Full wwPDB EM Validation Report (i)

Mar 31, 2025 – 06:48 PM JST

PDB ID	:	6KAF / pdb_00006kaf
EMDB ID	:	EMD-9957
Title	:	C2S2M2N2-type PSII-LHCII
Authors	:	Chang, S.H.; Shen, L.L.; Huang, Z.H.; Wang, W.D.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on	:	2019-06-22
Resolution	:	3.73 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

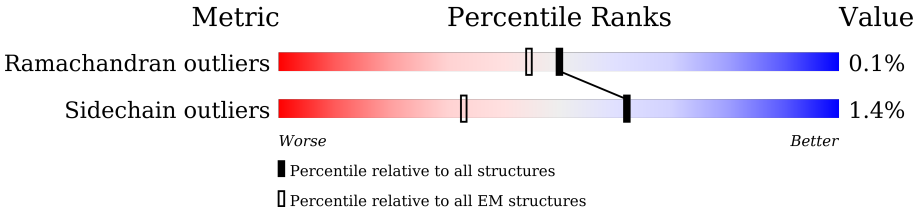
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	280	16% 79% 20%
1	r	280	15% 79% • 20%
2	A	352	94% • 5%
2	a	352	• 94% 5%
3	D	352	95% • •
3	d	352	95% • •
4	F	44	5% 68% 32%
4	f	44	5% 68% 32%
5	H	88	• 73% 27%

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Mol	Chain	Length	Quality of chain
5	h	88	73% 27%
6	I	37	86% 5% 8%
6	i	37	86% 5% 8%
7	J	50	32% 62% 38%
7	j	50	32% 62% 38%
8	K	46	78% 22%
8	k	46	78% 22%
9	L	38	5% 97%
9	l	38	5% 97%
10	M	34	94% 6%
10	m	34	6% 94% 6%
11	O	291	7% 72% 28%
11	o	291	8% 71% 28%
12	T	31	97%
12	t	31	97%
13	W	115	47% 53%
13	w	115	47% 53%
14	X	101	35% 65%
14	x	101	35% 65%
15	Z	62	100%
15	z	62	100%
16	Y	33	9% 91% 9%
16	y	33	9% 91% 9%
17	E	82	82% 17%
17	e	82	82% 17%

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Mol	Chain	Length	Quality of chain
18	1	257	30% 82% 15%
18	2	257	63% 81% 15%
18	3	257	58% 82% 15%
18	4	257	30% 82% 15%
18	5	257	63% 82% 15%
18	6	257	57% 83% 15%
18	G	257	6% 83% 15%
18	N	257	81% 16%
18	P	257	61% 82% 15%
18	Q	257	80% 83% 15%
18	U	257	82% 15%
18	V	257	69% 82% 15%
18	g	257	7% 83% 15%
18	n	257	82% 15%
18	p	257	60% 81% 15%
18	q	257	80% 83% 15%
18	u	257	83% 15%
18	v	257	68% 82% 15%
19	S	289	81% 18%
19	s	289	81% 18%
20	C	461	97%
20	c	461	97%
21	B	508	98%
21	b	508	5% 98%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	301	X	-	-	-
22	CLA	1	302	X	-	-	-
22	CLA	1	303	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	2	301	X	-	-	-
22	CLA	2	302	X	-	-	-
22	CLA	2	303	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	305	X	-	-	-
22	CLA	2	306	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	3	301	X	-	-	-
22	CLA	3	302	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	306	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	4	301	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	305	X	-	-	-
22	CLA	4	306	X	-	-	-
22	CLA	4	307	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	5	301	X	-	-	-
22	CLA	5	302	X	-	-	-
22	CLA	5	303	X	-	-	-
22	CLA	5	304	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	306	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	6	302	X	-	-	-
22	CLA	6	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	304	X	-	-	-
22	CLA	6	305	X	-	-	-
22	CLA	6	306	X	-	-	-
22	CLA	6	307	X	-	-	-
22	CLA	6	308	X	-	-	-
22	CLA	6	309	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	515	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	G	301	X	-	-	-
22	CLA	G	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	G	303	X	-	-	-
22	CLA	G	304	X	-	-	-
22	CLA	G	305	X	-	-	-
22	CLA	G	306	X	-	-	-
22	CLA	G	307	X	-	-	-
22	CLA	G	308	X	-	-	-
22	CLA	N	301	X	-	-	-
22	CLA	N	302	X	-	-	-
22	CLA	N	303	X	-	-	-
22	CLA	N	304	X	-	-	-
22	CLA	N	305	X	-	-	-
22	CLA	N	306	X	-	-	-
22	CLA	N	307	X	-	-	-
22	CLA	N	308	X	-	-	-
22	CLA	P	302	X	-	-	-
22	CLA	P	303	X	-	-	-
22	CLA	P	304	X	-	-	-
22	CLA	P	305	X	-	-	-
22	CLA	P	306	X	-	-	-
22	CLA	P	307	X	-	-	-
22	CLA	P	308	X	-	-	-
22	CLA	P	309	X	-	-	-
22	CLA	Q	301	X	-	-	-
22	CLA	Q	302	X	-	-	-
22	CLA	Q	303	X	-	-	-
22	CLA	Q	304	X	-	-	-
22	CLA	Q	305	X	-	-	-
22	CLA	Q	306	X	-	-	-
22	CLA	Q	307	X	-	-	-
22	CLA	Q	308	X	-	-	-
22	CLA	R	302	X	-	-	-
22	CLA	R	303	X	-	-	-
22	CLA	R	304	X	-	-	-
22	CLA	R	305	X	-	-	-
22	CLA	R	306	X	-	-	-
22	CLA	R	307	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	S	301	X	-	-	-
22	CLA	S	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	306	X	-	-	-
22	CLA	S	307	X	-	-	-
22	CLA	S	308	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	U	302	X	-	-	-
22	CLA	U	303	X	-	-	-
22	CLA	U	304	X	-	-	-
22	CLA	U	305	X	-	-	-
22	CLA	U	306	X	-	-	-
22	CLA	U	307	X	-	-	-
22	CLA	U	308	X	-	-	-
22	CLA	V	302	X	-	-	-
22	CLA	V	303	X	-	-	-
22	CLA	V	304	X	-	-	-
22	CLA	V	305	X	-	-	-
22	CLA	V	306	X	-	-	-
22	CLA	V	307	X	-	-	-
22	CLA	V	308	X	-	-	-
22	CLA	X	202	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	g	301	X	-	-	-
22	CLA	g	302	X	-	-	-
22	CLA	g	303	X	-	-	-
22	CLA	g	304	X	-	-	-
22	CLA	g	305	X	-	-	-
22	CLA	g	306	X	-	-	-
22	CLA	g	307	X	-	-	-
22	CLA	g	308	X	-	-	-
22	CLA	n	301	X	-	-	-
22	CLA	n	302	X	-	-	-
22	CLA	n	303	X	-	-	-
22	CLA	n	304	X	-	-	-
22	CLA	n	305	X	-	-	-
22	CLA	n	306	X	-	-	-
22	CLA	n	307	X	-	-	-
22	CLA	n	308	X	-	-	-
22	CLA	p	302	X	-	-	-
22	CLA	p	303	X	-	-	-
22	CLA	p	304	X	-	-	-
22	CLA	p	305	X	-	-	-
22	CLA	p	306	X	-	-	-
22	CLA	p	307	X	-	-	-
22	CLA	p	308	X	-	-	-
22	CLA	p	309	X	-	-	-
22	CLA	q	302	X	-	-	-
22	CLA	q	303	X	-	-	-
22	CLA	q	304	X	-	-	-
22	CLA	q	305	X	-	-	-
22	CLA	q	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	q	307	X	-	-	-
22	CLA	q	308	X	-	-	-
22	CLA	r	601	X	-	-	-
22	CLA	r	602	X	-	-	-
22	CLA	r	603	X	-	-	-
22	CLA	r	604	X	-	-	-
22	CLA	r	605	X	-	-	-
22	CLA	r	606	X	-	-	-
22	CLA	r	607	X	-	-	-
22	CLA	r	608	X	-	-	-
22	CLA	r	609	X	-	-	-
22	CLA	r	610	X	-	-	-
22	CLA	s	301	X	-	-	-
22	CLA	s	302	X	-	-	-
22	CLA	s	303	X	-	-	-
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	306	X	-	-	-
22	CLA	s	307	X	-	-	-
22	CLA	s	308	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	u	302	X	-	-	-
22	CLA	u	303	X	-	-	-
22	CLA	u	304	X	-	-	-
22	CLA	u	305	X	-	-	-
22	CLA	u	306	X	-	-	-
22	CLA	u	307	X	-	-	-
22	CLA	u	308	X	-	-	-
22	CLA	v	302	X	-	-	-
22	CLA	v	303	X	-	-	-
22	CLA	v	304	X	-	-	-
22	CLA	v	305	X	-	-	-
22	CLA	v	306	X	-	-	-
22	CLA	v	307	X	-	-	-
22	CLA	v	308	X	-	-	-
22	CLA	x	201	X	-	-	-
26	CHL	1	313	X	-	-	-
26	CHL	1	314	X	-	-	-
26	CHL	1	315	X	-	-	-
26	CHL	1	316	X	-	-	-
26	CHL	1	317	X	-	-	-
26	CHL	1	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	2	313	X	-	-	-
26	CHL	2	314	X	-	-	-
26	CHL	2	315	X	-	-	-
26	CHL	2	316	X	-	-	-
26	CHL	2	317	X	-	-	-
26	CHL	2	318	X	-	-	-
26	CHL	3	311	X	-	-	-
26	CHL	3	312	X	-	-	-
26	CHL	3	313	X	-	-	-
26	CHL	3	314	X	-	-	-
26	CHL	3	315	X	-	-	-
26	CHL	3	316	X	-	-	-
26	CHL	4	313	X	-	-	-
26	CHL	4	314	X	-	-	-
26	CHL	4	315	X	-	-	-
26	CHL	4	316	X	-	-	-
26	CHL	4	317	X	-	-	-
26	CHL	5	313	X	-	-	-
26	CHL	5	314	X	-	-	-
26	CHL	5	315	X	-	-	-
26	CHL	5	316	X	-	-	-
26	CHL	5	317	X	-	-	-
26	CHL	5	318	X	-	-	-
26	CHL	6	301	X	-	-	-
26	CHL	6	312	X	-	-	-
26	CHL	6	313	X	-	-	-
26	CHL	6	314	X	-	-	-
26	CHL	6	315	X	-	-	-
26	CHL	6	316	X	-	-	-
26	CHL	6	317	X	-	-	-
26	CHL	G	311	X	-	-	-
26	CHL	G	312	X	-	-	-
26	CHL	G	313	X	-	-	-
26	CHL	G	314	X	-	-	-
26	CHL	G	315	X	-	-	-
26	CHL	G	316	X	-	-	-
26	CHL	N	313	X	-	-	-
26	CHL	N	314	X	-	-	-
26	CHL	N	315	X	-	-	-
26	CHL	N	316	X	-	-	-
26	CHL	N	317	X	-	-	-
26	CHL	P	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	P	315	X	-	-	-
26	CHL	P	316	X	-	-	-
26	CHL	P	317	X	-	-	-
26	CHL	P	318	X	-	-	-
26	CHL	P	319	X	-	-	-
26	CHL	Q	311	X	-	-	-
26	CHL	Q	312	X	-	-	-
26	CHL	Q	313	X	-	-	-
26	CHL	Q	314	X	-	-	-
26	CHL	Q	315	X	-	-	-
26	CHL	Q	316	X	-	-	-
26	CHL	R	315	X	-	-	-
26	CHL	R	316	X	-	-	-
26	CHL	R	317	X	-	-	-
26	CHL	S	313	X	-	-	-
26	CHL	S	314	X	-	-	-
26	CHL	S	315	X	-	-	-
26	CHL	S	316	X	-	-	-
26	CHL	U	313	X	-	-	-
26	CHL	U	314	X	-	-	-
26	CHL	U	315	X	-	-	-
26	CHL	U	316	X	-	-	-
26	CHL	U	317	X	-	-	-
26	CHL	U	319	X	-	-	-
26	CHL	V	313	X	-	-	-
26	CHL	V	314	X	-	-	-
26	CHL	V	315	X	-	-	-
26	CHL	V	316	X	-	-	-
26	CHL	V	317	X	-	-	-
26	CHL	V	318	X	-	-	-
26	CHL	g	311	X	-	-	-
26	CHL	g	312	X	-	-	-
26	CHL	g	313	X	-	-	-
26	CHL	g	314	X	-	-	-
26	CHL	g	315	X	-	-	-
26	CHL	g	316	X	-	-	-
26	CHL	n	313	X	-	-	-
26	CHL	n	314	X	-	-	-
26	CHL	n	315	X	-	-	-
26	CHL	n	316	X	-	-	-
26	CHL	n	317	X	-	-	-
26	CHL	n	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	p	314	X	-	-	-
26	CHL	p	315	X	-	-	-
26	CHL	p	316	X	-	-	-
26	CHL	p	317	X	-	-	-
26	CHL	p	318	X	-	-	-
26	CHL	p	319	X	-	-	-
26	CHL	p	320	X	-	-	-
26	CHL	q	311	X	-	-	-
26	CHL	q	312	X	-	-	-
26	CHL	q	313	X	-	-	-
26	CHL	q	314	X	-	-	-
26	CHL	q	315	X	-	-	-
26	CHL	r	614	X	-	-	-
26	CHL	r	615	X	-	-	-
26	CHL	r	616	X	-	-	-
26	CHL	r	619	X	-	-	-
26	CHL	s	313	X	-	-	-
26	CHL	s	314	X	-	-	-
26	CHL	s	315	X	-	-	-
26	CHL	s	316	X	-	-	-
26	CHL	u	313	X	-	-	-
26	CHL	u	314	X	-	-	-
26	CHL	u	315	X	-	-	-
26	CHL	u	316	X	-	-	-
26	CHL	u	317	X	-	-	-
26	CHL	u	318	X	-	-	-
26	CHL	v	313	X	-	-	-
26	CHL	v	314	X	-	-	-
26	CHL	v	315	X	-	-	-
26	CHL	v	316	X	-	-	-
26	CHL	v	317	X	-	-	-
26	CHL	v	318	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 104363 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	r	223	1701	1081	286	329	5	0	0
1	R	223	1698	1080	285	328	5	0	0

- Molecule 2 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	a	333	2614	1707	430	462	15	0	0
2	A	333	2614	1707	430	462	15	0	0

- Molecule 3 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	341	2714	1791	447	464	12	0	0
3	D	341	2714	1791	447	464	12	0	0

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	f	30	243	165	41	36	1	0	0
4	F	30	243	165	41	36	1	0	0

- Molecule 5 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	h	64	488	327	72	87	2	0	0
5	H	64	488	327	72	87	2	0	0

- Molecule 6 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	i	34	275	189	41	43	2	0	0
6	I	34	275	189	41	43	2	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein J, PsbJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	j	31	245	168	36	39	2	0	0
7	J	31	245	168	36	39	2	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	k	36	288	203	41	44	0	0
8	K	36	288	203	41	44	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	l	37	306	205	50	51	0	0
9	L	37	306	205	50	51	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	m	32	248	168	35	45	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	M	32	248	168	35	45	0	0

- Molecule 11 is a protein called Oxygen-evolving enhancer protein 1 of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	o	210	1592	1016	254	318	4	0	0
11	O	210	1592	1016	254	318	4	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	t	30	247	171	36	38	2	0	0
12	T	30	247	171	36	38	2	0	0

- Molecule 13 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	w	54	417	269	67	79	2	0	0
13	W	54	417	269	67	79	2	0	0

- Molecule 14 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	x	35	242	159	39	44	0	0
14	X	35	242	159	39	44	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	z	62	465	319	69	76	1	0	0
15	Z	62	465	319	69	76	1	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein 30, Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	Y	30	208	137	34	37	0	0
16	y	30	208	137	34	37	0	0

- Molecule 17 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	E	68	555	366	90	99	0	0
17	e	68	555	366	90	99	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	1	218	1669	1081	271	312	5	0	0
18	2	218	1669	1081	271	312	5	0	0
18	3	219	1675	1084	272	314	5	0	0
18	4	218	1669	1081	271	312	5	0	0
18	5	218	1669	1081	271	312	5	0	0
18	6	219	1675	1084	272	314	5	0	0
18	v	218	1669	1081	271	312	5	0	0
18	p	218	1669	1081	271	312	5	0	0
18	q	219	1675	1084	272	314	5	0	0
18	V	218	1669	1081	271	312	5	0	0
18	P	218	1669	1081	271	312	5	0	0
18	Q	219	1675	1084	272	314	5	0	0
18	U	218	1669	1081	271	312	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	217	1661	1075	270	311	5	0	0
18	G	219	1675	1084	272	314	5	0	0
18	u	218	1669	1081	271	312	5	0	0
18	n	218	1669	1081	271	312	5	0	0
18	g	219	1675	1084	272	314	5	0	0

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	236	1797	1166	290	337	4	0	0
19	s	236	1797	1166	290	337	4	0	0

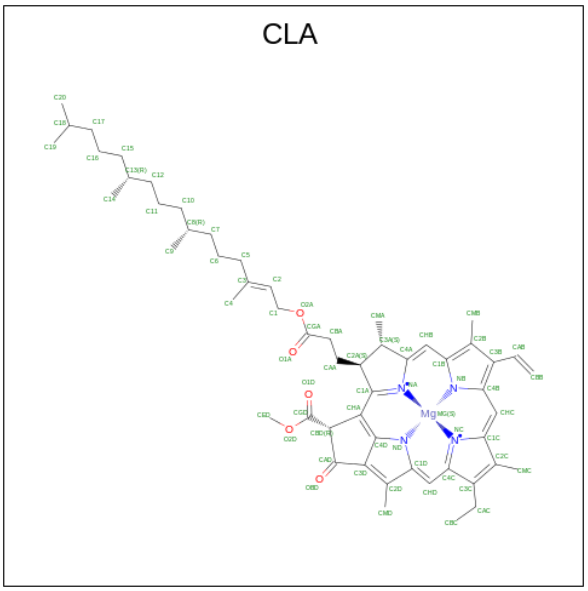
- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	C	450	3502	2290	585	610	17	0	0
20	c	450	3502	2290	585	610	17	0	0

- Molecule 21 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	B	503	3937	2575	658	692	12	0	0
21	b	503	3937	2575	658	692	12	0	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	d	1	65	55	1	4	5	0
22	x	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	50	40	1	4	5	0
22	A	1	60	50	1	4	5	0
22	1	1	65	55	1	4	5	0
22	1	1	65	55	1	4	5	0
22	1	1	50	40	1	4	5	0
22	1	1	60	50	1	4	5	0
22	1	1	60	50	1	4	5	0
22	1	1	60	50	1	4	5	0
22	1	1	65	55	1	4	5	0
22	1	1	48	38	1	4	5	0
22	2	1	65	55	1	4	5	0
22	2	1	65	55	1	4	5	0
22	2	1	50	40	1	4	5	0
22	2	1	65	55	1	4	5	0
22	2	1	60	50	1	4	5	0
22	2	1	60	50	1	4	5	0
22	2	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	2	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	v	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	p	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	p	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	q	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	V	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	V	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	P	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	Q	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	U	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	U	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	N	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	48	38	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	u	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	u	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	n	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	g	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	g	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	R	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	S	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms	AltConf
22	S	1	Total C Mg N O 49 39 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0
22	X	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0
22	b	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	s	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0

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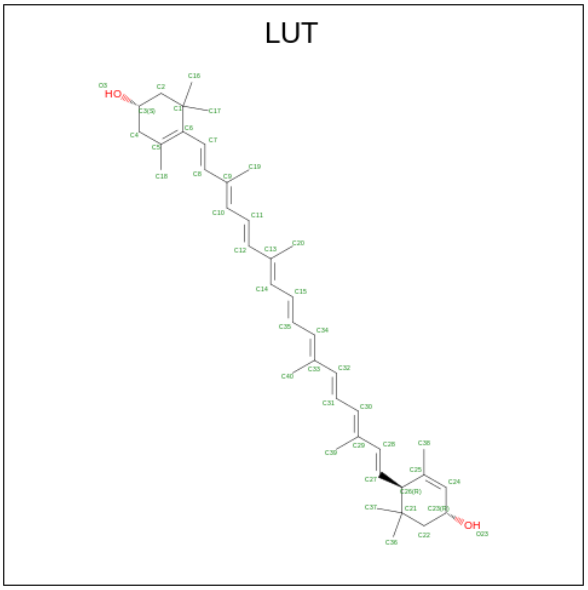
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	s	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	s	1	49	39	1	4	5	0

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	r	1	42	40	2	0
			Total	C	O	
23	1	1	42	40	2	0
			Total	C	O	
23	1	1	42	40	2	0
			Total	C	O	
23	2	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	2	1	42	40	2	0
23	4	1	42	40	2	0
23	4	1	42	40	2	0
23	5	1	42	40	2	0
23	5	1	42	40	2	0
23	v	1	42	40	2	0
23	v	1	42	40	2	0
23	p	1	42	40	2	0
23	p	1	42	40	2	0
23	V	1	42	40	2	0
23	V	1	42	40	2	0
23	P	1	42	40	2	0
23	P	1	42	40	2	0
23	U	1	42	40	2	0
23	U	1	42	40	2	0
23	N	1	42	40	2	0
23	N	1	42	40	2	0
23	u	1	42	40	2	0
23	u	1	42	40	2	0
23	n	1	42	40	2	0
23	n	1	42	40	2	0

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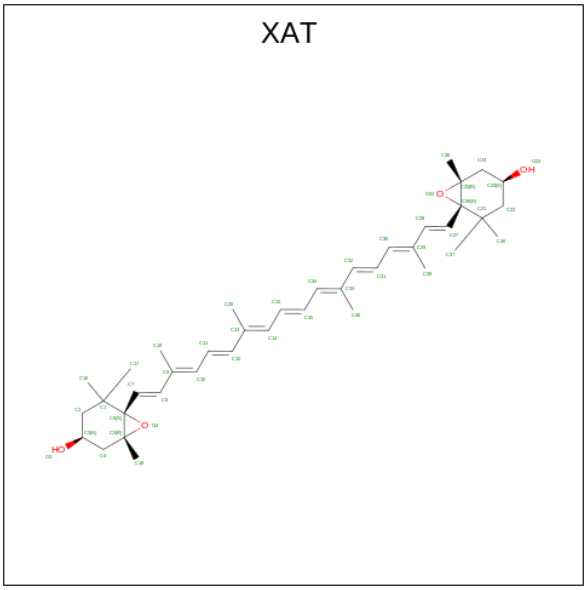
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	R	1	42	40	2	0
23	S	1	42	40	2	0
23	S	1	42	40	2	0
23	s	1	42	40	2	0
23	s	1	42	40	2	0

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	r	1	44	40	4	0
24	1	1	44	40	4	0
24	2	1	44	40	4	0
24	3	1	44	40	4	0
24	4	1	44	40	4	0
24	5	1	44	40	4	0

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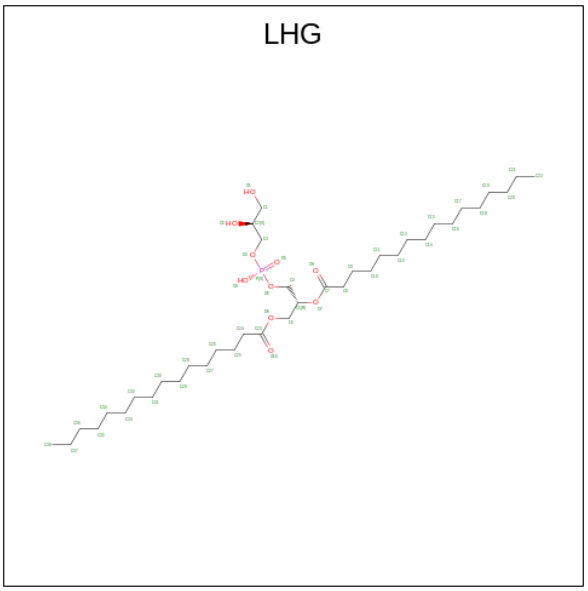
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	6	1	44	40	4	0
24	v	1	44	40	4	0
24	p	1	44	40	4	0
24	q	1	44	40	4	0
24	V	1	44	40	4	0
24	P	1	44	40	4	0
24	Q	1	44	40	4	0
24	U	1	44	40	4	0
24	N	1	44	40	4	0
24	G	1	44	40	4	0
24	u	1	44	40	4	0
24	n	1	44	40	4	0
24	g	1	44	40	4	0
24	R	1	44	40	4	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	r	1	42	31	10	1	0
25	a	1	43	32	10	1	0
25	d	1	46	35	10	1	0
25	d	1	49	38	10	1	0
25	l	1	49	38	10	1	0
25	A	1	43	32	10	1	0
25	L	1	49	38	10	1	0
25	1	1	49	38	10	1	0
25	2	1	49	38	10	1	0
25	3	1	49	38	10	1	0
25	4	1	49	38	10	1	0
25	5	1	49	38	10	1	0
25	6	1	49	38	10	1	0
25	v	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	p	1	49	38	10	1	0
25	q	1	49	38	10	1	0
25	V	1	49	38	10	1	0
25	P	1	49	38	10	1	0
25	Q	1	49	38	10	1	0
25	U	1	49	38	10	1	0
25	N	1	49	38	10	1	0
25	G	1	49	38	10	1	0
25	u	1	49	38	10	1	0
25	n	1	49	38	10	1	0
25	g	1	49	38	10	1	0
25	R	1	42	31	10	1	0
25	S	1	49	38	10	1	0
25	C	1	49	38	10	1	0
25	C	1	49	38	10	1	0
25	C	1	49	38	10	1	0
25	B	1	47	36	10	1	0
25	B	1	49	38	10	1	0
25	D	1	46	35	10	1	0
25	D	1	49	38	10	1	0
25	b	1	47	36	10	1	0

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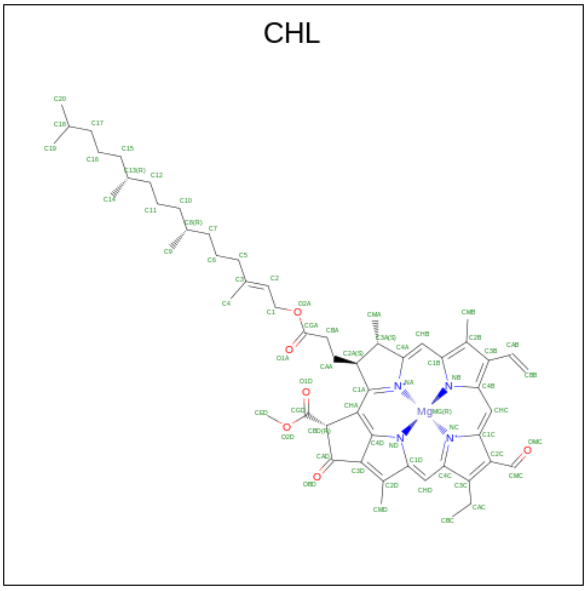
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	b	1	49	38	10	1	0
			Total	C	O	P	
25	c	1	49	38	10	1	0
			Total	C	O	P	
25	c	1	49	38	10	1	0
			Total	C	O	P	
25	c	1	49	38	10	1	0
			Total	C	O	P	
25	s	1	49	38	10	1	0

- Molecule 26 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	r	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	r	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
26	r	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	r	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	48	37	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	1	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	2	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	3	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	4	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	6	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	v	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	48	37	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	p	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	p	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	q	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	P	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	P	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	Q	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	G	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	u	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	g	1	61	50	1	4	6	0

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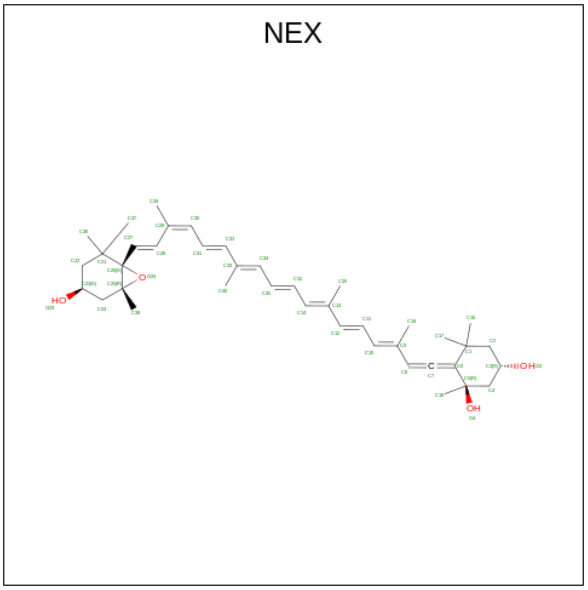
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	R	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
26	R	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
26	R	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
26	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	S	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
26	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
26	s	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
26	s	1	46	35	1	4	6	0

- Molecule 27 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	r	1	44	40	4	0
			Total	C	O	
27	r	1	44	40	4	0
			Total	C	O	
27	2	1	44	40	4	0
			Total	C	O	
27	5	1	44	40	4	0
			Total	C	O	
27	v	1	44	40	4	0
			Total	C	O	
27	p	1	44	40	4	0
			Total	C	O	
27	V	1	44	40	4	0
			Total	C	O	
27	P	1	44	40	4	0
			Total	C	O	
27	U	1	44	40	4	0
			Total	C	O	
27	N	1	44	40	4	0
			Total	C	O	
27	u	1	44	40	4	0
			Total	C	O	
27	u	1	44	40	4	0
			Total	C	O	
27	n	1	44	40	4	0
			Total	C	O	
27	R	1	44	40	4	0
			Total	C	O	
27	S	1	44	40	4	0
			Total	C	O	
27	s	1	44	40	4	0

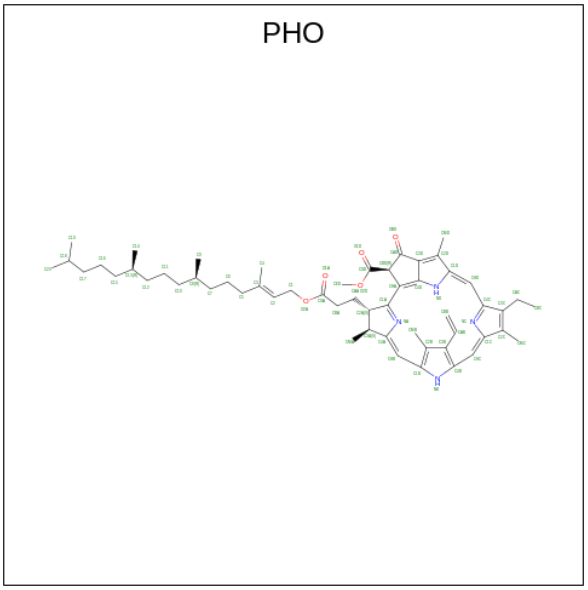
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
28	a	1	1	1	0
			Total	Fe	
28	A	1	1	1	0

- Molecule 29 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

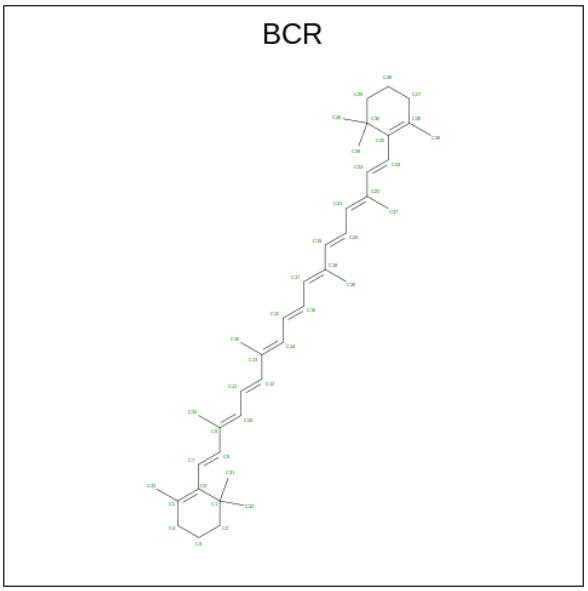
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
29	a	2	2	2	0
			Total	Cl	
29	A	2	2	2	0

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	a	1	64	55	4	5	0
			Total	C	N	O	
30	d	1	64	55	4	5	0
			Total	C	N	O	
30	A	1	64	55	4	5	0
			Total	C	N	O	
30	D	1	64	55	4	5	0

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
31	a	1	40	40	0
31	d	1	40	40	0
31	k	1	40	40	0
31	t	1	40	40	0
31	x	1	40	40	0
31	z	1	40	40	0
31	A	1	40	40	0
31	K	1	40	40	0
31	T	1	40	40	0
31	C	1	40	40	0
31	C	1	40	40	0
31	C	1	40	40	0
31	B	1	40	40	0
31	B	1	40	40	0

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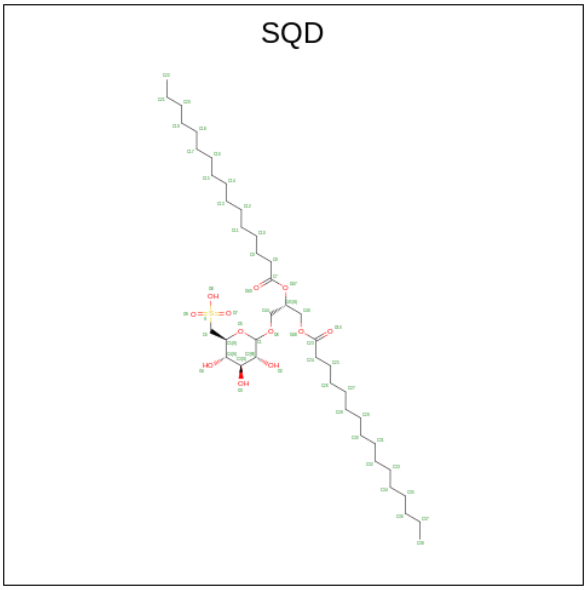
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
31	B	1	40	40	0
			Total	C	
31	D	1	40	40	0
			Total	C	
31	X	1	40	40	0
			Total	C	
31	b	1	40	40	0
			Total	C	
31	b	1	40	40	0
			Total	C	
31	b	1	40	40	0
			Total	C	
31	c	1	40	40	0
			Total	C	
31	c	1	40	40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	a	1	50	37	12	1	0
			Total	C	O	S	
32	a	1	54	41	12	1	0
			Total	C	O	S	
32	l	1	54	41	12	1	0

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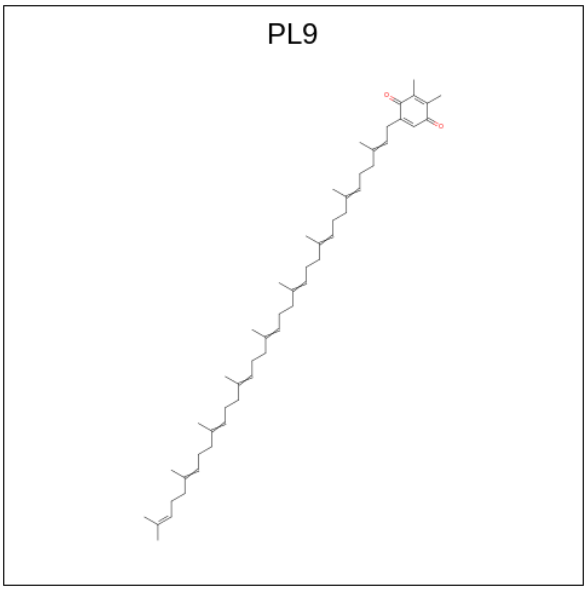
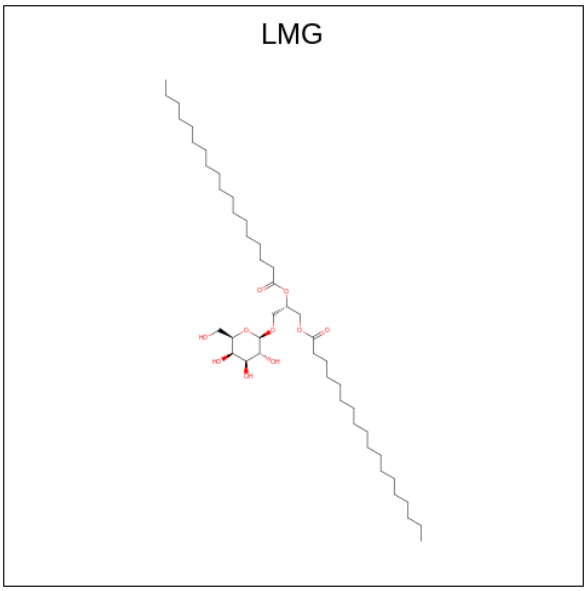
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	m	1	42	29	12	1	0
32	A	1	54	41	12	1	0
32	L	1	54	41	12	1	0
32	M	1	42	29	12	1	0
32	C	1	50	37	12	1	0

- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



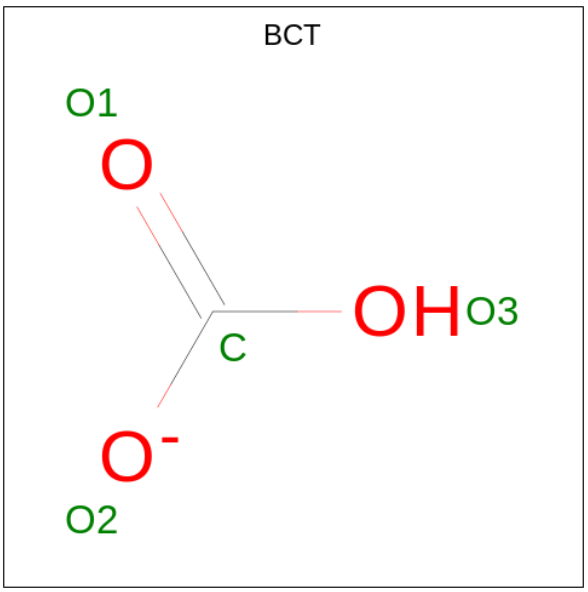
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	a	1	13	11	2	0
33	d	1	55	53	2	0
33	A	1	13	11	2	0
33	D	1	55	53	2	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



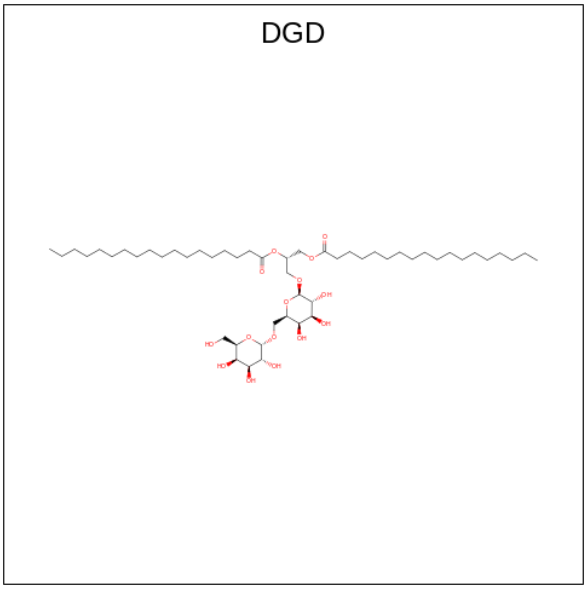
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	a	1	40	30	10	0
34	d	1	46	36	10	0
34	w	1	48	38	10	0
34	A	1	40	30	10	0
34	W	1	48	38	10	0
34	C	1	51	41	10	0
34	C	1	51	41	10	0
34	B	1	51	41	10	0
34	B	1	55	45	10	0
34	D	1	46	36	10	0
34	b	1	51	41	10	0
34	b	1	55	45	10	0
34	c	1	51	41	10	0
34	c	1	51	41	10	0

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



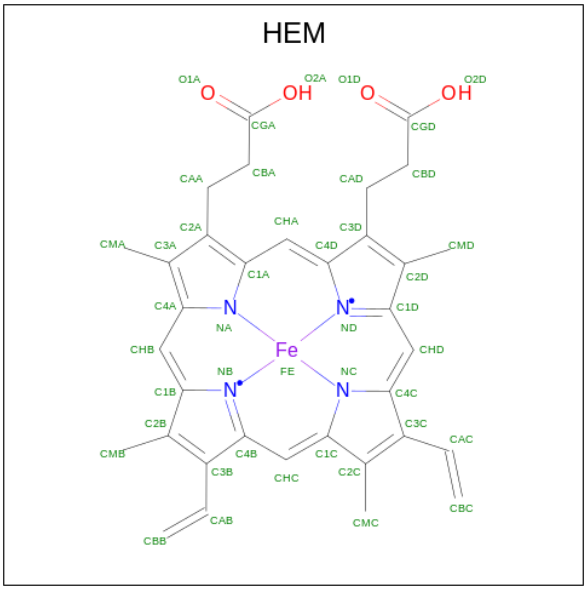
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	a	1	4	1	3	0
			Total	C	O	
35	D	1	4	1	3	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
36	a	1	59	44	15		0
36	A	1	59	44	15		0
36	J	1	60	45	15		0
36	C	1	55	40	15		0
36	C	1	62	47	15		0
36	B	1	62	47	15		0
36	b	1	62	47	15		0
36	c	1	55	40	15		0
36	c	1	62	47	15		0
36	c	1	60	45	15		0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
37	E	1	43	34	1	4	4	0

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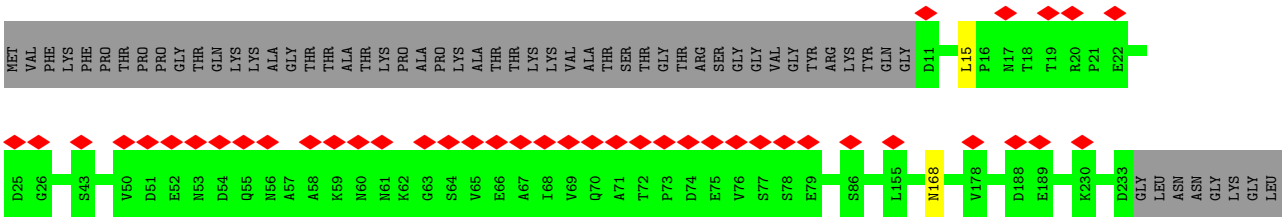
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
37	e	1	43	34	1	4	4	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

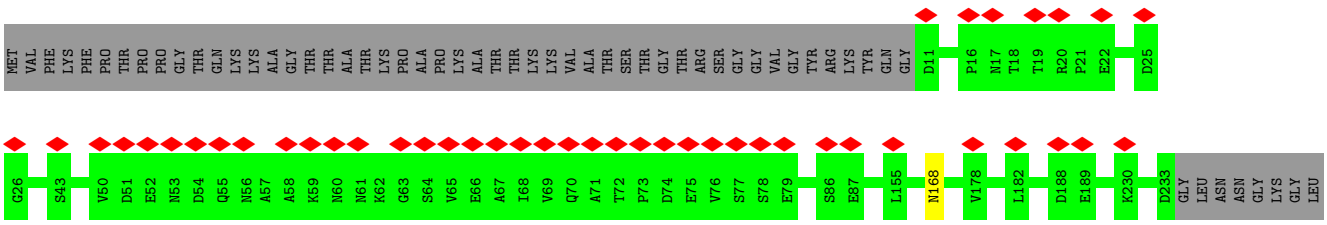
• Molecule 1: Chlorophyll a-b binding protein CP29

Chain r:



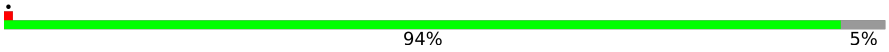
• Molecule 1: Chlorophyll a-b binding protein CP29

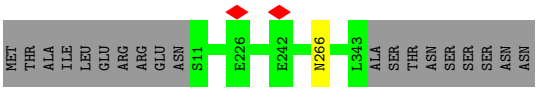
Chain R:



• Molecule 2: Photosystem II protein D1

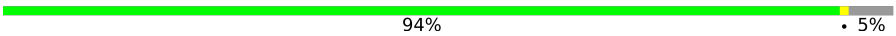
Chain a:

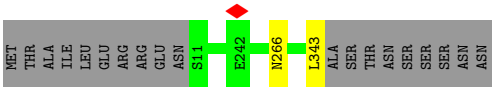




• Molecule 2: Photosystem II protein D1

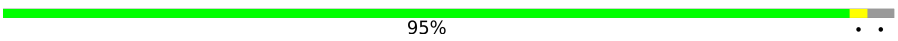
Chain A:

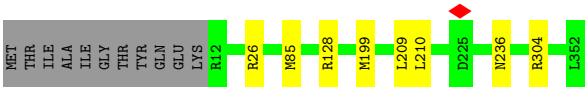




• Molecule 3: Photosystem II D2 protein

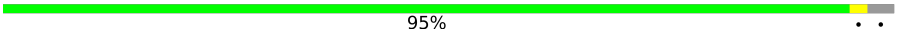
Chain d:

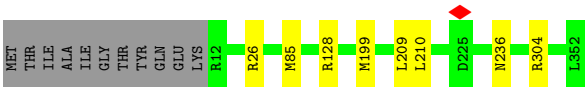




• Molecule 3: Photosystem II D2 protein

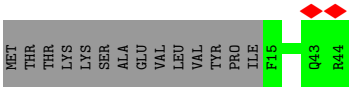
Chain D:





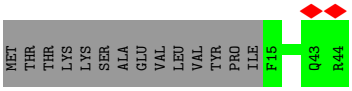
• Molecule 4: Cytochrome b559 subunit beta

Chain f:



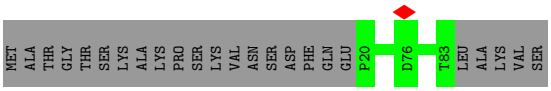
• Molecule 4: Cytochrome b559 subunit beta

Chain F:



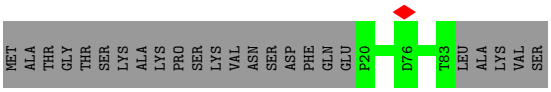
• Molecule 5: Photosystem II reaction center protein H

Chain h:



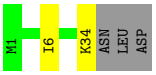
• Molecule 5: Photosystem II reaction center protein H

Chain H:



• Molecule 6: Photosystem II reaction center protein I

Chain i:

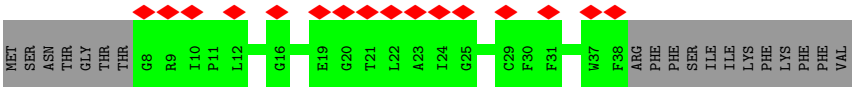


• Molecule 6: Photosystem II reaction center protein I

Chain I:

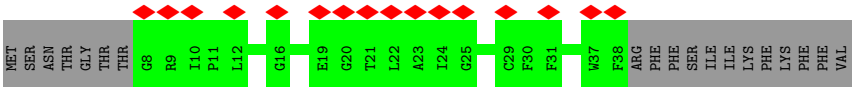
• Molecule 7: Photosystem II reaction center protein J, PsbJ

Chain j:



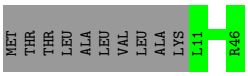
• Molecule 7: Photosystem II reaction center protein J, PsbJ

Chain J:



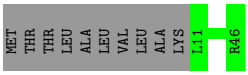
• Molecule 8: Photosystem II reaction center protein K

Chain k:



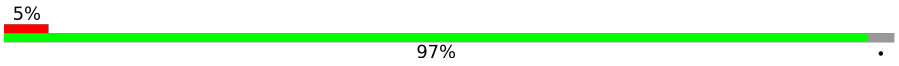
• Molecule 8: Photosystem II reaction center protein K

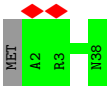
Chain K:



• Molecule 9: Photosystem II reaction center protein L

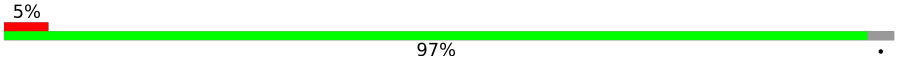
Chain l:

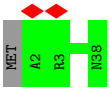




• Molecule 9: Photosystem II reaction center protein L

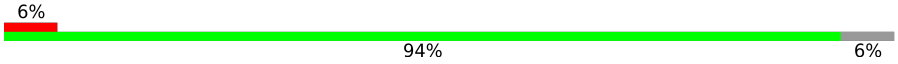
Chain L:

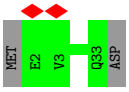




• Molecule 10: Photosystem II reaction center protein M

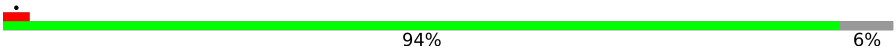
Chain m:

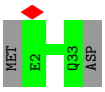




• Molecule 10: Photosystem II reaction center protein M

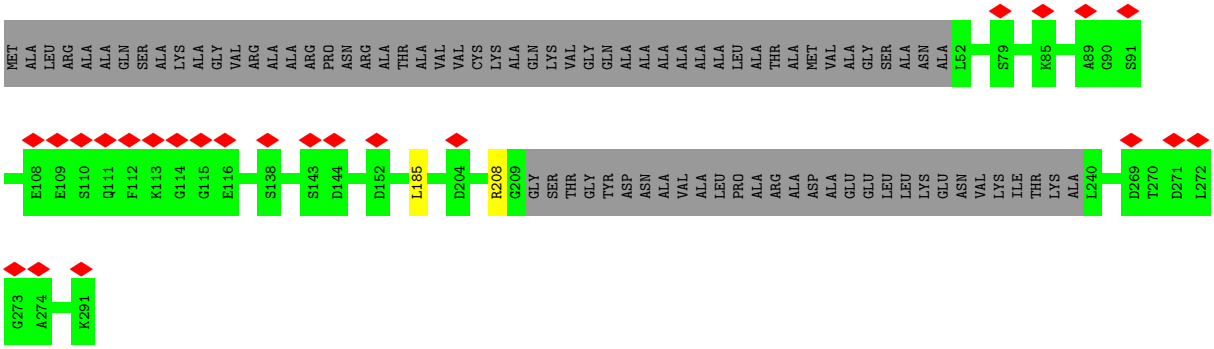
Chain M:





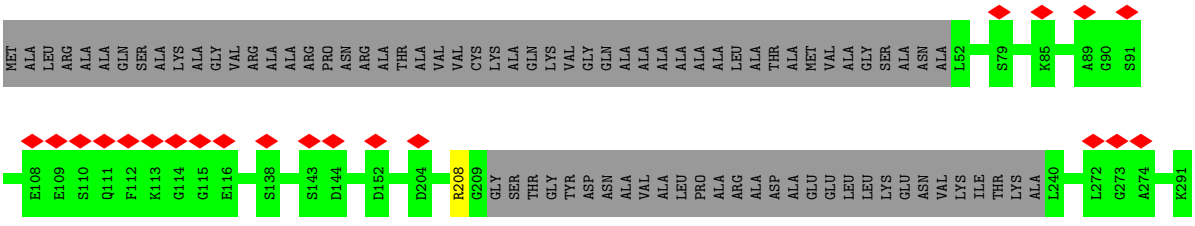
• Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II

Chain o:



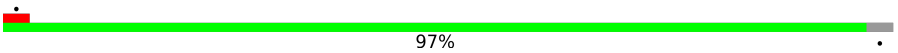
• Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II

Chain O:



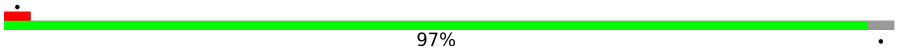
• Molecule 12: Photosystem II reaction center protein T

Chain t:



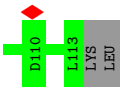
• Molecule 12: Photosystem II reaction center protein T

Chain T:



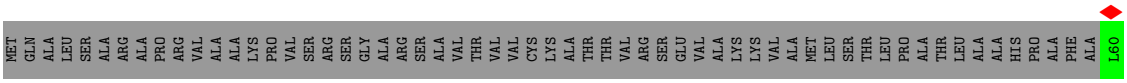
• Molecule 13: Photosystem II reaction center W protein, chloroplastic

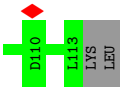
Chain w:



• Molecule 13: Photosystem II reaction center W protein, chloroplastic

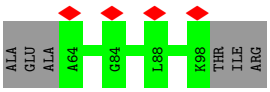
Chain W:





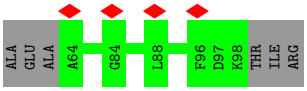
• Molecule 14: 4.1 kDa photosystem II subunit

Chain x:



• Molecule 14: 4.1 kDa photosystem II subunit

Chain X:



• Molecule 15: Photosystem II reaction center protein Z

Chain z: 

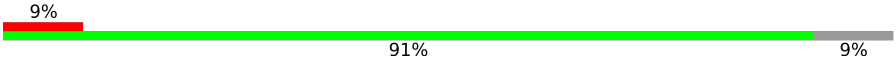
There are no outlier residues recorded for this chain.

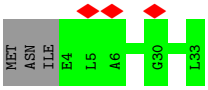
• Molecule 15: Photosystem II reaction center protein Z

Chain Z: 

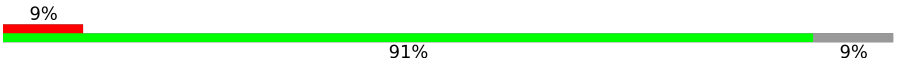
There are no outlier residues recorded for this chain.

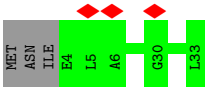
• Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain Y: 



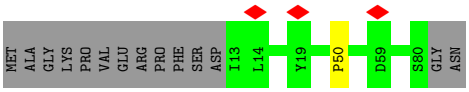
• Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain y: 



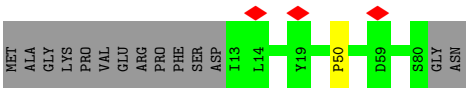
• Molecule 17: Cytochrome b559 subunit alpha

Chain E: 



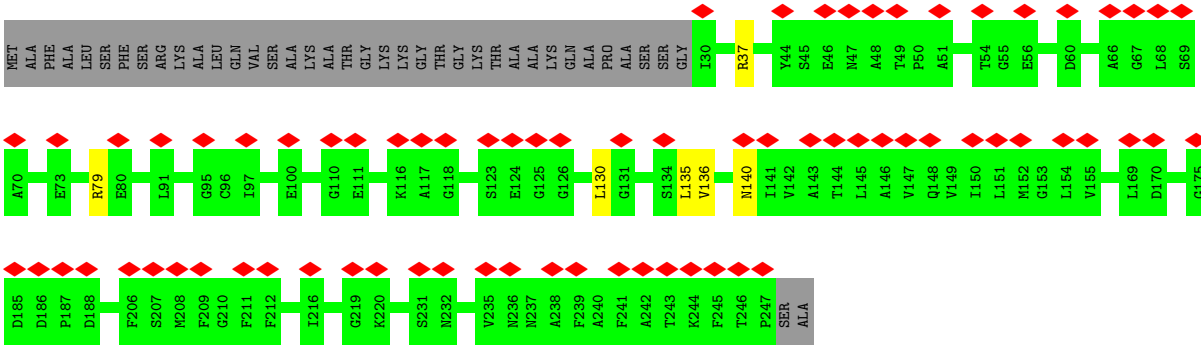
• Molecule 17: Cytochrome b559 subunit alpha

Chain e: 



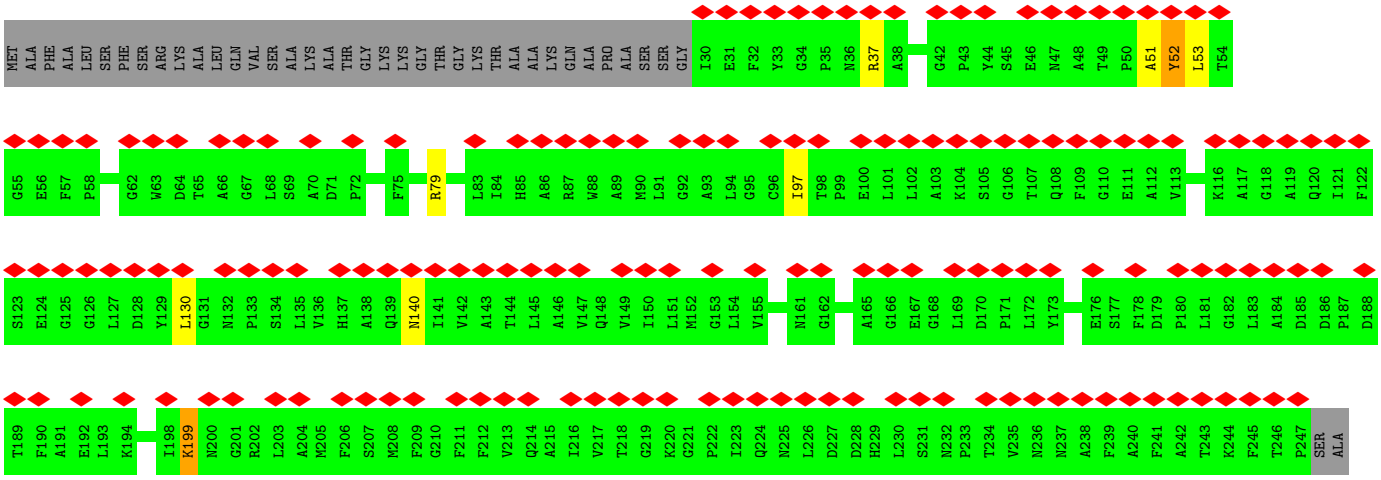
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 



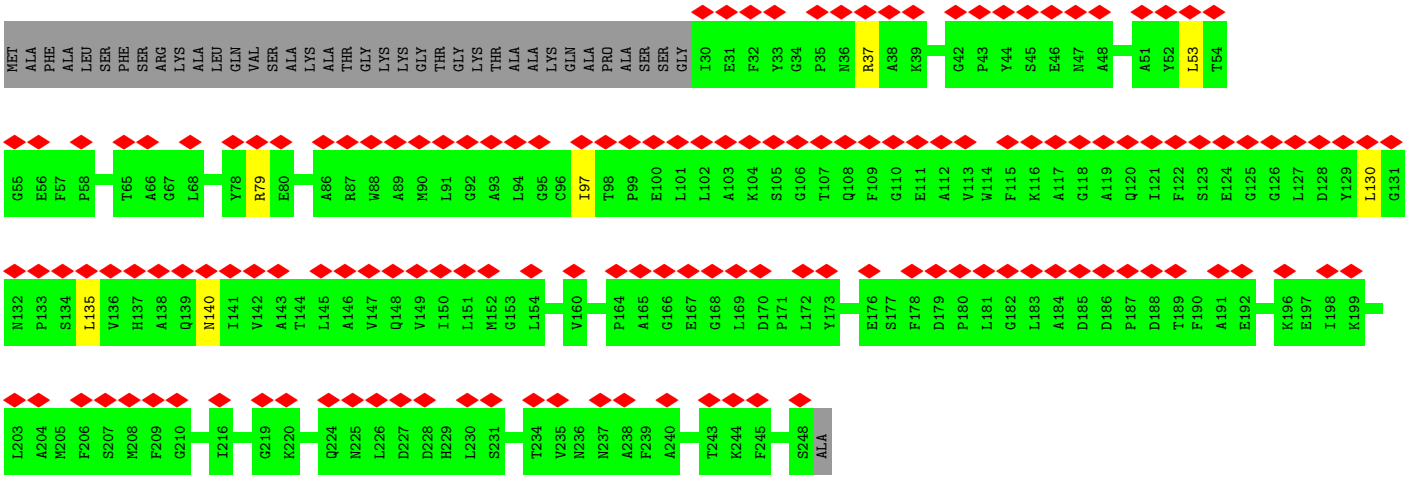
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



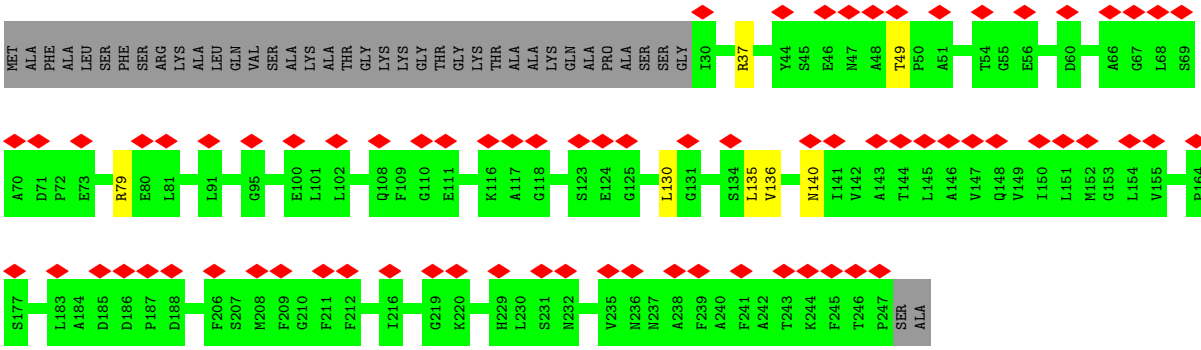
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



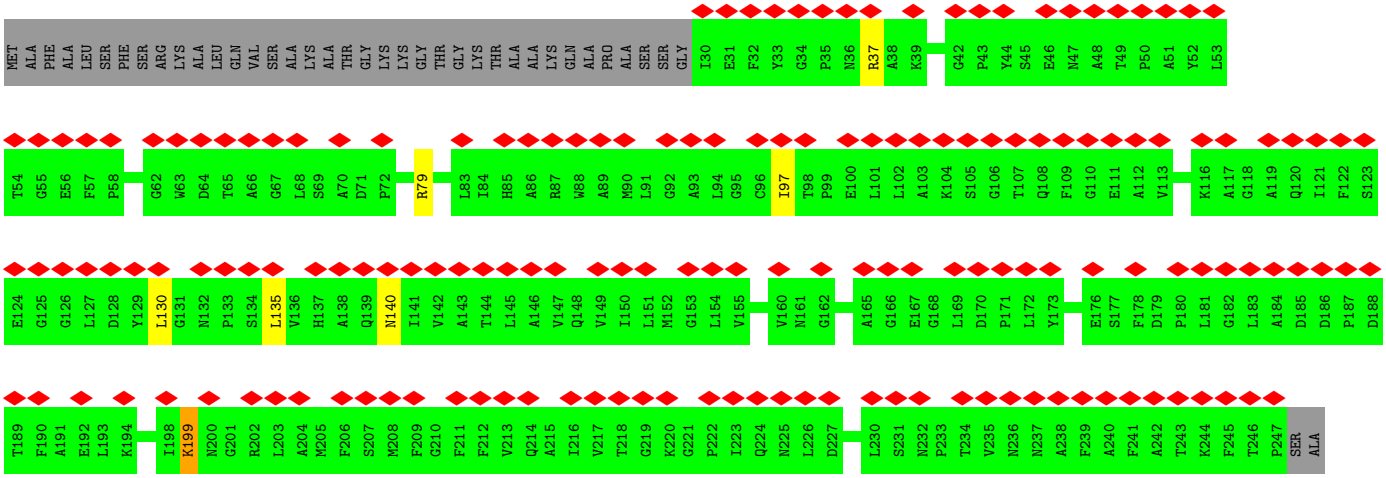
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



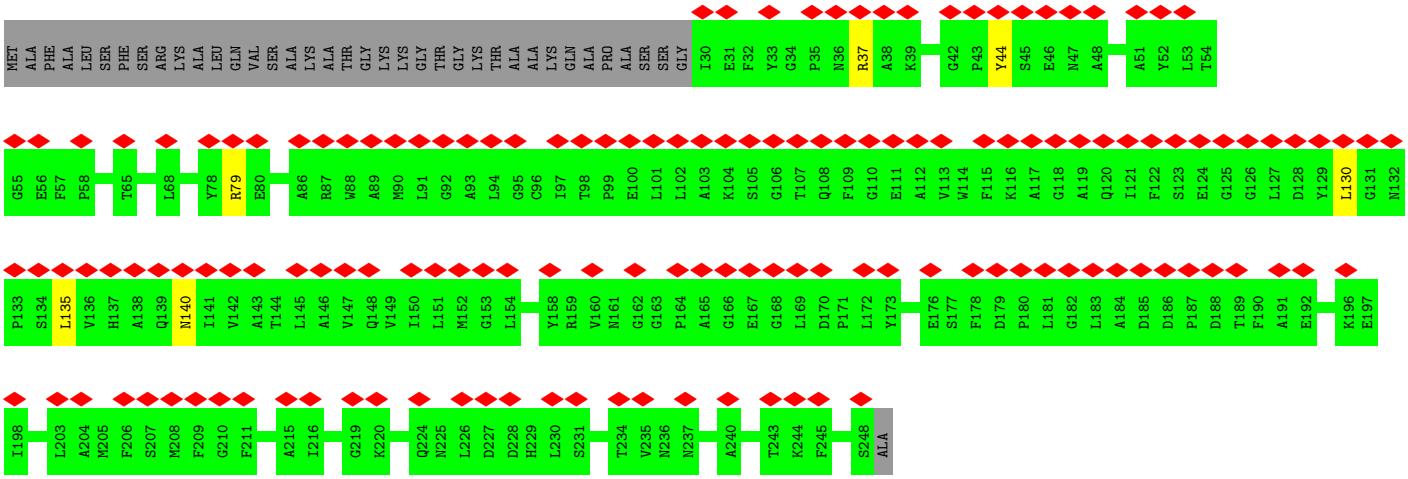
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



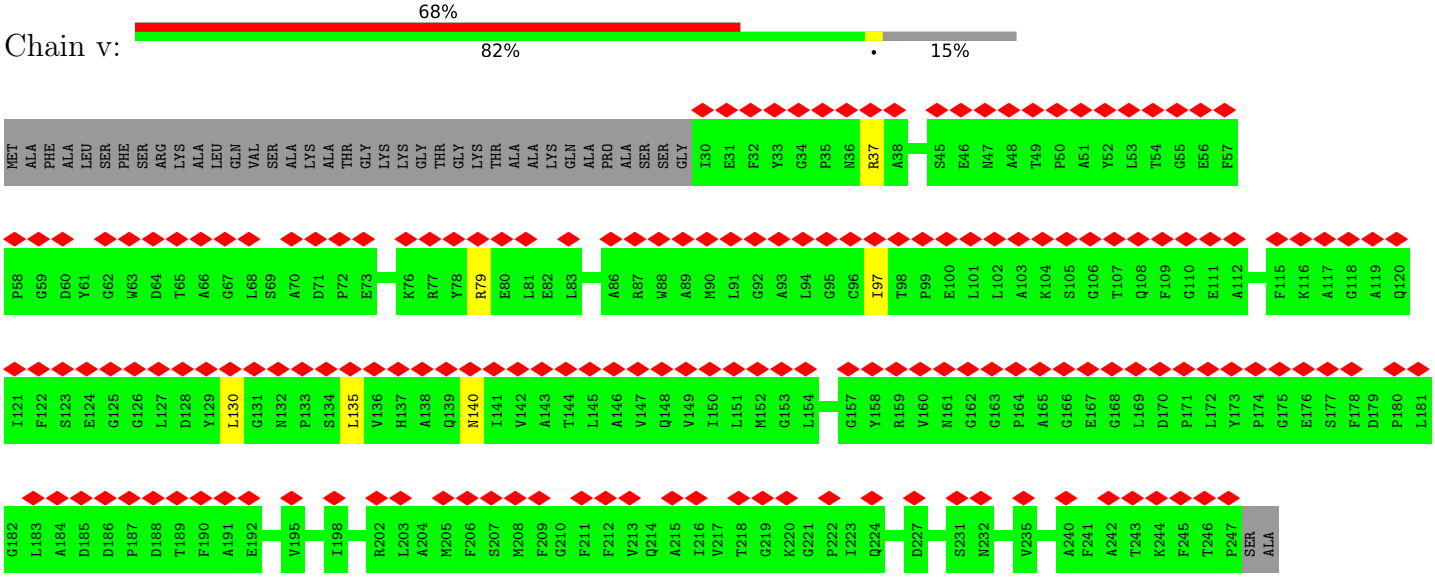
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



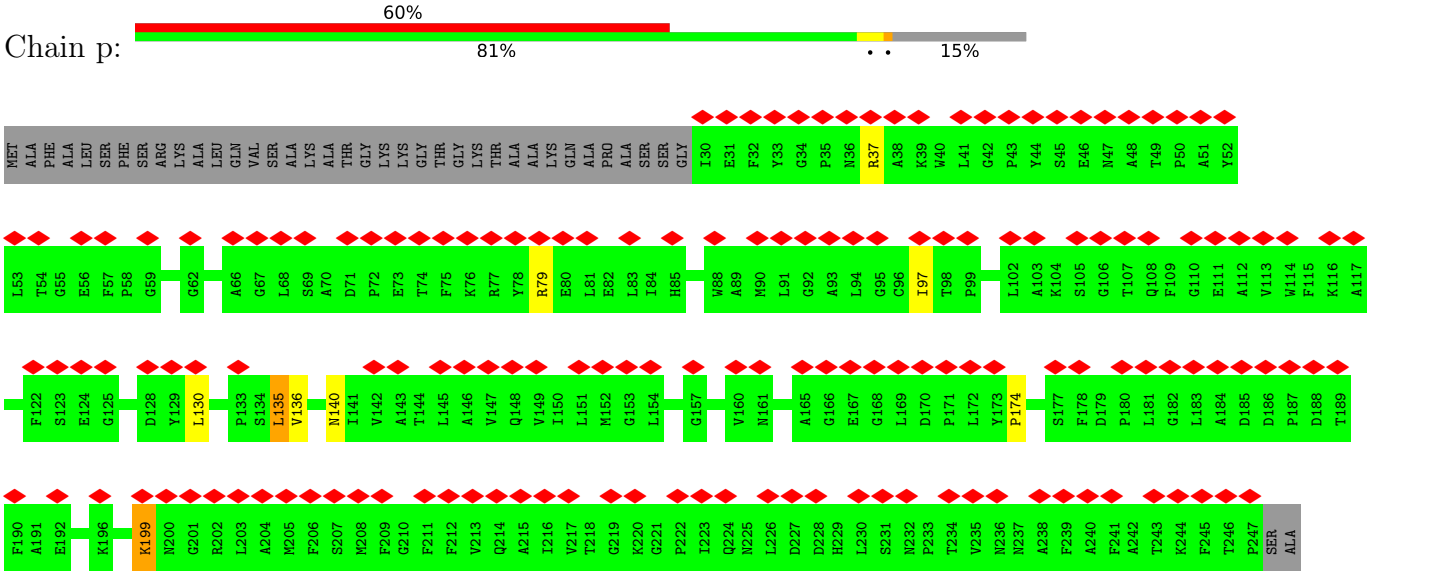
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain v:



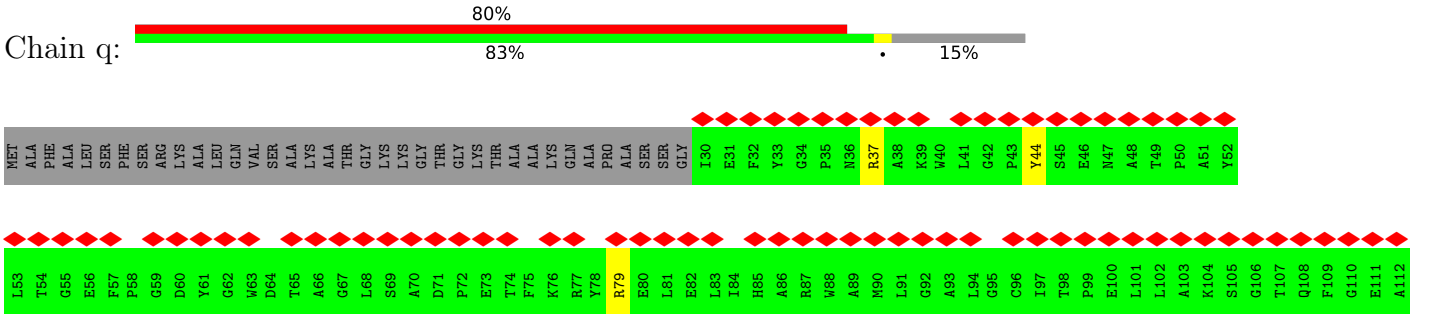
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain p:



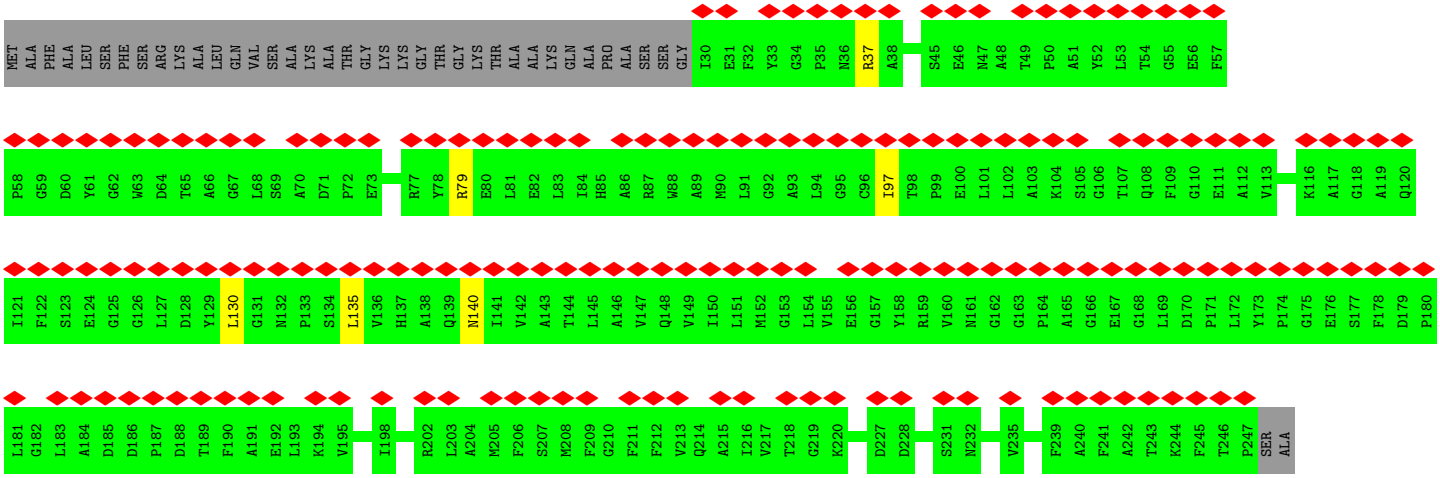
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain q:



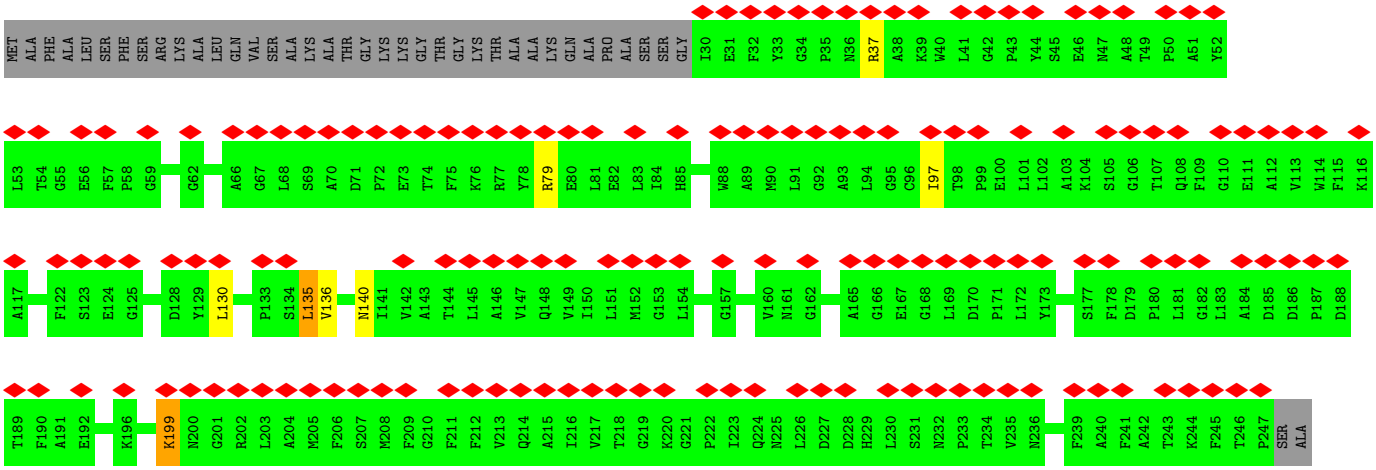
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain V:



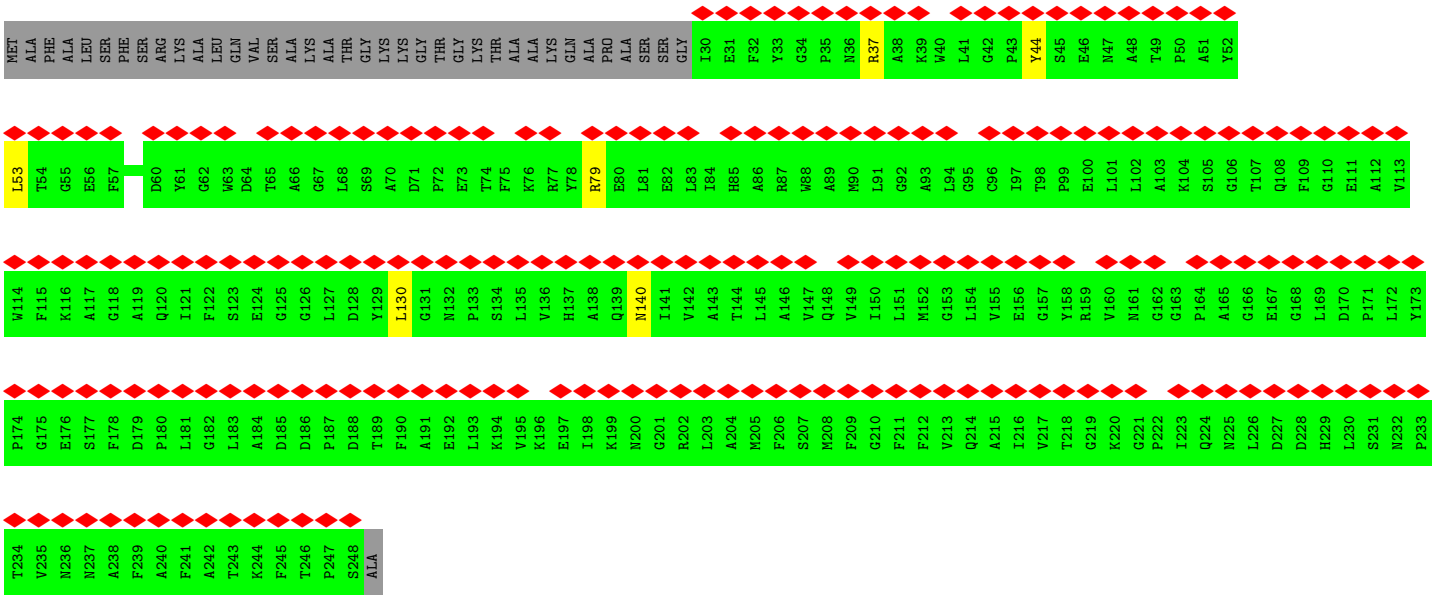
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain P:



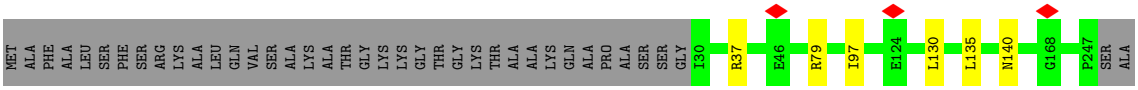
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain Q:



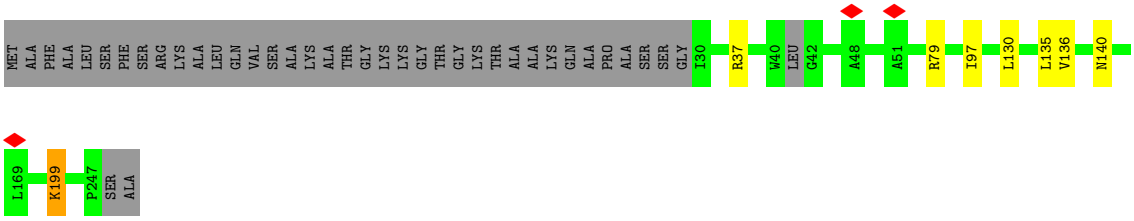
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain U:



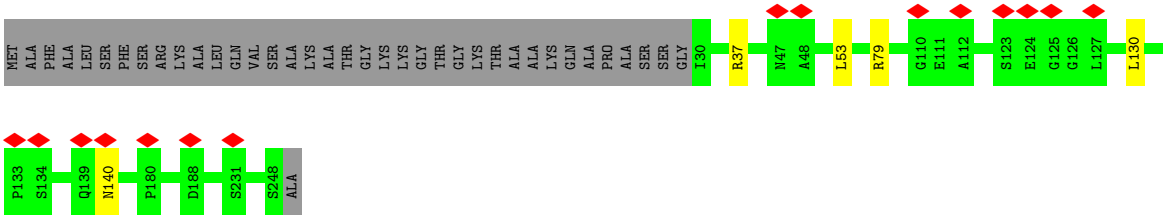
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain N:



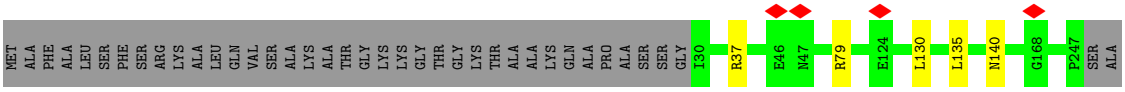
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain G:



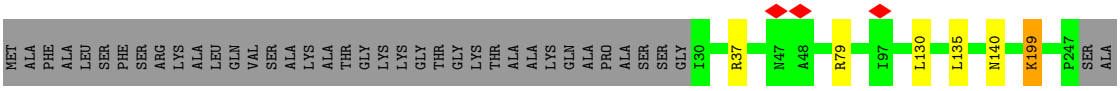
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain u:



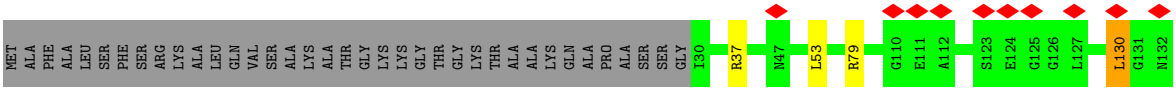
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

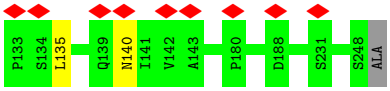
Chain n:



• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

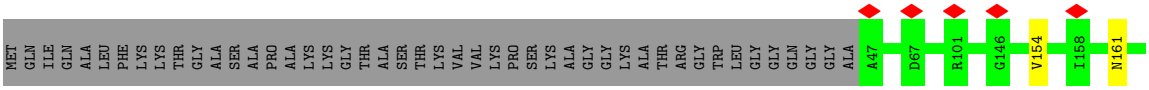
Chain g:

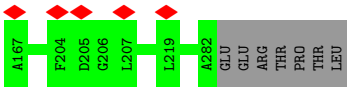




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

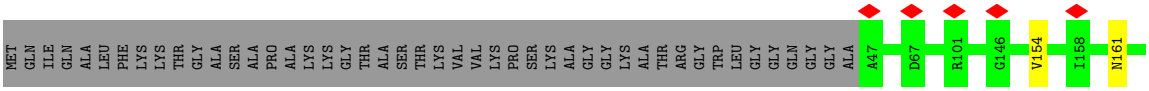
Chain S:

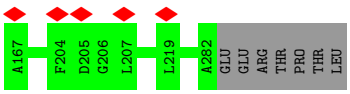




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

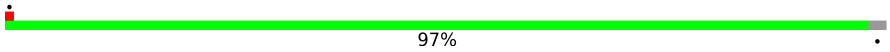
Chain s:

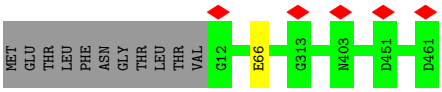




• Molecule 20: Photosystem II CP43 reaction center protein

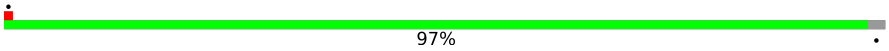
Chain C:

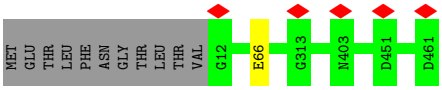




• Molecule 20: Photosystem II CP43 reaction center protein

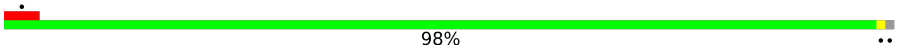
Chain c:

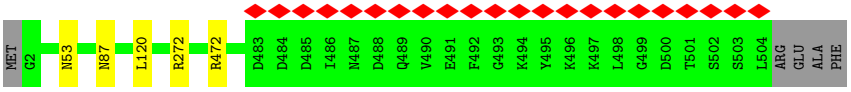




• Molecule 21: Photosystem II CP47 reaction center protein

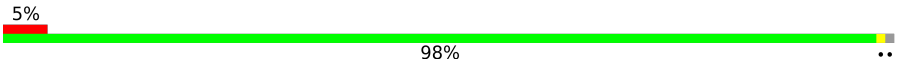
Chain B:

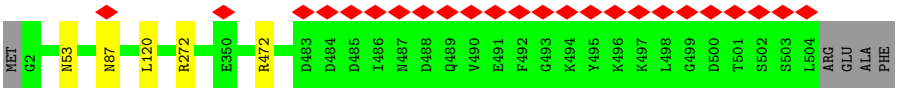




• Molecule 21: Photosystem II CP47 reaction center protein

Chain b:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.181	Depositor
Minimum map value	-1.592	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	392.1, 392.1, 392.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PHO, XAT, LHG, LMG, HEM, PL9, BCR, DGD, SQD, BCT, CHL, CL, LUT, NEX, FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	R	0.29	0/1736	0.55	0/2357
1	r	0.29	0/1739	0.55	0/2361
2	A	0.37	0/2696	0.55	1/3676 (0.0%)
2	a	0.37	0/2696	0.55	0/3676
3	D	0.38	0/2808	0.60	1/3830 (0.0%)
3	d	0.38	0/2808	0.60	1/3830 (0.0%)
4	F	0.31	0/250	0.51	0/338
4	f	0.32	0/250	0.52	0/338
5	H	0.33	0/499	0.55	0/683
5	h	0.32	0/499	0.55	0/683
6	I	0.42	0/283	0.58	0/383
6	i	0.42	0/283	0.58	0/383
7	J	0.28	0/254	0.49	0/345
7	j	0.27	0/254	0.48	0/345
8	K	0.40	0/300	0.65	0/414
8	k	0.40	0/300	0.64	0/414
9	L	0.33	0/314	0.51	0/427
9	l	0.33	0/314	0.51	0/427
10	M	0.30	0/252	0.53	0/345
10	m	0.30	0/252	0.54	0/345
11	O	0.30	0/1620	0.59	0/2184
11	o	0.30	0/1620	0.59	1/2184 (0.0%)
12	T	0.33	0/254	0.48	0/343
12	t	0.33	0/254	0.48	0/343
13	W	0.31	0/428	0.49	0/581
13	w	0.31	0/428	0.49	0/581
14	X	0.30	0/244	0.42	0/330
14	x	0.30	0/244	0.42	0/330
15	Z	0.29	0/476	0.49	0/654
15	z	0.29	0/476	0.49	0/654
16	Y	0.27	0/208	0.63	0/285
16	y	0.27	0/208	0.63	0/285

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	E	0.32	0/571	0.55	1/780 (0.1%)
17	e	0.32	0/571	0.56	1/780 (0.1%)
18	1	0.31	0/1717	0.56	1/2337 (0.0%)
18	2	0.33	0/1717	0.64	3/2337 (0.1%)
18	3	0.30	0/1723	0.57	2/2345 (0.1%)
18	4	0.31	0/1717	0.57	1/2337 (0.0%)
18	5	0.32	0/1717	0.60	2/2337 (0.1%)
18	6	0.31	0/1723	0.57	1/2345 (0.0%)
18	G	0.31	0/1723	0.59	2/2345 (0.1%)
18	N	0.33	0/1708	0.60	2/2323 (0.1%)
18	P	0.32	0/1717	0.60	3/2337 (0.1%)
18	Q	0.30	0/1723	0.58	2/2345 (0.1%)
18	U	0.33	0/1717	0.61	1/2337 (0.0%)
18	V	0.31	0/1717	0.57	1/2337 (0.0%)
18	g	0.31	0/1723	0.61	2/2345 (0.1%)
18	n	0.33	0/1717	0.62	2/2337 (0.1%)
18	p	0.32	0/1717	0.61	3/2337 (0.1%)
18	q	0.30	0/1723	0.58	1/2345 (0.0%)
18	u	0.33	0/1717	0.62	1/2337 (0.0%)
18	v	0.31	0/1717	0.58	1/2337 (0.0%)
19	S	0.33	0/1849	0.60	0/2521
19	s	0.33	0/1849	0.61	0/2521
20	C	0.34	0/3623	0.51	1/4936 (0.0%)
20	c	0.34	0/3623	0.51	1/4936 (0.0%)
21	B	0.33	0/4067	0.50	0/5533
21	b	0.33	0/4067	0.50	0/5533
All	All	0.33	0/76400	0.57	39/103994 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	r	0	1
18	1	0	1
18	2	0	2
18	3	0	1
18	4	0	2
18	5	0	1
18	6	0	2
18	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	P	0	1
18	Q	0	1
18	U	0	1
18	V	0	1
18	g	0	1
18	n	0	1
18	p	0	1
18	q	0	1
18	u	0	1
18	v	0	1
All	All	0	21

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	199	LYS	CD-CE-NZ	-8.78	91.50	111.70
18	5	199	LYS	CD-CE-NZ	-8.57	91.99	111.70
18	n	199	LYS	CD-CE-NZ	-8.17	92.92	111.70
18	p	199	LYS	CD-CE-NZ	-7.90	93.54	111.70
18	2	53	LEU	CA-CB-CG	7.88	133.43	115.30
18	N	199	LYS	CD-CE-NZ	-7.27	94.98	111.70
18	v	130	LEU	CA-CB-CG	7.13	131.71	115.30
18	q	130	LEU	CA-CB-CG	7.09	131.60	115.30
18	V	130	LEU	CA-CB-CG	7.08	131.59	115.30
18	P	199	LYS	CD-CE-NZ	-7.01	95.59	111.70
18	3	130	LEU	CA-CB-CG	6.97	131.32	115.30
18	G	130	LEU	CA-CB-CG	6.88	131.13	115.30
18	Q	130	LEU	CA-CB-CG	6.81	130.96	115.30
18	6	130	LEU	CA-CB-CG	6.67	130.63	115.30
18	u	130	LEU	CA-CB-CG	6.60	130.49	115.30
18	g	53	LEU	CA-CB-CG	6.48	130.21	115.30
18	n	130	LEU	CA-CB-CG	6.44	130.10	115.30
20	C	66	GLU	C-N-CA	6.23	137.27	121.70
18	P	130	LEU	CA-CB-CG	6.20	129.57	115.30
18	N	130	LEU	CA-CB-CG	6.20	129.56	115.30
18	G	53	LEU	CA-CB-CG	6.19	129.53	115.30
20	c	66	GLU	C-N-CA	6.12	137.01	121.70
18	2	130	LEU	CA-CB-CG	6.11	129.35	115.30
18	U	130	LEU	CA-CB-CG	6.11	129.34	115.30
2	A	343	LEU	CA-CB-CG	6.05	129.21	115.30
18	g	130	LEU	CA-CB-CG	6.00	129.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	130	LEU	CA-CB-CG	5.99	129.08	115.30
18	p	130	LEU	CA-CB-CG	5.98	129.06	115.30
18	5	130	LEU	CA-CB-CG	5.92	128.91	115.30
18	1	130	LEU	CA-CB-CG	5.91	128.89	115.30
17	e	50	PRO	C-N-CA	5.90	136.44	121.70
11	o	185	LEU	CA-CB-CG	5.45	127.84	115.30
18	P	135	LEU	CA-CB-CG	5.45	127.83	115.30
18	p	135	LEU	CA-CB-CG	5.45	127.83	115.30
3	d	209	LEU	CA-CB-CG	5.42	127.76	115.30
3	D	209	LEU	CA-CB-CG	5.39	127.70	115.30
18	3	53	LEU	CA-CB-CG	5.26	127.40	115.30
18	Q	53	LEU	CA-CB-CG	5.17	127.19	115.30
17	E	50	PRO	C-N-CA	5.16	134.60	121.70

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	1	135	LEU	Peptide
18	2	51	ALA	Peptide
18	2	52	TYR	Peptide
18	3	135	LEU	Peptide
18	4	135	LEU	Peptide
18	4	49	THR	Peptide
18	5	135	LEU	Peptide
18	6	135	LEU	Peptide
18	6	44	TYR	Peptide
18	N	135	LEU	Peptide
18	P	135	LEU	Peptide
18	Q	44	TYR	Peptide
18	U	135	LEU	Peptide
18	V	135	LEU	Peptide
18	g	135	LEU	Peptide
18	n	135	LEU	Peptide
18	p	135	LEU	Peptide
18	q	44	TYR	Peptide
1	r	15	LEU	Peptide
18	u	135	LEU	Peptide
18	v	135	LEU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	221/280 (79%)	201 (91%)	20 (9%)	0	100	100
1	r	221/280 (79%)	197 (89%)	24 (11%)	0	100	100
2	A	331/352 (94%)	314 (95%)	17 (5%)	0	100	100
2	a	331/352 (94%)	316 (96%)	15 (4%)	0	100	100
3	D	339/352 (96%)	304 (90%)	35 (10%)	0	100	100
3	d	339/352 (96%)	307 (91%)	32 (9%)	0	100	100
4	F	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
4	f	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
5	H	62/88 (70%)	61 (98%)	1 (2%)	0	100	100
5	h	62/88 (70%)	61 (98%)	1 (2%)	0	100	100
6	I	32/37 (86%)	29 (91%)	3 (9%)	0	100	100
6	i	32/37 (86%)	29 (91%)	3 (9%)	0	100	100
7	J	29/50 (58%)	27 (93%)	2 (7%)	0	100	100
7	j	29/50 (58%)	27 (93%)	2 (7%)	0	100	100
8	K	34/46 (74%)	30 (88%)	4 (12%)	0	100	100
8	k	34/46 (74%)	30 (88%)	4 (12%)	0	100	100
9	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
10	M	30/34 (88%)	30 (100%)	0	0	100	100
10	m	30/34 (88%)	30 (100%)	0	0	100	100
11	O	206/291 (71%)	176 (85%)	30 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	o	206/291 (71%)	175 (85%)	31 (15%)	0	100	100
12	T	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
12	t	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
13	W	52/115 (45%)	49 (94%)	3 (6%)	0	100	100
13	w	52/115 (45%)	49 (94%)	3 (6%)	0	100	100
14	X	33/101 (33%)	33 (100%)	0	0	100	100
14	x	33/101 (33%)	33 (100%)	0	0	100	100
15	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
15	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
16	Y	28/33 (85%)	26 (93%)	2 (7%)	0	100	100
16	y	28/33 (85%)	26 (93%)	2 (7%)	0	100	100
17	E	66/82 (80%)	58 (88%)	8 (12%)	0	100	100
17	e	66/82 (80%)	57 (86%)	9 (14%)	0	100	100
18	1	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	25	57
18	2	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	25	57
18	3	217/257 (84%)	191 (88%)	26 (12%)	0	100	100
18	4	216/257 (84%)	189 (88%)	26 (12%)	1 (0%)	25	57
18	5	216/257 (84%)	190 (88%)	26 (12%)	0	100	100
18	6	217/257 (84%)	190 (88%)	27 (12%)	0	100	100
18	G	217/257 (84%)	185 (85%)	32 (15%)	0	100	100
18	N	213/257 (83%)	188 (88%)	24 (11%)	1 (0%)	25	57
18	P	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	25	57
18	Q	217/257 (84%)	184 (85%)	33 (15%)	0	100	100
18	U	216/257 (84%)	187 (87%)	29 (13%)	0	100	100
18	V	216/257 (84%)	187 (87%)	29 (13%)	0	100	100
18	g	217/257 (84%)	183 (84%)	34 (16%)	0	100	100
18	n	216/257 (84%)	184 (85%)	32 (15%)	0	100	100
18	p	216/257 (84%)	186 (86%)	28 (13%)	2 (1%)	14	46
18	q	217/257 (84%)	186 (86%)	31 (14%)	0	100	100
18	u	216/257 (84%)	183 (85%)	33 (15%)	0	100	100
18	v	216/257 (84%)	186 (86%)	30 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	234/289 (81%)	201 (86%)	33 (14%)	0	100	100
19	s	234/289 (81%)	202 (86%)	32 (14%)	0	100	100
20	C	448/461 (97%)	429 (96%)	19 (4%)	0	100	100
20	c	448/461 (97%)	430 (96%)	18 (4%)	0	100	100
21	B	501/508 (99%)	472 (94%)	29 (6%)	0	100	100
21	b	501/508 (99%)	470 (94%)	31 (6%)	0	100	100
All	All	9485/11214 (85%)	8533 (90%)	945 (10%)	7 (0%)	50	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	2	52	TYR
18	p	136	VAL
18	P	136	VAL
18	1	136	VAL
18	N	136	VAL
18	p	174	PRO
18	4	136	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	175/218 (80%)	174 (99%)	1 (1%)	84	90
1	r	176/218 (81%)	175 (99%)	1 (1%)	84	90
2	A	272/289 (94%)	271 (100%)	1 (0%)	89	93
2	a	272/289 (94%)	271 (100%)	1 (0%)	89	93
3	D	272/281 (97%)	265 (97%)	7 (3%)	41	62
3	d	272/281 (97%)	265 (97%)	7 (3%)	41	62
4	F	24/37 (65%)	24 (100%)	0	100	100
4	f	24/37 (65%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	55/75 (73%)	55 (100%)	0	100	100
5	h	55/75 (73%)	55 (100%)	0	100	100
6	I	31/34 (91%)	29 (94%)	2 (6%)	14	41
6	i	31/34 (91%)	29 (94%)	2 (6%)	14	41
7	J	24/42 (57%)	24 (100%)	0	100	100
7	j	24/42 (57%)	24 (100%)	0	100	100
8	K	30/38 (79%)	30 (100%)	0	100	100
8	k	30/38 (79%)	30 (100%)	0	100	100
9	L	34/35 (97%)	34 (100%)	0	100	100
9	l	34/35 (97%)	34 (100%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	100	100
10	m	28/30 (93%)	28 (100%)	0	100	100
11	O	174/223 (78%)	173 (99%)	1 (1%)	84	90
11	o	174/223 (78%)	173 (99%)	1 (1%)	84	90
12	T	27/28 (96%)	27 (100%)	0	100	100
12	t	27/28 (96%)	27 (100%)	0	100	100
13	W	42/87 (48%)	42 (100%)	0	100	100
13	w	42/87 (48%)	42 (100%)	0	100	100
14	X	25/67 (37%)	25 (100%)	0	100	100
14	x	25/67 (37%)	25 (100%)	0	100	100
15	Z	52/52 (100%)	52 (100%)	0	100	100
15	z	52/52 (100%)	52 (100%)	0	100	100
16	Y	24/27 (89%)	24 (100%)	0	100	100
16	y	24/27 (89%)	24 (100%)	0	100	100
17	E	60/71 (84%)	60 (100%)	0	100	100
17	e	60/71 (84%)	60 (100%)	0	100	100
18	1	169/194 (87%)	166 (98%)	3 (2%)	54	71
18	2	169/194 (87%)	164 (97%)	5 (3%)	36	59
18	3	170/194 (88%)	166 (98%)	4 (2%)	44	64
18	4	169/194 (87%)	166 (98%)	3 (2%)	54	71
18	5	169/194 (87%)	164 (97%)	5 (3%)	36	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	6	170/194 (88%)	167 (98%)	3 (2%)	54	71
18	G	170/194 (88%)	167 (98%)	3 (2%)	54	71
18	N	168/194 (87%)	163 (97%)	5 (3%)	36	59
18	P	169/194 (87%)	164 (97%)	5 (3%)	36	59
18	Q	170/194 (88%)	167 (98%)	3 (2%)	54	71
18	U	169/194 (87%)	165 (98%)	4 (2%)	44	64
18	V	169/194 (87%)	165 (98%)	4 (2%)	44	64
18	g	170/194 (88%)	166 (98%)	4 (2%)	44	64
18	n	169/194 (87%)	165 (98%)	4 (2%)	44	64
18	p	169/194 (87%)	164 (97%)	5 (3%)	36	59
18	q	170/194 (88%)	167 (98%)	3 (2%)	54	71
18	u	169/194 (87%)	166 (98%)	3 (2%)	54	71
18	v	169/194 (87%)	165 (98%)	4 (2%)	44	64
19	S	181/217 (83%)	179 (99%)	2 (1%)	70	80
19	s	181/217 (83%)	179 (99%)	2 (1%)	70	80
20	C	352/362 (97%)	352 (100%)	0	100	100
20	c	352/362 (97%)	352 (100%)	0	100	100
21	B	403/407 (99%)	398 (99%)	5 (1%)	67	79
21	b	403/407 (99%)	398 (99%)	5 (1%)	67	79
All	All	7618/8732 (87%)	7510 (99%)	108 (1%)	62	76

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	r	168	ASN
2	a	266	ASN
3	d	26	ARG
3	d	85	MET
3	d	128	ARG
3	d	199	MET
3	d	210	LEU
3	d	236	ASN
3	d	304	ARG
6	i	6	ILE
6	i	34	LYS

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Mol	Chain	Res	Type
11	o	208	ARG
2	A	266	ASN
6	I	6	ILE
6	I	34	LYS
18	1	37	ARG
18	1	79	ARG
18	1	140	ASN
18	2	37	ARG
18	2	79	ARG
18	2	97	ILE
18	2	140	ASN
18	2	199	LYS
18	3	37	ARG
18	3	79	ARG
18	3	97	ILE
18	3	140	ASN
18	4	37	ARG
18	4	79	ARG
18	4	140	ASN
18	5	37	ARG
18	5	79	ARG
18	5	97	ILE
18	5	140	ASN
18	5	199	LYS
18	6	37	ARG
18	6	79	ARG
18	6	140	ASN
18	v	37	ARG
18	v	79	ARG
18	v	97	ILE
18	v	140	ASN
18	p	37	ARG
18	p	79	ARG
18	p	97	ILE
18	p	140	ASN
18	p	199	LYS
18	q	37	ARG
18	q	79	ARG
18	q	140	ASN
18	V	37	ARG
18	V	79	ARG
18	V	97	ILE

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Mol	Chain	Res	Type
18	V	140	ASN
18	P	37	ARG
18	P	79	ARG
18	P	97	ILE
18	P	140	ASN
18	P	199	LYS
18	Q	37	ARG
18	Q	79	ARG
18	Q	140	ASN
18	U	37	ARG
18	U	79	ARG
18	U	97	ILE
18	U	140	ASN
18	N	37	ARG
18	N	79	ARG
18	N	97	ILE
18	N	140	ASN
18	N	199	LYS
18	G	37	ARG
18	G	79	ARG
18	G	140	ASN
18	u	37	ARG
18	u	79	ARG
18	u	140	ASN
18	n	37	ARG
18	n	79	ARG
18	n	140	ASN
18	n	199	LYS
18	g	37	ARG
18	g	79	ARG
18	g	130	LEU
18	g	140	ASN
1	R	168	ASN
19	S	154	VAL
19	S	161	ASN
21	B	53	ASN
21	B	87	ASN
21	B	120	LEU
21	B	272	ARG
21	B	472	ARG
11	O	208	ARG
3	D	26	ARG

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Mol	Chain	Res	Type
3	D	85	MET
3	D	128	ARG
3	D	199	MET
3	D	210	LEU
3	D	236	ASN
3	D	304	ARG
21	b	53	ASN
21	b	87	ASN
21	b	120	LEU
21	b	272	ARG
21	b	472	ARG
19	s	154	VAL
19	s	161	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	r	55	GLN
1	r	56	ASN
1	r	168	ASN
2	a	181	ASN
2	a	266	ASN
2	a	296	ASN
2	a	338	ASN
3	d	83	ASN
3	d	98	GLN
3	d	129	GLN
3	d	142	ASN
3	d	194	ASN
3	d	236	ASN
3	d	239	GLN
3	d	255	GLN
3	d	292	ASN
3	d	350	ASN
4	f	40	GLN
5	h	69	ASN
11	o	266	GLN
2	A	181	ASN
2	A	195	HIS
2	A	266	ASN
2	A	296	ASN
2	A	338	ASN

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Mol	Chain	Res	Type
17	E	75	GLN
4	F	40	GLN
5	H	69	ASN
18	1	140	ASN
18	2	140	ASN
18	3	47	ASN
18	3	120	GLN
18	3	140	ASN
18	3	225	ASN
18	3	236	ASN
18	4	140	ASN
18	5	140	ASN
18	6	120	GLN
18	6	140	ASN
18	6	236	ASN
18	v	140	ASN
18	v	232	ASN
18	p	140	ASN
18	p	214	GLN
18	p	225	ASN
18	p	232	ASN
18	q	120	GLN
18	q	140	ASN
18	q	229	HIS
18	q	237	ASN
18	V	140	ASN
18	V	236	ASN
18	P	140	ASN
18	P	232	ASN
18	Q	120	GLN
18	Q	140	ASN
18	Q	161	ASN
18	Q	229	HIS
18	Q	237	ASN
18	U	140	ASN
18	N	140	ASN
18	N	229	HIS
18	G	47	ASN
18	G	120	GLN
18	G	140	ASN
18	u	140	ASN
18	n	140	ASN

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Mol	Chain	Res	Type
18	n	225	ASN
18	g	140	ASN
1	R	53	ASN
1	R	55	GLN
1	R	56	ASN
1	R	168	ASN
19	S	127	ASN
19	S	161	ASN
19	S	263	ASN
20	C	310	GLN
21	B	9	HIS
21	B	14	ASN
21	B	53	ASN
21	B	87	ASN
21	B	157	HIS
21	B	282	GLN
21	B	331	ASN
11	O	266	GLN
3	D	83	ASN
3	D	98	GLN
3	D	129	GLN
3	D	142	ASN
3	D	194	ASN
3	D	236	ASN
3	D	239	GLN
3	D	255	GLN
3	D	292	ASN
3	D	350	ASN
21	b	9	HIS
21	b	14	ASN
21	b	53	ASN
21	b	87	ASN
21	b	114	HIS
21	b	157	HIS
21	b	282	GLN
21	b	331	ASN
17	e	75	GLN
20	c	147	ASN
20	c	310	GLN
20	c	320	GLN
19	s	127	ASN
19	s	263	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 552 ligands modelled in this entry, 6 are monoatomic - leaving 546 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	LUT	s	310	19	42,43,43	0.79	0	51,60,60	1.72	13 (25%)
22	CLA	U	306	-	60,68,73	1.57	9 (15%)	70,107,113	1.43	8 (11%)
22	CLA	u	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.37	7 (9%)
26	CHL	U	314	-	50,58,74	2.15	14 (28%)	52,94,114	2.70	20 (38%)
31	BCR	X	201	-	41,41,41	4.79	24 (58%)	56,56,56	2.26	17 (30%)
26	CHL	6	301	-	66,74,74	1.91	16 (24%)	73,114,114	2.45	22 (30%)
22	CLA	c	511	20,8	65,73,73	1.48	9 (13%)	76,113,113	1.29	7 (9%)
26	CHL	u	317	18	66,74,74	1.86	15 (22%)	73,114,114	2.52	24 (32%)
26	CHL	G	316	-	61,69,74	1.95	15 (24%)	67,108,114	2.49	22 (32%)
26	CHL	2	314	-	48,56,74	2.38	17 (35%)	51,92,114	2.95	21 (41%)
22	CLA	g	305	22	60,68,73	1.52	8 (13%)	70,107,113	1.50	10 (14%)
22	CLA	n	306	-	60,68,73	1.49	6 (10%)	70,107,113	1.55	8 (11%)
37	HEM	e	101	4,17	41,50,50	1.59	5 (12%)	45,82,82	1.14	2 (4%)
22	CLA	C	512	20,8	65,73,73	1.48	9 (13%)	76,113,113	1.28	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	LUT	2	310	-	42,43,43	0.78	0	51,60,60	1.64	12 (23%)
24	XAT	p	312	-	39,47,47	2.59	18 (46%)	54,74,74	11.83	18 (33%)
26	CHL	V	318	-	66,74,74	1.94	16 (24%)	73,114,114	2.32	21 (28%)
22	CLA	3	306	22	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
22	CLA	5	302	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
26	CHL	P	318	-	66,74,74	1.85	14 (21%)	73,114,114	2.42	22 (30%)
23	LUT	5	309	-	42,43,43	0.76	0	51,60,60	1.75	13 (25%)
23	LUT	u	309	-	42,43,43	0.75	0	51,60,60	1.52	10 (19%)
22	CLA	Q	301	-	65,73,73	1.49	7 (10%)	76,113,113	1.42	7 (9%)
22	CLA	c	509	-	65,73,73	1.53	9 (13%)	76,113,113	1.52	9 (11%)
25	LHG	D	407	3	48,48,48	0.90	4 (8%)	51,54,54	1.07	3 (5%)
26	CHL	U	315	-	66,74,74	1.85	14 (21%)	73,114,114	2.47	23 (31%)
25	LHG	s	312	19	48,48,48	0.89	4 (8%)	51,54,54	1.14	3 (5%)
22	CLA	3	305	22	60,68,73	1.51	6 (10%)	70,107,113	1.52	10 (14%)
22	CLA	p	303	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	8 (10%)
26	CHL	3	315	18	66,74,74	1.89	16 (24%)	73,114,114	2.44	20 (27%)
26	CHL	N	315	-	50,58,74	2.17	16 (32%)	52,94,114	2.72	21 (40%)
22	CLA	s	309	-	49,57,73	1.67	8 (16%)	55,93,113	1.56	6 (10%)
22	CLA	c	507	-	65,73,73	1.52	9 (13%)	76,113,113	1.45	8 (10%)
23	LUT	4	309	-	42,43,43	0.73	0	51,60,60	1.60	11 (21%)
26	CHL	4	314	-	48,56,74	2.20	14 (29%)	51,92,114	2.87	21 (41%)
34	LMG	D	408	3	46,46,55	1.26	6 (13%)	54,54,63	1.02	2 (3%)
22	CLA	P	305	18	65,73,73	1.42	6 (9%)	76,113,113	1.45	8 (10%)
34	LMG	w	201	-	48,48,55	1.23	6 (12%)	56,56,63	1.12	4 (7%)
26	CHL	5	318	-	66,74,74	1.88	14 (21%)	73,114,114	2.37	23 (31%)
22	CLA	3	307	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
26	CHL	u	318	-	66,74,74	1.85	14 (21%)	73,114,114	2.38	21 (28%)
22	CLA	u	304	-	60,68,73	1.48	7 (11%)	70,107,113	1.55	7 (10%)
25	LHG	c	522	-	48,48,48	0.90	3 (6%)	51,54,54	1.07	2 (3%)
31	BCR	B	619	-	41,41,41	4.74	24 (58%)	56,56,56	2.26	22 (39%)
22	CLA	2	306	-	60,68,73	1.48	7 (11%)	70,107,113	1.56	8 (11%)
31	BCR	C	516	-	41,41,41	4.76	24 (58%)	56,56,56	2.30	20 (35%)
26	CHL	U	316	18	66,74,74	1.87	15 (22%)	73,114,114	2.56	24 (32%)
31	BCR	c	516	-	41,41,41	4.76	24 (58%)	56,56,56	2.30	21 (37%)
22	CLA	N	306	-	60,68,73	1.50	6 (10%)	70,107,113	1.55	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	G	308	-	48,56,73	1.71	7 (14%)	55,92,113	1.58	7 (12%)
24	XAT	G	309	-	39,47,47	2.53	17 (43%)	54,74,74	11.82	19 (35%)
26	CHL	1	317	18	66,74,74	1.90	15 (22%)	73,114,114	2.52	26 (35%)
22	CLA	Q	305	22	60,68,73	1.52	7 (11%)	70,107,113	1.41	7 (10%)
27	NEX	5	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.43	16 (32%)
23	LUT	S	310	-	42,43,43	0.77	0	51,60,60	1.69	14 (27%)
22	CLA	B	616	21	65,73,73	1.42	9 (13%)	76,113,113	1.45	9 (11%)
22	CLA	u	307	-	65,73,73	1.44	8 (12%)	76,113,113	1.46	8 (10%)
22	CLA	Q	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.54	8 (14%)
26	CHL	2	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.37	20 (27%)
22	CLA	q	303	-	50,58,73	1.69	6 (12%)	58,95,113	1.64	9 (15%)
26	CHL	n	317	-	66,74,74	1.92	17 (25%)	73,114,114	2.48	22 (30%)
22	CLA	B	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	6 (7%)
27	NEX	V	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.46	16 (32%)
31	BCR	B	620	-	41,41,41	4.75	24 (58%)	56,56,56	2.28	23 (41%)
26	CHL	U	317	-	66,74,74	1.86	14 (21%)	73,114,114	2.38	19 (26%)
22	CLA	C	504	-	65,73,73	1.49	10 (15%)	76,113,113	1.52	7 (9%)
22	CLA	6	302	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
22	CLA	B	610	-	65,73,73	1.48	8 (12%)	76,113,113	1.46	9 (11%)
31	BCR	C	518	-	41,41,41	4.75	24 (58%)	56,56,56	2.29	19 (33%)
34	LMG	d	407	3	46,46,55	1.26	6 (13%)	54,54,63	1.01	2 (3%)
26	CHL	2	317	-	66,74,74	1.86	13 (19%)	73,114,114	2.45	23 (31%)
26	CHL	g	311	-	66,74,74	1.89	15 (22%)	73,114,114	2.40	22 (30%)
31	BCR	A	409	-	41,41,41	4.74	24 (58%)	56,56,56	2.25	22 (39%)
23	LUT	P	310	-	42,43,43	0.73	0	51,60,60	1.67	14 (27%)
24	XAT	r	612	-	39,47,47	2.52	17 (43%)	54,74,74	11.45	25 (46%)
22	CLA	1	306	-	60,68,73	1.52	9 (15%)	70,107,113	1.45	9 (12%)
22	CLA	u	303	-	50,58,73	1.69	8 (16%)	58,95,113	1.59	8 (13%)
34	LMG	a	412	-	40,40,55	1.30	6 (15%)	48,48,63	1.16	2 (4%)
22	CLA	c	506	-	65,73,73	1.40	7 (10%)	76,113,113	1.65	9 (11%)
23	LUT	U	310	-	42,43,43	0.79	0	51,60,60	1.61	9 (17%)
25	LHG	N	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
26	CHL	g	313	-	50,58,74	2.19	14 (28%)	52,94,114	2.75	18 (34%)
25	LHG	v	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
25	LHG	p	313	-	48,48,48	0.90	4 (8%)	51,54,54	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	CLA	b	605	21	65,73,73	1.46	9 (13%)	76,113,113	1.75	11 (14%)
22	CLA	N	305	18	60,68,73	1.49	6 (10%)	70,107,113	1.93	13 (18%)
27	NEX	N	318	-	38,46,46	0.93	2 (5%)	50,70,70	2.40	17 (34%)
26	CHL	4	316	18	66,74,74	1.91	15 (22%)	73,114,114	2.48	26 (35%)
22	CLA	A	404	-	65,73,73	1.41	8 (12%)	76,113,113	1.59	8 (10%)
23	LUT	v	310	-	42,43,43	0.77	0	51,60,60	1.63	10 (19%)
27	NEX	u	319	-	38,46,46	0.93	1 (2%)	50,70,70	2.45	18 (36%)
32	SQD	l	102	9	53,54,54	0.93	4 (7%)	62,65,65	1.80	12 (19%)
22	CLA	3	301	-	65,73,73	1.47	7 (10%)	76,113,113	1.45	7 (9%)
26	CHL	S	314	-	46,54,74	2.28	16 (34%)	49,90,114	2.86	18 (36%)
26	CHL	n	315	-	50,58,74	2.22	16 (32%)	52,94,114	2.72	21 (40%)
35	BCT	a	414	-	2,3,3	1.35	0	2,3,3	0.20	0
30	PHO	A	407	-	51,69,69	1.09	5 (9%)	47,99,99	1.23	6 (12%)
22	CLA	a	405	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
22	CLA	s	304	19	45,53,73	1.75	6 (13%)	52,89,113	1.58	6 (11%)
23	LUT	V	309	-	42,43,43	0.78	0	51,60,60	1.63	13 (25%)
26	CHL	4	317	-	66,74,74	1.88	15 (22%)	73,114,114	2.41	22 (30%)
26	CHL	V	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.43	21 (28%)
33	PL9	A	410	-	13,13,55	3.64	7 (53%)	17,17,69	1.47	3 (17%)
33	PL9	D	405	-	55,55,55	1.54	6 (10%)	68,69,69	1.68	18 (26%)
26	CHL	6	317	-	61,69,74	1.99	13 (21%)	67,108,114	2.52	22 (32%)
22	CLA	r	602	-	60,68,73	1.53	6 (10%)	70,107,113	1.47	7 (10%)
22	CLA	6	303	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	7 (9%)
22	CLA	u	301	-	65,73,73	1.50	9 (13%)	76,113,113	1.41	6 (7%)
22	CLA	1	307	-	65,73,73	1.44	8 (12%)	76,113,113	1.47	9 (11%)
22	CLA	C	515	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	9 (11%)
22	CLA	G	307	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	7 (9%)
22	CLA	R	311	-	45,53,73	1.78	6 (13%)	52,89,113	1.65	6 (11%)
24	XAT	N	311	-	39,47,47	2.53	17 (43%)	54,74,74	11.91	18 (33%)
26	CHL	S	315	19	58,66,74	2.14	16 (27%)	63,104,114	2.44	20 (31%)
22	CLA	q	301	-	65,73,73	1.50	7 (10%)	76,113,113	1.42	7 (9%)
31	BCR	t	101	-	41,41,41	4.79	24 (58%)	56,56,56	2.38	22 (39%)
22	CLA	p	308	-	60,68,73	1.53	7 (11%)	70,107,113	1.50	6 (8%)
26	CHL	r	614	-	66,74,74	1.88	13 (19%)	73,114,114	2.43	22 (30%)
31	BCR	a	409	-	41,41,41	4.73	24 (58%)	56,56,56	2.22	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
27	NEX	s	317	19	38,46,46	0.87	1 (2%)	50,70,70	2.39	16 (32%)
22	CLA	6	307	22	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
30	PHO	D	401	-	51,69,69	1.03	4 (7%)	47,99,99	1.32	6 (12%)
22	CLA	1	305	-	60,68,73	1.49	6 (10%)	70,107,113	1.45	8 (11%)
25	LHG	3	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.11	2 (3%)
22	CLA	c	510	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	9 (11%)
22	CLA	U	305	-	60,68,73	1.52	7 (11%)	70,107,113	1.45	7 (10%)
22	CLA	n	305	18	60,68,73	1.51	7 (11%)	70,107,113	2.08	16 (22%)
22	CLA	R	307	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	6 (7%)
22	CLA	s	306	-	56,64,73	1.59	8 (14%)	65,102,113	1.51	10 (15%)
25	LHG	S	312	19	48,48,48	0.89	4 (8%)	51,54,54	1.13	3 (5%)
22	CLA	2	307	-	60,68,73	1.51	6 (10%)	70,107,113	1.50	7 (10%)
22	CLA	S	305	-	55,63,73	1.57	7 (12%)	64,101,113	1.49	7 (10%)
22	CLA	c	503	-	65,73,73	1.49	10 (15%)	76,113,113	1.51	7 (9%)
26	CHL	1	316	-	66,74,74	1.91	16 (24%)	73,114,114	2.45	22 (30%)
22	CLA	V	305	-	60,68,73	1.53	6 (10%)	70,107,113	1.48	7 (10%)
22	CLA	G	303	-	50,58,73	1.69	7 (14%)	58,95,113	1.62	7 (12%)
22	CLA	S	309	-	49,57,73	1.69	8 (16%)	55,93,113	1.55	6 (10%)
25	LHG	C	524	-	48,48,48	0.90	4 (8%)	51,54,54	1.13	2 (3%)
31	BCR	c	515	-	41,41,41	4.70	24 (58%)	56,56,56	2.67	23 (41%)
26	CHL	5	313	18	66,74,74	2.00	17 (25%)	73,114,114	2.39	21 (28%)
22	CLA	b	602	-	65,73,73	1.42	9 (13%)	76,113,113	1.44	7 (9%)
26	CHL	q	311	-	66,74,74	1.89	15 (22%)	73,114,114	2.43	22 (30%)
37	HEM	E	101	4,17	41,50,50	1.60	6 (14%)	45,82,82	1.15	2 (4%)
26	CHL	u	313	-	66,74,74	1.94	17 (25%)	73,114,114	2.37	23 (31%)
25	LHG	c	523	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
22	CLA	1	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	7 (12%)
31	BCR	T	101	-	41,41,41	4.79	24 (58%)	56,56,56	2.38	22 (39%)
26	CHL	g	312	-	48,56,74	2.27	14 (29%)	51,92,114	2.77	21 (41%)
31	BCR	b	620	-	41,41,41	4.77	24 (58%)	56,56,56	2.21	21 (37%)
22	CLA	4	308	-	48,56,73	1.69	6 (12%)	55,92,113	1.60	7 (12%)
33	PL9	d	404	-	55,55,55	1.54	6 (10%)	68,69,69	1.68	18 (26%)
22	CLA	q	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	8 (10%)
22	CLA	b	610	-	65,73,73	1.47	8 (12%)	76,113,113	1.45	9 (11%)
30	PHO	a	407	-	51,69,69	1.08	5 (9%)	47,99,99	1.23	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	CLA	b	614	-	65,73,73	1.43	9 (13%)	76,113,113	1.42	7 (9%)
23	LUT	U	309	-	42,43,43	0.74	0	51,60,60	1.54	10 (19%)
22	CLA	6	309	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)
22	CLA	3	303	-	50,58,73	1.68	7 (14%)	58,95,113	1.62	8 (13%)
24	XAT	n	311	-	39,47,47	2.53	18 (46%)	54,74,74	11.76	23 (42%)
25	LHG	n	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.03	2 (3%)
22	CLA	V	303	-	50,58,73	1.66	8 (16%)	58,95,113	1.66	8 (13%)
26	CHL	p	319	-	66,74,74	1.90	15 (22%)	73,114,114	2.37	22 (30%)
27	NEX	U	318	-	38,46,46	0.96	1 (2%)	50,70,70	2.38	12 (24%)
22	CLA	s	305	-	55,63,73	1.58	7 (12%)	64,101,113	1.49	8 (12%)
22	CLA	3	304	18	64,72,73	1.47	8 (12%)	74,111,113	1.52	9 (12%)
22	CLA	x	201	14	65,73,73	1.40	7 (10%)	76,113,113	1.53	8 (10%)
22	CLA	u	308	-	48,56,73	1.70	8 (16%)	55,92,113	1.57	7 (12%)
22	CLA	g	304	18	64,72,73	1.48	7 (10%)	74,111,113	1.50	8 (10%)
22	CLA	v	304	-	60,68,73	1.50	6 (10%)	70,107,113	1.52	7 (10%)
22	CLA	G	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.51	6 (7%)
22	CLA	B	604	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	7 (9%)
22	CLA	c	514	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	10 (13%)
25	LHG	2	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	q	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	8 (14%)
22	CLA	C	511	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	11 (14%)
34	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.07	2 (3%)
22	CLA	b	615	-	65,73,73	1.43	8 (12%)	76,113,113	1.49	7 (9%)
22	CLA	b	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.42	7 (9%)
22	CLA	6	305	18	64,72,73	1.47	7 (10%)	74,111,113	1.50	9 (12%)
22	CLA	v	306	-	60,68,73	1.55	8 (13%)	70,107,113	1.46	9 (12%)
22	CLA	C	507	-	65,73,73	1.39	7 (10%)	76,113,113	1.64	9 (11%)
30	PHO	d	401	-	51,69,69	1.03	4 (7%)	47,99,99	1.32	6 (12%)
22	CLA	C	509	20	65,73,73	1.46	9 (13%)	76,113,113	1.53	10 (13%)
22	CLA	b	613	-	65,73,73	1.44	8 (12%)	76,113,113	1.46	10 (13%)
26	CHL	r	616	-	61,69,74	2.02	17 (27%)	67,108,114	2.36	19 (28%)
26	CHL	s	313	-	46,54,74	2.34	16 (34%)	49,90,114	2.82	20 (40%)
22	CLA	B	602	-	65,73,73	1.43	9 (13%)	76,113,113	1.45	10 (13%)
26	CHL	u	314	-	48,56,74	2.22	16 (33%)	51,92,114	2.79	21 (41%)
22	CLA	R	305	-	48,56,73	1.73	6 (12%)	55,92,113	1.63	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CHL	s	316	-	46,54,74	2.37	16 (34%)	49,90,114	2.82	20 (40%)
34	LMG	A	411	-	40,40,55	1.30	6 (15%)	48,48,63	1.16	2 (4%)
22	CLA	b	611	-	65,73,73	1.48	8 (12%)	76,113,113	1.49	8 (10%)
26	CHL	P	317	-	66,74,74	1.93	17 (25%)	73,114,114	2.42	24 (32%)
26	CHL	N	316	-	66,74,74	1.86	15 (22%)	73,114,114	2.48	21 (28%)
22	CLA	r	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.46	6 (8%)
26	CHL	4	315	-	50,58,74	2.25	16 (32%)	52,94,114	2.67	19 (36%)
26	CHL	q	314	18	66,74,74	1.88	17 (25%)	73,114,114	2.48	20 (27%)
26	CHL	g	314	-	66,74,74	1.96	16 (24%)	73,114,114	2.41	23 (31%)
32	SQD	m	101	-	41,42,54	1.06	5 (12%)	50,53,65	1.75	11 (22%)
22	CLA	6	308	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
22	CLA	r	605	-	58,66,73	1.56	6 (10%)	67,104,113	1.53	6 (8%)
22	CLA	U	303	-	50,58,73	1.68	9 (18%)	58,95,113	1.56	7 (12%)
25	LHG	d	405	3	45,45,48	0.92	4 (8%)	48,51,54	1.07	2 (4%)
25	LHG	r	613	-	41,41,48	0.96	3 (7%)	44,47,54	1.09	2 (4%)
22	CLA	s	301	19	61,69,73	1.49	8 (13%)	71,108,113	1.53	11 (15%)
22	CLA	r	606	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
22	CLA	S	303	19	50,58,73	1.67	7 (14%)	58,95,113	1.63	8 (13%)
22	CLA	G	305	22	60,68,73	1.51	7 (11%)	70,107,113	1.53	8 (11%)
26	CHL	R	317	-	61,69,74	2.01	17 (27%)	67,108,114	2.38	20 (29%)
22	CLA	2	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.59	7 (12%)
22	CLA	b	607	-	65,73,73	1.48	9 (13%)	76,113,113	1.51	8 (10%)
26	CHL	n	314	-	48,56,74	2.35	17 (35%)	51,92,114	2.84	20 (39%)
23	LUT	N	310	-	42,43,43	0.78	0	51,60,60	1.69	15 (29%)
26	CHL	6	314	-	50,58,74	2.29	16 (32%)	52,94,114	2.62	22 (42%)
22	CLA	S	304	19	45,53,73	1.75	6 (13%)	52,89,113	1.58	6 (11%)
34	LMG	B	621	-	51,51,55	1.18	6 (11%)	59,59,63	1.44	6 (10%)
22	CLA	N	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	6 (7%)
22	CLA	1	302	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	7 (9%)
22	CLA	R	304	-	60,68,73	1.53	5 (8%)	70,107,113	1.48	6 (8%)
22	CLA	n	302	-	65,73,73	1.52	7 (10%)	76,113,113	1.37	7 (9%)
32	SQD	A	412	-	53,54,54	0.95	5 (9%)	62,65,65	1.50	10 (16%)
34	LMG	W	201	-	48,48,55	1.23	6 (12%)	56,56,63	1.12	4 (7%)
25	LHG	P	313	-	48,48,48	0.90	4 (8%)	51,54,54	1.07	2 (3%)
26	CHL	p	317	-	66,74,74	1.91	16 (24%)	73,114,114	2.41	21 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
26	CHL	v	316	-	66,74,74	1.89	16 (24%)	73,114,114	2.46	24 (32%)
26	CHL	q	313	-	50,58,74	2.18	16 (32%)	52,94,114	2.73	19 (36%)
22	CLA	v	305	-	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
22	CLA	s	307	-	49,57,73	1.66	7 (14%)	55,93,113	1.64	8 (14%)
25	LHG	A	413	2	42,42,48	0.93	3 (7%)	45,48,54	1.11	2 (4%)
27	NEX	S	317	19	38,46,46	0.88	1 (2%)	50,70,70	2.45	17 (34%)
24	XAT	3	309	-	39,47,47	2.56	18 (46%)	54,74,74	11.80	17 (31%)
26	CHL	V	317	18	66,74,74	1.91	15 (22%)	73,114,114	2.51	25 (34%)
22	CLA	B	614	-	65,73,73	1.44	9 (13%)	76,113,113	1.43	7 (9%)
22	CLA	P	304	-	50,58,73	1.67	8 (16%)	58,95,113	1.58	8 (13%)
22	CLA	3	302	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
22	CLA	5	303	-	50,58,73	1.67	8 (16%)	58,95,113	1.58	8 (13%)
26	CHL	Q	311	-	66,74,74	1.90	16 (24%)	73,114,114	2.44	23 (31%)
22	CLA	S	306	-	56,64,73	1.59	8 (14%)	65,102,113	1.51	8 (12%)
26	CHL	G	314	-	66,74,74	1.94	16 (24%)	73,114,114	2.32	21 (28%)
22	CLA	V	302	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
22	CLA	r	607	1	49,57,73	1.68	6 (12%)	55,93,113	1.66	9 (16%)
22	CLA	q	304	18	64,72,73	1.47	7 (10%)	74,111,113	1.63	8 (10%)
22	CLA	N	307	-	60,68,73	1.52	7 (11%)	70,107,113	1.48	7 (10%)
26	CHL	g	315	18	66,74,74	1.87	14 (21%)	73,114,114	2.44	20 (27%)
26	CHL	5	314	-	48,56,74	2.35	17 (35%)	51,92,114	2.83	20 (39%)
22	CLA	V	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	7 (9%)
22	CLA	X	202	14	65,73,73	1.40	7 (10%)	76,113,113	1.52	8 (10%)
27	NEX	P	301	18	38,46,46	0.94	1 (2%)	50,70,70	2.35	18 (36%)
22	CLA	P	307	-	60,68,73	1.48	6 (10%)	70,107,113	1.50	8 (11%)
26	CHL	r	615	-	56,64,74	2.05	15 (26%)	61,102,114	2.61	21 (34%)
26	CHL	S	316	-	46,54,74	2.36	16 (34%)	49,90,114	2.81	20 (40%)
23	LUT	5	310	-	42,43,43	0.77	0	51,60,60	1.64	12 (23%)
36	DGD	c	519	-	61,61,67	1.25	6 (9%)	75,75,81	1.17	3 (4%)
34	LMG	C	502	-	51,51,55	1.15	4 (7%)	59,59,63	1.16	3 (5%)
33	PL9	a	411	-	13,13,55	3.63	7 (53%)	17,17,69	1.48	3 (17%)
24	XAT	v	311	-	39,47,47	2.56	18 (46%)	54,74,74	12.01	19 (35%)
22	CLA	d	402	3	65,73,73	1.43	9 (13%)	76,113,113	1.39	8 (10%)
22	CLA	P	306	18	60,68,73	1.48	6 (10%)	70,107,113	2.01	12 (17%)
22	CLA	v	301	-	65,73,73	1.49	9 (13%)	76,113,113	1.35	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	S	301	19	61,69,73	1.48	7 (11%)	71,108,113	1.52	10 (14%)
26	CHL	p	315	-	48,56,74	2.41	17 (35%)	51,92,114	2.76	19 (37%)
26	CHL	n	316	-	66,74,74	1.91	15 (22%)	73,114,114	2.35	21 (28%)
26	CHL	P	316	-	50,58,74	2.24	16 (32%)	52,94,114	2.70	20 (38%)
22	CLA	P	302	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	7 (9%)
22	CLA	g	306	22	60,68,73	1.56	7 (11%)	70,107,113	1.39	6 (8%)
22	CLA	R	310	-	60,68,73	1.54	5 (8%)	70,107,113	1.55	9 (12%)
22	CLA	B	605	21	65,73,73	1.46	9 (13%)	76,113,113	1.76	13 (17%)
26	CHL	G	315	18	66,74,74	1.87	16 (24%)	73,114,114	2.42	20 (27%)
32	SQD	a	413	-	53,54,54	0.95	5 (9%)	62,65,65	1.51	9 (14%)
24	XAT	P	312	-	39,47,47	2.59	18 (46%)	54,74,74	11.98	19 (35%)
26	CHL	v	315	-	50,58,74	2.23	16 (32%)	52,94,114	2.70	21 (40%)
25	LHG	5	312	-	48,48,48	0.90	3 (6%)	51,54,54	1.07	2 (3%)
22	CLA	5	307	-	60,68,73	1.51	7 (11%)	70,107,113	1.48	7 (10%)
34	LMG	b	621	-	51,51,55	1.18	6 (11%)	59,59,63	1.44	7 (11%)
26	CHL	U	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.41	22 (30%)
25	LHG	q	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.05	2 (3%)
31	BCR	d	403	3	41,41,41	4.76	24 (58%)	56,56,56	2.26	23 (41%)
22	CLA	b	604	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	7 (9%)
24	XAT	4	311	-	39,47,47	2.54	17 (43%)	54,74,74	12.07	21 (38%)
26	CHL	g	316	-	61,69,74	1.97	16 (26%)	67,108,114	2.48	25 (37%)
22	CLA	b	609	-	65,73,73	1.45	8 (12%)	76,113,113	1.46	6 (7%)
22	CLA	U	307	-	65,73,73	1.45	9 (13%)	76,113,113	1.45	7 (9%)
22	CLA	3	308	-	48,56,73	1.71	6 (12%)	55,92,113	1.58	7 (12%)
22	CLA	R	302	27	49,57,73	1.73	7 (14%)	55,93,113	1.62	8 (14%)
22	CLA	5	306	-	60,68,73	1.47	7 (11%)	70,107,113	1.55	7 (10%)
22	CLA	R	303	-	60,68,73	1.52	6 (10%)	70,107,113	1.48	8 (11%)
22	CLA	S	307	-	49,57,73	1.66	7 (14%)	55,93,113	1.65	8 (14%)
22	CLA	U	301	-	65,73,73	1.49	9 (13%)	76,113,113	1.41	7 (9%)
22	CLA	n	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	7 (9%)
22	CLA	c	504	-	65,73,73	1.44	9 (13%)	76,113,113	1.43	7 (9%)
26	CHL	3	313	-	50,58,74	2.26	16 (32%)	52,94,114	2.63	21 (40%)
26	CHL	G	312	-	48,56,74	2.32	18 (37%)	51,92,114	2.82	20 (39%)
22	CLA	c	505	-	65,73,73	1.46	9 (13%)	76,113,113	1.45	7 (9%)
22	CLA	b	608	-	65,73,73	1.44	7 (10%)	76,113,113	1.52	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	CLA	4	305	-	60,68,73	1.51	7 (11%)	70,107,113	1.42	8 (11%)
22	CLA	V	301	-	65,73,73	1.51	9 (13%)	76,113,113	1.33	6 (7%)
36	DGD	C	520	-	63,63,67	1.22	6 (9%)	77,77,81	1.16	4 (5%)
22	CLA	1	301	-	65,73,73	1.48	9 (13%)	76,113,113	1.41	7 (9%)
26	CHL	5	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.36	21 (28%)
26	CHL	n	318	-	66,74,74	1.95	16 (24%)	73,114,114	2.35	23 (31%)
31	BCR	x	202	-	41,41,41	4.78	24 (58%)	56,56,56	2.27	18 (32%)
26	CHL	3	314	-	66,74,74	1.96	17 (25%)	73,114,114	2.38	20 (27%)
22	CLA	r	604	-	48,56,73	1.72	6 (12%)	55,92,113	1.63	8 (14%)
26	CHL	1	318	-	66,74,74	1.89	15 (22%)	73,114,114	2.39	22 (30%)
27	NEX	p	301	18	38,46,46	0.98	2 (5%)	50,70,70	2.43	19 (38%)
27	NEX	n	319	-	38,46,46	0.96	2 (5%)	50,70,70	2.64	17 (34%)
22	CLA	N	308	-	48,56,73	1.74	6 (12%)	55,92,113	1.54	7 (12%)
22	CLA	v	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	8 (10%)
22	CLA	B	613	-	65,73,73	1.43	8 (12%)	76,113,113	1.46	10 (13%)
22	CLA	n	307	-	60,68,73	1.51	7 (11%)	70,107,113	1.48	7 (10%)
22	CLA	V	308	-	48,56,73	1.69	6 (12%)	55,92,113	1.58	6 (10%)
24	XAT	g	309	-	39,47,47	2.53	17 (43%)	54,74,74	11.71	20 (37%)
25	LHG	6	311	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
25	LHG	V	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.10	2 (3%)
32	SQD	L	102	9	53,54,54	0.93	4 (7%)	62,65,65	1.80	12 (19%)
26	CHL	N	317	-	66,74,74	1.93	16 (24%)	73,114,114	2.33	22 (30%)
26	CHL	v	317	18	66,74,74	1.91	15 (22%)	73,114,114	2.52	25 (34%)
26	CHL	N	313	-	66,74,74	1.92	15 (22%)	73,114,114	2.41	22 (30%)
26	CHL	Q	313	-	50,58,74	2.20	16 (32%)	52,94,114	2.72	20 (38%)
25	LHG	G	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.10	2 (3%)
22	CLA	B	609	-	65,73,73	1.44	8 (12%)	76,113,113	1.45	6 (7%)
26	CHL	U	319	-	66,74,74	1.92	15 (22%)	73,114,114	2.39	21 (28%)
26	CHL	Q	314	-	66,74,74	1.93	16 (24%)	73,114,114	2.36	22 (30%)
24	XAT	U	311	-	39,47,47	2.51	17 (43%)	54,74,74	11.93	20 (37%)
36	DGD	c	518	-	63,63,67	1.22	6 (9%)	77,77,81	1.15	5 (6%)
23	LUT	v	309	-	42,43,43	0.79	0	51,60,60	1.65	12 (23%)
22	CLA	R	309	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	9 (16%)
22	CLA	s	302	-	45,53,73	1.81	6 (13%)	52,89,113	1.61	7 (13%)
22	CLA	s	303	19	50,58,73	1.67	7 (14%)	58,95,113	1.64	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	XAT	2	311	-	39,47,47	2.58	18 (46%)	54,74,74	11.93	19 (35%)
36	DGD	A	414	-	60,60,67	1.27	7 (11%)	74,74,81	1.25	6 (8%)
26	CHL	Q	312	-	48,56,74	2.29	15 (31%)	51,92,114	2.76	21 (41%)
27	NEX	r	617	-	38,46,46	1.01	3 (7%)	50,70,70	2.42	17 (34%)
22	CLA	5	308	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)
34	LMG	c	501	-	51,51,55	1.15	5 (9%)	59,59,63	1.16	3 (5%)
23	LUT	P	311	-	42,43,43	0.76	0	51,60,60	1.58	12 (23%)
22	CLA	B	608	-	65,73,73	1.43	7 (10%)	76,113,113	1.52	7 (9%)
22	CLA	U	308	-	48,56,73	1.71	8 (16%)	55,92,113	1.58	7 (12%)
22	CLA	N	302	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	7 (9%)
26	CHL	3	316	-	61,69,74	2.00	14 (22%)	67,108,114	2.48	23 (34%)
26	CHL	2	315	-	50,58,74	2.18	15 (30%)	52,94,114	2.77	19 (36%)
26	CHL	1	313	-	66,74,74	1.94	15 (22%)	73,114,114	2.37	23 (31%)
31	BCR	z	101	-	41,41,41	4.76	24 (58%)	56,56,56	2.32	20 (35%)
24	XAT	q	309	-	39,47,47	2.58	18 (46%)	54,74,74	11.94	18 (33%)
22	CLA	G	304	18	64,72,73	1.48	7 (10%)	74,111,113	1.53	9 (12%)
26	CHL	v	318	-	66,74,74	1.92	16 (24%)	73,114,114	2.32	21 (28%)
22	CLA	N	304	18	65,73,73	1.43	7 (10%)	76,113,113	1.53	9 (11%)
23	LUT	n	309	-	42,43,43	0.74	0	51,60,60	1.62	11 (21%)
27	NEX	v	319	-	38,46,46	0.89	1 (2%)	50,70,70	2.45	14 (28%)
26	CHL	5	315	-	50,58,74	2.17	15 (30%)	52,94,114	2.79	20 (38%)
26	CHL	V	314	-	48,56,74	2.30	17 (35%)	51,92,114	2.79	21 (41%)
25	LHG	b	622	-	46,46,48	0.91	4 (8%)	49,52,54	1.04	2 (4%)
22	CLA	A	406	-	50,58,73	1.65	10 (20%)	58,95,113	1.56	7 (12%)
25	LHG	B	622	-	46,46,48	0.91	4 (8%)	49,52,54	1.06	2 (4%)
26	CHL	1	314	22	48,56,74	2.25	14 (29%)	51,92,114	2.82	20 (39%)
26	CHL	S	313	-	46,54,74	2.33	16 (34%)	49,90,114	2.84	20 (40%)
22	CLA	b	612	-	65,73,73	1.48	7 (10%)	76,113,113	1.54	7 (9%)
22	CLA	6	304	-	50,58,73	1.68	7 (14%)	58,95,113	1.60	8 (13%)
22	CLA	g	302	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
22	CLA	g	303	-	50,58,73	1.69	7 (14%)	58,95,113	1.62	7 (12%)
23	LUT	1	309	-	42,43,43	0.72	0	51,60,60	1.57	10 (19%)
25	LHG	1	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	v	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
34	LMG	B	624	21	55,55,55	1.16	6 (10%)	63,63,63	1.07	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	SQD	C	501	-	49,50,54	1.00	5 (10%)	58,61,65	1.75	11 (18%)
26	CHL	G	311	-	66,74,74	1.87	15 (22%)	73,114,114	2.46	23 (31%)
22	CLA	B	603	-	65,73,73	1.45	9 (13%)	76,113,113	1.42	6 (7%)
22	CLA	G	306	22	60,68,73	1.54	6 (10%)	70,107,113	1.39	6 (8%)
22	CLA	n	308	-	48,56,73	1.75	6 (12%)	55,92,113	1.65	9 (16%)
23	LUT	p	311	-	42,43,43	0.76	0	51,60,60	1.54	12 (23%)
22	CLA	s	308	-	55,63,73	1.58	8 (14%)	64,101,113	1.51	7 (10%)
22	CLA	r	609	26	60,68,73	1.54	6 (10%)	70,107,113	1.58	11 (15%)
22	CLA	A	408	-	60,68,73	1.45	8 (13%)	70,107,113	1.67	8 (11%)
22	CLA	2	305	18	60,68,73	1.50	7 (11%)	70,107,113	2.03	15 (21%)
25	LHG	C	523	-	48,48,48	0.89	3 (6%)	51,54,54	1.07	2 (3%)
36	DGD	c	517	-	56,56,67	1.30	8 (14%)	70,70,81	1.19	5 (7%)
31	BCR	b	618	-	41,41,41	4.74	24 (58%)	56,56,56	2.46	23 (41%)
22	CLA	U	302	-	65,73,73	1.47	8 (12%)	76,113,113	1.39	6 (7%)
26	CHL	n	313	18	66,74,74	1.94	16 (24%)	73,114,114	2.40	24 (32%)
22	CLA	4	303	-	50,58,73	1.68	8 (16%)	58,95,113	1.56	8 (13%)
22	CLA	R	308	1	49,57,73	1.68	6 (12%)	55,93,113	1.66	8 (14%)
22	CLA	2	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	7 (9%)
25	LHG	b	623	21	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
22	CLA	n	304	18	65,73,73	1.42	7 (10%)	76,113,113	1.54	9 (11%)
23	LUT	2	309	-	42,43,43	0.76	0	51,60,60	1.68	14 (27%)
35	BCT	D	402	-	2,3,3	1.35	0	2,3,3	0.19	0
23	LUT	1	310	-	42,43,43	0.80	0	51,60,60	1.74	14 (27%)
22	CLA	B	611	-	65,73,73	1.47	8 (12%)	76,113,113	1.49	8 (10%)
22	CLA	V	306	-	60,68,73	1.56	7 (11%)	70,107,113	1.43	8 (11%)
36	DGD	b	601	21	63,63,67	1.23	7 (11%)	77,77,81	1.06	3 (3%)
22	CLA	g	307	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
22	CLA	4	306	-	60,68,73	1.56	8 (13%)	70,107,113	1.42	8 (11%)
22	CLA	c	508	20	65,73,73	1.47	9 (13%)	76,113,113	1.52	10 (13%)
24	XAT	1	311	-	39,47,47	2.54	17 (43%)	54,74,74	12.16	18 (33%)
22	CLA	Q	303	-	50,58,73	1.70	6 (12%)	58,95,113	1.58	8 (13%)
22	CLA	D	403	3	65,73,73	1.43	9 (13%)	76,113,113	1.39	8 (10%)
26	CHL	r	619	1	48,56,74	2.20	15 (31%)	51,92,114	2.82	19 (37%)
31	BCR	b	619	-	41,41,41	4.74	24 (58%)	56,56,56	2.27	20 (35%)
26	CHL	P	319	-	66,74,74	1.88	14 (21%)	73,114,114	2.40	20 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CHL	V	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.38	22 (30%)
36	DGD	C	519	-	56,56,67	1.30	8 (14%)	70,70,81	1.19	5 (7%)
26	CHL	N	314	-	48,56,74	2.33	16 (33%)	51,92,114	2.82	20 (39%)
22	CLA	c	512	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	9 (11%)
23	LUT	n	310	-	42,43,43	0.79	0	51,60,60	1.75	14 (27%)
23	LUT	r	611	1	42,43,43	0.75	0	51,60,60	1.66	10 (19%)
26	CHL	P	315	-	48,56,74	2.46	16 (33%)	51,92,114	2.76	19 (37%)
22	CLA	Q	306	22	60,68,73	1.54	5 (8%)	70,107,113	1.40	6 (8%)
22	CLA	5	304	18	65,73,73	1.45	9 (13%)	76,113,113	1.51	10 (13%)
22	CLA	B	615	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	7 (9%)
22	CLA	C	513	-	65,73,73	1.47	9 (13%)	76,113,113	1.53	9 (11%)
22	CLA	C	506	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	7 (9%)
23	LUT	S	311	-	42,43,43	0.77	0	51,60,60	1.64	17 (33%)
26	CHL	G	313	-	50,58,74	2.19	15 (30%)	52,94,114	2.72	18 (34%)
22	CLA	4	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.49	9 (11%)
22	CLA	r	610	-	45,53,73	1.79	6 (13%)	52,89,113	1.65	6 (11%)
22	CLA	C	514	-	65,73,73	1.44	10 (15%)	76,113,113	1.41	7 (9%)
26	CHL	R	315	-	66,74,74	1.88	13 (19%)	73,114,114	2.43	22 (30%)
26	CHL	6	313	-	48,56,74	2.37	17 (35%)	51,92,114	2.83	23 (45%)
26	CHL	Q	315	18	66,74,74	1.87	16 (24%)	73,114,114	2.47	21 (28%)
22	CLA	S	302	-	45,53,73	1.81	6 (13%)	52,89,113	1.61	7 (13%)
26	CHL	3	311	-	66,74,74	1.89	14 (21%)	73,114,114	2.46	23 (31%)
25	LHG	B	623	21	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
27	NEX	u	320	-	38,46,46	0.89	2 (5%)	50,70,70	2.32	18 (36%)
24	XAT	V	311	-	39,47,47	2.58	18 (46%)	54,74,74	12.00	18 (33%)
22	CLA	v	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	6 (10%)
22	CLA	N	303	-	50,58,73	1.65	7 (14%)	58,95,113	1.69	7 (12%)
22	CLA	2	304	18	65,73,73	1.45	9 (13%)	76,113,113	1.48	9 (11%)
22	CLA	p	306	18	60,68,73	1.49	6 (10%)	70,107,113	2.10	16 (22%)
22	CLA	S	308	-	55,63,73	1.59	7 (12%)	64,101,113	1.50	7 (10%)
22	CLA	c	502	-	65,73,73	1.48	9 (13%)	76,113,113	1.41	8 (10%)
36	DGD	B	601	21	63,63,67	1.22	7 (11%)	77,77,81	1.07	3 (3%)
22	CLA	4	301	-	65,73,73	1.47	9 (13%)	76,113,113	1.44	7 (9%)
32	SQD	M	101	-	41,42,54	1.06	5 (12%)	50,53,65	1.74	11 (22%)
26	CHL	q	312	-	48,56,74	2.36	17 (35%)	51,92,114	2.82	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CHL	v	313	-	66,74,74	1.92	16 (24%)	73,114,114	2.45	23 (31%)
22	CLA	2	303	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
26	CHL	p	318	-	66,74,74	1.84	14 (21%)	73,114,114	2.44	20 (27%)
22	CLA	q	306	22	60,68,73	1.53	5 (8%)	70,107,113	1.44	7 (10%)
24	XAT	R	313	-	39,47,47	2.54	17 (43%)	54,74,74	11.48	22 (40%)
26	CHL	v	314	-	48,56,74	2.23	15 (31%)	51,92,114	2.84	21 (41%)
23	LUT	4	310	-	42,43,43	0.83	1 (2%)	51,60,60	1.79	14 (27%)
26	CHL	V	315	-	50,58,74	2.29	16 (32%)	52,94,114	2.69	20 (38%)
36	DGD	J	101	-	61,61,67	1.26	6 (9%)	75,75,81	1.17	3 (4%)
22	CLA	R	306	-	58,66,73	1.56	6 (10%)	67,104,113	1.53	6 (8%)
22	CLA	q	302	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	7 (9%)
22	CLA	p	307	-	60,68,73	1.52	5 (8%)	70,107,113	1.46	8 (11%)
22	CLA	C	503	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	9 (11%)
26	CHL	Q	316	-	61,69,74	2.00	16 (26%)	67,108,114	2.48	22 (32%)
22	CLA	g	308	-	48,56,73	1.70	6 (12%)	55,92,113	1.56	7 (12%)
25	LHG	a	415	2	42,42,48	0.93	3 (7%)	45,48,54	1.10	2 (4%)
25	LHG	l	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	3 (5%)
31	BCR	K	101	-	41,41,41	4.72	24 (58%)	56,56,56	2.53	19 (33%)
31	BCR	D	404	3	41,41,41	4.77	24 (58%)	56,56,56	2.26	23 (41%)
22	CLA	P	309	-	48,56,73	1.69	6 (12%)	55,92,113	1.57	7 (12%)
22	CLA	p	309	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)
25	LHG	U	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.17	3 (5%)
22	CLA	n	303	-	50,58,73	1.69	6 (12%)	58,95,113	1.61	8 (13%)
25	LHG	4	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.07	2 (3%)
22	CLA	5	305	18	60,68,73	1.52	7 (11%)	70,107,113	2.04	13 (18%)
27	NEX	2	319	-	38,46,46	0.93	1 (2%)	50,70,70	2.45	14 (28%)
27	NEX	r	618	1,22	38,46,46	1.04	2 (5%)	50,70,70	2.49	16 (32%)
31	BCR	C	517	-	41,41,41	4.69	24 (58%)	56,56,56	2.67	24 (42%)
34	LMG	c	520	-	51,51,55	1.20	6 (11%)	59,59,63	1.08	2 (3%)
22	CLA	B	607	-	65,73,73	1.48	9 (13%)	76,113,113	1.50	9 (11%)
22	CLA	C	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.43	7 (9%)
32	SQD	a	410	-	49,50,54	1.01	5 (10%)	58,61,65	1.74	11 (18%)
22	CLA	P	308	-	60,68,73	1.53	7 (11%)	70,107,113	1.47	6 (8%)
22	CLA	2	301	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
22	CLA	a	406	-	50,58,73	1.65	10 (20%)	58,95,113	1.56	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CHL	p	320	-	66,74,74	1.87	14 (21%)	73,114,114	2.42	21 (28%)
22	CLA	u	306	-	60,68,73	1.54	10 (16%)	70,107,113	1.44	7 (10%)
22	CLA	p	304	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	8 (13%)
24	XAT	Q	309	-	39,47,47	2.60	18 (46%)	54,74,74	11.94	19 (35%)
22	CLA	G	302	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
26	CHL	1	315	-	50,58,74	2.23	16 (32%)	52,94,114	2.67	19 (36%)
26	CHL	R	316	-	56,64,74	2.05	14 (25%)	61,102,114	2.62	21 (34%)
22	CLA	1	304	-	60,68,73	1.49	8 (13%)	70,107,113	1.45	6 (8%)
26	CHL	2	313	18	66,74,74	1.99	17 (25%)	73,114,114	2.38	22 (30%)
26	CHL	2	318	-	66,74,74	1.88	14 (21%)	73,114,114	2.37	23 (31%)
31	BCR	B	618	-	41,41,41	4.74	24 (58%)	56,56,56	2.45	22 (39%)
22	CLA	u	305	-	60,68,73	1.52	7 (11%)	70,107,113	1.45	7 (10%)
22	CLA	1	303	-	50,58,73	1.66	9 (18%)	58,95,113	1.58	8 (13%)
22	CLA	Q	304	18	64,72,73	1.47	7 (10%)	74,111,113	1.53	9 (12%)
22	CLA	a	408	-	60,68,73	1.46	8 (13%)	70,107,113	1.68	8 (11%)
23	LUT	p	310	-	42,43,43	0.74	0	51,60,60	1.72	14 (27%)
26	CHL	6	312	-	66,74,74	1.90	15 (22%)	73,114,114	2.48	23 (31%)
26	CHL	s	315	19	58,66,74	2.14	16 (27%)	63,104,114	2.45	20 (31%)
26	CHL	p	316	-	50,58,74	2.23	16 (32%)	52,94,114	2.72	22 (42%)
26	CHL	q	315	-	61,69,74	2.01	16 (26%)	67,108,114	2.49	23 (34%)
23	LUT	N	309	-	42,43,43	0.72	0	51,60,60	1.55	11 (21%)
26	CHL	P	314	18	66,74,74	1.98	16 (24%)	73,114,114	2.40	22 (30%)
26	CHL	p	314	18	66,74,74	1.93	16 (24%)	73,114,114	2.42	23 (31%)
23	LUT	s	311	-	42,43,43	0.76	0	51,60,60	1.65	16 (31%)
22	CLA	6	306	22	60,68,73	1.51	6 (10%)	70,107,113	1.51	10 (14%)
22	CLA	B	612	-	65,73,73	1.49	7 (10%)	76,113,113	1.55	7 (9%)
22	CLA	b	617	21	65,73,73	1.51	10 (15%)	76,113,113	1.56	12 (15%)
22	CLA	r	601	27	49,57,73	1.73	7 (14%)	55,93,113	1.63	8 (14%)
26	CHL	5	317	-	66,74,74	1.86	12 (18%)	73,114,114	2.45	22 (30%)
25	LHG	g	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
24	XAT	u	311	-	39,47,47	2.54	18 (46%)	54,74,74	11.77	18 (33%)
23	LUT	R	312	-	42,43,43	0.73	0	51,60,60	1.52	11 (21%)
25	LHG	C	522	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
26	CHL	4	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.33	22 (30%)
22	CLA	a	404	-	65,73,73	1.40	8 (12%)	76,113,113	1.60	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	CLA	V	304	-	60,68,73	1.50	6 (10%)	70,107,113	1.52	8 (11%)
25	LHG	u	312	-	48,48,48	0.88	4 (8%)	51,54,54	1.13	3 (5%)
26	CHL	6	315	-	66,74,74	1.96	17 (25%)	73,114,114	2.39	22 (30%)
22	CLA	5	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
22	CLA	Q	302	-	65,73,73	1.45	6 (9%)	76,113,113	1.36	7 (9%)
36	DGD	a	416	-	60,60,67	1.27	7 (11%)	74,74,81	1.25	6 (8%)
26	CHL	u	316	-	66,74,74	1.90	14 (21%)	73,114,114	2.52	27 (36%)
24	XAT	5	311	-	39,47,47	2.58	18 (46%)	54,74,74	11.93	19 (35%)
22	CLA	4	304	-	60,68,73	1.50	8 (13%)	70,107,113	1.46	6 (8%)
26	CHL	u	315	-	50,58,74	2.14	13 (26%)	52,94,114	2.65	20 (38%)
25	LHG	L	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	3 (5%)
22	CLA	A	405	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	10 (13%)
23	LUT	V	310	-	42,43,43	0.78	0	51,60,60	1.62	12 (23%)
22	CLA	p	305	18	65,73,73	1.42	6 (9%)	76,113,113	1.46	8 (10%)
25	LHG	Q	310	-	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
25	LHG	R	314	-	41,41,48	0.96	3 (7%)	44,47,54	1.09	2 (4%)
22	CLA	q	305	22	60,68,73	1.51	7 (11%)	70,107,113	1.44	6 (8%)
25	LHG	c	521	-	48,48,48	0.90	4 (8%)	51,54,54	1.08	2 (3%)
27	NEX	R	301	1,22	38,46,46	1.03	2 (5%)	50,70,70	2.42	13 (26%)
22	CLA	C	508	-	65,73,73	1.51	9 (13%)	76,113,113	1.43	7 (9%)
22	CLA	v	303	-	50,58,73	1.67	7 (14%)	58,95,113	1.62	6 (10%)
22	CLA	p	302	-	65,73,73	1.43	7 (10%)	76,113,113	1.47	7 (9%)
22	CLA	B	617	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	8 (10%)
23	LUT	u	310	-	42,43,43	0.78	0	51,60,60	1.60	10 (19%)
22	CLA	g	301	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	7 (9%)
26	CHL	3	312	-	48,56,74	2.38	17 (35%)	51,92,114	2.80	23 (45%)
31	BCR	k	101	-	41,41,41	4.73	25 (60%)	56,56,56	2.52	19 (33%)
22	CLA	U	304	-	60,68,73	1.50	9 (15%)	70,107,113	1.48	8 (11%)
25	LHG	D	406	3	45,45,48	0.92	4 (8%)	48,51,54	1.08	2 (4%)
22	CLA	P	303	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	7 (9%)
22	CLA	b	603	-	65,73,73	1.45	9 (13%)	76,113,113	1.42	6 (7%)
26	CHL	6	316	18	66,74,74	1.89	17 (25%)	73,114,114	2.47	19 (26%)
25	LHG	d	406	3	48,48,48	0.90	4 (8%)	51,54,54	1.07	3 (5%)
22	CLA	r	608	-	49,57,73	1.68	6 (12%)	55,93,113	1.65	8 (14%)
22	CLA	C	510	-	65,73,73	1.53	9 (13%)	76,113,113	1.52	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	4	302	-	65,73,73	1.50	7 (10%)	76,113,113	1.34	7 (9%)
22	CLA	Q	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
24	XAT	6	310	-	39,47,47	2.56	18 (46%)	54,74,74	11.74	17 (31%)
34	LMG	b	624	21	55,55,55	1.17	6 (10%)	63,63,63	1.07	2 (3%)
26	CHL	s	314	-	46,54,74	2.29	16 (34%)	49,90,114	2.86	19 (38%)
22	CLA	c	513	-	65,73,73	1.43	9 (13%)	76,113,113	1.42	8 (10%)
22	CLA	b	616	21	65,73,73	1.43	9 (13%)	76,113,113	1.46	9 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LUT	s	310	19	-	2/29/67/67	0/2/2/2
22	CLA	U	306	-	1/1/14/20	10/31/109/115	-
22	CLA	u	302	-	1/1/15/20	14/37/115/115	-
26	CHL	U	314	-	3/3/16/26	10/20/118/137	-
31	BCR	X	201	-	-	9/29/63/63	0/2/2/2
26	CHL	6	301	-	3/3/20/26	20/39/137/137	-
22	CLA	c	511	20,8	1/1/15/20	18/37/115/115	-
26	CHL	u	317	18	3/3/20/26	11/39/137/137	-
26	CHL	G	316	-	3/3/19/26	13/33/131/137	-
26	CHL	2	314	-	3/3/16/26	9/18/116/137	-
22	CLA	g	305	22	1/1/14/20	10/31/109/115	-
22	CLA	n	306	-	1/1/14/20	9/31/109/115	-
37	HEM	e	101	4,17	-	3/12/54/54	-
22	CLA	C	512	20,8	1/1/15/20	20/37/115/115	-
23	LUT	2	310	-	-	1/29/67/67	0/2/2/2
24	XAT	p	312	-	-	7/31/93/93	0/4/4/4
26	CHL	V	318	-	3/3/20/26	17/39/137/137	-
22	CLA	3	306	22	1/1/14/20	16/31/109/115	-
22	CLA	5	302	-	1/1/15/20	16/37/115/115	-
26	CHL	P	318	-	3/3/20/26	17/39/137/137	-
23	LUT	5	309	-	-	4/29/67/67	0/2/2/2
23	LUT	u	309	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Q	301	-	1/1/15/20	14/37/115/115	-
22	CLA	c	509	-	1/1/15/20	9/37/115/115	-
25	LHG	D	407	3	-	18/53/53/53	-
26	CHL	U	315	-	3/3/20/26	14/39/137/137	-
25	LHG	s	312	19	-	17/53/53/53	-
22	CLA	3	305	22	1/1/14/20	9/31/109/115	-
22	CLA	p	303	-	1/1/15/20	6/37/115/115	-
26	CHL	3	315	18	3/3/20/26	21/39/137/137	-
26	CHL	N	315	-	3/3/16/26	7/20/118/137	-
22	CLA	s	309	-	1/1/11/20	2/18/96/115	-
22	CLA	c	507	-	1/1/15/20	20/37/115/115	-
23	LUT	4	309	-	-	2/29/67/67	0/2/2/2
26	CHL	4	314	-	3/3/16/26	10/18/116/137	-
34	LMG	D	408	3	-	17/41/61/70	0/1/1/1
22	CLA	P	305	18	1/1/15/20	10/37/115/115	-
34	LMG	w	201	-	-	22/43/63/70	0/1/1/1
26	CHL	5	318	-	3/3/20/26	16/39/137/137	-
22	CLA	3	307	-	1/1/15/20	10/37/115/115	-
26	CHL	u	318	-	3/3/20/26	20/39/137/137	-
22	CLA	u	304	-	1/1/14/20	5/31/109/115	-
25	LHG	c	522	-	-	24/53/53/53	-
31	BCR	B	619	-	-	14/29/63/63	0/2/2/2
22	CLA	2	306	-	1/1/14/20	11/31/109/115	-
31	BCR	C	516	-	-	8/29/63/63	0/2/2/2
26	CHL	U	316	18	3/3/20/26	11/39/137/137	-
31	BCR	c	516	-	-	11/29/63/63	0/2/2/2
22	CLA	N	306	-	1/1/14/20	9/31/109/115	-
22	CLA	G	308	-	1/1/11/20	9/17/95/115	-
26	CHL	1	317	18	3/3/20/26	19/39/137/137	-
24	XAT	G	309	-	-	10/31/93/93	0/4/4/4
22	CLA	Q	305	22	1/1/14/20	16/31/109/115	-
27	NEX	5	319	-	-	8/27/83/83	0/3/3/3
23	LUT	S	310	-	-	2/29/67/67	0/2/2/2
22	CLA	B	616	21	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	u	307	-	1/1/15/20	14/37/115/115	-
22	CLA	Q	308	-	1/1/11/20	9/17/95/115	-
26	CHL	2	316	-	3/3/20/26	17/39/137/137	-
22	CLA	q	303	-	1/1/12/20	8/19/97/115	-
26	CHL	n	317	-	3/3/20/26	17/39/137/137	-
22	CLA	B	606	-	1/1/15/20	18/37/115/115	-
27	NEX	V	319	-	-	6/27/83/83	0/3/3/3
31	BCR	B	620	-	-	12/29/63/63	0/2/2/2
26	CHL	U	317	-	3/3/20/26	18/39/137/137	-
22	CLA	C	504	-	1/1/15/20	21/37/115/115	-
22	CLA	6	302	-	1/1/15/20	17/37/115/115	-
22	CLA	B	610	-	1/1/15/20	16/37/115/115	-
31	BCR	C	518	-	-	11/29/63/63	0/2/2/2
34	LMG	d	407	3	-	17/41/61/70	0/1/1/1
26	CHL	2	317	-	3/3/20/26	11/39/137/137	-
26	CHL	g	311	-	3/3/20/26	21/39/137/137	-
31	BCR	A	409	-	-	3/29/63/63	0/2/2/2
23	LUT	P	310	-	-	2/29/67/67	0/2/2/2
24	XAT	r	612	-	-	7/31/93/93	0/4/4/4
22	CLA	1	306	-	1/1/14/20	14/31/109/115	-
22	CLA	u	303	-	1/1/12/20	6/19/97/115	-
34	LMG	a	412	-	-	8/35/55/70	0/1/1/1
22	CLA	c	506	-	1/1/15/20	19/37/115/115	-
26	CHL	g	313	-	3/3/16/26	8/20/118/137	-
23	LUT	U	310	-	-	3/29/67/67	0/2/2/2
25	LHG	N	312	-	-	16/53/53/53	-
25	LHG	v	312	-	-	19/53/53/53	-
25	LHG	p	313	-	-	22/53/53/53	-
22	CLA	b	605	21	1/1/15/20	16/37/115/115	-
22	CLA	N	305	18	1/1/14/20	12/31/109/115	-
27	NEX	N	318	-	-	9/27/83/83	0/3/3/3
26	CHL	4	316	18	3/3/20/26	14/39/137/137	-
22	CLA	A	404	-	1/1/15/20	15/37/115/115	-
23	LUT	v	310	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	NEX	u	319	-	-	7/27/83/83	0/3/3/3
32	SQD	l	102	9	-	21/49/69/69	0/1/1/1
22	CLA	3	301	-	1/1/15/20	14/37/115/115	-
26	CHL	S	314	-	3/3/16/26	7/15/113/137	-
26	CHL	n	315	-	3/3/16/26	10/20/118/137	-
30	PHO	A	407	-	-	10/37/103/103	0/5/6/6
22	CLA	a	405	-	1/1/15/20	10/37/115/115	-
22	CLA	s	304	19	1/1/11/20	9/13/91/115	-
23	LUT	V	309	-	-	2/29/67/67	0/2/2/2
26	CHL	4	317	-	3/3/20/26	14/39/137/137	-
26	CHL	V	313	-	3/3/20/26	19/39/137/137	-
33	PL9	A	410	-	-	0/5/18/73	0/1/1/1
33	PL9	D	405	-	-	9/53/73/73	0/1/1/1
26	CHL	6	317	-	3/3/19/26	16/33/131/137	-
22	CLA	r	602	-	1/1/14/20	7/31/109/115	-
22	CLA	6	303	-	1/1/15/20	12/37/115/115	-
22	CLA	u	301	-	-	7/37/115/115	-
22	CLA	1	307	-	1/1/15/20	11/37/115/115	-
22	CLA	C	515	-	1/1/15/20	10/37/115/115	-
22	CLA	G	307	-	1/1/15/20	12/37/115/115	-
22	CLA	R	311	-	1/1/11/20	8/13/91/115	-
24	XAT	N	311	-	-	8/31/93/93	0/4/4/4
26	CHL	S	315	19	3/3/18/26	15/30/128/137	-
22	CLA	q	301	-	-	15/37/115/115	-
31	BCR	t	101	-	-	12/29/63/63	0/2/2/2
22	CLA	p	308	-	1/1/14/20	11/31/109/115	-
26	CHL	r	614	-	3/3/20/26	20/39/137/137	-
31	BCR	a	409	-	-	2/29/63/63	0/2/2/2
27	NEX	s	317	19	-	4/27/83/83	0/3/3/3
22	CLA	6	307	22	1/1/14/20	16/31/109/115	-
30	PHO	D	401	-	-	11/37/103/103	0/5/6/6
22	CLA	1	305	-	1/1/14/20	8/31/109/115	-
25	LHG	3	310	-	-	18/53/53/53	-
22	CLA	c	510	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	U	305	-	1/1/14/20	10/31/109/115	-
22	CLA	n	305	18	1/1/14/20	11/31/109/115	-
22	CLA	R	307	-	1/1/15/20	16/37/115/115	-
22	CLA	s	306	-	1/1/13/20	5/27/105/115	-
25	LHG	S	312	19	-	17/53/53/53	-
22	CLA	2	307	-	1/1/14/20	8/31/109/115	-
22	CLA	S	305	-	1/1/13/20	6/25/103/115	-
22	CLA	c	503	-	1/1/15/20	20/37/115/115	-
26	CHL	1	316	-	3/3/20/26	21/39/137/137	-
22	CLA	V	305	-	1/1/14/20	8/31/109/115	-
22	CLA	G	303	-	1/1/12/20	10/19/97/115	-
22	CLA	S	309	-	1/1/11/20	2/18/96/115	-
25	LHG	C	524	-	-	13/53/53/53	-
31	BCR	c	515	-	-	14/29/63/63	0/2/2/2
26	CHL	5	313	18	3/3/20/26	21/39/137/137	-
22	CLA	b	602	-	1/1/15/20	17/37/115/115	-
26	CHL	q	311	-	3/3/20/26	17/39/137/137	-
37	HEM	E	101	4,17	-	2/12/54/54	-
26	CHL	u	313	-	3/3/20/26	14/39/137/137	-
25	LHG	c	523	-	-	17/53/53/53	-
22	CLA	1	308	-	1/1/11/20	11/17/95/115	-
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
26	CHL	g	312	-	3/3/16/26	10/18/116/137	-
31	BCR	b	620	-	-	12/29/63/63	0/2/2/2
22	CLA	4	308	-	1/1/11/20	11/17/95/115	-
33	PL9	d	404	-	-	9/53/73/73	0/1/1/1
22	CLA	q	307	-	1/1/15/20	15/37/115/115	-
22	CLA	b	610	-	1/1/15/20	16/37/115/115	-
30	PHO	a	407	-	-	10/37/103/103	0/5/6/6
22	CLA	b	614	-	1/1/15/20	16/37/115/115	-
23	LUT	U	309	-	-	4/29/67/67	0/2/2/2
22	CLA	6	309	-	1/1/11/20	10/17/95/115	-
22	CLA	3	303	-	1/1/12/20	10/19/97/115	-
24	XAT	n	311	-	-	9/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	n	312	-	-	19/53/53/53	-
22	CLA	V	303	-	1/1/12/20	6/19/97/115	-
26	CHL	p	319	-	3/3/20/26	15/39/137/137	-
27	NEX	U	318	-	-	3/27/83/83	0/3/3/3
22	CLA	s	305	-	1/1/13/20	5/25/103/115	-
22	CLA	3	304	18	1/1/14/20	15/36/114/115	-
22	CLA	x	201	14	1/1/15/20	10/37/115/115	-
22	CLA	u	308	-	1/1/11/20	10/17/95/115	-
22	CLA	g	304	18	1/1/14/20	8/36/114/115	-
22	CLA	v	304	-	1/1/14/20	14/31/109/115	-
22	CLA	G	301	-	1/1/15/20	19/37/115/115	-
22	CLA	B	604	-	1/1/15/20	15/37/115/115	-
22	CLA	c	514	-	1/1/15/20	9/37/115/115	-
25	LHG	2	312	-	-	24/53/53/53	-
22	CLA	q	308	-	1/1/11/20	11/17/95/115	-
22	CLA	C	511	-	1/1/15/20	14/37/115/115	-
34	LMG	C	521	-	-	19/46/66/70	0/1/1/1
22	CLA	b	615	-	1/1/15/20	18/37/115/115	-
22	CLA	b	606	-	1/1/15/20	18/37/115/115	-
22	CLA	6	305	18	1/1/14/20	19/36/114/115	-
22	CLA	v	306	-	1/1/14/20	13/31/109/115	-
22	CLA	C	507	-	1/1/15/20	19/37/115/115	-
30	PHO	d	401	-	-	11/37/103/103	0/5/6/6
22	CLA	C	509	20	1/1/15/20	14/37/115/115	-
22	CLA	b	613	-	1/1/15/20	16/37/115/115	-
26	CHL	r	616	-	3/3/19/26	16/33/131/137	-
26	CHL	s	313	-	3/3/16/26	7/15/113/137	-
22	CLA	B	602	-	1/1/15/20	19/37/115/115	-
26	CHL	u	314	-	3/3/16/26	11/18/116/137	-
22	CLA	R	305	-	1/1/11/20	7/17/95/115	-
26	CHL	s	316	-	3/3/16/26	11/15/113/137	-
34	LMG	A	411	-	-	11/35/55/70	0/1/1/1
22	CLA	b	611	-	1/1/15/20	14/37/115/115	-
26	CHL	P	317	-	3/3/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	N	316	-	3/3/20/26	17/39/137/137	-
22	CLA	r	603	-	1/1/14/20	11/31/109/115	-
26	CHL	4	315	-	3/3/16/26	6/20/118/137	-
26	CHL	q	314	18	3/3/20/26	23/39/137/137	-
26	CHL	g	314	-	3/3/20/26	20/39/137/137	-
32	SQD	m	101	-	-	21/37/57/69	0/1/1/1
22	CLA	6	308	-	1/1/15/20	10/37/115/115	-
22	CLA	r	605	-	1/1/13/20	7/29/107/115	-
22	CLA	U	303	-	1/1/12/20	5/19/97/115	-
25	LHG	d	405	3	-	26/50/50/53	-
25	LHG	r	613	-	-	19/46/46/53	-
22	CLA	s	301	19	1/1/14/20	16/33/111/115	-
22	CLA	r	606	-	1/1/15/20	16/37/115/115	-
22	CLA	S	303	19	1/1/12/20	6/19/97/115	-
22	CLA	G	305	22	1/1/14/20	10/31/109/115	-
26	CHL	R	317	-	3/3/19/26	16/33/131/137	-
22	CLA	2	308	-	1/1/11/20	6/17/95/115	-
22	CLA	b	607	-	-	13/37/115/115	-
26	CHL	n	314	-	3/3/16/26	10/18/116/137	-
23	LUT	N	310	-	-	1/29/67/67	0/2/2/2
26	CHL	6	314	-	3/3/16/26	11/20/118/137	-
22	CLA	S	304	19	1/1/11/20	9/13/91/115	-
34	LMG	B	621	-	-	20/46/66/70	0/1/1/1
22	CLA	N	301	-	1/1/15/20	13/37/115/115	-
22	CLA	1	302	-	1/1/15/20	14/37/115/115	-
22	CLA	R	304	-	1/1/14/20	11/31/109/115	-
22	CLA	n	302	-	1/1/15/20	16/37/115/115	-
32	SQD	A	412	-	-	21/49/69/69	0/1/1/1
34	LMG	W	201	-	-	21/43/63/70	0/1/1/1
25	LHG	P	313	-	-	24/53/53/53	-
26	CHL	p	317	-	3/3/20/26	14/39/137/137	-
26	CHL	v	316	-	3/3/20/26	15/39/137/137	-
26	CHL	q	313	-	3/3/16/26	9/20/118/137	-
22	CLA	v	305	-	1/1/14/20	7/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	s	307	-	1/1/11/20	6/18/96/115	-
25	LHG	A	413	2	-	27/47/47/53	-
27	NEX	S	317	19	-	4/27/83/83	0/3/3/3
24	XAT	3	309	-	-	8/31/93/93	0/4/4/4
26	CHL	V	317	18	3/3/20/26	14/39/137/137	-
22	CLA	B	614	-	1/1/15/20	14/37/115/115	-
22	CLA	P	304	-	1/1/12/20	10/19/97/115	-
22	CLA	3	302	-	1/1/15/20	13/37/115/115	-
22	CLA	5	303	-	1/1/12/20	5/19/97/115	-
26	CHL	Q	311	-	3/3/20/26	19/39/137/137	-
22	CLA	S	306	-	1/1/13/20	6/27/105/115	-
26	CHL	G	314	-	3/3/20/26	15/39/137/137	-
22	CLA	V	302	-	1/1/15/20	12/37/115/115	-
22	CLA	r	607	1	1/1/11/20	9/18/96/115	-
22	CLA	q	304	18	1/1/14/20	15/36/114/115	-
22	CLA	N	307	-	1/1/14/20	13/31/109/115	-
26	CHL	g	315	18	3/3/20/26	23/39/137/137	-
26	CHL	5	314	-	3/3/16/26	11/18/116/137	-
22	CLA	V	307	-	1/1/15/20	8/37/115/115	-
22	CLA	X	202	14	1/1/15/20	9/37/115/115	-
27	NEX	P	301	18	-	3/27/83/83	0/3/3/3
22	CLA	P	307	-	1/1/14/20	12/31/109/115	-
26	CHL	r	615	-	3/3/18/26	10/27/125/137	-
26	CHL	S	316	-	3/3/16/26	11/15/113/137	-
23	LUT	5	310	-	-	1/29/67/67	0/2/2/2
36	DGD	c	519	-	-	21/49/89/95	0/2/2/2
34	LMG	C	502	-	-	26/46/66/70	0/1/1/1
33	PL9	a	411	-	-	0/5/18/73	0/1/1/1
24	XAT	v	311	-	-	11/31/93/93	0/4/4/4
22	CLA	d	402	3	1/1/15/20	13/37/115/115	-
22	CLA	P	306	18	1/1/14/20	10/31/109/115	-
22	CLA	v	301	-	-	11/37/115/115	-
22	CLA	S	301	19	1/1/14/20	16/33/111/115	-
26	CHL	p	315	-	3/3/16/26	8/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	n	316	-	3/3/20/26	25/39/137/137	-
26	CHL	P	316	-	3/3/16/26	7/20/118/137	-
22	CLA	P	302	-	1/1/15/20	16/37/115/115	-
22	CLA	g	306	22	1/1/14/20	13/31/109/115	-
22	CLA	R	310	-	1/1/14/20	10/31/109/115	-
22	CLA	B	605	21	1/1/15/20	18/37/115/115	-
26	CHL	G	315	18	3/3/20/26	19/39/137/137	-
32	SQD	a	413	-	-	22/49/69/69	0/1/1/1
24	XAT	P	312	-	-	8/31/93/93	0/4/4/4
26	CHL	v	315	-	3/3/16/26	8/20/118/137	-
25	LHG	5	312	-	-	23/53/53/53	-
22	CLA	5	307	-	1/1/14/20	10/31/109/115	-
34	LMG	b	621	-	-	24/46/66/70	0/1/1/1
26	CHL	U	313	-	3/3/20/26	15/39/137/137	-
25	LHG	q	310	-	-	22/53/53/53	-
31	BCR	d	403	3	-	12/29/63/63	0/2/2/2
22	CLA	b	604	-	1/1/15/20	16/37/115/115	-
26	CHL	g	316	-	3/3/19/26	15/33/131/137	-
24	XAT	4	311	-	-	8/31/93/93	0/4/4/4
22	CLA	b	609	-	1/1/15/20	12/37/115/115	-
22	CLA	U	307	-	1/1/15/20	15/37/115/115	-
22	CLA	3	308	-	1/1/11/20	10/17/95/115	-
22	CLA	R	302	27	1/1/11/20	8/18/96/115	-
22	CLA	5	306	-	1/1/14/20	13/31/109/115	-
22	CLA	R	303	-	1/1/14/20	7/31/109/115	-
22	CLA	S	307	-	1/1/11/20	6/18/96/115	-
22	CLA	U	301	-	-	8/37/115/115	-
22	CLA	n	301	-	1/1/15/20	13/37/115/115	-
22	CLA	c	504	-	1/1/15/20	17/37/115/115	-
26	CHL	3	313	-	3/3/16/26	14/20/118/137	-
26	CHL	G	312	-	3/3/16/26	6/18/116/137	-
22	CLA	c	505	-	1/1/15/20	9/37/115/115	-
22	CLA	b	608	-	1/1/15/20	11/37/115/115	-
22	CLA	4	305	-	1/1/14/20	6/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	V	301	-	-	12/37/115/115	-
36	DGD	C	520	-	-	31/51/91/95	0/2/2/2
22	CLA	1	301	-	1/1/15/20	7/37/115/115	-
26	CHL	5	316	-	3/3/20/26	18/39/137/137	-
26	CHL	n	318	-	3/3/20/26	23/39/137/137	-
31	BCR	x	202	-	-	9/29/63/63	0/2/2/2
26	CHL	3	314	-	3/3/20/26	16/39/137/137	-
22	CLA	r	604	-	1/1/11/20	7/17/95/115	-
26	CHL	1	318	-	3/3/20/26	14/39/137/137	-
27	NEX	p	301	18	-	3/27/83/83	0/3/3/3
27	NEX	n	319	-	-	7/27/83/83	0/3/3/3
22	CLA	N	308	-	1/1/11/20	14/17/95/115	-
22	CLA	v	302	-	1/1/15/20	12/37/115/115	-
22	CLA	B	613	-	1/1/15/20	16/37/115/115	-
22	CLA	n	307	-	1/1/14/20	11/31/109/115	-
22	CLA	V	308	-	1/1/11/20	9/17/95/115	-
24	XAT	g	309	-	-	10/31/93/93	0/4/4/4
25	LHG	6	311	-	-	19/53/53/53	-
25	LHG	V	312	-	-	18/53/53/53	-
32	SQD	L	102	9	-	21/49/69/69	0/1/1/1
26	CHL	N	317	-	3/3/20/26	20/39/137/137	-
26	CHL	v	317	18	3/3/20/26	12/39/137/137	-
26	CHL	N	313	-	3/3/20/26	13/39/137/137	-
26	CHL	Q	313	-	3/3/16/26	9/20/118/137	-
25	LHG	G	310	-	-	19/53/53/53	-
22	CLA	B	609	-	1/1/15/20	12/37/115/115	-
26	CHL	U	319	-	3/3/20/26	20/39/137/137	-
26	CHL	Q	314	-	3/3/20/26	20/39/137/137	-
24	XAT	U	311	-	-	7/31/93/93	0/4/4/4
36	DGD	c	518	-	-	31/51/91/95	0/2/2/2
23	LUT	v	309	-	-	2/29/67/67	0/2/2/2
22	CLA	R	309	-	1/1/11/20	7/18/96/115	-
22	CLA	s	302	-	1/1/11/20	6/13/91/115	-
22	CLA	s	303	19	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	2	311	-	-	6/31/93/93	0/4/4/4
36	DGD	A	414	-	-	22/48/88/95	0/2/2/2
26	CHL	Q	312	-	3/3/16/26	14/18/116/137	-
27	NEX	r	617	-	-	2/27/83/83	0/3/3/3
22	CLA	5	308	-	1/1/11/20	3/17/95/115	-
34	LMG	c	501	-	-	25/46/66/70	0/1/1/1
23	LUT	P	311	-	-	3/29/67/67	0/2/2/2
22	CLA	B	608	-	1/1/15/20	14/37/115/115	-
22	CLA	U	308	-	1/1/11/20	10/17/95/115	-
22	CLA	N	302	-	1/1/15/20	20/37/115/115	-
26	CHL	3	316	-	3/3/19/26	16/33/131/137	-
26	CHL	2	315	-	3/3/16/26	5/20/118/137	-
26	CHL	1	313	-	3/3/20/26	12/39/137/137	-
31	BCR	z	101	-	-	8/29/63/63	0/2/2/2
24	XAT	q	309	-	-	12/31/93/93	0/4/4/4
22	CLA	G	304	18	1/1/14/20	10/36/114/115	-
26	CHL	v	318	-	3/3/20/26	20/39/137/137	-
22	CLA	N	304	18	1/1/15/20	17/37/115/115	-
23	LUT	n	309	-	-	0/29/67/67	0/2/2/2
27	NEX	v	319	-	-	4/27/83/83	0/3/3/3
26	CHL	5	315	-	3/3/16/26	6/20/118/137	-
26	CHL	V	314	-	3/3/16/26	11/18/116/137	-
26	CHL	S	313	-	3/3/16/26	7/15/113/137	-
22	CLA	A	406	-	1/1/12/20	7/19/97/115	-
26	CHL	1	314	22	3/3/16/26	14/18/116/137	-
25	LHG	B	622	-	-	21/51/51/53	-
25	LHG	b	622	-	-	22/51/51/53	-
22	CLA	b	612	-	1/1/15/20	13/37/115/115	-
22	CLA	6	304	-	1/1/12/20	11/19/97/115	-
22	CLA	g	302	-	1/1/15/20	13/37/115/115	-
22	CLA	g	303	-	1/1/12/20	11/19/97/115	-
23	LUT	1	309	-	-	2/29/67/67	0/2/2/2
25	LHG	1	312	-	-	14/53/53/53	-
22	CLA	v	307	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	B	624	21	-	21/50/70/70	0/1/1/1
32	SQD	C	501	-	-	27/45/65/69	0/1/1/1
26	CHL	G	311	-	3/3/20/26	18/39/137/137	-
22	CLA	B	603	-	1/1/15/20	14/37/115/115	-
22	CLA	G	306	22	1/1/14/20	9/31/109/115	-
22	CLA	n	308	-	1/1/11/20	11/17/95/115	-
23	LUT	p	311	-	-	3/29/67/67	0/2/2/2
22	CLA	s	308	-	1/1/13/20	7/25/103/115	-
22	CLA	r	609	26	1/1/14/20	10/31/109/115	-
22	CLA	A	408	-	1/1/14/20	12/31/109/115	-
22	CLA	2	305	18	1/1/14/20	11/31/109/115	-
25	LHG	C	523	-	-	24/53/53/53	-
36	DGD	c	517	-	-	22/44/84/95	0/2/2/2
31	BCR	b	618	-	-	8/29/63/63	0/2/2/2
22	CLA	U	302	-	1/1/15/20	12/37/115/115	-
26	CHL	n	313	18	3/3/20/26	19/39/137/137	-
22	CLA	4	303	-	1/1/12/20	9/19/97/115	-
22	CLA	R	308	1	1/1/11/20	10/18/96/115	-
22	CLA	2	302	-	1/1/15/20	14/37/115/115	-
25	LHG	b	623	21	-	24/53/53/53	-
22	CLA	n	304	18	1/1/15/20	14/37/115/115	-
23	LUT	2	309	-	-	4/29/67/67	0/2/2/2
23	LUT	1	310	-	-	0/29/67/67	0/2/2/2
22	CLA	B	611	-	1/1/15/20	14/37/115/115	-
22	CLA	V	306	-	1/1/14/20	7/31/109/115	-
36	DGD	b	601	21	-	21/51/91/95	0/2/2/2
22	CLA	g	307	-	1/1/15/20	12/37/115/115	-
22	CLA	4	306	-	1/1/14/20	16/31/109/115	-
22	CLA	c	508	20	1/1/15/20	14/37/115/115	-
24	XAT	1	311	-	-	7/31/93/93	0/4/4/4
22	CLA	Q	303	-	1/1/12/20	10/19/97/115	-
22	CLA	D	403	3	1/1/15/20	15/37/115/115	-
26	CHL	r	619	1	3/3/16/26	8/18/116/137	-
31	BCR	b	619	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	P	319	-	3/3/20/26	20/39/137/137	-
26	CHL	V	316	-	3/3/20/26	17/39/137/137	-
36	DGD	C	519	-	-	23/44/84/95	0/2/2/2
26	CHL	N	314	-	3/3/16/26	10/18/116/137	-
22	CLA	c	512	-	1/1/15/20	9/37/115/115	-
23	LUT	n	310	-	-	3/29/67/67	0/2/2/2
23	LUT	r	611	1	-	2/29/67/67	0/2/2/2
26	CHL	P	315	-	3/3/16/26	9/18/116/137	-
22	CLA	Q	306	22	1/1/14/20	11/31/109/115	-
22	CLA	5	304	18	1/1/15/20	12/37/115/115	-
22	CLA	B	615	-	1/1/15/20	17/37/115/115	-
22	CLA	C	513	-	1/1/15/20	10/37/115/115	-
22	CLA	C	506	-	1/1/15/20	13/37/115/115	-
23	LUT	S	311	-	-	8/29/67/67	0/2/2/2
26	CHL	G	313	-	3/3/16/26	7/20/118/137	-
22	CLA	4	307	-	1/1/15/20	7/37/115/115	-
22	CLA	r	610	-	1/1/11/20	8/13/91/115	-
22	CLA	C	514	-	1/1/15/20	12/37/115/115	-
26	CHL	R	315	-	3/3/20/26	20/39/137/137	-
26	CHL	6	313	-	3/3/16/26	8/18/116/137	-
26	CHL	Q	315	18	3/3/20/26	20/39/137/137	-
22	CLA	S	302	-	1/1/11/20	6/13/91/115	-
26	CHL	3	311	-	3/3/20/26	16/39/137/137	-
25	LHG	B	623	21	-	21/53/53/53	-
27	NEX	u	320	-	-	2/27/83/83	0/3/3/3
24	XAT	V	311	-	-	11/31/93/93	0/4/4/4
22	CLA	v	308	-	1/1/11/20	9/17/95/115	-
22	CLA	N	303	-	1/1/12/20	5/19/97/115	-
22	CLA	2	304	18	1/1/15/20	9/37/115/115	-
22	CLA	p	306	18	1/1/14/20	11/31/109/115	-
22	CLA	S	308	-	1/1/13/20	7/25/103/115	-
22	CLA	c	502	-	1/1/15/20	8/37/115/115	-
36	DGD	B	601	21	-	22/51/91/95	0/2/2/2
22	CLA	4	301	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	M	101	-	-	22/37/57/69	0/1/1/1
26	CHL	q	312	-	3/3/16/26	12/18/116/137	-
26	CHL	v	313	-	3/3/20/26	16/39/137/137	-
22	CLA	2	303	-	1/1/12/20	6/19/97/115	-
26	CHL	p	318	-	3/3/20/26	17/39/137/137	-
22	CLA	q	306	22	1/1/14/20	12/31/109/115	-
24	XAT	R	313	-	-	8/31/93/93	0/4/4/4
26	CHL	v	314	-	3/3/16/26	12/18/116/137	-
26	CHL	V	315	-	3/3/16/26	6/20/118/137	-
23	LUT	4	310	-	-	0/29/67/67	0/2/2/2
36	DGD	J	101	-	-	21/49/89/95	0/2/2/2
22	CLA	R	306	-	1/1/13/20	7/29/107/115	-
22	CLA	q	302	-	1/1/15/20	11/37/115/115	-
22	CLA	p	307	-	1/1/14/20	7/31/109/115	-
22	CLA	C	503	-	1/1/15/20	7/37/115/115	-
26	CHL	Q	316	-	3/3/19/26	12/33/131/137	-
22	CLA	g	308	-	1/1/11/20	8/17/95/115	-
25	LHG	a	415	2	-	26/47/47/53	-
25	LHG	l	101	-	-	27/53/53/53	-
31	BCR	K	101	-	-	13/29/63/63	0/2/2/2
31	BCR	D	404	3	-	13/29/63/63	0/2/2/2
22	CLA	P	309	-	1/1/11/20	10/17/95/115	-
22	CLA	p	309	-	1/1/11/20	6/17/95/115	-
25	LHG	U	312	-	-	29/53/53/53	-
22	CLA	n	303	-	1/1/12/20	7/19/97/115	-
25	LHG	4	312	-	-	18/53/53/53	-
22	CLA	5	305	18	1/1/14/20	11/31/109/115	-
27	NEX	2	319	-	-	7/27/83/83	0/3/3/3
27	NEX	r	618	1,22	-	7/27/83/83	0/3/3/3
31	BCR	C	517	-	-	14/29/63/63	0/2/2/2
34	LMG	c	520	-	-	21/46/66/70	0/1/1/1
22	CLA	B	607	-	1/1/15/20	13/37/115/115	-
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
32	SQD	a	410	-	-	25/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	308	-	1/1/14/20	13/31/109/115	-
22	CLA	2	301	-	1/1/15/20	11/37/115/115	-
22	CLA	a	406	-	1/1/12/20	8/19/97/115	-
26	CHL	p	320	-	3/3/20/26	18/39/137/137	-
22	CLA	u	306	-	1/1/14/20	10/31/109/115	-
22	CLA	p	304	-	1/1/12/20	10/19/97/115	-
24	XAT	Q	309	-	-	10/31/93/93	0/4/4/4
22	CLA	G	302	-	1/1/15/20	17/37/115/115	-
26	CHL	1	315	-	3/3/16/26	6/20/118/137	-
26	CHL	R	316	-	3/3/18/26	11/27/125/137	-
22	CLA	1	304	-	1/1/14/20	7/31/109/115	-
26	CHL	2	313	18	3/3/20/26	20/39/137/137	-
26	CHL	2	318	-	3/3/20/26	18/39/137/137	-
31	BCR	B	618	-	-	8/29/63/63	0/2/2/2
22	CLA	u	305	-	1/1/14/20	12/31/109/115	-
22	CLA	1	303	-	1/1/12/20	8/19/97/115	-
22	CLA	Q	304	18	1/1/14/20	14/36/114/115	-
22	CLA	a	408	-	1/1/14/20	11/31/109/115	-
26	CHL	6	312	-	3/3/20/26	16/39/137/137	-
26	CHL	s	315	19	3/3/18/26	15/30/128/137	-
23	LUT	p	310	-	-	2/29/67/67	0/2/2/2
26	CHL	p	316	-	3/3/16/26	7/20/118/137	-
26	CHL	q	315	-	3/3/19/26	12/33/131/137	-
23	LUT	N	309	-	-	2/29/67/67	0/2/2/2
26	CHL	P	314	18	3/3/20/26	14/39/137/137	-
26	CHL	p	314	18	3/3/20/26	13/39/137/137	-
23	LUT	s	311	-	-	7/29/67/67	0/2/2/2
22	CLA	6	306	22	1/1/14/20	13/31/109/115	-
22	CLA	B	612	-	1/1/15/20	15/37/115/115	-
22	CLA	b	617	21	1/1/15/20	12/37/115/115	-
22	CLA	r	601	27	1/1/11/20	7/18/96/115	-
26	CHL	5	317	-	3/3/20/26	15/39/137/137	-
25	LHG	g	310	-	-	20/53/53/53	-
24	XAT	u	311	-	-	7/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LUT	R	312	-	-	4/29/67/67	0/2/2/2
25	LHG	C	522	-	-	16/53/53/53	-
26	CHL	4	313	-	3/3/20/26	16/39/137/137	-
22	CLA	a	404	-	1/1/15/20	15/37/115/115	-
22	CLA	V	304	-	1/1/14/20	12/31/109/115	-
25	LHG	u	312	-	-	25/53/53/53	-
26	CHL	6	315	-	3/3/20/26	15/39/137/137	-
22	CLA	5	301	-	1/1/15/20	10/37/115/115	-
22	CLA	Q	302	-	1/1/15/20	11/37/115/115	-
36	DGD	a	416	-	-	24/48/88/95	0/2/2/2
26	CHL	u	316	-	3/3/20/26	23/39/137/137	-
24	XAT	5	311	-	-	6/31/93/93	0/4/4/4
22	CLA	4	304	-	1/1/14/20	9/31/109/115	-
26	CHL	u	315	-	3/3/16/26	8/20/118/137	-
25	LHG	L	101	-	-	28/53/53/53	-
22	CLA	A	405	-	1/1/15/20	10/37/115/115	-
23	LUT	V	310	-	-	0/29/67/67	0/2/2/2
22	CLA	p	305	18	1/1/15/20	11/37/115/115	-
25	LHG	Q	310	-	-	19/53/53/53	-
25	LHG	R	314	-	-	24/46/46/53	-
22	CLA	q	305	22	1/1/14/20	12/31/109/115	-
25	LHG	c	521	-	-	14/53/53/53	-
27	NEX	R	301	1,22	-	10/27/83/83	0/3/3/3
22	CLA	C	508	-	1/1/15/20	20/37/115/115	-
22	CLA	v	303	-	1/1/12/20	7/19/97/115	-
22	CLA	p	302	-	1/1/15/20	15/37/115/115	-
22	CLA	B	617	-	1/1/15/20	11/37/115/115	-
23	LUT	u	310	-	-	2/29/67/67	0/2/2/2
22	CLA	g	301	-	1/1/15/20	14/37/115/115	-
26	CHL	3	312	-	3/3/16/26	8/18/116/137	-
31	BCR	k	101	-	-	13/29/63/63	0/2/2/2
22	CLA	U	304	-	1/1/14/20	5/31/109/115	-
25	LHG	D	406	3	-	28/50/50/53	-
22	CLA	P	303	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	603	-	1/1/15/20	12/37/115/115	-
26	CHL	6	316	18	3/3/20/26	23/39/137/137	-
25	LHG	d	406	3	-	19/53/53/53	-
22	CLA	r	608	-	1/1/11/20	7/18/96/115	-
22	CLA	C	510	-	1/1/15/20	8/37/115/115	-
22	CLA	4	302	-	1/1/15/20	15/37/115/115	-
22	CLA	Q	307	-	1/1/15/20	10/37/115/115	-
24	XAT	6	310	-	-	8/31/93/93	0/4/4/4
34	LMG	b	624	21	-	22/50/70/70	0/1/1/1
26	CHL	s	314	-	3/3/16/26	6/15/113/137	-
22	CLA	c	513	-	1/1/15/20	8/37/115/115	-
22	CLA	b	616	21	1/1/15/20	9/37/115/115	-

All (5049) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	409	BCR	C26-C25	15.51	1.61	1.34
31	a	409	BCR	C26-C25	15.51	1.61	1.34
31	b	619	BCR	C5-C6	15.49	1.61	1.34
31	B	619	BCR	C5-C6	15.47	1.61	1.34
31	x	202	BCR	C5-C6	15.45	1.61	1.34
31	z	101	BCR	C5-C6	15.44	1.61	1.34
31	X	201	BCR	C5-C6	15.44	1.61	1.34
31	c	516	BCR	C26-C25	15.40	1.61	1.34
31	C	516	BCR	C5-C6	15.39	1.61	1.34
31	d	403	BCR	C26-C25	15.35	1.61	1.34
31	D	404	BCR	C26-C25	15.35	1.61	1.34
31	T	101	BCR	C5-C6	15.34	1.61	1.34
31	t	101	BCR	C5-C6	15.34	1.61	1.34
31	C	518	BCR	C26-C25	15.33	1.61	1.34
31	b	619	BCR	C26-C25	15.31	1.61	1.34
31	b	618	BCR	C5-C6	15.30	1.60	1.34
31	k	101	BCR	C5-C6	15.29	1.60	1.34
31	x	202	BCR	C26-C25	15.28	1.60	1.34
31	X	201	BCR	C26-C25	15.27	1.60	1.34
31	B	619	BCR	C26-C25	15.27	1.60	1.34
31	K	101	BCR	C5-C6	15.25	1.60	1.34
31	K	101	BCR	C26-C25	15.25	1.60	1.34
31	k	101	BCR	C26-C25	15.25	1.60	1.34
31	C	518	BCR	C5-C6	15.23	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	620	BCR	C5-C6	15.22	1.60	1.34
31	c	516	BCR	C5-C6	15.22	1.60	1.34
31	B	618	BCR	C5-C6	15.20	1.60	1.34
31	t	101	BCR	C26-C25	15.19	1.60	1.34
31	C	516	BCR	C26-C25	15.19	1.60	1.34
31	B	620	BCR	C5-C6	15.18	1.60	1.34
31	B	618	BCR	C26-C25	15.15	1.60	1.34
31	T	101	BCR	C26-C25	15.14	1.60	1.34
31	z	101	BCR	C26-C25	15.13	1.60	1.34
31	d	403	BCR	C5-C6	15.12	1.60	1.34
31	D	404	BCR	C5-C6	15.11	1.60	1.34
31	b	618	BCR	C26-C25	15.08	1.60	1.34
31	A	409	BCR	C5-C6	15.05	1.60	1.34
31	a	409	BCR	C5-C6	14.98	1.60	1.34
31	B	620	BCR	C26-C25	14.97	1.60	1.34
31	b	620	BCR	C26-C25	14.97	1.60	1.34
31	c	515	BCR	C5-C6	14.92	1.60	1.34
31	c	515	BCR	C26-C25	14.88	1.60	1.34
31	C	517	BCR	C5-C6	14.88	1.60	1.34
31	C	517	BCR	C26-C25	14.85	1.60	1.34
22	S	302	CLA	C4B-NB	8.04	1.42	1.35
33	a	411	PL9	C6-C5	8.00	1.53	1.35
22	s	302	CLA	C4B-NB	7.98	1.42	1.35
33	A	410	PL9	C6-C5	7.98	1.53	1.35
22	n	302	CLA	C4B-NB	7.97	1.42	1.35
31	B	618	BCR	C30-C25	-7.96	1.42	1.53
22	N	302	CLA	C4B-NB	7.94	1.42	1.35
31	b	618	BCR	C30-C25	-7.92	1.42	1.53
22	1	302	CLA	C4B-NB	7.76	1.42	1.35
22	4	306	CLA	C4B-NB	7.75	1.42	1.35
22	V	306	CLA	C4B-NB	7.74	1.42	1.35
22	4	302	CLA	C4B-NB	7.64	1.42	1.35
22	n	308	CLA	C4B-NB	7.63	1.42	1.35
22	5	305	CLA	C4B-NB	7.59	1.42	1.35
22	R	305	CLA	C4B-NB	7.58	1.42	1.35
22	R	302	CLA	C4B-NB	7.57	1.42	1.35
22	c	509	CLA	C4B-NB	7.56	1.42	1.35
22	r	601	CLA	C4B-NB	7.55	1.41	1.35
22	v	306	CLA	C4B-NB	7.54	1.41	1.35
22	Q	303	CLA	C4B-NB	7.54	1.41	1.35
22	N	308	CLA	C4B-NB	7.53	1.41	1.35
22	r	610	CLA	C4B-NB	7.52	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	C4B-NB	7.52	1.41	1.35
22	2	302	CLA	C4B-NB	7.51	1.41	1.35
22	g	306	CLA	C4B-NB	7.50	1.41	1.35
22	c	507	CLA	C4B-NB	7.49	1.41	1.35
22	R	309	CLA	C4B-NB	7.48	1.41	1.35
22	n	305	CLA	C4B-NB	7.46	1.41	1.35
22	R	311	CLA	C4B-NB	7.46	1.41	1.35
22	B	612	CLA	C4B-NB	7.44	1.41	1.35
22	2	305	CLA	C4B-NB	7.43	1.41	1.35
22	r	608	CLA	C4B-NB	7.41	1.41	1.35
22	q	303	CLA	C4B-NB	7.41	1.41	1.35
22	Q	306	CLA	C4B-NB	7.41	1.41	1.35
22	r	604	CLA	C4B-NB	7.40	1.41	1.35
22	r	609	CLA	C4B-NB	7.40	1.41	1.35
22	g	304	CLA	C4B-NB	7.39	1.41	1.35
22	G	304	CLA	C4B-NB	7.37	1.41	1.35
22	n	303	CLA	C4B-NB	7.37	1.41	1.35
22	G	303	CLA	C4B-NB	7.36	1.41	1.35
22	C	508	CLA	C4B-NB	7.36	1.41	1.35
22	U	306	CLA	C4B-NB	7.35	1.41	1.35
22	R	306	CLA	C4B-NB	7.35	1.41	1.35
22	q	306	CLA	C4B-NB	7.33	1.41	1.35
22	r	607	CLA	C4B-NB	7.33	1.41	1.35
22	B	610	CLA	C4B-NB	7.32	1.41	1.35
22	r	605	CLA	C4B-NB	7.31	1.41	1.35
22	b	610	CLA	C4B-NB	7.31	1.41	1.35
22	V	305	CLA	C4B-NB	7.31	1.41	1.35
22	p	309	CLA	C4B-NB	7.30	1.41	1.35
22	S	303	CLA	C4B-NB	7.30	1.41	1.35
22	R	310	CLA	C4B-NB	7.30	1.41	1.35
22	s	303	CLA	C4B-NB	7.30	1.41	1.35
22	5	308	CLA	C4B-NB	7.29	1.41	1.35
22	Q	304	CLA	C4B-NB	7.29	1.41	1.35
22	u	301	CLA	C4B-NB	7.29	1.41	1.35
22	b	612	CLA	C4B-NB	7.29	1.41	1.35
22	V	301	CLA	C4B-NB	7.28	1.41	1.35
22	P	308	CLA	C4B-NB	7.28	1.41	1.35
22	g	303	CLA	C4B-NB	7.28	1.41	1.35
22	R	304	CLA	C4B-NB	7.28	1.41	1.35
22	R	308	CLA	C4B-NB	7.28	1.41	1.35
22	S	309	CLA	C4B-NB	7.28	1.41	1.35
22	g	307	CLA	C4B-NB	7.27	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	304	CLA	C4B-NB	7.26	1.41	1.35
33	A	410	PL9	C2-C3	7.26	1.53	1.34
22	3	308	CLA	C4B-NB	7.26	1.41	1.35
22	6	309	CLA	C4B-NB	7.26	1.41	1.35
22	6	307	CLA	C4B-NB	7.26	1.41	1.35
22	G	307	CLA	C4B-NB	7.25	1.41	1.35
22	g	302	CLA	C4B-NB	7.25	1.41	1.35
22	p	308	CLA	C4B-NB	7.25	1.41	1.35
22	u	303	CLA	C4B-NB	7.24	1.41	1.35
22	q	301	CLA	C4B-NB	7.24	1.41	1.35
22	v	305	CLA	C4B-NB	7.24	1.41	1.35
22	q	304	CLA	C4B-NB	7.24	1.41	1.35
22	p	303	CLA	C4B-NB	7.24	1.41	1.35
22	G	306	CLA	C4B-NB	7.24	1.41	1.35
33	a	411	PL9	C2-C3	7.23	1.53	1.34
22	3	306	CLA	C4B-NB	7.23	1.41	1.35
22	p	306	CLA	C4B-NB	7.23	1.41	1.35
22	6	304	CLA	C4B-NB	7.23	1.41	1.35
22	u	302	CLA	C4B-NB	7.22	1.41	1.35
22	p	307	CLA	C4B-NB	7.21	1.41	1.35
22	N	305	CLA	C4B-NB	7.21	1.41	1.35
22	r	603	CLA	C4B-NB	7.21	1.41	1.35
22	P	309	CLA	C4B-NB	7.19	1.41	1.35
22	V	304	CLA	C4B-NB	7.19	1.41	1.35
22	U	301	CLA	C4B-NB	7.19	1.41	1.35
22	c	508	CLA	C4B-NB	7.19	1.41	1.35
22	6	305	CLA	C4B-NB	7.19	1.41	1.35
22	4	303	CLA	C4B-NB	7.19	1.41	1.35
31	c	515	BCR	C30-C25	-7.18	1.43	1.53
22	S	308	CLA	C4B-NB	7.18	1.41	1.35
22	V	302	CLA	C4B-NB	7.17	1.41	1.35
22	6	308	CLA	C4B-NB	7.17	1.41	1.35
22	Q	305	CLA	C4B-NB	7.17	1.41	1.35
22	3	305	CLA	C4B-NB	7.16	1.41	1.35
22	P	306	CLA	C4B-NB	7.16	1.41	1.35
22	U	302	CLA	C4B-NB	7.16	1.41	1.35
22	G	308	CLA	C4B-NB	7.16	1.41	1.35
22	S	301	CLA	C4B-NB	7.16	1.41	1.35
22	c	502	CLA	C4B-NB	7.16	1.41	1.35
22	3	303	CLA	C4B-NB	7.16	1.41	1.35
22	5	303	CLA	C4B-NB	7.15	1.41	1.35
22	4	308	CLA	C4B-NB	7.15	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	303	CLA	C4B-NB	7.15	1.41	1.35
22	N	307	CLA	C4B-NB	7.15	1.41	1.35
22	Q	307	CLA	C4B-NB	7.14	1.41	1.35
22	5	302	CLA	C4B-NB	7.13	1.41	1.35
22	5	307	CLA	C4B-NB	7.13	1.41	1.35
22	S	304	CLA	C4B-NB	7.13	1.41	1.35
22	q	307	CLA	C4B-NB	7.13	1.41	1.35
22	s	309	CLA	C4B-NB	7.13	1.41	1.35
22	Q	301	CLA	C4B-NB	7.13	1.41	1.35
22	2	307	CLA	C4B-NB	7.12	1.41	1.35
22	C	503	CLA	C4B-NB	7.12	1.41	1.35
22	s	301	CLA	C4B-NB	7.12	1.41	1.35
22	6	303	CLA	C4B-NB	7.11	1.41	1.35
22	U	308	CLA	C4B-NB	7.11	1.41	1.35
31	C	517	BCR	C30-C25	-7.11	1.44	1.53
22	p	304	CLA	C4B-NB	7.11	1.41	1.35
22	C	506	CLA	C4B-NB	7.11	1.41	1.35
22	S	307	CLA	C4B-NB	7.11	1.41	1.35
22	g	308	CLA	C4B-NB	7.11	1.41	1.35
22	v	302	CLA	C4B-NB	7.10	1.41	1.35
22	2	308	CLA	C4B-NB	7.10	1.41	1.35
22	C	509	CLA	C4B-NB	7.10	1.41	1.35
22	b	604	CLA	C4B-NB	7.10	1.41	1.35
22	S	306	CLA	C4B-NB	7.09	1.41	1.35
22	3	307	CLA	C4B-NB	7.09	1.41	1.35
22	s	306	CLA	C4B-NB	7.08	1.41	1.35
22	v	303	CLA	C4B-NB	7.08	1.41	1.35
22	V	307	CLA	C4B-NB	7.08	1.41	1.35
22	s	308	CLA	C4B-NB	7.08	1.41	1.35
22	1	308	CLA	C4B-NB	7.08	1.41	1.35
22	v	304	CLA	C4B-NB	7.07	1.41	1.35
22	g	305	CLA	C4B-NB	7.07	1.41	1.35
22	V	303	CLA	C4B-NB	7.07	1.41	1.35
22	n	307	CLA	C4B-NB	7.07	1.41	1.35
22	B	604	CLA	C4B-NB	7.07	1.41	1.35
22	P	304	CLA	C4B-NB	7.07	1.41	1.35
22	v	301	CLA	C4B-NB	7.06	1.41	1.35
22	R	307	CLA	C4B-NB	7.06	1.41	1.35
22	G	301	CLA	C4B-NB	7.06	1.41	1.35
22	n	306	CLA	C4B-NB	7.06	1.41	1.35
22	r	602	CLA	C4B-NB	7.06	1.41	1.35
22	q	305	CLA	C4B-NB	7.05	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	307	CLA	C4B-NB	7.05	1.41	1.35
22	V	308	CLA	C4B-NB	7.04	1.41	1.35
22	u	305	CLA	C4B-NB	7.04	1.41	1.35
22	6	306	CLA	C4B-NB	7.04	1.41	1.35
22	6	302	CLA	C4B-NB	7.04	1.41	1.35
22	3	301	CLA	C4B-NB	7.04	1.41	1.35
22	s	304	CLA	C4B-NB	7.03	1.41	1.35
22	r	606	CLA	C4B-NB	7.03	1.41	1.35
22	N	306	CLA	C4B-NB	7.03	1.41	1.35
22	G	302	CLA	C4B-NB	7.03	1.41	1.35
22	4	305	CLA	C4B-NB	7.02	1.41	1.35
22	v	307	CLA	C4B-NB	7.02	1.41	1.35
22	C	512	CLA	C4B-NB	7.02	1.41	1.35
22	2	303	CLA	C4B-NB	7.02	1.41	1.35
22	b	617	CLA	C4B-NB	7.02	1.41	1.35
22	B	607	CLA	C4B-NB	7.02	1.41	1.35
31	b	620	BCR	C30-C25	-7.01	1.44	1.53
22	1	306	CLA	C4B-NB	7.01	1.41	1.35
22	v	308	CLA	C4B-NB	7.01	1.41	1.35
22	1	303	CLA	C4B-NB	7.01	1.41	1.35
22	u	308	CLA	C4B-NB	7.01	1.41	1.35
22	b	607	CLA	C4B-NB	7.00	1.41	1.35
22	b	611	CLA	C4B-NB	7.00	1.41	1.35
31	B	620	BCR	C30-C25	-7.00	1.44	1.53
22	n	301	CLA	C4B-NB	7.00	1.41	1.35
22	G	305	CLA	C4B-NB	7.00	1.41	1.35
22	c	511	CLA	C4B-NB	6.99	1.41	1.35
22	U	305	CLA	C4B-NB	6.99	1.41	1.35
22	N	303	CLA	C4B-NB	6.99	1.41	1.35
22	4	307	CLA	C4B-NB	6.99	1.41	1.35
22	R	303	CLA	C4B-NB	6.98	1.41	1.35
22	g	301	CLA	C4B-NB	6.98	1.41	1.35
22	C	504	CLA	C4B-NB	6.97	1.41	1.35
22	b	606	CLA	C4B-NB	6.97	1.41	1.35
22	Q	302	CLA	C4B-NB	6.97	1.41	1.35
22	c	505	CLA	C4B-NB	6.96	1.41	1.35
22	C	513	CLA	C4B-NB	6.96	1.41	1.35
22	N	304	CLA	C4B-NB	6.96	1.41	1.35
22	U	304	CLA	C4B-NB	6.96	1.41	1.35
22	2	306	CLA	C4B-NB	6.96	1.41	1.35
22	P	303	CLA	C4B-NB	6.95	1.41	1.35
22	B	611	CLA	C4B-NB	6.95	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	503	CLA	C4B-NB	6.95	1.41	1.35
22	c	512	CLA	C4B-NB	6.94	1.41	1.35
22	u	306	CLA	C4B-NB	6.94	1.41	1.35
22	1	301	CLA	C4B-NB	6.93	1.41	1.35
22	N	301	CLA	C4B-NB	6.93	1.41	1.35
22	q	308	CLA	C4B-NB	6.93	1.41	1.35
31	z	101	BCR	C30-C25	-6.93	1.44	1.53
22	3	302	CLA	C4B-NB	6.92	1.41	1.35
22	5	301	CLA	C4B-NB	6.92	1.41	1.35
22	5	304	CLA	C4B-NB	6.91	1.41	1.35
22	p	305	CLA	C4B-NB	6.91	1.41	1.35
22	U	307	CLA	C4B-NB	6.90	1.41	1.35
22	s	305	CLA	C4B-NB	6.90	1.41	1.35
22	Q	308	CLA	C4B-NB	6.90	1.41	1.35
22	2	301	CLA	C4B-NB	6.89	1.41	1.35
22	P	307	CLA	C4B-NB	6.89	1.41	1.35
22	4	301	CLA	C4B-NB	6.89	1.41	1.35
22	B	609	CLA	C4B-NB	6.88	1.41	1.35
33	d	404	PL9	C2-C3	6.88	1.52	1.34
22	P	302	CLA	C4B-NB	6.87	1.41	1.35
22	q	302	CLA	C4B-NB	6.87	1.41	1.35
22	B	606	CLA	C4B-NB	6.86	1.41	1.35
22	4	304	CLA	C4B-NB	6.86	1.41	1.35
22	n	304	CLA	C4B-NB	6.86	1.41	1.35
22	S	305	CLA	C4B-NB	6.86	1.41	1.35
22	2	304	CLA	C4B-NB	6.86	1.41	1.35
33	D	405	PL9	C2-C3	6.86	1.52	1.34
22	b	609	CLA	C4B-NB	6.86	1.41	1.35
31	c	516	BCR	C30-C25	-6.86	1.44	1.53
31	C	516	BCR	C30-C25	-6.86	1.44	1.53
22	1	305	CLA	C4B-NB	6.84	1.41	1.35
31	C	518	BCR	C30-C25	-6.83	1.44	1.53
22	b	605	CLA	C4B-NB	6.83	1.41	1.35
22	P	305	CLA	C4B-NB	6.83	1.41	1.35
22	u	307	CLA	C4B-NB	6.83	1.41	1.35
22	B	615	CLA	C4B-NB	6.81	1.41	1.35
22	1	304	CLA	C4B-NB	6.80	1.41	1.35
22	1	307	CLA	C4B-NB	6.80	1.41	1.35
22	5	306	CLA	C4B-NB	6.80	1.41	1.35
31	b	619	BCR	C30-C25	-6.79	1.44	1.53
22	C	505	CLA	C4B-NB	6.79	1.41	1.35
22	b	615	CLA	C4B-NB	6.79	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C4B-NB	6.78	1.41	1.35
22	C	514	CLA	C4B-NB	6.78	1.41	1.35
31	x	202	BCR	C30-C25	-6.77	1.44	1.53
22	B	608	CLA	C4B-NB	6.77	1.41	1.35
22	u	304	CLA	C4B-NB	6.76	1.41	1.35
31	B	619	BCR	C30-C25	-6.76	1.44	1.53
22	B	605	CLA	C4B-NB	6.75	1.41	1.35
22	C	515	CLA	C4B-NB	6.75	1.41	1.35
22	p	302	CLA	C4B-NB	6.74	1.41	1.35
31	A	409	BCR	C30-C25	-6.71	1.44	1.53
31	X	201	BCR	C30-C25	-6.70	1.44	1.53
22	c	514	CLA	C4B-NB	6.70	1.41	1.35
31	a	409	BCR	C30-C25	-6.69	1.44	1.53
22	b	613	CLA	C4B-NB	6.69	1.41	1.35
22	c	513	CLA	C4B-NB	6.69	1.41	1.35
22	b	603	CLA	C4B-NB	6.69	1.41	1.35
22	x	201	CLA	C4B-NB	6.67	1.41	1.35
22	c	504	CLA	C4B-NB	6.66	1.41	1.35
22	X	202	CLA	C4B-NB	6.66	1.41	1.35
31	C	517	BCR	C29-C28	-6.62	1.36	1.52
31	c	515	BCR	C29-C28	-6.62	1.36	1.52
22	B	603	CLA	C4B-NB	6.62	1.41	1.35
22	B	613	CLA	C4B-NB	6.61	1.41	1.35
22	A	405	CLA	C4B-NB	6.60	1.41	1.35
22	a	406	CLA	C4B-NB	6.59	1.41	1.35
22	B	617	CLA	C4B-NB	6.59	1.41	1.35
22	a	405	CLA	C4B-NB	6.57	1.41	1.35
22	d	402	CLA	C4B-NB	6.57	1.41	1.35
22	A	406	CLA	C4B-NB	6.56	1.41	1.35
31	C	516	BCR	C29-C28	-6.56	1.36	1.52
31	z	101	BCR	C29-C28	-6.54	1.36	1.52
22	b	614	CLA	C4B-NB	6.54	1.41	1.35
22	B	614	CLA	C4B-NB	6.53	1.41	1.35
31	A	409	BCR	C29-C28	-6.52	1.36	1.52
31	k	101	BCR	C30-C25	-6.52	1.44	1.53
31	K	101	BCR	C30-C25	-6.52	1.44	1.53
31	a	409	BCR	C29-C28	-6.51	1.36	1.52
22	D	403	CLA	C4B-NB	6.51	1.41	1.35
31	B	618	BCR	C29-C28	-6.50	1.36	1.52
22	b	616	CLA	C4B-NB	6.50	1.41	1.35
22	B	602	CLA	C4B-NB	6.50	1.41	1.35
22	B	616	CLA	C4B-NB	6.48	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	618	BCR	C29-C28	-6.47	1.36	1.52
22	b	602	CLA	C4B-NB	6.45	1.41	1.35
31	C	518	BCR	C29-C28	-6.44	1.36	1.52
31	c	516	BCR	C29-C28	-6.43	1.36	1.52
31	X	201	BCR	C29-C28	-6.42	1.36	1.52
31	B	619	BCR	C29-C28	-6.41	1.36	1.52
31	D	404	BCR	C30-C25	-6.40	1.45	1.53
31	b	619	BCR	C29-C28	-6.40	1.36	1.52
31	b	620	BCR	C29-C28	-6.39	1.36	1.52
31	B	620	BCR	C29-C28	-6.38	1.36	1.52
31	t	101	BCR	C29-C28	-6.38	1.36	1.52
31	t	101	BCR	C30-C25	-6.37	1.45	1.53
31	d	403	BCR	C30-C25	-6.36	1.45	1.53
31	b	618	BCR	C2-C3	-6.36	1.36	1.52
31	x	202	BCR	C29-C28	-6.35	1.36	1.52
31	T	101	BCR	C29-C28	-6.35	1.36	1.52
22	a	408	CLA	C4B-NB	6.32	1.40	1.35
31	T	101	BCR	C30-C25	-6.31	1.45	1.53
31	k	101	BCR	C29-C28	-6.31	1.37	1.52
31	K	101	BCR	C29-C28	-6.30	1.37	1.52
22	c	506	CLA	C4B-NB	6.29	1.40	1.35
22	A	408	CLA	C4B-NB	6.27	1.40	1.35
31	c	516	BCR	C2-C3	-6.27	1.37	1.52
31	C	516	BCR	C2-C3	-6.27	1.37	1.52
31	B	618	BCR	C2-C3	-6.26	1.37	1.52
31	x	202	BCR	C2-C3	-6.26	1.37	1.52
31	B	619	BCR	C2-C3	-6.25	1.37	1.52
31	a	409	BCR	C2-C3	-6.25	1.37	1.52
31	z	101	BCR	C2-C3	-6.25	1.37	1.52
31	C	518	BCR	C2-C3	-6.24	1.37	1.52
31	B	620	BCR	C2-C3	-6.24	1.37	1.52
31	A	409	BCR	C2-C3	-6.24	1.37	1.52
31	t	101	BCR	C2-C3	-6.23	1.37	1.52
31	X	201	BCR	C2-C3	-6.23	1.37	1.52
31	T	101	BCR	C2-C3	-6.23	1.37	1.52
31	b	619	BCR	C2-C3	-6.23	1.37	1.52
31	D	404	BCR	C2-C3	-6.22	1.37	1.52
31	d	403	BCR	C2-C3	-6.21	1.37	1.52
31	b	620	BCR	C2-C3	-6.21	1.37	1.52
31	d	403	BCR	C29-C28	-6.20	1.37	1.52
31	D	404	BCR	C29-C28	-6.17	1.37	1.52
22	C	507	CLA	C4B-NB	6.16	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	409	BCR	C1-C6	-6.15	1.45	1.53
31	k	101	BCR	C2-C3	-6.15	1.37	1.52
22	A	404	CLA	C4B-NB	6.15	1.40	1.35
31	a	409	BCR	C1-C6	-6.14	1.45	1.53
31	C	517	BCR	C2-C3	-6.13	1.37	1.52
31	K	101	BCR	C2-C3	-6.12	1.37	1.52
22	C	511	CLA	C4B-NB	6.11	1.40	1.35
31	c	515	BCR	C2-C3	-6.09	1.37	1.52
22	a	404	CLA	C4B-NB	6.08	1.40	1.35
31	T	101	BCR	C8-C9	6.02	1.58	1.45
22	c	510	CLA	C4B-NB	6.01	1.40	1.35
31	t	101	BCR	C8-C9	6.00	1.58	1.45
31	c	515	BCR	C1-C6	-5.98	1.45	1.53
31	C	517	BCR	C1-C6	-5.95	1.45	1.53
31	D	404	BCR	C8-C9	5.83	1.58	1.45
31	B	620	BCR	C1-C6	-5.81	1.45	1.53
31	X	201	BCR	C1-C6	-5.81	1.45	1.53
31	b	618	BCR	C1-C6	-5.80	1.45	1.53
31	b	620	BCR	C1-C6	-5.80	1.45	1.53
31	d	403	BCR	C8-C9	5.80	1.58	1.45
31	b	620	BCR	C8-C9	5.80	1.58	1.45
31	C	516	BCR	C1-C6	-5.79	1.45	1.53
31	x	202	BCR	C1-C6	-5.78	1.45	1.53
31	X	201	BCR	C8-C9	5.76	1.58	1.45
31	B	620	BCR	C8-C9	5.75	1.58	1.45
31	x	202	BCR	C8-C9	5.73	1.58	1.45
31	z	101	BCR	C1-C6	-5.70	1.45	1.53
31	D	404	BCR	C1-C6	-5.65	1.46	1.53
31	K	101	BCR	C8-C9	5.65	1.58	1.45
31	B	618	BCR	C1-C6	-5.63	1.46	1.53
31	d	403	BCR	C1-C6	-5.63	1.46	1.53
31	k	101	BCR	C8-C9	5.63	1.58	1.45
31	c	516	BCR	C8-C9	5.60	1.58	1.45
31	C	518	BCR	C8-C9	5.58	1.57	1.45
31	z	101	BCR	C8-C9	5.56	1.57	1.45
31	B	619	BCR	C8-C9	5.53	1.57	1.45
31	t	101	BCR	C19-C18	5.53	1.57	1.45
31	C	516	BCR	C8-C9	5.53	1.57	1.45
31	b	619	BCR	C8-C9	5.52	1.57	1.45
31	T	101	BCR	C19-C18	5.51	1.57	1.45
26	P	315	CHL	C3B-C2B	5.50	1.48	1.40
26	P	315	CHL	CHC-C1C	5.50	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	618	BCR	C8-C9	5.48	1.57	1.45
26	1	317	CHL	O2D-CGD	5.46	1.46	1.33
26	4	316	CHL	O2D-CGD	5.44	1.46	1.33
31	b	618	BCR	C8-C9	5.44	1.57	1.45
31	A	409	BCR	C8-C9	5.42	1.57	1.45
31	c	515	BCR	C8-C9	5.38	1.57	1.45
31	C	517	BCR	C8-C9	5.37	1.57	1.45
31	a	409	BCR	C8-C9	5.36	1.57	1.45
26	p	315	CHL	C3B-C2B	5.36	1.47	1.40
26	v	317	CHL	O2D-CGD	5.36	1.46	1.33
26	n	314	CHL	C3B-C2B	5.35	1.47	1.40
31	k	101	BCR	C1-C6	-5.35	1.46	1.53
31	D	404	BCR	C29-C30	5.35	1.66	1.54
26	p	315	CHL	CHC-C1C	5.34	1.48	1.35
26	P	314	CHL	CHC-C1C	5.33	1.48	1.35
26	3	312	CHL	C3B-C2B	5.33	1.47	1.40
31	C	518	BCR	C1-C6	-5.33	1.46	1.53
31	X	201	BCR	C19-C18	5.32	1.57	1.45
26	6	313	CHL	C3B-C2B	5.32	1.47	1.40
31	T	101	BCR	C29-C30	5.32	1.66	1.54
31	t	101	BCR	C29-C30	5.32	1.66	1.54
31	x	202	BCR	C19-C18	5.31	1.57	1.45
31	d	403	BCR	C29-C30	5.31	1.66	1.54
31	c	516	BCR	C1-C6	-5.30	1.46	1.53
31	K	101	BCR	C1-C6	-5.29	1.46	1.53
26	V	317	CHL	O2D-CGD	5.29	1.46	1.33
31	K	101	BCR	C29-C30	5.25	1.66	1.54
31	b	619	BCR	C1-C6	-5.25	1.46	1.53
26	U	316	CHL	O2D-CGD	5.24	1.46	1.33
26	2	314	CHL	C3B-C2B	5.24	1.47	1.40
26	g	313	CHL	O2D-CGD	5.24	1.46	1.33
31	b	620	BCR	C19-C18	5.23	1.57	1.45
26	n	316	CHL	O2D-CGD	5.23	1.46	1.33
26	u	317	CHL	O2D-CGD	5.23	1.46	1.33
31	c	516	BCR	C19-C18	5.22	1.57	1.45
31	D	404	BCR	C19-C18	5.22	1.57	1.45
31	k	101	BCR	C29-C30	5.22	1.66	1.54
31	C	518	BCR	C19-C18	5.21	1.57	1.45
26	Q	312	CHL	O2D-CGD	5.21	1.45	1.33
26	n	314	CHL	CHC-C1C	5.20	1.48	1.35
26	p	314	CHL	CHC-C1C	5.20	1.48	1.35
26	q	312	CHL	O2D-CGD	5.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	403	BCR	C19-C18	5.19	1.57	1.45
26	2	314	CHL	CHC-C1C	5.19	1.48	1.35
26	3	312	CHL	CHC-C1C	5.18	1.48	1.35
31	B	620	BCR	C19-C18	5.18	1.57	1.45
26	5	314	CHL	C3B-C2B	5.18	1.47	1.40
26	s	313	CHL	O2D-CGD	5.17	1.45	1.33
26	g	316	CHL	O2D-CGD	5.17	1.45	1.33
26	s	314	CHL	O2D-CGD	5.16	1.45	1.33
31	z	101	BCR	C19-C18	5.16	1.57	1.45
26	V	316	CHL	O2D-CGD	5.16	1.45	1.33
26	n	315	CHL	O2D-CGD	5.16	1.45	1.33
31	B	619	BCR	C1-C6	-5.16	1.46	1.53
31	b	620	BCR	C29-C30	5.15	1.66	1.54
26	p	320	CHL	O2D-CGD	5.15	1.45	1.33
26	S	314	CHL	O2D-CGD	5.15	1.45	1.33
26	3	312	CHL	O2D-CGD	5.15	1.45	1.33
26	G	316	CHL	O2D-CGD	5.15	1.45	1.33
31	C	516	BCR	C19-C18	5.14	1.57	1.45
26	q	312	CHL	CHC-C1C	5.14	1.48	1.35
26	s	315	CHL	CHC-C1C	5.14	1.48	1.35
31	x	202	BCR	C29-C30	5.14	1.66	1.54
26	6	313	CHL	CHC-C1C	5.14	1.48	1.35
26	g	314	CHL	O2D-CGD	5.14	1.45	1.33
26	N	314	CHL	C3B-C2B	5.14	1.47	1.40
26	3	314	CHL	O2D-CGD	5.14	1.45	1.33
26	r	615	CHL	O2D-CGD	5.13	1.45	1.33
26	2	316	CHL	O2D-CGD	5.13	1.45	1.33
26	S	313	CHL	O2D-CGD	5.13	1.45	1.33
31	B	620	BCR	C29-C30	5.13	1.66	1.54
26	v	315	CHL	O2D-CGD	5.13	1.45	1.33
31	T	101	BCR	C1-C6	-5.13	1.46	1.53
26	G	312	CHL	CHC-C1C	5.13	1.48	1.35
26	5	313	CHL	CHC-C1C	5.13	1.48	1.35
26	p	315	CHL	O2D-CGD	5.12	1.45	1.33
26	S	315	CHL	CHC-C1C	5.12	1.48	1.35
26	G	312	CHL	O2D-CGD	5.12	1.45	1.33
26	R	315	CHL	O2D-CGD	5.12	1.45	1.33
26	6	315	CHL	O2D-CGD	5.12	1.45	1.33
26	G	313	CHL	O2D-CGD	5.12	1.45	1.33
31	X	201	BCR	C29-C30	5.12	1.65	1.54
26	Q	313	CHL	O2D-CGD	5.12	1.45	1.33
26	P	317	CHL	O2D-CGD	5.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	314	CHL	O2D-CGD	5.12	1.45	1.33
26	G	314	CHL	O2D-CGD	5.12	1.45	1.33
26	5	314	CHL	CHC-C1C	5.12	1.48	1.35
31	z	101	BCR	C29-C30	5.12	1.65	1.54
26	4	314	CHL	O2D-CGD	5.11	1.45	1.33
26	6	313	CHL	O2D-CGD	5.11	1.45	1.33
26	P	319	CHL	O2D-CGD	5.11	1.45	1.33
26	v	316	CHL	O2D-CGD	5.11	1.45	1.33
26	u	314	CHL	O2D-CGD	5.11	1.45	1.33
26	p	317	CHL	O2D-CGD	5.10	1.45	1.33
26	5	313	CHL	O2D-CGD	5.10	1.45	1.33
26	g	312	CHL	O2D-CGD	5.10	1.45	1.33
26	p	318	CHL	O2D-CGD	5.10	1.45	1.33
26	1	314	CHL	O2D-CGD	5.10	1.45	1.33
26	U	314	CHL	O2D-CGD	5.10	1.45	1.33
26	u	315	CHL	O2D-CGD	5.10	1.45	1.33
26	5	316	CHL	O2D-CGD	5.10	1.45	1.33
26	V	315	CHL	CHC-C1C	5.10	1.48	1.35
26	v	318	CHL	O2D-CGD	5.10	1.45	1.33
26	N	315	CHL	O2D-CGD	5.09	1.45	1.33
26	r	614	CHL	O2D-CGD	5.09	1.45	1.33
26	3	316	CHL	O2D-CGD	5.09	1.45	1.33
26	3	314	CHL	CHC-C1C	5.09	1.48	1.35
26	n	313	CHL	CHC-C1C	5.09	1.48	1.35
26	v	314	CHL	O2D-CGD	5.09	1.45	1.33
26	2	314	CHL	O2D-CGD	5.09	1.45	1.33
26	5	314	CHL	O2D-CGD	5.09	1.45	1.33
26	Q	316	CHL	O2D-CGD	5.09	1.45	1.33
26	R	316	CHL	O2D-CGD	5.09	1.45	1.33
26	6	314	CHL	CHC-C1C	5.09	1.48	1.35
26	P	314	CHL	O2D-CGD	5.09	1.45	1.33
26	U	315	CHL	O2D-CGD	5.09	1.45	1.33
26	V	315	CHL	O2D-CGD	5.09	1.45	1.33
26	P	316	CHL	O2D-CGD	5.09	1.45	1.33
26	S	316	CHL	CHC-C1C	5.08	1.48	1.35
26	1	318	CHL	O2D-CGD	5.08	1.45	1.33
26	u	316	CHL	O2D-CGD	5.08	1.45	1.33
26	r	616	CHL	O2D-CGD	5.08	1.45	1.33
26	G	315	CHL	O2D-CGD	5.08	1.45	1.33
31	C	516	BCR	C29-C30	5.08	1.65	1.54
26	q	313	CHL	O2D-CGD	5.08	1.45	1.33
26	V	314	CHL	O2D-CGD	5.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	311	CHL	O2D-CGD	5.08	1.45	1.33
26	N	313	CHL	O2D-CGD	5.08	1.45	1.33
26	p	314	CHL	O2D-CGD	5.07	1.45	1.33
26	6	317	CHL	O2D-CGD	5.07	1.45	1.33
26	5	318	CHL	O2D-CGD	5.07	1.45	1.33
26	q	314	CHL	O2D-CGD	5.07	1.45	1.33
26	P	318	CHL	O2D-CGD	5.07	1.45	1.33
26	N	314	CHL	O2D-CGD	5.07	1.45	1.33
26	6	314	CHL	O2D-CGD	5.07	1.45	1.33
26	S	315	CHL	O2D-CGD	5.07	1.45	1.33
26	4	315	CHL	O2D-CGD	5.07	1.45	1.33
26	q	312	CHL	C3B-C2B	5.07	1.47	1.40
26	V	318	CHL	O2D-CGD	5.07	1.45	1.33
26	n	314	CHL	O2D-CGD	5.07	1.45	1.33
26	R	317	CHL	O2D-CGD	5.07	1.45	1.33
26	g	314	CHL	CHC-C1C	5.07	1.48	1.35
26	Q	315	CHL	O2D-CGD	5.06	1.45	1.33
26	2	315	CHL	O2D-CGD	5.06	1.45	1.33
26	s	315	CHL	O2D-CGD	5.06	1.45	1.33
26	6	315	CHL	CHC-C1C	5.06	1.47	1.35
26	U	319	CHL	O2D-CGD	5.06	1.45	1.33
26	n	313	CHL	O2D-CGD	5.06	1.45	1.33
26	p	319	CHL	O2D-CGD	5.06	1.45	1.33
26	n	317	CHL	O2D-CGD	5.06	1.45	1.33
26	5	315	CHL	O2D-CGD	5.06	1.45	1.33
26	n	318	CHL	O2D-CGD	5.06	1.45	1.33
31	b	619	BCR	C19-C18	5.06	1.56	1.45
26	V	314	CHL	CHC-C1C	5.05	1.47	1.35
31	K	101	BCR	C19-C18	5.05	1.56	1.45
31	t	101	BCR	C1-C6	-5.05	1.46	1.53
26	p	316	CHL	O2D-CGD	5.05	1.45	1.33
26	2	313	CHL	CHC-C1C	5.05	1.47	1.35
26	r	619	CHL	O2D-CGD	5.04	1.45	1.33
26	u	313	CHL	O2D-CGD	5.04	1.45	1.33
26	2	318	CHL	O2D-CGD	5.04	1.45	1.33
26	4	317	CHL	O2D-CGD	5.04	1.45	1.33
26	Q	311	CHL	O2D-CGD	5.04	1.45	1.33
26	2	313	CHL	O2D-CGD	5.03	1.45	1.33
26	s	316	CHL	CHC-C1C	5.03	1.47	1.35
26	1	313	CHL	C3D-C4D	-5.03	1.32	1.44
31	b	619	BCR	C29-C30	5.03	1.65	1.54
26	3	315	CHL	O2D-CGD	5.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	311	CHL	O2D-CGD	5.03	1.45	1.33
26	N	317	CHL	O2D-CGD	5.03	1.45	1.33
26	N	314	CHL	CHC-C1C	5.02	1.47	1.35
26	3	313	CHL	O2D-CGD	5.02	1.45	1.33
26	U	313	CHL	O2D-CGD	5.02	1.45	1.33
31	B	619	BCR	C29-C30	5.02	1.65	1.54
26	s	316	CHL	O2D-CGD	5.02	1.45	1.33
26	q	315	CHL	O2D-CGD	5.01	1.45	1.33
26	5	317	CHL	O2D-CGD	5.01	1.45	1.33
26	4	313	CHL	O2D-CGD	5.01	1.45	1.33
26	2	317	CHL	O2D-CGD	5.01	1.45	1.33
26	1	315	CHL	O2D-CGD	5.01	1.45	1.33
31	k	101	BCR	C19-C18	5.01	1.56	1.45
31	a	409	BCR	C29-C30	5.01	1.65	1.54
31	B	619	BCR	C19-C18	5.01	1.56	1.45
26	g	315	CHL	O2D-CGD	5.01	1.45	1.33
26	6	312	CHL	O2D-CGD	5.00	1.45	1.33
31	c	516	BCR	C29-C30	5.00	1.65	1.54
26	v	313	CHL	O2D-CGD	5.00	1.45	1.33
26	P	315	CHL	C2C-C3C	5.00	1.47	1.36
26	V	313	CHL	O2D-CGD	5.00	1.45	1.33
31	A	409	BCR	C29-C30	4.99	1.65	1.54
26	u	318	CHL	O2D-CGD	4.99	1.45	1.33
31	C	517	BCR	C19-C18	4.99	1.56	1.45
26	1	313	CHL	O2D-CGD	4.99	1.45	1.33
26	n	317	CHL	C3D-C4D	-4.99	1.32	1.44
26	V	316	CHL	CHC-C1C	4.99	1.47	1.35
31	c	515	BCR	C19-C18	4.99	1.56	1.45
26	V	313	CHL	CHC-C1C	4.99	1.47	1.35
26	G	314	CHL	CHC-C1C	4.98	1.47	1.35
31	B	618	BCR	C29-C30	4.98	1.65	1.54
31	b	618	BCR	C29-C30	4.98	1.65	1.54
26	N	316	CHL	O2D-CGD	4.98	1.45	1.33
26	1	314	CHL	CHC-C1C	4.98	1.47	1.35
26	G	311	CHL	O2D-CGD	4.98	1.45	1.33
26	v	313	CHL	CHC-C1C	4.98	1.47	1.35
26	1	316	CHL	O2D-CGD	4.98	1.45	1.33
26	S	316	CHL	O2D-CGD	4.98	1.45	1.33
26	R	317	CHL	C3D-C4D	-4.98	1.32	1.44
26	Q	312	CHL	CHC-C1C	4.98	1.47	1.35
26	U	319	CHL	CHC-C1C	4.97	1.47	1.35
26	U	313	CHL	C3D-C4D	-4.97	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	314	CHL	C3B-C2B	4.97	1.47	1.40
26	2	314	CHL	C2C-C3C	4.97	1.47	1.36
31	C	518	BCR	C29-C30	4.96	1.65	1.54
26	3	313	CHL	CHC-C1C	4.96	1.47	1.35
26	6	314	CHL	C3B-C2B	4.96	1.47	1.40
26	4	313	CHL	CHC-C1C	4.96	1.47	1.35
26	Q	314	CHL	CHC-C1C	4.95	1.47	1.35
26	4	313	CHL	C3D-C4D	-4.95	1.33	1.44
31	c	515	BCR	C29-C30	4.95	1.65	1.54
26	s	315	CHL	C3B-C2B	4.95	1.47	1.40
26	U	313	CHL	CHC-C1C	4.95	1.47	1.35
31	C	517	BCR	C29-C30	4.95	1.65	1.54
26	U	317	CHL	O2D-CGD	4.95	1.45	1.33
26	n	313	CHL	C3B-C2B	4.95	1.47	1.40
26	6	301	CHL	C3D-C4D	-4.94	1.33	1.44
26	g	312	CHL	CHC-C1C	4.94	1.47	1.35
26	G	312	CHL	C3B-C2B	4.94	1.47	1.40
26	3	311	CHL	O2D-CGD	4.94	1.45	1.33
26	s	313	CHL	CHC-C1C	4.94	1.47	1.35
26	S	313	CHL	C3D-C4D	-4.94	1.33	1.44
26	r	616	CHL	CHC-C1C	4.94	1.47	1.35
26	r	616	CHL	C3D-C4D	-4.94	1.33	1.44
26	6	316	CHL	O2D-CGD	4.94	1.45	1.33
26	S	313	CHL	CHC-C1C	4.93	1.47	1.35
26	R	317	CHL	CHC-C1C	4.93	1.47	1.35
26	1	315	CHL	C3D-C4D	-4.93	1.33	1.44
26	p	315	CHL	C2C-C3C	4.93	1.47	1.36
26	S	315	CHL	C3B-C2B	4.93	1.47	1.40
26	P	315	CHL	C3D-C4D	-4.93	1.33	1.44
26	n	317	CHL	CHC-C1C	4.92	1.47	1.35
26	3	315	CHL	CHC-C1C	4.92	1.47	1.35
26	5	316	CHL	C3D-C4D	-4.92	1.33	1.44
26	1	313	CHL	CHC-C1C	4.91	1.47	1.35
24	r	612	XAT	C2-C3	-4.91	1.45	1.52
26	V	314	CHL	C3B-C2B	4.91	1.47	1.40
26	1	316	CHL	C3D-C4D	-4.91	1.33	1.44
26	V	318	CHL	CHC-C1C	4.91	1.47	1.35
26	6	301	CHL	O2D-CGD	4.91	1.45	1.33
26	p	317	CHL	CHC-C1C	4.91	1.47	1.35
26	g	311	CHL	CHC-C1C	4.91	1.47	1.35
26	V	313	CHL	C3D-C4D	-4.91	1.33	1.44
26	s	313	CHL	C3D-C4D	-4.91	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	619	CHL	CHC-C1C	4.91	1.47	1.35
26	P	315	CHL	O2D-CGD	4.91	1.45	1.33
26	n	318	CHL	C3D-C4D	-4.90	1.33	1.44
26	n	315	CHL	CHC-C1C	4.90	1.47	1.35
26	5	316	CHL	CHC-C1C	4.90	1.47	1.35
26	n	316	CHL	CHC-C1C	4.90	1.47	1.35
26	G	315	CHL	CHC-C1C	4.90	1.47	1.35
26	4	315	CHL	C3D-C4D	-4.90	1.33	1.44
26	4	315	CHL	CHC-C1C	4.90	1.47	1.35
26	N	315	CHL	CHC-C1C	4.90	1.47	1.35
26	Q	312	CHL	C3B-C2B	4.89	1.47	1.40
26	P	317	CHL	CHC-C1C	4.89	1.47	1.35
26	v	313	CHL	C3D-C4D	-4.89	1.33	1.44
26	p	315	CHL	C3D-C4D	-4.89	1.33	1.44
26	u	316	CHL	C3D-C4D	-4.89	1.33	1.44
26	N	316	CHL	C3D-C4D	-4.88	1.33	1.44
26	u	316	CHL	CHC-C1C	4.88	1.47	1.35
26	N	313	CHL	C3B-C2B	4.88	1.47	1.40
26	4	314	CHL	CHC-C1C	4.87	1.47	1.35
24	R	313	XAT	C8-C9	4.87	1.56	1.45
24	R	313	XAT	C2-C3	-4.87	1.45	1.52
26	1	315	CHL	CHC-C1C	4.87	1.47	1.35
26	g	315	CHL	CHC-C1C	4.87	1.47	1.35
26	5	314	CHL	C2C-C3C	4.87	1.47	1.36
26	2	316	CHL	C3D-C4D	-4.87	1.33	1.44
26	3	312	CHL	C2C-C3C	4.87	1.47	1.36
26	2	316	CHL	CHC-C1C	4.87	1.47	1.35
26	R	316	CHL	CHC-C1C	4.87	1.47	1.35
26	u	314	CHL	CHC-C1C	4.87	1.47	1.35
24	U	311	XAT	C22-C23	-4.87	1.45	1.52
37	e	101	HEM	C3C-C2C	-4.87	1.33	1.40
26	P	316	CHL	CHC-C1C	4.86	1.47	1.35
26	Q	314	CHL	C3B-C2B	4.86	1.47	1.40
26	u	313	CHL	CHC-C1C	4.86	1.47	1.35
26	p	316	CHL	CHC-C1C	4.86	1.47	1.35
26	v	316	CHL	C3D-C4D	-4.86	1.33	1.44
26	N	315	CHL	C3D-C4D	-4.86	1.33	1.44
26	g	313	CHL	CHC-C1C	4.86	1.47	1.35
26	r	615	CHL	CHC-C1C	4.85	1.47	1.35
26	P	317	CHL	C3D-C4D	-4.85	1.33	1.44
26	v	315	CHL	C3D-C4D	-4.85	1.33	1.44
31	a	409	BCR	C19-C18	4.85	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p	317	CHL	C3D-C4D	-4.85	1.33	1.44
26	6	313	CHL	CHD-C1D	4.85	1.47	1.38
26	4	316	CHL	C3D-C4D	-4.85	1.33	1.44
26	6	314	CHL	C3D-C4D	-4.85	1.33	1.44
26	v	314	CHL	CHC-C1C	4.85	1.47	1.35
26	3	313	CHL	C3D-C4D	-4.84	1.33	1.44
26	G	311	CHL	C3D-C4D	-4.84	1.33	1.44
26	u	315	CHL	CHC-C1C	4.84	1.47	1.35
26	N	317	CHL	C3D-C4D	-4.84	1.33	1.44
26	s	315	CHL	C2C-C3C	4.84	1.47	1.36
26	p	316	CHL	C3B-C2B	4.84	1.47	1.40
26	2	313	CHL	C3B-C2B	4.83	1.47	1.40
26	v	315	CHL	CHC-C1C	4.83	1.47	1.35
26	6	313	CHL	C2C-C3C	4.83	1.47	1.36
26	q	315	CHL	CHC-C1C	4.83	1.47	1.35
26	v	317	CHL	C3D-C4D	-4.83	1.33	1.44
26	u	313	CHL	C3D-C4D	-4.83	1.33	1.44
26	q	312	CHL	CHD-C1D	4.83	1.47	1.38
31	B	618	BCR	C19-C18	4.83	1.56	1.45
24	q	309	XAT	C8-C9	4.83	1.56	1.45
26	g	316	CHL	C3D-C4D	-4.83	1.33	1.44
26	3	314	CHL	C3B-C2B	4.83	1.47	1.40
26	6	315	CHL	C3B-C2B	4.82	1.47	1.40
24	Q	309	XAT	C8-C9	4.82	1.56	1.45
37	E	101	HEM	C3C-C2C	-4.82	1.33	1.40
26	v	316	CHL	CHC-C1C	4.82	1.47	1.35
26	6	312	CHL	CHC-C1C	4.82	1.47	1.35
26	V	315	CHL	C3D-C4D	-4.82	1.33	1.44
24	u	311	XAT	C22-C23	-4.82	1.45	1.52
26	V	315	CHL	C3B-C2B	4.82	1.47	1.40
26	5	313	CHL	C3B-C2B	4.82	1.47	1.40
24	r	612	XAT	C8-C9	4.82	1.56	1.45
26	2	313	CHL	C3D-C4D	-4.81	1.33	1.44
26	q	315	CHL	C3B-C2B	4.81	1.47	1.40
26	G	313	CHL	CHC-C1C	4.81	1.47	1.35
26	p	314	CHL	C3D-C4D	-4.81	1.33	1.44
26	U	314	CHL	C3D-C4D	-4.81	1.33	1.44
26	3	311	CHL	CHC-C1C	4.81	1.47	1.35
26	U	314	CHL	CHC-C1C	4.81	1.47	1.35
31	A	409	BCR	C19-C18	4.81	1.56	1.45
24	G	309	XAT	C28-C29	4.81	1.56	1.45
26	6	317	CHL	C3D-C4D	-4.81	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	318	CHL	C3D-C4D	-4.81	1.33	1.44
26	q	312	CHL	C2C-C3C	4.81	1.47	1.36
26	P	316	CHL	C3D-C4D	-4.81	1.33	1.44
26	S	315	CHL	C3D-C4D	-4.81	1.33	1.44
26	s	314	CHL	CHC-C1C	4.80	1.47	1.35
26	3	312	CHL	CHD-C1D	4.80	1.47	1.38
26	s	315	CHL	C3D-C4D	-4.80	1.33	1.44
26	V	317	CHL	C3D-C4D	-4.80	1.33	1.44
26	S	315	CHL	C2C-C3C	4.80	1.47	1.36
26	2	315	CHL	CHC-C1C	4.80	1.47	1.35
26	6	312	CHL	C3D-C4D	-4.80	1.33	1.44
26	3	311	CHL	C3D-C4D	-4.80	1.33	1.44
26	p	316	CHL	C3D-C4D	-4.80	1.33	1.44
26	U	315	CHL	C3D-C4D	-4.80	1.33	1.44
26	u	314	CHL	C3D-C4D	-4.80	1.33	1.44
26	n	315	CHL	C3D-C4D	-4.80	1.33	1.44
26	p	320	CHL	CHC-C1C	4.80	1.47	1.35
26	Q	311	CHL	CHC-C1C	4.79	1.47	1.35
31	b	618	BCR	C19-C18	4.79	1.56	1.45
26	5	313	CHL	C3D-C4D	-4.79	1.33	1.44
26	q	314	CHL	CHC-C1C	4.79	1.47	1.35
26	g	314	CHL	C3B-C2B	4.79	1.47	1.40
26	1	317	CHL	C3D-C4D	-4.79	1.33	1.44
26	s	316	CHL	C3D-C4D	-4.79	1.33	1.44
26	u	317	CHL	C3D-C4D	-4.79	1.33	1.44
26	q	313	CHL	C3D-C4D	-4.79	1.33	1.44
26	V	316	CHL	C3D-C4D	-4.79	1.33	1.44
26	3	314	CHL	C3D-C4D	-4.79	1.33	1.44
26	s	316	CHL	C3B-C2B	4.79	1.47	1.40
26	P	314	CHL	C3D-C4D	-4.78	1.33	1.44
26	6	315	CHL	C3D-C4D	-4.78	1.33	1.44
26	3	313	CHL	C3B-C2B	4.78	1.47	1.40
26	S	316	CHL	C3D-C4D	-4.78	1.33	1.44
26	Q	313	CHL	C3D-C4D	-4.78	1.33	1.44
26	Q	316	CHL	CHC-C1C	4.78	1.47	1.35
24	V	311	XAT	C8-C9	4.78	1.56	1.45
26	5	315	CHL	CHC-C1C	4.78	1.47	1.35
24	3	309	XAT	C28-C29	4.78	1.56	1.45
26	Q	311	CHL	C3D-C4D	-4.78	1.33	1.44
26	3	316	CHL	C3D-C4D	-4.77	1.33	1.44
24	R	313	XAT	C22-C23	-4.77	1.45	1.52
26	S	314	CHL	CHC-C1C	4.77	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p	314	CHL	C3B-C2B	4.77	1.47	1.40
26	2	318	CHL	C3D-C4D	-4.77	1.33	1.44
26	Q	316	CHL	C3D-C4D	-4.77	1.33	1.44
26	3	315	CHL	C2C-C3C	4.77	1.47	1.36
26	1	314	CHL	C3B-C2B	4.77	1.47	1.40
26	V	316	CHL	C3B-C2B	4.77	1.47	1.40
26	6	316	CHL	CHC-C1C	4.77	1.47	1.35
24	g	309	XAT	C22-C23	-4.77	1.45	1.52
26	N	316	CHL	CHC-C1C	4.77	1.47	1.35
26	N	314	CHL	C3D-C4D	-4.77	1.33	1.44
26	1	318	CHL	C3D-C4D	-4.77	1.33	1.44
26	6	301	CHL	CHC-C1C	4.76	1.47	1.35
26	U	316	CHL	C3D-C4D	-4.76	1.33	1.44
24	6	310	XAT	C28-C29	4.76	1.56	1.45
24	g	309	XAT	C8-C9	4.76	1.56	1.45
24	Q	309	XAT	C28-C29	4.76	1.56	1.45
26	V	317	CHL	CHC-C1C	4.76	1.47	1.35
26	G	312	CHL	C2C-C3C	4.76	1.46	1.36
26	q	313	CHL	CHC-C1C	4.76	1.47	1.35
26	G	316	CHL	C3D-C4D	-4.76	1.33	1.44
26	P	316	CHL	C3B-C2B	4.76	1.47	1.40
24	5	311	XAT	C8-C9	4.76	1.56	1.45
26	S	314	CHL	C2C-C3C	4.76	1.46	1.36
26	p	319	CHL	C3D-C4D	-4.75	1.33	1.44
26	n	318	CHL	CHC-C1C	4.75	1.47	1.35
26	5	317	CHL	C3D-C4D	-4.75	1.33	1.44
24	v	311	XAT	C8-C9	4.75	1.56	1.45
26	3	313	CHL	C2C-C3C	4.75	1.46	1.36
26	Q	316	CHL	C3B-C2B	4.75	1.47	1.40
24	g	309	XAT	C2-C3	-4.75	1.45	1.52
26	v	318	CHL	CHC-C1C	4.75	1.47	1.35
26	P	318	CHL	C3D-C4D	-4.75	1.33	1.44
26	N	313	CHL	C3D-C4D	-4.75	1.33	1.44
26	Q	315	CHL	CHC-C1C	4.75	1.47	1.35
26	4	317	CHL	C3D-C4D	-4.75	1.33	1.44
26	q	315	CHL	C3D-C4D	-4.75	1.33	1.44
26	s	314	CHL	C2C-C3C	4.75	1.46	1.36
24	r	612	XAT	C22-C23	-4.75	1.45	1.52
24	p	312	XAT	C28-C29	4.74	1.56	1.45
26	N	313	CHL	CHC-C1C	4.74	1.47	1.35
26	P	315	CHL	CHD-C1D	4.74	1.47	1.38
26	u	318	CHL	CHC-C1C	4.74	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	316	CHL	C2C-C3C	4.74	1.46	1.36
26	p	318	CHL	C3D-C4D	-4.74	1.33	1.44
26	u	315	CHL	C3D-C4D	-4.74	1.33	1.44
26	4	313	CHL	C3B-C2B	4.74	1.46	1.40
26	V	315	CHL	C2C-C3C	4.74	1.46	1.36
26	s	314	CHL	C3D-C4D	-4.74	1.33	1.44
26	G	313	CHL	C3D-C4D	-4.74	1.33	1.44
24	P	312	XAT	C8-C9	4.74	1.56	1.45
24	2	311	XAT	C8-C9	4.73	1.56	1.45
24	V	311	XAT	C28-C29	4.73	1.56	1.45
26	3	315	CHL	C3D-C4D	-4.73	1.33	1.44
24	G	309	XAT	C2-C3	-4.73	1.45	1.52
26	2	317	CHL	C3D-C4D	-4.73	1.33	1.44
26	U	319	CHL	C3D-C4D	-4.73	1.33	1.44
24	5	311	XAT	C28-C29	4.73	1.56	1.45
24	G	309	XAT	C8-C9	4.73	1.56	1.45
26	4	316	CHL	CHC-C1C	4.73	1.47	1.35
26	S	316	CHL	C2C-C3C	4.72	1.46	1.36
26	1	316	CHL	CHC-C1C	4.72	1.47	1.35
26	U	313	CHL	C3B-C2B	4.72	1.46	1.40
26	s	316	CHL	C2C-C3C	4.72	1.46	1.36
24	p	312	XAT	C8-C9	4.72	1.56	1.45
26	4	314	CHL	C3D-C4D	-4.72	1.33	1.44
26	r	614	CHL	CHC-C1C	4.72	1.47	1.35
26	g	315	CHL	C3D-C4D	-4.72	1.33	1.44
26	N	317	CHL	CHC-C1C	4.72	1.47	1.35
26	S	316	CHL	C3B-C2B	4.72	1.46	1.40
26	n	313	CHL	C3D-C4D	-4.72	1.33	1.44
26	6	314	CHL	C2C-C3C	4.72	1.46	1.36
26	R	315	CHL	CHC-C1C	4.72	1.47	1.35
26	5	315	CHL	C3D-C4D	-4.72	1.33	1.44
24	P	312	XAT	C28-C29	4.71	1.56	1.45
24	P	312	XAT	C32-C33	4.71	1.56	1.45
26	2	314	CHL	CHD-C1D	4.71	1.47	1.38
26	q	311	CHL	CHC-C1C	4.71	1.47	1.35
24	q	309	XAT	C22-C23	-4.71	1.45	1.52
24	n	311	XAT	C8-C9	4.71	1.56	1.45
24	3	309	XAT	C22-C23	-4.71	1.45	1.52
26	S	313	CHL	C3B-C2B	4.71	1.46	1.40
26	6	316	CHL	C3D-C4D	-4.71	1.33	1.44
26	2	317	CHL	CHC-C1C	4.71	1.47	1.35
26	P	318	CHL	CHC-C1C	4.71	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	311	XAT	C22-C23	-4.71	1.45	1.52
26	Q	315	CHL	C3D-C4D	-4.71	1.33	1.44
24	p	312	XAT	C2-C3	-4.71	1.45	1.52
26	U	317	CHL	CHC-C1C	4.70	1.47	1.35
26	V	313	CHL	C3B-C2B	4.70	1.46	1.40
26	q	311	CHL	C3D-C4D	-4.70	1.33	1.44
26	g	312	CHL	C2C-C3C	4.70	1.46	1.36
26	U	315	CHL	CHC-C1C	4.70	1.47	1.35
26	r	619	CHL	C3D-C4D	-4.70	1.33	1.44
31	t	101	BCR	C23-C22	4.70	1.56	1.45
26	1	318	CHL	CHC-C1C	4.70	1.47	1.35
24	1	311	XAT	C2-C3	-4.70	1.45	1.52
31	T	101	BCR	C23-C22	4.70	1.56	1.45
26	2	315	CHL	C3D-C4D	-4.70	1.33	1.44
26	g	312	CHL	C3B-C2B	4.70	1.46	1.40
26	s	313	CHL	C3B-C2B	4.70	1.46	1.40
24	v	311	XAT	C22-C23	-4.70	1.45	1.52
26	6	301	CHL	C3B-C2B	4.69	1.46	1.40
26	G	314	CHL	C3B-C2B	4.69	1.46	1.40
26	g	311	CHL	C3D-C4D	-4.69	1.33	1.44
24	G	309	XAT	C22-C23	-4.69	1.45	1.52
24	N	311	XAT	C28-C29	4.69	1.56	1.45
24	g	309	XAT	C28-C29	4.69	1.56	1.45
26	5	316	CHL	C3B-C2B	4.69	1.46	1.40
24	N	311	XAT	C22-C23	-4.69	1.45	1.52
26	v	315	CHL	C2C-C3C	4.69	1.46	1.36
24	q	309	XAT	C28-C29	4.69	1.56	1.45
24	n	311	XAT	C28-C29	4.69	1.56	1.45
26	1	317	CHL	CHC-C1C	4.69	1.47	1.35
26	v	318	CHL	C3D-C4D	-4.68	1.33	1.44
26	V	314	CHL	C2C-C3C	4.68	1.46	1.36
26	G	315	CHL	C3D-C4D	-4.68	1.33	1.44
24	1	311	XAT	C28-C29	4.68	1.56	1.45
26	S	314	CHL	C3D-C4D	-4.68	1.33	1.44
26	5	318	CHL	CHC-C1C	4.68	1.47	1.35
24	1	311	XAT	C22-C23	-4.68	1.45	1.52
26	u	313	CHL	C3B-C2B	4.68	1.46	1.40
26	q	314	CHL	C2C-C3C	4.68	1.46	1.36
26	n	316	CHL	C3D-C4D	-4.68	1.33	1.44
24	R	313	XAT	C28-C29	4.67	1.56	1.45
26	4	315	CHL	C2C-C3C	4.67	1.46	1.36
26	U	316	CHL	CHC-C1C	4.67	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	314	CHL	CHD-C1D	4.67	1.47	1.38
26	U	317	CHL	C3D-C4D	-4.67	1.33	1.44
24	r	612	XAT	C28-C29	4.67	1.56	1.45
26	1	315	CHL	C2C-C3C	4.67	1.46	1.36
24	n	311	XAT	C22-C23	-4.67	1.45	1.52
24	6	310	XAT	C8-C9	4.67	1.56	1.45
24	V	311	XAT	C32-C33	4.67	1.56	1.45
26	R	315	CHL	C3D-C4D	-4.67	1.33	1.44
26	4	317	CHL	CHC-C1C	4.66	1.46	1.35
24	6	310	XAT	C2-C3	-4.66	1.45	1.52
24	v	311	XAT	C28-C29	4.66	1.56	1.45
24	u	311	XAT	C28-C29	4.66	1.56	1.45
26	5	317	CHL	CHC-C1C	4.66	1.46	1.35
24	5	311	XAT	C32-C33	4.66	1.56	1.45
26	5	313	CHL	C2C-C3C	4.66	1.46	1.36
26	G	311	CHL	CHC-C1C	4.66	1.46	1.35
26	1	316	CHL	C3B-C2B	4.66	1.46	1.40
26	g	314	CHL	C2C-C3C	4.66	1.46	1.36
24	p	312	XAT	C32-C33	4.66	1.55	1.45
26	V	318	CHL	C2C-C3C	4.66	1.46	1.36
24	u	311	XAT	C8-C9	4.66	1.55	1.45
26	Q	312	CHL	C2C-C3C	4.65	1.46	1.36
26	v	317	CHL	CHC-C1C	4.65	1.46	1.35
26	u	317	CHL	CHC-C1C	4.65	1.46	1.35
26	6	314	CHL	CHD-C1D	4.65	1.47	1.38
24	p	312	XAT	C22-C23	-4.65	1.45	1.52
24	2	311	XAT	C28-C29	4.65	1.55	1.45
26	3	316	CHL	CHC-C1C	4.65	1.46	1.35
24	R	313	XAT	C32-C33	4.65	1.55	1.45
26	s	315	CHL	CHD-C1D	4.65	1.47	1.38
24	Q	309	XAT	C32-C33	4.65	1.55	1.45
26	G	314	CHL	C3D-C4D	-4.64	1.33	1.44
24	q	309	XAT	C2-C3	-4.64	1.45	1.52
26	N	314	CHL	CHD-C1D	4.64	1.47	1.38
26	r	614	CHL	C3D-C4D	-4.64	1.33	1.44
26	q	314	CHL	C3D-C4D	-4.64	1.33	1.44
26	v	315	CHL	C3B-C2B	4.64	1.46	1.40
24	3	309	XAT	C8-C9	4.64	1.55	1.45
26	5	314	CHL	CHD-C1D	4.64	1.47	1.38
26	V	318	CHL	C3D-C4D	-4.64	1.33	1.44
26	p	319	CHL	CHC-C1C	4.64	1.46	1.35
26	Q	316	CHL	C2C-C3C	4.64	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	311	XAT	C28-C29	4.64	1.55	1.45
24	2	311	XAT	C2-C3	-4.64	1.45	1.52
26	n	314	CHL	CHD-C1D	4.63	1.47	1.38
26	G	312	CHL	CHD-C1D	4.63	1.47	1.38
26	p	320	CHL	C3D-C4D	-4.63	1.33	1.44
26	n	314	CHL	C3D-C4D	-4.63	1.33	1.44
26	v	314	CHL	C3B-C2B	4.63	1.46	1.40
24	2	311	XAT	C22-C23	-4.63	1.45	1.52
26	r	614	CHL	C3B-C2B	4.63	1.46	1.40
24	4	311	XAT	C2-C3	-4.63	1.45	1.52
26	Q	314	CHL	C3D-C4D	-4.63	1.33	1.44
26	V	318	CHL	C3B-C2B	4.63	1.46	1.40
24	N	311	XAT	C8-C9	4.63	1.55	1.45
24	2	311	XAT	C32-C33	4.62	1.55	1.45
26	q	315	CHL	C2C-C3C	4.62	1.46	1.36
26	Q	313	CHL	CHC-C1C	4.62	1.46	1.35
26	1	313	CHL	C3B-C2B	4.62	1.46	1.40
24	P	312	XAT	C22-C23	-4.62	1.45	1.52
26	u	318	CHL	C3D-C4D	-4.62	1.33	1.44
26	g	316	CHL	CHC-C1C	4.62	1.46	1.35
26	P	319	CHL	C3D-C4D	-4.62	1.33	1.44
26	2	313	CHL	C2C-C3C	4.62	1.46	1.36
24	U	311	XAT	C28-C29	4.62	1.55	1.45
26	u	314	CHL	C3B-C2B	4.62	1.46	1.40
24	5	311	XAT	C2-C3	-4.62	1.45	1.52
26	n	315	CHL	C2C-C3C	4.62	1.46	1.36
31	b	620	BCR	C23-C22	4.62	1.55	1.45
26	S	315	CHL	CHD-C1D	4.61	1.47	1.38
26	G	314	CHL	C2C-C3C	4.61	1.46	1.36
26	2	315	CHL	C2C-C3C	4.61	1.46	1.36
26	3	316	CHL	C2C-C3C	4.61	1.46	1.36
26	3	313	CHL	CHD-C1D	4.61	1.47	1.38
24	V	311	XAT	C22-C23	-4.61	1.45	1.52
26	R	316	CHL	C3D-C4D	-4.61	1.33	1.44
24	P	312	XAT	C12-C13	4.61	1.55	1.45
26	6	317	CHL	C2C-C3C	4.61	1.46	1.36
24	r	612	XAT	C32-C33	4.61	1.55	1.45
24	U	311	XAT	C8-C9	4.60	1.55	1.45
26	p	319	CHL	C2C-C3C	4.60	1.46	1.36
24	1	311	XAT	C8-C9	4.60	1.55	1.45
26	P	316	CHL	C2C-C3C	4.60	1.46	1.36
26	6	315	CHL	C2C-C3C	4.60	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	314	CHL	C3B-C2B	4.60	1.46	1.40
26	G	316	CHL	CHC-C1C	4.60	1.46	1.35
26	U	319	CHL	C3B-C2B	4.60	1.46	1.40
24	q	309	XAT	C32-C33	4.59	1.55	1.45
26	v	318	CHL	C2C-C3C	4.59	1.46	1.36
26	Q	312	CHL	C3D-C4D	-4.59	1.33	1.44
26	5	315	CHL	C2C-C3C	4.59	1.46	1.36
24	4	311	XAT	C8-C9	4.59	1.55	1.45
24	v	311	XAT	C32-C33	4.59	1.55	1.45
26	2	315	CHL	C3B-C2B	4.59	1.46	1.40
24	3	309	XAT	C2-C3	-4.59	1.45	1.52
26	s	316	CHL	CHD-C1D	4.59	1.47	1.38
24	6	310	XAT	C22-C23	-4.59	1.45	1.52
26	g	313	CHL	C3B-C2B	4.59	1.46	1.40
26	R	315	CHL	C3B-C2B	4.58	1.46	1.40
26	p	318	CHL	CHC-C1C	4.58	1.46	1.35
26	N	317	CHL	C2C-C3C	4.58	1.46	1.36
26	p	315	CHL	CHD-C1D	4.58	1.47	1.38
26	2	316	CHL	C3B-C2B	4.58	1.46	1.40
26	3	314	CHL	C2C-C3C	4.58	1.46	1.36
26	r	615	CHL	C3D-C4D	-4.58	1.33	1.44
26	S	316	CHL	CHD-C1D	4.58	1.47	1.38
24	U	311	XAT	C2-C3	-4.58	1.45	1.52
26	1	315	CHL	C3B-C2B	4.58	1.46	1.40
26	1	314	CHL	C3D-C4D	-4.58	1.33	1.44
24	3	309	XAT	C32-C33	4.58	1.55	1.45
26	Q	315	CHL	C2C-C3C	4.58	1.46	1.36
24	u	311	XAT	C32-C33	4.57	1.55	1.45
26	S	314	CHL	C3B-C2B	4.57	1.46	1.40
26	s	314	CHL	C3B-C2B	4.57	1.46	1.40
24	Q	309	XAT	C22-C23	-4.57	1.45	1.52
26	g	312	CHL	CHD-C1D	4.57	1.47	1.38
26	3	316	CHL	CHD-C1D	4.57	1.47	1.38
26	q	312	CHL	C3D-C4D	-4.57	1.33	1.44
24	6	310	XAT	C12-C13	4.57	1.55	1.45
26	P	314	CHL	C2C-C3C	4.56	1.46	1.36
26	g	315	CHL	C3B-C2B	4.56	1.46	1.40
24	V	311	XAT	C2-C3	-4.56	1.45	1.52
26	2	318	CHL	CHC-C1C	4.56	1.46	1.35
26	R	316	CHL	C2C-C3C	4.56	1.46	1.36
24	P	312	XAT	C2-C3	-4.56	1.45	1.52
24	6	310	XAT	C32-C33	4.56	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	314	CHL	C2C-C3C	4.56	1.46	1.36
26	v	313	CHL	C3B-C2B	4.56	1.46	1.40
26	p	316	CHL	C2C-C3C	4.56	1.46	1.36
26	v	318	CHL	C3B-C2B	4.55	1.46	1.40
26	n	317	CHL	C3B-C2B	4.55	1.46	1.40
26	V	316	CHL	C2C-C3C	4.55	1.46	1.36
26	V	313	CHL	C2C-C3C	4.55	1.46	1.36
24	1	311	XAT	C32-C33	4.55	1.55	1.45
26	n	318	CHL	CHD-C1D	4.55	1.47	1.38
26	Q	315	CHL	C3B-C2B	4.55	1.46	1.40
26	n	318	CHL	C3B-C2B	4.55	1.46	1.40
26	6	317	CHL	CHC-C1C	4.54	1.46	1.35
26	N	314	CHL	C2C-C3C	4.54	1.46	1.36
24	5	311	XAT	C22-C23	-4.54	1.45	1.52
26	5	314	CHL	C3D-C4D	-4.54	1.33	1.44
26	4	314	CHL	C3B-C2B	4.54	1.46	1.40
24	Q	309	XAT	C2-C3	-4.54	1.45	1.52
31	B	620	BCR	C23-C22	4.54	1.55	1.45
24	Q	309	XAT	C12-C13	4.54	1.55	1.45
26	U	313	CHL	C2C-C3C	4.54	1.46	1.36
31	C	517	BCR	C3-C4	4.54	1.66	1.52
26	p	319	CHL	C3B-C2B	4.53	1.46	1.40
26	V	315	CHL	CHD-C1D	4.53	1.47	1.38
26	g	314	CHL	C3D-C4D	-4.53	1.33	1.44
26	6	317	CHL	CHD-C1D	4.53	1.47	1.38
24	4	311	XAT	C32-C33	4.53	1.55	1.45
24	g	309	XAT	C32-C33	4.53	1.55	1.45
31	t	101	BCR	C11-C10	4.53	1.57	1.43
24	3	309	XAT	C12-C13	4.53	1.55	1.45
24	N	311	XAT	C32-C33	4.53	1.55	1.45
26	6	316	CHL	C3B-C2B	4.53	1.46	1.40
24	V	311	XAT	C12-C13	4.53	1.55	1.45
26	5	313	CHL	CHD-C1D	4.53	1.47	1.38
26	5	315	CHL	C3B-C2B	4.52	1.46	1.40
24	5	311	XAT	C12-C13	4.52	1.55	1.45
26	P	317	CHL	C3B-C2B	4.52	1.46	1.40
31	X	201	BCR	C11-C10	4.52	1.57	1.43
26	P	319	CHL	C2C-C3C	4.52	1.46	1.36
26	p	316	CHL	CHD-C1D	4.52	1.47	1.38
26	Q	313	CHL	C2C-C3C	4.52	1.46	1.36
31	c	515	BCR	C3-C4	4.52	1.66	1.52
24	N	311	XAT	C2-C3	-4.52	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	317	CHL	C3B-C2B	4.52	1.46	1.40
26	4	315	CHL	C3B-C2B	4.52	1.46	1.40
24	v	311	XAT	C12-C13	4.52	1.55	1.45
26	n	318	CHL	C2C-C3C	4.51	1.46	1.36
24	v	311	XAT	C2-C3	-4.51	1.45	1.52
26	P	319	CHL	CHC-C1C	4.51	1.46	1.35
26	g	313	CHL	C3D-C4D	-4.51	1.34	1.44
26	1	313	CHL	C2C-C3C	4.51	1.46	1.36
31	T	101	BCR	C11-C10	4.51	1.57	1.43
26	v	317	CHL	C3B-C2B	4.51	1.46	1.40
26	r	615	CHL	C2C-C3C	4.51	1.46	1.36
26	s	313	CHL	O2A-CGA	4.51	1.45	1.30
26	1	318	CHL	C2C-C3C	4.50	1.46	1.36
26	1	317	CHL	O2A-CGA	4.50	1.46	1.33
26	V	317	CHL	C3B-C2B	4.50	1.46	1.40
24	p	312	XAT	C12-C13	4.50	1.55	1.45
26	v	316	CHL	C2C-C3C	4.50	1.46	1.36
26	G	315	CHL	C3B-C2B	4.50	1.46	1.40
26	2	316	CHL	C2C-C3C	4.50	1.46	1.36
26	S	314	CHL	O2A-CGA	4.50	1.45	1.30
26	v	316	CHL	C3B-C2B	4.49	1.46	1.40
24	n	311	XAT	C12-C13	4.49	1.55	1.45
26	u	313	CHL	C2C-C3C	4.49	1.46	1.36
26	P	317	CHL	CHD-C1D	4.49	1.47	1.38
26	s	314	CHL	O2A-CGA	4.49	1.45	1.30
26	4	315	CHL	CHD-C1D	4.49	1.47	1.38
26	N	317	CHL	CHD-C1D	4.49	1.47	1.38
26	4	316	CHL	C2C-C3C	4.49	1.46	1.36
24	u	311	XAT	C2-C3	-4.49	1.45	1.52
24	2	311	XAT	C12-C13	4.49	1.55	1.45
24	U	311	XAT	C32-C33	4.49	1.55	1.45
26	Q	312	CHL	CHD-C1D	4.49	1.47	1.38
26	v	314	CHL	C2C-C3C	4.49	1.46	1.36
26	2	313	CHL	CHD-C1D	4.49	1.47	1.38
26	2	318	CHL	C2C-C3C	4.49	1.46	1.36
24	R	313	XAT	C12-C13	4.49	1.55	1.45
26	2	314	CHL	C3D-C4D	-4.49	1.34	1.44
24	G	309	XAT	C32-C33	4.49	1.55	1.45
31	x	202	BCR	C11-C10	4.49	1.57	1.43
31	d	403	BCR	C11-C10	4.48	1.57	1.43
26	S	313	CHL	O2A-CGA	4.48	1.45	1.30
24	g	309	XAT	C12-C13	4.48	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	315	CHL	C2C-C3C	4.48	1.46	1.36
26	5	316	CHL	C2C-C3C	4.48	1.46	1.36
26	N	315	CHL	C2C-C3C	4.48	1.46	1.36
26	R	317	CHL	C2C-C3C	4.48	1.46	1.36
24	n	311	XAT	C2-C3	-4.48	1.45	1.52
26	r	616	CHL	CHD-C1D	4.48	1.47	1.38
26	5	317	CHL	O2A-CGA	4.48	1.46	1.33
26	G	313	CHL	C2C-C3C	4.48	1.46	1.36
26	S	316	CHL	O2A-CGA	4.48	1.45	1.30
31	B	620	BCR	C3-C4	4.48	1.66	1.52
26	2	317	CHL	O2A-CGA	4.48	1.46	1.33
26	r	616	CHL	C2C-C3C	4.48	1.46	1.36
31	D	404	BCR	C11-C10	4.47	1.57	1.43
26	r	616	CHL	C3B-C2B	4.47	1.46	1.40
26	6	312	CHL	C3B-C2B	4.47	1.46	1.40
26	R	317	CHL	CHD-C1D	4.47	1.47	1.38
24	u	311	XAT	C12-C13	4.47	1.55	1.45
26	v	313	CHL	C2C-C3C	4.47	1.46	1.36
26	P	317	CHL	C2C-C3C	4.47	1.46	1.36
26	P	316	CHL	CHD-C1D	4.47	1.47	1.38
26	s	313	CHL	CHD-C1D	4.47	1.47	1.38
31	b	620	BCR	C3-C4	4.47	1.66	1.52
31	c	516	BCR	C11-C10	4.46	1.57	1.43
31	X	201	BCR	C23-C22	4.46	1.55	1.45
26	4	317	CHL	C2C-C3C	4.46	1.46	1.36
26	n	315	CHL	C3B-C2B	4.46	1.46	1.40
26	U	314	CHL	C2C-C3C	4.46	1.46	1.36
26	v	314	CHL	C3D-C4D	-4.46	1.34	1.44
26	p	317	CHL	C3B-C2B	4.46	1.46	1.40
26	s	316	CHL	O2A-CGA	4.46	1.45	1.30
24	n	311	XAT	C32-C33	4.46	1.55	1.45
26	3	311	CHL	C2C-C3C	4.46	1.46	1.36
26	s	313	CHL	C2C-C3C	4.46	1.46	1.36
26	4	313	CHL	C2C-C3C	4.45	1.46	1.36
26	5	317	CHL	C3B-C2B	4.45	1.46	1.40
26	p	320	CHL	C3B-C2B	4.45	1.46	1.40
26	U	313	CHL	CHD-C1D	4.45	1.47	1.38
24	q	309	XAT	C12-C13	4.45	1.55	1.45
26	g	311	CHL	C3B-C2B	4.45	1.46	1.40
26	n	315	CHL	CHD-C1D	4.45	1.47	1.38
26	Q	314	CHL	C2C-C3C	4.45	1.46	1.36
26	g	312	CHL	C3D-C4D	-4.45	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	316	CHL	C3B-C2B	4.45	1.46	1.40
24	G	309	XAT	C12-C13	4.45	1.55	1.45
31	K	101	BCR	C3-C4	4.44	1.66	1.52
31	C	518	BCR	C11-C10	4.44	1.57	1.43
26	u	315	CHL	C3B-C2B	4.44	1.46	1.40
26	3	312	CHL	C3D-C4D	-4.44	1.34	1.44
31	t	101	BCR	C3-C4	4.44	1.66	1.52
26	G	313	CHL	O2A-CGA	4.44	1.46	1.33
26	6	313	CHL	C3D-C4D	-4.44	1.34	1.44
31	k	101	BCR	C2-C1	4.44	1.64	1.54
26	V	313	CHL	CHD-C1D	4.44	1.47	1.38
26	u	313	CHL	CHD-C1D	4.44	1.47	1.38
26	u	315	CHL	C2C-C3C	4.44	1.46	1.36
26	g	315	CHL	O2A-CGA	4.44	1.46	1.33
26	g	315	CHL	C2C-C3C	4.44	1.46	1.36
31	k	101	BCR	C3-C4	4.44	1.66	1.52
26	q	313	CHL	C2C-C3C	4.44	1.46	1.36
26	r	619	CHL	O2A-CGA	4.44	1.46	1.33
26	5	313	CHL	O2A-CGA	4.43	1.46	1.33
26	q	313	CHL	O2A-CGA	4.43	1.46	1.33
24	r	612	XAT	C12-C13	4.43	1.55	1.45
26	G	312	CHL	C3D-C4D	-4.43	1.34	1.44
26	1	318	CHL	C3B-C2B	4.43	1.46	1.40
26	6	316	CHL	O2A-CGA	4.43	1.46	1.33
31	D	404	BCR	C23-C22	4.43	1.55	1.45
31	z	101	BCR	C3-C4	4.43	1.66	1.52
31	C	516	BCR	C3-C4	4.43	1.66	1.52
26	u	315	CHL	O2A-CGA	4.43	1.46	1.33
26	U	319	CHL	C2C-C3C	4.43	1.46	1.36
26	N	316	CHL	C3B-C2B	4.43	1.46	1.40
26	2	313	CHL	O2A-CGA	4.43	1.46	1.33
26	6	312	CHL	C2C-C3C	4.43	1.46	1.36
24	4	311	XAT	C12-C13	4.42	1.55	1.45
31	K	101	BCR	C2-C1	4.42	1.64	1.54
26	Q	311	CHL	C2C-C3C	4.42	1.46	1.36
26	1	317	CHL	C2C-C3C	4.42	1.46	1.36
31	T	101	BCR	C3-C4	4.42	1.66	1.52
26	p	317	CHL	C2C-C3C	4.42	1.46	1.36
26	R	317	CHL	C3B-C2B	4.42	1.46	1.40
26	3	316	CHL	C3B-C2B	4.42	1.46	1.40
26	U	317	CHL	C2C-C3C	4.42	1.46	1.36
24	1	311	XAT	C12-C13	4.41	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	315	CHL	O2A-CGA	4.41	1.46	1.33
31	x	202	BCR	C23-C22	4.41	1.55	1.45
26	S	313	CHL	C2C-C3C	4.41	1.46	1.36
31	d	403	BCR	C23-C22	4.41	1.55	1.45
26	g	313	CHL	CHD-C1D	4.41	1.47	1.38
26	g	313	CHL	C2C-C3C	4.41	1.46	1.36
26	5	318	CHL	C2C-C3C	4.41	1.46	1.36
26	U	314	CHL	O2A-CGA	4.41	1.46	1.33
26	S	313	CHL	CHD-C1D	4.40	1.46	1.38
26	g	311	CHL	C2C-C3C	4.40	1.46	1.36
26	P	319	CHL	O2A-CGA	4.40	1.46	1.33
31	B	618	BCR	C3-C4	4.40	1.66	1.52
31	b	619	BCR	C3-C4	4.40	1.66	1.52
26	v	317	CHL	C2C-C3C	4.40	1.46	1.36
24	U	311	XAT	C12-C13	4.40	1.55	1.45
26	1	314	CHL	C2C-C3C	4.40	1.46	1.36
26	1	316	CHL	C2C-C3C	4.40	1.46	1.36
26	6	301	CHL	C2C-C3C	4.40	1.46	1.36
26	n	316	CHL	C2C-C3C	4.40	1.46	1.36
26	4	317	CHL	C3B-C2B	4.40	1.46	1.40
31	d	403	BCR	C3-C4	4.40	1.66	1.52
26	3	314	CHL	CHD-C1D	4.39	1.46	1.38
26	G	313	CHL	CHD-C1D	4.39	1.46	1.38
31	D	404	BCR	C3-C4	4.39	1.66	1.52
26	N	313	CHL	C2C-C3C	4.39	1.46	1.36
26	n	316	CHL	C3B-C2B	4.39	1.46	1.40
26	g	314	CHL	CHD-C1D	4.39	1.46	1.38
26	N	315	CHL	O2A-CGA	4.39	1.46	1.33
26	V	318	CHL	CHD-C1D	4.39	1.46	1.38
26	G	316	CHL	C2C-C3C	4.39	1.46	1.36
26	Q	313	CHL	C3B-C2B	4.39	1.46	1.40
26	Q	311	CHL	C3B-C2B	4.39	1.46	1.40
26	Q	313	CHL	CHD-C1D	4.38	1.46	1.38
26	V	317	CHL	C2C-C3C	4.38	1.46	1.36
26	5	316	CHL	CHD-C1D	4.38	1.46	1.38
26	n	315	CHL	O2A-CGA	4.38	1.46	1.33
26	4	316	CHL	C3B-C2B	4.38	1.46	1.40
26	Q	316	CHL	CHD-C1D	4.38	1.46	1.38
26	1	315	CHL	CHD-C1D	4.38	1.46	1.38
26	6	315	CHL	CHD-C1D	4.38	1.46	1.38
26	2	318	CHL	CHD-C1D	4.38	1.46	1.38
26	4	316	CHL	O2A-CGA	4.37	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	313	CHL	O2A-CGA	4.37	1.46	1.33
26	N	317	CHL	C3B-C2B	4.37	1.46	1.40
31	c	516	BCR	C3-C4	4.37	1.66	1.52
26	g	316	CHL	C2C-C3C	4.37	1.46	1.36
31	C	518	BCR	C3-C4	4.37	1.66	1.52
31	B	619	BCR	C3-C4	4.37	1.66	1.52
31	B	620	BCR	C11-C10	4.37	1.57	1.43
26	P	315	CHL	O2A-CGA	4.37	1.46	1.33
26	n	317	CHL	CHD-C1D	4.37	1.46	1.38
31	a	409	BCR	C3-C4	4.37	1.66	1.52
31	A	409	BCR	C3-C4	4.36	1.66	1.52
26	V	314	CHL	C3D-C4D	-4.36	1.34	1.44
26	2	316	CHL	CHD-C1D	4.36	1.46	1.38
26	q	313	CHL	CHD-C1D	4.36	1.46	1.38
26	v	317	CHL	O2A-CGA	4.36	1.46	1.33
31	b	618	BCR	C3-C4	4.36	1.66	1.52
31	b	620	BCR	C11-C10	4.36	1.57	1.43
24	N	311	XAT	C12-C13	4.36	1.55	1.45
26	3	311	CHL	C3B-C2B	4.36	1.46	1.40
26	G	314	CHL	CHD-C1D	4.36	1.46	1.38
26	G	315	CHL	O2A-CGA	4.36	1.46	1.33
26	P	314	CHL	CHD-C1D	4.36	1.46	1.38
26	n	317	CHL	C2C-C3C	4.36	1.46	1.36
26	R	316	CHL	C3B-C2B	4.36	1.46	1.40
26	U	314	CHL	C3B-C2B	4.35	1.46	1.40
26	g	316	CHL	O2A-CGA	4.35	1.46	1.33
26	r	619	CHL	C3B-C2B	4.35	1.46	1.40
26	V	317	CHL	O2A-CGA	4.35	1.46	1.33
26	V	314	CHL	O2A-CGA	4.35	1.46	1.33
26	q	315	CHL	CHD-C1D	4.34	1.46	1.38
26	q	311	CHL	C3B-C2B	4.34	1.46	1.40
26	v	318	CHL	CHD-C1D	4.34	1.46	1.38
31	C	518	BCR	C4-C5	-4.34	1.42	1.51
26	U	317	CHL	C3B-C2B	4.34	1.46	1.40
31	B	620	BCR	C2-C1	4.34	1.64	1.54
26	G	311	CHL	C2C-C3C	4.34	1.46	1.36
31	B	618	BCR	C4-C5	-4.34	1.42	1.51
26	q	311	CHL	C2C-C3C	4.34	1.46	1.36
31	X	201	BCR	C3-C4	4.34	1.66	1.52
26	r	615	CHL	C3B-C2B	4.34	1.46	1.40
26	6	301	CHL	CHD-C1D	4.34	1.46	1.38
26	1	317	CHL	C3B-C2B	4.34	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	315	CHL	O2A-CGA	4.34	1.46	1.33
31	z	101	BCR	C11-C10	4.33	1.56	1.43
26	v	313	CHL	CHD-C1D	4.33	1.46	1.38
26	4	313	CHL	CHD-C1D	4.33	1.46	1.38
26	g	316	CHL	CHD-C1D	4.33	1.46	1.38
31	x	202	BCR	C3-C4	4.33	1.66	1.52
26	p	320	CHL	C2C-C3C	4.33	1.46	1.36
26	4	315	CHL	O2A-CGA	4.33	1.46	1.33
31	C	516	BCR	C11-C10	4.33	1.56	1.43
26	Q	315	CHL	O2A-CGA	4.33	1.46	1.33
26	5	315	CHL	O2A-CGA	4.33	1.46	1.33
26	q	312	CHL	O2A-CGA	4.33	1.46	1.33
26	N	315	CHL	C3B-C2B	4.33	1.46	1.40
26	G	316	CHL	C3B-C2B	4.33	1.46	1.40
31	c	515	BCR	C23-C22	4.33	1.55	1.45
26	U	316	CHL	C2C-C3C	4.33	1.46	1.36
26	u	316	CHL	C2C-C3C	4.32	1.46	1.36
31	K	101	BCR	C11-C10	4.32	1.56	1.43
26	v	314	CHL	CHD-C1D	4.32	1.46	1.38
26	V	315	CHL	O2A-CGA	4.32	1.46	1.33
26	1	315	CHL	O2A-CGA	4.32	1.46	1.33
26	u	316	CHL	C3B-C2B	4.32	1.46	1.40
26	q	314	CHL	O2A-CGA	4.32	1.46	1.33
26	2	314	CHL	O2A-CGA	4.32	1.46	1.33
26	p	318	CHL	C3B-C2B	4.32	1.46	1.40
26	5	318	CHL	CHD-C1D	4.32	1.46	1.38
31	k	101	BCR	C11-C10	4.32	1.56	1.43
26	G	316	CHL	CHD-C1D	4.32	1.46	1.38
31	c	515	BCR	C11-C10	4.32	1.56	1.43
26	5	314	CHL	O2A-CGA	4.32	1.46	1.33
31	b	618	BCR	C4-C5	-4.31	1.42	1.51
26	N	317	CHL	O2A-CGA	4.31	1.45	1.33
26	3	315	CHL	C3B-C2B	4.31	1.46	1.40
26	R	316	CHL	O2A-CGA	4.31	1.45	1.33
26	1	314	CHL	CHD-C1D	4.31	1.46	1.38
31	b	620	BCR	C2-C1	4.31	1.64	1.54
26	1	314	CHL	O2A-CGA	4.31	1.45	1.33
26	v	315	CHL	CHD-C1D	4.31	1.46	1.38
26	G	311	CHL	C3B-C2B	4.31	1.46	1.40
26	4	314	CHL	C2C-C3C	4.31	1.46	1.36
31	b	619	BCR	C2-C1	4.31	1.64	1.54
26	P	319	CHL	C3B-C2B	4.31	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	614	CHL	C2C-C3C	4.31	1.46	1.36
31	C	516	BCR	C23-C22	4.31	1.55	1.45
26	v	315	CHL	O2A-CGA	4.31	1.45	1.33
26	n	313	CHL	C2C-C3C	4.31	1.46	1.36
26	P	318	CHL	O2A-CGA	4.31	1.45	1.33
26	Q	311	CHL	O2A-CGA	4.31	1.45	1.33
26	N	316	CHL	O2A-CGA	4.31	1.45	1.33
26	4	317	CHL	O2A-CGA	4.30	1.45	1.33
26	6	314	CHL	O2A-CGA	4.30	1.45	1.33
26	v	314	CHL	O2A-CGA	4.30	1.45	1.33
26	q	311	CHL	O2A-CGA	4.30	1.45	1.33
26	r	614	CHL	O2A-CGA	4.30	1.45	1.33
26	n	316	CHL	CHD-C1D	4.30	1.46	1.38
26	p	317	CHL	CHD-C1D	4.30	1.46	1.38
26	G	311	CHL	O2A-CGA	4.30	1.45	1.33
26	G	316	CHL	O2A-CGA	4.30	1.45	1.33
26	p	319	CHL	O2A-CGA	4.30	1.45	1.33
26	n	313	CHL	CHD-C1D	4.29	1.46	1.38
31	c	516	BCR	C4-C5	-4.29	1.42	1.51
26	r	615	CHL	O2A-CGA	4.29	1.45	1.33
31	C	517	BCR	C11-C10	4.29	1.56	1.43
26	P	316	CHL	O2A-CGA	4.29	1.45	1.33
26	S	315	CHL	O2A-CGA	4.29	1.45	1.33
26	s	315	CHL	O2A-CGA	4.29	1.45	1.33
31	z	101	BCR	C23-C22	4.29	1.55	1.45
26	G	312	CHL	O2A-CGA	4.29	1.45	1.33
31	B	619	BCR	C11-C10	4.29	1.56	1.43
26	2	315	CHL	O2A-CGA	4.29	1.45	1.33
26	Q	314	CHL	CHD-C1D	4.28	1.46	1.38
31	C	517	BCR	C23-C22	4.28	1.55	1.45
26	R	315	CHL	C2C-C3C	4.28	1.45	1.36
26	p	319	CHL	CHD-C1D	4.28	1.46	1.38
26	u	317	CHL	C3B-C2B	4.28	1.46	1.40
26	u	318	CHL	C2C-C3C	4.28	1.45	1.36
26	v	317	CHL	CHD-C1D	4.28	1.46	1.38
26	5	318	CHL	O2A-CGA	4.28	1.45	1.33
26	u	316	CHL	O2A-CGA	4.28	1.45	1.33
26	n	318	CHL	O2A-CGA	4.28	1.45	1.33
31	a	409	BCR	C4-C5	-4.28	1.42	1.51
31	b	619	BCR	C11-C10	4.28	1.56	1.43
26	u	318	CHL	C3B-C2B	4.28	1.46	1.40
26	4	314	CHL	O2A-CGA	4.27	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v	318	CHL	O2A-CGA	4.27	1.45	1.33
26	g	311	CHL	CHD-C1D	4.27	1.46	1.38
31	B	619	BCR	C2-C1	4.27	1.64	1.54
26	g	313	CHL	O2A-CGA	4.27	1.45	1.33
26	u	317	CHL	C2C-C3C	4.27	1.45	1.36
26	p	316	CHL	O2A-CGA	4.27	1.45	1.33
26	6	312	CHL	O2A-CGA	4.27	1.45	1.33
26	G	313	CHL	C3B-C2B	4.27	1.46	1.40
26	Q	312	CHL	O2A-CGA	4.27	1.45	1.33
31	d	403	BCR	C2-C1	4.26	1.64	1.54
26	V	318	CHL	O2A-CGA	4.26	1.45	1.33
26	r	616	CHL	O2A-CGA	4.26	1.45	1.33
26	5	318	CHL	C3B-C2B	4.26	1.46	1.40
26	1	316	CHL	CHD-C1D	4.26	1.46	1.38
31	B	618	BCR	C2-C1	4.26	1.63	1.54
31	c	516	BCR	C2-C1	4.26	1.63	1.54
31	C	517	BCR	C2-C1	4.26	1.63	1.54
31	c	516	BCR	C23-C22	4.26	1.55	1.45
26	u	316	CHL	CHD-C1D	4.26	1.46	1.38
26	6	313	CHL	O2A-CGA	4.26	1.45	1.33
26	V	316	CHL	CHD-C1D	4.26	1.46	1.38
26	p	318	CHL	O2A-CGA	4.25	1.45	1.33
31	C	518	BCR	C23-C22	4.25	1.55	1.45
26	u	314	CHL	O2A-CGA	4.25	1.45	1.33
26	R	315	CHL	CHD-C1D	4.25	1.46	1.38
26	g	312	CHL	O2A-CGA	4.25	1.45	1.33
26	q	315	CHL	O2A-CGA	4.25	1.45	1.33
26	5	317	CHL	C2C-C3C	4.25	1.45	1.36
26	P	315	CHL	CHD-C4C	4.25	1.48	1.39
26	3	311	CHL	O2A-CGA	4.25	1.45	1.33
26	3	312	CHL	O2A-CGA	4.25	1.45	1.33
26	2	318	CHL	O2A-CGA	4.25	1.45	1.33
26	P	317	CHL	O2A-CGA	4.25	1.45	1.33
31	D	404	BCR	C4-C5	-4.25	1.42	1.51
26	1	317	CHL	CHD-C1D	4.25	1.46	1.38
31	d	403	BCR	C4-C5	-4.25	1.42	1.51
26	r	615	CHL	CHD-C1D	4.24	1.46	1.38
26	6	301	CHL	O2A-CGA	4.24	1.45	1.33
31	C	518	BCR	C2-C1	4.24	1.63	1.54
26	p	314	CHL	C2C-C3C	4.24	1.45	1.36
26	p	314	CHL	O2A-CGA	4.24	1.45	1.33
26	U	319	CHL	CHD-C1D	4.24	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	317	CHL	O2A-CGA	4.24	1.45	1.33
26	R	317	CHL	O2A-CGA	4.24	1.45	1.33
26	r	614	CHL	CHD-C1D	4.24	1.46	1.38
31	c	515	BCR	C2-C1	4.24	1.63	1.54
31	d	403	BCR	C28-C27	4.24	1.65	1.52
31	D	404	BCR	C2-C1	4.24	1.63	1.54
26	U	319	CHL	O2A-CGA	4.24	1.45	1.33
31	A	409	BCR	C4-C5	-4.23	1.42	1.51
31	t	101	BCR	C2-C1	4.23	1.63	1.54
31	T	101	BCR	C2-C1	4.23	1.63	1.54
26	3	312	CHL	CHD-C4C	4.23	1.48	1.39
26	2	318	CHL	C3B-C2B	4.23	1.46	1.40
26	g	311	CHL	O2A-CGA	4.23	1.45	1.33
26	g	314	CHL	O2A-CGA	4.23	1.45	1.33
26	P	318	CHL	C2C-C3C	4.23	1.45	1.36
31	x	202	BCR	C2-C1	4.23	1.63	1.54
26	G	314	CHL	O2A-CGA	4.23	1.45	1.33
26	4	317	CHL	CHD-C1D	4.23	1.46	1.38
26	q	312	CHL	CHD-C4C	4.23	1.48	1.39
26	1	313	CHL	CHD-C1D	4.23	1.46	1.38
26	p	315	CHL	O2A-CGA	4.23	1.45	1.33
26	4	316	CHL	CHD-C1D	4.23	1.46	1.38
31	a	409	BCR	C11-C10	4.23	1.56	1.43
26	P	319	CHL	CHD-C1D	4.22	1.46	1.38
26	V	317	CHL	CHD-C1D	4.22	1.46	1.38
26	1	316	CHL	O2A-CGA	4.22	1.45	1.33
26	5	316	CHL	O2A-CGA	4.22	1.45	1.33
26	3	313	CHL	O2A-CGA	4.22	1.45	1.33
26	u	318	CHL	O2A-CGA	4.22	1.45	1.33
26	2	317	CHL	C2C-C3C	4.22	1.45	1.36
26	2	315	CHL	CHD-C1D	4.22	1.46	1.38
26	p	317	CHL	O2A-CGA	4.22	1.45	1.33
26	n	316	CHL	O2A-CGA	4.22	1.45	1.33
26	p	318	CHL	C2C-C3C	4.22	1.45	1.36
26	n	314	CHL	CHD-C4C	4.22	1.48	1.39
26	U	315	CHL	C2C-C3C	4.22	1.45	1.36
26	p	320	CHL	O2A-CGA	4.22	1.45	1.33
26	Q	316	CHL	O2A-CGA	4.22	1.45	1.33
31	B	618	BCR	C11-C10	4.22	1.56	1.43
31	A	409	BCR	C11-C10	4.22	1.56	1.43
31	A	409	BCR	C2-C1	4.21	1.63	1.54
26	U	316	CHL	C3B-C2B	4.21	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	316	CHL	O2A-CGA	4.21	1.45	1.33
26	Q	311	CHL	CHD-C1D	4.21	1.46	1.38
26	1	318	CHL	O2A-CGA	4.21	1.45	1.33
26	N	313	CHL	CHD-C1D	4.21	1.46	1.38
26	3	316	CHL	O2A-CGA	4.21	1.45	1.33
26	6	313	CHL	CHD-C4C	4.21	1.48	1.39
26	v	313	CHL	O2A-CGA	4.21	1.45	1.33
31	D	404	BCR	C28-C27	4.21	1.65	1.52
26	U	317	CHL	O2A-CGA	4.21	1.45	1.33
26	U	316	CHL	CHD-C1D	4.21	1.46	1.38
26	3	314	CHL	O2A-CGA	4.20	1.45	1.33
26	P	314	CHL	O2A-CGA	4.20	1.45	1.33
31	B	619	BCR	C23-C22	4.20	1.55	1.45
26	N	316	CHL	C2C-C3C	4.20	1.45	1.36
26	N	315	CHL	CHD-C1D	4.20	1.46	1.38
26	N	313	CHL	O2A-CGA	4.20	1.45	1.33
26	3	311	CHL	CHD-C1D	4.20	1.46	1.38
31	k	101	BCR	C28-C27	4.19	1.65	1.52
31	b	619	BCR	C23-C22	4.19	1.55	1.45
31	b	618	BCR	C11-C10	4.19	1.56	1.43
31	X	201	BCR	C2-C1	4.19	1.63	1.54
26	q	313	CHL	C3B-C2B	4.19	1.46	1.40
31	K	101	BCR	C28-C27	4.19	1.65	1.52
26	q	311	CHL	CHD-C1D	4.19	1.46	1.38
26	s	314	CHL	CHD-C1D	4.19	1.46	1.38
31	a	409	BCR	C2-C1	4.19	1.63	1.54
31	K	101	BCR	C23-C22	4.19	1.54	1.45
26	N	314	CHL	O2A-CGA	4.19	1.45	1.33
26	R	316	CHL	CHD-C1D	4.18	1.46	1.38
26	1	318	CHL	CHD-C1D	4.18	1.46	1.38
26	V	313	CHL	O2A-CGA	4.18	1.45	1.33
26	n	314	CHL	O2A-CGA	4.18	1.45	1.33
26	N	314	CHL	CHD-C4C	4.18	1.48	1.39
31	A	409	BCR	C23-C22	4.18	1.54	1.45
26	U	317	CHL	CHD-C1D	4.18	1.46	1.38
26	2	316	CHL	O2A-CGA	4.18	1.45	1.33
31	a	409	BCR	C23-C22	4.18	1.54	1.45
26	v	316	CHL	O2A-CGA	4.18	1.45	1.33
26	Q	314	CHL	O2A-CGA	4.17	1.45	1.33
26	1	313	CHL	O2A-CGA	4.17	1.45	1.33
26	u	313	CHL	O2A-CGA	4.17	1.45	1.33
26	6	317	CHL	C3B-C2B	4.17	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	317	CHL	O2A-CGA	4.17	1.45	1.33
26	u	314	CHL	C2C-C3C	4.17	1.45	1.36
26	r	619	CHL	C2C-C3C	4.17	1.45	1.36
31	z	101	BCR	C2-C1	4.17	1.63	1.54
26	u	314	CHL	CHD-C1D	4.17	1.46	1.38
26	U	313	CHL	O2A-CGA	4.17	1.45	1.33
26	P	318	CHL	C3B-C2B	4.17	1.46	1.40
26	6	315	CHL	O2A-CGA	4.16	1.45	1.33
26	n	313	CHL	O2A-CGA	4.16	1.45	1.33
31	b	618	BCR	C2-C1	4.16	1.63	1.54
31	K	101	BCR	C4-C5	-4.16	1.42	1.51
31	C	516	BCR	C2-C1	4.15	1.63	1.54
31	k	101	BCR	C4-C5	-4.15	1.42	1.51
26	4	313	CHL	O2A-CGA	4.15	1.45	1.33
26	S	314	CHL	CHD-C1D	4.14	1.46	1.38
26	U	315	CHL	C3B-C2B	4.14	1.46	1.40
31	b	618	BCR	C28-C27	4.14	1.65	1.52
26	U	315	CHL	CHD-C1D	4.14	1.46	1.38
26	U	316	CHL	O2A-CGA	4.13	1.45	1.33
26	p	315	CHL	CHD-C4C	4.13	1.48	1.39
26	S	315	CHL	CHD-C4C	4.13	1.48	1.39
26	6	312	CHL	CHD-C1D	4.13	1.46	1.38
26	u	317	CHL	O2A-CGA	4.13	1.45	1.33
31	k	101	BCR	C23-C22	4.13	1.54	1.45
26	n	318	CHL	CHD-C4C	4.13	1.48	1.39
26	G	311	CHL	CHD-C1D	4.13	1.46	1.38
31	b	620	BCR	C4-C5	-4.13	1.42	1.51
31	z	101	BCR	C4-C5	-4.13	1.42	1.51
26	u	317	CHL	CHD-C1D	4.12	1.46	1.38
31	x	202	BCR	C28-C27	4.12	1.65	1.52
26	U	315	CHL	O2A-CGA	4.12	1.45	1.33
26	5	314	CHL	CHD-C4C	4.12	1.48	1.39
26	6	314	CHL	CHD-C4C	4.12	1.48	1.39
31	B	618	BCR	C28-C27	4.11	1.65	1.52
31	b	620	BCR	C28-C27	4.11	1.65	1.52
26	p	314	CHL	CHD-C1D	4.11	1.46	1.38
26	3	316	CHL	CHD-C4C	4.10	1.48	1.39
26	s	315	CHL	CHD-C4C	4.10	1.48	1.39
31	B	620	BCR	C4-C5	-4.10	1.42	1.51
31	B	620	BCR	C28-C27	4.10	1.65	1.52
31	t	101	BCR	C28-C27	4.10	1.65	1.52
31	b	619	BCR	C4-C5	-4.10	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	314	CHL	CHD-C4C	4.09	1.48	1.39
26	5	313	CHL	CHD-C4C	4.09	1.48	1.39
26	2	314	CHL	CHD-C4C	4.09	1.48	1.39
26	V	315	CHL	CHD-C4C	4.09	1.48	1.39
31	b	619	BCR	C28-C27	4.09	1.65	1.52
26	g	312	CHL	CHD-C4C	4.09	1.48	1.39
26	r	619	CHL	CHD-C1D	4.08	1.46	1.38
31	B	619	BCR	C28-C27	4.08	1.65	1.52
26	5	315	CHL	CHD-C1D	4.08	1.46	1.38
31	C	516	BCR	C4-C5	-4.08	1.43	1.51
26	P	317	CHL	CHD-C4C	4.08	1.48	1.39
26	u	318	CHL	CHD-C1D	4.08	1.46	1.38
31	X	201	BCR	C28-C27	4.08	1.65	1.52
31	T	101	BCR	C28-C27	4.08	1.65	1.52
26	6	317	CHL	CHD-C4C	4.07	1.48	1.39
26	5	317	CHL	CHD-C1D	4.07	1.46	1.38
26	Q	312	CHL	CHD-C4C	4.07	1.48	1.39
26	G	312	CHL	CHD-C4C	4.07	1.48	1.39
26	N	317	CHL	CHD-C4C	4.07	1.48	1.39
26	2	313	CHL	CHD-C4C	4.07	1.48	1.39
31	c	516	BCR	C28-C27	4.06	1.65	1.52
31	t	101	BCR	C4-C5	-4.06	1.43	1.51
31	X	201	BCR	C4-C5	-4.06	1.43	1.51
26	3	313	CHL	CHD-C4C	4.06	1.48	1.39
31	C	518	BCR	C28-C27	4.06	1.65	1.52
26	g	314	CHL	CHD-C4C	4.06	1.48	1.39
26	P	318	CHL	CHD-C1D	4.06	1.46	1.38
31	B	619	BCR	C4-C5	-4.06	1.43	1.51
31	x	202	BCR	C4-C5	-4.05	1.43	1.51
26	p	318	CHL	CHD-C1D	4.04	1.46	1.38
31	C	517	BCR	C4-C5	-4.04	1.43	1.51
31	c	515	BCR	C4-C5	-4.04	1.43	1.51
31	A	409	BCR	C28-C27	4.04	1.65	1.52
26	3	314	CHL	CHD-C4C	4.03	1.48	1.39
26	S	316	CHL	CHD-C4C	4.03	1.48	1.39
26	r	616	CHL	CHD-C4C	4.03	1.48	1.39
26	s	316	CHL	CHD-C4C	4.03	1.48	1.39
31	T	101	BCR	C4-C5	-4.03	1.43	1.51
26	4	314	CHL	CHD-C1D	4.02	1.46	1.38
26	u	313	CHL	CHD-C4C	4.02	1.48	1.39
26	U	313	CHL	CHD-C4C	4.02	1.48	1.39
26	6	315	CHL	CHD-C4C	4.02	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	316	CHL	CHD-C1D	4.02	1.46	1.38
26	R	317	CHL	CHD-C4C	4.02	1.48	1.39
26	2	317	CHL	CHD-C1D	4.01	1.46	1.38
22	q	301	CLA	C1D-ND	4.01	1.42	1.37
26	V	316	CHL	CHD-C4C	4.01	1.48	1.39
31	a	409	BCR	C28-C27	4.01	1.65	1.52
26	n	313	CHL	CHD-C4C	4.00	1.48	1.39
26	V	314	CHL	CHD-C4C	3.99	1.48	1.39
31	C	517	BCR	C28-C27	3.99	1.65	1.52
26	n	315	CHL	CHD-C4C	3.99	1.48	1.39
26	q	315	CHL	CHD-C4C	3.98	1.48	1.39
26	N	313	CHL	CHD-C4C	3.98	1.48	1.39
26	p	320	CHL	CHD-C1D	3.98	1.46	1.38
31	c	515	BCR	C28-C27	3.97	1.64	1.52
26	2	318	CHL	CHD-C4C	3.97	1.48	1.39
26	p	316	CHL	CHD-C4C	3.97	1.48	1.39
26	V	313	CHL	CHD-C4C	3.97	1.48	1.39
26	P	316	CHL	CHD-C4C	3.96	1.48	1.39
31	B	618	BCR	C23-C22	3.96	1.54	1.45
26	5	318	CHL	CHD-C4C	3.95	1.48	1.39
26	s	313	CHL	CHD-C4C	3.95	1.48	1.39
26	Q	313	CHL	CHD-C4C	3.95	1.48	1.39
26	g	316	CHL	CHD-C4C	3.95	1.48	1.39
22	R	310	CLA	C1D-ND	3.95	1.42	1.37
26	q	311	CHL	CHD-C4C	3.95	1.48	1.39
26	2	316	CHL	CHD-C4C	3.95	1.48	1.39
26	v	316	CHL	CHD-C1D	3.95	1.46	1.38
26	Q	314	CHL	CHD-C4C	3.95	1.48	1.39
26	Q	316	CHL	CHD-C4C	3.95	1.48	1.39
26	G	314	CHL	CHD-C4C	3.94	1.48	1.39
26	5	316	CHL	CHD-C4C	3.94	1.48	1.39
31	t	101	BCR	C12-C13	3.94	1.54	1.45
26	n	316	CHL	CHD-C4C	3.94	1.48	1.39
26	U	314	CHL	CHD-C1D	3.94	1.46	1.38
26	u	316	CHL	CHD-C4C	3.94	1.48	1.39
31	T	101	BCR	C12-C13	3.93	1.54	1.45
22	Q	301	CLA	C1D-ND	3.93	1.42	1.37
26	p	317	CHL	CHD-C4C	3.93	1.48	1.39
22	R	302	CLA	C1D-ND	3.93	1.42	1.37
26	4	313	CHL	CHD-C4C	3.93	1.48	1.39
31	X	201	BCR	C12-C13	3.93	1.54	1.45
26	S	313	CHL	CHD-C4C	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	313	CHL	CHD-C4C	3.92	1.48	1.39
24	u	311	XAT	C31-C30	3.92	1.55	1.43
26	4	315	CHL	CHD-C4C	3.92	1.48	1.39
26	6	301	CHL	CHD-C4C	3.92	1.48	1.39
31	d	403	BCR	C12-C13	3.92	1.54	1.45
26	G	316	CHL	CHD-C4C	3.91	1.48	1.39
26	p	314	CHL	CHD-C4C	3.90	1.48	1.39
26	Q	311	CHL	CHD-C4C	3.90	1.48	1.39
26	U	319	CHL	CHD-C4C	3.90	1.48	1.39
22	V	301	CLA	C1D-ND	3.90	1.42	1.37
26	V	317	CHL	CHD-C4C	3.90	1.48	1.39
22	r	609	CLA	C1D-ND	3.90	1.42	1.37
26	G	313	CHL	CHD-C4C	3.90	1.48	1.39
31	x	202	BCR	C12-C13	3.90	1.54	1.45
26	V	318	CHL	CHD-C4C	3.90	1.48	1.39
31	D	404	BCR	C12-C13	3.89	1.54	1.45
26	1	316	CHL	CHD-C4C	3.89	1.48	1.39
26	4	316	CHL	CHD-C4C	3.89	1.48	1.39
26	g	313	CHL	CHD-C4C	3.89	1.48	1.39
24	V	311	XAT	C31-C30	3.88	1.55	1.43
22	n	308	CLA	C1D-ND	3.88	1.42	1.37
22	r	601	CLA	C1D-ND	3.88	1.42	1.37
26	1	313	CHL	CHD-C4C	3.88	1.48	1.39
26	v	315	CHL	CHD-C4C	3.88	1.48	1.39
26	U	316	CHL	CHD-C4C	3.88	1.48	1.39
26	p	319	CHL	CHD-C4C	3.87	1.48	1.39
31	C	516	BCR	C28-C27	3.87	1.64	1.52
26	1	315	CHL	CHD-C4C	3.87	1.48	1.39
36	a	416	DGD	O6E-C1E	3.87	1.51	1.41
24	P	312	XAT	C35-C34	3.87	1.55	1.43
31	b	618	BCR	C23-C22	3.87	1.54	1.45
26	u	314	CHL	CHD-C4C	3.87	1.48	1.39
26	v	314	CHL	CHD-C4C	3.87	1.48	1.39
31	T	101	BCR	C15-C14	3.87	1.55	1.43
26	r	614	CHL	CHD-C4C	3.87	1.48	1.39
26	6	312	CHL	CHD-C4C	3.86	1.48	1.39
36	A	414	DGD	O6E-C1E	3.86	1.51	1.41
31	z	101	BCR	C28-C27	3.86	1.64	1.52
24	p	312	XAT	C35-C34	3.86	1.55	1.43
22	g	306	CLA	C1D-ND	3.86	1.42	1.37
24	p	312	XAT	C31-C30	3.86	1.55	1.43
24	P	312	XAT	C31-C30	3.86	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v	317	CHL	CHD-C4C	3.85	1.48	1.39
26	v	313	CHL	CHD-C4C	3.85	1.48	1.39
26	1	317	CHL	CHD-C4C	3.85	1.48	1.39
24	R	313	XAT	C31-C30	3.85	1.55	1.43
26	v	318	CHL	CHD-C4C	3.84	1.48	1.39
24	Q	309	XAT	C35-C34	3.84	1.55	1.43
31	t	101	BCR	C15-C14	3.84	1.55	1.43
24	6	310	XAT	C35-C34	3.84	1.55	1.43
22	v	301	CLA	C1D-ND	3.84	1.42	1.37
24	R	313	XAT	C35-C34	3.84	1.55	1.43
26	n	317	CHL	CHD-C4C	3.83	1.48	1.39
26	3	311	CHL	CHD-C4C	3.83	1.48	1.39
26	R	315	CHL	CHD-C4C	3.83	1.48	1.39
24	3	309	XAT	C35-C34	3.83	1.55	1.43
24	v	311	XAT	C31-C30	3.83	1.55	1.43
24	U	311	XAT	C31-C30	3.83	1.55	1.43
22	3	301	CLA	C1D-ND	3.83	1.42	1.37
24	g	309	XAT	C31-C30	3.82	1.55	1.43
31	c	516	BCR	C12-C13	3.82	1.54	1.45
24	3	309	XAT	C15-C14	3.82	1.55	1.43
22	R	304	CLA	C1D-ND	3.82	1.42	1.37
24	Q	309	XAT	C15-C14	3.82	1.55	1.43
24	5	311	XAT	C31-C30	3.82	1.55	1.43
24	3	309	XAT	C31-C30	3.82	1.55	1.43
26	g	315	CHL	CHD-C1D	3.81	1.45	1.38
24	2	311	XAT	C31-C30	3.81	1.55	1.43
26	v	316	CHL	CHD-C4C	3.81	1.47	1.39
24	6	310	XAT	C15-C14	3.81	1.55	1.43
24	P	312	XAT	C15-C14	3.81	1.55	1.43
26	g	312	CHL	OBD-CAD	3.81	1.29	1.22
26	G	311	CHL	CHD-C4C	3.81	1.47	1.39
24	r	612	XAT	C31-C30	3.81	1.55	1.43
26	g	311	CHL	CHD-C4C	3.81	1.47	1.39
26	P	319	CHL	CHD-C4C	3.81	1.47	1.39
24	5	311	XAT	C35-C34	3.81	1.55	1.43
26	u	315	CHL	CHD-C1D	3.80	1.45	1.38
26	4	317	CHL	CHD-C4C	3.80	1.47	1.39
22	6	302	CLA	C1D-ND	3.80	1.42	1.37
26	U	315	CHL	CHD-C4C	3.80	1.47	1.39
24	Q	309	XAT	C31-C30	3.80	1.55	1.43
26	u	317	CHL	CHD-C4C	3.80	1.47	1.39
26	G	312	CHL	OBD-CAD	3.80	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	V	311	XAT	C35-C34	3.80	1.55	1.43
26	V	314	CHL	OBD-CAD	3.80	1.29	1.22
24	p	312	XAT	C15-C14	3.80	1.55	1.43
24	2	311	XAT	C15-C14	3.80	1.55	1.43
26	s	314	CHL	CHD-C4C	3.80	1.47	1.39
24	2	311	XAT	C35-C34	3.80	1.55	1.43
26	r	615	CHL	CHD-C4C	3.80	1.47	1.39
24	6	310	XAT	C31-C30	3.80	1.55	1.43
22	R	309	CLA	C1D-ND	3.79	1.42	1.37
26	R	316	CHL	CHD-C4C	3.79	1.47	1.39
26	S	314	CHL	CHD-C4C	3.79	1.47	1.39
26	1	318	CHL	CHD-C4C	3.79	1.47	1.39
26	1	314	CHL	CHD-C4C	3.78	1.47	1.39
24	4	311	XAT	C35-C34	3.78	1.55	1.43
26	G	315	CHL	CHD-C1D	3.78	1.45	1.38
22	r	603	CLA	C1D-ND	3.78	1.42	1.37
24	q	309	XAT	C11-C10	3.78	1.55	1.43
24	Q	309	XAT	C11-C10	3.78	1.55	1.43
24	q	309	XAT	C31-C30	3.78	1.55	1.43
24	4	311	XAT	C31-C30	3.78	1.55	1.43
26	v	314	CHL	OBD-CAD	3.78	1.29	1.22
24	5	311	XAT	C15-C14	3.78	1.55	1.43
24	1	311	XAT	C31-C30	3.78	1.55	1.43
24	P	312	XAT	C11-C10	3.78	1.55	1.43
24	G	309	XAT	C31-C30	3.77	1.55	1.43
24	1	311	XAT	C35-C34	3.77	1.55	1.43
24	q	309	XAT	C35-C34	3.77	1.55	1.43
24	V	311	XAT	C15-C14	3.77	1.55	1.43
22	p	304	CLA	C1D-ND	3.77	1.42	1.37
24	q	309	XAT	C15-C14	3.77	1.55	1.43
22	b	611	CLA	C1D-ND	3.77	1.42	1.37
24	r	612	XAT	C35-C34	3.77	1.55	1.43
24	1	311	XAT	C15-C14	3.76	1.55	1.43
24	u	311	XAT	C15-C14	3.76	1.55	1.43
26	3	312	CHL	OBD-CAD	3.76	1.29	1.22
24	N	311	XAT	C31-C30	3.76	1.55	1.43
31	C	518	BCR	C12-C13	3.76	1.54	1.45
22	3	308	CLA	C1D-ND	3.76	1.42	1.37
34	C	521	LMG	O6-C1	3.76	1.51	1.41
24	u	311	XAT	C35-C34	3.76	1.55	1.43
31	k	101	BCR	C12-C13	3.76	1.54	1.45
22	4	301	CLA	C1D-ND	3.75	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p	320	CHL	CHD-C4C	3.75	1.47	1.39
22	n	301	CLA	C1D-ND	3.75	1.42	1.37
24	V	311	XAT	C11-C10	3.75	1.55	1.43
26	r	619	CHL	CHD-C4C	3.75	1.47	1.39
22	G	301	CLA	C1D-ND	3.75	1.42	1.37
26	U	317	CHL	CHD-C4C	3.75	1.47	1.39
31	K	101	BCR	C12-C13	3.75	1.54	1.45
26	6	313	CHL	OBD-CAD	3.75	1.28	1.22
34	b	621	LMG	O6-C1	3.75	1.51	1.41
24	v	311	XAT	C35-C34	3.75	1.55	1.43
26	Q	312	CHL	OBD-CAD	3.75	1.28	1.22
22	r	610	CLA	C1D-ND	3.75	1.42	1.37
22	N	308	CLA	C1D-ND	3.75	1.42	1.37
26	2	315	CHL	CHD-C4C	3.74	1.47	1.39
24	4	311	XAT	C15-C14	3.74	1.55	1.43
34	b	624	LMG	O6-C1	3.74	1.51	1.41
24	R	313	XAT	C15-C14	3.74	1.55	1.43
22	B	611	CLA	C1D-ND	3.74	1.42	1.37
26	g	314	CHL	OBD-CAD	3.74	1.28	1.22
24	6	310	XAT	C11-C10	3.73	1.55	1.43
24	r	612	XAT	C11-C10	3.73	1.55	1.43
24	n	311	XAT	C31-C30	3.73	1.55	1.43
24	R	313	XAT	C11-C10	3.73	1.55	1.43
22	R	311	CLA	C1D-ND	3.73	1.42	1.37
31	b	620	BCR	C12-C13	3.73	1.54	1.45
22	R	306	CLA	C1D-ND	3.73	1.42	1.37
31	z	101	BCR	C12-C13	3.73	1.53	1.45
24	N	311	XAT	C35-C34	3.73	1.55	1.43
24	v	311	XAT	C11-C10	3.72	1.55	1.43
24	g	309	XAT	C35-C34	3.72	1.55	1.43
22	P	304	CLA	C1D-ND	3.72	1.42	1.37
22	Q	302	CLA	C1D-ND	3.72	1.42	1.37
22	G	306	CLA	C1D-ND	3.72	1.42	1.37
34	B	624	LMG	O6-C1	3.72	1.51	1.41
22	G	308	CLA	C1D-ND	3.72	1.42	1.37
24	n	311	XAT	C35-C34	3.72	1.55	1.43
24	r	612	XAT	C15-C14	3.72	1.55	1.43
24	p	312	XAT	C11-C10	3.72	1.55	1.43
22	v	302	CLA	C1D-ND	3.72	1.42	1.37
26	2	314	CHL	OBD-CAD	3.72	1.28	1.22
31	d	403	BCR	C15-C14	3.72	1.55	1.43
31	D	404	BCR	C15-C14	3.72	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	101	HEM	C3C-CAC	3.72	1.55	1.47
26	q	312	CHL	OBD-CAD	3.72	1.28	1.22
34	D	408	LMG	O6-C1	3.72	1.51	1.41
22	r	605	CLA	C1D-ND	3.71	1.42	1.37
22	r	608	CLA	C1D-ND	3.71	1.42	1.37
22	B	605	CLA	C1D-ND	3.71	1.42	1.37
34	d	407	LMG	O6-C1	3.71	1.51	1.41
24	G	309	XAT	C15-C14	3.71	1.55	1.43
24	5	311	XAT	C11-C10	3.71	1.55	1.43
24	g	309	XAT	C15-C14	3.71	1.55	1.43
22	N	301	CLA	C1D-ND	3.71	1.42	1.37
26	4	314	CHL	CHD-C4C	3.71	1.47	1.39
24	v	311	XAT	C15-C14	3.71	1.54	1.43
22	1	301	CLA	C1D-ND	3.71	1.42	1.37
22	6	307	CLA	C1D-ND	3.71	1.42	1.37
24	3	309	XAT	C11-C10	3.71	1.54	1.43
34	C	502	LMG	O6-C1	3.71	1.51	1.41
24	2	311	XAT	C11-C10	3.71	1.54	1.43
26	N	316	CHL	CHD-C4C	3.71	1.47	1.39
34	c	501	LMG	O6-C1	3.71	1.51	1.41
26	g	313	CHL	OBD-CAD	3.71	1.28	1.22
22	G	305	CLA	C1D-ND	3.70	1.42	1.37
22	g	301	CLA	C1D-ND	3.70	1.42	1.37
22	g	308	CLA	C1D-ND	3.70	1.42	1.37
22	4	302	CLA	C1D-ND	3.70	1.42	1.37
34	B	621	LMG	O6-C1	3.70	1.51	1.41
34	c	520	LMG	O6-C1	3.70	1.51	1.41
24	g	309	XAT	C11-C10	3.70	1.54	1.43
26	4	315	CHL	OBD-CAD	3.70	1.28	1.22
22	N	306	CLA	C1D-ND	3.70	1.42	1.37
37	e	101	HEM	C3C-CAC	3.70	1.55	1.47
26	u	314	CHL	OBD-CAD	3.70	1.28	1.22
26	n	315	CHL	OBD-CAD	3.70	1.28	1.22
26	3	315	CHL	CHD-C1D	3.69	1.45	1.38
26	S	314	CHL	OBD-CAD	3.69	1.28	1.22
26	5	314	CHL	OBD-CAD	3.69	1.28	1.22
22	q	302	CLA	C1D-ND	3.69	1.42	1.37
22	g	305	CLA	C1D-ND	3.69	1.42	1.37
22	G	307	CLA	C1D-ND	3.69	1.42	1.37
26	N	314	CHL	OBD-CAD	3.69	1.28	1.22
26	2	317	CHL	CHD-C4C	3.68	1.47	1.39
22	6	309	CLA	C1D-ND	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	309	XAT	C35-C34	3.68	1.54	1.43
31	C	516	BCR	C12-C13	3.68	1.53	1.45
22	S	305	CLA	C1D-ND	3.68	1.42	1.37
26	s	314	CHL	OBD-CAD	3.68	1.28	1.22
24	u	311	XAT	C11-C10	3.68	1.54	1.43
26	3	315	CHL	CHD-C4C	3.68	1.47	1.39
36	J	101	DGD	O6D-C1D	3.68	1.51	1.41
31	X	201	BCR	C15-C14	3.68	1.54	1.43
22	n	303	CLA	C1D-ND	3.68	1.42	1.37
26	1	314	CHL	OBD-CAD	3.68	1.28	1.22
22	U	305	CLA	C1D-ND	3.68	1.42	1.37
22	3	303	CLA	C1D-ND	3.68	1.42	1.37
26	5	315	CHL	CHD-C4C	3.68	1.47	1.39
22	V	306	CLA	C1D-ND	3.68	1.42	1.37
24	U	311	XAT	C15-C14	3.68	1.54	1.43
26	u	318	CHL	CHD-C4C	3.68	1.47	1.39
31	B	620	BCR	C12-C13	3.68	1.53	1.45
24	U	311	XAT	C35-C34	3.67	1.54	1.43
22	s	303	CLA	C1D-ND	3.67	1.42	1.37
26	5	317	CHL	CHD-C4C	3.67	1.47	1.39
31	A	409	BCR	C12-C13	3.67	1.53	1.45
24	4	311	XAT	C11-C10	3.67	1.54	1.43
22	u	305	CLA	C1D-ND	3.67	1.42	1.37
26	r	619	CHL	OBD-CAD	3.67	1.28	1.22
22	B	607	CLA	C1D-ND	3.67	1.42	1.37
31	c	516	BCR	C15-C14	3.66	1.54	1.43
22	s	304	CLA	C1D-ND	3.66	1.42	1.37
22	N	307	CLA	C1D-ND	3.66	1.42	1.37
34	A	411	LMG	O6-C1	3.66	1.51	1.41
24	G	309	XAT	C11-C10	3.66	1.54	1.43
22	g	307	CLA	C1D-ND	3.66	1.42	1.37
26	1	315	CHL	OBD-CAD	3.66	1.28	1.22
31	b	620	BCR	C15-C14	3.66	1.54	1.43
22	5	304	CLA	C1D-ND	3.66	1.42	1.37
22	s	302	CLA	C1D-ND	3.66	1.42	1.37
26	4	314	CHL	OBD-CAD	3.66	1.28	1.22
22	Q	308	CLA	C1D-ND	3.66	1.42	1.37
26	n	318	CHL	OBD-CAD	3.66	1.28	1.22
22	S	304	CLA	C1D-ND	3.66	1.42	1.37
24	N	311	XAT	C15-C14	3.65	1.54	1.43
31	x	202	BCR	C15-C14	3.65	1.54	1.43
26	G	313	CHL	OBD-CAD	3.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	409	BCR	C12-C13	3.65	1.53	1.45
24	U	311	XAT	C11-C10	3.65	1.54	1.43
36	c	518	DGD	O6E-C1E	3.65	1.51	1.41
26	U	315	CHL	OBD-CAD	3.65	1.28	1.22
26	n	314	CHL	OBD-CAD	3.65	1.28	1.22
22	G	303	CLA	C1D-ND	3.65	1.42	1.37
22	s	305	CLA	C1D-ND	3.65	1.42	1.37
22	b	607	CLA	C1D-ND	3.64	1.42	1.37
34	a	412	LMG	O6-C1	3.64	1.51	1.41
22	q	303	CLA	C1D-ND	3.64	1.42	1.37
22	n	307	CLA	C1D-ND	3.64	1.42	1.37
22	b	617	CLA	C1D-ND	3.64	1.42	1.37
24	n	311	XAT	C15-C14	3.64	1.54	1.43
22	P	307	CLA	C1D-ND	3.64	1.42	1.37
26	5	316	CHL	OBD-CAD	3.64	1.28	1.22
24	n	311	XAT	C11-C10	3.64	1.54	1.43
26	V	316	CHL	OBD-CAD	3.64	1.28	1.22
36	c	519	DGD	O6D-C1D	3.64	1.51	1.41
22	a	404	CLA	C4D-ND	-3.64	1.32	1.37
22	p	307	CLA	C1D-ND	3.64	1.42	1.37
26	5	313	CHL	OBD-CAD	3.64	1.28	1.22
26	q	313	CHL	OBD-CAD	3.64	1.28	1.22
22	q	308	CLA	C1D-ND	3.64	1.42	1.37
26	G	315	CHL	CHD-C4C	3.64	1.47	1.39
26	u	316	CHL	OBD-CAD	3.63	1.28	1.22
26	Q	314	CHL	OBD-CAD	3.63	1.28	1.22
22	5	301	CLA	C1D-ND	3.63	1.42	1.37
22	S	302	CLA	C1D-ND	3.63	1.42	1.37
22	a	406	CLA	C1D-ND	3.63	1.42	1.37
26	2	316	CHL	OBD-CAD	3.63	1.28	1.22
22	A	406	CLA	C1D-ND	3.63	1.42	1.37
22	1	302	CLA	C1D-ND	3.63	1.42	1.37
22	P	309	CLA	C1D-ND	3.63	1.42	1.37
26	P	316	CHL	OBD-CAD	3.63	1.28	1.22
26	Q	311	CHL	OBD-CAD	3.63	1.28	1.22
26	Q	313	CHL	OBD-CAD	3.63	1.28	1.22
22	2	308	CLA	C1D-ND	3.63	1.42	1.37
36	C	520	DGD	O6E-C1E	3.63	1.51	1.41
24	1	311	XAT	C11-C10	3.63	1.54	1.43
26	r	614	CHL	OBD-CAD	3.63	1.28	1.22
31	C	518	BCR	C15-C14	3.63	1.54	1.43
26	6	314	CHL	OBD-CAD	3.63	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	305	CLA	C1D-ND	3.63	1.42	1.37
22	N	303	CLA	C1D-ND	3.63	1.42	1.37
26	r	615	CHL	OBD-CAD	3.62	1.28	1.22
22	r	602	CLA	C1D-ND	3.62	1.42	1.37
26	5	315	CHL	OBD-CAD	3.62	1.28	1.22
22	V	308	CLA	C1D-ND	3.62	1.42	1.37
26	N	315	CHL	OBD-CAD	3.62	1.28	1.22
22	6	304	CLA	C1D-ND	3.62	1.42	1.37
22	s	307	CLA	C1D-ND	3.62	1.42	1.37
22	5	308	CLA	C1D-ND	3.62	1.42	1.37
22	Q	303	CLA	C1D-ND	3.62	1.42	1.37
26	P	319	CHL	OBD-CAD	3.62	1.28	1.22
22	6	306	CLA	C1D-ND	3.62	1.42	1.37
22	2	304	CLA	C1D-ND	3.62	1.42	1.37
26	Q	315	CHL	CHD-C1D	3.62	1.45	1.38
26	R	316	CHL	OBD-CAD	3.62	1.28	1.22
26	N	315	CHL	CHD-C4C	3.61	1.47	1.39
22	q	305	CLA	C1D-ND	3.61	1.42	1.37
22	b	608	CLA	C1D-ND	3.61	1.42	1.37
22	V	303	CLA	C1D-ND	3.61	1.42	1.37
26	6	315	CHL	OBD-CAD	3.61	1.28	1.22
26	p	316	CHL	OBD-CAD	3.61	1.28	1.22
22	u	302	CLA	C1D-ND	3.61	1.42	1.37
22	S	303	CLA	C1D-ND	3.61	1.42	1.37
36	a	416	DGD	O6D-C1D	3.61	1.51	1.41
26	3	313	CHL	OBD-CAD	3.61	1.28	1.22
36	A	414	DGD	O6D-C1D	3.61	1.51	1.41
26	N	317	CHL	OBD-CAD	3.61	1.28	1.22
22	R	303	CLA	C1D-ND	3.60	1.42	1.37
26	U	319	CHL	OBD-CAD	3.60	1.28	1.22
31	C	517	BCR	C12-C13	3.60	1.53	1.45
26	P	318	CHL	CHD-C4C	3.60	1.47	1.39
26	g	315	CHL	CHD-C4C	3.60	1.47	1.39
22	A	404	CLA	C4D-ND	-3.60	1.32	1.37
22	4	308	CLA	C1D-ND	3.60	1.42	1.37
22	R	305	CLA	C1D-ND	3.60	1.42	1.37
26	P	314	CHL	OBD-CAD	3.60	1.28	1.22
26	6	301	CHL	OBD-CAD	3.60	1.28	1.22
26	s	316	CHL	OBD-CAD	3.60	1.28	1.22
22	3	306	CLA	C1D-ND	3.60	1.42	1.37
22	u	301	CLA	C1D-ND	3.60	1.42	1.37
26	p	320	CHL	OBD-CAD	3.60	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	313	CHL	OBD-CAD	3.60	1.28	1.22
36	b	601	DGD	O6E-C1E	3.60	1.51	1.41
26	p	318	CHL	CHD-C4C	3.60	1.47	1.39
31	K	101	BCR	C15-C14	3.60	1.54	1.43
22	b	605	CLA	C1D-ND	3.60	1.42	1.37
26	G	314	CHL	OBD-CAD	3.60	1.28	1.22
31	c	515	BCR	C12-C13	3.60	1.53	1.45
26	G	311	CHL	OBD-CAD	3.60	1.28	1.22
22	v	308	CLA	C1D-ND	3.59	1.42	1.37
26	q	314	CHL	CHD-C4C	3.59	1.47	1.39
22	A	405	CLA	C1D-ND	3.59	1.42	1.37
31	k	101	BCR	C15-C14	3.59	1.54	1.43
22	B	608	CLA	C1D-ND	3.59	1.42	1.37
22	q	307	CLA	C1D-ND	3.59	1.42	1.37
26	n	313	CHL	OBD-CAD	3.59	1.28	1.22
26	2	313	CHL	OBD-CAD	3.59	1.28	1.22
26	V	315	CHL	OBD-CAD	3.59	1.28	1.22
22	R	308	CLA	C1D-ND	3.59	1.42	1.37
26	1	316	CHL	OBD-CAD	3.59	1.28	1.22
31	B	620	BCR	C15-C14	3.59	1.54	1.43
22	q	306	CLA	C1D-ND	3.59	1.42	1.37
26	6	316	CHL	CHD-C4C	3.59	1.47	1.39
26	S	316	CHL	OBD-CAD	3.59	1.28	1.22
26	p	319	CHL	OBD-CAD	3.59	1.28	1.22
26	R	315	CHL	OBD-CAD	3.59	1.28	1.22
22	s	306	CLA	C1D-ND	3.59	1.42	1.37
26	3	316	CHL	OBD-CAD	3.59	1.28	1.22
26	n	316	CHL	OBD-CAD	3.59	1.28	1.22
22	S	306	CLA	C1D-ND	3.59	1.42	1.37
26	6	312	CHL	OBD-CAD	3.59	1.28	1.22
22	v	303	CLA	C1D-ND	3.58	1.42	1.37
22	Q	304	CLA	C1D-ND	3.58	1.42	1.37
22	Q	306	CLA	C1D-ND	3.58	1.42	1.37
22	Q	307	CLA	C1D-ND	3.58	1.42	1.37
22	g	304	CLA	C1D-ND	3.58	1.42	1.37
26	6	317	CHL	OBD-CAD	3.58	1.28	1.22
22	6	308	CLA	C1D-ND	3.58	1.42	1.37
26	Q	315	CHL	CHD-C4C	3.58	1.47	1.39
22	g	302	CLA	C1D-ND	3.58	1.42	1.37
26	s	315	CHL	OBD-CAD	3.58	1.28	1.22
26	3	311	CHL	OBD-CAD	3.58	1.28	1.22
22	2	306	CLA	C1D-ND	3.58	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	313	CHL	OBD-CAD	3.57	1.28	1.22
22	n	302	CLA	C1D-ND	3.57	1.42	1.37
26	P	317	CHL	OBD-CAD	3.57	1.28	1.22
22	A	408	CLA	C1D-ND	3.57	1.42	1.37
22	V	302	CLA	C1D-ND	3.57	1.42	1.37
22	R	307	CLA	C1D-ND	3.57	1.42	1.37
22	3	307	CLA	C1D-ND	3.57	1.42	1.37
26	6	316	CHL	CHD-C1D	3.57	1.45	1.38
26	3	314	CHL	OBD-CAD	3.57	1.28	1.22
22	v	306	CLA	C1D-ND	3.56	1.42	1.37
22	p	305	CLA	C1D-ND	3.56	1.42	1.37
22	P	303	CLA	C1D-ND	3.56	1.42	1.37
26	u	313	CHL	OBD-CAD	3.56	1.28	1.22
26	1	318	CHL	OBD-CAD	3.56	1.28	1.22
26	U	314	CHL	OBD-CAD	3.56	1.28	1.22
26	p	315	CHL	OBD-CAD	3.56	1.28	1.22
22	4	306	CLA	C1D-ND	3.56	1.42	1.37
22	V	304	CLA	C1D-ND	3.56	1.42	1.37
31	B	619	BCR	C12-C13	3.56	1.53	1.45
22	r	604	CLA	C1D-ND	3.56	1.42	1.37
36	B	601	DGD	O6E-C1E	3.56	1.50	1.41
22	q	304	CLA	C1D-ND	3.56	1.42	1.37
26	5	318	CHL	OBD-CAD	3.56	1.28	1.22
26	u	315	CHL	OBD-CAD	3.56	1.28	1.22
26	2	315	CHL	OBD-CAD	3.56	1.28	1.22
26	4	317	CHL	OBD-CAD	3.56	1.28	1.22
22	1	308	CLA	C1D-ND	3.56	1.42	1.37
22	3	305	CLA	C1D-ND	3.56	1.42	1.37
26	V	318	CHL	OBD-CAD	3.55	1.28	1.22
26	S	315	CHL	OBD-CAD	3.55	1.28	1.22
22	U	308	CLA	C1D-ND	3.55	1.42	1.37
22	u	308	CLA	C1D-ND	3.55	1.42	1.37
22	S	307	CLA	C1D-ND	3.55	1.42	1.37
22	g	303	CLA	C1D-ND	3.55	1.42	1.37
22	p	309	CLA	C1D-ND	3.55	1.42	1.37
22	a	405	CLA	C4D-ND	-3.55	1.32	1.37
22	n	304	CLA	C1D-ND	3.55	1.42	1.37
26	g	311	CHL	OBD-CAD	3.55	1.28	1.22
22	a	405	CLA	C1D-ND	3.54	1.42	1.37
24	N	311	XAT	C11-C10	3.54	1.54	1.43
31	b	619	BCR	C12-C13	3.54	1.53	1.45
22	G	302	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	305	CLA	C1D-ND	3.54	1.42	1.37
22	N	302	CLA	C1D-ND	3.54	1.42	1.37
22	5	306	CLA	C1D-ND	3.54	1.42	1.37
26	g	316	CHL	OBD-CAD	3.54	1.28	1.22
31	b	619	BCR	C15-C14	3.54	1.54	1.43
26	2	318	CHL	OBD-CAD	3.54	1.28	1.22
26	v	313	CHL	OBD-CAD	3.54	1.28	1.22
22	U	302	CLA	C1D-ND	3.54	1.42	1.37
31	B	619	BCR	C15-C14	3.54	1.54	1.43
22	G	304	CLA	C1D-ND	3.54	1.42	1.37
31	C	516	BCR	C15-C14	3.54	1.54	1.43
26	q	311	CHL	OBD-CAD	3.54	1.28	1.22
31	c	515	BCR	C27-C26	-3.54	1.44	1.51
31	C	517	BCR	C27-C26	-3.54	1.44	1.51
26	P	315	CHL	OBD-CAD	3.54	1.28	1.22
26	U	314	CHL	CHD-C4C	3.53	1.47	1.39
26	v	317	CHL	OBD-CAD	3.53	1.28	1.22
22	p	303	CLA	C1D-ND	3.53	1.42	1.37
22	C	510	CLA	C4D-ND	-3.53	1.32	1.37
22	U	306	CLA	C1D-ND	3.53	1.42	1.37
26	V	317	CHL	OBD-CAD	3.53	1.28	1.22
22	n	306	CLA	C1D-ND	3.53	1.42	1.37
31	z	101	BCR	C15-C14	3.52	1.54	1.43
31	C	516	BCR	C27-C26	-3.52	1.44	1.51
22	1	305	CLA	C1D-ND	3.52	1.42	1.37
22	v	307	CLA	C1D-ND	3.52	1.42	1.37
26	v	316	CHL	OBD-CAD	3.52	1.28	1.22
22	5	307	CLA	C1D-ND	3.52	1.42	1.37
22	6	303	CLA	C1D-ND	3.52	1.42	1.37
22	2	301	CLA	C1D-ND	3.52	1.42	1.37
22	P	308	CLA	C1D-ND	3.52	1.42	1.37
26	v	315	CHL	OBD-CAD	3.52	1.28	1.22
26	v	318	CHL	OBD-CAD	3.52	1.28	1.22
22	b	604	CLA	C1D-ND	3.52	1.42	1.37
22	c	510	CLA	C4D-ND	-3.51	1.32	1.37
26	1	317	CHL	OBD-CAD	3.51	1.28	1.22
26	p	314	CHL	OBD-CAD	3.51	1.28	1.22
22	v	305	CLA	C1D-ND	3.51	1.42	1.37
22	V	307	CLA	C1D-ND	3.51	1.42	1.37
26	2	317	CHL	OBD-CAD	3.51	1.28	1.22
31	z	101	BCR	C27-C26	-3.50	1.44	1.51
22	3	302	CLA	C1D-ND	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	304	CLA	C1D-ND	3.50	1.42	1.37
22	c	512	CLA	C1D-ND	3.50	1.42	1.37
31	C	517	BCR	C15-C14	3.50	1.54	1.43
26	5	317	CHL	OBD-CAD	3.50	1.28	1.22
26	U	313	CHL	OBD-CAD	3.50	1.28	1.22
31	A	409	BCR	C15-C14	3.50	1.54	1.43
31	b	619	BCR	C27-C26	-3.50	1.44	1.51
22	c	503	CLA	C4D-ND	-3.50	1.32	1.37
26	4	316	CHL	OBD-CAD	3.50	1.28	1.22
34	W	201	LMG	O6-C1	3.50	1.50	1.41
22	a	408	CLA	C1D-ND	3.50	1.42	1.37
22	p	308	CLA	C1D-ND	3.50	1.42	1.37
36	J	101	DGD	O6E-C1E	3.49	1.50	1.41
22	U	301	CLA	C1D-ND	3.49	1.42	1.37
26	p	317	CHL	OBD-CAD	3.49	1.28	1.22
31	t	101	BCR	C24-C25	3.49	1.57	1.45
31	c	515	BCR	C15-C14	3.49	1.54	1.43
26	4	313	CHL	OBD-CAD	3.49	1.28	1.22
22	1	307	CLA	C1D-ND	3.49	1.42	1.37
22	r	606	CLA	C1D-ND	3.49	1.42	1.37
26	6	316	CHL	OBD-CAD	3.48	1.28	1.22
22	Q	305	CLA	C1D-ND	3.48	1.42	1.37
31	D	404	BCR	C24-C25	3.48	1.57	1.45
31	a	409	BCR	C15-C14	3.48	1.54	1.43
22	u	306	CLA	C1D-ND	3.48	1.42	1.37
26	1	313	CHL	OBD-CAD	3.48	1.28	1.22
26	s	313	CHL	OBD-CAD	3.48	1.28	1.22
31	T	101	BCR	C24-C25	3.48	1.57	1.45
22	C	504	CLA	C4D-ND	-3.48	1.32	1.37
22	2	302	CLA	C1D-ND	3.48	1.42	1.37
22	u	303	CLA	C1D-ND	3.48	1.42	1.37
22	B	610	CLA	C1D-ND	3.48	1.42	1.37
22	C	505	CLA	C1D-ND	3.48	1.42	1.37
31	B	618	BCR	C12-C13	3.48	1.53	1.45
22	3	304	CLA	C1D-ND	3.47	1.42	1.37
26	S	313	CHL	OBD-CAD	3.47	1.28	1.22
22	B	604	CLA	C1D-ND	3.47	1.42	1.37
22	b	610	CLA	C1D-ND	3.47	1.42	1.37
22	C	511	CLA	C4D-ND	-3.47	1.32	1.37
31	d	403	BCR	C24-C25	3.47	1.57	1.45
31	c	516	BCR	C27-C26	-3.47	1.44	1.51
31	B	619	BCR	C27-C26	-3.46	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	314	CHL	CHD-C1D	3.46	1.45	1.38
22	b	613	CLA	C4D-ND	-3.46	1.32	1.37
22	r	607	CLA	C1D-ND	3.46	1.42	1.37
26	G	316	CHL	OBD-CAD	3.46	1.28	1.22
22	1	303	CLA	C1D-ND	3.46	1.42	1.37
22	u	307	CLA	C1D-ND	3.46	1.42	1.37
22	V	305	CLA	C1D-ND	3.46	1.42	1.37
31	B	618	BCR	C15-C14	3.45	1.54	1.43
22	4	307	CLA	C1D-ND	3.45	1.42	1.37
34	w	201	LMG	O6-C1	3.45	1.50	1.41
26	U	317	CHL	OBD-CAD	3.45	1.28	1.22
22	5	302	CLA	C1D-ND	3.45	1.42	1.37
22	x	201	CLA	C1D-ND	3.45	1.42	1.37
26	r	616	CHL	OBD-CAD	3.45	1.28	1.22
22	b	609	CLA	C4D-ND	-3.45	1.33	1.37
22	U	307	CLA	C1D-ND	3.44	1.42	1.37
26	P	318	CHL	OBD-CAD	3.44	1.28	1.22
22	b	616	CLA	C1D-ND	3.44	1.42	1.37
22	5	302	CLA	C4D-ND	-3.44	1.33	1.37
26	u	315	CHL	CHD-C4C	3.44	1.47	1.39
22	c	509	CLA	C4D-ND	-3.44	1.33	1.37
22	S	309	CLA	C1D-ND	3.43	1.42	1.37
31	a	409	BCR	C24-C25	3.43	1.57	1.45
22	4	303	CLA	C1D-ND	3.43	1.42	1.37
26	u	318	CHL	OBD-CAD	3.43	1.28	1.22
22	N	304	CLA	C1D-ND	3.43	1.42	1.37
22	C	513	CLA	C1D-ND	3.43	1.42	1.37
36	c	519	DGD	O6E-C1E	3.43	1.50	1.41
22	c	504	CLA	C1D-ND	3.43	1.42	1.37
22	c	506	CLA	C1D-ND	3.43	1.42	1.37
22	6	305	CLA	C1D-ND	3.42	1.42	1.37
22	2	307	CLA	C1D-ND	3.42	1.42	1.37
22	B	602	CLA	C1D-ND	3.42	1.42	1.37
22	1	306	CLA	C1D-ND	3.42	1.42	1.37
22	C	507	CLA	C1D-ND	3.42	1.42	1.37
22	Q	301	CLA	C4D-ND	-3.42	1.33	1.37
22	s	309	CLA	C1D-ND	3.42	1.42	1.37
22	5	303	CLA	C1D-ND	3.42	1.42	1.37
31	b	618	BCR	C15-C14	3.42	1.54	1.43
22	B	613	CLA	C4D-ND	-3.42	1.33	1.37
22	B	617	CLA	C1D-ND	3.41	1.42	1.37
22	v	302	CLA	C4D-ND	-3.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	308	CLA	C1D-ND	3.41	1.42	1.37
31	C	518	BCR	C27-C26	-3.41	1.44	1.51
26	U	316	CHL	OBD-CAD	3.41	1.28	1.22
31	A	409	BCR	C24-C25	3.41	1.57	1.45
26	p	318	CHL	OBD-CAD	3.41	1.28	1.22
22	p	302	CLA	C1D-ND	3.41	1.42	1.37
22	X	202	CLA	C1D-ND	3.41	1.42	1.37
26	q	315	CHL	OBD-CAD	3.41	1.28	1.22
22	A	405	CLA	C4D-ND	-3.40	1.33	1.37
22	c	507	CLA	C4D-ND	-3.40	1.33	1.37
22	b	603	CLA	C1D-ND	3.40	1.42	1.37
26	3	315	CHL	OBD-CAD	3.40	1.28	1.22
22	2	303	CLA	C1D-ND	3.40	1.42	1.37
22	U	303	CLA	C1D-ND	3.39	1.42	1.37
22	C	508	CLA	C4D-ND	-3.39	1.33	1.37
22	B	609	CLA	C4D-ND	-3.39	1.33	1.37
22	c	504	CLA	C4D-ND	-3.39	1.33	1.37
22	S	308	CLA	C1D-ND	3.39	1.42	1.37
26	Q	316	CHL	OBD-CAD	3.39	1.28	1.22
22	2	301	CLA	C4D-ND	-3.39	1.33	1.37
22	B	606	CLA	C1D-ND	3.39	1.41	1.37
22	b	614	CLA	C1D-ND	3.38	1.41	1.37
22	B	614	CLA	C1D-ND	3.38	1.41	1.37
22	b	615	CLA	C1D-ND	3.38	1.41	1.37
31	b	618	BCR	C12-C13	3.38	1.53	1.45
22	3	301	CLA	C4D-ND	-3.38	1.33	1.37
22	u	304	CLA	C1D-ND	3.37	1.41	1.37
22	C	505	CLA	C4D-ND	-3.37	1.33	1.37
22	C	506	CLA	C4D-ND	-3.37	1.33	1.37
22	q	301	CLA	C4D-ND	-3.37	1.33	1.37
22	P	302	CLA	C1D-ND	3.36	1.41	1.37
26	P	315	CHL	MG-NA	-3.36	1.98	2.06
22	b	612	CLA	C1D-ND	3.36	1.41	1.37
22	B	606	CLA	C4D-ND	-3.36	1.33	1.37
22	b	606	CLA	C1D-ND	3.36	1.41	1.37
22	B	616	CLA	C1D-ND	3.36	1.41	1.37
22	c	514	CLA	C4D-ND	-3.36	1.33	1.37
26	u	317	CHL	OBD-CAD	3.36	1.28	1.22
26	n	317	CHL	OBD-CAD	3.36	1.28	1.22
22	5	305	CLA	C3D-C4D	3.35	1.51	1.44
26	R	317	CHL	OBD-CAD	3.35	1.28	1.22
22	V	302	CLA	C4D-ND	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	C4D-ND	-3.35	1.33	1.37
36	C	520	DGD	O6D-C1D	3.35	1.50	1.41
31	X	201	BCR	C24-C25	3.35	1.57	1.45
36	c	518	DGD	O6D-C1D	3.35	1.50	1.41
22	c	505	CLA	C4D-ND	-3.35	1.33	1.37
31	b	620	BCR	C24-C25	3.35	1.57	1.45
22	B	603	CLA	C1D-ND	3.35	1.41	1.37
22	B	614	CLA	C4D-ND	-3.35	1.33	1.37
22	b	602	CLA	C1D-ND	3.35	1.41	1.37
22	p	306	CLA	C3D-C4D	3.35	1.51	1.44
31	b	618	BCR	C27-C26	-3.35	1.44	1.51
31	x	202	BCR	C24-C25	3.35	1.57	1.45
22	d	402	CLA	C4D-ND	-3.34	1.33	1.37
31	b	619	BCR	C24-C25	3.34	1.57	1.45
22	B	615	CLA	C1D-ND	3.34	1.41	1.37
22	c	506	CLA	C4D-ND	-3.34	1.33	1.37
22	4	304	CLA	C1D-ND	3.34	1.41	1.37
31	b	620	BCR	C27-C26	-3.34	1.44	1.51
22	c	503	CLA	C1D-ND	3.34	1.41	1.37
22	c	511	CLA	C1D-ND	3.34	1.41	1.37
31	A	409	BCR	C27-C26	-3.34	1.44	1.51
31	B	619	BCR	C24-C25	3.33	1.56	1.45
22	A	406	CLA	C4D-ND	-3.33	1.33	1.37
22	b	606	CLA	C4D-ND	-3.33	1.33	1.37
22	B	617	CLA	C4D-ND	-3.33	1.33	1.37
31	C	518	BCR	C24-C25	3.33	1.56	1.45
31	B	620	BCR	C24-C25	3.33	1.56	1.45
22	1	301	CLA	C4D-ND	-3.33	1.33	1.37
22	B	612	CLA	C1D-ND	3.33	1.41	1.37
22	c	513	CLA	C4D-ND	-3.33	1.33	1.37
22	C	514	CLA	C4D-ND	-3.33	1.33	1.37
22	u	305	CLA	C4D-ND	-3.33	1.33	1.37
31	c	516	BCR	C24-C25	3.33	1.56	1.45
22	p	302	CLA	C4D-ND	-3.33	1.33	1.37
31	B	618	BCR	C27-C26	-3.32	1.44	1.51
31	T	101	BCR	C37-C22	3.32	1.57	1.50
22	4	301	CLA	C4D-ND	-3.32	1.33	1.37
22	b	614	CLA	C4D-ND	-3.32	1.33	1.37
22	D	403	CLA	C4D-ND	-3.32	1.33	1.37
22	b	602	CLA	C4D-ND	-3.32	1.33	1.37
22	C	504	CLA	C1D-ND	3.31	1.41	1.37
22	C	515	CLA	C4D-ND	-3.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	408	CLA	C4D-ND	-3.31	1.33	1.37
36	J	101	DGD	O2G-C1B	3.31	1.43	1.34
22	a	406	CLA	C4D-ND	-3.31	1.33	1.37
22	a	408	CLA	C4D-ND	-3.31	1.33	1.37
22	C	512	CLA	C1D-ND	3.31	1.41	1.37
22	6	302	CLA	C4D-ND	-3.31	1.33	1.37
22	A	404	CLA	C1D-ND	3.30	1.41	1.37
31	B	620	BCR	C27-C26	-3.30	1.44	1.51
22	5	301	CLA	C4D-ND	-3.30	1.33	1.37
22	G	301	CLA	C4D-ND	-3.30	1.33	1.37
22	s	301	CLA	CHC-C1C	3.30	1.43	1.35
22	u	304	CLA	C4D-ND	-3.30	1.33	1.37
26	q	314	CHL	OBD-CAD	3.30	1.28	1.22
31	a	409	BCR	C27-C26	-3.30	1.44	1.51
22	4	304	CLA	C4D-ND	-3.29	1.33	1.37
31	C	516	BCR	C24-C25	3.29	1.56	1.45
22	b	613	CLA	C1D-ND	3.29	1.41	1.37
22	n	305	CLA	C3D-C4D	3.29	1.51	1.44
22	C	510	CLA	CMB-C2B	-3.29	1.44	1.51
22	c	509	CLA	CMB-C2B	-3.28	1.44	1.51
22	c	514	CLA	C1D-ND	3.28	1.41	1.37
22	4	303	CLA	C4D-ND	-3.28	1.33	1.37
22	v	301	CLA	C4D-ND	-3.28	1.33	1.37
22	B	602	CLA	C4D-ND	-3.28	1.33	1.37
31	k	101	BCR	C27-C26	-3.28	1.44	1.51
22	V	301	CLA	C4D-ND	-3.27	1.33	1.37
22	v	307	CLA	C4D-ND	-3.27	1.33	1.37
22	u	306	CLA	C4D-ND	-3.27	1.33	1.37
31	t	101	BCR	C27-C26	-3.27	1.44	1.51
22	C	503	CLA	C1D-ND	3.27	1.41	1.37
22	S	301	CLA	CHC-C1C	3.27	1.43	1.35
22	C	514	CLA	C1D-ND	3.27	1.41	1.37
22	B	603	CLA	C4D-ND	-3.27	1.33	1.37
22	C	515	CLA	C1D-ND	3.27	1.41	1.37
31	z	101	BCR	C24-C25	3.27	1.56	1.45
22	c	507	CLA	CMB-C2B	-3.27	1.44	1.51
22	s	307	CLA	C4D-ND	-3.27	1.33	1.37
31	t	101	BCR	C37-C22	3.26	1.57	1.50
22	1	304	CLA	C4D-ND	-3.26	1.33	1.37
22	u	301	CLA	C4D-ND	-3.26	1.33	1.37
26	Q	315	CHL	OBD-CAD	3.26	1.28	1.22
22	U	301	CLA	C4D-ND	-3.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	C4D-ND	-3.26	1.33	1.37
22	3	302	CLA	C4D-ND	-3.26	1.33	1.37
36	c	519	DGD	O2G-C1B	3.26	1.43	1.34
22	2	307	CLA	C4D-ND	-3.26	1.33	1.37
22	b	603	CLA	C4D-ND	-3.25	1.33	1.37
22	2	302	CLA	C4D-ND	-3.25	1.33	1.37
22	g	301	CLA	C4D-ND	-3.25	1.33	1.37
22	x	201	CLA	C4D-ND	-3.25	1.33	1.37
22	C	508	CLA	CMB-C2B	-3.25	1.44	1.51
22	5	307	CLA	C4D-ND	-3.25	1.33	1.37
22	U	302	CLA	C4D-ND	-3.25	1.33	1.37
22	2	305	CLA	C3D-C4D	3.24	1.51	1.44
26	G	315	CHL	OBD-CAD	3.24	1.28	1.22
22	X	202	CLA	C4D-ND	-3.24	1.33	1.37
22	c	502	CLA	C1D-ND	3.24	1.41	1.37
22	V	307	CLA	C4D-ND	-3.24	1.33	1.37
22	P	302	CLA	C4D-ND	-3.24	1.33	1.37
26	N	316	CHL	OBD-CAD	3.24	1.28	1.22
22	B	612	CLA	C4D-ND	-3.24	1.33	1.37
22	b	604	CLA	C4D-ND	-3.24	1.33	1.37
22	1	304	CLA	C1D-ND	3.24	1.41	1.37
22	C	513	CLA	C4D-ND	-3.23	1.33	1.37
31	x	202	BCR	C27-C26	-3.23	1.44	1.51
31	K	101	BCR	C27-C26	-3.23	1.44	1.51
22	S	308	CLA	C4D-ND	-3.23	1.33	1.37
22	b	607	CLA	C4D-ND	-3.23	1.33	1.37
22	C	511	CLA	C1D-ND	3.23	1.41	1.37
31	X	201	BCR	C27-C26	-3.23	1.44	1.51
31	T	101	BCR	C20-C21	3.23	1.53	1.43
36	c	517	DGD	O6E-C1E	3.23	1.50	1.41
22	1	307	CLA	C4D-ND	-3.22	1.33	1.37
22	U	305	CLA	C4D-ND	-3.22	1.33	1.37
31	T	101	BCR	C27-C26	-3.22	1.44	1.51
22	B	608	CLA	C4D-ND	-3.22	1.33	1.37
22	b	617	CLA	C4D-ND	-3.22	1.33	1.37
22	u	301	CLA	CHC-C1C	3.22	1.43	1.35
22	B	604	CLA	C4D-ND	-3.22	1.33	1.37
22	1	303	CLA	C4D-ND	-3.22	1.33	1.37
36	b	601	DGD	O6D-C1D	3.22	1.50	1.41
22	S	305	CLA	C4D-ND	-3.21	1.33	1.37
22	U	301	CLA	CHC-C1C	3.21	1.43	1.35
36	B	601	DGD	O6D-C1D	3.21	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	C1D-ND	3.21	1.41	1.37
31	D	404	BCR	C27-C26	-3.21	1.44	1.51
22	s	305	CLA	C4D-ND	-3.21	1.33	1.37
36	C	520	DGD	O2G-C1B	3.21	1.43	1.34
22	Q	301	CLA	CHC-C1C	3.20	1.43	1.35
22	N	304	CLA	CHC-C1C	3.20	1.43	1.35
22	a	404	CLA	C1D-ND	3.20	1.41	1.37
31	C	517	BCR	C24-C25	3.20	1.56	1.45
36	C	519	DGD	O6E-C1E	3.20	1.50	1.41
31	t	101	BCR	C20-C21	3.20	1.53	1.43
31	c	515	BCR	C24-C25	3.20	1.56	1.45
22	c	508	CLA	C4D-ND	-3.20	1.33	1.37
22	b	611	CLA	C4D-ND	-3.20	1.33	1.37
26	g	315	CHL	OBD-CAD	3.20	1.28	1.22
22	1	306	CLA	C4D-ND	-3.20	1.33	1.37
22	b	610	CLA	C4D-ND	-3.19	1.33	1.37
31	k	101	BCR	C24-C25	3.19	1.56	1.45
22	B	613	CLA	C1D-ND	3.19	1.41	1.37
22	1	302	CLA	C4D-ND	-3.19	1.33	1.37
22	V	304	CLA	CHC-C1C	3.19	1.43	1.35
22	B	607	CLA	C4D-ND	-3.19	1.33	1.37
22	v	304	CLA	C4D-ND	-3.19	1.33	1.37
22	V	305	CLA	C4D-ND	-3.19	1.33	1.37
22	B	610	CLA	C4D-ND	-3.19	1.33	1.37
31	K	101	BCR	C24-C25	3.19	1.56	1.45
22	4	307	CLA	C4D-ND	-3.19	1.33	1.37
22	p	308	CLA	C4D-ND	-3.19	1.33	1.37
26	2	314	CHL	C3D-C2D	3.19	1.47	1.39
26	P	315	CHL	C3D-C2D	3.19	1.47	1.39
31	B	618	BCR	C24-C25	3.18	1.56	1.45
22	P	302	CLA	CHC-C1C	3.18	1.43	1.35
22	P	303	CLA	C4D-ND	-3.18	1.33	1.37
22	C	508	CLA	C1D-ND	3.18	1.41	1.37
22	c	507	CLA	C1D-ND	3.18	1.41	1.37
33	d	404	PL9	C6-C5	3.18	1.51	1.35
22	U	308	CLA	C4D-ND	-3.18	1.33	1.37
22	S	307	CLA	C4D-ND	-3.18	1.33	1.37
22	U	306	CLA	C4D-ND	-3.18	1.33	1.37
36	c	518	DGD	O2G-C1B	3.18	1.43	1.34
22	s	301	CLA	C1D-ND	3.18	1.41	1.37
22	c	510	CLA	C1D-ND	3.18	1.41	1.37
22	P	308	CLA	C4D-ND	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C4D-ND	-3.18	1.33	1.37
22	r	606	CLA	C4D-ND	-3.18	1.33	1.37
22	p	303	CLA	C4D-ND	-3.18	1.33	1.37
22	N	301	CLA	CHC-C1C	3.18	1.43	1.35
22	c	512	CLA	C4D-ND	-3.17	1.33	1.37
31	d	403	BCR	C27-C26	-3.17	1.44	1.51
33	D	405	PL9	C6-C5	3.17	1.51	1.35
22	U	304	CLA	C1D-ND	3.17	1.41	1.37
22	g	304	CLA	CHC-C1C	3.17	1.43	1.35
22	s	306	CLA	C4D-ND	-3.17	1.33	1.37
22	c	511	CLA	C4D-ND	-3.17	1.33	1.37
26	p	315	CHL	MG-NA	-3.17	1.98	2.06
22	6	303	CLA	C4D-ND	-3.17	1.33	1.37
22	g	303	CLA	C4D-ND	-3.17	1.33	1.37
31	D	404	BCR	C37-C22	3.17	1.57	1.50
22	n	301	CLA	CHC-C1C	3.17	1.43	1.35
22	Q	308	CLA	C4D-ND	-3.17	1.33	1.37
22	C	512	CLA	C4D-ND	-3.17	1.33	1.37
22	b	609	CLA	C1D-ND	3.16	1.41	1.37
32	M	101	SQD	O48-C23	3.16	1.42	1.33
22	s	301	CLA	C4D-ND	-3.16	1.33	1.37
22	5	306	CLA	C4D-ND	-3.16	1.33	1.37
22	R	307	CLA	C4D-ND	-3.16	1.33	1.37
33	a	411	PL9	C6-C1	3.16	1.53	1.45
22	n	304	CLA	CHC-C1C	3.16	1.43	1.35
33	A	410	PL9	C6-C1	3.16	1.53	1.45
22	r	602	CLA	C4D-ND	-3.16	1.33	1.37
34	d	407	LMG	O7-C10	3.16	1.43	1.34
22	R	303	CLA	C4D-ND	-3.16	1.33	1.37
22	4	302	CLA	C4D-ND	-3.16	1.33	1.37
22	S	301	CLA	C1D-ND	3.16	1.41	1.37
22	Q	307	CLA	C4D-ND	-3.15	1.33	1.37
22	U	307	CLA	C4D-ND	-3.15	1.33	1.37
31	B	619	BCR	C37-C22	3.15	1.57	1.50
36	c	517	DGD	O6D-C1D	3.15	1.49	1.41
22	6	308	CLA	C4D-ND	-3.15	1.33	1.37
22	v	304	CLA	CHC-C1C	3.15	1.43	1.35
22	p	302	CLA	CHC-C1C	3.15	1.43	1.35
37	e	101	HEM	CAB-C3B	3.15	1.56	1.47
22	1	305	CLA	C4D-ND	-3.15	1.33	1.37
22	v	303	CLA	C4D-ND	-3.15	1.33	1.37
31	b	618	BCR	C24-C25	3.15	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	611	CLA	C4D-ND	-3.15	1.33	1.37
32	m	101	SQD	O48-C23	3.14	1.42	1.33
22	3	308	CLA	C4D-ND	-3.14	1.33	1.37
26	6	317	CHL	C1D-C2D	3.14	1.51	1.45
22	V	304	CLA	C4D-ND	-3.14	1.33	1.37
31	c	516	BCR	C20-C21	3.14	1.53	1.43
22	Q	305	CLA	C4D-ND	-3.14	1.33	1.37
22	c	502	CLA	C4D-ND	-3.14	1.33	1.37
22	4	305	CLA	C4D-ND	-3.14	1.33	1.37
22	v	308	CLA	C4D-ND	-3.14	1.33	1.37
22	C	503	CLA	C4D-ND	-3.14	1.33	1.37
22	C	509	CLA	C4D-ND	-3.14	1.33	1.37
22	q	301	CLA	CHC-C1C	3.14	1.43	1.35
22	4	306	CLA	C4D-ND	-3.14	1.33	1.37
22	B	609	CLA	C1D-ND	3.14	1.41	1.37
37	E	101	HEM	CAB-C3B	3.14	1.56	1.47
22	u	308	CLA	C4D-ND	-3.14	1.33	1.37
22	v	305	CLA	C4D-ND	-3.13	1.33	1.37
34	D	408	LMG	O7-C10	3.13	1.43	1.34
36	C	519	DGD	O6D-C1D	3.13	1.49	1.41
36	a	416	DGD	O2G-C1B	3.13	1.43	1.34
31	d	403	BCR	C37-C22	3.13	1.57	1.50
22	S	306	CLA	C4D-ND	-3.13	1.33	1.37
22	q	307	CLA	C4D-ND	-3.13	1.33	1.37
22	N	301	CLA	C4D-ND	-3.13	1.33	1.37
22	S	301	CLA	C4D-ND	-3.13	1.33	1.37
32	a	410	SQD	O48-C23	3.13	1.42	1.33
22	q	303	CLA	C4D-ND	-3.13	1.33	1.37
36	A	414	DGD	O2G-C1B	3.13	1.43	1.34
22	Q	303	CLA	C4D-ND	-3.13	1.33	1.37
22	s	308	CLA	C4D-ND	-3.13	1.33	1.37
22	N	308	CLA	CHC-C1C	3.13	1.43	1.35
31	C	518	BCR	C20-C21	3.13	1.53	1.43
22	S	305	CLA	CHC-C1C	3.13	1.43	1.35
32	C	501	SQD	O48-C23	3.12	1.42	1.33
22	u	302	CLA	C4D-ND	-3.12	1.33	1.37
22	b	612	CLA	CHC-C1C	3.12	1.43	1.35
31	b	619	BCR	C37-C22	3.12	1.57	1.50
22	b	615	CLA	C4D-ND	-3.12	1.33	1.37
26	3	316	CHL	C1D-C2D	3.12	1.51	1.45
22	6	304	CLA	C4D-ND	-3.12	1.33	1.37
26	6	313	CHL	C3D-C2D	3.12	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	312	CHL	C3D-C2D	3.12	1.47	1.39
22	V	308	CLA	C4D-ND	-3.12	1.33	1.37
22	G	302	CLA	C4D-ND	-3.12	1.33	1.37
22	3	307	CLA	C4D-ND	-3.11	1.33	1.37
22	B	612	CLA	CHC-C1C	3.11	1.42	1.35
22	3	306	CLA	C4D-ND	-3.11	1.33	1.37
26	S	315	CHL	C3D-C2D	3.11	1.47	1.39
22	G	303	CLA	CHC-C1C	3.11	1.42	1.35
22	B	615	CLA	C4D-ND	-3.11	1.33	1.37
22	p	304	CLA	C4D-ND	-3.11	1.33	1.37
33	a	411	PL9	C5-C4	3.11	1.53	1.45
22	G	308	CLA	C4D-ND	-3.11	1.33	1.37
22	G	304	CLA	CHC-C1C	3.11	1.42	1.35
22	q	307	CLA	CHC-C1C	3.11	1.42	1.35
22	2	304	CLA	CHC-C1C	3.11	1.42	1.35
22	3	303	CLA	C4D-ND	-3.10	1.33	1.37
31	b	620	BCR	C37-C22	3.10	1.57	1.50
22	n	303	CLA	C4D-ND	-3.10	1.33	1.37
31	K	101	BCR	C37-C22	3.10	1.57	1.50
22	g	308	CLA	C4D-ND	-3.10	1.33	1.37
22	P	306	CLA	C3D-C4D	3.10	1.51	1.44
33	A	410	PL9	C5-C4	3.10	1.53	1.45
22	U	304	CLA	C4D-ND	-3.10	1.33	1.37
22	U	303	CLA	C4D-ND	-3.10	1.33	1.37
27	R	301	NEX	C7-C8	-3.10	1.26	1.32
22	q	308	CLA	C4D-ND	-3.10	1.33	1.37
22	c	503	CLA	CMB-C2B	-3.10	1.45	1.51
22	5	307	CLA	CHC-C1C	3.10	1.42	1.35
22	Q	307	CLA	CHC-C1C	3.09	1.42	1.35
22	u	307	CLA	C4D-ND	-3.09	1.33	1.37
22	s	305	CLA	CHC-C1C	3.09	1.42	1.35
22	6	307	CLA	C4D-ND	-3.09	1.33	1.37
26	3	312	CHL	C1D-C2D	3.09	1.51	1.45
22	s	309	CLA	C4D-ND	-3.09	1.33	1.37
22	n	302	CLA	C4D-ND	-3.09	1.33	1.37
31	b	620	BCR	C20-C21	3.09	1.53	1.43
26	P	315	CHL	C1D-C2D	3.09	1.51	1.45
22	V	307	CLA	CHC-C1C	3.09	1.42	1.35
26	s	316	CHL	C1D-C2D	3.09	1.51	1.45
26	p	315	CHL	C3D-C2D	3.08	1.47	1.39
22	u	303	CLA	CMB-C2B	-3.08	1.45	1.51
22	G	306	CLA	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	q	305	CLA	C4D-ND	-3.08	1.33	1.37
31	X	201	BCR	C37-C22	3.08	1.57	1.50
22	S	309	CLA	C4D-ND	-3.08	1.33	1.37
33	a	411	PL9	C2-C1	3.08	1.53	1.45
22	r	604	CLA	C4D-ND	-3.08	1.33	1.37
22	2	303	CLA	C4D-ND	-3.08	1.33	1.37
27	2	319	NEX	C7-C8	-3.08	1.26	1.32
22	2	306	CLA	C4D-ND	-3.08	1.33	1.37
22	2	308	CLA	C4D-ND	-3.08	1.33	1.37
31	B	620	BCR	C37-C22	3.08	1.57	1.50
26	s	315	CHL	C3D-C2D	3.08	1.47	1.39
22	5	303	CLA	C4D-ND	-3.08	1.33	1.37
22	v	307	CLA	CHC-C1C	3.08	1.42	1.35
22	G	303	CLA	C4D-ND	-3.08	1.33	1.37
31	a	409	BCR	C37-C22	3.08	1.57	1.50
22	Q	304	CLA	CHC-C1C	3.07	1.42	1.35
22	6	309	CLA	CHC-C1C	3.07	1.42	1.35
31	k	101	BCR	C37-C22	3.07	1.57	1.50
31	x	202	BCR	C37-C22	3.07	1.57	1.50
22	6	305	CLA	CHC-C1C	3.07	1.42	1.35
31	X	201	BCR	C20-C21	3.07	1.53	1.43
22	N	302	CLA	C4D-ND	-3.07	1.33	1.37
27	r	618	NEX	C7-C8	-3.07	1.26	1.32
22	G	308	CLA	CHC-C1C	3.07	1.42	1.35
22	P	309	CLA	C4D-ND	-3.07	1.33	1.37
22	g	308	CLA	CHC-C1C	3.07	1.42	1.35
22	g	301	CLA	CHC-C1C	3.07	1.42	1.35
22	V	303	CLA	C4D-ND	-3.06	1.33	1.37
33	A	410	PL9	C2-C1	3.06	1.53	1.45
22	G	301	CLA	CHC-C1C	3.06	1.42	1.35
26	5	314	CHL	C3D-C2D	3.06	1.47	1.39
31	D	404	BCR	C20-C21	3.06	1.52	1.43
22	6	302	CLA	CHC-C1C	3.06	1.42	1.35
22	R	305	CLA	C4D-ND	-3.06	1.33	1.37
22	3	304	CLA	CHC-C1C	3.06	1.42	1.35
31	A	409	BCR	C37-C22	3.06	1.57	1.50
27	U	318	NEX	C7-C8	-3.06	1.26	1.32
36	C	519	DGD	O2G-C1B	3.06	1.42	1.34
22	g	302	CLA	C4D-ND	-3.06	1.33	1.37
22	n	301	CLA	C4D-ND	-3.06	1.33	1.37
22	3	308	CLA	CHC-C1C	3.06	1.42	1.35
22	s	304	CLA	CHC-C1C	3.06	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	308	CLA	C4D-ND	-3.06	1.33	1.37
22	C	504	CLA	CMB-C2B	-3.06	1.45	1.51
22	5	301	CLA	CHC-C1C	3.06	1.42	1.35
22	V	306	CLA	C4D-ND	-3.06	1.33	1.37
22	C	506	CLA	C1D-ND	3.06	1.41	1.37
22	6	309	CLA	C4D-ND	-3.05	1.33	1.37
22	v	306	CLA	C4D-ND	-3.05	1.33	1.37
22	q	302	CLA	C4D-ND	-3.05	1.33	1.37
22	Q	305	CLA	CHC-C1C	3.05	1.42	1.35
22	p	309	CLA	C4D-ND	-3.05	1.33	1.37
22	2	307	CLA	CHC-C1C	3.05	1.42	1.35
22	A	408	CLA	CHC-C1C	3.05	1.42	1.35
22	4	308	CLA	C4D-ND	-3.05	1.33	1.37
26	q	312	CHL	C3D-C2D	3.05	1.47	1.39
22	p	307	CLA	C4D-ND	-3.05	1.33	1.37
22	n	303	CLA	CHC-C1C	3.04	1.42	1.35
31	x	202	BCR	C20-C21	3.04	1.52	1.43
22	u	303	CLA	C4D-ND	-3.04	1.33	1.37
22	n	307	CLA	CHC-C1C	3.04	1.42	1.35
22	S	309	CLA	CHC-C1C	3.04	1.42	1.35
26	N	314	CHL	C3D-C2D	3.04	1.47	1.39
22	5	304	CLA	CHC-C1C	3.04	1.42	1.35
31	B	620	BCR	C20-C21	3.04	1.52	1.43
22	q	306	CLA	C4D-ND	-3.04	1.33	1.37
22	N	303	CLA	C4D-ND	-3.04	1.33	1.37
31	z	101	BCR	C37-C22	3.04	1.57	1.50
31	d	403	BCR	C20-C21	3.04	1.52	1.43
22	q	305	CLA	CHC-C1C	3.04	1.42	1.35
22	u	305	CLA	CHC-C1C	3.04	1.42	1.35
26	S	316	CHL	C1D-C2D	3.04	1.51	1.45
22	r	605	CLA	CHC-C1C	3.04	1.42	1.35
22	v	308	CLA	CHC-C1C	3.03	1.42	1.35
22	2	301	CLA	CHC-C1C	3.03	1.42	1.35
22	u	304	CLA	CHC-C1C	3.03	1.42	1.35
31	c	515	BCR	C37-C22	3.03	1.57	1.50
24	Q	309	XAT	C4-C3	3.03	1.56	1.52
22	Q	308	CLA	CHC-C1C	3.03	1.42	1.35
22	S	303	CLA	C4D-ND	-3.03	1.33	1.37
31	C	517	BCR	C37-C22	3.03	1.57	1.50
31	C	516	BCR	C37-C22	3.03	1.57	1.50
22	r	601	CLA	CHC-C1C	3.03	1.42	1.35
26	6	313	CHL	C1D-C2D	3.03	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	305	CLA	CHC-C1C	3.03	1.42	1.35
22	S	304	CLA	C4D-ND	-3.03	1.33	1.37
22	P	305	CLA	C4D-ND	-3.03	1.33	1.37
22	r	603	CLA	CHC-C1C	3.03	1.42	1.35
22	V	301	CLA	CHC-C1C	3.03	1.42	1.35
36	B	601	DGD	O2G-C1B	3.03	1.42	1.34
27	r	617	NEX	C7-C8	-3.02	1.26	1.32
22	4	301	CLA	CHC-C1C	3.02	1.42	1.35
22	R	306	CLA	CHC-C1C	3.02	1.42	1.35
36	c	517	DGD	O2G-C1B	3.02	1.42	1.34
22	1	308	CLA	C4D-ND	-3.02	1.33	1.37
22	2	304	CLA	C4D-ND	-3.02	1.33	1.37
24	N	311	XAT	C38-C25	3.02	1.56	1.51
26	V	314	CHL	C3D-C2D	3.02	1.47	1.39
26	n	314	CHL	C3D-C2D	3.02	1.47	1.39
22	r	606	CLA	CHC-C1C	3.02	1.42	1.35
22	g	303	CLA	CHC-C1C	3.02	1.42	1.35
31	C	516	BCR	C20-C21	3.02	1.52	1.43
22	6	308	CLA	CHC-C1C	3.02	1.42	1.35
22	B	610	CLA	CHC-C1C	3.02	1.42	1.35
26	V	318	CHL	C3D-C2D	3.02	1.47	1.39
31	z	101	BCR	C20-C21	3.02	1.52	1.43
22	R	303	CLA	CHC-C1C	3.02	1.42	1.35
22	P	307	CLA	C4D-ND	-3.01	1.33	1.37
26	n	314	CHL	MG-NA	-3.01	1.99	2.06
22	b	610	CLA	CHC-C1C	3.01	1.42	1.35
22	n	307	CLA	C4D-ND	-3.01	1.33	1.37
22	P	309	CLA	CHC-C1C	3.01	1.42	1.35
22	v	302	CLA	CHC-C1C	3.01	1.42	1.35
22	Q	306	CLA	C4D-ND	-3.01	1.33	1.37
22	g	306	CLA	C4D-ND	-3.01	1.33	1.37
22	q	308	CLA	CHC-C1C	3.01	1.42	1.35
22	P	304	CLA	C4D-ND	-3.01	1.33	1.37
22	S	304	CLA	CHC-C1C	3.01	1.42	1.35
22	U	305	CLA	CHC-C1C	3.01	1.42	1.35
26	V	315	CHL	C3D-C2D	3.01	1.47	1.39
34	w	201	LMG	O7-C10	3.01	1.42	1.34
22	3	307	CLA	CHC-C1C	3.01	1.42	1.35
22	1	307	CLA	CHC-C1C	3.01	1.42	1.35
26	G	312	CHL	C3D-C2D	3.01	1.47	1.39
22	r	602	CLA	CHC-C1C	3.01	1.42	1.35
22	B	613	CLA	CHC-C1C	3.01	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	619	BCR	C20-C21	3.01	1.52	1.43
24	2	311	XAT	C24-C23	3.01	1.56	1.52
22	c	514	CLA	CHC-C1C	3.01	1.42	1.35
26	g	312	CHL	C3D-C2D	3.01	1.47	1.39
22	q	304	CLA	CHC-C1C	3.01	1.42	1.35
22	G	307	CLA	CHC-C1C	3.01	1.42	1.35
22	3	301	CLA	CHC-C1C	3.01	1.42	1.35
22	V	305	CLA	CHC-C1C	3.01	1.42	1.35
22	c	505	CLA	C1D-ND	3.00	1.41	1.37
26	v	318	CHL	C3D-C2D	3.00	1.47	1.39
22	C	510	CLA	C1D-ND	3.00	1.41	1.37
24	5	311	XAT	C24-C23	3.00	1.56	1.52
22	N	304	CLA	C4D-ND	-3.00	1.33	1.37
26	1	314	CHL	C3D-C2D	3.00	1.47	1.39
22	p	308	CLA	CHC-C1C	3.00	1.42	1.35
22	b	615	CLA	CHC-C1C	3.00	1.42	1.35
22	a	408	CLA	CHC-C1C	3.00	1.42	1.35
22	P	308	CLA	CHC-C1C	3.00	1.42	1.35
31	b	619	BCR	C20-C21	3.00	1.52	1.43
22	1	308	CLA	CHC-C1C	3.00	1.42	1.35
27	5	319	NEX	C7-C8	-3.00	1.27	1.32
22	V	302	CLA	CHC-C1C	3.00	1.42	1.35
22	p	309	CLA	CHC-C1C	3.00	1.42	1.35
22	N	307	CLA	CHC-C1C	3.00	1.42	1.35
22	2	308	CLA	CHC-C1C	3.00	1.42	1.35
22	3	305	CLA	C4D-ND	-3.00	1.33	1.37
22	4	307	CLA	CHC-C1C	3.00	1.42	1.35
22	v	301	CLA	CHC-C1C	3.00	1.42	1.35
27	n	319	NEX	C7-C8	-3.00	1.27	1.32
31	B	618	BCR	C37-C22	3.00	1.57	1.50
22	3	305	CLA	CHC-C1C	3.00	1.42	1.35
22	q	303	CLA	CHC-C1C	3.00	1.42	1.35
22	C	510	CLA	CHC-C1C	3.00	1.42	1.35
24	v	311	XAT	C4-C3	3.00	1.56	1.52
22	6	305	CLA	C4D-ND	-3.00	1.33	1.37
26	Q	312	CHL	C3D-C2D	2.99	1.47	1.39
24	Q	309	XAT	C38-C25	2.99	1.56	1.51
22	6	304	CLA	CHC-C1C	2.99	1.42	1.35
22	6	306	CLA	CHC-C1C	2.99	1.42	1.35
36	b	601	DGD	O2G-C1B	2.99	1.42	1.34
22	c	508	CLA	C1D-ND	2.99	1.41	1.37
22	c	509	CLA	C1D-ND	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	102	SQD	O48-C23	2.99	1.42	1.33
22	G	305	CLA	CHC-C1C	2.99	1.42	1.35
22	g	306	CLA	CHC-C1C	2.99	1.42	1.35
22	b	613	CLA	CHC-C1C	2.99	1.42	1.35
22	1	301	CLA	CHC-C1C	2.99	1.42	1.35
26	S	315	CHL	C1D-C2D	2.99	1.51	1.45
26	6	314	CHL	C3D-C2D	2.99	1.47	1.39
22	p	305	CLA	C4D-ND	-2.98	1.33	1.37
22	g	307	CLA	C4D-ND	-2.98	1.33	1.37
31	b	618	BCR	C37-C22	2.98	1.57	1.50
22	4	308	CLA	CHC-C1C	2.98	1.42	1.35
22	R	307	CLA	CHC-C1C	2.98	1.42	1.35
22	U	303	CLA	CMB-C2B	-2.98	1.45	1.51
32	l	102	SQD	O48-C23	2.98	1.42	1.33
22	R	304	CLA	CHC-C1C	2.98	1.42	1.35
26	V	313	CHL	C1D-C2D	2.98	1.51	1.45
22	r	608	CLA	CHC-C1C	2.98	1.42	1.35
22	s	303	CLA	C4D-ND	-2.98	1.33	1.37
34	b	624	LMG	O7-C10	2.98	1.42	1.34
22	c	504	CLA	CHC-C1C	2.98	1.42	1.35
22	p	305	CLA	CHC-C1C	2.98	1.42	1.35
22	g	307	CLA	CHC-C1C	2.98	1.42	1.35
26	n	318	CHL	C3D-C2D	2.98	1.47	1.39
31	t	101	BCR	C7-C6	2.98	1.55	1.45
22	c	511	CLA	CHC-C1C	2.98	1.42	1.35
22	c	509	CLA	CHC-C1C	2.98	1.42	1.35
22	N	305	CLA	CHC-C1C	2.98	1.42	1.35
22	C	505	CLA	CHC-C1C	2.98	1.42	1.35
22	C	515	CLA	CHC-C1C	2.97	1.42	1.35
26	3	313	CHL	C3D-C2D	2.97	1.47	1.39
22	Q	302	CLA	C4D-ND	-2.97	1.33	1.37
22	4	303	CLA	CHC-C1C	2.97	1.42	1.35
22	U	304	CLA	CHC-C1C	2.97	1.42	1.35
22	R	309	CLA	CHC-C1C	2.97	1.42	1.35
22	3	304	CLA	C4D-ND	-2.97	1.33	1.37
26	p	315	CHL	C1D-C2D	2.97	1.51	1.45
22	U	308	CLA	CHC-C1C	2.97	1.42	1.35
22	s	304	CLA	C4D-ND	-2.97	1.33	1.37
22	S	308	CLA	CHC-C1C	2.97	1.42	1.35
22	N	308	CLA	C4D-ND	-2.97	1.33	1.37
32	A	412	SQD	O48-C23	2.97	1.42	1.33
24	q	309	XAT	C38-C25	2.97	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	624	LMG	O7-C10	2.96	1.42	1.34
30	A	407	PHO	CAC-C3C	-2.96	1.47	1.52
22	G	307	CLA	C4D-ND	-2.96	1.33	1.37
22	X	202	CLA	CHC-C1C	2.96	1.42	1.35
22	D	403	CLA	CHC-C1C	2.96	1.42	1.35
26	S	316	CHL	C3D-C2D	2.96	1.47	1.39
33	A	410	PL9	C3-C4	2.96	1.53	1.49
26	u	316	CHL	C1D-C2D	2.96	1.51	1.45
22	3	303	CLA	CHC-C1C	2.96	1.42	1.35
26	N	317	CHL	C3D-C2D	2.96	1.47	1.39
22	V	308	CLA	CHC-C1C	2.96	1.42	1.35
22	1	304	CLA	CHC-C1C	2.96	1.42	1.35
22	C	512	CLA	CHC-C1C	2.96	1.42	1.35
22	r	609	CLA	CHC-C1C	2.96	1.42	1.35
22	v	305	CLA	CHC-C1C	2.96	1.42	1.35
22	u	308	CLA	CHC-C1C	2.96	1.42	1.35
22	r	608	CLA	C4D-ND	-2.96	1.33	1.37
22	5	304	CLA	C4D-ND	-2.96	1.33	1.37
22	B	615	CLA	CHC-C1C	2.96	1.42	1.35
22	b	604	CLA	CHC-C1C	2.96	1.42	1.35
22	4	304	CLA	CHC-C1C	2.96	1.42	1.35
22	r	603	CLA	C4D-ND	-2.96	1.33	1.37
26	5	313	CHL	C3D-C2D	2.95	1.47	1.39
22	x	201	CLA	CHC-C1C	2.95	1.42	1.35
22	B	605	CLA	CMB-C2B	-2.95	1.45	1.51
31	T	101	BCR	C7-C6	2.95	1.55	1.45
22	n	308	CLA	CHC-C1C	2.95	1.42	1.35
26	s	316	CHL	C3D-C2D	2.95	1.47	1.39
22	r	604	CLA	CHC-C1C	2.95	1.42	1.35
22	4	305	CLA	CHC-C1C	2.95	1.42	1.35
22	5	302	CLA	CHC-C1C	2.95	1.42	1.35
26	P	317	CHL	C1D-C2D	2.95	1.51	1.45
22	s	308	CLA	CHC-C1C	2.95	1.42	1.35
22	N	306	CLA	CHC-C1C	2.95	1.42	1.35
22	n	306	CLA	C4D-ND	-2.95	1.33	1.37
22	S	302	CLA	C4D-ND	-2.95	1.33	1.37
22	b	605	CLA	CMB-C2B	-2.95	1.45	1.51
22	6	306	CLA	C4D-ND	-2.95	1.33	1.37
22	r	610	CLA	CHC-C1C	2.95	1.42	1.35
22	d	402	CLA	CHC-C1C	2.95	1.42	1.35
22	S	307	CLA	CHC-C1C	2.95	1.42	1.35
22	G	302	CLA	CHC-C1C	2.95	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	C1D-ND	2.95	1.41	1.37
24	p	312	XAT	C24-C23	2.94	1.56	1.52
22	V	303	CLA	CHC-C1C	2.94	1.42	1.35
22	n	304	CLA	C4D-ND	-2.94	1.33	1.37
22	B	604	CLA	CHC-C1C	2.94	1.42	1.35
32	l	102	SQD	O47-C7	2.94	1.42	1.34
24	V	311	XAT	C4-C3	2.94	1.56	1.52
24	q	309	XAT	C4-C3	2.94	1.56	1.52
32	L	102	SQD	O47-C7	2.94	1.42	1.34
22	c	502	CLA	CHC-C1C	2.94	1.42	1.35
22	R	302	CLA	C4D-ND	-2.94	1.33	1.37
24	Q	309	XAT	C24-C23	2.94	1.56	1.52
22	6	303	CLA	CHC-C1C	2.94	1.42	1.35
26	U	313	CHL	C1D-C2D	2.94	1.51	1.45
22	B	605	CLA	C4D-ND	-2.94	1.33	1.37
22	s	302	CLA	C4D-ND	-2.94	1.33	1.37
26	Q	312	CHL	C1D-C2D	2.94	1.51	1.45
22	3	306	CLA	CHC-C1C	2.94	1.42	1.35
22	N	303	CLA	CHC-C1C	2.94	1.42	1.35
24	6	310	XAT	C4-C3	2.94	1.56	1.52
22	R	305	CLA	CHC-C1C	2.94	1.42	1.35
22	R	311	CLA	CHC-C1C	2.94	1.42	1.35
22	N	307	CLA	C4D-ND	-2.94	1.33	1.37
24	1	311	XAT	C38-C25	2.94	1.56	1.51
22	5	308	CLA	CHC-C1C	2.94	1.42	1.35
22	n	306	CLA	CHC-C1C	2.94	1.42	1.35
22	R	308	CLA	CHC-C1C	2.94	1.42	1.35
22	b	609	CLA	CHC-C1C	2.94	1.42	1.35
22	p	303	CLA	CHC-C1C	2.93	1.42	1.35
22	Q	306	CLA	CHC-C1C	2.93	1.42	1.35
26	G	312	CHL	C1D-C2D	2.93	1.51	1.45
34	W	201	LMG	O7-C10	2.93	1.42	1.34
22	a	406	CLA	CHC-C1C	2.93	1.42	1.35
22	s	307	CLA	CHC-C1C	2.93	1.42	1.35
22	C	507	CLA	CHC-C1C	2.93	1.42	1.35
22	C	503	CLA	CHC-C1C	2.93	1.42	1.35
24	6	310	XAT	C38-C25	2.93	1.56	1.51
24	v	311	XAT	C38-C25	2.93	1.56	1.51
26	q	315	CHL	C1D-C2D	2.93	1.51	1.45
22	5	306	CLA	CHC-C1C	2.93	1.42	1.35
22	p	307	CLA	CHC-C1C	2.93	1.42	1.35
32	a	413	SQD	O48-C23	2.93	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	V	311	XAT	C38-C25	2.93	1.56	1.51
22	U	303	CLA	CHC-C1C	2.93	1.42	1.35
22	B	614	CLA	CHC-C1C	2.93	1.42	1.35
22	G	306	CLA	CHC-C1C	2.93	1.42	1.35
24	4	311	XAT	C38-C25	2.93	1.56	1.51
22	5	305	CLA	CHC-C1C	2.93	1.42	1.35
22	g	305	CLA	CHC-C1C	2.93	1.42	1.35
22	u	303	CLA	CHC-C1C	2.93	1.42	1.35
26	g	313	CHL	C3D-C2D	2.92	1.47	1.39
22	U	307	CLA	CHC-C1C	2.92	1.42	1.35
22	n	305	CLA	CHC-C1C	2.92	1.42	1.35
26	5	313	CHL	C1D-C2D	2.92	1.51	1.45
22	P	303	CLA	CHC-C1C	2.92	1.42	1.35
26	4	315	CHL	C3D-C2D	2.92	1.47	1.39
22	A	406	CLA	CHC-C1C	2.92	1.42	1.35
27	p	301	NEX	C7-C8	-2.92	1.27	1.32
26	p	316	CHL	C3D-C2D	2.92	1.47	1.39
26	P	316	CHL	C3D-C2D	2.92	1.47	1.39
22	2	303	CLA	CHC-C1C	2.92	1.42	1.35
26	P	314	CHL	C3D-C2D	2.92	1.47	1.39
22	c	506	CLA	CHC-C1C	2.92	1.42	1.35
22	N	306	CLA	C4D-ND	-2.92	1.33	1.37
24	P	312	XAT	C4-C3	2.92	1.56	1.52
24	q	309	XAT	C18-C5	2.92	1.56	1.51
24	P	312	XAT	C38-C25	2.92	1.56	1.51
22	q	306	CLA	CHC-C1C	2.92	1.42	1.35
22	R	304	CLA	C4D-ND	-2.92	1.33	1.37
24	g	309	XAT	C38-C25	2.92	1.56	1.51
22	U	302	CLA	CHC-C1C	2.92	1.42	1.35
26	s	315	CHL	C1D-C2D	2.92	1.51	1.45
22	1	302	CLA	CHC-C1C	2.92	1.42	1.35
24	G	309	XAT	C38-C25	2.92	1.56	1.51
26	V	314	CHL	C1D-C2D	2.92	1.51	1.45
30	a	407	PHO	CAC-C3C	-2.92	1.47	1.52
31	C	517	BCR	C20-C21	2.92	1.52	1.43
22	2	306	CLA	CHC-C1C	2.92	1.42	1.35
22	5	303	CLA	CHC-C1C	2.92	1.42	1.35
22	g	302	CLA	CHC-C1C	2.92	1.42	1.35
32	a	410	SQD	O47-C7	2.91	1.42	1.34
26	s	313	CHL	C1D-C2D	2.91	1.51	1.45
22	r	607	CLA	CHC-C1C	2.91	1.42	1.35
22	r	605	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	314	CHL	MG-NA	-2.91	1.99	2.06
26	G	313	CHL	C3D-C2D	2.91	1.47	1.39
22	r	601	CLA	C4D-ND	-2.91	1.33	1.37
22	b	605	CLA	C4D-ND	-2.91	1.33	1.37
22	2	305	CLA	CHC-C1C	2.91	1.42	1.35
22	B	609	CLA	CHC-C1C	2.91	1.42	1.35
24	2	311	XAT	C4-C3	2.91	1.56	1.52
24	2	311	XAT	C38-C25	2.91	1.56	1.51
26	q	312	CHL	C1D-C2D	2.91	1.51	1.45
31	k	101	BCR	C20-C21	2.91	1.52	1.43
31	c	516	BCR	C37-C22	2.91	1.56	1.50
22	s	309	CLA	CHC-C1C	2.91	1.42	1.35
26	G	314	CHL	C3D-C2D	2.91	1.47	1.39
22	s	303	CLA	CHC-C1C	2.91	1.42	1.35
31	K	101	BCR	C20-C21	2.90	1.52	1.43
26	Q	316	CHL	C1D-C2D	2.90	1.51	1.45
22	R	310	CLA	CHC-C1C	2.90	1.42	1.35
22	u	302	CLA	CHC-C1C	2.90	1.42	1.35
22	B	606	CLA	CHC-C1C	2.90	1.42	1.35
22	c	512	CLA	CHC-C1C	2.90	1.42	1.35
22	1	305	CLA	CHC-C1C	2.90	1.42	1.35
26	v	315	CHL	C3D-C2D	2.90	1.47	1.39
22	4	302	CLA	CHC-C1C	2.90	1.42	1.35
32	a	413	SQD	O47-C7	2.90	1.42	1.34
22	u	306	CLA	CHC-C1C	2.90	1.42	1.35
31	c	515	BCR	C20-C21	2.90	1.52	1.43
24	4	311	XAT	C4-C3	2.90	1.56	1.52
26	2	313	CHL	C3D-C2D	2.90	1.47	1.39
26	g	314	CHL	C3D-C2D	2.90	1.47	1.39
22	P	306	CLA	CHC-C1C	2.90	1.42	1.35
22	R	306	CLA	C4D-ND	-2.90	1.33	1.37
26	q	311	CHL	C1D-C2D	2.90	1.51	1.45
26	Q	313	CHL	C3D-C2D	2.90	1.47	1.39
26	V	317	CHL	C1D-C2D	2.90	1.51	1.45
22	b	606	CLA	CHC-C1C	2.90	1.42	1.35
24	5	311	XAT	C4-C3	2.90	1.56	1.52
22	R	311	CLA	C4D-ND	-2.89	1.33	1.37
22	p	306	CLA	CHC-C1C	2.89	1.42	1.35
22	2	302	CLA	CHC-C1C	2.89	1.42	1.35
22	b	607	CLA	CHC-C1C	2.89	1.42	1.35
26	n	317	CHL	C3D-C2D	2.89	1.47	1.39
32	A	412	SQD	O47-C7	2.89	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	303	CLA	CHC-C1C	2.89	1.42	1.35
22	p	304	CLA	CHC-C1C	2.89	1.42	1.35
26	4	313	CHL	C3D-C2D	2.89	1.47	1.39
22	6	307	CLA	CHC-C1C	2.89	1.42	1.35
26	2	313	CHL	C1D-C2D	2.89	1.51	1.45
22	R	302	CLA	CHC-C1C	2.89	1.42	1.35
22	c	509	CLA	CMC-C2C	-2.89	1.44	1.50
26	n	313	CHL	C3D-C2D	2.89	1.47	1.39
31	C	518	BCR	C37-C22	2.89	1.56	1.50
24	3	309	XAT	C38-C25	2.89	1.56	1.51
32	C	501	SQD	O47-C7	2.89	1.42	1.34
22	c	510	CLA	CHC-C1C	2.89	1.42	1.35
26	g	313	CHL	C1D-C2D	2.89	1.51	1.45
22	R	309	CLA	C4D-ND	-2.88	1.33	1.37
26	S	313	CHL	C1D-C2D	2.88	1.51	1.45
22	Q	302	CLA	CHC-C1C	2.88	1.42	1.35
31	A	409	BCR	C20-C21	2.88	1.52	1.43
22	S	303	CLA	CHC-C1C	2.88	1.42	1.35
33	a	411	PL9	C3-C4	2.88	1.53	1.49
22	C	511	CLA	CHC-C1C	2.88	1.42	1.35
22	C	513	CLA	CHC-C1C	2.88	1.42	1.35
24	p	312	XAT	C38-C25	2.88	1.56	1.51
26	g	312	CHL	C1D-C2D	2.88	1.51	1.45
24	u	311	XAT	C38-C25	2.88	1.56	1.51
22	b	614	CLA	CHC-C1C	2.88	1.42	1.35
26	2	314	CHL	C1D-C2D	2.88	1.51	1.45
26	p	317	CHL	C1D-C2D	2.88	1.51	1.45
26	5	314	CHL	MG-NA	-2.87	1.99	2.06
22	3	302	CLA	CHC-C1C	2.87	1.42	1.35
26	1	315	CHL	C3D-C2D	2.87	1.47	1.39
26	5	316	CHL	C1D-C2D	2.87	1.51	1.45
22	P	304	CLA	CHC-C1C	2.87	1.42	1.35
22	N	305	CLA	C3D-C4D	2.87	1.50	1.44
26	g	316	CHL	C3D-C2D	2.87	1.47	1.39
27	u	319	NEX	C7-C8	-2.87	1.27	1.32
22	d	402	CLA	C1D-ND	2.87	1.41	1.37
26	2	313	CHL	MG-NA	-2.87	1.99	2.06
22	r	607	CLA	C4D-ND	-2.87	1.33	1.37
26	V	313	CHL	C3D-C2D	2.87	1.46	1.39
31	a	409	BCR	C20-C21	2.87	1.52	1.43
22	P	307	CLA	CHC-C1C	2.87	1.42	1.35
22	q	302	CLA	CHC-C1C	2.87	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	v	319	NEX	C7-C8	-2.87	1.27	1.32
22	r	610	CLA	C4D-ND	-2.87	1.33	1.37
22	G	304	CLA	C4D-ND	-2.87	1.33	1.37
26	6	312	CHL	C1D-C2D	2.87	1.51	1.45
24	3	309	XAT	C18-C5	2.86	1.56	1.51
24	Q	309	XAT	C18-C5	2.86	1.56	1.51
26	Q	314	CHL	C3D-C2D	2.86	1.46	1.39
26	Q	311	CHL	C1D-C2D	2.86	1.51	1.45
22	R	308	CLA	C4D-ND	-2.86	1.33	1.37
26	q	313	CHL	C1D-C2D	2.86	1.51	1.45
26	V	315	CHL	C1D-C2D	2.86	1.51	1.45
26	Q	313	CHL	C1D-C2D	2.86	1.51	1.45
26	q	315	CHL	C3D-C2D	2.86	1.46	1.39
22	B	608	CLA	CHC-C1C	2.86	1.42	1.35
22	B	603	CLA	CHC-C1C	2.86	1.42	1.35
22	V	306	CLA	CHC-C1C	2.86	1.42	1.35
26	S	315	CHL	MG-NA	-2.86	1.99	2.06
26	4	317	CHL	C3D-C2D	2.86	1.46	1.39
34	C	502	LMG	O7-C10	2.86	1.42	1.34
33	D	405	PL9	C2-C1	2.86	1.52	1.44
22	1	303	CLA	CHC-C1C	2.86	1.42	1.35
26	v	317	CHL	C3D-C2D	2.86	1.46	1.39
26	v	314	CHL	C1D-C2D	2.85	1.51	1.45
22	B	609	CLA	CMB-C2B	-2.85	1.45	1.51
26	U	316	CHL	C3D-C2D	2.85	1.46	1.39
26	2	316	CHL	C1D-C2D	2.85	1.51	1.45
26	g	316	CHL	C1D-C2D	2.85	1.51	1.45
22	b	608	CLA	CHC-C1C	2.85	1.42	1.35
26	s	315	CHL	MG-NA	-2.85	1.99	2.06
26	5	313	CHL	MG-NA	-2.85	1.99	2.06
26	n	317	CHL	C1D-C2D	2.85	1.50	1.45
22	b	602	CLA	CHC-C1C	2.85	1.42	1.35
26	3	316	CHL	C3D-C2D	2.85	1.46	1.39
31	b	620	BCR	C7-C6	2.85	1.55	1.45
22	B	607	CLA	CHC-C1C	2.85	1.42	1.35
26	Q	311	CHL	C3D-C2D	2.85	1.46	1.39
26	5	318	CHL	C3D-C2D	2.85	1.46	1.39
24	3	309	XAT	C4-C3	2.85	1.56	1.52
22	D	403	CLA	C1D-ND	2.85	1.41	1.37
26	s	313	CHL	C3D-C2D	2.85	1.46	1.39
26	5	314	CHL	C1D-C2D	2.84	1.50	1.45
26	Q	316	CHL	C3D-C2D	2.84	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	617	CLA	CHC-C1C	2.84	1.42	1.35
22	s	306	CLA	CHC-C1C	2.84	1.42	1.35
31	k	101	BCR	C7-C6	2.84	1.55	1.45
22	u	307	CLA	CHC-C1C	2.84	1.42	1.35
31	B	620	BCR	C7-C6	2.84	1.55	1.45
26	v	313	CHL	C1D-C2D	2.84	1.50	1.45
24	v	311	XAT	C18-C5	2.84	1.56	1.51
22	c	505	CLA	CHC-C1C	2.84	1.42	1.35
26	r	614	CHL	C3D-C2D	2.84	1.46	1.39
22	U	306	CLA	CHC-C1C	2.84	1.42	1.35
31	A	409	BCR	C39-C30	-2.84	1.48	1.53
22	S	306	CLA	CHC-C1C	2.84	1.42	1.35
33	d	404	PL9	C2-C1	2.84	1.52	1.44
22	a	404	CLA	CHC-C1C	2.84	1.42	1.35
22	N	302	CLA	CHC-C1C	2.84	1.42	1.35
26	v	314	CHL	C3D-C2D	2.84	1.46	1.39
26	2	314	CHL	MG-NA	-2.84	1.99	2.06
22	C	508	CLA	CHC-C1C	2.84	1.42	1.35
24	V	311	XAT	C18-C5	2.83	1.56	1.51
22	s	302	CLA	CHC-C1C	2.83	1.42	1.35
31	x	202	BCR	C7-C6	2.83	1.55	1.45
26	4	316	CHL	C3D-C2D	2.83	1.46	1.39
26	1	317	CHL	C3D-C2D	2.83	1.46	1.39
22	C	510	CLA	CMC-C2C	-2.83	1.44	1.50
22	Q	303	CLA	CHC-C1C	2.83	1.42	1.35
26	q	313	CHL	C3D-C2D	2.83	1.46	1.39
22	G	305	CLA	C4D-ND	-2.83	1.33	1.37
30	d	401	PHO	CAC-C3C	-2.83	1.47	1.52
26	p	319	CHL	C3D-C2D	2.83	1.46	1.39
26	5	316	CHL	C3D-C2D	2.83	1.46	1.39
26	V	317	CHL	C3D-C2D	2.83	1.46	1.39
26	6	317	CHL	C3D-C2D	2.83	1.46	1.39
26	r	616	CHL	C3D-C2D	2.83	1.46	1.39
31	X	201	BCR	C7-C6	2.83	1.55	1.45
26	u	314	CHL	C3D-C2D	2.83	1.46	1.39
26	n	315	CHL	C1D-C2D	2.83	1.50	1.45
22	B	602	CLA	CHC-C1C	2.83	1.42	1.35
27	N	318	NEX	C7-C8	-2.83	1.27	1.32
31	b	619	BCR	C7-C6	2.83	1.55	1.45
22	4	306	CLA	CHC-C1C	2.83	1.42	1.35
22	S	302	CLA	CHC-C1C	2.83	1.42	1.35
31	K	101	BCR	C7-C6	2.82	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	501	LMG	O7-C10	2.82	1.42	1.34
31	C	518	BCR	C7-C6	2.82	1.55	1.45
22	c	507	CLA	CHC-C1C	2.82	1.42	1.35
26	v	317	CHL	C1D-C2D	2.82	1.50	1.45
31	C	516	BCR	C7-C6	2.82	1.55	1.45
26	4	314	CHL	C3D-C2D	2.82	1.46	1.39
22	n	302	CLA	CHC-C1C	2.82	1.42	1.35
26	u	313	CHL	C1D-C2D	2.82	1.50	1.45
26	P	314	CHL	C1D-C2D	2.82	1.50	1.45
26	1	314	CHL	MG-NA	-2.82	1.99	2.06
26	G	316	CHL	C1D-C2D	2.82	1.50	1.45
31	B	618	BCR	C20-C21	2.82	1.52	1.43
22	1	303	CLA	CMB-C2B	-2.82	1.45	1.51
26	4	316	CHL	C1D-C2D	2.82	1.50	1.45
24	4	311	XAT	C18-C5	2.82	1.56	1.51
22	b	603	CLA	CHC-C1C	2.82	1.42	1.35
32	m	101	SQD	O47-C7	2.82	1.42	1.34
22	B	612	CLA	CMC-C2C	-2.81	1.44	1.50
26	1	318	CHL	C3D-C2D	2.81	1.46	1.39
31	B	619	BCR	C7-C6	2.81	1.55	1.45
26	R	315	CHL	C3D-C2D	2.81	1.46	1.39
26	S	313	CHL	C3D-C2D	2.81	1.46	1.39
26	r	615	CHL	C3D-C2D	2.81	1.46	1.39
26	2	318	CHL	C3D-C2D	2.81	1.46	1.39
26	V	316	CHL	C1D-C2D	2.81	1.50	1.45
30	D	401	PHO	CAC-C3C	-2.81	1.47	1.52
26	q	311	CHL	C3D-C2D	2.81	1.46	1.39
26	g	314	CHL	C1D-C2D	2.81	1.50	1.45
24	N	311	XAT	C24-C23	2.81	1.56	1.52
24	p	312	XAT	C18-C5	2.81	1.56	1.51
22	A	404	CLA	CHC-C1C	2.81	1.42	1.35
26	R	316	CHL	C3D-C2D	2.81	1.46	1.39
24	P	312	XAT	C24-C23	2.81	1.56	1.52
22	C	509	CLA	CHC-C1C	2.81	1.42	1.35
31	z	101	BCR	C7-C6	2.81	1.55	1.45
22	A	405	CLA	CHC-C1C	2.81	1.42	1.35
24	P	312	XAT	C18-C5	2.81	1.56	1.51
26	p	316	CHL	C1D-C2D	2.81	1.50	1.45
22	b	609	CLA	CMB-C2B	-2.81	1.45	1.51
22	C	504	CLA	C3B-C2B	-2.81	1.36	1.40
24	5	311	XAT	C38-C25	2.81	1.56	1.51
34	B	621	LMG	O7-C8	-2.81	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	508	CLA	CHC-C1C	2.81	1.42	1.35
22	3	303	CLA	CMB-C2B	-2.81	1.45	1.51
22	r	609	CLA	C4D-ND	-2.81	1.33	1.37
26	P	316	CHL	C1D-C2D	2.81	1.50	1.45
22	g	305	CLA	C4D-ND	-2.80	1.33	1.37
22	1	306	CLA	CHC-C1C	2.80	1.42	1.35
22	U	304	CLA	CMB-C2B	-2.80	1.45	1.51
22	C	514	CLA	CHC-C1C	2.80	1.42	1.35
24	1	311	XAT	C18-C5	2.80	1.56	1.51
24	U	311	XAT	C38-C25	2.80	1.56	1.51
22	a	405	CLA	CHC-C1C	2.80	1.42	1.35
26	2	316	CHL	C3D-C2D	2.80	1.46	1.39
26	N	313	CHL	C1D-C2D	2.80	1.50	1.45
26	P	319	CHL	C3D-C2D	2.80	1.46	1.39
26	3	311	CHL	C1D-C2D	2.80	1.50	1.45
24	1	311	XAT	C4-C3	2.80	1.56	1.52
26	R	317	CHL	C3D-C2D	2.80	1.46	1.39
24	g	309	XAT	C18-C5	2.80	1.56	1.51
34	C	521	LMG	O7-C10	2.80	1.42	1.34
22	g	304	CLA	C4D-ND	-2.80	1.33	1.37
22	C	506	CLA	CHC-C1C	2.80	1.42	1.35
26	G	316	CHL	C3D-C2D	2.80	1.46	1.39
26	u	317	CHL	C3D-C2D	2.80	1.46	1.39
26	6	314	CHL	C1D-C2D	2.80	1.50	1.45
31	c	515	BCR	C39-C30	-2.80	1.48	1.53
22	v	306	CLA	CHC-C1C	2.80	1.42	1.35
34	b	624	LMG	O8-C28	2.80	1.41	1.33
26	1	316	CHL	C1D-C2D	2.80	1.50	1.45
26	6	301	CHL	C1D-C2D	2.80	1.50	1.45
22	U	306	CLA	CMB-C2B	-2.80	1.45	1.51
32	M	101	SQD	O47-C7	2.79	1.42	1.34
26	N	317	CHL	C1D-C2D	2.79	1.50	1.45
26	n	318	CHL	C1D-C2D	2.79	1.50	1.45
22	4	303	CLA	CMB-C2B	-2.79	1.45	1.51
26	n	316	CHL	C3D-C2D	2.79	1.46	1.39
31	D	404	BCR	C7-C6	2.79	1.55	1.45
27	V	319	NEX	C7-C8	-2.79	1.27	1.32
26	R	317	CHL	C1D-C2D	2.79	1.50	1.45
31	t	101	BCR	C16-C17	2.79	1.52	1.43
24	u	311	XAT	C18-C5	2.79	1.56	1.51
22	G	303	CLA	CMB-C2B	-2.79	1.45	1.51
22	g	303	CLA	CMB-C2B	-2.79	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	311	XAT	C24-C23	2.79	1.56	1.52
26	2	318	CHL	C1D-C2D	2.79	1.50	1.45
31	c	516	BCR	C7-C6	2.79	1.55	1.45
34	a	412	LMG	O7-C10	2.79	1.42	1.34
34	C	521	LMG	O8-C28	2.79	1.41	1.33
34	B	624	LMG	O8-C28	2.79	1.41	1.33
24	6	310	XAT	C18-C5	2.79	1.56	1.51
26	v	313	CHL	C3D-C2D	2.79	1.46	1.39
24	G	309	XAT	C18-C5	2.79	1.56	1.51
26	p	314	CHL	C4B-CHC	2.78	1.48	1.41
31	a	409	BCR	C39-C30	-2.78	1.48	1.53
31	T	101	BCR	C16-C17	2.78	1.52	1.43
24	N	311	XAT	C4-C3	2.78	1.56	1.52
22	c	513	CLA	CHC-C1C	2.78	1.42	1.35
22	q	304	CLA	C4D-ND	-2.78	1.33	1.37
24	p	312	XAT	C4-C3	2.78	1.56	1.52
34	c	520	LMG	O7-C10	2.78	1.42	1.34
26	3	311	CHL	C3D-C2D	2.78	1.46	1.39
26	p	314	CHL	C3D-C2D	2.78	1.46	1.39
34	A	411	LMG	O7-C10	2.78	1.42	1.34
26	U	316	CHL	C1D-C2D	2.78	1.50	1.45
22	b	617	CLA	CHC-C1C	2.78	1.42	1.35
24	u	311	XAT	C4-C3	2.78	1.56	1.52
22	a	404	CLA	CMC-C2C	-2.78	1.44	1.50
26	N	313	CHL	C3D-C2D	2.78	1.46	1.39
34	a	412	LMG	O8-C28	2.78	1.41	1.33
26	1	313	CHL	C1D-C2D	2.78	1.50	1.45
31	b	618	BCR	C20-C21	2.78	1.52	1.43
26	4	313	CHL	C1D-C2D	2.78	1.50	1.45
24	V	311	XAT	C24-C23	2.78	1.56	1.52
22	a	405	CLA	CMB-C2B	-2.78	1.45	1.51
26	u	313	CHL	C3D-C2D	2.77	1.46	1.39
22	b	612	CLA	CMC-C2C	-2.77	1.44	1.50
26	G	313	CHL	C1D-C2D	2.77	1.50	1.45
26	V	315	CHL	MG-NA	-2.77	1.99	2.06
22	n	308	CLA	C4D-ND	-2.77	1.33	1.37
26	2	315	CHL	C3D-C2D	2.77	1.46	1.39
26	N	316	CHL	C1D-C2D	2.77	1.50	1.45
26	r	619	CHL	C3D-C2D	2.77	1.46	1.39
25	l	101	LHG	O7-C5	-2.77	1.39	1.46
26	3	313	CHL	C1D-C2D	2.77	1.50	1.45
26	5	318	CHL	C1D-C2D	2.77	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	620	BCR	C39-C30	-2.77	1.48	1.53
22	v	303	CLA	CMB-C2B	-2.77	1.45	1.51
24	5	311	XAT	C18-C5	2.77	1.56	1.51
26	g	311	CHL	C3D-C2D	2.77	1.46	1.39
25	c	522	LHG	O7-C5	-2.77	1.39	1.46
24	q	309	XAT	C24-C23	2.76	1.56	1.52
31	b	620	BCR	C39-C30	-2.76	1.48	1.53
26	5	315	CHL	C1D-C2D	2.76	1.50	1.45
22	A	404	CLA	CMC-C2C	-2.76	1.44	1.50
22	A	405	CLA	CMB-C2B	-2.76	1.45	1.51
22	B	604	CLA	CMB-C2B	-2.76	1.45	1.51
24	2	311	XAT	C18-C5	2.76	1.56	1.51
26	p	320	CHL	C3D-C2D	2.76	1.46	1.39
26	r	615	CHL	C1D-C2D	2.76	1.50	1.45
26	6	315	CHL	C1D-C2D	2.76	1.50	1.45
24	1	311	XAT	C24-C23	2.76	1.56	1.52
26	r	616	CHL	C1D-C2D	2.76	1.50	1.45
22	C	513	CLA	CMB-C2B	-2.76	1.45	1.51
22	R	310	CLA	C4D-ND	-2.76	1.33	1.37
22	N	303	CLA	CMB-C2B	-2.76	1.45	1.51
31	d	403	BCR	C16-C17	2.76	1.52	1.43
22	Q	304	CLA	C4D-ND	-2.76	1.33	1.37
31	C	517	BCR	C39-C30	-2.76	1.48	1.53
24	6	310	XAT	C24-C23	2.75	1.56	1.52
31	d	403	BCR	C7-C6	2.75	1.54	1.45
26	5	317	CHL	C1D-C2D	2.75	1.50	1.45
34	c	520	LMG	O8-C28	2.75	1.41	1.33
25	C	523	LHG	O7-C5	-2.75	1.39	1.46
22	b	604	CLA	CMB-C2B	-2.75	1.45	1.51
26	q	312	CHL	MG-NA	-2.75	1.99	2.06
26	1	313	CHL	C3D-C2D	2.75	1.46	1.39
26	3	314	CHL	C1D-C2D	2.75	1.50	1.45
34	A	411	LMG	O8-C28	2.75	1.41	1.33
26	n	316	CHL	C1D-C2D	2.75	1.50	1.45
26	3	315	CHL	C3D-C2D	2.75	1.46	1.39
26	G	314	CHL	C1D-C2D	2.75	1.50	1.45
31	C	517	BCR	C7-C6	2.75	1.54	1.45
24	U	311	XAT	C4-C3	2.75	1.56	1.52
24	U	311	XAT	C18-C5	2.75	1.56	1.51
24	R	313	XAT	C38-C25	2.74	1.56	1.51
22	V	301	CLA	CMB-C2B	-2.74	1.45	1.51
26	U	313	CHL	C3D-C2D	2.74	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	L	101	LHG	O7-C5	-2.74	1.39	1.46
26	1	318	CHL	C1D-C2D	2.74	1.50	1.45
26	V	318	CHL	C1D-C2D	2.74	1.50	1.45
26	g	311	CHL	C1D-C2D	2.74	1.50	1.45
26	v	315	CHL	C1D-C2D	2.74	1.50	1.45
26	G	311	CHL	C1D-C2D	2.74	1.50	1.45
22	B	616	CLA	CHC-C1C	2.74	1.42	1.35
26	4	313	CHL	MG-NA	-2.74	1.99	2.06
26	5	315	CHL	C3D-C2D	2.74	1.46	1.39
22	S	303	CLA	CMB-C2B	-2.74	1.45	1.51
22	v	301	CLA	CMB-C2B	-2.74	1.46	1.51
26	6	312	CHL	C3D-C2D	2.74	1.46	1.39
22	b	617	CLA	CMB-C2B	-2.74	1.46	1.51
31	D	404	BCR	C16-C17	2.73	1.51	1.43
26	s	316	CHL	MG-NA	-2.73	1.99	2.06
26	G	315	CHL	C3D-C2D	2.73	1.46	1.39
22	s	303	CLA	CMB-C2B	-2.73	1.46	1.51
31	c	515	BCR	C7-C6	2.73	1.54	1.45
22	U	306	CLA	C3B-C2B	-2.73	1.36	1.40
22	S	306	CLA	CMB-C2B	-2.73	1.46	1.51
24	n	311	XAT	C4-C3	2.73	1.56	1.52
26	1	317	CHL	C1D-C2D	2.73	1.50	1.45
26	U	319	CHL	C3D-C2D	2.73	1.46	1.39
22	B	611	CLA	CHC-C1C	2.73	1.42	1.35
22	6	304	CLA	CMB-C2B	-2.73	1.46	1.51
26	N	316	CHL	C3D-C2D	2.73	1.46	1.39
31	C	516	BCR	C39-C30	-2.73	1.48	1.53
26	u	318	CHL	C3D-C2D	2.73	1.46	1.39
26	Q	314	CHL	C1D-C2D	2.73	1.50	1.45
24	r	612	XAT	C38-C25	2.73	1.56	1.51
31	z	101	BCR	C39-C30	-2.73	1.48	1.53
22	s	306	CLA	CMB-C2B	-2.73	1.46	1.51
26	5	317	CHL	C3D-C2D	2.73	1.46	1.39
26	P	314	CHL	MG-NA	-2.72	1.99	2.06
25	U	312	LHG	O7-C5	-2.72	1.39	1.46
22	c	503	CLA	C3B-C2B	-2.72	1.36	1.40
26	2	317	CHL	C3D-C2D	2.72	1.46	1.39
26	1	314	CHL	C1D-C2D	2.72	1.50	1.45
22	1	301	CLA	CMB-C2B	-2.72	1.46	1.51
26	s	313	CHL	MG-NA	-2.72	1.99	2.06
26	2	315	CHL	C1D-C2D	2.72	1.50	1.45
26	n	315	CHL	C3D-C2D	2.72	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	315	CHL	C3D-C2D	2.72	1.46	1.39
22	b	611	CLA	CHC-C1C	2.72	1.41	1.35
24	3	309	XAT	C24-C23	2.72	1.56	1.52
24	4	311	XAT	C24-C23	2.72	1.56	1.52
31	c	516	BCR	C39-C30	-2.72	1.48	1.53
24	g	309	XAT	C24-C23	2.72	1.56	1.52
26	p	314	CHL	C1D-C2D	2.72	1.50	1.45
31	C	518	BCR	C39-C30	-2.72	1.48	1.53
26	P	314	CHL	C4B-CHC	2.72	1.48	1.41
25	d	405	LHG	O7-C5	-2.72	1.39	1.46
22	V	303	CLA	CMB-C2B	-2.72	1.46	1.51
26	S	314	CHL	C3D-C2D	2.72	1.46	1.39
26	P	318	CHL	C3D-C2D	2.71	1.46	1.39
26	3	314	CHL	C3D-C2D	2.71	1.46	1.39
26	U	317	CHL	C3D-C2D	2.71	1.46	1.39
26	s	314	CHL	C3D-C2D	2.71	1.46	1.39
26	6	314	CHL	MG-NA	-2.71	1.99	2.06
24	n	311	XAT	C18-C5	2.71	1.56	1.51
25	5	312	LHG	O7-C5	-2.71	1.39	1.46
26	u	317	CHL	C1D-C2D	2.71	1.50	1.45
25	D	407	LHG	O7-C5	-2.71	1.39	1.46
26	S	316	CHL	MG-NA	-2.71	1.99	2.06
22	C	508	CLA	C3B-C2B	-2.71	1.36	1.40
24	N	311	XAT	C18-C5	2.71	1.56	1.51
26	n	313	CHL	C1D-C2D	2.71	1.50	1.45
22	u	306	CLA	CMB-C2B	-2.71	1.46	1.51
25	D	406	LHG	O7-C5	-2.71	1.39	1.46
26	6	315	CHL	C3D-C2D	2.71	1.46	1.39
22	c	512	CLA	CMB-C2B	-2.71	1.46	1.51
26	U	319	CHL	C1D-C2D	2.71	1.50	1.45
34	b	621	LMG	O7-C8	-2.71	1.39	1.46
26	4	315	CHL	C1D-C2D	2.71	1.50	1.45
22	B	606	CLA	CMB-C2B	-2.70	1.46	1.51
25	d	406	LHG	O7-C5	-2.70	1.39	1.46
25	u	312	LHG	O7-C5	-2.70	1.39	1.46
22	C	503	CLA	CMB-C2B	-2.70	1.46	1.51
24	v	311	XAT	C24-C23	2.70	1.56	1.52
27	P	301	NEX	C7-C8	-2.70	1.27	1.32
22	4	301	CLA	CMB-C2B	-2.70	1.46	1.51
26	p	320	CHL	C1D-C2D	2.70	1.50	1.45
22	c	511	CLA	CMB-C2B	-2.70	1.46	1.51
26	R	316	CHL	C1D-C2D	2.70	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	317	CHL	C1D-C2D	2.70	1.50	1.45
22	b	612	CLA	CMB-C2B	-2.70	1.46	1.51
22	u	301	CLA	CMB-C2B	-2.69	1.46	1.51
26	N	314	CHL	C1D-C2D	2.69	1.50	1.45
26	u	314	CHL	C1D-C2D	2.69	1.50	1.45
22	B	612	CLA	CMB-C2B	-2.69	1.46	1.51
26	1	313	CHL	MG-NA	-2.69	1.99	2.06
22	b	616	CLA	CHC-C1C	2.69	1.41	1.35
26	U	315	CHL	C1D-C2D	2.69	1.50	1.45
26	P	319	CHL	C1D-C2D	2.69	1.50	1.45
22	n	303	CLA	CMB-C2B	-2.69	1.46	1.51
22	P	304	CLA	CMB-C2B	-2.69	1.46	1.51
22	Q	303	CLA	CMB-C2B	-2.69	1.46	1.51
26	2	317	CHL	C1D-C2D	2.69	1.50	1.45
26	p	318	CHL	C3D-C2D	2.69	1.46	1.39
31	B	619	BCR	C39-C30	-2.69	1.48	1.53
31	b	618	BCR	C39-C30	-2.69	1.48	1.53
26	r	614	CHL	C1D-C2D	2.69	1.50	1.45
26	Q	315	CHL	C3D-C2D	2.69	1.46	1.39
24	G	309	XAT	C24-C23	2.68	1.56	1.52
26	V	316	CHL	C3D-C2D	2.68	1.46	1.39
31	A	409	BCR	C7-C6	2.68	1.54	1.45
22	c	505	CLA	CMB-C2B	-2.68	1.46	1.51
26	P	317	CHL	C3D-C2D	2.68	1.46	1.39
26	P	315	CHL	C4B-CHC	2.68	1.48	1.41
26	g	315	CHL	C3D-C2D	2.68	1.46	1.39
26	3	314	CHL	MG-NA	-2.68	1.99	2.06
25	C	522	LHG	O7-C5	-2.68	1.39	1.46
22	c	507	CLA	C3B-C2B	-2.68	1.36	1.40
26	R	315	CHL	C1D-C2D	2.68	1.50	1.45
22	B	611	CLA	CMB-C2B	-2.68	1.46	1.51
22	N	302	CLA	CMB-C2B	-2.67	1.46	1.51
22	U	301	CLA	CMB-C2B	-2.67	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.67	1.46	1.51
26	v	316	CHL	C1D-C2D	2.67	1.50	1.45
26	u	315	CHL	C3D-C2D	2.67	1.46	1.39
26	q	314	CHL	C3D-C2D	2.67	1.46	1.39
31	a	409	BCR	C7-C6	2.67	1.54	1.45
26	U	319	CHL	MG-NA	-2.67	1.99	2.06
22	C	506	CLA	CMB-C2B	-2.67	1.46	1.51
31	x	202	BCR	C16-C17	2.67	1.51	1.43
31	b	619	BCR	C39-C30	-2.66	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	C4D-ND	-2.66	1.34	1.37
22	n	302	CLA	CMB-C2B	-2.66	1.46	1.51
25	c	521	LHG	O7-C5	-2.66	1.39	1.46
25	3	310	LHG	O7-C5	-2.66	1.39	1.46
22	b	611	CLA	CMB-C2B	-2.66	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.66	1.46	1.51
26	n	317	CHL	MG-NA	-2.66	2.00	2.06
26	v	318	CHL	C1D-C2D	2.66	1.50	1.45
31	B	618	BCR	C7-C6	2.66	1.54	1.45
22	a	406	CLA	CMB-C2B	-2.66	1.46	1.51
22	c	514	CLA	CMB-C2B	-2.66	1.46	1.51
26	S	314	CHL	C1D-C2D	2.66	1.50	1.45
22	B	615	CLA	CMB-C2B	-2.66	1.46	1.51
25	c	523	LHG	O7-C5	-2.66	1.39	1.46
26	P	318	CHL	C1D-C2D	2.66	1.50	1.45
22	B	605	CLA	CHC-C1C	2.66	1.41	1.35
26	n	313	CHL	MG-NA	-2.66	2.00	2.06
31	B	618	BCR	C39-C30	-2.66	1.48	1.53
22	B	616	CLA	C4D-ND	-2.65	1.34	1.37
26	u	315	CHL	C1D-ND	-2.65	1.34	1.37
26	4	314	CHL	C1D-C2D	2.65	1.50	1.45
26	S	313	CHL	MG-NA	-2.65	2.00	2.06
22	G	302	CLA	CMB-C2B	-2.65	1.46	1.51
31	X	201	BCR	C16-C17	2.65	1.51	1.43
26	p	317	CHL	C3D-C2D	2.65	1.46	1.39
22	b	606	CLA	CMB-C2B	-2.65	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.65	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.65	1.46	1.51
31	x	202	BCR	C39-C30	-2.65	1.48	1.53
34	b	621	LMG	O7-C10	2.65	1.41	1.34
26	4	315	CHL	MG-NA	-2.65	2.00	2.06
24	u	311	XAT	C24-C23	2.64	1.56	1.52
22	u	304	CLA	CMB-C2B	-2.64	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.64	1.46	1.51
25	C	524	LHG	O7-C5	-2.64	1.40	1.46
22	D	403	CLA	CMD-C2D	-2.64	1.45	1.50
22	b	613	CLA	CMB-C2B	-2.64	1.46	1.51
26	n	314	CHL	C1D-C2D	2.64	1.50	1.45
22	C	515	CLA	CMB-C2B	-2.64	1.46	1.51
22	d	402	CLA	CMD-C2D	-2.64	1.45	1.50
34	W	201	LMG	O8-C28	2.64	1.41	1.33
31	X	201	BCR	C39-C30	-2.64	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	619	CHL	C1D-C2D	2.64	1.50	1.45
26	3	313	CHL	MG-NA	-2.64	2.00	2.06
22	2	303	CLA	CMB-C2B	-2.64	1.46	1.51
22	U	307	CLA	CMB-C2B	-2.64	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.64	1.46	1.51
26	6	313	CHL	MG-NA	-2.64	2.00	2.06
22	6	303	CLA	CMB-C2B	-2.64	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.64	1.46	1.51
36	C	520	DGD	O1G-C1A	2.64	1.41	1.33
26	v	316	CHL	C3D-C2D	2.63	1.46	1.39
26	U	314	CHL	C3D-C2D	2.63	1.46	1.39
36	J	101	DGD	O1G-C1A	2.63	1.41	1.33
31	b	618	BCR	C7-C6	2.63	1.54	1.45
26	3	312	CHL	MG-NA	-2.63	2.00	2.06
22	b	605	CLA	CHC-C1C	2.63	1.41	1.35
22	q	302	CLA	CMB-C2B	-2.63	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.63	1.46	1.51
34	A	411	LMG	O7-C8	-2.63	1.40	1.46
22	d	402	CLA	CMB-C2B	-2.63	1.46	1.51
31	b	620	BCR	C16-C17	2.63	1.51	1.43
26	N	313	CHL	MG-NA	-2.63	2.00	2.06
22	g	305	CLA	CMB-C2B	-2.63	1.46	1.51
22	A	406	CLA	CMB-C2B	-2.63	1.46	1.51
22	P	302	CLA	CMB-C2B	-2.63	1.46	1.51
26	g	315	CHL	C1D-C2D	2.62	1.50	1.45
22	B	610	CLA	CMB-C2B	-2.62	1.46	1.51
26	1	315	CHL	C1D-C2D	2.62	1.50	1.45
34	w	201	LMG	O8-C28	2.62	1.41	1.33
22	g	302	CLA	CMB-C2B	-2.62	1.46	1.51
22	g	301	CLA	CMB-C2B	-2.62	1.46	1.51
22	5	303	CLA	CMB-C2B	-2.62	1.46	1.51
22	u	302	CLA	CMB-C2B	-2.62	1.46	1.51
22	3	302	CLA	CMB-C2B	-2.62	1.46	1.51
22	U	302	CLA	CMB-C2B	-2.62	1.46	1.51
26	6	316	CHL	C3D-C2D	2.62	1.46	1.39
22	C	510	CLA	C3B-C2B	-2.62	1.36	1.40
22	B	613	CLA	CMB-C2B	-2.62	1.46	1.51
34	a	412	LMG	O7-C8	-2.62	1.40	1.46
25	s	312	LHG	O7-C5	-2.62	1.40	1.46
22	2	305	CLA	C4D-ND	-2.62	1.34	1.37
22	G	301	CLA	CMB-C2B	-2.62	1.46	1.51
22	c	513	CLA	CMB-C2B	-2.61	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	u	308	CLA	CMB-C2B	-2.61	1.46	1.51
31	t	101	BCR	C39-C30	-2.61	1.48	1.53
36	c	519	DGD	O1G-C1A	2.61	1.41	1.33
26	n	316	CHL	MG-NA	-2.61	2.00	2.06
34	d	407	LMG	O8-C28	2.61	1.41	1.33
25	q	310	LHG	O7-C5	-2.61	1.40	1.46
26	p	315	CHL	C4B-CHC	2.61	1.48	1.41
27	u	320	NEX	C7-C8	-2.61	1.27	1.32
25	b	623	LHG	O7-C5	-2.61	1.40	1.46
24	n	311	XAT	C38-C25	2.61	1.55	1.51
25	6	311	LHG	O7-C5	-2.61	1.40	1.46
31	T	101	BCR	C39-C30	-2.61	1.48	1.53
22	U	308	CLA	CMB-C2B	-2.61	1.46	1.51
26	6	315	CHL	MG-NA	-2.61	2.00	2.06
26	g	314	CHL	MG-NA	-2.61	2.00	2.06
26	p	319	CHL	C1D-C2D	2.61	1.50	1.45
34	B	621	LMG	O7-C10	2.61	1.41	1.34
22	Q	301	CLA	CMB-C2B	-2.60	1.46	1.51
22	1	306	CLA	CMB-C2B	-2.60	1.46	1.51
25	B	623	LHG	O7-C5	-2.60	1.40	1.46
22	c	509	CLA	C3B-C2B	-2.60	1.36	1.40
22	S	308	CLA	CMB-C2B	-2.60	1.46	1.51
22	p	304	CLA	CMB-C2B	-2.60	1.46	1.51
26	p	318	CHL	C1D-C2D	2.60	1.50	1.45
25	V	312	LHG	O7-C5	-2.60	1.40	1.46
31	C	518	BCR	C16-C17	2.60	1.51	1.43
26	G	314	CHL	MG-NA	-2.59	2.00	2.06
26	Q	314	CHL	MG-NA	-2.59	2.00	2.06
22	N	301	CLA	CMB-C2B	-2.59	1.46	1.51
36	c	518	DGD	O1G-C1A	2.59	1.40	1.33
26	s	314	CHL	C1D-C2D	2.59	1.50	1.45
34	b	621	LMG	O8-C28	2.59	1.40	1.33
22	b	617	CLA	C3B-C2B	-2.59	1.36	1.40
31	c	516	BCR	C16-C17	2.59	1.51	1.43
25	S	312	LHG	O7-C5	-2.59	1.40	1.46
25	p	313	LHG	O7-C5	-2.59	1.40	1.46
22	u	307	CLA	CMB-C2B	-2.59	1.46	1.51
22	5	304	CLA	CMB-C2B	-2.59	1.46	1.51
34	D	408	LMG	O8-C28	2.59	1.40	1.33
25	P	313	LHG	O7-C5	-2.59	1.40	1.46
22	r	605	CLA	CMB-C2B	-2.59	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.59	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	305	CLA	CMB-C2B	-2.59	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.59	1.46	1.51
22	s	308	CLA	CMB-C2B	-2.58	1.46	1.51
22	R	311	CLA	CMB-C2B	-2.58	1.46	1.51
22	B	617	CLA	CMD-C2D	-2.58	1.45	1.50
26	P	315	CHL	C1D-ND	-2.58	1.34	1.37
26	2	313	CHL	C4B-CHC	2.58	1.48	1.41
22	C	514	CLA	CMB-C2B	-2.58	1.46	1.51
27	S	317	NEX	C7-C8	-2.58	1.27	1.32
26	1	315	CHL	MG-NA	-2.58	2.00	2.06
22	B	616	CLA	CMB-C2B	-2.58	1.46	1.51
26	V	316	CHL	MG-NA	-2.57	2.00	2.06
22	b	614	CLA	CMB-C2B	-2.57	1.46	1.51
22	4	305	CLA	CMB-C2B	-2.57	1.46	1.51
26	5	313	CHL	C4B-CHC	2.57	1.48	1.41
22	b	613	CLA	CMC-C2C	-2.57	1.45	1.50
36	C	519	DGD	O1G-C1G	-2.57	1.39	1.45
22	b	616	CLA	CMB-C2B	-2.57	1.46	1.51
31	K	101	BCR	C16-C17	2.57	1.51	1.43
34	C	502	LMG	O7-C8	-2.57	1.40	1.46
26	1	316	CHL	C3D-C2D	2.57	1.46	1.39
22	r	607	CLA	CMB-C2B	-2.57	1.46	1.51
22	B	603	CLA	CMB-C2B	-2.57	1.46	1.51
26	U	313	CHL	MG-NA	-2.56	2.00	2.06
22	4	306	CLA	CMB-C2B	-2.56	1.46	1.51
26	V	313	CHL	MG-NA	-2.56	2.00	2.06
26	q	315	CHL	MG-NA	-2.56	2.00	2.06
22	N	304	CLA	CMB-C2B	-2.56	1.46	1.51
22	r	610	CLA	CMB-C2B	-2.56	1.46	1.51
25	b	622	LHG	O7-C5	-2.56	1.40	1.46
22	G	305	CLA	CMB-C2B	-2.56	1.46	1.51
22	p	303	CLA	CMB-C2B	-2.56	1.46	1.51
22	b	603	CLA	CMB-C2B	-2.56	1.46	1.51
22	a	404	CLA	CMB-C2B	-2.56	1.46	1.51
22	q	301	CLA	CMB-C2B	-2.56	1.46	1.51
36	c	517	DGD	O1G-C1A	2.56	1.40	1.33
22	n	308	CLA	CMB-C2B	-2.56	1.46	1.51
26	G	315	CHL	C1D-C2D	2.56	1.50	1.45
22	2	301	CLA	CMB-C2B	-2.56	1.46	1.51
34	B	621	LMG	O1-C1	-2.56	1.35	1.40
22	N	305	CLA	C4D-ND	-2.56	1.34	1.37
31	D	404	BCR	C39-C30	-2.56	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	317	CHL	C1D-C2D	2.56	1.50	1.45
22	c	502	CLA	CMD-C2D	-2.55	1.45	1.50
22	r	604	CLA	CMB-C2B	-2.55	1.46	1.51
25	r	613	LHG	O8-C23	2.55	1.40	1.33
22	R	303	CLA	CMB-C2B	-2.55	1.46	1.51
34	B	621	LMG	O8-C28	2.55	1.40	1.33
22	4	304	CLA	CMB-C2B	-2.55	1.46	1.51
31	k	101	BCR	C16-C17	2.55	1.51	1.43
22	v	302	CLA	CMB-C2B	-2.55	1.46	1.51
26	5	316	CHL	MG-NA	-2.55	2.00	2.06
22	1	305	CLA	CMB-C2B	-2.55	1.46	1.51
34	c	501	LMG	O7-C8	-2.55	1.40	1.46
22	A	404	CLA	CMB-C2B	-2.55	1.46	1.51
22	G	307	CLA	CMB-C2B	-2.55	1.46	1.51
22	p	302	CLA	CMB-C2B	-2.55	1.46	1.51
22	g	307	CLA	CMB-C2B	-2.54	1.46	1.51
31	C	516	BCR	C16-C17	2.54	1.51	1.43
22	u	305	CLA	CMB-C2B	-2.54	1.46	1.51
26	6	301	CHL	C3D-C2D	2.54	1.46	1.39
31	B	620	BCR	C16-C17	2.54	1.51	1.43
26	Q	315	CHL	C1D-C2D	2.54	1.50	1.45
22	D	403	CLA	CMB-C2B	-2.54	1.46	1.51
36	c	517	DGD	O1G-C1G	-2.54	1.39	1.45
25	Q	310	LHG	O7-C5	-2.54	1.40	1.46
25	R	314	LHG	O8-C23	2.54	1.40	1.33
25	1	312	LHG	O7-C5	-2.54	1.40	1.46
22	R	306	CLA	CMB-C2B	-2.54	1.46	1.51
22	b	607	CLA	C3B-C2B	-2.54	1.36	1.40
22	Q	302	CLA	CMB-C2B	-2.54	1.46	1.51
22	n	301	CLA	CMB-C2B	-2.54	1.46	1.51
36	C	519	DGD	O1G-C1A	2.54	1.40	1.33
22	R	302	CLA	CMB-C2B	-2.53	1.46	1.51
25	B	622	LHG	O7-C5	-2.53	1.40	1.46
22	1	304	CLA	CMB-C2B	-2.53	1.46	1.51
26	n	313	CHL	C4B-CHC	2.53	1.48	1.41
22	S	309	CLA	CMB-C2B	-2.53	1.46	1.51
25	v	312	LHG	O7-C5	-2.53	1.40	1.46
22	C	503	CLA	CMD-C2D	-2.53	1.45	1.50
22	C	511	CLA	CMB-C2B	-2.53	1.46	1.51
31	b	619	BCR	C16-C17	2.53	1.51	1.43
22	B	613	CLA	CMC-C2C	-2.53	1.45	1.50
24	U	311	XAT	C24-C23	2.53	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	602	CLA	CMB-C2B	-2.53	1.46	1.51
26	n	318	CHL	MG-NA	-2.53	2.00	2.06
31	z	101	BCR	C16-C17	2.53	1.51	1.43
31	B	619	BCR	C16-C17	2.53	1.51	1.43
26	P	317	CHL	MG-NA	-2.53	2.00	2.06
22	5	301	CLA	CMB-C2B	-2.53	1.46	1.51
31	K	101	BCR	C39-C30	-2.53	1.48	1.53
22	q	303	CLA	CMB-C2B	-2.52	1.46	1.51
34	W	201	LMG	O7-C8	-2.52	1.40	1.46
22	B	602	CLA	CMB-C2B	-2.52	1.46	1.51
22	r	601	CLA	CMB-C2B	-2.52	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.52	1.46	1.51
27	r	618	NEX	C1-C6	-2.52	1.50	1.54
22	1	302	CLA	CMB-C2B	-2.52	1.46	1.51
22	c	503	CLA	CHC-C1C	2.52	1.41	1.35
22	2	304	CLA	CMB-C2B	-2.52	1.46	1.51
22	R	305	CLA	CMB-C2B	-2.52	1.46	1.51
26	u	318	CHL	C1D-C2D	2.52	1.50	1.45
25	b	623	LHG	O8-C23	2.52	1.40	1.33
22	V	307	CLA	CMB-C2B	-2.51	1.46	1.51
22	4	302	CLA	CMB-C2B	-2.51	1.46	1.51
26	U	314	CHL	C1D-ND	-2.51	1.34	1.37
22	S	302	CLA	CMB-C2B	-2.51	1.46	1.51
22	s	302	CLA	CMB-C2B	-2.51	1.46	1.51
25	B	623	LHG	O8-C23	2.51	1.40	1.33
22	v	306	CLA	CMB-C2B	-2.51	1.46	1.51
22	6	302	CLA	CMB-C2B	-2.51	1.46	1.51
22	C	504	CLA	CHC-C1C	2.51	1.41	1.35
22	b	605	CLA	C3B-C2B	-2.51	1.36	1.40
26	6	301	CHL	MG-NA	-2.51	2.00	2.06
22	1	308	CLA	CMB-C2B	-2.51	1.46	1.51
25	c	523	LHG	O8-C23	2.51	1.40	1.33
26	1	316	CHL	MG-NA	-2.51	2.00	2.06
26	v	315	CHL	MG-NA	-2.51	2.00	2.06
22	C	507	CLA	CMB-C2B	-2.51	1.46	1.51
25	C	524	LHG	O8-C23	2.51	1.40	1.33
26	6	317	CHL	MG-NA	-2.50	2.00	2.06
22	4	308	CLA	CMB-C2B	-2.50	1.46	1.51
22	v	307	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.50	1.46	1.51
22	P	303	CLA	CMB-C2B	-2.50	1.46	1.51
25	4	312	LHG	O8-C23	2.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	502	LMG	O8-C28	2.50	1.40	1.33
26	p	316	CHL	MG-NA	-2.50	2.00	2.06
31	k	101	BCR	C39-C30	-2.50	1.48	1.53
22	r	606	CLA	CMB-C2B	-2.50	1.46	1.51
24	g	309	XAT	C4-C3	2.50	1.55	1.52
22	V	302	CLA	CMB-C2B	-2.50	1.46	1.51
26	g	315	CHL	C4B-CHC	2.50	1.47	1.41
22	n	304	CLA	CMB-C2B	-2.50	1.46	1.51
26	6	317	CHL	C4C-C3C	2.50	1.49	1.45
36	a	416	DGD	O1G-C1A	2.50	1.40	1.33
26	2	316	CHL	MG-NA	-2.50	2.00	2.06
26	G	311	CHL	C3D-C2D	2.50	1.45	1.39
25	4	312	LHG	O7-C5	-2.50	1.40	1.46
25	1	312	LHG	O8-C23	2.50	1.40	1.33
26	3	316	CHL	MG-NA	-2.50	2.00	2.06
22	N	307	CLA	CMB-C2B	-2.50	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.50	1.46	1.51
36	A	414	DGD	O1G-C1A	2.49	1.40	1.33
26	p	315	CHL	C1D-ND	-2.49	1.34	1.37
34	c	520	LMG	O7-C8	-2.49	1.40	1.46
33	D	405	PL9	O1-C4	-2.49	1.17	1.23
22	5	305	CLA	C4D-ND	-2.49	1.34	1.37
31	d	403	BCR	C39-C30	-2.49	1.48	1.53
22	3	307	CLA	CMB-C2B	-2.49	1.46	1.51
34	b	624	LMG	O7-C8	-2.49	1.40	1.46
26	p	314	CHL	MG-NA	-2.49	2.00	2.06
22	3	305	CLA	CMB-C2B	-2.49	1.46	1.51
26	4	314	CHL	MG-NA	-2.49	2.00	2.06
22	V	308	CLA	CMB-C2B	-2.49	1.46	1.51
26	6	314	CHL	C1D-ND	-2.49	1.34	1.37
26	P	315	CHL	C1B-CHB	2.49	1.47	1.41
22	g	308	CLA	CMB-C2B	-2.49	1.46	1.51
25	2	312	LHG	O7-C5	-2.49	1.40	1.46
22	P	306	CLA	C4D-ND	-2.49	1.34	1.37
22	3	306	CLA	CMB-C2B	-2.49	1.46	1.51
27	s	317	NEX	C7-C8	-2.49	1.27	1.32
22	6	306	CLA	CMB-C2B	-2.49	1.46	1.51
22	N	308	CLA	CMB-C2B	-2.49	1.46	1.51
26	n	314	CHL	C4B-CHC	2.49	1.47	1.41
22	3	301	CLA	CMB-C2B	-2.49	1.46	1.51
22	R	310	CLA	CMB-C2B	-2.49	1.46	1.51
22	R	307	CLA	CMB-C2B	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	413	LHG	O7-C7	2.48	1.41	1.34
26	q	311	CHL	MG-NA	-2.48	2.00	2.06
22	G	308	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	602	CLA	CMB-C2B	-2.48	1.46	1.51
36	b	601	DGD	O1G-C1A	2.48	1.40	1.33
26	S	315	CHL	C4B-CHC	2.48	1.47	1.41
26	Q	316	CHL	MG-NA	-2.48	2.00	2.06
22	5	308	CLA	CMB-C2B	-2.48	1.46	1.51
34	w	201	LMG	O7-C8	-2.48	1.40	1.46
26	n	318	CHL	C4C-C3C	2.48	1.49	1.45
22	s	306	CLA	CMD-C2D	-2.48	1.45	1.50
25	n	312	LHG	O8-C23	2.48	1.40	1.33
22	6	307	CLA	CMB-C2B	-2.48	1.46	1.51
22	n	307	CLA	CMB-C2B	-2.48	1.46	1.51
22	P	309	CLA	CMB-C2B	-2.48	1.46	1.51
22	s	301	CLA	CMB-C2B	-2.48	1.46	1.51
25	a	415	LHG	O7-C7	2.48	1.41	1.34
22	c	506	CLA	CMB-C2B	-2.48	1.46	1.51
33	d	404	PL9	O1-C4	-2.48	1.18	1.23
25	n	312	LHG	O7-C5	-2.48	1.40	1.46
22	Q	306	CLA	CMB-C2B	-2.47	1.46	1.51
26	3	315	CHL	C1D-ND	-2.47	1.34	1.37
22	v	305	CLA	CMB-C2B	-2.47	1.46	1.51
22	V	305	CLA	CMB-C2B	-2.47	1.46	1.51
22	5	302	CLA	CMB-C2B	-2.47	1.46	1.51
34	C	521	LMG	O7-C8	-2.47	1.40	1.46
22	s	309	CLA	CMB-C2B	-2.47	1.46	1.51
34	c	501	LMG	O8-C28	2.47	1.40	1.33
24	G	309	XAT	C4-C3	2.47	1.55	1.52
22	P	308	CLA	CMB-C2B	-2.47	1.46	1.51
22	a	408	CLA	CMB-C2B	-2.47	1.46	1.51
26	P	316	CHL	MG-NA	-2.47	2.00	2.06
22	b	617	CLA	CMC-C2C	-2.47	1.45	1.50
22	B	607	CLA	C3B-C2B	-2.47	1.36	1.40
25	r	613	LHG	O7-C5	-2.47	1.40	1.46
22	2	307	CLA	CMB-C2B	-2.47	1.46	1.51
22	2	308	CLA	CMB-C2B	-2.47	1.46	1.51
36	B	601	DGD	O1G-C1A	2.47	1.40	1.33
26	3	315	CHL	C1D-C2D	2.47	1.50	1.45
22	2	302	CLA	CMB-C2B	-2.47	1.46	1.51
26	p	317	CHL	MG-NA	-2.47	2.00	2.06
26	4	315	CHL	C1D-ND	-2.47	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	316	CHL	C1D-ND	-2.47	1.34	1.37
24	r	612	XAT	C4-C3	2.46	1.55	1.52
22	p	307	CLA	CMB-C2B	-2.46	1.46	1.51
22	6	308	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.46	1.46	1.51
22	G	306	CLA	CMB-C2B	-2.46	1.46	1.51
22	A	408	CLA	CMB-C2B	-2.46	1.46	1.51
22	p	309	CLA	CMB-C2B	-2.46	1.46	1.51
26	6	313	CHL	C4C-C3C	2.46	1.49	1.45
25	v	312	LHG	O8-C23	2.46	1.40	1.33
22	s	307	CLA	CMB-C2B	-2.46	1.46	1.51
22	r	603	CLA	CMB-C2B	-2.46	1.46	1.51
26	v	313	CHL	MG-NA	-2.46	2.00	2.06
22	4	307	CLA	CMB-C2B	-2.45	1.46	1.51
26	U	315	CHL	C3D-C2D	2.45	1.45	1.39
26	2	314	CHL	C4B-CHC	2.45	1.47	1.41
22	V	306	CLA	CMB-C2B	-2.45	1.46	1.51
22	S	306	CLA	CMD-C2D	-2.45	1.45	1.50
22	1	307	CLA	CMB-C2B	-2.45	1.46	1.51
22	p	308	CLA	CMB-C2B	-2.45	1.46	1.51
36	B	601	DGD	O1G-C1G	-2.45	1.39	1.45
22	N	305	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	505	CLA	C3B-C2B	-2.45	1.37	1.40
26	6	316	CHL	C1D-C2D	2.45	1.50	1.45
22	u	306	CLA	CMD-C2D	-2.45	1.45	1.50
33	D	405	PL9	O2-C1	-2.45	1.18	1.24
25	q	310	LHG	O8-C23	2.45	1.40	1.33
22	5	305	CLA	CMB-C2B	-2.45	1.46	1.51
26	V	315	CHL	C1D-ND	-2.45	1.34	1.37
22	5	307	CLA	CMB-C2B	-2.44	1.46	1.51
26	u	316	CHL	MG-NA	-2.44	2.00	2.06
22	v	304	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.44	1.46	1.51
36	J	101	DGD	O1G-C1G	-2.44	1.39	1.45
27	R	301	NEX	C1-C6	-2.44	1.50	1.54
26	G	315	CHL	C4B-CHC	2.44	1.47	1.41
26	u	313	CHL	MG-NA	-2.44	2.00	2.06
26	q	314	CHL	C1D-C2D	2.44	1.50	1.45
22	n	305	CLA	C1D-ND	2.44	1.40	1.37
22	s	305	CLA	CMB-C2B	-2.44	1.46	1.51
22	r	609	CLA	CMB-C2B	-2.44	1.46	1.51
34	A	411	LMG	O1-C1	-2.44	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	313	XAT	C4-C3	2.44	1.55	1.52
26	s	315	CHL	C4B-CHC	2.44	1.47	1.41
22	q	306	CLA	CMB-C2B	-2.44	1.46	1.51
22	P	306	CLA	C1D-ND	2.43	1.40	1.37
22	q	305	CLA	CMB-C2B	-2.43	1.46	1.51
24	r	612	XAT	C18-C5	2.43	1.55	1.51
36	b	601	DGD	O1G-C1G	-2.43	1.39	1.45
25	5	312	LHG	O8-C23	2.43	1.40	1.33
25	c	522	LHG	O8-C23	2.43	1.40	1.33
22	C	512	CLA	CMD-C2D	-2.43	1.45	1.50
26	v	314	CHL	C4C-C3C	2.43	1.49	1.45
22	B	617	CLA	CMB-C2B	-2.43	1.46	1.51
22	S	301	CLA	CMB-C2B	-2.43	1.46	1.51
26	N	316	CHL	MG-NA	-2.43	2.00	2.06
26	g	312	CHL	MG-NA	-2.43	2.00	2.06
26	u	316	CHL	C3D-C2D	2.43	1.45	1.39
22	c	511	CLA	CMD-C2D	-2.43	1.45	1.50
22	p	306	CLA	C4D-ND	-2.43	1.34	1.37
26	V	313	CHL	C4B-CHC	2.43	1.47	1.41
26	q	314	CHL	C1D-ND	-2.42	1.34	1.37
22	X	202	CLA	CMB-C2B	-2.42	1.46	1.51
27	r	617	NEX	C1-C6	-2.42	1.50	1.54
26	N	317	CHL	MG-NA	-2.42	2.00	2.06
26	V	314	CHL	C4C-C3C	2.42	1.49	1.45
22	x	201	CLA	CMB-C2B	-2.42	1.46	1.51
22	2	305	CLA	CMB-C2B	-2.42	1.46	1.51
26	n	315	CHL	MG-NA	-2.42	2.00	2.06
22	q	308	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	506	CLA	C3B-C2B	-2.42	1.37	1.40
22	N	305	CLA	C1D-ND	2.42	1.40	1.37
25	g	310	LHG	O7-C5	-2.42	1.40	1.46
22	S	304	CLA	CMB-C2B	-2.42	1.46	1.51
25	s	312	LHG	O8-C23	2.42	1.40	1.33
22	A	404	CLA	CMD-C2D	-2.42	1.45	1.50
22	a	404	CLA	CMD-C2D	-2.42	1.45	1.50
22	B	605	CLA	C3B-C2B	-2.42	1.37	1.40
25	V	312	LHG	O8-C23	2.42	1.40	1.33
26	N	317	CHL	C4C-C3C	2.42	1.49	1.45
34	a	412	LMG	O1-C1	-2.42	1.36	1.40
26	s	313	CHL	C4B-CHC	2.42	1.47	1.41
22	Q	305	CLA	CMB-C2B	-2.42	1.46	1.51
22	S	307	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	314	LHG	O7-C5	-2.42	1.40	1.46
34	B	624	LMG	O7-C8	-2.42	1.40	1.46
22	v	308	CLA	CMB-C2B	-2.42	1.46	1.51
22	P	306	CLA	CMB-C2B	-2.42	1.46	1.51
26	1	313	CHL	C1D-ND	-2.42	1.34	1.37
24	R	313	XAT	C18-C5	2.41	1.55	1.51
22	U	306	CLA	CMD-C2D	-2.41	1.45	1.50
22	6	309	CLA	CMB-C2B	-2.41	1.46	1.51
26	3	312	CHL	C4C-C3C	2.41	1.49	1.45
26	Q	315	CHL	C4B-CHC	2.41	1.47	1.41
25	S	312	LHG	O8-C23	2.41	1.40	1.33
22	p	305	CLA	CMB-C2B	-2.41	1.46	1.51
25	C	523	LHG	O8-C23	2.41	1.40	1.33
22	Q	308	CLA	CMB-C2B	-2.41	1.46	1.51
33	d	404	PL9	O2-C1	-2.41	1.18	1.24
22	B	617	CLA	CMC-C2C	-2.41	1.45	1.50
22	s	304	CLA	CMB-C2B	-2.41	1.46	1.51
25	Q	310	LHG	O8-C23	2.41	1.40	1.33
25	g	310	LHG	O8-C23	2.41	1.40	1.33
26	6	313	CHL	C4B-CHC	2.41	1.47	1.41
26	3	314	CHL	C4B-CHC	2.41	1.47	1.41
26	q	312	CHL	C4C-C3C	2.41	1.49	1.45
26	3	312	CHL	C4B-CHC	2.41	1.47	1.41
25	2	312	LHG	O8-C23	2.41	1.40	1.33
26	V	318	CHL	MG-NA	-2.40	2.00	2.06
22	p	306	CLA	CMB-C2B	-2.40	1.46	1.51
22	u	306	CLA	C3B-C2B	-2.40	1.37	1.40
36	A	414	DGD	O1G-C1G	-2.40	1.39	1.45
26	p	315	CHL	C1B-CHB	2.40	1.47	1.41
26	3	313	CHL	C1D-ND	-2.40	1.34	1.37
26	N	314	CHL	C4C-C3C	2.40	1.49	1.45
22	R	308	CLA	CMB-C2B	-2.40	1.46	1.51
31	a	409	BCR	C16-C17	2.40	1.50	1.43
26	S	313	CHL	C4B-CHC	2.40	1.47	1.41
34	W	201	LMG	O1-C1	-2.40	1.36	1.40
26	1	315	CHL	C1D-ND	-2.40	1.34	1.37
31	A	409	BCR	C16-C17	2.40	1.50	1.43
22	R	304	CLA	CMB-C2B	-2.39	1.46	1.51
36	C	519	DGD	O5D-C1E	-2.39	1.36	1.40
36	c	517	DGD	O5D-C1E	-2.39	1.36	1.40
26	6	314	CHL	C4B-CHC	2.39	1.47	1.41
26	V	315	CHL	C4B-CHC	2.39	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	618	BCR	C16-C17	2.39	1.50	1.43
22	S	305	CLA	CMB-C2B	-2.39	1.46	1.51
22	3	308	CLA	CMB-C2B	-2.39	1.46	1.51
36	c	519	DGD	O1G-C1G	-2.39	1.39	1.45
26	3	316	CHL	C4C-C3C	2.39	1.49	1.45
26	6	316	CHL	C4B-CHC	2.39	1.47	1.41
22	Q	304	CLA	CMB-C2B	-2.38	1.46	1.51
26	Q	311	CHL	MG-NA	-2.38	2.00	2.06
26	N	315	CHL	C1D-C2D	2.38	1.50	1.45
34	d	407	LMG	O7-C8	-2.38	1.40	1.46
26	Q	313	CHL	C4C-C3C	2.38	1.49	1.45
34	D	408	LMG	O7-C8	-2.38	1.40	1.46
26	v	315	CHL	C1D-ND	-2.38	1.34	1.37
22	p	306	CLA	C1D-ND	2.38	1.40	1.37
22	R	309	CLA	CMB-C2B	-2.38	1.46	1.51
32	a	410	SQD	O2-C2	-2.38	1.37	1.43
22	g	306	CLA	CMB-C2B	-2.38	1.46	1.51
25	G	310	LHG	O8-C23	2.38	1.40	1.33
26	1	313	CHL	C4B-CHC	2.38	1.47	1.41
25	N	312	LHG	O8-C23	2.38	1.40	1.33
22	n	306	CLA	CMB-C2B	-2.38	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.38	1.45	1.50
22	P	305	CLA	CMB-C2B	-2.37	1.46	1.51
26	q	312	CHL	C4B-CHC	2.37	1.47	1.41
26	3	315	CHL	MG-NA	-2.37	2.00	2.06
26	6	314	CHL	C4C-C3C	2.37	1.49	1.45
31	c	515	BCR	C16-C17	2.37	1.50	1.43
22	Q	307	CLA	CMB-C2B	-2.37	1.46	1.51
26	g	312	CHL	C4C-C3C	2.37	1.49	1.45
26	3	315	CHL	C4B-CHC	2.37	1.47	1.41
26	v	313	CHL	C4B-CHC	2.37	1.47	1.41
22	n	305	CLA	CMB-C2B	-2.37	1.46	1.51
26	G	312	CHL	MG-NA	-2.37	2.00	2.06
26	s	314	CHL	C4C-C3C	2.37	1.49	1.45
25	p	313	LHG	O8-C23	2.37	1.40	1.33
22	q	304	CLA	CMB-C2B	-2.37	1.46	1.51
31	C	517	BCR	C16-C17	2.36	1.50	1.43
25	G	310	LHG	O7-C5	-2.36	1.40	1.46
34	w	201	LMG	O1-C1	-2.36	1.36	1.40
22	b	607	CLA	CMD-C2D	-2.36	1.45	1.50
34	c	520	LMG	O1-C1	-2.36	1.36	1.40
22	g	304	CLA	CMB-C2B	-2.36	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	312	CHL	C4B-CHC	2.36	1.47	1.41
26	v	318	CHL	C4C-C3C	2.36	1.49	1.45
26	3	313	CHL	C4B-CHC	2.36	1.47	1.41
25	D	407	LHG	O8-C23	2.36	1.40	1.33
25	N	312	LHG	O7-C5	-2.36	1.40	1.46
26	q	314	CHL	C4B-CHC	2.36	1.47	1.41
31	b	618	BCR	C16-C17	2.36	1.50	1.43
22	G	304	CLA	CMB-C2B	-2.36	1.46	1.51
26	6	315	CHL	C4B-CHC	2.36	1.47	1.41
26	N	314	CHL	C4B-CHC	2.36	1.47	1.41
26	S	314	CHL	C4C-C3C	2.36	1.49	1.45
25	l	101	LHG	O8-C23	2.36	1.40	1.33
26	2	318	CHL	MG-NA	-2.36	2.00	2.06
22	D	403	CLA	MG-ND	-2.36	2.01	2.05
25	A	413	LHG	O8-C6	-2.36	1.39	1.45
26	G	312	CHL	C4B-CHC	2.36	1.47	1.41
26	v	315	CHL	C4B-CHC	2.36	1.47	1.41
36	a	416	DGD	O1G-C1G	-2.35	1.39	1.45
26	P	316	CHL	C4B-CHC	2.35	1.47	1.41
26	5	318	CHL	MG-NA	-2.35	2.00	2.06
22	C	503	CLA	C3B-C2B	-2.35	1.37	1.40
26	5	314	CHL	C4B-CHC	2.35	1.47	1.41
22	P	307	CLA	CMB-C2B	-2.35	1.46	1.51
25	P	313	LHG	O8-C23	2.35	1.40	1.33
22	q	307	CLA	CMB-C2B	-2.35	1.46	1.51
22	b	613	CLA	CMD-C2D	-2.35	1.45	1.50
26	2	314	CHL	C4C-C3C	2.35	1.49	1.45
26	p	319	CHL	MG-NA	-2.35	2.00	2.06
22	A	405	CLA	CMD-C2D	-2.35	1.45	1.50
25	C	522	LHG	O8-C23	2.35	1.40	1.33
26	s	316	CHL	C4B-CHC	2.35	1.47	1.41
22	c	513	CLA	CMD-C2D	-2.35	1.45	1.50
26	v	317	CHL	C4B-CHC	2.35	1.47	1.41
22	B	609	CLA	CMD-C2D	-2.35	1.45	1.50
22	B	606	CLA	C3B-C2B	-2.35	1.37	1.40
26	g	314	CHL	C4B-CHC	2.35	1.47	1.41
26	N	315	CHL	C1D-ND	-2.35	1.34	1.37
33	A	410	PL9	O1-C4	-2.35	1.18	1.24
22	6	305	CLA	CMB-C2B	-2.35	1.46	1.51
25	L	101	LHG	O8-C23	2.35	1.40	1.33
26	r	616	CHL	C4B-CHC	2.34	1.47	1.41
22	V	304	CLA	CMB-C2B	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	521	LMG	O1-C1	-2.34	1.36	1.40
22	d	402	CLA	MG-ND	-2.34	2.01	2.05
26	S	316	CHL	C4B-CHC	2.34	1.47	1.41
22	2	306	CLA	CMB-C2B	-2.34	1.46	1.51
22	N	306	CLA	CMB-C2B	-2.34	1.46	1.51
22	r	608	CLA	CMB-C2B	-2.34	1.46	1.51
22	a	405	CLA	CMD-C2D	-2.34	1.45	1.50
30	a	407	PHO	CMC-C2C	-2.34	1.46	1.51
30	d	401	PHO	CMC-C2C	-2.34	1.46	1.51
32	C	501	SQD	O2-C2	-2.34	1.37	1.43
26	R	316	CHL	C4C-C3C	2.34	1.49	1.45
22	D	403	CLA	CMC-C2C	-2.34	1.45	1.50
26	3	313	CHL	C4C-C3C	2.34	1.49	1.45
26	V	315	CHL	C1B-CHB	2.34	1.47	1.41
25	a	415	LHG	O8-C6	-2.33	1.39	1.45
30	A	407	PHO	CMC-C2C	-2.33	1.46	1.51
26	5	317	CHL	MG-NA	-2.33	2.00	2.06
36	c	518	DGD	O1G-C1G	-2.33	1.39	1.45
26	Q	312	CHL	C4C-C3C	2.33	1.49	1.45
26	G	312	CHL	C4C-C3C	2.33	1.49	1.45
26	S	315	CHL	C1D-ND	-2.33	1.34	1.37
26	5	316	CHL	C1D-ND	-2.33	1.34	1.37
26	R	317	CHL	C4B-CHC	2.33	1.47	1.41
22	c	509	CLA	CMD-C2D	-2.33	1.45	1.50
22	B	613	CLA	CMD-C2D	-2.33	1.45	1.50
26	4	316	CHL	MG-NA	-2.33	2.00	2.06
26	g	314	CHL	C4C-C3C	2.33	1.49	1.45
26	Q	314	CHL	C4B-CHC	2.33	1.47	1.41
25	d	406	LHG	O8-C23	2.33	1.40	1.33
26	g	313	CHL	C4C-C3C	2.32	1.49	1.45
26	U	319	CHL	C4B-CHC	2.32	1.47	1.41
22	3	304	CLA	CMB-C2B	-2.32	1.46	1.51
22	b	606	CLA	C3B-C2B	-2.32	1.37	1.40
26	r	615	CHL	C4C-C3C	2.32	1.49	1.45
22	U	301	CLA	CMC-C2C	-2.32	1.45	1.50
22	d	402	CLA	CMC-C2C	-2.32	1.45	1.50
26	V	314	CHL	C4B-CHC	2.32	1.47	1.41
22	a	408	CLA	CMD-C2D	-2.32	1.45	1.50
26	g	316	CHL	MG-NA	-2.32	2.00	2.06
30	D	401	PHO	CMC-C2C	-2.32	1.46	1.51
25	3	310	LHG	O8-C6	-2.32	1.39	1.45
26	S	314	CHL	C4B-CHC	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	311	LHG	O8-C23	2.31	1.40	1.33
22	C	510	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	603	CLA	C3B-C2B	-2.31	1.37	1.40
22	S	309	CLA	CMD-C2D	-2.31	1.45	1.50
22	b	604	CLA	C3B-C2B	-2.31	1.37	1.40
22	A	408	CLA	CMD-C2D	-2.31	1.45	1.50
34	B	621	LMG	O1-C7	-2.31	1.39	1.43
26	4	313	CHL	C1D-ND	-2.31	1.34	1.37
26	V	316	CHL	C4B-CHC	2.31	1.47	1.41
26	2	318	CHL	C4C-C3C	2.31	1.49	1.45
26	v	316	CHL	MG-NA	-2.31	2.00	2.06
22	c	508	CLA	CMD-C2D	-2.31	1.45	1.50
22	R	303	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	614	CLA	CMC-C2C	-2.31	1.45	1.50
24	N	311	XAT	C20-C13	2.31	1.55	1.50
25	d	406	LHG	O8-C6	-2.31	1.39	1.45
22	u	304	CLA	CMC-C2C	-2.31	1.45	1.50
25	D	406	LHG	O8-C6	-2.31	1.39	1.45
36	C	520	DGD	O1G-C1G	-2.31	1.39	1.45
26	1	318	CHL	MG-NA	-2.31	2.00	2.06
22	b	607	CLA	CMC-C2C	-2.31	1.45	1.50
26	6	316	CHL	MG-NA	-2.31	2.00	2.06
25	c	521	LHG	O8-C23	2.31	1.40	1.33
22	C	509	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	607	CLA	CMC-C2C	-2.31	1.45	1.50
22	B	611	CLA	C3B-C2B	-2.31	1.37	1.40
22	b	609	CLA	CMD-C2D	-2.31	1.45	1.50
25	c	521	LHG	O8-C6	-2.31	1.39	1.45
25	N	312	LHG	O7-C7	2.30	1.40	1.34
26	R	315	CHL	C4C-C3C	2.30	1.49	1.45
26	2	316	CHL	C1D-ND	-2.30	1.35	1.37
26	s	314	CHL	C4B-CHC	2.30	1.47	1.41
33	a	411	PL9	O1-C4	-2.30	1.18	1.24
26	P	317	CHL	C4B-CHC	2.30	1.47	1.41
26	G	316	CHL	MG-NA	-2.30	2.00	2.06
22	B	604	CLA	C3B-C2B	-2.30	1.37	1.40
26	U	313	CHL	C4B-CHC	2.30	1.47	1.41
26	p	316	CHL	C4B-CHC	2.30	1.47	1.41
26	r	616	CHL	MG-NA	-2.30	2.00	2.06
22	u	301	CLA	CMC-C2C	-2.30	1.45	1.50
22	C	511	CLA	CMD-C2D	-2.30	1.45	1.50
26	r	614	CHL	C4B-CHC	2.30	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	407	LMG	O1-C1	-2.30	1.36	1.40
22	c	502	CLA	C3B-C2B	-2.30	1.37	1.40
25	6	311	LHG	O8-C6	-2.29	1.39	1.45
22	B	603	CLA	CMD-C2D	-2.29	1.45	1.50
34	D	408	LMG	O1-C1	-2.29	1.36	1.40
22	c	510	CLA	CMD-C2D	-2.29	1.45	1.50
26	Q	312	CHL	MG-NA	-2.29	2.00	2.06
26	5	314	CHL	C4C-C3C	2.29	1.49	1.45
22	u	303	CLA	C3B-C2B	-2.29	1.37	1.40
22	5	306	CLA	CMB-C2B	-2.29	1.46	1.51
22	C	507	CLA	CMD-C2D	-2.29	1.45	1.50
25	U	312	LHG	O8-C23	2.29	1.40	1.33
26	Q	315	CHL	C1D-ND	-2.29	1.35	1.37
26	u	316	CHL	C4B-CHC	2.29	1.47	1.41
24	q	309	XAT	C20-C13	2.29	1.55	1.50
26	P	314	CHL	C1D-ND	-2.29	1.35	1.37
26	N	314	CHL	C1D-ND	-2.29	1.35	1.37
25	D	407	LHG	O8-C6	-2.28	1.39	1.45
26	4	316	CHL	C4C-C3C	2.28	1.49	1.45
22	C	508	CLA	CMD-C2D	-2.28	1.46	1.50
26	3	311	CHL	C4B-CHC	2.28	1.47	1.41
25	d	405	LHG	O8-C6	-2.28	1.39	1.45
26	p	317	CHL	C4B-CHC	2.28	1.47	1.41
22	C	512	CLA	C3B-C2B	-2.28	1.37	1.40
26	Q	313	CHL	MG-NA	-2.28	2.00	2.06
26	G	314	CHL	C4B-CHC	2.28	1.47	1.41
30	D	401	PHO	CMD-C2D	-2.28	1.46	1.51
26	6	312	CHL	C4B-CHC	2.28	1.47	1.41
26	6	313	CHL	C1B-CHB	2.28	1.47	1.41
25	B	622	LHG	O8-C6	-2.28	1.40	1.45
26	v	314	CHL	C4B-CHC	2.28	1.47	1.41
26	6	316	CHL	C4C-C3C	2.28	1.49	1.45
25	4	312	LHG	O7-C7	2.28	1.40	1.34
26	S	316	CHL	C1D-ND	-2.28	1.35	1.37
26	V	317	CHL	C4B-CHC	2.28	1.47	1.41
26	S	316	CHL	C1B-CHB	2.28	1.47	1.41
26	6	312	CHL	MG-NA	-2.28	2.00	2.06
22	b	603	CLA	CMD-C2D	-2.28	1.46	1.50
24	5	311	XAT	C20-C13	2.28	1.55	1.50
22	C	514	CLA	CMD-C2D	-2.28	1.46	1.50
24	Q	309	XAT	C20-C13	2.28	1.55	1.50
25	3	310	LHG	O8-C23	2.27	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	622	LHG	O8-C6	-2.27	1.40	1.45
22	b	614	CLA	CMC-C2C	-2.27	1.46	1.50
22	C	504	CLA	CMC-C2C	-2.27	1.46	1.50
22	U	308	CLA	C3B-C2B	-2.27	1.37	1.40
26	n	314	CHL	C1B-CHB	2.27	1.47	1.41
26	2	315	CHL	MG-NA	-2.27	2.00	2.06
26	n	316	CHL	C4B-CHC	2.27	1.47	1.41
22	c	506	CLA	CMD-C2D	-2.27	1.46	1.50
26	3	312	CHL	C1B-CHB	2.27	1.47	1.41
22	u	308	CLA	C3B-C2B	-2.27	1.37	1.40
26	3	311	CHL	MG-NA	-2.27	2.00	2.06
26	s	316	CHL	C1B-CHB	2.27	1.47	1.41
26	2	315	CHL	C4B-CHC	2.27	1.47	1.41
22	U	304	CLA	CMC-C2C	-2.27	1.46	1.50
26	v	317	CHL	C4C-C3C	2.27	1.48	1.45
26	U	317	CHL	C4C-C3C	2.27	1.48	1.45
22	b	617	CLA	MG-ND	-2.27	2.01	2.05
22	R	302	CLA	CMC-C2C	-2.27	1.46	1.50
26	q	313	CHL	C4C-C3C	2.27	1.48	1.45
22	U	303	CLA	C3B-C2B	-2.27	1.37	1.40
26	p	319	CHL	C4C-C3C	2.27	1.48	1.45
26	p	318	CHL	MG-NA	-2.27	2.00	2.06
24	p	312	XAT	C20-C13	2.27	1.55	1.50
26	5	315	CHL	C4B-CHC	2.27	1.47	1.41
26	5	313	CHL	C1D-ND	-2.27	1.35	1.37
26	u	315	CHL	C4B-CHC	2.27	1.47	1.41
22	U	302	CLA	CMD-C2D	-2.27	1.46	1.50
24	V	311	XAT	C20-C13	2.26	1.55	1.50
26	5	318	CHL	C4C-C3C	2.26	1.48	1.45
26	V	318	CHL	C4C-C3C	2.26	1.48	1.45
22	r	602	CLA	CMD-C2D	-2.26	1.46	1.50
36	b	601	DGD	O2G-C2G	-2.26	1.40	1.46
32	l	102	SQD	O2-C2	-2.26	1.37	1.43
26	P	319	CHL	MG-NA	-2.26	2.00	2.06
22	n	303	CLA	CMD-C2D	-2.26	1.46	1.50
22	b	611	CLA	C3B-C2B	-2.26	1.37	1.40
26	4	317	CHL	MG-NA	-2.26	2.00	2.06
22	U	308	CLA	CMD-C2D	-2.26	1.46	1.50
24	R	313	XAT	C24-C23	2.26	1.55	1.52
22	u	308	CLA	CMD-C2D	-2.26	1.46	1.50
22	A	406	CLA	C3B-C2B	-2.26	1.37	1.40
22	c	507	CLA	CMD-C2D	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	519	DGD	O2G-C2G	-2.26	1.40	1.46
26	n	315	CHL	C4C-C3C	2.26	1.48	1.45
26	r	614	CHL	C4C-C3C	2.26	1.48	1.45
26	r	619	CHL	C4B-CHC	2.26	1.47	1.41
22	5	303	CLA	CMD-C2D	-2.26	1.46	1.50
26	S	315	CHL	C1B-CHB	2.26	1.47	1.41
30	d	401	PHO	CMD-C2D	-2.26	1.46	1.51
26	R	317	CHL	MG-NA	-2.26	2.00	2.06
22	g	307	CLA	CMD-C2D	-2.26	1.46	1.50
26	n	314	CHL	C1D-ND	-2.26	1.35	1.37
24	2	311	XAT	C40-C33	2.26	1.55	1.50
26	G	313	CHL	C4C-C3C	2.26	1.48	1.45
22	V	301	CLA	C3B-C2B	-2.26	1.37	1.40
26	u	313	CHL	C4B-CHC	2.26	1.47	1.41
26	1	314	CHL	C1D-ND	-2.26	1.35	1.37
25	P	313	LHG	O8-C6	-2.26	1.40	1.45
26	s	315	CHL	C1D-ND	-2.26	1.35	1.37
25	u	312	LHG	O8-C23	2.26	1.39	1.33
26	2	317	CHL	MG-NA	-2.26	2.00	2.06
26	V	317	CHL	MG-NA	-2.25	2.00	2.06
26	4	315	CHL	C4C-C3C	2.25	1.48	1.45
22	b	616	CLA	C3B-C2B	-2.25	1.37	1.40
26	1	315	CHL	C4B-CHC	2.25	1.47	1.41
26	s	316	CHL	C1D-ND	-2.25	1.35	1.37
22	s	309	CLA	CMD-C2D	-2.25	1.46	1.50
25	B	622	LHG	O8-C23	2.25	1.39	1.33
22	A	405	CLA	C3B-C2B	-2.25	1.37	1.40
24	r	612	XAT	C24-C23	2.25	1.55	1.52
36	c	517	DGD	O2G-C2G	-2.25	1.41	1.46
32	A	412	SQD	O2-C2	-2.25	1.37	1.43
26	P	319	CHL	C4C-C3C	2.25	1.48	1.45
26	n	317	CHL	C4C-C3C	2.25	1.48	1.45
25	d	406	LHG	O7-C7	2.25	1.40	1.34
24	P	312	XAT	C20-C13	2.25	1.55	1.50
22	a	406	CLA	C3B-C2B	-2.25	1.37	1.40
26	p	314	CHL	C1D-ND	-2.25	1.35	1.37
25	G	310	LHG	O7-C7	2.25	1.40	1.34
24	N	311	XAT	C40-C33	2.25	1.55	1.50
22	c	512	CLA	C3B-C2B	-2.25	1.37	1.40
22	G	307	CLA	CMD-C2D	-2.25	1.46	1.50
22	s	301	CLA	CMC-C2C	-2.25	1.46	1.50
26	1	317	CHL	MG-NA	-2.25	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	301	CLA	C3B-C2B	-2.25	1.37	1.40
22	c	513	CLA	MG-ND	-2.25	2.01	2.05
22	A	406	CLA	CMD-C2D	-2.25	1.46	1.50
26	5	316	CHL	C4B-CHC	2.25	1.47	1.41
22	c	512	CLA	CMD-C2D	-2.24	1.46	1.50
25	n	312	LHG	O7-C7	2.24	1.40	1.34
37	e	101	HEM	FE-NB	2.24	2.08	1.96
26	n	315	CHL	C4B-CHC	2.24	1.47	1.41
25	D	406	LHG	O8-C23	2.24	1.39	1.33
24	r	612	XAT	C20-C13	2.24	1.55	1.50
22	B	602	CLA	CMD-C2D	-2.24	1.46	1.50
22	b	602	CLA	CMD-C2D	-2.24	1.46	1.50
22	c	507	CLA	C3B-CAB	-2.24	1.43	1.47
22	c	511	CLA	C3B-C2B	-2.24	1.37	1.40
26	q	314	CHL	C4C-C3C	2.24	1.48	1.45
26	V	317	CHL	C4C-C3C	2.24	1.48	1.45
22	C	508	CLA	C3B-CAB	-2.24	1.43	1.47
24	n	311	XAT	C20-C13	2.24	1.55	1.50
22	2	302	CLA	CMD-C2D	-2.24	1.46	1.50
26	u	314	CHL	C4B-CHC	2.24	1.47	1.41
26	P	316	CHL	C4C-C3C	2.24	1.48	1.45
26	4	315	CHL	C4B-CHC	2.24	1.47	1.41
26	6	314	CHL	C1B-CHB	2.24	1.47	1.41
32	L	102	SQD	O2-C2	-2.24	1.37	1.43
22	g	305	CLA	C3B-C2B	-2.24	1.37	1.40
26	g	316	CHL	C4C-C3C	2.24	1.48	1.45
26	U	314	CHL	C4B-CHC	2.24	1.47	1.41
26	u	318	CHL	C4B-CHC	2.24	1.47	1.41
26	n	318	CHL	C1D-ND	-2.24	1.35	1.37
26	v	315	CHL	C1B-CHB	2.24	1.47	1.41
26	R	315	CHL	C4B-CHC	2.24	1.47	1.41
25	d	405	LHG	O8-C23	2.24	1.39	1.33
25	D	407	LHG	O7-C7	2.24	1.40	1.34
22	S	301	CLA	CMC-C2C	-2.24	1.46	1.50
26	g	311	CHL	C4B-CHC	2.24	1.47	1.41
26	U	316	CHL	MG-NA	-2.24	2.01	2.06
22	B	612	CLA	CMD-C2D	-2.24	1.46	1.50
26	U	313	CHL	C1D-ND	-2.24	1.35	1.37
26	G	314	CHL	C4C-C3C	2.24	1.48	1.45
22	b	612	CLA	CMD-C2D	-2.24	1.46	1.50
26	u	317	CHL	MG-NA	-2.24	2.01	2.06
26	r	616	CHL	C1D-ND	-2.24	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	317	CHL	C1D-ND	-2.24	1.35	1.37
22	C	505	CLA	MG-ND	-2.24	2.01	2.05
26	P	318	CHL	MG-NA	-2.23	2.01	2.06
26	q	315	CHL	C4B-CHC	2.23	1.47	1.41
22	4	306	CLA	CMD-C2D	-2.23	1.46	1.50
26	v	318	CHL	MG-NA	-2.23	2.01	2.06
26	s	316	CHL	C4C-C3C	2.23	1.48	1.45
22	c	503	CLA	CMC-C2C	-2.23	1.46	1.50
22	C	514	CLA	MG-ND	-2.23	2.01	2.05
26	V	315	CHL	C4C-C3C	2.23	1.48	1.45
25	v	312	LHG	O7-C7	2.23	1.40	1.34
22	B	616	CLA	C3B-C2B	-2.23	1.37	1.40
25	U	312	LHG	O8-C6	-2.23	1.40	1.45
22	n	307	CLA	CMD-C2D	-2.23	1.46	1.50
25	b	622	LHG	O8-C23	2.23	1.39	1.33
24	2	311	XAT	C20-C13	2.23	1.55	1.50
22	U	307	CLA	CMC-C2C	-2.23	1.46	1.50
32	a	413	SQD	O2-C2	-2.23	1.37	1.43
26	v	316	CHL	C4B-CHC	2.23	1.47	1.41
22	1	306	CLA	CMD-C2D	-2.23	1.46	1.50
25	B	622	LHG	O7-C7	2.23	1.40	1.34
26	s	313	CHL	C4C-C3C	2.23	1.48	1.45
25	C	522	LHG	O8-C6	-2.23	1.40	1.45
22	2	303	CLA	CMD-C2D	-2.23	1.46	1.50
22	n	304	CLA	CMD-C2D	-2.23	1.46	1.50
24	v	311	XAT	C20-C13	2.23	1.55	1.50
25	u	312	LHG	O8-C6	-2.22	1.40	1.45
26	R	317	CHL	C1D-ND	-2.22	1.35	1.37
26	2	316	CHL	C4B-CHC	2.22	1.47	1.41
22	n	305	CLA	C4D-ND	-2.22	1.34	1.37
26	6	315	CHL	C1D-ND	-2.22	1.35	1.37
26	S	316	CHL	C4C-C3C	2.22	1.48	1.45
36	B	601	DGD	O2G-C2G	-2.22	1.41	1.46
26	3	313	CHL	C1B-CHB	2.22	1.47	1.41
34	c	520	LMG	O1-C7	-2.22	1.39	1.43
25	1	312	LHG	O7-C7	2.22	1.40	1.34
26	g	312	CHL	C4B-CHC	2.22	1.47	1.41
24	3	309	XAT	C20-C13	2.22	1.55	1.50
26	U	314	CHL	C1D-C2D	2.22	1.49	1.45
24	6	310	XAT	C20-C13	2.22	1.55	1.50
25	g	310	LHG	O7-C7	2.22	1.40	1.34
26	S	313	CHL	C4C-C3C	2.22	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v	317	CHL	MG-NA	-2.22	2.01	2.06
22	a	405	CLA	C3B-C2B	-2.22	1.37	1.40
25	L	101	LHG	O8-C6	-2.22	1.40	1.45
26	V	313	CHL	C4C-C3C	2.22	1.48	1.45
26	R	317	CHL	C4C-C3C	2.22	1.48	1.45
34	b	621	LMG	O1-C1	-2.22	1.36	1.40
24	5	311	XAT	C40-C33	2.22	1.55	1.50
26	q	312	CHL	C1B-CHB	2.22	1.47	1.41
24	4	311	XAT	C20-C13	2.22	1.55	1.50
24	V	311	XAT	C40-C33	2.22	1.55	1.50
22	c	504	CLA	MG-ND	-2.22	2.01	2.05
26	4	313	CHL	C4B-CHC	2.22	1.47	1.41
26	G	311	CHL	C4B-CHC	2.22	1.47	1.41
22	C	504	CLA	CMD-C2D	-2.21	1.46	1.50
22	C	505	CLA	CMD-C2D	-2.21	1.46	1.50
37	E	101	HEM	FE-NB	2.21	2.07	1.96
26	3	314	CHL	C1D-ND	-2.21	1.35	1.37
26	G	316	CHL	C4C-C3C	2.21	1.48	1.45
23	4	310	LUT	C1-C6	-2.21	1.50	1.53
26	V	318	CHL	C4B-CHC	2.21	1.47	1.41
22	c	503	CLA	CMD-C2D	-2.21	1.46	1.50
24	p	312	XAT	C40-C33	2.21	1.55	1.50
26	s	315	CHL	C1B-CHB	2.21	1.47	1.41
25	p	313	LHG	O7-C7	2.21	1.40	1.34
22	1	304	CLA	MG-ND	-2.21	2.01	2.05
26	1	314	CHL	C4B-CHC	2.21	1.47	1.41
24	P	312	XAT	C40-C33	2.21	1.55	1.50
26	V	316	CHL	C4C-C3C	2.21	1.48	1.45
25	N	312	LHG	O8-C6	-2.21	1.40	1.45
34	b	624	LMG	O1-C1	-2.21	1.36	1.40
26	N	313	CHL	C4B-CHC	2.21	1.47	1.41
25	l	101	LHG	O8-C6	-2.21	1.40	1.45
26	G	314	CHL	C1D-ND	-2.21	1.35	1.37
22	S	307	CLA	CMD-C2D	-2.21	1.46	1.50
22	g	303	CLA	CMD-C2D	-2.21	1.46	1.50
22	C	513	CLA	C3B-C2B	-2.21	1.37	1.40
22	a	406	CLA	CMD-C2D	-2.20	1.46	1.50
22	c	504	CLA	CMD-C2D	-2.20	1.46	1.50
26	V	313	CHL	C1B-CHB	2.20	1.47	1.41
26	3	312	CHL	C2C-C1C	2.20	1.49	1.44
26	U	319	CHL	C1D-ND	-2.20	1.35	1.37
25	Q	310	LHG	O8-C6	-2.20	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p	316	CHL	C4C-C3C	2.20	1.48	1.45
22	B	611	CLA	CMD-C2D	-2.20	1.46	1.50
26	Q	311	CHL	C4B-CHC	2.20	1.47	1.41
25	p	313	LHG	O8-C6	-2.20	1.40	1.45
22	c	507	CLA	CMC-C2C	-2.20	1.46	1.50
22	C	503	CLA	CMC-C2C	-2.20	1.46	1.50
22	C	513	CLA	CMD-C2D	-2.20	1.46	1.50
26	Q	315	CHL	C4C-C3C	2.20	1.48	1.45
22	u	302	CLA	CMD-C2D	-2.20	1.46	1.50
25	V	312	LHG	O7-C7	2.20	1.40	1.34
22	P	303	CLA	CMD-C2D	-2.20	1.46	1.50
24	4	311	XAT	C40-C33	2.20	1.55	1.50
25	b	622	LHG	O7-C7	2.20	1.40	1.34
30	a	407	PHO	CBD-CGD	-2.20	1.49	1.52
22	b	616	CLA	C3B-CAB	-2.20	1.43	1.47
26	G	311	CHL	C4C-C3C	2.20	1.48	1.45
24	Q	309	XAT	C40-C33	2.20	1.55	1.50
26	U	316	CHL	C1D-ND	-2.20	1.35	1.37
22	2	305	CLA	C1D-ND	2.20	1.40	1.37
22	5	305	CLA	C1D-ND	2.20	1.40	1.37
30	A	407	PHO	CBD-CGD	-2.19	1.49	1.52
24	R	313	XAT	C20-C13	2.19	1.55	1.50
26	2	316	CHL	C4C-C3C	2.19	1.48	1.45
26	2	314	CHL	C1B-CHB	2.19	1.47	1.41
24	q	309	XAT	C40-C33	2.19	1.55	1.50
26	N	315	CHL	MG-NA	-2.19	2.01	2.06
24	n	311	XAT	C40-C33	2.19	1.55	1.50
26	G	312	CHL	C4D-CHA	2.19	1.46	1.38
26	1	317	CHL	C4C-C3C	2.19	1.48	1.45
26	U	315	CHL	MG-NA	-2.19	2.01	2.06
26	6	301	CHL	C4B-CHC	2.19	1.47	1.41
22	x	201	CLA	CMD-C2D	-2.19	1.46	1.50
26	N	314	CHL	C1B-CHB	2.19	1.47	1.41
26	G	315	CHL	C2C-C1C	2.19	1.49	1.44
22	c	502	CLA	CMC-C2C	-2.19	1.46	1.50
25	v	312	LHG	O8-C6	-2.19	1.40	1.45
26	N	316	CHL	C4B-CHC	2.19	1.47	1.41
25	c	521	LHG	O7-C7	2.19	1.40	1.34
22	B	615	CLA	CMD-C2D	-2.19	1.46	1.50
26	1	315	CHL	C4C-C3C	2.19	1.48	1.45
26	u	314	CHL	C4C-C3C	2.19	1.48	1.45
26	G	312	CHL	C2C-C1C	2.19	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	313	CHL	C1D-ND	-2.19	1.35	1.37
26	r	616	CHL	C4C-C3C	2.18	1.48	1.45
26	N	315	CHL	C4B-CHC	2.18	1.47	1.41
26	6	313	CHL	C4D-CHA	2.18	1.46	1.38
26	n	317	CHL	C4B-CHC	2.18	1.47	1.41
22	G	301	CLA	CMC-C2C	-2.18	1.46	1.50
22	2	301	CLA	CMC-C2C	-2.18	1.46	1.50
22	b	611	CLA	CMC-C2C	-2.18	1.46	1.50
24	6	310	XAT	C40-C33	2.18	1.55	1.50
22	P	308	CLA	CMD-C2D	-2.18	1.46	1.50
22	u	307	CLA	CMC-C2C	-2.18	1.46	1.50
22	b	615	CLA	CMD-C2D	-2.18	1.46	1.50
24	P	312	XAT	C28-C27	2.18	1.37	1.32
22	q	307	CLA	CMD-C2D	-2.18	1.46	1.50
22	C	515	CLA	CMD-C2D	-2.18	1.46	1.50
22	X	202	CLA	CMD-C2D	-2.18	1.46	1.50
22	a	408	CLA	CMC-C2C	-2.18	1.46	1.50
26	n	317	CHL	C1B-CHB	2.18	1.47	1.41
22	a	404	CLA	MG-ND	-2.18	2.01	2.05
22	N	302	CLA	CMD-C2D	-2.18	1.46	1.50
26	p	320	CHL	MG-NA	-2.18	2.01	2.06
25	2	312	LHG	O8-C6	-2.18	1.40	1.45
32	C	501	SQD	O3-C3	-2.18	1.37	1.43
22	A	404	CLA	MG-ND	-2.18	2.01	2.05
22	Q	305	CLA	CMD-C2D	-2.18	1.46	1.50
26	N	317	CHL	C1D-ND	-2.18	1.35	1.37
22	5	302	CLA	CMD-C2D	-2.18	1.46	1.50
22	b	611	CLA	CMD-C2D	-2.18	1.46	1.50
26	2	313	CHL	C1D-ND	-2.18	1.35	1.37
22	B	616	CLA	C3B-CAB	-2.17	1.43	1.47
26	2	314	CHL	C1D-ND	-2.17	1.35	1.37
22	B	609	CLA	MG-ND	-2.17	2.01	2.05
30	a	407	PHO	CMD-C2D	-2.17	1.46	1.51
26	1	316	CHL	C4B-CHC	2.17	1.47	1.41
26	p	317	CHL	C1D-ND	-2.17	1.35	1.37
36	b	601	DGD	O3G-C1D	-2.17	1.36	1.40
26	U	315	CHL	C4B-CHC	2.17	1.47	1.41
26	s	313	CHL	C1B-CHB	2.17	1.47	1.41
22	u	305	CLA	CMD-C2D	-2.17	1.46	1.50
34	b	621	LMG	O1-C7	-2.17	1.39	1.43
26	n	315	CHL	C1B-CHB	2.17	1.47	1.41
26	v	318	CHL	C1D-ND	-2.17	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	318	CHL	C1D-ND	-2.17	1.35	1.37
26	g	313	CHL	C4B-CHC	2.17	1.47	1.41
24	U	311	XAT	C28-C27	2.17	1.37	1.32
22	u	302	CLA	C3B-C2B	-2.17	1.37	1.40
26	p	314	CHL	C2C-C1C	2.17	1.49	1.44
22	C	506	CLA	CMD-C2D	-2.17	1.46	1.50
26	4	317	CHL	C4C-C3C	2.17	1.48	1.45
26	2	314	CHL	C4D-CHA	2.17	1.46	1.38
26	n	317	CHL	C1D-ND	-2.17	1.35	1.37
22	Q	301	CLA	CMD-C2D	-2.17	1.46	1.50
24	Q	309	XAT	C8-C7	2.17	1.37	1.32
24	1	311	XAT	C20-C13	2.17	1.55	1.50
24	3	309	XAT	C40-C33	2.17	1.55	1.50
26	U	314	CHL	MG-NA	-2.17	2.01	2.06
25	V	312	LHG	O8-C6	-2.17	1.40	1.45
26	Q	312	CHL	C1B-CHB	2.17	1.47	1.41
26	5	315	CHL	MG-NA	-2.17	2.01	2.06
24	v	311	XAT	C40-C33	2.17	1.55	1.50
22	b	608	CLA	CMD-C2D	-2.17	1.46	1.50
24	3	309	XAT	C28-C27	2.17	1.37	1.32
26	U	313	CHL	C4C-C3C	2.17	1.48	1.45
22	N	307	CLA	CMD-C2D	-2.17	1.46	1.50
26	Q	316	CHL	C4B-CHC	2.17	1.47	1.41
24	U	311	XAT	C40-C33	2.17	1.55	1.50
22	v	306	CLA	CMD-C2D	-2.16	1.46	1.50
26	u	317	CHL	C4C-C3C	2.16	1.48	1.45
25	G	310	LHG	O8-C6	-2.16	1.40	1.45
26	p	316	CHL	C1D-ND	-2.16	1.35	1.37
22	r	606	CLA	CMD-C2D	-2.16	1.46	1.50
26	n	314	CHL	C4C-C3C	2.16	1.48	1.45
22	b	603	CLA	C3B-C2B	-2.16	1.37	1.40
26	G	313	CHL	C4B-CHC	2.16	1.47	1.41
26	r	619	CHL	MG-NA	-2.16	2.01	2.06
26	3	312	CHL	C4D-CHA	2.16	1.46	1.38
22	R	305	CLA	CMD-C2D	-2.16	1.46	1.50
24	u	311	XAT	C28-C27	2.16	1.37	1.32
26	v	315	CHL	C4C-C3C	2.16	1.48	1.45
25	2	312	LHG	O7-C7	2.16	1.40	1.34
26	V	316	CHL	C1D-ND	-2.16	1.35	1.37
26	P	316	CHL	C1D-ND	-2.16	1.35	1.37
22	C	509	CLA	CMC-C2C	-2.16	1.46	1.50
26	4	314	CHL	C4B-CHC	2.16	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	315	CHL	C1B-CHB	2.16	1.47	1.41
26	3	315	CHL	C4C-C3C	2.16	1.48	1.45
30	A	407	PHO	CMB-C2B	-2.16	1.46	1.51
22	C	504	CLA	CAC-C3C	-2.16	1.45	1.51
22	p	308	CLA	CMD-C2D	-2.16	1.46	1.50
22	C	508	CLA	CMC-C2C	-2.16	1.46	1.50
26	V	316	CHL	C1B-CHB	2.16	1.47	1.41
26	5	315	CHL	C4C-C3C	2.16	1.48	1.45
22	b	603	CLA	C3B-CAB	-2.16	1.43	1.47
24	p	312	XAT	C28-C27	2.16	1.37	1.32
26	v	316	CHL	C1D-ND	-2.16	1.35	1.37
25	C	522	LHG	O7-C7	2.16	1.40	1.34
22	U	305	CLA	CMD-C2D	-2.16	1.46	1.50
26	n	313	CHL	C1B-CHB	2.16	1.47	1.41
25	B	623	LHG	O7-C7	2.16	1.40	1.34
22	V	307	CLA	CMD-C2D	-2.16	1.46	1.50
22	4	306	CLA	C3B-C2B	-2.16	1.37	1.40
30	A	407	PHO	CMD-C2D	-2.16	1.46	1.51
22	6	306	CLA	CMD-C2D	-2.16	1.46	1.50
24	R	313	XAT	C40-C33	2.16	1.55	1.50
25	R	314	LHG	O7-C7	2.16	1.40	1.34
24	G	309	XAT	C28-C27	2.16	1.37	1.32
26	P	314	CHL	C2C-C1C	2.16	1.49	1.44
22	c	514	CLA	CMD-C2D	-2.16	1.46	1.50
26	u	314	CHL	MG-NA	-2.16	2.01	2.06
22	r	604	CLA	CMD-C2D	-2.16	1.46	1.50
22	B	611	CLA	CMC-C2C	-2.16	1.46	1.50
26	u	313	CHL	C4C-C3C	2.15	1.48	1.45
25	b	623	LHG	O7-C7	2.15	1.40	1.34
26	S	314	CHL	MG-NA	-2.15	2.01	2.06
22	v	305	CLA	CMD-C2D	-2.15	1.46	1.50
24	1	311	XAT	C40-C33	2.15	1.55	1.50
26	S	315	CHL	C4C-C3C	2.15	1.48	1.45
22	U	304	CLA	C3B-C2B	-2.15	1.37	1.40
24	V	311	XAT	C28-C27	2.15	1.37	1.32
26	g	314	CHL	C1B-CHB	2.15	1.47	1.41
26	g	314	CHL	C1D-ND	-2.15	1.35	1.37
22	B	606	CLA	CMD-C2D	-2.15	1.46	1.50
24	G	309	XAT	C20-C13	2.15	1.55	1.50
26	v	313	CHL	C4C-C3C	2.15	1.48	1.45
22	4	304	CLA	MG-ND	-2.15	2.01	2.05
26	p	320	CHL	C4B-CHC	2.15	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	311	LHG	O7-C7	2.15	1.40	1.34
25	q	310	LHG	O8-C6	-2.15	1.40	1.45
22	C	509	CLA	C3B-C2B	-2.15	1.37	1.40
26	q	313	CHL	MG-NA	-2.15	2.01	2.06
25	a	415	LHG	O8-C23	2.15	1.39	1.33
22	S	303	CLA	CMC-C2C	-2.15	1.46	1.50
22	5	301	CLA	CMC-C2C	-2.15	1.46	1.50
34	C	521	LMG	O1-C7	-2.15	1.39	1.43
24	2	311	XAT	C28-C27	2.15	1.37	1.32
22	B	614	CLA	MG-ND	-2.15	2.01	2.05
22	v	303	CLA	CMD-C2D	-2.15	1.46	1.50
27	p	301	NEX	C1-C6	-2.15	1.50	1.54
26	6	315	CHL	C1B-CHB	2.15	1.47	1.41
22	p	303	CLA	CMD-C2D	-2.15	1.46	1.50
22	g	301	CLA	CMC-C2C	-2.15	1.46	1.50
22	b	616	CLA	CMD-C2D	-2.15	1.46	1.50
26	2	313	CHL	C1B-CHB	2.15	1.47	1.41
24	Q	309	XAT	C28-C27	2.15	1.37	1.32
26	4	316	CHL	C1D-ND	-2.15	1.35	1.37
26	6	301	CHL	C4C-C3C	2.15	1.48	1.45
32	C	501	SQD	O4-C4	-2.15	1.37	1.43
25	Q	310	LHG	O7-C7	2.15	1.40	1.34
22	b	606	CLA	CMC-C2C	-2.15	1.46	1.50
22	B	614	CLA	CMD-C2D	-2.15	1.46	1.50
22	s	301	CLA	CMD-C2D	-2.15	1.46	1.50
26	Q	314	CHL	C1D-ND	-2.15	1.35	1.37
26	q	311	CHL	C4B-CHC	2.14	1.47	1.41
22	A	405	CLA	MG-ND	-2.14	2.01	2.05
22	c	505	CLA	CMC-C2C	-2.14	1.46	1.50
22	3	305	CLA	CMD-C2D	-2.14	1.46	1.50
22	s	307	CLA	CMD-C2D	-2.14	1.46	1.50
32	a	410	SQD	O3-C3	-2.14	1.37	1.43
25	5	312	LHG	O8-C6	-2.14	1.40	1.45
26	5	316	CHL	C4C-C3C	2.14	1.48	1.45
22	R	302	CLA	CMD-C2D	-2.14	1.46	1.50
25	n	312	LHG	O8-C6	-2.14	1.40	1.45
22	b	606	CLA	CMD-C2D	-2.14	1.46	1.50
22	4	303	CLA	CMD-C2D	-2.14	1.46	1.50
26	v	314	CHL	C2C-C1C	2.14	1.49	1.44
26	1	318	CHL	C4C-C3C	2.14	1.48	1.45
26	N	313	CHL	C1D-ND	-2.14	1.35	1.37
26	6	315	CHL	C4C-C3C	2.14	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	615	CHL	C4B-CHC	2.14	1.46	1.41
25	C	524	LHG	O7-C7	2.14	1.40	1.34
26	3	315	CHL	C1B-CHB	2.14	1.46	1.41
22	u	307	CLA	CMD-C2D	-2.14	1.46	1.50
26	5	314	CHL	C1B-CHB	2.14	1.46	1.41
22	1	302	CLA	CMD-C2D	-2.14	1.46	1.50
22	4	302	CLA	CMD-C2D	-2.14	1.46	1.50
22	6	308	CLA	CMD-C2D	-2.14	1.46	1.50
22	S	301	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	610	CLA	CMD-C2D	-2.14	1.46	1.50
22	3	307	CLA	CMD-C2D	-2.14	1.46	1.50
26	u	313	CHL	C1D-ND	-2.14	1.35	1.37
24	u	311	XAT	C40-C33	2.14	1.55	1.50
26	R	316	CHL	C4B-CHC	2.14	1.46	1.41
22	s	302	CLA	CMD-C2D	-2.14	1.46	1.50
26	q	312	CHL	C4D-CHA	2.14	1.46	1.38
22	S	302	CLA	CMD-C2D	-2.14	1.46	1.50
22	C	513	CLA	CMC-C2C	-2.14	1.46	1.50
32	m	101	SQD	O2-C2	-2.14	1.37	1.43
26	Q	315	CHL	MG-NA	-2.14	2.01	2.06
22	v	301	CLA	C3B-C2B	-2.14	1.37	1.40
22	B	606	CLA	C3B-CAB	-2.13	1.43	1.47
22	B	608	CLA	CMC-C2C	-2.13	1.46	1.50
22	B	613	CLA	MG-ND	-2.13	2.01	2.05
33	D	405	PL9	C6-C1	2.13	1.52	1.48
22	V	306	CLA	CMD-C2D	-2.13	1.46	1.50
22	r	601	CLA	CMC-C2C	-2.13	1.46	1.50
22	c	505	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	512	CLA	CMC-C2C	-2.13	1.46	1.50
26	G	315	CHL	MG-NA	-2.13	2.01	2.06
22	C	506	CLA	C3B-CAB	-2.13	1.43	1.47
22	b	606	CLA	C3B-CAB	-2.13	1.43	1.47
22	b	614	CLA	MG-ND	-2.13	2.01	2.05
22	B	606	CLA	CMC-C2C	-2.13	1.46	1.50
36	B	601	DGD	O3G-C1D	-2.13	1.36	1.40
26	2	317	CHL	C4B-CHC	2.13	1.46	1.41
26	S	313	CHL	C1B-CHB	2.13	1.46	1.41
22	R	307	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	503	CLA	CAC-C3C	-2.13	1.45	1.51
25	3	310	LHG	O7-C7	2.13	1.40	1.34
26	p	319	CHL	C1D-ND	-2.13	1.35	1.37
22	S	303	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	514	CLA	CMC-C2C	-2.13	1.46	1.50
30	a	407	PHO	CMB-C2B	-2.13	1.46	1.51
34	A	411	LMG	O1-C7	-2.13	1.39	1.43
26	1	316	CHL	C1D-ND	-2.13	1.35	1.37
22	Q	307	CLA	CMD-C2D	-2.13	1.46	1.50
22	u	306	CLA	CMC-C2C	-2.13	1.46	1.50
22	s	308	CLA	CMD-C2D	-2.13	1.46	1.50
26	G	313	CHL	MG-NA	-2.13	2.01	2.06
34	B	624	LMG	O1-C1	-2.13	1.36	1.40
26	2	315	CHL	C4C-C3C	2.13	1.48	1.45
22	3	302	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	506	CLA	CMC-C2C	-2.13	1.46	1.50
22	A	408	CLA	CMC-C2C	-2.13	1.46	1.50
25	P	313	LHG	O7-C7	2.13	1.40	1.34
22	U	307	CLA	CMD-C2D	-2.13	1.46	1.50
25	A	413	LHG	O8-C23	2.13	1.39	1.33
22	c	508	CLA	CMC-C2C	-2.13	1.46	1.50
26	5	313	CHL	C1B-CHB	2.13	1.46	1.41
24	1	311	XAT	C28-C27	2.13	1.37	1.32
22	5	303	CLA	C3B-C2B	-2.13	1.37	1.40
26	u	317	CHL	C4B-CHC	2.13	1.46	1.41
22	u	303	CLA	CMC-C2C	-2.13	1.46	1.50
24	q	309	XAT	C8-C7	2.12	1.37	1.32
26	s	314	CHL	MG-NA	-2.12	2.01	2.06
22	U	306	CLA	CMC-C2C	-2.12	1.46	1.50
26	N	316	CHL	C1D-ND	-2.12	1.35	1.37
22	b	608	CLA	CMC-C2C	-2.12	1.46	1.50
22	q	301	CLA	CMC-C2C	-2.12	1.46	1.50
22	4	307	CLA	CMD-C2D	-2.12	1.46	1.50
22	C	507	CLA	CMC-C2C	-2.12	1.46	1.50
22	s	303	CLA	CMD-C2D	-2.12	1.46	1.50
22	U	304	CLA	CMD-C2D	-2.12	1.46	1.50
22	b	610	CLA	CMD-C2D	-2.12	1.46	1.50
22	c	514	CLA	C3B-CAB	-2.12	1.43	1.47
32	a	410	SQD	O4-C4	-2.12	1.38	1.43
22	1	301	CLA	CMC-C2C	-2.12	1.46	1.50
22	n	302	CLA	CMD-C2D	-2.12	1.46	1.50
26	V	314	CHL	MG-NA	-2.12	2.01	2.06
22	C	515	CLA	CMC-C2C	-2.12	1.46	1.50
22	u	301	CLA	C3B-C2B	-2.12	1.37	1.40
25	r	613	LHG	O7-C7	2.12	1.40	1.34
26	6	312	CHL	C1D-ND	-2.12	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	101	SQD	O2-C2	-2.12	1.38	1.43
26	g	311	CHL	MG-NA	-2.12	2.01	2.06
22	g	304	CLA	CMD-C2D	-2.12	1.46	1.50
22	s	304	CLA	CMD-C2D	-2.12	1.46	1.50
22	s	307	CLA	CMC-C2C	-2.12	1.46	1.50
22	2	304	CLA	C3B-C2B	-2.12	1.37	1.40
26	1	317	CHL	C4B-CHC	2.12	1.46	1.41
26	r	619	CHL	C4C-C3C	2.12	1.48	1.45
26	G	312	CHL	C1B-CHB	2.12	1.46	1.41
22	q	307	CLA	CMC-C2C	-2.12	1.46	1.50
26	U	317	CHL	C4B-CHC	2.12	1.46	1.41
24	g	309	XAT	C20-C13	2.12	1.55	1.50
26	q	314	CHL	MG-NA	-2.12	2.01	2.06
26	P	315	CHL	C2C-C1C	2.12	1.49	1.44
22	v	308	CLA	CMD-C2D	-2.12	1.46	1.50
26	P	318	CHL	C1D-ND	-2.12	1.35	1.37
22	B	604	CLA	C3B-CAB	-2.12	1.43	1.47
22	C	514	CLA	CMC-C2C	-2.12	1.46	1.50
25	q	310	LHG	O7-C7	2.12	1.40	1.34
22	s	303	CLA	CMC-C2C	-2.12	1.46	1.50
26	q	315	CHL	C4C-C3C	2.12	1.48	1.45
22	Q	308	CLA	CMD-C2D	-2.12	1.46	1.50
26	Q	316	CHL	C4C-C3C	2.12	1.48	1.45
22	a	406	CLA	MG-ND	-2.12	2.01	2.05
26	V	314	CHL	C4D-CHA	2.11	1.45	1.38
22	V	302	CLA	CMD-C2D	-2.11	1.46	1.50
26	1	316	CHL	C4C-C3C	2.11	1.48	1.45
22	C	506	CLA	CMC-C2C	-2.11	1.46	1.50
26	s	315	CHL	C4C-C3C	2.11	1.48	1.45
25	1	312	LHG	O8-C6	-2.11	1.40	1.45
24	5	311	XAT	C28-C27	2.11	1.37	1.32
25	g	310	LHG	O8-C6	-2.11	1.40	1.45
25	c	522	LHG	O8-C6	-2.11	1.40	1.45
26	6	315	CHL	C2C-C1C	2.11	1.49	1.44
22	S	305	CLA	CMC-C2C	-2.11	1.46	1.50
22	B	607	CLA	C3B-CAB	-2.11	1.43	1.47
32	A	412	SQD	O4-C4	-2.11	1.38	1.43
22	V	305	CLA	CMD-C2D	-2.11	1.46	1.50
22	N	303	CLA	CMD-C2D	-2.11	1.46	1.50
24	r	612	XAT	C40-C33	2.11	1.55	1.50
22	U	302	CLA	C3B-C2B	-2.11	1.37	1.40
22	4	301	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	CMD-C2D	-2.11	1.46	1.50
26	U	316	CHL	C4C-C3C	2.11	1.48	1.45
22	S	304	CLA	CMD-C2D	-2.11	1.46	1.50
22	C	515	CLA	C3B-CAB	-2.11	1.43	1.47
24	6	310	XAT	C28-C27	2.11	1.37	1.32
22	5	304	CLA	CMC-C2C	-2.11	1.46	1.50
22	p	305	CLA	CMC-C2C	-2.11	1.46	1.50
22	U	303	CLA	CMD-C2D	-2.11	1.46	1.50
22	u	304	CLA	CMD-C2D	-2.11	1.46	1.50
22	b	602	CLA	C3B-C2B	-2.11	1.37	1.40
22	c	508	CLA	C3B-C2B	-2.11	1.37	1.40
22	c	513	CLA	C3B-C2B	-2.11	1.37	1.40
36	c	519	DGD	O5D-C1E	-2.11	1.36	1.40
26	p	315	CHL	C2C-C1C	2.11	1.49	1.44
24	U	311	XAT	C20-C13	2.11	1.55	1.50
26	u	318	CHL	C4C-C3C	2.11	1.48	1.45
22	v	302	CLA	CMC-C2C	-2.11	1.46	1.50
22	q	301	CLA	CMD-C2D	-2.11	1.46	1.50
22	b	604	CLA	C3B-CAB	-2.11	1.43	1.47
26	u	314	CHL	C1D-ND	-2.11	1.35	1.37
26	v	313	CHL	C1B-CHB	2.11	1.46	1.41
22	B	603	CLA	C3B-CAB	-2.11	1.43	1.47
26	n	316	CHL	C1D-ND	-2.11	1.35	1.37
22	B	602	CLA	MG-ND	-2.11	2.01	2.05
26	n	313	CHL	C2C-C1C	2.11	1.49	1.44
22	2	304	CLA	CMC-C2C	-2.11	1.46	1.50
22	2	307	CLA	CMD-C2D	-2.11	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.11	1.46	1.50
22	u	303	CLA	CMD-C2D	-2.11	1.46	1.50
26	3	314	CHL	C1B-CHB	2.11	1.46	1.41
22	N	306	CLA	CMD-C2D	-2.11	1.46	1.50
22	1	306	CLA	MG-ND	-2.11	2.01	2.05
22	b	613	CLA	MG-ND	-2.11	2.01	2.05
22	b	602	CLA	CMC-C2C	-2.10	1.46	1.50
34	a	412	LMG	O1-C7	-2.10	1.39	1.43
26	u	313	CHL	C1B-CHB	2.10	1.46	1.41
22	V	303	CLA	CMD-C2D	-2.10	1.46	1.50
26	v	313	CHL	C1D-ND	-2.10	1.35	1.37
22	b	609	CLA	MG-ND	-2.10	2.01	2.05
26	P	316	CHL	C1B-CHB	2.10	1.46	1.41
22	B	605	CLA	CMD-C2D	-2.10	1.46	1.50
26	3	311	CHL	C1D-ND	-2.10	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	313	CHL	C1D-ND	-2.10	1.35	1.37
26	p	314	CHL	C1B-CHB	2.10	1.46	1.41
26	P	314	CHL	C1B-CHB	2.10	1.46	1.41
22	U	306	CLA	MG-ND	-2.10	2.01	2.05
26	g	315	CHL	MG-NA	-2.10	2.01	2.06
26	r	619	CHL	C1D-ND	-2.10	1.35	1.37
22	6	303	CLA	C3B-C2B	-2.10	1.37	1.40
26	G	313	CHL	C1B-CHB	2.10	1.46	1.41
26	5	313	CHL	C2C-C1C	2.10	1.49	1.44
26	5	316	CHL	C1B-CHB	2.10	1.46	1.41
26	5	314	CHL	C1D-ND	-2.10	1.35	1.37
22	b	602	CLA	MG-ND	-2.10	2.01	2.05
25	4	312	LHG	O8-C6	-2.10	1.40	1.45
22	S	308	CLA	CMD-C2D	-2.10	1.46	1.50
22	c	511	CLA	CMC-C2C	-2.10	1.46	1.50
24	q	309	XAT	C28-C27	2.10	1.37	1.32
22	4	307	CLA	CMC-C2C	-2.10	1.46	1.50
22	u	301	CLA	C3B-CAB	-2.10	1.43	1.47
26	4	316	CHL	C4B-CHC	2.10	1.46	1.41
36	A	414	DGD	O6E-C5E	2.10	1.49	1.44
22	6	303	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	602	CLA	C3B-C2B	-2.10	1.37	1.40
22	1	308	CLA	CMD-C2D	-2.10	1.46	1.50
22	R	306	CLA	CMD-C2D	-2.10	1.46	1.50
24	u	311	XAT	C20-C13	2.10	1.55	1.50
26	q	313	CHL	C4B-CHC	2.10	1.46	1.41
26	U	316	CHL	C4B-CHC	2.10	1.46	1.41
22	Q	303	CLA	CMD-C2D	-2.10	1.46	1.50
22	G	305	CLA	CMD-C2D	-2.10	1.46	1.50
26	U	313	CHL	C1B-CHB	2.10	1.46	1.41
36	C	520	DGD	O2G-C2G	-2.10	1.41	1.46
22	v	307	CLA	CMD-C2D	-2.10	1.46	1.50
32	A	412	SQD	O3-C3	-2.10	1.38	1.43
22	G	305	CLA	C3B-C2B	-2.10	1.37	1.40
26	v	318	CHL	C4B-CHC	2.10	1.46	1.41
26	n	318	CHL	C1B-CHB	2.10	1.46	1.41
22	N	304	CLA	CMD-C2D	-2.10	1.46	1.50
26	4	317	CHL	C1D-ND	-2.10	1.35	1.37
36	A	414	DGD	O2G-C2G	-2.10	1.41	1.46
22	q	308	CLA	CMD-C2D	-2.10	1.46	1.50
26	v	317	CHL	C1D-ND	-2.10	1.35	1.37
26	Q	314	CHL	C1B-CHB	2.10	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	313	CHL	C1B-CHB	2.10	1.46	1.41
22	U	301	CLA	C3B-CAB	-2.10	1.43	1.47
22	6	307	CLA	CMD-C2D	-2.09	1.46	1.50
22	v	307	CLA	CMC-C2C	-2.09	1.46	1.50
26	3	314	CHL	C4C-C3C	2.09	1.48	1.45
26	q	314	CHL	C2C-C1C	2.09	1.49	1.44
26	v	316	CHL	C4C-C3C	2.09	1.48	1.45
26	P	317	CHL	C1D-ND	-2.09	1.35	1.37
22	P	304	CLA	C3B-C2B	-2.09	1.37	1.40
36	J	101	DGD	O5D-C1E	-2.09	1.36	1.40
22	c	513	CLA	CMC-C2C	-2.09	1.46	1.50
24	4	311	XAT	C28-C27	2.09	1.37	1.32
22	S	307	CLA	CMC-C2C	-2.09	1.46	1.50
26	q	312	CHL	C1D-ND	-2.09	1.35	1.37
22	b	614	CLA	C3B-CAB	-2.09	1.43	1.47
26	S	313	CHL	C1D-ND	-2.09	1.35	1.37
22	1	307	CLA	CMD-C2D	-2.09	1.46	1.50
36	c	518	DGD	O2G-C2G	-2.09	1.41	1.46
22	1	305	CLA	CMD-C2D	-2.09	1.46	1.50
22	p	304	CLA	CMD-C2D	-2.09	1.46	1.50
32	a	413	SQD	O4-C4	-2.09	1.38	1.43
22	g	302	CLA	CMD-C2D	-2.09	1.46	1.50
22	A	406	CLA	MG-ND	-2.09	2.01	2.05
26	n	316	CHL	C4C-C3C	2.09	1.48	1.45
26	R	317	CHL	C2C-C1C	2.09	1.49	1.44
26	n	314	CHL	C4D-CHA	2.09	1.45	1.38
22	r	605	CLA	CMD-C2D	-2.09	1.46	1.50
26	p	316	CHL	C1B-CHB	2.09	1.46	1.41
26	q	315	CHL	C1B-CHB	2.09	1.46	1.41
26	V	314	CHL	C2C-C1C	2.09	1.49	1.44
22	v	301	CLA	CMC-C2C	-2.09	1.46	1.50
22	v	302	CLA	CMD-C2D	-2.09	1.46	1.50
22	G	302	CLA	CMD-C2D	-2.09	1.46	1.50
26	4	314	CHL	C1D-ND	-2.09	1.35	1.37
26	V	313	CHL	C1D-ND	-2.09	1.35	1.37
22	1	307	CLA	CMC-C2C	-2.09	1.46	1.50
26	2	313	CHL	C2C-C1C	2.09	1.49	1.44
26	5	314	CHL	C4D-CHA	2.09	1.45	1.38
37	E	101	HEM	CMB-C2B	2.09	1.55	1.50
26	Q	311	CHL	C4C-C3C	2.09	1.48	1.45
22	q	305	CLA	CMD-C2D	-2.09	1.46	1.50
24	g	309	XAT	C28-C27	2.08	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	404	PL9	C6-C1	2.08	1.52	1.48
26	2	313	CHL	C4C-C3C	2.08	1.48	1.45
22	V	308	CLA	CMD-C2D	-2.08	1.46	1.50
22	g	305	CLA	CMD-C2D	-2.08	1.46	1.50
26	6	312	CHL	C2C-C1C	2.08	1.49	1.44
32	a	413	SQD	O3-C3	-2.08	1.38	1.43
22	c	505	CLA	C3B-CAB	-2.08	1.43	1.47
24	v	311	XAT	C28-C27	2.08	1.37	1.32
24	N	311	XAT	C28-C27	2.08	1.37	1.32
22	v	301	CLA	CMD-C2D	-2.08	1.46	1.50
22	V	301	CLA	CMC-C2C	-2.08	1.46	1.50
22	N	307	CLA	CMC-C2C	-2.08	1.46	1.50
26	1	315	CHL	C1B-CHB	2.08	1.46	1.41
22	p	308	CLA	CMC-C2C	-2.08	1.46	1.50
26	2	315	CHL	C1D-ND	-2.08	1.35	1.37
26	N	316	CHL	C1B-CHB	2.08	1.46	1.41
34	D	408	LMG	O1-C7	-2.08	1.39	1.43
26	6	313	CHL	C2C-C1C	2.08	1.49	1.44
22	r	601	CLA	CMD-C2D	-2.08	1.46	1.50
22	p	302	CLA	CMD-C2D	-2.08	1.46	1.50
22	X	202	CLA	CMC-C2C	-2.08	1.46	1.50
26	N	315	CHL	C1B-CHB	2.08	1.46	1.41
22	P	308	CLA	CMC-C2C	-2.08	1.46	1.50
25	S	312	LHG	O7-C7	2.08	1.40	1.34
25	s	312	LHG	O7-C7	2.08	1.40	1.34
22	3	308	CLA	CMD-C2D	-2.08	1.46	1.50
26	1	316	CHL	C1B-CHB	2.08	1.46	1.41
22	B	610	CLA	C3B-C2B	-2.08	1.37	1.40
22	B	608	CLA	CMD-C2D	-2.08	1.46	1.50
26	3	314	CHL	C2C-C1C	2.08	1.49	1.44
36	a	416	DGD	O2G-C2G	-2.08	1.41	1.46
22	B	617	CLA	MG-ND	-2.08	2.01	2.05
30	d	401	PHO	CMB-C2B	-2.08	1.46	1.51
22	p	309	CLA	CMD-C2D	-2.08	1.46	1.50
22	V	307	CLA	CMC-C2C	-2.08	1.46	1.50
22	N	301	CLA	CMD-C2D	-2.08	1.46	1.50
27	N	318	NEX	O24-C25	-2.08	1.43	1.46
22	C	512	CLA	CMC-C2C	-2.08	1.46	1.50
22	3	307	CLA	CMC-C2C	-2.08	1.46	1.50
22	P	302	CLA	CMD-C2D	-2.08	1.46	1.50
22	n	301	CLA	CMD-C2D	-2.08	1.46	1.50
26	V	317	CHL	C1D-ND	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	303	CLA	C3B-C2B	-2.08	1.37	1.40
22	G	307	CLA	C3B-C2B	-2.08	1.37	1.40
22	R	308	CLA	CMD-C2D	-2.08	1.46	1.50
26	5	313	CHL	C4C-C3C	2.08	1.48	1.45
22	B	614	CLA	C3B-CAB	-2.07	1.43	1.47
22	1	301	CLA	C3B-C2B	-2.07	1.37	1.40
22	p	303	CLA	C3B-C2B	-2.07	1.37	1.40
22	u	306	CLA	MG-ND	-2.07	2.01	2.05
22	b	607	CLA	C3B-CAB	-2.07	1.43	1.47
22	3	304	CLA	CMD-C2D	-2.07	1.46	1.50
22	U	303	CLA	CMC-C2C	-2.07	1.46	1.50
22	b	604	CLA	CMC-C2C	-2.07	1.46	1.50
26	Q	315	CHL	C1B-CHB	2.07	1.46	1.41
22	V	301	CLA	CMD-C2D	-2.07	1.46	1.50
22	N	308	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	615	CLA	CMC-C2C	-2.07	1.46	1.50
25	B	623	LHG	O8-C6	-2.07	1.40	1.45
22	s	306	CLA	MG-ND	-2.07	2.01	2.05
22	b	603	CLA	CMC-C2C	-2.07	1.46	1.50
22	1	303	CLA	CMD-C2D	-2.07	1.46	1.50
22	1	306	CLA	CMC-C2C	-2.07	1.46	1.50
22	b	615	CLA	CMC-C2C	-2.07	1.46	1.50
22	1	306	CLA	C3B-C2B	-2.07	1.37	1.40
22	a	408	CLA	MG-ND	-2.07	2.01	2.05
22	B	610	CLA	CMC-C2C	-2.07	1.46	1.50
22	V	301	CLA	C3B-CAB	-2.07	1.43	1.47
26	n	313	CHL	C4C-C3C	2.07	1.48	1.45
22	1	303	CLA	C3B-C2B	-2.07	1.37	1.40
26	4	313	CHL	C4C-C3C	2.07	1.48	1.45
22	6	309	CLA	CMD-C2D	-2.07	1.46	1.50
22	S	305	CLA	CMD-C2D	-2.07	1.46	1.50
22	S	309	CLA	CMC-C2C	-2.07	1.46	1.50
22	2	303	CLA	CMC-C2C	-2.07	1.46	1.50
22	3	306	CLA	CMD-C2D	-2.07	1.46	1.50
22	G	308	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	605	CLA	C3B-CAB	-2.07	1.43	1.47
22	r	607	CLA	CMD-C2D	-2.07	1.46	1.50
22	v	301	CLA	C3B-CAB	-2.07	1.43	1.47
22	c	512	CLA	MG-ND	-2.07	2.01	2.05
26	g	311	CHL	C4C-C3C	2.07	1.48	1.45
24	n	311	XAT	C28-C27	2.07	1.37	1.32
22	A	405	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	n	307	CLA	CMC-C2C	-2.07	1.46	1.50
26	g	311	CHL	C2C-C1C	2.07	1.49	1.44
26	g	315	CHL	C4C-C3C	2.07	1.48	1.45
22	P	304	CLA	CMD-C2D	-2.07	1.46	1.50
36	a	416	DGD	O6E-C5E	2.07	1.49	1.44
22	b	605	CLA	C4B-CHC	-2.07	1.35	1.41
26	P	318	CHL	C4B-CHC	2.07	1.46	1.41
22	3	301	CLA	CMD-C2D	-2.07	1.46	1.50
26	q	311	CHL	C1D-ND	-2.07	1.35	1.37
26	r	615	CHL	C2C-C1C	2.07	1.49	1.44
22	C	511	CLA	CMC-C2C	-2.07	1.46	1.50
22	s	305	CLA	CMC-C2C	-2.07	1.46	1.50
26	r	616	CHL	C1B-CHB	2.07	1.46	1.41
22	c	514	CLA	C3B-C2B	-2.07	1.37	1.40
22	S	306	CLA	MG-ND	-2.07	2.01	2.05
22	d	402	CLA	C3B-CAB	-2.06	1.43	1.47
22	3	304	CLA	CMC-C2C	-2.06	1.46	1.50
22	u	301	CLA	CMD-C2D	-2.06	1.46	1.50
22	C	509	CLA	C3B-CAB	-2.06	1.43	1.47
22	b	610	CLA	CMC-C2C	-2.06	1.46	1.50
22	5	302	CLA	C3B-C2B	-2.06	1.37	1.40
22	4	305	CLA	CMD-C2D	-2.06	1.46	1.50
22	4	308	CLA	CMD-C2D	-2.06	1.46	1.50
22	6	304	CLA	CMC-C2C	-2.06	1.46	1.50
26	n	315	CHL	C1D-ND	-2.06	1.35	1.37
25	b	623	LHG	O8-C6	-2.06	1.40	1.45
26	Q	316	CHL	C1B-CHB	2.06	1.46	1.41
32	M	101	SQD	O4-C4	-2.06	1.38	1.43
26	n	317	CHL	C1C-NC	-2.06	1.34	1.37
22	B	605	CLA	C4B-CHC	-2.06	1.35	1.41
34	w	201	LMG	O1-C7	-2.06	1.40	1.43
22	B	616	CLA	CMD-C2D	-2.06	1.46	1.50
36	c	517	DGD	O3G-C1D	-2.06	1.36	1.40
22	u	302	CLA	CMC-C2C	-2.06	1.46	1.50
22	C	505	CLA	CMC-C2C	-2.06	1.46	1.50
26	G	315	CHL	C4C-C3C	2.06	1.48	1.45
26	p	317	CHL	C1B-CHB	2.06	1.46	1.41
22	a	406	CLA	C3B-CAB	-2.06	1.43	1.47
22	U	304	CLA	C3B-CAB	-2.06	1.43	1.47
22	b	605	CLA	C3B-CAB	-2.06	1.43	1.47
26	1	317	CHL	C1D-ND	-2.06	1.35	1.37
26	1	318	CHL	C4B-CHC	2.06	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	301	CLA	CMD-C2D	-2.06	1.46	1.50
22	s	306	CLA	CMC-C2C	-2.06	1.46	1.50
22	4	301	CLA	C3B-CAB	-2.06	1.43	1.47
22	u	307	CLA	C3B-CAB	-2.06	1.43	1.47
24	2	311	XAT	C8-C7	2.06	1.37	1.32
26	g	316	CHL	C4B-CHC	2.06	1.46	1.41
22	D	403	CLA	C3B-CAB	-2.06	1.43	1.47
27	u	320	NEX	O24-C25	-2.06	1.43	1.46
22	G	304	CLA	CMD-C2D	-2.06	1.46	1.50
22	1	301	CLA	C3B-CAB	-2.06	1.43	1.47
26	Q	313	CHL	C4B-CHC	2.06	1.46	1.41
22	B	604	CLA	CMC-C2C	-2.06	1.46	1.50
22	c	510	CLA	CMC-C2C	-2.06	1.46	1.50
37	e	101	HEM	CMB-C2B	2.06	1.55	1.50
26	P	317	CHL	C1B-CHB	2.06	1.46	1.41
22	x	201	CLA	CMC-C2C	-2.06	1.46	1.50
22	g	303	CLA	C3B-C2B	-2.06	1.37	1.40
22	S	309	CLA	C3B-C2B	-2.06	1.37	1.40
22	g	302	CLA	CMC-C2C	-2.06	1.46	1.50
37	E	101	HEM	CAA-C2A	2.06	1.55	1.52
22	c	509	CLA	MG-ND	-2.06	2.01	2.05
22	G	303	CLA	CMD-C2D	-2.06	1.46	1.50
22	s	309	CLA	C3B-C2B	-2.06	1.37	1.40
32	m	101	SQD	O4-C4	-2.06	1.38	1.43
22	u	308	CLA	C3B-CAB	-2.06	1.43	1.47
26	r	615	CHL	MG-NA	-2.06	2.01	2.06
22	P	307	CLA	CMD-C2D	-2.06	1.46	1.50
22	G	304	CLA	CMC-C2C	-2.05	1.46	1.50
26	6	301	CHL	C1D-ND	-2.05	1.35	1.37
30	D	401	PHO	CMB-C2B	-2.05	1.46	1.51
32	l	102	SQD	O3-C3	-2.05	1.38	1.43
26	2	316	CHL	C1B-CHB	2.05	1.46	1.41
22	6	302	CLA	CMD-C2D	-2.05	1.46	1.50
22	p	302	CLA	CMC-C2C	-2.05	1.46	1.50
22	U	307	CLA	C3B-C2B	-2.05	1.37	1.40
22	4	303	CLA	C3B-C2B	-2.05	1.37	1.40
22	a	405	CLA	MG-ND	-2.05	2.01	2.05
22	6	304	CLA	CMD-C2D	-2.05	1.46	1.50
22	V	302	CLA	CMC-C2C	-2.05	1.46	1.50
22	1	303	CLA	MG-ND	-2.05	2.01	2.05
22	5	307	CLA	CMD-C2D	-2.05	1.46	1.50
22	C	504	CLA	C4B-CHC	-2.05	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	313	CHL	C1B-CHB	2.05	1.46	1.41
26	G	314	CHL	C1B-CHB	2.05	1.46	1.41
22	n	302	CLA	CMC-C2C	-2.05	1.46	1.50
22	g	301	CLA	CMD-C2D	-2.05	1.46	1.50
34	W	201	LMG	O1-C7	-2.05	1.40	1.43
22	4	304	CLA	CMD-C2D	-2.05	1.46	1.50
22	S	308	CLA	CMC-C2C	-2.05	1.46	1.50
26	1	318	CHL	C1D-ND	-2.05	1.35	1.37
34	B	624	LMG	O1-C7	-2.05	1.40	1.43
22	v	303	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	602	CLA	CMC-C2C	-2.05	1.46	1.50
26	V	314	CHL	C1B-CHB	2.05	1.46	1.41
26	2	318	CHL	C1D-ND	-2.05	1.35	1.37
26	N	317	CHL	C1B-CHB	2.05	1.46	1.41
22	b	610	CLA	C3B-C2B	-2.05	1.37	1.40
24	P	312	XAT	C8-C7	2.05	1.37	1.32
22	4	301	CLA	CMD-C2D	-2.05	1.46	1.50
22	g	308	CLA	CMD-C2D	-2.05	1.46	1.50
22	c	511	CLA	C3B-CAB	-2.05	1.43	1.47
26	5	315	CHL	C1D-ND	-2.05	1.35	1.37
22	C	510	CLA	MG-ND	-2.05	2.01	2.05
22	G	306	CLA	CMD-C2D	-2.05	1.46	1.50
22	g	304	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	603	CLA	CMC-C2C	-2.05	1.46	1.50
27	n	319	NEX	O24-C25	-2.05	1.43	1.46
26	P	317	CHL	C4C-C3C	2.05	1.48	1.45
22	c	503	CLA	C4B-CHC	-2.05	1.35	1.41
26	U	319	CHL	C4C-C3C	2.05	1.48	1.45
22	q	302	CLA	C3B-C2B	-2.05	1.37	1.40
25	c	523	LHG	O7-C7	2.05	1.40	1.34
22	c	504	CLA	CMC-C2C	-2.05	1.46	1.50
24	G	309	XAT	C40-C33	2.05	1.55	1.50
26	U	317	CHL	MG-NA	-2.05	2.01	2.06
22	1	301	CLA	CMD-C2D	-2.05	1.46	1.50
22	5	307	CLA	CMC-C2C	-2.05	1.46	1.50
22	3	303	CLA	C3B-C2B	-2.05	1.37	1.40
22	P	309	CLA	CMD-C2D	-2.05	1.46	1.50
26	Q	311	CHL	C1D-ND	-2.05	1.35	1.37
22	P	305	CLA	CMC-C2C	-2.05	1.46	1.50
22	U	302	CLA	CMC-C2C	-2.05	1.46	1.50
22	N	301	CLA	CMC-C2C	-2.05	1.46	1.50
26	u	318	CHL	MG-NA	-2.04	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	309	XAT	C40-C33	2.04	1.55	1.50
22	n	308	CLA	CMD-C2D	-2.04	1.46	1.50
22	C	514	CLA	C3B-C2B	-2.04	1.37	1.40
22	a	405	CLA	CMC-C2C	-2.04	1.46	1.50
22	Q	307	CLA	CMC-C2C	-2.04	1.46	1.50
25	C	523	LHG	O8-C6	-2.04	1.40	1.45
26	p	317	CHL	C4C-C3C	2.04	1.48	1.45
22	q	303	CLA	CMD-C2D	-2.04	1.46	1.50
27	r	617	NEX	O24-C25	-2.04	1.43	1.46
22	q	302	CLA	CMD-C2D	-2.04	1.46	1.50
26	6	301	CHL	C1B-CHB	2.04	1.46	1.41
22	3	303	CLA	CMD-C2D	-2.04	1.46	1.50
22	5	304	CLA	CMD-C2D	-2.04	1.46	1.50
22	6	305	CLA	CMC-C2C	-2.04	1.46	1.50
24	V	311	XAT	C8-C7	2.04	1.37	1.32
26	4	313	CHL	C1B-CHB	2.04	1.46	1.41
25	s	312	LHG	O8-C6	-2.04	1.40	1.45
22	1	304	CLA	CMC-C2C	-2.04	1.46	1.50
22	n	305	CLA	C3D-C2D	2.04	1.44	1.39
26	p	318	CHL	C4B-CHC	2.04	1.46	1.41
26	N	313	CHL	C1B-CHB	2.04	1.46	1.41
26	Q	314	CHL	C4C-C3C	2.04	1.48	1.45
22	n	306	CLA	CMD-C2D	-2.04	1.46	1.50
36	C	519	DGD	O3G-C1D	-2.04	1.36	1.40
26	S	314	CHL	C1D-ND	-2.04	1.35	1.37
32	L	102	SQD	O3-C3	-2.04	1.38	1.43
22	P	303	CLA	CMC-C2C	-2.04	1.46	1.50
22	C	515	CLA	C3B-C2B	-2.04	1.37	1.40
24	5	311	XAT	C8-C7	2.04	1.37	1.32
26	u	316	CHL	C4C-C3C	2.04	1.48	1.45
22	2	305	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	615	CLA	C3B-CAB	-2.04	1.43	1.47
22	2	306	CLA	CMD-C2D	-2.04	1.46	1.50
22	Q	304	CLA	CMC-C2C	-2.04	1.46	1.50
22	S	306	CLA	CMC-C2C	-2.04	1.46	1.50
22	C	512	CLA	C3B-CAB	-2.04	1.43	1.47
22	4	301	CLA	C3B-C2B	-2.04	1.37	1.40
22	N	304	CLA	CMC-C2C	-2.04	1.46	1.50
22	s	309	CLA	CMC-C2C	-2.04	1.46	1.50
22	U	307	CLA	C3B-CAB	-2.04	1.43	1.47
22	b	615	CLA	C3B-CAB	-2.04	1.43	1.47
25	S	312	LHG	O8-C6	-2.04	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	MG-ND	-2.04	2.01	2.05
26	q	314	CHL	C1B-CHB	2.03	1.46	1.41
26	g	313	CHL	C1B-CHB	2.03	1.46	1.41
26	R	317	CHL	C1B-CHB	2.03	1.46	1.41
22	a	406	CLA	CMC-C2C	-2.03	1.46	1.50
22	1	303	CLA	CMC-C2C	-2.03	1.46	1.50
22	c	508	CLA	C3B-CAB	-2.03	1.43	1.47
22	U	301	CLA	CMD-C2D	-2.03	1.46	1.50
24	v	311	XAT	C8-C7	2.03	1.37	1.32
22	b	617	CLA	C3B-CAB	-2.03	1.43	1.47
22	s	305	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	408	CLA	MG-ND	-2.03	2.01	2.05
26	v	316	CHL	C1B-CHB	2.03	1.46	1.41
22	4	304	CLA	CMC-C2C	-2.03	1.46	1.50
22	Q	301	CLA	CMC-C2C	-2.03	1.46	1.50
22	2	302	CLA	C3B-C2B	-2.03	1.37	1.40
22	A	406	CLA	C3B-CAB	-2.03	1.43	1.47
26	V	318	CHL	C1B-CHB	2.03	1.46	1.41
24	3	309	XAT	C8-C7	2.03	1.37	1.32
22	P	302	CLA	CMC-C2C	-2.03	1.46	1.50
22	u	305	CLA	CMC-C2C	-2.03	1.46	1.50
22	g	306	CLA	CMD-C2D	-2.03	1.46	1.50
26	r	616	CHL	C2C-C1C	2.03	1.48	1.44
22	Q	304	CLA	CMD-C2D	-2.03	1.46	1.50
22	g	305	CLA	C3B-CAB	-2.03	1.43	1.47
22	V	303	CLA	CMC-C2C	-2.03	1.46	1.50
25	D	406	LHG	O7-C7	2.03	1.40	1.34
25	C	524	LHG	O8-C6	-2.03	1.40	1.45
26	G	316	CHL	C1D-ND	-2.03	1.35	1.37
22	r	608	CLA	CMD-C2D	-2.03	1.46	1.50
26	N	317	CHL	C4B-CHC	2.03	1.46	1.41
32	M	101	SQD	O3-C3	-2.03	1.38	1.43
22	2	304	CLA	C3B-CAB	-2.03	1.43	1.47
22	c	504	CLA	C3B-CAB	-2.03	1.43	1.47
22	2	308	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	406	CLA	CMC-C2C	-2.03	1.46	1.50
22	p	303	CLA	CMC-C2C	-2.03	1.46	1.50
26	G	316	CHL	C4B-CHC	2.03	1.46	1.41
22	N	302	CLA	CMC-C2C	-2.02	1.46	1.50
26	q	313	CHL	C1D-ND	-2.02	1.35	1.37
26	Q	316	CHL	C1D-ND	-2.02	1.35	1.37
22	5	306	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	306	CLA	CMC-C2C	-2.02	1.46	1.50
24	u	311	XAT	C8-C7	2.02	1.37	1.32
22	v	306	CLA	C3B-C2B	-2.02	1.37	1.40
34	d	407	LMG	O1-C7	-2.02	1.40	1.43
25	U	312	LHG	O7-C7	2.02	1.40	1.34
24	R	313	XAT	C8-C7	2.02	1.37	1.32
34	b	624	LMG	O1-C7	-2.02	1.40	1.43
32	m	101	SQD	O3-C3	-2.02	1.38	1.43
22	r	610	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	302	CLA	CMC-C2C	-2.02	1.46	1.50
22	3	301	CLA	CMC-C2C	-2.02	1.46	1.50
25	u	312	LHG	O7-C7	2.02	1.40	1.34
22	4	302	CLA	CMC-C2C	-2.02	1.46	1.50
26	p	319	CHL	C4B-CHC	2.02	1.46	1.41
22	G	303	CLA	C3B-C2B	-2.02	1.37	1.40
22	s	308	CLA	C3B-C2B	-2.02	1.37	1.40
22	s	301	CLA	MG-ND	-2.02	2.01	2.05
22	U	305	CLA	CMC-C2C	-2.02	1.46	1.50
22	C	505	CLA	C3B-CAB	-2.02	1.43	1.47
26	p	318	CHL	C1D-ND	-2.02	1.35	1.37
22	G	301	CLA	CMD-C2D	-2.02	1.46	1.50
26	v	318	CHL	C1B-CHB	2.02	1.46	1.41
24	6	310	XAT	C8-C7	2.02	1.37	1.32
22	2	304	CLA	CMD-C2D	-2.02	1.46	1.50
26	1	313	CHL	C4C-C3C	2.02	1.48	1.45
26	5	318	CHL	C1D-ND	-2.02	1.35	1.37
22	q	305	CLA	CMC-C2C	-2.02	1.46	1.50
22	4	303	CLA	MG-ND	-2.02	2.01	2.05
22	U	308	CLA	C3B-CAB	-2.02	1.43	1.47
25	d	405	LHG	O7-C7	2.02	1.40	1.34
22	5	304	CLA	C3B-CAB	-2.02	1.43	1.47
22	v	306	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	523	LHG	O8-C6	-2.02	1.40	1.45
22	c	502	CLA	C3B-CAB	-2.02	1.43	1.47
26	N	315	CHL	C4C-C3C	2.02	1.48	1.45
22	5	301	CLA	CMD-C2D	-2.02	1.46	1.50
26	q	311	CHL	C4C-C3C	2.02	1.48	1.45
26	p	320	CHL	C1D-ND	-2.02	1.35	1.37
22	r	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	R	311	CLA	CMD-C2D	-2.02	1.46	1.50
26	p	315	CHL	C4C-C3C	2.02	1.48	1.45
26	S	314	CHL	C1B-CHB	2.02	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	308	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	609	CLA	CMC-C2C	-2.01	1.46	1.50
26	s	314	CHL	C1D-ND	-2.01	1.35	1.37
22	1	304	CLA	CMD-C2D	-2.01	1.46	1.50
26	Q	311	CHL	C2C-C1C	2.01	1.48	1.44
26	s	314	CHL	C1B-CHB	2.01	1.46	1.41
22	Q	302	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	609	CLA	CMC-C2C	-2.01	1.46	1.50
22	B	616	CLA	CMC-C2C	-2.01	1.46	1.50
26	G	315	CHL	C1D-ND	-2.01	1.35	1.37
22	s	308	CLA	CMC-C2C	-2.01	1.46	1.50
26	u	315	CHL	MG-NA	-2.01	2.01	2.06
24	n	311	XAT	C8-C7	2.01	1.37	1.32
22	q	304	CLA	CMC-C2C	-2.01	1.46	1.50
26	6	316	CHL	C2C-C1C	2.01	1.48	1.44
22	Q	305	CLA	CMC-C2C	-2.01	1.46	1.50
26	u	314	CHL	C1B-CHB	2.01	1.46	1.41
22	6	305	CLA	C3D-C4D	2.01	1.48	1.44
26	4	317	CHL	C4B-CHC	2.01	1.46	1.41
26	G	311	CHL	C1D-ND	-2.01	1.35	1.37
22	5	303	CLA	CMC-C2C	-2.01	1.46	1.50
24	r	612	XAT	C8-C7	2.01	1.37	1.32
22	N	303	CLA	CMC-C2C	-2.01	1.46	1.50
22	n	304	CLA	CMC-C2C	-2.01	1.46	1.50
22	u	306	CLA	C3B-CAB	-2.01	1.43	1.47
26	n	318	CHL	C4B-CHC	2.01	1.46	1.41
22	1	307	CLA	MG-ND	-2.01	2.01	2.05
31	k	101	BCR	C32-C1	2.01	1.57	1.53
26	v	314	CHL	C1B-CHB	2.01	1.46	1.41
26	3	316	CHL	C4B-CHC	2.01	1.46	1.41
22	P	303	CLA	C3B-C2B	-2.01	1.37	1.40
22	r	609	CLA	CMC-C2C	-2.01	1.46	1.50
22	q	304	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	615	CLA	MG-ND	-2.01	2.01	2.05
26	g	316	CHL	C1D-ND	-2.01	1.35	1.37
26	U	315	CHL	C4C-C3C	2.01	1.48	1.45
22	g	306	CLA	CMC-C2C	-2.01	1.46	1.50
22	R	309	CLA	CMD-C2D	-2.01	1.46	1.50
22	n	301	CLA	CMC-C2C	-2.01	1.46	1.50
34	c	501	LMG	O1-C1	-2.01	1.36	1.40
22	G	308	CLA	C3B-CAB	-2.01	1.43	1.47
22	v	302	CLA	C3B-CAB	-2.01	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	304	CLA	CMC-C2C	-2.01	1.46	1.50
26	u	313	CHL	CMC-C2C	2.00	1.49	1.45
26	g	316	CHL	C1B-CHB	2.00	1.46	1.41
22	C	514	CLA	C3B-CAB	-2.00	1.43	1.47
26	G	311	CHL	MG-NA	-2.00	2.01	2.06
22	4	305	CLA	MG-ND	-2.00	2.01	2.05
26	R	316	CHL	C2C-C1C	2.00	1.48	1.44
22	3	302	CLA	C3B-C2B	-2.00	1.37	1.40
26	q	315	CHL	C1D-ND	-2.00	1.35	1.37
22	5	306	CLA	CMC-C2C	-2.00	1.46	1.50
22	v	304	CLA	CMD-C2D	-2.00	1.46	1.50
22	V	303	CLA	MG-ND	-2.00	2.01	2.05
26	G	312	CHL	CMC-C2C	2.00	1.49	1.45
22	3	304	CLA	C3D-C4D	2.00	1.48	1.44
26	P	319	CHL	C1D-ND	-2.00	1.35	1.37
22	b	616	CLA	C4B-CHC	-2.00	1.35	1.41
26	P	317	CHL	C2C-C1C	2.00	1.48	1.44
22	U	303	CLA	C3B-CAB	-2.00	1.43	1.47
22	4	306	CLA	CMC-C2C	-2.00	1.46	1.50
22	5	308	CLA	CMD-C2D	-2.00	1.46	1.50
22	V	304	CLA	CMC-C2C	-2.00	1.46	1.50
22	5	304	CLA	C3B-C2B	-2.00	1.37	1.40
26	6	316	CHL	C1B-CHB	2.00	1.46	1.41
22	2	306	CLA	CMC-C2C	-2.00	1.46	1.50
22	5	305	CLA	CMC-C2C	-2.00	1.46	1.50
22	b	604	CLA	CMD-C2D	-2.00	1.46	1.50
24	p	312	XAT	C8-C7	2.00	1.37	1.32

All (6389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	311	XAT	O4-C5-C4	60.27	158.66	113.38
24	2	311	XAT	O4-C5-C4	60.01	158.46	113.38
24	n	311	XAT	O24-C25-C24	59.81	158.31	113.38
24	N	311	XAT	O24-C25-C24	59.80	158.31	113.38
24	4	311	XAT	O4-C5-C4	59.80	158.31	113.38
24	Q	309	XAT	O4-C5-C4	59.77	158.28	113.38
24	q	309	XAT	O4-C5-C4	59.61	158.16	113.38
24	5	311	XAT	O4-C5-C4	59.57	158.13	113.38
24	V	311	XAT	O24-C25-C24	59.37	157.98	113.38
24	P	312	XAT	O24-C25-C24	59.35	157.97	113.38
24	1	311	XAT	O24-C25-C24	59.31	157.94	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	v	311	XAT	O24-C25-C24	59.18	157.84	113.38
24	G	309	XAT	O24-C25-C24	59.03	157.72	113.38
24	v	311	XAT	O4-C5-C4	58.85	157.59	113.38
24	4	311	XAT	O24-C25-C24	58.84	157.58	113.38
24	U	311	XAT	O24-C25-C24	58.82	157.57	113.38
24	V	311	XAT	O4-C5-C4	58.57	157.38	113.38
24	P	312	XAT	O4-C5-C4	58.52	157.35	113.38
24	U	311	XAT	O4-C5-C4	58.49	157.32	113.38
24	p	312	XAT	O4-C5-C4	58.42	157.27	113.38
24	u	311	XAT	O24-C25-C24	58.38	157.23	113.38
24	p	312	XAT	O24-C25-C24	58.11	157.03	113.38
24	3	309	XAT	O4-C5-C4	58.05	156.99	113.38
24	g	309	XAT	O24-C25-C24	57.98	156.94	113.38
24	3	309	XAT	O24-C25-C24	57.85	156.84	113.38
24	6	310	XAT	O4-C5-C4	57.76	156.77	113.38
24	5	311	XAT	O24-C25-C24	57.57	156.63	113.38
24	6	310	XAT	O24-C25-C24	57.53	156.60	113.38
24	q	309	XAT	O24-C25-C24	57.46	156.55	113.38
24	u	311	XAT	O4-C5-C4	57.28	156.41	113.38
24	Q	309	XAT	O24-C25-C24	57.27	156.40	113.38
24	2	311	XAT	O24-C25-C24	57.15	156.32	113.38
24	G	309	XAT	O4-C5-C4	57.05	156.24	113.38
24	g	309	XAT	O4-C5-C4	57.01	156.21	113.38
24	N	311	XAT	O4-C5-C4	56.93	156.15	113.38
24	R	313	XAT	O24-C25-C24	56.54	155.86	113.38
24	r	612	XAT	O4-C5-C4	56.22	155.62	113.38
24	r	612	XAT	O24-C25-C24	55.98	155.43	113.38
24	R	313	XAT	O4-C5-C4	55.96	155.42	113.38
24	n	311	XAT	O4-C5-C4	55.65	155.19	113.38
24	Q	309	XAT	C18-C5-C4	-13.45	99.14	114.28
24	u	311	XAT	C38-C25-C24	-13.32	99.30	114.28
24	1	311	XAT	C18-C5-C4	-13.13	99.51	114.28
24	4	311	XAT	C18-C5-C4	-13.09	99.55	114.28
24	p	312	XAT	C38-C25-C24	-13.09	99.55	114.28
24	n	311	XAT	O24-C25-C38	-12.99	99.49	115.06
24	P	312	XAT	C18-C5-C4	-12.99	99.67	114.28
24	U	311	XAT	C18-C5-C4	-12.98	99.68	114.28
24	5	311	XAT	C38-C25-C24	-12.98	99.68	114.28
24	v	311	XAT	C18-C5-C4	-12.93	99.73	114.28
24	N	311	XAT	C18-C5-C4	-12.93	99.74	114.28
24	q	309	XAT	C18-C5-C4	-12.92	99.74	114.28
24	2	311	XAT	C38-C25-C24	-12.92	99.75	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	311	XAT	C18-C5-C4	-12.92	99.75	114.28
24	1	311	XAT	C38-C25-C24	-12.91	99.75	114.28
24	u	311	XAT	C18-C5-C4	-12.91	99.76	114.28
24	2	311	XAT	C18-C5-C4	-12.89	99.78	114.28
24	4	311	XAT	C38-C25-C24	-12.83	99.85	114.28
24	N	311	XAT	C38-C25-C24	-12.83	99.85	114.28
24	V	311	XAT	C38-C25-C24	-12.82	99.85	114.28
24	V	311	XAT	C18-C5-C4	-12.81	99.87	114.28
24	U	311	XAT	C38-C25-C24	-12.81	99.87	114.28
24	p	312	XAT	C18-C5-C4	-12.70	99.99	114.28
24	R	313	XAT	C18-C5-C4	-12.70	99.99	114.28
24	3	309	XAT	C18-C5-C4	-12.67	100.03	114.28
24	N	311	XAT	O24-C25-C38	-12.60	99.96	115.06
24	P	312	XAT	C38-C25-C24	-12.60	100.11	114.28
24	6	310	XAT	C18-C5-C4	-12.60	100.11	114.28
24	q	309	XAT	O4-C5-C18	-12.59	99.97	115.06
24	P	312	XAT	O24-C25-C38	-12.58	99.98	115.06
24	2	311	XAT	O4-C5-C18	-12.57	99.99	115.06
24	r	612	XAT	C18-C5-C4	-12.57	100.14	114.28
24	v	311	XAT	C38-C25-C24	-12.57	100.14	114.28
24	G	309	XAT	C38-C25-C24	-12.56	100.15	114.28
24	Q	309	XAT	O4-C5-C18	-12.53	100.04	115.06
24	n	311	XAT	C18-C5-C4	-12.48	100.24	114.28
24	1	311	XAT	O4-C5-C18	-12.48	100.10	115.06
24	5	311	XAT	O4-C5-C18	-12.43	100.16	115.06
24	1	311	XAT	O24-C25-C38	-12.43	100.17	115.06
24	4	311	XAT	O4-C5-C18	-12.41	100.19	115.06
24	v	311	XAT	O24-C25-C38	-12.39	100.21	115.06
24	G	309	XAT	O24-C25-C38	-12.39	100.21	115.06
24	Q	309	XAT	C38-C25-C24	-12.39	100.34	114.28
24	V	311	XAT	O24-C25-C38	-12.38	100.22	115.06
24	G	309	XAT	C18-C5-C4	-12.37	100.37	114.28
24	g	309	XAT	C18-C5-C4	-12.32	100.42	114.28
24	v	311	XAT	O4-C5-C18	-12.32	100.30	115.06
24	q	309	XAT	C38-C25-C24	-12.30	100.44	114.28
24	n	311	XAT	C38-C25-C24	-12.30	100.44	114.28
24	6	310	XAT	C38-C25-C24	-12.30	100.44	114.28
24	3	309	XAT	C38-C25-C24	-12.28	100.46	114.28
24	U	311	XAT	O24-C25-C38	-12.27	100.35	115.06
24	g	309	XAT	C38-C25-C24	-12.27	100.48	114.28
24	4	311	XAT	O24-C25-C38	-12.20	100.44	115.06
24	V	311	XAT	O4-C5-C18	-12.16	100.49	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	612	XAT	C38-C25-C24	-12.11	100.66	114.28
24	3	309	XAT	O24-C25-C38	-12.03	100.64	115.06
24	g	309	XAT	O24-C25-C38	-12.00	100.68	115.06
24	R	313	XAT	C38-C25-C24	-11.98	100.80	114.28
24	P	312	XAT	O4-C5-C18	-11.95	100.74	115.06
24	6	310	XAT	O24-C25-C38	-11.93	100.76	115.06
24	p	312	XAT	O4-C5-C18	-11.91	100.79	115.06
24	5	311	XAT	O24-C25-C38	-11.87	100.83	115.06
24	3	309	XAT	O4-C5-C18	-11.86	100.85	115.06
24	U	311	XAT	O4-C5-C18	-11.85	100.86	115.06
24	u	311	XAT	O24-C25-C38	-11.81	100.91	115.06
24	6	310	XAT	O4-C5-C18	-11.80	100.91	115.06
24	p	312	XAT	O24-C25-C38	-11.79	100.94	115.06
24	Q	309	XAT	O24-C25-C38	-11.77	100.95	115.06
24	q	309	XAT	O24-C25-C38	-11.67	101.08	115.06
24	2	311	XAT	O24-C25-C38	-11.65	101.09	115.06
24	u	311	XAT	O4-C5-C18	-11.43	101.36	115.06
24	g	309	XAT	O4-C5-C18	-11.28	101.54	115.06
24	R	313	XAT	O24-C25-C38	-11.27	101.55	115.06
24	G	309	XAT	O4-C5-C18	-11.23	101.60	115.06
24	N	311	XAT	O4-C5-C18	-11.19	101.65	115.06
24	r	612	XAT	O24-C25-C38	-10.95	101.94	115.06
24	n	311	XAT	O4-C5-C18	-10.92	101.97	115.06
27	r	618	NEX	O24-C25-C24	10.78	121.48	113.38
24	r	612	XAT	O4-C5-C18	-10.24	102.79	115.06
27	R	301	NEX	O24-C25-C24	10.18	121.03	113.38
24	R	313	XAT	O4-C5-C18	-10.01	103.06	115.06
27	n	319	NEX	O24-C25-C24	9.95	120.85	113.38
27	U	318	NEX	O24-C25-C24	9.72	120.68	113.38
26	u	316	CHL	CMD-C2D-C1D	9.72	141.84	124.71
27	v	319	NEX	O24-C25-C24	9.55	120.56	113.38
26	U	315	CHL	CMD-C2D-C1D	9.22	140.96	124.71
26	6	301	CHL	CMD-C2D-C1D	9.17	140.87	124.71
26	P	317	CHL	CMD-C2D-C1D	9.05	140.67	124.71
26	G	311	CHL	CMD-C2D-C1D	9.04	140.64	124.71
26	1	316	CHL	CMD-C2D-C1D	9.03	140.63	124.71
27	s	317	NEX	O24-C25-C24	8.93	120.09	113.38
22	B	605	CLA	C4A-NA-C1A	8.88	110.70	106.71
26	6	315	CHL	CMD-C2D-C1D	8.88	140.36	124.71
27	5	319	NEX	O24-C25-C24	8.86	120.04	113.38
22	b	605	CLA	C4A-NA-C1A	8.85	110.69	106.71
27	V	319	NEX	O24-C25-C24	8.84	120.02	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	316	CHL	CMD-C2D-C1D	8.81	140.24	124.71
26	3	314	CHL	CMD-C2D-C1D	8.80	140.22	124.71
26	U	313	CHL	CMD-C2D-C1D	8.79	140.21	124.71
26	p	317	CHL	CMD-C2D-C1D	8.79	140.20	124.71
26	n	317	CHL	C2C-C3C-C4C	-8.78	100.23	106.49
27	r	617	NEX	O24-C25-C24	8.78	119.98	113.38
27	S	317	NEX	O24-C25-C24	8.77	119.97	113.38
26	n	315	CHL	CMD-C2D-C1D	8.77	140.16	124.71
22	p	306	CLA	C4A-NA-C1A	8.73	110.63	106.71
26	v	316	CHL	CMD-C2D-C1D	8.73	140.10	124.71
26	S	313	CHL	CMD-C2D-C1D	8.69	140.02	124.71
27	p	301	NEX	O24-C25-C24	8.68	119.90	113.38
26	6	317	CHL	CMD-C2D-C1D	8.67	140.00	124.71
22	C	504	CLA	C4A-NA-C1A	8.67	110.60	106.71
27	u	320	NEX	O24-C25-C24	8.65	119.88	113.38
26	s	313	CHL	CMD-C2D-C1D	8.63	139.93	124.71
26	V	313	CHL	CMD-C2D-C1D	8.63	139.93	124.71
27	2	319	NEX	O24-C25-C24	8.61	119.85	113.38
26	3	316	CHL	CMD-C2D-C1D	8.59	139.86	124.71
26	1	313	CHL	CMD-C2D-C1D	8.59	139.84	124.71
26	v	313	CHL	CMD-C2D-C1D	8.57	139.82	124.71
22	c	503	CLA	C4A-NA-C1A	8.54	110.55	106.71
26	Q	316	CHL	CMD-C2D-C1D	8.51	139.72	124.71
26	6	312	CHL	CMD-C2D-C1D	8.51	139.71	124.71
26	2	316	CHL	CMD-C2D-C1D	8.51	139.71	124.71
26	N	313	CHL	CMD-C2D-C1D	8.49	139.68	124.71
26	q	315	CHL	CMD-C2D-C1D	8.49	139.67	124.71
26	5	316	CHL	CMD-C2D-C1D	8.48	139.67	124.71
26	q	314	CHL	C2C-C3C-C4C	-8.47	100.45	106.49
26	6	316	CHL	C2C-C3C-C4C	-8.45	100.47	106.49
26	U	319	CHL	CMD-C2D-C1D	8.44	139.59	124.71
26	g	314	CHL	CMD-C2D-C1D	8.42	139.56	124.71
26	s	316	CHL	CMD-C2D-C1D	8.41	139.53	124.71
26	S	316	CHL	CMD-C2D-C1D	8.40	139.52	124.71
26	G	312	CHL	CMD-C2D-C1D	8.40	139.52	124.71
26	q	311	CHL	CMD-C2D-C1D	8.40	139.52	124.71
26	g	315	CHL	CMD-C2D-C1D	8.40	139.52	124.71
26	S	314	CHL	CMD-C2D-C1D	8.40	139.51	124.71
26	g	311	CHL	CMD-C2D-C1D	8.39	139.49	124.71
22	P	306	CLA	C4A-NA-C1A	8.39	110.48	106.71
26	n	316	CHL	CMD-C2D-C1D	8.38	139.49	124.71
26	5	317	CHL	CMD-C2D-C1D	8.38	139.49	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u	315	CHL	C2C-C3C-C4C	-8.38	100.52	106.49
26	2	317	CHL	CMD-C2D-C1D	8.38	139.48	124.71
26	N	316	CHL	CMD-C2D-C1D	8.38	139.48	124.71
26	3	311	CHL	CMD-C2D-C1D	8.38	139.47	124.71
26	s	314	CHL	CMD-C2D-C1D	8.37	139.47	124.71
26	P	318	CHL	CMD-C2D-C1D	8.36	139.45	124.71
26	R	317	CHL	CMD-C2D-C1D	8.36	139.44	124.71
26	Q	315	CHL	C2C-C3C-C4C	-8.36	100.53	106.49
26	r	615	CHL	CMD-C2D-C1D	8.35	139.44	124.71
26	p	318	CHL	CMD-C2D-C1D	8.35	139.43	124.71
26	p	320	CHL	CMD-C2D-C1D	8.33	139.40	124.71
26	u	313	CHL	CMD-C2D-C1D	8.33	139.40	124.71
26	2	315	CHL	CMD-C2D-C1D	8.32	139.38	124.71
26	v	314	CHL	CMD-C2D-C1D	8.32	139.38	124.71
26	q	313	CHL	CMD-C2D-C1D	8.31	139.36	124.71
22	5	305	CLA	C4A-NA-C1A	8.31	110.44	106.71
26	P	314	CHL	CMD-C2D-C1D	8.31	139.35	124.71
26	q	312	CHL	CMD-C2D-C1D	8.30	139.35	124.71
26	Q	314	CHL	CMD-C2D-C1D	8.30	139.34	124.71
22	n	305	CLA	C4A-NA-C1A	8.30	110.44	106.71
26	R	316	CHL	CMD-C2D-C1D	8.29	139.33	124.71
26	r	616	CHL	CMD-C2D-C1D	8.29	139.32	124.71
26	g	313	CHL	CMD-C2D-C1D	8.29	139.32	124.71
27	N	318	NEX	O24-C25-C24	8.28	119.60	113.38
26	2	313	CHL	CMD-C2D-C1D	8.28	139.31	124.71
26	3	315	CHL	C2C-C3C-C4C	-8.27	100.59	106.49
26	r	614	CHL	CMD-C2D-C1D	8.27	139.29	124.71
26	V	317	CHL	CMD-C2D-C1D	8.27	139.28	124.71
26	5	315	CHL	CMD-C2D-C1D	8.27	139.28	124.71
26	R	315	CHL	CMD-C2D-C1D	8.27	139.28	124.71
26	4	314	CHL	CMD-C2D-C1D	8.26	139.28	124.71
26	Q	311	CHL	CMD-C2D-C1D	8.25	139.26	124.71
26	p	314	CHL	CMD-C2D-C1D	8.24	139.24	124.71
26	4	313	CHL	CMD-C2D-C1D	8.24	139.23	124.71
26	V	314	CHL	CMD-C2D-C1D	8.23	139.22	124.71
26	6	313	CHL	CMD-C2D-C1D	8.23	139.22	124.71
26	5	314	CHL	CMD-C2D-C1D	8.23	139.22	124.71
22	2	305	CLA	C4A-NA-C1A	8.23	110.41	106.71
26	U	317	CHL	CMD-C2D-C1D	8.23	139.22	124.71
26	n	317	CHL	CMD-C2D-C1D	8.22	139.21	124.71
26	G	313	CHL	CMD-C2D-C1D	8.22	139.21	124.71
26	3	312	CHL	CMD-C2D-C1D	8.22	139.20	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	315	CHL	CHD-C1D-ND	-8.21	116.91	124.45
26	1	317	CHL	CMD-C2D-C1D	8.21	139.18	124.71
27	P	301	NEX	O24-C25-C24	8.21	119.55	113.38
26	r	619	CHL	CMD-C2D-C1D	8.21	139.18	124.71
26	5	313	CHL	CMD-C2D-C1D	8.21	139.18	124.71
26	p	315	CHL	CMD-C2D-C1D	8.20	139.17	124.71
26	p	316	CHL	CMD-C2D-C1D	8.20	139.17	124.71
26	Q	315	CHL	CMD-C2D-C1D	8.20	139.17	124.71
26	s	314	CHL	C2C-C3C-C4C	-8.19	100.65	106.49
26	G	315	CHL	CMD-C2D-C1D	8.19	139.14	124.71
26	g	315	CHL	C2C-C3C-C4C	-8.18	100.66	106.49
26	v	317	CHL	CMD-C2D-C1D	8.18	139.13	124.71
26	1	314	CHL	CMD-C2D-C1D	8.18	139.12	124.71
26	1	318	CHL	CMD-C2D-C1D	8.17	139.10	124.71
26	2	318	CHL	CMD-C2D-C1D	8.17	139.10	124.71
26	g	312	CHL	CMD-C2D-C1D	8.16	139.09	124.71
26	2	314	CHL	CMD-C2D-C1D	8.16	139.09	124.71
26	P	315	CHL	CMD-C2D-C1D	8.16	139.09	124.71
26	4	316	CHL	CMD-C2D-C1D	8.15	139.08	124.71
26	u	314	CHL	CMD-C2D-C1D	8.14	139.06	124.71
26	G	316	CHL	CMD-C2D-C1D	8.13	139.05	124.71
26	u	318	CHL	CMD-C2D-C1D	8.13	139.04	124.71
26	N	315	CHL	C2C-C3C-C4C	-8.13	100.70	106.49
26	Q	313	CHL	CMD-C2D-C1D	8.11	139.01	124.71
26	q	314	CHL	CMD-C2D-C1D	8.11	139.00	124.71
26	P	316	CHL	CMD-C2D-C1D	8.11	139.00	124.71
26	4	317	CHL	CMD-C2D-C1D	8.11	139.00	124.71
26	S	314	CHL	C2C-C3C-C4C	-8.09	100.72	106.49
26	N	314	CHL	CMD-C2D-C1D	8.09	138.97	124.71
26	n	314	CHL	CMD-C2D-C1D	8.08	138.96	124.71
26	G	314	CHL	CMD-C2D-C1D	8.08	138.96	124.71
26	s	315	CHL	CMD-C2D-C1D	8.06	138.92	124.71
26	g	316	CHL	CMD-C2D-C1D	8.06	138.92	124.71
26	Q	312	CHL	CMD-C2D-C1D	8.05	138.90	124.71
26	n	318	CHL	CMD-C2D-C1D	8.04	138.89	124.71
26	P	319	CHL	CMD-C2D-C1D	8.02	138.85	124.71
26	5	318	CHL	CMD-C2D-C1D	8.02	138.84	124.71
22	c	509	CLA	C4A-NA-C1A	8.01	110.31	106.71
26	N	317	CHL	CMD-C2D-C1D	8.01	138.82	124.71
26	S	315	CHL	CMD-C2D-C1D	8.00	138.82	124.71
26	U	314	CHL	C2C-C3C-C4C	-8.00	100.79	106.49
22	C	510	CLA	C4A-NA-C1A	7.98	110.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	316	CHL	CMD-C2D-C1D	7.98	138.78	124.71
26	1	315	CHL	CMD-C2D-C1D	7.98	138.78	124.71
22	r	609	CLA	C4A-NA-C1A	7.98	110.29	106.71
26	U	316	CHL	CMD-C2D-C1D	7.98	138.77	124.71
22	R	308	CLA	C4A-NA-C1A	7.96	110.28	106.71
26	p	319	CHL	CMD-C2D-C1D	7.96	138.74	124.71
22	B	612	CLA	C4A-NA-C1A	7.96	110.28	106.71
26	2	315	CHL	C2C-C3C-C4C	-7.95	100.82	106.49
26	3	315	CHL	CMD-C2D-C1D	7.94	138.71	124.71
26	n	313	CHL	CMD-C2D-C1D	7.94	138.71	124.71
22	b	617	CLA	C4A-NA-C1A	7.93	110.27	106.71
26	V	315	CHL	CMD-C2D-C1D	7.93	138.69	124.71
22	b	612	CLA	C4A-NA-C1A	7.92	110.27	106.71
26	u	317	CHL	CMD-C2D-C1D	7.92	138.67	124.71
26	4	315	CHL	CMD-C2D-C1D	7.92	138.66	124.71
26	N	316	CHL	C2C-C3C-C4C	-7.91	100.85	106.49
26	v	315	CHL	CMD-C2D-C1D	7.91	138.65	124.71
26	5	315	CHL	C2C-C3C-C4C	-7.90	100.86	106.49
26	3	313	CHL	CMD-C2D-C1D	7.88	138.60	124.71
26	G	315	CHL	C2C-C3C-C4C	-7.86	100.89	106.49
26	6	314	CHL	CMD-C2D-C1D	7.86	138.56	124.71
22	c	506	CLA	C4A-NA-C1A	7.85	110.23	106.71
26	N	315	CHL	CMD-C2D-C1D	7.84	138.54	124.71
22	q	304	CLA	C4A-NA-C1A	7.83	110.23	106.71
26	p	315	CHL	CHD-C1D-ND	-7.78	117.30	124.45
26	r	614	CHL	C2C-C3C-C4C	-7.78	100.94	106.49
26	U	314	CHL	CMD-C2D-C1D	7.77	138.41	124.71
26	R	316	CHL	C2C-C3C-C4C	-7.77	100.95	106.49
26	R	315	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
22	C	507	CLA	C4A-NA-C1A	7.75	110.19	106.71
22	n	305	CLA	CMD-C2D-C1D	-7.73	111.08	124.71
26	5	313	CHL	C2C-C3C-C4C	-7.73	100.98	106.49
22	b	607	CLA	C4A-NA-C1A	7.72	110.17	106.71
26	1	314	CHL	C2C-C3C-C4C	-7.72	100.99	106.49
26	4	314	CHL	C2C-C3C-C4C	-7.71	100.99	106.49
26	V	318	CHL	CMD-C2D-C1D	7.71	138.30	124.71
22	C	509	CLA	C4A-NA-C1A	7.70	110.17	106.71
22	3	305	CLA	C4A-NA-C1A	7.68	110.16	106.71
22	r	607	CLA	C4A-NA-C1A	7.67	110.16	106.71
22	p	303	CLA	C4A-NA-C1A	7.66	110.15	106.71
26	p	318	CHL	C2C-C3C-C4C	-7.65	101.04	106.49
26	r	615	CHL	C2C-C3C-C4C	-7.63	101.05	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	318	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
22	B	607	CLA	C4A-NA-C1A	7.62	110.13	106.71
22	G	305	CLA	C4A-NA-C1A	7.62	110.13	106.71
22	2	305	CLA	CMD-C2D-C1D	-7.61	111.30	124.71
22	b	608	CLA	C4A-NA-C1A	7.60	110.12	106.71
26	v	318	CHL	CMD-C2D-C1D	7.60	138.10	124.71
22	n	308	CLA	C4A-NA-C1A	7.59	110.12	106.71
26	v	315	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
22	2	307	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	N	305	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	g	305	CLA	C4A-NA-C1A	7.57	110.11	106.71
26	u	317	CHL	C2C-C3C-C4C	-7.57	101.09	106.49
26	U	319	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
22	R	310	CLA	C4A-NA-C1A	7.56	110.10	106.71
26	r	619	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
26	v	318	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
22	p	306	CLA	CMD-C2D-C1D	-7.55	111.41	124.71
22	c	505	CLA	C4A-NA-C1A	7.55	110.10	106.71
26	v	316	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
26	2	314	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
22	r	605	CLA	C4A-NA-C1A	7.50	110.08	106.71
22	g	307	CLA	C4A-NA-C1A	7.50	110.08	106.71
26	1	315	CHL	C2C-C3C-C4C	-7.50	101.14	106.49
22	B	606	CLA	C4A-NA-C1A	7.50	110.08	106.71
22	c	508	CLA	C4A-NA-C1A	7.49	110.08	106.71
22	5	305	CLA	CMD-C2D-C1D	-7.49	111.51	124.71
26	U	316	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
26	P	316	CHL	C2C-C3C-C4C	-7.48	101.15	106.49
31	k	101	BCR	C24-C23-C22	-7.48	114.93	126.23
22	5	307	CLA	C4A-NA-C1A	7.48	110.07	106.71
26	v	313	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
22	G	307	CLA	C4A-NA-C1A	7.47	110.06	106.71
22	R	306	CLA	C4A-NA-C1A	7.47	110.06	106.71
22	C	506	CLA	C4A-NA-C1A	7.46	110.06	106.71
26	p	314	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
22	6	306	CLA	C4A-NA-C1A	7.45	110.06	106.71
22	V	305	CLA	C4A-NA-C1A	7.45	110.06	106.71
26	4	315	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
22	s	308	CLA	C4A-NA-C1A	7.43	110.05	106.71
26	5	317	CHL	C2C-C3C-C4C	-7.43	101.19	106.49
22	r	604	CLA	C4A-NA-C1A	7.42	110.04	106.71
22	p	308	CLA	C4A-NA-C1A	7.41	110.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	606	CLA	C4A-NA-C1A	7.41	110.04	106.71
31	K	101	BCR	C24-C23-C22	-7.41	115.03	126.23
22	R	305	CLA	C4A-NA-C1A	7.41	110.04	106.71
26	2	313	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
22	B	608	CLA	C4A-NA-C1A	7.40	110.03	106.71
22	P	308	CLA	C4A-NA-C1A	7.40	110.03	106.71
26	S	313	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
31	C	517	BCR	C15-C14-C13	-7.39	116.76	127.31
26	s	316	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
26	6	317	CHL	C2C-C3C-C4C	-7.37	101.23	106.49
26	p	319	CHL	C2C-C3C-C4C	-7.37	101.24	106.49
22	U	307	CLA	C4A-NA-C1A	7.37	110.02	106.71
26	s	313	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
26	n	315	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
26	N	314	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
26	U	315	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
22	C	515	CLA	C4A-NA-C1A	7.36	110.01	106.71
22	b	615	CLA	C4A-NA-C1A	7.36	110.01	106.71
26	g	312	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
22	B	603	CLA	C4A-NA-C1A	7.34	110.01	106.71
26	n	313	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
22	N	303	CLA	C4A-NA-C1A	7.34	110.01	106.71
26	u	318	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
22	r	603	CLA	C4A-NA-C1A	7.34	110.00	106.71
26	g	316	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
26	2	314	CHL	CHD-C1D-ND	-7.33	117.72	124.45
31	c	515	BCR	C15-C14-C13	-7.33	116.85	127.31
26	P	319	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
26	G	316	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
26	v	317	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
22	1	306	CLA	C4A-NA-C1A	7.31	109.99	106.71
26	3	313	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
22	N	307	CLA	C4A-NA-C1A	7.31	109.99	106.71
26	4	316	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
26	P	314	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
26	4	317	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
26	V	315	CHL	C2C-C3C-C4C	-7.30	101.29	106.49
22	v	306	CLA	C4A-NA-C1A	7.29	109.98	106.71
26	5	314	CHL	C2C-C3C-C4C	-7.29	101.29	106.49
22	n	307	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	P	303	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	S	308	CLA	C4A-NA-C1A	7.28	109.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	C4A-NA-C1A	7.27	109.98	106.71
26	V	318	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
22	c	514	CLA	C4A-NA-C1A	7.27	109.97	106.71
26	p	316	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
26	6	314	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
22	u	307	CLA	C4A-NA-C1A	7.27	109.97	106.71
26	S	316	CHL	C2C-C3C-C4C	-7.26	101.31	106.49
22	b	603	CLA	C4A-NA-C1A	7.26	109.97	106.71
26	V	313	CHL	C2C-C3C-C4C	-7.26	101.31	106.49
22	c	507	CLA	C4A-NA-C1A	7.25	109.97	106.71
26	1	317	CHL	C2C-C3C-C4C	-7.24	101.33	106.49
22	2	308	CLA	C4A-NA-C1A	7.24	109.96	106.71
26	U	317	CHL	C2C-C3C-C4C	-7.23	101.33	106.49
26	n	314	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
26	Q	312	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
26	u	314	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
22	V	307	CLA	C4A-NA-C1A	7.20	109.94	106.71
26	S	315	CHL	CHD-C1D-ND	-7.20	117.84	124.45
26	v	314	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
22	P	306	CLA	CMD-C2D-C1D	-7.19	112.03	124.71
26	n	316	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
22	Q	304	CLA	C4A-NA-C1A	7.19	109.94	106.71
22	v	303	CLA	C4A-NA-C1A	7.19	109.94	106.71
26	V	314	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
26	s	315	CHL	CHD-C1D-ND	-7.18	117.86	124.45
22	5	306	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	Q	303	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	n	306	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	R	304	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	5	303	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	C	513	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	R	311	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	G	304	CLA	C4A-NA-C1A	7.16	109.93	106.71
26	V	316	CHL	C2C-C3C-C4C	-7.16	101.38	106.49
26	G	314	CHL	C2C-C3C-C4C	-7.16	101.38	106.49
26	u	315	CHL	CMD-C2D-C1D	7.16	137.33	124.71
22	U	304	CLA	C4A-NA-C1A	7.15	109.92	106.71
26	1	318	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
22	r	610	CLA	C4A-NA-C1A	7.14	109.92	106.71
22	b	616	CLA	C4A-NA-C1A	7.13	109.91	106.71
26	U	316	CHL	O2D-CGD-CBD	7.12	123.93	111.27
22	p	305	CLA	C4A-NA-C1A	7.12	109.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	307	CLA	C4A-NA-C1A	7.12	109.91	106.71
26	6	312	CHL	C2C-C3C-C4C	-7.12	101.42	106.49
26	v	317	CHL	O2D-CGD-CBD	7.12	123.92	111.27
26	S	316	CHL	CHD-C1D-ND	-7.12	117.91	124.45
22	2	306	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	U	308	CLA	C4A-NA-C1A	7.11	109.90	106.71
26	s	316	CHL	CHD-C1D-ND	-7.10	117.93	124.45
26	g	313	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
26	3	316	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
22	5	304	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	R	302	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	r	601	CLA	C4A-NA-C1A	7.09	109.89	106.71
22	v	305	CLA	C4A-NA-C1A	7.09	109.89	106.71
26	V	313	CHL	CHD-C1D-ND	-7.08	117.94	124.45
22	5	308	CLA	C4A-NA-C1A	7.08	109.89	106.71
22	p	307	CLA	C4A-NA-C1A	7.08	109.89	106.71
26	2	317	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
26	2	318	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
22	u	306	CLA	C4A-NA-C1A	7.07	109.89	106.71
26	5	316	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
22	N	306	CLA	C4A-NA-C1A	7.07	109.88	106.71
26	1	317	CHL	O2D-CGD-CBD	7.06	123.82	111.27
22	g	304	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	B	613	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	C	514	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	4	308	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	4	307	CLA	C4A-NA-C1A	7.05	109.87	106.71
22	u	302	CLA	C4A-NA-C1A	7.04	109.87	106.71
26	G	313	CHL	C2C-C3C-C4C	-7.04	101.47	106.49
22	b	611	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	C	503	CLA	C4A-NA-C1A	7.03	109.87	106.71
26	g	314	CHL	C2C-C3C-C4C	-7.03	101.48	106.49
22	s	307	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	C	508	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	v	307	CLA	C4A-NA-C1A	7.03	109.86	106.71
22	q	307	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	B	610	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	c	512	CLA	C4A-NA-C1A	7.02	109.86	106.71
26	Q	316	CHL	C2C-C3C-C4C	-7.02	101.48	106.49
22	c	513	CLA	C4A-NA-C1A	7.02	109.86	106.71
26	3	311	CHL	C2C-C3C-C4C	-7.02	101.48	106.49
26	u	316	CHL	C2C-C3C-C4C	-7.02	101.48	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	320	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
22	2	304	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	V	306	CLA	C4A-NA-C1A	7.01	109.86	106.71
26	2	316	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
26	n	318	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
22	q	306	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	g	306	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	2	303	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	u	308	CLA	C4A-NA-C1A	7.00	109.86	106.71
22	n	304	CLA	C4A-NA-C1A	7.00	109.86	106.71
26	Q	314	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
22	U	302	CLA	C4A-NA-C1A	7.00	109.85	106.71
26	G	311	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
26	2	314	CHL	C4A-NA-C1A	6.99	109.85	106.71
26	s	313	CHL	CHD-C1D-ND	-6.99	118.03	124.45
26	N	317	CHL	C2C-C3C-C4C	-6.99	101.51	106.49
22	B	611	CLA	C4A-NA-C1A	6.98	109.84	106.71
26	5	314	CHL	CHD-C1D-ND	-6.98	118.04	124.45
22	a	405	CLA	C4A-NA-C1A	6.98	109.84	106.71
26	6	313	CHL	CHD-C1D-ND	-6.98	118.04	124.45
26	V	317	CHL	C2C-C3C-C4C	-6.98	101.52	106.49
22	P	304	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	A	405	CLA	C4A-NA-C1A	6.97	109.84	106.71
22	N	305	CLA	CMD-C2D-C1D	-6.97	112.43	124.71
22	3	304	CLA	C4A-NA-C1A	6.97	109.84	106.71
26	Q	311	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
22	4	306	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	6	308	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	Q	307	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	x	201	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	V	308	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	b	613	CLA	C4A-NA-C1A	6.95	109.83	106.71
26	g	311	CHL	C2C-C3C-C4C	-6.95	101.53	106.49
22	s	309	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	q	308	CLA	C4A-NA-C1A	6.94	109.83	106.71
22	B	616	CLA	C4A-NA-C1A	6.94	109.82	106.71
22	c	502	CLA	C4A-NA-C1A	6.94	109.82	106.71
22	S	307	CLA	C4A-NA-C1A	6.93	109.82	106.71
26	R	317	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
26	q	315	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
22	u	305	CLA	C4A-NA-C1A	6.93	109.82	106.71
26	4	313	CHL	C2C-C3C-C4C	-6.93	101.55	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	301	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
26	p	317	CHL	C2C-C3C-C4C	-6.92	101.55	106.49
26	6	315	CHL	C2C-C3C-C4C	-6.92	101.56	106.49
22	5	302	CLA	C4A-NA-C1A	6.92	109.82	106.71
22	V	303	CLA	C4A-NA-C1A	6.92	109.82	106.71
26	3	314	CHL	C2C-C3C-C4C	-6.92	101.56	106.49
26	q	312	CHL	C2C-C3C-C4C	-6.91	101.56	106.49
22	b	610	CLA	C4A-NA-C1A	6.91	109.81	106.71
26	5	318	CHL	C2C-C3C-C4C	-6.91	101.56	106.49
26	3	312	CHL	CHD-C1D-ND	-6.90	118.11	124.45
22	X	202	CLA	C4A-NA-C1A	6.90	109.81	106.71
26	5	313	CHL	CHD-C1D-ND	-6.90	118.11	124.45
22	G	303	CLA	C4A-NA-C1A	6.90	109.81	106.71
22	u	303	CLA	C4A-NA-C1A	6.90	109.81	106.71
26	U	313	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
26	1	313	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
22	v	308	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	1	308	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	U	306	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	3	308	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	P	305	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	q	303	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	P	307	CLA	C4A-NA-C1A	6.87	109.80	106.71
24	r	612	XAT	C26-C27-C28	-6.87	111.47	125.99
31	C	518	BCR	C11-C10-C9	-6.87	117.51	127.31
22	U	305	CLA	C4A-NA-C1A	6.87	109.79	106.71
26	5	316	CHL	CHD-C1D-ND	-6.86	118.15	124.45
26	1	316	CHL	C2C-C3C-C4C	-6.86	101.60	106.49
26	1	313	CHL	CHD-C1D-ND	-6.86	118.15	124.45
22	3	306	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	S	309	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	1	307	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	a	408	CLA	C4A-NA-C1A	6.85	109.79	106.71
22	c	510	CLA	C4A-NA-C1A	6.85	109.78	106.71
26	r	616	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
31	c	516	BCR	C11-C10-C9	-6.83	117.56	127.31
26	S	313	CHL	CHD-C1D-ND	-6.83	118.17	124.45
22	Q	306	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	v	302	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	C	511	CLA	C4A-NA-C1A	6.82	109.77	106.71
26	2	316	CHL	CHD-C1D-ND	-6.82	118.19	124.45
22	N	308	CLA	C4A-NA-C1A	6.81	109.77	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	408	CLA	C4A-NA-C1A	6.81	109.77	106.71
22	b	609	CLA	C4A-NA-C1A	6.81	109.77	106.71
22	r	608	CLA	C4A-NA-C1A	6.80	109.77	106.71
22	N	304	CLA	C4A-NA-C1A	6.80	109.77	106.71
22	4	304	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	6	307	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	p	304	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	R	309	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	1	304	CLA	C4A-NA-C1A	6.80	109.76	106.71
26	V	315	CHL	CHD-C1D-ND	-6.79	118.21	124.45
22	6	309	CLA	C4A-NA-C1A	6.79	109.76	106.71
26	V	317	CHL	O2D-CGD-CBD	6.78	123.31	111.27
24	N	311	XAT	C15-C14-C13	-6.78	117.64	127.31
26	q	315	CHL	CHD-C1D-ND	-6.78	118.23	124.45
26	s	315	CHL	C2C-C3C-C4C	-6.78	101.66	106.49
22	s	304	CLA	C4A-NA-C1A	6.78	109.75	106.71
22	s	302	CLA	C4A-NA-C1A	6.77	109.75	106.71
26	3	316	CHL	CHD-C1D-ND	-6.77	118.23	124.45
22	a	404	CLA	C4A-NA-C1A	6.76	109.75	106.71
22	V	302	CLA	C4A-NA-C1A	6.76	109.74	106.71
26	q	313	CHL	C2C-C3C-C4C	-6.75	101.68	106.49
26	2	313	CHL	CHD-C1D-ND	-6.75	118.25	124.45
22	B	609	CLA	C4A-NA-C1A	6.75	109.74	106.71
26	3	314	CHL	CHD-C1D-ND	-6.74	118.26	124.45
22	Q	308	CLA	C4A-NA-C1A	6.74	109.74	106.71
26	n	318	CHL	CHD-C1D-ND	-6.74	118.26	124.45
22	S	302	CLA	C4A-NA-C1A	6.74	109.73	106.71
26	6	314	CHL	CHD-C1D-ND	-6.73	118.27	124.45
26	P	314	CHL	CHD-C1D-ND	-6.73	118.27	124.45
26	Q	313	CHL	C2C-C3C-C4C	-6.73	101.69	106.49
22	R	307	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	617	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	6	305	CLA	C4A-NA-C1A	6.73	109.73	106.71
26	p	315	CHL	C2C-C3C-C4C	-6.73	101.69	106.49
22	B	602	CLA	C4A-NA-C1A	6.72	109.73	106.71
26	4	313	CHL	CHD-C1D-ND	-6.72	118.28	124.45
26	v	313	CHL	CHD-C1D-ND	-6.72	118.28	124.45
26	P	317	CHL	CHD-C1D-ND	-6.72	118.28	124.45
22	b	602	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	g	303	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	B	614	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	r	606	CLA	C4A-NA-C1A	6.70	109.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	304	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	G	312	CHL	C2C-C3C-C4C	-6.70	101.72	106.49
22	p	309	CLA	C4A-NA-C1A	6.69	109.71	106.71
26	N	317	CHL	CHD-C1D-ND	-6.68	118.31	124.45
22	A	404	CLA	C4A-NA-C1A	6.68	109.71	106.71
26	6	313	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
26	u	313	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
26	q	312	CHL	CHD-C1D-ND	-6.67	118.32	124.45
26	U	313	CHL	CHD-C1D-ND	-6.67	118.32	124.45
26	S	315	CHL	C2C-C3C-C4C	-6.67	101.73	106.49
26	P	317	CHL	C2C-C3C-C4C	-6.66	101.74	106.49
22	S	303	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	G	306	CLA	C4A-NA-C1A	6.66	109.70	106.71
26	g	314	CHL	CHD-C1D-ND	-6.65	118.34	124.45
26	6	317	CHL	CHD-C1D-ND	-6.65	118.34	124.45
26	q	311	CHL	CHD-C1D-ND	-6.64	118.35	124.45
22	P	309	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	G	308	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	1	305	CLA	C4A-NA-C1A	6.63	109.69	106.71
26	3	315	CHL	CHD-C1D-ND	-6.63	118.36	124.45
26	6	315	CHL	CHD-C1D-ND	-6.63	118.36	124.45
22	s	303	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	q	302	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	3	302	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	s	305	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	6	303	CLA	C4A-NA-C1A	6.60	109.67	106.71
26	N	313	CHL	CHD-C1D-ND	-6.60	118.39	124.45
26	q	311	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
26	n	317	CHL	CHD-C1D-ND	-6.59	118.40	124.45
22	A	406	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	c	504	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	N	302	CLA	C4A-NA-C1A	6.58	109.67	106.71
22	U	303	CLA	C4A-NA-C1A	6.58	109.66	106.71
26	3	312	CHL	C2C-C3C-C4C	-6.58	101.80	106.49
22	C	505	CLA	C4A-NA-C1A	6.58	109.66	106.71
26	G	312	CHL	CHD-C1D-ND	-6.57	118.42	124.45
26	4	316	CHL	O2D-CGD-CBD	6.57	122.94	111.27
26	P	315	CHL	C2C-C3C-C4C	-6.57	101.81	106.49
22	2	302	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	q	305	CLA	C4A-NA-C1A	6.56	109.66	106.71
26	Q	316	CHL	CHD-C1D-ND	-6.56	118.43	124.45
22	3	303	CLA	C4A-NA-C1A	6.55	109.65	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	302	CLA	C4A-NA-C1A	6.55	109.65	106.71
26	3	313	CHL	CHD-C1D-ND	-6.55	118.44	124.45
26	p	317	CHL	CHD-C1D-ND	-6.55	118.44	124.45
26	u	316	CHL	CHD-C1D-ND	-6.54	118.44	124.45
22	Q	305	CLA	C4A-NA-C1A	6.53	109.64	106.71
26	u	313	CHL	CHD-C1D-ND	-6.53	118.45	124.45
22	R	303	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	S	305	CLA	C4A-NA-C1A	6.52	109.64	106.71
26	N	316	CHL	CHD-C1D-ND	-6.52	118.46	124.45
22	g	308	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	a	406	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	u	304	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	b	614	CLA	C4A-NA-C1A	6.51	109.63	106.71
26	n	314	CHL	CHD-C1D-ND	-6.50	118.48	124.45
26	r	616	CHL	CHD-C1D-ND	-6.49	118.49	124.45
26	n	314	CHL	C1B-CHB-C4A	-6.49	117.26	130.12
26	p	316	CHL	CHD-C1D-ND	-6.49	118.49	124.45
27	u	319	NEX	O24-C25-C24	6.48	118.25	113.38
22	n	303	CLA	C4A-NA-C1A	6.48	109.62	106.71
26	3	311	CHL	CHD-C1D-ND	-6.48	118.50	124.45
22	g	302	CLA	C4A-NA-C1A	6.47	109.62	106.71
26	1	314	CHL	CHD-C1D-ND	-6.47	118.51	124.45
22	4	305	CLA	C4A-NA-C1A	6.45	109.61	106.71
26	v	315	CHL	CHD-C1D-ND	-6.44	118.53	124.45
26	N	314	CHL	CHD-C1D-ND	-6.44	118.54	124.45
22	V	304	CLA	C4A-NA-C1A	6.43	109.60	106.71
26	g	313	CHL	CHD-C1D-ND	-6.42	118.55	124.45
22	G	302	CLA	C4A-NA-C1A	6.42	109.59	106.71
26	R	317	CHL	CHD-C1D-ND	-6.42	118.56	124.45
26	6	312	CHL	CHD-C1D-ND	-6.41	118.56	124.45
26	V	316	CHL	CHD-C1D-ND	-6.41	118.56	124.45
26	n	315	CHL	CHD-C1D-ND	-6.40	118.57	124.45
26	G	314	CHL	CHD-C1D-ND	-6.40	118.58	124.45
22	v	304	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	r	602	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	4	302	CLA	C4A-NA-C1A	6.39	109.58	106.71
26	G	313	CHL	CHD-C1D-ND	-6.39	118.59	124.45
26	Q	312	CHL	CHD-C1D-ND	-6.38	118.59	124.45
26	Q	311	CHL	CHD-C1D-ND	-6.38	118.59	124.45
26	4	315	CHL	CHD-C1D-ND	-6.37	118.60	124.45
26	N	313	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
26	V	314	CHL	CHD-C1D-ND	-6.36	118.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u	317	CHL	O2D-CGD-CBD	6.36	122.57	111.27
22	b	604	CLA	C4A-NA-C1A	6.36	109.57	106.71
22	B	604	CLA	C4A-NA-C1A	6.36	109.56	106.71
26	P	316	CHL	CHD-C1D-ND	-6.35	118.62	124.45
26	1	316	CHL	CHD-C1D-ND	-6.35	118.62	124.45
26	g	312	CHL	CHD-C1D-ND	-6.35	118.62	124.45
26	Q	314	CHL	CHD-C1D-ND	-6.34	118.63	124.45
22	1	303	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	Q	302	CLA	C4A-NA-C1A	6.34	109.56	106.71
26	1	315	CHL	CHD-C1D-ND	-6.32	118.64	124.45
26	U	316	CHL	CHD-C1D-ND	-6.32	118.65	124.45
26	6	301	CHL	CHD-C1D-ND	-6.32	118.65	124.45
26	u	314	CHL	CHD-C1D-ND	-6.30	118.66	124.45
26	Q	315	CHL	CHD-C1D-ND	-6.30	118.67	124.45
24	R	313	XAT	C26-C27-C28	-6.29	112.69	125.99
26	p	314	CHL	CHD-C1D-ND	-6.29	118.68	124.45
31	C	516	BCR	C15-C14-C13	-6.28	118.34	127.31
26	v	316	CHL	CHD-C1D-ND	-6.28	118.68	124.45
26	n	313	CHL	CHD-C1D-ND	-6.27	118.69	124.45
26	V	317	CHL	CHD-C1D-ND	-6.26	118.70	124.45
31	z	101	BCR	C15-C14-C13	-6.25	118.39	127.31
26	q	313	CHL	CHD-C1D-ND	-6.24	118.72	124.45
26	Q	313	CHL	CHD-C1D-ND	-6.24	118.72	124.45
22	6	304	CLA	C4A-NA-C1A	6.23	109.51	106.71
26	U	319	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	R	313	XAT	C6-C7-C8	-6.21	112.86	125.99
26	n	316	CHL	CHD-C1D-ND	-6.21	118.75	124.45
26	2	314	CHL	C1B-CHB-C4A	-6.21	117.83	130.12
26	u	317	CHL	CHD-C1D-ND	-6.20	118.75	124.45
26	G	316	CHL	CHD-C1D-ND	-6.20	118.76	124.45
26	4	316	CHL	CHD-C1D-ND	-6.19	118.76	124.45
26	N	314	CHL	C1B-CHB-C4A	-6.18	117.88	130.12
26	p	320	CHL	CHD-C1D-ND	-6.18	118.78	124.45
26	q	314	CHL	CHD-C1D-ND	-6.17	118.78	124.45
26	V	318	CHL	CHD-C1D-ND	-6.17	118.79	124.45
26	1	317	CHL	CHD-C1D-ND	-6.15	118.80	124.45
26	g	315	CHL	CHD-C1D-ND	-6.14	118.81	124.45
22	c	511	CLA	C4A-NA-C1A	6.14	109.47	106.71
26	g	316	CHL	CHD-C1D-ND	-6.14	118.82	124.45
22	S	306	CLA	C4A-NA-C1A	6.13	109.46	106.71
22	U	301	CLA	C4A-NA-C1A	6.12	109.46	106.71
26	1	318	CHL	CHD-C1D-ND	-6.12	118.83	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	301	CLA	C4A-NA-C1A	6.12	109.46	106.71
26	v	317	CHL	CHD-C1D-ND	-6.12	118.83	124.45
22	v	301	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	d	402	CLA	C4A-NA-C1A	6.09	109.45	106.71
26	2	317	CHL	CHD-C1D-ND	-6.09	118.86	124.45
22	p	302	CLA	C4A-NA-C1A	6.09	109.44	106.71
24	r	612	XAT	C6-C7-C8	-6.08	113.13	125.99
26	g	311	CHL	CHD-C1D-ND	-6.07	118.87	124.45
26	2	318	CHL	CHD-C1D-ND	-6.06	118.88	124.45
22	n	305	CLA	CMD-C2D-C3D	6.06	141.55	127.61
22	2	305	CLA	CMD-C2D-C3D	6.05	141.53	127.61
26	5	317	CHL	CHD-C1D-ND	-6.05	118.90	124.45
26	p	319	CHL	CHD-C1D-ND	-6.05	118.90	124.45
31	B	620	BCR	C16-C17-C18	-6.03	118.70	127.31
22	1	302	CLA	C4A-NA-C1A	6.03	109.42	106.71
22	s	301	CLA	C4A-NA-C1A	6.03	109.42	106.71
26	5	318	CHL	CHD-C1D-ND	-6.03	118.92	124.45
26	6	316	CHL	CHD-C1D-ND	-6.03	118.92	124.45
22	P	306	CLA	CMD-C2D-C3D	6.02	141.47	127.61
26	G	315	CHL	CHD-C1D-ND	-6.02	118.92	124.45
22	p	306	CLA	CMD-C2D-C3D	6.02	141.45	127.61
22	D	403	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	V	301	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	s	306	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	n	301	CLA	C4A-NA-C1A	6.01	109.41	106.71
26	r	615	CHL	CHD-C1D-ND	-6.00	118.94	124.45
22	4	303	CLA	C4A-NA-C1A	6.00	109.40	106.71
22	u	301	CLA	C4A-NA-C1A	6.00	109.40	106.71
22	C	512	CLA	C4A-NA-C1A	5.99	109.40	106.71
22	2	301	CLA	C4A-NA-C1A	5.99	109.40	106.71
26	r	614	CHL	CHD-C1D-ND	-5.98	118.96	124.45
26	2	315	CHL	CHD-C1D-ND	-5.98	118.96	124.45
22	5	305	CLA	CMD-C2D-C3D	5.97	141.36	127.61
26	4	314	CHL	CHD-C1D-ND	-5.97	118.97	124.45
26	4	317	CHL	CHD-C1D-ND	-5.97	118.97	124.45
26	P	318	CHL	CHD-C1D-ND	-5.97	118.97	124.45
26	5	314	CHL	C1B-CHB-C4A	-5.96	118.31	130.12
26	R	316	CHL	CHD-C1D-ND	-5.95	118.99	124.45
26	r	619	CHL	CHD-C1D-ND	-5.94	119.00	124.45
31	b	620	BCR	C16-C17-C18	-5.93	118.85	127.31
26	q	314	CHL	C3C-C4C-NC	5.91	117.20	110.57
22	S	301	CLA	C4A-NA-C1A	5.91	109.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	315	CHL	CHD-C1D-ND	-5.90	119.04	124.45
22	1	301	CLA	C4A-NA-C1A	5.89	109.35	106.71
22	P	302	CLA	C4A-NA-C1A	5.89	109.35	106.71
22	3	301	CLA	C4A-NA-C1A	5.88	109.35	106.71
26	u	315	CHL	C3C-C4C-NC	5.88	117.17	110.57
26	P	319	CHL	CHD-C1D-ND	-5.88	119.05	124.45
31	C	517	BCR	C1-C6-C5	-5.87	114.34	122.61
26	R	315	CHL	CHD-C1D-ND	-5.87	119.06	124.45
26	U	317	CHL	CHD-C1D-ND	-5.85	119.08	124.45
26	v	318	CHL	CHD-C1D-ND	-5.84	119.08	124.45
26	P	315	CHL	C1B-CHB-C4A	-5.84	118.55	130.12
31	c	515	BCR	C1-C6-C5	-5.83	114.40	122.61
26	U	315	CHL	CHD-C1D-ND	-5.83	119.10	124.45
26	G	311	CHL	CHD-C1D-ND	-5.82	119.11	124.45
22	q	301	CLA	C4A-NA-C1A	5.80	109.31	106.71
26	u	318	CHL	CHD-C1D-ND	-5.78	119.14	124.45
26	Q	315	CHL	C3C-C4C-NC	5.76	117.04	110.57
22	N	301	CLA	C4A-NA-C1A	5.76	109.30	106.71
26	6	316	CHL	C3C-C4C-NC	5.76	117.03	110.57
22	A	408	CLA	CMB-C2B-C1B	-5.73	119.66	128.46
26	n	318	CHL	O2D-CGD-CBD	5.73	121.44	111.27
22	N	305	CLA	CMD-C2D-C3D	5.72	140.76	127.61
22	g	301	CLA	C4A-NA-C1A	5.71	109.27	106.71
26	v	314	CHL	CHD-C1D-ND	-5.71	119.21	124.45
26	p	318	CHL	CHD-C1D-ND	-5.71	119.21	124.45
24	V	311	XAT	C15-C14-C13	-5.70	119.18	127.31
22	5	301	CLA	C4A-NA-C1A	5.69	109.27	106.71
27	V	319	NEX	C11-C10-C9	-5.68	119.21	127.31
22	a	408	CLA	CMB-C2B-C1B	-5.68	119.74	128.46
22	6	302	CLA	C4A-NA-C1A	5.67	109.26	106.71
31	x	202	BCR	C11-C10-C9	-5.66	119.23	127.31
26	s	314	CHL	CHD-C1D-ND	-5.66	119.26	124.45
26	3	312	CHL	C1B-CHB-C4A	-5.65	118.93	130.12
26	S	314	CHL	CHD-C1D-ND	-5.64	119.27	124.45
24	n	311	XAT	C6-C7-C8	-5.64	114.07	125.99
26	G	315	CHL	C3C-C4C-NC	5.64	116.89	110.57
31	x	202	BCR	C7-C8-C9	-5.63	117.72	126.23
22	g	301	CLA	CMB-C2B-C1B	-5.63	119.81	128.46
26	g	315	CHL	C3C-C4C-NC	5.59	116.84	110.57
26	6	313	CHL	C1B-CHB-C4A	-5.58	119.06	130.12
31	X	201	BCR	C7-C8-C9	-5.58	117.80	126.23
22	Q	301	CLA	C4A-NA-C1A	5.58	109.21	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	201	BCR	C11-C10-C9	-5.58	119.35	127.31
31	C	516	BCR	C16-C17-C18	-5.56	119.38	127.31
31	z	101	BCR	C16-C17-C18	-5.54	119.41	127.31
26	p	315	CHL	C1B-CHB-C4A	-5.53	119.16	130.12
26	U	314	CHL	C3C-C4C-NC	5.53	116.77	110.57
26	3	315	CHL	C3C-C4C-NC	5.52	116.76	110.57
26	v	313	CHL	O2D-CGD-CBD	5.52	121.07	111.27
27	u	319	NEX	C38-C25-C26	-5.51	113.03	122.26
26	g	312	CHL	O2D-CGD-CBD	5.50	121.04	111.27
22	G	301	CLA	C4A-NA-C1A	5.49	109.18	106.71
26	N	315	CHL	CHD-C1D-ND	-5.48	119.41	124.45
26	5	318	CHL	O2D-CGD-CBD	5.47	121.00	111.27
26	R	316	CHL	C3C-C4C-NC	5.45	116.69	110.57
26	s	314	CHL	C3C-C4C-NC	5.44	116.68	110.57
26	q	312	CHL	C1B-CHB-C4A	-5.44	119.35	130.12
26	N	315	CHL	C3C-C4C-NC	5.44	116.67	110.57
24	Q	309	XAT	C15-C14-C13	-5.43	119.56	127.31
26	S	314	CHL	C3C-C4C-NC	5.43	116.66	110.57
26	Q	313	CHL	O2D-CGD-CBD	5.43	120.92	111.27
31	t	101	BCR	C24-C23-C22	-5.42	118.05	126.23
26	5	315	CHL	C3C-C4C-NC	5.41	116.64	110.57
22	u	304	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
26	V	313	CHL	O2D-CGD-CBD	5.41	120.88	111.27
26	p	318	CHL	C3C-C4C-NC	5.41	116.63	110.57
24	G	309	XAT	C6-C7-C8	-5.39	114.60	125.99
26	q	314	CHL	C2D-C1D-ND	5.38	114.07	110.10
24	6	310	XAT	C6-C7-C8	-5.38	114.63	125.99
22	G	301	CLA	CMB-C2B-C1B	-5.36	120.22	128.46
26	3	311	CHL	O2D-CGD-CBD	5.35	120.78	111.27
26	q	312	CHL	C4A-NA-C1A	5.35	109.11	106.71
26	P	318	CHL	C3C-C4C-NC	5.35	116.57	110.57
26	r	615	CHL	C3C-C4C-NC	5.32	116.53	110.57
24	q	309	XAT	C15-C14-C13	-5.31	119.72	127.31
27	n	319	NEX	C15-C14-C13	-5.31	119.73	127.31
26	q	313	CHL	O2D-CGD-CBD	5.31	120.70	111.27
31	K	101	BCR	C16-C17-C18	-5.30	119.74	127.31
31	T	101	BCR	C24-C23-C22	-5.30	118.23	126.23
26	S	316	CHL	O2D-CGD-CBD	5.29	120.67	111.27
24	g	309	XAT	C6-C7-C8	-5.29	114.80	125.99
26	P	315	CHL	C4A-NA-C1A	5.29	109.08	106.71
26	s	316	CHL	O2D-CGD-CBD	5.29	120.67	111.27
26	v	314	CHL	C3C-C4C-NC	5.29	116.50	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	618	BCR	C15-C14-C13	-5.29	119.77	127.31
26	2	315	CHL	C3C-C4C-NC	5.27	116.49	110.57
26	q	312	CHL	O2D-CGD-CBD	5.27	120.64	111.27
27	n	319	NEX	C11-C10-C9	-5.27	119.79	127.31
26	2	318	CHL	O2D-CGD-CBD	5.27	120.63	111.27
26	G	311	CHL	O2D-CGD-CBD	5.27	120.63	111.27
26	6	312	CHL	O2D-CGD-CBD	5.26	120.62	111.27
26	n	314	CHL	C4A-NA-C1A	5.26	109.07	106.71
26	U	314	CHL	CHD-C1D-ND	-5.26	119.62	124.45
26	G	312	CHL	O2D-CGD-CBD	5.25	120.60	111.27
31	C	518	BCR	C16-C17-C18	-5.25	119.82	127.31
31	B	619	BCR	C16-C17-C18	-5.25	119.82	127.31
31	b	618	BCR	C15-C14-C13	-5.24	119.83	127.31
26	u	317	CHL	C3C-C4C-NC	5.24	116.44	110.57
22	C	507	CLA	CMB-C2B-C1B	-5.24	120.41	128.46
31	K	101	BCR	C1-C6-C5	-5.23	115.25	122.61
26	p	316	CHL	O2D-CGD-CBD	5.22	120.54	111.27
31	k	101	BCR	C1-C6-C5	-5.21	115.27	122.61
26	p	314	CHL	O2D-CGD-CBD	5.21	120.52	111.27
26	6	316	CHL	C2D-C1D-ND	5.21	113.94	110.10
26	2	317	CHL	C3C-C4C-NC	5.20	116.41	110.57
26	U	316	CHL	C3C-C4C-NC	5.20	116.41	110.57
26	R	315	CHL	O2D-CGD-CBD	5.20	120.52	111.27
26	u	318	CHL	C3C-C4C-NC	5.20	116.41	110.57
22	c	506	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
26	N	317	CHL	O2D-CGD-CBD	5.20	120.51	111.27
26	r	614	CHL	O2D-CGD-CBD	5.20	120.51	111.27
26	p	320	CHL	C3C-C4C-NC	5.20	116.40	110.57
26	g	316	CHL	O2D-CGD-CBD	5.20	120.50	111.27
26	Q	315	CHL	C2D-C1D-ND	5.20	113.93	110.10
31	c	516	BCR	C16-C17-C18	-5.19	119.90	127.31
26	r	619	CHL	C3C-C4C-NC	5.19	116.39	110.57
31	b	618	BCR	C11-C10-C9	-5.19	119.90	127.31
26	4	314	CHL	O2D-CGD-CBD	5.19	120.48	111.27
26	4	314	CHL	C3C-C4C-NC	5.18	116.38	110.57
31	k	101	BCR	C16-C17-C18	-5.18	119.92	127.31
27	u	319	NEX	C15-C14-C13	-5.18	119.92	127.31
26	P	314	CHL	O2D-CGD-CBD	5.18	120.47	111.27
26	6	314	CHL	O2D-CGD-CBD	5.18	120.47	111.27
26	U	317	CHL	C3C-C4C-NC	5.17	116.37	110.57
31	b	619	BCR	C16-C17-C18	-5.17	119.93	127.31
26	q	315	CHL	O2D-CGD-CBD	5.16	120.44	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	314	CHL	O2D-CGD-CBD	5.16	120.44	111.27
26	v	316	CHL	C3C-C4C-NC	5.16	116.36	110.57
26	n	317	CHL	O2D-CGD-CBD	5.16	120.44	111.27
26	S	314	CHL	O2D-CGD-CBD	5.16	120.43	111.27
22	b	609	CLA	CMB-C2B-C1B	-5.15	120.54	128.46
22	A	404	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
27	2	319	NEX	C11-C10-C9	-5.15	119.96	127.31
22	a	404	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
26	3	313	CHL	O2D-CGD-CBD	5.15	120.41	111.27
26	G	311	CHL	C3C-C4C-NC	5.14	116.34	110.57
31	x	202	BCR	C16-C17-C18	-5.14	119.97	127.31
26	3	311	CHL	C3C-C4C-NC	5.14	116.33	110.57
26	6	312	CHL	C3C-C4C-NC	5.13	116.33	110.57
26	V	315	CHL	O2D-CGD-CBD	5.13	120.39	111.27
26	Q	315	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
26	g	315	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
31	c	515	BCR	C4-C5-C6	-5.13	115.28	122.73
26	P	319	CHL	C3C-C4C-NC	5.12	116.32	110.57
26	N	316	CHL	C3C-C4C-NC	5.12	116.31	110.57
31	B	618	BCR	C11-C10-C9	-5.12	120.00	127.31
22	x	201	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
31	X	201	BCR	C16-C17-C18	-5.11	120.01	127.31
26	p	319	CHL	O2D-CGD-CBD	5.11	120.36	111.27
31	c	515	BCR	C33-C5-C6	-5.11	118.79	124.53
26	6	313	CHL	C4A-NA-C1A	5.11	109.00	106.71
26	q	314	CHL	C3D-C2D-C1D	-5.11	98.86	105.83
26	3	314	CHL	C1B-CHB-C4A	-5.11	120.00	130.12
26	Q	311	CHL	O2D-CGD-CBD	5.11	120.34	111.27
26	5	317	CHL	C3C-C4C-NC	5.10	116.30	110.57
24	4	311	XAT	C35-C34-C33	-5.10	120.03	127.31
26	g	311	CHL	C3C-C4C-NC	5.10	116.29	110.57
27	N	318	NEX	C38-C25-C26	-5.10	113.71	122.26
26	4	315	CHL	O2D-CGD-CBD	5.10	120.33	111.27
26	v	318	CHL	C3C-C4C-NC	5.10	116.28	110.57
26	4	317	CHL	C3C-C4C-NC	5.09	116.28	110.57
26	4	317	CHL	O2D-CGD-CBD	5.09	120.31	111.27
22	6	302	CLA	CMB-C2B-C1B	-5.08	120.65	128.46
31	C	517	BCR	C33-C5-C6	-5.08	118.82	124.53
26	5	314	CHL	C4A-NA-C1A	5.08	108.99	106.71
26	P	316	CHL	O2D-CGD-CBD	5.08	120.30	111.27
22	X	202	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
26	r	614	CHL	C3C-C4C-NC	5.08	116.27	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	605	CLA	CAA-C2A-C3A	-5.08	98.87	112.78
26	v	315	CHL	O2D-CGD-CBD	5.08	120.29	111.27
31	C	517	BCR	C4-C5-C6	-5.08	115.36	122.73
24	Q	309	XAT	C11-C10-C9	-5.07	120.07	127.31
26	R	315	CHL	C3C-C4C-NC	5.07	116.25	110.57
22	b	605	CLA	CAA-C2A-C3A	-5.07	98.90	112.78
26	6	316	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
26	G	315	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
26	1	317	CHL	C3C-C4C-NC	5.06	116.24	110.57
26	g	313	CHL	C3C-C4C-NC	5.06	116.24	110.57
22	P	302	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
26	V	318	CHL	O2D-CGD-CBD	5.05	120.25	111.27
24	3	309	XAT	C6-C7-C8	-5.05	115.32	125.99
24	q	309	XAT	C11-C10-C9	-5.04	120.11	127.31
31	B	618	BCR	C16-C17-C18	-5.04	120.11	127.31
26	g	311	CHL	O2D-CGD-CBD	5.04	120.23	111.27
26	S	315	CHL	O2D-CGD-CBD	5.04	120.22	111.27
26	1	316	CHL	O2D-CGD-CBD	5.04	120.22	111.27
31	b	618	BCR	C38-C26-C25	-5.04	118.87	124.53
27	S	317	NEX	C11-C10-C9	-5.03	120.12	127.31
26	n	313	CHL	C3C-C4C-NC	5.03	116.22	110.57
31	K	101	BCR	C20-C21-C22	-5.03	120.13	127.31
22	B	609	CLA	CMB-C2B-C1B	-5.03	120.73	128.46
31	b	618	BCR	C16-C17-C18	-5.03	120.13	127.31
26	p	319	CHL	C3C-C4C-NC	5.03	116.21	110.57
31	k	101	BCR	C20-C21-C22	-5.03	120.14	127.31
26	N	313	CHL	O2D-CGD-CBD	5.03	120.20	111.27
27	2	319	NEX	C38-C25-C26	-5.02	113.84	122.26
27	V	319	NEX	C27-C28-C29	-5.02	117.74	125.53
27	2	319	NEX	C27-C28-C29	-5.02	117.74	125.53
26	g	314	CHL	C1B-CHB-C4A	-5.02	120.19	130.12
26	p	317	CHL	O2D-CGD-CBD	5.01	120.18	111.27
26	4	316	CHL	C3C-C4C-NC	5.01	116.19	110.57
22	Q	301	CLA	CMB-C2B-C1B	-5.01	120.76	128.46
27	U	318	NEX	C15-C14-C13	-5.01	120.16	127.31
27	u	319	NEX	C11-C10-C9	-5.01	120.16	127.31
22	2	306	CLA	CMB-C2B-C1B	-5.01	120.77	128.46
26	1	315	CHL	O2D-CGD-CBD	5.00	120.15	111.27
22	3	301	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
31	T	101	BCR	C11-C10-C9	-4.99	120.18	127.31
26	N	315	CHL	O2D-CGD-CBD	4.99	120.14	111.27
26	1	318	CHL	C3C-C4C-NC	4.99	116.17	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	319	NEX	C11-C10-C9	-4.99	120.19	127.31
26	Q	312	CHL	O2D-CGD-CBD	4.98	120.12	111.27
24	R	313	XAT	C18-C5-C6	-4.98	113.91	122.26
27	P	301	NEX	C38-C25-C26	-4.98	113.92	122.26
27	S	317	NEX	C38-C25-C26	-4.97	113.92	122.26
26	U	315	CHL	C3C-C4C-NC	4.97	116.15	110.57
26	n	317	CHL	C3C-C4C-NC	4.97	116.15	110.57
32	L	102	SQD	O9-S-C6	4.97	112.85	106.94
26	v	314	CHL	O2D-CGD-CBD	4.97	120.11	111.27
31	t	101	BCR	C11-C10-C9	-4.97	120.21	127.31
26	Q	311	CHL	C3C-C4C-NC	4.97	116.15	110.57
26	v	318	CHL	O2D-CGD-CBD	4.97	120.09	111.27
26	P	319	CHL	O2D-CGD-CBD	4.97	120.09	111.27
22	q	304	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
26	2	316	CHL	O2D-CGD-CBD	4.96	120.08	111.27
27	5	319	NEX	C27-C28-C29	-4.96	117.84	125.53
26	3	315	CHL	C3D-C2D-C1D	-4.96	99.07	105.83
26	6	315	CHL	C1B-CHB-C4A	-4.96	120.30	130.12
26	V	314	CHL	O2D-CGD-CBD	4.95	120.07	111.27
26	s	315	CHL	O2D-CGD-CBD	4.95	120.07	111.27
26	1	314	CHL	O2D-CGD-CBD	4.95	120.06	111.27
26	N	316	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
26	5	316	CHL	O2D-CGD-CBD	4.94	120.05	111.27
26	1	313	CHL	O2D-CGD-CBD	4.94	120.05	111.27
22	5	301	CLA	CMB-C2B-C1B	-4.94	120.87	128.46
24	N	311	XAT	C6-C7-C8	-4.94	115.55	125.99
26	S	313	CHL	O2D-CGD-CBD	4.94	120.05	111.27
26	p	318	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
26	p	314	CHL	C3C-C4C-NC	4.94	116.11	110.57
31	t	101	BCR	C33-C5-C6	-4.94	118.98	124.53
26	5	313	CHL	O2D-CGD-CBD	4.93	120.03	111.27
26	n	313	CHL	O2D-CGD-CBD	4.93	120.03	111.27
26	2	313	CHL	O2D-CGD-CBD	4.93	120.03	111.27
27	v	319	NEX	C27-C28-C29	-4.93	117.88	125.53
26	U	313	CHL	O2D-CGD-CBD	4.93	120.03	111.27
26	u	314	CHL	C3C-C4C-NC	4.93	116.10	110.57
26	V	317	CHL	C3C-C4C-NC	4.93	116.10	110.57
26	G	316	CHL	C3C-C4C-NC	4.92	116.09	110.57
22	p	302	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
22	N	301	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
27	s	317	NEX	C38-C25-C26	-4.92	114.01	122.26
26	v	317	CHL	C3C-C4C-NC	4.92	116.09	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	u	320	NEX	C38-C25-C26	-4.92	114.02	122.26
32	l	102	SQD	O9-S-C6	4.91	112.78	106.94
27	v	319	NEX	C11-C10-C9	-4.91	120.30	127.31
26	v	313	CHL	C3C-C4C-NC	4.91	116.08	110.57
26	G	313	CHL	C3C-C4C-NC	4.91	116.08	110.57
27	r	617	NEX	C38-C25-C26	-4.91	114.03	122.26
26	Q	316	CHL	O2D-CGD-CBD	4.91	119.99	111.27
26	g	313	CHL	O2D-CGD-CBD	4.90	119.98	111.27
26	G	312	CHL	C4A-NA-C1A	4.90	108.91	106.71
26	4	313	CHL	O2D-CGD-CBD	4.90	119.98	111.27
31	b	619	BCR	C1-C6-C5	-4.90	115.71	122.61
24	U	311	XAT	C6-C7-C8	-4.90	115.64	125.99
22	n	306	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
26	V	318	CHL	C3C-C4C-NC	4.89	116.05	110.57
26	P	318	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
26	1	318	CHL	O2D-CGD-CBD	4.88	119.94	111.27
26	g	316	CHL	C3C-C4C-NC	4.88	116.04	110.57
27	N	318	NEX	C15-C14-C13	-4.88	120.35	127.31
31	T	101	BCR	C33-C5-C6	-4.88	119.05	124.53
26	s	313	CHL	O2D-CGD-CBD	4.88	119.93	111.27
27	u	319	NEX	O24-C25-C38	4.88	120.90	115.06
31	b	619	BCR	C15-C14-C13	-4.88	120.35	127.31
31	D	404	BCR	C24-C23-C22	-4.87	118.87	126.23
26	6	317	CHL	O2D-CGD-CBD	4.87	119.93	111.27
26	R	316	CHL	O2D-CGD-CBD	4.87	119.93	111.27
22	3	304	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
26	G	315	CHL	C2D-C1D-ND	4.87	113.69	110.10
22	A	408	CLA	CMB-C2B-C3B	4.86	133.78	124.68
31	B	619	BCR	C1-C6-C5	-4.86	115.76	122.61
26	p	317	CHL	C3C-C4C-NC	4.86	116.03	110.57
27	U	318	NEX	C38-C25-C26	-4.86	114.11	122.26
27	V	319	NEX	C38-C25-C26	-4.86	114.11	122.26
36	C	519	DGD	O2G-C1B-C2B	4.86	121.97	111.50
26	3	312	CHL	C4A-NA-C1A	4.86	108.89	106.71
31	B	619	BCR	C15-C14-C13	-4.85	120.39	127.31
26	V	314	CHL	C3C-C4C-NC	4.85	116.01	110.57
36	c	517	DGD	O2G-C1B-C2B	4.85	121.95	111.50
31	B	618	BCR	C38-C26-C25	-4.85	119.09	124.53
31	d	403	BCR	C24-C23-C22	-4.85	118.91	126.23
22	2	301	CLA	CMB-C2B-C1B	-4.85	121.02	128.46
22	a	408	CLA	CMB-C2B-C3B	4.84	133.74	124.68
26	2	317	CHL	O2D-CGD-CBD	4.84	119.87	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	301	CHL	O2D-CGD-CBD	4.84	119.87	111.27
26	6	313	CHL	O2D-CGD-CBD	4.84	119.87	111.27
26	U	319	CHL	C3C-C4C-NC	4.84	116.00	110.57
26	2	317	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
27	5	319	NEX	C38-C25-C26	-4.84	114.15	122.26
26	2	318	CHL	C3C-C4C-NC	4.84	116.00	110.57
22	5	306	CLA	CMB-C2B-C1B	-4.83	121.03	128.46
22	B	617	CLA	CMB-C2B-C1B	-4.83	121.04	128.46
24	u	311	XAT	C6-C7-C8	-4.83	115.79	125.99
22	n	301	CLA	CMB-C2B-C1B	-4.83	121.05	128.46
27	n	319	NEX	C17-C1-C6	-4.82	106.16	110.47
26	U	317	CHL	O2D-CGD-CBD	4.82	119.84	111.27
31	d	403	BCR	C30-C25-C26	-4.82	115.82	122.61
26	v	315	CHL	C3C-C4C-NC	4.82	115.98	110.57
26	5	317	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
31	A	409	BCR	C11-C10-C9	-4.82	120.43	127.31
26	5	318	CHL	C3C-C4C-NC	4.82	115.97	110.57
26	p	320	CHL	C3D-C2D-C1D	-4.81	99.27	105.83
26	g	315	CHL	C2D-C1D-ND	4.81	113.65	110.10
27	p	301	NEX	C38-C25-C26	-4.81	114.21	122.26
26	q	313	CHL	C3C-C4C-NC	4.80	115.96	110.57
26	3	311	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
26	Q	312	CHL	C3C-C4C-NC	4.80	115.95	110.57
26	v	316	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
26	5	317	CHL	O2D-CGD-CBD	4.79	119.78	111.27
31	a	409	BCR	C1-C6-C5	-4.79	115.87	122.61
22	c	510	CLA	CMB-C2B-C1B	-4.79	121.11	128.46
26	3	316	CHL	O2D-CGD-CBD	4.79	119.77	111.27
26	R	316	CHL	C3D-C2D-C1D	-4.79	99.30	105.83
31	t	101	BCR	C20-C21-C22	-4.78	120.48	127.31
26	G	316	CHL	O2D-CGD-CBD	4.78	119.77	111.27
24	v	311	XAT	C15-C14-C13	-4.78	120.49	127.31
27	u	319	NEX	C31-C30-C29	-4.78	120.49	127.31
31	T	101	BCR	C7-C8-C9	-4.78	119.02	126.23
26	P	317	CHL	O2D-CGD-CBD	4.77	119.75	111.27
27	R	301	NEX	C17-C1-C6	-4.77	106.20	110.47
22	C	511	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
31	D	404	BCR	C30-C25-C26	-4.77	115.90	122.61
24	r	612	XAT	C18-C5-C6	-4.77	114.27	122.26
22	v	304	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
22	N	306	CLA	CMB-C2B-C1B	-4.76	121.14	128.46
26	5	315	CHL	O2D-CGD-CBD	4.76	119.73	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	315	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
26	3	312	CHL	O2D-CGD-CBD	4.76	119.73	111.27
26	u	317	CHL	C3D-C2D-C1D	-4.76	99.33	105.83
27	2	319	NEX	C35-C34-C33	-4.76	120.52	127.31
26	u	318	CHL	O2D-CGD-CBD	4.75	119.72	111.27
24	p	312	XAT	C6-C7-C8	-4.75	115.94	125.99
26	R	317	CHL	C3C-C4C-NC	4.75	115.90	110.57
31	A	409	BCR	C1-C6-C5	-4.75	115.92	122.61
26	G	313	CHL	O2D-CGD-CBD	4.75	119.70	111.27
24	q	309	XAT	C26-C27-C28	-4.75	115.96	125.99
26	g	311	CHL	C3D-C2D-C1D	-4.74	99.36	105.83
27	n	319	NEX	C38-C25-C26	-4.74	114.31	122.26
22	V	304	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
31	c	515	BCR	C11-C10-C9	-4.74	120.54	127.31
26	P	318	CHL	CHD-C4C-C3C	-4.74	117.87	124.84
26	r	619	CHL	C3D-C2D-C1D	-4.74	99.37	105.83
26	r	615	CHL	C3D-C2D-C1D	-4.73	99.37	105.83
31	t	101	BCR	C7-C8-C9	-4.73	119.08	126.23
27	r	617	NEX	C15-C14-C13	-4.73	120.56	127.31
24	6	310	XAT	C15-C14-C13	-4.73	120.56	127.31
26	1	315	CHL	C3C-C4C-NC	4.72	115.87	110.57
26	p	318	CHL	CHD-C4C-C3C	-4.72	117.90	124.84
26	2	313	CHL	C3C-C4C-NC	4.72	115.87	110.57
26	1	316	CHL	C3C-C4C-NC	4.72	115.86	110.57
26	n	317	CHL	C3D-C2D-C1D	-4.72	99.39	105.83
26	3	315	CHL	C2D-C1D-ND	4.72	113.58	110.10
32	l	102	SQD	O5-C5-C4	4.72	118.26	109.69
22	6	305	CLA	CMB-C2B-C1B	-4.72	121.22	128.46
26	q	311	CHL	C3C-C4C-NC	4.71	115.86	110.57
27	p	301	NEX	C27-C28-C29	-4.71	118.22	125.53
26	1	314	CHL	C3C-C4C-NC	4.71	115.86	110.57
31	C	517	BCR	C27-C26-C25	-4.71	115.89	122.73
24	6	310	XAT	C26-C27-C28	-4.71	116.03	125.99
26	r	615	CHL	O2D-CGD-CBD	4.71	119.64	111.27
27	P	301	NEX	C27-C28-C29	-4.71	118.22	125.53
26	g	312	CHL	C3C-C4C-NC	4.70	115.85	110.57
26	2	317	CHL	CHD-C4C-C3C	-4.70	117.93	124.84
27	5	319	NEX	C35-C34-C33	-4.70	120.60	127.31
31	a	409	BCR	C11-C10-C9	-4.70	120.60	127.31
31	b	618	BCR	C24-C23-C22	-4.70	119.14	126.23
22	q	301	CLA	CMB-C2B-C1B	-4.69	121.25	128.46
22	g	301	CLA	CMB-C2B-C3B	4.69	133.46	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	312	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
26	2	315	CHL	O2D-CGD-CBD	4.69	119.60	111.27
26	U	316	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
31	T	101	BCR	C20-C21-C22	-4.69	120.62	127.31
32	C	501	SQD	C1-O5-C5	4.69	122.89	113.69
26	5	313	CHL	C3C-C4C-NC	4.68	115.82	110.57
26	n	314	CHL	O2D-CGD-CBD	4.68	119.59	111.27
24	3	309	XAT	C15-C14-C13	-4.68	120.63	127.31
31	x	202	BCR	C15-C14-C13	-4.68	120.63	127.31
32	a	410	SQD	C1-O5-C5	4.68	122.88	113.69
27	v	319	NEX	C38-C25-C26	-4.68	114.42	122.26
26	P	314	CHL	C3C-C4C-NC	4.68	115.82	110.57
26	P	319	CHL	C3D-C2D-C1D	-4.68	99.45	105.83
26	r	619	CHL	O2D-CGD-CBD	4.68	119.58	111.27
26	4	314	CHL	C3D-C2D-C1D	-4.68	99.45	105.83
26	Q	313	CHL	C3C-C4C-NC	4.68	115.81	110.57
26	g	315	CHL	CHD-C4C-C3C	-4.67	117.97	124.84
26	v	314	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
26	U	319	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
31	c	515	BCR	C27-C26-C25	-4.67	115.95	122.73
26	P	316	CHL	C3C-C4C-NC	4.66	115.80	110.57
26	u	315	CHL	CHD-C4C-C3C	-4.66	117.99	124.84
26	r	616	CHL	C3C-C4C-NC	4.66	115.80	110.57
32	L	102	SQD	O5-C5-C4	4.66	118.16	109.69
26	g	314	CHL	C3D-C2D-C1D	-4.66	99.47	105.83
22	G	304	CLA	CMB-C2B-C1B	-4.66	121.31	128.46
31	X	201	BCR	C15-C14-C13	-4.65	120.67	127.31
27	u	320	NEX	C15-C14-C13	-4.65	120.67	127.31
26	1	318	CHL	C3D-C2D-C1D	-4.65	99.48	105.83
26	V	313	CHL	C3C-C4C-NC	4.64	115.78	110.57
26	u	314	CHL	C3D-C2D-C1D	-4.64	99.49	105.83
26	2	314	CHL	O2D-CGD-CBD	4.64	119.52	111.27
26	5	316	CHL	C3C-C4C-NC	4.64	115.77	110.57
22	n	303	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
26	u	313	CHL	C3C-C4C-NC	4.64	115.77	110.57
24	P	312	XAT	C15-C14-C13	-4.64	120.69	127.31
26	U	319	CHL	O2D-CGD-CBD	4.63	119.50	111.27
26	Q	314	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
22	u	301	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
26	Q	316	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
26	V	316	CHL	C3C-C4C-NC	4.63	115.76	110.57
26	u	316	CHL	C3C-C4C-NC	4.63	115.76	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	317	CHL	C3C-C4C-NC	4.63	115.76	110.57
26	r	616	CHL	O2D-CGD-CBD	4.63	119.49	111.27
26	N	314	CHL	O2D-CGD-CBD	4.63	119.49	111.27
26	R	315	CHL	C3D-C2D-C1D	-4.63	99.52	105.83
26	P	318	CHL	O2D-CGD-CBD	4.63	119.49	111.27
26	2	315	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
31	K	101	BCR	C15-C14-C13	-4.62	120.71	127.31
26	n	313	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
26	G	313	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
22	s	303	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
26	S	313	CHL	C3C-C4C-NC	4.62	115.75	110.57
26	G	311	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
26	2	316	CHL	C3C-C4C-NC	4.62	115.75	110.57
27	V	319	NEX	C15-C14-C13	-4.62	120.72	127.31
31	A	409	BCR	C15-C14-C13	-4.62	120.72	127.31
26	G	314	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
26	q	315	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
26	u	318	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
26	p	317	CHL	C3D-C2D-C1D	-4.61	99.53	105.83
26	G	314	CHL	C3C-C4C-NC	4.61	115.75	110.57
26	6	301	CHL	C3C-C4C-NC	4.61	115.74	110.57
26	g	313	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
26	4	317	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
26	5	314	CHL	O2D-CGD-CBD	4.61	119.46	111.27
26	p	314	CHL	CHD-C4C-C3C	-4.61	118.06	124.84
27	u	320	NEX	C11-C10-C9	-4.61	120.73	127.31
26	5	315	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
26	Q	314	CHL	C3C-C4C-NC	4.61	115.74	110.57
26	Q	316	CHL	C3C-C4C-NC	4.61	115.74	110.57
23	r	611	LUT	C35-C34-C33	-4.61	120.73	127.31
26	6	312	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
26	n	316	CHL	C3C-C4C-NC	4.60	115.73	110.57
26	q	311	CHL	O2D-CGD-CBD	4.60	119.44	111.27
26	q	314	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
26	4	315	CHL	C3C-C4C-NC	4.60	115.73	110.57
26	Q	315	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
26	1	314	CHL	C1B-CHB-C4A	-4.59	121.02	130.12
26	r	614	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
26	n	316	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
26	n	315	CHL	C3C-C4C-NC	4.59	115.72	110.57
26	U	317	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
26	N	313	CHL	C3D-C2D-C1D	-4.59	99.57	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	507	CLA	CMB-C2B-C3B	4.58	133.25	124.68
31	C	517	BCR	C11-C10-C9	-4.58	120.77	127.31
26	p	319	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
26	4	316	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
22	Q	304	CLA	CMB-C2B-C1B	-4.57	121.43	128.46
26	1	317	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
26	U	313	CHL	C3C-C4C-NC	4.57	115.70	110.57
22	c	506	CLA	CMB-C2B-C3B	4.57	133.22	124.68
26	G	312	CHL	C3C-C4C-NC	4.57	115.69	110.57
26	u	315	CHL	CHD-C1D-ND	-4.57	120.26	124.45
26	1	314	CHL	C3D-C2D-C1D	-4.57	99.60	105.83
26	p	318	CHL	O2D-CGD-CBD	4.56	119.38	111.27
26	V	316	CHL	C3D-C2D-C1D	-4.56	99.60	105.83
26	p	314	CHL	C3D-C2D-C1D	-4.56	99.60	105.83
26	R	317	CHL	O2D-CGD-CBD	4.56	119.37	111.27
26	R	317	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
26	6	315	CHL	C3C-C4C-NC	4.56	115.68	110.57
26	V	314	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
26	s	313	CHL	C3C-C4C-NC	4.56	115.68	110.57
26	3	311	CHL	CHD-C4C-C3C	-4.55	118.14	124.84
26	V	317	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
26	1	316	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
26	1	313	CHL	C3C-C4C-NC	4.55	115.67	110.57
24	q	309	XAT	C31-C30-C29	-4.55	120.82	127.31
26	q	313	CHL	C3D-C2D-C1D	-4.55	99.63	105.83
26	Q	311	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
26	v	315	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
22	4	301	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
26	u	314	CHL	O2D-CGD-CBD	4.54	119.33	111.27
22	N	303	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
26	6	317	CHL	C3C-C4C-NC	4.54	115.66	110.57
31	B	618	BCR	C24-C23-C22	-4.54	119.38	126.23
26	p	315	CHL	C4A-NA-C1A	4.54	108.75	106.71
26	N	316	CHL	O2D-CGD-CBD	4.54	119.33	111.27
26	p	320	CHL	CHD-C4C-C3C	-4.54	118.17	124.84
26	S	314	CHL	C3D-C2D-C1D	-4.53	99.64	105.83
26	q	311	CHL	C3D-C2D-C1D	-4.53	99.64	105.83
31	K	101	BCR	C4-C5-C6	-4.53	116.15	122.73
31	c	516	BCR	C1-C6-C5	-4.53	116.23	122.61
32	m	101	SQD	O9-S-C6	4.53	112.32	106.94
26	v	313	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
26	G	312	CHL	C3D-C2D-C1D	-4.53	99.65	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	608	CLA	CMB-C2B-C1B	-4.53	121.51	128.46
26	p	316	CHL	C3C-C4C-NC	4.52	115.64	110.57
26	4	314	CHL	CHD-C4C-C3C	-4.52	118.19	124.84
22	6	304	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
22	R	309	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
31	a	409	BCR	C15-C14-C13	-4.52	120.86	127.31
26	P	314	CHL	C3D-C2D-C1D	-4.52	99.67	105.83
27	N	318	NEX	C27-C28-C29	-4.52	118.52	125.53
26	2	314	CHL	C3D-C2D-C1D	-4.52	99.67	105.83
26	V	313	CHL	C3D-C2D-C1D	-4.51	99.67	105.83
26	1	313	CHL	C3D-C2D-C1D	-4.51	99.67	105.83
26	4	313	CHL	C3C-C4C-NC	4.51	115.63	110.57
26	3	316	CHL	C3C-C4C-NC	4.51	115.63	110.57
31	k	101	BCR	C15-C14-C13	-4.51	120.87	127.31
22	B	608	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
31	C	517	BCR	C24-C23-C22	-4.51	119.42	126.23
26	g	314	CHL	C3C-C4C-NC	4.51	115.63	110.57
26	S	313	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
26	v	318	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
26	3	314	CHL	C3C-C4C-NC	4.50	115.62	110.57
26	q	315	CHL	C3C-C4C-NC	4.50	115.62	110.57
26	5	317	CHL	CHD-C4C-C3C	-4.50	118.22	124.84
26	6	316	CHL	CHD-C4C-C3C	-4.50	118.22	124.84
26	v	317	CHL	C3D-C2D-C1D	-4.50	99.70	105.83
26	s	313	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
26	s	316	CHL	C3C-C4C-NC	4.49	115.61	110.57
22	G	301	CLA	CMB-C2B-C3B	4.49	133.08	124.68
26	r	619	CHL	CHD-C4C-C3C	-4.49	118.24	124.84
26	u	313	CHL	O2D-CGD-CBD	4.49	119.25	111.27
26	r	616	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
26	q	314	CHL	C1D-ND-C4D	-4.49	103.15	106.33
26	2	316	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
26	g	314	CHL	O2D-CGD-CBD	4.49	119.24	111.27
26	s	314	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
26	4	313	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
32	M	101	SQD	O9-S-C6	4.49	112.27	106.94
26	S	316	CHL	C3C-C4C-NC	4.48	115.60	110.57
27	s	317	NEX	C11-C10-C9	-4.48	120.91	127.31
26	P	317	CHL	C3D-C2D-C1D	-4.48	99.71	105.83
23	U	310	LUT	C35-C34-C33	-4.48	120.92	127.31
24	n	311	XAT	C18-C5-C6	-4.47	114.76	122.26
24	Q	309	XAT	C26-C27-C28	-4.47	116.54	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	307	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
24	1	311	XAT	C35-C34-C33	-4.47	120.94	127.31
26	G	316	CHL	C3D-C2D-C1D	-4.47	99.74	105.83
26	V	318	CHL	C3D-C2D-C1D	-4.47	99.74	105.83
26	2	313	CHL	C3D-C2D-C1D	-4.46	99.74	105.83
26	u	316	CHL	O2D-CGD-CBD	4.46	119.20	111.27
31	c	515	BCR	C16-C17-C18	-4.46	120.94	127.31
22	b	608	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
26	N	314	CHL	C4A-NA-C1A	4.46	108.71	106.71
26	n	313	CHL	CHD-C4C-C3C	-4.46	118.29	124.84
31	c	515	BCR	C24-C23-C22	-4.46	119.50	126.23
26	u	313	CHL	C3D-C2D-C1D	-4.46	99.75	105.83
22	U	301	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
26	Q	312	CHL	C3D-C2D-C1D	-4.46	99.75	105.83
22	S	303	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
27	r	618	NEX	C2-C1-C6	4.45	113.54	109.21
26	N	313	CHL	C3C-C4C-NC	4.45	115.56	110.57
26	N	314	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
31	k	101	BCR	C4-C5-C6	-4.45	116.27	122.73
26	6	301	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
26	p	316	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
26	n	314	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
26	n	316	CHL	O2D-CGD-CBD	4.45	119.17	111.27
26	u	316	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	5	314	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	5	313	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	3	313	CHL	C3C-C4C-NC	4.44	115.56	110.57
26	U	313	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
22	S	307	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
26	5	316	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
32	m	101	SQD	O7-S-C6	4.44	112.22	106.94
26	p	315	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
27	v	319	NEX	C15-C14-C13	-4.44	120.97	127.31
26	6	317	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	N	316	CHL	CHD-C4C-C3C	-4.44	118.32	124.84
22	S	301	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
32	M	101	SQD	O7-S-C6	4.43	112.21	106.94
26	Q	315	CHL	C1D-ND-C4D	-4.43	103.19	106.33
27	r	617	NEX	C11-C10-C9	-4.43	120.99	127.31
26	U	314	CHL	CHD-C4C-C3C	-4.43	118.33	124.84
26	2	318	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
26	n	315	CHL	C3D-C2D-C1D	-4.43	99.79	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	320	CHL	C2D-C1D-ND	4.43	113.37	110.10
27	p	301	NEX	C15-C14-C13	-4.43	120.99	127.31
26	V	315	CHL	C1B-CHB-C4A	-4.43	121.35	130.12
27	s	317	NEX	C35-C34-C33	-4.43	120.99	127.31
26	s	316	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
26	q	312	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
27	N	318	NEX	C11-C10-C9	-4.42	121.00	127.31
26	5	318	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
26	P	315	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
26	g	316	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
27	n	319	NEX	C27-C28-C29	-4.41	118.69	125.53
27	r	617	NEX	C27-C28-C29	-4.41	118.69	125.53
27	P	301	NEX	O24-C25-C38	4.41	120.34	115.06
26	6	316	CHL	C1D-ND-C4D	-4.41	103.20	106.33
22	g	304	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
26	N	317	CHL	C3D-C2D-C1D	-4.41	99.82	105.83
26	n	318	CHL	C3D-C2D-C1D	-4.40	99.82	105.83
26	N	315	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
26	3	312	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
26	3	316	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
26	S	316	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
31	C	518	BCR	C1-C6-C5	-4.40	116.42	122.61
22	V	303	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
22	s	301	CLA	CMB-C2B-C1B	-4.40	121.71	128.46
33	d	404	PL9	C7-C8-C9	-4.39	119.48	126.79
26	s	315	CHL	C3D-C2D-C1D	-4.39	99.84	105.83
26	Q	313	CHL	C3D-C2D-C1D	-4.39	99.84	105.83
26	v	316	CHL	CHD-C4C-C3C	-4.39	118.39	124.84
27	p	301	NEX	C2-C1-C6	4.39	113.47	109.21
26	S	315	CHL	C3D-C2D-C1D	-4.39	99.85	105.83
26	V	315	CHL	C3D-C2D-C1D	-4.38	99.85	105.83
27	S	317	NEX	C35-C34-C33	-4.38	121.06	127.31
26	u	317	CHL	C2D-C1D-ND	4.38	113.33	110.10
26	5	315	CHL	CHD-C4C-C3C	-4.38	118.41	124.84
25	G	310	LHG	O7-C7-C8	4.37	120.92	111.50
23	N	310	LUT	C35-C34-C33	-4.37	121.07	127.31
26	3	314	CHL	C3D-C2D-C1D	-4.37	99.87	105.83
26	6	313	CHL	C3D-C2D-C1D	-4.37	99.87	105.83
26	U	315	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
26	g	312	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
26	Q	314	CHL	C1B-CHB-C4A	-4.36	121.48	130.12
33	D	405	PL9	C7-C8-C9	-4.36	119.53	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	309	XAT	C26-C27-C28	-4.36	116.78	125.99
26	N	317	CHL	C3C-C4C-NC	4.36	115.46	110.57
26	n	315	CHL	O2D-CGD-CBD	4.35	119.00	111.27
26	2	317	CHL	C2D-C1D-ND	4.35	113.31	110.10
24	V	311	XAT	C6-C7-C8	-4.35	116.80	125.99
22	A	404	CLA	CMB-C2B-C3B	4.35	132.82	124.68
22	a	404	CLA	CMB-C2B-C3B	4.35	132.81	124.68
26	6	315	CHL	C3D-C2D-C1D	-4.35	99.90	105.83
31	C	517	BCR	C16-C17-C18	-4.34	121.11	127.31
26	G	314	CHL	C1B-CHB-C4A	-4.34	121.52	130.12
26	N	316	CHL	C2D-C1D-ND	4.34	113.30	110.10
31	c	515	BCR	C38-C26-C25	-4.34	119.65	124.53
26	V	315	CHL	C3C-C4C-NC	4.34	115.44	110.57
36	c	519	DGD	O2G-C1B-C2B	4.34	120.85	111.50
24	g	309	XAT	C26-C27-C28	-4.34	116.83	125.99
26	P	316	CHL	C3D-C2D-C1D	-4.33	99.92	105.83
27	R	301	NEX	C2-C1-C6	4.33	113.42	109.21
22	6	302	CLA	CMB-C2B-C3B	4.33	132.78	124.68
27	R	301	NEX	C38-C25-C26	-4.33	115.00	122.26
36	J	101	DGD	O2G-C1B-C2B	4.33	120.83	111.50
24	v	311	XAT	C6-C7-C8	-4.33	116.84	125.99
22	N	304	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
22	b	613	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
22	u	304	CLA	CMB-C2B-C3B	4.32	132.75	124.68
22	2	306	CLA	CMB-C2B-C3B	4.32	132.75	124.68
32	L	102	SQD	O7-S-C6	4.31	112.06	106.94
26	U	314	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
26	p	318	CHL	C2D-C1D-ND	4.31	113.28	110.10
22	q	303	CLA	CMB-C2B-C1B	-4.31	121.85	128.46
22	B	612	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
26	1	315	CHL	C3D-C2D-C1D	-4.30	99.96	105.83
27	r	618	NEX	C38-C25-C26	-4.30	115.06	122.26
25	g	310	LHG	O7-C7-C8	4.30	120.76	111.50
23	u	310	LUT	C35-C34-C33	-4.30	121.18	127.31
22	n	305	CLA	C4D-C3D-CAD	-4.29	103.03	108.10
27	R	301	NEX	C27-C28-C29	-4.29	118.87	125.53
22	b	614	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
26	Q	311	CHL	CHD-C4C-C3C	-4.29	118.54	124.84
23	5	310	LUT	C35-C34-C33	-4.29	121.19	127.31
22	x	201	CLA	CMB-C2B-C3B	4.29	132.70	124.68
26	U	315	CHL	O2D-CGD-CBD	4.28	118.88	111.27
26	Q	314	CHL	O2D-CGD-CBD	4.28	118.87	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	315	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
22	C	511	CLA	CMB-C2B-C3B	4.28	132.68	124.68
25	C	524	LHG	O7-C7-C8	4.27	120.71	111.50
24	r	612	XAT	C38-C25-C26	-4.27	115.10	122.26
26	G	312	CHL	C1B-CHB-C4A	-4.27	121.66	130.12
26	3	314	CHL	O2D-CGD-CBD	4.27	118.85	111.27
24	N	311	XAT	C18-C5-C6	-4.27	115.11	122.26
26	v	314	CHL	CHD-C4C-C3C	-4.27	118.57	124.84
22	X	202	CLA	CMB-C2B-C3B	4.26	132.66	124.68
23	P	310	LUT	C35-C34-C33	-4.26	121.23	127.31
26	4	315	CHL	C3D-C2D-C1D	-4.26	100.02	105.83
22	G	303	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
25	N	312	LHG	O7-C7-C8	4.25	120.67	111.50
22	B	613	CLA	CMB-C2B-C1B	-4.25	121.92	128.46
31	C	517	BCR	C38-C26-C25	-4.25	119.75	124.53
31	b	619	BCR	C4-C5-C6	-4.25	116.56	122.73
31	c	515	BCR	C7-C8-C9	-4.25	119.81	126.23
26	U	316	CHL	C2D-C1D-ND	4.25	113.24	110.10
22	b	612	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
22	n	306	CLA	CMB-C2B-C3B	4.25	132.62	124.68
31	t	101	BCR	C30-C25-C26	-4.25	116.63	122.61
31	b	620	BCR	C38-C26-C25	-4.24	119.76	124.53
22	c	512	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
23	1	309	LUT	C15-C14-C13	-4.24	121.26	127.31
22	p	306	CLA	C4D-C3D-CAD	-4.24	103.10	108.10
22	P	302	CLA	CMB-C2B-C3B	4.24	132.61	124.68
26	v	316	CHL	C2D-C1D-ND	4.24	113.23	110.10
22	1	301	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
26	S	314	CHL	CHD-C4C-C3C	-4.23	118.62	124.84
26	3	312	CHL	C3C-C4C-NC	4.23	115.32	110.57
32	l	102	SQD	O7-S-C6	4.23	111.97	106.94
27	S	317	NEX	C15-C14-C13	-4.23	121.27	127.31
22	B	614	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
24	R	313	XAT	C15-C14-C13	-4.23	121.27	127.31
31	A	409	BCR	C16-C17-C18	-4.23	121.28	127.31
26	6	314	CHL	C3C-C4C-NC	4.23	115.31	110.57
31	T	101	BCR	C30-C25-C26	-4.23	116.66	122.61
22	q	304	CLA	CMB-C2B-C3B	4.23	132.59	124.68
26	u	317	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
22	c	510	CLA	CMB-C2B-C3B	4.23	132.58	124.68
22	5	301	CLA	CMB-C2B-C3B	4.22	132.58	124.68
23	4	309	LUT	C15-C14-C13	-4.22	121.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	311	CHL	C2D-C1D-ND	4.22	113.22	110.10
26	U	316	CHL	CHD-C4C-C3C	-4.22	118.63	124.84
31	a	409	BCR	C16-C17-C18	-4.22	121.29	127.31
24	5	311	XAT	C31-C30-C29	-4.22	121.29	127.31
26	V	316	CHL	C1B-CHB-C4A	-4.22	121.77	130.12
27	r	618	NEX	C27-C28-C29	-4.22	118.99	125.53
31	B	620	BCR	C38-C26-C25	-4.22	119.79	124.53
22	5	306	CLA	CMB-C2B-C3B	4.22	132.57	124.68
23	4	310	LUT	C7-C8-C9	-4.21	119.87	126.23
22	4	303	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
26	g	311	CHL	CHD-C4C-C3C	-4.21	118.66	124.84
26	5	317	CHL	C3B-C4B-NB	4.21	114.65	109.21
26	s	314	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
26	N	315	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
24	G	309	XAT	C15-C14-C13	-4.20	121.31	127.31
32	l	102	SQD	O47-C7-C8	4.20	120.56	111.50
32	L	102	SQD	O47-C7-C8	4.20	120.56	111.50
22	C	513	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
26	u	314	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
27	u	320	NEX	C27-C28-C29	-4.20	119.02	125.53
26	2	314	CHL	C3C-C4C-NC	4.20	115.28	110.57
22	3	301	CLA	CMB-C2B-C3B	4.20	132.53	124.68
26	G	311	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
26	2	315	CHL	CHD-C4C-C3C	-4.19	118.67	124.84
22	n	304	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
24	g	309	XAT	C15-C14-C13	-4.19	121.32	127.31
22	3	303	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
22	p	302	CLA	CMB-C2B-C3B	4.19	132.52	124.68
31	B	619	BCR	C4-C5-C6	-4.19	116.64	122.73
26	s	315	CHL	C3C-C4C-NC	4.19	115.27	110.57
31	C	517	BCR	C7-C8-C9	-4.19	119.91	126.23
26	G	314	CHL	O2D-CGD-CBD	4.19	118.71	111.27
27	V	319	NEX	C35-C34-C33	-4.18	121.34	127.31
26	1	317	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
26	6	313	CHL	C3C-C4C-NC	4.18	115.26	110.57
22	C	510	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
26	6	315	CHL	O2D-CGD-CBD	4.18	118.70	111.27
26	5	317	CHL	C2D-C1D-ND	4.18	113.18	110.10
23	n	309	LUT	C7-C8-C9	-4.18	119.92	126.23
27	5	319	NEX	C15-C14-C13	-4.18	121.35	127.31
27	s	317	NEX	C15-C14-C13	-4.18	121.35	127.31
26	5	314	CHL	C3C-C4C-NC	4.18	115.26	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u	318	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
26	r	619	CHL	C2D-C1D-ND	4.18	113.18	110.10
26	u	318	CHL	C2D-C1D-ND	4.18	113.18	110.10
26	R	315	CHL	CAC-C3C-C4C	4.17	130.23	124.81
22	b	604	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
26	P	314	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
26	v	316	CHL	O2D-CGD-CBD	4.17	118.68	111.27
27	r	618	NEX	C15-C14-C13	-4.17	121.36	127.31
25	c	523	LHG	O7-C7-C8	4.17	120.48	111.50
24	2	311	XAT	C15-C14-C13	-4.17	121.36	127.31
25	v	312	LHG	O7-C7-C8	4.16	120.47	111.50
26	u	315	CHL	C3D-C2D-C1D	-4.16	100.15	105.83
22	B	617	CLA	CMB-C2B-C3B	4.16	132.46	124.68
26	r	615	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
31	z	101	BCR	C24-C23-C22	-4.16	119.95	126.23
26	4	317	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
23	n	310	LUT	C35-C34-C33	-4.16	121.38	127.31
26	n	318	CHL	C3C-C4C-NC	4.16	115.23	110.57
22	3	304	CLA	CMB-C2B-C3B	4.16	132.46	124.68
34	B	624	LMG	O7-C10-C11	4.16	120.46	111.50
24	5	311	XAT	C26-C27-C28	-4.15	117.21	125.99
26	3	315	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
31	B	618	BCR	C4-C5-C6	-4.15	116.70	122.73
26	P	318	CHL	C2D-C1D-ND	4.15	113.16	110.10
31	B	620	BCR	C1-C6-C5	-4.15	116.77	122.61
26	q	312	CHL	C3C-C4C-NC	4.15	115.22	110.57
31	D	404	BCR	C4-C5-C6	-4.15	116.71	122.73
26	3	313	CHL	C3D-C2D-C1D	-4.14	100.18	105.83
31	d	403	BCR	C33-C5-C6	-4.14	119.88	124.53
22	s	307	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
22	b	615	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
26	u	316	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
31	d	403	BCR	C4-C5-C6	-4.14	116.73	122.73
26	P	319	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
26	R	316	CHL	CHD-C4C-C3C	-4.13	118.76	124.84
27	N	318	NEX	O24-C25-C38	4.13	120.01	115.06
22	1	303	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
22	N	306	CLA	CMB-C2B-C3B	4.13	132.41	124.68
22	B	604	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
34	b	624	LMG	O7-C10-C11	4.13	120.40	111.50
26	P	319	CHL	C3B-C4B-NB	4.13	114.55	109.21
22	g	303	CLA	CMB-C2B-C1B	-4.12	122.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	305	CLA	C4D-C3D-CAD	-4.12	103.23	108.10
26	6	317	CHL	C3B-C4B-NB	4.12	114.54	109.21
32	C	501	SQD	C44-O6-C1	4.12	121.79	113.74
25	S	312	LHG	O7-C7-C8	4.12	120.38	111.50
27	2	319	NEX	O24-C25-C38	4.12	119.99	115.06
31	t	101	BCR	C38-C26-C25	-4.12	119.90	124.53
22	2	301	CLA	CMB-C2B-C3B	4.12	132.38	124.68
26	S	315	CHL	C3C-C4C-NC	4.12	115.19	110.57
26	v	314	CHL	C2D-C1D-ND	4.12	113.14	110.10
25	s	312	LHG	O7-C7-C8	4.11	120.36	111.50
24	R	313	XAT	C38-C25-C26	-4.11	115.37	122.26
25	2	312	LHG	O7-C7-C8	4.11	120.36	111.50
22	c	509	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
31	T	101	BCR	C38-C26-C25	-4.11	119.91	124.53
24	u	311	XAT	C18-C5-C6	-4.11	115.37	122.26
31	b	618	BCR	C4-C5-C6	-4.11	116.76	122.73
23	p	310	LUT	C15-C14-C13	-4.11	121.45	127.31
31	t	101	BCR	C16-C17-C18	-4.11	121.45	127.31
31	B	620	BCR	C15-C14-C13	-4.11	121.45	127.31
31	B	619	BCR	C11-C10-C9	-4.11	121.45	127.31
24	r	612	XAT	C15-C14-C13	-4.10	121.45	127.31
24	Q	309	XAT	C31-C30-C29	-4.10	121.45	127.31
26	p	320	CHL	O2D-CGD-CBD	4.10	118.56	111.27
26	V	317	CHL	CHD-C4C-C3C	-4.10	118.81	124.84
34	c	501	LMG	O7-C10-C11	4.10	120.34	111.50
27	r	617	NEX	C2-C1-C6	4.10	113.19	109.21
22	B	615	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
23	R	312	LUT	C35-C34-C33	-4.10	121.46	127.31
22	N	301	CLA	CMB-C2B-C3B	4.10	132.34	124.68
24	2	311	XAT	C38-C25-C26	-4.09	115.40	122.26
24	P	312	XAT	C6-C7-C8	-4.09	117.34	125.99
26	6	312	CHL	C2D-C1D-ND	4.09	113.12	110.10
26	s	316	CHL	C1B-CHB-C4A	-4.09	122.02	130.12
34	C	502	LMG	O7-C10-C11	4.09	120.31	111.50
24	P	312	XAT	C31-C30-C29	-4.09	121.48	127.31
24	G	309	XAT	C31-C30-C29	-4.09	121.48	127.31
26	q	311	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
31	D	404	BCR	C33-C5-C6	-4.08	119.94	124.53
26	6	316	CHL	O2D-CGD-CBD	4.08	118.52	111.27
24	V	311	XAT	C31-C30-C29	-4.08	121.48	127.31
27	2	319	NEX	C15-C14-C13	-4.08	121.48	127.31
24	v	311	XAT	C31-C30-C29	-4.08	121.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	620	BCR	C1-C6-C5	-4.08	116.87	122.61
24	N	311	XAT	C26-C27-C28	-4.07	117.38	125.99
26	4	316	CHL	CHD-C4C-C3C	-4.07	118.85	124.84
22	Q	301	CLA	CMB-C2B-C3B	4.07	132.30	124.68
27	u	319	NEX	C35-C34-C33	-4.07	121.50	127.31
26	P	319	CHL	C2D-C1D-ND	4.07	113.10	110.10
27	P	301	NEX	C15-C14-C13	-4.07	121.51	127.31
24	3	309	XAT	C11-C10-C9	-4.07	121.51	127.31
26	S	316	CHL	C1B-CHB-C4A	-4.06	122.07	130.12
23	5	309	LUT	C35-C34-C33	-4.06	121.51	127.31
26	p	317	CHL	CHD-C4C-C3C	-4.06	118.87	124.84
26	n	314	CHL	C3C-C4C-NC	4.06	115.12	110.57
26	R	316	CHL	C2D-C1D-ND	4.06	113.09	110.10
26	G	315	CHL	C1D-ND-C4D	-4.06	103.45	106.33
27	p	301	NEX	O24-C25-C38	4.06	119.92	115.06
26	r	614	CHL	CAC-C3C-C4C	4.06	130.07	124.81
31	b	619	BCR	C33-C5-C6	-4.05	119.98	124.53
22	U	303	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
27	N	318	NEX	C35-C34-C33	-4.05	121.53	127.31
26	n	317	CHL	CAC-C3C-C4C	4.04	130.05	124.81
31	X	201	BCR	C38-C26-C25	-4.04	119.99	124.53
25	R	314	LHG	O7-C7-C8	4.04	120.21	111.50
26	N	314	CHL	C3C-C4C-NC	4.04	115.10	110.57
25	V	312	LHG	O7-C7-C8	4.04	120.20	111.50
31	A	409	BCR	C33-C5-C6	-4.04	120.00	124.53
26	4	314	CHL	C2D-C1D-ND	4.04	113.08	110.10
24	3	309	XAT	C35-C34-C33	-4.03	121.56	127.31
26	u	314	CHL	C2D-C1D-ND	4.03	113.07	110.10
26	N	313	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
26	4	317	CHL	C3B-C4B-NB	4.03	114.41	109.21
24	G	309	XAT	C26-C27-C28	-4.02	117.49	125.99
26	g	315	CHL	C1D-ND-C4D	-4.02	103.48	106.33
26	r	614	CHL	CHD-C4C-C3C	-4.02	118.93	124.84
24	5	311	XAT	C38-C25-C26	-4.02	115.52	122.26
22	R	303	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
31	C	516	BCR	C24-C23-C22	-4.02	120.16	126.23
22	u	305	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
26	u	317	CHL	C1D-ND-C4D	-4.02	103.48	106.33
22	b	609	CLA	CMB-C2B-C3B	4.02	132.19	124.68
26	R	315	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
31	c	516	BCR	C15-C14-C13	-4.01	121.59	127.31
23	v	309	LUT	C7-C8-C9	-4.01	120.18	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	309	XAT	C18-C5-C6	-4.01	115.55	122.26
26	u	316	CHL	CMD-C2D-C3D	-4.01	118.40	127.61
26	v	313	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
26	V	316	CHL	O2D-CGD-CBD	4.00	118.38	111.27
23	V	309	LUT	C7-C8-C9	-4.00	120.19	126.23
22	V	304	CLA	CMB-C2B-C3B	4.00	132.17	124.68
22	C	507	CLA	O2D-CGD-O1D	-4.00	116.01	123.84
26	2	317	CHL	C3B-C4B-NB	4.00	114.38	109.21
27	v	319	NEX	C35-C34-C33	-4.00	121.60	127.31
22	2	305	CLA	C4D-C3D-CAD	-4.00	103.38	108.10
26	6	314	CHL	C3D-C2D-C1D	-4.00	100.38	105.83
23	5	309	LUT	C15-C14-C13	-4.00	121.61	127.31
34	w	201	LMG	O7-C10-C11	4.00	120.11	111.50
22	c	506	CLA	O2D-CGD-O1D	-3.99	116.03	123.84
26	1	318	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
26	2	318	CHL	C3B-C4B-NB	3.99	114.37	109.21
26	G	316	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
31	B	618	BCR	C1-C6-C5	-3.99	117.00	122.61
22	v	304	CLA	CMB-C2B-C3B	3.99	132.14	124.68
22	n	301	CLA	CMB-C2B-C3B	3.99	132.13	124.68
26	v	317	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
31	z	101	BCR	C38-C26-C25	-3.98	120.06	124.53
32	a	410	SQD	C44-O6-C1	3.98	121.52	113.74
22	P	306	CLA	C4D-C3D-CAD	-3.98	103.40	108.10
24	6	310	XAT	C38-C25-C26	-3.98	115.59	122.26
26	Q	313	CHL	CAC-C3C-C4C	3.98	129.97	124.81
24	R	313	XAT	C35-C15-C14	-3.98	115.33	123.47
31	a	409	BCR	C33-C5-C6	-3.98	120.06	124.53
22	6	305	CLA	CMB-C2B-C3B	3.98	132.12	124.68
31	T	101	BCR	C16-C17-C18	-3.97	121.64	127.31
26	p	315	CHL	C3C-C4C-NC	3.97	115.02	110.57
27	S	317	NEX	C31-C30-C29	-3.97	121.64	127.31
22	r	606	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
26	U	319	CHL	CHD-C4C-C3C	-3.97	119.00	124.84
24	Q	309	XAT	C38-C25-C26	-3.97	115.61	122.26
27	p	301	NEX	C35-C34-C33	-3.96	121.65	127.31
26	r	615	CHL	C2D-C1D-ND	3.96	113.02	110.10
24	n	311	XAT	C26-C27-C28	-3.96	117.62	125.99
26	G	313	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
23	s	310	LUT	C35-C34-C33	-3.96	121.66	127.31
31	A	409	BCR	C7-C8-C9	-3.96	120.25	126.23
24	2	311	XAT	C31-C30-C29	-3.96	121.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	314	CHL	CAC-C3C-C4C	3.96	129.94	124.81
22	G	304	CLA	CMB-C2B-C3B	3.96	132.08	124.68
25	U	312	LHG	O7-C7-C8	3.95	120.02	111.50
23	p	310	LUT	C35-C34-C33	-3.95	121.67	127.31
22	U	305	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
26	U	316	CHL	C1D-ND-C4D	-3.95	103.53	106.33
26	3	315	CHL	O2D-CGD-CBD	3.95	118.28	111.27
26	n	316	CHL	CHD-C4C-C3C	-3.95	119.04	124.84
22	D	403	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
31	b	619	BCR	C11-C10-C9	-3.95	121.68	127.31
24	1	311	XAT	C31-C30-C29	-3.94	121.68	127.31
26	4	317	CHL	C2D-C1D-ND	3.94	113.01	110.10
31	K	101	BCR	C30-C25-C26	-3.94	117.06	122.61
24	1	311	XAT	C6-C7-C8	-3.94	117.66	125.99
25	n	312	LHG	O7-C7-C8	3.94	119.99	111.50
32	C	501	SQD	O47-C7-C8	3.94	119.99	111.50
24	p	312	XAT	C26-C27-C28	-3.94	117.67	125.99
26	g	313	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
22	B	609	CLA	CMB-C2B-C3B	3.94	132.04	124.68
26	g	316	CHL	C3B-C4B-NB	3.93	114.30	109.21
26	1	316	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
26	q	311	CHL	C2D-C1D-ND	3.93	113.00	110.10
26	U	317	CHL	C3B-C4B-NB	3.93	114.29	109.21
32	A	412	SQD	O7-S-C6	3.93	111.61	106.94
26	P	317	CHL	C1B-CHB-C4A	-3.93	122.33	130.12
26	g	316	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
26	U	317	CHL	CHD-C4C-C3C	-3.93	119.07	124.84
24	5	311	XAT	C6-C7-C8	-3.93	117.69	125.99
36	A	414	DGD	O2G-C1B-C2B	3.93	119.97	111.50
26	Q	311	CHL	C2D-C1D-ND	3.93	113.00	110.10
36	a	416	DGD	O2G-C1B-C2B	3.92	119.96	111.50
22	R	309	CLA	CMB-C2B-C3B	3.92	132.02	124.68
27	V	319	NEX	O24-C25-C38	3.92	119.76	115.06
34	b	621	LMG	O7-C10-C11	3.92	119.96	111.50
26	1	318	CHL	C3B-C4B-NB	3.92	114.28	109.21
26	6	312	CHL	C1D-ND-C4D	-3.92	103.55	106.33
24	5	311	XAT	C15-C14-C13	-3.92	121.72	127.31
24	q	309	XAT	C38-C25-C26	-3.92	115.69	122.26
31	k	101	BCR	C30-C25-C26	-3.92	117.09	122.61
22	P	307	CLA	CMB-C2B-C3B	3.92	132.01	124.68
24	v	311	XAT	C26-C27-C28	-3.92	117.71	125.99
26	U	314	CHL	O2D-CGD-CBD	3.92	118.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	413	SQD	O7-S-C6	3.92	111.59	106.94
26	U	317	CHL	C2D-C1D-ND	3.91	112.99	110.10
25	r	613	LHG	O7-C7-C8	3.91	119.94	111.50
23	1	310	LUT	C7-C8-C9	-3.91	120.32	126.23
31	B	619	BCR	C23-C24-C25	-3.91	116.22	127.20
24	g	309	XAT	C31-C30-C29	-3.91	121.73	127.31
26	G	316	CHL	C3B-C4B-NB	3.91	114.27	109.21
24	3	309	XAT	C38-C25-C26	-3.91	115.71	122.26
24	2	311	XAT	C35-C34-C33	-3.91	121.73	127.31
25	6	311	LHG	O7-C7-C8	3.91	119.92	111.50
26	5	318	CHL	CHD-C4C-C3C	-3.91	119.10	124.84
27	u	319	NEX	C26-C27-C28	-3.91	117.73	125.99
31	b	619	BCR	C23-C24-C25	-3.90	116.24	127.20
22	r	602	CLA	CMB-C2B-C1B	-3.90	122.46	128.46
26	v	316	CHL	C1D-ND-C4D	-3.90	103.56	106.33
24	U	311	XAT	C15-C14-C13	-3.90	121.74	127.31
31	K	101	BCR	C33-C5-C6	-3.90	120.15	124.53
26	N	316	CHL	C1D-ND-C4D	-3.90	103.56	106.33
34	B	621	LMG	O7-C10-C11	3.90	119.91	111.50
25	u	312	LHG	O7-C7-C8	3.90	119.91	111.50
22	v	303	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
31	x	202	BCR	C38-C26-C25	-3.90	120.15	124.53
22	u	303	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
24	G	309	XAT	C18-C5-C6	-3.90	115.73	122.26
31	C	518	BCR	C15-C14-C13	-3.89	121.75	127.31
24	4	311	XAT	C6-C7-C8	-3.89	117.76	125.99
23	2	310	LUT	C35-C34-C33	-3.89	121.75	127.31
22	R	307	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
26	v	314	CHL	C3B-C4B-NB	3.89	114.23	109.21
25	Q	310	LHG	O7-C7-C8	3.88	119.87	111.50
26	g	313	CHL	CAC-C3C-C4C	3.88	129.85	124.81
22	r	608	CLA	CMB-C2B-C3B	3.88	131.94	124.68
22	S	301	CLA	CMB-C2B-C3B	3.88	131.94	124.68
34	B	621	LMG	C1-C2-C3	3.88	118.08	110.00
25	P	313	LHG	O7-C7-C8	3.88	119.86	111.50
24	N	311	XAT	C11-C10-C9	-3.88	121.77	127.31
26	g	311	CHL	C2D-C1D-ND	3.88	112.96	110.10
22	u	301	CLA	CMB-C2B-C3B	3.88	131.93	124.68
23	U	309	LUT	C35-C34-C33	-3.88	121.78	127.31
34	W	201	LMG	O7-C10-C11	3.87	119.85	111.50
26	p	320	CHL	C1D-ND-C4D	-3.87	103.58	106.33
23	v	310	LUT	C7-C8-C9	-3.87	120.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	311	XAT	C26-C27-C28	-3.87	117.81	125.99
31	k	101	BCR	C33-C5-C6	-3.87	120.18	124.53
22	U	304	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
23	N	309	LUT	C7-C8-C9	-3.87	120.39	126.23
22	q	307	CLA	CMB-C2B-C1B	-3.86	122.52	128.46
26	2	317	CHL	C1D-ND-C4D	-3.86	103.59	106.33
26	Q	311	CHL	C1D-ND-C4D	-3.86	103.59	106.33
31	b	618	BCR	C8-C7-C6	-3.86	116.35	127.20
26	1	317	CHL	C2D-C1D-ND	3.86	112.95	110.10
27	s	317	NEX	C31-C30-C29	-3.86	121.80	127.31
22	d	402	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
26	r	619	CHL	CAC-C3C-C4C	3.86	129.82	124.81
22	Q	304	CLA	CMB-C2B-C3B	3.86	131.90	124.68
25	C	523	LHG	O7-C7-C8	3.86	119.82	111.50
26	n	318	CHL	CAC-C3C-C4C	3.86	129.81	124.81
26	R	315	CHL	C2D-C1D-ND	3.86	112.94	110.10
34	A	411	LMG	O7-C10-C11	3.85	119.81	111.50
22	P	305	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
22	n	307	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
34	a	412	LMG	O7-C10-C11	3.85	119.80	111.50
26	u	314	CHL	CAC-C3C-C4C	3.85	129.81	124.81
26	3	311	CHL	C1D-ND-C4D	-3.85	103.60	106.33
26	V	317	CHL	C2D-C1D-ND	3.85	112.94	110.10
22	s	301	CLA	CMB-C2B-C3B	3.85	131.88	124.68
26	q	313	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
26	p	319	CHL	C3B-C4B-NB	3.85	114.19	109.21
22	q	301	CLA	CMB-C2B-C3B	3.85	131.88	124.68
22	C	505	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
32	C	501	SQD	O9-S-C6	3.85	111.51	106.94
27	5	319	NEX	O24-C25-C38	3.85	119.67	115.06
31	B	618	BCR	C7-C8-C9	-3.85	120.42	126.23
27	2	319	NEX	C39-C29-C30	-3.85	117.54	122.92
26	G	311	CHL	C3B-C4B-NB	3.85	114.18	109.21
25	4	312	LHG	O7-C7-C8	3.84	119.78	111.50
27	S	317	NEX	O24-C25-C38	3.84	119.66	115.06
24	u	311	XAT	C15-C14-C13	-3.84	121.83	127.31
25	c	522	LHG	O7-C7-C8	3.84	119.78	111.50
26	U	319	CHL	C2D-C1D-ND	3.84	112.93	110.10
31	B	620	BCR	C38-C26-C27	3.84	120.99	113.62
26	N	313	CHL	C2D-C1D-ND	3.84	112.93	110.10
26	3	316	CHL	C3B-C4B-NB	3.84	114.17	109.21
22	p	306	CLA	CMB-C2B-C1B	-3.84	122.57	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	p	312	XAT	C38-C25-C26	-3.83	115.83	122.26
22	Q	307	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
26	5	315	CHL	C2D-C1D-ND	3.83	112.93	110.10
22	c	508	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
22	C	509	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
25	D	406	LHG	O7-C7-C8	3.83	119.75	111.50
32	a	410	SQD	O47-C7-C8	3.83	119.75	111.50
26	Q	313	CHL	C3B-C4B-NB	3.82	114.15	109.21
26	5	318	CHL	C3B-C4B-NB	3.82	114.15	109.21
26	q	311	CHL	C1D-ND-C4D	-3.82	103.62	106.33
26	q	313	CHL	CAC-C3C-C4C	3.82	129.77	124.81
26	2	313	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
26	Q	316	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
26	5	313	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
34	b	621	LMG	C4-C3-C2	3.82	117.49	110.82
22	v	301	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
24	4	311	XAT	C26-C27-C28	-3.81	117.93	125.99
27	S	317	NEX	C27-C28-C29	-3.81	119.61	125.53
24	n	311	XAT	C15-C14-C13	-3.81	121.87	127.31
26	1	314	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
27	U	318	NEX	C27-C28-C29	-3.81	119.62	125.53
25	d	405	LHG	O7-C7-C8	3.81	119.71	111.50
26	6	301	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
22	b	614	CLA	CMB-C2B-C3B	3.81	131.80	124.68
31	d	403	BCR	C7-C8-C9	-3.81	120.48	126.23
25	l	101	LHG	O7-C7-C8	3.81	119.70	111.50
26	2	318	CHL	CHD-C4C-C3C	-3.81	119.25	124.84
26	Q	314	CHL	CHD-C4C-C3C	-3.81	119.25	124.84
22	1	307	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
26	1	318	CHL	C2D-C1D-ND	3.80	112.91	110.10
22	V	301	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
27	s	317	NEX	O24-C25-C38	3.80	119.61	115.06
22	6	308	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
22	c	504	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
26	3	315	CHL	C1D-ND-C4D	-3.80	103.64	106.33
26	u	318	CHL	C3B-C4B-NB	3.80	114.12	109.21
34	B	621	LMG	C4-C3-C2	3.80	117.45	110.82
22	v	308	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
26	p	319	CHL	CHD-C4C-C3C	-3.80	119.26	124.84
31	B	619	BCR	C33-C5-C6	-3.80	120.27	124.53
22	B	608	CLA	CMB-C2B-C3B	3.80	131.78	124.68
31	D	404	BCR	C27-C26-C25	-3.79	117.22	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	a	416	DGD	O6E-C5E-C4E	3.79	116.58	109.69
22	B	614	CLA	CMB-C2B-C3B	3.79	131.77	124.68
26	p	318	CHL	C3B-C4B-NB	3.79	114.11	109.21
26	u	315	CHL	O2D-CGD-CBD	3.79	118.00	111.27
26	n	313	CHL	CAC-C3C-C4C	3.79	129.73	124.81
24	v	311	XAT	C35-C34-C33	-3.79	121.90	127.31
26	u	317	CHL	CAC-C3C-C4C	3.79	129.72	124.81
26	5	317	CHL	C1D-ND-C4D	-3.78	103.65	106.33
26	4	316	CHL	C2D-C1D-ND	3.78	112.89	110.10
31	d	403	BCR	C27-C26-C25	-3.78	117.24	122.73
26	1	317	CHL	C3B-C4B-NB	3.78	114.10	109.21
24	u	311	XAT	C27-C28-C29	-3.78	119.67	125.53
26	q	315	CHL	CHD-C4C-C3C	-3.78	119.29	124.84
26	r	614	CHL	C2D-C1D-ND	3.78	112.89	110.10
31	z	101	BCR	C30-C25-C26	-3.78	117.29	122.61
26	n	316	CHL	C2D-C1D-ND	3.78	112.89	110.10
26	P	317	CHL	CHD-C4C-C3C	-3.78	119.29	124.84
31	D	404	BCR	C7-C8-C9	-3.78	120.53	126.23
32	a	410	SQD	O9-S-C6	3.78	111.43	106.94
22	4	307	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
25	L	101	LHG	O7-C7-C8	3.77	119.63	111.50
31	z	101	BCR	C1-C6-C5	-3.77	117.30	122.61
22	U	301	CLA	CMB-C2B-C3B	3.77	131.74	124.68
26	U	317	CHL	CAC-C3C-C4C	3.77	129.70	124.81
25	q	310	LHG	O7-C7-C8	3.77	119.63	111.50
36	C	520	DGD	O2G-C1B-C2B	3.77	119.62	111.50
26	V	318	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
26	q	314	CHL	O2D-CGD-CBD	3.77	117.97	111.27
22	n	303	CLA	CMB-C2B-C3B	3.77	131.73	124.68
26	v	318	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
22	2	307	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
31	c	516	BCR	C23-C24-C25	-3.77	116.63	127.20
26	V	316	CHL	CHD-C4C-C3C	-3.76	119.31	124.84
26	g	312	CHL	C1B-CHB-C4A	-3.76	122.67	130.12
31	C	518	BCR	C23-C24-C25	-3.76	116.64	127.20
25	3	310	LHG	O7-C7-C8	3.76	119.61	111.50
26	N	317	CHL	C3B-C4B-NB	3.76	114.07	109.21
27	P	301	NEX	C35-C34-C33	-3.76	121.94	127.31
26	2	315	CHL	C2D-C1D-ND	3.76	112.87	110.10
25	1	312	LHG	O7-C7-C8	3.76	119.60	111.50
22	g	304	CLA	CMB-C2B-C3B	3.76	131.71	124.68
26	g	313	CHL	C2D-C1D-ND	3.76	112.87	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	317	CHL	C1D-ND-C4D	-3.76	103.67	106.33
31	a	409	BCR	C7-C8-C9	-3.76	120.56	126.23
22	2	302	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
26	v	317	CHL	C2D-C1D-ND	3.75	112.87	110.10
22	S	302	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
31	C	516	BCR	C1-C6-C5	-3.75	117.33	122.61
23	V	309	LUT	C35-C34-C33	-3.75	121.96	127.31
26	G	315	CHL	O2D-CGD-CBD	3.75	117.93	111.27
24	4	311	XAT	C31-C30-C29	-3.75	121.96	127.31
24	6	310	XAT	C35-C34-C33	-3.75	121.96	127.31
27	U	318	NEX	C31-C30-C29	-3.75	121.96	127.31
26	4	314	CHL	C3B-C4B-NB	3.75	114.05	109.21
22	b	608	CLA	CMB-C2B-C3B	3.75	131.69	124.68
26	r	615	CHL	C3B-C4B-NB	3.74	114.05	109.21
24	V	311	XAT	C35-C34-C33	-3.74	121.97	127.31
27	v	319	NEX	C39-C29-C30	-3.74	117.68	122.92
24	2	311	XAT	C6-C7-C8	-3.74	118.08	125.99
32	L	102	SQD	C1-O5-C5	3.74	121.03	113.69
22	s	306	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
36	A	414	DGD	O6E-C5E-C4E	3.74	116.49	109.69
31	D	404	BCR	C38-C26-C25	-3.74	120.33	124.53
26	G	311	CHL	C2D-C1D-ND	3.74	112.86	110.10
22	N	305	CLA	C4D-C3D-CAD	-3.74	103.69	108.10
31	D	404	BCR	C1-C6-C5	-3.74	117.35	122.61
23	4	310	LUT	C35-C34-C33	-3.74	121.98	127.31
24	g	309	XAT	C38-C25-C26	-3.74	116.00	122.26
26	U	315	CHL	C3B-C4B-NB	3.74	114.04	109.21
22	b	605	CLA	CHB-C4A-NA	3.74	129.68	124.51
26	U	319	CHL	C1B-CHB-C4A	-3.74	122.72	130.12
23	2	309	LUT	C35-C34-C33	-3.73	121.98	127.31
31	T	101	BCR	C1-C6-C5	-3.73	117.36	122.61
26	u	316	CHL	C1D-ND-C4D	-3.73	103.69	106.33
22	S	307	CLA	CMB-C2B-C3B	3.73	131.66	124.68
26	G	316	CHL	C2D-C1D-ND	3.73	112.85	110.10
36	c	518	DGD	O2G-C1B-C2B	3.73	119.54	111.50
22	R	304	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
22	b	607	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
31	b	620	BCR	C38-C26-C27	3.73	120.77	113.62
22	R	310	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
31	C	516	BCR	C38-C26-C25	-3.72	120.35	124.53
22	s	302	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
26	Q	312	CHL	CHD-C4C-C3C	-3.72	119.37	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	p	305	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
24	U	311	XAT	C18-C5-C6	-3.72	116.02	122.26
22	S	306	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
26	p	320	CHL	C3B-C4B-NB	3.72	114.02	109.21
27	s	317	NEX	C27-C28-C29	-3.72	119.76	125.53
31	C	516	BCR	C8-C7-C6	-3.72	116.76	127.20
26	R	316	CHL	C3B-C4B-NB	3.72	114.02	109.21
26	u	318	CHL	CAC-C3C-C4C	3.72	129.63	124.81
31	z	101	BCR	C4-C5-C6	-3.72	117.33	122.73
22	q	303	CLA	CMB-C2B-C3B	3.72	131.63	124.68
31	z	101	BCR	C8-C7-C6	-3.71	116.77	127.20
25	p	313	LHG	O7-C7-C8	3.71	119.50	111.50
26	q	311	CHL	C3B-C4B-NB	3.71	114.01	109.21
31	d	403	BCR	C1-C6-C5	-3.71	117.38	122.61
32	C	501	SQD	O7-S-C6	3.71	111.35	106.94
32	M	101	SQD	O47-C7-C8	3.71	119.50	111.50
24	6	310	XAT	C11-C10-C9	-3.71	122.01	127.31
23	r	611	LUT	C7-C8-C9	-3.71	120.63	126.23
26	g	311	CHL	C3B-C4B-NB	3.71	114.01	109.21
26	p	314	CHL	C2D-C1D-ND	3.71	112.84	110.10
31	c	515	BCR	C30-C25-C26	-3.71	117.39	122.61
32	A	412	SQD	O9-S-O7	-3.71	101.11	113.95
26	v	314	CHL	CAC-C3C-C4C	3.71	129.62	124.81
26	n	313	CHL	C3B-C4B-NB	3.70	114.00	109.21
32	m	101	SQD	O47-C7-C8	3.70	119.48	111.50
22	G	305	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
26	4	316	CHL	C3B-C4B-NB	3.70	114.00	109.21
26	G	311	CHL	CAC-C3C-C4C	3.70	129.62	124.81
23	S	310	LUT	C35-C34-C33	-3.70	122.03	127.31
26	n	317	CHL	OMC-CMC-C2C	-3.70	117.32	125.69
31	X	201	BCR	C1-C6-C5	-3.70	117.40	122.61
22	B	605	CLA	CHB-C4A-NA	3.70	129.63	124.51
26	S	314	CHL	C2D-C1D-ND	3.70	112.83	110.10
26	U	316	CHL	C3B-C4B-NB	3.69	113.99	109.21
22	V	307	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	S	308	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
24	6	310	XAT	C18-C5-C6	-3.69	116.07	122.26
22	3	307	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
31	K	101	BCR	C38-C26-C27	3.69	120.71	113.62
27	u	320	NEX	O24-C25-C38	3.69	119.48	115.06
22	5	307	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
23	P	311	LUT	C15-C14-C13	-3.69	122.04	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	k	101	BCR	C38-C26-C27	3.69	120.70	113.62
22	v	307	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
24	P	312	XAT	C18-C5-C6	-3.69	116.08	122.26
22	C	515	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
31	C	516	BCR	C4-C5-C6	-3.69	117.38	122.73
24	P	312	XAT	C26-C27-C28	-3.69	118.20	125.99
32	a	410	SQD	O9-S-O7	-3.69	101.19	113.95
26	g	311	CHL	CAC-C3C-C4C	3.68	129.59	124.81
26	n	318	CHL	C3B-C4B-NB	3.68	113.97	109.21
31	C	518	BCR	C4-C5-C6	-3.68	117.38	122.73
26	v	318	CHL	C3B-C4B-NB	3.68	113.97	109.21
26	G	313	CHL	C2D-C1D-ND	3.68	112.81	110.10
32	a	413	SQD	O47-C7-C8	3.68	119.43	111.50
26	s	314	CHL	C2D-C1D-ND	3.68	112.81	110.10
31	d	403	BCR	C38-C26-C25	-3.68	120.40	124.53
26	v	317	CHL	CAC-C3C-C4C	3.67	129.58	124.81
22	4	301	CLA	CMB-C2B-C3B	3.67	131.55	124.68
26	U	315	CHL	CMD-C2D-C3D	-3.67	119.16	127.61
31	x	202	BCR	C1-C6-C5	-3.67	117.44	122.61
32	l	102	SQD	C1-O5-C5	3.67	120.90	113.69
31	C	517	BCR	C30-C25-C26	-3.67	117.44	122.61
26	P	315	CHL	C3C-C4C-NC	3.67	114.69	110.57
25	A	413	LHG	O7-C7-C8	3.67	119.41	111.50
26	v	317	CHL	C1D-ND-C4D	-3.67	103.73	106.33
31	a	409	BCR	C33-C5-C4	3.67	120.66	113.62
22	S	305	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
22	1	302	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
27	U	318	NEX	O24-C25-C38	3.66	119.44	115.06
32	a	410	SQD	O7-S-C6	3.66	111.29	106.94
22	p	308	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
26	u	313	CHL	CHD-C4C-C3C	-3.66	119.46	124.84
22	N	304	CLA	CMB-C2B-C3B	3.66	131.53	124.68
27	r	618	NEX	C5-C6-C1	3.66	123.33	119.70
25	5	312	LHG	O7-C7-C8	3.66	119.39	111.50
22	4	304	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
24	3	309	XAT	C18-C5-C6	-3.66	116.13	122.26
22	q	305	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	n	313	CHL	C2D-C1D-ND	3.66	112.80	110.10
26	6	317	CHL	C3D-C4D-ND	3.66	116.15	110.24
32	A	412	SQD	O47-C7-C8	3.66	119.38	111.50
31	A	409	BCR	C33-C5-C4	3.66	120.64	113.62
22	c	514	CLA	CMB-C2B-C1B	-3.66	122.85	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	302	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
31	t	101	BCR	C38-C26-C27	3.65	120.64	113.62
32	C	501	SQD	O9-S-O7	-3.65	101.31	113.95
22	b	613	CLA	CMB-C2B-C3B	3.65	131.51	124.68
22	6	304	CLA	CMB-C2B-C3B	3.65	131.51	124.68
32	m	101	SQD	O9-S-O7	-3.65	101.31	113.95
26	g	315	CHL	O2D-CGD-CBD	3.65	117.75	111.27
26	u	318	CHL	C1D-ND-C4D	-3.65	103.74	106.33
26	p	319	CHL	C2D-C1D-ND	3.65	112.79	110.10
25	a	415	LHG	O7-C7-C8	3.65	119.36	111.50
26	g	314	CHL	C4A-NA-C1A	3.65	108.35	106.71
26	6	315	CHL	CHD-C4C-C3C	-3.65	119.48	124.84
26	6	301	CHL	C1B-CHB-C4A	-3.65	122.90	130.12
26	u	314	CHL	C1D-ND-C4D	-3.65	103.75	106.33
22	N	302	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
26	q	313	CHL	C3B-C4B-NB	3.64	113.92	109.21
22	s	308	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
31	D	404	BCR	C11-C10-C9	-3.64	122.11	127.31
26	u	317	CHL	C3B-C4B-NB	3.64	113.92	109.21
31	B	620	BCR	C33-C5-C4	3.64	120.61	113.62
22	B	615	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
26	N	316	CHL	CAC-C3C-C4C	3.64	129.53	124.81
26	1	316	CHL	C3B-C4B-NB	3.64	113.91	109.21
32	l	102	SQD	C4-C3-C2	3.64	117.17	110.82
22	4	302	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
24	q	309	XAT	C35-C34-C33	-3.64	122.12	127.31
32	L	102	SQD	O9-S-O7	-3.64	101.37	113.95
26	R	317	CHL	CHD-C4C-C3C	-3.63	119.50	124.84
27	R	301	NEX	C39-C29-C30	-3.63	117.83	122.92
26	5	315	CHL	C3B-C4B-NB	3.63	113.91	109.21
22	b	617	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
26	V	313	CHL	CHD-C4C-C3C	-3.63	119.50	124.84
22	n	304	CLA	CMB-C2B-C3B	3.63	131.47	124.68
22	B	607	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
22	V	306	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
26	V	317	CHL	C3B-C4B-NB	3.63	113.90	109.21
23	v	309	LUT	C35-C34-C33	-3.63	122.13	127.31
31	A	409	BCR	C4-C5-C6	-3.63	117.47	122.73
32	M	101	SQD	O9-S-O7	-3.63	101.40	113.95
22	3	308	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
24	5	311	XAT	C11-C10-C9	-3.62	122.14	127.31
25	c	521	LHG	O7-C7-C8	3.62	119.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Q	311	CHL	C3B-C4B-NB	3.62	113.89	109.21
26	G	313	CHL	C3B-C4B-NB	3.62	113.89	109.21
32	a	413	SQD	O9-S-O7	-3.62	101.43	113.95
27	r	617	NEX	C35-C34-C33	-3.62	122.15	127.31
26	u	314	CHL	C3B-C4B-NB	3.62	113.89	109.21
27	U	318	NEX	C35-C34-C33	-3.62	122.15	127.31
22	P	303	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
27	r	617	NEX	O24-C25-C38	3.61	119.39	115.06
26	2	315	CHL	C3B-C4B-NB	3.61	113.88	109.21
31	b	620	BCR	C33-C5-C4	3.61	120.56	113.62
23	N	309	LUT	C35-C34-C33	-3.61	122.16	127.31
24	R	313	XAT	C35-C34-C33	-3.61	122.16	127.31
22	s	305	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
31	t	101	BCR	C1-C6-C5	-3.61	117.53	122.61
22	N	303	CLA	CMB-C2B-C3B	3.61	131.43	124.68
26	6	314	CHL	C1B-CHB-C4A	-3.61	122.98	130.12
26	r	619	CHL	C3B-C4B-NB	3.60	113.87	109.21
26	G	313	CHL	CAC-C3C-C4C	3.60	129.48	124.81
26	U	314	CHL	C2D-C1D-ND	3.60	112.76	110.10
26	4	315	CHL	C1B-CHB-C4A	-3.60	122.99	130.12
24	u	311	XAT	C38-C25-C26	-3.60	116.23	122.26
26	n	317	CHL	CHD-C4C-C3C	-3.60	119.55	124.84
26	n	318	CHL	C1B-CHB-C4A	-3.60	122.99	130.12
26	N	316	CHL	C3B-C4B-NB	3.60	113.86	109.21
26	G	316	CHL	C1D-ND-C4D	-3.60	103.78	106.33
31	c	516	BCR	C4-C5-C6	-3.59	117.51	122.73
27	n	319	NEX	C35-C34-C33	-3.59	122.18	127.31
25	C	522	LHG	O7-C7-C8	3.59	119.24	111.50
26	N	313	CHL	C3B-C4B-NB	3.59	113.85	109.21
31	d	403	BCR	C11-C10-C9	-3.59	122.19	127.31
23	4	309	LUT	C7-C8-C9	-3.59	120.81	126.23
22	p	307	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
23	n	310	LUT	C15-C14-C13	-3.59	122.19	127.31
34	B	621	LMG	O6-C1-C2	3.59	117.94	110.35
26	6	301	CHL	CMD-C2D-C3D	-3.59	119.36	127.61
26	u	315	CHL	C2D-C1D-ND	3.59	112.75	110.10
26	6	312	CHL	C3B-C4B-NB	3.59	113.85	109.21
31	B	620	BCR	C4-C5-C6	-3.59	117.53	122.73
26	U	316	CHL	CAC-C3C-C4C	3.58	129.46	124.81
23	u	309	LUT	C35-C34-C33	-3.58	122.19	127.31
34	c	520	LMG	O7-C10-C11	3.58	119.22	111.50
22	B	613	CLA	CMB-C2B-C3B	3.58	131.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	l	102	SQD	O9-S-O7	-3.58	101.55	113.95
26	1	317	CHL	C1D-ND-C4D	-3.58	103.79	106.33
26	Q	311	CHL	C3D-C4D-ND	3.58	116.03	110.24
22	a	406	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
24	p	312	XAT	C18-C5-C6	-3.58	116.26	122.26
26	6	317	CHL	C1D-ND-C4D	-3.58	103.79	106.33
26	N	317	CHL	CAC-C3C-C4C	3.58	129.45	124.81
22	N	305	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	P	308	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
22	B	611	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
25	B	622	LHG	O7-C7-C8	3.58	119.21	111.50
22	R	306	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
22	A	406	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
22	c	507	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
26	v	314	CHL	C1D-ND-C4D	-3.57	103.80	106.33
23	n	309	LUT	C35-C34-C33	-3.57	122.21	127.31
26	1	316	CHL	C1B-CHB-C4A	-3.57	123.04	130.12
24	U	311	XAT	C38-C25-C26	-3.57	116.28	122.26
26	U	313	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
24	V	311	XAT	C11-C10-C9	-3.57	122.22	127.31
31	a	409	BCR	C4-C5-C6	-3.57	117.56	122.73
22	r	605	CLA	CMB-C2B-C1B	-3.56	122.98	128.46
31	b	620	BCR	C30-C25-C26	-3.56	117.59	122.61
26	p	314	CHL	CAC-C3C-C4C	3.56	129.43	124.81
22	b	615	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
34	C	521	LMG	O7-C10-C11	3.56	119.18	111.50
31	b	620	BCR	C8-C7-C6	-3.56	117.20	127.20
26	1	314	CHL	CAC-C3C-C4C	3.56	129.43	124.81
22	6	309	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
27	v	319	NEX	O24-C25-C38	3.56	119.32	115.06
26	Q	315	CHL	O2D-CGD-CBD	3.56	117.59	111.27
23	s	310	LUT	C35-C15-C14	-3.56	116.19	123.47
26	4	316	CHL	C1D-ND-C4D	-3.56	103.81	106.33
26	p	318	CHL	C1D-ND-C4D	-3.56	103.81	106.33
26	G	314	CHL	CHD-C4C-C3C	-3.56	119.61	124.84
22	g	303	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
26	V	314	CHL	C3B-C4B-NB	3.55	113.81	109.21
22	1	304	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
26	Q	314	CHL	C2D-C1D-ND	3.55	112.72	110.10
22	P	306	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
26	r	615	CHL	CAC-C3C-C4C	3.55	129.42	124.81
26	3	311	CHL	C3B-C4B-NB	3.55	113.80	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	313	CHL	CHD-C4C-C3C	-3.55	119.62	124.84
31	B	618	BCR	C20-C21-C22	-3.55	122.24	127.31
27	V	319	NEX	C39-C29-C30	-3.55	117.95	122.92
26	6	317	CHL	CHD-C4C-C3C	-3.55	119.62	124.84
26	Q	313	CHL	CHD-C4C-C3C	-3.55	119.62	124.84
26	p	318	CHL	CAC-C3C-C4C	3.55	129.41	124.81
26	g	316	CHL	CAC-C3C-C4C	3.55	129.41	124.81
31	b	618	BCR	C20-C21-C22	-3.55	122.25	127.31
26	4	313	CHL	CAC-C3C-C4C	3.55	129.41	124.81
24	n	311	XAT	C38-C25-C26	-3.55	116.31	122.26
26	U	316	CHL	C3D-C4D-ND	3.55	115.98	110.24
23	1	310	LUT	C35-C34-C33	-3.55	122.25	127.31
22	C	508	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
23	4	310	LUT	C2-C3-C4	3.55	115.16	110.30
31	b	618	BCR	C27-C26-C25	-3.54	117.58	122.73
26	S	315	CHL	C1B-CHB-C4A	-3.54	123.10	130.12
24	G	309	XAT	C35-C34-C33	-3.54	122.25	127.31
22	Q	305	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
26	g	316	CHL	C2D-C1D-ND	3.54	112.71	110.10
24	Q	309	XAT	C35-C34-C33	-3.54	122.26	127.31
23	5	309	LUT	C11-C10-C9	-3.54	122.26	127.31
26	3	314	CHL	CHD-C4C-C3C	-3.54	119.64	124.84
26	v	313	CHL	CAC-C3C-C4C	3.54	129.40	124.81
31	T	101	BCR	C38-C26-C27	3.54	120.42	113.62
31	D	404	BCR	C38-C26-C27	3.54	120.42	113.62
26	6	301	CHL	C3B-C4B-NB	3.54	113.78	109.21
26	P	318	CHL	C3B-C4B-NB	3.54	113.78	109.21
23	v	310	LUT	C35-C34-C33	-3.54	122.26	127.31
24	1	311	XAT	C15-C14-C13	-3.54	122.26	127.31
31	b	620	BCR	C4-C5-C6	-3.54	117.60	122.73
26	q	311	CHL	C3D-C4D-ND	3.54	115.96	110.24
26	V	317	CHL	CAC-C3C-C4C	3.54	129.40	124.81
23	N	310	LUT	C15-C14-C13	-3.54	122.26	127.31
22	s	303	CLA	CMB-C2B-C3B	3.54	131.29	124.68
24	g	309	XAT	C11-C10-C9	-3.53	122.27	127.31
26	G	311	CHL	C1D-ND-C4D	-3.53	103.82	106.33
26	1	313	CHL	CHD-C4C-C3C	-3.53	119.64	124.84
22	r	607	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
26	4	317	CHL	CAC-C3C-C4C	3.53	129.40	124.81
22	R	311	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
26	V	313	CHL	CAC-C3C-C4C	3.53	129.39	124.81
31	B	618	BCR	C33-C5-C4	3.53	120.40	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q	313	CHL	C2D-C1D-ND	3.53	112.71	110.10
26	r	619	CHL	C1D-ND-C4D	-3.53	103.83	106.33
24	2	311	XAT	C26-C27-C28	-3.53	118.53	125.99
31	X	201	BCR	C20-C21-C22	-3.53	122.27	127.31
26	v	317	CHL	C3D-C4D-ND	3.53	115.95	110.24
22	r	610	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	n	305	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
26	n	314	CHL	CAC-C3C-C4C	3.53	129.39	124.81
26	Q	316	CHL	C2D-C1D-ND	3.53	112.70	110.10
26	V	314	CHL	C4A-NA-C1A	3.53	108.29	106.71
26	v	317	CHL	C3B-C4B-NB	3.53	113.77	109.21
27	R	301	NEX	C5-C6-C1	3.53	123.20	119.70
22	N	307	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
26	V	314	CHL	CAC-C3C-C4C	3.53	129.39	124.81
22	b	611	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
26	U	315	CHL	C1D-ND-C4D	-3.53	103.83	106.33
24	V	311	XAT	C18-C5-C6	-3.53	116.35	122.26
23	U	310	LUT	C15-C14-C13	-3.53	122.28	127.31
22	V	303	CLA	CMB-C2B-C3B	3.52	131.27	124.68
26	R	315	CHL	C3B-C4B-NB	3.52	113.77	109.21
31	C	517	BCR	C20-C21-C22	-3.52	122.28	127.31
26	S	314	CHL	C3B-C4B-NB	3.52	113.77	109.21
26	u	316	CHL	C3B-C4B-NB	3.52	113.76	109.21
26	1	314	CHL	C3B-C4B-NB	3.52	113.76	109.21
24	G	309	XAT	C11-C10-C9	-3.52	122.28	127.31
32	L	102	SQD	C4-C3-C2	3.52	116.97	110.82
23	v	310	LUT	C15-C14-C13	-3.52	122.29	127.31
23	5	309	LUT	C7-C8-C9	-3.52	120.92	126.23
22	u	307	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	v	316	CHL	C3B-C4B-NB	3.52	113.76	109.21
24	2	311	XAT	C11-C10-C9	-3.52	122.29	127.31
26	Q	316	CHL	C3B-C4B-NB	3.52	113.76	109.21
22	g	305	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
26	2	318	CHL	CAC-C3C-C4C	3.52	129.37	124.81
26	3	316	CHL	C3D-C4D-ND	3.52	115.92	110.24
26	r	616	CHL	CHD-C4C-C3C	-3.52	119.67	124.84
27	5	319	NEX	C39-C29-C30	-3.52	118.00	122.92
26	V	317	CHL	C3D-C4D-ND	3.52	115.92	110.24
26	G	316	CHL	CAC-C3C-C4C	3.51	129.37	124.81
31	d	403	BCR	C38-C26-C27	3.51	120.36	113.62
26	5	318	CHL	C2D-C1D-ND	3.51	112.69	110.10
26	V	316	CHL	CAC-C3C-C4C	3.51	129.37	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v	315	CHL	CHD-C4C-C3C	-3.51	119.68	124.84
26	g	313	CHL	C3B-C4B-NB	3.51	113.75	109.21
26	g	312	CHL	C3B-C4B-NB	3.51	113.74	109.21
31	C	516	BCR	C30-C25-C26	-3.51	117.67	122.61
22	p	304	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
31	k	101	BCR	C27-C26-C25	-3.51	117.64	122.73
31	B	620	BCR	C8-C7-C6	-3.51	117.36	127.20
26	s	314	CHL	C3B-C4B-NB	3.51	113.74	109.21
26	u	317	CHL	C3D-C4D-ND	3.51	115.91	110.24
26	4	317	CHL	C1D-ND-C4D	-3.51	103.84	106.33
31	B	618	BCR	C27-C26-C25	-3.50	117.64	122.73
26	6	312	CHL	C3D-C4D-ND	3.50	115.90	110.24
26	4	313	CHL	CHD-C4C-C3C	-3.50	119.69	124.84
22	1	305	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
31	K	101	BCR	C11-C10-C9	-3.50	122.31	127.31
22	V	305	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
26	5	317	CHL	CAC-C3C-C4C	3.50	129.35	124.81
22	5	305	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
24	G	309	XAT	C38-C25-C26	-3.50	116.39	122.26
31	B	618	BCR	C8-C7-C6	-3.50	117.37	127.20
26	G	314	CHL	C2D-C1D-ND	3.50	112.68	110.10
26	V	314	CHL	CHD-C4C-C3C	-3.50	119.70	124.84
31	K	101	BCR	C7-C8-C9	-3.50	120.95	126.23
22	4	306	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
34	b	621	LMG	O6-C5-C4	3.49	116.04	109.69
32	a	410	SQD	O6-C1-C2	3.49	113.76	108.30
26	Q	312	CHL	C1B-CHB-C4A	-3.49	123.20	130.12
22	b	610	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
27	p	301	NEX	C39-C29-C30	-3.49	118.03	122.92
26	3	316	CHL	CHD-C4C-C3C	-3.49	119.71	124.84
22	P	304	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
26	p	317	CHL	C2D-C1D-ND	3.49	112.67	110.10
26	r	614	CHL	C3B-C4B-NB	3.49	113.72	109.21
26	p	317	CHL	C1B-CHB-C4A	-3.49	123.21	130.12
31	T	101	BCR	C33-C5-C4	3.49	120.31	113.62
31	x	202	BCR	C20-C21-C22	-3.49	122.34	127.31
22	B	610	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	P	310	LUT	C15-C14-C13	-3.48	122.34	127.31
26	g	316	CHL	C1D-ND-C4D	-3.48	103.86	106.33
26	q	315	CHL	C2D-C1D-ND	3.48	112.67	110.10
31	B	620	BCR	C24-C23-C22	-3.48	120.98	126.23
24	q	309	XAT	C35-C15-C14	-3.48	116.35	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q	314	CHL	C3B-C4B-NB	3.48	113.70	109.21
24	5	311	XAT	C35-C34-C33	-3.48	122.35	127.31
26	P	317	CHL	CMD-C2D-C3D	-3.48	119.62	127.61
27	N	318	NEX	C39-C29-C30	-3.48	118.05	122.92
23	r	611	LUT	C15-C14-C13	-3.47	122.35	127.31
26	1	314	CHL	C2D-C1D-ND	3.47	112.66	110.10
26	g	312	CHL	CHD-C4C-C3C	-3.47	119.73	124.84
26	r	615	CHL	CHB-C4A-NA	3.47	129.31	124.51
22	1	301	CLA	CMB-C2B-C3B	3.47	131.18	124.68
24	4	311	XAT	C15-C14-C13	-3.47	122.35	127.31
31	K	101	BCR	C27-C26-C25	-3.47	117.69	122.73
23	u	310	LUT	C15-C14-C13	-3.47	122.36	127.31
26	s	315	CHL	C1B-CHB-C4A	-3.47	123.24	130.12
26	2	317	CHL	O2A-CGA-CBA	3.47	122.80	111.91
31	x	202	BCR	C23-C24-C25	-3.47	117.46	127.20
26	n	315	CHL	CHD-C4C-C3C	-3.47	119.74	124.84
26	g	315	CHL	CAC-C3C-C4C	3.47	129.31	124.81
24	q	309	XAT	C6-C7-C8	-3.46	118.67	125.99
22	n	304	CLA	CHB-C4A-NA	3.46	129.30	124.51
22	5	304	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
22	s	307	CLA	CMB-C2B-C3B	3.46	131.16	124.68
31	B	619	BCR	C8-C7-C6	-3.46	117.48	127.20
22	U	307	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
26	6	314	CHL	CAC-C3C-C4C	3.46	129.30	124.81
22	G	308	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
24	p	312	XAT	C35-C34-C33	-3.46	122.37	127.31
26	1	316	CHL	CAC-C3C-C4C	3.46	129.30	124.81
30	A	407	PHO	CMB-C2B-C3B	3.46	131.15	124.68
26	P	318	CHL	CAC-C3C-C4C	3.46	129.30	124.81
22	2	305	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	3	302	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
31	B	620	BCR	C30-C25-C26	-3.46	117.74	122.61
26	1	318	CHL	CAC-C3C-C4C	3.46	129.30	124.81
23	p	311	LUT	C15-C14-C13	-3.46	122.38	127.31
26	v	318	CHL	C2D-C1D-ND	3.46	112.65	110.10
22	q	307	CLA	CMB-C2B-C3B	3.46	131.14	124.68
26	U	315	CHL	CAC-C3C-C4C	3.46	129.29	124.81
31	C	518	BCR	C27-C26-C25	-3.45	117.72	122.73
26	1	315	CHL	CHD-C4C-C3C	-3.45	119.76	124.84
24	4	311	XAT	C38-C25-C26	-3.45	116.47	122.26
31	C	516	BCR	C16-C15-C14	-3.45	116.40	123.47
31	b	619	BCR	C38-C26-C25	-3.45	120.66	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	308	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
22	g	302	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
22	V	302	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
22	4	305	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
31	b	618	BCR	C7-C8-C9	-3.44	121.03	126.23
22	1	308	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
26	6	316	CHL	C3B-C4B-NB	3.44	113.66	109.21
22	r	609	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
22	g	308	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
26	4	316	CHL	C3D-C4D-ND	3.44	115.81	110.24
26	5	318	CHL	CAC-C3C-C4C	3.44	129.28	124.81
26	4	314	CHL	CAC-C3C-C4C	3.44	129.27	124.81
26	P	319	CHL	C1D-ND-C4D	-3.44	103.89	106.33
31	k	101	BCR	C11-C10-C9	-3.44	122.40	127.31
26	5	315	CHL	C1D-ND-C4D	-3.44	103.89	106.33
22	r	603	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
26	g	316	CHL	C3D-C4D-ND	3.44	115.80	110.24
26	2	316	CHL	CHD-C4C-C3C	-3.43	119.79	124.84
26	N	313	CHL	C1D-ND-C4D	-3.43	103.89	106.33
22	P	309	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	a	408	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
26	Q	315	CHL	C3B-C4B-NB	3.43	113.65	109.21
30	a	407	PHO	CMB-C2B-C3B	3.43	131.10	124.68
31	c	516	BCR	C27-C26-C25	-3.43	117.75	122.73
31	c	516	BCR	C7-C8-C9	-3.43	121.05	126.23
26	r	616	CHL	CAC-C3C-C4C	3.43	129.26	124.81
22	4	308	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
26	2	318	CHL	C2D-C1D-ND	3.43	112.63	110.10
26	R	316	CHL	CAC-C3C-C4C	3.43	129.26	124.81
36	A	414	DGD	C1E-O6E-C5E	3.43	120.42	113.69
22	A	405	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
26	U	314	CHL	C3B-C4B-NB	3.43	113.64	109.21
26	U	319	CHL	CAC-C3C-C4C	3.43	129.26	124.81
22	6	307	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	S	303	CLA	CMB-C2B-C3B	3.43	131.09	124.68
23	2	310	LUT	C7-C8-C9	-3.43	121.06	126.23
26	U	315	CHL	C2D-C1D-ND	3.43	112.63	110.10
26	s	313	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
31	B	619	BCR	C15-C16-C17	-3.42	116.46	123.47
26	6	315	CHL	CMD-C2D-C3D	-3.42	119.74	127.61
22	Q	307	CLA	CMB-C2B-C3B	3.42	131.08	124.68
22	N	308	CLA	CMB-C2B-C1B	-3.42	123.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	201	BCR	C23-C24-C25	-3.42	117.59	127.20
26	3	311	CHL	C3D-C4D-ND	3.42	115.77	110.24
22	s	309	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
26	1	316	CHL	CMD-C2D-C3D	-3.42	119.75	127.61
26	R	317	CHL	CAC-C3C-C4C	3.42	129.25	124.81
24	5	311	XAT	C18-C5-C6	-3.42	116.53	122.26
26	5	316	CHL	CHD-C4C-C3C	-3.42	119.82	124.84
26	N	313	CHL	C1B-CHB-C4A	-3.42	123.35	130.12
22	3	303	CLA	CMB-C2B-C3B	3.42	131.07	124.68
32	m	101	SQD	C44-O6-C1	3.42	120.41	113.74
31	b	619	BCR	C8-C7-C6	-3.42	117.61	127.20
22	q	306	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
26	U	313	CHL	CAC-C3C-C4C	3.42	129.24	124.81
26	n	316	CHL	C3B-C4B-NB	3.41	113.62	109.21
23	4	309	LUT	C35-C34-C33	-3.41	122.44	127.31
31	k	101	BCR	C38-C26-C25	-3.41	120.69	124.53
22	5	303	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
36	a	416	DGD	C1E-O6E-C5E	3.41	120.39	113.69
26	2	317	CHL	CAC-C3C-C4C	3.41	129.24	124.81
31	D	404	BCR	C33-C5-C4	3.41	120.17	113.62
22	3	306	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
31	C	518	BCR	C20-C21-C22	-3.41	122.44	127.31
22	5	302	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
24	U	311	XAT	C26-C27-C28	-3.40	118.79	125.99
26	6	317	CHL	CAC-C3C-C4C	3.40	129.23	124.81
26	V	318	CHL	C3B-C4B-NB	3.40	113.61	109.21
22	2	308	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
26	n	317	CHL	C2D-C1D-ND	3.40	112.61	110.10
26	q	315	CHL	C3B-C4B-NB	3.40	113.61	109.21
22	Q	303	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
26	p	316	CHL	C1B-CHB-C4A	-3.40	123.39	130.12
26	5	318	CHL	C3D-C4D-ND	3.40	115.74	110.24
31	C	518	BCR	C7-C8-C9	-3.40	121.10	126.23
26	G	316	CHL	C3D-C4D-ND	3.40	115.73	110.24
22	p	309	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
31	C	518	BCR	C21-C20-C19	-3.40	112.61	123.22
26	6	301	CHL	CAC-C3C-C4C	3.40	129.22	124.81
22	b	604	CLA	CMB-C2B-C3B	3.40	131.03	124.68
26	g	312	CHL	CAC-C3C-C4C	3.40	129.22	124.81
25	b	623	LHG	O7-C7-C8	3.39	118.82	111.50
26	1	317	CHL	C3D-C4D-ND	3.39	115.73	110.24
24	N	311	XAT	C35-C15-C14	-3.39	116.52	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	305	CLA	CMB-C2B-C3B	3.39	131.03	124.68
22	V	308	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	Q	312	CHL	CAC-C3C-C4C	3.39	129.21	124.81
22	r	601	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
22	c	512	CLA	CMB-C2B-C3B	3.39	131.02	124.68
31	b	620	BCR	C15-C14-C13	-3.39	122.47	127.31
31	c	515	BCR	C20-C21-C22	-3.39	122.47	127.31
22	v	306	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
26	Q	312	CHL	C3B-C4B-NB	3.39	113.59	109.21
26	1	317	CHL	CAC-C3C-C4C	3.39	129.21	124.81
22	u	305	CLA	CMB-C2B-C3B	3.39	131.01	124.68
26	G	311	CHL	CMD-C2D-C3D	-3.39	119.83	127.61
26	u	313	CHL	CAC-C3C-C4C	3.39	129.20	124.81
22	B	604	CLA	CMB-C2B-C3B	3.38	131.01	124.68
22	b	615	CLA	CMB-C2B-C3B	3.38	131.01	124.68
27	r	617	NEX	C39-C29-C30	-3.38	118.18	122.92
26	G	314	CHL	CAC-C3C-C4C	3.38	129.20	124.81
23	2	309	LUT	C15-C14-C13	-3.38	122.48	127.31
26	P	318	CHL	C1D-ND-C4D	-3.38	103.93	106.33
26	v	318	CHL	CAC-C3C-C4C	3.38	129.20	124.81
27	U	318	NEX	C11-C10-C9	-3.38	122.49	127.31
31	t	101	BCR	C33-C5-C4	3.38	120.11	113.62
26	u	316	CHL	CAC-C3C-C4C	3.38	129.19	124.81
31	c	516	BCR	C33-C5-C4	3.38	120.11	113.62
23	P	311	LUT	C35-C34-C33	-3.38	122.49	127.31
32	M	101	SQD	C44-O6-C1	3.38	120.34	113.74
26	Q	313	CHL	C3D-C4D-ND	3.38	115.70	110.24
26	u	315	CHL	C3B-C4B-NB	3.38	113.58	109.21
26	u	313	CHL	C2D-C1D-ND	3.38	112.59	110.10
25	B	623	LHG	O7-C7-C8	3.38	118.78	111.50
26	N	316	CHL	C3D-C4D-ND	3.38	115.70	110.24
30	d	401	PHO	CMB-C2B-C3B	3.38	130.99	124.68
30	D	401	PHO	CMB-C2B-C3B	3.38	130.99	124.68
26	p	317	CHL	C3B-C4B-NB	3.38	113.57	109.21
31	k	101	BCR	C7-C8-C9	-3.37	121.14	126.23
25	b	622	LHG	O7-C7-C8	3.37	118.77	111.50
24	P	312	XAT	C38-C25-C26	-3.37	116.61	122.26
26	Q	311	CHL	CAC-C3C-C4C	3.37	129.19	124.81
31	a	409	BCR	C8-C7-C6	-3.37	117.73	127.20
22	C	513	CLA	CMB-C2B-C3B	3.37	130.99	124.68
26	V	316	CHL	C2D-C1D-ND	3.37	112.59	110.10
26	R	316	CHL	CHB-C4A-NA	3.37	129.17	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	405	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
27	n	319	NEX	C2-C1-C6	3.37	112.48	109.21
26	Q	315	CHL	C3D-C4D-ND	3.37	115.69	110.24
26	u	313	CHL	C3B-C4B-NB	3.37	113.56	109.21
26	3	313	CHL	C1B-CHB-C4A	-3.37	123.45	130.12
26	S	313	CHL	CAC-C3C-C4C	3.37	129.18	124.81
22	4	303	CLA	CMB-C2B-C3B	3.37	130.98	124.68
31	B	619	BCR	C38-C26-C25	-3.37	120.75	124.53
22	B	615	CLA	CMB-C2B-C3B	3.37	130.98	124.68
27	P	301	NEX	C39-C29-C30	-3.37	118.21	122.92
26	5	318	CHL	C1D-ND-C4D	-3.36	103.94	106.33
26	u	316	CHL	C2D-C1D-ND	3.36	112.58	110.10
26	u	314	CHL	C3D-C4D-ND	3.36	115.68	110.24
31	d	403	BCR	C33-C5-C4	3.36	120.08	113.62
22	B	605	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
22	B	617	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
26	5	316	CHL	CAC-C3C-C4C	3.36	129.17	124.81
26	N	315	CHL	C3B-C4B-NB	3.36	113.56	109.21
22	D	403	CLA	CMB-C2B-C3B	3.36	130.96	124.68
26	u	316	CHL	C3D-C4D-ND	3.36	115.67	110.24
22	v	302	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
26	v	316	CHL	C3D-C4D-ND	3.36	115.67	110.24
22	b	605	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
27	u	319	NEX	C24-C23-C22	-3.35	104.29	110.77
26	P	317	CHL	C3B-C4B-NB	3.35	113.54	109.21
22	B	612	CLA	CMB-C2B-C3B	3.35	130.95	124.68
31	b	620	BCR	C27-C26-C25	-3.35	117.86	122.73
22	b	602	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
26	3	314	CHL	CMD-C2D-C3D	-3.35	119.91	127.61
22	B	604	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
27	p	301	NEX	C11-C10-C9	-3.35	122.53	127.31
26	5	313	CHL	C1B-CHB-C4A	-3.35	123.48	130.12
26	q	314	CHL	C3D-C4D-ND	3.35	115.66	110.24
26	N	315	CHL	C2D-C1D-ND	3.35	112.57	110.10
26	U	313	CHL	C3D-C4D-ND	3.35	115.66	110.24
22	q	308	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
22	q	304	CLA	CHB-C4A-NA	3.35	129.14	124.51
26	4	314	CHL	C1D-ND-C4D	-3.35	103.96	106.33
22	G	307	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
26	2	316	CHL	CAC-C3C-C4C	3.35	129.15	124.81
31	c	516	BCR	C21-C20-C19	-3.35	112.77	123.22
26	s	316	CHL	CAC-C3C-C4C	3.35	129.15	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	305	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
26	4	316	CHL	CAC-C3C-C4C	3.34	129.15	124.81
31	b	619	BCR	C15-C16-C17	-3.34	116.62	123.47
26	p	316	CHL	CHD-C4C-C3C	-3.34	119.93	124.84
26	v	315	CHL	C2D-C1D-ND	3.34	112.57	110.10
24	1	311	XAT	C38-C25-C26	-3.34	116.66	122.26
26	4	317	CHL	C3D-C4D-ND	3.34	115.64	110.24
22	d	402	CLA	CMB-C2B-C3B	3.34	130.93	124.68
22	3	305	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
26	6	317	CHL	C2D-C1D-ND	3.34	112.57	110.10
23	n	310	LUT	C7-C8-C9	-3.34	121.19	126.23
26	P	314	CHL	C1B-CHB-C4A	-3.34	123.50	130.12
22	G	302	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
32	C	501	SQD	O6-C1-C2	3.34	113.52	108.30
22	b	604	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
31	A	409	BCR	C38-C26-C25	-3.34	120.78	124.53
22	5	308	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
23	5	310	LUT	C7-C8-C9	-3.34	121.19	126.23
24	v	311	XAT	C38-C25-C26	-3.34	116.67	122.26
22	r	606	CLA	CMB-C2B-C3B	3.34	130.92	124.68
22	Q	306	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
23	s	310	LUT	C7-C8-C9	-3.34	121.19	126.23
26	u	313	CHL	C3D-C4D-ND	3.34	115.63	110.24
22	R	303	CLA	CMB-C2B-C3B	3.34	130.92	124.68
22	p	303	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
26	Q	312	CHL	C2D-C1D-ND	3.33	112.56	110.10
22	2	303	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
22	g	307	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
26	P	316	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	6	316	CHL	C3D-C4D-ND	3.33	115.63	110.24
26	S	316	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	P	316	CHL	CHD-C4C-C3C	-3.33	119.94	124.84
24	V	311	XAT	C38-C25-C26	-3.33	116.68	122.26
26	s	313	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	2	313	CHL	C3B-C4B-NB	3.33	113.52	109.21
26	n	316	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	G	314	CHL	C3B-C4B-NB	3.33	113.51	109.21
26	P	314	CHL	C2D-C1D-ND	3.33	112.56	110.10
26	r	616	CHL	C1B-CHB-C4A	-3.33	123.53	130.12
22	6	303	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
26	p	319	CHL	CAC-C3C-C4C	3.33	129.13	124.81
22	6	306	CLA	O2D-CGD-O1D	-3.33	117.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	K	101	BCR	C38-C26-C25	-3.33	120.79	124.53
26	P	319	CHL	CHB-C4A-NA	3.33	129.11	124.51
24	q	309	XAT	C30-C31-C32	-3.33	112.84	123.22
22	c	513	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
26	V	318	CHL	C2D-C1D-ND	3.33	112.56	110.10
31	z	101	BCR	C16-C15-C14	-3.33	116.66	123.47
26	p	318	CHL	CHB-C4A-NA	3.33	129.11	124.51
26	U	317	CHL	C1D-ND-C4D	-3.32	103.97	106.33
22	6	306	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
31	x	202	BCR	C4-C5-C6	-3.32	117.90	122.73
26	V	313	CHL	C3D-C4D-ND	3.32	115.61	110.24
22	S	304	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	b	612	CLA	CMB-C2B-C3B	3.32	130.90	124.68
22	S	305	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
22	Q	308	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
27	R	301	NEX	C35-C34-C33	-3.32	122.57	127.31
22	S	309	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	p	306	CLA	CMB-C2B-C3B	3.32	130.89	124.68
26	G	315	CHL	CAC-C3C-C4C	3.32	129.12	124.81
26	5	317	CHL	C3D-C4D-ND	3.32	115.61	110.24
26	5	316	CHL	C3B-C4B-NB	3.32	113.50	109.21
24	v	311	XAT	C18-C5-C6	-3.32	116.70	122.26
23	n	310	LUT	C18-C5-C4	3.32	120.51	114.36
26	U	319	CHL	C3B-C4B-NB	3.32	113.50	109.21
22	G	303	CLA	CMB-C2B-C3B	3.32	130.89	124.68
26	2	316	CHL	C3B-C4B-NB	3.32	113.50	109.21
22	3	305	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
26	1	316	CHL	C2D-C1D-ND	3.32	112.55	110.10
26	v	313	CHL	C2D-C1D-ND	3.32	112.55	110.10
26	3	316	CHL	CAC-C3C-C4C	3.32	129.11	124.81
26	2	318	CHL	C3D-C4D-ND	3.32	115.60	110.24
26	5	317	CHL	O2A-CGA-CBA	3.32	122.32	111.91
31	X	201	BCR	C4-C5-C6	-3.32	117.92	122.73
26	4	317	CHL	CHB-C4A-NA	3.31	129.10	124.51
26	n	315	CHL	C3B-C4B-NB	3.31	113.50	109.21
31	a	409	BCR	C24-C23-C22	-3.31	121.23	126.23
27	u	320	NEX	C39-C29-C30	-3.31	118.28	122.92
26	1	318	CHL	C1D-ND-C4D	-3.31	103.98	106.33
22	5	304	CLA	CHB-C4A-NA	3.31	129.09	124.51
26	3	314	CHL	CAC-C3C-C4C	3.31	129.11	124.81
31	b	618	BCR	C1-C6-C5	-3.31	117.95	122.61
22	C	505	CLA	CMB-C2B-C3B	3.31	130.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B	601	DGD	O2G-C1B-C2B	3.31	118.63	111.50
26	g	314	CHL	C2D-C1D-ND	3.31	112.54	110.10
26	P	316	CHL	C1B-CHB-C4A	-3.31	123.57	130.12
31	A	409	BCR	C24-C23-C22	-3.31	121.24	126.23
31	b	620	BCR	C24-C23-C22	-3.31	121.24	126.23
22	s	304	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
26	n	317	CHL	C3B-C4B-NB	3.30	113.48	109.21
31	B	620	BCR	C27-C26-C25	-3.30	117.94	122.73
26	6	315	CHL	CAC-C3C-C4C	3.30	129.09	124.81
26	U	313	CHL	CMD-C2D-C3D	-3.30	120.02	127.61
26	p	320	CHL	C3D-C4D-ND	3.30	115.58	110.24
26	V	314	CHL	C1B-CHB-C4A	-3.30	123.58	130.12
26	p	315	CHL	CED-O2D-CGD	3.30	123.40	115.94
22	Q	302	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
23	S	310	LUT	C7-C8-C9	-3.30	121.25	126.23
24	v	311	XAT	C11-C10-C9	-3.30	122.61	127.31
26	n	316	CHL	C1B-CHB-C4A	-3.30	123.59	130.12
26	s	314	CHL	C1D-ND-C4D	-3.29	104.00	106.33
26	1	313	CHL	CAC-C3C-C4C	3.29	129.08	124.81
26	Q	314	CHL	C3B-C4B-NB	3.29	113.47	109.21
22	R	310	CLA	CHB-C4A-NA	3.29	129.06	124.51
31	A	409	BCR	C8-C7-C6	-3.29	117.96	127.20
22	P	305	CLA	CMB-C2B-C3B	3.29	130.84	124.68
26	v	316	CHL	CAC-C3C-C4C	3.29	129.08	124.81
26	g	314	CHL	CAC-C3C-C4C	3.29	129.08	124.81
22	C	514	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
26	n	315	CHL	CMD-C2D-C3D	-3.29	120.05	127.61
26	s	316	CHL	CHD-C4C-C3C	-3.29	120.01	124.84
26	2	314	CHL	CAC-C3C-C4C	3.29	129.07	124.81
26	V	318	CHL	CAC-C3C-C4C	3.28	129.07	124.81
22	s	305	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
23	1	310	LUT	C3-C4-C5	-3.28	105.32	111.85
26	n	315	CHL	CAC-C3C-C4C	3.28	129.07	124.81
22	c	504	CLA	CMB-C2B-C3B	3.28	130.82	124.68
31	C	518	BCR	C33-C5-C4	3.28	119.92	113.62
31	c	516	BCR	C20-C21-C22	-3.28	122.63	127.31
26	G	312	CHL	CAC-C3C-C4C	3.28	129.07	124.81
26	Q	313	CHL	C2D-C1D-ND	3.28	112.52	110.10
22	2	304	CLA	CHB-C4A-NA	3.28	129.05	124.51
22	B	602	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
24	4	311	XAT	C18-C5-C6	-3.28	116.77	122.26
24	U	311	XAT	C31-C30-C29	-3.28	122.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	316	CHL	CAC-C3C-C4C	3.28	129.06	124.81
23	v	309	LUT	C15-C14-C13	-3.28	122.64	127.31
24	V	311	XAT	C26-C27-C28	-3.27	119.07	125.99
34	b	621	LMG	C1-C2-C3	3.27	116.81	110.00
26	q	311	CHL	CAC-C3C-C4C	3.27	129.05	124.81
22	R	308	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
26	p	314	CHL	C1D-ND-C4D	-3.27	104.01	106.33
26	v	317	CHL	O2A-CGA-CBA	3.27	122.17	111.91
26	S	313	CHL	C3D-C4D-ND	3.27	115.53	110.24
31	b	618	BCR	C33-C5-C4	3.27	119.89	113.62
26	2	317	CHL	C3D-C4D-ND	3.27	115.52	110.24
26	5	316	CHL	C3D-C4D-ND	3.27	115.52	110.24
22	r	602	CLA	CMB-C2B-C3B	3.27	130.79	124.68
26	n	315	CHL	C1B-CHB-C4A	-3.26	123.66	130.12
26	S	316	CHL	CHD-C4C-C3C	-3.26	120.04	124.84
27	P	301	NEX	C17-C1-C6	-3.26	107.55	110.47
26	g	311	CHL	C1D-ND-C4D	-3.26	104.02	106.33
26	V	314	CHL	C2D-C1D-ND	3.26	112.51	110.10
26	p	314	CHL	C3D-C4D-ND	3.26	115.51	110.24
26	v	313	CHL	C3D-C4D-ND	3.26	115.50	110.24
26	R	315	CHL	C1D-ND-C4D	-3.26	104.02	106.33
26	P	315	CHL	O2D-CGD-CBD	3.25	117.05	111.27
26	V	317	CHL	O2A-CGA-CBA	3.25	122.11	111.91
26	P	319	CHL	CAC-C3C-C4C	3.25	129.03	124.81
22	1	307	CLA	CMB-C2B-C3B	3.25	130.76	124.68
26	V	316	CHL	C3B-C4B-NB	3.25	113.41	109.21
22	p	309	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
22	b	617	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
26	3	315	CHL	C3D-C4D-ND	3.25	115.49	110.24
22	1	303	CLA	CMB-C2B-C3B	3.25	130.76	124.68
22	c	505	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
23	V	310	LUT	C35-C34-C33	-3.25	122.67	127.31
26	q	312	CHL	O2D-CGD-O1D	-3.25	117.49	123.84
26	q	313	CHL	C3D-C4D-ND	3.25	115.49	110.24
31	C	517	BCR	C8-C7-C6	-3.25	118.08	127.20
32	C	501	SQD	O5-C5-C4	3.25	115.59	109.69
26	1	315	CHL	C3B-C4B-NB	3.25	113.41	109.21
26	5	315	CHL	C3D-C4D-ND	3.25	115.49	110.24
26	5	313	CHL	CAC-C3C-C4C	3.25	129.02	124.81
26	2	316	CHL	C3D-C4D-ND	3.24	115.49	110.24
22	n	307	CLA	CMB-C2B-C3B	3.24	130.75	124.68
26	2	316	CHL	C2D-C1D-ND	3.24	112.49	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	312	XAT	C35-C34-C33	-3.24	122.68	127.31
22	S	305	CLA	CMB-C2B-C3B	3.24	130.75	124.68
26	G	315	CHL	C3B-C4B-NB	3.24	113.40	109.21
31	c	515	BCR	C8-C7-C6	-3.24	118.10	127.20
22	C	503	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
26	V	316	CHL	CMD-C2D-C3D	-3.24	120.16	127.61
22	R	307	CLA	CMB-C2B-C3B	3.24	130.74	124.68
26	3	315	CHL	C3B-C4B-NB	3.24	113.40	109.21
26	G	312	CHL	C3B-C4B-NB	3.24	113.39	109.21
26	g	312	CHL	C2D-C1D-ND	3.23	112.49	110.10
26	N	313	CHL	C3D-C4D-ND	3.23	115.47	110.24
24	2	311	XAT	C27-C28-C29	-3.23	120.51	125.53
22	U	304	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
24	2	311	XAT	C18-C5-C6	-3.23	116.84	122.26
22	u	304	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
26	q	315	CHL	C1B-CHB-C4A	-3.23	123.72	130.12
26	1	318	CHL	C3D-C4D-ND	3.23	115.46	110.24
31	b	619	BCR	C38-C26-C27	3.23	119.82	113.62
22	v	308	CLA	CMB-C2B-C3B	3.23	130.72	124.68
32	l	102	SQD	C44-O6-C1	3.23	120.05	113.74
22	q	302	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
22	R	302	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
27	n	319	NEX	C39-C29-C30	-3.23	118.40	122.92
32	A	412	SQD	O9-S-C6	3.23	110.77	106.94
26	S	314	CHL	C1D-ND-C4D	-3.23	104.04	106.33
27	S	317	NEX	C17-C1-C6	-3.23	107.58	110.47
26	R	317	CHL	C1B-CHB-C4A	-3.22	123.73	130.12
22	4	304	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
36	b	601	DGD	O2G-C1B-C2B	3.22	118.45	111.50
26	N	317	CHL	C3D-C4D-ND	3.22	115.45	110.24
22	P	309	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
26	1	314	CHL	C4A-NA-C1A	3.22	108.15	106.71
27	u	319	NEX	C2-C1-C6	3.22	112.34	109.21
26	G	313	CHL	C3D-C4D-ND	3.22	115.44	110.24
26	p	315	CHL	O2D-CGD-CBD	3.22	116.99	111.27
22	A	408	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
32	a	410	SQD	O5-C5-C4	3.22	115.54	109.69
26	Q	314	CHL	CAC-C3C-C4C	3.22	128.98	124.81
26	G	312	CHL	CHD-C4C-C3C	-3.22	120.11	124.84
26	p	317	CHL	CAC-C3C-C4C	3.22	128.98	124.81
26	S	313	CHL	C3B-C4B-NB	3.22	113.37	109.21
22	c	502	CLA	CMB-C2B-C1B	-3.22	123.52	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	D	408	LMG	O7-C10-C11	3.22	118.43	111.50
26	5	314	CHL	CAC-C3C-C4C	3.21	128.98	124.81
22	1	304	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
31	z	101	BCR	C33-C5-C4	3.21	119.79	113.62
22	2	307	CLA	CMB-C2B-C3B	3.21	130.69	124.68
26	6	313	CHL	CAC-C3C-C4C	3.21	128.98	124.81
22	p	305	CLA	CMB-C2B-C3B	3.21	130.69	124.68
27	S	317	NEX	C2-C1-C6	3.21	112.33	109.21
22	C	506	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
26	6	317	CHL	CMD-C2D-C3D	-3.21	120.23	127.61
22	c	508	CLA	CMB-C2B-C3B	3.21	130.68	124.68
22	N	304	CLA	CHB-C4A-NA	3.21	128.95	124.51
26	g	314	CHL	CHD-C4C-C3C	-3.21	120.13	124.84
22	u	306	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
31	B	619	BCR	C38-C26-C27	3.20	119.77	113.62
22	6	308	CLA	CMB-C2B-C3B	3.20	130.67	124.68
22	g	303	CLA	CMB-C2B-C3B	3.20	130.67	124.68
22	4	307	CLA	CMB-C2B-C3B	3.20	130.67	124.68
26	P	317	CHL	CAC-C3C-C4C	3.20	128.97	124.81
26	U	315	CHL	C3D-C4D-ND	3.20	115.42	110.24
22	2	304	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
26	4	315	CHL	C3B-C4B-NB	3.20	113.35	109.21
26	4	315	CHL	CHD-C4C-C3C	-3.20	120.14	124.84
31	C	516	BCR	C33-C5-C4	3.20	119.76	113.62
22	G	305	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
24	N	311	XAT	C38-C25-C26	-3.20	116.90	122.26
23	p	310	LUT	C11-C10-C9	-3.20	122.75	127.31
31	C	516	BCR	C21-C20-C19	-3.20	113.24	123.22
22	p	306	CLA	CHB-C4A-NA	3.20	128.93	124.51
24	Q	309	XAT	C18-C5-C6	-3.20	116.91	122.26
26	p	317	CHL	CMD-C2D-C3D	-3.20	120.26	127.61
26	3	316	CHL	C1D-ND-C4D	-3.19	104.07	106.33
26	U	319	CHL	C1D-ND-C4D	-3.19	104.07	106.33
31	b	618	BCR	C23-C24-C25	-3.19	118.24	127.20
26	s	313	CHL	C3D-C4D-ND	3.19	115.40	110.24
26	r	615	CHL	C1D-ND-C4D	-3.19	104.07	106.33
27	n	319	NEX	O24-C25-C38	3.19	118.87	115.06
23	1	310	LUT	C15-C14-C13	-3.19	122.76	127.31
26	2	313	CHL	C1B-CHB-C4A	-3.19	123.81	130.12
26	U	313	CHL	C3B-C4B-NB	3.18	113.33	109.21
22	u	303	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
26	n	317	CHL	C3D-C4D-ND	3.18	115.39	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	318	CHL	C1D-ND-C4D	-3.18	104.07	106.33
26	q	313	CHL	C1D-ND-C4D	-3.18	104.07	106.33
26	R	316	CHL	C1D-ND-C4D	-3.18	104.07	106.33
22	u	308	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
31	B	620	BCR	C20-C21-C22	-3.18	122.77	127.31
26	Q	316	CHL	C3D-C4D-ND	3.18	115.39	110.24
26	n	316	CHL	C1D-ND-C4D	-3.18	104.07	106.33
26	S	313	CHL	CMD-C2D-C3D	-3.18	120.29	127.61
26	r	614	CHL	C1D-ND-C4D	-3.18	104.08	106.33
26	p	316	CHL	C3B-C4B-NB	3.18	113.32	109.21
26	Q	313	CHL	C1C-C2C-C3C	-3.18	104.59	107.11
26	V	315	CHL	C4A-NA-C1A	3.18	108.14	106.71
34	d	407	LMG	O7-C10-C11	3.18	118.35	111.50
26	4	313	CHL	C3B-C4B-NB	3.18	113.32	109.21
31	B	618	BCR	C23-C24-C25	-3.18	118.28	127.20
26	G	315	CHL	C3D-C4D-ND	3.18	115.38	110.24
31	z	101	BCR	C21-C20-C19	-3.18	113.30	123.22
26	s	314	CHL	C3D-C4D-ND	3.18	115.38	110.24
22	U	308	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
32	L	102	SQD	C44-O6-C1	3.17	119.94	113.74
26	n	318	CHL	C3D-C4D-ND	3.17	115.37	110.24
26	3	316	CHL	CMD-C2D-C3D	-3.17	120.32	127.61
26	q	312	CHL	CAC-C3C-C4C	3.17	128.93	124.81
26	N	317	CHL	C1B-CHB-C4A	-3.17	123.84	130.12
24	n	311	XAT	C35-C34-C33	-3.17	122.78	127.31
26	v	313	CHL	C3B-C4B-NB	3.17	113.31	109.21
26	p	314	CHL	C3B-C4B-NB	3.17	113.31	109.21
26	P	316	CHL	C3B-C4B-NB	3.17	113.31	109.21
26	Q	315	CHL	CAC-C3C-C4C	3.17	128.92	124.81
22	C	509	CLA	CMB-C2B-C3B	3.17	130.61	124.68
26	g	315	CHL	C3B-C4B-NB	3.17	113.31	109.21
23	s	310	LUT	C30-C31-C32	-3.17	113.33	123.22
31	C	517	BCR	C33-C5-C4	3.17	119.70	113.62
26	q	315	CHL	C3D-C4D-ND	3.16	115.36	110.24
26	3	316	CHL	C2D-C1D-ND	3.16	112.43	110.10
26	4	315	CHL	CAC-C3C-C4C	3.16	128.91	124.81
26	G	311	CHL	CHB-C4A-NA	3.16	128.88	124.51
26	r	619	CHL	C3D-C4D-ND	3.16	115.35	110.24
22	5	307	CLA	CMB-C2B-C3B	3.16	130.59	124.68
26	u	313	CHL	C1D-ND-C4D	-3.16	104.09	106.33
26	g	314	CHL	C3B-C4B-NB	3.16	113.29	109.21
31	x	202	BCR	C38-C26-C27	3.16	119.68	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	604	CLA	CMB-C2B-C1B	-3.15	123.61	128.46
26	1	313	CHL	C3D-C4D-ND	3.15	115.34	110.24
26	S	314	CHL	C3D-C4D-ND	3.15	115.34	110.24
24	1	311	XAT	C18-C5-C6	-3.15	116.97	122.26
24	q	309	XAT	C18-C5-C6	-3.15	116.97	122.26
26	U	317	CHL	CHB-C4A-NA	3.15	128.87	124.51
22	3	305	CLA	CHB-C4A-NA	3.15	128.87	124.51
26	S	316	CHL	C3D-C4D-ND	3.15	115.34	110.24
26	q	314	CHL	CAC-C3C-C4C	3.15	128.90	124.81
22	R	305	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
24	r	612	XAT	C10-C11-C12	-3.15	113.38	123.22
26	2	313	CHL	CAC-C3C-C4C	3.15	128.90	124.81
26	s	316	CHL	C3D-C4D-ND	3.15	115.33	110.24
26	s	313	CHL	CMD-C2D-C3D	-3.15	120.37	127.61
22	1	306	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
22	U	302	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
23	2	309	LUT	C11-C10-C9	-3.15	122.82	127.31
31	z	101	BCR	C29-C30-C25	3.15	115.33	110.48
26	u	318	CHL	CHB-C4A-NA	3.15	128.86	124.51
22	s	305	CLA	CMB-C2B-C3B	3.15	130.57	124.68
31	b	619	BCR	C27-C26-C25	-3.15	118.16	122.73
31	z	101	BCR	C27-C26-C25	-3.15	118.16	122.73
26	v	315	CHL	C3D-C4D-ND	3.14	115.32	110.24
22	3	308	CLA	CMB-C2B-C3B	3.14	130.56	124.68
26	P	314	CHL	C3D-C4D-ND	3.14	115.32	110.24
26	p	320	CHL	CAC-C3C-C4C	3.14	128.89	124.81
26	Q	316	CHL	CAC-C3C-C4C	3.14	128.89	124.81
22	b	608	CLA	CHB-C4A-NA	3.14	128.86	124.51
26	6	301	CHL	C3D-C4D-ND	3.14	115.32	110.24
26	P	319	CHL	C3D-C4D-ND	3.14	115.32	110.24
26	p	317	CHL	C3D-C4D-ND	3.14	115.32	110.24
27	r	618	NEX	C39-C29-C30	-3.14	118.52	122.92
22	R	310	CLA	CMB-C2B-C3B	3.14	130.55	124.68
31	c	515	BCR	C33-C5-C4	3.14	119.64	113.62
26	V	313	CHL	C2D-C1D-ND	3.14	112.42	110.10
24	g	309	XAT	C35-C34-C33	-3.14	122.83	127.31
22	N	308	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
26	V	313	CHL	CMD-C2D-C3D	-3.14	120.40	127.61
26	1	315	CHL	C1B-CHB-C4A	-3.14	123.91	130.12
26	N	314	CHL	C3B-C4B-NB	3.14	113.27	109.21
26	G	313	CHL	C1D-ND-C4D	-3.14	104.11	106.33
26	3	313	CHL	C3D-C4D-ND	3.14	115.31	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	316	CHL	O2A-CGA-CBA	3.13	121.75	111.91
31	x	202	BCR	C30-C25-C26	-3.13	118.20	122.61
23	u	309	LUT	C15-C14-C13	-3.13	122.84	127.31
24	u	311	XAT	C26-C27-C28	-3.13	119.37	125.99
26	V	313	CHL	C3B-C4B-NB	3.13	113.26	109.21
26	2	315	CHL	C1D-ND-C4D	-3.13	104.11	106.33
22	3	307	CLA	CMB-C2B-C3B	3.13	130.53	124.68
26	G	311	CHL	C1C-C2C-C3C	-3.13	104.63	107.11
25	d	406	LHG	O7-C7-C8	3.13	118.25	111.50
26	g	315	CHL	C3D-C4D-ND	3.13	115.30	110.24
31	b	619	BCR	C20-C21-C22	-3.13	122.85	127.31
26	G	311	CHL	C3D-C4D-ND	3.13	115.29	110.24
31	B	619	BCR	C27-C26-C25	-3.12	118.19	122.73
22	q	307	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
26	N	317	CHL	C2D-C1D-ND	3.12	112.41	110.10
26	1	315	CHL	C3D-C4D-ND	3.12	115.29	110.24
22	G	306	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
22	R	304	CLA	CMB-C2B-C3B	3.12	130.52	124.68
26	V	315	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
26	1	316	CHL	C3D-C4D-ND	3.12	115.28	110.24
26	1	317	CHL	O1D-CGD-CBD	-3.12	118.10	124.48
31	c	516	BCR	C38-C26-C25	-3.12	121.03	124.53
26	p	317	CHL	C1D-ND-C4D	-3.12	104.12	106.33
26	v	317	CHL	O2D-CGD-O1D	-3.12	117.75	123.84
22	Q	303	CLA	C1B-CHB-C4A	-3.12	123.95	130.12
26	p	320	CHL	CHB-C4A-NA	3.11	128.82	124.51
26	v	315	CHL	C1B-CHB-C4A	-3.11	123.95	130.12
26	n	316	CHL	C3D-C4D-ND	3.11	115.27	110.24
22	v	304	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
31	C	516	BCR	C23-C24-C25	-3.11	118.47	127.20
26	3	313	CHL	CHD-C4C-C3C	-3.11	120.27	124.84
26	v	315	CHL	C3B-C4B-NB	3.11	113.23	109.21
26	6	301	CHL	C2D-C1D-ND	3.11	112.40	110.10
26	2	318	CHL	C1C-C2C-C3C	-3.11	104.65	107.11
22	p	306	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	5	304	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
26	R	315	CHL	C3D-C4D-ND	3.11	115.26	110.24
23	V	310	LUT	C7-C8-C9	-3.11	121.54	126.23
22	6	309	CLA	CMB-C2B-C3B	3.10	130.49	124.68
22	v	303	CLA	CMB-C2B-C3B	3.10	130.48	124.68
31	C	518	BCR	C38-C26-C25	-3.10	121.04	124.53
24	U	311	XAT	C27-C28-C29	-3.10	120.72	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u	318	CHL	C3D-C4D-ND	3.10	115.25	110.24
26	p	318	CHL	C3D-C4D-ND	3.10	115.25	110.24
26	1	313	CHL	CMD-C2D-C3D	-3.10	120.48	127.61
26	5	313	CHL	C3B-C4B-NB	3.10	113.22	109.21
22	V	307	CLA	CMB-C2B-C3B	3.10	130.48	124.68
27	u	319	NEX	C27-C28-C29	-3.10	120.72	125.53
31	C	516	BCR	C20-C21-C22	-3.10	122.89	127.31
24	G	309	XAT	C30-C31-C32	-3.10	113.55	123.22
22	b	616	CLA	CHB-C4A-NA	3.10	128.80	124.51
26	g	313	CHL	C1D-ND-C4D	-3.10	104.13	106.33
26	Q	312	CHL	C3D-C4D-ND	3.10	115.25	110.24
26	P	314	CHL	C3B-C4B-NB	3.10	113.21	109.21
22	q	305	CLA	CMB-C2B-C3B	3.10	130.47	124.68
26	s	313	CHL	C3B-C4B-NB	3.10	113.21	109.21
26	6	312	CHL	CAC-C3C-C4C	3.10	128.83	124.81
22	v	301	CLA	CMB-C2B-C3B	3.10	130.47	124.68
26	5	317	CHL	CHB-C4A-NA	3.10	128.79	124.51
25	D	407	LHG	O7-C7-C8	3.09	118.17	111.50
23	P	311	LUT	C31-C30-C29	-3.09	122.89	127.31
22	v	307	CLA	CMB-C2B-C3B	3.09	130.47	124.68
26	U	319	CHL	C3D-C4D-ND	3.09	115.24	110.24
22	U	306	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
22	4	304	CLA	CMB-C2B-C3B	3.09	130.46	124.68
22	N	305	CLA	CMB-C2B-C3B	3.09	130.46	124.68
31	z	101	BCR	C23-C24-C25	-3.09	118.53	127.20
26	P	318	CHL	C3D-C4D-ND	3.09	115.23	110.24
31	c	516	BCR	C30-C25-C26	-3.09	118.26	122.61
23	S	311	LUT	C35-C34-C33	-3.09	122.90	127.31
31	X	201	BCR	C38-C26-C27	3.09	119.55	113.62
26	5	318	CHL	C1C-C2C-C3C	-3.09	104.66	107.11
31	K	101	BCR	C8-C7-C6	-3.09	118.54	127.20
23	1	309	LUT	C7-C8-C9	-3.09	121.57	126.23
22	p	308	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
26	r	614	CHL	C3D-C4D-ND	3.08	115.23	110.24
26	p	319	CHL	C3D-C4D-ND	3.08	115.23	110.24
22	V	301	CLA	CMB-C2B-C3B	3.08	130.45	124.68
31	b	618	BCR	C21-C20-C19	-3.08	113.59	123.22
26	s	315	CHL	CHD-C4C-C3C	-3.08	120.31	124.84
31	k	101	BCR	C8-C7-C6	-3.08	118.54	127.20
27	2	319	NEX	C11-C12-C13	-3.08	117.76	126.42
26	P	317	CHL	C2D-C1D-ND	3.08	112.38	110.10
26	N	315	CHL	CAC-C3C-C4C	3.08	128.81	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	616	CLA	CHB-C4A-NA	3.08	128.77	124.51
22	4	308	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
26	n	313	CHL	C3D-C4D-ND	3.08	115.22	110.24
26	v	313	CHL	CMD-C2D-C3D	-3.08	120.53	127.61
31	B	620	BCR	C10-C11-C12	-3.08	113.62	123.22
26	V	315	CHL	CAC-C3C-C4C	3.08	128.80	124.81
32	M	101	SQD	C4-C3-C2	3.07	116.19	110.82
26	S	313	CHL	C2D-C1D-ND	3.07	112.37	110.10
22	n	308	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
26	s	316	CHL	C3B-C4B-NB	3.07	113.18	109.21
22	q	308	CLA	CHB-C4A-NA	3.07	128.76	124.51
26	v	314	CHL	C3D-C4D-ND	3.07	115.21	110.24
22	V	304	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
27	r	618	NEX	C5-C4-C3	3.07	115.38	111.75
22	p	308	CLA	CMB-C2B-C3B	3.07	130.42	124.68
26	g	313	CHL	C3D-C4D-ND	3.07	115.20	110.24
26	2	315	CHL	C3D-C4D-ND	3.07	115.20	110.24
22	p	305	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	C	506	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	B	608	CLA	CHB-C4A-NA	3.07	128.75	124.51
22	c	505	CLA	CHB-C4A-NA	3.07	128.75	124.51
23	2	310	LUT	C11-C10-C9	-3.07	122.93	127.31
26	U	316	CHL	O1D-CGD-CBD	-3.07	118.21	124.48
22	1	308	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
26	5	316	CHL	C2D-C1D-ND	3.07	112.36	110.10
31	b	618	BCR	C38-C26-C27	3.07	119.51	113.62
26	5	316	CHL	CMD-C2D-C3D	-3.07	120.56	127.61
31	t	101	BCR	C4-C5-C6	-3.07	118.28	122.73
26	1	316	CHL	C1D-ND-C4D	-3.06	104.16	106.33
31	C	518	BCR	C30-C25-C26	-3.06	118.30	122.61
26	5	318	CHL	C4-C3-C5	3.06	120.42	115.27
26	U	313	CHL	C2D-C1D-ND	3.06	112.36	110.10
22	p	307	CLA	CMB-C2B-C3B	3.06	130.41	124.68
26	R	317	CHL	C3B-C4B-NB	3.06	113.17	109.21
22	n	304	CLA	CMA-C3A-C4A	-3.06	103.54	111.77
23	n	309	LUT	C15-C14-C13	-3.06	122.94	127.31
31	B	620	BCR	C23-C24-C25	-3.06	118.60	127.20
31	B	618	BCR	C38-C26-C27	3.06	119.50	113.62
26	P	317	CHL	C3D-C4D-ND	3.06	115.19	110.24
26	S	315	CHL	CHD-C4C-C3C	-3.06	120.34	124.84
23	V	309	LUT	C15-C14-C13	-3.06	122.94	127.31
33	D	405	PL9	C17-C18-C19	-3.06	120.30	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	m	101	SQD	C4-C3-C2	3.06	116.16	110.82
26	3	312	CHL	CAC-C3C-C4C	3.06	128.78	124.81
26	V	318	CHL	C3D-C4D-ND	3.06	115.18	110.24
26	2	316	CHL	CMD-C2D-C3D	-3.06	120.58	127.61
31	T	101	BCR	C4-C5-C6	-3.06	118.29	122.73
26	2	313	CHL	C3D-C4D-ND	3.06	115.18	110.24
22	5	304	CLA	CMB-C2B-C3B	3.06	130.40	124.68
26	U	316	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
22	r	609	CLA	CHB-C4A-NA	3.05	128.74	124.51
26	v	314	CHL	CHB-C4A-NA	3.05	128.74	124.51
22	U	303	CLA	CMB-C2B-C3B	3.05	130.39	124.68
22	N	303	CLA	CHB-C4A-NA	3.05	128.73	124.51
31	X	201	BCR	C30-C25-C26	-3.05	118.31	122.61
31	z	101	BCR	C20-C21-C22	-3.05	122.95	127.31
31	T	101	BCR	C27-C26-C25	-3.05	118.30	122.73
22	5	305	CLA	CHB-C4A-NA	3.05	128.73	124.51
26	4	315	CHL	C3D-C4D-ND	3.05	115.17	110.24
26	6	314	CHL	C3D-C4D-ND	3.05	115.17	110.24
26	V	315	CHL	C3D-C4D-ND	3.05	115.17	110.24
23	5	310	LUT	C11-C10-C9	-3.05	122.96	127.31
26	S	316	CHL	C3B-C4B-NB	3.05	113.15	109.21
26	4	314	CHL	C3D-C4D-ND	3.05	115.17	110.24
26	5	313	CHL	C4-C3-C5	3.05	120.40	115.27
26	q	311	CHL	C4-C3-C5	3.05	120.40	115.27
23	V	310	LUT	C15-C35-C34	-3.05	117.23	123.47
26	P	316	CHL	C3D-C4D-ND	3.05	115.17	110.24
26	N	313	CHL	C1C-C2C-C3C	-3.04	104.70	107.11
26	n	315	CHL	C3D-C4D-ND	3.04	115.16	110.24
26	P	318	CHL	CHB-C4A-NA	3.04	128.72	124.51
26	n	315	CHL	C2D-C1D-ND	3.04	112.35	110.10
23	1	310	LUT	C16-C1-C6	-3.04	105.36	110.30
22	c	510	CLA	CHB-C4A-NA	3.04	128.72	124.51
26	u	317	CHL	O2A-CGA-CBA	3.04	121.46	111.91
32	l	102	SQD	C3-C4-C5	3.04	115.67	110.24
26	V	318	CHL	C1B-CHB-C4A	-3.04	124.09	130.12
23	R	312	LUT	C15-C14-C13	-3.04	122.97	127.31
26	v	316	CHL	CMD-C2D-C3D	-3.04	120.62	127.61
26	q	311	CHL	CHB-C4A-NA	3.04	128.72	124.51
26	Q	316	CHL	C1D-ND-C4D	-3.04	104.17	106.33
26	g	311	CHL	C3D-C4D-ND	3.04	115.16	110.24
26	2	318	CHL	C4-C3-C5	3.04	120.38	115.27
26	U	317	CHL	C3D-C4D-ND	3.04	115.15	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	306	CLA	CHB-C4A-NA	3.04	128.71	124.51
22	N	304	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
26	1	313	CHL	C2D-C1D-ND	3.04	112.34	110.10
26	r	619	CHL	CHB-C4A-NA	3.04	128.71	124.51
22	x	201	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	n	304	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	C	511	CLA	CHB-C4A-NA	3.04	128.71	124.51
26	Q	313	CHL	C1D-ND-C4D	-3.04	104.18	106.33
22	C	515	CLA	CMB-C2B-C3B	3.04	130.36	124.68
26	6	313	CHL	C3B-C4B-NB	3.04	113.13	109.21
22	p	305	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
31	c	515	BCR	C21-C20-C19	-3.03	113.75	123.22
22	s	309	CLA	CMB-C2B-C3B	3.03	130.35	124.68
26	u	313	CHL	C1C-C2C-C3C	-3.03	104.71	107.11
31	b	618	BCR	C40-C30-C25	-3.03	105.38	110.30
22	P	308	CLA	CMB-C2B-C3B	3.03	130.35	124.68
26	s	315	CHL	CAC-C3C-C4C	3.03	128.75	124.81
22	P	306	CLA	CMB-C2B-C3B	3.03	130.35	124.68
24	g	309	XAT	C30-C31-C32	-3.03	113.75	123.22
22	2	304	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	U	314	CHL	C3D-C4D-ND	3.03	115.14	110.24
26	4	313	CHL	C3D-C4D-ND	3.03	115.14	110.24
26	3	314	CHL	C3B-C4B-NB	3.03	113.13	109.21
22	6	309	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	4	310	LUT	C15-C14-C13	-3.03	122.99	127.31
31	b	620	BCR	C23-C24-C25	-3.03	118.69	127.20
22	6	306	CLA	CHB-C4A-NA	3.03	128.70	124.51
26	S	316	CHL	CMD-C2D-C3D	-3.03	120.65	127.61
31	b	618	BCR	C15-C16-C17	-3.03	117.27	123.47
26	3	311	CHL	CHB-C4A-NA	3.03	128.70	124.51
26	v	313	CHL	C1D-ND-C4D	-3.03	104.19	106.33
23	S	310	LUT	C30-C31-C32	-3.02	113.78	123.22
26	U	316	CHL	CHB-C4A-NA	3.02	128.69	124.51
23	V	310	LUT	C15-C14-C13	-3.02	122.99	127.31
27	u	320	NEX	C35-C34-C33	-3.02	122.99	127.31
22	P	305	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
26	5	313	CHL	C3D-C4D-ND	3.02	115.13	110.24
27	n	319	NEX	C16-C1-C6	3.02	113.18	110.47
26	p	315	CHL	C3D-C4D-ND	3.02	115.13	110.24
22	1	304	CLA	CMB-C2B-C3B	3.02	130.33	124.68
26	g	315	CHL	O2A-CGA-CBA	3.02	121.39	111.91
26	6	317	CHL	CHB-C4A-NA	3.02	128.69	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	514	CLA	CMB-C2B-C3B	3.02	130.33	124.68
23	s	311	LUT	C15-C14-C13	-3.02	123.00	127.31
24	3	309	XAT	C31-C30-C29	-3.02	123.00	127.31
26	P	319	CHL	C1C-C2C-C3C	-3.02	104.72	107.11
22	C	513	CLA	CHB-C4A-NA	3.02	128.69	124.51
26	n	313	CHL	C1D-ND-C4D	-3.02	104.19	106.33
22	R	308	CLA	CHB-C4A-NA	3.02	128.69	124.51
31	D	404	BCR	C8-C7-C6	-3.02	118.73	127.20
26	6	301	CHL	C1D-ND-C4D	-3.02	104.19	106.33
26	1	318	CHL	CHB-C4A-NA	3.02	128.68	124.51
22	P	303	CLA	CMB-C2B-C3B	3.01	130.32	124.68
26	1	313	CHL	C3B-C4B-NB	3.01	113.11	109.21
33	d	404	PL9	C17-C18-C19	-3.01	120.40	127.66
26	6	316	CHL	CAC-C3C-C4C	3.01	128.72	124.81
26	v	317	CHL	O1D-CGD-CBD	-3.01	118.32	124.48
26	s	316	CHL	CMD-C2D-C3D	-3.01	120.68	127.61
26	3	313	CHL	C3B-C4B-NB	3.01	113.11	109.21
24	G	309	XAT	C10-C11-C12	-3.01	113.82	123.22
26	v	318	CHL	C3D-C4D-ND	3.01	115.11	110.24
22	V	301	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
23	n	309	LUT	C18-C5-C6	-3.01	121.15	124.53
22	X	202	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	2	308	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	G	308	CLA	CMB-C2B-C3B	3.01	130.30	124.68
22	g	308	CLA	CMB-C2B-C3B	3.01	130.30	124.68
22	Q	304	CLA	CHB-C4A-NA	3.00	128.67	124.51
23	n	309	LUT	C11-C10-C9	-3.00	123.02	127.31
26	R	317	CHL	C2D-C1D-ND	3.00	112.32	110.10
36	J	101	DGD	O1G-C1A-C2A	3.00	121.33	111.91
31	a	409	BCR	C38-C26-C25	-3.00	121.16	124.53
27	P	301	NEX	C11-C10-C9	-3.00	123.03	127.31
31	T	101	BCR	C20-C19-C18	-3.00	117.98	126.42
26	r	616	CHL	C3B-C4B-NB	3.00	113.09	109.21
22	U	301	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
26	5	314	CHL	C3B-C4B-NB	3.00	113.09	109.21
26	2	313	CHL	C4A-NA-C1A	3.00	108.06	106.71
26	r	615	CHL	C3D-C4D-ND	3.00	115.09	110.24
33	D	405	PL9	C22-C23-C24	-3.00	120.44	127.66
25	c	523	LHG	O8-C23-C24	3.00	121.32	111.91
26	V	316	CHL	C3D-C4D-ND	3.00	115.09	110.24
22	3	308	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
31	d	403	BCR	C8-C7-C6	-3.00	118.78	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	404	PL9	C22-C23-C24	-3.00	120.44	127.66
26	v	313	CHL	C1-C2-C3	-3.00	120.86	126.04
26	3	313	CHL	CAC-C3C-C4C	3.00	128.70	124.81
26	Q	312	CHL	O2D-CGD-O1D	-3.00	117.98	123.84
26	N	315	CHL	C3D-C4D-ND	3.00	115.08	110.24
22	c	507	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
26	U	314	CHL	C1D-ND-C4D	-2.99	104.21	106.33
31	C	516	BCR	C29-C30-C25	2.99	115.09	110.48
26	N	317	CHL	CHD-C4C-C3C	-2.99	120.44	124.84
22	Q	305	CLA	CMB-C2B-C3B	2.99	130.28	124.68
26	G	311	CHL	C4-C3-C5	2.99	120.30	115.27
26	6	315	CHL	C3B-C4B-NB	2.99	113.08	109.21
33	D	405	PL9	C12-C13-C14	-2.99	120.46	127.66
26	3	312	CHL	C3B-C4B-NB	2.99	113.08	109.21
26	q	311	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
33	d	404	PL9	C12-C13-C14	-2.99	120.46	127.66
26	U	317	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
23	4	309	LUT	C31-C30-C29	-2.99	123.05	127.31
22	b	610	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
32	L	102	SQD	C3-C4-C5	2.99	115.57	110.24
22	n	305	CLA	CMB-C2B-C3B	2.99	130.26	124.68
26	s	315	CHL	C3D-C4D-ND	2.99	115.07	110.24
26	3	315	CHL	O2A-CGA-CBA	2.98	121.28	111.91
26	1	315	CHL	CAC-C3C-C4C	2.98	128.68	124.81
26	N	313	CHL	CMD-C2D-C3D	-2.98	120.75	127.61
22	B	616	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
26	p	316	CHL	C3D-C4D-ND	2.98	115.06	110.24
22	U	308	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	c	512	CLA	CHB-C4A-NA	2.98	128.63	124.51
24	Q	309	XAT	C7-C8-C9	-2.98	120.90	125.53
22	B	610	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
36	c	519	DGD	O1G-C1A-C2A	2.98	121.26	111.91
22	B	611	CLA	CHB-C4A-NA	2.98	128.63	124.51
22	P	306	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	4	314	CHL	O2D-CGD-O1D	-2.98	118.01	123.84
22	4	307	CLA	CHB-C4A-NA	2.98	128.63	124.51
27	5	319	NEX	C11-C12-C13	-2.98	118.05	126.42
24	r	612	XAT	C35-C15-C14	-2.98	117.38	123.47
26	q	315	CHL	C1D-ND-C4D	-2.98	104.22	106.33
26	2	317	CHL	CHB-C4A-NA	2.98	128.63	124.51
36	A	414	DGD	C3E-C4E-C5E	2.97	115.55	110.24
26	p	319	CHL	C1D-ND-C4D	-2.97	104.22	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	305	CLA	CMB-C2B-C3B	2.97	130.24	124.68
22	C	509	CLA	CHB-C4A-NA	2.97	128.62	124.51
26	Q	316	CHL	CMD-C2D-C3D	-2.97	120.77	127.61
26	S	315	CHL	C3D-C4D-ND	2.97	115.05	110.24
26	6	316	CHL	O2A-CGA-CBA	2.97	121.24	111.91
31	C	517	BCR	C21-C20-C19	-2.97	113.94	123.22
26	P	314	CHL	CAC-C3C-C4C	2.97	128.67	124.81
22	2	305	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	U	304	CLA	CMB-C2B-C3B	2.97	130.23	124.68
25	Q	310	LHG	O8-C23-C24	2.97	121.22	111.91
22	g	305	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
31	A	409	BCR	C20-C21-C22	-2.97	123.07	127.31
26	V	317	CHL	O1D-CGD-CBD	-2.97	118.41	124.48
26	q	313	CHL	C1C-C2C-C3C	-2.97	104.76	107.11
22	n	305	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
27	r	618	NEX	C35-C34-C33	-2.97	123.08	127.31
22	b	611	CLA	CHB-C4A-NA	2.97	128.61	124.51
26	U	313	CHL	C1B-CHB-C4A	-2.97	124.24	130.12
22	g	304	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
26	q	315	CHL	CMD-C2D-C3D	-2.96	120.79	127.61
22	5	301	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
24	N	311	XAT	C10-C11-C12	-2.96	113.97	123.22
22	S	308	CLA	CMB-C2B-C3B	2.96	130.22	124.68
22	5	303	CLA	CHB-C4A-NA	2.96	128.61	124.51
22	V	303	CLA	CHB-C4A-NA	2.96	128.61	124.51
26	r	614	CHL	C4-C3-C5	2.96	120.25	115.27
22	n	303	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
22	C	508	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	u	302	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
22	g	306	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
23	P	310	LUT	C11-C10-C9	-2.96	123.09	127.31
22	Q	308	CLA	CHB-C4A-NA	2.96	128.60	124.51
23	S	311	LUT	C15-C14-C13	-2.96	123.09	127.31
26	R	317	CHL	C3D-C4D-ND	2.96	115.02	110.24
26	S	315	CHL	CAC-C3C-C4C	2.96	128.65	124.81
22	r	605	CLA	CMB-C2B-C3B	2.96	130.21	124.68
26	P	315	CHL	C3D-C4D-ND	2.96	115.02	110.24
24	u	311	XAT	C11-C10-C9	-2.96	123.09	127.31
22	5	308	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	b	610	CLA	CMB-C2B-C3B	2.96	130.21	124.68
31	k	101	BCR	C33-C5-C4	2.95	119.29	113.62
22	N	307	CLA	CMB-C2B-C3B	2.95	130.21	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	318	CHL	C2D-C1D-ND	2.95	112.28	110.10
22	p	304	CLA	CMB-C2B-C3B	2.95	130.21	124.68
26	s	314	CHL	CMD-C2D-C3D	-2.95	120.82	127.61
26	G	312	CHL	CMD-C2D-C3D	-2.95	120.82	127.61
22	u	303	CLA	CMB-C2B-C3B	2.95	130.20	124.68
22	G	301	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
26	S	316	CHL	C4A-NA-C1A	2.95	108.03	106.71
22	P	305	CLA	CHB-C4A-NA	2.95	128.59	124.51
26	U	313	CHL	C1D-ND-C4D	-2.95	104.24	106.33
22	c	506	CLA	CHB-C4A-NA	2.95	128.59	124.51
24	g	309	XAT	C10-C11-C12	-2.95	114.01	123.22
26	s	313	CHL	C2D-C1D-ND	2.95	112.28	110.10
26	u	315	CHL	C3D-C4D-ND	2.95	115.01	110.24
24	P	312	XAT	C11-C10-C9	-2.95	123.10	127.31
31	B	619	BCR	C20-C21-C22	-2.95	123.10	127.31
22	c	508	CLA	CHB-C4A-NA	2.95	128.59	124.51
26	G	312	CHL	O2D-CGD-O1D	-2.95	118.07	123.84
26	U	315	CHL	O2A-CGA-CBA	2.95	121.16	111.91
26	q	312	CHL	C3B-C4B-NB	2.95	113.02	109.21
22	Q	308	CLA	CMB-C2B-C3B	2.95	130.19	124.68
26	1	317	CHL	O2D-CGD-O1D	-2.95	118.08	123.84
22	u	301	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
31	t	101	BCR	C20-C19-C18	-2.95	118.14	126.42
26	q	311	CHL	CMD-C2D-C3D	-2.95	120.84	127.61
32	a	413	SQD	O9-S-C6	2.95	110.44	106.94
22	1	308	CLA	CMB-C2B-C3B	2.94	130.19	124.68
26	4	314	CHL	C1B-CHB-C4A	-2.94	124.29	130.12
26	u	313	CHL	CMD-C2D-C3D	-2.94	120.84	127.61
26	S	314	CHL	CMD-C2D-C3D	-2.94	120.84	127.61
26	1	313	CHL	C1-C2-C3	-2.94	120.95	126.04
22	D	403	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
26	s	315	CHL	C4A-NA-C1A	2.94	108.03	106.71
22	C	507	CLA	CHB-C4A-NA	2.94	128.58	124.51
31	d	403	BCR	C30-C25-C24	2.94	124.10	115.78
22	2	305	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	3	302	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	q	308	CLA	CMB-C2B-C3B	2.94	130.18	124.68
23	1	309	LUT	C31-C30-C29	-2.94	123.11	127.31
22	u	308	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	n	305	CLA	CHB-C4A-NA	2.94	128.58	124.51
22	b	603	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
26	u	315	CHL	CAC-C3C-C4C	2.94	128.62	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	313	CHL	C2D-C1D-ND	2.94	112.27	110.10
26	q	312	CHL	CMD-C2D-C3D	-2.94	120.86	127.61
23	2	309	LUT	C30-C31-C32	-2.94	114.05	123.22
31	K	101	BCR	C33-C5-C4	2.94	119.26	113.62
26	6	312	CHL	CMD-C2D-C3D	-2.94	120.86	127.61
31	b	620	BCR	C15-C16-C17	-2.94	117.46	123.47
22	a	408	CLA	CHB-C4A-NA	2.94	128.57	124.51
26	v	315	CHL	CAC-C3C-C4C	2.94	128.62	124.81
22	3	306	CLA	CMB-C2B-C3B	2.94	130.17	124.68
22	s	306	CLA	CMB-C2B-C3B	2.94	130.17	124.68
26	p	319	CHL	C1C-C2C-C3C	-2.93	104.78	107.11
22	6	307	CLA	CMB-C2B-C3B	2.93	130.17	124.68
22	B	610	CLA	CMB-C2B-C3B	2.93	130.17	124.68
31	c	515	BCR	C23-C24-C25	-2.93	118.96	127.20
23	S	310	LUT	C35-C15-C14	-2.93	117.46	123.47
26	G	312	CHL	C2D-C1D-ND	2.93	112.27	110.10
24	N	311	XAT	C35-C34-C33	-2.93	123.12	127.31
22	2	307	CLA	CHB-C4A-NA	2.93	128.57	124.51
26	u	315	CHL	CMB-C2B-C3B	2.93	130.16	124.68
23	U	310	LUT	C38-C25-C24	-2.93	117.29	123.56
31	B	618	BCR	C21-C20-C19	-2.93	114.07	123.22
22	q	306	CLA	CMB-C2B-C3B	2.93	130.16	124.68
26	3	315	CHL	CAC-C3C-C4C	2.93	128.61	124.81
22	g	305	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	q	315	CHL	CAC-C3C-C4C	2.93	128.61	124.81
26	U	314	CHL	CAC-C3C-C4C	2.93	128.61	124.81
26	6	312	CHL	CHB-C4A-NA	2.93	128.56	124.51
22	r	607	CLA	CMB-C2B-C3B	2.93	130.16	124.68
22	a	406	CLA	CMB-C2B-C3B	2.93	130.16	124.68
22	N	307	CLA	CHB-C4A-NA	2.93	128.56	124.51
24	R	313	XAT	C10-C11-C12	-2.93	114.08	123.22
26	p	315	CHL	CHD-C4C-C3C	-2.93	120.54	124.84
26	p	316	CHL	C2D-C1D-ND	2.93	112.26	110.10
22	2	304	CLA	CMB-C2B-C3B	2.93	130.15	124.68
33	d	404	PL9	C42-C43-C44	-2.93	120.61	127.66
31	C	517	BCR	C23-C24-C25	-2.93	118.98	127.20
22	b	606	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
31	a	409	BCR	C20-C21-C22	-2.93	123.14	127.31
22	B	602	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	u	313	CHL	C1-C2-C3	-2.93	120.98	126.04
22	P	308	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
31	D	404	BCR	C30-C25-C24	2.92	124.05	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u	317	CHL	CHB-C4A-NA	2.92	128.55	124.51
26	Q	316	CHL	O2A-CGA-CBA	2.92	121.08	111.91
26	R	316	CHL	C3D-C4D-ND	2.92	114.97	110.24
22	4	308	CLA	CHB-C4A-NA	2.92	128.55	124.51
36	a	416	DGD	C3E-C4E-C5E	2.92	115.45	110.24
26	s	316	CHL	C4A-NA-C1A	2.92	108.02	106.71
22	R	306	CLA	CHB-C4A-NA	2.92	128.55	124.51
22	V	305	CLA	CMB-C2B-C3B	2.92	130.14	124.68
26	g	311	CHL	C1C-C2C-C3C	-2.92	104.80	107.11
26	P	314	CHL	O2A-CGA-CBA	2.92	121.06	111.91
36	c	518	DGD	O1G-C1A-C2A	2.92	121.06	111.91
22	r	603	CLA	CMB-C2B-C3B	2.92	130.14	124.68
26	r	616	CHL	C3D-C4D-ND	2.92	114.96	110.24
26	6	313	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
22	b	615	CLA	CHB-C4A-NA	2.92	128.54	124.51
33	d	404	PL9	C37-C38-C39	-2.92	120.64	127.66
22	u	307	CLA	CMB-C2B-C3B	2.92	130.13	124.68
22	S	306	CLA	CMB-C2B-C3B	2.92	130.13	124.68
22	r	605	CLA	CHB-C4A-NA	2.92	128.54	124.51
22	s	308	CLA	CMB-C2B-C3B	2.91	130.13	124.68
27	s	317	NEX	C17-C1-C6	-2.91	107.86	110.47
26	S	315	CHL	C4A-NA-C1A	2.91	108.02	106.71
22	6	302	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
22	G	303	CLA	CHB-C4A-NA	2.91	128.54	124.51
26	r	616	CHL	C2D-C1D-ND	2.91	112.25	110.10
33	D	405	PL9	C37-C38-C39	-2.91	120.65	127.66
22	A	406	CLA	CMB-C2B-C3B	2.91	130.12	124.68
31	t	101	BCR	C27-C26-C25	-2.91	118.50	122.73
22	r	607	CLA	CHB-C4A-NA	2.91	128.54	124.51
26	g	312	CHL	C3D-C4D-ND	2.91	114.95	110.24
26	Q	313	CHL	O2A-CGA-CBA	2.91	121.04	111.91
24	U	311	XAT	C10-C11-C12	-2.91	114.14	123.22
22	G	305	CLA	CHB-C4A-NA	2.91	128.54	124.51
22	b	602	CLA	CHB-C4A-NA	2.91	128.54	124.51
22	B	603	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
31	c	516	BCR	C8-C7-C6	-2.91	119.03	127.20
30	D	401	PHO	O2D-CGD-O1D	-2.91	118.15	123.84
22	B	605	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
22	1	307	CLA	CHB-C4A-NA	2.91	128.53	124.51
26	Q	311	CHL	CHB-C4A-NA	2.91	128.53	124.51
25	C	524	LHG	O8-C23-C24	2.91	121.03	111.91
22	4	308	CLA	CMB-C2B-C3B	2.91	130.11	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	315	CHL	C3B-C4B-NB	2.91	112.97	109.21
33	D	405	PL9	C42-C43-C44	-2.90	120.67	127.66
22	b	617	CLA	CHB-C4A-NA	2.90	128.53	124.51
22	2	304	CLA	CMA-C3A-C4A	-2.90	103.97	111.77
22	d	402	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
26	q	315	CHL	O2A-CGA-CBA	2.90	121.01	111.91
26	n	316	CHL	CMD-C2D-C3D	-2.90	120.94	127.61
26	V	317	CHL	C1C-C2C-C3C	-2.90	104.81	107.11
26	V	313	CHL	C1D-ND-C4D	-2.90	104.28	106.33
26	U	319	CHL	CMD-C2D-C3D	-2.90	120.95	127.61
26	Q	314	CHL	C3D-C4D-ND	2.90	114.92	110.24
26	R	317	CHL	CMD-C2D-C3D	-2.90	120.95	127.61
22	b	617	CLA	C2A-C1A-CHA	2.90	128.93	123.86
22	b	616	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
22	B	610	CLA	CHB-C4A-NA	2.90	128.52	124.51
31	b	620	BCR	C10-C11-C12	-2.90	114.18	123.22
22	G	308	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	R	306	CLA	CMB-C2B-C3B	2.90	130.10	124.68
26	2	313	CHL	CMD-C2D-C3D	-2.89	120.95	127.61
22	B	611	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	q	305	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	V	308	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	U	307	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
26	g	311	CHL	C4-C3-C5	2.89	120.14	115.27
26	N	315	CHL	O2A-CGA-CBA	2.89	120.98	111.91
26	U	314	CHL	O2A-CGA-CBA	2.89	120.98	111.91
26	N	313	CHL	CAC-C3C-C4C	2.89	128.56	124.81
26	1	318	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
22	b	610	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	g	314	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
26	g	312	CHL	O2A-CGA-CBA	2.89	120.98	111.91
22	b	605	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
26	N	314	CHL	O2A-CGA-CBA	2.89	120.98	111.91
27	v	319	NEX	C11-C12-C13	-2.89	118.30	126.42
22	r	603	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	B	613	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	r	609	CLA	CMB-C2B-C3B	2.89	130.08	124.68
22	b	613	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	3	312	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
26	S	315	CHL	C3B-C4B-NB	2.89	112.94	109.21
23	2	309	LUT	C10-C11-C12	-2.89	114.21	123.22
26	u	314	CHL	CMB-C2B-C3B	2.89	130.08	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	314	CHL	CMB-C2B-C3B	2.89	130.08	124.68
26	r	616	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
26	U	313	CHL	C1-C2-C3	-2.89	121.05	126.04
22	V	308	CLA	CHB-C4A-NA	2.89	128.50	124.51
22	B	611	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
26	5	313	CHL	C2D-C1D-ND	2.88	112.23	110.10
22	2	303	CLA	CHB-C4A-NA	2.88	128.50	124.51
22	b	611	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	g	308	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
30	d	401	PHO	O2D-CGD-O1D	-2.88	118.20	123.84
22	Q	306	CLA	CMB-C2B-C3B	2.88	130.07	124.68
26	P	314	CHL	CMD-C2D-C3D	-2.88	120.98	127.61
24	4	311	XAT	C27-C28-C29	-2.88	121.06	125.53
27	R	301	NEX	O24-C25-C38	2.88	118.51	115.06
31	B	618	BCR	C40-C30-C25	-2.88	105.63	110.30
22	B	606	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	4	313	CHL	C1-C2-C3	-2.88	121.06	126.04
22	5	303	CLA	CMB-C2B-C3B	2.88	130.06	124.68
22	A	408	CLA	CHB-C4A-NA	2.88	128.49	124.51
22	b	602	CLA	CMB-C2B-C3B	2.88	130.06	124.68
31	A	409	BCR	C30-C25-C26	-2.88	118.56	122.61
22	c	505	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	1	317	CHL	C1-O2A-CGA	2.88	123.99	116.44
26	G	316	CHL	CHB-C4A-NA	2.88	128.49	124.51
22	C	504	CLA	CHB-C4A-NA	2.88	128.49	124.51
26	U	315	CHL	CHB-C4A-NA	2.88	128.49	124.51
31	b	619	BCR	C33-C5-C4	2.88	119.14	113.62
22	3	307	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	u	310	LUT	C38-C25-C24	-2.87	117.41	123.56
36	C	520	DGD	O1G-C1A-C2A	2.87	120.93	111.91
22	v	303	CLA	CHB-C4A-NA	2.87	128.49	124.51
22	q	303	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
27	S	317	NEX	C39-C29-C30	-2.87	118.90	122.92
26	s	315	CHL	C3B-C4B-NB	2.87	112.92	109.21
26	1	313	CHL	C1B-CHB-C4A	-2.87	124.43	130.12
31	C	518	BCR	C8-C7-C6	-2.87	119.14	127.20
31	b	620	BCR	C30-C25-C24	2.87	123.90	115.78
31	c	516	BCR	C15-C16-C17	-2.87	117.59	123.47
26	6	313	CHL	O2A-CGA-CBA	2.87	120.92	111.91
26	1	317	CHL	CHB-C4A-NA	2.87	128.48	124.51
26	q	313	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
22	n	307	CLA	CHB-C4A-NA	2.87	128.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	314	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
22	4	305	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	1	305	CLA	CMB-C2B-C3B	2.87	130.05	124.68
32	a	413	SQD	O8-S-C6	2.87	110.31	105.74
22	n	308	CLA	CHB-C4A-NA	2.87	128.48	124.51
22	3	303	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
22	u	303	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
22	B	615	CLA	CHB-C4A-NA	2.87	128.48	124.51
22	b	611	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
31	C	518	BCR	C15-C16-C17	-2.87	117.60	123.47
23	V	310	LUT	C38-C25-C24	-2.87	117.43	123.56
26	5	313	CHL	C4A-NA-C1A	2.86	107.99	106.71
22	u	307	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	s	301	CLA	CHB-C4A-NA	2.86	128.47	124.51
26	u	314	CHL	O2D-CGD-O1D	-2.86	118.24	123.84
34	A	411	LMG	O8-C28-C29	2.86	120.90	111.91
22	b	617	CLA	O1D-CGD-CBD	2.86	130.34	124.48
22	P	304	CLA	CMB-C2B-C3B	2.86	130.04	124.68
26	G	312	CHL	C1C-C2C-C3C	-2.86	104.84	107.11
27	R	301	NEX	C28-C29-C30	2.86	123.33	118.94
23	S	310	LUT	C18-C5-C6	-2.86	121.31	124.53
26	g	312	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
22	g	304	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	P	310	LUT	C7-C8-C9	-2.86	121.92	126.23
22	5	307	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	B	612	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	g	301	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
26	4	313	CHL	C2D-C1D-ND	2.86	112.21	110.10
31	C	516	BCR	C27-C26-C25	-2.86	118.58	122.73
22	1	305	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	p	303	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	B	606	CLA	CHB-C4A-NA	2.86	128.46	124.51
26	n	314	CHL	O2A-CGA-CBA	2.86	120.87	111.91
26	U	314	CHL	CMB-C2B-C3B	2.86	130.02	124.68
25	L	101	LHG	O8-C23-C24	2.85	120.87	111.91
23	U	309	LUT	C15-C14-C13	-2.85	123.24	127.31
22	X	202	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	p	310	LUT	C3-C4-C5	-2.85	106.17	111.85
22	U	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	5	313	CHL	CMD-C2D-C3D	-2.85	121.05	127.61
23	N	309	LUT	C15-C14-C13	-2.85	123.24	127.31
23	R	312	LUT	C7-C8-C9	-2.85	121.93	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	307	CLA	CHB-C4A-NA	2.85	128.45	124.51
26	2	316	CHL	C1D-ND-C4D	-2.85	104.31	106.33
26	n	317	CHL	C1D-ND-C4D	-2.85	104.31	106.33
23	p	310	LUT	C31-C30-C29	-2.85	123.24	127.31
23	s	311	LUT	C35-C34-C33	-2.85	123.24	127.31
26	q	315	CHL	C1C-C2C-C3C	-2.85	104.85	107.11
26	4	313	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
26	p	315	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
26	6	314	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
26	q	313	CHL	O2A-CGA-CBA	2.85	120.85	111.91
22	R	311	CLA	CHB-C4A-NA	2.85	128.45	124.51
22	B	607	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
26	V	317	CHL	O2D-CGD-O1D	-2.85	118.27	123.84
22	v	306	CLA	CHB-C4A-NA	2.85	128.45	124.51
26	p	315	CHL	O2A-CGA-CBA	2.85	120.84	111.91
23	u	309	LUT	C16-C1-C6	-2.85	105.68	110.30
26	4	317	CHL	C1C-C2C-C3C	-2.85	104.86	107.11
26	Q	311	CHL	C1C-C2C-C3C	-2.85	104.86	107.11
26	p	316	CHL	CMD-C2D-C3D	-2.85	121.07	127.61
22	b	607	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
22	x	201	CLA	CHB-C4A-NA	2.85	128.45	124.51
22	n	307	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
22	b	612	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
26	6	315	CHL	C3D-C4D-ND	2.85	114.84	110.24
26	P	319	CHL	O2A-CGA-CBA	2.84	120.83	111.91
26	G	314	CHL	C3D-C4D-ND	2.84	114.84	110.24
31	X	201	BCR	C33-C5-C4	2.84	119.08	113.62
26	1	315	CHL	C2D-C1D-ND	2.84	112.20	110.10
22	V	307	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	4	310	LUT	C18-C5-C6	-2.84	121.33	124.53
26	3	312	CHL	C1C-C2C-C3C	-2.84	104.86	107.11
26	P	316	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
22	g	306	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
31	C	516	BCR	C10-C11-C12	-2.84	114.35	123.22
22	b	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	C	513	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	1	308	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	5	306	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	R	311	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	B	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	u	317	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
24	V	311	XAT	C27-C28-C29	-2.84	121.12	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	620	BCR	C15-C16-C17	-2.84	117.66	123.47
22	3	302	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	C	503	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	3	316	CHL	C1C-C2C-C3C	-2.84	104.86	107.11
23	P	310	LUT	C3-C4-C5	-2.84	106.20	111.85
26	V	317	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
26	n	315	CHL	O2A-CGA-CBA	2.84	120.81	111.91
22	c	512	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	v	314	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
31	D	404	BCR	C16-C17-C18	-2.84	123.26	127.31
27	u	319	NEX	C17-C1-C6	-2.84	107.93	110.47
26	n	318	CHL	CHD-C4C-C3C	-2.84	120.67	124.84
22	R	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	b	602	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	4	315	CHL	O2A-CGA-CBA	2.84	120.81	111.91
31	c	515	BCR	C11-C12-C13	-2.83	118.45	126.42
22	P	309	CLA	CMB-C2B-C3B	2.83	129.98	124.68
31	z	101	BCR	C33-C5-C6	-2.83	121.34	124.53
26	P	315	CHL	CHD-C1D-C2D	2.83	131.43	125.48
26	Q	311	CHL	C4-C3-C5	2.83	120.04	115.27
26	s	313	CHL	C1B-CHB-C4A	-2.83	124.50	130.12
22	P	304	CLA	CHB-C4A-NA	2.83	128.43	124.51
31	b	618	BCR	C30-C25-C26	-2.83	118.62	122.61
23	v	310	LUT	C3-C4-C5	-2.83	106.21	111.85
26	1	315	CHL	O2A-CGA-CBA	2.83	120.80	111.91
26	2	315	CHL	CMD-C2D-C3D	-2.83	121.10	127.61
34	a	412	LMG	O8-C28-C29	2.83	120.80	111.91
26	P	315	CHL	CMD-C2D-C3D	-2.83	121.10	127.61
26	r	619	CHL	CMB-C2B-C3B	2.83	129.98	124.68
22	N	302	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	p	312	XAT	C15-C14-C13	-2.83	123.27	127.31
22	V	302	CLA	CMB-C2B-C3B	2.83	129.97	124.68
25	C	522	LHG	O8-C23-C24	2.83	120.79	111.91
22	N	308	CLA	CMB-C2B-C3B	2.83	129.97	124.68
26	p	320	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
22	B	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	p	316	CHL	O2A-CGA-CBA	2.83	120.79	111.91
22	2	306	CLA	CHB-C4A-NA	2.83	128.42	124.51
26	4	316	CHL	O1D-CGD-CBD	-2.83	118.70	124.48
22	r	610	CLA	CMB-C2B-C3B	2.83	129.97	124.68
26	2	318	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
26	Q	311	CHL	CMD-C2D-C3D	-2.83	121.11	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	316	CHL	C1D-ND-C4D	-2.83	104.33	106.33
24	r	612	XAT	C4-C3-C2	-2.83	105.31	110.77
26	3	311	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
22	R	303	CLA	CHB-C4A-NA	2.83	128.42	124.51
22	2	308	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	4	305	CLA	CMB-C2B-C3B	2.83	129.97	124.68
26	p	318	CHL	CMB-C2B-C3B	2.83	129.97	124.68
22	b	606	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	S	311	LUT	C31-C30-C29	-2.83	123.28	127.31
22	C	515	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
22	5	305	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
32	A	412	SQD	C4-C3-C2	2.83	115.76	110.82
22	G	302	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	S	304	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	r	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	3	311	CHL	C1-C2-C3	-2.82	121.16	126.04
23	2	309	LUT	C7-C8-C9	-2.82	121.97	126.23
22	B	602	CLA	CMB-C2B-C3B	2.82	129.96	124.68
24	q	309	XAT	C10-C11-C12	-2.82	114.41	123.22
26	5	315	CHL	CHB-C4A-NA	2.82	128.41	124.51
26	6	314	CHL	C3B-C4B-NB	2.82	112.86	109.21
31	B	618	BCR	C15-C16-C17	-2.82	117.70	123.47
26	3	314	CHL	C3D-C4D-ND	2.82	114.80	110.24
22	r	610	CLA	CHB-C4A-NA	2.82	128.41	124.51
22	G	307	CLA	CHB-C4A-NA	2.82	128.41	124.51
26	n	314	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
31	a	409	BCR	C30-C25-C26	-2.82	118.64	122.61
26	2	313	CHL	C4-C3-C5	2.82	120.01	115.27
25	l	101	LHG	O8-C23-C24	2.82	120.75	111.91
22	2	301	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
26	v	317	CHL	CHB-C4A-NA	2.82	128.41	124.51
26	6	314	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
26	q	312	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
23	4	310	LUT	C18-C5-C4	2.82	119.57	114.36
22	p	309	CLA	CMB-C2B-C3B	2.82	129.95	124.68
26	r	614	CHL	CMD-C2D-C3D	-2.82	121.14	127.61
22	c	514	CLA	CAA-C2A-C3A	-2.82	105.07	112.78
22	u	302	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	g	313	CHL	CMD-C2D-C3D	-2.82	121.14	127.61
23	n	310	LUT	C38-C25-C24	-2.82	117.53	123.56
26	Q	316	CHL	C1B-CHB-C4A	-2.82	124.54	130.12
31	z	101	BCR	C10-C11-C12	-2.82	114.43	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	201	BCR	C33-C5-C6	-2.81	121.37	124.53
26	V	317	CHL	CHB-C4A-NA	2.81	128.40	124.51
22	Q	304	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	g	311	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
31	B	618	BCR	C30-C25-C26	-2.81	118.65	122.61
22	R	305	CLA	CHB-C4A-NA	2.81	128.40	124.51
22	r	601	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	Q	313	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
26	Q	316	CHL	C1C-C2C-C3C	-2.81	104.88	107.11
22	5	304	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
24	Q	309	XAT	C30-C31-C32	-2.81	114.45	123.22
31	x	202	BCR	C33-C5-C4	2.81	119.01	113.62
22	v	301	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
26	p	314	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
31	B	619	BCR	C33-C5-C4	2.81	119.01	113.62
26	6	312	CHL	C1-C2-C3	-2.81	121.19	126.04
26	Q	314	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
26	3	311	CHL	CAC-C3C-C4C	2.81	128.45	124.81
26	q	315	CHL	CMB-C2B-C3B	2.81	129.93	124.68
26	N	313	CHL	CMB-C2B-C3B	2.81	129.93	124.68
26	V	313	CHL	C1B-CHB-C4A	-2.81	124.56	130.12
26	n	317	CHL	C1B-CHB-C4A	-2.81	124.56	130.12
23	1	310	LUT	C31-C30-C29	-2.81	123.31	127.31
31	C	517	BCR	C11-C12-C13	-2.81	118.53	126.42
26	S	313	CHL	C1D-ND-C4D	-2.81	104.34	106.33
22	C	509	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	u	305	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
26	6	315	CHL	O2A-CGA-CBA	2.81	120.71	111.91
26	v	314	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
26	V	314	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
22	v	308	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	3	305	CLA	CMB-C2B-C3B	2.80	129.93	124.68
23	1	309	LUT	C38-C25-C24	-2.80	117.56	123.56
22	5	308	CLA	CMB-C2B-C3B	2.80	129.93	124.68
22	6	306	CLA	CMB-C2B-C3B	2.80	129.92	124.68
22	c	508	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	A	405	CLA	CMB-C2B-C3B	2.80	129.92	124.68
26	v	314	CHL	O2A-CGA-CBA	2.80	120.70	111.91
31	B	620	BCR	C30-C25-C24	2.80	123.71	115.78
22	V	306	CLA	CHB-C4A-NA	2.80	128.39	124.51
24	5	311	XAT	C10-C11-C12	-2.80	114.47	123.22
26	5	315	CHL	CMD-C2D-C3D	-2.80	121.17	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	303	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
25	c	522	LHG	O8-C23-C24	2.80	120.70	111.91
33	d	404	PL9	C40-C39-C41	2.80	119.98	115.27
26	4	316	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
26	v	317	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
22	Q	302	CLA	CMB-C2B-C3B	2.80	129.91	124.68
26	v	314	CHL	C1C-C2C-C3C	-2.80	104.89	107.11
26	5	314	CHL	CHD-C4C-C3C	-2.80	120.73	124.84
22	N	306	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	B	607	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	S	301	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	c	503	CLA	CHB-C4A-NA	2.80	128.38	124.51
26	u	315	CHL	C1D-ND-C4D	-2.80	104.35	106.33
22	v	305	CLA	CMB-C2B-C3B	2.80	129.91	124.68
31	d	403	BCR	C16-C17-C18	-2.80	123.32	127.31
26	4	314	CHL	C4D-CHA-C1A	-2.80	117.85	121.25
26	3	312	CHL	O2A-CGA-CBA	2.79	120.68	111.91
22	R	304	CLA	CHB-C4A-NA	2.79	128.38	124.51
26	5	314	CHL	CMB-C2B-C3B	2.79	129.91	124.68
22	p	304	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
26	S	314	CHL	CHB-C4A-NA	2.79	128.38	124.51
22	c	512	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
26	6	315	CHL	C2D-C1D-ND	2.79	112.16	110.10
26	P	316	CHL	C2D-C1D-ND	2.79	112.16	110.10
25	C	523	LHG	O8-C23-C24	2.79	120.67	111.91
26	1	317	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
22	U	305	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	B	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	6	307	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	R	315	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
26	1	314	CHL	C3D-C4D-ND	2.79	114.75	110.24
22	6	304	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	6	308	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	r	615	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
22	b	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	G	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	2	308	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	c	502	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	s	311	LUT	C31-C30-C29	-2.79	123.33	127.31
26	V	314	CHL	O2A-CGA-CBA	2.79	120.65	111.91
22	r	601	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	r	604	CLA	CHB-C4A-NA	2.79	128.37	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	r	602	CLA	CHB-C4A-NA	2.79	128.37	124.51
26	p	314	CHL	O2A-CGA-CBA	2.79	120.65	111.91
26	N	317	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
26	Q	316	CHL	CMB-C2B-C3B	2.79	129.89	124.68
22	G	304	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	U	311	XAT	C11-C10-C9	-2.79	123.33	127.31
22	N	304	CLA	CMA-C3A-C4A	-2.78	104.29	111.77
26	U	317	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
22	U	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
26	G	316	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
22	p	307	CLA	CHB-C4A-NA	2.78	128.36	124.51
22	B	614	CLA	CHB-C4A-NA	2.78	128.36	124.51
24	u	311	XAT	C31-C30-C29	-2.78	123.34	127.31
26	1	317	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
36	C	520	DGD	C4E-C3E-C2E	2.78	115.68	110.82
26	u	313	CHL	C1B-CHB-C4A	-2.78	124.61	130.12
26	v	315	CHL	O2A-CGA-CBA	2.78	120.64	111.91
26	G	313	CHL	C1C-C2C-C3C	-2.78	104.91	107.11
22	G	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
26	1	313	CHL	O2A-CGA-CBA	2.78	120.63	111.91
22	C	510	CLA	CMB-C2B-C3B	2.78	129.88	124.68
26	1	316	CHL	C1C-C2C-C3C	-2.78	104.91	107.11
22	b	604	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
26	G	315	CHL	C4-C3-C5	2.78	119.94	115.27
22	c	513	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	1	311	XAT	C11-C10-C9	-2.78	123.35	127.31
26	P	316	CHL	O2A-CGA-CBA	2.78	120.62	111.91
26	3	313	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
22	v	307	CLA	CHB-C4A-NA	2.78	128.35	124.51
22	q	308	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	5	302	CLA	CMB-C2B-C3B	2.78	129.87	124.68
27	U	318	NEX	C39-C29-C30	-2.77	119.04	122.92
26	P	318	CHL	CMB-C2B-C3B	2.77	129.87	124.68
26	V	317	CHL	CMB-C2B-C3B	2.77	129.87	124.68
26	s	315	CHL	CMD-C2D-C3D	-2.77	121.23	127.61
23	p	311	LUT	C31-C30-C29	-2.77	123.35	127.31
22	S	309	CLA	CMB-C2B-C3B	2.77	129.86	124.68
22	s	304	CLA	CMB-C2B-C3B	2.77	129.86	124.68
23	4	310	LUT	C31-C30-C29	-2.77	123.36	127.31
26	3	314	CHL	C2D-C1D-ND	2.77	112.15	110.10
26	2	314	CHL	CMD-C2D-C3D	-2.77	121.24	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	315	CHL	O2A-CGA-CBA	2.77	120.60	111.91
26	G	314	CHL	CMB-C2B-C3B	2.77	129.86	124.68
26	G	314	CHL	O2A-CGA-CBA	2.77	120.60	111.91
22	3	304	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	5	315	CHL	CMB-C2B-C3B	2.77	129.86	124.68
26	3	312	CHL	CHD-C4C-C3C	-2.77	120.77	124.84
23	s	310	LUT	C18-C5-C6	-2.77	121.42	124.53
22	P	304	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
26	3	311	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
22	b	607	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	r	616	CHL	CMB-C2B-C3B	2.77	129.86	124.68
22	G	304	CLA	CHB-C4A-NA	2.77	128.34	124.51
22	C	507	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
24	R	313	XAT	C4-C3-C2	-2.77	105.43	110.77
22	g	302	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
32	C	501	SQD	O8-S-C6	2.76	110.14	105.74
31	C	516	BCR	C33-C5-C6	-2.76	121.42	124.53
22	V	303	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	P	317	CHL	C1D-ND-C4D	-2.76	104.37	106.33
22	a	405	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	g	303	CLA	CHB-C4A-NA	2.76	128.33	124.51
24	N	311	XAT	C31-C30-C29	-2.76	123.37	127.31
23	2	310	LUT	C38-C25-C24	-2.76	117.65	123.56
36	B	601	DGD	O1G-C1A-C2A	2.76	120.58	111.91
22	Q	307	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	1	312	LHG	O8-C23-C24	2.76	120.58	111.91
26	5	315	CHL	O2A-CGA-CBA	2.76	120.58	111.91
26	g	316	CHL	CMD-C2D-C3D	-2.76	121.26	127.61
22	S	308	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	5	317	CHL	CMD-C2D-C3D	-2.76	121.26	127.61
22	v	302	CLA	CMB-C2B-C3B	2.76	129.84	124.68
26	1	315	CHL	CMD-C2D-C3D	-2.76	121.26	127.61
24	Q	309	XAT	C10-C11-C12	-2.76	114.60	123.22
22	C	513	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
22	R	308	CLA	CMB-C2B-C3B	2.76	129.84	124.68
24	4	311	XAT	C11-C12-C13	-2.76	118.66	126.42
26	g	312	CHL	O2D-CGD-O1D	-2.76	118.44	123.84
22	B	604	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
26	2	314	CHL	O2A-CGA-CBA	2.76	120.57	111.91
27	s	317	NEX	C39-C29-C30	-2.76	119.06	122.92
26	N	314	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
26	p	320	CHL	CMB-C2B-C3B	2.76	129.84	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	405	PL9	C40-C39-C41	2.76	119.91	115.27
22	R	303	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	p	309	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	q	305	CLA	CHB-C4A-NA	2.76	128.33	124.51
26	N	314	CHL	CMB-C2B-C3B	2.76	129.84	124.68
22	S	306	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	p	304	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	p	308	CLA	CHB-C4A-NA	2.76	128.33	124.51
27	2	319	NEX	C28-C29-C30	2.76	123.17	118.94
26	4	314	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
26	V	315	CHL	C2D-C1D-ND	2.76	112.14	110.10
26	G	313	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
31	x	202	BCR	C33-C5-C6	-2.76	121.43	124.53
22	S	302	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	s	308	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
26	V	314	CHL	O2D-CGD-O1D	-2.76	118.45	123.84
22	g	307	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	C	506	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
31	A	409	BCR	C23-C24-C25	-2.76	119.46	127.20
22	S	309	CLA	CHB-C4A-NA	2.76	128.32	124.51
36	b	601	DGD	O1G-C1A-C2A	2.76	120.56	111.91
22	2	304	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
22	C	514	CLA	CMB-C2B-C3B	2.76	129.83	124.68
26	v	318	CHL	C1C-C2C-C3C	-2.76	104.93	107.11
26	1	314	CHL	CMD-C2D-C3D	-2.76	121.28	127.61
24	u	311	XAT	C10-C11-C12	-2.76	114.62	123.22
22	B	608	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
31	k	101	BCR	C10-C11-C12	-2.76	114.62	123.22
22	g	307	CLA	CMB-C2B-C3B	2.75	129.83	124.68
26	R	316	CHL	CMB-C2B-C3B	2.75	129.83	124.68
26	P	317	CHL	C1C-C2C-C3C	-2.75	104.93	107.11
22	A	405	CLA	CHB-C4A-NA	2.75	128.32	124.51
26	n	314	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
22	3	303	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	V	305	CLA	CHB-C4A-NA	2.75	128.32	124.51
26	3	316	CHL	CMB-C2B-C3B	2.75	129.83	124.68
22	N	305	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
26	n	318	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
22	P	308	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	C	515	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	s	303	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	s	306	CLA	O2D-CGD-O1D	-2.75	118.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	u	306	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	2	303	CLA	CMB-C2B-C3B	2.75	129.82	124.68
22	c	506	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
22	c	509	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
22	C	505	CLA	CHB-C4A-NA	2.75	128.31	124.51
26	2	313	CHL	O2A-CGA-CBA	2.75	120.53	111.91
26	S	316	CHL	C2D-C1D-ND	2.75	112.13	110.10
26	2	317	CHL	CMD-C2D-C3D	-2.75	121.29	127.61
26	P	314	CHL	CMB-C2B-C3B	2.75	129.82	124.68
22	v	303	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	u	316	CHL	C4-C3-C5	2.75	119.89	115.27
22	3	306	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	R	309	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
26	u	318	CHL	C1C-C2C-C3C	-2.75	104.94	107.11
23	5	309	LUT	C30-C31-C32	-2.75	114.65	123.22
22	N	307	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
25	r	613	LHG	O8-C23-C24	2.74	120.52	111.91
25	6	311	LHG	O8-C23-C24	2.74	120.52	111.91
22	P	303	CLA	CHB-C4A-NA	2.74	128.31	124.51
26	V	314	CHL	CAA-C2A-C3A	-2.74	105.27	112.78
31	a	409	BCR	C21-C20-C19	-2.74	114.66	123.22
26	r	614	CHL	OMC-CMC-C2C	-2.74	119.49	125.69
26	R	315	CHL	OMC-CMC-C2C	-2.74	119.49	125.69
27	n	319	NEX	C11-C12-C13	-2.74	118.72	126.42
26	5	318	CHL	CMB-C2B-C3B	2.74	129.81	124.68
22	C	510	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	4	304	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	5	314	CHL	O2A-CGA-CBA	2.74	120.50	111.91
22	6	304	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	p	307	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
26	P	315	CHL	CMB-C2B-C3B	2.74	129.80	124.68
23	S	310	LUT	C16-C1-C6	-2.74	105.86	110.30
22	B	607	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
23	v	310	LUT	C15-C35-C34	-2.74	117.87	123.47
22	p	303	CLA	CMB-C2B-C3B	2.74	129.80	124.68
22	V	304	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	v	314	CHL	CMB-C2B-C3B	2.74	129.80	124.68
26	p	316	CHL	CMB-C2B-C3B	2.74	129.80	124.68
23	5	310	LUT	C38-C25-C24	-2.74	117.70	123.56
26	4	315	CHL	CMD-C2D-C3D	-2.74	121.32	127.61
22	u	302	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	1	317	CHL	CMB-C2B-C3B	2.73	129.79	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	313	CHL	C4-C3-C5	2.73	119.87	115.27
26	4	316	CHL	C1C-C2C-C3C	-2.73	104.94	107.11
22	6	305	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	4	316	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
26	S	315	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
26	N	316	CHL	O2A-CGA-CBA	2.73	120.48	111.91
22	v	306	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	s	316	CHL	C2D-C1D-ND	2.73	112.12	110.10
22	c	504	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	v	310	LUT	C31-C30-C29	-2.73	123.41	127.31
26	G	312	CHL	CMB-C2B-C3B	2.73	129.79	124.68
26	g	312	CHL	CMB-C2B-C3B	2.73	129.79	124.68
26	V	313	CHL	C1-C2-C3	-2.73	121.32	126.04
26	2	315	CHL	CMB-C2B-C3B	2.73	129.79	124.68
26	2	314	CHL	C3B-C4B-NB	2.73	112.74	109.21
23	1	310	LUT	C38-C25-C24	-2.73	117.72	123.56
26	Q	315	CHL	CHB-C4A-NA	2.73	128.29	124.51
22	G	307	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	p	320	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
26	R	317	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
26	2	315	CHL	O2A-CGA-CBA	2.73	120.47	111.91
26	r	616	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
22	6	307	CLA	CHB-C4A-NA	2.73	128.28	124.51
26	U	314	CHL	CHB-C4A-NA	2.73	128.28	124.51
22	q	307	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
22	U	306	CLA	CHB-C4A-NA	2.73	128.28	124.51
22	4	303	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
27	u	319	NEX	C11-C12-C13	-2.72	118.76	126.42
26	6	314	CHL	CMB-C2B-C3B	2.72	129.78	124.68
22	G	301	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	s	302	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	3	306	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	R	302	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	s	309	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
27	n	319	NEX	C15-C35-C34	-2.72	117.89	123.47
22	c	507	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	2	314	CHL	CMB-C2B-C3B	2.72	129.77	124.68
26	v	317	CHL	C1C-C2C-C3C	-2.72	104.95	107.11
24	Q	309	XAT	C35-C15-C14	-2.72	117.90	123.47
22	P	309	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	3	316	CHL	CHB-C4A-NA	2.72	128.28	124.51
26	3	312	CHL	CMB-C2B-C3B	2.72	129.77	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	v	312	LHG	O8-C23-C24	2.72	120.45	111.91
22	c	509	CLA	CMB-C2B-C3B	2.72	129.77	124.68
26	u	315	CHL	O2A-CGA-CBA	2.72	120.45	111.91
22	s	309	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	5	318	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
27	V	319	NEX	C24-C23-C22	-2.72	105.52	110.77
22	1	305	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	c	514	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	Q	312	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
22	C	508	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	N	317	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
22	3	301	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
26	r	615	CHL	CMB-C2B-C3B	2.72	129.77	124.68
26	4	313	CHL	C1B-CHB-C4A	-2.72	124.73	130.12
27	V	319	NEX	C11-C12-C13	-2.72	118.78	126.42
22	6	308	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	u	317	CHL	C1-C2-C3	-2.72	121.34	126.04
26	Q	312	CHL	O2A-CGA-CBA	2.72	120.44	111.91
22	q	302	CLA	CMB-C2B-C3B	2.72	129.76	124.68
24	4	311	XAT	C15-C35-C34	-2.72	117.91	123.47
22	v	304	CLA	CHB-C4A-NA	2.72	128.27	124.51
27	r	618	NEX	C17-C1-C6	-2.72	108.04	110.47
26	2	316	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
24	u	311	XAT	C15-C35-C34	-2.72	117.91	123.47
27	R	301	NEX	C24-C23-C22	-2.72	105.53	110.77
22	B	616	CLA	CMB-C2B-C3B	2.72	129.76	124.68
22	1	304	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	u	314	CHL	CHB-C4A-NA	2.72	128.27	124.51
34	d	407	LMG	O8-C28-C29	2.72	120.43	111.91
22	V	305	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	6	304	CLA	CHB-C4A-NA	2.71	128.27	124.51
22	R	306	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	3	302	CLA	O2A-CGA-O1A	-2.71	116.74	123.59
26	p	320	CHL	O2A-CGA-CBA	2.71	120.42	111.91
22	r	601	CLA	CMB-C2B-C3B	2.71	129.75	124.68
22	3	307	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	4	301	CLA	CHB-C4A-NA	2.71	128.26	124.51
31	K	101	BCR	C10-C11-C12	-2.71	114.75	123.22
26	5	313	CHL	O2A-CGA-CBA	2.71	120.42	111.91
26	R	316	CHL	CMD-C2D-C3D	-2.71	121.38	127.61
26	Q	311	CHL	O2A-CGA-CBA	2.71	120.42	111.91
26	G	315	CHL	O2A-CGA-CBA	2.71	120.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	318	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
22	p	302	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
22	A	404	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
33	d	404	PL9	C53-C6-C1	2.71	120.53	114.99
26	s	314	CHL	CMB-C2B-C3B	2.71	129.75	124.68
26	5	316	CHL	C1D-ND-C4D	-2.71	104.41	106.33
32	A	412	SQD	O8-S-C6	2.71	110.06	105.74
22	2	305	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
32	m	101	SQD	O5-C5-C4	2.71	114.61	109.69
25	R	314	LHG	O8-C23-C24	2.71	120.41	111.91
26	U	313	CHL	C1C-C2C-C3C	-2.71	104.97	107.11
22	v	305	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	5	304	CLA	CMA-C3A-C4A	-2.71	104.50	111.77
23	1	309	LUT	C35-C34-C33	-2.71	123.45	127.31
22	2	307	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	4	303	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	n	306	CLA	CHB-C4A-NA	2.71	128.25	124.51
26	P	318	CHL	CMD-C2D-C3D	-2.71	121.39	127.61
26	G	316	CHL	C1C-C2C-C3C	-2.71	104.97	107.11
22	S	303	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	6	303	CLA	CMB-C2B-C3B	2.70	129.74	124.68
31	b	619	BCR	C30-C25-C26	-2.70	118.80	122.61
26	n	313	CHL	CHB-C4A-NA	2.70	128.25	124.51
26	6	301	CHL	CMB-C2B-C3B	2.70	129.74	124.68
26	2	317	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
26	6	317	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
22	B	617	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	R	313	XAT	C30-C31-C32	-2.70	114.78	123.22
26	6	312	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
26	N	315	CHL	C1D-ND-C4D	-2.70	104.42	106.33
22	1	301	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
23	p	311	LUT	C38-C25-C24	-2.70	117.78	123.56
22	3	308	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
22	1	306	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	r	605	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
26	Q	312	CHL	C1D-ND-C4D	-2.70	104.42	106.33
22	V	302	CLA	CHB-C4A-NA	2.70	128.25	124.51
33	D	405	PL9	C53-C6-C1	2.70	120.51	114.99
26	n	317	CHL	CMD-C2D-C3D	-2.70	121.40	127.61
22	Q	306	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
22	a	405	CLA	CMB-C2B-C3B	2.70	129.73	124.68
26	g	314	CHL	O2A-CGA-CBA	2.70	120.38	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	302	CLA	CMB-C2B-C3B	2.70	129.73	124.68
22	G	305	CLA	O2D-CGD-CBD	2.70	116.06	111.27
34	D	408	LMG	O8-C28-C29	2.70	120.38	111.91
24	U	311	XAT	C15-C35-C34	-2.70	117.94	123.47
26	p	319	CHL	C4-C3-C5	2.70	119.81	115.27
22	b	616	CLA	CMB-C2B-C3B	2.70	129.73	124.68
25	c	521	LHG	O8-C23-C24	2.70	120.37	111.91
26	P	317	CHL	O2A-CGA-CBA	2.70	120.37	111.91
22	b	607	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
22	U	307	CLA	CHB-C4A-NA	2.70	128.24	124.51
22	C	514	CLA	CHB-C4A-NA	2.70	128.24	124.51
22	c	513	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	1	318	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
26	P	316	CHL	CMB-C2B-C3B	2.69	129.72	124.68
22	4	306	CLA	CHB-C4A-NA	2.69	128.24	124.51
26	g	315	CHL	CHB-C4A-NA	2.69	128.24	124.51
26	s	314	CHL	CHB-C4A-NA	2.69	128.24	124.51
22	Q	303	CLA	CMB-C2B-C3B	2.69	129.72	124.68
26	S	314	CHL	CMB-C2B-C3B	2.69	129.72	124.68
22	5	304	CLA	C1-C2-C3	-2.69	121.39	126.04
22	b	608	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
24	r	612	XAT	C39-C29-C28	2.69	122.32	118.08
27	p	301	NEX	C17-C1-C6	-2.69	108.06	110.47
26	Q	314	CHL	O2A-CGA-CBA	2.69	120.36	111.91
22	G	306	CLA	CMB-C2B-C3B	2.69	129.72	124.68
31	t	101	BCR	C11-C12-C13	-2.69	118.85	126.42
24	v	311	XAT	C10-C11-C12	-2.69	114.82	123.22
23	v	310	LUT	C38-C25-C24	-2.69	117.80	123.56
26	P	315	CHL	O2A-CGA-CBA	2.69	120.35	111.91
22	u	308	CLA	CMB-C2B-C3B	2.69	129.71	124.68
26	g	313	CHL	CMB-C2B-C3B	2.69	129.71	124.68
32	M	101	SQD	O5-C5-C4	2.69	114.58	109.69
22	Q	307	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	S	312	LHG	O8-C23-C24	2.69	120.35	111.91
25	s	312	LHG	O8-C23-C24	2.69	120.35	111.91
22	N	304	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
26	V	318	CHL	O2A-CGA-CBA	2.69	120.35	111.91
26	s	315	CHL	O2A-CGA-CBA	2.69	120.35	111.91
31	T	101	BCR	C30-C25-C24	2.69	123.39	115.78
22	A	406	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	q	307	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	b	614	CLA	CHB-C4A-NA	2.69	128.23	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	311	XAT	C11-C12-C13	-2.69	118.86	126.42
22	p	304	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	p	316	CHL	C4A-NA-C1A	2.69	107.92	106.71
26	5	315	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
26	4	314	CHL	CMB-C2B-C3B	2.69	129.71	124.68
26	U	317	CHL	CMB-C2B-C3B	2.69	129.71	124.68
26	S	315	CHL	O2A-CGA-CBA	2.69	120.34	111.91
22	V	306	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	n	316	CHL	C2A-C3A-C4A	-2.69	97.53	101.87
22	u	303	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	s	307	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	u	318	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
22	1	303	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
22	B	608	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
26	V	313	CHL	O2A-CGA-CBA	2.69	120.34	111.91
31	A	409	BCR	C21-C20-C19	-2.69	114.83	123.22
22	a	404	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	Q	305	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
26	u	316	CHL	C4D-CHA-C1A	-2.68	117.98	121.25
22	a	406	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	u	313	CHL	O2A-CGA-CBA	2.68	120.33	111.91
23	s	311	LUT	C18-C5-C6	-2.68	121.52	124.53
26	p	315	CHL	CMB-C2B-C3B	2.68	129.70	124.68
26	P	314	CHL	C1D-ND-C4D	-2.68	104.43	106.33
26	N	316	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
26	p	317	CHL	C1C-C2C-C3C	-2.68	104.98	107.11
26	6	313	CHL	CHD-C4C-C3C	-2.68	120.90	124.84
26	5	316	CHL	O2A-CGA-CBA	2.68	120.32	111.91
22	v	306	CLA	CMB-C2B-C3B	2.68	129.69	124.68
26	v	316	CHL	CMB-C2B-C3B	2.68	129.69	124.68
26	Q	314	CHL	CMB-C2B-C3B	2.68	129.69	124.68
22	S	309	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	B	603	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	6	313	CHL	C1C-C2C-C3C	-2.68	104.99	107.11
26	V	318	CHL	CMB-C2B-C3B	2.68	129.69	124.68
26	u	314	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
26	6	317	CHL	C4-C3-C5	2.68	119.78	115.27
26	p	317	CHL	O2A-CGA-CBA	2.68	120.31	111.91
26	r	619	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
31	x	202	BCR	C27-C26-C25	-2.68	118.84	122.73
31	X	201	BCR	C27-C26-C25	-2.68	118.84	122.73
26	2	316	CHL	O2A-CGA-CBA	2.68	120.31	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Q	312	CHL	CMB-C2B-C3B	2.68	129.69	124.68
26	V	315	CHL	CMD-C2D-C3D	-2.68	121.46	127.61
26	g	311	CHL	C1B-CHB-C4A	-2.68	124.82	130.12
22	q	303	CLA	CHB-C4A-NA	2.68	128.21	124.51
26	3	316	CHL	C4-C3-C5	2.68	119.77	115.27
31	T	101	BCR	C11-C12-C13	-2.67	118.90	126.42
22	S	301	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
26	4	317	CHL	CMD-C2D-C3D	-2.67	121.46	127.61
26	N	314	CHL	OMC-CMC-C2C	-2.67	119.64	125.69
22	P	303	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
27	R	301	NEX	C11-C12-C13	-2.67	118.91	126.42
22	N	308	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	G	308	CLA	CHB-C4A-NA	2.67	128.21	124.51
26	6	313	CHL	CMB-C2B-C3B	2.67	129.68	124.68
33	d	404	PL9	C20-C19-C21	2.67	119.77	115.27
22	v	305	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	q	306	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	P	311	LUT	C11-C10-C9	-2.67	123.50	127.31
26	v	316	CHL	O2A-CGA-CBA	2.67	120.29	111.91
22	S	307	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
26	U	316	CHL	CMB-C2B-C3B	2.67	129.68	124.68
26	G	312	CHL	O2A-CGA-CBA	2.67	120.29	111.91
22	q	304	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
26	n	314	CHL	C3B-C4B-NB	2.67	112.66	109.21
23	4	310	LUT	C38-C25-C24	-2.67	117.84	123.56
22	R	310	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	V	310	LUT	C31-C30-C29	-2.67	123.50	127.31
26	R	315	CHL	C4-C3-C5	2.67	119.76	115.27
26	4	313	CHL	CMB-C2B-C3B	2.67	129.67	124.68
23	5	309	LUT	C3-C4-C5	-2.67	106.53	111.85
22	n	301	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
26	V	316	CHL	O2A-CGA-CBA	2.67	120.28	111.91
23	r	611	LUT	C18-C5-C6	-2.67	121.53	124.53
22	G	302	CLA	CMB-C2B-C3B	2.67	129.67	124.68
26	p	318	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
26	4	316	CHL	CMB-C2B-C3B	2.67	129.67	124.68
22	c	513	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
26	6	316	CHL	CHB-C4A-NA	2.67	128.20	124.51
31	t	101	BCR	C30-C25-C24	2.67	123.32	115.78
26	r	614	CHL	CMB-C2B-C3B	2.67	129.67	124.68
22	6	309	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
31	a	409	BCR	C16-C15-C14	-2.67	118.01	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	602	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
31	a	409	BCR	C23-C24-C25	-2.67	119.72	127.20
22	P	304	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
26	v	313	CHL	O2A-CGA-CBA	2.66	120.27	111.91
31	A	409	BCR	C16-C15-C14	-2.66	118.02	123.47
24	6	310	XAT	C31-C30-C29	-2.66	123.51	127.31
33	a	411	PL9	C6-C1-C2	2.66	119.85	117.13
26	2	315	CHL	C1B-CHB-C4A	-2.66	124.84	130.12
24	Q	309	XAT	C6-C7-C8	-2.66	120.36	125.99
26	U	313	CHL	O2A-CGA-CBA	2.66	120.27	111.91
22	n	304	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
23	U	309	LUT	C16-C1-C6	-2.66	105.98	110.30
23	2	310	LUT	C15-C14-C13	-2.66	123.51	127.31
22	r	606	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	u	315	CHL	CHB-C4A-NA	2.66	128.19	124.51
26	4	313	CHL	O2A-CGA-CBA	2.66	120.26	111.91
27	v	319	NEX	C28-C29-C30	2.66	123.03	118.94
26	u	313	CHL	C4-C3-C5	2.66	119.75	115.27
23	2	309	LUT	C35-C15-C14	-2.66	118.02	123.47
33	A	410	PL9	C6-C1-C2	2.66	119.84	117.13
23	S	311	LUT	C18-C5-C6	-2.66	121.54	124.53
23	N	310	LUT	C38-C25-C24	-2.66	117.87	123.56
22	v	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	S	307	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	v	303	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
22	r	604	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	5	301	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	q	304	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	g	311	CHL	O2A-CGA-CBA	2.66	120.25	111.91
22	g	301	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	R	307	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	U	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	s	306	CLA	CHB-C4A-NA	2.66	128.19	124.51
32	a	413	SQD	C4-C3-C2	2.66	115.46	110.82
26	R	316	CHL	C4-C3-C5	2.66	119.74	115.27
22	g	306	CLA	CMB-C2B-C3B	2.66	129.65	124.68
32	a	410	SQD	O8-S-C6	2.66	109.97	105.74
22	R	302	CLA	O2A-CGA-O1A	-2.66	116.89	123.59
26	U	315	CHL	C4-C3-C5	2.65	119.74	115.27
22	1	301	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	s	301	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
26	N	317	CHL	C1D-ND-C4D	-2.65	104.45	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	314	CHL	CAA-C2A-C3A	-2.65	105.51	112.78
27	P	301	NEX	C24-C23-C22	-2.65	105.65	110.77
31	B	619	BCR	C30-C25-C26	-2.65	118.88	122.61
22	V	303	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
26	G	314	CHL	CMD-C2D-C3D	-2.65	121.51	127.61
26	G	313	CHL	O2A-CGA-CBA	2.65	120.23	111.91
22	g	308	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	G	311	CHL	O2A-CGA-CBA	2.65	120.23	111.91
26	v	315	CHL	C1D-ND-C4D	-2.65	104.45	106.33
27	r	617	NEX	C4-C3-C2	-2.65	105.66	110.77
27	r	617	NEX	C17-C1-C6	-2.65	108.10	110.47
22	r	606	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	U	308	CLA	CMB-C2B-C3B	2.65	129.63	124.68
22	2	302	CLA	CMB-C2B-C3B	2.65	129.63	124.68
22	p	302	CLA	CHB-C4A-NA	2.65	128.17	124.51
22	1	306	CLA	CMB-C2B-C3B	2.65	129.63	124.68
30	a	407	PHO	O1D-CGD-CBD	2.65	129.15	124.74
22	b	603	CLA	CHB-C4A-NA	2.65	128.17	124.51
27	p	301	NEX	C24-C23-C22	-2.65	105.67	110.77
23	u	309	LUT	C38-C25-C24	-2.64	117.90	123.56
22	2	301	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
27	U	318	NEX	C26-C27-C28	-2.64	120.40	125.99
27	v	319	NEX	C24-C23-C22	-2.64	105.67	110.77
22	2	305	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
26	R	317	CHL	CMB-C2B-C3B	2.64	129.62	124.68
26	p	319	CHL	CMB-C2B-C3B	2.64	129.62	124.68
25	U	312	LHG	O8-C23-C24	2.64	120.20	111.91
26	1	314	CHL	CMB-C2B-C3B	2.64	129.62	124.68
26	u	317	CHL	CMB-C2B-C3B	2.64	129.62	124.68
22	1	303	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	5	316	CHL	CMB-C2B-C3B	2.64	129.61	124.68
22	1	306	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
27	5	319	NEX	C24-C23-C22	-2.64	105.68	110.77
27	N	318	NEX	C24-C23-C22	-2.64	105.68	110.77
26	g	316	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
36	c	518	DGD	C4E-C3E-C2E	2.64	115.43	110.82
22	P	307	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
32	a	413	SQD	C44-O6-C1	2.64	118.89	113.74
31	d	403	BCR	C1-C6-C7	2.64	123.24	115.78
26	q	315	CHL	C4-C3-C5	2.64	119.71	115.27
25	2	312	LHG	O8-C23-C24	2.64	120.18	111.91
25	3	310	LHG	O8-C23-C24	2.64	120.18	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	s	307	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
26	1	314	CHL	O2D-CGD-O1D	-2.64	118.69	123.84
26	q	312	CHL	CMB-C2B-C3B	2.64	129.61	124.68
22	5	302	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	n	315	CHL	C1D-ND-C4D	-2.64	104.46	106.33
22	r	609	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
22	P	304	CLA	C1-C2-C3	-2.63	122.49	126.75
22	r	602	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
26	4	314	CHL	O2A-CGA-CBA	2.63	120.17	111.91
26	U	313	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
26	4	316	CHL	CHB-C4A-NA	2.63	128.15	124.51
22	S	306	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	R	307	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	5	316	CHL	C1B-CHB-C4A	-2.63	124.91	130.12
23	5	309	LUT	C10-C11-C12	-2.63	115.01	123.22
23	s	311	LUT	C10-C11-C12	-2.63	115.01	123.22
22	U	308	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	4	315	CHL	C2D-C1D-ND	2.63	112.04	110.10
22	s	304	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	4	302	CLA	CMB-C2B-C3B	2.63	129.60	124.68
22	n	303	CLA	C1-C2-C3	-2.63	122.50	126.75
22	v	301	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	q	302	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	b	610	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
26	s	315	CHL	C2D-C1D-ND	2.63	112.04	110.10
26	n	317	CHL	O2A-CGA-CBA	2.63	120.15	111.91
22	1	303	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	Q	308	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
25	5	312	LHG	O8-C23-C24	2.63	120.15	111.91
22	3	302	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
26	3	314	CHL	CMB-C2B-C3B	2.62	129.59	124.68
22	5	305	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	6	309	CLA	CHB-C4A-NA	2.62	128.14	124.51
25	b	623	LHG	O8-C23-C24	2.62	120.14	111.91
26	g	314	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
23	s	311	LUT	C3-C4-C5	-2.62	106.63	111.85
26	p	314	CHL	CMB-C2B-C3B	2.62	129.59	124.68
22	q	301	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
22	U	302	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	4	301	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
22	N	301	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
22	s	302	CLA	CHB-C4A-NA	2.62	128.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	314	CHL	CHD-C4C-C3C	-2.62	120.99	124.84
22	c	511	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	P	311	LUT	C38-C25-C24	-2.62	117.95	123.56
22	S	304	CLA	CHB-C4A-NA	2.62	128.13	124.51
27	5	319	NEX	C35-C15-C14	-2.62	118.11	123.47
22	s	308	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	S	306	CLA	C2D-C1D-ND	-2.62	108.17	110.10
22	b	608	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	B	623	LHG	O8-C23-C24	2.62	120.12	111.91
26	G	316	CHL	CMB-C2B-C3B	2.62	129.58	124.68
22	S	302	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	C	512	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
26	V	314	CHL	C3D-C4D-ND	2.62	114.47	110.24
23	4	310	LUT	C11-C10-C9	-2.62	123.58	127.31
22	c	505	CLA	CMB-C2B-C3B	2.62	129.57	124.68
22	B	610	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
22	s	306	CLA	C2D-C1D-ND	-2.62	108.18	110.10
26	N	316	CHL	CMB-C2B-C3B	2.62	129.57	124.68
22	U	303	CLA	CHB-C4A-NA	2.61	128.13	124.51
24	6	310	XAT	C10-C11-C12	-2.61	115.06	123.22
22	4	305	CLA	CHB-C4A-NA	2.61	128.13	124.51
26	2	316	CHL	CMB-C2B-C3B	2.61	129.57	124.68
26	2	318	CHL	CMB-C2B-C3B	2.61	129.57	124.68
26	2	315	CHL	CAC-C3C-C4C	2.61	128.20	124.81
22	C	514	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
23	5	310	LUT	C15-C14-C13	-2.61	123.58	127.31
22	N	305	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	u	317	CHL	O1D-CGD-CBD	-2.61	119.14	124.48
22	P	302	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	R	302	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	N	316	CHL	CHB-C4A-NA	2.61	128.12	124.51
22	d	402	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
22	R	308	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
26	n	318	CHL	O2A-CGA-CBA	2.61	120.09	111.91
22	3	301	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
26	u	316	CHL	CAA-CBA-CGA	-2.61	105.63	113.25
26	S	313	CHL	C1B-CHB-C4A	-2.61	124.95	130.12
26	N	313	CHL	O2A-CGA-CBA	2.61	120.09	111.91
26	G	311	CHL	C1-C2-C3	-2.61	121.53	126.04
26	6	315	CHL	CMB-C2B-C3B	2.61	129.55	124.68
26	U	316	CHL	C1-C2-C3	-2.61	121.54	126.04
25	u	312	LHG	O8-C23-C24	2.61	120.08	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	603	CLA	CMB-C2B-C3B	2.61	129.55	124.68
22	n	306	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	N	310	LUT	C18-C5-C4	2.60	119.18	114.36
22	P	302	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	5	306	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	S	308	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	g	314	CHL	C3D-C4D-ND	2.60	114.44	110.24
26	6	301	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	S	314	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	N	315	CHL	CMD-C2D-C3D	-2.60	121.63	127.61
23	p	311	LUT	C35-C34-C33	-2.60	123.60	127.31
26	Q	314	CHL	C1D-ND-C4D	-2.60	104.49	106.33
22	N	301	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	D	404	BCR	C1-C6-C7	2.60	123.13	115.78
26	U	314	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
26	G	316	CHL	O2A-CGA-CBA	2.60	120.06	111.91
23	v	309	LUT	C38-C25-C24	-2.60	118.00	123.56
22	R	303	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
26	n	316	CHL	CMB-C2B-C3B	2.60	129.54	124.68
22	5	307	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	V	312	LHG	O8-C23-C24	2.60	120.06	111.91
26	1	316	CHL	O1D-CGD-CBD	-2.60	119.17	124.48
36	B	601	DGD	O6E-C5E-C4E	2.60	114.41	109.69
22	2	306	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
26	1	313	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	s	315	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
22	v	307	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	Q	305	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	U	305	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	1	313	CHL	C1D-ND-C4D	-2.59	104.49	106.33
24	r	612	XAT	C35-C34-C33	-2.59	123.61	127.31
26	3	314	CHL	O2A-CGA-CBA	2.59	120.05	111.91
26	Q	315	CHL	O2A-CGA-CBA	2.59	120.05	111.91
27	r	617	NEX	C11-C12-C13	-2.59	119.13	126.42
26	r	616	CHL	C4-C3-C5	2.59	119.63	115.27
26	V	314	CHL	CMB-C2B-C3B	2.59	129.53	124.68
26	g	313	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
22	C	515	CLA	CBA-CAA-C2A	2.59	121.51	113.86
26	g	315	CHL	CMD-C2D-C3D	-2.59	121.65	127.61
22	r	606	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
32	a	413	SQD	C1-O5-C5	2.59	118.78	113.69
23	S	311	LUT	C3-C4-C5	-2.59	106.69	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	405	PL9	C20-C19-C21	2.59	119.63	115.27
22	5	307	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
22	5	308	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	G	306	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
23	S	310	LUT	C15-C14-C13	-2.59	123.62	127.31
32	m	101	SQD	O48-C23-C24	2.59	120.03	111.91
22	4	302	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	G	303	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
22	A	408	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
22	r	608	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
36	C	519	DGD	O1G-C1A-C2A	2.59	120.03	111.91
22	D	403	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
22	C	506	CLA	CMB-C2B-C3B	2.59	129.52	124.68
25	4	312	LHG	O8-C23-C24	2.59	120.02	111.91
26	v	318	CHL	O2A-CGA-CBA	2.59	120.02	111.91
32	l	102	SQD	O6-C1-C2	2.59	112.34	108.30
27	P	301	NEX	C2-C1-C6	2.58	111.72	109.21
26	5	316	CHL	C1C-C2C-C3C	-2.58	105.06	107.11
22	6	303	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
30	A	407	PHO	O1D-CGD-CBD	2.58	129.04	124.74
31	c	516	BCR	C33-C5-C6	-2.58	121.63	124.53
36	c	517	DGD	O1G-C1A-C2A	2.58	120.01	111.91
22	d	402	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	3	313	CHL	C2D-C1D-ND	2.58	112.01	110.10
22	1	308	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
22	6	303	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	G	306	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
26	p	319	CHL	CMD-C2D-C3D	-2.58	121.68	127.61
26	v	318	CHL	C1D-ND-C4D	-2.58	104.50	106.33
26	v	318	CHL	CMB-C2B-C3B	2.58	129.50	124.68
22	A	404	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
22	N	303	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
22	v	308	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
27	S	317	NEX	C24-C23-C22	-2.58	105.79	110.77
32	M	101	SQD	O48-C23-C24	2.58	120.00	111.91
26	V	316	CHL	CMB-C2B-C3B	2.58	129.50	124.68
22	c	510	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	n	310	LUT	C18-C5-C6	-2.58	121.63	124.53
26	u	314	CHL	O2A-CGA-CBA	2.58	120.00	111.91
22	V	301	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
26	v	313	CHL	C4-C3-C5	2.58	119.61	115.27
26	G	312	CHL	CAA-C2A-C3A	-2.58	105.72	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	302	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	n	302	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
26	6	312	CHL	CMB-C2B-C3B	2.58	129.50	124.68
22	P	307	CLA	CHB-C4A-NA	2.58	128.07	124.51
26	6	312	CHL	C4-C3-C5	2.58	119.61	115.27
26	R	315	CHL	O2A-CGA-CBA	2.58	119.99	111.91
27	2	319	NEX	C24-C23-C22	-2.58	105.80	110.77
23	P	311	LUT	C3-C4-C5	-2.58	106.72	111.85
26	5	315	CHL	CAC-C3C-C4C	2.57	128.15	124.81
22	G	305	CLA	CMB-C2B-C3B	2.57	129.49	124.68
22	5	303	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
26	p	314	CHL	C1B-CHB-C4A	-2.57	125.02	130.12
23	p	311	LUT	C3-C4-C5	-2.57	106.73	111.85
23	v	309	LUT	C18-C5-C6	-2.57	121.64	124.53
34	w	201	LMG	C6-C5-C4	-2.57	106.98	113.00
26	n	318	CHL	C1C-C2C-C3C	-2.57	105.07	107.11
22	6	302	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
22	u	307	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	s	309	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	1	313	CHL	CMB-C2B-C3B	2.57	129.49	124.68
26	S	315	CHL	C1C-C2C-C3C	-2.57	105.07	107.11
26	P	319	CHL	CMD-C2D-C3D	-2.57	121.70	127.61
25	P	313	LHG	O8-C23-C24	2.57	119.98	111.91
26	n	318	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
33	D	405	PL9	C27-C28-C29	-2.57	121.47	127.66
22	s	303	CLA	C1-C2-C3	-2.57	122.59	126.75
22	U	306	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	U	319	CHL	CMB-C2B-C3B	2.57	129.49	124.68
22	R	305	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
23	U	310	LUT	C16-C1-C6	-2.57	106.13	110.30
26	p	319	CHL	C1B-CHB-C4A	-2.57	125.03	130.12
22	u	308	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	p	313	LHG	O8-C23-C24	2.57	119.97	111.91
23	N	310	LUT	C7-C8-C9	-2.57	122.35	126.23
22	3	304	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	2	302	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	2	318	CHL	CHB-C4A-NA	2.57	128.06	124.51
22	b	609	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	a	404	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	n	313	CHL	CMB-C2B-C3B	2.57	129.48	124.68
22	C	511	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	A	404	CLA	CHB-C4A-NA	2.57	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	314	CHL	CAC-C3C-C4C	2.57	128.14	124.81
26	1	316	CHL	C4-C3-C5	2.57	119.59	115.27
22	B	609	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
26	6	312	CHL	O2A-CGA-CBA	2.56	119.96	111.91
22	b	605	CLA	C2A-C1A-CHA	2.56	128.34	123.86
23	S	311	LUT	C10-C11-C12	-2.56	115.21	123.22
26	S	315	CHL	C2D-C1D-ND	2.56	111.99	110.10
26	6	301	CHL	O2A-CGA-CBA	2.56	119.96	111.91
26	g	316	CHL	CHB-C4A-NA	2.56	128.06	124.51
22	C	503	CLA	CMB-C2B-C3B	2.56	129.47	124.68
22	P	302	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
27	u	319	NEX	C15-C35-C34	-2.56	118.22	123.47
31	d	403	BCR	C20-C21-C22	-2.56	123.65	127.31
26	6	314	CHL	O2A-CGA-CBA	2.56	119.95	111.91
22	3	308	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	v	315	CHL	CMD-C2D-C3D	-2.56	121.72	127.61
22	N	306	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	q	306	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
23	S	310	LUT	C1-C2-C3	2.56	119.43	113.64
26	s	316	CHL	CMB-C2B-C3B	2.56	129.47	124.68
26	g	313	CHL	C1B-CHB-C4A	-2.56	125.04	130.12
22	a	404	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	5	314	CHL	C2D-C1D-ND	2.56	111.99	110.10
22	C	510	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	6	315	CHL	C4-C3-C5	2.56	119.58	115.27
22	u	306	CLA	CMB-C2B-C3B	2.56	129.47	124.68
22	r	607	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
26	1	316	CHL	CMB-C2B-C3B	2.56	129.47	124.68
23	r	611	LUT	C35-C15-C14	-2.56	118.23	123.47
27	U	318	NEX	C15-C35-C34	-2.56	118.23	123.47
22	4	306	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
23	1	309	LUT	C3-C4-C5	-2.56	106.76	111.85
26	P	319	CHL	CMB-C2B-C3B	2.56	129.46	124.68
22	1	307	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
26	N	314	CHL	O2D-CGD-O1D	-2.56	118.84	123.84
25	N	312	LHG	O8-C23-C24	2.56	119.93	111.91
27	r	618	NEX	C24-C23-C22	-2.56	105.84	110.77
26	R	317	CHL	C4-C3-C5	2.56	119.57	115.27
22	g	306	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
22	Q	307	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
24	r	612	XAT	C28-C29-C30	-2.56	115.02	118.94
31	C	518	BCR	C33-C5-C6	-2.55	121.66	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	301	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
30	D	401	PHO	O1D-CGD-CBD	2.55	128.99	124.74
22	3	306	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
22	6	303	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
26	V	314	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
26	S	314	CHL	CAC-C3C-C4C	2.55	128.12	124.81
23	N	309	LUT	C11-C10-C9	-2.55	123.67	127.31
26	q	311	CHL	C1-C2-C3	-2.55	121.63	126.04
22	p	302	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
22	A	405	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
33	D	405	PL9	C32-C33-C34	-2.55	121.51	127.66
23	V	309	LUT	C18-C5-C6	-2.55	121.66	124.53
23	u	310	LUT	C16-C1-C6	-2.55	106.16	110.30
26	R	315	CHL	CHB-C4A-NA	2.55	128.04	124.51
26	G	315	CHL	CHB-C4A-NA	2.55	128.04	124.51
22	2	303	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
22	U	308	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
22	u	308	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
26	4	317	CHL	O2A-CGA-CBA	2.55	119.91	111.91
26	U	316	CHL	C2A-C1A-CHA	-2.55	119.40	123.86
33	d	404	PL9	C32-C33-C34	-2.55	121.52	127.66
31	D	404	BCR	C20-C21-C22	-2.55	123.67	127.31
23	U	310	LUT	C39-C29-C28	2.55	122.09	118.08
22	1	302	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	V	319	NEX	C28-C29-C30	2.55	122.85	118.94
26	2	313	CHL	C1-C2-C3	-2.55	121.64	126.04
26	q	311	CHL	O2A-CGA-CBA	2.55	119.91	111.91
22	V	307	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	R	302	CLA	CMB-C2B-C3B	2.55	129.44	124.68
22	3	302	CLA	CHB-C4A-NA	2.55	128.03	124.51
27	r	618	NEX	O24-C25-C38	2.55	118.11	115.06
26	R	315	CHL	CMB-C2B-C3B	2.55	129.44	124.68
22	R	304	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	2	306	CLA	C2A-C1A-CHA	2.55	128.31	123.86
23	V	309	LUT	C38-C25-C24	-2.54	118.11	123.56
26	n	314	CHL	O2D-CGD-O1D	-2.54	118.86	123.84
22	P	306	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
22	B	603	CLA	CMB-C2B-C3B	2.54	129.44	124.68
22	r	608	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	s	310	LUT	C11-C10-C9	-2.54	123.68	127.31
26	N	317	CHL	O2A-CGA-CBA	2.54	119.89	111.91
22	S	305	CLA	C1B-CHB-C4A	-2.54	125.08	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	302	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	c	509	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	3	311	CHL	CMB-C2B-C3B	2.54	129.43	124.68
26	n	313	CHL	CMD-C2D-C3D	-2.54	121.77	127.61
26	3	311	CHL	C4-C3-C5	2.54	119.55	115.27
26	G	315	CHL	CMB-C2B-C3B	2.54	129.43	124.68
34	B	621	LMG	O8-C28-C29	2.54	119.88	111.91
26	s	315	CHL	CMB-C2B-C3B	2.54	129.43	124.68
26	S	315	CHL	CMB-C2B-C3B	2.54	129.43	124.68
26	r	614	CHL	O2A-CGA-CBA	2.54	119.87	111.91
23	S	310	LUT	C11-C10-C9	-2.54	123.69	127.31
26	g	315	CHL	CMB-C2B-C3B	2.54	129.43	124.68
22	b	611	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
25	g	310	LHG	O8-C23-C24	2.54	119.87	111.91
22	G	306	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	s	310	LUT	C16-C1-C6	-2.54	106.18	110.30
27	s	317	NEX	C24-C23-C22	-2.54	105.87	110.77
22	r	609	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
26	G	311	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
22	S	303	CLA	CHB-C4A-NA	2.54	128.02	124.51
26	u	316	CHL	C1B-CHB-C4A	-2.54	125.09	130.12
23	V	309	LUT	C11-C10-C9	-2.54	123.69	127.31
22	s	305	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
23	2	310	LUT	C18-C5-C6	-2.54	121.68	124.53
26	p	315	CHL	C3B-C4B-NB	2.53	112.49	109.21
22	B	611	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
26	U	316	CHL	CMD-C2D-C3D	-2.53	121.78	127.61
26	P	315	CHL	CHD-C4C-C3C	-2.53	121.11	124.84
26	s	313	CHL	C1D-ND-C4D	-2.53	104.53	106.33
22	u	305	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	D	403	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	s	310	LUT	C21-C26-C27	-2.53	109.50	112.70
26	2	316	CHL	C1B-CHB-C4A	-2.53	125.10	130.12
22	c	514	CLA	CBA-CAA-C2A	2.53	121.33	113.86
22	R	307	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
23	r	611	LUT	C11-C10-C9	-2.53	123.70	127.31
22	5	303	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
24	P	312	XAT	C10-C11-C12	-2.53	115.32	123.22
23	1	309	LUT	C15-C35-C34	-2.53	118.29	123.47
22	a	405	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	4	307	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	Q	301	CLA	C1B-CHB-C4A	-2.53	125.11	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	N	309	LUT	C16-C1-C6	-2.53	106.20	110.30
22	Q	303	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	4	303	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	b	622	LHG	O8-C23-C24	2.53	119.84	111.91
26	u	318	CHL	CMB-C2B-C3B	2.53	129.41	124.68
31	B	619	BCR	C7-C8-C9	-2.53	122.42	126.23
34	C	521	LMG	O8-C28-C29	2.53	119.84	111.91
26	G	313	CHL	CHB-C4A-NA	2.53	128.01	124.51
26	Q	312	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
31	X	201	BCR	C24-C23-C22	-2.53	122.42	126.23
26	P	317	CHL	C4-C3-C5	2.53	119.52	115.27
26	3	313	CHL	O2A-CGA-CBA	2.53	119.83	111.91
31	c	516	BCR	C38-C26-C27	2.53	118.47	113.62
26	R	316	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
26	Q	313	CHL	O2D-CGD-O1D	-2.53	118.90	123.84
26	v	317	CHL	CMB-C2B-C3B	2.52	129.40	124.68
27	u	319	NEX	C4-C3-C2	-2.52	105.90	110.77
33	a	411	PL9	C7-C3-C2	-2.52	119.98	123.30
33	d	404	PL9	C15-C14-C16	2.52	119.52	115.27
26	q	311	CHL	C4D-CHA-C1A	-2.52	118.18	121.25
22	R	309	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	n	305	CLA	CAD-C3D-C2D	2.52	152.97	140.80
27	n	319	NEX	C24-C23-C22	-2.52	105.90	110.77
26	4	317	CHL	CMB-C2B-C3B	2.52	129.40	124.68
26	U	313	CHL	CMB-C2B-C3B	2.52	129.40	124.68
26	p	315	CHL	CHD-C1D-C2D	2.52	130.77	125.48
23	n	310	LUT	C22-C23-C24	-2.52	108.87	111.74
26	U	316	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
26	P	317	CHL	CMB-C2B-C3B	2.52	129.39	124.68
22	V	302	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
33	D	405	PL9	C25-C24-C26	2.52	119.51	115.27
26	Q	316	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
23	s	310	LUT	C1-C2-C3	2.52	119.33	113.64
26	v	317	CHL	C4-C3-C5	2.52	119.51	115.27
22	c	514	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
26	4	316	CHL	C1-O2A-CGA	2.52	123.05	116.44
22	N	308	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
22	V	308	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
22	a	408	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
22	2	307	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
22	V	306	CLA	CMB-C2B-C3B	2.52	129.38	124.68
33	A	410	PL9	C7-C3-C2	-2.51	119.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	r	617	NEX	C24-C23-C22	-2.51	105.92	110.77
23	p	310	LUT	C38-C25-C24	-2.51	118.18	123.56
23	U	310	LUT	C7-C8-C9	-2.51	122.44	126.23
33	d	404	PL9	C27-C28-C29	-2.51	121.61	127.66
26	N	316	CHL	C4-C3-C5	2.51	119.50	115.27
22	Q	301	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
30	d	401	PHO	O1D-CGD-CBD	2.51	128.92	124.74
23	5	310	LUT	C18-C5-C6	-2.51	121.71	124.53
34	W	201	LMG	C6-C5-C4	-2.51	107.12	113.00
22	r	604	CLA	CMB-C2B-C3B	2.51	129.38	124.68
22	s	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	r	615	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
26	v	315	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
30	a	407	PHO	O2D-CGD-O1D	-2.51	118.93	123.84
22	R	305	CLA	CMB-C2B-C3B	2.51	129.37	124.68
22	Q	306	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	2	311	XAT	C10-C11-C12	-2.51	115.39	123.22
26	q	314	CHL	CHB-C4A-NA	2.51	127.98	124.51
26	2	314	CHL	CHD-C4C-C3C	-2.51	121.15	124.84
22	P	308	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
26	S	316	CHL	O2D-CGD-O1D	-2.51	118.94	123.84
33	d	404	PL9	C25-C24-C26	2.51	119.49	115.27
22	2	303	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
22	c	503	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
23	S	310	LUT	C10-C11-C12	-2.51	115.39	123.22
23	u	310	LUT	C39-C29-C28	2.51	122.03	118.08
31	d	403	BCR	C35-C13-C12	2.51	122.03	118.08
26	q	312	CHL	C2D-C1D-ND	2.51	111.95	110.10
22	c	510	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
27	2	319	NEX	C35-C15-C14	-2.51	118.34	123.47
22	G	307	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
26	u	316	CHL	O2A-CGA-CBA	2.51	119.77	111.91
22	c	502	CLA	CMB-C2B-C3B	2.50	129.36	124.68
25	B	622	LHG	O8-C23-C24	2.50	119.77	111.91
23	n	309	LUT	C31-C30-C29	-2.50	123.74	127.31
23	s	310	LUT	C15-C14-C13	-2.50	123.74	127.31
31	b	619	BCR	C7-C8-C9	-2.50	122.45	126.23
26	v	313	CHL	CMB-C2B-C3B	2.50	129.36	124.68
26	2	315	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
31	c	515	BCR	C16-C15-C14	-2.50	118.35	123.47
26	S	316	CHL	CMB-C2B-C3B	2.50	129.36	124.68
22	B	603	CLA	C1B-CHB-C4A	-2.50	125.16	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	310	LHG	O8-C23-C24	2.50	119.76	111.91
34	c	501	LMG	O8-C28-C29	2.50	119.76	111.91
22	g	306	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	N	309	LUT	C30-C31-C32	-2.50	115.42	123.22
22	s	302	CLA	CMB-C2B-C3B	2.50	129.35	124.68
26	2	317	CHL	CMB-C2B-C3B	2.50	129.35	124.68
26	s	316	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
22	b	603	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	g	307	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
26	6	301	CHL	C4-C3-C5	2.50	119.47	115.27
32	L	102	SQD	O6-C1-C2	2.50	112.20	108.30
30	A	407	PHO	O2D-CGD-O1D	-2.50	118.96	123.84
26	3	313	CHL	C4A-NA-C1A	2.50	107.83	106.71
22	C	504	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
22	A	404	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	q	302	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	n	305	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
34	c	520	LMG	O8-C28-C29	2.49	119.73	111.91
26	P	319	CHL	C4-C3-C5	2.49	119.47	115.27
23	p	310	LUT	C8-C7-C6	-2.49	120.20	127.20
22	G	302	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	A	408	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	4	308	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	C	505	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	p	304	CLA	C1-C2-C3	-2.49	122.72	126.75
30	d	401	PHO	C4A-C3A-C2A	-2.49	100.47	102.84
22	Q	301	CLA	CHB-C4A-NA	2.49	127.96	124.51
26	r	619	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
22	5	305	CLA	CAD-C3D-C2D	2.49	152.82	140.80
22	p	308	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	g	307	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
26	q	314	CHL	O2A-CGA-CBA	2.49	119.72	111.91
33	d	404	PL9	C35-C34-C36	2.49	119.46	115.27
27	N	318	NEX	C16-C1-C6	2.49	112.70	110.47
26	p	319	CHL	CHB-C4A-NA	2.49	127.95	124.51
26	n	318	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
22	4	302	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	v	308	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
26	V	318	CHL	C1D-ND-C4D	-2.49	104.57	106.33
26	V	318	CHL	C4-C3-C5	2.49	119.45	115.27
22	S	302	CLA	CMB-C2B-C3B	2.49	129.33	124.68
26	p	317	CHL	CMB-C2B-C3B	2.49	129.33	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	313	CHL	CMB-C2B-C3B	2.49	129.33	124.68
26	n	316	CHL	CED-O2D-CGD	2.48	121.56	115.94
26	1	318	CHL	O2A-CGA-CBA	2.48	119.70	111.91
26	v	318	CHL	C1B-CHB-C4A	-2.48	125.20	130.12
22	2	304	CLA	C1-C2-C3	-2.48	121.75	126.04
26	3	311	CHL	O2A-CGA-CBA	2.48	119.70	111.91
22	r	608	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
26	P	318	CHL	O2A-CGA-CBA	2.48	119.70	111.91
33	D	405	PL9	C15-C14-C16	2.48	119.45	115.27
22	G	304	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
22	C	511	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
26	G	315	CHL	C1C-C2C-C3C	-2.48	105.14	107.11
27	u	320	NEX	C28-C29-C30	2.48	122.75	118.94
27	u	320	NEX	C24-C23-C22	-2.48	105.98	110.77
23	r	611	LUT	C38-C25-C24	-2.48	118.25	123.56
26	1	316	CHL	O2A-CGA-CBA	2.48	119.69	111.91
23	v	309	LUT	C11-C10-C9	-2.48	123.77	127.31
22	n	303	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
22	B	616	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
23	1	310	LUT	C10-C11-C12	-2.48	115.48	123.22
31	D	404	BCR	C35-C13-C12	2.48	121.98	118.08
26	6	313	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
23	4	309	LUT	C38-C25-C24	-2.48	118.25	123.56
24	N	311	XAT	C30-C31-C32	-2.48	115.48	123.22
26	G	314	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
22	C	506	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
23	s	311	LUT	C20-C13-C12	2.48	121.98	118.08
22	b	615	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
26	p	318	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
26	G	312	CHL	C3D-C4D-ND	2.48	114.25	110.24
23	p	310	LUT	C7-C8-C9	-2.48	122.49	126.23
22	S	301	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
22	U	302	CLA	CMB-C2B-C3B	2.48	129.31	124.68
22	c	504	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
26	r	616	CHL	O2A-CGA-CBA	2.48	119.68	111.91
22	U	305	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
22	N	305	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
26	n	314	CHL	C2D-C1D-ND	2.48	111.93	110.10
23	R	312	LUT	C18-C5-C6	-2.47	121.75	124.53
31	b	620	BCR	C34-C9-C8	2.47	121.98	118.08
26	3	315	CHL	C4-C3-C5	2.47	119.43	115.27
22	5	302	CLA	O2D-CGD-O1D	-2.47	119.00	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	306	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
26	s	314	CHL	C1C-C2C-C3C	-2.47	105.15	107.11
34	C	502	LMG	O8-C28-C29	2.47	119.67	111.91
26	Q	311	CHL	C1-C2-C3	-2.47	121.77	126.04
26	Q	311	CHL	C2A-C1A-CHA	-2.47	119.53	123.86
23	u	310	LUT	C3-C4-C5	-2.47	106.93	111.85
26	q	313	CHL	CHB-C4A-NA	2.47	127.93	124.51
22	n	307	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
22	n	308	CLA	CMB-C2B-C3B	2.47	129.30	124.68
23	r	611	LUT	C30-C31-C32	-2.47	115.50	123.22
26	g	314	CHL	CMB-C2B-C3B	2.47	129.30	124.68
26	G	314	CHL	C1D-ND-C4D	-2.47	104.58	106.33
22	R	309	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
26	G	315	CHL	CMD-C2D-C3D	-2.47	121.93	127.61
22	C	515	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
23	2	310	LUT	C3-C4-C5	-2.47	106.94	111.85
26	Q	316	CHL	C4-C3-C5	2.47	119.42	115.27
24	3	309	XAT	C10-C11-C12	-2.47	115.51	123.22
27	n	319	NEX	C31-C30-C29	-2.47	123.79	127.31
26	R	317	CHL	O2A-CGA-CBA	2.47	119.65	111.91
26	P	315	CHL	CED-O2D-CGD	2.47	121.52	115.94
26	6	317	CHL	CMB-C2B-C3B	2.47	129.29	124.68
23	2	309	LUT	C38-C25-C24	-2.47	118.28	123.56
22	N	303	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
22	a	404	CLA	CAA-C2A-C3A	-2.47	106.03	112.78
26	r	614	CHL	CHB-C4A-NA	2.47	127.92	124.51
26	p	320	CHL	C4-C3-C5	2.47	119.42	115.27
22	Q	304	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
26	1	315	CHL	CMB-C2B-C3B	2.46	129.29	124.68
26	4	314	CHL	CHB-C4A-NA	2.46	127.92	124.51
22	s	301	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
33	D	405	PL9	C35-C34-C36	2.46	119.41	115.27
26	N	313	CHL	C2A-C3A-C4A	-2.46	97.89	101.87
23	V	310	LUT	C3-C4-C5	-2.46	106.95	111.85
26	V	317	CHL	C1-C2-C3	-2.46	121.79	126.04
22	2	302	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	6	305	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
26	Q	314	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
26	U	315	CHL	CMB-C2B-C3B	2.46	129.28	124.68
26	n	317	CHL	CMB-C2B-C3B	2.46	129.28	124.68
31	b	618	BCR	C33-C5-C6	-2.46	121.77	124.53
22	r	603	CLA	O2D-CGD-O1D	-2.46	119.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	u	305	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
26	V	318	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
26	P	314	CHL	C1-C2-C3	-2.46	121.79	126.04
32	A	412	SQD	C44-O6-C1	2.46	118.54	113.74
23	P	310	LUT	C30-C31-C32	-2.46	115.55	123.22
26	p	318	CHL	O2A-CGA-CBA	2.46	119.61	111.91
26	g	314	CHL	C4-C3-C5	2.46	119.40	115.27
22	V	307	CLA	O2A-CGA-O1A	-2.46	117.40	123.59
26	1	318	CHL	CMB-C2B-C3B	2.45	129.27	124.68
26	4	317	CHL	C4-C3-C5	2.45	119.40	115.27
22	N	302	CLA	CHB-C4A-NA	2.45	127.91	124.51
26	u	317	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
26	g	316	CHL	CMB-C2B-C3B	2.45	129.27	124.68
25	d	405	LHG	O8-C23-C24	2.45	119.61	111.91
31	d	403	BCR	C37-C22-C23	2.45	121.94	118.08
23	R	312	LUT	C38-C25-C24	-2.45	118.31	123.56
22	N	307	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
26	3	312	CHL	C2D-C1D-ND	2.45	111.91	110.10
26	u	317	CHL	CMD-C2D-C3D	-2.45	121.97	127.61
22	Q	302	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	s	304	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
31	C	518	BCR	C38-C26-C27	2.45	118.33	113.62
26	4	315	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
26	n	313	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
26	g	316	CHL	C4-C3-C5	2.45	119.39	115.27
26	P	314	CHL	O2A-CGA-O1A	-2.45	117.41	123.59
22	5	306	CLA	C2A-C1A-CHA	2.45	128.14	123.86
22	b	616	CLA	C2A-C1A-CHA	2.45	128.14	123.86
31	B	620	BCR	C34-C9-C8	2.45	121.94	118.08
26	g	311	CHL	C1-C2-C3	-2.45	121.81	126.04
26	1	315	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
31	k	101	BCR	C16-C15-C14	-2.45	118.46	123.47
26	u	316	CHL	CMB-C2B-C3B	2.45	129.26	124.68
26	G	316	CHL	C4-C3-C5	2.45	119.39	115.27
24	4	311	XAT	C11-C10-C9	-2.45	123.81	127.31
22	B	605	CLA	C2A-C1A-CHA	2.45	128.14	123.86
22	b	609	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
26	2	317	CHL	C1-C2-C3	-2.45	121.81	126.04
22	A	404	CLA	CAA-CBA-CGA	-2.45	106.10	113.25
22	u	306	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
22	b	609	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	q	312	CHL	C4D-CHA-C1A	-2.45	118.27	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	312	CHL	C2A-C1A-CHA	-2.45	119.58	123.86
22	A	406	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	B	607	CLA	CMB-C2B-C3B	2.45	129.26	124.68
22	Q	302	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
25	D	406	LHG	O8-C23-C24	2.45	119.58	111.91
22	U	304	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	S	305	CLA	CHB-C4A-NA	2.45	127.89	124.51
26	p	315	CHL	C2D-C1D-ND	2.45	111.91	110.10
36	A	414	DGD	O1G-C1A-C2A	2.44	119.58	111.91
31	B	620	BCR	C33-C5-C6	-2.44	121.78	124.53
27	r	617	NEX	C28-C29-C30	2.44	122.69	118.94
32	m	101	SQD	O6-C1-C2	2.44	112.12	108.30
24	n	311	XAT	C39-C29-C28	2.44	121.93	118.08
26	5	313	CHL	C1-C2-C3	-2.44	121.82	126.04
26	P	315	CHL	CAC-C3C-C4C	2.44	127.98	124.81
22	p	306	CLA	CAD-C3D-C2D	2.44	152.59	140.80
26	6	313	CHL	C2D-C1D-ND	2.44	111.90	110.10
23	V	309	LUT	C3-C4-C5	-2.44	106.99	111.85
22	g	303	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	n	301	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	3	316	CHL	O2A-CGA-CBA	2.44	119.57	111.91
22	q	303	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
26	N	314	CHL	C2D-C1D-ND	2.44	111.90	110.10
27	u	320	NEX	C15-C35-C34	-2.44	118.47	123.47
22	u	307	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	B	609	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	p	311	LUT	C11-C10-C9	-2.44	123.83	127.31
36	a	416	DGD	O1G-C1A-C2A	2.44	119.57	111.91
26	p	315	CHL	CAC-C3C-C4C	2.44	127.98	124.81
34	W	201	LMG	O8-C28-C29	2.44	119.56	111.91
22	1	302	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
22	a	408	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
22	U	306	CLA	C2A-C1A-CHA	2.44	128.12	123.86
24	v	311	XAT	C30-C31-C32	-2.44	115.61	123.22
34	w	201	LMG	O6-C5-C4	2.44	114.12	109.69
26	Q	311	CHL	CMB-C2B-C3B	2.44	129.24	124.68
26	u	317	CHL	C2A-C1A-CHA	-2.44	119.59	123.86
22	b	606	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
23	4	310	LUT	C16-C1-C6	-2.44	106.34	110.30
26	g	312	CHL	C4A-NA-C1A	2.44	107.80	106.71
26	Q	315	CHL	CMD-C2D-C3D	-2.44	122.01	127.61
23	S	311	LUT	C20-C13-C12	2.44	121.92	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	616	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
34	b	624	LMG	O8-C28-C29	2.44	119.56	111.91
22	3	304	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
22	5	308	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	s	311	LUT	C7-C8-C9	-2.44	122.55	126.23
23	s	310	LUT	C10-C11-C12	-2.44	115.61	123.22
22	B	615	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
22	s	305	CLA	CHB-C4A-NA	2.44	127.88	124.51
36	b	601	DGD	O6E-C5E-C4E	2.44	114.12	109.69
26	u	313	CHL	CMB-C2B-C3B	2.44	129.23	124.68
23	1	310	LUT	C18-C5-C4	2.43	118.87	114.36
26	N	313	CHL	C4D-CHA-C1A	-2.43	118.29	121.25
22	a	406	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
37	E	101	HEM	CMB-C2B-C1B	-2.43	121.33	125.04
22	r	607	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	4	310	LUT	C22-C23-C24	-2.43	108.97	111.74
22	6	307	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	r	615	CHL	C4-C3-C5	2.43	119.36	115.27
26	g	312	CHL	C1D-ND-C4D	-2.43	104.61	106.33
26	5	317	CHL	CMB-C2B-C3B	2.43	129.23	124.68
24	4	311	XAT	C30-C31-C32	-2.43	115.63	123.22
24	n	311	XAT	C11-C12-C13	-2.43	119.59	126.42
22	C	507	CLA	O1D-CGD-CBD	2.43	129.46	124.48
23	5	310	LUT	C22-C23-C24	-2.43	108.98	111.74
31	D	404	BCR	C37-C22-C23	2.43	121.90	118.08
23	U	309	LUT	C22-C23-C24	2.43	114.50	111.74
26	v	317	CHL	C2A-C1A-CHA	-2.43	119.61	123.86
26	n	318	CHL	C1D-ND-C4D	-2.43	104.61	106.33
26	U	316	CHL	C4-C3-C5	2.43	119.36	115.27
26	Q	314	CHL	C4-C3-C5	2.43	119.35	115.27
26	4	313	CHL	C1C-C2C-C3C	-2.43	105.19	107.11
23	5	309	LUT	C35-C15-C14	-2.43	118.50	123.47
22	c	506	CLA	O1D-CGD-CBD	2.43	129.45	124.48
31	B	620	BCR	C11-C10-C9	-2.43	123.85	127.31
22	c	505	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	S	304	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	p	303	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
26	V	313	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
22	R	304	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
25	D	407	LHG	O8-C23-C24	2.42	119.52	111.91
22	q	301	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
26	q	313	CHL	O2D-CGD-O1D	-2.42	119.10	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	404	CLA	CAA-CBA-CGA	-2.42	106.17	113.25
26	3	312	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
26	g	315	CHL	OMC-CMC-C2C	-2.42	120.21	125.69
26	N	313	CHL	C1-C2-C3	-2.42	121.85	126.04
26	3	312	CHL	C3D-C4D-ND	2.42	114.16	110.24
26	6	313	CHL	C3D-C4D-ND	2.42	114.16	110.24
22	G	307	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	1	310	LUT	C22-C23-C24	-2.42	108.98	111.74
26	q	311	CHL	C2A-C1A-CHA	-2.42	119.62	123.86
26	2	313	CHL	CMB-C2B-C3B	2.42	129.21	124.68
22	q	306	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	4	307	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	a	405	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	B	609	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	3	311	CHL	O2D-CGD-O1D	-2.42	119.11	123.84
26	q	312	CHL	O2A-CGA-CBA	2.42	119.50	111.91
26	U	319	CHL	O2A-CGA-CBA	2.42	119.50	111.91
26	3	313	CHL	C1C-C2C-C3C	-2.42	105.19	107.11
31	b	618	BCR	C16-C15-C14	-2.42	118.52	123.47
22	r	609	CLA	C2A-C1A-CHA	2.42	128.09	123.86
34	B	624	LMG	O8-C28-C29	2.42	119.49	111.91
26	1	316	CHL	CGD-CBD-CAD	-2.42	102.91	110.73
23	P	310	LUT	C35-C15-C14	-2.42	118.52	123.47
31	t	101	BCR	C15-C16-C17	-2.42	118.52	123.47
22	B	614	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
22	c	511	CLA	CHB-C4A-NA	2.42	127.85	124.51
34	b	621	LMG	O8-C28-C29	2.42	119.49	111.91
22	5	307	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
23	u	310	LUT	C7-C8-C9	-2.41	122.59	126.23
22	A	405	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	A	406	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	q	302	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	u	304	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	N	309	LUT	C18-C5-C6	-2.41	121.82	124.53
26	6	314	CHL	C4A-NA-C1A	2.41	107.79	106.71
26	U	315	CHL	C4D-CHA-C1A	-2.41	118.31	121.25
34	w	201	LMG	O8-C28-C29	2.41	119.48	111.91
22	q	307	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
26	V	315	CHL	CMB-C2B-C3B	2.41	129.19	124.68
25	n	312	LHG	O8-C23-C24	2.41	119.48	111.91
22	b	617	CLA	CMB-C2B-C3B	2.41	129.19	124.68
22	b	607	CLA	CMB-C2B-C3B	2.41	129.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	313	CHL	CMB-C2B-C3B	2.41	129.19	124.68
22	U	301	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	u	302	CLA	CMB-C2B-C3B	2.41	129.19	124.68
22	r	609	CLA	C1-C2-C3	-2.41	121.87	126.04
22	B	610	CLA	C4-C3-C5	2.41	119.33	115.27
26	3	315	CHL	CHB-C4A-NA	2.41	127.84	124.51
26	6	315	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
26	q	314	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
27	2	319	NEX	C30-C31-C32	-2.41	115.70	123.22
26	v	318	CHL	C4-C3-C5	2.41	119.32	115.27
22	S	303	CLA	C1-C2-C3	-2.41	122.85	126.75
26	2	314	CHL	OMC-CMC-C2C	-2.41	120.24	125.69
22	c	502	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	S	303	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
31	T	101	BCR	C15-C16-C17	-2.41	118.54	123.47
26	n	318	CHL	CMB-C2B-C3B	2.41	129.18	124.68
22	X	202	CLA	O2D-CGD-CBD	2.41	115.55	111.27
26	p	315	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
26	p	316	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
34	b	621	LMG	C1-O6-C5	2.41	118.41	113.69
23	U	309	LUT	C30-C31-C32	-2.41	115.71	123.22
23	P	310	LUT	C38-C25-C24	-2.40	118.41	123.56
22	x	201	CLA	O2D-CGD-CBD	2.40	115.54	111.27
26	n	313	CHL	C4-C3-C5	2.40	119.32	115.27
26	q	312	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
22	b	612	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	v	307	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
22	v	304	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
33	D	405	PL9	C30-C29-C31	2.40	119.31	115.27
22	C	503	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
34	W	201	LMG	O6-C5-C4	2.40	114.06	109.69
26	v	313	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
25	A	413	LHG	O8-C23-C24	2.40	119.44	111.91
23	N	310	LUT	C1-C2-C3	2.40	119.07	113.64
26	p	314	CHL	C4-C3-C5	2.40	119.31	115.27
26	P	317	CHL	C4D-CHA-C1A	-2.40	118.33	121.25
22	r	603	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	4	307	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
26	6	312	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
22	C	510	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	V	310	LUT	C10-C11-C12	-2.40	115.73	123.22
22	N	302	CLA	CMB-C2B-C3B	2.40	129.17	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	313	CHL	CMB-C2B-C3B	2.40	129.17	124.68
25	q	310	LHG	O8-C23-C24	2.40	119.44	111.91
22	3	307	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
26	6	301	CHL	CGD-CBD-CAD	-2.40	102.97	110.73
26	N	317	CHL	C4-C3-C5	2.40	119.30	115.27
22	B	612	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
33	d	404	PL9	C30-C29-C31	2.40	119.30	115.27
22	r	605	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
22	1	307	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
22	V	307	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
27	u	320	NEX	C16-C1-C6	2.40	112.62	110.47
27	5	319	NEX	C17-C1-C6	-2.40	108.33	110.47
26	5	314	CHL	C3D-C4D-ND	2.39	114.11	110.24
26	G	311	CHL	C4D-CHA-C1A	-2.39	118.33	121.25
31	b	620	BCR	C20-C21-C22	-2.39	123.89	127.31
26	s	314	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
25	d	406	LHG	O8-C23-C24	2.39	119.42	111.91
24	g	309	XAT	C15-C35-C34	-2.39	118.57	123.47
26	3	314	CHL	C4-C3-C5	2.39	119.30	115.27
31	A	409	BCR	C38-C26-C27	2.39	118.21	113.62
27	5	319	NEX	C28-C29-C30	2.39	122.61	118.94
22	Q	306	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	1	317	CHL	C4-C3-C5	2.39	119.30	115.27
23	r	611	LUT	C10-C11-C12	-2.39	115.75	123.22
22	g	305	CLA	CMB-C2B-C3B	2.39	129.15	124.68
22	R	306	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	u	317	CHL	C4-C3-C5	2.39	119.30	115.27
23	4	309	LUT	C3-C4-C5	-2.39	107.09	111.85
22	v	305	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
27	r	617	NEX	C19-C9-C10	-2.39	119.57	122.92
26	Q	313	CHL	CHB-C4A-NA	2.39	127.82	124.51
24	R	313	XAT	C19-C9-C8	2.39	121.84	118.08
22	U	306	CLA	CMB-C2B-C3B	2.39	129.15	124.68
22	C	509	CLA	C2A-C1A-CHA	2.39	128.04	123.86
22	N	301	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	S	314	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
23	s	311	LUT	C38-C25-C24	-2.39	118.44	123.56
25	a	415	LHG	O8-C23-C24	2.39	119.41	111.91
26	1	317	CHL	O2A-CGA-CBA	2.39	119.41	111.91
26	R	317	CHL	C1D-ND-C4D	-2.39	104.64	106.33
22	N	307	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
31	C	518	BCR	C10-C11-C12	-2.39	115.76	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	307	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
37	e	101	HEM	CMB-C2B-C1B	-2.39	121.40	125.04
22	A	405	CLA	C2A-C1A-CHA	2.39	128.04	123.86
26	P	314	CHL	C4-C3-C5	2.39	119.29	115.27
26	5	318	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
22	1	304	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	n	302	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	B	606	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
22	c	508	CLA	C2A-C1A-CHA	2.39	128.03	123.86
22	Q	308	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
31	b	620	BCR	C33-C5-C6	-2.39	121.85	124.53
22	B	605	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
26	1	314	CHL	C4D-CHA-C1A	-2.39	118.34	121.25
22	C	508	CLA	CMB-C2B-C3B	2.39	129.14	124.68
23	u	309	LUT	C3-C4-C5	-2.39	107.10	111.85
22	g	301	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	2	303	CLA	C1-C2-C3	-2.39	122.89	126.75
23	P	311	LUT	C7-C8-C9	-2.39	122.63	126.23
30	D	401	PHO	C1B-NB-C4B	2.38	111.99	107.09
22	5	305	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
22	C	512	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
26	N	317	CHL	CMB-C2B-C3B	2.38	129.14	124.68
26	S	315	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
31	t	101	BCR	C1-C6-C7	2.38	122.52	115.78
36	J	101	DGD	O6D-C5D-C4D	2.38	114.02	109.69
22	Q	305	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	c	508	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
26	V	317	CHL	C2A-C1A-CHA	-2.38	119.69	123.86
23	4	309	LUT	C18-C5-C6	-2.38	121.85	124.53
26	N	314	CHL	C3D-C4D-ND	2.38	114.09	110.24
22	2	305	CLA	CAD-C3D-C2D	2.38	152.29	140.80
26	r	619	CHL	CAA-C2A-C3A	-2.38	106.26	112.78
31	B	620	BCR	C21-C20-C19	-2.38	115.79	123.22
26	q	314	CHL	CMD-C2D-C3D	-2.38	122.14	127.61
26	p	318	CHL	C1-C2-C3	-2.38	121.93	126.04
32	M	101	SQD	O6-C1-C2	2.38	112.02	108.30
23	s	310	LUT	C39-C29-C28	2.38	121.83	118.08
22	Q	303	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	6	316	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
22	R	310	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
22	n	303	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	c	507	CLA	CMB-C2B-C3B	2.38	129.13	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	313	CHL	C4A-NA-C1A	2.38	107.78	106.71
31	c	515	BCR	C36-C18-C19	2.38	121.82	118.08
22	u	304	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
26	v	313	CHL	C1B-CHB-C4A	-2.38	125.41	130.12
26	n	316	CHL	O2A-CGA-CBA	2.38	119.37	111.91
23	S	310	LUT	C39-C29-C28	2.38	121.82	118.08
22	a	406	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
27	N	318	NEX	C17-C1-C6	-2.38	108.34	110.47
26	P	316	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
22	V	308	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
22	R	308	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
31	x	202	BCR	C24-C23-C22	-2.38	122.65	126.23
22	P	305	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
22	u	301	CLA	CHB-C4A-NA	2.37	127.80	124.51
22	s	305	CLA	C1-C2-C3	-2.37	121.94	126.04
26	U	315	CHL	C1-C2-C3	-2.37	121.94	126.04
22	4	304	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
26	n	315	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
22	b	605	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	d	401	PHO	C1B-NB-C4B	2.37	111.97	107.09
22	C	509	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
26	u	313	CHL	CHB-C4A-NA	2.37	127.79	124.51
22	b	614	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	p	305	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
26	g	314	CHL	CED-O2D-CGD	2.37	121.30	115.94
26	p	317	CHL	C4D-CHA-C1A	-2.37	118.36	121.25
31	K	101	BCR	C16-C15-C14	-2.37	118.62	123.47
26	3	314	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
26	n	317	CHL	C4-C3-C5	2.37	119.26	115.27
22	q	304	CLA	O1D-CGD-CBD	2.37	129.33	124.48
22	S	301	CLA	C1-C2-C3	-2.37	121.94	126.04
22	v	301	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	s	306	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
26	N	315	CHL	CMB-C2B-C3B	2.37	129.11	124.68
22	Q	304	CLA	O1D-CGD-CBD	2.37	129.33	124.48
24	U	311	XAT	C35-C34-C33	-2.37	123.93	127.31
22	6	308	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
23	5	309	LUT	C15-C35-C34	-2.37	118.62	123.47
26	5	317	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
26	n	314	CHL	C4D-CHA-C1A	-2.37	118.37	121.25
26	5	318	CHL	CHB-C4A-NA	2.37	127.78	124.51
22	b	614	CLA	O2D-CGD-O1D	-2.37	119.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	q	308	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
26	v	317	CHL	OMC-CMC-C2C	-2.37	120.34	125.69
26	p	317	CHL	O1D-CGD-CBD	-2.37	119.64	124.48
22	a	405	CLA	C2A-C1A-CHA	2.37	128.00	123.86
22	q	301	CLA	CHB-C4A-NA	2.36	127.78	124.51
26	2	314	CHL	CHD-C1D-C2D	2.36	130.44	125.48
22	B	605	CLA	CAA-CBA-CGA	-2.36	106.35	113.25
22	u	301	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
26	5	313	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
22	4	306	CLA	CMB-C2B-C3B	2.36	129.10	124.68
30	D	401	PHO	C4A-C3A-C2A	-2.36	100.59	102.84
22	r	607	CLA	C2A-C1A-CHA	2.36	127.99	123.86
26	n	318	CHL	C4-C3-C5	2.36	119.24	115.27
22	s	301	CLA	C1-C2-C3	-2.36	121.96	126.04
24	p	312	XAT	C11-C10-C9	-2.36	123.94	127.31
22	2	305	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	c	511	CLA	CMB-C2B-C1B	-2.36	124.84	128.46
26	4	316	CHL	C4-C3-C5	2.36	119.24	115.27
23	s	311	LUT	C18-C5-C4	2.36	118.72	114.36
26	p	316	CHL	OMC-CMC-C2C	-2.36	120.36	125.69
26	g	314	CHL	C1-C2-C3	-2.36	121.97	126.04
22	c	509	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	6	316	CHL	CMB-C2B-C3B	2.36	129.09	124.68
22	6	308	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	4	315	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
22	r	610	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
24	5	311	XAT	C30-C31-C32	-2.36	115.86	123.22
23	S	311	LUT	C7-C8-C9	-2.36	122.67	126.23
22	B	614	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
26	r	614	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
26	6	317	CHL	C2A-C1A-CHA	-2.36	119.74	123.86
22	s	303	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
27	p	301	NEX	C11-C12-C13	-2.35	119.80	126.42
26	S	313	CHL	CMB-C2B-C3B	2.35	129.08	124.68
22	n	302	CLA	CMB-C2B-C3B	2.35	129.08	124.68
26	g	313	CHL	O2A-CGA-CBA	2.35	119.29	111.91
22	B	616	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
24	r	612	XAT	C27-C28-C29	2.35	129.18	125.53
31	C	517	BCR	C16-C15-C14	-2.35	118.65	123.47
26	v	317	CHL	C4D-CHA-C1A	-2.35	118.39	121.25
22	V	301	CLA	CHB-C4A-NA	2.35	127.77	124.51
31	K	101	BCR	C21-C20-C19	-2.35	115.88	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	320	CHL	CED-O2D-CGD	2.35	121.26	115.94
22	n	308	CLA	C2A-C1A-CHA	2.35	127.97	123.86
26	s	315	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
31	C	517	BCR	C36-C18-C19	2.35	121.78	118.08
26	u	318	CHL	C4-C3-C5	2.35	119.22	115.27
22	v	306	CLA	C2A-C1A-CHA	2.35	127.97	123.86
27	N	318	NEX	C11-C12-C13	-2.35	119.81	126.42
22	C	512	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	u	315	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
22	4	305	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
26	V	316	CHL	C4-C3-C5	2.35	119.22	115.27
26	v	316	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
22	g	305	CLA	O2D-CGD-CBD	2.35	115.44	111.27
23	p	310	LUT	C30-C31-C32	-2.35	115.89	123.22
26	v	318	CHL	CMD-C2D-C3D	-2.35	122.22	127.61
26	q	312	CHL	C3D-C4D-ND	2.35	114.03	110.24
23	2	310	LUT	C18-C5-C4	2.35	118.70	114.36
26	p	316	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
26	u	316	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
22	v	306	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
26	4	316	CHL	O2A-CGA-CBA	2.35	119.27	111.91
22	b	602	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
36	C	520	DGD	C1E-C2E-C3E	2.35	114.88	110.00
22	6	305	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
26	g	316	CHL	O2A-CGA-CBA	2.34	119.27	111.91
31	k	101	BCR	C21-C20-C19	-2.34	115.90	123.22
22	2	308	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
22	c	503	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
26	5	317	CHL	C1-C2-C3	-2.34	121.99	126.04
26	6	301	CHL	O1D-CGD-CBD	-2.34	119.69	124.48
22	N	306	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
26	3	311	CHL	C2A-C1A-CHA	-2.34	119.76	123.86
22	p	306	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	Q	303	CLA	C1-C2-C3	-2.34	122.96	126.75
26	q	311	CHL	CMB-C2B-C3B	2.34	129.06	124.68
26	6	317	CHL	O2A-CGA-CBA	2.34	119.26	111.91
26	3	315	CHL	CMD-C2D-C3D	-2.34	122.23	127.61
22	S	304	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	C	508	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
26	N	315	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
22	R	308	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
24	P	312	XAT	C30-C31-C32	-2.34	115.92	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	308	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
24	p	312	XAT	C30-C31-C32	-2.34	115.92	123.22
31	b	620	BCR	C11-C10-C9	-2.34	123.97	127.31
26	p	319	CHL	O2A-CGA-CBA	2.34	119.25	111.91
22	2	306	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
26	2	314	CHL	C2D-C1D-ND	2.34	111.83	110.10
26	4	315	CHL	CMB-C2B-C3B	2.34	129.05	124.68
22	n	308	CLA	O2D-CGD-CBD	2.34	115.42	111.27
26	V	318	CHL	C1-C2-C3	-2.34	122.00	126.04
26	N	316	CHL	OMC-CMC-C2C	-2.34	120.41	125.69
22	6	305	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
22	P	302	CLA	CHD-C1D-ND	-2.33	122.31	124.45
22	V	304	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	c	514	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	S	301	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
26	P	316	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
26	v	316	CHL	C4-C3-C5	2.33	119.19	115.27
23	U	309	LUT	C35-C15-C14	-2.33	118.70	123.47
22	b	616	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
26	2	313	CHL	C1D-ND-C4D	-2.33	104.68	106.33
26	Q	311	CHL	C4D-CHA-C1A	-2.33	118.42	121.25
26	1	318	CHL	C4-C3-C5	2.33	119.19	115.27
26	u	316	CHL	C1-C2-C3	-2.33	122.02	126.04
22	C	513	CLA	C2A-C1A-CHA	2.33	127.93	123.86
22	n	308	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
26	Q	315	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
22	x	201	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
26	U	316	CHL	O2A-CGA-O1A	-2.33	117.72	123.59
26	N	313	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
26	S	316	CHL	C1C-C2C-C3C	-2.33	105.27	107.11
31	B	618	BCR	C16-C15-C14	-2.33	118.71	123.47
22	C	505	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
26	p	314	CHL	O1D-CGD-CBD	-2.33	119.73	124.48
26	q	315	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
26	u	314	CHL	C1C-C2C-C3C	-2.33	105.27	107.11
26	p	314	CHL	C1-C2-C3	-2.32	122.02	126.04
26	G	316	CHL	C1-C2-C3	-2.32	122.02	126.04
24	n	311	XAT	C19-C9-C8	2.32	121.74	118.08
22	b	617	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
22	G	308	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	5	309	LUT	C38-C25-C24	-2.32	118.59	123.56
27	V	319	NEX	C16-C1-C6	2.32	112.55	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	x	202	BCR	C34-C9-C10	-2.32	119.67	122.92
22	b	611	CLA	C2A-C1A-CHA	2.32	127.92	123.86
23	v	310	LUT	C10-C11-C12	-2.32	115.97	123.22
22	r	607	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
22	B	611	CLA	C2A-C1A-CHA	2.32	127.92	123.86
23	u	310	LUT	C22-C23-C24	-2.32	109.10	111.74
26	U	314	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
26	n	318	CHL	O1D-CGD-CBD	-2.32	119.73	124.48
23	N	309	LUT	C10-C11-C12	-2.32	115.97	123.22
22	g	304	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	v	309	LUT	C16-C1-C6	-2.32	106.54	110.30
26	V	317	CHL	C4D-CHA-C1A	-2.32	118.43	121.25
26	4	316	CHL	C1B-CHB-C4A	-2.32	125.52	130.12
22	G	301	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	U	304	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	P	318	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
31	b	618	BCR	C10-C11-C12	-2.32	115.98	123.22
26	n	313	CHL	O2A-CGA-CBA	2.32	119.18	111.91
27	v	319	NEX	C17-C1-C6	-2.32	108.40	110.47
26	R	315	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
31	C	516	BCR	C34-C9-C8	2.32	121.73	118.08
22	p	309	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
22	C	515	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
26	P	315	CHL	C3B-C4B-NB	2.32	112.21	109.21
22	b	613	CLA	CAA-CBA-CGA	-2.32	106.48	113.25
26	3	313	CHL	CMB-C2B-C3B	2.32	129.01	124.68
32	a	410	SQD	O48-C23-C24	2.32	119.18	111.91
26	Q	315	CHL	C4-C3-C5	2.32	119.17	115.27
22	1	306	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
22	B	613	CLA	CAA-CBA-CGA	-2.32	106.48	113.25
26	v	313	CHL	CHB-C4A-NA	2.32	127.72	124.51
22	S	309	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
22	b	602	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
24	G	309	XAT	C15-C35-C34	-2.32	118.73	123.47
27	2	319	NEX	C17-C1-C6	-2.32	108.40	110.47
23	S	311	LUT	C38-C25-C24	-2.32	118.60	123.56
22	5	306	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
27	u	319	NEX	C39-C29-C30	-2.32	119.68	122.92
26	6	316	CHL	C4-C3-C5	2.31	119.17	115.27
33	D	405	PL9	C45-C44-C46	2.31	119.17	115.27
22	1	305	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
26	V	316	CHL	C4D-CHA-C1A	-2.31	118.43	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	612	XAT	C19-C9-C8	2.31	121.72	118.08
22	B	602	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
26	P	316	CHL	C4A-NA-C1A	2.31	107.75	106.71
26	n	316	CHL	C4D-CHA-C1A	-2.31	118.43	121.25
23	2	310	LUT	C31-C30-C29	-2.31	124.01	127.31
23	p	311	LUT	C10-C11-C12	-2.31	116.00	123.22
31	A	409	BCR	C10-C11-C12	-2.31	116.00	123.22
22	3	305	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	1	307	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
26	6	316	CHL	CMD-C2D-C3D	-2.31	122.30	127.61
26	1	315	CHL	C1D-ND-C4D	-2.31	104.69	106.33
26	u	314	CHL	C1B-CHB-C4A	-2.31	125.54	130.12
26	g	312	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
34	B	621	LMG	C8-O7-C10	-2.31	112.11	117.79
23	1	310	LUT	C18-C5-C6	-2.31	121.94	124.53
23	v	309	LUT	C1-C2-C3	2.31	118.86	113.64
27	N	318	NEX	C31-C30-C29	-2.31	124.02	127.31
26	v	316	CHL	C1-C2-C3	-2.31	122.05	126.04
22	b	605	CLA	CBA-CAA-C2A	2.31	120.67	113.86
22	s	301	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	5	309	LUT	C39-C29-C28	2.30	121.71	118.08
23	S	311	LUT	C18-C5-C4	2.30	118.62	114.36
31	D	404	BCR	C23-C24-C25	-2.30	120.73	127.20
32	C	501	SQD	O48-C23-C24	2.30	119.14	111.91
24	P	312	XAT	C27-C28-C29	-2.30	121.96	125.53
22	3	301	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	5	303	CLA	C1-C2-C3	-2.30	123.03	126.75
26	2	317	CHL	O2A-CGA-O1A	-2.30	117.78	123.59
22	v	302	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	N	310	LUT	C2-C3-C4	2.30	113.45	110.30
23	U	309	LUT	C10-C11-C12	-2.30	116.04	123.22
22	X	202	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	s	304	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
24	n	311	XAT	C20-C13-C12	2.30	121.70	118.08
26	V	315	CHL	OMC-CMC-C2C	-2.30	120.49	125.69
26	v	313	CHL	O1D-CGD-CBD	-2.30	119.78	124.48
24	g	309	XAT	C36-C21-C26	2.30	116.25	110.05
22	r	609	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
31	a	409	BCR	C38-C26-C27	2.30	118.03	113.62
22	2	302	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
26	6	314	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
23	1	309	LUT	C10-C11-C12	-2.30	116.04	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	406	CLA	C2D-C1D-ND	-2.30	108.41	110.10
22	r	609	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	c	512	CLA	C2A-C1A-CHA	2.30	127.88	123.86
23	n	310	LUT	C1-C6-C5	-2.30	119.38	122.61
22	n	306	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
31	C	517	BCR	C29-C30-C25	2.30	114.02	110.48
26	Q	311	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
22	R	311	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
26	N	315	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
26	p	314	CHL	C4D-CHA-C1A	-2.30	118.45	121.25
26	V	317	CHL	O2A-CGA-O1A	-2.29	117.80	123.59
26	P	318	CHL	C4-C3-C5	2.29	119.13	115.27
26	1	314	CHL	C1D-ND-C4D	-2.29	104.70	106.33
22	3	307	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
22	c	504	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
24	p	312	XAT	C31-C30-C29	-2.29	124.04	127.31
27	u	320	NEX	C11-C12-C13	-2.29	119.97	126.42
36	c	519	DGD	O6D-C5D-C4D	2.29	113.86	109.69
23	s	311	LUT	C15-C35-C34	-2.29	118.78	123.47
26	U	316	CHL	C4D-CHA-C1A	-2.29	118.46	121.25
23	N	310	LUT	C11-C10-C9	-2.29	124.04	127.31
22	g	305	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	U	315	CHL	C4D-C3D-CAD	2.29	110.80	108.10
23	s	311	LUT	C30-C31-C32	-2.29	116.06	123.22
32	L	102	SQD	O48-C23-C24	2.29	119.10	111.91
26	Q	315	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
26	1	317	CHL	C1-C2-C3	-2.29	122.08	126.04
22	3	305	CLA	O2D-CGD-CBD	2.29	115.34	111.27
27	N	318	NEX	C30-C31-C32	-2.29	116.07	123.22
22	c	507	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	U	317	CHL	O2A-CGA-CBA	2.29	119.09	111.91
24	R	313	XAT	C39-C29-C28	2.29	121.68	118.08
22	C	509	CLA	CHD-C1D-ND	-2.29	122.35	124.45
31	T	101	BCR	C1-C6-C7	2.29	122.25	115.78
31	c	515	BCR	C29-C30-C25	2.29	114.00	110.48
26	U	315	CHL	OMC-CMC-C2C	-2.29	120.52	125.69
26	U	315	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
24	r	612	XAT	C31-C32-C33	-2.29	119.99	126.42
22	2	301	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	S	306	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
32	C	501	SQD	O5-C1-C2	2.29	115.19	110.35
22	a	406	CLA	C2D-C1D-ND	-2.29	108.42	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g	311	CHL	CMB-C2B-C3B	2.29	128.96	124.68
22	R	308	CLA	C2A-C1A-CHA	2.29	127.86	123.86
23	V	309	LUT	C31-C30-C29	-2.28	124.05	127.31
23	n	310	LUT	C11-C10-C9	-2.28	124.05	127.31
26	n	315	CHL	CMB-C2B-C3B	2.28	128.95	124.68
32	m	101	SQD	O8-S-C6	2.28	109.38	105.74
22	5	301	CLA	CHB-C4A-NA	2.28	127.67	124.51
26	4	315	CHL	C4A-NA-C1A	2.28	107.73	106.71
26	N	316	CHL	C2A-C1A-CHA	-2.28	119.86	123.86
22	1	301	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
22	q	303	CLA	C1-C2-C3	-2.28	123.06	126.75
26	p	318	CHL	C4-C3-C5	2.28	119.11	115.27
33	d	404	PL9	C45-C44-C46	2.28	119.11	115.27
23	N	310	LUT	C18-C5-C6	-2.28	121.96	124.53
26	1	315	CHL	O2D-CGD-O1D	-2.28	119.37	123.84
32	M	101	SQD	O8-S-C6	2.28	109.38	105.74
26	s	313	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
34	C	502	LMG	C8-O7-C10	-2.28	112.17	117.79
22	Q	302	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
32	L	102	SQD	O48-C23-O10	-2.28	117.83	123.59
26	6	313	CHL	CAA-C2A-C3A	-2.28	106.53	112.78
26	2	313	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
22	C	513	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	u	303	CLA	O2D-CGD-CBD	2.28	115.32	111.27
26	4	317	CHL	C2A-C1A-CHA	-2.28	119.87	123.86
26	Q	316	CHL	C1-C2-C3	-2.28	122.10	126.04
22	6	306	CLA	O2D-CGD-CBD	2.28	115.32	111.27
31	B	618	BCR	C10-C11-C12	-2.28	116.10	123.22
22	1	305	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
22	2	307	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
23	S	311	LUT	C30-C31-C32	-2.28	116.11	123.22
36	c	517	DGD	C6D-C5D-C4D	-2.28	107.33	112.09
23	P	310	LUT	C31-C30-C29	-2.28	124.06	127.31
26	3	313	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
22	4	306	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
23	P	311	LUT	C22-C23-C24	-2.28	109.15	111.74
22	P	306	CLA	CAD-C3D-C2D	2.28	151.79	140.80
26	V	316	CHL	CED-O2D-CGD	2.28	121.09	115.94
22	v	302	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
26	R	317	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
31	d	403	BCR	C10-C11-C12	-2.28	116.11	123.22
31	a	409	BCR	C37-C22-C23	2.28	121.67	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	409	BCR	C37-C22-C23	2.28	121.67	118.08
26	U	314	CHL	OMC-CMC-C2C	-2.28	120.54	125.69
31	A	409	BCR	C15-C16-C17	-2.28	118.81	123.47
31	z	101	BCR	C34-C9-C8	2.28	121.66	118.08
26	G	316	CHL	C2A-C1A-CHA	-2.28	119.88	123.86
31	d	403	BCR	C23-C24-C25	-2.28	120.81	127.20
27	N	318	NEX	C15-C35-C34	-2.28	118.81	123.47
27	p	301	NEX	C30-C31-C32	-2.28	116.12	123.22
32	l	102	SQD	O48-C23-O10	-2.27	117.85	123.59
26	V	315	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
26	5	318	CHL	O1D-CGD-CBD	-2.27	119.83	124.48
24	R	313	XAT	C16-C1-C6	2.27	116.18	110.05
27	p	301	NEX	C28-C29-C30	2.27	122.43	118.94
26	P	315	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
26	q	314	CHL	CMB-C2B-C3B	2.27	128.93	124.68
26	S	313	CHL	O2D-CGD-O1D	-2.27	119.40	123.84
22	p	305	CLA	CMA-C3A-C4A	-2.27	105.67	111.77
26	U	317	CHL	C4-C3-C5	2.27	119.09	115.27
24	q	309	XAT	C36-C21-C26	2.27	116.17	110.05
26	P	316	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
22	5	302	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	q	303	CLA	C2A-C1A-CHA	2.27	127.83	123.86
23	5	310	LUT	C35-C15-C14	-2.27	118.83	123.47
22	q	305	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	P	307	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
27	S	317	NEX	C26-C27-C28	-2.27	121.20	125.99
23	2	310	LUT	C22-C23-C24	-2.27	109.16	111.74
22	P	303	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	n	305	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	a	406	CLA	C1-C2-C3	-2.27	123.08	126.75
22	U	307	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	q	308	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	c	512	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	6	302	CLA	CHB-C4A-NA	2.27	127.64	124.51
22	P	309	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	R	302	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
26	p	319	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
26	n	317	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
26	u	318	CHL	O2A-CGA-CBA	2.27	119.02	111.91
26	2	314	CHL	C1D-CHD-C4C	-2.26	121.17	126.06
22	C	507	CLA	C3A-C2A-C1A	2.26	104.73	101.34
31	c	516	BCR	C10-C11-C12	-2.26	116.15	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	u	307	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
26	v	317	CHL	C1-C2-C3	-2.26	122.13	126.04
22	c	506	CLA	C3A-C2A-C1A	2.26	104.73	101.34
24	1	311	XAT	C30-C31-C32	-2.26	116.16	123.22
26	p	320	CHL	C1-C2-C3	-2.26	122.13	126.04
26	U	317	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
26	v	316	CHL	C1B-CHB-C4A	-2.26	125.64	130.12
22	s	307	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	p	311	LUT	C15-C35-C34	-2.26	118.84	123.47
24	n	311	XAT	C35-C15-C14	-2.26	118.84	123.47
26	U	319	CHL	C2A-C3A-C4A	-2.26	98.22	101.87
26	Q	315	CHL	C2A-C1A-CHA	-2.26	119.91	123.86
23	p	311	LUT	C7-C8-C9	-2.26	122.82	126.23
23	p	311	LUT	C22-C23-C24	-2.26	109.17	111.74
24	3	309	XAT	C36-C21-C26	2.26	116.15	110.05
22	S	303	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
26	3	312	CHL	CAA-C2A-C3A	-2.26	106.59	112.78
26	6	314	CHL	OMC-CMC-C2C	-2.26	120.58	125.69
22	c	502	CLA	C2D-C1D-ND	-2.26	108.44	110.10
22	B	602	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
26	v	314	CHL	CAA-C2A-C3A	-2.26	106.59	112.78
22	B	607	CLA	O2D-CGD-CBD	2.26	115.28	111.27
27	s	317	NEX	C26-C27-C28	-2.26	121.22	125.99
31	b	620	BCR	C37-C22-C23	2.26	121.64	118.08
22	G	305	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	S	302	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
26	V	316	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
32	l	102	SQD	O48-C23-C24	2.26	118.99	111.91
22	R	310	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
22	Q	307	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
22	4	305	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
22	b	607	CLA	O2D-CGD-CBD	2.25	115.28	111.27
22	3	303	CLA	C1-C2-C3	-2.25	123.10	126.75
22	c	503	CLA	C2A-C1A-CHA	2.25	127.80	123.86
22	u	306	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
22	r	602	CLA	CHD-C1D-ND	-2.25	122.38	124.45
23	2	310	LUT	C1-C2-C3	2.25	118.73	113.64
22	B	615	CLA	O2D-CGD-CBD	2.25	115.27	111.27
27	5	319	NEX	C30-C31-C32	-2.25	116.19	123.22
32	a	413	SQD	O48-C23-O10	-2.25	117.91	123.59
22	S	307	CLA	C1B-CHB-C4A	-2.25	125.66	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	317	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
26	n	313	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
26	2	318	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
22	q	307	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
31	a	409	BCR	C10-C11-C12	-2.25	116.19	123.22
22	c	513	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	6	304	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
26	5	314	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
22	V	305	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
24	r	612	XAT	C16-C1-C6	2.25	116.12	110.05
27	r	618	NEX	C15-C35-C34	-2.25	118.87	123.47
22	a	408	CLA	O2D-CGD-CBD	2.25	115.27	111.27
22	4	302	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
26	N	317	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
36	c	517	DGD	O2G-C1B-O1B	-2.25	118.27	123.70
26	g	313	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
26	G	311	CHL	CMB-C2B-C3B	2.25	128.88	124.68
32	a	410	SQD	O5-C1-C2	2.25	115.11	110.35
26	V	317	CHL	C4-C3-C5	2.25	119.05	115.27
26	g	311	CHL	CHB-C4A-NA	2.25	127.62	124.51
22	V	302	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
26	u	318	CHL	O2D-CGD-O1D	-2.25	119.45	123.84
26	r	616	CHL	C1D-ND-C4D	-2.25	104.74	106.33
22	1	302	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	n	307	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
22	c	513	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
26	S	313	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
26	q	315	CHL	C1-C2-C3	-2.24	122.16	126.04
22	6	306	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
22	C	503	CLA	C2D-C1D-ND	-2.24	108.45	110.10
33	D	405	PL9	C51-C49-C50	2.24	119.56	114.60
22	G	302	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
36	C	519	DGD	C6D-C5D-C4D	-2.24	107.41	112.09
22	n	305	CLA	C3D-C4D-ND	2.24	113.86	110.24
22	n	303	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
22	4	306	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	S	310	LUT	C18-C5-C4	2.24	118.51	114.36
31	C	516	BCR	C11-C10-C9	-2.24	124.11	127.31
26	6	315	CHL	C1-C2-C3	-2.24	122.17	126.04
23	p	311	LUT	C18-C5-C6	-2.24	122.01	124.53
26	V	313	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
22	C	504	CLA	C2A-C1A-CHA	2.24	127.77	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	305	CLA	C4D-CHA-C1A	2.24	123.97	121.25
26	U	319	CHL	C4D-CHA-C1A	-2.24	118.53	121.25
36	C	519	DGD	O2G-C1B-O1B	-2.24	118.29	123.70
22	C	514	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	S	311	LUT	C35-C15-C14	-2.24	118.89	123.47
31	d	403	BCR	C16-C15-C14	-2.24	118.89	123.47
23	u	309	LUT	C10-C11-C12	-2.24	116.24	123.22
27	S	317	NEX	C16-C1-C6	2.24	112.47	110.47
34	c	501	LMG	C8-O7-C10	-2.24	112.28	117.79
22	s	303	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
22	c	508	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	6	313	CHL	CAA-C2A-C1A	2.24	119.30	111.97
23	5	310	LUT	C18-C5-C4	2.24	118.50	114.36
31	B	619	BCR	C24-C23-C22	-2.23	122.86	126.23
22	p	306	CLA	C2A-C1A-CHA	2.23	127.77	123.86
23	v	309	LUT	C3-C4-C5	-2.23	107.40	111.85
22	b	604	CLA	CHB-C4A-NA	2.23	127.60	124.51
27	P	301	NEX	C28-C29-C30	2.23	122.37	118.94
22	b	612	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
26	u	315	CHL	CED-O2D-CGD	2.23	120.98	115.94
23	N	310	LUT	C16-C1-C6	-2.23	106.68	110.30
22	S	308	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
26	5	318	CHL	C1B-CHB-C4A	-2.23	125.70	130.12
23	p	310	LUT	C15-C35-C34	-2.23	118.91	123.47
31	a	409	BCR	C15-C16-C17	-2.23	118.91	123.47
22	q	303	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
22	g	302	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
26	S	315	CHL	CHD-C1D-C2D	2.23	130.16	125.48
26	P	317	CHL	O1D-CGD-CBD	-2.23	119.92	124.48
26	u	317	CHL	C4D-CHA-C1A	-2.23	118.54	121.25
22	s	302	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
26	g	316	CHL	O1D-CGD-CBD	-2.23	119.93	124.48
22	p	302	CLA	CHD-C1D-ND	-2.23	122.41	124.45
26	r	616	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
26	5	315	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
22	2	301	CLA	C1-C2-C3	-2.23	122.19	126.04
22	N	305	CLA	C2A-C1A-CHA	2.23	127.75	123.86
36	c	518	DGD	C1E-C2E-C3E	2.23	114.63	110.00
26	g	316	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
22	b	617	CLA	CHA-C4D-ND	2.23	137.15	132.50
26	P	314	CHL	O1D-CGD-CBD	-2.23	119.93	124.48
23	R	312	LUT	C35-C15-C14	-2.23	118.92	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	407	PHO	OBD-CAD-CBD	-2.22	122.56	125.82
26	U	313	CHL	C4D-CHA-C1A	-2.22	118.54	121.25
26	2	318	CHL	O1D-CGD-CBD	-2.22	119.93	124.48
26	P	316	CHL	C1D-ND-C4D	-2.22	104.75	106.33
31	D	404	BCR	C10-C11-C12	-2.22	116.28	123.22
23	R	312	LUT	C30-C31-C32	-2.22	116.28	123.22
26	s	316	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
36	C	519	DGD	C6E-C5E-C4E	-2.22	107.80	113.00
23	p	311	LUT	C16-C1-C6	-2.22	106.69	110.30
26	v	316	CHL	C2A-C1A-CHA	-2.22	119.97	123.86
22	b	615	CLA	O2D-CGD-CBD	2.22	115.22	111.27
23	1	310	LUT	C15-C35-C34	-2.22	118.92	123.47
23	R	312	LUT	C10-C11-C12	-2.22	116.29	123.22
31	X	201	BCR	C34-C9-C10	-2.22	119.81	122.92
26	5	314	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
22	s	308	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	p	307	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	u	303	CLA	C1-C2-C3	-2.22	123.16	126.75
26	N	315	CHL	C1B-CHB-C4A	-2.22	125.72	130.12
24	6	310	XAT	C36-C21-C26	2.22	116.03	110.05
23	S	310	LUT	C21-C26-C27	-2.22	109.90	112.70
22	B	612	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
26	p	316	CHL	C1D-ND-C4D	-2.22	104.76	106.33
22	2	305	CLA	C3D-C4D-ND	2.22	113.82	110.24
27	N	318	NEX	C28-C29-C30	2.22	122.34	118.94
22	4	301	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	B	605	CLA	CMB-C2B-C3B	2.22	128.82	124.68
22	B	605	CLA	CBA-CAA-C2A	2.22	120.40	113.86
36	c	517	DGD	C6E-C5E-C4E	-2.22	107.81	113.00
26	u	315	CHL	CMD-C2D-C3D	-2.22	122.52	127.61
26	4	313	CHL	CHB-C4A-NA	2.22	127.58	124.51
26	P	319	CHL	O2D-CGD-O1D	-2.21	119.51	123.84
22	r	601	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
22	U	302	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
26	4	316	CHL	C1-C2-C3	-2.21	122.22	126.04
26	P	314	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
23	v	309	LUT	C31-C30-C29	-2.21	124.15	127.31
26	Q	314	CHL	C1-C2-C3	-2.21	122.22	126.04
22	3	305	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
26	N	313	CHL	C4-C3-C5	2.21	118.99	115.27
23	S	311	LUT	C19-C9-C8	2.21	121.56	118.08
22	r	604	CLA	O2A-CGA-O1A	-2.21	118.01	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	310	LUT	C8-C7-C6	-2.21	120.99	127.20
26	g	315	CHL	C2A-C1A-CHA	-2.21	119.99	123.86
22	N	303	CLA	C1-C2-C3	-2.21	123.18	126.75
24	v	311	XAT	C27-C28-C29	-2.21	122.10	125.53
23	V	310	LUT	C18-C5-C4	2.21	118.45	114.36
22	Q	305	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
32	A	412	SQD	O6-C1-C2	2.21	111.75	108.30
27	R	301	NEX	C4-C3-C2	-2.21	106.51	110.77
23	n	309	LUT	C30-C31-C32	-2.21	116.32	123.22
22	3	303	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
26	4	316	CHL	CED-O2D-CGD	2.21	120.93	115.94
26	3	315	CHL	C1B-CHB-C4A	-2.21	125.74	130.12
22	g	304	CLA	O1D-CGD-CBD	2.21	129.00	124.48
22	N	304	CLA	C1-C2-C3	-2.21	122.22	126.04
26	N	314	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
26	2	315	CHL	CHB-C4A-NA	2.21	127.56	124.51
26	s	313	CHL	OMC-CMC-C2C	-2.21	120.70	125.69
26	u	316	CHL	C4D-C3D-CAD	2.21	110.70	108.10
22	S	305	CLA	C1-C2-C3	-2.21	122.23	126.04
22	N	304	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
22	b	617	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
33	d	404	PL9	C51-C49-C50	2.21	119.47	114.60
27	S	317	NEX	C11-C12-C13	-2.21	120.22	126.42
22	6	306	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
22	U	307	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
26	G	313	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
23	v	309	LUT	C18-C5-C4	2.20	118.44	114.36
26	v	318	CHL	CHB-C4A-NA	2.20	127.56	124.51
26	5	317	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
22	Q	303	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
26	u	313	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
22	B	606	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
23	n	310	LUT	C3-C4-C5	-2.20	107.47	111.85
26	n	318	CHL	C1-C2-C3	-2.20	122.23	126.04
22	S	301	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
22	b	605	CLA	CMB-C2B-C3B	2.20	128.80	124.68
26	V	318	CHL	O1D-CGD-CBD	-2.20	119.98	124.48
26	p	320	CHL	C2A-C1A-CHA	-2.20	120.01	123.86
26	n	313	CHL	C4D-CHA-C1A	-2.20	118.57	121.25
23	P	310	LUT	C10-C11-C12	-2.20	116.35	123.22
22	C	504	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
23	V	309	LUT	C18-C5-C4	2.20	118.43	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	315	CHL	CHD-C1D-C2D	2.20	130.09	125.48
26	u	316	CHL	CHB-C4A-NA	2.20	127.55	124.51
31	K	101	BCR	C23-C24-C25	-2.20	121.03	127.20
26	2	313	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
23	4	310	LUT	C1-C6-C5	-2.20	119.52	122.61
26	V	315	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
23	u	309	LUT	C7-C8-C9	-2.20	122.92	126.23
22	C	514	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
31	k	101	BCR	C23-C24-C25	-2.20	121.03	127.20
26	1	316	CHL	C4D-CHA-C1A	-2.20	118.58	121.25
22	6	305	CLA	O1D-CGD-CBD	2.20	128.98	124.48
24	u	311	XAT	C35-C34-C33	-2.20	124.18	127.31
23	5	310	LUT	C1-C2-C3	2.20	118.60	113.64
31	C	516	BCR	C38-C26-C27	2.20	117.83	113.62
24	n	311	XAT	C36-C21-C26	2.20	115.97	110.05
22	C	510	CLA	C4-C3-C5	2.19	118.96	115.27
30	A	407	PHO	C1B-NB-C4B	2.19	111.60	107.09
22	Q	308	CLA	C2A-C1A-CHA	2.19	127.70	123.86
22	b	606	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
26	V	316	CHL	C2A-C3A-C4A	-2.19	98.33	101.87
22	q	308	CLA	C2A-C1A-CHA	2.19	127.69	123.86
23	V	309	LUT	C16-C1-C6	-2.19	106.74	110.30
23	V	309	LUT	C1-C2-C3	2.19	118.59	113.64
24	n	311	XAT	C27-C28-C29	-2.19	122.13	125.53
31	z	101	BCR	C11-C10-C9	-2.19	124.18	127.31
23	P	311	LUT	C18-C5-C6	-2.19	122.07	124.53
22	2	305	CLA	C4D-CHA-C1A	2.19	123.92	121.25
23	u	309	LUT	C30-C31-C32	-2.19	116.38	123.22
26	n	313	CHL	C4A-NA-C1A	2.19	107.69	106.71
33	a	411	PL9	C11-C9-C10	2.19	119.44	114.60
22	5	305	CLA	C3D-C4D-ND	2.19	113.78	110.24
26	4	313	CHL	C1D-ND-C4D	-2.19	104.78	106.33
32	A	412	SQD	O48-C23-O10	-2.19	118.06	123.59
31	b	619	BCR	C24-C23-C22	-2.19	122.93	126.23
26	v	316	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
26	g	312	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
26	v	315	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
22	Q	307	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
31	B	619	BCR	C30-C25-C24	2.19	121.97	115.78
22	C	508	CLA	O1D-CGD-CBD	2.19	128.96	124.48
31	C	517	BCR	C37-C22-C23	2.19	121.53	118.08
26	5	313	CHL	C4D-CHA-C1A	-2.19	118.58	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u	316	CHL	C2A-C1A-CHA	-2.19	120.03	123.86
23	S	311	LUT	C16-C1-C6	-2.19	106.75	110.30
26	n	313	CHL	C1B-CHB-C4A	-2.19	125.78	130.12
22	c	511	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
22	u	305	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
22	u	302	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
24	1	311	XAT	C27-C28-C29	-2.19	122.14	125.53
24	2	311	XAT	C30-C31-C32	-2.19	116.40	123.22
30	A	407	PHO	OBD-CAD-CBD	-2.19	122.62	125.82
27	r	618	NEX	C28-C29-C30	2.19	122.29	118.94
22	P	307	CLA	C2A-C1A-CHA	2.18	127.68	123.86
31	T	101	BCR	C2-C1-C6	2.18	113.84	110.48
22	C	503	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
22	U	301	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
26	g	316	CHL	C1-C2-C3	-2.18	122.27	126.04
22	R	305	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
26	p	314	CHL	O2A-CGA-O1A	-2.18	118.08	123.59
26	u	317	CHL	O2A-CGA-O1A	-2.18	118.08	123.59
26	G	314	CHL	C2A-C3A-C4A	-2.18	98.34	101.87
26	n	316	CHL	C1C-C2C-C3C	-2.18	105.38	107.11
24	Q	309	XAT	C36-C21-C26	2.18	115.94	110.05
22	V	305	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
26	g	316	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
22	N	305	CLA	C4D-CHA-C1A	2.18	123.91	121.25
26	n	314	CHL	C3D-C4D-ND	2.18	113.77	110.24
22	B	617	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
30	a	407	PHO	C1B-NB-C4B	2.18	111.57	107.09
24	v	311	XAT	C36-C21-C26	2.18	115.94	110.05
27	r	618	NEX	C20-C13-C14	-2.18	119.87	122.92
26	u	315	CHL	C1C-C2C-C3C	-2.18	105.38	107.11
26	Q	314	CHL	C2A-C3A-C4A	-2.18	98.35	101.87
31	B	620	BCR	C7-C8-C9	-2.18	122.94	126.23
27	v	319	NEX	C30-C31-C32	-2.18	116.41	123.22
22	n	304	CLA	C2D-C1D-ND	-2.18	108.50	110.10
22	c	506	CLA	C2A-C1A-CHA	2.18	127.67	123.86
26	5	313	CHL	C1D-ND-C4D	-2.18	104.79	106.33
22	b	613	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
26	3	314	CHL	C4A-NA-C1A	2.18	107.69	106.71
22	c	507	CLA	O1D-CGD-CBD	2.18	128.94	124.48
26	V	313	CHL	O1D-CGD-CBD	-2.18	120.03	124.48
26	6	314	CHL	CHD-C1D-C2D	2.18	130.05	125.48
36	a	416	DGD	O6E-C1E-C2E	2.18	114.96	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	407	PHO	CMD-C2D-C3D	2.18	128.75	124.68
23	4	309	LUT	C11-C10-C9	-2.18	124.20	127.31
26	6	313	CHL	CHD-C1D-C2D	2.18	130.05	125.48
22	V	306	CLA	C2A-C1A-CHA	2.18	127.67	123.86
24	g	309	XAT	C40-C33-C32	2.18	121.51	118.08
26	N	315	CHL	CHB-C4A-NA	2.18	127.52	124.51
23	s	310	LUT	C18-C5-C4	2.18	118.39	114.36
27	P	301	NEX	C30-C31-C32	-2.18	116.42	123.22
26	6	301	CHL	C1-C2-C3	-2.18	122.28	126.04
22	q	306	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
23	n	310	LUT	C10-C11-C12	-2.18	116.42	123.22
27	s	317	NEX	C2-C1-C6	2.18	111.33	109.21
22	r	608	CLA	C2A-C1A-CHA	2.18	127.66	123.86
22	4	306	CLA	C2A-C1A-CHA	2.18	127.66	123.86
26	v	317	CHL	O2A-CGA-O1A	-2.18	118.10	123.59
26	5	317	CHL	C2A-C1A-CHA	-2.18	120.06	123.86
26	g	311	CHL	O1D-CGD-CBD	-2.18	120.03	124.48
23	2	309	LUT	C3-C4-C5	-2.18	107.52	111.85
32	A	412	SQD	C1-O5-C5	2.17	117.96	113.69
26	S	316	CHL	C1D-ND-C4D	-2.17	104.79	106.33
26	s	316	CHL	C1D-ND-C4D	-2.17	104.79	106.33
22	r	609	CLA	C3A-C2A-C1A	2.17	104.60	101.34
31	t	101	BCR	C36-C18-C17	-2.17	119.88	122.92
22	C	512	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
24	1	311	XAT	C16-C1-C6	2.17	115.92	110.05
22	p	305	CLA	C1-C2-C3	-2.17	122.28	126.04
22	B	617	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
22	C	510	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
25	u	312	LHG	C5-O7-C7	-2.17	112.44	117.79
26	3	315	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
24	R	313	XAT	C24-C23-C22	-2.17	106.58	110.77
22	q	302	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	6	315	CHL	C1D-ND-C4D	-2.17	104.79	106.33
23	p	310	LUT	C16-C1-C6	-2.17	106.78	110.30
23	V	309	LUT	C30-C31-C32	-2.17	116.44	123.22
22	V	306	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
23	n	309	LUT	C16-C1-C6	-2.17	106.78	110.30
26	P	314	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
22	b	616	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	1	313	CHL	O2A-CGA-O1A	-2.17	118.11	123.59
26	5	316	CHL	O1D-CGD-CBD	-2.17	120.04	124.48
22	c	508	CLA	O2A-CGA-O1A	-2.17	118.11	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	314	CHL	C3D-C4D-ND	2.17	113.75	110.24
26	Q	316	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
22	6	302	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	u	306	CLA	C2A-C1A-CHA	2.17	127.65	123.86
22	U	303	CLA	C1-C2-C3	-2.17	123.24	126.75
22	n	305	CLA	C2A-C1A-CHA	2.17	127.65	123.86
26	s	313	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
26	2	315	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
22	6	306	CLA	C2A-C1A-CHA	2.17	127.65	123.86
26	4	313	CHL	O2A-CGA-O1A	-2.17	118.12	123.59
30	a	407	PHO	CMD-C2D-C3D	2.17	128.73	124.68
22	G	308	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	U	309	LUT	C8-C7-C6	-2.17	121.11	127.20
26	N	317	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
22	S	301	CLA	C2A-C1A-CHA	2.17	127.65	123.86
31	D	404	BCR	C16-C15-C14	-2.17	119.03	123.47
31	c	515	BCR	C37-C22-C23	2.17	121.49	118.08
31	a	409	BCR	C27-C26-C25	-2.17	119.59	122.73
27	N	318	NEX	C26-C27-C28	-2.17	121.41	125.99
33	A	410	PL9	C11-C9-C10	2.17	119.39	114.60
27	P	301	NEX	C31-C30-C29	-2.17	124.22	127.31
22	4	307	CLA	CAC-C3C-C4C	2.17	127.62	124.81
27	u	320	NEX	C19-C9-C10	-2.17	119.89	122.92
26	2	317	CHL	C2A-C1A-CHA	-2.17	120.07	123.86
23	P	310	LUT	C8-C7-C6	-2.17	121.12	127.20
36	A	414	DGD	O6E-C1E-C2E	2.16	114.93	110.35
23	N	310	LUT	C8-C7-C6	-2.16	121.12	127.20
23	s	311	LUT	C39-C29-C28	2.16	121.49	118.08
26	g	316	CHL	C1B-CHB-C4A	-2.16	125.83	130.12
22	n	305	CLA	C3A-C2A-C1A	2.16	104.58	101.34
26	6	312	CHL	C4D-CHA-C1A	-2.16	118.62	121.25
22	C	515	CLA	C2A-C1A-CHA	2.16	127.64	123.86
24	G	309	XAT	C36-C21-C26	2.16	115.89	110.05
23	u	309	LUT	C18-C5-C6	-2.16	122.10	124.53
26	Q	314	CHL	CED-O2D-CGD	2.16	120.83	115.94
23	v	310	LUT	C16-C1-C6	-2.16	106.79	110.30
24	4	311	XAT	C16-C1-C6	2.16	115.88	110.05
26	6	317	CHL	C1-C2-C3	-2.16	122.30	126.04
22	s	301	CLA	C2A-C1A-CHA	2.16	127.64	123.86
22	q	301	CLA	CHD-C1D-ND	-2.16	122.47	124.45
22	C	509	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
23	V	310	LUT	C1-C2-C3	2.16	118.52	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	315	CHL	O1D-CGD-CBD	-2.16	120.06	124.48
26	q	311	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
22	r	601	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	1	313	CHL	O1D-CGD-CBD	-2.16	120.06	124.48
26	2	318	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
22	G	302	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
31	b	619	BCR	C30-C25-C24	2.16	121.89	115.78
22	p	303	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	5	314	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
23	U	310	LUT	C18-C5-C6	-2.16	122.10	124.53
22	3	302	CLA	C1-O2A-CGA	2.16	122.10	116.44
26	u	318	CHL	C1-C2-C3	-2.16	122.31	126.04
23	U	309	LUT	C38-C25-C24	-2.16	118.94	123.56
26	u	313	CHL	C2A-C1A-CHA	-2.16	120.09	123.86
31	A	409	BCR	C27-C26-C25	-2.16	119.60	122.73
26	G	315	CHL	C2A-C1A-CHA	-2.16	120.09	123.86
22	s	301	CLA	CMA-C3A-C4A	-2.15	105.98	111.77
23	n	309	LUT	C10-C11-C12	-2.15	116.50	123.22
26	G	311	CHL	C2A-C1A-CHA	-2.15	120.09	123.86
26	n	315	CHL	OMC-CMC-C2C	-2.15	120.82	125.69
27	r	618	NEX	C26-C27-C28	-2.15	121.44	125.99
26	1	317	CHL	C2A-C1A-CHA	-2.15	120.09	123.86
26	6	314	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
26	q	314	CHL	C4-C3-C5	2.15	118.89	115.27
23	S	310	LUT	C38-C25-C24	-2.15	118.95	123.56
22	p	306	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
26	2	317	CHL	CBC-CAC-C3C	-2.15	106.50	112.43
24	p	312	XAT	C20-C13-C12	2.15	121.47	118.08
22	c	514	CLA	C2A-C1A-CHA	2.15	127.62	123.86
23	u	310	LUT	C18-C5-C6	-2.15	122.11	124.53
26	1	317	CHL	C4D-CHA-C1A	-2.15	118.63	121.25
22	B	616	CLA	C2A-C1A-CHA	2.15	127.62	123.86
27	u	320	NEX	C17-C1-C6	-2.15	108.55	110.47
23	1	309	LUT	C18-C5-C6	-2.15	122.11	124.53
27	P	301	NEX	C19-C9-C10	-2.15	119.91	122.92
22	b	610	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	b	611	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
24	n	311	XAT	C28-C29-C30	-2.15	115.64	118.94
26	G	312	CHL	C4D-CHA-C1A	-2.15	118.64	121.25
22	R	309	CLA	C2A-C1A-CHA	2.15	127.61	123.86
22	B	611	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
22	c	509	CLA	CAA-C2A-C3A	-2.15	106.90	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R	315	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
22	S	308	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
22	P	309	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
31	C	517	BCR	C15-C16-C17	-2.15	119.08	123.47
22	s	308	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
26	P	317	CHL	CED-O2D-CGD	2.14	120.78	115.94
22	n	308	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
24	v	311	XAT	C35-C15-C14	-2.14	119.08	123.47
26	u	313	CHL	C4D-CHA-C1A	-2.14	118.64	121.25
26	Q	315	CHL	CED-O2D-CGD	2.14	120.78	115.94
22	U	305	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	c	502	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
26	3	316	CHL	C2A-C1A-CHA	-2.14	120.11	123.86
22	P	307	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
26	3	312	CHL	CHD-C1D-C2D	2.14	129.97	125.48
26	S	313	CHL	C1C-C2C-C3C	-2.14	105.42	107.11
26	3	312	CHL	CAA-C2A-C1A	2.14	118.99	111.97
26	G	316	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
23	n	310	LUT	C1-C2-C3	2.14	118.47	113.64
26	1	318	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
26	4	316	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
23	s	311	LUT	C19-C9-C8	2.14	121.45	118.08
22	R	302	CLA	CAC-C3C-C4C	2.14	127.58	124.81
22	P	303	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
31	c	515	BCR	C7-C6-C5	-2.14	116.28	121.46
26	g	316	CHL	C2A-C1A-CHA	-2.14	120.12	123.86
26	n	315	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
22	C	507	CLA	C2A-C1A-CHA	2.14	127.60	123.86
22	b	613	CLA	C2A-C1A-CHA	2.14	127.60	123.86
26	1	318	CHL	C2A-C1A-CHA	-2.14	120.12	123.86
31	c	516	BCR	C34-C9-C10	-2.14	119.93	122.92
22	C	511	CLA	C11-C12-C13	-2.14	109.01	115.92
26	v	318	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
26	5	314	CHL	CHD-C1D-C2D	2.14	129.96	125.48
26	G	316	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
26	S	313	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
26	3	311	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
31	T	101	BCR	C29-C30-C25	2.14	113.77	110.48
22	p	303	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
26	6	317	CHL	O2D-CGD-O1D	-2.13	119.66	123.84
26	6	314	CHL	C2D-C1D-ND	2.13	111.68	110.10
22	3	304	CLA	O1D-CGD-CBD	2.13	128.85	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	U	310	LUT	C10-C11-C12	-2.13	116.56	123.22
26	R	316	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
26	q	314	CHL	C2A-C1A-CHA	-2.13	120.13	123.86
22	c	504	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	Q	315	CHL	CMB-C2B-C3B	2.13	128.67	124.68
23	R	312	LUT	C11-C10-C9	-2.13	124.27	127.31
26	S	313	CHL	CHB-C4A-NA	2.13	127.46	124.51
26	1	314	CHL	O2A-CGA-CBA	2.13	118.60	111.91
26	S	316	CHL	CHD-C1D-C2D	2.13	129.95	125.48
26	v	315	CHL	OMC-CMC-C2C	-2.13	120.86	125.69
23	u	309	LUT	C8-C7-C6	-2.13	121.21	127.20
22	x	201	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
26	P	317	CHL	C1-C2-C3	-2.13	122.36	126.04
23	V	310	LUT	C16-C1-C6	-2.13	106.84	110.30
26	Q	313	CHL	C1B-CHB-C4A	-2.13	125.90	130.12
22	S	307	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
27	r	617	NEX	C31-C30-C29	-2.13	124.27	127.31
22	B	616	CLA	C2D-C1D-ND	-2.13	108.53	110.10
22	v	305	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	5	301	CLA	C1-C2-C3	-2.13	122.36	126.04
22	c	510	CLA	C11-C12-C13	-2.13	109.03	115.92
26	s	316	CHL	CHD-C1D-C2D	2.13	129.95	125.48
24	N	311	XAT	C40-C33-C32	2.13	121.43	118.08
22	B	613	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
24	5	311	XAT	C16-C1-C6	2.13	115.79	110.05
26	6	313	CHL	O2A-CGA-O1A	-2.13	118.22	123.59
26	1	314	CHL	CED-O2D-CGD	2.13	120.75	115.94
26	3	316	CHL	C1-C2-C3	-2.13	122.36	126.04
22	b	610	CLA	C4-C3-C5	2.13	118.85	115.27
22	C	505	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	p	312	XAT	C35-C15-C14	-2.13	119.11	123.47
22	B	617	CLA	C2D-C1D-ND	-2.13	108.54	110.10
24	V	311	XAT	C10-C11-C12	-2.13	116.58	123.22
32	m	101	SQD	O48-C23-O10	-2.13	118.22	123.59
27	u	320	NEX	C4-C3-C2	-2.13	106.67	110.77
22	B	613	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
22	4	301	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	P	304	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	2	309	LUT	C8-C7-C6	-2.12	121.23	127.20
26	g	316	CHL	C4D-CHA-C1A	-2.12	118.66	121.25
24	U	311	XAT	C36-C21-C26	2.12	115.78	110.05
31	B	618	BCR	C33-C5-C6	-2.12	122.14	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Q	304	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	2	316	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
26	v	316	CHL	CHB-C4A-NA	2.12	127.45	124.51
22	N	305	CLA	CAD-C3D-C2D	2.12	151.05	140.80
26	n	313	CHL	C1-C2-C3	-2.12	122.37	126.04
26	3	315	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
23	1	310	LUT	C11-C10-C9	-2.12	124.28	127.31
36	c	518	DGD	O5D-C1E-C2E	2.12	111.62	108.30
23	N	309	LUT	C38-C25-C24	-2.12	119.02	123.56
22	6	307	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
22	3	304	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
31	C	518	BCR	C34-C9-C10	-2.12	119.95	122.92
22	4	305	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
26	v	315	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
22	n	305	CLA	OBD-CAD-C3D	2.12	133.62	128.52
22	R	310	CLA	C1-C2-C3	-2.12	122.38	126.04
23	N	309	LUT	C35-C15-C14	-2.12	119.13	123.47
26	4	316	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
22	v	302	CLA	CHD-C1D-ND	-2.12	122.51	124.45
26	V	313	CHL	C4-C3-C5	2.12	118.83	115.27
26	4	313	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
26	U	319	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
26	n	317	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
22	d	402	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
32	M	101	SQD	O48-C23-O10	-2.12	118.25	123.59
26	n	317	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
22	4	307	CLA	C1-C2-C3	-2.12	122.38	126.04
26	u	314	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
24	U	311	XAT	C30-C31-C32	-2.12	116.61	123.22
22	1	305	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
22	c	510	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
22	b	613	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
24	2	311	XAT	C16-C1-C6	2.12	115.76	110.05
22	n	306	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	6	316	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
26	N	317	CHL	C1-C2-C3	-2.11	122.39	126.04
22	V	304	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
26	g	314	CHL	C4D-CHA-C1A	-2.11	118.68	121.25
22	b	617	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	4	311	XAT	C36-C21-C26	2.11	115.75	110.05
23	r	611	LUT	C31-C30-C29	-2.11	124.30	127.31
22	s	301	CLA	CAA-C2A-C3A	-2.11	106.99	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	517	BCR	C7-C6-C5	-2.11	116.34	121.46
22	N	306	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	s	317	NEX	C11-C12-C13	-2.11	120.49	126.42
23	R	312	LUT	C16-C1-C6	-2.11	106.88	110.30
22	U	306	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	3	304	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	4	310	LUT	C1-C2-C3	2.11	118.41	113.64
27	V	319	NEX	C30-C31-C32	-2.11	116.63	123.22
22	B	605	CLA	O2D-CGD-CBD	2.11	115.02	111.27
23	N	310	LUT	C10-C11-C12	-2.11	116.64	123.22
31	t	101	BCR	C34-C9-C10	-2.11	119.97	122.92
22	6	306	CLA	C3A-C2A-C1A	2.11	104.50	101.34
26	3	311	CHL	C4D-CHA-C1A	-2.11	118.68	121.25
26	V	316	CHL	C1-C2-C3	-2.11	122.40	126.04
22	C	504	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
26	Q	313	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
22	p	306	CLA	C4D-CHA-C1A	2.11	123.81	121.25
27	5	319	NEX	C26-C27-C28	-2.11	121.54	125.99
26	S	314	CHL	C4D-CHA-C1A	-2.11	118.69	121.25
25	D	407	LHG	C6-C5-C4	-2.11	106.81	111.79
24	g	309	XAT	C16-C1-C6	2.11	115.73	110.05
23	n	309	LUT	C18-C5-C4	2.11	118.25	114.36
22	c	509	CLA	C4-C3-C5	2.10	118.81	115.27
26	3	314	CHL	C1D-ND-C4D	-2.10	104.84	106.33
26	R	315	CHL	O1D-CGD-CBD	-2.10	120.18	124.48
22	1	303	CLA	C1-C2-C3	-2.10	123.35	126.75
31	b	620	BCR	C21-C20-C19	-2.10	116.65	123.22
26	5	318	CHL	O2A-CGA-CBA	2.10	118.51	111.91
37	e	101	HEM	CAA-CBA-CGA	-2.10	107.86	113.76
22	X	202	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
22	1	306	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
26	r	615	CHL	C1B-CHB-C4A	-2.10	125.95	130.12
31	T	101	BCR	C34-C9-C10	-2.10	119.98	122.92
23	5	309	LUT	C16-C1-C6	-2.10	106.89	110.30
26	5	318	CHL	C2A-C1A-CHA	-2.10	120.18	123.86
31	x	202	BCR	C30-C25-C24	2.10	121.72	115.78
23	v	309	LUT	C30-C31-C32	-2.10	116.66	123.22
23	s	311	LUT	C16-C1-C6	-2.10	106.89	110.30
26	p	318	CHL	C1-O2A-CGA	2.10	121.96	116.44
26	4	314	CHL	CED-O2D-CGD	2.10	120.69	115.94
22	V	303	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
22	A	408	CLA	O2D-CGD-CBD	2.10	115.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	s	307	CLA	C2A-C1A-CHA	2.10	127.53	123.86
26	6	314	CHL	O1D-CGD-CBD	-2.10	120.19	124.48
26	u	315	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
26	g	311	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
22	B	616	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	2	309	LUT	C39-C29-C28	2.10	121.38	118.08
26	p	317	CHL	CAA-CBA-CGA	-2.10	107.12	113.25
31	D	404	BCR	C15-C14-C13	-2.10	124.32	127.31
26	2	318	CHL	O2A-CGA-CBA	2.10	118.49	111.91
22	b	606	CLA	CMB-C2B-C3B	2.10	128.60	124.68
23	N	310	LUT	C22-C23-C24	-2.10	109.35	111.74
26	6	301	CHL	C4D-CHA-C1A	-2.10	118.70	121.25
27	V	319	NEX	C31-C30-C29	-2.10	124.32	127.31
31	d	403	BCR	C21-C20-C19	-2.10	116.67	123.22
22	C	511	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
23	4	309	LUT	C15-C35-C34	-2.10	119.18	123.47
22	6	303	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	n	306	CLA	C2A-C1A-CHA	2.10	127.52	123.86
26	q	313	CHL	O1D-CGD-CBD	-2.10	120.20	124.48
24	u	311	XAT	C30-C31-C32	-2.10	116.68	123.22
26	6	315	CHL	CED-O2D-CGD	2.09	120.67	115.94
27	p	301	NEX	C35-C15-C14	-2.09	119.18	123.47
26	6	315	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
22	v	304	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
31	z	101	BCR	C38-C26-C27	2.09	117.64	113.62
22	v	302	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	B	608	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	g	302	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	b	604	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	c	509	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
24	n	311	XAT	C40-C33-C32	2.09	121.38	118.08
26	p	319	CHL	C1-C2-C3	-2.09	122.42	126.04
22	D	403	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
26	U	314	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
22	B	613	CLA	C2A-C1A-CHA	2.09	127.52	123.86
26	p	314	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
24	p	312	XAT	C16-C1-C6	2.09	115.69	110.05
26	1	318	CHL	C1-C2-C3	-2.09	122.42	126.04
26	V	314	CHL	C1D-ND-C4D	-2.09	104.85	106.33
31	B	618	BCR	C29-C30-C25	2.09	113.70	110.48
31	T	101	BCR	C36-C18-C17	-2.09	119.99	122.92
26	3	313	CHL	O1D-CGD-CBD	-2.09	120.20	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	316	CHL	O1D-CGD-CBD	-2.09	120.21	124.48
22	U	304	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	p	307	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	r	601	CLA	C2A-C1A-CHA	2.09	127.51	123.86
22	C	510	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	3	305	CLA	C2A-C1A-CHA	2.09	127.51	123.86
26	Q	312	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
26	2	314	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
31	D	404	BCR	C21-C20-C19	-2.09	116.70	123.22
26	u	314	CHL	C2A-C1A-CHA	-2.09	120.21	123.86
26	2	313	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
22	N	302	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	5	316	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
26	v	313	CHL	C1C-C2C-C3C	-2.09	105.46	107.11
22	Q	302	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
31	t	101	BCR	C2-C1-C6	2.09	113.69	110.48
26	v	315	CHL	C4A-NA-C1A	2.09	107.64	106.71
26	U	314	CHL	CED-O2D-CGD	2.09	120.66	115.94
31	a	409	BCR	C1-C6-C7	2.09	121.68	115.78
26	R	316	CHL	O2A-CGA-CBA	2.09	118.45	111.91
22	g	305	CLA	C3A-C2A-C1A	2.09	104.46	101.34
24	G	309	XAT	C16-C1-C6	2.09	115.68	110.05
26	2	318	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
26	S	315	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
26	2	316	CHL	O2D-CGD-O1D	-2.09	119.76	123.84
23	U	309	LUT	C20-C13-C12	2.08	121.36	118.08
26	n	315	CHL	O2D-CGD-O1D	-2.08	119.76	123.84
31	B	620	BCR	C37-C22-C23	2.08	121.36	118.08
27	P	301	NEX	O4-C5-C18	-2.08	105.68	109.39
26	u	316	CHL	OMC-CMC-C2C	-2.08	120.97	125.69
22	1	302	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	b	605	CLA	O2D-CGD-CBD	2.08	114.97	111.27
23	P	310	LUT	C39-C29-C28	2.08	121.36	118.08
22	4	303	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	u	316	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
22	p	303	CLA	C2A-C1A-CHA	2.08	127.50	123.86
22	U	308	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	3	313	CHL	C1D-ND-C4D	-2.08	104.86	106.33
24	R	313	XAT	C36-C21-C26	2.08	115.67	110.05
23	P	311	LUT	C10-C11-C12	-2.08	116.72	123.22
22	s	307	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	n	311	XAT	C15-C35-C34	-2.08	119.21	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	409	BCR	C1-C6-C7	2.08	121.66	115.78
26	V	318	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
26	3	316	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
27	U	318	NEX	C11-C12-C13	-2.08	120.57	126.42
23	4	309	LUT	C16-C1-C6	-2.08	106.93	110.30
22	1	306	CLA	C2A-C1A-CHA	2.08	127.50	123.86
26	p	314	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
26	4	315	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
26	6	312	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
26	G	313	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
22	R	310	CLA	C2A-C1A-CHA	2.08	127.49	123.86
26	N	316	CHL	O2D-CGD-O1D	-2.08	119.78	123.84
23	u	310	LUT	C10-C11-C12	-2.08	116.73	123.22
27	p	301	NEX	O24-C25-C26	-2.08	57.24	58.96
26	1	315	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
22	b	613	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	c	515	BCR	C30-C25-C24	2.08	121.66	115.78
22	4	303	CLA	C1-C2-C3	-2.08	123.39	126.75
27	n	319	NEX	C28-C29-C30	2.08	122.13	118.94
23	R	312	LUT	C31-C30-C29	-2.08	124.35	127.31
26	p	319	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
26	N	316	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
22	g	304	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	V	303	CLA	C1-C2-C3	-2.08	123.39	126.75
26	P	317	CHL	C2A-C3A-C4A	-2.08	98.52	101.87
22	p	309	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	5	304	CLA	C2A-C1A-CHA	2.08	127.49	123.86
26	q	314	CHL	CED-O2D-CGD	2.08	120.63	115.94
26	R	316	CHL	C1B-CHB-C4A	-2.07	126.01	130.12
22	d	402	CLA	C2D-C1D-ND	-2.07	108.58	110.10
23	P	311	LUT	C16-C1-C6	-2.07	106.93	110.30
23	U	310	LUT	C3-C4-C5	-2.07	107.72	111.85
26	Q	313	CHL	C2A-C1A-CHA	-2.07	120.23	123.86
27	p	301	NEX	C31-C30-C29	-2.07	124.35	127.31
26	v	314	CHL	C4D-CHA-C1A	-2.07	118.72	121.25
26	s	313	CHL	C4D-CHA-C1A	-2.07	118.72	121.25
31	b	619	BCR	C10-C11-C12	-2.07	116.75	123.22
27	s	317	NEX	C4-C3-C2	-2.07	106.77	110.77
22	2	305	CLA	C2A-C1A-CHA	2.07	127.48	123.86
33	D	405	PL9	C12-C11-C9	-2.07	106.16	112.98
26	g	312	CHL	O2A-CGA-O1A	-2.07	118.36	123.59
23	p	310	LUT	C10-C11-C12	-2.07	116.75	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	315	CHL	C2D-C1D-ND	2.07	111.63	110.10
22	G	305	CLA	C3A-C2A-C1A	2.07	104.44	101.34
24	P	312	XAT	C36-C21-C26	2.07	115.64	110.05
22	1	306	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
22	b	616	CLA	C2D-C1D-ND	-2.07	108.58	110.10
22	B	614	CLA	C2A-C1A-CHA	2.07	127.48	123.86
26	4	317	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
26	P	318	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
26	v	318	CHL	O2D-CGD-O1D	-2.07	119.79	123.84
22	B	613	CLA	O1D-CGD-CBD	2.07	128.72	124.48
23	N	310	LUT	C30-C31-C32	-2.07	116.76	123.22
33	d	404	PL9	C12-C11-C9	-2.07	106.17	112.98
23	5	310	LUT	C16-C1-C6	-2.07	106.94	110.30
22	s	305	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	2	318	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
22	r	607	CLA	C3A-C2A-C1A	2.07	104.44	101.34
22	P	306	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	g	315	CHL	C1C-C2C-C3C	-2.07	105.47	107.11
23	p	310	LUT	C1-C2-C3	2.07	118.31	113.64
31	d	403	BCR	C15-C14-C13	-2.07	124.36	127.31
22	u	304	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
22	B	604	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	P	311	LUT	C15-C35-C34	-2.07	119.24	123.47
26	s	315	CHL	C4D-CHA-C1A	-2.07	118.73	121.25
22	5	308	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
26	r	615	CHL	C1-O2A-CGA	2.07	121.87	116.44
26	v	315	CHL	CMB-C2B-C3B	2.07	128.54	124.68
26	2	317	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
22	N	306	CLA	C2A-C1A-CHA	2.07	127.47	123.86
22	1	303	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
22	5	302	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
31	B	619	BCR	C10-C11-C12	-2.07	116.77	123.22
31	b	619	BCR	C34-C9-C8	2.07	121.33	118.08
24	2	311	XAT	C35-C15-C14	-2.07	119.24	123.47
26	r	614	CHL	O1D-CGD-CBD	-2.07	120.26	124.48
22	c	510	CLA	O1D-CGD-CBD	2.06	128.71	124.48
22	c	503	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
26	U	315	CHL	C2A-C1A-CHA	-2.06	120.25	123.86
27	s	317	NEX	O24-C25-C26	-2.06	57.25	58.96
26	v	316	CHL	CED-O2D-CGD	2.06	120.61	115.94
27	V	319	NEX	O24-C25-C26	-2.06	57.25	58.96
22	B	605	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	p	306	CLA	C3A-C2A-C1A	2.06	104.43	101.34
22	p	304	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
26	3	312	CHL	O2A-CGA-O1A	-2.06	118.39	123.59
24	n	311	XAT	C16-C1-C6	2.06	115.61	110.05
24	R	313	XAT	C17-C1-C6	-2.06	104.48	110.05
22	s	302	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
22	2	306	CLA	CHA-C1A-NA	-2.06	121.68	126.40
26	r	614	CHL	C1C-C2C-C3C	-2.06	105.48	107.11
22	4	302	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
26	q	315	CHL	O1D-CGD-CBD	-2.06	120.27	124.48
22	p	306	CLA	C3D-C4D-ND	2.06	113.57	110.24
26	R	316	CHL	C1-O2A-CGA	2.06	121.85	116.44
22	g	305	CLA	C2A-C1A-CHA	2.06	127.46	123.86
31	x	202	BCR	C15-C16-C17	-2.06	119.25	123.47
26	P	318	CHL	C1-O2A-CGA	2.06	121.85	116.44
23	2	309	LUT	C31-C30-C29	-2.06	124.37	127.31
23	5	310	LUT	C3-C4-C5	-2.06	107.75	111.85
22	n	304	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	V	309	LUT	C35-C15-C14	-2.06	119.26	123.47
26	1	317	CHL	C1B-CHB-C4A	-2.06	126.04	130.12
27	p	301	NEX	C5-C4-C3	-2.06	109.31	111.75
37	E	101	HEM	CAA-CBA-CGA	-2.06	107.99	113.76
22	R	305	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
22	B	606	CLA	CMB-C2B-C3B	2.06	128.53	124.68
31	b	618	BCR	C11-C12-C13	-2.06	120.64	126.42
26	1	316	CHL	C1-C2-C3	-2.06	122.49	126.04
22	1	308	CLA	C2A-C1A-CHA	2.06	127.45	123.86
26	N	314	CHL	O2A-CGA-O1A	-2.06	118.41	123.59
26	g	314	CHL	O2D-CGD-O1D	-2.06	119.82	123.84
22	c	513	CLA	C1-C2-C3	-2.05	122.49	126.04
22	p	307	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	s	314	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
31	C	517	BCR	C30-C25-C24	2.05	121.59	115.78
26	3	315	CHL	OMC-CMC-C2C	-2.05	121.04	125.69
24	V	311	XAT	C36-C21-C26	2.05	115.59	110.05
26	1	318	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
26	n	316	CHL	O1D-CGD-CBD	-2.05	120.28	124.48
27	u	320	NEX	C26-C27-C28	-2.05	121.65	125.99
22	c	508	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
25	S	312	LHG	C5-O7-C7	-2.05	112.74	117.79
22	B	610	CLA	CHD-C1D-ND	-2.05	122.57	124.45
26	q	315	CHL	C4D-CHA-C1A	-2.05	118.75	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R	315	CHL	C1-C2-C3	-2.05	122.50	126.04
22	4	308	CLA	C2A-C1A-CHA	2.05	127.44	123.86
26	N	315	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
23	S	311	LUT	C39-C29-C28	2.05	121.31	118.08
23	5	309	LUT	C31-C30-C29	-2.05	124.39	127.31
22	Q	304	CLA	CHD-C1D-ND	-2.05	122.57	124.45
27	5	319	NEX	C16-C1-C6	2.05	112.31	110.47
22	B	607	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	u	316	CHL	CED-O2D-CGD	2.05	120.57	115.94
26	v	313	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
24	P	312	XAT	C16-C1-C6	2.05	115.57	110.05
26	3	314	CHL	C4D-CHA-C1A	-2.05	118.76	121.25
22	R	305	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
23	p	310	LUT	C35-C15-C14	-2.05	119.28	123.47
22	Q	308	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
26	5	315	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
26	v	316	CHL	OMC-CMC-C2C	-2.04	121.06	125.69
22	2	308	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
22	B	607	CLA	O2A-C1-C2	-2.04	103.26	108.64
23	2	309	LUT	C16-C1-C6	-2.04	106.98	110.30
31	t	101	BCR	C29-C30-C25	2.04	113.63	110.48
22	S	307	CLA	C2A-C1A-CHA	2.04	127.43	123.86
22	c	505	CLA	C3C-C4C-NC	-2.04	108.28	110.57
27	v	319	NEX	C16-C1-C6	2.04	112.30	110.47
22	G	304	CLA	O1D-CGD-CBD	2.04	128.66	124.48
27	u	319	NEX	O24-C25-C26	-2.04	57.27	58.96
22	C	506	CLA	C3C-C4C-NC	-2.04	108.28	110.57
22	b	613	CLA	O1D-CGD-CBD	2.04	128.66	124.48
22	5	304	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	n	314	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
26	Q	312	CHL	C4A-NA-C1A	2.04	107.62	106.71
22	p	306	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	r	619	CHL	C4D-CHA-C1A	-2.04	118.77	121.25
27	V	319	NEX	C15-C35-C34	-2.04	119.29	123.47
22	B	602	CLA	C2D-C1D-ND	-2.04	108.60	110.10
22	v	306	CLA	C1-C2-C3	-2.04	122.51	126.04
26	Q	311	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
25	d	406	LHG	C6-C5-C4	-2.04	106.96	111.79
22	R	303	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	d	401	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
22	U	304	CLA	O2D-CGD-CBD	2.04	114.89	111.27
23	P	310	LUT	C1-C2-C3	2.04	118.25	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	S	311	LUT	C8-C7-C6	-2.04	121.47	127.20
25	s	312	LHG	C5-O7-C7	-2.04	112.77	117.79
26	3	316	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
26	P	318	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
22	R	309	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
23	N	310	LUT	C39-C29-C28	2.04	121.29	118.08
26	r	619	CHL	C1C-C2C-C3C	-2.04	105.50	107.11
23	S	311	LUT	C11-C10-C9	-2.04	124.40	127.31
22	6	309	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
26	1	317	CHL	CED-O2D-CGD	2.04	120.55	115.94
22	q	304	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	g	305	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	D	401	PHO	O2A-CGA-O1A	-2.04	118.45	123.59
31	B	619	BCR	C34-C9-C8	2.04	121.29	118.08
26	n	313	CHL	C1C-C2C-C3C	-2.04	105.50	107.11
22	1	307	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
26	q	315	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
26	4	317	CHL	C4D-CHA-C1A	-2.04	118.77	121.25
22	V	304	CLA	CHD-C1D-ND	-2.03	122.58	124.45
26	5	317	CHL	O1D-CGD-CBD	-2.03	120.32	124.48
26	6	314	CHL	C4D-CHA-C1A	-2.03	118.77	121.25
27	n	319	NEX	C4-C3-C2	-2.03	106.84	110.77
22	2	301	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
26	V	314	CHL	CHB-C4A-NA	2.03	127.33	124.51
26	U	319	CHL	C1-O2A-CGA	2.03	121.78	116.44
24	V	311	XAT	C16-C1-C6	2.03	115.54	110.05
22	r	608	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	V	306	CLA	O1D-CGD-CBD	2.03	128.65	124.48
23	n	309	LUT	C8-C7-C6	-2.03	121.49	127.20
23	s	311	LUT	C11-C10-C9	-2.03	124.41	127.31
22	u	307	CLA	CAC-C3C-C4C	2.03	127.45	124.81
22	P	306	CLA	O1D-CGD-CBD	2.03	128.64	124.48
26	n	318	CHL	C4A-NA-C1A	2.03	107.62	106.71
22	r	604	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
23	2	309	LUT	C15-C35-C34	-2.03	119.31	123.47
22	b	605	CLA	CMC-C2C-C3C	2.03	131.63	126.12
26	4	313	CHL	O2D-CGD-O1D	-2.03	119.86	123.84
26	P	317	CHL	CAA-CBA-CGA	-2.03	107.31	113.25
22	b	610	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	c	502	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
24	6	310	XAT	C16-C1-C6	2.03	115.53	110.05
22	B	602	CLA	C2A-C1A-CHA	2.03	127.41	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	301	CLA	CHD-C1D-ND	-2.03	122.59	124.45
27	P	301	NEX	C11-C12-C13	-2.03	120.71	126.42
23	N	309	LUT	C31-C30-C29	-2.03	124.41	127.31
26	G	311	CHL	C4D-C3D-CAD	2.03	110.49	108.10
22	c	511	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	U	311	XAT	C40-C33-C32	2.03	121.28	118.08
22	3	307	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
22	u	308	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	B	610	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	P	318	CHL	C1-C2-C3	-2.03	122.53	126.04
22	N	305	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
22	3	305	CLA	C3A-C2A-C1A	2.03	104.38	101.34
24	3	309	XAT	C16-C1-C6	2.03	115.52	110.05
22	B	613	CLA	CHA-C1A-NA	-2.03	121.75	126.40
26	2	317	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
26	2	316	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
22	C	512	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	b	607	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	N	302	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
31	B	619	BCR	C20-C19-C18	-2.03	120.72	126.42
22	C	511	CLA	O1D-CGD-CBD	2.03	128.63	124.48
22	G	304	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	A	405	CLA	C1-C2-C3	-2.03	122.54	126.04
22	v	306	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
26	1	313	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
22	b	617	CLA	CAA-C2A-C1A	2.03	118.62	111.97
26	Q	314	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
26	1	313	CHL	C6-C5-C3	-2.03	108.14	113.45
22	C	509	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
22	R	309	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	u	302	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
22	c	507	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	D	403	CLA	C2D-C1D-ND	-2.02	108.61	110.10
26	U	313	CHL	C2A-C1A-CHA	-2.02	120.32	123.86
26	q	312	CHL	CHD-C1D-C2D	2.02	129.73	125.48
22	S	306	CLA	CHA-C1A-NA	-2.02	121.76	126.40
23	P	310	LUT	C16-C1-C6	-2.02	107.02	110.30
22	b	614	CLA	C2A-C1A-CHA	2.02	127.40	123.86
22	3	306	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
22	r	604	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
22	1	307	CLA	CAC-C3C-C4C	2.02	127.44	124.81
26	G	314	CHL	C4D-CHA-C1A	-2.02	118.79	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	V	310	LUT	C22-C23-C24	-2.02	109.44	111.74
22	s	306	CLA	CHA-C1A-NA	-2.02	121.77	126.40
26	p	316	CHL	O2A-CGA-O1A	-2.02	118.49	123.59
22	n	302	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
26	6	313	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
25	L	101	LHG	C5-O7-C7	-2.02	112.81	117.79
22	6	304	CLA	C1-C2-C3	-2.02	123.48	126.75
31	B	619	BCR	C11-C12-C13	-2.02	120.74	126.42
26	1	313	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
22	n	301	CLA	C2D-C1D-ND	-2.02	108.61	110.10
22	C	503	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	G	315	CHL	C1B-CHB-C4A	-2.02	126.12	130.12
26	5	316	CHL	O2D-CGD-O1D	-2.02	119.89	123.84
26	5	315	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
22	G	303	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	G	304	CLA	CHD-C1D-ND	-2.02	122.60	124.45
27	S	317	NEX	O24-C25-C26	-2.02	57.29	58.96
26	V	317	CHL	C1B-CHB-C4A	-2.02	126.12	130.12
24	r	612	XAT	C17-C1-C6	-2.02	104.59	110.05
27	p	301	NEX	C26-C27-C28	-2.02	121.72	125.99
22	P	305	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
22	c	511	CLA	CMB-C2B-C3B	2.02	128.45	124.68
26	3	316	CHL	O1D-CGD-CBD	-2.02	120.36	124.48
23	n	310	LUT	C30-C31-C32	-2.02	116.92	123.22
22	R	303	CLA	C2D-C1D-ND	-2.02	108.62	110.10
26	5	317	CHL	O2D-CGD-O1D	-2.02	119.89	123.84
22	C	503	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
26	P	319	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
22	c	512	CLA	CHA-C1A-NA	-2.02	121.78	126.40
26	v	314	CHL	C1B-CHB-C4A	-2.02	126.12	130.12
26	G	314	CHL	C1-C2-C3	-2.02	122.56	126.04
31	b	618	BCR	C29-C30-C25	2.02	113.58	110.48
22	2	302	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	3	313	CHL	C4D-CHA-C1A	-2.02	118.80	121.25
22	1	301	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	U	301	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	C	512	CLA	CMB-C2B-C3B	2.01	128.45	124.68
26	5	318	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
26	s	314	CHL	O2A-CGA-CBA	2.01	120.50	114.03
31	B	620	BCR	C1-C6-C7	2.01	121.48	115.78
31	c	516	BCR	C30-C25-C24	2.01	121.48	115.78
22	C	511	CLA	CHD-C1D-ND	-2.01	122.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	308	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
27	u	320	NEX	O24-C25-C26	-2.01	57.29	58.96
26	Q	312	CHL	CAA-C2A-C1A	2.01	118.57	111.97
23	1	310	LUT	C30-C31-C32	-2.01	116.93	123.22
26	p	317	CHL	C2A-C3A-C4A	-2.01	98.62	101.87
24	4	311	XAT	C7-C8-C9	-2.01	122.41	125.53
26	u	318	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
26	N	317	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
24	r	612	XAT	C36-C21-C26	2.01	115.48	110.05
26	6	315	CHL	C4A-NA-C1A	2.01	107.61	106.71
26	n	314	CHL	CAA-C2A-C3A	-2.01	107.27	112.78
26	N	315	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
22	B	602	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
26	G	314	CHL	CED-O2D-CGD	2.01	120.49	115.94
22	C	513	CLA	CHA-C1A-NA	-2.01	121.79	126.40
24	5	311	XAT	C40-C33-C32	2.01	121.25	118.08
22	g	303	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	c	514	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	n	317	CHL	CHB-C4A-NA	2.01	127.29	124.51
26	Q	316	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
24	r	612	XAT	C20-C13-C12	2.01	121.25	118.08
27	S	317	NEX	C31-C32-C33	-2.01	120.77	126.42
23	1	309	LUT	C16-C1-C6	-2.01	107.04	110.30
22	B	605	CLA	CMC-C2C-C3C	2.01	131.57	126.12
26	s	316	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
22	S	302	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
22	C	504	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
34	b	621	LMG	C8-O7-C10	-2.01	112.84	117.79
27	r	617	NEX	C26-C27-C28	-2.01	121.75	125.99
22	2	304	CLA	C2A-C1A-CHA	2.01	127.37	123.86
26	U	319	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
27	u	319	NEX	C31-C32-C33	-2.01	120.77	126.42
22	b	606	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
26	q	312	CHL	CAA-C2A-C3A	-2.01	107.28	112.78
26	r	614	CHL	C1B-CHB-C4A	-2.01	126.14	130.12
24	r	612	XAT	C24-C23-C22	-2.01	106.89	110.77
22	3	308	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	2	310	LUT	C16-C1-C6	-2.01	107.04	110.30
23	4	309	LUT	C10-C11-C12	-2.01	116.95	123.22
22	a	405	CLA	C1-C2-C3	-2.01	122.57	126.04
31	X	201	BCR	C15-C16-C17	-2.01	119.36	123.47
24	5	311	XAT	C36-C21-C26	2.01	115.46	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	503	CLA	C1-C2-C3	-2.01	122.57	126.04
22	C	511	CLA	C2A-C1A-CHA	2.01	127.37	123.86
22	s	306	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
26	q	313	CHL	C1B-CHB-C4A	-2.01	126.14	130.12
26	r	615	CHL	O1D-CGD-CBD	-2.01	120.38	124.48
22	A	405	CLA	CHA-C1A-NA	-2.01	121.80	126.40
22	V	302	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
22	s	306	CLA	CAC-C3C-C4C	2.00	127.41	124.81
26	g	314	CHL	C1D-ND-C4D	-2.00	104.91	106.33
26	g	315	CHL	O2A-CGA-O1A	-2.00	118.53	123.59
22	b	608	CLA	C2A-C1A-CHA	2.00	127.36	123.86
22	6	305	CLA	CHD-C1D-ND	-2.00	122.61	124.45
26	S	316	CHL	O1D-CGD-CBD	-2.00	120.38	124.48
23	4	310	LUT	C30-C31-C32	-2.00	116.96	123.22
27	P	301	NEX	O24-C25-C26	-2.00	57.30	58.96
22	2	305	CLA	C3A-C2A-C1A	2.00	104.34	101.34
26	5	316	CHL	C2A-C1A-CHA	-2.00	120.36	123.86
26	3	312	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
26	n	315	CHL	CED-O2D-CGD	2.00	120.47	115.94
22	N	308	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	g	301	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
31	c	516	BCR	C24-C23-C22	-2.00	123.21	126.23
26	4	314	CHL	C1C-C2C-C3C	-2.00	105.53	107.11
23	v	310	LUT	C18-C5-C4	2.00	118.06	114.36
26	r	615	CHL	O2A-CGA-CBA	2.00	118.19	111.91
22	Q	301	CLA	CHD-C1D-ND	-2.00	122.61	124.45
22	A	405	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
22	P	305	CLA	C1-C2-C3	-2.00	122.58	126.04
22	n	302	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	U	312	LHG	C5-O7-C7	-2.00	112.86	117.79
22	r	606	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	5	305	CLA	C4D-CHA-C1A	2.00	123.68	121.25
22	5	303	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	l	101	LHG	C5-O7-C7	-2.00	112.87	117.79
26	6	317	CHL	O1D-CGD-CBD	-2.00	120.39	124.48
26	R	317	CHL	C4D-CHA-C1A	-2.00	118.81	121.25

All (612) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	r	601	CLA	ND
22	r	602	CLA	ND

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Mol	Chain	Res	Type	Atom
22	r	603	CLA	ND
22	r	604	CLA	ND
22	r	605	CLA	ND
22	r	606	CLA	ND
22	r	607	CLA	ND
22	r	608	CLA	ND
22	r	609	CLA	ND
22	r	610	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	406	CLA	ND
22	a	408	CLA	ND
22	d	402	CLA	ND
22	x	201	CLA	ND
22	A	404	CLA	ND
22	A	405	CLA	ND
22	A	406	CLA	ND
22	A	408	CLA	ND
22	1	301	CLA	ND
22	1	302	CLA	ND
22	1	303	CLA	ND
22	1	304	CLA	ND
22	1	305	CLA	ND
22	1	306	CLA	ND
22	1	307	CLA	ND
22	1	308	CLA	ND
22	2	301	CLA	ND
22	2	302	CLA	ND
22	2	303	CLA	ND
22	2	304	CLA	ND
22	2	305	CLA	ND
22	2	306	CLA	ND
22	2	307	CLA	ND
22	2	308	CLA	ND
22	3	301	CLA	ND
22	3	302	CLA	ND
22	3	303	CLA	ND
22	3	304	CLA	ND
22	3	305	CLA	ND
22	3	306	CLA	ND
22	3	307	CLA	ND
22	3	308	CLA	ND

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Mol	Chain	Res	Type	Atom
22	4	301	CLA	ND
22	4	302	CLA	ND
22	4	303	CLA	ND
22	4	304	CLA	ND
22	4	305	CLA	ND
22	4	306	CLA	ND
22	4	307	CLA	ND
22	4	308	CLA	ND
22	5	301	CLA	ND
22	5	302	CLA	ND
22	5	303	CLA	ND
22	5	304	CLA	ND
22	5	305	CLA	ND
22	5	306	CLA	ND
22	5	307	CLA	ND
22	5	308	CLA	ND
22	6	302	CLA	ND
22	6	303	CLA	ND
22	6	304	CLA	ND
22	6	305	CLA	ND
22	6	306	CLA	ND
22	6	307	CLA	ND
22	6	308	CLA	ND
22	6	309	CLA	ND
22	v	302	CLA	ND
22	v	303	CLA	ND
22	v	304	CLA	ND
22	v	305	CLA	ND
22	v	306	CLA	ND
22	v	307	CLA	ND
22	v	308	CLA	ND
22	p	302	CLA	ND
22	p	303	CLA	ND
22	p	304	CLA	ND
22	p	305	CLA	ND
22	p	306	CLA	ND
22	p	307	CLA	ND
22	p	308	CLA	ND
22	p	309	CLA	ND
22	q	302	CLA	ND
22	q	303	CLA	ND
22	q	304	CLA	ND

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Mol	Chain	Res	Type	Atom
22	q	305	CLA	ND
22	q	306	CLA	ND
22	q	307	CLA	ND
22	q	308	CLA	ND
22	V	302	CLA	ND
22	V	303	CLA	ND
22	V	304	CLA	ND
22	V	305	CLA	ND
22	V	306	CLA	ND
22	V	307	CLA	ND
22	V	308	CLA	ND
22	P	302	CLA	ND
22	P	303	CLA	ND
22	P	304	CLA	ND
22	P	305	CLA	ND
22	P	306	CLA	ND
22	P	307	CLA	ND
22	P	308	CLA	ND
22	P	309	CLA	ND
22	Q	301	CLA	ND
22	Q	302	CLA	ND
22	Q	303	CLA	ND
22	Q	304	CLA	ND
22	Q	305	CLA	ND
22	Q	306	CLA	ND
22	Q	307	CLA	ND
22	Q	308	CLA	ND
22	U	302	CLA	ND
22	U	303	CLA	ND
22	U	304	CLA	ND
22	U	305	CLA	ND
22	U	306	CLA	ND
22	U	307	CLA	ND
22	U	308	CLA	ND
22	N	301	CLA	ND
22	N	302	CLA	ND
22	N	303	CLA	ND
22	N	304	CLA	ND
22	N	305	CLA	ND
22	N	306	CLA	ND
22	N	307	CLA	ND
22	N	308	CLA	ND

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Mol	Chain	Res	Type	Atom
22	G	301	CLA	ND
22	G	302	CLA	ND
22	G	303	CLA	ND
22	G	304	CLA	ND
22	G	305	CLA	ND
22	G	306	CLA	ND
22	G	307	CLA	ND
22	G	308	CLA	ND
22	u	302	CLA	ND
22	u	303	CLA	ND
22	u	304	CLA	ND
22	u	305	CLA	ND
22	u	306	CLA	ND
22	u	307	CLA	ND
22	u	308	CLA	ND
22	n	301	CLA	ND
22	n	302	CLA	ND
22	n	303	CLA	ND
22	n	304	CLA	ND
22	n	305	CLA	ND
22	n	306	CLA	ND
22	n	307	CLA	ND
22	n	308	CLA	ND
22	g	301	CLA	ND
22	g	302	CLA	ND
22	g	303	CLA	ND
22	g	304	CLA	ND
22	g	305	CLA	ND
22	g	306	CLA	ND
22	g	307	CLA	ND
22	g	308	CLA	ND
22	R	302	CLA	ND
22	R	303	CLA	ND
22	R	304	CLA	ND
22	R	305	CLA	ND
22	R	306	CLA	ND
22	R	307	CLA	ND
22	R	308	CLA	ND
22	R	309	CLA	ND
22	R	310	CLA	ND
22	R	311	CLA	ND
22	S	301	CLA	ND

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Mol	Chain	Res	Type	Atom
22	S	302	CLA	ND
22	S	303	CLA	ND
22	S	304	CLA	ND
22	S	305	CLA	ND
22	S	306	CLA	ND
22	S	307	CLA	ND
22	S	308	CLA	ND
22	S	309	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	C	514	CLA	ND
22	C	515	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	609	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	B	617	CLA	ND
22	D	403	CLA	ND
22	X	202	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	b	617	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	c	514	CLA	ND
22	s	301	CLA	ND
22	s	302	CLA	ND
22	s	303	CLA	ND
22	s	304	CLA	ND
22	s	305	CLA	ND
22	s	306	CLA	ND
22	s	307	CLA	ND
22	s	308	CLA	ND
22	s	309	CLA	ND
26	r	614	CHL	NC
26	r	614	CHL	ND
26	r	614	CHL	NA
26	r	615	CHL	NC
26	r	615	CHL	ND
26	r	615	CHL	NA
26	r	616	CHL	NC
26	r	616	CHL	ND

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Mol	Chain	Res	Type	Atom
26	r	616	CHL	NA
26	r	619	CHL	NC
26	r	619	CHL	ND
26	r	619	CHL	NA
26	1	313	CHL	NC
26	1	313	CHL	ND
26	1	313	CHL	NA
26	1	314	CHL	NC
26	1	314	CHL	ND
26	1	314	CHL	NA
26	1	315	CHL	NC
26	1	315	CHL	ND
26	1	315	CHL	NA
26	1	316	CHL	NC
26	1	316	CHL	ND
26	1	316	CHL	NA
26	1	317	CHL	NC
26	1	317	CHL	ND
26	1	317	CHL	NA
26	1	318	CHL	NC
26	1	318	CHL	ND
26	1	318	CHL	NA
26	2	313	CHL	NC
26	2	313	CHL	ND
26	2	313	CHL	NA
26	2	314	CHL	NC
26	2	314	CHL	ND
26	2	314	CHL	NA
26	2	315	CHL	NC
26	2	315	CHL	ND
26	2	315	CHL	NA
26	2	316	CHL	NC
26	2	316	CHL	ND
26	2	316	CHL	NA
26	2	317	CHL	NC
26	2	317	CHL	ND
26	2	317	CHL	NA
26	2	318	CHL	NC
26	2	318	CHL	ND
26	2	318	CHL	NA
26	3	311	CHL	NC
26	3	311	CHL	ND

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Mol	Chain	Res	Type	Atom
26	3	311	CHL	NA
26	3	312	CHL	NC
26	3	312	CHL	ND
26	3	312	CHL	NA
26	3	313	CHL	NC
26	3	313	CHL	ND
26	3	313	CHL	NA
26	3	314	CHL	NC
26	3	314	CHL	ND
26	3	314	CHL	NA
26	3	315	CHL	NC
26	3	315	CHL	ND
26	3	315	CHL	NA
26	3	316	CHL	NC
26	3	316	CHL	ND
26	3	316	CHL	NA
26	4	313	CHL	NC
26	4	313	CHL	ND
26	4	313	CHL	NA
26	4	314	CHL	NC
26	4	314	CHL	ND
26	4	314	CHL	NA
26	4	315	CHL	NC
26	4	315	CHL	ND
26	4	315	CHL	NA
26	4	316	CHL	NC
26	4	316	CHL	ND
26	4	316	CHL	NA
26	4	317	CHL	NC
26	4	317	CHL	ND
26	4	317	CHL	NA
26	5	313	CHL	NC
26	5	313	CHL	ND
26	5	313	CHL	NA
26	5	314	CHL	NC
26	5	314	CHL	ND
26	5	314	CHL	NA
26	5	315	CHL	NC
26	5	315	CHL	ND
26	5	315	CHL	NA
26	5	316	CHL	NC
26	5	316	CHL	ND

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Mol	Chain	Res	Type	Atom
26	5	316	CHL	NA
26	5	317	CHL	NC
26	5	317	CHL	ND
26	5	317	CHL	NA
26	5	318	CHL	NC
26	5	318	CHL	ND
26	5	318	CHL	NA
26	6	301	CHL	NC
26	6	301	CHL	ND
26	6	301	CHL	NA
26	6	312	CHL	NC
26	6	312	CHL	ND
26	6	312	CHL	NA
26	6	313	CHL	NC
26	6	313	CHL	ND
26	6	313	CHL	NA
26	6	314	CHL	NC
26	6	314	CHL	ND
26	6	314	CHL	NA
26	6	315	CHL	NC
26	6	315	CHL	ND
26	6	315	CHL	NA
26	6	316	CHL	NC
26	6	316	CHL	ND
26	6	316	CHL	NA
26	6	317	CHL	NC
26	6	317	CHL	ND
26	6	317	CHL	NA
26	v	313	CHL	NC
26	v	313	CHL	ND
26	v	313	CHL	NA
26	v	314	CHL	NC
26	v	314	CHL	ND
26	v	314	CHL	NA
26	v	315	CHL	NC
26	v	315	CHL	ND
26	v	315	CHL	NA
26	v	316	CHL	NC
26	v	316	CHL	ND
26	v	316	CHL	NA
26	v	317	CHL	NC
26	v	317	CHL	ND

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Mol	Chain	Res	Type	Atom
26	v	317	CHL	NA
26	v	318	CHL	NC
26	v	318	CHL	ND
26	v	318	CHL	NA
26	p	314	CHL	NC
26	p	314	CHL	ND
26	p	314	CHL	NA
26	p	315	CHL	NC
26	p	315	CHL	ND
26	p	315	CHL	NA
26	p	316	CHL	NC
26	p	316	CHL	ND
26	p	316	CHL	NA
26	p	317	CHL	NC
26	p	317	CHL	ND
26	p	317	CHL	NA
26	p	318	CHL	NC
26	p	318	CHL	ND
26	p	318	CHL	NA
26	p	319	CHL	NC
26	p	319	CHL	ND
26	p	319	CHL	NA
26	p	320	CHL	NC
26	p	320	CHL	ND
26	p	320	CHL	NA
26	q	311	CHL	NC
26	q	311	CHL	ND
26	q	311	CHL	NA
26	q	312	CHL	NC
26	q	312	CHL	ND
26	q	312	CHL	NA
26	q	313	CHL	NC
26	q	313	CHL	ND
26	q	313	CHL	NA
26	q	314	CHL	NC
26	q	314	CHL	ND
26	q	314	CHL	NA
26	q	315	CHL	NC
26	q	315	CHL	ND
26	q	315	CHL	NA
26	V	313	CHL	NC
26	V	313	CHL	ND

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Mol	Chain	Res	Type	Atom
26	V	313	CHL	NA
26	V	314	CHL	NC
26	V	314	CHL	ND
26	V	314	CHL	NA
26	V	315	CHL	NC
26	V	315	CHL	ND
26	V	315	CHL	NA
26	V	316	CHL	NC
26	V	316	CHL	ND
26	V	316	CHL	NA
26	V	317	CHL	NC
26	V	317	CHL	ND
26	V	317	CHL	NA
26	V	318	CHL	NC
26	V	318	CHL	ND
26	V	318	CHL	NA
26	P	314	CHL	NC
26	P	314	CHL	ND
26	P	314	CHL	NA
26	P	315	CHL	NC
26	P	315	CHL	ND
26	P	315	CHL	NA
26	P	316	CHL	NC
26	P	316	CHL	ND
26	P	316	CHL	NA
26	P	317	CHL	NC
26	P	317	CHL	ND
26	P	317	CHL	NA
26	P	318	CHL	NC
26	P	318	CHL	ND
26	P	318	CHL	NA
26	P	319	CHL	NC
26	P	319	CHL	ND
26	P	319	CHL	NA
26	Q	311	CHL	NC
26	Q	311	CHL	ND
26	Q	311	CHL	NA
26	Q	312	CHL	NC
26	Q	312	CHL	ND
26	Q	312	CHL	NA
26	Q	313	CHL	NC
26	Q	313	CHL	ND

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Mol	Chain	Res	Type	Atom
26	Q	313	CHL	NA
26	Q	314	CHL	NC
26	Q	314	CHL	ND
26	Q	314	CHL	NA
26	Q	315	CHL	NC
26	Q	315	CHL	ND
26	Q	315	CHL	NA
26	Q	316	CHL	NC
26	Q	316	CHL	ND
26	Q	316	CHL	NA
26	U	313	CHL	NC
26	U	313	CHL	ND
26	U	313	CHL	NA
26	U	314	CHL	NC
26	U	314	CHL	ND
26	U	314	CHL	NA
26	U	315	CHL	NC
26	U	315	CHL	ND
26	U	315	CHL	NA
26	U	316	CHL	NC
26	U	316	CHL	ND
26	U	316	CHL	NA
26	U	317	CHL	NC
26	U	317	CHL	ND
26	U	317	CHL	NA
26	U	319	CHL	NC
26	U	319	CHL	ND
26	U	319	CHL	NA
26	N	313	CHL	NC
26	N	313	CHL	ND
26	N	313	CHL	NA
26	N	314	CHL	NC
26	N	314	CHL	ND
26	N	314	CHL	NA
26	N	315	CHL	NC
26	N	315	CHL	ND
26	N	315	CHL	NA
26	N	316	CHL	NC
26	N	316	CHL	ND
26	N	316	CHL	NA
26	N	317	CHL	NC
26	N	317	CHL	ND

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Mol	Chain	Res	Type	Atom
26	N	317	CHL	NA
26	G	311	CHL	NC
26	G	311	CHL	ND
26	G	311	CHL	NA
26	G	312	CHL	NC
26	G	312	CHL	ND
26	G	312	CHL	NA
26	G	313	CHL	NC
26	G	313	CHL	ND
26	G	313	CHL	NA
26	G	314	CHL	NC
26	G	314	CHL	ND
26	G	314	CHL	NA
26	G	315	CHL	NC
26	G	315	CHL	ND
26	G	315	CHL	NA
26	G	316	CHL	NC
26	G	316	CHL	ND
26	G	316	CHL	NA
26	u	313	CHL	NC
26	u	313	CHL	ND
26	u	313	CHL	NA
26	u	314	CHL	NC
26	u	314	CHL	ND
26	u	314	CHL	NA
26	u	315	CHL	NC
26	u	315	CHL	ND
26	u	315	CHL	NA
26	u	316	CHL	NC
26	u	316	CHL	ND
26	u	316	CHL	NA
26	u	317	CHL	NC
26	u	317	CHL	ND
26	u	317	CHL	NA
26	u	318	CHL	NC
26	u	318	CHL	ND
26	u	318	CHL	NA
26	n	313	CHL	NC
26	n	313	CHL	ND
26	n	313	CHL	NA
26	n	314	CHL	NC
26	n	314	CHL	ND

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Mol	Chain	Res	Type	Atom
26	n	314	CHL	NA
26	n	315	CHL	NC
26	n	315	CHL	ND
26	n	315	CHL	NA
26	n	316	CHL	NC
26	n	316	CHL	ND
26	n	316	CHL	NA
26	n	317	CHL	NC
26	n	317	CHL	ND
26	n	317	CHL	NA
26	n	318	CHL	NC
26	n	318	CHL	ND
26	n	318	CHL	NA
26	g	311	CHL	NC
26	g	311	CHL	ND
26	g	311	CHL	NA
26	g	312	CHL	NC
26	g	312	CHL	ND
26	g	312	CHL	NA
26	g	313	CHL	NC
26	g	313	CHL	ND
26	g	313	CHL	NA
26	g	314	CHL	NC
26	g	314	CHL	ND
26	g	314	CHL	NA
26	g	315	CHL	NC
26	g	315	CHL	ND
26	g	315	CHL	NA
26	g	316	CHL	NC
26	g	316	CHL	ND
26	g	316	CHL	NA
26	R	315	CHL	NC
26	R	315	CHL	ND
26	R	315	CHL	NA
26	R	316	CHL	NC
26	R	316	CHL	ND
26	R	316	CHL	NA
26	R	317	CHL	NC
26	R	317	CHL	ND
26	R	317	CHL	NA
26	S	313	CHL	NC
26	S	313	CHL	ND

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Mol	Chain	Res	Type	Atom
26	S	313	CHL	NA
26	S	314	CHL	NC
26	S	314	CHL	ND
26	S	314	CHL	NA
26	S	315	CHL	NC
26	S	315	CHL	ND
26	S	315	CHL	NA
26	S	316	CHL	NC
26	S	316	CHL	ND
26	S	316	CHL	NA
26	s	313	CHL	NC
26	s	313	CHL	ND
26	s	313	CHL	NA
26	s	314	CHL	NC
26	s	314	CHL	ND
26	s	314	CHL	NA
26	s	315	CHL	NC
26	s	315	CHL	ND
26	s	315	CHL	NA
26	s	316	CHL	NC
26	s	316	CHL	ND
26	s	316	CHL	NA

All (6713) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	r	604	CLA	C1A-C2A-CAA-CBA
22	r	606	CLA	CBD-CGD-O2D-CED
22	r	606	CLA	C2-C3-C5-C6
22	r	606	CLA	C4-C3-C5-C6
22	r	607	CLA	C1A-C2A-CAA-CBA
22	r	607	CLA	C3A-C2A-CAA-CBA
22	r	608	CLA	CBD-CGD-O2D-CED
22	r	609	CLA	CBD-CGD-O2D-CED
22	r	610	CLA	C1A-C2A-CAA-CBA
22	r	610	CLA	C3A-C2A-CAA-CBA
22	a	404	CLA	CHA-CBD-CGD-O1D
22	a	404	CLA	CHA-CBD-CGD-O2D
22	a	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
22	a	406	CLA	CHA-CBD-CGD-O1D
22	a	406	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	404	CLA	CHA-CBD-CGD-O1D
22	A	404	CLA	CHA-CBD-CGD-O2D
22	A	405	CLA	CHA-CBD-CGD-O1D
22	A	405	CLA	CHA-CBD-CGD-O2D
22	A	406	CLA	CHA-CBD-CGD-O1D
22	A	406	CLA	CHA-CBD-CGD-O2D
22	1	302	CLA	CHA-CBD-CGD-O1D
22	1	302	CLA	CHA-CBD-CGD-O2D
22	1	302	CLA	CBD-CGD-O2D-CED
22	1	303	CLA	CHA-CBD-CGD-O1D
22	1	303	CLA	CHA-CBD-CGD-O2D
22	1	303	CLA	CAD-CBD-CGD-O1D
22	1	303	CLA	CBD-CGD-O2D-CED
22	1	304	CLA	CBD-CGD-O2D-CED
22	1	305	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	CBD-CGD-O2D-CED
22	1	308	CLA	C1A-C2A-CAA-CBA
22	1	308	CLA	C3A-C2A-CAA-CBA
22	1	308	CLA	CHA-CBD-CGD-O1D
22	1	308	CLA	CHA-CBD-CGD-O2D
22	1	308	CLA	CAD-CBD-CGD-O1D
22	2	301	CLA	CBD-CGD-O2D-CED
22	2	303	CLA	CBD-CGD-O2D-CED
22	2	304	CLA	CBD-CGD-O2D-CED
22	2	305	CLA	CHA-CBD-CGD-O1D
22	2	305	CLA	CHA-CBD-CGD-O2D
22	2	308	CLA	CBD-CGD-O2D-CED
22	3	301	CLA	CBD-CGD-O2D-CED
22	3	302	CLA	CBA-CGA-O2A-C1
22	3	302	CLA	O1A-CGA-O2A-C1
22	3	302	CLA	CHA-CBD-CGD-O1D
22	3	302	CLA	CHA-CBD-CGD-O2D
22	3	302	CLA	CAD-CBD-CGD-O1D
22	3	302	CLA	C6-C7-C8-C9
22	3	303	CLA	C1A-C2A-CAA-CBA
22	3	303	CLA	C3A-C2A-CAA-CBA
22	3	304	CLA	CBD-CGD-O2D-CED
22	3	305	CLA	CBD-CGD-O2D-CED
22	3	307	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CHA-CBD-CGD-O1D
22	3	308	CLA	CHA-CBD-CGD-O2D
22	3	308	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	3	308	CLA	CAD-CBD-CGD-O2D
22	4	302	CLA	CHA-CBD-CGD-O1D
22	4	302	CLA	CHA-CBD-CGD-O2D
22	4	303	CLA	CHA-CBD-CGD-O1D
22	4	303	CLA	CHA-CBD-CGD-O2D
22	4	303	CLA	CAD-CBD-CGD-O1D
22	4	303	CLA	CAD-CBD-CGD-O2D
22	4	303	CLA	CBD-CGD-O2D-CED
22	4	305	CLA	CBD-CGD-O2D-CED
22	4	307	CLA	CBD-CGD-O2D-CED
22	4	308	CLA	C1A-C2A-CAA-CBA
22	4	308	CLA	C3A-C2A-CAA-CBA
22	4	308	CLA	CHA-CBD-CGD-O1D
22	4	308	CLA	CHA-CBD-CGD-O2D
22	4	308	CLA	CAD-CBD-CGD-O1D
22	5	301	CLA	CBD-CGD-O2D-CED
22	5	304	CLA	CBD-CGD-O2D-CED
22	5	305	CLA	CHA-CBD-CGD-O1D
22	5	305	CLA	CHA-CBD-CGD-O2D
22	5	307	CLA	CBD-CGD-O2D-CED
22	5	308	CLA	CBD-CGD-O2D-CED
22	6	302	CLA	CBD-CGD-O2D-CED
22	6	303	CLA	CHA-CBD-CGD-O1D
22	6	303	CLA	CHA-CBD-CGD-O2D
22	6	304	CLA	C1A-C2A-CAA-CBA
22	6	304	CLA	C3A-C2A-CAA-CBA
22	6	304	CLA	CBD-CGD-O2D-CED
22	6	305	CLA	CBD-CGD-O2D-CED
22	6	306	CLA	CBD-CGD-O2D-CED
22	6	308	CLA	CBD-CGD-O2D-CED
22	6	309	CLA	CHA-CBD-CGD-O1D
22	6	309	CLA	CHA-CBD-CGD-O2D
22	6	309	CLA	CAD-CBD-CGD-O1D
22	6	309	CLA	CAD-CBD-CGD-O2D
22	v	303	CLA	C1A-C2A-CAA-CBA
22	v	304	CLA	C1A-C2A-CAA-CBA
22	v	304	CLA	CBD-CGD-O2D-CED
22	v	305	CLA	CBD-CGD-O2D-CED
22	v	307	CLA	CBD-CGD-O2D-CED
22	v	308	CLA	C1A-C2A-CAA-CBA
22	v	308	CLA	C3A-C2A-CAA-CBA
22	p	302	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	p	304	CLA	C1A-C2A-CAA-CBA
22	p	304	CLA	C3A-C2A-CAA-CBA
22	p	304	CLA	CHA-CBD-CGD-O1D
22	p	304	CLA	CBD-CGD-O2D-CED
22	p	306	CLA	CHA-CBD-CGD-O1D
22	p	306	CLA	CHA-CBD-CGD-O2D
22	p	308	CLA	CBD-CGD-O2D-CED
22	p	309	CLA	C1A-C2A-CAA-CBA
22	p	309	CLA	C3A-C2A-CAA-CBA
22	p	309	CLA	CBD-CGD-O2D-CED
22	q	302	CLA	CHA-CBD-CGD-O1D
22	q	302	CLA	CHA-CBD-CGD-O2D
22	q	303	CLA	C1A-C2A-CAA-CBA
22	q	303	CLA	C3A-C2A-CAA-CBA
22	q	304	CLA	CBD-CGD-O2D-CED
22	q	305	CLA	CBD-CGD-O2D-CED
22	q	307	CLA	CBD-CGD-O2D-CED
22	q	308	CLA	C3A-C2A-CAA-CBA
22	q	308	CLA	CHA-CBD-CGD-O1D
22	q	308	CLA	CHA-CBD-CGD-O2D
22	q	308	CLA	CBD-CGD-O2D-CED
22	V	303	CLA	C1A-C2A-CAA-CBA
22	V	303	CLA	C3A-C2A-CAA-CBA
22	V	304	CLA	C1A-C2A-CAA-CBA
22	V	304	CLA	CBD-CGD-O2D-CED
22	V	305	CLA	CBD-CGD-O2D-CED
22	V	306	CLA	CBD-CGD-O2D-CED
22	V	308	CLA	C2A-CAA-CBA-CGA
22	P	302	CLA	CBD-CGD-O2D-CED
22	P	304	CLA	C1A-C2A-CAA-CBA
22	P	304	CLA	C3A-C2A-CAA-CBA
22	P	304	CLA	CHA-CBD-CGD-O1D
22	P	304	CLA	CHA-CBD-CGD-O2D
22	P	304	CLA	CAD-CBD-CGD-O1D
22	P	306	CLA	CHA-CBD-CGD-O1D
22	P	306	CLA	CHA-CBD-CGD-O2D
22	P	308	CLA	CBD-CGD-O2D-CED
22	P	309	CLA	C1A-C2A-CAA-CBA
22	P	309	CLA	C3A-C2A-CAA-CBA
22	P	309	CLA	CBD-CGD-O2D-CED
22	Q	301	CLA	CBD-CGD-O2D-CED
22	Q	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	Q	303	CLA	C3A-C2A-CAA-CBA
22	Q	303	CLA	CHA-CBD-CGD-O1D
22	Q	303	CLA	CHA-CBD-CGD-O2D
22	Q	304	CLA	CBD-CGD-O2D-CED
22	Q	304	CLA	O1D-CGD-O2D-CED
22	Q	305	CLA	CHA-CBD-CGD-O1D
22	Q	305	CLA	CHA-CBD-CGD-O2D
22	Q	305	CLA	CBD-CGD-O2D-CED
22	Q	305	CLA	O1D-CGD-O2D-CED
22	Q	308	CLA	C3A-C2A-CAA-CBA
22	Q	308	CLA	CHA-CBD-CGD-O1D
22	Q	308	CLA	CHA-CBD-CGD-O2D
22	U	301	CLA	CBD-CGD-O2D-CED
22	U	305	CLA	CBD-CGD-O2D-CED
22	U	305	CLA	O1D-CGD-O2D-CED
22	U	307	CLA	CBD-CGD-O2D-CED
22	U	308	CLA	CHA-CBD-CGD-O1D
22	U	308	CLA	CAD-CBD-CGD-O1D
22	U	308	CLA	CAD-CBD-CGD-O2D
22	N	302	CLA	CHA-CBD-CGD-O1D
22	N	302	CLA	CHA-CBD-CGD-O2D
22	N	302	CLA	CAD-CBD-CGD-O1D
22	N	302	CLA	CBD-CGD-O2D-CED
22	N	303	CLA	CHA-CBD-CGD-O1D
22	N	303	CLA	CHA-CBD-CGD-O2D
22	N	303	CLA	CAD-CBD-CGD-O1D
22	N	304	CLA	CBD-CGD-O2D-CED
22	N	305	CLA	CHA-CBD-CGD-O1D
22	N	305	CLA	CHA-CBD-CGD-O2D
22	N	306	CLA	CBD-CGD-O2D-CED
22	N	308	CLA	C1A-C2A-CAA-CBA
22	N	308	CLA	CAD-CBD-CGD-O1D
22	N	308	CLA	CAD-CBD-CGD-O2D
22	G	301	CLA	C2-C3-C5-C6
22	G	301	CLA	C4-C3-C5-C6
22	G	302	CLA	CHA-CBD-CGD-O1D
22	G	302	CLA	CHA-CBD-CGD-O2D
22	G	302	CLA	CAD-CBD-CGD-O1D
22	G	302	CLA	CBD-CGD-O2D-CED
22	G	303	CLA	C1A-C2A-CAA-CBA
22	G	303	CLA	C3A-C2A-CAA-CBA
22	G	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	G	303	CLA	CHA-CBD-CGD-O2D
22	G	304	CLA	CBD-CGD-O2D-CED
22	G	304	CLA	O1D-CGD-O2D-CED
22	G	305	CLA	CBD-CGD-O2D-CED
22	G	307	CLA	CBD-CGD-O2D-CED
22	G	307	CLA	O1D-CGD-O2D-CED
22	G	308	CLA	CHA-CBD-CGD-O1D
22	G	308	CLA	CHA-CBD-CGD-O2D
22	G	308	CLA	CAD-CBD-CGD-O1D
22	u	301	CLA	CBD-CGD-O2D-CED
22	u	305	CLA	CBD-CGD-O2D-CED
22	u	305	CLA	O1D-CGD-O2D-CED
22	u	307	CLA	CBD-CGD-O2D-CED
22	u	308	CLA	CHA-CBD-CGD-O1D
22	u	308	CLA	CHA-CBD-CGD-O2D
22	u	308	CLA	CAD-CBD-CGD-O1D
22	u	308	CLA	CAD-CBD-CGD-O2D
22	n	303	CLA	CHA-CBD-CGD-O1D
22	n	303	CLA	CHA-CBD-CGD-O2D
22	n	305	CLA	CHA-CBD-CGD-O1D
22	n	305	CLA	CHA-CBD-CGD-O2D
22	n	306	CLA	CBD-CGD-O2D-CED
22	n	308	CLA	C1A-C2A-CAA-CBA
22	n	308	CLA	C3A-C2A-CAA-CBA
22	n	308	CLA	CBD-CGD-O2D-CED
22	g	301	CLA	C2-C3-C5-C6
22	g	301	CLA	C4-C3-C5-C6
22	g	302	CLA	CHA-CBD-CGD-O1D
22	g	302	CLA	CHA-CBD-CGD-O2D
22	g	302	CLA	CAD-CBD-CGD-O1D
22	g	302	CLA	CBD-CGD-O2D-CED
22	g	303	CLA	C3A-C2A-CAA-CBA
22	g	303	CLA	CAD-CBD-CGD-O1D
22	g	303	CLA	CAD-CBD-CGD-O2D
22	g	304	CLA	CBD-CGD-O2D-CED
22	g	304	CLA	O1D-CGD-O2D-CED
22	g	305	CLA	C1A-C2A-CAA-CBA
22	g	305	CLA	C3A-C2A-CAA-CBA
22	g	305	CLA	CBD-CGD-O2D-CED
22	g	307	CLA	CBD-CGD-O2D-CED
22	g	307	CLA	O1D-CGD-O2D-CED
22	g	308	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	g	308	CLA	CHA-CBD-CGD-O2D
22	g	308	CLA	CAD-CBD-CGD-O1D
22	g	308	CLA	CAD-CBD-CGD-O2D
22	R	304	CLA	CBD-CGD-O2D-CED
22	R	305	CLA	C1A-C2A-CAA-CBA
22	R	307	CLA	CBD-CGD-O2D-CED
22	R	308	CLA	C1A-C2A-CAA-CBA
22	R	308	CLA	C3A-C2A-CAA-CBA
22	R	309	CLA	CBD-CGD-O2D-CED
22	R	310	CLA	C1A-C2A-CAA-CBA
22	R	310	CLA	C3A-C2A-CAA-CBA
22	R	310	CLA	CHA-CBD-CGD-O1D
22	R	310	CLA	CHA-CBD-CGD-O2D
22	R	310	CLA	CBD-CGD-O2D-CED
22	R	311	CLA	C1A-C2A-CAA-CBA
22	R	311	CLA	C3A-C2A-CAA-CBA
22	S	301	CLA	C1A-C2A-CAA-CBA
22	S	302	CLA	CBD-CGD-O2D-CED
22	S	303	CLA	CBD-CGD-O2D-CED
22	S	304	CLA	C1A-C2A-CAA-CBA
22	S	304	CLA	C3A-C2A-CAA-CBA
22	S	304	CLA	CBD-CGD-O2D-CED
22	S	305	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	C2-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
22	C	507	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	C2-C3-C5-C6
22	C	510	CLA	C4-C3-C5-C6
22	C	513	CLA	CHA-CBD-CGD-O1D
22	C	513	CLA	CHA-CBD-CGD-O2D
22	C	513	CLA	CBD-CGD-O2D-CED
22	C	514	CLA	CBD-CGD-O2D-CED
22	C	515	CLA	C1A-C2A-CAA-CBA
22	B	604	CLA	CAD-CBD-CGD-O1D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	C2-C3-C5-C6
22	B	604	CLA	C4-C3-C5-C6
22	B	605	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	CAD-CBD-CGD-O2D
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O2D
22	B	608	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	C1A-C2A-CAA-CBA
22	B	613	CLA	C1A-C2A-CAA-CBA
22	B	613	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CBD-CGD-O2D-CED
22	B	615	CLA	C2-C3-C5-C6
22	B	615	CLA	C4-C3-C5-C6
22	B	615	CLA	C6-C7-C8-C9
22	B	616	CLA	CHA-CBD-CGD-O1D
22	B	616	CLA	CHA-CBD-CGD-O2D
22	B	617	CLA	CAD-CBD-CGD-O1D
22	B	617	CLA	CAD-CBD-CGD-O2D
22	X	202	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	CAD-CBD-CGD-O1D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	C2-C3-C5-C6
22	b	604	CLA	C4-C3-C5-C6
22	b	605	CLA	CAD-CBD-CGD-O1D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	C2-C3-C5-C6
22	b	610	CLA	C4-C3-C5-C6
22	b	610	CLA	C6-C7-C8-C9
22	b	611	CLA	C1A-C2A-CAA-CBA
22	b	613	CLA	C1A-C2A-CAA-CBA
22	b	613	CLA	C3A-C2A-CAA-CBA
22	b	615	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CHA-CBD-CGD-O1D
22	b	616	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	504	CLA	C2-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	C2-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6
22	c	509	CLA	C2-C3-C5-C6
22	c	509	CLA	C4-C3-C5-C6
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CHA-CBD-CGD-O1D
22	c	512	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	C2A-CAA-CBA-CGA
22	c	513	CLA	CBD-CGD-O2D-CED
22	c	514	CLA	C1A-C2A-CAA-CBA
22	s	301	CLA	C1A-C2A-CAA-CBA
22	s	301	CLA	C3A-C2A-CAA-CBA
22	s	302	CLA	CBD-CGD-O2D-CED
22	s	303	CLA	CBD-CGD-O2D-CED
22	s	304	CLA	C1A-C2A-CAA-CBA
22	s	304	CLA	C3A-C2A-CAA-CBA
22	s	304	CLA	CBD-CGD-O2D-CED
22	s	305	CLA	CBD-CGD-O2D-CED
23	1	309	LUT	C1-C6-C7-C8
23	2	309	LUT	C27-C28-C29-C30
23	2	309	LUT	C27-C28-C29-C39
23	4	309	LUT	C1-C6-C7-C8
23	5	309	LUT	C27-C28-C29-C30
23	5	309	LUT	C27-C28-C29-C39
23	U	309	LUT	C1-C6-C7-C8
23	S	311	LUT	C11-C12-C13-C20
23	S	311	LUT	C27-C28-C29-C30
23	S	311	LUT	C27-C28-C29-C39
23	s	311	LUT	C27-C28-C29-C30
23	s	311	LUT	C27-C28-C29-C39
24	r	612	XAT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	r	612	XAT	C27-C28-C29-C39
24	r	612	XAT	C31-C32-C33-C34
24	r	612	XAT	C31-C32-C33-C40
24	1	311	XAT	C9-C10-C11-C12
24	1	311	XAT	C31-C32-C33-C34
24	1	311	XAT	C31-C32-C33-C40
24	2	311	XAT	C7-C8-C9-C10
24	2	311	XAT	C7-C8-C9-C19
24	3	309	XAT	C7-C8-C9-C10
24	3	309	XAT	C7-C8-C9-C19
24	3	309	XAT	C31-C32-C33-C40
24	4	311	XAT	C9-C10-C11-C12
24	4	311	XAT	C31-C32-C33-C34
24	4	311	XAT	C31-C32-C33-C40
24	5	311	XAT	C7-C8-C9-C10
24	5	311	XAT	C7-C8-C9-C19
24	5	311	XAT	C11-C12-C13-C14
24	5	311	XAT	C11-C12-C13-C20
24	6	310	XAT	C7-C8-C9-C10
24	6	310	XAT	C7-C8-C9-C19
24	6	310	XAT	C31-C32-C33-C34
24	6	310	XAT	C31-C32-C33-C40
24	v	311	XAT	C7-C8-C9-C10
24	v	311	XAT	C7-C8-C9-C19
24	v	311	XAT	C27-C28-C29-C30
24	v	311	XAT	C27-C28-C29-C39
24	v	311	XAT	C31-C32-C33-C40
24	p	312	XAT	C27-C28-C29-C30
24	p	312	XAT	C27-C28-C29-C39
24	p	312	XAT	C31-C32-C33-C40
24	q	309	XAT	C7-C8-C9-C19
24	q	309	XAT	C13-C14-C15-C35
24	q	309	XAT	C31-C32-C33-C34
24	q	309	XAT	C31-C32-C33-C40
24	V	311	XAT	C7-C8-C9-C10
24	V	311	XAT	C7-C8-C9-C19
24	V	311	XAT	C11-C12-C13-C14
24	V	311	XAT	C11-C12-C13-C20
24	V	311	XAT	C27-C28-C29-C30
24	V	311	XAT	C27-C28-C29-C39
24	P	312	XAT	C11-C12-C13-C14
24	P	312	XAT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
24	P	312	XAT	C31-C32-C33-C34
24	P	312	XAT	C31-C32-C33-C40
24	Q	309	XAT	C7-C8-C9-C10
24	Q	309	XAT	C7-C8-C9-C19
24	Q	309	XAT	C31-C32-C33-C34
24	Q	309	XAT	C31-C32-C33-C40
24	U	311	XAT	C7-C8-C9-C10
24	U	311	XAT	C7-C8-C9-C19
24	U	311	XAT	C11-C12-C13-C14
24	U	311	XAT	C11-C12-C13-C20
24	U	311	XAT	C31-C32-C33-C34
24	U	311	XAT	C31-C32-C33-C40
24	N	311	XAT	C7-C8-C9-C19
24	N	311	XAT	C9-C10-C11-C12
24	G	309	XAT	C7-C8-C9-C10
24	G	309	XAT	C7-C8-C9-C19
24	G	309	XAT	C11-C12-C13-C14
24	G	309	XAT	C11-C12-C13-C20
24	G	309	XAT	C27-C28-C29-C39
24	G	309	XAT	C31-C32-C33-C34
24	G	309	XAT	C31-C32-C33-C40
24	u	311	XAT	C7-C8-C9-C10
24	u	311	XAT	C7-C8-C9-C19
24	u	311	XAT	C11-C12-C13-C14
24	u	311	XAT	C11-C12-C13-C20
24	n	311	XAT	C27-C28-C29-C30
24	n	311	XAT	C27-C28-C29-C39
24	g	309	XAT	C7-C8-C9-C10
24	g	309	XAT	C7-C8-C9-C19
24	g	309	XAT	C11-C12-C13-C14
24	g	309	XAT	C11-C12-C13-C20
24	g	309	XAT	C27-C28-C29-C39
24	g	309	XAT	C31-C32-C33-C34
24	g	309	XAT	C31-C32-C33-C40
24	R	313	XAT	C27-C28-C29-C30
24	R	313	XAT	C27-C28-C29-C39
25	r	613	LHG	C4-O6-P-O5
25	a	415	LHG	C2-C3-O3-P
25	a	415	LHG	C4-O6-P-O3
25	a	415	LHG	C4-O6-P-O4
25	a	415	LHG	C4-O6-P-O5
25	a	415	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	d	405	LHG	O1-C1-C2-C3
25	d	405	LHG	C3-O3-P-O4
25	d	405	LHG	C3-O3-P-O5
25	d	406	LHG	C4-O6-P-O4
25	l	101	LHG	C3-O3-P-O4
25	l	101	LHG	C3-O3-P-O5
25	l	101	LHG	C4-O6-P-O4
25	A	413	LHG	C2-C3-O3-P
25	A	413	LHG	C4-O6-P-O3
25	A	413	LHG	C4-O6-P-O4
25	A	413	LHG	C4-O6-P-O5
25	A	413	LHG	C8-C7-O7-C5
25	L	101	LHG	O1-C1-C2-O2
25	L	101	LHG	C3-O3-P-O4
25	L	101	LHG	C3-O3-P-O5
25	L	101	LHG	C4-O6-P-O4
25	1	312	LHG	O1-C1-C2-C3
25	1	312	LHG	O2-C2-C3-O3
25	1	312	LHG	C4-O6-P-O5
25	2	312	LHG	O1-C1-C2-C3
25	2	312	LHG	C4-O6-P-O5
25	3	310	LHG	C4-O6-P-O5
25	4	312	LHG	C4-O6-P-O5
25	5	312	LHG	C4-O6-P-O5
25	6	311	LHG	O1-C1-C2-C3
25	6	311	LHG	C4-O6-P-O5
25	v	312	LHG	C3-O3-P-O4
25	v	312	LHG	C4-O6-P-O5
25	p	313	LHG	O1-C1-C2-O2
25	p	313	LHG	O1-C1-C2-C3
25	p	313	LHG	C1-C2-C3-O3
25	p	313	LHG	C4-O6-P-O5
25	q	310	LHG	C1-C2-C3-O3
25	q	310	LHG	C4-O6-P-O5
25	V	312	LHG	O1-C1-C2-O2
25	V	312	LHG	O1-C1-C2-C3
25	V	312	LHG	C3-O3-P-O4
25	V	312	LHG	C3-O3-P-O5
25	V	312	LHG	C4-O6-P-O5
25	Q	310	LHG	O1-C1-C2-C3
25	Q	310	LHG	C4-O6-P-O5
25	U	312	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
25	G	310	LHG	O1-C1-C2-C3
25	G	310	LHG	C4-O6-P-O5
25	u	312	LHG	C3-O3-P-O5
25	n	312	LHG	C1-C2-C3-O3
25	n	312	LHG	C4-O6-P-O5
25	g	310	LHG	O1-C1-C2-C3
25	g	310	LHG	C4-O6-P-O5
25	R	314	LHG	O1-C1-C2-C3
25	R	314	LHG	O2-C2-C3-O3
25	R	314	LHG	C3-O3-P-O4
25	R	314	LHG	C3-O3-P-O5
25	R	314	LHG	C3-O3-P-O6
25	R	314	LHG	C4-O6-P-O5
25	S	312	LHG	C4-O6-P-O5
25	C	522	LHG	C24-C23-O8-C6
25	C	524	LHG	O1-C1-C2-C3
25	C	524	LHG	C1-C2-C3-O3
25	C	524	LHG	O9-C7-O7-C5
25	C	524	LHG	C8-C7-O7-C5
25	B	622	LHG	C4-O6-P-O4
25	B	623	LHG	O1-C1-C2-C3
25	B	623	LHG	O2-C2-C3-O3
25	B	623	LHG	C3-O3-P-O4
25	B	623	LHG	C4-O6-P-O4
25	B	623	LHG	C4-O6-P-O5
25	B	623	LHG	O7-C5-C6-O8
25	D	406	LHG	C3-O3-P-O4
25	D	407	LHG	C4-O6-P-O4
25	b	622	LHG	C3-O3-P-O6
25	b	622	LHG	C4-O6-P-O4
25	b	622	LHG	C4-O6-P-O5
25	b	623	LHG	O1-C1-C2-O2
25	b	623	LHG	O1-C1-C2-C3
25	b	623	LHG	O2-C2-C3-O3
25	b	623	LHG	C3-O3-P-O4
25	b	623	LHG	C4-O6-P-O4
25	b	623	LHG	C4-O6-P-O5
25	b	623	LHG	O7-C5-C6-O8
25	c	521	LHG	O1-C1-C2-C3
25	c	521	LHG	C4-O6-P-O5
25	c	523	LHG	O1-C1-C2-C3
25	c	523	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	c	523	LHG	O9-C7-O7-C5
25	s	312	LHG	C4-O6-P-O5
26	r	614	CHL	C1C-C2C-CMC-OMC
26	r	614	CHL	C3C-C2C-CMC-OMC
26	1	314	CHL	C3C-C2C-CMC-OMC
26	1	314	CHL	CHA-CBD-CGD-O1D
26	1	314	CHL	CHA-CBD-CGD-O2D
26	1	314	CHL	CAD-CBD-CGD-O1D
26	1	314	CHL	CAD-CBD-CGD-O2D
26	1	314	CHL	CBD-CGD-O2D-CED
26	1	315	CHL	C1C-C2C-CMC-OMC
26	1	317	CHL	C1C-C2C-CMC-OMC
26	1	317	CHL	C3C-C2C-CMC-OMC
26	2	313	CHL	C2-C3-C5-C6
26	2	313	CHL	C4-C3-C5-C6
26	2	314	CHL	C1C-C2C-CMC-OMC
26	2	314	CHL	C3C-C2C-CMC-OMC
26	2	314	CHL	CHA-CBD-CGD-O1D
26	2	314	CHL	CHA-CBD-CGD-O2D
26	2	314	CHL	CBD-CGD-O2D-CED
26	2	315	CHL	CBD-CGD-O2D-CED
26	2	316	CHL	C1C-C2C-CMC-OMC
26	2	316	CHL	C3C-C2C-CMC-OMC
26	2	316	CHL	CHA-CBD-CGD-O1D
26	2	316	CHL	CHA-CBD-CGD-O2D
26	2	318	CHL	C3C-C2C-CMC-OMC
26	3	312	CHL	CHA-CBD-CGD-O1D
26	3	312	CHL	CHA-CBD-CGD-O2D
26	3	312	CHL	CAD-CBD-CGD-O1D
26	3	313	CHL	C3A-C2A-CAA-CBA
26	3	313	CHL	C1C-C2C-CMC-OMC
26	3	314	CHL	CBD-CGD-O2D-CED
26	3	315	CHL	C1C-C2C-CMC-OMC
26	3	315	CHL	C3C-C2C-CMC-OMC
26	3	316	CHL	C1A-C2A-CAA-CBA
26	3	316	CHL	C1C-C2C-CMC-OMC
26	3	316	CHL	C3C-C2C-CMC-OMC
26	3	316	CHL	CHA-CBD-CGD-O1D
26	3	316	CHL	CHA-CBD-CGD-O2D
26	4	314	CHL	CHA-CBD-CGD-O1D
26	4	314	CHL	CHA-CBD-CGD-O2D
26	4	314	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	4	314	CHL	CAD-CBD-CGD-O2D
26	4	314	CHL	CBD-CGD-O2D-CED
26	4	315	CHL	C1C-C2C-CMC-OMC
26	4	316	CHL	C1A-C2A-CAA-CBA
26	4	316	CHL	C1C-C2C-CMC-OMC
26	4	316	CHL	C3C-C2C-CMC-OMC
26	4	317	CHL	C3C-C2C-CMC-OMC
26	5	313	CHL	C2-C3-C5-C6
26	5	313	CHL	C4-C3-C5-C6
26	5	314	CHL	C1C-C2C-CMC-OMC
26	5	314	CHL	C3C-C2C-CMC-OMC
26	5	314	CHL	CHA-CBD-CGD-O1D
26	5	314	CHL	CHA-CBD-CGD-O2D
26	5	314	CHL	CAD-CBD-CGD-O1D
26	5	314	CHL	CBD-CGD-O2D-CED
26	5	316	CHL	C1C-C2C-CMC-OMC
26	5	316	CHL	C3C-C2C-CMC-OMC
26	5	316	CHL	CHA-CBD-CGD-O1D
26	5	316	CHL	CHA-CBD-CGD-O2D
26	5	318	CHL	C3C-C2C-CMC-OMC
26	5	318	CHL	C14-C13-C15-C16
26	6	301	CHL	C3C-C2C-CMC-OMC
26	6	301	CHL	C11-C10-C8-C9
26	6	313	CHL	CHA-CBD-CGD-O1D
26	6	313	CHL	CHA-CBD-CGD-O2D
26	6	313	CHL	CAD-CBD-CGD-O1D
26	6	314	CHL	C1C-C2C-CMC-OMC
26	6	315	CHL	C2A-CAA-CBA-CGA
26	6	315	CHL	CBD-CGD-O2D-CED
26	6	316	CHL	C1A-C2A-CAA-CBA
26	6	316	CHL	C1C-C2C-CMC-OMC
26	6	316	CHL	C3C-C2C-CMC-OMC
26	6	317	CHL	C1A-C2A-CAA-CBA
26	6	317	CHL	C1C-C2C-CMC-OMC
26	6	317	CHL	C3C-C2C-CMC-OMC
26	v	313	CHL	C3C-C2C-CMC-OMC
26	v	314	CHL	C3C-C2C-CMC-OMC
26	v	314	CHL	CHA-CBD-CGD-O1D
26	v	314	CHL	CHA-CBD-CGD-O2D
26	v	314	CHL	CAD-CBD-CGD-O1D
26	v	314	CHL	CAD-CBD-CGD-O2D
26	v	315	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	v	316	CHL	C1C-C2C-CMC-OMC
26	v	316	CHL	C3C-C2C-CMC-OMC
26	v	317	CHL	C1C-C2C-CMC-OMC
26	v	317	CHL	C3C-C2C-CMC-OMC
26	v	317	CHL	C11-C10-C8-C9
26	v	318	CHL	C1C-C2C-CMC-OMC
26	v	318	CHL	C3C-C2C-CMC-OMC
26	v	318	CHL	C6-C7-C8-C9
26	p	315	CHL	CHA-CBD-CGD-O1D
26	p	315	CHL	CHA-CBD-CGD-O2D
26	p	315	CHL	CAD-CBD-CGD-O1D
26	p	315	CHL	CBD-CGD-O2D-CED
26	p	316	CHL	C1C-C2C-CMC-OMC
26	p	317	CHL	CHA-CBD-CGD-O1D
26	p	318	CHL	CBD-CGD-O2D-CED
26	p	319	CHL	C1C-C2C-CMC-OMC
26	p	319	CHL	C3C-C2C-CMC-OMC
26	p	320	CHL	C11-C10-C8-C9
26	q	311	CHL	C2-C3-C5-C6
26	q	311	CHL	C4-C3-C5-C6
26	q	312	CHL	C2A-CAA-CBA-CGA
26	q	312	CHL	C3C-C2C-CMC-OMC
26	q	312	CHL	CHA-CBD-CGD-O1D
26	q	312	CHL	CHA-CBD-CGD-O2D
26	q	312	CHL	CAD-CBD-CGD-O1D
26	q	312	CHL	CAD-CBD-CGD-O2D
26	q	313	CHL	CHA-CBD-CGD-O1D
26	q	313	CHL	CHA-CBD-CGD-O2D
26	q	314	CHL	C1A-C2A-CAA-CBA
26	q	314	CHL	C3C-C2C-CMC-OMC
26	q	315	CHL	C1C-C2C-CMC-OMC
26	q	315	CHL	C3C-C2C-CMC-OMC
26	V	313	CHL	C3C-C2C-CMC-OMC
26	V	314	CHL	C3C-C2C-CMC-OMC
26	V	314	CHL	CHA-CBD-CGD-O1D
26	V	314	CHL	CHA-CBD-CGD-O2D
26	V	314	CHL	CAD-CBD-CGD-O1D
26	V	315	CHL	C1C-C2C-CMC-OMC
26	V	316	CHL	C3C-C2C-CMC-OMC
26	V	317	CHL	C3C-C2C-CMC-OMC
26	V	318	CHL	C3C-C2C-CMC-OMC
26	V	318	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	P	315	CHL	CHA-CBD-CGD-O1D
26	P	315	CHL	CHA-CBD-CGD-O2D
26	P	315	CHL	CAD-CBD-CGD-O1D
26	P	316	CHL	C1C-C2C-CMC-OMC
26	P	317	CHL	C2A-CAA-CBA-CGA
26	P	317	CHL	CHA-CBD-CGD-O1D
26	P	317	CHL	CHA-CBD-CGD-O2D
26	P	317	CHL	C11-C10-C8-C9
26	P	318	CHL	C3C-C2C-CMC-OMC
26	P	319	CHL	C1A-C2A-CAA-CBA
26	P	319	CHL	C3C-C2C-CMC-OMC
26	Q	312	CHL	C1A-C2A-CAA-CBA
26	Q	312	CHL	C3C-C2C-CMC-OMC
26	Q	312	CHL	CHA-CBD-CGD-O1D
26	Q	312	CHL	CHA-CBD-CGD-O2D
26	Q	312	CHL	CAD-CBD-CGD-O1D
26	Q	312	CHL	CAD-CBD-CGD-O2D
26	Q	313	CHL	CHA-CBD-CGD-O1D
26	Q	313	CHL	CHA-CBD-CGD-O2D
26	Q	314	CHL	C3C-C2C-CMC-OMC
26	Q	314	CHL	C11-C10-C8-C9
26	Q	315	CHL	C1A-C2A-CAA-CBA
26	Q	315	CHL	C1C-C2C-CMC-OMC
26	Q	315	CHL	C3C-C2C-CMC-OMC
26	Q	315	CHL	C11-C10-C8-C9
26	Q	316	CHL	C1C-C2C-CMC-OMC
26	Q	316	CHL	C3C-C2C-CMC-OMC
26	U	314	CHL	C1C-C2C-CMC-OMC
26	U	314	CHL	CHA-CBD-CGD-O1D
26	U	314	CHL	CHA-CBD-CGD-O2D
26	U	315	CHL	C1C-C2C-CMC-OMC
26	U	315	CHL	C3C-C2C-CMC-OMC
26	U	315	CHL	CHA-CBD-CGD-O1D
26	U	315	CHL	CHA-CBD-CGD-O2D
26	U	316	CHL	C1C-C2C-CMC-OMC
26	U	316	CHL	C3C-C2C-CMC-OMC
26	U	316	CHL	C6-C7-C8-C9
26	U	317	CHL	C1C-C2C-CMC-OMC
26	U	317	CHL	C3C-C2C-CMC-OMC
26	U	317	CHL	C14-C13-C15-C16
26	U	319	CHL	C1A-C2A-CAA-CBA
26	U	319	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	U	319	CHL	C1C-C2C-CMC-OMC
26	U	319	CHL	C3C-C2C-CMC-OMC
26	U	319	CHL	CHA-CBD-CGD-O1D
26	U	319	CHL	CHA-CBD-CGD-O2D
26	U	319	CHL	C11-C10-C8-C9
26	N	313	CHL	C3C-C2C-CMC-OMC
26	N	314	CHL	C1C-C2C-CMC-OMC
26	N	314	CHL	C3C-C2C-CMC-OMC
26	N	314	CHL	CHA-CBD-CGD-O1D
26	N	314	CHL	CHA-CBD-CGD-O2D
26	N	314	CHL	CAD-CBD-CGD-O1D
26	N	314	CHL	CAD-CBD-CGD-O2D
26	N	314	CHL	CBD-CGD-O2D-CED
26	N	315	CHL	C1C-C2C-CMC-OMC
26	N	316	CHL	C1C-C2C-CMC-OMC
26	N	316	CHL	C3C-C2C-CMC-OMC
26	N	316	CHL	CHA-CBD-CGD-O1D
26	N	316	CHL	CHA-CBD-CGD-O2D
26	N	317	CHL	C1C-C2C-CMC-OMC
26	N	317	CHL	C3C-C2C-CMC-OMC
26	G	311	CHL	C2-C3-C5-C6
26	G	311	CHL	C4-C3-C5-C6
26	G	312	CHL	CHA-CBD-CGD-O1D
26	G	312	CHL	CHA-CBD-CGD-O2D
26	G	312	CHL	CAD-CBD-CGD-O1D
26	G	312	CHL	CAD-CBD-CGD-O2D
26	G	313	CHL	C3C-C2C-CMC-OMC
26	G	314	CHL	C1C-C2C-CMC-OMC
26	G	314	CHL	C3C-C2C-CMC-OMC
26	G	314	CHL	CBD-CGD-O2D-CED
26	G	315	CHL	C1A-C2A-CAA-CBA
26	G	316	CHL	C1A-C2A-CAA-CBA
26	G	316	CHL	C1C-C2C-CMC-OMC
26	G	316	CHL	C3C-C2C-CMC-OMC
26	u	314	CHL	CHA-CBD-CGD-O1D
26	u	314	CHL	CHA-CBD-CGD-O2D
26	u	314	CHL	CAD-CBD-CGD-O1D
26	u	314	CHL	CAD-CBD-CGD-O2D
26	u	315	CHL	C1C-C2C-CMC-OMC
26	u	315	CHL	CHA-CBD-CGD-O1D
26	u	315	CHL	CHA-CBD-CGD-O2D
26	u	316	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	u	316	CHL	C3C-C2C-CMC-OMC
26	u	316	CHL	CHA-CBD-CGD-O1D
26	u	317	CHL	C1C-C2C-CMC-OMC
26	u	317	CHL	C3C-C2C-CMC-OMC
26	u	317	CHL	C6-C7-C8-C9
26	u	318	CHL	C1C-C2C-CMC-OMC
26	u	318	CHL	C3C-C2C-CMC-OMC
26	n	313	CHL	C1C-C2C-CMC-OMC
26	n	313	CHL	C3C-C2C-CMC-OMC
26	n	314	CHL	C3C-C2C-CMC-OMC
26	n	314	CHL	CHA-CBD-CGD-O1D
26	n	314	CHL	CHA-CBD-CGD-O2D
26	n	314	CHL	CAD-CBD-CGD-O1D
26	n	314	CHL	CAD-CBD-CGD-O2D
26	n	314	CHL	CBD-CGD-O2D-CED
26	n	315	CHL	C1C-C2C-CMC-OMC
26	n	316	CHL	C1A-C2A-CAA-CBA
26	n	316	CHL	C1C-C2C-CMC-OMC
26	n	316	CHL	C3C-C2C-CMC-OMC
26	n	316	CHL	CHA-CBD-CGD-O2D
26	n	317	CHL	C1C-C2C-CMC-OMC
26	n	317	CHL	C3C-C2C-CMC-OMC
26	n	317	CHL	CHA-CBD-CGD-O1D
26	n	317	CHL	CHA-CBD-CGD-O2D
26	n	318	CHL	C1C-C2C-CMC-OMC
26	n	318	CHL	C3C-C2C-CMC-OMC
26	g	312	CHL	C1C-C2C-CMC-OMC
26	g	312	CHL	C3C-C2C-CMC-OMC
26	g	312	CHL	CHA-CBD-CGD-O1D
26	g	312	CHL	CHA-CBD-CGD-O2D
26	g	313	CHL	C3C-C2C-CMC-OMC
26	g	314	CHL	C3C-C2C-CMC-OMC
26	g	315	CHL	C1C-C2C-CMC-OMC
26	g	315	CHL	C3C-C2C-CMC-OMC
26	g	316	CHL	C1A-C2A-CAA-CBA
26	g	316	CHL	C1C-C2C-CMC-OMC
26	g	316	CHL	C3C-C2C-CMC-OMC
26	R	315	CHL	C1C-C2C-CMC-OMC
26	R	315	CHL	C3C-C2C-CMC-OMC
26	R	316	CHL	C3C-C2C-CMC-OMC
26	R	316	CHL	CHA-CBD-CGD-O1D
26	S	313	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	S	313	CHL	C3C-C2C-CMC-OMC
26	S	316	CHL	C1A-C2A-CAA-CBA
26	S	316	CHL	CHA-CBD-CGD-O1D
26	S	316	CHL	CHA-CBD-CGD-O2D
26	s	313	CHL	C1C-C2C-CMC-OMC
26	s	313	CHL	C3C-C2C-CMC-OMC
26	s	316	CHL	C1A-C2A-CAA-CBA
26	s	316	CHL	C3C-C2C-CMC-OMC
26	s	316	CHL	CHA-CBD-CGD-O1D
26	s	316	CHL	CHA-CBD-CGD-O2D
27	r	618	NEX	C7-C8-C9-C10
27	r	618	NEX	C7-C8-C9-C19
27	r	618	NEX	O24-C26-C27-C28
27	2	319	NEX	C7-C8-C9-C19
27	2	319	NEX	C11-C12-C13-C14
27	2	319	NEX	C11-C12-C13-C20
27	5	319	NEX	C7-C8-C9-C10
27	5	319	NEX	C7-C8-C9-C19
27	5	319	NEX	C11-C12-C13-C14
27	5	319	NEX	C11-C12-C13-C20
27	v	319	NEX	C11-C12-C13-C14
27	v	319	NEX	C11-C12-C13-C20
27	V	319	NEX	C7-C8-C9-C19
27	V	319	NEX	C11-C12-C13-C14
27	V	319	NEX	C11-C12-C13-C20
27	N	318	NEX	C7-C8-C9-C10
27	N	318	NEX	C7-C8-C9-C19
27	n	319	NEX	C7-C8-C9-C10
27	n	319	NEX	C7-C8-C9-C19
27	n	319	NEX	C11-C12-C13-C20
27	R	301	NEX	C7-C8-C9-C10
27	R	301	NEX	C7-C8-C9-C19
27	R	301	NEX	C11-C12-C13-C14
27	R	301	NEX	C11-C12-C13-C20
27	R	301	NEX	O24-C26-C27-C28
27	S	317	NEX	C7-C8-C9-C10
27	S	317	NEX	C7-C8-C9-C19
27	s	317	NEX	C7-C8-C9-C10
27	s	317	NEX	C7-C8-C9-C19
31	a	409	BCR	C7-C8-C9-C10
31	a	409	BCR	C7-C8-C9-C34
31	d	403	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	d	403	BCR	C11-C12-C13-C14
31	d	403	BCR	C11-C12-C13-C35
31	d	403	BCR	C15-C16-C17-C18
31	d	403	BCR	C17-C18-C19-C20
31	d	403	BCR	C36-C18-C19-C20
31	d	403	BCR	C21-C22-C23-C24
31	d	403	BCR	C37-C22-C23-C24
31	d	403	BCR	C23-C24-C25-C30
31	k	101	BCR	C11-C12-C13-C14
31	k	101	BCR	C11-C12-C13-C35
31	k	101	BCR	C17-C18-C19-C20
31	k	101	BCR	C36-C18-C19-C20
31	k	101	BCR	C21-C22-C23-C24
31	k	101	BCR	C37-C22-C23-C24
31	t	101	BCR	C7-C8-C9-C10
31	t	101	BCR	C17-C18-C19-C20
31	t	101	BCR	C36-C18-C19-C20
31	t	101	BCR	C21-C22-C23-C24
31	t	101	BCR	C37-C22-C23-C24
31	t	101	BCR	C23-C24-C25-C26
31	x	202	BCR	C7-C8-C9-C10
31	x	202	BCR	C7-C8-C9-C34
31	x	202	BCR	C11-C12-C13-C14
31	x	202	BCR	C11-C12-C13-C35
31	z	101	BCR	C11-C12-C13-C35
31	A	409	BCR	C7-C8-C9-C10
31	A	409	BCR	C7-C8-C9-C34
31	K	101	BCR	C11-C12-C13-C14
31	K	101	BCR	C11-C12-C13-C35
31	K	101	BCR	C17-C18-C19-C20
31	K	101	BCR	C36-C18-C19-C20
31	K	101	BCR	C21-C22-C23-C24
31	K	101	BCR	C37-C22-C23-C24
31	T	101	BCR	C17-C18-C19-C20
31	T	101	BCR	C36-C18-C19-C20
31	T	101	BCR	C21-C22-C23-C24
31	T	101	BCR	C37-C22-C23-C24
31	T	101	BCR	C23-C24-C25-C26
31	C	516	BCR	C11-C12-C13-C35
31	C	516	BCR	C13-C14-C15-C16
31	C	517	BCR	C17-C18-C19-C20
31	C	517	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	C	517	BCR	C21-C22-C23-C24
31	C	517	BCR	C37-C22-C23-C24
31	C	518	BCR	C7-C8-C9-C10
31	C	518	BCR	C7-C8-C9-C34
31	C	518	BCR	C17-C18-C19-C20
31	C	518	BCR	C36-C18-C19-C20
31	C	518	BCR	C21-C22-C23-C24
31	C	518	BCR	C37-C22-C23-C24
31	C	518	BCR	C23-C24-C25-C30
31	B	618	BCR	C11-C12-C13-C14
31	B	618	BCR	C11-C12-C13-C35
31	B	619	BCR	C1-C6-C7-C8
31	B	619	BCR	C7-C8-C9-C10
31	B	619	BCR	C7-C8-C9-C34
31	B	619	BCR	C17-C18-C19-C20
31	B	619	BCR	C36-C18-C19-C20
31	B	619	BCR	C21-C22-C23-C24
31	B	619	BCR	C37-C22-C23-C24
31	B	620	BCR	C11-C12-C13-C14
31	B	620	BCR	C11-C12-C13-C35
31	B	620	BCR	C17-C18-C19-C20
31	B	620	BCR	C36-C18-C19-C20
31	B	620	BCR	C37-C22-C23-C24
31	D	404	BCR	C1-C6-C7-C8
31	D	404	BCR	C11-C12-C13-C14
31	D	404	BCR	C11-C12-C13-C35
31	D	404	BCR	C15-C16-C17-C18
31	D	404	BCR	C17-C18-C19-C20
31	D	404	BCR	C36-C18-C19-C20
31	D	404	BCR	C21-C22-C23-C24
31	D	404	BCR	C37-C22-C23-C24
31	D	404	BCR	C23-C24-C25-C30
31	X	201	BCR	C7-C8-C9-C10
31	X	201	BCR	C7-C8-C9-C34
31	X	201	BCR	C11-C12-C13-C14
31	X	201	BCR	C11-C12-C13-C35
31	b	619	BCR	C1-C6-C7-C8
31	b	619	BCR	C7-C8-C9-C10
31	b	619	BCR	C7-C8-C9-C34
31	b	619	BCR	C13-C14-C15-C16
31	b	619	BCR	C17-C18-C19-C20
31	b	619	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	b	619	BCR	C21-C22-C23-C24
31	b	619	BCR	C37-C22-C23-C24
31	b	620	BCR	C11-C12-C13-C14
31	b	620	BCR	C11-C12-C13-C35
31	b	620	BCR	C36-C18-C19-C20
31	b	620	BCR	C21-C22-C23-C24
31	b	620	BCR	C37-C22-C23-C24
31	c	515	BCR	C17-C18-C19-C20
31	c	515	BCR	C36-C18-C19-C20
31	c	515	BCR	C21-C22-C23-C24
31	c	515	BCR	C37-C22-C23-C24
31	c	516	BCR	C7-C8-C9-C10
31	c	516	BCR	C7-C8-C9-C34
31	c	516	BCR	C17-C18-C19-C20
31	c	516	BCR	C36-C18-C19-C20
31	c	516	BCR	C21-C22-C23-C24
31	c	516	BCR	C37-C22-C23-C24
31	c	516	BCR	C23-C24-C25-C30
32	a	410	SQD	C45-C44-O6-C1
32	a	410	SQD	O5-C1-O6-C44
32	a	410	SQD	C5-C6-S-O7
32	a	410	SQD	C5-C6-S-O8
32	a	410	SQD	C5-C6-S-O9
32	a	413	SQD	C5-C6-S-O9
32	l	102	SQD	C2-C1-O6-C44
32	l	102	SQD	O5-C1-O6-C44
32	l	102	SQD	O49-C7-O47-C45
32	l	102	SQD	C8-C7-O47-C45
32	m	101	SQD	O49-C7-O47-C45
32	m	101	SQD	O5-C5-C6-S
32	A	412	SQD	C5-C6-S-O7
32	A	412	SQD	C5-C6-S-O8
32	A	412	SQD	C5-C6-S-O9
32	L	102	SQD	C2-C1-O6-C44
32	L	102	SQD	O5-C1-O6-C44
32	L	102	SQD	O49-C7-O47-C45
32	L	102	SQD	C8-C7-O47-C45
32	M	101	SQD	O49-C7-O47-C45
32	M	101	SQD	O5-C5-C6-S
32	C	501	SQD	C45-C44-O6-C1
32	C	501	SQD	O5-C1-O6-C44
32	C	501	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
32	C	501	SQD	C5-C6-S-O8
34	C	521	LMG	C2-C1-O1-C7
34	C	521	LMG	O6-C1-O1-C7
34	B	624	LMG	O6-C1-O1-C7
34	B	624	LMG	C11-C10-O7-C8
34	b	624	LMG	O6-C1-O1-C7
34	b	624	LMG	C11-C10-O7-C8
34	c	520	LMG	C2-C1-O1-C7
34	c	520	LMG	O6-C1-O1-C7
36	a	416	DGD	C2D-C1D-O3G-C3G
36	a	416	DGD	O6D-C1D-O3G-C3G
36	A	414	DGD	C2D-C1D-O3G-C3G
36	A	414	DGD	O6D-C1D-O3G-C3G
36	A	414	DGD	C2E-C1E-O5D-C6D
36	J	101	DGD	C2B-C1B-O2G-C2G
36	C	519	DGD	C2B-C1B-O2G-C2G
36	C	520	DGD	C2E-C1E-O5D-C6D
36	C	520	DGD	O6E-C1E-O5D-C6D
36	c	517	DGD	C2B-C1B-O2G-C2G
36	c	518	DGD	C2E-C1E-O5D-C6D
36	c	518	DGD	O6E-C1E-O5D-C6D
36	c	519	DGD	C2B-C1B-O2G-C2G
37	E	101	HEM	C2A-CAA-CBA-CGA
37	e	101	HEM	C2A-CAA-CBA-CGA
22	r	602	CLA	O1D-CGD-O2D-CED
22	r	608	CLA	O1D-CGD-O2D-CED
22	1	305	CLA	O1D-CGD-O2D-CED
22	1	307	CLA	O1D-CGD-O2D-CED
22	3	303	CLA	O1D-CGD-O2D-CED
22	3	304	CLA	O1D-CGD-O2D-CED
22	3	307	CLA	O1D-CGD-O2D-CED
22	4	305	CLA	O1D-CGD-O2D-CED
22	6	304	CLA	O1D-CGD-O2D-CED
22	6	305	CLA	O1D-CGD-O2D-CED
22	6	306	CLA	O1D-CGD-O2D-CED
22	6	308	CLA	O1D-CGD-O2D-CED
22	v	303	CLA	O1D-CGD-O2D-CED
22	v	305	CLA	O1D-CGD-O2D-CED
22	p	308	CLA	O1D-CGD-O2D-CED
22	q	305	CLA	O1D-CGD-O2D-CED
22	q	307	CLA	O1D-CGD-O2D-CED
22	V	303	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	V	305	CLA	O1D-CGD-O2D-CED
22	V	307	CLA	O1D-CGD-O2D-CED
22	P	308	CLA	O1D-CGD-O2D-CED
22	Q	307	CLA	O1D-CGD-O2D-CED
22	g	305	CLA	O1D-CGD-O2D-CED
22	R	303	CLA	O1D-CGD-O2D-CED
22	R	309	CLA	O1D-CGD-O2D-CED
22	S	302	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	B	608	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
22	B	614	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
22	b	614	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	s	302	CLA	O1D-CGD-O2D-CED
22	r	606	CLA	O1D-CGD-O2D-CED
22	r	609	CLA	O1D-CGD-O2D-CED
22	3	305	CLA	O1D-CGD-O2D-CED
22	4	302	CLA	O1D-CGD-O2D-CED
22	4	307	CLA	O1D-CGD-O2D-CED
22	5	307	CLA	O1D-CGD-O2D-CED
22	6	303	CLA	O1D-CGD-O2D-CED
22	v	306	CLA	O1D-CGD-O2D-CED
22	q	304	CLA	O1D-CGD-O2D-CED
22	G	305	CLA	O1D-CGD-O2D-CED
22	G	306	CLA	O1D-CGD-O2D-CED
22	n	301	CLA	O1D-CGD-O2D-CED
22	n	307	CLA	O1D-CGD-O2D-CED
22	R	307	CLA	O1D-CGD-O2D-CED
22	R	310	CLA	O1D-CGD-O2D-CED
22	S	308	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	602	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	s	308	CLA	O1D-CGD-O2D-CED
22	r	602	CLA	CBD-CGD-O2D-CED
22	r	603	CLA	CBD-CGD-O2D-CED
22	x	201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	1	301	CLA	CBD-CGD-O2D-CED
22	2	302	CLA	CBD-CGD-O2D-CED
22	2	306	CLA	CBD-CGD-O2D-CED
22	2	307	CLA	CBD-CGD-O2D-CED
22	3	302	CLA	CBD-CGD-O2D-CED
22	3	303	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CBD-CGD-O2D-CED
22	4	301	CLA	CBD-CGD-O2D-CED
22	4	302	CLA	CBD-CGD-O2D-CED
22	4	304	CLA	CBD-CGD-O2D-CED
22	4	306	CLA	CBD-CGD-O2D-CED
22	5	302	CLA	CBD-CGD-O2D-CED
22	5	306	CLA	CBD-CGD-O2D-CED
22	6	303	CLA	CBD-CGD-O2D-CED
22	6	309	CLA	CBD-CGD-O2D-CED
22	v	301	CLA	CBD-CGD-O2D-CED
22	v	303	CLA	CBD-CGD-O2D-CED
22	v	306	CLA	CBD-CGD-O2D-CED
22	v	308	CLA	CBD-CGD-O2D-CED
22	p	305	CLA	CBD-CGD-O2D-CED
22	p	307	CLA	CBD-CGD-O2D-CED
22	q	301	CLA	CBD-CGD-O2D-CED
22	q	302	CLA	CBD-CGD-O2D-CED
22	V	301	CLA	CBD-CGD-O2D-CED
22	V	303	CLA	CBD-CGD-O2D-CED
22	V	307	CLA	CBD-CGD-O2D-CED
22	V	308	CLA	CBD-CGD-O2D-CED
22	P	303	CLA	CBD-CGD-O2D-CED
22	P	304	CLA	CBD-CGD-O2D-CED
22	P	305	CLA	CBD-CGD-O2D-CED
22	P	307	CLA	CBD-CGD-O2D-CED
22	Q	307	CLA	CBD-CGD-O2D-CED
22	Q	308	CLA	CBD-CGD-O2D-CED
22	U	308	CLA	CBD-CGD-O2D-CED
22	N	301	CLA	CBD-CGD-O2D-CED
22	N	308	CLA	CBD-CGD-O2D-CED
22	G	303	CLA	CBD-CGD-O2D-CED
22	G	306	CLA	CBD-CGD-O2D-CED
22	G	308	CLA	CBD-CGD-O2D-CED
22	u	303	CLA	CBD-CGD-O2D-CED
22	u	304	CLA	CBD-CGD-O2D-CED
22	u	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	n	301	CLA	CBD-CGD-O2D-CED
22	n	302	CLA	CBD-CGD-O2D-CED
22	n	303	CLA	CBD-CGD-O2D-CED
22	n	304	CLA	CBD-CGD-O2D-CED
22	n	307	CLA	CBD-CGD-O2D-CED
22	g	303	CLA	CBD-CGD-O2D-CED
22	g	306	CLA	CBD-CGD-O2D-CED
22	g	308	CLA	CBD-CGD-O2D-CED
22	R	303	CLA	CBD-CGD-O2D-CED
22	S	308	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	CBD-CGD-O2D-CED
22	B	617	CLA	CBD-CGD-O2D-CED
22	b	602	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	s	308	CLA	CBD-CGD-O2D-CED
26	r	616	CHL	CBD-CGD-O2D-CED
26	r	619	CHL	CBD-CGD-O2D-CED
26	3	312	CHL	CBD-CGD-O2D-CED
26	3	315	CHL	CBD-CGD-O2D-CED
26	3	316	CHL	CBD-CGD-O2D-CED
26	5	315	CHL	CBD-CGD-O2D-CED
26	6	313	CHL	CBD-CGD-O2D-CED
26	6	316	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	6	317	CHL	CBD-CGD-O2D-CED
26	P	315	CHL	CBD-CGD-O2D-CED
26	P	318	CHL	CBD-CGD-O2D-CED
26	Q	314	CHL	CBD-CGD-O2D-CED
26	Q	315	CHL	CBD-CGD-O2D-CED
26	G	313	CHL	CBD-CGD-O2D-CED
26	G	315	CHL	CBD-CGD-O2D-CED
26	u	314	CHL	CBD-CGD-O2D-CED
26	g	313	CHL	CBD-CGD-O2D-CED
26	g	314	CHL	CBD-CGD-O2D-CED
26	g	315	CHL	CBD-CGD-O2D-CED
26	R	317	CHL	CBD-CGD-O2D-CED
22	2	302	CLA	O1A-CGA-O2A-C1
22	P	306	CLA	O1A-CGA-O2A-C1
22	n	308	CLA	O1A-CGA-O2A-C1
25	2	312	LHG	O10-C23-O8-C6
25	5	312	LHG	O10-C23-O8-C6
25	C	522	LHG	O10-C23-O8-C6
25	c	521	LHG	O10-C23-O8-C6
26	G	315	CHL	O1A-CGA-O2A-C1
34	C	502	LMG	O10-C28-O8-C9
34	B	621	LMG	O10-C28-O8-C9
34	c	501	LMG	O10-C28-O8-C9
36	J	101	DGD	O1A-C1A-O1G-C1G
36	c	519	DGD	O1A-C1A-O1G-C1G
22	r	603	CLA	O1D-CGD-O2D-CED
22	2	304	CLA	O1D-CGD-O2D-CED
22	2	307	CLA	O1D-CGD-O2D-CED
22	P	303	CLA	O1D-CGD-O2D-CED
22	P	305	CLA	O1D-CGD-O2D-CED
22	Q	301	CLA	O1D-CGD-O2D-CED
22	U	307	CLA	O1D-CGD-O2D-CED
22	N	301	CLA	O1D-CGD-O2D-CED
22	n	306	CLA	O1D-CGD-O2D-CED
22	g	306	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
22	B	617	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
26	3	315	CHL	O1D-CGD-O2D-CED
26	6	316	CHL	O1D-CGD-O2D-CED
26	Q	314	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	2	303	CLA	O1D-CGD-O2D-CED
22	3	301	CLA	O1D-CGD-O2D-CED
22	5	301	CLA	O1D-CGD-O2D-CED
22	5	308	CLA	O1D-CGD-O2D-CED
22	6	302	CLA	O1D-CGD-O2D-CED
22	v	307	CLA	O1D-CGD-O2D-CED
22	p	302	CLA	O1D-CGD-O2D-CED
22	p	305	CLA	O1D-CGD-O2D-CED
22	p	309	CLA	O1D-CGD-O2D-CED
22	P	302	CLA	O1D-CGD-O2D-CED
22	N	302	CLA	O1D-CGD-O2D-CED
22	N	304	CLA	O1D-CGD-O2D-CED
22	N	306	CLA	O1D-CGD-O2D-CED
22	G	302	CLA	O1D-CGD-O2D-CED
22	n	308	CLA	O1D-CGD-O2D-CED
22	g	302	CLA	O1D-CGD-O2D-CED
22	S	303	CLA	O1D-CGD-O2D-CED
22	S	305	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
22	s	303	CLA	O1D-CGD-O2D-CED
22	s	304	CLA	O1D-CGD-O2D-CED
22	s	305	CLA	O1D-CGD-O2D-CED
26	1	314	CHL	O1D-CGD-O2D-CED
26	2	314	CHL	O1D-CGD-O2D-CED
26	3	314	CHL	O1D-CGD-O2D-CED
26	6	315	CHL	O1D-CGD-O2D-CED
26	p	315	CHL	O1D-CGD-O2D-CED
26	n	314	CHL	O1D-CGD-O2D-CED
22	P	303	CLA	CBA-CGA-O2A-C1
22	P	306	CLA	CBA-CGA-O2A-C1
22	n	308	CLA	CBA-CGA-O2A-C1
25	2	312	LHG	C24-C23-O8-C6
25	5	312	LHG	C24-C23-O8-C6
25	c	521	LHG	C24-C23-O8-C6
36	J	101	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
36	c	519	DGD	C2A-C1A-O1G-C1G
22	r	601	CLA	CBD-CGD-O2D-CED
22	a	404	CLA	CBD-CGD-O2D-CED
22	a	406	CLA	CBD-CGD-O2D-CED
22	A	404	CLA	CBD-CGD-O2D-CED
22	A	406	CLA	CBD-CGD-O2D-CED
22	1	306	CLA	CBD-CGD-O2D-CED
22	3	306	CLA	CBD-CGD-O2D-CED
22	5	303	CLA	CBD-CGD-O2D-CED
22	6	307	CLA	CBD-CGD-O2D-CED
22	q	306	CLA	CBD-CGD-O2D-CED
22	V	302	CLA	CBD-CGD-O2D-CED
22	U	302	CLA	CBD-CGD-O2D-CED
22	U	304	CLA	CBD-CGD-O2D-CED
22	N	307	CLA	CBD-CGD-O2D-CED
22	u	302	CLA	CBD-CGD-O2D-CED
22	S	307	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
26	2	317	CHL	CBD-CGD-O2D-CED
26	5	317	CHL	CBD-CGD-O2D-CED
26	6	301	CHL	CBD-CGD-O2D-CED
26	q	311	CHL	CBD-CGD-O2D-CED
26	q	314	CHL	CBD-CGD-O2D-CED
26	N	316	CHL	CBD-CGD-O2D-CED
26	n	315	CHL	CBD-CGD-O2D-CED
26	g	316	CHL	CBD-CGD-O2D-CED
30	a	407	PHO	CBD-CGD-O2D-CED
30	d	401	PHO	CBD-CGD-O2D-CED
30	A	407	PHO	CBD-CGD-O2D-CED
30	D	401	PHO	CBD-CGD-O2D-CED
22	r	601	CLA	O1A-CGA-O2A-C1
22	r	607	CLA	O1A-CGA-O2A-C1
22	1	305	CLA	O1A-CGA-O2A-C1
22	2	305	CLA	O1A-CGA-O2A-C1
22	4	305	CLA	O1A-CGA-O2A-C1
22	5	302	CLA	O1A-CGA-O2A-C1
22	6	305	CLA	O1A-CGA-O2A-C1
22	v	305	CLA	O1A-CGA-O2A-C1
22	p	306	CLA	O1A-CGA-O2A-C1
22	q	304	CLA	O1A-CGA-O2A-C1
22	V	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	V	308	CLA	O1A-CGA-O2A-C1
22	P	303	CLA	O1A-CGA-O2A-C1
22	U	305	CLA	O1A-CGA-O2A-C1
22	N	302	CLA	O1A-CGA-O2A-C1
22	N	306	CLA	O1A-CGA-O2A-C1
22	G	302	CLA	O1A-CGA-O2A-C1
22	u	305	CLA	O1A-CGA-O2A-C1
22	g	302	CLA	O1A-CGA-O2A-C1
22	R	302	CLA	O1A-CGA-O2A-C1
22	R	308	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	O1A-CGA-O2A-C1
22	C	512	CLA	O1A-CGA-O2A-C1
22	c	507	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	O1A-CGA-O2A-C1
25	B	622	LHG	O10-C23-O8-C6
25	b	622	LHG	O10-C23-O8-C6
30	a	407	PHO	O1A-CGA-O2A-C1
30	A	407	PHO	O1A-CGA-O2A-C1
32	m	101	SQD	O10-C23-O48-C46
32	M	101	SQD	O10-C23-O48-C46
36	a	416	DGD	O1A-C1A-O1G-C1G
36	A	414	DGD	O1A-C1A-O1G-C1G
22	1	303	CLA	O1D-CGD-O2D-CED
22	5	304	CLA	O1D-CGD-O2D-CED
22	p	304	CLA	O1D-CGD-O2D-CED
22	V	304	CLA	O1D-CGD-O2D-CED
22	P	309	CLA	O1D-CGD-O2D-CED
22	u	307	CLA	O1D-CGD-O2D-CED
22	R	304	CLA	O1D-CGD-O2D-CED
22	C	513	CLA	O1D-CGD-O2D-CED
22	C	514	CLA	O1D-CGD-O2D-CED
26	4	314	CHL	O1D-CGD-O2D-CED
26	N	314	CHL	O1D-CGD-O2D-CED
34	A	411	LMG	O6-C5-C6-O5
22	1	304	CLA	O1D-CGD-O2D-CED
22	2	301	CLA	O1D-CGD-O2D-CED
22	2	308	CLA	O1D-CGD-O2D-CED
22	4	303	CLA	O1D-CGD-O2D-CED
22	5	306	CLA	O1D-CGD-O2D-CED
22	v	304	CLA	O1D-CGD-O2D-CED
22	q	308	CLA	O1D-CGD-O2D-CED
22	V	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	U	301	CLA	O1D-CGD-O2D-CED
22	S	304	CLA	O1D-CGD-O2D-CED
26	2	315	CHL	O1D-CGD-O2D-CED
26	5	314	CHL	O1D-CGD-O2D-CED
26	p	318	CHL	O1D-CGD-O2D-CED
26	G	314	CHL	O1D-CGD-O2D-CED
36	A	414	DGD	O6D-C5D-C6D-O5D
22	R	308	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	CBD-CGD-O2D-CED
22	s	307	CLA	CBD-CGD-O2D-CED
26	p	320	CHL	CBD-CGD-O2D-CED
26	s	316	CHL	CBD-CGD-O2D-CED
26	Q	315	CHL	C13-C15-C16-C17
22	x	201	CLA	O1D-CGD-O2D-CED
22	1	302	CLA	O1D-CGD-O2D-CED
22	v	301	CLA	O1D-CGD-O2D-CED
22	u	301	CLA	O1D-CGD-O2D-CED
22	u	308	CLA	O1D-CGD-O2D-CED
22	X	202	CLA	O1D-CGD-O2D-CED
25	D	406	LHG	O9-C7-O7-C5
34	B	624	LMG	O9-C10-O7-C8
34	b	624	LMG	O9-C10-O7-C8
36	J	101	DGD	O1B-C1B-O2G-C2G
36	C	519	DGD	O1B-C1B-O2G-C2G
36	c	517	DGD	O1B-C1B-O2G-C2G
36	c	519	DGD	O1B-C1B-O2G-C2G
22	5	302	CLA	O1D-CGD-O2D-CED
22	x	201	CLA	C3-C5-C6-C7
22	1	307	CLA	C3-C5-C6-C7
22	p	302	CLA	C3-C5-C6-C7
22	P	307	CLA	C3-C5-C6-C7
22	P	308	CLA	C3-C5-C6-C7
22	Q	304	CLA	C3-C5-C6-C7
22	U	307	CLA	C3-C5-C6-C7
22	G	307	CLA	C3-C5-C6-C7
22	u	307	CLA	C3-C5-C6-C7
22	g	307	CLA	C3-C5-C6-C7
22	R	304	CLA	C3-C5-C6-C7
22	R	310	CLA	C3-C5-C6-C7
22	C	505	CLA	C3-C5-C6-C7
22	B	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C3-C5-C6-C7
22	B	615	CLA	C3-C5-C6-C7
22	X	202	CLA	C3-C5-C6-C7
22	b	615	CLA	C3-C5-C6-C7
22	c	504	CLA	C3-C5-C6-C7
26	r	616	CHL	C3-C5-C6-C7
26	5	313	CHL	C3-C5-C6-C7
26	p	314	CHL	C3-C5-C6-C7
26	p	317	CHL	C3-C5-C6-C7
26	q	314	CHL	C3-C5-C6-C7
26	q	315	CHL	C3-C5-C6-C7
26	V	317	CHL	C3-C5-C6-C7
26	P	314	CHL	C3-C5-C6-C7
26	N	313	CHL	C3-C5-C6-C7
26	n	313	CHL	C3-C5-C6-C7
26	n	316	CHL	C3-C5-C6-C7
26	R	317	CHL	C3-C5-C6-C7
26	S	315	CHL	C3-C5-C6-C7
26	s	315	CHL	C3-C5-C6-C7
30	d	401	PHO	C3-C5-C6-C7
30	D	401	PHO	C3-C5-C6-C7
22	r	607	CLA	CBA-CGA-O2A-C1
22	1	305	CLA	CBA-CGA-O2A-C1
22	2	302	CLA	CBA-CGA-O2A-C1
22	4	302	CLA	CBA-CGA-O2A-C1
22	4	305	CLA	CBA-CGA-O2A-C1
22	5	302	CLA	CBA-CGA-O2A-C1
22	6	303	CLA	CBA-CGA-O2A-C1
22	v	305	CLA	CBA-CGA-O2A-C1
22	p	306	CLA	CBA-CGA-O2A-C1
22	q	304	CLA	CBA-CGA-O2A-C1
22	V	305	CLA	CBA-CGA-O2A-C1
22	V	308	CLA	CBA-CGA-O2A-C1
22	Q	302	CLA	CBA-CGA-O2A-C1
22	U	305	CLA	CBA-CGA-O2A-C1
22	N	302	CLA	CBA-CGA-O2A-C1
22	N	306	CLA	CBA-CGA-O2A-C1
22	G	302	CLA	CBA-CGA-O2A-C1
22	u	302	CLA	CBA-CGA-O2A-C1
22	n	306	CLA	CBA-CGA-O2A-C1
22	g	302	CLA	CBA-CGA-O2A-C1
22	R	302	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	R	308	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
22	c	511	CLA	CBA-CGA-O2A-C1
25	B	622	LHG	C24-C23-O8-C6
25	b	622	LHG	C24-C23-O8-C6
26	G	311	CHL	CBA-CGA-O2A-C1
26	G	315	CHL	CBA-CGA-O2A-C1
30	a	407	PHO	CBA-CGA-O2A-C1
30	A	407	PHO	CBA-CGA-O2A-C1
34	C	502	LMG	C29-C28-O8-C9
34	B	621	LMG	C29-C28-O8-C9
34	c	501	LMG	C29-C28-O8-C9
36	a	416	DGD	C2A-C1A-O1G-C1G
36	A	414	DGD	C2A-C1A-O1G-C1G
36	C	520	DGD	O6E-C5E-C6E-O5E
36	c	518	DGD	O6E-C5E-C6E-O5E
25	d	405	LHG	C8-C7-O7-C5
25	D	406	LHG	C8-C7-O7-C5
25	c	523	LHG	C8-C7-O7-C5
32	m	101	SQD	C8-C7-O47-C45
32	M	101	SQD	C8-C7-O47-C45
22	2	306	CLA	O1D-CGD-O2D-CED
22	3	308	CLA	O1D-CGD-O2D-CED
22	4	304	CLA	O1D-CGD-O2D-CED
22	q	301	CLA	O1D-CGD-O2D-CED
22	V	301	CLA	O1D-CGD-O2D-CED
22	U	308	CLA	O1D-CGD-O2D-CED
22	N	308	CLA	O1D-CGD-O2D-CED
22	u	304	CLA	O1D-CGD-O2D-CED
22	n	303	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
26	r	616	CHL	O1D-CGD-O2D-CED
26	P	315	CHL	O1D-CGD-O2D-CED
26	P	318	CHL	O1D-CGD-O2D-CED
26	R	317	CHL	O1D-CGD-O2D-CED
22	r	607	CLA	CBD-CGD-O2D-CED
26	S	316	CHL	CBD-CGD-O2D-CED
22	U	302	CLA	O1A-CGA-O2A-C1
36	a	416	DGD	O6D-C5D-C6D-O5D
36	a	416	DGD	C4D-C5D-C6D-O5D
36	A	414	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
22	P	302	CLA	C4-C3-C5-C6
22	C	508	CLA	C4-C3-C5-C6
22	b	615	CLA	C4-C3-C5-C6
22	c	505	CLA	C4-C3-C5-C6
26	r	614	CHL	C4-C3-C5-C6
26	Q	311	CHL	C4-C3-C5-C6
26	g	311	CHL	C4-C3-C5-C6
22	C	508	CLA	C2-C3-C5-C6
22	b	615	CLA	C2-C3-C5-C6
26	r	614	CHL	C2-C3-C5-C6
26	g	311	CHL	C2-C3-C5-C6
22	C	509	CLA	CBD-CGD-O2D-CED
26	5	318	CHL	CBD-CGD-O2D-CED
26	G	316	CHL	CBD-CGD-O2D-CED
22	P	306	CLA	C2A-CAA-CBA-CGA
22	N	308	CLA	C2A-CAA-CBA-CGA
22	G	301	CLA	C2A-CAA-CBA-CGA
22	g	301	CLA	C2A-CAA-CBA-CGA
22	C	514	CLA	C2A-CAA-CBA-CGA
22	b	602	CLA	C2A-CAA-CBA-CGA
22	b	608	CLA	C2A-CAA-CBA-CGA
26	r	616	CHL	C2A-CAA-CBA-CGA
26	1	314	CHL	C2A-CAA-CBA-CGA
26	2	314	CHL	C2A-CAA-CBA-CGA
26	2	315	CHL	C2A-CAA-CBA-CGA
26	2	316	CHL	C2A-CAA-CBA-CGA
26	3	314	CHL	C2A-CAA-CBA-CGA
26	3	315	CHL	C2A-CAA-CBA-CGA
26	5	314	CHL	C2A-CAA-CBA-CGA
26	5	316	CHL	C2A-CAA-CBA-CGA
26	6	316	CHL	C2A-CAA-CBA-CGA
26	v	314	CHL	C2A-CAA-CBA-CGA
26	V	314	CHL	C2A-CAA-CBA-CGA
26	V	315	CHL	C2A-CAA-CBA-CGA
26	V	316	CHL	C2A-CAA-CBA-CGA
26	Q	312	CHL	C2A-CAA-CBA-CGA
26	U	314	CHL	C2A-CAA-CBA-CGA
26	U	315	CHL	C2A-CAA-CBA-CGA
26	G	314	CHL	C2A-CAA-CBA-CGA
26	n	316	CHL	C2A-CAA-CBA-CGA
26	g	312	CHL	C2A-CAA-CBA-CGA
26	R	317	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	Q	310	LHG	O10-C23-O8-C6
34	b	621	LMG	O10-C28-O8-C9
22	4	301	CLA	O1D-CGD-O2D-CED
26	5	315	CHL	O1D-CGD-O2D-CED
22	r	603	CLA	C3-C5-C6-C7
22	p	307	CLA	C3-C5-C6-C7
22	V	301	CLA	C3-C5-C6-C7
22	V	306	CLA	C3-C5-C6-C7
22	P	302	CLA	C3-C5-C6-C7
22	B	607	CLA	C3-C5-C6-C7
22	b	605	CLA	C3-C5-C6-C7
22	b	607	CLA	C3-C5-C6-C7
22	r	601	CLA	CBA-CGA-O2A-C1
22	A	405	CLA	CBA-CGA-O2A-C1
22	2	305	CLA	CBA-CGA-O2A-C1
22	6	305	CLA	CBA-CGA-O2A-C1
22	6	306	CLA	CBA-CGA-O2A-C1
22	p	303	CLA	CBA-CGA-O2A-C1
22	U	302	CLA	CBA-CGA-O2A-C1
22	u	305	CLA	CBA-CGA-O2A-C1
22	R	309	CLA	CBA-CGA-O2A-C1
22	C	507	CLA	CBA-CGA-O2A-C1
22	C	508	CLA	CBA-CGA-O2A-C1
22	c	507	CLA	CBA-CGA-O2A-C1
25	Q	310	LHG	C24-C23-O8-C6
32	l	102	SQD	C24-C23-O48-C46
32	m	101	SQD	C24-C23-O48-C46
32	L	102	SQD	C24-C23-O48-C46
32	M	101	SQD	C24-C23-O48-C46
34	d	407	LMG	C29-C28-O8-C9
34	D	408	LMG	C29-C28-O8-C9
22	1	301	CLA	O1D-CGD-O2D-CED
22	Q	308	CLA	O1D-CGD-O2D-CED
26	3	312	CHL	O1D-CGD-O2D-CED
26	G	315	CHL	O1D-CGD-O2D-CED
22	P	306	CLA	CBD-CGD-O2D-CED
22	U	303	CLA	CBD-CGD-O2D-CED
26	V	314	CHL	CBD-CGD-O2D-CED
26	Q	312	CHL	CBD-CGD-O2D-CED
22	2	302	CLA	O1D-CGD-O2D-CED
22	3	302	CLA	O1D-CGD-O2D-CED
22	q	302	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	P	307	CLA	O1D-CGD-O2D-CED
22	G	308	CLA	O1D-CGD-O2D-CED
22	g	308	CLA	O1D-CGD-O2D-CED
26	6	313	CHL	O1D-CGD-O2D-CED
26	u	314	CHL	O1D-CGD-O2D-CED
25	d	405	LHG	O9-C7-O7-C5
22	3	305	CLA	O1A-CGA-O2A-C1
22	4	302	CLA	O1A-CGA-O2A-C1
22	6	303	CLA	O1A-CGA-O2A-C1
22	6	306	CLA	O1A-CGA-O2A-C1
22	p	303	CLA	O1A-CGA-O2A-C1
22	u	302	CLA	O1A-CGA-O2A-C1
22	g	304	CLA	O1A-CGA-O2A-C1
26	q	311	CHL	O1A-CGA-O2A-C1
26	G	311	CHL	O1A-CGA-O2A-C1
34	d	407	LMG	O10-C28-O8-C9
34	D	408	LMG	O10-C28-O8-C9
22	6	309	CLA	O1D-CGD-O2D-CED
26	g	314	CHL	O1D-CGD-O2D-CED
24	V	311	XAT	C13-C14-C15-C35
24	N	311	XAT	C33-C34-C35-C15
31	t	101	BCR	C13-C14-C15-C16
31	z	101	BCR	C13-C14-C15-C16
31	T	101	BCR	C13-C14-C15-C16
31	C	517	BCR	C13-C14-C15-C16
31	B	619	BCR	C13-C14-C15-C16
31	B	620	BCR	C15-C16-C17-C18
31	b	618	BCR	C9-C10-C11-C12
31	c	516	BCR	C9-C10-C11-C12
34	a	412	LMG	O6-C5-C6-O5
36	B	601	DGD	O6E-C5E-C6E-O5E
22	a	405	CLA	CBD-CGD-O2D-CED
22	a	408	CLA	CBD-CGD-O2D-CED
22	A	405	CLA	CBD-CGD-O2D-CED
22	N	305	CLA	CBD-CGD-O2D-CED
22	n	305	CLA	CBD-CGD-O2D-CED
22	R	302	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	CBD-CGD-O2D-CED
22	b	611	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
26	1	316	CHL	CBD-CGD-O2D-CED
26	2	313	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	2	318	CHL	CBD-CGD-O2D-CED
26	5	313	CHL	CBD-CGD-O2D-CED
26	q	312	CHL	CBD-CGD-O2D-CED
26	q	313	CHL	CBD-CGD-O2D-CED
26	P	316	CHL	CBD-CGD-O2D-CED
26	Q	311	CHL	CBD-CGD-O2D-CED
26	Q	313	CHL	CBD-CGD-O2D-CED
26	N	315	CHL	CBD-CGD-O2D-CED
22	P	304	CLA	O1D-CGD-O2D-CED
22	g	303	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
26	r	619	CHL	O1D-CGD-O2D-CED
25	C	523	LHG	O2-C2-C3-O3
25	C	524	LHG	O2-C2-C3-O3
25	c	521	LHG	O2-C2-C3-O3
25	c	522	LHG	O2-C2-C3-O3
25	c	523	LHG	O2-C2-C3-O3
22	2	307	CLA	C3-C5-C6-C7
22	4	307	CLA	C3-C5-C6-C7
22	q	301	CLA	C3-C5-C6-C7
22	N	307	CLA	C3-C5-C6-C7
26	5	316	CHL	C3-C5-C6-C7
26	G	315	CHL	C3-C5-C6-C7
22	a	405	CLA	CBA-CGA-O2A-C1
22	3	304	CLA	CBA-CGA-O2A-C1
22	q	302	CLA	CBA-CGA-O2A-C1
22	Q	304	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	CBA-CGA-O2A-C1
22	b	608	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	CBA-CGA-O2A-C1
26	6	312	CHL	CBA-CGA-O2A-C1
26	g	311	CHL	CBA-CGA-O2A-C1
32	a	413	SQD	C24-C23-O48-C46
34	b	621	LMG	C29-C28-O8-C9
22	Q	302	CLA	O1A-CGA-O2A-C1
22	n	306	CLA	O1A-CGA-O2A-C1
36	b	601	DGD	O6E-C5E-C6E-O5E
34	C	502	LMG	C4-C5-C6-O5
22	v	308	CLA	O1D-CGD-O2D-CED
22	p	307	CLA	O1D-CGD-O2D-CED
22	V	308	CLA	O1D-CGD-O2D-CED
22	n	302	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	n	304	CLA	O1D-CGD-O2D-CED
26	Q	315	CHL	O1D-CGD-O2D-CED
25	r	613	LHG	C8-C7-O7-C5
32	C	501	SQD	C8-C7-O47-C45
22	2	305	CLA	CBD-CGD-O2D-CED
22	p	306	CLA	CBD-CGD-O2D-CED
22	S	301	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
26	v	314	CHL	CBD-CGD-O2D-CED
26	p	316	CHL	CBD-CGD-O2D-CED
26	U	314	CHL	CBD-CGD-O2D-CED
26	n	317	CHL	CBD-CGD-O2D-CED
34	A	411	LMG	C4-C5-C6-O5
36	c	518	DGD	C4E-C5E-C6E-O5E
26	g	315	CHL	O1D-CGD-O2D-CED
22	a	405	CLA	O1A-CGA-O2A-C1
34	c	501	LMG	C4-C5-C6-O5
36	C	520	DGD	C4E-C5E-C6E-O5E
22	c	503	CLA	O1D-CGD-O2D-CED
22	5	305	CLA	CBD-CGD-O2D-CED
22	p	303	CLA	CBD-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
26	2	317	CHL	C10-C11-C12-C13
22	C	513	CLA	C3-C5-C6-C7
22	c	512	CLA	C3-C5-C6-C7
26	6	315	CHL	C3-C5-C6-C7
26	U	319	CHL	C3-C5-C6-C7
22	3	305	CLA	CBA-CGA-O2A-C1
22	g	304	CLA	CBA-CGA-O2A-C1
26	q	311	CHL	CBA-CGA-O2A-C1
32	A	412	SQD	C24-C23-O48-C46
22	C	504	CLA	O1D-CGD-O2D-CED
25	a	415	LHG	O9-C7-O7-C5
25	A	413	LHG	O9-C7-O7-C5
36	B	601	DGD	C4E-C5E-C6E-O5E
22	R	309	CLA	O1A-CGA-O2A-C1
22	C	507	CLA	O1A-CGA-O2A-C1
26	6	312	CHL	O1A-CGA-O2A-C1
26	g	311	CHL	O1A-CGA-O2A-C1
34	c	501	LMG	O6-C5-C6-O5
22	R	307	CLA	C4-C3-C5-C6
22	B	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	R	307	CLA	C2-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
22	V	302	CLA	C2A-CAA-CBA-CGA
22	Q	305	CLA	C2A-CAA-CBA-CGA
22	g	303	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	C2A-CAA-CBA-CGA
22	B	613	CLA	C2A-CAA-CBA-CGA
22	b	613	CLA	C2A-CAA-CBA-CGA
22	c	505	CLA	C2A-CAA-CBA-CGA
26	5	315	CHL	C2A-CAA-CBA-CGA
26	Q	314	CHL	C2A-CAA-CBA-CGA
26	Q	315	CHL	C2A-CAA-CBA-CGA
26	G	312	CHL	C2A-CAA-CBA-CGA
26	u	314	CHL	C2A-CAA-CBA-CGA
26	s	314	CHL	C2A-CAA-CBA-CGA
22	3	306	CLA	O1D-CGD-O2D-CED
22	4	306	CLA	O1D-CGD-O2D-CED
22	G	303	CLA	O1D-CGD-O2D-CED
26	6	317	CHL	O1D-CGD-O2D-CED
34	w	201	LMG	O6-C5-C6-O5
34	W	201	LMG	O6-C5-C6-O5
34	C	521	LMG	O6-C5-C6-O5
22	A	405	CLA	O1A-CGA-O2A-C1
22	q	302	CLA	O1A-CGA-O2A-C1
22	Q	304	CLA	O1A-CGA-O2A-C1
22	B	602	CLA	O1A-CGA-O2A-C1
22	b	608	CLA	O1A-CGA-O2A-C1
22	c	506	CLA	O1A-CGA-O2A-C1
36	c	519	DGD	C4E-C5E-C6E-O5E
26	g	313	CHL	O1D-CGD-O2D-CED
22	r	608	CLA	CBA-CGA-O2A-C1
22	x	201	CLA	CBA-CGA-O2A-C1
22	u	306	CLA	CBA-CGA-O2A-C1
22	C	515	CLA	CBA-CGA-O2A-C1
22	B	613	CLA	CBA-CGA-O2A-C1
22	b	613	CLA	CBA-CGA-O2A-C1
26	6	301	CHL	CBA-CGA-O2A-C1
26	V	313	CHL	CBA-CGA-O2A-C1
26	Q	311	CHL	CBA-CGA-O2A-C1
26	U	313	CHL	CBA-CGA-O2A-C1
26	u	313	CHL	CBA-CGA-O2A-C1
26	g	314	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	c	517	DGD	C2A-C1A-O1G-C1G
34	C	502	LMG	O6-C5-C6-O5
36	J	101	DGD	C4E-C5E-C6E-O5E
36	b	601	DGD	C4E-C5E-C6E-O5E
22	u	303	CLA	O1D-CGD-O2D-CED
26	3	316	CHL	O1D-CGD-O2D-CED
26	G	313	CHL	O1D-CGD-O2D-CED
22	3	304	CLA	O1A-CGA-O2A-C1
32	a	410	SQD	C8-C7-O47-C45
22	a	404	CLA	O1D-CGD-O2D-CED
22	A	404	CLA	O1D-CGD-O2D-CED
22	6	307	CLA	O1D-CGD-O2D-CED
22	u	302	CLA	O1D-CGD-O2D-CED
26	n	315	CHL	O1D-CGD-O2D-CED
26	r	614	CHL	CBD-CGD-O2D-CED
26	R	315	CHL	CBD-CGD-O2D-CED
26	5	317	CHL	O1D-CGD-O2D-CED
26	q	314	CHL	O1D-CGD-O2D-CED
25	d	406	LHG	C1-C2-C3-O3
25	1	312	LHG	C1-C2-C3-O3
25	P	313	LHG	C1-C2-C3-O3
25	R	314	LHG	C1-C2-C3-O3
25	B	623	LHG	C1-C2-C3-O3
25	D	407	LHG	C1-C2-C3-O3
25	b	623	LHG	C1-C2-C3-O3
25	r	613	LHG	O9-C7-O7-C5
22	a	408	CLA	O1A-CGA-O2A-C1
22	u	306	CLA	O1A-CGA-O2A-C1
22	S	308	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	O1A-CGA-O2A-C1
22	b	613	CLA	O1A-CGA-O2A-C1
26	6	301	CHL	O1A-CGA-O2A-C1
26	v	313	CHL	O1A-CGA-O2A-C1
26	U	313	CHL	O1A-CGA-O2A-C1
26	u	313	CHL	O1A-CGA-O2A-C1
26	g	314	CHL	O1A-CGA-O2A-C1
36	c	517	DGD	O1A-C1A-O1G-C1G
22	r	609	CLA	C3-C5-C6-C7
22	a	408	CLA	CBA-CGA-O2A-C1
22	A	408	CLA	CBA-CGA-O2A-C1
22	1	302	CLA	CBA-CGA-O2A-C1
22	p	304	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	q	303	CLA	CBA-CGA-O2A-C1
22	q	306	CLA	CBA-CGA-O2A-C1
22	U	306	CLA	CBA-CGA-O2A-C1
22	G	303	CLA	CBA-CGA-O2A-C1
22	u	308	CLA	CBA-CGA-O2A-C1
22	S	303	CLA	CBA-CGA-O2A-C1
22	S	306	CLA	CBA-CGA-O2A-C1
22	S	308	CLA	CBA-CGA-O2A-C1
22	B	607	CLA	CBA-CGA-O2A-C1
22	B	611	CLA	CBA-CGA-O2A-C1
22	X	202	CLA	CBA-CGA-O2A-C1
22	b	602	CLA	CBA-CGA-O2A-C1
22	b	607	CLA	CBA-CGA-O2A-C1
22	b	611	CLA	CBA-CGA-O2A-C1
22	b	617	CLA	CBA-CGA-O2A-C1
22	c	514	CLA	CBA-CGA-O2A-C1
22	s	301	CLA	CBA-CGA-O2A-C1
22	s	303	CLA	CBA-CGA-O2A-C1
22	s	306	CLA	CBA-CGA-O2A-C1
22	s	308	CLA	CBA-CGA-O2A-C1
25	3	310	LHG	C24-C23-O8-C6
25	6	311	LHG	C24-C23-O8-C6
26	1	313	CHL	CBA-CGA-O2A-C1
26	1	316	CHL	CBA-CGA-O2A-C1
26	3	311	CHL	CBA-CGA-O2A-C1
26	v	313	CHL	CBA-CGA-O2A-C1
26	p	319	CHL	CBA-CGA-O2A-C1
26	g	315	CHL	CBA-CGA-O2A-C1
26	S	315	CHL	CBA-CGA-O2A-C1
36	C	519	DGD	C2A-C1A-O1G-C1G
34	w	201	LMG	C4-C5-C6-O5
22	r	601	CLA	O1D-CGD-O2D-CED
24	4	311	XAT	C33-C34-C35-C15
24	v	311	XAT	C9-C10-C11-C12
24	Q	309	XAT	C29-C30-C31-C32
24	N	311	XAT	C13-C14-C15-C35
24	u	311	XAT	C9-C10-C11-C12
31	k	101	BCR	C9-C10-C11-C12
31	K	101	BCR	C9-C10-C11-C12
31	C	518	BCR	C9-C10-C11-C12
31	c	515	BCR	C13-C14-C15-C16
34	c	520	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	U	306	CLA	C5-C6-C7-C8
22	C	503	CLA	C15-C16-C17-C18
22	B	606	CLA	C13-C15-C16-C17
26	4	316	CHL	C8-C10-C11-C12
26	6	301	CHL	C13-C15-C16-C17
36	C	519	DGD	O1A-C1A-O1G-C1G
34	a	412	LMG	C4-C5-C6-O5
34	W	201	LMG	C4-C5-C6-O5
22	C	504	CLA	C8-C10-C11-C12
22	C	507	CLA	C5-C6-C7-C8
22	b	613	CLA	C15-C16-C17-C18
26	4	317	CHL	C13-C15-C16-C17
26	v	317	CHL	C13-C15-C16-C17
26	v	318	CHL	C13-C15-C16-C17
26	V	317	CHL	C8-C10-C11-C12
26	P	318	CHL	C13-C15-C16-C17
26	n	317	CHL	C13-C15-C16-C17
25	a	415	LHG	O2-C2-C3-O3
25	A	413	LHG	O2-C2-C3-O3
25	p	313	LHG	O2-C2-C3-O3
25	q	310	LHG	O2-C2-C3-O3
25	n	312	LHG	O2-C2-C3-O3
34	C	521	LMG	C28-C29-C30-C31
22	6	309	CLA	O2A-C1-C2-C3
22	q	308	CLA	O2A-C1-C2-C3
22	g	308	CLA	O2A-C1-C2-C3
32	m	101	SQD	C2-C1-O6-C44
32	M	101	SQD	C2-C1-O6-C44
36	a	416	DGD	C2E-C1E-O5D-C6D
32	a	413	SQD	O6-C44-C45-O47
22	p	304	CLA	O1A-CGA-O2A-C1
22	q	306	CLA	O1A-CGA-O2A-C1
22	U	306	CLA	O1A-CGA-O2A-C1
22	S	306	CLA	O1A-CGA-O2A-C1
22	b	611	CLA	O1A-CGA-O2A-C1
22	s	306	CLA	O1A-CGA-O2A-C1
22	s	308	CLA	O1A-CGA-O2A-C1
26	Q	311	CHL	C2-C3-C5-C6
22	v	305	CLA	C6-C7-C8-C9
22	V	305	CLA	C6-C7-C8-C9
22	P	303	CLA	C6-C7-C8-C9
22	U	302	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	U	305	CLA	C6-C7-C8-C9
22	u	305	CLA	C6-C7-C8-C9
22	n	304	CLA	C14-C13-C15-C16
22	C	508	CLA	C14-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C9
22	B	602	CLA	C14-C13-C15-C16
22	B	603	CLA	C11-C12-C13-C14
22	B	603	CLA	C14-C13-C15-C16
22	B	605	CLA	C6-C7-C8-C9
22	B	606	CLA	C14-C13-C15-C16
22	B	610	CLA	C6-C7-C8-C9
22	B	614	CLA	C11-C10-C8-C9
22	b	602	CLA	C14-C13-C15-C16
22	b	603	CLA	C14-C13-C15-C16
22	b	605	CLA	C6-C7-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	b	615	CLA	C6-C7-C8-C9
22	c	507	CLA	C14-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C9
26	1	316	CHL	C11-C10-C8-C9
26	1	317	CHL	C6-C7-C8-C9
26	1	317	CHL	C14-C13-C15-C16
26	1	318	CHL	C14-C13-C15-C16
26	2	316	CHL	C11-C10-C8-C9
26	2	318	CHL	C14-C13-C15-C16
26	4	316	CHL	C6-C7-C8-C9
26	4	317	CHL	C14-C13-C15-C16
26	5	316	CHL	C11-C10-C8-C9
26	5	317	CHL	C11-C10-C8-C9
26	6	316	CHL	C6-C7-C8-C9
26	v	316	CHL	C11-C10-C8-C9
26	v	317	CHL	C11-C12-C13-C14
26	v	318	CHL	C14-C13-C15-C16
26	p	318	CHL	C6-C7-C8-C9
26	V	317	CHL	C11-C10-C8-C9
26	P	318	CHL	C6-C7-C8-C9
26	P	319	CHL	C14-C13-C15-C16
26	U	316	CHL	C14-C13-C15-C16
26	U	317	CHL	C6-C7-C8-C9
26	U	317	CHL	C11-C10-C8-C9
26	N	316	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	N	317	CHL	C6-C7-C8-C9
26	G	311	CHL	C11-C12-C13-C14
26	G	314	CHL	C11-C10-C8-C9
26	u	316	CHL	C11-C12-C13-C14
26	u	318	CHL	C6-C7-C8-C9
26	u	318	CHL	C14-C13-C15-C16
26	n	318	CHL	C6-C7-C8-C9
26	g	311	CHL	C11-C12-C13-C14
22	A	406	CLA	O1D-CGD-O2D-CED
22	1	306	CLA	O1D-CGD-O2D-CED
22	5	303	CLA	O1D-CGD-O2D-CED
22	N	307	CLA	O1D-CGD-O2D-CED
26	q	311	CHL	O1D-CGD-O2D-CED
30	D	401	PHO	O1D-CGD-O2D-CED
26	s	313	CHL	CBD-CGD-O2D-CED
22	c	507	CLA	C13-C15-C16-C17
26	2	318	CHL	C8-C10-C11-C12
26	q	311	CHL	C15-C16-C17-C18
26	g	314	CHL	C13-C15-C16-C17
22	G	302	CLA	C2A-CAA-CBA-CGA
22	g	302	CLA	C2A-CAA-CBA-CGA
22	g	308	CLA	C2A-CAA-CBA-CGA
22	B	602	CLA	C2A-CAA-CBA-CGA
26	4	314	CHL	C2A-CAA-CBA-CGA
26	P	315	CHL	C2A-CAA-CBA-CGA
26	S	314	CHL	C2A-CAA-CBA-CGA
23	N	309	LUT	C31-C32-C33-C40
23	n	310	LUT	C7-C8-C9-C19
23	s	311	LUT	C11-C12-C13-C20
24	2	311	XAT	C11-C12-C13-C20
24	3	309	XAT	C11-C12-C13-C20
24	6	310	XAT	C11-C12-C13-C20
24	v	311	XAT	C11-C12-C13-C20
24	q	309	XAT	C11-C12-C13-C20
24	V	311	XAT	C31-C32-C33-C40
24	n	311	XAT	C11-C12-C13-C20
24	n	311	XAT	C31-C32-C33-C40
27	N	318	NEX	C11-C12-C13-C20
27	u	319	NEX	C11-C12-C13-C20
31	d	403	BCR	C7-C8-C9-C34
31	k	101	BCR	C7-C8-C9-C34
31	t	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
31	K	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C7-C8-C9-C34
31	C	517	BCR	C7-C8-C9-C34
31	B	619	BCR	C11-C12-C13-C35
31	D	404	BCR	C7-C8-C9-C34
31	b	618	BCR	C11-C12-C13-C35
24	2	311	XAT	C11-C12-C13-C14
24	6	310	XAT	C11-C12-C13-C14
24	v	311	XAT	C11-C12-C13-C14
24	v	311	XAT	C31-C32-C33-C34
24	q	309	XAT	C7-C8-C9-C10
24	q	309	XAT	C11-C12-C13-C14
24	V	311	XAT	C31-C32-C33-C34
24	n	311	XAT	C11-C12-C13-C14
24	n	311	XAT	C31-C32-C33-C34
31	d	403	BCR	C7-C8-C9-C10
31	k	101	BCR	C7-C8-C9-C10
31	K	101	BCR	C7-C8-C9-C10
31	T	101	BCR	C7-C8-C9-C10
31	C	517	BCR	C7-C8-C9-C10
31	D	404	BCR	C7-C8-C9-C10
31	b	618	BCR	C11-C12-C13-C14
31	c	515	BCR	C7-C8-C9-C10
25	5	312	LHG	C8-C7-O7-C5
34	C	521	LMG	C4-C5-C6-O5
25	d	406	LHG	C7-C8-C9-C10
25	D	407	LHG	C7-C8-C9-C10
22	A	408	CLA	O1A-CGA-O2A-C1
22	G	303	CLA	O1A-CGA-O2A-C1
22	B	611	CLA	O1A-CGA-O2A-C1
26	3	311	CHL	O1A-CGA-O2A-C1
32	A	412	SQD	O10-C23-O48-C46
22	p	305	CLA	C15-C16-C17-C18
22	P	307	CLA	C8-C10-C11-C12
22	N	301	CLA	C15-C16-C17-C18
22	n	301	CLA	C15-C16-C17-C18
22	n	304	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
22	B	612	CLA	C5-C6-C7-C8
22	X	202	CLA	C8-C10-C11-C12
26	5	313	CHL	C10-C11-C12-C13
26	5	317	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	6	312	CHL	C13-C15-C16-C17
26	P	318	CHL	C5-C6-C7-C8
26	P	318	CHL	C8-C10-C11-C12
26	R	315	CHL	C13-C15-C16-C17
26	R	317	CHL	C8-C10-C11-C12
22	U	304	CLA	O1D-CGD-O2D-CED
22	S	307	CLA	O1D-CGD-O2D-CED
26	6	301	CHL	O1D-CGD-O2D-CED
26	g	316	CHL	O1D-CGD-O2D-CED
30	d	401	PHO	O1D-CGD-O2D-CED
30	a	407	PHO	O1D-CGD-O2D-CED
22	p	306	CLA	C3-C5-C6-C7
22	B	609	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
26	2	316	CHL	C3-C5-C6-C7
22	1	303	CLA	CBA-CGA-O2A-C1
22	6	304	CLA	CBA-CGA-O2A-C1
22	U	308	CLA	CBA-CGA-O2A-C1
22	G	304	CLA	CBA-CGA-O2A-C1
22	S	301	CLA	CBA-CGA-O2A-C1
22	c	503	CLA	CBA-CGA-O2A-C1
26	q	314	CHL	CBA-CGA-O2A-C1
26	g	316	CHL	CBA-CGA-O2A-C1
26	s	315	CHL	CBA-CGA-O2A-C1
22	r	609	CLA	C5-C6-C7-C8
22	1	307	CLA	C10-C11-C12-C13
22	2	305	CLA	C8-C10-C11-C12
22	5	301	CLA	C10-C11-C12-C13
22	q	301	CLA	C8-C10-C11-C12
22	Q	302	CLA	C15-C16-C17-C18
22	U	302	CLA	C13-C15-C16-C17
22	N	306	CLA	C10-C11-C12-C13
22	G	301	CLA	C13-C15-C16-C17
22	C	509	CLA	C5-C6-C7-C8
22	B	603	CLA	C13-C15-C16-C17
22	B	610	CLA	C5-C6-C7-C8
22	B	613	CLA	C15-C16-C17-C18
22	b	612	CLA	C15-C16-C17-C18
22	c	502	CLA	C15-C16-C17-C18
22	c	504	CLA	C5-C6-C7-C8
22	c	507	CLA	C10-C11-C12-C13
26	1	313	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	4	313	CHL	C10-C11-C12-C13
26	5	313	CHL	C8-C10-C11-C12
26	5	318	CHL	C8-C10-C11-C12
26	v	317	CHL	C5-C6-C7-C8
26	v	317	CHL	C8-C10-C11-C12
26	p	318	CHL	C13-C15-C16-C17
26	p	319	CHL	C13-C15-C16-C17
26	V	313	CHL	C13-C15-C16-C17
26	V	316	CHL	C8-C10-C11-C12
26	V	317	CHL	C5-C6-C7-C8
26	P	317	CHL	C13-C15-C16-C17
26	Q	315	CHL	C8-C10-C11-C12
26	U	319	CHL	C5-C6-C7-C8
26	N	313	CHL	C13-C15-C16-C17
26	N	316	CHL	C8-C10-C11-C12
26	G	311	CHL	C8-C10-C11-C12
26	u	318	CHL	C13-C15-C16-C17
26	g	311	CHL	C8-C10-C11-C12
36	c	519	DGD	O6E-C5E-C6E-O5E
25	P	313	LHG	C23-C24-C25-C26
25	U	312	LHG	C23-C24-C25-C26
25	G	310	LHG	C23-C24-C25-C26
25	u	312	LHG	C23-C24-C25-C26
25	g	310	LHG	C23-C24-C25-C26
32	A	412	SQD	C7-C8-C9-C10
30	A	407	PHO	O1D-CGD-O2D-CED
22	c	505	CLA	O1D-CGD-O2D-CED
22	x	201	CLA	C8-C10-C11-C12
22	1	306	CLA	C5-C6-C7-C8
22	2	301	CLA	C10-C11-C12-C13
22	2	302	CLA	C8-C10-C11-C12
22	3	304	CLA	C13-C15-C16-C17
22	5	306	CLA	C8-C10-C11-C12
22	6	303	CLA	C8-C10-C11-C12
22	v	302	CLA	C10-C11-C12-C13
22	v	305	CLA	C5-C6-C7-C8
22	q	305	CLA	C5-C6-C7-C8
22	V	302	CLA	C13-C15-C16-C17
22	V	306	CLA	C10-C11-C12-C13
22	Q	301	CLA	C8-C10-C11-C12
22	Q	304	CLA	C8-C10-C11-C12
22	u	306	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	508	CLA	C10-C11-C12-C13
22	C	512	CLA	C10-C11-C12-C13
22	C	515	CLA	C13-C15-C16-C17
22	B	602	CLA	C13-C15-C16-C17
22	B	612	CLA	C15-C16-C17-C18
22	b	606	CLA	C13-C15-C16-C17
22	b	608	CLA	C8-C10-C11-C12
22	b	608	CLA	C10-C11-C12-C13
22	c	506	CLA	C5-C6-C7-C8
22	c	508	CLA	C5-C6-C7-C8
22	c	509	CLA	C5-C6-C7-C8
22	c	511	CLA	C10-C11-C12-C13
22	c	514	CLA	C13-C15-C16-C17
26	2	317	CHL	C5-C6-C7-C8
26	2	318	CHL	C5-C6-C7-C8
26	3	314	CHL	C13-C15-C16-C17
26	5	313	CHL	C15-C16-C17-C18
26	5	316	CHL	C15-C16-C17-C18
26	5	317	CHL	C13-C15-C16-C17
26	5	318	CHL	C13-C15-C16-C17
26	6	315	CHL	C13-C15-C16-C17
26	p	314	CHL	C13-C15-C16-C17
26	p	318	CHL	C5-C6-C7-C8
26	V	317	CHL	C13-C15-C16-C17
26	V	318	CHL	C13-C15-C16-C17
26	P	314	CHL	C10-C11-C12-C13
26	P	314	CHL	C15-C16-C17-C18
26	P	319	CHL	C8-C10-C11-C12
26	P	319	CHL	C13-C15-C16-C17
26	Q	311	CHL	C15-C16-C17-C18
26	Q	315	CHL	C15-C16-C17-C18
26	U	316	CHL	C8-C10-C11-C12
26	G	314	CHL	C13-C15-C16-C17
26	u	316	CHL	C13-C15-C16-C17
26	u	317	CHL	C8-C10-C11-C12
26	u	318	CHL	C5-C6-C7-C8
26	n	316	CHL	C8-C10-C11-C12
26	g	311	CHL	C13-C15-C16-C17
26	g	314	CHL	C8-C10-C11-C12
26	2	317	CHL	O1D-CGD-O2D-CED
26	N	316	CHL	O1D-CGD-O2D-CED
25	l	101	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
25	1	312	LHG	O1-C1-C2-O2
25	2	312	LHG	O1-C1-C2-O2
25	g	310	LHG	O1-C1-C2-O2
25	R	314	LHG	O1-C1-C2-O2
25	B	623	LHG	O1-C1-C2-O2
22	1	302	CLA	O1A-CGA-O2A-C1
32	a	413	SQD	O10-C23-O48-C46
25	r	613	LHG	C23-C24-C25-C26
25	l	101	LHG	C7-C8-C9-C10
25	L	101	LHG	C7-C8-C9-C10
25	1	312	LHG	C23-C24-C25-C26
25	6	311	LHG	C23-C24-C25-C26
25	N	312	LHG	C23-C24-C25-C26
25	n	312	LHG	C23-C24-C25-C26
25	R	314	LHG	C23-C24-C25-C26
32	a	413	SQD	C7-C8-C9-C10
32	C	501	SQD	C23-C24-C25-C26
34	w	201	LMG	C10-C11-C12-C13
34	W	201	LMG	C10-C11-C12-C13
34	C	502	LMG	C10-C11-C12-C13
34	c	501	LMG	C10-C11-C12-C13
22	s	301	CLA	CBD-CGD-O2D-CED
22	a	404	CLA	C8-C10-C11-C12
22	x	201	CLA	C15-C16-C17-C18
22	2	304	CLA	C10-C11-C12-C13
22	3	304	CLA	C10-C11-C12-C13
22	4	307	CLA	C10-C11-C12-C13
22	G	302	CLA	C15-C16-C17-C18
22	C	512	CLA	C15-C16-C17-C18
22	B	605	CLA	C5-C6-C7-C8
22	B	612	CLA	C13-C15-C16-C17
22	b	612	CLA	C5-C6-C7-C8
26	1	313	CHL	C8-C10-C11-C12
26	2	317	CHL	C13-C15-C16-C17
26	3	311	CHL	C8-C10-C11-C12
26	4	313	CHL	C13-C15-C16-C17
26	4	313	CHL	C15-C16-C17-C18
26	6	312	CHL	C8-C10-C11-C12
26	v	313	CHL	C8-C10-C11-C12
26	v	318	CHL	C5-C6-C7-C8
26	v	318	CHL	C15-C16-C17-C18
26	p	319	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	V	318	CHL	C15-C16-C17-C18
26	Q	314	CHL	C13-C15-C16-C17
26	U	313	CHL	C13-C15-C16-C17
26	n	317	CHL	C8-C10-C11-C12
26	g	315	CHL	C15-C16-C17-C18
22	4	303	CLA	CBA-CGA-O2A-C1
22	Q	303	CLA	CBA-CGA-O2A-C1
22	N	305	CLA	CBA-CGA-O2A-C1
22	C	504	CLA	CBA-CGA-O2A-C1
22	B	614	CLA	CBA-CGA-O2A-C1
22	a	406	CLA	O1D-CGD-O2D-CED
22	q	306	CLA	O1D-CGD-O2D-CED
22	U	302	CLA	O1D-CGD-O2D-CED
22	a	404	CLA	C5-C6-C7-C8
22	A	404	CLA	C5-C6-C7-C8
22	5	305	CLA	C8-C10-C11-C12
22	q	302	CLA	C15-C16-C17-C18
22	P	306	CLA	C8-C10-C11-C12
22	U	307	CLA	C8-C10-C11-C12
22	G	301	CLA	C8-C10-C11-C12
22	u	307	CLA	C8-C10-C11-C12
22	g	301	CLA	C15-C16-C17-C18
22	B	603	CLA	C5-C6-C7-C8
22	D	403	CLA	C13-C15-C16-C17
22	b	603	CLA	C5-C6-C7-C8
22	b	612	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
26	r	616	CHL	C8-C10-C11-C12
26	1	313	CHL	C15-C16-C17-C18
26	1	316	CHL	C15-C16-C17-C18
26	2	313	CHL	C15-C16-C17-C18
26	v	317	CHL	C15-C16-C17-C18
26	P	317	CHL	C15-C16-C17-C18
26	U	313	CHL	C8-C10-C11-C12
26	U	319	CHL	C8-C10-C11-C12
26	u	317	CHL	C15-C16-C17-C18
26	n	316	CHL	C5-C6-C7-C8
26	g	314	CHL	C15-C16-C17-C18
26	R	315	CHL	C8-C10-C11-C12
25	3	310	LHG	C23-C24-C25-C26
25	4	312	LHG	C23-C24-C25-C26
25	B	622	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	G	301	CLA	CBD-CGD-O2D-CED
26	S	315	CHL	C8-C10-C11-C12
26	s	315	CHL	C8-C10-C11-C12
22	u	302	CLA	C13-C15-C16-C17
22	g	307	CLA	C8-C10-C11-C12
22	S	301	CLA	C8-C10-C11-C12
22	B	614	CLA	C13-C15-C16-C17
22	b	609	CLA	C8-C10-C11-C12
26	1	317	CHL	C8-C10-C11-C12
26	1	317	CHL	C13-C15-C16-C17
26	1	317	CHL	C15-C16-C17-C18
26	2	318	CHL	C13-C15-C16-C17
26	4	313	CHL	C8-C10-C11-C12
26	4	316	CHL	C13-C15-C16-C17
26	p	320	CHL	C15-C16-C17-C18
26	P	319	CHL	C15-C16-C17-C18
26	n	317	CHL	C15-C16-C17-C18
22	3	304	CLA	C6-C7-C8-C10
22	v	307	CLA	C12-C13-C15-C16
22	q	307	CLA	C11-C12-C13-C15
22	q	307	CLA	C12-C13-C15-C16
22	Q	304	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	B	603	CLA	C11-C12-C13-C15
26	1	317	CHL	C6-C7-C8-C10
26	2	313	CHL	C6-C7-C8-C10
26	5	317	CHL	C6-C7-C8-C10
26	U	315	CHL	C6-C7-C8-C10
26	U	319	CHL	C12-C13-C15-C16
26	n	316	CHL	C12-C13-C15-C16
26	g	315	CHL	C6-C7-C8-C10
26	S	315	CHL	C6-C7-C8-C10
26	s	315	CHL	C6-C7-C8-C10
22	b	609	CLA	C3-C5-C6-C7
26	1	316	CHL	C3-C5-C6-C7
22	q	303	CLA	O1A-CGA-O2A-C1
22	u	308	CLA	O1A-CGA-O2A-C1
22	B	607	CLA	O1A-CGA-O2A-C1
22	X	202	CLA	O1A-CGA-O2A-C1
22	b	602	CLA	O1A-CGA-O2A-C1
22	c	514	CLA	O1A-CGA-O2A-C1
22	s	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	3	310	LHG	O10-C23-O8-C6
25	6	311	LHG	O10-C23-O8-C6
26	p	319	CHL	O1A-CGA-O2A-C1
26	S	315	CHL	O1A-CGA-O2A-C1
24	1	311	XAT	C29-C30-C31-C32
24	3	309	XAT	C9-C10-C11-C12
24	6	310	XAT	C9-C10-C11-C12
24	v	311	XAT	C29-C30-C31-C32
24	q	309	XAT	C9-C10-C11-C12
24	q	309	XAT	C29-C30-C31-C32
24	V	311	XAT	C29-C30-C31-C32
24	P	312	XAT	C9-C10-C11-C12
24	P	312	XAT	C29-C30-C31-C32
24	Q	309	XAT	C9-C10-C11-C12
24	U	311	XAT	C9-C10-C11-C12
24	G	309	XAT	C9-C10-C11-C12
24	n	311	XAT	C29-C30-C31-C32
24	g	309	XAT	C9-C10-C11-C12
31	k	101	BCR	C19-C20-C21-C22
31	K	101	BCR	C15-C16-C17-C18
31	K	101	BCR	C19-C20-C21-C22
31	B	618	BCR	C9-C10-C11-C12
31	B	619	BCR	C19-C20-C21-C22
31	b	619	BCR	C19-C20-C21-C22
31	c	515	BCR	C9-C10-C11-C12
22	1	308	CLA	CBA-CGA-O2A-C1
22	5	305	CLA	CBA-CGA-O2A-C1
22	G	308	CLA	CBA-CGA-O2A-C1
26	R	315	CHL	CBA-CGA-O2A-C1
22	a	406	CLA	C2A-CAA-CBA-CGA
22	6	304	CLA	C2A-CAA-CBA-CGA
22	6	306	CLA	C2A-CAA-CBA-CGA
22	p	306	CLA	C2A-CAA-CBA-CGA
22	N	301	CLA	C2A-CAA-CBA-CGA
22	N	303	CLA	C2A-CAA-CBA-CGA
22	C	504	CLA	C2A-CAA-CBA-CGA
22	c	503	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
22	s	308	CLA	C2A-CAA-CBA-CGA
26	3	312	CHL	C2A-CAA-CBA-CGA
26	6	313	CHL	C2A-CAA-CBA-CGA
26	v	315	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	v	316	CHL	C2A-CAA-CBA-CGA
26	p	317	CHL	C2A-CAA-CBA-CGA
26	q	314	CHL	C2A-CAA-CBA-CGA
26	G	313	CHL	C2A-CAA-CBA-CGA
26	n	314	CHL	C2A-CAA-CBA-CGA
22	V	302	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	O1D-CGD-O2D-CED
22	b	604	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
26	p	320	CHL	O1D-CGD-O2D-CED
22	r	605	CLA	C8-C10-C11-C12
22	a	408	CLA	C10-C11-C12-C13
22	x	201	CLA	C13-C15-C16-C17
22	A	404	CLA	C8-C10-C11-C12
22	2	301	CLA	C8-C10-C11-C12
22	4	306	CLA	C8-C10-C11-C12
22	5	301	CLA	C8-C10-C11-C12
22	5	302	CLA	C15-C16-C17-C18
22	U	301	CLA	C8-C10-C11-C12
22	G	307	CLA	C8-C10-C11-C12
22	u	301	CLA	C8-C10-C11-C12
22	g	301	CLA	C8-C10-C11-C12
22	R	306	CLA	C8-C10-C11-C12
22	C	509	CLA	C13-C15-C16-C17
22	C	515	CLA	C15-C16-C17-C18
22	B	605	CLA	C8-C10-C11-C12
22	B	609	CLA	C8-C10-C11-C12
22	B	613	CLA	C10-C11-C12-C13
22	B	614	CLA	C15-C16-C17-C18
22	X	202	CLA	C13-C15-C16-C17
22	b	613	CLA	C10-C11-C12-C13
22	b	614	CLA	C13-C15-C16-C17
22	c	514	CLA	C15-C16-C17-C18
22	s	301	CLA	C8-C10-C11-C12
26	1	318	CHL	C15-C16-C17-C18
26	2	316	CHL	C15-C16-C17-C18
26	p	318	CHL	C8-C10-C11-C12
26	U	317	CHL	C5-C6-C7-C8
26	N	313	CHL	C8-C10-C11-C12
26	N	313	CHL	C10-C11-C12-C13
26	u	313	CHL	C8-C10-C11-C12
26	u	313	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	b	617	CLA	O1A-CGA-O2A-C1
26	1	316	CHL	O1A-CGA-O2A-C1
26	6	312	CHL	CBD-CGD-O2D-CED
26	n	318	CHL	CBD-CGD-O2D-CED
36	c	519	DGD	O6E-C1E-O5D-C6D
22	d	402	CLA	C13-C15-C16-C17
22	5	301	CLA	C13-C15-C16-C17
22	5	301	CLA	C15-C16-C17-C18
22	b	603	CLA	C13-C15-C16-C17
26	5	318	CHL	C15-C16-C17-C18
26	G	315	CHL	C15-C16-C17-C18
26	u	316	CHL	C8-C10-C11-C12
26	u	318	CHL	C15-C16-C17-C18
36	J	101	DGD	O6E-C5E-C6E-O5E
25	d	406	LHG	O2-C2-C3-O3
25	C	522	LHG	O2-C2-C3-O3
25	B	622	LHG	O2-C2-C3-O3
25	D	407	LHG	O2-C2-C3-O3
25	b	622	LHG	O2-C2-C3-O3
32	C	501	SQD	O49-C7-O47-C45
22	A	408	CLA	C10-C11-C12-C13
22	4	306	CLA	C5-C6-C7-C8
22	5	305	CLA	C5-C6-C7-C8
22	6	306	CLA	C5-C6-C7-C8
22	p	302	CLA	C8-C10-C11-C12
22	V	304	CLA	C5-C6-C7-C8
22	P	302	CLA	C8-C10-C11-C12
22	g	306	CLA	C10-C11-C12-C13
22	C	515	CLA	C5-C6-C7-C8
22	b	614	CLA	C15-C16-C17-C18
22	c	507	CLA	C5-C6-C7-C8
22	c	508	CLA	C13-C15-C16-C17
26	2	318	CHL	C15-C16-C17-C18
26	3	315	CHL	C8-C10-C11-C12
26	6	316	CHL	C15-C16-C17-C18
26	p	314	CHL	C10-C11-C12-C13
26	p	317	CHL	C8-C10-C11-C12
26	P	317	CHL	C8-C10-C11-C12
26	P	318	CHL	C15-C16-C17-C18
26	U	316	CHL	C13-C15-C16-C17
26	G	314	CHL	C8-C10-C11-C12
26	G	316	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	n	318	CHL	C15-C16-C17-C18
30	a	407	PHO	C5-C6-C7-C8
22	b	614	CLA	CBA-CGA-O2A-C1
26	v	318	CHL	CBD-CGD-O2D-CED
22	R	308	CLA	O1D-CGD-O2D-CED
22	r	608	CLA	O1A-CGA-O2A-C1
22	x	201	CLA	O1A-CGA-O2A-C1
22	G	304	CLA	O1A-CGA-O2A-C1
22	S	303	CLA	O1A-CGA-O2A-C1
22	C	515	CLA	O1A-CGA-O2A-C1
22	b	607	CLA	O1A-CGA-O2A-C1
22	s	301	CLA	O1A-CGA-O2A-C1
26	1	313	CHL	O1A-CGA-O2A-C1
26	V	313	CHL	O1A-CGA-O2A-C1
26	Q	311	CHL	O1A-CGA-O2A-C1
26	g	315	CHL	O1A-CGA-O2A-C1
26	g	316	CHL	O1A-CGA-O2A-C1
32	l	102	SQD	O10-C23-O48-C46
25	b	622	LHG	C7-C8-C9-C10
22	q	304	CLA	C8-C10-C11-C12
22	N	301	CLA	C8-C10-C11-C12
22	S	308	CLA	C5-C6-C7-C8
22	C	508	CLA	C8-C10-C11-C12
22	C	510	CLA	C5-C6-C7-C8
22	b	602	CLA	C13-C15-C16-C17
22	b	605	CLA	C8-C10-C11-C12
22	b	614	CLA	C8-C10-C11-C12
26	1	313	CHL	C10-C11-C12-C13
26	1	316	CHL	C13-C15-C16-C17
26	3	314	CHL	C8-C10-C11-C12
26	3	315	CHL	C15-C16-C17-C18
26	5	316	CHL	C13-C15-C16-C17
26	p	317	CHL	C13-C15-C16-C17
26	p	320	CHL	C8-C10-C11-C12
26	q	314	CHL	C15-C16-C17-C18
26	Q	314	CHL	C8-C10-C11-C12
22	U	308	CLA	O1A-CGA-O2A-C1
22	S	301	CLA	O1A-CGA-O2A-C1
22	B	614	CLA	O1A-CGA-O2A-C1
26	s	315	CHL	O1A-CGA-O2A-C1
32	L	102	SQD	O10-C23-O48-C46
34	C	521	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
22	r	602	CLA	C8-C10-C11-C12
22	2	305	CLA	C5-C6-C7-C8
22	v	304	CLA	C8-C10-C11-C12
22	p	302	CLA	C10-C11-C12-C13
22	P	305	CLA	C13-C15-C16-C17
22	Q	305	CLA	C5-C6-C7-C8
22	n	301	CLA	C8-C10-C11-C12
22	C	508	CLA	C13-C15-C16-C17
22	C	511	CLA	C13-C15-C16-C17
22	B	608	CLA	C10-C11-C12-C13
22	B	609	CLA	C13-C15-C16-C17
22	B	614	CLA	C8-C10-C11-C12
22	b	609	CLA	C13-C15-C16-C17
22	c	510	CLA	C13-C15-C16-C17
22	c	514	CLA	C5-C6-C7-C8
22	s	308	CLA	C5-C6-C7-C8
26	r	614	CHL	C8-C10-C11-C12
26	1	318	CHL	C13-C15-C16-C17
26	2	316	CHL	C8-C10-C11-C12
26	2	317	CHL	C8-C10-C11-C12
26	3	311	CHL	C13-C15-C16-C17
26	4	313	CHL	C5-C6-C7-C8
26	6	301	CHL	C15-C16-C17-C18
26	v	313	CHL	C13-C15-C16-C17
26	q	311	CHL	C13-C15-C16-C17
26	q	315	CHL	C8-C10-C11-C12
26	N	316	CHL	C13-C15-C16-C17
26	N	317	CHL	C8-C10-C11-C12
26	G	311	CHL	C13-C15-C16-C17
26	n	318	CHL	C8-C10-C11-C12
26	R	316	CHL	C5-C6-C7-C8
30	A	407	PHO	C5-C6-C7-C8
25	r	613	LHG	C3-O3-P-O6
25	r	613	LHG	C4-O6-P-O3
25	a	415	LHG	C3-O3-P-O6
25	d	405	LHG	C4-O6-P-O3
25	l	101	LHG	C3-O3-P-O6
25	A	413	LHG	C3-O3-P-O6
25	L	101	LHG	C3-O3-P-O6
25	V	312	LHG	C3-O3-P-O6
25	Q	310	LHG	C4-O6-P-O3
25	U	312	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
25	U	312	LHG	C4-O6-P-O3
25	G	310	LHG	C4-O6-P-O3
25	u	312	LHG	C3-O3-P-O6
25	u	312	LHG	C4-O6-P-O3
25	g	310	LHG	C4-O6-P-O3
25	S	312	LHG	C4-O6-P-O3
25	C	523	LHG	C3-O3-P-O6
25	C	523	LHG	C4-O6-P-O3
25	B	622	LHG	C3-O3-P-O6
25	B	622	LHG	C4-O6-P-O3
25	B	623	LHG	C4-O6-P-O3
25	D	406	LHG	C4-O6-P-O3
25	b	622	LHG	C4-O6-P-O3
25	b	623	LHG	C4-O6-P-O3
25	c	522	LHG	C3-O3-P-O6
25	c	522	LHG	C4-O6-P-O3
25	c	523	LHG	C4-O6-P-O3
25	s	312	LHG	C4-O6-P-O3
25	d	405	LHG	C23-C24-C25-C26
22	n	307	CLA	C3-C5-C6-C7
22	5	307	CLA	CBA-CGA-O2A-C1
22	v	302	CLA	CBA-CGA-O2A-C1
22	U	303	CLA	CBA-CGA-O2A-C1
22	n	303	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	CBA-CGA-O2A-C1
22	c	504	CLA	CBA-CGA-O2A-C1
26	2	313	CHL	CBA-CGA-O2A-C1
22	b	605	CLA	CBD-CGD-O2D-CED
22	U	302	CLA	C5-C6-C7-C8
22	u	305	CLA	C5-C6-C7-C8
22	c	507	CLA	C8-C10-C11-C12
26	2	313	CHL	C8-C10-C11-C12
26	2	316	CHL	C13-C15-C16-C17
26	3	315	CHL	C10-C11-C12-C13
26	v	316	CHL	C8-C10-C11-C12
26	U	317	CHL	C13-C15-C16-C17
22	3	308	CLA	O2A-C1-C2-C3
22	Q	308	CLA	O2A-C1-C2-C3
22	G	308	CLA	O2A-C1-C2-C3
25	q	310	LHG	C7-C8-C9-C10
34	B	624	LMG	C10-C11-C12-C13
34	b	624	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	s	307	CLA	O1D-CGD-O2D-CED
26	s	316	CHL	O1D-CGD-O2D-CED
25	C	523	LHG	C1-C2-C3-O3
25	B	622	LHG	C1-C2-C3-O3
25	b	622	LHG	C1-C2-C3-O3
25	c	521	LHG	C1-C2-C3-O3
25	c	522	LHG	C1-C2-C3-O3
25	5	312	LHG	O9-C7-O7-C5
34	C	521	LMG	O9-C10-O7-C8
22	C	506	CLA	C4-C3-C5-C6
26	s	315	CHL	C4-C3-C5-C6
22	c	505	CLA	C2-C3-C5-C6
22	5	304	CLA	C15-C16-C17-C18
26	6	315	CHL	C8-C10-C11-C12
26	P	314	CHL	C8-C10-C11-C12
26	U	313	CHL	C15-C16-C17-C18
26	S	313	CHL	CBD-CGD-O2D-CED
22	Q	303	CLA	O1A-CGA-O2A-C1
22	3	305	CLA	C2A-CAA-CBA-CGA
22	n	301	CLA	C2A-CAA-CBA-CGA
22	n	308	CLA	C2A-CAA-CBA-CGA
22	S	308	CLA	C2A-CAA-CBA-CGA
22	C	509	CLA	C2A-CAA-CBA-CGA
22	b	603	CLA	C2A-CAA-CBA-CGA
26	p	314	CHL	C2A-CAA-CBA-CGA
26	P	314	CHL	C2A-CAA-CBA-CGA
22	u	307	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C19
22	q	305	CLA	C3-C5-C6-C7
22	q	308	CLA	CBA-CGA-O2A-C1
22	P	304	CLA	CBA-CGA-O2A-C1
22	P	307	CLA	CBA-CGA-O2A-C1
26	4	313	CHL	CBA-CGA-O2A-C1
26	5	313	CHL	CBA-CGA-O2A-C1
26	p	317	CHL	CBA-CGA-O2A-C1
26	V	317	CHL	CBA-CGA-O2A-C1
26	G	316	CHL	CBA-CGA-O2A-C1
26	u	316	CHL	CBA-CGA-O2A-C1
26	u	316	CHL	C15-C16-C17-C18
22	C	512	CLA	CBD-CGD-O2D-CED
26	5	317	CHL	C8-C10-C11-C12
26	Q	311	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	Q	316	CHL	C8-C10-C11-C12
26	N	317	CHL	C15-C16-C17-C18
24	2	311	XAT	C9-C10-C11-C12
24	2	311	XAT	C29-C30-C31-C32
24	5	311	XAT	C9-C10-C11-C12
24	V	311	XAT	C9-C10-C11-C12
24	G	309	XAT	C29-C30-C31-C32
24	g	309	XAT	C29-C30-C31-C32
31	x	202	BCR	C13-C14-C15-C16
31	C	517	BCR	C9-C10-C11-C12
31	C	518	BCR	C19-C20-C21-C22
31	X	201	BCR	C13-C14-C15-C16
31	b	620	BCR	C15-C16-C17-C18
31	c	516	BCR	C19-C20-C21-C22
36	J	101	DGD	C1A-C2A-C3A-C4A
25	P	313	LHG	C17-C18-C19-C20
25	Q	310	LHG	C11-C10-C9-C8
22	r	607	CLA	O1D-CGD-O2D-CED
22	C	509	CLA	O1D-CGD-O2D-CED
22	B	605	CLA	CBD-CGD-O2D-CED
34	c	520	LMG	C11-C10-O7-C8
22	5	304	CLA	C10-C11-C12-C13
22	U	305	CLA	C5-C6-C7-C8
22	C	505	CLA	C10-C11-C12-C13
22	B	610	CLA	C13-C15-C16-C17
22	b	615	CLA	C15-C16-C17-C18
22	c	504	CLA	C10-C11-C12-C13
22	v	307	CLA	C3-C5-C6-C7
25	6	311	LHG	C25-C26-C27-C28
25	V	312	LHG	C24-C25-C26-C27
25	u	312	LHG	C16-C17-C18-C19
25	c	522	LHG	C15-C16-C17-C18
32	a	413	SQD	C9-C10-C11-C12
32	A	412	SQD	C9-C10-C11-C12
34	b	621	LMG	C13-C14-C15-C16
34	b	621	LMG	C36-C37-C38-C39
36	C	520	DGD	C4B-C5B-C6B-C7B
36	c	517	DGD	C7B-C8B-C9B-CAB
36	c	518	DGD	C4B-C5B-C6B-C7B
26	S	316	CHL	O1D-CGD-O2D-CED
22	p	308	CLA	C11-C12-C13-C14
22	g	306	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C16-C17-C18-C19
22	B	610	CLA	C16-C17-C18-C20
22	b	603	CLA	C16-C17-C18-C19
22	b	606	CLA	C16-C17-C18-C19
26	r	616	CHL	C11-C12-C13-C15
26	1	317	CHL	C16-C17-C18-C20
26	6	316	CHL	C16-C17-C18-C20
26	U	319	CHL	C16-C17-C18-C19
26	N	316	CHL	C16-C17-C18-C20
26	n	316	CHL	C16-C17-C18-C19
26	n	317	CHL	C16-C17-C18-C19
26	n	318	CHL	C16-C17-C18-C19
22	3	308	CLA	CBA-CGA-O2A-C1
22	n	305	CLA	CBA-CGA-O2A-C1
22	B	617	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	C2A-C1A-O1G-C1G
25	3	310	LHG	C25-C26-C27-C28
25	P	313	LHG	C26-C27-C28-C29
25	Q	310	LHG	C17-C18-C19-C20
25	C	523	LHG	C15-C16-C17-C18
25	C	524	LHG	C16-C17-C18-C19
25	b	623	LHG	C11-C12-C13-C14
32	l	102	SQD	C12-C13-C14-C15
32	C	501	SQD	C29-C30-C31-C32
34	B	621	LMG	C17-C18-C19-C20
34	B	621	LMG	C37-C38-C39-C40
34	B	624	LMG	C11-C12-C13-C14
36	J	101	DGD	C2A-C3A-C4A-C5A
36	C	519	DGD	C7B-C8B-C9B-CAB
26	5	318	CHL	O1D-CGD-O2D-CED
26	G	316	CHL	O1D-CGD-O2D-CED
34	c	520	LMG	O9-C10-O7-C8
26	5	316	CHL	C8-C10-C11-C12
26	3	313	CHL	CBD-CGD-O2D-CED
25	U	312	LHG	C24-C25-C26-C27
32	l	102	SQD	C10-C11-C12-C13
34	w	201	LMG	C29-C30-C31-C32
34	W	201	LMG	C29-C30-C31-C32
34	C	502	LMG	C15-C16-C17-C18
34	B	621	LMG	C29-C30-C31-C32
34	B	621	LMG	C36-C37-C38-C39
34	b	624	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	5	305	CLA	O1A-CGA-O2A-C1
22	b	614	CLA	O1A-CGA-O2A-C1
26	q	314	CHL	O1A-CGA-O2A-C1
25	d	405	LHG	C24-C25-C26-C27
25	L	101	LHG	C11-C12-C13-C14
25	U	312	LHG	C10-C11-C12-C13
25	N	312	LHG	C26-C27-C28-C29
25	G	310	LHG	C25-C26-C27-C28
25	b	623	LHG	C25-C26-C27-C28
32	a	413	SQD	C14-C15-C16-C17
32	L	102	SQD	C12-C13-C14-C15
34	B	621	LMG	C35-C36-C37-C38
34	b	621	LMG	C38-C39-C40-C41
34	c	501	LMG	C15-C16-C17-C18
36	C	520	DGD	C9B-CAB-CBB-CCB
36	B	601	DGD	CCA-CDA-CEA-CFA
22	P	306	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
22	p	306	CLA	C5-C6-C7-C8
22	B	602	CLA	C8-C10-C11-C12
26	r	614	CHL	C15-C16-C17-C18
25	P	313	LHG	O2-C2-C3-O3
25	p	313	LHG	C24-C25-C26-C27
25	V	312	LHG	C25-C26-C27-C28
25	P	313	LHG	C24-C25-C26-C27
25	R	314	LHG	C16-C17-C18-C19
26	R	316	CHL	C3-C5-C6-C7
22	U	303	CLA	O1D-CGD-O2D-CED
22	B	611	CLA	O1D-CGD-O2D-CED
36	J	101	DGD	C2E-C1E-O5D-C6D
36	c	518	DGD	C2D-C1D-O3G-C3G
36	c	519	DGD	C2E-C1E-O5D-C6D
22	r	609	CLA	CBA-CGA-O2A-C1
22	2	303	CLA	CBA-CGA-O2A-C1
25	d	405	LHG	C12-C13-C14-C15
25	g	310	LHG	C32-C33-C34-C35
25	b	622	LHG	C24-C25-C26-C27
32	L	102	SQD	C10-C11-C12-C13
34	d	407	LMG	C11-C12-C13-C14
34	w	201	LMG	C11-C12-C13-C14
34	C	502	LMG	C37-C38-C39-C40
36	c	517	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
22	d	402	CLA	C15-C16-C17-C18
22	g	306	CLA	C8-C10-C11-C12
22	R	310	CLA	C10-C11-C12-C13
22	D	403	CLA	C15-C16-C17-C18
26	6	301	CHL	C8-C10-C11-C12
26	U	313	CHL	C5-C6-C7-C8
22	4	303	CLA	O1A-CGA-O2A-C1
22	5	307	CLA	O1A-CGA-O2A-C1
22	6	304	CLA	O1A-CGA-O2A-C1
22	P	307	CLA	O1A-CGA-O2A-C1
22	N	305	CLA	O1A-CGA-O2A-C1
22	C	504	CLA	O1A-CGA-O2A-C1
22	c	503	CLA	O1A-CGA-O2A-C1
26	5	313	CHL	O1A-CGA-O2A-C1
22	6	307	CLA	C11-C12-C13-C15
22	v	304	CLA	C11-C12-C13-C14
22	G	301	CLA	C16-C17-C18-C20
22	G	305	CLA	C11-C12-C13-C15
22	n	304	CLA	C16-C17-C18-C20
22	n	305	CLA	C11-C12-C13-C14
22	C	504	CLA	C16-C17-C18-C20
22	b	610	CLA	C16-C17-C18-C20
26	2	313	CHL	C16-C17-C18-C19
26	3	316	CHL	C11-C12-C13-C15
26	4	316	CHL	C16-C17-C18-C19
26	5	313	CHL	C16-C17-C18-C19
26	6	317	CHL	C11-C12-C13-C14
26	v	317	CHL	C16-C17-C18-C19
26	v	317	CHL	C16-C17-C18-C20
26	q	314	CHL	C16-C17-C18-C19
26	Q	316	CHL	C11-C12-C13-C15
26	N	317	CHL	C16-C17-C18-C20
26	g	311	CHL	C16-C17-C18-C20
26	R	315	CHL	C16-C17-C18-C20
22	N	305	CLA	O1D-CGD-O2D-CED
26	V	314	CHL	O1D-CGD-O2D-CED
26	Q	312	CHL	O1D-CGD-O2D-CED
22	r	605	CLA	C4-C3-C5-C6
22	4	302	CLA	C4-C3-C5-C6
26	3	314	CHL	C4-C3-C5-C6
26	6	315	CHL	C4-C3-C5-C6
26	S	315	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	5	312	LHG	C28-C29-C30-C31
25	B	623	LHG	C11-C12-C13-C14
25	B	623	LHG	C25-C26-C27-C28
34	B	621	LMG	C13-C14-C15-C16
34	B	621	LMG	C38-C39-C40-C41
36	C	519	DGD	C4A-C5A-C6A-C7A
22	P	302	CLA	C2-C3-C5-C6
26	n	316	CHL	C2-C3-C5-C6
22	2	304	CLA	C11-C12-C13-C14
22	4	306	CLA	C11-C10-C8-C9
22	5	304	CLA	C11-C12-C13-C14
22	U	307	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	b	612	CLA	C11-C10-C8-C9
22	c	508	CLA	C6-C7-C8-C9
26	v	316	CHL	C14-C13-C15-C16
26	V	313	CHL	C11-C12-C13-C14
26	V	316	CHL	C14-C13-C15-C16
26	Q	311	CHL	C6-C7-C8-C9
26	N	316	CHL	C14-C13-C15-C16
26	G	311	CHL	C6-C7-C8-C9
26	n	318	CHL	C11-C10-C8-C9
26	g	311	CHL	C6-C7-C8-C9
26	g	314	CHL	C11-C10-C8-C9
26	g	314	CHL	C14-C13-C15-C16
26	g	315	CHL	C11-C10-C8-C9
22	b	611	CLA	O1D-CGD-O2D-CED
25	6	311	LHG	C12-C13-C14-C15
25	p	313	LHG	C26-C27-C28-C29
25	q	310	LHG	C11-C12-C13-C14
25	V	312	LHG	C31-C32-C33-C34
25	G	310	LHG	C10-C11-C12-C13
25	g	310	LHG	C10-C11-C12-C13
25	S	312	LHG	C15-C16-C17-C18
25	C	523	LHG	C14-C15-C16-C17
25	D	406	LHG	C12-C13-C14-C15
25	s	312	LHG	C15-C16-C17-C18
32	a	410	SQD	C24-C25-C26-C27
32	a	413	SQD	C12-C13-C14-C15
32	A	412	SQD	C24-C25-C26-C27
34	d	407	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
34	B	624	LMG	C37-C38-C39-C40
34	D	408	LMG	C11-C12-C13-C14
34	c	501	LMG	C37-C38-C39-C40
36	c	517	DGD	C4A-C5A-C6A-C7A
22	C	512	CLA	C13-C15-C16-C17
26	u	313	CHL	C15-C16-C17-C18
26	g	316	CHL	C8-C10-C11-C12
26	R	315	CHL	C15-C16-C17-C18
22	A	406	CLA	C2A-CAA-CBA-CGA
22	2	306	CLA	C2A-CAA-CBA-CGA
22	3	301	CLA	C2A-CAA-CBA-CGA
22	6	302	CLA	C2A-CAA-CBA-CGA
22	P	309	CLA	C2A-CAA-CBA-CGA
26	u	315	CHL	C2A-CAA-CBA-CGA
26	u	316	CHL	C2A-CAA-CBA-CGA
26	n	313	CHL	C2A-CAA-CBA-CGA
26	S	316	CHL	C2A-CAA-CBA-CGA
26	s	316	CHL	C2A-CAA-CBA-CGA
22	1	303	CLA	O1A-CGA-O2A-C1
22	1	308	CLA	O1A-CGA-O2A-C1
22	G	308	CLA	O1A-CGA-O2A-C1
22	c	504	CLA	O1A-CGA-O2A-C1
26	G	316	CHL	O1A-CGA-O2A-C1
26	R	315	CHL	O1A-CGA-O2A-C1
24	1	311	XAT	C11-C12-C13-C20
24	4	311	XAT	C11-C12-C13-C20
24	p	312	XAT	C11-C12-C13-C20
24	Q	309	XAT	C11-C12-C13-C20
24	N	311	XAT	C11-C12-C13-C20
31	t	101	BCR	C11-C12-C13-C35
31	z	101	BCR	C36-C18-C19-C20
31	T	101	BCR	C11-C12-C13-C35
31	C	516	BCR	C36-C18-C19-C20
31	b	619	BCR	C11-C12-C13-C35
31	c	515	BCR	C7-C8-C9-C34
31	c	515	BCR	C11-C12-C13-C35
25	5	312	LHG	C24-C25-C26-C27
25	p	313	LHG	C31-C32-C33-C34
25	D	406	LHG	C24-C25-C26-C27
32	a	413	SQD	C24-C25-C26-C27
36	a	416	DGD	C5B-C6B-C7B-C8B
36	A	414	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
36	c	518	DGD	C7A-C8A-C9A-CAA
36	c	518	DGD	C8B-C9B-CAB-CBB
25	r	613	LHG	O1-C1-C2-C3
25	a	415	LHG	O1-C1-C2-C3
25	l	101	LHG	O1-C1-C2-C3
25	A	413	LHG	O1-C1-C2-C3
25	L	101	LHG	O1-C1-C2-C3
25	q	310	LHG	O1-C1-C2-C3
25	P	313	LHG	O1-C1-C2-C3
25	u	312	LHG	O1-C1-C2-C3
25	n	312	LHG	O1-C1-C2-C3
25	C	522	LHG	O1-C1-C2-C3
25	B	622	LHG	O1-C1-C2-C3
25	D	406	LHG	O1-C1-C2-C3
25	b	622	LHG	O1-C1-C2-C3
23	S	311	LUT	C11-C12-C13-C14
24	1	311	XAT	C11-C12-C13-C14
24	3	309	XAT	C11-C12-C13-C14
24	4	311	XAT	C11-C12-C13-C14
24	p	312	XAT	C11-C12-C13-C14
24	Q	309	XAT	C11-C12-C13-C14
24	N	311	XAT	C11-C12-C13-C14
24	G	309	XAT	C27-C28-C29-C30
31	t	101	BCR	C11-C12-C13-C14
31	z	101	BCR	C11-C12-C13-C14
31	z	101	BCR	C17-C18-C19-C20
31	T	101	BCR	C11-C12-C13-C14
31	C	516	BCR	C11-C12-C13-C14
31	C	516	BCR	C17-C18-C19-C20
31	B	620	BCR	C21-C22-C23-C24
22	N	306	CLA	C3-C5-C6-C7
22	a	408	CLA	O1D-CGD-O2D-CED
25	R	314	LHG	O9-C7-O7-C5
34	W	201	LMG	O9-C10-O7-C8
22	6	302	CLA	C8-C10-C11-C12
22	6	307	CLA	C10-C11-C12-C13
22	P	306	CLA	C5-C6-C7-C8
22	b	610	CLA	C5-C6-C7-C8
26	1	313	CHL	C5-C6-C7-C8
26	2	313	CHL	C10-C11-C12-C13
26	q	311	CHL	C8-C10-C11-C12
26	U	316	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	G	315	CHL	C13-C15-C16-C17
25	R	314	LHG	C8-C7-O7-C5
34	W	201	LMG	C11-C10-O7-C8
25	p	313	LHG	C9-C10-C11-C12
25	p	313	LHG	C15-C16-C17-C18
32	L	102	SQD	C14-C15-C16-C17
32	M	101	SQD	C27-C28-C29-C30
36	C	519	DGD	CAB-CBB-CCB-CDB
36	C	520	DGD	C7A-C8A-C9A-CAA
22	r	610	CLA	CBD-CGD-O2D-CED
25	r	613	LHG	C7-C8-C9-C10
25	v	312	LHG	C23-C24-C25-C26
25	R	314	LHG	C7-C8-C9-C10
25	D	406	LHG	C23-C24-C25-C26
36	c	519	DGD	C1A-C2A-C3A-C4A
25	a	415	LHG	C30-C31-C32-C33
25	l	101	LHG	C11-C12-C13-C14
25	A	413	LHG	C30-C31-C32-C33
25	p	313	LHG	C25-C26-C27-C28
25	P	313	LHG	C11-C10-C9-C8
25	Q	310	LHG	C9-C10-C11-C12
25	Q	310	LHG	C14-C15-C16-C17
25	c	522	LHG	C14-C15-C16-C17
25	c	523	LHG	C16-C17-C18-C19
32	l	102	SQD	C14-C15-C16-C17
32	A	412	SQD	C12-C13-C14-C15
34	C	521	LMG	C35-C36-C37-C38
34	B	624	LMG	C14-C15-C16-C17
34	b	624	LMG	C14-C15-C16-C17
34	b	624	LMG	C37-C38-C39-C40
36	c	519	DGD	C2A-C3A-C4A-C5A
22	r	603	CLA	C11-C12-C13-C14
22	r	603	CLA	C11-C12-C13-C15
22	6	307	CLA	C11-C12-C13-C14
22	P	308	CLA	C11-C12-C13-C14
22	P	308	CLA	C11-C12-C13-C15
22	Q	305	CLA	C11-C12-C13-C14
22	G	305	CLA	C11-C12-C13-C14
22	R	304	CLA	C11-C12-C13-C14
22	R	304	CLA	C11-C12-C13-C15
22	B	610	CLA	C16-C17-C18-C19
22	b	603	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	C16-C17-C18-C20
22	b	610	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C20
26	r	616	CHL	C11-C12-C13-C14
26	6	301	CHL	C16-C17-C18-C19
26	6	301	CHL	C16-C17-C18-C20
26	p	314	CHL	C16-C17-C18-C20
26	q	311	CHL	C16-C17-C18-C19
26	q	311	CHL	C16-C17-C18-C20
26	V	317	CHL	C16-C17-C18-C19
26	P	314	CHL	C16-C17-C18-C20
26	P	318	CHL	C16-C17-C18-C19
26	P	318	CHL	C16-C17-C18-C20
26	Q	311	CHL	C16-C17-C18-C19
26	Q	315	CHL	C16-C17-C18-C19
26	Q	315	CHL	C16-C17-C18-C20
26	N	316	CHL	C16-C17-C18-C19
26	N	317	CHL	C16-C17-C18-C19
26	n	316	CHL	C16-C17-C18-C20
26	n	318	CHL	C16-C17-C18-C20
26	g	311	CHL	C16-C17-C18-C19
26	R	317	CHL	C11-C12-C13-C14
26	R	317	CHL	C11-C12-C13-C15
36	a	416	DGD	O6E-C1E-O5D-C6D
36	A	414	DGD	O6E-C1E-O5D-C6D
36	J	101	DGD	O6E-C1E-O5D-C6D
22	3	301	CLA	C8-C10-C11-C12
22	3	302	CLA	C8-C10-C11-C12
22	V	301	CLA	C10-C11-C12-C13
22	c	510	CLA	C8-C10-C11-C12
22	c	511	CLA	C13-C15-C16-C17
26	p	317	CHL	C15-C16-C17-C18
26	V	313	CHL	C8-C10-C11-C12
26	V	313	CHL	C10-C11-C12-C13
26	U	317	CHL	C15-C16-C17-C18
26	P	316	CHL	O1D-CGD-O2D-CED
26	Q	313	CHL	O1D-CGD-O2D-CED
25	1	312	LHG	C25-C26-C27-C28
25	v	312	LHG	C25-C26-C27-C28
25	N	312	LHG	C25-C26-C27-C28
25	u	312	LHG	C25-C26-C27-C28
25	B	622	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	C	519	DGD	C4B-C5B-C6B-C7B
22	r	605	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
26	4	317	CHL	CBD-CGD-O2D-CED
25	r	613	LHG	C15-C16-C17-C18
25	6	311	LHG	C27-C28-C29-C30
25	B	622	LHG	C9-C10-C11-C12
32	l	102	SQD	C9-C10-C11-C12
32	m	101	SQD	C9-C10-C11-C12
32	m	101	SQD	C27-C28-C29-C30
32	A	412	SQD	C17-C18-C19-C20
32	M	101	SQD	C9-C10-C11-C12
34	C	502	LMG	C16-C17-C18-C19
25	V	312	LHG	C23-C24-C25-C26
25	C	522	LHG	C23-C24-C25-C26
22	q	304	CLA	C10-C11-C12-C13
22	n	301	CLA	C5-C6-C7-C8
22	C	511	CLA	C8-C10-C11-C12
26	V	316	CHL	C13-C15-C16-C17
26	2	313	CHL	O1A-CGA-O2A-C1
26	4	313	CHL	O1A-CGA-O2A-C1
25	v	312	LHG	C24-C25-C26-C27
32	a	413	SQD	C28-C29-C30-C31
34	d	407	LMG	C13-C14-C15-C16
34	D	408	LMG	C13-C14-C15-C16
36	A	414	DGD	C7B-C8B-C9B-CAB
26	2	318	CHL	O1D-CGD-O2D-CED
22	5	307	CLA	C3-C5-C6-C7
26	u	316	CHL	C3-C5-C6-C7
22	4	306	CLA	CBA-CGA-O2A-C1
22	Q	305	CLA	CBA-CGA-O2A-C1
22	n	302	CLA	CBA-CGA-O2A-C1
22	B	608	CLA	CBA-CGA-O2A-C1
22	b	612	CLA	CBA-CGA-O2A-C1
25	A	413	LHG	C31-C32-C33-C34
32	A	412	SQD	C14-C15-C16-C17
32	L	102	SQD	C9-C10-C11-C12
34	b	621	LMG	C37-C38-C39-C40
36	c	517	DGD	C4B-C5B-C6B-C7B
22	a	405	CLA	O1D-CGD-O2D-CED
22	R	302	CLA	O1D-CGD-O2D-CED
26	2	313	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	5	313	CHL	O1D-CGD-O2D-CED
26	q	313	CHL	O1D-CGD-O2D-CED
26	N	315	CHL	O1D-CGD-O2D-CED
22	r	601	CLA	C3A-C2A-CAA-CBA
22	v	303	CLA	C3A-C2A-CAA-CBA
22	S	301	CLA	C3A-C2A-CAA-CBA
22	C	514	CLA	C3A-C2A-CAA-CBA
22	C	515	CLA	C3A-C2A-CAA-CBA
22	B	611	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA
22	c	513	CLA	C3A-C2A-CAA-CBA
22	c	514	CLA	C3A-C2A-CAA-CBA
26	r	614	CHL	C3A-C2A-CAA-CBA
26	1	316	CHL	C3A-C2A-CAA-CBA
26	2	316	CHL	C3A-C2A-CAA-CBA
26	5	316	CHL	C3A-C2A-CAA-CBA
26	Q	312	CHL	C3A-C2A-CAA-CBA
26	U	319	CHL	C3A-C2A-CAA-CBA
26	u	316	CHL	C3A-C2A-CAA-CBA
26	n	316	CHL	C3A-C2A-CAA-CBA
26	g	313	CHL	C3A-C2A-CAA-CBA
26	R	315	CHL	C3A-C2A-CAA-CBA
22	A	405	CLA	C8-C10-C11-C12
22	6	305	CLA	C13-C15-C16-C17
22	U	306	CLA	C10-C11-C12-C13
25	a	415	LHG	C31-C32-C33-C34
25	l	101	LHG	C25-C26-C27-C28
25	A	413	LHG	C25-C26-C27-C28
25	u	312	LHG	C13-C14-C15-C16
25	u	312	LHG	C30-C31-C32-C33
25	C	522	LHG	C24-C25-C26-C27
25	D	406	LHG	C28-C29-C30-C31
32	M	101	SQD	C11-C10-C9-C8
34	c	501	LMG	C16-C17-C18-C19
36	a	416	DGD	C7B-C8B-C9B-CAB
36	c	518	DGD	C9B-CAB-CBB-CCB
22	A	405	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	O1D-CGD-O2D-CED
26	Q	311	CHL	O1D-CGD-O2D-CED
22	v	302	CLA	O1A-CGA-O2A-C1
22	C	505	CLA	O1A-CGA-O2A-C1
22	3	306	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	6	306	CLA	C11-C12-C13-C14
22	6	306	CLA	C11-C12-C13-C15
22	p	308	CLA	C11-C12-C13-C15
22	Q	305	CLA	C11-C12-C13-C15
22	g	306	CLA	C11-C12-C13-C15
22	C	504	CLA	C16-C17-C18-C19
22	B	603	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C20
26	r	614	CHL	C16-C17-C18-C19
26	r	614	CHL	C16-C17-C18-C20
26	1	317	CHL	C16-C17-C18-C19
26	3	315	CHL	C16-C17-C18-C19
26	3	315	CHL	C16-C17-C18-C20
26	3	316	CHL	C11-C12-C13-C14
26	4	316	CHL	C16-C17-C18-C20
26	6	316	CHL	C16-C17-C18-C19
26	6	317	CHL	C11-C12-C13-C15
26	p	318	CHL	C16-C17-C18-C19
26	p	318	CHL	C16-C17-C18-C20
26	q	314	CHL	C16-C17-C18-C20
26	V	317	CHL	C16-C17-C18-C20
26	P	314	CHL	C16-C17-C18-C19
26	Q	316	CHL	C11-C12-C13-C14
26	U	319	CHL	C16-C17-C18-C20
26	G	315	CHL	C16-C17-C18-C20
25	a	415	LHG	C25-C26-C27-C28
25	l	101	LHG	C32-C33-C34-C35
25	P	313	LHG	C25-C26-C27-C28
25	G	310	LHG	C27-C28-C29-C30
25	n	312	LHG	C14-C15-C16-C17
32	A	412	SQD	C28-C29-C30-C31
34	w	201	LMG	C13-C14-C15-C16
34	C	521	LMG	C12-C13-C14-C15
34	B	624	LMG	C22-C23-C24-C25
36	C	520	DGD	C8B-C9B-CAB-CBB
22	r	604	CLA	O2A-C1-C2-C3
22	2	308	CLA	O2A-C1-C2-C3
22	R	305	CLA	O2A-C1-C2-C3
34	c	520	LMG	C7-C8-C9-O8
22	4	308	CLA	CBD-CGD-O2D-CED
22	D	403	CLA	CBD-CGD-O2D-CED
26	U	317	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	b	621	LMG	C4-C5-C6-O5
25	2	312	LHG	C16-C17-C18-C19
25	B	622	LHG	C24-C25-C26-C27
32	m	101	SQD	C11-C10-C9-C8
34	b	621	LMG	C30-C31-C32-C33
22	1	306	CLA	C3-C5-C6-C7
22	V	307	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
22	s	308	CLA	C3-C5-C6-C7
25	a	415	LHG	C7-C8-C9-C10
25	A	413	LHG	C7-C8-C9-C10
34	b	621	LMG	C28-C29-C30-C31
25	S	312	LHG	C11-C12-C13-C14
25	D	407	LHG	C26-C27-C28-C29
34	W	201	LMG	C11-C12-C13-C14
22	Q	301	CLA	C10-C11-C12-C13
22	1	302	CLA	C4-C3-C5-C6
22	2	302	CLA	C4-C3-C5-C6
22	3	306	CLA	C4-C3-C5-C6
22	5	302	CLA	C4-C3-C5-C6
22	6	307	CLA	C4-C3-C5-C6
22	v	302	CLA	C4-C3-C5-C6
22	v	306	CLA	C4-C3-C5-C6
22	q	307	CLA	C4-C3-C5-C6
22	u	302	CLA	C4-C3-C5-C6
26	n	316	CHL	C4-C3-C5-C6
22	g	305	CLA	CBA-CGA-O2A-C1
22	B	610	CLA	CBA-CGA-O2A-C1
22	B	612	CLA	CBA-CGA-O2A-C1
22	b	610	CLA	CBA-CGA-O2A-C1
26	3	314	CHL	CBA-CGA-O2A-C1
22	1	302	CLA	C2-C3-C5-C6
22	2	302	CLA	C2-C3-C5-C6
22	3	306	CLA	C2-C3-C5-C6
22	4	306	CLA	C2-C3-C5-C6
22	5	302	CLA	C2-C3-C5-C6
22	v	302	CLA	C2-C3-C5-C6
22	u	302	CLA	C2-C3-C5-C6
22	u	307	CLA	C2-C3-C5-C6
26	6	315	CHL	C2-C3-C5-C6
26	q	314	CHL	C2-C3-C5-C6
26	S	315	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	s	315	CHL	C2-C3-C5-C6
25	l	101	LHG	C8-C7-O7-C5
25	L	101	LHG	C8-C7-O7-C5
34	w	201	LMG	C11-C10-O7-C8
22	r	602	CLA	C2A-CAA-CBA-CGA
22	5	303	CLA	C2A-CAA-CBA-CGA
22	p	309	CLA	C2A-CAA-CBA-CGA
22	R	303	CLA	C2A-CAA-CBA-CGA
25	d	405	LHG	O1-C1-C2-O2
25	Q	310	LHG	O1-C1-C2-O2
25	G	310	LHG	O1-C1-C2-O2
25	n	312	LHG	O1-C1-C2-O2
25	C	522	LHG	O1-C1-C2-O2
25	C	524	LHG	O1-C1-C2-O2
25	c	521	LHG	O1-C1-C2-O2
25	3	310	LHG	C27-C28-C29-C30
25	n	312	LHG	C25-C26-C27-C28
25	s	312	LHG	C11-C12-C13-C14
32	a	410	SQD	C25-C26-C27-C28
34	b	621	LMG	C15-C16-C17-C18
34	b	621	LMG	C17-C18-C19-C20
34	b	621	LMG	C35-C36-C37-C38
36	c	518	DGD	C2B-C3B-C4B-C5B
36	c	519	DGD	C9A-CAA-CBA-CCA
22	U	303	CLA	O1A-CGA-O2A-C1
22	n	303	CLA	O1A-CGA-O2A-C1
22	B	617	CLA	O1A-CGA-O2A-C1
26	p	317	CHL	O1A-CGA-O2A-C1
26	V	317	CHL	O1A-CGA-O2A-C1
22	A	408	CLA	C11-C12-C13-C14
26	Q	311	CHL	C16-C17-C18-C20
26	R	315	CHL	C16-C17-C18-C19
22	B	608	CLA	C8-C10-C11-C12
22	b	610	CLA	C13-C15-C16-C17
25	5	312	LHG	C11-C10-C9-C8
34	C	502	LMG	C36-C37-C38-C39
36	C	520	DGD	C2B-C3B-C4B-C5B
22	6	308	CLA	C3-C5-C6-C7
22	Q	301	CLA	C3-C5-C6-C7
22	4	308	CLA	CBA-CGA-O2A-C1
25	L	101	LHG	C9-C10-C11-C12
34	C	521	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	q	308	CLA	O1A-CGA-O2A-C1
22	P	304	CLA	O1A-CGA-O2A-C1
22	n	305	CLA	O1A-CGA-O2A-C1
26	u	316	CHL	O1A-CGA-O2A-C1
32	m	101	SQD	C23-C24-C25-C26
32	M	101	SQD	C23-C24-C25-C26
25	C	522	LHG	C1-C2-C3-O3
25	d	406	LHG	C26-C27-C28-C29
25	V	312	LHG	C32-C33-C34-C35
34	c	520	LMG	C21-C22-C23-C24
36	A	414	DGD	C7A-C8A-C9A-CAA
34	w	201	LMG	O9-C10-O7-C8
26	1	317	CHL	C2-C1-O2A-CGA
25	L	101	LHG	C32-C33-C34-C35
25	1	312	LHG	C26-C27-C28-C29
25	n	312	LHG	C27-C28-C29-C30
25	C	522	LHG	C14-C15-C16-C17
32	m	101	SQD	C25-C26-C27-C28
34	b	621	LMG	C16-C17-C18-C19
22	5	302	CLA	C10-C11-C12-C13
22	N	304	CLA	C8-C10-C11-C12
22	C	511	CLA	C10-C11-C12-C13
22	B	615	CLA	C15-C16-C17-C18
26	5	313	CHL	C5-C6-C7-C8
26	p	318	CHL	C15-C16-C17-C18
22	3	308	CLA	O1A-CGA-O2A-C1
22	B	610	CLA	O1A-CGA-O2A-C1
22	b	610	CLA	O1A-CGA-O2A-C1
36	c	518	DGD	O1A-C1A-O1G-C1G
25	d	405	LHG	C33-C34-C35-C36
25	g	310	LHG	C28-C29-C30-C31
25	g	310	LHG	C33-C34-C35-C36
32	M	101	SQD	C25-C26-C27-C28
34	b	624	LMG	C22-C23-C24-C25
22	c	503	CLA	C16-C17-C18-C19
22	c	507	CLA	C16-C17-C18-C20
25	u	312	LHG	C7-C8-C9-C10
22	3	307	CLA	C3-C5-C6-C7
22	S	308	CLA	C3-C5-C6-C7
23	r	611	LUT	C1-C6-C7-C8
23	r	611	LUT	C5-C6-C7-C8
23	1	309	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	4	309	LUT	C5-C6-C7-C8
23	U	309	LUT	C5-C6-C7-C8
23	R	312	LUT	C5-C6-C7-C8
31	d	403	BCR	C5-C6-C7-C8
31	k	101	BCR	C23-C24-C25-C26
31	t	101	BCR	C5-C6-C7-C8
31	x	202	BCR	C23-C24-C25-C26
31	x	202	BCR	C23-C24-C25-C30
31	z	101	BCR	C1-C6-C7-C8
31	K	101	BCR	C23-C24-C25-C26
31	T	101	BCR	C5-C6-C7-C8
31	C	516	BCR	C1-C6-C7-C8
31	C	517	BCR	C1-C6-C7-C8
31	C	517	BCR	C23-C24-C25-C26
31	C	518	BCR	C23-C24-C25-C26
31	B	618	BCR	C5-C6-C7-C8
31	B	619	BCR	C23-C24-C25-C26
31	B	619	BCR	C23-C24-C25-C30
31	B	620	BCR	C23-C24-C25-C26
31	B	620	BCR	C23-C24-C25-C30
31	D	404	BCR	C5-C6-C7-C8
31	X	201	BCR	C23-C24-C25-C26
31	X	201	BCR	C23-C24-C25-C30
31	b	618	BCR	C5-C6-C7-C8
31	b	619	BCR	C23-C24-C25-C26
31	b	619	BCR	C23-C24-C25-C30
31	b	620	BCR	C23-C24-C25-C26
31	b	620	BCR	C23-C24-C25-C30
31	c	515	BCR	C1-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C26
31	c	516	BCR	C23-C24-C25-C26
25	D	407	LHG	C33-C34-C35-C36
25	c	521	LHG	C11-C12-C13-C14
34	C	502	LMG	C18-C19-C20-C21
34	c	520	LMG	C12-C13-C14-C15
36	C	520	DGD	CCA-CDA-CEA-CFA
26	p	316	CHL	O1D-CGD-O2D-CED
22	p	307	CLA	CBA-CGA-O2A-C1
25	d	405	LHG	C24-C23-O8-C6
25	D	406	LHG	C24-C23-O8-C6
26	r	614	CHL	CBA-CGA-O2A-C1
26	1	314	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	V	318	CHL	CBA-CGA-O2A-C1
22	d	402	CLA	C10-C11-C12-C13
22	G	302	CLA	C5-C6-C7-C8
22	G	306	CLA	C5-C6-C7-C8
22	b	605	CLA	C5-C6-C7-C8
22	c	510	CLA	C10-C11-C12-C13
26	4	317	CHL	C8-C10-C11-C12
26	5	317	CHL	C15-C16-C17-C18
26	v	313	CHL	C10-C11-C12-C13
26	p	320	CHL	C13-C15-C16-C17
26	V	318	CHL	C5-C6-C7-C8
26	Q	311	CHL	C8-C10-C11-C12
26	u	313	CHL	C5-C6-C7-C8
34	d	407	LMG	C11-C10-O7-C8
25	d	405	LHG	C11-C12-C13-C14
25	l	101	LHG	C9-C10-C11-C12
25	3	310	LHG	C31-C32-C33-C34
25	6	311	LHG	C31-C32-C33-C34
25	6	311	LHG	C32-C33-C34-C35
25	Q	310	LHG	C26-C27-C28-C29
25	g	310	LHG	C27-C28-C29-C30
25	b	622	LHG	C9-C10-C11-C12
36	J	101	DGD	C7B-C8B-C9B-CAB
22	1	308	CLA	O2A-C1-C2-C3
22	4	308	CLA	O2A-C1-C2-C3
22	v	308	CLA	O2A-C1-C2-C3
22	n	302	CLA	O1A-CGA-O2A-C1
22	s	301	CLA	C14-C13-C15-C16
25	2	312	LHG	C23-C24-C25-C26
25	U	312	LHG	C7-C8-C9-C10
25	c	521	LHG	C23-C24-C25-C26
34	D	408	LMG	C28-C29-C30-C31
25	u	312	LHG	C10-C11-C12-C13
34	c	501	LMG	C18-C19-C20-C21
22	R	303	CLA	C8-C10-C11-C12
22	B	612	CLA	C10-C11-C12-C13
22	D	403	CLA	C10-C11-C12-C13
26	1	316	CHL	C8-C10-C11-C12
26	6	317	CHL	C8-C10-C11-C12
26	G	314	CHL	C15-C16-C17-C18
25	S	312	LHG	C32-C33-C34-C35
22	4	306	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	u	307	CLA	C4-C3-C5-C6
26	q	314	CHL	C4-C3-C5-C6
26	Q	315	CHL	C4-C3-C5-C6
33	d	404	PL9	C30-C29-C31-C32
26	q	312	CHL	O1D-CGD-O2D-CED
22	r	605	CLA	C2-C3-C5-C6
22	2	304	CLA	C11-C12-C13-C15
22	2	307	CLA	C11-C10-C8-C7
22	3	301	CLA	C11-C10-C8-C7
22	3	302	CLA	C11-C10-C8-C7
22	3	304	CLA	C12-C13-C15-C16
22	4	302	CLA	C2-C3-C5-C6
22	4	306	CLA	C11-C10-C8-C7
22	5	304	CLA	C11-C12-C13-C15
22	5	307	CLA	C2-C3-C5-C6
22	6	302	CLA	C11-C10-C8-C7
22	6	305	CLA	C6-C7-C8-C10
22	6	307	CLA	C2-C3-C5-C6
22	v	302	CLA	C12-C13-C15-C16
22	v	306	CLA	C2-C3-C5-C6
22	q	307	CLA	C2-C3-C5-C6
22	Q	307	CLA	C2-C3-C5-C6
22	U	307	CLA	C2-C3-C5-C6
22	U	307	CLA	C11-C10-C8-C7
22	n	307	CLA	C6-C7-C8-C10
22	C	503	CLA	C11-C10-C8-C7
22	C	504	CLA	C12-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C15
22	C	514	CLA	C6-C7-C8-C10
22	B	606	CLA	C12-C13-C15-C16
22	B	610	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	B	613	CLA	C6-C7-C8-C10
22	b	605	CLA	C6-C7-C8-C10
22	b	606	CLA	C12-C13-C15-C16
22	b	612	CLA	C11-C10-C8-C7
22	b	613	CLA	C6-C7-C8-C10
22	c	503	CLA	C2-C3-C5-C6
22	c	504	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C12-C13-C15
26	r	615	CHL	C2-C3-C5-C6
26	1	317	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	2	318	CHL	C11-C10-C8-C7
26	2	318	CHL	C12-C13-C15-C16
26	3	314	CHL	C2-C3-C5-C6
26	6	312	CHL	C6-C7-C8-C10
26	v	318	CHL	C12-C13-C15-C16
26	V	313	CHL	C11-C12-C13-C15
26	V	316	CHL	C12-C13-C15-C16
26	P	319	CHL	C12-C13-C15-C16
26	Q	311	CHL	C6-C7-C8-C10
26	Q	315	CHL	C2-C3-C5-C6
26	N	316	CHL	C12-C13-C15-C16
26	G	311	CHL	C6-C7-C8-C10
26	G	311	CHL	C12-C13-C15-C16
26	g	311	CHL	C6-C7-C8-C10
26	g	315	CHL	C11-C10-C8-C7
33	d	404	PL9	C28-C29-C31-C32
33	D	405	PL9	C28-C29-C31-C32
26	p	319	CHL	C3-C5-C6-C7
22	2	303	CLA	O1A-CGA-O2A-C1
22	4	306	CLA	O1A-CGA-O2A-C1
22	4	308	CLA	O1A-CGA-O2A-C1
22	Q	305	CLA	O1A-CGA-O2A-C1
22	g	305	CLA	O1A-CGA-O2A-C1
22	B	608	CLA	O1A-CGA-O2A-C1
22	b	612	CLA	O1A-CGA-O2A-C1
26	3	314	CHL	O1A-CGA-O2A-C1
25	v	312	LHG	C30-C31-C32-C33
25	b	622	LHG	C10-C11-C12-C13
32	a	410	SQD	C30-C31-C32-C33
32	a	413	SQD	C10-C11-C12-C13
32	L	102	SQD	C15-C16-C17-C18
36	C	520	DGD	C7B-C8B-C9B-CAB
22	1	302	CLA	C13-C15-C16-C17
22	5	306	CLA	C5-C6-C7-C8
22	C	508	CLA	C5-C6-C7-C8
26	1	316	CHL	C5-C6-C7-C8
26	2	317	CHL	C15-C16-C17-C18
26	n	313	CHL	C10-C11-C12-C13
24	5	311	XAT	C29-C30-C31-C32
24	Q	309	XAT	C13-C14-C15-C35
24	n	311	XAT	C9-C10-C11-C12
27	r	618	NEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	k	101	BCR	C15-C16-C17-C18
31	B	619	BCR	C15-C16-C17-C18
31	c	515	BCR	C15-C16-C17-C18
22	v	304	CLA	C11-C12-C13-C15
22	N	305	CLA	C11-C12-C13-C14
22	n	304	CLA	C16-C17-C18-C19
22	C	508	CLA	C16-C17-C18-C20
26	2	313	CHL	C16-C17-C18-C20
26	5	313	CHL	C16-C17-C18-C20
26	v	316	CHL	C16-C17-C18-C19
26	G	316	CHL	C11-C12-C13-C15
22	n	305	CLA	O1D-CGD-O2D-CED
25	C	523	LHG	O9-C7-O7-C5
25	c	522	LHG	O9-C7-O7-C5
32	a	410	SQD	O49-C7-O47-C45
34	B	621	LMG	O9-C10-O7-C8
22	1	306	CLA	CBA-CGA-O2A-C1
22	5	303	CLA	CBA-CGA-O2A-C1
22	6	309	CLA	CBA-CGA-O2A-C1
22	G	307	CLA	CBA-CGA-O2A-C1
22	n	304	CLA	CBA-CGA-O2A-C1
22	g	307	CLA	CBA-CGA-O2A-C1
26	3	313	CHL	CBA-CGA-O2A-C1
26	6	315	CHL	CBA-CGA-O2A-C1
26	P	317	CHL	CBA-CGA-O2A-C1
26	Q	315	CHL	CBA-CGA-O2A-C1
26	u	317	CHL	CBA-CGA-O2A-C1
25	d	405	LHG	C26-C27-C28-C29
32	a	410	SQD	C9-C10-C11-C12
36	a	416	DGD	C7A-C8A-C9A-CAA
22	1	304	CLA	C2A-CAA-CBA-CGA
22	v	304	CLA	C2A-CAA-CBA-CGA
22	q	301	CLA	C2A-CAA-CBA-CGA
22	V	304	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	B	603	CLA	C2A-CAA-CBA-CGA
22	c	502	CLA	C2A-CAA-CBA-CGA
26	p	315	CHL	C2A-CAA-CBA-CGA
26	Q	313	CHL	C2A-CAA-CBA-CGA
22	S	301	CLA	O1D-CGD-O2D-CED
22	a	405	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	3	301	CLA	C15-C16-C17-C18
22	v	304	CLA	C5-C6-C7-C8
22	n	307	CLA	C5-C6-C7-C8
22	B	607	CLA	C5-C6-C7-C8
22	b	607	CLA	C5-C6-C7-C8
26	r	614	CHL	C13-C15-C16-C17
26	3	314	CHL	C15-C16-C17-C18
26	q	314	CHL	C13-C15-C16-C17
25	L	101	LHG	C25-C26-C27-C28
25	U	312	LHG	C16-C17-C18-C19
25	n	312	LHG	C28-C29-C30-C31
25	c	521	LHG	C24-C25-C26-C27
34	c	501	LMG	C36-C37-C38-C39
22	p	303	CLA	O1D-CGD-O2D-CED
25	4	312	LHG	C25-C26-C27-C28
36	b	601	DGD	C3A-C4A-C5A-C6A
34	d	407	LMG	C28-C29-C30-C31
36	A	414	DGD	C1A-C2A-C3A-C4A
22	2	305	CLA	O1D-CGD-O2D-CED
22	A	404	CLA	C13-C15-C16-C17
22	P	302	CLA	C5-C6-C7-C8
22	R	307	CLA	C10-C11-C12-C13
22	c	512	CLA	C8-C10-C11-C12
26	4	317	CHL	C15-C16-C17-C18
25	2	312	LHG	C9-C10-C11-C12
25	S	312	LHG	C16-C17-C18-C19
32	l	102	SQD	C27-C28-C29-C30
22	B	617	CLA	C3-C5-C6-C7
22	b	606	CLA	CBA-CGA-O2A-C1
26	6	317	CHL	CBA-CGA-O2A-C1
22	n	305	CLA	C11-C12-C13-C15
26	V	316	CHL	C16-C17-C18-C19
36	c	518	DGD	O6D-C1D-O3G-C3G
26	V	313	CHL	C5-C6-C7-C8
26	n	317	CHL	O1D-CGD-O2D-CED
25	d	405	LHG	C28-C29-C30-C31
25	U	312	LHG	C25-C26-C27-C28
32	l	102	SQD	C15-C16-C17-C18
32	C	501	SQD	C9-C10-C11-C12
25	3	310	LHG	C8-C7-O7-C5
25	V	312	LHG	C8-C7-O7-C5
25	C	523	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	B	623	LHG	C8-C7-O7-C5
25	b	623	LHG	C8-C7-O7-C5
25	c	522	LHG	C8-C7-O7-C5
34	C	502	LMG	C11-C10-O7-C8
34	B	621	LMG	C11-C10-O7-C8
34	D	408	LMG	C11-C10-O7-C8
34	c	501	LMG	C11-C10-O7-C8
25	N	312	LHG	O6-C4-C5-O7
25	N	312	LHG	C10-C11-C12-C13
25	u	312	LHG	C9-C10-C11-C12
25	u	312	LHG	C12-C13-C14-C15
25	s	312	LHG	C32-C33-C34-C35
36	b	601	DGD	O6D-C5D-C6D-O5D
22	g	307	CLA	C5-C6-C7-C8
22	c	506	CLA	C15-C16-C17-C18
26	3	316	CHL	C8-C10-C11-C12
26	q	314	CHL	C8-C10-C11-C12
22	R	306	CLA	CBD-CGD-O2D-CED
26	1	315	CHL	CBD-CGD-O2D-CED
26	3	311	CHL	CBD-CGD-O2D-CED
26	V	318	CHL	CBD-CGD-O2D-CED
32	C	501	SQD	C25-C26-C27-C28
36	J	101	DGD	C9A-CAA-CBA-CCA
36	c	517	DGD	C8B-C9B-CAB-CBB
25	l	101	LHG	O9-C7-O7-C5
25	L	101	LHG	O9-C7-O7-C5
25	3	310	LHG	O9-C7-O7-C5
25	B	623	LHG	O9-C7-O7-C5
34	d	407	LMG	O9-C10-O7-C8
25	D	407	LHG	C17-C18-C19-C20
25	c	521	LHG	C14-C15-C16-C17
32	L	102	SQD	C27-C28-C29-C30
32	a	410	SQD	C2-C1-O6-C44
32	C	501	SQD	C2-C1-O6-C44
36	C	520	DGD	C2D-C1D-O3G-C3G
26	Q	314	CHL	C15-C16-C17-C18
25	a	415	LHG	O7-C5-C6-O8
25	l	101	LHG	O7-C5-C6-O8
25	A	413	LHG	O7-C5-C6-O8
25	L	101	LHG	O7-C5-C6-O8
25	5	312	LHG	O7-C5-C6-O8
32	m	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
32	A	412	SQD	O6-C44-C45-O47
32	M	101	SQD	O47-C45-C46-O48
34	B	624	LMG	O1-C7-C8-O7
34	b	624	LMG	O1-C7-C8-O7
26	S	315	CHL	CBD-CGD-O2D-CED
22	p	307	CLA	O1A-CGA-O2A-C1
25	d	405	LHG	O10-C23-O8-C6
22	G	301	CLA	C16-C17-C18-C19
26	v	318	CHL	C16-C17-C18-C19
26	n	317	CHL	C16-C17-C18-C20
25	d	405	LHG	C15-C16-C17-C18
25	G	310	LHG	C32-C33-C34-C35
25	D	406	LHG	C26-C27-C28-C29
36	C	519	DGD	C8B-C9B-CAB-CBB
22	c	511	CLA	C5-C6-C7-C8
26	r	615	CHL	C5-C6-C7-C8
26	3	315	CHL	C13-C15-C16-C17
26	4	316	CHL	C15-C16-C17-C18
26	6	316	CHL	C13-C15-C16-C17
26	G	311	CHL	C15-C16-C17-C18
22	5	307	CLA	C4-C3-C5-C6
22	Q	307	CLA	C4-C3-C5-C6
22	U	307	CLA	C4-C3-C5-C6
22	c	503	CLA	C4-C3-C5-C6
26	r	615	CHL	C4-C3-C5-C6
33	D	405	PL9	C30-C29-C31-C32
22	N	302	CLA	C2-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
32	L	102	SQD	C29-C30-C31-C32
36	b	601	DGD	C7B-C8B-C9B-CAB
22	A	404	CLA	C11-C12-C13-C14
22	2	307	CLA	C11-C10-C8-C9
22	3	302	CLA	C11-C10-C8-C9
22	3	304	CLA	C6-C7-C8-C9
22	3	304	CLA	C14-C13-C15-C16
22	6	305	CLA	C6-C7-C8-C9
22	v	302	CLA	C14-C13-C15-C16
22	v	307	CLA	C14-C13-C15-C16
22	q	307	CLA	C11-C12-C13-C14
22	q	307	CLA	C14-C13-C15-C16
22	V	302	CLA	C14-C13-C15-C16
22	Q	304	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	u	305	CLA	C11-C10-C8-C9
22	n	307	CLA	C6-C7-C8-C9
22	g	301	CLA	C11-C12-C13-C14
22	C	504	CLA	C14-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C14
22	C	506	CLA	C11-C12-C13-C14
22	C	507	CLA	C14-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	b	613	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C12-C13-C14
22	c	507	CLA	C6-C7-C8-C9
22	s	301	CLA	C6-C7-C8-C9
26	2	313	CHL	C6-C7-C8-C9
26	2	313	CHL	C14-C13-C15-C16
26	5	313	CHL	C14-C13-C15-C16
26	6	312	CHL	C6-C7-C8-C9
26	v	313	CHL	C6-C7-C8-C9
26	V	313	CHL	C6-C7-C8-C9
26	U	315	CHL	C6-C7-C8-C9
26	G	311	CHL	C14-C13-C15-C16
26	n	316	CHL	C14-C13-C15-C16
26	g	311	CHL	C14-C13-C15-C16
26	S	315	CHL	C6-C7-C8-C9
30	a	407	PHO	C11-C10-C8-C9
30	A	407	PHO	C11-C10-C8-C9
26	4	315	CHL	CBD-CGD-O2D-CED
26	u	318	CHL	CBD-CGD-O2D-CED
25	b	622	LHG	C12-C13-C14-C15
22	u	306	CLA	C3-C5-C6-C7
22	C	504	CLA	C3-C5-C6-C7
26	3	314	CHL	C3-C5-C6-C7
22	B	607	CLA	O1D-CGD-O2D-CED
22	A	405	CLA	C2A-CAA-CBA-CGA
22	4	304	CLA	C2A-CAA-CBA-CGA
22	v	301	CLA	C2A-CAA-CBA-CGA
22	V	301	CLA	C2A-CAA-CBA-CGA
22	Q	301	CLA	C2A-CAA-CBA-CGA
22	N	302	CLA	C2A-CAA-CBA-CGA
22	S	301	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	C2A-CAA-CBA-CGA
22	c	506	CLA	C2A-CAA-CBA-CGA
22	s	301	CLA	C2A-CAA-CBA-CGA
26	N	314	CHL	C2A-CAA-CBA-CGA
26	g	314	CHL	C2A-CAA-CBA-CGA
25	4	312	LHG	C29-C30-C31-C32
25	4	312	LHG	C31-C32-C33-C34
32	A	412	SQD	C10-C11-C12-C13
36	B	601	DGD	C3A-C4A-C5A-C6A
23	U	309	LUT	C11-C12-C13-C20
23	R	312	LUT	C7-C8-C9-C19
24	P	312	XAT	C7-C8-C9-C19
22	p	306	CLA	O1D-CGD-O2D-CED
26	s	313	CHL	O1D-CGD-O2D-CED
22	G	307	CLA	C5-C6-C7-C8
22	C	511	CLA	C5-C6-C7-C8
26	3	311	CHL	C10-C11-C12-C13
25	d	406	LHG	C17-C18-C19-C20
25	U	312	LHG	C13-C14-C15-C16
25	D	406	LHG	C10-C11-C12-C13
34	d	407	LMG	C15-C16-C17-C18
34	W	201	LMG	C32-C33-C34-C35
34	C	502	LMG	C19-C20-C21-C22
24	3	309	XAT	C31-C32-C33-C34
24	N	311	XAT	C7-C8-C9-C10
24	g	309	XAT	C27-C28-C29-C30
27	n	319	NEX	C11-C12-C13-C14
31	B	619	BCR	C11-C12-C13-C14
22	n	304	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	O1A-CGA-O2A-C1
25	D	406	LHG	O10-C23-O8-C6
26	r	614	CHL	O1A-CGA-O2A-C1
26	1	314	CHL	O1A-CGA-O2A-C1
26	V	318	CHL	O1A-CGA-O2A-C1
22	r	601	CLA	C1A-C2A-CAA-CBA
22	r	602	CLA	C1A-C2A-CAA-CBA
22	r	606	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	C1A-C2A-CAA-CBA
22	A	405	CLA	C1A-C2A-CAA-CBA
22	A	408	CLA	C1A-C2A-CAA-CBA
22	1	304	CLA	C1A-C2A-CAA-CBA
22	2	301	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	2	304	CLA	C1A-C2A-CAA-CBA
22	2	305	CLA	C1A-C2A-CAA-CBA
22	4	304	CLA	C1A-C2A-CAA-CBA
22	5	301	CLA	C1A-C2A-CAA-CBA
22	5	304	CLA	C1A-C2A-CAA-CBA
22	p	305	CLA	C1A-C2A-CAA-CBA
22	q	301	CLA	C1A-C2A-CAA-CBA
22	q	308	CLA	C1A-C2A-CAA-CBA
22	P	305	CLA	C1A-C2A-CAA-CBA
22	Q	301	CLA	C1A-C2A-CAA-CBA
22	Q	305	CLA	C1A-C2A-CAA-CBA
22	Q	308	CLA	C1A-C2A-CAA-CBA
22	N	304	CLA	C1A-C2A-CAA-CBA
22	N	305	CLA	C1A-C2A-CAA-CBA
22	G	301	CLA	C1A-C2A-CAA-CBA
22	G	304	CLA	C1A-C2A-CAA-CBA
22	n	304	CLA	C1A-C2A-CAA-CBA
22	n	305	CLA	C1A-C2A-CAA-CBA
22	g	303	CLA	C1A-C2A-CAA-CBA
22	R	303	CLA	C1A-C2A-CAA-CBA
22	R	307	CLA	C1A-C2A-CAA-CBA
22	S	305	CLA	C1A-C2A-CAA-CBA
22	C	510	CLA	C1A-C2A-CAA-CBA
22	C	514	CLA	C1A-C2A-CAA-CBA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	b	607	CLA	C1A-C2A-CAA-CBA
22	c	509	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	s	305	CLA	C1A-C2A-CAA-CBA
26	r	614	CHL	C1A-C2A-CAA-CBA
26	1	314	CHL	C1A-C2A-CAA-CBA
26	1	316	CHL	C1A-C2A-CAA-CBA
26	1	317	CHL	C1A-C2A-CAA-CBA
26	1	318	CHL	C1A-C2A-CAA-CBA
26	2	316	CHL	C1A-C2A-CAA-CBA
26	2	318	CHL	C1A-C2A-CAA-CBA
26	3	312	CHL	C1A-C2A-CAA-CBA
26	3	313	CHL	C1A-C2A-CAA-CBA
26	3	315	CHL	C1A-C2A-CAA-CBA
26	4	314	CHL	C1A-C2A-CAA-CBA
26	4	317	CHL	C1A-C2A-CAA-CBA
26	5	316	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	5	318	CHL	C1A-C2A-CAA-CBA
26	6	313	CHL	C1A-C2A-CAA-CBA
26	6	314	CHL	C1A-C2A-CAA-CBA
26	v	314	CHL	C1A-C2A-CAA-CBA
26	p	318	CHL	C1A-C2A-CAA-CBA
26	V	317	CHL	C1A-C2A-CAA-CBA
26	U	316	CHL	C1A-C2A-CAA-CBA
26	U	317	CHL	C1A-C2A-CAA-CBA
26	N	314	CHL	C1A-C2A-CAA-CBA
26	u	314	CHL	C1A-C2A-CAA-CBA
26	u	316	CHL	C1A-C2A-CAA-CBA
26	u	317	CHL	C1A-C2A-CAA-CBA
26	u	318	CHL	C1A-C2A-CAA-CBA
26	n	314	CHL	C1A-C2A-CAA-CBA
26	g	311	CHL	C1A-C2A-CAA-CBA
26	g	312	CHL	C1A-C2A-CAA-CBA
26	g	313	CHL	C1A-C2A-CAA-CBA
26	g	315	CHL	C1A-C2A-CAA-CBA
26	R	315	CHL	C1A-C2A-CAA-CBA
22	A	408	CLA	C11-C12-C13-C15
22	3	306	CLA	C11-C12-C13-C15
22	N	301	CLA	C16-C17-C18-C20
22	N	302	CLA	C16-C17-C18-C19
22	u	307	CLA	C16-C17-C18-C19
22	n	301	CLA	C16-C17-C18-C20
26	p	314	CHL	C16-C17-C18-C19
26	V	318	CHL	C16-C17-C18-C19
26	P	319	CHL	C16-C17-C18-C19
25	b	623	LHG	O9-C7-O7-C5
34	C	502	LMG	O9-C10-O7-C8
34	c	501	LMG	O9-C10-O7-C8
25	d	406	LHG	C8-C7-O7-C5
25	P	313	LHG	C8-C7-O7-C5
32	a	413	SQD	C17-C18-C19-C20
34	c	501	LMG	C19-C20-C21-C22
36	B	601	DGD	C9A-CAA-CBA-CCA
24	4	311	XAT	C29-C30-C31-C32
31	x	202	BCR	C9-C10-C11-C12
31	C	517	BCR	C15-C16-C17-C18
31	C	517	BCR	C19-C20-C21-C22
31	c	515	BCR	C19-C20-C21-C22
22	V	305	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C8-C10-C11-C12
25	d	405	LHG	C3-O3-P-O6
25	d	406	LHG	C4-O6-P-O3
25	l	101	LHG	C4-O6-P-O3
25	L	101	LHG	C4-O6-P-O3
25	2	312	LHG	C4-O6-P-O3
25	4	312	LHG	C4-O6-P-O3
25	5	312	LHG	C4-O6-P-O3
25	v	312	LHG	C3-O3-P-O6
25	B	623	LHG	C3-O3-P-O6
25	D	406	LHG	C3-O3-P-O6
25	D	407	LHG	C4-O6-P-O3
25	b	623	LHG	C3-O3-P-O6
25	s	312	LHG	C16-C17-C18-C19
34	C	521	LMG	C10-C11-C12-C13
36	c	518	DGD	C1A-C2A-C3A-C4A
36	c	518	DGD	C1B-C2B-C3B-C4B
22	g	306	CLA	C3-C5-C6-C7
22	B	614	CLA	C3-C5-C6-C7
26	v	314	CHL	O1D-CGD-O2D-CED
22	r	609	CLA	O1A-CGA-O2A-C1
22	P	303	CLA	C5-C6-C7-C8
22	B	602	CLA	C15-C16-C17-C18
22	c	510	CLA	C5-C6-C7-C8
26	6	316	CHL	C8-C10-C11-C12
22	u	303	CLA	CBA-CGA-O2A-C1
22	B	606	CLA	CBA-CGA-O2A-C1
25	S	312	LHG	C24-C23-O8-C6
25	D	406	LHG	O6-C4-C5-C6
22	5	305	CLA	O1D-CGD-O2D-CED
25	N	312	LHG	C9-C10-C11-C12
34	w	201	LMG	C30-C31-C32-C33
36	a	416	DGD	C1A-C2A-C3A-C4A
36	C	520	DGD	C1B-C2B-C3B-C4B
25	d	406	LHG	C33-C34-C35-C36
36	c	519	DGD	C7B-C8B-C9B-CAB
36	A	414	DGD	O6E-C5E-C6E-O5E
22	C	512	CLA	C5-C6-C7-C8
34	W	201	LMG	C30-C31-C32-C33
26	r	614	CHL	O1D-CGD-O2D-CED
32	l	102	SQD	C29-C30-C31-C32
26	6	312	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	3	310	LHG	C24-C25-C26-C27
36	a	416	DGD	C6A-C7A-C8A-C9A
36	b	601	DGD	C4D-C5D-C6D-O5D
25	s	312	LHG	C24-C23-O8-C6
36	a	416	DGD	O6E-C5E-C6E-O5E
25	d	406	LHG	O9-C7-O7-C5
34	D	408	LMG	O9-C10-O7-C8
34	C	502	LMG	C14-C15-C16-C17
34	c	501	LMG	C14-C15-C16-C17
22	3	305	CLA	C5-C6-C7-C8
22	p	305	CLA	C8-C10-C11-C12
26	6	315	CHL	C15-C16-C17-C18
36	B	601	DGD	O6D-C5D-C6D-O5D
34	w	201	LMG	C32-C33-C34-C35
25	D	407	LHG	C8-C7-O7-C5
22	1	306	CLA	O1A-CGA-O2A-C1
22	5	303	CLA	O1A-CGA-O2A-C1
22	6	309	CLA	O1A-CGA-O2A-C1
26	3	313	CHL	O1A-CGA-O2A-C1
26	P	317	CHL	O1A-CGA-O2A-C1
26	Q	315	CHL	O1A-CGA-O2A-C1
26	u	317	CHL	O1A-CGA-O2A-C1
25	d	406	LHG	C11-C12-C13-C14
25	G	310	LHG	C24-C25-C26-C27
36	A	414	DGD	C2B-C3B-C4B-C5B
22	6	302	CLA	C15-C16-C17-C18
22	v	303	CLA	C2A-CAA-CBA-CGA
22	V	302	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
26	R	315	CHL	O1D-CGD-O2D-CED
22	N	305	CLA	C3-C5-C6-C7
25	A	413	LHG	C4-C5-C6-O8
25	6	311	LHG	C24-C25-C26-C27
25	v	312	LHG	C4-C5-C6-O8
25	Q	310	LHG	C4-C5-C6-O8
25	R	314	LHG	C4-C5-C6-O8
32	m	101	SQD	C44-C45-C46-O48
32	A	412	SQD	O6-C44-C45-C46
32	A	412	SQD	C11-C12-C13-C14
32	M	101	SQD	C44-C45-C46-O48
34	w	201	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	C	502	LMG	O1-C7-C8-C9
34	C	521	LMG	O1-C7-C8-C9
34	b	621	LMG	C7-C8-C9-O8
34	c	501	LMG	O1-C7-C8-C9
34	c	501	LMG	C7-C8-C9-O8
34	c	520	LMG	O1-C7-C8-C9
36	C	519	DGD	O1G-C1G-C2G-C3G
36	C	520	DGD	C5B-C6B-C7B-C8B
36	c	517	DGD	O1G-C1G-C2G-C3G
36	c	518	DGD	C7B-C8B-C9B-CAB
22	5	302	CLA	C13-C15-C16-C17
22	b	612	CLA	C10-C11-C12-C13
26	g	315	CHL	C13-C15-C16-C17
25	q	310	LHG	C24-C25-C26-C27
25	R	314	LHG	C28-C29-C30-C31
25	D	406	LHG	C15-C16-C17-C18
26	6	315	CHL	O1A-CGA-O2A-C1
26	6	317	CHL	O1A-CGA-O2A-C1
34	C	502	LMG	C8-C7-O1-C1
34	c	501	LMG	C8-C7-O1-C1
36	C	520	DGD	C2G-C3G-O3G-C1D
36	c	518	DGD	C2G-C3G-O3G-C1D
25	1	312	LHG	C11-C12-C13-C14
36	C	520	DGD	CDA-CEA-CFA-CGA
36	b	601	DGD	CCA-CDA-CEA-CFA
22	U	306	CLA	CBD-CGD-O2D-CED
22	P	308	CLA	C8-C10-C11-C12
22	c	505	CLA	C5-C6-C7-C8
25	D	406	LHG	C35-C36-C37-C38
34	b	624	LMG	O6-C5-C6-O5
25	c	522	LHG	C23-C24-C25-C26
25	s	312	LHG	C25-C26-C27-C28
25	s	312	LHG	C35-C36-C37-C38
34	D	408	LMG	C15-C16-C17-C18
36	a	416	DGD	C2B-C3B-C4B-C5B
22	v	306	CLA	C3-C5-C6-C7
22	N	305	CLA	C11-C12-C13-C15
22	B	611	CLA	C16-C17-C18-C20
30	D	401	PHO	C10-C11-C12-C13
25	D	407	LHG	C11-C12-C13-C14
34	D	408	LMG	O6-C5-C6-O5
36	C	519	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
36	c	517	DGD	O6E-C5E-C6E-O5E
25	r	613	LHG	O1-C1-C2-O2
25	D	406	LHG	O1-C1-C2-O2
25	c	523	LHG	O1-C1-C2-O2
22	5	308	CLA	O2A-C1-C2-C3
22	U	308	CLA	O2A-C1-C2-C3
22	u	308	CLA	O2A-C1-C2-C3
34	c	520	LMG	C35-C36-C37-C38
36	A	414	DGD	C6A-C7A-C8A-C9A
22	q	305	CLA	C8-C10-C11-C12
25	p	313	LHG	C23-C24-C25-C26
34	A	411	LMG	C28-C29-C30-C31
36	C	519	DGD	C1B-C2B-C3B-C4B
36	b	601	DGD	C1A-C2A-C3A-C4A
36	c	517	DGD	C1B-C2B-C3B-C4B
22	G	304	CLA	C16-C17-C18-C19
25	d	406	LHG	C35-C36-C37-C38
22	Q	306	CLA	C8-C10-C11-C12
30	d	401	PHO	C10-C11-C12-C13
34	d	407	LMG	O6-C5-C6-O5
34	B	624	LMG	O6-C5-C6-O5
22	Q	302	CLA	C4-C3-C5-C6
22	N	302	CLA	C4-C3-C5-C6
26	2	317	CHL	C4-C3-C5-C6
26	V	316	CHL	C4-C3-C5-C6
26	n	318	CHL	C4-C3-C5-C6
26	R	317	CHL	C4-C3-C5-C6
33	d	404	PL9	C15-C14-C16-C17
33	D	405	PL9	C15-C14-C16-C17
26	V	316	CHL	C2-C3-C5-C6
33	d	404	PL9	C13-C14-C16-C17
25	g	310	LHG	C7-C8-C9-C10
22	a	408	CLA	C11-C12-C13-C14
22	q	301	CLA	C16-C17-C18-C20
22	q	305	CLA	C11-C12-C13-C14
26	G	315	CHL	C16-C17-C18-C19
26	G	316	CHL	C11-C12-C13-C14
22	r	604	CLA	CBA-CGA-O2A-C1
22	5	306	CLA	CBA-CGA-O2A-C1
22	Q	306	CLA	CBA-CGA-O2A-C1
22	B	605	CLA	CBA-CGA-O2A-C1
22	b	605	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	a	415	LHG	C24-C23-O8-C6
25	A	413	LHG	C24-C23-O8-C6
26	3	316	CHL	CBA-CGA-O2A-C1
26	P	316	CHL	CBA-CGA-O2A-C1
26	n	315	CHL	CBA-CGA-O2A-C1
26	g	312	CHL	CBD-CGD-O2D-CED
22	n	302	CLA	C15-C16-C17-C18
22	C	507	CLA	C13-C15-C16-C17
22	C	507	CLA	C15-C16-C17-C18
22	X	202	CLA	C15-C16-C17-C18
22	b	602	CLA	C5-C6-C7-C8
22	b	604	CLA	C15-C16-C17-C18
26	U	315	CHL	C8-C10-C11-C12
25	S	312	LHG	C25-C26-C27-C28
36	c	519	DGD	CBB-CCB-CDB-CEB
32	l	102	SQD	C46-C45-O47-C7
32	L	102	SQD	C46-C45-O47-C7
22	s	301	CLA	O1D-CGD-O2D-CED
22	a	405	CLA	C2A-CAA-CBA-CGA
22	q	301	CLA	C13-C15-C16-C17
22	c	506	CLA	C13-C15-C16-C17
26	Q	311	CHL	C10-C11-C12-C13
26	n	318	CHL	C13-C15-C16-C17
22	4	305	CLA	C2-C1-O2A-CGA
22	p	306	CLA	C2-C1-O2A-CGA
26	r	616	CHL	C2-C1-O2A-CGA
26	R	317	CHL	C2-C1-O2A-CGA
25	d	405	LHG	C10-C11-C12-C13
36	c	518	DGD	C8A-C9A-CAA-CBA
22	G	301	CLA	O1D-CGD-O2D-CED
26	U	314	CHL	O1D-CGD-O2D-CED
26	S	313	CHL	O1D-CGD-O2D-CED
22	C	504	CLA	C10-C11-C12-C13
22	C	506	CLA	C5-C6-C7-C8
25	B	623	LHG	C5-C4-O6-P
25	D	407	LHG	C19-C20-C21-C22
34	C	521	LMG	C11-C12-C13-C14
22	6	307	CLA	CBA-CGA-O2A-C1
22	R	305	CLA	CBA-CGA-O2A-C1
26	v	318	CHL	CBA-CGA-O2A-C1
26	U	316	CHL	CBA-CGA-O2A-C1
26	R	317	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	4	312	LHG	O6-C4-C5-O7
22	b	611	CLA	C16-C17-C18-C19
26	V	316	CHL	C16-C17-C18-C20
26	g	316	CHL	C11-C12-C13-C15
26	1	318	CHL	CBD-CGD-O2D-CED
25	B	622	LHG	C27-C28-C29-C30
34	c	501	LMG	C32-C33-C34-C35
26	v	316	CHL	C13-C15-C16-C17
26	q	314	CHL	C10-C11-C12-C13
22	r	610	CLA	O1D-CGD-O2D-CED
26	v	318	CHL	O1D-CGD-O2D-CED
22	G	307	CLA	O1A-CGA-O2A-C1
22	g	307	CLA	O1A-CGA-O2A-C1
22	b	606	CLA	O1A-CGA-O2A-C1
25	S	312	LHG	O10-C23-O8-C6
37	E	101	HEM	C3D-CAD-CBD-CGD
32	C	501	SQD	C30-C31-C32-C33
34	B	624	LMG	C28-C29-C30-C31
34	b	624	LMG	C28-C29-C30-C31
22	1	306	CLA	C10-C11-C12-C13
22	6	307	CLA	C8-C10-C11-C12
22	N	301	CLA	C5-C6-C7-C8
22	B	606	CLA	C5-C6-C7-C8
22	b	614	CLA	C10-C11-C12-C13
22	b	617	CLA	C10-C11-C12-C13
26	2	313	CHL	C5-C6-C7-C8
25	S	312	LHG	C35-C36-C37-C38
25	R	314	LHG	O7-C5-C6-O8
34	d	407	LMG	O1-C7-C8-O7
34	D	408	LMG	O1-C7-C8-O7
25	d	406	LHG	C19-C20-C21-C22
25	5	312	LHG	C13-C14-C15-C16
25	b	622	LHG	C27-C28-C29-C30
32	C	501	SQD	C24-C25-C26-C27
25	V	312	LHG	O9-C7-O7-C5
25	D	407	LHG	O9-C7-O7-C5
22	A	405	CLA	C13-C15-C16-C17
22	N	302	CLA	C15-C16-C17-C18
22	B	602	CLA	C5-C6-C7-C8
22	c	505	CLA	C15-C16-C17-C18
26	p	319	CHL	C8-C10-C11-C12
22	B	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	O1A-CGA-O2A-C1
25	s	312	LHG	O10-C23-O8-C6
26	3	316	CHL	O1A-CGA-O2A-C1
22	n	302	CLA	C16-C17-C18-C19
30	d	401	PHO	CHA-CBD-CGD-O1D
30	d	401	PHO	CHA-CBD-CGD-O2D
30	D	401	PHO	CHA-CBD-CGD-O1D
30	D	401	PHO	CHA-CBD-CGD-O2D
26	4	317	CHL	O1D-CGD-O2D-CED
25	C	524	LHG	C19-C20-C21-C22
34	b	621	LMG	C22-C23-C24-C25
36	c	518	DGD	C3A-C4A-C5A-C6A
26	r	616	CHL	C4-C3-C5-C6
25	U	312	LHG	C12-C13-C14-C15
36	B	601	DGD	C4D-C5D-C6D-O5D
22	r	606	CLA	C11-C10-C8-C7
22	a	404	CLA	C11-C12-C13-C15
22	d	402	CLA	C11-C12-C13-C15
22	A	404	CLA	C11-C12-C13-C15
22	3	301	CLA	C11-C12-C13-C15
22	3	306	CLA	C6-C7-C8-C10
22	5	302	CLA	C11-C10-C8-C7
22	5	304	CLA	C6-C7-C8-C10
22	6	302	CLA	C11-C12-C13-C15
22	6	305	CLA	C11-C12-C13-C15
22	v	305	CLA	C6-C7-C8-C10
22	p	302	CLA	C11-C12-C13-C15
22	q	301	CLA	C6-C7-C8-C10
22	q	304	CLA	C11-C12-C13-C15
22	V	301	CLA	C11-C12-C13-C15
22	V	302	CLA	C12-C13-C15-C16
22	Q	304	CLA	C12-C13-C15-C16
22	Q	305	CLA	C11-C10-C8-C7
22	N	304	CLA	C11-C10-C8-C7
22	N	307	CLA	C6-C7-C8-C10
22	n	304	CLA	C12-C13-C15-C16
22	n	306	CLA	C11-C10-C8-C7
22	g	301	CLA	C11-C12-C13-C15
22	g	306	CLA	C11-C10-C8-C7
22	R	307	CLA	C11-C10-C8-C7
22	S	301	CLA	C6-C7-C8-C10
22	S	301	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C6-C7-C8-C10
22	C	507	CLA	C6-C7-C8-C10
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C12-C13-C15
22	B	602	CLA	C12-C13-C15-C16
22	B	603	CLA	C12-C13-C15-C16
22	B	607	CLA	C6-C7-C8-C10
22	B	612	CLA	C6-C7-C8-C10
22	B	613	CLA	C11-C12-C13-C15
22	B	616	CLA	C11-C12-C13-C15
22	B	617	CLA	C12-C13-C15-C16
22	D	403	CLA	C11-C12-C13-C15
22	b	607	CLA	C6-C7-C8-C10
22	b	612	CLA	C6-C7-C8-C10
22	b	613	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C10-C8-C7
22	b	616	CLA	C6-C7-C8-C10
22	c	503	CLA	C6-C7-C8-C10
22	c	503	CLA	C11-C10-C8-C7
22	c	503	CLA	C12-C13-C15-C16
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C12-C13-C15-C16
22	c	507	CLA	C6-C7-C8-C10
22	s	301	CLA	C6-C7-C8-C10
26	1	313	CHL	C11-C12-C13-C15
26	1	318	CHL	C12-C13-C15-C16
26	2	313	CHL	C12-C13-C15-C16
26	2	316	CHL	C12-C13-C15-C16
26	2	317	CHL	C2-C3-C5-C6
26	3	311	CHL	C6-C7-C8-C10
26	4	316	CHL	C6-C7-C8-C10
26	4	317	CHL	C12-C13-C15-C16
26	5	313	CHL	C12-C13-C15-C16
26	5	316	CHL	C12-C13-C15-C16
26	5	317	CHL	C11-C10-C8-C7
26	6	315	CHL	C12-C13-C15-C16
26	v	313	CHL	C6-C7-C8-C10
26	v	313	CHL	C11-C12-C13-C15
26	v	316	CHL	C12-C13-C15-C16
26	v	317	CHL	C11-C10-C8-C7
26	p	320	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	q	311	CHL	C12-C13-C15-C16
26	q	314	CHL	C12-C13-C15-C16
26	V	313	CHL	C6-C7-C8-C10
26	V	313	CHL	C12-C13-C15-C16
26	P	314	CHL	C12-C13-C15-C16
26	Q	311	CHL	C12-C13-C15-C16
26	Q	314	CHL	C11-C10-C8-C7
26	U	317	CHL	C12-C13-C15-C16
26	N	313	CHL	C11-C12-C13-C15
26	N	316	CHL	C6-C7-C8-C10
26	G	311	CHL	C11-C12-C13-C15
26	G	314	CHL	C12-C13-C15-C16
26	G	315	CHL	C12-C13-C15-C16
26	u	313	CHL	C11-C12-C13-C15
26	u	316	CHL	C12-C13-C15-C16
26	u	318	CHL	C11-C12-C13-C15
26	n	313	CHL	C11-C12-C13-C15
26	n	317	CHL	C6-C7-C8-C10
26	n	318	CHL	C2-C3-C5-C6
26	g	311	CHL	C12-C13-C15-C16
26	R	317	CHL	C2-C3-C5-C6
30	a	407	PHO	C11-C10-C8-C7
30	A	407	PHO	C11-C10-C8-C7
33	D	405	PL9	C13-C14-C16-C17
25	b	623	LHG	O7-C7-C8-C9
22	3	306	CLA	C3-C5-C6-C7
34	B	621	LMG	C19-C20-C21-C22
22	r	606	CLA	C14-C13-C15-C16
22	a	404	CLA	C11-C12-C13-C14
22	d	402	CLA	C11-C12-C13-C14
22	3	301	CLA	C6-C7-C8-C9
22	3	301	CLA	C11-C12-C13-C14
22	3	306	CLA	C6-C7-C8-C9
22	5	302	CLA	C11-C10-C8-C9
22	5	307	CLA	C11-C10-C8-C9
22	6	302	CLA	C11-C12-C13-C14
22	6	303	CLA	C11-C10-C8-C9
22	6	305	CLA	C11-C12-C13-C14
22	v	306	CLA	C11-C10-C8-C9
22	q	301	CLA	C11-C12-C13-C14
22	q	304	CLA	C11-C12-C13-C14
22	V	301	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	P	302	CLA	C11-C12-C13-C14
22	P	305	CLA	C6-C7-C8-C9
22	Q	304	CLA	C11-C12-C13-C14
22	Q	304	CLA	C14-C13-C15-C16
22	Q	306	CLA	C6-C7-C8-C9
22	N	302	CLA	C14-C13-C15-C16
22	N	307	CLA	C6-C7-C8-C9
22	G	301	CLA	C11-C12-C13-C14
22	G	306	CLA	C11-C10-C8-C9
22	G	307	CLA	C14-C13-C15-C16
22	g	306	CLA	C11-C10-C8-C9
22	g	307	CLA	C14-C13-C15-C16
22	R	307	CLA	C14-C13-C15-C16
22	S	301	CLA	C6-C7-C8-C9
22	C	510	CLA	C11-C12-C13-C14
22	C	512	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	613	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C12-C13-C14
22	c	503	CLA	C14-C13-C15-C16
22	c	506	CLA	C14-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C14
26	1	313	CHL	C11-C12-C13-C14
26	1	318	CHL	C6-C7-C8-C9
26	2	313	CHL	C11-C12-C13-C14
26	2	317	CHL	C11-C12-C13-C14
26	2	318	CHL	C6-C7-C8-C9
26	2	318	CHL	C11-C10-C8-C9
26	3	311	CHL	C6-C7-C8-C9
26	4	313	CHL	C11-C12-C13-C14
26	v	313	CHL	C11-C12-C13-C14
26	p	314	CHL	C11-C12-C13-C14
26	p	320	CHL	C14-C13-C15-C16
26	q	311	CHL	C14-C13-C15-C16
26	q	314	CHL	C14-C13-C15-C16
26	V	313	CHL	C14-C13-C15-C16
26	P	314	CHL	C14-C13-C15-C16
26	Q	311	CHL	C14-C13-C15-C16
26	U	313	CHL	C11-C12-C13-C14
26	U	315	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	U	319	CHL	C14-C13-C15-C16
26	u	313	CHL	C11-C12-C13-C14
26	n	313	CHL	C11-C12-C13-C14
26	n	316	CHL	C11-C10-C8-C9
26	s	315	CHL	C6-C7-C8-C9
25	C	523	LHG	C23-C24-C25-C26
25	l	101	LHG	C30-C31-C32-C33
25	6	311	LHG	C11-C12-C13-C14
25	C	523	LHG	C16-C17-C18-C19
22	r	603	CLA	CBA-CGA-O2A-C1
22	3	306	CLA	CBA-CGA-O2A-C1
22	R	306	CLA	CBA-CGA-O2A-C1
26	r	616	CHL	CBA-CGA-O2A-C1
26	3	315	CHL	CBA-CGA-O2A-C1
22	R	307	CLA	C8-C10-C11-C12
26	v	318	CHL	C8-C10-C11-C12
22	a	404	CLA	C2A-CAA-CBA-CGA
22	1	301	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	O1D-CGD-O2D-CED
26	1	316	CHL	O1D-CGD-O2D-CED
22	u	303	CLA	O1A-CGA-O2A-C1
22	b	605	CLA	O1A-CGA-O2A-C1
31	C	517	BCR	C11-C12-C13-C35
22	V	302	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
26	v	316	CHL	C16-C17-C18-C20
25	4	312	LHG	O1-C1-C2-C3
31	b	620	BCR	C17-C18-C19-C20
34	C	502	LMG	C32-C33-C34-C35
22	U	306	CLA	C3-C5-C6-C7
22	b	605	CLA	O1D-CGD-O2D-CED
22	n	304	CLA	C15-C16-C17-C18
25	2	312	LHG	C28-C29-C30-C31
36	a	416	DGD	C8B-C9B-CAB-CBB
22	A	406	CLA	CBA-CGA-O2A-C1
22	G	305	CLA	CBA-CGA-O2A-C1
25	c	522	LHG	C24-C23-O8-C6
26	v	316	CHL	CBA-CGA-O2A-C1
26	p	316	CHL	CBA-CGA-O2A-C1
34	C	502	LMG	C22-C23-C24-C25
34	b	624	LMG	C24-C25-C26-C27
22	B	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	U	317	CHL	C8-C10-C11-C12
22	B	605	CLA	O1D-CGD-O2D-CED
36	A	414	DGD	CAB-CBB-CCB-CDB
22	d	402	CLA	CBD-CGD-O2D-CED
34	B	621	LMG	C30-C31-C32-C33
22	B	602	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C19
22	a	404	CLA	C13-C15-C16-C17
22	A	408	CLA	C8-C10-C11-C12
22	6	305	CLA	C8-C10-C11-C12
22	B	614	CLA	C10-C11-C12-C13
26	g	315	CHL	C5-C6-C7-C8
25	a	415	LHG	O6-C4-C5-C6
25	d	405	LHG	O6-C4-C5-C6
25	l	101	LHG	O6-C4-C5-C6
25	A	413	LHG	O6-C4-C5-C6
25	L	101	LHG	O6-C4-C5-C6
25	d	405	LHG	C25-C26-C27-C28
34	B	624	LMG	C24-C25-C26-C27
36	B	601	DGD	C7B-C8B-C9B-CAB
34	a	412	LMG	C28-C29-C30-C31
36	C	520	DGD	C1A-C2A-C3A-C4A
34	D	408	LMG	C33-C34-C35-C36
34	c	520	LMG	C11-C12-C13-C14
25	u	312	LHG	C24-C23-O8-C6
26	4	317	CHL	CBA-CGA-O2A-C1
36	C	520	DGD	C2A-C1A-O1G-C1G
22	1	308	CLA	CBD-CGD-O2D-CED
22	3	305	CLA	C10-C11-C12-C13
22	B	611	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
34	c	520	LMG	O6-C5-C6-O5
22	c	511	CLA	O1D-CGD-O2D-CED
26	3	313	CHL	O1D-CGD-O2D-CED
22	C	514	CLA	C4-C3-C5-C6
26	p	320	CHL	C4-C3-C5-C6
26	Q	314	CHL	C4-C3-C5-C6
26	g	314	CHL	C4-C3-C5-C6
22	Q	302	CLA	C2-C3-C5-C6
26	r	616	CHL	C2-C3-C5-C6
26	Q	314	CHL	C2-C3-C5-C6
25	G	310	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	R	304	CLA	C8-C10-C11-C12
25	P	313	LHG	O9-C7-O7-C5
22	S	301	CLA	C14-C13-C15-C16
26	P	316	CHL	O1A-CGA-O2A-C1
25	C	522	LHG	C25-C26-C27-C28
22	N	304	CLA	C16-C17-C18-C20
30	D	401	PHO	C16-C17-C18-C19
34	B	624	LMG	C32-C33-C34-C35
26	n	313	CHL	C8-C10-C11-C12
22	a	404	CLA	CBA-CGA-O2A-C1
22	3	303	CLA	CBA-CGA-O2A-C1
25	N	312	LHG	C24-C23-O8-C6
26	V	316	CHL	CBA-CGA-O2A-C1
26	U	317	CHL	CBA-CGA-O2A-C1
26	u	318	CHL	CBA-CGA-O2A-C1
34	B	624	LMG	C29-C28-O8-C9
36	C	519	DGD	O6D-C5D-C6D-O5D
34	b	621	LMG	C29-C30-C31-C32
25	a	415	LHG	C5-C4-O6-P
25	l	101	LHG	C2-C3-O3-P
25	A	413	LHG	C5-C4-O6-P
25	L	101	LHG	C2-C3-O3-P
25	b	623	LHG	C5-C4-O6-P
25	c	522	LHG	C2-C3-O3-P
22	Q	306	CLA	O1A-CGA-O2A-C1
26	n	315	CHL	O1A-CGA-O2A-C1
22	N	308	CLA	C3A-C2A-CAA-CBA
26	6	314	CHL	C3A-C2A-CAA-CBA
26	P	319	CHL	C3A-C2A-CAA-CBA
26	g	311	CHL	C3A-C2A-CAA-CBA
26	g	316	CHL	C3A-C2A-CAA-CBA
26	S	316	CHL	C3A-C2A-CAA-CBA
26	s	316	CHL	C3A-C2A-CAA-CBA
26	U	315	CHL	C10-C11-C12-C13
25	L	101	LHG	C16-C17-C18-C19
32	m	101	SQD	C12-C13-C14-C15
24	r	612	XAT	C29-C30-C31-C32
24	4	311	XAT	C13-C14-C15-C35
31	X	201	BCR	C9-C10-C11-C12
31	b	619	BCR	C15-C16-C17-C18
25	d	406	LHG	C12-C13-C14-C15
25	U	312	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	g	310	LHG	C9-C10-C11-C12
25	D	407	LHG	C18-C19-C20-C21
22	P	305	CLA	C15-C16-C17-C18
22	C	514	CLA	C5-C6-C7-C8
22	c	507	CLA	C15-C16-C17-C18
26	6	316	CHL	C5-C6-C7-C8
26	v	313	CHL	C5-C6-C7-C8
26	N	316	CHL	C15-C16-C17-C18
26	U	316	CHL	O1A-CGA-O2A-C1
25	G	310	LHG	C33-C34-C35-C36
36	C	520	DGD	C8A-C9A-CAA-CBA
22	q	301	CLA	C16-C17-C18-C19
22	U	307	CLA	C16-C17-C18-C20
30	D	401	PHO	C16-C17-C18-C20
37	e	101	HEM	C3D-CAD-CBD-CGD
22	A	404	CLA	CBA-CGA-O2A-C1
22	Q	307	CLA	CBA-CGA-O2A-C1
25	C	523	LHG	C24-C23-O8-C6
25	N	312	LHG	C29-C30-C31-C32
25	n	312	LHG	C12-C13-C14-C15
25	C	524	LHG	C26-C27-C28-C29
22	b	606	CLA	C5-C6-C7-C8
22	c	510	CLA	C15-C16-C17-C18
22	c	514	CLA	C10-C11-C12-C13
26	p	318	CHL	C10-C11-C12-C13
26	V	318	CHL	C8-C10-C11-C12
25	a	415	LHG	C4-C5-C6-O8
25	l	101	LHG	C4-C5-C6-O8
25	L	101	LHG	C4-C5-C6-O8
25	3	310	LHG	C4-C5-C6-O8
25	V	312	LHG	C4-C5-C6-O8
25	B	623	LHG	C4-C5-C6-O8
25	b	623	LHG	C4-C5-C6-O8
32	a	413	SQD	O6-C44-C45-C46
32	l	102	SQD	C44-C45-C46-O48
32	L	102	SQD	C44-C45-C46-O48
34	d	407	LMG	O1-C7-C8-C9
34	d	407	LMG	C7-C8-C9-O8
34	w	201	LMG	O1-C7-C8-C9
34	W	201	LMG	C7-C8-C9-O8
34	C	502	LMG	C7-C8-C9-O8
34	C	521	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
34	B	624	LMG	O1-C7-C8-C9
34	D	408	LMG	O1-C7-C8-C9
34	D	408	LMG	C7-C8-C9-O8
34	b	624	LMG	O1-C7-C8-C9
36	a	416	DGD	O1G-C1G-C2G-C3G
36	A	414	DGD	O1G-C1G-C2G-C3G
36	C	520	DGD	C3A-C4A-C5A-C6A
22	6	307	CLA	O1A-CGA-O2A-C1
25	a	415	LHG	O10-C23-O8-C6
25	A	413	LHG	O10-C23-O8-C6
26	6	312	CHL	O1D-CGD-O2D-CED
34	B	621	LMG	C15-C16-C17-C18
36	c	518	DGD	CDB-CEB-CFB-CGB
36	c	517	DGD	O6D-C5D-C6D-O5D
22	b	602	CLA	C3-C5-C6-C7
22	5	306	CLA	O1A-CGA-O2A-C1
22	C	504	CLA	C5-C6-C7-C8
26	N	317	CHL	C13-C15-C16-C17
22	g	304	CLA	C4-C3-C5-C6
22	D	403	CLA	C4-C3-C5-C6
26	U	313	CHL	C4-C3-C5-C6
22	c	507	CLA	C16-C17-C18-C19
26	U	317	CHL	O1D-CGD-O2D-CED
25	l	101	LHG	C16-C17-C18-C19
34	B	621	LMG	C21-C22-C23-C24
22	g	304	CLA	C16-C17-C18-C19
36	a	416	DGD	C9B-CAB-CBB-CCB
26	1	315	CHL	O1D-CGD-O2D-CED
26	V	318	CHL	O1D-CGD-O2D-CED
26	p	314	CHL	C8-C10-C11-C12
25	3	310	LHG	C4-O6-P-O3
25	R	314	LHG	C4-O6-P-O3
26	r	615	CHL	C3C-C2C-CMC-OMC
26	1	315	CHL	C3C-C2C-CMC-OMC
26	1	316	CHL	C3C-C2C-CMC-OMC
26	1	318	CHL	C3C-C2C-CMC-OMC
26	3	313	CHL	C3C-C2C-CMC-OMC
26	4	314	CHL	C3C-C2C-CMC-OMC
26	4	315	CHL	C3C-C2C-CMC-OMC
26	5	313	CHL	C3C-C2C-CMC-OMC
26	6	314	CHL	C3C-C2C-CMC-OMC
26	v	315	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	p	314	CHL	C3C-C2C-CMC-OMC
26	p	316	CHL	C3C-C2C-CMC-OMC
26	p	318	CHL	C3C-C2C-CMC-OMC
26	q	313	CHL	C3C-C2C-CMC-OMC
26	V	315	CHL	C3C-C2C-CMC-OMC
26	P	314	CHL	C3C-C2C-CMC-OMC
26	P	316	CHL	C3C-C2C-CMC-OMC
26	Q	313	CHL	C3C-C2C-CMC-OMC
26	U	313	CHL	C3C-C2C-CMC-OMC
26	U	314	CHL	C3C-C2C-CMC-OMC
26	N	315	CHL	C3C-C2C-CMC-OMC
26	G	311	CHL	C3C-C2C-CMC-OMC
26	u	315	CHL	C3C-C2C-CMC-OMC
26	n	315	CHL	C3C-C2C-CMC-OMC
26	S	315	CHL	C3C-C2C-CMC-OMC
26	S	316	CHL	C3C-C2C-CMC-OMC
26	s	315	CHL	C3C-C2C-CMC-OMC
25	B	622	LHG	C23-C24-C25-C26
22	r	604	CLA	O1A-CGA-O2A-C1
22	R	305	CLA	O1A-CGA-O2A-C1
22	6	307	CLA	C3-C5-C6-C7
22	4	301	CLA	C2A-CAA-CBA-CGA
26	p	320	CHL	C2A-CAA-CBA-CGA
26	N	315	CHL	C2A-CAA-CBA-CGA
26	G	315	CHL	C2A-CAA-CBA-CGA
25	6	311	LHG	O1-C1-C2-O2
25	b	622	LHG	O1-C1-C2-O2
22	a	408	CLA	C8-C10-C11-C12
22	u	302	CLA	C5-C6-C7-C8
22	g	302	CLA	C5-C6-C7-C8
25	1	312	LHG	C13-C14-C15-C16
25	D	406	LHG	C27-C28-C29-C30
25	D	407	LHG	C12-C13-C14-C15
34	B	621	LMG	C18-C19-C20-C21
25	a	415	LHG	O6-C4-C5-O7
25	A	413	LHG	O6-C4-C5-O7
25	U	312	LHG	O6-C4-C5-O7
25	u	312	LHG	O6-C4-C5-O7
25	n	312	LHG	O6-C4-C5-O7
25	R	314	LHG	O6-C4-C5-O7
25	D	406	LHG	O6-C4-C5-O7
22	g	303	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
34	a	412	LMG	C39-C40-C41-C42
22	r	603	CLA	O1A-CGA-O2A-C1
26	v	318	CHL	O1A-CGA-O2A-C1
22	C	508	CLA	C16-C17-C18-C19
26	V	318	CHL	C16-C17-C18-C20
26	g	316	CHL	C11-C12-C13-C14
22	C	508	CLA	C15-C16-C17-C18
34	D	408	LMG	C16-C17-C18-C19
36	C	520	DGD	CDB-CEB-CFB-CGB
22	b	602	CLA	CAA-CBA-CGA-O2A
25	a	415	LHG	C9-C10-C11-C12
25	3	310	LHG	C15-C16-C17-C18
22	3	306	CLA	O1A-CGA-O2A-C1
22	Q	304	CLA	C15-C16-C17-C18
34	c	501	LMG	C22-C23-C24-C25
26	3	311	CHL	C3-C5-C6-C7
25	r	613	LHG	O7-C5-C6-O8
25	2	312	LHG	O7-C5-C6-O8
25	3	310	LHG	O7-C5-C6-O8
25	V	312	LHG	O7-C5-C6-O8
25	N	312	LHG	O7-C5-C6-O8
34	C	502	LMG	O1-C7-C8-O7
34	b	621	LMG	O7-C8-C9-O8
36	C	519	DGD	O1G-C1G-C2G-O2G
36	c	517	DGD	O1G-C1G-C2G-O2G
22	b	602	CLA	C15-C16-C17-C18
22	r	605	CLA	O1D-CGD-O2D-CED
25	u	312	LHG	C8-C7-O7-C5
26	4	315	CHL	O1D-CGD-O2D-CED
26	n	318	CHL	O1D-CGD-O2D-CED
22	q	305	CLA	C11-C12-C13-C15
22	N	301	CLA	C16-C17-C18-C19
22	N	304	CLA	C16-C17-C18-C19
22	B	602	CLA	C16-C17-C18-C19
26	v	318	CHL	C16-C17-C18-C20
26	P	319	CHL	C16-C17-C18-C20
30	d	401	PHO	C16-C17-C18-C19
30	d	401	PHO	C16-C17-C18-C20
22	N	307	CLA	C5-C6-C7-C8
22	B	609	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
25	2	312	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	d	405	LHG	C27-C28-C29-C30
25	c	522	LHG	C17-C18-C19-C20
34	B	624	LMG	C21-C22-C23-C24
36	c	519	DGD	CCA-CDA-CEA-CFA
26	5	317	CHL	C4-C3-C5-C6
26	q	315	CHL	C4-C3-C5-C6
26	Q	316	CHL	C4-C3-C5-C6
22	n	304	CLA	C2-C1-O2A-CGA
22	S	301	CLA	C2-C1-O2A-CGA
22	C	509	CLA	C2-C1-O2A-CGA
22	b	609	CLA	C2-C1-O2A-CGA
22	c	508	CLA	C2-C1-O2A-CGA
22	c	514	CLA	C2-C1-O2A-CGA
26	N	313	CHL	C2-C1-O2A-CGA
26	N	317	CHL	C2-C1-O2A-CGA
26	n	313	CHL	C2-C1-O2A-CGA
26	n	318	CHL	C2-C1-O2A-CGA
22	U	306	CLA	O1D-CGD-O2D-CED
26	p	320	CHL	C2-C3-C5-C6
25	A	413	LHG	C9-C10-C11-C12
22	q	302	CLA	C5-C6-C7-C8
26	V	317	CHL	C15-C16-C17-C18
36	B	601	DGD	C1A-C2A-C3A-C4A
22	6	305	CLA	C11-C10-C8-C9
22	p	305	CLA	C11-C10-C8-C9
22	q	304	CLA	C14-C13-C15-C16
22	V	307	CLA	C14-C13-C15-C16
22	P	307	CLA	C6-C7-C8-C9
22	U	305	CLA	C11-C10-C8-C9
22	N	304	CLA	C14-C13-C15-C16
22	G	301	CLA	C6-C7-C8-C9
22	u	302	CLA	C6-C7-C8-C9
22	u	307	CLA	C14-C13-C15-C16
22	n	302	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C12-C13-C14
22	B	608	CLA	C11-C10-C8-C9
22	B	617	CLA	C14-C13-C15-C16
22	b	617	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	c	511	CLA	C6-C7-C8-C9
22	s	301	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	1	317	CHL	C11-C12-C13-C14
26	2	316	CHL	C14-C13-C15-C16
26	3	311	CHL	C11-C12-C13-C14
26	3	311	CHL	C14-C13-C15-C16
26	5	316	CHL	C14-C13-C15-C16
26	5	317	CHL	C6-C7-C8-C9
26	6	312	CHL	C11-C12-C13-C14
26	6	312	CHL	C14-C13-C15-C16
26	v	313	CHL	C14-C13-C15-C16
26	p	317	CHL	C14-C13-C15-C16
26	p	319	CHL	C11-C12-C13-C14
26	q	311	CHL	C11-C12-C13-C14
26	q	314	CHL	C11-C12-C13-C14
26	V	318	CHL	C14-C13-C15-C16
26	P	314	CHL	C11-C12-C13-C14
26	Q	311	CHL	C11-C12-C13-C14
26	Q	314	CHL	C11-C12-C13-C14
26	N	313	CHL	C11-C12-C13-C14
26	G	314	CHL	C14-C13-C15-C16
26	u	317	CHL	C14-C13-C15-C16
26	g	315	CHL	C14-C13-C15-C16
26	R	315	CHL	C11-C12-C13-C14
26	R	315	CHL	C14-C13-C15-C16
25	c	523	LHG	C19-C20-C21-C22
34	d	407	LMG	C12-C13-C14-C15
36	A	414	DGD	C8B-C9B-CAB-CBB
36	c	518	DGD	C5B-C6B-C7B-C8B
22	D	403	CLA	O1D-CGD-O2D-CED
22	v	302	CLA	C5-C6-C7-C8
22	b	615	CLA	C8-C10-C11-C12
22	b	617	CLA	C13-C15-C16-C17
26	5	313	CHL	C13-C15-C16-C17
25	4	312	LHG	C2-C3-O3-P
25	5	312	LHG	C2-C3-O3-P
25	Q	310	LHG	C2-C3-O3-P
25	R	314	LHG	C2-C3-O3-P
22	R	306	CLA	O1A-CGA-O2A-C1
26	3	315	CHL	O1A-CGA-O2A-C1
26	R	317	CHL	O1A-CGA-O2A-C1
25	L	101	LHG	C30-C31-C32-C33
22	p	302	CLA	C2A-CAA-CBA-CGA
22	P	302	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	U	301	CLA	C2A-CAA-CBA-CGA
22	S	305	CLA	C2A-CAA-CBA-CGA
22	a	408	CLA	C11-C12-C13-C15
26	u	316	CHL	C16-C17-C18-C19
23	2	309	LUT	C1-C6-C7-C8
23	2	309	LUT	C5-C6-C7-C8
23	v	309	LUT	C5-C6-C7-C8
23	V	309	LUT	C5-C6-C7-C8
23	u	309	LUT	C1-C6-C7-C8
23	u	309	LUT	C5-C6-C7-C8
23	R	312	LUT	C1-C6-C7-C8
31	k	101	BCR	C1-C6-C7-C8
31	t	101	BCR	C23-C24-C25-C30
31	z	101	BCR	C5-C6-C7-C8
31	K	101	BCR	C1-C6-C7-C8
31	T	101	BCR	C23-C24-C25-C30
31	C	516	BCR	C5-C6-C7-C8
31	B	620	BCR	C5-C6-C7-C8
31	b	618	BCR	C1-C6-C7-C8
31	b	620	BCR	C1-C6-C7-C8
31	b	620	BCR	C5-C6-C7-C8
22	r	606	CLA	C8-C10-C11-C12
22	U	302	CLA	C15-C16-C17-C18
22	b	604	CLA	C5-C6-C7-C8
26	R	315	CHL	C10-C11-C12-C13
34	b	624	LMG	C32-C33-C34-C35
25	d	406	LHG	C18-C19-C20-C21
25	D	406	LHG	C31-C32-C33-C34
25	c	522	LHG	C16-C17-C18-C19
23	s	311	LUT	C11-C12-C13-C14
24	p	312	XAT	C31-C32-C33-C34
27	u	319	NEX	C11-C12-C13-C14
31	b	619	BCR	C11-C12-C13-C14
22	v	307	CLA	C10-C11-C12-C13
22	P	302	CLA	C15-C16-C17-C18
22	P	308	CLA	C5-C6-C7-C8
22	C	511	CLA	C15-C16-C17-C18
22	b	615	CLA	C5-C6-C7-C8
26	5	317	CHL	C5-C6-C7-C8
26	G	315	CHL	C5-C6-C7-C8
25	5	312	LHG	C25-C26-C27-C28
34	C	502	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
36	c	517	DGD	C1A-C2A-C3A-C4A
25	U	312	LHG	C8-C7-O7-C5
34	d	407	LMG	C30-C31-C32-C33
36	c	518	DGD	CDA-CEA-CFA-CGA
22	N	308	CLA	O2A-C1-C2-C3
22	B	617	CLA	C13-C15-C16-C17
26	p	316	CHL	O1A-CGA-O2A-C1
22	U	307	CLA	C16-C17-C18-C19
34	A	411	LMG	C10-C11-C12-C13
22	2	301	CLA	C15-C16-C17-C18
26	U	315	CHL	C15-C16-C17-C18
32	a	413	SQD	C16-C17-C18-C19
34	b	621	LMG	C11-C12-C13-C14
36	C	520	DGD	CAB-CBB-CCB-CDB
22	4	308	CLA	O1D-CGD-O2D-CED
26	1	318	CHL	O1D-CGD-O2D-CED
26	S	315	CHL	O1D-CGD-O2D-CED
22	B	604	CLA	C5-C6-C7-C8
22	B	617	CLA	C10-C11-C12-C13
25	r	613	LHG	O6-C4-C5-C6
25	G	310	LHG	O6-C4-C5-C6
25	g	310	LHG	O6-C4-C5-C6
25	c	523	LHG	O6-C4-C5-C6
26	u	318	CHL	O1D-CGD-O2D-CED
32	M	101	SQD	C12-C13-C14-C15
22	r	606	CLA	C12-C13-C15-C16
22	1	306	CLA	C11-C10-C8-C7
22	3	302	CLA	C6-C7-C8-C10
22	5	307	CLA	C11-C10-C8-C7
22	6	303	CLA	C11-C10-C8-C7
22	6	305	CLA	C11-C10-C8-C7
22	6	308	CLA	C12-C13-C15-C16
22	v	306	CLA	C11-C10-C8-C7
22	p	305	CLA	C11-C10-C8-C7
22	q	301	CLA	C11-C12-C13-C15
22	q	304	CLA	C12-C13-C15-C16
22	q	306	CLA	C6-C7-C8-C10
22	V	305	CLA	C6-C7-C8-C10
22	V	307	CLA	C12-C13-C15-C16
22	P	302	CLA	C11-C12-C13-C15
22	P	303	CLA	C11-C10-C8-C7
22	P	305	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	Q	301	CLA	C11-C12-C13-C15
22	Q	304	CLA	C11-C12-C13-C15
22	Q	306	CLA	C6-C7-C8-C10
22	U	305	CLA	C6-C7-C8-C10
22	N	302	CLA	C12-C13-C15-C16
22	G	301	CLA	C6-C7-C8-C10
22	G	301	CLA	C11-C12-C13-C15
22	G	302	CLA	C11-C10-C8-C7
22	G	302	CLA	C12-C13-C15-C16
22	G	306	CLA	C11-C10-C8-C7
22	G	307	CLA	C12-C13-C15-C16
22	u	305	CLA	C6-C7-C8-C10
22	u	307	CLA	C12-C13-C15-C16
22	n	302	CLA	C12-C13-C15-C16
22	n	304	CLA	C11-C12-C13-C15
22	g	301	CLA	C6-C7-C8-C10
22	g	301	CLA	C12-C13-C15-C16
22	g	307	CLA	C12-C13-C15-C16
22	R	307	CLA	C12-C13-C15-C16
22	C	508	CLA	C12-C13-C15-C16
22	C	509	CLA	C12-C13-C15-C16
22	C	512	CLA	C6-C7-C8-C10
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C6-C7-C8-C10
22	B	605	CLA	C6-C7-C8-C10
22	B	605	CLA	C11-C10-C8-C7
22	B	608	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C10-C8-C7
22	B	615	CLA	C6-C7-C8-C10
22	B	616	CLA	C6-C7-C8-C10
22	b	602	CLA	C12-C13-C15-C16
22	b	604	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	b	610	CLA	C6-C7-C8-C10
22	b	616	CLA	C11-C12-C13-C15
22	b	617	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
22	c	508	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	s	301	CLA	C11-C12-C13-C15
26	r	614	CHL	C11-C12-C13-C15
26	r	614	CHL	C12-C13-C15-C16
26	1	316	CHL	C12-C13-C15-C16
26	1	317	CHL	C11-C12-C13-C15
26	2	313	CHL	C11-C12-C13-C15
26	2	316	CHL	C11-C10-C8-C7
26	3	311	CHL	C11-C12-C13-C15
26	3	311	CHL	C12-C13-C15-C16
26	4	313	CHL	C11-C12-C13-C15
26	4	317	CHL	C11-C12-C13-C15
26	5	318	CHL	C11-C12-C13-C15
26	5	318	CHL	C12-C13-C15-C16
26	6	312	CHL	C12-C13-C15-C16
26	6	316	CHL	C6-C7-C8-C10
26	6	316	CHL	C11-C12-C13-C15
26	v	313	CHL	C12-C13-C15-C16
26	v	318	CHL	C6-C7-C8-C10
26	p	314	CHL	C11-C12-C13-C15
26	p	320	CHL	C12-C13-C15-C16
26	q	311	CHL	C11-C12-C13-C15
26	q	314	CHL	C11-C12-C13-C15
26	q	315	CHL	C2-C3-C5-C6
26	V	318	CHL	C6-C7-C8-C10
26	P	317	CHL	C11-C10-C8-C7
26	P	317	CHL	C12-C13-C15-C16
26	Q	311	CHL	C11-C12-C13-C15
26	Q	315	CHL	C11-C10-C8-C7
26	Q	315	CHL	C12-C13-C15-C16
26	Q	316	CHL	C2-C3-C5-C6
26	U	313	CHL	C11-C12-C13-C15
26	U	315	CHL	C12-C13-C15-C16
26	U	316	CHL	C6-C7-C8-C10
26	N	313	CHL	C12-C13-C15-C16
26	N	317	CHL	C6-C7-C8-C10
26	N	317	CHL	C11-C12-C13-C15
26	u	316	CHL	C11-C12-C13-C15
26	u	318	CHL	C12-C13-C15-C16
26	n	318	CHL	C11-C12-C13-C15
26	g	311	CHL	C11-C12-C13-C15
26	g	314	CHL	C2-C3-C5-C6
26	g	315	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	R	315	CHL	C11-C12-C13-C15
26	R	315	CHL	C12-C13-C15-C16
26	4	317	CHL	O1A-CGA-O2A-C1
25	v	312	LHG	C29-C30-C31-C32
22	r	606	CLA	C10-C11-C12-C13
22	P	302	CLA	C10-C11-C12-C13
22	N	304	CLA	C13-C15-C16-C17
22	c	503	CLA	C8-C10-C11-C12
24	R	313	XAT	C13-C14-C15-C35
27	R	301	NEX	C29-C30-C31-C32
31	C	518	BCR	C15-C16-C17-C18
31	c	516	BCR	C15-C16-C17-C18
22	N	302	CLA	C16-C17-C18-C20
22	n	301	CLA	C16-C17-C18-C19
26	R	316	CHL	C6-C7-C8-C9
25	p	313	LHG	C16-C17-C18-C19
25	q	310	LHG	C28-C29-C30-C31
32	a	413	SQD	C29-C30-C31-C32
32	m	101	SQD	C26-C27-C28-C29
25	4	312	LHG	C13-C14-C15-C16
25	C	522	LHG	C11-C10-C9-C8
26	Q	316	CHL	C10-C11-C12-C13
26	G	316	CHL	C5-C6-C7-C8
26	v	316	CHL	O1A-CGA-O2A-C1
22	A	404	CLA	C2A-CAA-CBA-CGA
22	u	308	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
26	P	319	CHL	C2A-CAA-CBA-CGA
25	B	622	LHG	C29-C30-C31-C32
32	M	101	SQD	C26-C27-C28-C29
22	D	403	CLA	C5-C6-C7-C8
34	D	408	LMG	C30-C31-C32-C33
36	b	601	DGD	C2A-C3A-C4A-C5A
26	2	318	CHL	C3-C5-C6-C7
22	r	605	CLA	CBA-CGA-O2A-C1
22	q	307	CLA	CBA-CGA-O2A-C1
32	C	501	SQD	C24-C23-O48-C46
34	b	624	LMG	C29-C28-O8-C9
32	A	412	SQD	C29-C30-C31-C32
25	1	312	LHG	C19-C20-C21-C22
25	n	312	LHG	C29-C30-C31-C32
25	R	314	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	D	407	LHG	C28-C29-C30-C31
26	3	311	CHL	C5-C6-C7-C8
26	g	315	CHL	C10-C11-C12-C13
25	d	406	LHG	C28-C29-C30-C31
36	C	520	DGD	C9A-CAA-CBA-CCA
22	1	303	CLA	CAD-CBD-CGD-O2D
22	1	308	CLA	CAD-CBD-CGD-O2D
22	2	301	CLA	CAD-CBD-CGD-O2D
22	2	308	CLA	CAD-CBD-CGD-O2D
22	4	308	CLA	CAD-CBD-CGD-O2D
22	6	302	CLA	CAD-CBD-CGD-O2D
22	v	304	CLA	CAD-CBD-CGD-O2D
22	p	305	CLA	CAD-CBD-CGD-O2D
22	N	307	CLA	CAD-CBD-CGD-O2D
22	G	305	CLA	CAD-CBD-CGD-O2D
22	G	308	CLA	CAD-CBD-CGD-O2D
22	u	304	CLA	CAD-CBD-CGD-O2D
22	g	305	CLA	CAD-CBD-CGD-O2D
22	R	304	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	s	303	CLA	CAD-CBD-CGD-O2D
26	5	313	CHL	CAD-CBD-CGD-O2D
26	5	314	CHL	CAD-CBD-CGD-O2D
26	p	315	CHL	CAD-CBD-CGD-O2D
26	V	314	CHL	CAD-CBD-CGD-O2D
26	P	315	CHL	CAD-CBD-CGD-O2D
26	P	319	CHL	CAD-CBD-CGD-O2D
26	Q	316	CHL	CAD-CBD-CGD-O2D
26	U	313	CHL	CAD-CBD-CGD-O2D
26	u	313	CHL	CAD-CBD-CGD-O2D
22	6	306	CLA	C3-C5-C6-C7
22	1	301	CLA	C15-C16-C17-C18
36	J	101	DGD	CCA-CDA-CEA-CFA
25	c	522	LHG	O10-C23-O8-C6
26	U	317	CHL	O1A-CGA-O2A-C1
22	1	307	CLA	CBA-CGA-O2A-C1
22	2	306	CLA	CBA-CGA-O2A-C1
22	v	307	CLA	CBA-CGA-O2A-C1
26	p	320	CHL	CBA-CGA-O2A-C1
22	R	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	d	402	CLA	C4-C3-C5-C6
22	6	305	CLA	C4-C3-C5-C6
22	p	302	CLA	C4-C3-C5-C6
26	6	301	CHL	C4-C3-C5-C6
33	d	404	PL9	C45-C44-C46-C47
33	D	405	PL9	C45-C44-C46-C47
22	n	302	CLA	C16-C17-C18-C20
26	R	316	CHL	C6-C7-C8-C10
34	W	201	LMG	C17-C18-C19-C20
36	C	520	DGD	O6D-C1D-O3G-C3G
22	b	606	CLA	C15-C16-C17-C18
26	5	317	CHL	C2-C3-C5-C6
26	6	301	CHL	C2-C3-C5-C6
33	D	405	PL9	C43-C44-C46-C47
25	2	312	LHG	C2-C3-O3-P
25	6	311	LHG	C4-C5-C6-O8
25	N	312	LHG	C4-C5-C6-O8
25	g	310	LHG	C4-C5-C6-O8
25	c	523	LHG	C2-C3-O3-P
26	r	616	CHL	O1A-CGA-O2A-C1
25	d	405	LHG	O6-C4-C5-O7
25	P	313	LHG	O6-C4-C5-O7
25	G	310	LHG	O6-C4-C5-O7
25	c	523	LHG	O6-C4-C5-O7
22	6	302	CLA	C5-C6-C7-C8
22	c	503	CLA	C10-C11-C12-C13
22	2	301	CLA	C2A-CAA-CBA-CGA
22	5	301	CLA	C2A-CAA-CBA-CGA
22	u	301	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	C2A-CAA-CBA-CGA
34	b	624	LMG	O10-C28-O8-C9
26	u	316	CHL	C16-C17-C18-C20
25	u	312	LHG	O9-C7-O7-C5
22	r	609	CLA	CHA-CBD-CGD-O1D
22	r	609	CLA	CHA-CBD-CGD-O2D
22	r	610	CLA	CHA-CBD-CGD-O1D
22	r	610	CLA	CHA-CBD-CGD-O2D
22	2	301	CLA	CHA-CBD-CGD-O1D
22	5	306	CLA	CHA-CBD-CGD-O1D
22	5	306	CLA	CHA-CBD-CGD-O2D
22	6	307	CLA	CHA-CBD-CGD-O1D
22	v	306	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	v	306	CLA	CHA-CBD-CGD-O2D
22	v	308	CLA	CHA-CBD-CGD-O1D
22	v	308	CLA	CHA-CBD-CGD-O2D
22	p	304	CLA	CHA-CBD-CGD-O2D
22	q	303	CLA	CHA-CBD-CGD-O1D
22	q	303	CLA	CHA-CBD-CGD-O2D
22	q	305	CLA	CHA-CBD-CGD-O1D
22	q	305	CLA	CHA-CBD-CGD-O2D
22	V	308	CLA	CHA-CBD-CGD-O1D
22	V	308	CLA	CHA-CBD-CGD-O2D
22	Q	302	CLA	CHA-CBD-CGD-O1D
22	U	308	CLA	CHA-CBD-CGD-O2D
22	u	303	CLA	CHA-CBD-CGD-O1D
22	u	303	CLA	CHA-CBD-CGD-O2D
22	n	302	CLA	CHA-CBD-CGD-O1D
22	R	311	CLA	CHA-CBD-CGD-O1D
22	R	311	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	C	511	CLA	CHA-CBD-CGD-O1D
22	C	511	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O1D
22	B	603	CLA	CHA-CBD-CGD-O2D
22	B	610	CLA	CHA-CBD-CGD-O1D
22	B	610	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O2D
22	b	610	CLA	CHA-CBD-CGD-O1D
22	b	610	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
26	r	619	CHL	CHA-CBD-CGD-O1D
26	r	619	CHL	CHA-CBD-CGD-O2D
26	p	317	CHL	CHA-CBD-CGD-O2D
26	u	316	CHL	CHA-CBD-CGD-O2D
26	n	316	CHL	CHA-CBD-CGD-O1D
26	R	316	CHL	CHA-CBD-CGD-O2D
22	a	404	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	u	312	LHG	O10-C23-O8-C6
25	C	523	LHG	O10-C23-O8-C6
26	u	318	CHL	O1A-CGA-O2A-C1
34	B	624	LMG	O10-C28-O8-C9
36	C	520	DGD	O1A-C1A-O1G-C1G
22	V	308	CLA	O2A-C1-C2-C3
22	n	308	CLA	O2A-C1-C2-C3
34	w	201	LMG	C2-C1-O1-C7
26	n	316	CHL	C15-C16-C17-C18
36	B	601	DGD	C2A-C3A-C4A-C5A
25	v	312	LHG	O7-C5-C6-O8
32	a	410	SQD	O6-C44-C45-O47
32	l	102	SQD	O47-C45-C46-O48
32	L	102	SQD	O47-C45-C46-O48
32	C	501	SQD	O6-C44-C45-O47
34	w	201	LMG	O1-C7-C8-O7
34	w	201	LMG	O7-C8-C9-O8
34	C	521	LMG	O1-C7-C8-O7
34	c	501	LMG	O1-C7-C8-O7
34	c	501	LMG	O7-C8-C9-O8
34	c	520	LMG	O1-C7-C8-O7
36	a	416	DGD	O1G-C1G-C2G-O2G
36	A	414	DGD	O1G-C1G-C2G-O2G
36	b	601	DGD	O2G-C2G-C3G-O3G
22	4	307	CLA	CBA-CGA-O2A-C1
25	2	312	LHG	C26-C27-C28-C29
26	3	311	CHL	O1D-CGD-O2D-CED
22	d	402	CLA	C5-C6-C7-C8
22	G	306	CLA	C10-C11-C12-C13
22	g	306	CLA	C5-C6-C7-C8
26	Q	316	CHL	C5-C6-C7-C8
26	u	313	CHL	C10-C11-C12-C13
22	A	404	CLA	O1A-CGA-O2A-C1
22	A	406	CLA	O1A-CGA-O2A-C1
22	3	303	CLA	O1A-CGA-O2A-C1
22	G	305	CLA	O1A-CGA-O2A-C1
26	V	316	CHL	O1A-CGA-O2A-C1
25	3	310	LHG	O1-C1-C2-O2
25	d	405	LHG	C31-C32-C33-C34
36	A	414	DGD	C9B-CAB-CBB-CCB
22	a	404	CLA	C3-C5-C6-C7
22	Q	305	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	N	317	CHL	C4-C3-C5-C6
26	n	317	CHL	C4-C3-C5-C6
26	R	316	CHL	C4-C3-C5-C6
25	L	101	LHG	C24-C25-C26-C27
22	g	303	CLA	O1A-CGA-O2A-C1
25	N	312	LHG	O10-C23-O8-C6
26	n	317	CHL	C2-C3-C5-C6
26	R	316	CHL	C2-C3-C5-C6
33	d	404	PL9	C43-C44-C46-C47
33	d	404	PL9	C4-C3-C7-C8
33	D	405	PL9	C4-C3-C7-C8
25	D	406	LHG	C11-C12-C13-C14
36	c	518	DGD	C9A-CAA-CBA-CCA
25	U	312	LHG	O9-C7-O7-C5
22	2	305	CLA	C10-C11-C12-C13
22	1	306	CLA	C11-C10-C8-C9
22	3	307	CLA	C14-C13-C15-C16
22	q	304	CLA	C6-C7-C8-C9
22	q	304	CLA	C11-C10-C8-C9
22	q	305	CLA	C11-C10-C8-C9
22	q	306	CLA	C6-C7-C8-C9
22	U	307	CLA	C14-C13-C15-C16
22	N	305	CLA	C6-C7-C8-C9
22	g	301	CLA	C6-C7-C8-C9
22	g	301	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
26	3	314	CHL	C11-C10-C8-C9
26	6	301	CHL	C14-C13-C15-C16
26	6	315	CHL	C11-C10-C8-C9
26	n	313	CHL	C6-C7-C8-C9
26	g	315	CHL	C11-C12-C13-C14
32	M	101	SQD	C45-C46-O48-C23
36	C	519	DGD	C4D-C5D-C6D-O5D
25	C	523	LHG	C17-C18-C19-C20
32	a	410	SQD	C27-C28-C29-C30
32	C	501	SQD	C14-C15-C16-C17
32	a	413	SQD	C5-C6-S-O8
32	m	101	SQD	C4-C5-C6-S
32	M	101	SQD	C4-C5-C6-S
25	l	101	LHG	C24-C25-C26-C27
25	V	312	LHG	C9-C10-C11-C12
26	3	313	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	P	319	CHL	C10-C11-C12-C13
22	Q	307	CLA	O1A-CGA-O2A-C1
27	N	318	NEX	C31-C32-C33-C40
31	B	618	BCR	C7-C8-C9-C34
32	m	101	SQD	C45-C46-O48-C23
25	v	312	LHG	C31-C32-C33-C34
22	u	305	CLA	C8-C10-C11-C12
22	B	612	CLA	C8-C10-C11-C12
34	c	501	LMG	C35-C36-C37-C38
23	N	309	LUT	C31-C32-C33-C34
23	n	310	LUT	C7-C8-C9-C10
22	a	408	CLA	C1A-C2A-CAA-CBA
22	1	301	CLA	C1A-C2A-CAA-CBA
22	3	304	CLA	C1A-C2A-CAA-CBA
22	4	301	CLA	C1A-C2A-CAA-CBA
22	v	301	CLA	C1A-C2A-CAA-CBA
22	P	302	CLA	C1A-C2A-CAA-CBA
22	U	301	CLA	C1A-C2A-CAA-CBA
22	N	301	CLA	C1A-C2A-CAA-CBA
22	u	301	CLA	C1A-C2A-CAA-CBA
22	u	304	CLA	C1A-C2A-CAA-CBA
22	g	301	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
26	v	318	CHL	C1A-C2A-CAA-CBA
26	p	319	CHL	C1A-C2A-CAA-CBA
32	a	413	SQD	C23-C24-C25-C26
22	u	302	CLA	C15-C16-C17-C18
26	1	318	CHL	C5-C6-C7-C8
26	2	313	CHL	C13-C15-C16-C17
22	Q	303	CLA	CBD-CGD-O2D-CED
25	v	312	LHG	C24-C23-O8-C6
26	v	315	CHL	CBA-CGA-O2A-C1
26	q	315	CHL	CBA-CGA-O2A-C1
34	b	624	LMG	C21-C22-C23-C24
36	J	101	DGD	C3A-C4A-C5A-C6A
22	2	306	CLA	O1A-CGA-O2A-C1
22	B	603	CLA	C15-C16-C17-C18
26	G	311	CHL	C5-C6-C7-C8
25	d	406	LHG	C3-O3-P-O6
26	P	319	CHL	CBD-CGD-O2D-CED
22	B	608	CLA	C4-C3-C5-C6
26	v	316	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	G	305	CLA	C3-C5-C6-C7
22	S	306	CLA	C3-C5-C6-C7
22	C	515	CLA	C3-C5-C6-C7
25	r	613	LHG	C2-C3-O3-P
25	C	523	LHG	C2-C3-O3-P
25	b	623	LHG	C15-C16-C17-C18
25	c	521	LHG	C25-C26-C27-C28
34	w	201	LMG	C12-C13-C14-C15
26	p	320	CHL	O1A-CGA-O2A-C1
25	r	613	LHG	C3-O3-P-O5
25	a	415	LHG	C3-O3-P-O4
25	a	415	LHG	C3-O3-P-O5
25	d	405	LHG	C4-O6-P-O4
25	d	405	LHG	C4-O6-P-O5
25	d	406	LHG	C4-O6-P-O5
25	l	101	LHG	C4-O6-P-O5
25	A	413	LHG	C3-O3-P-O4
25	A	413	LHG	C3-O3-P-O5
25	L	101	LHG	C4-O6-P-O5
25	v	312	LHG	C3-O3-P-O5
25	U	312	LHG	C4-O6-P-O4
25	U	312	LHG	C4-O6-P-O5
25	u	312	LHG	C4-O6-P-O4
25	u	312	LHG	C4-O6-P-O5
25	C	523	LHG	C3-O3-P-O4
25	C	523	LHG	C3-O3-P-O5
25	C	523	LHG	C4-O6-P-O4
25	C	523	LHG	C4-O6-P-O5
25	B	622	LHG	C3-O3-P-O4
25	B	623	LHG	C3-O3-P-O5
25	D	406	LHG	C3-O3-P-O5
25	D	406	LHG	C4-O6-P-O4
25	D	406	LHG	C4-O6-P-O5
25	D	407	LHG	C4-O6-P-O5
25	b	623	LHG	C3-O3-P-O5
25	c	522	LHG	C3-O3-P-O5
25	c	522	LHG	C4-O6-P-O4
25	c	522	LHG	C4-O6-P-O5
25	c	523	LHG	C4-O6-P-O5
22	5	304	CLA	C16-C17-C18-C20
22	q	307	CLA	C16-C17-C18-C20
22	u	305	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	q	315	CHL	C11-C12-C13-C15
34	c	520	LMG	C10-C11-C12-C13
32	a	410	SQD	C14-C15-C16-C17
34	w	201	LMG	O6-C1-O1-C7
22	a	406	CLA	CBA-CGA-O2A-C1
22	6	308	CLA	CBA-CGA-O2A-C1
22	C	510	CLA	CBA-CGA-O2A-C1
25	L	101	LHG	C24-C23-O8-C6
25	1	312	LHG	O6-C4-C5-C6
25	4	312	LHG	O6-C4-C5-C6
25	5	312	LHG	O6-C4-C5-C6
25	P	313	LHG	O6-C4-C5-C6
25	U	312	LHG	O6-C4-C5-C6
25	N	312	LHG	O6-C4-C5-C6
25	u	312	LHG	O6-C4-C5-C6
25	n	312	LHG	O6-C4-C5-C6
25	R	314	LHG	O6-C4-C5-C6
22	r	605	CLA	O1A-CGA-O2A-C1
32	a	413	SQD	O47-C7-C8-C9
22	S	309	CLA	C2A-CAA-CBA-CGA
22	A	404	CLA	C3-C5-C6-C7
25	q	310	LHG	C26-C27-C28-C29
25	D	406	LHG	C25-C26-C27-C28
36	J	101	DGD	C3B-C4B-C5B-C6B
25	C	522	LHG	C8-C7-O7-C5
22	b	604	CLA	C16-C17-C18-C19
25	P	313	LHG	C18-C19-C20-C21
22	1	302	CLA	CAD-CBD-CGD-O1D
22	4	302	CLA	CAD-CBD-CGD-O1D
22	6	303	CLA	CAD-CBD-CGD-O1D
22	v	306	CLA	CAD-CBD-CGD-O1D
22	v	308	CLA	CAD-CBD-CGD-O1D
22	p	304	CLA	CAD-CBD-CGD-O1D
22	q	302	CLA	CAD-CBD-CGD-O1D
22	q	303	CLA	CAD-CBD-CGD-O1D
22	q	308	CLA	CAD-CBD-CGD-O1D
22	V	308	CLA	CAD-CBD-CGD-O1D
22	Q	302	CLA	CAD-CBD-CGD-O1D
22	Q	303	CLA	CAD-CBD-CGD-O1D
22	Q	308	CLA	CAD-CBD-CGD-O1D
22	G	303	CLA	CAD-CBD-CGD-O1D
22	n	302	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	n	303	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	511	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	510	CLA	CAD-CBD-CGD-O1D
26	r	619	CHL	CAD-CBD-CGD-O1D
26	2	314	CHL	CAD-CBD-CGD-O1D
26	g	312	CHL	CAD-CBD-CGD-O1D
27	2	319	NEX	C7-C8-C9-C10
27	V	319	NEX	C7-C8-C9-C10
30	a	407	PHO	CAD-CBD-CGD-O1D
30	A	407	PHO	CAD-CBD-CGD-O1D
32	l	102	SQD	C5-C6-S-O7
32	L	102	SQD	C5-C6-S-O7
32	C	501	SQD	C5-C6-S-O9
36	c	517	DGD	C4D-C5D-C6D-O5D
25	B	623	LHG	O7-C7-C8-C9
22	B	610	CLA	C15-C16-C17-C18
25	P	313	LHG	C31-C32-C33-C34
36	a	416	DGD	CAB-CBB-CCB-CDB
25	R	314	LHG	C12-C13-C14-C15
26	G	314	CHL	C3-C5-C6-C7
22	B	606	CLA	C15-C16-C17-C18
26	P	319	CHL	O1D-CGD-O2D-CED
25	P	313	LHG	C24-C23-O8-C6
25	U	312	LHG	C24-C23-O8-C6
26	6	316	CHL	CBA-CGA-O2A-C1
26	u	315	CHL	CBA-CGA-O2A-C1
22	c	513	CLA	CAA-CBA-CGA-O2A
22	d	402	CLA	O1D-CGD-O2D-CED
25	C	522	LHG	O9-C7-O7-C5
25	p	313	LHG	C27-C28-C29-C30
22	C	507	CLA	C4-C3-C5-C6
22	c	506	CLA	C4-C3-C5-C6
22	r	609	CLA	C3A-C2A-CAA-CBA
22	1	307	CLA	C6-C7-C8-C10
22	2	302	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	2	304	CLA	C12-C13-C15-C16
22	3	307	CLA	C11-C10-C8-C7
22	3	307	CLA	C12-C13-C15-C16
22	4	302	CLA	C12-C13-C15-C16
22	4	304	CLA	C11-C10-C8-C7
22	6	308	CLA	C11-C10-C8-C7
22	q	304	CLA	C6-C7-C8-C10
22	q	305	CLA	C11-C10-C8-C7
22	P	303	CLA	C6-C7-C8-C10
22	P	307	CLA	C6-C7-C8-C10
22	U	302	CLA	C6-C7-C8-C10
22	U	307	CLA	C12-C13-C15-C16
22	u	302	CLA	C12-C13-C15-C16
22	g	305	CLA	C6-C7-C8-C10
22	C	509	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	b	602	CLA	C11-C12-C13-C15
22	b	615	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
22	c	510	CLA	C6-C7-C8-C10
22	c	511	CLA	C6-C7-C8-C10
22	c	511	CLA	C11-C10-C8-C7
25	r	613	LHG	O6-C4-C5-O7
25	l	101	LHG	O6-C4-C5-O7
25	L	101	LHG	O6-C4-C5-O7
25	1	312	LHG	O6-C4-C5-O7
25	5	312	LHG	O6-C4-C5-O7
25	q	310	LHG	O6-C4-C5-O7
25	Q	310	LHG	C7-C8-C9-C10
25	g	310	LHG	O6-C4-C5-O7
26	1	316	CHL	C11-C10-C8-C7
26	1	318	CHL	C11-C12-C13-C15
26	2	317	CHL	C11-C12-C13-C15
26	2	318	CHL	C11-C12-C13-C15
26	3	314	CHL	C12-C13-C15-C16
26	3	315	CHL	C12-C13-C15-C16
26	5	313	CHL	C11-C12-C13-C15
26	5	317	CHL	C11-C12-C13-C15
26	6	301	CHL	C12-C13-C15-C16
26	6	312	CHL	C11-C12-C13-C15
26	v	316	CHL	C11-C10-C8-C7
26	p	317	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	p	318	CHL	C6-C7-C8-C10
26	p	319	CHL	C11-C12-C13-C15
26	P	314	CHL	C11-C12-C13-C15
26	P	318	CHL	C6-C7-C8-C10
26	Q	314	CHL	C12-C13-C15-C16
26	u	317	CHL	C6-C7-C8-C10
26	u	318	CHL	C6-C7-C8-C10
26	n	313	CHL	C12-C13-C15-C16
26	g	315	CHL	C11-C12-C13-C15
30	d	401	PHO	C11-C12-C13-C15
30	D	401	PHO	C11-C12-C13-C15
25	N	312	LHG	C14-C15-C16-C17
34	A	411	LMG	C32-C33-C34-C35
22	c	507	CLA	C3-C5-C6-C7
23	N	310	LUT	C29-C30-C31-C32
25	2	312	LHG	C27-C28-C29-C30
25	C	524	LHG	C33-C34-C35-C36
25	B	622	LHG	C13-C14-C15-C16
22	C	515	CLA	C10-C11-C12-C13
26	p	317	CHL	C5-C6-C7-C8
36	C	519	DGD	C1A-C2A-C3A-C4A
26	S	314	CHL	O1D-CGD-O2D-CED
26	s	314	CHL	O1D-CGD-O2D-CED
25	2	312	LHG	C8-C7-O7-C5
25	s	312	LHG	C8-C7-O7-C5
25	c	523	LHG	C26-C27-C28-C29
25	U	312	LHG	O10-C23-O8-C6
26	v	315	CHL	O1A-CGA-O2A-C1
25	2	312	LHG	O2-C2-C3-O3
25	4	312	LHG	C9-C10-C11-C12
25	U	312	LHG	C29-C30-C31-C32
25	D	407	LHG	C35-C36-C37-C38
26	g	311	CHL	C5-C6-C7-C8
22	p	308	CLA	C2A-CAA-CBA-CGA
26	q	313	CHL	C2A-CAA-CBA-CGA
22	u	305	CLA	C11-C12-C13-C15
22	4	306	CLA	C3-C5-C6-C7
26	3	315	CHL	C3-C5-C6-C7
36	C	520	DGD	O6D-C5D-C6D-O5D
22	P	309	CLA	O2A-C1-C2-C3
25	5	312	LHG	C4-C5-C6-O8
25	B	622	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	r	615	CHL	C1C-C2C-CMC-OMC
26	1	314	CHL	C1C-C2C-CMC-OMC
26	1	316	CHL	C1C-C2C-CMC-OMC
26	1	318	CHL	C1C-C2C-CMC-OMC
26	2	318	CHL	C1C-C2C-CMC-OMC
26	4	314	CHL	C1C-C2C-CMC-OMC
26	4	317	CHL	C1C-C2C-CMC-OMC
26	5	313	CHL	C1C-C2C-CMC-OMC
26	5	318	CHL	C1C-C2C-CMC-OMC
26	6	301	CHL	C1C-C2C-CMC-OMC
26	v	313	CHL	C1C-C2C-CMC-OMC
26	v	314	CHL	C1C-C2C-CMC-OMC
26	p	314	CHL	C1C-C2C-CMC-OMC
26	p	318	CHL	C1C-C2C-CMC-OMC
26	q	312	CHL	C1C-C2C-CMC-OMC
26	q	313	CHL	C1C-C2C-CMC-OMC
26	q	314	CHL	C1C-C2C-CMC-OMC
26	V	313	CHL	C1C-C2C-CMC-OMC
26	V	314	CHL	C1C-C2C-CMC-OMC
26	V	316	CHL	C1C-C2C-CMC-OMC
26	V	317	CHL	C1C-C2C-CMC-OMC
26	V	318	CHL	C1C-C2C-CMC-OMC
26	P	314	CHL	C1C-C2C-CMC-OMC
26	P	318	CHL	C1C-C2C-CMC-OMC
26	P	319	CHL	C1C-C2C-CMC-OMC
26	Q	312	CHL	C1C-C2C-CMC-OMC
26	Q	313	CHL	C1C-C2C-CMC-OMC
26	Q	314	CHL	C1C-C2C-CMC-OMC
26	U	313	CHL	C1C-C2C-CMC-OMC
26	N	313	CHL	C1C-C2C-CMC-OMC
26	G	311	CHL	C1C-C2C-CMC-OMC
26	G	313	CHL	C1C-C2C-CMC-OMC
26	G	315	CHL	C1C-C2C-CMC-OMC
26	n	314	CHL	C1C-C2C-CMC-OMC
26	g	313	CHL	C1C-C2C-CMC-OMC
26	g	314	CHL	C1C-C2C-CMC-OMC
26	R	316	CHL	C1C-C2C-CMC-OMC
26	S	315	CHL	C1C-C2C-CMC-OMC
26	S	316	CHL	C1C-C2C-CMC-OMC
26	s	315	CHL	C1C-C2C-CMC-OMC
26	s	316	CHL	C1C-C2C-CMC-OMC
34	W	201	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	B	601	DGD	C1G-C2G-C3G-O3G
36	b	601	DGD	C1G-C2G-C3G-O3G
25	6	311	LHG	O7-C5-C6-O8
25	p	313	LHG	O7-C5-C6-O8
25	Q	310	LHG	O7-C5-C6-O8
34	d	407	LMG	O7-C8-C9-O8
34	W	201	LMG	O1-C7-C8-O7
34	W	201	LMG	O7-C8-C9-O8
34	C	502	LMG	O7-C8-C9-O8
34	C	521	LMG	O7-C8-C9-O8
34	D	408	LMG	O7-C8-C9-O8
34	c	520	LMG	O7-C8-C9-O8
36	B	601	DGD	O2G-C2G-C3G-O3G
34	B	621	LMG	C16-C17-C18-C19
25	v	312	LHG	O10-C23-O8-C6
26	q	315	CHL	O1A-CGA-O2A-C1
22	V	304	CLA	C8-C10-C11-C12
22	N	304	CLA	C15-C16-C17-C18
26	3	316	CHL	C10-C11-C12-C13
26	p	319	CHL	C5-C6-C7-C8
36	c	518	DGD	C3B-C4B-C5B-C6B
36	c	519	DGD	C3B-C4B-C5B-C6B
25	S	312	LHG	C2-C3-O3-P
25	s	312	LHG	C2-C3-O3-P
25	b	623	LHG	C12-C13-C14-C15
22	q	307	CLA	O1A-CGA-O2A-C1
26	r	619	CHL	O1A-CGA-O2A-C1
22	P	305	CLA	C5-C6-C7-C8
26	g	311	CHL	C15-C16-C17-C18
22	6	303	CLA	C4-C3-C5-C6
26	p	317	CHL	C4-C3-C5-C6
26	G	314	CHL	C4-C3-C5-C6
22	n	307	CLA	CBA-CGA-O2A-C1
22	C	506	CLA	CBA-CGA-O2A-C1
26	r	619	CHL	CBA-CGA-O2A-C1
22	g	304	CLA	C2-C3-C5-C6
26	N	317	CHL	C2-C3-C5-C6
22	1	308	CLA	O1D-CGD-O2D-CED
22	C	514	CLA	CAA-CBA-CGA-O2A
32	A	412	SQD	O47-C7-C8-C9
25	U	312	LHG	C32-C33-C34-C35
36	b	601	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
22	v	301	CLA	C10-C11-C12-C13
22	U	305	CLA	C8-C10-C11-C12
22	r	606	CLA	C11-C10-C8-C9
22	5	304	CLA	C6-C7-C8-C9
22	6	302	CLA	C6-C7-C8-C9
22	6	308	CLA	C14-C13-C15-C16
22	Q	301	CLA	C11-C12-C13-C14
22	Q	305	CLA	C11-C10-C8-C9
22	G	302	CLA	C11-C10-C8-C9
22	G	302	CLA	C14-C13-C15-C16
22	n	302	CLA	C11-C10-C8-C9
22	n	306	CLA	C11-C10-C8-C9
22	R	307	CLA	C11-C10-C8-C9
22	C	507	CLA	C6-C7-C8-C9
22	B	604	CLA	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	B	607	CLA	C6-C7-C8-C9
22	B	610	CLA	C14-C13-C15-C16
22	B	612	CLA	C6-C7-C8-C9
22	B	616	CLA	C6-C7-C8-C9
22	b	604	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C12-C13-C14
22	c	502	CLA	C11-C10-C8-C9
22	c	508	CLA	C14-C13-C15-C16
26	r	614	CHL	C14-C13-C15-C16
26	1	313	CHL	C6-C7-C8-C9
26	1	316	CHL	C14-C13-C15-C16
26	Q	314	CHL	C14-C13-C15-C16
26	Q	315	CHL	C14-C13-C15-C16
26	N	313	CHL	C14-C13-C15-C16
26	N	317	CHL	C11-C10-C8-C9
26	G	315	CHL	C14-C13-C15-C16
26	n	317	CHL	C6-C7-C8-C9
26	n	318	CHL	C11-C12-C13-C14
22	a	406	CLA	O1A-CGA-O2A-C1
26	s	314	CHL	CBD-CGD-O2D-CED
34	b	621	LMG	O9-C10-O7-C8
32	a	410	SQD	C18-C19-C20-C21
26	6	316	CHL	O1A-CGA-O2A-C1
22	5	306	CLA	C2A-CAA-CBA-CGA
25	P	313	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
25	5	312	LHG	C16-C17-C18-C19
32	C	501	SQD	C18-C19-C20-C21
26	g	312	CHL	O1D-CGD-O2D-CED
25	q	310	LHG	C30-C31-C32-C33
25	b	622	LHG	C29-C30-C31-C32
26	g	315	CHL	C3-C5-C6-C7
22	B	604	CLA	C15-C16-C17-C18
26	R	317	CHL	C10-C11-C12-C13
25	q	310	LHG	C27-C28-C29-C30
36	c	519	DGD	C3A-C4A-C5A-C6A
25	U	312	LHG	C30-C31-C32-C33
25	2	312	LHG	O9-C7-O7-C5
34	b	624	LMG	C13-C14-C15-C16
26	u	315	CHL	O1A-CGA-O2A-C1
22	Q	305	CLA	C2-C3-C5-C6
26	n	313	CHL	C16-C17-C18-C20
22	G	306	CLA	C8-C10-C11-C12
22	r	601	CLA	C1-C2-C3-C4
22	r	607	CLA	C1-C2-C3-C4
22	r	608	CLA	C1-C2-C3-C4
22	R	302	CLA	C1-C2-C3-C4
22	R	308	CLA	C1-C2-C3-C4
22	R	309	CLA	C1-C2-C3-C4
22	S	307	CLA	C1-C2-C3-C4
22	s	307	CLA	C1-C2-C3-C4
26	1	315	CHL	C1-C2-C3-C4
26	2	315	CHL	C1-C2-C3-C4
26	3	313	CHL	C1-C2-C3-C4
26	4	315	CHL	C1-C2-C3-C4
26	5	315	CHL	C1-C2-C3-C4
26	6	314	CHL	C1-C2-C3-C4
26	v	315	CHL	C1-C2-C3-C4
26	p	316	CHL	C1-C2-C3-C4
26	q	313	CHL	C1-C2-C3-C4
26	V	315	CHL	C1-C2-C3-C4
26	P	316	CHL	C1-C2-C3-C4
26	Q	313	CHL	C1-C2-C3-C4
26	U	314	CHL	C1-C2-C3-C4
26	N	315	CHL	C1-C2-C3-C4
26	G	313	CHL	C1-C2-C3-C4
26	u	315	CHL	C1-C2-C3-C4
26	n	315	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	g	313	CHL	C1-C2-C3-C4
25	P	313	LHG	O10-C23-O8-C6
26	u	314	CHL	O1A-CGA-O2A-C1
25	G	310	LHG	C9-C10-C11-C12
22	B	615	CLA	C5-C6-C7-C8
25	a	415	LHG	C4-C5-O7-C7
25	A	413	LHG	C4-C5-O7-C7
25	2	312	LHG	O6-C4-C5-C6
25	p	313	LHG	O6-C4-C5-C6
25	a	415	LHG	C1-C2-C3-O3
25	A	413	LHG	C1-C2-C3-O3
22	r	606	CLA	C2A-CAA-CBA-CGA
22	Q	308	CLA	C2A-CAA-CBA-CGA
22	U	304	CLA	C2A-CAA-CBA-CGA
22	u	304	CLA	C2A-CAA-CBA-CGA
22	R	307	CLA	C2A-CAA-CBA-CGA
22	S	304	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	C2A-CAA-CBA-CGA
22	b	604	CLA	C2A-CAA-CBA-CGA
22	s	309	CLA	C2A-CAA-CBA-CGA
26	P	318	CHL	C2A-CAA-CBA-CGA
26	g	315	CHL	C2A-CAA-CBA-CGA
25	6	311	LHG	O9-C7-O7-C5
25	q	310	LHG	O9-C7-O7-C5
25	s	312	LHG	O9-C7-O7-C5
22	P	303	CLA	C13-C15-C16-C17
22	d	402	CLA	C2-C1-O2A-CGA
22	6	305	CLA	C2-C1-O2A-CGA
22	p	308	CLA	C2-C1-O2A-CGA
22	P	306	CLA	C2-C1-O2A-CGA
22	g	302	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA
22	C	515	CLA	C2-C1-O2A-CGA
22	B	609	CLA	C2-C1-O2A-CGA
22	D	403	CLA	C2-C1-O2A-CGA
22	c	506	CLA	C2-C1-O2A-CGA
22	s	301	CLA	C2-C1-O2A-CGA
26	n	315	CHL	C2-C1-O2A-CGA
25	P	313	LHG	C9-C10-C11-C12
34	A	411	LMG	C39-C40-C41-C42
22	u	306	CLA	C11-C12-C13-C15
22	b	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	1	307	CLA	O1A-CGA-O2A-C1
22	C	510	CLA	O1A-CGA-O2A-C1
25	L	101	LHG	O10-C23-O8-C6
22	q	307	CLA	C3-C5-C6-C7
22	Q	307	CLA	C3-C5-C6-C7
25	2	312	LHG	C35-C36-C37-C38
25	C	522	LHG	C9-C10-C11-C12
22	6	305	CLA	C10-C11-C12-C13
32	C	501	SQD	C10-C11-C12-C13
22	Q	303	CLA	O1D-CGD-O2D-CED
26	6	314	CHL	CBA-CGA-O2A-C1
26	u	314	CHL	CBA-CGA-O2A-C1
27	R	301	NEX	C13-C14-C15-C35
22	v	307	CLA	O1A-CGA-O2A-C1
22	V	304	CLA	O1A-CGA-O2A-C1
25	2	312	LHG	O6-C4-C5-O7
25	p	313	LHG	O6-C4-C5-O7
25	S	312	LHG	O8-C23-C24-C25
22	S	309	CLA	O2A-C1-C2-C3
22	s	309	CLA	O2A-C1-C2-C3
26	P	318	CHL	C4-C3-C5-C6
26	R	315	CHL	C4-C3-C5-C6
25	b	623	LHG	C28-C29-C30-C31
26	r	615	CHL	O1D-CGD-O2D-CED
23	v	309	LUT	C1-C6-C7-C8
23	V	309	LUT	C1-C6-C7-C8
23	S	310	LUT	C5-C6-C7-C8
31	B	620	BCR	C1-C6-C7-C8
22	6	305	CLA	C2-C3-C5-C6
22	4	307	CLA	O1A-CGA-O2A-C1
25	4	312	LHG	C7-C8-C9-C10
22	2	308	CLA	CBA-CGA-O2A-C1
22	V	302	CLA	CBA-CGA-O2A-C1
34	W	201	LMG	C29-C28-O8-C9
25	s	312	LHG	O8-C23-C24-C25
26	s	315	CHL	O1D-CGD-O2D-CED
25	6	311	LHG	C8-C7-O7-C5
25	q	310	LHG	C8-C7-O7-C5
34	b	621	LMG	C11-C10-O7-C8
34	W	201	LMG	O6-C1-O1-C7
36	C	519	DGD	O6E-C1E-O5D-C6D
25	b	622	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
32	A	412	SQD	C16-C17-C18-C19
22	b	610	CLA	C15-C16-C17-C18
22	b	612	CLA	C8-C10-C11-C12
34	W	201	LMG	C2-C1-O1-C7
25	d	406	LHG	C30-C31-C32-C33
25	D	406	LHG	C13-C14-C15-C16
34	B	621	LMG	C22-C23-C24-C25
22	C	511	CLA	CBA-CGA-O2A-C1
22	c	509	CLA	CBA-CGA-O2A-C1
25	6	311	LHG	C4-O6-P-O3
25	q	310	LHG	C4-O6-P-O3
25	n	312	LHG	C4-O6-P-O3
25	C	524	LHG	C3-O3-P-O6
25	C	524	LHG	C4-O6-P-O3
25	D	407	LHG	C3-O3-P-O6
25	c	521	LHG	C4-O6-P-O3
25	c	523	LHG	C3-O3-P-O6
32	A	412	SQD	C23-C24-C25-C26
25	2	312	LHG	C12-C13-C14-C15
25	S	312	LHG	C11-C10-C9-C8
36	C	519	DGD	C2B-C3B-C4B-C5B
25	C	522	LHG	C11-C12-C13-C14
26	p	318	CHL	C4-C3-C5-C6
26	u	316	CHL	C4-C3-C5-C6
22	3	301	CLA	C6-C7-C8-C10
22	V	302	CLA	C11-C10-C8-C7
22	N	305	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	C	509	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C12-C13-C15
22	c	508	CLA	C6-C7-C8-C10
22	c	511	CLA	C11-C12-C13-C15
26	V	318	CHL	C12-C13-C15-C16
26	g	314	CHL	C12-C13-C15-C16
22	C	511	CLA	O1A-CGA-O2A-C1
22	4	304	CLA	C11-C10-C8-C9
22	6	308	CLA	C11-C10-C8-C9
22	p	302	CLA	C11-C12-C13-C14
22	q	301	CLA	C6-C7-C8-C9
22	P	303	CLA	C11-C10-C8-C9
22	N	304	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	n	304	CLA	C11-C12-C13-C14
22	g	305	CLA	C6-C7-C8-C9
22	S	301	CLA	C11-C12-C13-C14
22	C	509	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C9
22	B	616	CLA	C11-C12-C13-C14
22	b	607	CLA	C6-C7-C8-C9
22	b	612	CLA	C6-C7-C8-C9
22	b	616	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C10-C8-C9
26	3	314	CHL	C14-C13-C15-C16
26	4	317	CHL	C11-C12-C13-C14
26	5	313	CHL	C11-C12-C13-C14
26	5	318	CHL	C11-C12-C13-C14
26	6	315	CHL	C14-C13-C15-C16
26	6	316	CHL	C11-C12-C13-C14
26	P	317	CHL	C14-C13-C15-C16
26	N	317	CHL	C11-C12-C13-C14
26	u	316	CHL	C14-C13-C15-C16
26	n	313	CHL	C14-C13-C15-C16
26	g	315	CHL	C6-C7-C8-C9
26	3	314	CHL	C10-C11-C12-C13
24	q	309	XAT	C33-C34-C35-C15
24	R	313	XAT	C33-C34-C35-C15
27	r	618	NEX	C29-C30-C31-C32
27	R	301	NEX	C9-C10-C11-C12
31	B	620	BCR	C13-C14-C15-C16
22	Q	307	CLA	C16-C17-C18-C20
32	a	410	SQD	C11-C10-C9-C8
34	B	624	LMG	C12-C13-C14-C15
34	B	624	LMG	C13-C14-C15-C16
36	c	517	DGD	C2B-C3B-C4B-C5B
22	c	510	CLA	CBA-CGA-O2A-C1
25	l	101	LHG	C24-C23-O8-C6
22	G	301	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	O1A-CGA-O2A-C1
34	W	201	LMG	O10-C28-O8-C9
25	n	312	LHG	C11-C12-C13-C14
26	S	314	CHL	CBD-CGD-O2D-CED
22	s	304	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	6	317	CHL	C2C-C3C-CAC-CBC
36	A	414	DGD	C4A-C5A-C6A-C7A
32	m	101	SQD	C7-C8-C9-C10
22	2	308	CLA	O1A-CGA-O2A-C1
22	n	307	CLA	O1A-CGA-O2A-C1
22	C	506	CLA	O1A-CGA-O2A-C1
26	6	314	CHL	O1A-CGA-O2A-C1
26	N	317	CHL	O1A-CGA-O2A-C1
24	u	311	XAT	C31-C32-C33-C40
27	2	319	NEX	C31-C32-C33-C40
27	5	319	NEX	C31-C32-C33-C40
31	b	618	BCR	C36-C18-C19-C20
22	5	304	CLA	C16-C17-C18-C19
22	R	310	CLA	CBA-CGA-O2A-C1
26	v	314	CHL	CBA-CGA-O2A-C1
25	U	312	LHG	O1-C1-C2-C3
25	q	310	LHG	C2-C3-O3-P
25	B	623	LHG	C2-C3-O3-P
22	6	308	CLA	O1A-CGA-O2A-C1
27	N	318	NEX	C11-C12-C13-C14
31	c	515	BCR	C11-C12-C13-C14
22	s	301	CLA	C12-C13-C15-C16
22	4	301	CLA	C15-C16-C17-C18
25	S	312	LHG	C8-C7-O7-C5
22	3	304	CLA	C4-C3-C5-C6
26	1	316	CHL	C4-C3-C5-C6
26	g	315	CHL	C4-C3-C5-C6
25	A	413	LHG	O1-C1-C2-O2
22	C	514	CLA	C2-C3-C5-C6
22	D	403	CLA	C2-C3-C5-C6
26	U	313	CHL	C2-C3-C5-C6
26	G	314	CHL	C2-C3-C5-C6
34	b	624	LMG	C12-C13-C14-C15
22	q	306	CLA	C11-C12-C13-C15
22	q	307	CLA	C16-C17-C18-C19
26	q	315	CHL	C11-C12-C13-C14
22	N	304	CLA	CBA-CGA-O2A-C1
22	N	307	CLA	CBA-CGA-O2A-C1
22	G	301	CLA	CBA-CGA-O2A-C1
22	c	505	CLA	CBA-CGA-O2A-C1
26	N	317	CHL	CBA-CGA-O2A-C1
32	a	410	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
22	V	302	CLA	O1A-CGA-O2A-C1
26	V	313	CHL	CBD-CGD-O2D-CED
22	R	311	CLA	O1D-CGD-O2D-CED
25	C	523	LHG	C11-C12-C13-C14
34	c	501	LMG	C13-C14-C15-C16
26	V	313	CHL	O1D-CGD-O2D-CED
25	n	312	LHG	C11-C10-C9-C8
36	c	518	DGD	O6D-C5D-C6D-O5D
22	V	304	CLA	CBA-CGA-O2A-C1
22	D	403	CLA	CBA-CGA-O2A-C1
36	c	519	DGD	C5A-C6A-C7A-C8A
22	p	305	CLA	C2A-CAA-CBA-CGA
22	q	305	CLA	C2A-CAA-CBA-CGA
22	P	308	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	C2A-CAA-CBA-CGA
36	c	517	DGD	O6E-C1E-O5D-C6D
22	R	304	CLA	C5-C6-C7-C8
23	n	310	LUT	C29-C30-C31-C32
23	S	311	LUT	C33-C34-C35-C15
23	s	311	LUT	C33-C34-C35-C15
24	n	311	XAT	C33-C34-C35-C15
31	x	202	BCR	C15-C16-C17-C18
31	z	101	BCR	C19-C20-C21-C22
31	C	516	BCR	C19-C20-C21-C22
34	C	502	LMG	C13-C14-C15-C16
25	q	310	LHG	O6-C4-C5-C6
22	N	304	CLA	O1A-CGA-O2A-C1
22	s	301	CLA	CAA-CBA-CGA-O2A
22	B	603	CLA	C10-C11-C12-C13
25	3	310	LHG	C32-C33-C34-C35
25	N	312	LHG	C11-C10-C9-C8
26	3	316	CHL	C2C-C3C-CAC-CBC
26	s	315	CHL	CBD-CGD-O2D-CED
32	a	410	SQD	C7-C8-C9-C10
22	C	508	CLA	C3-C5-C6-C7
25	s	312	LHG	C11-C10-C9-C8
36	C	520	DGD	C3B-C4B-C5B-C6B
22	1	305	CLA	C4-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
26	v	313	CHL	C4-C3-C5-C6
33	d	404	PL9	C35-C34-C36-C37
22	C	506	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	l	102	SQD	C16-C17-C18-C19
26	p	317	CHL	C2-C3-C5-C6
26	g	315	CHL	C2-C3-C5-C6
22	N	307	CLA	O1A-CGA-O2A-C1
22	R	310	CLA	O1A-CGA-O2A-C1
32	a	413	SQD	C13-C14-C15-C16
26	Q	311	CHL	C5-C6-C7-C8
25	S	312	LHG	O9-C7-O7-C5
25	U	312	LHG	C9-C10-C11-C12
36	c	518	DGD	CAB-CBB-CCB-CDB
22	1	305	CLA	C2-C1-O2A-CGA
22	2	302	CLA	C2-C1-O2A-CGA
22	G	304	CLA	C2-C1-O2A-CGA
22	G	306	CLA	C2-C1-O2A-CGA
22	R	302	CLA	C2-C1-O2A-CGA
22	C	504	CLA	C2-C1-O2A-CGA
22	B	611	CLA	C2-C1-O2A-CGA
26	v	315	CHL	C2-C1-O2A-CGA
26	g	314	CHL	C2-C1-O2A-CGA
25	c	522	LHG	C25-C26-C27-C28
34	d	407	LMG	C16-C17-C18-C19
36	a	416	DGD	C4A-C5A-C6A-C7A
22	b	616	CLA	C5-C6-C7-C8
26	g	316	CHL	C5-C6-C7-C8
32	a	410	SQD	C10-C11-C12-C13
22	5	307	CLA	C2A-CAA-CBA-CGA
22	q	308	CLA	C2A-CAA-CBA-CGA
22	N	304	CLA	C2A-CAA-CBA-CGA
22	G	303	CLA	C2A-CAA-CBA-CGA
22	S	303	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
22	B	615	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
22	b	615	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
25	P	313	LHG	O7-C5-C6-O8
22	b	603	CLA	C15-C16-C17-C18
25	b	623	LHG	C2-C3-O3-P
34	w	201	LMG	C16-C17-C18-C19
36	c	518	DGD	C6B-C7B-C8B-C9B
22	r	604	CLA	C3A-C2A-CAA-CBA
22	R	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	q	314	CHL	C3A-C2A-CAA-CBA
30	d	401	PHO	C3A-C2A-CAA-CBA
30	D	401	PHO	C3A-C2A-CAA-CBA
22	r	606	CLA	C16-C17-C18-C20
25	B	623	LHG	C28-C29-C30-C31
32	a	410	SQD	C26-C27-C28-C29
26	G	313	CHL	O2A-C1-C2-C3
26	n	315	CHL	O2A-C1-C2-C3
22	b	616	CLA	CBD-CGD-O2D-CED
32	C	501	SQD	C28-C29-C30-C31
31	X	201	BCR	C15-C16-C17-C18
25	r	613	LHG	C28-C29-C30-C31
25	q	310	LHG	C9-C10-C11-C12
26	N	317	CHL	C2C-C3C-CAC-CBC
22	a	408	CLA	C4-C3-C5-C6
22	g	307	CLA	C4-C3-C5-C6
26	P	317	CHL	C4-C3-C5-C6
33	D	405	PL9	C35-C34-C36-C37
36	B	601	DGD	C1B-C2B-C3B-C4B
26	v	316	CHL	C2-C3-C5-C6
22	V	301	CLA	C8-C10-C11-C12
22	S	301	CLA	CAA-CBA-CGA-O2A
22	1	305	CLA	C6-C7-C8-C9
22	6	305	CLA	C14-C13-C15-C16
22	B	605	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C10-C8-C9
26	4	316	CHL	C14-C13-C15-C16
26	p	320	CHL	C11-C12-C13-C14
26	q	311	CHL	C6-C7-C8-C9
26	V	316	CHL	C11-C10-C8-C9
26	V	316	CHL	C11-C12-C13-C14
26	G	311	CHL	C11-C10-C8-C9
26	u	318	CHL	C11-C12-C13-C14
26	g	311	CHL	C11-C10-C8-C9
26	g	314	CHL	C11-C12-C13-C14
22	s	305	CLA	C5-C6-C7-C8
25	l	101	LHG	O10-C23-O8-C6
34	b	624	LMG	C30-C31-C32-C33
26	6	315	CHL	C10-C11-C12-C13
25	r	613	LHG	C4-C5-C6-O8
25	p	313	LHG	C4-C5-C6-O8
27	r	617	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
27	r	618	NEX	C39-C29-C30-C31
27	2	319	NEX	C39-C29-C30-C31
27	5	319	NEX	C39-C29-C30-C31
27	v	319	NEX	C39-C29-C30-C31
27	p	301	NEX	C39-C29-C30-C31
27	V	319	NEX	C39-C29-C30-C31
27	P	301	NEX	C39-C29-C30-C31
27	U	318	NEX	C39-C29-C30-C31
27	N	318	NEX	C39-C29-C30-C31
27	u	319	NEX	C39-C29-C30-C31
27	u	320	NEX	C39-C29-C30-C31
27	n	319	NEX	C39-C29-C30-C31
27	R	301	NEX	C39-C29-C30-C31
27	S	317	NEX	C39-C29-C30-C31
27	s	317	NEX	C39-C29-C30-C31
36	c	518	DGD	O1B-C1B-O2G-C2G
25	c	523	LHG	C11-C10-C9-C8
32	L	102	SQD	C16-C17-C18-C19
22	3	306	CLA	C2A-CAA-CBA-CGA
22	B	606	CLA	C2A-CAA-CBA-CGA
34	D	408	LMG	C12-C13-C14-C15
26	v	314	CHL	O1A-CGA-O2A-C1
25	B	623	LHG	C26-C27-C28-C29
34	b	624	LMG	C15-C16-C17-C18
22	u	306	CLA	C11-C12-C13-C14
25	C	523	LHG	C25-C26-C27-C28
24	q	309	XAT	C27-C28-C29-C39
24	R	313	XAT	C7-C8-C9-C19
34	c	520	LMG	C33-C34-C35-C36
22	C	504	CLA	C15-C16-C17-C18
25	v	312	LHG	C9-C10-C11-C12
25	U	312	LHG	C26-C27-C28-C29
23	R	312	LUT	C7-C8-C9-C10
34	C	521	LMG	C9-C8-O7-C10
34	c	520	LMG	C9-C8-O7-C10
22	C	509	CLA	C10-C11-C12-C13
22	B	613	CLA	C8-C10-C11-C12
26	q	315	CHL	C5-C6-C7-C8
22	B	606	CLA	C4-C3-C5-C6
22	r	609	CLA	C1A-C2A-CAA-CBA
22	2	302	CLA	C1A-C2A-CAA-CBA
22	2	306	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	3	308	CLA	C1A-C2A-CAA-CBA
22	5	302	CLA	C1A-C2A-CAA-CBA
22	5	305	CLA	C1A-C2A-CAA-CBA
22	5	306	CLA	C1A-C2A-CAA-CBA
22	p	302	CLA	C1A-C2A-CAA-CBA
22	V	301	CLA	C1A-C2A-CAA-CBA
22	U	304	CLA	C1A-C2A-CAA-CBA
22	n	301	CLA	C1A-C2A-CAA-CBA
22	g	304	CLA	C1A-C2A-CAA-CBA
22	R	302	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	C1A-C2A-CAA-CBA
22	B	604	CLA	C1A-C2A-CAA-CBA
22	b	604	CLA	C1A-C2A-CAA-CBA
22	c	504	CLA	C1A-C2A-CAA-CBA
26	P	318	CHL	C1A-C2A-CAA-CBA
22	4	306	CLA	C6-C7-C8-C10
22	6	306	CLA	C6-C7-C8-C10
22	v	301	CLA	C6-C7-C8-C10
22	p	308	CLA	C11-C10-C8-C7
22	q	304	CLA	C11-C10-C8-C7
22	N	304	CLA	C11-C12-C13-C15
22	n	302	CLA	C11-C10-C8-C7
22	g	307	CLA	C2-C3-C5-C6
22	b	609	CLA	C11-C12-C13-C15
22	c	502	CLA	C11-C10-C8-C7
26	5	316	CHL	C11-C10-C8-C7
26	6	316	CHL	C12-C13-C15-C16
26	p	320	CHL	C6-C7-C8-C10
26	V	317	CHL	C11-C10-C8-C7
26	P	319	CHL	C11-C12-C13-C15
26	G	314	CHL	C6-C7-C8-C10
26	n	313	CHL	C6-C7-C8-C10
34	a	412	LMG	C10-C11-C12-C13
22	c	509	CLA	O1A-CGA-O2A-C1
32	a	413	SQD	C30-C31-C32-C33
36	b	601	DGD	C9B-CAB-CBB-CCB
26	5	315	CHL	C3C-C2C-CMC-OMC
26	p	320	CHL	C3C-C2C-CMC-OMC
26	G	315	CHL	C3C-C2C-CMC-OMC
25	Q	310	LHG	C25-C26-C27-C28
34	c	520	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	C10-C11-C12-C13
25	L	101	LHG	C31-C32-C33-C34
32	A	412	SQD	C32-C33-C34-C35
34	A	411	LMG	C40-C41-C42-C43
34	B	624	LMG	C15-C16-C17-C18
22	b	616	CLA	O1D-CGD-O2D-CED
22	3	303	CLA	C2A-CAA-CBA-CGA
22	5	304	CLA	C2A-CAA-CBA-CGA
22	q	307	CLA	C2A-CAA-CBA-CGA
22	P	305	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
22	s	303	CLA	C2A-CAA-CBA-CGA
26	S	313	CHL	C2A-CAA-CBA-CGA
26	s	313	CHL	C2A-CAA-CBA-CGA
22	a	405	CLA	C13-C15-C16-C17
22	4	302	CLA	C13-C15-C16-C17
22	b	613	CLA	C8-C10-C11-C12
36	J	101	DGD	C5A-C6A-C7A-C8A
26	N	315	CHL	O2A-C1-C2-C3
26	n	318	CHL	CBA-CGA-O2A-C1
34	w	201	LMG	C29-C28-O8-C9
34	B	624	LMG	C30-C31-C32-C33
25	l	101	LHG	C31-C32-C33-C34
22	Q	307	CLA	C16-C17-C18-C19
22	R	307	CLA	C16-C17-C18-C20
22	g	302	CLA	C15-C16-C17-C18
26	V	316	CHL	C15-C16-C17-C18
26	U	313	CHL	C10-C11-C12-C13
34	a	412	LMG	C32-C33-C34-C35
36	c	518	DGD	C5A-C6A-C7A-C8A
22	A	408	CLA	C4-C3-C5-C6
26	6	316	CHL	C4-C3-C5-C6
26	p	319	CHL	C4-C3-C5-C6
26	U	317	CHL	C4-C3-C5-C6
22	Q	302	CLA	C8-C10-C11-C12
22	B	611	CLA	C15-C16-C17-C18
32	M	101	SQD	C7-C8-C9-C10
22	6	303	CLA	C2-C3-C5-C6
26	1	316	CHL	C2-C3-C5-C6
26	P	318	CHL	C2-C3-C5-C6
34	b	621	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	m	101	SQD	C29-C30-C31-C32
36	b	601	DGD	CBA-CCA-CDA-CEA
22	C	509	CLA	C8-C10-C11-C12
22	c	505	CLA	O1A-CGA-O2A-C1
26	q	315	CHL	O1D-CGD-O2D-CED
25	V	312	LHG	C13-C14-C15-C16
36	B	601	DGD	C9B-CAB-CBB-CCB
25	v	312	LHG	O9-C7-O7-C5
27	r	617	NEX	C28-C29-C30-C31
27	r	618	NEX	C28-C29-C30-C31
27	2	319	NEX	C28-C29-C30-C31
27	5	319	NEX	C28-C29-C30-C31
27	v	319	NEX	C28-C29-C30-C31
27	p	301	NEX	C28-C29-C30-C31
27	V	319	NEX	C28-C29-C30-C31
27	P	301	NEX	C28-C29-C30-C31
27	U	318	NEX	C28-C29-C30-C31
27	N	318	NEX	C28-C29-C30-C31
27	u	319	NEX	C28-C29-C30-C31
27	u	320	NEX	C28-C29-C30-C31
27	n	319	NEX	C28-C29-C30-C31
27	R	301	NEX	C28-C29-C30-C31
27	S	317	NEX	C28-C29-C30-C31
27	s	317	NEX	C28-C29-C30-C31
22	v	306	CLA	C8-C10-C11-C12
22	u	306	CLA	C10-C11-C12-C13
22	c	508	CLA	C8-C10-C11-C12
22	d	402	CLA	CBA-CGA-O2A-C1
26	U	319	CHL	C15-C16-C17-C18
23	p	311	LUT	C9-C10-C11-C12
23	u	310	LUT	C29-C30-C31-C32
24	Q	309	XAT	C33-C34-C35-C15
22	U	302	CLA	C8-C10-C11-C12
22	b	604	CLA	C8-C10-C11-C12
26	4	313	CHL	C16-C17-C18-C20
25	u	312	LHG	C24-C25-C26-C27
25	n	312	LHG	C13-C14-C15-C16
32	a	410	SQD	C31-C32-C33-C34
22	4	302	CLA	C5-C6-C7-C8
22	R	307	CLA	C15-C16-C17-C18
22	D	403	CLA	O1A-CGA-O2A-C1
25	l	101	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	L	101	LHG	C1-C2-C3-O3
25	S	312	LHG	C1-C2-C3-O3
22	q	303	CLA	C2-C1-O2A-CGA
22	q	304	CLA	C2-C1-O2A-CGA
22	V	305	CLA	C2-C1-O2A-CGA
22	U	305	CLA	C2-C1-O2A-CGA
22	G	302	CLA	C2-C1-O2A-CGA
22	u	305	CLA	C2-C1-O2A-CGA
22	b	611	CLA	C2-C1-O2A-CGA
26	3	313	CHL	C2-C1-O2A-CGA
26	6	314	CHL	C2-C1-O2A-CGA
26	q	314	CHL	C2-C1-O2A-CGA
26	P	319	CHL	C2-C1-O2A-CGA
26	S	315	CHL	C2-C1-O2A-CGA
26	s	315	CHL	C2-C1-O2A-CGA
22	a	408	CLA	C2-C3-C5-C6
22	3	304	CLA	C2-C3-C5-C6
26	p	318	CHL	C2-C3-C5-C6
26	P	317	CHL	C2-C3-C5-C6
26	u	316	CHL	C2-C3-C5-C6
22	C	513	CLA	O1A-CGA-O2A-C1
26	n	318	CHL	O1A-CGA-O2A-C1
34	w	201	LMG	O10-C28-O8-C9
22	1	302	CLA	C5-C6-C7-C8
36	J	101	DGD	C8A-C9A-CAA-CBA
32	a	410	SQD	C23-C24-C25-C26
22	x	201	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
25	C	523	LHG	C19-C20-C21-C22
26	S	316	CHL	CAA-CBA-CGA-O2A
36	b	601	DGD	C1B-C2B-C3B-C4B
22	P	309	CLA	O1A-CGA-O2A-C1
22	B	604	CLA	C13-C15-C16-C17
22	Q	307	CLA	C2A-CAA-CBA-CGA
22	G	307	CLA	C2A-CAA-CBA-CGA
22	p	302	CLA	C16-C17-C18-C20
26	s	316	CHL	CAA-CBA-CGA-O2A
26	5	315	CHL	O2A-C1-C2-C3
26	2	314	CHL	C2-C1-O2A-CGA
36	C	519	DGD	C2A-C3A-C4A-C5A
36	b	601	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
25	b	623	LHG	O9-C7-C8-C9
22	d	402	CLA	O1A-CGA-O2A-C1
22	V	303	CLA	O1A-CGA-O2A-C1
26	Q	314	CHL	O1A-CGA-O2A-C1
23	2	310	LUT	C1-C6-C7-C8
23	5	309	LUT	C1-C6-C7-C8
23	5	310	LUT	C1-C6-C7-C8
23	p	310	LUT	C1-C6-C7-C8
23	p	311	LUT	C1-C6-C7-C8
23	p	311	LUT	C5-C6-C7-C8
23	P	310	LUT	C1-C6-C7-C8
23	P	310	LUT	C5-C6-C7-C8
23	P	311	LUT	C1-C6-C7-C8
23	U	310	LUT	C1-C6-C7-C8
23	U	310	LUT	C5-C6-C7-C8
23	u	310	LUT	C1-C6-C7-C8
23	S	310	LUT	C1-C6-C7-C8
23	S	311	LUT	C1-C6-C7-C8
23	s	310	LUT	C1-C6-C7-C8
23	s	310	LUT	C5-C6-C7-C8
23	s	311	LUT	C1-C6-C7-C8
31	A	409	BCR	C1-C6-C7-C8
25	2	312	LHG	C24-C25-C26-C27
25	4	312	LHG	C19-C20-C21-C22
22	B	603	CLA	CAA-CBA-CGA-O2A
25	c	522	LHG	C11-C12-C13-C14
36	c	519	DGD	C5B-C6B-C7B-C8B
26	s	316	CHL	CAA-CBA-CGA-O1A
25	3	310	LHG	O1-C1-C2-C3
23	P	311	LUT	C9-C10-C11-C12
24	r	612	XAT	C33-C34-C35-C15
27	u	319	NEX	C29-C30-C31-C32
31	D	404	BCR	C19-C20-C21-C22
31	b	618	BCR	C13-C14-C15-C16
22	V	303	CLA	CBA-CGA-O2A-C1
22	6	302	CLA	C4-C3-C5-C6
22	B	607	CLA	C4-C3-C5-C6
26	P	319	CHL	C4-C3-C5-C6
24	u	311	XAT	C31-C32-C33-C34
31	C	517	BCR	C11-C12-C13-C14
22	r	603	CLA	C5-C6-C7-C8
30	A	407	PHO	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	d	402	CLA	C2-C3-C5-C6
22	R	306	CLA	C2-C3-C5-C6
22	B	602	CLA	CAA-CBA-CGA-O2A
26	6	301	CHL	C3-C5-C6-C7
26	S	313	CHL	CAA-CBA-CGA-O2A
26	p	315	CHL	C2-C1-O2A-CGA
26	N	317	CHL	C4C-C3C-CAC-CBC
26	v	318	CHL	C10-C11-C12-C13
26	Q	314	CHL	CBA-CGA-O2A-C1
26	s	313	CHL	CAA-CBA-CGA-O2A
26	Q	316	CHL	O1A-CGA-O2A-C1
22	3	305	CLA	C11-C12-C13-C15
26	r	614	CHL	C5-C6-C7-C8
26	n	316	CHL	C13-C15-C16-C17
26	S	313	CHL	CAA-CBA-CGA-O1A
26	S	316	CHL	CAA-CBA-CGA-O1A
22	s	306	CLA	C2A-CAA-CBA-CGA
22	P	309	CLA	CBA-CGA-O2A-C1
22	C	513	CLA	CBA-CGA-O2A-C1
25	5	312	LHG	C7-C8-C9-C10
26	S	314	CHL	CAA-CBA-CGA-O2A
26	s	314	CHL	CAA-CBA-CGA-O2A
26	V	313	CHL	C16-C17-C18-C20
32	a	413	SQD	C11-C12-C13-C14
36	c	519	DGD	C8A-C9A-CAA-CBA
22	1	307	CLA	C8-C10-C11-C12
22	n	301	CLA	C13-C15-C16-C17
22	b	604	CLA	C13-C15-C16-C17
26	G	316	CHL	C4-C3-C5-C6
34	C	521	LMG	C40-C41-C42-C43
22	1	306	CLA	C6-C7-C8-C10
22	v	302	CLA	C11-C12-C13-C15
22	p	302	CLA	C2-C3-C5-C6
22	n	305	CLA	C6-C7-C8-C10
22	C	507	CLA	C2-C3-C5-C6
22	C	512	CLA	C2-C3-C5-C6
22	B	608	CLA	C2-C3-C5-C6
26	1	313	CHL	C6-C7-C8-C10
26	v	317	CHL	C11-C12-C13-C15
26	q	311	CHL	C6-C7-C8-C10
26	Q	314	CHL	C11-C12-C13-C15
26	U	317	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	V	307	CLA	CBA-CGA-O2A-C1
26	Q	316	CHL	CBA-CGA-O2A-C1
32	C	501	SQD	C11-C10-C9-C8
25	a	415	LHG	O1-C1-C2-O2
25	u	312	LHG	O1-C1-C2-O2
32	M	101	SQD	C29-C30-C31-C32
23	5	309	LUT	C9-C10-C11-C12
23	U	310	LUT	C29-C30-C31-C32
22	r	608	CLA	CAA-CBA-CGA-O2A
22	C	512	CLA	CAA-CBA-CGA-O2A
26	n	316	CHL	CAA-CBA-CGA-O2A
36	C	519	DGD	C2E-C1E-O5D-C6D
36	c	517	DGD	C2E-C1E-O5D-C6D
22	R	311	CLA	CAA-CBA-CGA-O2A
32	L	102	SQD	C11-C10-C9-C8
25	b	622	LHG	O7-C5-C6-O8
34	a	412	LMG	O7-C8-C9-O8
36	c	517	DGD	O2G-C2G-C3G-O3G
36	c	519	DGD	O1G-C1G-C2G-O2G
22	b	602	CLA	CAA-CBA-CGA-O1A
26	5	314	CHL	C2-C1-O2A-CGA
26	1	315	CHL	O2A-C1-C2-C3
26	2	315	CHL	O2A-C1-C2-C3
26	3	313	CHL	O2A-C1-C2-C3
26	4	315	CHL	O2A-C1-C2-C3
26	6	314	CHL	O2A-C1-C2-C3
26	v	315	CHL	O2A-C1-C2-C3
26	V	315	CHL	O2A-C1-C2-C3
26	Q	313	CHL	O2A-C1-C2-C3
26	g	313	CHL	O2A-C1-C2-C3
22	p	303	CLA	CAA-CBA-CGA-O2A
22	u	306	CLA	CAA-CBA-CGA-O2A
26	u	316	CHL	CAA-CBA-CGA-O2A
22	Q	301	CLA	C15-C16-C17-C18
22	C	503	CLA	C13-C15-C16-C17
22	c	502	CLA	C13-C15-C16-C17
26	6	317	CHL	C10-C11-C12-C13
30	a	407	PHO	C13-C15-C16-C17
26	v	318	CHL	C2C-C3C-CAC-CBC
22	r	606	CLA	C16-C17-C18-C19
26	u	313	CHL	C16-C17-C18-C20
26	s	313	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	p	313	LHG	C24-C23-O8-C6
22	u	302	CLA	CAA-CBA-CGA-O2A
22	n	308	CLA	CAA-CBA-CGA-O2A
22	R	309	CLA	CAA-CBA-CGA-O2A
22	c	511	CLA	CAA-CBA-CGA-O2A
25	u	312	LHG	O8-C23-C24-C25
26	5	316	CHL	CAA-CBA-CGA-O2A
26	G	315	CHL	CAA-CBA-CGA-O2A
26	q	312	CHL	C2-C1-O2A-CGA
22	B	602	CLA	C4-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
22	b	608	CLA	C4-C3-C5-C6
26	3	311	CHL	C4-C3-C5-C6
26	u	313	CHL	C4-C3-C5-C6
26	g	316	CHL	C4-C3-C5-C6
30	a	407	PHO	C4-C3-C5-C6
22	6	306	CLA	C8-C10-C11-C12
25	1	312	LHG	C4-O6-P-O3
25	p	313	LHG	C4-O6-P-O3
22	A	408	CLA	C2-C3-C5-C6
22	c	506	CLA	C2-C3-C5-C6
26	p	319	CHL	C2-C3-C5-C6
26	R	315	CHL	C2-C3-C5-C6
25	D	406	LHG	C30-C31-C32-C33
36	C	520	DGD	C5A-C6A-C7A-C8A
22	q	306	CLA	CAA-CBA-CGA-O2A
22	P	303	CLA	CAA-CBA-CGA-O2A
25	P	313	LHG	O8-C23-C24-C25
34	w	201	LMG	O7-C10-C11-C12
34	c	501	LMG	O8-C28-C29-C30
34	A	411	LMG	C36-C37-C38-C39
34	c	520	LMG	C40-C41-C42-C43
22	S	301	CLA	C12-C13-C15-C16
22	1	302	CLA	C6-C7-C8-C9
22	1	307	CLA	C6-C7-C8-C9
22	2	301	CLA	C14-C13-C15-C16
22	2	302	CLA	C14-C13-C15-C16
22	2	304	CLA	C14-C13-C15-C16
22	3	301	CLA	C11-C10-C8-C9
22	3	307	CLA	C11-C10-C8-C9
22	4	302	CLA	C14-C13-C15-C16
22	6	302	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	v	301	CLA	C6-C7-C8-C9
22	u	302	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	C	514	CLA	C6-C7-C8-C9
26	r	614	CHL	C11-C12-C13-C14
26	1	313	CHL	C11-C10-C8-C9
26	2	318	CHL	C11-C12-C13-C14
26	3	315	CHL	C14-C13-C15-C16
26	4	313	CHL	C11-C10-C8-C9
26	p	320	CHL	C6-C7-C8-C9
26	P	317	CHL	C11-C12-C13-C14
25	g	310	LHG	C24-C25-C26-C27
26	S	314	CHL	CAA-CBA-CGA-O1A
22	V	304	CLA	C3A-C2A-CAA-CBA
22	R	302	CLA	C3A-C2A-CAA-CBA
22	B	608	CLA	C3A-C2A-CAA-CBA
26	6	316	CHL	C3A-C2A-CAA-CBA
26	Q	315	CHL	C3A-C2A-CAA-CBA
22	3	304	CLA	C16-C17-C18-C19
32	l	102	SQD	C11-C10-C9-C8
22	5	302	CLA	CAA-CBA-CGA-O2A
22	v	304	CLA	CAA-CBA-CGA-O2A
22	Q	302	CLA	CAA-CBA-CGA-O2A
22	N	306	CLA	CAA-CBA-CGA-O2A
26	r	615	CHL	CBD-CGD-O2D-CED
26	n	318	CHL	C2C-C3C-CAC-CBC
22	r	603	CLA	CAD-CBD-CGD-O2D
22	A	408	CLA	CAD-CBD-CGD-O2D
22	3	302	CLA	CAD-CBD-CGD-O2D
22	4	304	CLA	CAD-CBD-CGD-O2D
22	5	301	CLA	CAD-CBD-CGD-O2D
22	5	302	CLA	CAD-CBD-CGD-O2D
22	6	306	CLA	CAD-CBD-CGD-O2D
22	v	302	CLA	CAD-CBD-CGD-O2D
22	p	308	CLA	CAD-CBD-CGD-O2D
22	q	306	CLA	CAD-CBD-CGD-O2D
22	q	307	CLA	CAD-CBD-CGD-O2D
22	V	304	CLA	CAD-CBD-CGD-O2D
22	P	302	CLA	CAD-CBD-CGD-O2D
22	P	304	CLA	CAD-CBD-CGD-O2D
22	P	305	CLA	CAD-CBD-CGD-O2D
22	P	308	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	P	309	CLA	CAD-CBD-CGD-O2D
22	Q	301	CLA	CAD-CBD-CGD-O2D
22	U	304	CLA	CAD-CBD-CGD-O2D
22	N	301	CLA	CAD-CBD-CGD-O2D
22	N	302	CLA	CAD-CBD-CGD-O2D
22	N	303	CLA	CAD-CBD-CGD-O2D
22	N	304	CLA	CAD-CBD-CGD-O2D
22	N	306	CLA	CAD-CBD-CGD-O2D
22	n	301	CLA	CAD-CBD-CGD-O2D
22	n	306	CLA	CAD-CBD-CGD-O2D
22	g	306	CLA	CAD-CBD-CGD-O2D
22	S	303	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	B	602	CLA	CAD-CBD-CGD-O2D
22	c	511	CLA	CAD-CBD-CGD-O2D
26	3	312	CHL	CAD-CBD-CGD-O2D
26	6	313	CHL	CAD-CBD-CGD-O2D
26	n	315	CHL	CAD-CBD-CGD-O2D
34	c	520	LMG	C7-C8-O7-C10
22	q	306	CLA	C11-C12-C13-C14
22	R	307	CLA	C16-C17-C18-C19
25	n	312	LHG	C24-C25-C26-C27
25	c	522	LHG	C19-C20-C21-C22
36	c	517	DGD	C2A-C3A-C4A-C5A
26	6	312	CHL	C5-C6-C7-C8
26	N	317	CHL	C5-C6-C7-C8
22	Q	306	CLA	C2A-CAA-CBA-CGA
25	C	524	LHG	C11-C10-C9-C8
22	r	606	CLA	C5-C6-C7-C8
22	S	307	CLA	C2-C1-O2A-CGA
22	C	512	CLA	C2-C1-O2A-CGA
26	4	316	CHL	C2-C1-O2A-CGA
26	s	314	CHL	CAA-CBA-CGA-O1A
25	v	312	LHG	C11-C12-C13-C14
32	a	413	SQD	C32-C33-C34-C35
22	4	302	CLA	CAA-CBA-CGA-O2A
22	6	304	CLA	CAA-CBA-CGA-O2A
22	V	304	CLA	CAA-CBA-CGA-O2A
25	U	312	LHG	O8-C23-C24-C25
25	N	312	LHG	O8-C23-C24-C25
26	r	616	CHL	CAA-CBA-CGA-O2A
26	2	316	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
34	W	201	LMG	O7-C10-C11-C12
36	b	601	DGD	O2G-C1B-C2B-C3B
25	6	311	LHG	C14-C15-C16-C17
25	p	313	LHG	C34-C35-C36-C37
22	R	306	CLA	C4-C3-C5-C6
26	3	315	CHL	C4-C3-C5-C6
26	6	312	CHL	C4-C3-C5-C6
26	u	318	CHL	C4-C3-C5-C6
26	r	615	CHL	C6-C7-C8-C10
22	S	304	CLA	CAA-CBA-CGA-O2A
26	1	314	CHL	C2-C1-O2A-CGA
34	W	201	LMG	C16-C17-C18-C19
26	V	315	CHL	O1D-CGD-O2D-CED
22	C	504	CLA	C2-C3-C5-C6
22	B	607	CLA	C2-C3-C5-C6
22	b	607	CLA	C2-C3-C5-C6
26	6	316	CHL	C2-C3-C5-C6
26	v	313	CHL	C2-C3-C5-C6
22	r	603	CLA	CAA-CBA-CGA-O2A
22	v	306	CLA	CAA-CBA-CGA-O2A
22	N	301	CLA	CAA-CBA-CGA-O2A
22	N	307	CLA	CAA-CBA-CGA-O2A
22	G	302	CLA	CAA-CBA-CGA-O2A
22	n	301	CLA	CAA-CBA-CGA-O2A
26	1	316	CHL	CAA-CBA-CGA-O2A
26	3	313	CHL	CAA-CBA-CGA-O2A
26	R	317	CHL	CAA-CBA-CGA-O2A
26	s	315	CHL	CAA-CBA-CGA-O2A
25	c	523	LHG	C18-C19-C20-C21
23	U	309	LUT	C11-C12-C13-C14
24	P	312	XAT	C7-C8-C9-C10
31	B	618	BCR	C7-C8-C9-C10
25	q	310	LHG	C12-C13-C14-C15
24	r	612	XAT	O4-C6-C7-C8
24	3	309	XAT	O24-C26-C27-C28
24	6	310	XAT	O24-C26-C27-C28
24	N	311	XAT	O24-C26-C27-C28
24	R	313	XAT	O4-C6-C7-C8
24	R	313	XAT	O24-C26-C27-C28
25	2	312	LHG	C4-C5-C6-O8
25	G	310	LHG	C2-C3-O3-P
25	B	622	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
25	b	622	LHG	C4-C5-C6-O8
27	p	301	NEX	O24-C26-C27-C28
27	P	301	NEX	O24-C26-C27-C28
27	U	318	NEX	O24-C26-C27-C28
27	N	318	NEX	O24-C26-C27-C28
27	u	319	NEX	O24-C26-C27-C28
27	n	319	NEX	O24-C26-C27-C28
32	C	501	SQD	O6-C44-C45-C46
34	b	621	LMG	O1-C7-C8-C9
22	r	610	CLA	CAA-CBA-CGA-O2A
26	V	314	CHL	O1A-CGA-O2A-C1
25	Q	310	LHG	O6-C4-C5-O7
25	c	521	LHG	O6-C4-C5-O7
26	r	616	CHL	C10-C11-C12-C13
22	1	306	CLA	CAA-CBA-CGA-O2A
22	4	306	CLA	CAA-CBA-CGA-O2A
22	v	302	CLA	CAA-CBA-CGA-O2A
22	P	307	CLA	CAA-CBA-CGA-O2A
22	U	302	CLA	CAA-CBA-CGA-O2A
26	P	315	CHL	CAA-CBA-CGA-O2A
26	g	314	CHL	CAA-CBA-CGA-O2A
22	R	308	CLA	O2A-C1-C2-C3
26	q	313	CHL	O2A-C1-C2-C3
22	s	304	CLA	CAA-CBA-CGA-O2A
22	a	404	CLA	O2A-C1-C2-C3
22	A	404	CLA	O2A-C1-C2-C3
22	c	510	CLA	O2A-C1-C2-C3
26	r	615	CHL	O2A-C1-C2-C3
26	U	319	CHL	O2A-C1-C2-C3
26	n	316	CHL	O2A-C1-C2-C3
26	R	316	CHL	O2A-C1-C2-C3
25	r	613	LHG	C17-C18-C19-C20
22	2	304	CLA	C2A-CAA-CBA-CGA
22	6	307	CLA	C2A-CAA-CBA-CGA
22	p	304	CLA	C2A-CAA-CBA-CGA
22	U	307	CLA	C2A-CAA-CBA-CGA
22	G	304	CLA	C2A-CAA-CBA-CGA
22	g	307	CLA	C2A-CAA-CBA-CGA
22	2	302	CLA	CAA-CBA-CGA-O2A
26	S	315	CHL	CAA-CBA-CGA-O2A
34	C	502	LMG	O8-C28-C29-C30
36	b	601	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
25	p	313	LHG	O10-C23-O8-C6
22	R	311	CLA	CAA-CBA-CGA-O1A
22	S	304	CLA	CAA-CBA-CGA-O1A
36	B	601	DGD	C6B-C7B-C8B-C9B
25	s	312	LHG	C1-C2-C3-O3
22	R	311	CLA	CBD-CGD-O2D-CED
26	n	316	CHL	CBD-CGD-O2D-CED
22	r	604	CLA	CHA-CBD-CGD-O1D
22	r	604	CLA	CHA-CBD-CGD-O2D
22	1	306	CLA	CHA-CBD-CGD-O1D
22	1	306	CLA	CHA-CBD-CGD-O2D
22	2	303	CLA	CHA-CBD-CGD-O2D
22	2	306	CLA	CHA-CBD-CGD-O1D
22	2	306	CLA	CHA-CBD-CGD-O2D
22	3	303	CLA	CHA-CBD-CGD-O1D
22	3	305	CLA	CHA-CBD-CGD-O1D
22	3	306	CLA	CHA-CBD-CGD-O1D
22	3	306	CLA	CHA-CBD-CGD-O2D
22	4	306	CLA	CHA-CBD-CGD-O1D
22	6	304	CLA	CHA-CBD-CGD-O1D
22	6	304	CLA	CHA-CBD-CGD-O2D
22	6	307	CLA	CHA-CBD-CGD-O2D
22	v	301	CLA	CHA-CBD-CGD-O1D
22	V	301	CLA	CHA-CBD-CGD-O2D
22	V	306	CLA	CHA-CBD-CGD-O1D
22	V	306	CLA	CHA-CBD-CGD-O2D
22	P	307	CLA	CHA-CBD-CGD-O1D
22	Q	302	CLA	CHA-CBD-CGD-O2D
22	Q	306	CLA	CHA-CBD-CGD-O1D
22	Q	306	CLA	CHA-CBD-CGD-O2D
22	U	301	CLA	CHA-CBD-CGD-O1D
22	U	301	CLA	CHA-CBD-CGD-O2D
22	U	303	CLA	CHA-CBD-CGD-O1D
22	N	308	CLA	CHA-CBD-CGD-O1D
22	N	308	CLA	CHA-CBD-CGD-O2D
22	G	301	CLA	CHA-CBD-CGD-O1D
22	G	301	CLA	CHA-CBD-CGD-O2D
22	u	301	CLA	CHA-CBD-CGD-O2D
22	n	302	CLA	CHA-CBD-CGD-O2D
22	g	301	CLA	CHA-CBD-CGD-O1D
22	g	301	CLA	CHA-CBD-CGD-O2D
22	g	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	g	303	CLA	CHA-CBD-CGD-O2D
22	R	304	CLA	CHA-CBD-CGD-O2D
22	R	305	CLA	CHA-CBD-CGD-O1D
22	R	305	CLA	CHA-CBD-CGD-O2D
22	S	302	CLA	CHA-CBD-CGD-O1D
22	S	302	CLA	CHA-CBD-CGD-O2D
22	S	304	CLA	CHA-CBD-CGD-O1D
22	S	304	CLA	CHA-CBD-CGD-O2D
22	S	307	CLA	CHA-CBD-CGD-O1D
22	S	307	CLA	CHA-CBD-CGD-O2D
22	C	514	CLA	CHA-CBD-CGD-O1D
22	B	604	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	B	611	CLA	CHA-CBD-CGD-O2D
22	B	612	CLA	CHA-CBD-CGD-O1D
22	B	612	CLA	CHA-CBD-CGD-O2D
22	B	613	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CHA-CBD-CGD-O2D
22	b	604	CLA	CHA-CBD-CGD-O2D
22	b	608	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CHA-CBD-CGD-O2D
22	b	614	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	c	513	CLA	CHA-CBD-CGD-O1D
22	s	302	CLA	CHA-CBD-CGD-O1D
22	s	302	CLA	CHA-CBD-CGD-O2D
22	s	304	CLA	CHA-CBD-CGD-O1D
22	s	304	CLA	CHA-CBD-CGD-O2D
22	s	307	CLA	CHA-CBD-CGD-O1D
22	s	307	CLA	CHA-CBD-CGD-O2D
26	6	312	CHL	CHA-CBD-CGD-O2D
26	6	317	CHL	CHA-CBD-CGD-O1D
26	6	317	CHL	CHA-CBD-CGD-O2D
26	n	313	CHL	CHA-CBD-CGD-O1D
26	n	313	CHL	CHA-CBD-CGD-O2D
26	g	311	CHL	CHA-CBD-CGD-O1D
26	g	311	CHL	CHA-CBD-CGD-O2D
26	g	316	CHL	CHA-CBD-CGD-O1D
26	g	316	CHL	CHA-CBD-CGD-O2D
22	r	610	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	q	302	CLA	C4-C3-C5-C6
22	5	306	CLA	CAA-CBA-CGA-O2A
22	p	307	CLA	CAA-CBA-CGA-O2A
22	P	308	CLA	CAA-CBA-CGA-O2A
22	N	302	CLA	CAA-CBA-CGA-O2A
22	R	304	CLA	CAA-CBA-CGA-O2A
34	B	621	LMG	O8-C28-C29-C30
25	g	310	LHG	C29-C30-C31-C32
26	3	315	CHL	C2-C3-C5-C6
22	b	611	CLA	C15-C16-C17-C18
26	p	319	CHL	C2C-C3C-CAC-CBC
22	p	305	CLA	C13-C15-C16-C17
22	2	306	CLA	CAA-CBA-CGA-O2A
22	3	306	CLA	CAA-CBA-CGA-O2A
22	q	301	CLA	CAA-CBA-CGA-O2A
22	g	302	CLA	CAA-CBA-CGA-O2A
22	C	503	CLA	CAA-CBA-CGA-O2A
26	3	315	CHL	CAA-CBA-CGA-O2A
32	a	410	SQD	O47-C7-C8-C9
36	B	601	DGD	O2G-C1B-C2B-C3B
25	B	622	LHG	O7-C5-C6-O8
25	c	522	LHG	O7-C5-C6-O8
34	A	411	LMG	O7-C8-C9-O8
34	b	621	LMG	O1-C7-C8-O7
36	J	101	DGD	O1G-C1G-C2G-O2G
36	C	519	DGD	O2G-C2G-C3G-O3G
22	v	304	CLA	O1A-CGA-O2A-C1
34	a	412	LMG	C40-C41-C42-C43
22	c	513	CLA	C5-C6-C7-C8
26	n	313	CHL	C13-C15-C16-C17
34	c	520	LMG	C20-C21-C22-C23
36	a	416	DGD	C3B-C4B-C5B-C6B
26	4	313	CHL	O1D-CGD-O2D-CED
22	2	307	CLA	CAA-CBA-CGA-O2A
22	4	301	CLA	CAA-CBA-CGA-O2A
22	5	305	CLA	CAA-CBA-CGA-O2A
22	6	307	CLA	CAA-CBA-CGA-O2A
22	n	302	CLA	CAA-CBA-CGA-O2A
22	g	306	CLA	CAA-CBA-CGA-O2A
22	R	303	CLA	CAA-CBA-CGA-O2A
22	c	502	CLA	CAA-CBA-CGA-O2A
26	6	314	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	C	501	SQD	O47-C7-C8-C9
26	n	318	CHL	C4C-C3C-CAC-CBC
26	u	313	CHL	C2A-CAA-CBA-CGA
22	s	304	CLA	CAA-CBA-CGA-O1A
25	4	312	LHG	O1-C1-C2-O2
25	B	622	LHG	O1-C1-C2-O2
22	p	305	CLA	C10-C11-C12-C13
22	r	602	CLA	CAA-CBA-CGA-O2A
22	1	301	CLA	CAA-CBA-CGA-O2A
22	1	302	CLA	CAA-CBA-CGA-O2A
22	Q	306	CLA	CAA-CBA-CGA-O2A
22	N	308	CLA	CAA-CBA-CGA-O2A
22	u	307	CLA	CAA-CBA-CGA-O2A
26	n	317	CHL	CAA-CBA-CGA-O2A
34	b	621	LMG	C12-C13-C14-C15
22	4	305	CLA	C8-C10-C11-C12
22	1	304	CLA	C11-C10-C8-C7
22	6	302	CLA	C6-C7-C8-C10
22	6	305	CLA	C12-C13-C15-C16
22	G	307	CLA	C2-C3-C5-C6
26	5	316	CHL	C2-C3-C5-C6
26	6	301	CHL	C11-C10-C8-C7
26	u	318	CHL	C2-C3-C5-C6
22	p	308	CLA	CAA-CBA-CGA-O2A
22	n	306	CLA	CAA-CBA-CGA-O2A
22	S	306	CLA	CAA-CBA-CGA-O2A
25	C	523	LHG	O8-C23-C24-C25
26	u	314	CHL	C2-C1-O2A-CGA
22	6	306	CLA	C6-C7-C8-C9
22	p	308	CLA	C11-C10-C8-C9
22	V	302	CLA	C11-C10-C8-C9
22	n	305	CLA	C6-C7-C8-C9
22	X	202	CLA	C6-C7-C8-C9
22	b	602	CLA	C11-C12-C13-C14
22	b	609	CLA	C11-C12-C13-C14
26	1	318	CHL	C11-C12-C13-C14
26	4	313	CHL	C6-C7-C8-C9
26	5	317	CHL	C11-C12-C13-C14
30	d	401	PHO	C11-C12-C13-C14
30	D	401	PHO	C11-C12-C13-C14
22	R	309	CLA	CAA-CBA-CGA-O1A
22	r	607	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	V	314	CHL	CBA-CGA-O2A-C1
34	A	411	LMG	C29-C28-O8-C9
22	U	306	CLA	CAA-CBA-CGA-O2A
25	G	310	LHG	O8-C23-C24-C25
36	B	601	DGD	O1G-C1A-C2A-C3A
25	u	312	LHG	O10-C23-C24-C25
22	p	302	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C20
36	b	601	DGD	C5B-C6B-C7B-C8B
26	5	318	CHL	C3-C5-C6-C7
25	v	312	LHG	C8-C7-O7-C5
36	c	518	DGD	C2B-C1B-O2G-C2G
22	2	307	CLA	C2A-CAA-CBA-CGA
22	6	308	CLA	C2A-CAA-CBA-CGA
22	v	307	CLA	C2A-CAA-CBA-CGA
22	V	307	CLA	C2A-CAA-CBA-CGA
22	Q	303	CLA	C2A-CAA-CBA-CGA
32	m	101	SQD	O49-C7-C8-C9
34	c	501	LMG	O10-C28-C29-C30
34	b	624	LMG	C29-C30-C31-C32
22	s	302	CLA	CAA-CBA-CGA-O2A
22	r	603	CLA	CAA-CBA-CGA-O1A
22	v	302	CLA	CAA-CBA-CGA-O1A
22	v	306	CLA	CAA-CBA-CGA-O1A
22	q	306	CLA	CAA-CBA-CGA-O1A
22	N	301	CLA	CAA-CBA-CGA-O1A
22	u	302	CLA	CAA-CBA-CGA-O1A
26	r	616	CHL	CAA-CBA-CGA-O1A
26	3	313	CHL	CAA-CBA-CGA-O1A
34	w	201	LMG	O9-C10-C11-C12
36	B	601	DGD	CDA-CEA-CFA-CGA
22	C	512	CLA	C4-C3-C5-C6
26	Q	312	CHL	O1A-CGA-O2A-C1
33	d	404	PL9	C33-C34-C36-C37
26	n	318	CHL	C5-C6-C7-C8
26	G	312	CHL	CBD-CGD-O2D-CED
36	J	101	DGD	C6A-C7A-C8A-C9A
22	Q	302	CLA	CAA-CBA-CGA-O1A
32	M	101	SQD	O49-C7-C8-C9
23	s	311	LUT	C7-C8-C9-C10
24	R	313	XAT	C7-C8-C9-C10
27	N	318	NEX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
31	b	618	BCR	C17-C18-C19-C20
36	c	519	DGD	C6A-C7A-C8A-C9A
22	N	308	CLA	CBA-CGA-O2A-C1
22	a	406	CLA	C1A-C2A-CAA-CBA
22	1	307	CLA	C1A-C2A-CAA-CBA
22	2	303	CLA	C1A-C2A-CAA-CBA
22	3	301	CLA	C1A-C2A-CAA-CBA
22	4	303	CLA	C1A-C2A-CAA-CBA
22	6	302	CLA	C1A-C2A-CAA-CBA
22	6	305	CLA	C1A-C2A-CAA-CBA
22	6	309	CLA	C1A-C2A-CAA-CBA
22	P	303	CLA	C1A-C2A-CAA-CBA
22	P	307	CLA	C1A-C2A-CAA-CBA
22	N	307	CLA	C1A-C2A-CAA-CBA
22	G	305	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
26	r	616	CHL	C1A-C2A-CAA-CBA
26	4	313	CHL	C1A-C2A-CAA-CBA
26	5	314	CHL	C1A-C2A-CAA-CBA
26	6	301	CHL	C1A-C2A-CAA-CBA
26	q	312	CHL	C1A-C2A-CAA-CBA
26	U	315	CHL	C1A-C2A-CAA-CBA
26	G	311	CHL	C1A-C2A-CAA-CBA
26	g	314	CHL	C1A-C2A-CAA-CBA
26	R	317	CHL	C1A-C2A-CAA-CBA
26	S	314	CHL	C1A-C2A-CAA-CBA
22	1	306	CLA	CAA-CBA-CGA-O1A
22	U	302	CLA	CAA-CBA-CGA-O1A
22	n	301	CLA	CAA-CBA-CGA-O1A
26	2	316	CHL	CAA-CBA-CGA-O1A
26	5	316	CHL	CAA-CBA-CGA-O1A
26	P	315	CHL	CAA-CBA-CGA-O1A
26	R	317	CHL	CAA-CBA-CGA-O1A
36	b	601	DGD	O1A-C1A-C2A-C3A
22	B	615	CLA	CAA-CBA-CGA-O2A
32	M	101	SQD	C13-C14-C15-C16
26	n	316	CHL	O1A-CGA-O2A-C1
22	Q	305	CLA	C2-C1-O2A-CGA
22	Q	306	CLA	C2-C1-O2A-CGA
22	N	302	CLA	C2-C1-O2A-CGA
22	c	511	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	s	307	CLA	C2-C1-O2A-CGA
26	1	318	CHL	C2-C1-O2A-CGA
26	6	317	CHL	C4C-C3C-CAC-CBC
22	N	302	CLA	C10-C11-C12-C13
22	4	306	CLA	CAA-CBA-CGA-O1A
22	5	306	CLA	CAA-CBA-CGA-O1A
22	v	304	CLA	CAA-CBA-CGA-O1A
22	p	303	CLA	CAA-CBA-CGA-O1A
22	G	302	CLA	CAA-CBA-CGA-O1A
22	n	308	CLA	CAA-CBA-CGA-O1A
26	G	315	CHL	CAA-CBA-CGA-O1A
26	u	316	CHL	CAA-CBA-CGA-O1A
26	n	316	CHL	CAA-CBA-CGA-O1A
34	W	201	LMG	O9-C10-C11-C12
34	C	502	LMG	O10-C28-C29-C30
36	B	601	DGD	O1A-C1A-C2A-C3A
25	b	623	LHG	C26-C27-C28-C29
32	a	410	SQD	O6-C44-C45-C46
36	C	519	DGD	C1G-C2G-C3G-O3G
36	c	517	DGD	C1G-C2G-C3G-O3G
22	U	307	CLA	CAA-CBA-CGA-O2A
22	s	306	CLA	CAA-CBA-CGA-O2A
25	U	312	LHG	C19-C20-C21-C22
22	3	307	CLA	C2A-CAA-CBA-CGA
22	u	307	CLA	C2A-CAA-CBA-CGA
22	n	307	CLA	C2A-CAA-CBA-CGA
22	B	614	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C2A-CAA-CBA-CGA
22	s	305	CLA	C2A-CAA-CBA-CGA
36	a	416	DGD	C4B-C5B-C6B-C7B
36	C	519	DGD	CDB-CEB-CFB-CGB
26	3	314	CHL	C16-C17-C18-C19
26	u	318	CHL	C16-C17-C18-C20
22	r	608	CLA	CAA-CBA-CGA-O1A
22	3	306	CLA	CAA-CBA-CGA-O1A
22	6	304	CLA	CAA-CBA-CGA-O1A
22	p	307	CLA	CAA-CBA-CGA-O1A
22	P	308	CLA	CAA-CBA-CGA-O1A
22	N	307	CLA	CAA-CBA-CGA-O1A
22	c	511	CLA	CAA-CBA-CGA-O1A
25	P	313	LHG	O10-C23-C24-C25
22	N	301	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	q	312	CHL	O1A-CGA-O2A-C1
22	4	304	CLA	CAA-CBA-CGA-O2A
22	4	306	CLA	C10-C11-C12-C13
25	r	613	LHG	C5-C4-O6-P
25	5	312	LHG	C5-C4-O6-P
25	R	314	LHG	C5-C4-O6-P
22	V	304	CLA	CAA-CBA-CGA-O1A
22	u	306	CLA	CAA-CBA-CGA-O1A
22	n	306	CLA	CAA-CBA-CGA-O1A
22	g	302	CLA	CAA-CBA-CGA-O1A
22	C	512	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	CAA-CBA-CGA-O1A
25	U	312	LHG	O10-C23-C24-C25
25	N	312	LHG	O10-C23-C24-C25
22	P	308	CLA	C2-C3-C5-C6
22	N	308	CLA	O1A-CGA-O2A-C1
26	5	318	CHL	O1A-CGA-O2A-C1
25	3	310	LHG	C3-O3-P-O5
25	4	312	LHG	C3-O3-P-O5
25	5	312	LHG	C3-O3-P-O5
25	5	312	LHG	C4-O6-P-O4
25	P	313	LHG	C4-O6-P-O5
25	G	310	LHG	C3-O3-P-O5
25	g	310	LHG	C3-O3-P-O5
25	g	310	LHG	C4-O6-P-O4
25	S	312	LHG	C3-O3-P-O5
25	C	522	LHG	C4-O6-P-O5
25	b	622	LHG	C3-O3-P-O4
25	s	312	LHG	C3-O3-P-O5
25	q	310	LHG	C23-C24-C25-C26
26	3	316	CHL	C4C-C3C-CAC-CBC
36	c	518	DGD	CCA-CDA-CEA-CFA
22	2	306	CLA	CAA-CBA-CGA-O1A
22	5	305	CLA	CAA-CBA-CGA-O1A
22	P	303	CLA	CAA-CBA-CGA-O1A
22	N	302	CLA	CAA-CBA-CGA-O1A
22	S	306	CLA	CAA-CBA-CGA-O1A
22	C	503	CLA	CAA-CBA-CGA-O1A
25	G	310	LHG	O10-C23-C24-C25
26	6	314	CHL	CAA-CBA-CGA-O1A
26	s	315	CHL	CAA-CBA-CGA-O1A
36	B	601	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
22	b	609	CLA	CAA-CBA-CGA-O2A
26	6	316	CHL	CAA-CBA-CGA-O2A
22	c	512	CLA	O1A-CGA-O2A-C1
34	A	411	LMG	O10-C28-O8-C9
36	A	414	DGD	C3B-C4B-C5B-C6B
36	J	101	DGD	CBB-CCB-CDB-CEB
22	S	302	CLA	CAA-CBA-CGA-O2A
23	p	310	LUT	C5-C6-C7-C8
23	P	311	LUT	C5-C6-C7-C8
23	S	311	LUT	C5-C6-C7-C8
31	B	618	BCR	C1-C6-C7-C8
36	C	520	DGD	C2A-C3A-C4A-C5A
22	q	302	CLA	C13-C15-C16-C17
22	1	302	CLA	CAA-CBA-CGA-O1A
22	p	308	CLA	CAA-CBA-CGA-O1A
22	U	306	CLA	CAA-CBA-CGA-O1A
22	R	304	CLA	CAA-CBA-CGA-O1A
26	1	316	CHL	CAA-CBA-CGA-O1A
26	3	315	CHL	CAA-CBA-CGA-O1A
26	g	314	CHL	CAA-CBA-CGA-O1A
26	S	315	CHL	CAA-CBA-CGA-O1A
34	B	621	LMG	O10-C28-C29-C30
36	b	601	DGD	O1B-C1B-C2B-C3B
25	5	312	LHG	C35-C36-C37-C38
25	P	313	LHG	C27-C28-C29-C30
26	1	317	CHL	O1A-CGA-O2A-C1
26	U	314	CHL	O1A-CGA-O2A-C1
25	4	312	LHG	O8-C23-C24-C25
26	P	314	CHL	CAA-CBA-CGA-O2A
22	G	301	CLA	C5-C6-C7-C8
22	B	613	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C20
22	N	307	CLA	C2A-CAA-CBA-CGA
22	P	307	CLA	CAA-CBA-CGA-O1A
22	N	306	CLA	CAA-CBA-CGA-O1A
22	P	302	CLA	C13-C15-C16-C17
22	Q	304	CLA	C10-C11-C12-C13
22	P	309	CLA	CAA-CBA-CGA-O2A
26	6	301	CHL	CAA-CBA-CGA-O2A
22	G	304	CLA	C13-C15-C16-C17
22	r	602	CLA	CAA-CBA-CGA-O1A
22	2	307	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	A	407	PHO	C4-C3-C5-C6
22	1	305	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
22	p	306	CLA	C11-C12-C13-C14
22	D	403	CLA	C16-C17-C18-C19
22	s	302	CLA	CAA-CBA-CGA-O1A
22	p	302	CLA	CAD-CBD-CGD-O1D
22	p	309	CLA	CAD-CBD-CGD-O1D
22	U	306	CLA	CAD-CBD-CGD-O1D
22	G	305	CLA	CAD-CBD-CGD-O1D
22	u	306	CLA	CAD-CBD-CGD-O1D
22	n	308	CLA	CAD-CBD-CGD-O1D
22	g	305	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O1D
26	r	615	CHL	CAD-CBD-CGD-O1D
26	u	317	CHL	CAD-CBD-CGD-O1D
26	n	318	CHL	CAD-CBD-CGD-O1D
26	S	314	CHL	CAD-CBD-CGD-O1D
26	s	314	CHL	CAD-CBD-CGD-O1D
27	u	319	NEX	C7-C8-C9-C10
32	l	102	SQD	O5-C5-C6-S
32	L	102	SQD	O5-C5-C6-S
32	C	501	SQD	O5-C5-C6-S
22	1	301	CLA	CAA-CBA-CGA-O1A
22	2	302	CLA	CAA-CBA-CGA-O1A
22	4	302	CLA	CAA-CBA-CGA-O1A
22	5	302	CLA	CAA-CBA-CGA-O1A
25	C	523	LHG	O10-C23-C24-C25
36	J	101	DGD	C5B-C6B-C7B-C8B
22	3	303	CLA	CAA-CBA-CGA-O2A
22	6	302	CLA	CAA-CBA-CGA-O2A
22	v	301	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
25	c	522	LHG	O8-C23-C24-C25
22	1	304	CLA	C11-C10-C8-C9
22	N	304	CLA	C11-C12-C13-C14
22	B	609	CLA	C11-C12-C13-C14
22	b	610	CLA	C14-C13-C15-C16
22	c	508	CLA	C11-C10-C8-C9
26	Q	314	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	B	601	DGD	C4B-C5B-C6B-C7B
25	q	310	LHG	O1-C1-C2-O2
22	A	408	CLA	CBD-CGD-O2D-CED
34	C	521	LMG	C20-C21-C22-C23
22	3	304	CLA	C5-C6-C7-C8
26	U	319	CHL	C13-C15-C16-C17
22	4	301	CLA	CAA-CBA-CGA-O1A
22	6	307	CLA	CAA-CBA-CGA-O1A
22	N	308	CLA	CAA-CBA-CGA-O1A
22	g	306	CLA	CAA-CBA-CGA-O1A
26	n	317	CHL	CAA-CBA-CGA-O1A
25	A	413	LHG	C15-C16-C17-C18
25	R	314	LHG	C19-C20-C21-C22
22	v	304	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
26	U	314	CHL	CBA-CGA-O2A-C1
26	n	316	CHL	CBA-CGA-O2A-C1
22	1	307	CLA	CAA-CBA-CGA-O2A
22	3	301	CLA	CAA-CBA-CGA-O2A
22	3	307	CLA	CAA-CBA-CGA-O2A
22	v	303	CLA	CAA-CBA-CGA-O2A
22	V	306	CLA	CAA-CBA-CGA-O2A
22	Q	301	CLA	CAA-CBA-CGA-O2A
22	U	301	CLA	CAA-CBA-CGA-O2A
22	n	307	CLA	CAA-CBA-CGA-O2A
22	R	308	CLA	CAA-CBA-CGA-O2A
22	C	507	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
26	1	314	CHL	CAA-CBA-CGA-O2A
26	1	317	CHL	CAA-CBA-CGA-O2A
26	p	314	CHL	CAA-CBA-CGA-O2A
26	u	313	CHL	CAA-CBA-CGA-O2A
26	n	313	CHL	CAA-CBA-CGA-O2A
22	r	606	CLA	C15-C16-C17-C18
22	C	506	CLA	C8-C10-C11-C12
22	V	307	CLA	O1A-CGA-O2A-C1
36	B	601	DGD	C8A-C9A-CAA-CBA
22	4	307	CLA	CAA-CBA-CGA-O2A
22	5	301	CLA	CAA-CBA-CGA-O2A
22	v	308	CLA	CAA-CBA-CGA-O2A
22	p	302	CLA	CAA-CBA-CGA-O2A
22	P	302	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	G	306	CLA	CAA-CBA-CGA-O2A
22	S	305	CLA	CAA-CBA-CGA-O2A
22	b	611	CLA	CAA-CBA-CGA-O2A
25	q	310	LHG	O8-C23-C24-C25
26	V	313	CHL	CAA-CBA-CGA-O2A
26	U	313	CHL	CAA-CBA-CGA-O2A
26	N	313	CHL	CAA-CBA-CGA-O2A
32	M	101	SQD	O47-C7-C8-C9
22	R	307	CLA	C5-C6-C7-C8
26	1	317	CHL	C10-C11-C12-C13
25	V	312	LHG	C34-C35-C36-C37
25	Q	310	LHG	C24-C25-C26-C27
26	Q	312	CHL	C2-C1-O2A-CGA
32	C	501	SQD	C7-C8-C9-C10
22	q	301	CLA	CAA-CBA-CGA-O1A
22	Q	306	CLA	CAA-CBA-CGA-O1A
22	R	303	CLA	CAA-CBA-CGA-O1A
25	g	310	LHG	C2-C3-O3-P
22	G	307	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
26	2	318	CHL	C4-C3-C5-C6
26	5	318	CHL	C4-C3-C5-C6
26	V	318	CHL	C4-C3-C5-C6
22	v	301	CLA	C13-C15-C16-C17
25	C	523	LHG	C12-C13-C14-C15
22	x	201	CLA	C6-C7-C8-C10
22	2	302	CLA	C3A-C2A-CAA-CBA
22	2	306	CLA	C3A-C2A-CAA-CBA
22	5	302	CLA	C3A-C2A-CAA-CBA
22	5	306	CLA	C3A-C2A-CAA-CBA
22	v	304	CLA	C3A-C2A-CAA-CBA
22	C	513	CLA	C11-C12-C13-C15
22	B	605	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C11-C12-C13-C15
22	B	606	CLA	C2-C3-C5-C6
22	B	609	CLA	C11-C12-C13-C15
22	b	603	CLA	C12-C13-C15-C16
22	b	613	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
26	r	619	CHL	C3A-C2A-CAA-CBA
26	3	316	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	4	316	CHL	C12-C13-C15-C16
26	5	318	CHL	C11-C10-C8-C7
26	6	317	CHL	C3A-C2A-CAA-CBA
26	V	316	CHL	C6-C7-C8-C10
26	Q	314	CHL	C6-C7-C8-C10
26	U	315	CHL	C3A-C2A-CAA-CBA
26	U	317	CHL	C6-C7-C8-C10
26	U	319	CHL	C11-C10-C8-C7
26	G	315	CHL	C3A-C2A-CAA-CBA
26	G	316	CHL	C3A-C2A-CAA-CBA
26	n	318	CHL	C6-C7-C8-C10
33	D	405	PL9	C33-C34-C36-C37
22	3	301	CLA	CAA-CBA-CGA-O1A
22	6	302	CLA	CAA-CBA-CGA-O1A
22	V	301	CLA	CAA-CBA-CGA-O1A
22	n	302	CLA	CAA-CBA-CGA-O1A
37	e	101	HEM	CAA-CBA-CGA-O1A
32	L	102	SQD	C28-C29-C30-C31
22	r	607	CLA	CAA-CBA-CGA-O2A
22	A	404	CLA	CAA-CBA-CGA-O2A
22	1	304	CLA	CAA-CBA-CGA-O2A
22	2	301	CLA	CAA-CBA-CGA-O2A
22	V	301	CLA	CAA-CBA-CGA-O2A
22	B	611	CLA	CAA-CBA-CGA-O2A
22	c	506	CLA	CAA-CBA-CGA-O2A
25	Q	310	LHG	O8-C23-C24-C25
25	b	622	LHG	O8-C23-C24-C25
26	4	313	CHL	CAA-CBA-CGA-O2A
26	g	312	CHL	CAA-CBA-CGA-O2A
32	l	102	SQD	C28-C29-C30-C31
23	S	311	LUT	C7-C8-C9-C10
24	1	311	XAT	C27-C28-C29-C30
24	q	309	XAT	C27-C28-C29-C30
27	5	319	NEX	C31-C32-C33-C34
31	B	618	BCR	C17-C18-C19-C20
22	C	507	CLA	CAA-CBA-CGA-O1A
22	B	615	CLA	CAA-CBA-CGA-O1A
22	b	611	CLA	CAA-CBA-CGA-O1A
26	n	313	CHL	CAA-CBA-CGA-O1A
32	C	501	SQD	O49-C7-C8-C9
24	v	311	XAT	C13-C14-C15-C35
24	p	312	XAT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	b	620	BCR	C13-C14-C15-C16
32	C	501	SQD	C26-C27-C28-C29
34	C	502	LMG	C31-C32-C33-C34
26	u	318	CHL	C16-C17-C18-C19
22	a	404	CLA	CAA-CBA-CGA-O2A
22	2	305	CLA	CAA-CBA-CGA-O2A
25	5	312	LHG	O8-C23-C24-C25
26	4	316	CHL	CAA-CBA-CGA-O2A
26	N	316	CHL	CAA-CBA-CGA-O2A
32	m	101	SQD	O47-C7-C8-C9
22	3	303	CLA	CAA-CBA-CGA-O1A
22	v	301	CLA	CAA-CBA-CGA-O1A
22	v	303	CLA	CAA-CBA-CGA-O1A
22	U	307	CLA	CAA-CBA-CGA-O1A
22	u	307	CLA	CAA-CBA-CGA-O1A
22	n	307	CLA	CAA-CBA-CGA-O1A
22	b	615	CLA	CAA-CBA-CGA-O1A
22	b	617	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
22	s	306	CLA	CAA-CBA-CGA-O1A
25	c	522	LHG	O10-C23-C24-C25
26	4	313	CHL	CAA-CBA-CGA-O1A
26	V	313	CHL	CAA-CBA-CGA-O1A
36	a	416	DGD	CDB-CEB-CFB-CGB
22	v	307	CLA	C8-C10-C11-C12
22	Q	301	CLA	C13-C15-C16-C17
25	L	101	LHG	O2-C2-C3-O3
22	u	301	CLA	CAA-CBA-CGA-O2A
26	P	318	CHL	CAA-CBA-CGA-O2A
26	U	319	CHL	CAA-CBA-CGA-O2A
36	C	520	DGD	O1G-C1A-C2A-C3A
25	c	522	LHG	C30-C31-C32-C33
26	P	319	CHL	C2C-C3C-CAC-CBC
22	3	307	CLA	CAA-CBA-CGA-O1A
22	4	304	CLA	CAA-CBA-CGA-O1A
22	R	308	CLA	CAA-CBA-CGA-O1A
22	B	611	CLA	CAA-CBA-CGA-O1A
25	4	312	LHG	O10-C23-C24-C25
26	1	317	CHL	CAA-CBA-CGA-O1A
26	p	314	CHL	CAA-CBA-CGA-O1A
26	N	313	CHL	CAA-CBA-CGA-O1A
22	U	308	CLA	C2A-CAA-CBA-CGA

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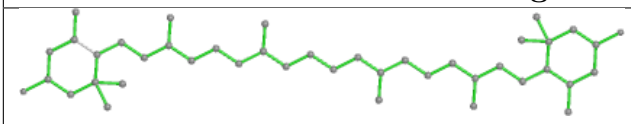
Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C2A-CAA-CBA-CGA
26	p	318	CHL	C2A-CAA-CBA-CGA
26	v	318	CHL	C4C-C3C-CAC-CBC
22	q	306	CLA	C8-C10-C11-C12
22	u	307	CLA	C5-C6-C7-C8
22	S	305	CLA	C5-C6-C7-C8
22	S	306	CLA	C5-C6-C7-C8
22	b	615	CLA	C13-C15-C16-C17
26	Q	312	CHL	CBA-CGA-O2A-C1
36	C	520	DGD	C6B-C7B-C8B-C9B
22	A	408	CLA	C3-C5-C6-C7
22	Q	301	CLA	CAA-CBA-CGA-O1A
26	N	316	CHL	CAA-CBA-CGA-O1A
22	P	308	CLA	C4-C3-C5-C6
25	v	312	LHG	C12-C13-C14-C15
22	G	304	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	CAA-CBA-CGA-O2A
26	2	313	CHL	CAA-CBA-CGA-O2A
22	S	302	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

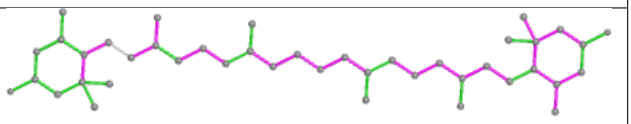
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

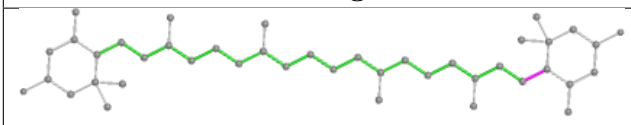
Ligand LUT s 310



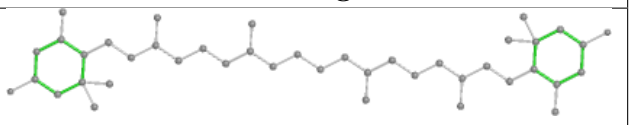
Bond lengths



Bond angles

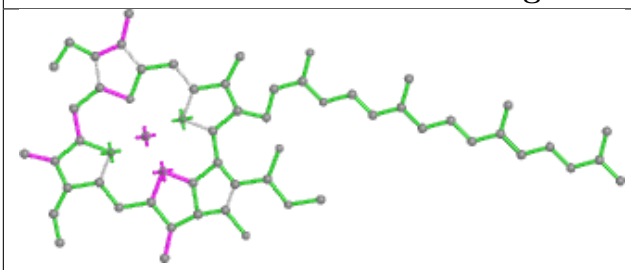


Torsions

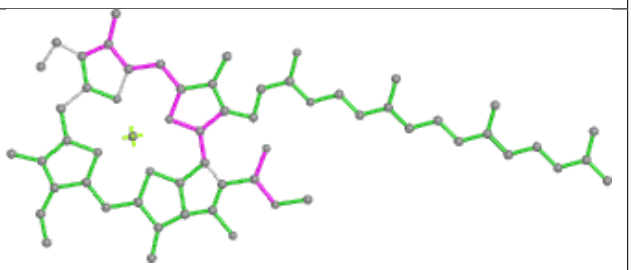


Rings

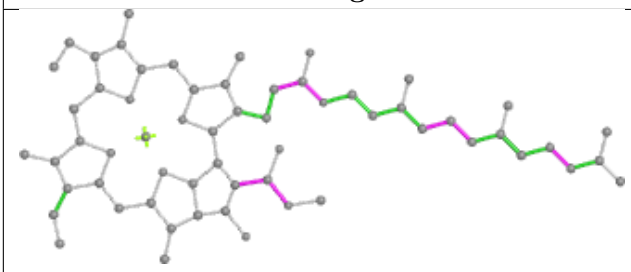
Ligand CLA U 306



Bond lengths



Bond angles



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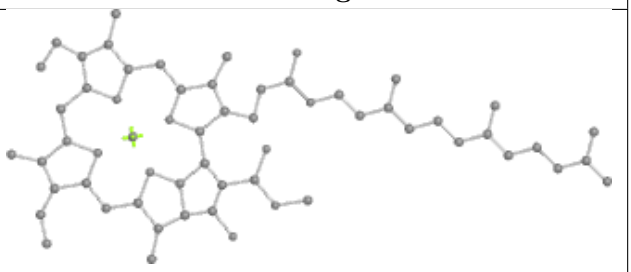
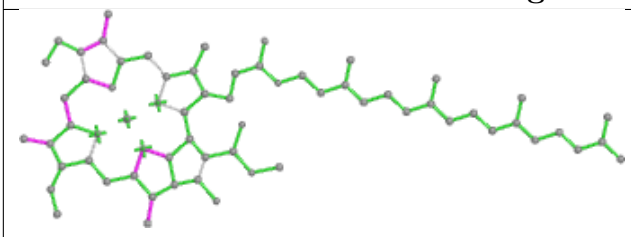
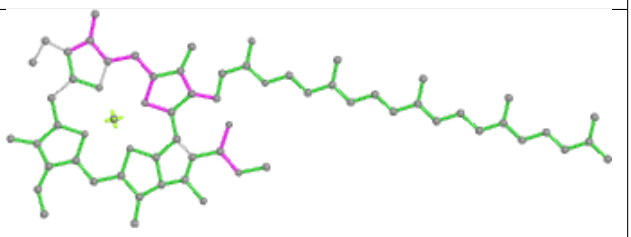


Rings

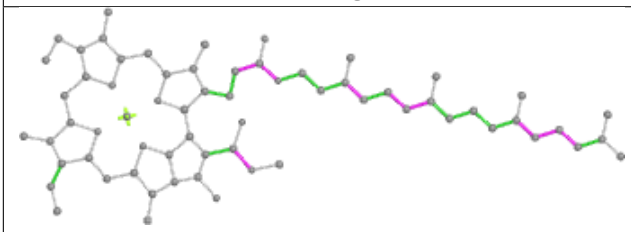
Ligand CLA u 302



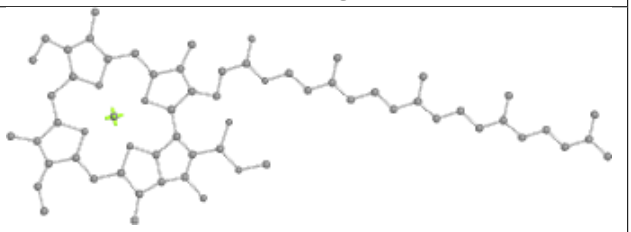
Bond lengths



Bond angles

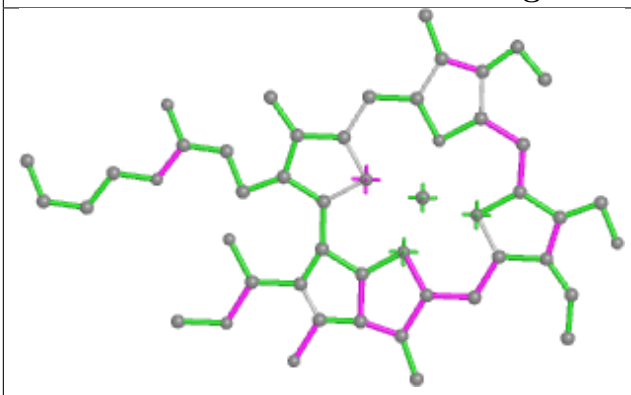


Torsions

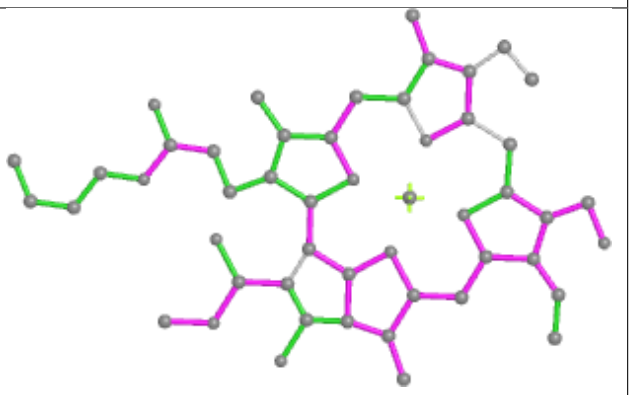


Rings

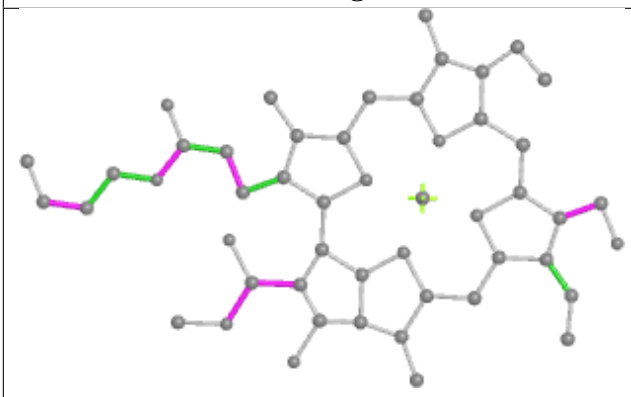
Ligand CHL U 314



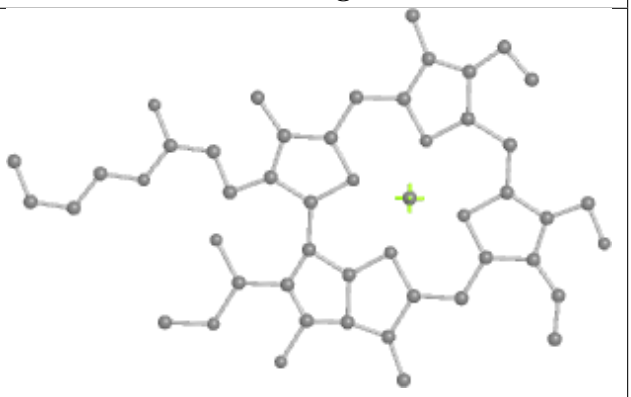
Bond lengths



Bond angles

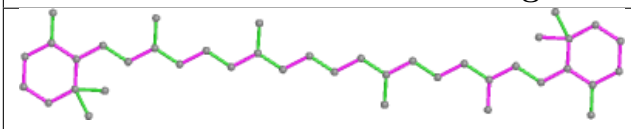


Torsions

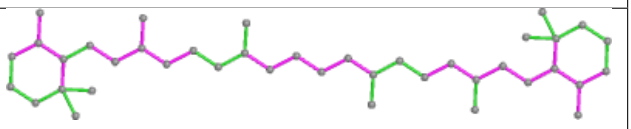


Rings

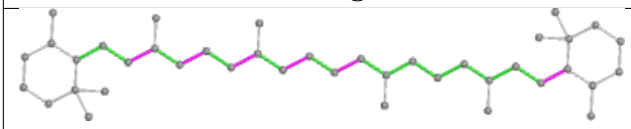
Ligand BCR X 201



Bond lengths



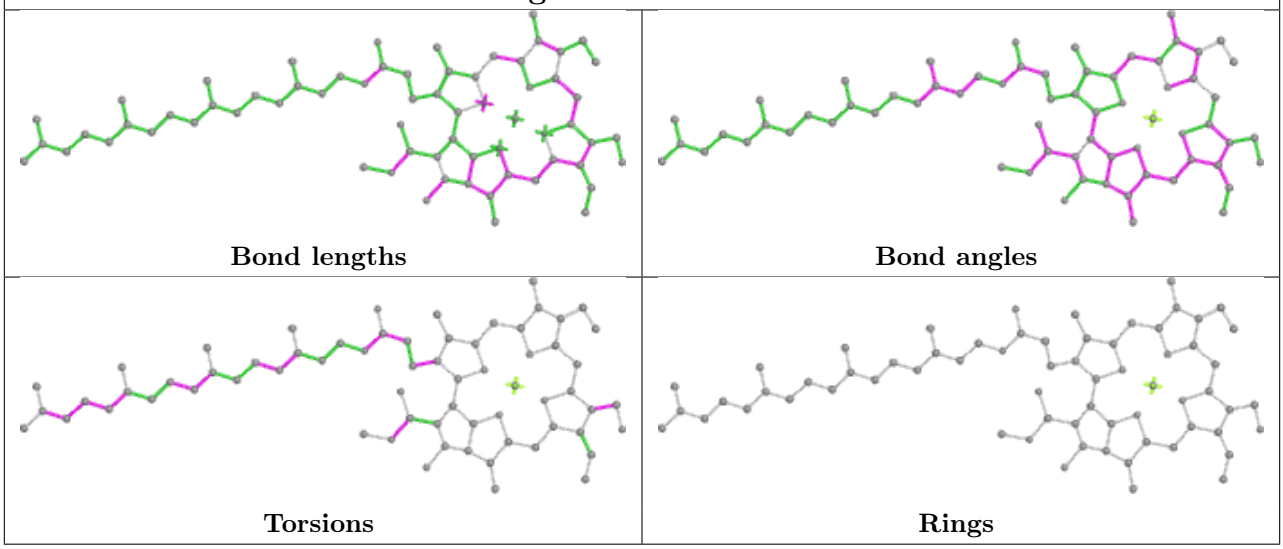
Bond angles



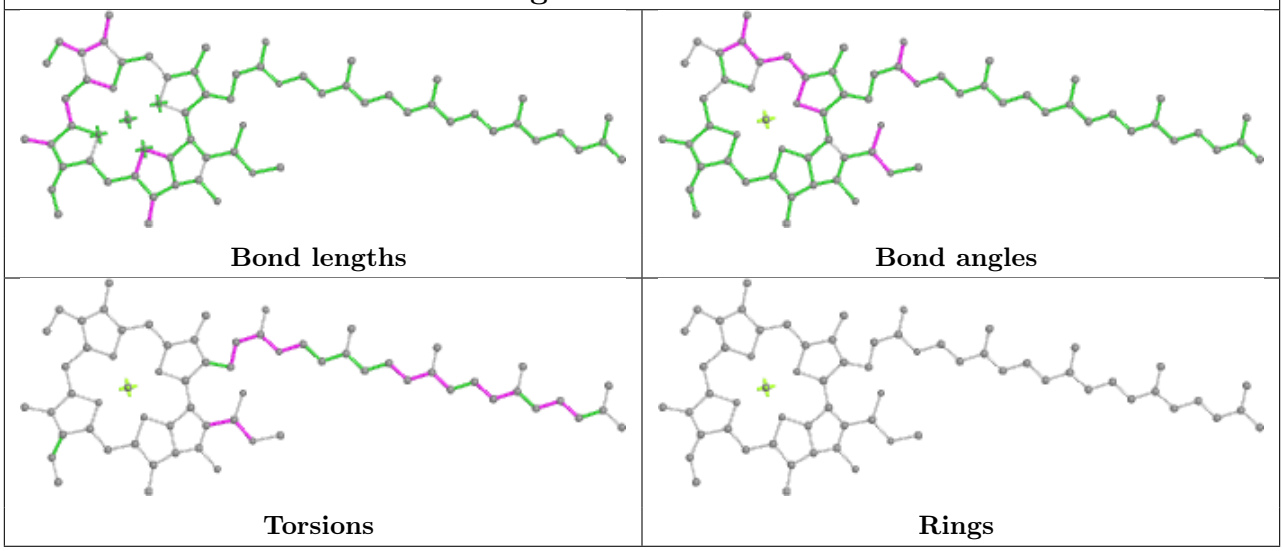
Torsions

Rings

Ligand CHL 6 301



Ligand CLA c 511



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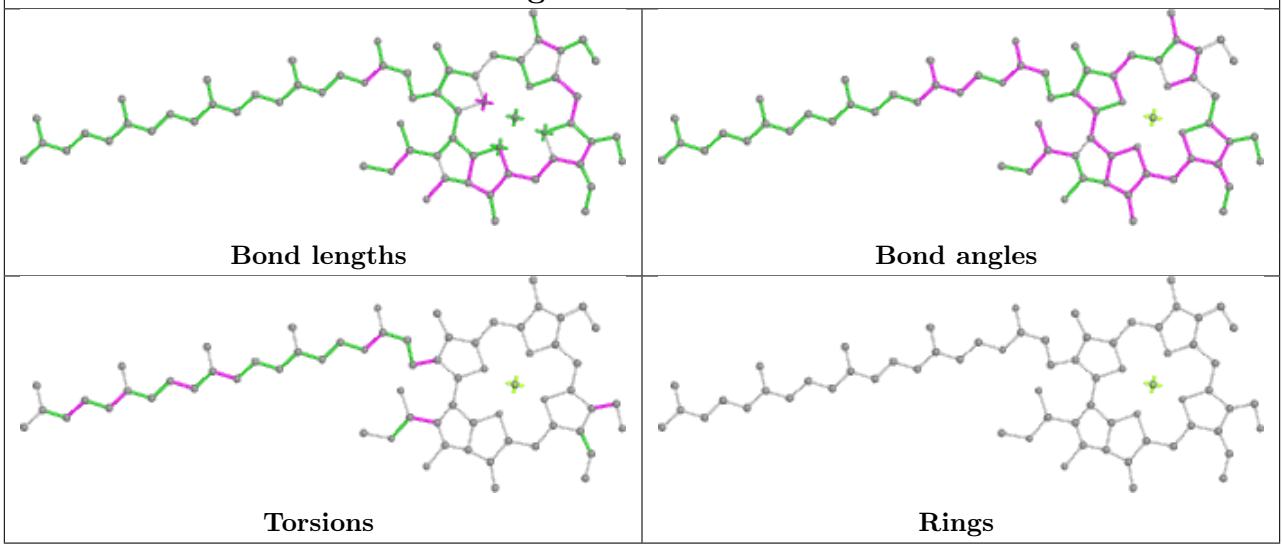
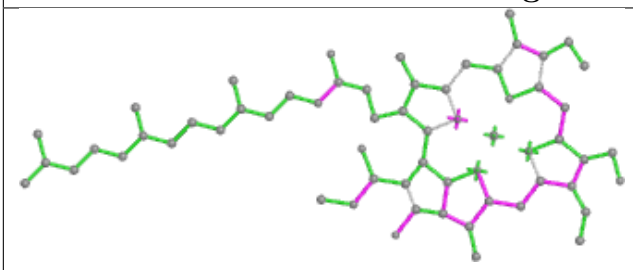
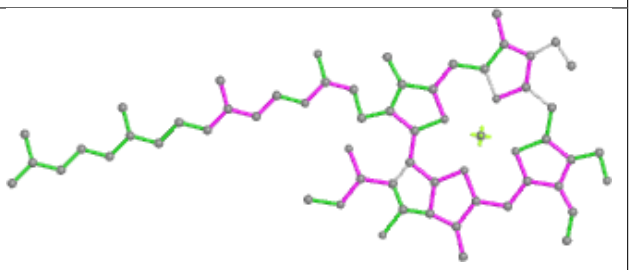


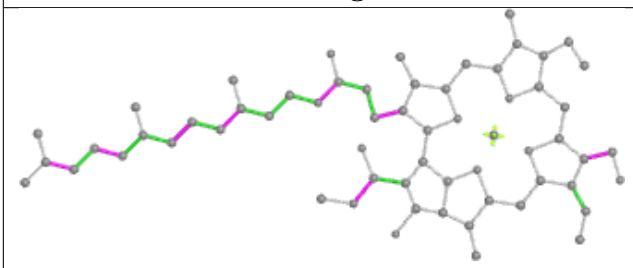
Ligand CHL G 316



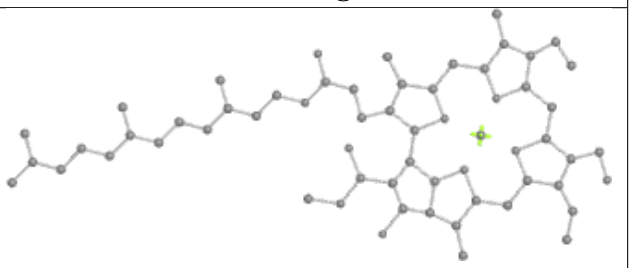
Bond lengths



Bond angles

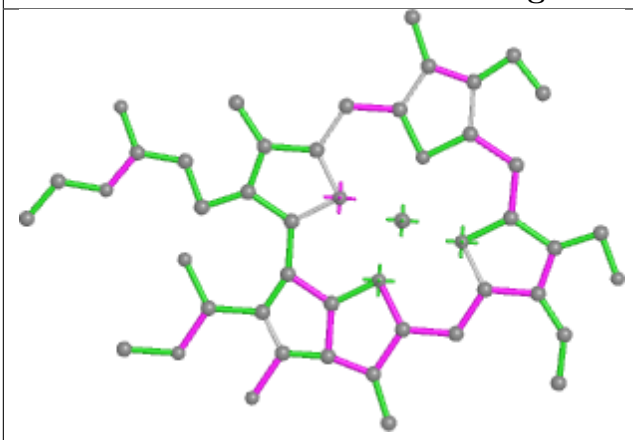


Torsions

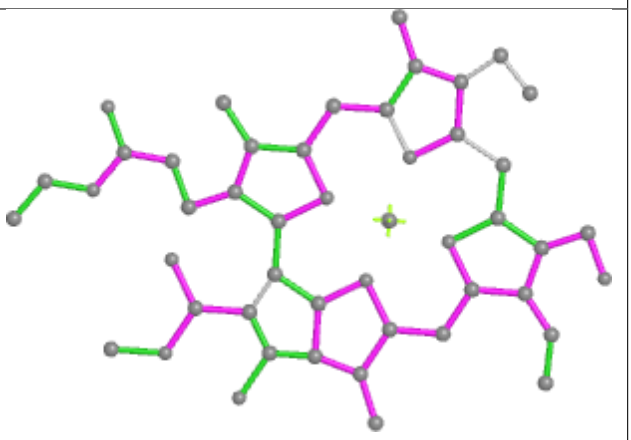


Rings

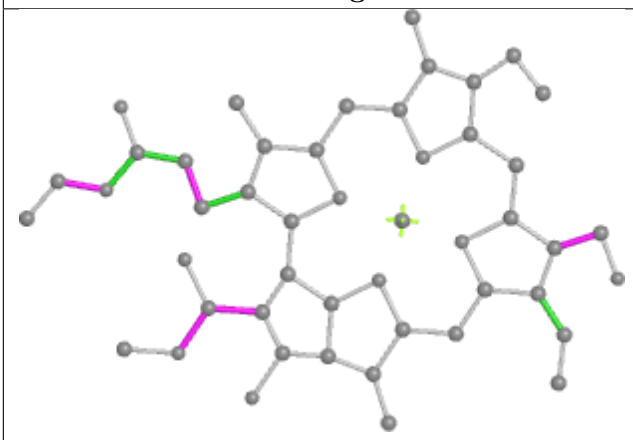
Ligand CHL 2 314



Bond lengths



Bond angles



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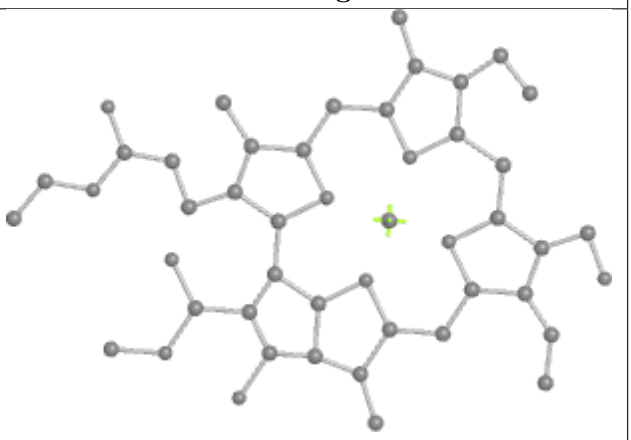
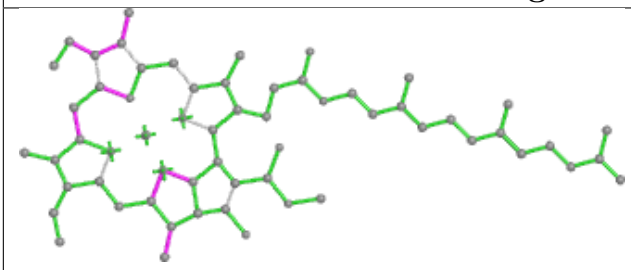
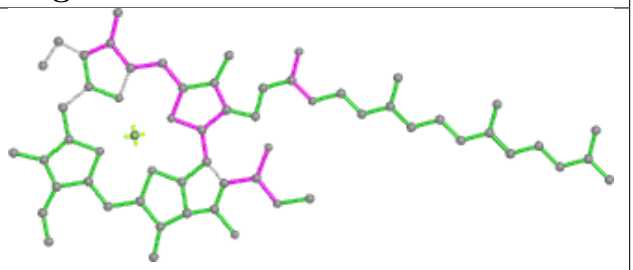
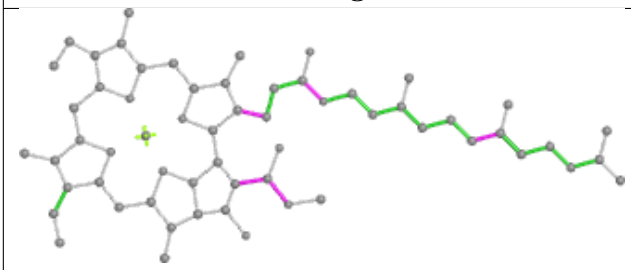
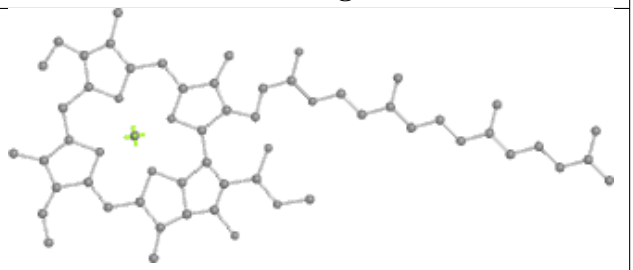


Rings

Ligand CLA g 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

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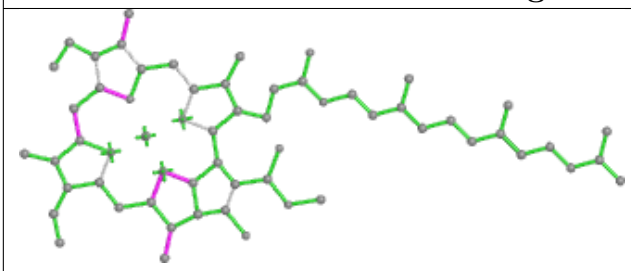
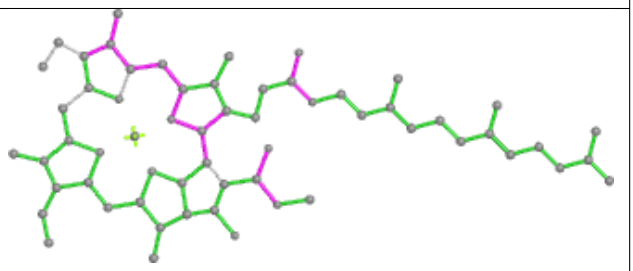
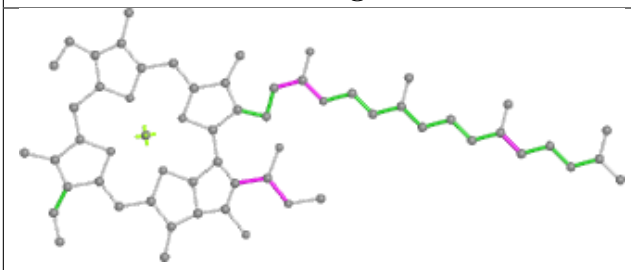
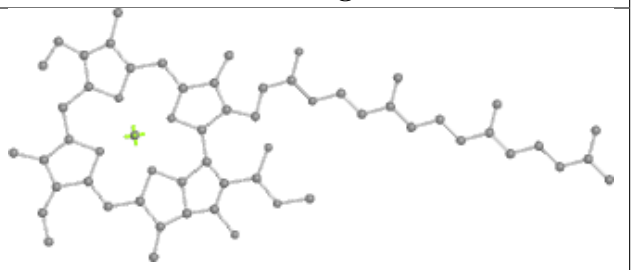
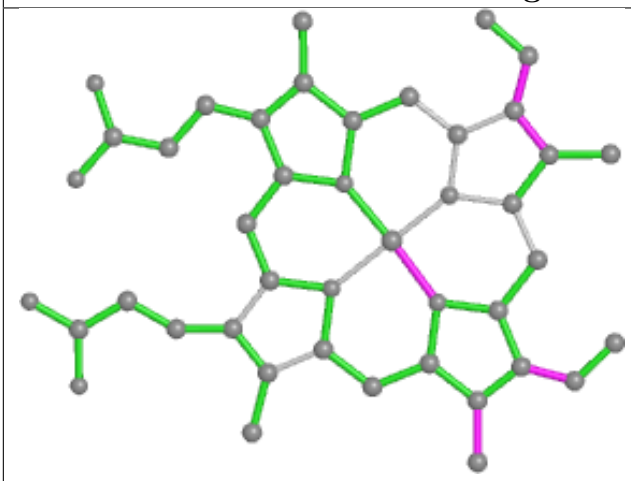
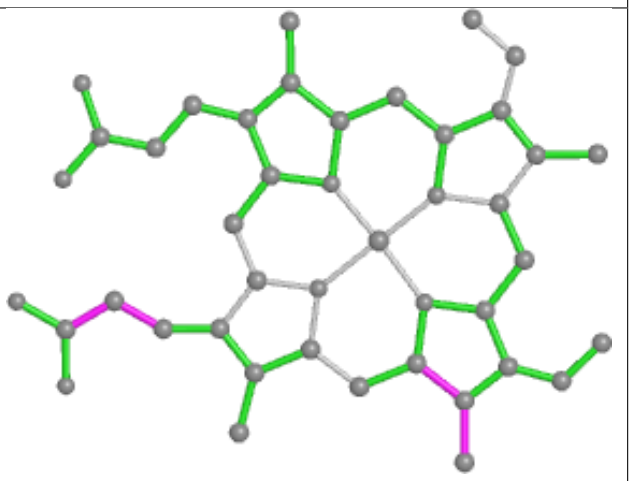
 Bond lengths	 Bond angles
 Torsions	 Rings

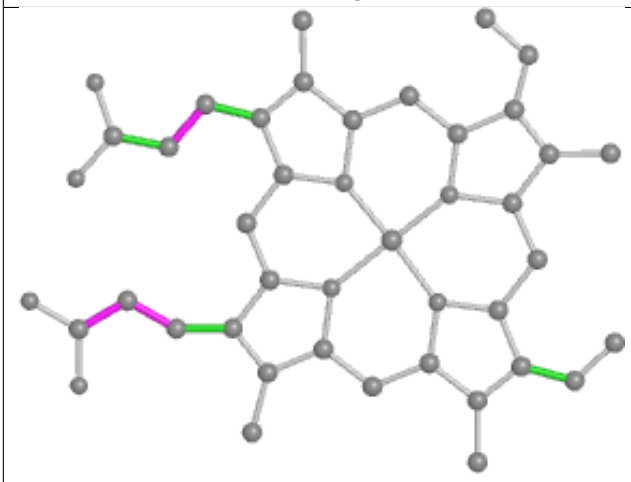
Ligand HEM e 101



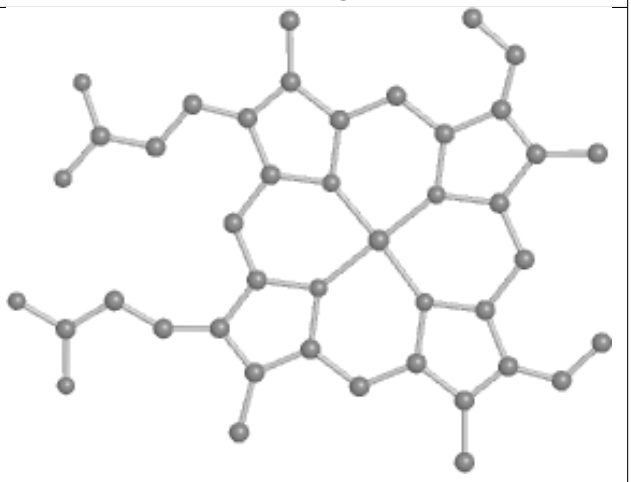
Bond lengths



Bond angles

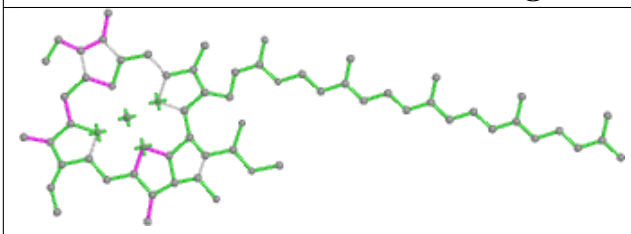


Torsions



Rings

Ligand CLA C 512



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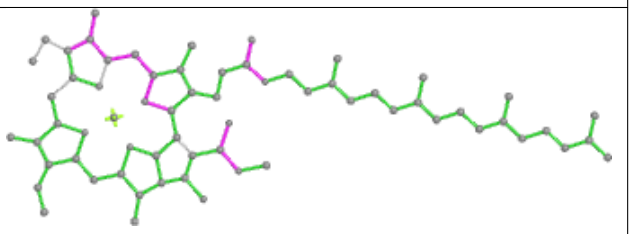
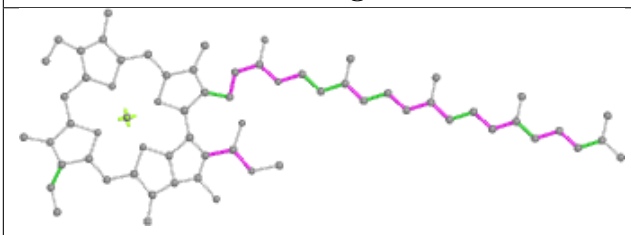


Bond angles



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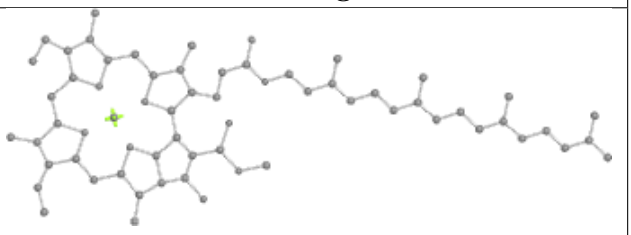
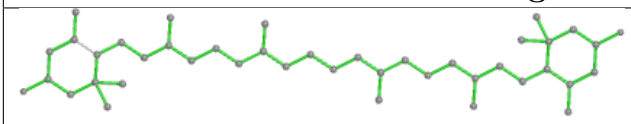
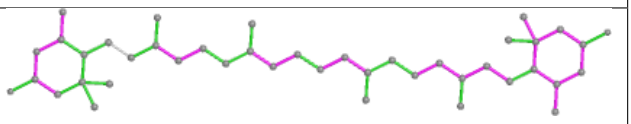
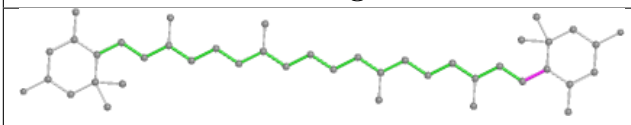
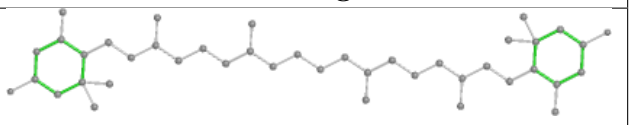


Rings

Ligand LUT 2 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

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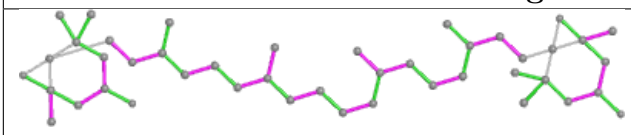
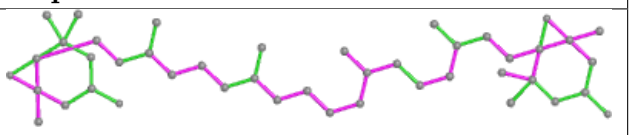
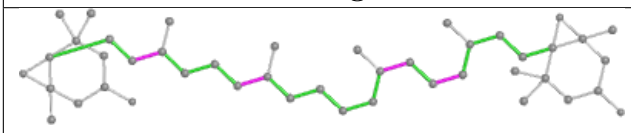
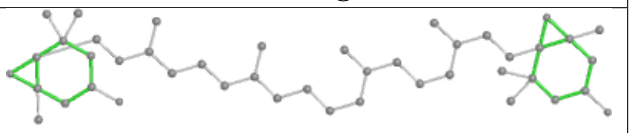
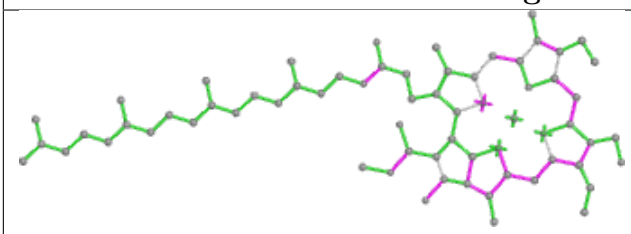
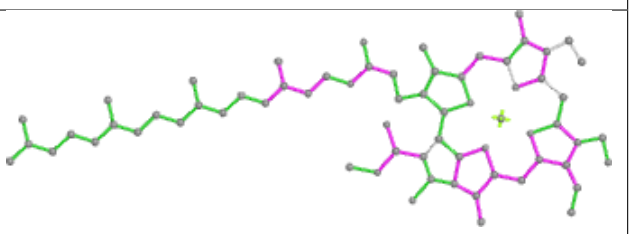
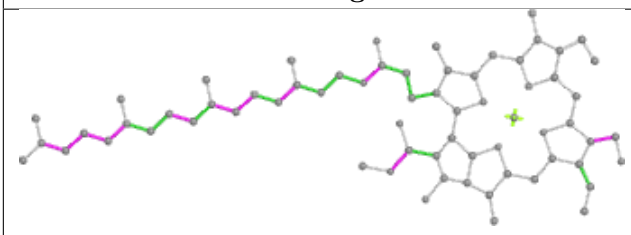
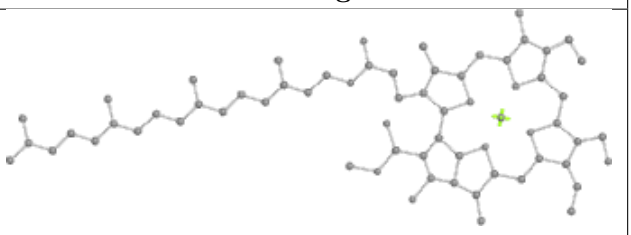
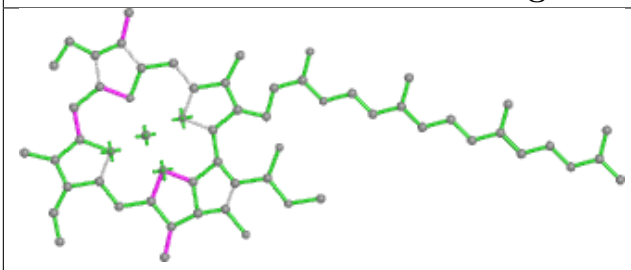
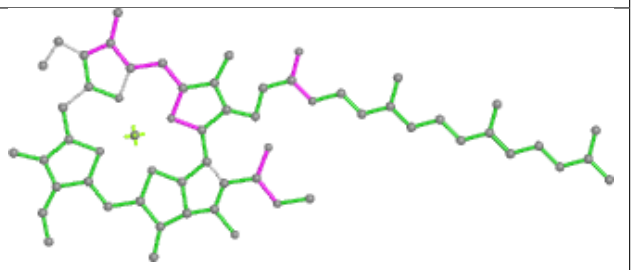
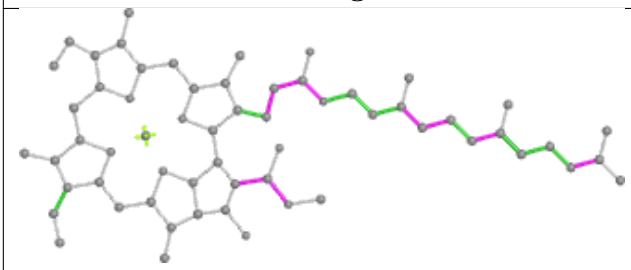
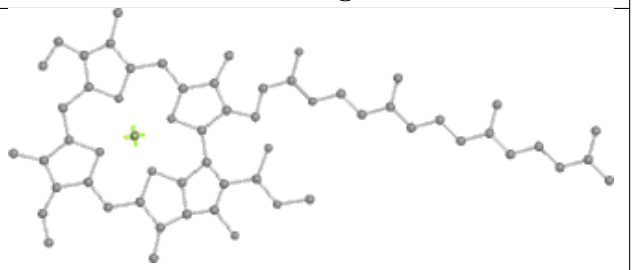
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL V 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

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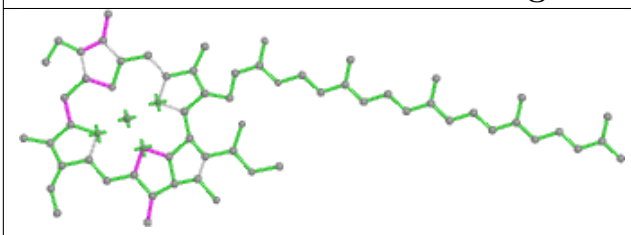
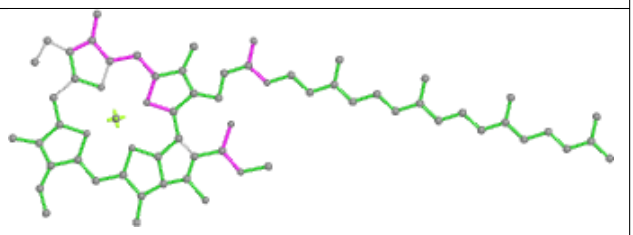
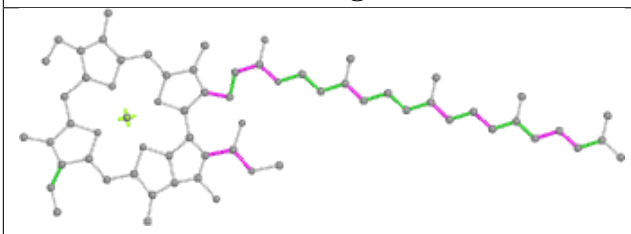
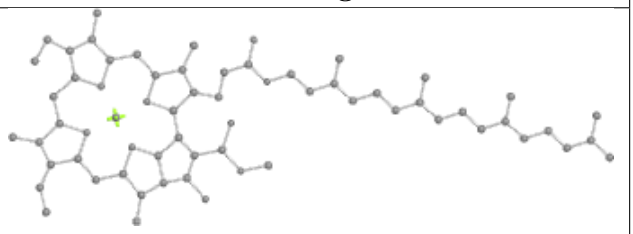
 Bond lengths	 Bond angles
 Torsions	 Rings

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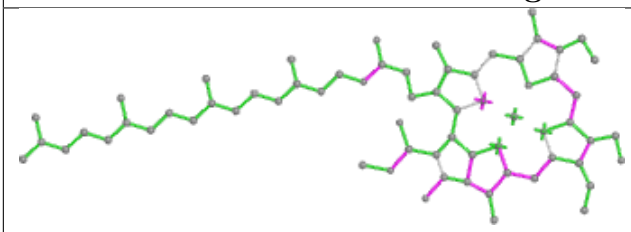
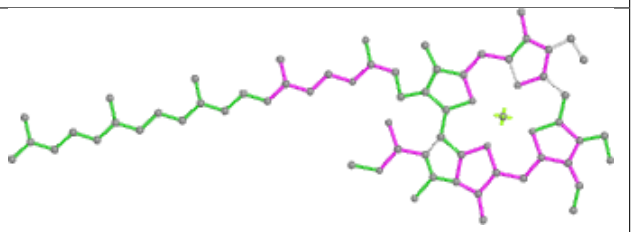
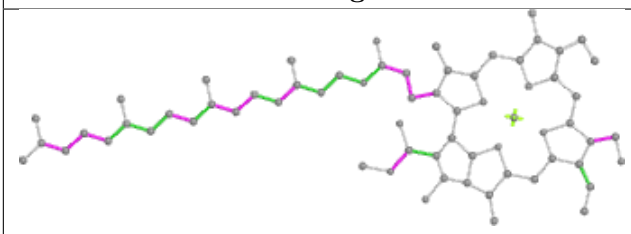
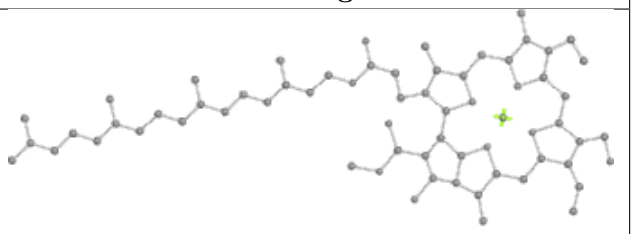
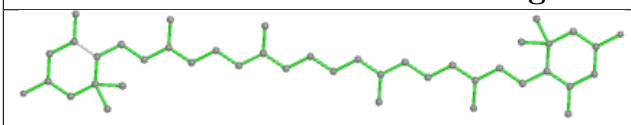
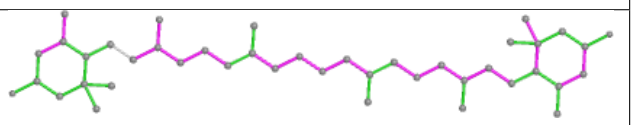
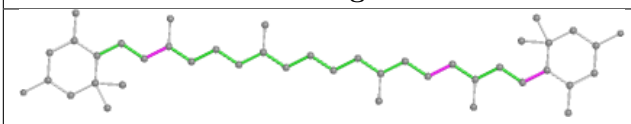
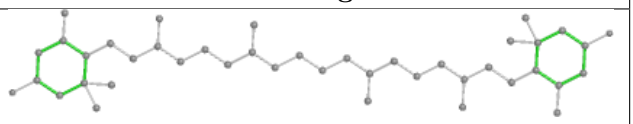
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 5 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

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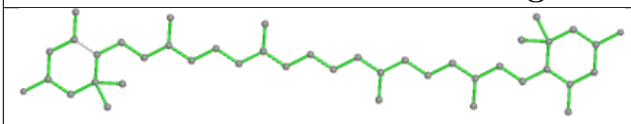
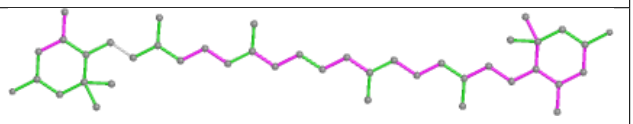
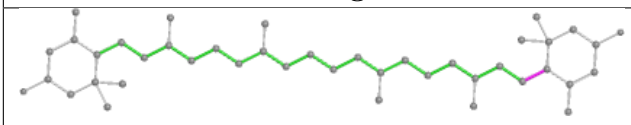
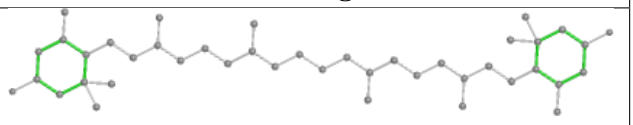
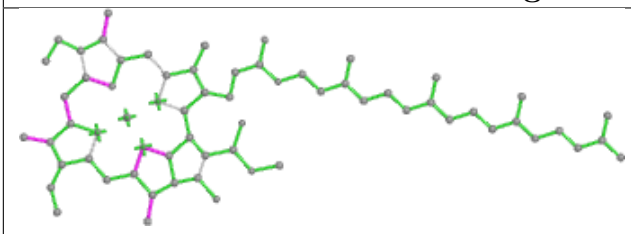
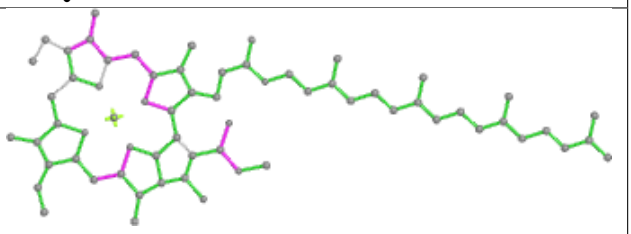
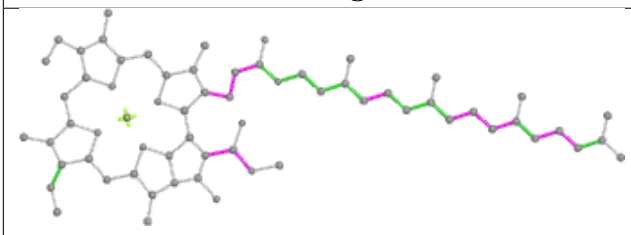
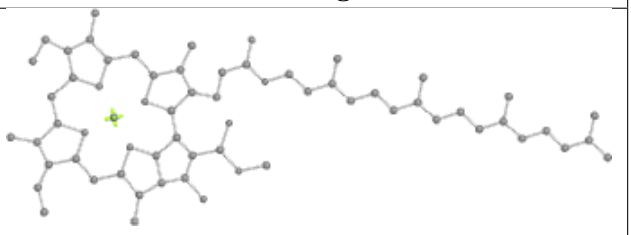
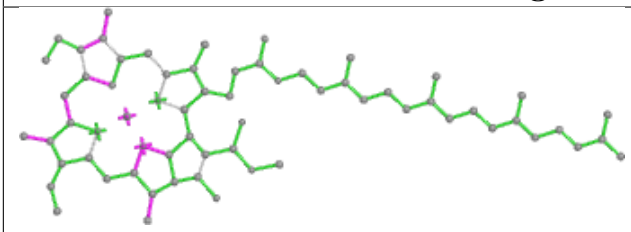
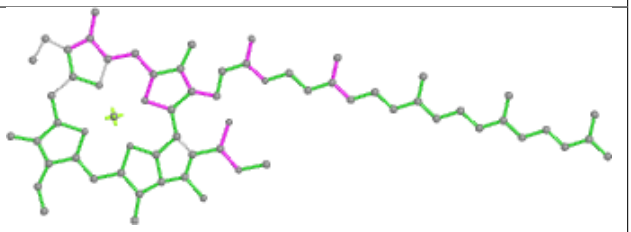
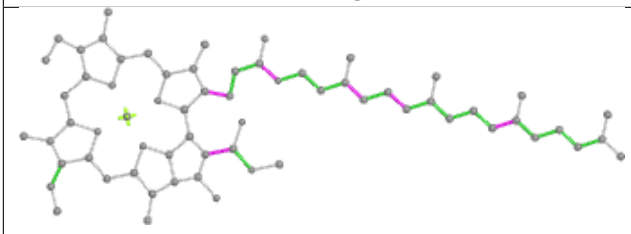
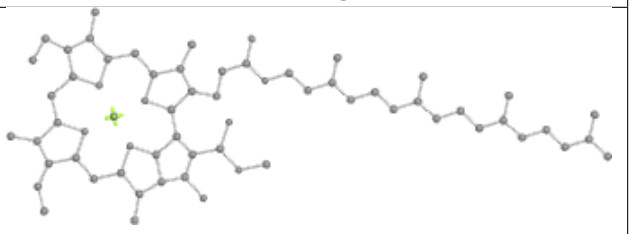
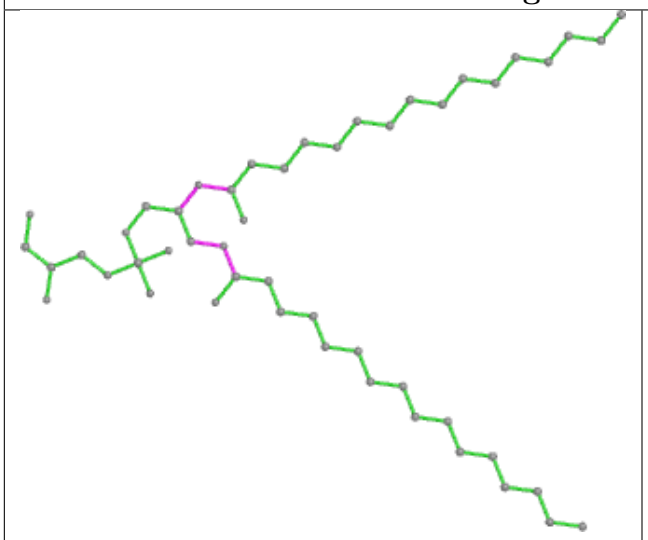
 Bond lengths	 Bond angles
 Torsions	 Rings

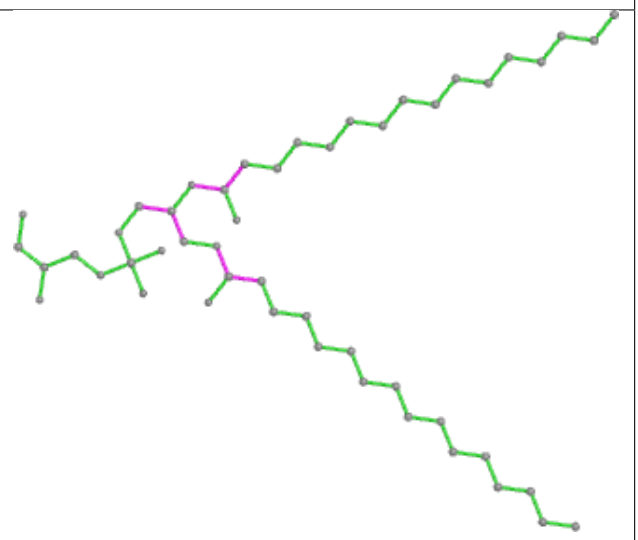
Ligand CLA Q 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

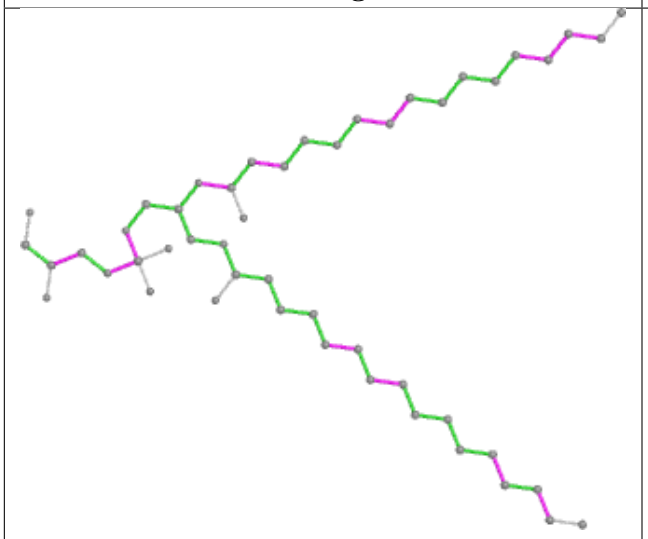
Ligand LHG D 407



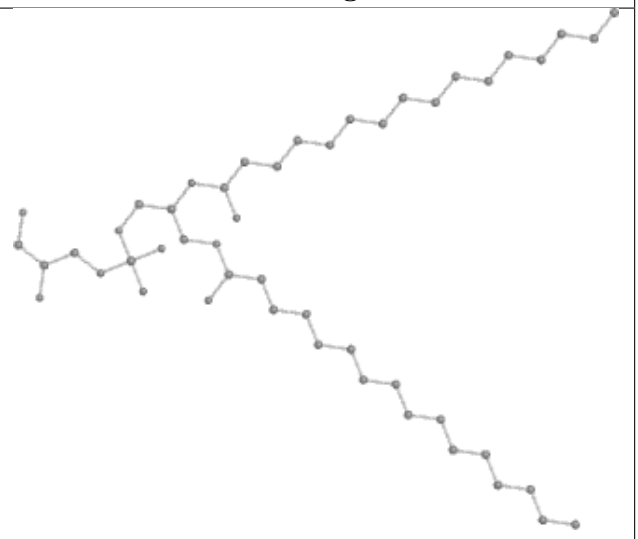
Bond lengths



Bond angles

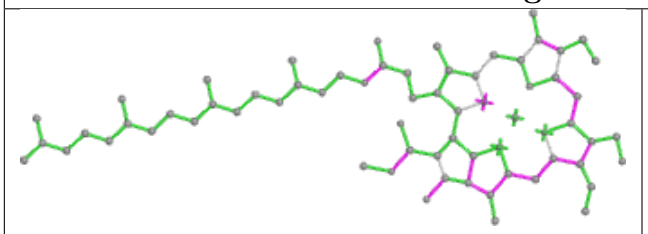


Torsions



Rings

Ligand CHL U 315



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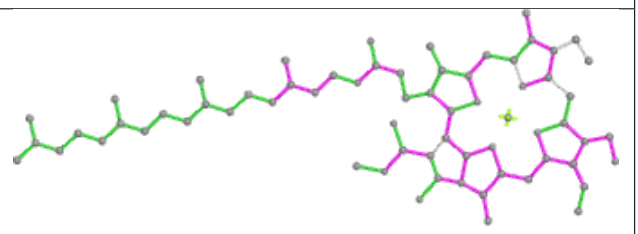
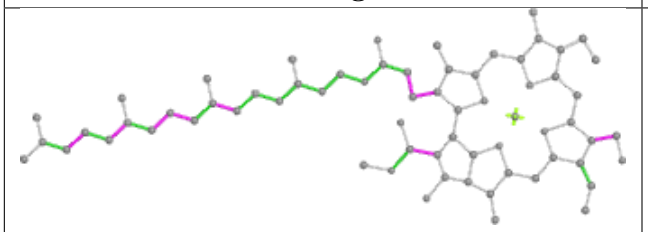


Bond angles



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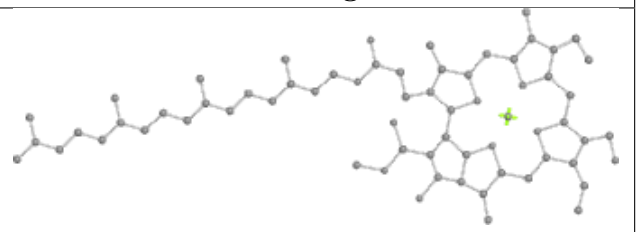
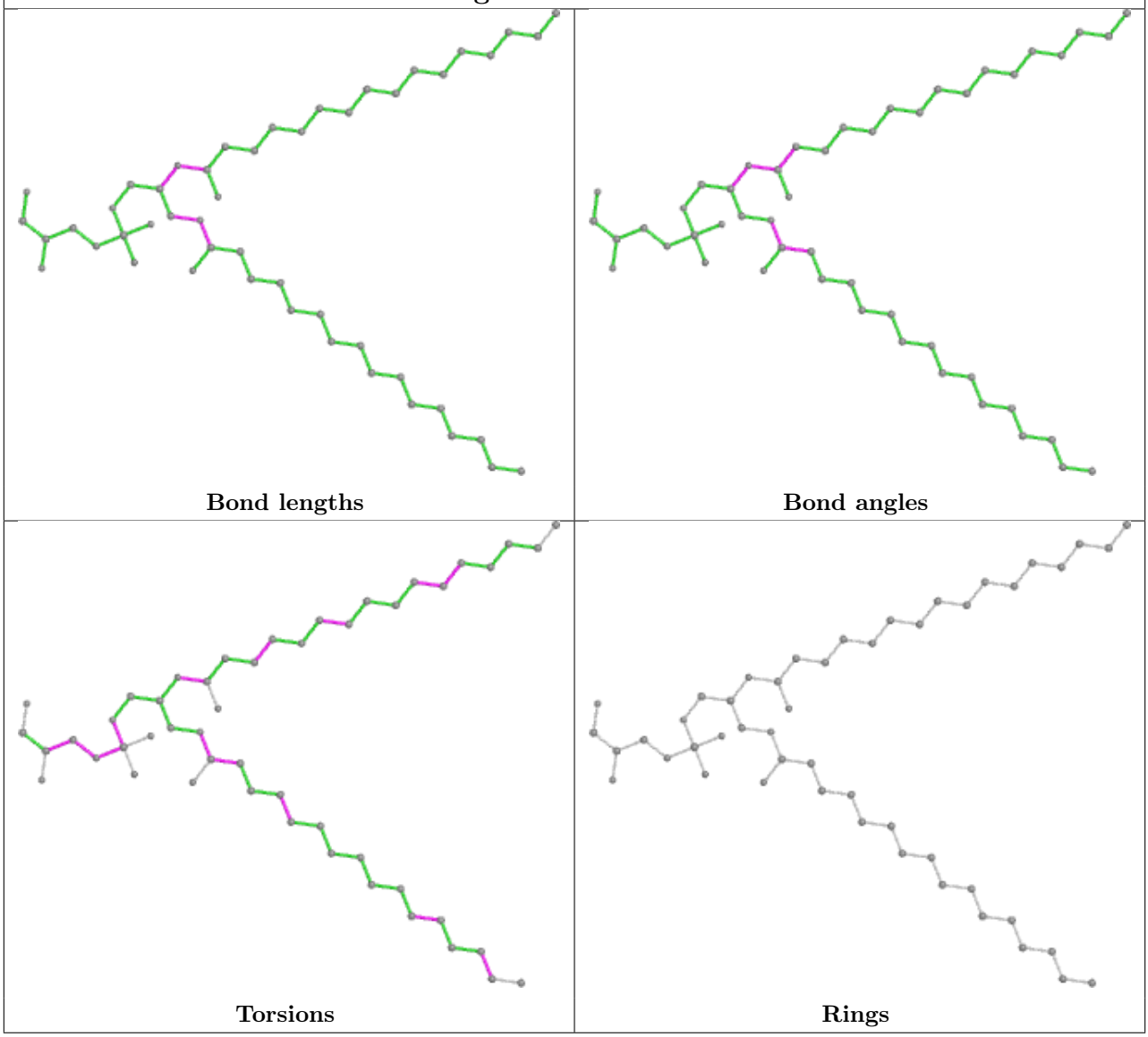
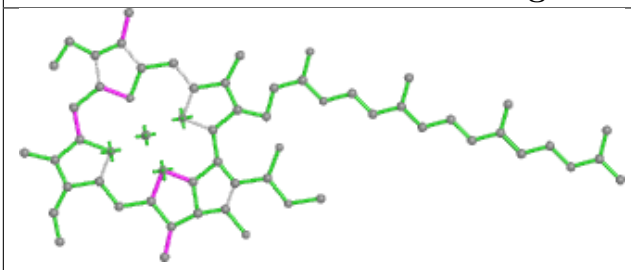
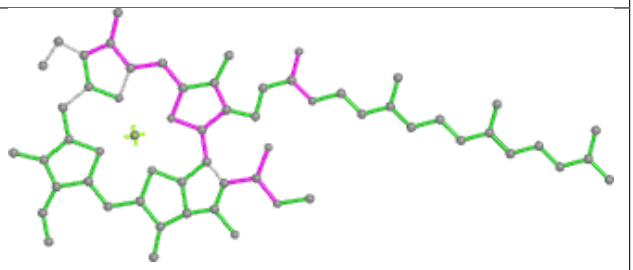
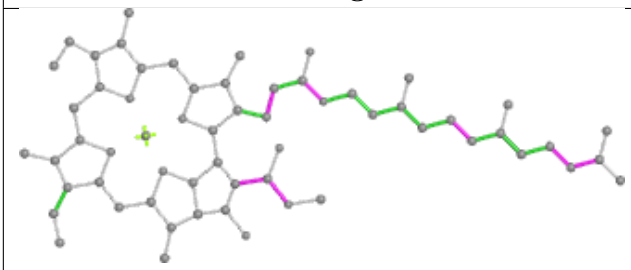
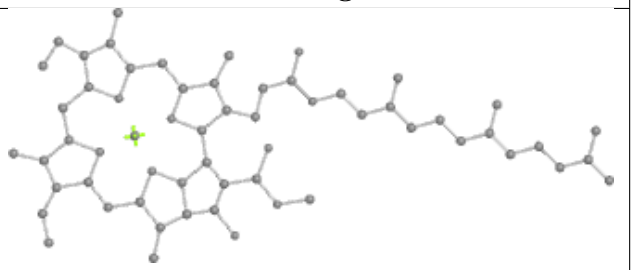
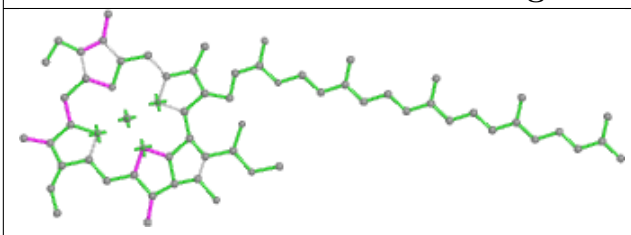
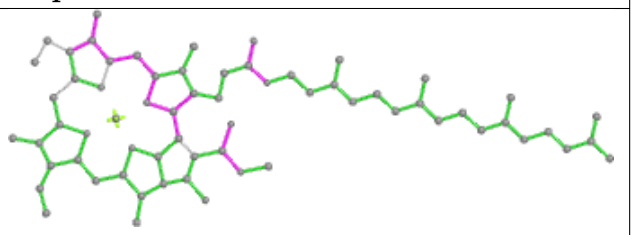
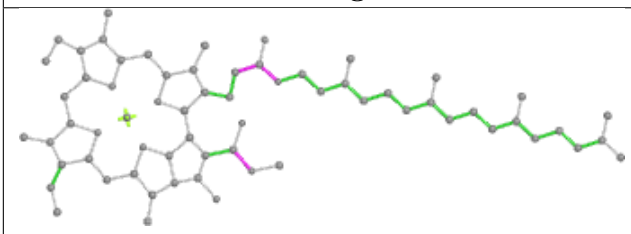
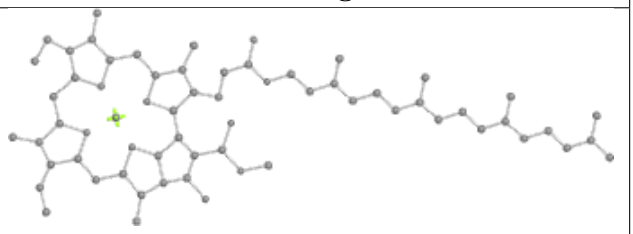


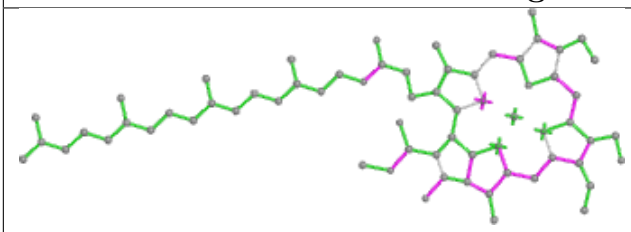
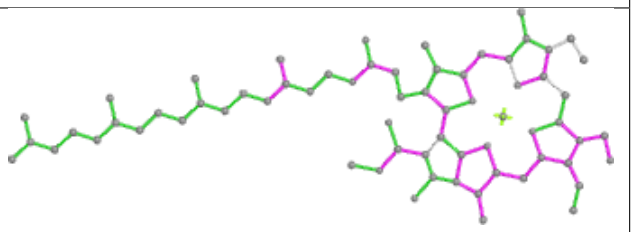
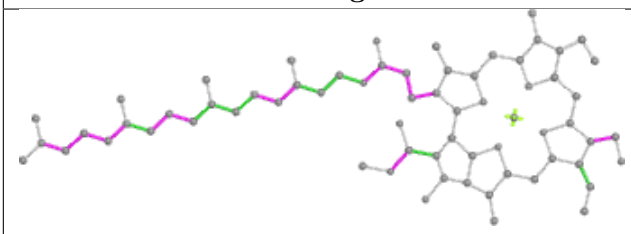
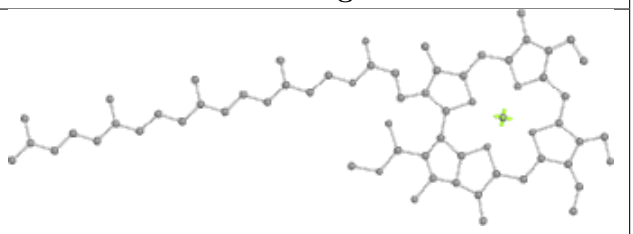
Rings

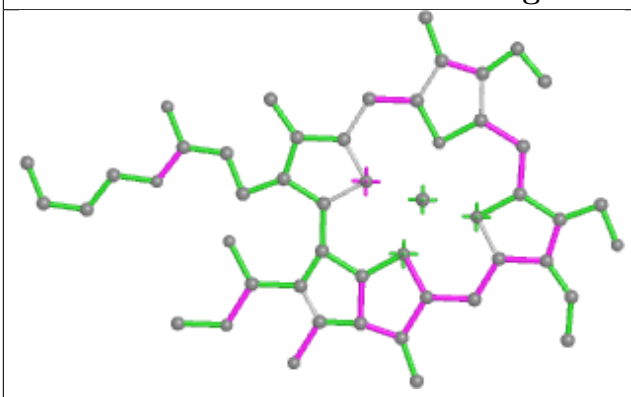
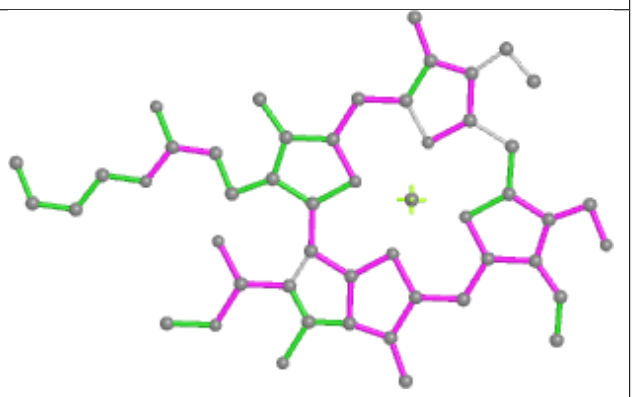
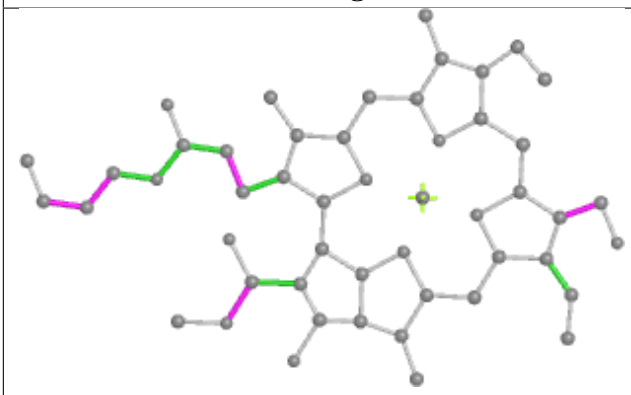
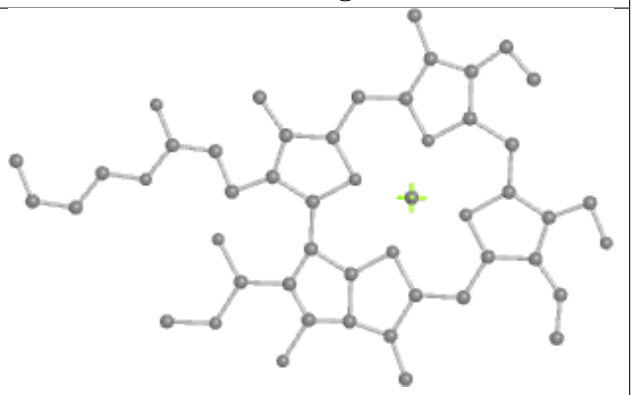
Ligand LHG s 312

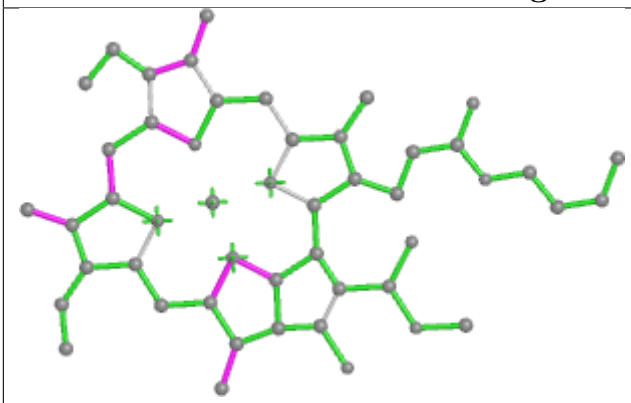
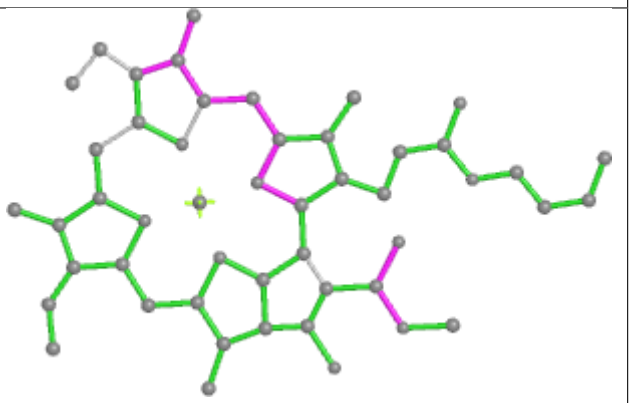
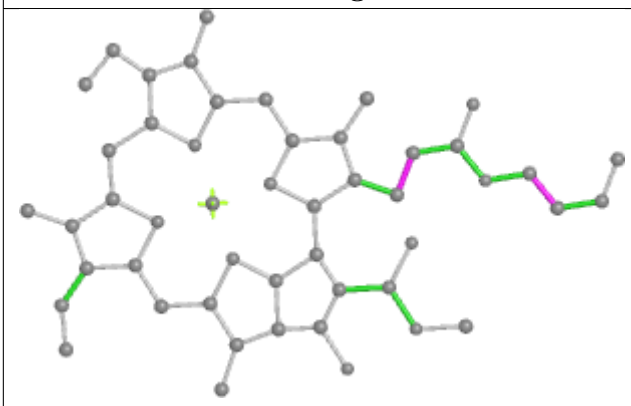
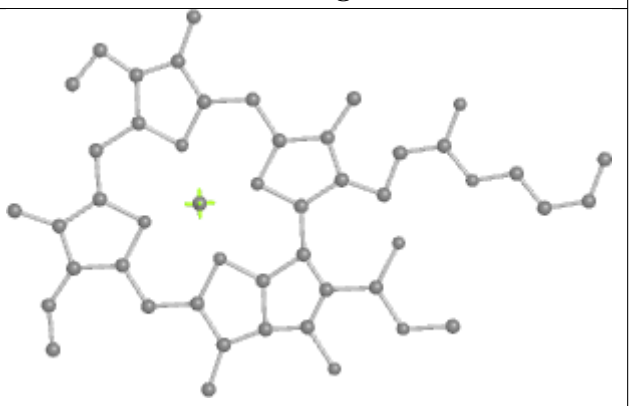


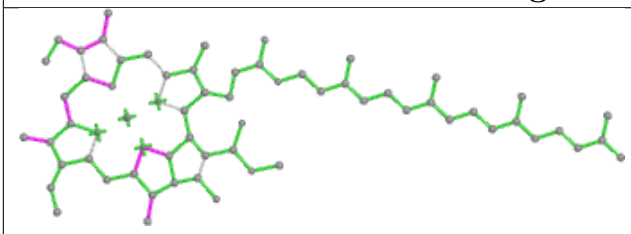
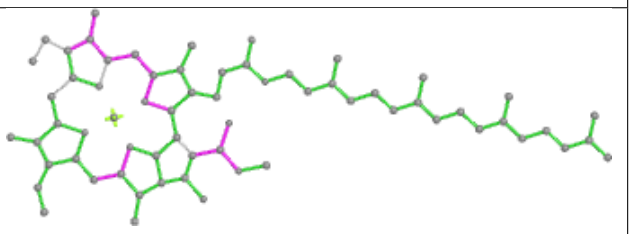
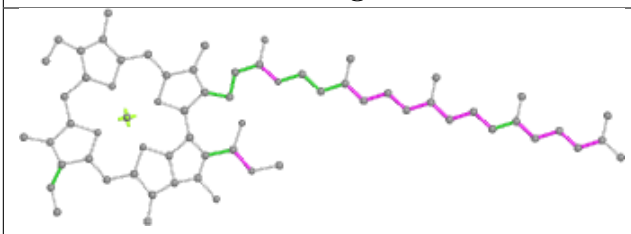
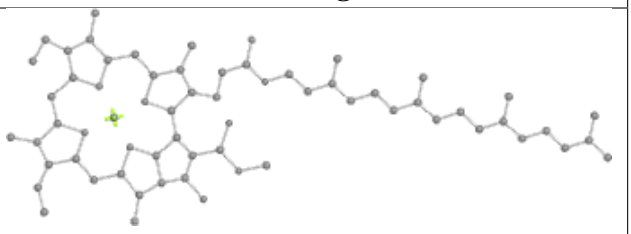
Ligand CLA 3 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

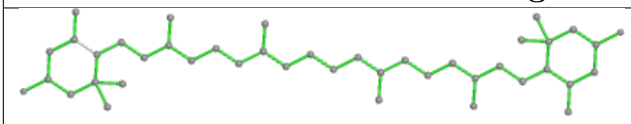
Ligand CHL 3 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

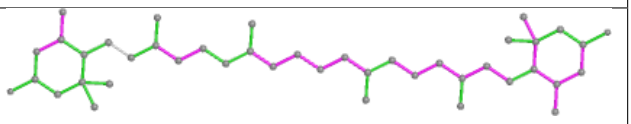
Ligand CLA s 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

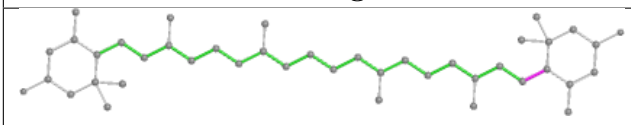
Ligand LUT 4 309



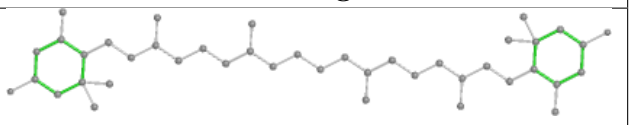
Bond lengths



Bond angles

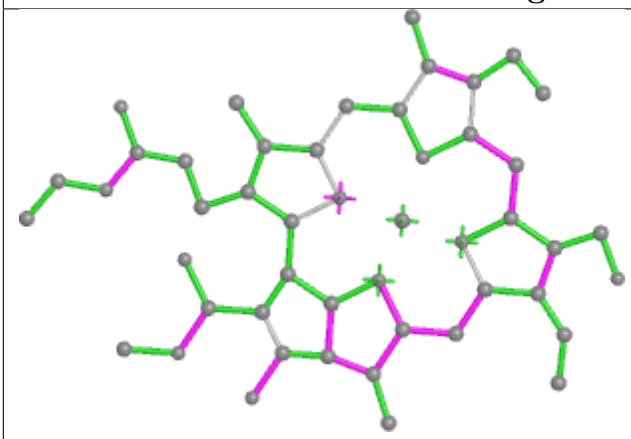


Torsions

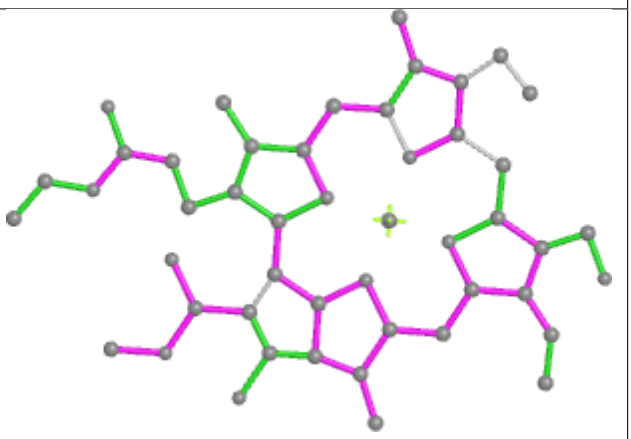


Rings

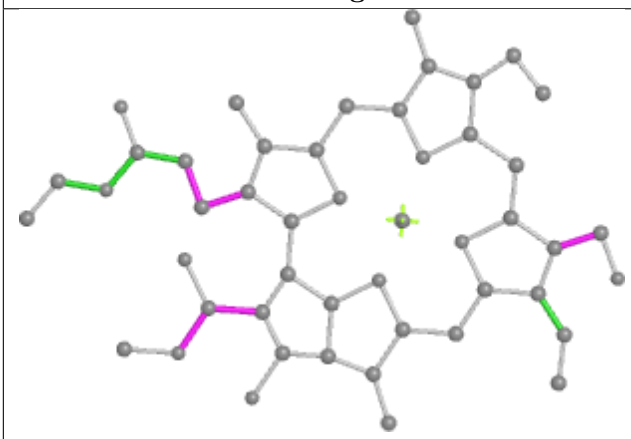
Ligand CHL 4 314



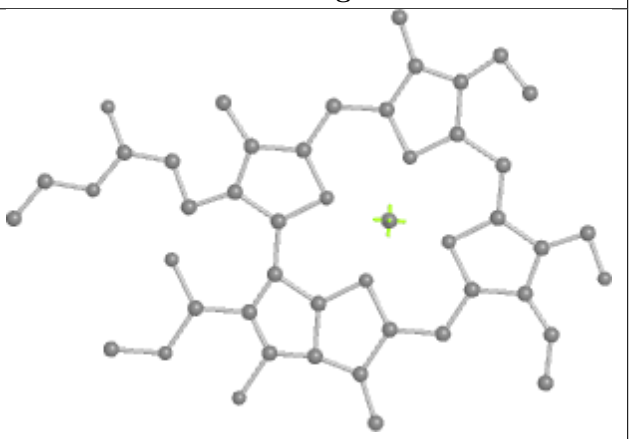
Bond lengths



Bond angles

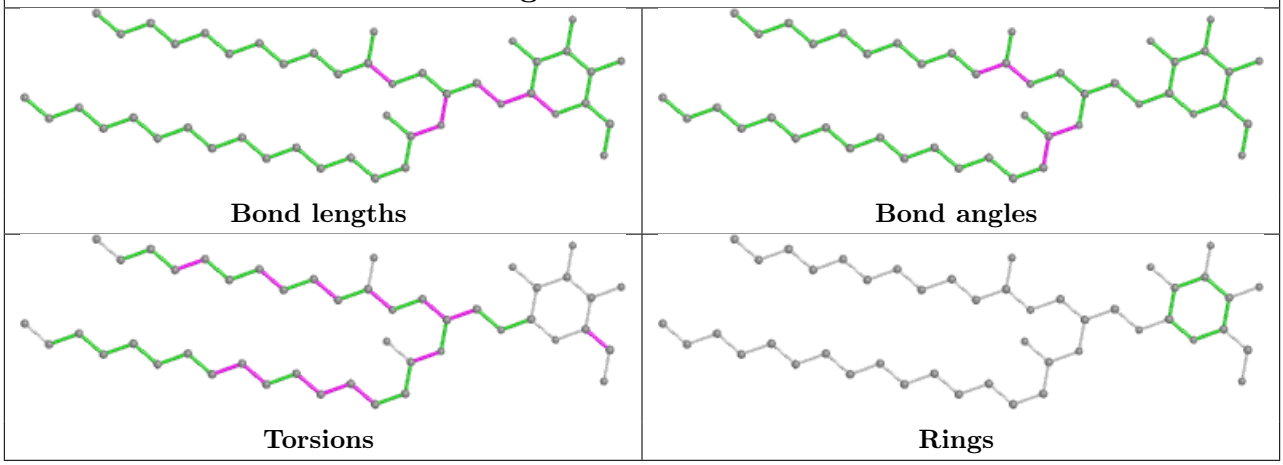


Torsions

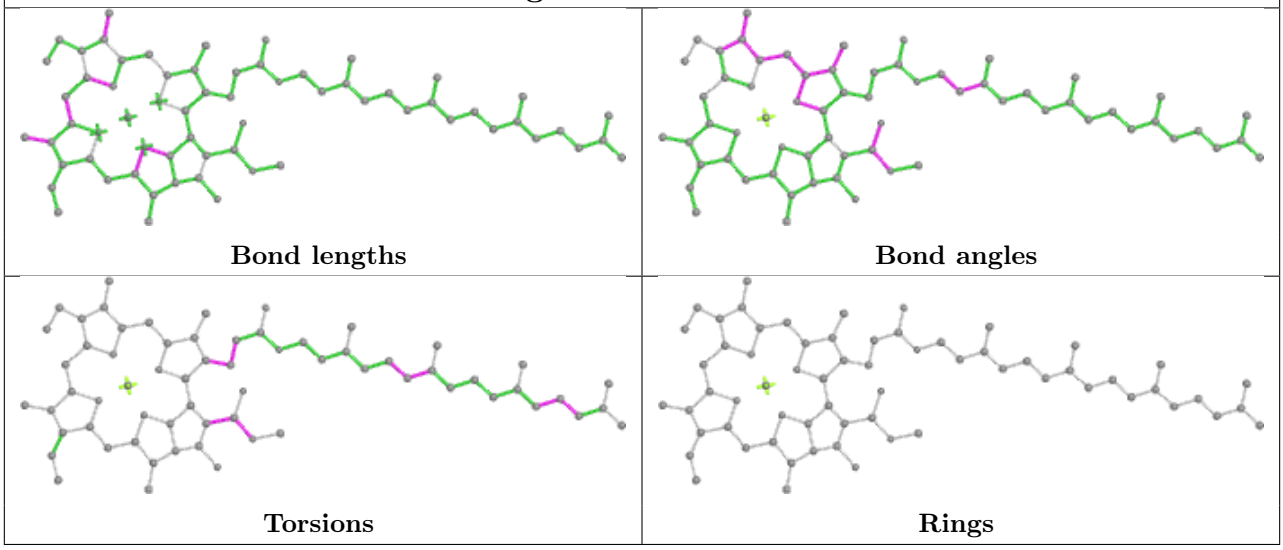


Rings

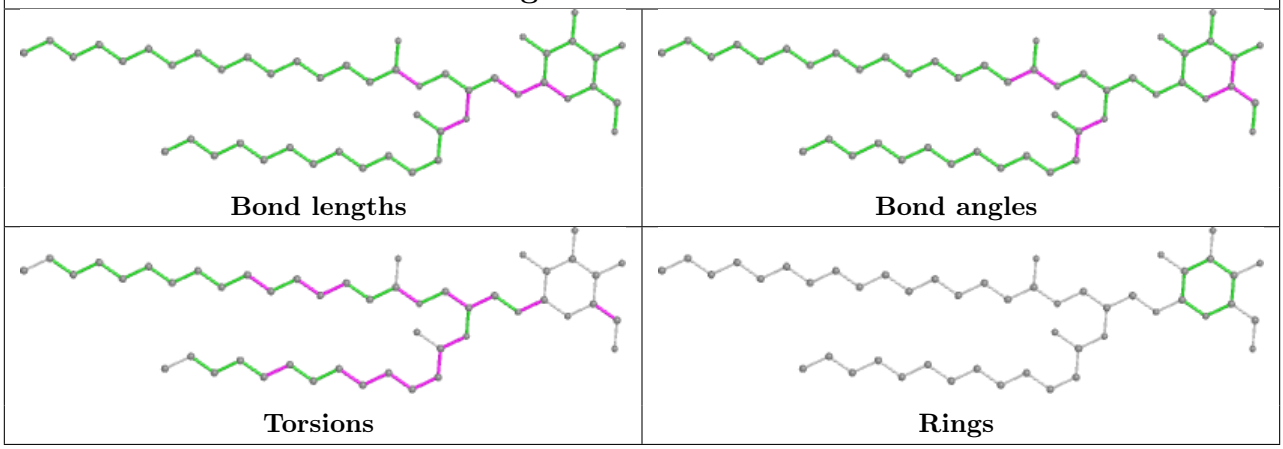
Ligand LMG D 408



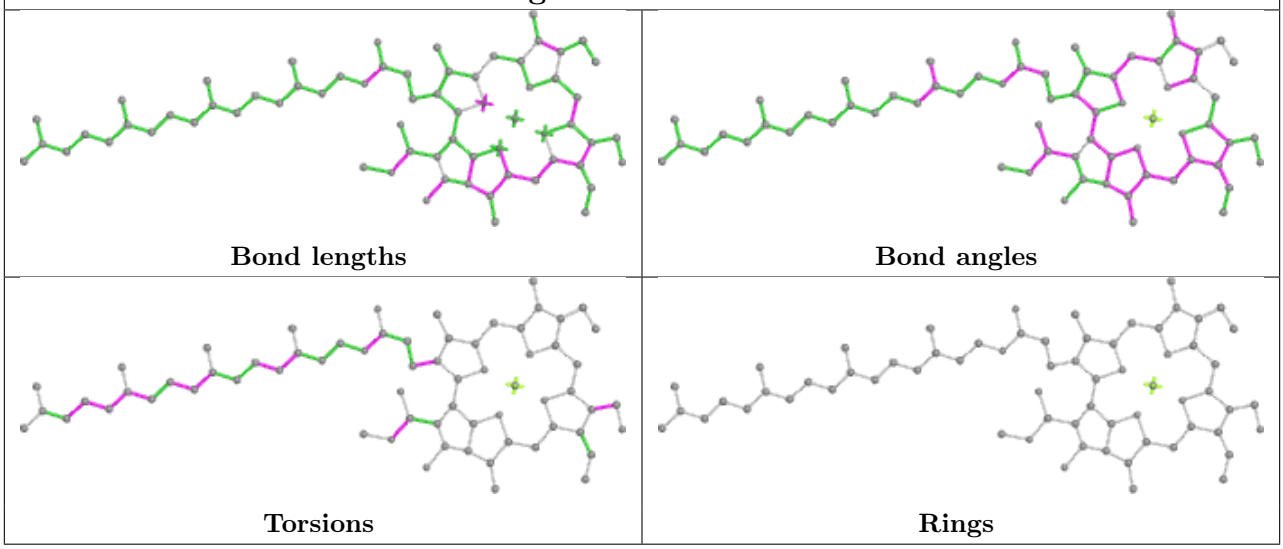
Ligand CLA P 305



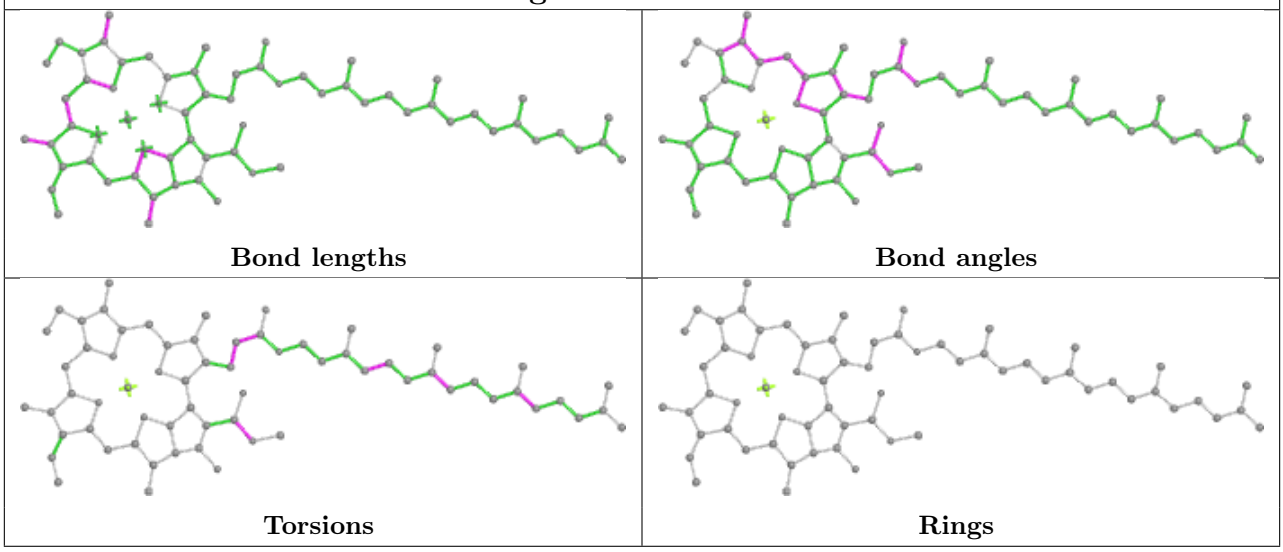
Ligand LMG w 201



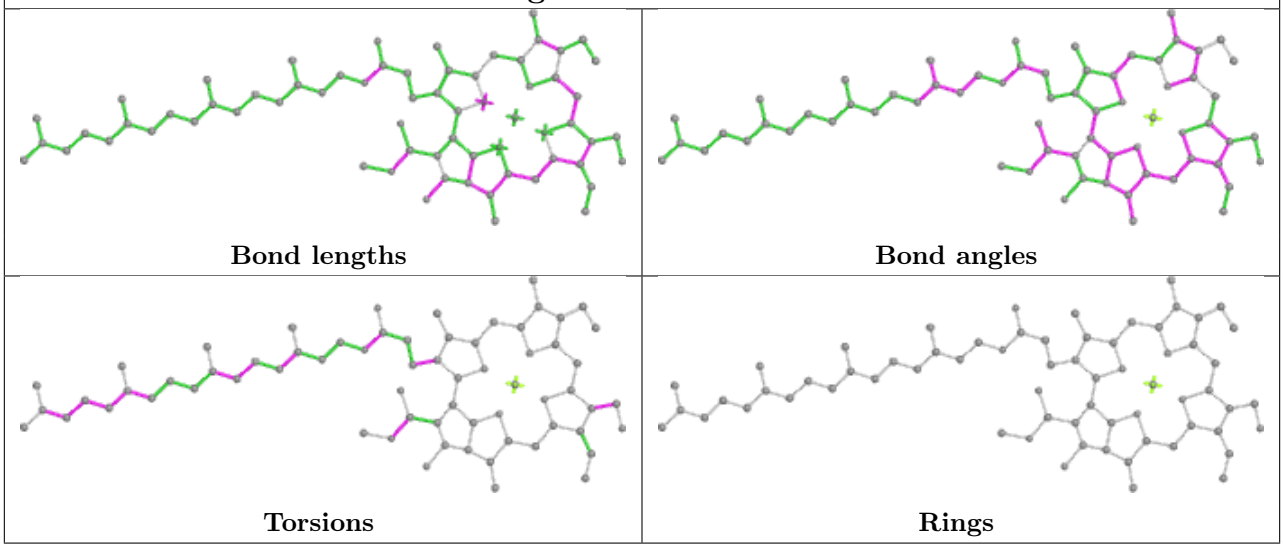
Ligand CHL 5 318

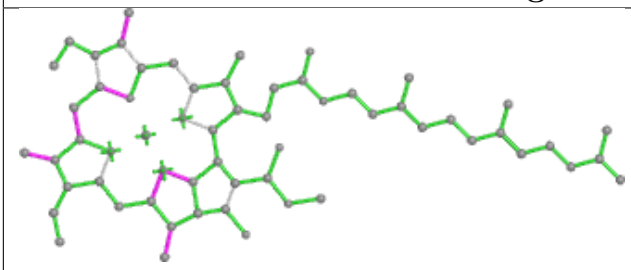
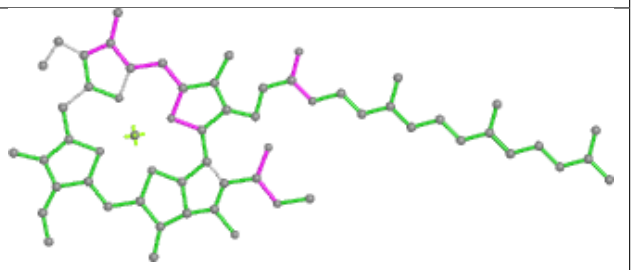
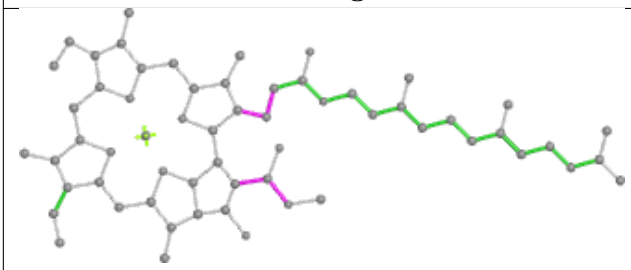
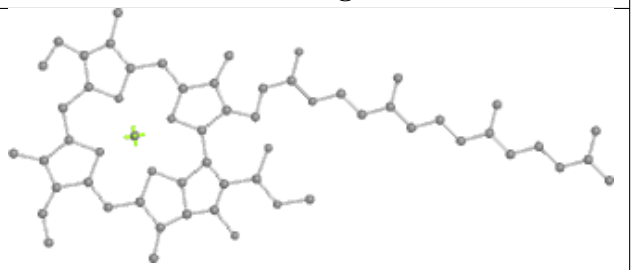


Ligand CLA 3 307

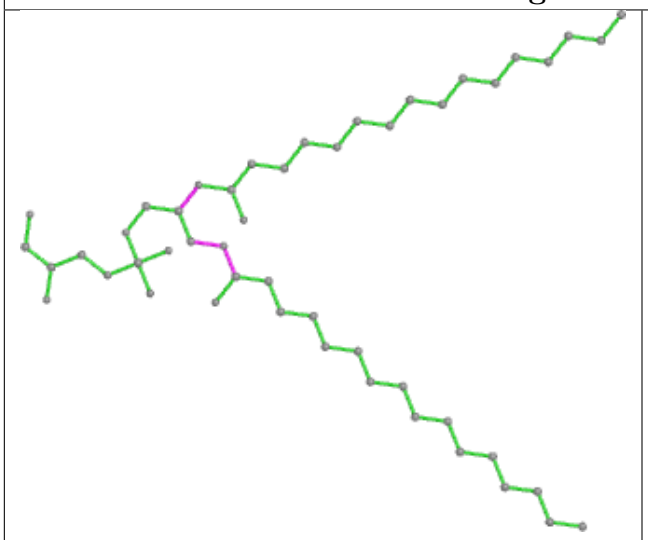


Ligand CHL u 318

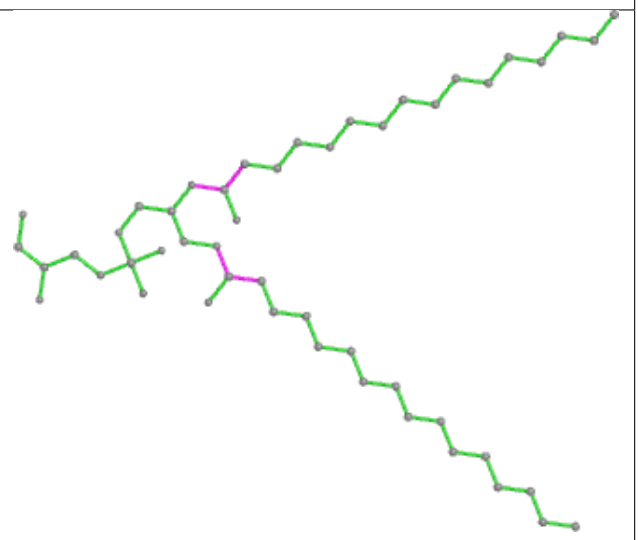


Ligand CLA u 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

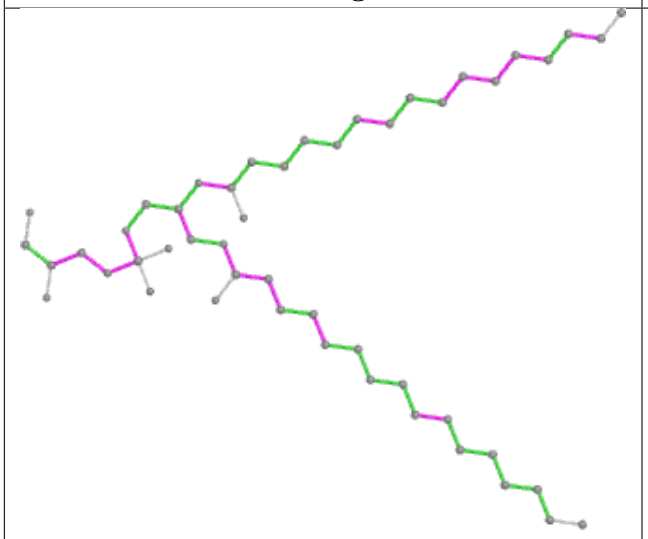
Ligand LHG c 522



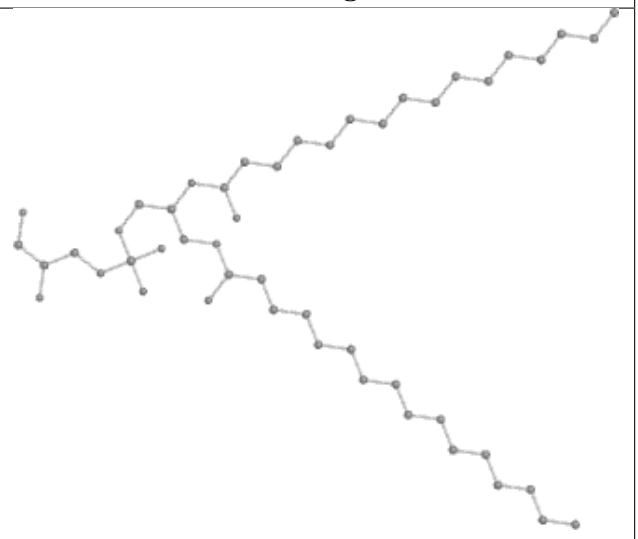
Bond lengths



Bond angles

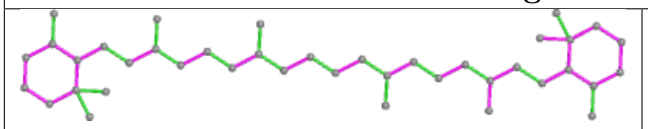


Torsions

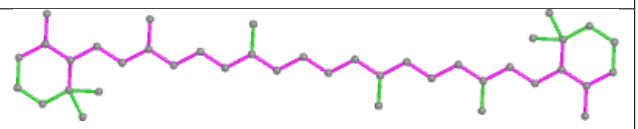


Rings

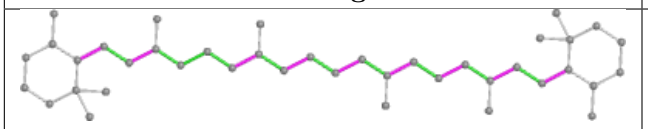
Ligand BCR B 619



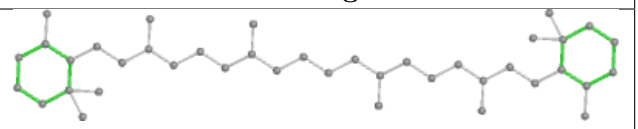
Bond lengths



Bond angles

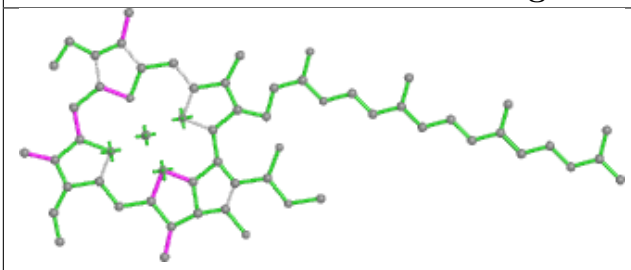


Torsions

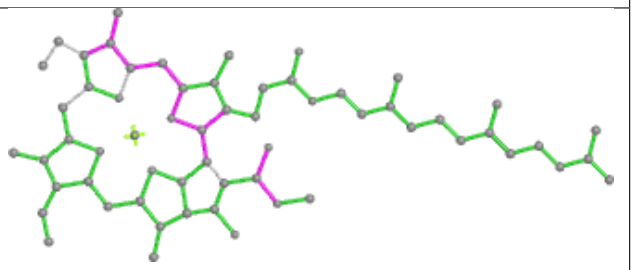


Rings

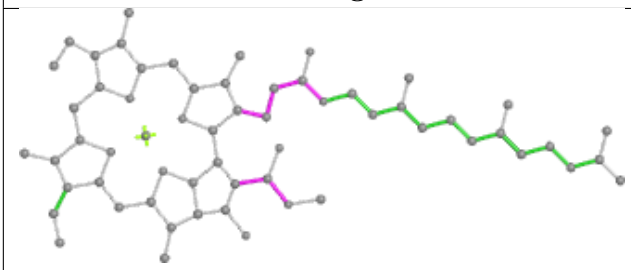
Ligand CLA 2 306



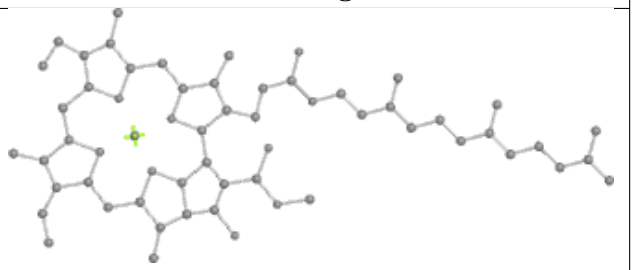
Bond lengths



Bond angles

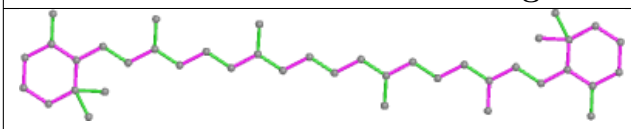


Torsions

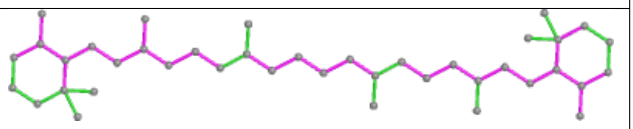


Rings

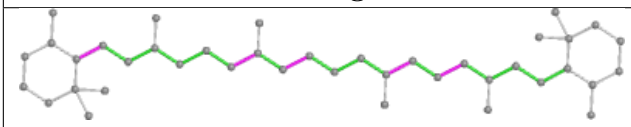
Ligand BCR C 516



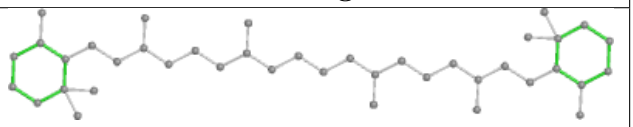
Bond lengths



Bond angles

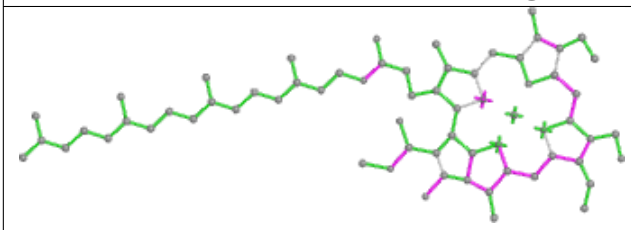


Torsions

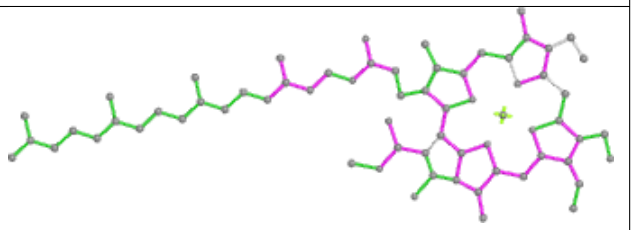


Rings

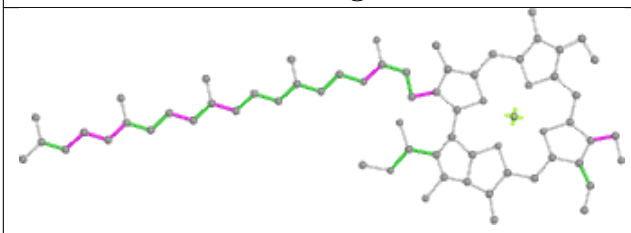
Ligand CHL U 316



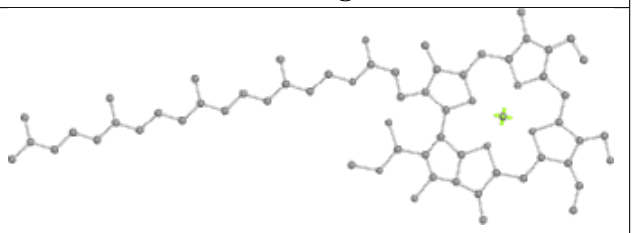
Bond lengths



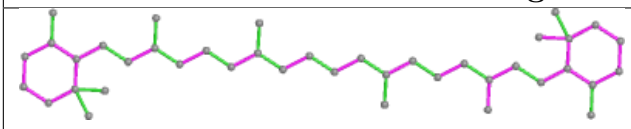
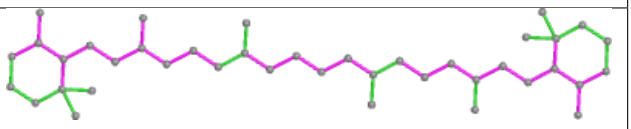
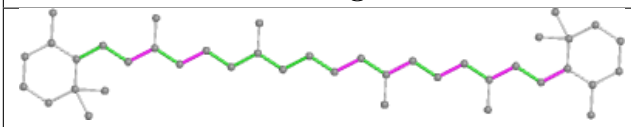
Bond angles

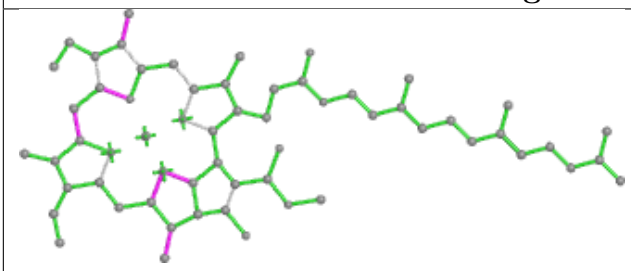
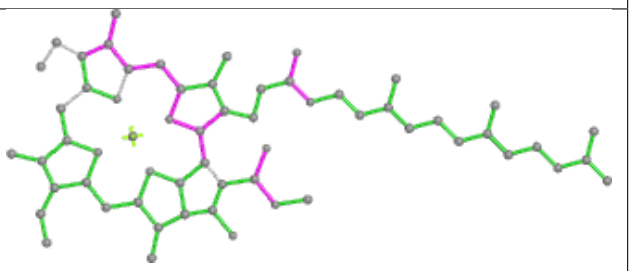
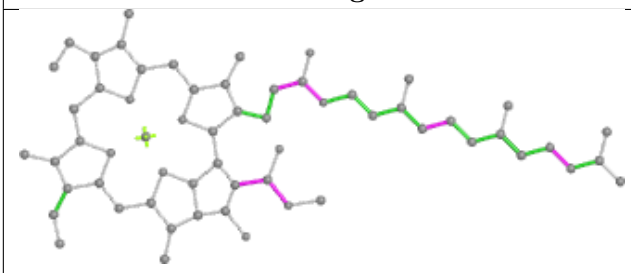
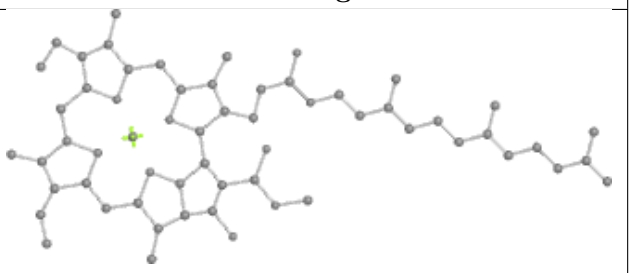


Torsions

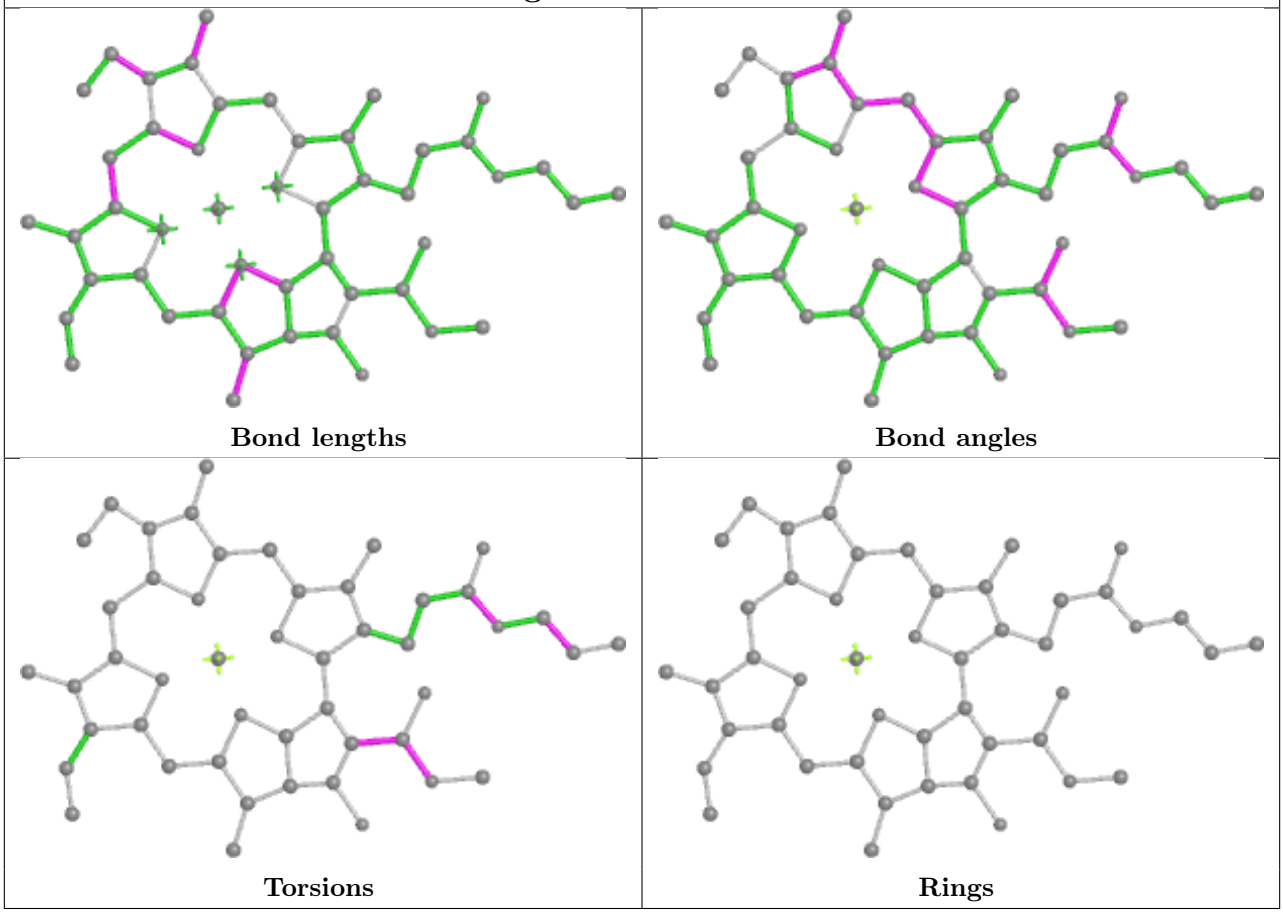


Rings

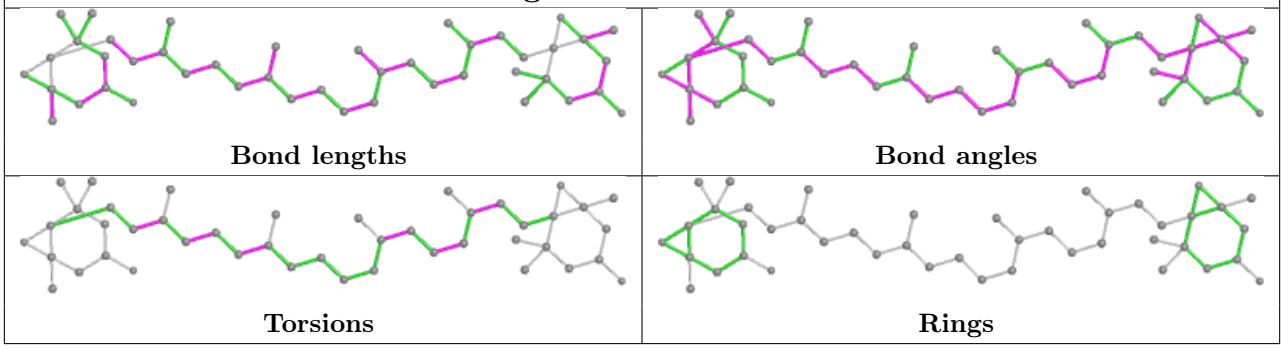
Ligand BCR c 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

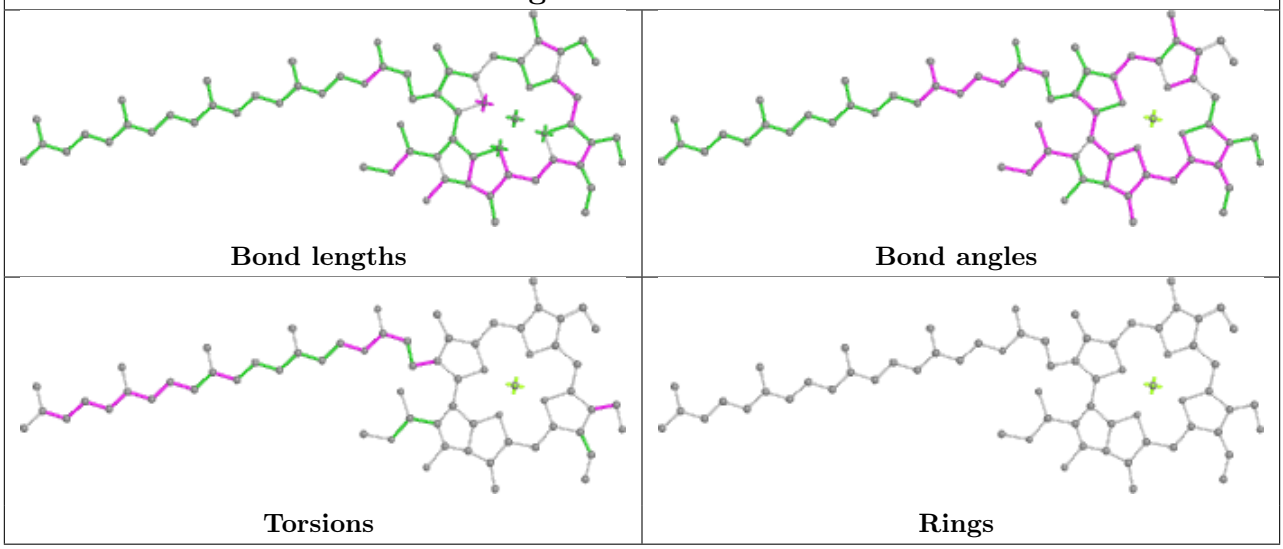
Ligand CLA G 308



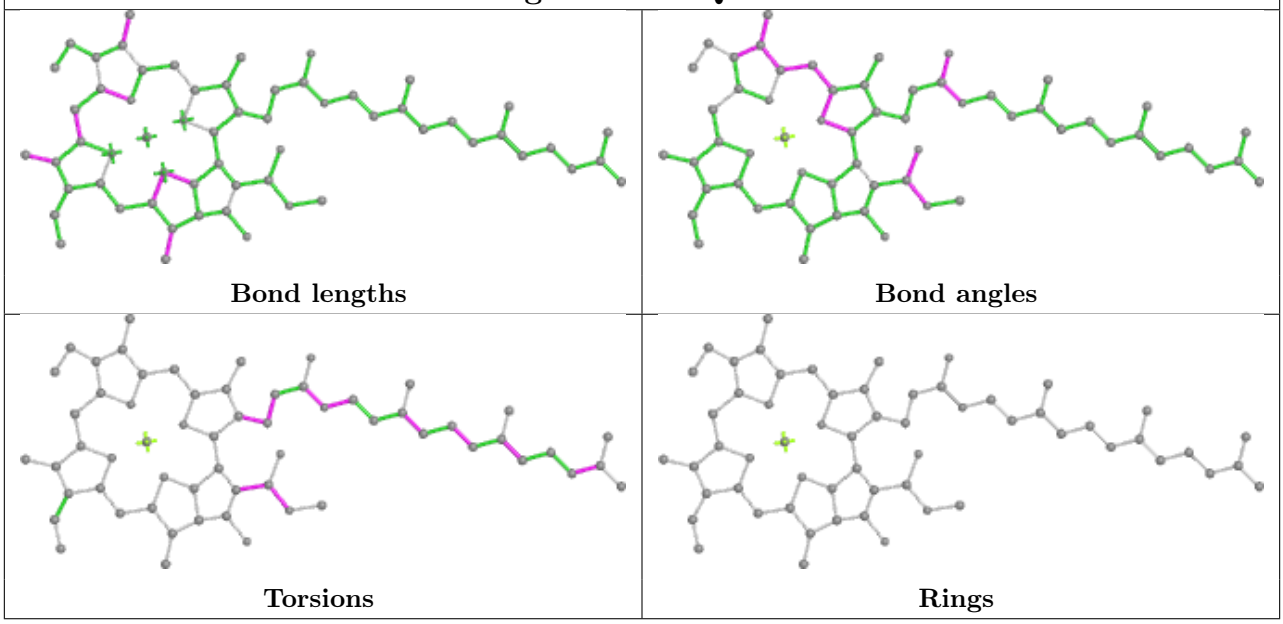
Ligand XAT G 309



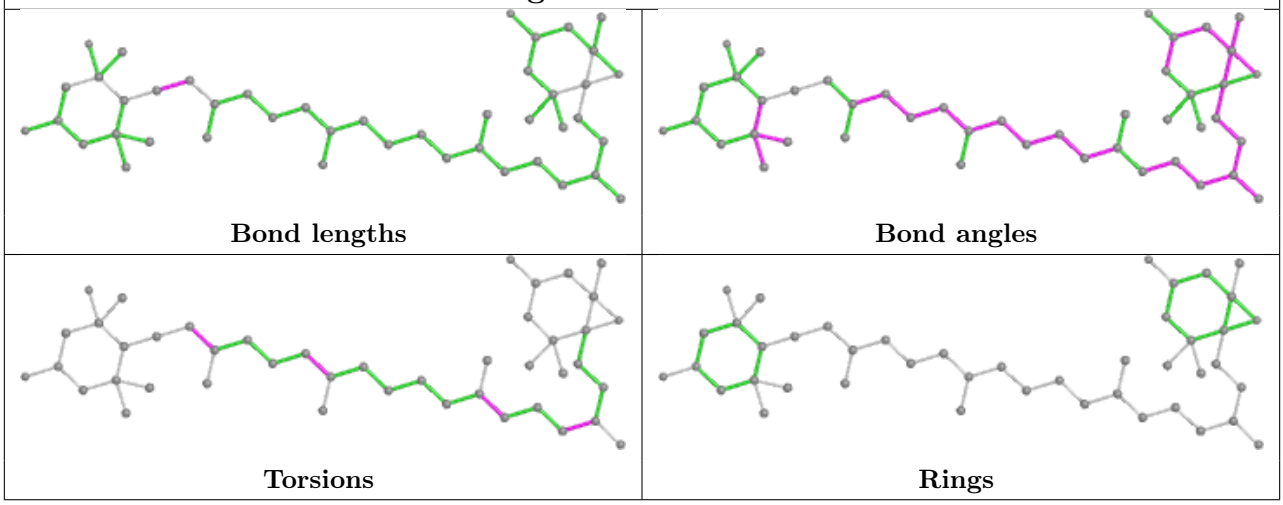
Ligand CHL 1 317



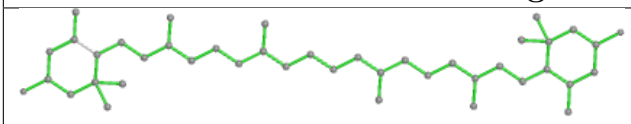
Ligand CLA Q 305



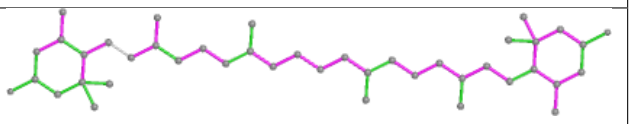
Ligand NEX 5 319



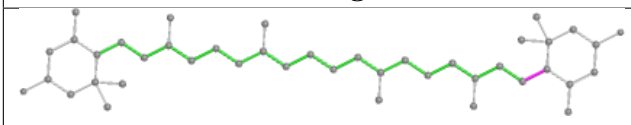
Ligand LUT S 310



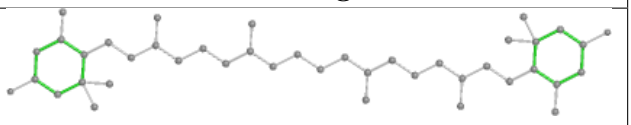
Bond lengths



Bond angles

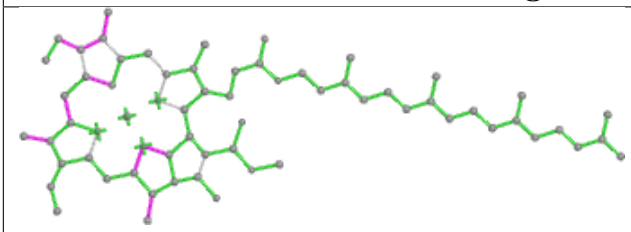


Torsions

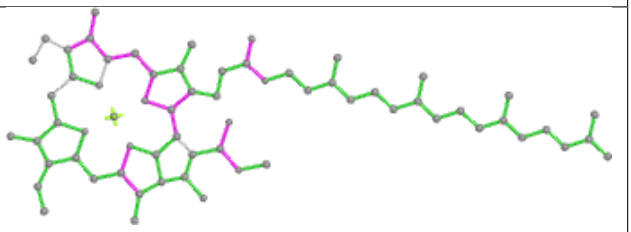


Rings

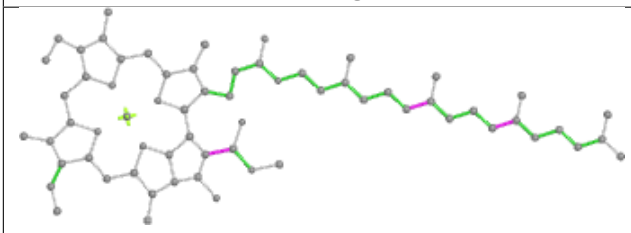
Ligand CLA B 616



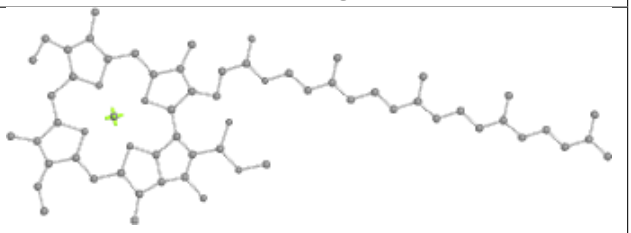
Bond lengths



Bond angles

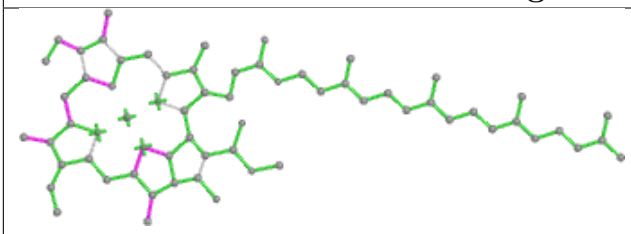


Torsions

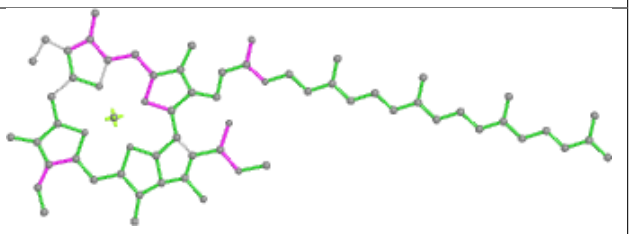


Rings

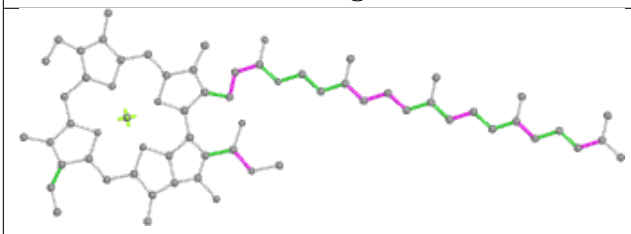
Ligand CLA u 307



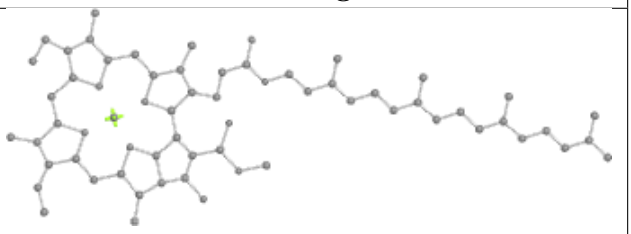
Bond lengths



Bond angles

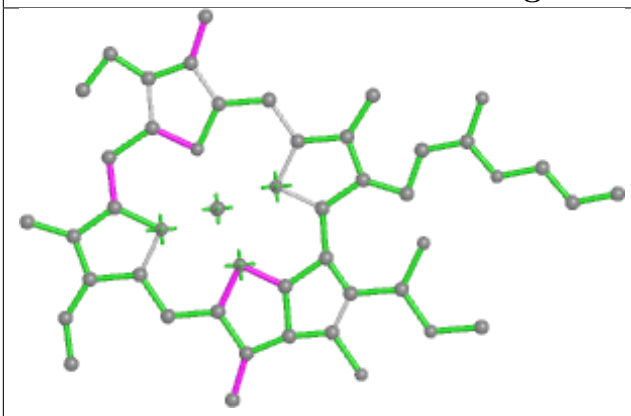


Torsions

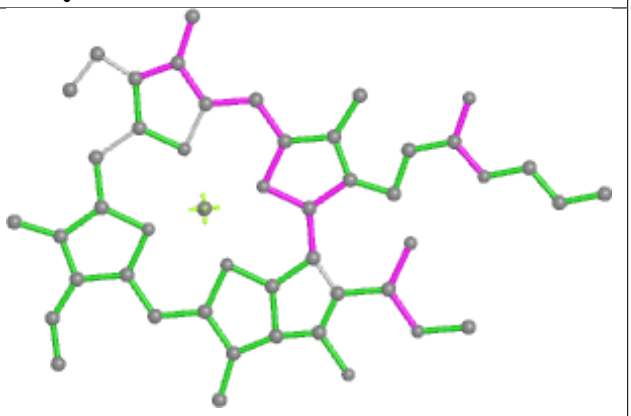


Rings

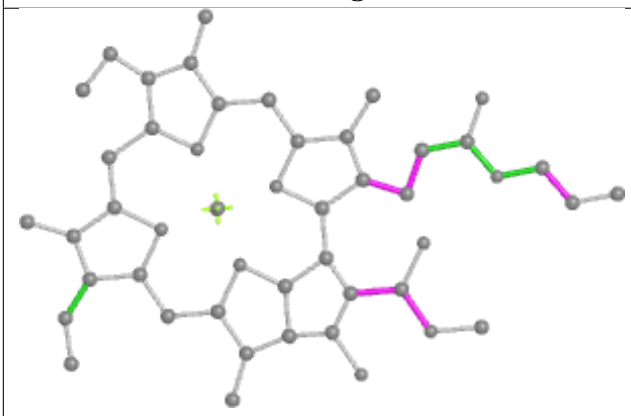
Ligand CLA Q 308



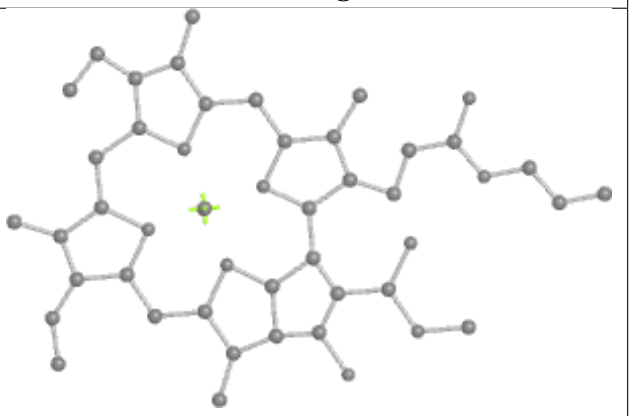
Bond lengths



Bond angles

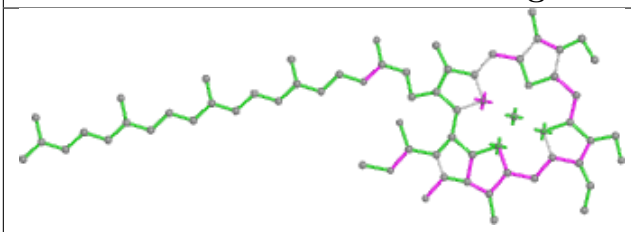


Torsions

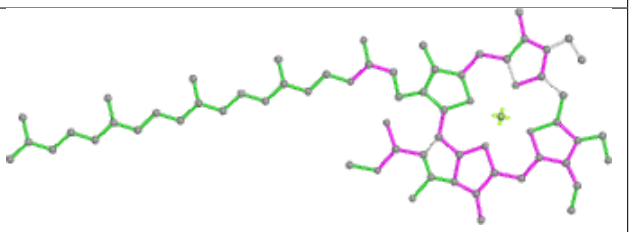


Rings

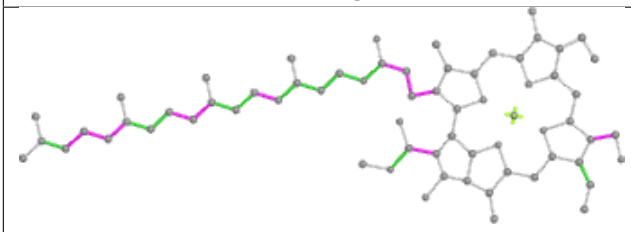
Ligand CHL 2 316



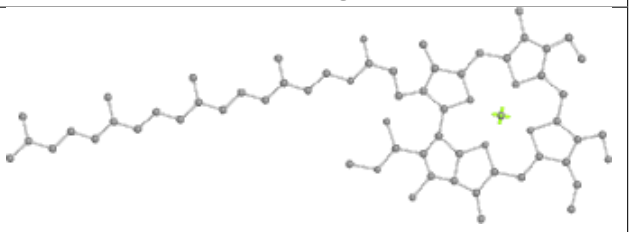
Bond lengths



Bond angles

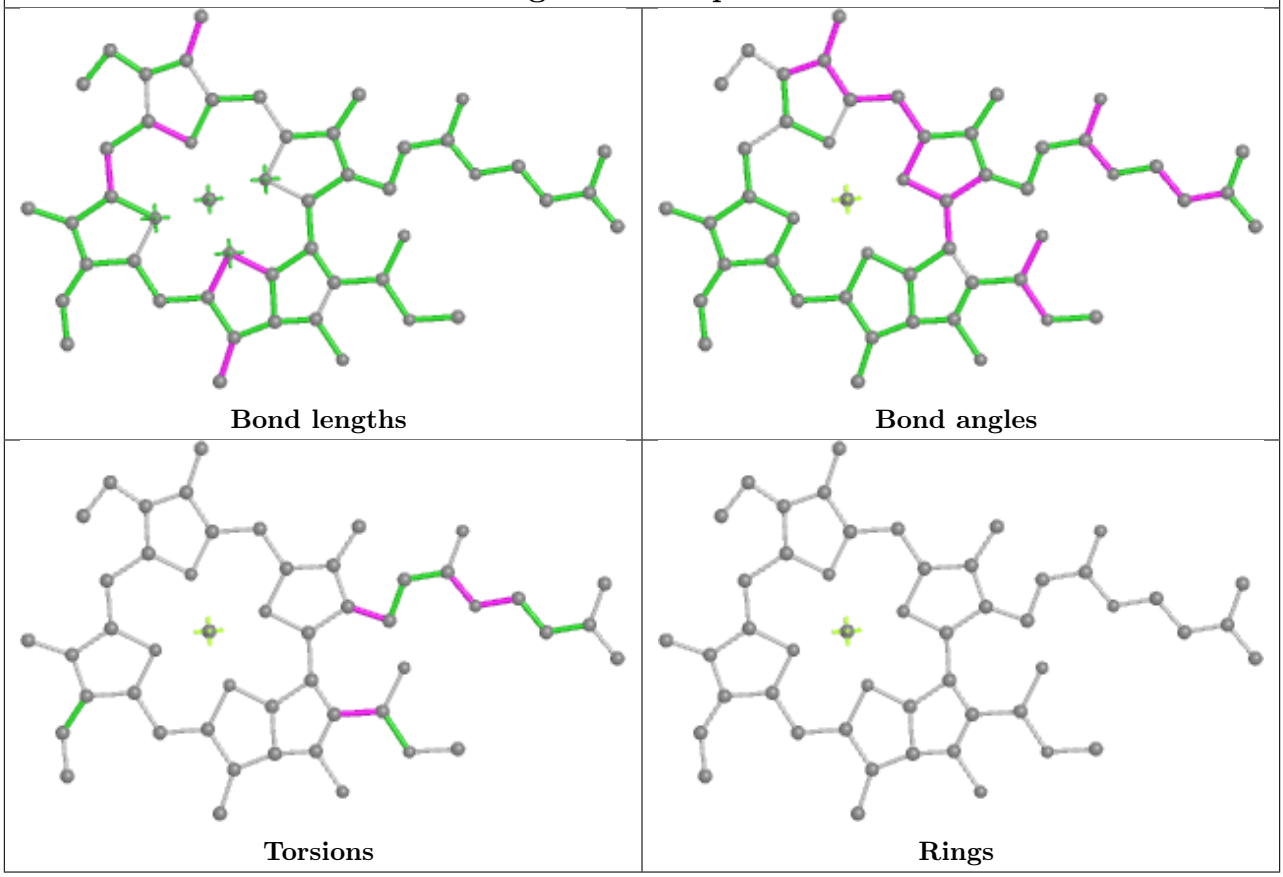


Torsions

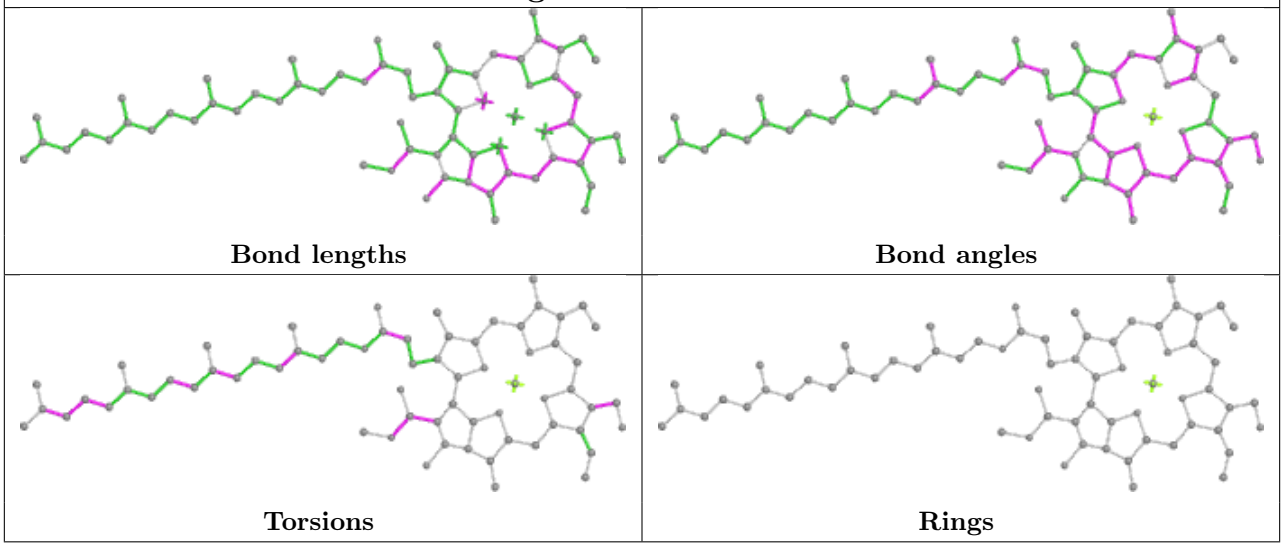


Rings

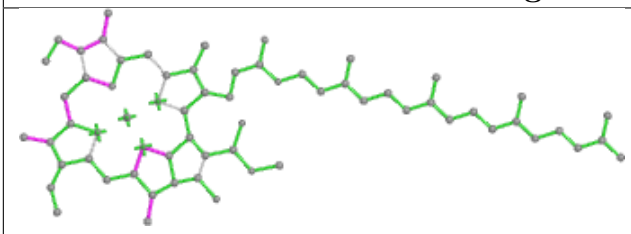
Ligand CLA q 303



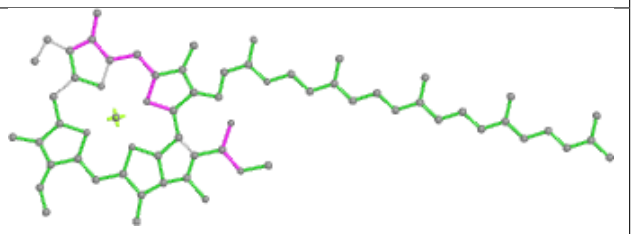
Ligand CHL n 317



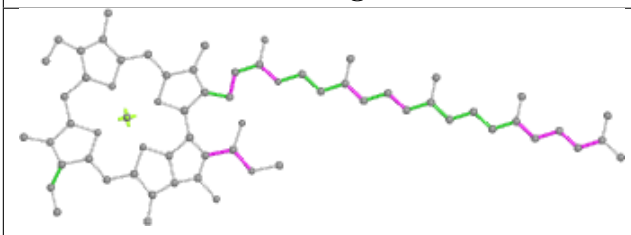
Ligand CLA B 606



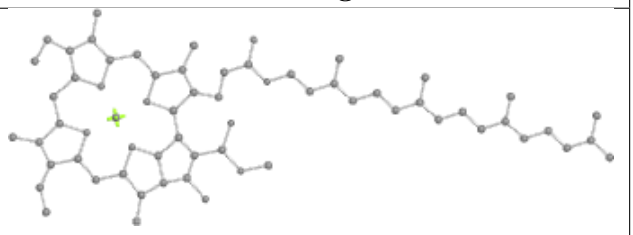
Bond lengths



Bond angles

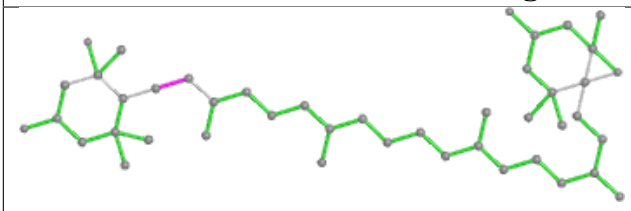


Torsions

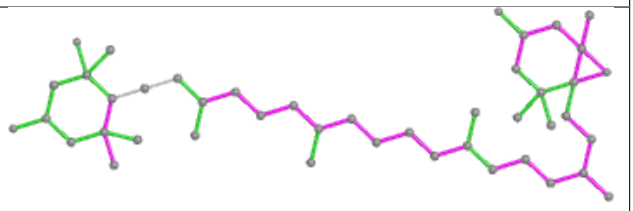


Rings

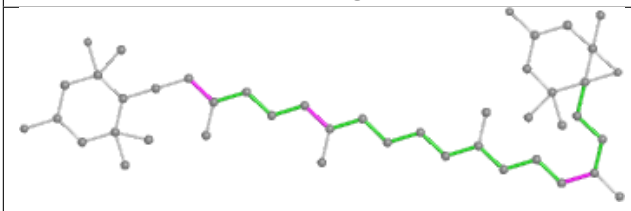
Ligand NEX V 319



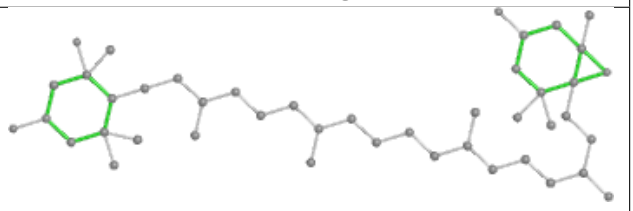
Bond lengths



Bond angles

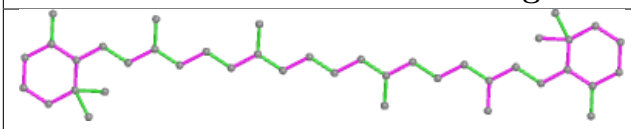


Torsions

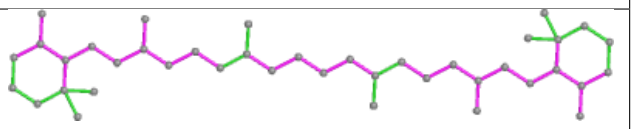


Rings

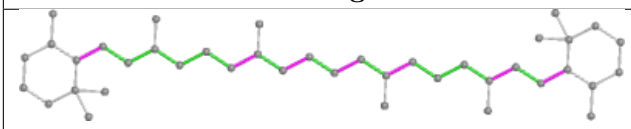
Ligand BCR B 620



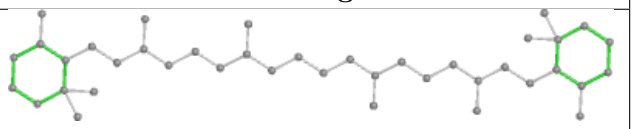
Bond lengths



Bond angles

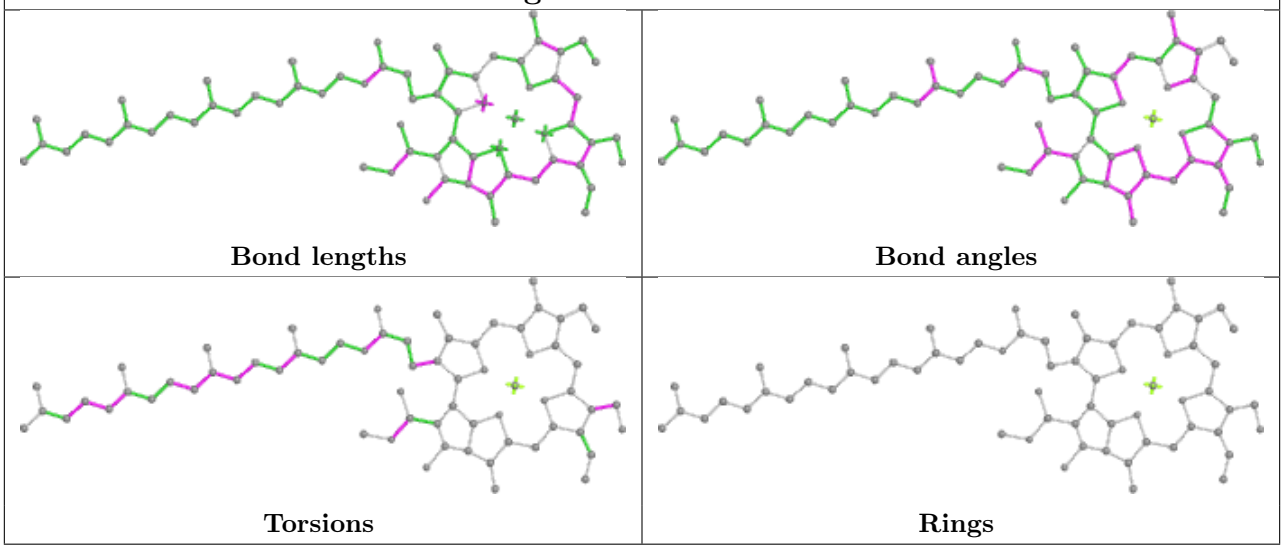


Torsions

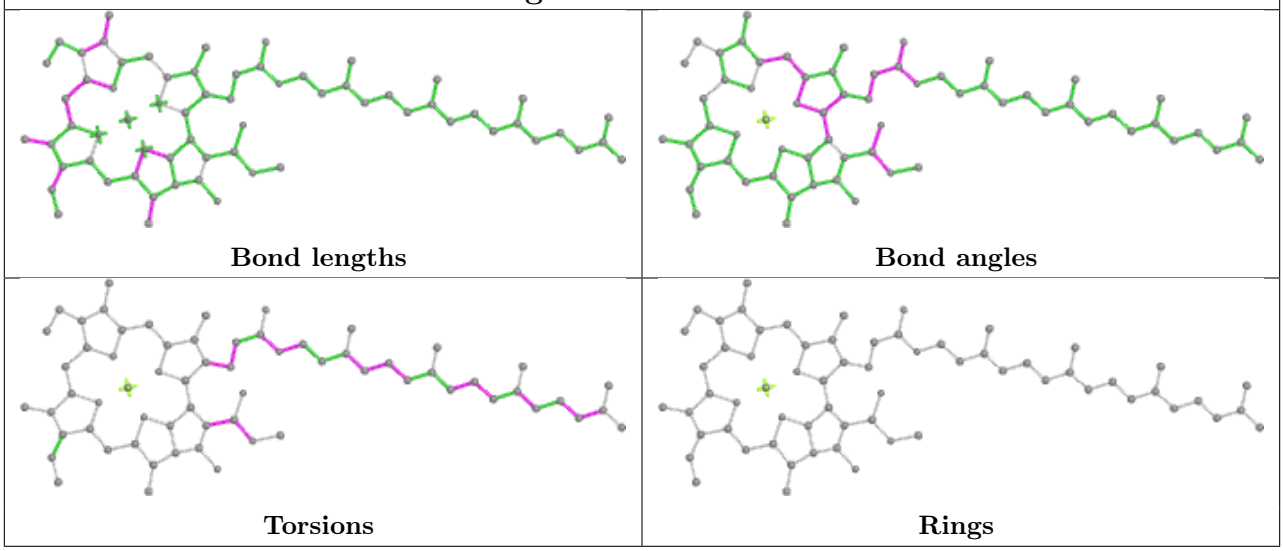


Rings

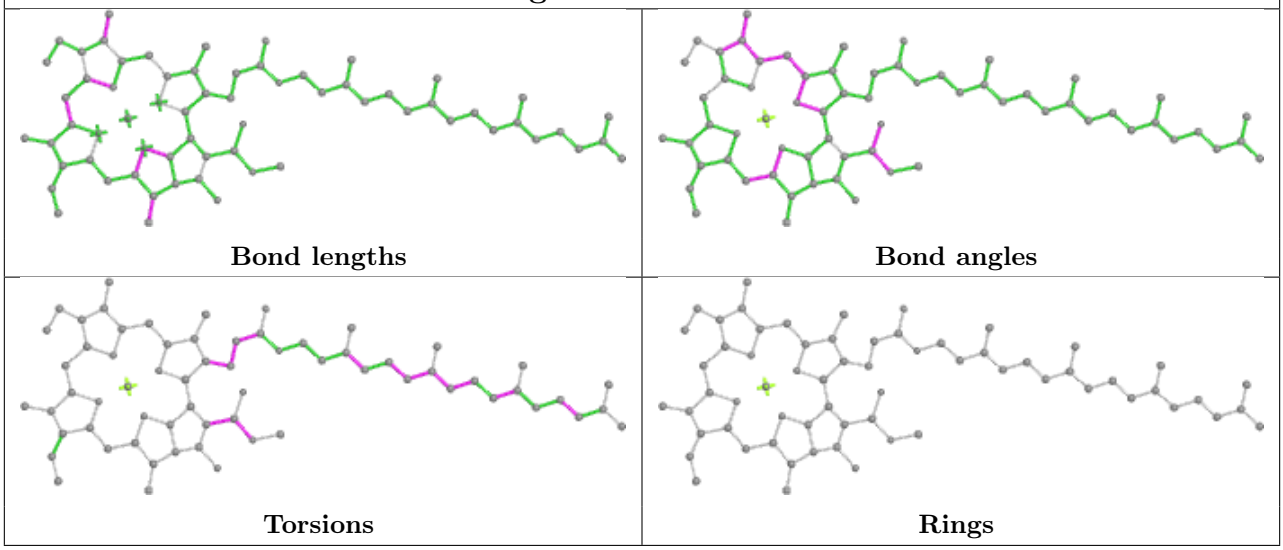
Ligand CHL U 317

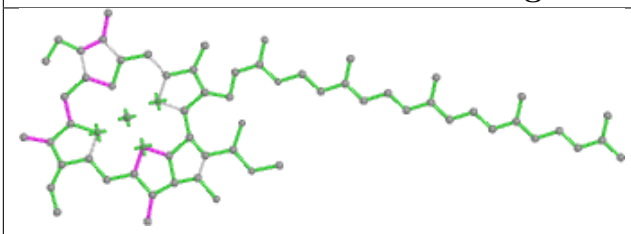
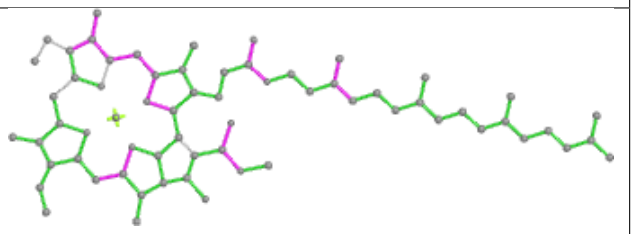
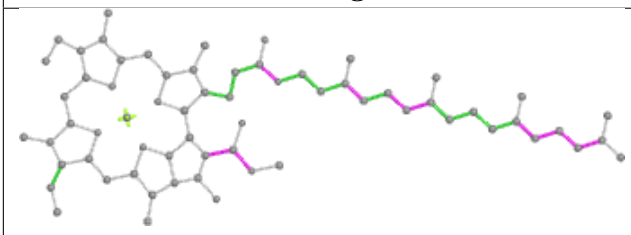
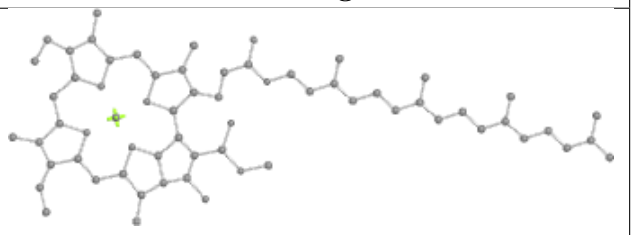


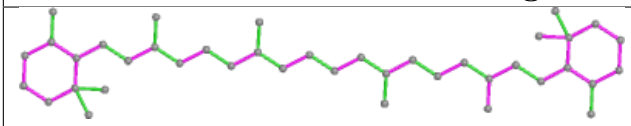
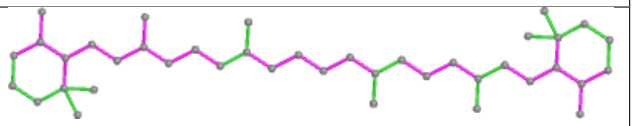
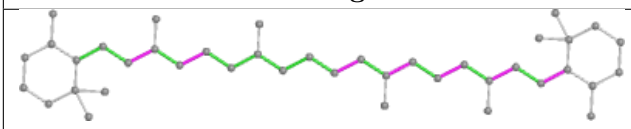
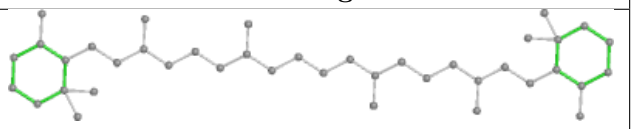
Ligand CLA C 504

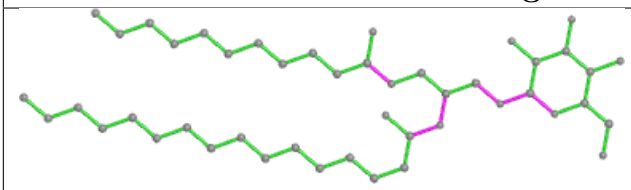
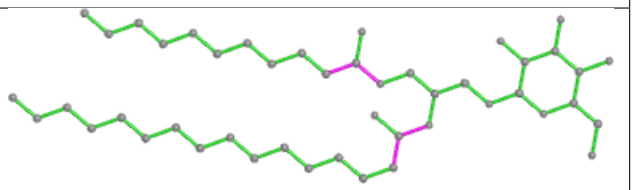
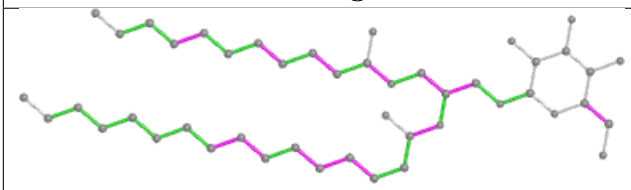
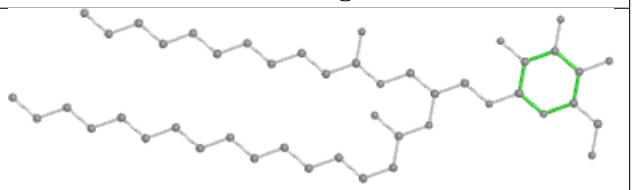


Ligand CLA 6 302

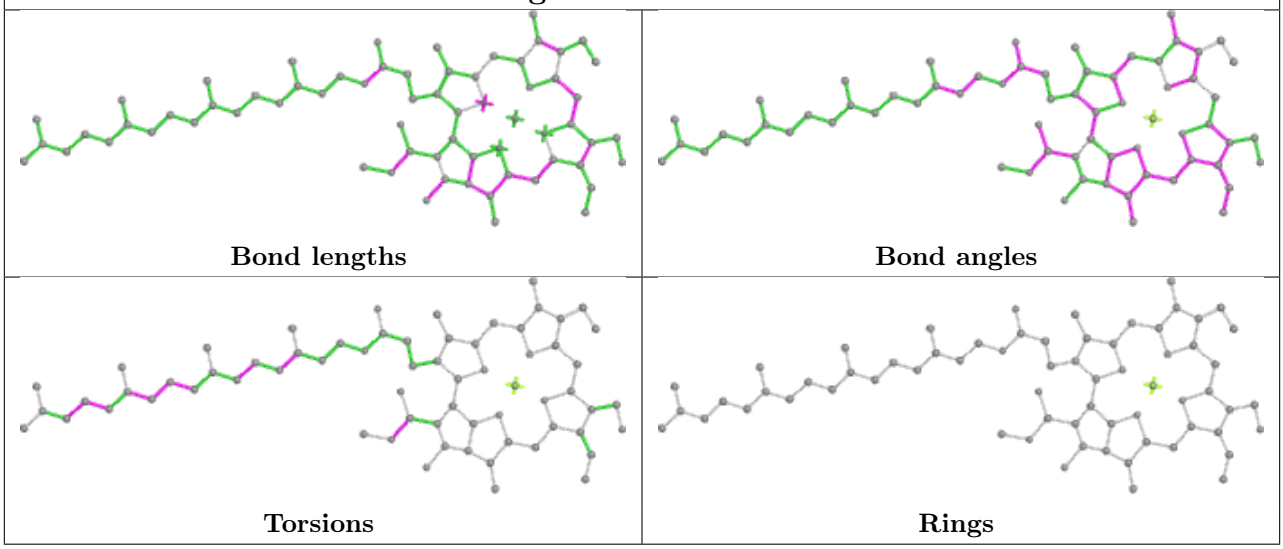


Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

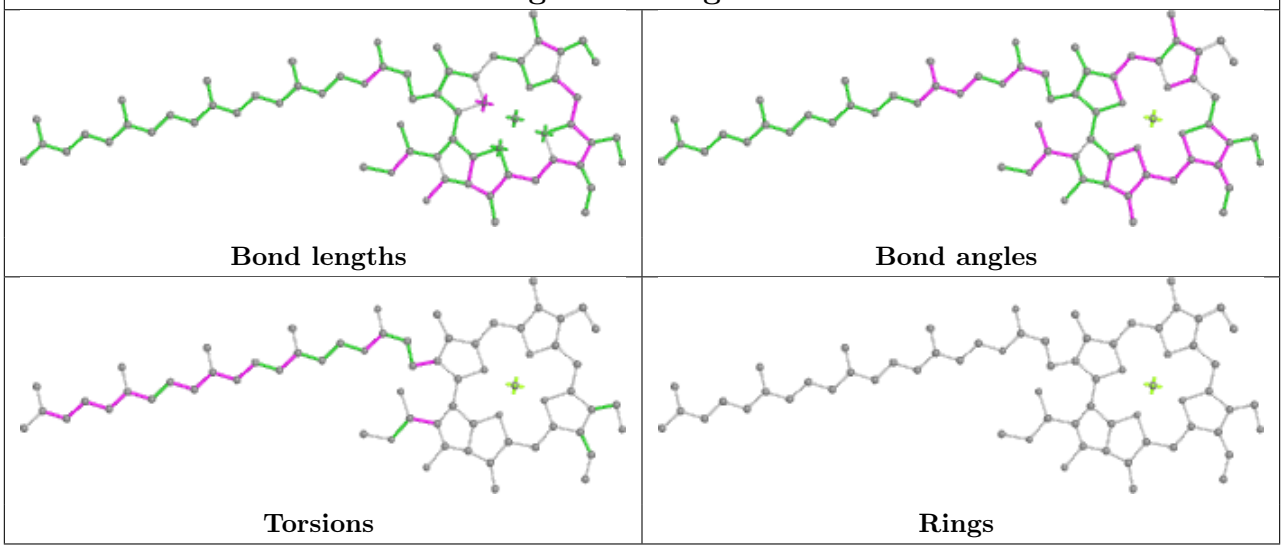
Ligand BCR C 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

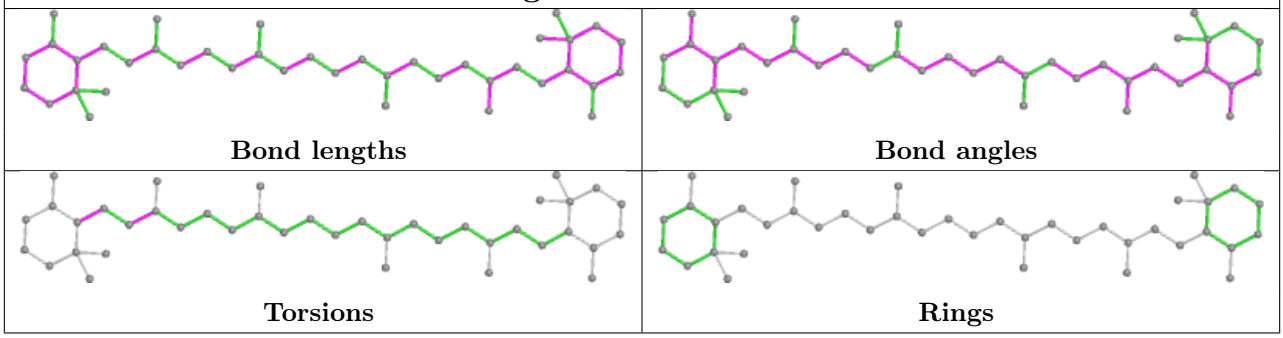
Ligand CHL 2 317

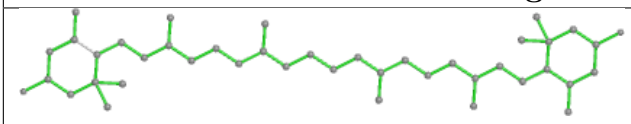
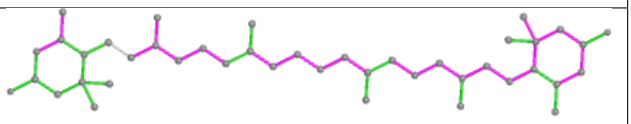
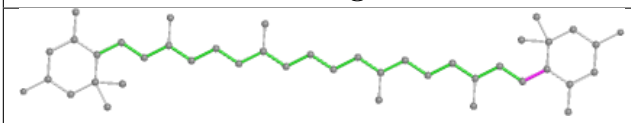
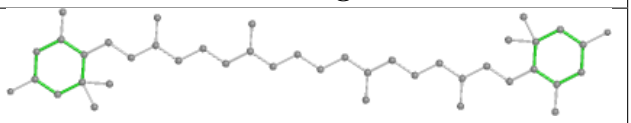


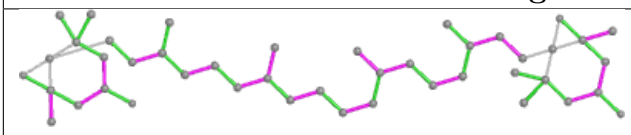
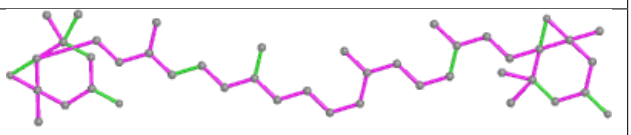
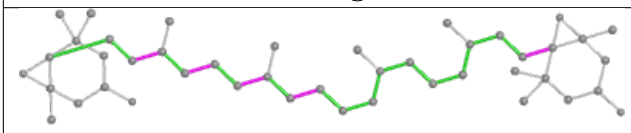
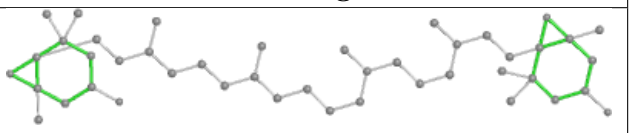
Ligand CHL g 311

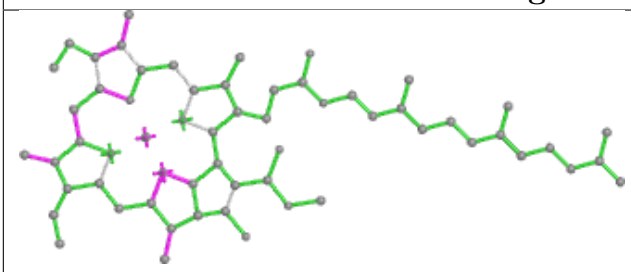
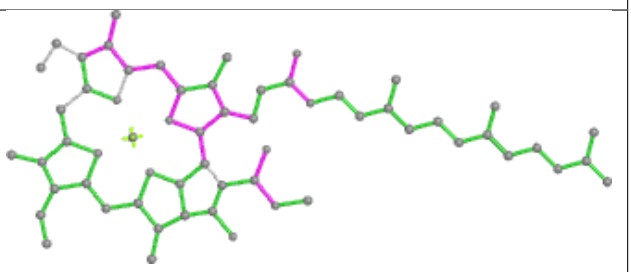
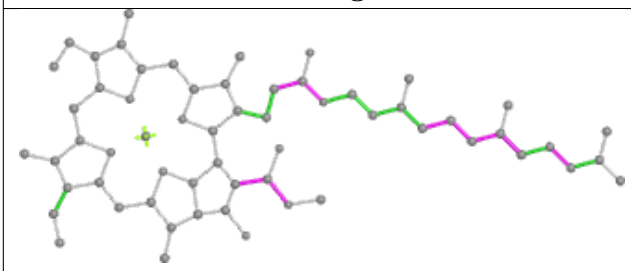
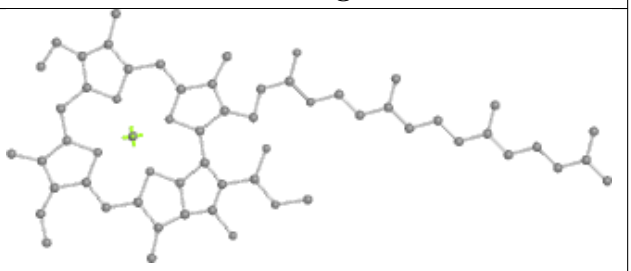


Ligand BCR A 409

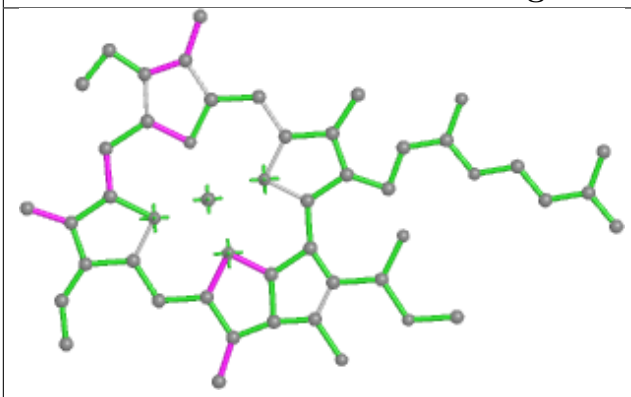


Ligand LUT P 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

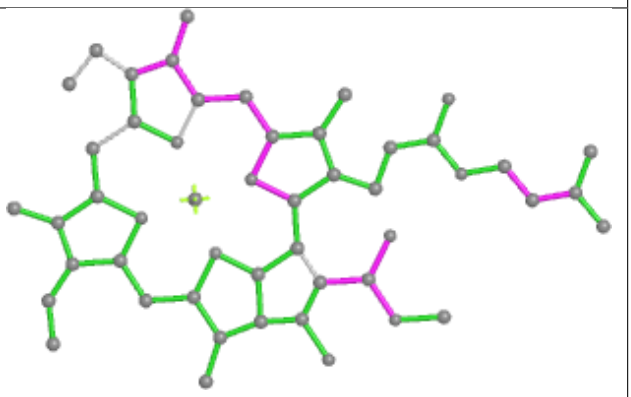
Ligand XAT r 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

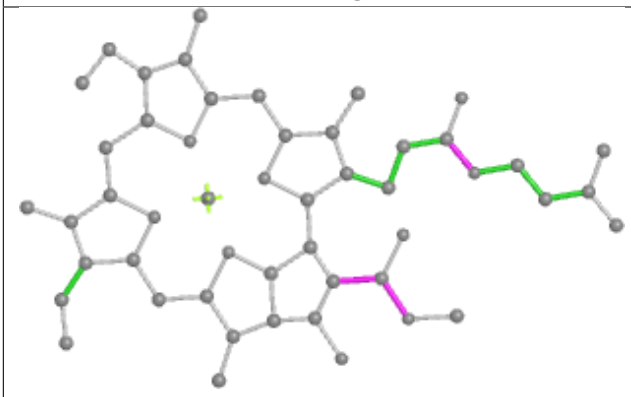
Ligand CLA u 303



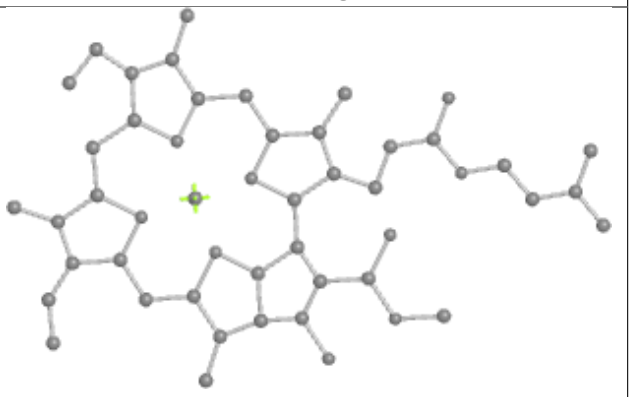
Bond lengths



Bond angles

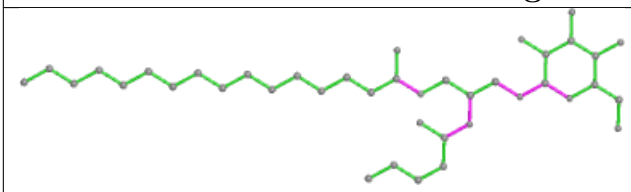


Torsions

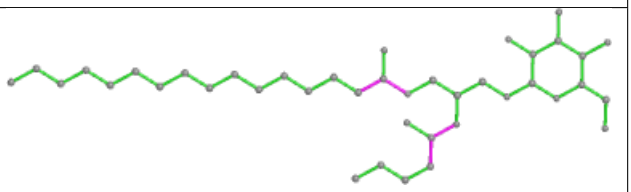


Rings

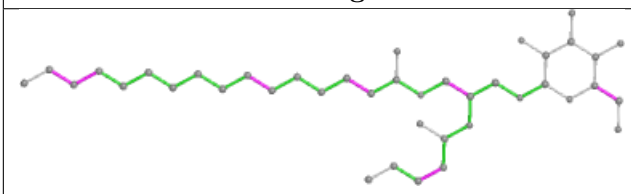
Ligand LMG a 412



Bond lengths



Bond angles



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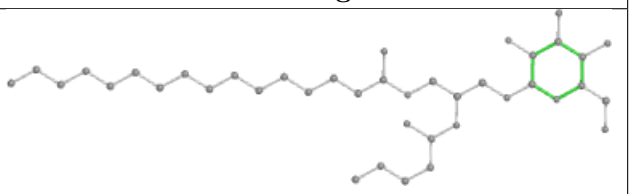
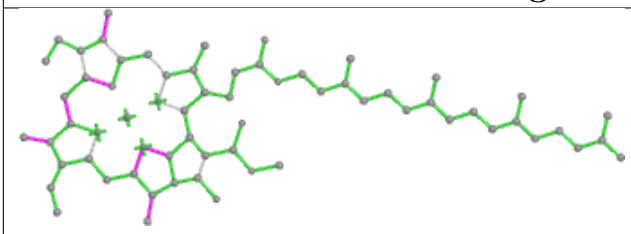
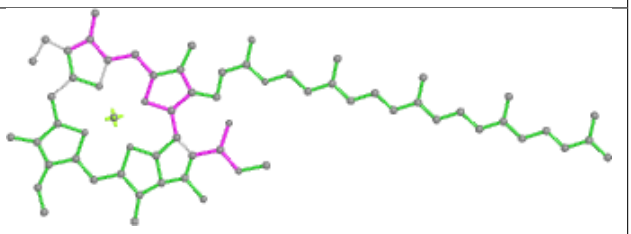
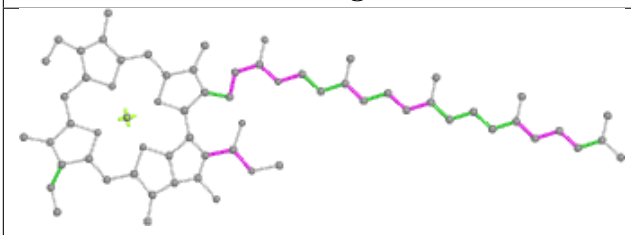
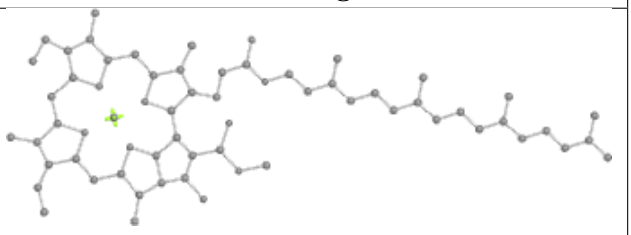
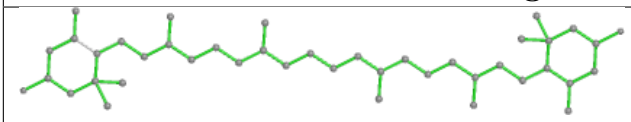
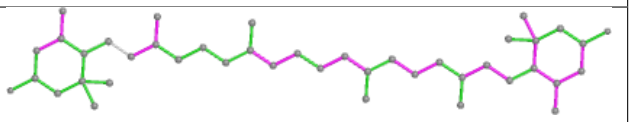
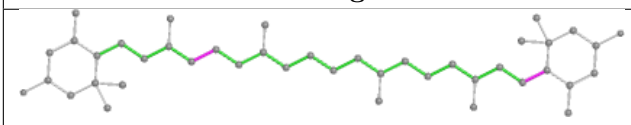
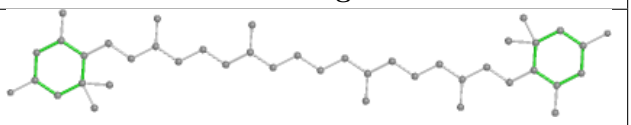
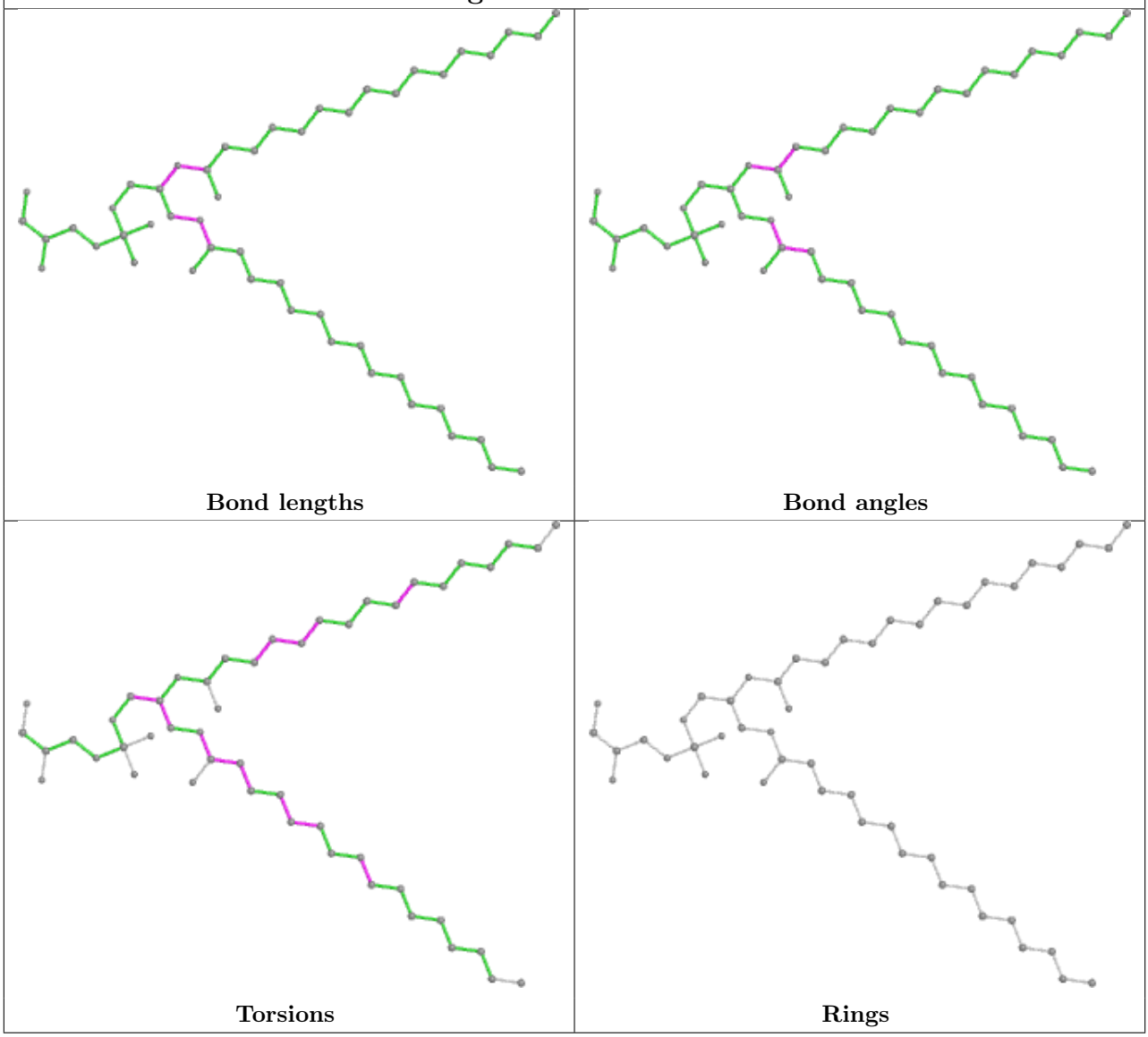


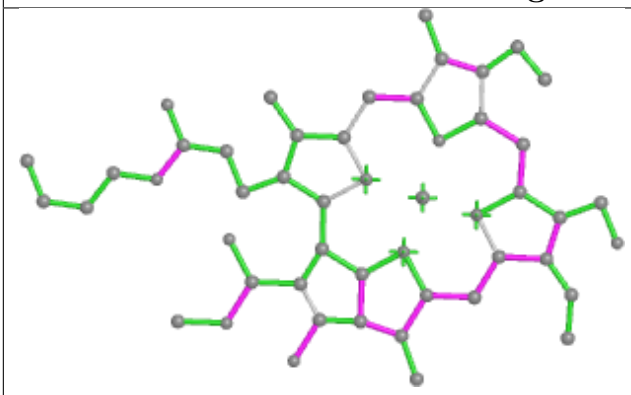
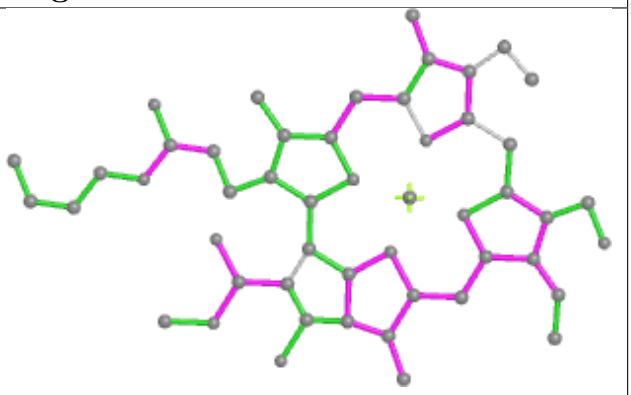
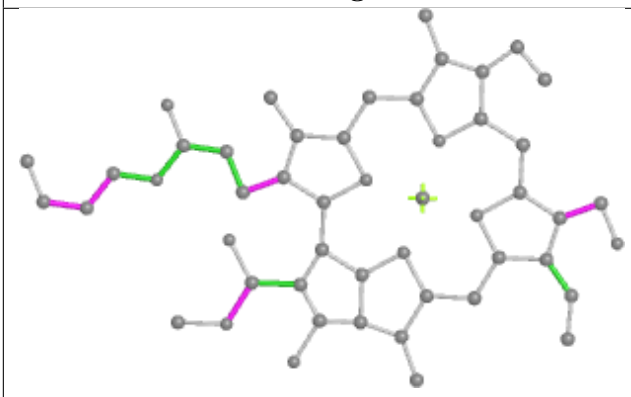
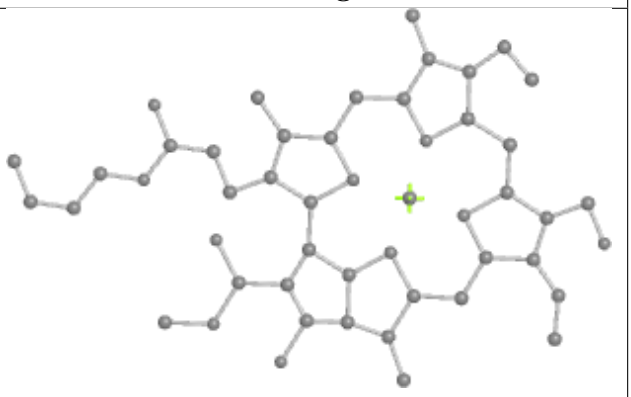
Rings

Ligand CLA c 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

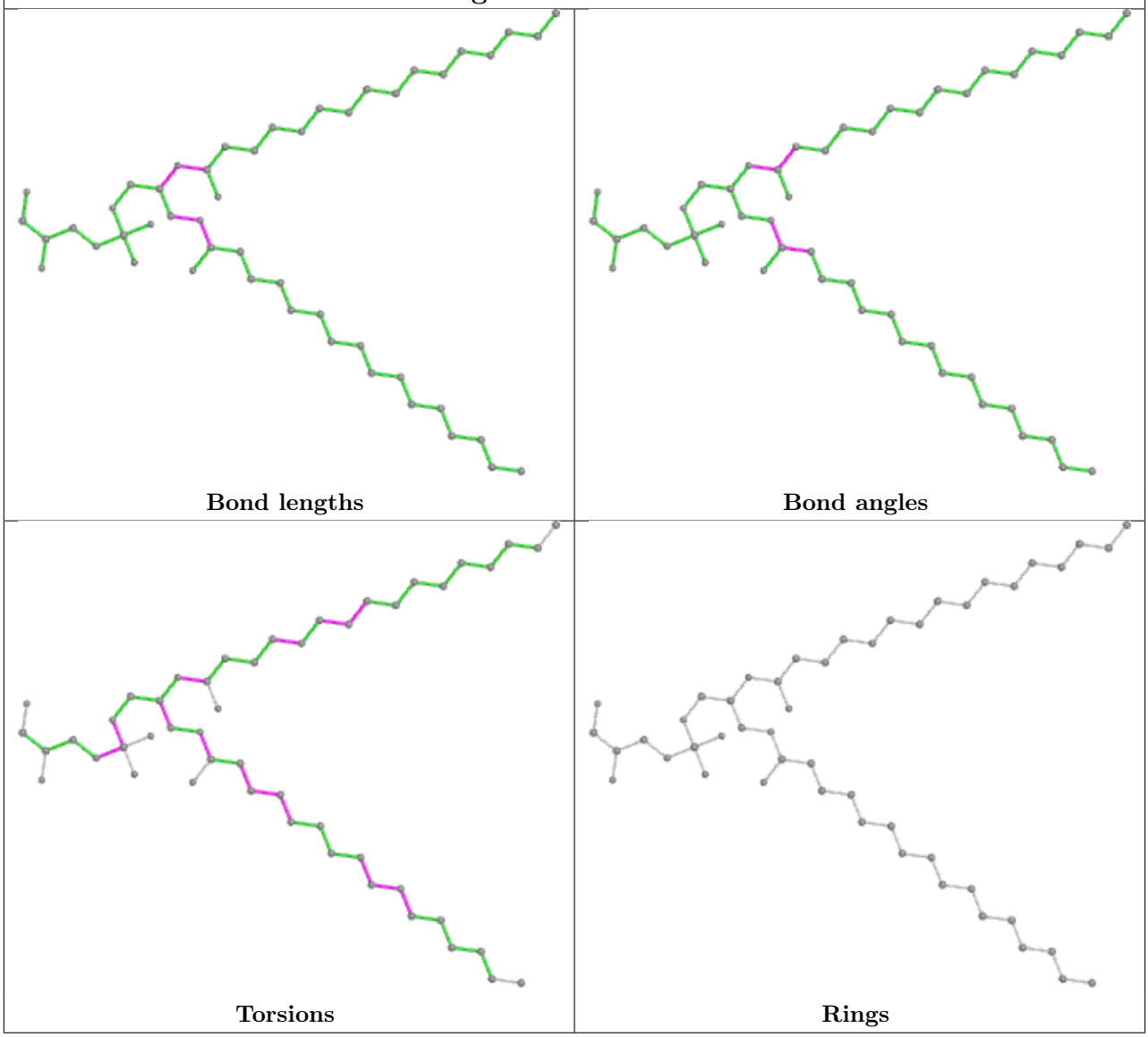
Ligand LUT U 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG N 312

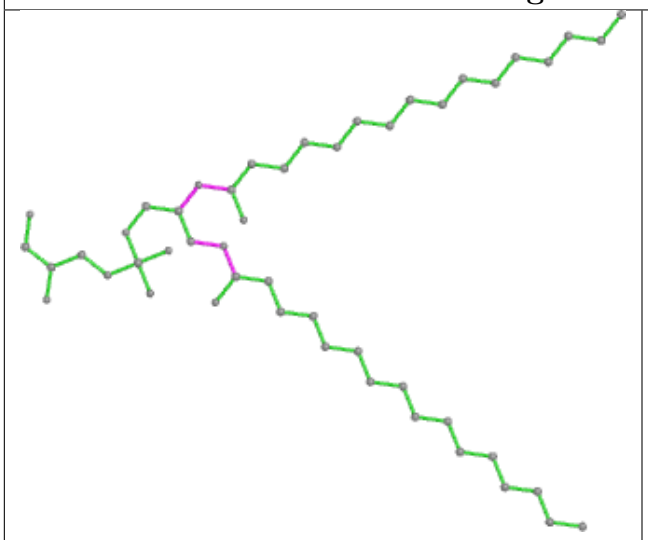


Ligand CHL g 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

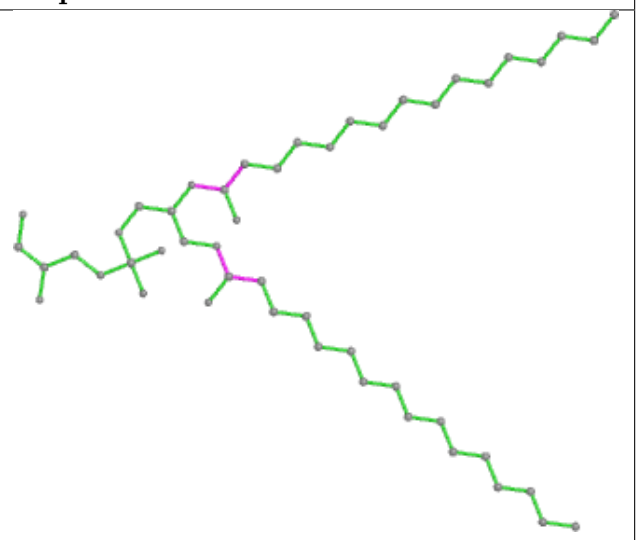
Ligand LHG v 312



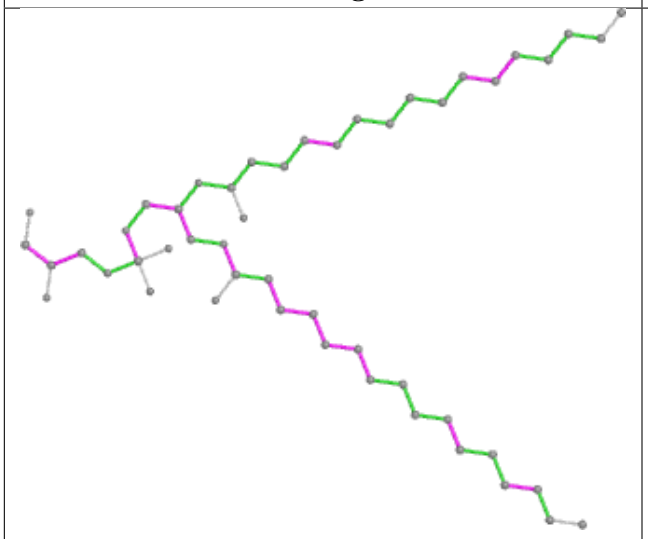
Ligand LHG p 313



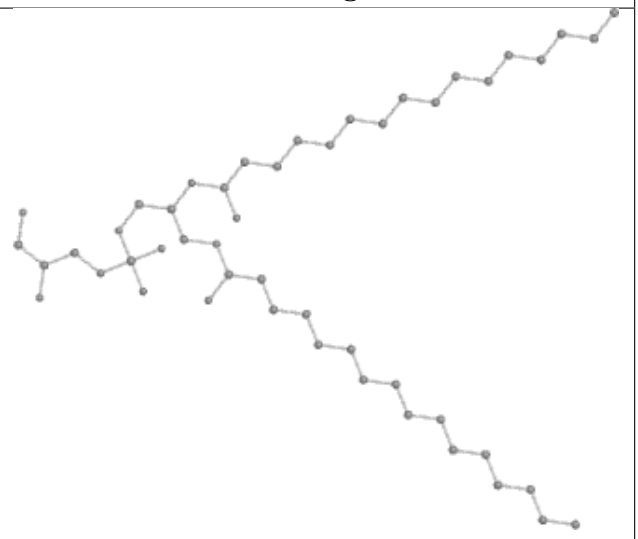
Bond lengths



Bond angles

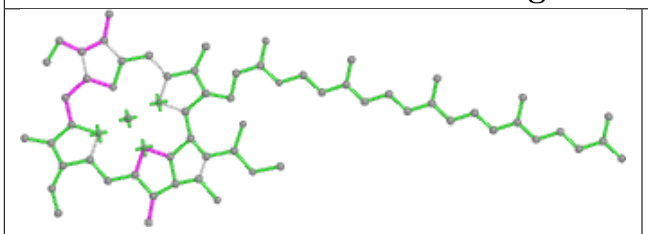


Torsions

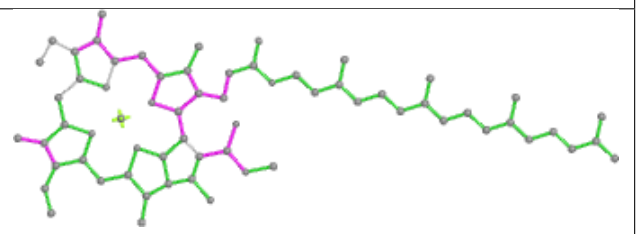


Rings

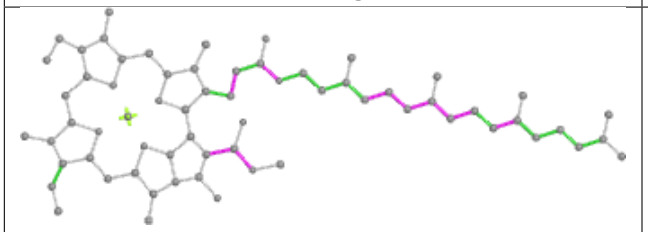
Ligand CLA b 605



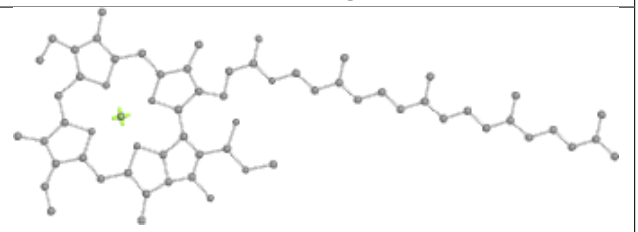
Bond lengths



Bond angles

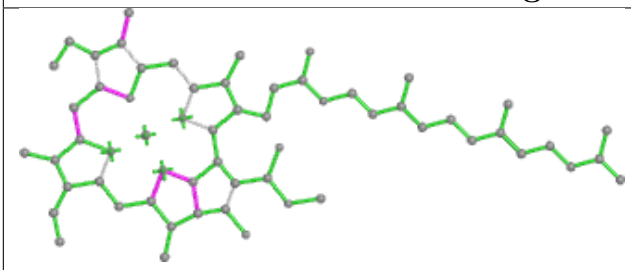


Torsions

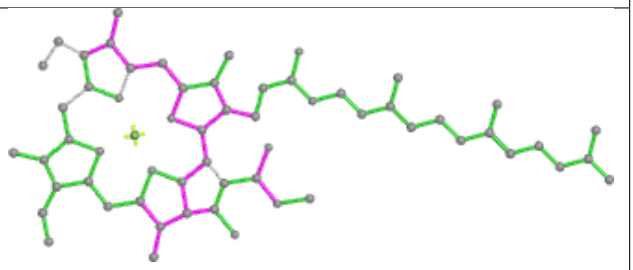


Rings

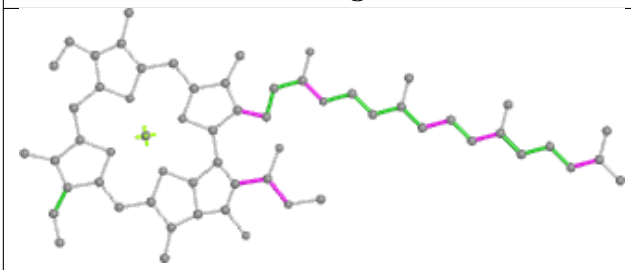
Ligand CLA N 305



Bond lengths



Bond angles



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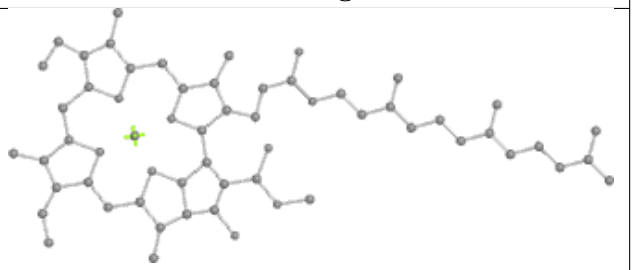
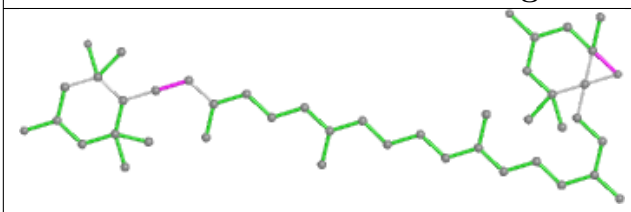


Rings

Ligand NEX N 318



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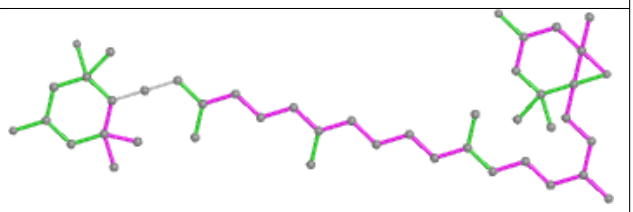
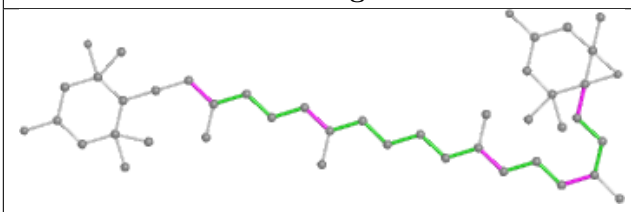


Bond angles



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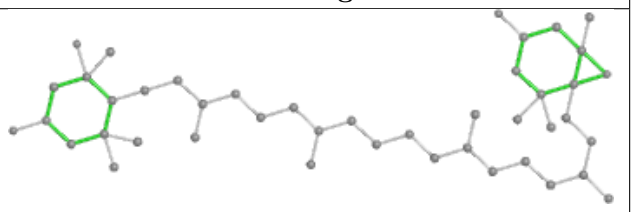
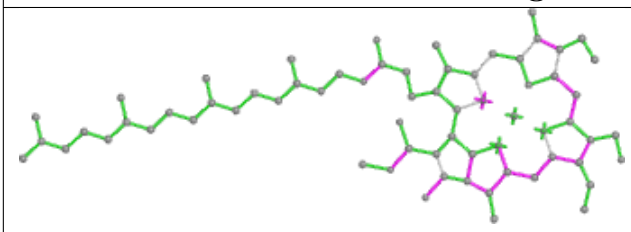


Rings

Ligand CHL 4 316



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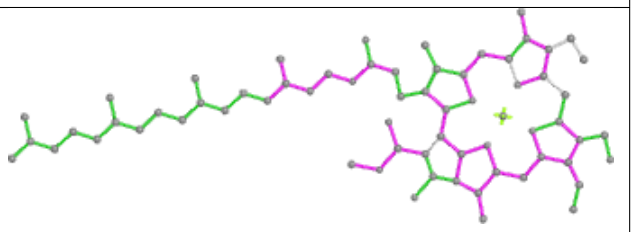
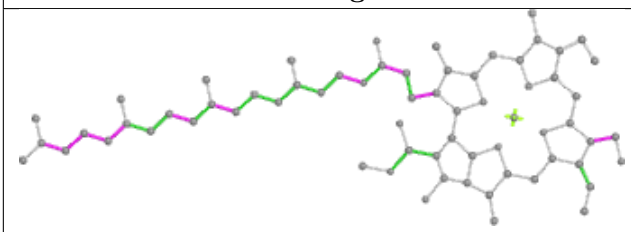
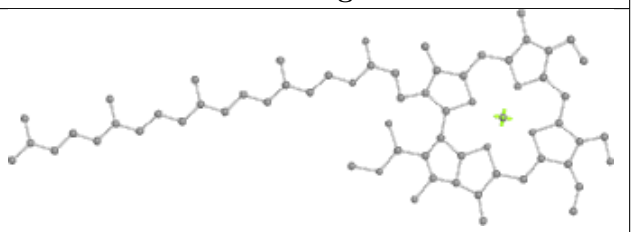


Bond angles

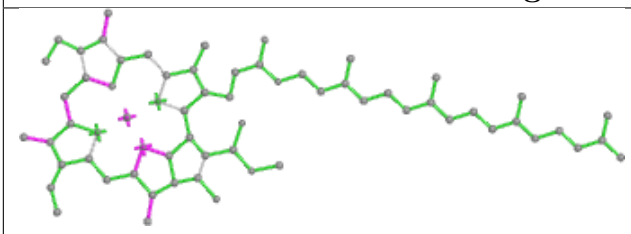


Torsions

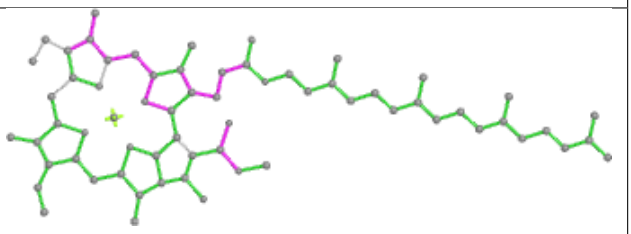


Rings

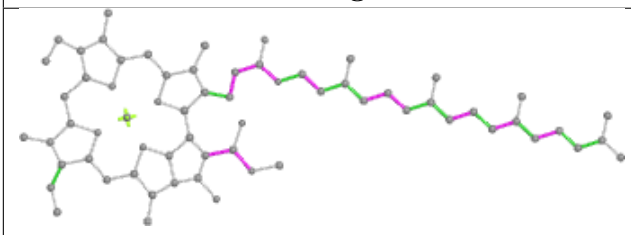
Ligand CLA A 404



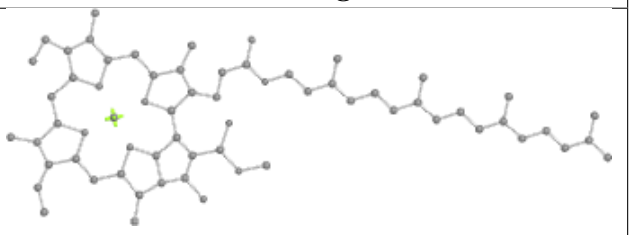
Bond lengths



Bond angles

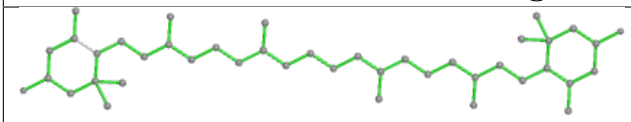


Torsions



Rings

Ligand LUT v 310



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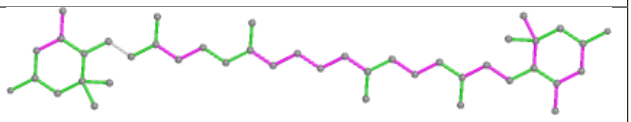
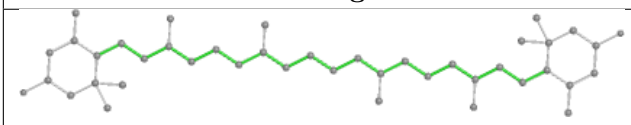


Bond angles



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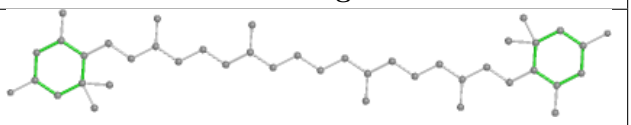
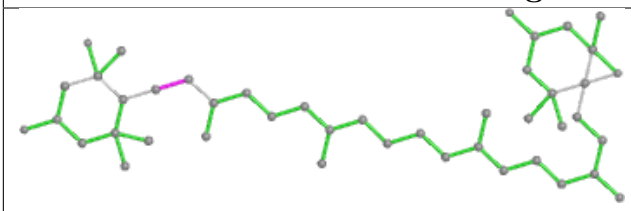


Rings

Ligand NEX u 319



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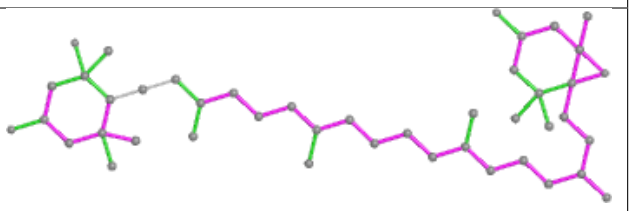
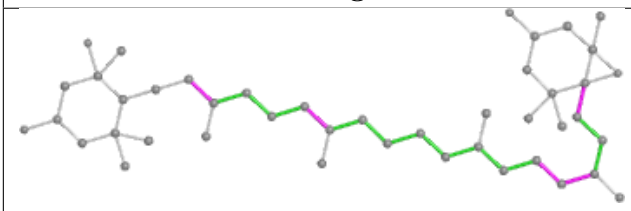


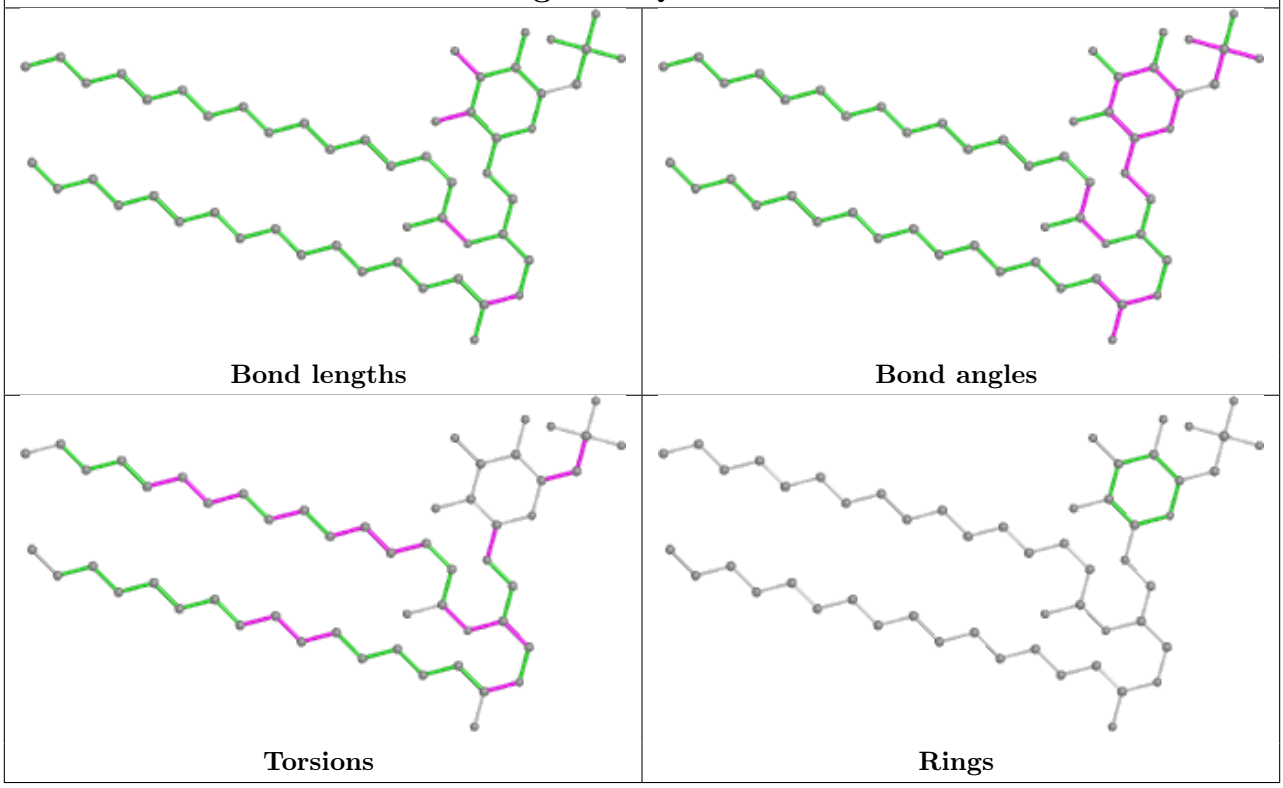
Bond angles



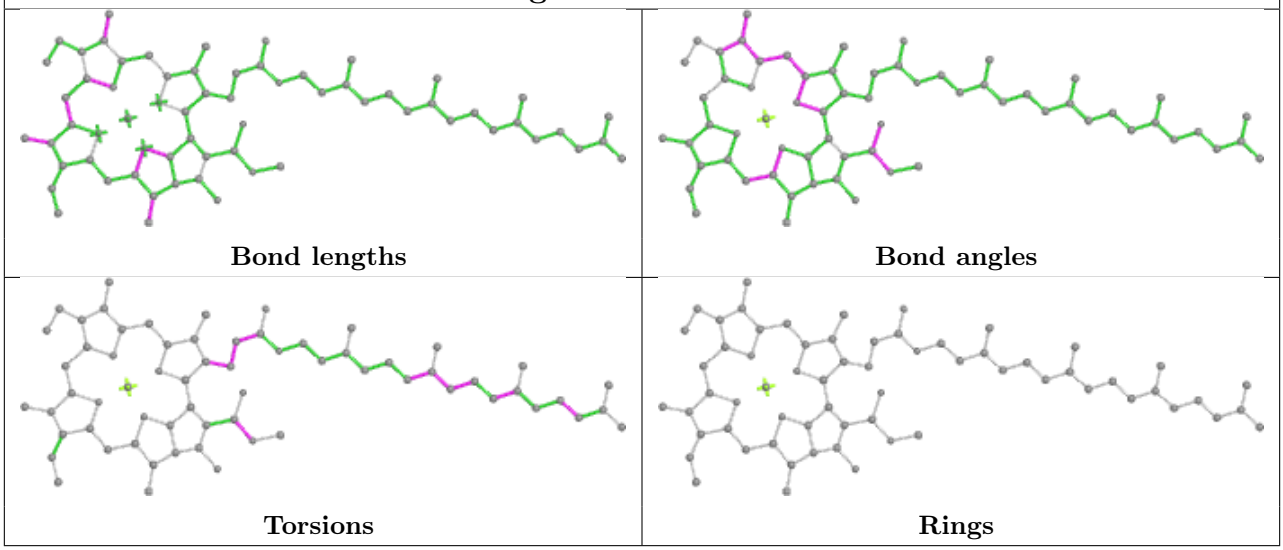
Torsions

Rings

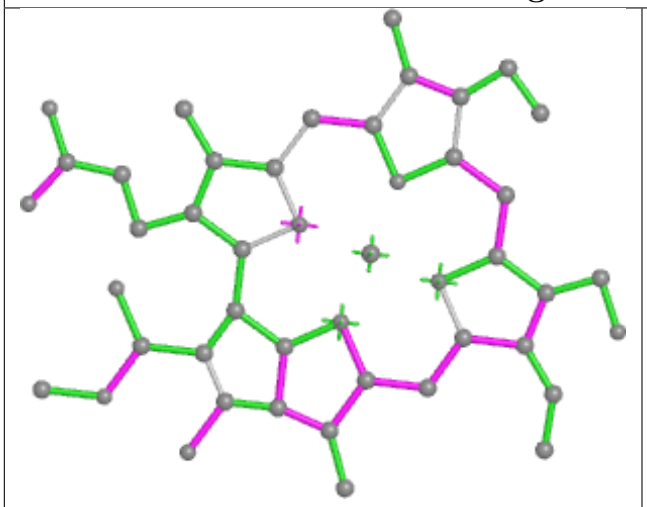
Ligand SQD l 102



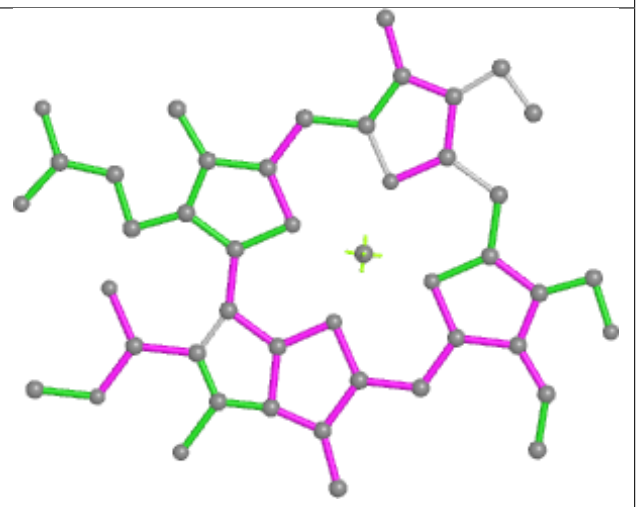
Ligand CLA 3 301



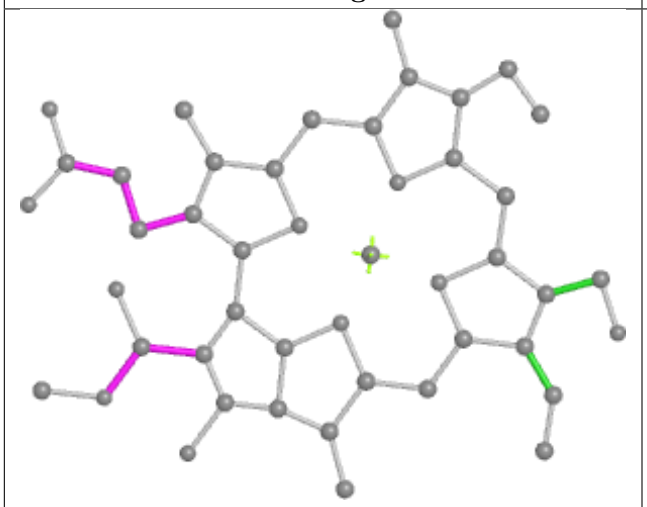
Ligand CHL S 314



Bond lengths



Bond angles



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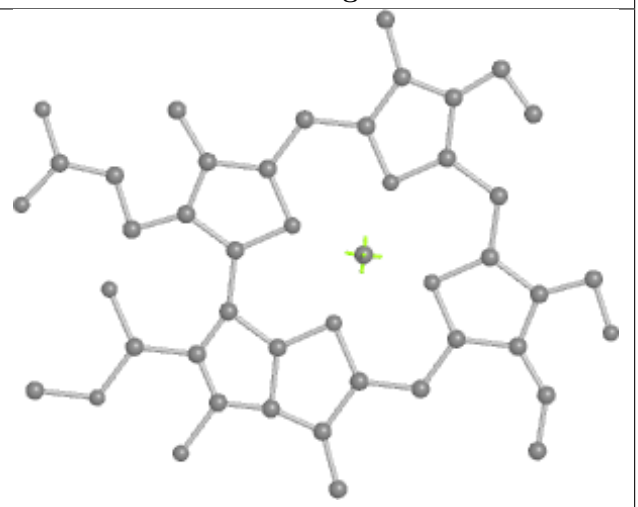
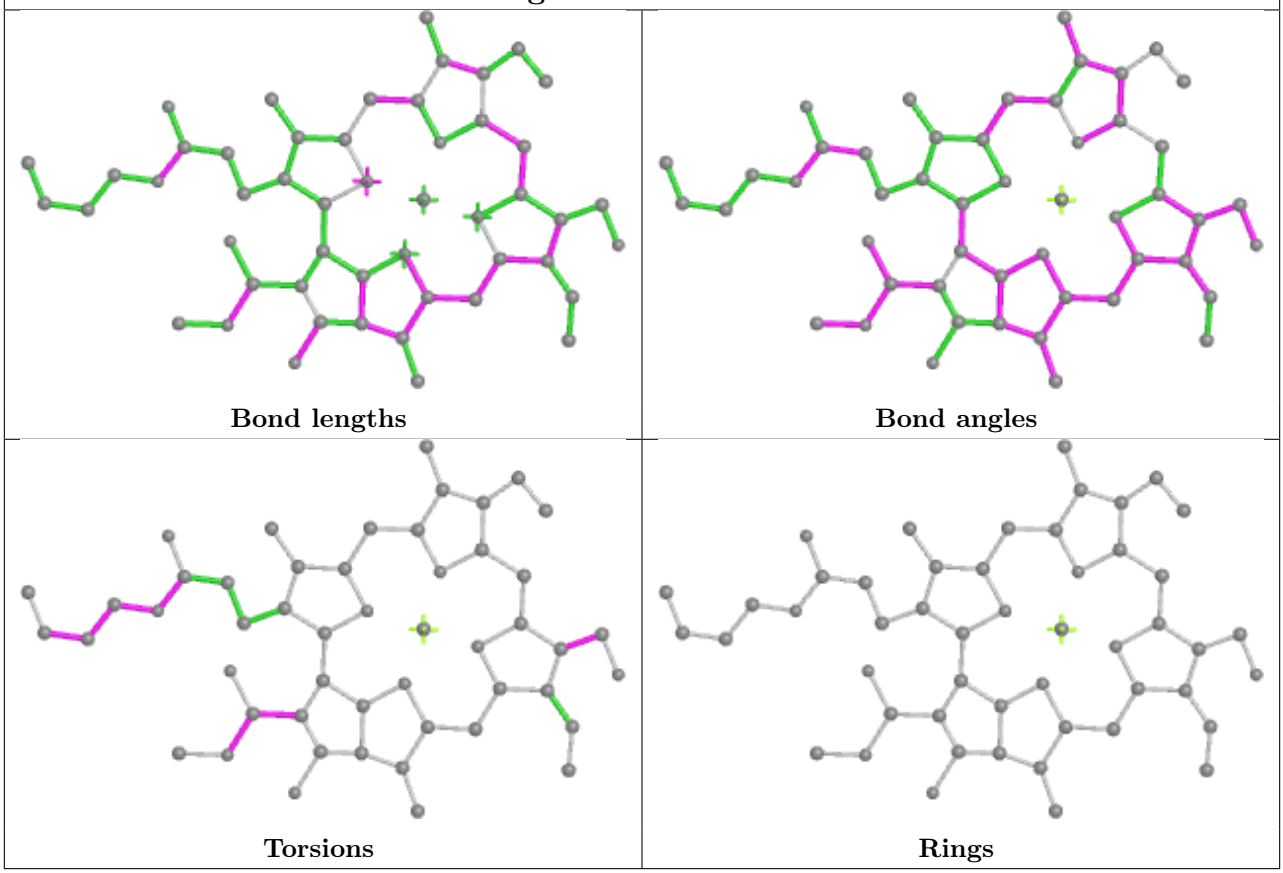
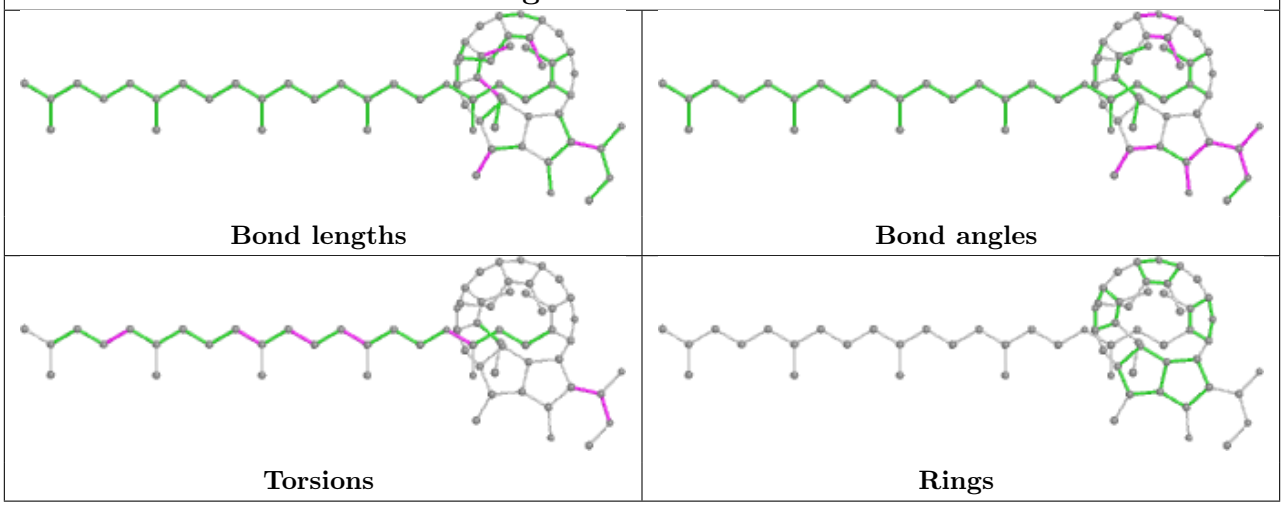


Rings

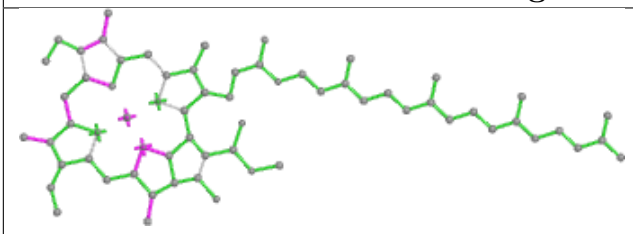
Ligand CHL n 315



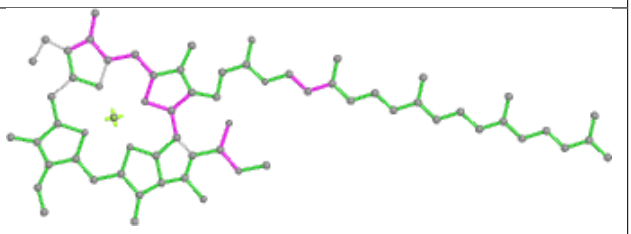
Ligand PHO A 407



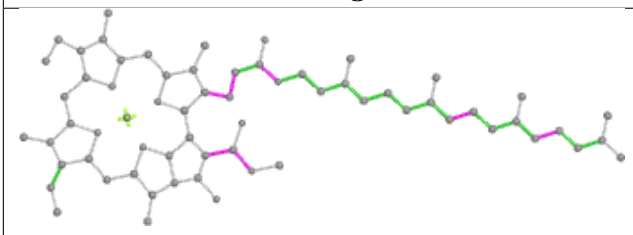
Ligand CLA a 405



Bond lengths



Bond angles



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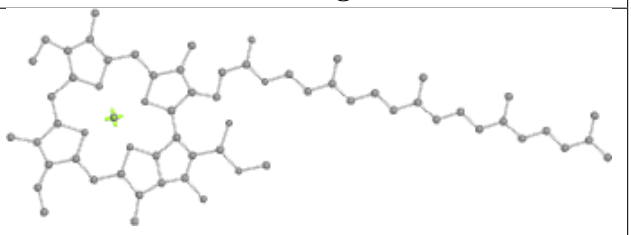
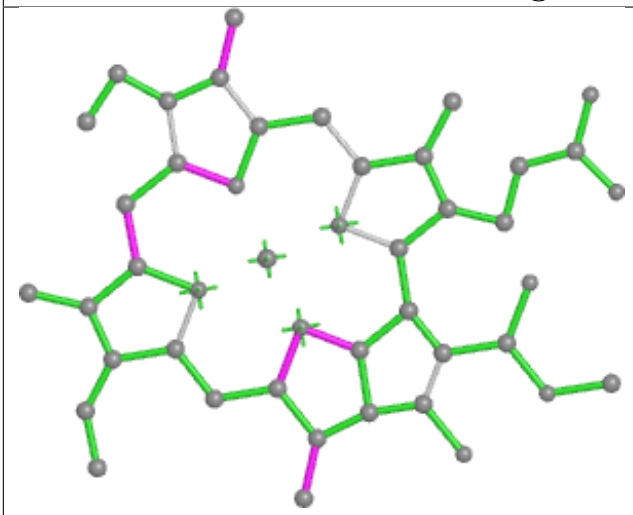
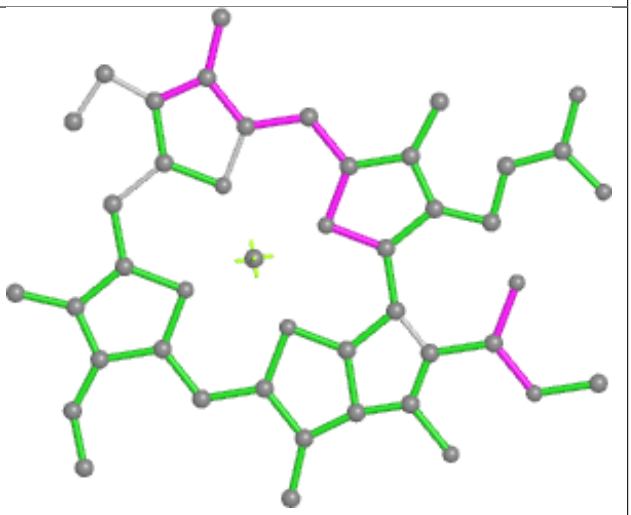


Rings

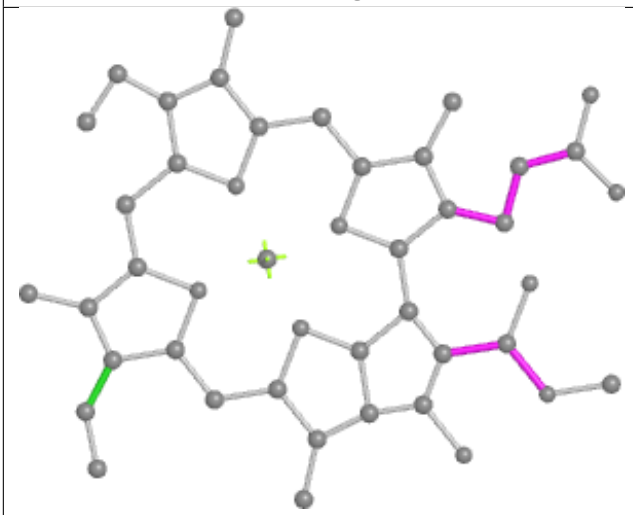
Ligand CLA s 304



Bond lengths



Bond angles



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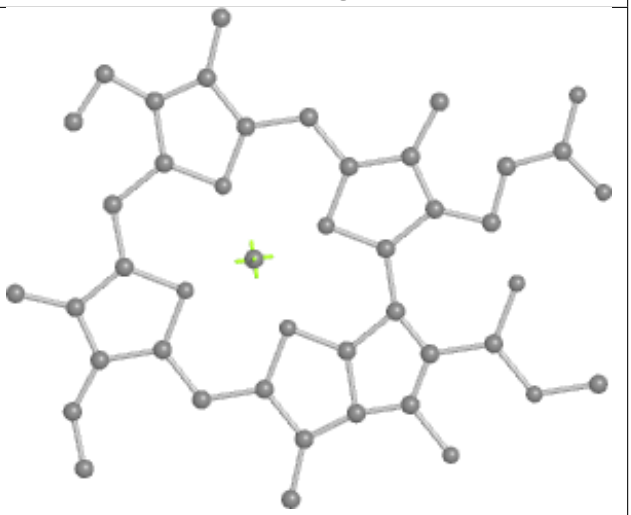
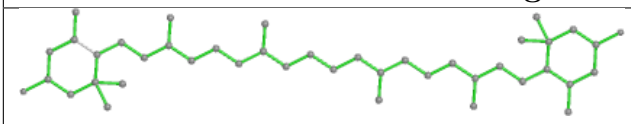


Rings

Ligand LUT V 309



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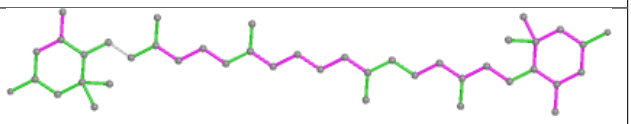
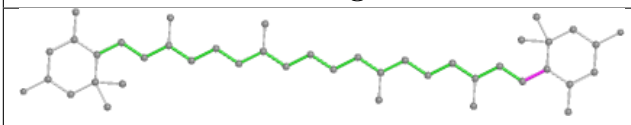


Bond angles



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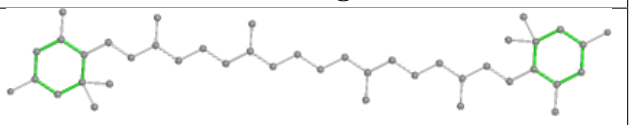
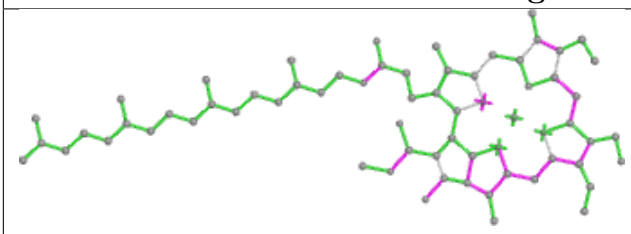


Rings

Ligand CHL 4 317



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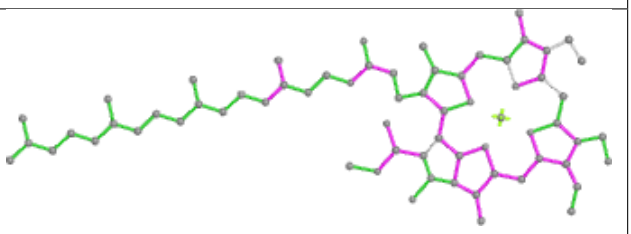
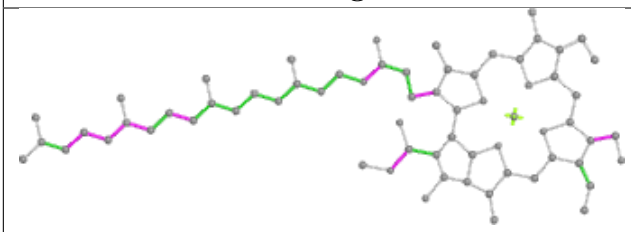


Bond angles



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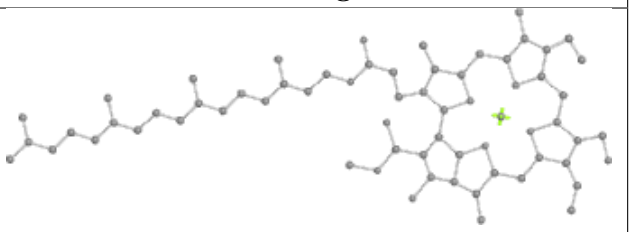
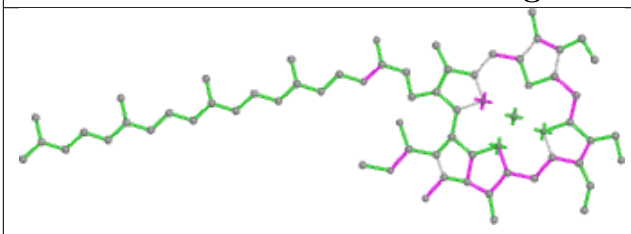
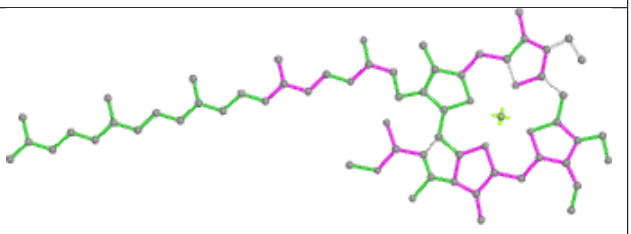


Rings

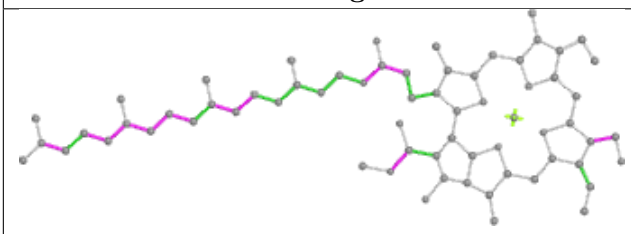
Ligand CHL V 313



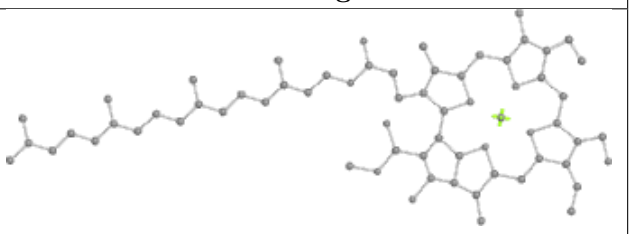
Bond lengths



Bond angles

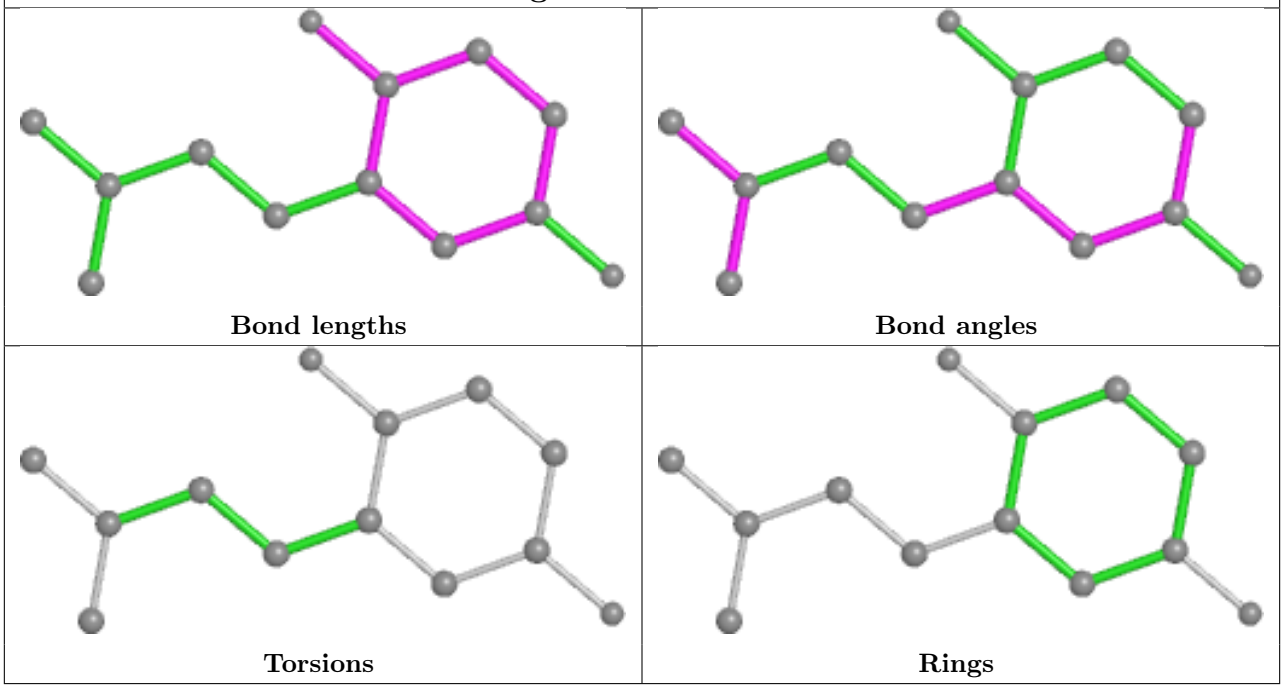


Torsions

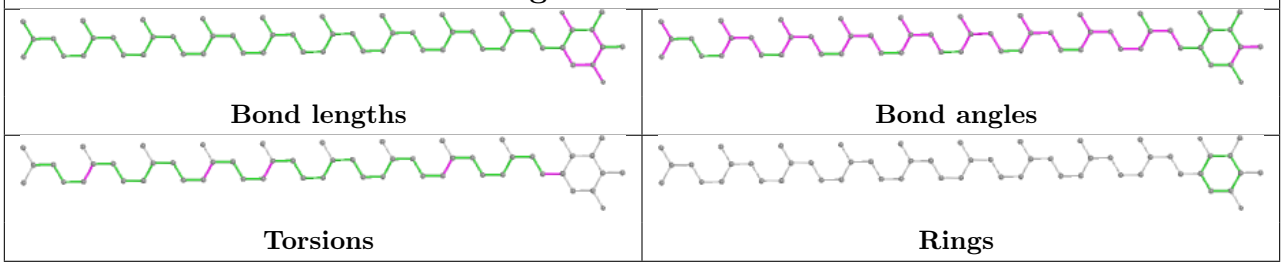


Rings

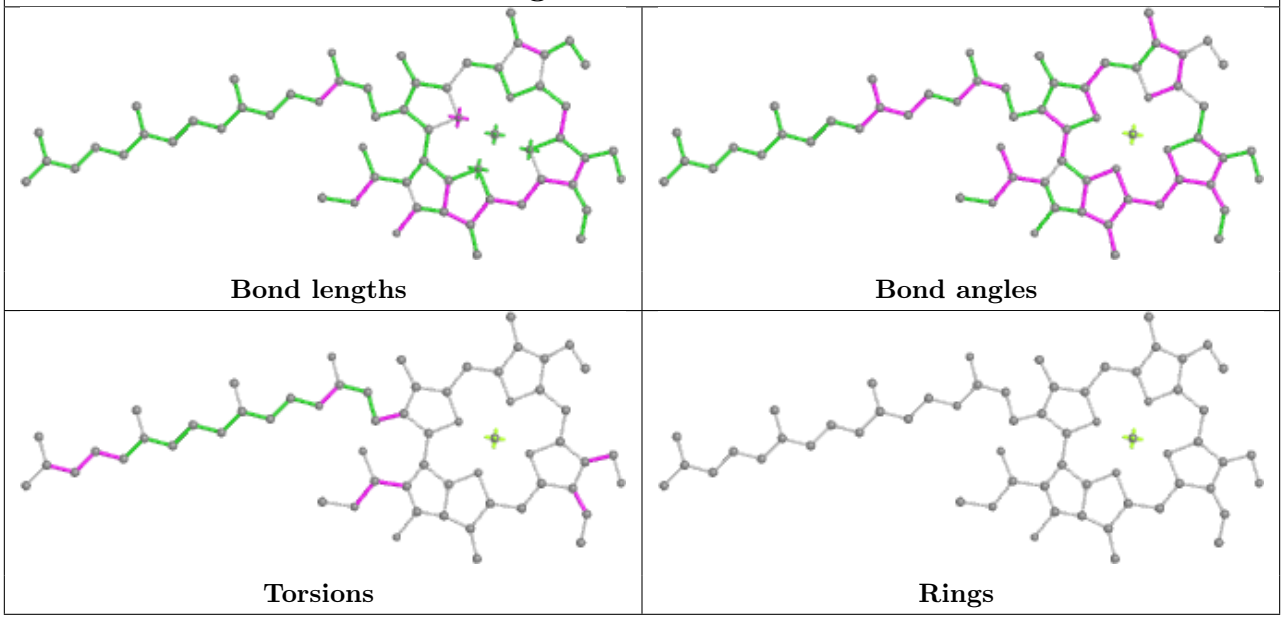
Ligand PL9 A 410

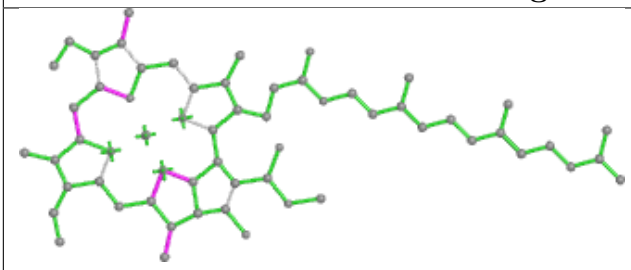
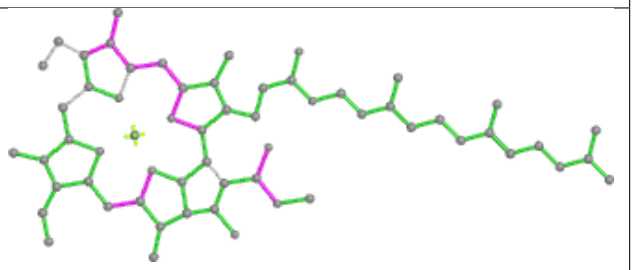
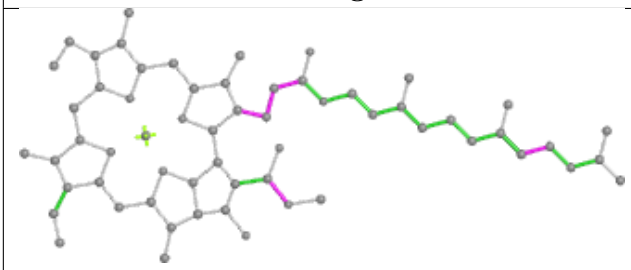
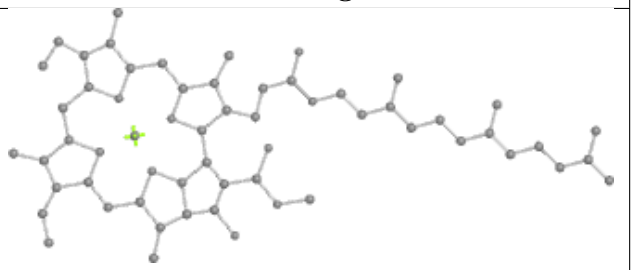


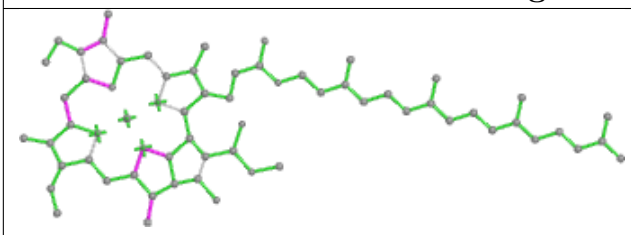
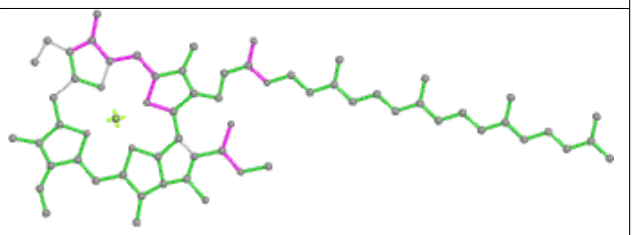
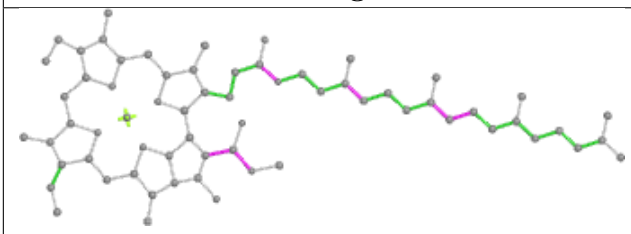
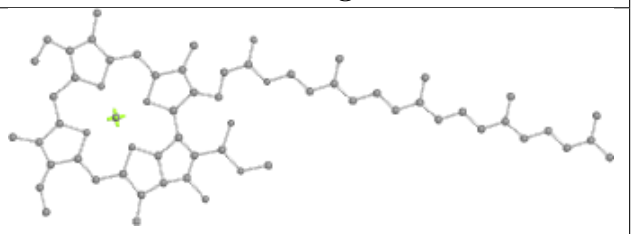
Ligand PL9 D 405



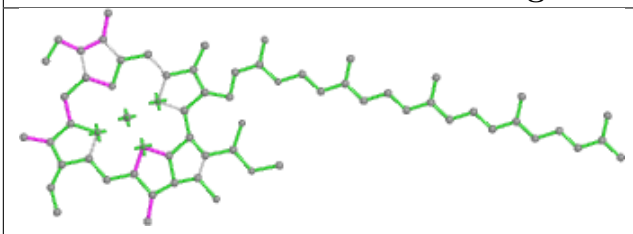
Ligand CHL 6 317



Ligand CLA r 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA u 301



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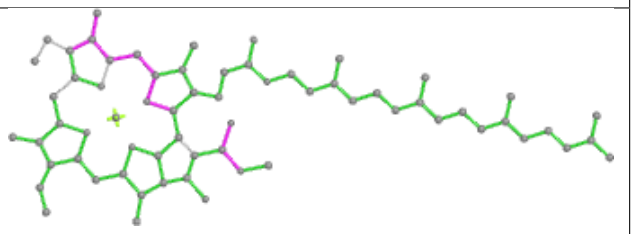

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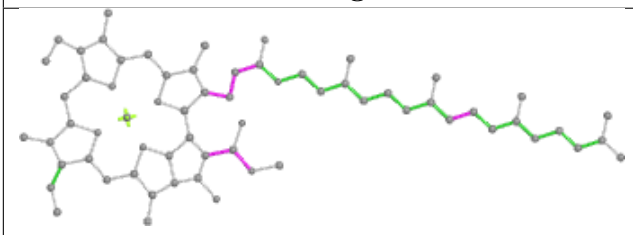

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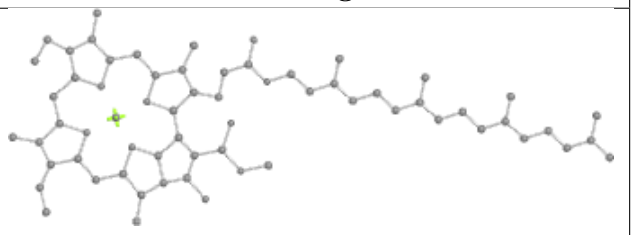
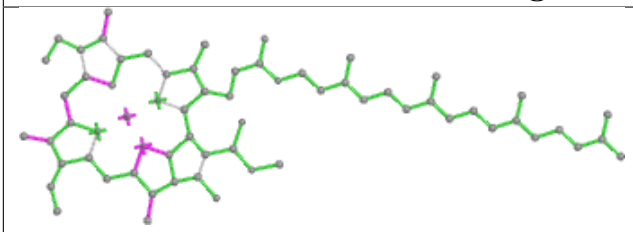


Rings

Ligand CLA 1 307



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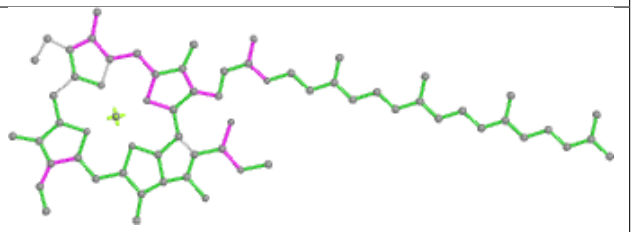

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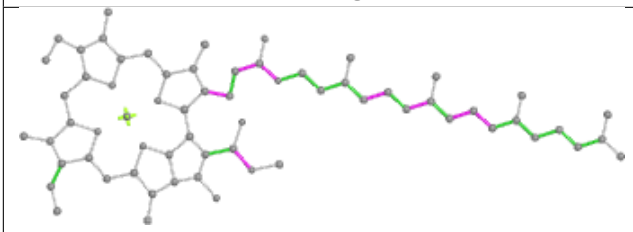

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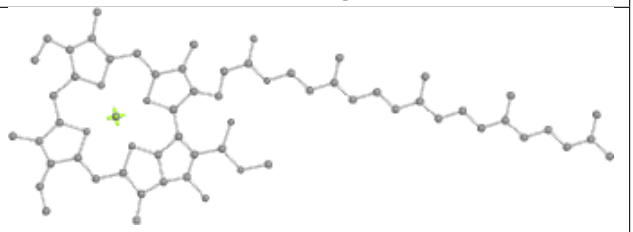
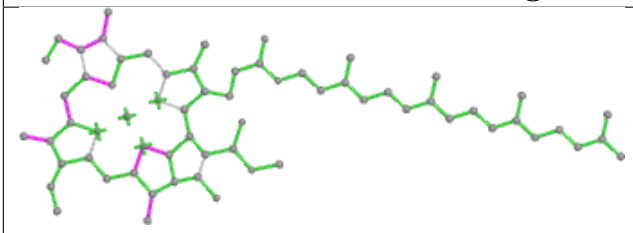


Rings

Ligand CLA C 515



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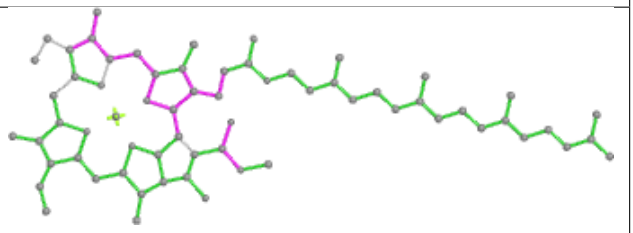

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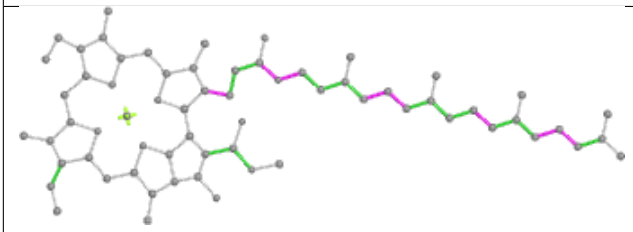

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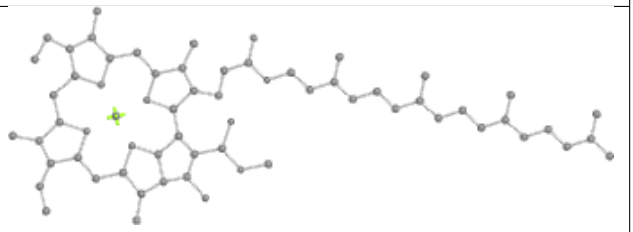
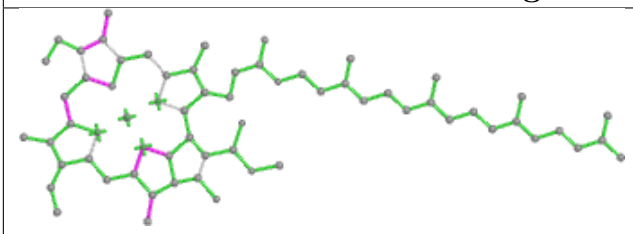


Rings

Ligand CLA G 307



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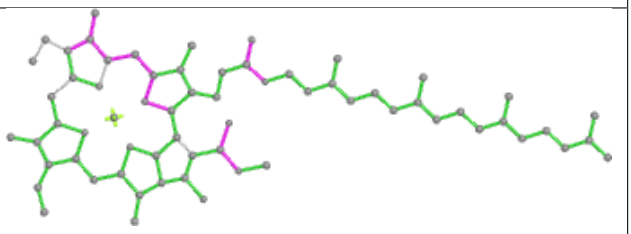

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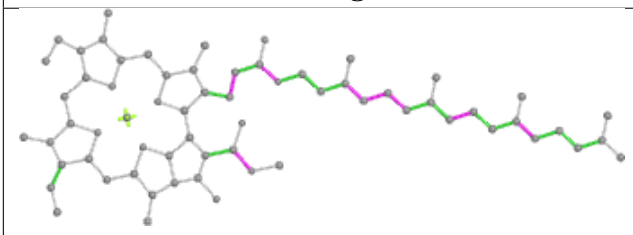

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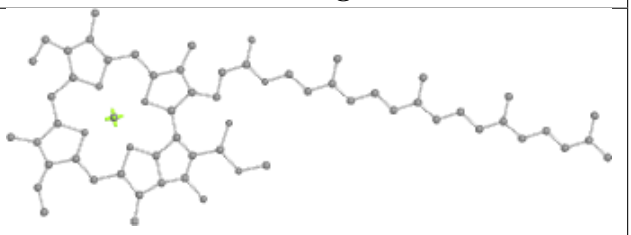
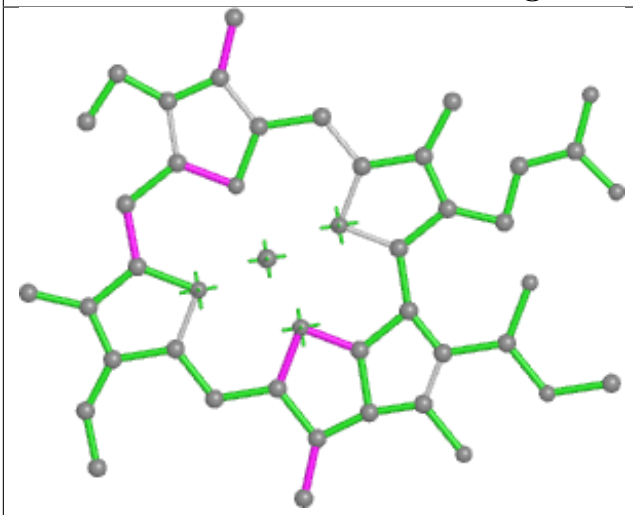


Rings

Ligand CLA R 311



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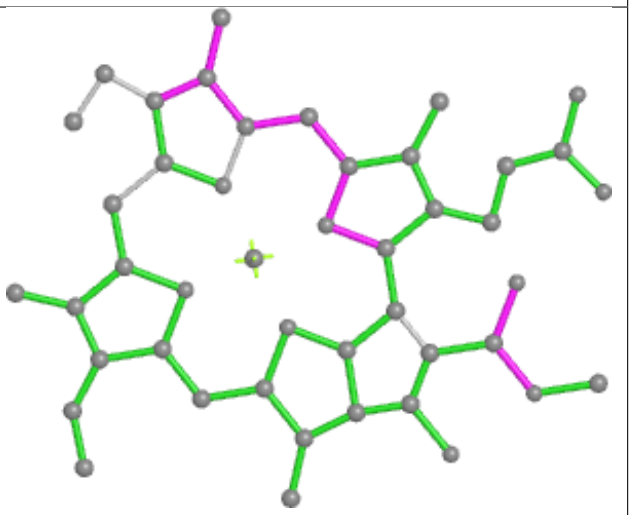

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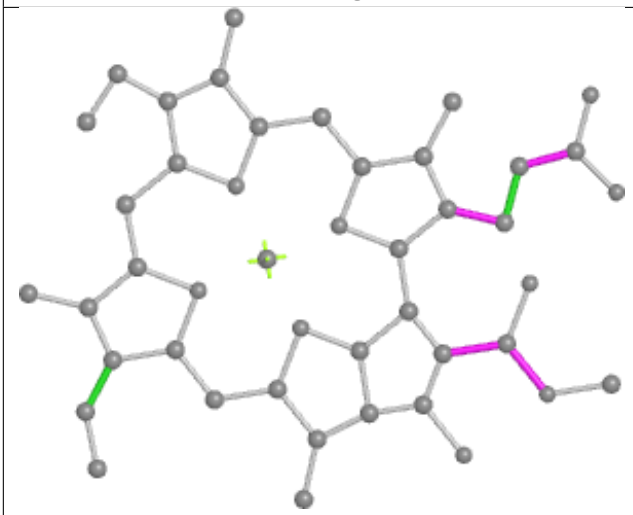

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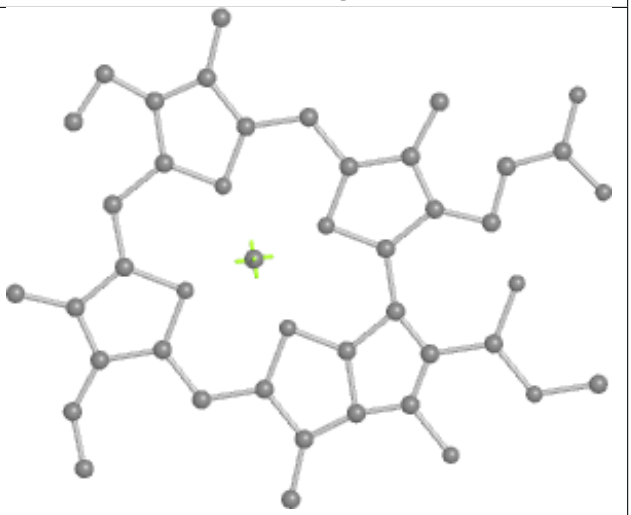
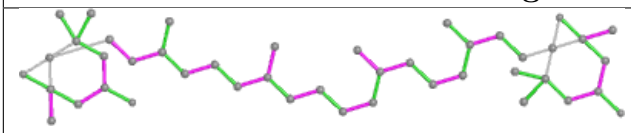


Rings

Ligand XAT N 311



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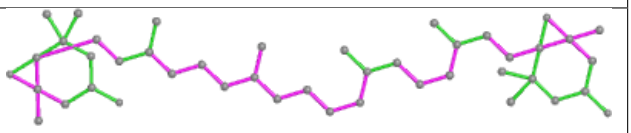

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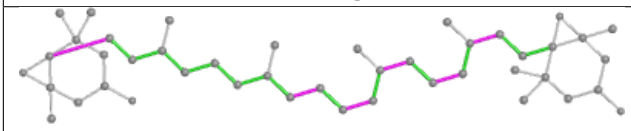

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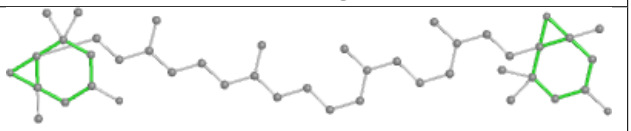
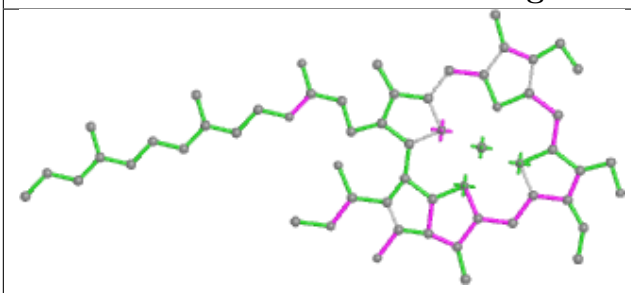


Rings

Ligand CHL S 315



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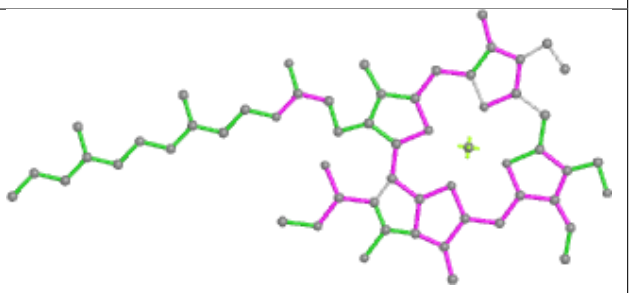

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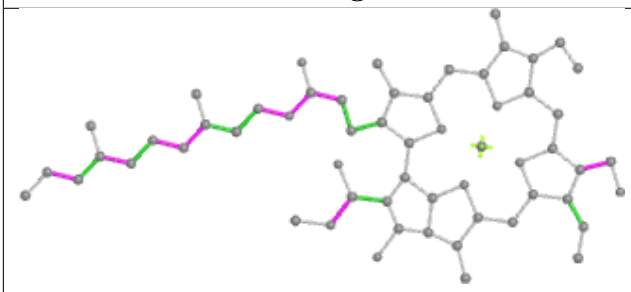

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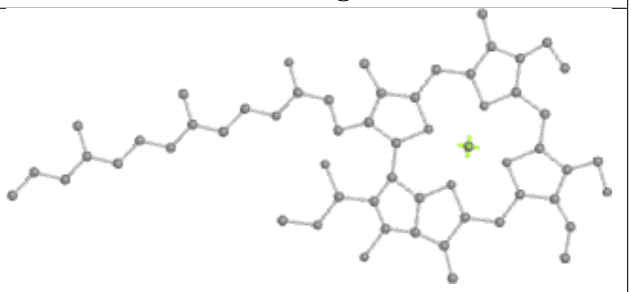
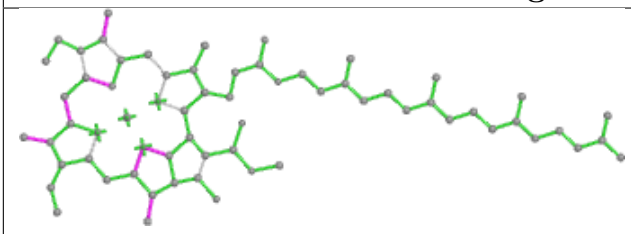


Rings

Ligand CLA q 301



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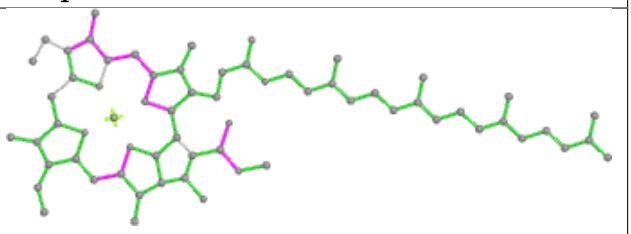

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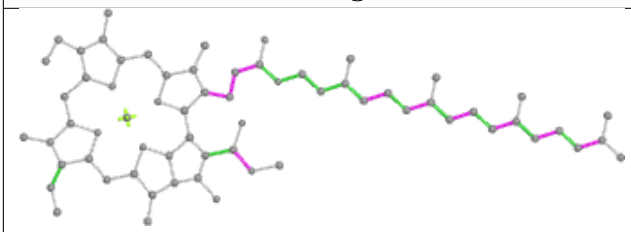

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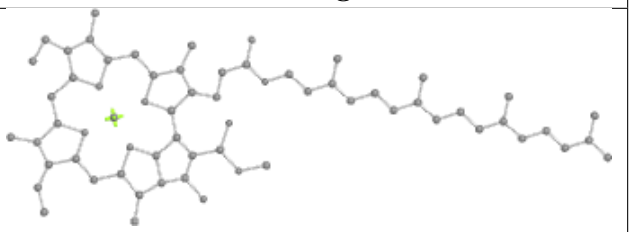
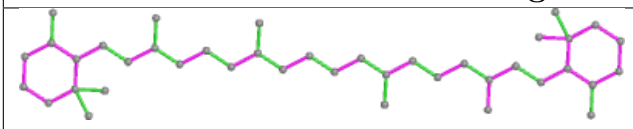


Rings

Ligand BCR t 101



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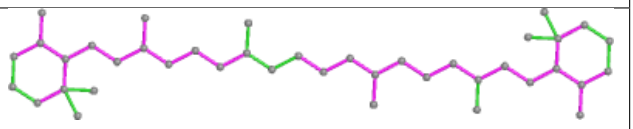

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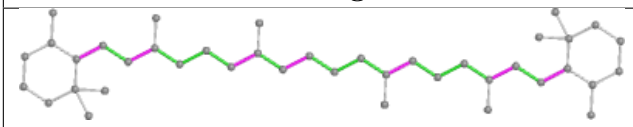

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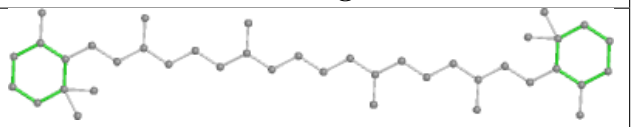
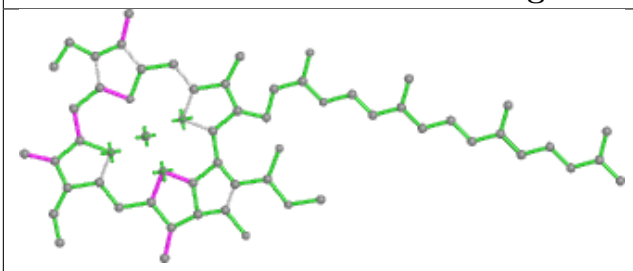


Rings

Ligand CLA p 308



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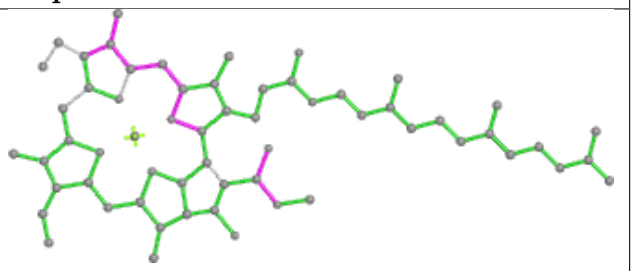

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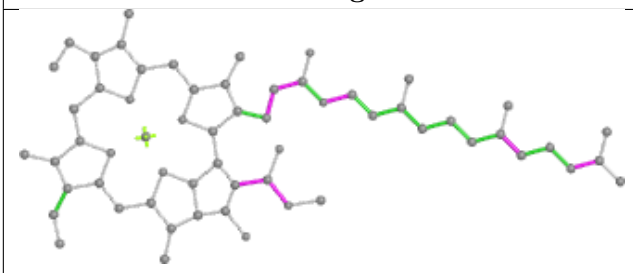

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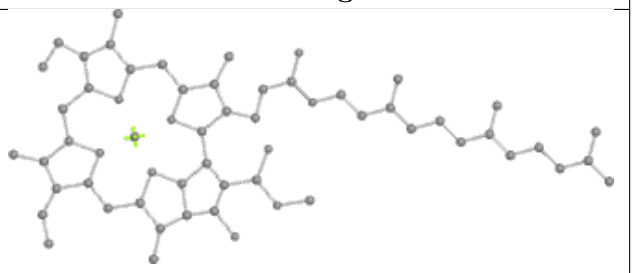
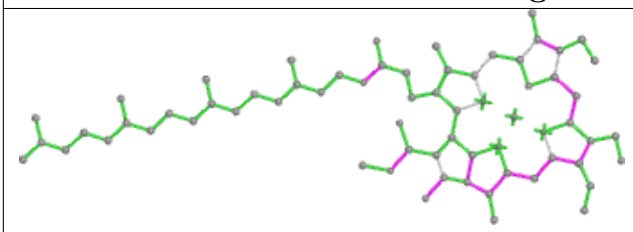


Rings

Ligand CHL r 614



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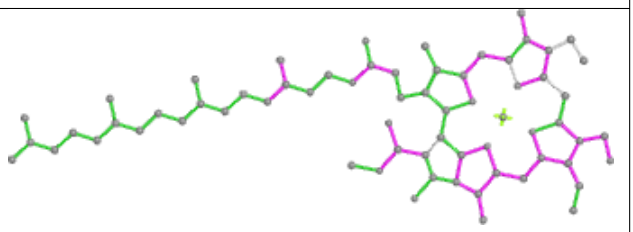

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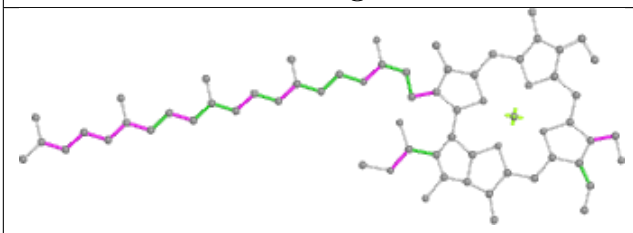

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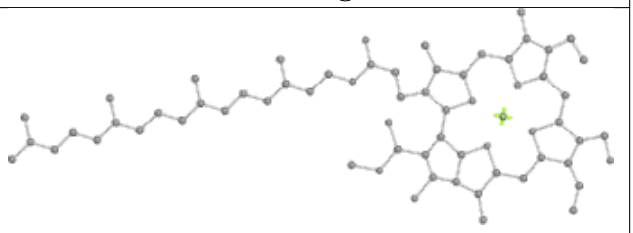
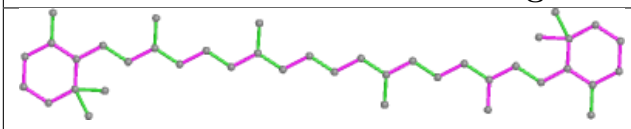


Rings

Ligand BCR a 409



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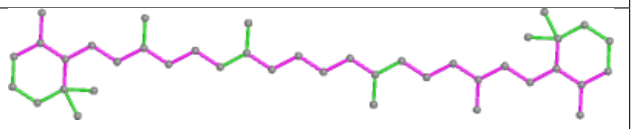
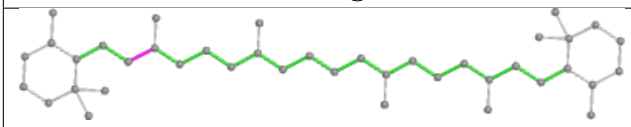


Bond angles



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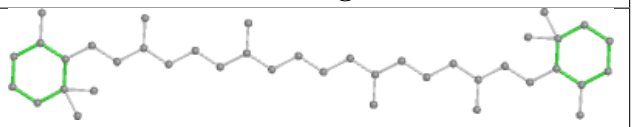
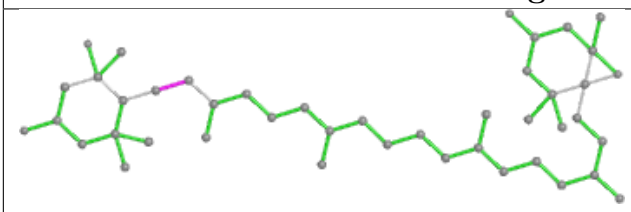


Rings

Ligand NEX s 317



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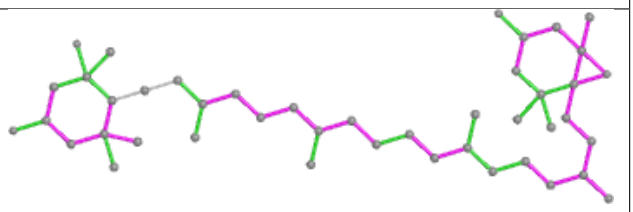
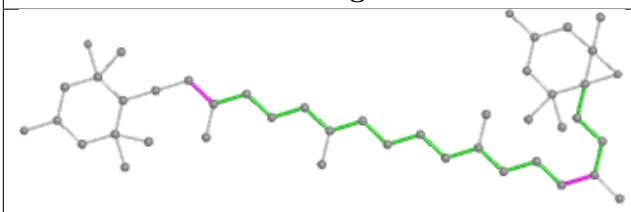


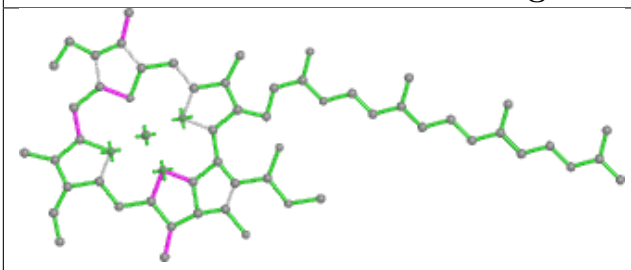
Bond angles



Torsions

Rings

Ligand CLA 6 307



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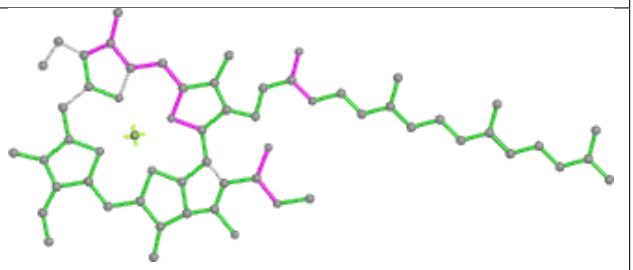

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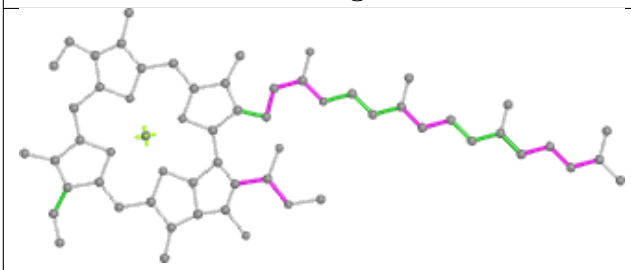

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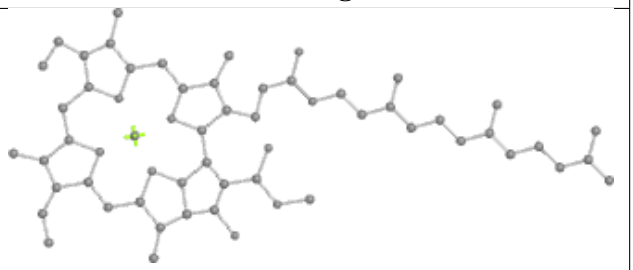
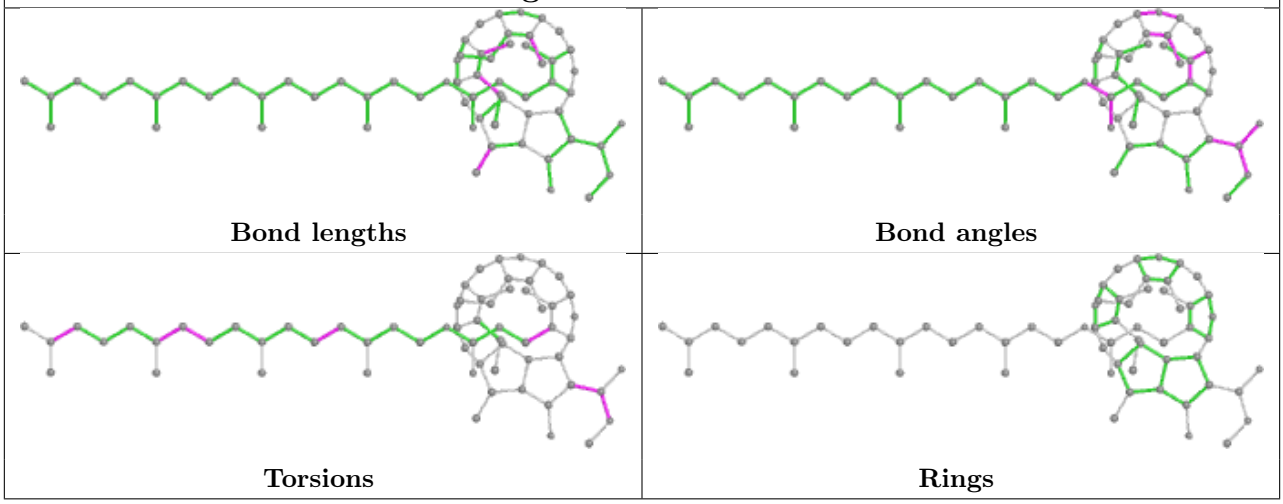
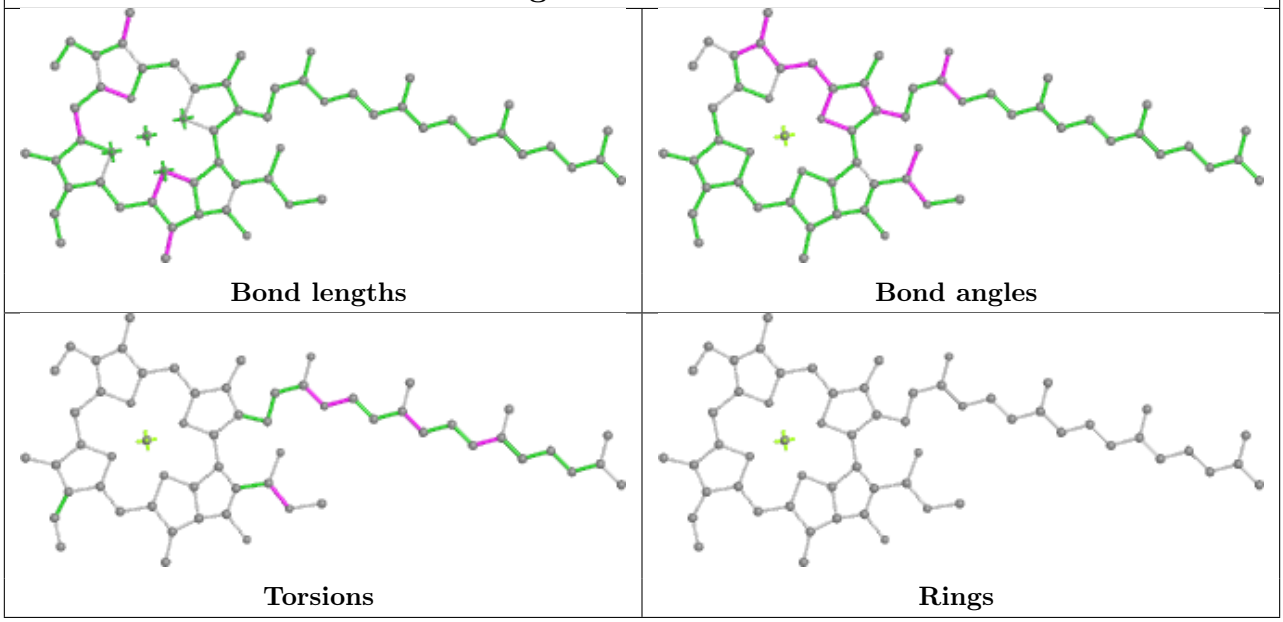


Rings

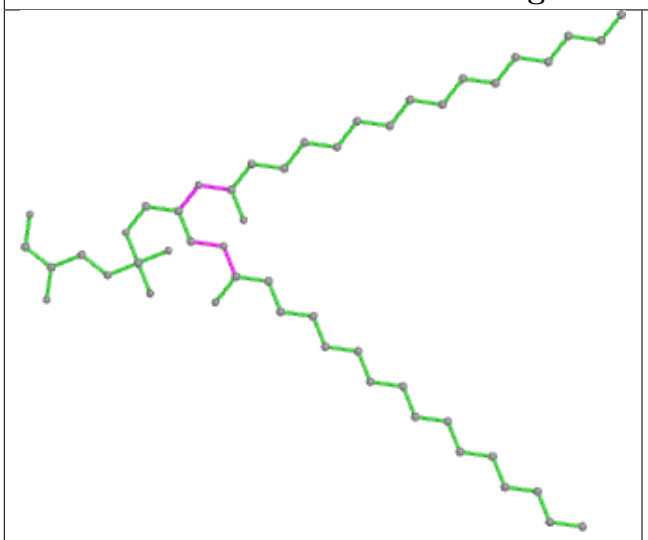
Ligand PHO D 401



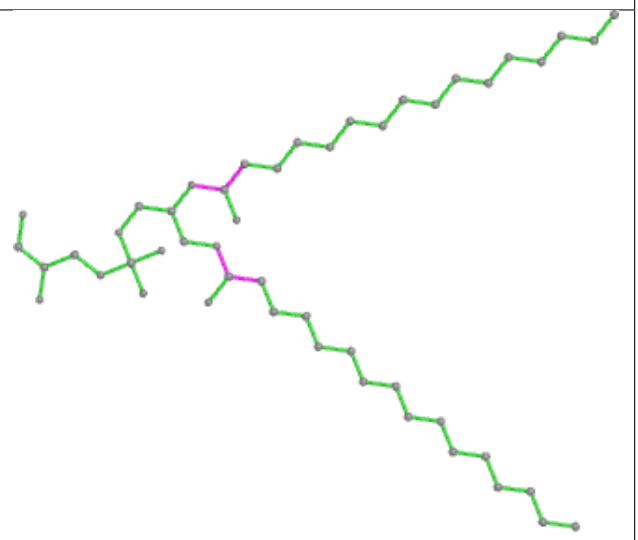
Ligand CLA 1 305



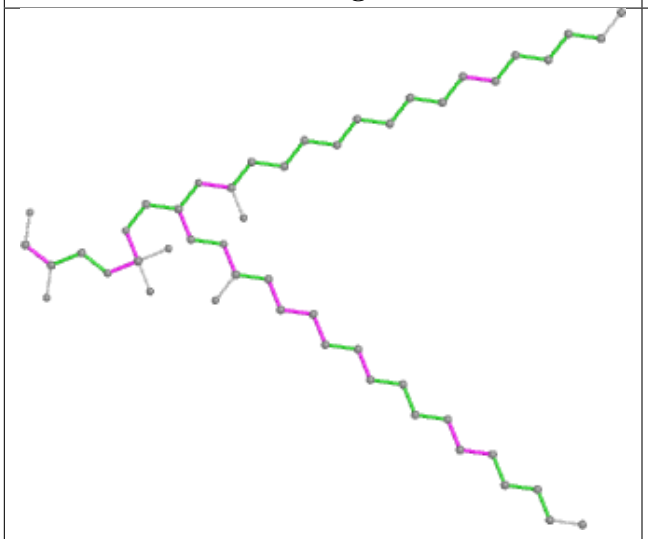
Ligand LHG 3 310



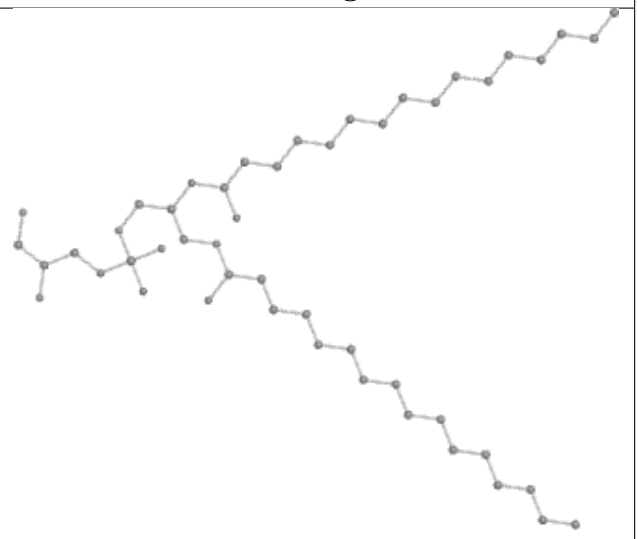
Bond lengths



Bond angles

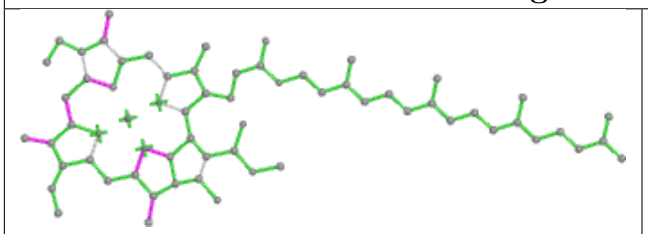


Torsions

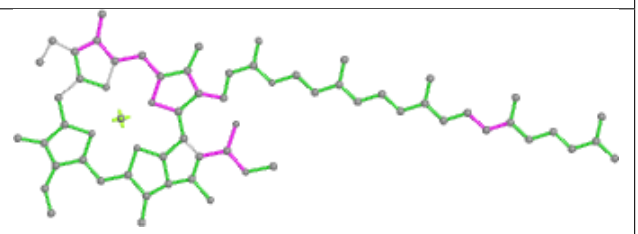


Rings

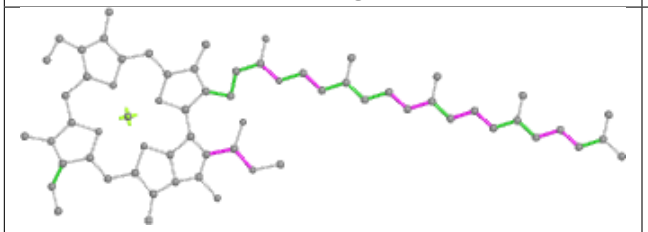
Ligand CLA c 510



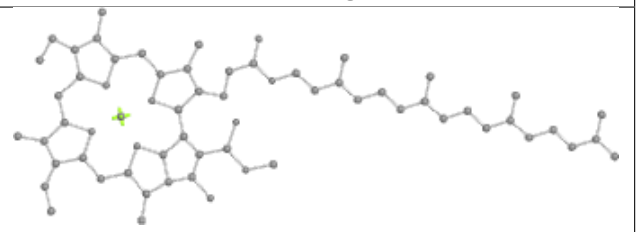
Bond lengths



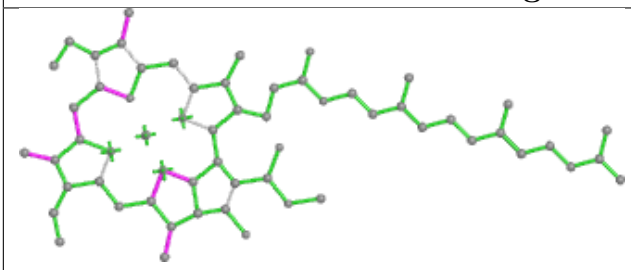
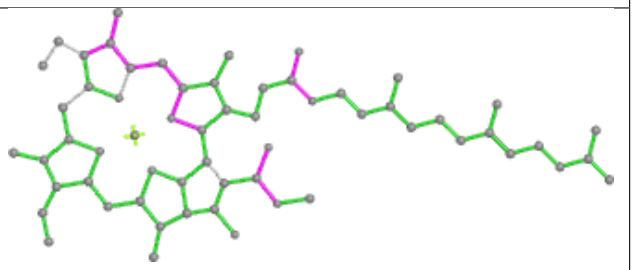
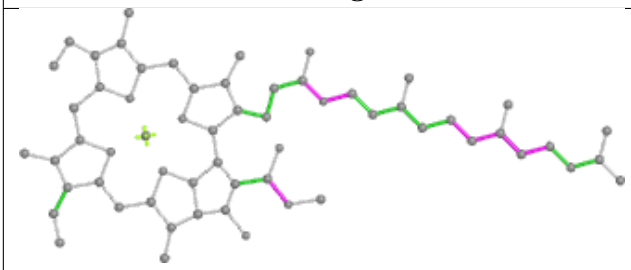
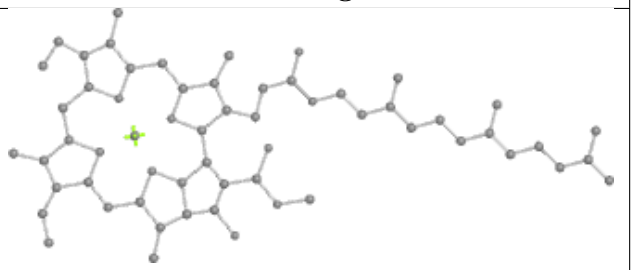
Bond angles

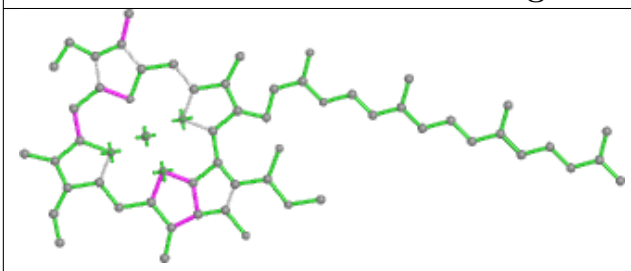
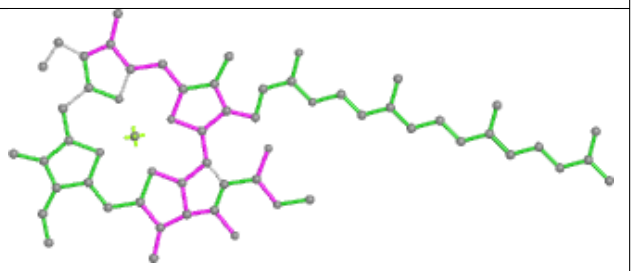
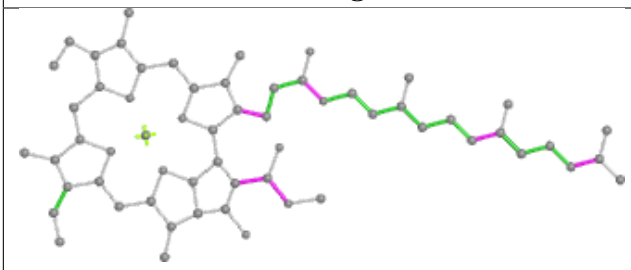
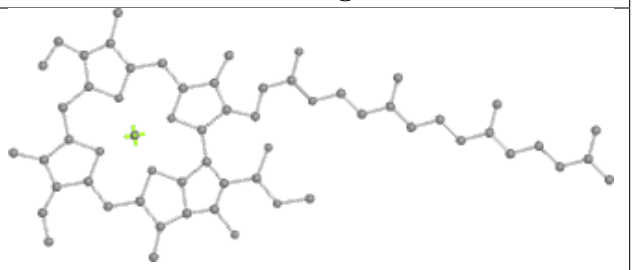


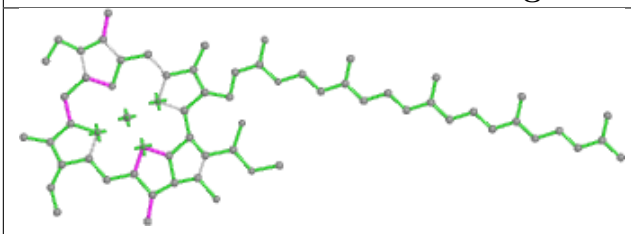
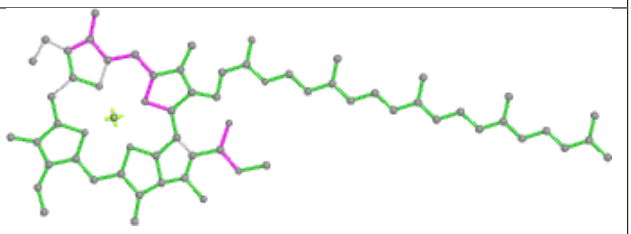
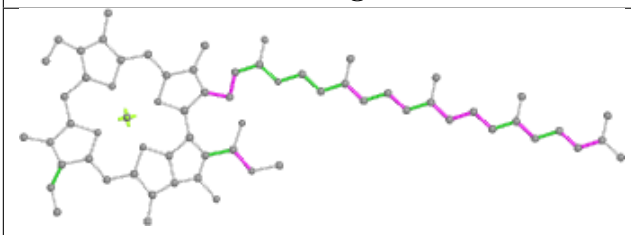
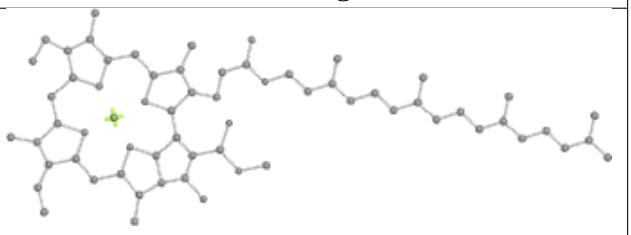
Torsions

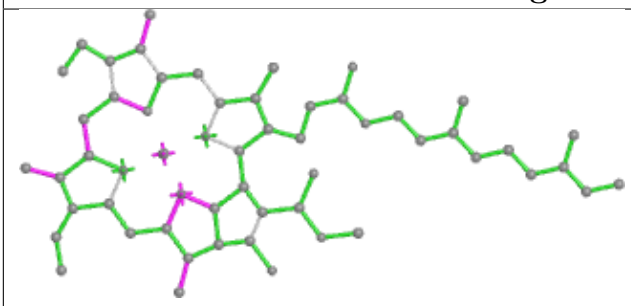
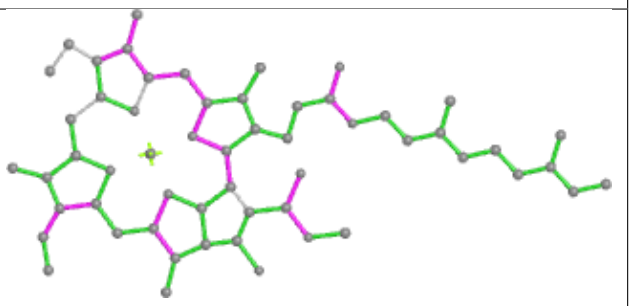
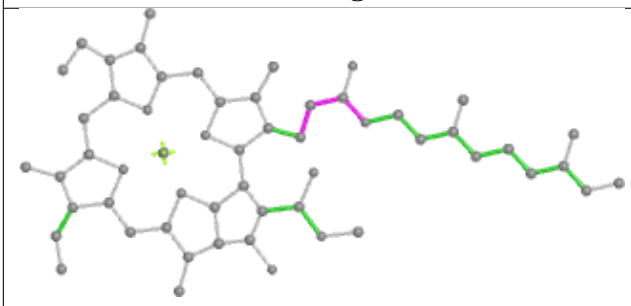
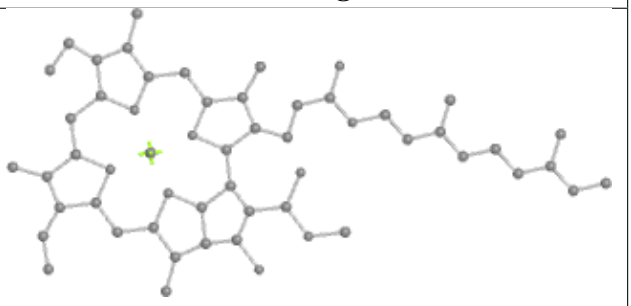


Rings

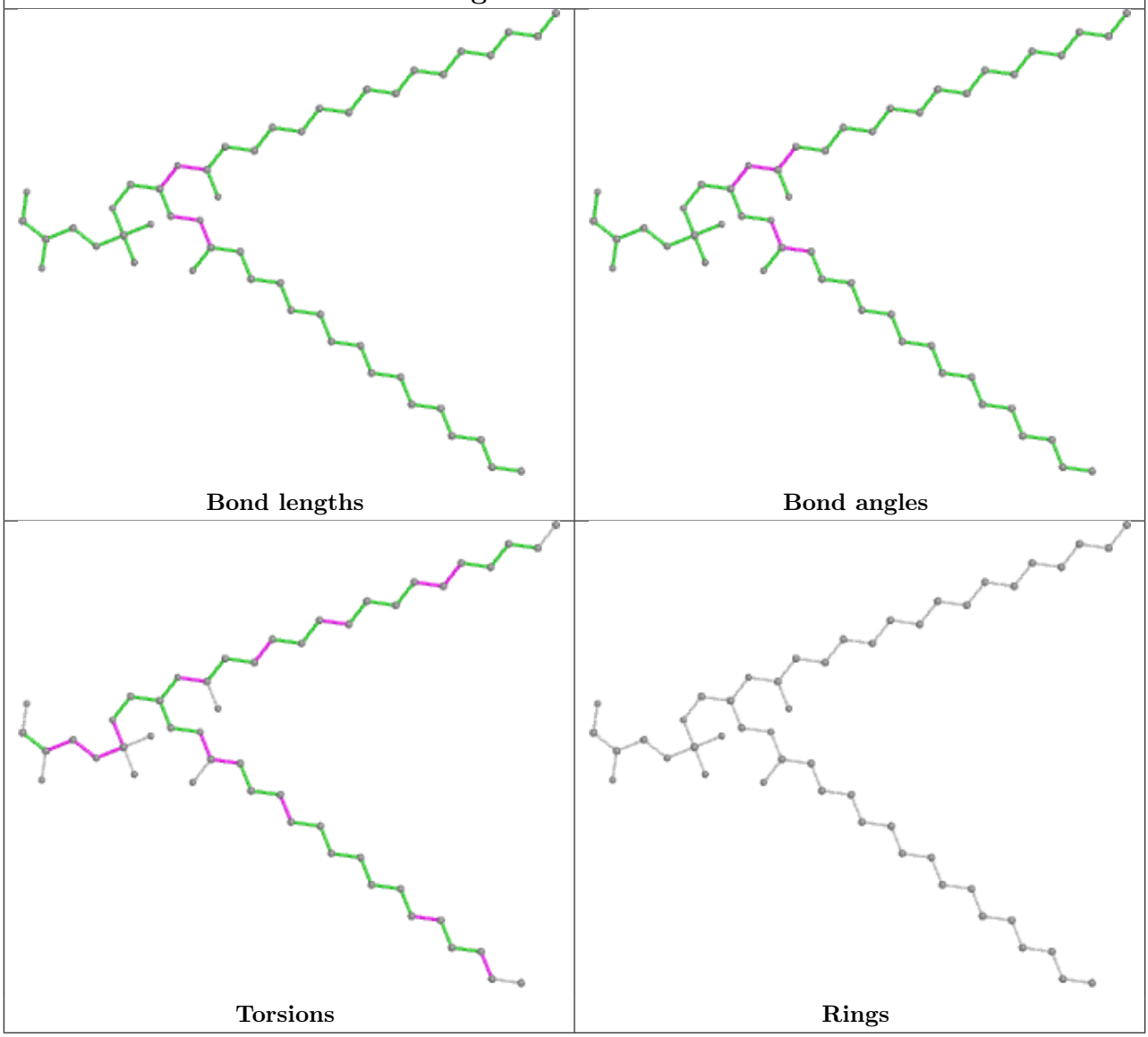
Ligand CLA U 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

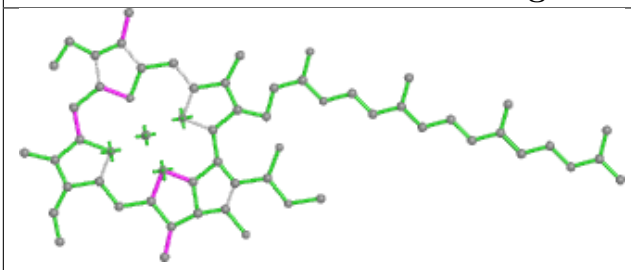
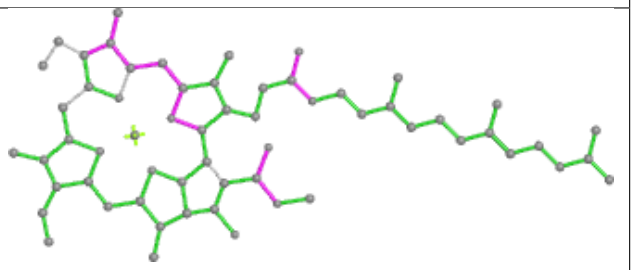
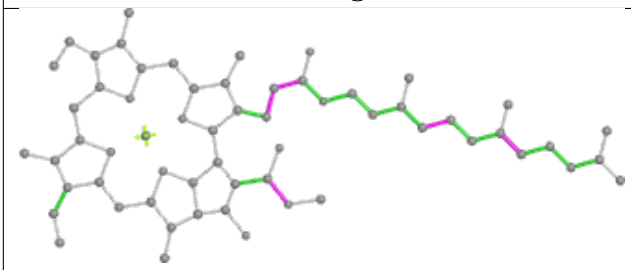
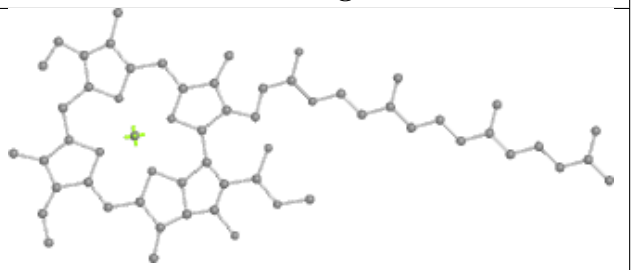
Ligand CLA n 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

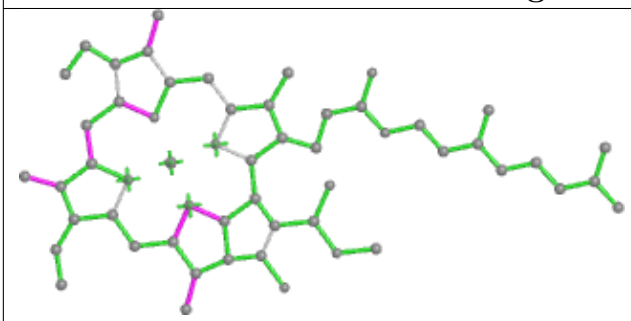
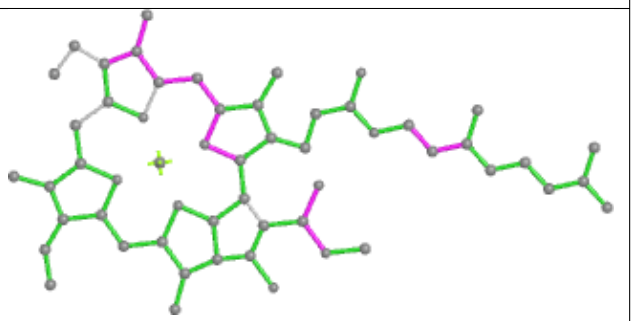
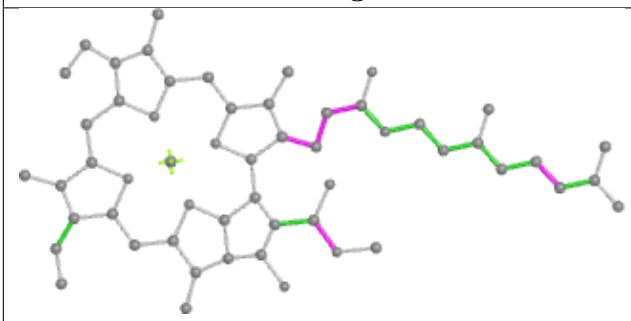
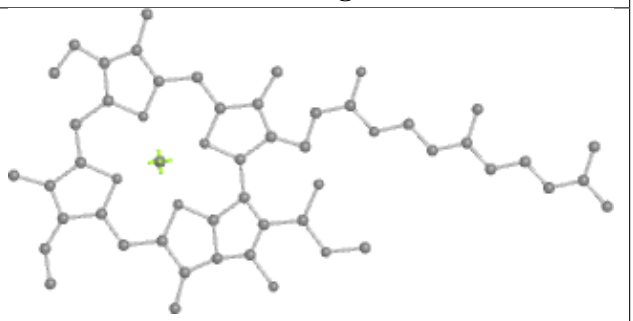
Ligand CLA R 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

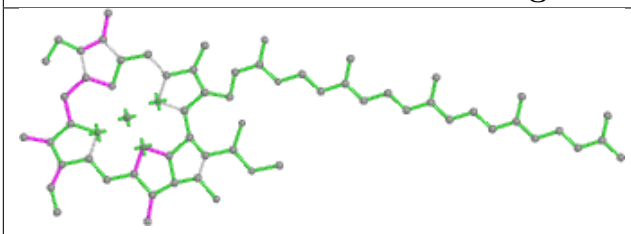
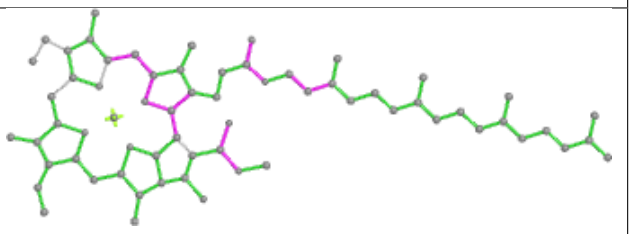
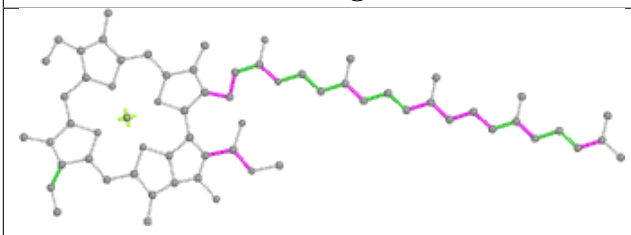
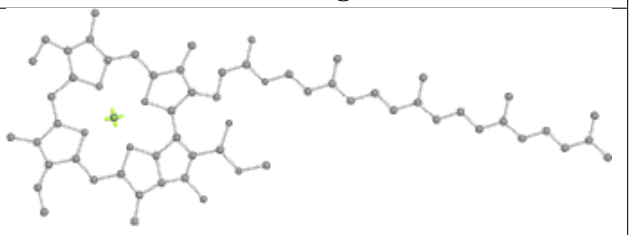
Ligand CLA s 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

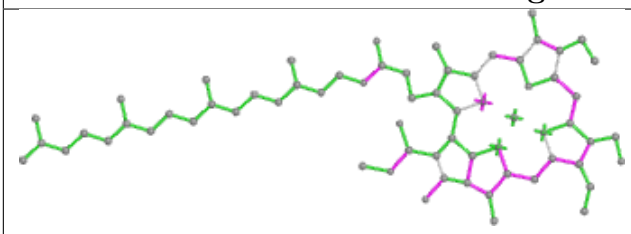
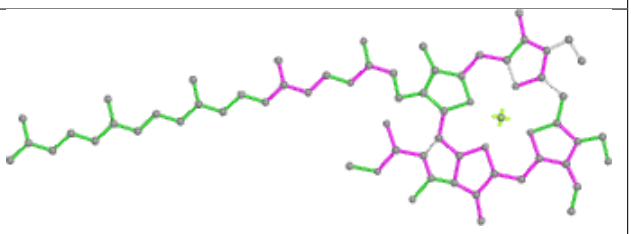
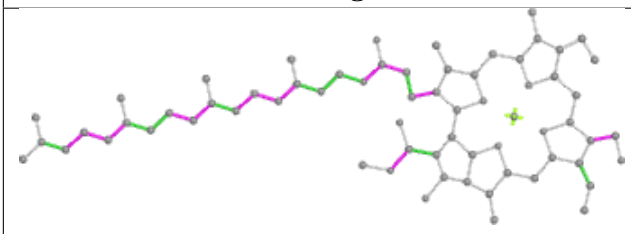
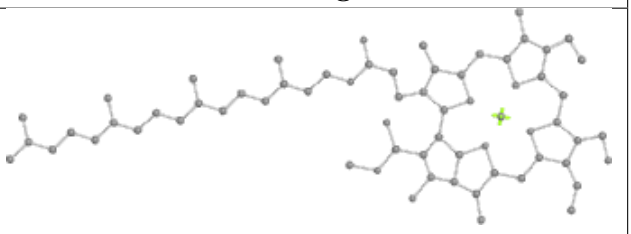
Ligand LHG S 312



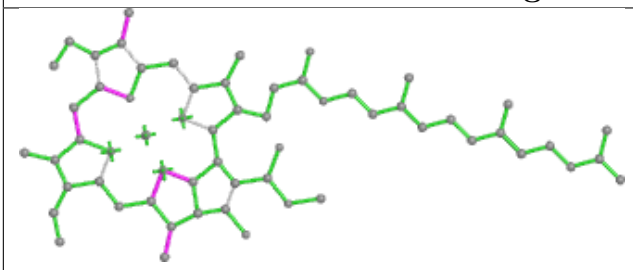
Ligand CLA 2 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

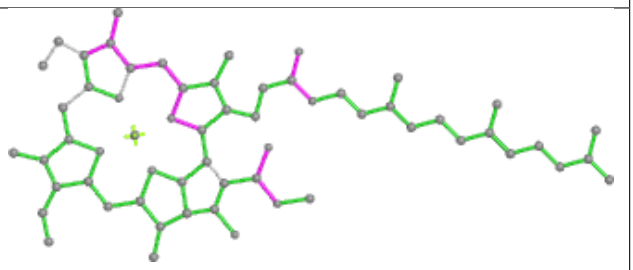
Ligand CLA c 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 1 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

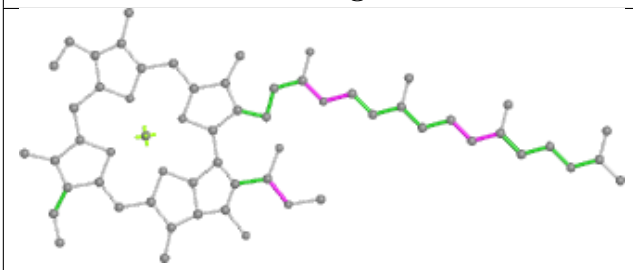
Ligand CLA V 305



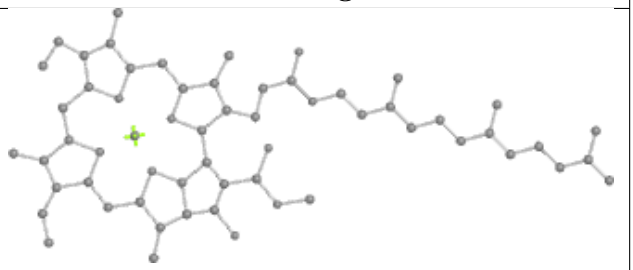
Bond lengths



Bond angles

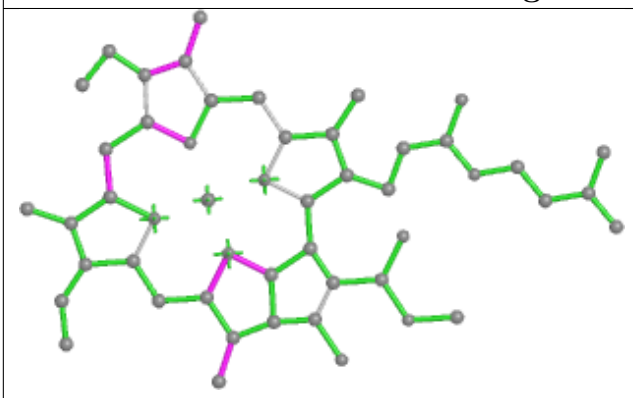


Torsions

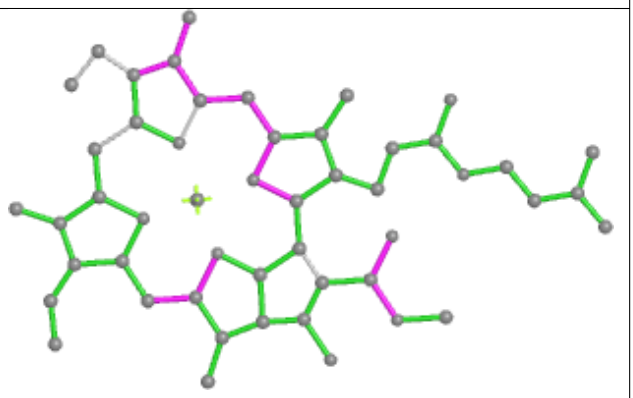


Rings

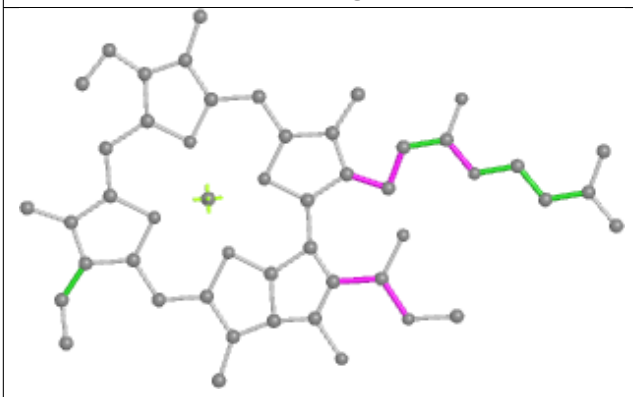
Ligand CLA G 303



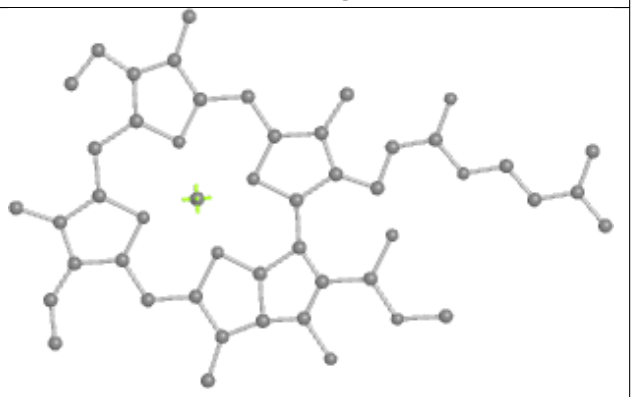
Bond lengths



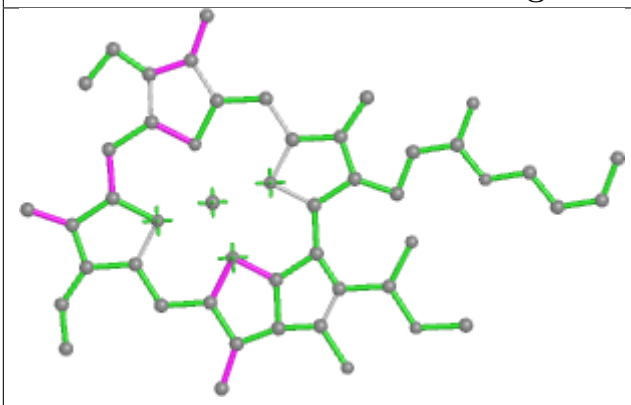
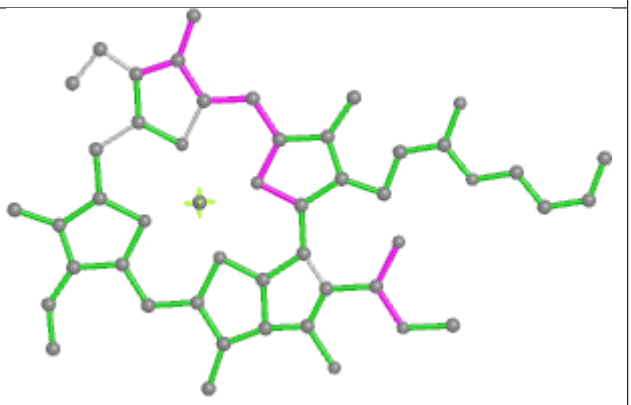
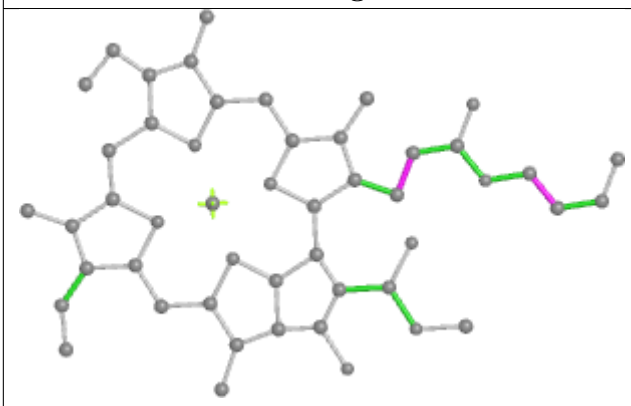
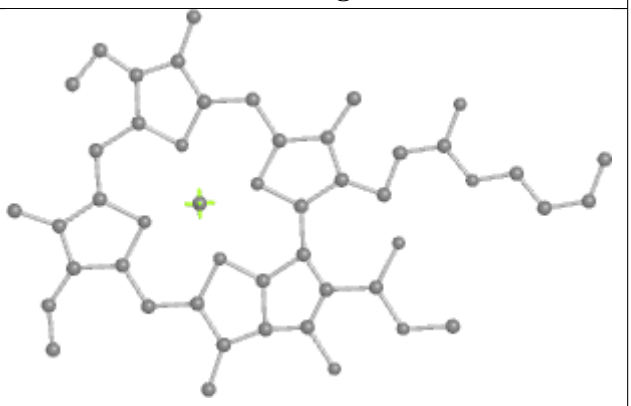
Bond angles



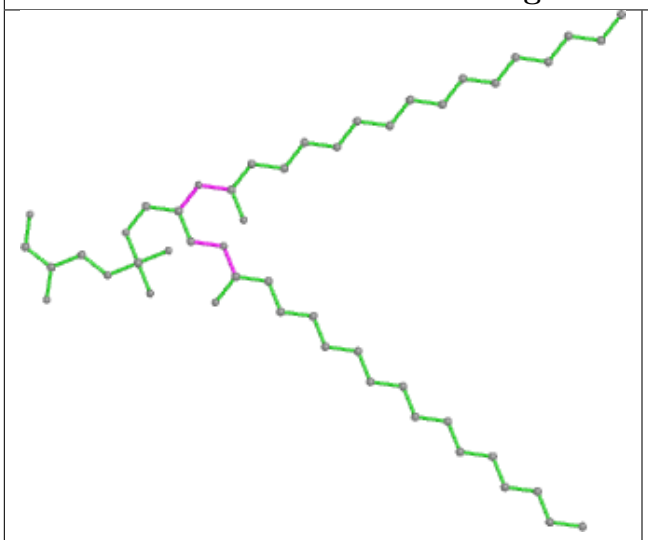
Torsions



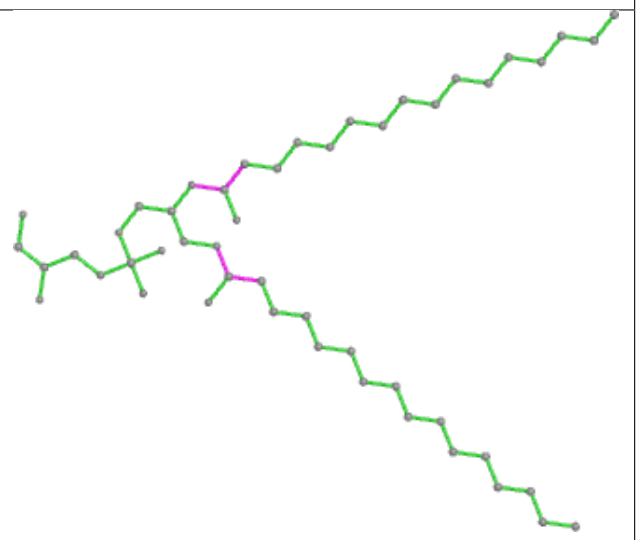
Rings

Ligand CLA S 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

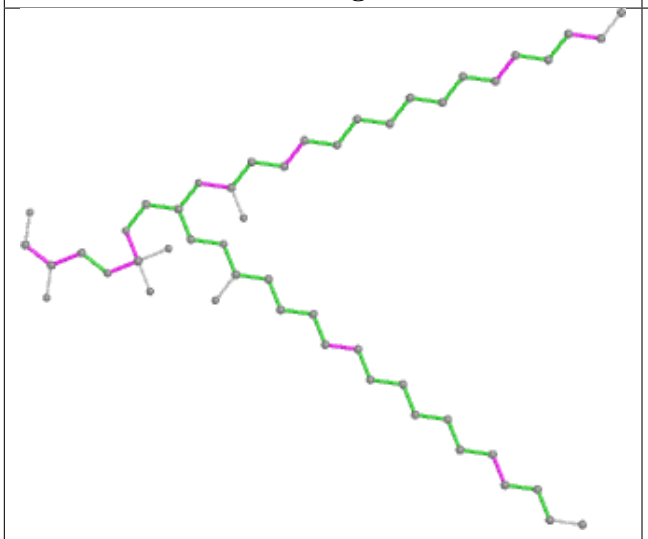
Ligand LHG C 524



Bond lengths



Bond angles



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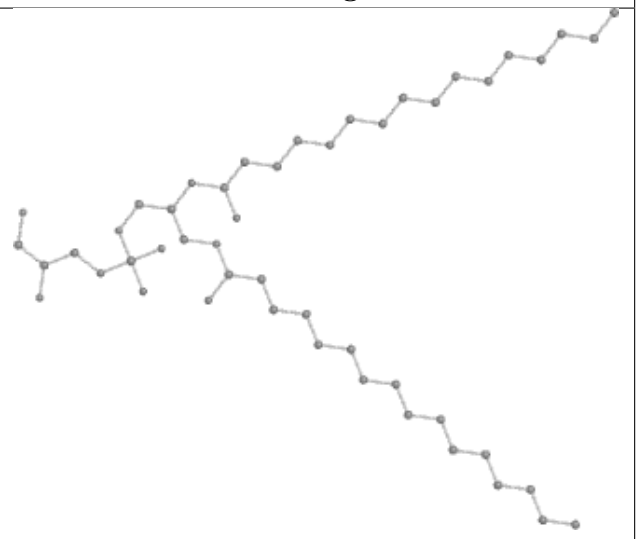
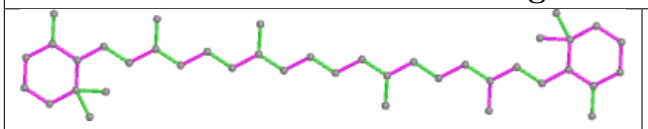
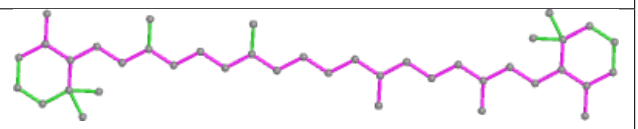


Rings

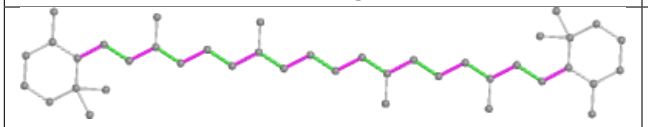
Ligand BCR c 515



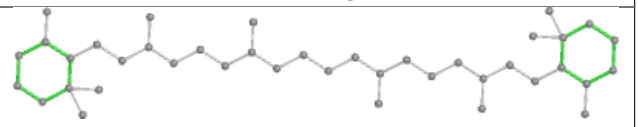
Bond lengths



Bond angles

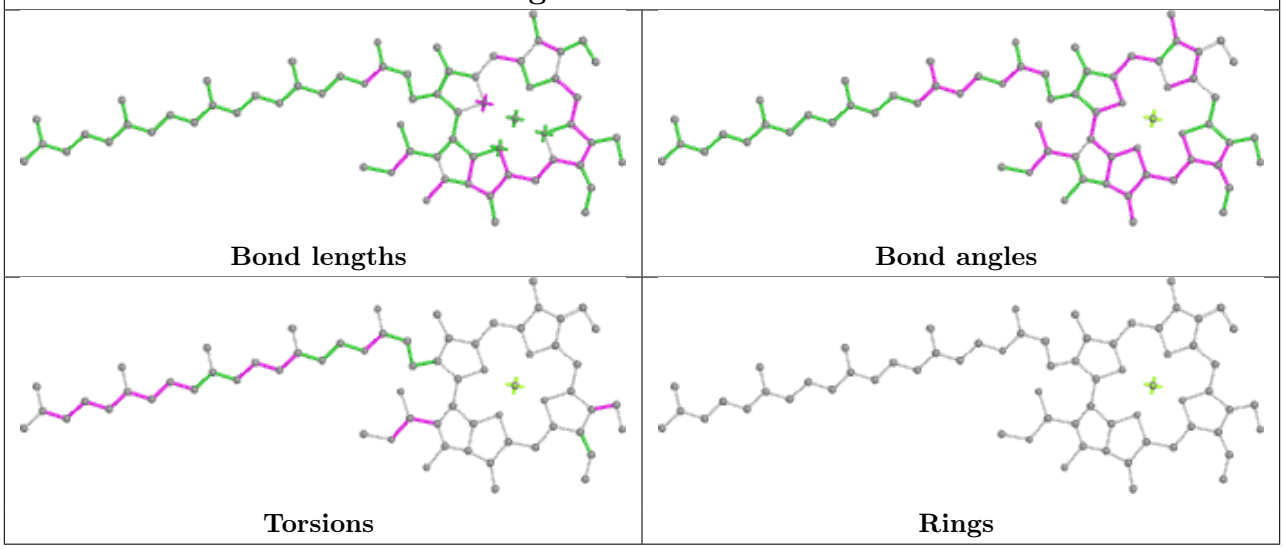


Torsions

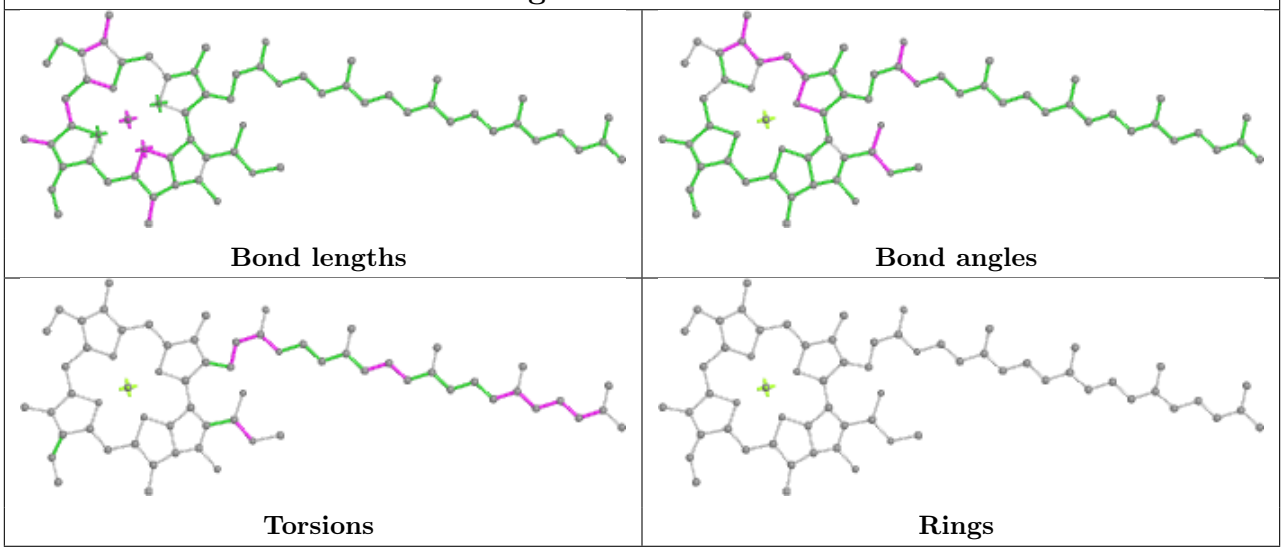


Rings

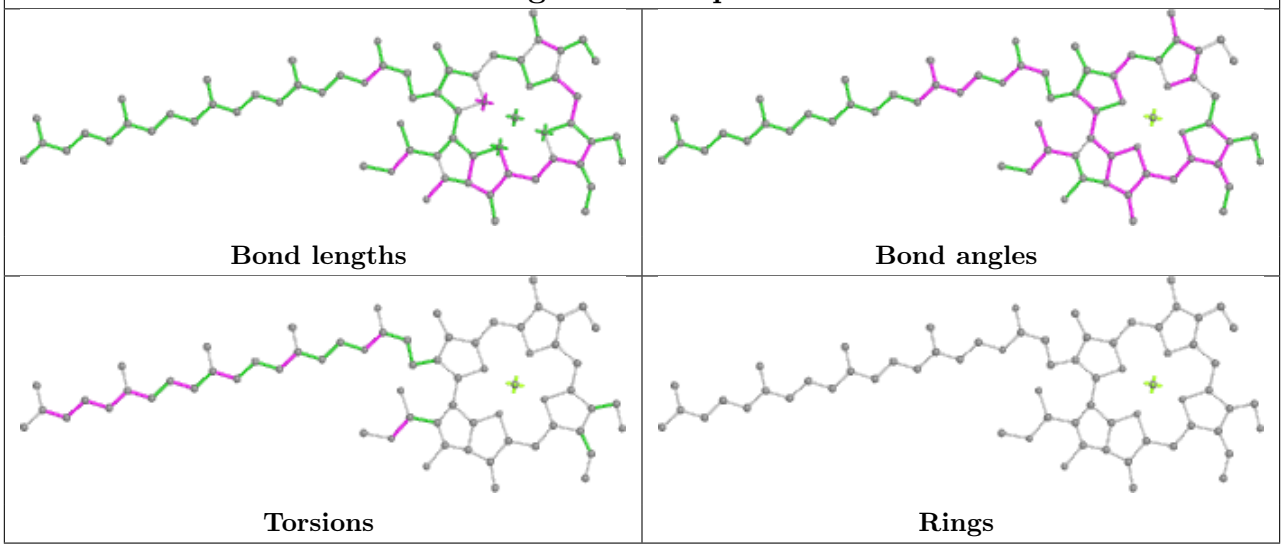
Ligand CHL 5 313



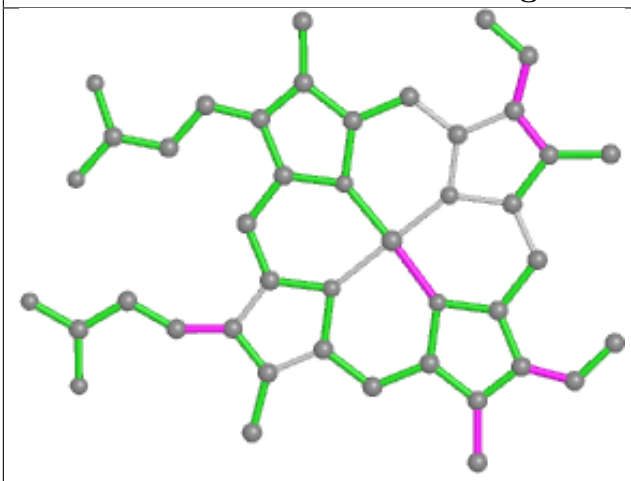
Ligand CLA b 602



Ligand CHL q 311



Ligand HEM E 101



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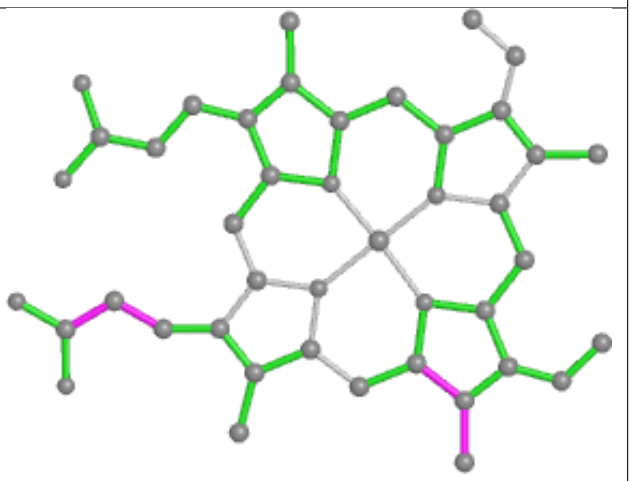
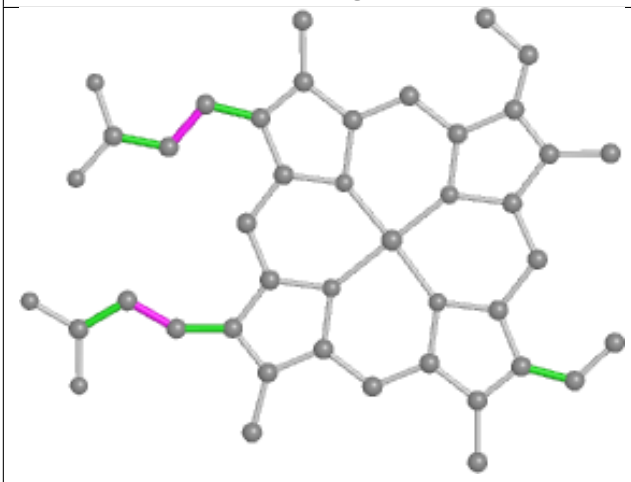


Bond angles



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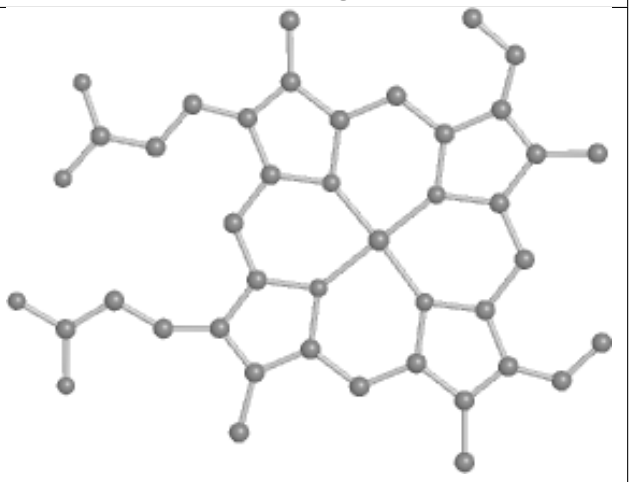
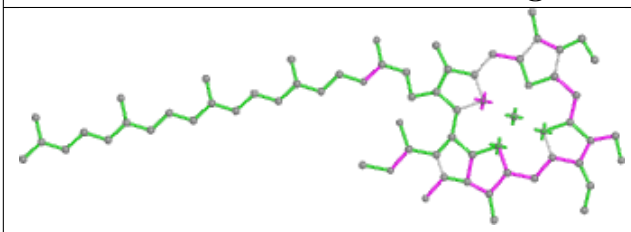


Rings

Ligand CHL u 313



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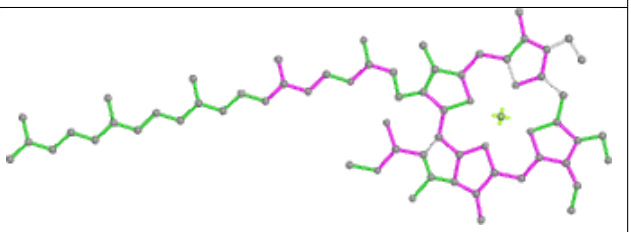

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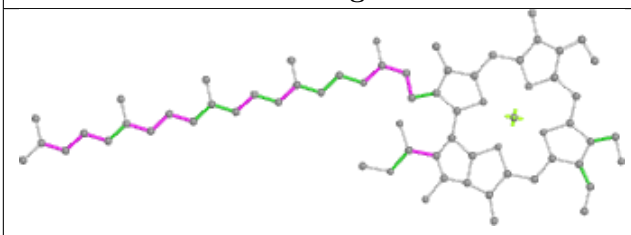

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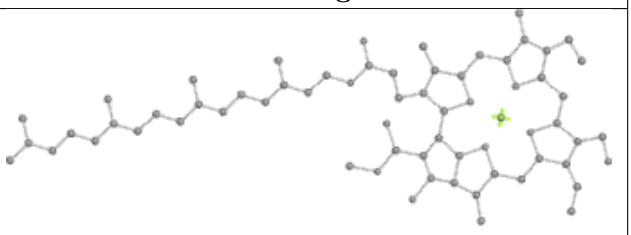
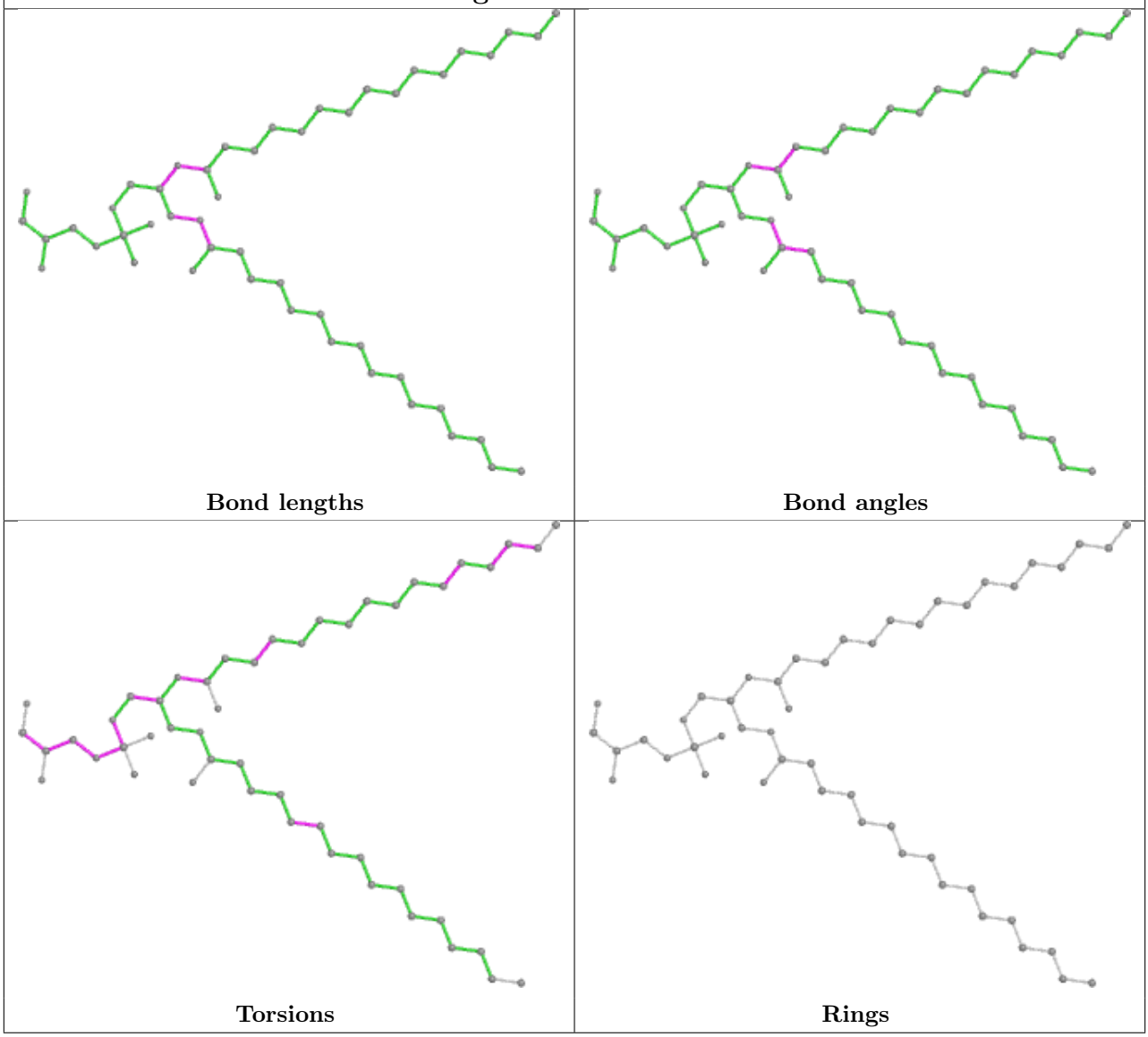
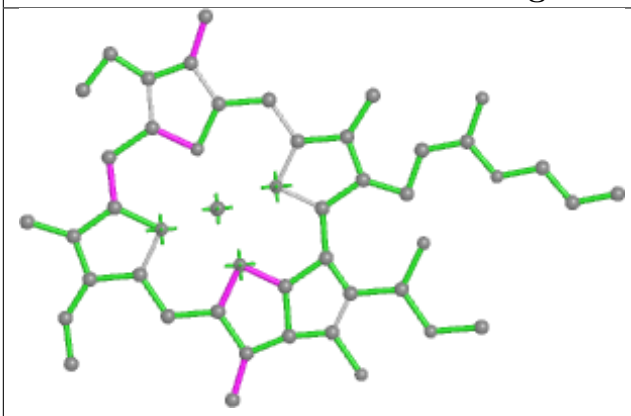


Rings

Ligand LHG c 523



Ligand CLA 1 308



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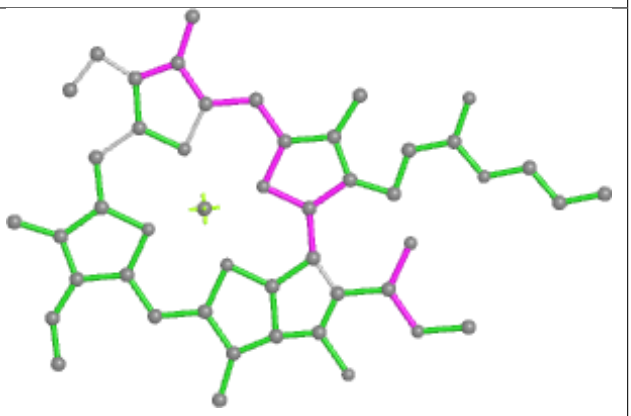

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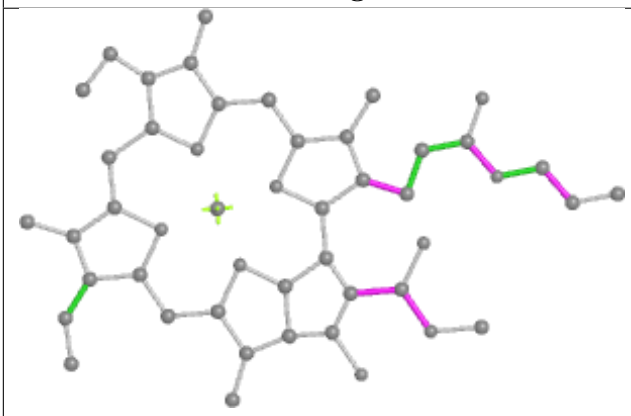

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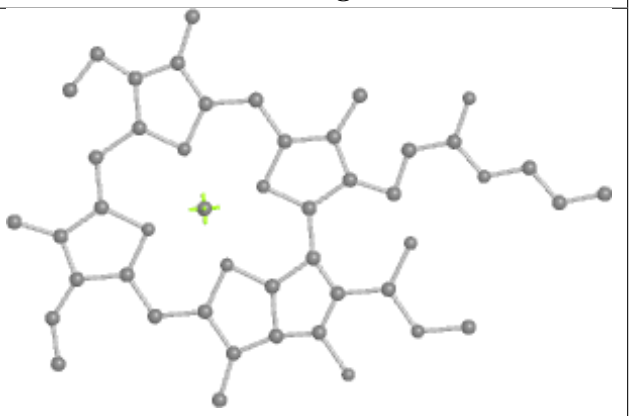
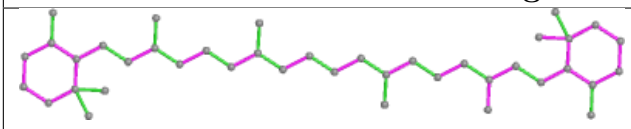


Rings

Ligand BCR T 101



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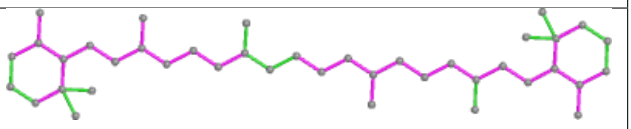
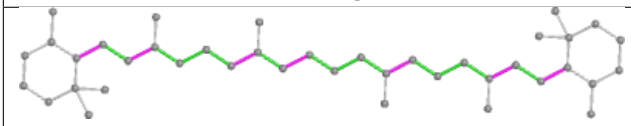


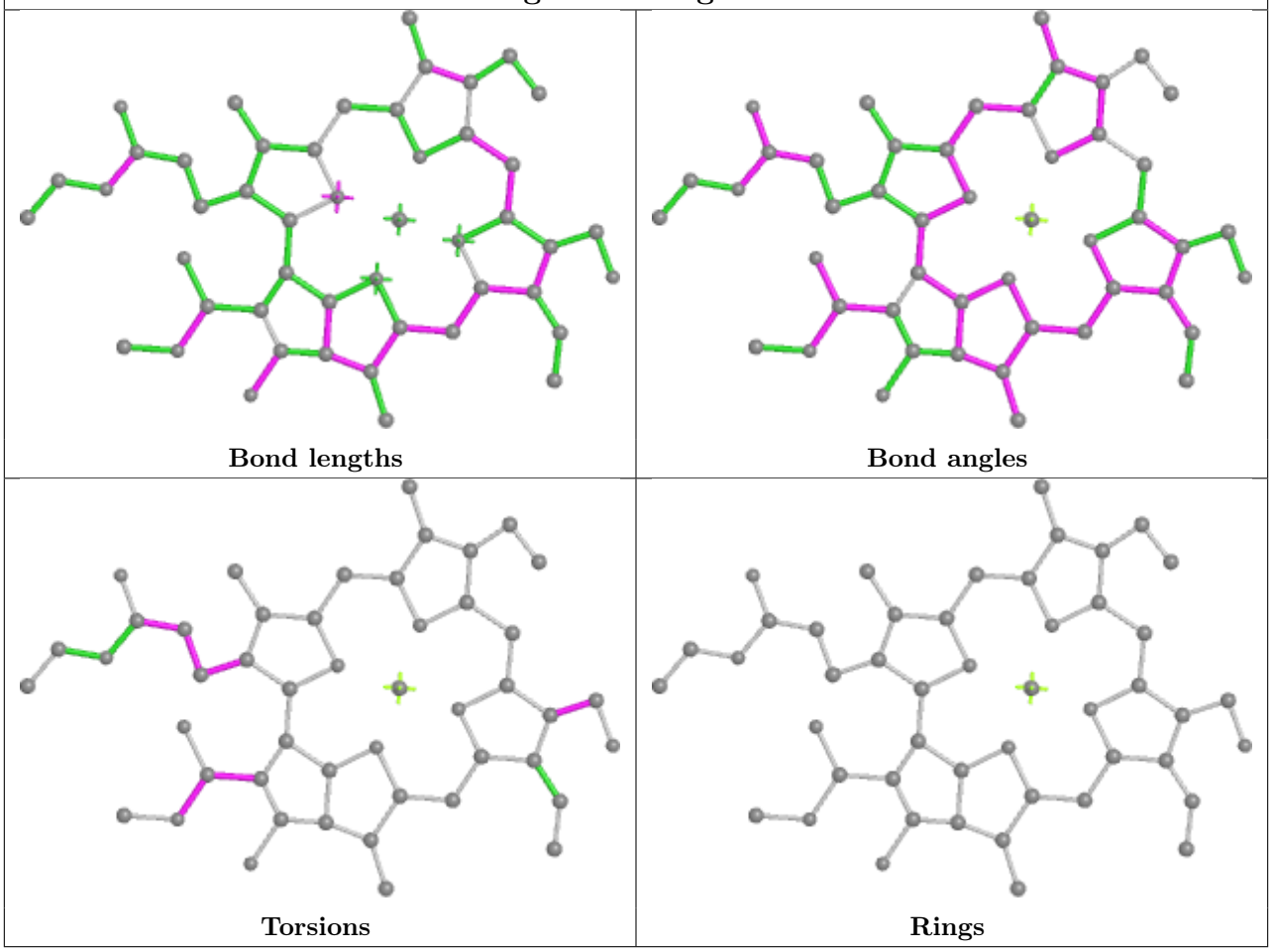
Bond angles



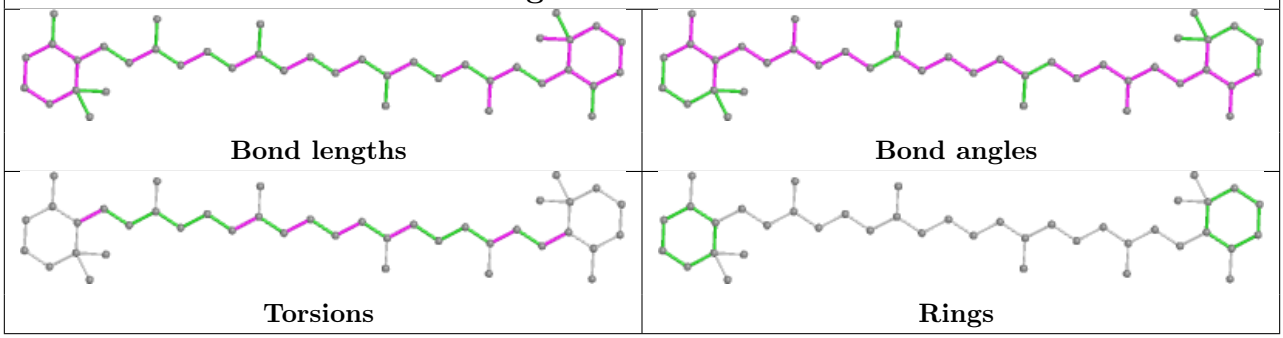
Torsions

Rings

Ligand CHL g 312



Ligand BCR b 620



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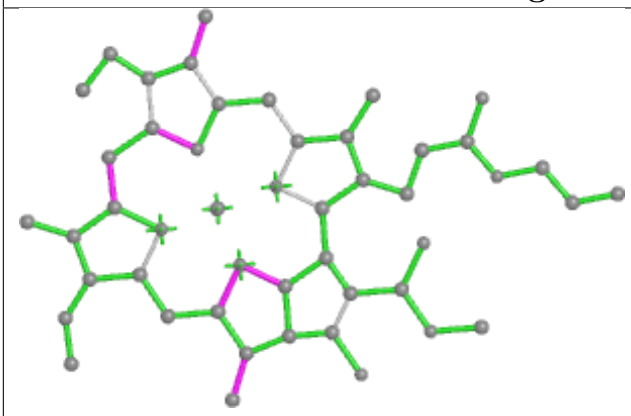

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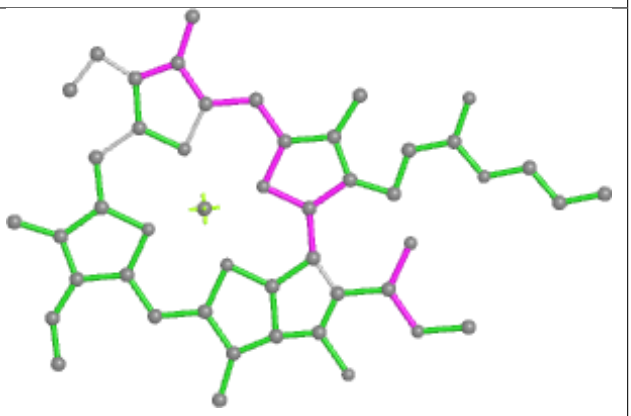
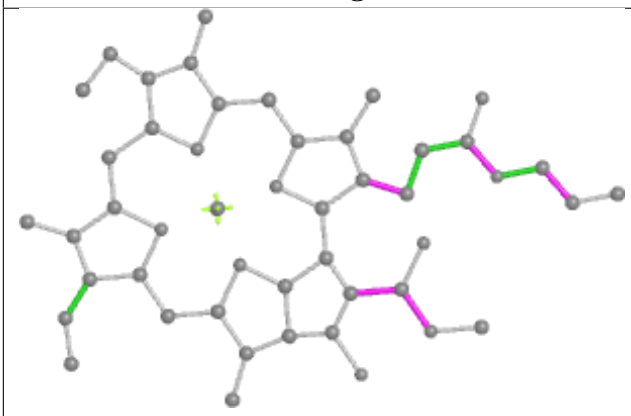


Bond angles



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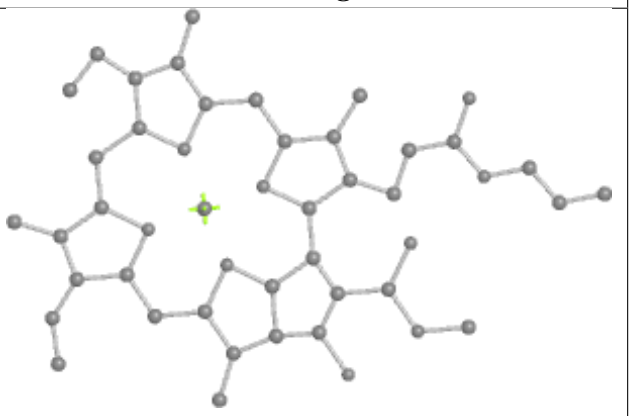
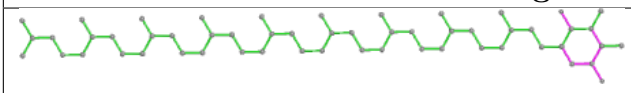


Rings

Ligand PL9 d 404



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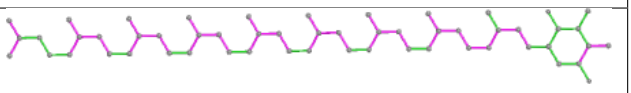
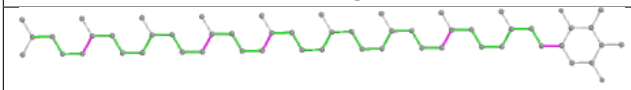


Bond angles



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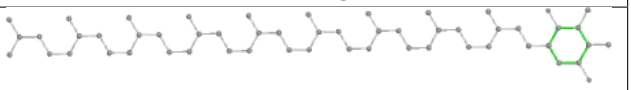
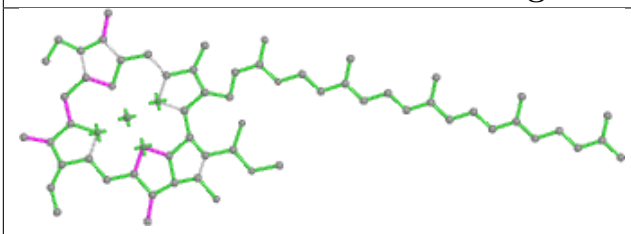


Rings

Ligand CLA q 307



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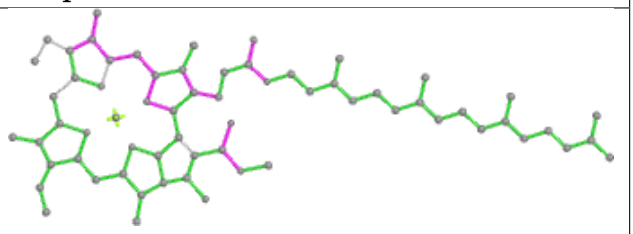

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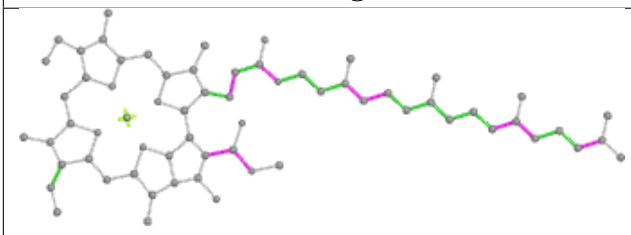

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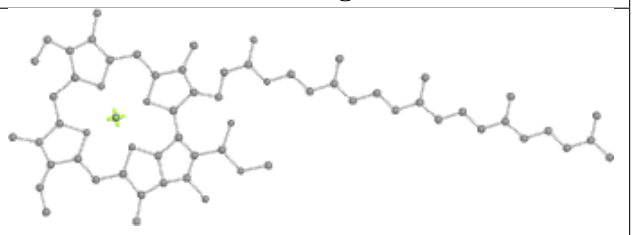
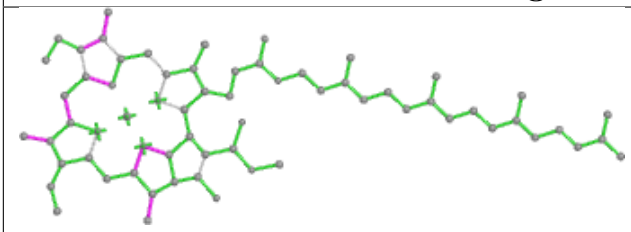


Rings

Ligand CLA b 610



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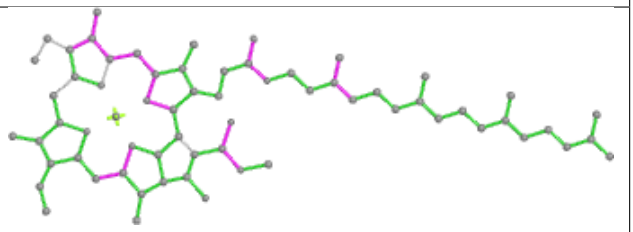
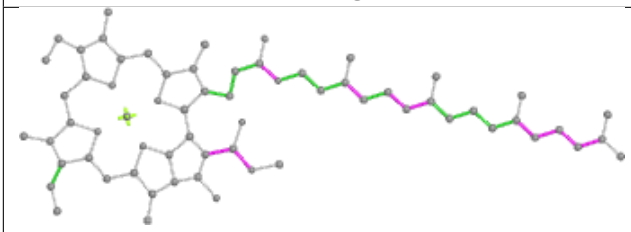


Bond angles



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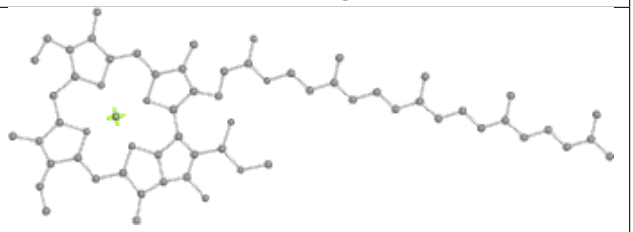
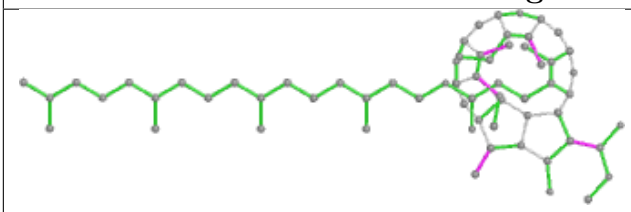


Rings

Ligand PHO a 407



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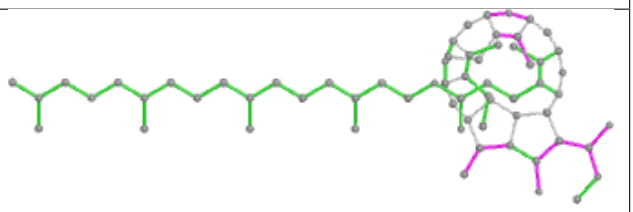
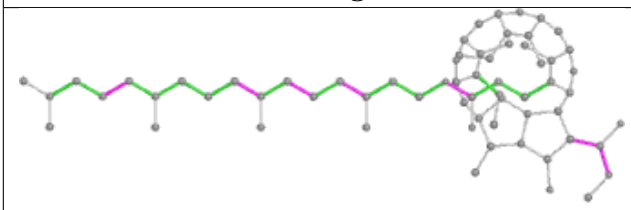


Bond angles



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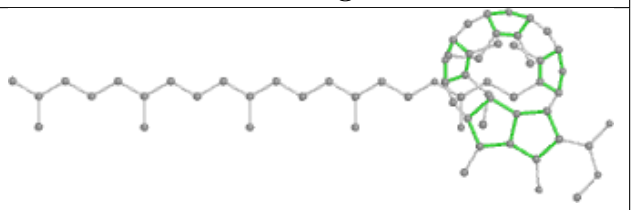
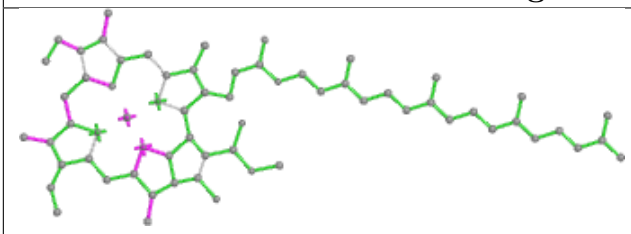
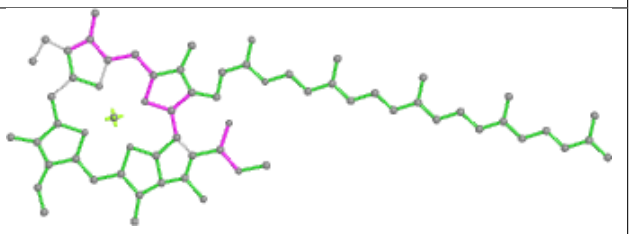
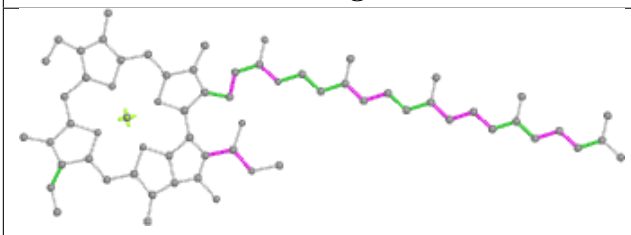
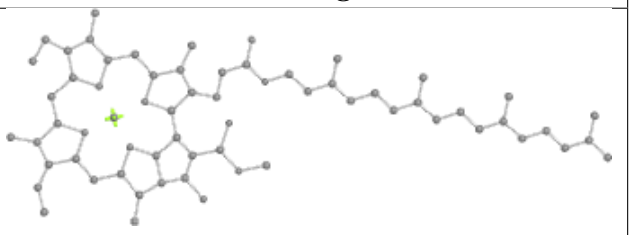
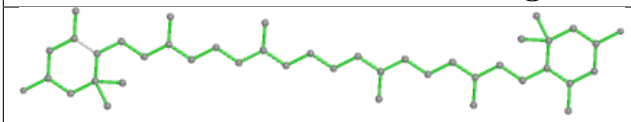
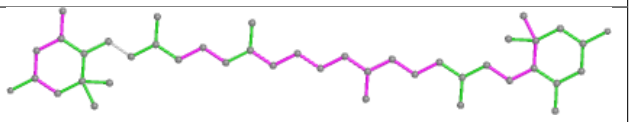
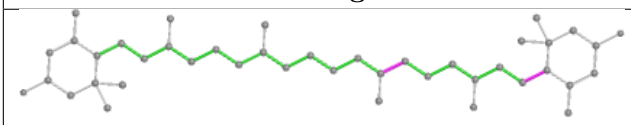
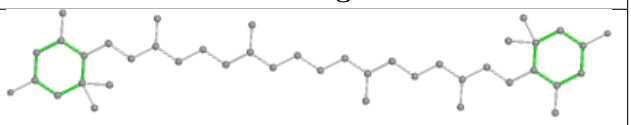
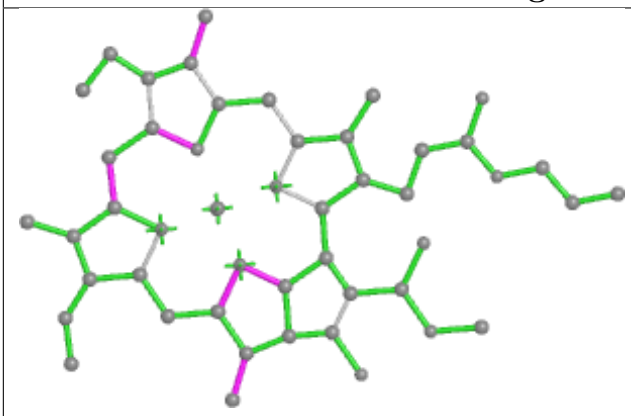
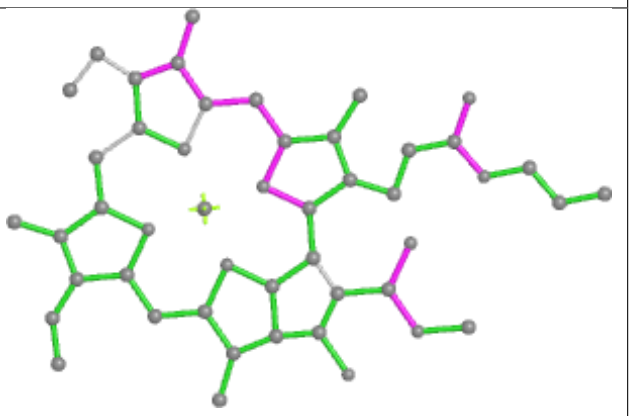
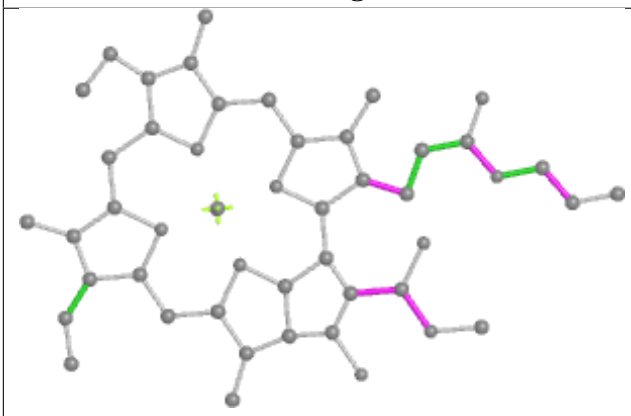
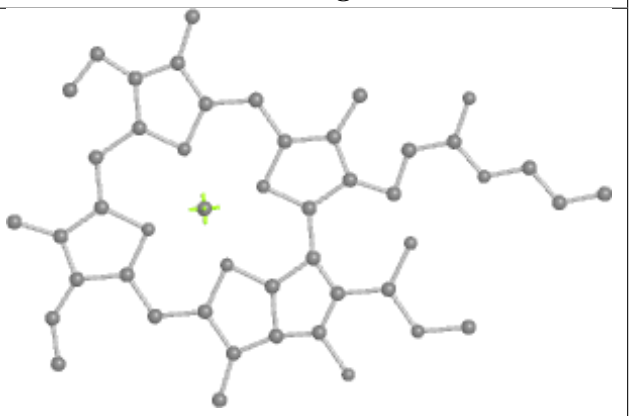


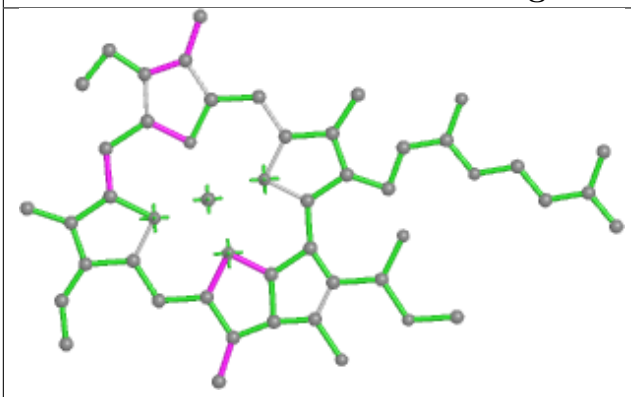
Rings

Ligand CLA b 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

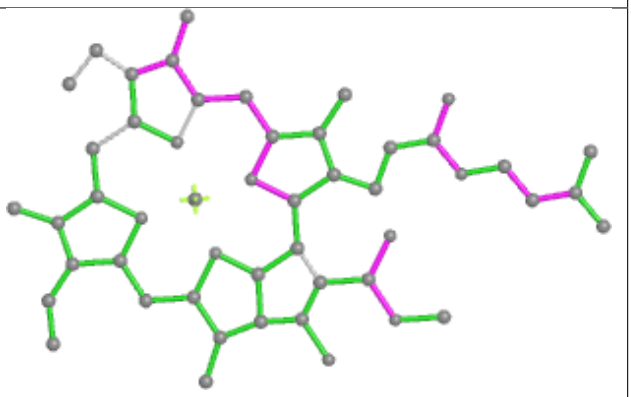
Ligand LUT U 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

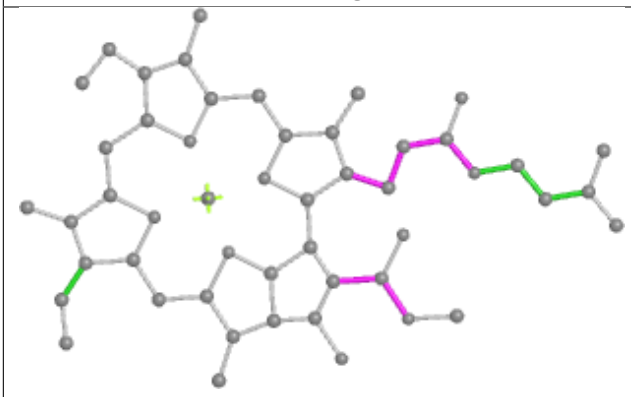
Ligand CLA 3 303



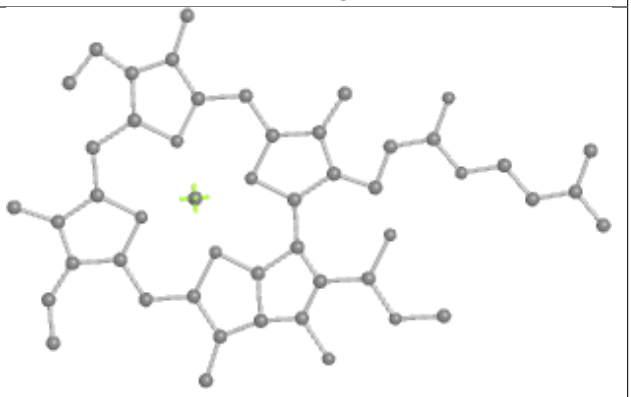
Bond lengths



Bond angles

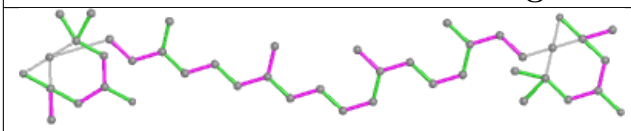


Torsions

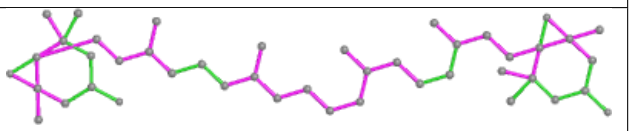


Rings

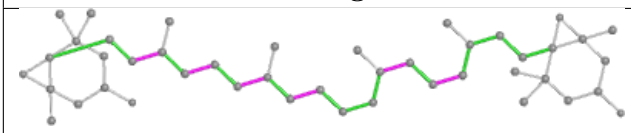
Ligand XAT n 311



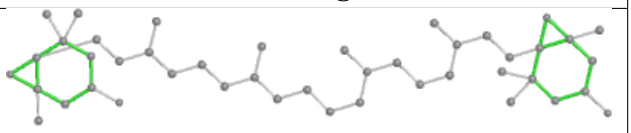
Bond lengths



Bond angles

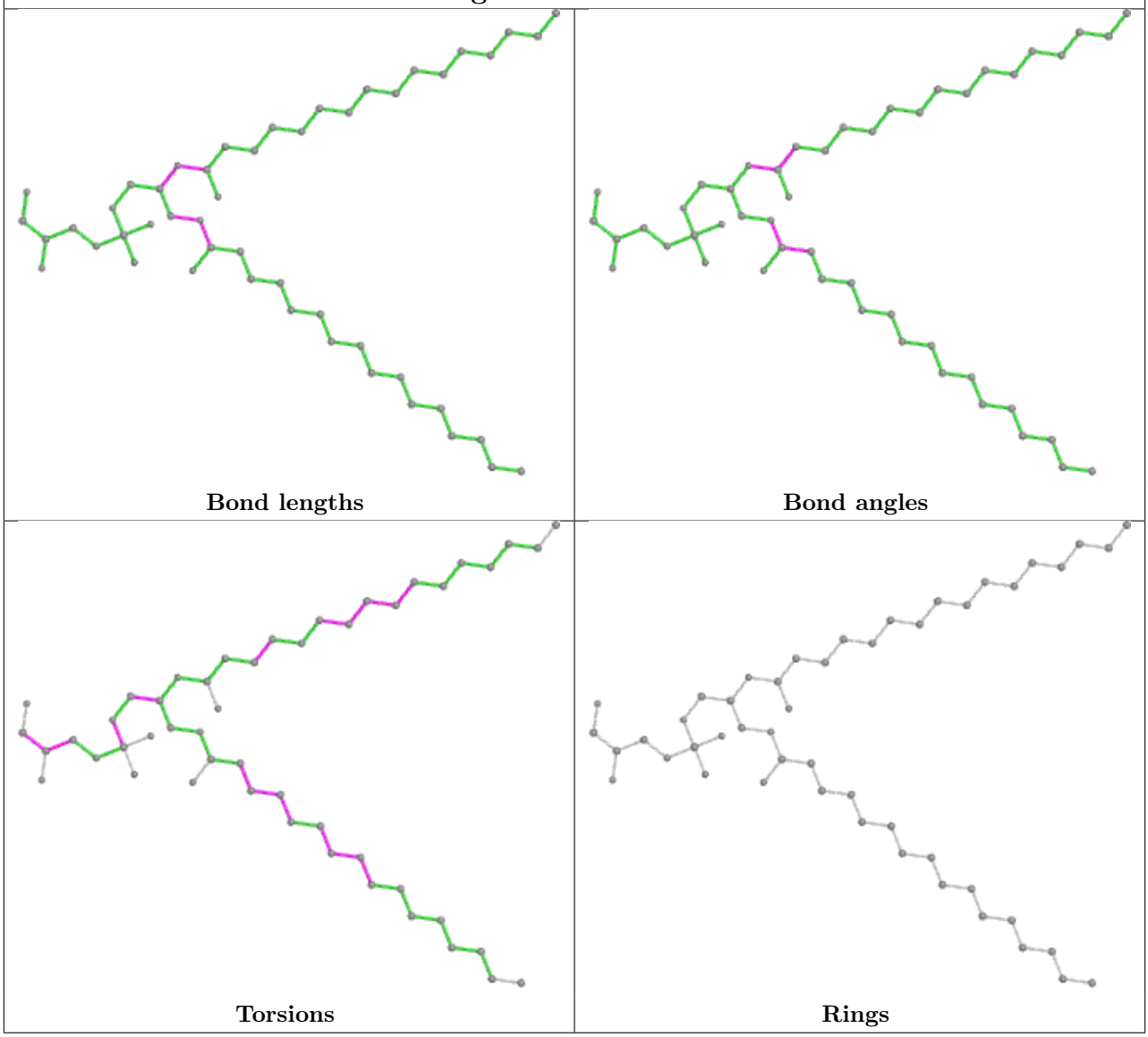


Torsions

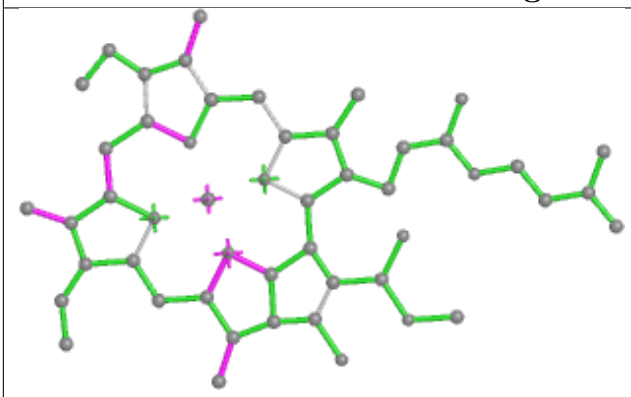


Rings

Ligand LHG n 312



Ligand CLA V 303



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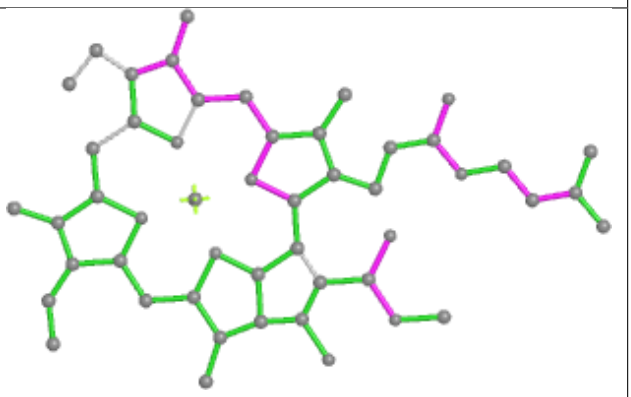
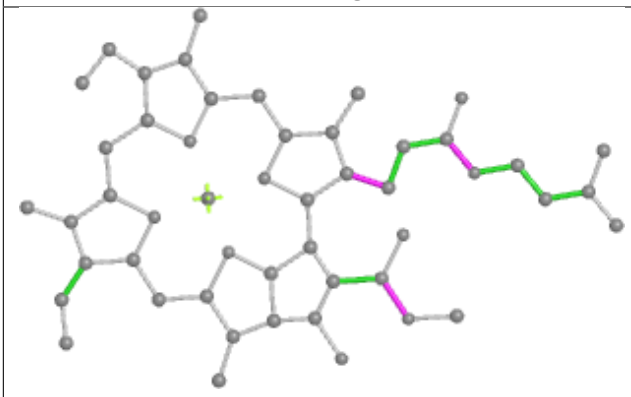


Bond angles



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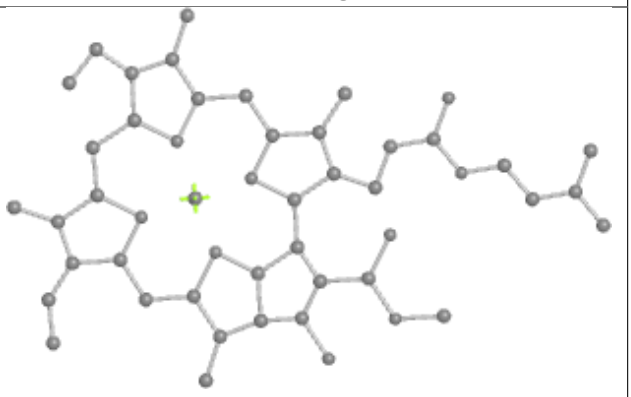
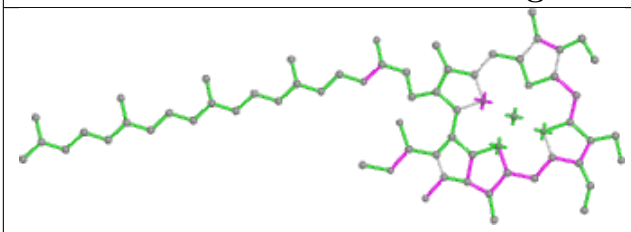


Rings

Ligand CHL p 319



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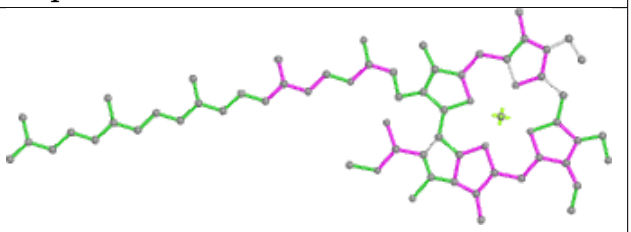

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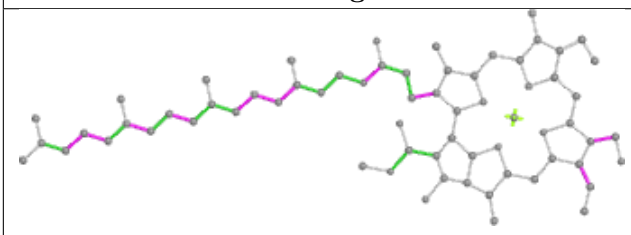
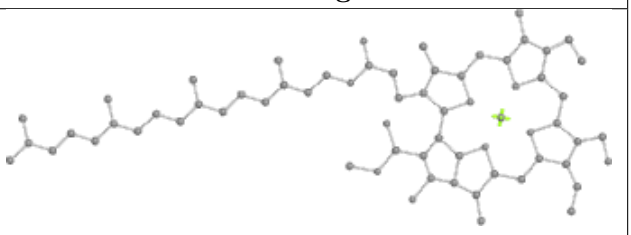
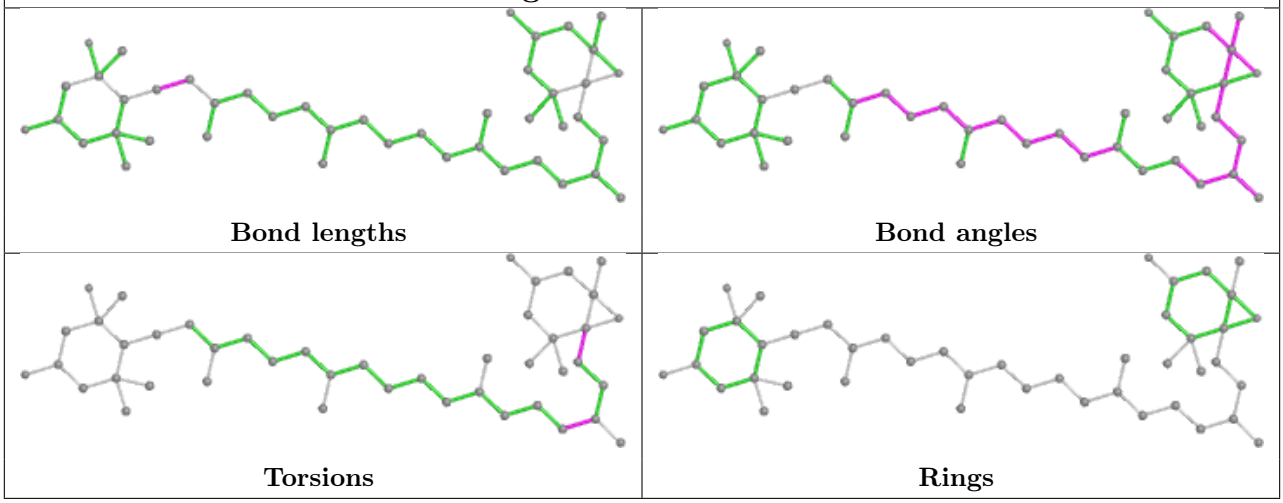


Torsions

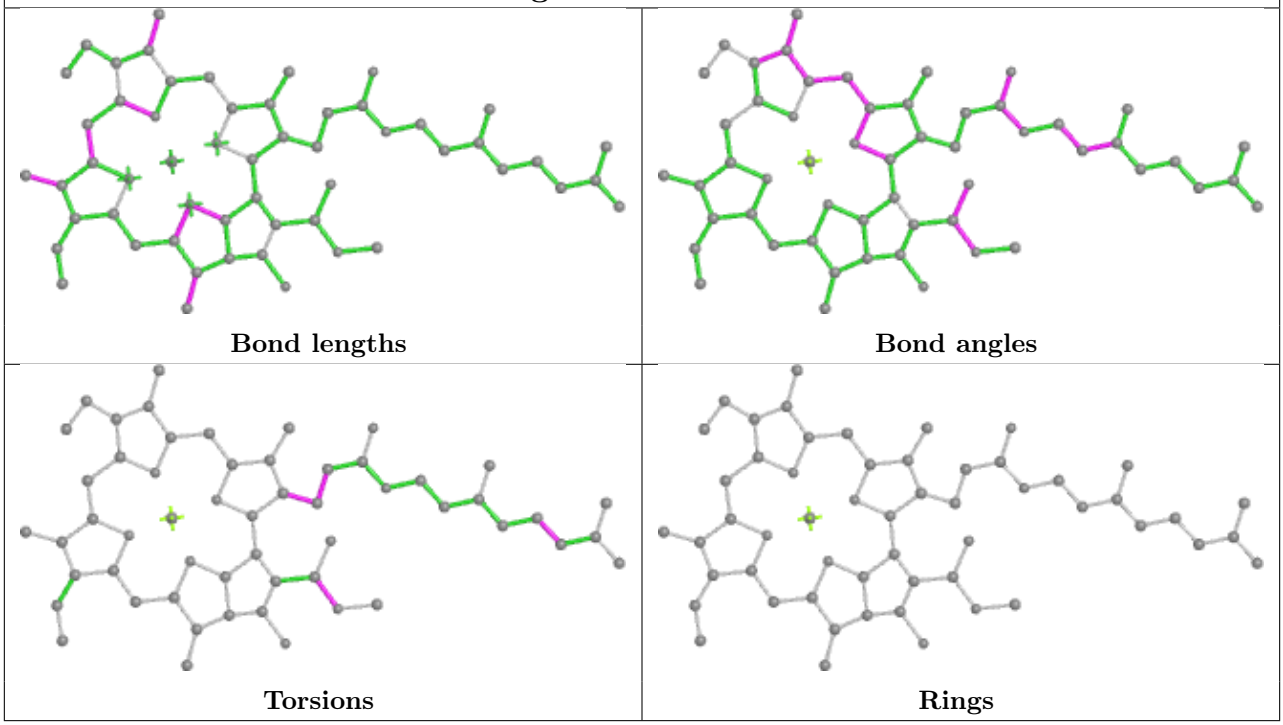


Rings

Ligand NEX U 318



Ligand CLA s 305



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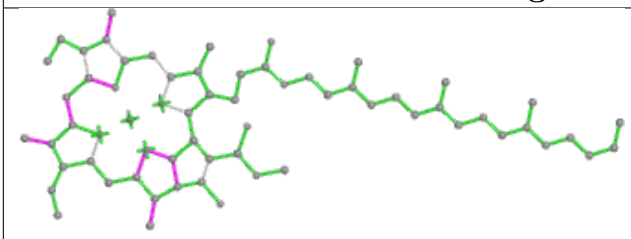
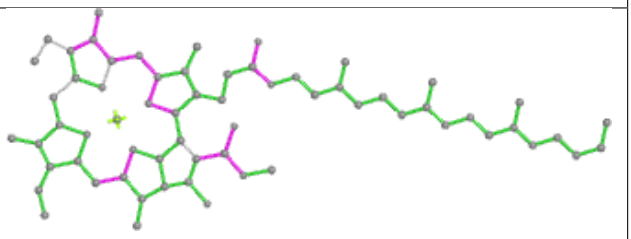
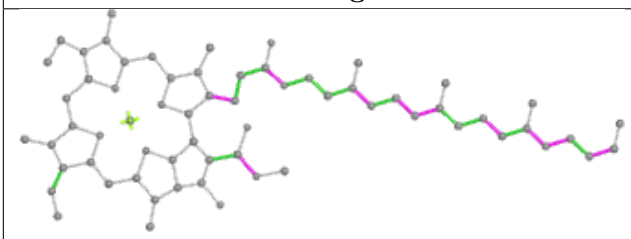
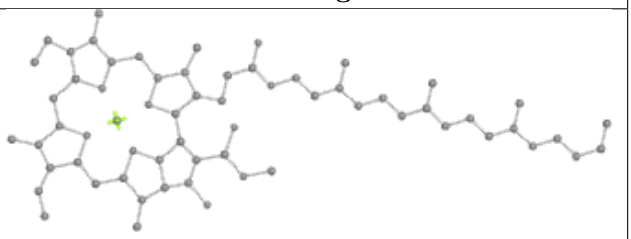
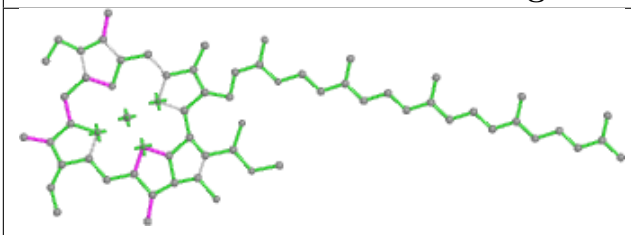
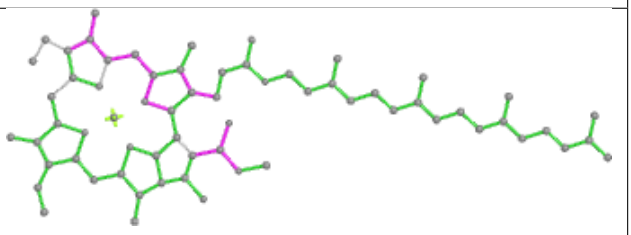
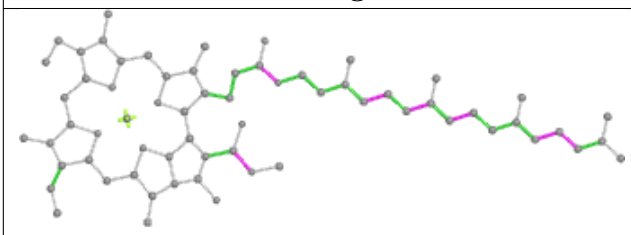
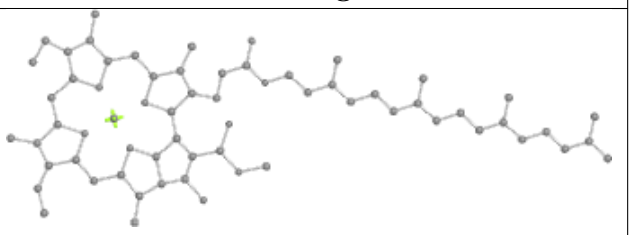
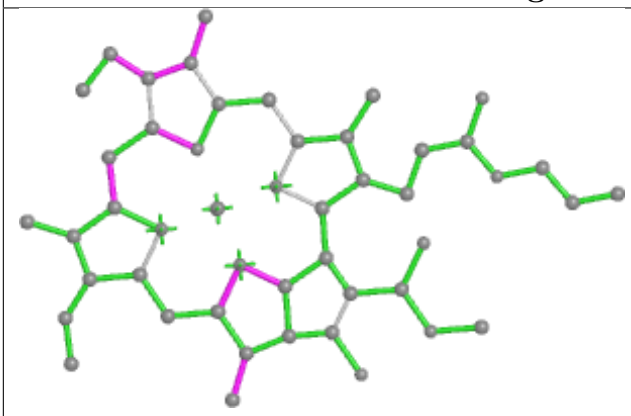
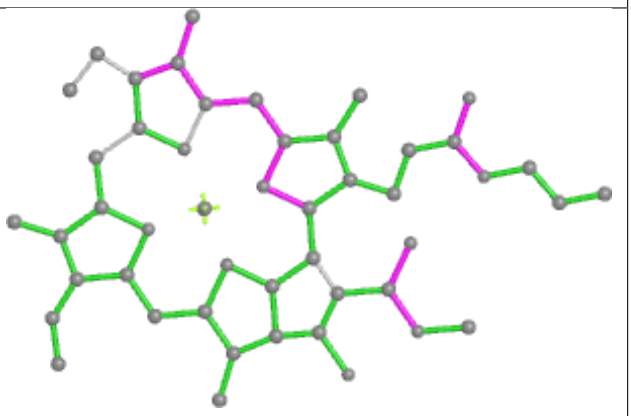
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA x 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

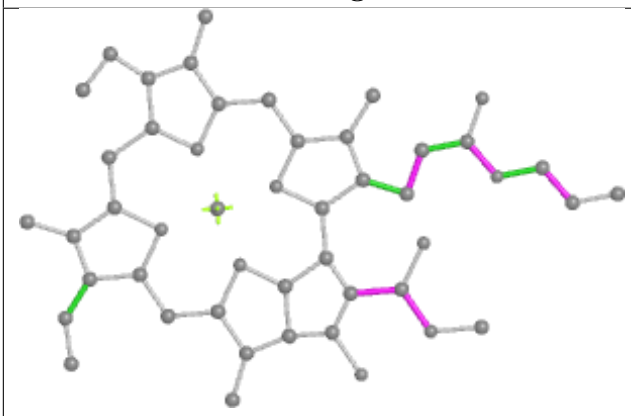
Ligand CLA u 308



Bond lengths



Bond angles



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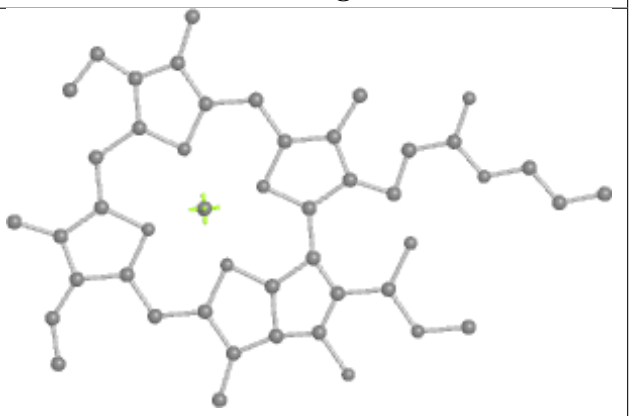
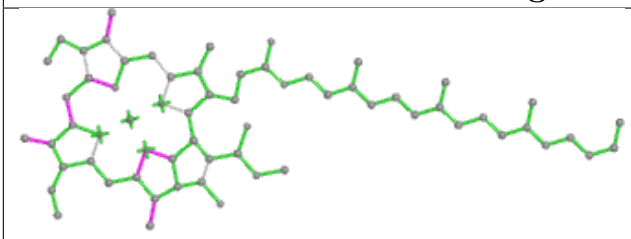


Rings

Ligand CLA g 304



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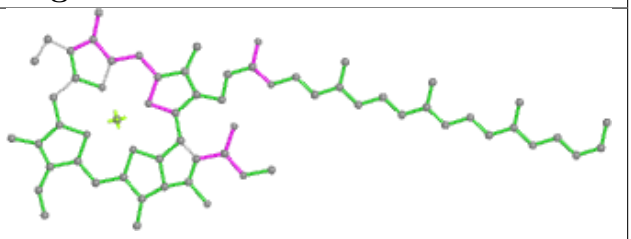
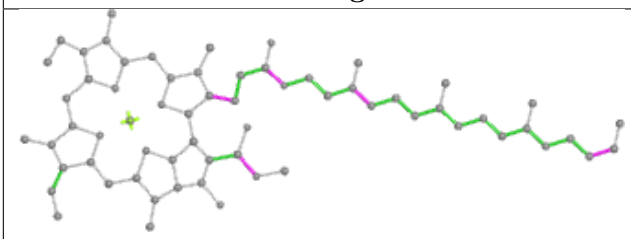


Bond angles



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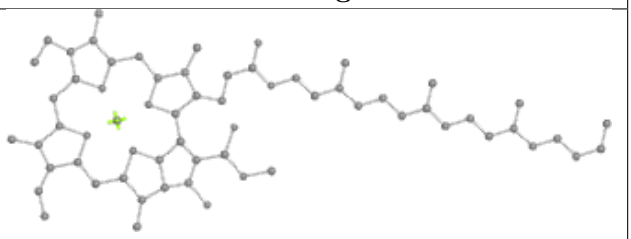
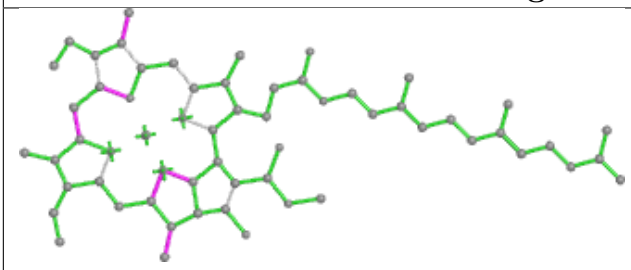
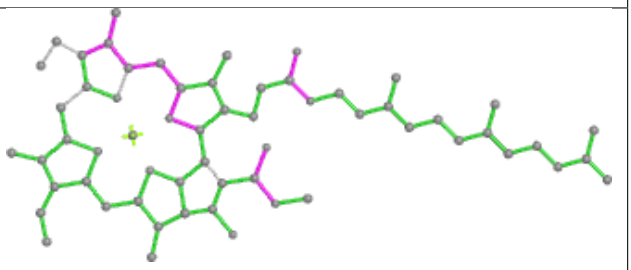
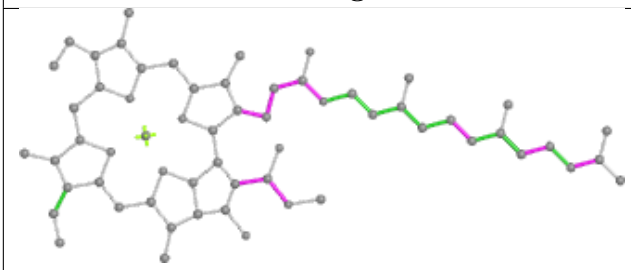
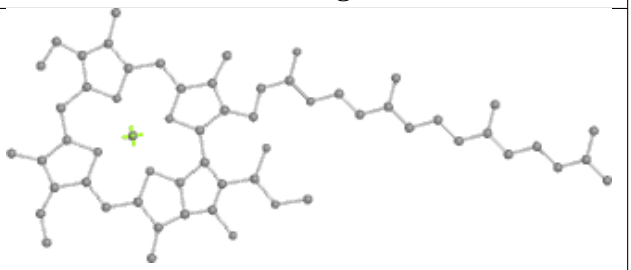
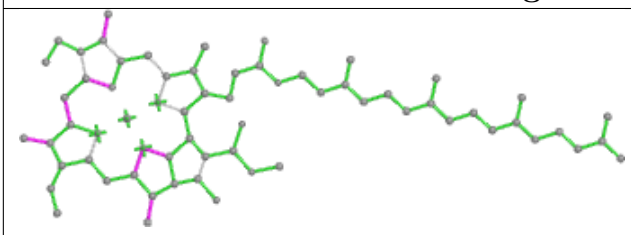
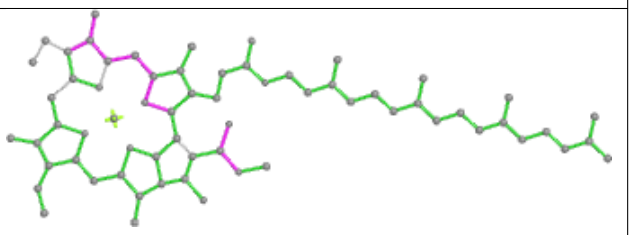
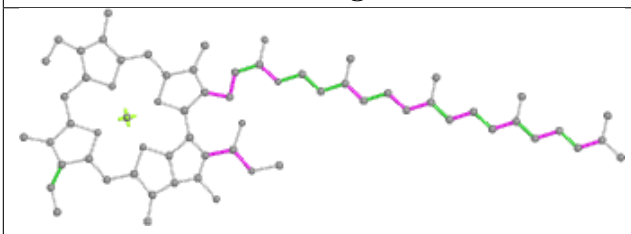
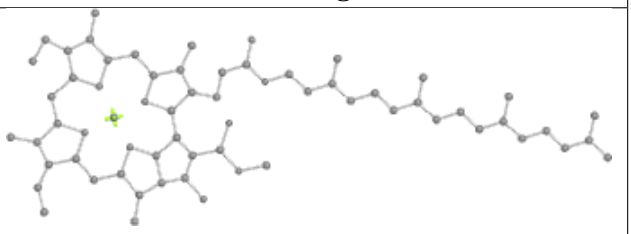


Rings

Ligand CLA v 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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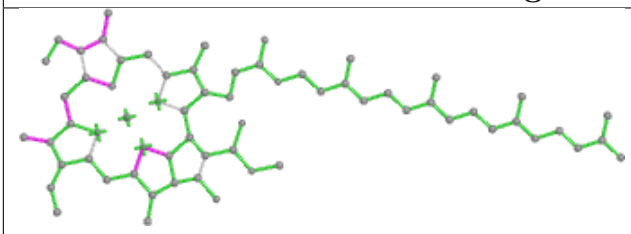
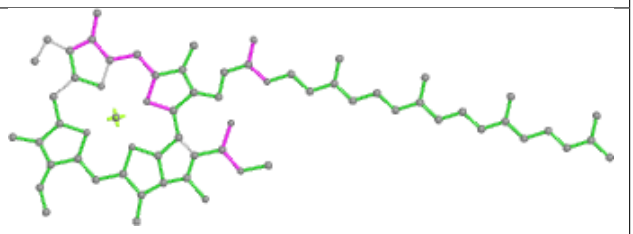
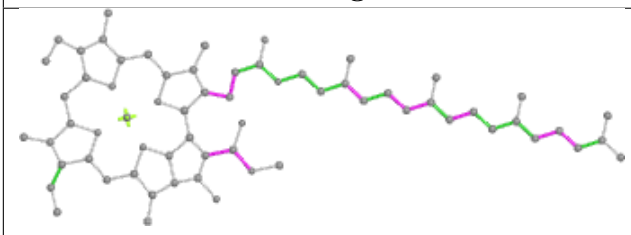
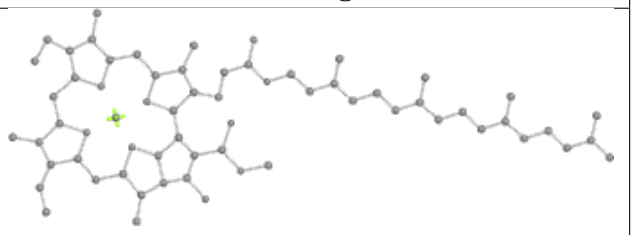
 Bond lengths	 Bond angles
 Torsions	 Rings

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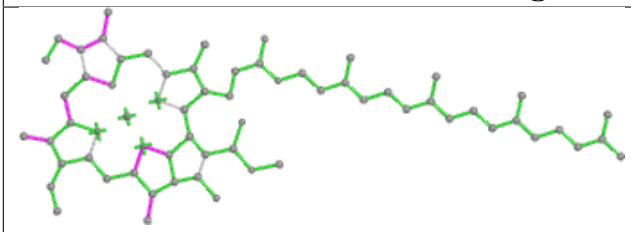
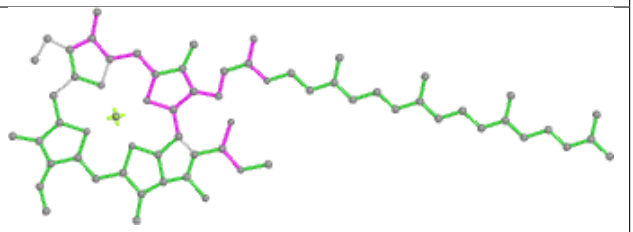
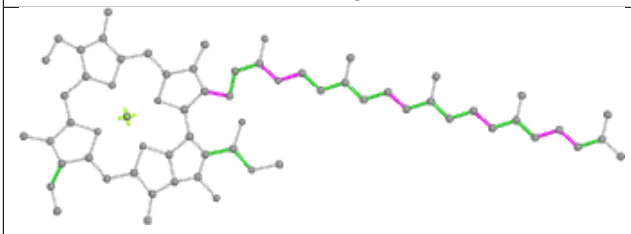
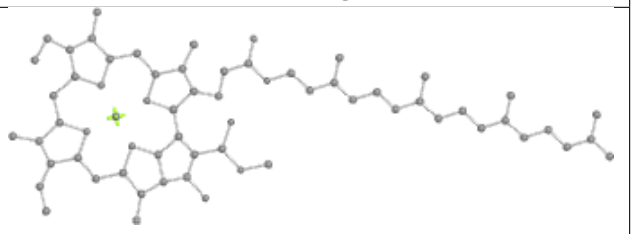
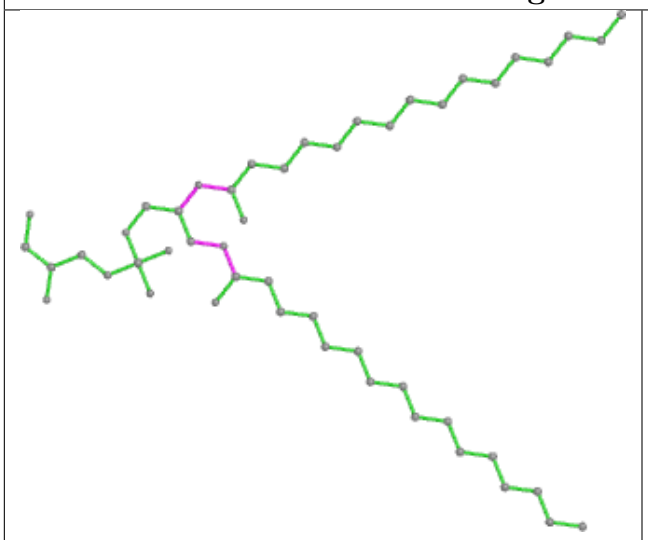
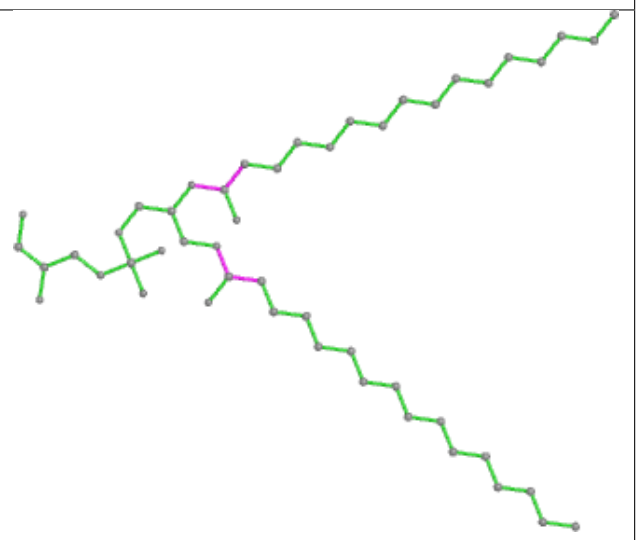
 Bond lengths	 Bond angles
 Torsions	 Rings

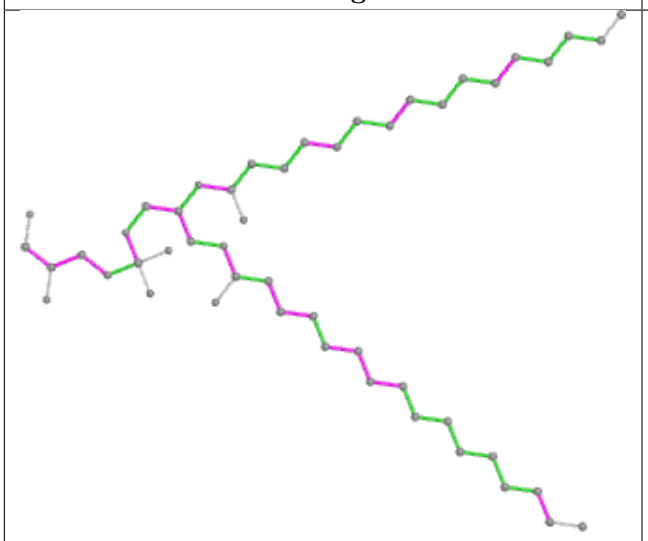
Ligand LHG 2 312



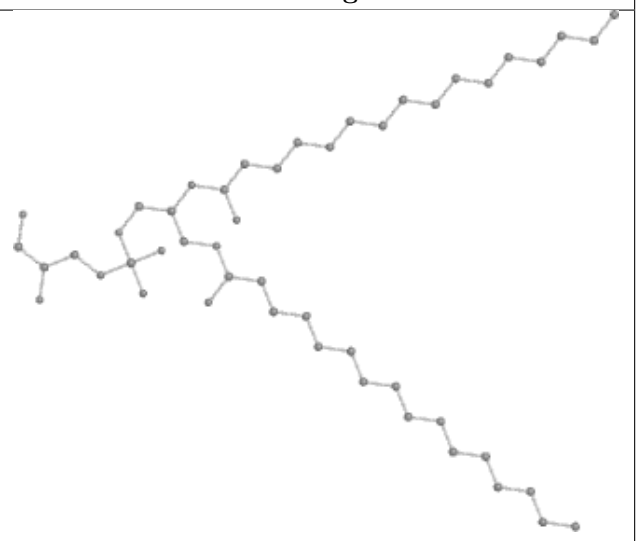
Bond lengths



Bond angles

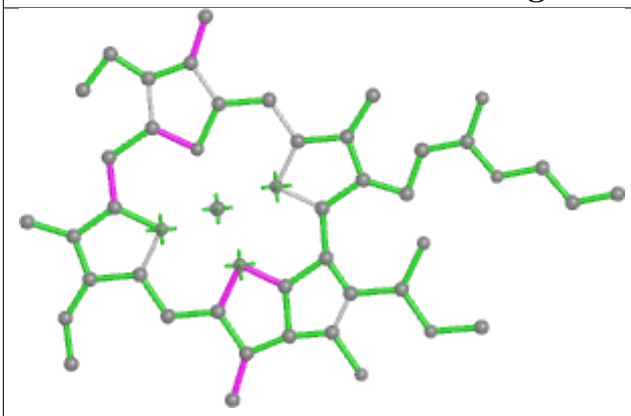


Torsions



Rings

Ligand CLA q 308



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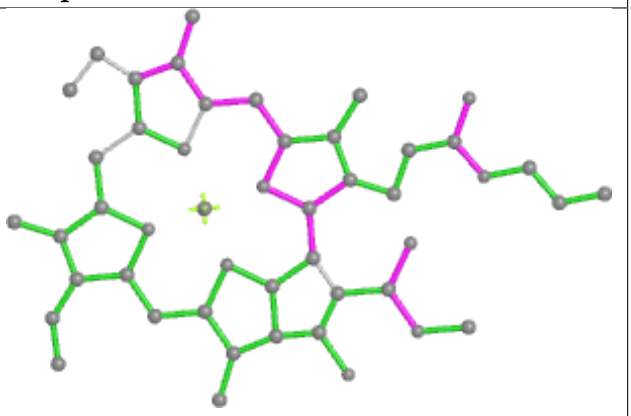
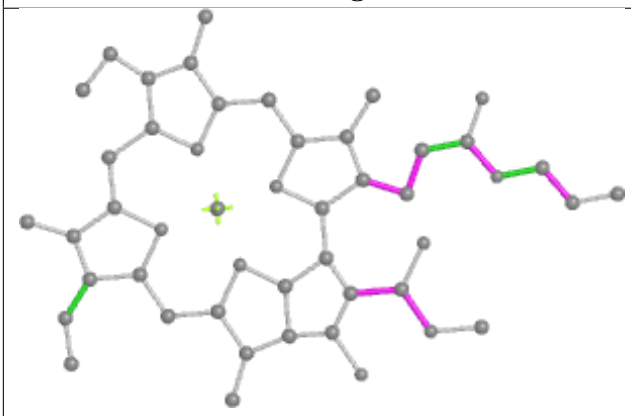


Bond angles



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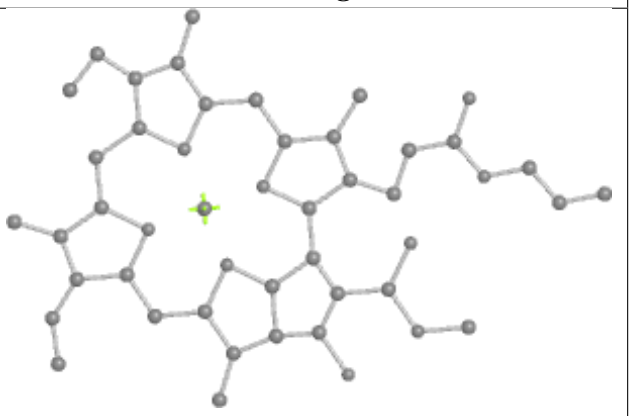
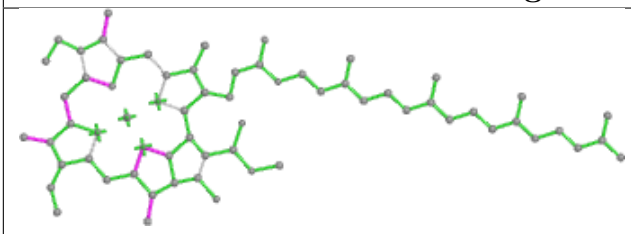
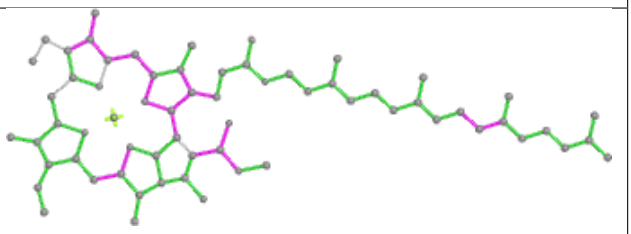


Rings

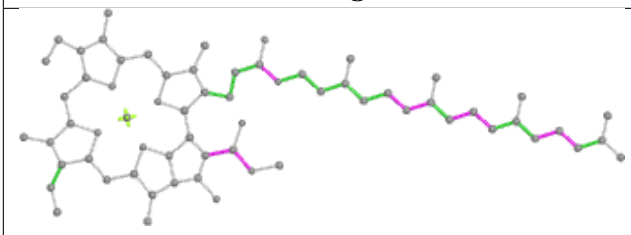
Ligand CLA C 511



Bond lengths



Bond angles



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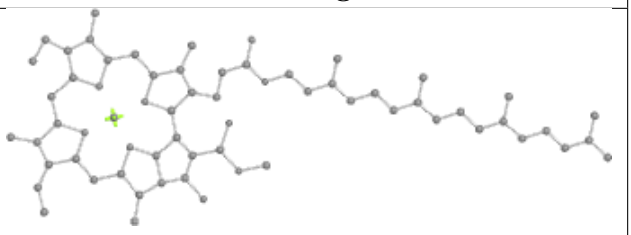
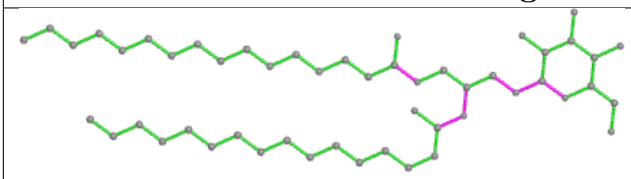
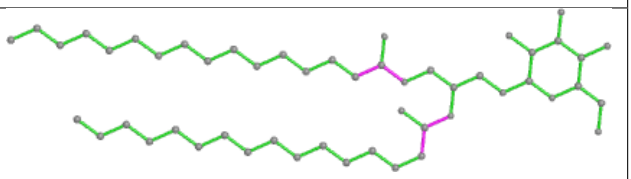


Rings

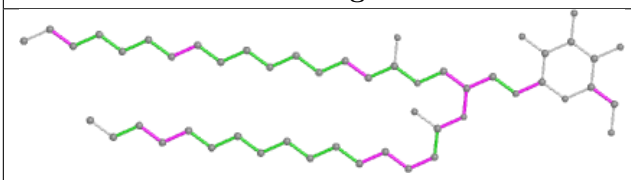
Ligand LMG C 521



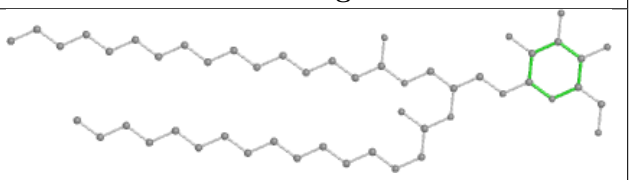
Bond lengths



Bond angles

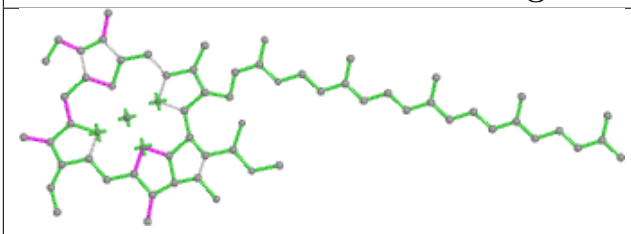


Torsions

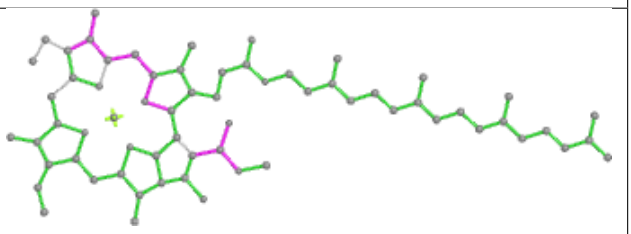


Rings

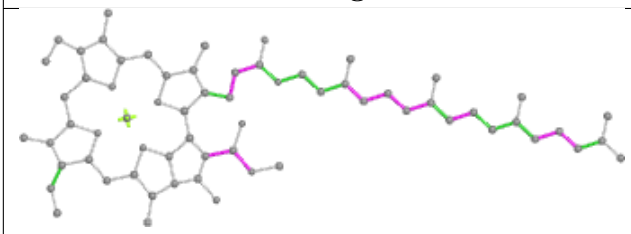
Ligand CLA b 615



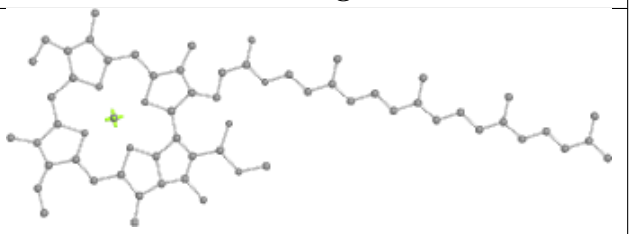
Bond lengths



Bond angles

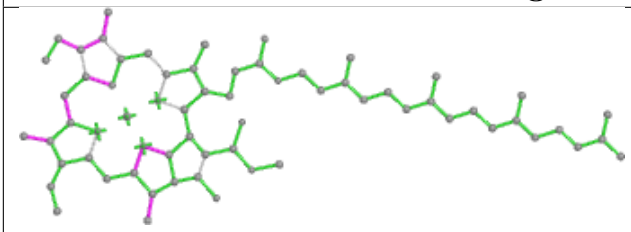


Torsions

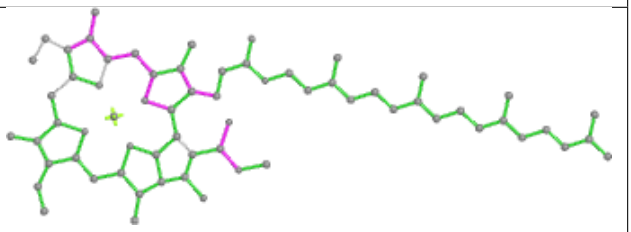


Rings

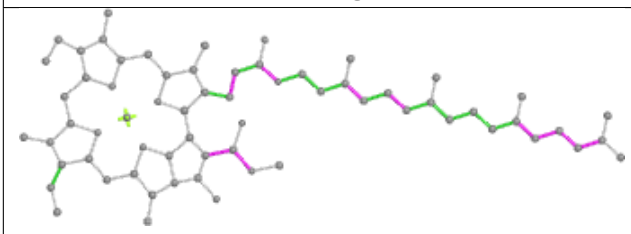
Ligand CLA b 606



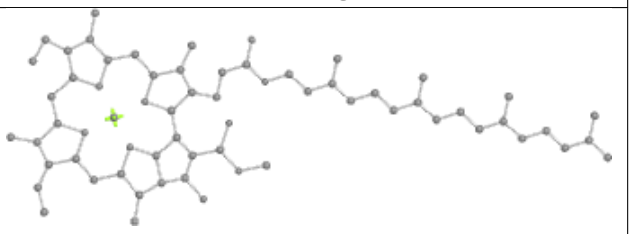
Bond lengths



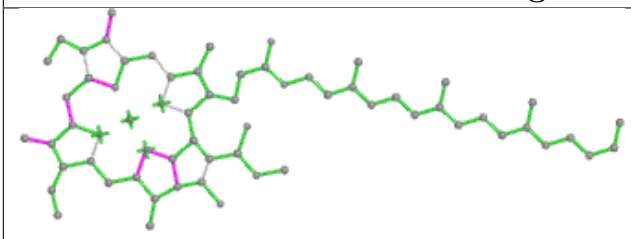
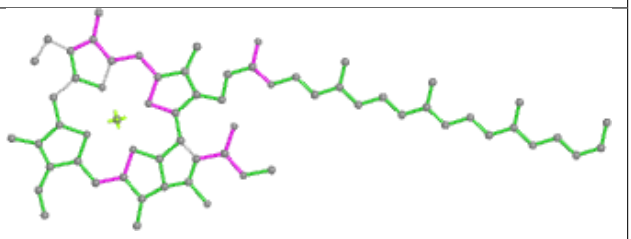
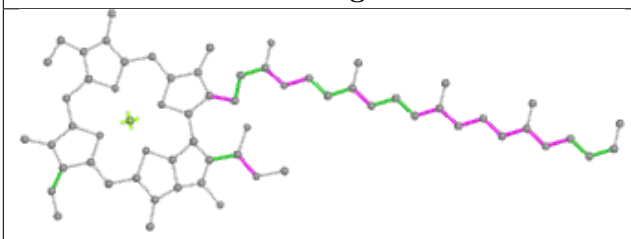
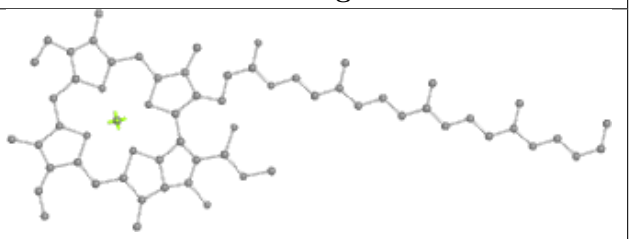
Bond angles

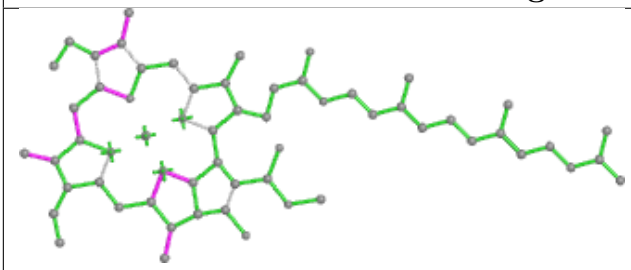
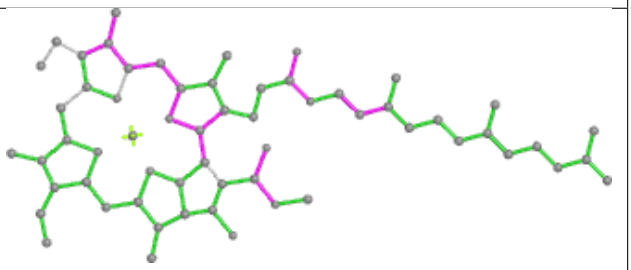
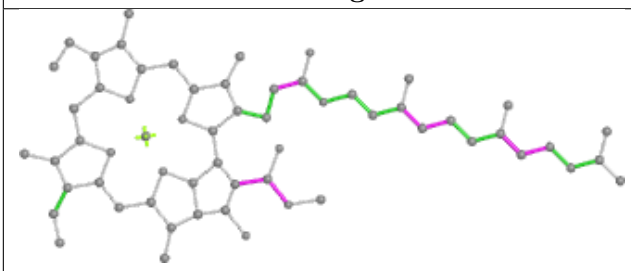
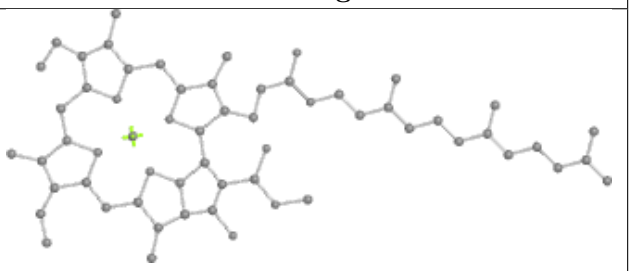


Torsions

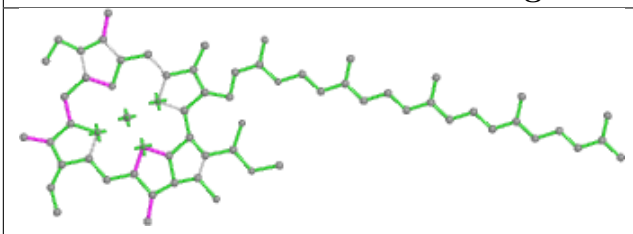


Rings

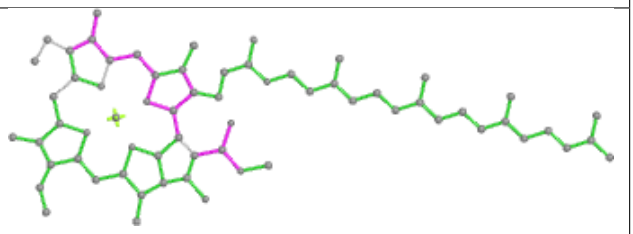
Ligand CLA 6 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

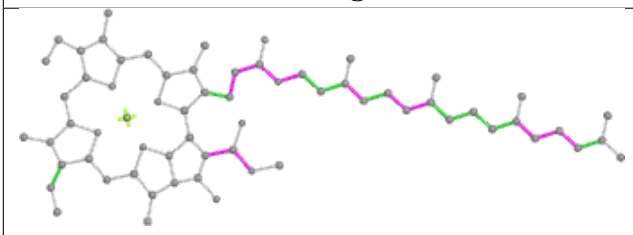
Ligand CLA C 507



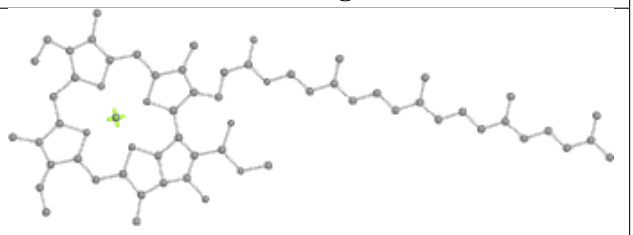
Bond lengths



Bond angles

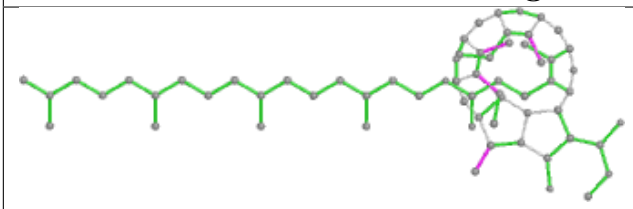


Torsions

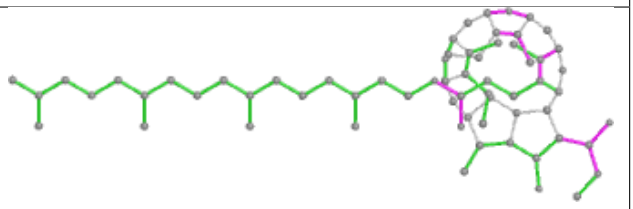


Rings

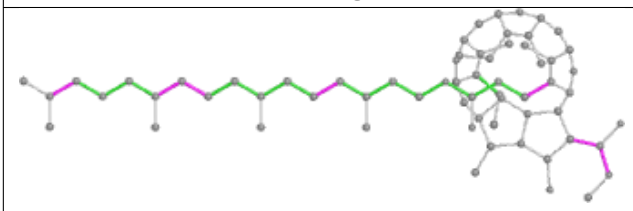
Ligand PHO d 401



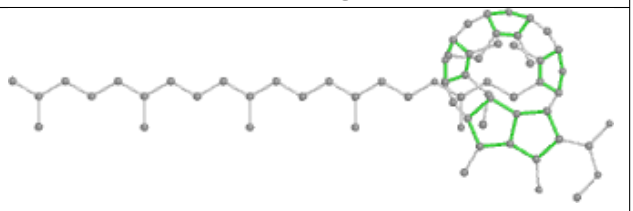
Bond lengths



Bond angles

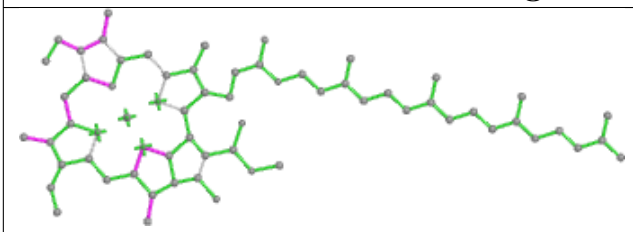


Torsions

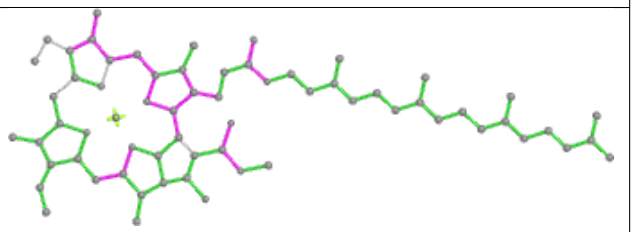


Rings

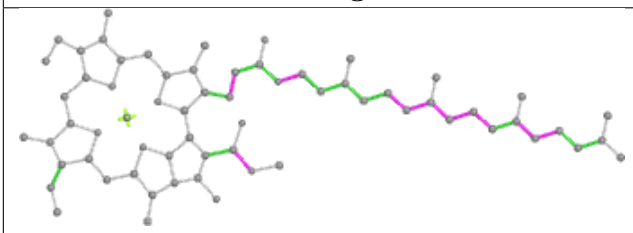
Ligand CLA C 509



Bond lengths



Bond angles



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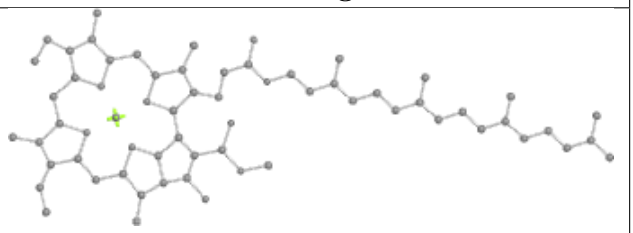
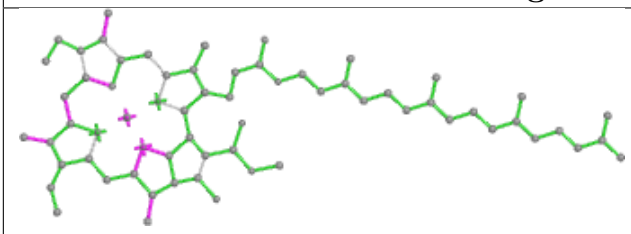
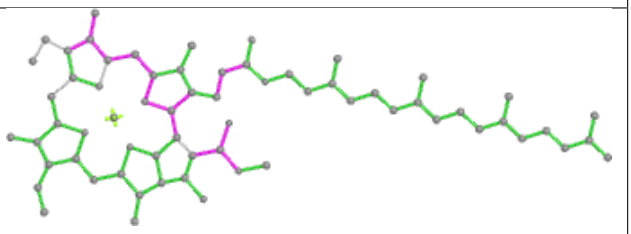
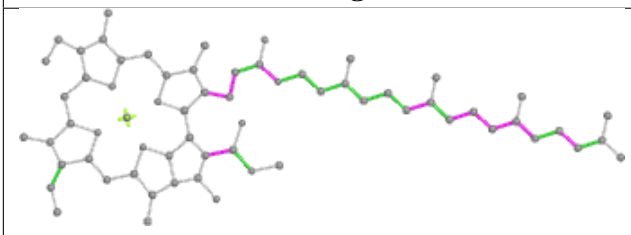
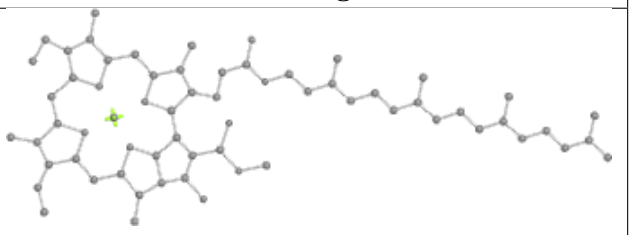
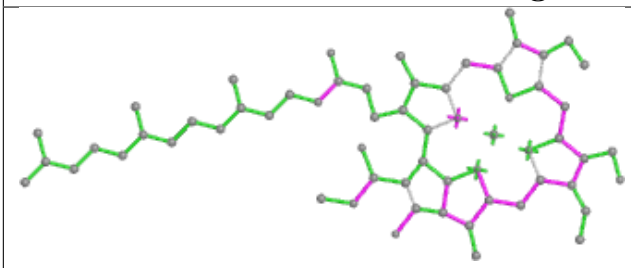
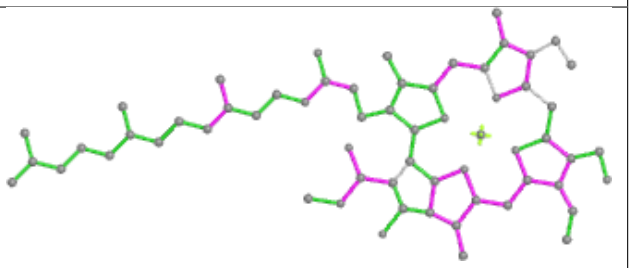
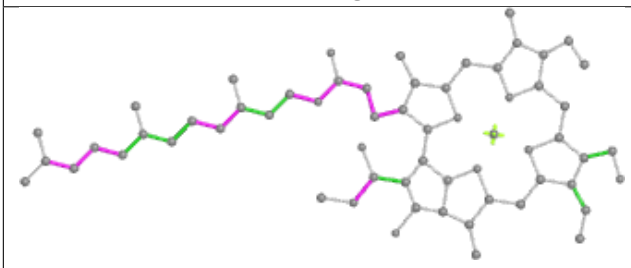
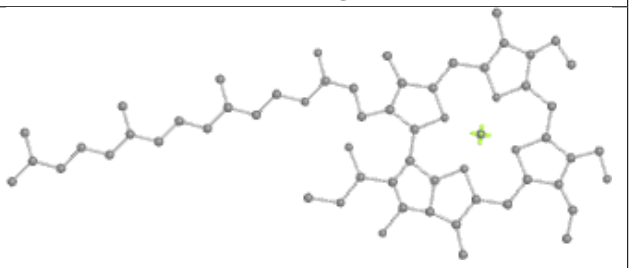
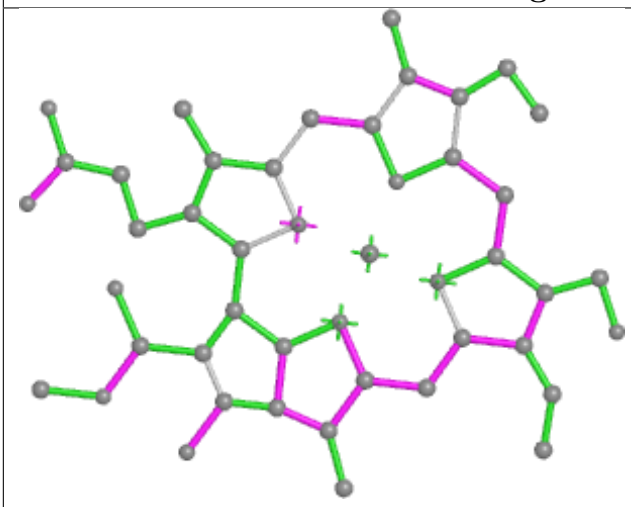


Rings

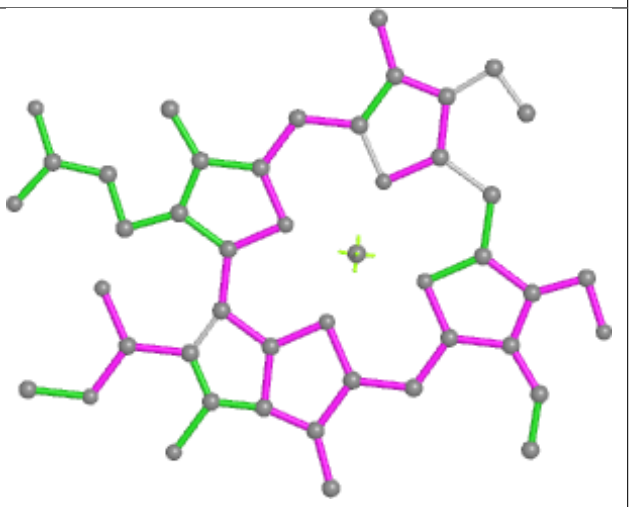
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

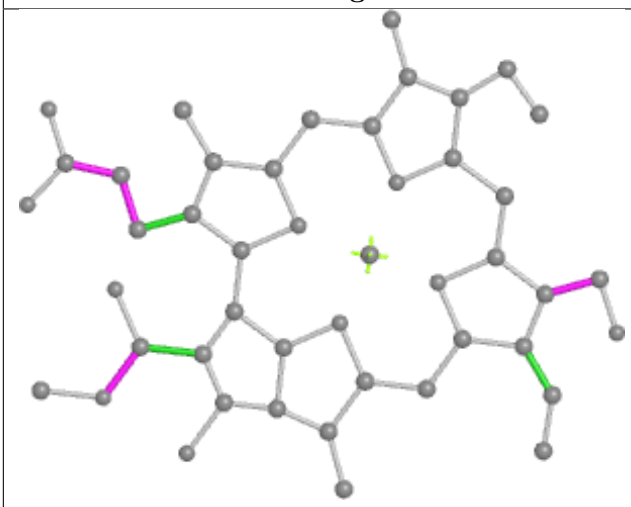
Ligand CHL s 313



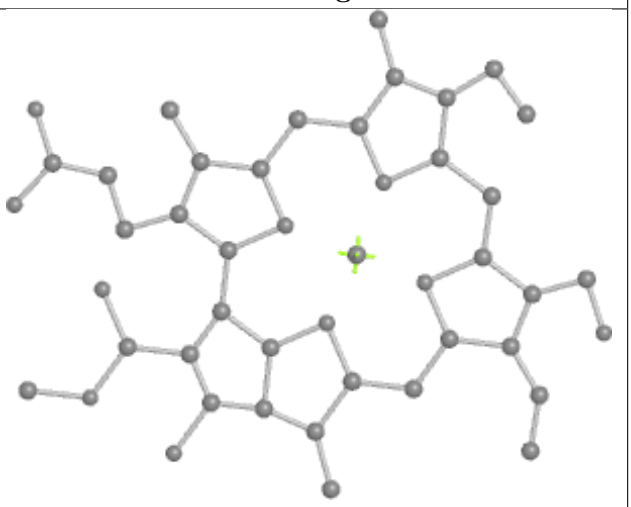
Bond lengths



Bond angles

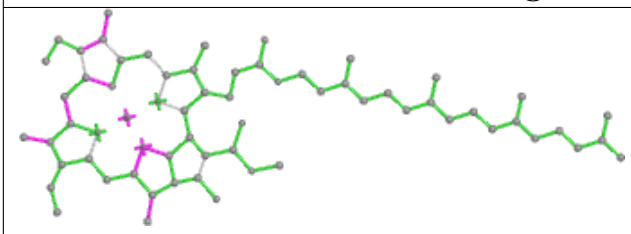


Torsions

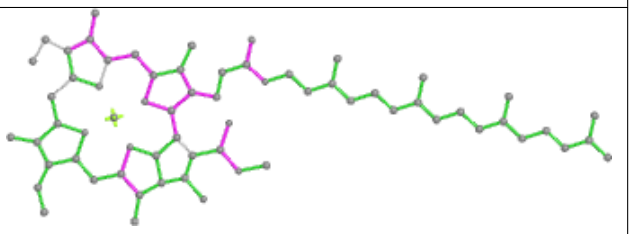


Rings

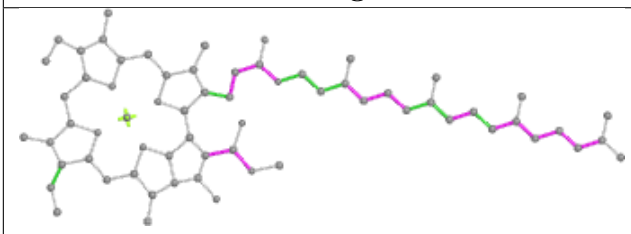
Ligand CLA B 602



Bond lengths



Bond angles



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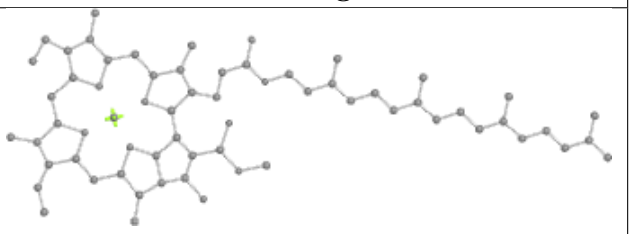
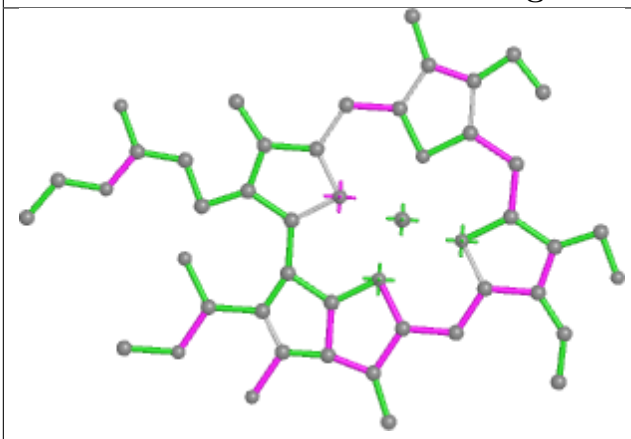
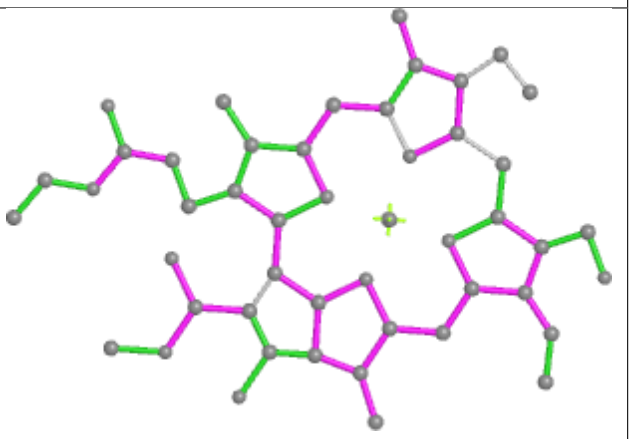
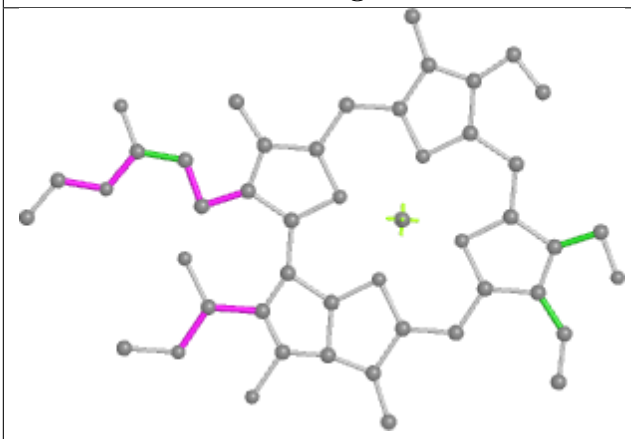
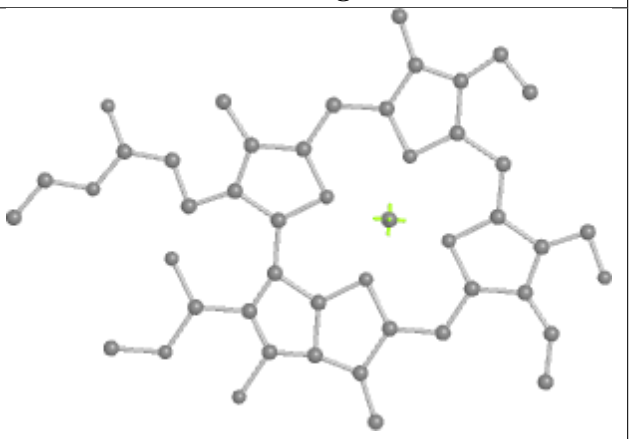
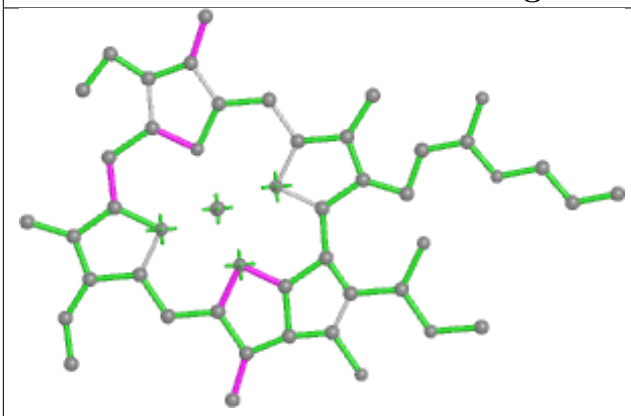
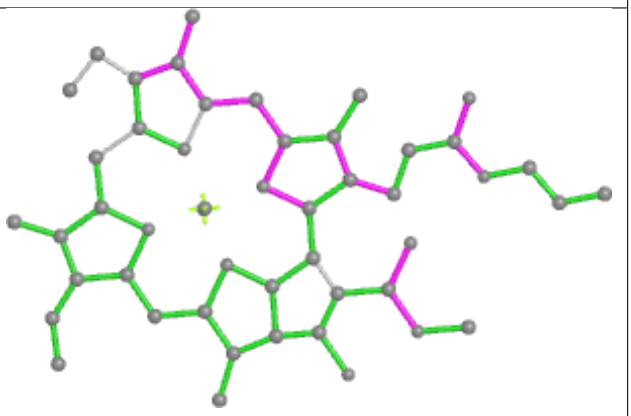
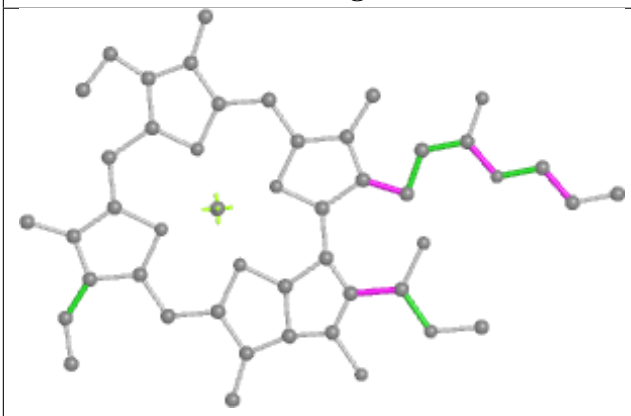
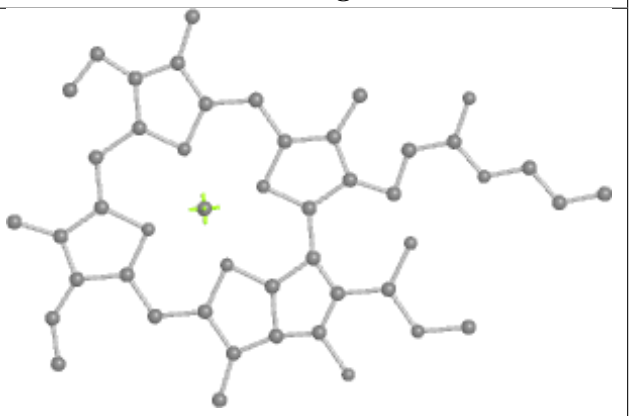
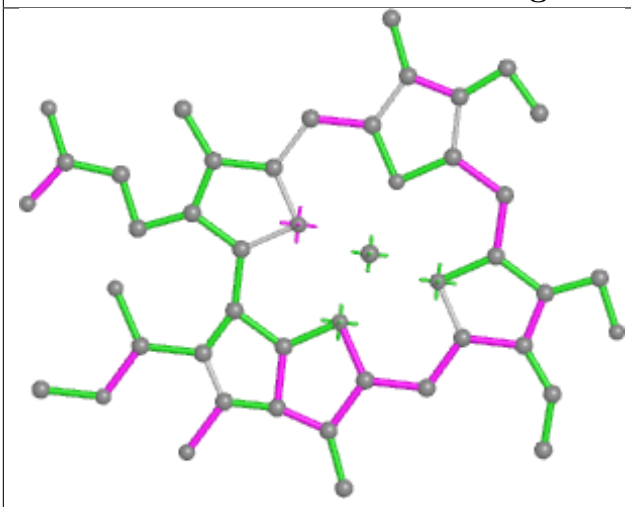


Rings

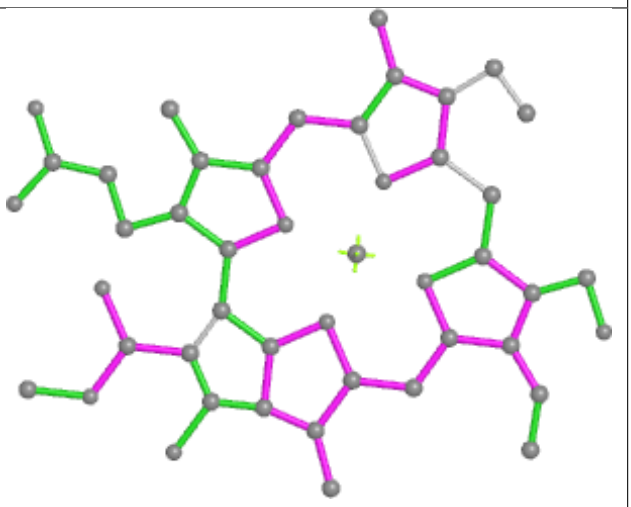
Ligand CHL u 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

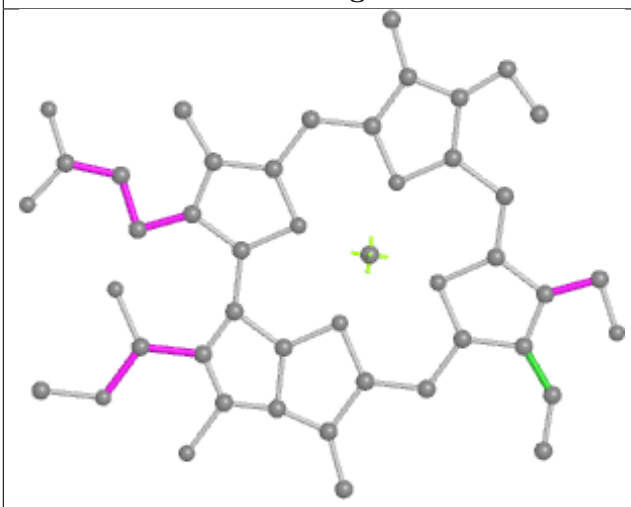
Ligand CHL s 316



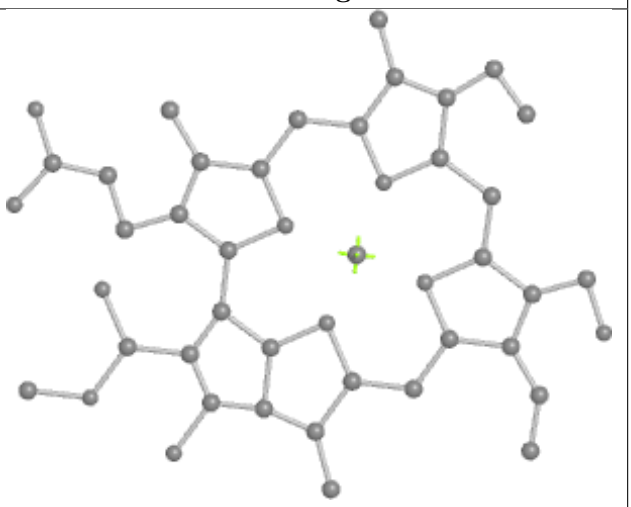
Bond lengths



Bond angles

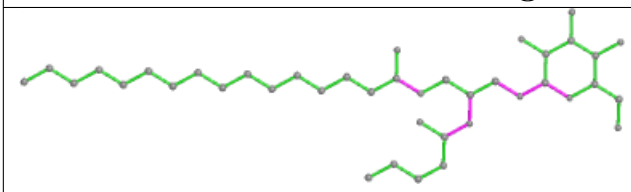


Torsions

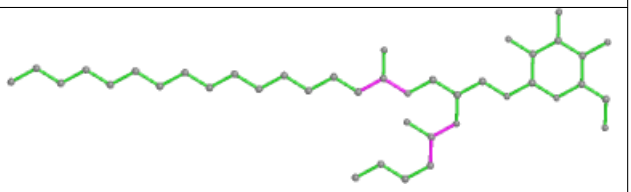


Rings

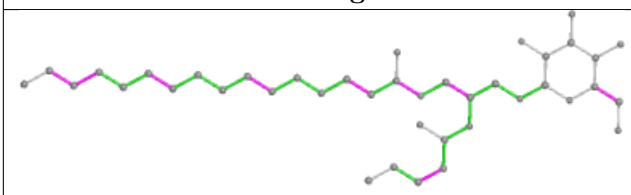
Ligand LMG A 411



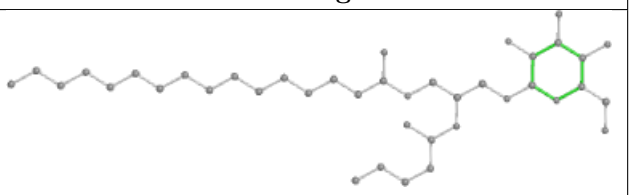
Bond lengths



Bond angles

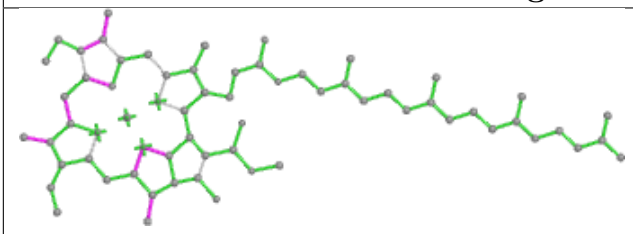


Torsions

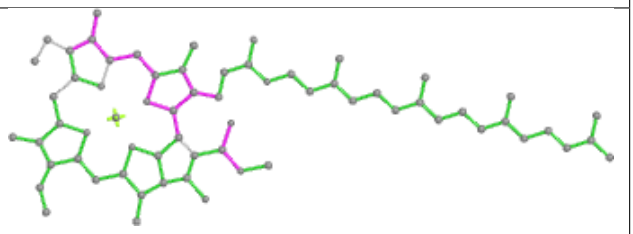


Rings

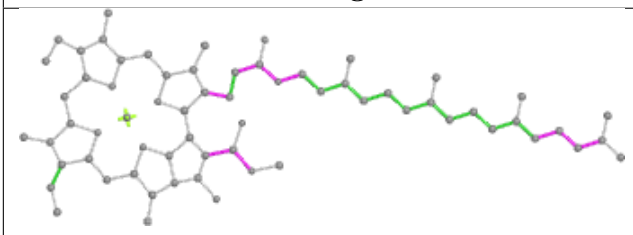
Ligand CLA b 611



Bond lengths



Bond angles



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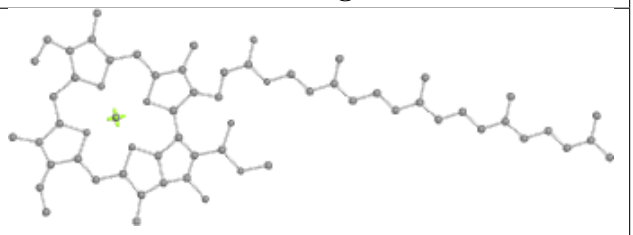
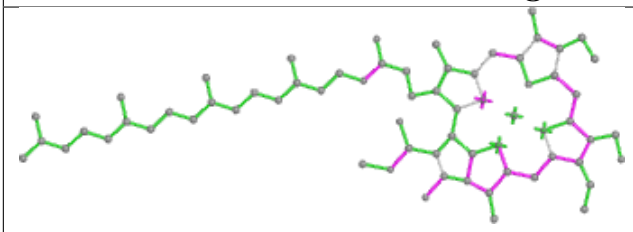
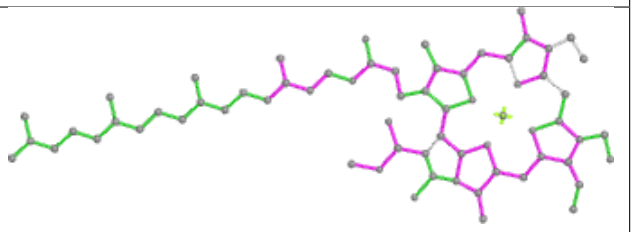


Rings

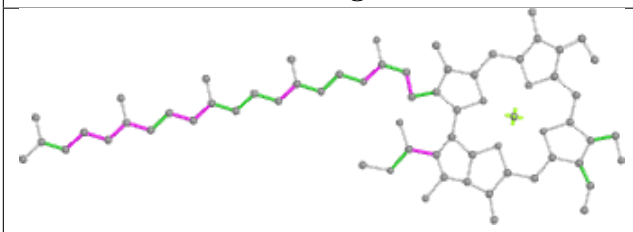
Ligand CHL P 317



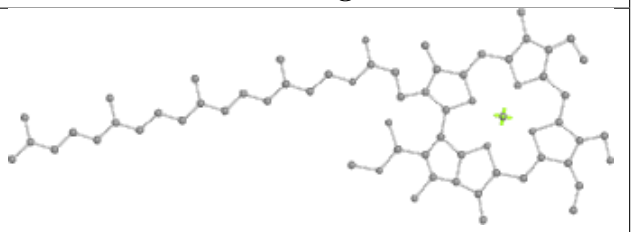
Bond lengths



Bond angles

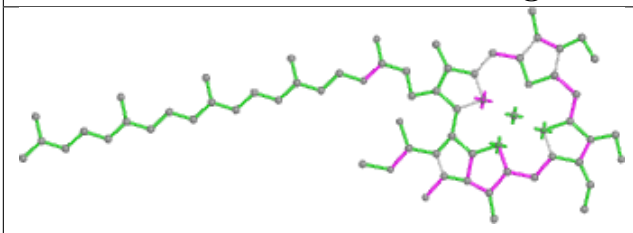


Torsions



Rings

Ligand CHL N 316



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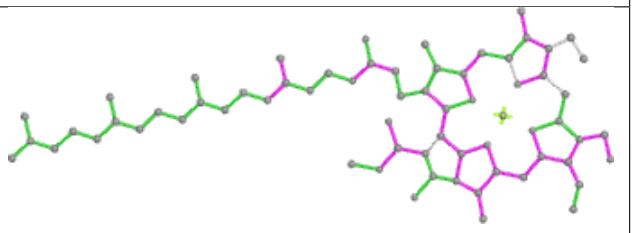
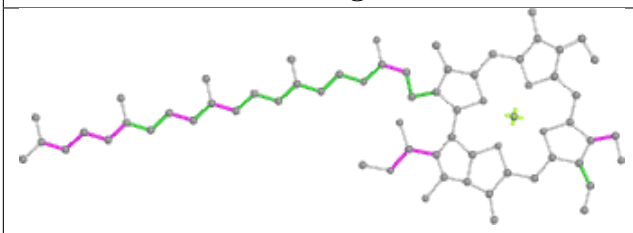
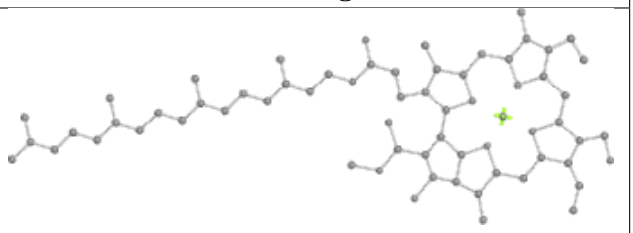


Bond angles

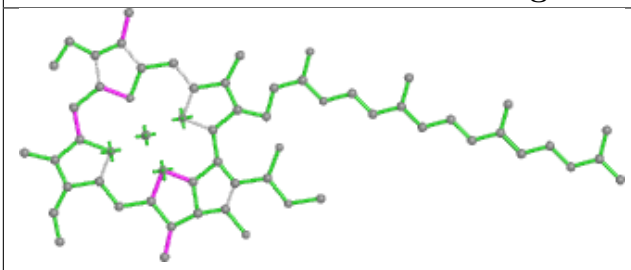


Torsions

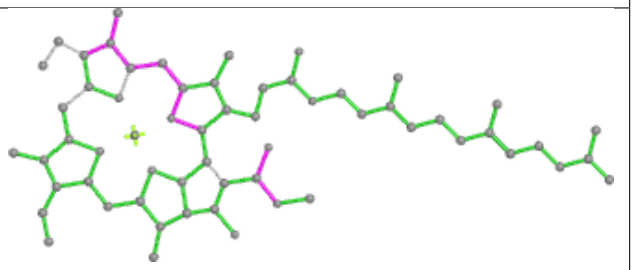


Rings

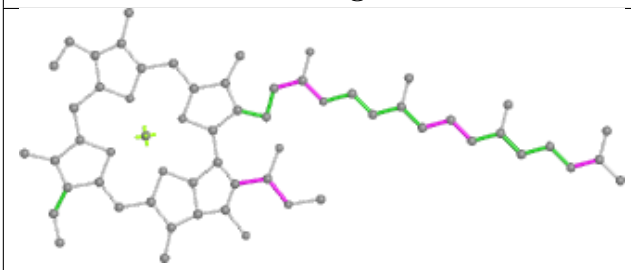
Ligand CLA r 603



Bond lengths



Bond angles



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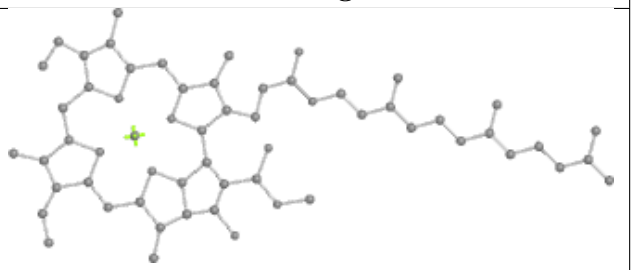
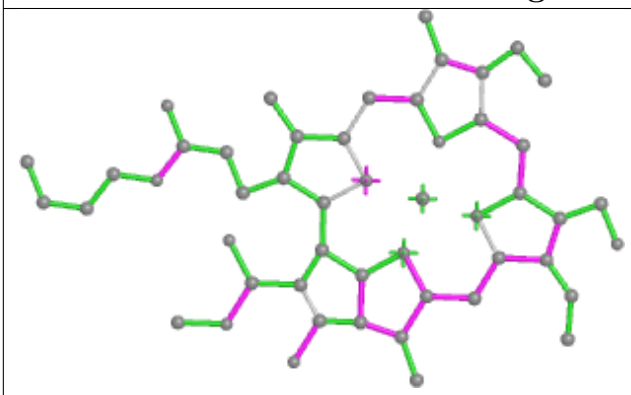
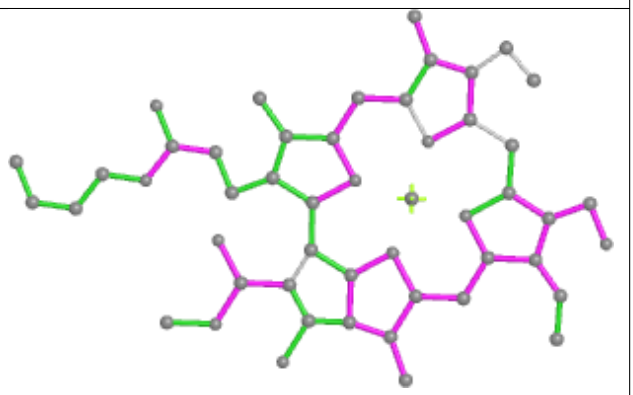


Rings

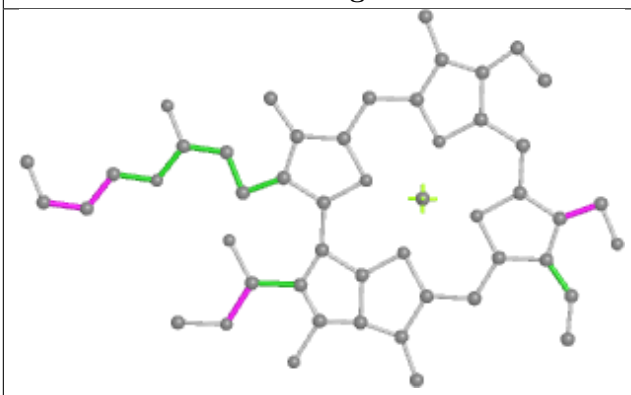
Ligand CHL 4 315



Bond lengths



Bond angles



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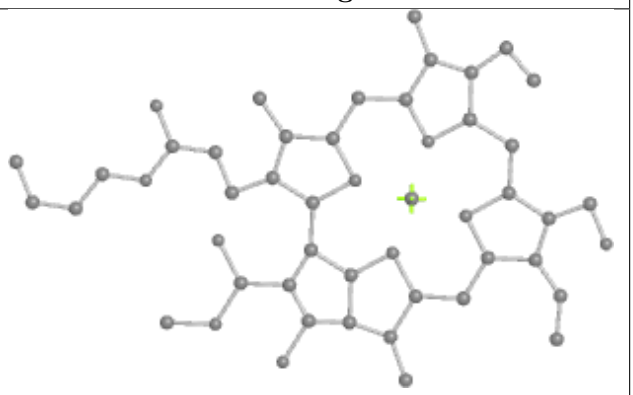
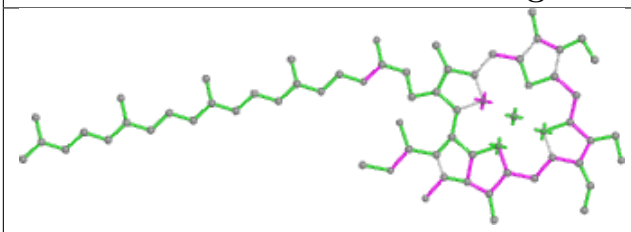
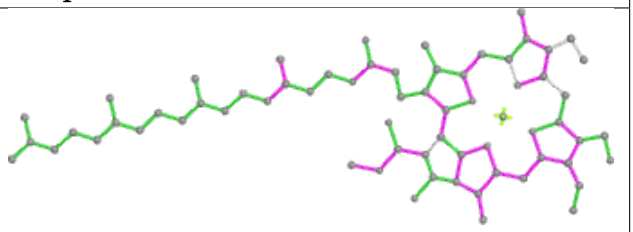
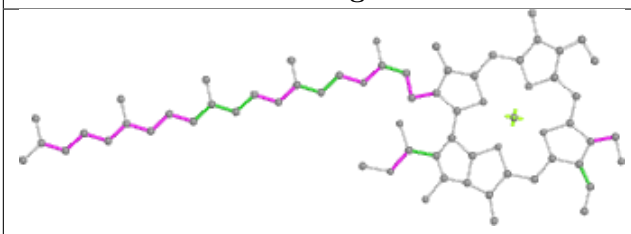
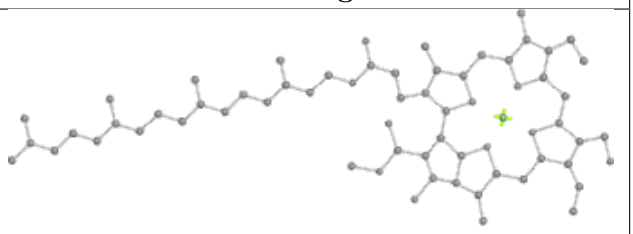
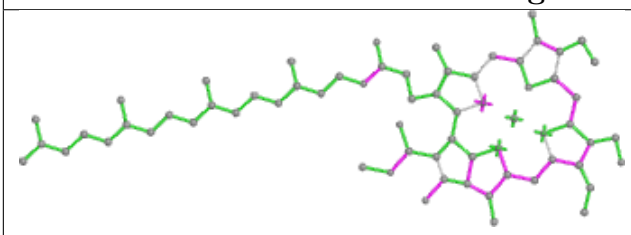
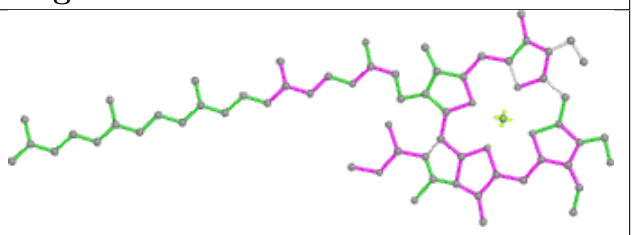
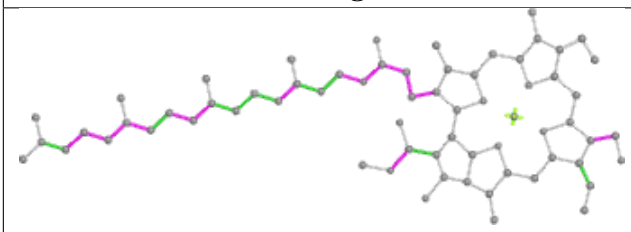
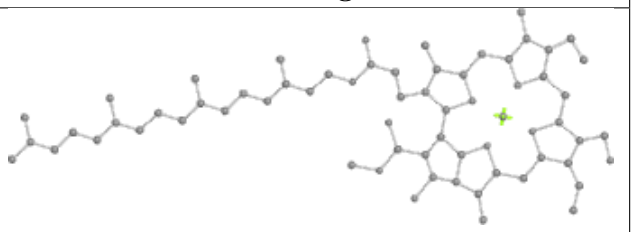
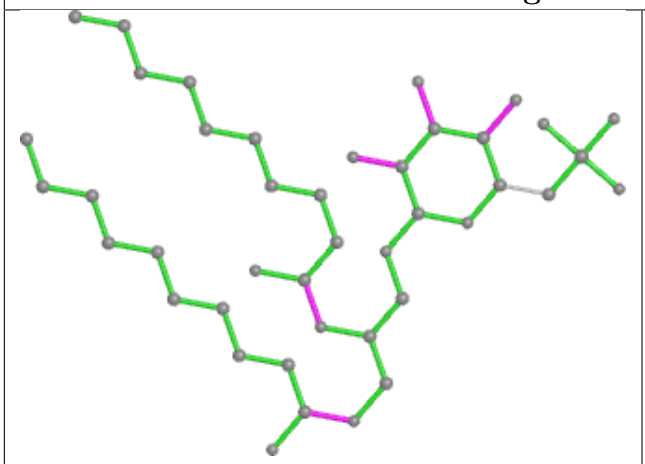


Rings

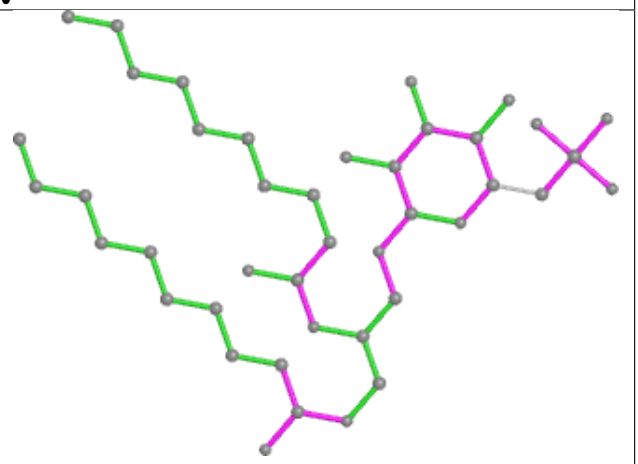
Ligand CHL q 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL g 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

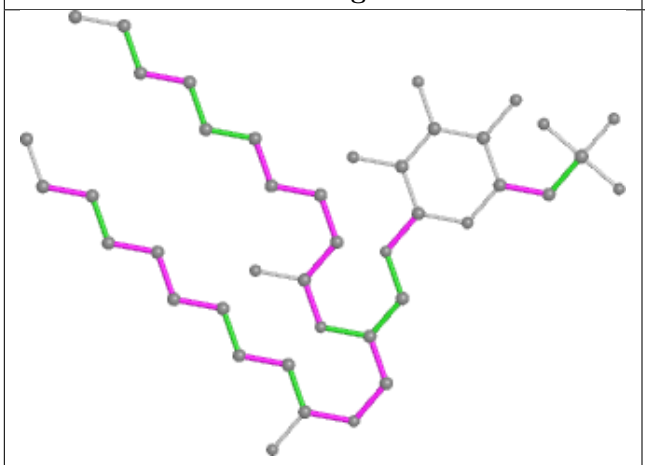
Ligand SQD m 101



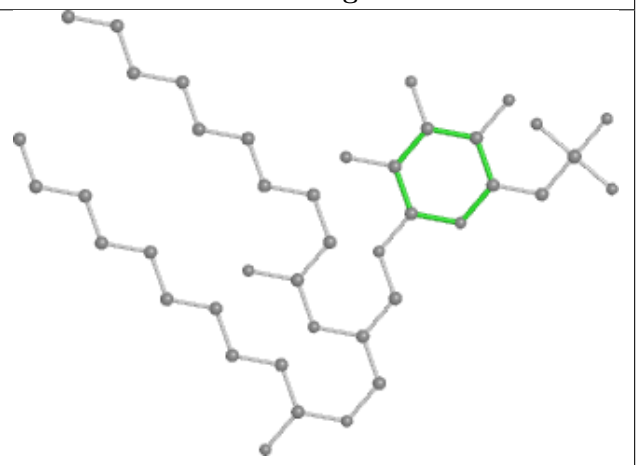
Bond lengths



Bond angles

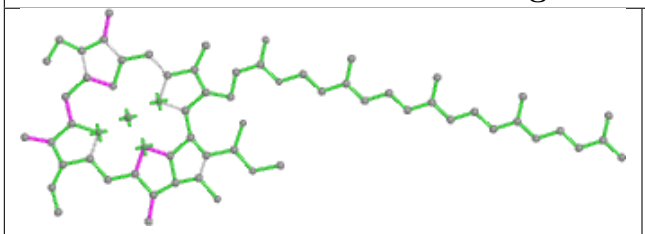


Torsions

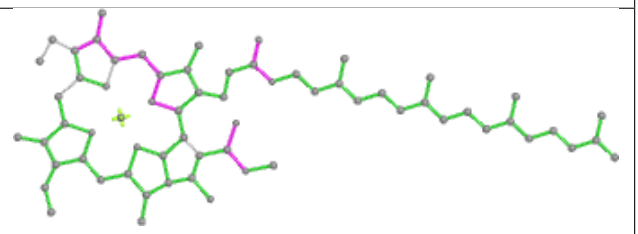


Rings

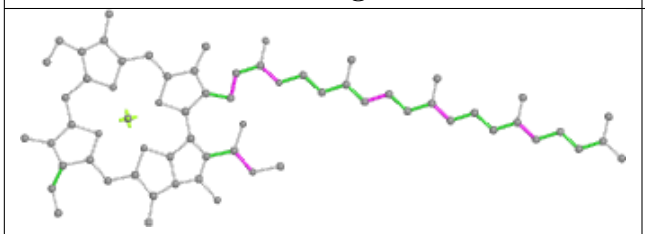
Ligand CLA 6 308



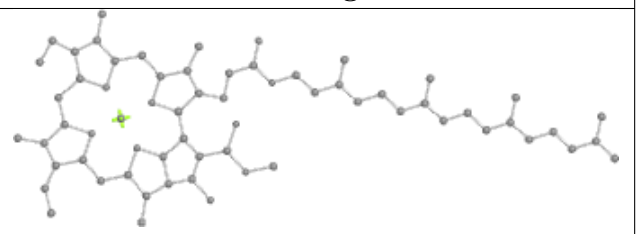
Bond lengths



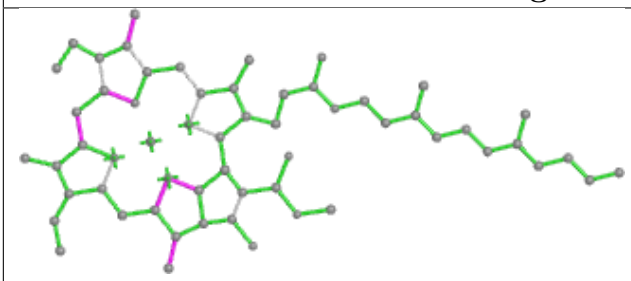
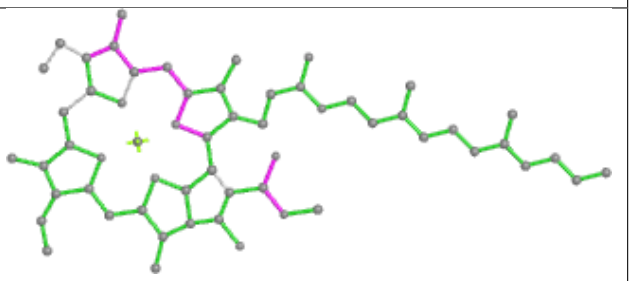
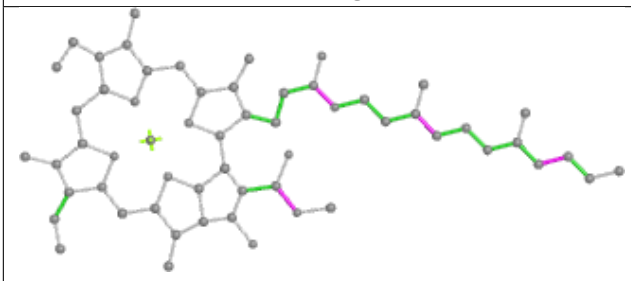
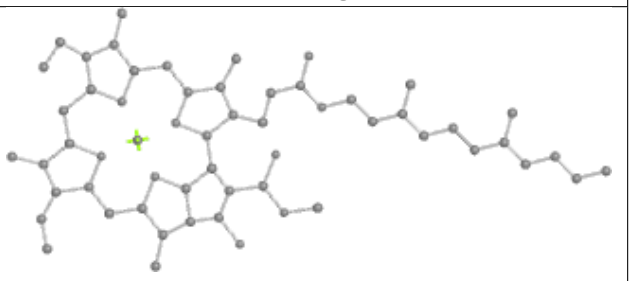
Bond angles

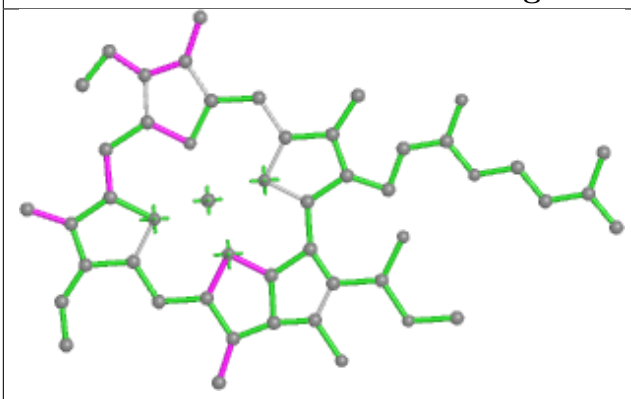
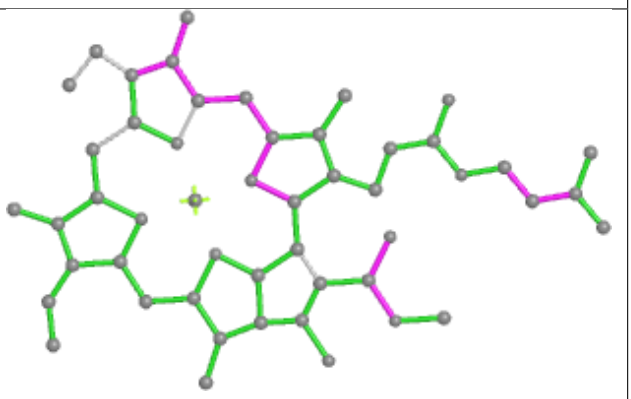
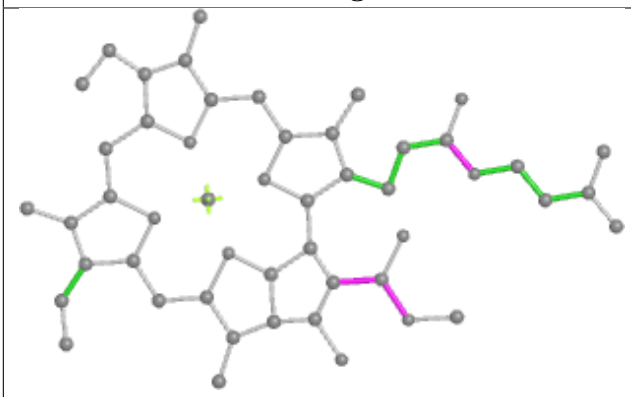
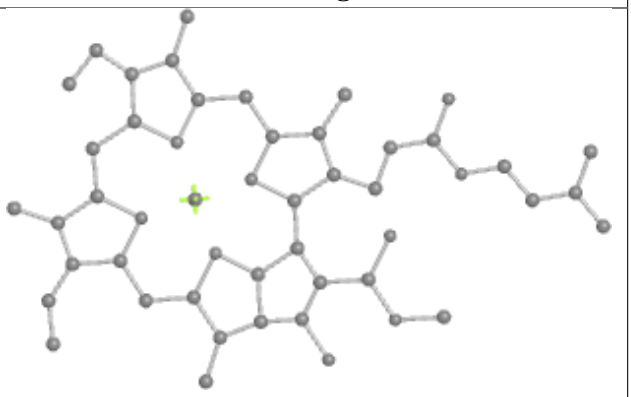


Torsions

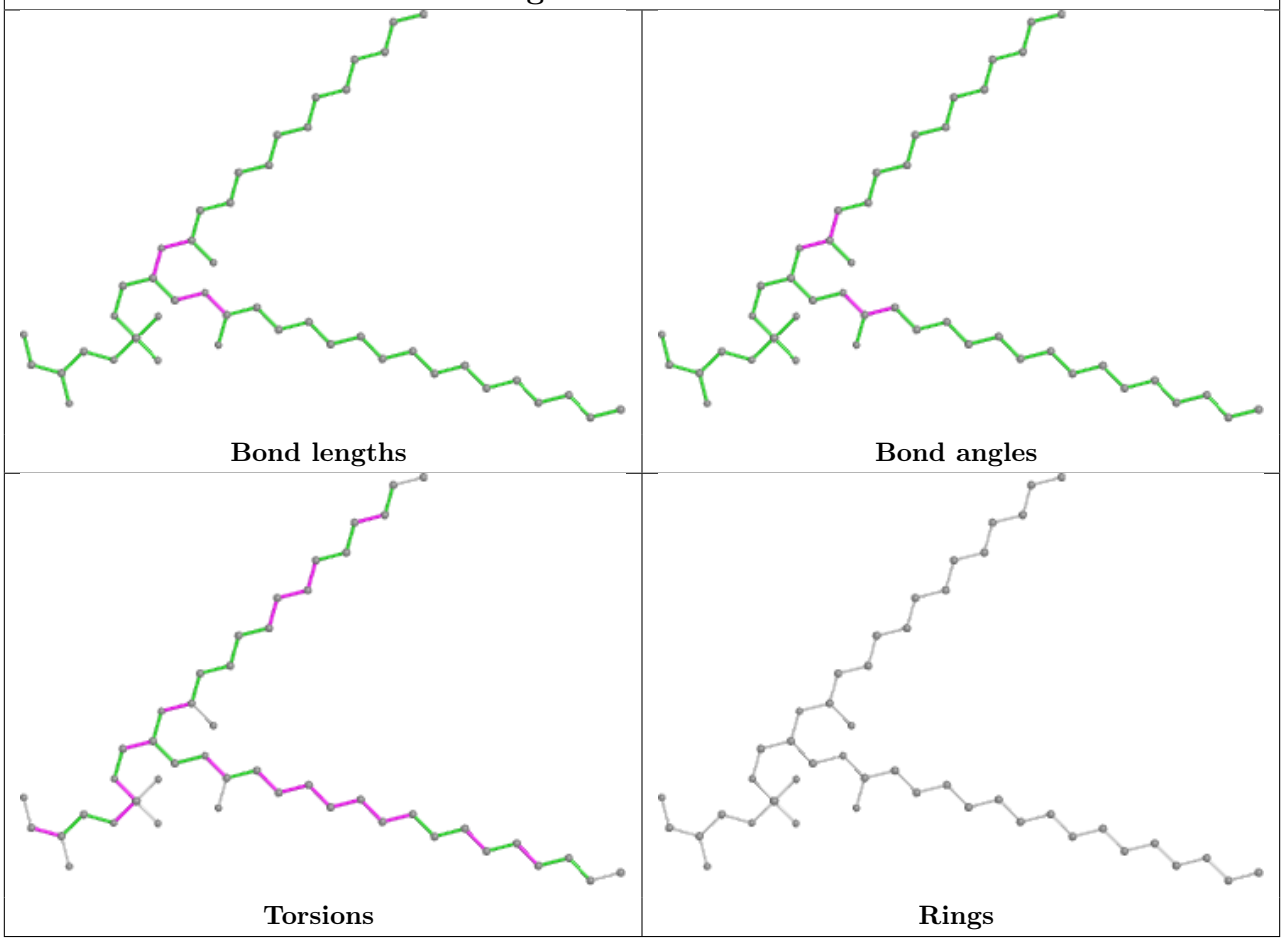


Rings

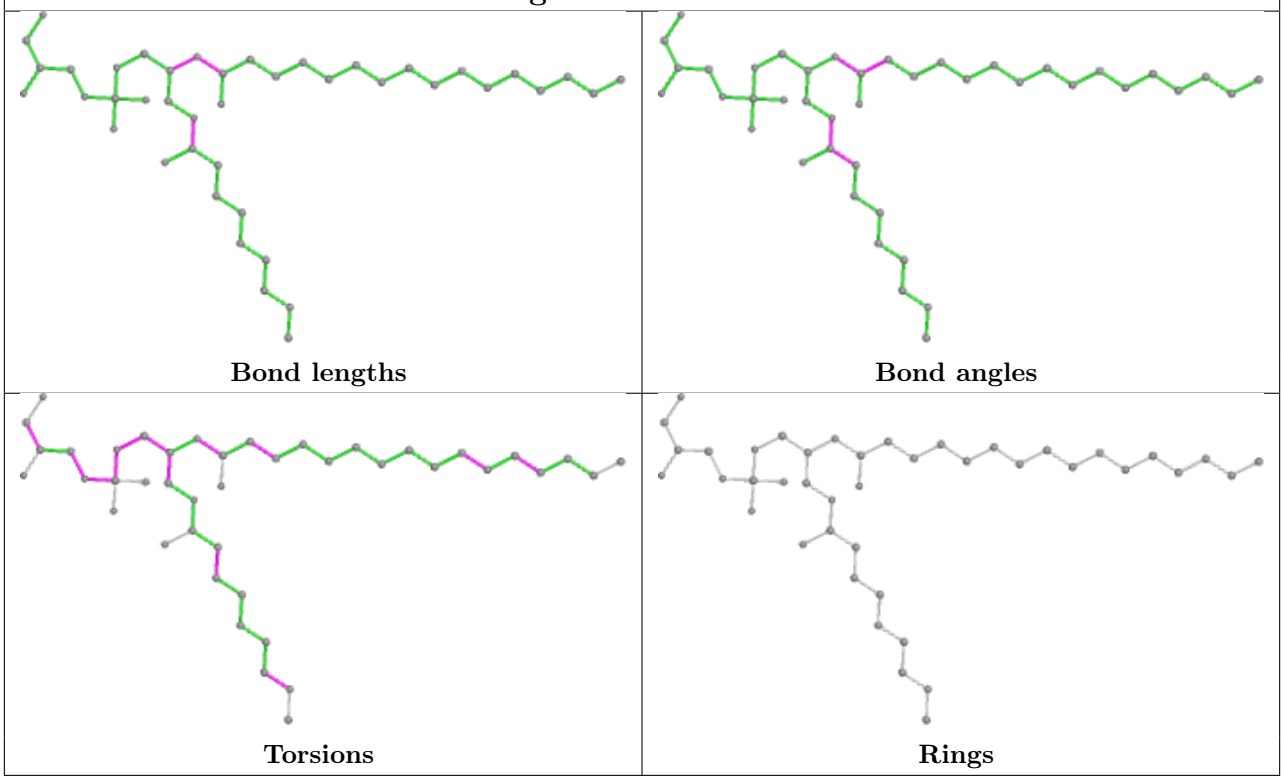
Ligand CLA r 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

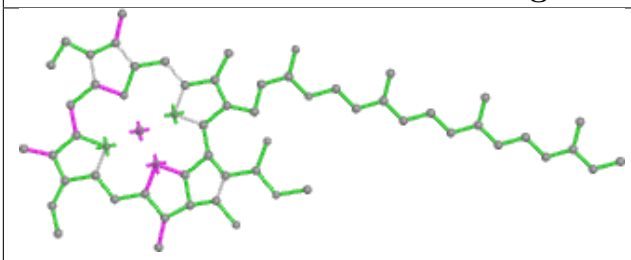
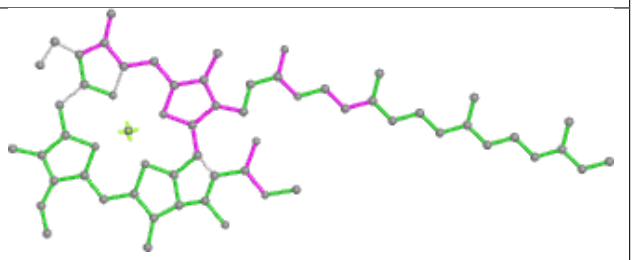
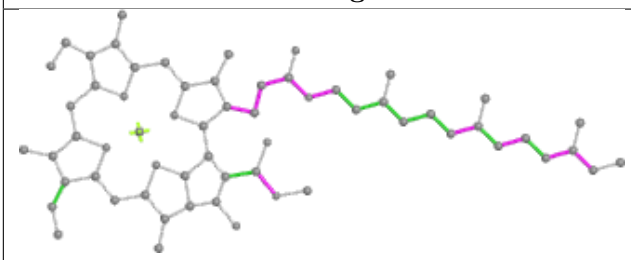
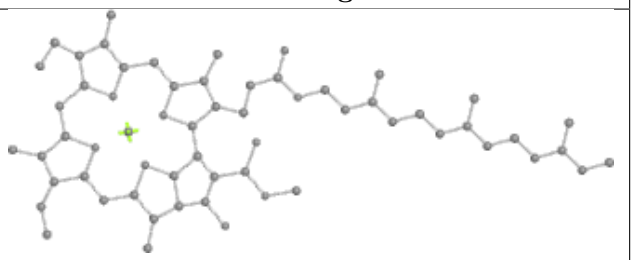
Ligand CLA U 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

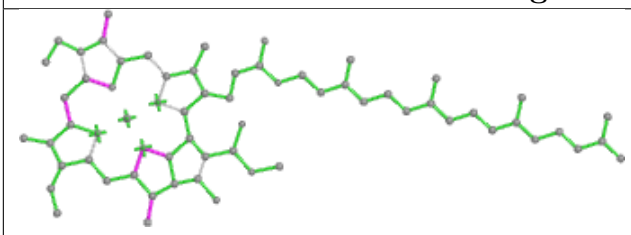
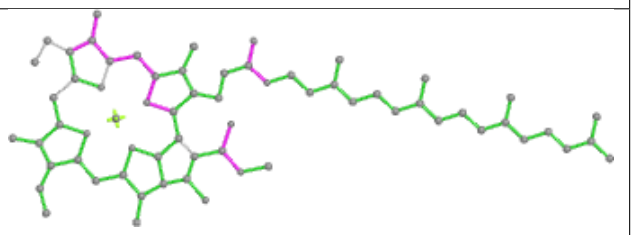
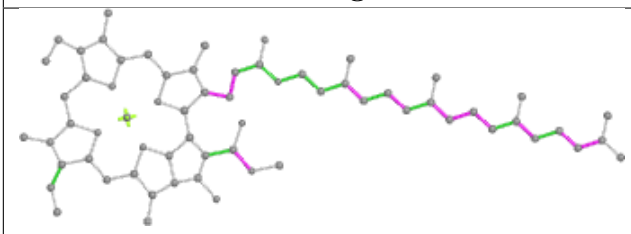
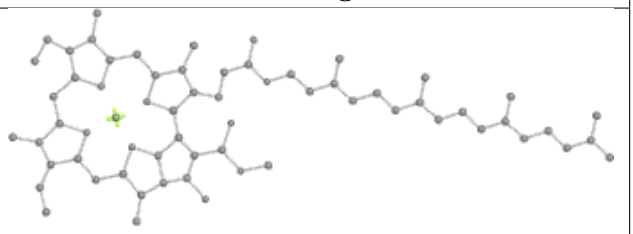
Ligand LHG d 405

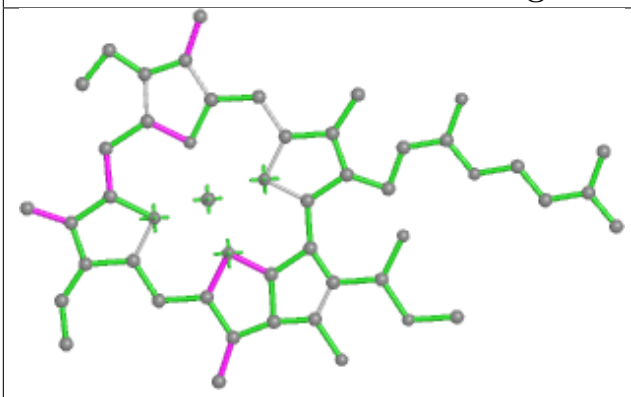
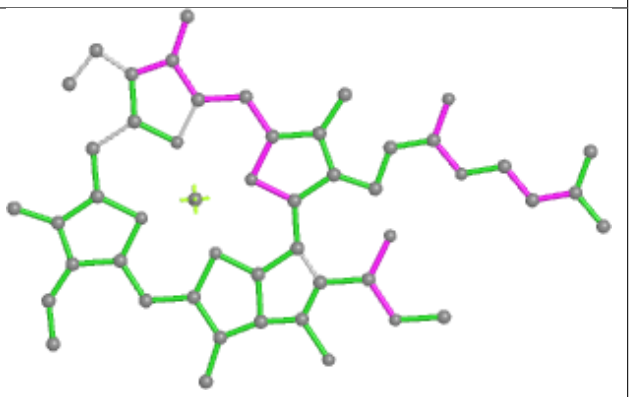
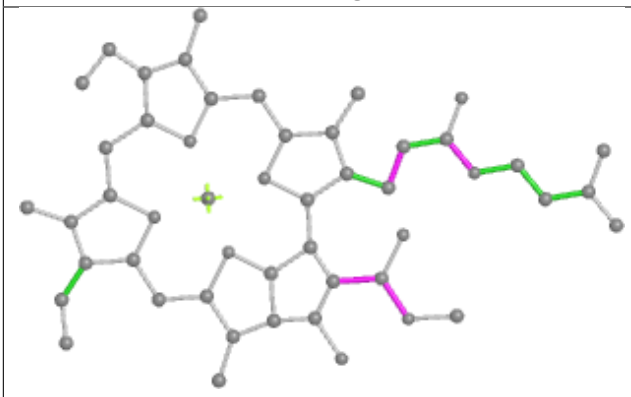
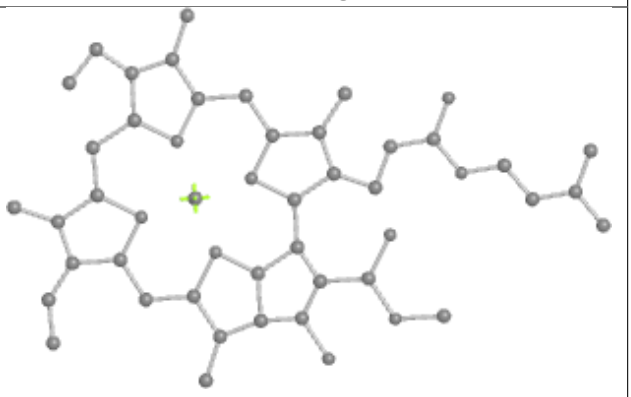


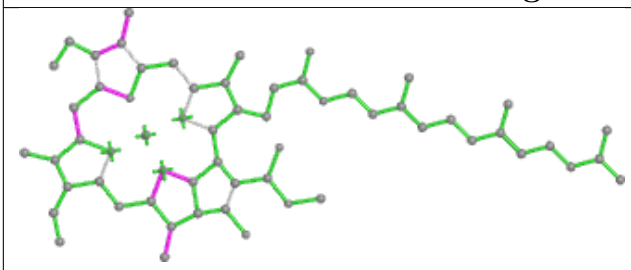
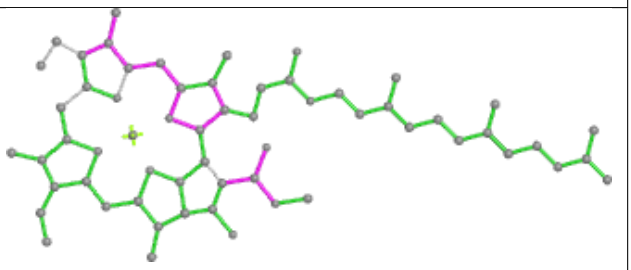
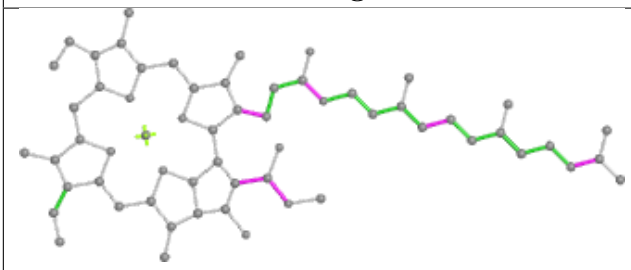
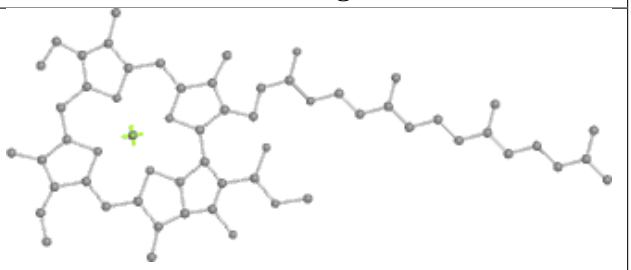
Ligand LHG r 613



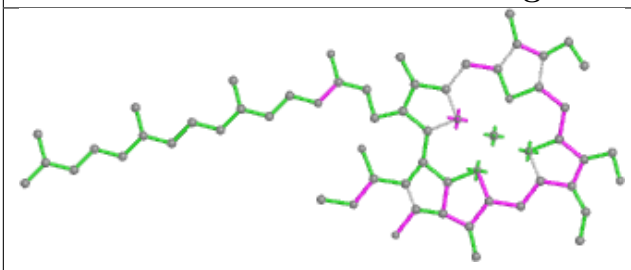
Ligand CLA s 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL R 317



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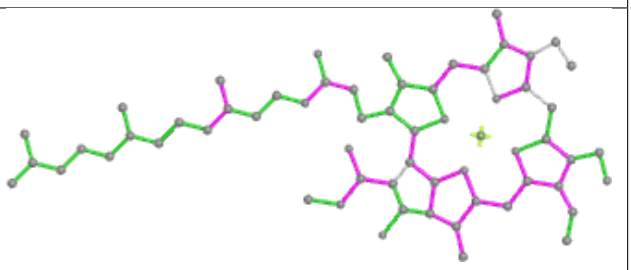

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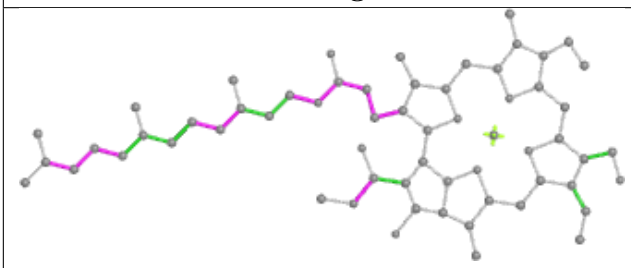

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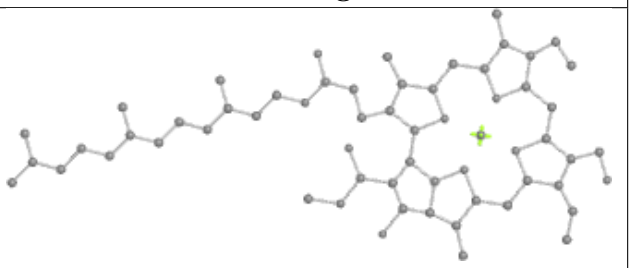
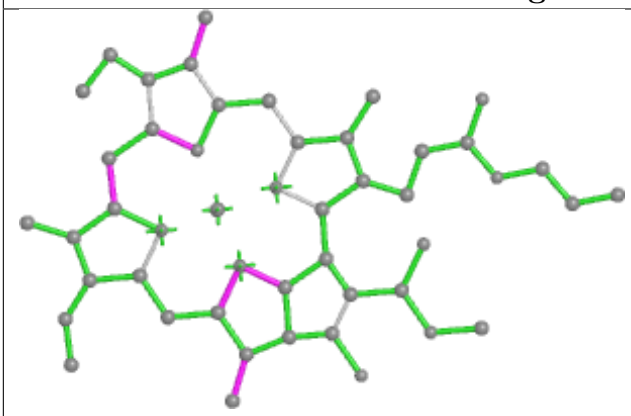


Rings

Ligand CLA 2 308



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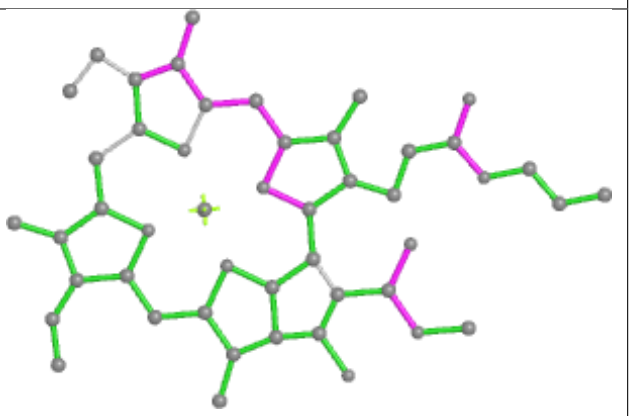
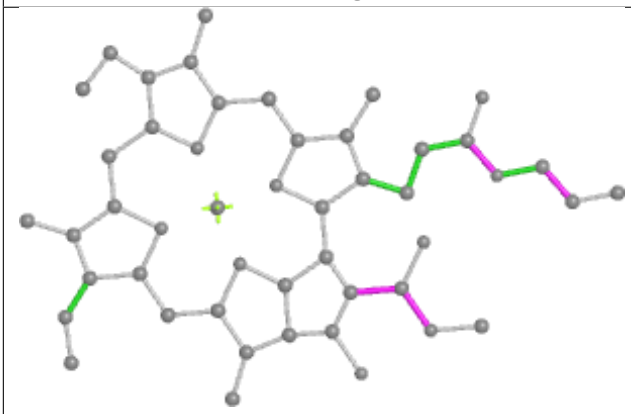


Bond angles



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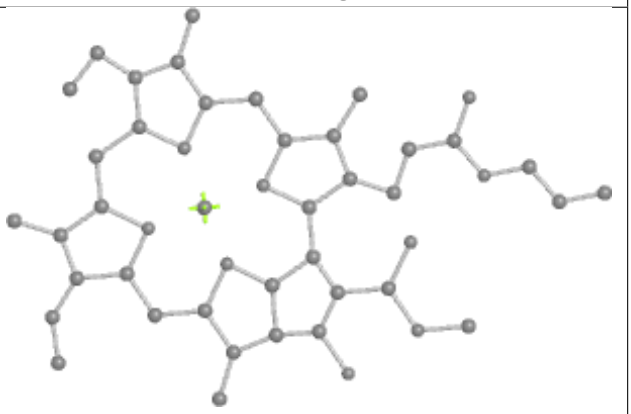
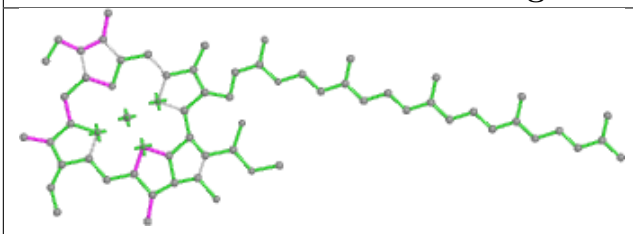


Rings

Ligand CLA b 607



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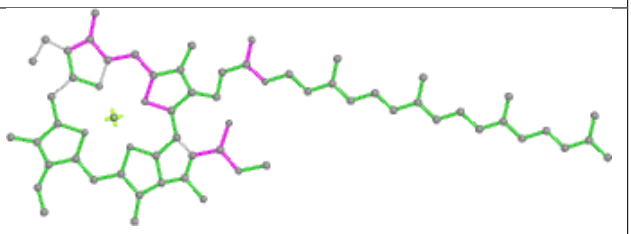
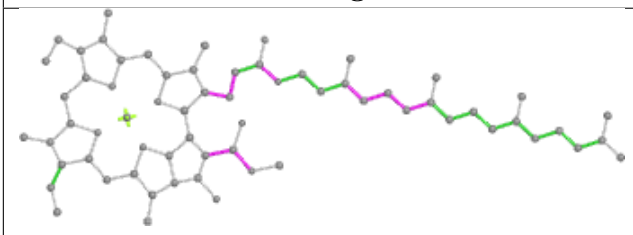


Bond angles



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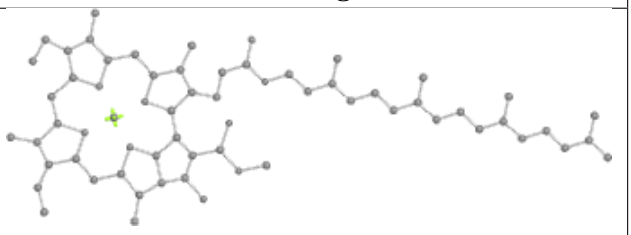
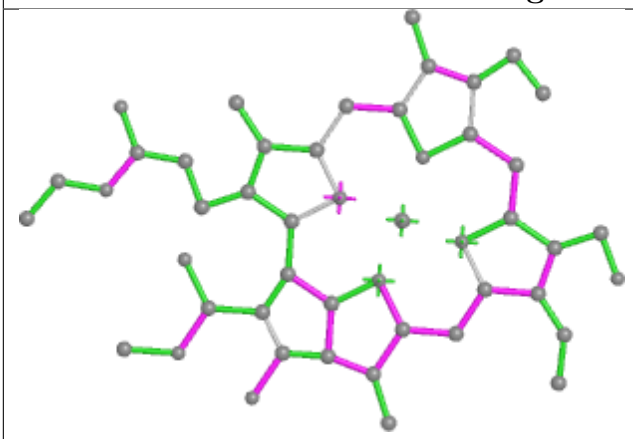


Rings

Ligand CHL n 314



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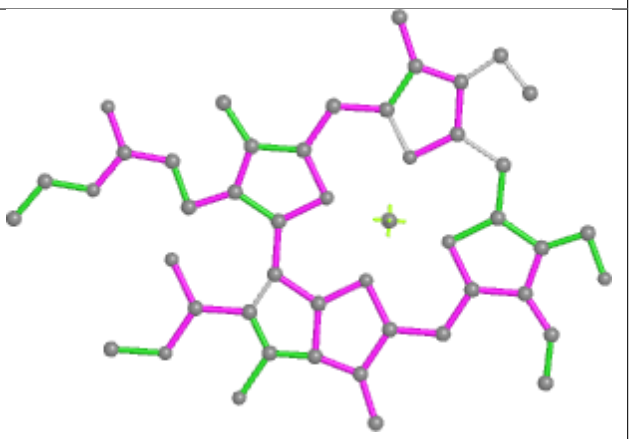

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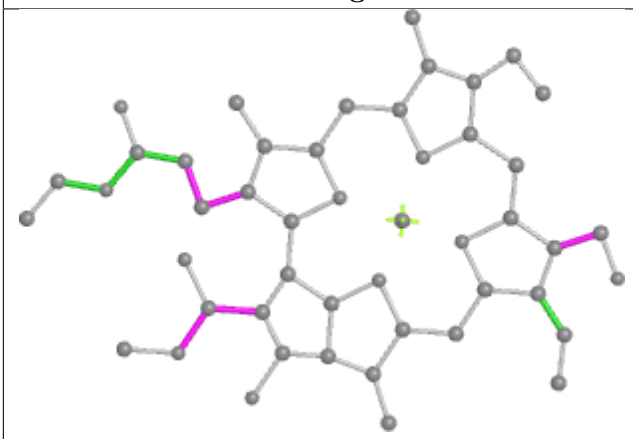

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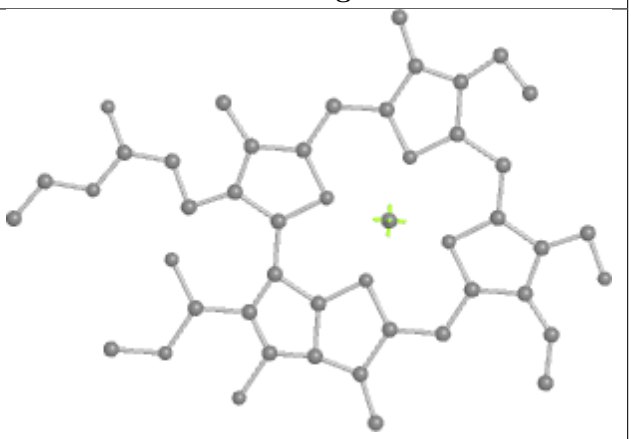
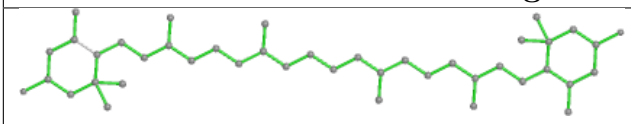
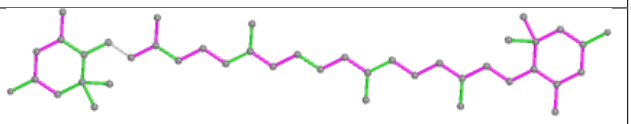


Rings

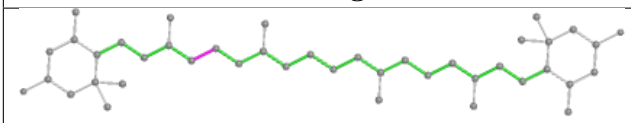
Ligand LUT N 310



Bond lengths



Bond angles



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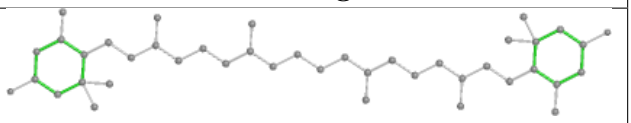
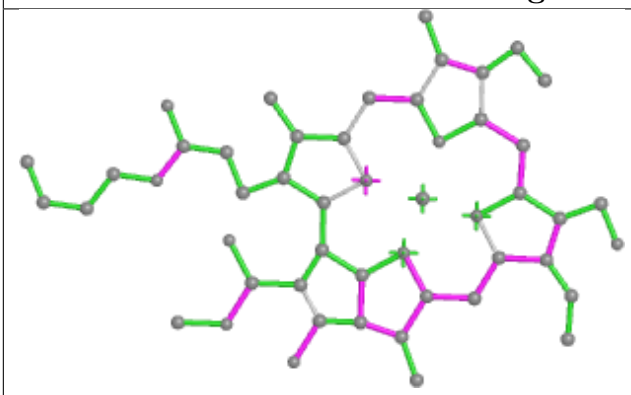


Rings

Ligand CHL 6 314



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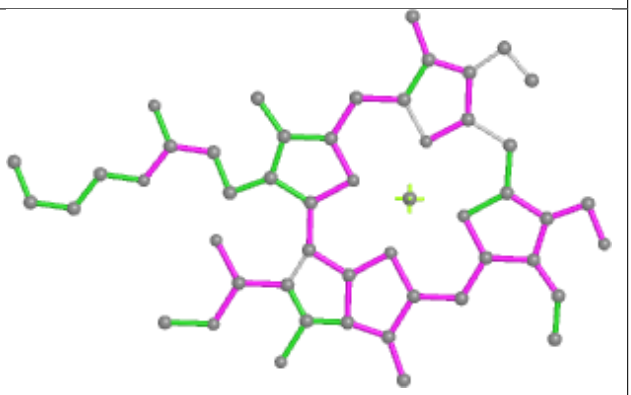

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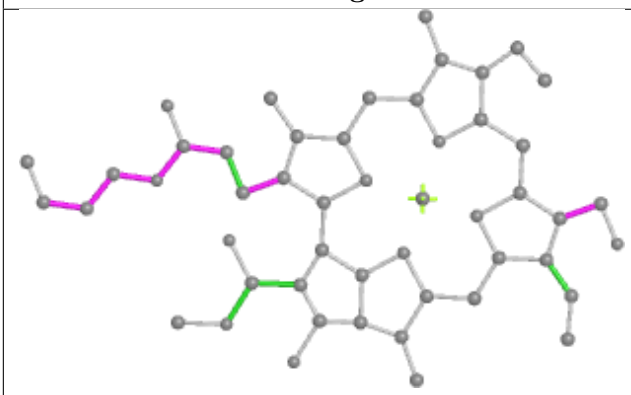

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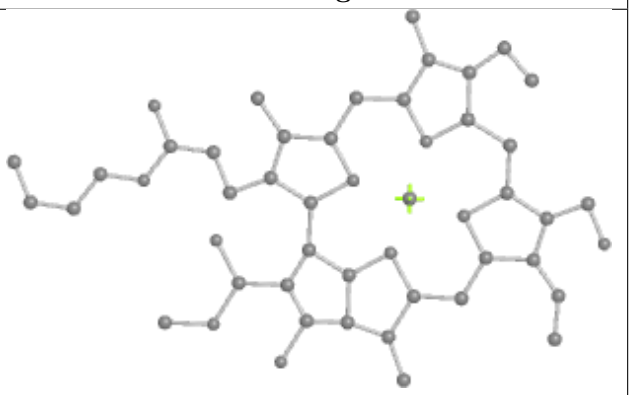
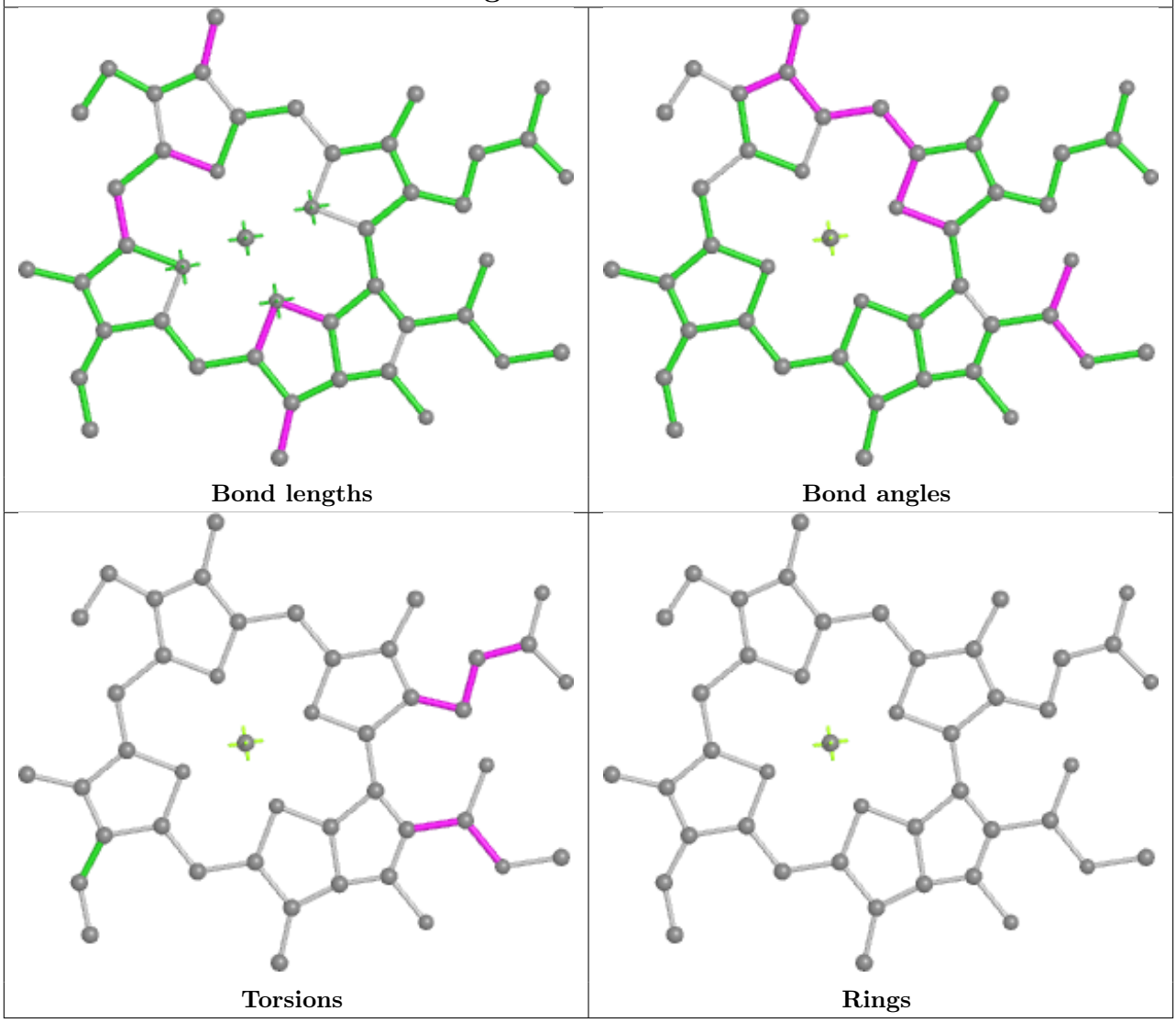
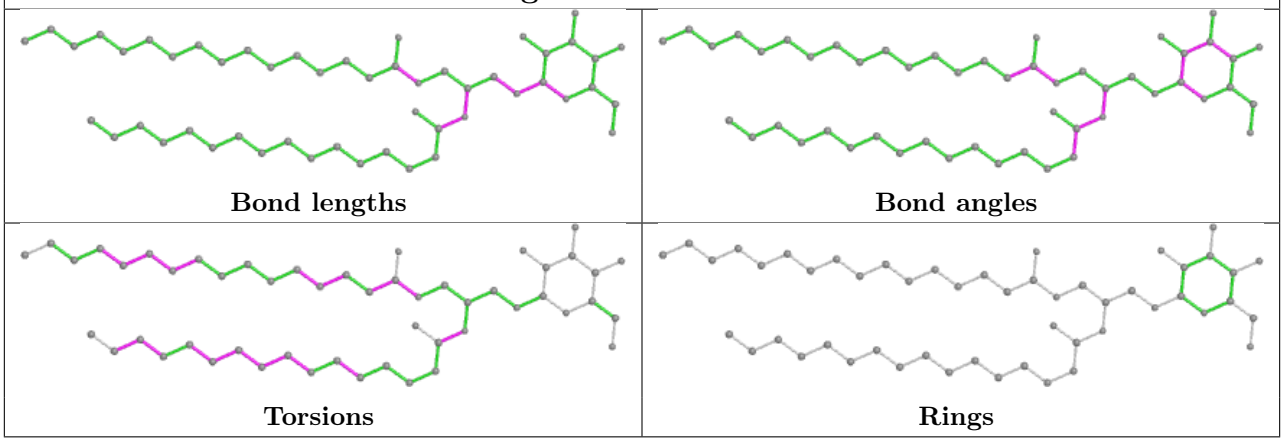


Rings

Ligand CLA S 304



Ligand LMG B 621



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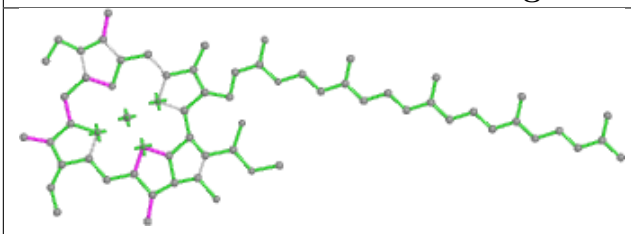
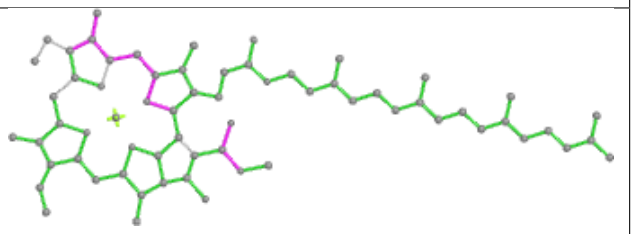
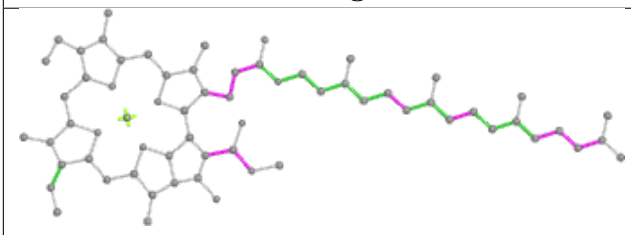
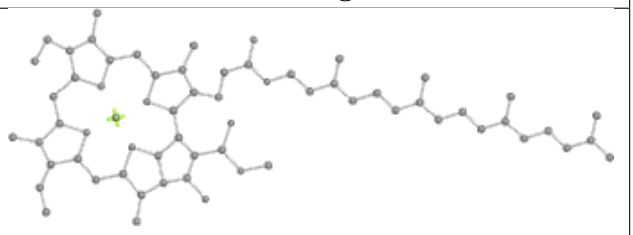
 Bond lengths	 Bond angles
 Torsions	 Rings

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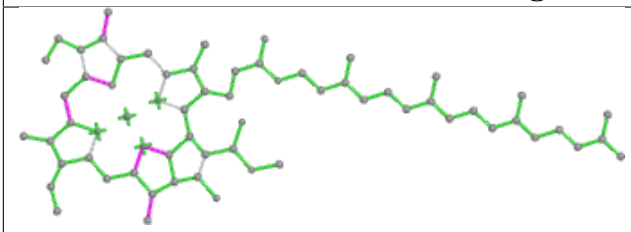
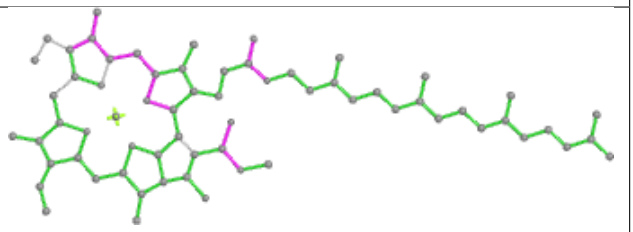
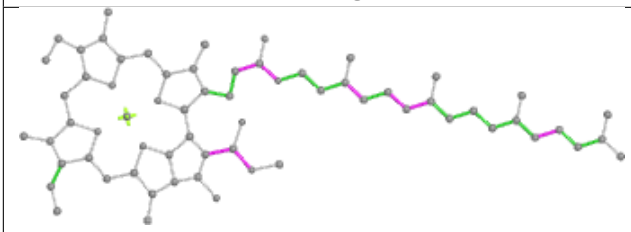
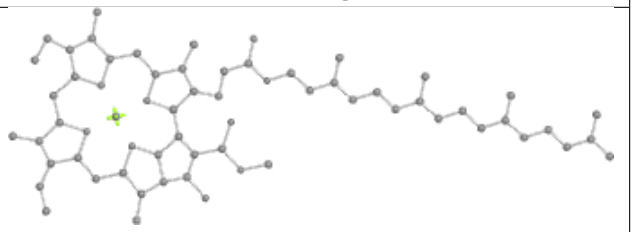
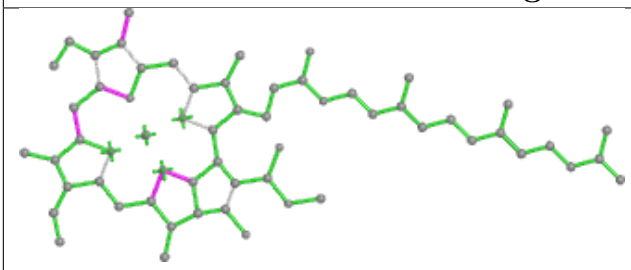
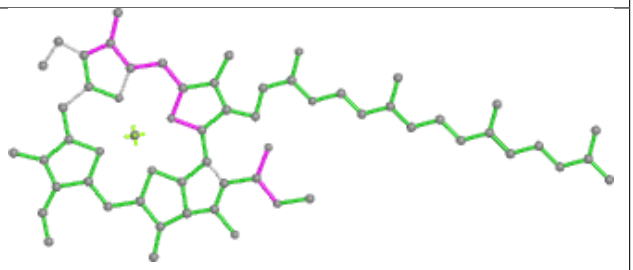
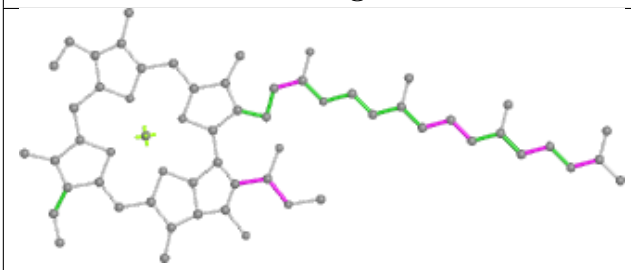
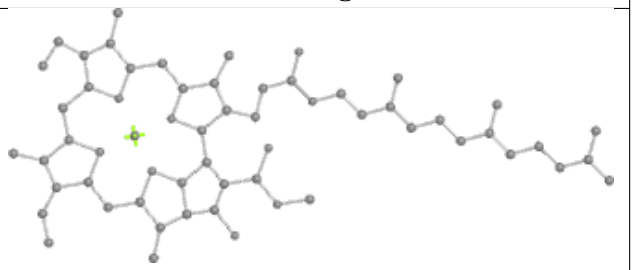
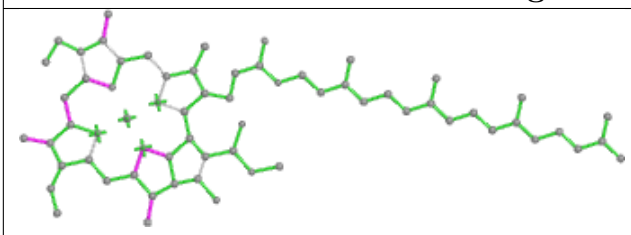
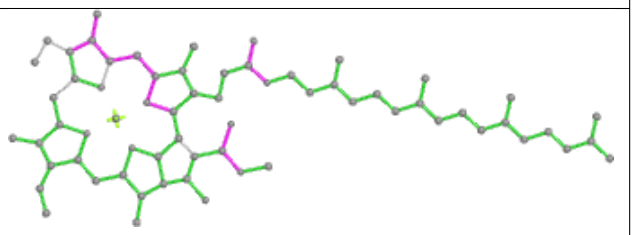
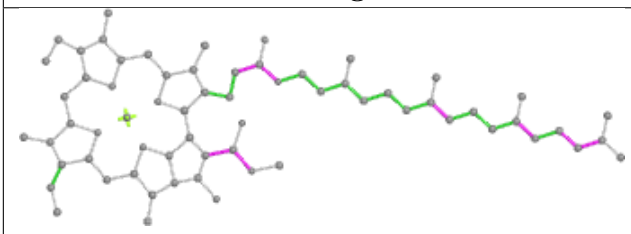
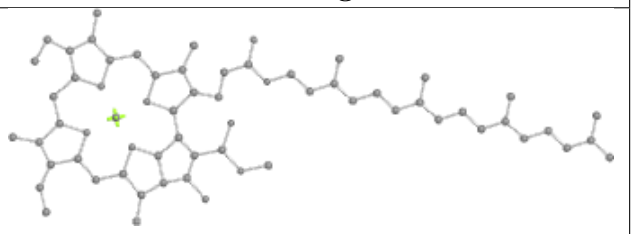
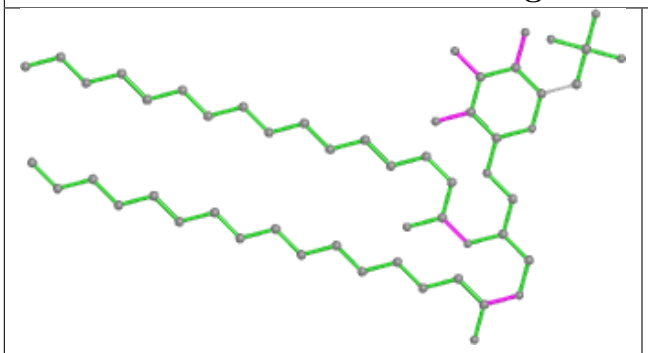
 Bond lengths	 Bond angles
 Torsions	 Rings

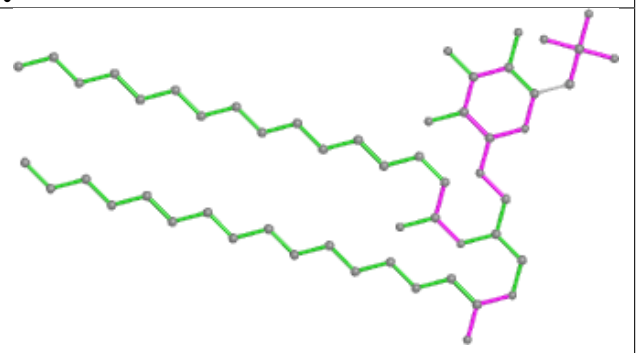
Ligand CLA R 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

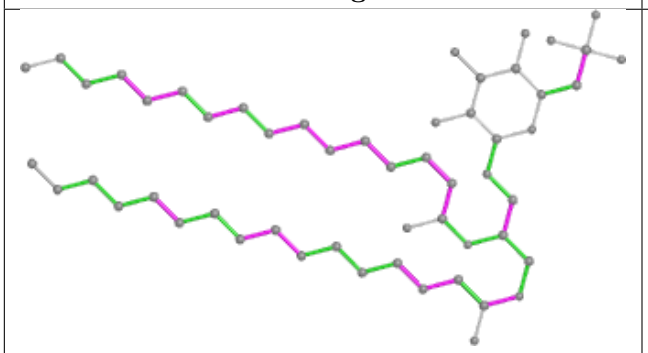
Ligand SQD A 412



Bond lengths



Bond angles



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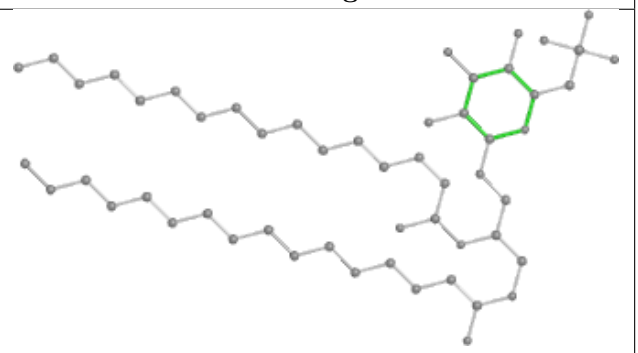
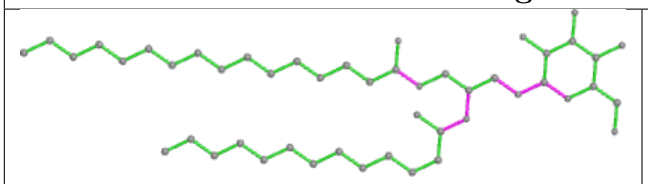
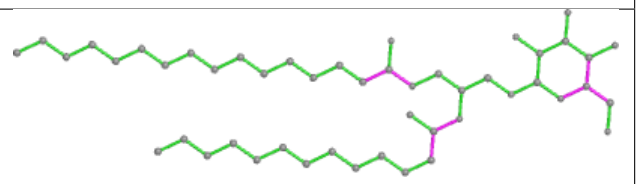


Rings

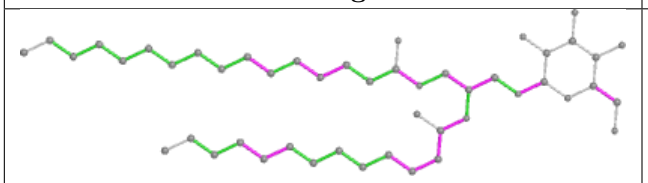
Ligand LMG W 201



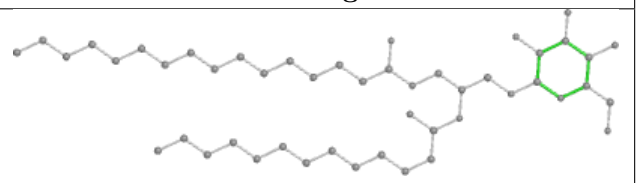
Bond lengths



Bond angles

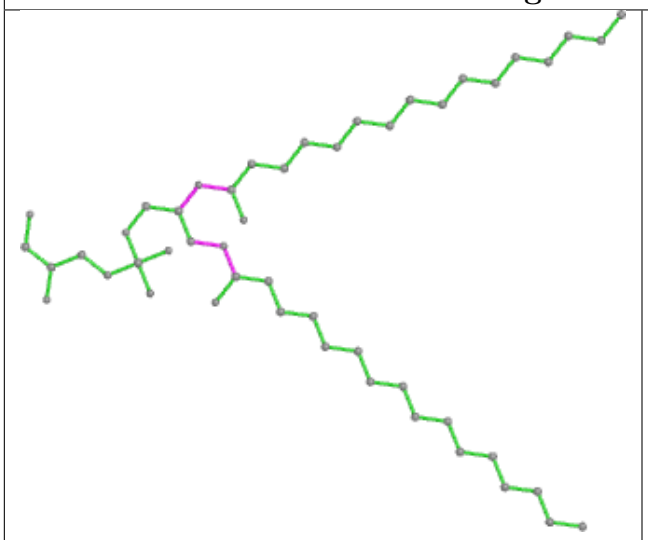


Torsions

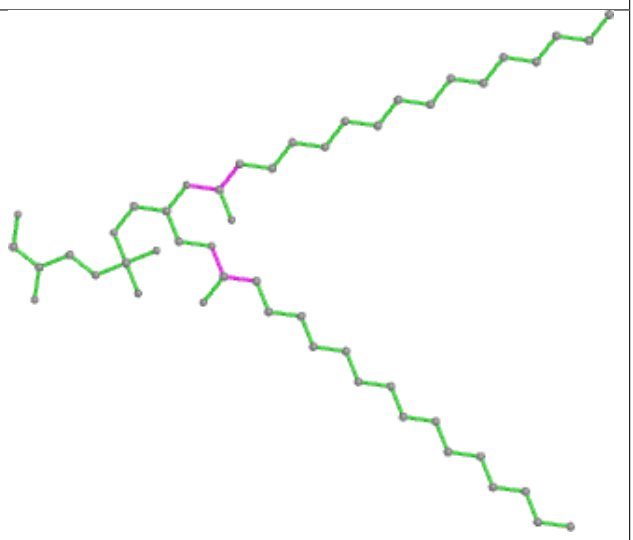


Rings

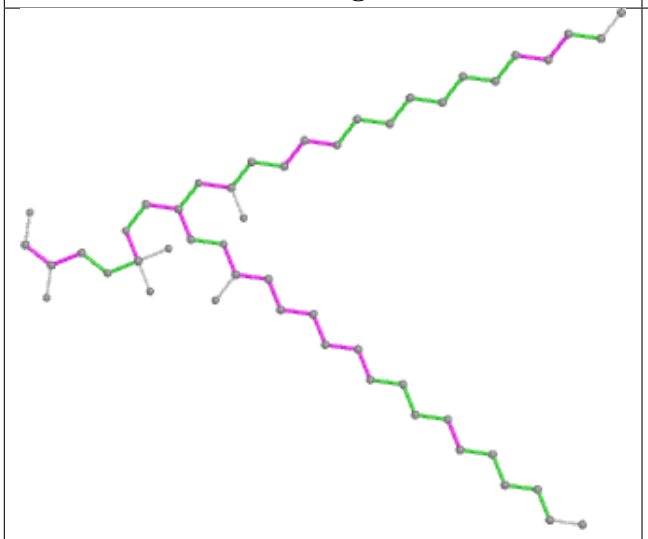
Ligand LHG P 313



Bond lengths



Bond angles



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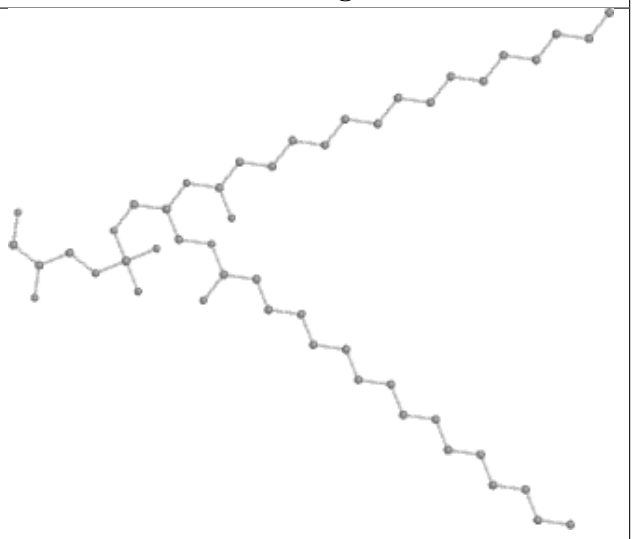
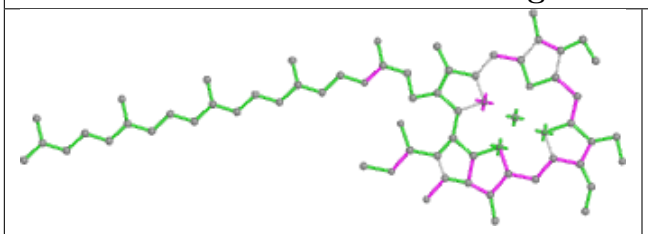
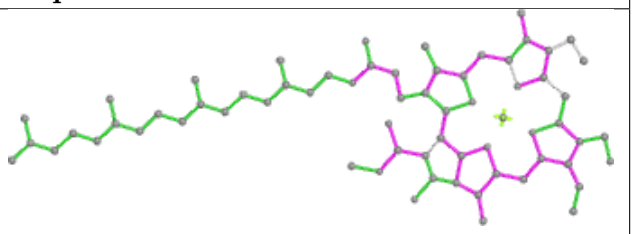


Rings

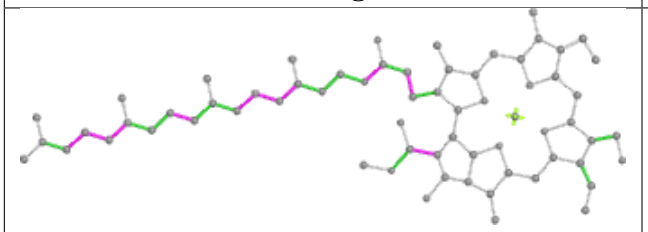
Ligand CHL p 317



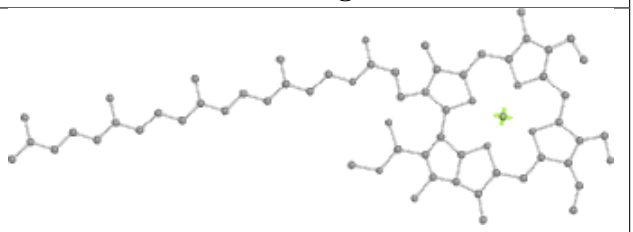
Bond lengths



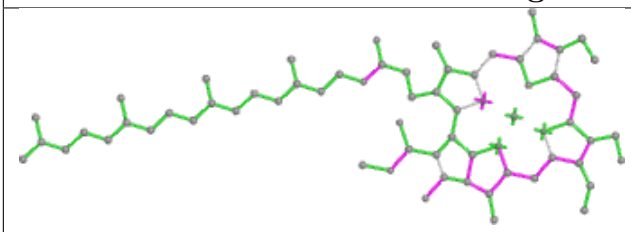
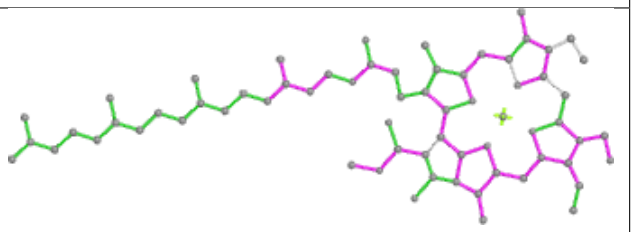
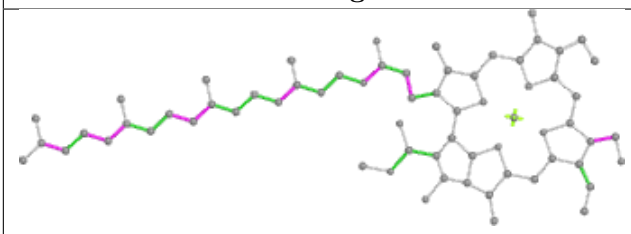
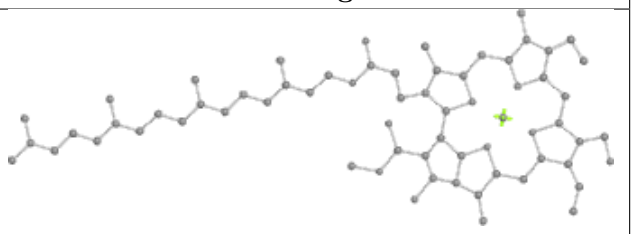
Bond angles

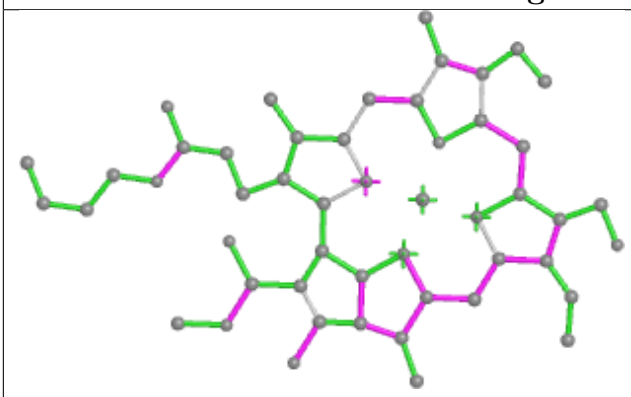
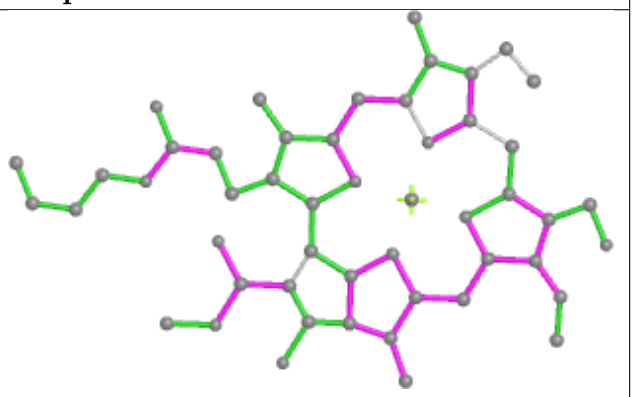
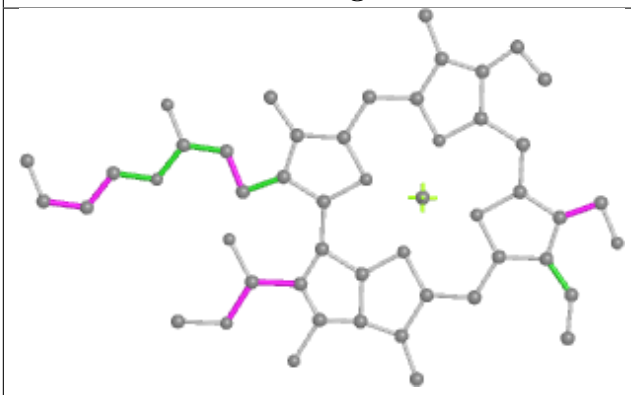
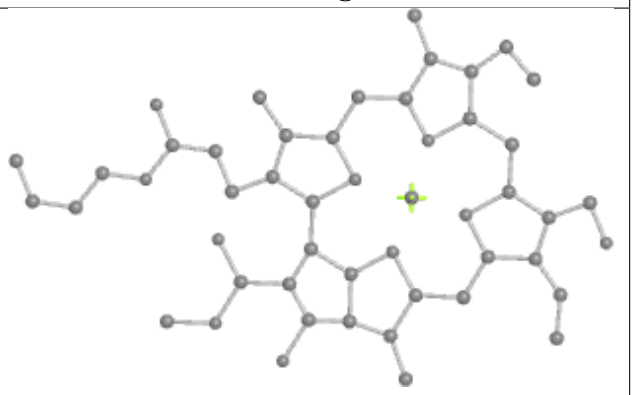


Torsions

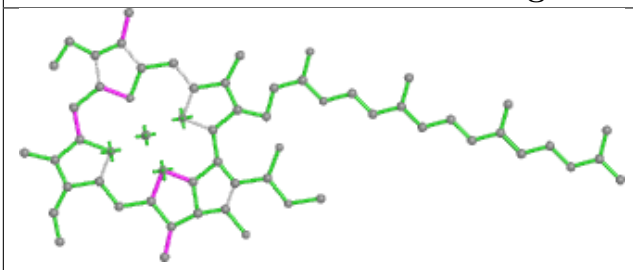


Rings

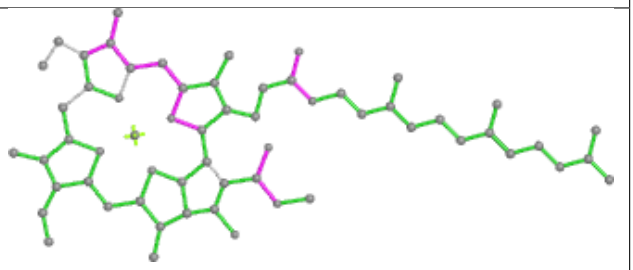
Ligand CHL v 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL q 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

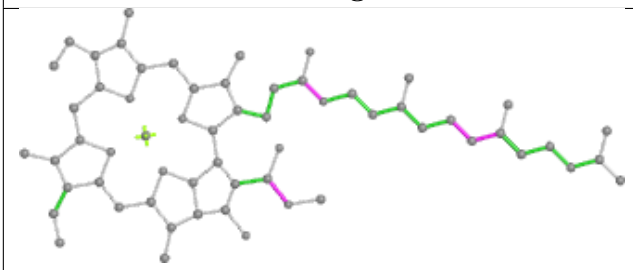
Ligand CLA v 305



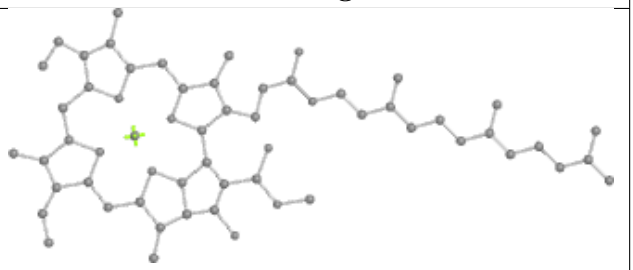
Bond lengths



Bond angles

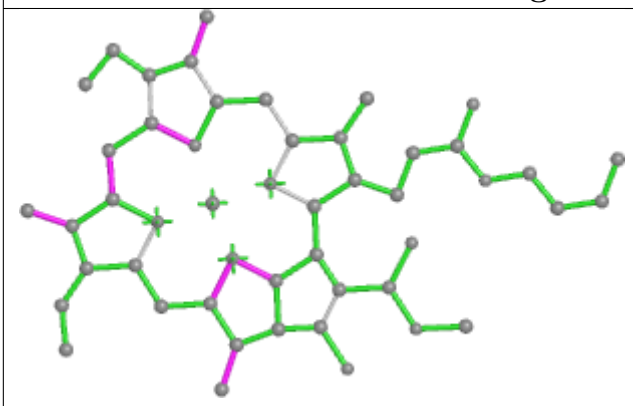


Torsions

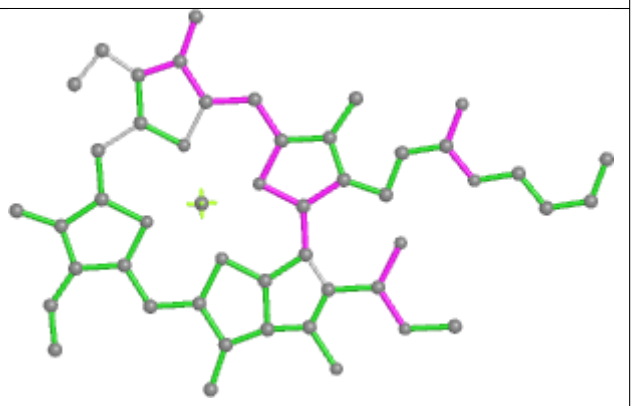


Rings

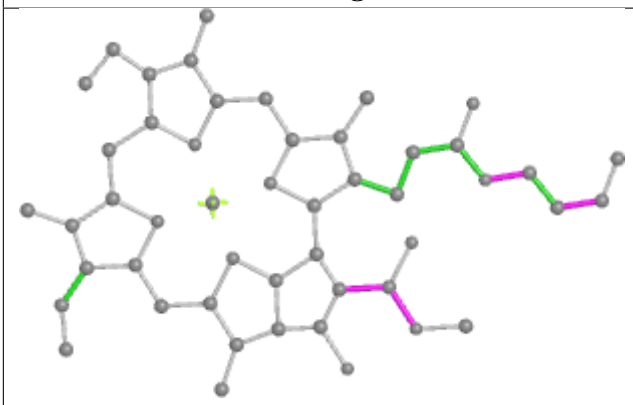
Ligand CLA s 307



Bond lengths



Bond angles



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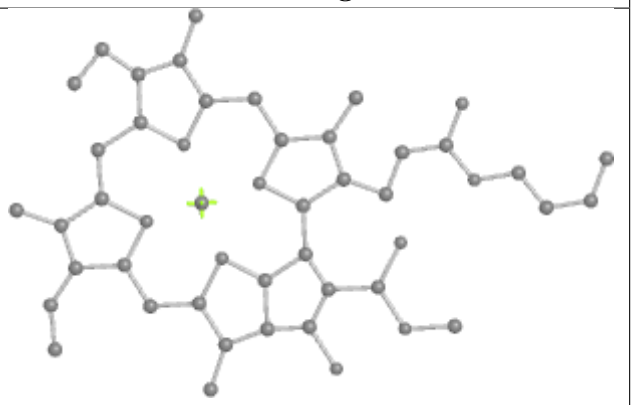
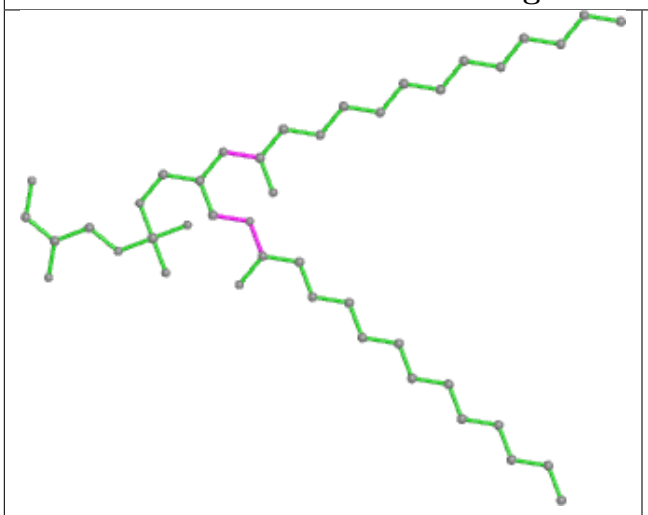


Rings

Ligand LHG A 413



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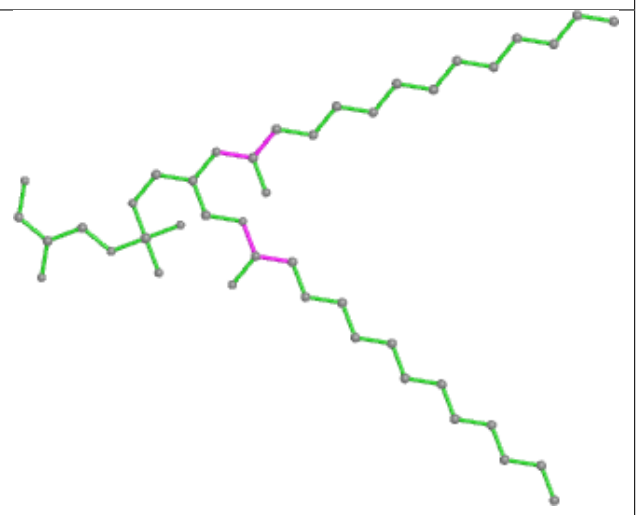
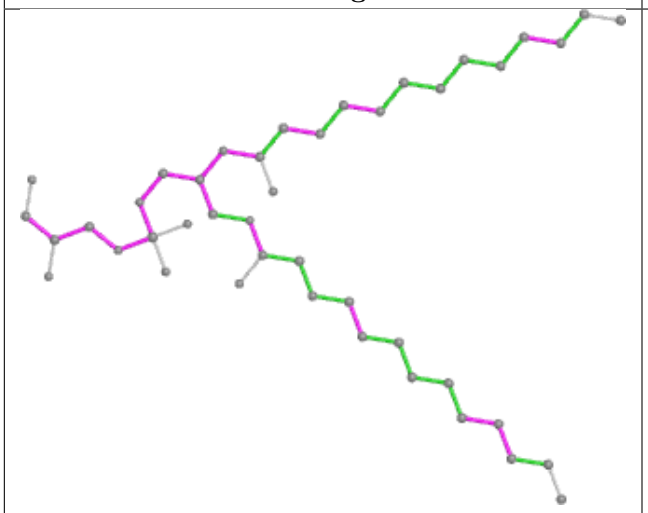


Bond angles



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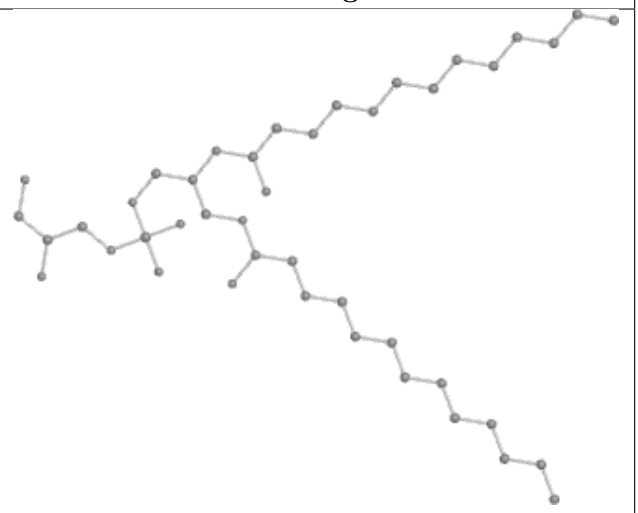
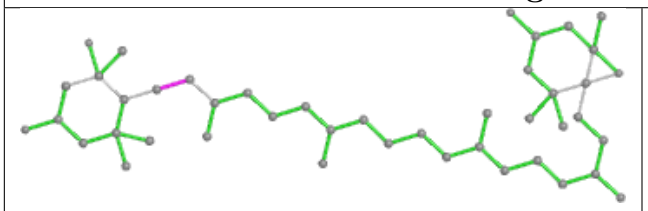


Rings

Ligand NEX S 317



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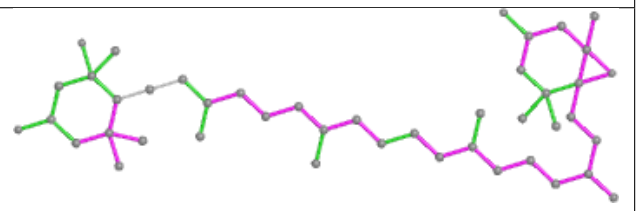
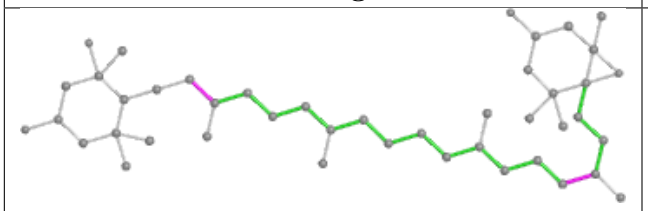


Bond angles



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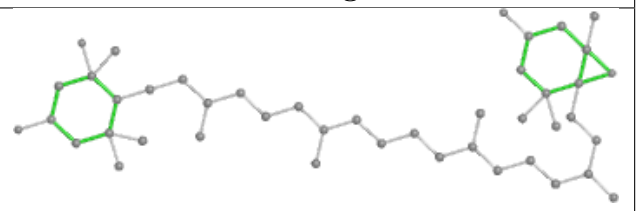
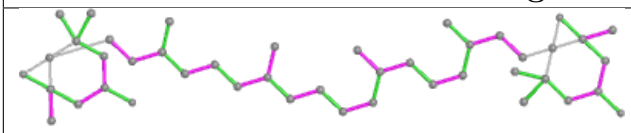
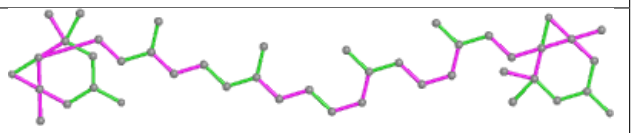


Rings

Ligand XAT 3 309



Bond lengths



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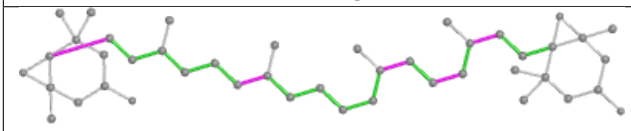

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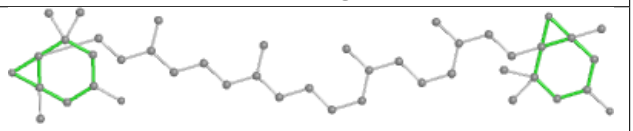
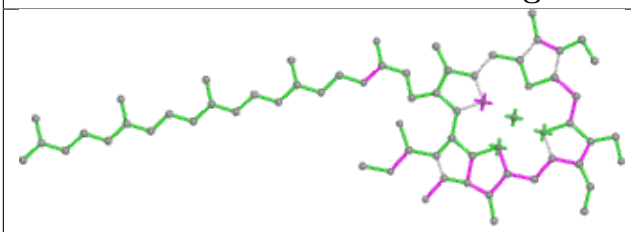


Rings

Ligand CHL V 317



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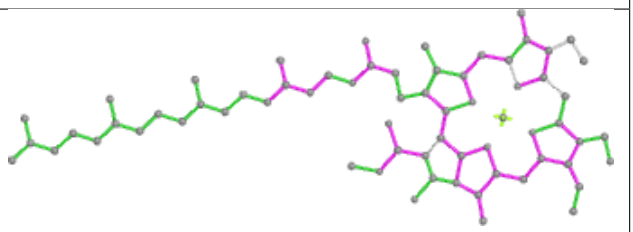
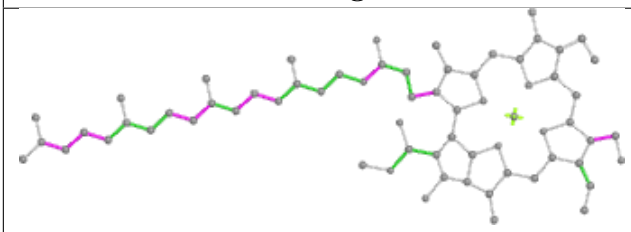


Bond angles



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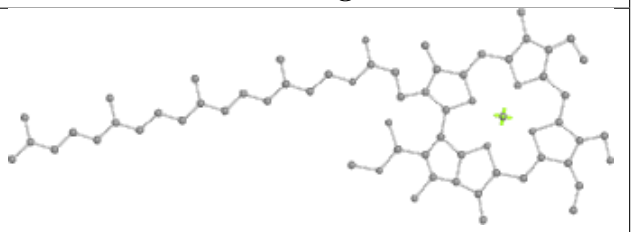
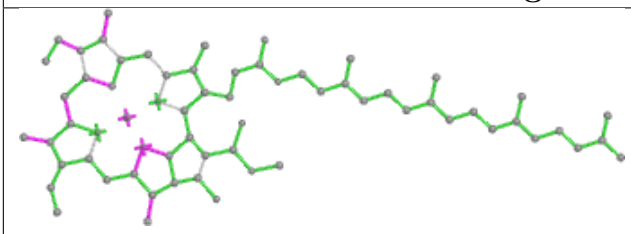
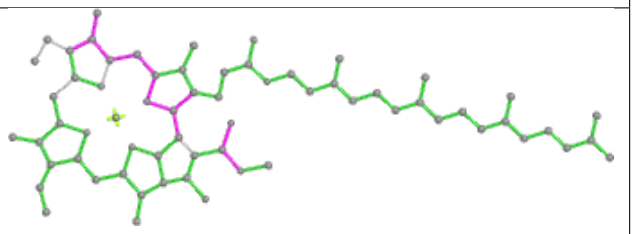


Rings

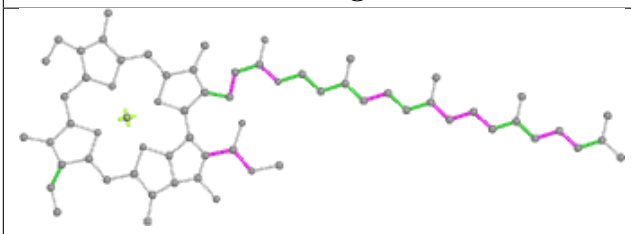
Ligand CLA B 614



Bond lengths



Bond angles



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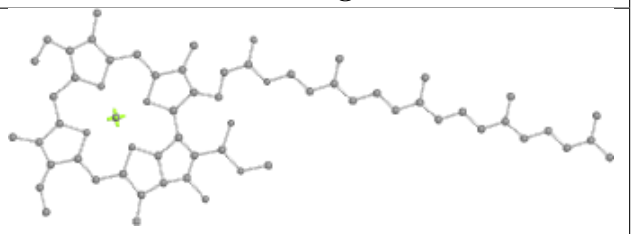
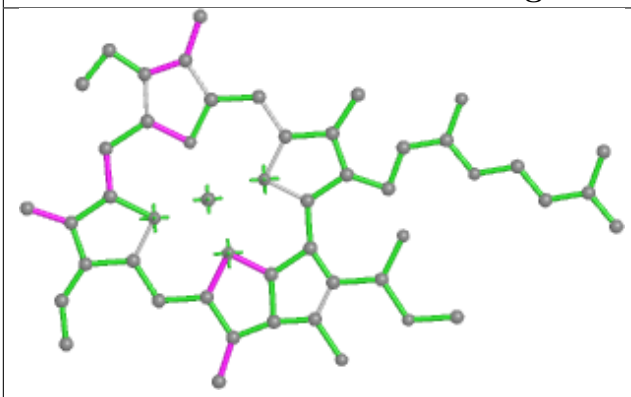


Rings

Ligand CLA P 304



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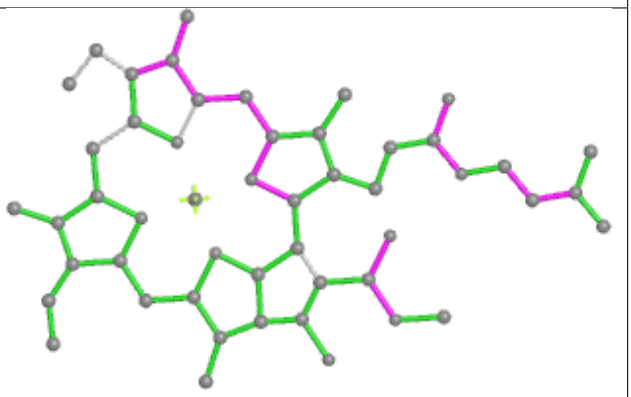
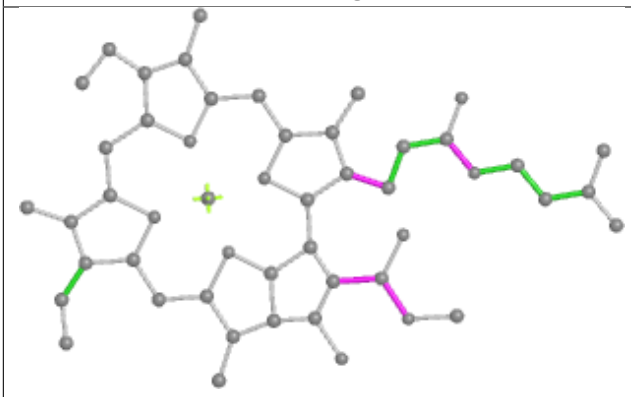


Bond angles



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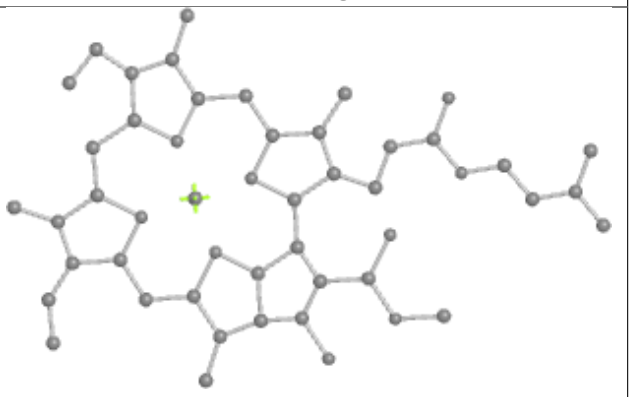
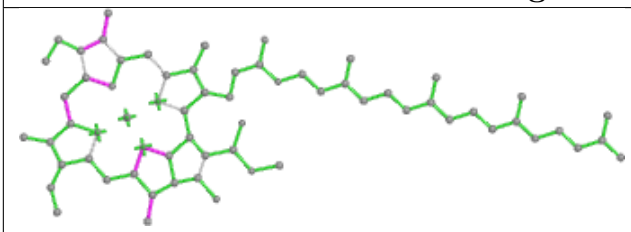


Rings

Ligand CLA 3 302



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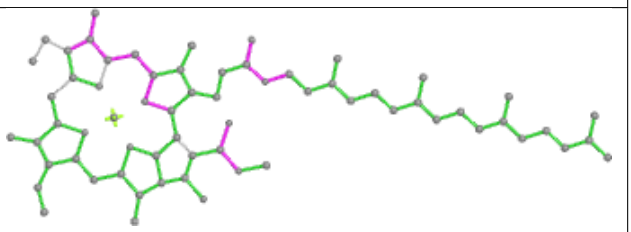
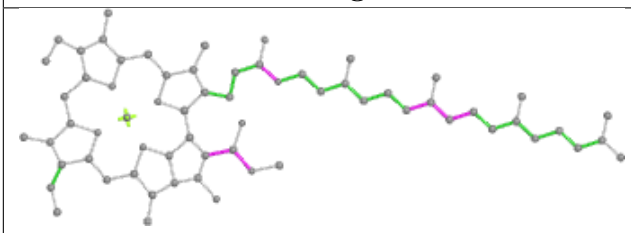


Bond angles



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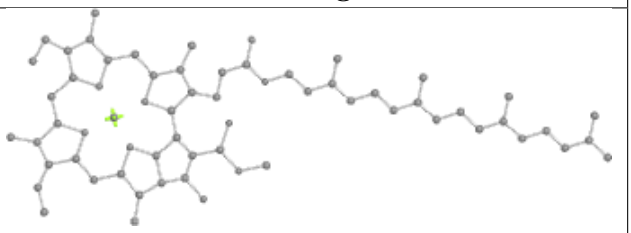
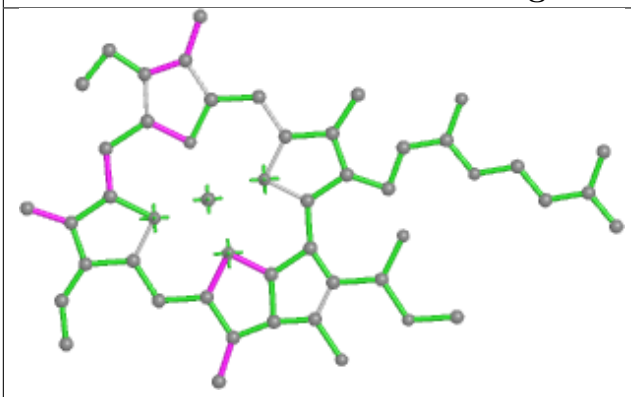
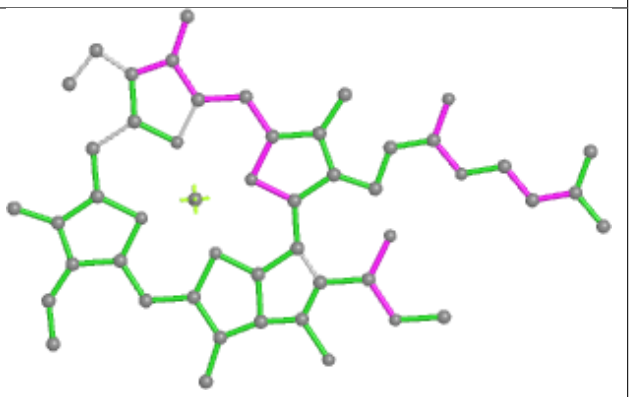


Rings

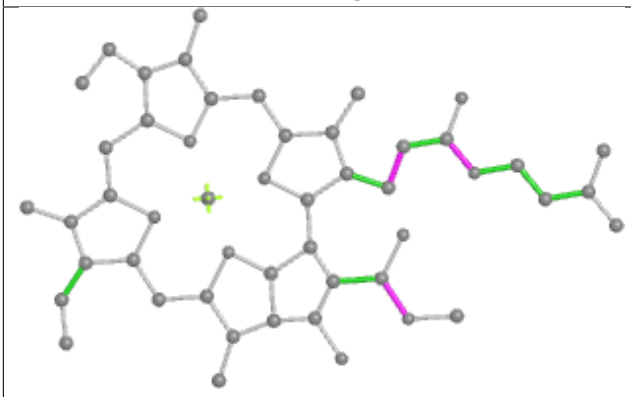
Ligand CLA 5 303



Bond lengths



Bond angles



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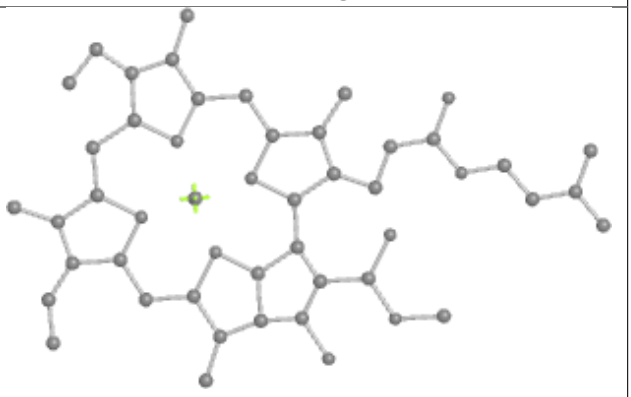
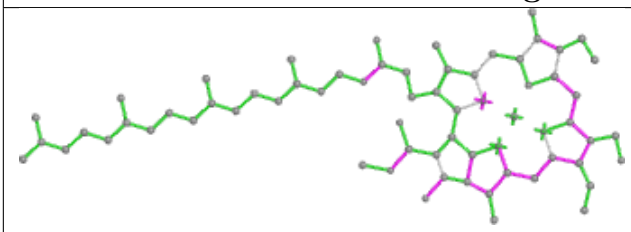
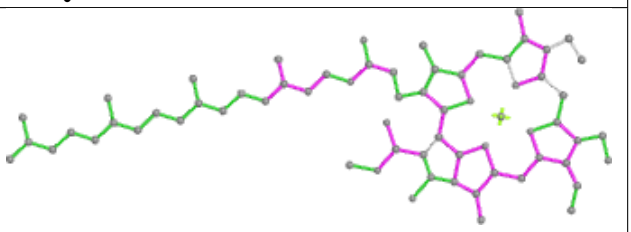


Rings

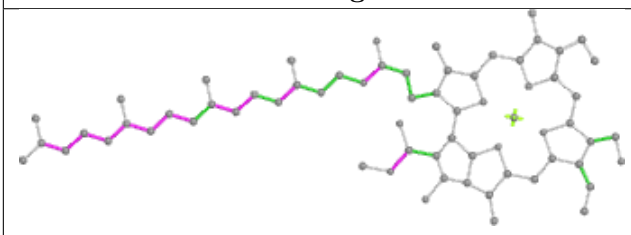
Ligand CHL Q 311



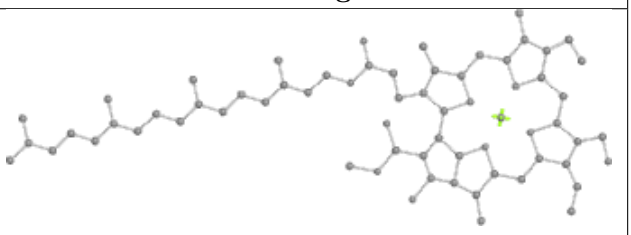
Bond lengths



Bond angles

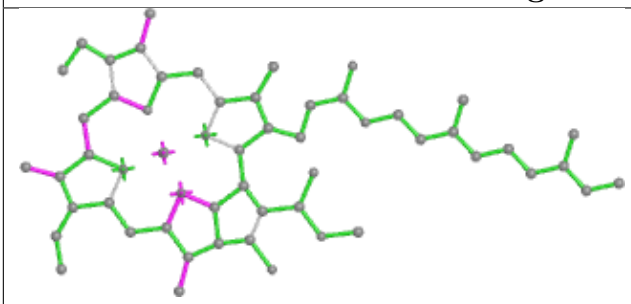


Torsions

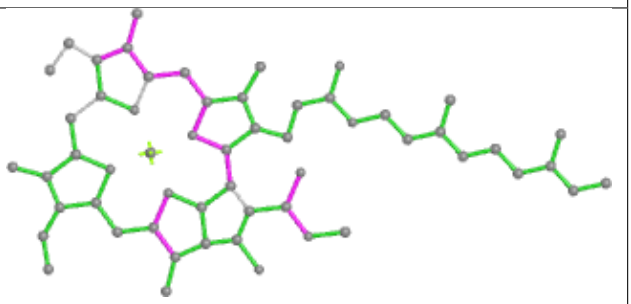


Rings

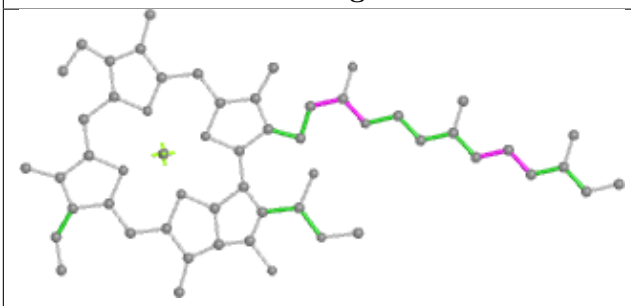
Ligand CLA S 306



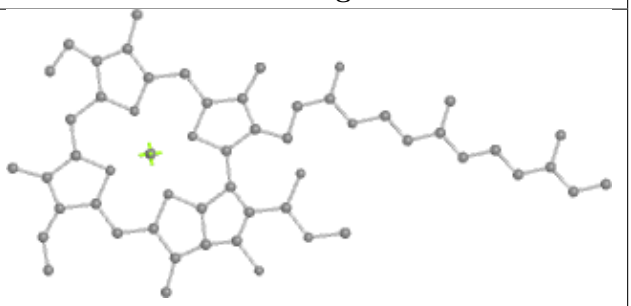
Bond lengths



Bond angles

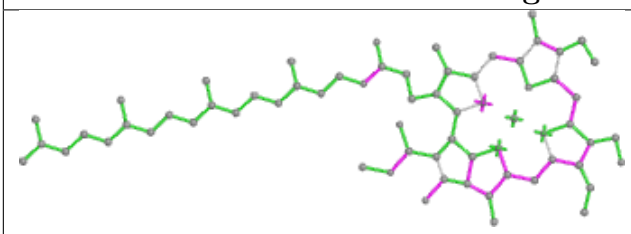


Torsions

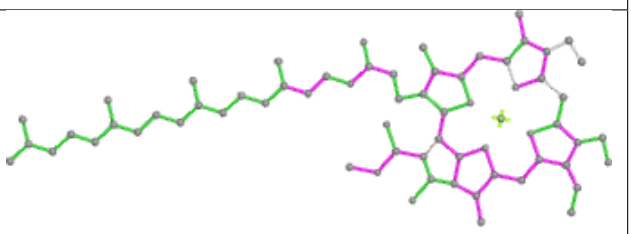


Rings

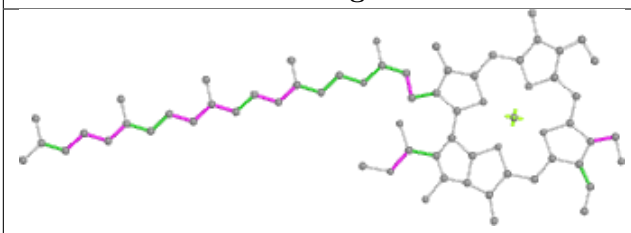
Ligand CHL G 314



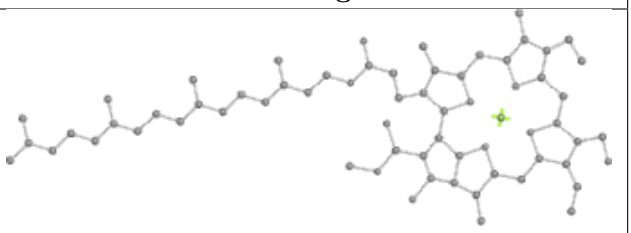
Bond lengths



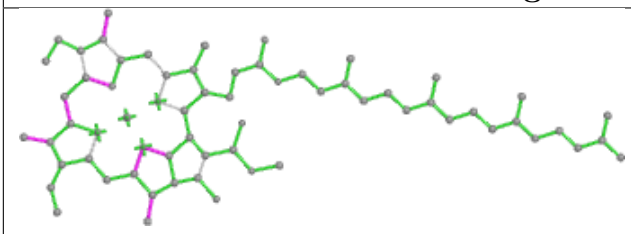
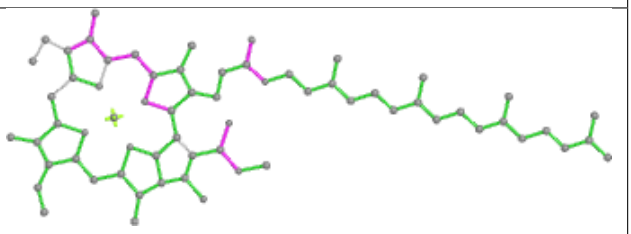
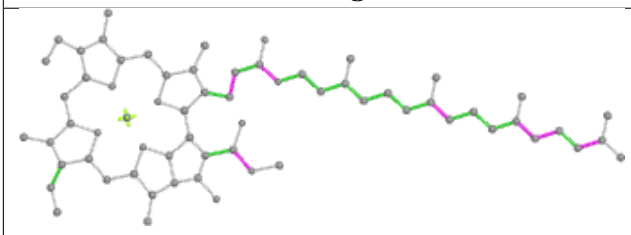
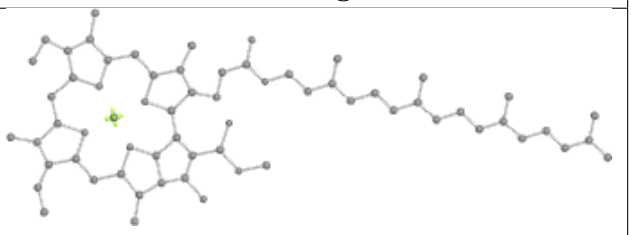
Bond angles

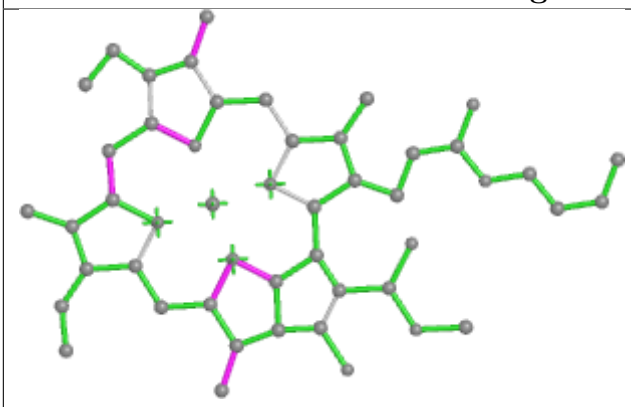
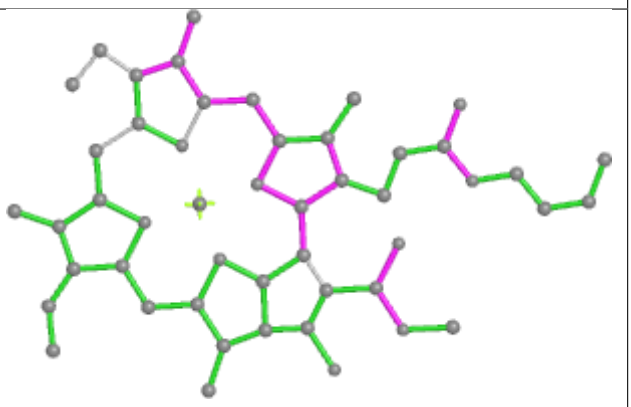
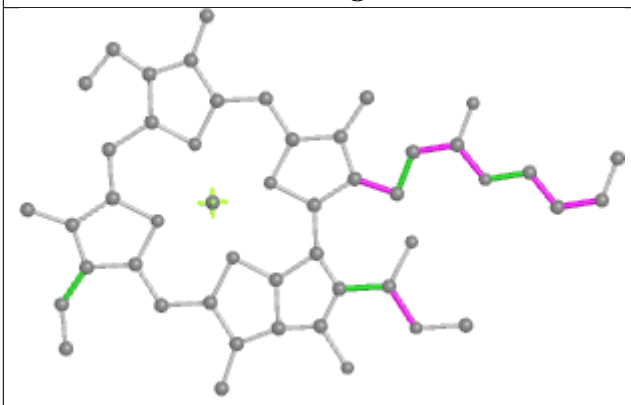
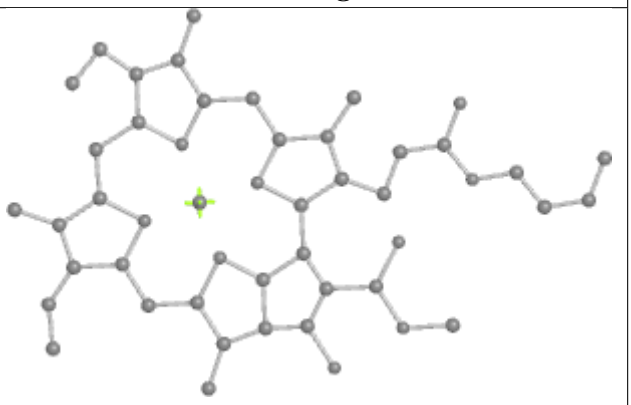


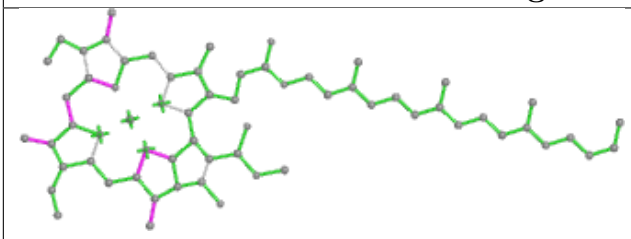
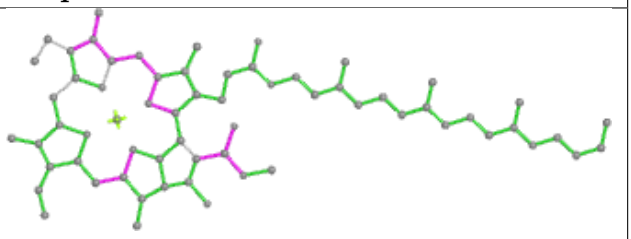
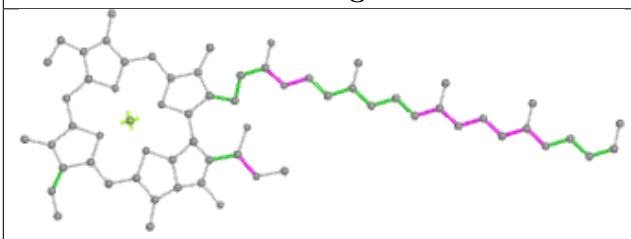
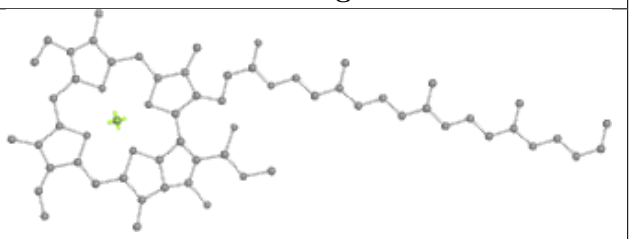
Torsions

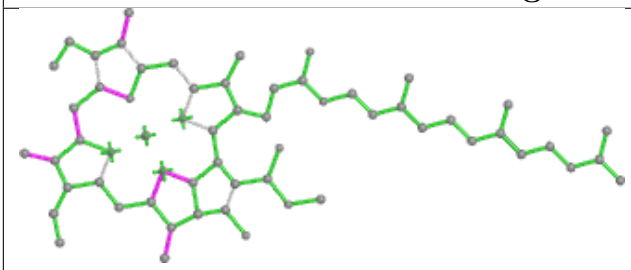
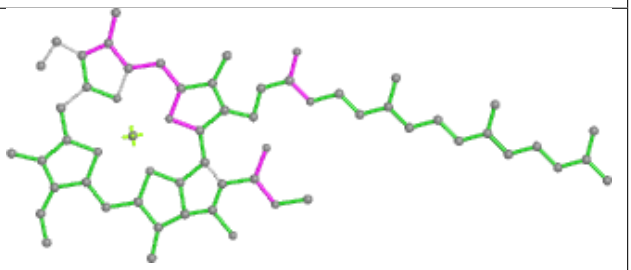
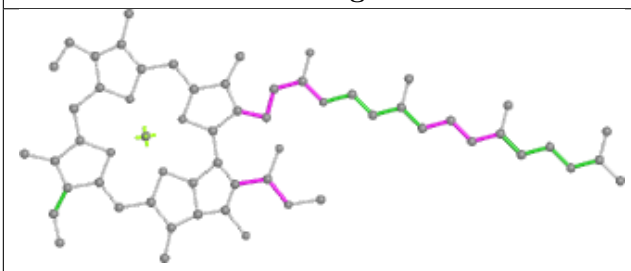
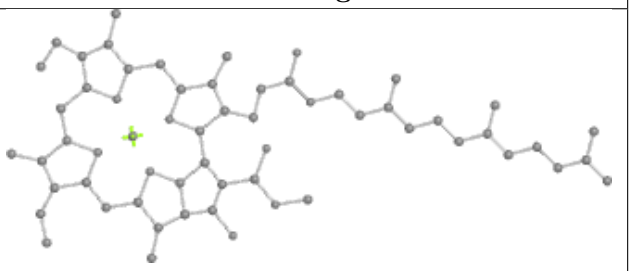


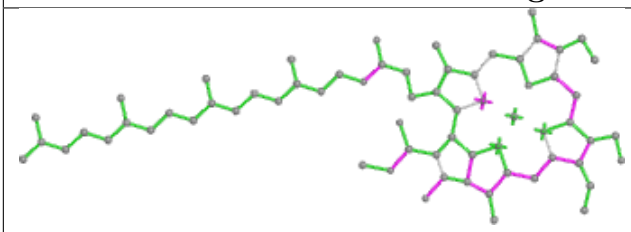
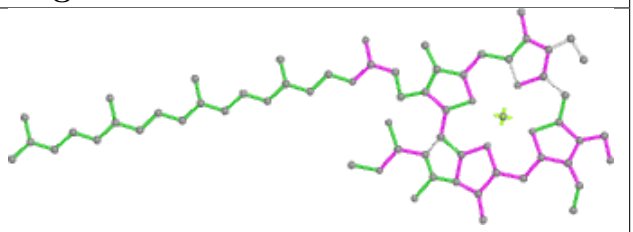
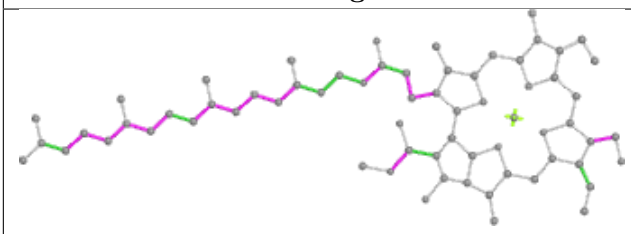
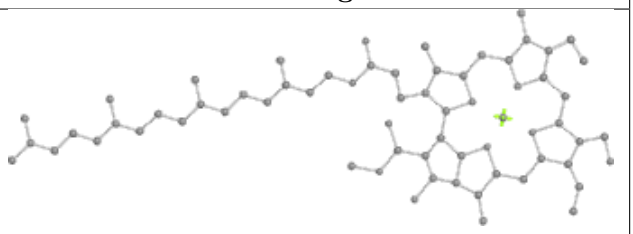
Rings

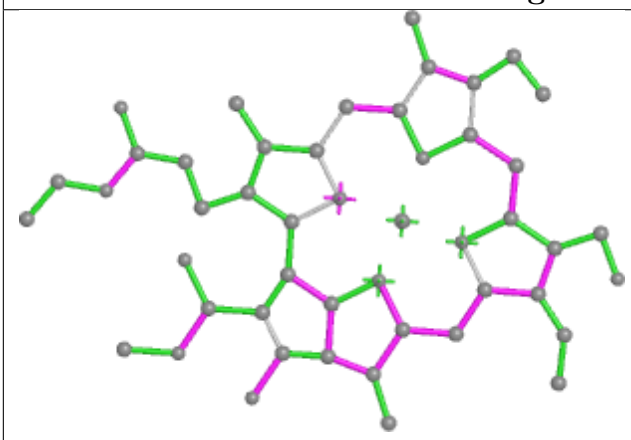
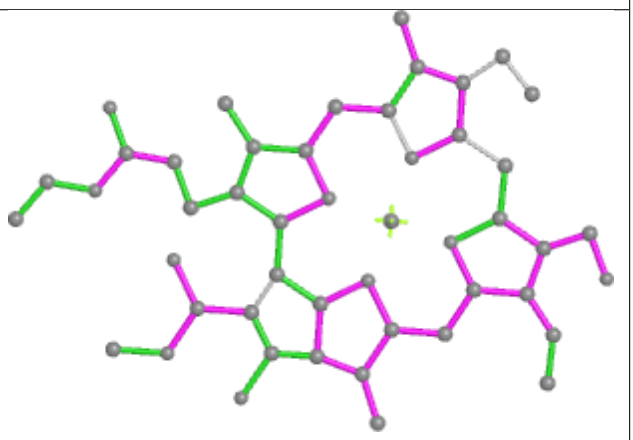
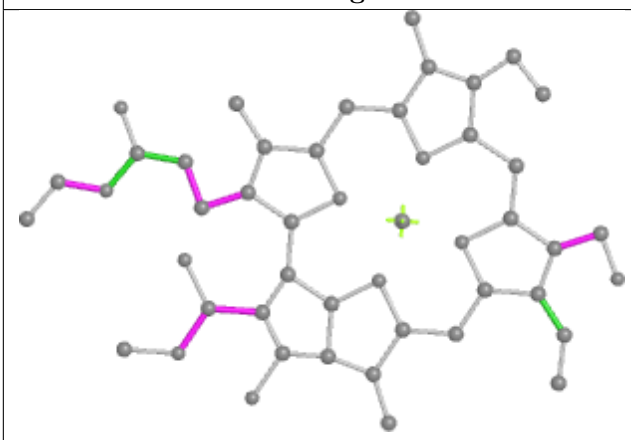
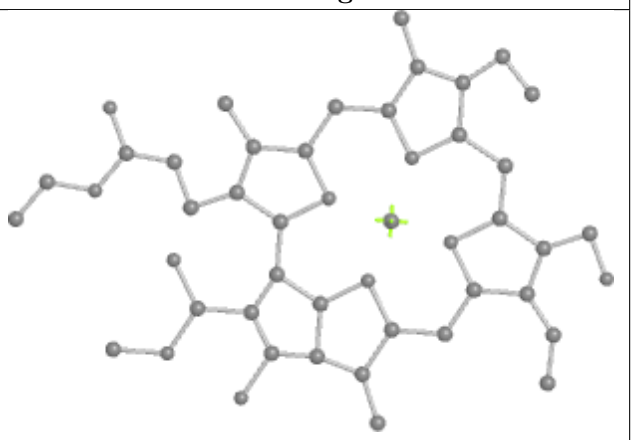
Ligand CLA V 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

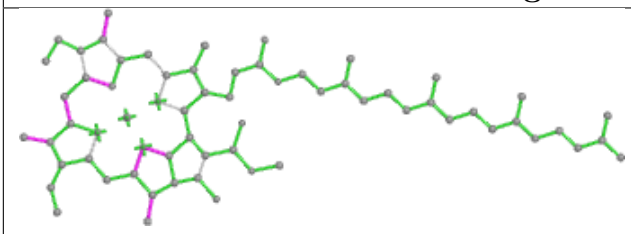
Ligand CLA q 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

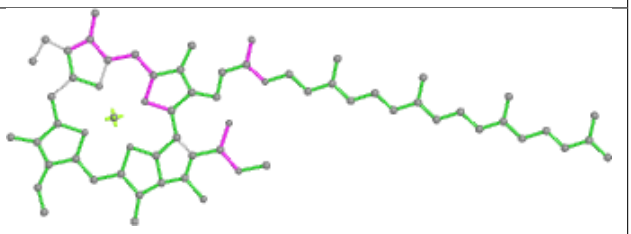
Ligand CHL g 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 5 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

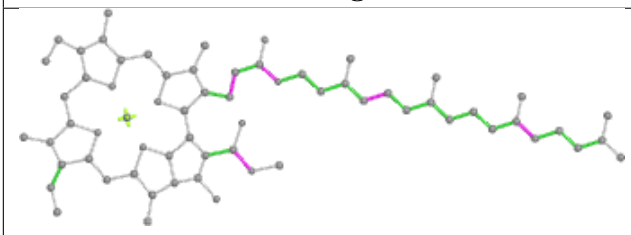
Ligand CLA V 307



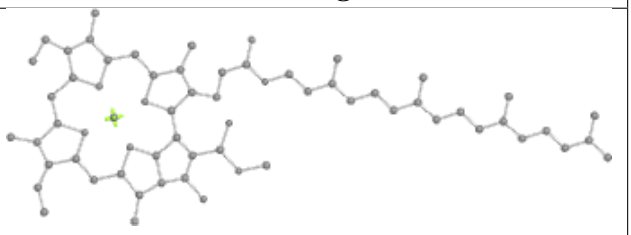
Bond lengths



Bond angles

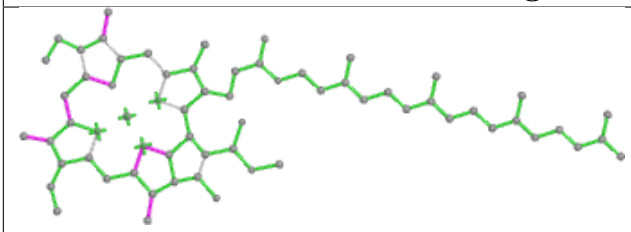


Torsions

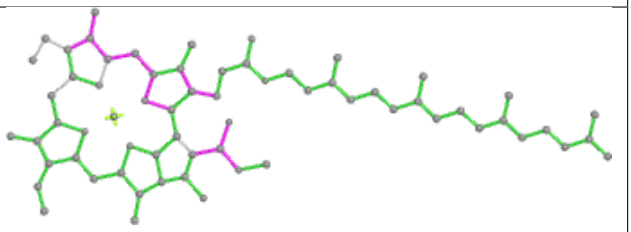


Rings

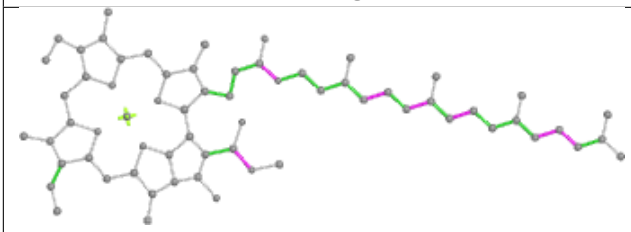
Ligand CLA X 202



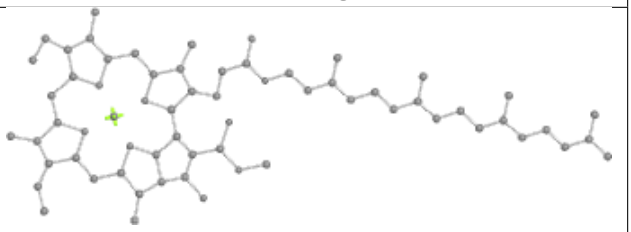
Bond lengths



Bond angles

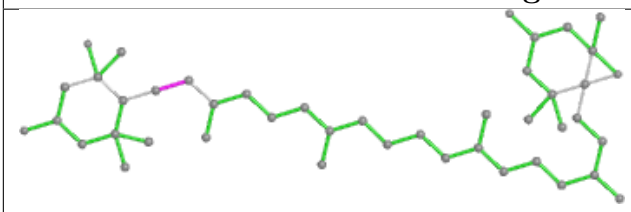


Torsions

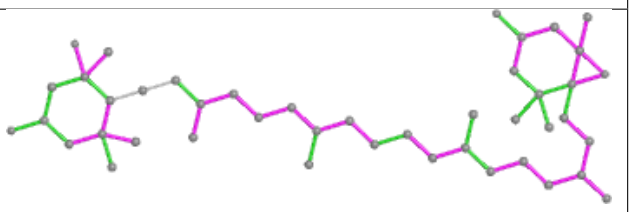


Rings

Ligand NEX P 301



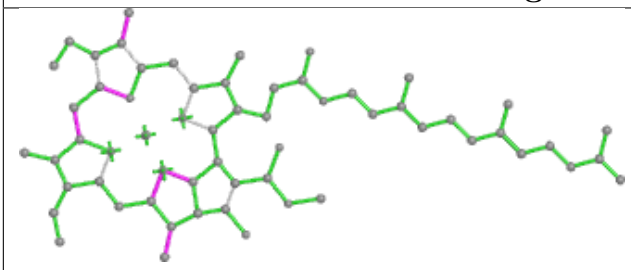
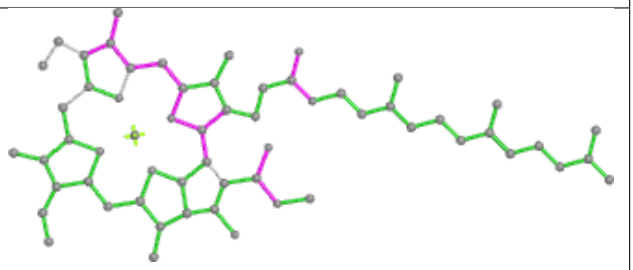
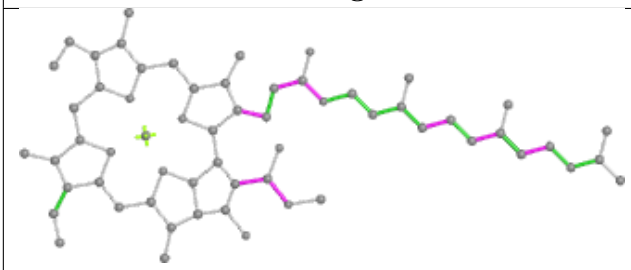
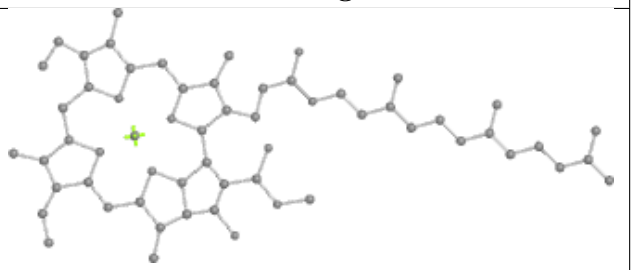
Bond lengths

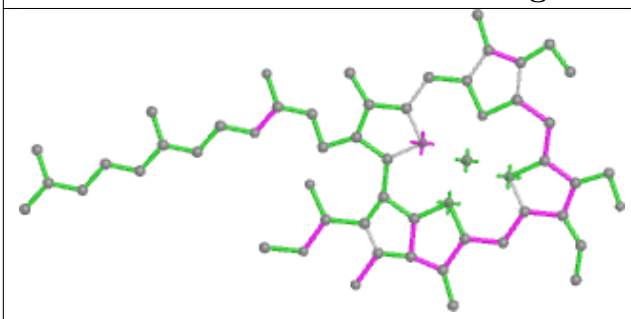
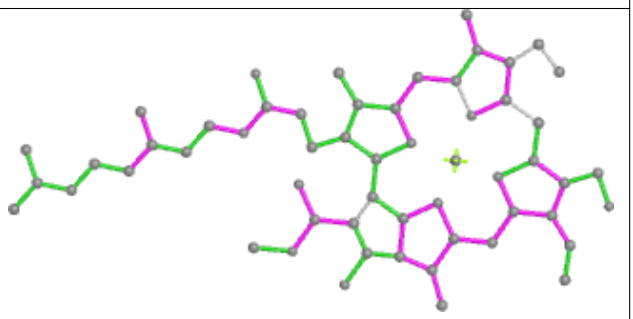
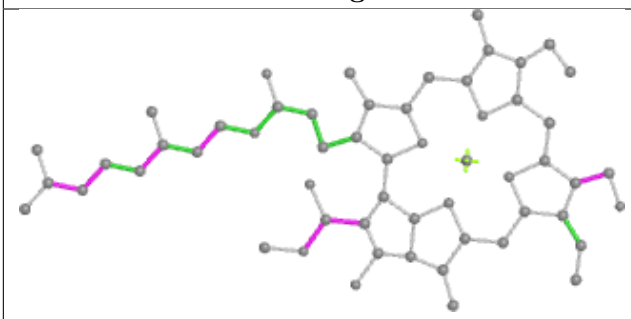
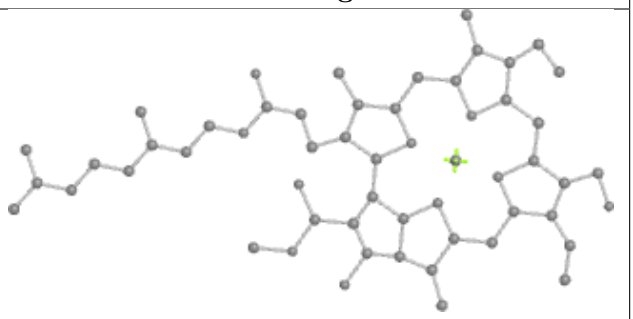


Bond angles

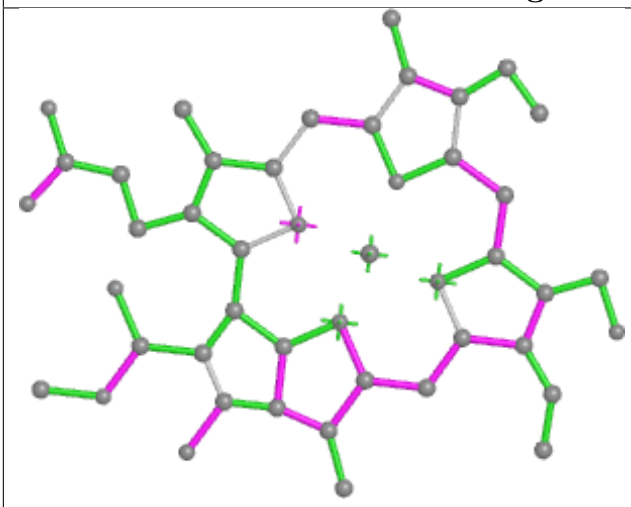
Torsions

Rings

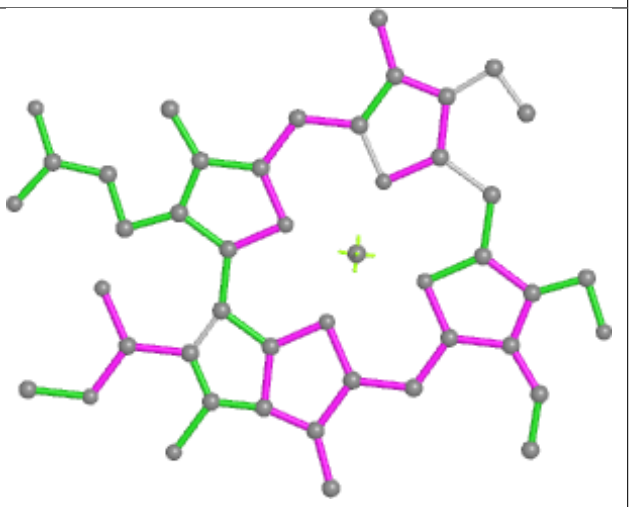
Ligand CLA P 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

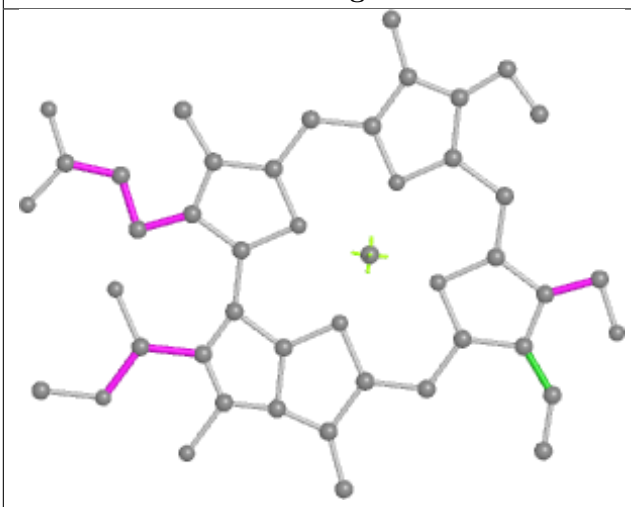
Ligand CHL S 316



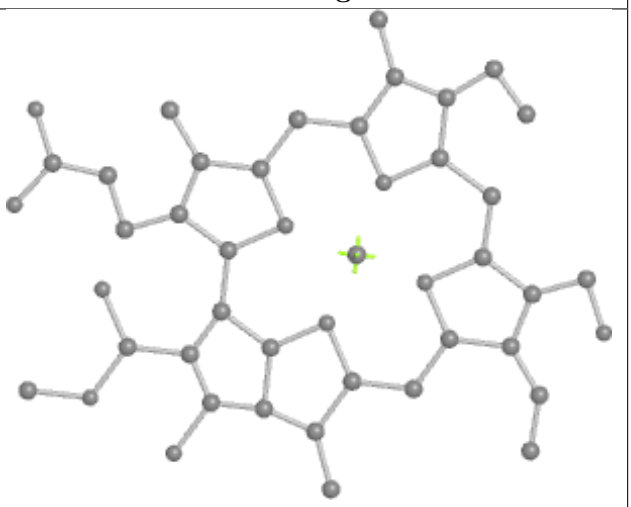
Bond lengths



Bond angles

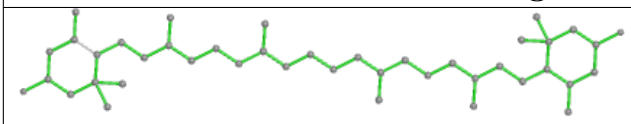


Torsions

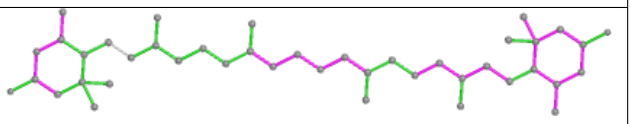


Rings

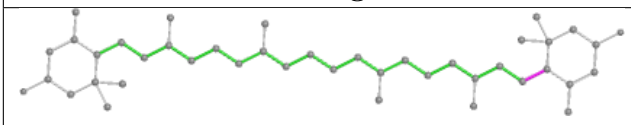
Ligand LUT 5 310



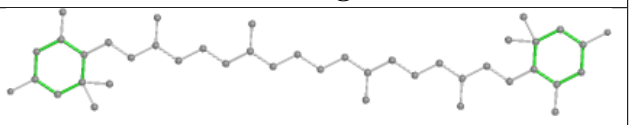
Bond lengths



Bond angles

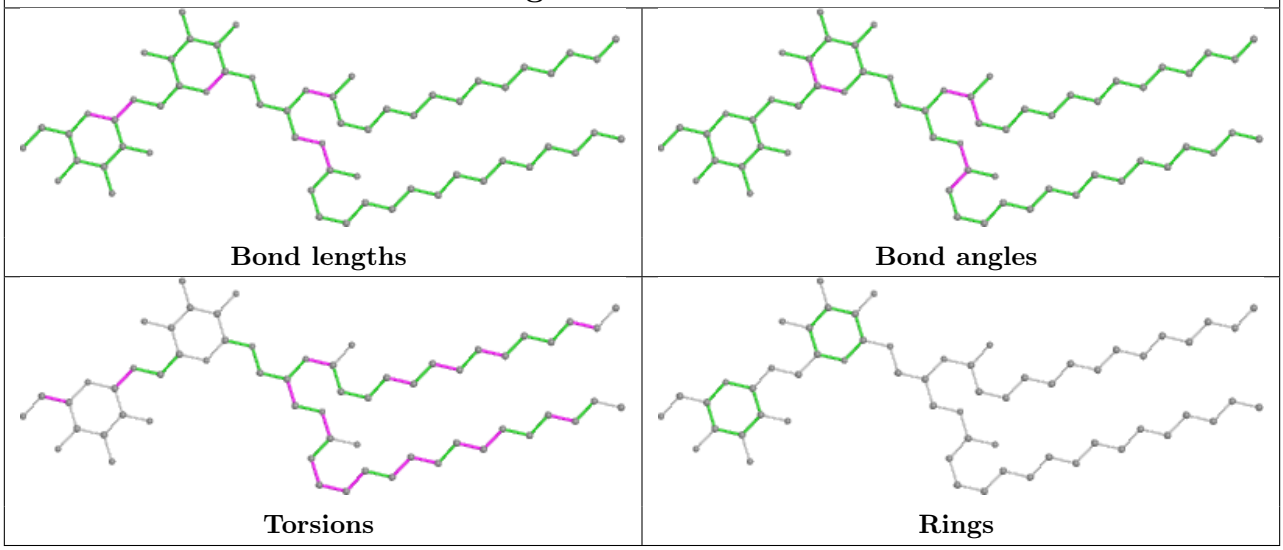


Torsions

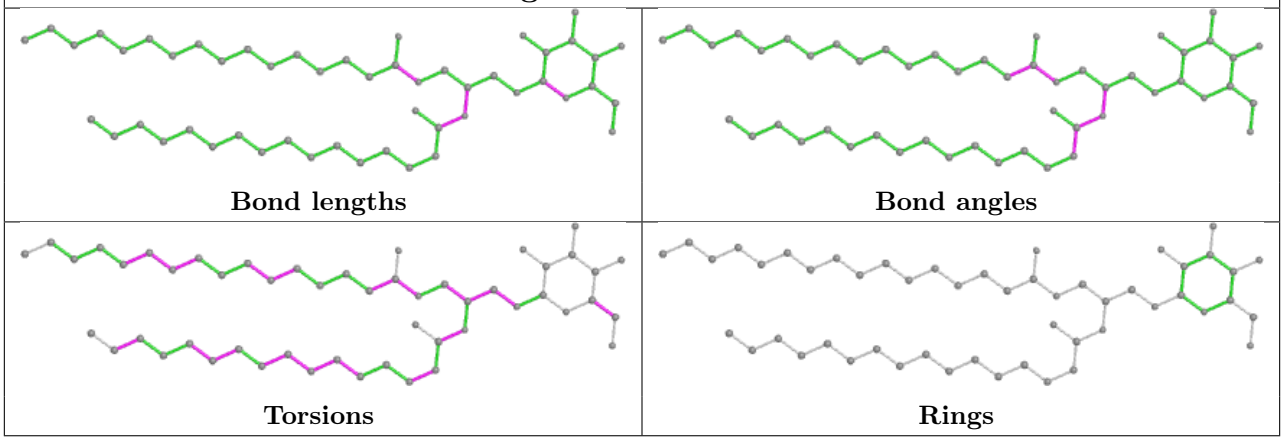


Rings

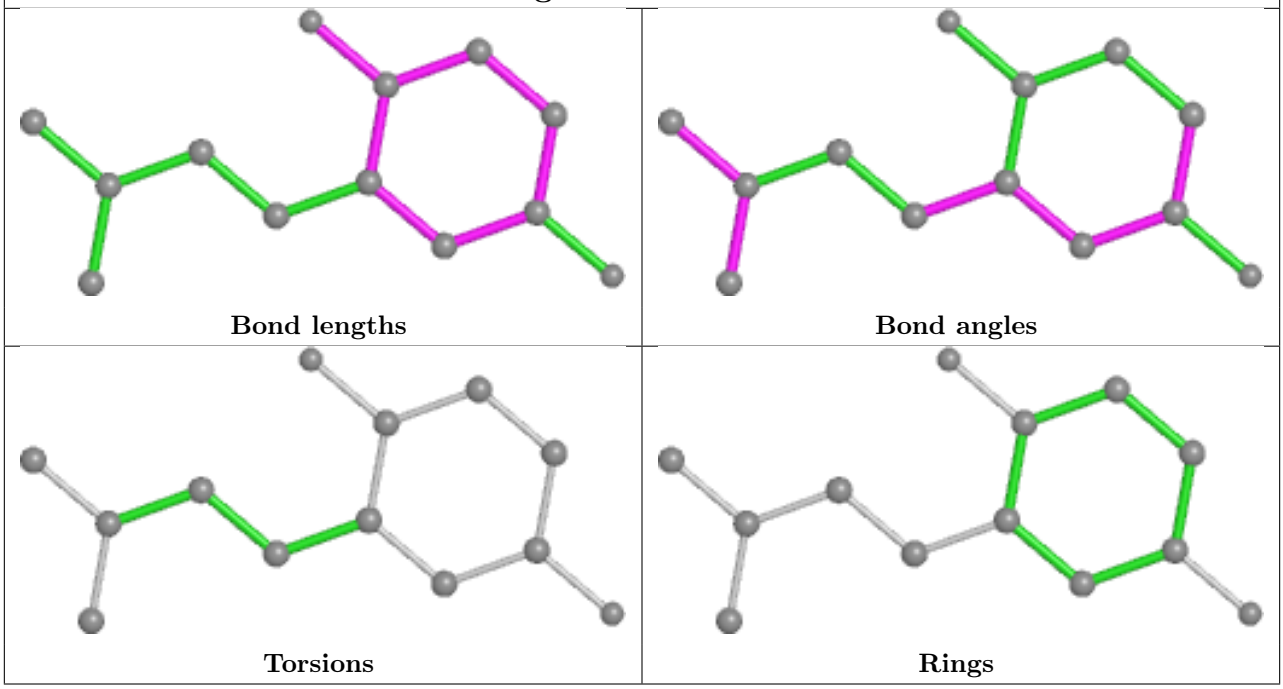
Ligand DGD c 519



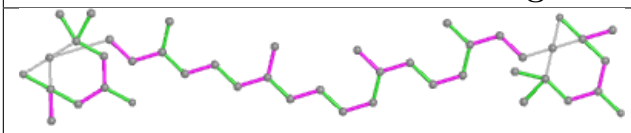
Ligand LMG C 502



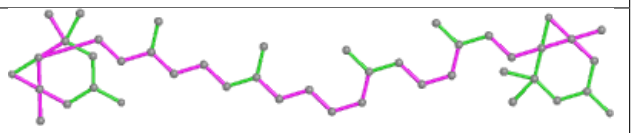
Ligand PL9 a 411



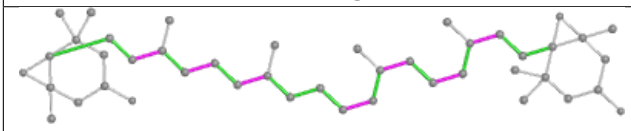
Ligand XAT v 311



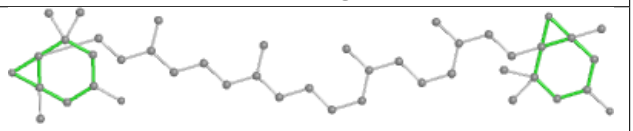
Bond lengths



Bond angles

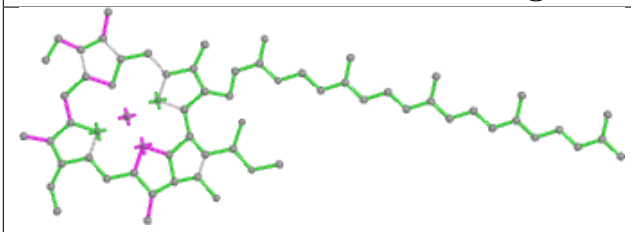


Torsions

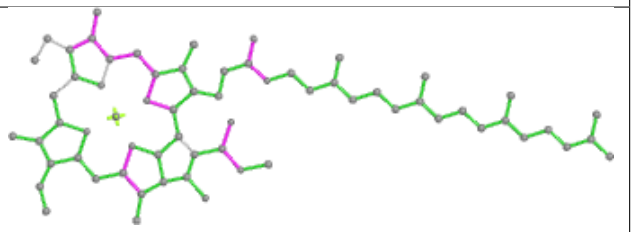


Rings

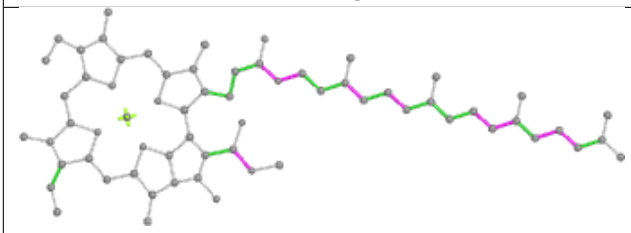
Ligand CLA d 402



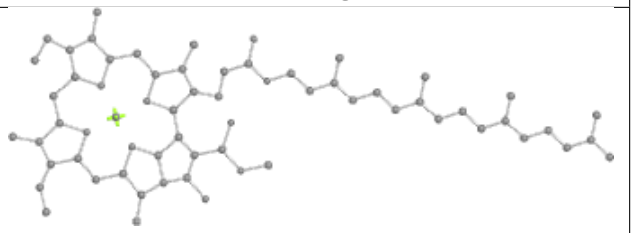
Bond lengths



Bond angles

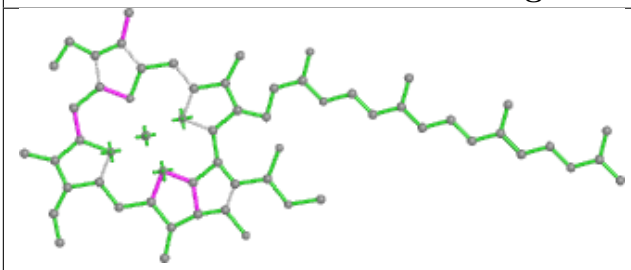


Torsions

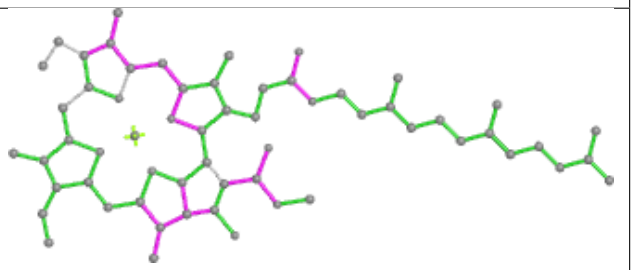


Rings

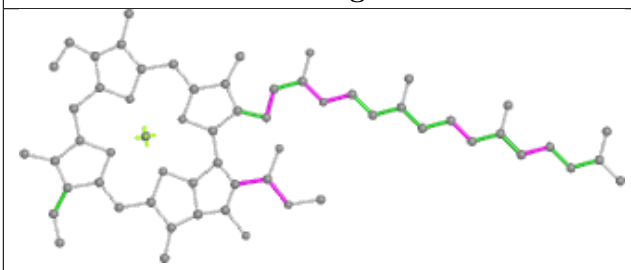
Ligand CLA P 306



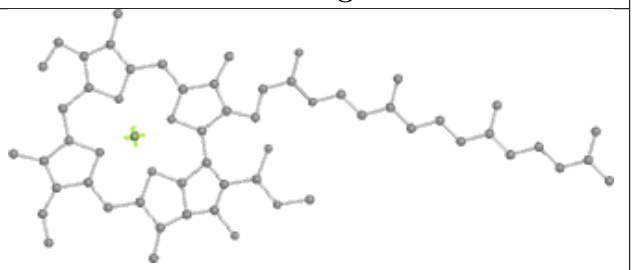
Bond lengths



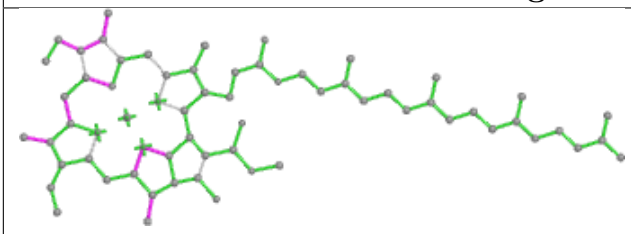
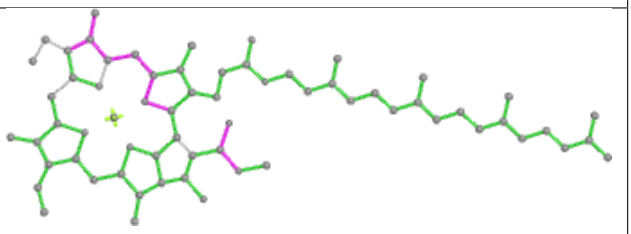
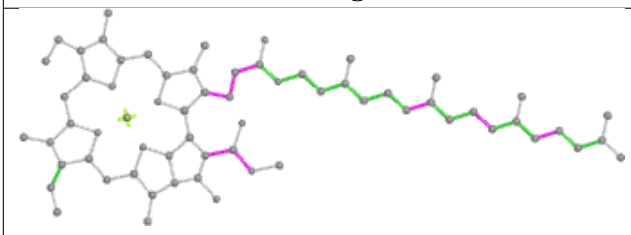
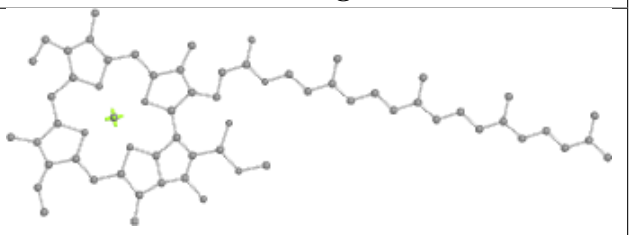
Bond angles

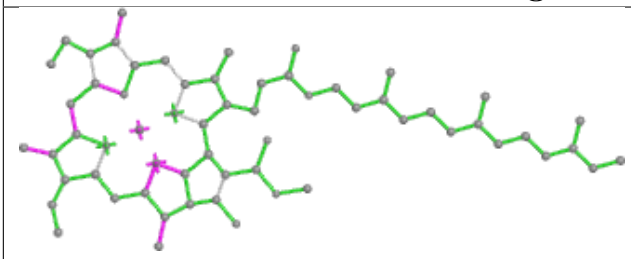
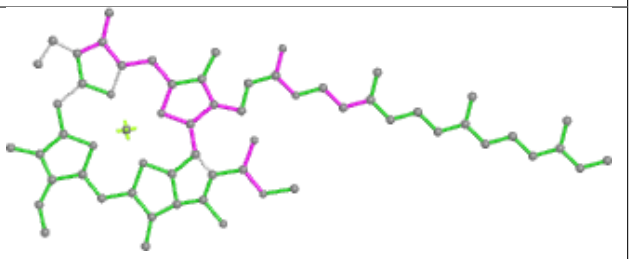
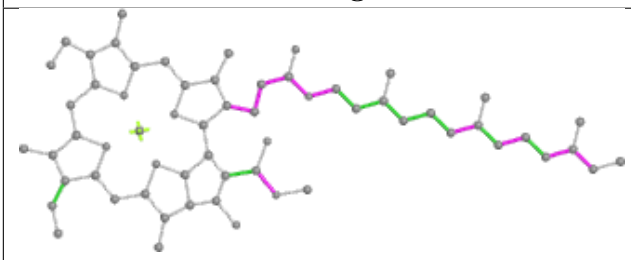
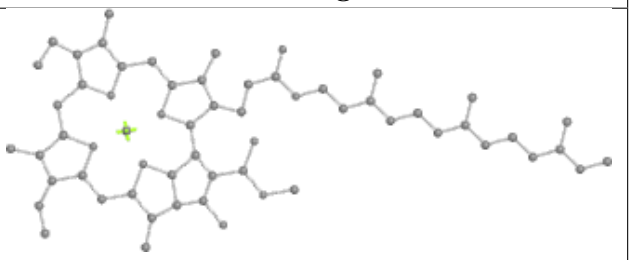


Torsions

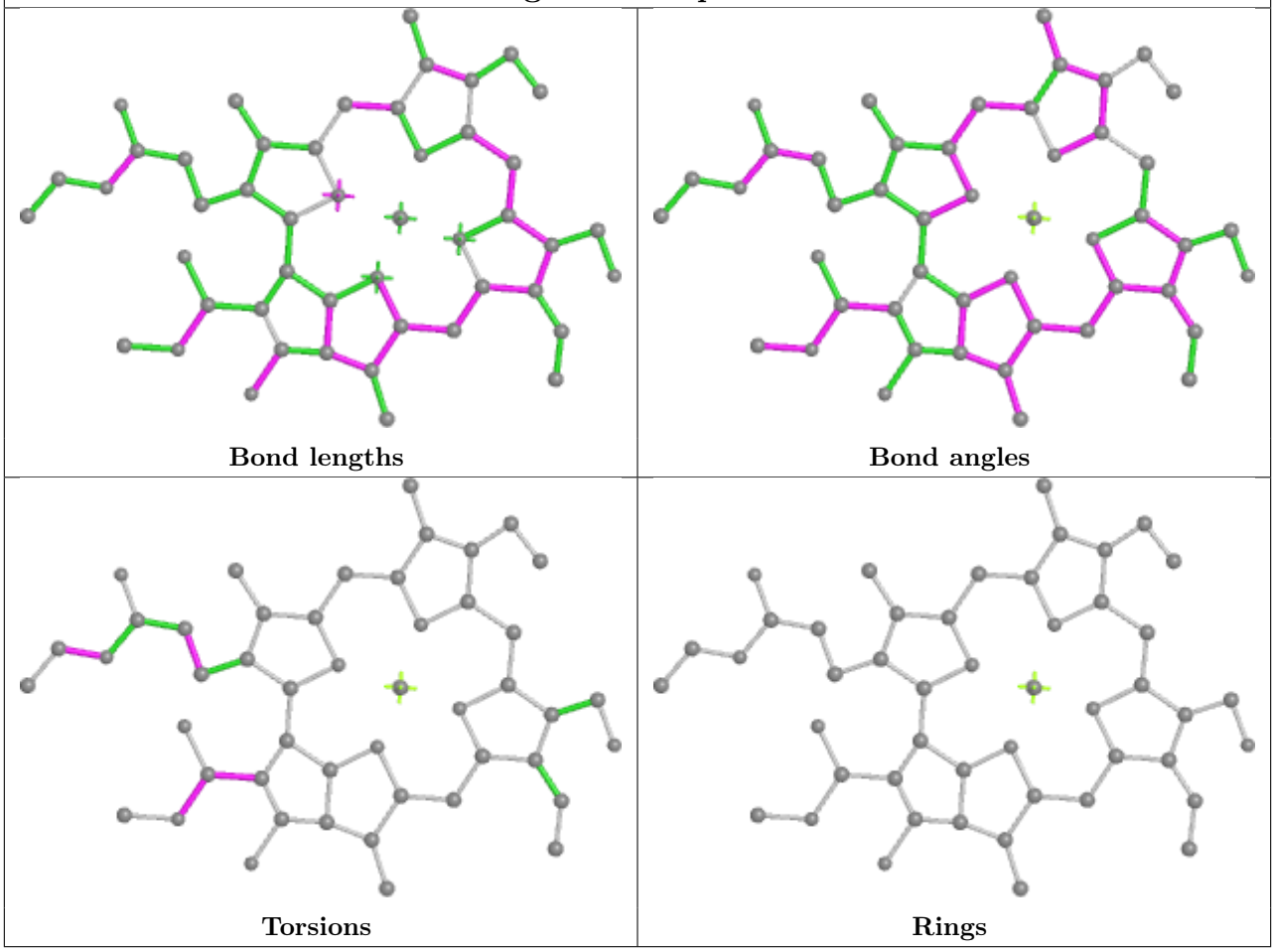


Rings

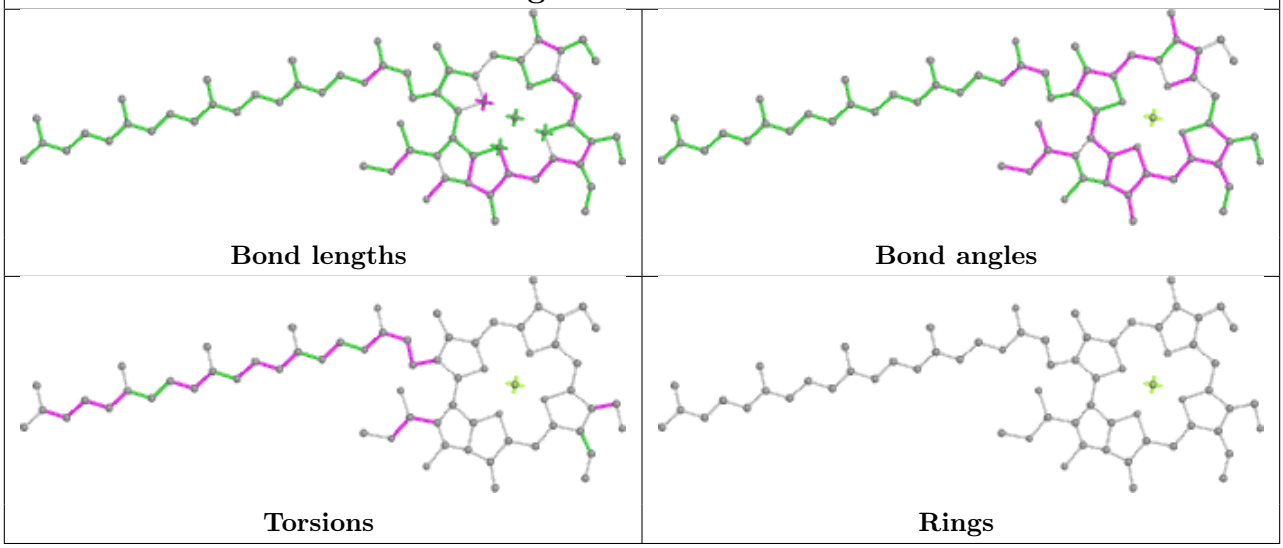
Ligand CLA v 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

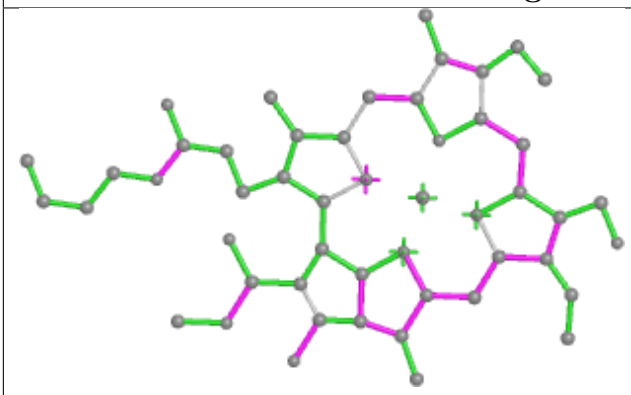
Ligand CHL p 315



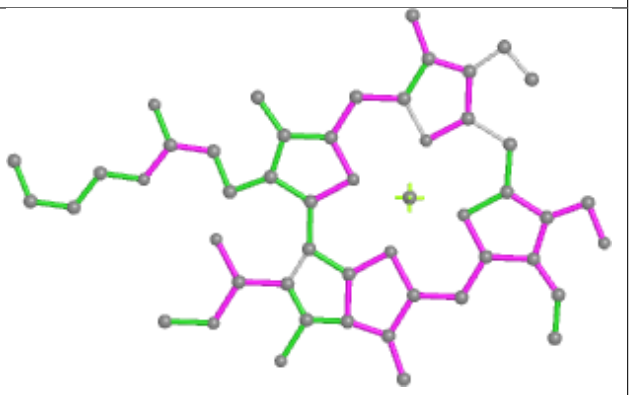
Ligand CHL n 316



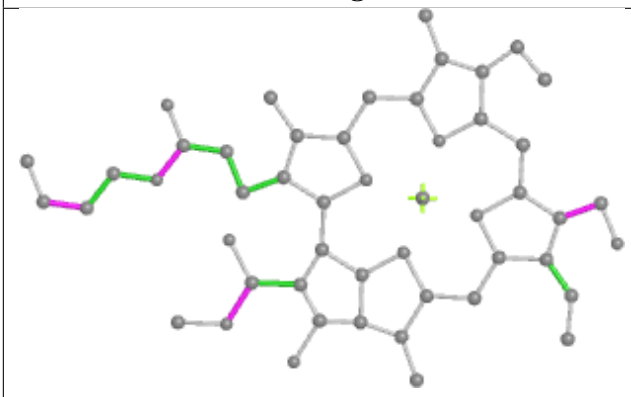
Ligand CHL P 316



Bond lengths



Bond angles



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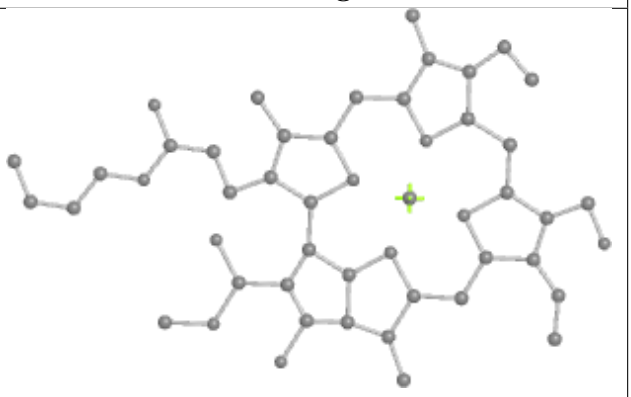
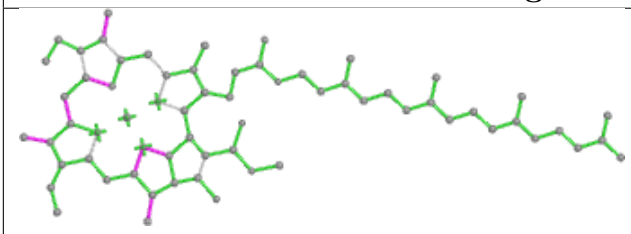
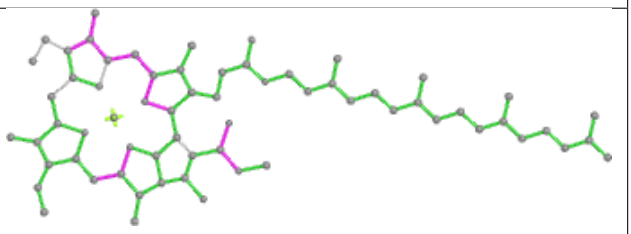


Rings

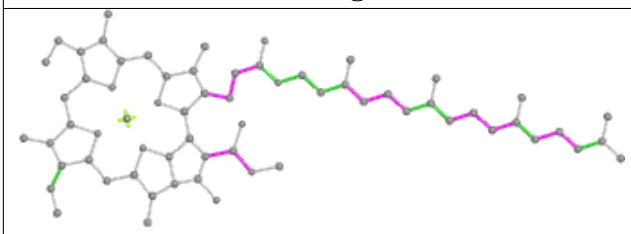
Ligand CLA P 302



Bond lengths



Bond angles



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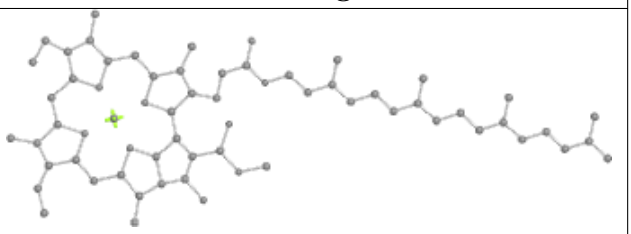
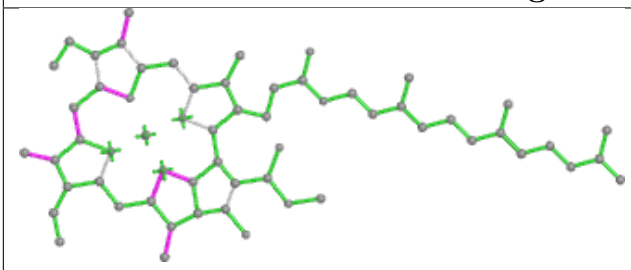
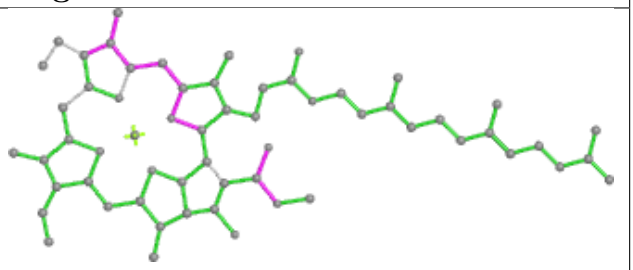
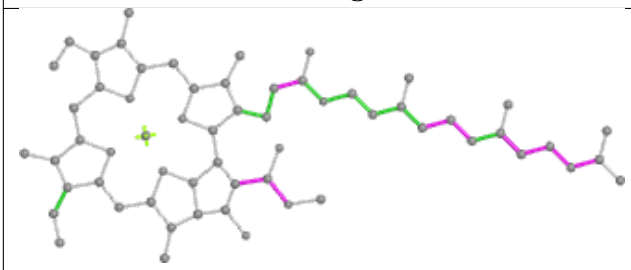
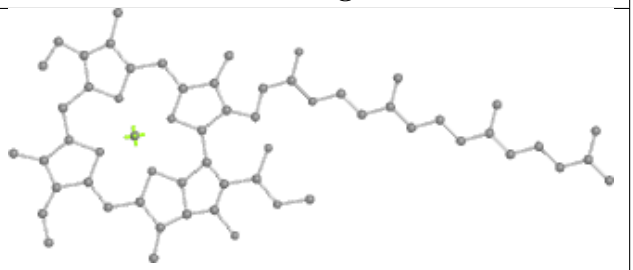


Rings

Ligand CLA g 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

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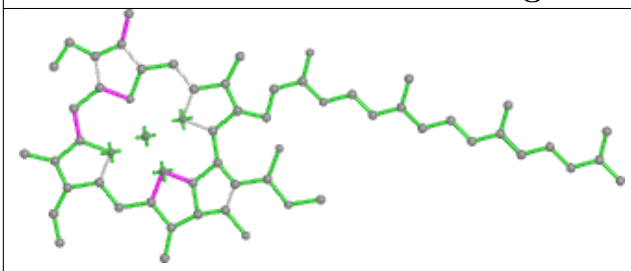
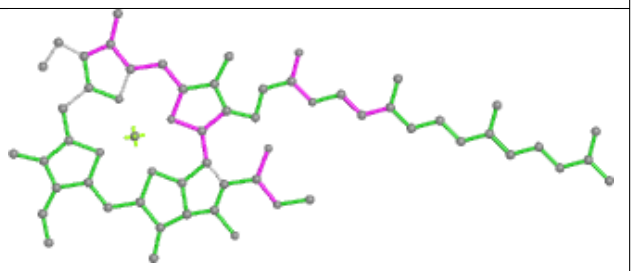
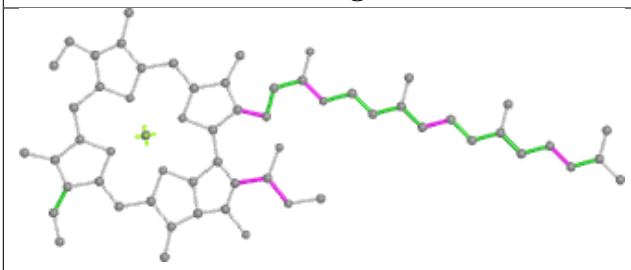
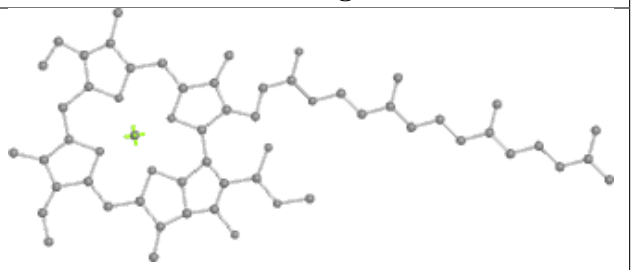
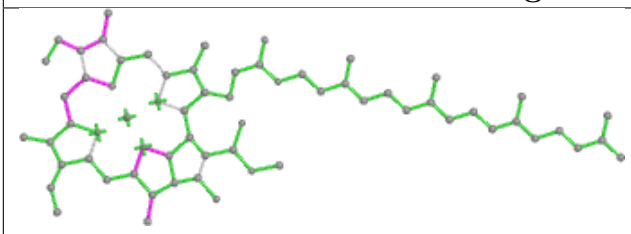
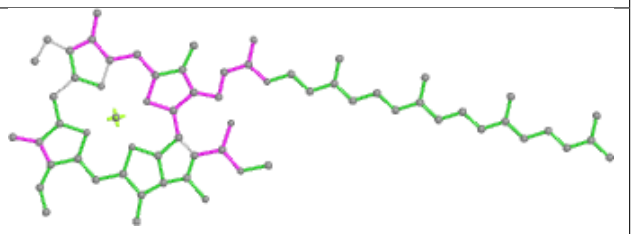
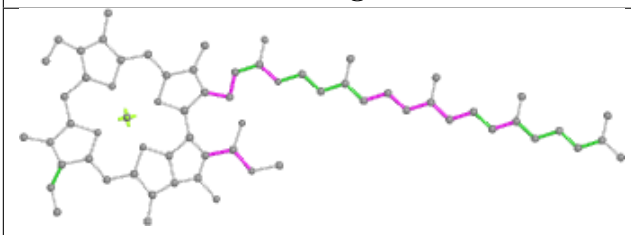
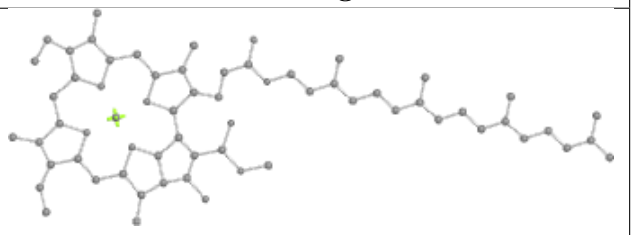
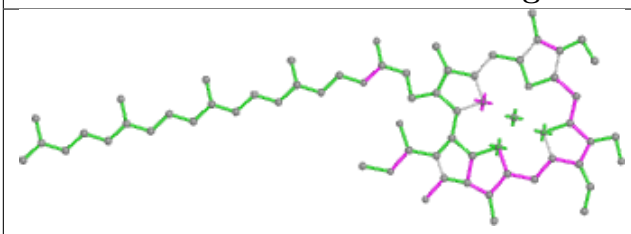
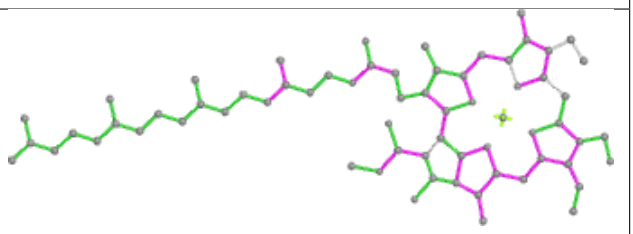
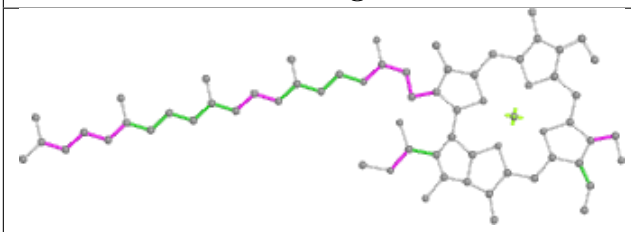
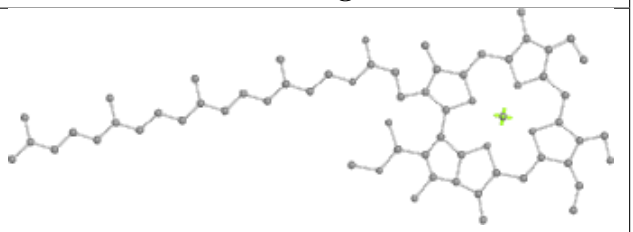
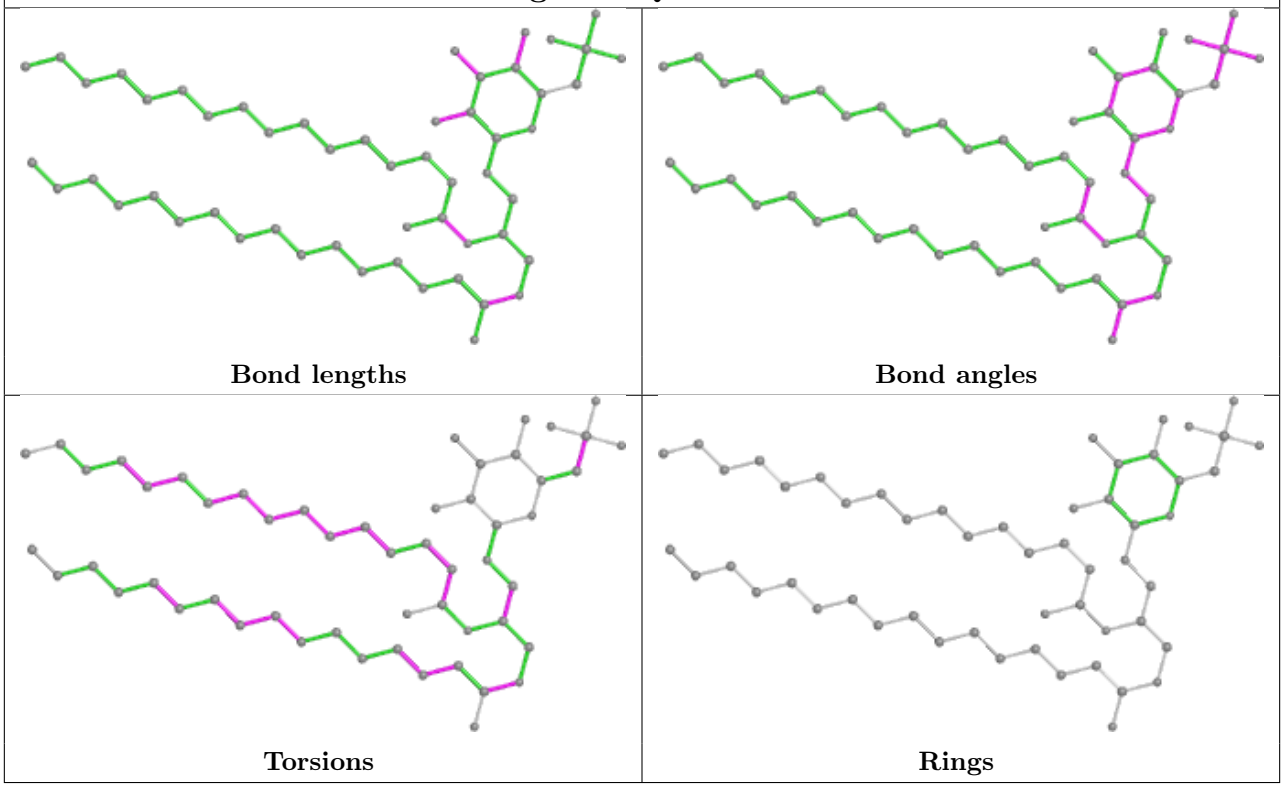
 Bond lengths	 Bond angles
 Torsions	 Rings

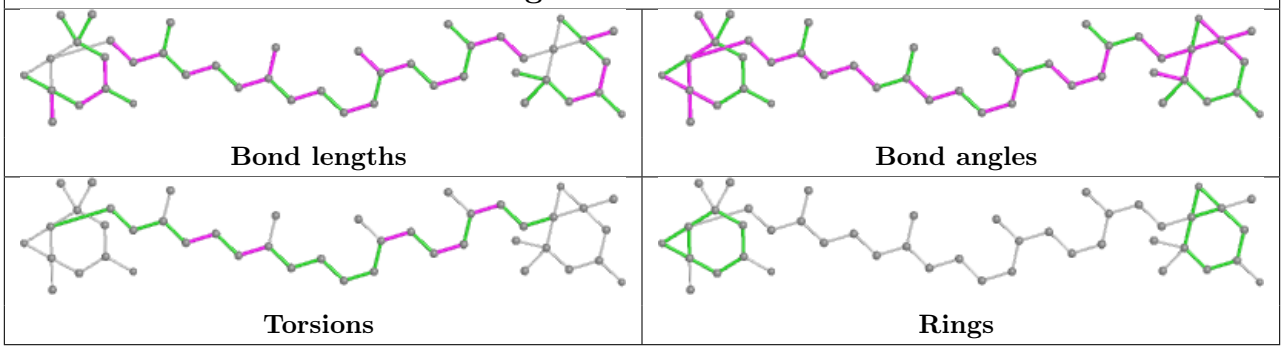
Ligand CLA B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

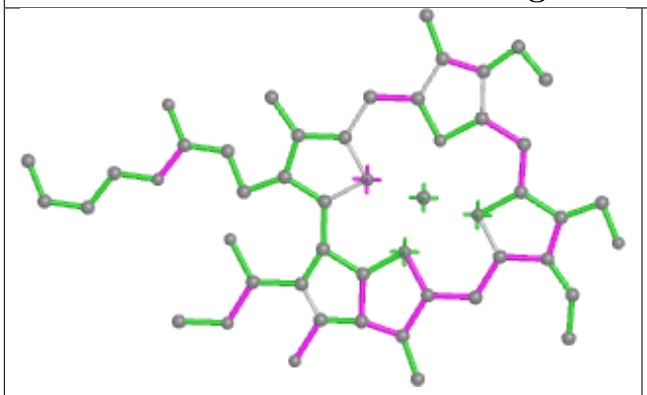
Ligand SQD a 413



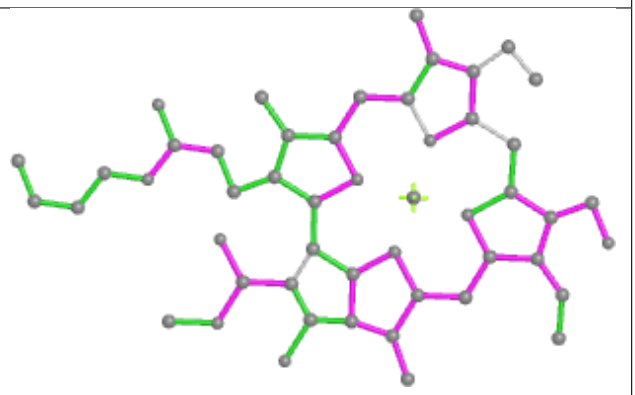
Ligand XAT P 312



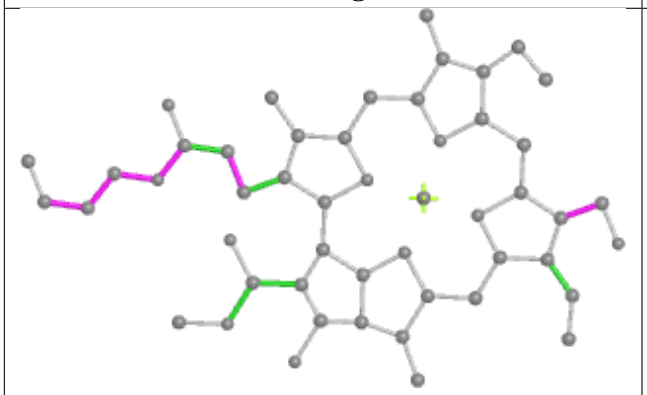
Ligand CHL v 315



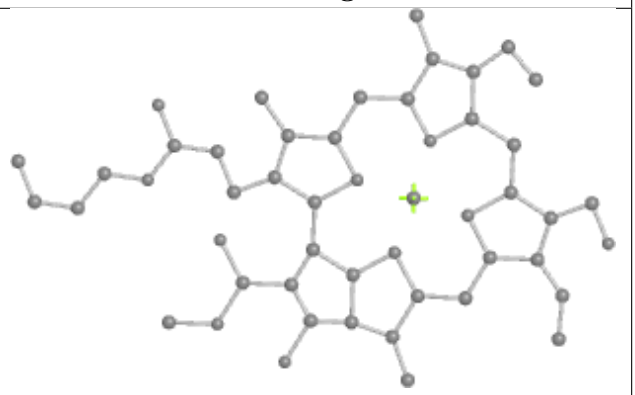
Bond lengths



Bond angles

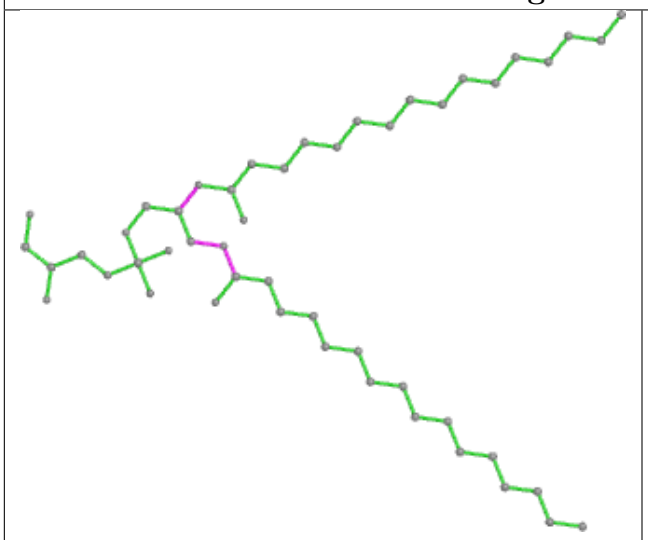


Torsions

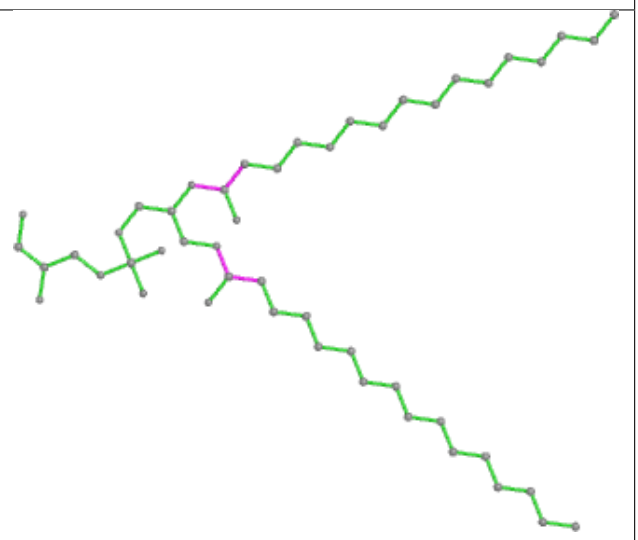


Rings

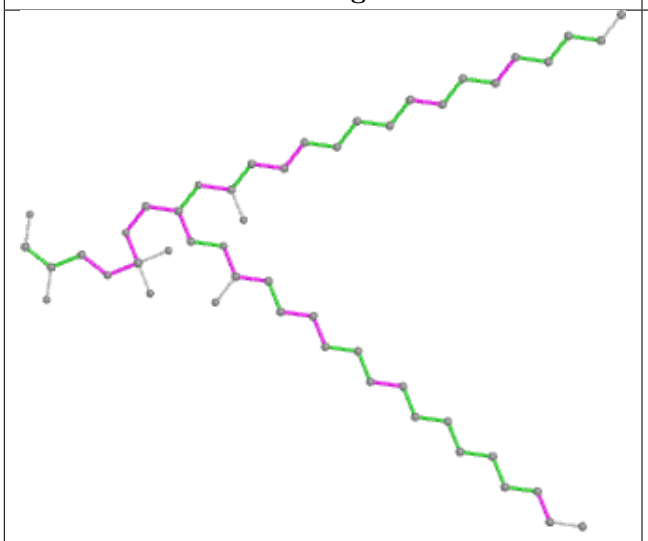
Ligand LHG 5 312



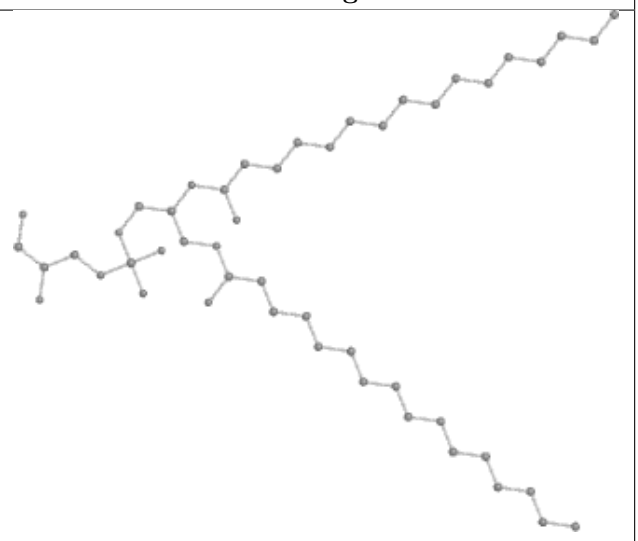
Bond lengths



Bond angles

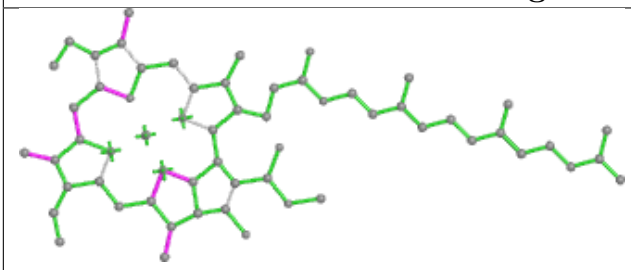


Torsions



Rings

Ligand CLA 5 307



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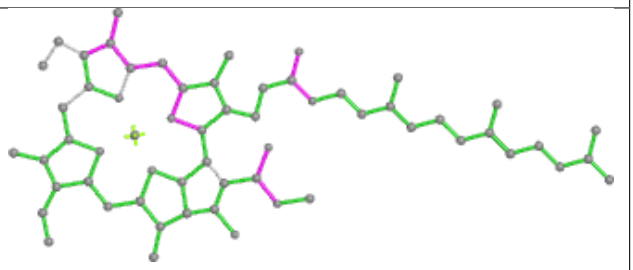
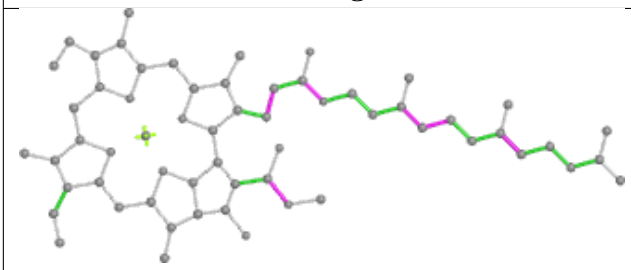
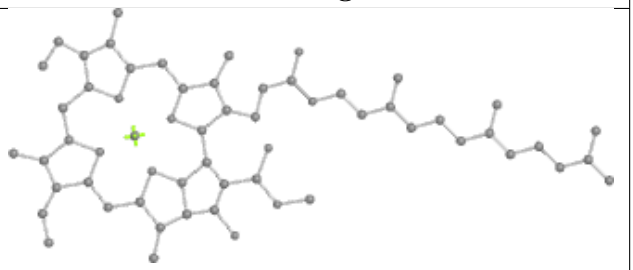


Bond angles

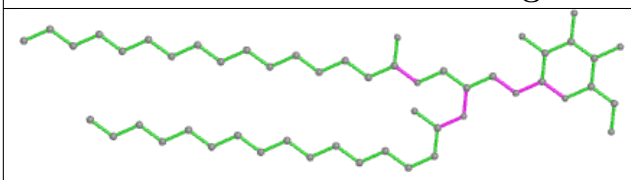


Torsions

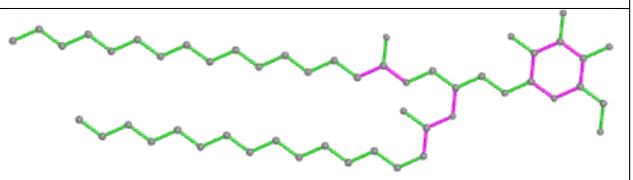


Rings

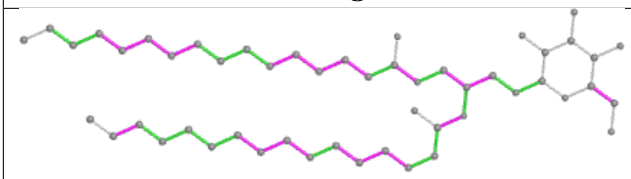
Ligand LMG b 621



Bond lengths



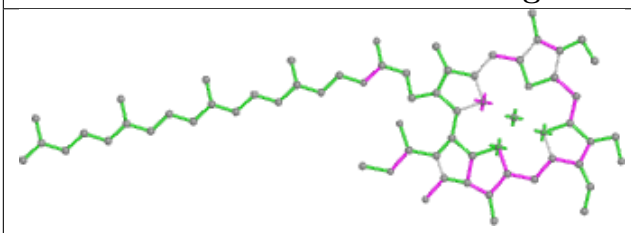
Bond angles



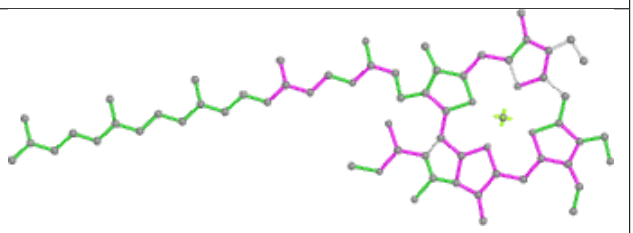
Torsions

Rings

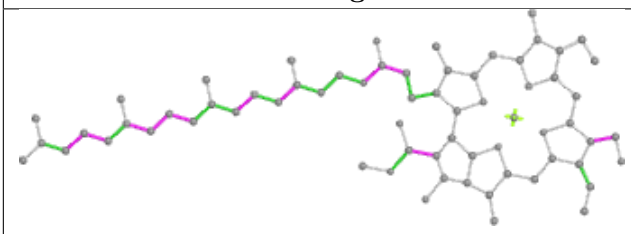
Ligand CHL U 313



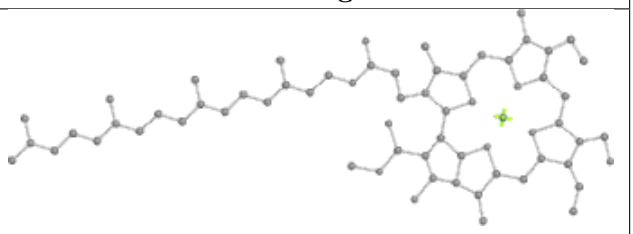
Bond lengths



Bond angles

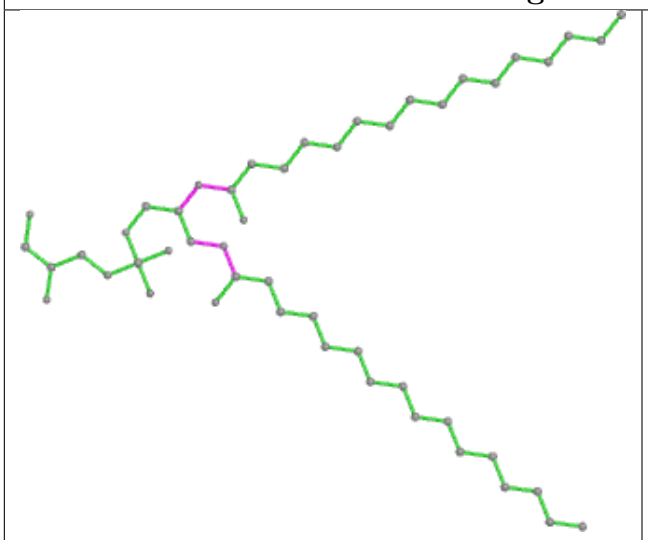


Torsions

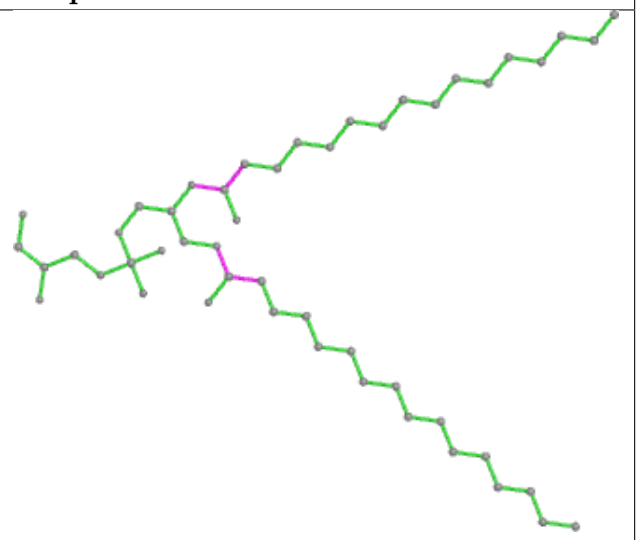


Rings

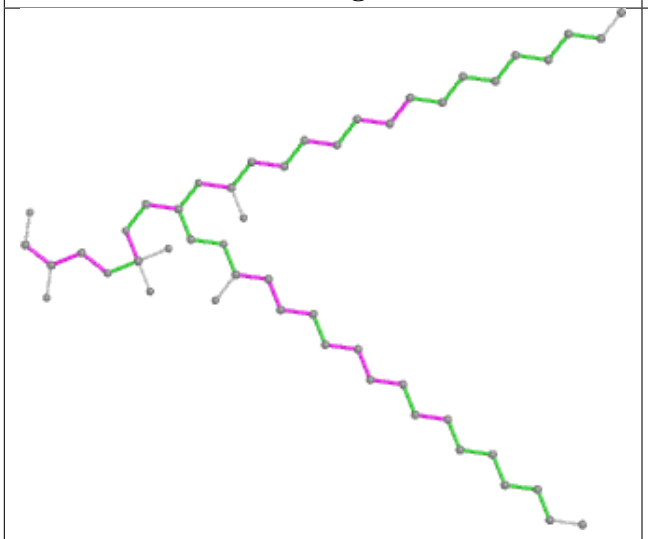
Ligand LHG q 310



Bond lengths



Bond angles



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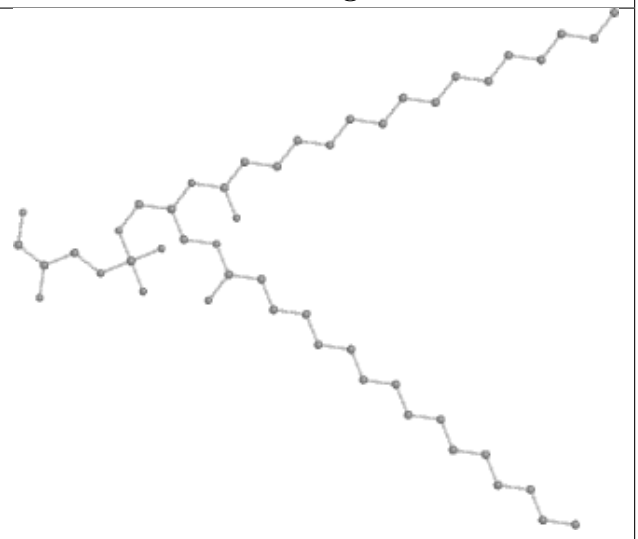
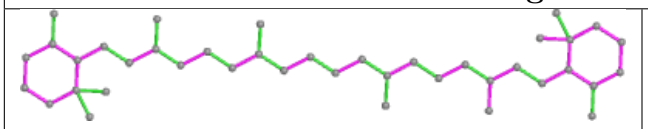
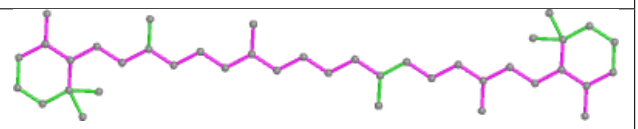


Rings

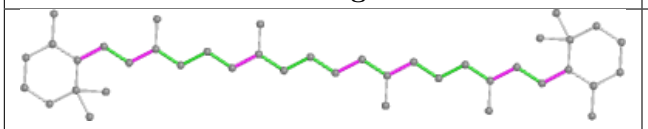
Ligand BCR d 403



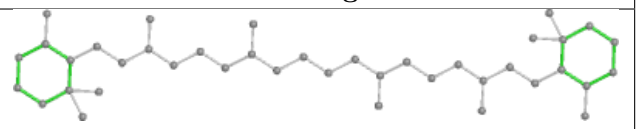
Bond lengths



Bond angles

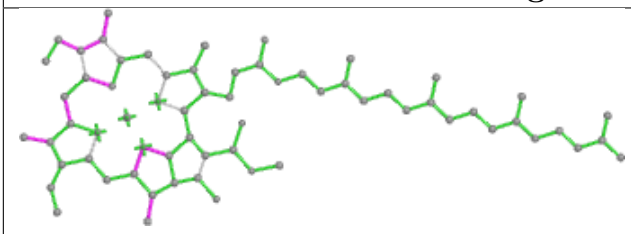


Torsions

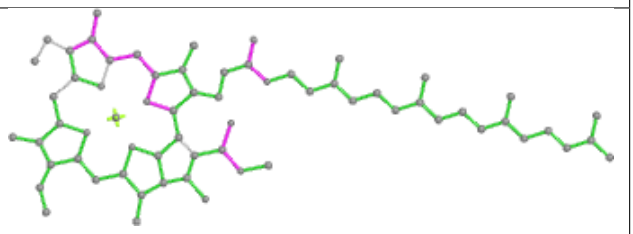


Rings

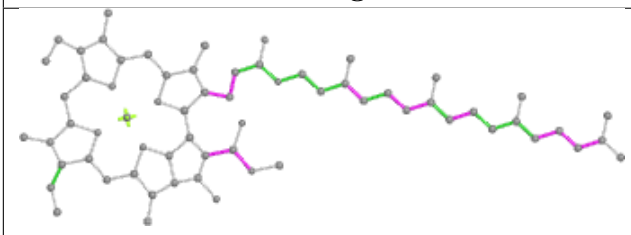
Ligand CLA b 604



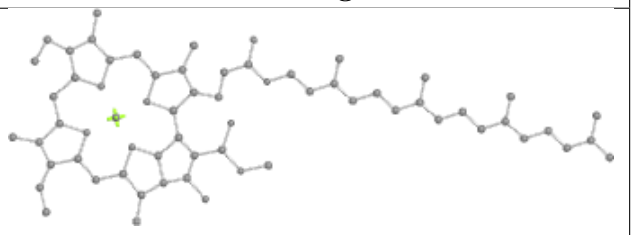
Bond lengths



Bond angles

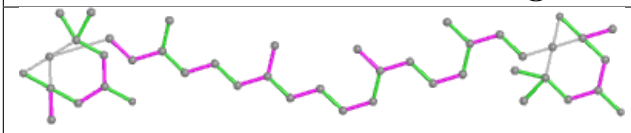


Torsions

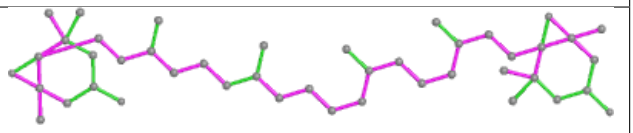


Rings

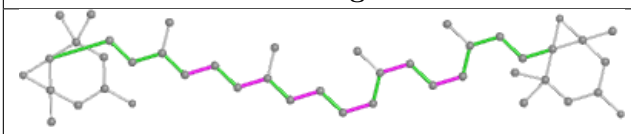
Ligand XAT 4 311



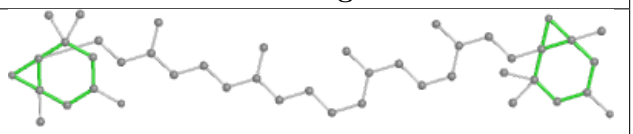
Bond lengths



Bond angles

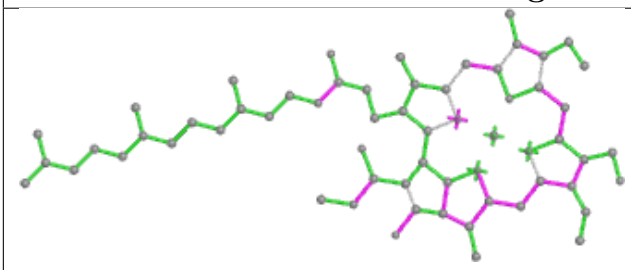


Torsions



Rings

Ligand CHL g 316



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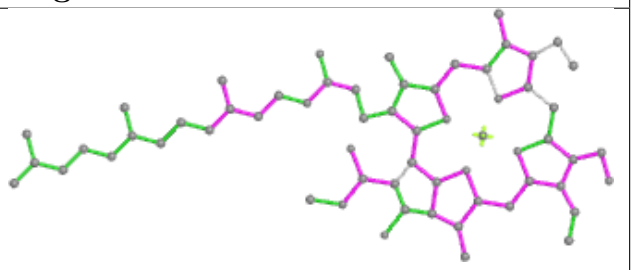
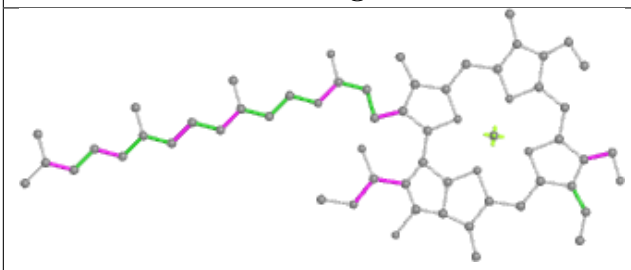


Bond angles



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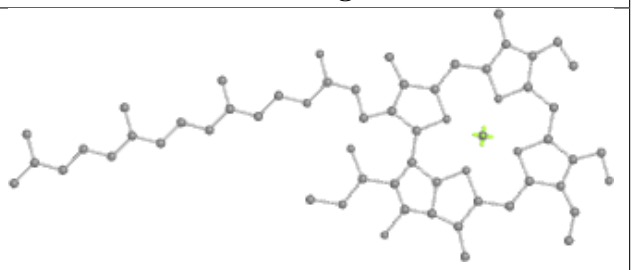
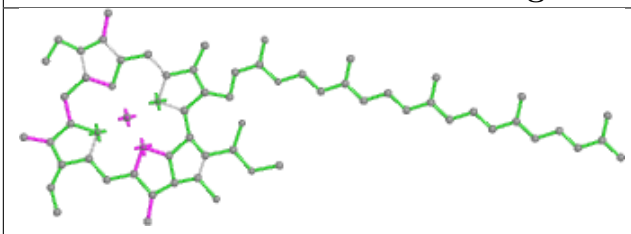
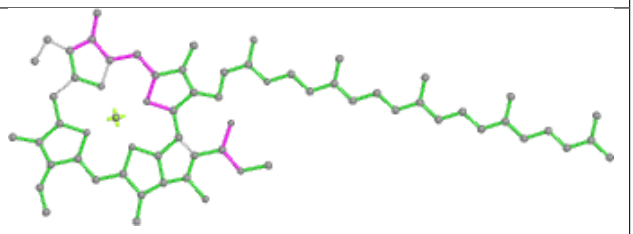
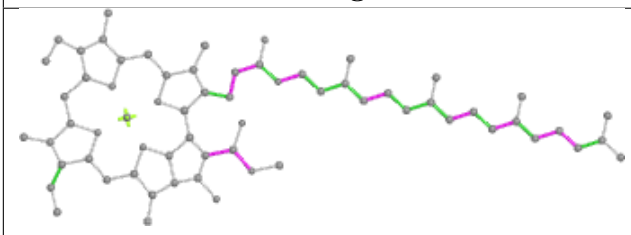
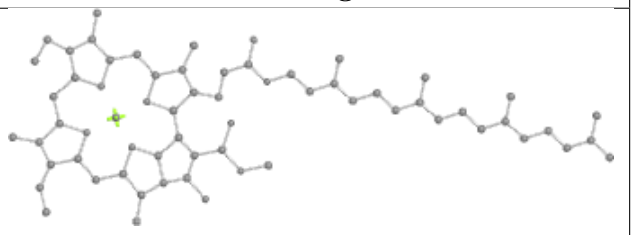
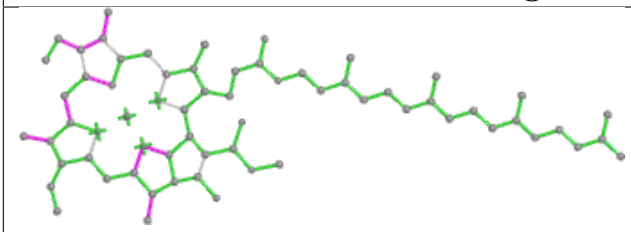
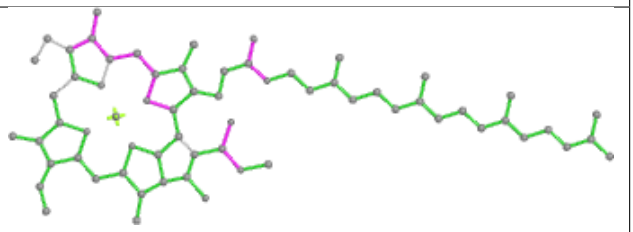
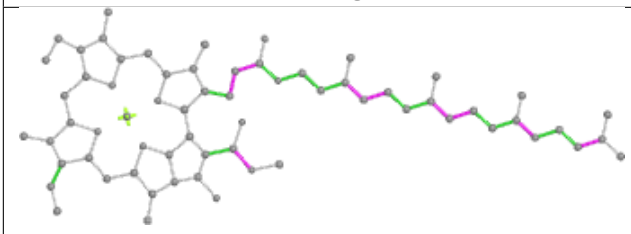
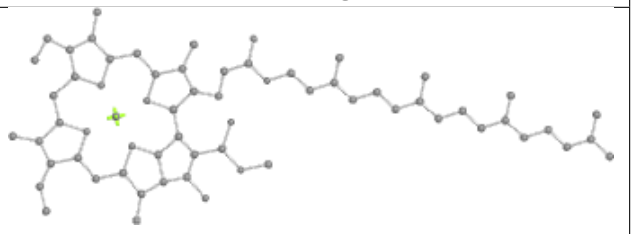
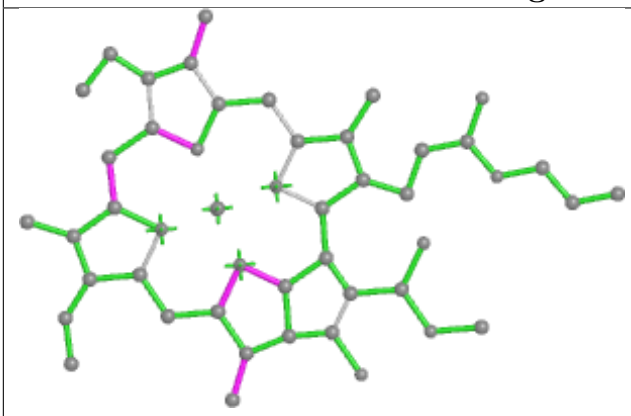
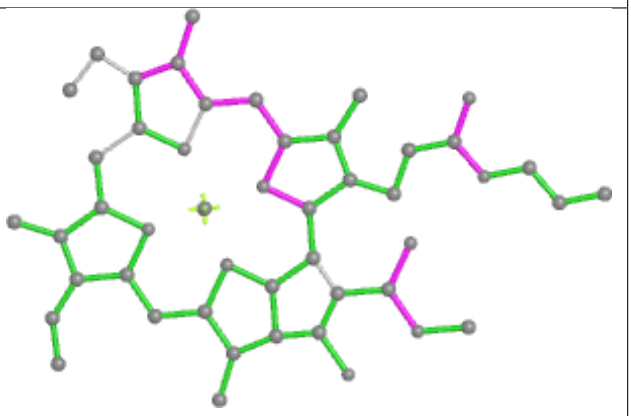
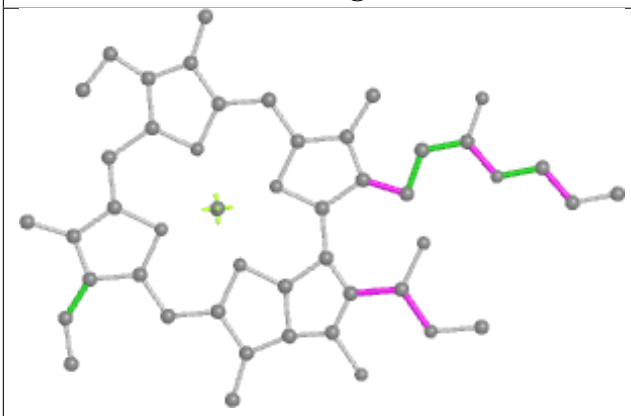
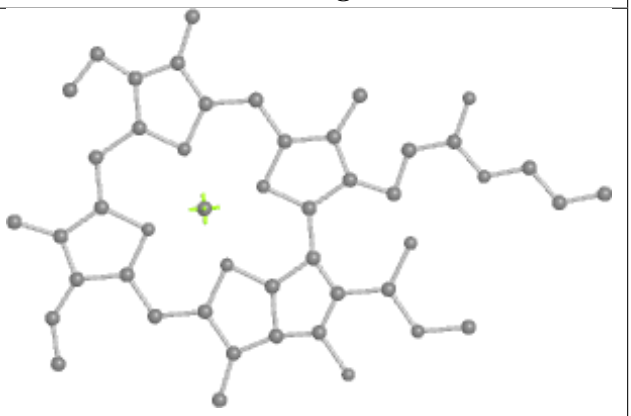
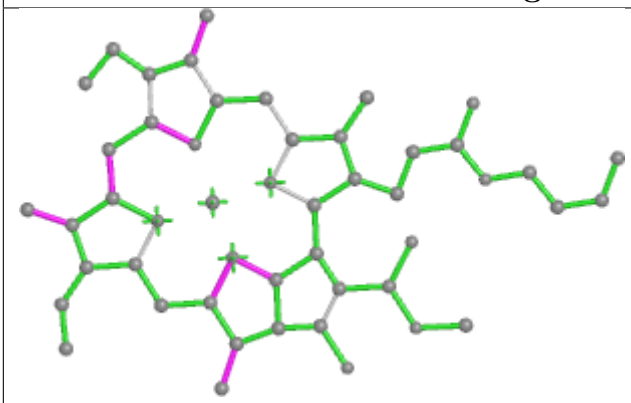
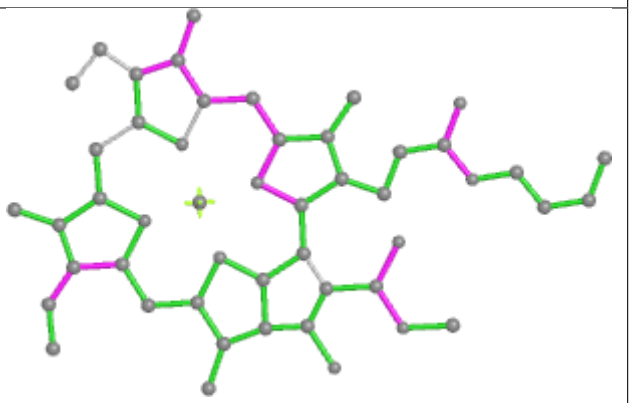
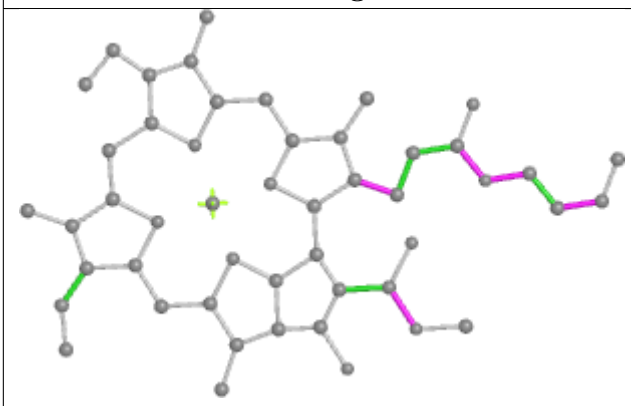
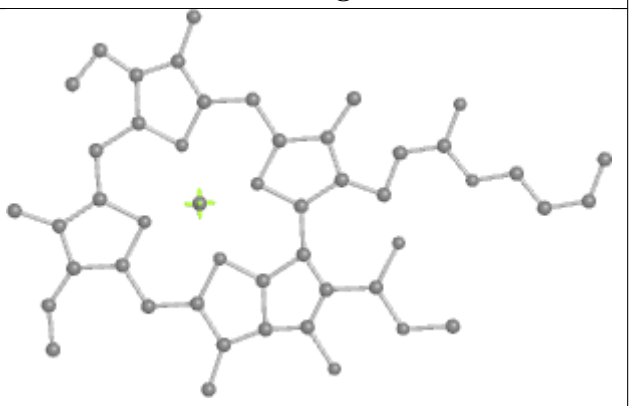


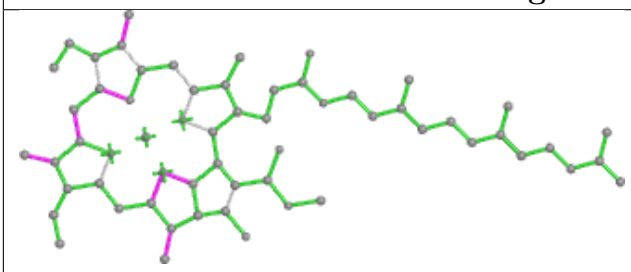
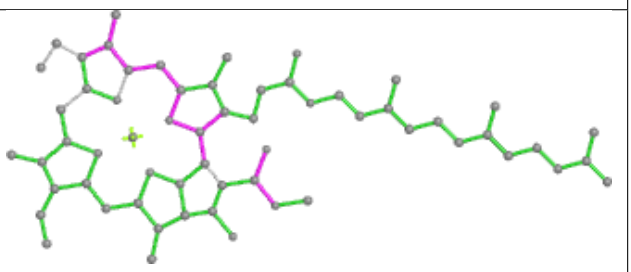
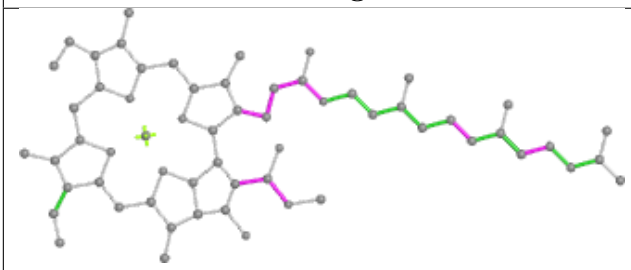
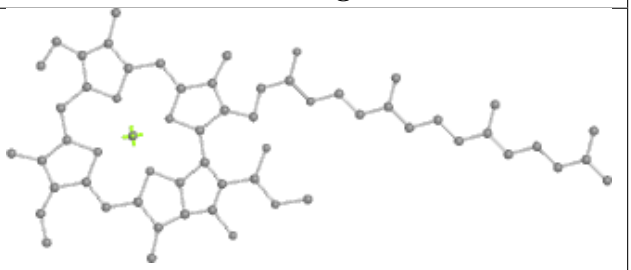
Rings

Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

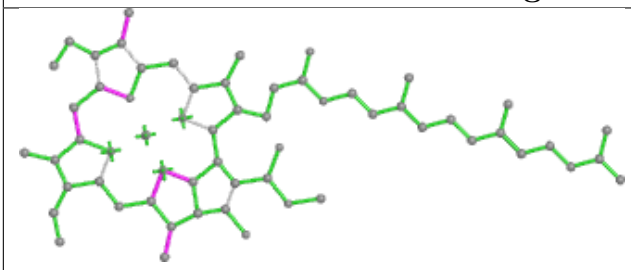
Ligand CLA U 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

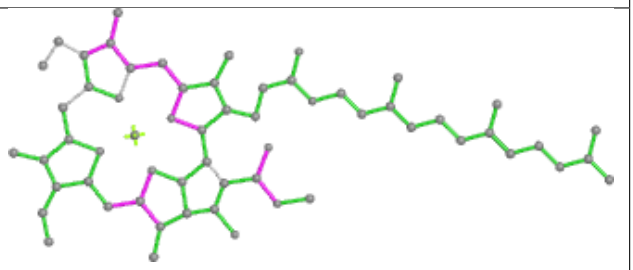
Ligand CLA R 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

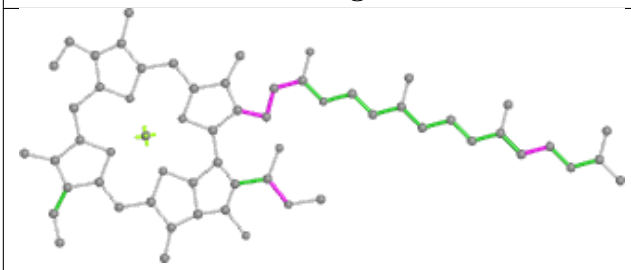
Ligand CLA R 303



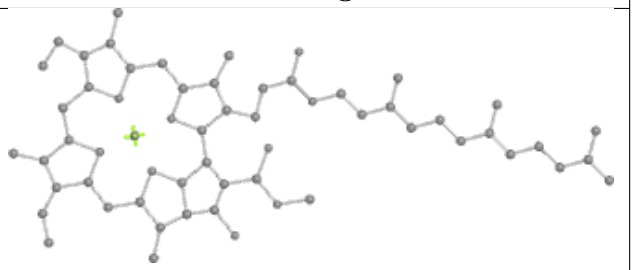
Bond lengths



Bond angles

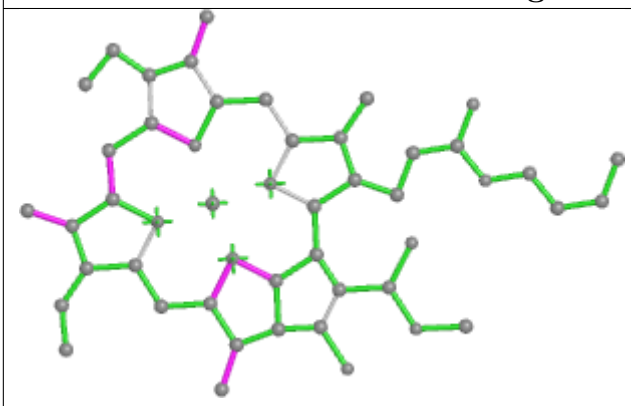


Torsions

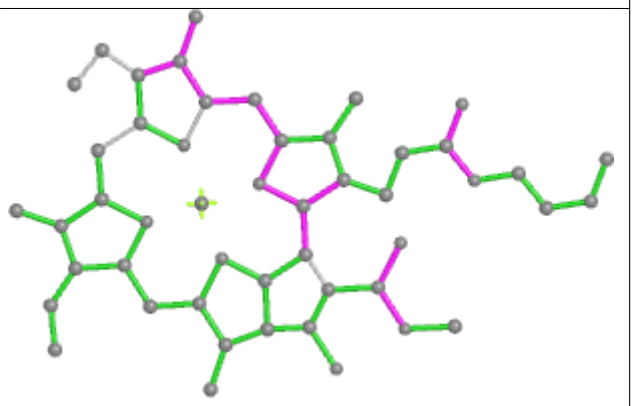


Rings

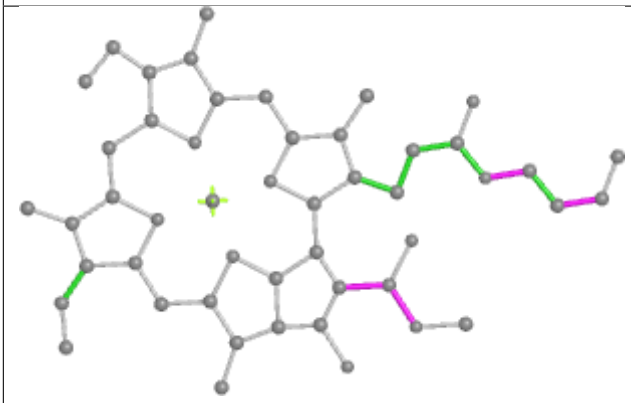
Ligand CLA S 307



Bond lengths



Bond angles



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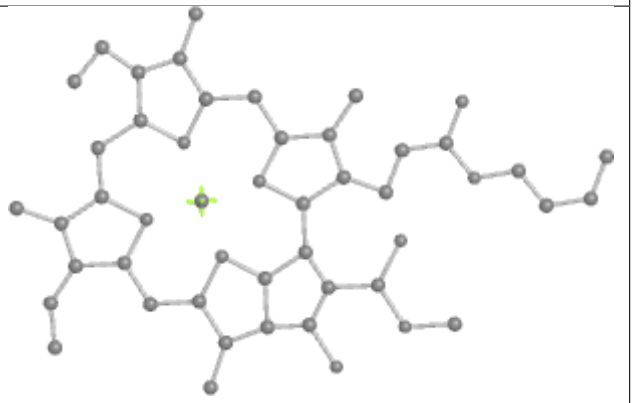
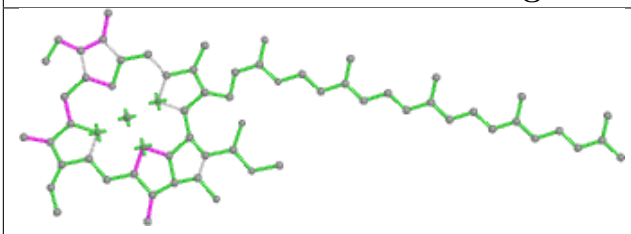
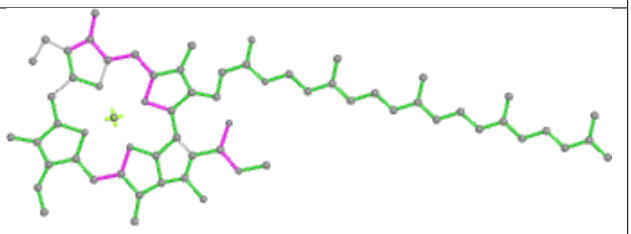


Rings

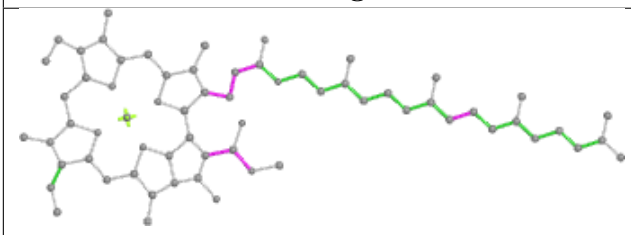
Ligand CLA U 301



Bond lengths



Bond angles



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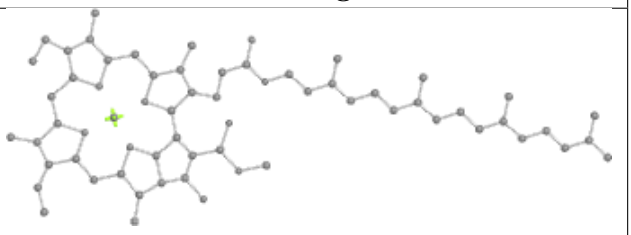
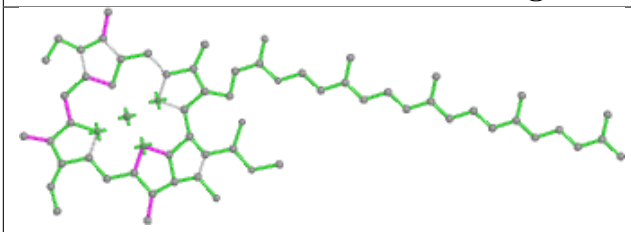
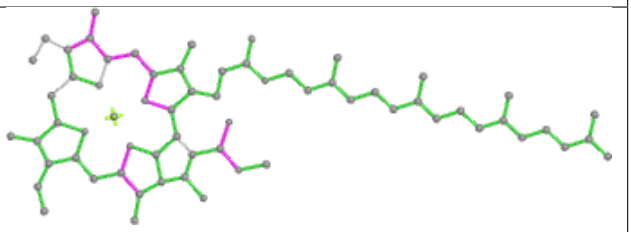


Rings

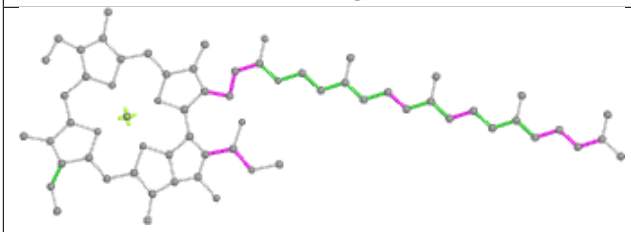
Ligand CLA n 301



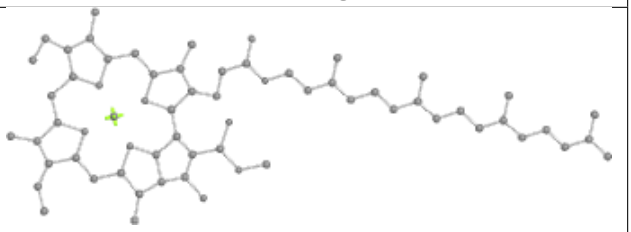
Bond lengths



Bond angles

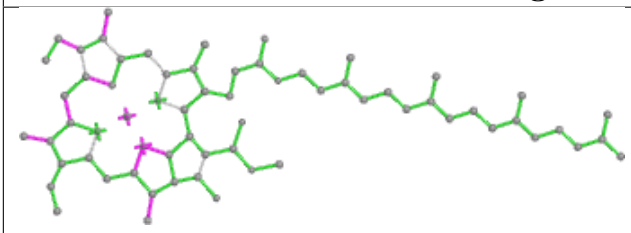


Torsions

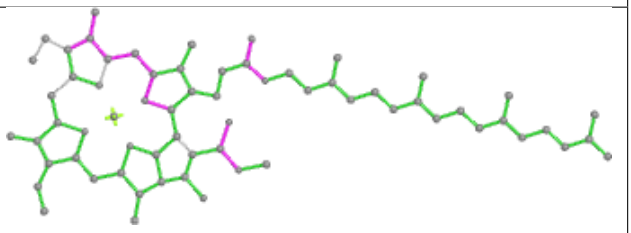


Rings

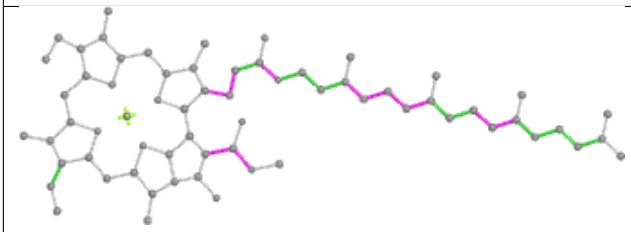
Ligand CLA c 504



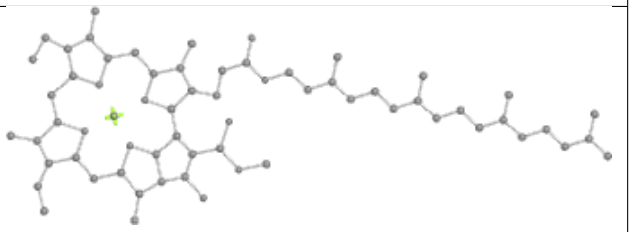
Bond lengths



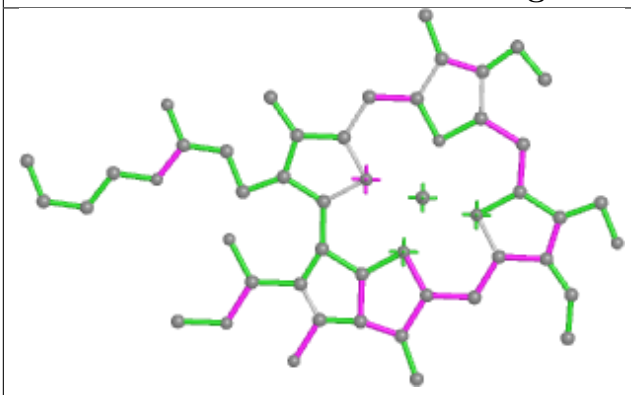
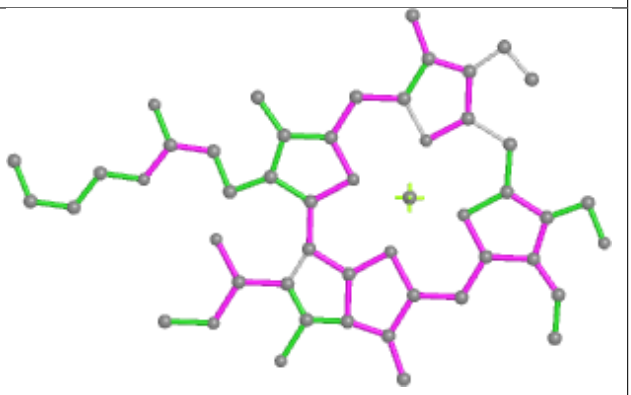
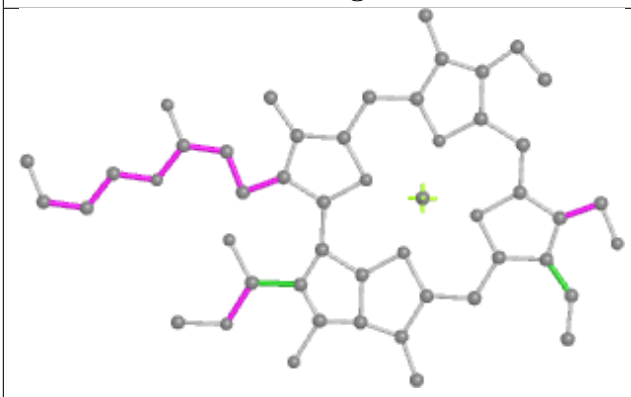
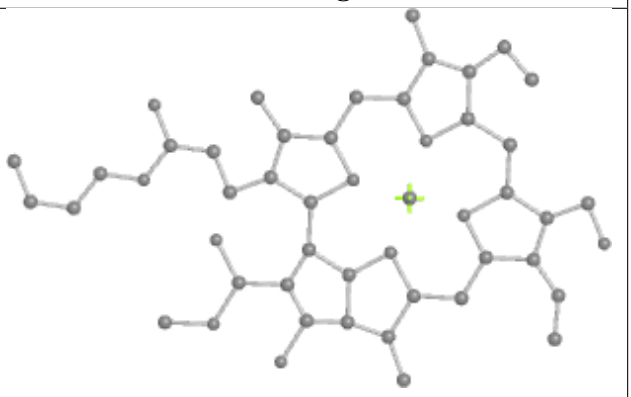
Bond angles



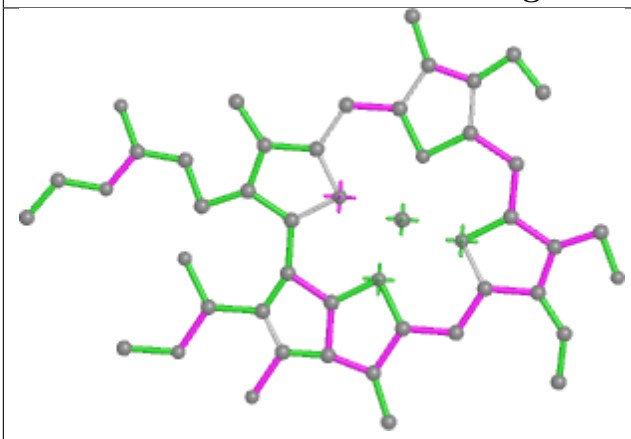
Torsions



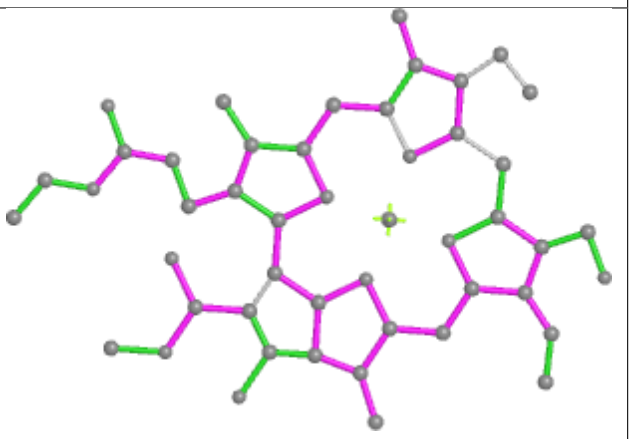
Rings

Ligand CHL 3 313	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

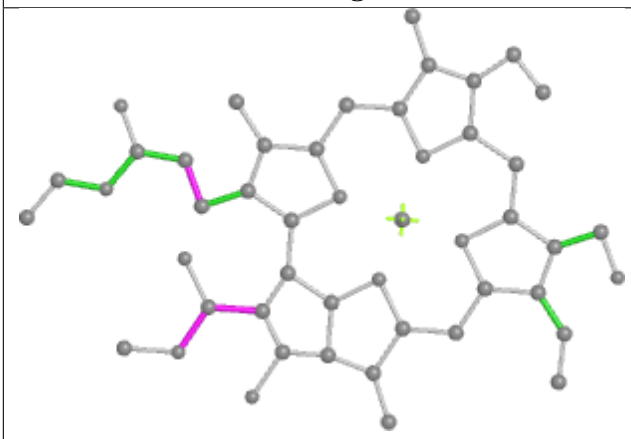
Ligand CHL G 312



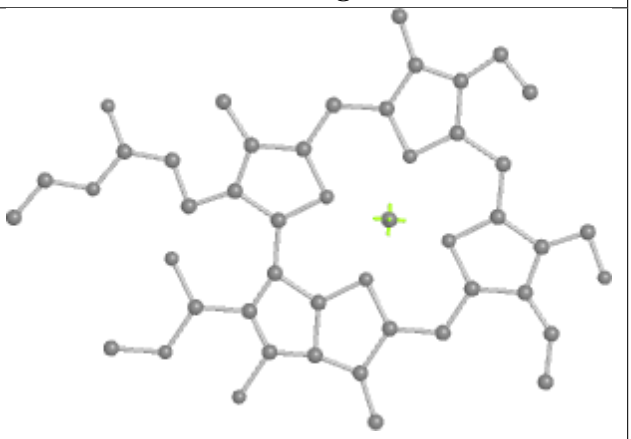
Bond lengths



Bond angles

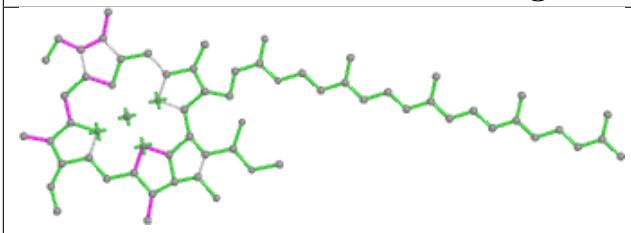


Torsions

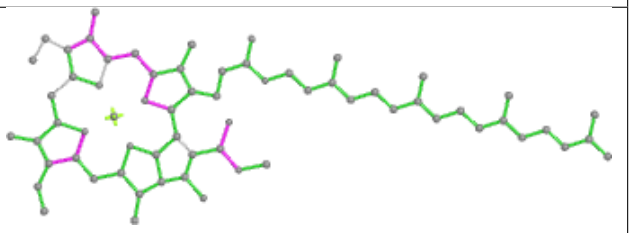


Rings

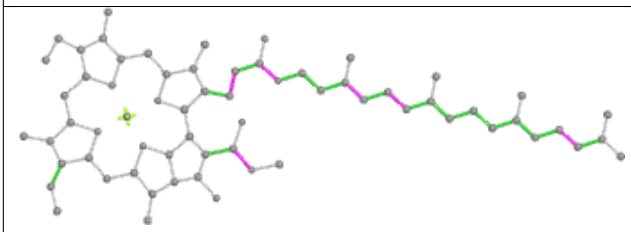
Ligand CLA c 505



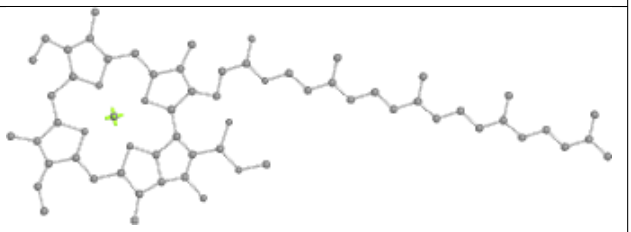
Bond lengths



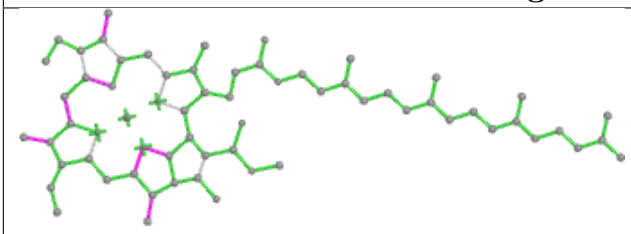
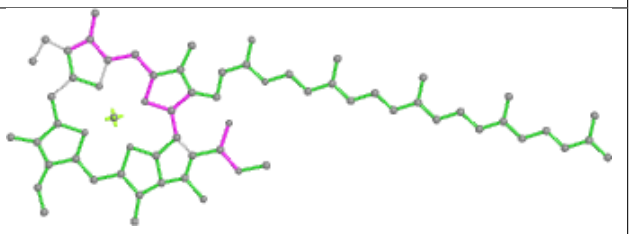
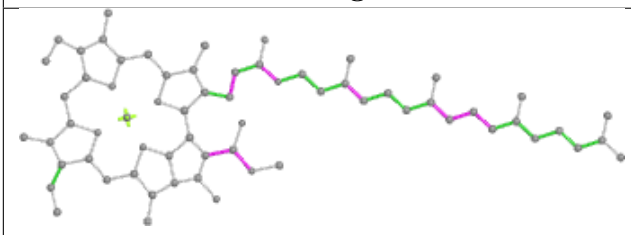
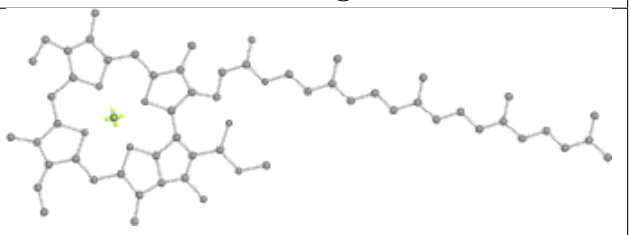
Bond angles

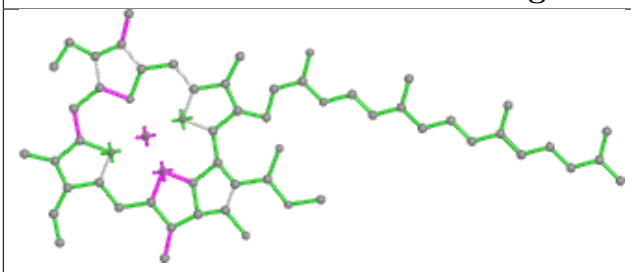
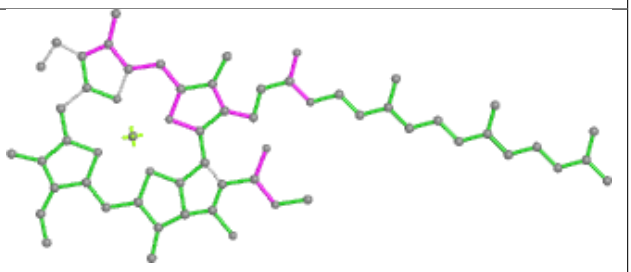
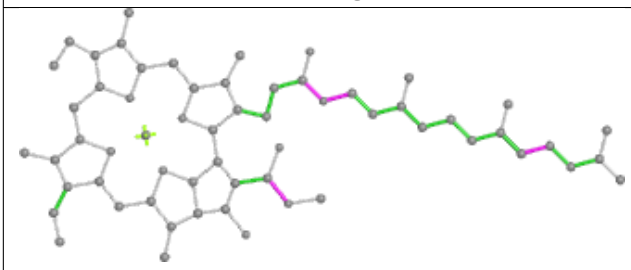
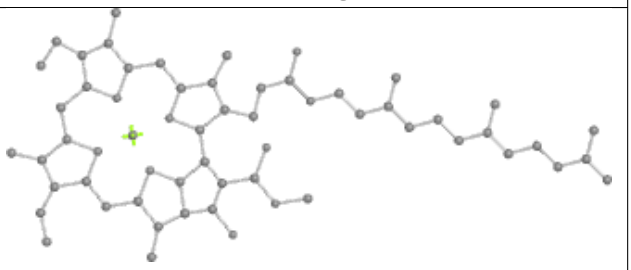


Torsions

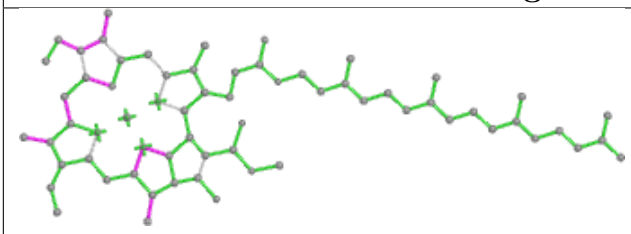


Rings

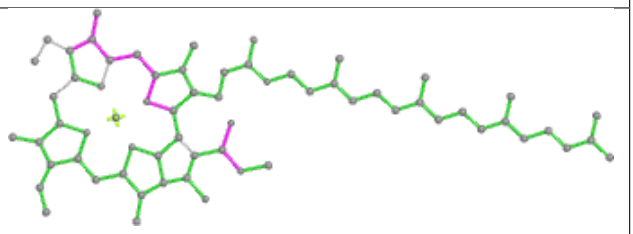
Ligand CLA b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

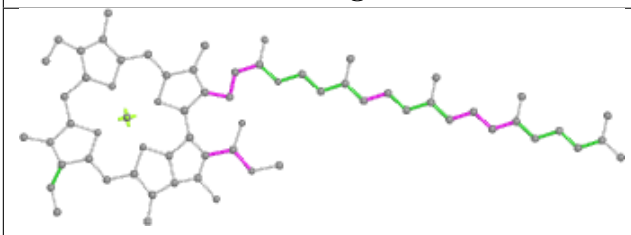
Ligand CLA V 301



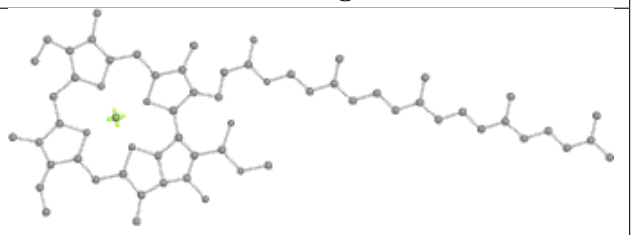
Bond lengths



Bond angles

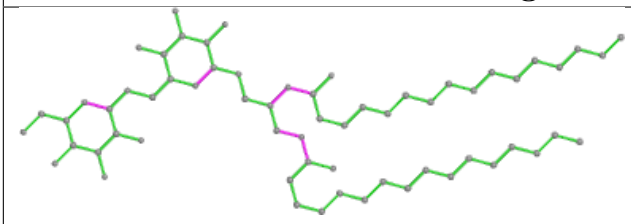


Torsions

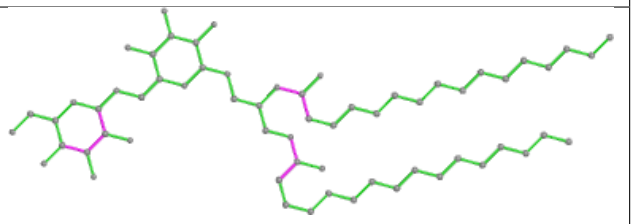


Rings

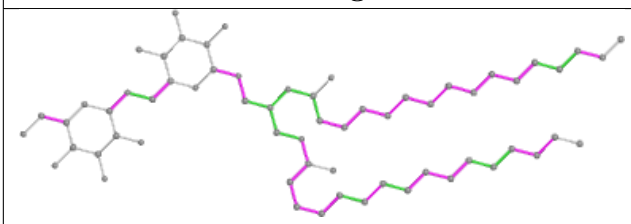
Ligand DGD C 520



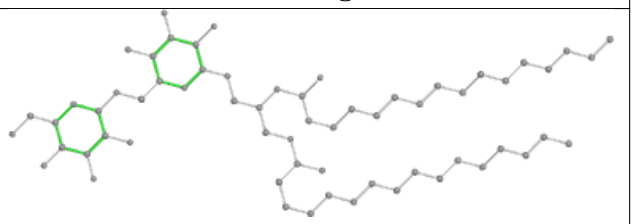
Bond lengths



Bond angles

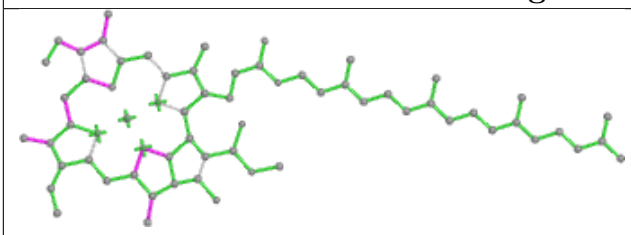


Torsions

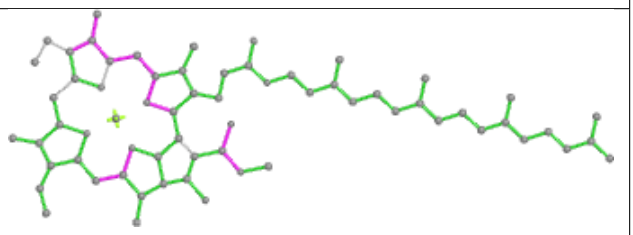


Rings

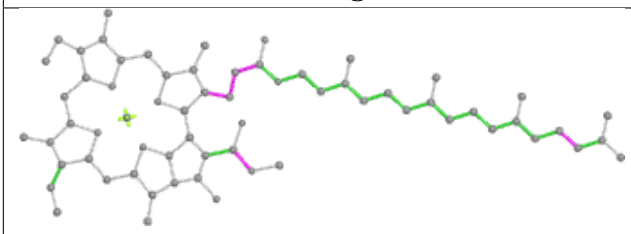
Ligand CLA 1 301



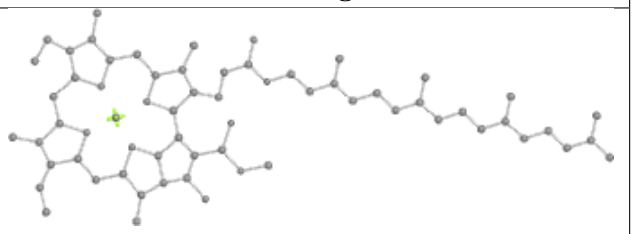
Bond lengths



Bond angles

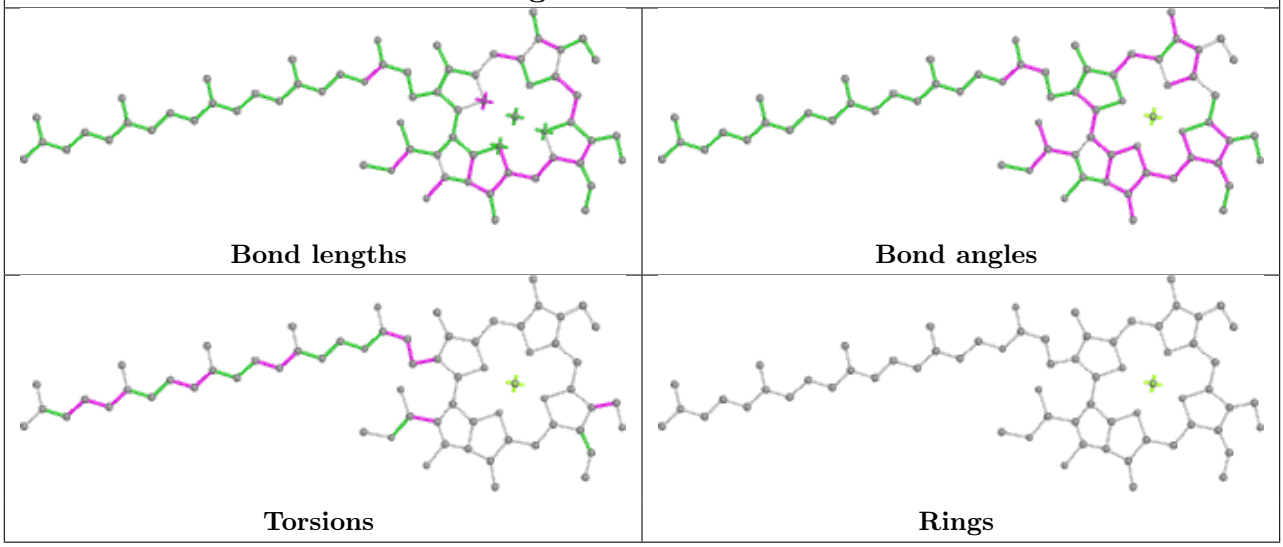


Torsions

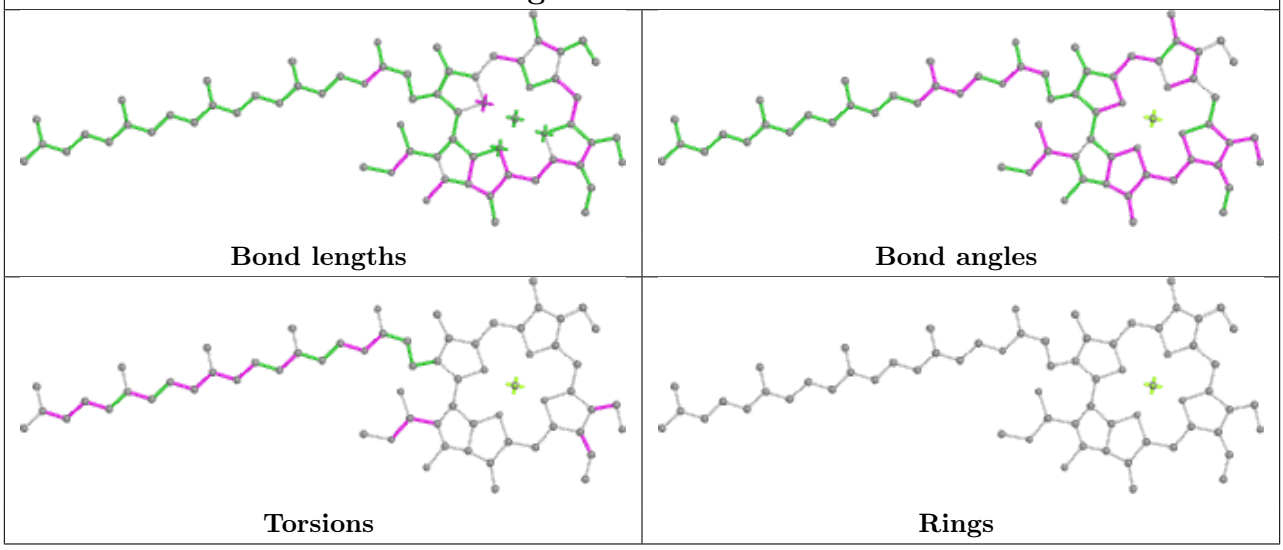


Rings

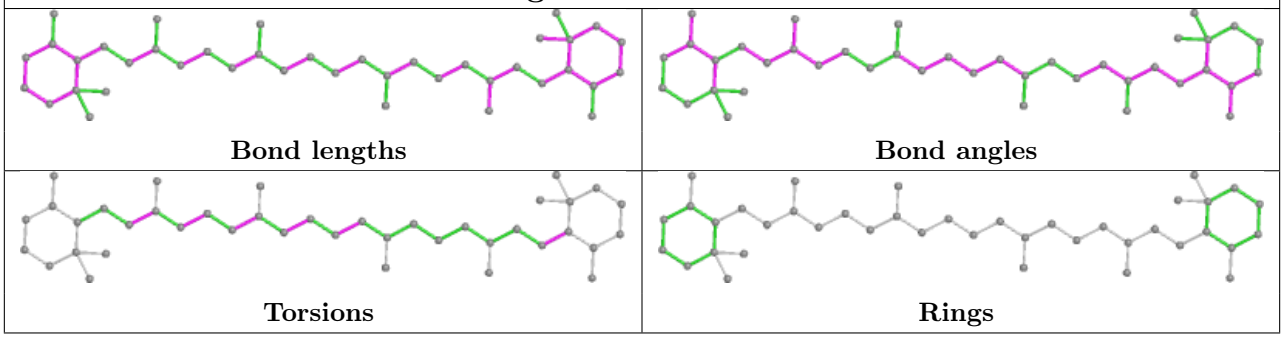
Ligand CHL 5 316

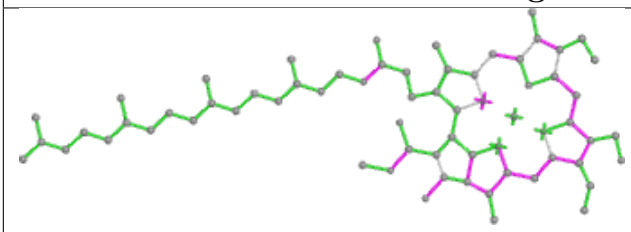
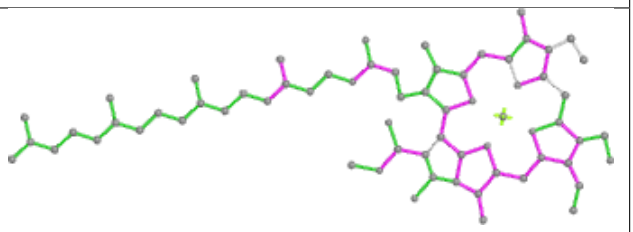
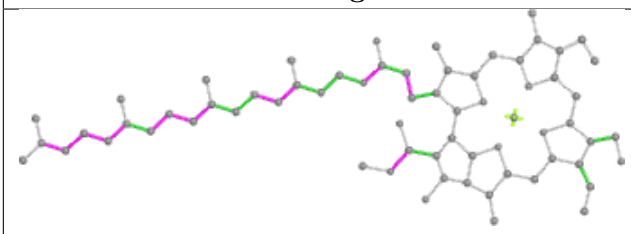
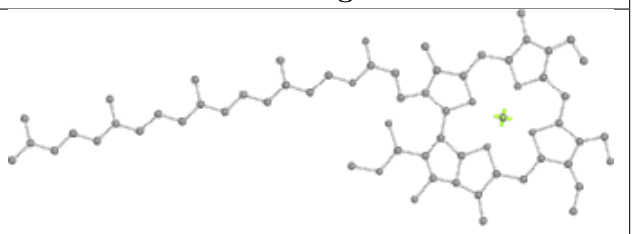


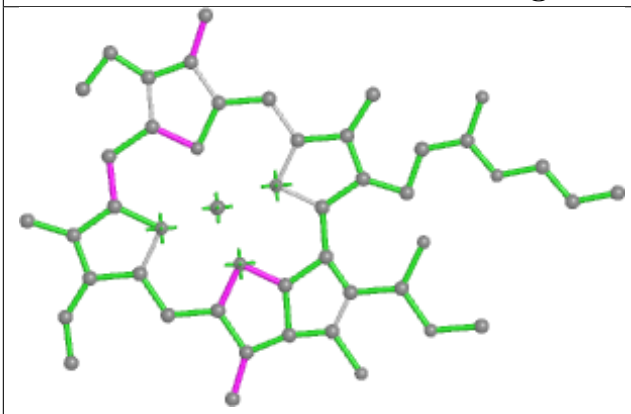
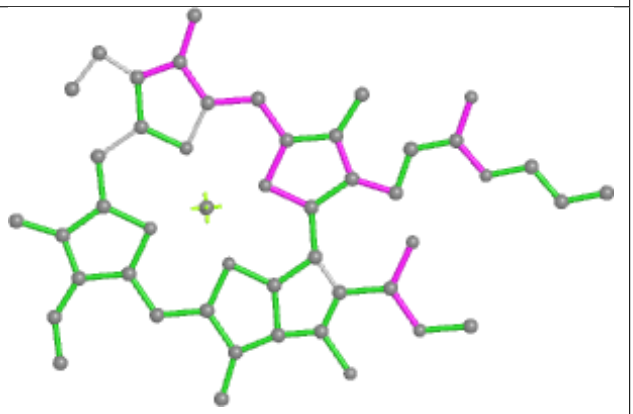
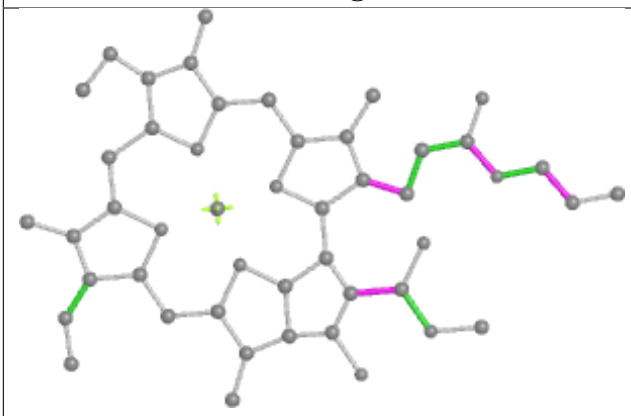
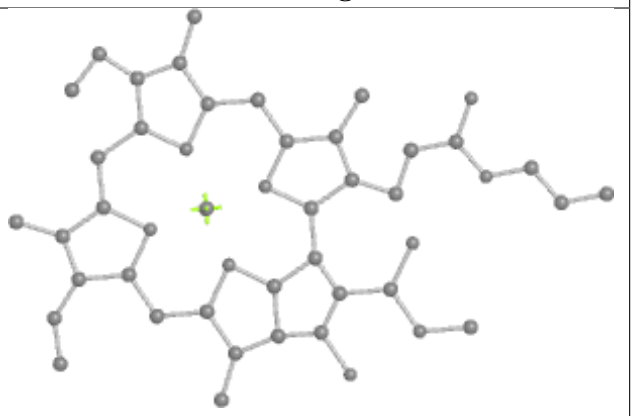
Ligand CHL n 318



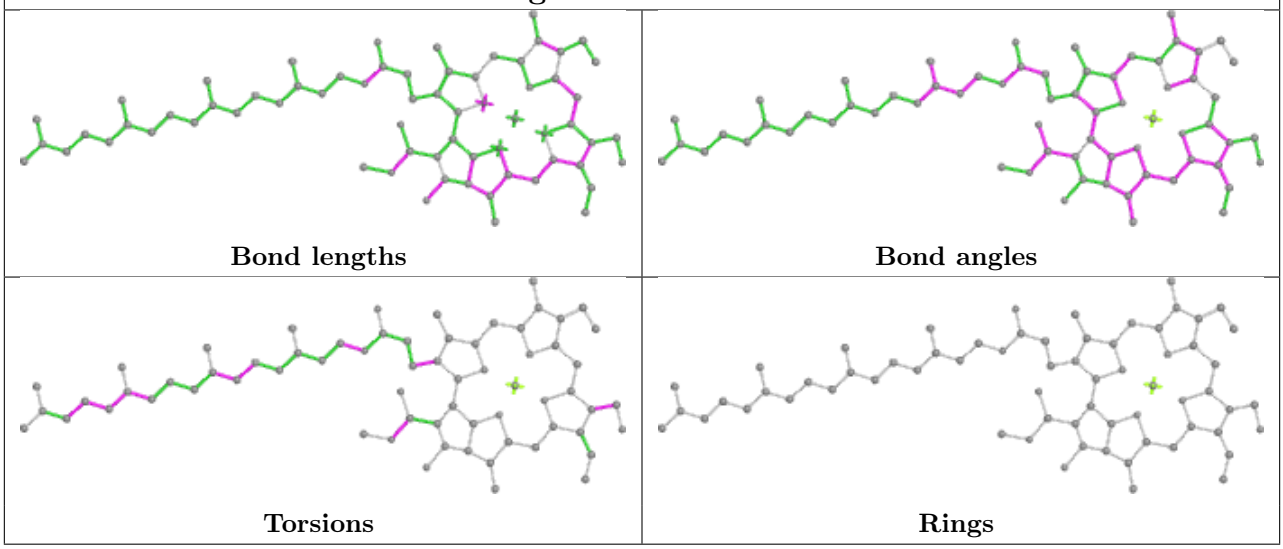
Ligand BCR x 202



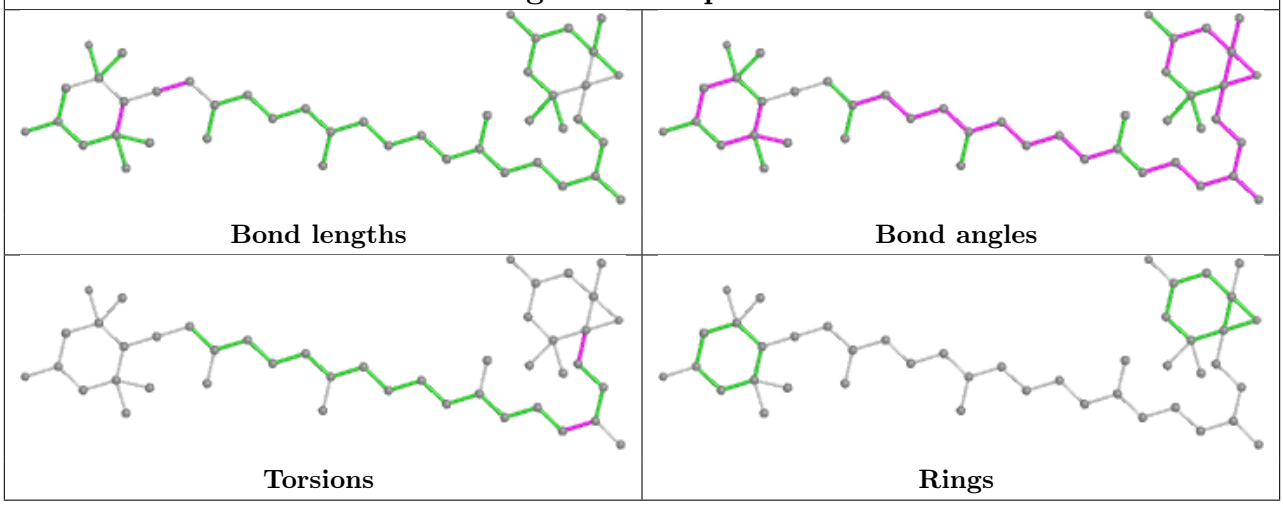
Ligand CHL 3 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

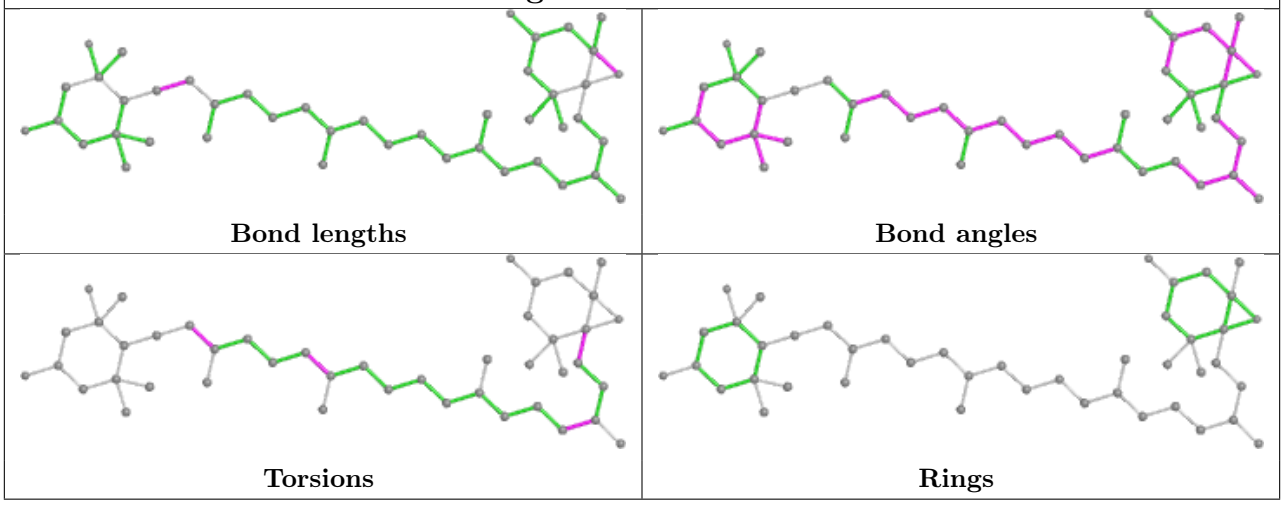
Ligand CHL 1 318



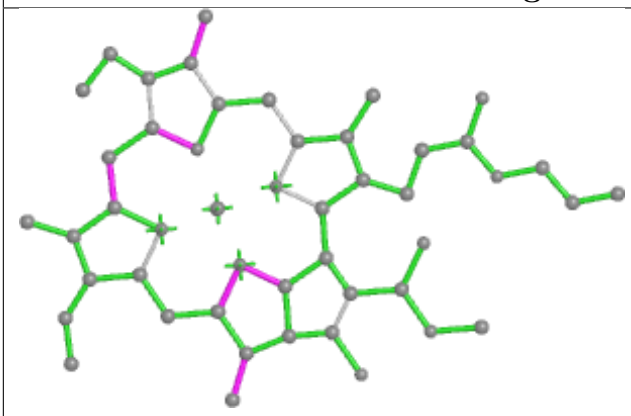
Ligand NEX p 301



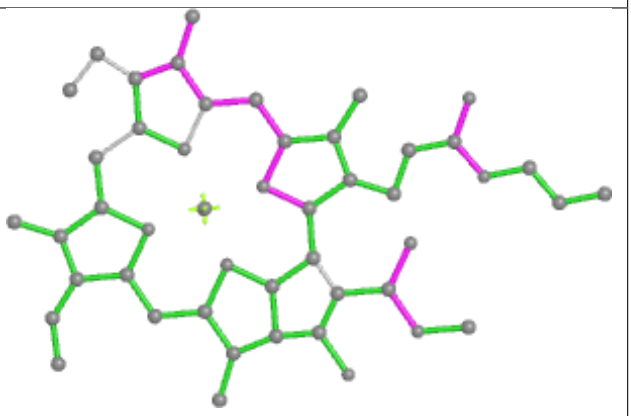
Ligand NEX n 319



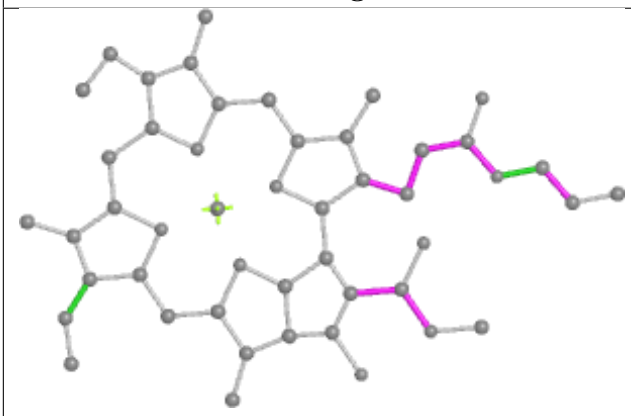
Ligand CLA N 308



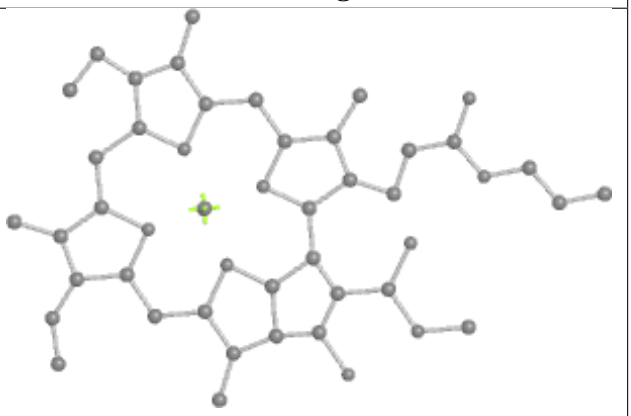
Bond lengths



Bond angles

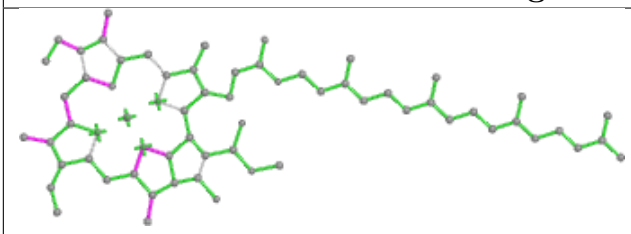


Torsions

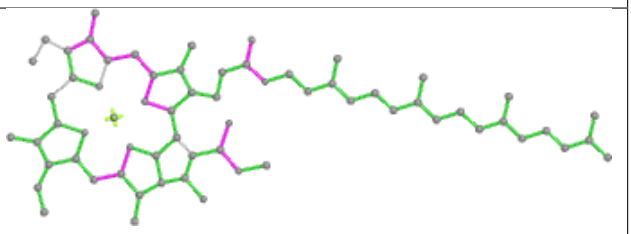


Rings

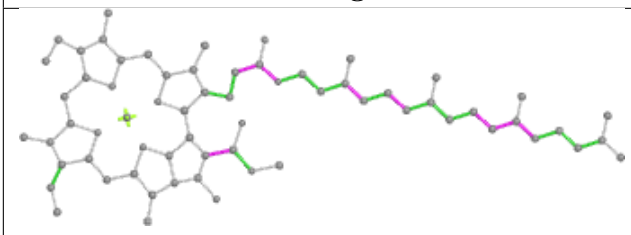
Ligand CLA v 302



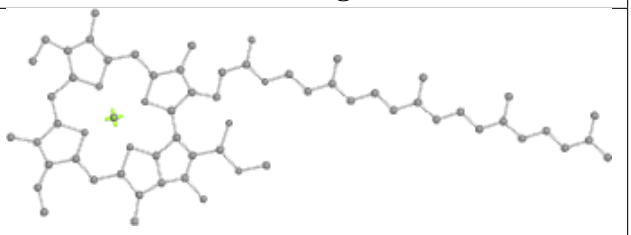
Bond lengths



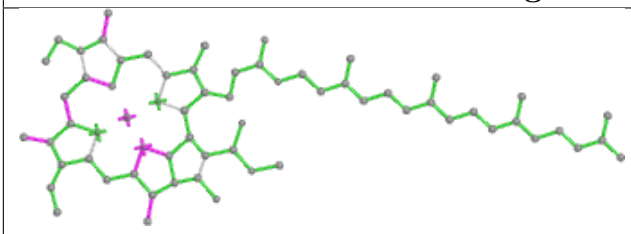
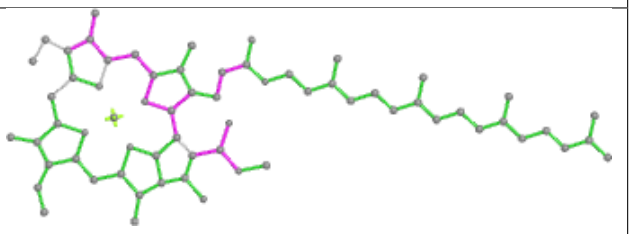
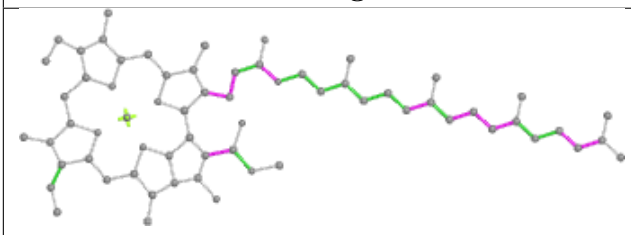
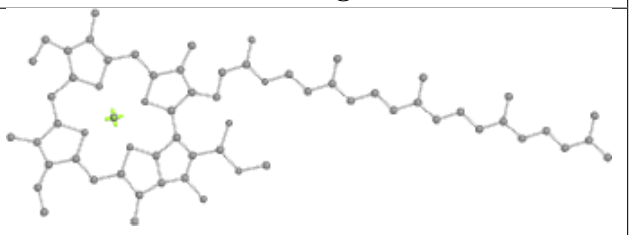
Bond angles

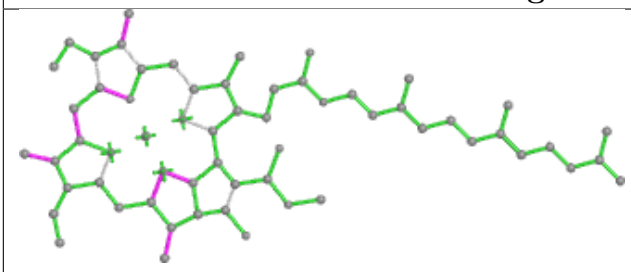
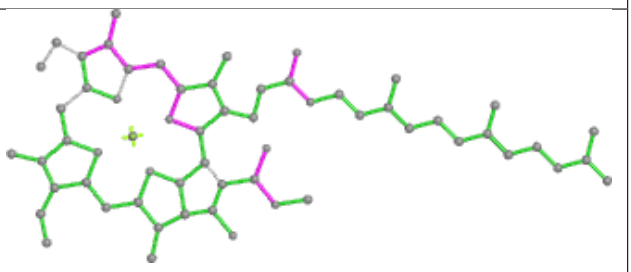
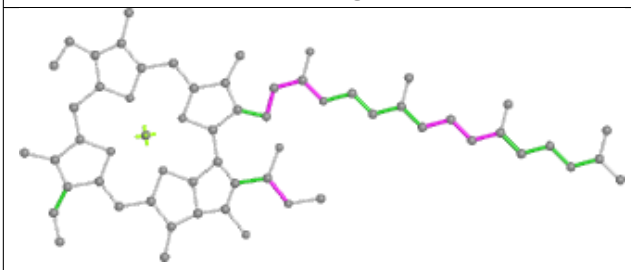
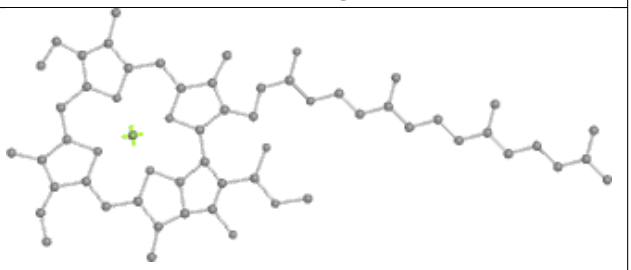


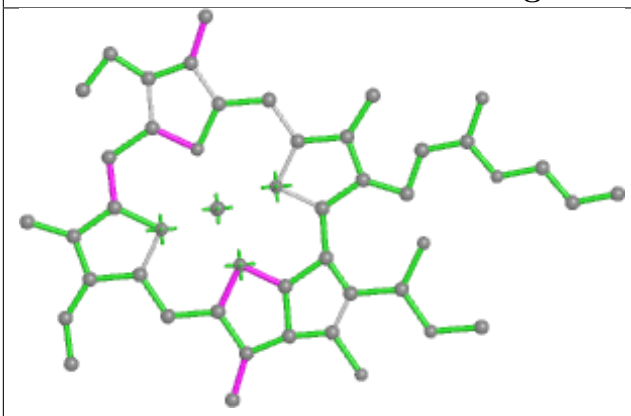
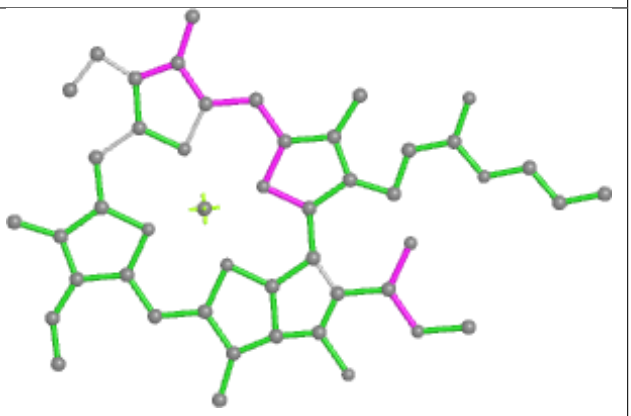
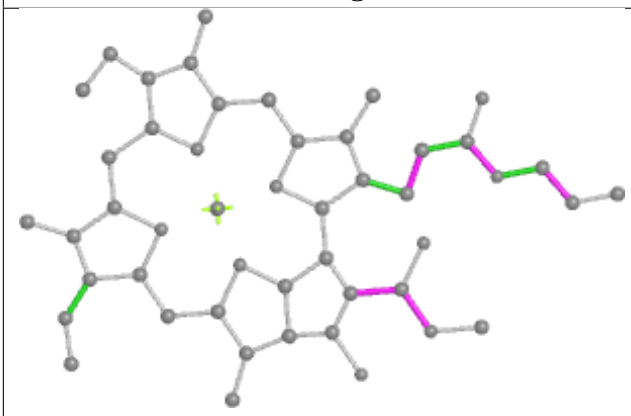
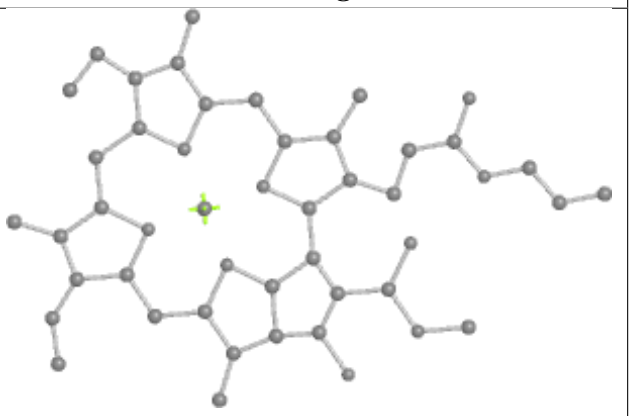
Torsions

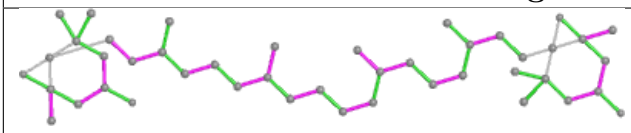
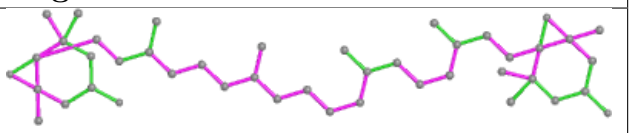
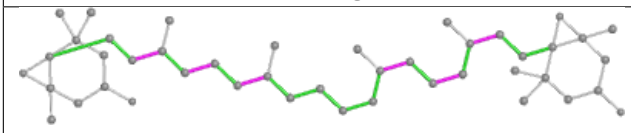
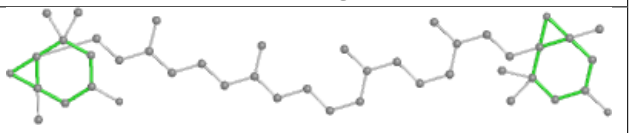


Rings

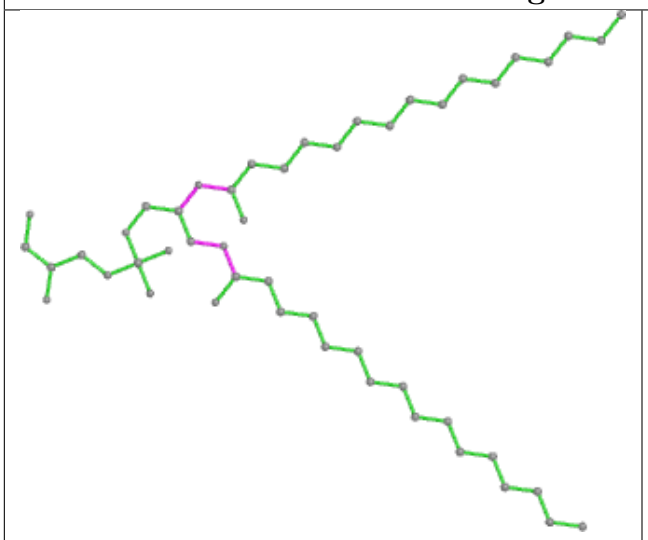
Ligand CLA B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

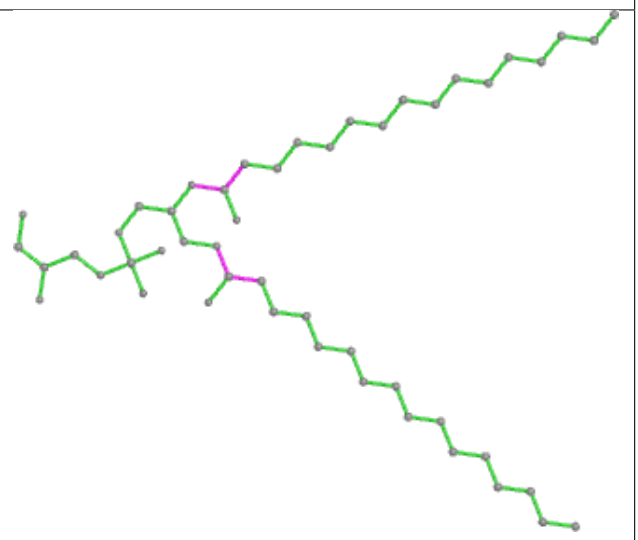
Ligand CLA V 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT g 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

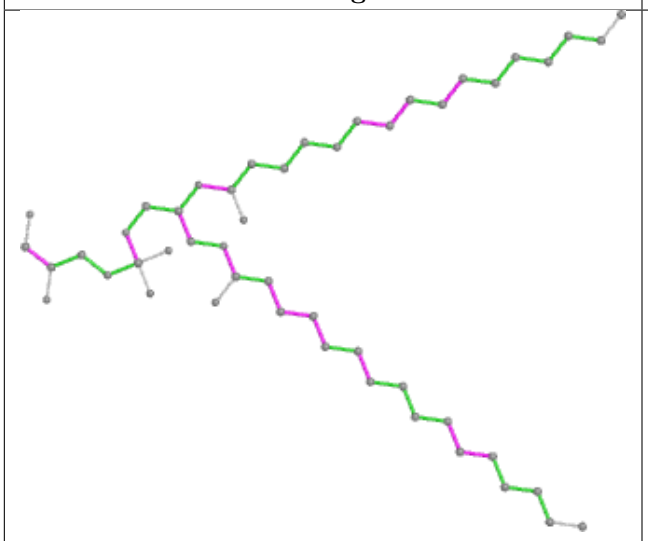
Ligand LHG 6 311



Bond lengths



Bond angles



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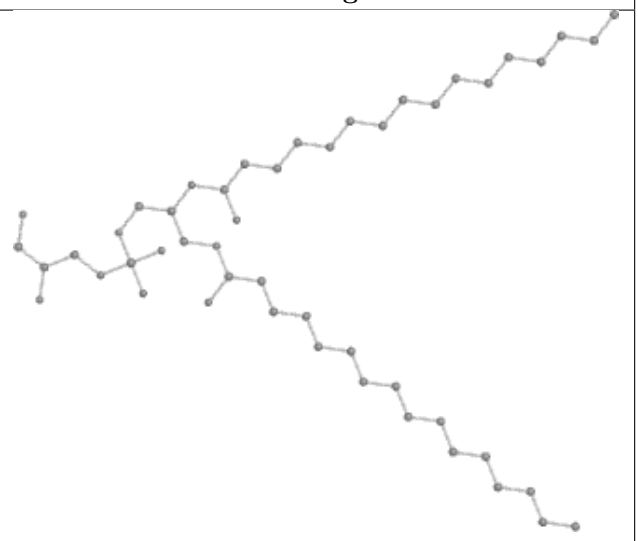
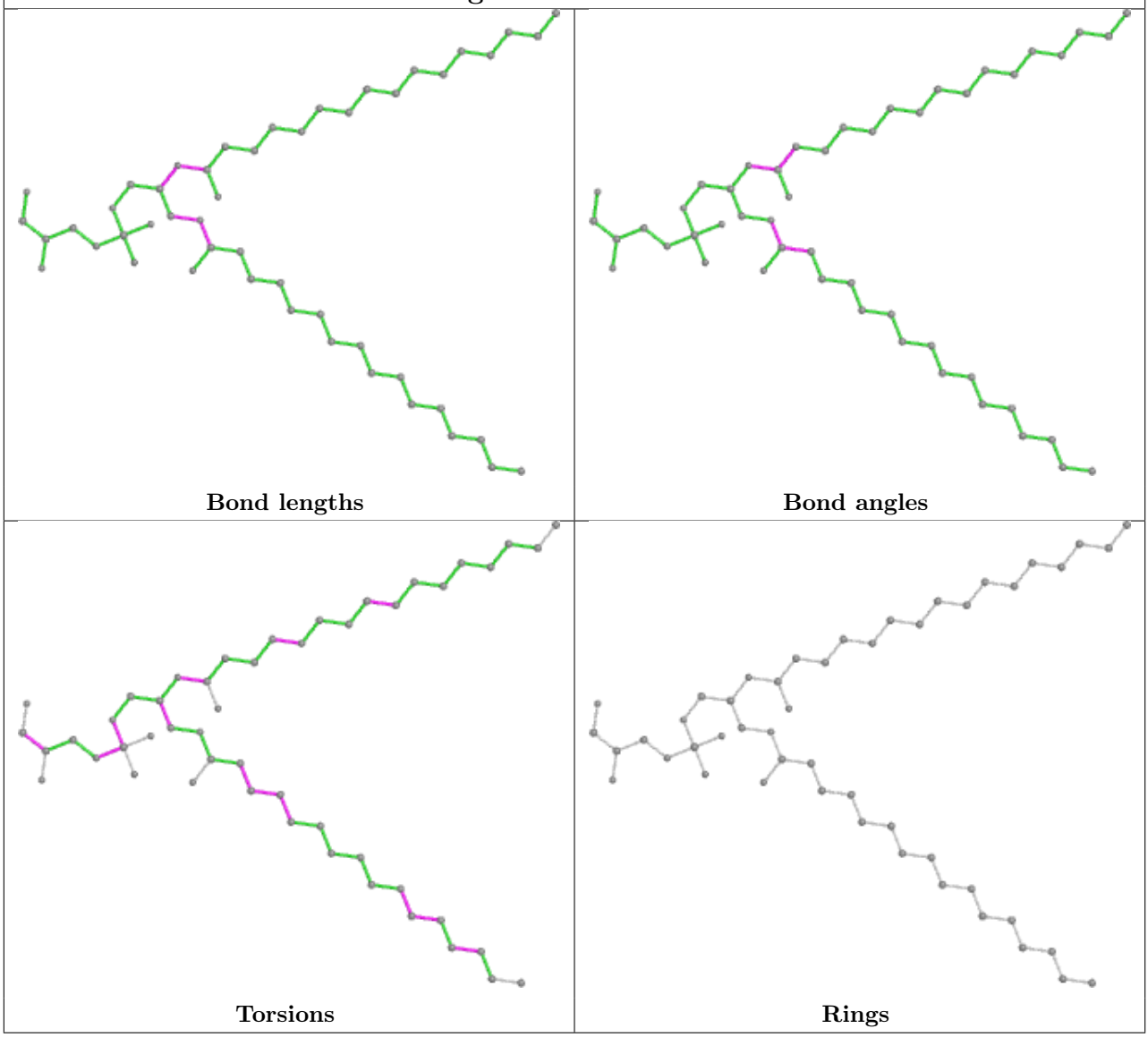
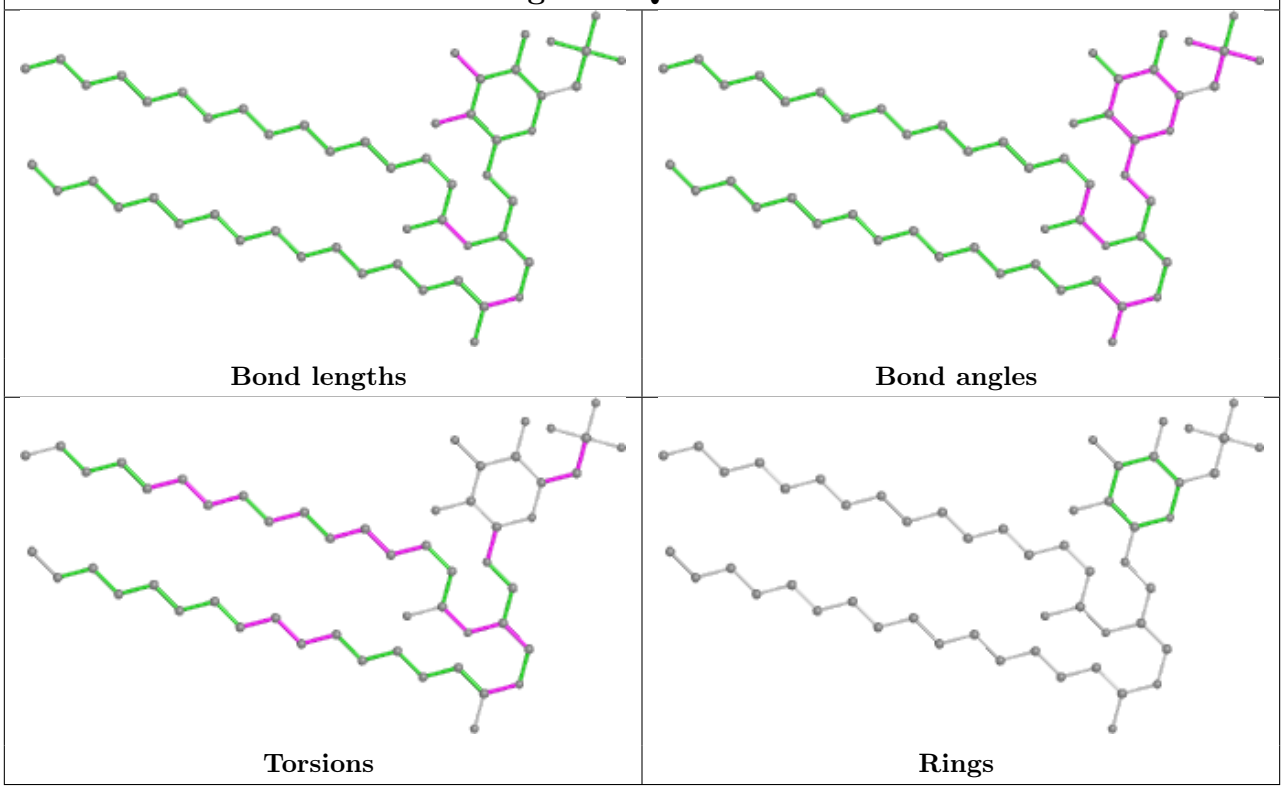


Rings

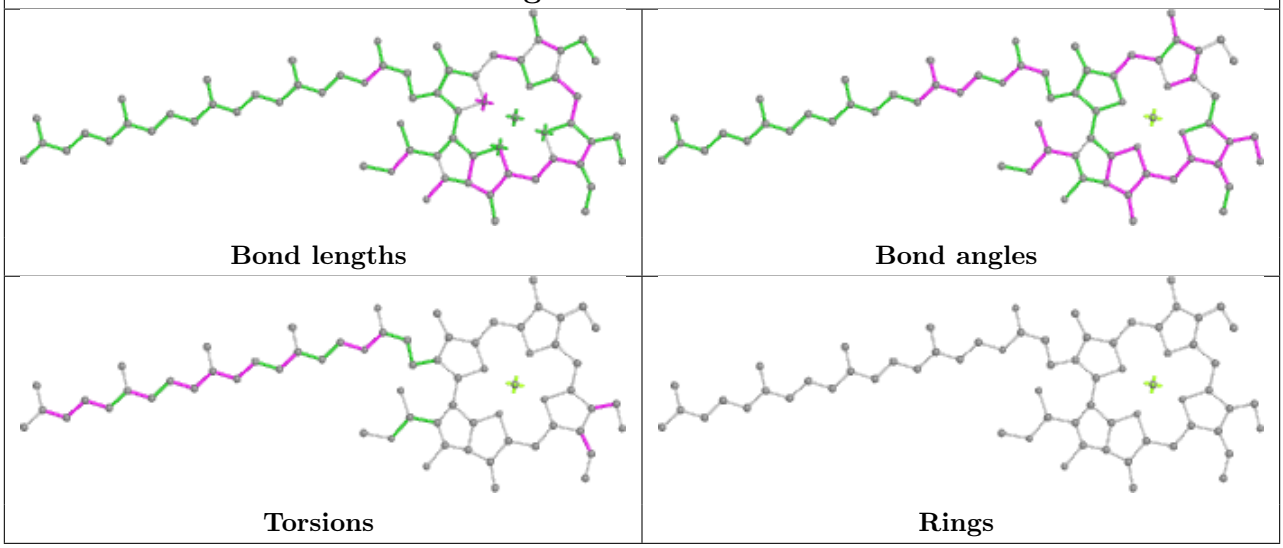
Ligand LHG V 312

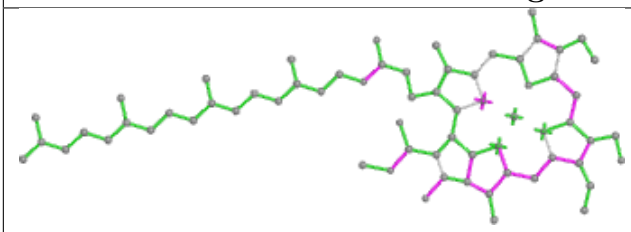
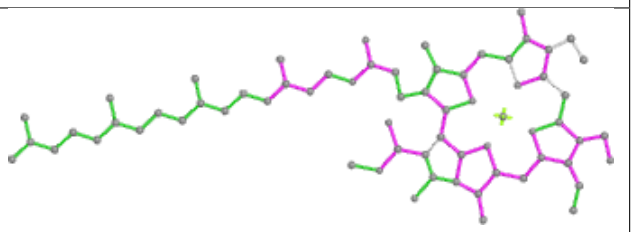
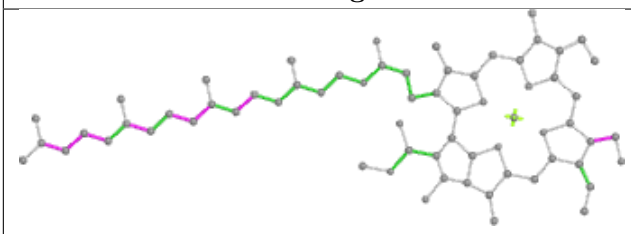
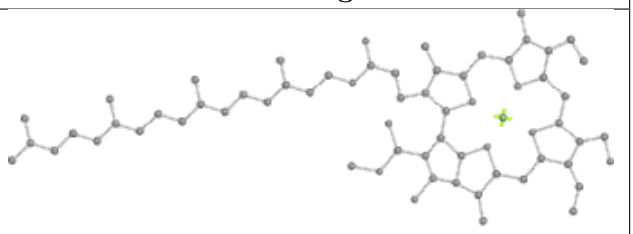


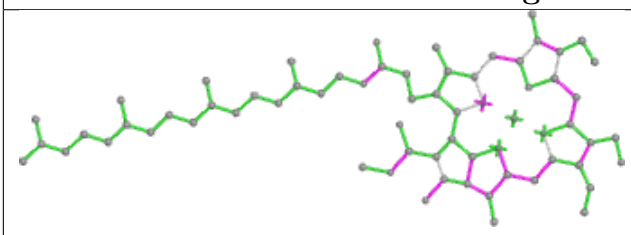
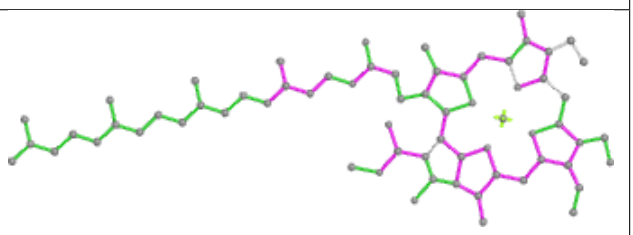
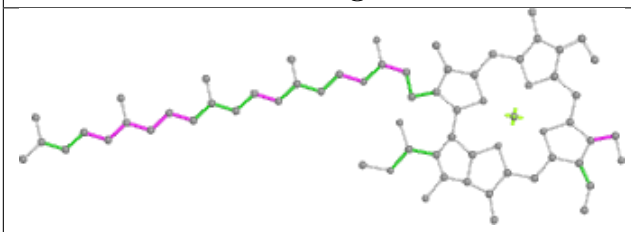
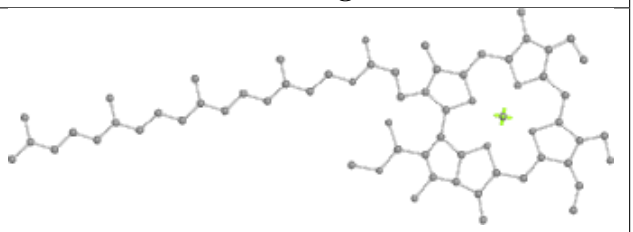
Ligand SQD L 102

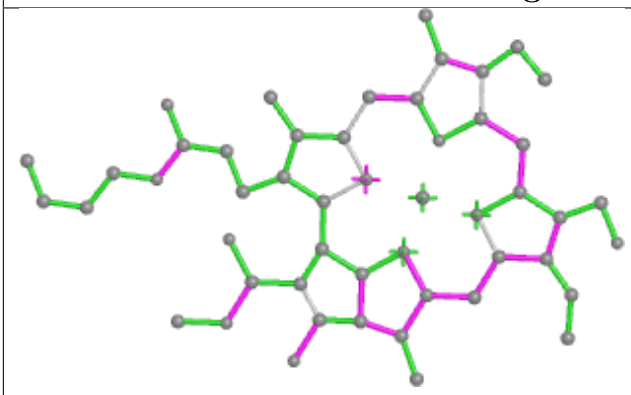
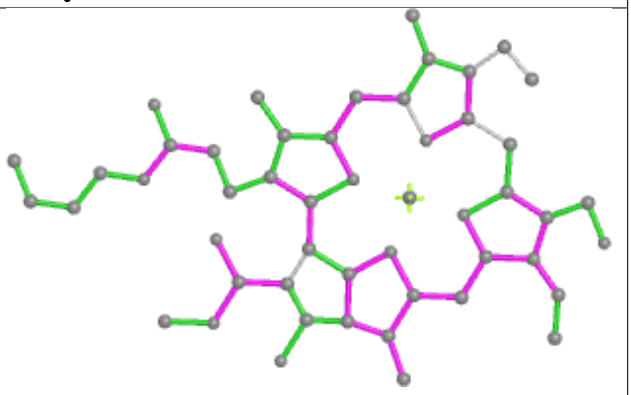
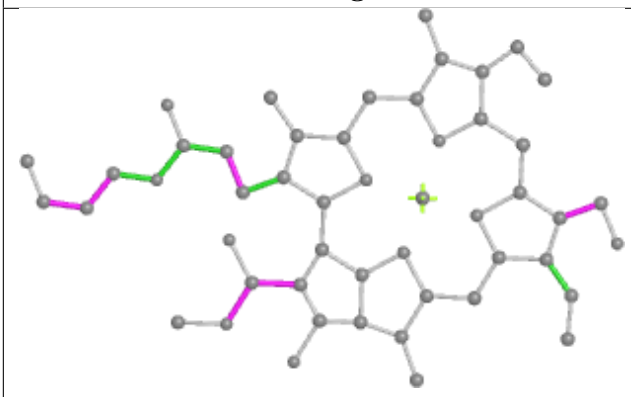
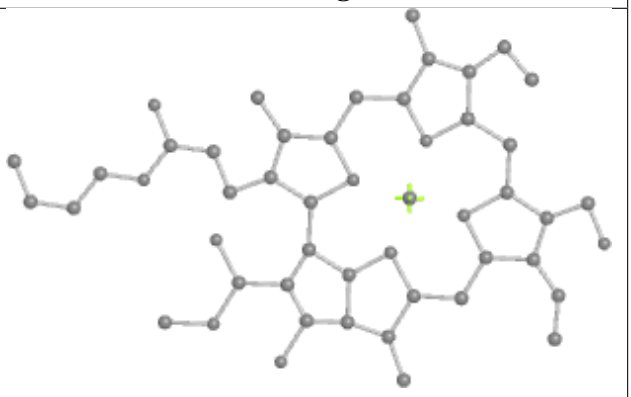


Ligand CHL N 317

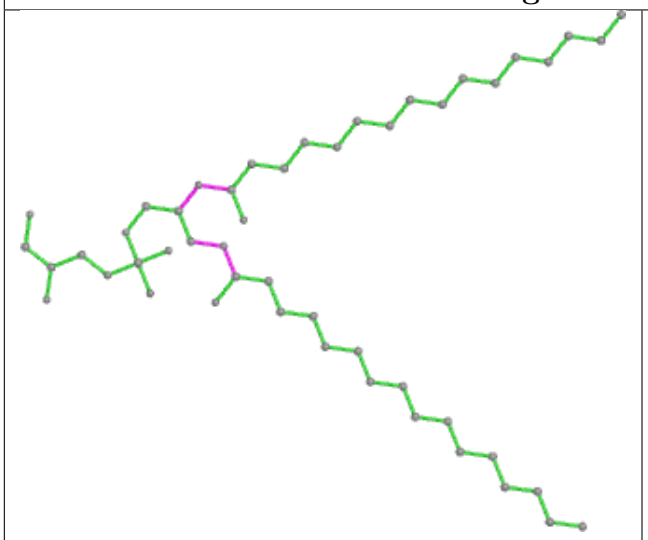


Ligand CHL v 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

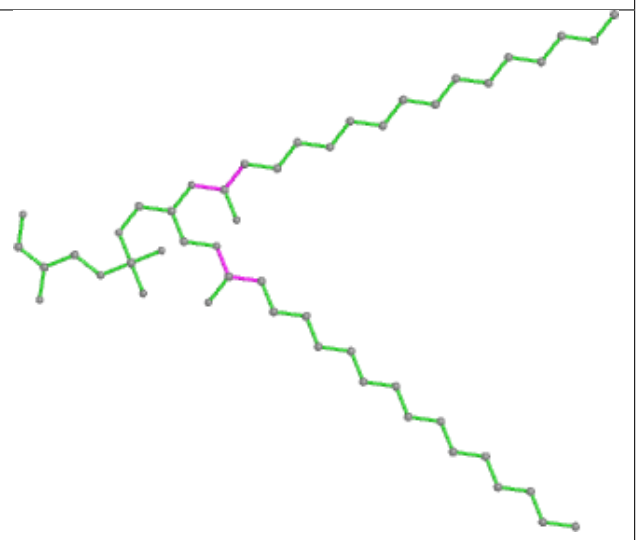
Ligand CHL N 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Q 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

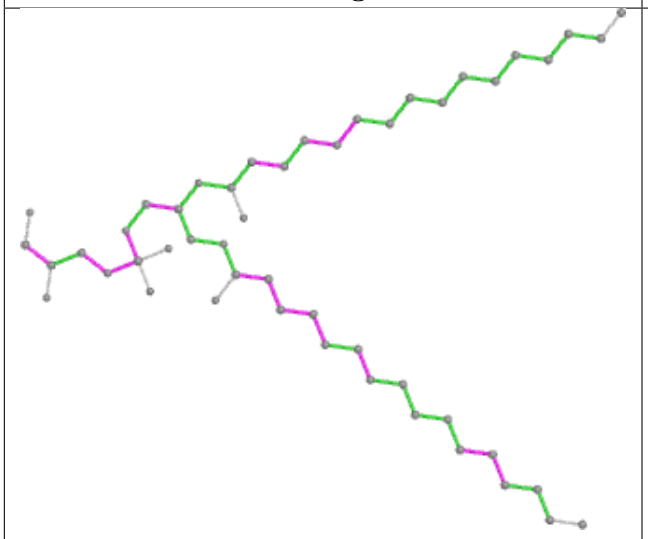
Ligand LHG G 310



Bond lengths



Bond angles



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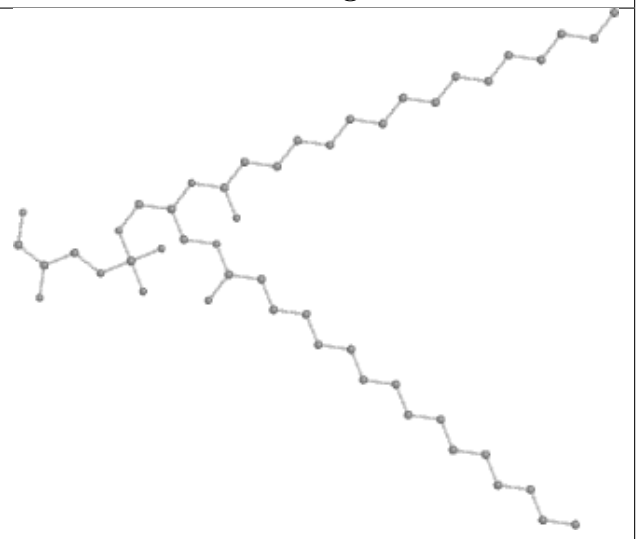
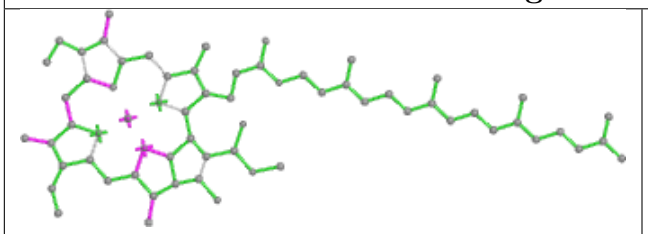
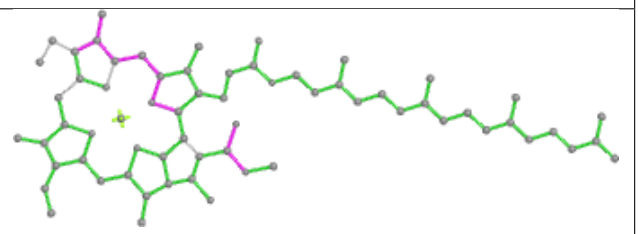


Rings

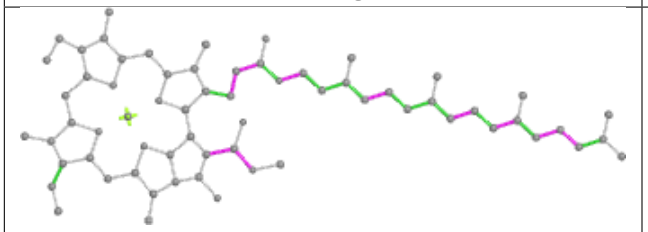
Ligand CLA B 609



Bond lengths



Bond angles



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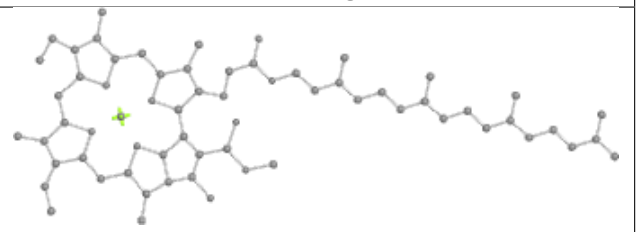
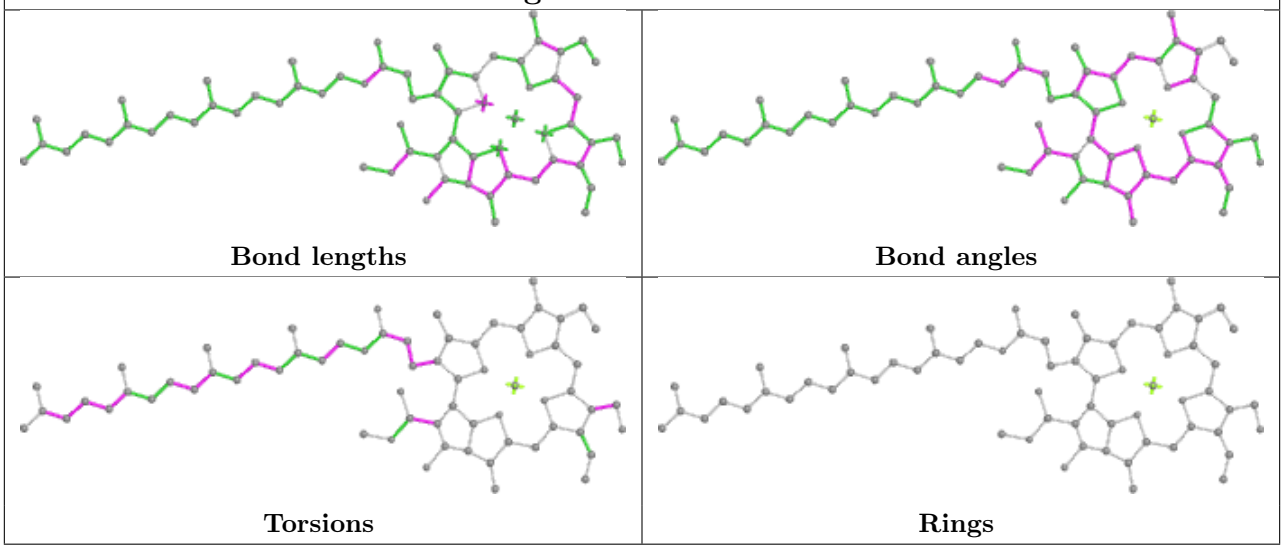
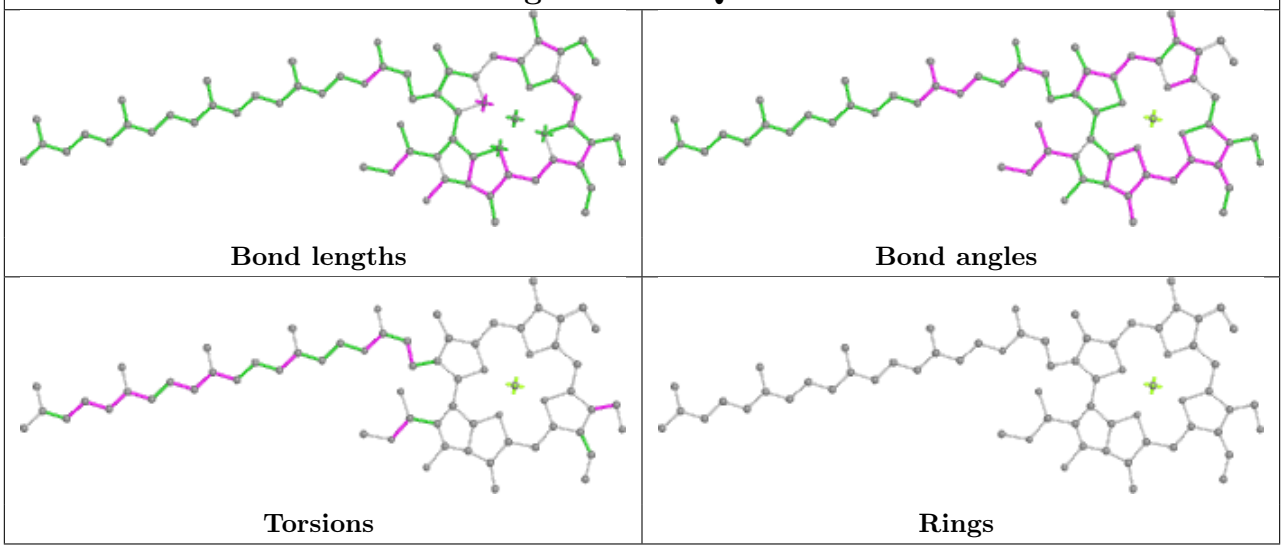


Rings

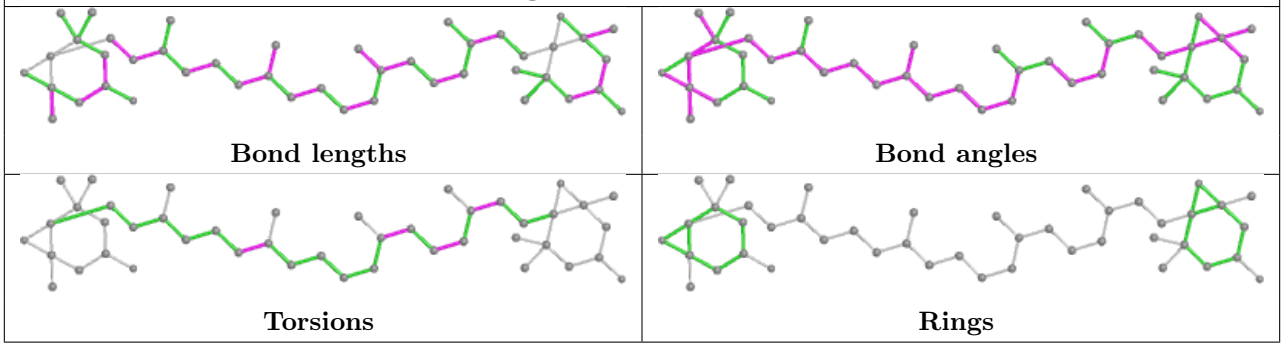
Ligand CHL U 319

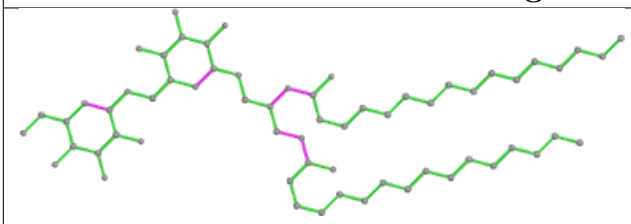
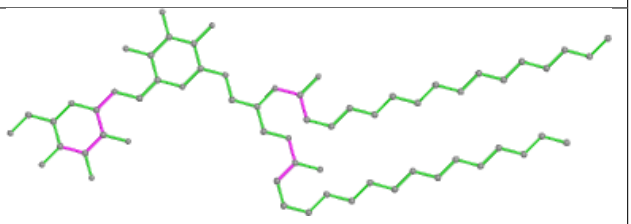
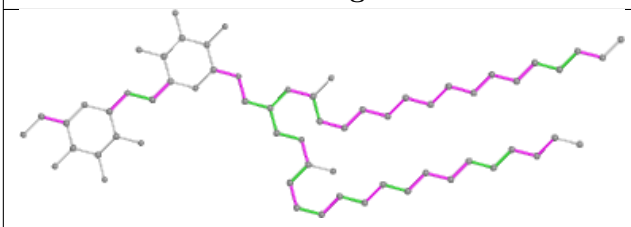
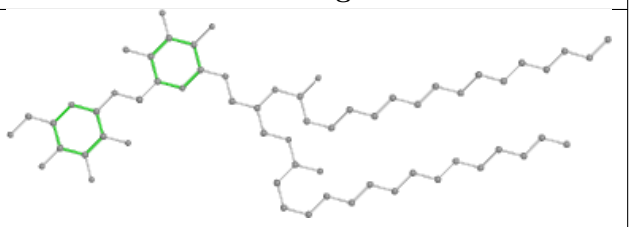


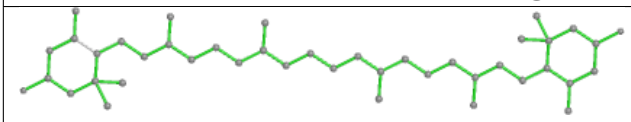
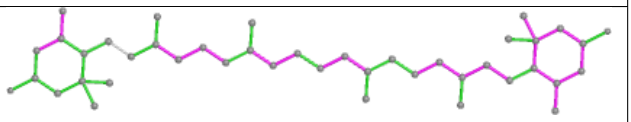
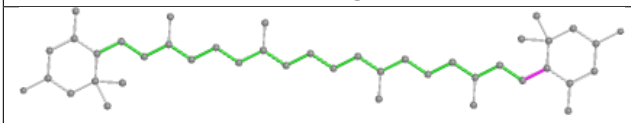
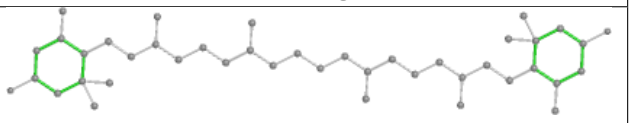
Ligand CHL Q 314

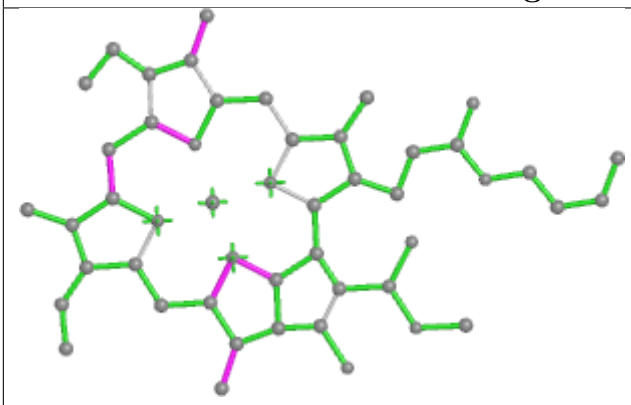
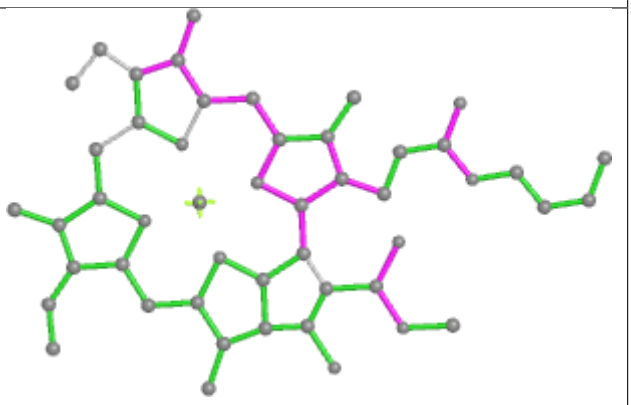
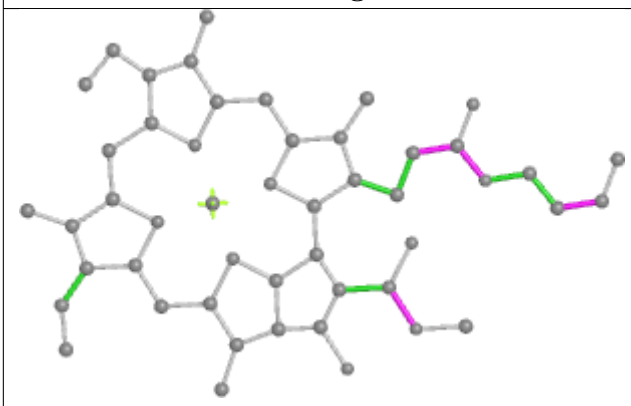
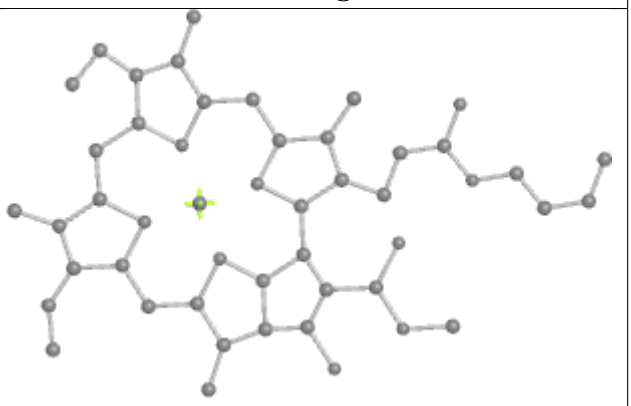


Ligand XAT U 311

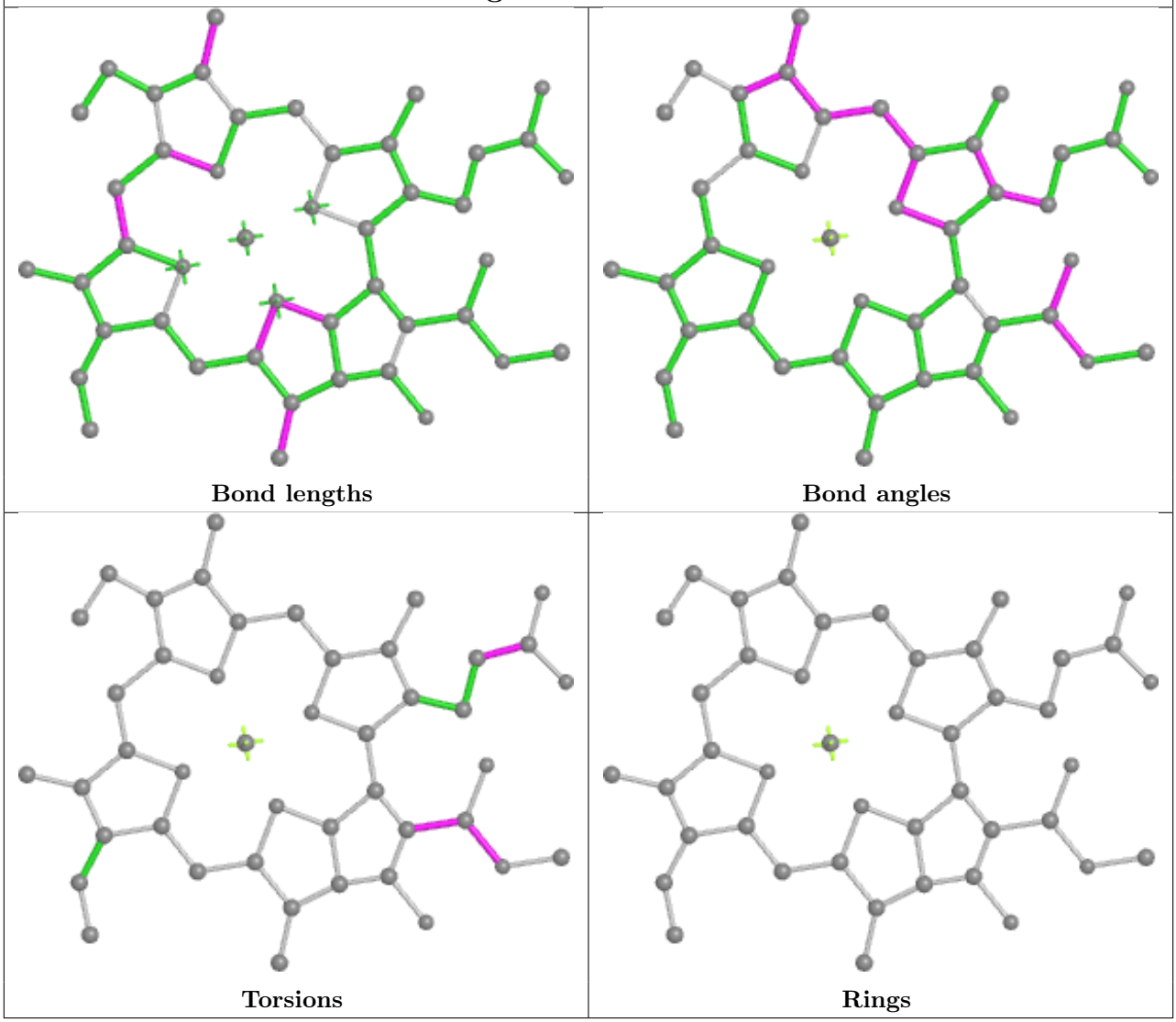


Ligand DGD c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

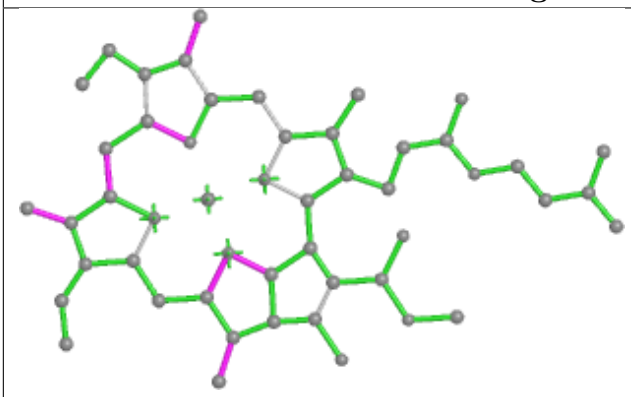
Ligand LUT v 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

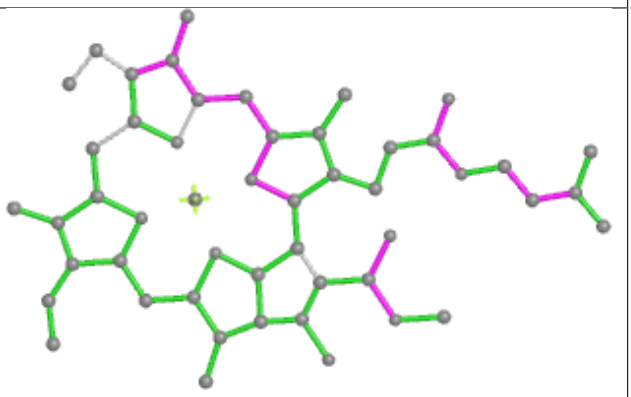
Ligand CLA s 302



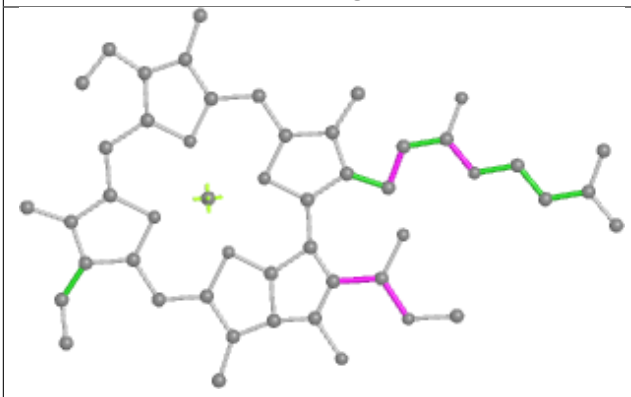
Ligand CLA s 303



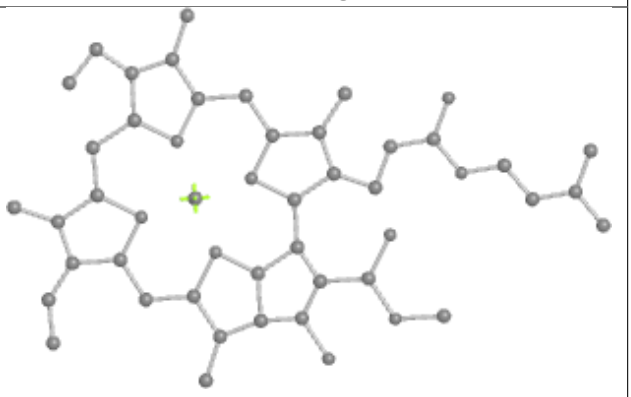
Bond lengths



Bond angles

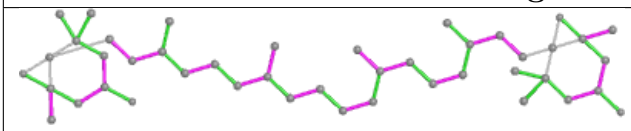


Torsions

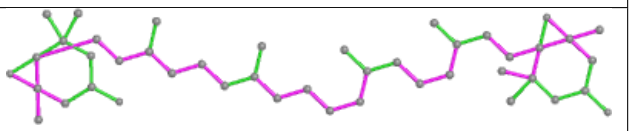


Rings

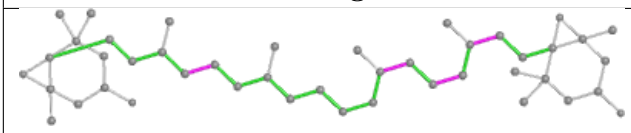
Ligand XAT 2 311



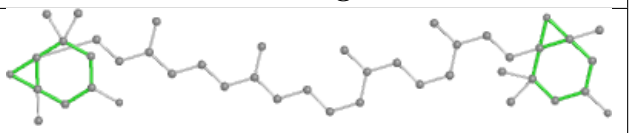
Bond lengths



Bond angles

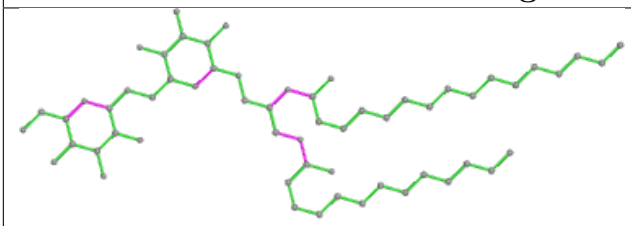


Torsions



Rings

Ligand DGD A 414



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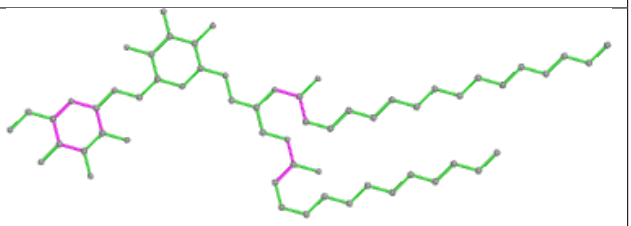

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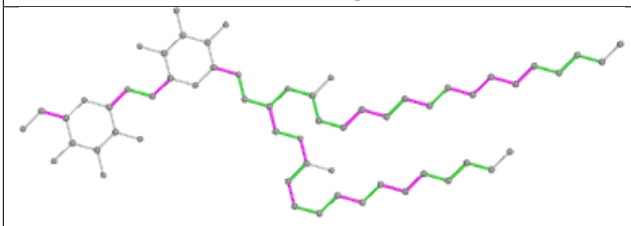

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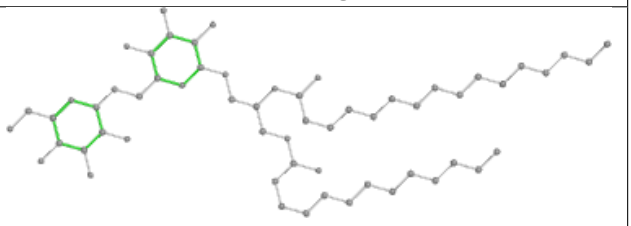
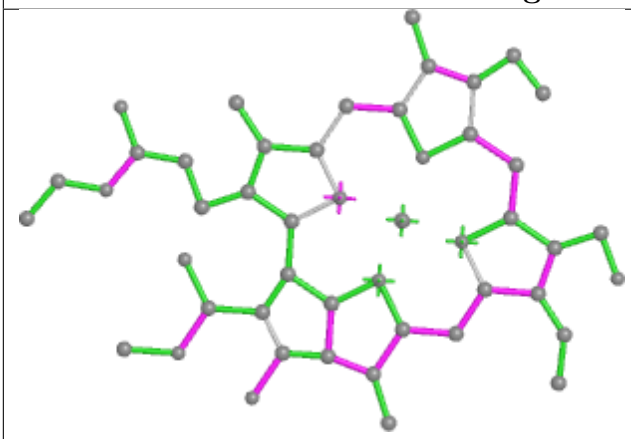


Rings

Ligand CHL Q 312



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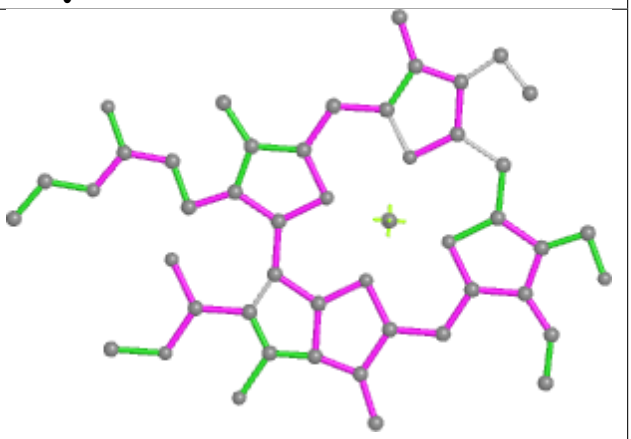
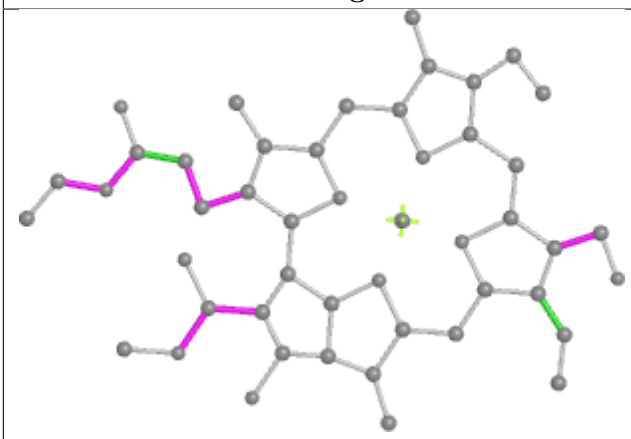


Bond angles



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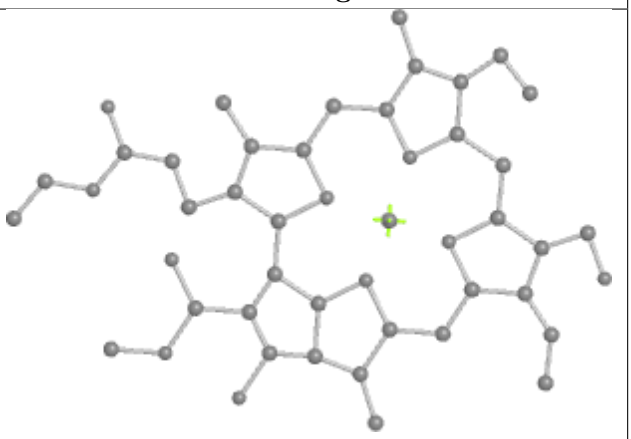
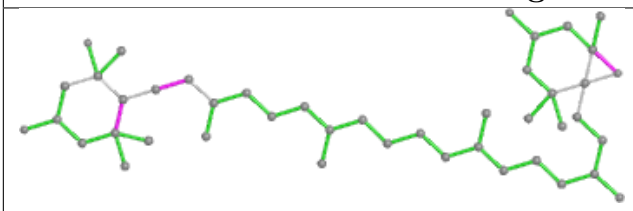


Rings

Ligand NEX r 617



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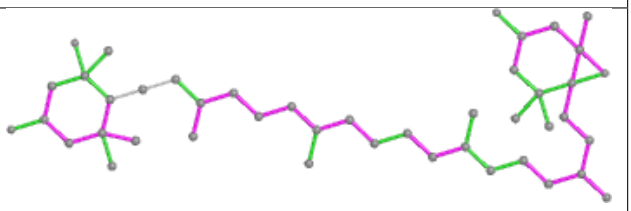
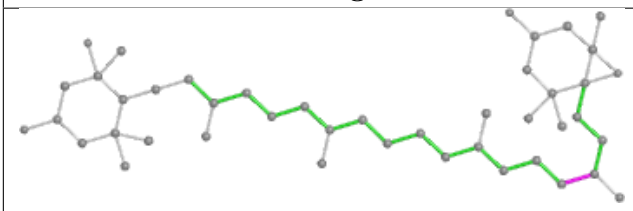


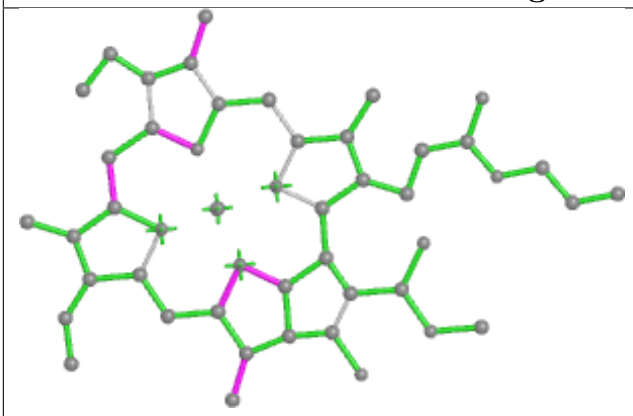
Bond angles



Torsions

Rings

Ligand CLA 5 308



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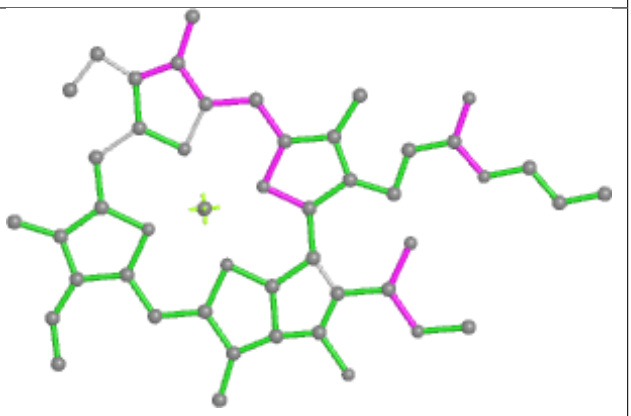

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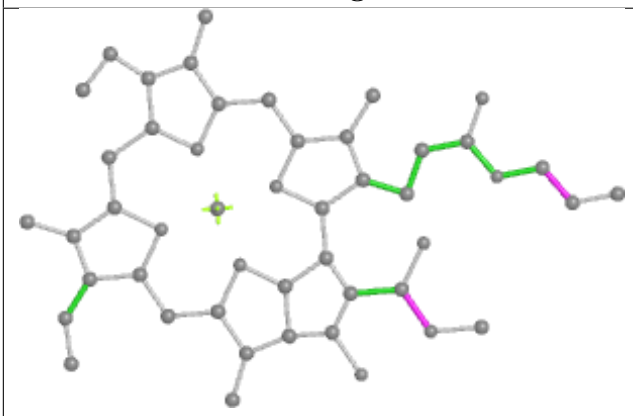

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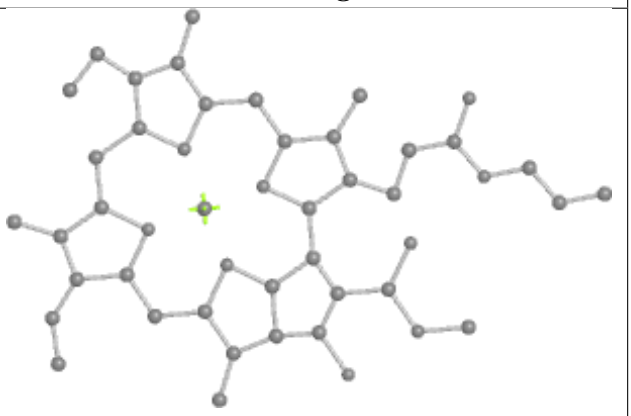
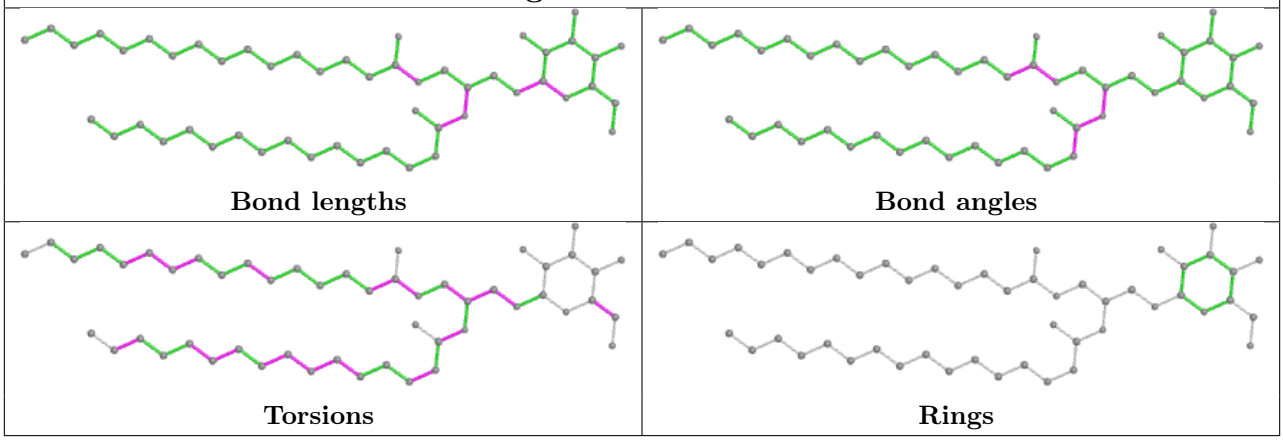


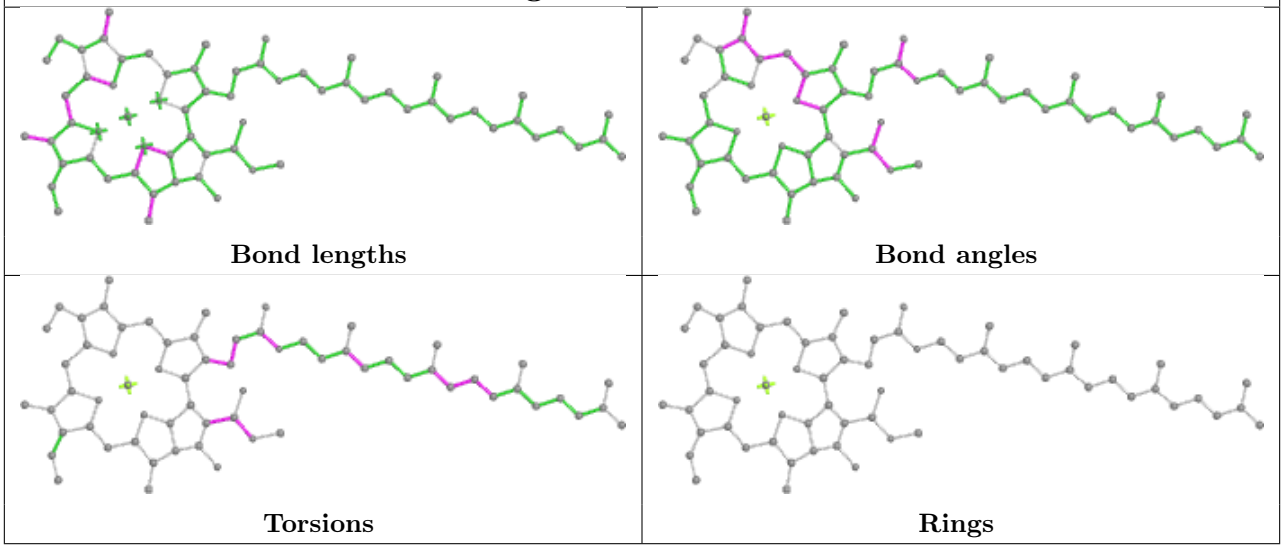
Rings

Ligand LMG c 501

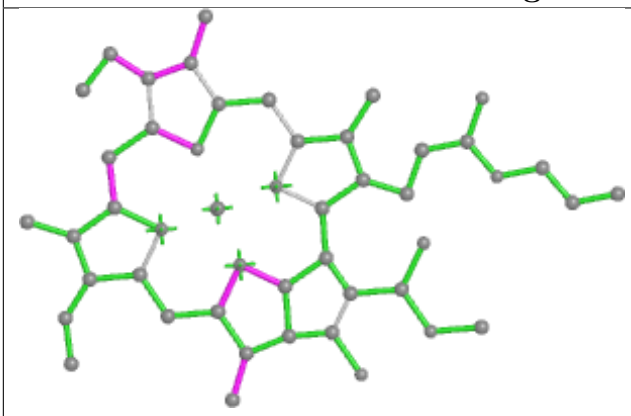


Ligand LUT P 311

Ligand CLA B 608



Ligand CLA U 308



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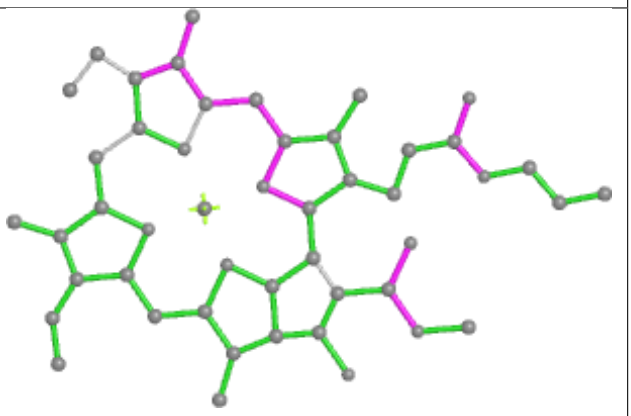
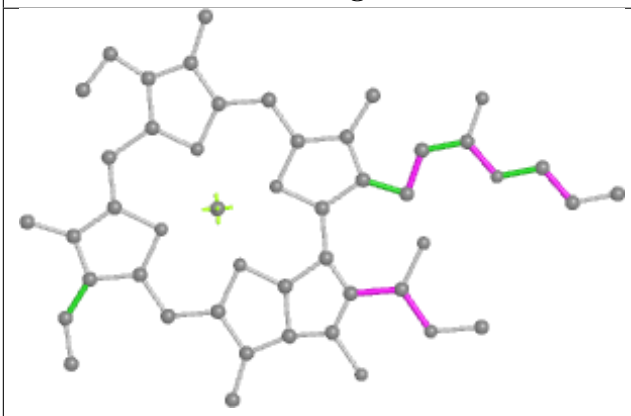


Bond angles



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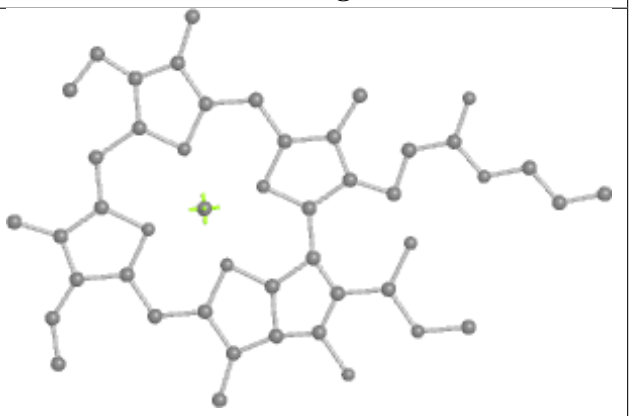
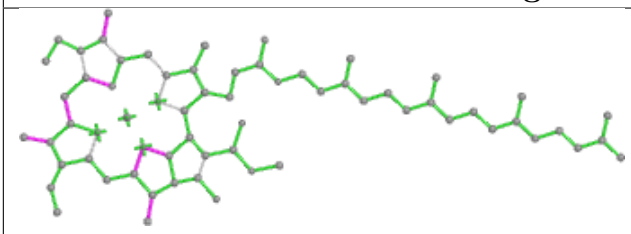


Rings

Ligand CLA N 302



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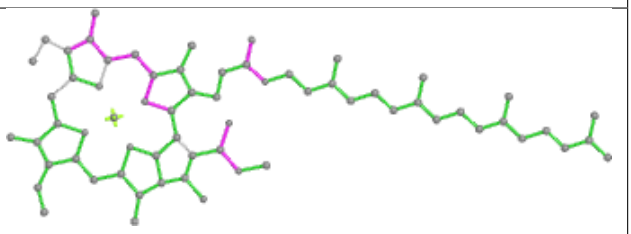

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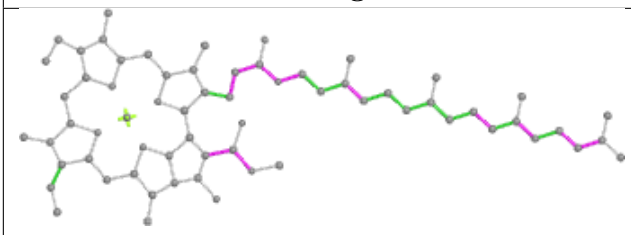

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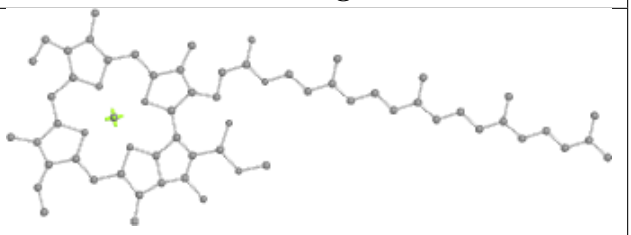
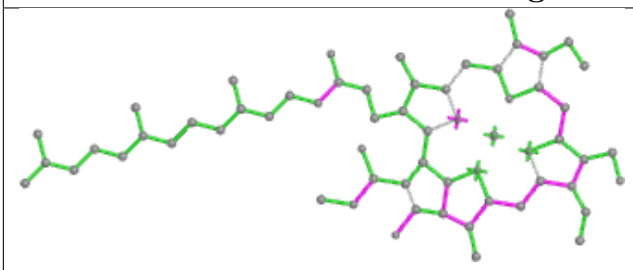


Rings

Ligand CHL 3 316



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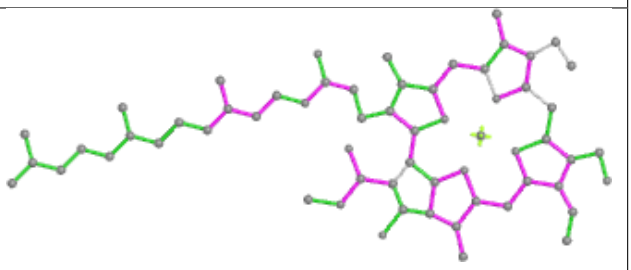

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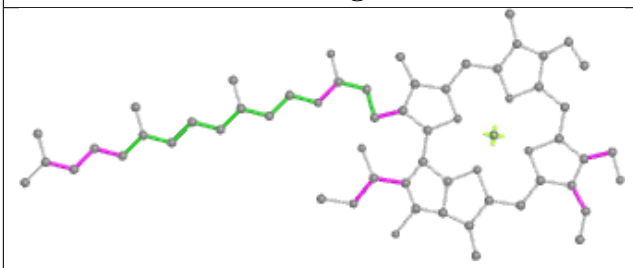

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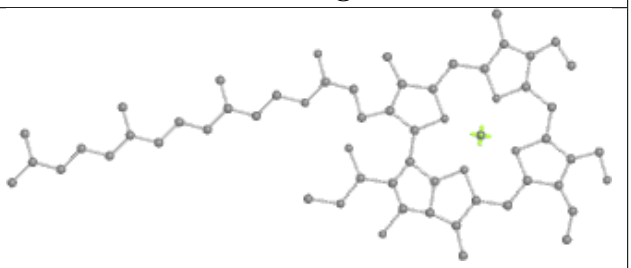
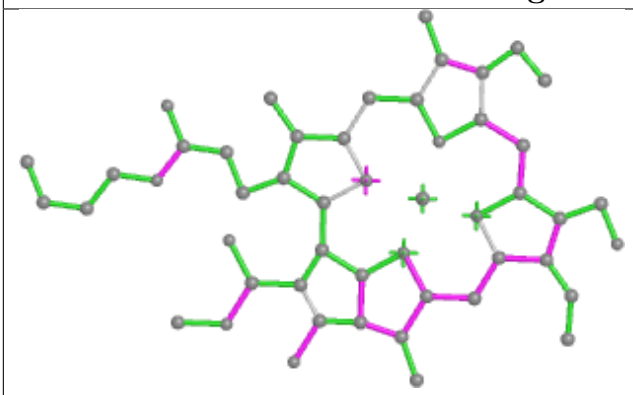
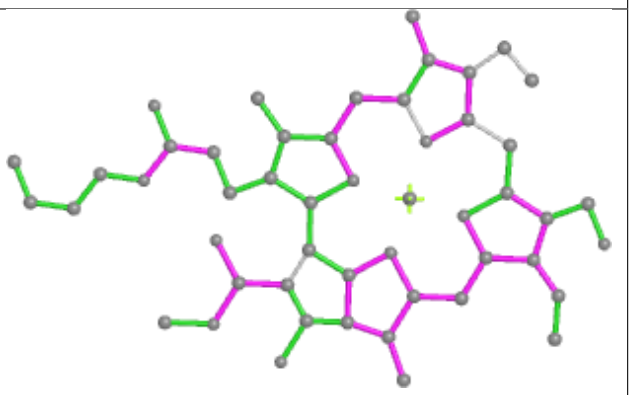


Rings

Ligand CHL 2 315



Bond lengths



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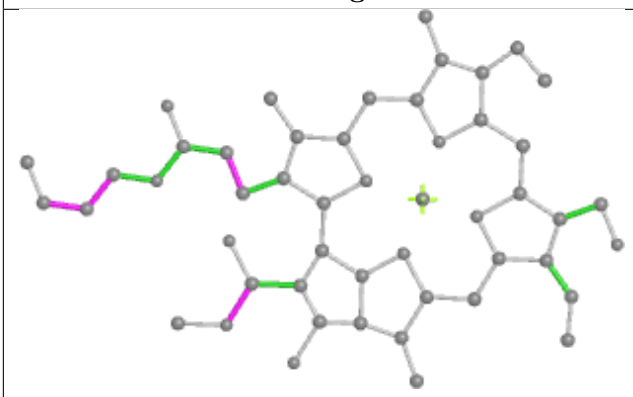
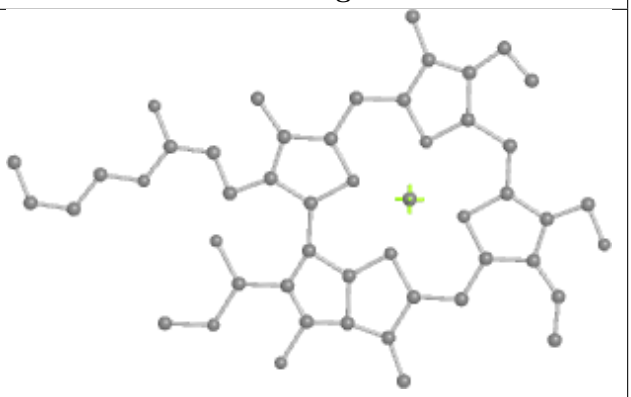
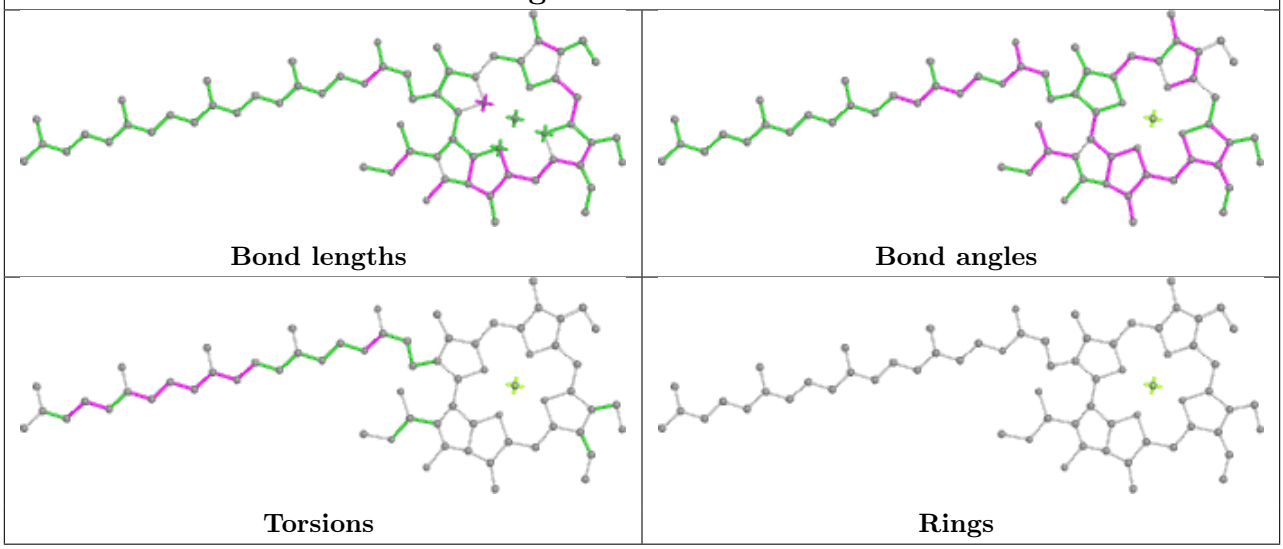


Torsions

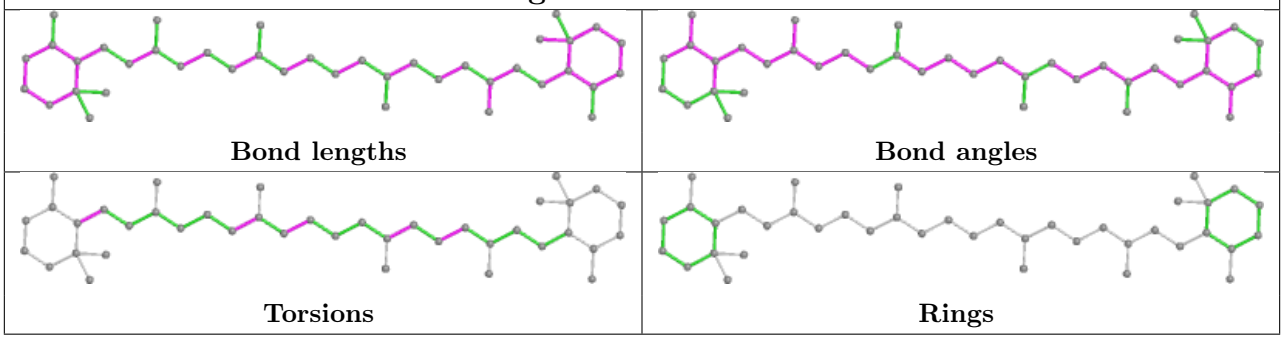


Rings

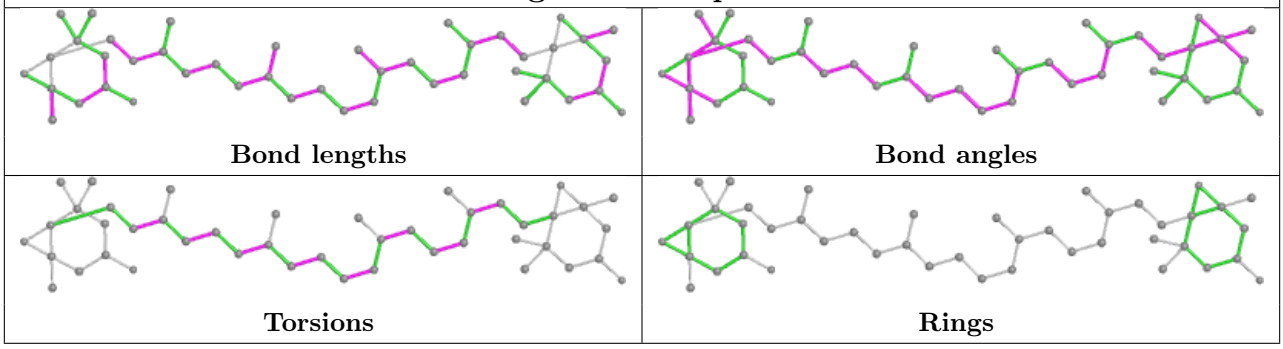
Ligand CHL 1 313



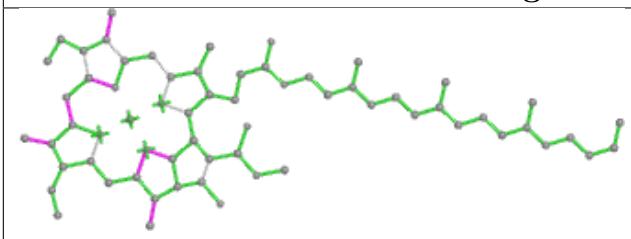
Ligand BCR z 101



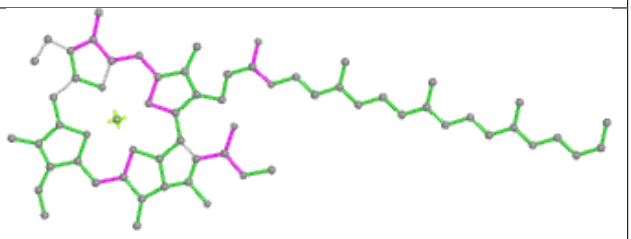
Ligand XAT q 309



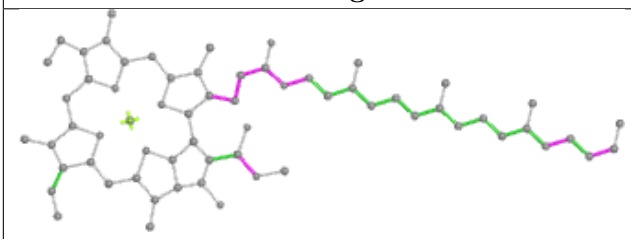
Ligand CLA G 304



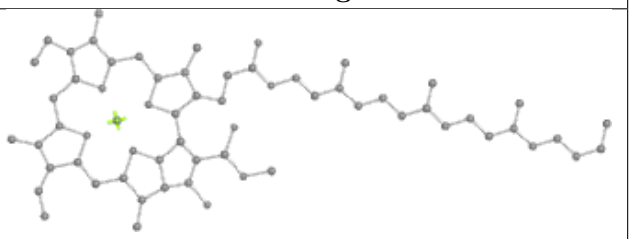
Bond lengths



Bond angles

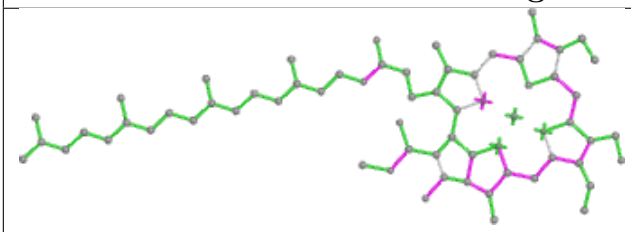


Torsions

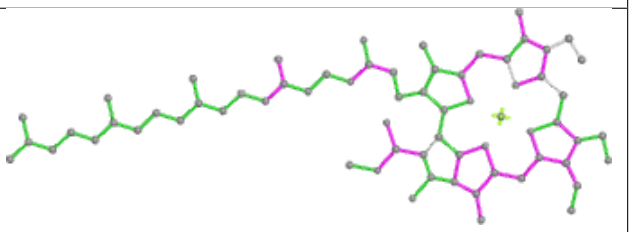


Rings

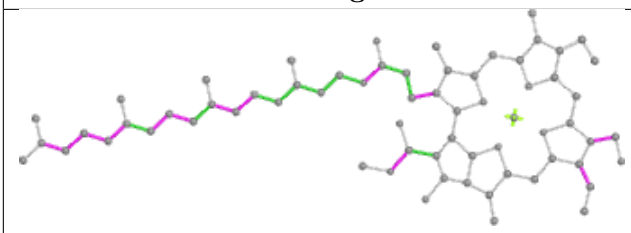
Ligand CHL v 318



Bond lengths



Bond angles



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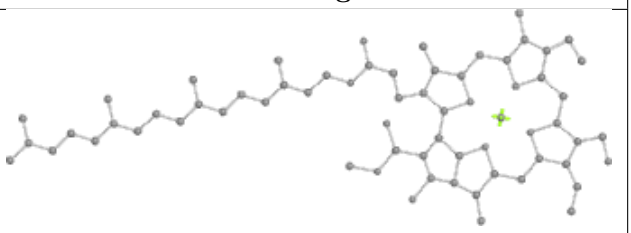
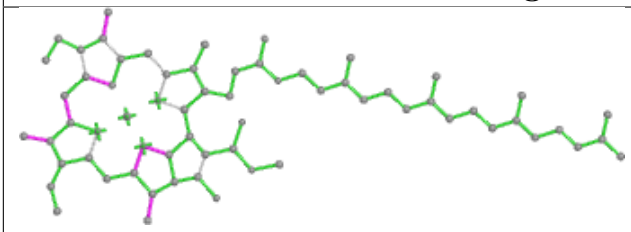
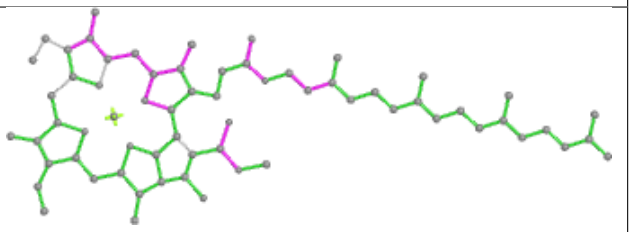


Rings

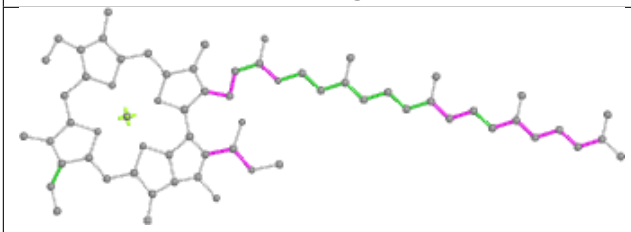
Ligand CLA N 304



Bond lengths



Bond angles



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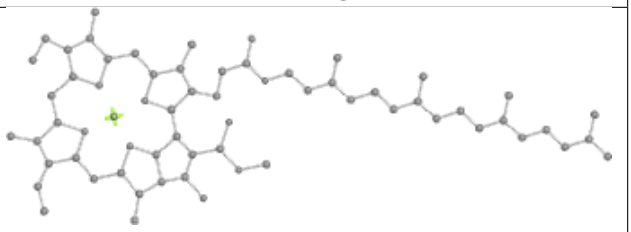
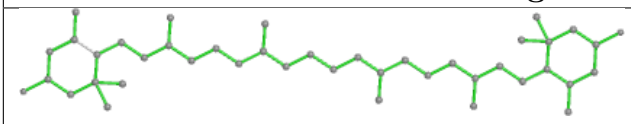
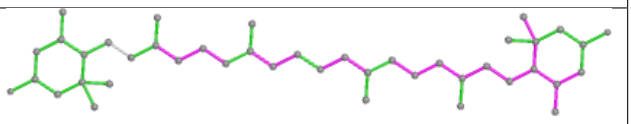
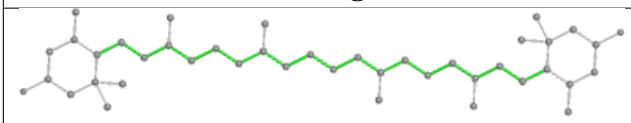
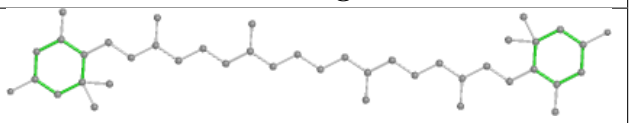
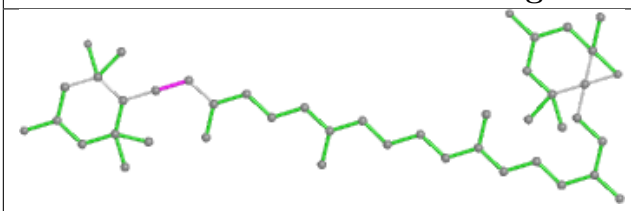
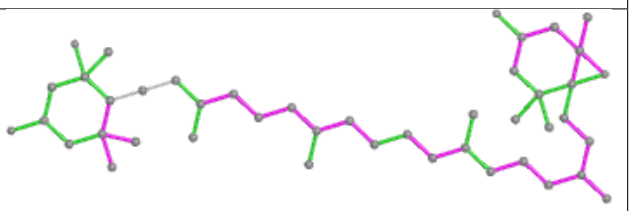
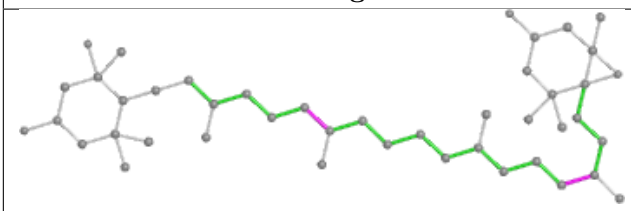
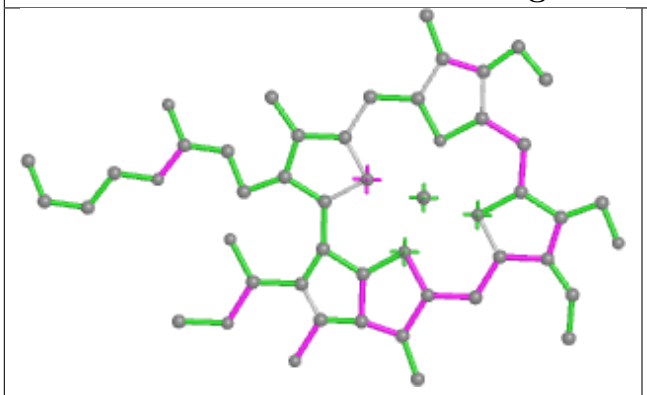


Rings

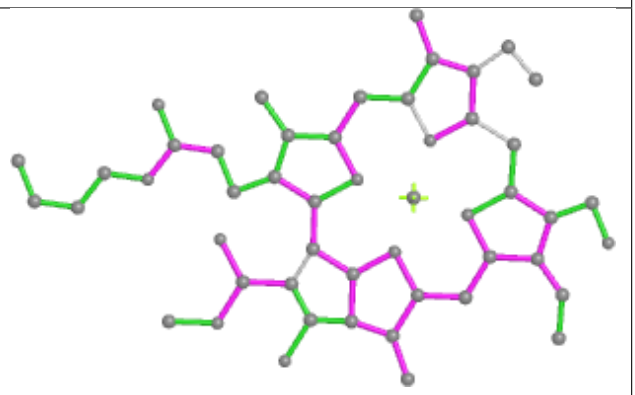
Ligand LUT n 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX v 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

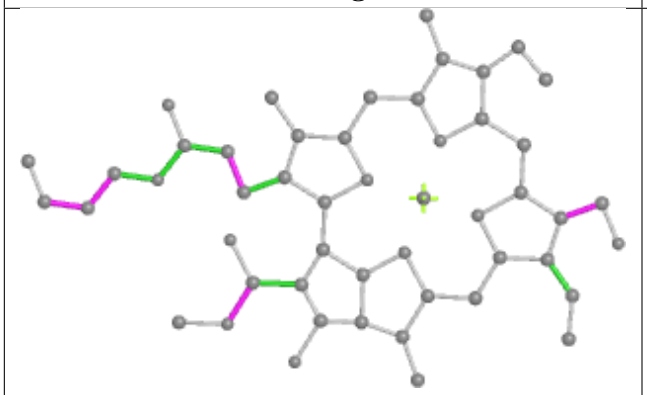
Ligand CHL 5 315



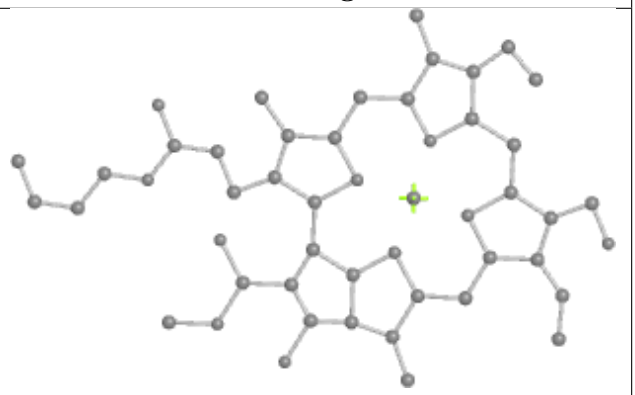
Bond lengths



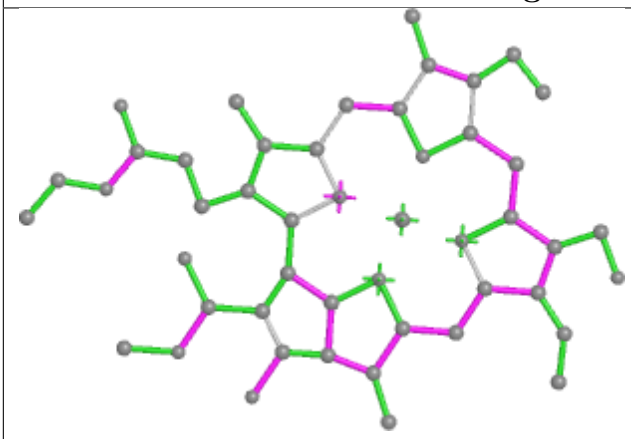
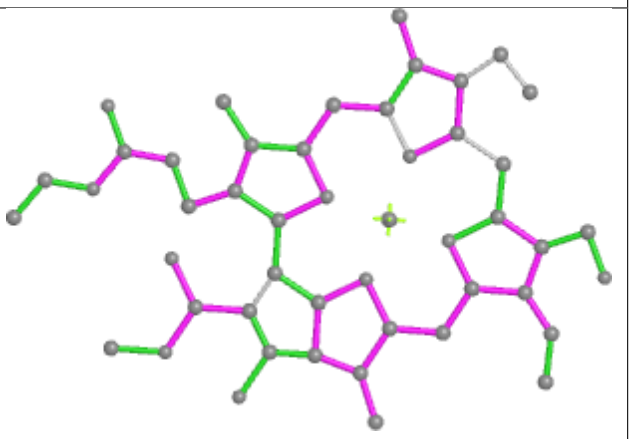
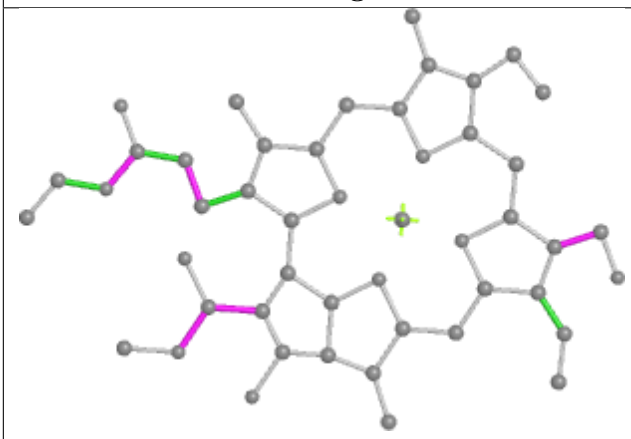
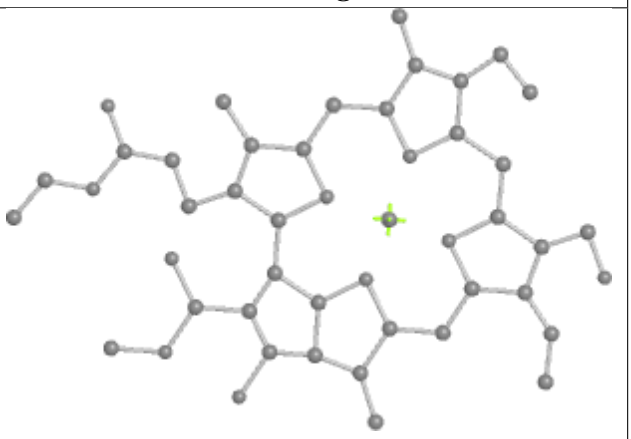
Bond angles



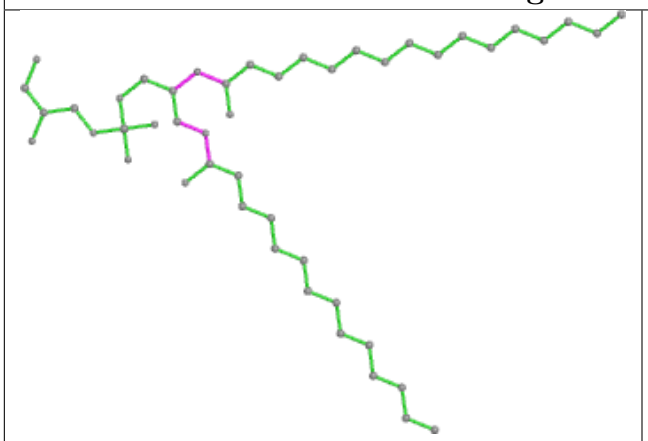
Torsions



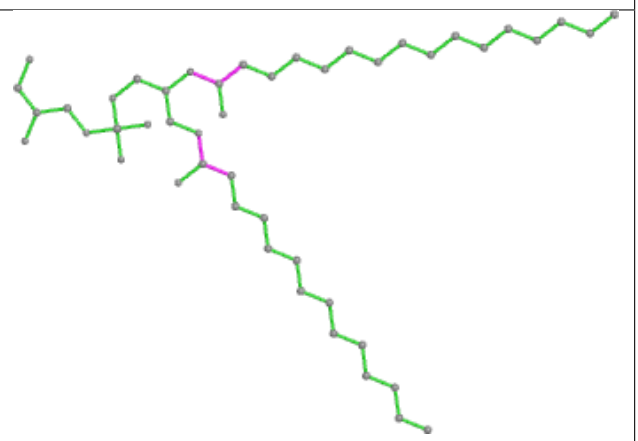
Rings

Ligand CHL V 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

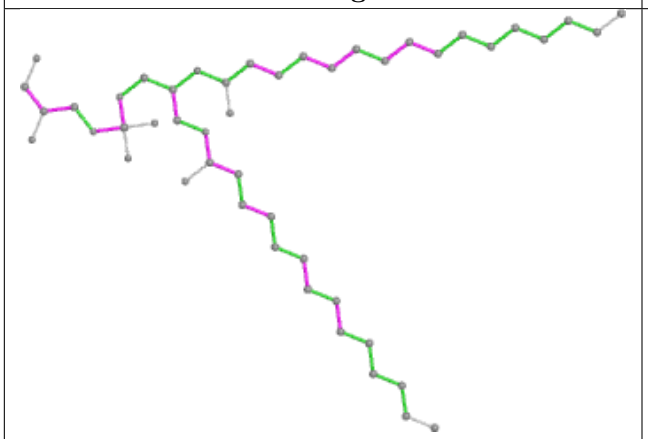
Ligand LHG b 622



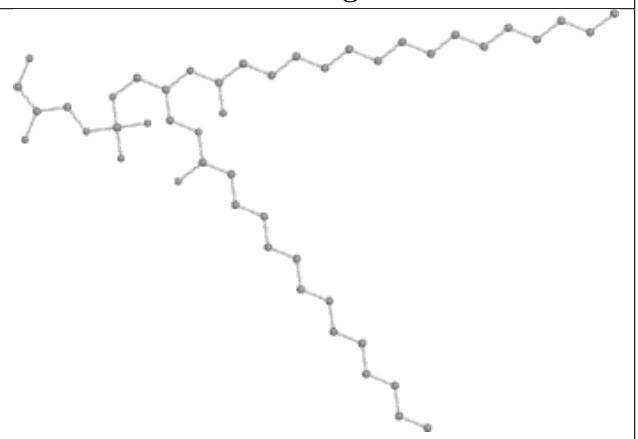
Bond lengths



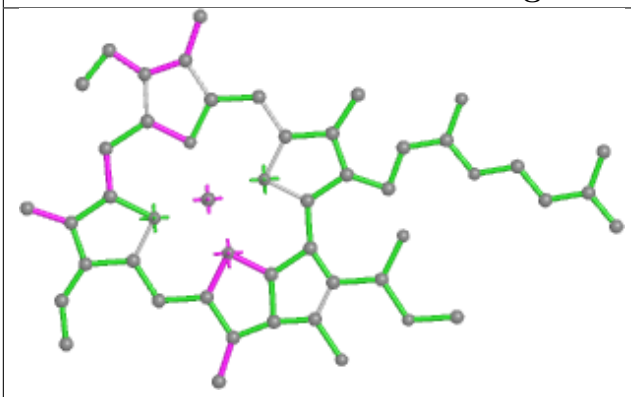
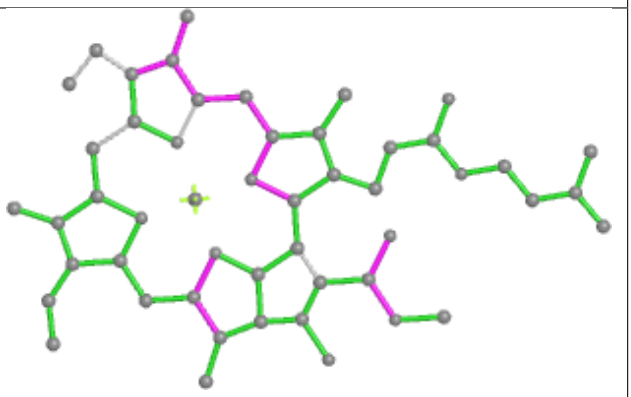
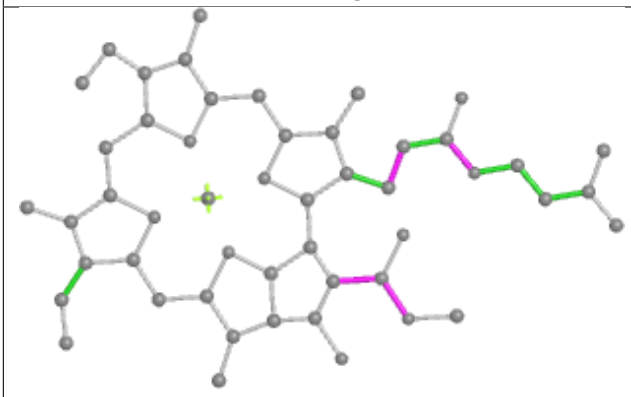
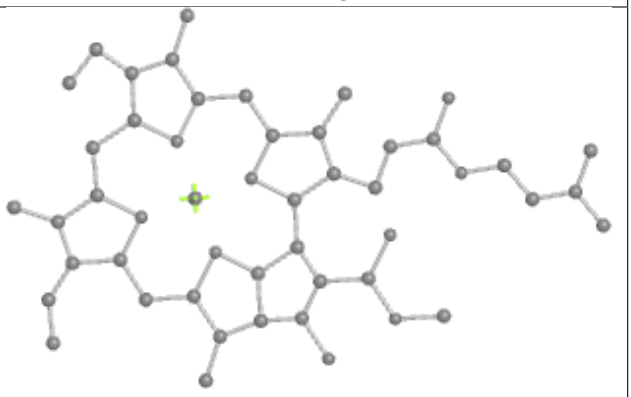
Bond angles

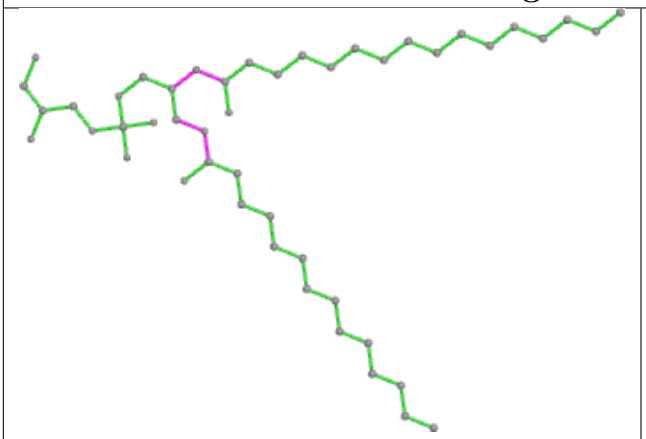
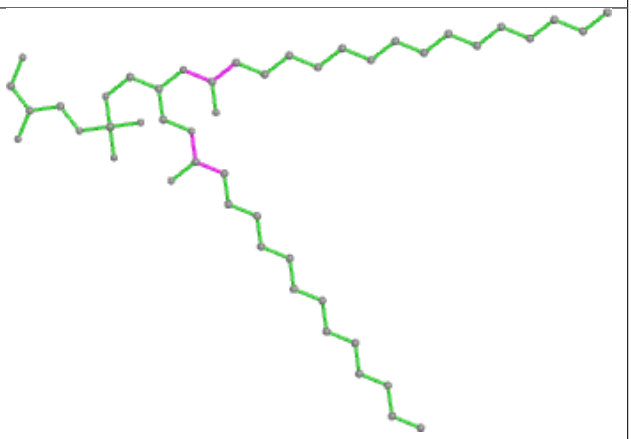
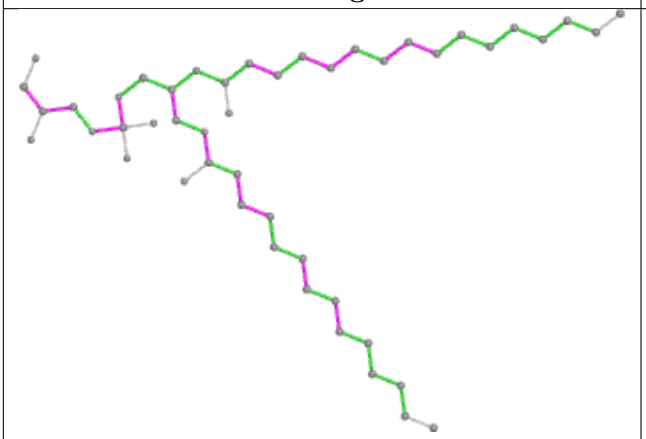
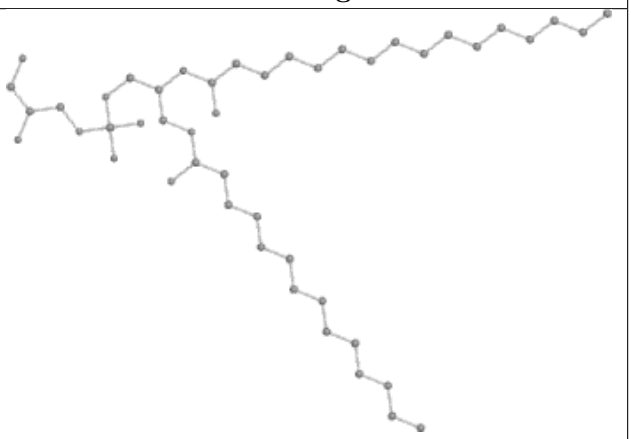


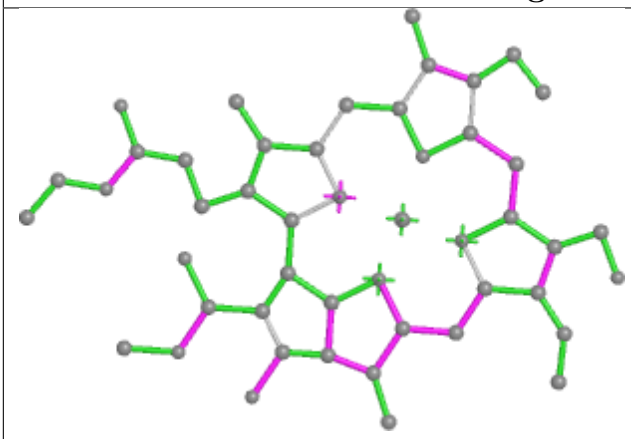
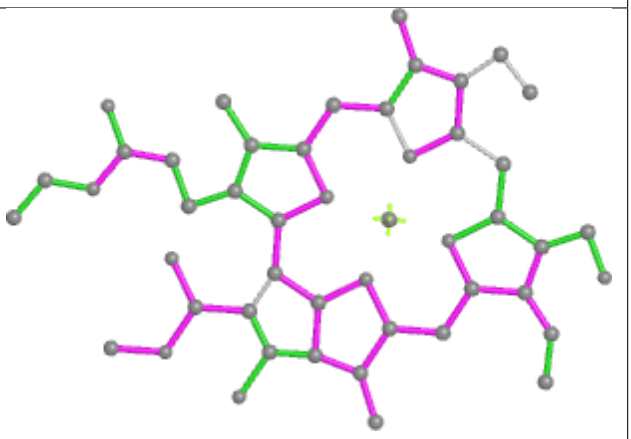
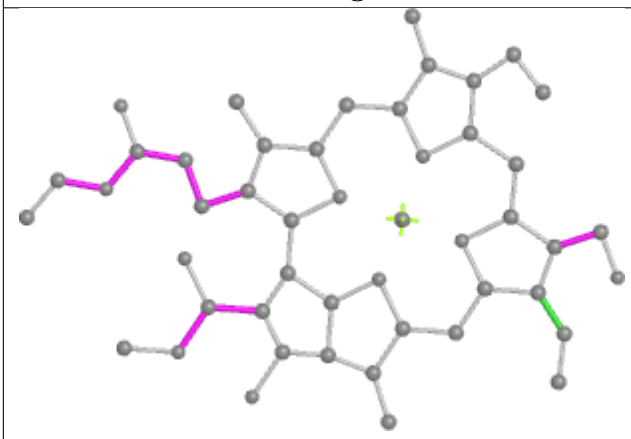
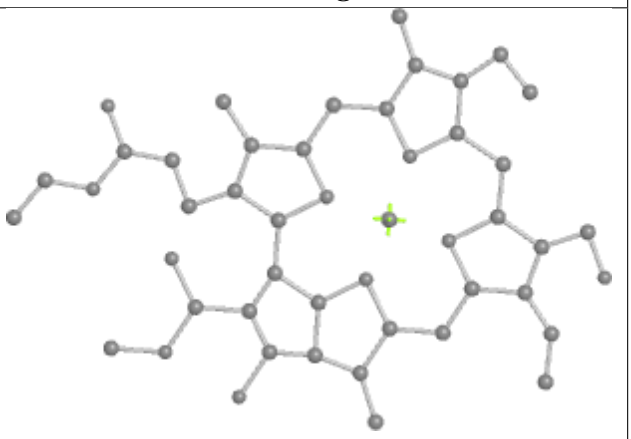
Torsions



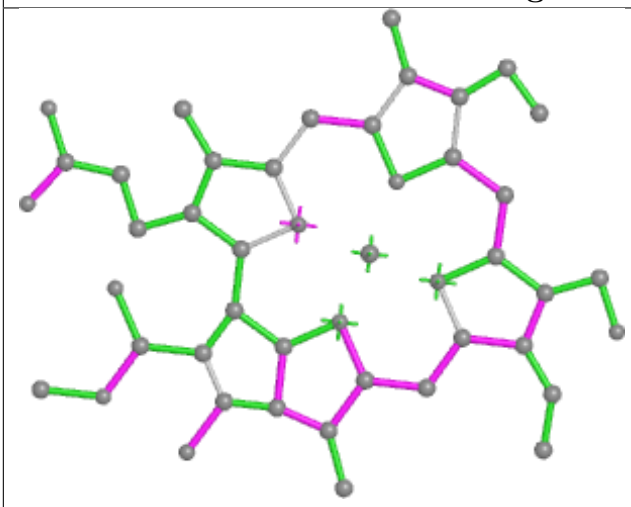
Rings

Ligand CLA A 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG B 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 1 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL S 313



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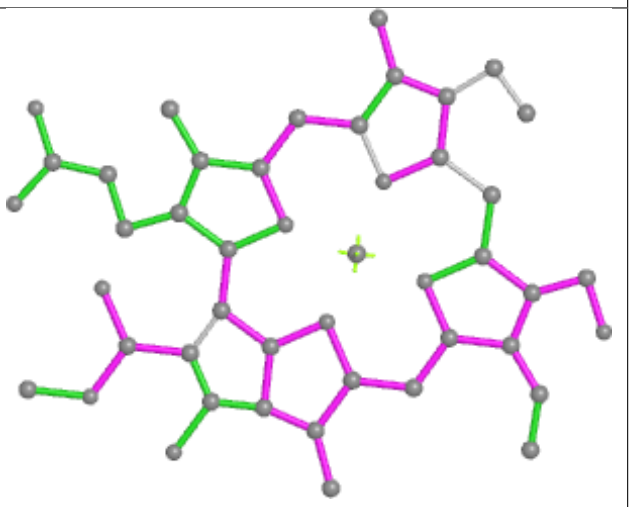
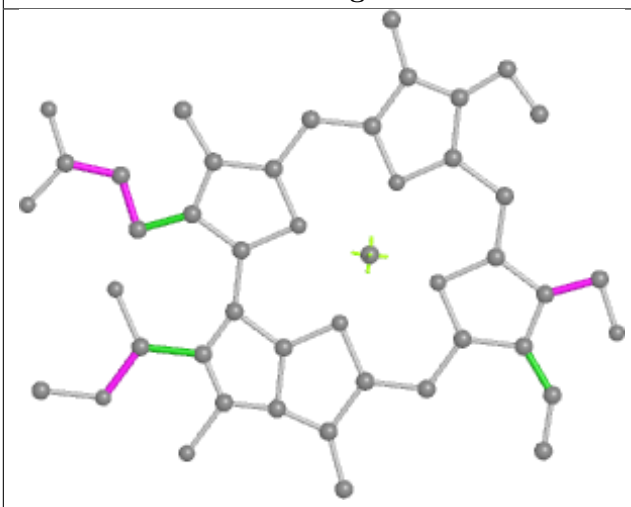
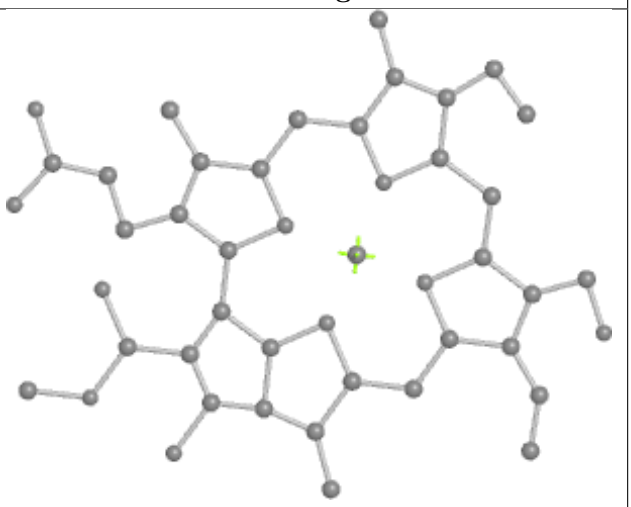


Bond angles

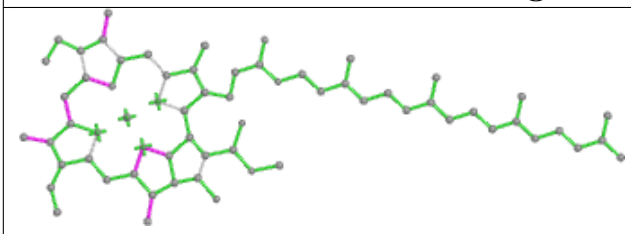


Torsions

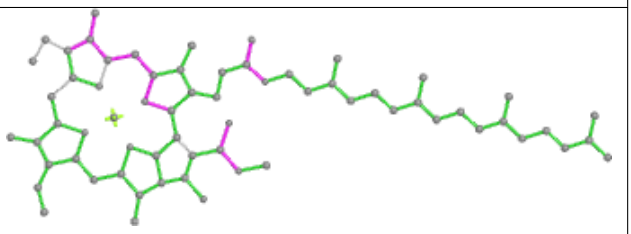


Rings

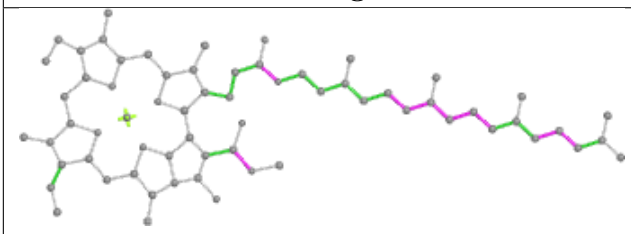
Ligand CLA b 612



Bond lengths



Bond angles



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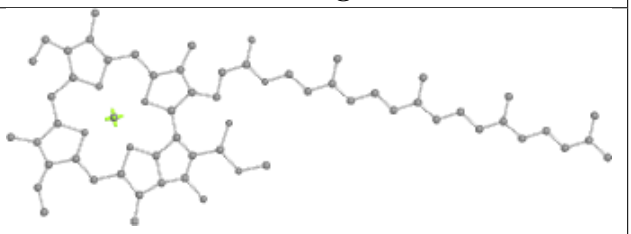
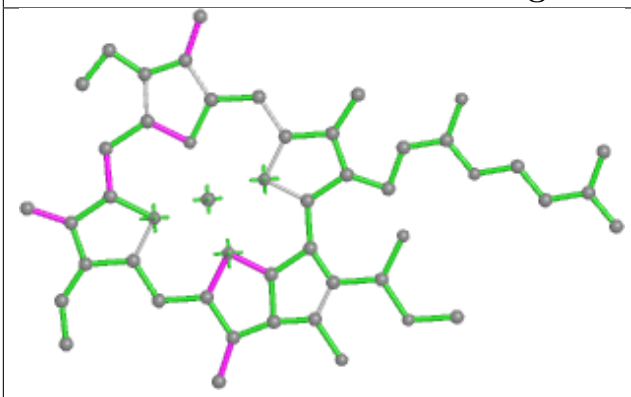
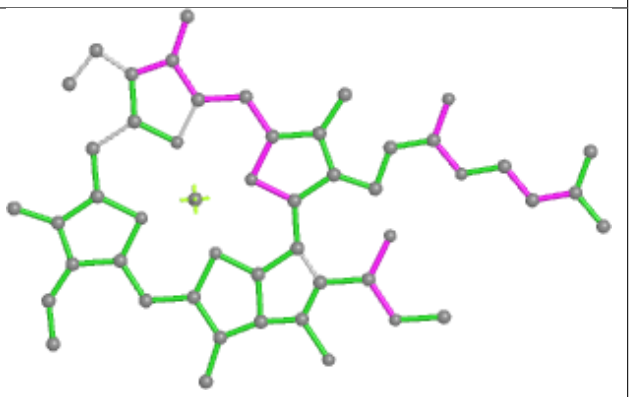
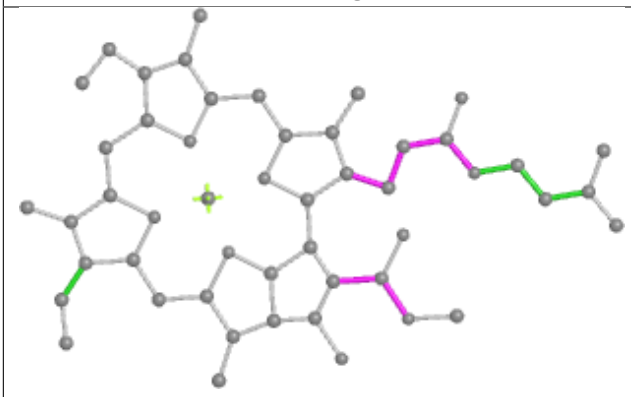
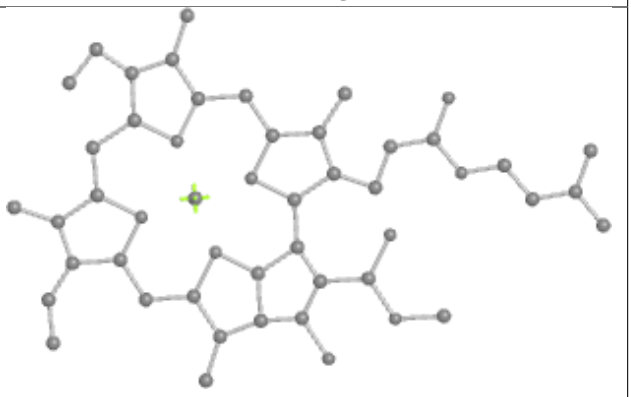
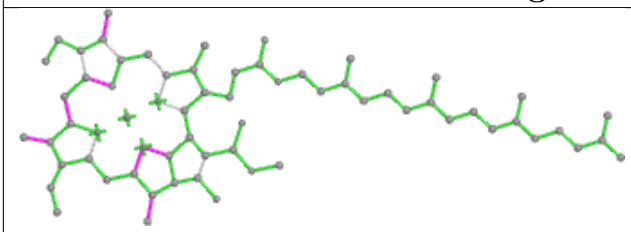
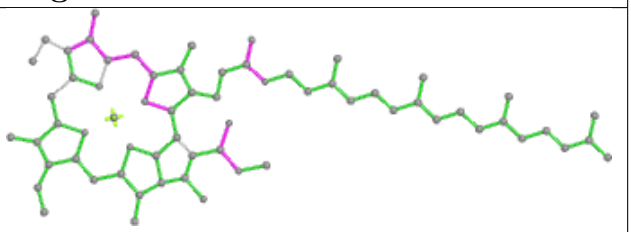
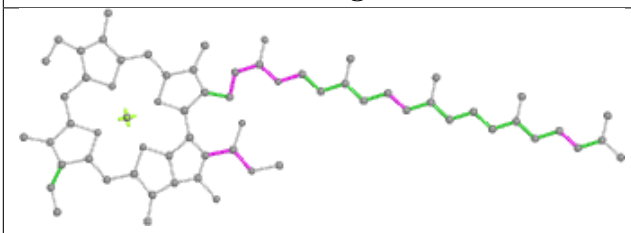
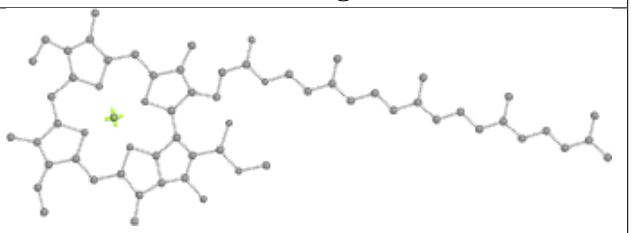
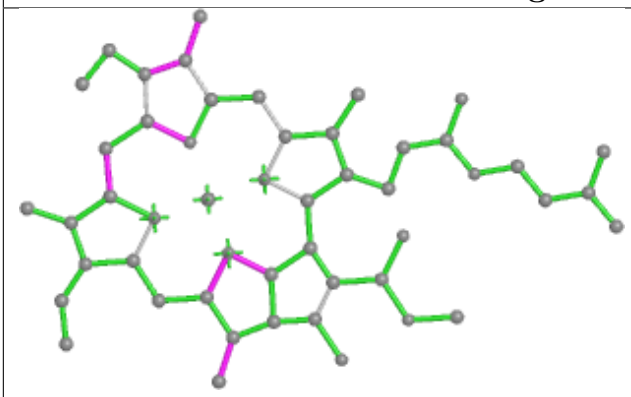
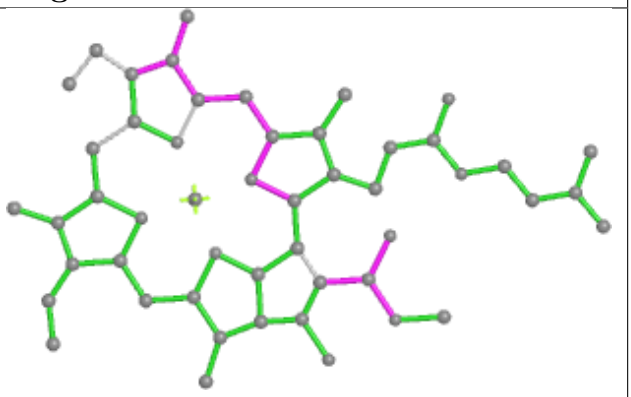
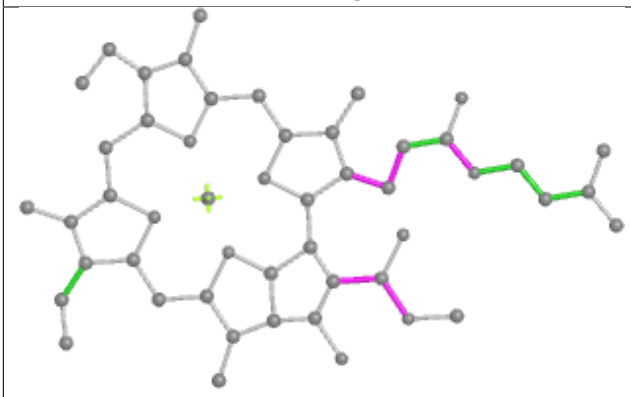
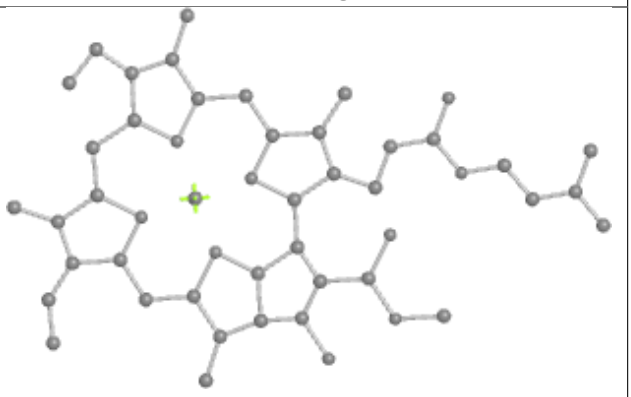
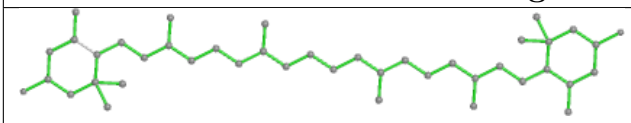
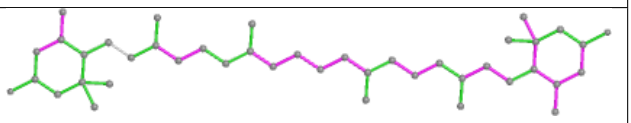
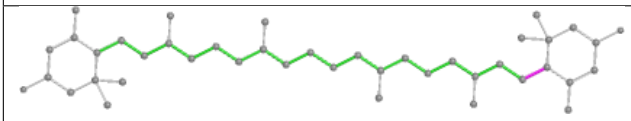
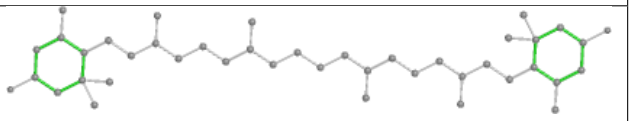


Rings

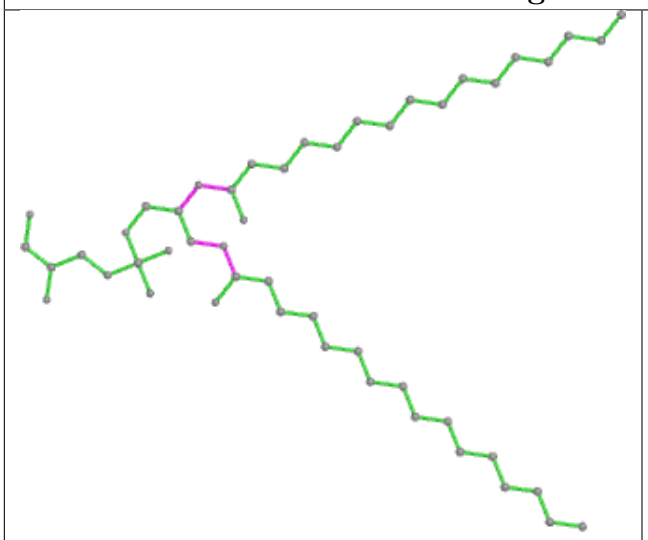
Ligand CLA 6 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

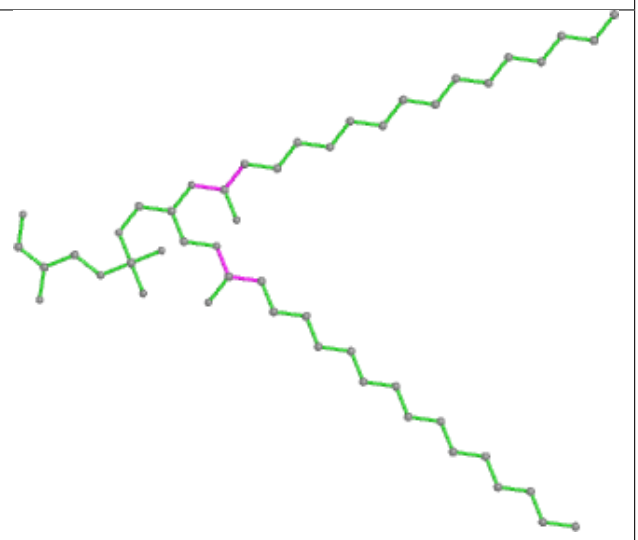
Ligand CLA g 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 1 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

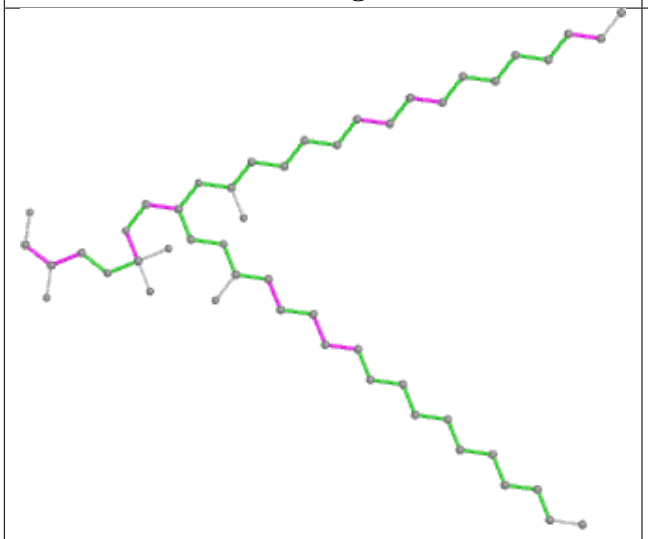
Ligand LHG 1 312



Bond lengths



Bond angles



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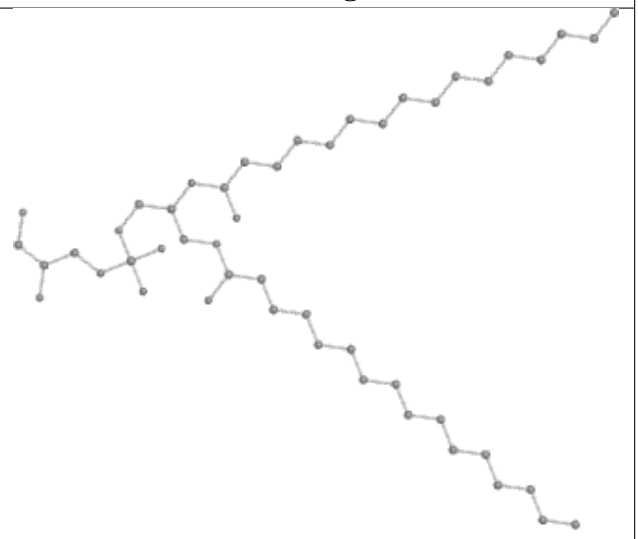
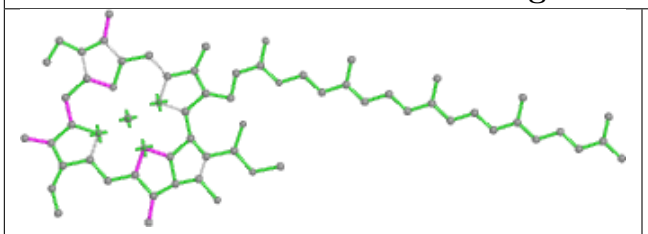
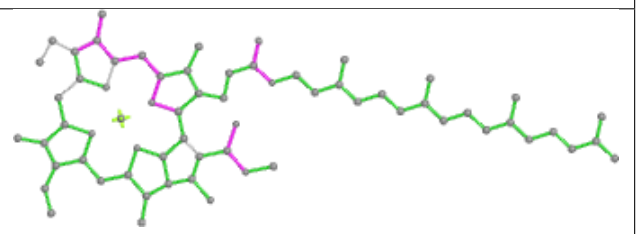


Rings

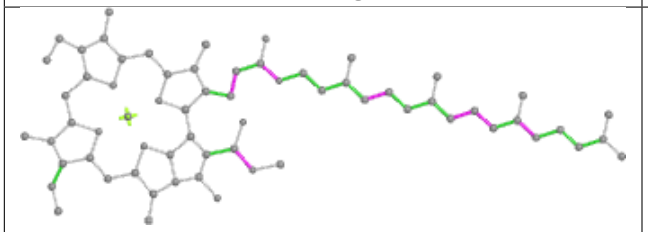
Ligand CLA v 307



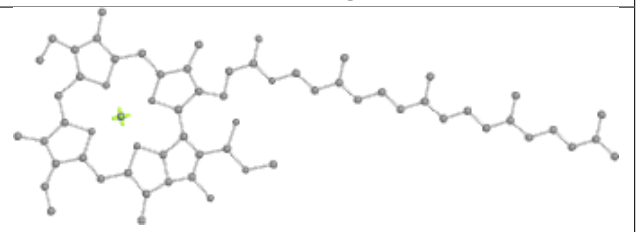
Bond lengths



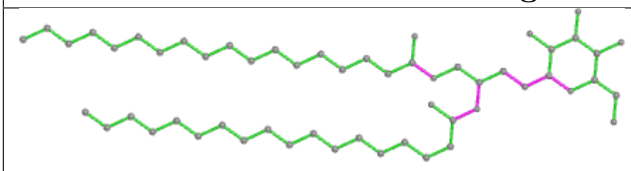
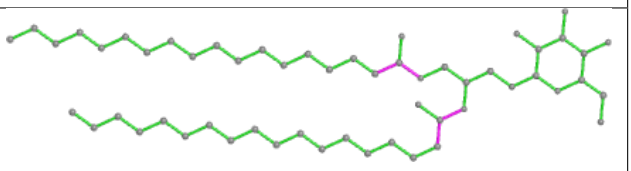
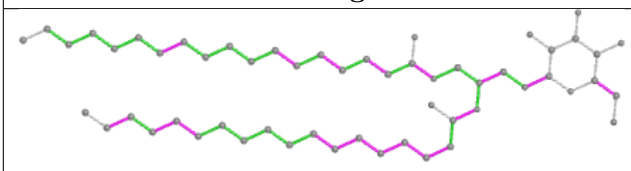
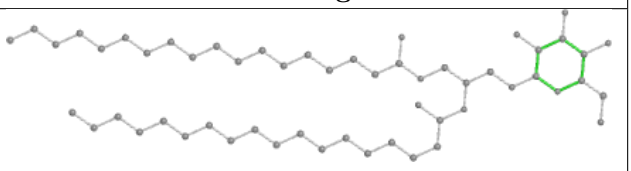
Bond angles

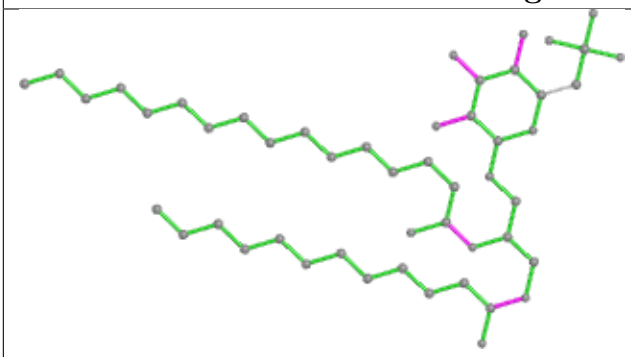
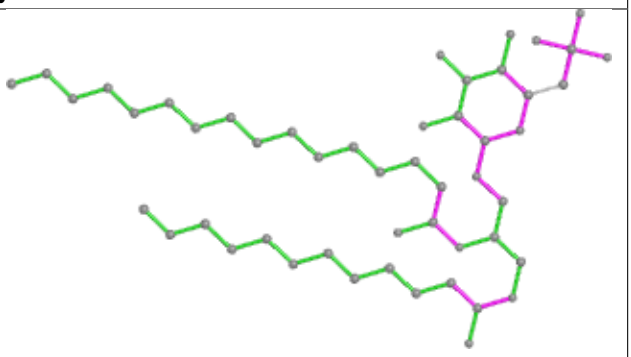
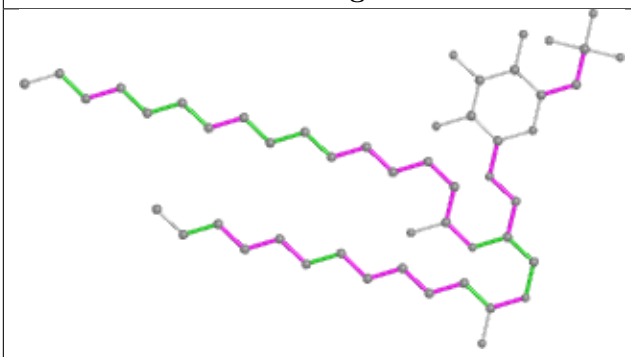
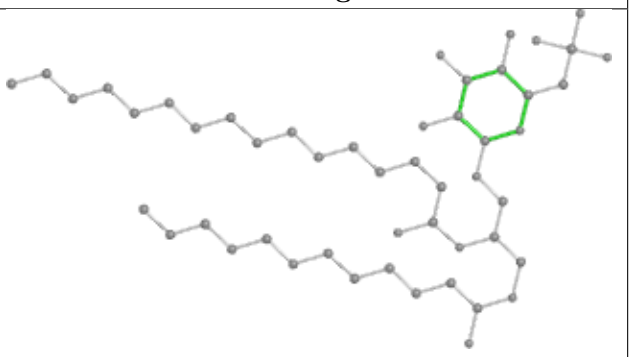


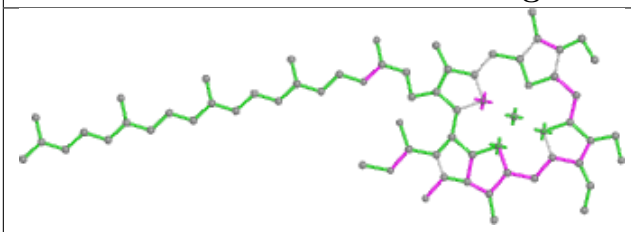
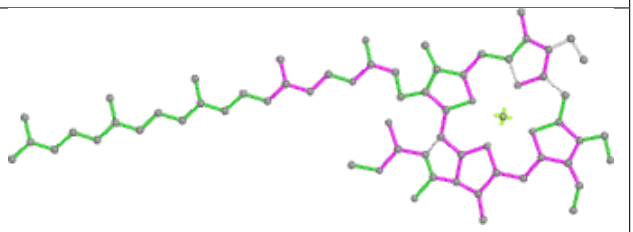
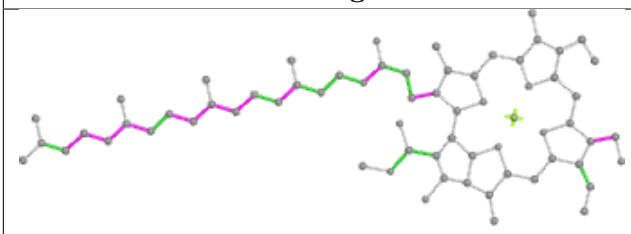
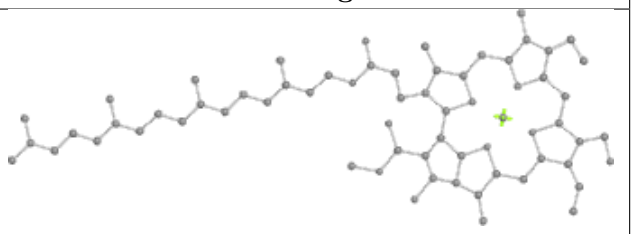
Torsions



Rings

Ligand LMG B 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

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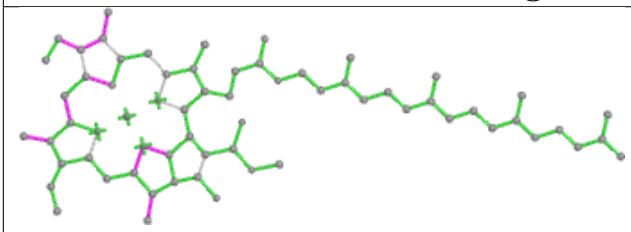
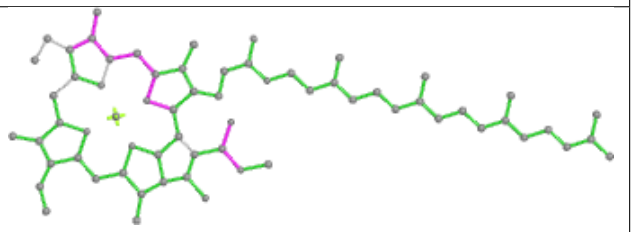
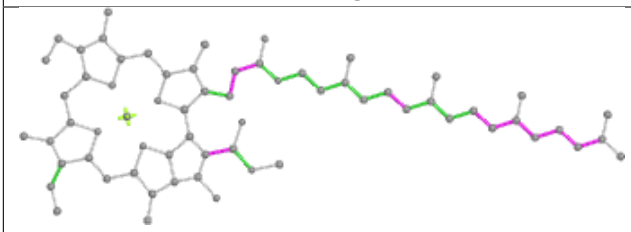
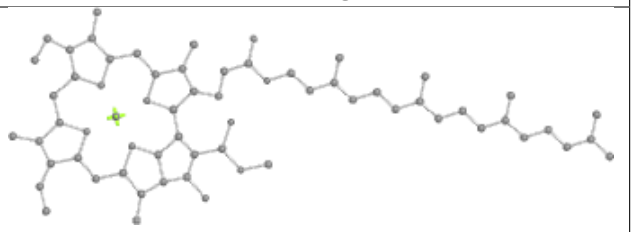
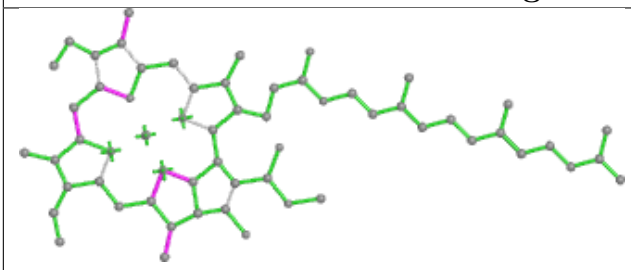
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 306



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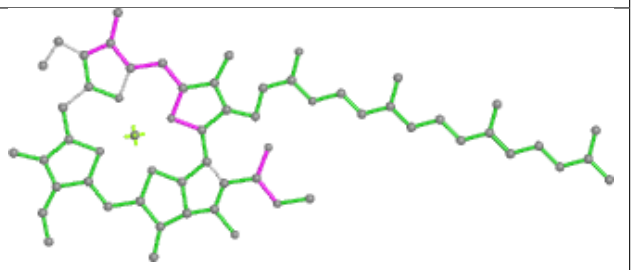

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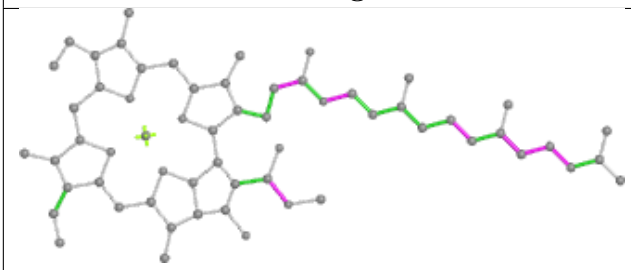

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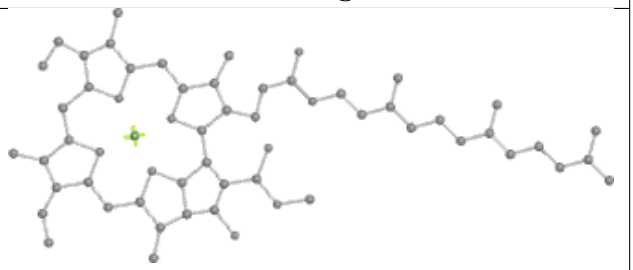
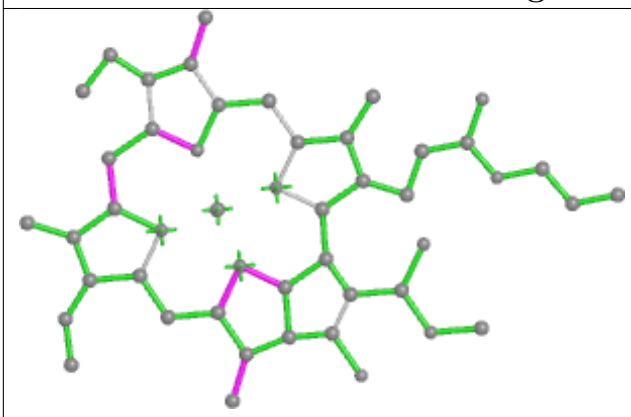


Rings

Ligand CLA n 308



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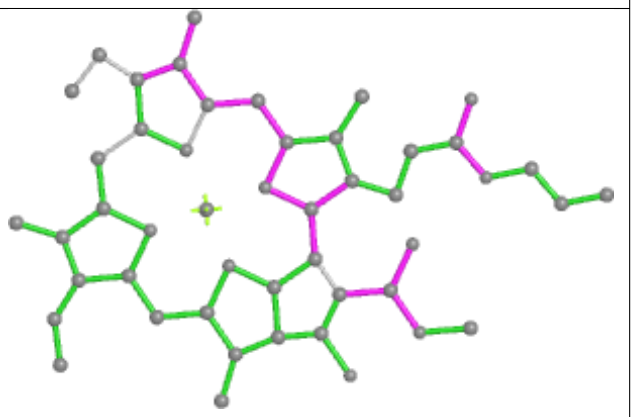

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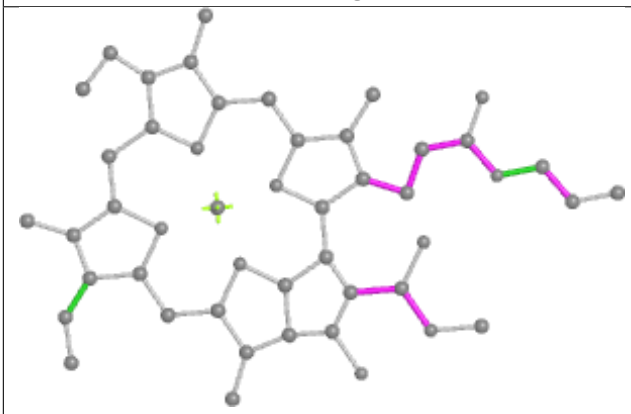

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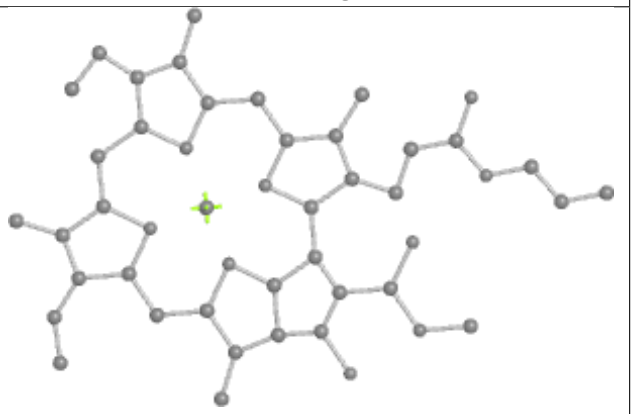
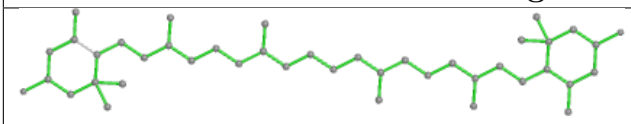


Rings

Ligand LUT p 311



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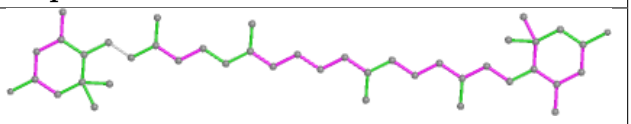

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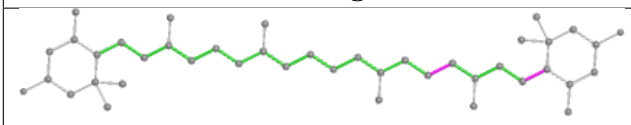

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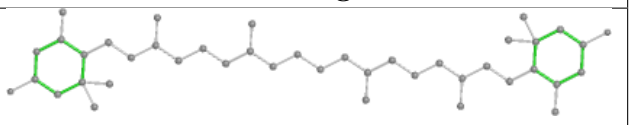
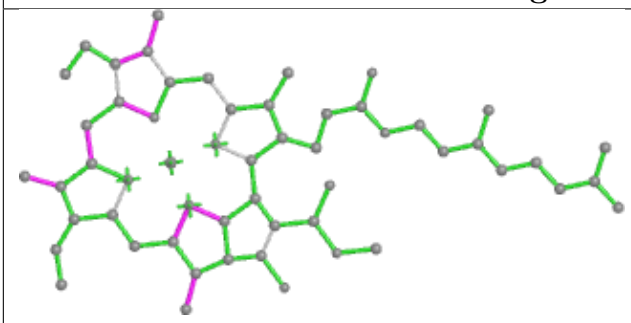


Rings

Ligand CLA s 308



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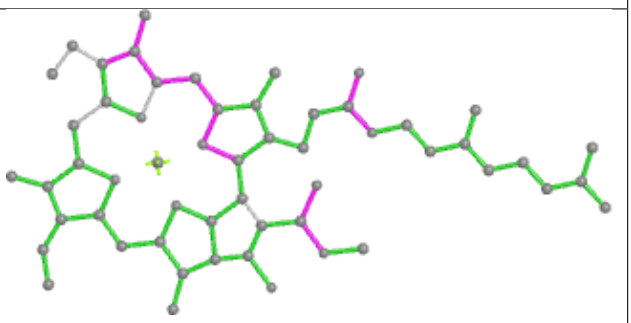
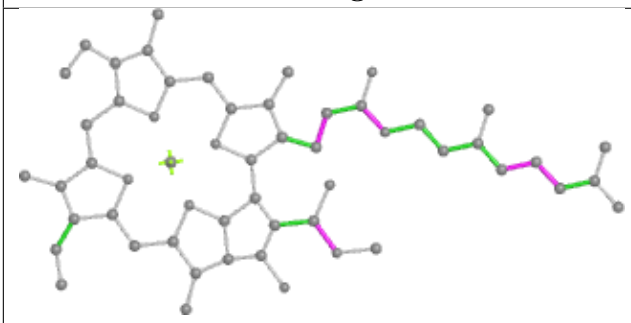


Bond angles



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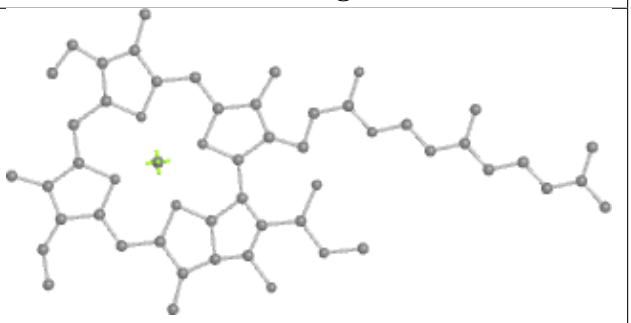
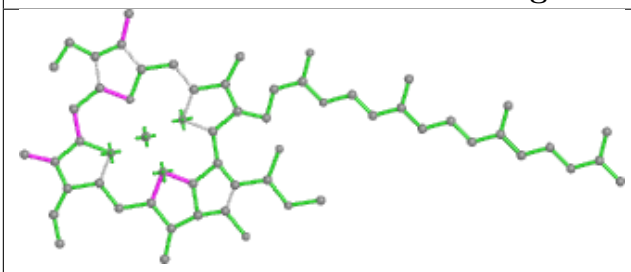


Rings

Ligand CLA r 609



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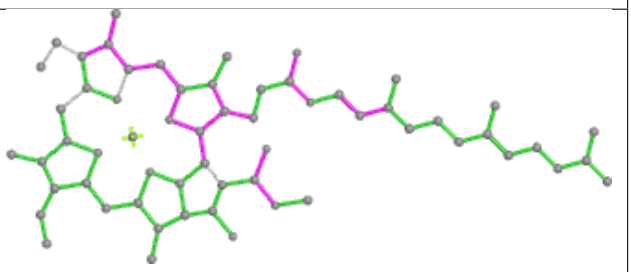
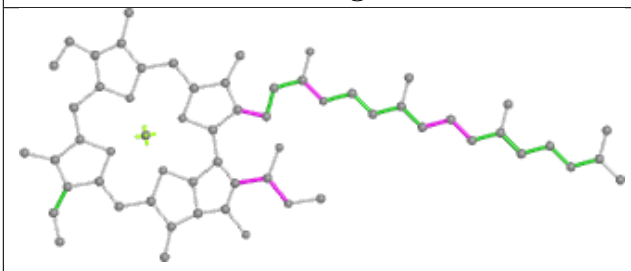


Bond angles



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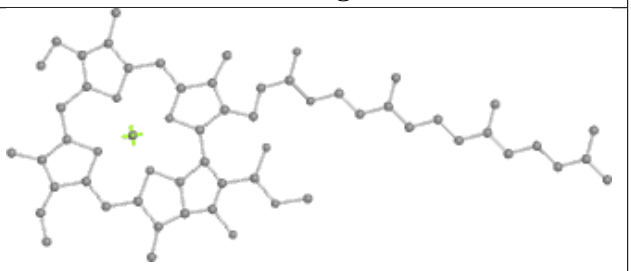
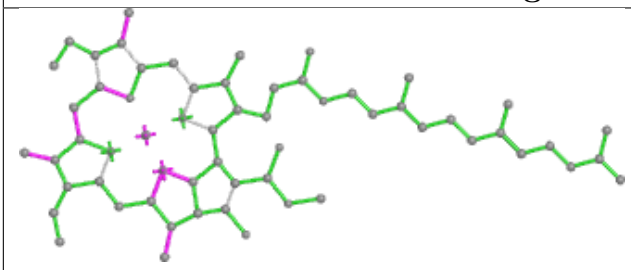
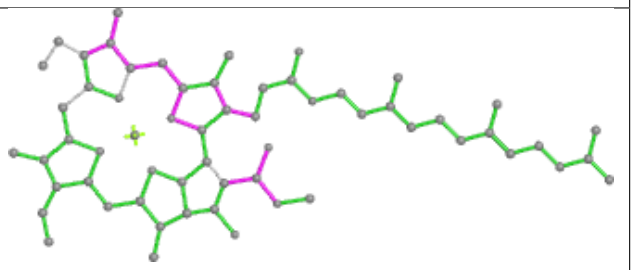
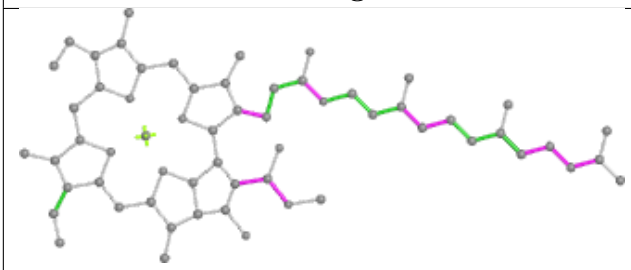
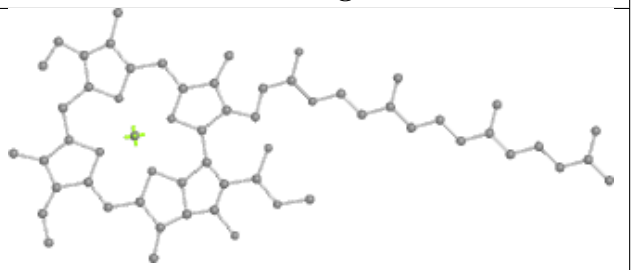
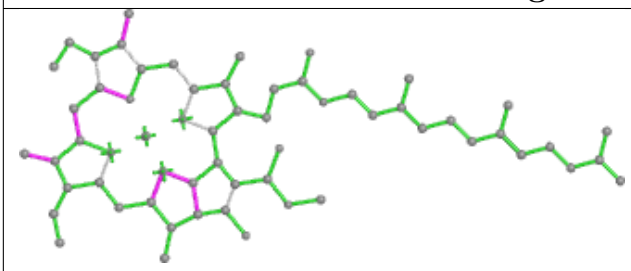
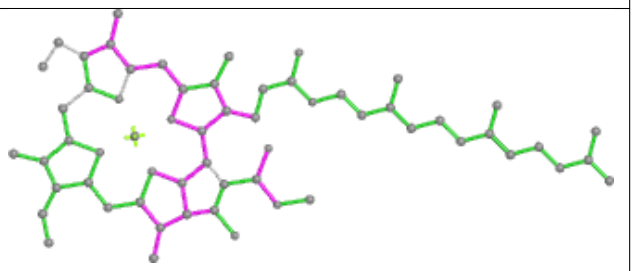
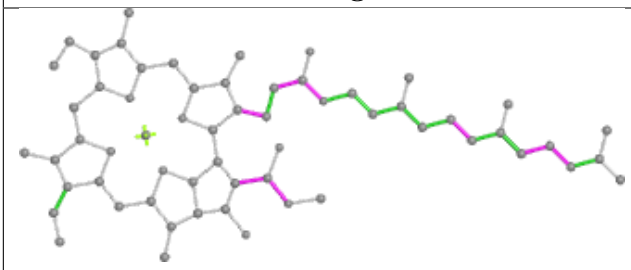
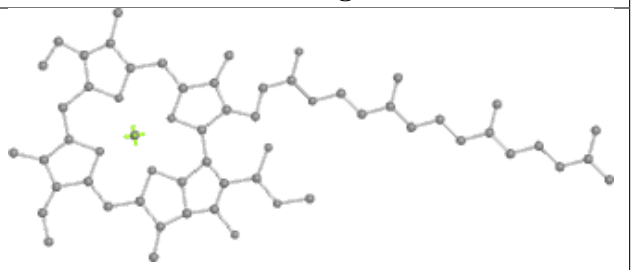
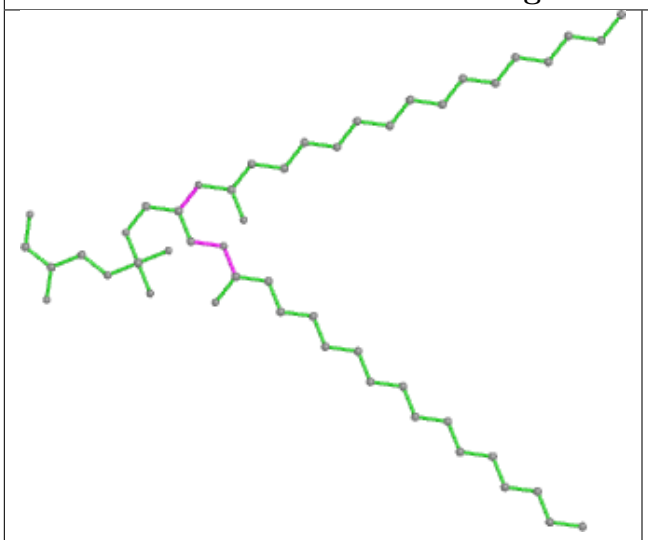


Rings

Ligand CLA A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG C 523



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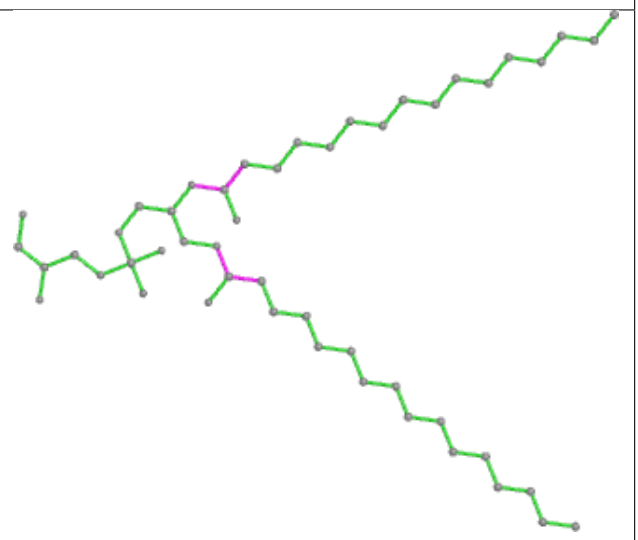
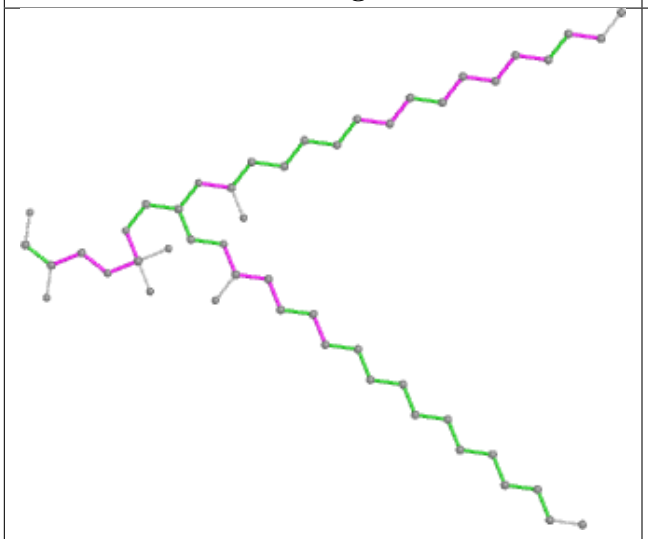


Bond angles



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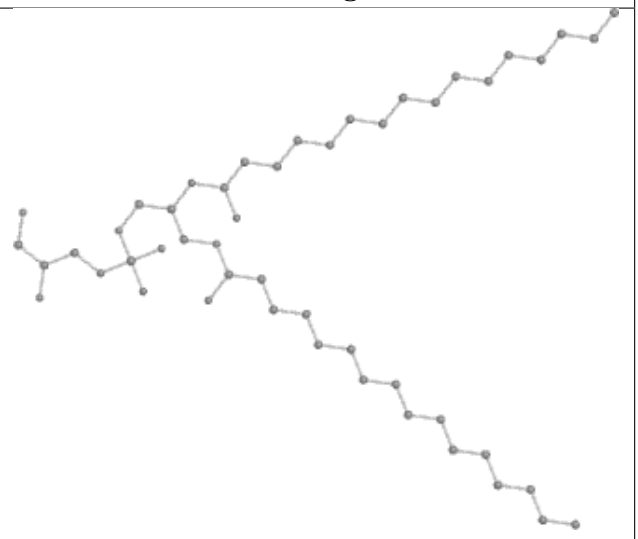
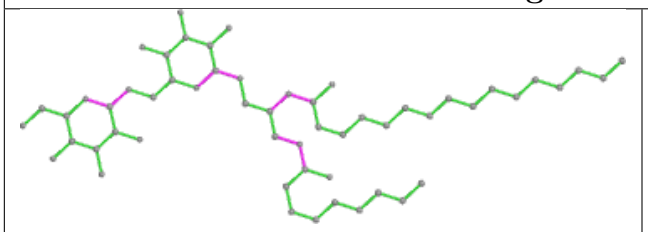


Rings

Ligand DGD c 517



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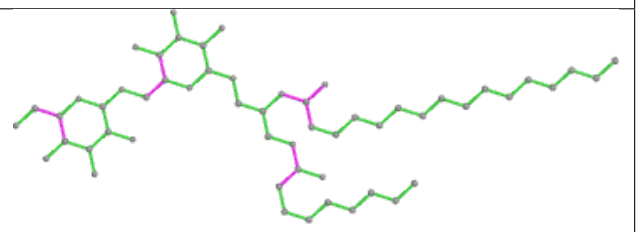
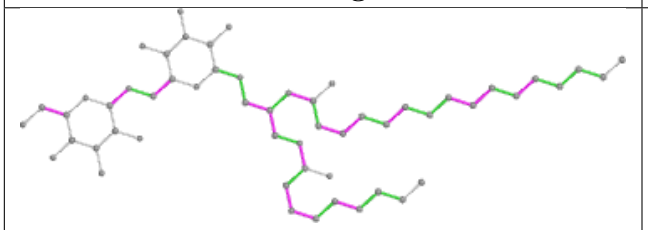


Bond angles



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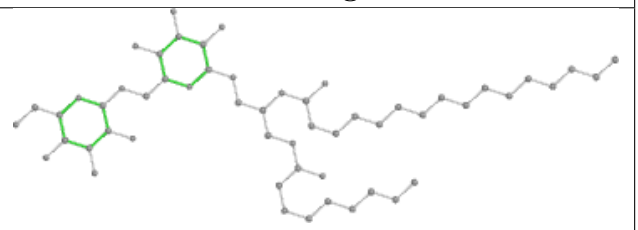
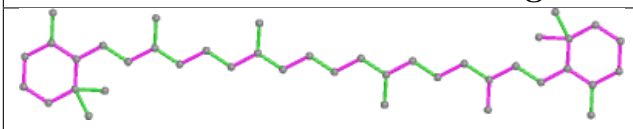


Rings

Ligand BCR b 618



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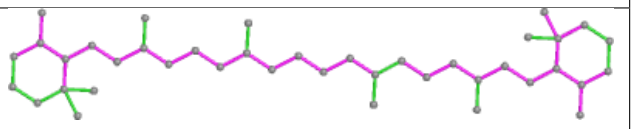

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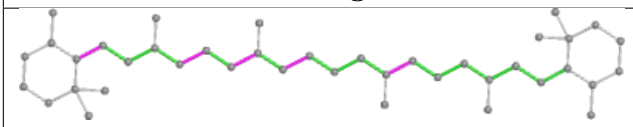

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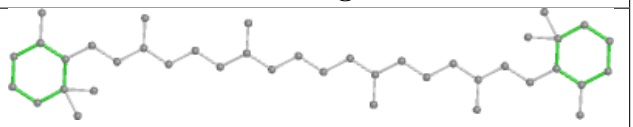
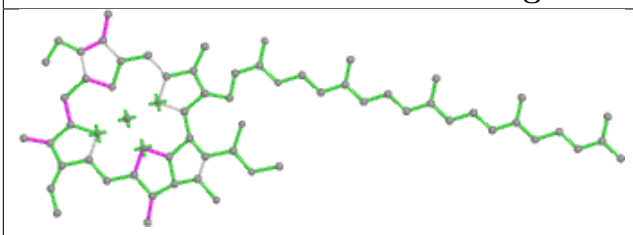


Rings

Ligand CLA U 302



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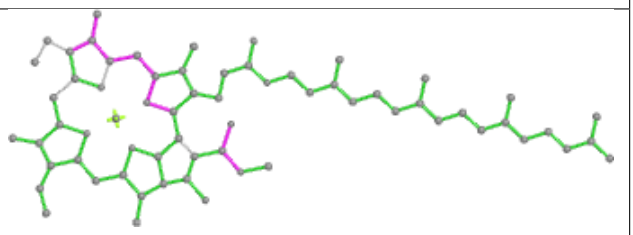

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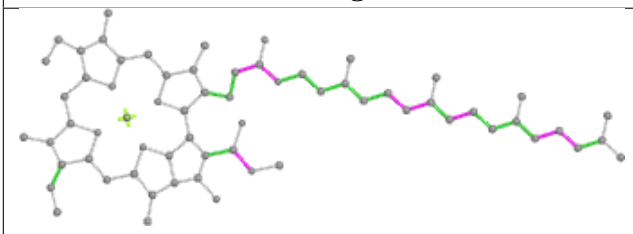

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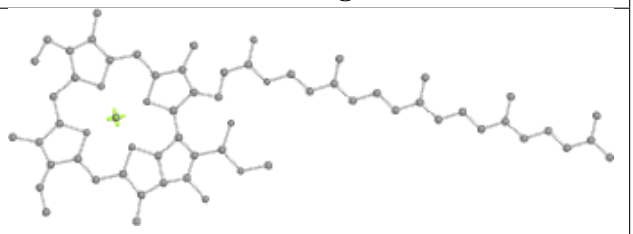
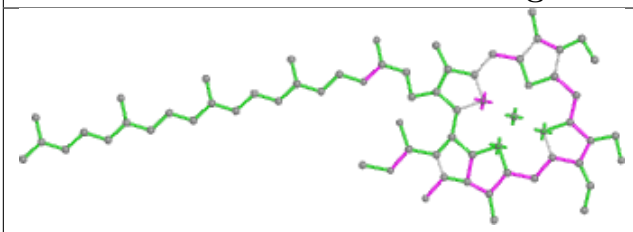


Rings

Ligand CHL n 313



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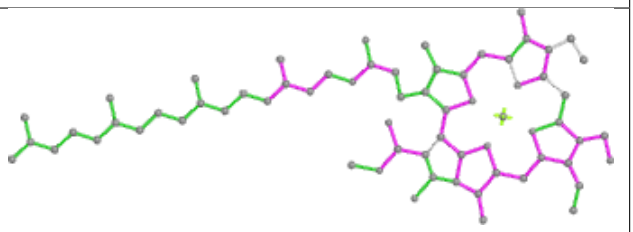
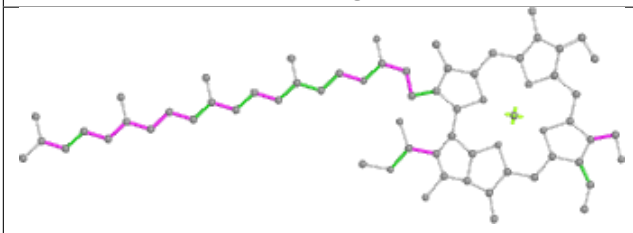
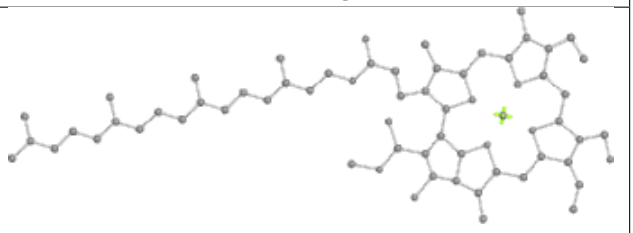


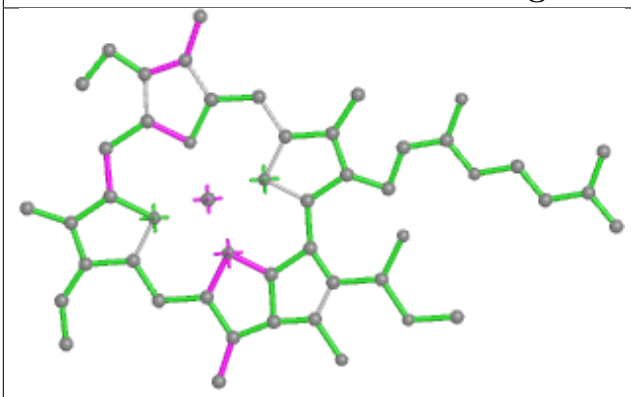
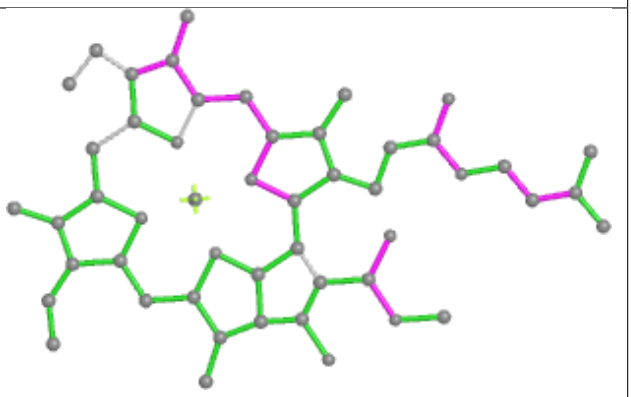
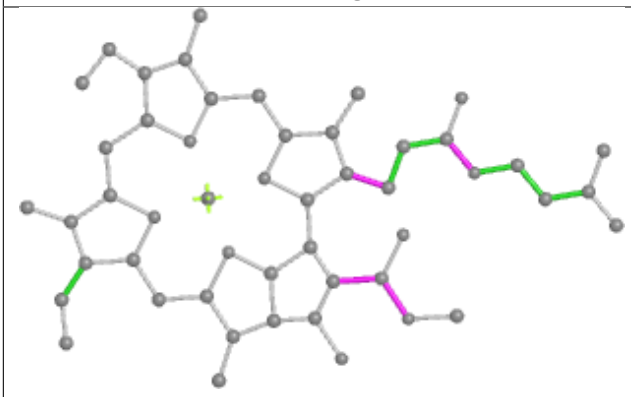
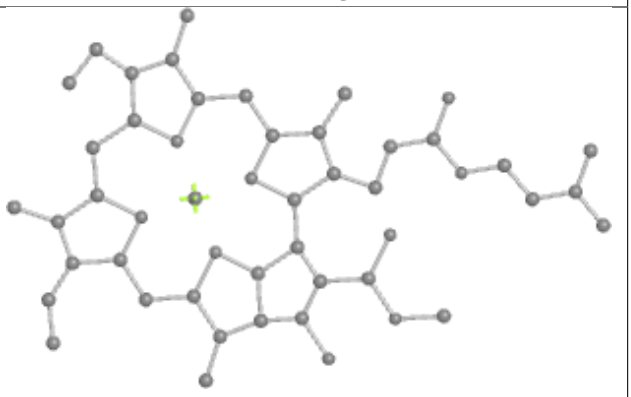
Bond angles



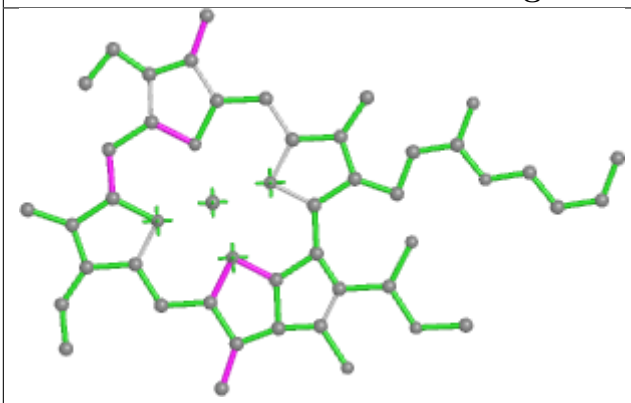
Torsions



Rings

Ligand CLA 4 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 308



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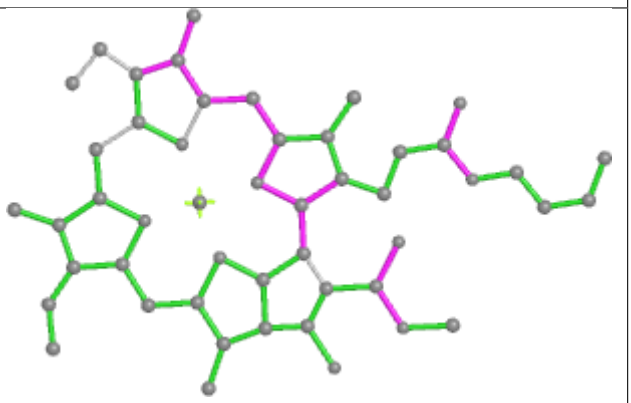
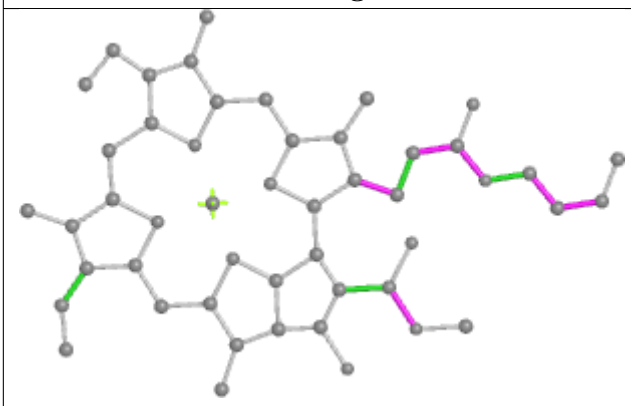


Bond angles



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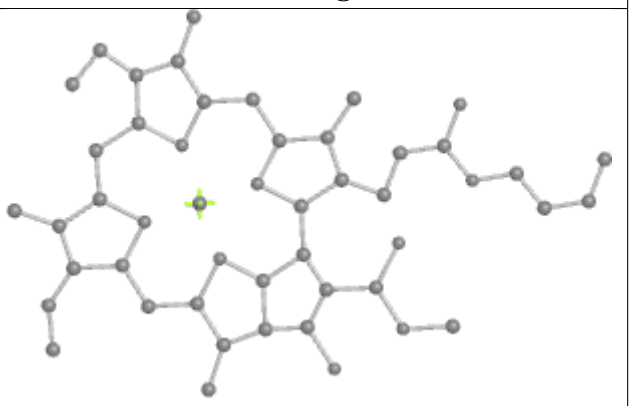
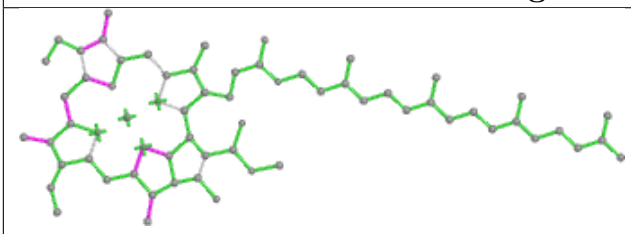


Rings

Ligand CLA 2 302



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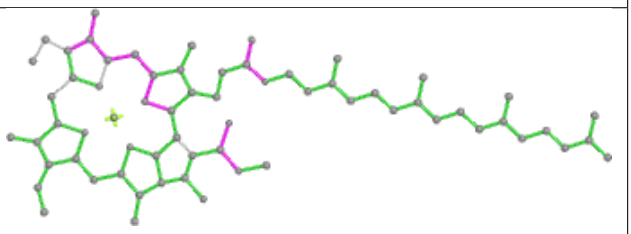
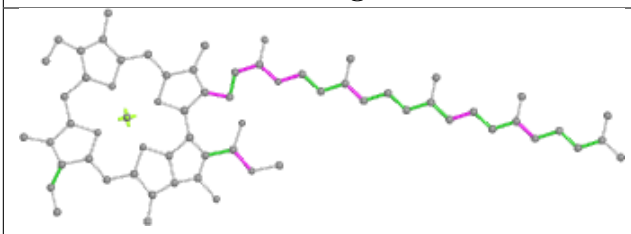


Bond angles



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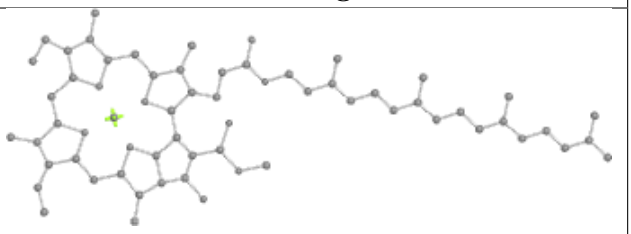
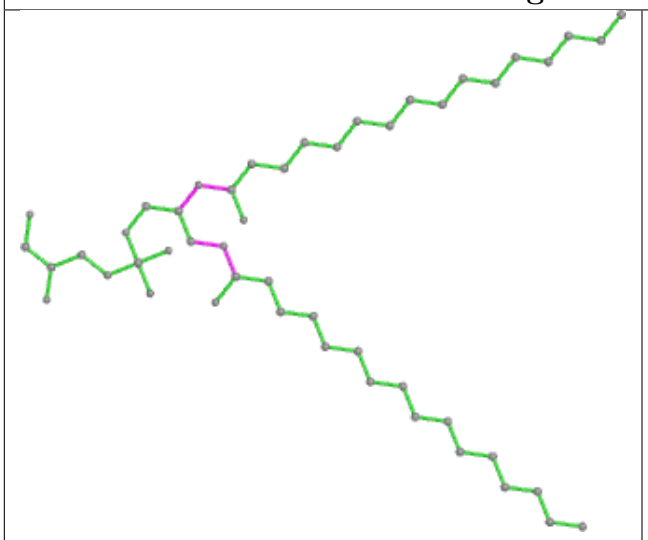


Rings

Ligand LHG b 623



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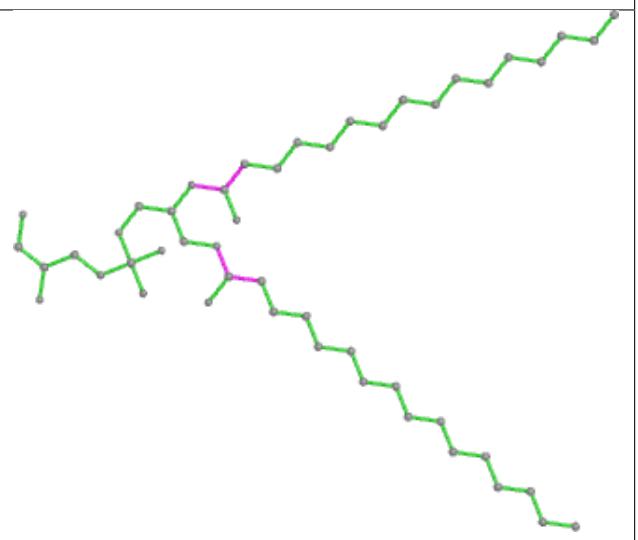

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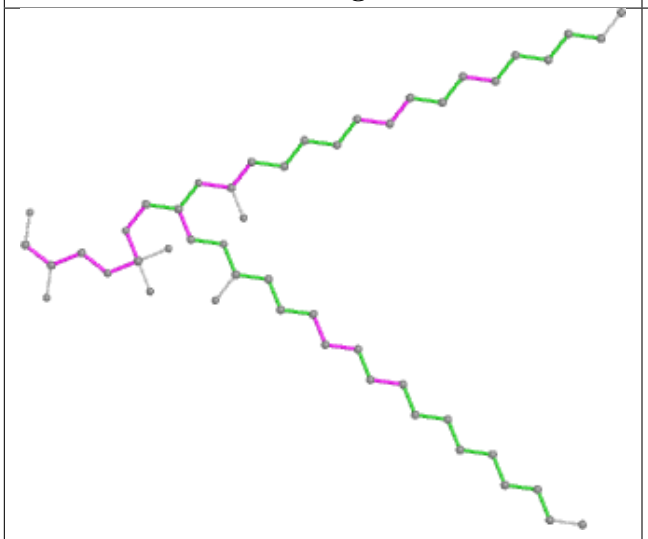

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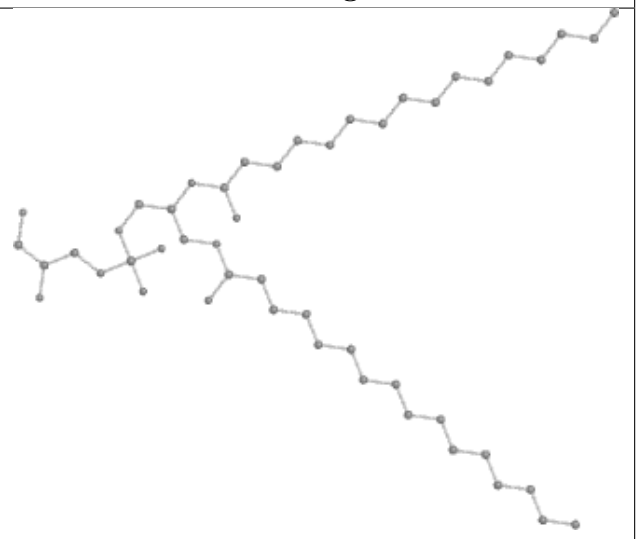
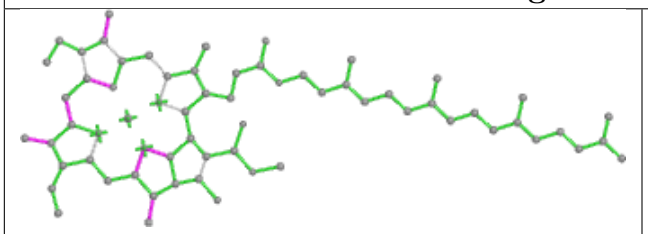


Rings

Ligand CLA n 304



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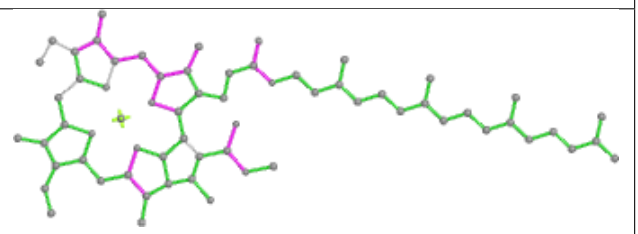
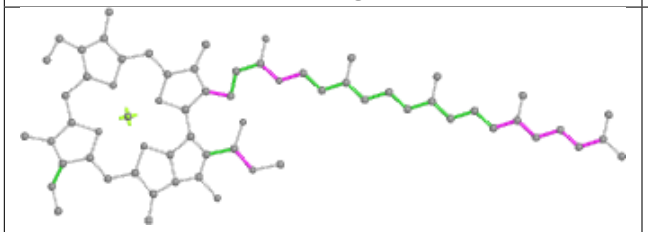


Bond angles



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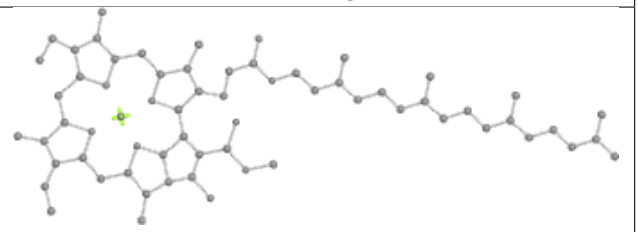
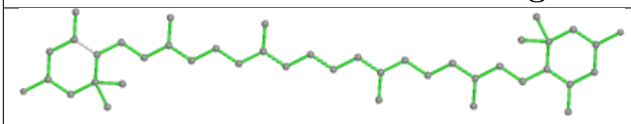
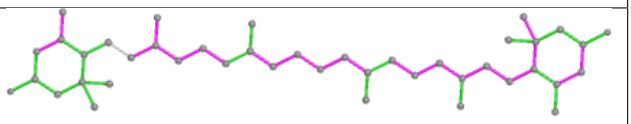
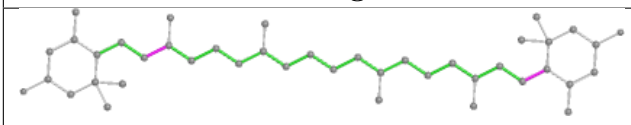
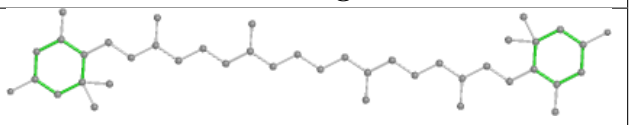
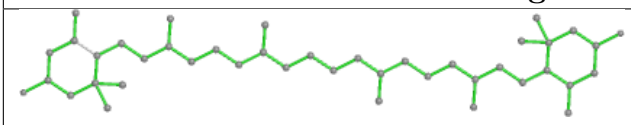
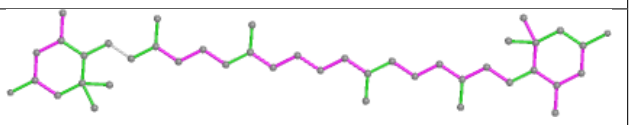
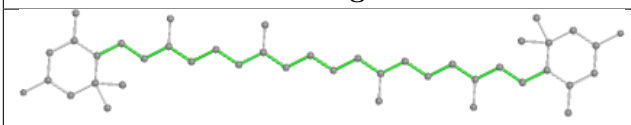
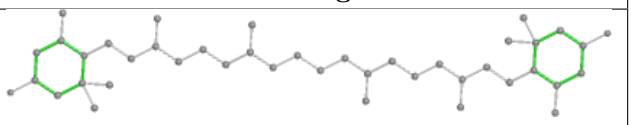
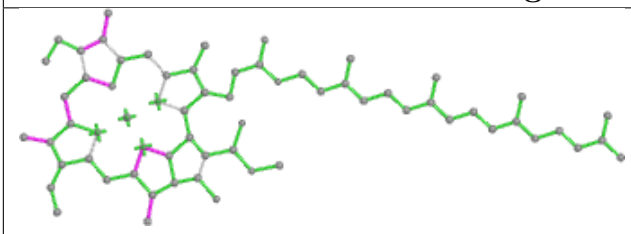
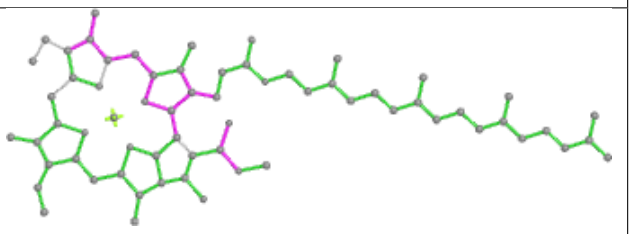
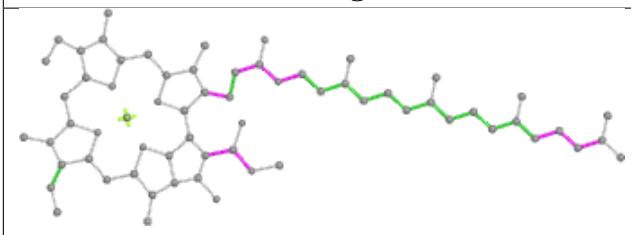
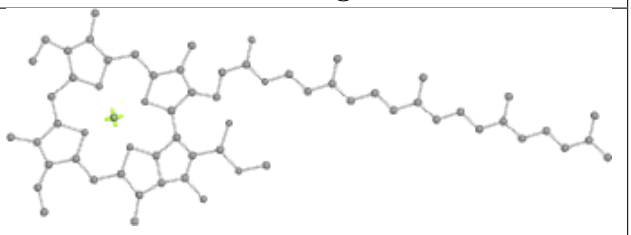
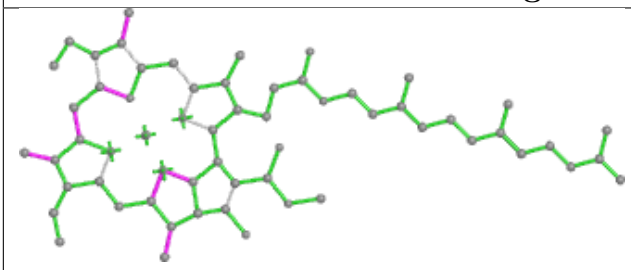
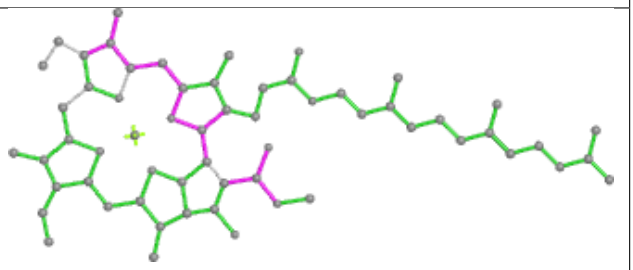
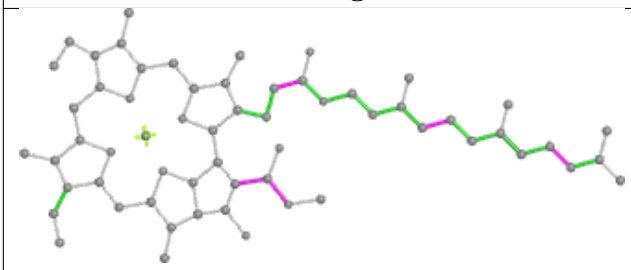
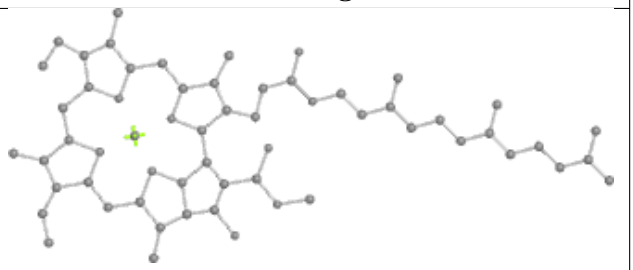


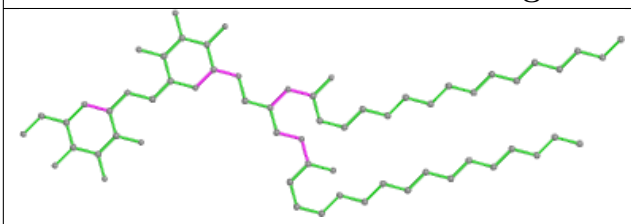
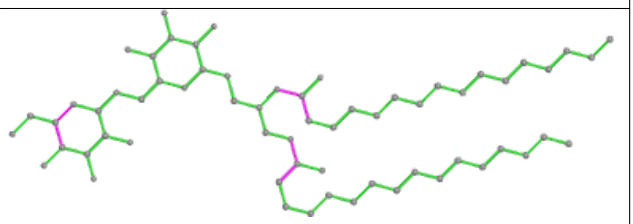
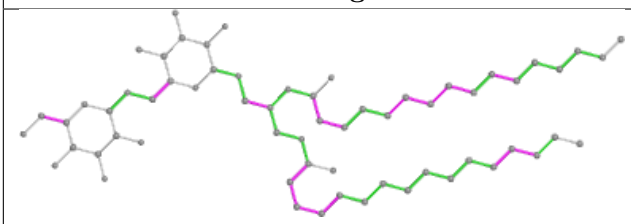
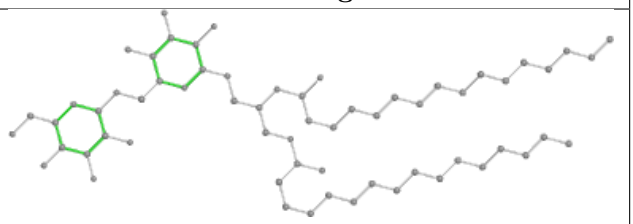
Rings

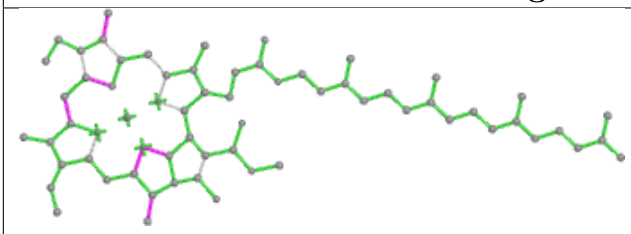
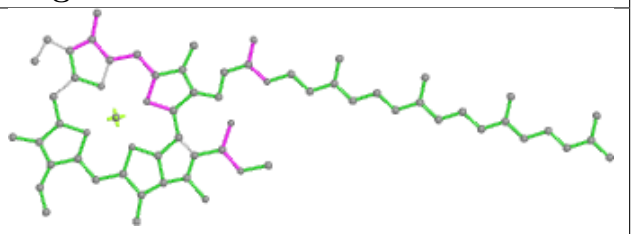
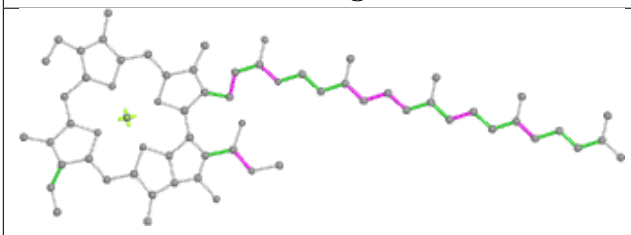
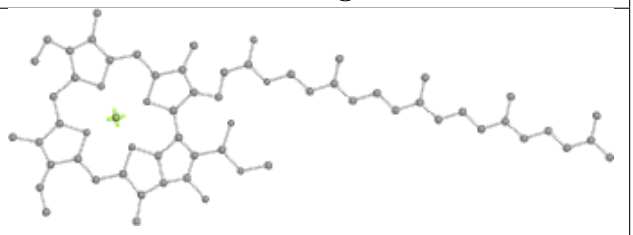
Ligand LUT 2 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

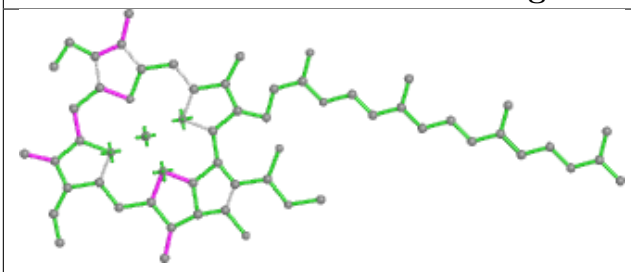
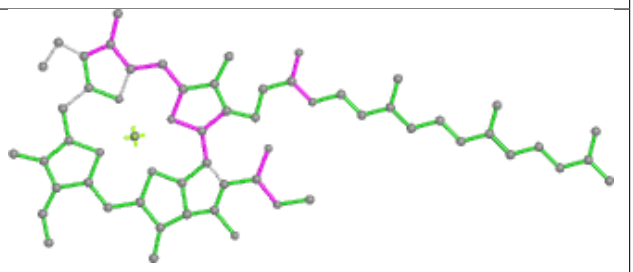
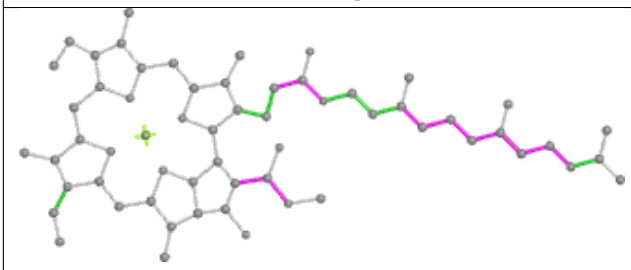
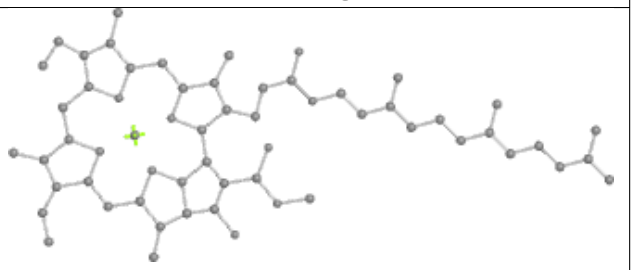
Ligand LUT 1 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

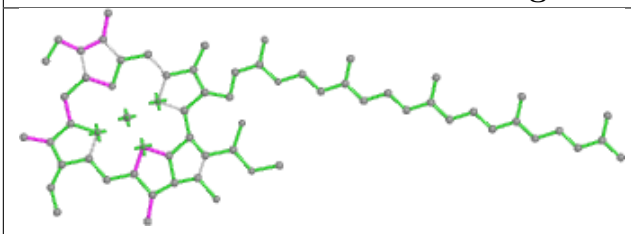
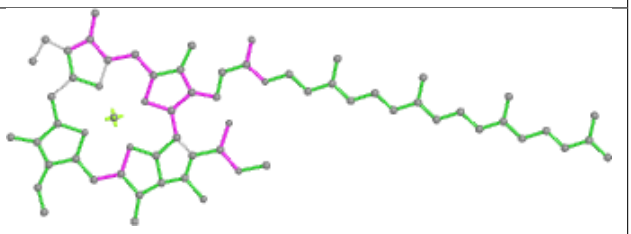
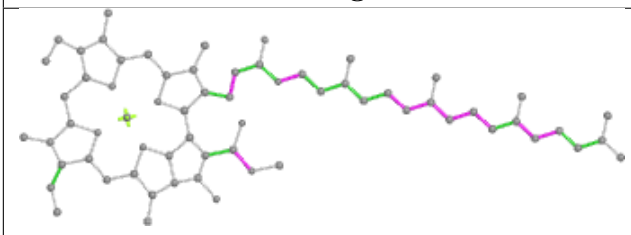
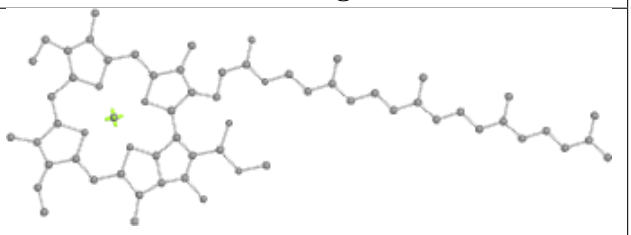
Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

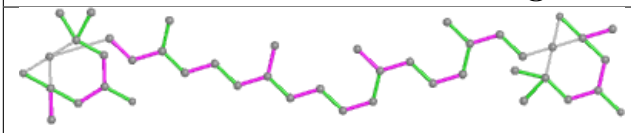
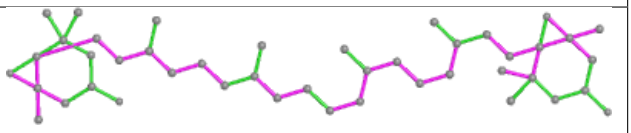
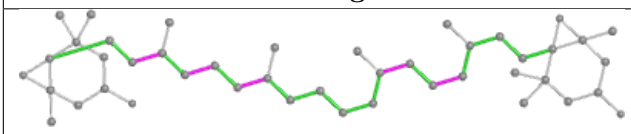
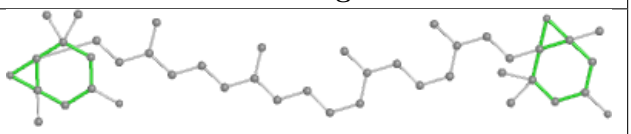
Ligand CLA V 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

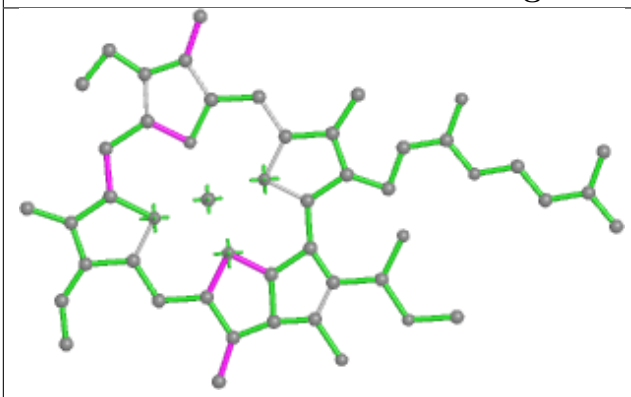
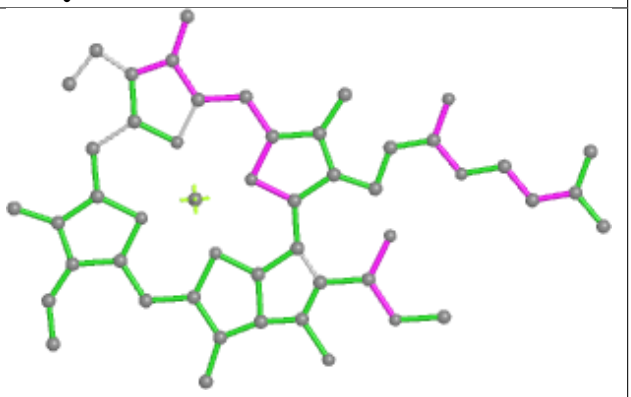
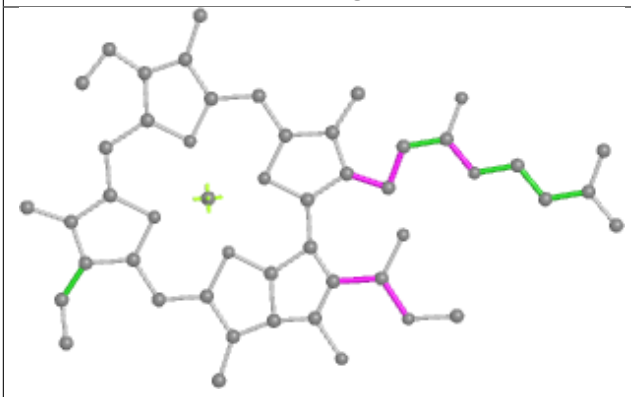
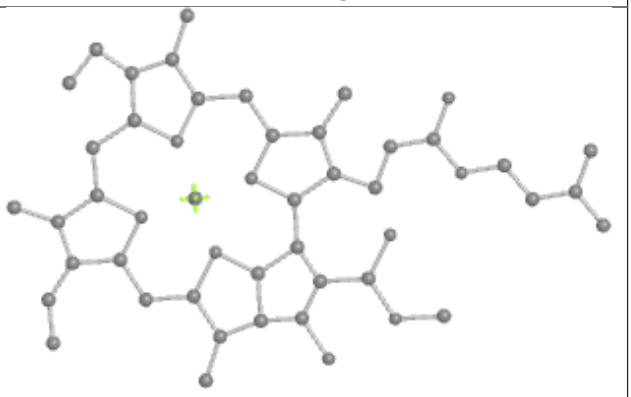
Ligand DGD b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

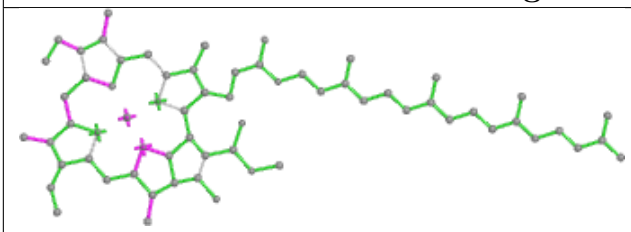
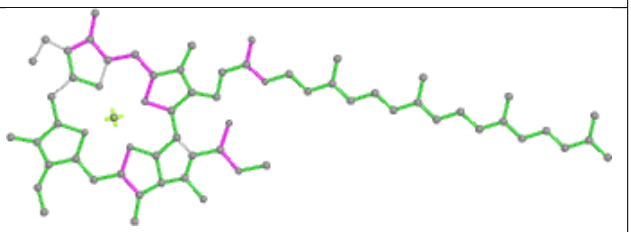
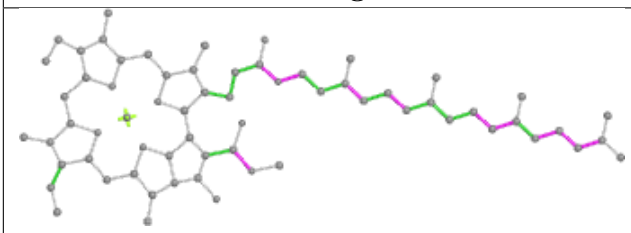
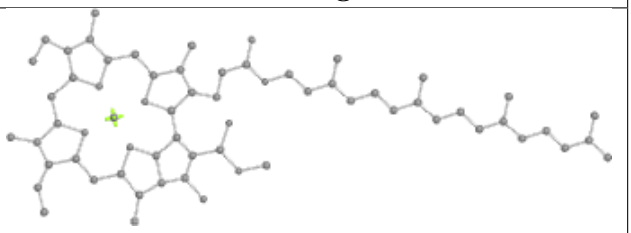
Ligand CLA g 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

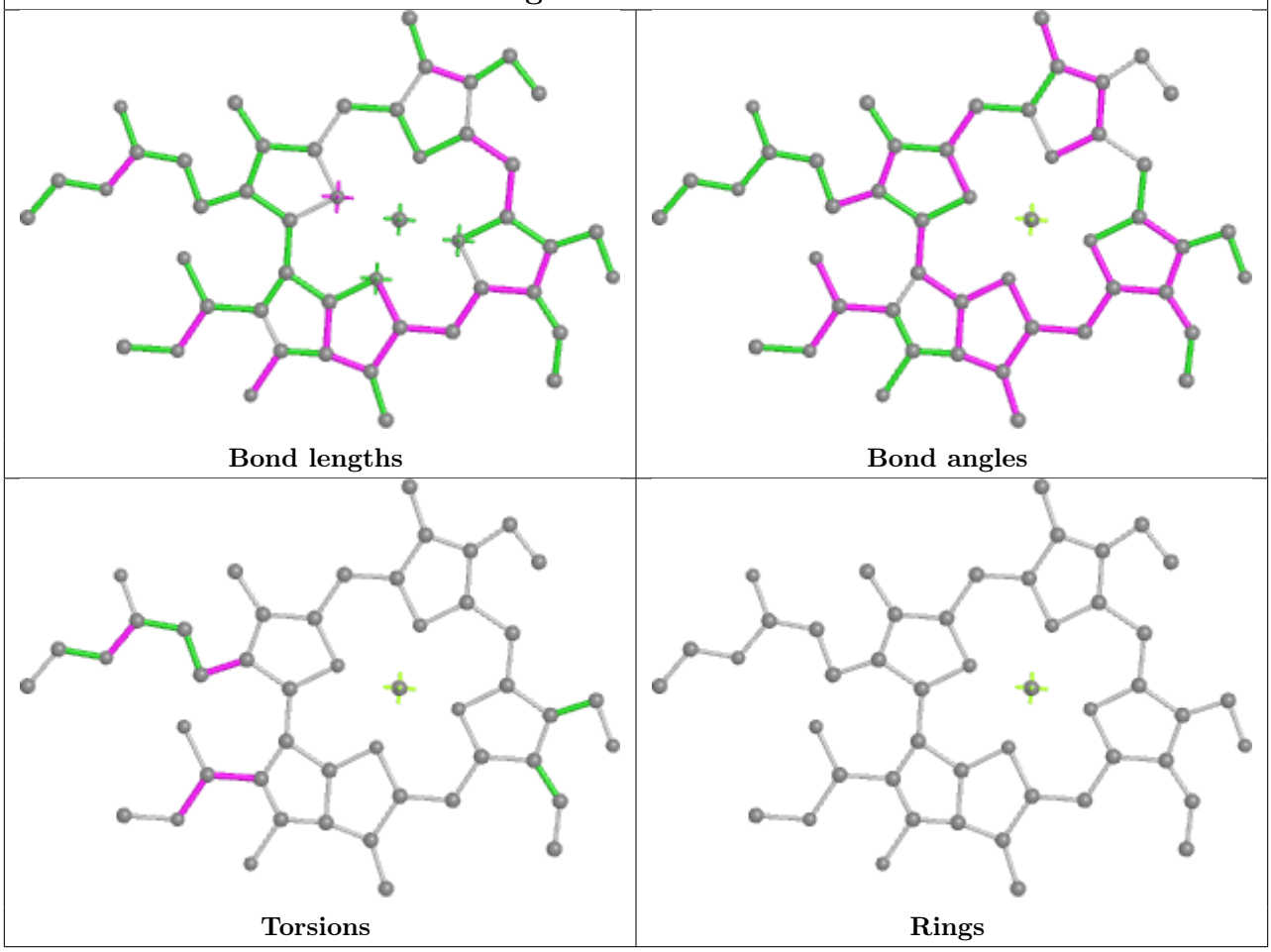
Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 1 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

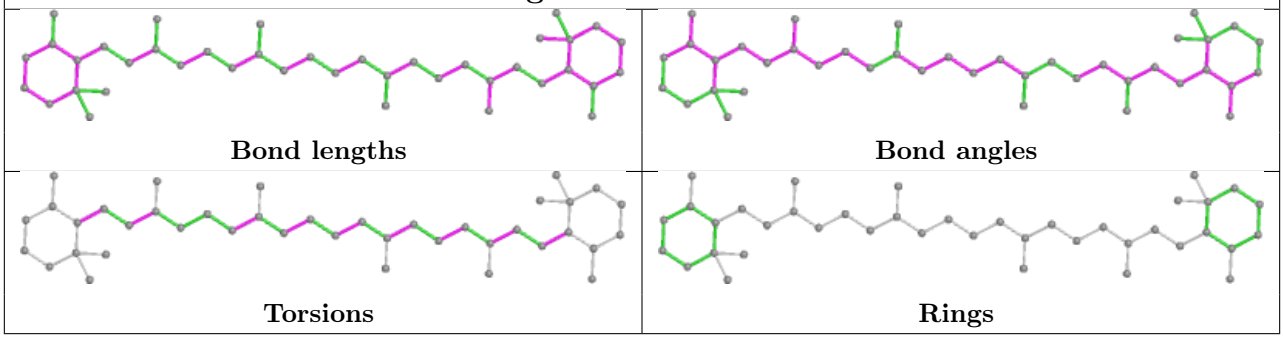
Ligand CLA Q 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

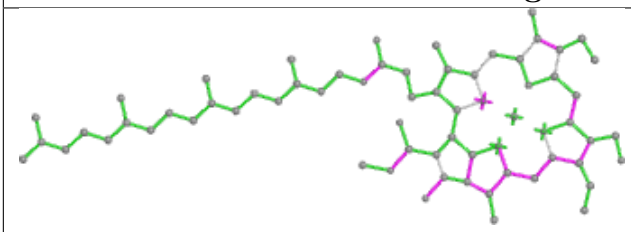
Ligand CHL r 619



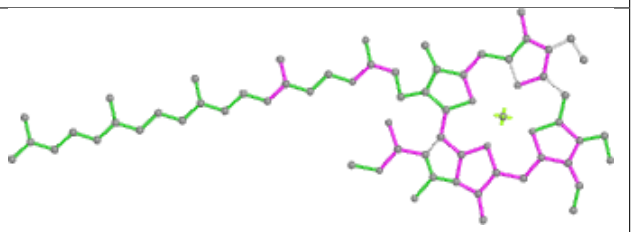
Ligand BCR b 619



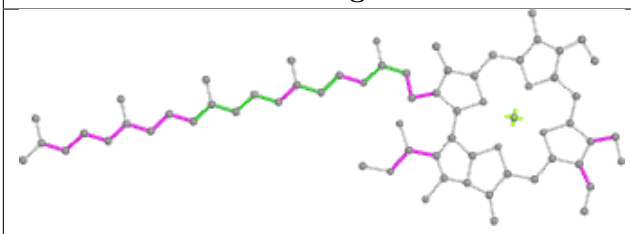
Ligand CHL P 319



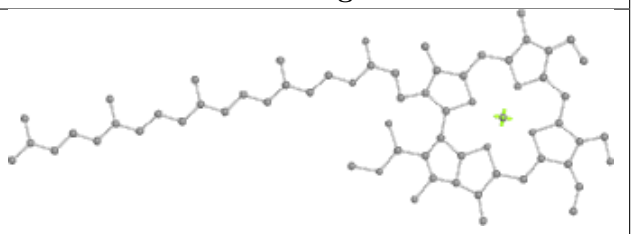
Bond lengths



Bond angles

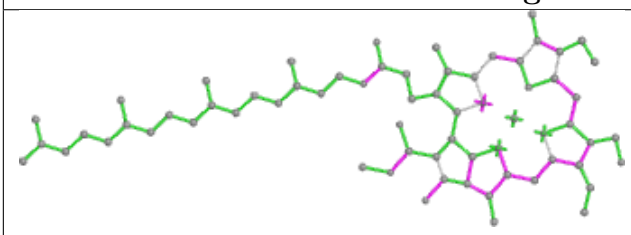


Torsions



Rings

Ligand CHL V 316



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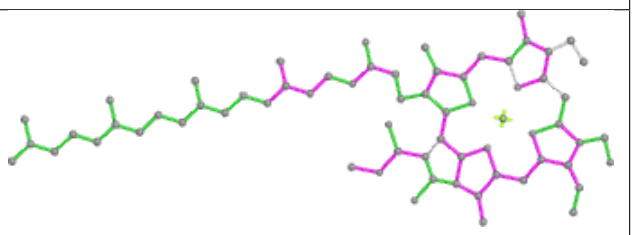
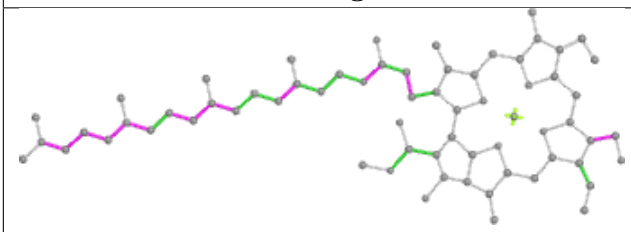


Bond angles



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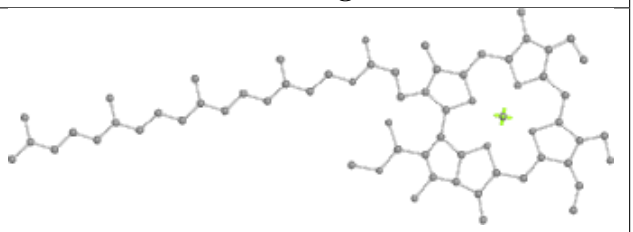
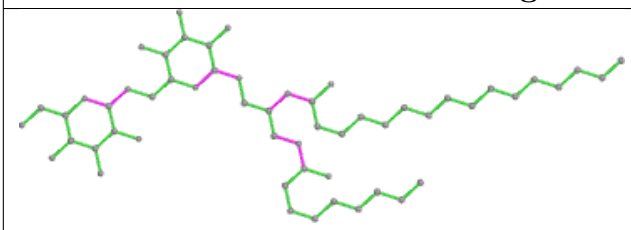
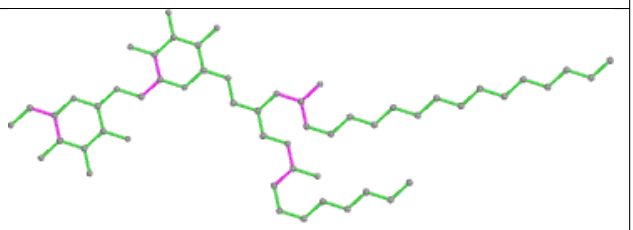


Rings

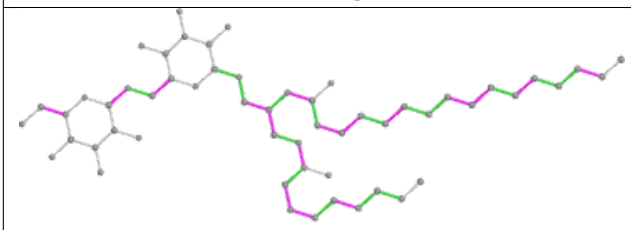
Ligand DGD C 519



Bond lengths



Bond angles



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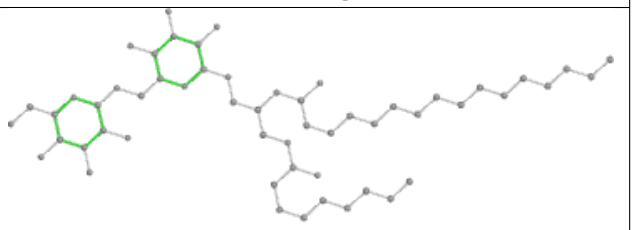
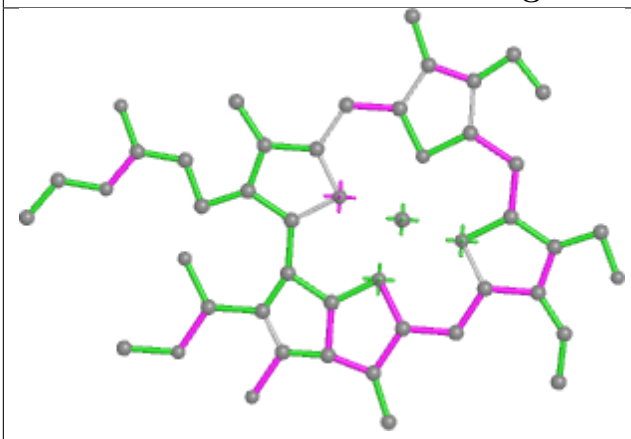


Rings

Ligand CHL N 314



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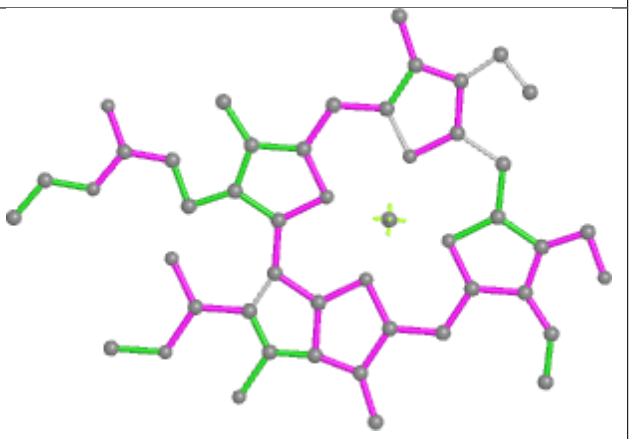
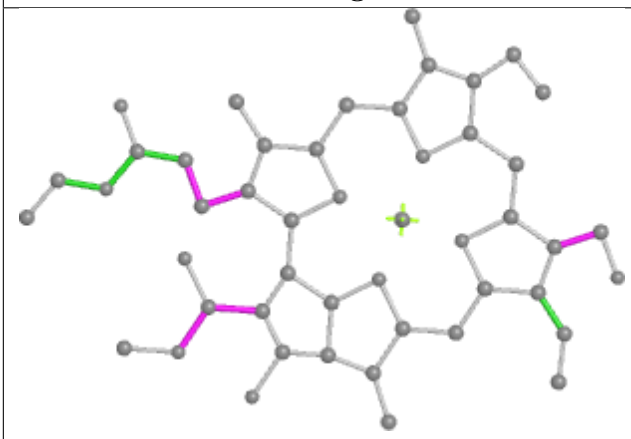


Bond angles



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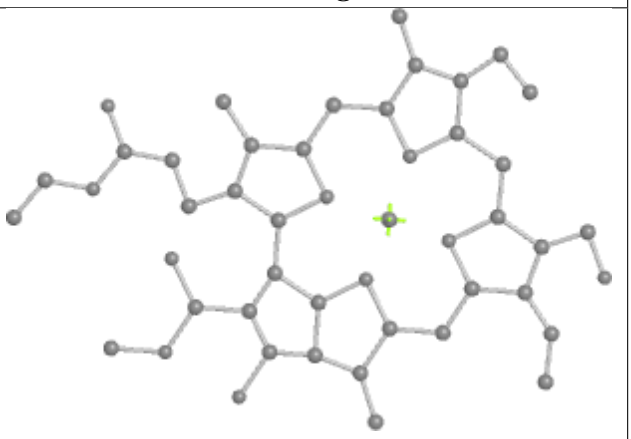
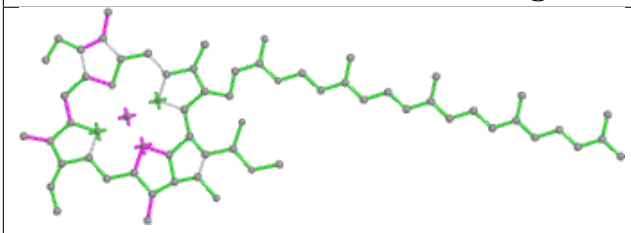


Rings

Ligand CLA c 512



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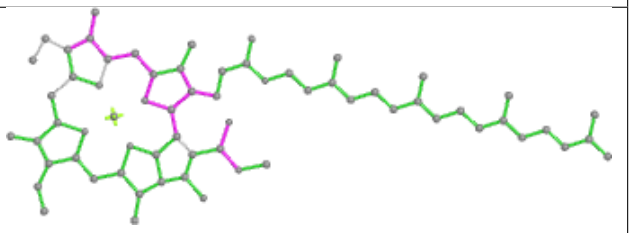
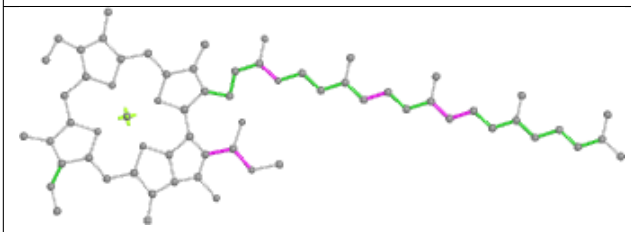


Bond angles



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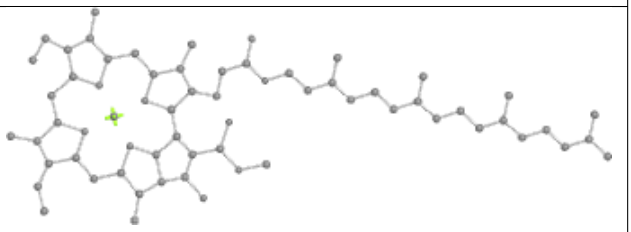
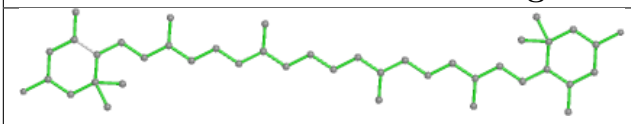
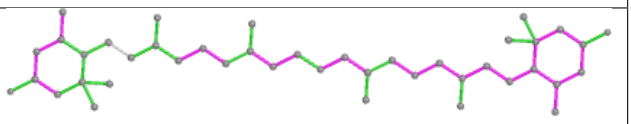


Rings

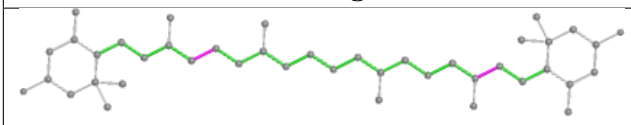
Ligand LUT n 310



Bond lengths



Bond angles



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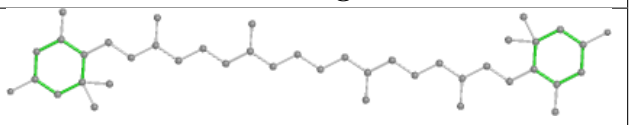
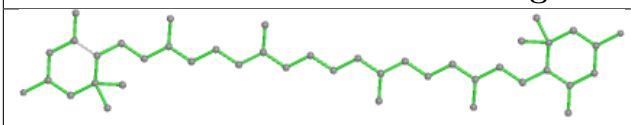


Rings

Ligand LUT r 611



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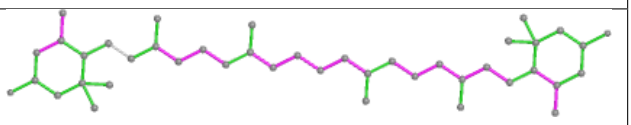
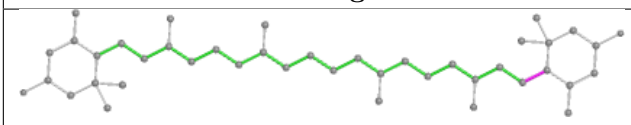


Bond angles



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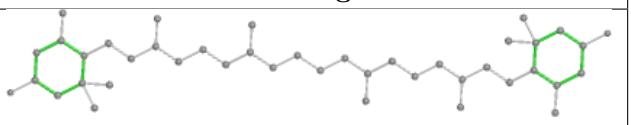
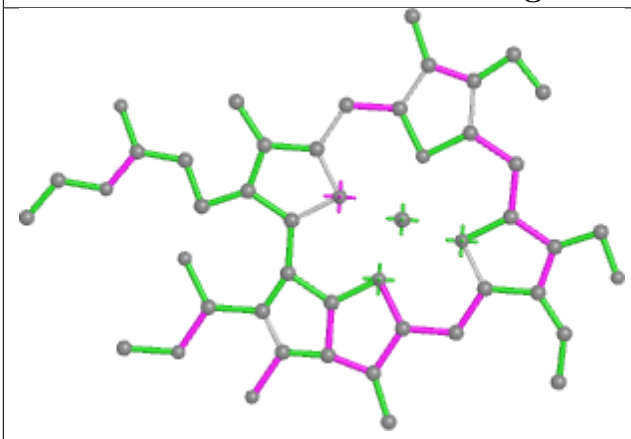


Rings

Ligand CHL P 315



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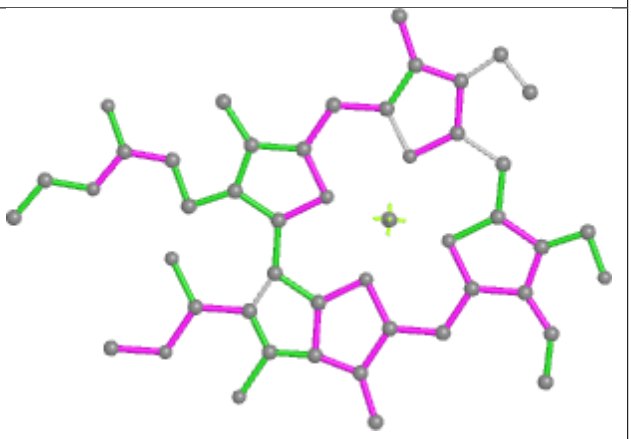
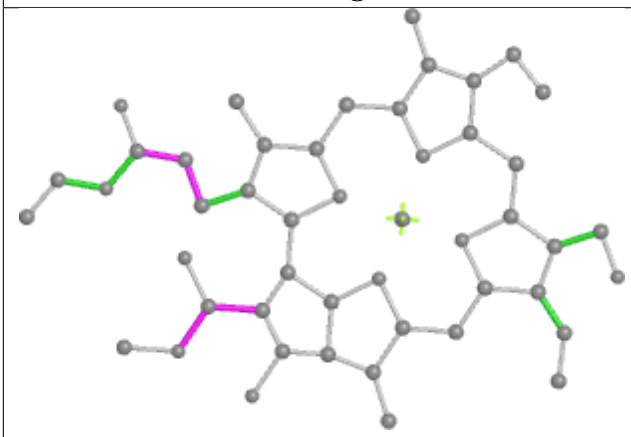


Bond angles



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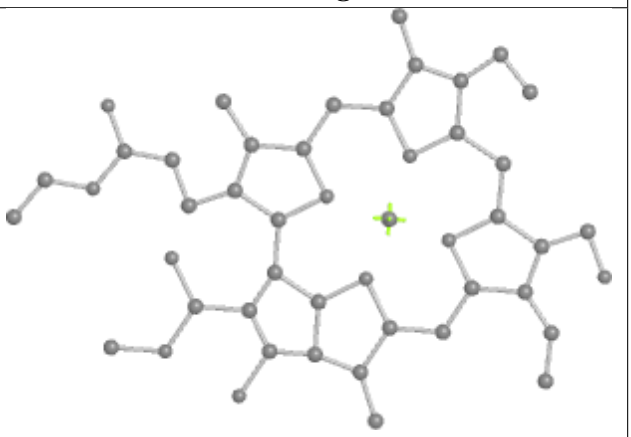
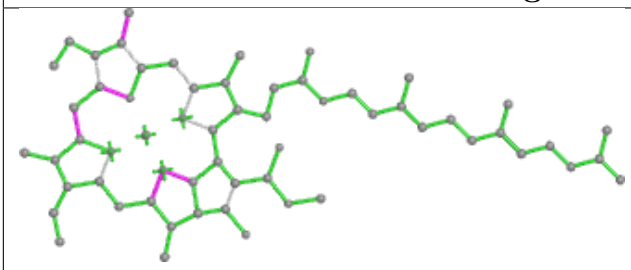
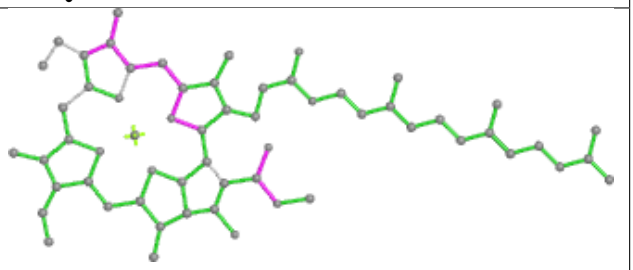
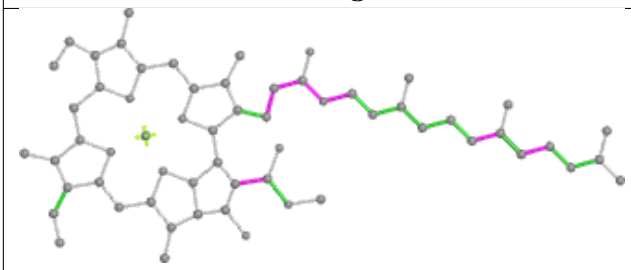
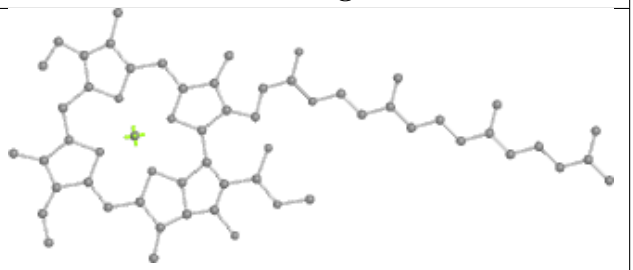
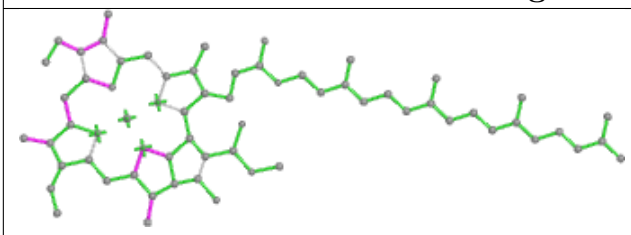
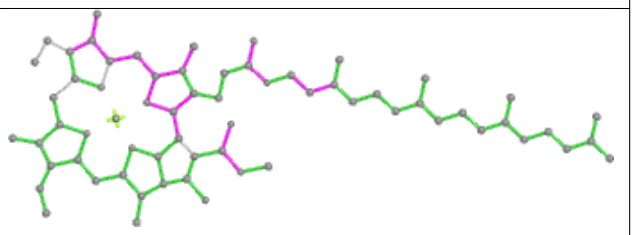
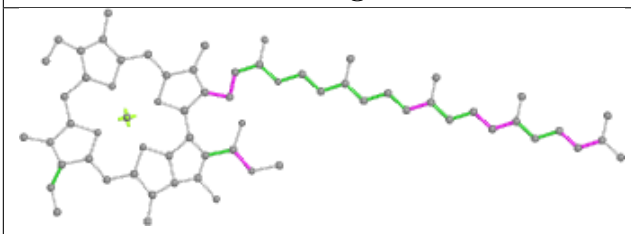
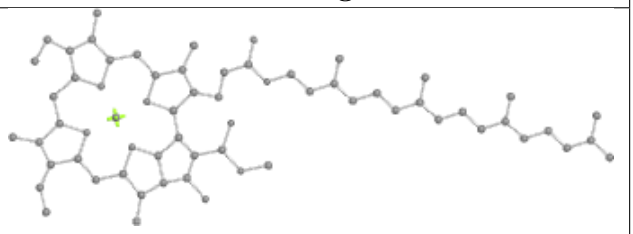
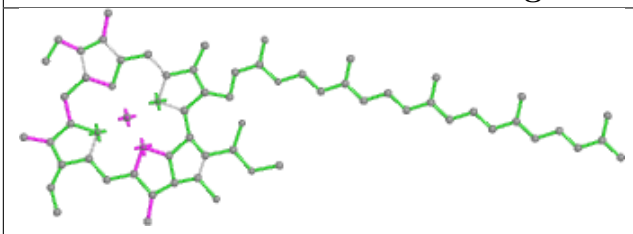


Rings

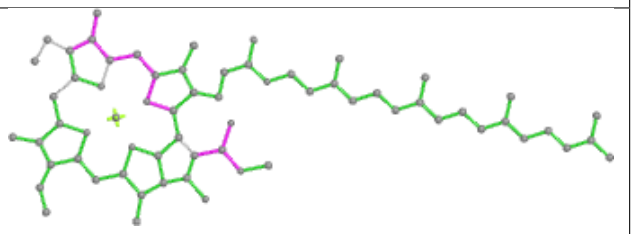
Ligand CLA Q 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

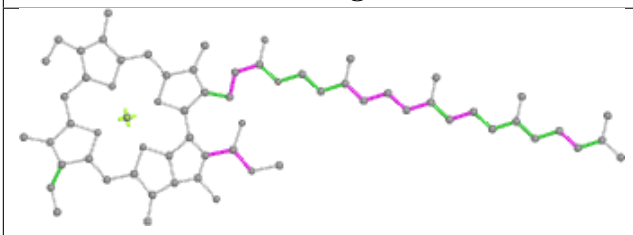
Ligand CLA B 615



Bond lengths



Bond angles



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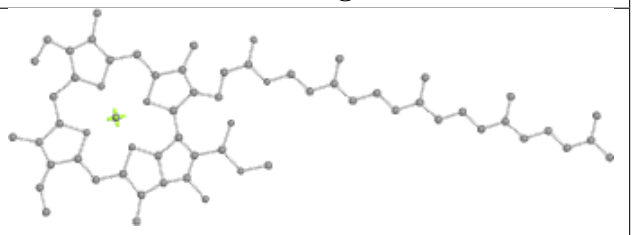
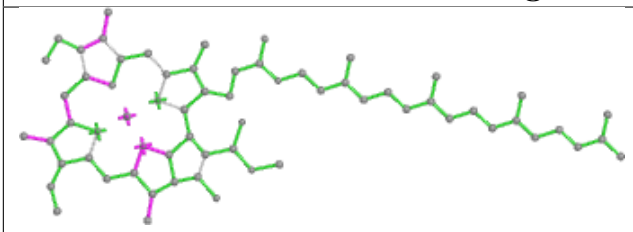
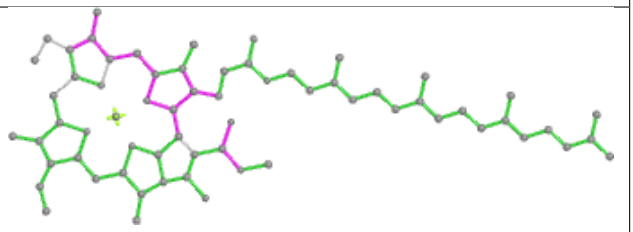


Rings

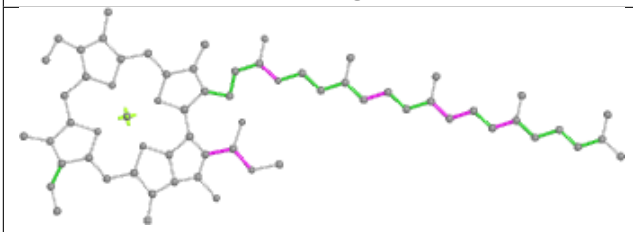
Ligand CLA C 513



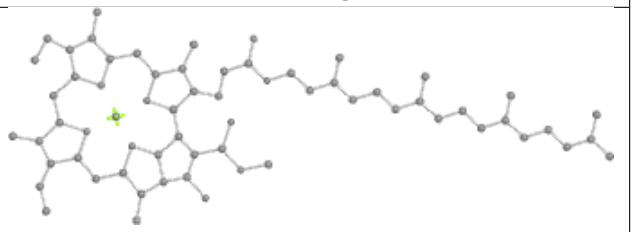
Bond lengths



Bond angles

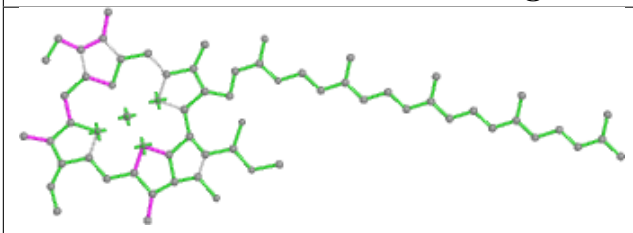


Torsions

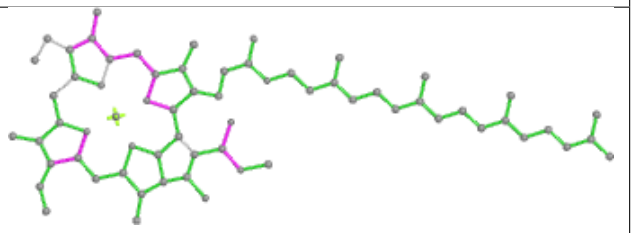


Rings

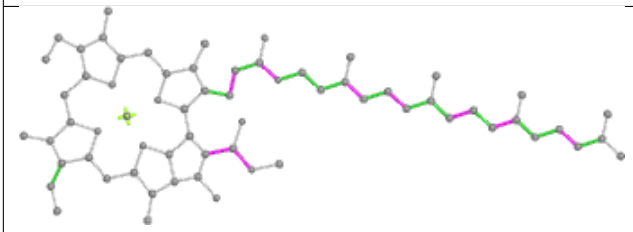
Ligand CLA C 506



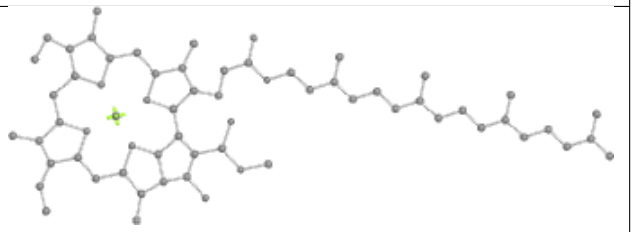
Bond lengths



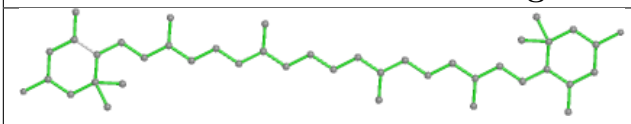
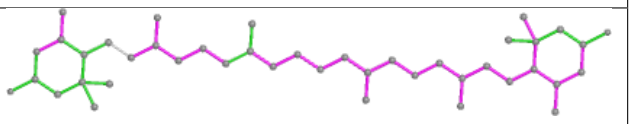
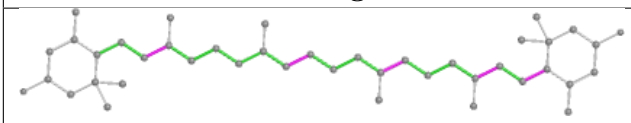
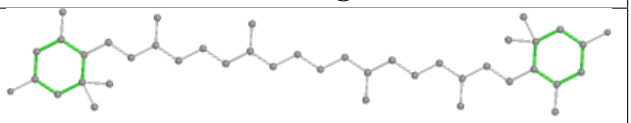
Bond angles

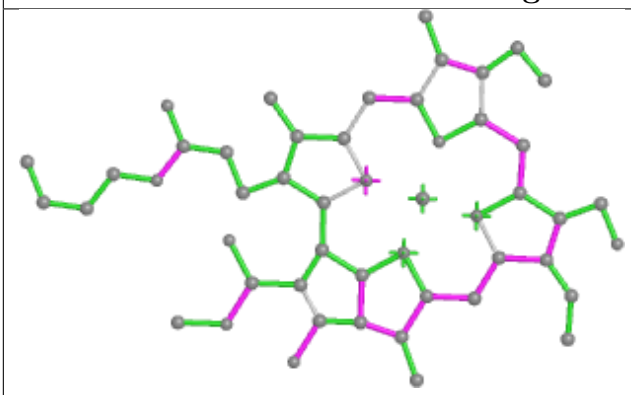
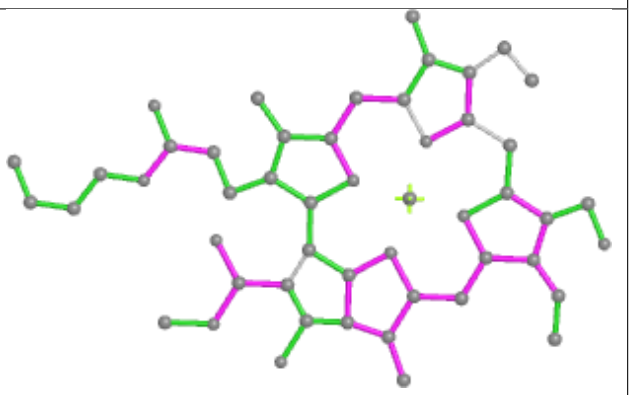
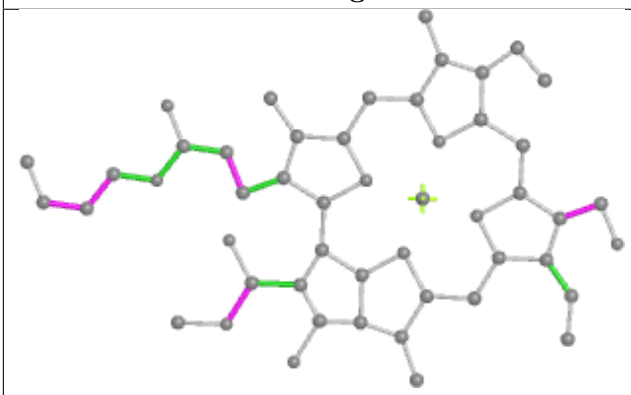
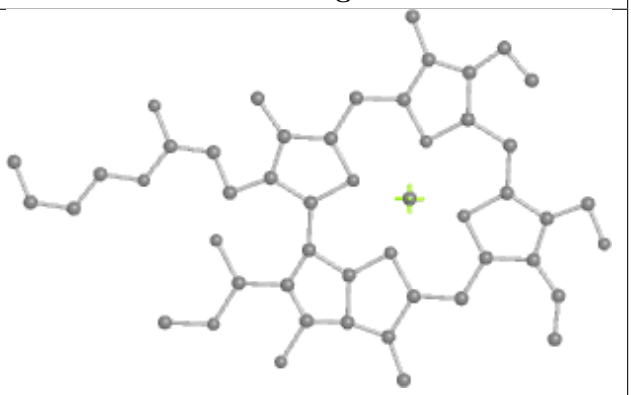


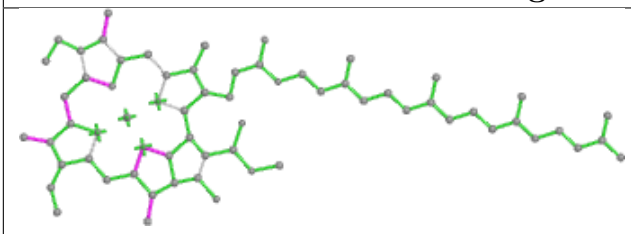
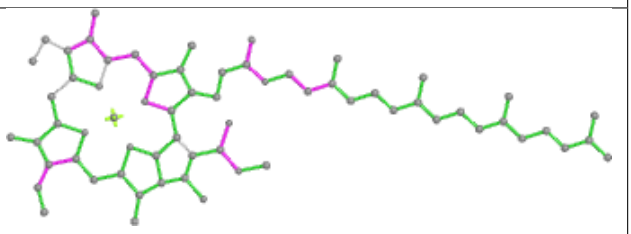
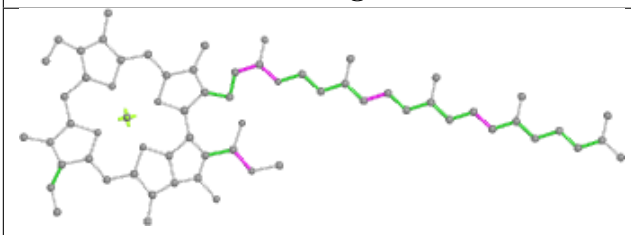
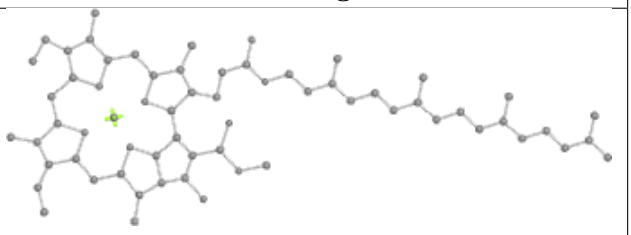
Torsions



Rings

Ligand LUT S 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

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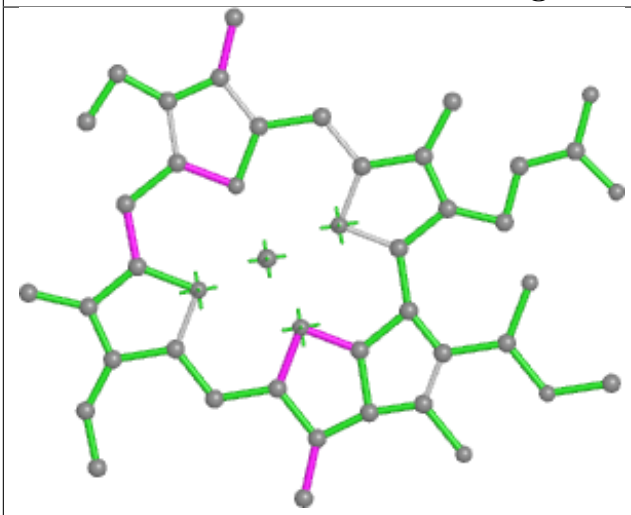
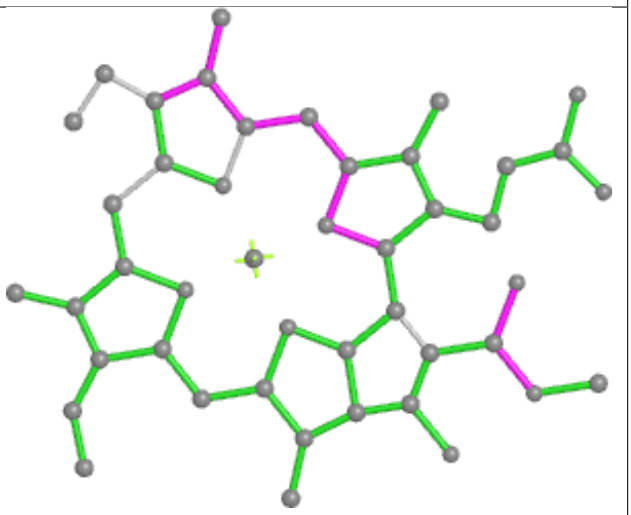
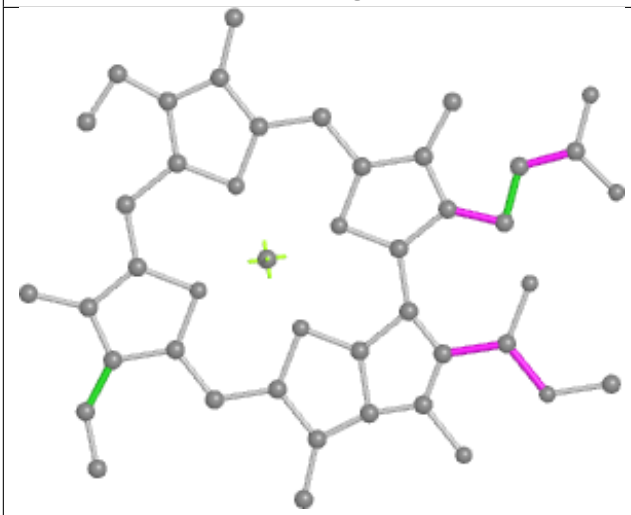
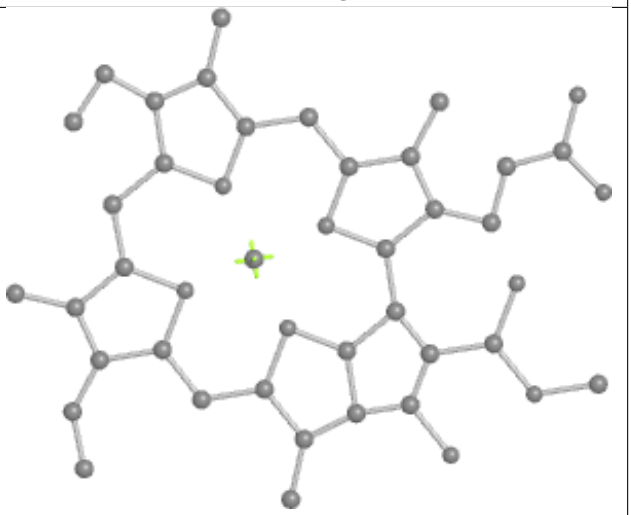
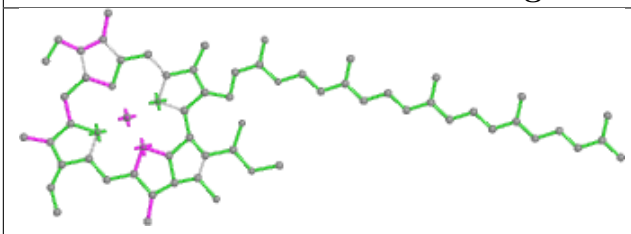
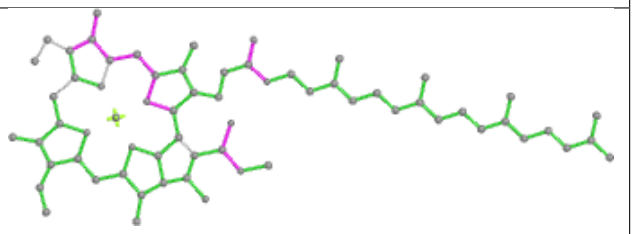
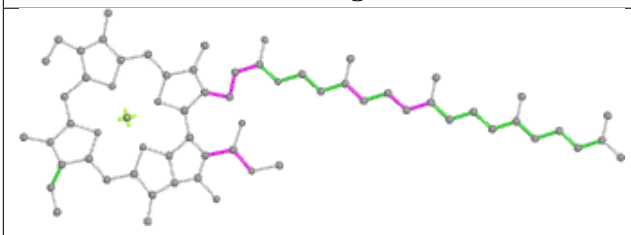
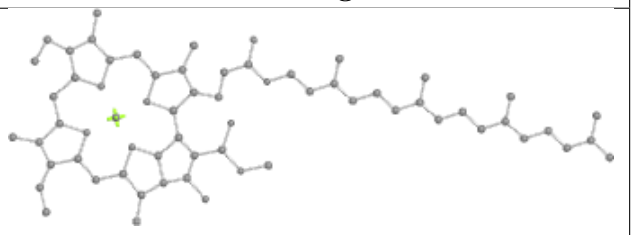
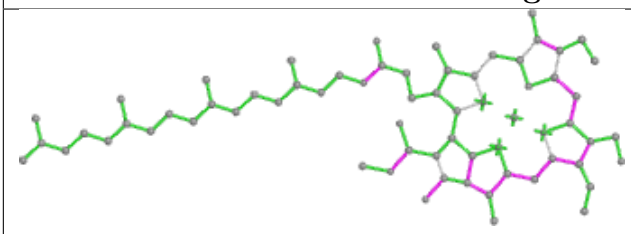
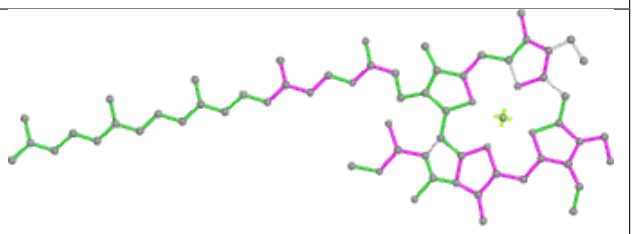
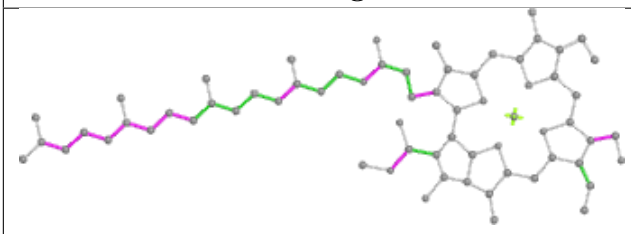
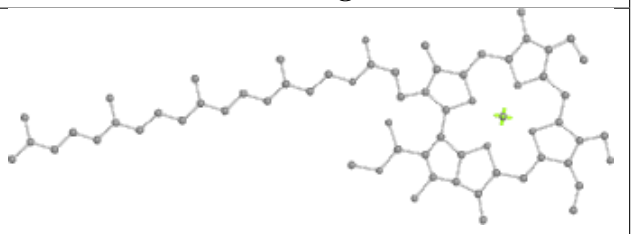
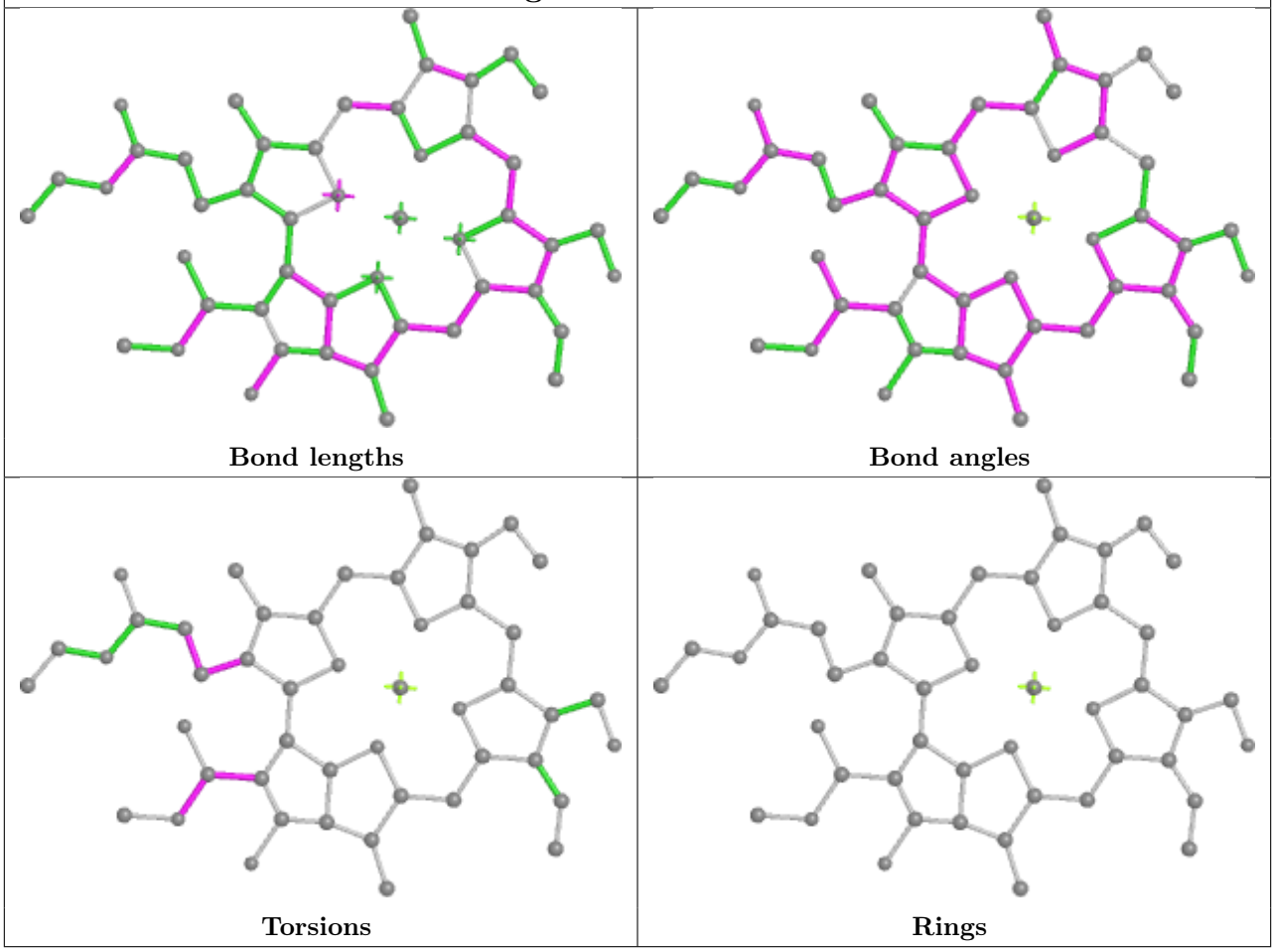
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL R 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 313



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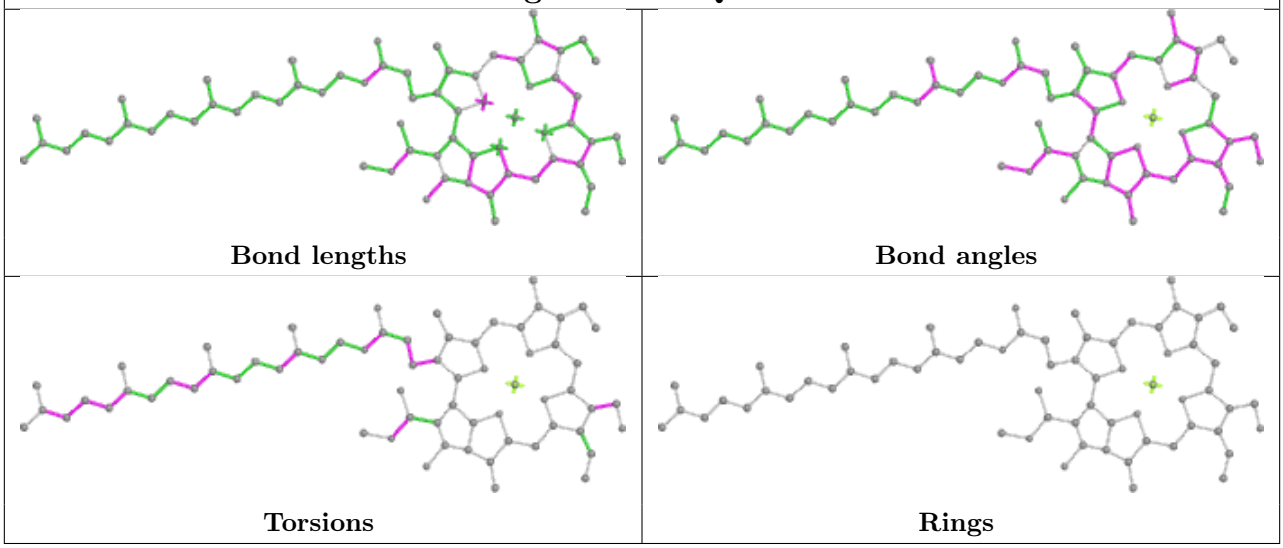

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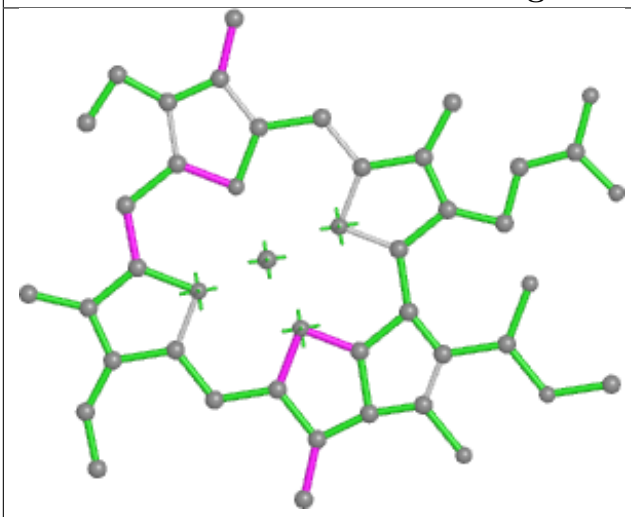
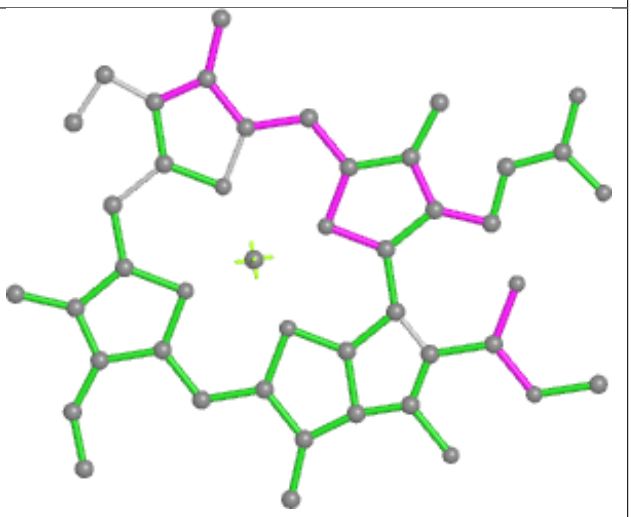
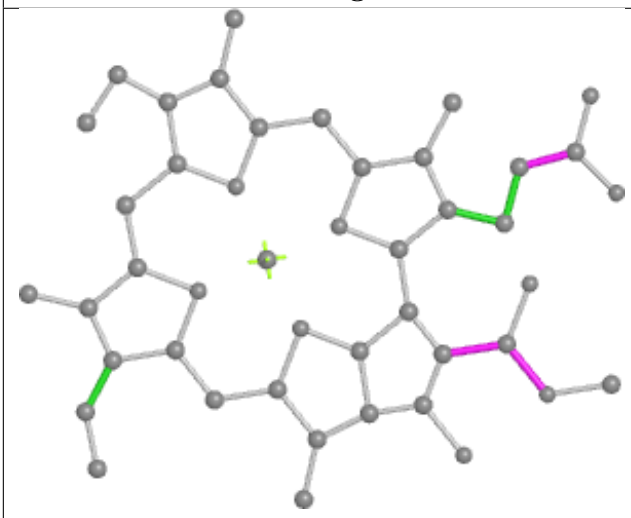


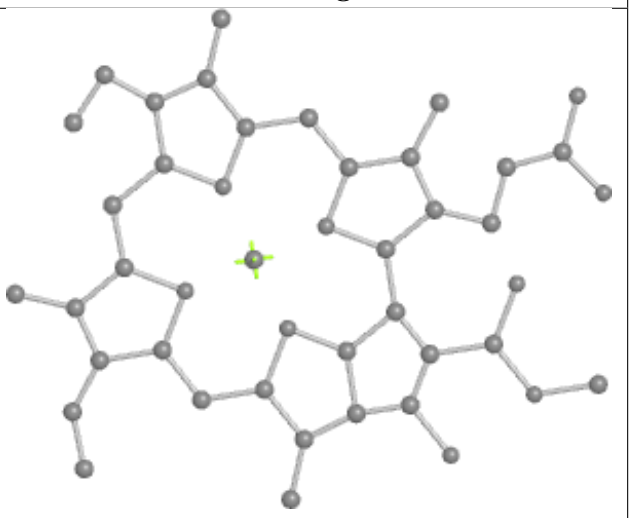
Bond lengths



Bond angles

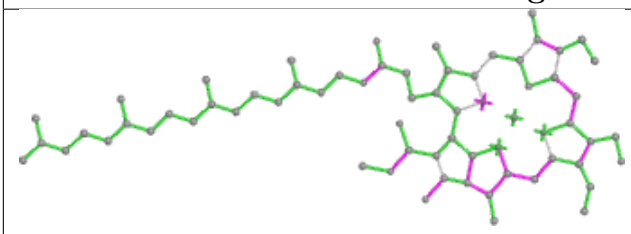


Torsions

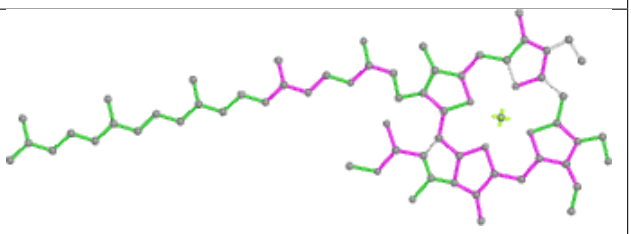


Rings

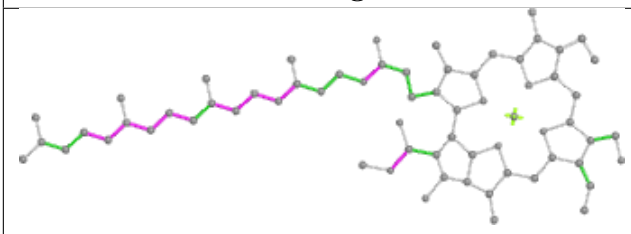
Ligand CHL 3 311



Bond lengths



Bond angles



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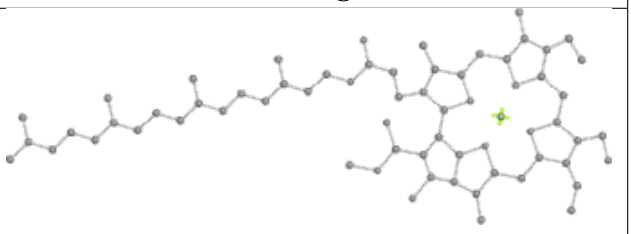
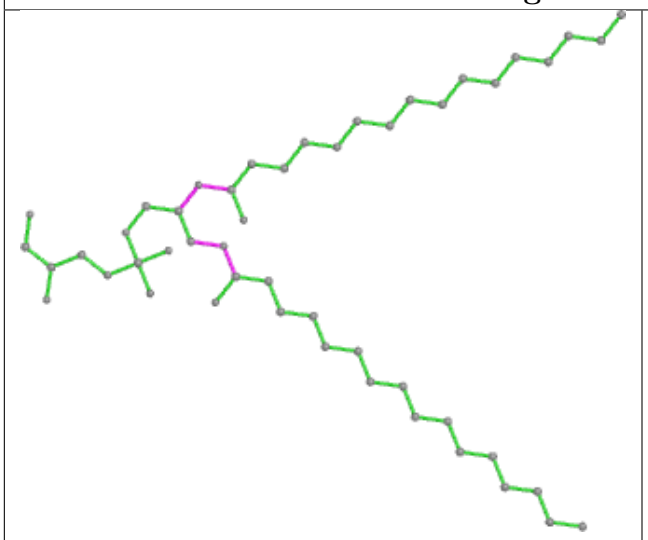
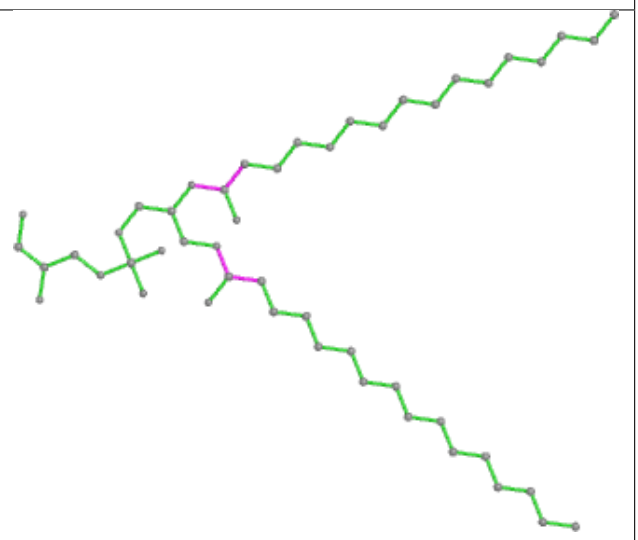


Rings

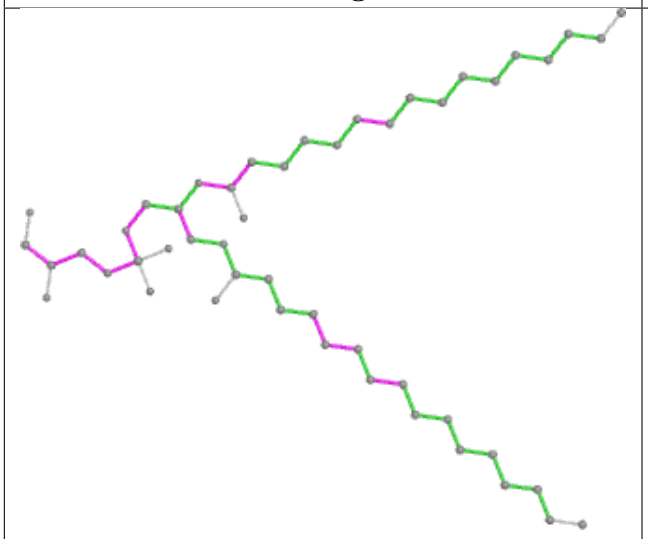
Ligand LHG B 623



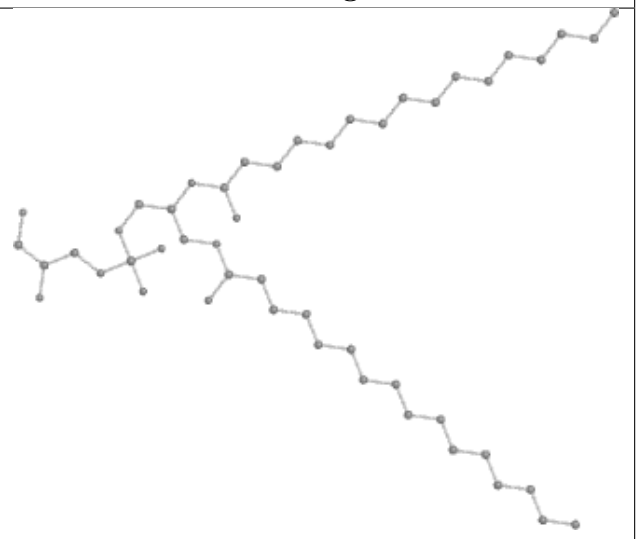
Bond lengths



Bond angles

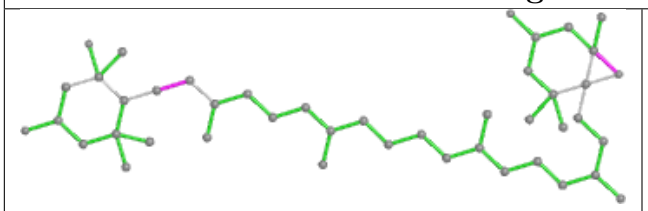


Torsions



Rings

Ligand NEX u 320



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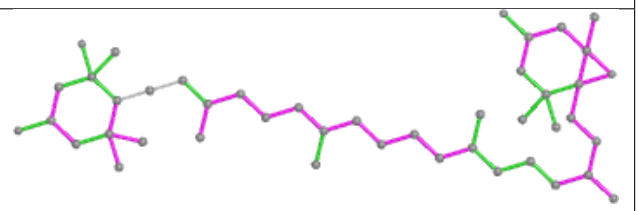
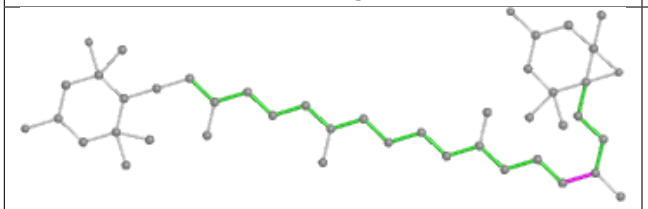
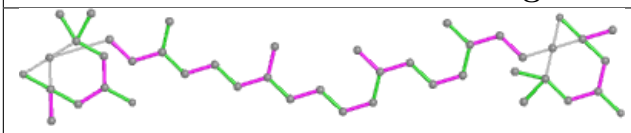
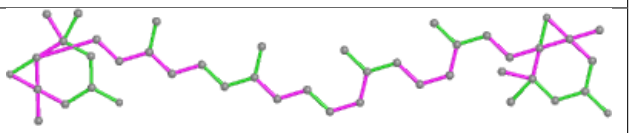
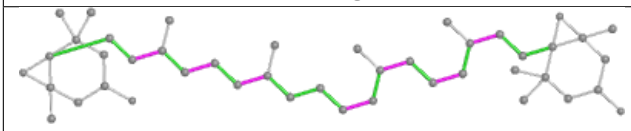
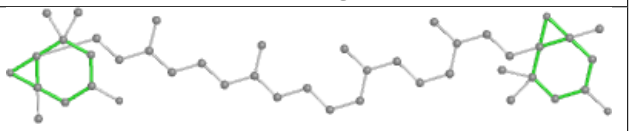


Bond angles



Torsions

Rings

Ligand XAT V 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

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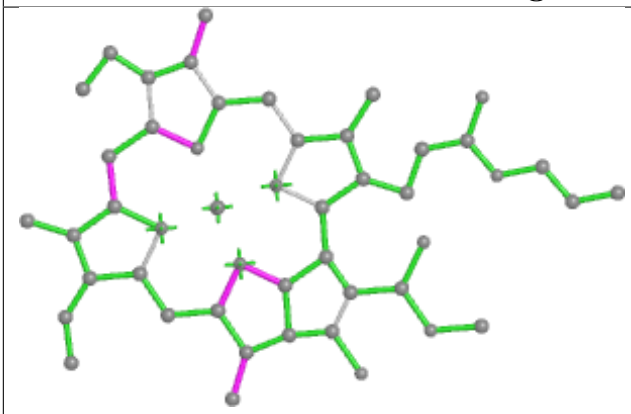
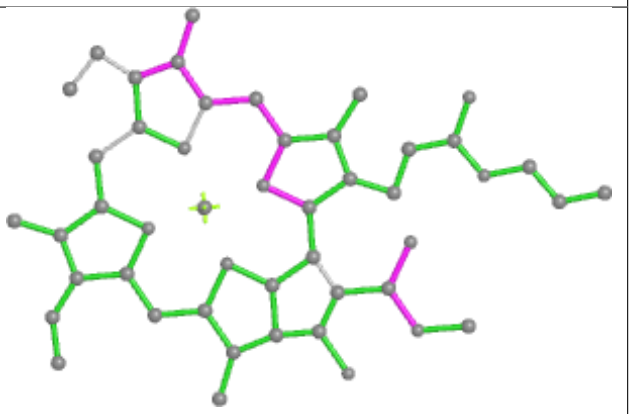
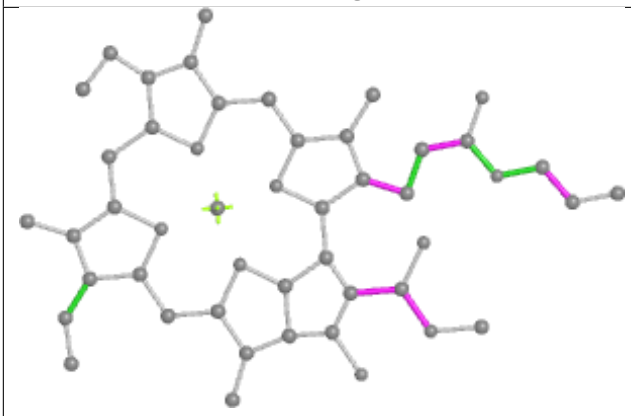
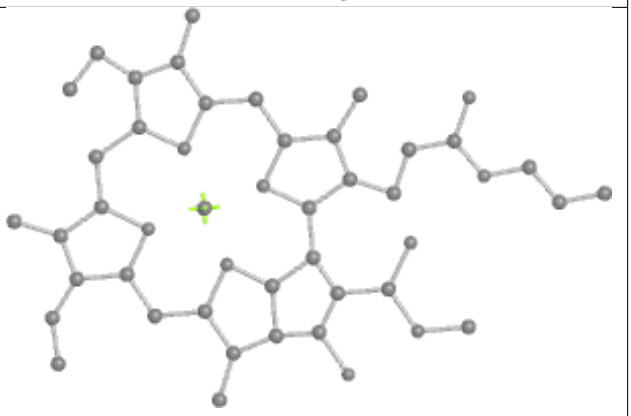
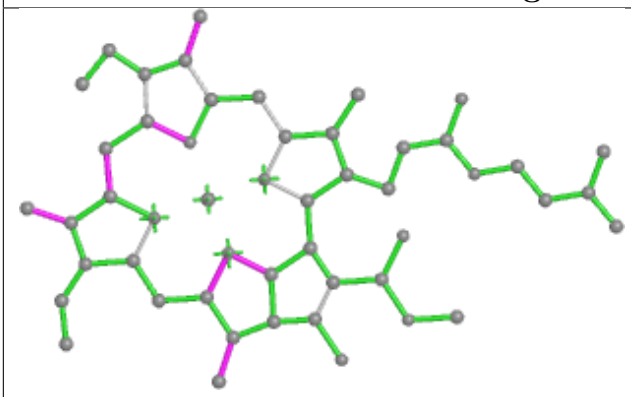
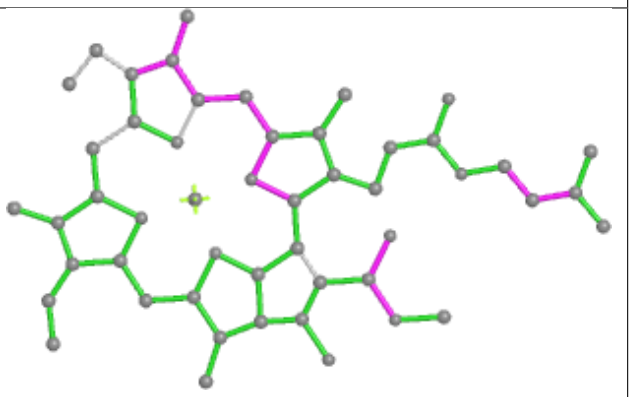
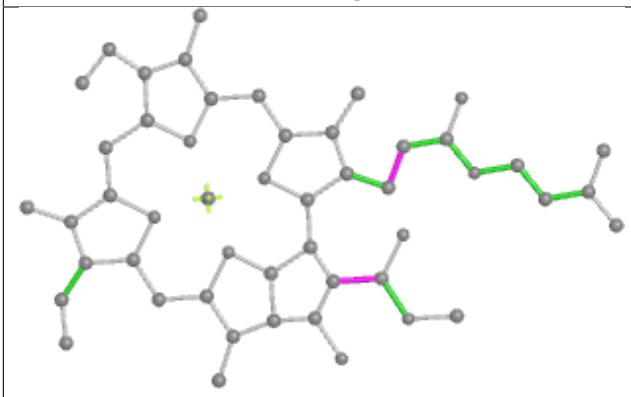
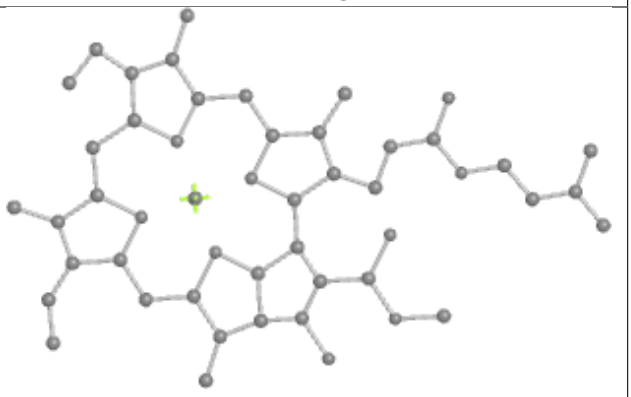
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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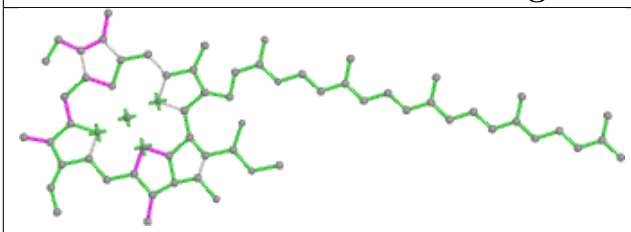
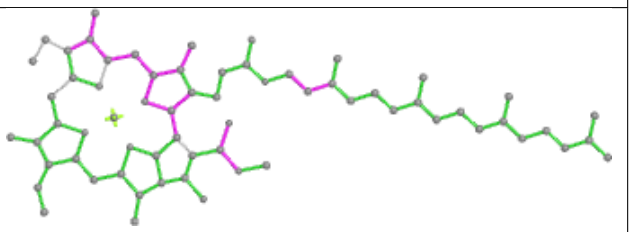
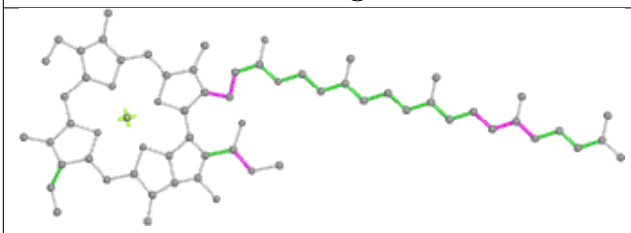
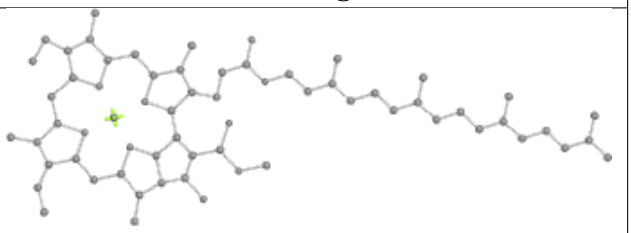
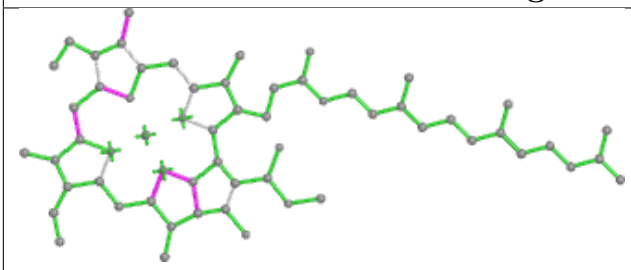
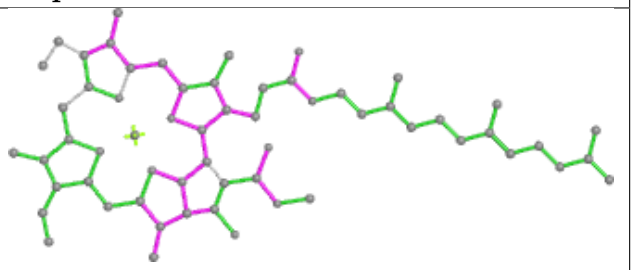
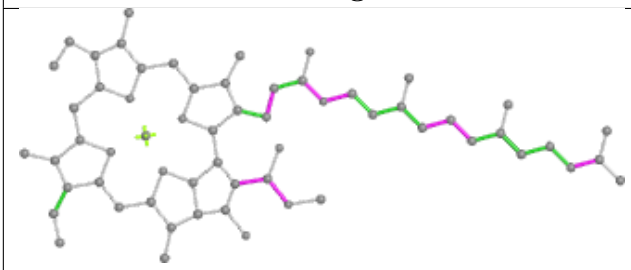
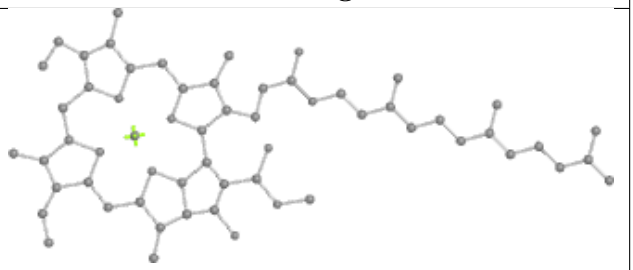
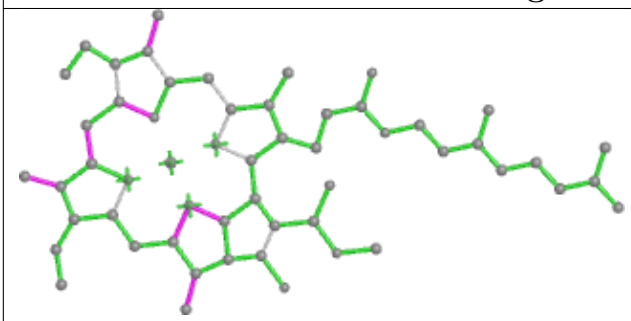
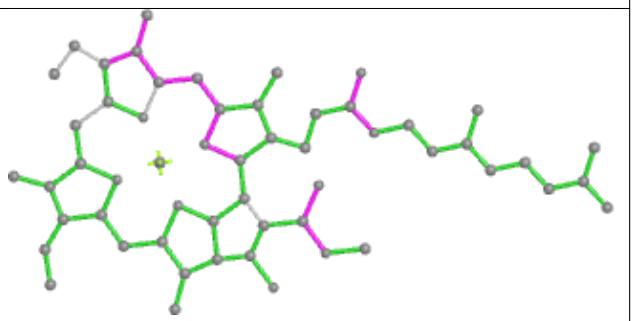
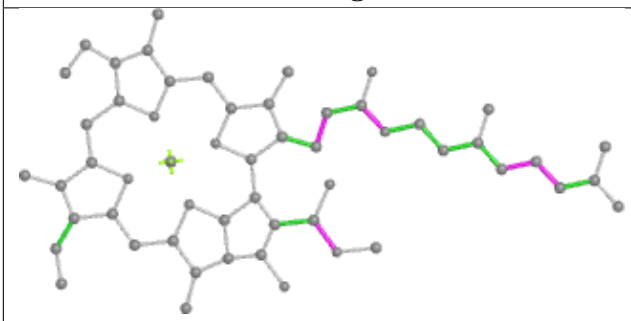
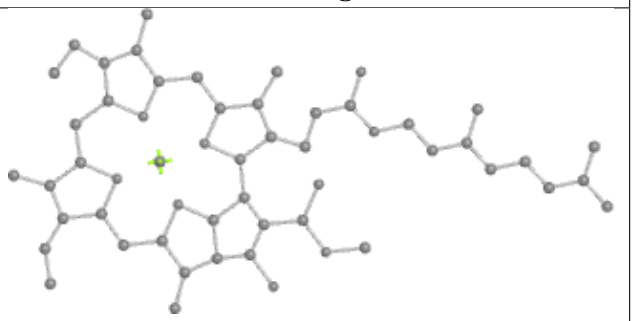
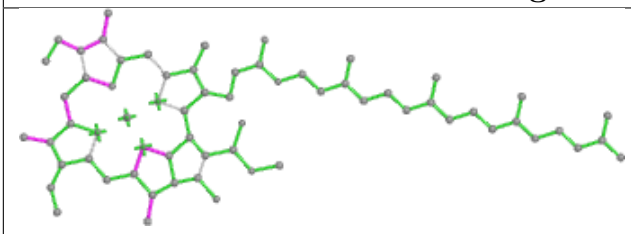
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 502



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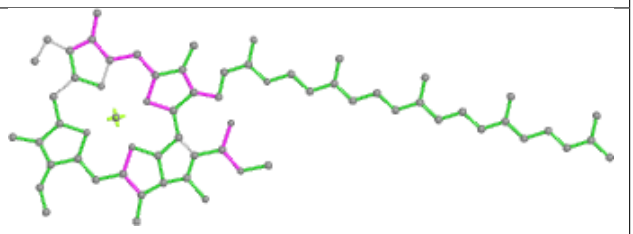
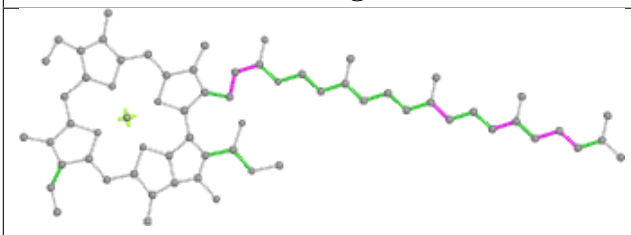


Bond angles



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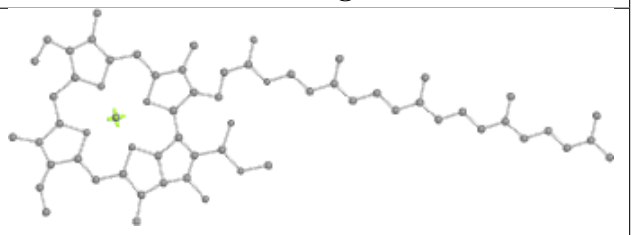
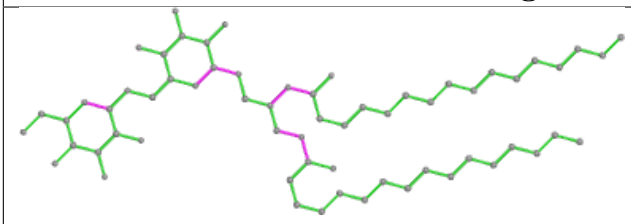


Rings

Ligand DGD B 601



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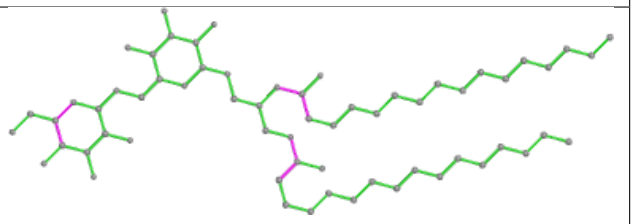
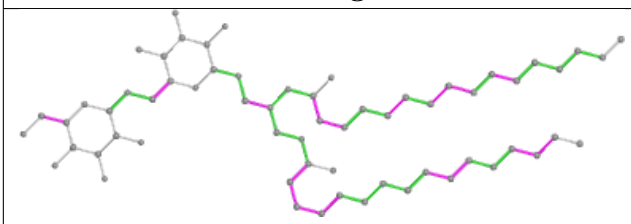


Bond angles



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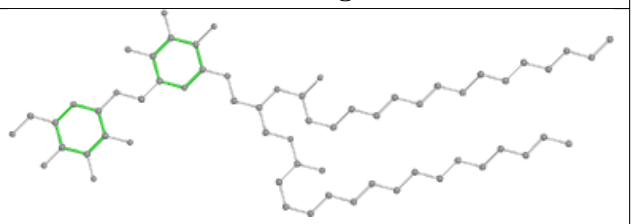
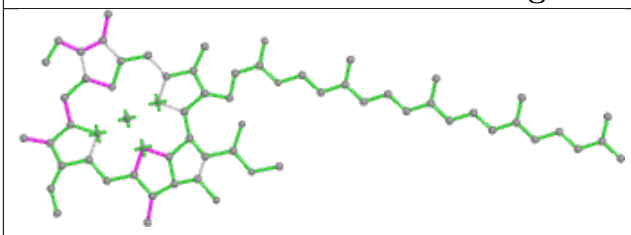


Rings

Ligand CLA 4 301



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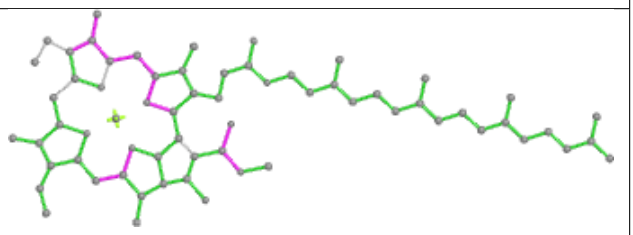
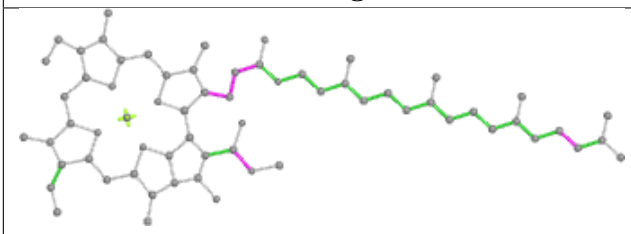


Bond angles



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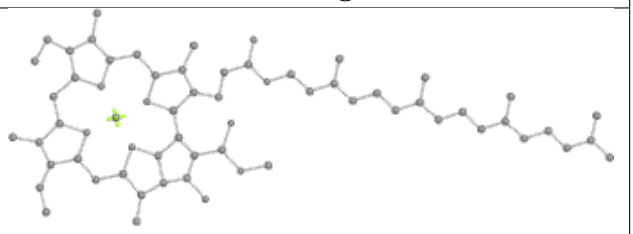
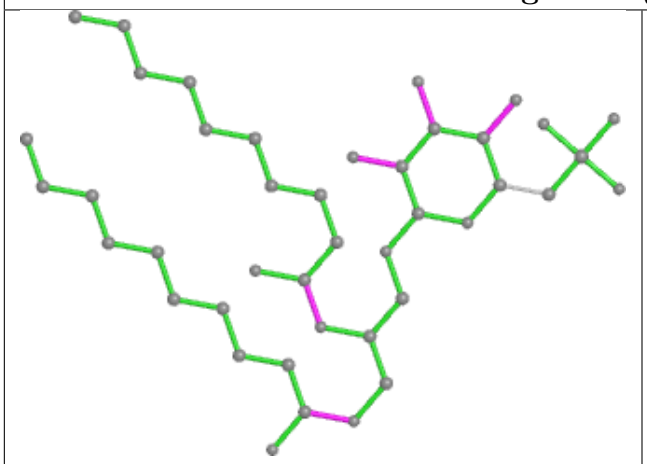


Rings

Ligand SQD M 101



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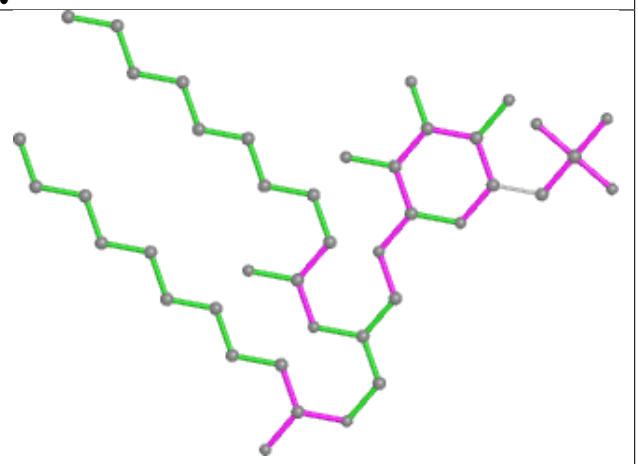

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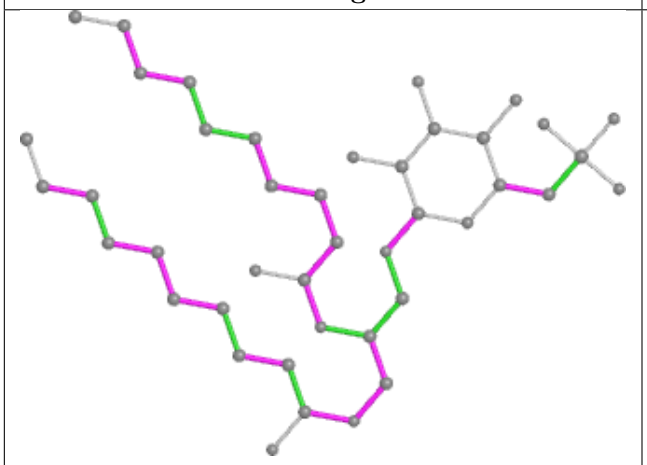

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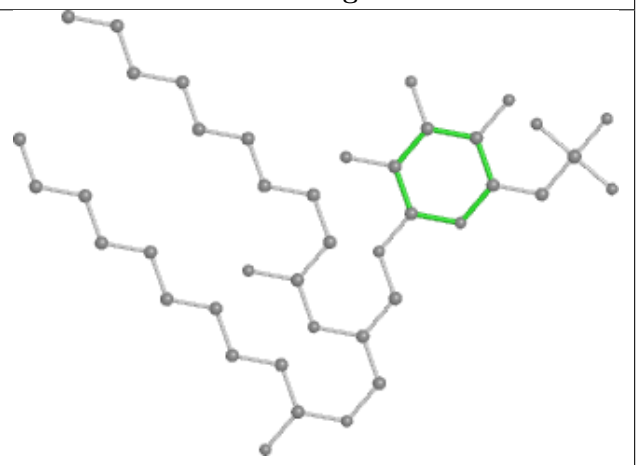
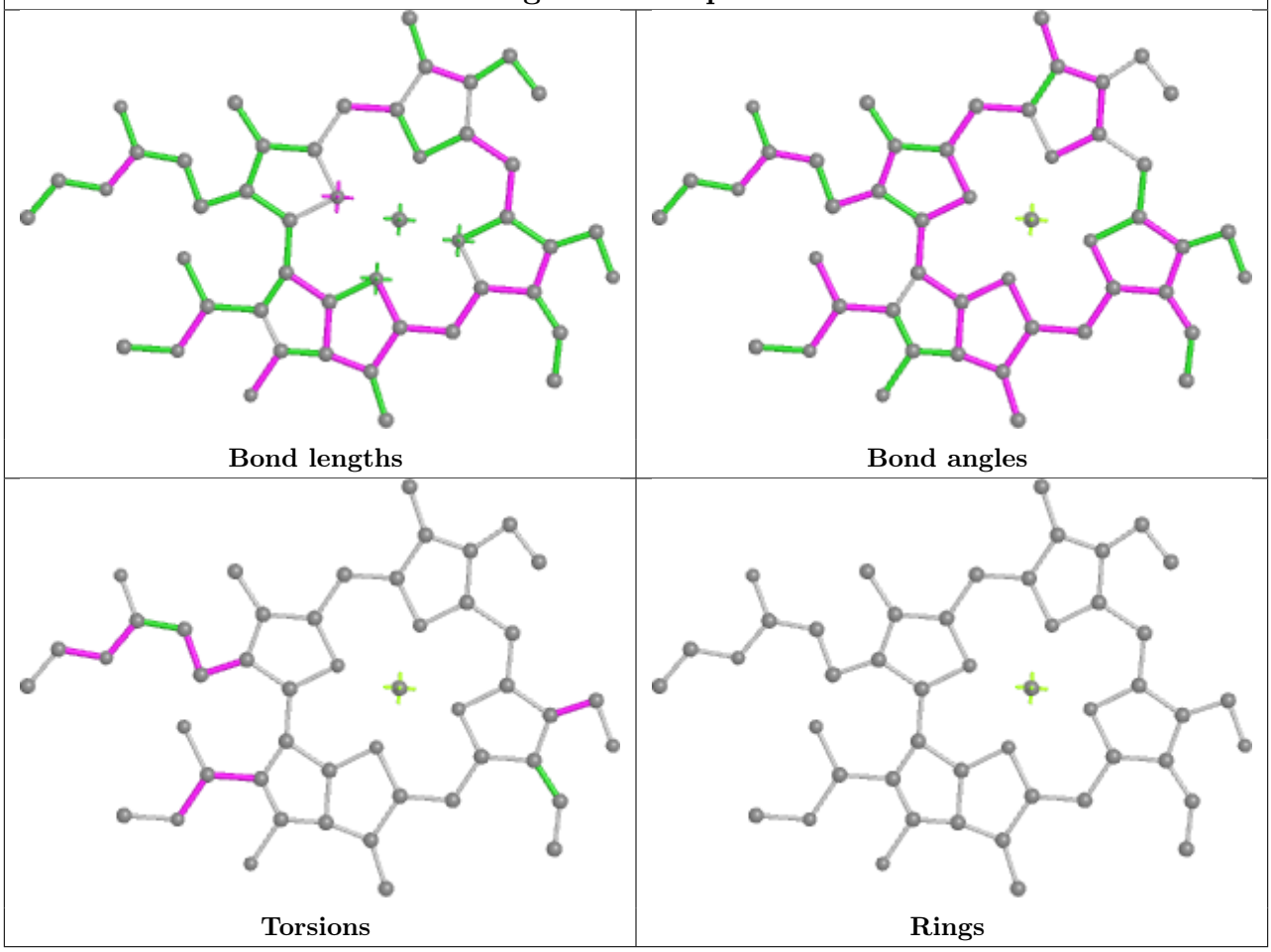
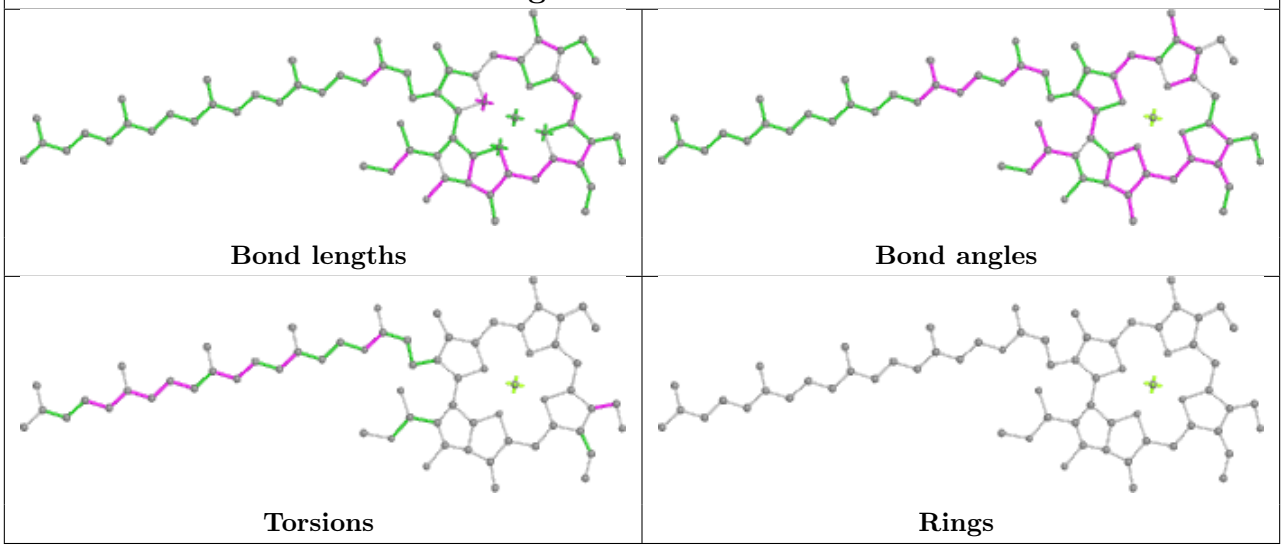


Rings

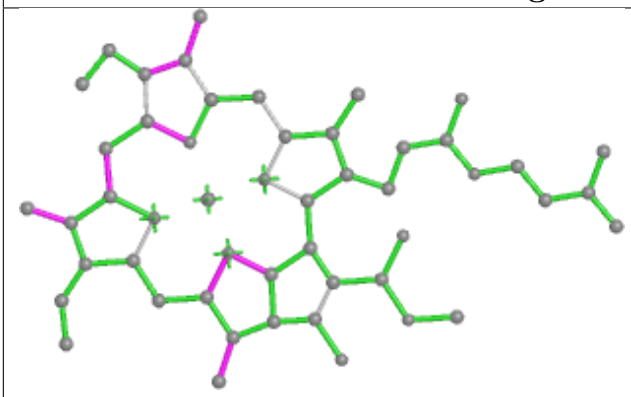
Ligand CHL q 312



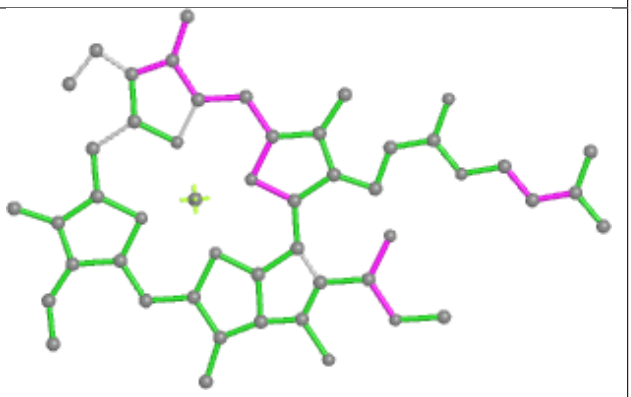
Ligand CHL v 313



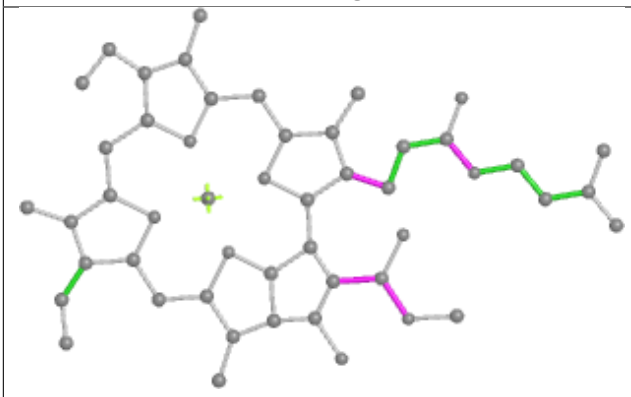
Ligand CLA 2 303



Bond lengths



Bond angles



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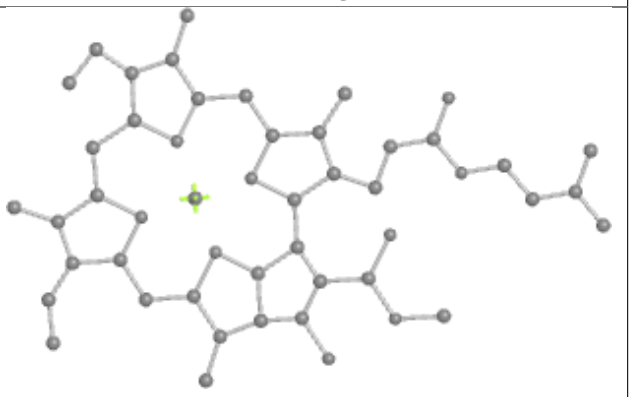
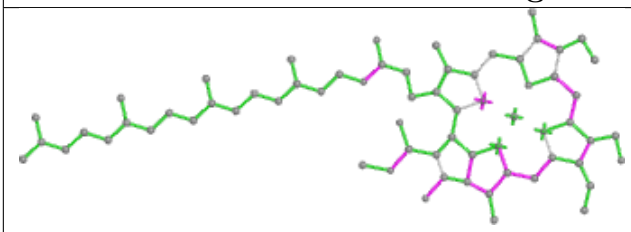
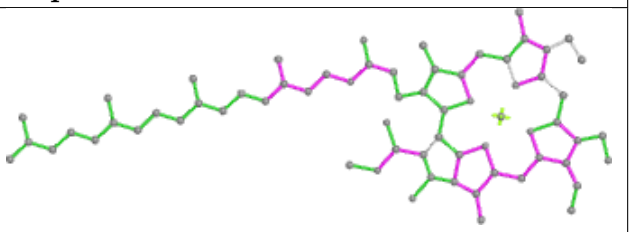


Rings

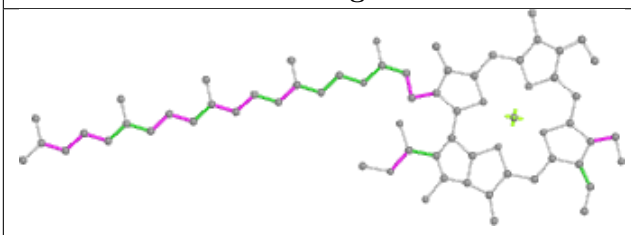
Ligand CHL p 318



Bond lengths



Bond angles



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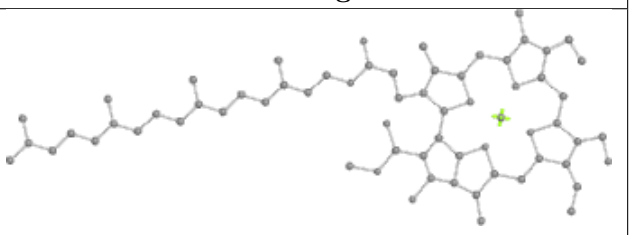
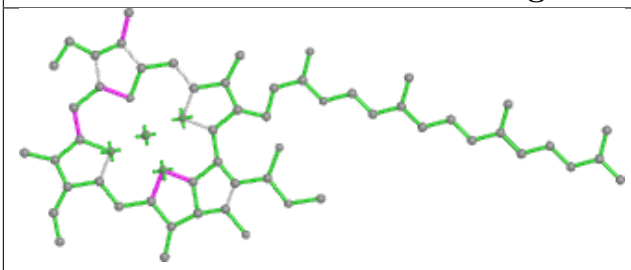
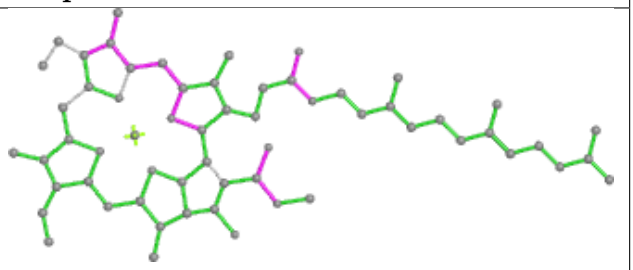
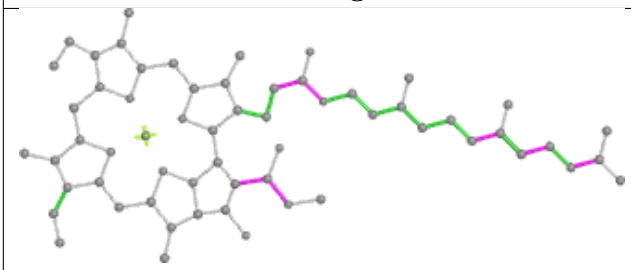
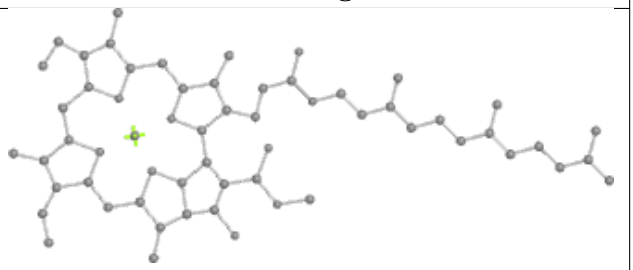
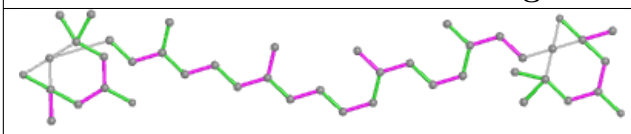
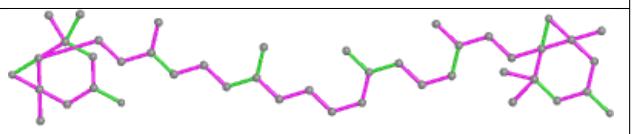
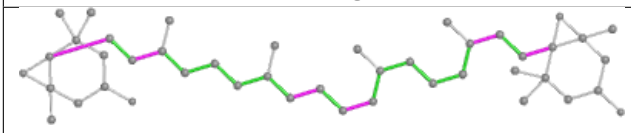
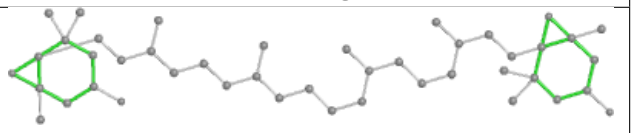
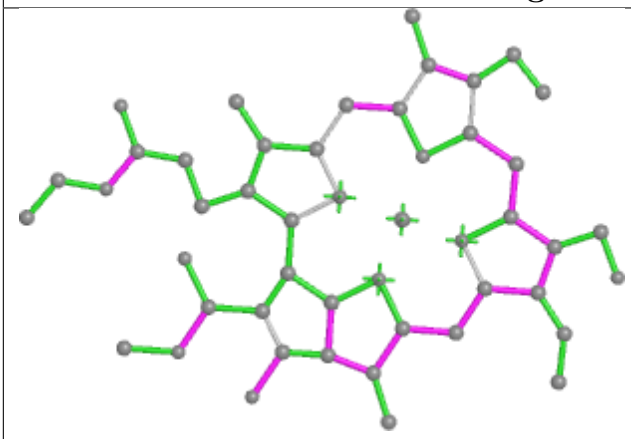


Rings

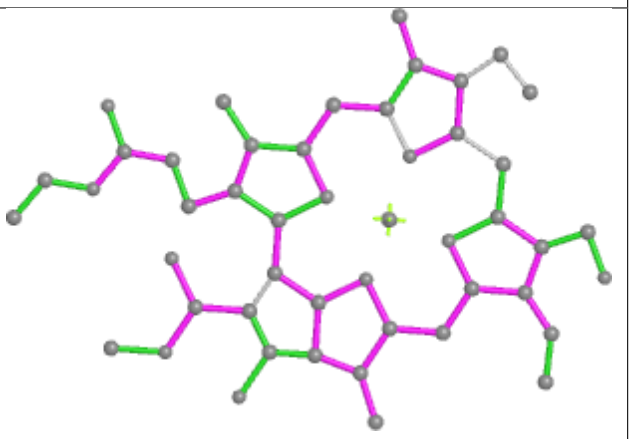
Ligand CLA q 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT R 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

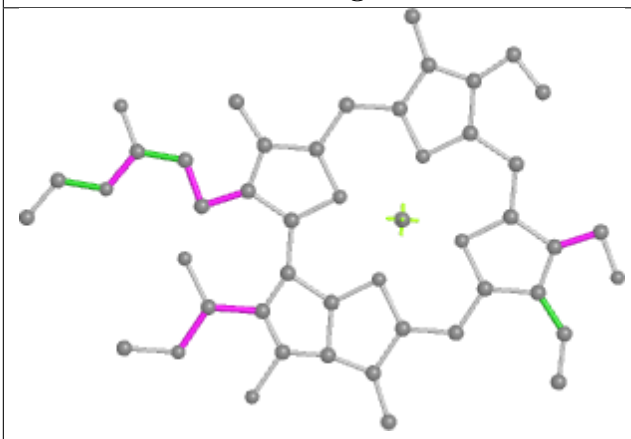
Ligand CHL v 314



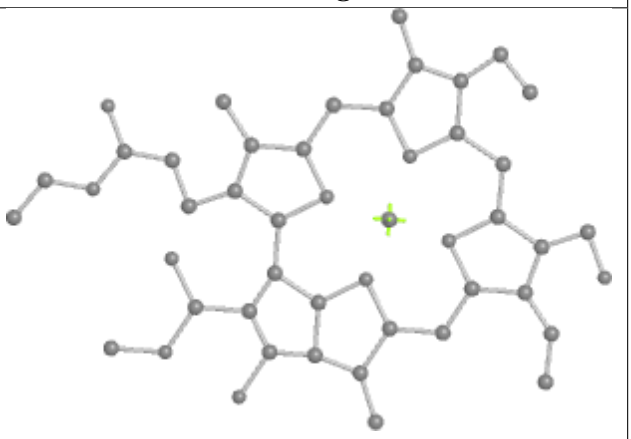
Bond lengths



Bond angles

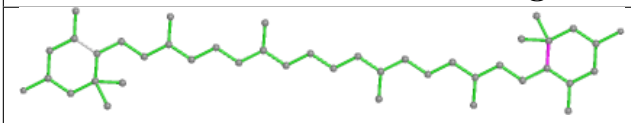


Torsions

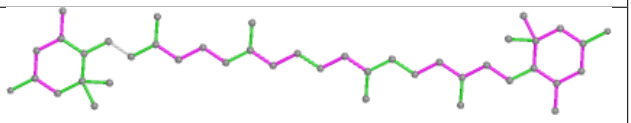


Rings

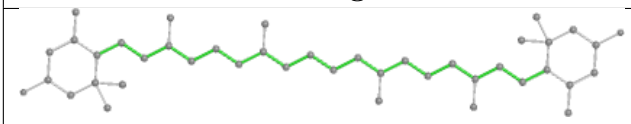
Ligand LUT 4 310



Bond lengths



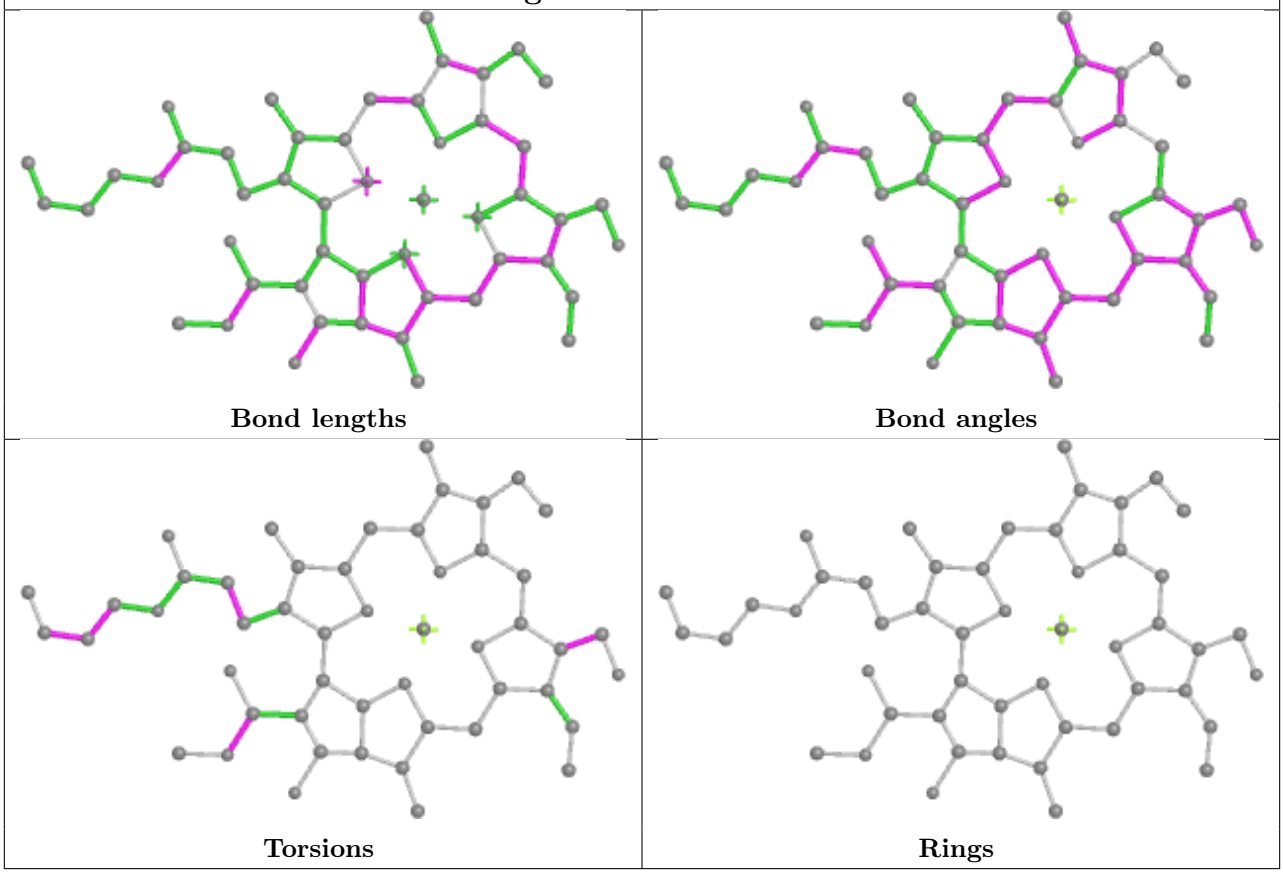
Bond angles



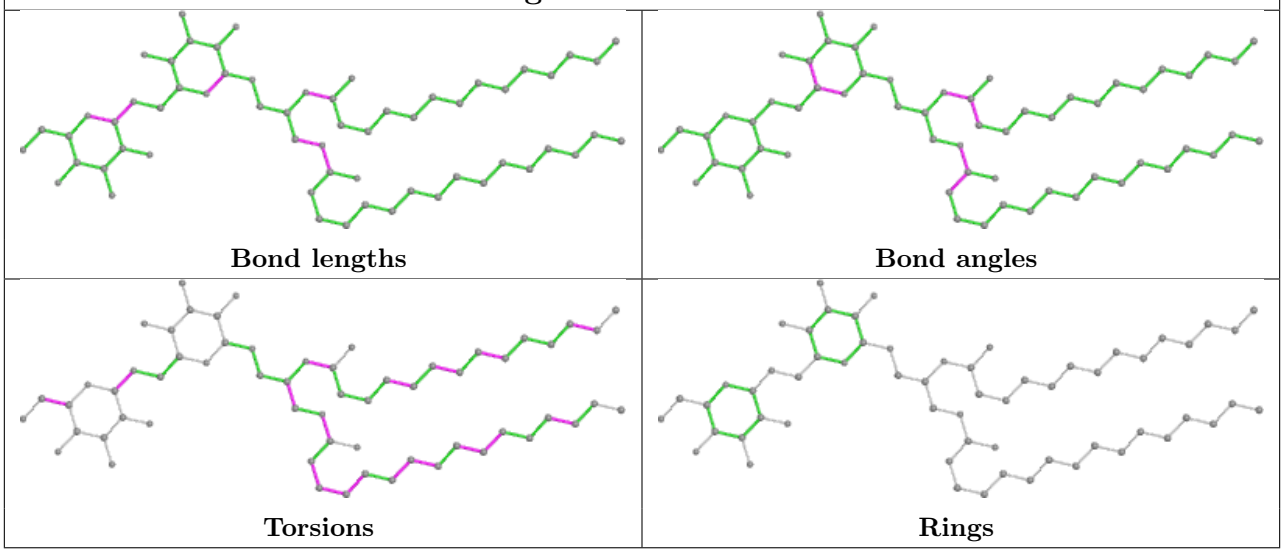
Torsions

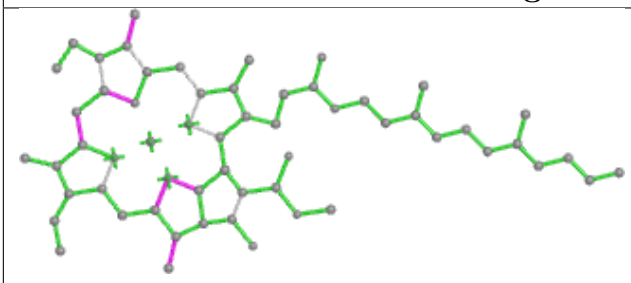
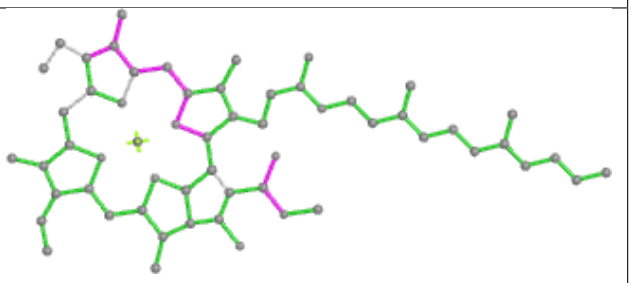
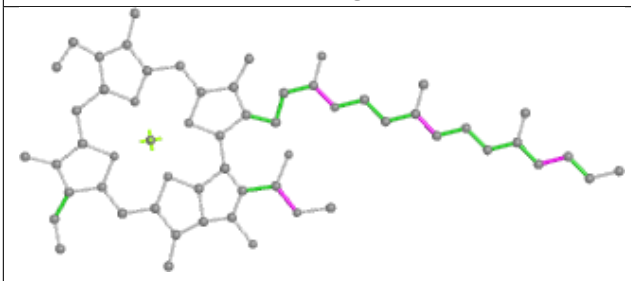
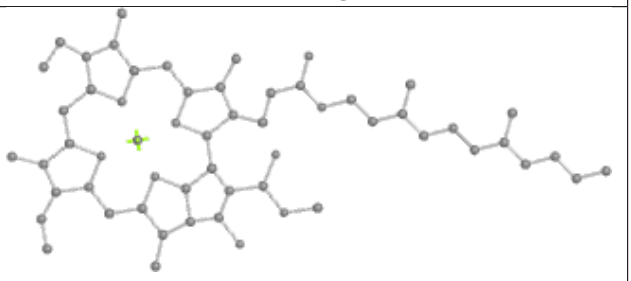
Rings

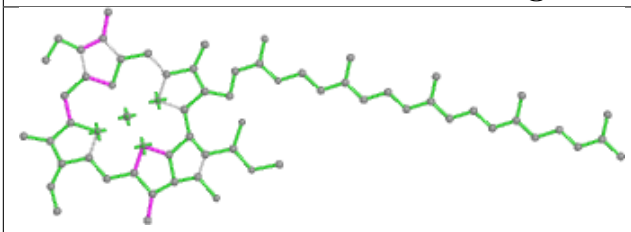
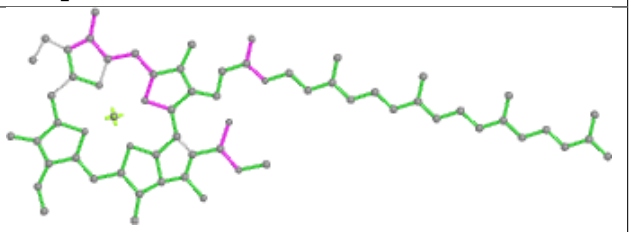
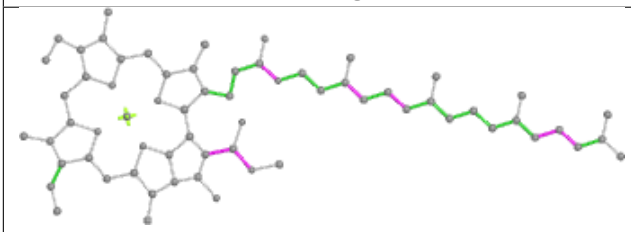
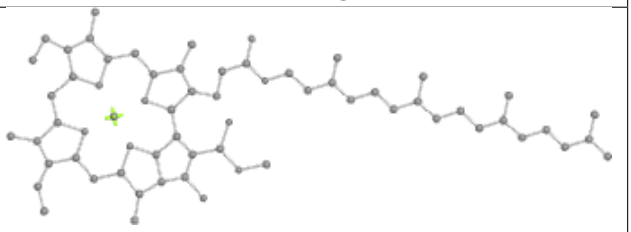
Ligand CHL V 315

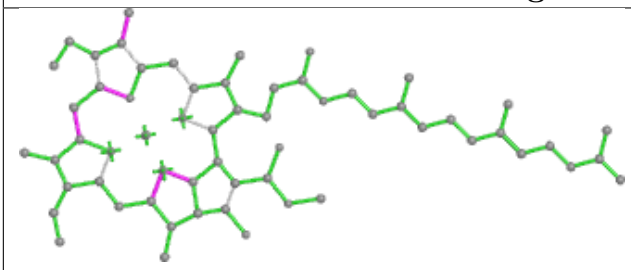
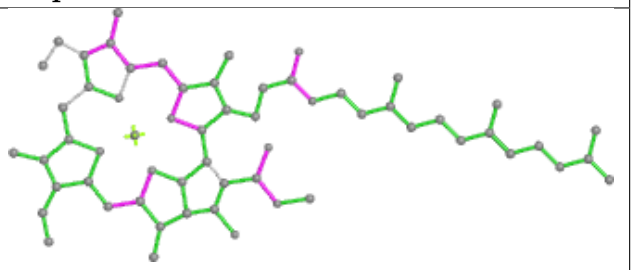
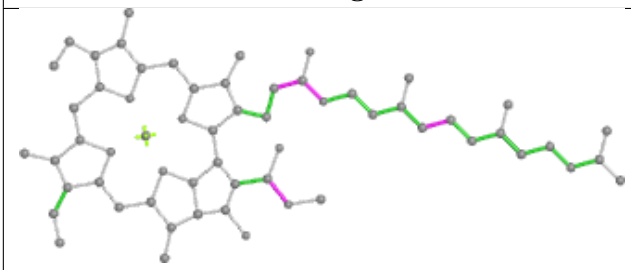
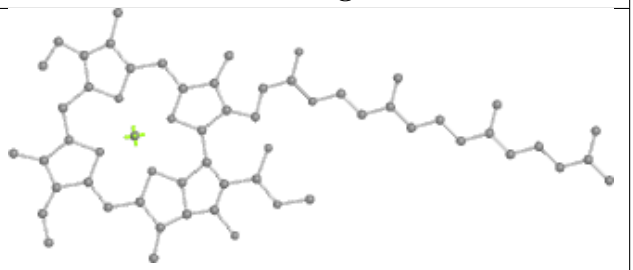


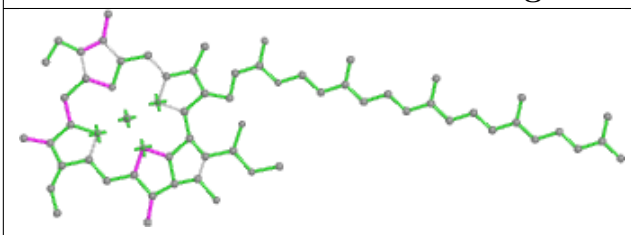
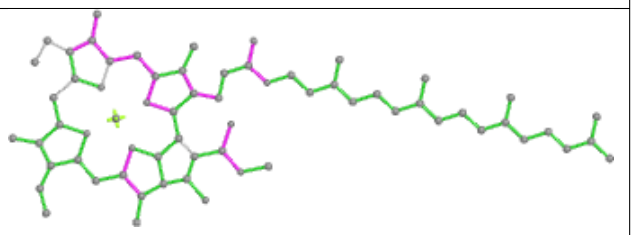
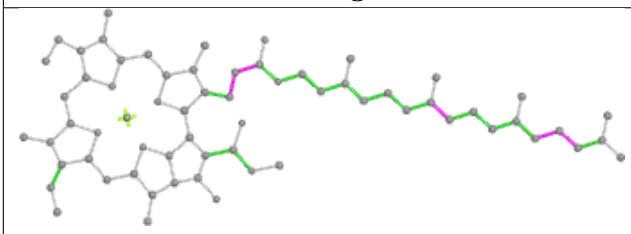
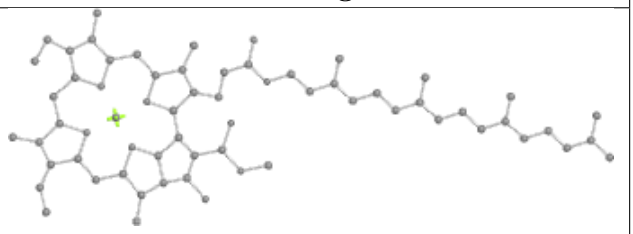
Ligand DGD J 101



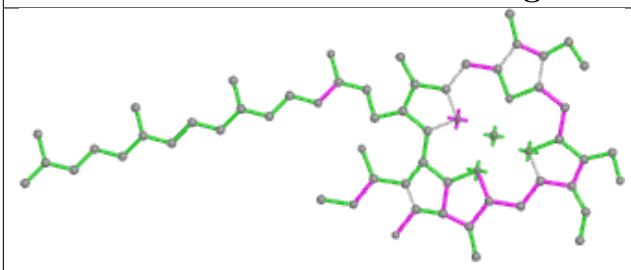
Ligand CLA R 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

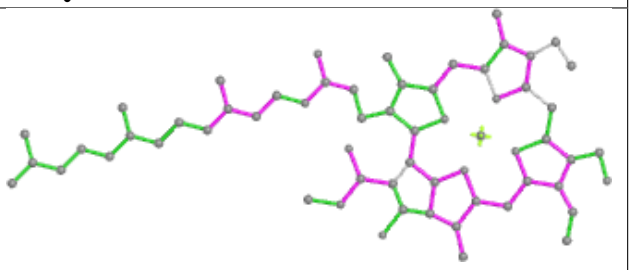
Ligand CLA p 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

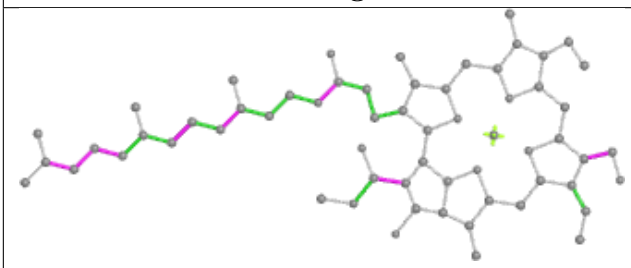
Ligand CHL Q 316



Bond lengths



Bond angles



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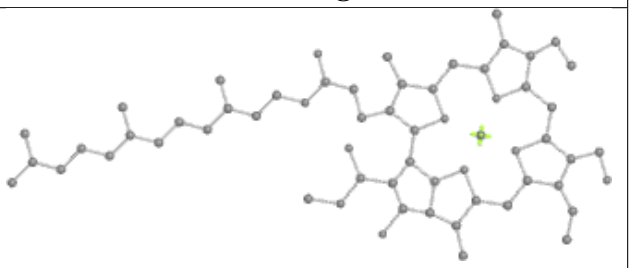
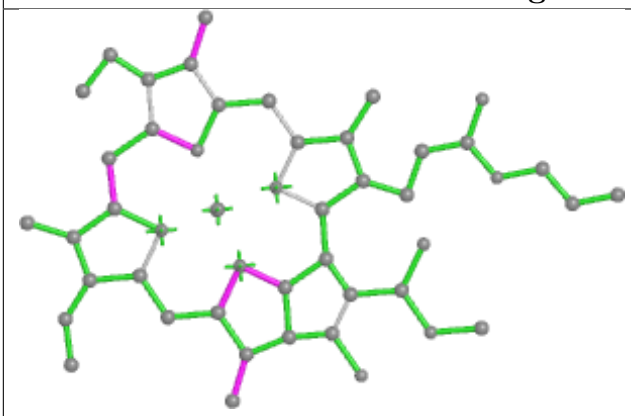
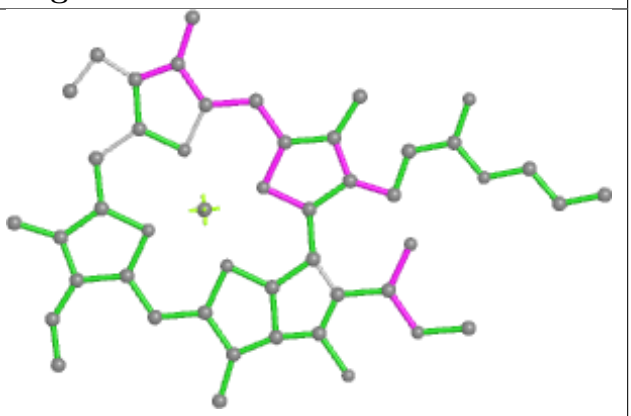


Rings

Ligand CLA g 308



Bond lengths



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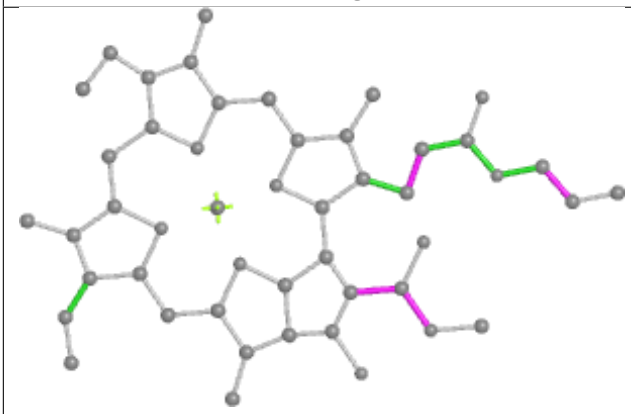

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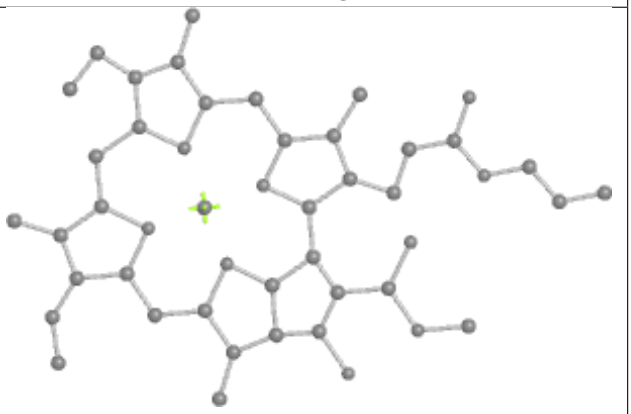
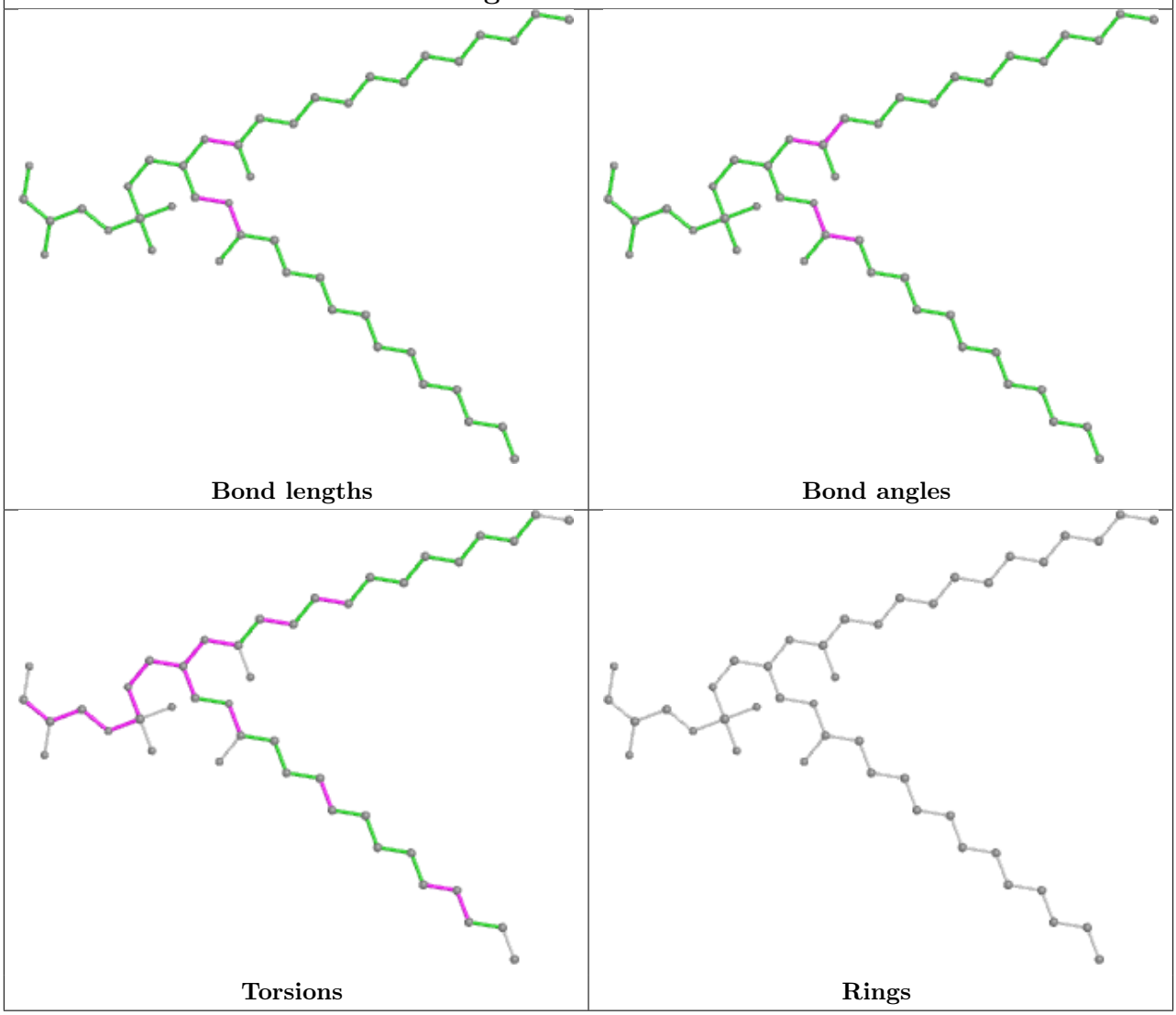
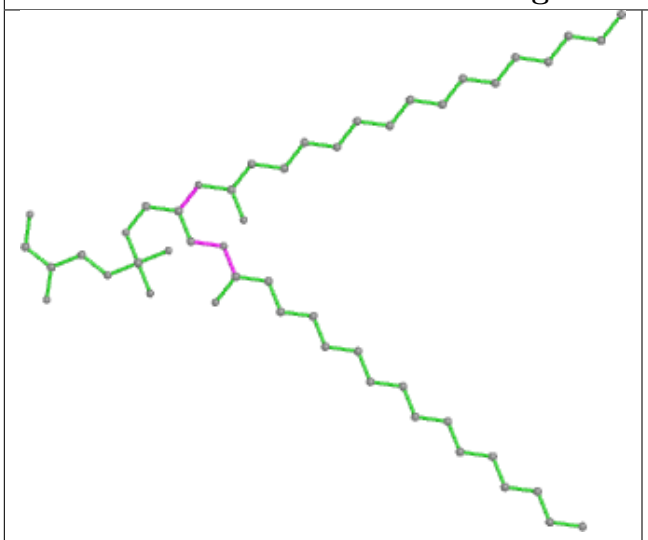


Rings

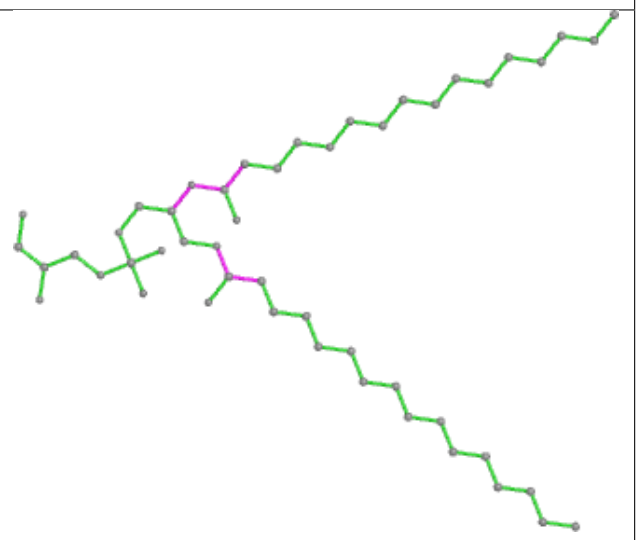
Ligand LHG a 415



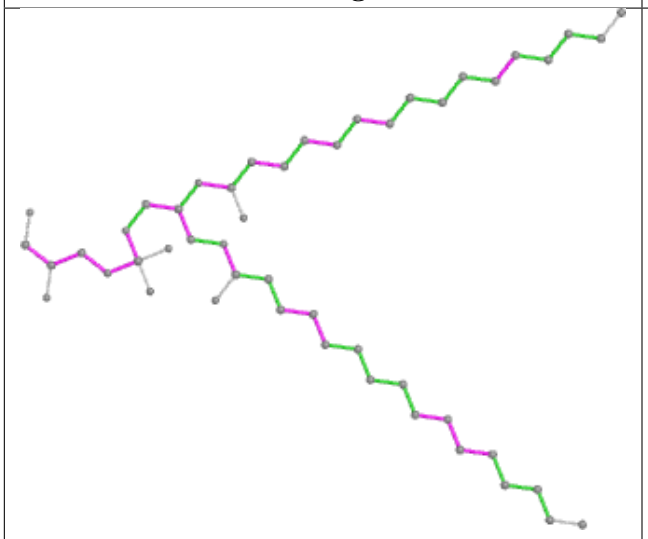
Ligand LHG l 101



Bond lengths



Bond angles



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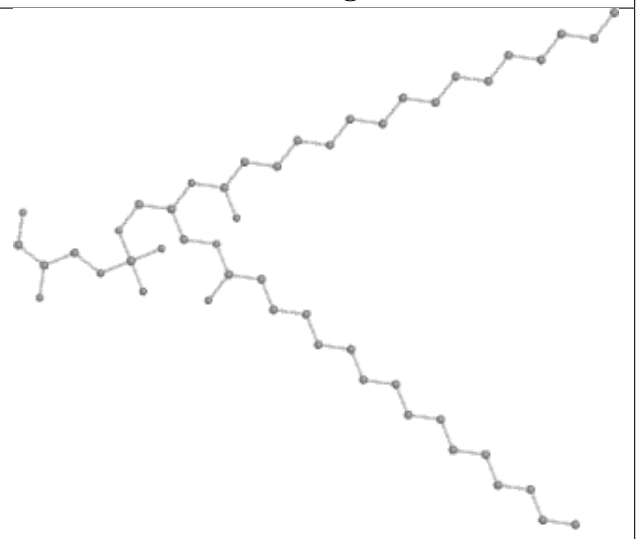
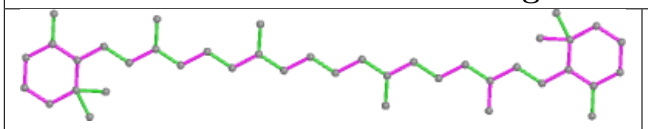


Rings

Ligand BCR K 101



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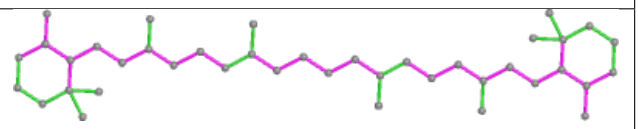
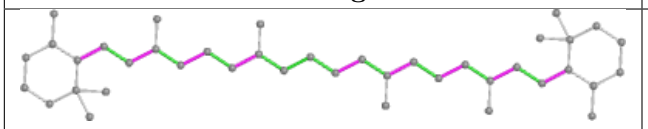
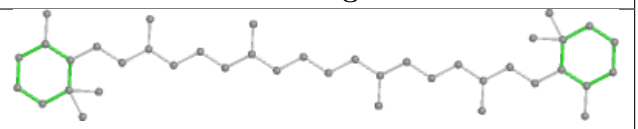


Bond angles

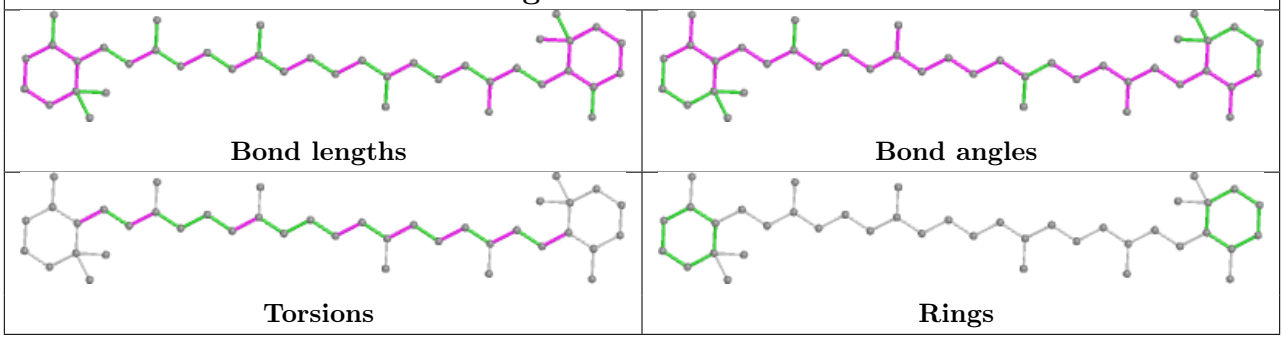


Torsions

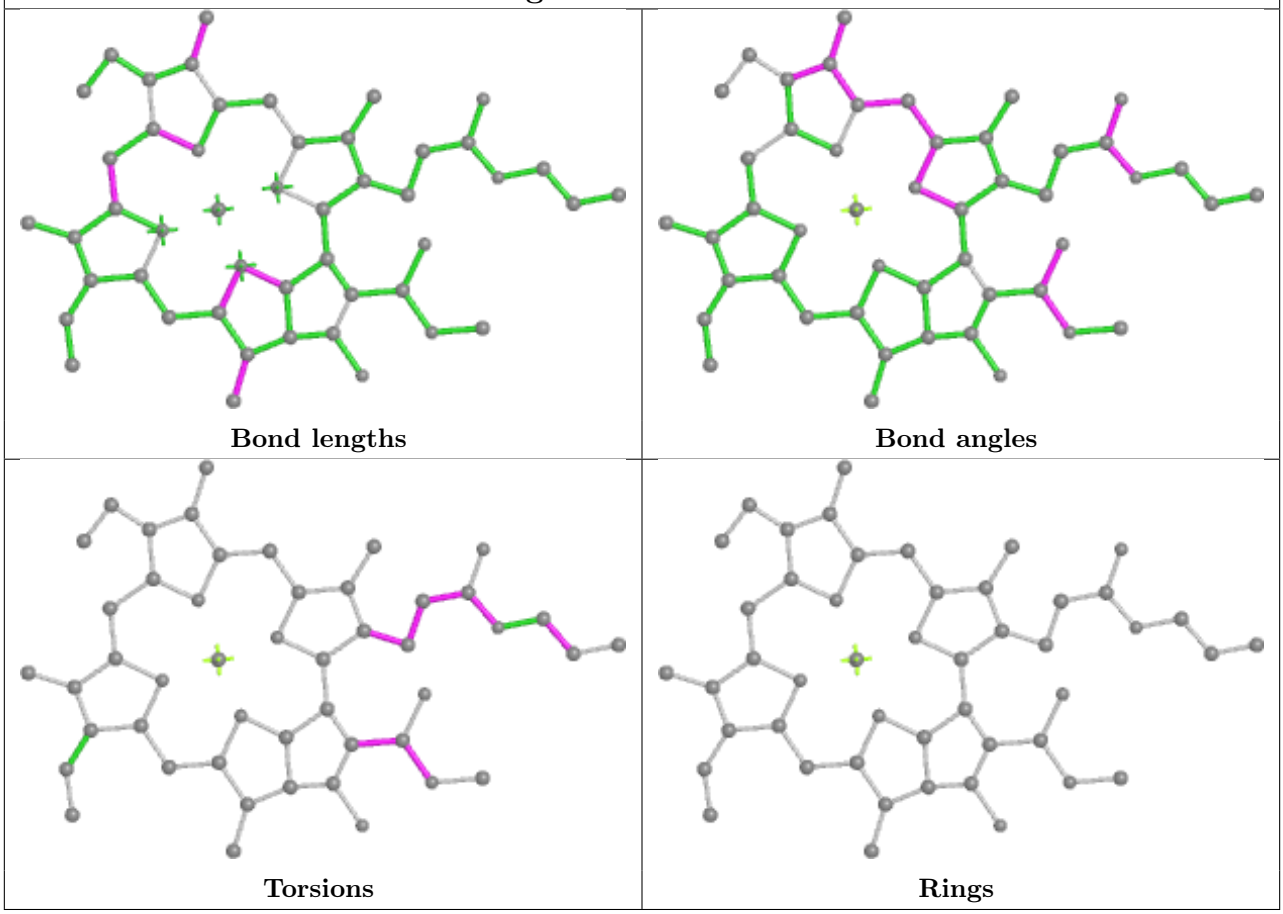


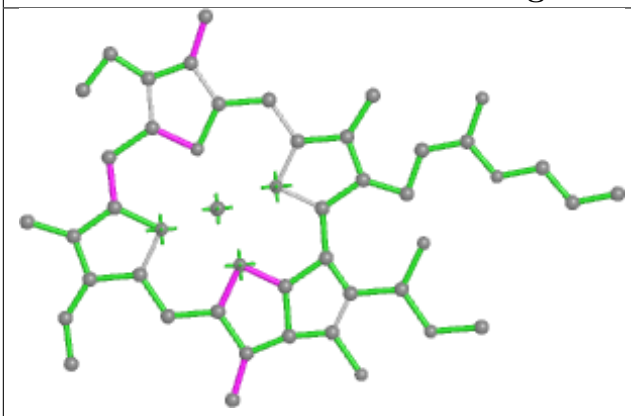
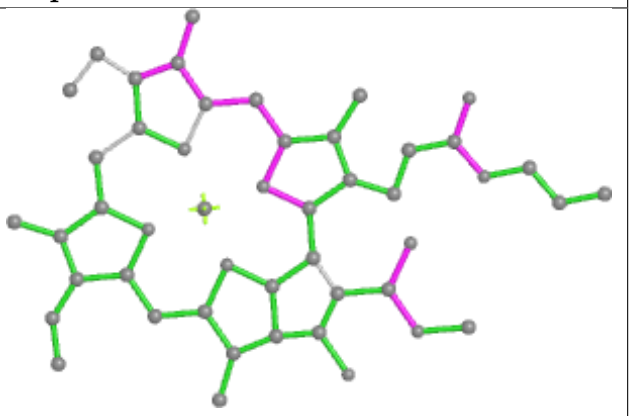
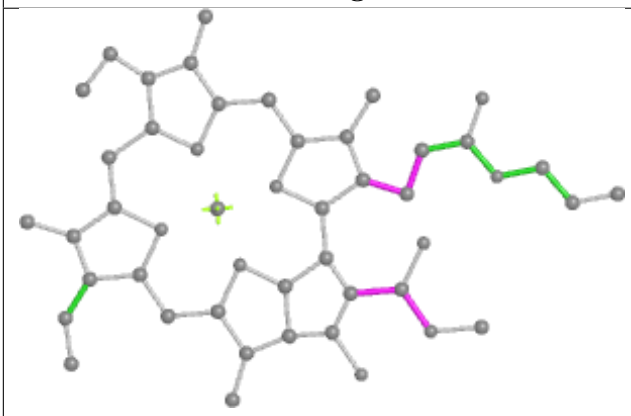
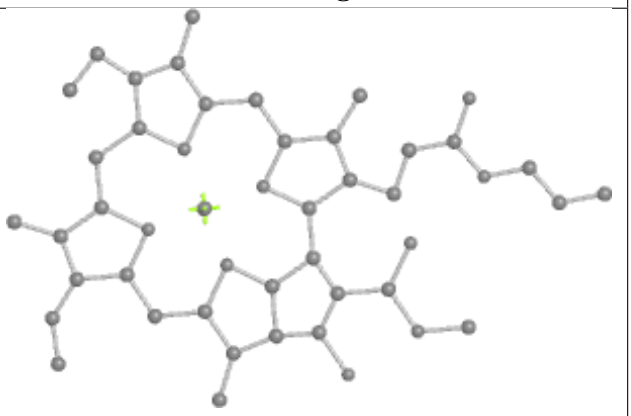
Rings

Ligand BCR D 404

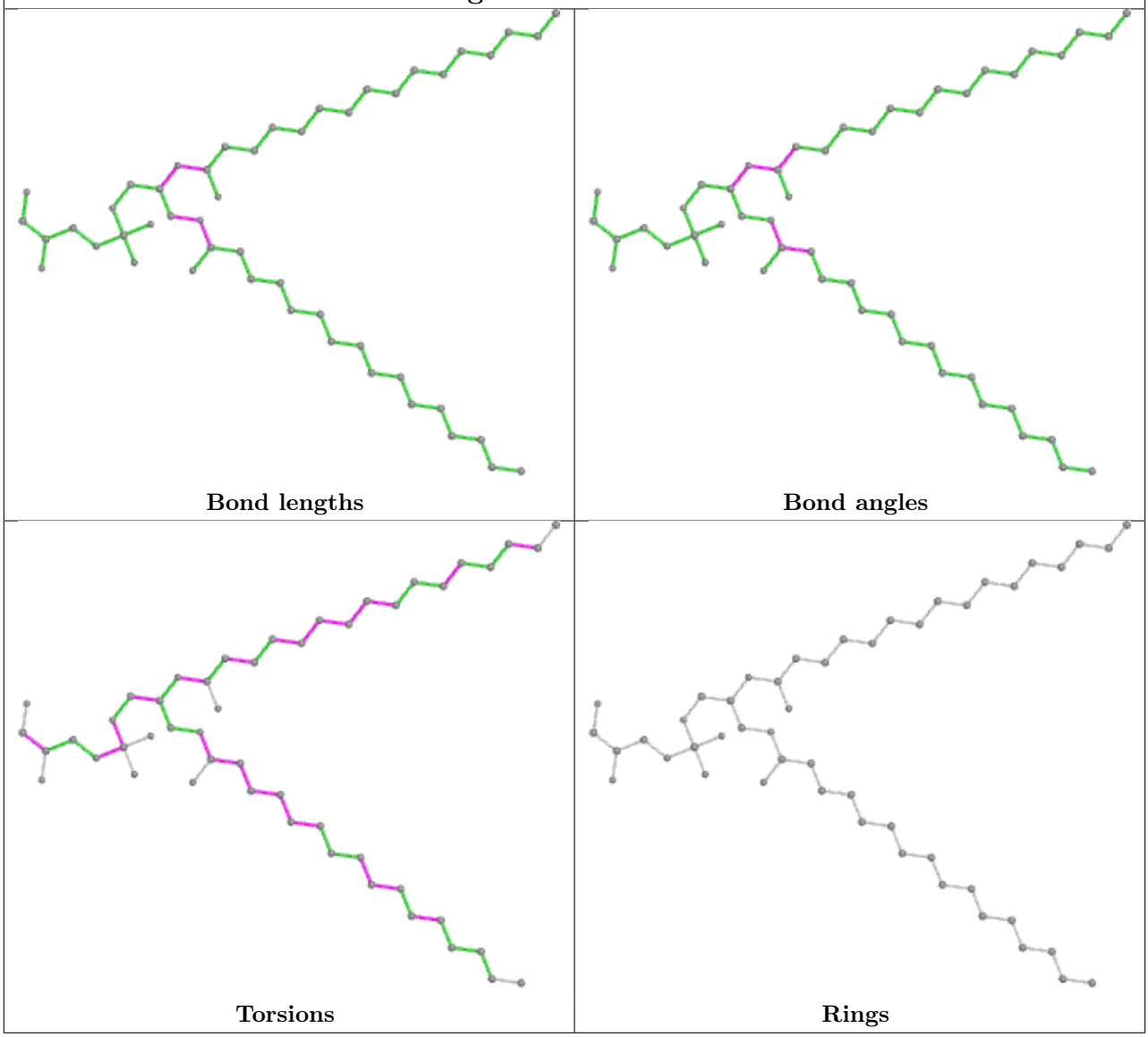


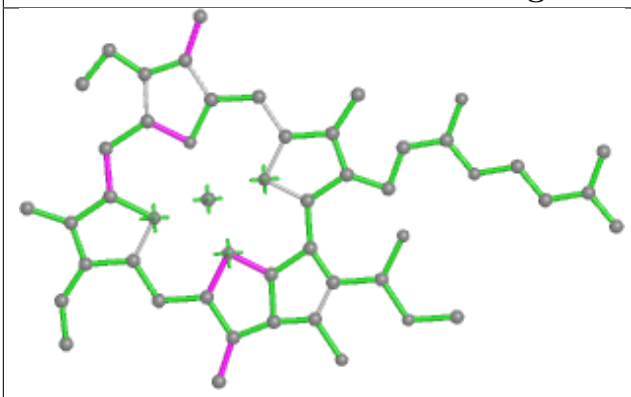
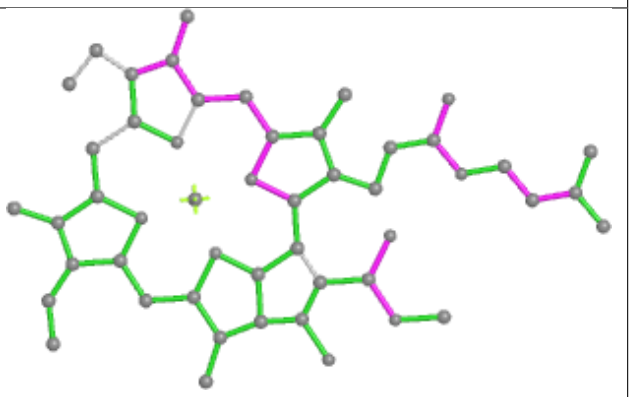
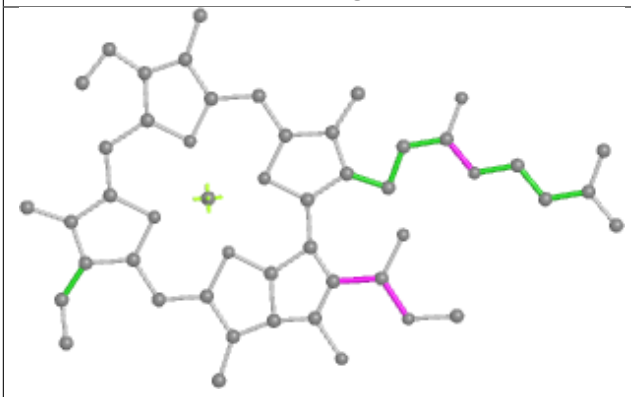
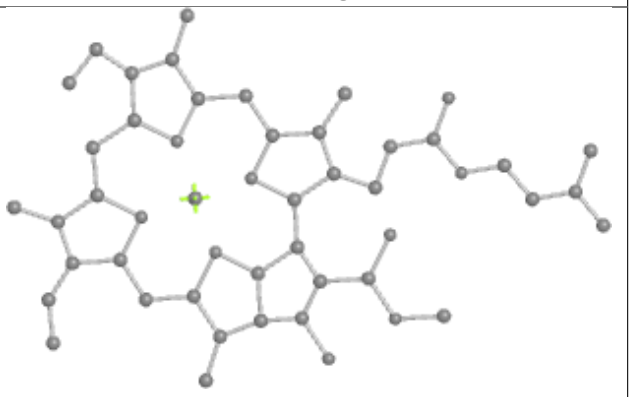
Ligand CLA P 309



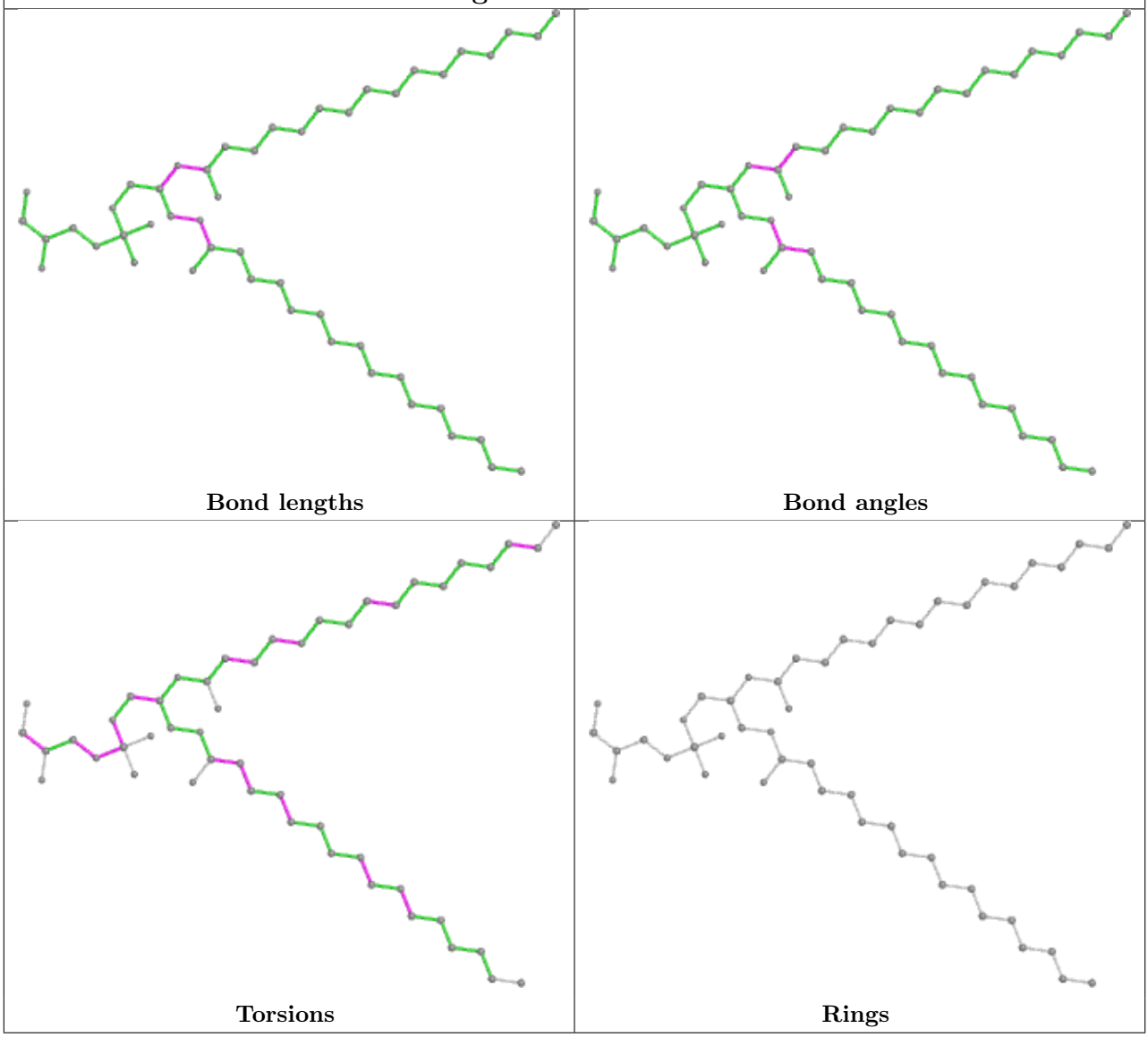
Ligand CLA p 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG U 312

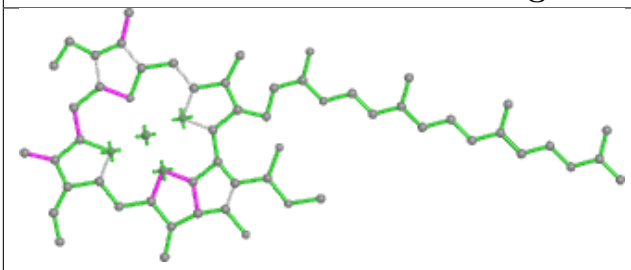


Ligand CLA n 303	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

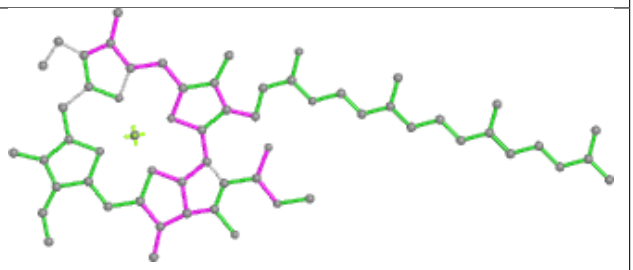
Ligand LHG 4 312



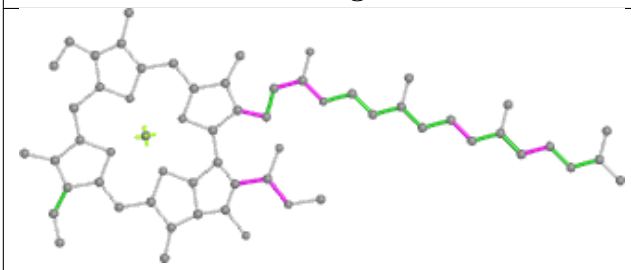
Ligand CLA 5 305



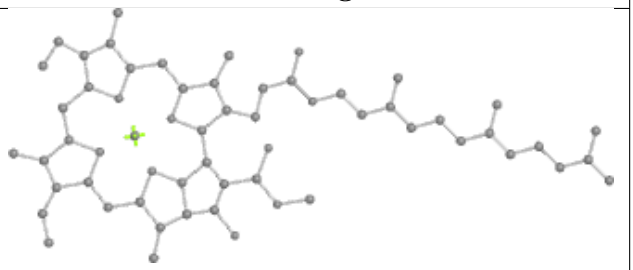
Bond lengths



Bond angles

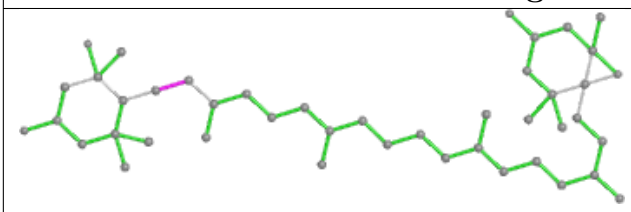


Torsions

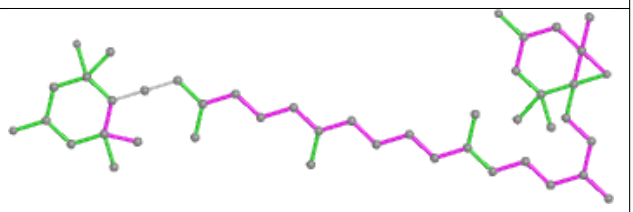


Rings

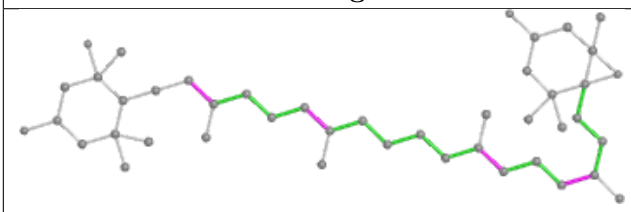
Ligand NEX 2 319



Bond lengths



Bond angles



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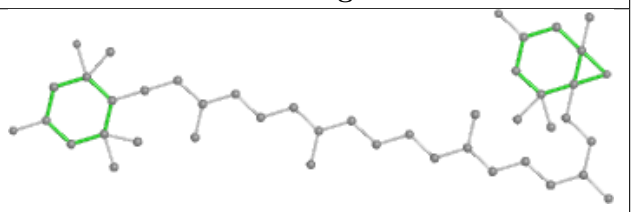
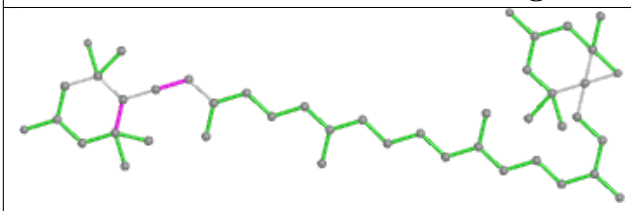
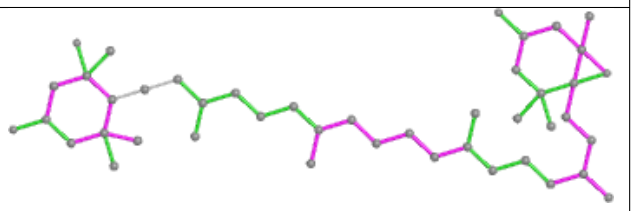


Rings

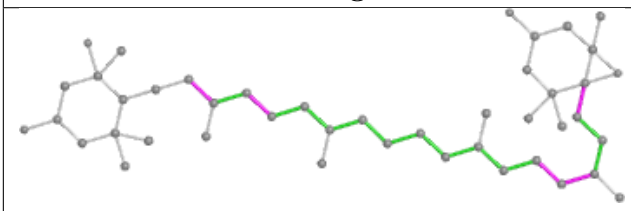
Ligand NEX r 618



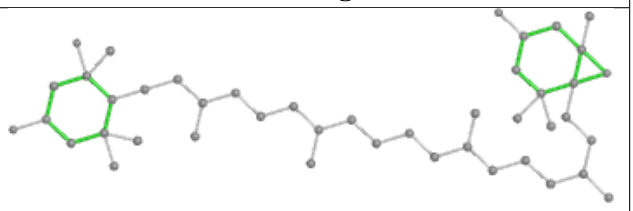
Bond lengths



Bond angles

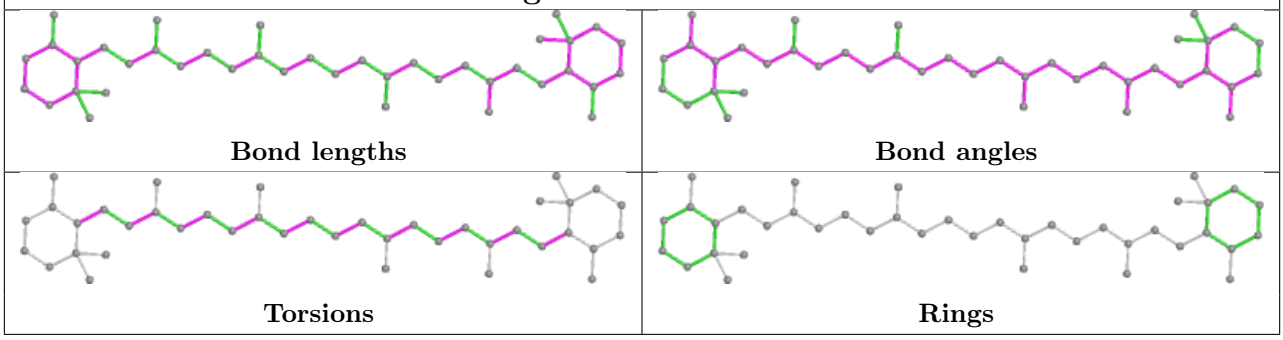


Torsions

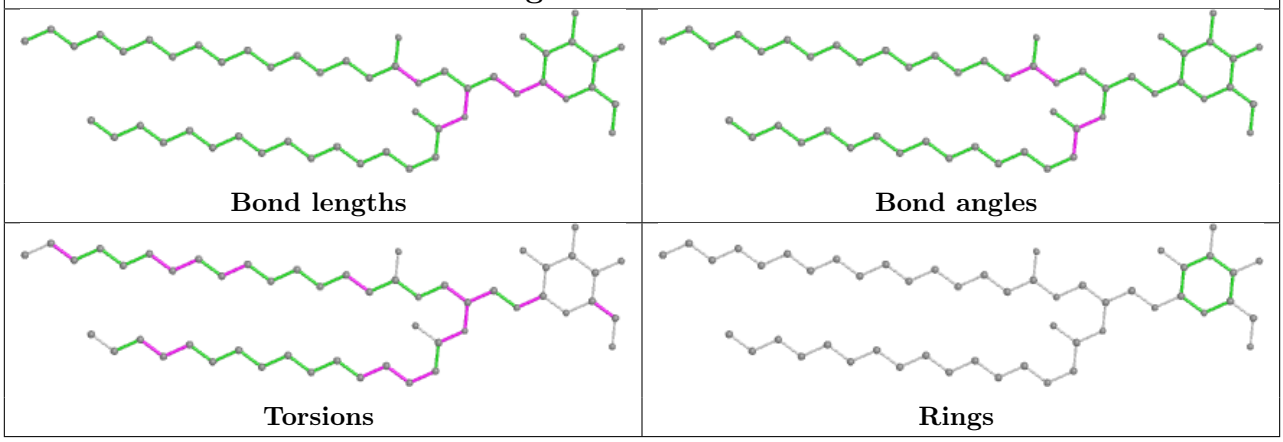


Rings

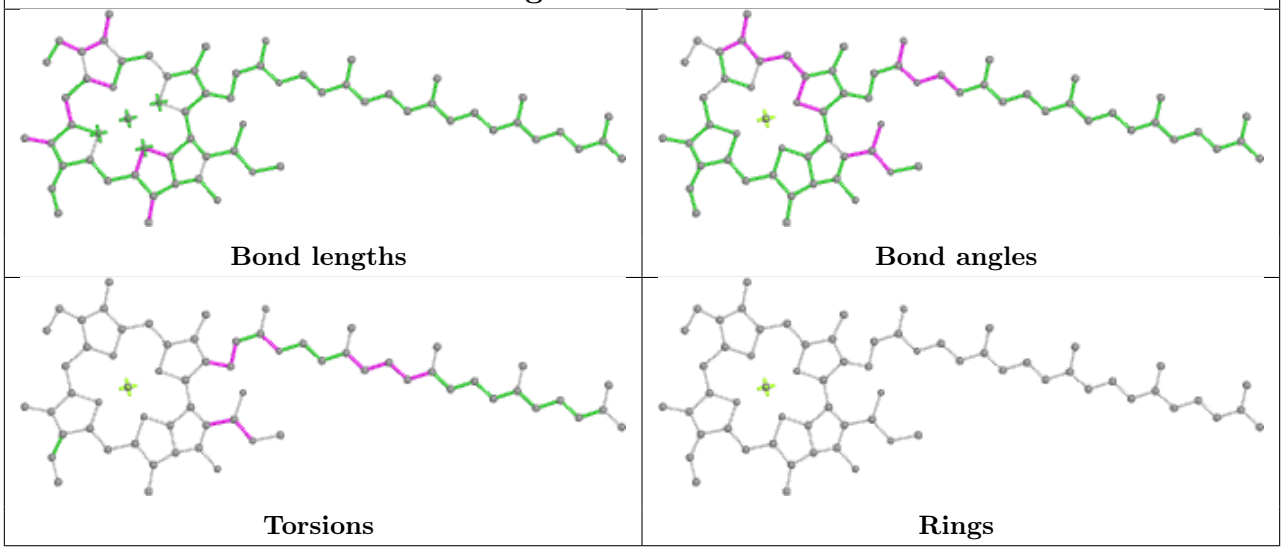
Ligand BCR C 517

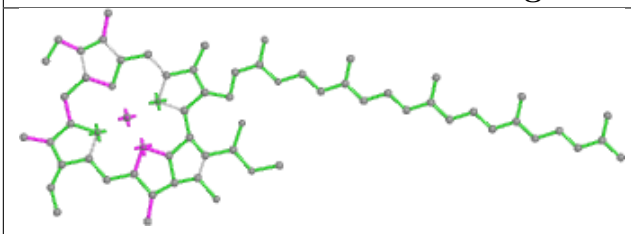
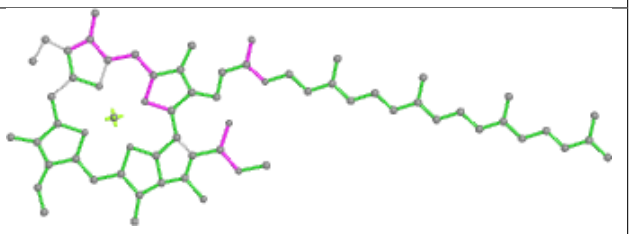
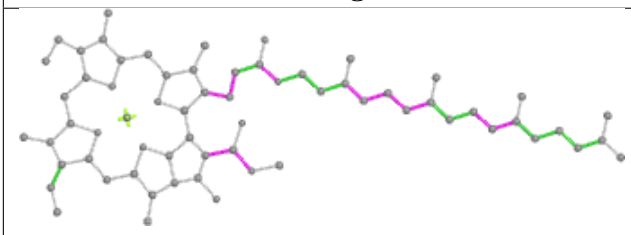
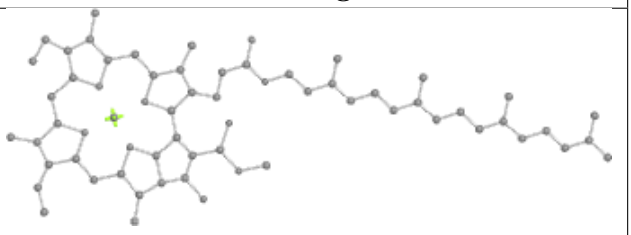


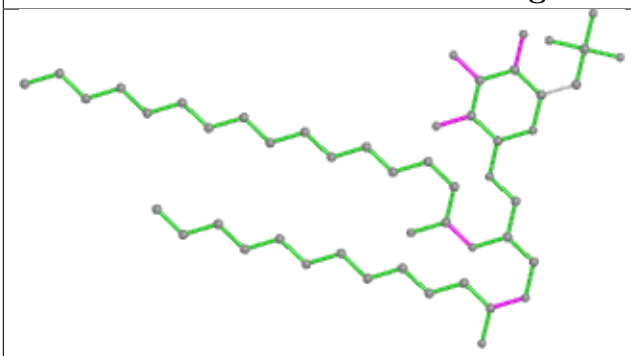
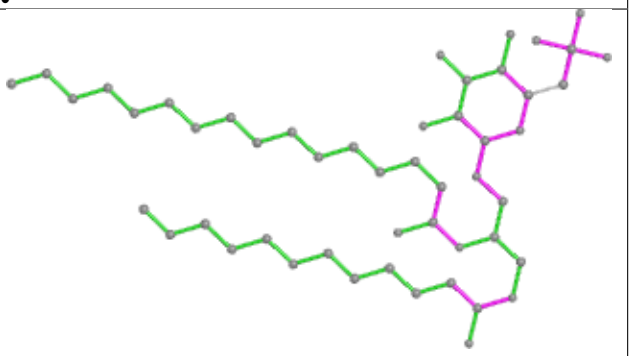
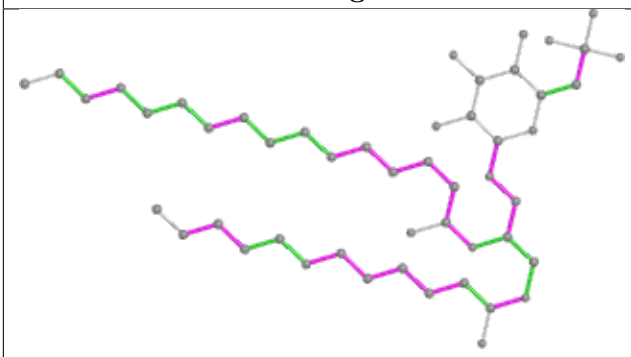
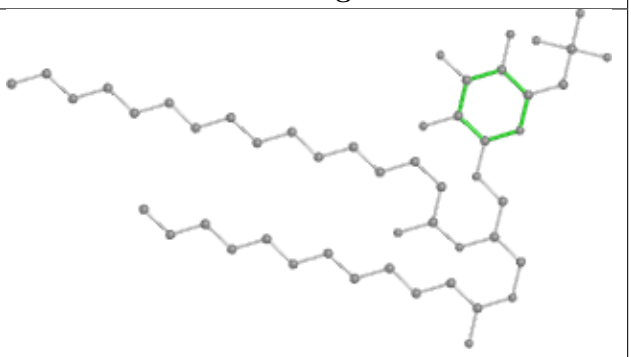
Ligand LMG c 520

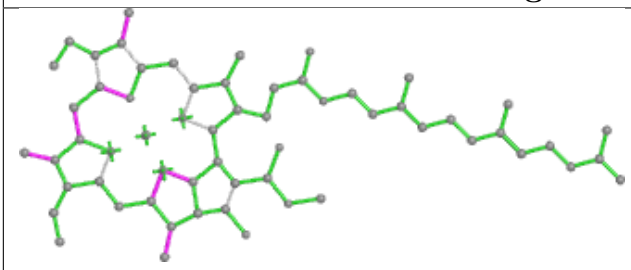
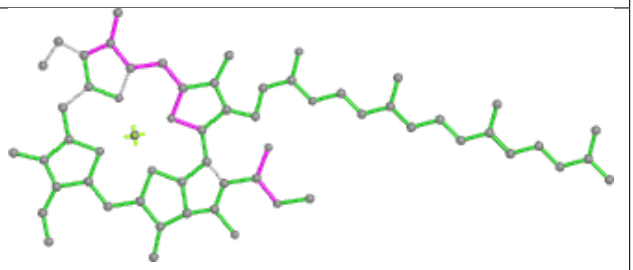
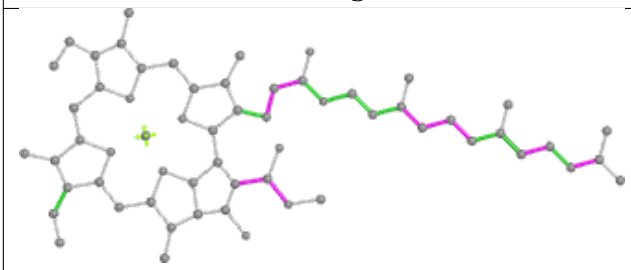
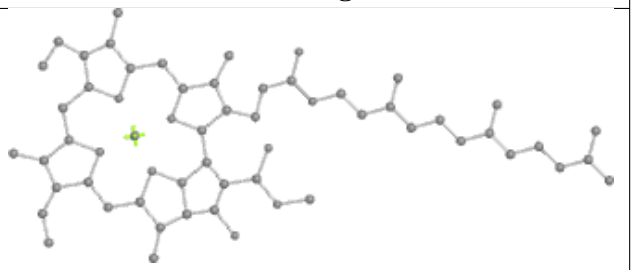


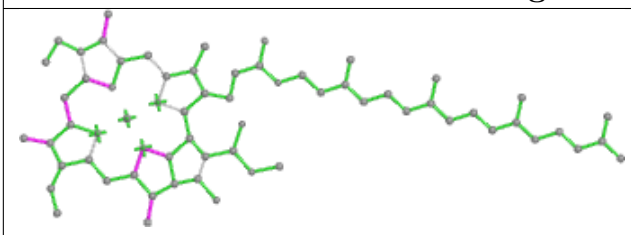
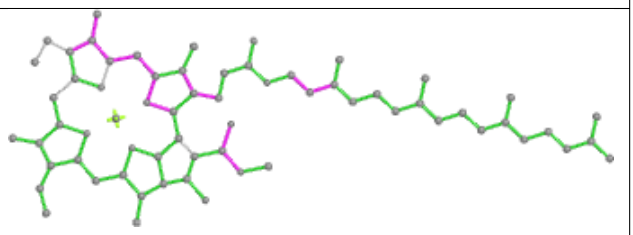
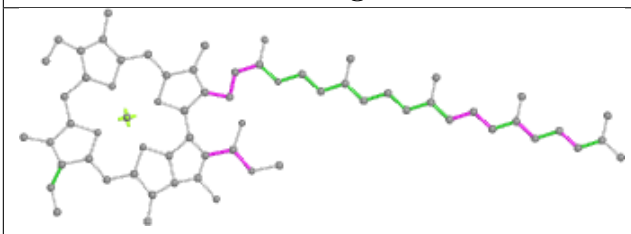
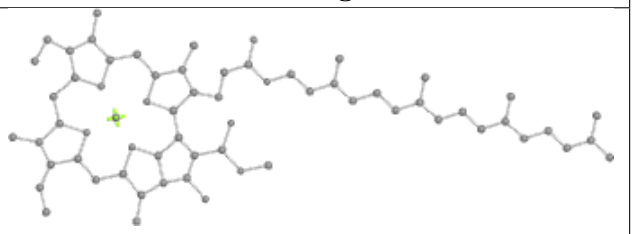
Ligand CLA B 607



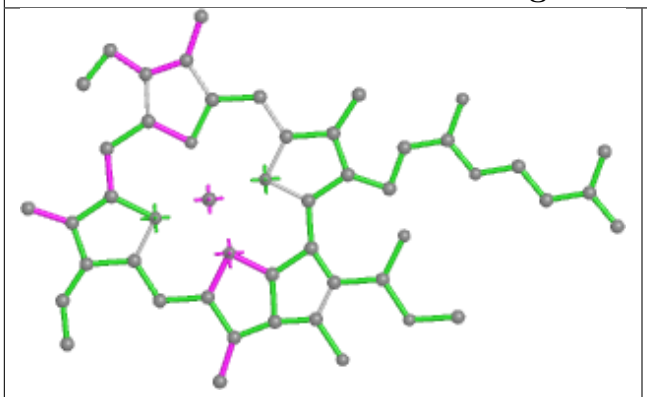
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

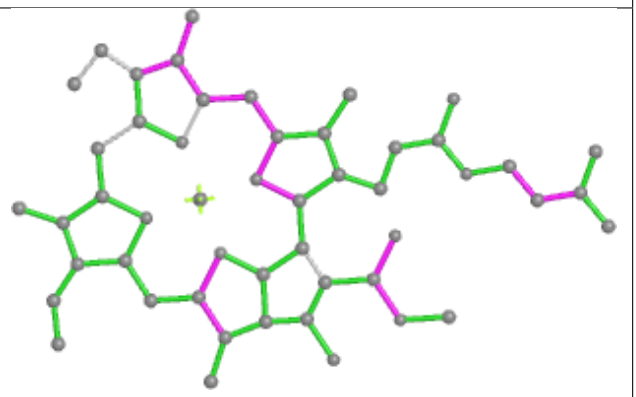
Ligand CLA P 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

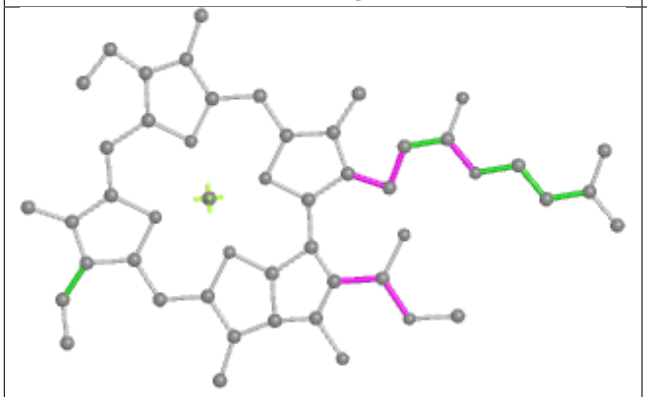
Ligand CLA a 406



Bond lengths



Bond angles



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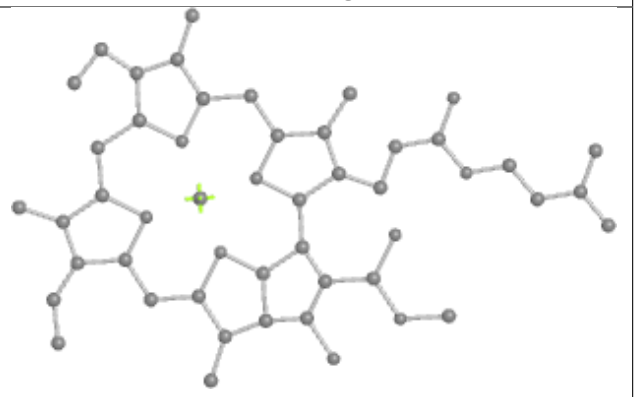
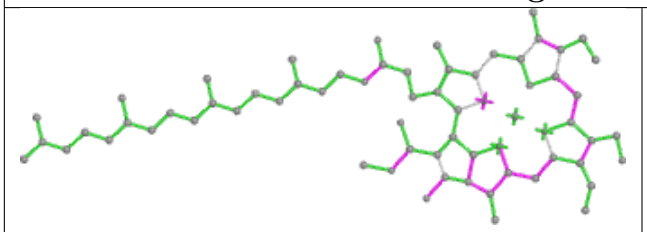
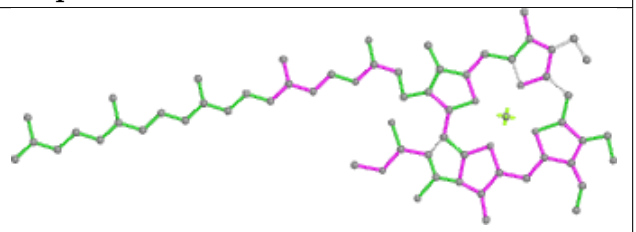


Rings

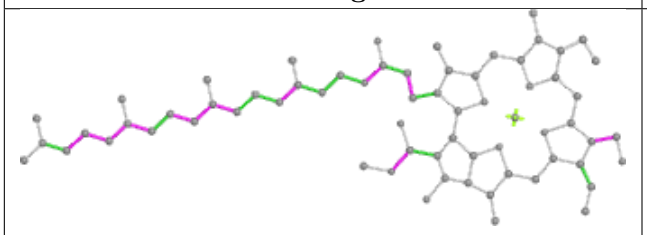
Ligand CHL p 320



Bond lengths



Bond angles



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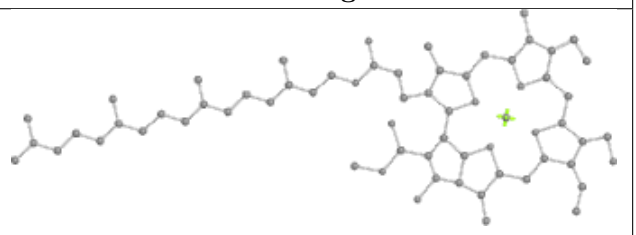
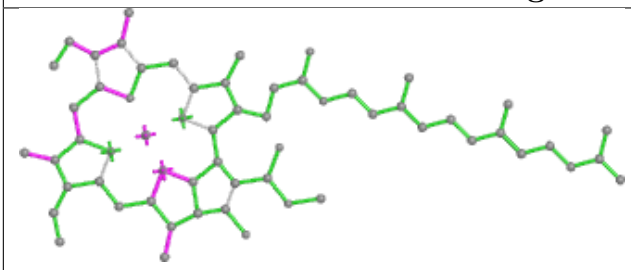
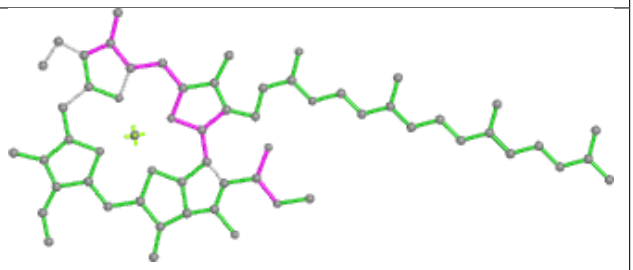
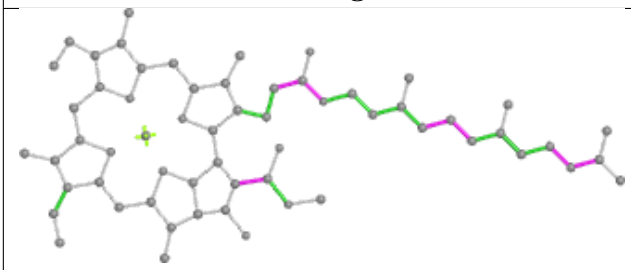
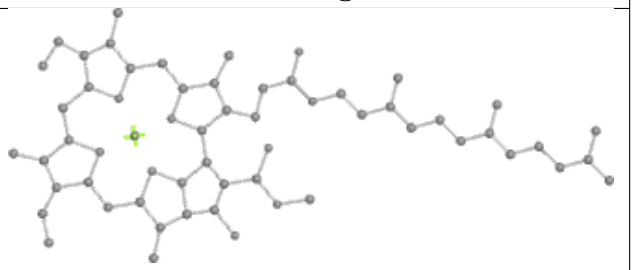
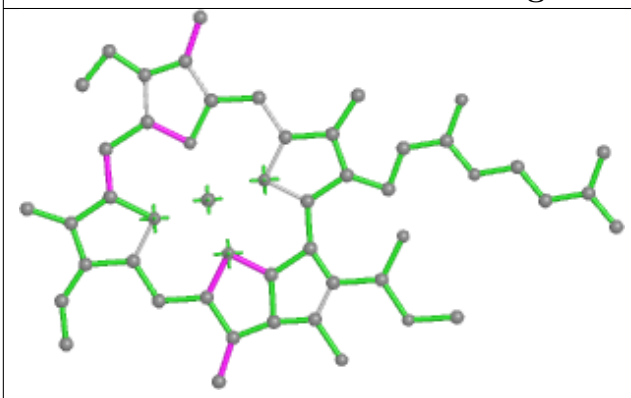
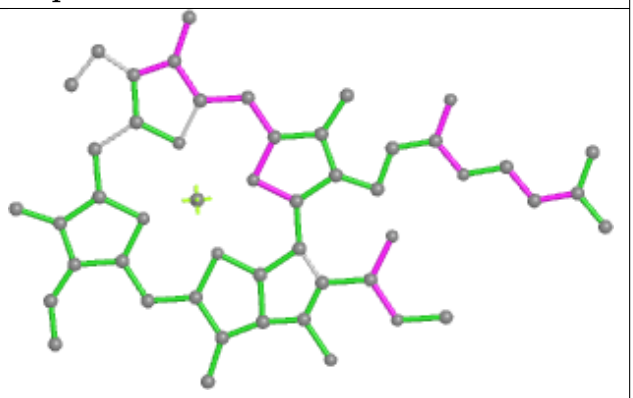
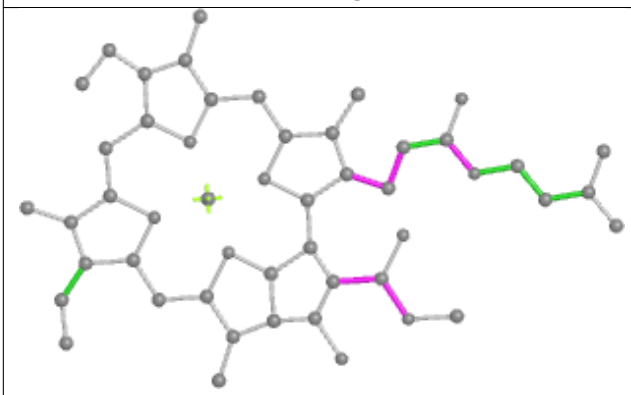
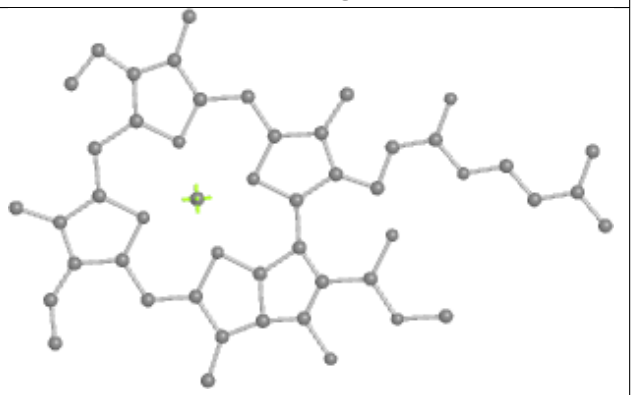
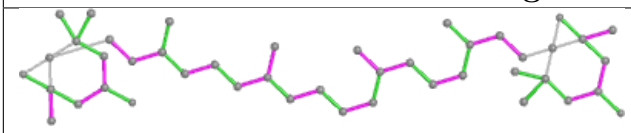
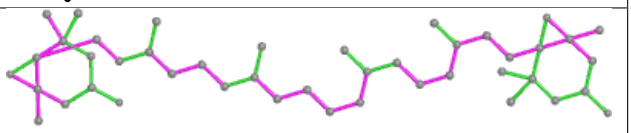
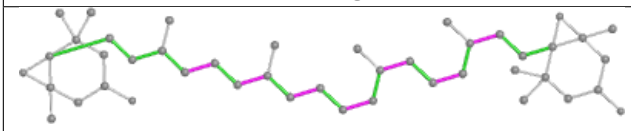
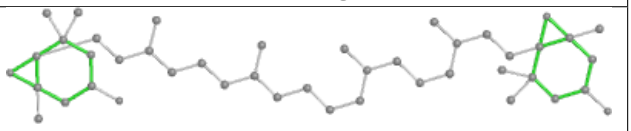
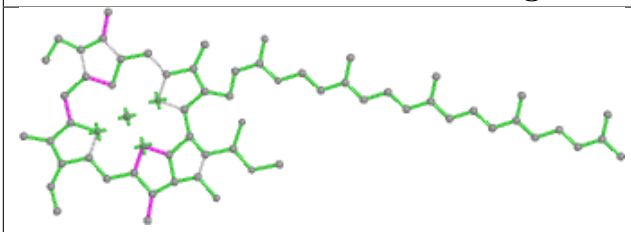
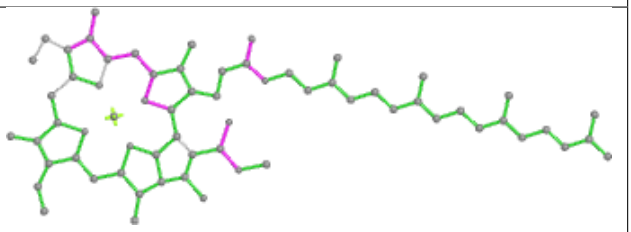
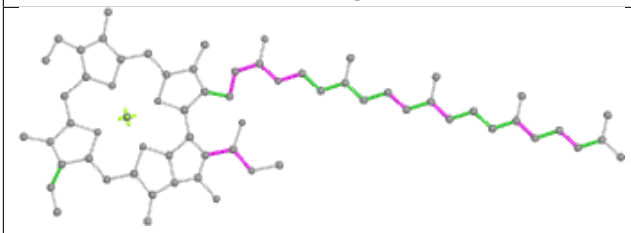
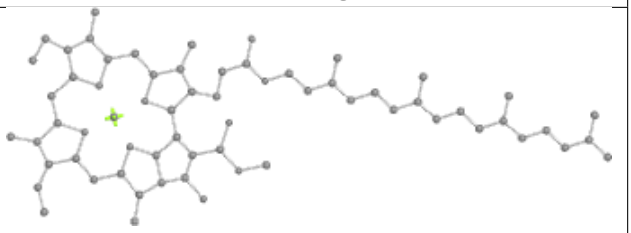


Rings

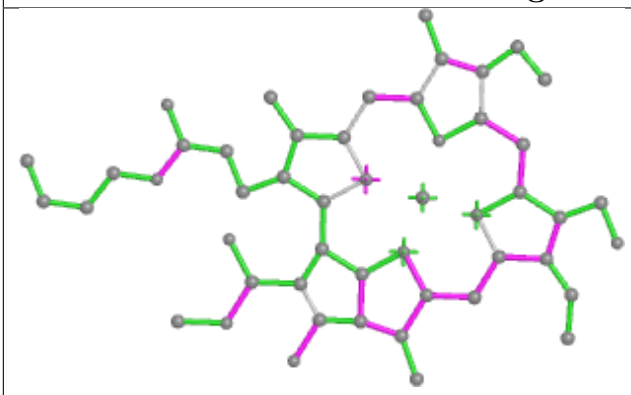
Ligand CLA u 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

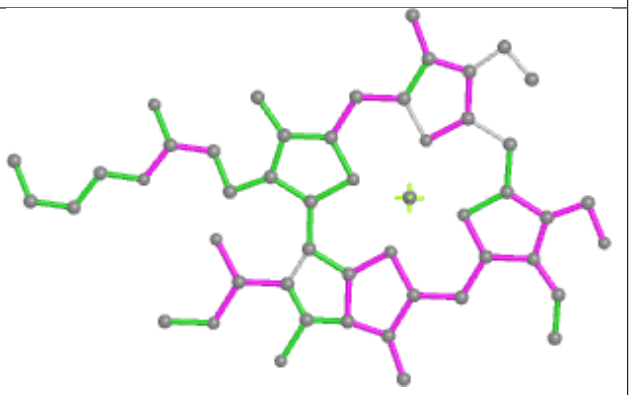
Ligand XAT Q 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

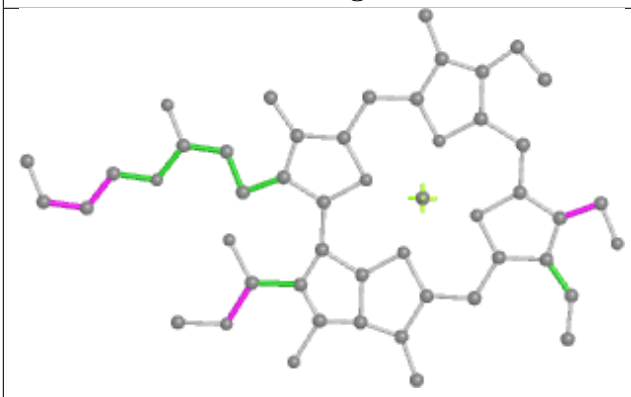
Ligand CHL 1 315



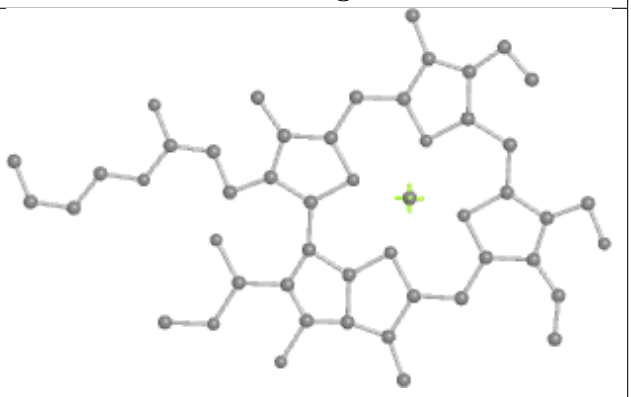
Bond lengths



Bond angles

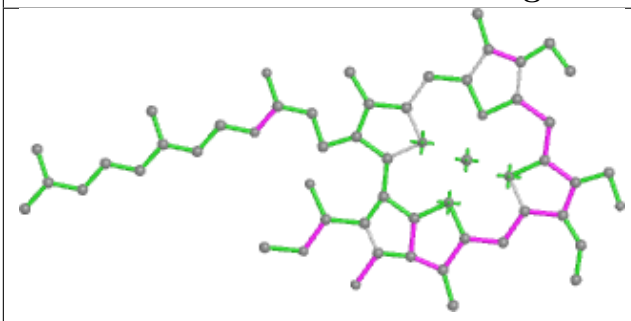


Torsions

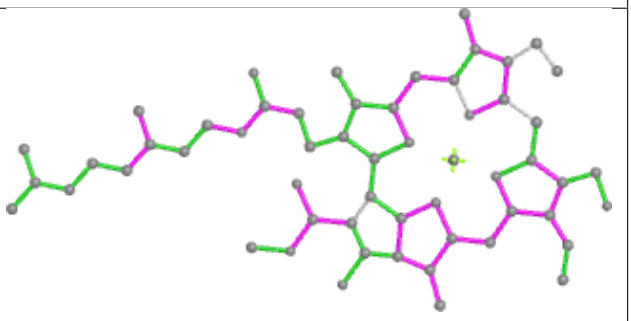


Rings

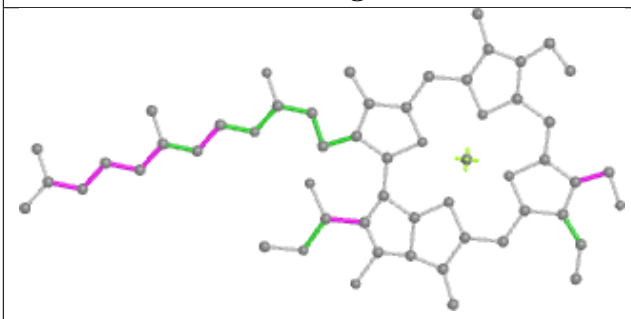
Ligand CHL R 316



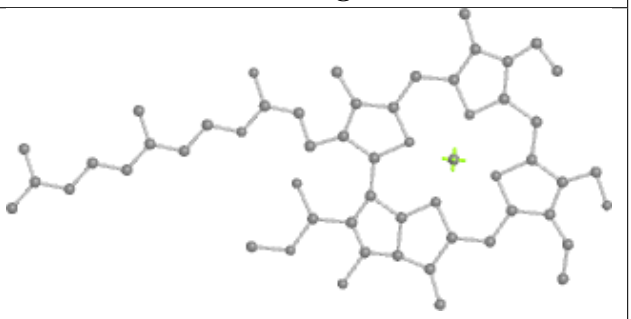
Bond lengths



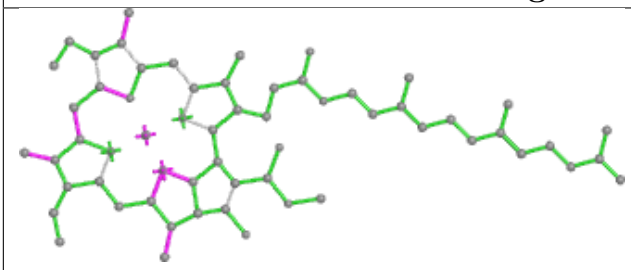
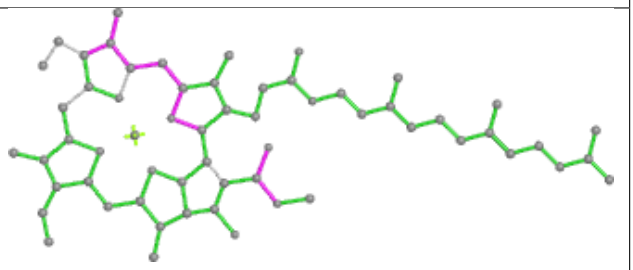
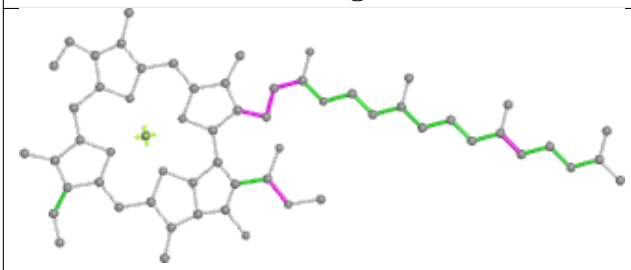
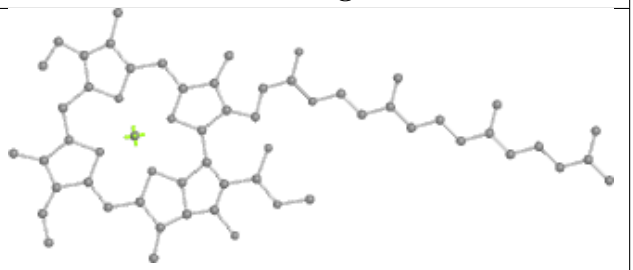
Bond angles

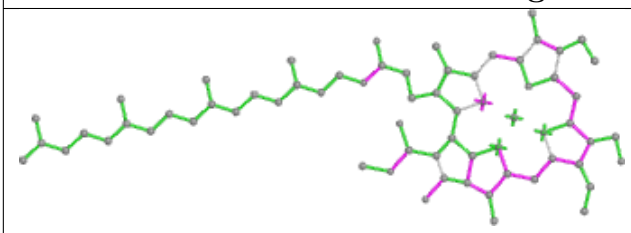
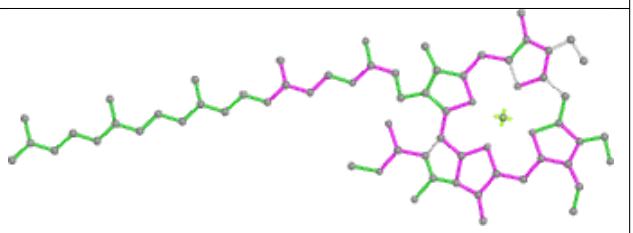
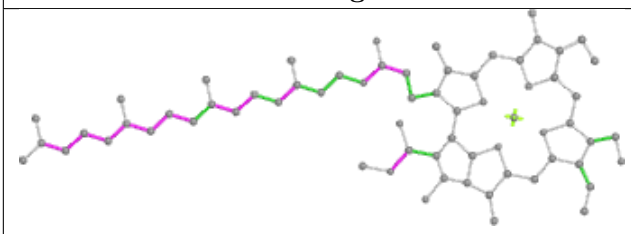
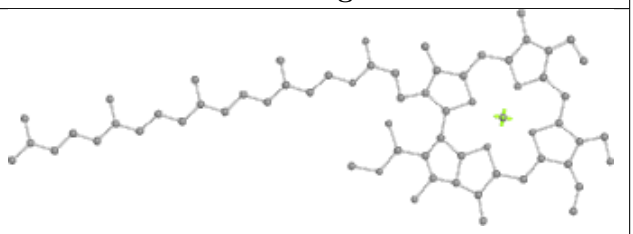


Torsions

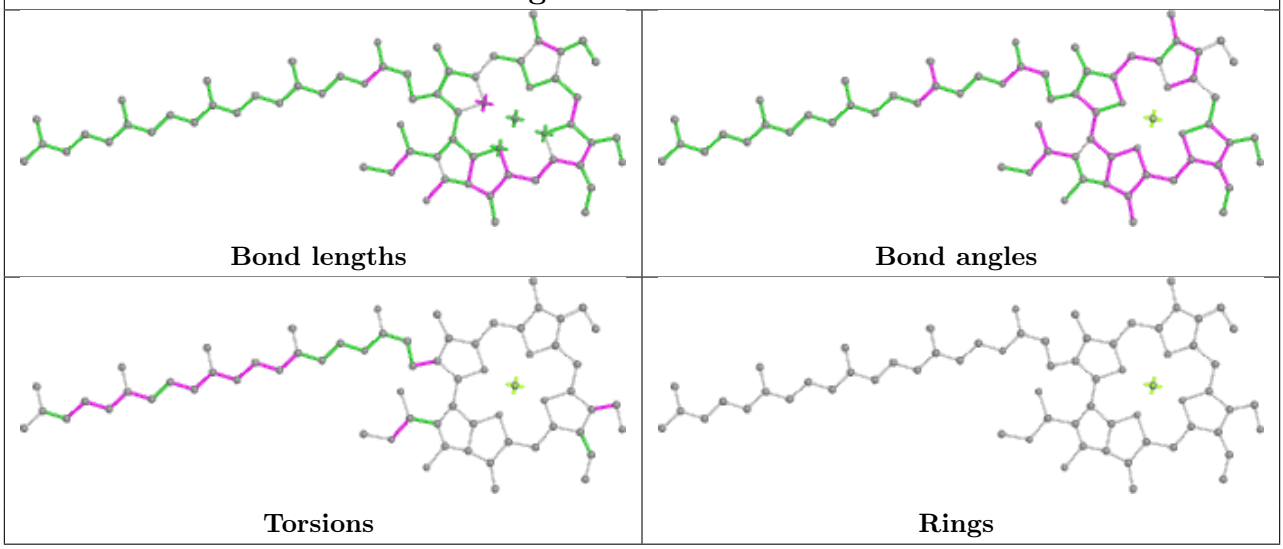


Rings

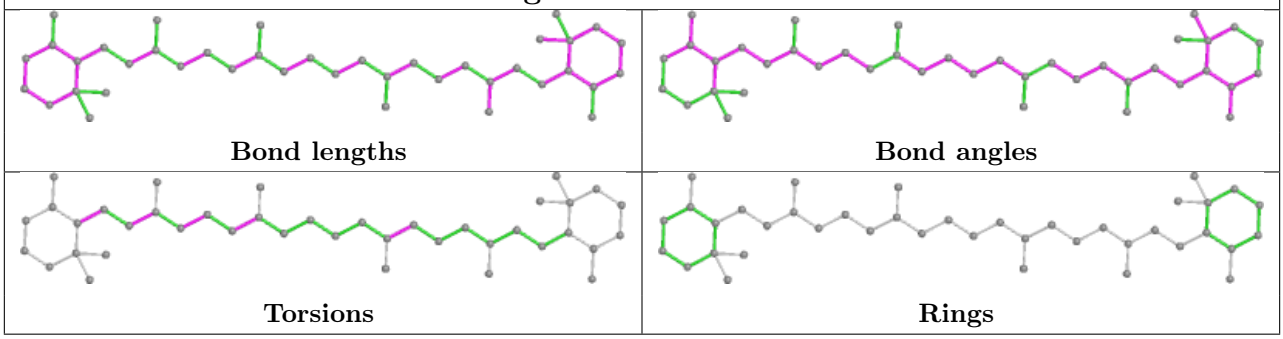
Ligand CLA 1 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

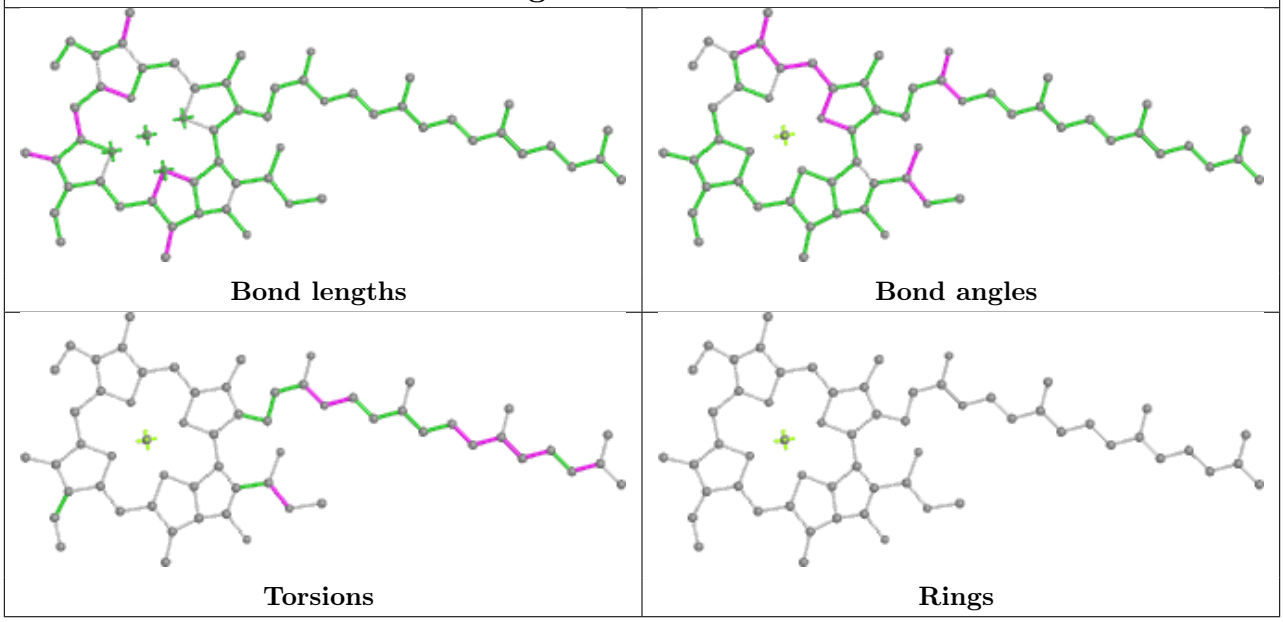
Ligand CHL 2 318



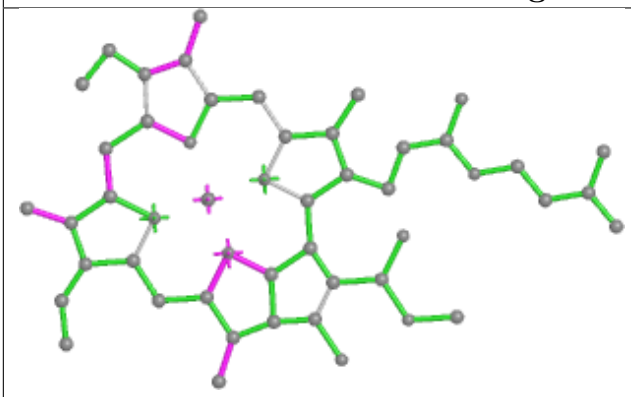
Ligand BCR B 618



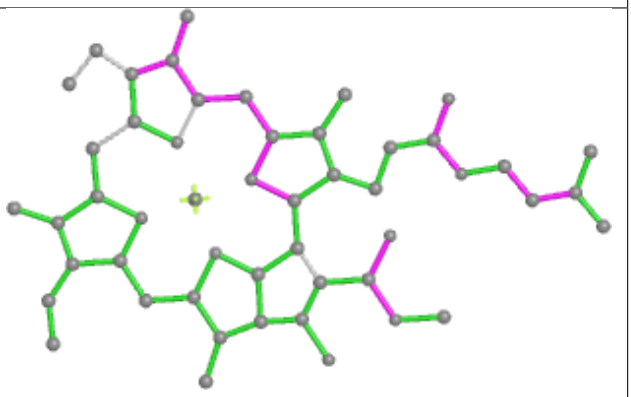
Ligand CLA u 305



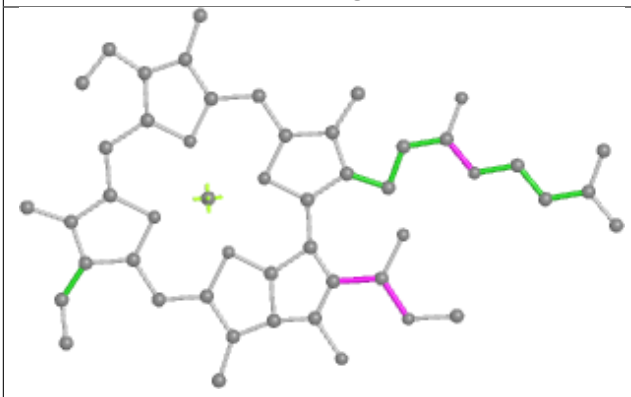
Ligand CLA 1 303



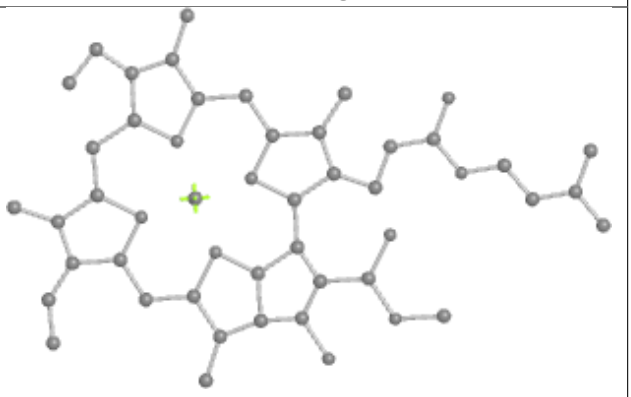
Bond lengths



Bond angles

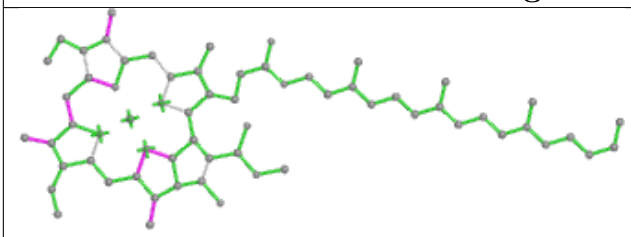


Torsions

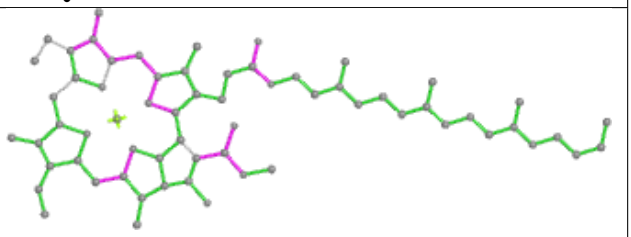


Rings

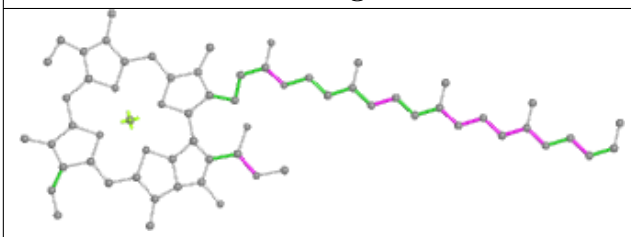
Ligand CLA Q 304



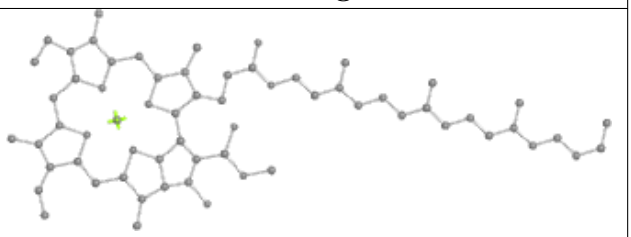
Bond lengths



Bond angles

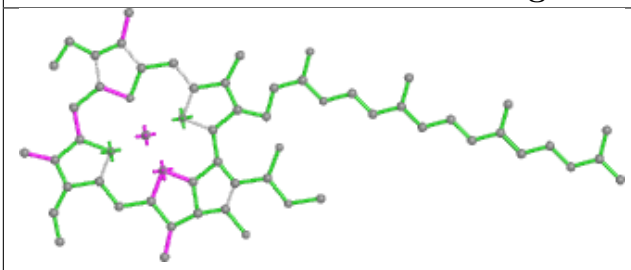


Torsions

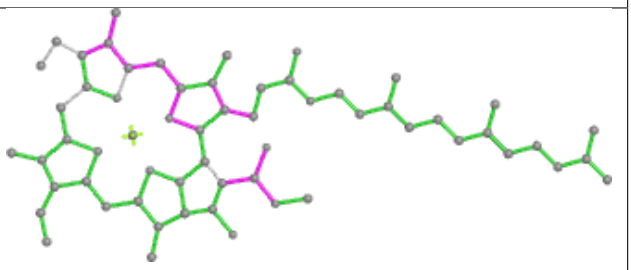


Rings

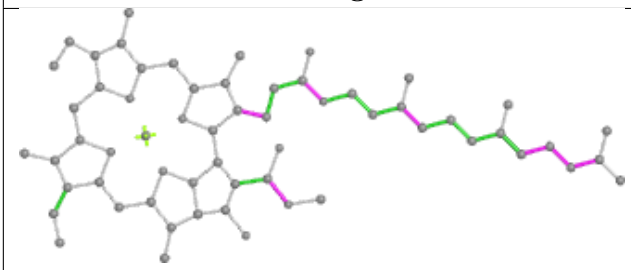
Ligand CLA a 408



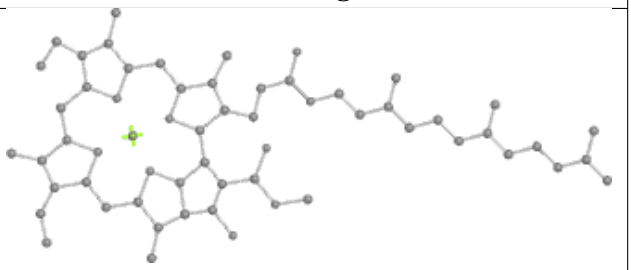
Bond lengths



Bond angles

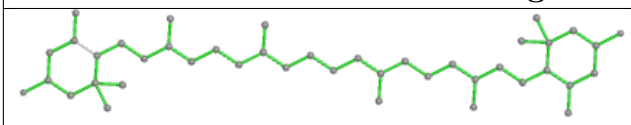


Torsions



Rings

Ligand LUT p 310



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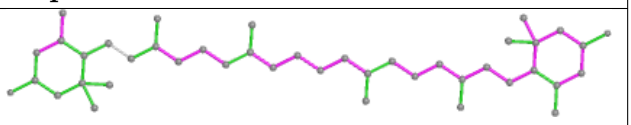
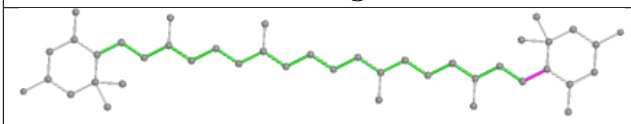


Bond angles



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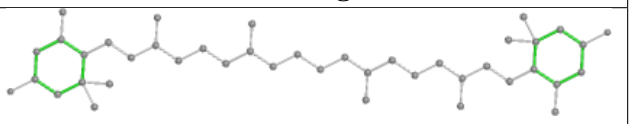
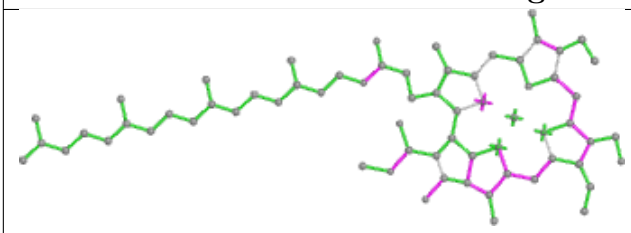


Rings

Ligand CHL 6 312



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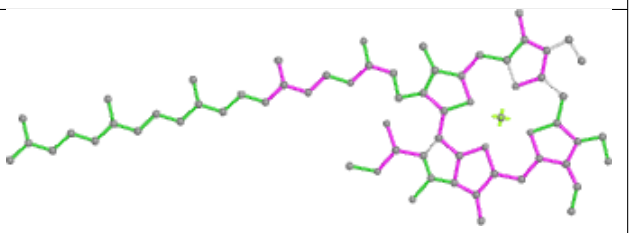

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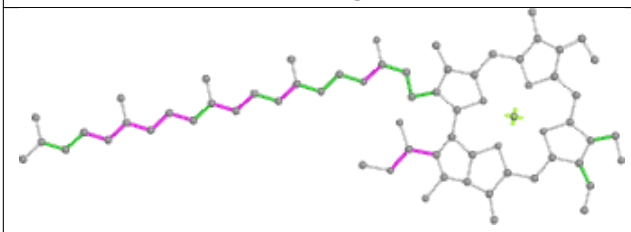

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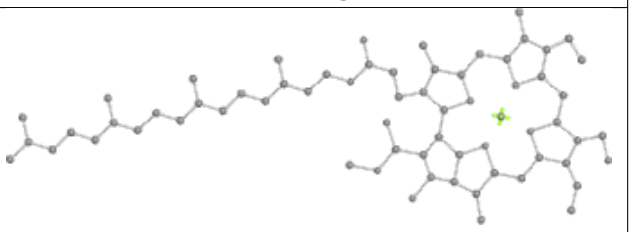
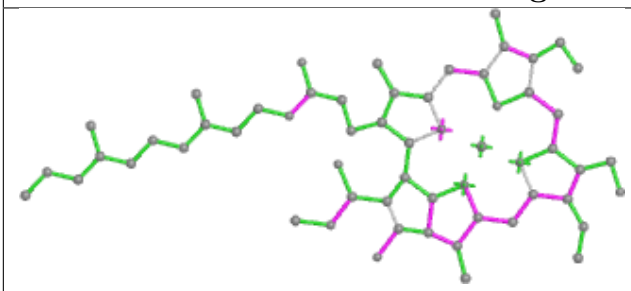


Rings

Ligand CHL s 315



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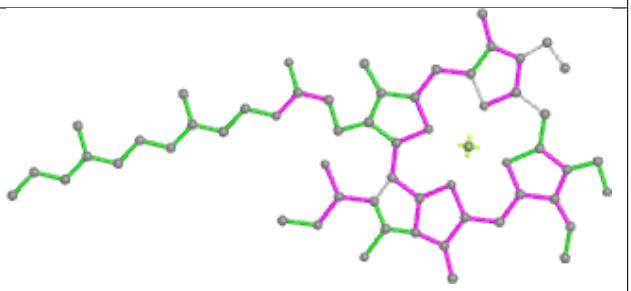
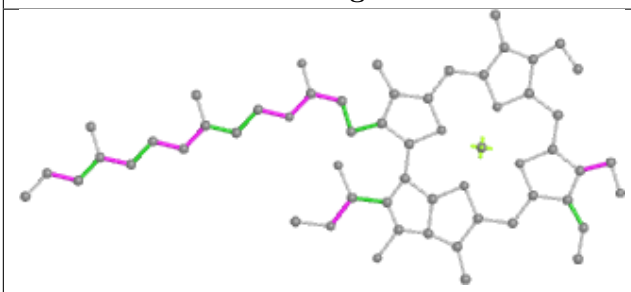


Bond angles



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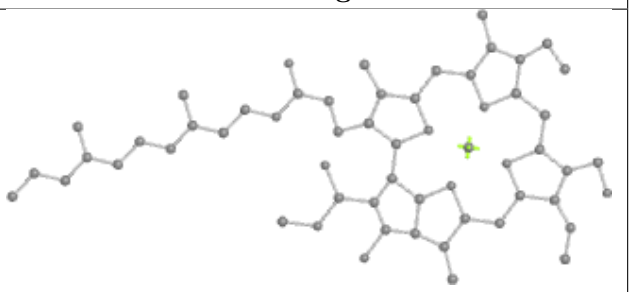
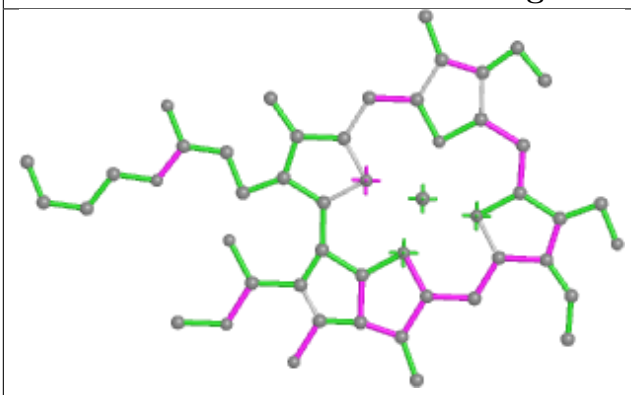


Rings

Ligand CHL p 316



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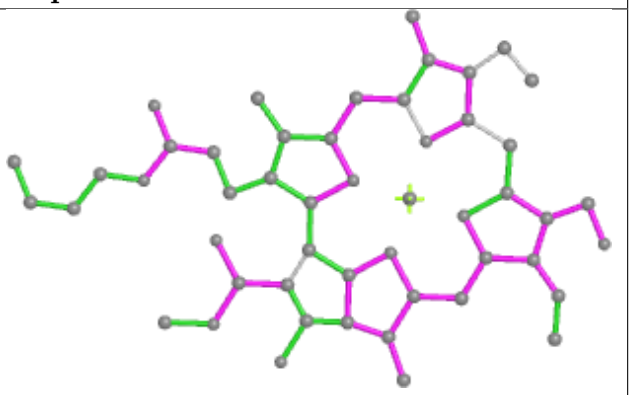
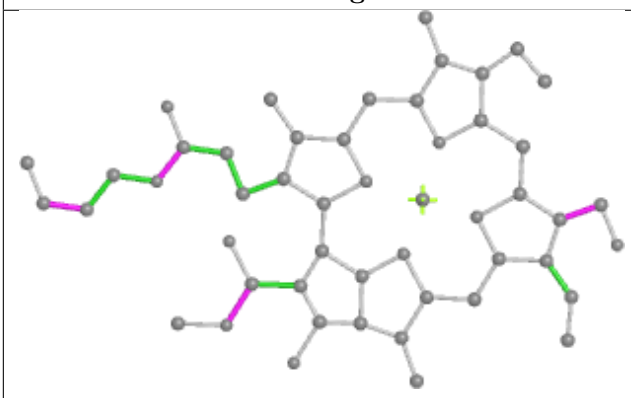


Bond angles



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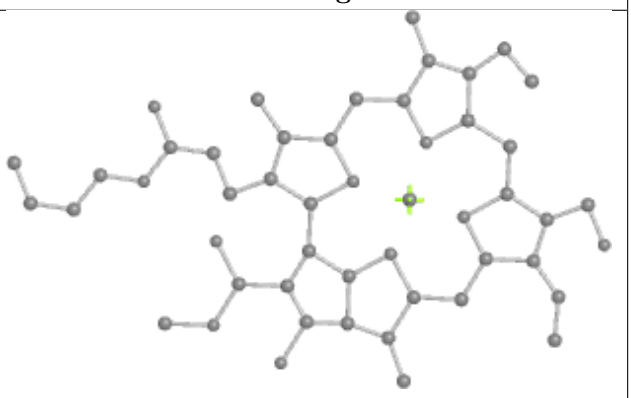
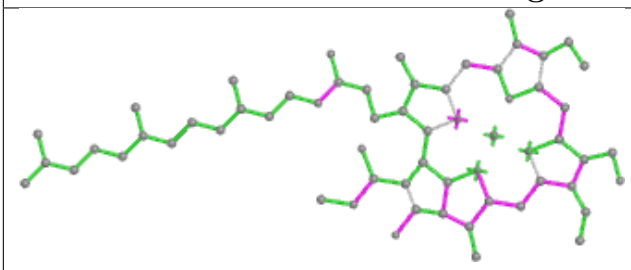


Rings

Ligand CHL q 315



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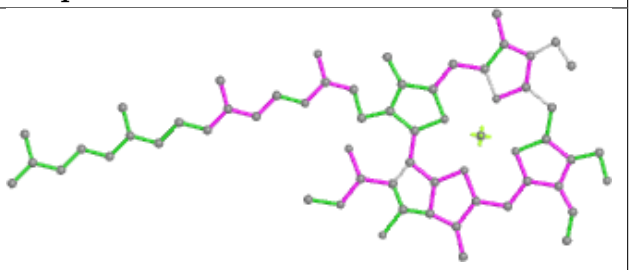

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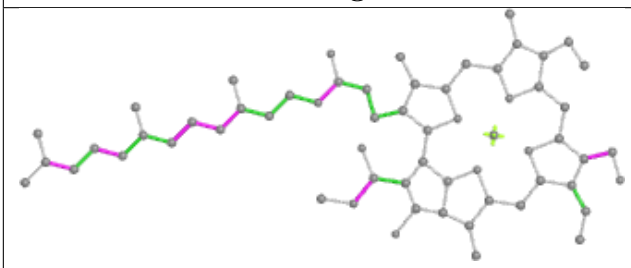

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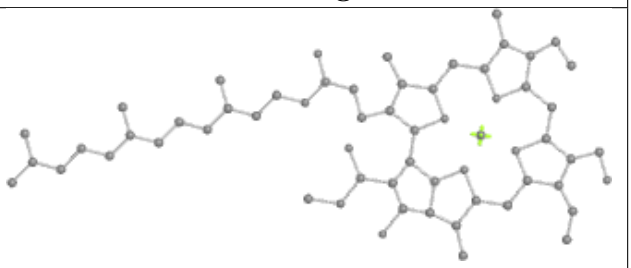
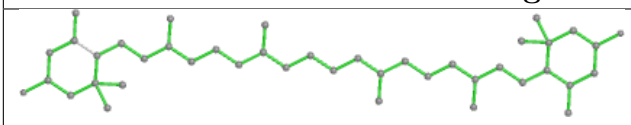


Rings

Ligand LUT N 309



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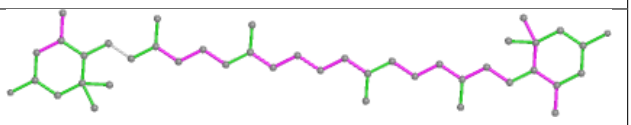
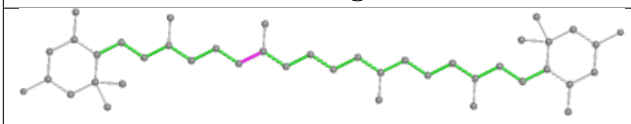


Bond angles



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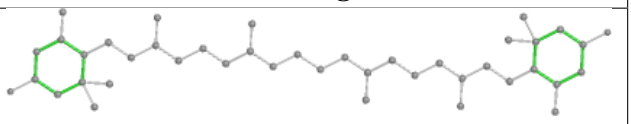
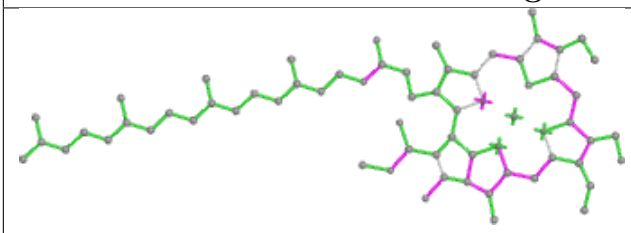


Rings

Ligand CHL P 314



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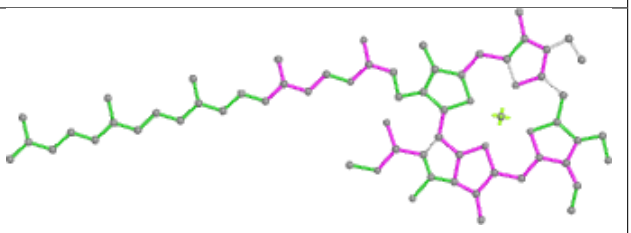
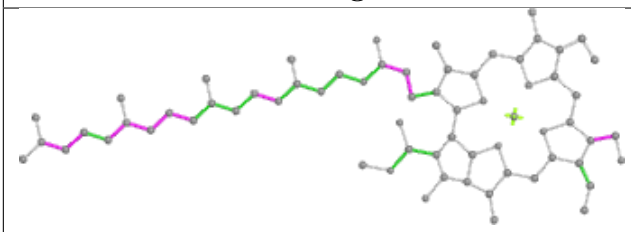
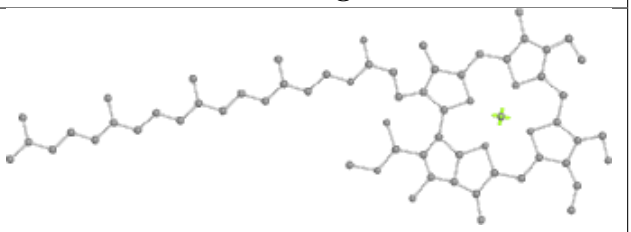


Bond angles

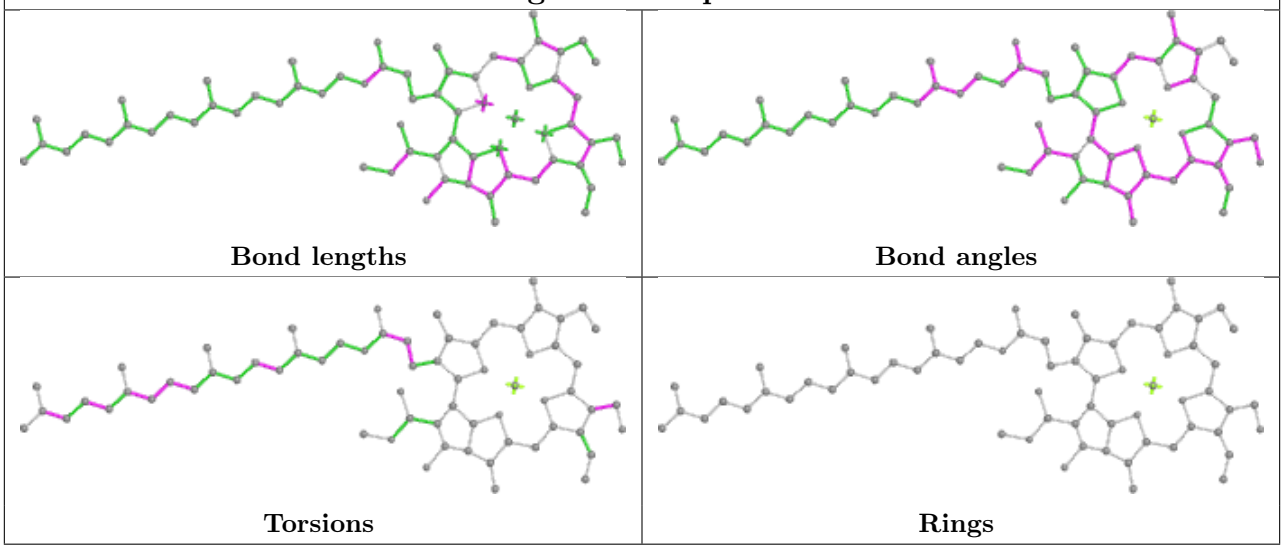


Torsions

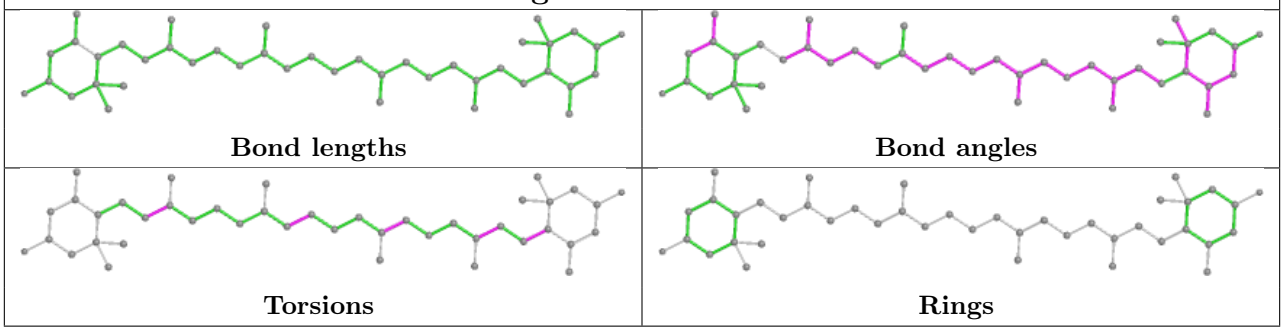


Rings

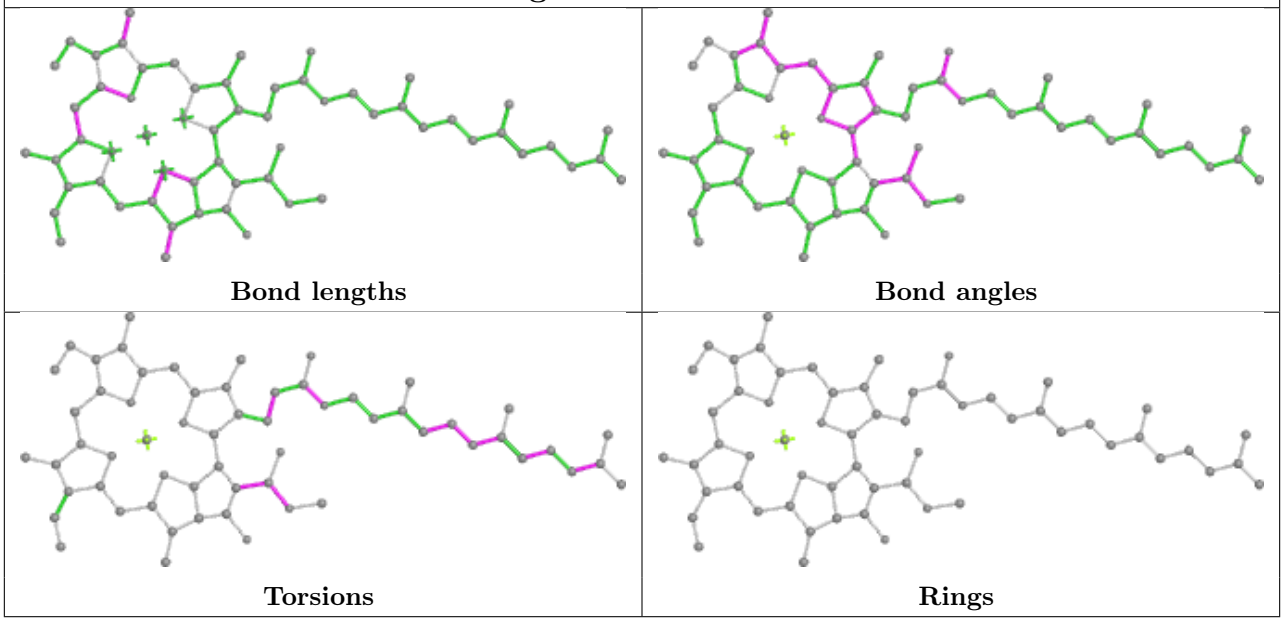
Ligand CHL p 314

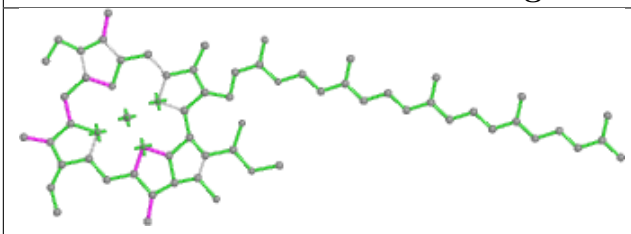
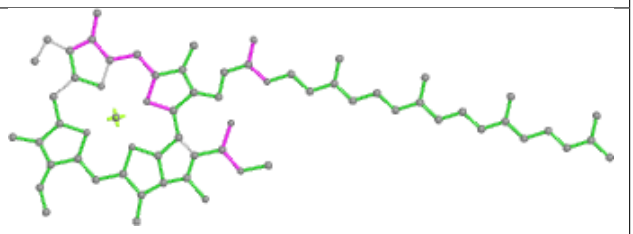
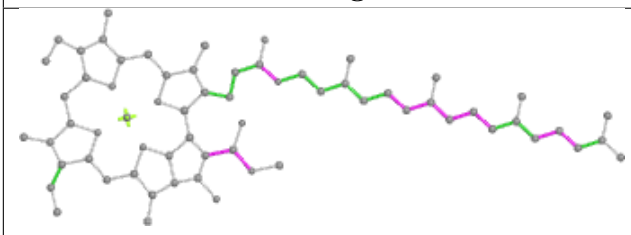
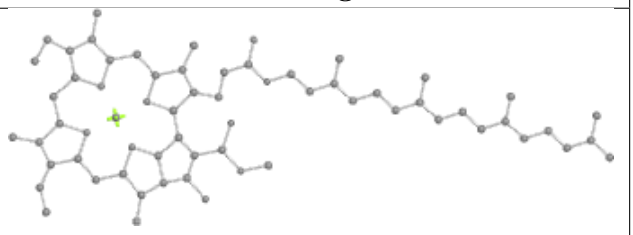


Ligand LUT s 311



Ligand CLA 6 306



Ligand CLA B 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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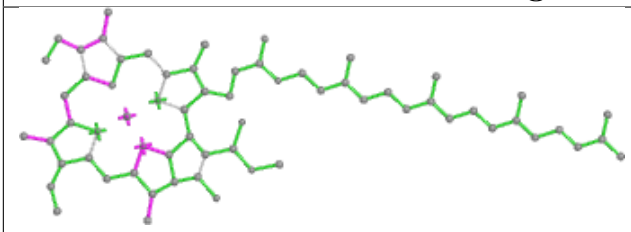
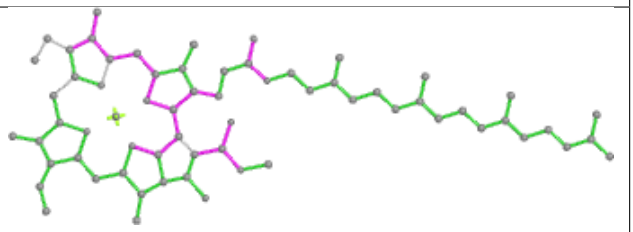
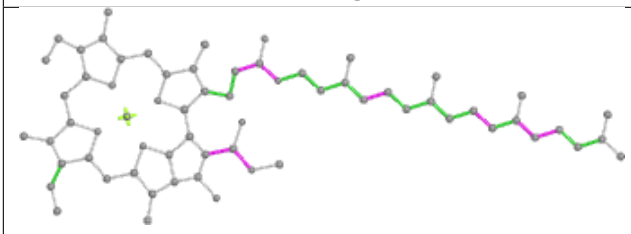
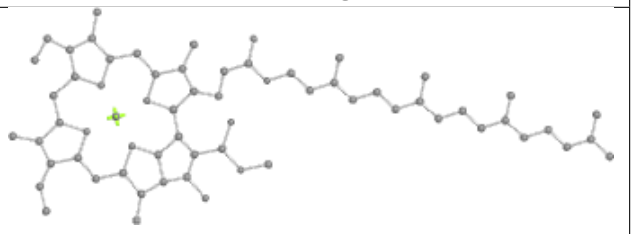
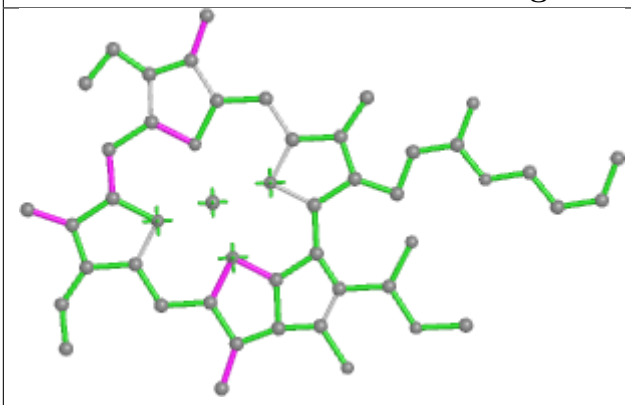
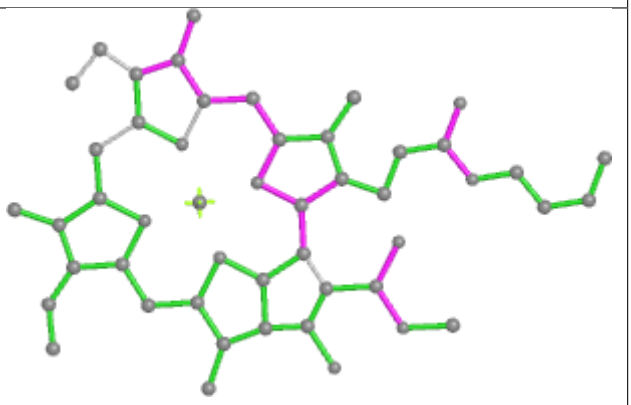
 Bond lengths	 Bond angles
 Torsions	 Rings

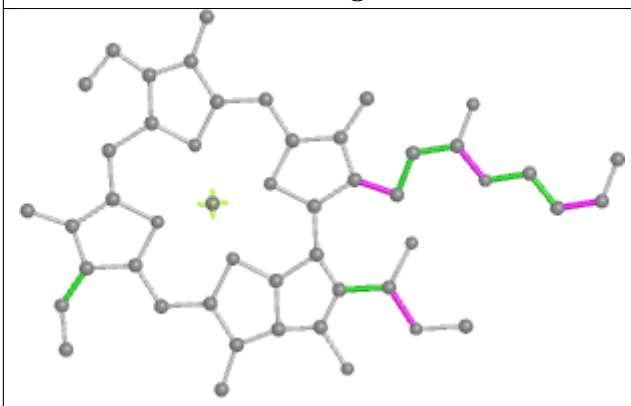
Ligand CLA r 601



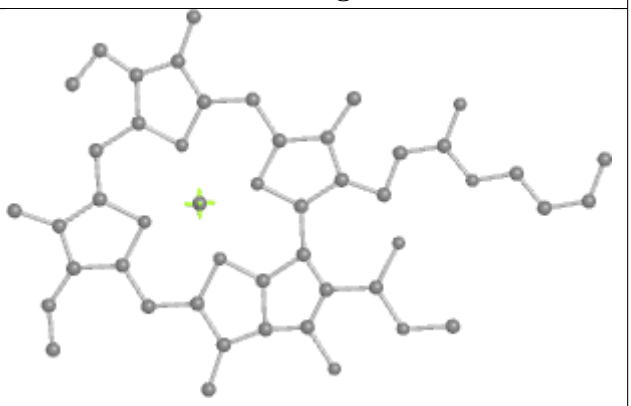
Bond lengths



Bond angles

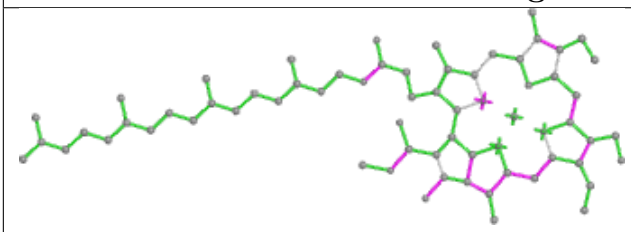


Torsions



Rings

Ligand CHL 5 317



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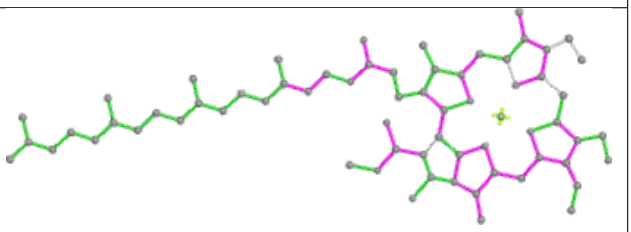
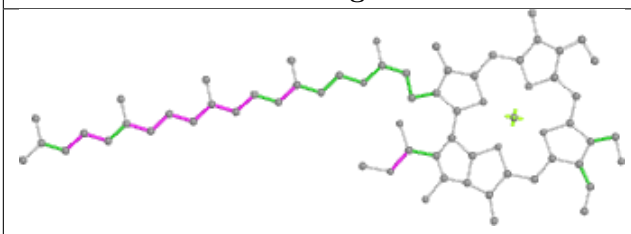


Bond angles



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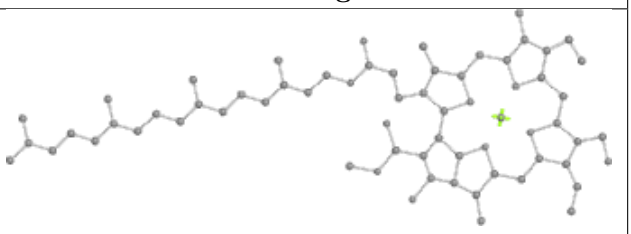
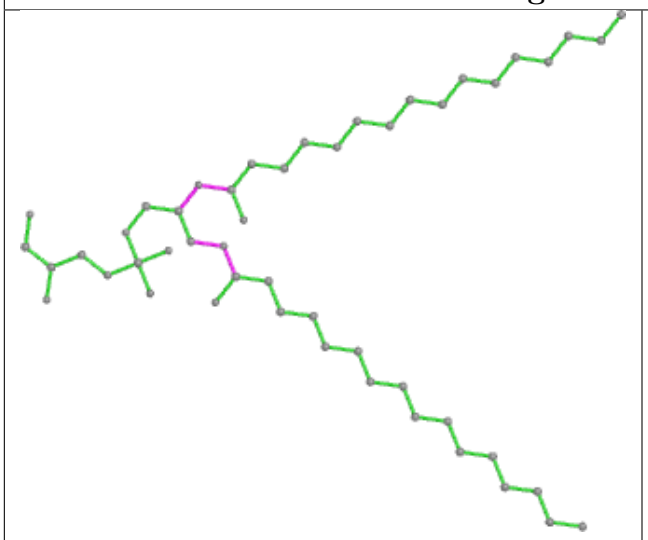


Rings

Ligand LHG g 310



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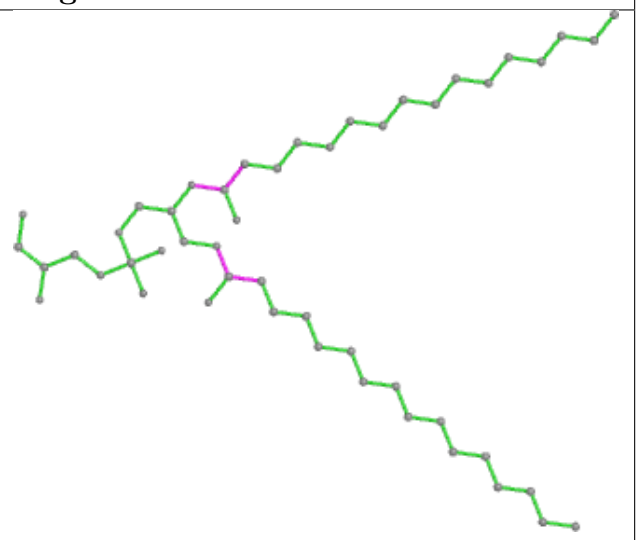
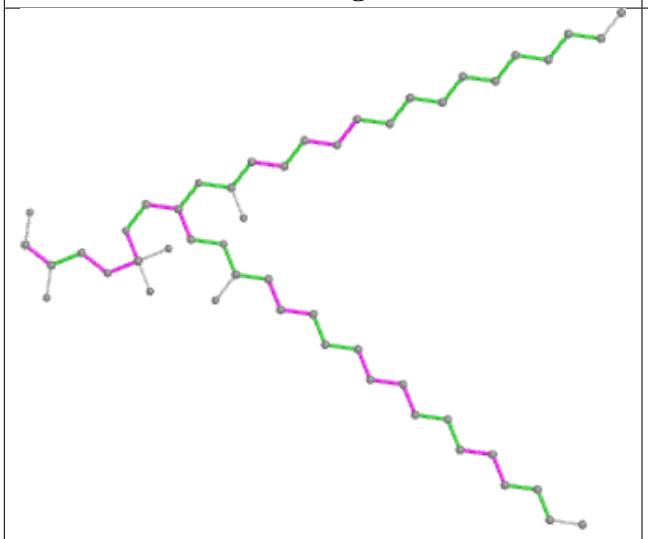
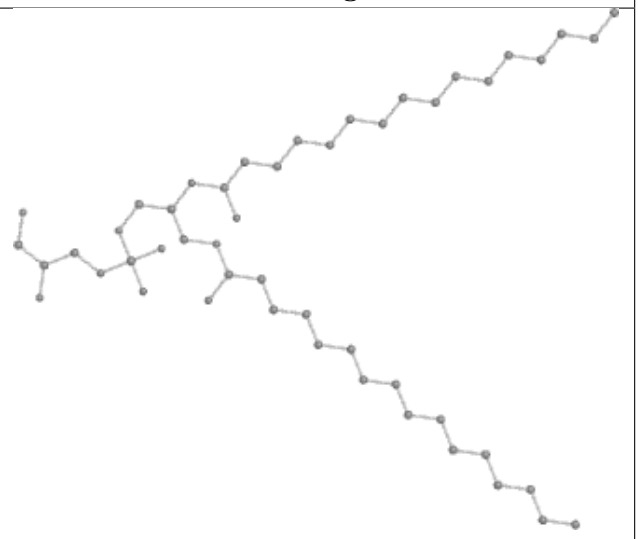


Bond angles

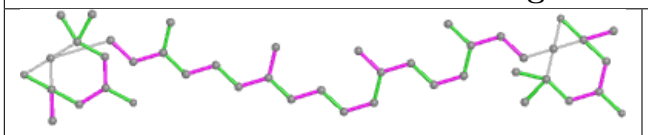


Torsions

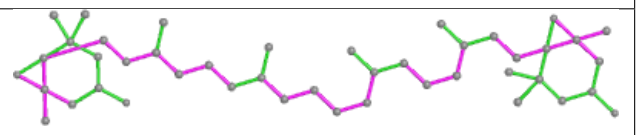


Rings

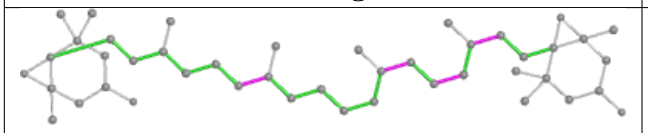
Ligand XAT u 311



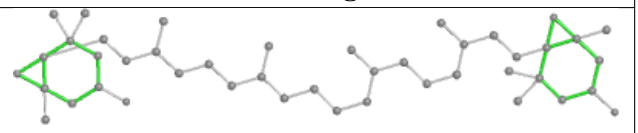
Bond lengths



Bond angles

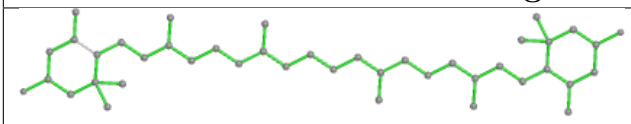


Torsions

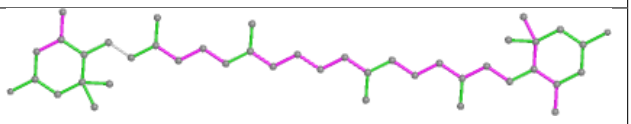


Rings

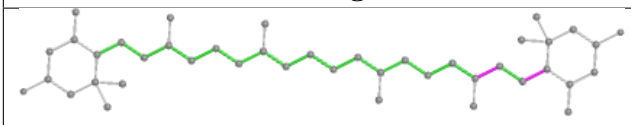
Ligand LUT R 312



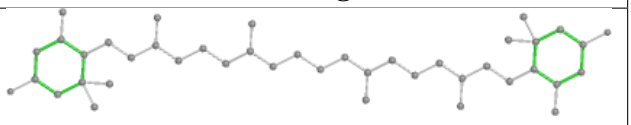
Bond lengths



Bond angles

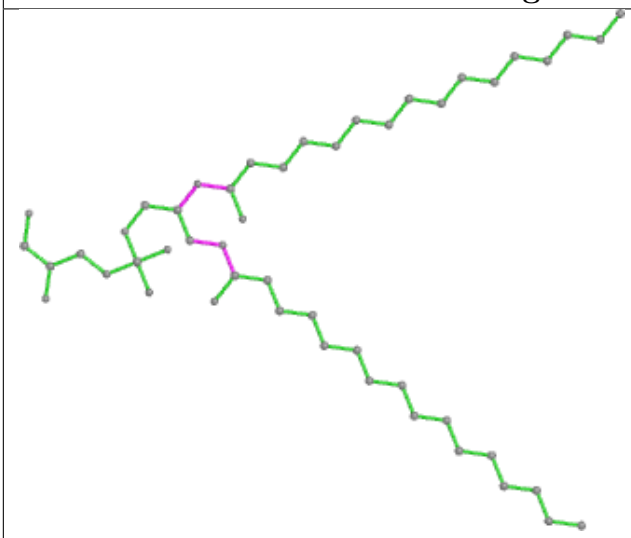


Torsions

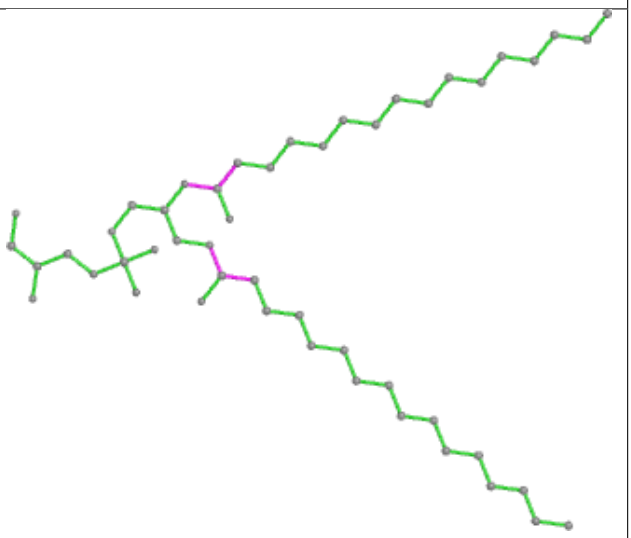


Rings

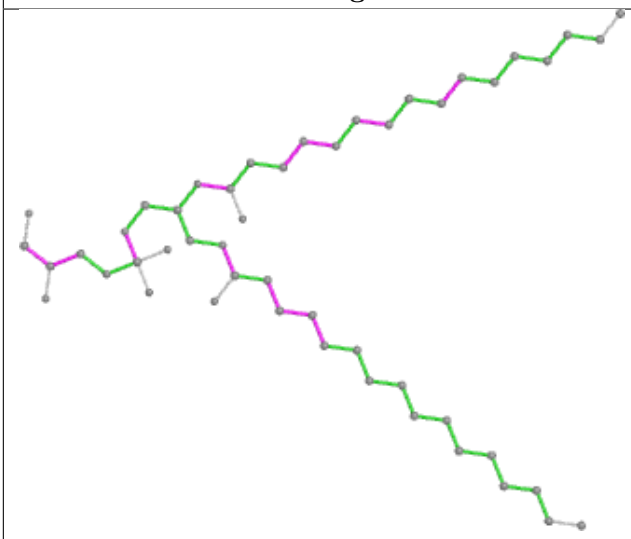
Ligand LHG C 522



Bond lengths



Bond angles



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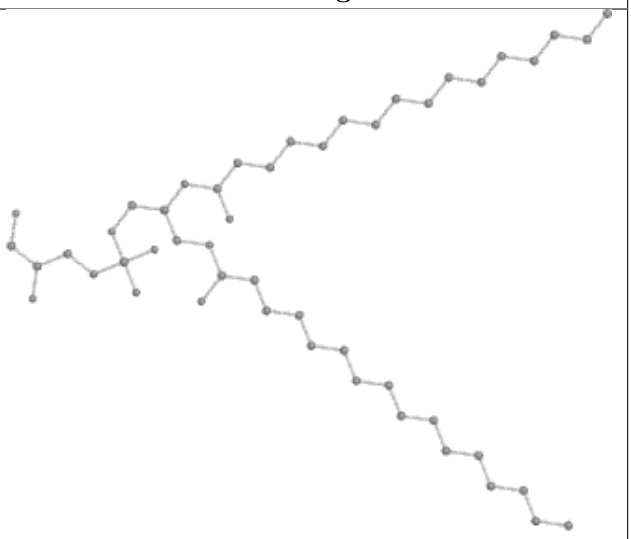
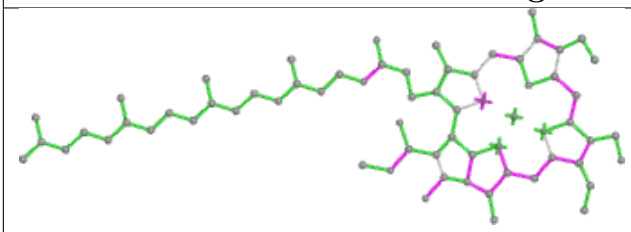
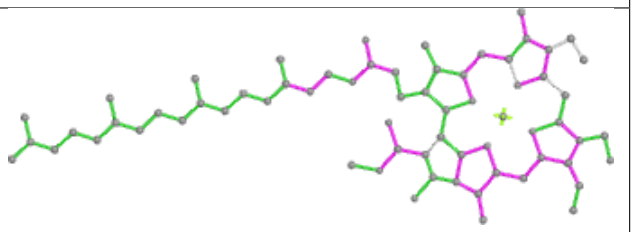
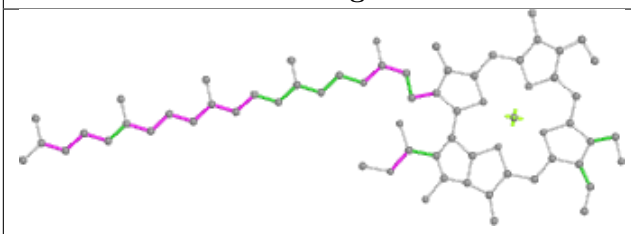
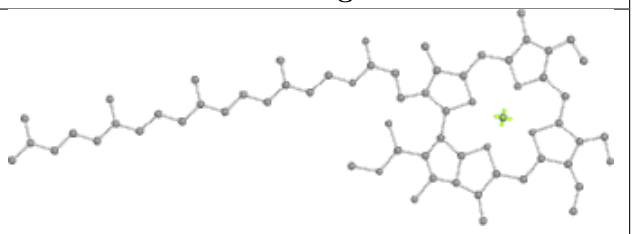
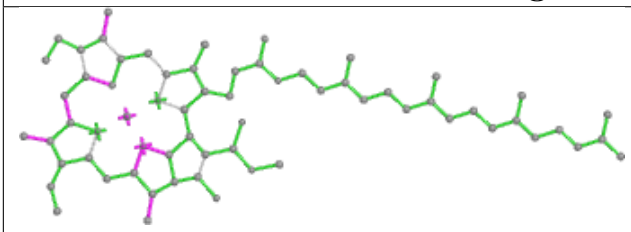
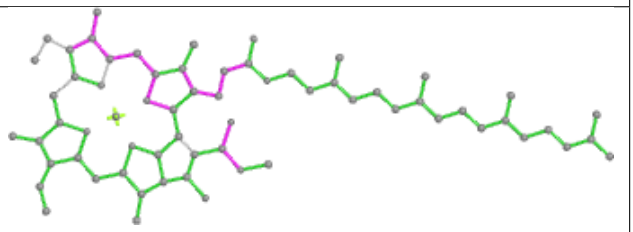
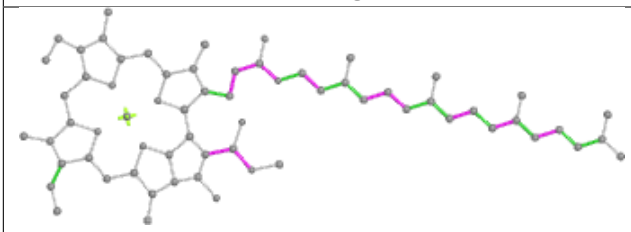
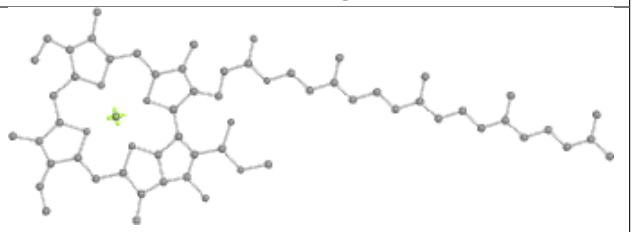
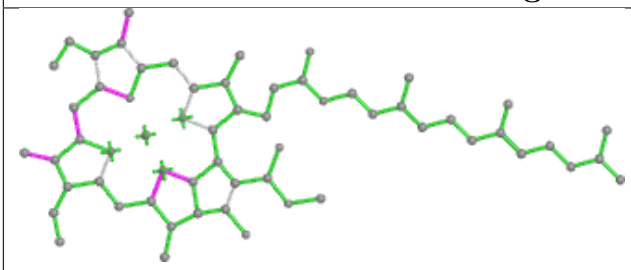
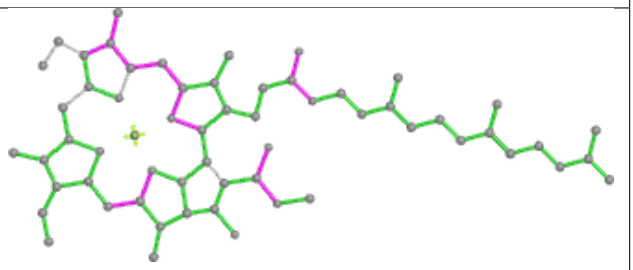
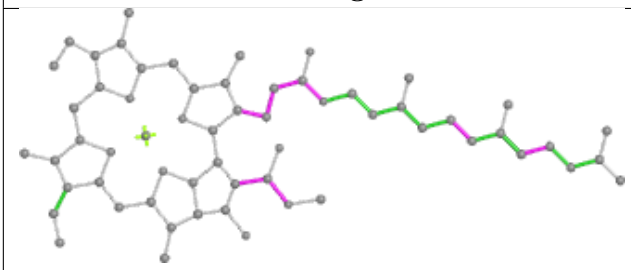
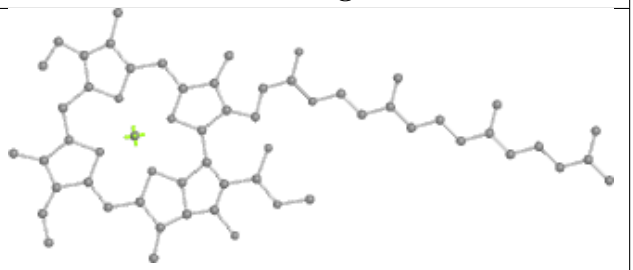


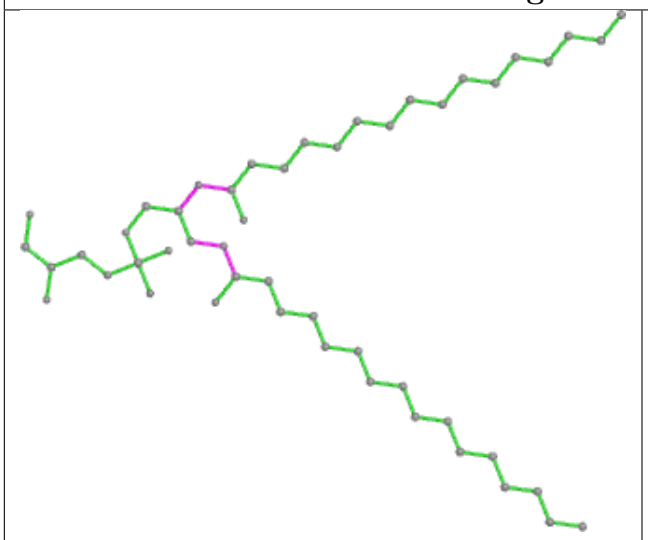
Rings

Ligand CHL 4 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

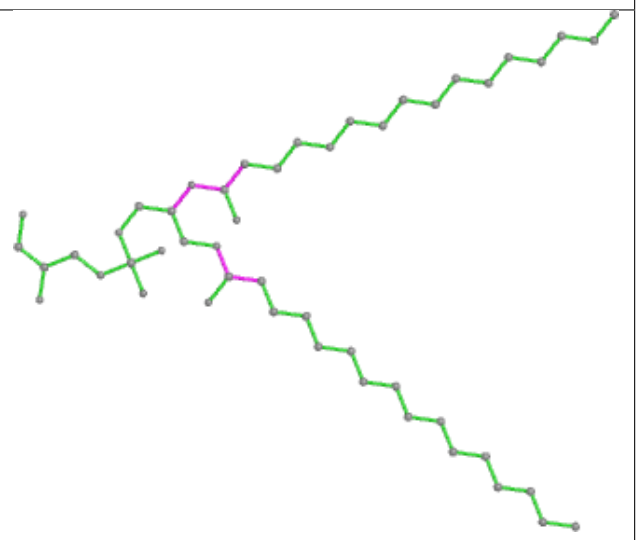
Ligand CLA a 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

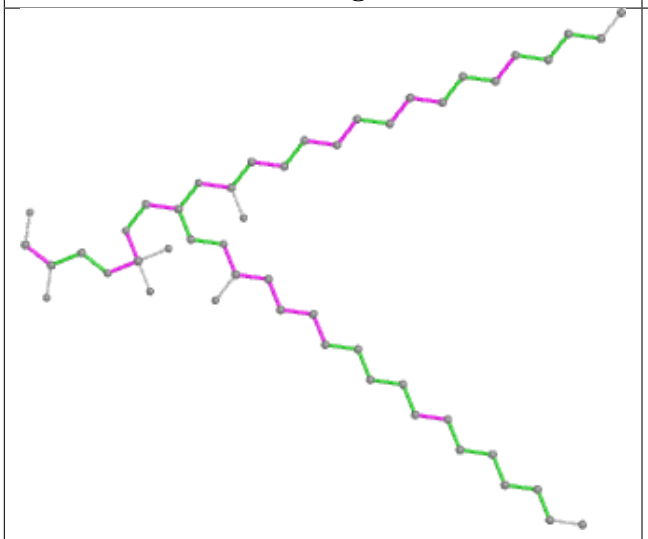
Ligand LHG u 312



Bond lengths



Bond angles



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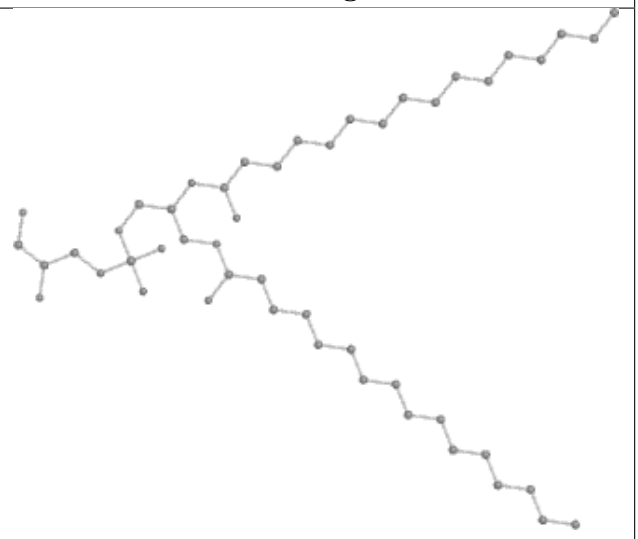
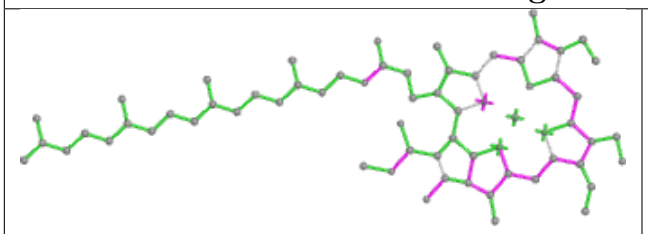


Rings

Ligand CHL 6 315



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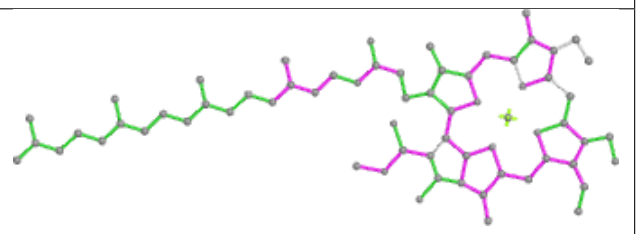
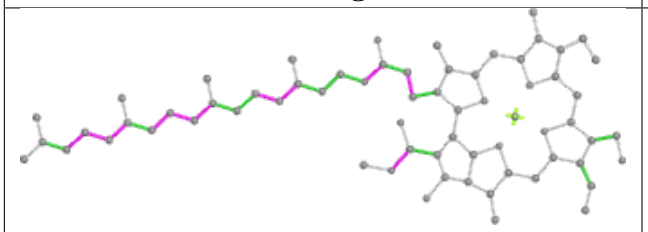


Bond angles



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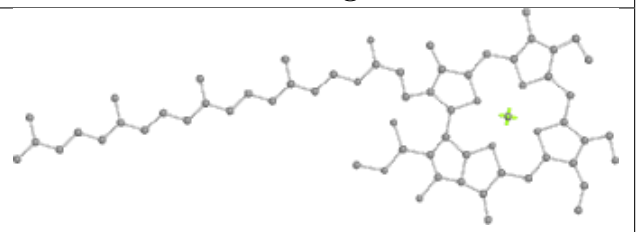
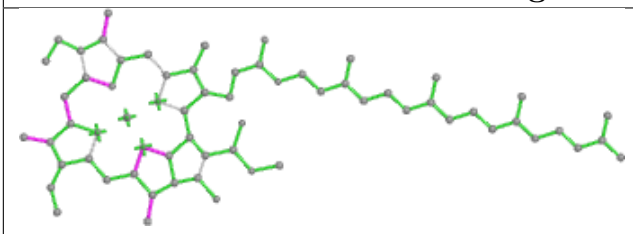


Rings

Ligand CLA 5 301



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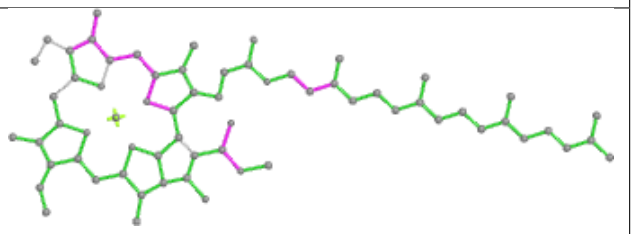
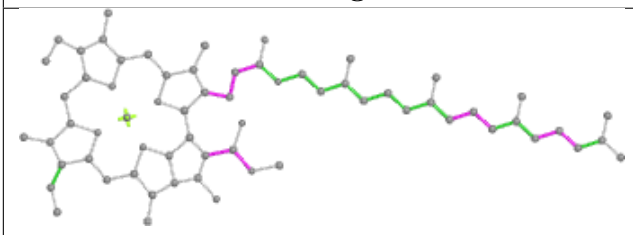


Bond angles



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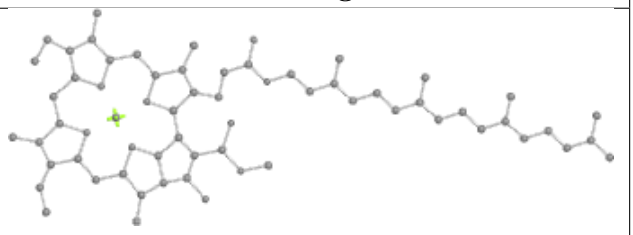
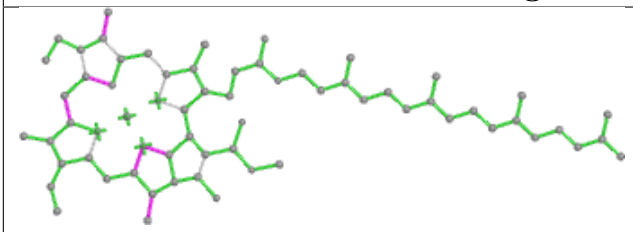
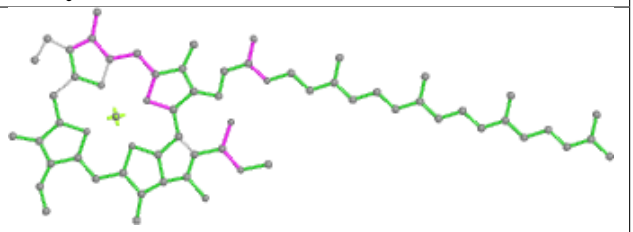


Rings

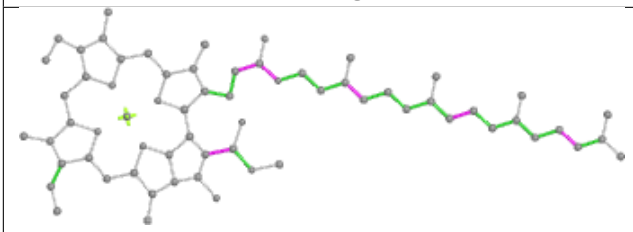
Ligand CLA Q 302



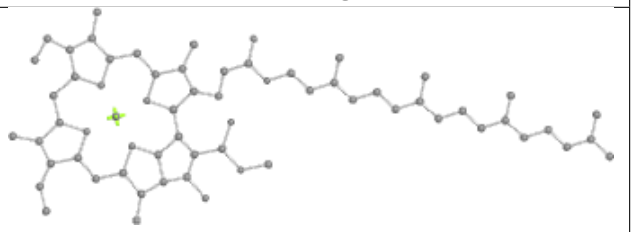
Bond lengths



Bond angles

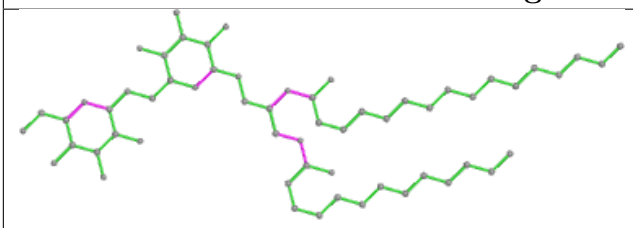


Torsions

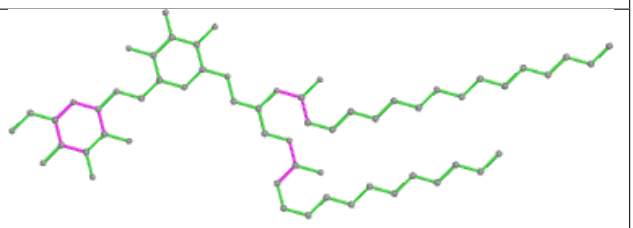


Rings

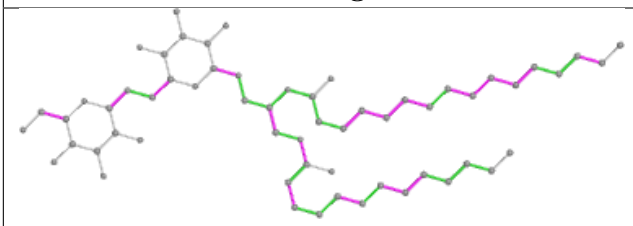
Ligand DGD a 416



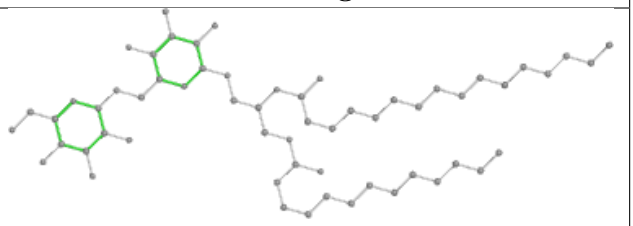
Bond lengths



Bond angles

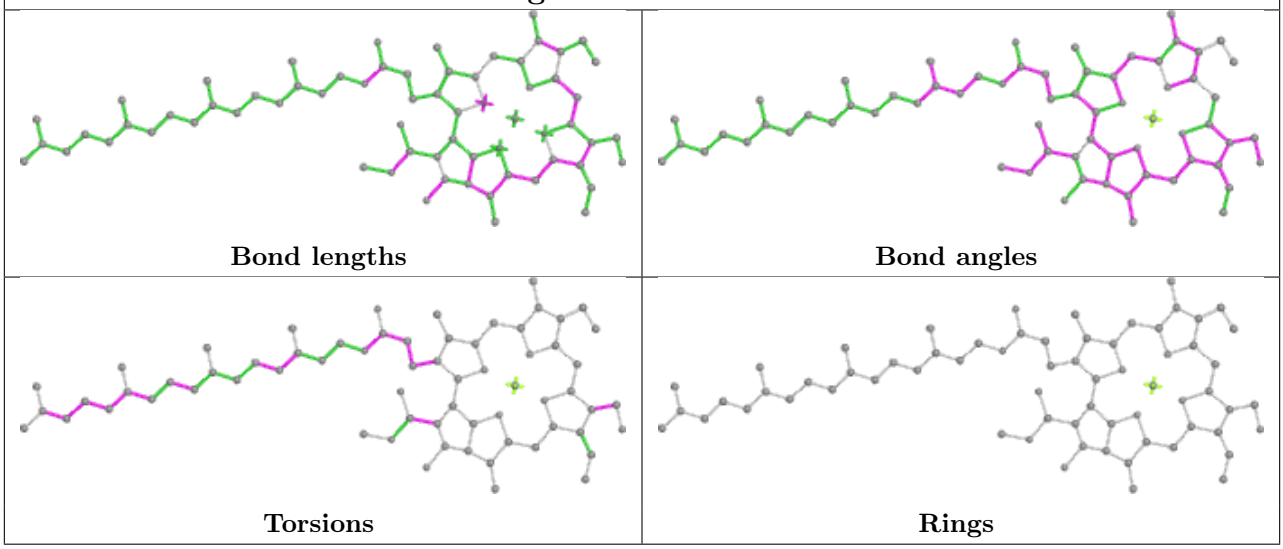


Torsions

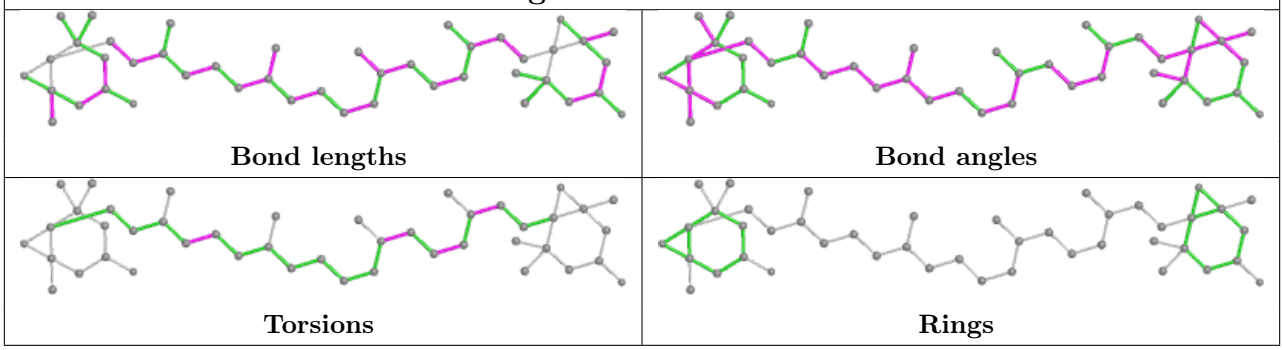


Rings

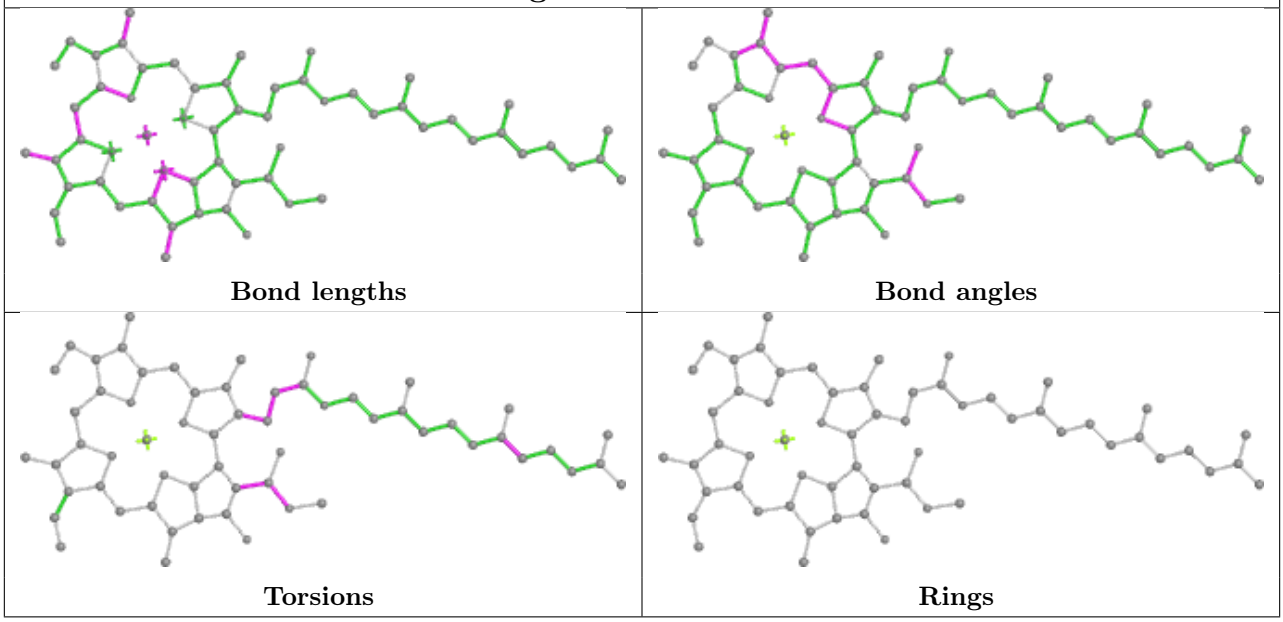
Ligand CHL u 316



Ligand XAT 5 311



Ligand CLA 4 304



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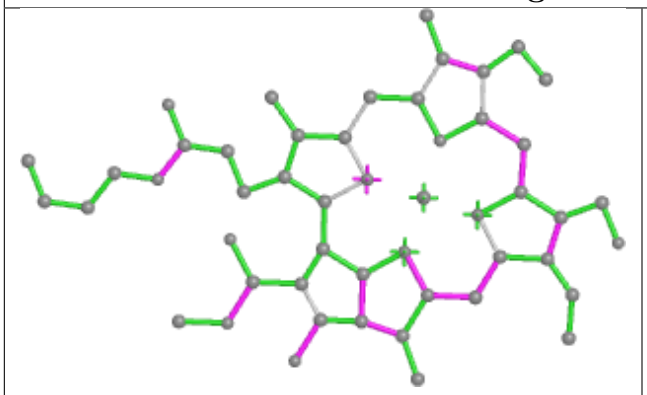
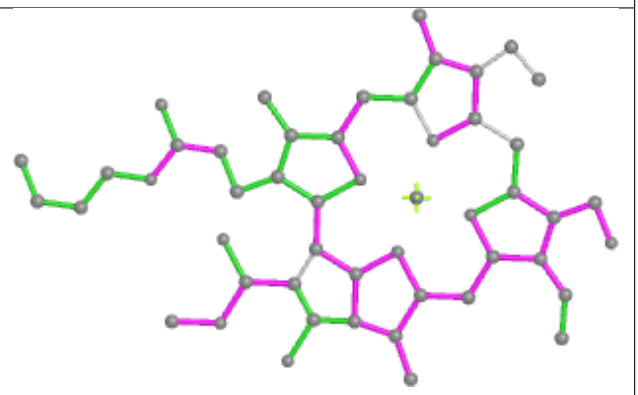
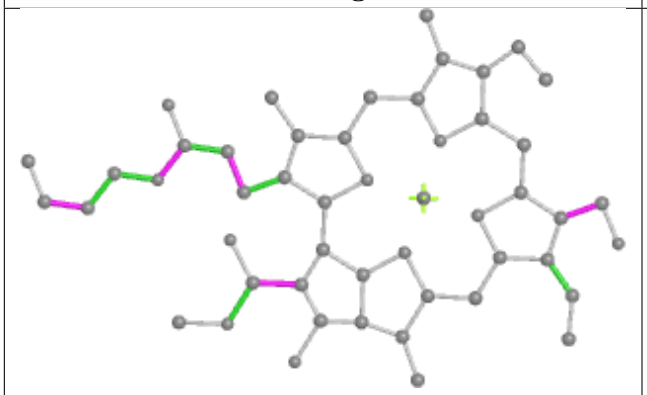


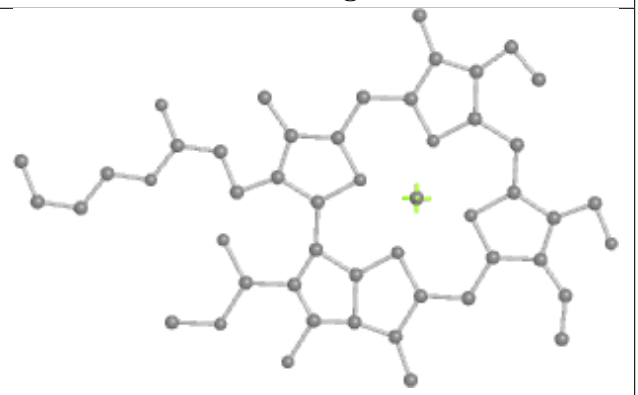
Bond lengths



Bond angles

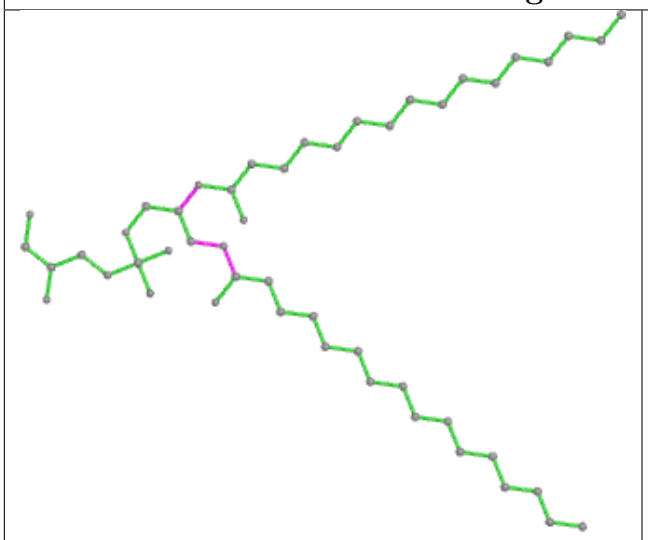


Torsions

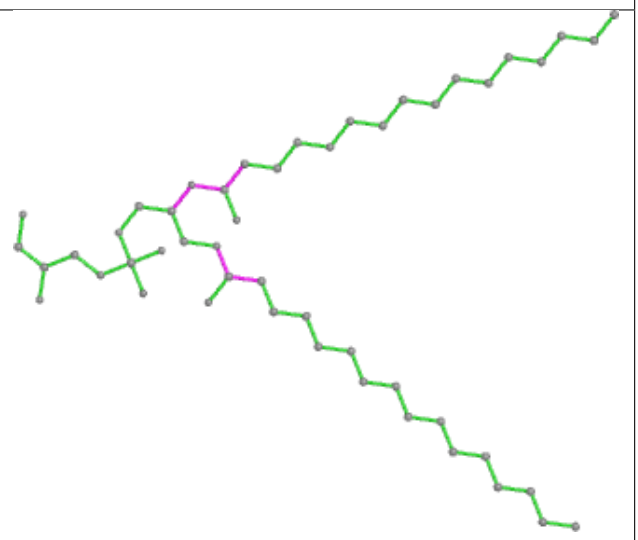


Rings

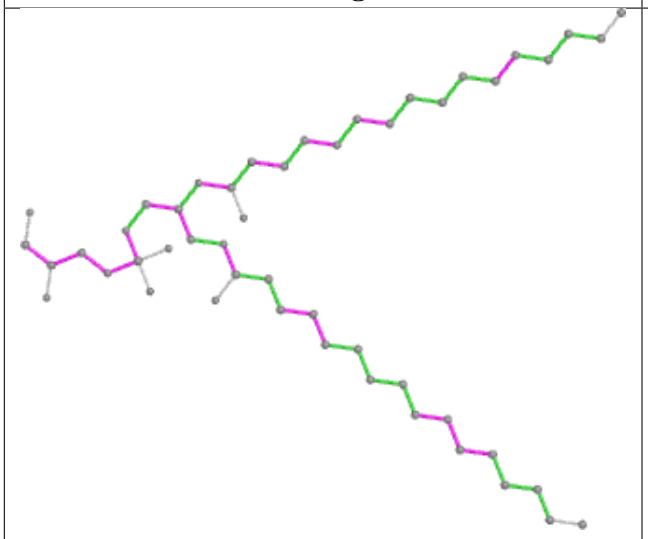
Ligand LHG L 101



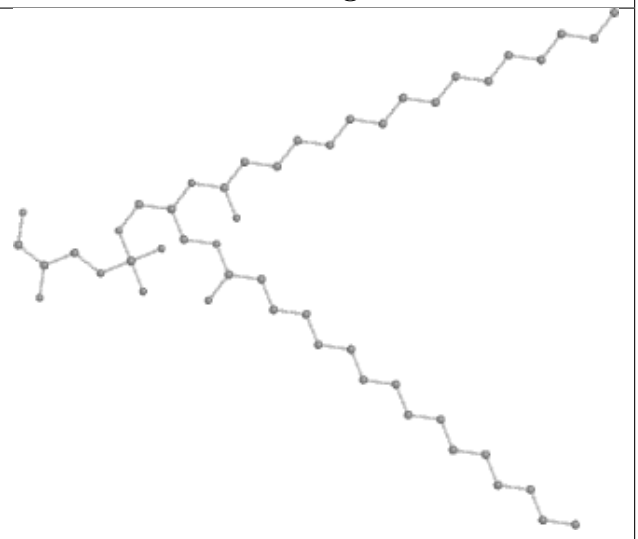
Bond lengths



Bond angles

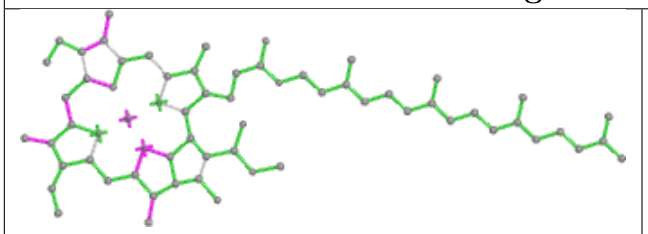


Torsions

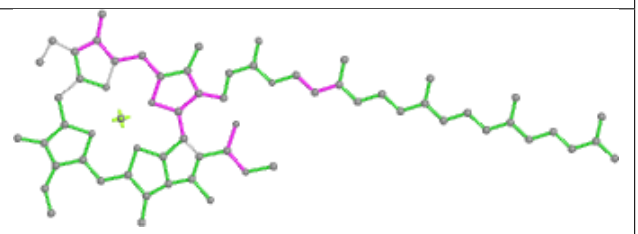


Rings

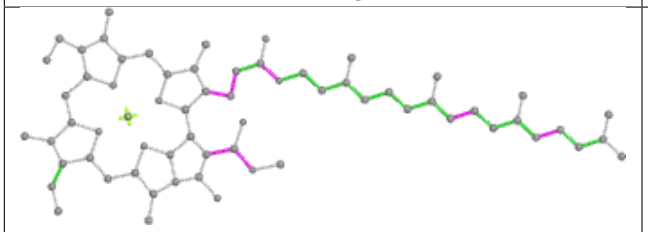
Ligand CLA A 405



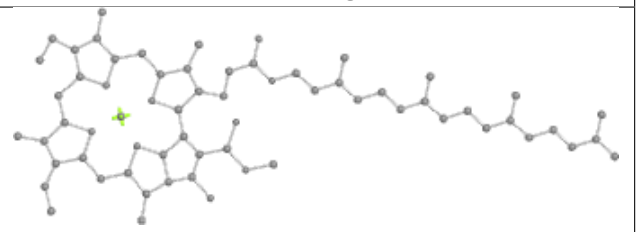
Bond lengths



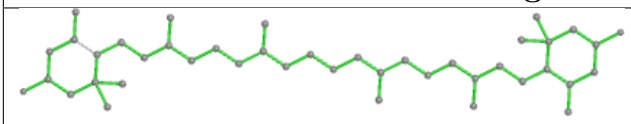
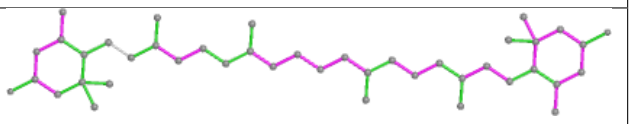
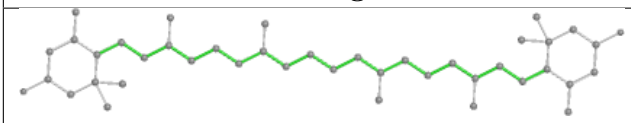
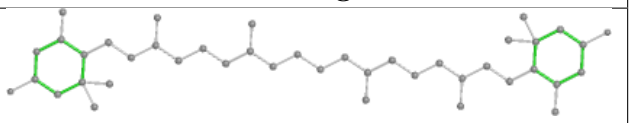
Bond angles

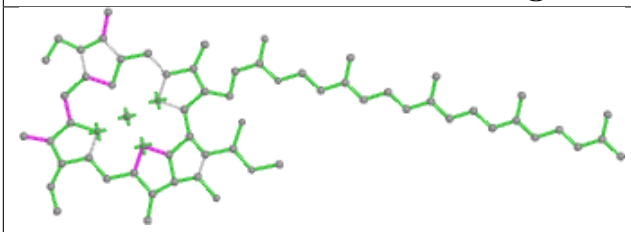
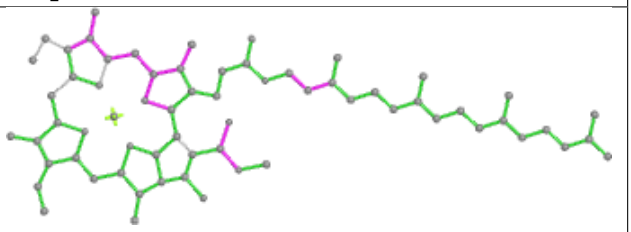
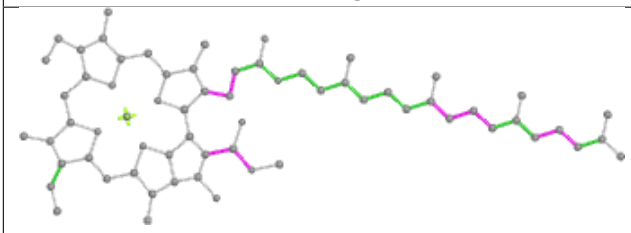
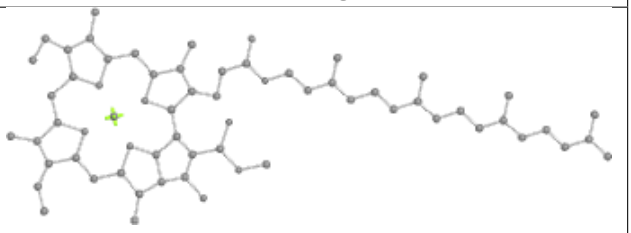


Torsions

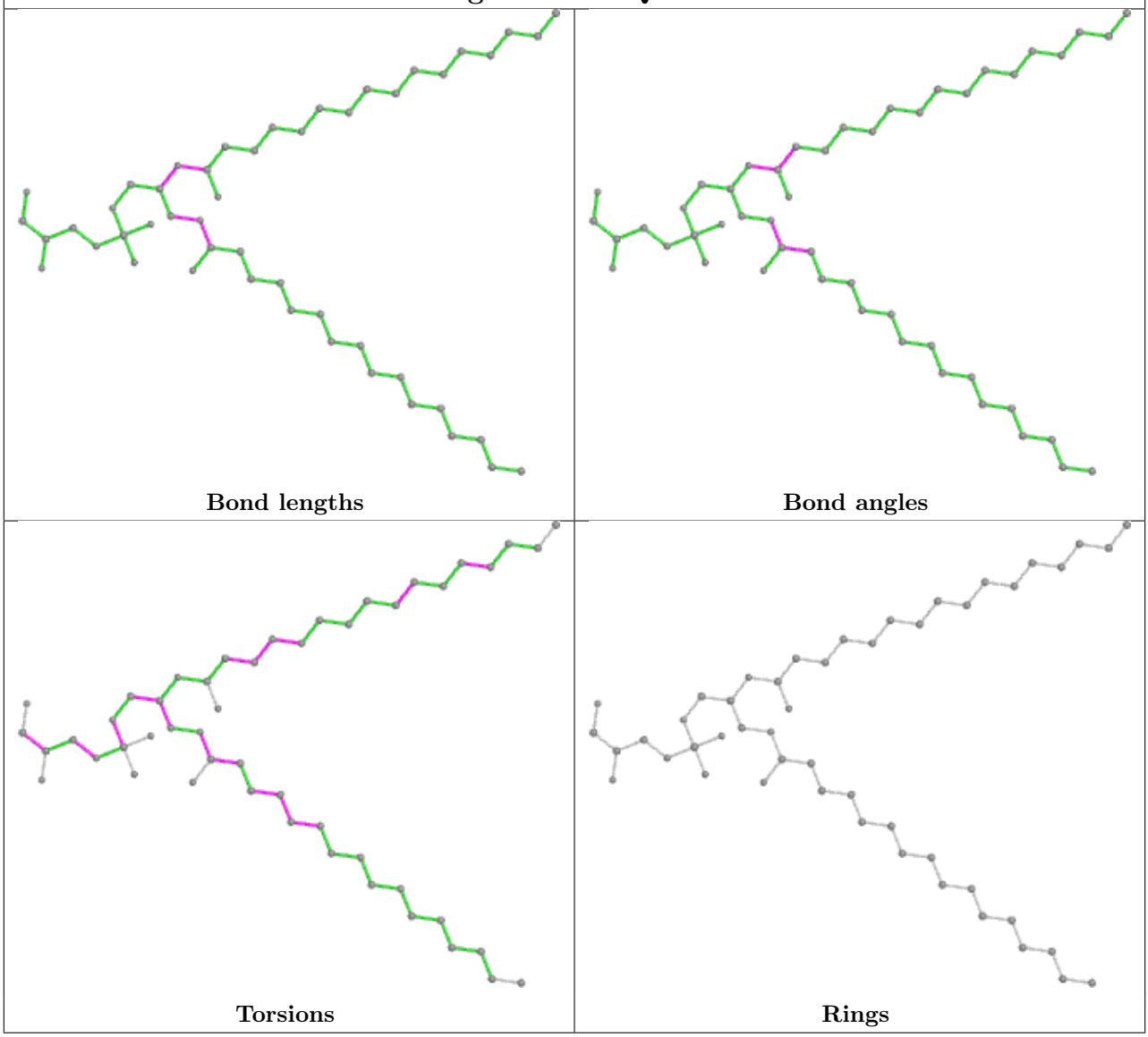


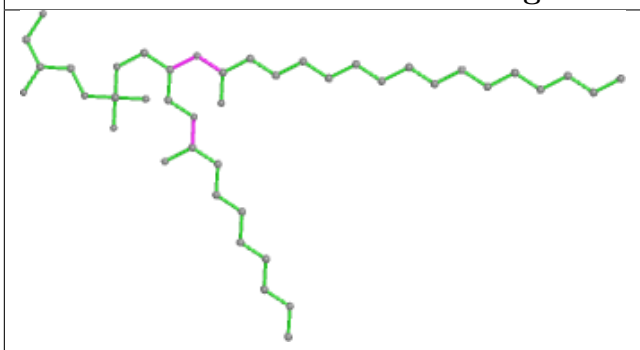
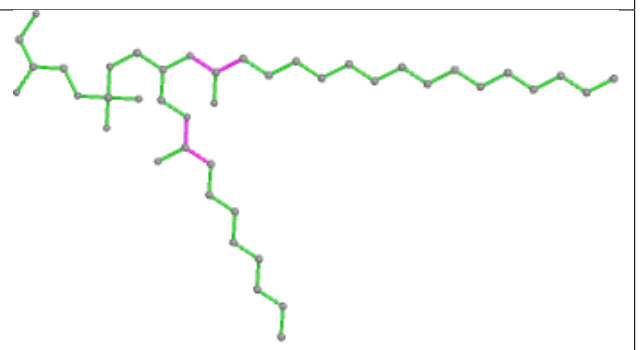
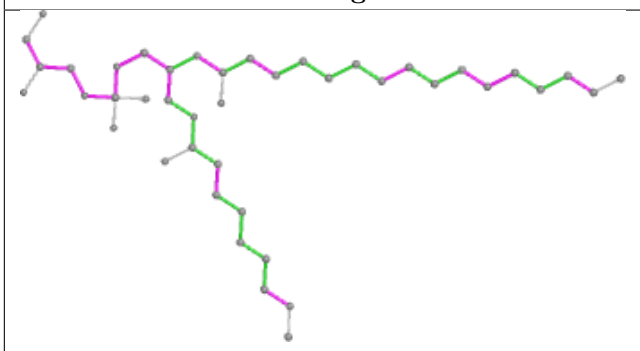
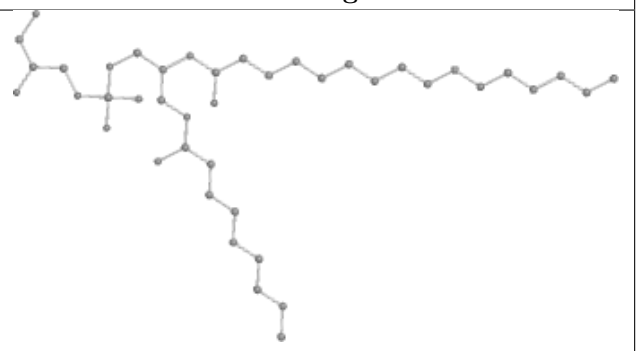
Rings

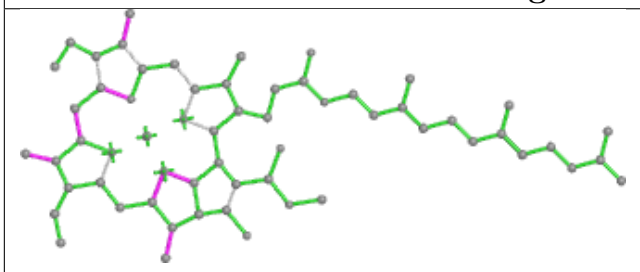
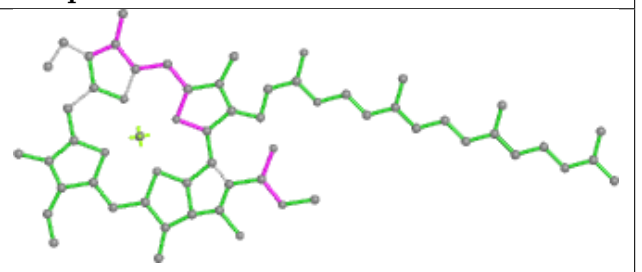
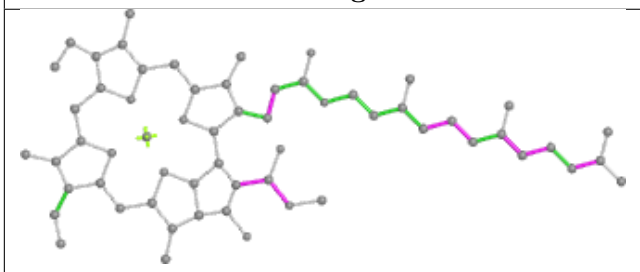
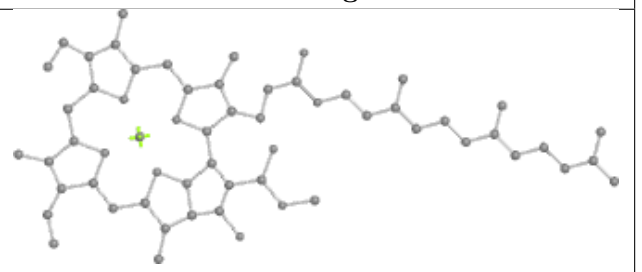
Ligand LUT V 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

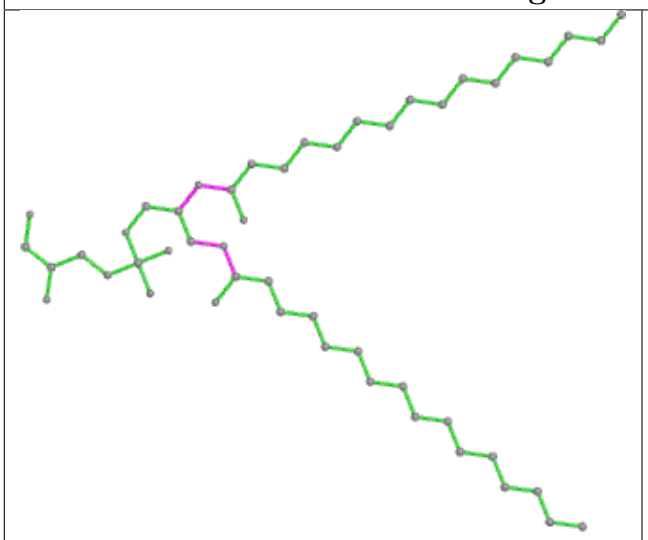
Ligand LHG Q 310



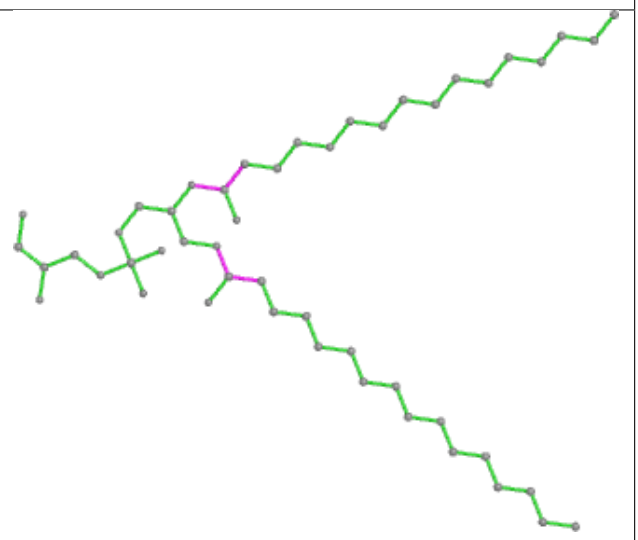
Ligand LHG R 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

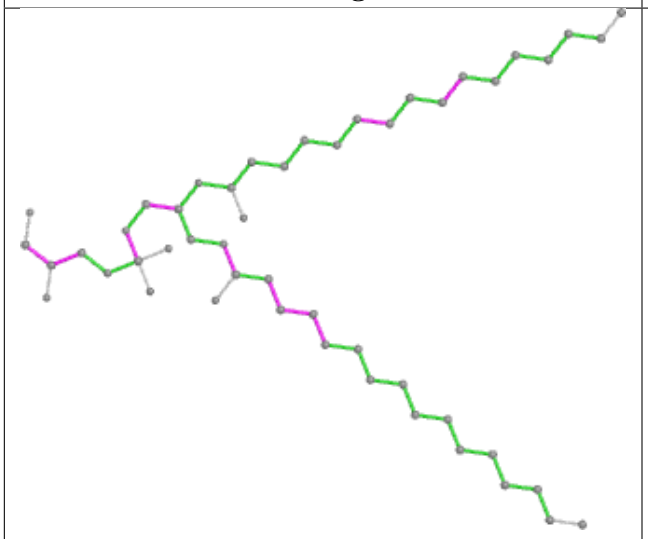
Ligand LHG c 521



Bond lengths



Bond angles



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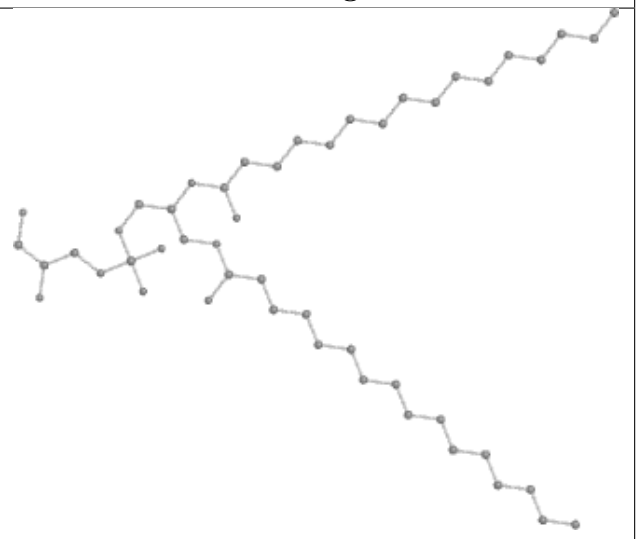
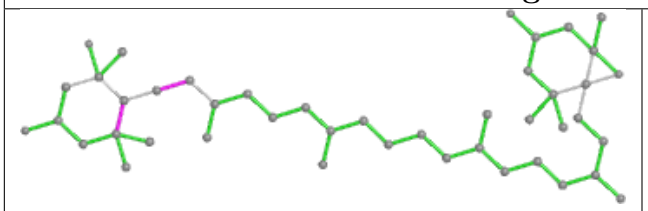


Rings

Ligand NEX R 301



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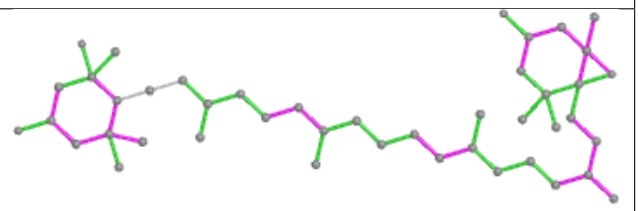

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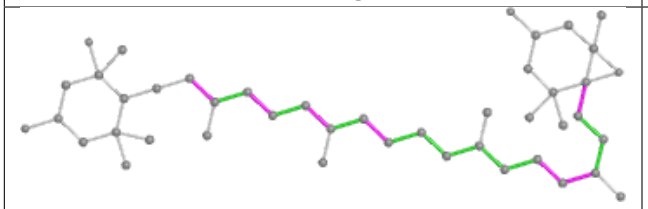
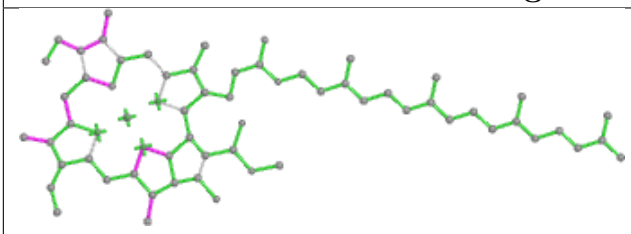
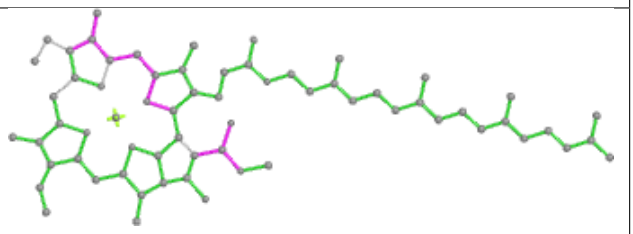
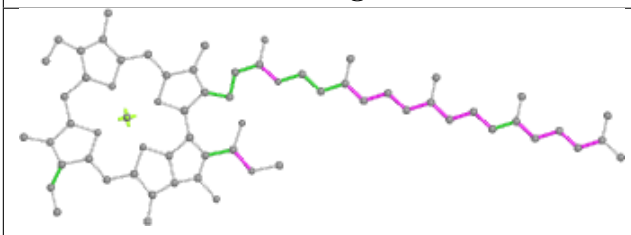
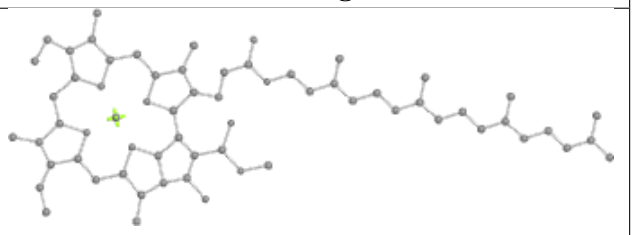


Torsions

Rings

Ligand CLA C 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

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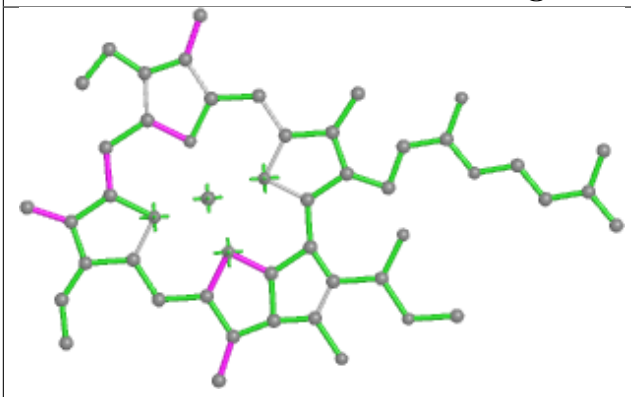
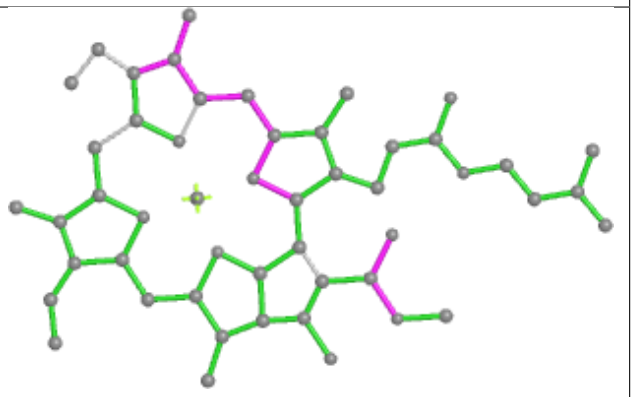
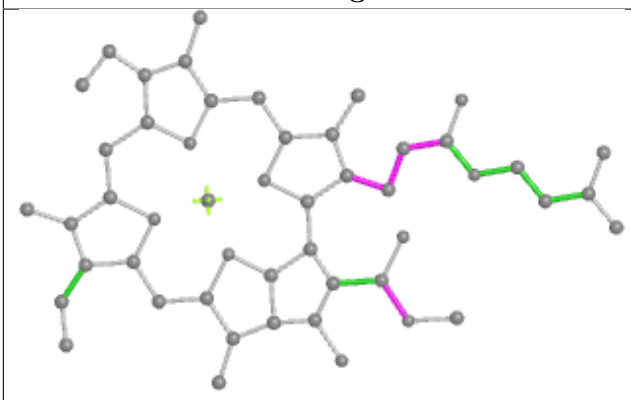
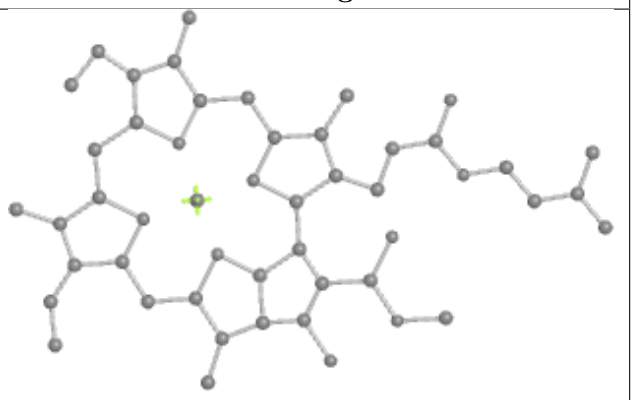
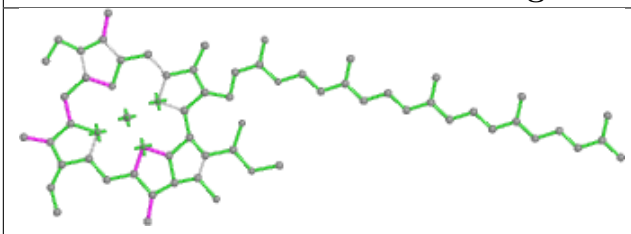
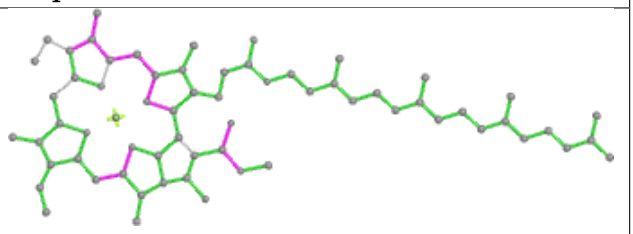
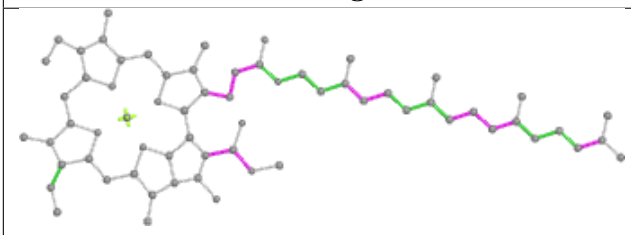
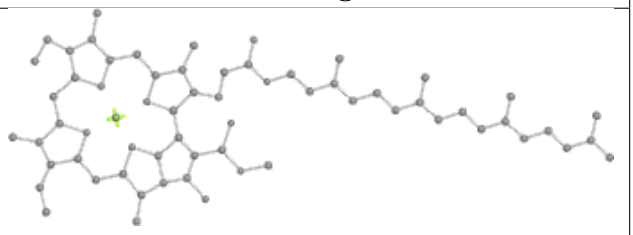
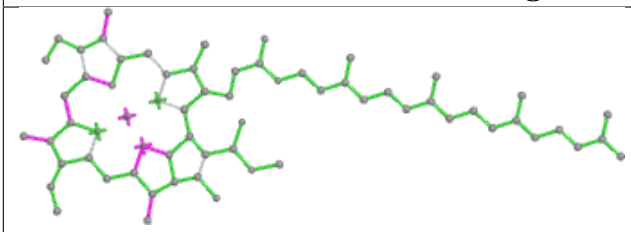
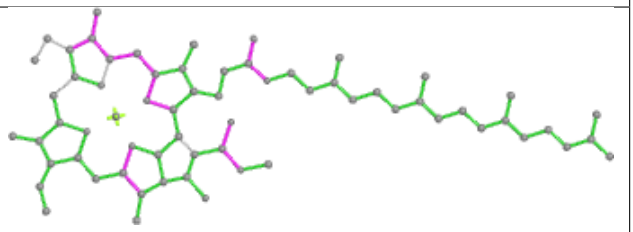
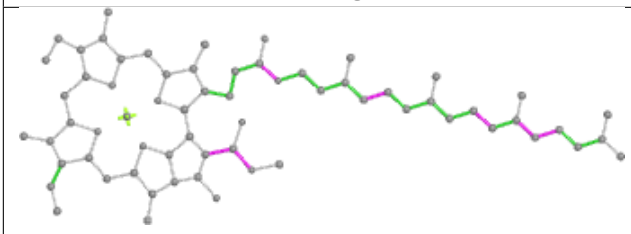
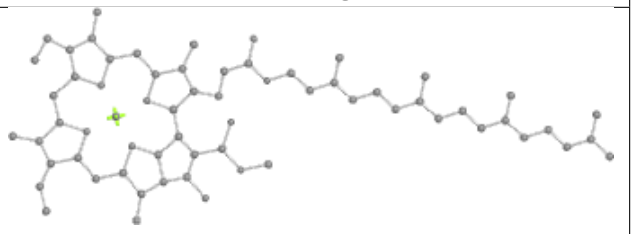
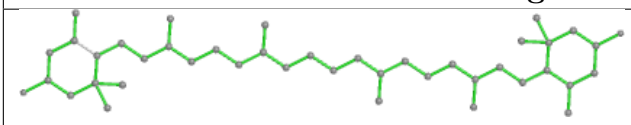
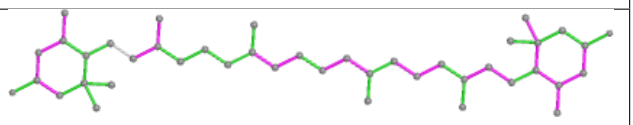
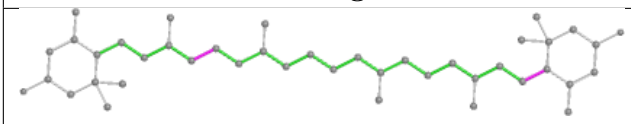
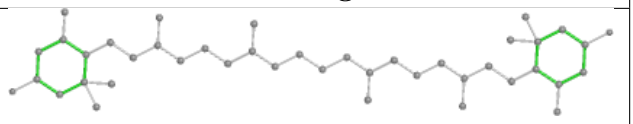
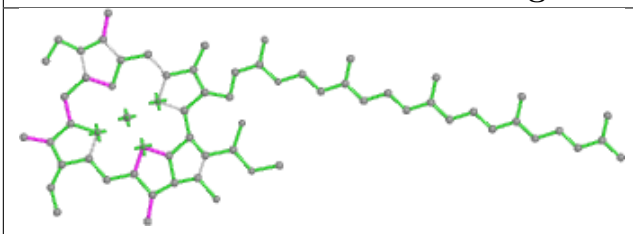
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT u 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 301



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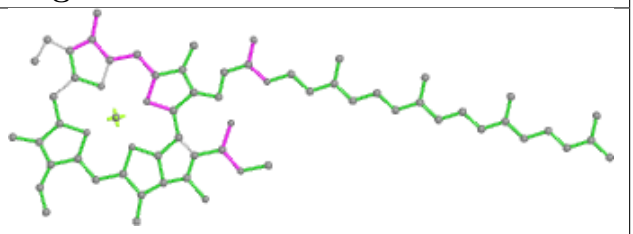
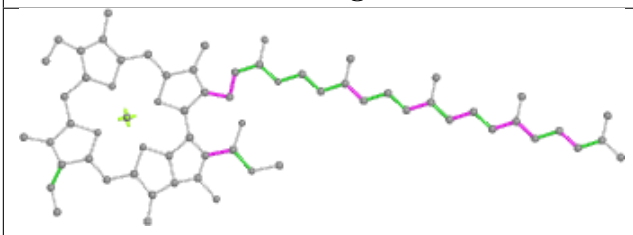
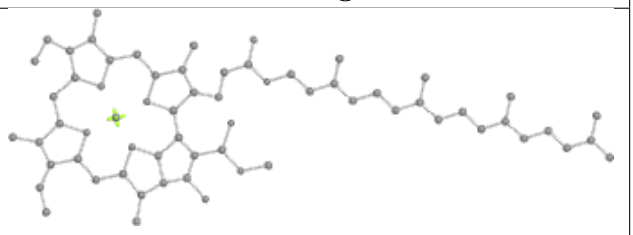


Bond angles

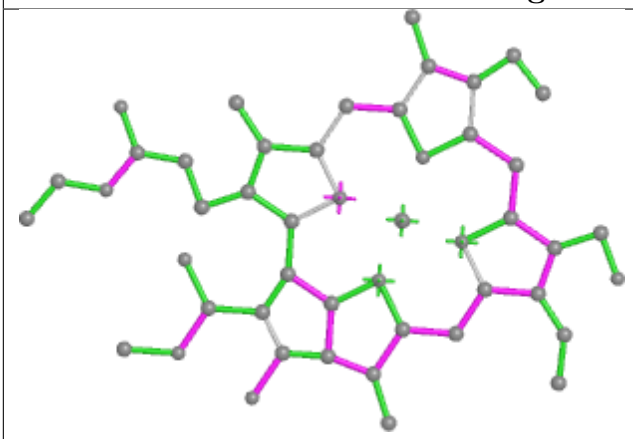


Torsions



Rings

Ligand CHL 3 312



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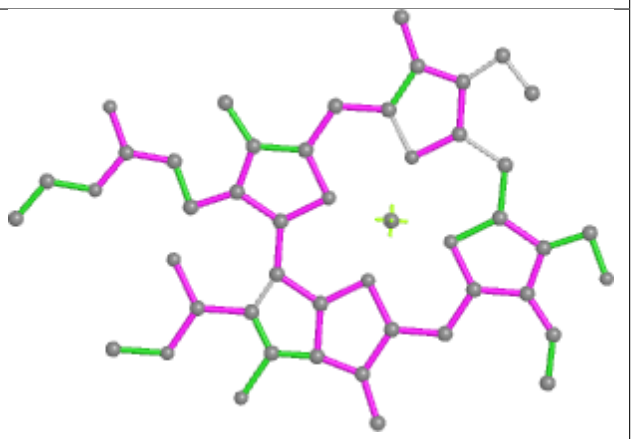

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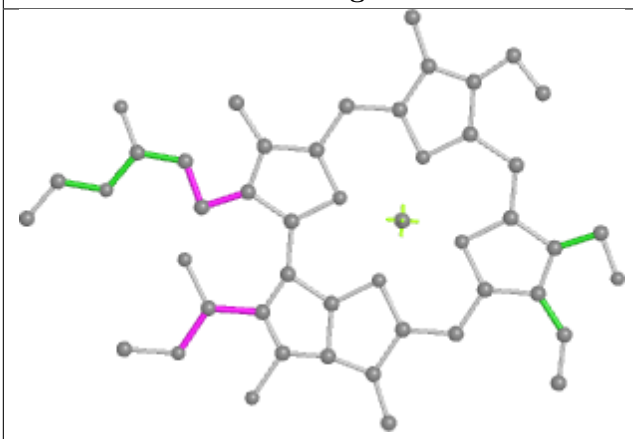

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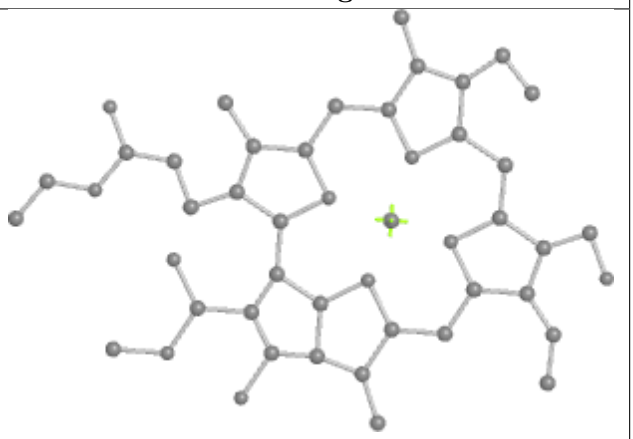
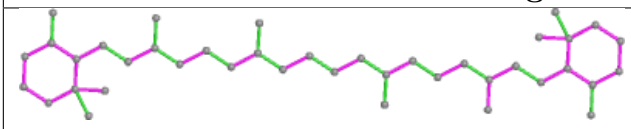
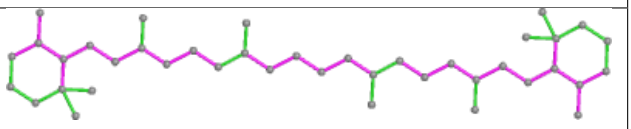
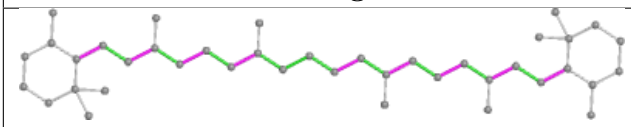
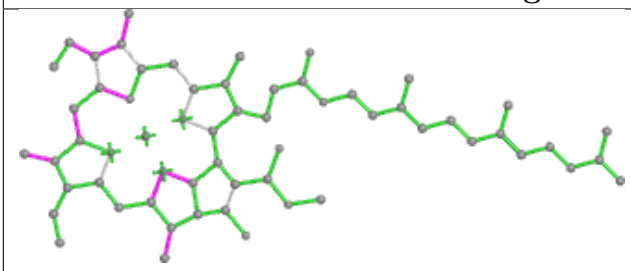
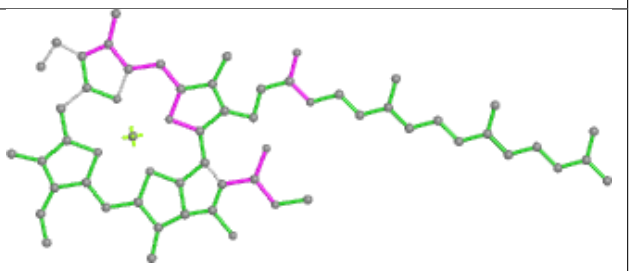
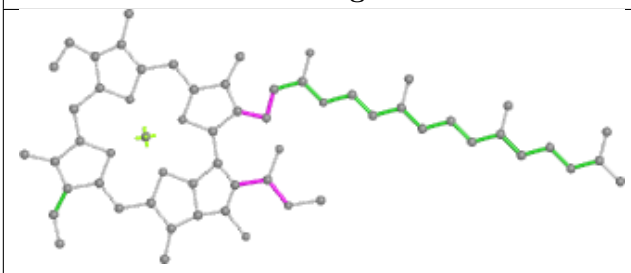
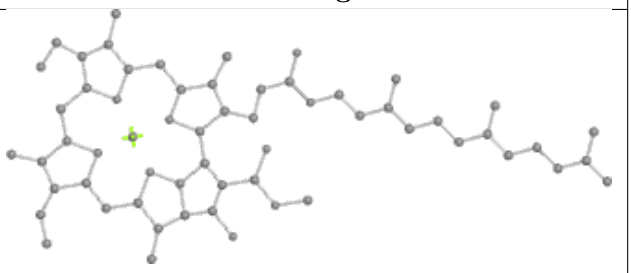
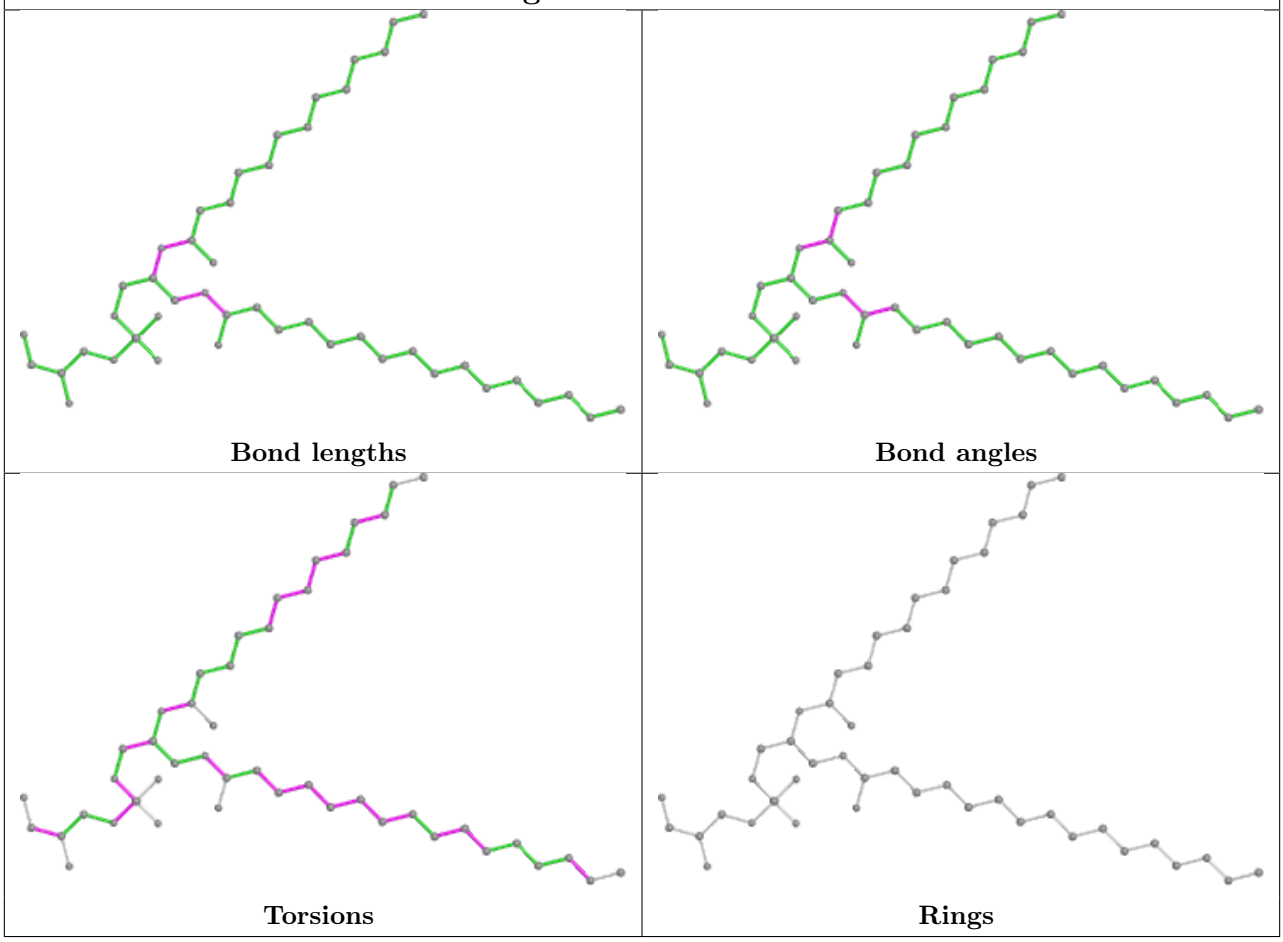


Rings

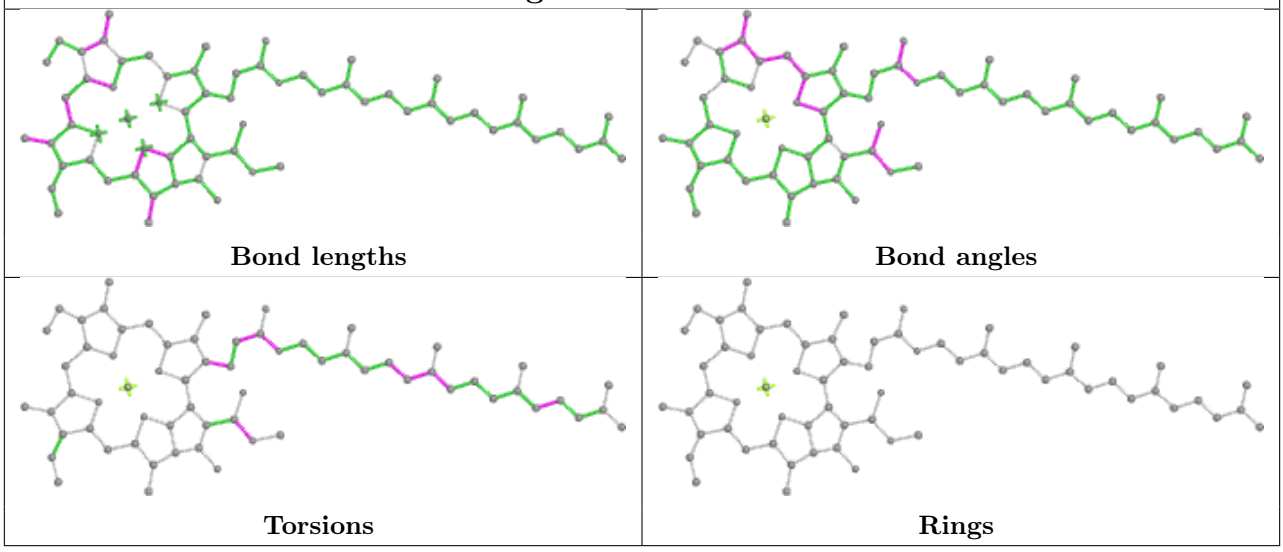
Ligand BCR k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

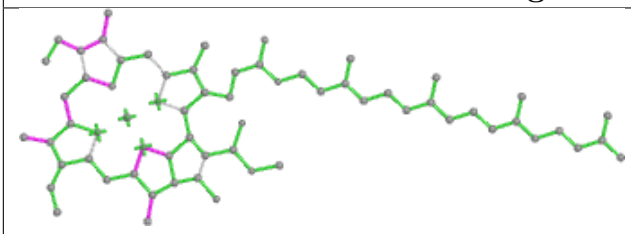
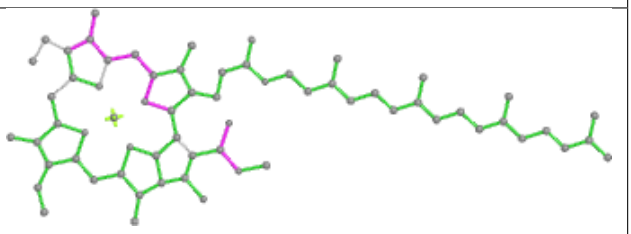
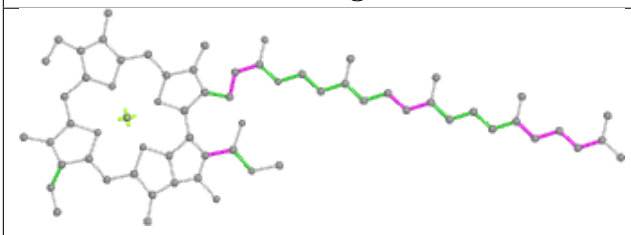
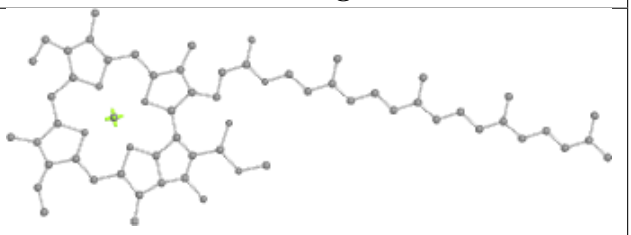
Ligand CLA U 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

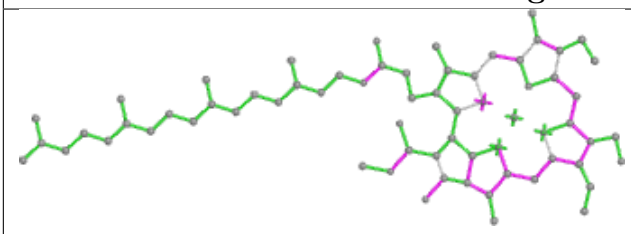
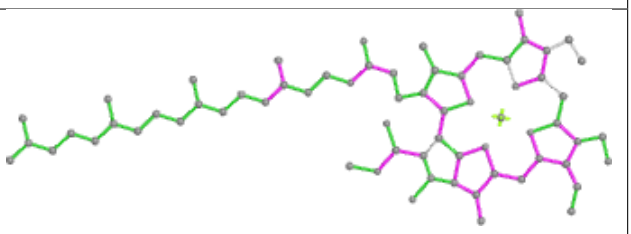
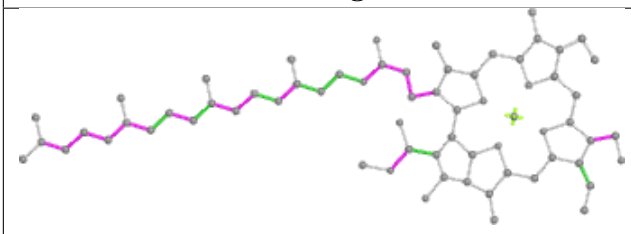
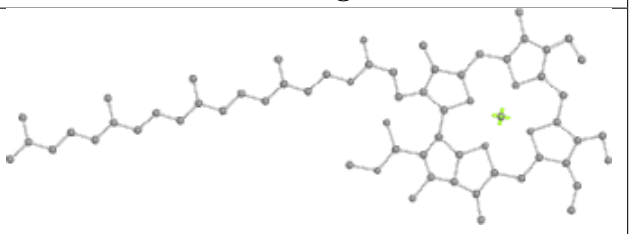
Ligand LHG D 406



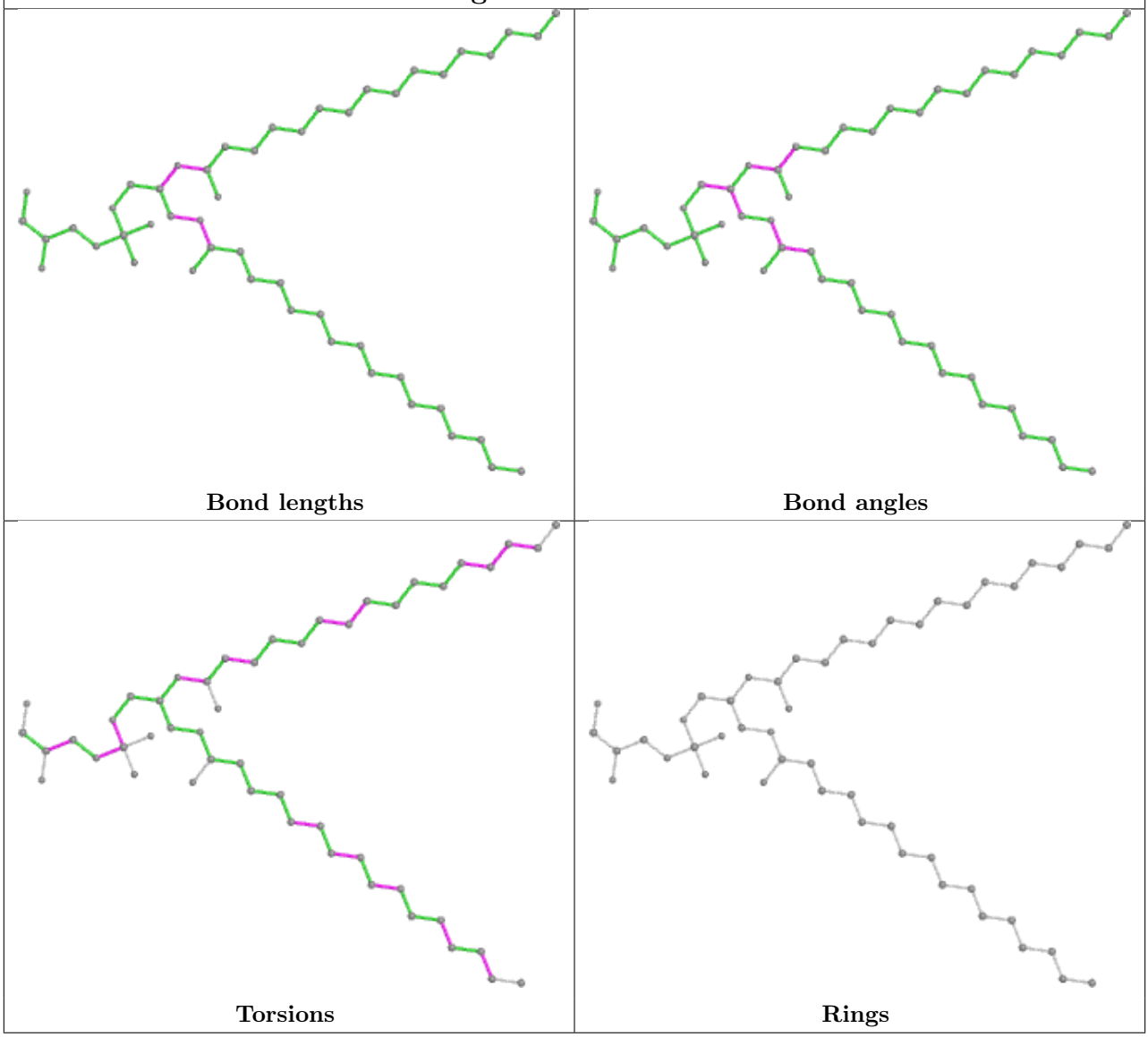
Ligand CLA P 303

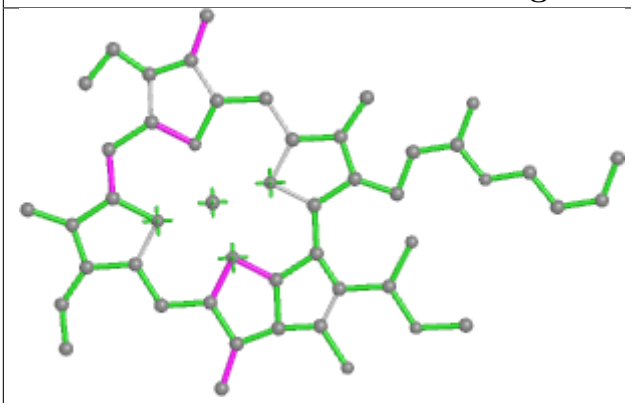
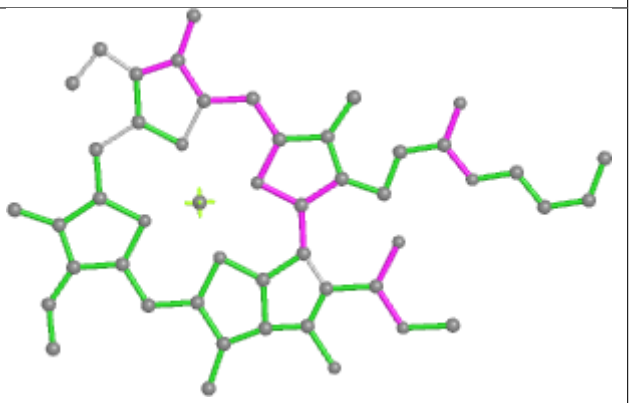
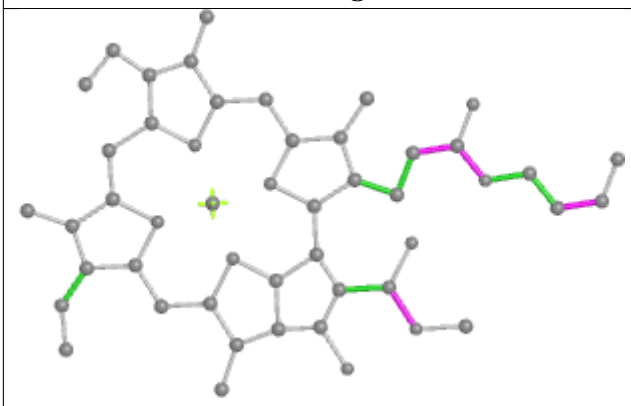
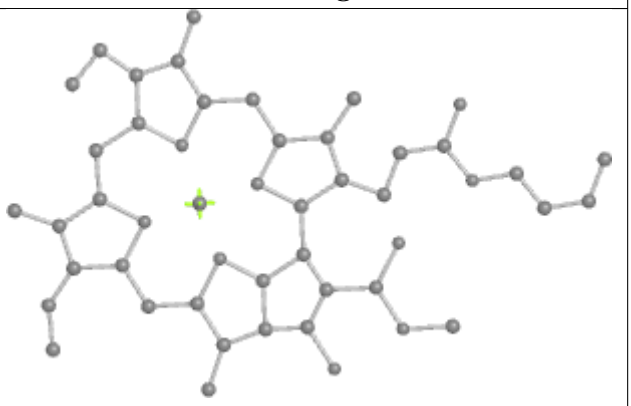


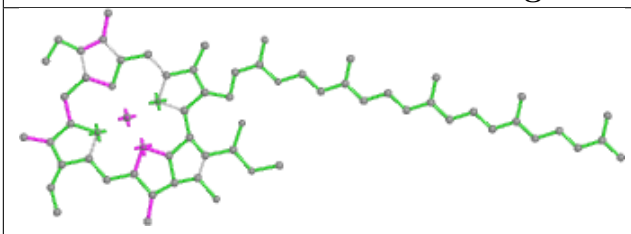
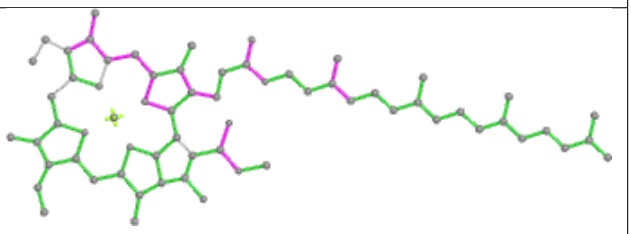
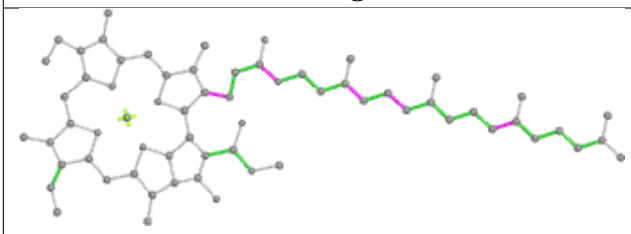
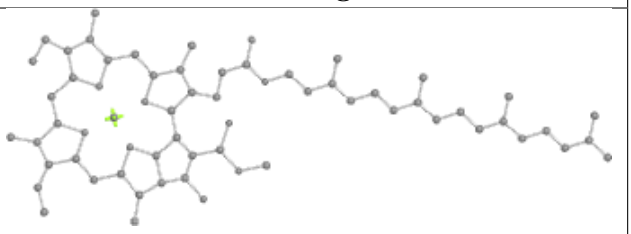
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

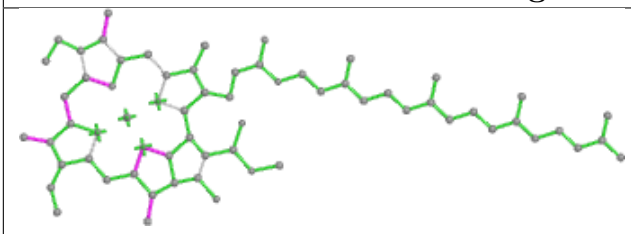
Ligand LHG d 406



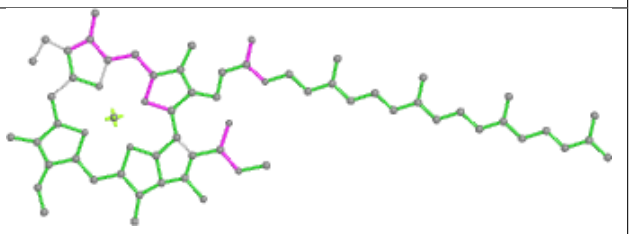
Ligand CLA r 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

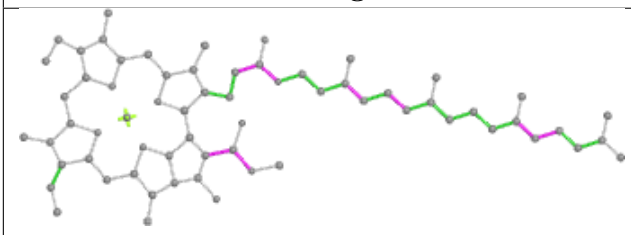
Ligand CLA 4 302



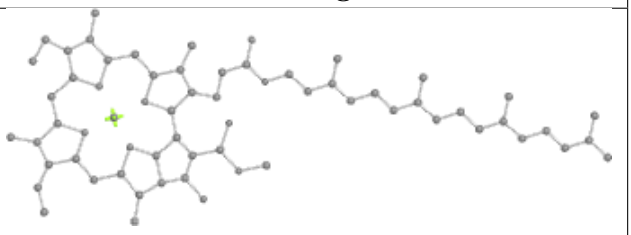
Bond lengths



Bond angles

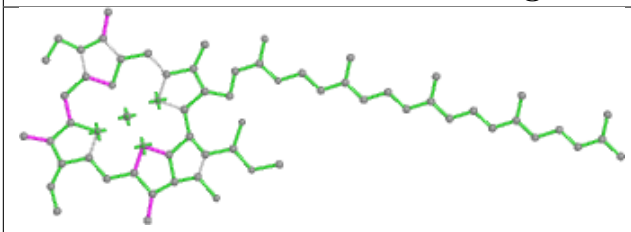


Torsions

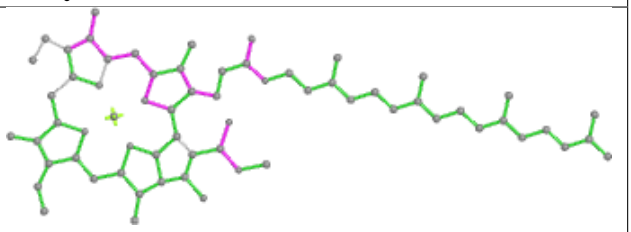


Rings

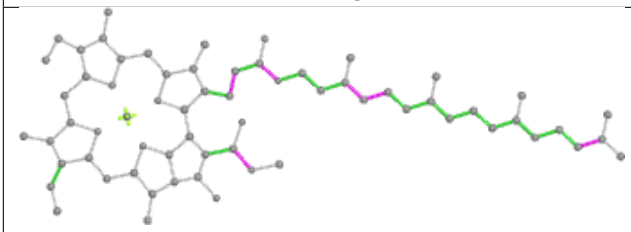
Ligand CLA Q 307



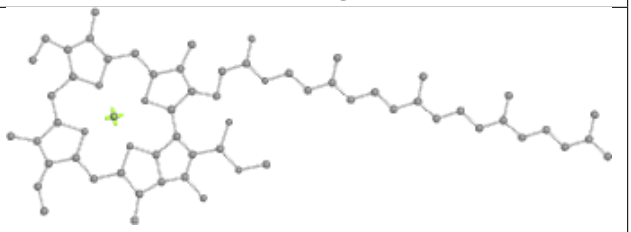
Bond lengths



Bond angles

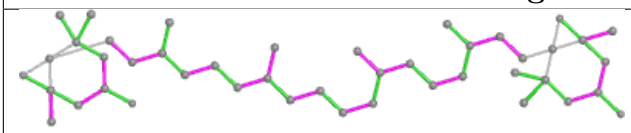


Torsions

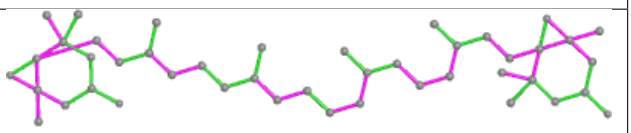


Rings

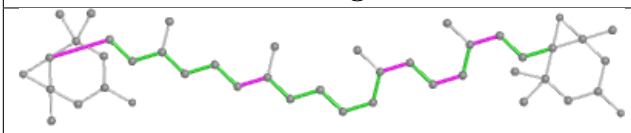
Ligand XAT 6 310



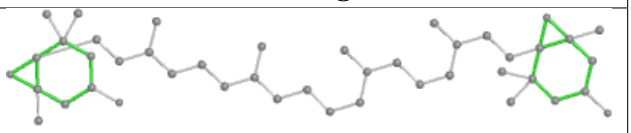
Bond lengths



Bond angles

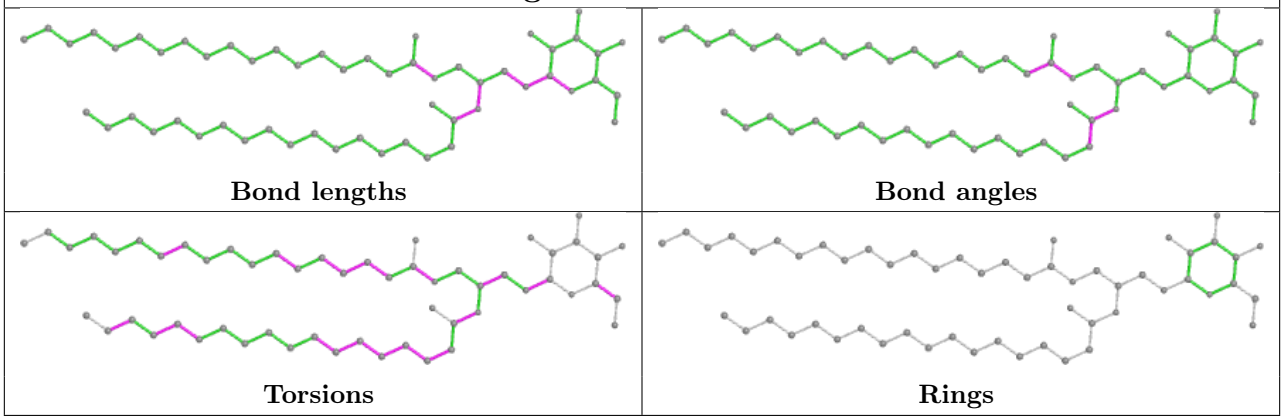


Torsions

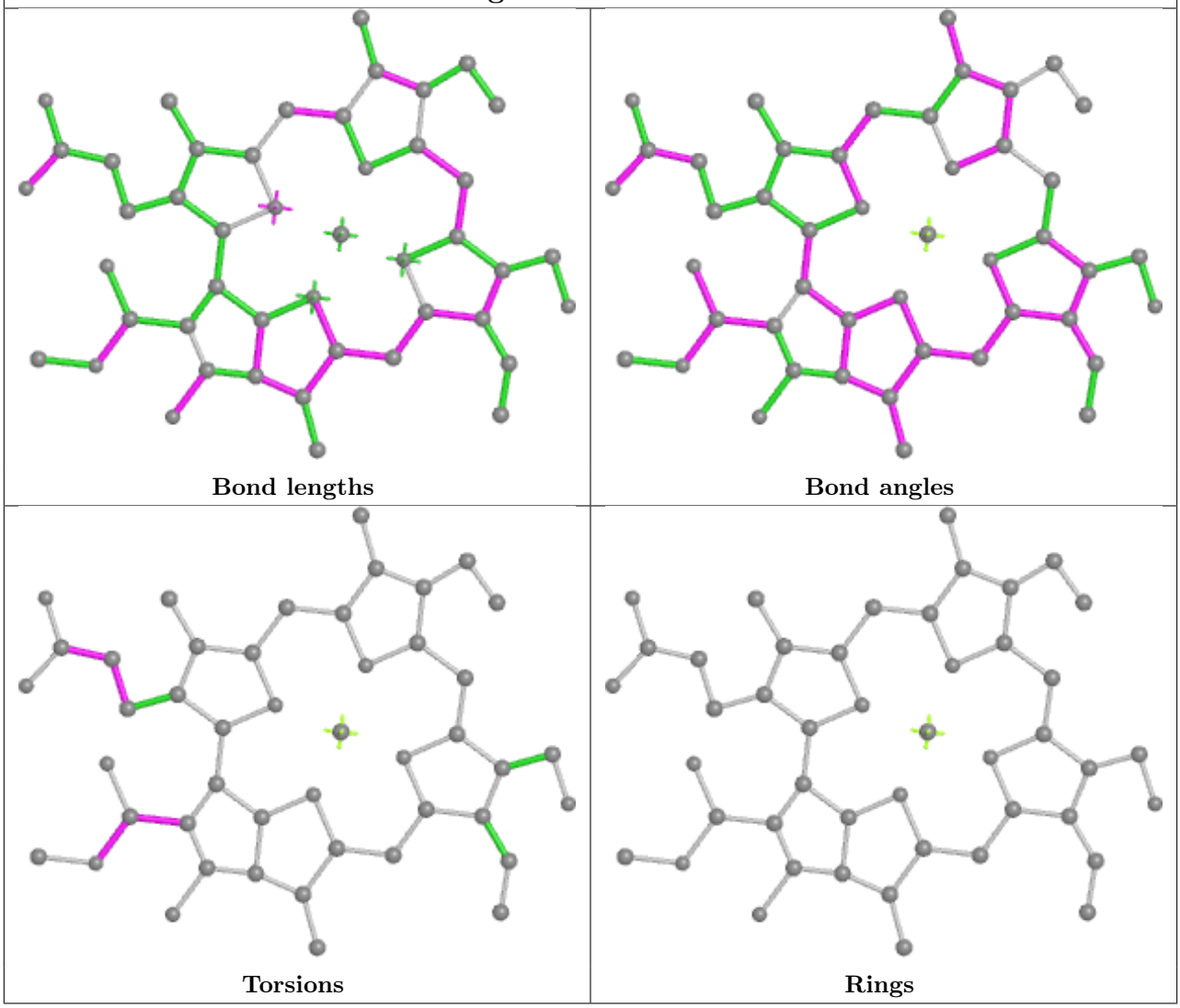


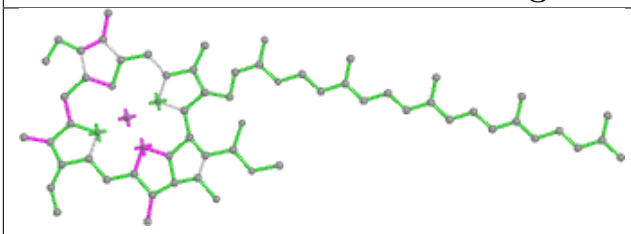
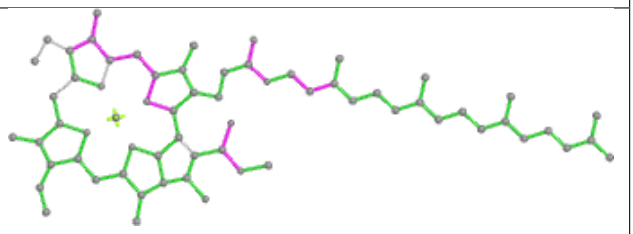
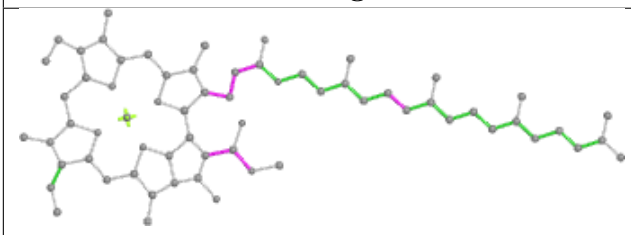
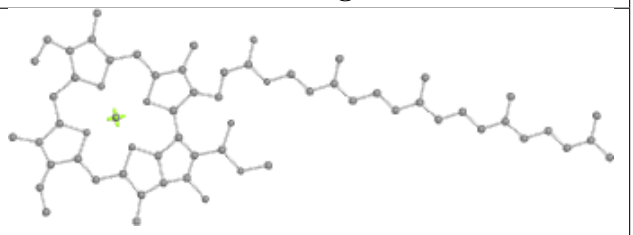
Rings

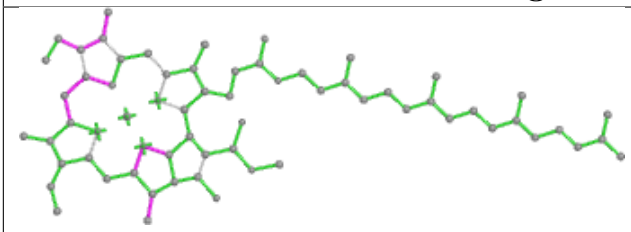
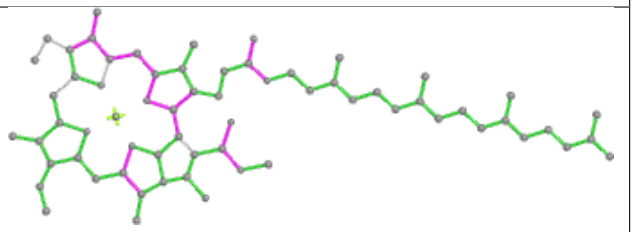
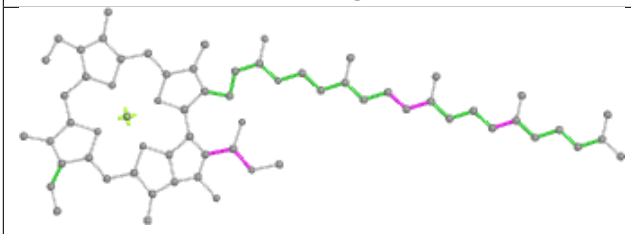
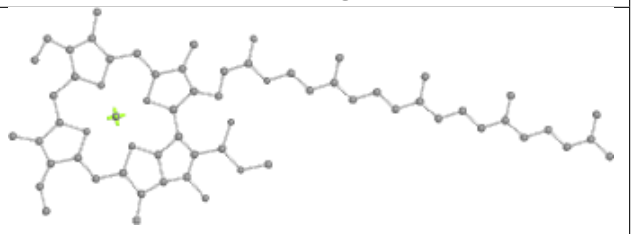
Ligand LMG b 624



Ligand CHL s 314



Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

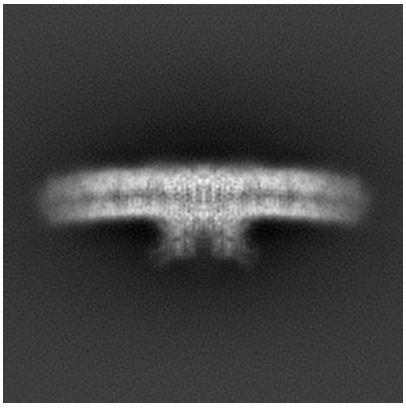
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9957. These allow visual inspection of the internal detail of the map and identification of artifacts.

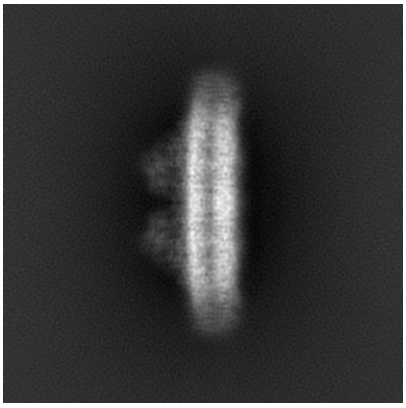
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

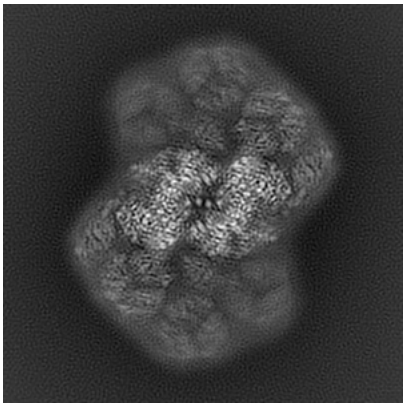
6.1.1 Primary map



X



Y

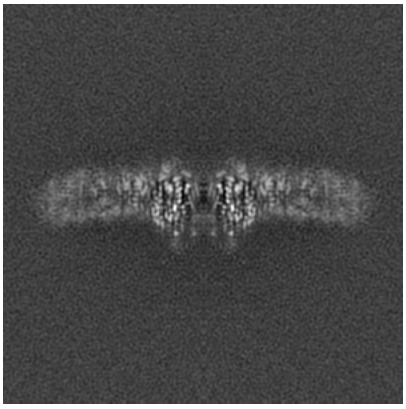


Z

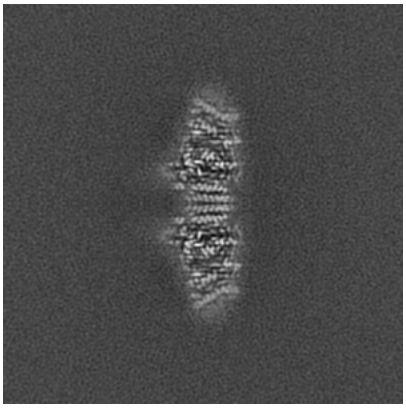
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

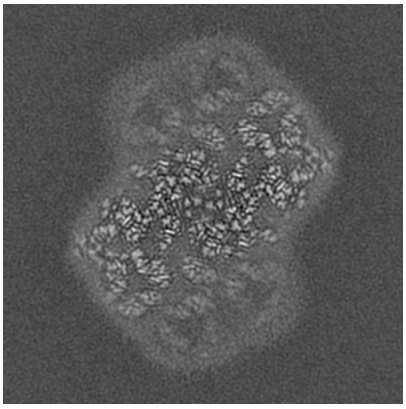
6.2.1 Primary map



X Index: 150



Y Index: 150

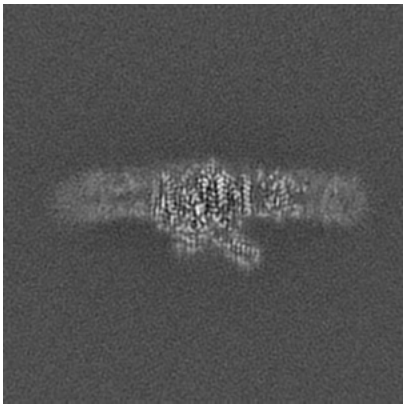


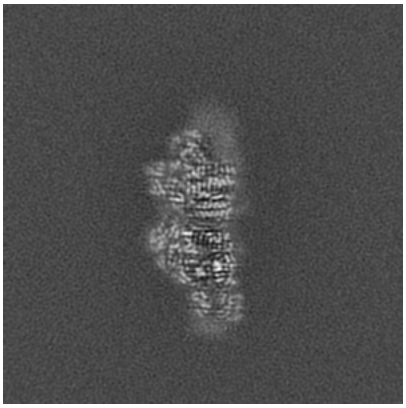
Z Index: 150

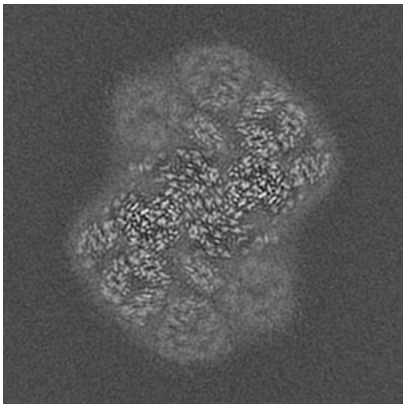
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 180

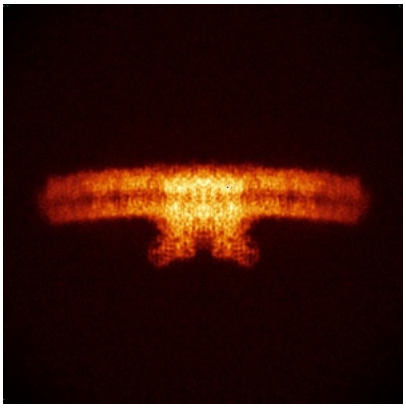

Y Index: 131

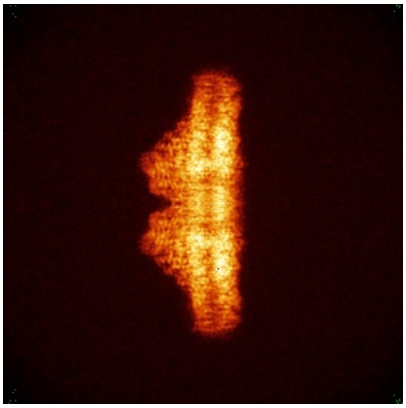

Z Index: 164

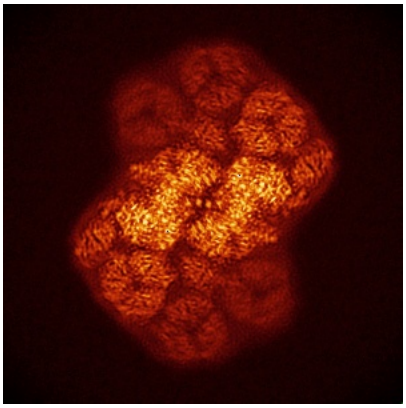
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

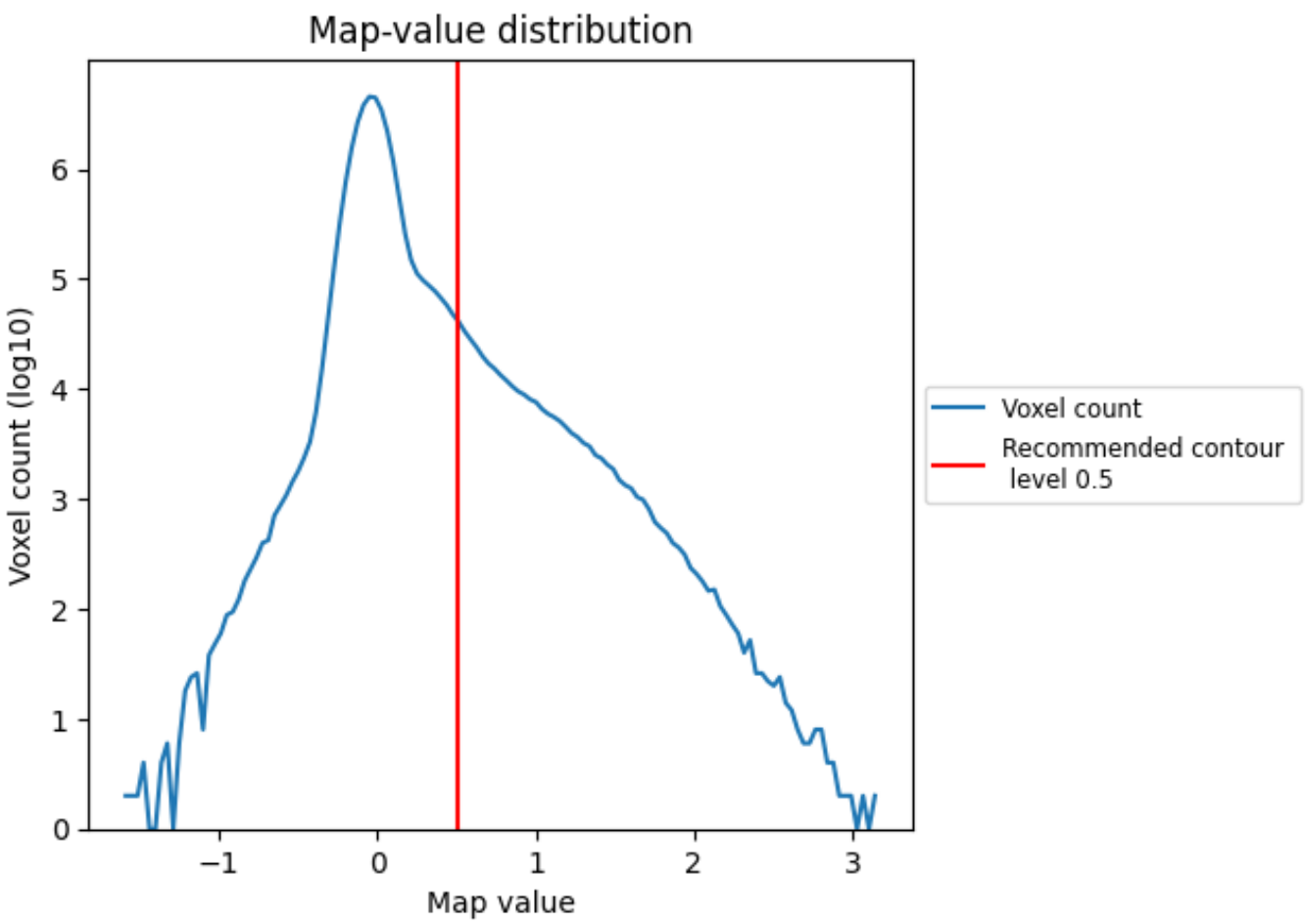
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

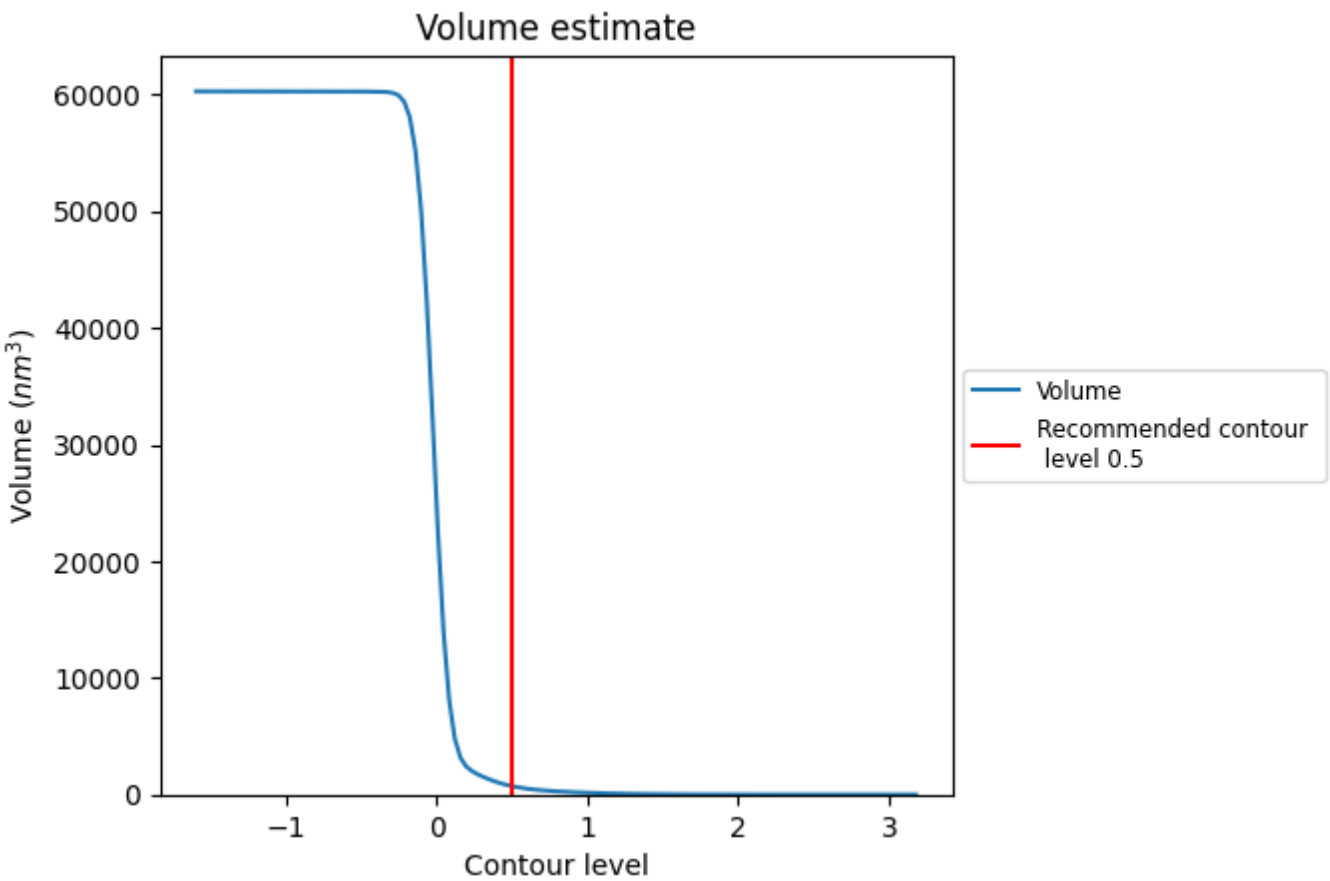
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

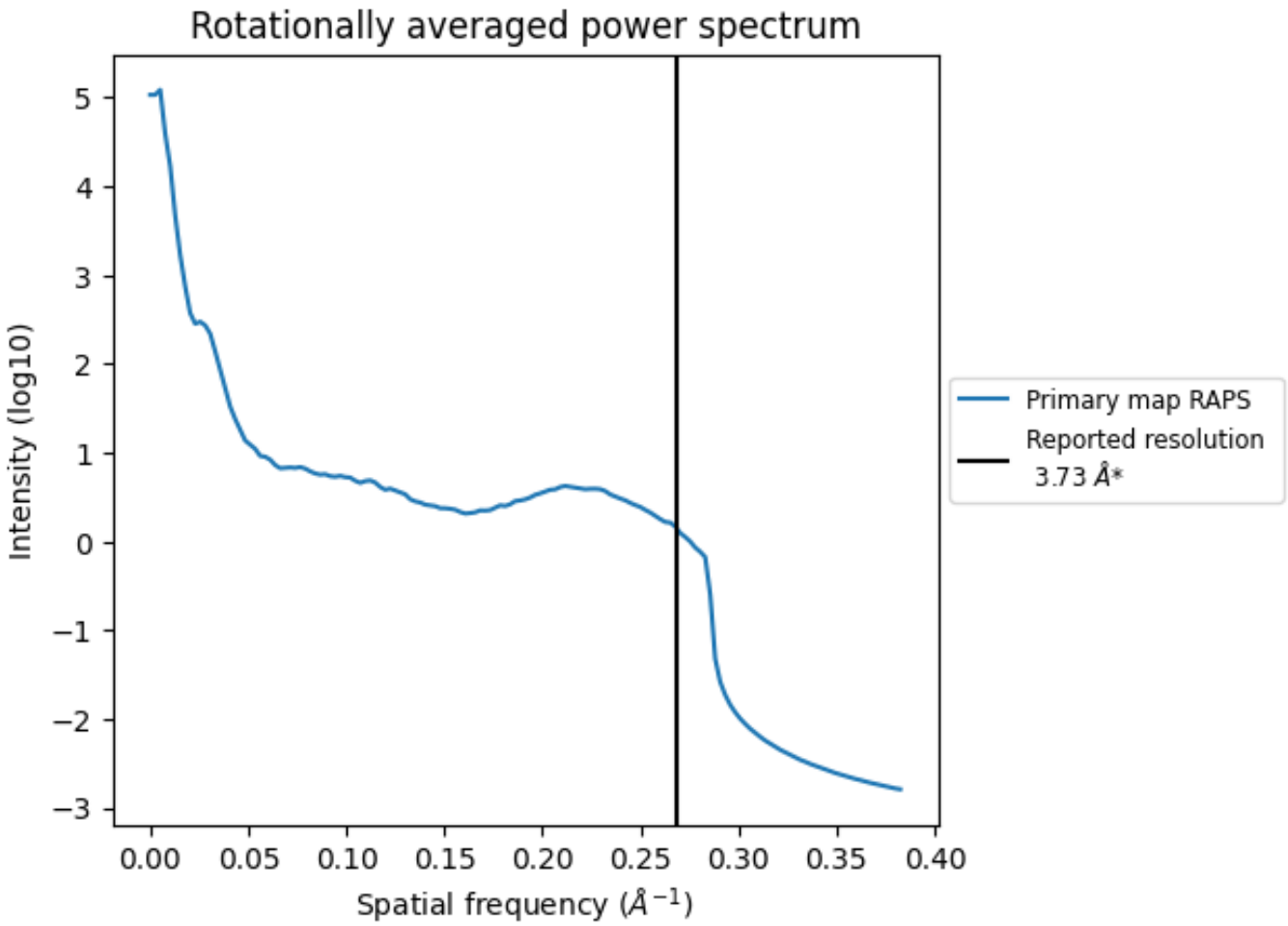
7.2 Volume estimate (i)



The volume at the recommended contour level is 727 nm^3; this corresponds to an approximate mass of 657 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.268 Å^{-1}

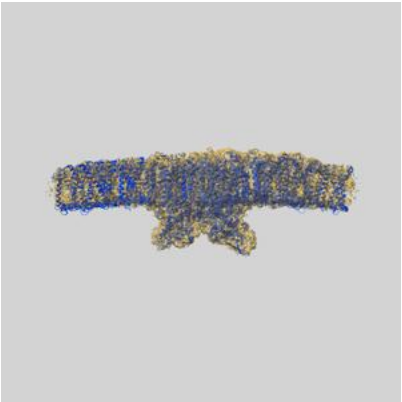
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

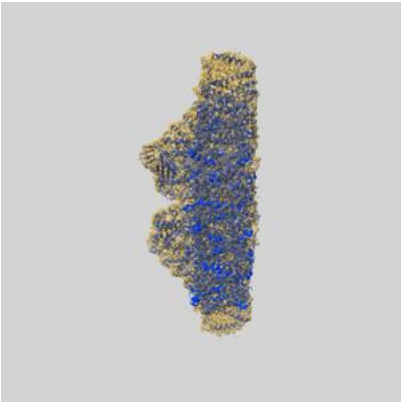
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9957 and PDB model 6KAF. Per-residue inclusion information can be found in section 3 on page 53.

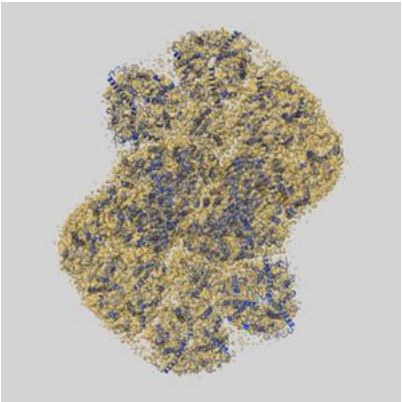
9.1 Map-model overlay (i)



X



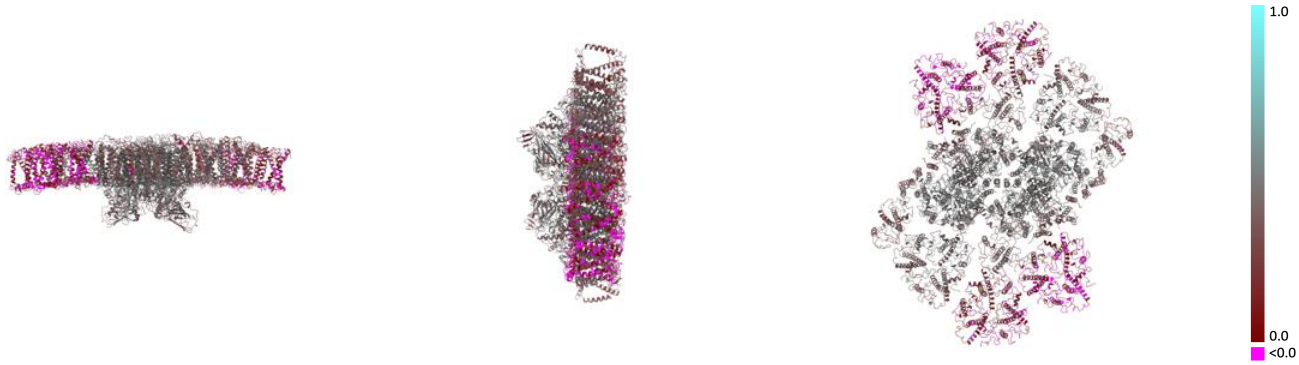
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

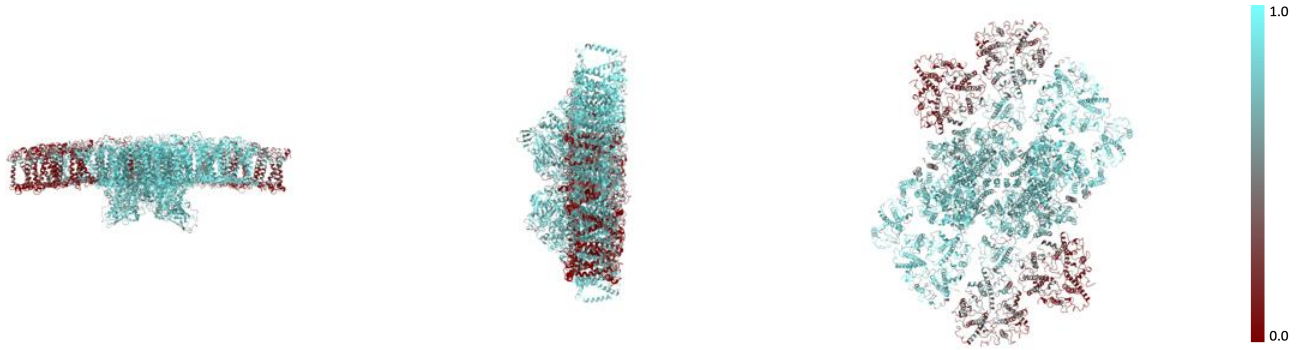
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

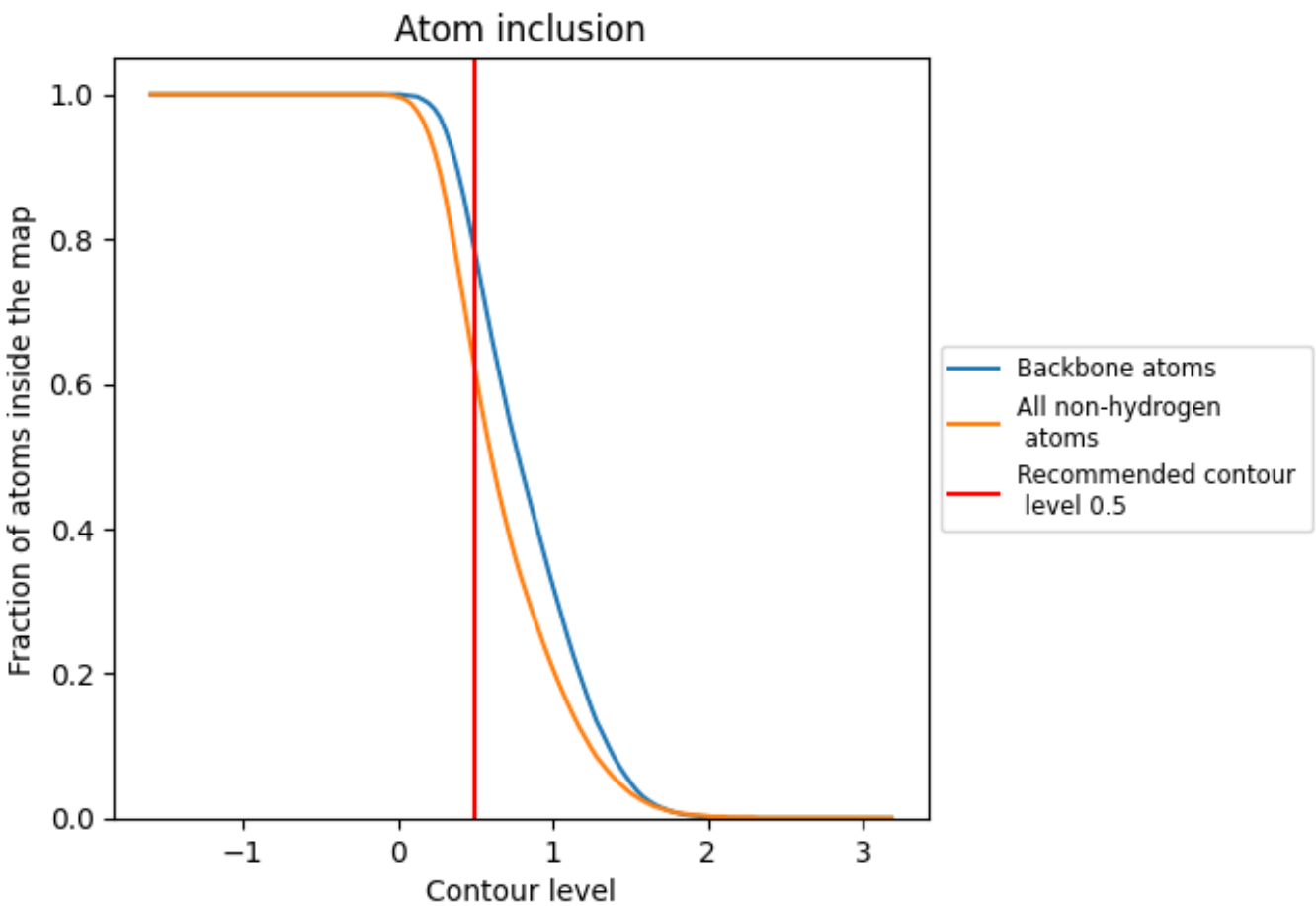
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6150	0.3260
1	0.4690	0.2180
2	0.2680	0.1130
3	0.2680	0.1030
4	0.4800	0.2330
5	0.2690	0.1100
6	0.2770	0.1120
A	0.8490	0.4710
B	0.7780	0.4420
C	0.8260	0.4680
D	0.8310	0.4580
E	0.7560	0.3920
F	0.7560	0.3190
G	0.7130	0.3870
H	0.8090	0.4290
I	0.9010	0.4840
J	0.4170	0.2730
K	0.8150	0.4280
L	0.7390	0.4530
M	0.7010	0.4110
N	0.7720	0.4060
O	0.7120	0.3810
P	0.2560	0.0890
Q	0.1050	0.0300
R	0.6320	0.3760
S	0.7690	0.3680
T	0.6880	0.4350
U	0.7830	0.4490
V	0.2130	0.0700
W	0.7840	0.4360
X	0.6850	0.3900
Y	0.6120	0.3520
Z	0.7730	0.3730
a	0.8460	0.4710
b	0.7770	0.4400

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Chain	Atom inclusion	Q-score
c	0.8220	0.4660
d	0.8320	0.4570
e	0.7540	0.3870
f	0.7600	0.3190
g	0.7080	0.3760
h	0.8160	0.4260
i	0.9010	0.4870
j	0.4120	0.2370
k	0.8150	0.4320
l	0.7360	0.4490
m	0.7010	0.4070
n	0.7640	0.3960
o	0.7120	0.3830
p	0.2400	0.0800
q	0.1080	0.0270
r	0.6390	0.3800
s	0.7680	0.3660
t	0.6880	0.4350
u	0.7850	0.4490
v	0.2150	0.0810
w	0.7790	0.4330
x	0.6850	0.3930
y	0.6120	0.3550
z	0.7630	0.3830