Full wwPDB EM Validation Report

May 11, 2025 – 08:37 AM JST

PDB ID	:	9IS4 / pdb_00009is4
EMDB ID	:	EMD-60830
Title	:	Cryo-EM structure of a TEF30-associated intermediate C2S-type PSII-LHCII supercomplex from Chlamydomonas reinhardtii
Authors	:	Wang, Y.; Wang, C.; Li, A.; Liu, Z.
Deposited on	:	2024-07-16
Resolution	:	2.90 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 ⓘ 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 ⓘ) were used in the production of this report:

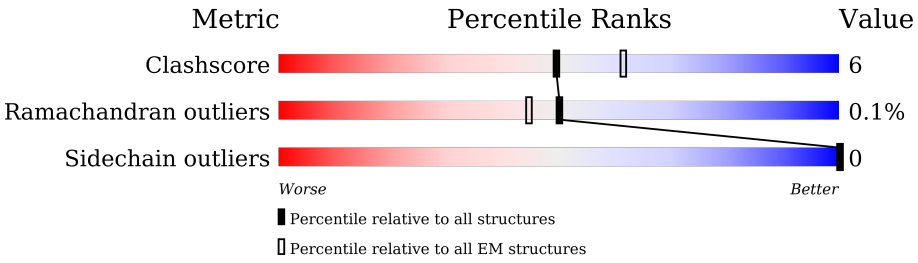
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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.



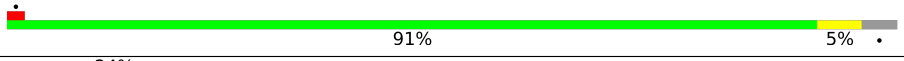
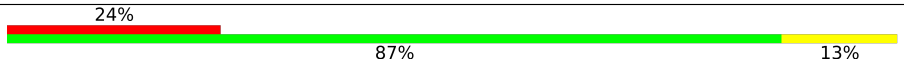
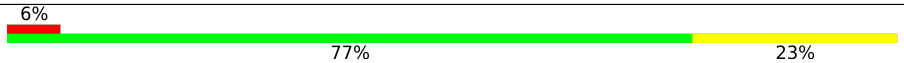
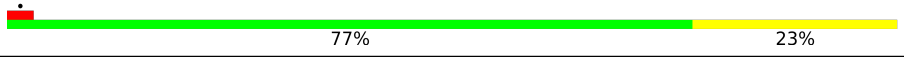
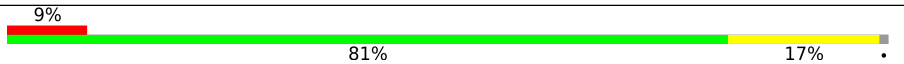
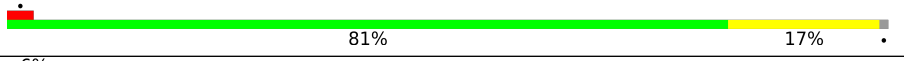
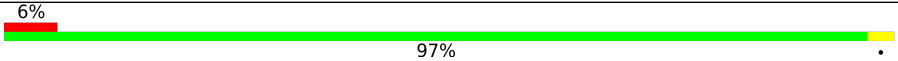
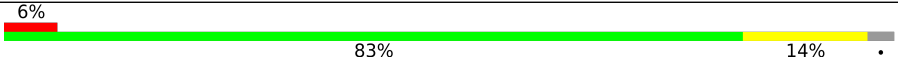
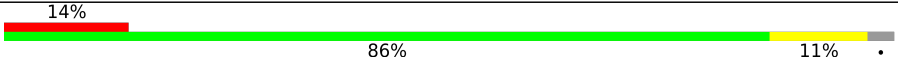
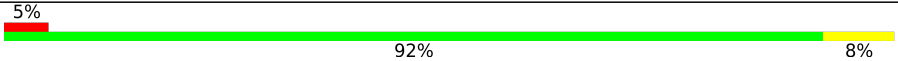
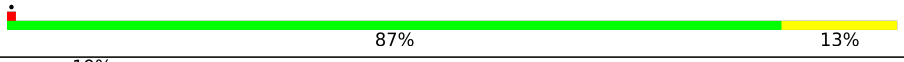
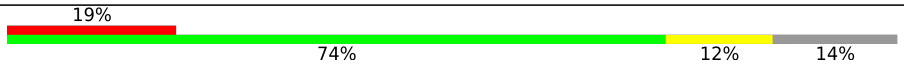
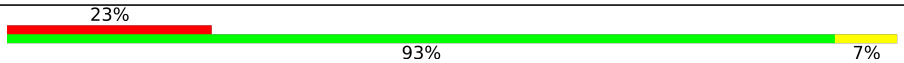
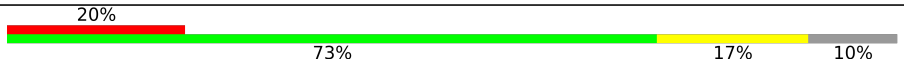
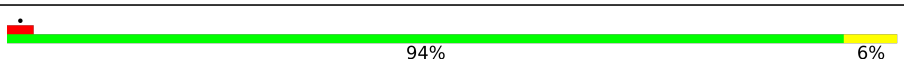
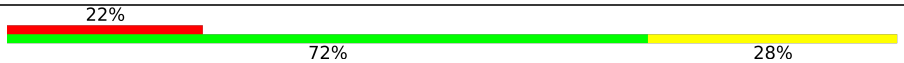
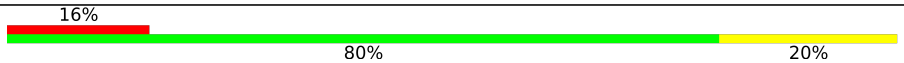
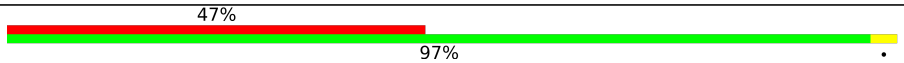
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	159	12% 84% 16%
2	A	335	7% 80% 14% 6%
2	a	335	82% 9% 9%
3	B	481	93% 7%
3	b	481	89% 11%
4	C	449	90% 10%
4	c	449	88% 10%
5	D	351	5% 91% 8%

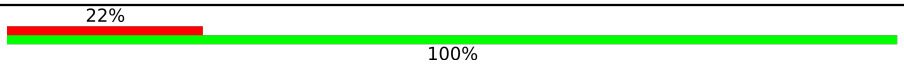
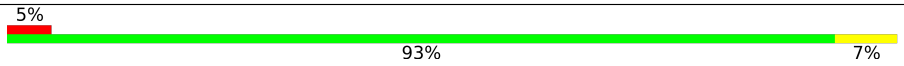
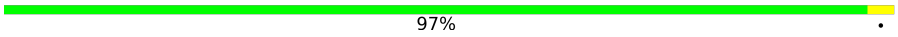
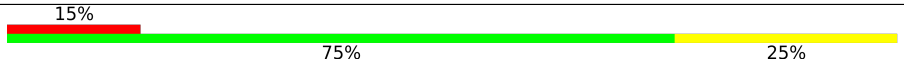
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	d	351	
6	E	75	
6	e	75	
7	F	31	
7	f	31	
8	G	219	
9	H	69	
9	h	69	
10	I	35	
10	i	35	
11	K	37	
11	k	37	
12	L	37	
12	l	37	
13	M	31	
13	m	31	
14	N	219	
15	O	240	
16	S	250	
17	T	30	
17	t	30	
18	V	32	
18	v	32	
19	W	56	
20	X	32	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
20	x	32	
21	Y	220	
22	Z	61	
22	z	61	
23	r	201	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	402	X	-	-	-
25	CLA	A	403	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	B	501	X	-	-	-
25	CLA	B	502	X	-	-	-
25	CLA	B	503	X	-	-	-
25	CLA	B	504	X	-	-	-
25	CLA	B	505	X	-	-	-
25	CLA	B	506	X	-	-	-
25	CLA	B	507	X	-	-	-
25	CLA	B	508	X	-	-	-
25	CLA	B	509	X	-	-	-
25	CLA	B	510	X	-	-	-
25	CLA	B	511	X	-	-	-
25	CLA	B	512	X	-	-	-
25	CLA	B	513	X	-	-	-
25	CLA	B	514	X	-	-	-
25	CLA	B	515	X	-	-	-
25	CLA	B	516	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	604	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	613	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	303	X	-	-	-
25	CLA	N	304	X	-	-	-
25	CLA	N	305	X	-	-	-
25	CLA	N	311	X	-	-	-
25	CLA	N	312	X	-	-	-
25	CLA	N	313	X	-	-	-
25	CLA	N	314	X	-	-	-
25	CLA	N	315	X	-	-	-
25	CLA	S	602	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	605	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	613	X	-	-	-
25	CLA	S	614	X	-	-	-
25	CLA	Y	304	X	-	-	-
25	CLA	Y	305	X	-	-	-
25	CLA	Y	306	X	-	-	-
25	CLA	Y	311	X	-	-	-
25	CLA	Y	312	X	-	-	-
25	CLA	Y	313	X	-	-	-
25	CLA	Y	314	X	-	-	-
25	CLA	Y	315	X	-	-	-
25	CLA	a	402	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	a	403	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	b	501	X	-	-	-
25	CLA	b	502	X	-	-	-
25	CLA	b	503	X	-	-	-
25	CLA	b	504	X	-	-	-
25	CLA	b	505	X	-	-	-
25	CLA	b	506	X	-	-	-
25	CLA	b	507	X	-	-	-
25	CLA	b	508	X	-	-	-
25	CLA	b	509	X	-	-	-
25	CLA	b	510	X	-	-	-
25	CLA	b	511	X	-	-	-
25	CLA	b	512	X	-	-	-
25	CLA	b	513	X	-	-	-
25	CLA	b	514	X	-	-	-
25	CLA	b	515	X	-	-	-
25	CLA	b	516	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	r	301	X	-	-	-
25	CLA	r	302	X	-	-	-
25	CLA	r	303	X	-	-	-
25	CLA	r	307	X	-	-	-
25	CLA	r	308	X	-	-	-
33	BCT	a	409	-	-	X	-
36	CHL	G	601	X	-	-	-
36	CHL	G	605	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CHL	G	606	X	-	-	-
36	CHL	G	607	X	-	-	-
36	CHL	G	608	X	-	-	-
36	CHL	G	609	X	-	-	-
36	CHL	G	619	X	-	-	-
36	CHL	N	302	X	-	-	-
36	CHL	N	306	X	-	-	-
36	CHL	N	307	X	-	-	-
36	CHL	N	308	X	-	-	-
36	CHL	N	309	X	-	-	-
36	CHL	N	310	X	-	-	-
36	CHL	S	601	X	-	-	-
36	CHL	S	606	X	-	-	-
36	CHL	S	607	X	-	-	-
36	CHL	S	608	X	-	-	-
36	CHL	Y	303	X	-	-	-
36	CHL	Y	307	X	-	-	-
36	CHL	Y	308	X	-	-	-
36	CHL	Y	309	X	-	-	-
36	CHL	Y	310	X	-	-	-
36	CHL	r	304	X	-	-	-
36	CHL	r	305	X	-	-	-
36	CHL	r	306	X	-	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 55146 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 PDZ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	159	Total	C	N	O	S	0	0
			1285	803	231	245	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	315	Total	C	N	O	S	0	0
			2465	1620	407	423	15		
2	a	304	Total	C	N	O	S	0	0
			2375	1561	392	407	15		

- Molecule 3 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		
3	b	481	Total	C	N	O	S	0	0
			3763	2468	631	652	12		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		
4	c	438	Total	C	N	O	S	0	0
			3431	2249	571	594	17		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	337	Total 2686	C 1777	N 439	O 458	S 12	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	75	Total 610	C 399	N 101	O 110	0	0
6	e	71	Total 575	C 376	N 94	O 105	0	0

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total 251	C 171	N 42	O 37	S 1	0	0
7	f	31	Total 251	C 171	N 42	O 37	S 1	0	0

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	219	Total 1667	C 1082	N 272	O 308	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	68	Total 519	C 347	N 77	O 93	S 2	0	0
9	h	68	Total 519	C 346	N 77	O 94	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	35	Total 283	C 193	N 43	O 45	S 2	0	0
10	i	34	Total 275	C 189	N 41	O 43	S 2	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total 297	C 209	N 43	O 45	0	0
11	k	37	Total 296	C 209	N 43	O 44	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total 301	C 202	N 49	O 50	0	0
12	l	37	Total 306	C 205	N 50	O 51	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	30	Total 230	C 158	N 32	O 40	0	0
13	m	30	Total 232	C 158	N 33	O 41	0	0

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	219	Total 1672	C 1081	N 272	O 314	S 5	0	0

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	207	Total 1565	C 1001	N 246	O 314	S 4	0	0

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	250	Total 1894	C 1225	N 310	O 355	S 4	0	0

- Molecule 17 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		
17	t	27	Total	C	N	O	S	0	0
			220	154	30	35	1		

- Molecule 18 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	32	Total	C	N	O	0	0
			224	147	37	40		
18	v	32	Total	C	N	O	0	0
			224	147	37	40		

- Molecule 19 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	56	Total	C	N	O	S	0	0
			434	281	70	81	2		

- Molecule 20 is a protein called Chloroplast photosystem II subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	X	32	Total	C	N	O	0	0
			214	140	35	39		
20	x	32	Total	C	N	O	0	0
			214	140	35	39		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	220	Total	C	N	O	S	0	0
			1686	1100	271	310	5		

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
22	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

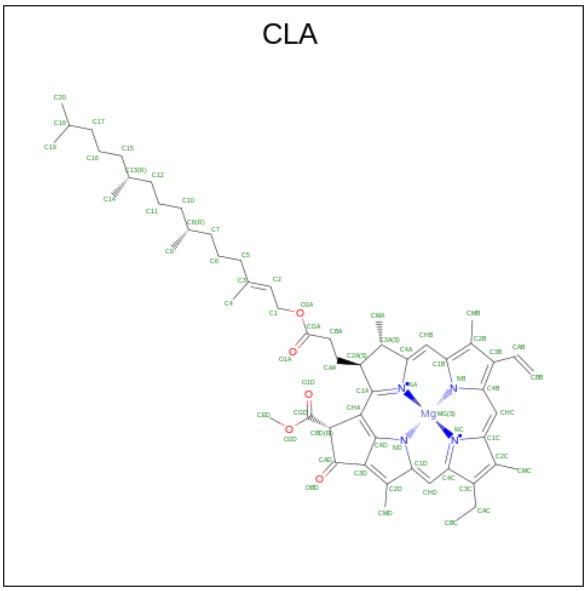
- Molecule 23 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	r	160	Total	C	N	O	S	0	0
			1235	795	208	227	5		

- Molecule 24 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 25 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
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	B	1	Total C Mg N O 65 55 1 4 5	0
25	C	1	Total C Mg N O 65 55 1 4 5	0
25	C	1	Total C Mg N O 65 55 1 4 5	0
25	C	1	Total C Mg N O 65 55 1 4 5	0
25	C	1	Total C Mg N O 65 55 1 4 5	0
25	C	1	Total C Mg N O 65 55 1 4 5	0
25	C	1	Total C Mg N O 65 55 1 4 5	0
25	C	1	Total C Mg N O 65 55 1 4 5	0
25	C	1	Total C Mg N O 65 55 1 4 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

Continued on next page...

Continued from previous page...

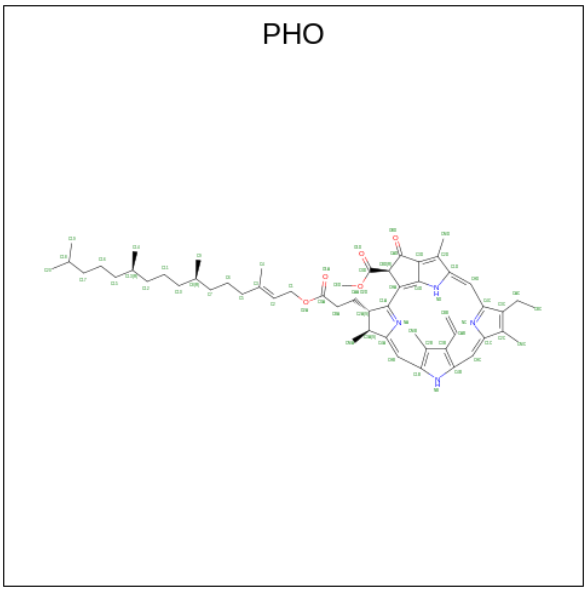
Mol	Chain	Residues	Atoms	AltConf
25	a	1	Total C Mg N O 65 55 1 4 5	0
25	a	1	Total C Mg N O 49 39 1 4 5	0
25	a	1	Total C Mg N O 60 50 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 45 35 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 45 35 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0

Continued on next page...

Continued from previous page...

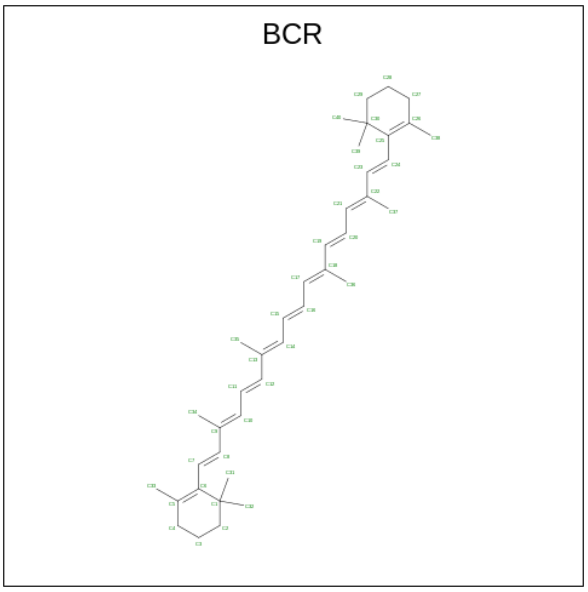
Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	c	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 41	C 33	Mg 1	N 4	O 3	0

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



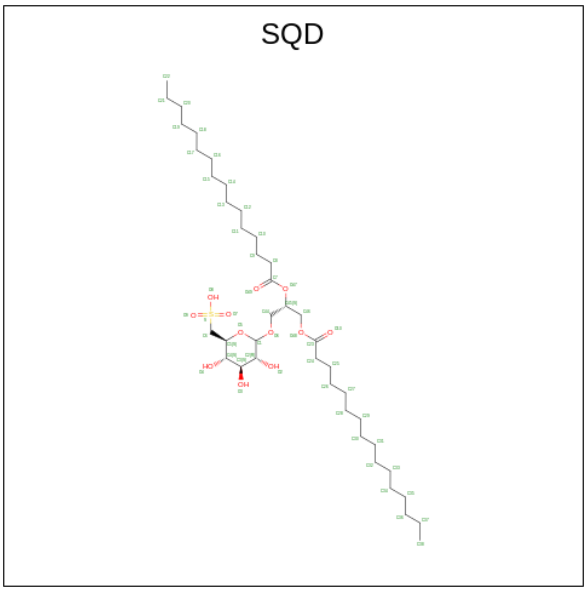
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



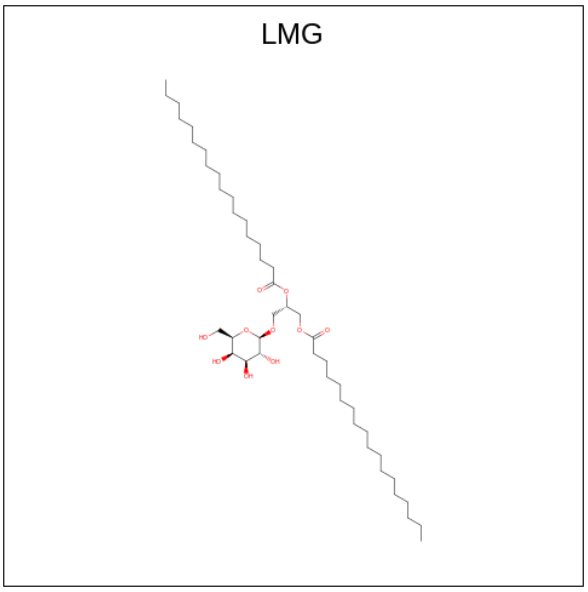
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	D	1	Total C 40 40	0
27	H	1	Total C 40 40	0
27	V	1	Total C 40 40	0
27	a	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	d	1	Total C 40 40	0
27	h	1	Total C 40 40	0
27	k	1	Total C 40 40	0
27	t	1	Total C 40 40	0
27	v	1	Total C 40 40	0
27	z	1	Total C 40 40	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



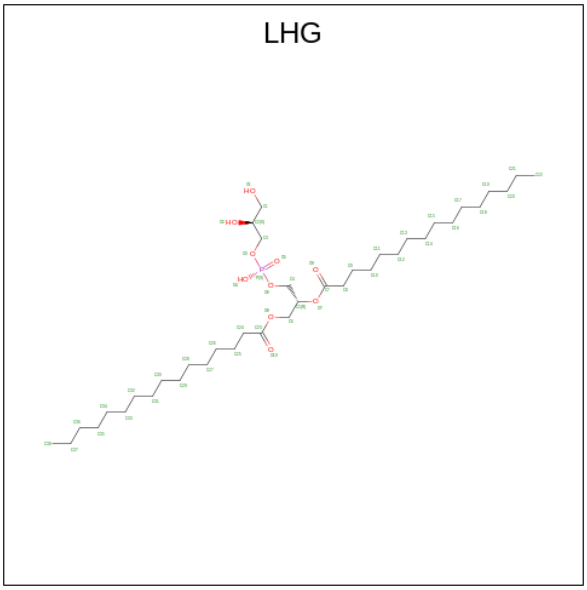
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	S	0
			51	38	12	1	
28	a	1	Total	C	O	S	0
			51	38	12	1	
28	t	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C O 51 41 10	0
29	C	1	Total C O 51 41 10	0
29	D	1	Total C O 46 36 10	0
29	H	1	Total C O 48 38 10	0
29	W	1	Total C O 48 38 10	0
29	a	1	Total C O 46 36 10	0
29	b	1	Total C O 42 32 10	0
29	c	1	Total C O 40 30 10	0
29	d	1	Total C O 41 31 10	0
29	d	1	Total C O 48 38 10	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



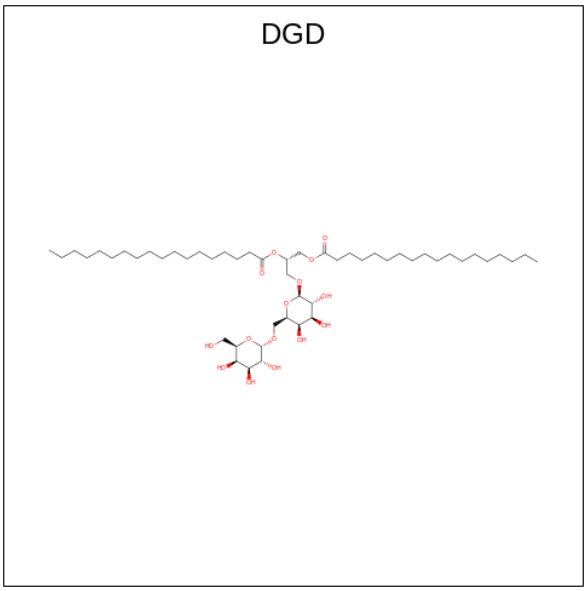
Mol	Chain	Residues	Atoms	AltConf
30	B	1	Total C O P 44 33 10 1	0

Continued on next page...

Continued from previous page...

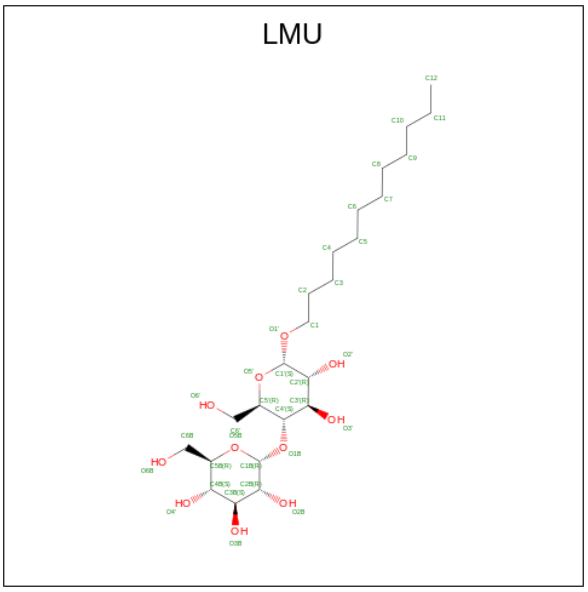
Mol	Chain	Residues	Atoms				AltConf
30	C	1	Total	C	O	P	0
			47	36	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			39	28	10	1	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	S	1	Total	C	O	P	0
			45	34	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			43	32	10	1	
30	a	1	Total	C	O	P	0
			44	33	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			44	33	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



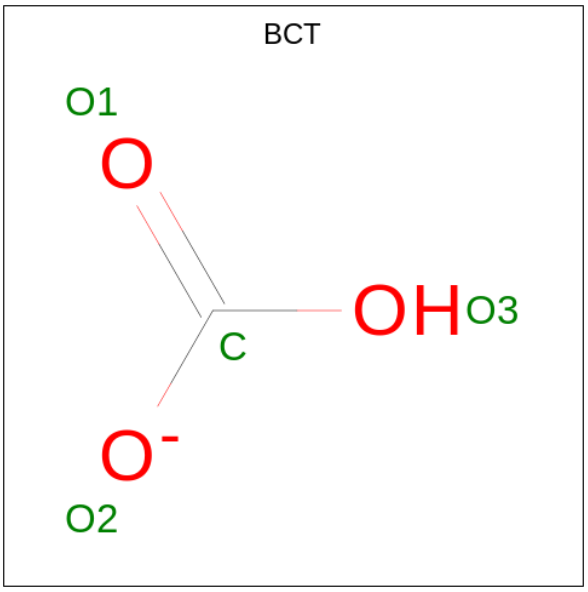
Mol	Chain	Residues	Atoms	AltConf
31	C	1	Total C O 55 40 15	0
31	C	1	Total C O 62 47 15	0
31	C	1	Total C O 59 44 15	0
31	W	1	Total C O 66 51 15	0
31	Y	1	Total C O 66 51 15	0
31	c	1	Total C O 53 38 15	0
31	c	1	Total C O 49 34 15	0
31	c	1	Total C O 59 44 15	0

- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



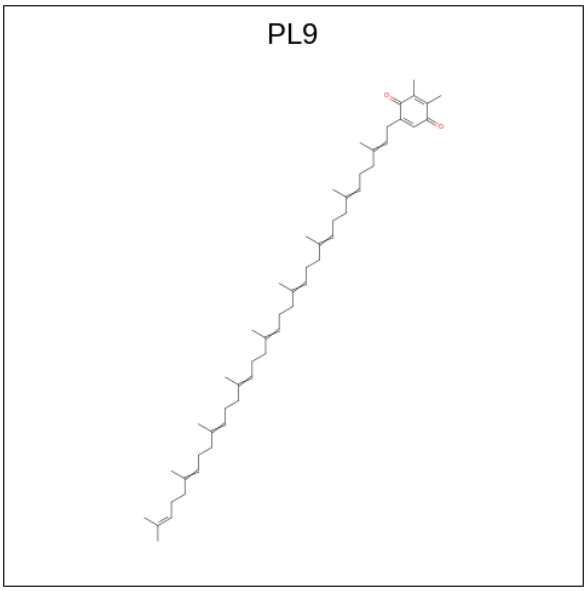
Mol	Chain	Residues	Atoms	AltConf
32	C	1	Total C O 35 24 11	0
32	C	1	Total C O 35 24 11	0
32	S	1	Total C O 35 24 11	0
32	c	1	Total C O 35 24 11	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



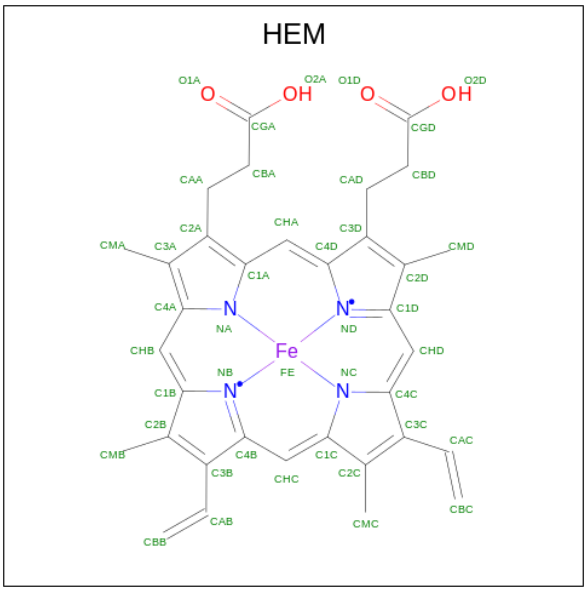
Mol	Chain	Residues	Atoms	AltConf
33	D	1	Total C O 4 1 3	0
33	a	1	Total C O 4 1 3	0

- Molecule 34 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



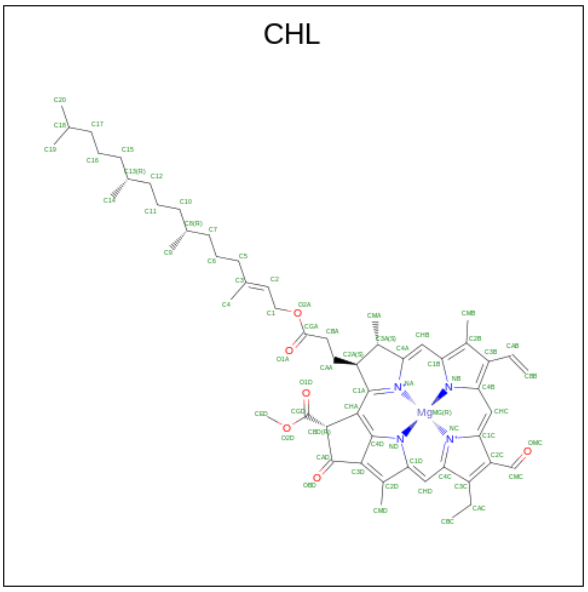
Mol	Chain	Residues	Atoms	AltConf
34	D	1	Total C O 55 53 2	0
34	d	1	Total C O 55 53 2	0

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
35	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 36 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
36	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

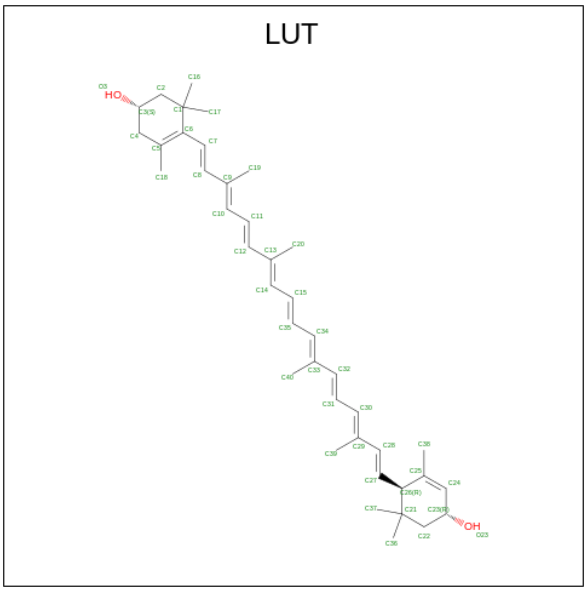
Mol	Chain	Residues	Atoms					AltConf
36	G	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
36	G	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
36	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
36	G	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
36	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
36	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
36	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
36	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
36	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
36	S	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
36	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
36	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
36	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
36	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
36	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
36	r	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
36	r	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
36	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 37 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



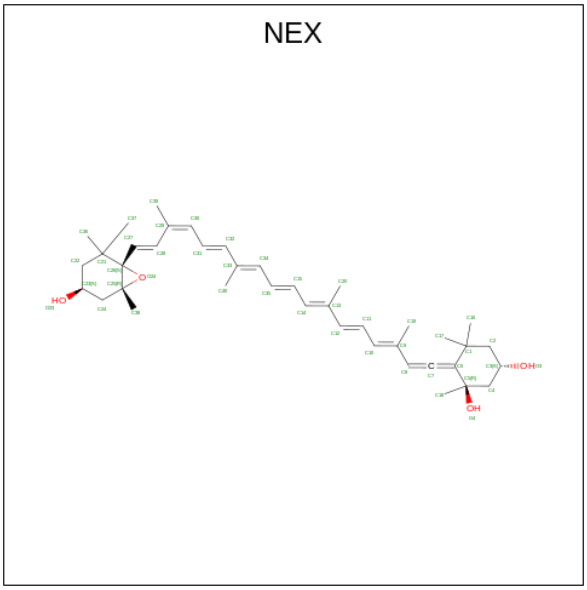
Mol	Chain	Residues	Atoms			AltConf
37	G	1	Total	C	O	0
			42	40	2	
37	G	1	Total	C	O	0
			42	40	2	
37	N	1	Total	C	O	0
			42	40	2	
37	N	1	Total	C	O	0
			42	40	2	
37	S	1	Total	C	O	0
			42	40	2	
37	S	1	Total	C	O	0
			42	40	2	
37	Y	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

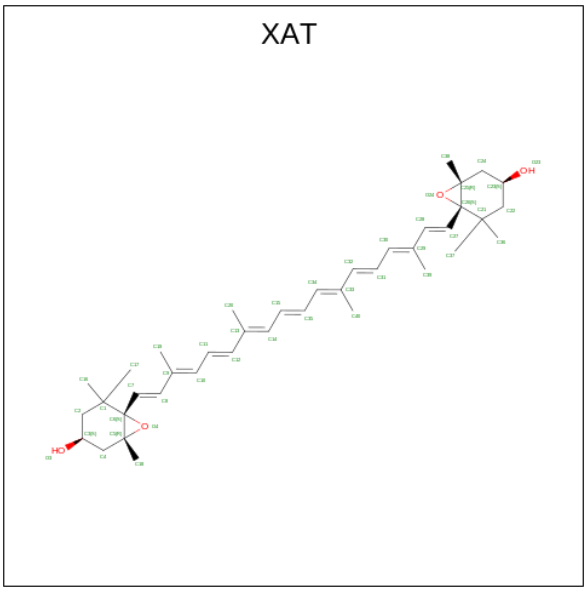
Mol	Chain	Residues	Atoms	AltConf
37	Y	1	Total C O 42 40 2	0

- Molecule 38 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: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
38	G	1	Total C O 44 40 4	0
38	N	1	Total C O 44 40 4	0
38	S	1	Total C O 44 40 4	0
38	Y	1	Total C O 44 40 4	0
38	r	1	Total C O 44 40 4	0

- Molecule 39 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: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



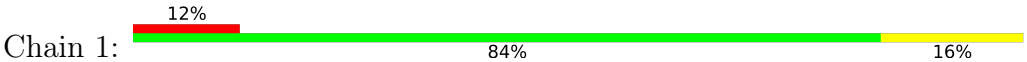
Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			44	40	4	
39	N	1	Total	C	O	0
			44	40	4	
39	Y	1	Total	C	O	0
			44	40	4	
39	r	1	Total	C	O	0
			44	40	4	

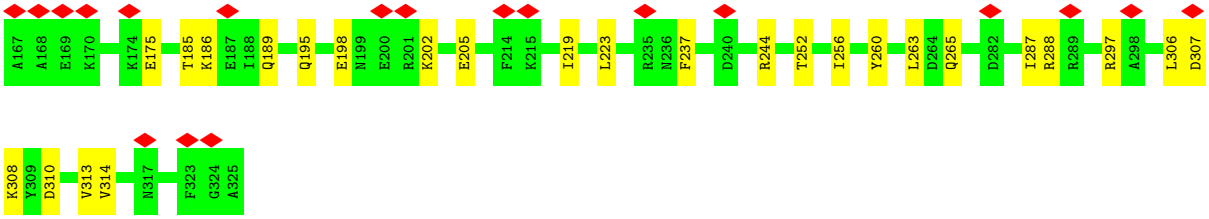
3 Residue-property plots (i)

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: PDZ domain-containing protein

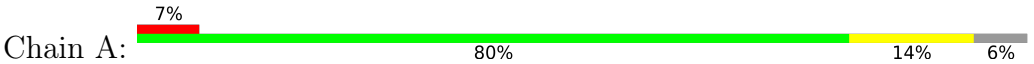
Chain 1:

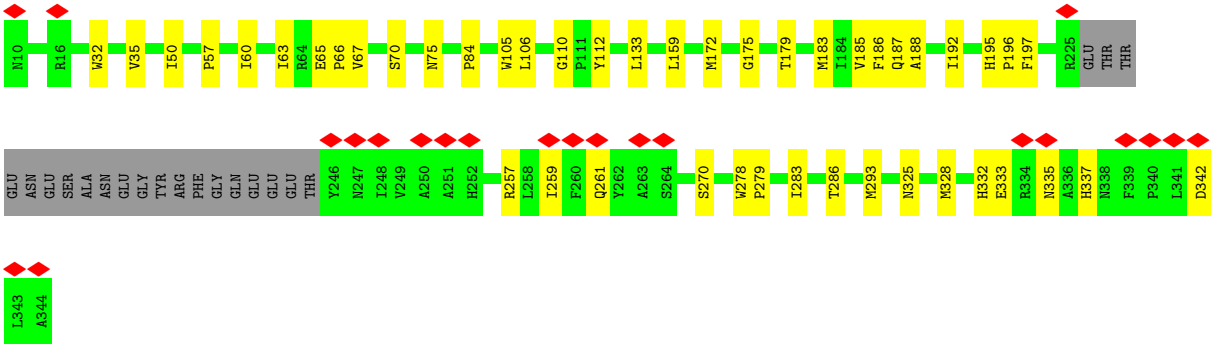




• Molecule 2: Photosystem II protein D1

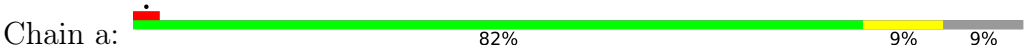
Chain A:

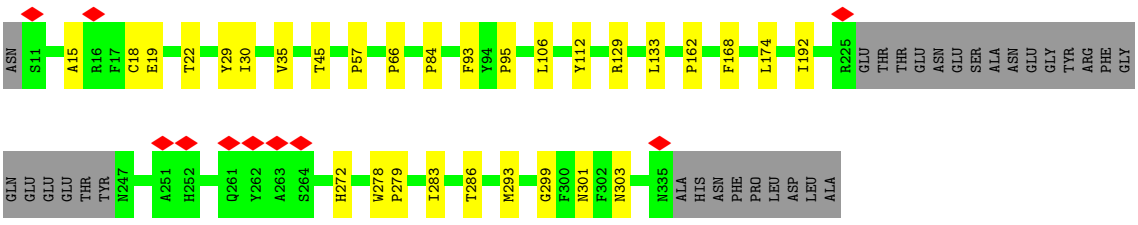




• Molecule 2: Photosystem II protein D1

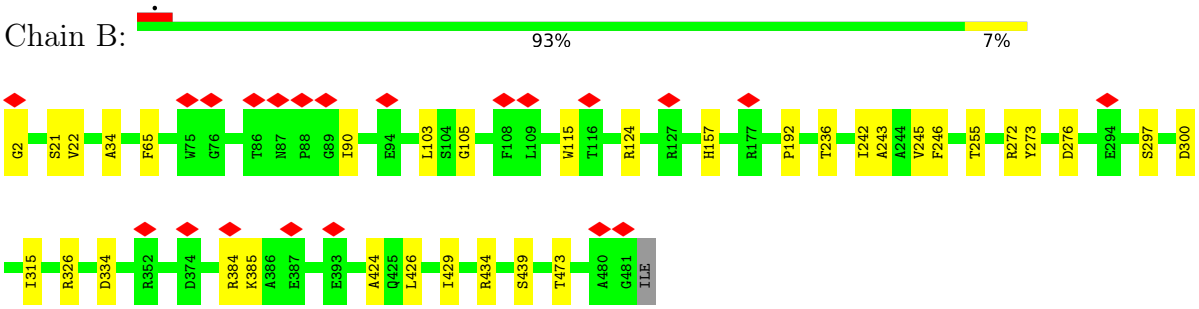
Chain a:





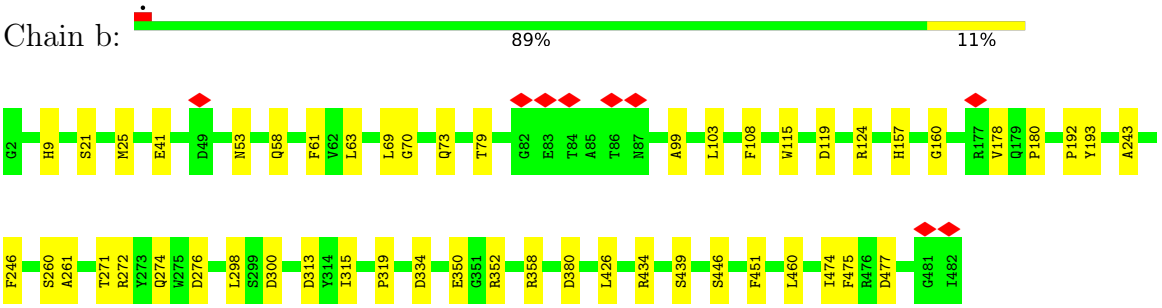
• Molecule 3: Photosystem II CP47 reaction center protein

Chain B:



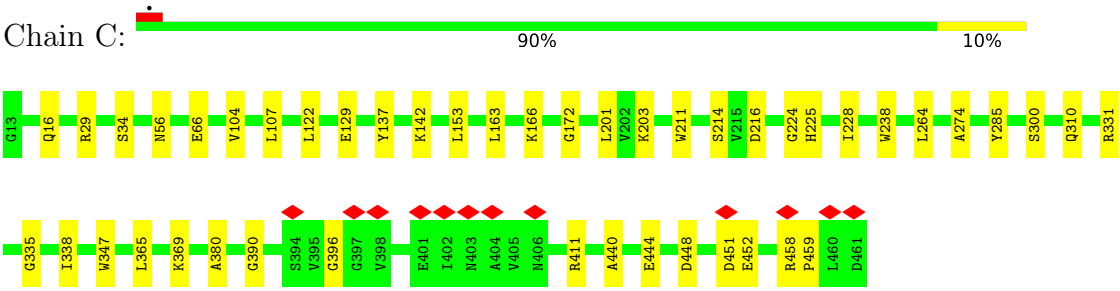
• Molecule 3: Photosystem II CP47 reaction center protein

Chain b:



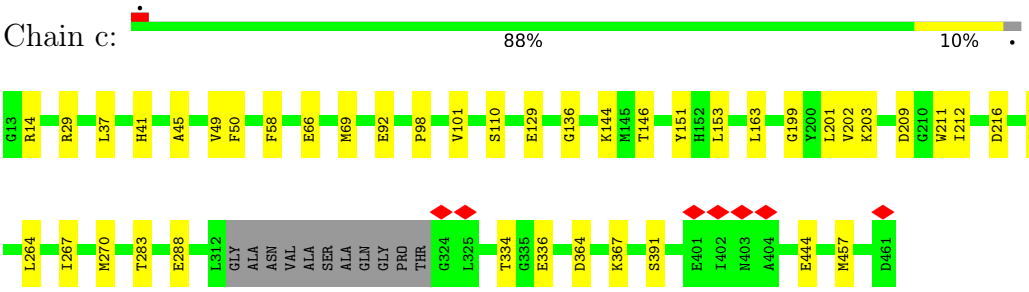
• Molecule 4: Photosystem II CP43 reaction center protein

Chain C:



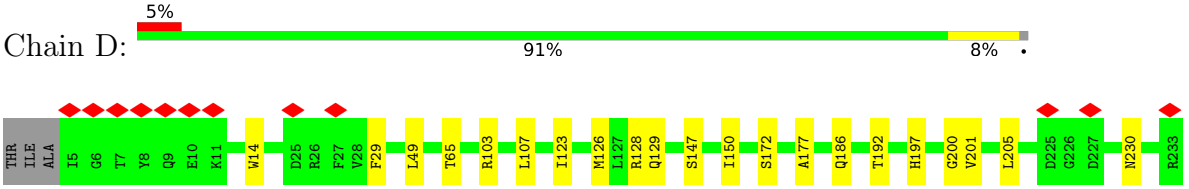
• Molecule 4: Photosystem II CP43 reaction center protein

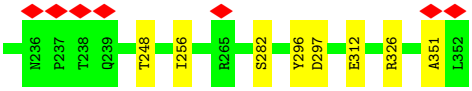
Chain c:



• Molecule 5: Photosystem II D2 protein

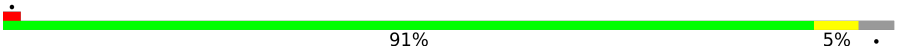
Chain D:

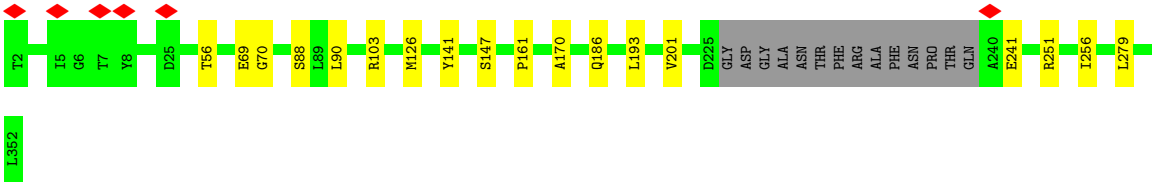




• Molecule 5: Photosystem II D2 protein

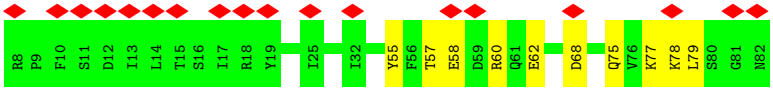
Chain d:





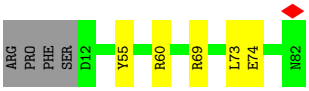
• Molecule 6: Cytochrome b559 subunit alpha

Chain E:



• Molecule 6: Cytochrome b559 subunit alpha

Chain e:

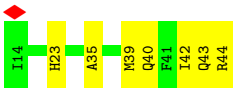


• Molecule 7: Cytochrome b559 subunit beta

Chain F:

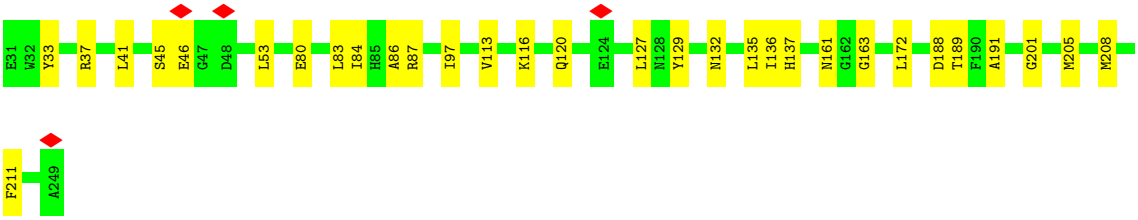
• Molecule 7: Cytochrome b559 subunit beta

Chain f:

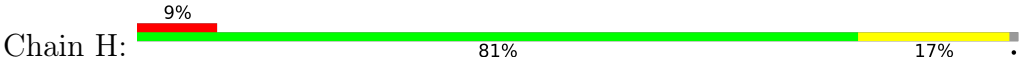


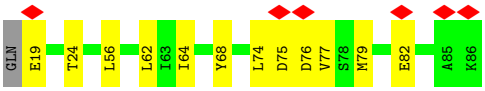
• Molecule 8: Chlorophyll a-b binding protein, chloroplastic

Chain G:

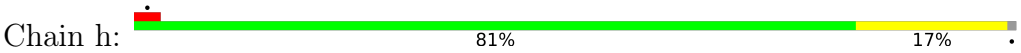


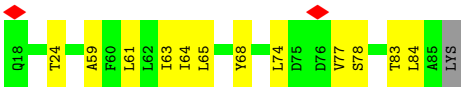
• Molecule 9: Photosystem II reaction center protein H



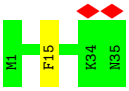


• Molecule 9: Photosystem II reaction center protein H

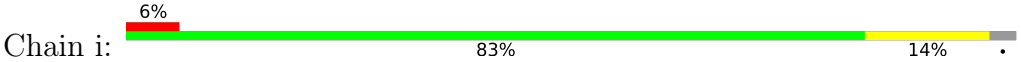


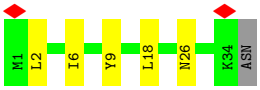


• Molecule 10: Photosystem II reaction center protein I

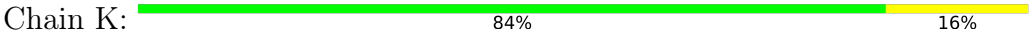


• Molecule 10: Photosystem II reaction center protein I

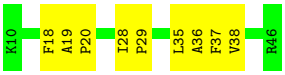




• Molecule 11: Photosystem II reaction center protein K

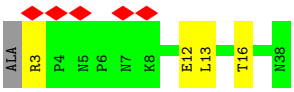


• Molecule 11: Photosystem II reaction center protein K



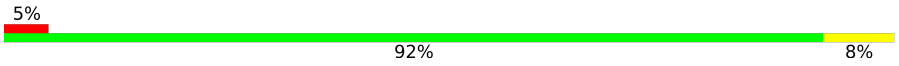
• Molecule 12: Photosystem II reaction center protein L

Chain L:



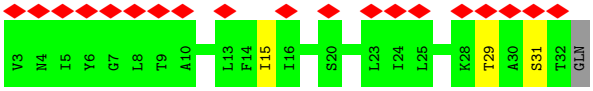
• Molecule 12: Photosystem II reaction center protein L

Chain l:



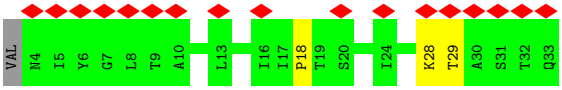
• Molecule 13: Photosystem II reaction center protein M

Chain M:



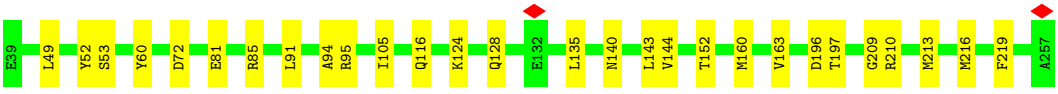
• Molecule 13: Photosystem II reaction center protein M

Chain m:



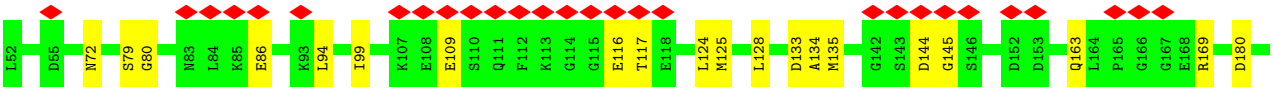
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

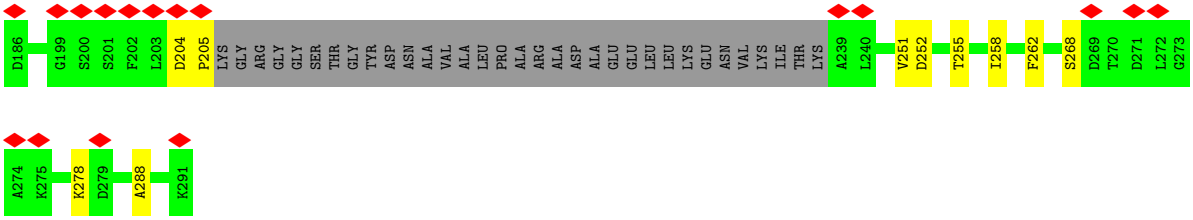
Chain N:



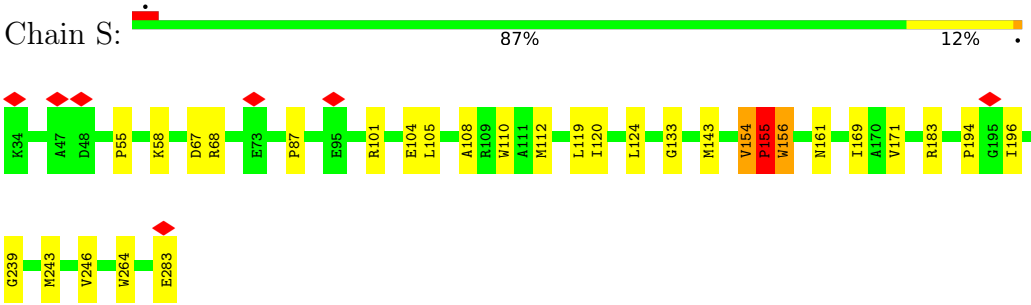
• Molecule 15: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:

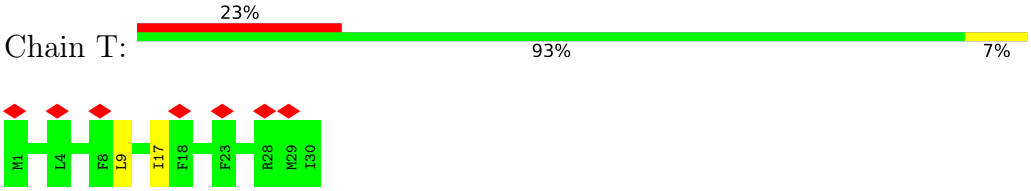




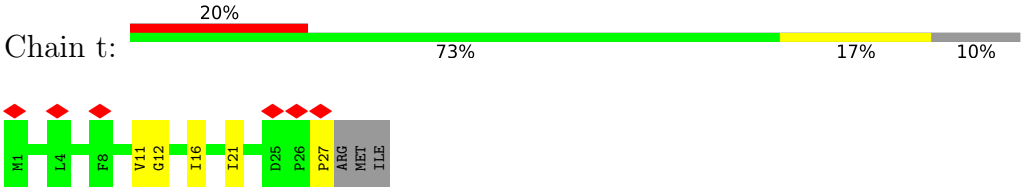
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic



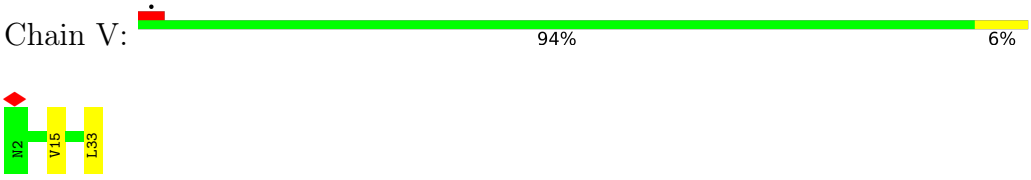
• Molecule 17: Photosystem II reaction center protein T



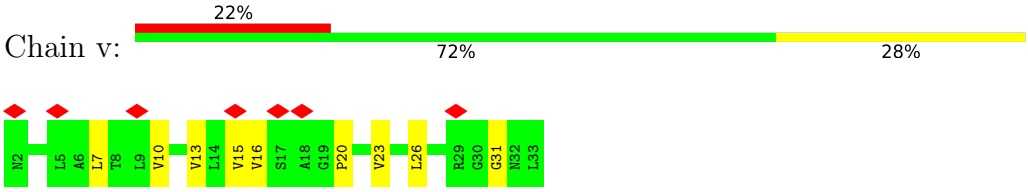
• Molecule 17: Photosystem II reaction center protein T



• Molecule 18: Photosystem II reaction center protein Psb30

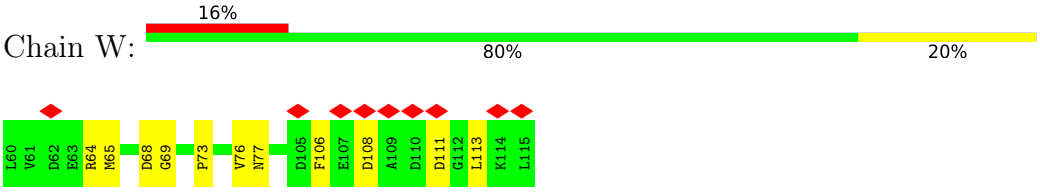


• Molecule 18: Photosystem II reaction center protein Psb30



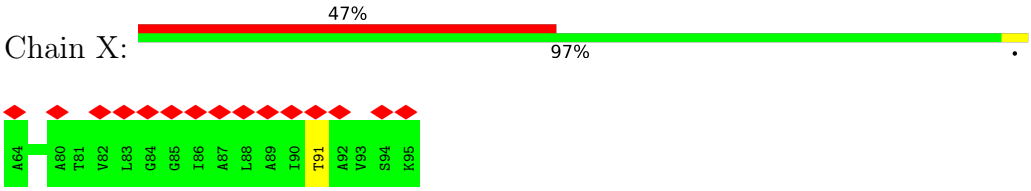
• Molecule 19: Photosystem II reaction center W protein, chloroplastic

Chain W:



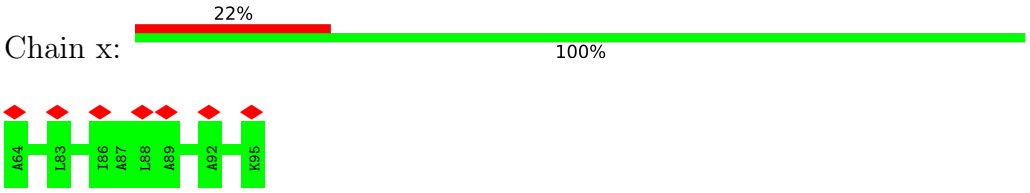
• Molecule 20: Chloroplast photosystem II subunit X

Chain X:



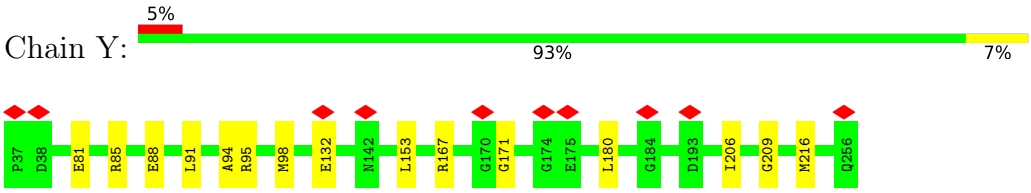
• Molecule 20: Chloroplast photosystem II subunit X

Chain x:



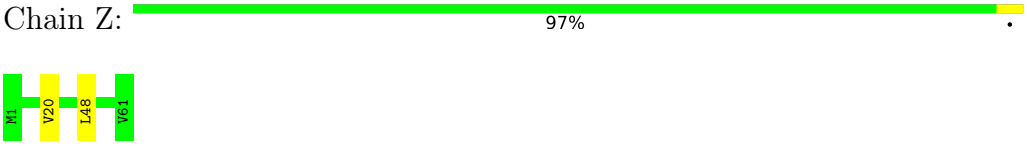
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain Y:



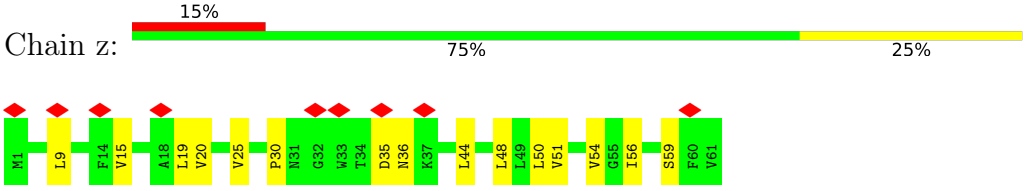
• Molecule 22: Photosystem II reaction center protein Z

Chain Z:



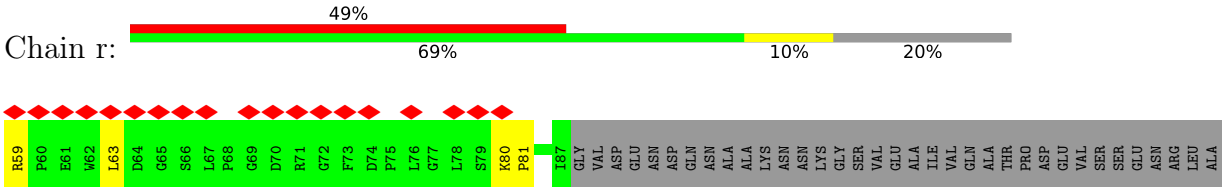
• Molecule 22: Photosystem II reaction center protein Z

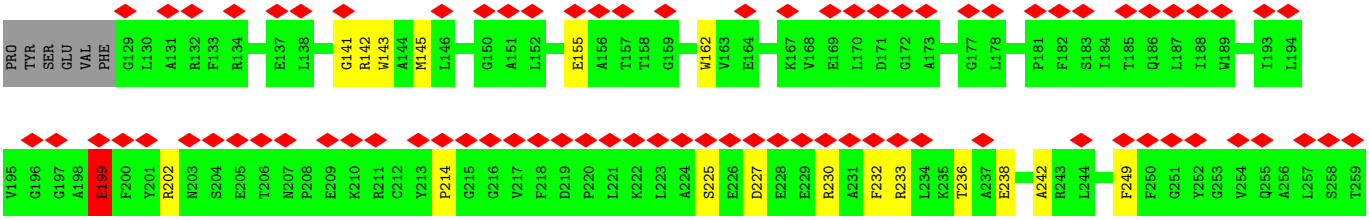
Chain z:



• Molecule 23: Chlorophyll a-b binding protein CP29

Chain r:




PRO TYR SER GLU VAL PHE G129 L130 A131 R132 F133 R134 E137 L138 G141 R142 W143 A144 M145 L146 G150 A151 L152 E155 A156 T157 T158 G159 W162 V163 E164 K167 V168 E169 L170 D171 G172 A173 G177 L178 P181 F182 S183 I184 T185 Q186 L187 I188 W189 I193 L194
V195 G196 G197 A198 E199 F200 Y201 R202 N203 S204 E205 T206 N207 P208 E209 K210 R211 C212 Y213 P214 G215 G216 V217 F218 D219 P220 L221 K222 L223 A224 S225 E226 D227 E228 E229 R230 A231 F232 R233 L234 K235 T236 A237 E238 A242 R243 L244 F249 F250 G251 Y252 G253 V254 Q255 A256 L257 S258 T259

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97962	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	39.154	Depositor
Minimum map value	-20.689	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.163	Depositor
Recommended contour level	6.8	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: FE2, SQD, LMU, PL9, NEX, PHO, CHL, LHG, BCR, LMG, LUT, BCT, DGD, HEM, CLA, XAT

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	1	0.11	0/1307	0.29	0/1755
2	A	0.16	0/2544	0.28	0/3470
2	a	0.18	0/2450	0.29	0/3340
3	B	0.14	0/3883	0.27	0/5286
3	b	0.17	0/3891	0.29	0/5297
4	C	0.15	0/3619	0.27	0/4931
4	c	0.15	0/3550	0.31	0/4834
5	D	0.16	0/2866	0.29	0/3909
5	d	0.17	0/2777	0.28	0/3787
6	E	0.12	0/628	0.29	0/857
6	e	0.13	0/591	0.29	0/807
7	F	0.12	0/258	0.27	0/349
7	f	0.15	0/258	0.26	0/349
8	G	0.14	0/1717	0.29	0/2337
9	H	0.13	0/530	0.28	0/725
9	h	0.31	0/530	0.46	0/726
10	I	0.14	0/291	0.23	0/394
10	i	0.15	0/283	0.32	0/383
11	K	0.17	0/309	0.32	0/425
11	k	0.17	0/308	0.41	0/425
12	L	0.12	0/309	0.21	0/420
12	l	0.15	0/314	0.25	0/427
13	M	0.13	0/234	0.25	0/321
13	m	0.14	0/236	0.30	0/323
14	N	0.14	0/1720	0.28	0/2341
15	O	0.11	0/1593	0.29	0/2150
16	S	0.16	0/1948	0.42	3/2653 (0.1%)
17	T	0.10	0/254	0.22	0/343
17	t	0.13	0/227	0.24	0/308
18	V	0.10	0/224	0.22	0/307
18	v	0.13	0/224	0.34	0/307
19	W	0.12	0/445	0.27	0/603

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	X	0.11	0/215	0.22	0/292
20	x	0.13	0/215	0.24	0/292
21	Y	0.14	0/1739	0.26	0/2364
22	Z	0.13	0/469	0.26	0/644
22	z	0.13	0/469	0.34	0/644
23	r	0.16	0/1264	0.39	2/1711 (0.1%)
All	All	0.15	0/44689	0.30	5/60836 (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
16	S	0	1
23	r	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	S	155	PRO	CA-N-CD	-6.95	102.27	112.00
16	S	155	PRO	CA-C-N	5.51	132.07	121.54
16	S	155	PRO	C-N-CA	5.51	132.07	121.54
23	r	225	SER	CB-CA-C	-5.21	110.55	116.54
23	r	199	GLU	CA-CB-CG	5.17	124.45	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	S	154	VAL	Peptide
23	r	199	GLU	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1285	0	1254	16	0
2	A	2465	0	2396	34	0
2	a	2375	0	2316	20	0
3	B	3755	0	3642	29	0
3	b	3763	0	3653	35	0
4	C	3498	0	3372	36	0
4	c	3431	0	3308	34	0
5	D	2771	0	2655	28	0
5	d	2686	0	2585	15	0
6	E	610	0	599	8	0
6	e	575	0	565	4	0
7	F	251	0	263	5	0
7	f	251	0	263	7	0
8	G	1667	0	1606	22	0
9	H	519	0	549	13	0
9	h	519	0	544	9	0
10	I	283	0	293	1	0
10	i	275	0	287	4	0
11	K	297	0	308	5	0
11	k	296	0	308	8	0
12	L	301	0	310	4	0
12	l	306	0	315	3	0
13	M	230	0	252	3	0
13	m	232	0	251	3	0
14	N	1672	0	1611	18	0
15	O	1565	0	1562	20	0
16	S	1894	0	1838	30	0
17	T	247	0	260	2	0
17	t	220	0	227	4	0
18	V	224	0	256	3	0
18	v	224	0	256	7	0
19	W	434	0	411	9	0
20	X	214	0	240	1	0
20	x	214	0	240	0	0
21	Y	1686	0	1623	11	0
22	Z	458	0	490	2	0
22	z	458	0	490	11	0
23	r	1235	0	1221	17	0
24	A	1	0	0	0	0
24	a	1	0	0	0	0
25	A	174	0	170	1	0
25	B	1040	0	1152	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	845	0	936	12	0
25	D	195	0	216	4	0
25	G	432	0	416	2	0
25	N	461	0	463	5	0
25	S	471	0	363	9	0
25	Y	502	0	535	0	0
25	a	174	0	170	2	0
25	b	1000	0	1074	19	0
25	c	808	0	861	14	0
25	d	172	0	175	4	0
25	r	241	0	193	3	0
26	A	64	0	74	2	0
26	D	64	0	74	1	0
26	a	64	0	74	2	0
26	d	64	0	74	1	0
27	A	40	0	56	5	0
27	B	80	0	112	6	0
27	C	120	0	168	12	0
27	D	40	0	56	3	0
27	H	40	0	56	5	0
27	V	40	0	56	4	0
27	a	40	0	56	2	0
27	b	120	0	168	4	0
27	c	40	0	56	4	0
27	d	40	0	56	2	0
27	h	40	0	56	5	0
27	k	40	0	56	4	0
27	t	40	0	56	3	0
27	v	40	0	56	8	0
27	z	40	0	56	3	0
28	A	51	0	69	2	0
28	a	51	0	69	0	0
28	t	54	0	78	0	0
29	B	51	0	72	2	0
29	C	51	0	72	0	0
29	D	46	0	62	0	0
29	H	48	0	66	2	0
29	W	48	0	66	1	0
29	a	46	0	62	0	0
29	b	42	0	54	0	0
29	c	40	0	46	0	0
29	d	89	0	118	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	44	0	61	1	0
30	C	47	0	67	0	0
30	D	88	0	122	2	0
30	G	49	0	74	0	0
30	L	49	0	74	1	0
30	N	49	0	74	1	0
30	S	45	0	63	2	0
30	Y	49	0	74	2	0
30	a	87	0	117	1	0
30	b	49	0	74	1	0
30	d	93	0	135	4	0
30	l	49	0	74	4	0
31	C	176	0	226	1	0
31	W	66	0	96	0	0
31	Y	66	0	96	1	0
31	c	161	0	196	3	0
32	C	70	0	92	3	0
32	S	35	0	46	0	0
32	c	35	0	46	0	0
33	D	4	0	0	0	0
33	a	4	0	0	2	0
34	D	55	0	80	0	0
34	d	55	0	80	1	0
35	F	43	0	30	5	0
35	f	43	0	30	4	0
36	G	378	0	336	9	0
36	N	360	0	348	13	0
36	S	182	0	125	10	0
36	Y	274	0	239	8	0
36	r	133	0	91	4	0
37	G	84	0	112	4	0
37	N	84	0	112	4	0
37	S	84	0	112	8	0
37	Y	84	0	112	6	0
38	G	44	0	56	3	0
38	N	44	0	56	1	0
38	S	44	0	56	1	0
38	Y	44	0	56	4	0
38	r	44	0	56	3	0
39	G	44	0	56	2	0
39	N	44	0	56	3	0
39	Y	44	0	56	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	r	44	0	56	3	0
All	All	55146	0	55711	611	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (611) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:208:MET:HE2	37:G:616:LUT:H10	1.55	0.89
2:A:185:VAL:HG13	2:A:332:HIS:HE1	1.37	0.89
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.66	0.77
4:c:264:LEU:HD21	25:c:508:CLA:HAB	1.66	0.77
36:G:606:CHL:HHC	36:G:606:CHL:HBB1	1.66	0.76
9:h:78:SER:HB2	9:h:83:THR:HG22	1.68	0.76
36:G:608:CHL:HHC	36:G:608:CHL:HBB1	1.66	0.75
36:N:306:CHL:HHC	36:N:306:CHL:HBB1	1.68	0.75
5:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.69	0.74
36:Y:310:CHL:HHC	36:Y:310:CHL:HBB1	1.68	0.74
14:N:152:THR:HG22	36:N:306:CHL:HAC1	1.69	0.73
21:Y:216:MET:HE2	37:Y:317:LUT:H10	1.70	0.73
5:d:186:GLN:HB2	25:d:403:CLA:HBC1	1.69	0.73
16:S:246:VAL:HG11	37:S:616:LUT:H12	1.70	0.73
2:A:133:LEU:HD23	5:D:256:ILE:HG12	1.70	0.71
4:C:264:LEU:HD21	25:C:508:CLA:HAB	1.72	0.70
6:E:60:ARG:NH1	6:E:79:LEU:O	2.25	0.70
3:B:384:ARG:NH2	15:O:204:ASP:O	2.25	0.70
5:D:192:THR:HG23	25:D:404:CLA:HBC2	1.73	0.70
36:Y:309:CHL:HHC	36:Y:309:CHL:HBB1	1.73	0.70
2:A:172:MET:HE3	2:A:179:THR:HG22	1.75	0.69
36:Y:308:CHL:HHC	36:Y:308:CHL:HBB1	1.74	0.69
3:B:192:PRO:HG3	9:H:68:TYR:CD1	2.27	0.69
4:C:310:GLN:HE22	4:C:369:LYS:HA	1.58	0.69
36:N:310:CHL:HBB1	36:N:310:CHL:HHC	1.73	0.69
4:c:153:LEU:HD21	25:c:506:CLA:HAB	1.74	0.69
36:r:304:CHL:HHC	36:r:304:CHL:HBB1	1.76	0.68
3:B:272:ARG:NH1	3:B:276:ASP:OD2	2.26	0.68
2:A:185:VAL:HG13	2:A:332:HIS:CE1	2.25	0.68
23:r:141:GLY:HA3	23:r:242:ALA:HB1	1.75	0.67
4:C:300:SER:OG	4:C:380:ALA:O	2.13	0.67
2:a:29:TYR:O	2:a:129:ARG:NH1	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:G:609:CHL:HHC	36:G:609:CHL:HBB1	1.76	0.66
9:H:82:GLU:N	9:H:82:GLU:OE1	2.27	0.66
4:c:444:GLU:N	4:c:444:GLU:OE1	2.28	0.66
13:M:31:SER:OG	13:m:28:LYS:NZ	2.27	0.66
36:S:607:CHL:HHC	36:S:607:CHL:HBB1	1.77	0.66
25:b:504:CLA:HAA2	25:b:512:CLA:H141	1.78	0.66
16:S:58:LYS:NZ	30:S:618:LHG:O1	2.30	0.65
18:v:26:LEU:HD21	22:z:25:VAL:HA	1.79	0.65
1:1:287:ILE:O	1:1:297:ARG:NH2	2.30	0.65
4:C:142:LYS:NZ	19:W:111:ASP:O	2.31	0.63
9:h:74:LEU:HB2	9:h:77:VAL:HG22	1.81	0.63
2:a:299:GLY:O	4:c:391:SER:OG	2.17	0.63
18:v:15:VAL:HG23	27:v:101:BCR:HC8	1.81	0.63
36:r:305:CHL:HHC	36:r:305:CHL:HBB1	1.81	0.63
16:S:55:PRO:O	16:S:68:ARG:NH1	2.32	0.63
2:A:270:SER:OG	28:A:407:SQD:O49	2.16	0.62
25:b:505:CLA:H8	25:b:512:CLA:H203	1.81	0.62
23:r:80:LYS:NZ	23:r:81:PRO:O	2.31	0.62
3:b:243:ALA:HA	3:b:246:PHE:CE2	2.33	0.62
2:A:332:HIS:CD2	2:A:333:GLU:HG2	2.35	0.62
1:1:313:VAL:HG23	1:1:314:VAL:HG23	1.79	0.62
14:N:196:ASP:OD1	14:N:197:THR:N	2.33	0.62
25:b:502:CLA:H42	29:d:410:LMG:H112	1.81	0.61
18:V:15:VAL:HG13	27:V:101:BCR:H10C	1.82	0.61
3:B:124:ARG:NH1	9:H:19:GLU:O	2.33	0.61
3:b:272:ARG:NH1	3:b:276:ASP:OD2	2.33	0.61
5:d:279:LEU:HD22	26:d:402:PHO:HBC3	1.81	0.61
23:r:202:ARG:NH2	25:r:307:CLA:O1D	2.33	0.61
5:D:126:MET:HE3	5:D:150:ILE:HD12	1.83	0.61
36:S:606:CHL:HHC	36:S:606:CHL:HBB1	1.83	0.61
8:G:87:ARG:NH1	36:G:608:CHL:OBD	2.34	0.60
16:S:161:ASN:ND2	36:S:606:CHL:OBD	2.33	0.60
16:S:101:ARG:NH1	16:S:104:GLU:OE1	2.35	0.60
21:Y:94:ALA:HB1	21:Y:209:GLY:HA3	1.83	0.60
30:d:408:LHG:H322	17:t:21:ILE:HD11	1.82	0.60
16:S:108:ALA:O	16:S:112:MET:HG3	2.03	0.59
4:C:34:SER:OG	4:C:129:GLU:OE2	2.15	0.59
16:S:171:VAL:HG11	36:S:606:CHL:HED2	1.86	0.58
3:b:41:GLU:OE2	3:b:61:PHE:N	2.32	0.58
4:c:216:ASP:HA	4:c:283:THR:HG21	1.85	0.58
5:D:172:SER:HB2	5:D:177:ALA:HB1	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:201:LEU:HD11	27:c:514:BCR:H373	1.85	0.58
36:N:309:CHL:HHC	36:N:309:CHL:HBB1	1.86	0.58
5:d:193:LEU:O	12:l:35:TYR:OH	2.15	0.58
11:K:13:GLU:OE1	11:K:13:GLU:N	2.29	0.57
15:O:251:VAL:HG23	15:O:258:ILE:HG22	1.84	0.57
3:b:434:ARG:HG3	3:b:439:SER:HB2	1.85	0.57
3:B:192:PRO:HG3	9:H:68:TYR:CE1	2.39	0.57
8:G:33:TYR:CE2	8:G:191:ALA:HB1	2.40	0.57
8:G:188:ASP:OD1	8:G:189:THR:N	2.37	0.57
14:N:135:LEU:HD21	25:N:305:CLA:HAA2	1.85	0.57
36:N:307:CHL:HHC	36:N:307:CHL:HBB1	1.85	0.57
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.87	0.57
31:c:515:DGD:O4E	31:c:515:DGD:O5E	2.20	0.57
11:k:36:ALA:HB2	27:k:101:BCR:H391	1.87	0.57
12:l:13:LEU:N	13:m:29:THR:OG1	2.37	0.57
23:r:227:ASP:OD2	23:r:230:ARG:N	2.38	0.57
27:v:101:BCR:H382	27:v:101:BCR:H23C	1.86	0.57
12:L:13:LEU:N	13:M:29:THR:OG1	2.34	0.56
5:d:241:GLU:OE1	5:d:241:GLU:N	2.29	0.56
2:A:50:ILE:HG22	27:A:406:BCR:H271	1.86	0.56
3:b:350:GLU:OE1	3:b:352:ARG:NH1	2.37	0.56
1:1:306:LEU:O	1:1:310:ASP:N	2.37	0.56
25:b:516:CLA:OBD	9:h:24:THR:HG21	2.05	0.56
38:Y:318:NEX:H183	38:Y:318:NEX:H192	1.88	0.56
3:B:192:PRO:HG3	9:H:68:TYR:HD1	1.71	0.56
3:B:424:ALA:HB2	3:B:429:ILE:HD11	1.88	0.56
15:O:124:LEU:HD23	19:W:64:ARG:HH22	1.71	0.56
4:C:122:LEU:HD11	25:C:511:CLA:H92	1.88	0.56
4:C:153:LEU:HD21	25:C:506:CLA:HAB	1.85	0.56
4:C:444:GLU:OE1	4:C:444:GLU:N	2.31	0.56
14:N:94:ALA:HB1	14:N:209:GLY:HA3	1.86	0.56
15:O:252:ASP:OD1	15:O:255:THR:OG1	2.24	0.56
4:c:267:ILE:HA	4:c:270:MET:HE3	1.87	0.56
30:D:408:LHG:H291	17:T:17:ILE:HG23	1.88	0.56
35:f:101:HEM:HBC2	35:f:101:HEM:HMC2	1.87	0.56
4:C:107:LEU:HD23	27:C:516:BCR:HC8	1.88	0.55
6:E:58:GLU:N	6:E:58:GLU:OE1	2.39	0.55
4:c:199:GLY:HA2	4:c:202:VAL:HG12	1.87	0.55
16:S:133:GLY:HA3	25:S:604:CLA:HED3	1.88	0.55
23:r:142:ARG:NE	23:r:238:GLU:OE2	2.39	0.55
8:G:163:GLY:H	36:G:608:CHL:HMC	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:43:GLN:N	7:F:43:GLN:OE1	2.39	0.55
28:A:407:SQD:O8	5:D:230:ASN:ND2	2.35	0.55
3:B:326:ARG:NH2	5:D:297:ASP:OD2	2.39	0.55
27:V:101:BCR:H343	22:Z:20:VAL:HG21	1.87	0.55
4:c:334:THR:OG1	4:c:336:GLU:OE1	2.24	0.55
7:f:35:ALA:O	7:f:39:MET:HG3	2.06	0.55
2:a:30:ILE:O	2:a:30:ILE:HG13	2.07	0.55
2:a:133:LEU:HD23	5:d:256:ILE:HG12	1.88	0.55
22:z:9:LEU:HD13	22:z:54:VAL:HG21	1.89	0.55
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.89	0.54
2:a:272:HIS:CE1	33:a:409:BCT:O2	2.60	0.54
2:A:335:ASN:HA	5:D:351:ALA:HB2	1.88	0.54
14:N:216:MET:HG2	37:N:317:LUT:H12	1.88	0.54
16:S:143:MET:HE1	36:S:606:CHL:HMD3	1.89	0.54
36:S:608:CHL:HHC	36:S:608:CHL:HBB1	1.90	0.54
4:c:224:GLY:HA3	27:c:514:BCR:H402	1.90	0.54
14:N:95:ARG:NH1	36:N:309:CHL:OBD	2.33	0.54
2:A:187:GLN:HG2	2:A:192:ILE:HG22	1.89	0.54
16:S:169:ILE:HG12	36:S:607:CHL:HBC1	1.89	0.54
6:e:74:GLU:OE1	6:e:74:GLU:N	2.31	0.54
38:r:310:NEX:H192	38:r:310:NEX:H183	1.90	0.54
9:h:61:LEU:HD23	9:h:64:ILE:HD11	1.90	0.54
5:D:123:ILE:HD11	29:H:102:LMG:H402	1.90	0.53
16:S:154:VAL:HB	25:S:605:CLA:C4D	2.38	0.53
14:N:116:GLN:OE1	14:N:116:GLN:N	2.42	0.53
13:M:15:ILE:HD11	17:T:9:LEU:HD21	1.91	0.53
11:k:35:LEU:HB2	27:v:101:BCR:H351	1.90	0.53
22:z:56:ILE:O	22:z:59:SER:OG	2.26	0.53
1:1:175:GLU:OE2	1:1:185:THR:OG1	2.25	0.53
2:A:195:HIS:CD2	2:A:197:PHE:HB2	2.44	0.53
16:S:194:PRO:HG2	16:S:196:ILE:HB	1.90	0.53
4:c:14:ARG:O	4:c:29:ARG:NH1	2.41	0.53
23:r:141:GLY:O	23:r:145:MET:HG3	2.08	0.53
9:H:19:GLU:OE2	12:L:3:ARG:NH2	2.41	0.53
21:Y:167:ARG:NH2	36:Y:310:CHL:O1D	2.41	0.53
23:r:59:ARG:NH2	23:r:63:LEU:O	2.42	0.53
2:A:337:HIS:NE2	2:A:342:ASP:OD1	2.37	0.53
16:S:196:ILE:HD11	16:S:215:PRO:HA	1.91	0.53
4:c:129:GLU:OE1	4:c:129:GLU:N	2.41	0.53
8:G:86:ALA:HB1	8:G:201:GLY:HA3	1.91	0.53
27:B:517:BCR:H373	17:t:11:VAL:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:452:GLU:OE2	5:D:248:THR:OG1	2.27	0.52
9:H:75:ASP:OD1	9:H:76:ASP:N	2.43	0.52
15:O:133:ASP:OD1	15:O:134:ALA:N	2.42	0.52
4:C:104:VAL:HG21	27:C:514:BCR:HC42	1.90	0.52
3:b:70:GLY:HA2	3:b:178:VAL:HG11	1.91	0.52
18:v:20:PRO:HA	18:v:23:VAL:HG12	1.91	0.52
29:d:409:LMG:O6	7:f:40:GLN:NE2	2.43	0.52
1:1:288:ARG:NH2	1:1:310:ASP:OD2	2.41	0.52
8:G:113:VAL:HG23	8:G:116:LYS:HB2	1.92	0.52
16:S:154:VAL:HG12	16:S:155:PRO:HD2	1.92	0.52
39:Y:302:XAT:H10	30:Y:319:LHG:H211	1.90	0.52
4:c:66:GLU:N	4:c:66:GLU:OE1	2.39	0.52
18:v:15:VAL:CG2	27:v:101:BCR:HC8	2.40	0.52
30:a:410:LHG:O3	30:a:410:LHG:O1	2.28	0.52
3:b:157:HIS:HE1	25:b:506:CLA:NA	2.07	0.52
4:C:274:ALA:HB2	25:C:502:CLA:HMD1	1.92	0.51
32:C:522:LMU:H101	31:Y:301:DGD:HAH2	1.93	0.51
21:Y:91:LEU:HD23	21:Y:180:LEU:HD22	1.93	0.51
25:c:508:CLA:H2	25:c:510:CLA:H12	1.92	0.51
15:O:125:MET:HE2	15:O:163:GLN:HB3	1.92	0.51
3:b:73:GLN:HG2	3:b:79:THR:HG22	1.92	0.51
14:N:105:ILE:HD11	14:N:219:PHE:HZ	1.76	0.51
16:S:283:GLU:OE1	16:S:283:GLU:N	2.41	0.51
30:B:520:LHG:H111	30:L:101:LHG:HC92	1.91	0.51
5:D:312:GLU:HG2	15:O:205:PRO:HG3	1.93	0.51
36:N:308:CHL:HHC	36:N:308:CHL:HBB1	1.93	0.51
4:C:365:LEU:O	4:C:369:LYS:HG2	2.11	0.51
8:G:83:LEU:HD23	8:G:172:LEU:HD22	1.93	0.51
2:A:259:ILE:HG23	2:A:261:GLN:HG2	1.92	0.51
22:z:48:LEU:O	22:z:51:VAL:HG22	2.10	0.51
16:S:264:TRP:HB2	37:S:615:LUT:H22	1.93	0.50
2:a:162:PRO:HB3	2:a:168:PHE:HA	1.93	0.50
3:b:9:HIS:HB2	25:b:511:CLA:HBA1	1.93	0.50
2:A:185:VAL:CG1	2:A:332:HIS:HE1	2.19	0.50
25:b:510:CLA:HBB1	27:h:101:BCR:HC22	1.93	0.50
4:c:151:TYR:CD2	25:c:512:CLA:HAB	2.47	0.50
16:S:67:ASP:OD1	16:S:68:ARG:N	2.43	0.50
2:a:192:ILE:HD12	2:a:293:MET:HE1	1.93	0.50
30:D:408:LHG:HC62	12:L:16:THR:HG23	1.92	0.50
39:Y:302:XAT:H171	30:Y:319:LHG:H221	1.93	0.50
31:c:517:DGD:O3D	29:d:409:LMG:O3	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:250:ARG:NH1	10:i:26:ASN:O	2.45	0.50
21:Y:81:GLU:O	21:Y:85:ARG:HG2	2.12	0.50
4:c:136:GLY:O	4:c:144:LYS:NZ	2.45	0.50
4:C:29:ARG:NH1	25:C:511:CLA:OBD	2.44	0.49
5:d:161:PRO:HB3	5:d:170:ALA:HB2	1.93	0.49
15:O:268:SER:N	15:O:278:LYS:O	2.44	0.49
2:a:272:HIS:HE1	33:a:409:BCT:O2	1.96	0.49
25:N:305:CLA:H61	16:S:155:PRO:HG3	1.94	0.49
2:a:278:TRP:HB3	2:a:279:PRO:HD3	1.93	0.49
25:S:605:CLA:H2A	25:S:605:CLA:O2D	2.13	0.49
15:O:99:ILE:HD12	15:O:135:MET:HE1	1.94	0.49
25:c:511:CLA:H171	22:z:20:VAL:HG23	1.94	0.49
2:A:67:VAL:HG12	5:D:312:GLU:HB2	1.94	0.49
2:A:337:HIS:O	5:D:351:ALA:HB1	2.12	0.49
14:N:128:GLN:HG3	14:N:135:LEU:HD13	1.94	0.49
9:H:74:LEU:HB2	9:H:77:VAL:HG22	1.95	0.48
2:a:283:ILE:HA	2:a:286:THR:HG22	1.94	0.48
3:B:105:GLY:HA3	27:B:517:BCR:H271	1.95	0.48
4:C:331:ARG:NH1	4:C:335:GLY:O	2.46	0.48
5:D:296:TYR:OH	5:D:326:ARG:NH1	2.44	0.48
1:1:219:ILE:HG21	1:1:263:LEU:HD11	1.95	0.48
4:C:216:ASP:OD1	4:C:216:ASP:N	2.45	0.48
14:N:160:MET:HA	14:N:163:VAL:HG22	1.94	0.48
2:a:301:ASN:OD1	2:a:303:ASN:ND2	2.46	0.48
4:c:98:PRO:HA	4:c:101:VAL:HG22	1.95	0.48
4:c:163:LEU:HD22	25:c:501:CLA:C2D	2.43	0.48
25:c:501:CLA:HBA2	25:c:501:CLA:H3A	1.60	0.48
2:A:60:ILE:HD12	2:A:84:PRO:HD2	1.95	0.48
36:Y:303:CHL:HHC	36:Y:303:CHL:HBB1	1.95	0.48
25:b:511:CLA:H2A	25:b:511:CLA:O1D	2.13	0.48
36:G:605:CHL:HHC	36:G:605:CHL:HBB1	1.95	0.48
25:c:511:CLA:H93	27:k:101:BCR:H272	1.95	0.48
25:S:602:CLA:H3A	25:S:602:CLA:HBA2	1.50	0.48
4:C:224:GLY:C	27:C:515:BCR:H383	2.39	0.48
8:G:41:LEU:HB2	8:G:45:SER:HB2	1.96	0.48
25:b:502:CLA:H43	9:h:65:LEU:HA	1.95	0.48
2:A:32:TRP:O	2:A:35:VAL:HG12	2.14	0.48
3:B:385:LYS:NZ	15:O:204:ASP:OD1	2.38	0.48
2:a:84:PRO:HA	2:a:112:TYR:CG	2.48	0.48
25:b:501:CLA:HMD1	27:h:101:BCR:H272	1.95	0.48
7:F:18:ARG:NH2	35:F:101:HEM:O2A	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:r:249:PHE:CZ	39:r:309:XAT:H10	2.49	0.48
11:K:29:PRO:O	11:K:32:PHE:HB2	2.14	0.47
16:S:105:LEU:HD23	16:S:210:LEU:HB3	1.96	0.47
3:b:99:ALA:HB1	25:b:506:CLA:H51	1.96	0.47
30:d:407:LHG:H111	30:l:101:LHG:H102	1.95	0.47
5:D:129:GLN:NE2	26:D:402:PHO:OBD	2.47	0.47
7:F:23:HIS:NE2	35:F:101:HEM:C4B	2.81	0.47
1:1:237:PHE:O	1:1:244:ARG:NH1	2.47	0.47
2:A:278:TRP:HB3	2:A:279:PRO:HD3	1.97	0.47
3:B:236:THR:HB	3:B:473:THR:HG21	1.94	0.47
6:E:55:TYR:O	6:E:60:ARG:NH2	2.45	0.47
4:c:224:GLY:C	27:c:514:BCR:H383	2.39	0.47
25:c:506:CLA:H122	25:c:506:CLA:H162	1.50	0.47
2:A:257:ARG:O	5:D:128:ARG:NH2	2.48	0.47
25:S:605:CLA:HBD	25:S:605:CLA:HBA1	1.96	0.47
3:b:474:ILE:HD11	30:b:521:LHG:HC5	1.96	0.47
23:r:199:GLU:OE2	25:r:307:CLA:C4A	2.61	0.47
1:1:252:THR:O	1:1:256:ILE:HG12	2.14	0.47
5:D:29:PHE:O	5:D:128:ARG:NH1	2.47	0.47
21:Y:88:GLU:HA	21:Y:180:LEU:HD21	1.96	0.47
25:d:401:CLA:H3A	25:d:401:CLA:HBA2	1.54	0.47
11:k:37:PHE:HB3	27:v:101:BCR:H272	1.96	0.47
3:B:242:ILE:HA	3:B:245:VAL:HG22	1.97	0.47
5:D:126:MET:HE1	5:D:147:SER:HA	1.97	0.47
7:f:39:MET:O	7:f:42:ILE:HG22	2.14	0.47
2:A:106:LEU:HD11	27:A:406:BCR:H402	1.95	0.47
3:B:243:ALA:HA	3:B:246:PHE:CD2	2.50	0.47
25:C:513:CLA:H62	25:C:513:CLA:H41	1.69	0.47
5:D:65:THR:O	5:D:65:THR:OG1	2.33	0.47
6:E:57:THR:OG1	6:E:58:GLU:OE1	2.33	0.47
8:G:129:TYR:HB2	8:G:136:ILE:HD12	1.97	0.47
25:G:611:CLA:H3A	25:G:611:CLA:HBA2	1.46	0.47
16:S:154:VAL:CG1	16:S:155:PRO:HD2	2.44	0.47
36:Y:303:CHL:HBA1	36:Y:303:CHL:H3A	1.75	0.47
27:b:518:BCR:H351	27:b:518:BCR:H15C	1.73	0.47
3:B:103:LEU:HB2	25:B:506:CLA:H62	1.97	0.47
3:B:315:ILE:HG21	3:B:426:LEU:HD22	1.97	0.47
11:K:30:VAL:O	11:K:33:ILE:HG22	2.15	0.47
5:d:141:TYR:OH	30:d:407:LHG:O4	2.28	0.47
27:A:406:BCR:H15C	27:A:406:BCR:H351	1.78	0.47
4:C:129:GLU:OE1	4:C:137:TYR:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:G:617:NEX:H15	38:G:617:NEX:H201	1.73	0.47
18:V:15:VAL:CG1	27:V:101:BCR:H10C	2.44	0.47
7:f:23:HIS:HE1	35:f:101:HEM:C4D	2.32	0.47
18:v:13:VAL:HA	18:v:16:VAL:HG12	1.97	0.47
19:W:68:ASP:OD1	19:W:69:GLY:N	2.48	0.47
27:z:101:BCR:H15C	27:z:101:BCR:H351	1.78	0.47
27:v:101:BCR:H23C	27:v:101:BCR:H19C	1.96	0.46
35:F:101:HEM:HBC2	35:F:101:HEM:CHD	2.45	0.46
30:d:407:LHG:H111	30:l:101:LHG:HC81	1.96	0.46
4:C:225:HIS:HA	4:C:228:ILE:HG22	1.97	0.46
27:C:515:BCR:H382	27:C:515:BCR:H23C	1.97	0.46
5:d:126:MET:HE1	5:d:147:SER:HA	1.98	0.46
25:B:515:CLA:H61	25:B:515:CLA:H92	1.76	0.46
11:K:29:PRO:HA	11:K:32:PHE:HD2	1.80	0.46
27:a:406:BCR:H15C	27:a:406:BCR:H351	1.79	0.46
4:c:92:GLU:N	4:c:92:GLU:OE1	2.48	0.46
3:B:90:ILE:HD11	25:B:506:CLA:H202	1.97	0.46
3:b:41:GLU:OE1	3:b:63:LEU:N	2.45	0.46
3:b:334:ASP:OD1	3:b:334:ASP:N	2.46	0.46
27:h:101:BCR:H11C	27:h:101:BCR:H341	1.74	0.46
1:1:263:LEU:O	1:1:265:GLN:NE2	2.45	0.46
3:B:243:ALA:HA	3:B:246:PHE:CE2	2.51	0.46
25:N:312:CLA:HBD	25:N:313:CLA:OBD	2.16	0.46
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.74	0.46
8:G:132:ASN:HB3	8:G:135:LEU:HD13	1.98	0.46
39:G:620:XAT:H202	21:Y:153:LEU:HD21	1.98	0.46
27:H:101:BCR:H341	27:H:101:BCR:H11C	1.77	0.46
36:S:601:CHL:HBB1	36:S:601:CHL:HHC	1.98	0.46
25:S:610:CLA:HAB	37:S:615:LUT:H32	1.98	0.46
27:z:101:BCR:HC8	27:z:101:BCR:H321	1.98	0.46
12:l:25:ILE:HD13	13:m:18:PRO:HB2	1.97	0.46
1:1:202:LYS:O	1:1:205:GLU:HG3	2.16	0.46
1:1:307:ASP:OD1	1:1:308:LYS:N	2.49	0.46
15:O:94:LEU:HD11	15:O:288:ALA:HB1	1.97	0.46
16:S:110:TRP:CD1	25:S:609:CLA:HMD3	2.51	0.46
27:C:514:BCR:H11C	27:C:514:BCR:H341	1.82	0.46
4:c:211:TRP:CE3	4:c:212:ILE:HG12	2.51	0.46
4:C:16:GLN:OE1	5:D:230:ASN:ND2	2.41	0.45
4:C:166:LYS:HD3	25:C:502:CLA:H192	1.98	0.45
2:a:15:ALA:O	2:a:19:GLU:HG2	2.16	0.45
3:b:451:PHE:HE2	25:b:504:CLA:HMA3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:405:BCR:H15C	27:d:405:BCR:H351	1.86	0.45
5:D:103:ARG:NH2	6:E:77:LYS:HG3	2.31	0.45
8:G:205:MET:HE2	25:G:602:CLA:HMC3	1.97	0.45
36:G:606:CHL:OMC	37:G:616:LUT:H163	2.16	0.45
21:Y:171:GLY:H	36:Y:309:CHL:HMC	1.80	0.45
4:c:457:MET:HE2	5:d:251:ARG:NH2	2.31	0.45
5:d:103:ARG:HG2	6:e:73:LEU:HD12	1.98	0.45
17:t:12:GLY:O	17:t:16:ILE:HG12	2.16	0.45
4:C:66:GLU:OE1	4:C:66:GLU:N	2.44	0.45
3:b:192:PRO:HG3	9:h:68:TYR:CD1	2.52	0.45
4:c:50:PHE:HB2	4:c:110:SER:OG	2.15	0.45
4:C:166:LYS:NZ	4:C:172:GLY:O	2.49	0.45
18:V:33:LEU:HD23	18:V:33:LEU:H	1.82	0.45
9:H:56:LEU:HB3	27:H:101:BCR:H14C	1.99	0.45
16:S:87:PRO:O	37:S:616:LUT:O23	2.28	0.45
16:S:155:PRO:O	16:S:156:TRP:CG	2.70	0.45
2:A:283:ILE:HA	2:A:286:THR:HG22	1.98	0.45
37:G:616:LUT:H15	37:G:616:LUT:H201	1.82	0.45
38:N:318:NEX:H35	38:N:318:NEX:H401	1.79	0.45
3:b:298:LEU:HD23	3:b:298:LEU:HA	1.86	0.45
23:r:230:ARG:HD2	23:r:233:ARG:HE	1.82	0.45
16:S:110:TRP:HD1	25:S:609:CLA:HMD3	1.82	0.45
5:d:56:THR:OG1	5:d:69:GLU:OE2	2.30	0.45
5:d:70:GLY:O	7:f:44:ARG:NH1	2.49	0.45
27:D:406:BCR:H20C	27:D:406:BCR:H361	1.81	0.45
36:N:302:CHL:H141	36:N:302:CHL:H161	1.72	0.45
16:S:108:ALA:HB1	16:S:239:GLY:HA3	1.98	0.45
39:Y:302:XAT:H31	39:Y:302:XAT:H391	1.80	0.45
25:B:513:CLA:H2	25:B:513:CLA:HED3	2.00	0.44
27:H:101:BCR:H20C	27:H:101:BCR:H361	1.86	0.44
15:O:116:GLU:N	15:O:116:GLU:OE1	2.50	0.44
21:Y:95:ARG:HA	21:Y:98:MET:HE3	1.99	0.44
3:b:271:THR:HB	3:b:274:GLN:HG3	2.00	0.44
25:b:503:CLA:H3A	25:b:503:CLA:HBA2	1.52	0.44
25:b:507:CLA:HBA2	25:b:507:CLA:H3A	1.62	0.44
6:e:55:TYR:O	6:e:60:ARG:NH2	2.50	0.44
27:t:101:BCR:H11C	27:t:101:BCR:H341	1.79	0.44
4:c:146:THR:HG21	4:c:244:PRO:HD3	1.99	0.44
4:c:203:LYS:HG2	4:c:209:ASP:HB3	1.99	0.44
39:N:301:XAT:H35	39:N:301:XAT:H401	1.82	0.44
37:Y:317:LUT:H15	37:Y:317:LUT:H201	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:53:ASN:OD1	3:b:58:GLN:NE2	2.50	0.44
3:b:380:ASP:OD1	3:b:380:ASP:N	2.50	0.44
1:1:186:LYS:HE2	17:t:27:PRO:HG2	1.99	0.44
27:B:517:BCR:H11C	27:B:517:BCR:H341	1.88	0.44
36:N:310:CHL:H91	36:N:310:CHL:H112	1.79	0.44
30:N:319:LHG:O3	30:N:319:LHG:O1	2.35	0.44
15:O:180:ASP:N	15:O:180:ASP:OD1	2.49	0.44
27:t:101:BCR:H15C	27:t:101:BCR:H351	1.74	0.44
38:S:617:NEX:H35	38:S:617:NEX:H401	1.74	0.44
9:h:59:ALA:O	9:h:63:ILE:HG12	2.18	0.44
2:A:186:PHE:HE1	2:A:293:MET:SD	2.41	0.44
25:B:504:CLA:H92	25:B:504:CLA:H61	1.77	0.44
25:B:508:CLA:HMB2	5:D:126:MET:SD	2.58	0.44
2:A:84:PRO:HA	2:A:112:TYR:CG	2.52	0.44
38:G:617:NEX:H35	38:G:617:NEX:H401	1.83	0.44
7:f:42:ILE:HG13	7:f:43:GLN:H	1.83	0.44
2:A:325:ASN:HA	2:A:328:MET:HE3	1.99	0.44
27:B:518:BCR:H331	27:B:518:BCR:HC8	2.00	0.44
4:C:390:GLY:HA2	4:C:396:GLY:HA2	1.98	0.44
27:C:515:BCR:H11C	27:C:515:BCR:H341	1.84	0.44
38:G:617:NEX:H11	38:G:617:NEX:H191	1.75	0.44
15:O:109:GLU:HG3	15:O:117:THR:HG22	1.99	0.44
37:Y:317:LUT:H11	37:Y:317:LUT:H191	1.88	0.44
34:d:406:PL9:H322	30:l:101:LHG:H211	2.00	0.44
23:r:155:GLU:OE2	23:r:162:TRP:N	2.51	0.44
27:v:101:BCR:H24C	27:v:101:BCR:H371	1.56	0.44
14:N:124:LYS:HA	36:N:308:CHL:HED2	2.00	0.44
25:N:303:CLA:H141	25:N:303:CLA:H162	1.79	0.44
38:Y:318:NEX:H15	38:Y:318:NEX:H201	1.75	0.44
3:b:21:SER:OG	3:b:115:TRP:HB2	2.17	0.44
8:G:120:GLN:HB2	8:G:127:LEU:HD12	1.99	0.43
37:G:615:LUT:H11	37:G:615:LUT:H191	1.84	0.43
14:N:81:GLU:O	14:N:85:ARG:HG2	2.18	0.43
14:N:210:ARG:HA	14:N:213:MET:HE3	2.00	0.43
19:W:108:ASP:OD1	19:W:108:ASP:N	2.47	0.43
25:a:402:CLA:HBD	25:d:401:CLA:HAC2	1.99	0.43
3:b:460:LEU:HD23	3:b:460:LEU:HA	1.90	0.43
31:c:515:DGD:HO5E	31:c:515:DGD:HO4E	1.63	0.43
23:r:214:PRO:HB3	36:r:306:CHL:HBC2	2.00	0.43
25:B:509:CLA:H92	25:B:509:CLA:H62	1.70	0.43
4:C:104:VAL:HG23	27:C:516:BCR:H332	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:68:ASP:OD1	6:E:68:ASP:N	2.46	0.43
39:Y:302:XAT:H11	39:Y:302:XAT:H191	1.88	0.43
4:c:58:PHE:HE1	25:c:504:CLA:HED3	1.84	0.43
25:B:501:CLA:HBB2	27:H:101:BCR:H351	1.99	0.43
4:C:203:LYS:NZ	4:C:214:SER:OG	2.40	0.43
25:C:504:CLA:H141	25:C:504:CLA:H161	1.77	0.43
25:C:509:CLA:H141	25:C:509:CLA:H161	1.77	0.43
8:G:37:ARG:NH2	8:G:53:LEU:O	2.51	0.43
29:H:102:LMG:H111	29:H:102:LMG:H142	1.69	0.43
16:S:183:ARG:HG3	36:S:608:CHL:CHD	2.48	0.43
19:W:106:PHE:HD2	19:W:111:ASP:HB3	1.83	0.43
2:a:18:CYS:O	2:a:22:THR:HG22	2.18	0.43
2:a:174:LEU:HD22	26:a:404:PHO:H143	2.00	0.43
27:b:519:BCR:H15C	27:b:519:BCR:H351	1.76	0.43
29:B:519:LMG:H421	29:B:519:LMG:H392	1.84	0.43
2:A:188:ALA:HB2	2:A:328:MET:HB3	2.01	0.43
5:D:200:GLY:HA3	5:D:282:SER:OG	2.18	0.43
11:K:38:VAL:HG21	27:V:101:BCR:H19C	2.01	0.43
19:W:65:MET:HE2	19:W:77:ASN:HD21	1.84	0.43
38:Y:318:NEX:H35	38:Y:318:NEX:H401	1.79	0.43
2:a:45:THR:HB	26:a:404:PHO:H93	2.00	0.43
27:b:517:BCR:H15C	27:b:517:BCR:H351	1.72	0.43
1:1:189:GLN:HG2	4:c:457:MET:O	2.18	0.43
2:a:93:PHE:CE2	2:a:95:PRO:HG3	2.54	0.43
18:v:7:LEU:HA	18:v:10:VAL:HG22	2.00	0.43
18:v:31:GLY:HA2	22:z:30:PRO:HD3	2.01	0.43
3:B:2:GLY:N	12:L:12:GLU:OE2	2.51	0.43
4:C:238:TRP:HE3	32:C:522:LMU:H61	1.83	0.43
25:C:502:CLA:H92	25:C:512:CLA:H42	2.00	0.43
27:C:514:BCR:H20C	27:C:514:BCR:H361	1.89	0.43
8:G:46:GLU:N	8:G:46:GLU:OE1	2.52	0.43
22:Z:48:LEU:HD23	22:Z:48:LEU:HA	1.87	0.43
3:b:193:TYR:O	9:h:84:LEU:HD23	2.19	0.43
5:d:201:VAL:HG22	25:d:403:CLA:C1B	2.49	0.43
29:d:410:LMG:H111	29:d:410:LMG:H141	1.80	0.43
2:A:159:LEU:HD23	31:C:517:DGD:HBT1	2.01	0.43
29:B:519:LMG:H392	29:B:519:LMG:H361	1.75	0.43
4:C:163:LEU:HD22	25:C:501:CLA:C2D	2.48	0.43
4:C:440:ALA:HB1	19:W:113:LEU:HG	2.01	0.43
36:N:306:CHL:HED3	16:S:124:LEU:HD21	2.01	0.43
29:W:201:LMG:O5	29:W:201:LMG:O4	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:25:MET:HE1	3:b:108:PHE:CD1	2.54	0.43
3:b:260:SER:OG	3:b:261:ALA:N	2.52	0.43
3:B:157:HIS:HE1	25:B:506:CLA:NA	2.17	0.43
4:C:338:ILE:HG21	4:C:347:TRP:HB2	2.01	0.43
8:G:97:ILE:HD11	8:G:211:PHE:CZ	2.54	0.43
37:N:317:LUT:H11	37:N:317:LUT:H191	1.88	0.43
38:Y:318:NEX:H11	38:Y:318:NEX:H191	1.82	0.43
7:f:23:HIS:HE1	35:f:101:HEM:ND	2.16	0.43
32:C:522:LMU:H61	32:C:522:LMU:H92	1.73	0.42
3:b:103:LEU:HD22	25:b:506:CLA:H41	2.00	0.42
25:c:506:CLA:H71	25:c:506:CLA:H111	1.80	0.42
11:k:18:PHE:CE2	22:z:9:LEU:HD23	2.54	0.42
1:1:195:GLN:O	1:1:198:GLU:HG3	2.19	0.42
2:A:195:HIS:ND1	2:A:196:PRO:HD2	2.34	0.42
3:B:297:SER:OG	3:B:300:ASP:OD2	2.32	0.42
7:F:16:THR:HG23	7:F:19:TRP:H	1.84	0.42
8:G:97:ILE:HD11	8:G:211:PHE:HZ	1.84	0.42
36:G:607:CHL:HHC	36:G:607:CHL:HBB1	2.01	0.42
14:N:60:TYR:OH	14:N:72:ASP:OD2	2.30	0.42
37:N:317:LUT:H15	37:N:317:LUT:H201	1.83	0.42
37:S:616:LUT:H15	37:S:616:LUT:H201	1.84	0.42
25:b:502:CLA:H143	25:b:502:CLA:H162	1.79	0.42
4:c:45:ALA:O	4:c:49:VAL:HG22	2.19	0.42
4:C:458:ARG:HG3	4:C:459:PRO:HD2	2.01	0.42
27:C:516:BCR:H24C	27:C:516:BCR:H371	1.70	0.42
15:O:144:ASP:OD1	15:O:145:GLY:N	2.53	0.42
2:a:106:LEU:HD21	27:a:406:BCR:H402	2.01	0.42
2:A:63:ILE:HG13	2:A:65:GLU:HG2	1.99	0.42
3:b:477:ASP:OD1	3:b:477:ASP:N	2.51	0.42
5:d:88:SER:OG	6:e:69:ARG:NH2	2.53	0.42
2:A:57:PRO:HB2	2:A:66:PRO:HB2	2.02	0.42
25:B:502:CLA:H43	9:H:64:ILE:HG22	2.01	0.42
27:B:517:BCR:H24C	27:B:517:BCR:H371	1.78	0.42
4:C:448:ASP:OD2	4:C:451:ASP:N	2.53	0.42
27:c:514:BCR:H341	27:c:514:BCR:H11C	1.80	0.42
27:h:101:BCR:H15C	27:h:101:BCR:H351	1.80	0.42
23:r:232:PHE:O	23:r:236:THR:HG23	2.19	0.42
3:B:21:SER:OG	3:B:115:TRP:HB2	2.19	0.42
4:C:201:LEU:O	4:C:211:TRP:NE1	2.46	0.42
36:N:302:CHL:HBA1	36:N:302:CHL:H3A	1.87	0.42
25:a:405:CLA:H42	10:i:9:TYR:HE1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:r:233:ARG:O	23:r:236:THR:OG1	2.29	0.42
27:v:101:BCR:H20C	27:v:101:BCR:H361	1.44	0.42
25:D:405:CLA:O1D	25:D:405:CLA:H2A	2.19	0.42
10:i:2:LEU:O	10:i:6:ILE:HG12	2.20	0.42
23:r:249:PHE:CE1	39:r:309:XAT:H12	2.54	0.42
25:B:501:CLA:H142	25:B:501:CLA:H112	1.90	0.42
16:S:243:MET:HE3	25:S:602:CLA:HMC3	2.02	0.42
3:b:119:ASP:OD1	3:b:124:ARG:NH2	2.53	0.42
25:B:502:CLA:H122	25:B:502:CLA:H162	1.89	0.42
25:B:512:CLA:HBA1	25:B:512:CLA:H3A	1.91	0.42
21:Y:206:ILE:HD12	21:Y:206:ILE:HA	1.95	0.42
37:Y:317:LUT:H35	37:Y:317:LUT:H401	1.81	0.42
25:c:509:CLA:H93	25:c:509:CLA:H111	1.78	0.42
27:k:101:BCR:H11C	27:k:101:BCR:H341	1.91	0.42
27:t:101:BCR:H24C	27:t:101:BCR:H371	1.89	0.42
5:D:49:LEU:HD13	27:D:406:BCR:C15	2.50	0.42
7:F:36:ILE:HA	7:F:39:MET:HE3	2.02	0.42
23:r:143:TRP:CE2	36:r:306:CHL:HED2	2.55	0.42
25:B:503:CLA:H41	25:B:503:CLA:H61	1.88	0.41
27:C:515:BCR:H20C	27:C:515:BCR:H361	1.94	0.41
14:N:49:LEU:HB2	14:N:53:SER:HB3	2.02	0.41
15:O:79:SER:OG	15:O:80:GLY:N	2.53	0.41
16:S:119:LEU:HD23	16:S:119:LEU:HA	1.90	0.41
2:a:57:PRO:HB2	2:a:66:PRO:HB2	2.02	0.41
39:r:309:XAT:H401	39:r:309:XAT:H35	1.77	0.41
2:A:183:MET:HB3	25:A:402:CLA:HBC2	2.02	0.41
3:B:315:ILE:HG22	3:B:426:LEU:HB3	2.02	0.41
8:G:33:TYR:HE2	8:G:191:ALA:HB1	1.83	0.41
8:G:161:ASN:HD22	14:N:52:TYR:HA	1.85	0.41
3:b:313:ASP:OD1	3:b:358:ARG:NH1	2.53	0.41
27:b:519:BCR:H11C	27:b:519:BCR:H341	1.80	0.41
38:r:310:NEX:H11	38:r:310:NEX:H191	1.80	0.41
3:B:255:THR:HG21	25:B:502:CLA:HED1	2.03	0.41
4:C:56:ASN:C	4:C:56:ASN:HD22	2.28	0.41
39:G:620:XAT:H11	39:G:620:XAT:H191	1.87	0.41
15:O:72:ASN:ND2	15:O:128:LEU:HB3	2.36	0.41
37:Y:316:LUT:H35	37:Y:316:LUT:H401	1.77	0.41
2:A:261:GLN:OE1	2:A:261:GLN:HA	2.20	0.41
25:C:504:CLA:H93	25:C:504:CLA:H111	1.87	0.41
15:O:163:GLN:HA	15:O:169:ARG:HA	2.03	0.41
36:Y:310:CHL:H143	36:Y:310:CHL:H161	1.72	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:319:PRO:HB3	3:b:446:SER:HB3	2.02	0.41
27:h:101:BCR:H24C	27:h:101:BCR:H371	1.85	0.41
38:r:310:NEX:H15	38:r:310:NEX:H201	1.74	0.41
27:B:518:BCR:H11C	27:B:518:BCR:H341	1.87	0.41
5:D:14:TRP:NE1	20:X:91:THR:OG1	2.51	0.41
5:D:103:ARG:O	5:D:107:LEU:HB2	2.20	0.41
5:D:197:HIS:O	5:D:201:VAL:HG12	2.21	0.41
6:E:75:GLN:HA	6:E:78:LYS:HG2	2.01	0.41
8:G:83:LEU:HD12	8:G:83:LEU:HA	1.90	0.41
39:Y:302:XAT:H35	39:Y:302:XAT:H401	1.81	0.41
3:b:474:ILE:HG23	3:b:475:PHE:CD1	2.55	0.41
25:b:510:CLA:H2	25:b:510:CLA:H61	1.71	0.41
27:k:101:BCR:H371	27:k:101:BCR:H24C	1.66	0.41
14:N:91:LEU:HD12	14:N:91:LEU:HA	1.90	0.41
14:N:140:ASN:HB3	14:N:143:LEU:HD13	2.03	0.41
39:N:301:XAT:H31	39:N:301:XAT:H391	1.87	0.41
19:W:65:MET:HE2	19:W:65:MET:HB3	2.00	0.41
4:c:37:LEU:HD12	4:c:37:LEU:HA	1.86	0.41
25:c:506:CLA:H171	25:c:506:CLA:H51	2.03	0.41
27:d:405:BCR:H20C	27:d:405:BCR:H361	1.88	0.41
11:k:28:ILE:H	11:k:28:ILE:HD12	1.86	0.41
11:k:35:LEU:HA	11:k:38:VAL:HG12	2.02	0.41
22:z:15:VAL:HG11	22:z:50:LEU:HD12	2.02	0.41
27:z:101:BCR:H20C	27:z:101:BCR:H361	1.84	0.41
25:B:516:CLA:OBD	9:H:24:THR:HG21	2.21	0.41
8:G:80:GLU:O	8:G:84:ILE:HG12	2.21	0.41
36:N:306:CHL:H102	16:S:120:ILE:HD11	2.03	0.41
36:S:601:CHL:O1D	30:S:618:LHG:H121	2.21	0.41
19:W:73:PRO:O	19:W:76:VAL:HG22	2.21	0.41
3:b:193:TYR:HB2	9:h:83:THR:OG1	2.21	0.41
3:b:300:ASP:N	3:b:300:ASP:OD1	2.51	0.41
4:c:288:GLU:OE1	4:c:288:GLU:N	2.52	0.41
22:z:19:LEU:HD11	22:z:44:LEU:HD12	2.03	0.41
27:A:406:BCR:HC31	10:I:15:PHE:HE1	1.85	0.41
6:E:62:GLU:OE1	6:E:62:GLU:HA	2.20	0.41
37:S:615:LUT:H11	37:S:615:LUT:H191	1.89	0.41
22:z:35:ASP:OD1	22:z:36:ASN:N	2.53	0.41
1:1:223:LEU:HD21	1:1:260:TYR:CZ	2.56	0.41
2:A:175:GLY:O	2:A:179:THR:HG23	2.20	0.41
25:B:506:CLA:H112	25:B:506:CLA:H152	1.87	0.41
4:C:104:VAL:HG11	27:C:514:BCR:HC32	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:285:TYR:O	4:C:411:ARG:NH2	2.53	0.41
25:D:405:CLA:H42	9:H:62:LEU:HD11	2.03	0.41
27:H:101:BCR:H351	27:H:101:BCR:H15C	1.76	0.41
25:N:305:CLA:H92	25:N:305:CLA:H62	1.96	0.41
37:S:615:LUT:H15	37:S:615:LUT:H201	1.86	0.41
37:S:616:LUT:H401	37:S:616:LUT:H35	1.77	0.41
3:b:69:LEU:HD12	25:b:505:CLA:HBA1	2.03	0.41
4:c:37:LEU:HG	4:c:41:HIS:CE1	2.55	0.41
4:c:267:ILE:HG12	25:c:502:CLA:HAC1	2.02	0.41
11:k:19:ALA:N	11:k:20:PRO:HD2	2.36	0.41
27:D:406:BCR:H15C	27:D:406:BCR:H351	1.85	0.41
36:G:601:CHL:H62	36:G:601:CHL:H41	1.96	0.41
39:Y:302:XAT:H373	39:Y:302:XAT:H23	1.92	0.41
11:k:28:ILE:N	11:k:29:PRO:HD2	2.36	0.41
2:A:105:TRP:NE1	2:A:110:GLY:HA3	2.35	0.40
26:A:404:PHO:HAB	5:D:205:LEU:HD13	2.03	0.40
25:B:514:CLA:H112	25:B:514:CLA:H91	1.90	0.40
9:H:79:MET:HE2	9:H:79:MET:HA	2.02	0.40
37:N:316:LUT:H401	37:N:316:LUT:H35	1.79	0.40
21:Y:132:GLU:OE1	21:Y:132:GLU:N	2.50	0.40
5:d:90:LEU:HD12	5:d:90:LEU:HA	1.89	0.40
30:l:101:LHG:H141	30:l:101:LHG:H111	1.93	0.40
23:r:145:MET:HE3	25:r:308:CLA:HMC2	2.02	0.40
3:B:34:ALA:HB2	25:B:505:CLA:HMD2	2.04	0.40
2:a:35:VAL:HG11	10:i:18:LEU:HD23	2.02	0.40
4:c:364:ASP:HB3	4:c:367:LYS:HB2	2.03	0.40
22:z:50:LEU:HD23	22:z:50:LEU:HA	1.77	0.40
1:1:307:ASP:OD1	1:1:307:ASP:C	2.65	0.40
26:A:404:PHO:H61	26:A:404:PHO:H2	1.77	0.40
3:B:65:PHE:HE1	25:B:504:CLA:HED2	1.86	0.40
3:B:273:TYR:HA	3:B:276:ASP:HB2	2.03	0.40
3:B:334:ASP:OD1	3:B:334:ASP:C	2.65	0.40
25:B:516:CLA:H11	25:B:516:CLA:H52	1.75	0.40
8:G:135:LEU:O	8:G:137:HIS:N	2.51	0.40
25:b:506:CLA:HBA2	25:b:506:CLA:H3A	1.36	0.40
2:A:70:SER:O	2:A:75:ASN:HB2	2.21	0.40
3:B:22:VAL:HG13	25:B:514:CLA:HMB3	2.03	0.40
39:N:301:XAT:H201	39:N:301:XAT:H15	1.78	0.40
15:O:86:GLU:OE1	15:O:86:GLU:N	2.54	0.40
37:Y:316:LUT:H11	37:Y:316:LUT:H191	1.88	0.40
3:b:160:GLY:HA3	3:b:180:PRO:HB3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:406:BCR:H20C	27:A:406:BCR:H361	1.90	0.40
3:B:434:ARG:HB2	3:B:439:SER:HB2	2.04	0.40
15:O:99:ILE:HG23	15:O:262:PHE:CE1	2.56	0.40
3:b:315:ILE:HG22	3:b:426:LEU:HB3	2.04	0.40
4:c:69:MET:HE3	4:c:69:MET:HB2	1.93	0.40

There are no symmetry-related clashes.

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	1	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
2	A	311/335 (93%)	304 (98%)	7 (2%)	0	100	100
2	a	300/335 (90%)	295 (98%)	5 (2%)	0	100	100
3	B	478/481 (99%)	472 (99%)	6 (1%)	0	100	100
3	b	479/481 (100%)	468 (98%)	11 (2%)	0	100	100
4	C	447/449 (100%)	440 (98%)	7 (2%)	0	100	100
4	c	434/449 (97%)	418 (96%)	16 (4%)	0	100	100
5	D	346/351 (99%)	341 (99%)	5 (1%)	0	100	100
5	d	333/351 (95%)	325 (98%)	8 (2%)	0	100	100
6	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	e	69/75 (92%)	67 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	G	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
9	H	66/69 (96%)	66 (100%)	0	0	100	100
9	h	66/69 (96%)	63 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	33/35 (94%)	33 (100%)	0	0	100	100
10	i	32/35 (91%)	31 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	L	34/37 (92%)	34 (100%)	0	0	100	100
12	l	35/37 (95%)	35 (100%)	0	0	100	100
13	M	28/31 (90%)	28 (100%)	0	0	100	100
13	m	28/31 (90%)	28 (100%)	0	0	100	100
14	N	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	25	56
15	O	203/240 (85%)	197 (97%)	6 (3%)	0	100	100
16	S	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	16	45
17	T	28/30 (93%)	28 (100%)	0	0	100	100
17	t	25/30 (83%)	25 (100%)	0	0	100	100
18	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
18	v	30/32 (94%)	30 (100%)	0	0	100	100
19	W	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
20	X	30/32 (94%)	30 (100%)	0	0	100	100
20	x	30/32 (94%)	30 (100%)	0	0	100	100
21	Y	218/220 (99%)	213 (98%)	5 (2%)	0	100	100
22	Z	59/61 (97%)	59 (100%)	0	0	100	100
22	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
23	r	156/201 (78%)	148 (95%)	8 (5%)	0	100	100
All	All	5481/5736 (96%)	5351 (98%)	127 (2%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	S	155	PRO
16	S	156	TRP
14	N	144	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	1	132/132 (100%)	132 (100%)	0	100	100
2	A	256/273 (94%)	256 (100%)	0	100	100
2	a	247/273 (90%)	247 (100%)	0	100	100
3	B	382/383 (100%)	382 (100%)	0	100	100
3	b	383/383 (100%)	383 (100%)	0	100	100
4	C	352/352 (100%)	352 (100%)	0	100	100
4	c	346/352 (98%)	346 (100%)	0	100	100
5	D	278/280 (99%)	278 (100%)	0	100	100
5	d	270/280 (96%)	270 (100%)	0	100	100
6	E	66/66 (100%)	66 (100%)	0	100	100
6	e	62/66 (94%)	62 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	G	164/164 (100%)	164 (100%)	0	100	100
9	H	58/59 (98%)	58 (100%)	0	100	100
9	h	58/59 (98%)	58 (100%)	0	100	100
10	I	32/32 (100%)	32 (100%)	0	100	100
10	i	31/32 (97%)	31 (100%)	0	100	100
11	K	31/31 (100%)	31 (100%)	0	100	100
11	k	31/31 (100%)	31 (100%)	0	100	100
12	L	34/34 (100%)	34 (100%)	0	100	100
12	l	34/34 (100%)	34 (100%)	0	100	100
13	M	26/27 (96%)	26 (100%)	0	100	100
13	m	26/27 (96%)	26 (100%)	0	100	100
14	N	169/169 (100%)	169 (100%)	0	100	100
15	O	171/195 (88%)	171 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	S	188/188 (100%)	188 (100%)	0	100	100
17	T	27/27 (100%)	27 (100%)	0	100	100
17	t	24/27 (89%)	24 (100%)	0	100	100
18	V	26/26 (100%)	26 (100%)	0	100	100
18	v	26/26 (100%)	26 (100%)	0	100	100
19	W	44/44 (100%)	44 (100%)	0	100	100
20	X	22/22 (100%)	22 (100%)	0	100	100
20	x	22/22 (100%)	22 (100%)	0	100	100
21	Y	169/169 (100%)	169 (100%)	0	100	100
22	Z	51/51 (100%)	51 (100%)	0	100	100
22	z	51/51 (100%)	51 (100%)	0	100	100
23	r	127/161 (79%)	127 (100%)	0	100	100
All	All	4466/4598 (97%)	4466 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	192	ASN
2	A	108	ASN
2	A	304	GLN
2	A	332	HIS
4	C	106	HIS
4	C	310	GLN
5	D	106	GLN
8	G	105	ASN
14	N	148	ASN
21	Y	147	GLN
2	a	322	ASN
2	a	332	HIS
3	b	179	GLN
4	c	370	ASN
5	d	164	GLN
7	f	43	GLN

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 223 ligands modelled in this entry, 2 are monoatomic - leaving 221 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	$\#\|Z\| > 2$
25	CLA	B	514	-	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
38	NEX	N	318	-	38,46,46	0.98	2 (5%)	50,70,70	2.26	12 (24%)
30	LHG	Y	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.05	3 (5%)
39	XAT	r	309	-	39,47,47	0.89	0	54,74,74	2.74	19 (35%)
25	CLA	C	511	4	65,73,73	1.51	6 (9%)	76,113,113	1.32	7 (9%)
25	CLA	B	509	-	65,73,73	1.51	5 (7%)	76,113,113	1.28	8 (10%)
25	CLA	a	403	-	49,57,73	1.72	7 (14%)	55,93,113	1.45	8 (14%)
25	CLA	b	502	-	65,73,73	1.49	6 (9%)	76,113,113	1.29	9 (11%)
27	BCR	h	101	-	41,41,41	0.72	0	56,56,56	2.03	13 (23%)
25	CLA	c	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.20	7 (9%)
25	CLA	S	613	16	49,57,73	1.77	7 (14%)	55,93,113	1.38	8 (14%)
36	CHL	N	308	-	66,74,74	1.89	15 (22%)	73,114,114	2.75	22 (30%)
30	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	4 (7%)
37	LUT	N	316	-	42,43,43	0.77	0	51,60,60	1.63	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	PL9	D	407	-	55,55,55	1.26	4 (7%)	68,69,69	1.54	13 (19%)
25	CLA	B	512	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
25	CLA	D	405	-	65,73,73	1.51	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	S	611	30	49,57,73	1.70	6 (12%)	55,93,113	1.44	7 (12%)
25	CLA	Y	315	-	54,62,73	1.64	6 (11%)	62,99,113	1.34	7 (11%)
25	CLA	S	604	-	49,57,73	1.73	6 (12%)	55,93,113	1.43	8 (14%)
25	CLA	Y	304	21	65,73,73	1.48	6 (9%)	76,113,113	1.27	7 (9%)
27	BCR	H	101	-	41,41,41	0.73	0	56,56,56	2.01	14 (25%)
27	BCR	C	516	-	41,41,41	0.75	0	56,56,56	2.04	19 (33%)
27	BCR	d	405	-	41,41,41	0.76	1 (2%)	56,56,56	2.14	18 (32%)
27	BCR	v	101	-	41,41,41	0.75	0	56,56,56	2.52	19 (33%)
25	CLA	D	404	-	65,73,73	1.51	7 (10%)	76,113,113	1.29	9 (11%)
25	CLA	S	602	16	49,57,73	1.74	7 (14%)	55,93,113	1.38	9 (16%)
25	CLA	a	405	-	60,68,73	1.54	6 (10%)	70,107,113	1.35	7 (10%)
36	CHL	S	601	16	46,54,74	2.27	14 (30%)	49,90,114	3.29	20 (40%)
25	CLA	r	307	23	45,53,73	1.92	7 (15%)	52,89,113	1.40	7 (13%)
31	DGD	Y	301	-	67,67,67	0.84	2 (2%)	81,81,81	0.90	3 (3%)
25	CLA	b	514	-	45,53,73	1.80	6 (13%)	52,89,113	1.44	7 (13%)
30	LHG	S	618	25	44,44,48	0.95	2 (4%)	47,50,54	1.12	3 (6%)
29	LMG	D	410	-	46,46,55	0.97	2 (4%)	54,54,63	1.02	3 (5%)
32	LMU	c	519	-	36,36,36	1.16	2 (5%)	47,47,47	0.93	1 (2%)
36	CHL	Y	308	-	46,54,74	2.29	16 (34%)	49,90,114	3.24	18 (36%)
25	CLA	c	503	-	65,73,73	1.51	6 (9%)	76,113,113	1.32	8 (10%)
25	CLA	Y	305	-	65,73,73	1.50	6 (9%)	76,113,113	1.31	6 (7%)
28	SQD	A	407	-	50,51,54	1.20	4 (8%)	59,62,65	1.19	4 (6%)
27	BCR	V	101	-	41,41,41	0.79	1 (2%)	56,56,56	1.89	17 (30%)
25	CLA	B	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	7 (9%)
25	CLA	r	301	23	60,68,73	1.60	6 (10%)	70,107,113	1.30	7 (10%)
27	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	1.94	16 (28%)
38	NEX	Y	318	-	38,46,46	0.96	1 (2%)	50,70,70	2.34	12 (24%)
34	PL9	d	406	-	55,55,55	1.27	5 (9%)	68,69,69	1.55	13 (19%)
26	PHO	D	402	-	51,69,69	1.00	4 (7%)	47,99,99	1.17	5 (10%)
29	LMG	d	410	-	48,48,55	0.94	2 (4%)	56,56,63	1.05	4 (7%)
25	CLA	Y	314	21	65,73,73	1.52	6 (9%)	76,113,113	1.29	7 (9%)
36	CHL	G	608	-	44,52,74	2.24	14 (31%)	46,87,114	3.25	18 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	C	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.22	7 (9%)
25	CLA	c	501	-	65,73,73	1.53	7 (10%)	76,113,113	1.26	9 (11%)
25	CLA	b	501	-	65,73,73	1.53	7 (10%)	76,113,113	1.25	7 (9%)
28	SQD	a	407	-	50,51,54	1.20	4 (8%)	59,62,65	1.13	4 (6%)
29	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	0.97	3 (5%)
25	CLA	S	610	16	49,57,73	1.72	7 (14%)	55,93,113	1.36	8 (14%)
25	CLA	C	507	-	65,73,73	1.48	6 (9%)	76,113,113	1.34	7 (9%)
29	LMG	H	102	-	48,48,55	0.97	2 (4%)	56,56,63	1.04	3 (5%)
36	CHL	r	304	-	44,52,74	2.25	14 (31%)	46,87,114	3.29	18 (39%)
25	CLA	A	402	-	65,73,73	1.51	7 (10%)	76,113,113	1.28	6 (7%)
25	CLA	C	504	-	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
36	CHL	N	310	14	66,74,74	1.93	15 (22%)	73,114,114	2.75	21 (28%)
25	CLA	B	501	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	7 (9%)
37	LUT	Y	317	-	42,43,43	0.80	0	51,60,60	1.68	11 (21%)
27	BCR	B	517	-	41,41,41	0.72	0	56,56,56	2.64	19 (33%)
30	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
25	CLA	G	613	8	65,73,73	1.51	5 (7%)	76,113,113	1.29	7 (9%)
25	CLA	d	404	-	42,50,73	1.86	6 (14%)	48,85,113	1.51	7 (14%)
37	LUT	S	616	-	42,43,43	0.82	0	51,60,60	1.74	17 (33%)
31	DGD	c	516	-	50,50,67	0.96	2 (4%)	64,64,81	1.04	3 (4%)
25	CLA	C	513	-	65,73,73	1.48	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	D	401	-	65,73,73	1.50	7 (10%)	76,113,113	1.35	10 (13%)
25	CLA	b	507	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	8 (10%)
25	CLA	N	315	-	42,50,73	1.87	6 (14%)	48,85,113	1.36	7 (14%)
32	LMU	C	523	-	36,36,36	1.16	2 (5%)	47,47,47	0.98	2 (4%)
25	CLA	c	502	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	9 (11%)
30	LHG	D	409	-	38,38,48	1.03	2 (5%)	41,44,54	1.09	2 (4%)
36	CHL	S	607	-	43,51,74	2.28	15 (34%)	45,86,114	3.33	18 (40%)
25	CLA	b	509	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	c	506	-	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
37	LUT	G	616	-	42,43,43	0.80	0	51,60,60	1.64	12 (23%)
25	CLA	C	502	-	65,73,73	1.50	8 (12%)	76,113,113	1.30	7 (9%)
25	CLA	B	508	-	65,73,73	1.51	6 (9%)	76,113,113	1.26	8 (10%)
25	CLA	c	512	-	56,64,73	1.63	7 (12%)	65,102,113	1.38	7 (10%)
30	LHG	b	521	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	G	614	-	42,50,73	1.85	6 (14%)	48,85,113	1.42	7 (14%)
31	DGD	c	517	-	60,60,67	0.88	2 (3%)	74,74,81	1.00	3 (4%)
32	LMU	S	619	-	36,36,36	1.15	2 (5%)	47,47,47	0.92	1 (2%)
25	CLA	S	612	16	45,53,73	1.79	6 (13%)	52,89,113	1.45	7 (13%)
36	CHL	N	307	-	46,54,74	2.30	16 (34%)	49,90,114	3.21	18 (36%)
30	LHG	a	411	-	43,43,48	0.99	2 (4%)	46,49,54	1.02	3 (6%)
39	XAT	N	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.73	20 (37%)
33	BCT	D	403	24	2,3,3	1.26	0	2,3,3	4.14	2 (100%)
36	CHL	G	619	-	66,74,74	1.90	15 (22%)	73,114,114	2.76	22 (30%)
31	DGD	C	519	-	60,60,67	0.89	2 (3%)	74,74,81	0.89	3 (4%)
27	BCR	b	517	-	41,41,41	0.75	1 (2%)	56,56,56	1.93	16 (28%)
25	CLA	c	507	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
29	LMG	W	201	-	48,48,55	0.95	2 (4%)	56,56,63	1.07	4 (7%)
25	CLA	Y	306	-	58,66,73	1.58	5 (8%)	67,104,113	1.38	9 (13%)
25	CLA	C	509	-	65,73,73	1.49	5 (7%)	76,113,113	1.33	6 (7%)
25	CLA	S	605	16	50,58,73	1.72	7 (14%)	58,95,113	1.43	8 (13%)
30	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	3 (5%)
39	XAT	Y	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.76	19 (35%)
25	CLA	S	609	16	41,49,73	1.89	7 (17%)	47,84,113	1.45	7 (14%)
27	BCR	k	101	-	41,41,41	0.74	1 (2%)	56,56,56	2.08	16 (28%)
25	CLA	G	603	-	65,73,73	1.52	7 (10%)	76,113,113	1.29	7 (9%)
28	SQD	t	102	-	53,54,54	1.18	4 (7%)	62,65,65	1.05	5 (8%)
38	NEX	r	310	-	38,46,46	0.99	1 (2%)	50,70,70	2.36	14 (28%)
25	CLA	N	313	14	45,53,73	1.83	7 (15%)	52,89,113	1.42	6 (11%)
26	PHO	a	404	-	51,69,69	1.02	4 (7%)	47,99,99	1.19	6 (12%)
36	CHL	G	606	-	43,51,74	2.24	15 (34%)	45,86,114	3.33	19 (42%)
27	BCR	b	519	-	41,41,41	0.75	0	56,56,56	2.01	15 (26%)
25	CLA	b	512	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
30	LHG	N	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
25	CLA	N	311	14	65,73,73	1.49	6 (9%)	76,113,113	1.22	7 (9%)
25	CLA	G	602	8	65,73,73	1.49	6 (9%)	76,113,113	1.27	7 (9%)
25	CLA	B	503	-	65,73,73	1.51	6 (9%)	76,113,113	1.26	7 (9%)
25	CLA	B	507	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	6 (7%)
25	CLA	G	612	8	43,51,73	1.83	7 (16%)	49,86,113	1.41	6 (12%)
25	CLA	C	512	-	65,73,73	1.53	7 (10%)	76,113,113	1.25	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	a	402	-	65,73,73	1.50	7 (10%)	76,113,113	1.28	8 (10%)
36	CHL	Y	303	21	66,74,74	1.90	14 (21%)	73,114,114	2.73	22 (30%)
37	LUT	Y	316	-	42,43,43	0.77	0	51,60,60	1.67	13 (25%)
27	BCR	B	518	-	41,41,41	0.76	0	56,56,56	1.93	13 (23%)
25	CLA	G	611	30	45,53,73	1.79	6 (13%)	52,89,113	1.47	6 (11%)
25	CLA	r	308	23	41,49,73	1.95	7 (17%)	47,84,113	1.48	6 (12%)
27	BCR	c	514	-	41,41,41	0.76	1 (2%)	56,56,56	1.97	14 (25%)
25	CLA	r	302	-	46,54,73	1.80	6 (13%)	53,90,113	1.47	7 (13%)
36	CHL	S	608	-	49,57,74	2.20	15 (30%)	52,93,114	3.13	20 (38%)
36	CHL	S	606	-	44,52,74	2.22	15 (34%)	46,87,114	3.32	19 (41%)
31	DGD	W	202	-	67,67,67	0.84	2 (2%)	81,81,81	0.96	5 (6%)
39	XAT	G	620	-	39,47,47	0.91	1 (2%)	54,74,74	4.21	23 (42%)
35	HEM	f	101	7,6	41,50,50	1.48	3 (7%)	45,82,82	1.44	6 (13%)
38	NEX	G	617	-	38,46,46	0.97	1 (2%)	50,70,70	2.40	15 (30%)
25	CLA	S	614	-	48,56,73	1.77	7 (14%)	55,92,113	1.36	8 (14%)
25	CLA	B	515	-	65,73,73	1.50	5 (7%)	76,113,113	1.25	6 (7%)
36	CHL	Y	310	21	66,74,74	1.95	15 (22%)	73,114,114	2.68	22 (30%)
25	CLA	b	506	-	65,73,73	1.50	6 (9%)	76,113,113	1.28	7 (9%)
25	CLA	b	515	-	65,73,73	1.50	7 (10%)	76,113,113	1.28	6 (7%)
35	HEM	F	101	7,6	41,50,50	1.55	6 (14%)	45,82,82	1.12	3 (6%)
25	CLA	G	610	8	65,73,73	1.51	5 (7%)	76,113,113	1.26	7 (9%)
25	CLA	Y	312	30	65,73,73	1.51	6 (9%)	76,113,113	1.28	8 (10%)
25	CLA	C	503	-	65,73,73	1.50	5 (7%)	76,113,113	1.28	8 (10%)
25	CLA	B	502	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	8 (10%)
25	CLA	d	403	-	65,73,73	1.51	7 (10%)	76,113,113	1.34	9 (11%)
31	DGD	c	515	-	54,54,67	0.92	2 (3%)	68,68,81	1.03	4 (5%)
25	CLA	b	513	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
25	CLA	B	506	-	65,73,73	1.51	7 (10%)	76,113,113	1.26	8 (10%)
27	BCR	C	514	-	41,41,41	0.79	1 (2%)	56,56,56	1.89	14 (25%)
36	CHL	N	306	14	66,74,74	1.90	15 (22%)	73,114,114	2.74	21 (28%)
25	CLA	C	506	-	65,73,73	1.51	6 (9%)	76,113,113	1.29	9 (11%)
29	LMG	d	409	-	41,41,55	1.03	2 (4%)	49,49,63	1.08	3 (6%)
30	LHG	a	410	-	42,42,48	0.99	2 (4%)	45,48,54	1.12	2 (4%)
36	CHL	G	607	-	50,58,74	2.19	15 (30%)	52,94,114	3.17	20 (38%)
29	LMG	B	519	-	51,51,55	0.92	2 (3%)	59,59,63	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	A	403	-	49,57,73	1.73	7 (14%)	55,93,113	1.45	8 (14%)
27	BCR	A	406	-	41,41,41	0.76	0	56,56,56	1.92	12 (21%)
36	CHL	N	302	14	66,74,74	1.91	15 (22%)	73,114,114	2.76	22 (30%)
29	LMG	b	520	-	42,42,55	1.00	2 (4%)	50,50,63	1.03	3 (6%)
25	CLA	b	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.25	7 (9%)
25	CLA	d	401	-	65,73,73	1.54	7 (10%)	76,113,113	1.33	10 (13%)
25	CLA	N	312	30	49,57,73	1.74	6 (12%)	55,93,113	1.39	6 (10%)
27	BCR	z	101	-	41,41,41	0.72	0	56,56,56	2.09	17 (30%)
30	LHG	G	618	25	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
25	CLA	b	516	-	45,53,73	1.78	7 (15%)	52,89,113	1.54	6 (11%)
25	CLA	B	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	6 (7%)
25	CLA	B	511	-	65,73,73	1.51	7 (10%)	76,113,113	1.29	9 (11%)
27	BCR	a	406	-	41,41,41	0.78	1 (2%)	56,56,56	1.91	17 (30%)
25	CLA	Y	311	21	65,73,73	1.51	6 (9%)	76,113,113	1.25	7 (9%)
29	LMG	a	408	-	46,46,55	0.98	2 (4%)	54,54,63	1.06	3 (5%)
29	LMG	c	518	-	39,39,55	1.05	2 (5%)	46,46,63	1.05	3 (6%)
36	CHL	r	306	-	46,54,74	2.29	15 (32%)	49,90,114	3.19	18 (36%)
37	LUT	G	615	-	42,43,43	0.77	0	51,60,60	1.67	13 (25%)
25	CLA	C	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	8 (10%)
25	CLA	A	405	-	60,68,73	1.54	6 (10%)	70,107,113	1.37	9 (12%)
38	NEX	S	617	-	38,46,46	0.96	1 (2%)	50,70,70	2.31	13 (26%)
25	CLA	C	508	-	65,73,73	1.51	7 (10%)	76,113,113	1.27	7 (9%)
25	CLA	c	504	-	60,68,73	1.59	7 (11%)	70,107,113	1.29	8 (11%)
25	CLA	S	603	-	42,50,73	1.85	6 (14%)	48,85,113	1.52	8 (16%)
30	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
25	CLA	N	304	-	65,73,73	1.51	7 (10%)	76,113,113	1.28	7 (9%)
25	CLA	b	504	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
37	LUT	N	317	-	42,43,43	0.82	0	51,60,60	1.72	13 (25%)
25	CLA	G	604	-	42,50,73	1.85	6 (14%)	48,85,113	1.46	7 (14%)
30	LHG	B	520	-	43,43,48	0.98	2 (4%)	46,49,54	1.06	3 (6%)
30	LHG	C	521	-	46,46,48	0.96	2 (4%)	49,52,54	1.01	3 (6%)
36	CHL	N	309	-	50,58,74	2.18	15 (30%)	52,94,114	3.16	19 (36%)
25	CLA	N	303	14	65,73,73	1.50	6 (9%)	76,113,113	1.30	9 (11%)
36	CHL	Y	307	21	46,54,74	2.29	15 (32%)	49,90,114	3.24	18 (36%)
25	CLA	c	510	-	65,73,73	1.52	6 (9%)	76,113,113	1.31	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
33	BCT	a	409	24	2,3,3	1.27	0	2,3,3	4.16	1 (50%)
25	CLA	B	504	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	10 (13%)
25	CLA	c	511	4	65,73,73	1.51	6 (9%)	76,113,113	1.34	9 (11%)
37	LUT	S	615	-	42,43,43	0.80	0	51,60,60	1.66	12 (23%)
25	CLA	b	511	-	65,73,73	1.50	8 (12%)	76,113,113	1.30	8 (10%)
36	CHL	G	601	8	66,74,74	1.90	15 (22%)	73,114,114	2.74	21 (28%)
36	CHL	r	305	-	43,51,74	2.30	14 (32%)	45,86,114	3.31	18 (40%)
30	LHG	d	407	-	43,43,48	0.96	2 (4%)	46,49,54	1.08	4 (8%)
25	CLA	N	314	14	65,73,73	1.52	6 (9%)	76,113,113	1.29	7 (9%)
25	CLA	b	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	6 (7%)
25	CLA	c	509	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
25	CLA	B	516	-	65,73,73	1.51	6 (9%)	76,113,113	1.30	6 (7%)
26	PHO	A	404	-	51,69,69	1.02	4 (7%)	47,99,99	1.12	5 (10%)
32	LMU	C	522	-	36,36,36	1.15	2 (5%)	47,47,47	0.96	1 (2%)
25	CLA	B	513	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	6 (7%)
25	CLA	c	513	-	42,50,73	1.83	5 (11%)	48,85,113	1.43	7 (14%)
31	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	0.99	4 (5%)
36	CHL	G	605	8	43,51,74	2.27	14 (32%)	45,86,114	3.41	18 (40%)
36	CHL	Y	309	-	50,58,74	2.21	15 (30%)	52,94,114	3.09	19 (36%)
25	CLA	C	501	-	65,73,73	1.52	7 (10%)	76,113,113	1.26	7 (9%)
27	BCR	b	518	-	41,41,41	0.73	0	56,56,56	1.93	16 (28%)
36	CHL	G	609	8	66,74,74	1.92	15 (22%)	73,114,114	2.75	21 (28%)
27	BCR	t	101	-	41,41,41	0.72	1 (2%)	56,56,56	2.00	16 (28%)
31	DGD	C	517	-	56,56,67	0.90	2 (3%)	70,70,81	1.04	4 (5%)
25	CLA	N	305	-	65,73,73	1.51	6 (9%)	76,113,113	1.29	8 (10%)
27	BCR	D	406	-	41,41,41	0.74	0	56,56,56	2.06	20 (35%)
25	CLA	r	303	-	49,57,73	1.75	6 (12%)	55,93,113	1.43	8 (14%)
25	CLA	c	508	-	65,73,73	1.51	7 (10%)	76,113,113	1.25	7 (9%)
25	CLA	Y	313	21	65,73,73	1.50	6 (9%)	76,113,113	1.29	6 (7%)
25	CLA	b	508	-	65,73,73	1.52	7 (10%)	76,113,113	1.29	8 (10%)
26	PHO	d	402	-	51,69,69	1.01	4 (7%)	47,99,99	1.21	5 (10%)

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
25	CLA	B	514	-	1/1/15/20	13/37/115/115	-
38	NEX	N	318	-	-	2/27/83/83	0/3/3/3
30	LHG	Y	319	25	-	13/53/53/53	-
39	XAT	r	309	-	-	0/31/93/93	0/4/4/4
25	CLA	C	511	4	1/1/15/20	8/37/115/115	-
25	CLA	B	509	-	1/1/15/20	13/37/115/115	-
25	CLA	a	403	-	1/1/11/20	7/18/96/115	-
25	CLA	b	502	-	1/1/15/20	13/37/115/115	-
27	BCR	h	101	-	-	2/29/63/63	0/2/2/2
25	CLA	c	505	-	1/1/15/20	16/37/115/115	-
25	CLA	S	613	16	1/1/11/20	6/18/96/115	-
36	CHL	N	308	-	3/3/20/26	24/39/137/137	-
30	LHG	l	101	-	-	7/53/53/53	-
37	LUT	N	316	-	-	0/29/67/67	0/2/2/2
34	PL9	D	407	-	-	3/53/73/73	0/1/1/1
25	CLA	B	512	-	1/1/15/20	11/37/115/115	-
25	CLA	D	405	-	1/1/15/20	18/37/115/115	-
25	CLA	S	611	30	1/1/11/20	4/18/96/115	-
25	CLA	Y	315	-	1/1/12/20	5/24/102/115	-
25	CLA	S	604	-	1/1/11/20	6/18/96/115	-
25	CLA	Y	304	21	1/1/15/20	9/37/115/115	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	BCR	C	516	-	-	1/29/63/63	0/2/2/2
27	BCR	d	405	-	-	4/29/63/63	0/2/2/2
27	BCR	v	101	-	-	5/29/63/63	0/2/2/2
25	CLA	D	404	-	1/1/15/20	8/37/115/115	-
25	CLA	S	602	16	1/1/11/20	7/18/96/115	-
25	CLA	a	405	-	1/1/14/20	5/31/109/115	-
36	CHL	S	601	16	3/3/16/26	6/15/113/137	-
25	CLA	r	307	23	1/1/11/20	6/13/91/115	-
31	DGD	Y	301	-	-	9/55/95/95	0/2/2/2
25	CLA	b	514	-	1/1/11/20	4/13/91/115	-
30	LHG	S	618	25	-	8/49/49/53	-
29	LMG	D	410	-	-	6/41/61/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMU	c	519	-	-	6/21/61/61	0/2/2/2
36	CHL	Y	308	-	3/3/16/26	5/15/113/137	-
25	CLA	c	503	-	1/1/15/20	14/37/115/115	-
25	CLA	Y	305	-	1/1/15/20	17/37/115/115	-
28	SQD	A	407	-	-	7/46/66/69	0/1/1/1
27	BCR	V	101	-	-	4/29/63/63	0/2/2/2
25	CLA	B	505	-	1/1/15/20	8/37/115/115	-
25	CLA	r	301	23	1/1/14/20	7/31/109/115	-
27	BCR	C	515	-	-	6/29/63/63	0/2/2/2
38	NEX	Y	318	-	-	3/27/83/83	0/3/3/3
34	PL9	d	406	-	-	4/53/73/73	0/1/1/1
26	PHO	D	402	-	-	10/37/103/103	0/5/6/6
29	LMG	d	410	-	-	12/43/63/70	0/1/1/1
25	CLA	Y	314	21	1/1/15/20	13/37/115/115	-
36	CHL	G	608	-	3/3/15/26	3/13/111/137	-
25	CLA	C	505	-	1/1/15/20	9/37/115/115	-
25	CLA	c	501	-	1/1/15/20	15/37/115/115	-
25	CLA	b	501	-	1/1/15/20	17/37/115/115	-
28	SQD	a	407	-	-	5/46/66/69	0/1/1/1
29	LMG	C	520	-	-	5/46/66/70	0/1/1/1
25	CLA	S	610	16	1/1/11/20	5/18/96/115	-
25	CLA	C	507	-	1/1/15/20	5/37/115/115	-
29	LMG	H	102	-	-	8/43/63/70	0/1/1/1
36	CHL	r	304	-	3/3/15/26	3/13/111/137	-
25	CLA	A	402	-	1/1/15/20	12/37/115/115	-
25	CLA	C	504	-	1/1/15/20	9/37/115/115	-
36	CHL	N	310	14	3/3/20/26	14/39/137/137	-
25	CLA	B	501	-	1/1/15/20	11/37/115/115	-
37	LUT	Y	317	-	-	0/29/67/67	0/2/2/2
27	BCR	B	517	-	-	8/29/63/63	0/2/2/2
30	LHG	L	101	-	-	8/53/53/53	-
25	CLA	G	613	8	1/1/15/20	13/37/115/115	-
25	CLA	d	404	-	1/1/10/20	6/10/88/115	-
37	LUT	S	616	-	-	0/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	c	516	-	-	5/38/78/95	0/2/2/2
25	CLA	C	513	-	1/1/15/20	16/37/115/115	-
25	CLA	D	401	-	1/1/15/20	7/37/115/115	-
25	CLA	b	507	-	1/1/15/20	14/37/115/115	-
25	CLA	N	315	-	1/1/10/20	4/10/88/115	-
36	CHL	S	607	-	3/3/15/26	2/12/110/137	-
25	CLA	c	502	-	1/1/15/20	17/37/115/115	-
30	LHG	D	409	-	-	7/43/43/53	-
32	LMU	C	523	-	-	8/21/61/61	0/2/2/2
25	CLA	b	509	-	1/1/15/20	16/37/115/115	-
25	CLA	c	506	-	1/1/15/20	19/37/115/115	-
37	LUT	G	616	-	-	0/29/67/67	0/2/2/2
25	CLA	C	502	-	1/1/15/20	11/37/115/115	-
25	CLA	B	508	-	1/1/15/20	16/37/115/115	-
25	CLA	c	512	-	1/1/13/20	4/27/105/115	-
30	LHG	b	521	-	-	9/53/53/53	-
25	CLA	G	614	-	1/1/10/20	1/10/88/115	-
31	DGD	c	517	-	-	9/48/88/95	0/2/2/2
32	LMU	S	619	-	-	7/21/61/61	0/2/2/2
25	CLA	S	612	16	1/1/11/20	2/13/91/115	-
36	CHL	N	307	-	3/3/16/26	7/15/113/137	-
30	LHG	a	411	-	-	8/48/48/53	-
39	XAT	N	301	-	-	0/31/93/93	0/4/4/4
36	CHL	G	619	-	3/3/20/26	19/39/137/137	-
31	DGD	C	519	-	-	3/48/88/95	0/2/2/2
27	BCR	b	517	-	-	4/29/63/63	0/2/2/2
25	CLA	c	507	-	1/1/15/20	13/37/115/115	-
29	LMG	W	201	-	-	9/43/63/70	0/1/1/1
25	CLA	Y	306	-	1/1/13/20	6/29/107/115	-
25	CLA	C	509	-	1/1/15/20	9/37/115/115	-
25	CLA	S	605	16	1/1/12/20	6/19/97/115	-
30	LHG	d	408	-	-	7/53/53/53	-
39	XAT	Y	302	-	-	0/31/93/93	0/4/4/4
25	CLA	S	609	16	1/1/10/20	5/8/86/115	-
27	BCR	k	101	-	-	1/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	603	-	1/1/15/20	17/37/115/115	-
28	SQD	t	102	-	-	5/49/69/69	0/1/1/1
38	NEX	r	310	-	-	3/27/83/83	0/3/3/3
25	CLA	N	313	14	1/1/11/20	3/13/91/115	-
36	CHL	G	606	-	3/3/15/26	1/12/110/137	-
26	PHO	a	404	-	-	9/37/103/103	0/5/6/6
27	BCR	b	519	-	-	4/29/63/63	0/2/2/2
25	CLA	b	512	-	1/1/15/20	14/37/115/115	-
30	LHG	N	319	25	-	10/53/53/53	-
25	CLA	N	311	14	1/1/15/20	7/37/115/115	-
25	CLA	G	602	8	1/1/15/20	12/37/115/115	-
25	CLA	B	503	-	1/1/15/20	6/37/115/115	-
25	CLA	B	507	-	1/1/15/20	8/37/115/115	-
25	CLA	G	612	8	1/1/10/20	2/11/89/115	-
25	CLA	C	512	-	1/1/15/20	6/37/115/115	-
25	CLA	a	402	-	1/1/15/20	9/37/115/115	-
36	CHL	Y	303	21	3/3/20/26	18/39/137/137	-
37	LUT	Y	316	-	-	0/29/67/67	0/2/2/2
27	BCR	B	518	-	-	2/29/63/63	0/2/2/2
25	CLA	G	611	30	1/1/11/20	5/13/91/115	-
25	CLA	r	308	23	1/1/10/20	3/8/86/115	-
27	BCR	c	514	-	-	5/29/63/63	0/2/2/2
25	CLA	r	302	-	1/1/11/20	3/15/93/115	-
36	CHL	S	608	-	3/3/16/26	10/19/117/137	-
36	CHL	S	606	-	3/3/15/26	6/13/111/137	-
31	DGD	W	202	-	-	7/55/95/95	0/2/2/2
39	XAT	G	620	-	-	0/31/93/93	0/4/4/4
35	HEM	f	101	7,6	-	1/12/54/54	-
38	NEX	G	617	-	-	2/27/83/83	0/3/3/3
25	CLA	S	614	-	1/1/11/20	5/17/95/115	-
25	CLA	B	515	-	1/1/15/20	3/37/115/115	-
36	CHL	Y	310	21	3/3/20/26	19/39/137/137	-
25	CLA	b	506	-	1/1/15/20	17/37/115/115	-
25	CLA	b	515	-	1/1/15/20	14/37/115/115	-
35	HEM	F	101	7,6	-	0/12/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	610	8	1/1/15/20	8/37/115/115	-
25	CLA	Y	312	30	1/1/15/20	5/37/115/115	-
25	CLA	C	503	-	1/1/15/20	8/37/115/115	-
25	CLA	B	502	-	1/1/15/20	5/37/115/115	-
25	CLA	d	403	-	1/1/15/20	12/37/115/115	-
31	DGD	c	515	-	-	3/42/82/95	0/2/2/2
25	CLA	b	513	-	1/1/15/20	6/37/115/115	-
25	CLA	B	506	-	1/1/15/20	7/37/115/115	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
36	CHL	N	306	14	3/3/20/26	19/39/137/137	-
25	CLA	C	506	-	1/1/15/20	9/37/115/115	-
29	LMG	d	409	-	-	6/36/56/70	0/1/1/1
30	LHG	a	410	-	-	8/47/47/53	-
36	CHL	G	607	-	3/3/16/26	8/20/118/137	-
29	LMG	B	519	-	-	2/46/66/70	0/1/1/1
25	CLA	A	403	-	1/1/11/20	5/18/96/115	-
27	BCR	A	406	-	-	0/29/63/63	0/2/2/2
36	CHL	N	302	14	3/3/20/26	15/39/137/137	-
29	LMG	b	520	-	-	5/37/57/70	0/1/1/1
25	CLA	b	505	-	1/1/15/20	18/37/115/115	-
25	CLA	d	401	-	1/1/15/20	14/37/115/115	-
25	CLA	N	312	30	1/1/11/20	9/18/96/115	-
27	BCR	z	101	-	-	6/29/63/63	0/2/2/2
30	LHG	G	618	25	-	9/53/53/53	-
25	CLA	b	516	-	1/1/11/20	4/13/91/115	-
25	CLA	B	510	-	1/1/15/20	12/37/115/115	-
25	CLA	B	511	-	1/1/15/20	7/37/115/115	-
27	BCR	a	406	-	-	2/29/63/63	0/2/2/2
25	CLA	Y	311	21	1/1/15/20	7/37/115/115	-
29	LMG	a	408	-	-	5/41/61/70	0/1/1/1
29	LMG	c	518	-	-	5/32/52/70	0/1/1/1
36	CHL	r	306	-	3/3/16/26	5/15/113/137	-
37	LUT	G	615	-	-	0/29/67/67	0/2/2/2
25	CLA	C	510	-	1/1/15/20	14/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	405	-	1/1/14/20	4/31/109/115	-
38	NEX	S	617	-	-	3/27/83/83	0/3/3/3
25	CLA	C	508	-	1/1/15/20	10/37/115/115	-
25	CLA	c	504	-	1/1/14/20	8/31/109/115	-
25	CLA	S	603	-	1/1/10/20	2/10/88/115	-
30	LHG	D	408	-	-	10/53/53/53	-
25	CLA	N	304	-	1/1/15/20	10/37/115/115	-
25	CLA	b	504	-	1/1/15/20	17/37/115/115	-
37	LUT	N	317	-	-	0/29/67/67	0/2/2/2
25	CLA	G	604	-	1/1/10/20	2/10/88/115	-
36	CHL	Y	307	21	3/3/16/26	3/15/113/137	-
36	CHL	N	309	-	3/3/16/26	5/20/118/137	-
30	LHG	B	520	-	-	12/48/48/53	-
25	CLA	N	303	14	1/1/15/20	10/37/115/115	-
30	LHG	C	521	-	-	11/51/51/53	-
25	CLA	c	510	-	1/1/15/20	10/37/115/115	-
25	CLA	b	510	-	1/1/15/20	14/37/115/115	-
37	LUT	S	615	-	-	0/29/67/67	0/2/2/2
25	CLA	B	504	-	1/1/15/20	18/37/115/115	-
25	CLA	c	511	4	1/1/15/20	14/37/115/115	-
25	CLA	b	511	-	1/1/15/20	20/37/115/115	-
36	CHL	G	601	8	3/3/20/26	15/39/137/137	-
36	CHL	r	305	-	3/3/15/26	3/12/110/137	-
30	LHG	d	407	-	-	7/48/48/53	-
25	CLA	N	314	14	1/1/15/20	11/37/115/115	-
25	CLA	b	503	-	1/1/15/20	12/37/115/115	-
25	CLA	c	509	-	1/1/15/20	15/37/115/115	-
25	CLA	B	516	-	1/1/15/20	11/37/115/115	-
26	PHO	A	404	-	-	7/37/103/103	0/5/6/6
32	LMU	C	522	-	-	9/21/61/61	0/2/2/2
25	CLA	B	513	-	1/1/15/20	5/37/115/115	-
25	CLA	c	513	-	1/1/10/20	5/10/88/115	-
36	CHL	Y	309	-	3/3/16/26	7/20/118/137	-
36	CHL	G	605	8	3/3/15/26	2/12/110/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	C	518	-	-	10/51/91/95	0/2/2/2
25	CLA	C	501	-	1/1/15/20	14/37/115/115	-
36	CHL	G	609	8	3/3/20/26	19/39/137/137	-
27	BCR	b	518	-	-	2/29/63/63	0/2/2/2
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
31	DGD	C	517	-	-	6/44/84/95	0/2/2/2
25	CLA	N	305	-	1/1/15/20	13/37/115/115	-
27	BCR	D	406	-	-	2/29/63/63	0/2/2/2
25	CLA	r	303	-	1/1/11/20	9/18/96/115	-
25	CLA	c	508	-	1/1/15/20	13/37/115/115	-
25	CLA	Y	313	21	1/1/15/20	9/37/115/115	-
25	CLA	b	508	-	1/1/15/20	10/37/115/115	-
26	PHO	d	402	-	-	8/37/103/103	0/5/6/6

All (1194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	308	CLA	C4B-NB	8.30	1.42	1.35
25	r	307	CLA	C4B-NB	8.16	1.42	1.35
25	r	301	CLA	C4B-NB	8.01	1.42	1.35
25	r	303	CLA	C4B-NB	7.89	1.42	1.35
25	d	401	CLA	C4B-NB	7.86	1.42	1.35
25	S	613	CLA	C4B-NB	7.85	1.42	1.35
25	S	609	CLA	C4B-NB	7.79	1.42	1.35
25	r	302	CLA	C4B-NB	7.77	1.42	1.35
25	c	501	CLA	C4B-NB	7.77	1.42	1.35
25	b	501	CLA	C4B-NB	7.76	1.42	1.35
25	S	614	CLA	C4B-NB	7.74	1.42	1.35
25	C	512	CLA	C4B-NB	7.74	1.42	1.35
25	N	313	CLA	C4B-NB	7.74	1.42	1.35
25	C	501	CLA	C4B-NB	7.72	1.42	1.35
25	G	610	CLA	C4B-NB	7.72	1.42	1.35
25	G	603	CLA	C4B-NB	7.71	1.42	1.35
25	N	315	CLA	C4B-NB	7.71	1.42	1.35
25	d	404	CLA	C4B-NB	7.71	1.42	1.35
25	S	602	CLA	C4B-NB	7.70	1.42	1.35
25	S	603	CLA	C4B-NB	7.70	1.42	1.35
25	S	605	CLA	C4B-NB	7.70	1.42	1.35
25	N	314	CLA	C4B-NB	7.68	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	C4B-NB	7.68	1.42	1.35
25	D	405	CLA	C4B-NB	7.66	1.42	1.35
25	c	504	CLA	C4B-NB	7.66	1.42	1.35
25	N	312	CLA	C4B-NB	7.65	1.42	1.35
25	C	504	CLA	C4B-NB	7.64	1.42	1.35
25	S	604	CLA	C4B-NB	7.63	1.42	1.35
25	B	509	CLA	C4B-NB	7.63	1.42	1.35
25	Y	314	CLA	C4B-NB	7.63	1.42	1.35
25	G	604	CLA	C4B-NB	7.62	1.42	1.35
25	N	305	CLA	C4B-NB	7.62	1.42	1.35
25	b	508	CLA	C4B-NB	7.62	1.42	1.35
25	Y	311	CLA	C4B-NB	7.62	1.42	1.35
25	B	514	CLA	C4B-NB	7.62	1.42	1.35
25	B	508	CLA	C4B-NB	7.61	1.42	1.35
25	B	506	CLA	C4B-NB	7.61	1.42	1.35
25	G	614	CLA	C4B-NB	7.61	1.42	1.35
25	S	610	CLA	C4B-NB	7.61	1.42	1.35
25	B	511	CLA	C4B-NB	7.61	1.42	1.35
25	G	612	CLA	C4B-NB	7.60	1.42	1.35
25	c	511	CLA	C4B-NB	7.60	1.42	1.35
25	c	512	CLA	C4B-NB	7.60	1.42	1.35
25	C	511	CLA	C4B-NB	7.60	1.42	1.35
25	G	613	CLA	C4B-NB	7.60	1.42	1.35
25	C	508	CLA	C4B-NB	7.59	1.42	1.35
25	A	403	CLA	C4B-NB	7.59	1.42	1.35
25	B	504	CLA	C4B-NB	7.58	1.42	1.35
25	B	502	CLA	C4B-NB	7.58	1.42	1.35
25	N	303	CLA	C4B-NB	7.58	1.42	1.35
25	Y	312	CLA	C4B-NB	7.57	1.42	1.35
25	N	304	CLA	C4B-NB	7.56	1.42	1.35
25	B	515	CLA	C4B-NB	7.56	1.42	1.35
25	c	505	CLA	C4B-NB	7.56	1.42	1.35
25	b	509	CLA	C4B-NB	7.56	1.42	1.35
25	C	506	CLA	C4B-NB	7.56	1.42	1.35
25	D	404	CLA	C4B-NB	7.56	1.42	1.35
25	Y	313	CLA	C4B-NB	7.55	1.41	1.35
25	C	510	CLA	C4B-NB	7.55	1.41	1.35
25	B	510	CLA	C4B-NB	7.55	1.41	1.35
25	c	513	CLA	C4B-NB	7.53	1.41	1.35
25	c	503	CLA	C4B-NB	7.53	1.41	1.35
25	B	507	CLA	C4B-NB	7.53	1.41	1.35
25	B	501	CLA	C4B-NB	7.52	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	514	CLA	C4B-NB	7.52	1.41	1.35
25	d	403	CLA	C4B-NB	7.51	1.41	1.35
25	b	515	CLA	C4B-NB	7.51	1.41	1.35
25	b	507	CLA	C4B-NB	7.51	1.41	1.35
25	c	508	CLA	C4B-NB	7.51	1.41	1.35
25	b	503	CLA	C4B-NB	7.50	1.41	1.35
25	C	505	CLA	C4B-NB	7.50	1.41	1.35
25	c	506	CLA	C4B-NB	7.50	1.41	1.35
25	B	503	CLA	C4B-NB	7.49	1.41	1.35
25	C	503	CLA	C4B-NB	7.49	1.41	1.35
25	B	513	CLA	C4B-NB	7.49	1.41	1.35
25	a	403	CLA	C4B-NB	7.49	1.41	1.35
25	S	612	CLA	C4B-NB	7.49	1.41	1.35
25	G	611	CLA	C4B-NB	7.49	1.41	1.35
25	b	511	CLA	C4B-NB	7.49	1.41	1.35
25	Y	306	CLA	C4B-NB	7.48	1.41	1.35
25	B	505	CLA	C4B-NB	7.46	1.41	1.35
25	b	506	CLA	C4B-NB	7.45	1.41	1.35
25	c	502	CLA	C4B-NB	7.45	1.41	1.35
25	C	509	CLA	C4B-NB	7.44	1.41	1.35
25	A	402	CLA	C4B-NB	7.44	1.41	1.35
25	D	401	CLA	C4B-NB	7.43	1.41	1.35
25	C	513	CLA	C4B-NB	7.43	1.41	1.35
25	N	311	CLA	C4B-NB	7.43	1.41	1.35
25	Y	305	CLA	C4B-NB	7.43	1.41	1.35
25	c	509	CLA	C4B-NB	7.42	1.41	1.35
25	B	516	CLA	C4B-NB	7.42	1.41	1.35
25	b	504	CLA	C4B-NB	7.42	1.41	1.35
25	b	502	CLA	C4B-NB	7.41	1.41	1.35
25	b	513	CLA	C4B-NB	7.40	1.41	1.35
25	b	505	CLA	C4B-NB	7.39	1.41	1.35
25	A	405	CLA	C4B-NB	7.37	1.41	1.35
25	c	507	CLA	C4B-NB	7.36	1.41	1.35
25	a	402	CLA	C4B-NB	7.35	1.41	1.35
25	G	602	CLA	C4B-NB	7.35	1.41	1.35
25	C	507	CLA	C4B-NB	7.34	1.41	1.35
25	Y	315	CLA	C4B-NB	7.34	1.41	1.35
25	B	512	CLA	C4B-NB	7.33	1.41	1.35
25	a	405	CLA	C4B-NB	7.32	1.41	1.35
25	S	611	CLA	C4B-NB	7.31	1.41	1.35
25	b	516	CLA	C4B-NB	7.31	1.41	1.35
25	C	502	CLA	C4B-NB	7.31	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	512	CLA	C4B-NB	7.30	1.41	1.35
25	b	510	CLA	C4B-NB	7.27	1.41	1.35
25	Y	304	CLA	C4B-NB	7.20	1.41	1.35
36	N	307	CHL	CHC-C1C	5.25	1.48	1.35
36	Y	308	CHL	CHC-C1C	5.20	1.48	1.35
36	r	305	CHL	O2D-CGD	5.18	1.45	1.33
36	Y	307	CHL	O2D-CGD	5.17	1.45	1.33
36	r	304	CHL	O2D-CGD	5.17	1.45	1.33
36	G	605	CHL	O2D-CGD	5.15	1.45	1.33
36	G	601	CHL	O2D-CGD	5.14	1.45	1.33
36	G	606	CHL	O2D-CGD	5.13	1.45	1.33
36	S	607	CHL	O2D-CGD	5.13	1.45	1.33
36	G	607	CHL	O2D-CGD	5.13	1.45	1.33
36	N	308	CHL	O2D-CGD	5.13	1.45	1.33
36	G	609	CHL	O2D-CGD	5.12	1.45	1.33
36	Y	308	CHL	O2D-CGD	5.12	1.45	1.33
36	r	306	CHL	O2D-CGD	5.12	1.45	1.33
36	Y	309	CHL	CHC-C1C	5.11	1.48	1.35
36	G	619	CHL	O2D-CGD	5.11	1.45	1.33
36	N	310	CHL	O2D-CGD	5.10	1.45	1.33
36	N	302	CHL	O2D-CGD	5.10	1.45	1.33
36	G	606	CHL	CHC-C1C	5.09	1.48	1.35
36	S	606	CHL	CHC-C1C	5.09	1.48	1.35
36	N	307	CHL	O2D-CGD	5.08	1.45	1.33
36	Y	309	CHL	O2D-CGD	5.08	1.45	1.33
36	S	601	CHL	O2D-CGD	5.08	1.45	1.33
36	S	607	CHL	CHC-C1C	5.07	1.48	1.35
36	Y	310	CHL	O2D-CGD	5.07	1.45	1.33
36	N	309	CHL	CHC-C1C	5.06	1.48	1.35
36	G	608	CHL	O2D-CGD	5.06	1.45	1.33
36	N	306	CHL	O2D-CGD	5.06	1.45	1.33
36	Y	303	CHL	O2D-CGD	5.06	1.45	1.33
36	Y	310	CHL	CHC-C1C	5.06	1.47	1.35
36	r	305	CHL	CHC-C1C	5.05	1.47	1.35
36	G	608	CHL	CHC-C1C	5.05	1.47	1.35
36	N	309	CHL	O2D-CGD	5.04	1.45	1.33
36	N	302	CHL	CHC-C1C	5.04	1.47	1.35
36	Y	307	CHL	CHC-C1C	5.04	1.47	1.35
36	G	619	CHL	CHC-C1C	5.03	1.47	1.35
36	S	601	CHL	CHC-C1C	5.02	1.47	1.35
36	G	607	CHL	CHC-C1C	5.02	1.47	1.35
36	Y	303	CHL	CHC-C1C	5.01	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	608	CHL	CHC-C1C	5.00	1.47	1.35
36	N	308	CHL	CHC-C1C	5.00	1.47	1.35
36	N	310	CHL	CHC-C1C	5.00	1.47	1.35
36	N	306	CHL	CHC-C1C	4.99	1.47	1.35
36	r	304	CHL	CHC-C1C	4.99	1.47	1.35
36	S	606	CHL	O2D-CGD	4.98	1.45	1.33
36	r	306	CHL	CHC-C1C	4.97	1.47	1.35
36	Y	310	CHL	C3D-C4D	-4.94	1.33	1.44
36	G	605	CHL	CHC-C1C	4.93	1.47	1.35
36	Y	310	CHL	C3B-C2B	4.93	1.47	1.40
36	Y	309	CHL	C3B-C2B	4.93	1.47	1.40
36	G	601	CHL	CHC-C1C	4.92	1.47	1.35
36	G	609	CHL	CHC-C1C	4.91	1.47	1.35
36	N	307	CHL	C3D-C4D	-4.91	1.33	1.44
36	G	609	CHL	C3D-C4D	-4.90	1.33	1.44
36	r	305	CHL	C3B-C2B	4.90	1.47	1.40
36	N	310	CHL	C3B-C2B	4.90	1.47	1.40
36	N	310	CHL	C3D-C4D	-4.89	1.33	1.44
36	Y	303	CHL	C3D-C4D	-4.88	1.33	1.44
36	N	309	CHL	C3D-C4D	-4.88	1.33	1.44
36	S	608	CHL	O2D-CGD	4.88	1.45	1.33
36	G	605	CHL	C3B-C2B	4.87	1.47	1.40
36	Y	308	CHL	C3D-C4D	-4.86	1.33	1.44
36	S	607	CHL	C3B-C2B	4.86	1.47	1.40
36	N	302	CHL	C3D-C4D	-4.84	1.33	1.44
36	Y	309	CHL	C3D-C4D	-4.84	1.33	1.44
36	G	608	CHL	C3B-C2B	4.84	1.47	1.40
36	G	601	CHL	C3D-C4D	-4.83	1.33	1.44
36	S	601	CHL	C3D-C4D	-4.83	1.33	1.44
36	S	608	CHL	C3D-C4D	-4.82	1.33	1.44
36	G	608	CHL	C3D-C4D	-4.82	1.33	1.44
36	G	619	CHL	C3D-C4D	-4.82	1.33	1.44
36	S	607	CHL	C3D-C4D	-4.81	1.33	1.44
36	N	306	CHL	C3D-C4D	-4.81	1.33	1.44
36	G	606	CHL	C3D-C4D	-4.81	1.33	1.44
36	G	607	CHL	C3D-C4D	-4.81	1.33	1.44
36	G	609	CHL	C3B-C2B	4.80	1.47	1.40
36	r	305	CHL	C3D-C4D	-4.80	1.33	1.44
36	r	306	CHL	C3B-C2B	4.80	1.47	1.40
36	S	606	CHL	C3D-C4D	-4.79	1.33	1.44
36	Y	307	CHL	C3D-C4D	-4.78	1.33	1.44
36	Y	307	CHL	C3B-C2B	4.78	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	608	CHL	C3B-C2B	4.78	1.47	1.40
36	r	304	CHL	C3B-C2B	4.77	1.47	1.40
36	N	308	CHL	C3D-C4D	-4.75	1.33	1.44
36	r	304	CHL	C3D-C4D	-4.75	1.33	1.44
36	r	306	CHL	C3D-C4D	-4.75	1.33	1.44
36	G	605	CHL	C3D-C4D	-4.75	1.33	1.44
36	N	306	CHL	C3B-C2B	4.73	1.46	1.40
36	G	606	CHL	C3B-C2B	4.70	1.46	1.40
36	S	606	CHL	C3B-C2B	4.69	1.46	1.40
36	N	309	CHL	C3B-C2B	4.68	1.46	1.40
35	F	101	HEM	C3C-C2C	-4.67	1.33	1.40
36	G	619	CHL	C3B-C2B	4.66	1.46	1.40
36	N	302	CHL	C3B-C2B	4.66	1.46	1.40
36	G	607	CHL	C3B-C2B	4.66	1.46	1.40
36	N	308	CHL	C3B-C2B	4.64	1.46	1.40
36	Y	309	CHL	C2C-C3C	4.63	1.46	1.36
36	Y	303	CHL	C3B-C2B	4.62	1.46	1.40
36	S	601	CHL	C3B-C2B	4.60	1.46	1.40
36	N	307	CHL	C3B-C2B	4.60	1.46	1.40
28	t	102	SQD	O8-S	4.60	1.63	1.47
36	Y	310	CHL	C2C-C3C	4.60	1.46	1.36
28	A	407	SQD	O8-S	4.59	1.63	1.47
36	G	609	CHL	C2C-C3C	4.59	1.46	1.36
36	G	608	CHL	C2C-C3C	4.58	1.46	1.36
36	G	601	CHL	C3B-C2B	4.58	1.46	1.40
28	a	407	SQD	O8-S	4.58	1.63	1.47
36	Y	308	CHL	C3B-C2B	4.56	1.46	1.40
36	N	306	CHL	C2C-C3C	4.56	1.46	1.36
36	r	305	CHL	C2C-C3C	4.54	1.46	1.36
36	r	306	CHL	C2C-C3C	4.54	1.46	1.36
36	G	605	CHL	C2C-C3C	4.54	1.46	1.36
36	S	601	CHL	C2C-C3C	4.53	1.46	1.36
36	S	607	CHL	C2C-C3C	4.52	1.46	1.36
36	G	601	CHL	C2C-C3C	4.50	1.46	1.36
36	N	307	CHL	C2C-C3C	4.50	1.46	1.36
36	Y	307	CHL	O2A-CGA	4.49	1.45	1.30
36	G	607	CHL	C2C-C3C	4.49	1.46	1.36
36	S	608	CHL	C2C-C3C	4.48	1.46	1.36
36	Y	308	CHL	O2A-CGA	4.48	1.45	1.30
36	N	309	CHL	C2C-C3C	4.48	1.46	1.36
36	Y	307	CHL	C2C-C3C	4.48	1.46	1.36
36	G	619	CHL	C2C-C3C	4.48	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	601	CHL	O2A-CGA	4.47	1.45	1.30
36	Y	303	CHL	C2C-C3C	4.47	1.46	1.36
36	N	308	CHL	C2C-C3C	4.47	1.46	1.36
36	N	307	CHL	O2A-CGA	4.47	1.45	1.30
36	N	302	CHL	C2C-C3C	4.46	1.46	1.36
36	N	310	CHL	C2C-C3C	4.46	1.46	1.36
36	r	306	CHL	O2A-CGA	4.46	1.45	1.30
36	Y	308	CHL	C2C-C3C	4.45	1.46	1.36
36	r	304	CHL	C2C-C3C	4.45	1.46	1.36
36	Y	310	CHL	CHD-C1D	4.38	1.46	1.38
36	G	606	CHL	C2C-C3C	4.37	1.46	1.36
36	G	609	CHL	O2A-CGA	4.35	1.46	1.33
36	r	306	CHL	CHD-C1D	4.33	1.46	1.38
36	r	305	CHL	CHD-C1D	4.33	1.46	1.38
36	S	606	CHL	C2C-C3C	4.32	1.46	1.36
36	G	601	CHL	CHD-C1D	4.30	1.46	1.38
36	G	601	CHL	O2A-CGA	4.30	1.45	1.33
36	G	609	CHL	CHD-C1D	4.29	1.46	1.38
36	G	607	CHL	O2A-CGA	4.29	1.45	1.33
36	Y	303	CHL	CHD-C1D	4.29	1.46	1.38
36	Y	310	CHL	O2A-CGA	4.29	1.45	1.33
31	C	519	DGD	O1G-C1A	4.28	1.45	1.33
36	N	310	CHL	CHD-C1D	4.28	1.46	1.38
29	C	520	LMG	O8-C28	4.28	1.45	1.33
36	Y	309	CHL	CHD-C1D	4.27	1.46	1.38
36	G	608	CHL	CHD-C1D	4.27	1.46	1.38
36	N	302	CHL	CHD-C1D	4.27	1.46	1.38
36	r	304	CHL	CHD-C1D	4.26	1.46	1.38
36	N	310	CHL	O2A-CGA	4.26	1.45	1.33
30	a	411	LHG	O8-C23	4.26	1.45	1.33
36	S	608	CHL	O2A-CGA	4.26	1.45	1.33
31	c	516	DGD	O1G-C1A	4.25	1.45	1.33
36	S	607	CHL	CHD-C1D	4.25	1.46	1.38
28	t	102	SQD	O48-C23	4.25	1.45	1.33
29	d	409	LMG	O8-C28	4.25	1.45	1.33
28	a	407	SQD	O48-C23	4.25	1.45	1.33
29	a	408	LMG	O8-C28	4.25	1.45	1.33
36	S	601	CHL	CHD-C1D	4.24	1.46	1.38
36	Y	307	CHL	CHD-C1D	4.24	1.46	1.38
36	N	302	CHL	O2A-CGA	4.24	1.45	1.33
29	c	518	LMG	O8-C28	4.24	1.45	1.33
36	N	309	CHL	O2A-CGA	4.24	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	518	DGD	O1G-C1A	4.24	1.45	1.33
30	C	521	LHG	O8-C23	4.24	1.45	1.33
36	G	619	CHL	O2A-CGA	4.23	1.45	1.33
36	Y	309	CHL	O2A-CGA	4.23	1.45	1.33
36	N	306	CHL	O2A-CGA	4.23	1.45	1.33
36	N	308	CHL	O2A-CGA	4.23	1.45	1.33
29	D	410	LMG	O8-C28	4.22	1.45	1.33
30	B	520	LHG	O8-C23	4.22	1.45	1.33
36	Y	303	CHL	O2A-CGA	4.22	1.45	1.33
29	H	102	LMG	O8-C28	4.21	1.45	1.33
36	G	607	CHL	CHD-C1D	4.21	1.46	1.38
29	B	519	LMG	O8-C28	4.21	1.45	1.33
31	Y	301	DGD	O1G-C1A	4.21	1.45	1.33
31	c	515	DGD	O1G-C1A	4.21	1.45	1.33
30	L	101	LHG	O8-C23	4.20	1.45	1.33
29	b	520	LMG	O8-C28	4.19	1.45	1.33
28	t	102	SQD	O47-C7	4.19	1.46	1.34
36	S	608	CHL	CHD-C1D	4.19	1.46	1.38
30	N	319	LHG	O8-C23	4.18	1.45	1.33
30	D	408	LHG	O8-C23	4.18	1.45	1.33
29	d	410	LMG	O8-C28	4.17	1.45	1.33
36	N	307	CHL	CHD-C1D	4.17	1.46	1.38
30	b	521	LHG	O8-C23	4.17	1.45	1.33
30	a	410	LHG	O8-C23	4.17	1.45	1.33
28	A	407	SQD	O48-C23	4.17	1.45	1.33
36	N	309	CHL	CHD-C1D	4.17	1.46	1.38
36	G	605	CHL	CHD-C1D	4.16	1.46	1.38
30	a	410	LHG	O7-C7	4.16	1.46	1.34
29	H	102	LMG	O7-C10	4.16	1.46	1.34
30	D	409	LHG	O8-C23	4.16	1.45	1.33
36	Y	308	CHL	CHD-C1D	4.16	1.46	1.38
31	W	202	DGD	O1G-C1A	4.16	1.45	1.33
29	W	201	LMG	O8-C28	4.16	1.45	1.33
31	C	517	DGD	O1G-C1A	4.16	1.45	1.33
29	D	410	LMG	O7-C10	4.16	1.46	1.34
31	c	517	DGD	O1G-C1A	4.16	1.45	1.33
36	S	606	CHL	CHD-C1D	4.15	1.46	1.38
30	Y	319	LHG	O8-C23	4.15	1.45	1.33
29	C	520	LMG	O7-C10	4.14	1.46	1.34
36	G	619	CHL	CHD-C1D	4.14	1.46	1.38
30	l	101	LHG	O8-C23	4.13	1.45	1.33
30	G	618	LHG	O8-C23	4.13	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	407	LHG	O8-C23	4.12	1.45	1.33
30	d	408	LHG	O8-C23	4.12	1.45	1.33
36	N	306	CHL	CHD-C1D	4.12	1.46	1.38
30	C	521	LHG	O7-C7	4.12	1.45	1.34
28	a	407	SQD	O47-C7	4.11	1.45	1.34
34	D	407	PL9	C7-C3	-4.10	1.47	1.51
29	a	408	LMG	O7-C10	4.09	1.45	1.34
29	B	519	LMG	O7-C10	4.09	1.45	1.34
30	S	618	LHG	O8-C23	4.08	1.45	1.33
25	r	307	CLA	C1D-ND	4.08	1.42	1.37
30	b	521	LHG	O7-C7	4.08	1.45	1.34
30	D	409	LHG	O7-C7	4.07	1.45	1.34
30	a	411	LHG	O7-C7	4.07	1.45	1.34
29	W	201	LMG	O7-C10	4.06	1.45	1.34
28	A	407	SQD	O47-C7	4.06	1.45	1.34
29	c	518	LMG	O7-C10	4.06	1.45	1.34
31	C	519	DGD	O2G-C1B	4.06	1.45	1.34
36	N	308	CHL	CHD-C1D	4.05	1.46	1.38
31	Y	301	DGD	O2G-C1B	4.05	1.45	1.34
31	C	518	DGD	O2G-C1B	4.05	1.45	1.34
31	c	517	DGD	O2G-C1B	4.05	1.45	1.34
29	d	410	LMG	O7-C10	4.05	1.45	1.34
31	c	516	DGD	O2G-C1B	4.05	1.45	1.34
34	d	406	PL9	C7-C3	-4.04	1.47	1.51
30	D	408	LHG	O7-C7	4.04	1.45	1.34
31	c	515	DGD	O2G-C1B	4.03	1.45	1.34
29	d	409	LMG	O7-C10	4.03	1.45	1.34
30	Y	319	LHG	O7-C7	4.01	1.45	1.34
31	W	202	DGD	O2G-C1B	4.01	1.45	1.34
31	C	517	DGD	O2G-C1B	4.01	1.45	1.34
36	G	606	CHL	CHD-C1D	4.01	1.46	1.38
30	S	618	LHG	O7-C7	4.01	1.45	1.34
25	r	308	CLA	C1D-ND	4.01	1.42	1.37
30	B	520	LHG	O7-C7	4.01	1.45	1.34
30	L	101	LHG	O7-C7	4.01	1.45	1.34
30	N	319	LHG	O7-C7	3.99	1.45	1.34
30	l	101	LHG	O7-C7	3.99	1.45	1.34
30	G	618	LHG	O7-C7	3.99	1.45	1.34
35	f	101	HEM	C3C-C2C	-3.98	1.34	1.40
29	b	520	LMG	O7-C10	3.96	1.45	1.34
30	d	407	LHG	O7-C7	3.95	1.45	1.34
30	d	408	LHG	O7-C7	3.95	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	301	CLA	C1D-ND	3.93	1.42	1.37
25	B	516	CLA	C1D-ND	3.93	1.42	1.37
25	N	311	CLA	C1D-ND	3.91	1.42	1.37
25	b	507	CLA	C1D-ND	3.89	1.42	1.37
36	Y	310	CHL	CHD-C4C	3.89	1.48	1.39
25	d	404	CLA	C1D-ND	3.88	1.42	1.37
25	B	507	CLA	C1D-ND	3.88	1.42	1.37
25	B	514	CLA	C1D-ND	3.87	1.42	1.37
25	Y	311	CLA	C1D-ND	3.87	1.42	1.37
25	S	605	CLA	C1D-ND	3.87	1.42	1.37
25	r	302	CLA	C1D-ND	3.87	1.42	1.37
36	r	305	CHL	CHD-C4C	3.87	1.48	1.39
36	r	304	CHL	CHD-C4C	3.87	1.48	1.39
25	Y	314	CLA	C1D-ND	3.86	1.42	1.37
36	G	601	CHL	CHD-C4C	3.85	1.48	1.39
25	C	503	CLA	C1D-ND	3.85	1.42	1.37
25	D	405	CLA	C1D-ND	3.85	1.42	1.37
25	S	609	CLA	C1D-ND	3.84	1.42	1.37
36	r	306	CHL	CHD-C4C	3.83	1.48	1.39
25	Y	313	CLA	C1D-ND	3.82	1.42	1.37
25	B	510	CLA	C1D-ND	3.81	1.42	1.37
25	S	614	CLA	C1D-ND	3.81	1.42	1.37
25	c	511	CLA	C1D-ND	3.81	1.42	1.37
36	N	302	CHL	CHD-C4C	3.81	1.47	1.39
25	N	314	CLA	C1D-ND	3.81	1.42	1.37
25	Y	304	CLA	C1D-ND	3.81	1.42	1.37
25	b	516	CLA	C1D-ND	3.80	1.42	1.37
25	G	613	CLA	C1D-ND	3.80	1.42	1.37
25	G	604	CLA	C1D-ND	3.80	1.42	1.37
36	Y	303	CHL	CHD-C4C	3.80	1.47	1.39
25	A	403	CLA	C1D-ND	3.80	1.42	1.37
36	G	605	CHL	CHD-C4C	3.79	1.47	1.39
25	c	513	CLA	C1D-ND	3.79	1.42	1.37
36	Y	309	CHL	CHD-C4C	3.79	1.47	1.39
25	D	401	CLA	C1D-ND	3.79	1.42	1.37
25	N	313	CLA	C1D-ND	3.79	1.42	1.37
25	c	504	CLA	C1D-ND	3.79	1.42	1.37
25	C	510	CLA	C1D-ND	3.79	1.42	1.37
25	c	508	CLA	C1D-ND	3.79	1.42	1.37
36	G	609	CHL	CHD-C4C	3.79	1.47	1.39
25	c	510	CLA	C1D-ND	3.78	1.42	1.37
36	Y	307	CHL	CHD-C4C	3.78	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	612	CLA	C1D-ND	3.78	1.42	1.37
25	r	303	CLA	C1D-ND	3.78	1.42	1.37
25	c	506	CLA	C1D-ND	3.78	1.42	1.37
25	G	614	CLA	C1D-ND	3.78	1.42	1.37
25	Y	315	CLA	C1D-ND	3.78	1.42	1.37
25	G	610	CLA	C1D-ND	3.78	1.42	1.37
25	S	611	CLA	C1D-ND	3.78	1.42	1.37
25	G	602	CLA	C1D-ND	3.78	1.42	1.37
25	C	502	CLA	C1D-ND	3.78	1.42	1.37
36	S	601	CHL	CHD-C4C	3.77	1.47	1.39
25	S	613	CLA	C1D-ND	3.77	1.42	1.37
36	N	310	CHL	CHD-C4C	3.77	1.47	1.39
25	S	604	CLA	C1D-ND	3.77	1.42	1.37
25	b	501	CLA	C1D-ND	3.77	1.42	1.37
36	S	608	CHL	CHD-C4C	3.77	1.47	1.39
25	C	511	CLA	C1D-ND	3.77	1.42	1.37
25	C	509	CLA	C1D-ND	3.76	1.42	1.37
25	Y	306	CLA	C1D-ND	3.76	1.42	1.37
36	G	608	CHL	CHD-C4C	3.76	1.47	1.39
36	N	309	CHL	CHD-C4C	3.76	1.47	1.39
25	N	315	CLA	C1D-ND	3.76	1.42	1.37
25	c	507	CLA	C1D-ND	3.76	1.42	1.37
25	B	509	CLA	C1D-ND	3.75	1.42	1.37
36	Y	308	CHL	CHD-C4C	3.75	1.47	1.39
25	C	507	CLA	C1D-ND	3.75	1.42	1.37
25	a	405	CLA	C1D-ND	3.75	1.42	1.37
25	N	312	CLA	C1D-ND	3.75	1.42	1.37
25	b	515	CLA	C1D-ND	3.75	1.42	1.37
25	C	508	CLA	C1D-ND	3.75	1.42	1.37
25	C	506	CLA	C1D-ND	3.75	1.42	1.37
25	c	501	CLA	C1D-ND	3.75	1.42	1.37
25	B	506	CLA	C1D-ND	3.74	1.42	1.37
25	N	304	CLA	C1D-ND	3.74	1.42	1.37
25	G	603	CLA	C1D-ND	3.74	1.42	1.37
36	G	607	CHL	CHD-C4C	3.74	1.47	1.39
25	B	515	CLA	C1D-ND	3.74	1.42	1.37
25	d	401	CLA	C1D-ND	3.74	1.42	1.37
25	c	503	CLA	C1D-ND	3.74	1.42	1.37
25	A	402	CLA	C1D-ND	3.74	1.42	1.37
25	B	501	CLA	C1D-ND	3.73	1.42	1.37
25	b	504	CLA	C1D-ND	3.73	1.42	1.37
25	G	611	CLA	C1D-ND	3.73	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	501	CLA	C1D-ND	3.73	1.42	1.37
25	b	511	CLA	C1D-ND	3.73	1.42	1.37
25	c	509	CLA	C1D-ND	3.73	1.42	1.37
36	r	306	CHL	OBD-CAD	3.73	1.28	1.22
25	S	612	CLA	C1D-ND	3.73	1.42	1.37
36	G	619	CHL	CHD-C4C	3.73	1.47	1.39
25	S	602	CLA	C1D-ND	3.72	1.42	1.37
36	S	607	CHL	CHD-C4C	3.72	1.47	1.39
25	B	505	CLA	C1D-ND	3.72	1.42	1.37
25	Y	305	CLA	C1D-ND	3.72	1.42	1.37
25	B	511	CLA	C1D-ND	3.71	1.42	1.37
36	G	605	CHL	OBD-CAD	3.71	1.28	1.22
36	N	307	CHL	CHD-C4C	3.71	1.47	1.39
25	N	303	CLA	C1D-ND	3.71	1.42	1.37
25	N	305	CLA	C1D-ND	3.71	1.42	1.37
25	A	405	CLA	C1D-ND	3.71	1.42	1.37
25	C	504	CLA	C1D-ND	3.71	1.42	1.37
36	r	305	CHL	OBD-CAD	3.70	1.28	1.22
25	S	610	CLA	C1D-ND	3.70	1.42	1.37
25	a	402	CLA	C1D-ND	3.70	1.42	1.37
36	N	306	CHL	CHD-C4C	3.70	1.47	1.39
25	b	509	CLA	C1D-ND	3.70	1.42	1.37
25	B	513	CLA	C1D-ND	3.70	1.42	1.37
25	b	513	CLA	C1D-ND	3.70	1.42	1.37
25	C	512	CLA	C1D-ND	3.70	1.42	1.37
25	b	505	CLA	C1D-ND	3.70	1.42	1.37
25	Y	312	CLA	C1D-ND	3.69	1.42	1.37
36	G	606	CHL	OBD-CAD	3.69	1.28	1.22
36	r	304	CHL	OBD-CAD	3.69	1.28	1.22
25	B	512	CLA	C1D-ND	3.69	1.42	1.37
36	Y	308	CHL	OBD-CAD	3.69	1.28	1.22
36	N	302	CHL	OBD-CAD	3.68	1.28	1.22
25	a	403	CLA	C1D-ND	3.68	1.42	1.37
35	f	101	HEM	C3C-CAC	3.68	1.55	1.47
25	S	603	CLA	C1D-ND	3.68	1.42	1.37
25	b	514	CLA	C1D-ND	3.68	1.42	1.37
36	G	607	CHL	OBD-CAD	3.67	1.28	1.22
36	N	307	CHL	OBD-CAD	3.67	1.28	1.22
25	B	502	CLA	C1D-ND	3.67	1.42	1.37
36	N	308	CHL	CHD-C4C	3.67	1.47	1.39
25	B	504	CLA	C1D-ND	3.67	1.42	1.37
25	b	506	CLA	C1D-ND	3.67	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	508	CLA	C1D-ND	3.67	1.42	1.37
36	S	607	CHL	OBD-CAD	3.66	1.28	1.22
36	S	606	CHL	OBD-CAD	3.66	1.28	1.22
25	b	510	CLA	C1D-ND	3.66	1.42	1.37
36	N	310	CHL	OBD-CAD	3.66	1.28	1.22
25	B	503	CLA	C1D-ND	3.66	1.42	1.37
36	Y	307	CHL	OBD-CAD	3.65	1.28	1.22
35	F	101	HEM	C3C-CAC	3.65	1.55	1.47
25	b	502	CLA	C1D-ND	3.65	1.42	1.37
36	S	606	CHL	CHD-C4C	3.65	1.47	1.39
25	c	512	CLA	C1D-ND	3.65	1.42	1.37
36	G	601	CHL	OBD-CAD	3.65	1.28	1.22
25	c	502	CLA	C1D-ND	3.64	1.42	1.37
36	N	306	CHL	OBD-CAD	3.63	1.28	1.22
36	G	619	CHL	OBD-CAD	3.63	1.28	1.22
25	C	505	CLA	C1D-ND	3.63	1.42	1.37
25	C	513	CLA	C1D-ND	3.62	1.42	1.37
36	Y	303	CHL	OBD-CAD	3.62	1.28	1.22
36	G	606	CHL	CHD-C4C	3.62	1.47	1.39
36	N	309	CHL	OBD-CAD	3.62	1.28	1.22
36	Y	309	CHL	OBD-CAD	3.61	1.28	1.22
36	N	308	CHL	OBD-CAD	3.60	1.28	1.22
25	b	512	CLA	C1D-ND	3.60	1.42	1.37
36	Y	310	CHL	OBD-CAD	3.59	1.28	1.22
25	b	503	CLA	C1D-ND	3.59	1.42	1.37
36	G	608	CHL	OBD-CAD	3.58	1.28	1.22
36	G	609	CHL	OBD-CAD	3.57	1.28	1.22
36	S	601	CHL	OBD-CAD	3.56	1.28	1.22
25	d	403	CLA	C1D-ND	3.55	1.42	1.37
25	B	508	CLA	C1D-ND	3.54	1.42	1.37
34	d	406	PL9	C3-C4	-3.53	1.43	1.49
25	D	404	CLA	C1D-ND	3.52	1.42	1.37
25	c	505	CLA	C1D-ND	3.49	1.42	1.37
34	D	407	PL9	C3-C4	-3.44	1.43	1.49
32	c	519	LMU	O5'-C1'	3.43	1.50	1.41
36	S	608	CHL	OBD-CAD	3.42	1.28	1.22
32	S	619	LMU	O5B-C1B	3.36	1.50	1.41
38	G	617	NEX	C7-C8	-3.35	1.26	1.32
32	C	523	LMU	O5B-C1B	3.34	1.50	1.41
38	S	617	NEX	C7-C8	-3.32	1.26	1.32
32	C	522	LMU	O5B-C1B	3.31	1.50	1.41
32	S	619	LMU	O5'-C1'	3.31	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	519	LMU	O5B-C1B	3.28	1.50	1.41
32	C	522	LMU	O5'-C1'	3.27	1.50	1.41
25	a	402	CLA	C4D-ND	-3.26	1.33	1.37
25	A	402	CLA	C4D-ND	-3.25	1.33	1.37
38	Y	318	NEX	C7-C8	-3.24	1.26	1.32
32	C	523	LMU	O5'-C1'	3.23	1.50	1.41
25	b	512	CLA	C4D-ND	-3.21	1.33	1.37
25	b	505	CLA	C4D-ND	-3.21	1.33	1.37
25	a	403	CLA	C4D-ND	-3.21	1.33	1.37
25	c	503	CLA	C4D-ND	-3.19	1.33	1.37
25	c	506	CLA	C4D-ND	-3.19	1.33	1.37
25	d	401	CLA	C4D-ND	-3.18	1.33	1.37
25	B	508	CLA	C4D-ND	-3.17	1.33	1.37
25	d	403	CLA	C4D-ND	-3.17	1.33	1.37
25	G	613	CLA	C4D-ND	-3.17	1.33	1.37
25	C	513	CLA	C4D-ND	-3.17	1.33	1.37
38	r	310	NEX	C7-C8	-3.17	1.26	1.32
25	b	508	CLA	C4D-ND	-3.16	1.33	1.37
25	S	613	CLA	C4D-ND	-3.15	1.33	1.37
25	G	602	CLA	C4D-ND	-3.15	1.33	1.37
25	a	405	CLA	C4D-ND	-3.15	1.33	1.37
25	c	508	CLA	C4D-ND	-3.15	1.33	1.37
25	c	513	CLA	C4D-ND	-3.14	1.33	1.37
25	B	506	CLA	C4D-ND	-3.13	1.33	1.37
25	C	508	CLA	C4D-ND	-3.13	1.33	1.37
25	c	504	CLA	C4D-ND	-3.13	1.33	1.37
25	B	504	CLA	C4D-ND	-3.13	1.33	1.37
38	N	318	NEX	C7-C8	-3.13	1.26	1.32
25	D	401	CLA	C4D-ND	-3.13	1.33	1.37
25	b	501	CLA	C4D-ND	-3.12	1.33	1.37
25	B	509	CLA	C4D-ND	-3.12	1.33	1.37
25	Y	312	CLA	C4D-ND	-3.12	1.33	1.37
25	B	505	CLA	C4D-ND	-3.12	1.33	1.37
25	c	501	CLA	C4D-ND	-3.12	1.33	1.37
25	b	504	CLA	C4D-ND	-3.11	1.33	1.37
25	Y	304	CLA	C4D-ND	-3.11	1.33	1.37
25	b	506	CLA	C4D-ND	-3.11	1.33	1.37
25	B	516	CLA	C4D-ND	-3.11	1.33	1.37
25	b	509	CLA	C4D-ND	-3.11	1.33	1.37
25	C	503	CLA	C4D-ND	-3.10	1.33	1.37
25	A	403	CLA	C4D-ND	-3.09	1.33	1.37
25	A	405	CLA	C4D-ND	-3.09	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	305	CLA	C4D-ND	-3.09	1.33	1.37
25	d	404	CLA	C4D-ND	-3.09	1.33	1.37
25	S	604	CLA	C4D-ND	-3.09	1.33	1.37
25	c	507	CLA	C4D-ND	-3.08	1.33	1.37
25	c	502	CLA	C4D-ND	-3.08	1.33	1.37
25	C	506	CLA	C4D-ND	-3.08	1.33	1.37
25	Y	314	CLA	C4D-ND	-3.08	1.33	1.37
25	N	303	CLA	C4D-ND	-3.08	1.33	1.37
25	C	504	CLA	C4D-ND	-3.07	1.33	1.37
25	C	502	CLA	C4D-ND	-3.07	1.33	1.37
25	b	514	CLA	C4D-ND	-3.07	1.33	1.37
25	D	404	CLA	C4D-ND	-3.07	1.33	1.37
25	B	511	CLA	C4D-ND	-3.07	1.33	1.37
25	c	505	CLA	C4D-ND	-3.06	1.33	1.37
25	c	510	CLA	C4D-ND	-3.06	1.33	1.37
25	S	602	CLA	CHC-C1C	3.06	1.42	1.35
25	S	610	CLA	CHC-C1C	3.06	1.42	1.35
25	D	405	CLA	C4D-ND	-3.05	1.33	1.37
25	b	516	CLA	C4D-ND	-3.05	1.33	1.37
25	B	515	CLA	C4D-ND	-3.05	1.33	1.37
25	N	312	CLA	CHC-C1C	3.05	1.42	1.35
25	b	512	CLA	CHC-C1C	3.04	1.42	1.35
25	b	507	CLA	C4D-ND	-3.03	1.33	1.37
25	N	314	CLA	C4D-ND	-3.03	1.33	1.37
25	b	502	CLA	C4D-ND	-3.03	1.33	1.37
25	G	610	CLA	CHC-C1C	3.03	1.42	1.35
25	N	312	CLA	C4D-ND	-3.03	1.33	1.37
25	S	609	CLA	C4D-ND	-3.03	1.33	1.37
25	B	503	CLA	C4D-ND	-3.03	1.33	1.37
25	G	614	CLA	C4D-ND	-3.03	1.33	1.37
25	c	512	CLA	C4D-ND	-3.03	1.33	1.37
25	Y	312	CLA	CHC-C1C	3.03	1.42	1.35
25	N	311	CLA	C4D-ND	-3.03	1.33	1.37
25	c	505	CLA	CHC-C1C	3.02	1.42	1.35
25	Y	315	CLA	C4D-ND	-3.02	1.33	1.37
25	N	315	CLA	CHC-C1C	3.02	1.42	1.35
36	r	304	CHL	C1D-C2D	3.02	1.51	1.45
25	G	611	CLA	CHC-C1C	3.01	1.42	1.35
25	G	604	CLA	CHC-C1C	3.01	1.42	1.35
25	B	502	CLA	C4D-ND	-3.01	1.33	1.37
25	C	509	CLA	C4D-ND	-3.01	1.33	1.37
36	r	305	CHL	C1D-C2D	3.01	1.51	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	611	CLA	C4D-ND	-3.01	1.33	1.37
25	S	611	CLA	CHC-C1C	3.01	1.42	1.35
25	b	507	CLA	CHC-C1C	3.01	1.42	1.35
25	r	301	CLA	CHC-C1C	3.01	1.42	1.35
25	B	507	CLA	C4D-ND	-3.01	1.33	1.37
25	r	303	CLA	C4D-ND	-3.01	1.33	1.37
25	S	614	CLA	CHC-C1C	3.00	1.42	1.35
25	b	510	CLA	C4D-ND	-3.00	1.33	1.37
25	B	503	CLA	CHC-C1C	3.00	1.42	1.35
25	B	507	CLA	CHC-C1C	3.00	1.42	1.35
25	G	604	CLA	C4D-ND	-3.00	1.33	1.37
25	G	610	CLA	C4D-ND	-3.00	1.33	1.37
25	C	510	CLA	CHC-C1C	3.00	1.42	1.35
25	c	511	CLA	C4D-ND	-3.00	1.33	1.37
25	C	505	CLA	CHC-C1C	3.00	1.42	1.35
25	c	508	CLA	CHC-C1C	3.00	1.42	1.35
25	S	602	CLA	C4D-ND	-3.00	1.33	1.37
25	B	513	CLA	CHC-C1C	3.00	1.42	1.35
25	G	611	CLA	C4D-ND	-3.00	1.33	1.37
25	b	513	CLA	CHC-C1C	3.00	1.42	1.35
25	r	301	CLA	C4D-ND	-3.00	1.33	1.37
25	N	304	CLA	C4D-ND	-3.00	1.33	1.37
25	S	612	CLA	C4D-ND	-3.00	1.33	1.37
25	c	501	CLA	CHC-C1C	2.99	1.42	1.35
25	D	404	CLA	CHC-C1C	2.99	1.42	1.35
25	B	501	CLA	C4D-ND	-2.99	1.33	1.37
25	b	503	CLA	C4D-ND	-2.99	1.33	1.37
25	c	510	CLA	CHC-C1C	2.99	1.42	1.35
25	N	303	CLA	CHC-C1C	2.99	1.42	1.35
25	b	511	CLA	C4D-ND	-2.99	1.33	1.37
25	Y	306	CLA	C4D-ND	-2.99	1.33	1.37
35	F	101	HEM	CAB-C3B	2.99	1.55	1.47
25	C	510	CLA	C4D-ND	-2.98	1.33	1.37
25	S	610	CLA	C4D-ND	-2.98	1.33	1.37
25	B	514	CLA	CHC-C1C	2.98	1.42	1.35
36	r	306	CHL	C1D-C2D	2.98	1.51	1.45
25	A	402	CLA	CHC-C1C	2.98	1.42	1.35
25	B	513	CLA	C4D-ND	-2.98	1.33	1.37
25	Y	305	CLA	C4D-ND	-2.98	1.33	1.37
25	c	506	CLA	CHC-C1C	2.98	1.42	1.35
25	Y	306	CLA	CHC-C1C	2.98	1.42	1.35
25	B	511	CLA	CHC-C1C	2.98	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	CHC-C1C	2.98	1.42	1.35
25	C	512	CLA	C4D-ND	-2.98	1.33	1.37
25	c	503	CLA	CHC-C1C	2.98	1.42	1.35
25	r	303	CLA	CHC-C1C	2.98	1.42	1.35
25	d	403	CLA	CHC-C1C	2.98	1.42	1.35
25	N	305	CLA	CHC-C1C	2.98	1.42	1.35
25	b	503	CLA	CHC-C1C	2.97	1.42	1.35
25	Y	315	CLA	CHC-C1C	2.97	1.42	1.35
25	B	502	CLA	CHC-C1C	2.97	1.42	1.35
25	C	511	CLA	C4D-ND	-2.97	1.33	1.37
25	Y	311	CLA	C4D-ND	-2.97	1.33	1.37
25	G	603	CLA	C4D-ND	-2.97	1.33	1.37
25	B	505	CLA	CHC-C1C	2.97	1.42	1.35
25	c	504	CLA	CHC-C1C	2.97	1.42	1.35
25	G	614	CLA	CHC-C1C	2.96	1.42	1.35
25	S	604	CLA	CHC-C1C	2.96	1.42	1.35
25	N	315	CLA	C4D-ND	-2.96	1.33	1.37
25	b	502	CLA	CHC-C1C	2.96	1.42	1.35
25	C	508	CLA	CHC-C1C	2.96	1.42	1.35
25	N	304	CLA	CHC-C1C	2.96	1.42	1.35
25	b	514	CLA	CHC-C1C	2.96	1.42	1.35
25	C	504	CLA	CHC-C1C	2.96	1.42	1.35
25	B	510	CLA	CHC-C1C	2.95	1.42	1.35
25	S	603	CLA	CHC-C1C	2.95	1.42	1.35
36	Y	310	CHL	C1D-C2D	2.95	1.51	1.45
25	Y	313	CLA	C4D-ND	-2.95	1.33	1.37
25	B	506	CLA	CHC-C1C	2.95	1.42	1.35
25	C	501	CLA	C4D-ND	-2.95	1.33	1.37
25	C	501	CLA	CHC-C1C	2.95	1.42	1.35
25	a	405	CLA	CHC-C1C	2.95	1.42	1.35
25	b	505	CLA	CHC-C1C	2.95	1.42	1.35
25	A	405	CLA	CHC-C1C	2.95	1.42	1.35
25	B	510	CLA	C4D-ND	-2.94	1.33	1.37
25	C	507	CLA	C4D-ND	-2.94	1.33	1.37
25	b	513	CLA	C4D-ND	-2.94	1.33	1.37
25	B	509	CLA	CHC-C1C	2.94	1.42	1.35
25	c	507	CLA	CHC-C1C	2.94	1.42	1.35
25	Y	311	CLA	CHC-C1C	2.94	1.42	1.35
25	N	313	CLA	CHC-C1C	2.94	1.42	1.35
25	S	605	CLA	C4D-ND	-2.94	1.33	1.37
25	B	512	CLA	CHC-C1C	2.94	1.42	1.35
25	c	511	CLA	CHC-C1C	2.93	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	501	CLA	CHC-C1C	2.93	1.42	1.35
25	C	511	CLA	CHC-C1C	2.93	1.42	1.35
36	N	310	CHL	C1D-C2D	2.93	1.51	1.45
25	b	516	CLA	CHC-C1C	2.93	1.42	1.35
25	S	609	CLA	CHC-C1C	2.92	1.42	1.35
25	C	512	CLA	CHC-C1C	2.92	1.42	1.35
25	B	514	CLA	C4D-ND	-2.92	1.33	1.37
25	G	612	CLA	C4D-ND	-2.92	1.33	1.37
25	a	402	CLA	CHC-C1C	2.92	1.42	1.35
25	r	308	CLA	CHC-C1C	2.92	1.42	1.35
25	C	509	CLA	CHC-C1C	2.92	1.42	1.35
25	S	614	CLA	C4D-ND	-2.92	1.33	1.37
25	Y	314	CLA	CHC-C1C	2.92	1.42	1.35
25	b	509	CLA	CHC-C1C	2.91	1.42	1.35
25	b	510	CLA	CHC-C1C	2.91	1.42	1.35
25	c	509	CLA	C4D-ND	-2.91	1.33	1.37
28	t	102	SQD	C6-S	-2.91	1.66	1.77
36	Y	303	CHL	C1D-C2D	2.91	1.51	1.45
25	c	509	CLA	CHC-C1C	2.91	1.42	1.35
36	G	601	CHL	C1D-C2D	2.91	1.51	1.45
25	c	512	CLA	CHC-C1C	2.91	1.42	1.35
25	C	507	CLA	CHC-C1C	2.91	1.42	1.35
25	Y	304	CLA	CHC-C1C	2.91	1.42	1.35
25	G	612	CLA	CHC-C1C	2.91	1.42	1.35
25	N	314	CLA	CHC-C1C	2.91	1.42	1.35
25	d	404	CLA	CHC-C1C	2.91	1.42	1.35
25	C	513	CLA	CHC-C1C	2.90	1.42	1.35
36	G	605	CHL	C1D-C2D	2.90	1.51	1.45
25	G	613	CLA	CHC-C1C	2.90	1.42	1.35
36	N	302	CHL	C1D-C2D	2.90	1.51	1.45
25	b	515	CLA	C4D-ND	-2.90	1.33	1.37
25	r	308	CLA	C4D-ND	-2.90	1.33	1.37
25	B	512	CLA	C4D-ND	-2.90	1.33	1.37
25	a	403	CLA	CHC-C1C	2.90	1.42	1.35
25	c	513	CLA	CHC-C1C	2.90	1.42	1.35
25	N	311	CLA	CHC-C1C	2.90	1.42	1.35
25	S	613	CLA	CHC-C1C	2.90	1.42	1.35
25	c	502	CLA	CHC-C1C	2.89	1.42	1.35
25	S	612	CLA	CHC-C1C	2.89	1.42	1.35
25	B	508	CLA	CHC-C1C	2.89	1.42	1.35
25	r	302	CLA	CHC-C1C	2.89	1.42	1.35
25	S	603	CLA	C4D-ND	-2.89	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	609	CHL	C1D-C2D	2.89	1.51	1.45
25	b	506	CLA	CHC-C1C	2.89	1.42	1.35
25	C	505	CLA	C4D-ND	-2.89	1.33	1.37
25	Y	313	CLA	CHC-C1C	2.89	1.42	1.35
25	B	516	CLA	CHC-C1C	2.89	1.42	1.35
25	C	503	CLA	CHC-C1C	2.89	1.42	1.35
25	D	405	CLA	CHC-C1C	2.88	1.42	1.35
25	G	602	CLA	CHC-C1C	2.88	1.42	1.35
36	S	601	CHL	C1D-C2D	2.87	1.51	1.45
25	B	504	CLA	CHC-C1C	2.87	1.42	1.35
25	b	508	CLA	CHC-C1C	2.87	1.42	1.35
25	G	603	CLA	CHC-C1C	2.87	1.42	1.35
36	Y	307	CHL	C1D-C2D	2.87	1.51	1.45
25	b	511	CLA	CHC-C1C	2.87	1.42	1.35
25	A	403	CLA	CHC-C1C	2.87	1.42	1.35
25	d	401	CLA	CHC-C1C	2.86	1.42	1.35
25	N	313	CLA	C4D-ND	-2.85	1.33	1.37
25	r	302	CLA	C4D-ND	-2.85	1.33	1.37
36	N	306	CHL	C1D-C2D	2.85	1.50	1.45
25	B	501	CLA	CHC-C1C	2.85	1.42	1.35
36	Y	308	CHL	C1D-C2D	2.84	1.50	1.45
36	S	607	CHL	C1D-C2D	2.84	1.50	1.45
25	Y	305	CLA	CHC-C1C	2.84	1.42	1.35
25	B	515	CLA	CHC-C1C	2.84	1.42	1.35
28	A	407	SQD	C6-S	-2.84	1.66	1.77
25	b	508	CLA	CMB-C2B	-2.83	1.45	1.51
25	b	515	CLA	CHC-C1C	2.83	1.42	1.35
36	Y	309	CHL	C1D-C2D	2.83	1.50	1.45
36	N	309	CHL	C1D-C2D	2.83	1.50	1.45
25	r	307	CLA	CHC-C1C	2.82	1.42	1.35
36	G	607	CHL	C1D-C2D	2.82	1.50	1.45
36	G	619	CHL	C1D-C2D	2.82	1.50	1.45
35	f	101	HEM	CAB-C3B	2.82	1.55	1.47
25	r	307	CLA	C4D-ND	-2.82	1.33	1.37
25	D	401	CLA	CHC-C1C	2.81	1.42	1.35
36	G	608	CHL	C1D-C2D	2.81	1.50	1.45
25	C	502	CLA	CHC-C1C	2.81	1.42	1.35
25	S	605	CLA	CHC-C1C	2.80	1.42	1.35
25	r	307	CLA	MG-NA	2.78	2.12	2.06
36	S	608	CHL	C1D-C2D	2.77	1.50	1.45
28	a	407	SQD	C6-S	-2.76	1.67	1.77
26	A	404	PHO	CAC-C3C	-2.76	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	308	CHL	C1D-C2D	2.76	1.50	1.45
25	b	504	CLA	CHC-C1C	2.75	1.42	1.35
34	d	406	PL9	C6-C1	-2.75	1.43	1.48
36	S	606	CHL	C1D-C2D	2.72	1.50	1.45
36	N	307	CHL	C1D-C2D	2.69	1.50	1.45
26	a	404	PHO	CAC-C3C	-2.69	1.47	1.52
25	B	508	CLA	CMB-C2B	-2.68	1.46	1.51
36	r	305	CHL	C3D-C2D	2.67	1.46	1.39
25	b	511	CLA	CMB-C2B	-2.67	1.46	1.51
26	d	402	PHO	CAC-C3C	-2.67	1.47	1.52
36	S	606	CHL	C3D-C2D	2.67	1.46	1.39
36	r	304	CHL	C3D-C2D	2.66	1.46	1.39
25	C	502	CLA	CMB-C2B	-2.64	1.46	1.51
36	G	606	CHL	C1D-C2D	2.64	1.50	1.45
25	b	509	CLA	CMB-C2B	-2.63	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.63	1.46	1.51
36	Y	310	CHL	C3D-C2D	2.62	1.46	1.39
25	d	401	CLA	CMB-C2B	-2.62	1.46	1.51
26	D	402	PHO	CAC-C3C	-2.61	1.47	1.52
36	N	307	CHL	C3D-C2D	2.61	1.46	1.39
36	Y	307	CHL	C3D-C2D	2.60	1.46	1.39
36	S	607	CHL	C3D-C2D	2.60	1.46	1.39
36	G	609	CHL	C3D-C2D	2.60	1.46	1.39
36	N	307	CHL	C4B-CHC	2.59	1.48	1.41
36	G	606	CHL	C3D-C2D	2.59	1.46	1.39
36	r	306	CHL	C3D-C2D	2.59	1.46	1.39
36	G	607	CHL	C3D-C2D	2.58	1.46	1.39
25	C	506	CLA	CMB-C2B	-2.58	1.46	1.51
25	b	503	CLA	CMB-C2B	-2.57	1.46	1.51
36	N	302	CHL	C3D-C2D	2.57	1.46	1.39
25	c	506	CLA	CMB-C2B	-2.57	1.46	1.51
36	G	601	CHL	C3D-C2D	2.57	1.46	1.39
36	G	608	CHL	C3D-C2D	2.56	1.46	1.39
36	Y	308	CHL	C3D-C2D	2.56	1.46	1.39
36	G	605	CHL	C3D-C2D	2.56	1.46	1.39
25	B	503	CLA	CMB-C2B	-2.56	1.46	1.51
36	S	601	CHL	C3D-C2D	2.55	1.46	1.39
36	Y	303	CHL	C3D-C2D	2.55	1.46	1.39
36	N	308	CHL	C3D-C2D	2.55	1.46	1.39
36	Y	308	CHL	C4B-CHC	2.55	1.48	1.41
25	b	513	CLA	CMB-C2B	-2.55	1.46	1.51
25	S	605	CLA	CMB-C2B	-2.55	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	504	CLA	CMB-C2B	-2.55	1.46	1.51
36	G	619	CHL	C3D-C2D	2.54	1.46	1.39
36	N	310	CHL	C3D-C2D	2.54	1.46	1.39
25	a	403	CLA	CMB-C2B	-2.54	1.46	1.51
25	D	401	CLA	CMB-C2B	-2.54	1.46	1.51
36	N	306	CHL	C3D-C2D	2.54	1.46	1.39
25	C	511	CLA	CMB-C2B	-2.54	1.46	1.51
36	Y	309	CHL	C3D-C2D	2.54	1.46	1.39
36	S	608	CHL	C3D-C2D	2.53	1.46	1.39
25	Y	305	CLA	CMB-C2B	-2.53	1.46	1.51
25	c	508	CLA	CMB-C2B	-2.53	1.46	1.51
25	G	603	CLA	CMB-C2B	-2.52	1.46	1.51
25	b	506	CLA	CMB-C2B	-2.52	1.46	1.51
25	c	501	CLA	CMB-C2B	-2.52	1.46	1.51
36	Y	309	CHL	C4B-CHC	2.52	1.48	1.41
25	B	510	CLA	CMB-C2B	-2.51	1.46	1.51
25	A	403	CLA	CMB-C2B	-2.51	1.46	1.51
25	b	510	CLA	CMB-C2B	-2.51	1.46	1.51
36	N	309	CHL	C3D-C2D	2.51	1.46	1.39
25	b	505	CLA	CMB-C2B	-2.50	1.46	1.51
25	S	604	CLA	CMB-C2B	-2.50	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.50	1.46	1.51
25	B	511	CLA	CMB-C2B	-2.50	1.46	1.51
25	b	515	CLA	CMB-C2B	-2.49	1.46	1.51
25	b	514	CLA	CMB-C2B	-2.49	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.49	1.46	1.51
25	c	504	CLA	CMB-C2B	-2.49	1.46	1.51
25	C	508	CLA	CMB-C2B	-2.49	1.46	1.51
25	C	504	CLA	CMB-C2B	-2.49	1.46	1.51
36	G	606	CHL	C4B-CHC	2.48	1.47	1.41
25	S	603	CLA	CMB-C2B	-2.48	1.46	1.51
25	r	307	CLA	C1B-NB	2.48	1.37	1.35
25	N	313	CLA	CMB-C2B	-2.48	1.46	1.51
25	S	611	CLA	CMB-C2B	-2.48	1.46	1.51
25	b	502	CLA	CMB-C2B	-2.48	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.48	1.46	1.51
36	S	606	CHL	C4B-CHC	2.48	1.47	1.41
25	G	602	CLA	CMB-C2B	-2.48	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.48	1.46	1.51
25	b	507	CLA	CMB-C2B	-2.48	1.46	1.51
25	G	613	CLA	CMB-C2B	-2.47	1.46	1.51
25	r	301	CLA	CMB-C2B	-2.47	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	613	CLA	CMB-C2B	-2.47	1.46	1.51
25	d	403	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	504	CLA	CMB-C2B	-2.47	1.46	1.51
25	C	501	CLA	CMB-C2B	-2.47	1.46	1.51
25	Y	304	CLA	CMB-C2B	-2.47	1.46	1.51
25	a	402	CLA	CMB-C2B	-2.47	1.46	1.51
25	C	509	CLA	CMB-C2B	-2.47	1.46	1.51
25	N	305	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	506	CLA	CMB-C2B	-2.47	1.46	1.51
25	Y	315	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	507	CLA	CMB-C2B	-2.46	1.46	1.51
25	Y	312	CLA	CMB-C2B	-2.46	1.46	1.51
25	N	304	CLA	CMB-C2B	-2.46	1.46	1.51
25	N	315	CLA	CMB-C2B	-2.46	1.46	1.51
34	D	407	PL9	C6-C1	-2.46	1.44	1.48
25	B	514	CLA	CMB-C2B	-2.46	1.46	1.51
25	S	614	CLA	CMB-C2B	-2.46	1.46	1.51
25	Y	314	CLA	CMB-C2B	-2.46	1.46	1.51
25	B	501	CLA	CMB-C2B	-2.46	1.46	1.51
25	b	516	CLA	CMB-C2B	-2.46	1.46	1.51
25	N	312	CLA	CMB-C2B	-2.46	1.46	1.51
25	Y	313	CLA	CMB-C2B	-2.46	1.46	1.51
25	B	512	CLA	CMB-C2B	-2.45	1.46	1.51
25	S	602	CLA	CMB-C2B	-2.45	1.46	1.51
36	G	608	CHL	C4B-CHC	2.45	1.47	1.41
25	b	501	CLA	CMB-C2B	-2.45	1.46	1.51
25	d	404	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	513	CLA	CMB-C2B	-2.45	1.46	1.51
25	D	405	CLA	CMB-C2B	-2.45	1.46	1.51
25	a	405	CLA	CMB-C2B	-2.45	1.46	1.51
25	A	402	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	516	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	503	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	512	CLA	CMB-C2B	-2.44	1.46	1.51
36	N	309	CHL	C4B-CHC	2.44	1.47	1.41
25	G	614	CLA	CMB-C2B	-2.44	1.46	1.51
25	N	314	CLA	CMB-C2B	-2.44	1.46	1.51
25	G	611	CLA	CMB-C2B	-2.44	1.46	1.51
36	S	601	CHL	C4B-CHC	2.44	1.47	1.41
25	Y	306	CLA	CMB-C2B	-2.44	1.46	1.51
25	r	303	CLA	CMB-C2B	-2.44	1.46	1.51
36	N	307	CHL	MG-NA	-2.44	2.00	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	607	CHL	C4B-CHC	2.44	1.47	1.41
25	c	511	CLA	CMB-C2B	-2.44	1.46	1.51
25	S	609	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	502	CLA	CMB-C2B	-2.43	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.43	1.46	1.51
25	G	604	CLA	CMB-C2B	-2.43	1.46	1.51
25	Y	311	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	507	CLA	CMB-C2B	-2.43	1.46	1.51
36	N	306	CHL	C4B-CHC	2.43	1.47	1.41
25	D	404	CLA	CMB-C2B	-2.43	1.46	1.51
36	N	310	CHL	MG-NA	-2.43	2.00	2.06
25	C	505	CLA	CMB-C2B	-2.42	1.46	1.51
25	r	302	CLA	CMB-C2B	-2.42	1.46	1.51
36	Y	310	CHL	C4B-CHC	2.42	1.47	1.41
25	r	308	CLA	CMB-C2B	-2.42	1.46	1.51
25	A	405	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	509	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.41	1.46	1.51
25	N	311	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	505	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
25	G	612	CLA	CMB-C2B	-2.40	1.46	1.51
25	N	303	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	513	CLA	CMB-C2B	-2.40	1.46	1.51
25	S	610	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.39	1.46	1.51
36	Y	303	CHL	C4B-CHC	2.39	1.47	1.41
25	c	513	CLA	CMB-C2B	-2.39	1.46	1.51
25	S	612	CLA	CMB-C2B	-2.39	1.46	1.51
36	Y	307	CHL	C4B-CHC	2.38	1.47	1.41
36	G	619	CHL	C4B-CHC	2.38	1.47	1.41
36	N	302	CHL	C4B-CHC	2.38	1.47	1.41
36	r	305	CHL	C4B-CHC	2.38	1.47	1.41
36	S	607	CHL	MG-NA	-2.37	2.00	2.06
25	B	515	CLA	CMB-C2B	-2.37	1.46	1.51
36	N	308	CHL	C4B-CHC	2.37	1.47	1.41
36	S	608	CHL	C4B-CHC	2.37	1.47	1.41
25	r	307	CLA	CMB-C2B	-2.37	1.46	1.51
25	G	610	CLA	CMB-C2B	-2.37	1.46	1.51
36	G	605	CHL	C4B-CHC	2.36	1.47	1.41
36	G	607	CHL	C4B-CHC	2.36	1.47	1.41
36	N	310	CHL	C4B-CHC	2.36	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	r	304	CHL	C4B-CHC	2.35	1.47	1.41
36	r	305	CHL	C4C-C3C	2.35	1.49	1.45
36	r	304	CHL	MG-NA	-2.35	2.00	2.06
36	r	306	CHL	C4B-CHC	2.35	1.47	1.41
36	r	305	CHL	MG-NA	-2.35	2.00	2.06
36	Y	310	CHL	MG-NA	-2.35	2.00	2.06
25	d	403	CLA	CMC-C2C	-2.34	1.45	1.50
34	d	406	PL9	C53-C6	-2.34	1.45	1.50
36	S	608	CHL	C4C-C3C	2.34	1.49	1.45
36	r	306	CHL	MG-NA	-2.33	2.00	2.06
36	Y	310	CHL	C4C-C3C	2.32	1.49	1.45
36	Y	308	CHL	MG-NA	-2.32	2.00	2.06
36	G	607	CHL	MG-NA	-2.32	2.00	2.06
36	G	609	CHL	C4C-C3C	2.32	1.49	1.45
25	D	404	CLA	CMD-C2D	-2.32	1.45	1.50
36	G	619	CHL	MG-NA	-2.31	2.00	2.06
36	Y	309	CHL	MG-NA	-2.31	2.00	2.06
36	G	609	CHL	C4B-CHC	2.31	1.47	1.41
36	r	304	CHL	C4C-C3C	2.31	1.49	1.45
36	G	601	CHL	C4B-CHC	2.31	1.47	1.41
36	S	606	CHL	MG-NA	-2.30	2.00	2.06
35	F	101	HEM	FE-NB	2.30	2.08	1.96
36	N	309	CHL	MG-NA	-2.30	2.00	2.06
36	G	605	CHL	C4C-C3C	2.29	1.49	1.45
36	G	605	CHL	MG-NA	-2.29	2.00	2.06
36	G	608	CHL	MG-NA	-2.28	2.00	2.06
36	N	306	CHL	MG-NA	-2.27	2.00	2.06
36	G	606	CHL	MG-NA	-2.27	2.00	2.06
27	a	406	BCR	C30-C25	-2.25	1.50	1.53
36	S	608	CHL	MG-NA	-2.25	2.00	2.06
36	G	609	CHL	MG-NA	-2.25	2.00	2.06
25	c	505	CLA	CMD-C2D	-2.25	1.46	1.50
36	G	601	CHL	C4C-C3C	2.25	1.48	1.45
36	N	307	CHL	C1B-CHB	2.24	1.47	1.41
36	N	308	CHL	MG-NA	-2.24	2.01	2.06
36	N	310	CHL	C4C-C3C	2.24	1.48	1.45
36	N	310	CHL	C1B-CHB	2.24	1.47	1.41
36	Y	310	CHL	C1B-CHB	2.24	1.47	1.41
36	G	619	CHL	C4C-C3C	2.23	1.48	1.45
38	N	318	NEX	C1-C6	-2.23	1.50	1.54
25	C	505	CLA	CMD-C2D	-2.23	1.46	1.50
36	G	607	CHL	C4C-C3C	2.23	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Y	303	CHL	MG-NA	-2.23	2.01	2.06
34	D	407	PL9	C53-C6	-2.22	1.46	1.50
36	Y	309	CHL	C4C-C3C	2.21	1.48	1.45
25	A	402	CLA	CMC-C2C	-2.21	1.46	1.50
25	b	508	CLA	CMD-C2D	-2.21	1.46	1.50
36	S	607	CHL	C1B-CHB	2.21	1.47	1.41
25	b	516	CLA	CMC-C2C	-2.21	1.46	1.50
36	S	606	CHL	C4C-C3C	2.21	1.48	1.45
36	G	605	CHL	C1B-CHB	2.21	1.47	1.41
36	S	606	CHL	C1B-CHB	2.21	1.47	1.41
36	Y	307	CHL	C4C-C3C	2.20	1.48	1.45
25	b	503	CLA	CMD-C2D	-2.20	1.46	1.50
36	N	302	CHL	MG-NA	-2.20	2.01	2.06
25	A	402	CLA	CMD-C2D	-2.20	1.46	1.50
25	d	403	CLA	CMD-C2D	-2.20	1.46	1.50
36	S	601	CHL	C4C-C3C	2.19	1.48	1.45
26	d	402	PHO	CMD-C2D	-2.19	1.46	1.51
26	A	404	PHO	CMC-C2C	-2.19	1.46	1.51
35	F	101	HEM	FE-ND	2.18	2.07	1.96
25	a	402	CLA	CMC-C2C	-2.18	1.46	1.50
36	Y	308	CHL	C1B-CHB	2.18	1.47	1.41
25	d	401	CLA	C3B-C2B	-2.18	1.37	1.40
36	r	306	CHL	C4C-C3C	2.18	1.48	1.45
25	B	503	CLA	CMD-C2D	-2.18	1.46	1.50
26	D	402	PHO	CMD-C2D	-2.18	1.46	1.51
27	C	515	BCR	C30-C25	-2.18	1.50	1.53
36	Y	303	CHL	C4C-C3C	2.17	1.48	1.45
36	N	302	CHL	C4C-C3C	2.17	1.48	1.45
36	r	304	CHL	C1B-CHB	2.17	1.47	1.41
25	B	512	CLA	CMD-C2D	-2.17	1.46	1.50
25	b	512	CLA	CMD-C2D	-2.17	1.46	1.50
36	G	606	CHL	C1B-CHB	2.17	1.47	1.41
25	B	504	CLA	CMD-C2D	-2.17	1.46	1.50
36	r	305	CHL	C1B-CHB	2.16	1.47	1.41
36	G	608	CHL	C4C-C3C	2.16	1.48	1.45
26	D	402	PHO	CMC-C2C	-2.16	1.46	1.51
36	Y	309	CHL	C1B-CHB	2.16	1.47	1.41
36	G	609	CHL	C1B-CHB	2.16	1.47	1.41
36	G	608	CHL	C1B-CHB	2.15	1.47	1.41
36	N	309	CHL	C4C-C3C	2.15	1.48	1.45
26	A	404	PHO	CMD-C2D	-2.15	1.46	1.51
26	a	404	PHO	CMC-C2C	-2.15	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	308	CHL	C4C-C3C	2.15	1.48	1.45
36	G	601	CHL	MG-NA	-2.15	2.01	2.06
36	N	306	CHL	C1B-CHB	2.15	1.47	1.41
25	S	613	CLA	C3B-C2B	-2.15	1.37	1.40
36	N	309	CHL	C1B-CHB	2.15	1.47	1.41
25	C	501	CLA	CMD-C2D	-2.14	1.46	1.50
25	G	603	CLA	C3B-C2B	-2.14	1.37	1.40
36	r	306	CHL	C1B-CHB	2.14	1.46	1.41
25	C	512	CLA	C3B-C2B	-2.14	1.37	1.40
25	D	404	CLA	CMC-C2C	-2.14	1.46	1.50
26	d	402	PHO	CMC-C2C	-2.14	1.46	1.51
36	S	601	CHL	MG-NA	-2.14	2.01	2.06
25	a	402	CLA	CMD-C2D	-2.13	1.46	1.50
25	b	506	CLA	CMD-C2D	-2.13	1.46	1.50
36	S	608	CHL	C1B-CHB	2.13	1.46	1.41
36	N	308	CHL	C1B-CHB	2.13	1.46	1.41
39	G	620	XAT	O24-C25	-2.12	1.43	1.46
36	S	607	CHL	C4C-C3C	2.12	1.48	1.45
36	Y	307	CHL	MG-NA	-2.12	2.01	2.06
25	S	610	CLA	CMD-C2D	-2.12	1.46	1.50
36	Y	307	CHL	C1B-CHB	2.12	1.46	1.41
25	d	401	CLA	CMD-C2D	-2.12	1.46	1.50
26	a	404	PHO	CMD-C2D	-2.11	1.46	1.51
25	b	501	CLA	C3B-C2B	-2.11	1.37	1.40
36	G	607	CHL	C1B-CHB	2.11	1.46	1.41
25	c	512	CLA	CMD-C2D	-2.11	1.46	1.50
25	a	403	CLA	CMD-C2D	-2.11	1.46	1.50
25	N	311	CLA	CMD-C2D	-2.11	1.46	1.50
36	N	306	CHL	C4C-C3C	2.11	1.48	1.45
26	A	404	PHO	CMB-C2B	-2.11	1.46	1.51
36	G	619	CHL	C1B-CHB	2.11	1.46	1.41
25	B	516	CLA	CMC-C2C	-2.11	1.46	1.50
25	B	508	CLA	CMD-C2D	-2.10	1.46	1.50
25	C	512	CLA	CMD-C2D	-2.10	1.46	1.50
25	S	614	CLA	CMD-C2D	-2.10	1.46	1.50
25	c	507	CLA	CMD-C2D	-2.10	1.46	1.50
25	Y	313	CLA	CMD-C2D	-2.10	1.46	1.50
25	c	510	CLA	CMD-C2D	-2.10	1.46	1.50
25	c	501	CLA	C3B-C2B	-2.10	1.37	1.40
25	r	308	CLA	C3B-C2B	-2.10	1.37	1.40
25	N	305	CLA	CMD-C2D	-2.10	1.46	1.50
25	C	513	CLA	CMD-C2D	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	307	CHL	C4C-C3C	2.09	1.48	1.45
27	V	101	BCR	C1-C6	-2.09	1.50	1.53
25	c	504	CLA	C3B-C2B	-2.09	1.37	1.40
26	a	404	PHO	CMB-C2B	-2.09	1.46	1.51
25	G	614	CLA	CMD-C2D	-2.08	1.46	1.50
25	b	502	CLA	CMD-C2D	-2.08	1.46	1.50
25	N	315	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	509	CLA	CMD-C2D	-2.08	1.46	1.50
25	C	501	CLA	C3B-C2B	-2.08	1.37	1.40
26	d	402	PHO	CMB-C2B	-2.08	1.46	1.51
36	N	307	CHL	C2C-C1C	2.08	1.49	1.44
25	A	405	CLA	CMD-C2D	-2.07	1.46	1.50
25	S	609	CLA	C3B-C2B	-2.07	1.37	1.40
25	G	603	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	505	CLA	CMD-C2D	-2.07	1.46	1.50
25	c	501	CLA	CMD-C2D	-2.07	1.46	1.50
25	Y	315	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	501	CLA	CMD-C2D	-2.07	1.46	1.50
25	c	508	CLA	CMD-C2D	-2.07	1.46	1.50
36	N	302	CHL	C1B-CHB	2.07	1.46	1.41
36	Y	308	CHL	C2C-C1C	2.07	1.49	1.44
25	b	512	CLA	CMC-C2C	-2.07	1.46	1.50
36	Y	308	CHL	C4C-C3C	2.07	1.48	1.45
25	C	511	CLA	CMD-C2D	-2.07	1.46	1.50
25	D	401	CLA	CMD-C2D	-2.07	1.46	1.50
25	b	510	CLA	CMD-C2D	-2.07	1.46	1.50
25	A	403	CLA	CMD-C2D	-2.06	1.46	1.50
27	b	517	BCR	C30-C25	-2.06	1.50	1.53
25	S	613	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	515	CLA	CMD-C2D	-2.06	1.46	1.50
26	D	402	PHO	CMB-C2B	-2.06	1.46	1.51
35	F	101	HEM	CMB-C2B	2.06	1.55	1.50
25	b	509	CLA	CMD-C2D	-2.06	1.46	1.50
25	N	312	CLA	CMD-C2D	-2.06	1.46	1.50
25	B	510	CLA	CMD-C2D	-2.06	1.46	1.50
27	c	514	BCR	C30-C25	-2.06	1.50	1.53
25	C	510	CLA	CMD-C2D	-2.06	1.46	1.50
25	Y	305	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	504	CLA	CMD-C2D	-2.06	1.46	1.50
25	c	502	CLA	CMD-C2D	-2.06	1.46	1.50
25	C	506	CLA	CMD-C2D	-2.06	1.46	1.50
25	S	602	CLA	CMD-C2D	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	511	CLA	CMD-C2D	-2.06	1.46	1.50
25	B	501	CLA	CMD-C2D	-2.06	1.46	1.50
25	G	612	CLA	CMD-C2D	-2.05	1.46	1.50
25	N	304	CLA	C3B-C2B	-2.05	1.37	1.40
25	b	511	CLA	C3B-C2B	-2.05	1.37	1.40
25	b	513	CLA	CMD-C2D	-2.05	1.46	1.50
25	N	304	CLA	CMD-C2D	-2.05	1.46	1.50
25	b	516	CLA	CMD-C2D	-2.05	1.46	1.50
25	C	508	CLA	CMD-C2D	-2.05	1.46	1.50
25	Y	304	CLA	CMD-C2D	-2.05	1.46	1.50
25	D	405	CLA	CMD-C2D	-2.05	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.05	1.46	1.50
25	b	514	CLA	CMD-C2D	-2.05	1.46	1.50
36	G	606	CHL	C2C-C1C	2.05	1.49	1.44
39	N	301	XAT	O4-C5	-2.05	1.43	1.46
25	B	513	CLA	CMD-C2D	-2.05	1.46	1.50
25	B	506	CLA	CMD-C2D	-2.05	1.46	1.50
25	S	611	CLA	CMD-C2D	-2.04	1.46	1.50
39	Y	302	XAT	O4-C5	-2.04	1.43	1.46
25	c	503	CLA	CMD-C2D	-2.04	1.46	1.50
25	C	502	CLA	C3B-C2B	-2.04	1.37	1.40
25	S	604	CLA	CMD-C2D	-2.04	1.46	1.50
25	B	505	CLA	CMD-C2D	-2.04	1.46	1.50
25	S	612	CLA	CMD-C2D	-2.04	1.46	1.50
25	B	511	CLA	CMC-C2C	-2.04	1.46	1.50
27	C	514	BCR	C30-C25	-2.04	1.51	1.53
25	B	507	CLA	CMD-C2D	-2.04	1.46	1.50
25	B	511	CLA	CMD-C2D	-2.04	1.46	1.50
25	S	614	CLA	C3B-C2B	-2.04	1.37	1.40
25	a	403	CLA	C3B-C2B	-2.04	1.37	1.40
27	k	101	BCR	C1-C6	-2.03	1.51	1.53
25	Y	312	CLA	CMD-C2D	-2.03	1.46	1.50
25	b	511	CLA	CMC-C2C	-2.03	1.46	1.50
25	B	502	CLA	CMD-C2D	-2.03	1.46	1.50
25	r	302	CLA	CMD-C2D	-2.03	1.46	1.50
25	G	602	CLA	CMD-C2D	-2.03	1.46	1.50
36	G	606	CHL	C4C-C3C	2.03	1.48	1.45
25	d	404	CLA	CMD-C2D	-2.03	1.46	1.50
25	G	611	CLA	CMD-C2D	-2.03	1.46	1.50
25	N	313	CLA	C3B-C2B	-2.03	1.37	1.40
25	c	512	CLA	C3B-C2B	-2.03	1.37	1.40
34	d	406	PL9	C52-C5	-2.03	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	t	101	BCR	C30-C25	-2.03	1.51	1.53
25	c	508	CLA	CMC-C2C	-2.03	1.46	1.50
25	N	314	CLA	CMD-C2D	-2.03	1.46	1.50
25	a	405	CLA	CMD-C2D	-2.02	1.46	1.50
25	C	507	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	508	CLA	C3B-C2B	-2.02	1.37	1.40
25	B	514	CLA	CMD-C2D	-2.02	1.46	1.50
25	C	508	CLA	CMC-C2C	-2.02	1.46	1.50
25	b	515	CLA	C3B-C2B	-2.02	1.37	1.40
25	C	502	CLA	CMD-C2D	-2.02	1.46	1.50
25	C	504	CLA	CMD-C2D	-2.02	1.46	1.50
25	C	502	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	506	CLA	CMC-C2C	-2.02	1.46	1.50
25	Y	314	CLA	CMD-C2D	-2.02	1.46	1.50
25	S	605	CLA	CMD-C2D	-2.02	1.46	1.50
25	r	301	CLA	CMD-C2D	-2.02	1.46	1.50
25	N	303	CLA	CMD-C2D	-2.01	1.46	1.50
25	A	403	CLA	C3B-C2B	-2.01	1.37	1.40
25	S	602	CLA	C3B-C2B	-2.01	1.37	1.40
25	G	604	CLA	CMD-C2D	-2.01	1.46	1.50
25	r	308	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	507	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	504	CLA	CMD-C2D	-2.01	1.46	1.50
25	N	313	CLA	CMD-C2D	-2.01	1.46	1.50
25	c	511	CLA	CMD-C2D	-2.01	1.46	1.50
25	S	605	CLA	C3B-C2B	-2.01	1.37	1.40
25	S	603	CLA	CMD-C2D	-2.01	1.46	1.50
36	S	607	CHL	C2C-C1C	2.01	1.48	1.44
25	Y	311	CLA	CMD-C2D	-2.01	1.46	1.50
25	S	609	CLA	CMD-C2D	-2.01	1.46	1.50
27	d	405	BCR	C1-C6	-2.01	1.51	1.53
36	S	606	CHL	C2C-C1C	2.01	1.48	1.44
36	G	601	CHL	C1B-CHB	2.00	1.46	1.41
25	D	401	CLA	CMC-C2C	-2.00	1.46	1.50
25	G	612	CLA	C3B-C2B	-2.00	1.37	1.40
25	b	503	CLA	CMC-C2C	-2.00	1.46	1.50
25	S	610	CLA	CMC-C2C	-2.00	1.46	1.50
25	r	303	CLA	CMD-C2D	-2.00	1.46	1.50

All (2053) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	G	620	XAT	C37-C21-C36	-16.15	83.54	107.37
39	G	620	XAT	C37-C21-C22	-13.76	85.08	108.98
27	B	517	BCR	C16-C17-C18	-9.63	113.57	127.31
36	G	605	CHL	C1D-ND-C4D	-9.02	99.93	106.33
36	S	601	CHL	C1D-ND-C4D	-8.88	100.03	106.33
36	N	306	CHL	C1D-ND-C4D	-8.84	100.05	106.33
39	N	301	XAT	O24-C25-C24	8.78	119.98	113.38
36	G	619	CHL	C1D-ND-C4D	-8.71	100.14	106.33
36	G	606	CHL	C1D-ND-C4D	-8.71	100.15	106.33
36	G	607	CHL	C1D-ND-C4D	-8.70	100.16	106.33
36	N	309	CHL	C1D-ND-C4D	-8.68	100.17	106.33
36	Y	307	CHL	C1D-ND-C4D	-8.68	100.17	106.33
36	N	308	CHL	C1D-ND-C4D	-8.63	100.20	106.33
36	Y	308	CHL	C1D-ND-C4D	-8.62	100.21	106.33
36	N	310	CHL	CMD-C2D-C1D	8.61	139.89	124.71
36	r	304	CHL	C1D-ND-C4D	-8.61	100.22	106.33
36	N	302	CHL	C1D-ND-C4D	-8.60	100.23	106.33
36	S	607	CHL	C1D-ND-C4D	-8.53	100.28	106.33
36	r	306	CHL	CMD-C2D-C1D	8.53	139.74	124.71
36	S	601	CHL	CMD-C2D-C1D	8.53	139.74	124.71
36	Y	303	CHL	C1D-ND-C4D	-8.52	100.28	106.33
36	G	601	CHL	C1D-ND-C4D	-8.52	100.29	106.33
36	N	309	CHL	CMD-C2D-C1D	8.51	139.71	124.71
39	Y	302	XAT	O24-C25-C24	8.48	119.75	113.38
36	r	306	CHL	C1D-ND-C4D	-8.48	100.31	106.33
36	N	302	CHL	CMD-C2D-C1D	8.47	139.65	124.71
36	G	601	CHL	CMD-C2D-C1D	8.47	139.64	124.71
36	Y	309	CHL	C1D-ND-C4D	-8.46	100.33	106.33
36	G	605	CHL	CMD-C2D-C1D	8.46	139.62	124.71
36	Y	303	CHL	CMD-C2D-C1D	8.46	139.62	124.71
36	r	305	CHL	C1D-ND-C4D	-8.45	100.33	106.33
36	G	609	CHL	CMD-C2D-C1D	8.45	139.60	124.71
36	N	307	CHL	C1D-ND-C4D	-8.44	100.34	106.33
36	N	306	CHL	CMD-C2D-C1D	8.44	139.58	124.71
36	S	608	CHL	CMD-C2D-C1D	8.44	139.58	124.71
36	G	608	CHL	C1D-ND-C4D	-8.43	100.35	106.33
36	N	310	CHL	C1D-ND-C4D	-8.43	100.35	106.33
36	Y	307	CHL	CMD-C2D-C1D	8.43	139.56	124.71
36	Y	310	CHL	CMD-C2D-C1D	8.43	139.56	124.71
36	Y	308	CHL	CMD-C2D-C1D	8.41	139.54	124.71
36	G	609	CHL	C1D-ND-C4D	-8.40	100.36	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	r	305	CHL	CMD-C2D-C1D	8.40	139.52	124.71
36	Y	309	CHL	CMD-C2D-C1D	8.39	139.49	124.71
36	G	608	CHL	CMD-C2D-C1D	8.38	139.48	124.71
36	G	619	CHL	CMD-C2D-C1D	8.36	139.45	124.71
36	N	308	CHL	CMD-C2D-C1D	8.34	139.42	124.71
36	S	606	CHL	C1D-ND-C4D	-8.34	100.41	106.33
36	G	607	CHL	CMD-C2D-C1D	8.34	139.40	124.71
36	r	304	CHL	CMD-C2D-C1D	8.34	139.40	124.71
36	S	607	CHL	CMD-C2D-C1D	8.25	139.26	124.71
36	S	608	CHL	C1D-ND-C4D	-8.23	100.48	106.33
38	S	617	NEX	O24-C25-C24	8.08	119.45	113.38
27	v	101	BCR	C16-C17-C18	-8.08	115.77	127.31
39	G	620	XAT	O24-C25-C24	8.07	119.44	113.38
38	Y	318	NEX	O24-C25-C24	8.04	119.42	113.38
36	N	307	CHL	CMD-C2D-C1D	8.04	138.89	124.71
36	N	307	CHL	C2C-C3C-C4C	-8.02	100.77	106.49
38	G	617	NEX	O24-C25-C24	8.01	119.40	113.38
36	S	606	CHL	C2C-C3C-C4C	-7.99	100.80	106.49
36	N	308	CHL	C2C-C3C-C4C	-7.93	100.83	106.49
38	r	310	NEX	O24-C25-C24	7.91	119.32	113.38
36	Y	310	CHL	C1D-ND-C4D	-7.91	100.72	106.33
36	G	606	CHL	C2C-C3C-C4C	-7.91	100.85	106.49
36	S	606	CHL	CMD-C2D-C1D	7.88	138.60	124.71
36	Y	308	CHL	C2C-C3C-C4C	-7.88	100.87	106.49
36	N	306	CHL	C2C-C3C-C4C	-7.81	100.92	106.49
36	S	608	CHL	C2C-C3C-C4C	-7.81	100.92	106.49
36	G	606	CHL	CMD-C2D-C1D	7.77	138.41	124.71
36	G	609	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
36	S	601	CHL	C2C-C3C-C4C	-7.75	100.96	106.49
36	G	607	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
36	G	619	CHL	C2C-C3C-C4C	-7.68	101.01	106.49
36	Y	310	CHL	C2C-C3C-C4C	-7.67	101.03	106.49
39	r	309	XAT	O24-C25-C24	7.66	119.13	113.38
36	G	608	CHL	C2C-C3C-C4C	-7.62	101.06	106.49
36	N	309	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
36	Y	309	CHL	C2C-C3C-C4C	-7.57	101.10	106.49
36	r	305	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
36	G	605	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
36	S	607	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
36	Y	307	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
36	N	302	CHL	C2C-C3C-C4C	-7.47	101.17	106.49
36	G	601	CHL	C2C-C3C-C4C	-7.42	101.20	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	N	310	CHL	C2C-C3C-C4C	-7.37	101.24	106.49
39	r	309	XAT	O4-C5-C4	7.36	118.91	113.38
36	r	304	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
36	r	306	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
38	N	318	NEX	O24-C25-C24	7.31	118.88	113.38
36	N	310	CHL	CHD-C1D-ND	-7.27	117.77	124.45
27	B	517	BCR	C24-C23-C22	-7.27	115.25	126.23
36	Y	303	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
36	N	308	CHL	C2D-C1D-ND	7.16	115.38	110.10
36	G	605	CHL	C2D-C1D-ND	7.15	115.37	110.10
39	G	620	XAT	C37-C21-C26	-7.13	90.80	110.05
36	N	306	CHL	C2D-C1D-ND	7.09	115.33	110.10
36	Y	310	CHL	CHD-C1D-ND	-7.06	117.97	124.45
36	G	606	CHL	C2D-C1D-ND	7.02	115.28	110.10
36	S	601	CHL	C2D-C1D-ND	6.98	115.25	110.10
39	Y	302	XAT	O4-C5-C4	6.96	118.61	113.38
36	G	607	CHL	C2D-C1D-ND	6.96	115.23	110.10
36	Y	307	CHL	C2D-C1D-ND	6.94	115.22	110.10
36	G	619	CHL	C2D-C1D-ND	6.93	115.21	110.10
36	N	309	CHL	C2D-C1D-ND	6.87	115.16	110.10
36	G	609	CHL	CHD-C1D-ND	-6.84	118.17	124.45
36	G	608	CHL	C2D-C1D-ND	6.82	115.13	110.10
36	S	606	CHL	C2D-C1D-ND	6.80	115.12	110.10
36	G	605	CHL	CHD-C1D-ND	-6.75	118.25	124.45
36	S	607	CHL	C2D-C1D-ND	6.73	115.07	110.10
36	Y	308	CHL	C2D-C1D-ND	6.72	115.06	110.10
36	N	302	CHL	CHD-C1D-ND	-6.72	118.28	124.45
36	N	302	CHL	C2D-C1D-ND	6.72	115.05	110.10
36	Y	309	CHL	C2D-C1D-ND	6.71	115.05	110.10
36	r	304	CHL	C2D-C1D-ND	6.71	115.05	110.10
39	G	620	XAT	C18-C5-C6	-6.70	111.03	122.26
39	N	301	XAT	O4-C5-C4	6.69	118.41	113.38
36	G	609	CHL	C2D-C1D-ND	6.69	115.03	110.10
38	N	318	NEX	C38-C25-C26	-6.68	111.06	122.26
36	r	306	CHL	CHD-C1D-ND	-6.68	118.31	124.45
39	G	620	XAT	C36-C21-C22	6.68	120.59	108.98
38	r	310	NEX	C38-C25-C26	-6.66	111.09	122.26
36	S	608	CHL	C2D-C1D-ND	6.66	115.02	110.10
36	r	306	CHL	C2D-C1D-ND	6.66	115.01	110.10
36	Y	303	CHL	C2D-C1D-ND	6.66	115.01	110.10
36	S	601	CHL	CHD-C1D-ND	-6.65	118.35	124.45
36	G	601	CHL	C2D-C1D-ND	6.65	115.00	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	r	305	CHL	CHD-C1D-ND	-6.62	118.37	124.45
38	G	617	NEX	C38-C25-C26	-6.62	111.17	122.26
36	r	305	CHL	C2D-C1D-ND	6.61	114.97	110.10
36	S	607	CHL	CHD-C1D-ND	-6.59	118.40	124.45
36	N	310	CHL	C2D-C1D-ND	6.57	114.95	110.10
38	S	617	NEX	C38-C25-C26	-6.57	111.25	122.26
39	r	309	XAT	C18-C5-C6	-6.57	111.25	122.26
39	N	301	XAT	C18-C5-C6	-6.55	111.28	122.26
36	N	307	CHL	C2D-C1D-ND	6.55	114.93	110.10
36	N	307	CHL	CHD-C1D-ND	-6.54	118.45	124.45
39	r	309	XAT	C38-C25-C26	-6.53	111.31	122.26
36	Y	303	CHL	CHD-C1D-ND	-6.53	118.46	124.45
38	Y	318	NEX	C38-C25-C26	-6.51	111.35	122.26
36	r	304	CHL	CHD-C1D-ND	-6.51	118.47	124.45
36	Y	308	CHL	CHD-C1D-ND	-6.51	118.47	124.45
36	G	601	CHL	CHD-C1D-ND	-6.50	118.48	124.45
36	N	306	CHL	CHD-C1D-ND	-6.50	118.48	124.45
39	G	620	XAT	O4-C5-C4	6.48	118.25	113.38
39	Y	302	XAT	C18-C5-C6	-6.47	111.41	122.26
39	G	620	XAT	C38-C25-C26	-6.45	111.45	122.26
36	N	309	CHL	CHD-C1D-ND	-6.45	118.53	124.45
39	N	301	XAT	C38-C25-C26	-6.43	111.49	122.26
39	Y	302	XAT	C38-C25-C26	-6.42	111.51	122.26
36	Y	307	CHL	CHD-C1D-ND	-6.40	118.57	124.45
36	G	607	CHL	CHD-C1D-ND	-6.38	118.59	124.45
25	b	512	CLA	C4A-NA-C1A	6.37	109.57	106.71
36	G	619	CHL	CHD-C1D-ND	-6.34	118.62	124.45
36	S	608	CHL	CHD-C1D-ND	-6.32	118.64	124.45
36	G	608	CHL	CHD-C1D-ND	-6.25	118.71	124.45
36	Y	309	CHL	CHD-C1D-ND	-6.24	118.72	124.45
36	Y	310	CHL	C2D-C1D-ND	6.22	114.69	110.10
36	S	606	CHL	O2D-CGD-CBD	6.14	122.18	111.27
36	N	308	CHL	CHD-C1D-ND	-6.11	118.83	124.45
36	S	606	CHL	CHD-C1D-ND	-6.10	118.85	124.45
27	v	101	BCR	C24-C23-C22	-6.01	117.15	126.23
36	G	606	CHL	CHD-C1D-ND	-5.96	118.98	124.45
25	c	502	CLA	C4A-NA-C1A	5.74	109.29	106.71
27	d	405	BCR	C28-C27-C26	-5.69	103.91	114.08
25	C	511	CLA	C4A-NA-C1A	5.69	109.26	106.71
25	C	502	CLA	C4A-NA-C1A	5.66	109.25	106.71
25	B	512	CLA	C4A-NA-C1A	5.61	109.23	106.71
27	k	101	BCR	C20-C21-C22	-5.56	119.37	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	403	CLA	C4A-NA-C1A	5.56	109.21	106.71
36	G	606	CHL	C3C-C4C-NC	5.55	116.80	110.57
33	a	409	BCT	O2-C-O1	5.55	133.94	119.55
36	N	308	CHL	C3C-C4C-NC	5.54	116.78	110.57
25	b	510	CLA	C4A-NA-C1A	5.52	109.19	106.71
25	B	513	CLA	C4A-NA-C1A	5.52	109.19	106.71
33	D	403	BCT	O2-C-O1	5.50	133.81	119.55
27	h	101	BCR	C11-C10-C9	-5.50	119.46	127.31
27	h	101	BCR	C7-C8-C9	-5.48	117.95	126.23
36	S	606	CHL	C3C-C4C-NC	5.48	116.71	110.57
25	c	509	CLA	C4A-NA-C1A	5.48	109.17	106.71
36	N	306	CHL	C3C-C4C-NC	5.45	116.69	110.57
25	b	513	CLA	C4A-NA-C1A	5.45	109.16	106.71
36	Y	308	CHL	C3C-C4C-NC	5.43	116.67	110.57
36	N	307	CHL	C3C-C4C-NC	5.41	116.64	110.57
27	k	101	BCR	C24-C23-C22	-5.36	118.14	126.23
25	G	611	CLA	C4A-NA-C1A	5.35	109.11	106.71
36	G	619	CHL	C3C-C4C-NC	5.35	116.57	110.57
36	G	609	CHL	C3C-C4C-NC	5.34	116.56	110.57
36	G	607	CHL	C3C-C4C-NC	5.33	116.55	110.57
36	G	605	CHL	C3C-C4C-NC	5.30	116.51	110.57
36	Y	307	CHL	C3C-C4C-NC	5.29	116.51	110.57
25	c	507	CLA	C4A-NA-C1A	5.28	109.08	106.71
36	N	309	CHL	C3C-C4C-NC	5.28	116.49	110.57
36	Y	310	CHL	O2D-CGD-CBD	5.26	120.62	111.27
36	G	605	CHL	C3D-C4D-ND	5.26	118.75	110.24
25	Y	312	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	C	507	CLA	C4A-NA-C1A	5.26	109.07	106.71
36	S	601	CHL	C3C-C4C-NC	5.26	116.47	110.57
36	S	601	CHL	C3D-C4D-ND	5.26	118.74	110.24
25	C	509	CLA	C4A-NA-C1A	5.25	109.07	106.71
36	N	307	CHL	C3D-C4D-ND	5.25	118.73	110.24
36	S	608	CHL	C3C-C4C-NC	5.25	116.45	110.57
36	S	607	CHL	C3C-C4C-NC	5.25	116.45	110.57
36	r	304	CHL	C3D-C4D-ND	5.24	118.72	110.24
25	B	510	CLA	C4A-NA-C1A	5.23	109.06	106.71
36	G	608	CHL	C3C-C4C-NC	5.22	116.42	110.57
36	N	308	CHL	C3D-C2D-C1D	-5.21	98.72	105.83
36	Y	308	CHL	C3D-C4D-ND	5.21	118.67	110.24
27	H	101	BCR	C11-C10-C9	-5.20	119.89	127.31
25	D	404	CLA	C4A-NA-C1A	5.20	109.04	106.71
36	r	305	CHL	C3C-C4C-NC	5.20	116.40	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	G	609	CHL	O2D-CGD-CBD	5.19	120.49	111.27
36	G	601	CHL	C3C-C4C-NC	5.18	116.38	110.57
36	r	304	CHL	C3C-C4C-NC	5.18	116.38	110.57
36	N	307	CHL	O2D-CGD-CBD	5.17	120.46	111.27
36	r	305	CHL	C3D-C4D-ND	5.17	118.60	110.24
27	C	516	BCR	C20-C21-C22	-5.17	119.93	127.31
36	N	302	CHL	C3D-C4D-ND	5.17	118.60	110.24
36	N	302	CHL	C3C-C4C-NC	5.17	116.37	110.57
27	C	516	BCR	C24-C23-C22	-5.17	118.43	126.23
36	G	606	CHL	C3D-C4D-ND	5.17	118.60	110.24
36	Y	303	CHL	C3D-C4D-ND	5.16	118.58	110.24
36	S	607	CHL	C3D-C4D-ND	5.15	118.57	110.24
36	N	306	CHL	C3D-C2D-C1D	-5.15	98.80	105.83
27	c	514	BCR	C15-C14-C13	-5.15	119.96	127.31
36	N	306	CHL	C3D-C4D-ND	5.15	118.57	110.24
36	G	601	CHL	C3D-C4D-ND	5.15	118.56	110.24
25	S	611	CLA	C4A-NA-C1A	5.14	109.02	106.71
36	S	607	CHL	O2D-CGD-CBD	5.14	120.41	111.27
36	r	306	CHL	C3C-C4C-NC	5.14	116.34	110.57
36	Y	309	CHL	C3C-C4C-NC	5.14	116.34	110.57
36	G	619	CHL	C3D-C4D-ND	5.14	118.56	110.24
36	N	309	CHL	C3D-C4D-ND	5.14	118.55	110.24
36	N	310	CHL	C3D-C4D-ND	5.14	118.55	110.24
36	r	306	CHL	C3D-C4D-ND	5.14	118.55	110.24
36	N	310	CHL	O2D-CGD-CBD	5.12	120.38	111.27
36	N	310	CHL	C3C-C4C-NC	5.12	116.31	110.57
36	G	609	CHL	C3D-C4D-ND	5.11	118.51	110.24
36	G	607	CHL	C3D-C4D-ND	5.10	118.49	110.24
36	G	608	CHL	C3D-C2D-C1D	-5.09	98.88	105.83
36	G	609	CHL	C3D-C2D-C1D	-5.09	98.89	105.83
36	G	605	CHL	C3D-C2D-C1D	-5.08	98.89	105.83
36	S	608	CHL	C3D-C2D-C1D	-5.08	98.90	105.83
25	b	516	CLA	C4A-NA-C1A	5.08	108.99	106.71
36	Y	307	CHL	C3D-C4D-ND	5.08	118.45	110.24
36	Y	307	CHL	C3D-C2D-C1D	-5.08	98.90	105.83
36	Y	310	CHL	C3C-C4C-NC	5.08	116.27	110.57
36	G	607	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
36	S	608	CHL	O2D-CGD-CBD	5.06	120.25	111.27
36	S	601	CHL	C3D-C2D-C1D	-5.05	98.93	105.83
36	N	309	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
25	C	510	CLA	C4A-NA-C1A	5.04	108.97	106.71
25	c	511	CLA	C4A-NA-C1A	5.04	108.97	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Y	309	CHL	C3D-C4D-ND	5.03	118.38	110.24
25	D	401	CLA	C4A-NA-C1A	5.03	108.97	106.71
36	G	619	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
27	b	517	BCR	C15-C14-C13	-5.02	120.14	127.31
36	N	310	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
36	Y	309	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
25	b	509	CLA	C4A-NA-C1A	5.02	108.96	106.71
27	v	101	BCR	C20-C19-C18	-5.02	112.31	126.42
36	N	302	CHL	O2D-CGD-CBD	5.02	120.19	111.27
38	G	617	NEX	C15-C14-C13	-5.01	120.16	127.31
36	Y	310	CHL	C3D-C4D-ND	5.01	118.34	110.24
36	r	306	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
36	Y	303	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
36	S	606	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
36	G	608	CHL	C3D-C4D-ND	4.99	118.32	110.24
36	S	606	CHL	C3D-C4D-ND	4.99	118.31	110.24
25	N	314	CLA	C4A-NA-C1A	4.98	108.95	106.71
36	Y	310	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
36	G	601	CHL	C3D-C2D-C1D	-4.98	99.04	105.83
36	G	606	CHL	C3D-C2D-C1D	-4.98	99.04	105.83
36	N	302	CHL	C3D-C2D-C1D	-4.98	99.04	105.83
25	r	301	CLA	C4A-NA-C1A	4.98	108.94	106.71
27	H	101	BCR	C7-C8-C9	-4.98	118.72	126.23
27	z	101	BCR	C11-C10-C9	-4.97	120.21	127.31
36	N	308	CHL	C3D-C4D-ND	4.96	118.26	110.24
36	r	304	CHL	C3D-C2D-C1D	-4.96	99.07	105.83
36	S	607	CHL	C3D-C2D-C1D	-4.96	99.07	105.83
25	r	308	CLA	C4A-NA-C1A	4.96	108.93	106.71
36	Y	308	CHL	O2D-CGD-CBD	4.95	120.06	111.27
25	B	516	CLA	C4A-NA-C1A	4.95	108.93	106.71
25	S	604	CLA	C4A-NA-C1A	4.95	108.93	106.71
36	r	305	CHL	C3D-C2D-C1D	-4.94	99.08	105.83
25	d	404	CLA	C4A-NA-C1A	4.94	108.93	106.71
36	r	304	CHL	O2D-CGD-CBD	4.94	120.04	111.27
25	c	510	CLA	C4A-NA-C1A	4.93	108.92	106.71
25	b	515	CLA	C4A-NA-C1A	4.92	108.92	106.71
25	G	613	CLA	C4A-NA-C1A	4.92	108.92	106.71
36	Y	308	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
36	Y	303	CHL	C3C-C4C-NC	4.92	116.09	110.57
25	Y	314	CLA	C4A-NA-C1A	4.91	108.91	106.71
36	Y	303	CHL	O2D-CGD-CBD	4.91	119.99	111.27
36	N	309	CHL	O2D-CGD-CBD	4.90	119.98	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	d	406	PL9	C7-C3-C4	4.90	120.86	116.88
25	C	506	CLA	C4A-NA-C1A	4.90	108.91	106.71
25	B	505	CLA	C4A-NA-C1A	4.90	108.91	106.71
36	r	305	CHL	O2D-CGD-CBD	4.90	119.97	111.27
36	S	608	CHL	C3D-C4D-ND	4.89	118.14	110.24
34	D	407	PL9	C7-C3-C4	4.88	120.84	116.88
38	r	310	NEX	C15-C14-C13	-4.87	120.36	127.31
27	z	101	BCR	C16-C17-C18	-4.87	120.36	127.31
36	G	619	CHL	O2D-CGD-CBD	4.87	119.92	111.27
25	C	501	CLA	C4A-NA-C1A	4.85	108.89	106.71
25	r	303	CLA	C4A-NA-C1A	4.85	108.89	106.71
39	G	620	XAT	C15-C14-C13	-4.85	120.39	127.31
39	r	309	XAT	C6-C7-C8	-4.84	115.77	125.99
27	b	518	BCR	C15-C14-C13	-4.83	120.41	127.31
36	Y	307	CHL	O2D-CGD-CBD	4.83	119.85	111.27
25	b	505	CLA	C4A-NA-C1A	4.82	108.87	106.71
36	N	307	CHL	C3D-C2D-C1D	-4.81	99.26	105.83
25	D	405	CLA	C4A-NA-C1A	4.81	108.87	106.71
25	N	312	CLA	C4A-NA-C1A	4.81	108.87	106.71
36	G	606	CHL	O2D-CGD-CBD	4.81	119.82	111.27
36	G	605	CHL	O2D-CGD-CBD	4.81	119.81	111.27
25	C	513	CLA	C4A-NA-C1A	4.80	108.86	106.71
27	D	406	BCR	C7-C8-C9	4.80	133.49	126.23
27	k	101	BCR	C11-C10-C9	-4.80	120.46	127.31
25	S	603	CLA	C4A-NA-C1A	4.79	108.86	106.71
25	N	305	CLA	C4A-NA-C1A	4.77	108.85	106.71
25	Y	305	CLA	C4A-NA-C1A	4.77	108.85	106.71
27	V	101	BCR	C16-C17-C18	-4.77	120.51	127.31
25	B	501	CLA	C4A-NA-C1A	4.76	108.84	106.71
36	Y	309	CHL	O2D-CGD-CBD	4.74	119.69	111.27
25	d	401	CLA	C4A-NA-C1A	4.74	108.84	106.71
25	c	512	CLA	C4A-NA-C1A	4.74	108.83	106.71
25	b	511	CLA	C4A-NA-C1A	4.73	108.83	106.71
36	G	601	CHL	O2D-CGD-CBD	4.72	119.66	111.27
25	B	509	CLA	C4A-NA-C1A	4.72	108.83	106.71
25	a	405	CLA	C4A-NA-C1A	4.72	108.83	106.71
25	N	304	CLA	C4A-NA-C1A	4.72	108.83	106.71
25	C	504	CLA	C4A-NA-C1A	4.72	108.83	106.71
36	G	608	CHL	O2D-CGD-CBD	4.71	119.64	111.27
27	B	517	BCR	C19-C18-C17	4.71	126.17	118.94
27	C	515	BCR	C15-C14-C13	-4.71	120.59	127.31
36	G	607	CHL	O2D-CGD-CBD	4.69	119.60	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	517	BCR	C16-C15-C14	-4.68	113.88	123.47
25	A	405	CLA	C4A-NA-C1A	4.67	108.81	106.71
25	c	506	CLA	C4A-NA-C1A	4.67	108.81	106.71
38	Y	318	NEX	C15-C14-C13	-4.67	120.65	127.31
27	H	101	BCR	C16-C17-C18	-4.65	120.67	127.31
27	t	101	BCR	C15-C14-C13	-4.65	120.67	127.31
25	G	603	CLA	C4A-NA-C1A	4.64	108.79	106.71
25	c	504	CLA	C4A-NA-C1A	4.62	108.78	106.71
25	N	303	CLA	C4A-NA-C1A	4.61	108.78	106.71
25	b	504	CLA	C4A-NA-C1A	4.61	108.78	106.71
36	N	308	CHL	O2D-CGD-CBD	4.59	119.43	111.27
25	Y	306	CLA	C4A-NA-C1A	4.59	108.77	106.71
36	S	601	CHL	O2D-CGD-CBD	4.59	119.43	111.27
25	Y	313	CLA	C4A-NA-C1A	4.59	108.77	106.71
25	a	403	CLA	C4A-NA-C1A	4.59	108.77	106.71
36	N	306	CHL	O2D-CGD-CBD	4.58	119.41	111.27
38	G	617	NEX	C11-C10-C9	-4.58	120.78	127.31
38	S	617	NEX	C35-C34-C33	-4.56	120.80	127.31
25	S	613	CLA	C4A-NA-C1A	4.56	108.76	106.71
25	B	515	CLA	C4A-NA-C1A	4.55	108.75	106.71
36	r	306	CHL	O2D-CGD-CBD	4.53	119.33	111.27
39	G	620	XAT	O4-C5-C18	4.53	120.49	115.06
25	c	501	CLA	C4A-NA-C1A	4.52	108.74	106.71
25	B	514	CLA	C4A-NA-C1A	4.52	108.74	106.71
25	C	512	CLA	C4A-NA-C1A	4.52	108.74	106.71
25	A	402	CLA	C4A-NA-C1A	4.50	108.73	106.71
39	Y	302	XAT	C15-C14-C13	-4.50	120.89	127.31
25	b	503	CLA	C4A-NA-C1A	4.49	108.73	106.71
25	A	403	CLA	C4A-NA-C1A	4.49	108.72	106.71
39	r	309	XAT	C35-C34-C33	-4.48	120.92	127.31
25	B	502	CLA	C4A-NA-C1A	4.48	108.72	106.71
25	b	508	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
25	S	602	CLA	C4A-NA-C1A	4.47	108.72	106.71
25	b	501	CLA	C4A-NA-C1A	4.47	108.72	106.71
25	b	507	CLA	C4A-NA-C1A	4.45	108.70	106.71
27	b	519	BCR	C16-C17-C18	-4.45	120.97	127.31
25	b	506	CLA	C4A-NA-C1A	4.44	108.70	106.71
39	N	301	XAT	O4-C5-C18	4.42	120.35	115.06
25	B	503	CLA	C4A-NA-C1A	4.42	108.69	106.71
38	N	318	NEX	O24-C25-C38	4.42	120.35	115.06
25	C	503	CLA	C4A-NA-C1A	4.41	108.69	106.71
27	b	519	BCR	C15-C14-C13	-4.41	121.02	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	406	BCR	C11-C10-C9	-4.41	121.02	127.31
39	r	309	XAT	O4-C5-C18	4.40	120.33	115.06
25	c	508	CLA	C4A-NA-C1A	4.40	108.68	106.71
39	N	301	XAT	C6-C7-C8	-4.40	116.69	125.99
39	G	620	XAT	C6-C7-C8	-4.40	116.70	125.99
25	C	508	CLA	C4A-NA-C1A	4.40	108.68	106.71
25	B	511	CLA	C4A-NA-C1A	4.39	108.68	106.71
27	v	101	BCR	C37-C22-C21	-4.38	116.79	122.92
27	B	518	BCR	C16-C17-C18	-4.37	121.08	127.31
27	z	101	BCR	C33-C5-C6	-4.37	119.62	124.53
25	A	405	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
27	V	101	BCR	C33-C5-C6	-4.36	119.63	124.53
27	c	514	BCR	C24-C23-C22	-4.36	119.65	126.23
29	d	410	LMG	O7-C10-C11	4.36	120.89	111.50
39	Y	302	XAT	C6-C7-C8	-4.35	116.80	125.99
25	Y	304	CLA	C4A-NA-C1A	4.35	108.66	106.71
25	B	506	CLA	C4A-NA-C1A	4.34	108.66	106.71
27	d	405	BCR	C16-C17-C18	-4.34	121.11	127.31
27	h	101	BCR	C16-C17-C18	-4.34	121.12	127.31
38	r	310	NEX	C27-C28-C29	-4.34	118.80	125.53
25	b	514	CLA	C4A-NA-C1A	4.33	108.65	106.71
36	G	606	CHL	CHD-C4C-C3C	-4.31	118.50	124.84
31	W	202	DGD	O2G-C1B-C2B	4.31	120.79	111.50
37	S	616	LUT	C35-C34-C33	-4.30	121.17	127.31
27	t	101	BCR	C30-C25-C26	-4.30	116.55	122.61
25	B	507	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
36	N	308	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
25	c	513	CLA	C4A-NA-C1A	4.29	108.64	106.71
36	Y	308	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
27	H	101	BCR	C15-C14-C13	-4.29	121.19	127.31
25	G	604	CLA	C4A-NA-C1A	4.27	108.62	106.71
25	S	612	CLA	C4A-NA-C1A	4.27	108.62	106.71
30	S	618	LHG	O7-C7-C8	4.26	120.69	111.50
39	r	309	XAT	C26-C27-C28	-4.26	116.99	125.99
38	G	617	NEX	C27-C28-C29	-4.26	118.92	125.53
25	G	610	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
25	S	610	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
25	Y	306	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
37	Y	316	LUT	C35-C34-C33	-4.25	121.25	127.31
25	B	512	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
29	D	410	LMG	O7-C10-C11	4.24	120.64	111.50
39	r	309	XAT	O24-C25-C38	4.24	120.13	115.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	406	BCR	C16-C17-C18	-4.23	121.27	127.31
30	L	101	LHG	O7-C7-C8	4.23	120.61	111.50
25	B	507	CLA	C4A-NA-C1A	4.23	108.61	106.71
27	t	101	BCR	C11-C10-C9	-4.22	121.28	127.31
25	N	313	CLA	C4A-NA-C1A	4.22	108.60	106.71
25	G	602	CLA	C4A-NA-C1A	4.22	108.60	106.71
27	d	405	BCR	C27-C26-C25	-4.20	116.63	122.73
31	C	518	DGD	O2G-C1B-C2B	4.20	120.55	111.50
27	D	406	BCR	C16-C17-C18	-4.20	121.32	127.31
25	b	516	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
25	b	502	CLA	C4A-NA-C1A	4.20	108.59	106.71
25	B	508	CLA	C4A-NA-C1A	4.19	108.59	106.71
27	A	406	BCR	C15-C14-C13	-4.19	121.33	127.31
25	B	504	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
25	B	508	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
27	t	101	BCR	C3-C4-C5	-4.18	106.61	114.08
25	a	405	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
30	a	410	LHG	O7-C7-C8	4.16	120.47	111.50
38	Y	318	NEX	C27-C28-C29	-4.16	119.08	125.53
25	b	513	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
39	N	301	XAT	C15-C14-C13	-4.16	121.38	127.31
27	v	101	BCR	C23-C22-C21	4.15	125.32	118.94
39	Y	302	XAT	O4-C5-C18	4.15	120.03	115.06
31	c	517	DGD	O2G-C1B-C2B	4.15	120.44	111.50
27	A	406	BCR	C16-C17-C18	-4.15	121.39	127.31
25	G	614	CLA	C4A-NA-C1A	4.15	108.57	106.71
36	N	306	CHL	CHD-C4C-C3C	-4.15	118.75	124.84
38	N	318	NEX	C27-C28-C29	-4.14	119.10	125.53
29	a	408	LMG	O7-C10-C11	4.14	120.42	111.50
36	G	619	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
38	G	617	NEX	O24-C25-C38	4.13	120.00	115.06
25	Y	315	CLA	C4A-NA-C1A	4.13	108.56	106.71
27	z	101	BCR	C20-C21-C22	-4.13	121.42	127.31
28	A	407	SQD	O47-C7-C8	4.13	120.39	111.50
36	N	307	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
27	B	517	BCR	C23-C22-C21	4.12	125.27	118.94
25	G	612	CLA	C4A-NA-C1A	4.11	108.56	106.71
36	N	309	CHL	CHD-C4C-C3C	-4.11	118.79	124.84
27	v	101	BCR	C19-C18-C17	4.11	125.25	118.94
27	B	518	BCR	C1-C6-C5	-4.10	116.83	122.61
38	S	617	NEX	C27-C28-C29	-4.10	119.17	125.53
25	B	513	CLA	CMB-C2B-C1B	-4.09	122.17	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	513	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
25	C	510	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
27	a	406	BCR	C24-C23-C22	-4.09	120.06	126.23
29	W	201	LMG	O7-C10-C11	4.08	120.30	111.50
38	r	310	NEX	O24-C25-C38	4.08	119.94	115.06
25	N	303	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
37	N	316	LUT	C35-C34-C33	-4.08	121.49	127.31
30	N	319	LHG	O7-C7-C8	4.08	120.29	111.50
25	a	402	CLA	C4A-NA-C1A	4.07	108.54	106.71
29	d	409	LMG	O7-C10-C11	4.07	120.28	111.50
36	S	601	CHL	CHD-C4C-C3C	-4.07	118.85	124.84
25	r	302	CLA	C4A-NA-C1A	4.07	108.53	106.71
25	c	509	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
27	z	101	BCR	C24-C23-C22	-4.06	120.10	126.23
27	t	101	BCR	C33-C5-C6	-4.06	119.97	124.53
36	S	607	CHL	CHD-C4C-C3C	-4.06	118.87	124.84
38	Y	318	NEX	C35-C34-C33	-4.06	121.52	127.31
39	G	620	XAT	C35-C34-C33	-4.06	121.52	127.31
27	A	406	BCR	C7-C8-C9	-4.06	120.10	126.23
36	G	607	CHL	CHD-C4C-C3C	-4.05	118.88	124.84
36	r	306	CHL	CHD-C4C-C3C	-4.05	118.88	124.84
37	S	615	LUT	C35-C34-C33	-4.05	121.53	127.31
25	G	604	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
37	G	615	LUT	C35-C34-C33	-4.05	121.53	127.31
30	d	408	LHG	O7-C7-C8	4.05	120.22	111.50
25	A	402	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
29	B	519	LMG	O7-C10-C11	4.04	120.22	111.50
27	a	406	BCR	C15-C14-C13	-4.04	121.54	127.31
39	Y	302	XAT	C31-C30-C29	-4.04	121.54	127.31
27	A	406	BCR	C24-C23-C22	-4.03	120.14	126.23
27	B	518	BCR	C15-C14-C13	-4.02	121.57	127.31
31	C	517	DGD	O2G-C1B-C2B	4.02	120.17	111.50
25	B	506	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
27	k	101	BCR	C7-C8-C9	-4.02	120.16	126.23
36	S	606	CHL	CHD-C4C-C3C	-4.02	118.94	124.84
29	H	102	LMG	O7-C10-C11	4.02	120.16	111.50
25	c	503	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
27	b	518	BCR	C16-C17-C18	-4.01	121.59	127.31
25	C	508	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
27	h	101	BCR	C20-C21-C22	-4.01	121.59	127.31
36	Y	307	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
25	b	509	CLA	CMB-C2B-C1B	-4.00	122.32	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	506	CLA	CMB-C2B-C1B	-3.99	122.32	128.46
25	b	502	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
36	G	608	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
27	D	406	BCR	C34-C9-C8	3.99	124.36	118.08
31	c	516	DGD	O2G-C1B-C2B	3.99	120.10	111.50
27	C	514	BCR	C7-C8-C9	-3.98	120.22	126.23
25	C	509	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
36	S	606	CHL	CAC-C3C-C4C	3.98	129.97	124.81
30	D	408	LHG	O7-C7-C8	3.97	120.05	111.50
29	C	520	LMG	O7-C10-C11	3.97	120.05	111.50
27	c	514	BCR	C7-C8-C9	-3.97	120.24	126.23
36	Y	309	CHL	CHD-C4C-C3C	-3.97	119.01	124.84
27	z	101	BCR	C15-C14-C13	-3.96	121.65	127.31
25	b	508	CLA	C4A-NA-C1A	3.96	108.49	106.71
27	b	519	BCR	C11-C10-C9	-3.96	121.66	127.31
27	C	514	BCR	C16-C17-C18	-3.96	121.67	127.31
25	Y	304	CLA	CMB-C2B-C1B	-3.96	122.39	128.46
30	C	521	LHG	O7-C7-C8	3.95	120.02	111.50
27	b	519	BCR	C20-C21-C22	-3.94	121.68	127.31
25	Y	311	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
25	r	302	CLA	CMB-C2B-C1B	-3.94	122.42	128.46
25	B	502	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
36	r	304	CHL	CHD-C4C-C3C	-3.93	119.07	124.84
38	S	617	NEX	O24-C25-C38	3.93	119.76	115.06
30	G	618	LHG	O7-C7-C8	3.92	119.96	111.50
30	D	409	LHG	O7-C7-C8	3.92	119.95	111.50
25	c	510	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
31	c	515	DGD	O2G-C1B-C2B	3.92	119.95	111.50
27	C	514	BCR	C30-C25-C26	-3.92	117.10	122.61
25	b	507	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
36	G	605	CHL	CHD-C4C-C3C	-3.91	119.09	124.84
25	B	504	CLA	C4A-NA-C1A	3.91	108.46	106.71
30	B	520	LHG	O7-C7-C8	3.91	119.92	111.50
29	b	520	LMG	O7-C10-C11	3.90	119.92	111.50
25	a	402	CLA	CMB-C2B-C1B	-3.90	122.46	128.46
25	b	514	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
27	C	515	BCR	C24-C23-C22	-3.90	120.34	126.23
25	r	303	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
25	c	513	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
25	c	508	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
30	Y	319	LHG	O7-C7-C8	3.89	119.88	111.50
25	C	503	CLA	CMB-C2B-C1B	-3.89	122.49	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	603	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
36	S	608	CHL	CHD-C4C-C3C	-3.88	119.13	124.84
36	N	302	CHL	CHD-C4C-C3C	-3.88	119.13	124.84
25	C	505	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
31	C	519	DGD	O2G-C1B-C2B	3.88	119.86	111.50
25	S	605	CLA	C4A-NA-C1A	3.88	108.45	106.71
38	N	318	NEX	C15-C14-C13	-3.87	121.78	127.31
38	Y	318	NEX	O24-C25-C38	3.87	119.70	115.06
25	c	505	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
25	D	401	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
27	h	101	BCR	C15-C14-C13	-3.87	121.79	127.31
25	S	609	CLA	C4A-NA-C1A	3.87	108.44	106.71
39	Y	302	XAT	C35-C34-C33	-3.86	121.79	127.31
27	C	516	BCR	C11-C10-C9	-3.86	121.80	127.31
27	b	518	BCR	C11-C10-C9	-3.85	121.81	127.31
30	d	407	LHG	O7-C7-C8	3.85	119.80	111.50
25	b	504	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
25	B	511	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
29	c	518	LMG	O7-C10-C11	3.84	119.78	111.50
25	N	311	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
25	S	612	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
30	l	101	LHG	O7-C7-C8	3.84	119.77	111.50
36	Y	303	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
25	b	503	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
28	t	102	SQD	O47-C7-C8	3.83	119.77	111.50
25	B	514	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
25	Y	311	CLA	C4A-NA-C1A	3.83	108.43	106.71
25	C	504	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
25	r	301	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
25	b	512	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
25	c	503	CLA	C4A-NA-C1A	3.82	108.42	106.71
27	c	514	BCR	C16-C17-C18	-3.82	121.86	127.31
25	N	305	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
39	N	301	XAT	C35-C34-C33	-3.81	121.87	127.31
36	r	305	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
25	b	511	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
30	a	411	LHG	O7-C7-C8	3.80	119.70	111.50
27	H	101	BCR	C20-C21-C22	-3.80	121.89	127.31
25	b	506	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
27	z	101	BCR	C3-C4-C5	-3.79	107.30	114.08
27	v	101	BCR	C16-C15-C14	-3.79	115.71	123.47
38	N	318	NEX	C35-C34-C33	-3.79	121.90	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	506	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	Y	313	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
27	B	517	BCR	C27-C26-C25	-3.78	117.24	122.73
25	B	503	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
25	b	505	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
25	S	611	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
38	r	310	NEX	C35-C34-C33	-3.78	121.92	127.31
39	G	620	XAT	C31-C30-C29	-3.78	121.92	127.31
25	Y	315	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
25	d	404	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
36	G	601	CHL	CAC-C3C-C4C	3.77	129.70	124.81
25	B	509	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
25	G	602	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
36	G	601	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
25	G	611	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
25	b	510	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
25	D	405	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
27	B	517	BCR	C21-C20-C19	-3.76	111.48	123.22
31	Y	301	DGD	O2G-C1B-C2B	3.76	119.61	111.50
27	b	518	BCR	C20-C21-C22	-3.76	121.94	127.31
37	Y	317	LUT	C35-C34-C33	-3.76	121.94	127.31
39	Y	302	XAT	O24-C25-C38	3.76	119.56	115.06
27	v	101	BCR	C3-C4-C5	-3.75	107.37	114.08
38	Y	318	NEX	C11-C10-C9	-3.75	121.96	127.31
25	G	610	CLA	C4A-NA-C1A	3.75	108.39	106.71
25	S	604	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
36	r	304	CHL	CAC-C3C-C4C	3.74	129.66	124.81
27	B	517	BCR	C33-C5-C6	-3.74	120.33	124.53
25	A	405	CLA	CMB-C2B-C3B	3.73	131.66	124.68
25	G	614	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
27	C	514	BCR	C11-C10-C9	-3.73	121.98	127.31
27	c	514	BCR	C11-C10-C9	-3.73	121.99	127.31
27	b	519	BCR	C24-C23-C22	-3.73	120.60	126.23
25	A	403	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
25	G	613	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
25	a	403	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
38	S	617	NEX	C15-C14-C13	-3.71	122.02	127.31
25	S	605	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
25	c	511	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
25	B	512	CLA	CMB-C2B-C3B	3.69	131.59	124.68
25	Y	312	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
27	C	514	BCR	C24-C23-C22	-3.69	120.67	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d	405	BCR	C20-C21-C22	-3.69	122.05	127.31
27	z	101	BCR	C7-C8-C9	-3.68	120.67	126.23
28	a	407	SQD	O47-C7-C8	3.68	119.44	111.50
25	r	307	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
25	B	507	CLA	CMB-C2B-C3B	3.68	131.56	124.68
25	c	509	CLA	CMB-C2B-C3B	3.68	131.56	124.68
36	S	608	CHL	CAC-C3C-C4C	3.67	129.58	124.81
25	c	512	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	d	403	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	B	505	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
27	v	101	BCR	C30-C25-C26	-3.66	117.46	122.61
27	B	518	BCR	C20-C21-C22	-3.66	122.09	127.31
27	B	517	BCR	C28-C27-C26	-3.66	107.54	114.08
25	S	610	CLA	CMB-C2B-C3B	3.65	131.51	124.68
25	G	610	CLA	CMB-C2B-C3B	3.65	131.51	124.68
27	k	101	BCR	C28-C27-C26	-3.65	107.56	114.08
27	B	518	BCR	C24-C23-C22	-3.65	120.72	126.23
25	a	405	CLA	CMB-C2B-C3B	3.64	131.49	124.68
27	b	517	BCR	C3-C4-C5	-3.64	107.58	114.08
25	Y	305	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
25	C	507	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
37	G	615	LUT	C11-C10-C9	-3.63	122.12	127.31
37	G	616	LUT	C35-C34-C33	-3.63	122.13	127.31
36	N	310	CHL	CAC-C3C-C4C	3.63	129.52	124.81
36	r	305	CHL	CAC-C3C-C4C	3.63	129.52	124.81
27	c	514	BCR	C3-C4-C5	-3.63	107.60	114.08
25	N	311	CLA	C4A-NA-C1A	3.63	108.34	106.71
36	G	609	CHL	CHD-C4C-C3C	-3.63	119.51	124.84
37	G	616	LUT	C15-C14-C13	-3.62	122.14	127.31
25	b	516	CLA	CMB-C2B-C3B	3.62	131.45	124.68
27	b	517	BCR	C16-C17-C18	-3.62	122.14	127.31
25	N	315	CLA	C4A-NA-C1A	3.62	108.33	106.71
25	S	614	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
28	a	407	SQD	O7-S-C6	3.61	111.23	106.94
27	b	519	BCR	C7-C8-C9	-3.61	120.79	126.23
39	N	301	XAT	O24-C25-C38	3.59	119.36	115.06
37	S	616	LUT	C15-C14-C13	-3.59	122.18	127.31
25	c	507	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
27	v	101	BCR	C33-C5-C6	-3.59	120.50	124.53
25	C	513	CLA	CMB-C2B-C3B	3.58	131.38	124.68
36	G	609	CHL	CAC-C3C-C4C	3.58	129.46	124.81
25	B	513	CLA	CMB-C2B-C3B	3.58	131.37	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Y	317	LUT	C15-C14-C13	-3.58	122.21	127.31
25	B	504	CLA	CMB-C2B-C3B	3.57	131.37	124.68
36	G	607	CHL	CAC-C3C-C4C	3.57	129.45	124.81
25	B	510	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
27	C	514	BCR	C15-C14-C13	-3.57	122.22	127.31
25	B	515	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
27	d	405	BCR	C24-C23-C22	-3.57	120.85	126.23
25	B	501	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
27	b	517	BCR	C11-C10-C9	-3.56	122.23	127.31
27	C	516	BCR	C7-C8-C9	-3.56	120.86	126.23
27	B	518	BCR	C38-C26-C25	-3.56	120.53	124.53
30	b	521	LHG	O7-C7-C8	3.55	119.16	111.50
25	C	511	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
25	Y	314	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
36	Y	310	CHL	CAC-C3C-C4C	3.55	129.41	124.81
27	C	515	BCR	C16-C17-C18	-3.55	122.25	127.31
28	A	407	SQD	O7-S-C6	3.55	111.15	106.94
25	b	513	CLA	CMB-C2B-C3B	3.54	131.31	124.68
25	C	509	CLA	CMB-C2B-C3B	3.54	131.31	124.68
36	G	606	CHL	CAC-C3C-C4C	3.54	129.41	124.81
25	C	510	CLA	CMB-C2B-C3B	3.54	131.31	124.68
25	N	313	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
25	N	314	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
25	Y	306	CLA	CMB-C2B-C3B	3.53	131.29	124.68
27	D	406	BCR	C20-C21-C22	-3.53	122.27	127.31
36	Y	307	CHL	CAC-C3C-C4C	3.53	129.39	124.81
27	C	515	BCR	C11-C10-C9	-3.53	122.28	127.31
27	B	517	BCR	C36-C18-C17	-3.52	118.00	122.92
25	B	516	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
36	N	308	CHL	CAC-C3C-C4C	3.51	129.37	124.81
36	G	601	CHL	C3B-C4B-NB	3.51	113.75	109.21
39	Y	302	XAT	C26-C27-C28	-3.51	118.58	125.99
37	S	615	LUT	C18-C5-C6	-3.51	120.59	124.53
25	c	502	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
39	N	301	XAT	C26-C27-C28	-3.50	118.58	125.99
36	N	307	CHL	CAC-C3C-C4C	3.50	129.36	124.81
39	G	620	XAT	C26-C27-C28	-3.50	118.60	125.99
25	c	503	CLA	CMB-C2B-C3B	3.50	131.22	124.68
25	b	501	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
27	d	405	BCR	C1-C6-C5	-3.50	117.69	122.61
27	v	101	BCR	C36-C18-C17	-3.50	118.03	122.92
27	H	101	BCR	C3-C4-C5	-3.49	107.84	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	401	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
39	r	309	XAT	C15-C14-C13	-3.48	122.34	127.31
27	d	405	BCR	C11-C10-C9	-3.48	122.34	127.31
27	h	101	BCR	C3-C4-C5	-3.48	107.87	114.08
27	A	406	BCR	C20-C21-C22	-3.47	122.35	127.31
27	h	101	BCR	C24-C23-C22	-3.47	120.98	126.23
37	N	317	LUT	C35-C34-C33	-3.47	122.36	127.31
25	N	304	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
25	C	502	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
36	N	302	CHL	CAC-C3C-C4C	3.46	129.30	124.81
27	C	514	BCR	C20-C21-C22	-3.46	122.38	127.31
27	A	406	BCR	C33-C5-C6	-3.46	120.65	124.53
27	B	517	BCR	C38-C26-C27	3.46	120.26	113.62
37	N	317	LUT	C7-C8-C9	-3.46	121.01	126.23
27	d	405	BCR	C15-C14-C13	-3.46	122.38	127.31
25	C	512	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
25	Y	304	CLA	CMB-C2B-C3B	3.45	131.14	124.68
36	Y	307	CHL	C3B-C4B-NB	3.45	113.67	109.21
25	b	508	CLA	CMB-C2B-C3B	3.45	131.13	124.68
25	N	303	CLA	CMB-C2B-C3B	3.45	131.13	124.68
36	N	310	CHL	CHD-C4C-C3C	-3.45	119.77	124.84
25	D	404	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
25	c	501	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
25	c	510	CLA	CMB-C2B-C3B	3.44	131.12	124.68
25	b	511	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
25	A	402	CLA	CMB-C2B-C3B	3.44	131.11	124.68
36	Y	303	CHL	C3B-C4B-NB	3.44	113.65	109.21
37	N	317	LUT	C15-C14-C13	-3.44	122.41	127.31
25	r	307	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
27	a	406	BCR	C7-C8-C9	-3.43	121.06	126.23
25	G	603	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
27	B	517	BCR	C37-C22-C21	-3.42	118.13	122.92
36	G	619	CHL	CAC-C3C-C4C	3.42	129.25	124.81
25	S	602	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
36	N	302	CHL	C1-C2-C3	-3.42	120.13	126.04
25	G	612	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	b	502	CLA	CMB-C2B-C3B	3.42	131.07	124.68
38	r	310	NEX	C11-C10-C9	-3.41	122.44	127.31
25	N	312	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
38	G	617	NEX	C35-C34-C33	-3.41	122.44	127.31
36	Y	308	CHL	CAC-C3C-C4C	3.41	129.24	124.81
25	N	315	CLA	CMB-C2B-C1B	-3.41	123.23	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	r	306	CHL	C3B-C4B-NB	3.40	113.61	109.21
27	D	406	BCR	C24-C23-C22	-3.40	121.09	126.23
25	c	504	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
36	G	605	CHL	C3B-C4B-NB	3.40	113.60	109.21
25	S	609	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
25	c	513	CLA	CMB-C2B-C3B	3.40	131.03	124.68
25	B	506	CLA	CMB-C2B-C3B	3.39	131.03	124.68
25	C	508	CLA	CMB-C2B-C3B	3.39	131.03	124.68
37	G	616	LUT	C7-C8-C9	-3.39	121.11	126.23
25	r	302	CLA	CMB-C2B-C3B	3.39	131.02	124.68
36	S	607	CHL	CAC-C3C-C4C	3.38	129.20	124.81
25	C	501	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
36	G	609	CHL	C3B-C4B-NB	3.38	113.58	109.21
36	S	608	CHL	C3B-C4B-NB	3.38	113.58	109.21
25	G	604	CLA	CMB-C2B-C3B	3.38	131.01	124.68
25	Y	311	CLA	CMB-C2B-C3B	3.37	130.99	124.68
27	C	515	BCR	C30-C25-C26	-3.37	117.87	122.61
36	Y	303	CHL	C1-C2-C3	-3.37	120.22	126.04
36	S	601	CHL	CAC-C3C-C4C	3.37	129.18	124.81
27	b	517	BCR	C24-C23-C22	-3.37	121.15	126.23
25	S	603	CLA	CMB-C2B-C3B	3.37	130.97	124.68
27	B	518	BCR	C4-C5-C6	-3.36	117.85	122.73
25	c	506	CLA	CMB-C2B-C3B	3.36	130.96	124.68
36	G	607	CHL	C3B-C4B-NB	3.35	113.54	109.21
36	G	605	CHL	CAC-C3C-C4C	3.35	129.16	124.81
27	d	405	BCR	C7-C8-C9	-3.35	121.17	126.23
36	N	302	CHL	C3B-C4B-NB	3.35	113.54	109.21
25	c	505	CLA	C1B-CHB-C4A	-3.34	123.49	130.12
25	a	402	CLA	CMB-C2B-C3B	3.34	130.93	124.68
27	b	518	BCR	C7-C8-C9	-3.34	121.19	126.23
27	a	406	BCR	C30-C25-C26	-3.34	117.91	122.61
27	c	514	BCR	C30-C25-C26	-3.34	117.91	122.61
36	r	304	CHL	C3B-C4B-NB	3.34	113.52	109.21
27	V	101	BCR	C7-C8-C9	-3.33	121.20	126.23
36	S	601	CHL	C3B-C4B-NB	3.33	113.52	109.21
39	G	620	XAT	O24-C25-C38	3.33	119.05	115.06
25	B	508	CLA	CMB-C2B-C3B	3.33	130.91	124.68
37	Y	317	LUT	C7-C8-C9	-3.33	121.20	126.23
36	Y	310	CHL	CHD-C4C-C3C	-3.33	119.94	124.84
25	N	311	CLA	CMB-C2B-C3B	3.33	130.91	124.68
25	c	508	CLA	CMB-C2B-C3B	3.33	130.91	124.68
36	N	309	CHL	CAC-C3C-C4C	3.33	129.13	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	401	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
34	D	407	PL9	C7-C3-C2	-3.32	118.93	123.30
36	G	619	CHL	C3B-C4B-NB	3.32	113.50	109.21
36	N	306	CHL	C3B-C4B-NB	3.32	113.50	109.21
27	b	517	BCR	C20-C21-C22	-3.32	122.58	127.31
27	D	406	BCR	C3-C4-C5	-3.32	108.16	114.08
25	c	511	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
27	C	515	BCR	C33-C5-C4	3.31	119.98	113.62
31	c	516	DGD	O1G-C1A-C2A	3.31	120.07	111.38
25	c	505	CLA	CMB-C2B-C3B	3.31	130.87	124.68
37	S	615	LUT	C15-C14-C13	-3.31	122.58	127.31
37	N	316	LUT	C15-C14-C13	-3.31	122.59	127.31
25	B	502	CLA	CMB-C2B-C3B	3.30	130.86	124.68
27	D	406	BCR	C15-C14-C13	-3.30	122.60	127.31
25	a	403	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
25	b	514	CLA	CMB-C2B-C3B	3.29	130.84	124.68
25	r	303	CLA	CMB-C2B-C3B	3.29	130.84	124.68
25	S	614	CLA	C4A-NA-C1A	3.29	108.18	106.71
39	G	620	XAT	C36-C21-C26	3.28	118.91	110.05
25	C	505	CLA	CMB-C2B-C3B	3.28	130.82	124.68
25	G	602	CLA	CMB-C2B-C3B	3.28	130.82	124.68
25	D	401	CLA	CMB-C2B-C3B	3.28	130.81	124.68
25	b	507	CLA	CMB-C2B-C3B	3.28	130.81	124.68
37	G	615	LUT	C7-C8-C9	-3.28	121.28	126.23
25	S	612	CLA	CMB-C2B-C3B	3.28	130.81	124.68
27	C	516	BCR	C28-C27-C26	-3.28	108.22	114.08
27	t	101	BCR	C27-C26-C25	-3.28	117.97	122.73
25	C	504	CLA	CMB-C2B-C3B	3.28	130.81	124.68
27	a	406	BCR	C11-C10-C9	-3.28	122.63	127.31
25	b	515	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
37	Y	316	LUT	C15-C14-C13	-3.28	122.63	127.31
37	Y	316	LUT	C7-C8-C9	-3.27	121.29	126.23
25	S	613	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
36	N	308	CHL	C3B-C4B-NB	3.27	113.44	109.21
25	B	511	CLA	CMB-C2B-C3B	3.27	130.79	124.68
34	d	406	PL9	C7-C3-C2	-3.27	119.00	123.30
25	A	403	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
27	k	101	BCR	C33-C5-C6	-3.27	120.86	124.53
37	S	615	LUT	C21-C26-C27	-3.26	108.57	112.70
27	C	515	BCR	C33-C5-C6	-3.26	120.86	124.53
25	Y	313	CLA	CMB-C2B-C3B	3.26	130.78	124.68
25	C	503	CLA	CMB-C2B-C3B	3.26	130.77	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	506	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
37	N	316	LUT	C18-C5-C6	-3.25	120.87	124.53
25	c	503	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
37	G	616	LUT	C18-C5-C6	-3.25	120.88	124.53
36	r	305	CHL	C3B-C4B-NB	3.25	113.41	109.21
25	b	510	CLA	CMB-C2B-C3B	3.24	130.75	124.68
37	S	615	LUT	C7-C8-C9	-3.24	121.33	126.23
25	b	506	CLA	CMB-C2B-C3B	3.24	130.75	124.68
25	D	405	CLA	CMB-C2B-C3B	3.24	130.74	124.68
37	N	316	LUT	C7-C8-C9	-3.24	121.34	126.23
37	N	316	LUT	C11-C10-C9	-3.24	122.69	127.31
36	N	309	CHL	C3B-C4B-NB	3.24	113.39	109.21
25	d	404	CLA	CMB-C2B-C3B	3.23	130.72	124.68
25	a	402	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
25	N	311	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
25	Y	315	CLA	CMB-C2B-C3B	3.23	130.71	124.68
34	d	406	PL9	C7-C8-C9	-3.23	121.42	126.79
36	G	608	CHL	CAC-C3C-C4C	3.22	128.99	124.81
27	d	405	BCR	C38-C26-C27	3.22	119.81	113.62
27	c	514	BCR	C33-C5-C6	-3.22	120.91	124.53
25	r	308	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
25	C	505	CLA	C4A-NA-C1A	3.22	108.15	106.71
25	B	504	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
25	C	507	CLA	CMB-C2B-C3B	3.22	130.69	124.68
25	b	509	CLA	CMB-C2B-C3B	3.21	130.69	124.68
25	r	301	CLA	CMB-C2B-C3B	3.21	130.69	124.68
36	Y	303	CHL	CAC-C3C-C4C	3.21	128.98	124.81
25	b	512	CLA	CMB-C2B-C3B	3.21	130.69	124.68
27	v	101	BCR	C20-C21-C22	3.20	131.88	127.31
27	a	406	BCR	C3-C4-C5	-3.20	108.36	114.08
25	a	403	CLA	CMB-C2B-C3B	3.20	130.66	124.68
25	D	404	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
37	Y	316	LUT	C11-C10-C9	-3.20	122.75	127.31
25	C	505	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
25	c	512	CLA	CMB-C2B-C3B	3.19	130.66	124.68
25	D	405	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
25	c	507	CLA	CMB-C2B-C3B	3.19	130.65	124.68
27	V	101	BCR	C33-C5-C4	3.19	119.75	113.62
37	G	615	LUT	C15-C14-C13	-3.19	122.76	127.31
25	b	504	CLA	CMB-C2B-C3B	3.19	130.65	124.68
25	b	503	CLA	CMB-C2B-C3B	3.19	130.64	124.68
25	S	614	CLA	C1B-CHB-C4A	-3.19	123.81	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	305	CLA	CMB-C2B-C3B	3.18	130.64	124.68
27	b	518	BCR	C33-C5-C6	-3.18	120.95	124.53
25	A	403	CLA	CMB-C2B-C3B	3.18	130.63	124.68
25	B	514	CLA	CMB-C2B-C3B	3.18	130.63	124.68
27	V	101	BCR	C24-C23-C22	-3.18	121.43	126.23
27	B	517	BCR	C7-C8-C9	-3.18	121.43	126.23
25	B	509	CLA	CMB-C2B-C3B	3.18	130.62	124.68
25	b	502	CLA	C1B-CHB-C4A	-3.18	123.83	130.12
25	G	614	CLA	CMB-C2B-C3B	3.17	130.61	124.68
25	B	508	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
25	G	610	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
27	b	519	BCR	C38-C26-C25	-3.17	120.97	124.53
36	Y	309	CHL	CAC-C3C-C4C	3.17	128.92	124.81
36	S	606	CHL	O2D-CGD-O1D	-3.17	117.65	123.84
36	S	607	CHL	C3B-C4B-NB	3.17	113.30	109.21
25	B	503	CLA	CMB-C2B-C3B	3.17	130.60	124.68
25	G	613	CLA	CMB-C2B-C3B	3.17	130.60	124.68
25	d	403	CLA	CMB-C2B-C3B	3.16	130.60	124.68
27	a	406	BCR	C33-C5-C6	-3.16	120.98	124.53
25	G	611	CLA	CMB-C2B-C3B	3.16	130.59	124.68
25	S	610	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
25	S	611	CLA	CMB-C2B-C3B	3.16	130.59	124.68
36	Y	309	CHL	C3B-C4B-NB	3.15	113.29	109.21
26	d	402	PHO	CMB-C2B-C3B	3.15	130.58	124.68
25	b	505	CLA	CMB-C2B-C3B	3.15	130.58	124.68
25	S	604	CLA	CMB-C2B-C3B	3.15	130.57	124.68
27	t	101	BCR	C16-C17-C18	-3.15	122.81	127.31
25	Y	311	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
25	c	511	CLA	CMB-C2B-C3B	3.15	130.57	124.68
26	D	402	PHO	CMB-C2B-C3B	3.15	130.56	124.68
39	N	301	XAT	C31-C30-C29	-3.14	122.82	127.31
25	S	614	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
25	b	504	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
25	c	507	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
37	Y	317	LUT	C18-C5-C6	-3.14	121.00	124.53
27	b	517	BCR	C30-C25-C26	-3.14	118.20	122.61
27	b	518	BCR	C24-C23-C22	-3.14	121.50	126.23
36	G	601	CHL	C4-C3-C5	3.13	120.54	115.27
38	S	617	NEX	C31-C30-C29	-3.13	122.84	127.31
36	G	608	CHL	C3B-C4B-NB	3.13	113.26	109.21
25	S	605	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
25	r	307	CLA	CMB-C2B-C3B	3.13	130.54	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	N	306	CHL	CAC-C3C-C4C	3.13	128.87	124.81
27	C	516	BCR	C10-C11-C12	-3.13	113.44	123.22
25	b	501	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
27	C	515	BCR	C3-C4-C5	-3.13	108.49	114.08
27	b	519	BCR	C33-C5-C6	-3.13	121.02	124.53
25	B	516	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	b	508	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
25	a	403	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
36	N	310	CHL	C3B-C4B-NB	3.12	113.25	109.21
27	B	518	BCR	C11-C10-C9	-3.12	122.85	127.31
25	S	605	CLA	CMB-C2B-C3B	3.12	130.52	124.68
27	C	516	BCR	C33-C5-C6	-3.12	121.02	124.53
25	C	506	CLA	CMB-C2B-C3B	3.12	130.51	124.68
27	k	101	BCR	C15-C16-C17	-3.12	117.09	123.47
27	H	101	BCR	C24-C23-C22	-3.12	121.53	126.23
25	Y	305	CLA	CMB-C2B-C3B	3.11	130.50	124.68
25	b	503	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
37	Y	316	LUT	C18-C5-C6	-3.11	121.03	124.53
25	G	602	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
25	B	507	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
25	d	404	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
25	B	505	CLA	CMB-C2B-C3B	3.10	130.47	124.68
25	r	302	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
36	N	308	CHL	C4-C3-C5	3.09	120.48	115.27
25	B	515	CLA	CMB-C2B-C3B	3.09	130.46	124.68
25	D	401	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
25	S	605	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
25	B	503	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
25	S	609	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
25	b	502	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
25	c	508	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
36	G	606	CHL	C3B-C4B-NB	3.07	113.19	109.21
25	D	405	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	Y	304	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	S	602	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
27	D	406	BCR	C33-C5-C4	3.07	119.52	113.62
25	A	403	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	Y	312	CLA	CMB-C2B-C3B	3.07	130.43	124.68
37	Y	317	LUT	C16-C1-C6	-3.07	105.32	110.30
25	r	308	CLA	C1B-CHB-C4A	-3.07	124.05	130.12
36	S	606	CHL	C3B-C4B-NB	3.06	113.17	109.21
25	B	501	CLA	CMB-C2B-C3B	3.06	130.41	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	511	CLA	CMB-C2B-C3B	3.06	130.40	124.68
25	d	403	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
27	k	101	BCR	C15-C14-C13	-3.06	122.95	127.31
25	C	512	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
38	N	318	NEX	C11-C10-C9	-3.06	122.95	127.31
36	r	306	CHL	CAC-C3C-C4C	3.05	128.77	124.81
26	a	404	PHO	CMB-C2B-C3B	3.05	130.39	124.68
25	A	405	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	S	613	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
37	N	317	LUT	C11-C10-C9	-3.05	122.96	127.31
36	Y	310	CHL	C3B-C4B-NB	3.05	113.15	109.21
27	C	516	BCR	C16-C17-C18	-3.05	122.96	127.31
27	c	514	BCR	C20-C21-C22	-3.05	122.96	127.31
25	d	404	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
39	Y	302	XAT	C11-C10-C9	-3.05	122.96	127.31
25	d	401	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
36	N	310	CHL	C1-C2-C3	-3.04	120.78	126.04
27	k	101	BCR	C16-C17-C18	-3.04	122.97	127.31
25	Y	315	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
39	G	620	XAT	C11-C10-C9	-3.04	122.97	127.31
25	a	405	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
37	N	317	LUT	C18-C5-C4	3.04	119.98	114.36
25	A	402	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
37	G	615	LUT	C21-C26-C27	-3.03	108.87	112.70
25	N	314	CLA	CMB-C2B-C3B	3.03	130.35	124.68
27	z	101	BCR	C30-C25-C26	-3.03	118.35	122.61
25	Y	314	CLA	CMB-C2B-C3B	3.03	130.34	124.68
27	b	519	BCR	C3-C4-C5	-3.02	108.68	114.08
25	C	506	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
25	b	506	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
27	D	406	BCR	C30-C25-C26	-3.02	118.36	122.61
27	B	518	BCR	C3-C4-C5	-3.02	108.69	114.08
25	N	312	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
25	C	508	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
25	B	506	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
27	V	101	BCR	C16-C15-C14	-3.01	117.30	123.47
27	h	101	BCR	C38-C26-C25	-3.01	121.15	124.53
25	c	513	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
25	c	501	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
25	b	514	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
27	b	519	BCR	C28-C27-C26	-3.00	108.72	114.08
25	S	613	CLA	O2D-CGD-O1D	-3.00	117.97	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	501	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
25	N	315	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
25	b	514	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
37	G	615	LUT	C18-C5-C6	-3.00	121.16	124.53
27	b	518	BCR	C28-C27-C26	-3.00	108.72	114.08
38	S	617	NEX	C26-C27-C28	-3.00	119.66	125.99
25	A	405	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
25	C	508	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
25	C	507	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	D	401	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	b	510	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	G	614	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
25	D	404	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	C	504	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
25	c	506	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
26	A	404	PHO	CMB-C2B-C3B	2.99	130.26	124.68
25	C	511	CLA	CMB-C2B-C3B	2.99	130.26	124.68
27	D	406	BCR	C8-C9-C10	-2.98	114.36	118.94
25	D	404	CLA	CMB-C2B-C3B	2.98	130.26	124.68
25	c	508	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
25	B	511	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
25	r	301	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
27	b	517	BCR	C7-C8-C9	-2.98	121.73	126.23
27	C	515	BCR	C8-C7-C6	-2.98	118.83	127.20
25	Y	306	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
25	S	614	CLA	CMB-C2B-C3B	2.98	130.25	124.68
25	B	510	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
25	B	510	CLA	CMB-C2B-C3B	2.98	130.25	124.68
25	b	507	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
37	N	316	LUT	C21-C26-C27	-2.98	108.94	112.70
30	l	101	LHG	O8-C23-C24	2.98	121.24	111.91
38	G	617	NEX	C39-C29-C30	-2.97	118.76	122.92
25	B	502	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
36	S	601	CHL	C2A-C1A-CHA	-2.97	118.66	123.86
25	B	516	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
25	G	612	CLA	CMB-C2B-C3B	2.97	130.23	124.68
28	a	407	SQD	O9-S-C6	2.97	110.47	106.94
25	c	507	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	c	512	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	C	512	CLA	CMB-C2B-C3B	2.96	130.21	124.68
25	C	503	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
27	v	101	BCR	C27-C26-C25	-2.96	118.44	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	D	407	PL9	C7-C8-C9	-2.95	121.87	126.79
25	G	613	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
32	C	522	LMU	C1B-O1B-C4'	-2.95	110.66	117.96
25	c	510	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
25	C	510	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
27	v	101	BCR	C28-C27-C26	-2.95	108.81	114.08
25	Y	305	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
37	N	317	LUT	C18-C5-C6	-2.95	121.22	124.53
25	B	511	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	S	609	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
27	D	406	BCR	C33-C5-C6	-2.95	121.22	124.53
25	S	602	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
25	Y	315	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
25	b	501	CLA	CMB-C2B-C3B	2.94	130.19	124.68
25	N	313	CLA	CMB-C2B-C3B	2.94	130.19	124.68
25	N	305	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
25	B	502	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	b	508	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	B	514	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	B	509	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	C	511	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	b	511	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
37	Y	316	LUT	C21-C26-C27	-2.93	108.99	112.70
25	C	501	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	d	403	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	G	604	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
26	d	402	PHO	O1D-CGD-CBD	2.93	129.62	124.74
25	c	504	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
27	C	516	BCR	C15-C14-C13	-2.93	123.13	127.31
25	G	603	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
29	W	201	LMG	C8-O7-C10	-2.92	110.59	117.79
25	N	304	CLA	CMB-C2B-C3B	2.92	130.15	124.68
25	C	513	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
25	c	504	CLA	CMB-C2B-C3B	2.92	130.15	124.68
25	c	501	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
27	C	514	BCR	C27-C26-C25	-2.92	118.49	122.73
27	v	101	BCR	C33-C5-C4	2.92	119.22	113.62
25	G	614	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
25	N	314	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	Y	314	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	C	513	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
25	b	515	CLA	C1B-CHB-C4A	-2.91	124.35	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	S	617	NEX	C11-C10-C9	-2.91	123.15	127.31
25	S	604	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
25	C	501	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
25	b	516	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
27	B	517	BCR	C11-C10-C9	-2.91	123.16	127.31
39	N	301	XAT	C11-C10-C9	-2.91	123.16	127.31
25	S	609	CLA	CMB-C2B-C3B	2.91	130.12	124.68
36	Y	303	CHL	CHB-C4A-NA	2.91	128.53	124.51
25	S	612	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
27	b	517	BCR	C33-C5-C6	-2.91	121.27	124.53
27	t	101	BCR	C38-C26-C27	2.91	119.20	113.62
34	D	407	PL9	C40-C39-C41	2.91	120.16	115.27
25	S	610	CLA	C4A-NA-C1A	2.90	108.01	106.71
27	H	101	BCR	C38-C26-C25	-2.90	121.27	124.53
25	N	305	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
38	Y	318	NEX	C26-C27-C28	-2.90	119.85	125.99
25	Y	313	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
27	C	516	BCR	C33-C5-C4	2.90	119.19	113.62
25	Y	306	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	B	514	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	B	512	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
36	S	608	CHL	O2D-CGD-O1D	-2.90	118.17	123.84
34	d	406	PL9	C40-C39-C41	2.90	120.15	115.27
25	B	503	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
36	Y	308	CHL	C3B-C4B-NB	2.90	112.95	109.21
25	b	505	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
25	C	509	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
37	S	615	LUT	C11-C10-C9	-2.89	123.18	127.31
36	Y	310	CHL	CMB-C2B-C3B	2.89	130.09	124.68
25	b	504	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	c	509	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
25	B	501	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	C	515	BCR	C7-C8-C9	-2.89	121.87	126.23
25	G	613	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
25	r	303	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
37	Y	317	LUT	C11-C10-C9	-2.89	123.19	127.31
25	N	312	CLA	CMB-C2B-C3B	2.89	130.08	124.68
36	N	308	CHL	CHB-C4A-NA	2.88	128.50	124.51
25	N	313	CLA	C1B-CHB-C4A	-2.88	124.40	130.12
25	N	315	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	C	509	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	c	512	CLA	O2D-CGD-O1D	-2.88	118.20	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	612	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	B	510	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	b	510	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	S	602	CLA	CMB-C2B-C3B	2.88	130.07	124.68
25	a	405	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	b	503	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	N	314	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
25	B	507	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	b	515	CLA	CMB-C2B-C3B	2.87	130.06	124.68
31	c	517	DGD	O1G-C1A-C2A	2.87	120.93	111.91
25	C	506	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	b	509	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
25	Y	314	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
31	W	202	DGD	C2G-O2G-C1B	-2.87	110.73	117.79
25	N	312	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
25	r	303	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	c	518	LMG	O8-C28-C29	2.87	120.90	111.91
25	C	503	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
25	r	302	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
36	G	619	CHL	C1-C2-C3	-2.86	121.09	126.04
25	b	516	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
25	S	603	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
25	S	611	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
25	b	512	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
25	C	507	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
27	C	516	BCR	C3-C4-C5	-2.86	108.97	114.08
37	S	616	LUT	C21-C26-C27	-2.86	109.08	112.70
25	c	510	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
27	C	515	BCR	C1-C6-C5	-2.86	118.58	122.61
25	N	304	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
25	G	612	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	B	515	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
25	N	304	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	b	515	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	G	603	CLA	CMB-C2B-C3B	2.86	130.02	124.68
25	B	505	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
29	d	409	LMG	C8-O7-C10	-2.86	110.76	117.79
25	N	303	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
37	S	616	LUT	C7-C8-C9	-2.85	121.92	126.23
30	d	407	LHG	O8-C23-C24	2.85	120.86	111.91
36	Y	308	CHL	C2A-C1A-CHA	-2.85	118.87	123.86
27	v	101	BCR	C21-C20-C19	2.85	132.12	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	303	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
25	c	502	CLA	CMB-C2B-C3B	2.85	130.01	124.68
27	D	406	BCR	C38-C26-C27	2.85	119.09	113.62
27	d	405	BCR	C33-C5-C4	2.85	119.09	113.62
25	Y	305	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	N	315	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	c	504	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	c	505	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	N	302	CHL	C2A-C1A-CHA	-2.85	118.88	123.86
25	B	508	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	B	513	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
27	b	519	BCR	C33-C5-C4	2.85	119.09	113.62
25	Y	312	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
25	C	505	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	G	610	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
39	r	309	XAT	C10-C11-C12	-2.84	114.34	123.22
25	S	603	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
37	S	616	LUT	C16-C1-C6	-2.84	105.70	110.30
27	A	406	BCR	C33-C5-C4	2.83	119.06	113.62
25	C	512	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
36	Y	310	CHL	C4-C3-C5	2.83	120.03	115.27
36	r	305	CHL	CMB-C2B-C3B	2.83	129.97	124.68
38	Y	318	NEX	C31-C30-C29	-2.83	123.28	127.31
39	r	309	XAT	C31-C30-C29	-2.82	123.28	127.31
25	c	509	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	r	307	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	N	313	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
36	G	605	CHL	C2A-C1A-CHA	-2.82	118.92	123.86
36	G	609	CHL	C2A-C1A-CHA	-2.82	118.92	123.86
25	C	501	CLA	CMB-C2B-C3B	2.82	129.95	124.68
38	r	310	NEX	C26-C27-C28	-2.82	120.03	125.99
38	N	318	NEX	C39-C29-C30	-2.82	118.97	122.92
36	G	607	CHL	CHB-C4A-NA	2.82	128.41	124.51
36	N	310	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
25	b	513	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	G	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	r	308	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	a	408	LMG	O8-C28-C29	2.81	120.73	111.91
25	C	510	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
36	G	619	CHL	CMB-C2B-C3B	2.81	129.93	124.68
36	Y	303	CHL	CMB-C2B-C3B	2.81	129.93	124.68
36	G	609	CHL	CMB-C2B-C3B	2.81	129.93	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	517	BCR	C30-C25-C26	-2.81	118.66	122.61
25	c	505	CLA	C4A-NA-C1A	2.80	107.97	106.71
25	Y	304	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	B	505	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
38	N	318	NEX	C24-C23-C22	-2.80	105.37	110.77
25	c	501	CLA	CMB-C2B-C3B	2.80	129.92	124.68
36	G	607	CHL	CMB-C2B-C3B	2.80	129.91	124.68
27	z	101	BCR	C33-C5-C4	2.80	118.99	113.62
25	Y	313	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
25	C	502	CLA	CMB-C2B-C3B	2.80	129.91	124.68
25	d	401	CLA	CMB-C2B-C3B	2.80	129.91	124.68
27	C	516	BCR	C15-C16-C17	-2.80	117.74	123.47
27	B	518	BCR	C7-C8-C9	-2.80	122.01	126.23
27	b	518	BCR	C38-C26-C27	2.79	118.98	113.62
25	b	507	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	G	611	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
27	t	101	BCR	C33-C5-C4	2.79	118.97	113.62
30	S	618	LHG	C5-O7-C7	-2.78	110.94	117.79
25	Y	311	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
27	d	405	BCR	C29-C30-C25	2.78	114.77	110.48
25	c	502	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	b	501	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	r	302	CLA	CHB-C4A-NA	2.78	128.36	124.51
36	G	606	CHL	C2A-C1A-CHA	-2.78	119.00	123.86
38	Y	318	NEX	C24-C23-C22	-2.78	105.41	110.77
29	H	102	LMG	O8-C28-C29	2.78	120.62	111.91
36	N	302	CHL	C4-C3-C5	2.78	119.94	115.27
25	b	509	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	C	504	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
31	C	517	DGD	O1G-C1A-C2A	2.77	120.61	111.91
25	B	509	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	B	506	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
27	d	405	BCR	C30-C25-C26	-2.77	118.71	122.61
31	C	518	DGD	O1G-C1A-C2A	2.77	120.60	111.91
25	B	512	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
30	B	520	LHG	O8-C23-C24	2.77	120.60	111.91
25	B	504	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
27	B	517	BCR	C33-C5-C4	2.77	118.94	113.62
25	G	611	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
25	B	515	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
36	N	302	CHL	CMB-C2B-C3B	2.77	129.85	124.68
36	r	306	CHL	CMD-C2D-C3D	-2.77	121.25	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	r	304	CHL	CMB-C2B-C3B	2.77	129.85	124.68
27	k	101	BCR	C10-C11-C12	-2.76	114.59	123.22
25	B	516	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
37	S	616	LUT	C18-C5-C6	-2.76	121.42	124.53
25	b	515	CLA	CHB-C4A-NA	2.76	128.33	124.51
36	S	601	CHL	CMB-C2B-C3B	2.76	129.85	124.68
25	S	611	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
27	D	406	BCR	C38-C26-C25	-2.76	121.43	124.53
26	D	402	PHO	O2D-CGD-O1D	-2.76	118.45	123.84
30	Y	319	LHG	O8-C23-C24	2.75	120.55	111.91
30	L	101	LHG	C5-O7-C7	-2.75	111.01	117.79
26	d	402	PHO	C1-C2-C3	-2.75	121.28	126.04
38	S	617	NEX	C24-C23-C22	-2.75	105.45	110.77
27	t	101	BCR	C28-C27-C26	-2.75	109.16	114.08
38	N	318	NEX	C26-C27-C28	-2.75	120.17	125.99
26	A	404	PHO	O1D-CGD-CBD	2.75	129.32	124.74
25	S	612	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
26	a	404	PHO	O1D-CGD-CBD	2.75	129.32	124.74
36	N	307	CHL	C3B-C4B-NB	2.75	112.77	109.21
25	N	311	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
36	N	309	CHL	O2A-CGA-CBA	2.75	120.54	111.91
25	c	506	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
27	b	518	BCR	C38-C26-C25	-2.75	121.44	124.53
27	v	101	BCR	C38-C26-C27	2.75	118.89	113.62
25	G	603	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
25	G	604	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
37	Y	317	LUT	C21-C26-C27	-2.75	109.23	112.70
30	d	408	LHG	O8-C23-C24	2.74	120.52	111.91
36	G	609	CHL	C4-C3-C5	2.74	119.89	115.27
25	b	513	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	C	502	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
36	N	307	CHL	C2A-C1A-CHA	-2.74	119.07	123.86
36	G	619	CHL	O2A-CGA-CBA	2.74	120.51	111.91
38	r	310	NEX	C31-C30-C29	-2.74	123.40	127.31
36	N	302	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
25	c	511	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
25	S	604	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
25	S	610	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
36	Y	303	CHL	C2A-C1A-CHA	-2.74	119.08	123.86
34	D	407	PL9	C22-C23-C24	-2.74	121.07	127.66
37	S	615	LUT	C35-C15-C14	-2.74	117.87	123.47
36	G	601	CHL	CMD-C2D-C3D	-2.74	121.32	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	S	601	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
36	N	308	CHL	CMB-C2B-C3B	2.73	129.79	124.68
36	S	608	CHL	O2A-CGA-CBA	2.73	120.47	111.91
36	G	601	CHL	C2A-C1A-CHA	-2.73	119.09	123.86
28	t	102	SQD	O48-C23-C24	2.73	120.47	111.91
25	r	308	CLA	CMB-C2B-C3B	2.73	129.78	124.68
37	S	616	LUT	C18-C5-C4	2.73	119.41	114.36
36	Y	308	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
26	d	402	PHO	O2D-CGD-O1D	-2.72	118.51	123.84
36	N	309	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
36	Y	307	CHL	CMB-C2B-C3B	2.72	129.77	124.68
36	G	619	CHL	C4-C3-C5	2.72	119.85	115.27
27	V	101	BCR	C10-C11-C12	-2.72	114.73	123.22
29	C	520	LMG	O8-C28-C29	2.72	120.44	111.91
25	C	502	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
37	N	317	LUT	C16-C1-C6	-2.72	105.89	110.30
36	r	306	CHL	CMB-C2B-C3B	2.72	129.76	124.68
36	Y	309	CHL	CMB-C2B-C3B	2.72	129.76	124.68
25	c	512	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	c	502	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
36	Y	303	CHL	CMD-C2D-C3D	-2.71	121.37	127.61
26	a	404	PHO	C1-C2-C3	-2.71	121.36	126.04
25	C	507	CLA	CHB-C4A-NA	2.71	128.26	124.51
27	a	406	BCR	C20-C21-C22	-2.71	123.44	127.31
25	a	402	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
36	N	310	CHL	O2A-CGA-CBA	2.71	120.40	111.91
27	B	518	BCR	C38-C26-C27	2.71	118.82	113.62
36	G	607	CHL	O2A-CGA-CBA	2.71	120.40	111.91
36	G	605	CHL	CMB-C2B-C3B	2.71	129.74	124.68
36	N	309	CHL	CMB-C2B-C3B	2.71	129.74	124.68
36	r	305	CHL	CMD-C2D-C3D	-2.70	121.40	127.61
31	W	202	DGD	O1G-C1A-C2A	2.70	120.39	111.91
25	Y	312	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
36	Y	310	CHL	CMD-C2D-C3D	-2.70	121.40	127.61
38	N	318	NEX	C31-C30-C29	-2.70	123.46	127.31
36	G	619	CHL	CHB-C4A-NA	2.70	128.25	124.51
31	C	517	DGD	C2G-O2G-C1B	-2.70	111.14	117.79
35	f	101	HEM	C4B-CHC-C1C	2.70	126.12	122.56
36	G	601	CHL	CMB-C2B-C3B	2.70	129.72	124.68
30	a	410	LHG	O8-C23-C24	2.70	120.37	111.91
27	D	406	BCR	C10-C11-C12	-2.69	114.81	123.22
39	Y	302	XAT	C27-C28-C29	-2.69	121.35	125.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	301	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
25	S	613	CLA	CMB-C2B-C3B	2.69	129.72	124.68
27	b	518	BCR	C33-C5-C4	2.69	118.79	113.62
25	c	503	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
27	C	514	BCR	C1-C6-C5	-2.69	118.82	122.61
27	C	514	BCR	C38-C26-C27	2.69	118.79	113.62
36	G	608	CHL	CMB-C2B-C3B	2.69	129.71	124.68
27	V	101	BCR	C38-C26-C25	-2.69	121.51	124.53
27	t	101	BCR	C20-C21-C22	-2.69	123.47	127.31
27	v	101	BCR	C8-C7-C6	-2.69	119.65	127.20
36	S	607	CHL	CMB-C2B-C3B	2.68	129.70	124.68
36	r	304	CHL	C2A-C1A-CHA	-2.68	119.17	123.86
25	c	507	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	a	404	PHO	O2D-CGD-O1D	-2.68	118.60	123.84
38	Y	318	NEX	C39-C29-C30	-2.68	119.17	122.92
39	Y	302	XAT	C4-C3-C2	-2.67	105.61	110.77
31	Y	301	DGD	O1G-C1A-C2A	2.67	120.30	111.91
36	G	609	CHL	O2A-CGA-CBA	2.67	120.30	111.91
36	N	306	CHL	CMB-C2B-C3B	2.67	129.68	124.68
27	d	405	BCR	C4-C5-C6	-2.67	118.85	122.73
36	N	306	CHL	C1-C2-C3	-2.67	121.42	126.04
27	b	517	BCR	C38-C26-C27	2.67	118.74	113.62
31	c	515	DGD	O1G-C1A-C2A	2.67	120.28	111.91
38	G	617	NEX	C24-C23-C22	-2.67	105.62	110.77
27	b	519	BCR	C38-C26-C27	2.67	118.74	113.62
34	d	406	PL9	C22-C23-C24	-2.67	121.24	127.66
26	D	402	PHO	O1D-CGD-CBD	2.66	129.18	124.74
36	N	309	CHL	C2A-C1A-CHA	-2.66	119.20	123.86
25	C	511	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
25	c	509	CLA	CHB-C4A-NA	2.66	128.19	124.51
36	G	605	CHL	CMD-C2D-C3D	-2.66	121.49	127.61
25	d	401	CLA	C1-C2-C3	-2.66	121.44	126.04
35	f	101	HEM	C1B-NB-C4B	2.66	107.82	105.07
36	N	306	CHL	C2A-C1A-CHA	-2.66	119.21	123.86
36	S	608	CHL	CMB-C2B-C3B	2.66	129.65	124.68
28	a	407	SQD	O48-C23-C24	2.66	120.25	111.91
30	L	101	LHG	O8-C23-C24	2.66	120.24	111.91
27	V	101	BCR	C8-C7-C6	-2.65	119.75	127.20
36	G	609	CHL	CMD-C2D-C3D	-2.65	121.51	127.61
38	r	310	NEX	C39-C29-C30	-2.65	119.21	122.92
39	G	620	XAT	C4-C3-C2	-2.65	105.65	110.77
37	G	615	LUT	C35-C15-C14	-2.65	118.04	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	h	101	BCR	C28-C27-C26	-2.65	109.34	114.08
38	G	617	NEX	C26-C27-C28	-2.65	120.39	125.99
36	N	310	CHL	CMB-C2B-C3B	2.65	129.63	124.68
36	S	608	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
36	N	307	CHL	CMB-C2B-C3B	2.65	129.63	124.68
36	Y	309	CHL	O2A-CGA-CBA	2.65	120.22	111.91
36	Y	310	CHL	C1B-CHB-C4A	-2.65	124.87	130.12
36	Y	303	CHL	O2A-CGA-CBA	2.64	120.21	111.91
36	Y	309	CHL	CMD-C2D-C3D	-2.64	121.53	127.61
36	r	304	CHL	CMD-C2D-C3D	-2.64	121.53	127.61
36	Y	307	CHL	CHB-C4A-NA	2.64	128.17	124.51
36	Y	307	CHL	CMD-C2D-C3D	-2.64	121.54	127.61
25	b	512	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
29	a	408	LMG	C8-O7-C10	-2.64	111.30	117.79
25	c	513	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
30	N	319	LHG	O8-C23-C24	2.63	120.17	111.91
26	A	404	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
36	G	619	CHL	C2A-C1A-CHA	-2.63	119.26	123.86
35	f	101	HEM	C4D-ND-C1D	2.63	107.79	105.07
36	G	601	CHL	O2A-CGA-CBA	2.63	120.16	111.91
36	r	305	CHL	C2A-C1A-CHA	-2.63	119.26	123.86
30	G	618	LHG	O8-C23-C24	2.63	120.16	111.91
36	G	619	CHL	CMD-C2D-C3D	-2.63	121.57	127.61
37	N	316	LUT	C35-C15-C14	-2.63	118.09	123.47
25	b	516	CLA	CHB-C4A-NA	2.63	128.14	124.51
32	C	523	LMU	C1B-O1B-C4'	-2.63	111.46	117.96
25	c	501	CLA	C1-C2-C3	-2.63	121.50	126.04
36	G	606	CHL	CMB-C2B-C3B	2.63	129.59	124.68
25	G	603	CLA	CHB-C4A-NA	2.62	128.14	124.51
36	S	607	CHL	C2A-C1A-CHA	-2.62	119.28	123.86
25	B	510	CLA	CHB-C4A-NA	2.62	128.14	124.51
25	B	512	CLA	CHB-C4A-NA	2.62	128.14	124.51
36	S	601	CHL	CHB-C4A-NA	2.62	128.13	124.51
25	B	513	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	N	313	CLA	CHB-C4A-NA	2.61	128.13	124.51
36	Y	303	CHL	C4-C3-C5	2.61	119.67	115.27
36	S	608	CHL	C2A-C1A-CHA	-2.61	119.29	123.86
37	Y	316	LUT	C35-C15-C14	-2.61	118.12	123.47
25	S	612	CLA	CHB-C4A-NA	2.61	128.12	124.51
31	c	515	DGD	C2G-O2G-C1B	-2.61	111.37	117.79
35	f	101	HEM	C3B-C2B-C1B	2.61	108.42	106.49
36	N	306	CHL	CMD-C2D-C3D	-2.61	121.62	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	406	BCR	C28-C27-C26	-2.60	109.43	114.08
36	N	308	CHL	O2A-CGA-CBA	2.60	120.08	111.91
36	Y	307	CHL	C2A-C1A-CHA	-2.60	119.31	123.86
25	S	603	CLA	CHB-C4A-NA	2.60	128.11	124.51
27	V	101	BCR	C28-C27-C26	-2.60	109.44	114.08
30	D	409	LHG	O8-C23-C24	2.60	120.06	111.91
36	N	306	CHL	O2A-CGA-CBA	2.60	120.06	111.91
36	G	608	CHL	CMD-C2D-C3D	-2.59	121.64	127.61
25	G	612	CLA	CHB-C4A-NA	2.59	128.10	124.51
36	N	310	CHL	C2A-C1A-CHA	-2.59	119.32	123.86
39	Y	302	XAT	C18-C5-C4	2.59	117.20	114.28
38	r	310	NEX	C24-C23-C22	-2.59	105.77	110.77
25	B	516	CLA	CHB-C4A-NA	2.59	128.09	124.51
31	C	519	DGD	O1G-C1A-C2A	2.59	120.03	111.91
36	G	607	CHL	CMD-C2D-C3D	-2.59	121.67	127.61
37	G	616	LUT	C18-C5-C4	2.58	119.14	114.36
25	Y	313	CLA	CHB-C4A-NA	2.58	128.09	124.51
29	d	409	LMG	O8-C28-C29	2.58	120.01	111.91
25	b	510	CLA	CHB-C4A-NA	2.58	128.08	124.51
36	N	309	CHL	CHB-C4A-NA	2.58	128.08	124.51
27	a	406	BCR	C38-C26-C27	2.58	118.58	113.62
36	S	607	CHL	CMD-C2D-C3D	-2.58	121.67	127.61
27	k	101	BCR	C33-C5-C4	2.58	118.58	113.62
27	B	518	BCR	C33-C5-C4	2.58	118.57	113.62
36	N	302	CHL	O2A-CGA-CBA	2.58	120.00	111.91
27	C	515	BCR	C20-C21-C22	-2.58	123.63	127.31
39	r	309	XAT	C24-C23-C22	-2.58	105.80	110.77
28	A	407	SQD	O48-C23-C24	2.58	119.99	111.91
36	G	605	CHL	CHB-C4A-NA	2.57	128.07	124.51
25	Y	305	CLA	CHB-C4A-NA	2.57	128.07	124.51
36	Y	308	CHL	CMB-C2B-C3B	2.57	129.49	124.68
36	N	310	CHL	C4-C3-C5	2.57	119.60	115.27
36	r	304	CHL	CHB-C4A-NA	2.57	128.07	124.51
27	H	101	BCR	C28-C27-C26	-2.57	109.49	114.08
39	G	620	XAT	C18-C5-C4	2.57	117.17	114.28
30	S	618	LHG	O8-C23-C24	2.56	119.95	111.91
37	Y	317	LUT	C18-C5-C4	2.56	119.10	114.36
30	D	408	LHG	O8-C23-C24	2.56	119.95	111.91
27	C	514	BCR	C3-C4-C5	-2.56	109.50	114.08
27	c	514	BCR	C27-C26-C25	-2.56	119.02	122.73
34	d	406	PL9	C27-C28-C29	-2.55	121.51	127.66
39	G	620	XAT	C38-C25-C24	2.55	117.15	114.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	515	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	a	411	LHG	O8-C23-C24	2.55	119.92	111.91
25	C	512	CLA	CHB-C4A-NA	2.55	128.04	124.51
36	G	601	CHL	CHB-C4A-NA	2.55	128.04	124.51
36	G	601	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
29	d	410	LMG	O8-C28-C29	2.55	119.91	111.91
30	d	408	LHG	C5-O7-C7	-2.55	111.51	117.79
38	S	617	NEX	C39-C29-C30	-2.55	119.35	122.92
36	r	306	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
36	S	606	CHL	CMB-C2B-C3B	2.54	129.44	124.68
30	C	521	LHG	O8-C23-C24	2.54	119.88	111.91
25	Y	306	CLA	C1-C2-C3	-2.54	121.65	126.04
31	C	518	DGD	C2G-O2G-C1B	-2.54	111.54	117.79
29	b	520	LMG	O8-C28-C29	2.54	119.88	111.91
36	r	304	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
27	H	101	BCR	C38-C26-C27	2.54	118.49	113.62
25	b	504	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	b	513	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	B	511	CLA	C1-C2-C3	-2.53	121.66	126.04
37	G	616	LUT	C16-C1-C6	-2.53	106.19	110.30
38	G	617	NEX	C31-C30-C29	-2.53	123.70	127.31
36	G	609	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
37	G	616	LUT	C11-C10-C9	-2.53	123.70	127.31
25	A	402	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
34	D	407	PL9	C27-C28-C29	-2.52	121.58	127.66
36	G	609	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
37	G	616	LUT	C21-C26-C27	-2.52	109.51	112.70
25	N	304	CLA	CHB-C4A-NA	2.52	128.00	124.51
36	r	305	CHL	CHB-C4A-NA	2.52	128.00	124.51
36	G	605	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
27	h	101	BCR	C38-C26-C27	2.52	118.46	113.62
36	Y	310	CHL	C2A-C1A-CHA	-2.51	119.46	123.86
27	C	514	BCR	C28-C27-C26	-2.51	109.59	114.08
37	G	616	LUT	C31-C30-C29	-2.51	123.72	127.31
36	r	306	CHL	C2A-C1A-CHA	-2.51	119.47	123.86
36	N	310	CHL	C1B-CHB-C4A	-2.51	125.15	130.12
36	Y	310	CHL	O2D-CGD-O1D	-2.51	118.94	123.84
36	G	609	CHL	C1-C2-C3	-2.51	121.71	126.04
34	d	406	PL9	C20-C19-C21	2.51	119.49	115.27
36	N	307	CHL	CMD-C2D-C3D	-2.51	121.85	127.61
27	a	406	BCR	C33-C5-C4	2.51	118.43	113.62
39	N	301	XAT	C27-C28-C29	-2.51	121.64	125.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	G	607	CHL	C2A-C1A-CHA	-2.50	119.48	123.86
27	A	406	BCR	C3-C4-C5	-2.50	109.61	114.08
30	l	101	LHG	C5-O7-C7	-2.50	111.63	117.79
27	V	101	BCR	C3-C4-C5	-2.50	109.61	114.08
39	N	301	XAT	C4-C3-C2	-2.50	105.94	110.77
36	N	308	CHL	CMD-C2D-C3D	-2.50	121.86	127.61
36	S	608	CHL	CHB-C4A-NA	2.49	127.96	124.51
36	N	310	CHL	O2D-CGD-O1D	-2.49	118.96	123.84
36	S	607	CHL	O2D-CGD-O1D	-2.49	118.96	123.84
35	f	101	HEM	C4C-CHD-C1D	2.49	125.85	122.56
37	N	317	LUT	C21-C26-C27	-2.49	109.56	112.70
27	z	101	BCR	C27-C26-C25	-2.49	119.12	122.73
25	B	513	CLA	CHB-C4A-NA	2.48	127.95	124.51
29	d	410	LMG	C8-O7-C10	-2.48	111.67	117.79
36	Y	303	CHL	C1C-C2C-C3C	-2.48	105.14	107.11
36	S	606	CHL	C2A-C1A-CHA	-2.48	119.52	123.86
25	r	307	CLA	C4A-NA-C1A	2.48	107.82	106.71
25	D	405	CLA	CHB-C4A-NA	2.48	127.94	124.51
37	S	616	LUT	C11-C10-C9	-2.48	123.77	127.31
36	G	606	CHL	CHB-C4A-NA	2.48	127.94	124.51
39	r	309	XAT	C19-C9-C8	2.47	121.97	118.08
27	C	515	BCR	C4-C5-C6	-2.47	119.15	122.73
27	C	516	BCR	C38-C26-C27	2.47	118.36	113.62
37	S	615	LUT	C8-C7-C6	-2.47	120.27	127.20
27	V	101	BCR	C15-C14-C13	-2.47	123.79	127.31
27	d	405	BCR	C16-C15-C14	-2.47	118.42	123.47
32	c	519	LMU	C1B-O1B-C4'	-2.47	111.86	117.96
27	t	101	BCR	C24-C23-C22	-2.47	122.51	126.23
25	C	509	CLA	CHB-C4A-NA	2.47	127.92	124.51
31	c	517	DGD	C2G-O2G-C1B	-2.46	111.72	117.79
34	D	407	PL9	C20-C19-C21	2.46	119.42	115.27
27	D	406	BCR	C1-C6-C5	-2.46	119.14	122.61
30	B	520	LHG	C5-O7-C7	-2.46	111.72	117.79
39	r	309	XAT	C35-C15-C14	-2.46	118.43	123.47
25	B	504	CLA	CHB-C4A-NA	2.46	127.91	124.51
36	N	307	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
27	b	517	BCR	C15-C16-C17	-2.45	118.45	123.47
36	S	601	CHL	C4A-NA-C1A	-2.45	105.60	106.71
39	N	301	XAT	C18-C5-C4	2.45	117.04	114.28
29	b	520	LMG	C8-O7-C10	-2.45	111.76	117.79
36	N	310	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
30	d	407	LHG	C5-O7-C7	-2.45	111.77	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	S	616	LUT	C3-C4-C5	-2.44	106.98	111.85
36	N	306	CHL	CHB-C4A-NA	2.44	127.89	124.51
36	S	607	CHL	CHB-C4A-NA	2.44	127.89	124.51
27	B	517	BCR	C3-C4-C5	-2.44	109.72	114.08
25	S	605	CLA	CHB-C4A-NA	2.44	127.88	124.51
36	Y	308	CHL	CHB-C4A-NA	2.44	127.88	124.51
25	B	504	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
29	D	410	LMG	C8-O7-C10	-2.43	111.81	117.79
37	S	615	LUT	C30-C31-C32	-2.43	115.64	123.22
29	D	410	LMG	O8-C28-C29	2.42	119.50	111.91
25	B	504	CLA	C1-C2-C3	-2.42	121.86	126.04
36	Y	310	CHL	O2A-CGA-CBA	2.42	119.50	111.91
27	D	406	BCR	C4-C5-C6	-2.42	119.22	122.73
36	S	606	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
27	t	101	BCR	C7-C8-C9	-2.42	122.58	126.23
37	Y	317	LUT	C31-C30-C29	-2.42	123.86	127.31
39	G	620	XAT	C27-C28-C29	-2.42	121.78	125.53
36	S	606	CHL	CHB-C4A-NA	2.42	127.85	124.51
36	Y	307	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
27	d	405	BCR	C3-C4-C5	-2.41	109.77	114.08
25	b	501	CLA	CHB-C4A-NA	2.41	127.84	124.51
27	b	517	BCR	C27-C26-C25	-2.41	119.23	122.73
36	r	306	CHL	CHB-C4A-NA	2.41	127.84	124.51
25	S	614	CLA	CHD-C1D-ND	-2.41	122.24	124.45
25	b	505	CLA	CHD-C1D-ND	-2.40	122.24	124.45
25	B	507	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	B	504	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
25	b	505	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
27	a	406	BCR	C40-C30-C25	-2.40	106.41	110.30
29	B	519	LMG	O8-C28-C29	2.40	119.43	111.91
25	c	502	CLA	CHB-C4A-NA	2.40	127.82	124.51
27	c	514	BCR	C15-C16-C17	-2.39	118.57	123.47
30	b	521	LHG	O8-C23-C24	2.39	119.42	111.91
36	Y	303	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
25	a	405	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	c	502	CLA	C1-C2-C3	-2.39	121.91	126.04
25	Y	312	CLA	CHB-C4A-NA	2.39	127.81	124.51
39	r	309	XAT	C4-C3-C2	-2.39	106.16	110.77
29	H	102	LMG	C8-O7-C10	-2.39	111.92	117.79
36	N	309	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
25	b	503	CLA	CHB-C4A-NA	2.38	127.81	124.51
27	d	405	BCR	C10-C11-C12	-2.38	115.78	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	G	601	CHL	C1-C2-C3	-2.38	121.93	126.04
39	Y	302	XAT	C15-C35-C34	-2.38	118.60	123.47
25	D	401	CLA	CHB-C4A-NA	2.38	127.80	124.51
36	N	308	CHL	C1-C2-C3	-2.38	121.93	126.04
36	N	306	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
25	Y	304	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	d	404	CLA	CHB-C4A-NA	2.38	127.80	124.51
27	B	517	BCR	C15-C16-C17	2.37	128.33	123.47
25	C	506	CLA	CHB-C4A-NA	2.37	127.79	124.51
36	G	605	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
25	S	613	CLA	CHD-C1D-ND	-2.37	122.28	124.45
36	N	302	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
25	N	305	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	d	401	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
25	c	511	CLA	CHB-C4A-NA	2.37	127.78	124.51
27	B	517	BCR	C8-C7-C6	-2.37	120.56	127.20
25	C	501	CLA	CHB-C4A-NA	2.36	127.78	124.51
35	f	101	HEM	CMC-C2C-C3C	2.36	129.10	124.68
30	G	618	LHG	C5-O7-C7	-2.36	111.97	117.79
36	Y	307	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
27	z	101	BCR	C28-C27-C26	-2.36	109.86	114.08
25	C	510	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	b	502	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	b	517	BCR	C33-C5-C4	2.36	118.14	113.62
25	C	513	CLA	CHB-C4A-NA	2.36	127.77	124.51
38	Y	318	NEX	C38-C25-C24	2.36	116.93	114.28
25	c	503	CLA	CHB-C4A-NA	2.36	127.77	124.51
36	G	609	CHL	CHB-C4A-NA	2.35	127.77	124.51
25	G	614	CLA	CHB-C4A-NA	2.35	127.77	124.51
27	V	101	BCR	C38-C26-C27	2.35	118.13	113.62
36	r	305	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
36	N	306	CHL	C4-C3-C5	2.35	119.23	115.27
30	D	408	LHG	C5-O7-C7	-2.35	112.01	117.79
25	b	506	CLA	CHB-C4A-NA	2.35	127.76	124.51
38	r	310	NEX	C19-C9-C10	-2.35	119.63	122.92
28	t	102	SQD	O8-S-C6	2.35	109.48	105.74
25	S	602	CLA	CHB-C4A-NA	2.35	127.76	124.51
27	k	101	BCR	C35-C13-C12	2.35	121.77	118.08
31	C	519	DGD	C2G-O2G-C1B	-2.34	112.02	117.79
38	G	617	NEX	C15-C35-C34	-2.34	118.67	123.47
36	N	302	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
25	B	514	CLA	CHB-C4A-NA	2.34	127.75	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	314	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	B	508	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	C	511	CLA	CHB-C4A-NA	2.34	127.75	124.51
27	C	516	BCR	C27-C26-C25	-2.34	119.34	122.73
25	b	507	CLA	CHB-C4A-NA	2.34	127.74	124.51
36	N	302	CHL	CHB-C4A-NA	2.34	127.74	124.51
25	G	602	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	b	514	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	A	403	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
25	c	506	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	b	502	CLA	CHD-C1D-ND	-2.33	122.31	124.45
36	r	305	CHL	C1C-C2C-C3C	-2.33	105.26	107.11
25	b	504	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
27	C	515	BCR	C15-C16-C17	-2.33	118.70	123.47
25	a	403	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	S	611	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	a	402	CLA	CHB-C4A-NA	2.33	127.73	124.51
37	Y	316	LUT	C30-C31-C32	-2.33	115.95	123.22
25	c	504	CLA	CHD-C1D-ND	-2.33	122.31	124.45
25	C	502	CLA	CHB-C4A-NA	2.33	127.73	124.51
27	a	406	BCR	C38-C26-C25	-2.33	121.91	124.53
25	A	405	CLA	CHB-C4A-NA	2.33	127.73	124.51
36	G	619	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
37	N	317	LUT	C1-C2-C3	2.33	118.90	113.64
25	B	509	CLA	CHB-C4A-NA	2.32	127.73	124.51
36	N	308	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
27	C	516	BCR	C36-C18-C19	2.32	121.74	118.08
39	G	620	XAT	C15-C35-C34	-2.32	118.72	123.47
25	N	312	CLA	CHB-C4A-NA	2.32	127.72	124.51
38	N	318	NEX	C38-C25-C24	2.32	116.89	114.28
25	B	505	CLA	CHB-C4A-NA	2.32	127.72	124.51
36	G	601	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
25	B	502	CLA	CHB-C4A-NA	2.32	127.72	124.51
36	G	608	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
36	Y	308	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
25	r	307	CLA	CHB-C4A-NA	2.31	127.71	124.51
25	B	502	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	c	503	CLA	C1-C2-C3	-2.31	122.04	126.04
27	H	101	BCR	C23-C24-C25	-2.31	120.71	127.20
37	Y	316	LUT	C18-C5-C4	2.31	118.64	114.36
37	S	616	LUT	C38-C25-C24	-2.31	118.62	123.56
37	S	616	LUT	C8-C7-C6	-2.31	120.72	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	F	101	HEM	CBA-CAA-C2A	-2.31	108.68	112.62
37	N	317	LUT	C31-C30-C29	-2.31	124.02	127.31
27	C	515	BCR	C21-C20-C19	-2.31	116.02	123.22
25	B	503	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	B	511	CLA	CHB-C4A-NA	2.31	127.70	124.51
28	A	407	SQD	O8-S-C6	2.31	109.41	105.74
26	d	402	PHO	CMC-C2C-C3C	2.31	129.29	124.94
39	Y	302	XAT	C24-C23-C22	-2.30	106.33	110.77
36	r	304	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
37	Y	316	LUT	C8-C7-C6	-2.30	120.74	127.20
37	G	615	LUT	C8-C7-C6	-2.30	120.75	127.20
29	B	519	LMG	C8-O7-C10	-2.30	112.14	117.79
37	S	616	LUT	C35-C15-C14	-2.30	118.77	123.47
38	S	617	NEX	C38-C25-C24	2.30	116.86	114.28
25	G	611	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	C	508	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	Y	306	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	N	315	CLA	CHD-C1D-ND	-2.29	122.34	124.45
25	b	511	CLA	CHB-C4A-NA	2.29	127.69	124.51
36	S	601	CHL	OMC-CMC-C2C	-2.29	120.50	125.69
36	N	309	CHL	C1C-C2C-C3C	-2.29	105.29	107.11
25	b	513	CLA	C1-C2-C3	-2.29	122.08	126.04
25	N	305	CLA	CHD-C1D-ND	-2.29	122.35	124.45
36	Y	309	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
27	c	514	BCR	C33-C5-C4	2.29	118.01	113.62
25	S	613	CLA	CHB-C4A-NA	2.29	127.67	124.51
36	G	606	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
35	F	101	HEM	C4D-ND-C1D	2.28	107.43	105.07
25	Y	314	CLA	CHB-C4A-NA	2.28	127.67	124.51
36	Y	309	CHL	O2D-CGD-O1D	-2.28	119.37	123.84
36	Y	310	CHL	C1C-C2C-C3C	-2.28	105.30	107.11
25	B	501	CLA	CHB-C4A-NA	2.28	127.67	124.51
25	S	604	CLA	CHD-C1D-ND	-2.28	122.36	124.45
27	b	517	BCR	C38-C26-C25	-2.28	121.97	124.53
25	A	403	CLA	CHB-C4A-NA	2.28	127.67	124.51
25	D	401	CLA	CHD-C1D-ND	-2.28	122.36	124.45
27	C	515	BCR	C27-C26-C25	-2.28	119.42	122.73
25	C	513	CLA	C1-C2-C3	-2.28	122.10	126.04
36	G	607	CHL	C1C-C2C-C3C	-2.28	105.31	107.11
25	c	504	CLA	CHB-C4A-NA	2.28	127.66	124.51
27	b	518	BCR	C3-C4-C5	-2.28	110.01	114.08
27	a	406	BCR	C8-C7-C6	-2.28	120.80	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	N	317	LUT	C38-C25-C24	-2.28	118.68	123.56
27	z	101	BCR	C34-C9-C10	-2.28	119.73	122.92
27	D	406	BCR	C27-C26-C25	-2.28	119.42	122.73
25	G	613	CLA	CHB-C4A-NA	2.28	127.66	124.51
25	d	403	CLA	CHB-C4A-NA	2.28	127.66	124.51
25	S	609	CLA	CHB-C4A-NA	2.28	127.66	124.51
36	S	606	CHL	CMD-C2D-C3D	-2.28	122.38	127.61
27	h	101	BCR	C34-C9-C10	-2.28	119.74	122.92
25	D	404	CLA	C1-C2-C3	-2.27	122.11	126.04
25	c	508	CLA	CHB-C4A-NA	2.27	127.66	124.51
27	a	406	BCR	C27-C26-C25	-2.27	119.43	122.73
25	B	506	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	C	504	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	d	401	CLA	CHB-C4A-NA	2.27	127.65	124.51
39	N	301	XAT	C15-C35-C34	-2.27	118.82	123.47
36	S	607	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
36	N	306	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
27	t	101	BCR	C8-C7-C6	-2.27	120.83	127.20
27	C	516	BCR	C8-C7-C6	-2.27	120.83	127.20
25	b	512	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	c	501	CLA	CHB-C4A-NA	2.27	127.64	124.51
25	Y	306	CLA	CHD-C1D-ND	-2.27	122.37	124.45
27	b	517	BCR	C28-C27-C26	-2.26	110.03	114.08
27	V	101	BCR	C37-C22-C23	2.26	121.64	118.08
36	N	302	CHL	C4A-NA-C1A	-2.26	105.69	106.71
36	Y	310	CHL	C1-C2-C3	-2.26	122.13	126.04
25	c	510	CLA	CHB-C4A-NA	2.26	127.63	124.51
25	A	402	CLA	CHB-C4A-NA	2.26	127.63	124.51
25	Y	315	CLA	CHB-C4A-NA	2.25	127.63	124.51
37	S	616	LUT	C10-C11-C12	-2.25	116.18	123.22
25	G	604	CLA	CHD-C1D-ND	-2.25	122.38	124.45
25	N	303	CLA	CHD-C1D-ND	-2.25	122.38	124.45
36	G	619	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
25	N	303	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	d	404	CLA	CHD-C1D-ND	-2.25	122.39	124.45
25	r	303	CLA	CHB-C4A-NA	2.25	127.62	124.51
25	N	315	CLA	CHB-C4A-NA	2.25	127.62	124.51
27	b	518	BCR	C30-C25-C26	-2.25	119.44	122.61
34	d	406	PL9	C12-C13-C14	-2.25	122.25	127.66
37	N	316	LUT	C8-C7-C6	-2.25	120.89	127.20
36	N	307	CHL	OMC-CMC-C2C	-2.25	120.60	125.69
36	G	607	CHL	O2D-CGD-O1D	-2.25	119.44	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	508	CLA	CHB-C4A-NA	2.25	127.62	124.51
25	C	503	CLA	CHB-C4A-NA	2.24	127.61	124.51
27	d	405	BCR	C33-C5-C6	-2.24	122.01	124.53
31	Y	301	DGD	O6D-C5D-C6D	2.24	111.19	106.67
25	D	404	CLA	CHB-C4A-NA	2.24	127.61	124.51
25	C	506	CLA	C1-C2-C3	-2.24	122.17	126.04
36	G	608	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
25	c	513	CLA	CHB-C4A-NA	2.24	127.61	124.51
38	r	310	NEX	C38-C25-C24	2.24	116.80	114.28
27	D	406	BCR	C8-C7-C6	2.24	133.49	127.20
25	S	614	CLA	CHB-C4A-NA	2.24	127.61	124.51
30	N	319	LHG	C5-O7-C7	-2.24	112.28	117.79
25	c	512	CLA	C1-C2-C3	-2.24	122.17	126.04
25	B	501	CLA	CHD-C1D-ND	-2.24	122.40	124.45
25	B	505	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	G	604	CLA	CHB-C4A-NA	2.23	127.60	124.51
28	t	102	SQD	O9-S-C6	2.23	109.59	106.94
34	d	406	PL9	C31-C32-C33	-2.23	104.55	111.88
36	Y	303	CHL	C4A-NA-C1A	-2.23	105.70	106.71
25	D	405	CLA	CHD-C1D-ND	-2.23	122.40	124.45
27	a	406	BCR	C16-C15-C14	-2.23	118.91	123.47
37	Y	317	LUT	C38-C25-C24	-2.23	118.79	123.56
27	A	406	BCR	C8-C7-C6	-2.23	120.94	127.20
37	N	317	LUT	C10-C11-C12	-2.23	116.26	123.22
25	c	502	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
25	S	604	CLA	CHB-C4A-NA	2.22	127.58	124.51
29	C	520	LMG	C8-O7-C10	-2.22	112.32	117.79
36	G	619	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
27	b	517	BCR	C8-C7-C6	-2.22	120.97	127.20
36	S	601	CHL	C1C-C2C-C3C	-2.22	105.36	107.11
25	b	509	CLA	CHB-C4A-NA	2.21	127.57	124.51
25	b	512	CLA	C16-C15-C13	-2.21	108.77	115.92
25	N	314	CLA	CHD-C1D-ND	-2.21	122.42	124.45
34	d	406	PL9	O1-C4-C3	-2.21	118.28	120.72
38	G	617	NEX	C17-C1-C6	-2.21	108.50	110.47
27	b	519	BCR	C8-C7-C6	-2.21	121.00	127.20
25	B	504	CLA	CAA-CBA-CGA	-2.21	106.80	113.25
29	W	201	LMG	O8-C28-C29	2.21	118.84	111.91
25	Y	311	CLA	CHB-C4A-NA	2.21	127.56	124.51
36	G	608	CHL	C2A-C1A-CHA	-2.21	120.00	123.86
25	S	610	CLA	CHD-C1D-ND	-2.20	122.43	124.45
37	G	615	LUT	C18-C5-C4	2.20	118.44	114.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	G	606	CHL	CMD-C2D-C3D	-2.20	122.55	127.61
37	N	316	LUT	C38-C25-C24	-2.20	118.85	123.56
25	B	511	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
25	d	401	CLA	CHD-C1D-ND	-2.20	122.43	124.45
37	G	615	LUT	C30-C31-C32	-2.20	116.36	123.22
37	G	616	LUT	C38-C25-C24	-2.20	118.85	123.56
27	v	101	BCR	C1-C6-C5	-2.20	119.52	122.61
39	N	301	XAT	C24-C23-C22	-2.20	106.53	110.77
28	t	102	SQD	O7-S-C6	2.20	109.55	106.94
31	c	515	DGD	O6D-C5D-C6D	2.20	111.10	106.67
34	D	407	PL9	C12-C13-C14	-2.20	122.37	127.66
36	N	308	CHL	O2D-CGD-O1D	-2.20	119.55	123.84
25	S	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	r	303	CLA	CHD-C1D-ND	-2.19	122.44	124.45
34	D	407	PL9	C31-C32-C33	-2.19	104.67	111.88
25	S	602	CLA	O2D-CGD-CBD	2.19	115.17	111.27
25	S	603	CLA	CAA-C2A-C3A	-2.19	108.78	114.26
27	c	514	BCR	C38-C26-C27	2.19	117.83	113.62
26	a	404	PHO	O2A-CGA-O1A	-2.19	118.06	123.59
25	b	504	CLA	CHD-C1D-ND	-2.19	122.44	124.45
27	C	516	BCR	C35-C13-C12	2.19	121.53	118.08
27	z	101	BCR	C38-C26-C27	2.19	117.83	113.62
37	S	616	LUT	C31-C30-C29	-2.19	124.19	127.31
34	D	407	PL9	O1-C4-C3	-2.19	118.31	120.72
25	C	504	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	G	610	CLA	CHB-C4A-NA	2.19	127.54	124.51
36	S	608	CHL	C1C-C2C-C3C	-2.19	105.38	107.11
27	h	101	BCR	C23-C24-C25	-2.19	121.06	127.20
25	B	509	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
27	H	101	BCR	C33-C5-C6	-2.19	122.07	124.53
27	b	518	BCR	C8-C7-C6	-2.19	121.06	127.20
27	b	518	BCR	C27-C26-C25	-2.18	119.56	122.73
27	a	406	BCR	C21-C20-C19	-2.18	116.41	123.22
25	C	505	CLA	CHB-C4A-NA	2.18	127.53	124.51
27	z	101	BCR	C36-C18-C17	-2.18	119.87	122.92
25	Y	315	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	N	311	CLA	CHB-C4A-NA	2.18	127.53	124.51
25	A	405	CLA	C1-C2-C3	-2.18	122.28	126.04
25	N	305	CLA	C1-C2-C3	-2.18	122.28	126.04
25	C	506	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
36	Y	309	CHL	C2A-C1A-CHA	-2.17	120.06	123.86
37	Y	316	LUT	C38-C25-C24	-2.17	118.91	123.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	514	BCR	C33-C5-C4	2.17	117.79	113.62
29	c	518	LMG	C8-O7-C10	-2.17	112.44	117.79
27	k	101	BCR	C36-C18-C19	2.17	121.50	118.08
25	b	507	CLA	CHD-C1D-ND	-2.17	122.46	124.45
32	C	523	LMU	O5'-C5'-C4'	2.17	114.33	109.75
37	N	316	LUT	C30-C31-C32	-2.17	116.44	123.22
25	Y	314	CLA	CHD-C1D-ND	-2.17	122.46	124.45
37	Y	316	LUT	C10-C11-C12	-2.17	116.45	123.22
37	N	317	LUT	C8-C7-C6	-2.17	121.11	127.20
25	d	401	CLA	O2D-CGD-CBD	2.17	115.12	111.27
25	N	311	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
25	r	301	CLA	CHB-C4A-NA	2.17	127.51	124.51
25	c	511	CLA	C1-C2-C3	-2.16	122.30	126.04
25	d	403	CLA	C1-C2-C3	-2.16	122.31	126.04
25	G	602	CLA	C1-C2-C3	-2.16	122.31	126.04
27	A	406	BCR	C38-C26-C25	-2.16	122.10	124.53
25	c	508	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
36	r	306	CHL	O2D-CGD-O1D	-2.16	119.62	123.84
36	N	308	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
26	A	404	PHO	CMC-C2C-C3C	2.15	129.00	124.94
25	b	501	CLA	CHD-C1D-ND	-2.15	122.48	124.45
25	A	403	CLA	O2D-CGD-CBD	2.15	115.09	111.27
30	a	411	LHG	C5-O7-C7	-2.15	112.49	117.79
27	H	101	BCR	C34-C9-C10	-2.15	119.91	122.92
37	G	615	LUT	C38-C25-C24	-2.15	118.96	123.56
31	C	518	DGD	O6D-C5D-C6D	2.15	111.00	106.67
25	b	508	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
25	Y	312	CLA	C1-C2-C3	-2.15	122.33	126.04
25	Y	311	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
25	a	405	CLA	CHD-C1D-ND	-2.14	122.48	124.45
27	V	101	BCR	C20-C21-C22	-2.14	124.25	127.31
25	A	405	CLA	CHD-C1D-ND	-2.14	122.49	124.45
25	c	511	CLA	CHD-C1D-ND	-2.14	122.49	124.45
27	A	406	BCR	C16-C15-C14	-2.14	119.09	123.47
34	d	406	PL9	O2-C1-C6	2.14	124.29	120.59
30	C	521	LHG	C5-O7-C7	-2.14	112.53	117.79
27	c	514	BCR	C21-C20-C19	-2.14	116.55	123.22
25	G	613	CLA	CHD-C1D-ND	-2.14	122.49	124.45
36	Y	308	CHL	OMC-CMC-C2C	-2.14	120.86	125.69
39	r	309	XAT	C38-C25-C24	2.14	116.68	114.28
25	C	506	CLA	CHD-C1D-ND	-2.14	122.49	124.45
25	b	514	CLA	CHD-C1D-ND	-2.14	122.49	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	S	617	NEX	C35-C15-C14	-2.14	119.10	123.47
25	C	510	CLA	C1-C2-C3	-2.13	122.35	126.04
36	G	606	CHL	OMC-CMC-C2C	-2.13	120.87	125.69
27	k	101	BCR	C37-C22-C21	-2.13	119.94	122.92
34	D	407	PL9	O2-C1-C6	2.13	124.28	120.59
27	b	518	BCR	C15-C16-C17	-2.13	119.11	123.47
36	Y	310	CHL	OMC-CMC-C2C	-2.13	120.87	125.69
25	B	508	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
25	B	514	CLA	CHD-C1D-ND	-2.13	122.50	124.45
27	t	101	BCR	C15-C16-C17	-2.13	119.11	123.47
25	b	511	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	c	503	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	G	614	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	r	302	CLA	C2A-C1A-CHA	2.13	127.58	123.86
37	S	615	LUT	C18-C5-C4	2.13	118.29	114.36
25	S	610	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
25	S	605	CLA	C1-C2-C3	-2.12	123.31	126.75
25	S	609	CLA	CAA-C2A-C3A	-2.12	111.14	116.10
27	k	101	BCR	C27-C26-C25	-2.12	119.65	122.73
25	r	308	CLA	CAA-C2A-C3A	-2.12	111.15	116.10
38	G	617	NEX	C38-C25-C24	2.12	116.67	114.28
31	W	202	DGD	O6D-C5D-C6D	2.12	110.94	106.67
26	D	402	PHO	C1-C2-C3	-2.12	122.38	126.04
25	B	503	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	a	403	CLA	O2D-CGD-CBD	2.12	115.03	111.27
25	b	508	CLA	C1-C2-C3	-2.12	122.38	126.04
25	C	513	CLA	CHD-C1D-ND	-2.12	122.51	124.45
25	G	603	CLA	CHD-C1D-ND	-2.11	122.51	124.45
25	b	502	CLA	O2D-CGD-CBD	2.11	115.02	111.27
25	b	507	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
25	C	502	CLA	C1-C2-C3	-2.11	122.39	126.04
25	B	511	CLA	CHD-C1D-ND	-2.11	122.51	124.45
30	Y	319	LHG	C5-O7-C7	-2.11	112.59	117.79
27	k	101	BCR	C38-C26-C27	2.11	117.67	113.62
25	b	505	CLA	CHB-C4A-NA	2.11	127.43	124.51
27	h	101	BCR	C33-C5-C6	-2.11	122.16	124.53
35	F	101	HEM	C1B-NB-C4B	2.11	107.25	105.07
25	B	506	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
36	S	606	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
25	C	508	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
37	S	615	LUT	C38-C25-C24	-2.11	119.05	123.56
26	D	402	PHO	CMC-C2C-C3C	2.11	128.91	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	G	620	XAT	C10-C11-C12	-2.10	116.65	123.22
36	N	308	CHL	OMC-CMC-C2C	-2.10	120.93	125.69
36	S	601	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
25	c	505	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	c	505	CLA	CHB-C4A-NA	2.10	127.41	124.51
27	C	514	BCR	C33-C5-C6	-2.10	122.17	124.53
25	b	509	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
32	S	619	LMU	C1B-O1B-C4'	-2.10	112.78	117.96
25	b	513	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
25	C	510	CLA	CHD-C1D-ND	-2.09	122.53	124.45
25	c	501	CLA	CHD-C1D-ND	-2.09	122.53	124.45
27	b	519	BCR	C1-C6-C5	-2.09	119.67	122.61
30	d	407	LHG	O8-C23-O10	-2.09	118.31	123.59
37	G	616	LUT	C10-C11-C12	-2.09	116.70	123.22
27	H	101	BCR	C35-C13-C14	-2.09	120.00	122.92
27	b	519	BCR	C34-C9-C10	-2.09	120.00	122.92
27	C	516	BCR	C21-C20-C19	-2.08	116.71	123.22
37	S	615	LUT	C10-C11-C12	-2.08	116.71	123.22
29	d	410	LMG	O7-C10-O9	-2.08	118.67	123.70
34	d	406	PL9	C37-C38-C39	-2.08	122.64	127.66
25	a	403	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
31	c	516	DGD	C2G-O2G-C1B	-2.08	112.67	117.79
25	S	610	CLA	CHB-C4A-NA	2.08	127.39	124.51
25	c	509	CLA	C1-C2-C3	-2.08	122.45	126.04
25	D	404	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
25	S	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	B	518	BCR	C28-C27-C26	-2.07	110.37	114.08
38	r	310	NEX	C15-C35-C34	-2.07	119.23	123.47
25	B	514	CLA	C1-C2-C3	-2.07	122.46	126.04
25	a	402	CLA	CHD-C1D-ND	-2.07	122.55	124.45
34	D	407	PL9	O2-C1-C2	-2.07	117.04	121.78
39	N	301	XAT	C30-C31-C32	-2.07	116.76	123.22
25	D	401	CLA	O2D-CGD-CBD	2.07	114.94	111.27
25	B	506	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	b	511	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
25	c	506	CLA	CHD-C1D-ND	-2.07	122.56	124.45
25	G	610	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
25	S	611	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
31	W	202	DGD	O2G-C1B-O1B	-2.06	118.72	123.70
25	C	505	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
34	d	406	PL9	O2-C1-C2	-2.06	117.06	121.78
25	A	405	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	613	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
37	G	615	LUT	C31-C30-C29	-2.06	124.37	127.31
39	N	301	XAT	C10-C11-C12	-2.06	116.79	123.22
39	Y	302	XAT	C38-C25-C24	2.06	116.59	114.28
36	N	307	CHL	CHB-C4A-NA	2.06	127.36	124.51
25	B	508	CLA	CHD-C1D-ND	-2.06	122.56	124.45
27	z	101	BCR	C20-C19-C18	-2.05	120.64	126.42
25	C	511	CLA	C1-C2-C3	-2.05	122.49	126.04
36	G	607	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
25	c	510	CLA	C1-C2-C3	-2.05	122.49	126.04
25	C	503	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	C	501	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	C	503	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	b	502	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	Y	312	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	c	504	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
36	G	606	CHL	C1C-C2C-C3C	-2.05	105.49	107.11
25	d	403	CLA	O2D-CGD-CBD	2.05	114.91	111.27
39	r	309	XAT	C18-C5-C4	2.05	116.58	114.28
25	c	506	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
25	S	604	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
25	D	405	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
27	C	516	BCR	C4-C5-C6	-2.04	119.76	122.73
37	Y	317	LUT	C30-C31-C32	-2.04	116.84	123.22
25	b	509	CLA	C1-C2-C3	-2.04	122.51	126.04
25	S	614	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	S	605	CLA	O2D-CGD-CBD	2.04	114.89	111.27
25	C	504	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	B	502	CLA	O2D-CGD-CBD	2.04	114.89	111.27
25	c	501	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	N	303	CLA	C1-C2-C3	-2.04	122.52	126.04
26	a	404	PHO	CMC-C2C-C3C	2.04	128.78	124.94
25	B	509	CLA	CHD-C1D-ND	-2.03	122.58	124.45
25	Y	304	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	W	201	LMG	C7-O1-C1	-2.03	109.77	113.74
25	C	507	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
37	G	616	LUT	C30-C31-C32	-2.03	116.87	123.22
27	z	101	BCR	C16-C15-C14	-2.03	119.31	123.47
25	r	303	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	b	506	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
27	V	101	BCR	C35-C13-C12	2.03	121.28	118.08
25	c	513	CLA	CHD-C1D-ND	-2.03	122.59	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	G	617	NEX	C30-C31-C32	-2.03	116.89	123.22
25	a	402	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
36	Y	309	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
25	N	304	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	D	404	CLA	O2D-CGD-CBD	2.03	114.87	111.27
25	c	502	CLA	CHD-C1D-ND	-2.03	122.59	124.45
37	S	616	LUT	C30-C31-C32	-2.02	116.90	123.22
25	r	301	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
37	S	616	LUT	C15-C35-C34	-2.02	119.33	123.47
39	r	309	XAT	C20-C13-C12	2.02	121.26	118.08
27	D	406	BCR	C16-C15-C14	-2.02	119.33	123.47
31	C	517	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
34	D	407	PL9	C37-C38-C39	-2.02	122.80	127.66
37	Y	316	LUT	C16-C1-C6	-2.02	107.03	110.30
25	Y	306	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	D	401	CLA	C1-C2-C3	-2.01	122.56	126.04
25	r	307	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
27	V	101	BCR	C11-C10-C9	-2.01	124.44	127.31
30	l	101	LHG	O8-C23-O10	-2.01	118.52	123.59
25	N	303	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	S	603	CLA	CHD-C1D-ND	-2.01	122.61	124.45
36	S	608	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
25	d	403	CLA	CHD-C1D-ND	-2.01	122.61	124.45
37	N	316	LUT	C10-C11-C12	-2.01	116.94	123.22
37	G	615	LUT	C39-C29-C28	2.01	121.24	118.08
37	N	316	LUT	C18-C5-C4	2.01	118.08	114.36
26	A	404	PHO	O2A-CGA-O1A	-2.01	118.52	123.59
25	c	511	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
39	N	301	XAT	C19-C9-C8	2.01	121.24	118.08
33	D	403	BCT	O3-C-O1	-2.01	114.34	119.55
39	Y	302	XAT	C10-C11-C12	-2.01	116.96	123.22
25	D	401	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
36	G	608	CHL	C1B-CHB-C4A	-2.00	126.15	130.12
37	S	616	LUT	C39-C29-C28	2.00	121.23	118.08
25	S	612	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
25	b	510	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
27	t	101	BCR	C11-C12-C13	-2.00	120.80	126.42
25	c	507	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (184) chirality outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
25	A	402	CLA	ND
25	A	403	CLA	ND
25	A	405	CLA	ND
25	B	501	CLA	ND
25	B	502	CLA	ND
25	B	503	CLA	ND
25	B	504	CLA	ND
25	B	505	CLA	ND
25	B	506	CLA	ND
25	B	507	CLA	ND
25	B	508	CLA	ND
25	B	509	CLA	ND
25	B	510	CLA	ND
25	B	511	CLA	ND
25	B	512	CLA	ND
25	B	513	CLA	ND
25	B	514	CLA	ND
25	B	515	CLA	ND
25	B	516	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	401	CLA	ND
25	D	404	CLA	ND
25	D	405	CLA	ND
25	G	602	CLA	ND
25	G	603	CLA	ND
25	G	604	CLA	ND
25	G	610	CLA	ND
25	G	611	CLA	ND
25	G	612	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
25	G	613	CLA	ND
25	G	614	CLA	ND
25	N	303	CLA	ND
25	N	304	CLA	ND
25	N	305	CLA	ND
25	N	311	CLA	ND
25	N	312	CLA	ND
25	N	313	CLA	ND
25	N	314	CLA	ND
25	N	315	CLA	ND
25	S	602	CLA	ND
25	S	603	CLA	ND
25	S	604	CLA	ND
25	S	605	CLA	ND
25	S	609	CLA	ND
25	S	610	CLA	ND
25	S	611	CLA	ND
25	S	612	CLA	ND
25	S	613	CLA	ND
25	S	614	CLA	ND
25	Y	304	CLA	ND
25	Y	305	CLA	ND
25	Y	306	CLA	ND
25	Y	311	CLA	ND
25	Y	312	CLA	ND
25	Y	313	CLA	ND
25	Y	314	CLA	ND
25	Y	315	CLA	ND
25	a	402	CLA	ND
25	a	403	CLA	ND
25	a	405	CLA	ND
25	b	501	CLA	ND
25	b	502	CLA	ND
25	b	503	CLA	ND
25	b	504	CLA	ND
25	b	505	CLA	ND
25	b	506	CLA	ND
25	b	507	CLA	ND
25	b	508	CLA	ND
25	b	509	CLA	ND
25	b	510	CLA	ND
25	b	511	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
25	b	512	CLA	ND
25	b	513	CLA	ND
25	b	514	CLA	ND
25	b	515	CLA	ND
25	b	516	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	401	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND
25	r	301	CLA	ND
25	r	302	CLA	ND
25	r	303	CLA	ND
25	r	307	CLA	ND
25	r	308	CLA	ND
36	G	601	CHL	NA
36	G	601	CHL	NC
36	G	601	CHL	ND
36	G	605	CHL	NA
36	G	605	CHL	NC
36	G	605	CHL	ND
36	G	606	CHL	NA
36	G	606	CHL	NC
36	G	606	CHL	ND
36	G	607	CHL	NA
36	G	607	CHL	NC
36	G	607	CHL	ND
36	G	608	CHL	NA
36	G	608	CHL	NC
36	G	608	CHL	ND
36	G	609	CHL	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
36	G	609	CHL	NC
36	G	609	CHL	ND
36	G	619	CHL	NA
36	G	619	CHL	NC
36	G	619	CHL	ND
36	N	302	CHL	NA
36	N	302	CHL	NC
36	N	302	CHL	ND
36	N	306	CHL	NA
36	N	306	CHL	NC
36	N	306	CHL	ND
36	N	307	CHL	NA
36	N	307	CHL	NC
36	N	307	CHL	ND
36	N	308	CHL	NA
36	N	308	CHL	NC
36	N	308	CHL	ND
36	N	309	CHL	NA
36	N	309	CHL	NC
36	N	309	CHL	ND
36	N	310	CHL	NA
36	N	310	CHL	NC
36	N	310	CHL	ND
36	S	601	CHL	NA
36	S	601	CHL	NC
36	S	601	CHL	ND
36	S	606	CHL	NA
36	S	606	CHL	NC
36	S	606	CHL	ND
36	S	607	CHL	NA
36	S	607	CHL	NC
36	S	607	CHL	ND
36	S	608	CHL	NA
36	S	608	CHL	NC
36	S	608	CHL	ND
36	Y	303	CHL	NA
36	Y	303	CHL	NC
36	Y	303	CHL	ND
36	Y	307	CHL	NA
36	Y	307	CHL	NC
36	Y	307	CHL	ND
36	Y	308	CHL	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
36	Y	308	CHL	NC
36	Y	308	CHL	ND
36	Y	309	CHL	NA
36	Y	309	CHL	NC
36	Y	309	CHL	ND
36	Y	310	CHL	NA
36	Y	310	CHL	NC
36	Y	310	CHL	ND
36	r	304	CHL	NA
36	r	304	CHL	NC
36	r	304	CHL	ND
36	r	305	CHL	NA
36	r	305	CHL	NC
36	r	305	CHL	ND
36	r	306	CHL	NA
36	r	306	CHL	NC
36	r	306	CHL	ND

All (1697) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	501	CLA	CHA-CBD-CGD-O1D
25	B	501	CLA	CHA-CBD-CGD-O2D
25	B	501	CLA	CAD-CBD-CGD-O1D
25	B	504	CLA	C1A-C2A-CAA-CBA
25	B	504	CLA	CHA-CBD-CGD-O1D
25	B	507	CLA	CBD-CGD-O2D-CED
25	B	509	CLA	C1A-C2A-CAA-CBA
25	B	509	CLA	C3A-C2A-CAA-CBA
25	B	512	CLA	C1A-C2A-CAA-CBA
25	B	514	CLA	CHA-CBD-CGD-O1D
25	B	514	CLA	CHA-CBD-CGD-O2D
25	B	514	CLA	CAD-CBD-CGD-O1D
25	C	501	CLA	CHA-CBD-CGD-O1D
25	C	501	CLA	CHA-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O1D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O2D
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CHA-CBD-CGD-O1D
25	C	513	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C11-C12-C13-C14
25	D	404	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C3A-C2A-CAA-CBA
25	D	405	CLA	CHA-CBD-CGD-O1D
25	D	405	CLA	CAD-CBD-CGD-O1D
25	D	405	CLA	CAD-CBD-CGD-O2D
25	D	405	CLA	C11-C12-C13-C14
25	G	603	CLA	C1A-C2A-CAA-CBA
25	G	603	CLA	C3A-C2A-CAA-CBA
25	G	603	CLA	C14-C13-C15-C16
25	G	611	CLA	C3A-C2A-CAA-CBA
25	N	305	CLA	CHA-CBD-CGD-O1D
25	N	305	CLA	CHA-CBD-CGD-O2D
25	N	305	CLA	CAD-CBD-CGD-O1D
25	N	305	CLA	CBD-CGD-O2D-CED
25	N	311	CLA	CBD-CGD-O2D-CED
25	N	312	CLA	C1A-C2A-CAA-CBA
25	N	312	CLA	C3A-C2A-CAA-CBA
25	N	315	CLA	C1A-C2A-CAA-CBA
25	S	602	CLA	C3A-C2A-CAA-CBA
25	S	602	CLA	CHA-CBD-CGD-O1D
25	S	602	CLA	CHA-CBD-CGD-O2D
25	S	605	CLA	C1A-C2A-CAA-CBA
25	S	613	CLA	CBD-CGD-O2D-CED
25	Y	314	CLA	CHA-CBD-CGD-O1D
25	Y	314	CLA	CHA-CBD-CGD-O2D
25	a	403	CLA	C1A-C2A-CAA-CBA
25	a	403	CLA	C3A-C2A-CAA-CBA
25	b	501	CLA	C1A-C2A-CAA-CBA
25	b	501	CLA	CBD-CGD-O2D-CED
25	b	503	CLA	C3A-C2A-CAA-CBA
25	b	504	CLA	C1A-C2A-CAA-CBA
25	b	504	CLA	CHA-CBD-CGD-O1D
25	b	504	CLA	CHA-CBD-CGD-O2D
25	b	504	CLA	CAD-CBD-CGD-O1D
25	b	505	CLA	C1A-C2A-CAA-CBA
25	b	505	CLA	CBD-CGD-O2D-CED
25	b	506	CLA	C3A-C2A-CAA-CBA
25	b	506	CLA	CHA-CBD-CGD-O1D
25	b	506	CLA	CAD-CBD-CGD-O1D
25	b	506	CLA	CAD-CBD-CGD-O2D
25	b	507	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	507	CLA	C3A-C2A-CAA-CBA
25	b	509	CLA	C1A-C2A-CAA-CBA
25	b	509	CLA	C3A-C2A-CAA-CBA
25	b	509	CLA	CHA-CBD-CGD-O1D
25	b	509	CLA	CHA-CBD-CGD-O2D
25	b	509	CLA	CBD-CGD-O2D-CED
25	b	511	CLA	CAD-CBD-CGD-O1D
25	b	511	CLA	CAD-CBD-CGD-O2D
25	b	512	CLA	C1A-C2A-CAA-CBA
25	b	512	CLA	C3A-C2A-CAA-CBA
25	c	501	CLA	C3A-C2A-CAA-CBA
25	c	502	CLA	C2A-CAA-CBA-CGA
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	CHA-CBD-CGD-O1D
25	c	503	CLA	CHA-CBD-CGD-O2D
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	505	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	508	CLA	C2A-CAA-CBA-CGA
25	c	511	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CAD-CBD-CGD-O1D
25	c	511	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CHA-CBD-CGD-O1D
25	c	513	CLA	CHA-CBD-CGD-O2D
25	d	401	CLA	C1A-C2A-CAA-CBA
25	d	401	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	CHA-CBD-CGD-O1D
25	d	404	CLA	CAD-CBD-CGD-O1D
25	d	404	CLA	CAD-CBD-CGD-O2D
25	r	301	CLA	CHA-CBD-CGD-O1D
25	r	301	CLA	CHA-CBD-CGD-O2D
25	r	302	CLA	CBD-CGD-O2D-CED
25	r	307	CLA	CBD-CGD-O2D-CED
25	r	308	CLA	CBD-CGD-O2D-CED
27	B	517	BCR	C17-C18-C19-C20
27	B	517	BCR	C36-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	B	517	BCR	C21-C22-C23-C24
27	B	517	BCR	C37-C22-C23-C24
27	B	517	BCR	C23-C24-C25-C26
27	B	518	BCR	C7-C8-C9-C10
27	B	518	BCR	C7-C8-C9-C34
27	C	514	BCR	C23-C24-C25-C26
27	C	515	BCR	C7-C8-C9-C34
27	C	515	BCR	C21-C22-C23-C24
27	C	515	BCR	C37-C22-C23-C24
27	C	515	BCR	C23-C24-C25-C26
27	D	406	BCR	C7-C8-C9-C10
27	D	406	BCR	C7-C8-C9-C34
27	V	101	BCR	C21-C22-C23-C24
27	V	101	BCR	C37-C22-C23-C24
27	b	517	BCR	C7-C8-C9-C10
27	b	517	BCR	C7-C8-C9-C34
27	c	514	BCR	C21-C22-C23-C24
27	c	514	BCR	C37-C22-C23-C24
27	d	405	BCR	C37-C22-C23-C24
27	t	101	BCR	C5-C6-C7-C8
27	t	101	BCR	C23-C24-C25-C26
27	z	101	BCR	C1-C6-C7-C8
27	z	101	BCR	C5-C6-C7-C8
27	z	101	BCR	C21-C22-C23-C24
27	z	101	BCR	C37-C22-C23-C24
29	W	201	LMG	O1-C7-C8-O7
29	a	408	LMG	O6-C1-O1-C7
29	c	518	LMG	C19-C20-C21-C22
29	d	410	LMG	O7-C8-C9-O8
30	B	520	LHG	C3-O3-P-O4
30	B	520	LHG	C4-O6-P-O4
30	C	521	LHG	C4-O6-P-O4
30	D	409	LHG	C4-O6-P-O3
30	D	409	LHG	C4-O6-P-O5
30	G	618	LHG	C4-O6-P-O4
30	G	618	LHG	C4-O6-P-O5
30	L	101	LHG	C4-O6-P-O3
30	L	101	LHG	C4-O6-P-O4
30	L	101	LHG	C4-O6-P-O5
30	N	319	LHG	C4-O6-P-O4
30	N	319	LHG	C4-O6-P-O5
30	S	618	LHG	C4-O6-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	Y	319	LHG	C4-O6-P-O3
30	Y	319	LHG	C4-O6-P-O4
30	Y	319	LHG	C4-O6-P-O5
30	a	411	LHG	C3-O3-P-O6
30	a	411	LHG	C4-O6-P-O3
30	b	521	LHG	C3-O3-P-O5
30	b	521	LHG	C3-O3-P-O6
30	b	521	LHG	C4-O6-P-O4
30	d	407	LHG	C3-O3-P-O6
30	d	407	LHG	C4-O6-P-O4
30	d	408	LHG	C3-O3-P-O5
30	l	101	LHG	C3-O3-P-O6
31	C	519	DGD	C4D-C5D-C6D-O5D
31	c	516	DGD	C2E-C1E-O5D-C6D
32	S	619	LMU	O5B-C1B-O1B-C4'
36	G	619	CHL	C3C-C2C-CMC-OMC
36	S	606	CHL	C3C-C2C-CMC-OMC
36	S	606	CHL	CHA-CBD-CGD-O1D
36	S	606	CHL	CHA-CBD-CGD-O2D
36	S	608	CHL	CHA-CBD-CGD-O1D
36	S	608	CHL	CHA-CBD-CGD-O2D
36	S	608	CHL	CAD-CBD-CGD-O1D
36	S	608	CHL	CAD-CBD-CGD-O2D
25	r	303	CLA	O1D-CGD-O2D-CED
25	B	505	CLA	O1D-CGD-O2D-CED
25	G	612	CLA	O1D-CGD-O2D-CED
25	B	501	CLA	CBD-CGD-O2D-CED
25	B	505	CLA	CBD-CGD-O2D-CED
25	B	509	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	D	405	CLA	CBD-CGD-O2D-CED
25	G	612	CLA	CBD-CGD-O2D-CED
25	N	314	CLA	CBD-CGD-O2D-CED
25	b	507	CLA	CBD-CGD-O2D-CED
25	b	511	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
25	r	303	CLA	CBD-CGD-O2D-CED
26	d	402	PHO	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	S	608	CHL	CBD-CGD-O2D-CED
36	r	306	CHL	CBD-CGD-O2D-CED
25	A	402	CLA	O1A-CGA-O2A-C1
25	B	513	CLA	O1A-CGA-O2A-C1
25	C	506	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
25	r	302	CLA	O1D-CGD-O2D-CED
25	B	507	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	O1D-CGD-O2D-CED
25	N	311	CLA	O1D-CGD-O2D-CED
25	b	505	CLA	O1D-CGD-O2D-CED
25	r	308	CLA	O1D-CGD-O2D-CED
25	B	513	CLA	CBA-CGA-O2A-C1
25	b	508	CLA	CBA-CGA-O2A-C1
25	B	514	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	G	602	CLA	CBD-CGD-O2D-CED
25	G	613	CLA	CBD-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED
25	Y	314	CLA	CBD-CGD-O2D-CED
25	b	515	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
36	N	309	CHL	CBD-CGD-O2D-CED
25	B	516	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
25	N	312	CLA	O1A-CGA-O2A-C1
25	S	613	CLA	O1A-CGA-O2A-C1
25	Y	312	CLA	O1A-CGA-O2A-C1
25	b	508	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	O1A-CGA-O2A-C1
25	d	401	CLA	O1A-CGA-O2A-C1
25	r	303	CLA	O1A-CGA-O2A-C1
26	a	404	PHO	O1A-CGA-O2A-C1
25	S	613	CLA	O1D-CGD-O2D-CED
25	b	501	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	r	307	CLA	O1D-CGD-O2D-CED
25	N	305	CLA	O1D-CGD-O2D-CED
25	b	509	CLA	O1D-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	504	CLA	CBD-CGD-O2D-CED
25	Y	304	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	G	605	CHL	CBD-CGD-O2D-CED
36	G	608	CHL	CBD-CGD-O2D-CED
25	b	507	CLA	O1D-CGD-O2D-CED
25	c	501	CLA	O1D-CGD-O2D-CED
25	c	504	CLA	O1D-CGD-O2D-CED
25	c	502	CLA	O1D-CGD-O2D-CED
25	G	613	CLA	C3-C5-C6-C7
25	Y	314	CLA	C3-C5-C6-C7
25	b	502	CLA	C3-C5-C6-C7
25	b	503	CLA	C3-C5-C6-C7
25	c	512	CLA	C3-C5-C6-C7
26	A	404	PHO	C3-C5-C6-C7
26	a	404	PHO	C3-C5-C6-C7
25	A	402	CLA	CBA-CGA-O2A-C1
25	B	516	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	N	312	CLA	CBA-CGA-O2A-C1
25	Y	305	CLA	CBA-CGA-O2A-C1
25	d	401	CLA	CBA-CGA-O2A-C1
26	a	404	PHO	CBA-CGA-O2A-C1
25	N	314	CLA	O1D-CGD-O2D-CED
36	r	306	CHL	O1D-CGD-O2D-CED
25	N	312	CLA	CBD-CGD-O2D-CED
36	S	601	CHL	CBD-CGD-O2D-CED
25	c	506	CLA	O1A-CGA-O2A-C1
25	B	505	CLA	C4-C3-C5-C6
25	b	505	CLA	C4-C3-C5-C6
25	b	515	CLA	C4-C3-C5-C6
25	G	610	CLA	CBD-CGD-O2D-CED
25	B	506	CLA	C2A-CAA-CBA-CGA
25	B	513	CLA	C2A-CAA-CBA-CGA
25	C	509	CLA	C2A-CAA-CBA-CGA
25	b	506	CLA	C2A-CAA-CBA-CGA
25	b	511	CLA	C2A-CAA-CBA-CGA
36	G	619	CHL	C2A-CAA-CBA-CGA
36	N	306	CHL	C2A-CAA-CBA-CGA
36	N	307	CHL	C2A-CAA-CBA-CGA
36	S	601	CHL	C2A-CAA-CBA-CGA
36	Y	307	CHL	C2A-CAA-CBA-CGA
36	Y	308	CHL	C2A-CAA-CBA-CGA
25	b	508	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	D	402	PHO	C3-C5-C6-C7
25	C	513	CLA	CBA-CGA-O2A-C1
25	S	613	CLA	CBA-CGA-O2A-C1
25	Y	312	CLA	CBA-CGA-O2A-C1
25	b	502	CLA	CBA-CGA-O2A-C1
25	b	505	CLA	CBA-CGA-O2A-C1
25	b	509	CLA	CBA-CGA-O2A-C1
25	b	511	CLA	CBA-CGA-O2A-C1
25	c	508	CLA	CBA-CGA-O2A-C1
25	r	303	CLA	CBA-CGA-O2A-C1
25	b	506	CLA	CBD-CGD-O2D-CED
25	b	508	CLA	CBD-CGD-O2D-CED
25	B	509	CLA	O1D-CGD-O2D-CED
26	d	402	PHO	O1D-CGD-O2D-CED
36	S	608	CHL	O1D-CGD-O2D-CED
25	B	510	CLA	O1A-CGA-O2A-C1
25	C	509	CLA	O1A-CGA-O2A-C1
25	C	512	CLA	O1A-CGA-O2A-C1
25	S	611	CLA	O1A-CGA-O2A-C1
25	Y	305	CLA	O1A-CGA-O2A-C1
25	b	502	CLA	O1A-CGA-O2A-C1
25	b	505	CLA	O1A-CGA-O2A-C1
25	b	509	CLA	O1A-CGA-O2A-C1
25	b	511	CLA	O1A-CGA-O2A-C1
27	v	101	BCR	C19-C20-C21-C22
25	S	604	CLA	CBD-CGD-O2D-CED
25	Y	311	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
26	D	402	PHO	CBD-CGD-O2D-CED
36	r	304	CHL	CBD-CGD-O2D-CED
25	B	501	CLA	O1D-CGD-O2D-CED
25	b	511	CLA	O1D-CGD-O2D-CED
25	B	504	CLA	C3-C5-C6-C7
25	C	509	CLA	CBA-CGA-O2A-C1
25	S	611	CLA	CBA-CGA-O2A-C1
26	A	404	PHO	CBA-CGA-O2A-C1
26	d	402	PHO	CBA-CGA-O2A-C1
25	C	510	CLA	O1A-CGA-O2A-C1
25	d	404	CLA	O1D-CGD-O2D-CED
29	a	408	LMG	C11-C10-O7-C8
29	d	409	LMG	C11-C10-O7-C8
25	a	403	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	C	523	LMU	O5'-C5'-C6'-O6'
31	C	519	DGD	O6D-C5D-C6D-O5D
36	Y	309	CHL	CBD-CGD-O2D-CED
25	B	510	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
32	C	522	LMU	O5'-C5'-C6'-O6'
29	a	408	LMG	O9-C10-O7-C8
26	A	404	PHO	O1A-CGA-O2A-C1
25	b	505	CLA	C2-C3-C5-C6
36	G	607	CHL	CBD-CGD-O2D-CED
31	C	518	DGD	O6D-C5D-C6D-O5D
25	B	516	CLA	C2A-CAA-CBA-CGA
36	G	607	CHL	C2A-CAA-CBA-CGA
25	D	405	CLA	O1D-CGD-O2D-CED
25	c	504	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
26	d	402	PHO	O1A-CGA-O2A-C1
29	W	201	LMG	O6-C1-O1-C7
31	c	516	DGD	O6E-C1E-O5D-C6D
34	D	407	PL9	C39-C41-C42-C43
25	B	514	CLA	O1D-CGD-O2D-CED
25	G	613	CLA	O1D-CGD-O2D-CED
29	d	409	LMG	O9-C10-O7-C8
25	G	603	CLA	CBA-CGA-O2A-C1
25	N	314	CLA	CBA-CGA-O2A-C1
25	a	403	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	b	510	CLA	CBA-CGA-O2A-C1
25	B	506	CLA	C8-C10-C11-C12
25	B	501	CLA	C8-C10-C11-C12
30	b	521	LHG	O2-C2-C3-O3
31	c	517	DGD	C4D-C5D-C6D-O5D
25	S	614	CLA	CBA-CGA-O2A-C1
36	G	601	CHL	C4-C3-C5-C6
25	b	515	CLA	C2-C3-C5-C6
25	B	504	CLA	C6-C7-C8-C9
25	B	506	CLA	C6-C7-C8-C9
25	B	508	CLA	C11-C10-C8-C9
25	C	504	CLA	C11-C12-C13-C14
25	C	512	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	509	CLA	C6-C7-C8-C9
25	b	510	CLA	C11-C12-C13-C14
25	b	511	CLA	C11-C12-C13-C14
25	b	515	CLA	C6-C7-C8-C9
25	c	507	CLA	C14-C13-C15-C16
36	N	302	CHL	C14-C13-C15-C16
36	N	306	CHL	C6-C7-C8-C9
36	N	308	CHL	C6-C7-C8-C9
36	N	308	CHL	C14-C13-C15-C16
36	Y	310	CHL	C14-C13-C15-C16
25	b	515	CLA	O1D-CGD-O2D-CED
36	Y	308	CHL	CBD-CGD-O2D-CED
25	C	510	CLA	C2A-CAA-CBA-CGA
25	c	506	CLA	C2A-CAA-CBA-CGA
36	N	308	CHL	C2A-CAA-CBA-CGA
27	H	101	BCR	C7-C8-C9-C34
27	b	519	BCR	C7-C8-C9-C34
27	b	519	BCR	C37-C22-C23-C24
27	h	101	BCR	C7-C8-C9-C34
27	t	101	BCR	C7-C8-C9-C34
27	H	101	BCR	C7-C8-C9-C10
27	h	101	BCR	C7-C8-C9-C10
27	t	101	BCR	C7-C8-C9-C10
32	C	522	LMU	C4'-C5'-C6'-O6'
31	C	518	DGD	C1B-C2B-C3B-C4B
25	G	603	CLA	O1A-CGA-O2A-C1
36	Y	310	CHL	C13-C15-C16-C17
25	c	511	CLA	O1D-CGD-O2D-CED
25	S	610	CLA	CBA-CGA-O2A-C1
25	B	516	CLA	C8-C10-C11-C12
25	Y	311	CLA	C5-C6-C7-C8
25	a	405	CLA	C10-C11-C12-C13
25	b	502	CLA	C8-C10-C11-C12
36	N	302	CHL	C5-C6-C7-C8
36	N	302	CHL	C15-C16-C17-C18
36	Y	310	CHL	C8-C10-C11-C12
30	B	520	LHG	C23-C24-C25-C26
31	C	517	DGD	C1B-C2B-C3B-C4B
25	S	609	CLA	O1D-CGD-O2D-CED
25	B	510	CLA	C15-C16-C17-C18
25	C	504	CLA	C10-C11-C12-C13
25	G	613	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	502	CLA	C13-C15-C16-C17
36	G	609	CHL	C15-C16-C17-C18
36	G	619	CHL	C8-C10-C11-C12
36	N	306	CHL	C8-C10-C11-C12
36	Y	303	CHL	C5-C6-C7-C8
34	d	406	PL9	C47-C48-C49-C51
25	B	514	CLA	C8-C10-C11-C12
25	C	503	CLA	C15-C16-C17-C18
25	C	507	CLA	C13-C15-C16-C17
25	b	502	CLA	C5-C6-C7-C8
25	C	505	CLA	CBA-CGA-O2A-C1
25	b	513	CLA	CBA-CGA-O2A-C1
25	Y	314	CLA	O1D-CGD-O2D-CED
25	d	401	CLA	C2-C1-O2A-CGA
25	B	509	CLA	C5-C6-C7-C8
36	G	601	CHL	C8-C10-C11-C12
36	G	608	CHL	C2A-CAA-CBA-CGA
36	r	304	CHL	C2A-CAA-CBA-CGA
36	S	608	CHL	O2A-C1-C2-C3
25	B	504	CLA	C8-C10-C11-C12
36	Y	303	CHL	C8-C10-C11-C12
25	C	504	CLA	O1D-CGD-O2D-CED
25	C	510	CLA	C6-C7-C8-C10
25	C	513	CLA	C6-C7-C8-C10
25	G	610	CLA	C11-C12-C13-C15
25	b	512	CLA	C6-C7-C8-C10
25	b	515	CLA	C6-C7-C8-C10
25	c	508	CLA	C11-C12-C13-C15
36	N	302	CHL	C11-C10-C8-C7
36	N	308	CHL	C11-C12-C13-C15
36	Y	310	CHL	C12-C13-C15-C16
25	a	403	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	O1D-CGD-O2D-CED
25	G	602	CLA	O1D-CGD-O2D-CED
25	Y	304	CLA	O1D-CGD-O2D-CED
36	G	608	CHL	O1D-CGD-O2D-CED
36	N	309	CHL	O1D-CGD-O2D-CED
25	C	506	CLA	C13-C15-C16-C17
25	a	402	CLA	C13-C15-C16-C17
36	N	310	CHL	C8-C10-C11-C12
25	N	314	CLA	O1A-CGA-O2A-C1
25	b	510	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	504	CLA	CBD-CGD-O2D-CED
36	N	302	CHL	CBD-CGD-O2D-CED
25	C	510	CLA	C15-C16-C17-C18
34	d	406	PL9	C39-C41-C42-C43
30	d	408	LHG	C7-C8-C9-C10
30	B	520	LHG	O2-C2-C3-O3
36	G	609	CHL	C3-C5-C6-C7
36	N	306	CHL	C3-C5-C6-C7
36	S	606	CHL	C2A-CAA-CBA-CGA
36	N	306	CHL	C13-C15-C16-C17
36	N	310	CHL	C15-C16-C17-C18
32	c	519	LMU	C3'-C4'-O1B-C1B
25	S	614	CLA	O1A-CGA-O2A-C1
25	a	405	CLA	O1A-CGA-O2A-C1
25	B	515	CLA	C5-C6-C7-C8
25	C	502	CLA	O1D-CGD-O2D-CED
36	G	605	CHL	O1D-CGD-O2D-CED
25	C	505	CLA	O1A-CGA-O2A-C1
36	S	601	CHL	O1D-CGD-O2D-CED
25	B	501	CLA	C13-C15-C16-C17
25	B	503	CLA	C13-C15-C16-C17
25	b	511	CLA	C5-C6-C7-C8
25	c	509	CLA	C8-C10-C11-C12
36	G	619	CHL	C10-C11-C12-C13
30	B	520	LHG	C3-O3-P-O6
30	B	520	LHG	C4-O6-P-O3
30	C	521	LHG	C4-O6-P-O3
30	G	618	LHG	C4-O6-P-O3
30	L	101	LHG	C3-O3-P-O6
30	N	319	LHG	C4-O6-P-O3
30	Y	319	LHG	C3-O3-P-O6
30	b	521	LHG	C4-O6-P-O3
30	d	407	LHG	C4-O6-P-O3
25	D	405	CLA	C3-C5-C6-C7
25	N	312	CLA	O1D-CGD-O2D-CED
25	b	513	CLA	O1A-CGA-O2A-C1
31	c	517	DGD	O6D-C5D-C6D-O5D
25	G	610	CLA	O1D-CGD-O2D-CED
30	B	520	LHG	C1-C2-C3-O3
25	B	505	CLA	C2-C3-C5-C6
25	N	304	CLA	C15-C16-C17-C18
25	A	402	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	514	CLA	C2A-CAA-CBA-CGA
25	N	314	CLA	C2A-CAA-CBA-CGA
25	S	613	CLA	C2A-CAA-CBA-CGA
25	b	505	CLA	C2A-CAA-CBA-CGA
25	b	507	CLA	C2A-CAA-CBA-CGA
36	G	609	CHL	C16-C17-C18-C19
36	Y	303	CHL	C16-C17-C18-C19
31	C	517	DGD	O6E-C5E-C6E-O5E
25	b	507	CLA	C3-C5-C6-C7
25	b	505	CLA	C13-C15-C16-C17
25	c	510	CLA	C8-C10-C11-C12
36	G	609	CHL	C10-C11-C12-C13
25	b	508	CLA	O1D-CGD-O2D-CED
36	G	601	CHL	CBD-CGD-O2D-CED
30	C	521	LHG	C32-C33-C34-C35
30	N	319	LHG	C33-C34-C35-C36
32	C	523	LMU	C4-C5-C6-C7
25	C	501	CLA	C16-C17-C18-C19
36	G	601	CHL	C16-C17-C18-C20
36	G	619	CHL	C16-C17-C18-C20
36	N	302	CHL	C16-C17-C18-C20
36	N	310	CHL	C16-C17-C18-C20
36	Y	310	CHL	C16-C17-C18-C20
25	B	514	CLA	CBA-CGA-O2A-C1
31	c	517	DGD	C3B-C4B-C5B-C6B
36	G	619	CHL	C15-C16-C17-C18
28	t	102	SQD	C31-C32-C33-C34
25	b	506	CLA	O1D-CGD-O2D-CED
25	S	610	CLA	O1A-CGA-O2A-C1
29	d	410	LMG	C15-C16-C17-C18
36	N	310	CHL	C13-C15-C16-C17
30	d	408	LHG	O2-C2-C3-O3
25	G	602	CLA	C3-C5-C6-C7
25	c	509	CLA	CBA-CGA-O2A-C1
30	B	520	LHG	C28-C29-C30-C31
30	C	521	LHG	C12-C13-C14-C15
25	D	401	CLA	C16-C17-C18-C20
36	N	306	CHL	C16-C17-C18-C19
25	S	604	CLA	O1D-CGD-O2D-CED
25	Y	311	CLA	O1D-CGD-O2D-CED
34	D	407	PL9	C15-C14-C16-C17
25	B	505	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	510	CLA	C14-C13-C15-C16
25	D	405	CLA	C11-C10-C8-C9
25	D	405	CLA	C14-C13-C15-C16
25	G	603	CLA	C11-C12-C13-C14
25	b	504	CLA	C11-C12-C13-C14
25	b	505	CLA	C11-C12-C13-C14
25	b	510	CLA	C11-C10-C8-C9
25	b	515	CLA	C11-C10-C8-C9
25	c	502	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
25	c	508	CLA	C6-C7-C8-C9
25	B	513	CLA	C15-C16-C17-C18
25	S	614	CLA	C2A-CAA-CBA-CGA
25	r	302	CLA	C2A-CAA-CBA-CGA
27	C	514	BCR	C7-C8-C9-C34
27	z	101	BCR	C7-C8-C9-C34
27	b	519	BCR	C7-C8-C9-C10
27	z	101	BCR	C7-C8-C9-C10
36	Y	303	CHL	C13-C15-C16-C17
29	c	518	LMG	C10-C11-C12-C13
29	b	520	LMG	C11-C12-C13-C14
30	d	407	LHG	C29-C30-C31-C32
31	C	518	DGD	C4B-C5B-C6B-C7B
32	C	523	LMU	C6-C7-C8-C9
25	A	405	CLA	C11-C12-C13-C14
25	A	405	CLA	C11-C12-C13-C15
25	C	501	CLA	C16-C17-C18-C20
25	D	405	CLA	C16-C17-C18-C19
25	G	602	CLA	C16-C17-C18-C19
25	G	602	CLA	C16-C17-C18-C20
25	G	613	CLA	C16-C17-C18-C20
25	N	303	CLA	C16-C17-C18-C19
25	N	303	CLA	C16-C17-C18-C20
25	r	301	CLA	C11-C12-C13-C14
25	r	301	CLA	C11-C12-C13-C15
36	G	601	CHL	C16-C17-C18-C19
36	N	302	CHL	C16-C17-C18-C19
36	G	609	CHL	C5-C6-C7-C8
31	W	202	DGD	C2A-C3A-C4A-C5A
36	G	619	CHL	CBD-CGD-O2D-CED
36	r	305	CHL	CBD-CGD-O2D-CED
36	r	304	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	D	408	LHG	C7-C8-C9-C10
25	b	506	CLA	CBA-CGA-O2A-C1
29	H	102	LMG	C29-C30-C31-C32
26	D	402	PHO	O1D-CGD-O2D-CED
25	A	402	CLA	C3A-C2A-CAA-CBA
25	B	516	CLA	C3A-C2A-CAA-CBA
25	C	513	CLA	C3A-C2A-CAA-CBA
25	N	304	CLA	C3A-C2A-CAA-CBA
25	S	605	CLA	C3A-C2A-CAA-CBA
25	Y	305	CLA	C3A-C2A-CAA-CBA
25	b	501	CLA	C3A-C2A-CAA-CBA
25	b	504	CLA	C3A-C2A-CAA-CBA
25	c	507	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	C3A-C2A-CAA-CBA
25	b	509	CLA	C5-C6-C7-C8
32	S	619	LMU	O1'-C1-C2-C3
25	c	513	CLA	O1D-CGD-O2D-CED
25	D	405	CLA	C16-C17-C18-C20
25	G	613	CLA	C16-C17-C18-C19
36	G	609	CHL	C16-C17-C18-C20
36	G	619	CHL	C16-C17-C18-C19
36	N	310	CHL	C16-C17-C18-C19
36	Y	310	CHL	C16-C17-C18-C19
25	b	503	CLA	CBD-CGD-O2D-CED
25	C	509	CLA	O2A-C1-C2-C3
25	C	510	CLA	C4-C3-C5-C6
26	A	404	PHO	C4-C3-C5-C6
25	C	510	CLA	C2-C3-C5-C6
25	G	613	CLA	C2-C3-C5-C6
26	A	404	PHO	C2-C3-C5-C6
34	D	407	PL9	C13-C14-C16-C17
36	G	601	CHL	C2A-CAA-CBA-CGA
25	d	401	CLA	C15-C16-C17-C18
29	W	201	LMG	C29-C30-C31-C32
25	Y	313	CLA	C3-C5-C6-C7
29	d	409	LMG	C28-C29-C30-C31
25	B	504	CLA	CBD-CGD-O2D-CED
32	C	523	LMU	C7-C8-C9-C10
25	C	509	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
25	c	508	CLA	C2-C1-O2A-CGA
32	C	523	LMU	C4'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	a	407	SQD	C33-C34-C35-C36
36	N	302	CHL	C13-C15-C16-C17
36	Y	303	CHL	C15-C16-C17-C18
25	B	514	CLA	O1A-CGA-O2A-C1
25	c	509	CLA	O1A-CGA-O2A-C1
32	c	519	LMU	C1-C2-C3-C4
32	c	519	LMU	C5'-C4'-O1B-C1B
26	d	402	PHO	C3-C5-C6-C7
27	B	517	BCR	C23-C24-C25-C30
27	C	514	BCR	C1-C6-C7-C8
27	C	514	BCR	C5-C6-C7-C8
27	C	514	BCR	C23-C24-C25-C30
27	C	515	BCR	C23-C24-C25-C30
27	V	101	BCR	C23-C24-C25-C26
27	a	406	BCR	C23-C24-C25-C26
27	b	517	BCR	C23-C24-C25-C26
27	c	514	BCR	C23-C24-C25-C26
27	c	514	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C26
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C23-C24-C25-C30
27	v	101	BCR	C23-C24-C25-C26
27	v	101	BCR	C23-C24-C25-C30
25	B	507	CLA	CBA-CGA-O2A-C1
25	Y	315	CLA	CBA-CGA-O2A-C1
25	b	510	CLA	C15-C16-C17-C18
26	a	404	PHO	C8-C10-C11-C12
36	G	619	CHL	C13-C15-C16-C17
28	a	407	SQD	C8-C7-O47-C45
25	C	513	CLA	C4-C3-C5-C6
25	G	613	CLA	C4-C3-C5-C6
25	B	505	CLA	C11-C12-C13-C15
25	B	510	CLA	C12-C13-C15-C16
25	C	501	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C12-C13-C15
25	D	405	CLA	C11-C10-C8-C7
25	D	405	CLA	C12-C13-C15-C16
25	G	602	CLA	C11-C12-C13-C15
25	G	603	CLA	C6-C7-C8-C10
25	G	603	CLA	C11-C12-C13-C15
25	Y	311	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	Y	314	CLA	C11-C10-C8-C7
25	b	505	CLA	C11-C12-C13-C15
25	b	510	CLA	C11-C10-C8-C7
25	b	515	CLA	C11-C10-C8-C7
25	c	502	CLA	C12-C13-C15-C16
25	c	506	CLA	C12-C13-C15-C16
25	c	508	CLA	C6-C7-C8-C10
25	c	509	CLA	C12-C13-C15-C16
34	d	406	PL9	C13-C14-C16-C17
36	G	609	CHL	C12-C13-C15-C16
25	c	508	CLA	C3-C5-C6-C7
25	b	506	CLA	O1A-CGA-O2A-C1
25	B	508	CLA	C13-C15-C16-C17
36	N	308	CHL	CBD-CGD-O2D-CED
25	D	401	CLA	C16-C17-C18-C19
29	b	520	LMG	O9-C10-O7-C8
29	B	519	LMG	C10-C11-C12-C13
29	a	408	LMG	C10-C11-C12-C13
30	d	407	LHG	C23-C24-C25-C26
36	G	609	CHL	C2C-C3C-CAC-CBC
25	C	505	CLA	C2A-CAA-CBA-CGA
25	b	508	CLA	C2A-CAA-CBA-CGA
36	Y	309	CHL	O1D-CGD-O2D-CED
36	G	607	CHL	O1D-CGD-O2D-CED
25	A	405	CLA	C3-C5-C6-C7
25	Y	305	CLA	C13-C15-C16-C17
28	A	407	SQD	C8-C7-O47-C45
29	b	520	LMG	C11-C10-O7-C8
36	Y	310	CHL	CBD-CGD-O2D-CED
28	A	407	SQD	O49-C7-O47-C45
29	C	520	LMG	O7-C8-C9-O8
29	H	102	LMG	O7-C8-C9-O8
30	N	319	LHG	C25-C26-C27-C28
36	N	306	CHL	C16-C17-C18-C20
29	D	410	LMG	O6-C5-C6-O5
29	b	520	LMG	O6-C5-C6-O5
25	C	503	CLA	C8-C10-C11-C12
34	d	406	PL9	C15-C14-C16-C17
25	B	508	CLA	C2-C3-C5-C6
36	G	601	CHL	C2-C3-C5-C6
25	B	502	CLA	C11-C10-C8-C9
25	C	501	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	510	CLA	C6-C7-C8-C9
25	C	513	CLA	C6-C7-C8-C9
25	D	404	CLA	C11-C12-C13-C14
25	G	602	CLA	C11-C12-C13-C14
25	G	610	CLA	C11-C12-C13-C14
25	G	613	CLA	C14-C13-C15-C16
25	N	314	CLA	C11-C12-C13-C14
25	Y	311	CLA	C11-C12-C13-C14
25	Y	314	CLA	C11-C10-C8-C9
25	b	512	CLA	C6-C7-C8-C9
25	b	513	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C12-C13-C14
36	G	609	CHL	C14-C13-C15-C16
36	G	619	CHL	C6-C7-C8-C9
36	N	302	CHL	C11-C10-C8-C9
36	N	308	CHL	C11-C12-C13-C14
36	Y	310	CHL	C11-C12-C13-C14
25	Y	305	CLA	C3-C5-C6-C7
25	G	603	CLA	C2A-CAA-CBA-CGA
25	G	611	CLA	C2A-CAA-CBA-CGA
25	Y	314	CLA	C2A-CAA-CBA-CGA
25	b	516	CLA	C2A-CAA-CBA-CGA
31	C	517	DGD	C3A-C4A-C5A-C6A
32	C	522	LMU	C3-C4-C5-C6
29	a	408	LMG	O6-C5-C6-O5
32	S	619	LMU	O5'-C5'-C6'-O6'
25	a	403	CLA	O1D-CGD-O2D-CED
25	B	507	CLA	O1A-CGA-O2A-C1
25	Y	315	CLA	O1A-CGA-O2A-C1
25	A	402	CLA	C1A-C2A-CAA-CBA
25	B	516	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	G	611	CLA	C1A-C2A-CAA-CBA
25	N	304	CLA	C1A-C2A-CAA-CBA
25	S	602	CLA	C1A-C2A-CAA-CBA
25	Y	305	CLA	C1A-C2A-CAA-CBA
25	Y	306	CLA	C1A-C2A-CAA-CBA
25	Y	315	CLA	C1A-C2A-CAA-CBA
25	b	503	CLA	C1A-C2A-CAA-CBA
25	b	506	CLA	C1A-C2A-CAA-CBA
25	b	514	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	507	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	r	303	CLA	C1A-C2A-CAA-CBA
29	W	201	LMG	C11-C10-O7-C8
30	C	521	LHG	C8-C7-O7-C5
30	l	101	LHG	C8-C7-O7-C5
28	A	407	SQD	C25-C26-C27-C28
25	C	506	CLA	C5-C6-C7-C8
36	G	601	CHL	C15-C16-C17-C18
30	S	618	LHG	C4-O6-P-O3
29	c	518	LMG	O6-C5-C6-O5
25	B	512	CLA	C10-C11-C12-C13
29	d	409	LMG	C10-C11-C12-C13
29	d	410	LMG	O6-C5-C6-O5
32	S	619	LMU	O5B-C5B-C6B-O6B
25	b	503	CLA	C8-C10-C11-C12
36	Y	303	CHL	C16-C17-C18-C20
28	A	407	SQD	C10-C11-C12-C13
36	Y	308	CHL	O1D-CGD-O2D-CED
31	C	518	DGD	O6E-C5E-C6E-O5E
25	N	303	CLA	C3-C5-C6-C7
25	N	315	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	C2-C3-C5-C6
25	c	506	CLA	C5-C6-C7-C8
36	N	310	CHL	C5-C6-C7-C8
25	Y	313	CLA	C8-C10-C11-C12
25	N	304	CLA	C16-C17-C18-C20
29	H	102	LMG	O6-C5-C6-O5
29	H	102	LMG	C7-C8-C9-O8
29	W	201	LMG	O1-C7-C8-C9
30	C	521	LHG	C4-C5-C6-O8
32	c	519	LMU	C3-C4-C5-C6
31	Y	301	DGD	O6E-C5E-C6E-O5E
31	c	517	DGD	C5D-C6D-O5D-C1E
30	a	411	LHG	C14-C15-C16-C17
36	Y	310	CHL	C2C-C3C-CAC-CBC
32	c	519	LMU	O5'-C5'-C6'-O6'
25	B	504	CLA	C5-C6-C7-C8
25	B	508	CLA	C4-C3-C5-C6
25	c	511	CLA	C4-C3-C5-C6
29	H	102	LMG	C10-C11-C12-C13
36	G	601	CHL	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	N	302	CHL	CBA-CGA-O2A-C1
36	G	609	CHL	CBD-CGD-O2D-CED
25	C	510	CLA	C8-C10-C11-C12
36	Y	310	CHL	C15-C16-C17-C18
29	d	409	LMG	O6-C5-C6-O5
36	G	609	CHL	C8-C10-C11-C12
25	b	511	CLA	C2-C1-O2A-CGA
36	G	609	CHL	C13-C15-C16-C17
25	B	504	CLA	CBA-CGA-O2A-C1
30	a	410	LHG	O6-C4-C5-O7
28	A	407	SQD	O47-C7-C8-C9
28	A	407	SQD	C28-C29-C30-C31
25	B	506	CLA	C5-C6-C7-C8
36	N	302	CHL	O1D-CGD-O2D-CED
28	a	407	SQD	O49-C7-O47-C45
25	B	507	CLA	C5-C6-C7-C8
36	N	302	CHL	O1A-CGA-O2A-C1
26	D	402	PHO	CHA-CBD-CGD-O1D
26	D	402	PHO	CHA-CBD-CGD-O2D
26	a	404	PHO	C4-C3-C5-C6
25	B	502	CLA	C11-C10-C8-C7
25	B	508	CLA	C6-C7-C8-C10
25	B	508	CLA	C11-C10-C8-C7
25	B	515	CLA	C12-C13-C15-C16
25	C	510	CLA	C12-C13-C15-C16
25	C	512	CLA	C6-C7-C8-C10
25	D	401	CLA	C11-C12-C13-C15
25	G	613	CLA	C12-C13-C15-C16
25	N	314	CLA	C11-C12-C13-C15
25	Y	313	CLA	C11-C12-C13-C15
25	b	503	CLA	C11-C12-C13-C15
25	b	506	CLA	C11-C10-C8-C7
25	b	508	CLA	C11-C12-C13-C15
25	b	509	CLA	C6-C7-C8-C10
25	b	510	CLA	C11-C12-C13-C15
25	b	512	CLA	C11-C10-C8-C7
25	b	513	CLA	C6-C7-C8-C10
25	c	505	CLA	C12-C13-C15-C16
25	c	509	CLA	C6-C7-C8-C10
36	N	308	CHL	C6-C7-C8-C10
36	N	308	CHL	C12-C13-C15-C16
36	Y	310	CHL	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	508	CLA	C6-C7-C8-C9
25	B	508	CLA	C11-C12-C13-C14
25	B	510	CLA	C11-C12-C13-C14
25	B	515	CLA	C14-C13-C15-C16
25	B	516	CLA	C14-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C9
25	C	510	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
25	D	401	CLA	C11-C12-C13-C14
25	D	404	CLA	C11-C10-C8-C9
25	N	305	CLA	C11-C12-C13-C14
25	Y	305	CLA	C11-C12-C13-C14
25	Y	314	CLA	C14-C13-C15-C16
25	b	506	CLA	C11-C10-C8-C9
25	b	512	CLA	C11-C10-C8-C9
25	c	501	CLA	C6-C7-C8-C9
25	c	503	CLA	C11-C10-C8-C9
25	c	505	CLA	C14-C13-C15-C16
25	c	508	CLA	C11-C10-C8-C9
25	c	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C12-C13-C14
25	d	401	CLA	C11-C12-C13-C14
26	a	404	PHO	C11-C12-C13-C14
36	G	601	CHL	C11-C10-C8-C9
36	G	601	CHL	C11-C12-C13-C14
25	c	511	CLA	CBA-CGA-O2A-C1
29	W	201	LMG	C29-C28-O8-C9
36	N	308	CHL	C13-C15-C16-C17
25	C	501	CLA	C2A-CAA-CBA-CGA
25	b	504	CLA	O1D-CGD-O2D-CED
25	N	304	CLA	C16-C17-C18-C19
27	d	405	BCR	C21-C22-C23-C24
36	G	619	CHL	O1D-CGD-O2D-CED
30	C	521	LHG	O9-C7-O7-C5
25	C	501	CLA	CBA-CGA-O2A-C1
25	S	604	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	C	501	CLA	C8-C10-C11-C12
32	C	522	LMU	C4-C5-C6-C7
25	C	503	CLA	C5-C6-C7-C8
30	C	521	LHG	O6-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	411	LHG	O6-C4-C5-C6
31	C	518	DGD	C1A-C2A-C3A-C4A
29	d	410	LMG	C12-C13-C14-C15
25	B	516	CLA	C5-C6-C7-C8
36	N	308	CHL	O1D-CGD-O2D-CED
26	a	404	PHO	C2-C3-C5-C6
30	S	618	LHG	C23-C24-C25-C26
36	G	601	CHL	O1D-CGD-O2D-CED
32	C	523	LMU	C3-C4-C5-C6
36	Y	303	CHL	C3-C5-C6-C7
25	B	503	CLA	C16-C17-C18-C20
25	A	403	CLA	CBA-CGA-O2A-C1
25	N	305	CLA	CBA-CGA-O2A-C1
25	Y	306	CLA	CBA-CGA-O2A-C1
25	a	402	CLA	CBA-CGA-O2A-C1
30	b	521	LHG	C23-C24-C25-C26
25	B	512	CLA	C3A-C2A-CAA-CBA
25	b	505	CLA	C3A-C2A-CAA-CBA
25	c	505	CLA	C3A-C2A-CAA-CBA
25	c	506	CLA	C3A-C2A-CAA-CBA
32	C	522	LMU	C9-C10-C11-C12
32	S	619	LMU	C4-C5-C6-C7
25	B	509	CLA	CBA-CGA-O2A-C1
36	N	310	CHL	CBA-CGA-O2A-C1
25	d	403	CLA	C8-C10-C11-C12
28	t	102	SQD	O6-C44-C45-C46
29	C	520	LMG	C7-C8-C9-O8
29	B	519	LMG	C37-C38-C39-C40
25	B	504	CLA	O1A-CGA-O2A-C1
36	r	305	CHL	O1D-CGD-O2D-CED
36	G	607	CHL	C3C-C2C-CMC-OMC
36	N	307	CHL	C3C-C2C-CMC-OMC
36	N	308	CHL	C3C-C2C-CMC-OMC
36	S	601	CHL	C3C-C2C-CMC-OMC
36	S	607	CHL	C3C-C2C-CMC-OMC
36	Y	310	CHL	C3C-C2C-CMC-OMC
36	N	309	CHL	C2A-CAA-CBA-CGA
30	D	409	LHG	O6-C4-C5-O7
36	G	601	CHL	O1A-CGA-O2A-C1
25	A	402	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	O1A-CGA-O2A-C1
31	c	515	DGD	C4B-C5B-C6B-C7B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	N	319	LHG	O7-C5-C6-O8
31	Y	301	DGD	O2G-C2G-C3G-O3G
30	G	618	LHG	C32-C33-C34-C35
25	C	504	CLA	C15-C16-C17-C18
29	d	410	LMG	C33-C34-C35-C36
29	W	201	LMG	O9-C10-O7-C8
30	l	101	LHG	O9-C7-O7-C5
25	c	510	CLA	C2-C1-O2A-CGA
25	C	513	CLA	C11-C10-C8-C9
25	Y	313	CLA	C11-C12-C13-C14
25	b	502	CLA	C11-C10-C8-C9
25	b	504	CLA	C14-C13-C15-C16
25	b	508	CLA	C11-C12-C13-C14
25	c	501	CLA	C11-C12-C13-C14
25	c	501	CLA	C14-C13-C15-C16
25	c	511	CLA	C14-C13-C15-C16
26	A	404	PHO	C6-C7-C8-C9
36	G	609	CHL	C11-C10-C8-C9
36	N	302	CHL	C11-C12-C13-C14
36	Y	310	CHL	C6-C7-C8-C9
25	B	503	CLA	C16-C17-C18-C19
27	V	101	BCR	C23-C24-C25-C30
27	a	406	BCR	C23-C24-C25-C30
25	B	504	CLA	O1D-CGD-O2D-CED
27	C	515	BCR	C7-C8-C9-C10
27	b	519	BCR	C21-C22-C23-C24
36	r	305	CHL	C1A-C2A-CAA-CBA
25	A	405	CLA	C5-C6-C7-C8
25	B	502	CLA	C13-C15-C16-C17
32	C	522	LMU	C6-C7-C8-C9
30	N	319	LHG	C23-C24-C25-C26
25	S	614	CLA	O2A-C1-C2-C3
25	C	501	CLA	O1A-CGA-O2A-C1
30	L	101	LHG	O6-C4-C5-C6
30	a	410	LHG	O6-C4-C5-C6
28	t	102	SQD	O47-C7-C8-C9
25	B	507	CLA	C11-C12-C13-C15
25	B	516	CLA	C12-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C10
25	C	508	CLA	C6-C7-C8-C10
25	C	508	CLA	C11-C12-C13-C15
25	C	511	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C11-C12-C13-C15
25	D	404	CLA	C11-C10-C8-C7
25	G	603	CLA	C12-C13-C15-C16
25	N	304	CLA	C6-C7-C8-C10
25	N	311	CLA	C12-C13-C15-C16
25	N	314	CLA	C12-C13-C15-C16
25	Y	305	CLA	C11-C12-C13-C15
25	Y	314	CLA	C12-C13-C15-C16
25	b	502	CLA	C11-C10-C8-C7
25	b	504	CLA	C11-C12-C13-C15
25	b	504	CLA	C12-C13-C15-C16
25	b	506	CLA	C12-C13-C15-C16
25	b	511	CLA	C6-C7-C8-C10
25	b	515	CLA	C12-C13-C15-C16
25	c	501	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C12-C13-C15
25	c	503	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	507	CLA	C6-C7-C8-C10
25	c	510	CLA	C11-C12-C13-C15
25	c	511	CLA	C12-C13-C15-C16
25	d	401	CLA	C11-C12-C13-C15
26	D	402	PHO	C6-C7-C8-C10
26	a	404	PHO	C11-C12-C13-C15
26	d	402	PHO	C11-C10-C8-C7
36	G	601	CHL	C11-C10-C8-C7
36	G	601	CHL	C11-C12-C13-C15
36	G	619	CHL	C11-C12-C13-C15
36	N	302	CHL	C11-C12-C13-C15
36	N	306	CHL	C11-C12-C13-C15
36	Y	303	CHL	C12-C13-C15-C16
36	Y	310	CHL	C6-C7-C8-C10
29	W	201	LMG	O10-C28-O8-C9
36	N	307	CHL	CBD-CGD-O2D-CED
25	C	508	CLA	C13-C15-C16-C17
25	D	404	CLA	C10-C11-C12-C13
25	b	515	CLA	C3-C5-C6-C7
36	Y	303	CHL	CBA-CGA-O2A-C1
25	b	503	CLA	O1D-CGD-O2D-CED
36	N	306	CHL	C15-C16-C17-C18
25	A	402	CLA	CAD-CBD-CGD-O2D
25	A	403	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	501	CLA	CAD-CBD-CGD-O2D
25	B	506	CLA	CAD-CBD-CGD-O2D
25	B	508	CLA	CAD-CBD-CGD-O2D
25	B	514	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	508	CLA	CAD-CBD-CGD-O2D
25	G	610	CLA	CAD-CBD-CGD-O2D
25	N	312	CLA	CAD-CBD-CGD-O2D
25	a	402	CLA	CAD-CBD-CGD-O2D
25	a	405	CLA	CAD-CBD-CGD-O2D
25	b	516	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	508	CLA	CAD-CBD-CGD-O2D
25	d	401	CLA	CAD-CBD-CGD-O2D
25	d	403	CLA	CAD-CBD-CGD-O2D
26	A	404	PHO	CAD-CBD-CGD-O2D
36	G	606	CHL	CAD-CBD-CGD-O2D
36	N	306	CHL	CAD-CBD-CGD-O2D
36	Y	310	CHL	O1D-CGD-O2D-CED
36	G	609	CHL	C4C-C3C-CAC-CBC
25	b	501	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
25	c	507	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	C11-C12-C13-C14
31	C	518	DGD	O6D-C1D-O3G-C3G
31	C	518	DGD	O6E-C1E-O5D-C6D
29	d	410	LMG	C7-C8-C9-O8
30	N	319	LHG	C4-C5-C6-O8
31	W	202	DGD	O1G-C1G-C2G-C3G
36	Y	303	CHL	CBD-CGD-O2D-CED
30	a	411	LHG	O6-C4-C5-O7
25	S	602	CLA	O2A-C1-C2-C3
25	r	303	CLA	O2A-C1-C2-C3
35	f	101	HEM	C4B-C3B-CAB-CBB
25	G	613	CLA	C2A-CAA-CBA-CGA
36	Y	309	CHL	C2A-CAA-CBA-CGA
25	B	508	CLA	C16-C17-C18-C20
36	N	306	CHL	O1D-CGD-O2D-CED
25	B	504	CLA	CHA-CBD-CGD-O2D
25	B	509	CLA	CHA-CBD-CGD-O1D
25	B	509	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	510	CLA	CHA-CBD-CGD-O1D
25	B	510	CLA	CHA-CBD-CGD-O2D
25	C	511	CLA	CHA-CBD-CGD-O2D
25	D	405	CLA	CHA-CBD-CGD-O2D
25	N	304	CLA	CHA-CBD-CGD-O1D
25	N	304	CLA	CHA-CBD-CGD-O2D
25	S	603	CLA	CHA-CBD-CGD-O1D
25	S	603	CLA	CHA-CBD-CGD-O2D
25	S	605	CLA	CHA-CBD-CGD-O1D
25	S	605	CLA	CHA-CBD-CGD-O2D
25	S	609	CLA	CHA-CBD-CGD-O1D
25	S	609	CLA	CHA-CBD-CGD-O2D
25	b	501	CLA	CHA-CBD-CGD-O1D
25	b	506	CLA	CHA-CBD-CGD-O2D
25	b	510	CLA	CHA-CBD-CGD-O1D
25	b	510	CLA	CHA-CBD-CGD-O2D
25	b	513	CLA	CHA-CBD-CGD-O1D
25	b	513	CLA	CHA-CBD-CGD-O2D
25	c	501	CLA	CHA-CBD-CGD-O1D
25	c	505	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CHA-CBD-CGD-O2D
25	d	404	CLA	CHA-CBD-CGD-O2D
25	r	303	CLA	CHA-CBD-CGD-O1D
25	r	303	CLA	CHA-CBD-CGD-O2D
25	B	509	CLA	O1A-CGA-O2A-C1
25	S	604	CLA	O1A-CGA-O2A-C1
25	a	402	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
36	N	310	CHL	O1A-CGA-O2A-C1
29	H	102	LMG	C11-C12-C13-C14
30	L	101	LHG	C28-C29-C30-C31
31	Y	301	DGD	C6A-C7A-C8A-C9A
31	Y	301	DGD	CAA-CBA-CCA-CDA
31	W	202	DGD	O1G-C1G-C2G-O2G
31	W	202	DGD	C3A-C4A-C5A-C6A
36	N	306	CHL	CBD-CGD-O2D-CED
25	Y	306	CLA	O1A-CGA-O2A-C1
25	b	511	CLA	C16-C17-C18-C19
29	d	409	LMG	C11-C12-C13-C14
31	C	517	DGD	C7B-C8B-C9B-CAB
36	N	302	CHL	C3-C5-C6-C7
25	D	405	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	Y	314	CLA	C8-C10-C11-C12
25	C	509	CLA	C4-C3-C5-C6
25	b	503	CLA	C4-C3-C5-C6
25	A	403	CLA	O1A-CGA-O2A-C1
25	N	305	CLA	O1A-CGA-O2A-C1
25	A	402	CLA	C14-C13-C15-C16
25	B	511	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	C	508	CLA	C6-C7-C8-C9
25	c	507	CLA	C6-C7-C8-C9
26	d	402	PHO	C11-C10-C8-C9
36	Y	303	CHL	C11-C10-C8-C9
36	Y	303	CHL	C14-C13-C15-C16
36	G	609	CHL	O1D-CGD-O2D-CED
36	Y	303	CHL	O1A-CGA-O2A-C1
25	A	402	CLA	O1D-CGD-O2D-CED
25	B	514	CLA	C16-C17-C18-C20
32	S	619	LMU	C2-C3-C4-C5
27	b	518	BCR	C7-C8-C9-C34
27	C	514	BCR	C7-C8-C9-C10
25	B	511	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	C1A-C2A-CAA-CBA
25	B	512	CLA	C16-C17-C18-C19
25	b	509	CLA	C2-C1-O2A-CGA
25	c	505	CLA	C2-C1-O2A-CGA
25	b	512	CLA	CBA-CGA-O2A-C1
27	k	101	BCR	C9-C10-C11-C12
25	N	315	CLA	O1D-CGD-O2D-CED
36	N	307	CHL	O1D-CGD-O2D-CED
30	a	410	LHG	C3-O3-P-O6
30	a	410	LHG	C4-O6-P-O3
30	d	408	LHG	C3-O3-P-O6
30	d	408	LHG	C4-O6-P-O3
25	C	513	CLA	C2-C3-C5-C6
29	D	410	LMG	C12-C13-C14-C15
25	b	501	CLA	O1A-CGA-O2A-C1
30	B	520	LHG	C3-O3-P-O5
30	L	101	LHG	C3-O3-P-O5
30	S	618	LHG	C4-O6-P-O5
30	Y	319	LHG	C3-O3-P-O4
30	a	411	LHG	C3-O3-P-O4
30	a	411	LHG	C4-O6-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	b	521	LHG	C4-O6-P-O5
30	d	407	LHG	C3-O3-P-O4
30	l	101	LHG	C3-O3-P-O4
25	G	603	CLA	C16-C17-C18-C20
25	b	508	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C20
25	S	604	CLA	O2A-C1-C2-C3
29	H	102	LMG	C29-C28-O8-C9
36	Y	303	CHL	O1D-CGD-O2D-CED
25	b	510	CLA	C3-C5-C6-C7
31	C	517	DGD	C2A-C3A-C4A-C5A
36	Y	310	CHL	C4C-C3C-CAC-CBC
25	B	504	CLA	C16-C17-C18-C19
36	N	308	CHL	C16-C17-C18-C20
25	B	504	CLA	CAD-CBD-CGD-O1D
25	B	509	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	S	609	CLA	CAD-CBD-CGD-O1D
25	S	614	CLA	CAD-CBD-CGD-O1D
25	b	509	CLA	CAD-CBD-CGD-O1D
25	c	503	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	c	513	CLA	CAD-CBD-CGD-O1D
36	S	606	CHL	CAD-CBD-CGD-O1D
25	N	305	CLA	C5-C6-C7-C8
25	c	502	CLA	O1A-CGA-O2A-C1
25	c	507	CLA	O1A-CGA-O2A-C1
29	D	410	LMG	C16-C17-C18-C19
30	d	408	LHG	C1-C2-C3-O3
32	C	523	LMU	C5-C6-C7-C8
25	b	512	CLA	C16-C17-C18-C20
25	Y	315	CLA	C4-C3-C5-C6
25	B	504	CLA	C12-C13-C15-C16
25	B	506	CLA	C6-C7-C8-C10
25	C	506	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C10-C8-C7
25	G	602	CLA	C6-C7-C8-C10
25	G	610	CLA	C11-C10-C8-C7
25	b	510	CLA	C6-C7-C8-C10
25	c	503	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	C11-C12-C13-C15
25	r	301	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	C	521	LHG	O6-C4-C5-O7
30	L	101	LHG	O6-C4-C5-O7
36	G	609	CHL	C11-C12-C13-C15
36	G	619	CHL	C12-C13-C15-C16
36	N	310	CHL	C11-C12-C13-C15
29	d	410	LMG	C19-C20-C21-C22
25	c	509	CLA	C2A-CAA-CBA-CGA
25	B	508	CLA	C16-C17-C18-C19
31	Y	301	DGD	C1G-C2G-C3G-O3G
36	G	607	CHL	C1C-C2C-CMC-OMC
36	G	619	CHL	C1C-C2C-CMC-OMC
36	N	307	CHL	C1C-C2C-CMC-OMC
36	N	308	CHL	C1C-C2C-CMC-OMC
36	S	601	CHL	C1C-C2C-CMC-OMC
36	S	606	CHL	C1C-C2C-CMC-OMC
36	S	607	CHL	C1C-C2C-CMC-OMC
28	t	102	SQD	O6-C44-C45-O47
31	c	516	DGD	O2G-C2G-C3G-O3G
25	B	503	CLA	C10-C11-C12-C13
30	a	410	LHG	C33-C34-C35-C36
31	W	202	DGD	C2B-C3B-C4B-C5B
31	c	517	DGD	C9B-CAB-CBB-CCB
31	C	518	DGD	C5D-C6D-O5D-C1E
25	b	505	CLA	C8-C10-C11-C12
25	c	501	CLA	C8-C10-C11-C12
25	B	508	CLA	C15-C16-C17-C18
25	D	405	CLA	CBA-CGA-O2A-C1
25	b	504	CLA	CBA-CGA-O2A-C1
30	G	618	LHG	C17-C18-C19-C20
25	a	403	CLA	O2A-C1-C2-C3
25	Y	306	CLA	C8-C10-C11-C12
25	B	507	CLA	C11-C12-C13-C14
25	B	509	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C12-C13-C14
25	N	304	CLA	C6-C7-C8-C9
25	N	311	CLA	C14-C13-C15-C16
25	Y	304	CLA	C14-C13-C15-C16
25	Y	306	CLA	C6-C7-C8-C9
25	b	506	CLA	C14-C13-C15-C16
25	b	511	CLA	C6-C7-C8-C9
25	b	515	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	N	306	CHL	C11-C12-C13-C14
36	N	308	CHL	C11-C10-C8-C9
36	Y	303	CHL	C11-C12-C13-C14
25	b	511	CLA	C16-C17-C18-C20
29	H	102	LMG	O10-C28-O8-C9
25	b	506	CLA	C8-C10-C11-C12
25	b	508	CLA	C16-C17-C18-C19
25	S	605	CLA	O1A-CGA-O2A-C1
25	b	512	CLA	O1A-CGA-O2A-C1
25	c	504	CLA	C10-C11-C12-C13
25	S	602	CLA	C1-C2-C3-C4
25	S	610	CLA	C1-C2-C3-C4
25	S	611	CLA	C1-C2-C3-C4
25	S	613	CLA	C1-C2-C3-C4
36	N	309	CHL	C1-C2-C3-C4
25	B	512	CLA	O1A-CGA-O2A-C1
25	D	405	CLA	O1A-CGA-O2A-C1
25	C	505	CLA	C8-C10-C11-C12
25	B	501	CLA	C2A-CAA-CBA-CGA
25	N	303	CLA	C2A-CAA-CBA-CGA
25	S	602	CLA	C2A-CAA-CBA-CGA
25	Y	304	CLA	C2A-CAA-CBA-CGA
25	B	512	CLA	CBA-CGA-O2A-C1
25	S	605	CLA	CBA-CGA-O2A-C1
25	B	513	CLA	C2-C1-O2A-CGA
36	N	310	CHL	C2-C1-O2A-CGA
25	C	513	CLA	C16-C17-C18-C19
25	D	401	CLA	C15-C16-C17-C18
25	b	504	CLA	O1A-CGA-O2A-C1
25	N	312	CLA	O2A-C1-C2-C3
25	Y	305	CLA	C4-C3-C5-C6
36	Y	309	CHL	O1A-CGA-O2A-C1
36	Y	309	CHL	CBA-CGA-O2A-C1
25	B	514	CLA	C16-C17-C18-C19
25	G	602	CLA	C2A-CAA-CBA-CGA
25	b	501	CLA	C2A-CAA-CBA-CGA
25	b	504	CLA	C2A-CAA-CBA-CGA
30	C	521	LHG	O7-C5-C6-O8
30	C	521	LHG	C3-O3-P-O6
30	D	408	LHG	C3-O3-P-O6
30	D	408	LHG	C4-O6-P-O3
30	D	409	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	G	618	LHG	C3-O3-P-O6
30	N	319	LHG	C3-O3-P-O6
30	S	618	LHG	C3-O3-P-O6
30	l	101	LHG	C4-O6-P-O3
25	B	504	CLA	C16-C17-C18-C20
31	c	516	DGD	C1G-C2G-C3G-O3G
36	G	619	CHL	C4-C3-C5-C6
25	B	511	CLA	C13-C15-C16-C17
25	A	402	CLA	C12-C13-C15-C16
25	B	508	CLA	C11-C12-C13-C15
25	B	511	CLA	C6-C7-C8-C10
25	C	509	CLA	C2-C3-C5-C6
25	b	502	CLA	C6-C7-C8-C10
25	b	511	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C12-C13-C15
36	Y	303	CHL	C11-C10-C8-C7
25	B	504	CLA	C14-C13-C15-C16
25	C	504	CLA	C14-C13-C15-C16
25	b	503	CLA	C11-C12-C13-C14
36	G	609	CHL	C11-C12-C13-C14
36	G	619	CHL	C14-C13-C15-C16
25	A	402	CLA	C15-C16-C17-C18
25	C	510	CLA	C13-C15-C16-C17
27	C	516	BCR	C9-C10-C11-C12
25	b	507	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C19
36	N	308	CHL	C16-C17-C18-C19
30	d	407	LHG	C7-C8-C9-C10
25	G	603	CLA	C16-C17-C18-C19
29	D	410	LMG	C18-C19-C20-C21
30	b	521	LHG	C1-C2-C3-O3
36	N	310	CHL	C4-C3-C5-C6
31	Y	301	DGD	CDA-CEA-CFA-CGA
25	S	610	CLA	C2A-CAA-CBA-CGA
25	B	512	CLA	C16-C17-C18-C20
30	Y	319	LHG	C27-C28-C29-C30
26	a	404	PHO	C5-C6-C7-C8
25	C	508	CLA	CBD-CGD-O2D-CED
25	b	515	CLA	C16-C17-C18-C20
28	A	407	SQD	O49-C7-C8-C9
25	c	510	CLA	C4-C3-C5-C6
25	B	508	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	510	CLA	C2-C3-C5-C6
25	N	303	CLA	C8-C10-C11-C12
25	b	504	CLA	C5-C6-C7-C8
36	N	306	CHL	C5-C6-C7-C8
25	B	510	CLA	C2-C1-O2A-CGA
25	b	506	CLA	C2-C1-O2A-CGA
25	B	508	CLA	C2A-CAA-CBA-CGA
25	Y	305	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
25	d	401	CLA	C2A-CAA-CBA-CGA
25	B	508	CLA	O1D-CGD-O2D-CED
25	B	504	CLA	C3A-C2A-CAA-CBA
25	N	305	CLA	C3A-C2A-CAA-CBA
25	G	602	CLA	C8-C10-C11-C12
25	A	403	CLA	O2A-C1-C2-C3
25	Y	315	CLA	C2-C3-C5-C6
25	B	505	CLA	C6-C7-C8-C9
25	B	516	CLA	C11-C10-C8-C9
25	b	502	CLA	C6-C7-C8-C9
25	b	504	CLA	C11-C10-C8-C9
25	b	510	CLA	C6-C7-C8-C9
25	b	511	CLA	C11-C10-C8-C9
25	d	403	CLA	C11-C12-C13-C14
36	N	310	CHL	C11-C12-C13-C14
30	B	520	LHG	C31-C32-C33-C34
25	C	502	CLA	C13-C15-C16-C17
25	Y	304	CLA	C13-C15-C16-C17
25	c	510	CLA	C10-C11-C12-C13
27	B	517	BCR	C20-C21-C22-C37
27	v	101	BCR	C20-C21-C22-C37
30	Y	319	LHG	C4-C5-C6-O8
38	G	617	NEX	C39-C29-C30-C31
38	N	318	NEX	C39-C29-C30-C31
38	S	617	NEX	C39-C29-C30-C31
38	Y	318	NEX	C39-C29-C30-C31
38	r	310	NEX	C39-C29-C30-C31
31	c	515	DGD	C4E-C5E-C6E-O5E
25	B	503	CLA	C2A-CAA-CBA-CGA
36	S	608	CHL	C2A-CAA-CBA-CGA
25	b	512	CLA	C16-C17-C18-C19
25	b	515	CLA	C16-C17-C18-C19
25	d	403	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	515	CLA	C13-C15-C16-C17
29	b	520	LMG	C17-C18-C19-C20
31	c	516	DGD	CCB-CDB-CEB-CFB
36	N	308	CHL	C4-C3-C5-C6
25	N	305	CLA	C1A-C2A-CAA-CBA
25	r	307	CLA	C1A-C2A-CAA-CBA
36	N	308	CHL	C1A-C2A-CAA-CBA
25	C	502	CLA	C11-C12-C13-C15
25	N	303	CLA	C6-C7-C8-C10
25	b	501	CLA	C6-C7-C8-C10
25	b	511	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C12-C13-C15
36	Y	303	CHL	C11-C12-C13-C15
25	Y	313	CLA	C15-C16-C17-C18
25	d	403	CLA	C10-C11-C12-C13
25	B	505	CLA	C13-C15-C16-C17
25	N	314	CLA	C10-C11-C12-C13
25	S	611	CLA	O2A-C1-C2-C3
26	D	402	PHO	C15-C16-C17-C18
30	D	408	LHG	C14-C15-C16-C17
25	B	511	CLA	C2-C3-C5-C6
36	G	619	CHL	C2-C3-C5-C6
36	N	310	CHL	C10-C11-C12-C13
27	B	517	BCR	C20-C21-C22-C23
27	v	101	BCR	C20-C21-C22-C23
38	G	617	NEX	C28-C29-C30-C31
38	N	318	NEX	C28-C29-C30-C31
38	S	617	NEX	C28-C29-C30-C31
38	Y	318	NEX	C28-C29-C30-C31
38	r	310	NEX	C28-C29-C30-C31
30	Y	319	LHG	O7-C5-C6-O8
36	N	307	CHL	CAA-CBA-CGA-O2A
25	Y	313	CLA	C10-C11-C12-C13
25	C	505	CLA	C13-C15-C16-C17
25	C	508	CLA	O1D-CGD-O2D-CED
30	G	618	LHG	C16-C17-C18-C19
25	A	403	CLA	C2-C1-O2A-CGA
25	C	505	CLA	C2-C1-O2A-CGA
25	N	314	CLA	C2-C1-O2A-CGA
25	c	507	CLA	C2-C1-O2A-CGA
36	Y	310	CHL	C2-C1-O2A-CGA
25	d	401	CLA	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	Y	304	CLA	C10-C11-C12-C13
36	N	307	CHL	CAA-CBA-CGA-O1A
25	C	513	CLA	C16-C17-C18-C20
25	C	508	CLA	C11-C10-C8-C9
25	b	501	CLA	C14-C13-C15-C16
30	N	319	LHG	C11-C10-C9-C8
29	c	518	LMG	C11-C12-C13-C14
27	b	517	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C30
25	a	402	CLA	C15-C16-C17-C18
25	B	511	CLA	C4-C3-C5-C6
25	a	405	CLA	C4-C3-C5-C6
25	b	507	CLA	C4-C3-C5-C6
25	c	502	CLA	C4-C3-C5-C6
25	G	604	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C10-C11-C12-C13
25	Y	305	CLA	C2-C3-C5-C6
36	N	310	CHL	C2-C3-C5-C6
36	r	306	CHL	CAA-CBA-CGA-O2A
30	d	408	LHG	C23-C24-C25-C26
25	C	502	CLA	C8-C10-C11-C12
25	N	311	CLA	C8-C10-C11-C12
32	C	523	LMU	C1-C2-C3-C4
30	G	618	LHG	O6-C4-C5-O7
25	N	313	CLA	CAA-CBA-CGA-O2A
25	b	509	CLA	C2A-CAA-CBA-CGA
25	b	501	CLA	C16-C17-C18-C20
30	G	618	LHG	O6-C4-C5-C6
25	Y	314	CLA	O1A-CGA-O2A-C1
25	B	516	CLA	C11-C10-C8-C7
25	c	507	CLA	C12-C13-C15-C16
30	b	521	LHG	C25-C26-C27-C28
25	c	506	CLA	CAA-CBA-CGA-O2A
25	C	511	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
29	d	410	LMG	C29-C28-O8-C9
29	c	518	LMG	C12-C13-C14-C15
25	c	501	CLA	C15-C16-C17-C18
25	c	506	CLA	C10-C11-C12-C13
25	d	401	CLA	CAA-CBA-CGA-O2A
36	S	608	CHL	CAA-CBA-CGA-O2A
31	Y	301	DGD	O6D-C5D-C6D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	512	CLA	C2A-CAA-CBA-CGA
25	C	509	CLA	C13-C15-C16-C17
25	N	303	CLA	CBA-CGA-O2A-C1
29	D	410	LMG	O7-C10-C11-C12
25	G	611	CLA	CAA-CBA-CGA-O2A
25	b	503	CLA	C2-C3-C5-C6
30	D	408	LHG	C33-C34-C35-C36
31	C	519	DGD	C7A-C8A-C9A-CAA
25	a	402	CLA	C16-C17-C18-C20
25	Y	314	CLA	CBA-CGA-O2A-C1
25	b	509	CLA	CAA-CBA-CGA-O2A
25	B	512	CLA	C11-C10-C8-C9
25	C	506	CLA	C11-C10-C8-C9
25	G	602	CLA	C6-C7-C8-C9
25	G	610	CLA	C11-C10-C8-C9
25	N	303	CLA	C6-C7-C8-C9
25	N	314	CLA	C14-C13-C15-C16
25	b	501	CLA	C6-C7-C8-C9
25	b	505	CLA	C6-C7-C8-C9
25	c	502	CLA	C11-C10-C8-C9
25	c	506	CLA	C14-C13-C15-C16
25	r	301	CLA	C6-C7-C8-C9
26	D	402	PHO	C6-C7-C8-C9
36	G	619	CHL	C11-C12-C13-C14
25	c	506	CLA	C3-C5-C6-C7
25	N	313	CLA	CAA-CBA-CGA-O1A
25	S	612	CLA	CAA-CBA-CGA-O2A
30	Y	319	LHG	C23-C24-C25-C26
25	r	307	CLA	C3A-C2A-CAA-CBA
36	N	308	CHL	C3A-C2A-CAA-CBA
31	Y	301	DGD	C2A-C3A-C4A-C5A
25	N	303	CLA	O1A-CGA-O2A-C1
31	c	515	DGD	O6D-C5D-C6D-O5D
25	d	403	CLA	CAA-CBA-CGA-O2A
30	a	411	LHG	C25-C26-C27-C28
25	r	307	CLA	CAA-CBA-CGA-O2A
25	B	507	CLA	CAD-CBD-CGD-O2D
25	B	511	CLA	CAD-CBD-CGD-O2D
25	B	512	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
25	G	614	CLA	CAD-CBD-CGD-O2D
25	N	305	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	N	311	CLA	CAD-CBD-CGD-O2D
25	N	313	CLA	CAD-CBD-CGD-O2D
25	N	315	CLA	CAD-CBD-CGD-O2D
25	S	604	CLA	CAD-CBD-CGD-O2D
25	Y	306	CLA	CAD-CBD-CGD-O2D
25	Y	311	CLA	CAD-CBD-CGD-O2D
25	b	502	CLA	CAD-CBD-CGD-O2D
25	b	503	CLA	CAD-CBD-CGD-O2D
25	b	504	CLA	CAD-CBD-CGD-O2D
25	b	512	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
25	b	501	CLA	C16-C17-C18-C19
25	A	402	CLA	C13-C15-C16-C17
30	l	101	LHG	C14-C15-C16-C17
25	B	502	CLA	C2-C1-O2A-CGA
25	b	516	CLA	CAA-CBA-CGA-O2A
36	Y	307	CHL	CAA-CBA-CGA-O2A
25	G	603	CLA	CAA-CBA-CGA-O2A
25	Y	305	CLA	CAA-CBA-CGA-O2A
25	b	511	CLA	CAA-CBA-CGA-O2A
29	C	520	LMG	O7-C10-C11-C12
30	D	409	LHG	O8-C23-C24-C25
25	C	504	CLA	C13-C15-C16-C17
25	c	502	CLA	C2-C3-C5-C6
31	c	517	DGD	O2G-C1B-C2B-C3B
36	N	308	CHL	CAA-CBA-CGA-O2A
30	S	618	LHG	C11-C12-C13-C14
36	N	308	CHL	O1A-CGA-O2A-C1
27	b	518	BCR	C7-C8-C9-C10
26	D	402	PHO	C2C-C3C-CAC-CBC
38	S	617	NEX	O24-C26-C27-C28
38	Y	318	NEX	O24-C26-C27-C28
38	r	310	NEX	O24-C26-C27-C28
36	Y	308	CHL	CAA-CBA-CGA-O2A
32	C	522	LMU	O1'-C1-C2-C3
25	c	503	CLA	O1A-CGA-O2A-C1
25	b	512	CLA	CAA-CBA-CGA-O2A
25	c	508	CLA	CAA-CBA-CGA-O2A
30	D	408	LHG	C12-C13-C14-C15
36	G	607	CHL	O2A-C1-C2-C3
36	N	309	CHL	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	Y	309	CHL	O2A-C1-C2-C3
25	S	612	CLA	CAA-CBA-CGA-O1A
36	Y	307	CHL	CAA-CBA-CGA-O1A
36	Y	308	CHL	CAA-CBA-CGA-O1A
25	b	514	CLA	CBD-CGD-O2D-CED
29	C	520	LMG	C35-C36-C37-C38
25	C	512	CLA	O2A-C1-C2-C3
25	N	304	CLA	O2A-C1-C2-C3
25	c	505	CLA	O2A-C1-C2-C3
25	c	506	CLA	O2A-C1-C2-C3
36	N	306	CHL	O2A-C1-C2-C3
29	d	410	LMG	O10-C28-O8-C9
25	N	311	CLA	C2A-CAA-CBA-CGA
25	b	503	CLA	C2A-CAA-CBA-CGA
25	b	501	CLA	CAA-CBA-CGA-O2A
25	b	502	CLA	CAA-CBA-CGA-O2A
25	c	503	CLA	CAA-CBA-CGA-O2A
25	c	509	CLA	CAA-CBA-CGA-O2A
30	a	410	LHG	O8-C23-C24-C25
25	G	611	CLA	CAA-CBA-CGA-O1A
25	b	516	CLA	CAA-CBA-CGA-O1A
36	r	306	CHL	CAA-CBA-CGA-O1A
29	d	410	LMG	C32-C33-C34-C35
25	Y	304	CLA	O1A-CGA-O2A-C1
25	C	503	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	510	CLA	CHA-CBD-CGD-O1D
25	C	510	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	CHA-CBD-CGD-O2D
25	D	401	CLA	CHA-CBD-CGD-O1D
25	D	401	CLA	CHA-CBD-CGD-O2D
25	G	603	CLA	CHA-CBD-CGD-O1D
25	G	603	CLA	CHA-CBD-CGD-O2D
25	G	613	CLA	CHA-CBD-CGD-O1D
25	G	613	CLA	CHA-CBD-CGD-O2D
25	Y	305	CLA	CHA-CBD-CGD-O1D
25	Y	305	CLA	CHA-CBD-CGD-O2D
25	b	501	CLA	CHA-CBD-CGD-O2D
25	b	505	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	507	CLA	CHA-CBD-CGD-O1D
25	c	501	CLA	CHA-CBD-CGD-O2D
25	c	505	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O2D
25	d	401	CLA	CHA-CBD-CGD-O2D
25	r	308	CLA	CHA-CBD-CGD-O2D
25	Y	304	CLA	CBA-CGA-O2A-C1
30	D	409	LHG	O6-C4-C5-C6
25	c	504	CLA	C11-C12-C13-C15
31	C	518	DGD	O1G-C1A-C2A-C3A
31	W	202	DGD	O2G-C1B-C2B-C3B
25	B	502	CLA	C3-C5-C6-C7
30	B	520	LHG	C9-C10-C11-C12
25	a	402	CLA	CAA-CBA-CGA-O2A
25	b	507	CLA	CAA-CBA-CGA-O2A
26	d	402	PHO	CHA-CBD-CGD-O1D
36	N	308	CHL	CBA-CGA-O2A-C1
25	B	512	CLA	C11-C10-C8-C7
25	Y	305	CLA	C12-C13-C15-C16
36	G	609	CHL	C6-C7-C8-C10
25	N	305	CLA	C16-C17-C18-C19
25	a	402	CLA	C16-C17-C18-C19
30	Y	319	LHG	C11-C10-C9-C8
25	b	510	CLA	CAA-CBA-CGA-O2A
25	C	502	CLA	C11-C12-C13-C14
25	G	603	CLA	C6-C7-C8-C9
25	Y	305	CLA	C14-C13-C15-C16
25	b	507	CLA	C11-C12-C13-C14
25	c	505	CLA	C11-C12-C13-C14
28	a	407	SQD	C4-C5-C6-S
25	Y	311	CLA	C16-C17-C18-C20
26	D	402	PHO	C16-C17-C18-C19
25	N	312	CLA	C2A-CAA-CBA-CGA
25	b	514	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	CAA-CBA-CGA-O1A
31	c	517	DGD	O1B-C1B-C2B-C3B
25	d	403	CLA	C16-C17-C18-C19
25	C	513	CLA	C13-C15-C16-C17
25	r	307	CLA	CAA-CBA-CGA-O1A
25	b	511	CLA	CAA-CBA-CGA-O1A
25	c	508	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	d	403	CLA	CAA-CBA-CGA-O1A
28	t	102	SQD	O49-C7-C8-C9
36	N	308	CHL	CAA-CBA-CGA-O1A
25	B	510	CLA	C1A-C2A-CAA-CBA
25	c	509	CLA	C1A-C2A-CAA-CBA
36	G	619	CHL	C1A-C2A-CAA-CBA
36	Y	303	CHL	C1A-C2A-CAA-CBA
36	r	306	CHL	C1A-C2A-CAA-CBA
30	B	520	LHG	C7-C8-C9-C10
25	b	509	CLA	CAA-CBA-CGA-O1A
25	d	401	CLA	CAA-CBA-CGA-O1A
36	Y	309	CHL	C2-C1-O2A-CGA
30	D	408	LHG	C13-C14-C15-C16
25	c	503	CLA	CBA-CGA-O2A-C1
25	Y	305	CLA	CAA-CBA-CGA-O1A
25	b	512	CLA	CAA-CBA-CGA-O1A
25	c	503	CLA	CAA-CBA-CGA-O1A
29	D	410	LMG	O9-C10-C11-C12
36	S	608	CHL	CAA-CBA-CGA-O1A
25	G	610	CLA	C2A-CAA-CBA-CGA
30	S	618	LHG	C13-C14-C15-C16
25	Y	312	CLA	C16-C17-C18-C19
25	b	510	CLA	CAA-CBA-CGA-O1A
25	b	511	CLA	C8-C10-C11-C12
25	B	501	CLA	CAA-CBA-CGA-O2A
25	Y	313	CLA	CAA-CBA-CGA-O2A
25	b	501	CLA	CAA-CBA-CGA-O1A
30	D	409	LHG	O10-C23-C24-C25
25	C	502	CLA	O1A-CGA-O2A-C1
30	Y	319	LHG	C30-C31-C32-C33
30	D	408	LHG	C3-O3-P-O5
30	S	618	LHG	C3-O3-P-O5
29	W	201	LMG	C28-C29-C30-C31
25	c	509	CLA	CAA-CBA-CGA-O1A
30	a	410	LHG	O10-C23-C24-C25
25	S	610	CLA	O2A-C1-C2-C3
25	B	506	CLA	C13-C15-C16-C17
32	C	522	LMU	C7-C8-C9-C10
25	G	603	CLA	CAA-CBA-CGA-O1A
25	a	402	CLA	CAA-CBA-CGA-O1A
25	b	502	CLA	CAA-CBA-CGA-O1A
31	C	518	DGD	O1A-C1A-C2A-C3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	505	CLA	CAA-CBA-CGA-O2A
25	C	502	CLA	CBA-CGA-O2A-C1
29	C	520	LMG	O9-C10-C11-C12
30	a	410	LHG	C29-C30-C31-C32
25	B	510	CLA	CAA-CBA-CGA-O2A
29	d	410	LMG	O7-C10-C11-C12
36	N	306	CHL	C10-C11-C12-C13
31	c	517	DGD	C7A-C8A-C9A-CAA
25	C	505	CLA	CAD-CBD-CGD-O1D
25	C	513	CLA	CAD-CBD-CGD-O1D
25	G	604	CLA	CAD-CBD-CGD-O1D
25	b	501	CLA	CAD-CBD-CGD-O1D
25	b	505	CLA	CAD-CBD-CGD-O1D
25	b	507	CLA	CAD-CBD-CGD-O1D
25	c	510	CLA	CAA-CBA-CGA-O2A
36	N	306	CHL	CAA-CBA-CGA-O2A
36	N	308	CHL	C5-C6-C7-C8
25	C	505	CLA	C11-C10-C8-C9
25	Y	312	CLA	C6-C7-C8-C9
25	Y	313	CLA	C14-C13-C15-C16
25	c	505	CLA	C6-C7-C8-C9
25	c	507	CLA	C11-C12-C13-C14
25	d	403	CLA	C11-C10-C8-C9
36	G	609	CHL	C6-C7-C8-C9
28	a	407	SQD	C10-C11-C12-C13
25	C	505	CLA	C16-C17-C18-C19
25	C	501	CLA	CAA-CBA-CGA-O2A
25	Y	304	CLA	CAA-CBA-CGA-O2A
30	Y	319	LHG	C17-C18-C19-C20
25	G	602	CLA	CAA-CBA-CGA-O2A
30	D	408	LHG	O8-C23-C24-C25
25	C	501	CLA	CAA-CBA-CGA-O1A
25	B	503	CLA	C4-C3-C5-C6
36	Y	310	CHL	C4-C3-C5-C6
25	c	503	CLA	C13-C15-C16-C17
25	B	504	CLA	C6-C7-C8-C10
25	B	509	CLA	C2-C3-C5-C6
25	B	510	CLA	C3A-C2A-CAA-CBA
25	C	513	CLA	C11-C10-C8-C7
25	D	405	CLA	C11-C12-C13-C15
25	Y	312	CLA	C11-C10-C8-C7
25	b	507	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	505	CLA	C6-C7-C8-C10
25	c	509	CLA	C11-C12-C13-C15
25	c	511	CLA	C6-C7-C8-C10
25	r	303	CLA	C3A-C2A-CAA-CBA
36	N	306	CHL	C6-C7-C8-C10
36	N	308	CHL	C2-C3-C5-C6
25	Y	313	CLA	CAA-CBA-CGA-O1A
25	b	507	CLA	CAA-CBA-CGA-O1A
30	D	408	LHG	O10-C23-C24-C25
25	b	514	CLA	CAA-CBA-CGA-O2A
31	Y	301	DGD	O1G-C1A-C2A-C3A
36	G	607	CHL	CAA-CBA-CGA-O2A
27	c	514	BCR	C7-C8-C9-C10
25	B	501	CLA	CAA-CBA-CGA-O1A
36	G	607	CHL	CAA-CBA-CGA-O1A
32	C	522	LMU	C2-C1-O1'-C1'
32	c	519	LMU	C2-C1-O1'-C1'
25	N	303	CLA	CAA-CBA-CGA-O2A
25	c	512	CLA	CAA-CBA-CGA-O2A
31	c	517	DGD	O6E-C1E-O5D-C6D
25	c	505	CLA	C10-C11-C12-C13
36	Y	310	CHL	C5-C6-C7-C8
30	Y	319	LHG	C26-C27-C28-C29
25	B	514	CLA	C13-C15-C16-C17
30	l	101	LHG	O8-C23-C24-C25
31	C	517	DGD	O1G-C1A-C2A-C3A
25	b	505	CLA	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
31	W	202	DGD	O1B-C1B-C2B-C3B
36	N	306	CHL	CAA-CBA-CGA-O1A
25	r	301	CLA	C2A-CAA-CBA-CGA
36	S	601	CHL	CAA-CBA-CGA-O1A
29	d	410	LMG	C36-C37-C38-C39
32	S	619	LMU	C3-C4-C5-C6
25	b	512	CLA	C8-C10-C11-C12
25	c	502	CLA	C5-C6-C7-C8
25	B	509	CLA	C4-C3-C5-C6
25	D	404	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

152 monomers are involved in 298 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	514	CLA	2	0
38	N	318	NEX	1	0
30	Y	319	LHG	2	0
39	r	309	XAT	3	0
25	C	511	CLA	2	0
25	B	509	CLA	1	0
25	b	502	CLA	3	0
27	h	101	BCR	5	0
36	N	308	CHL	2	0
30	l	101	LHG	4	0
37	N	316	LUT	1	0
25	B	512	CLA	1	0
25	D	405	CLA	2	0
25	S	604	CLA	1	0
27	H	101	BCR	5	0
27	C	516	BCR	3	0
27	d	405	BCR	2	0
27	v	101	BCR	8	0
25	D	404	CLA	2	0
25	S	602	CLA	2	0
25	a	405	CLA	1	0
36	S	601	CHL	2	0
25	r	307	CLA	2	0
31	Y	301	DGD	1	0
30	S	618	LHG	2	0
36	Y	308	CHL	1	0
28	A	407	SQD	2	0
27	V	101	BCR	4	0
25	B	505	CLA	1	0
27	C	515	BCR	5	0
38	Y	318	NEX	4	0
34	d	406	PL9	1	0
26	D	402	PHO	1	0
29	d	410	LMG	2	0
36	G	608	CHL	3	0
25	c	501	CLA	2	0
25	b	501	CLA	1	0
25	S	610	CLA	1	0
29	H	102	LMG	2	0
36	r	304	CHL	1	0
25	A	402	CLA	1	0
25	C	504	CLA	2	0
36	N	310	CHL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	501	CLA	2	0
37	Y	317	LUT	4	0
27	B	517	BCR	4	0
30	L	101	LHG	1	0
37	S	616	LUT	4	0
25	C	513	CLA	1	0
25	b	507	CLA	1	0
25	c	502	CLA	1	0
36	S	607	CHL	2	0
25	c	506	CLA	4	0
37	G	616	LUT	3	0
25	C	502	CLA	3	0
25	B	508	CLA	1	0
25	c	512	CLA	1	0
30	b	521	LHG	1	0
31	c	517	DGD	1	0
36	N	307	CHL	1	0
39	N	301	XAT	3	0
27	b	517	BCR	1	0
29	W	201	LMG	1	0
25	C	509	CLA	1	0
25	S	605	CLA	3	0
30	d	408	LHG	1	0
39	Y	302	XAT	6	0
25	S	609	CLA	2	0
27	k	101	BCR	4	0
38	r	310	NEX	3	0
25	N	313	CLA	1	0
26	a	404	PHO	2	0
36	G	606	CHL	2	0
27	b	519	BCR	2	0
25	b	512	CLA	2	0
30	N	319	LHG	1	0
25	G	602	CLA	1	0
25	B	503	CLA	1	0
25	C	512	CLA	1	0
25	a	402	CLA	1	0
36	Y	303	CHL	2	0
37	Y	316	LUT	2	0
27	B	518	BCR	2	0
25	G	611	CLA	1	0
25	r	308	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	c	514	BCR	4	0
36	S	608	CHL	2	0
36	S	606	CHL	4	0
39	G	620	XAT	2	0
35	f	101	HEM	4	0
38	G	617	NEX	3	0
25	B	515	CLA	1	0
36	Y	310	CHL	3	0
25	b	506	CLA	4	0
35	F	101	HEM	5	0
25	B	502	CLA	3	0
25	d	403	CLA	2	0
31	c	515	DGD	2	0
25	B	506	CLA	4	0
27	C	514	BCR	4	0
36	N	306	CHL	4	0
25	C	506	CLA	1	0
29	d	409	LMG	2	0
30	a	410	LHG	1	0
36	G	607	CHL	1	0
29	B	519	LMG	2	0
27	A	406	BCR	5	0
36	N	302	CHL	2	0
25	b	505	CLA	2	0
25	d	401	CLA	2	0
25	N	312	CLA	1	0
27	z	101	BCR	3	0
25	b	516	CLA	1	0
27	a	406	BCR	2	0
36	r	306	CHL	2	0
37	G	615	LUT	1	0
38	S	617	NEX	1	0
25	C	508	CLA	1	0
25	c	504	CLA	1	0
30	D	408	LHG	2	0
25	b	504	CLA	2	0
37	N	317	LUT	3	0
30	B	520	LHG	1	0
36	N	309	CHL	2	0
25	N	303	CLA	1	0
25	c	510	CLA	1	0
25	b	510	CLA	2	0

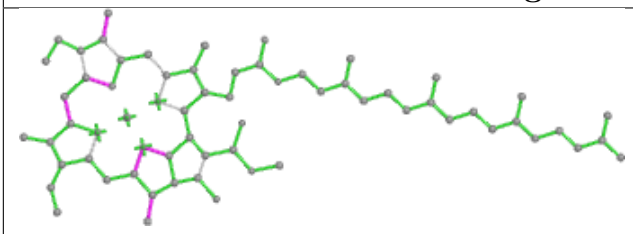
Continued on next page...

Continued from previous page...

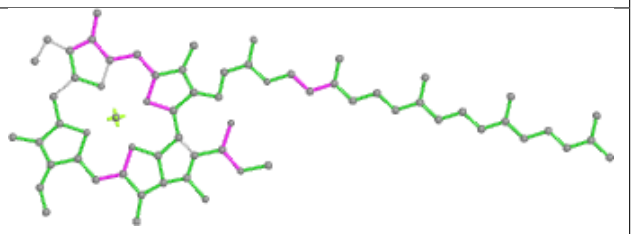
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	409	BCT	2	0
25	B	504	CLA	2	0
25	c	511	CLA	2	0
37	S	615	LUT	4	0
25	b	511	CLA	2	0
36	G	601	CHL	1	0
36	r	305	CHL	1	0
30	d	407	LHG	3	0
25	b	503	CLA	1	0
25	c	509	CLA	1	0
25	B	516	CLA	2	0
26	A	404	PHO	2	0
32	C	522	LMU	3	0
25	B	513	CLA	1	0
36	G	605	CHL	1	0
36	Y	309	CHL	2	0
25	C	501	CLA	1	0
27	b	518	BCR	1	0
36	G	609	CHL	1	0
27	t	101	BCR	3	0
31	C	517	DGD	1	0
25	N	305	CLA	3	0
27	D	406	BCR	3	0
25	c	508	CLA	2	0
26	d	402	PHO	1	0

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.

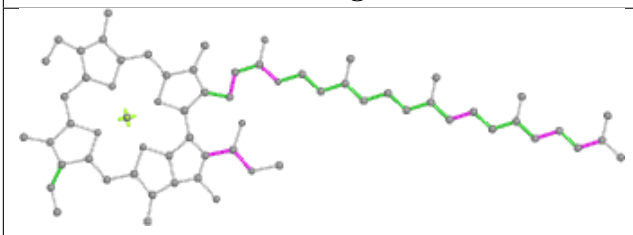
Ligand CLA B 514



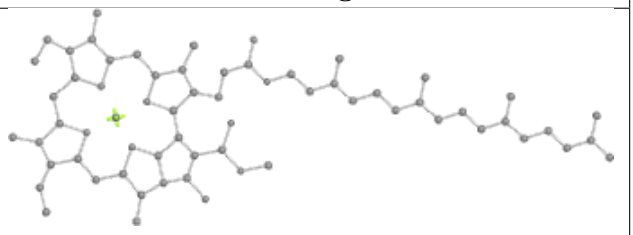
Bond lengths



Bond angles

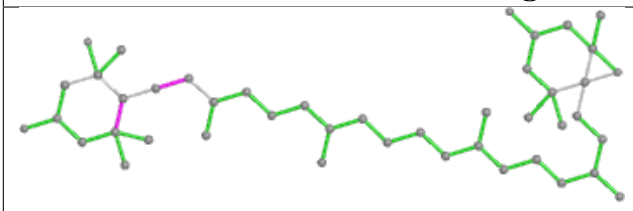


Torsions

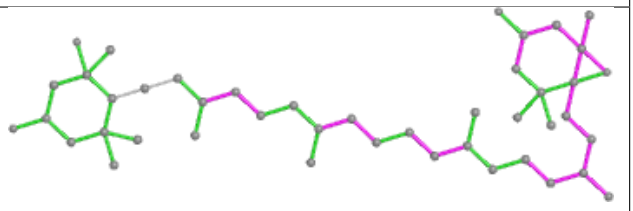


Rings

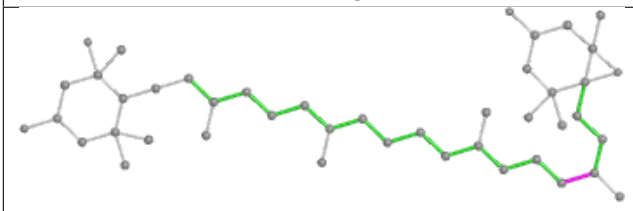
Ligand NEX N 318



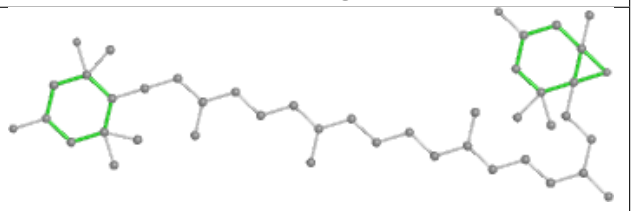
Bond lengths



Bond angles

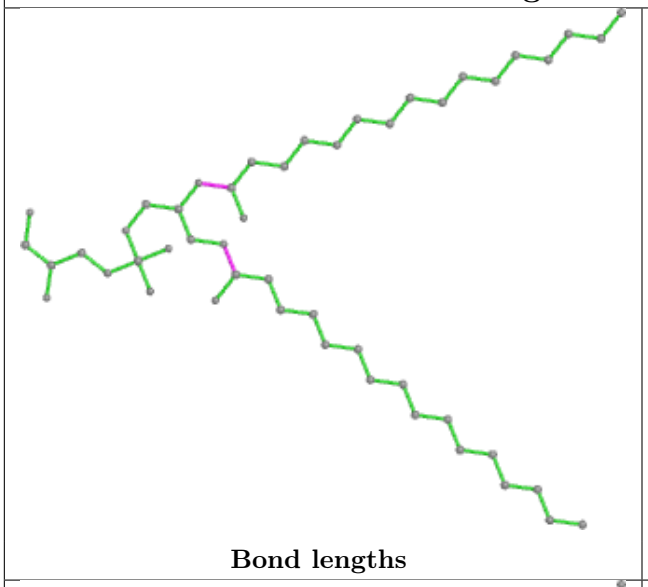


Torsions

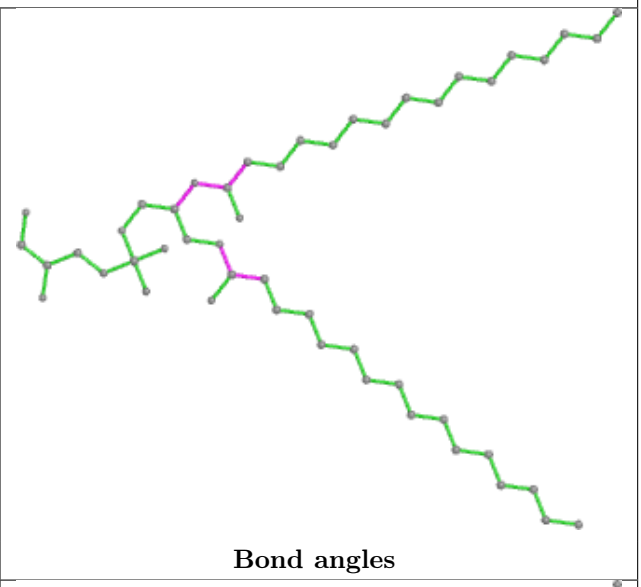


Rings

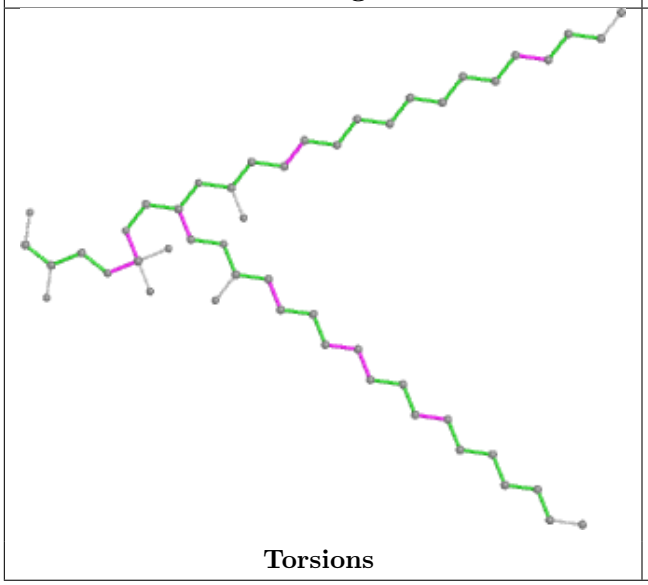
Ligand LHG Y 319



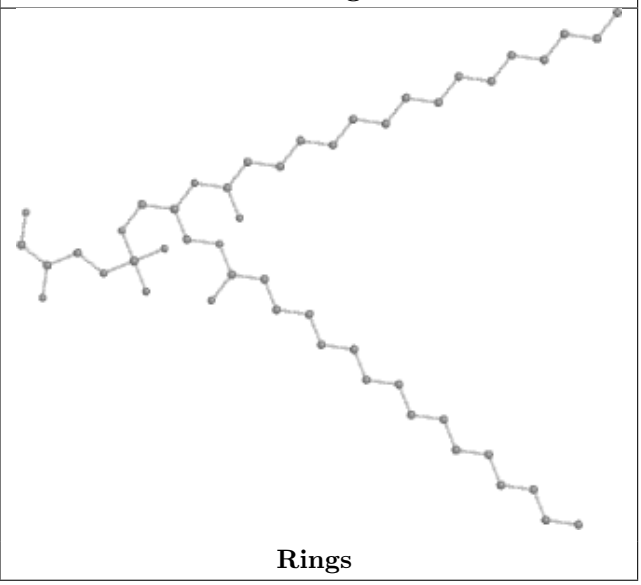
Bond lengths



Bond angles

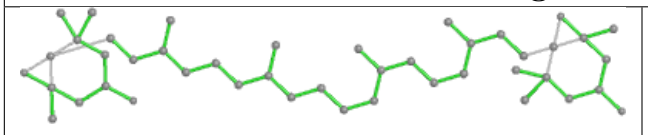


Torsions

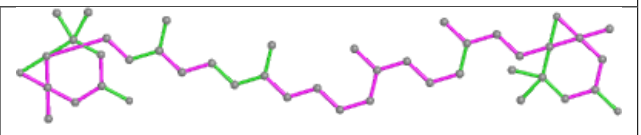


Rings

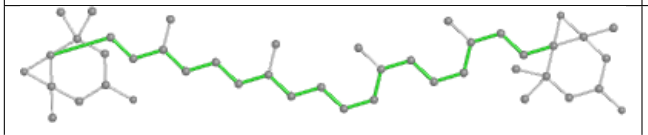
Ligand XAT r 309



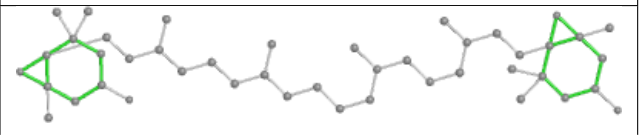
Bond lengths



Bond angles

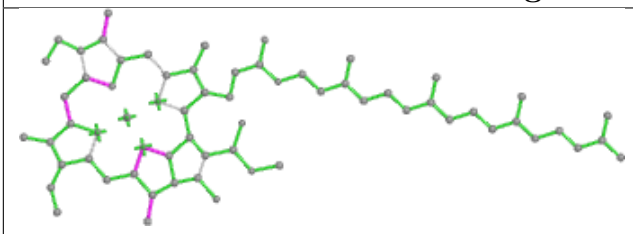


Torsions

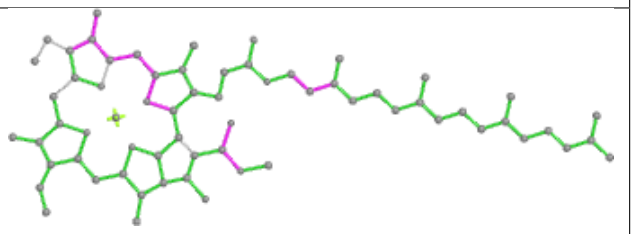


Rings

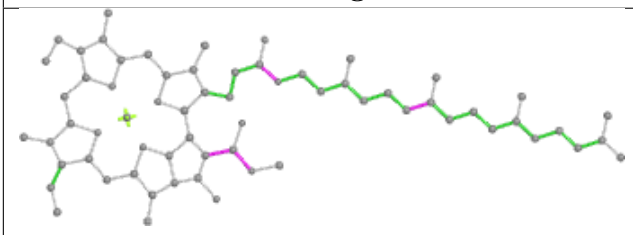
Ligand CLA C 511



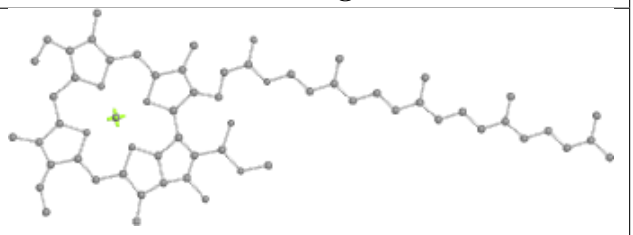
Bond lengths



Bond angles

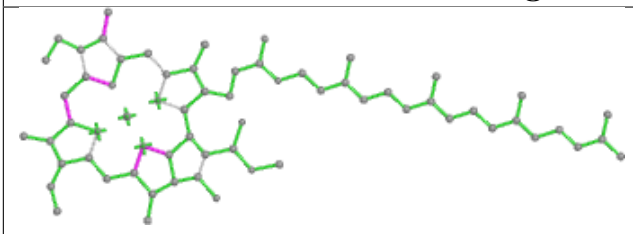


Torsions

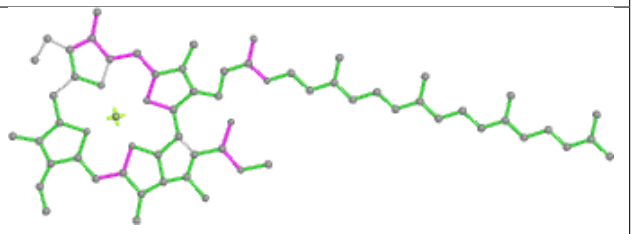


Rings

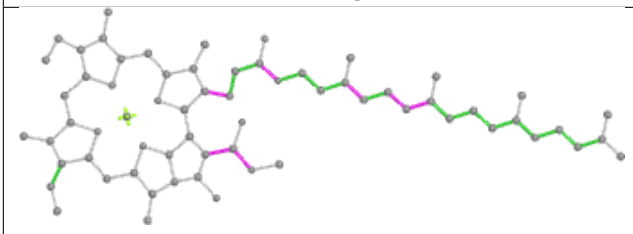
Ligand CLA B 509



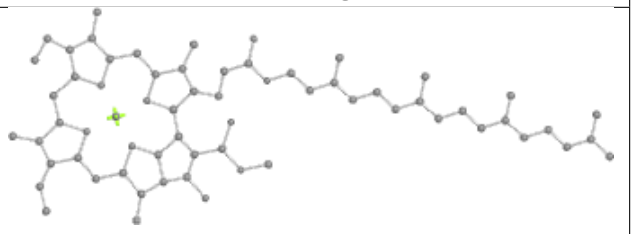
Bond lengths



Bond angles

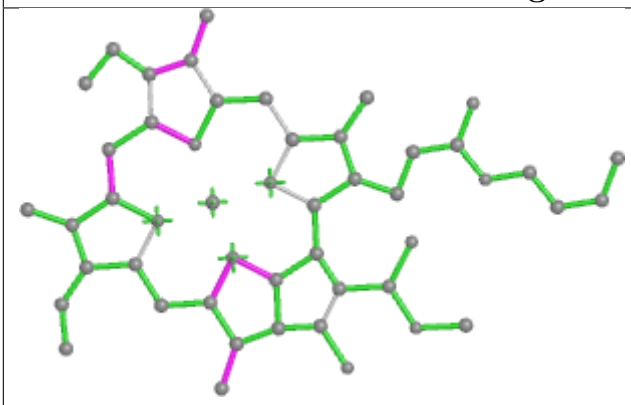


Torsions

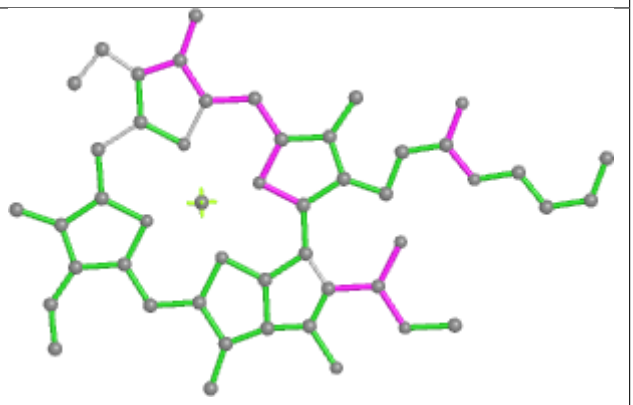


Rings

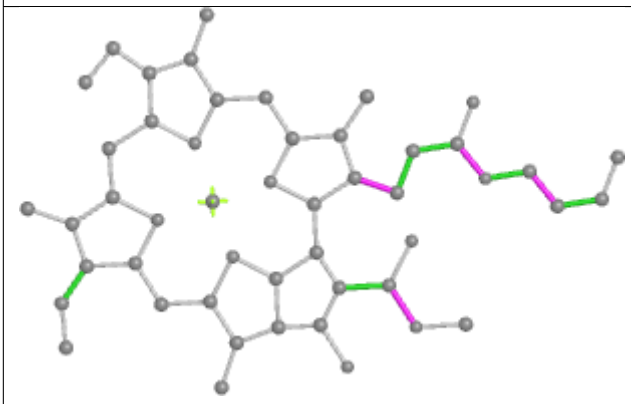
Ligand CLA a 403



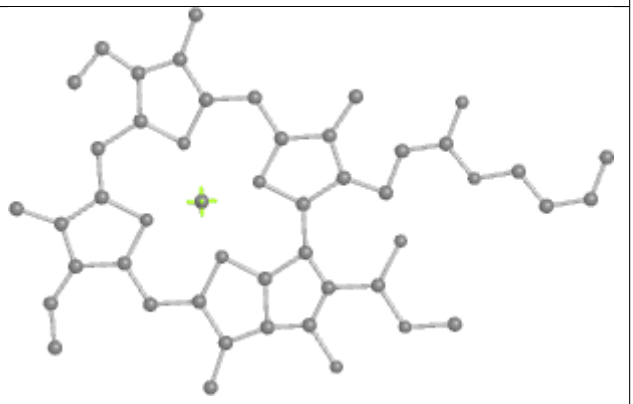
Bond lengths



Bond angles

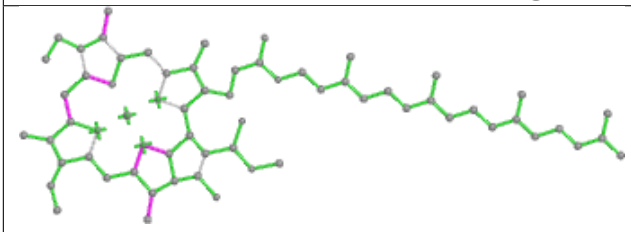


Torsions

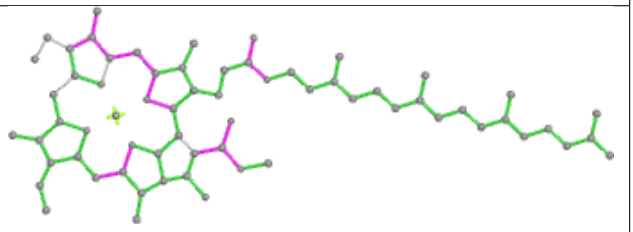


Rings

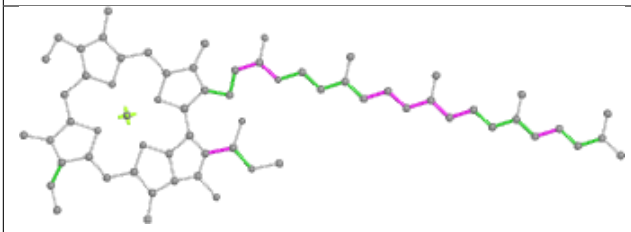
Ligand CLA b 502



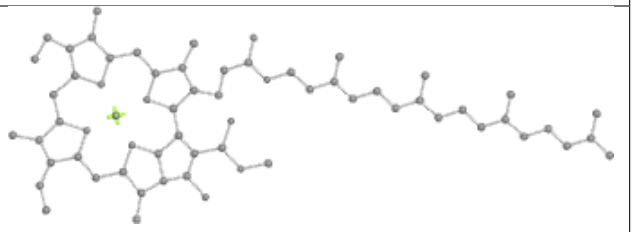
Bond lengths



Bond angles

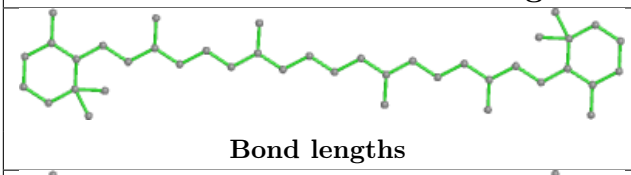


Torsions

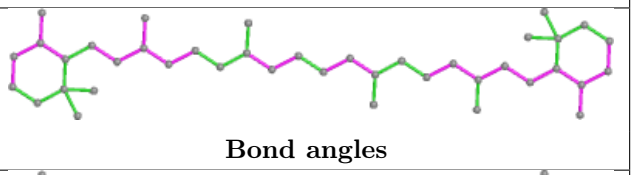


Rings

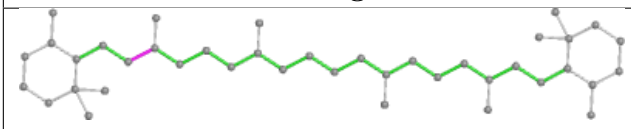
Ligand BCR h 101



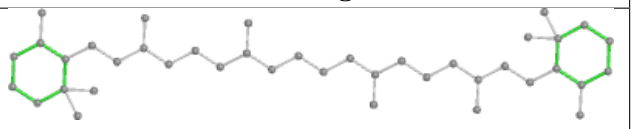
Bond lengths



Bond angles

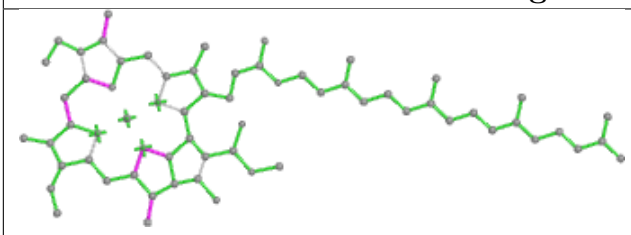


Torsions

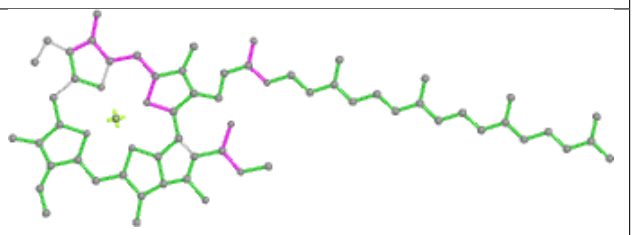


Rings

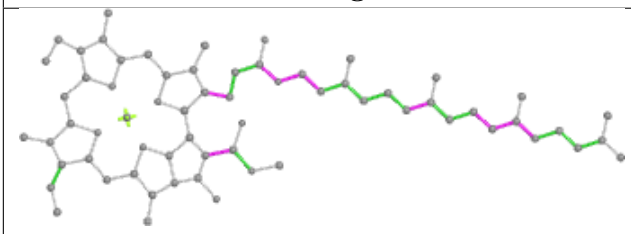
Ligand CLA c 505



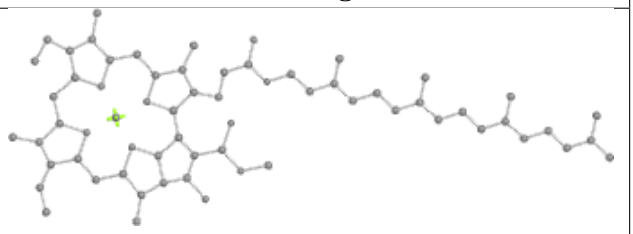
Bond lengths



Bond angles

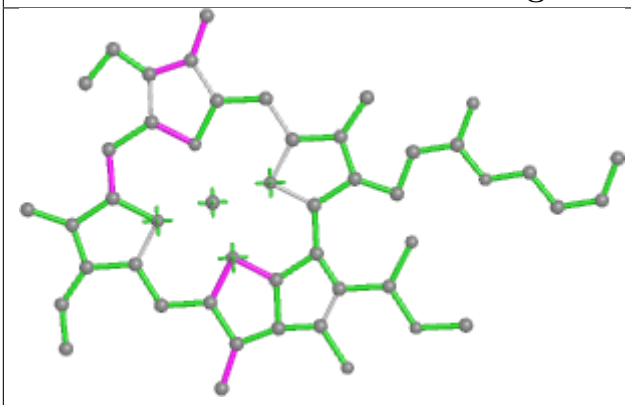


Torsions

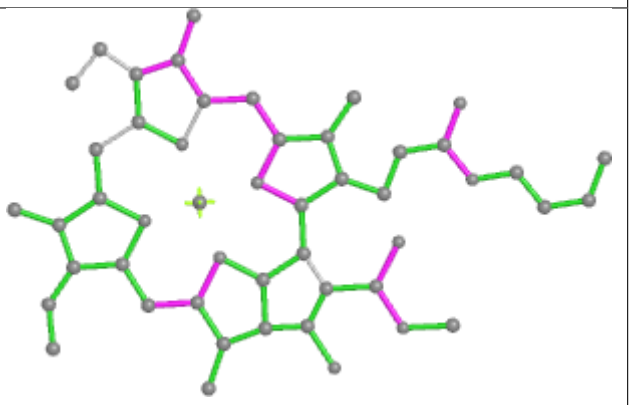


Rings

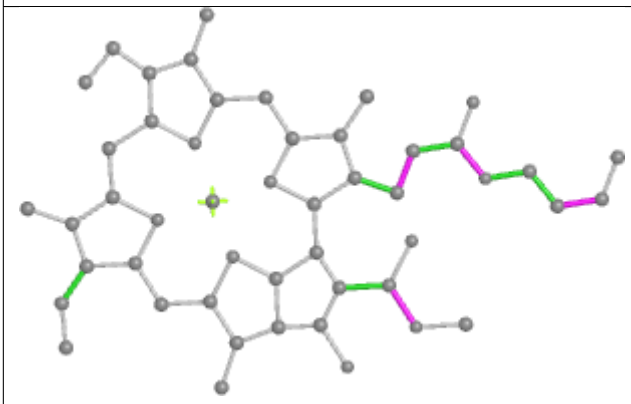
Ligand CLA S 613



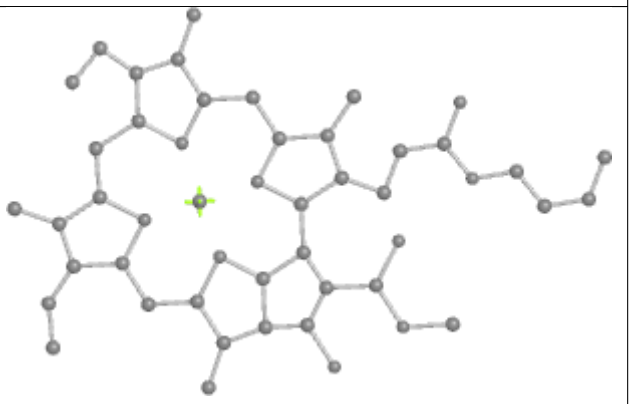
Bond lengths



Bond angles

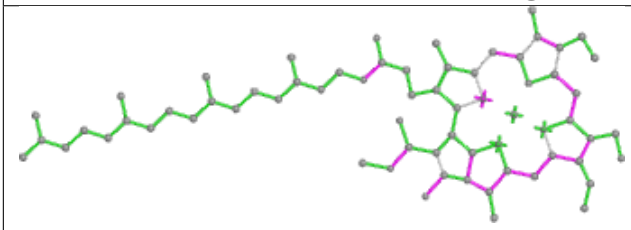


Torsions

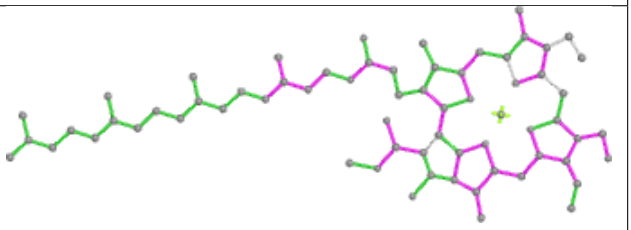


Rings

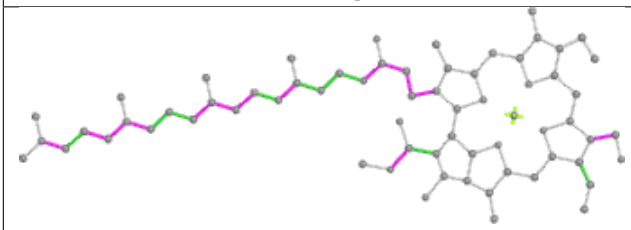
Ligand CHL N 308



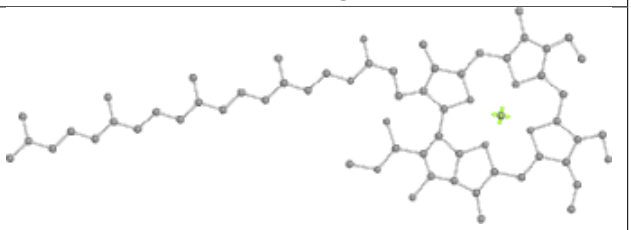
Bond lengths



Bond angles

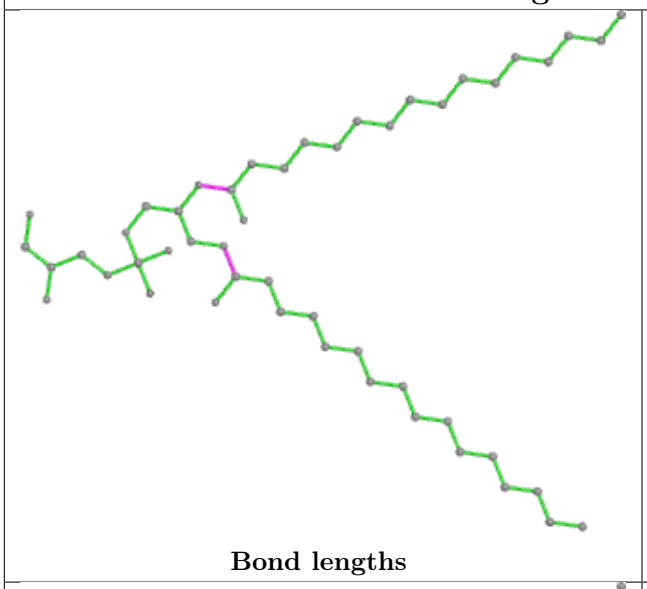


Torsions

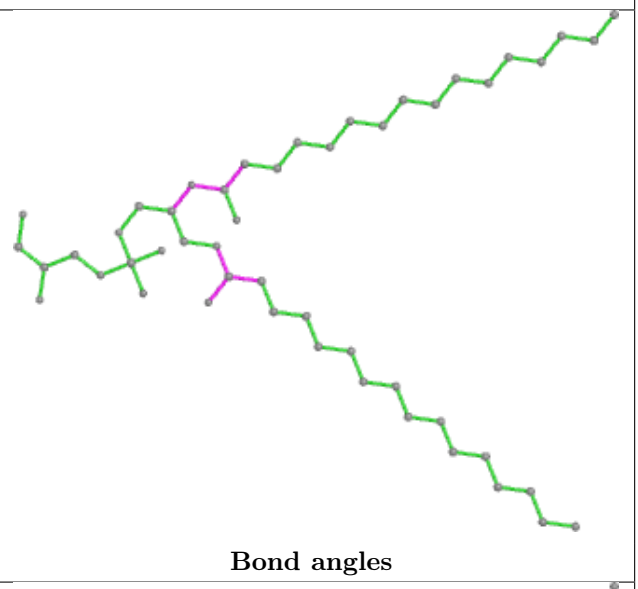


Rings

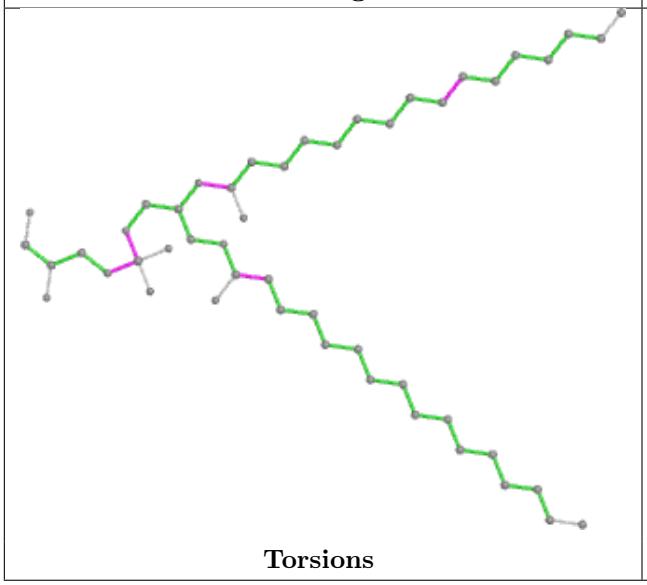
Ligand LHG l 101



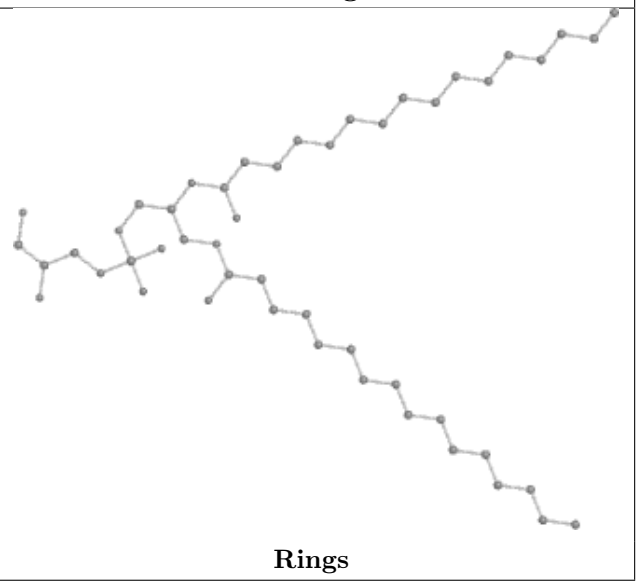
Bond lengths



Bond angles

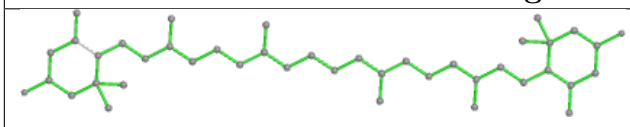


Torsions

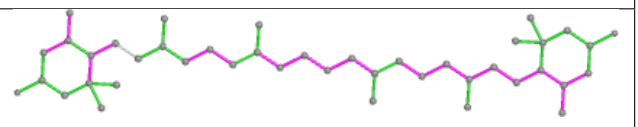


Rings

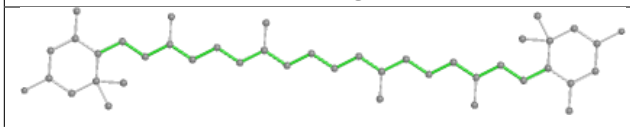
Ligand LUT N 316



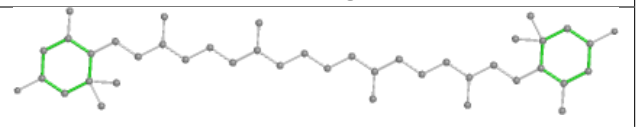
Bond lengths



Bond angles

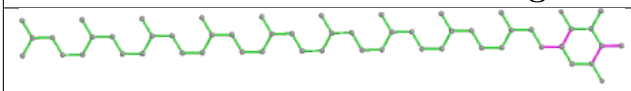


Torsions

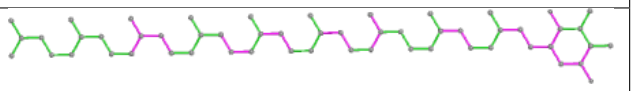


Rings

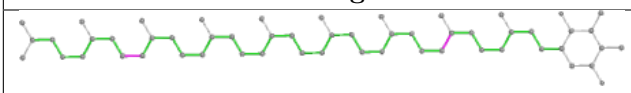
Ligand PL9 D 407



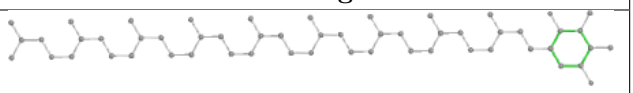
Bond lengths



Bond angles

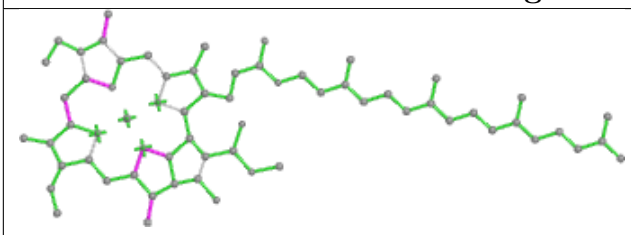


Torsions

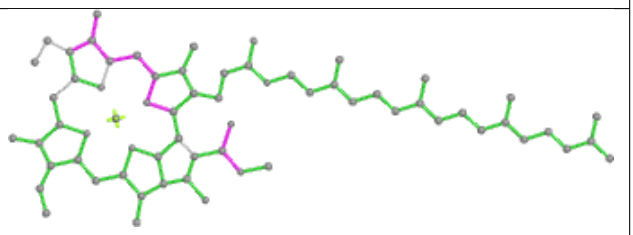


Rings

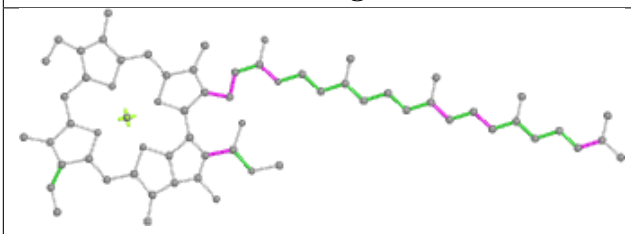
Ligand CLA B 512



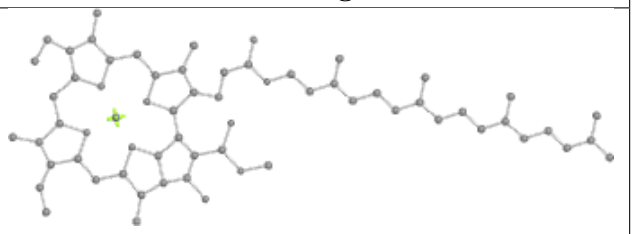
Bond lengths



Bond angles

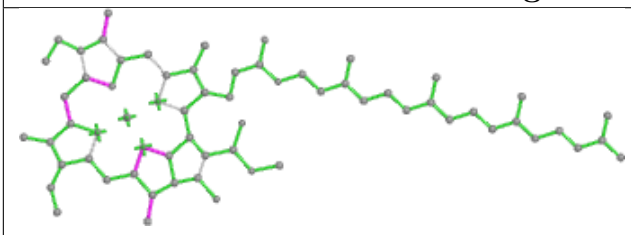


Torsions

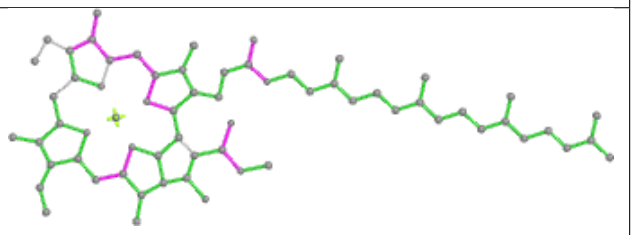


Rings

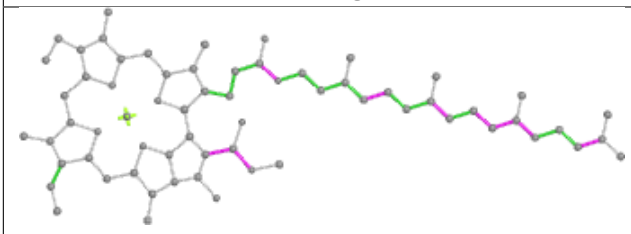
Ligand CLA D 405



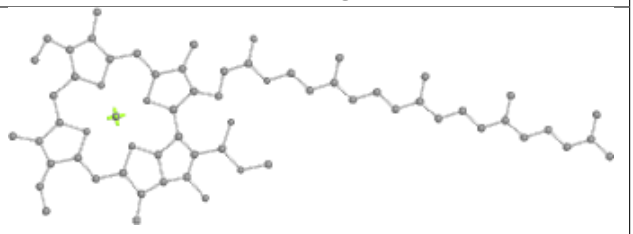
Bond lengths



Bond angles

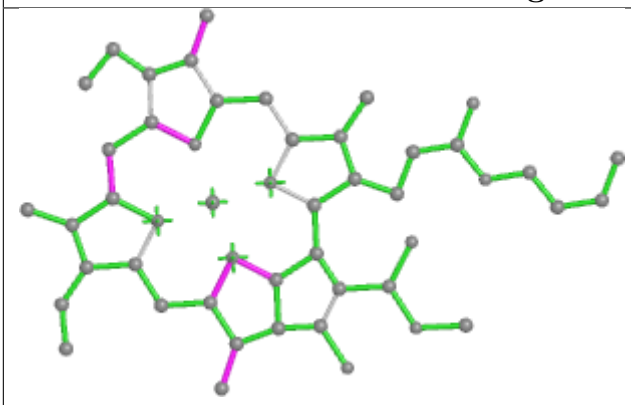


Torsions

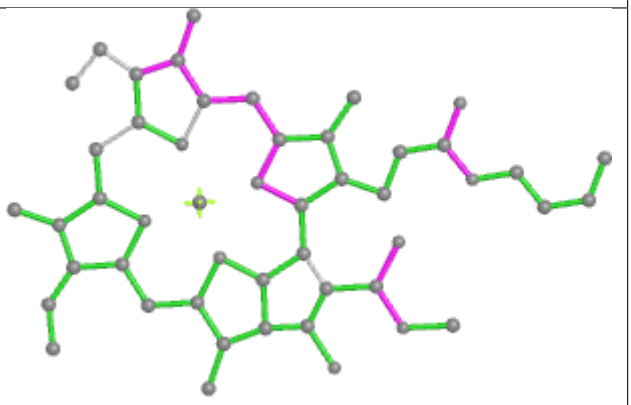


Rings

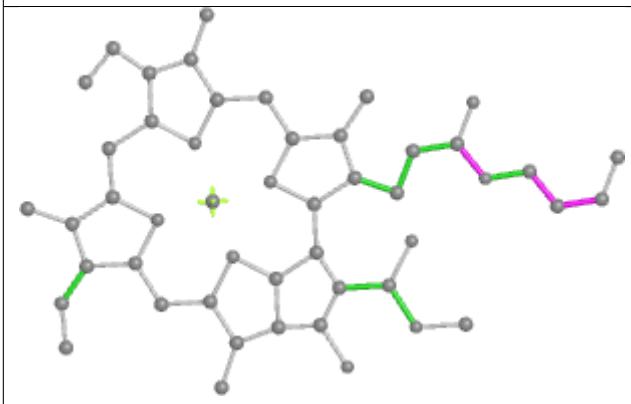
Ligand CLA S 611



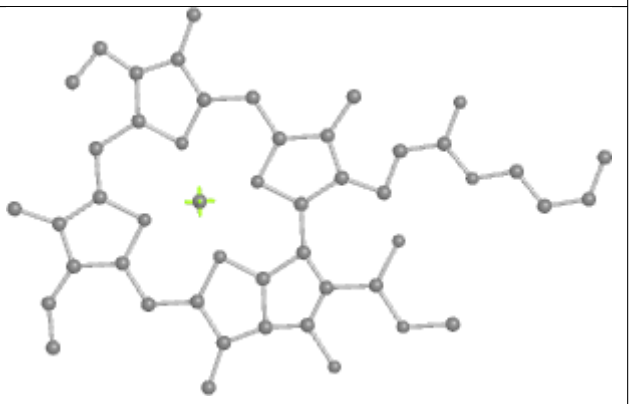
Bond lengths



Bond angles

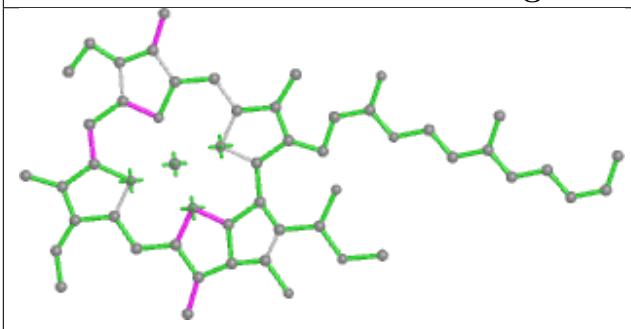


Torsions

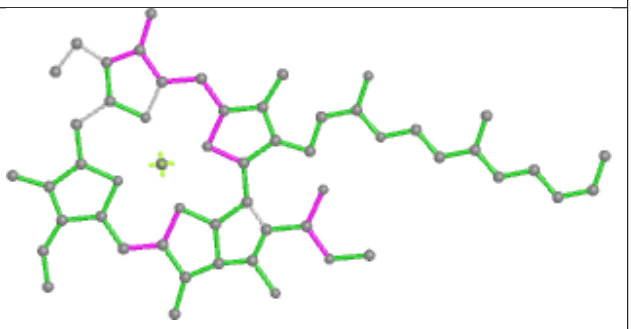


Rings

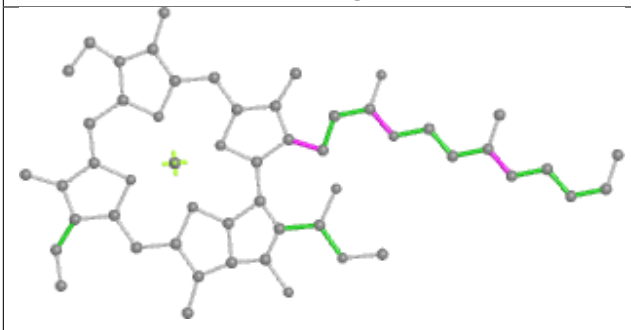
Ligand CLA Y 315



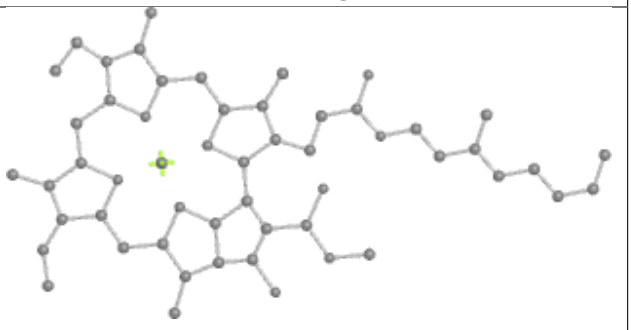
Bond lengths



Bond angles

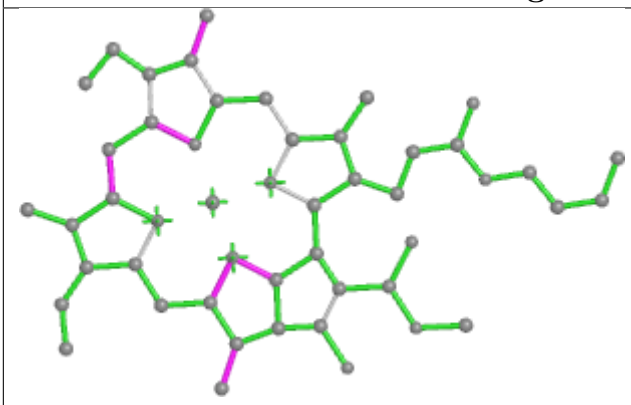


Torsions

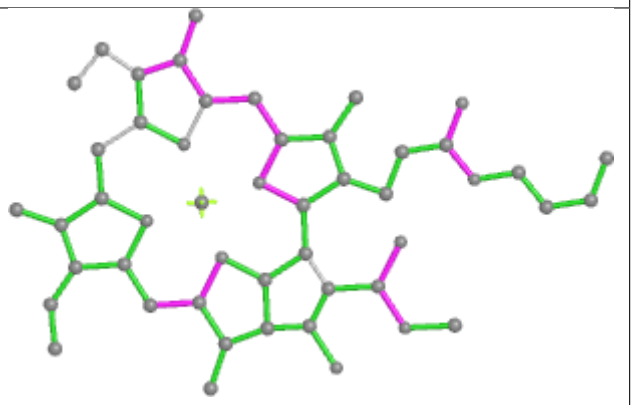


Rings

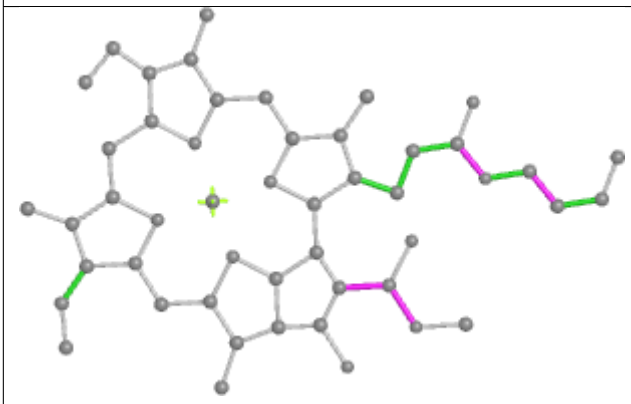
Ligand CLA S 604



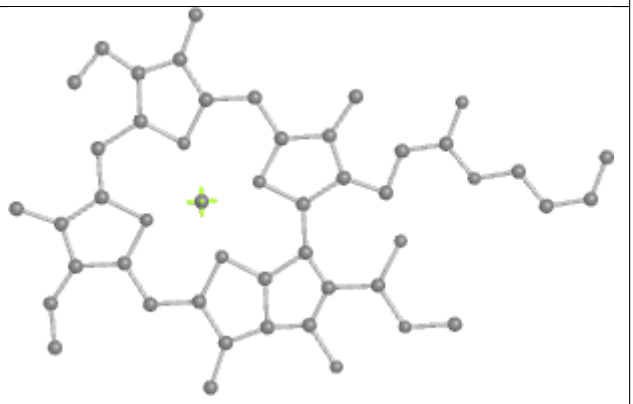
Bond lengths



Bond angles

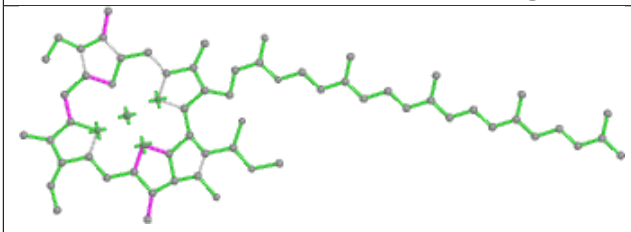


Torsions

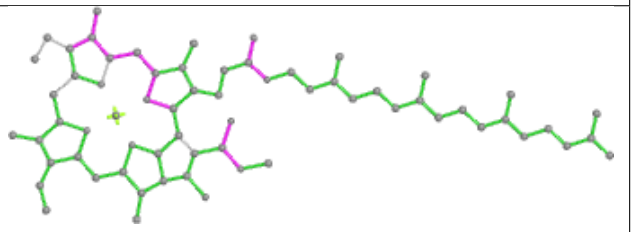


Rings

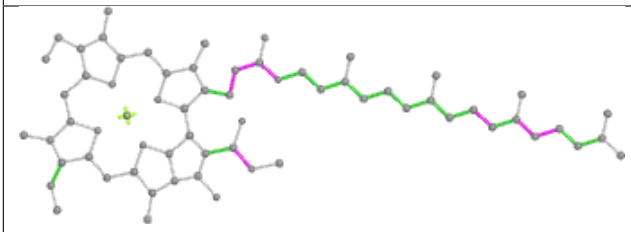
Ligand CLA Y 304



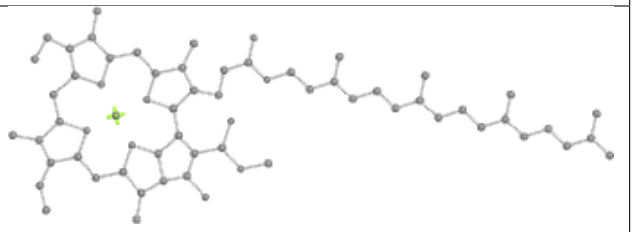
Bond lengths



Bond angles

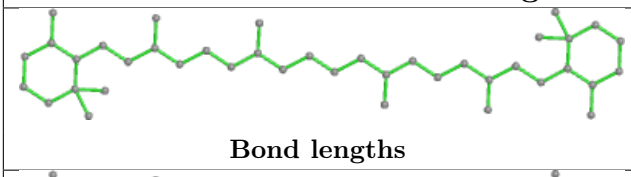


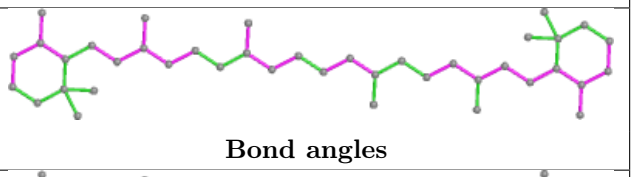
Torsions

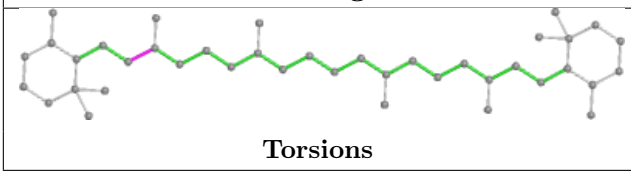


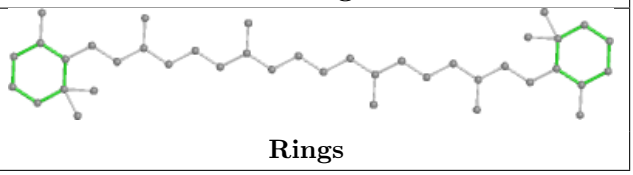
Rings

Ligand BCR H 101

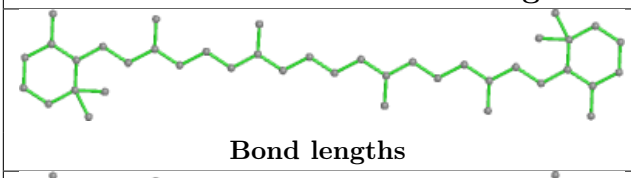

Bond lengths

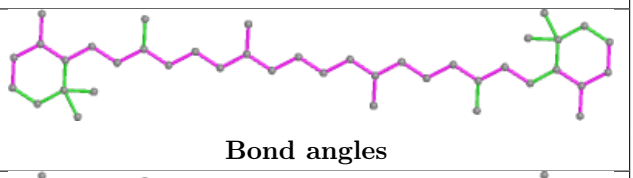

Bond angles

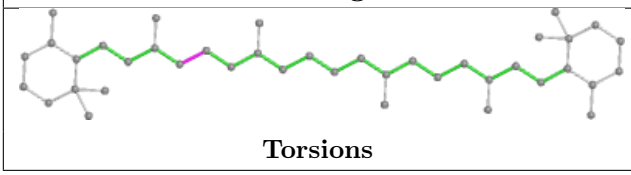

Torsions

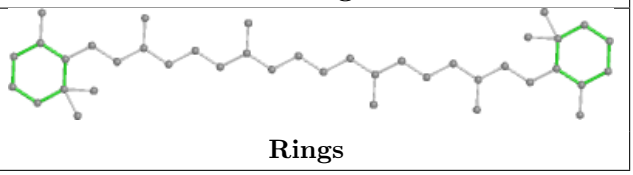

Rings

Ligand BCR C 516

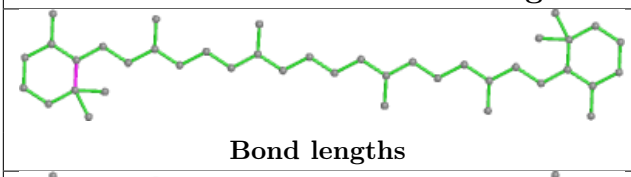

Bond lengths

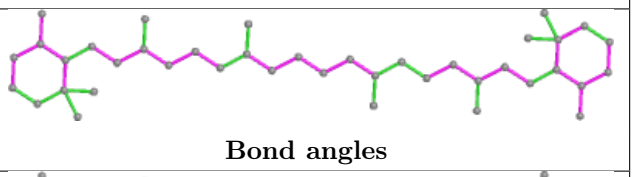

Bond angles

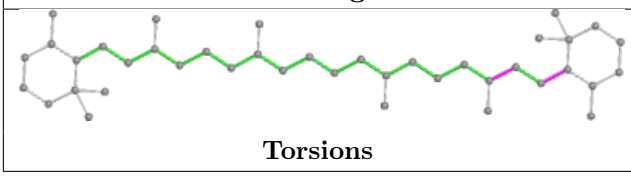

Torsions

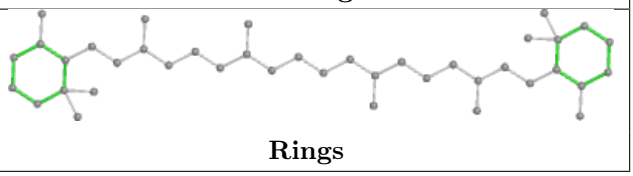

Rings

Ligand BCR d 405

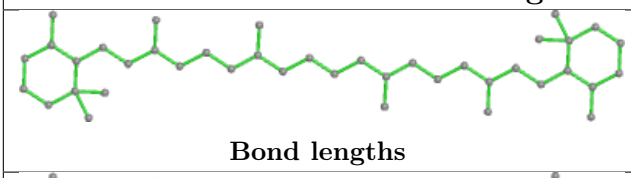

Bond lengths

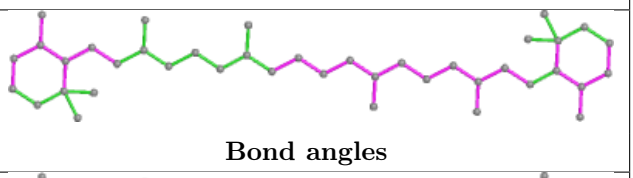

Bond angles

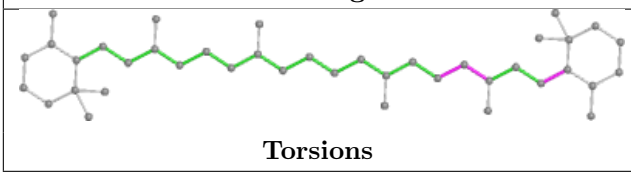

Torsions

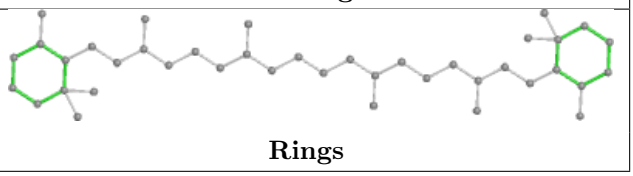

Rings

Ligand BCR v 101

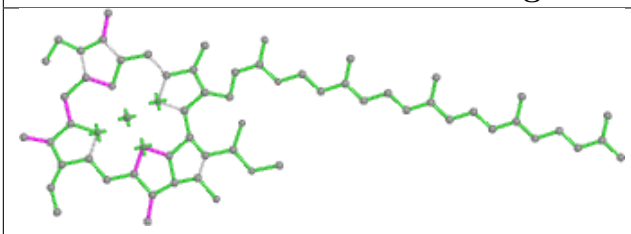

Bond lengths


Bond angles

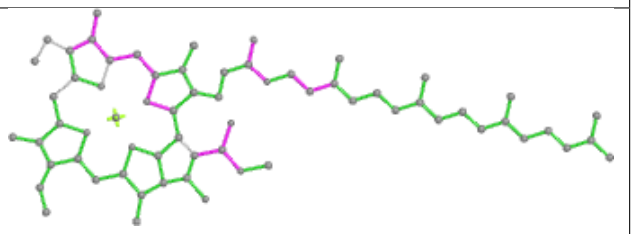

Torsions


Rings

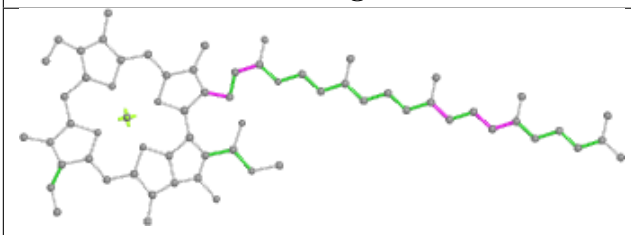
Ligand CLA D 404



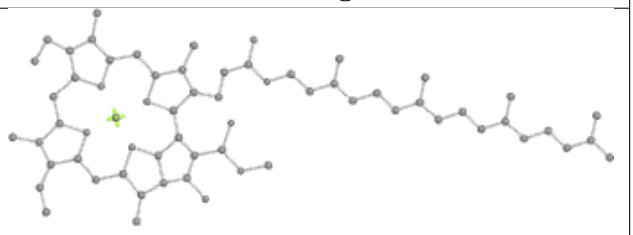
Bond lengths



Bond angles

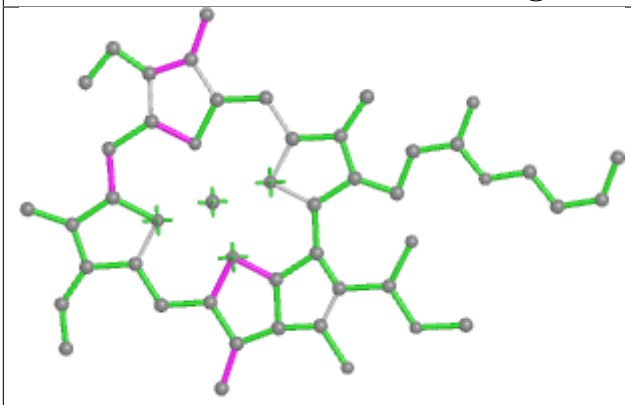


Torsions

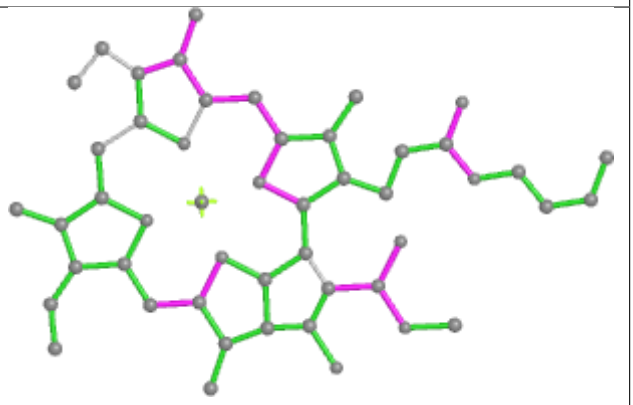


Rings

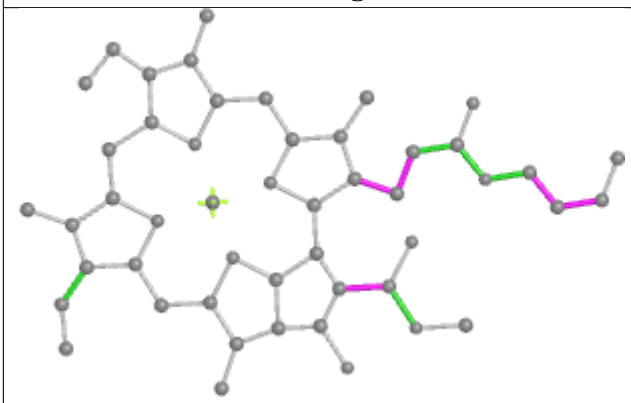
Ligand CLA S 602



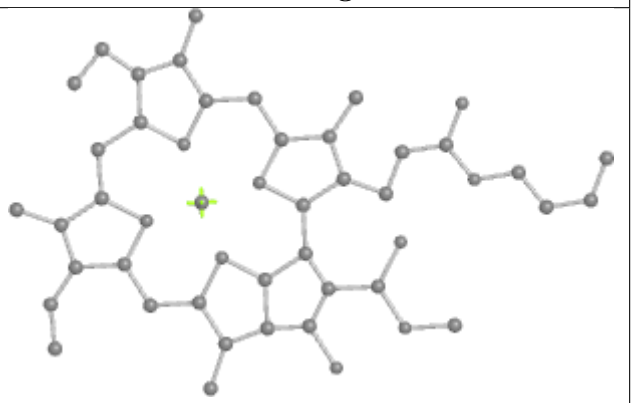
Bond lengths



Bond angles

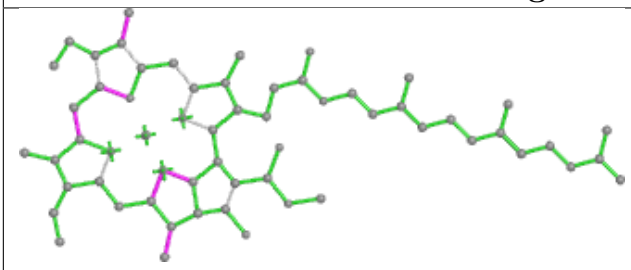


Torsions

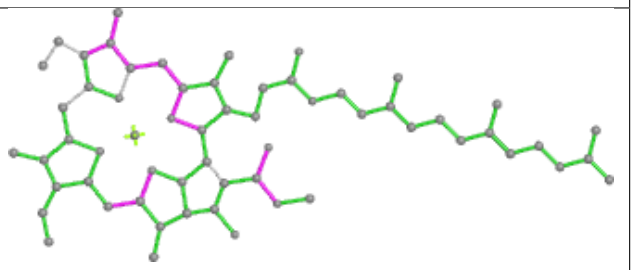


Rings

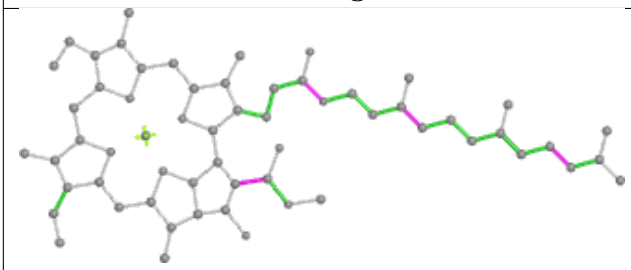
Ligand CLA a 405



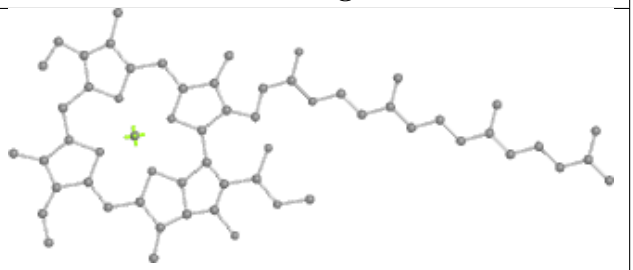
Bond lengths



Bond angles

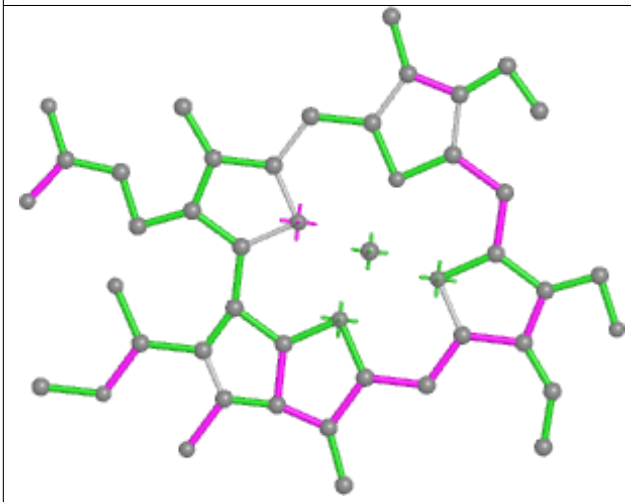


Torsions

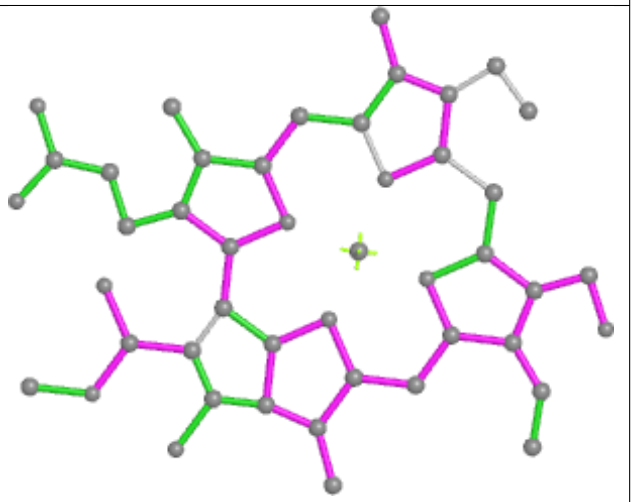


Rings

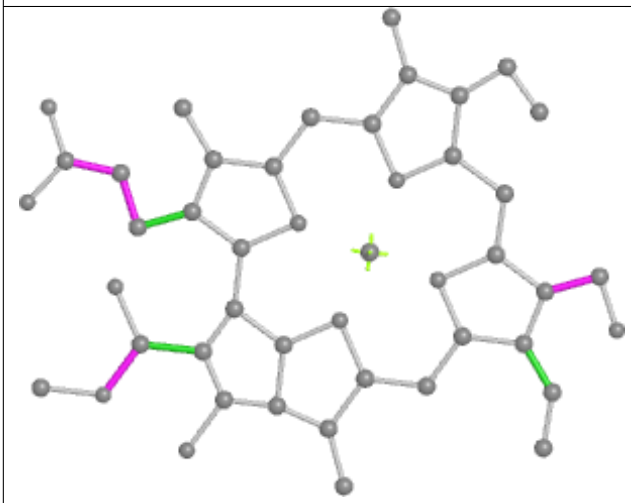
Ligand CHL S 601



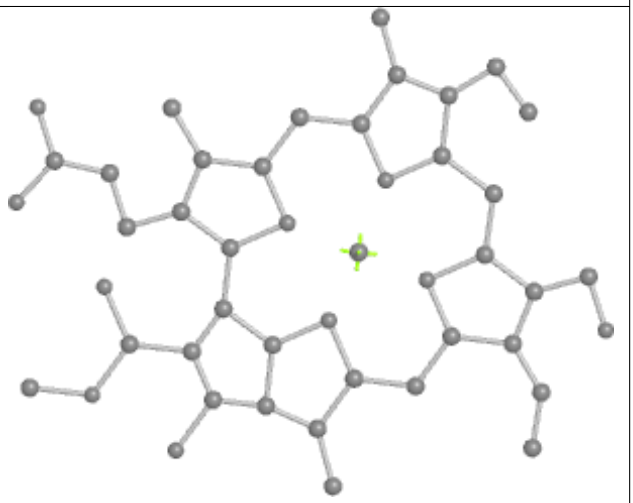
Bond lengths



Bond angles

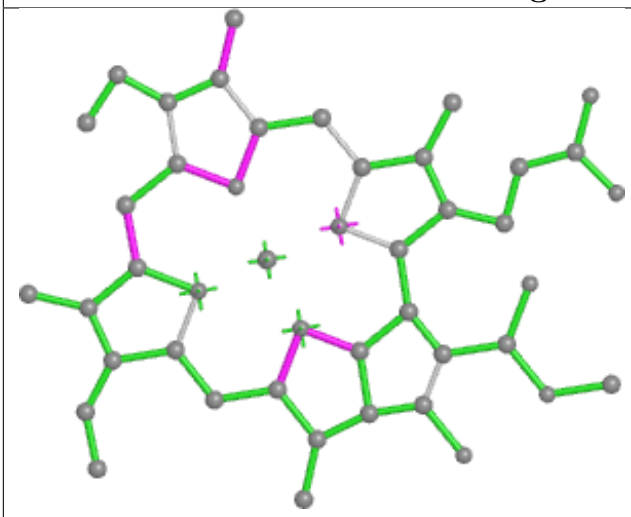


Torsions

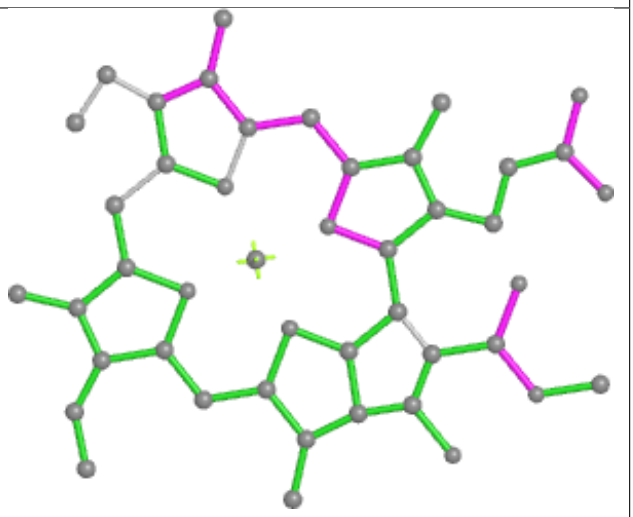


Rings

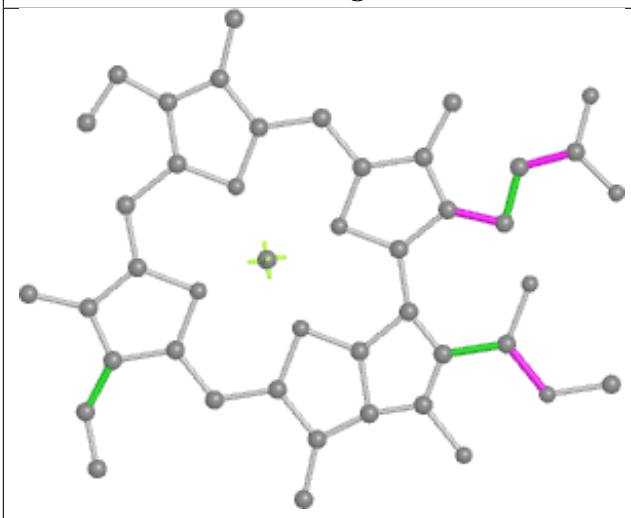
Ligand CLA r 307



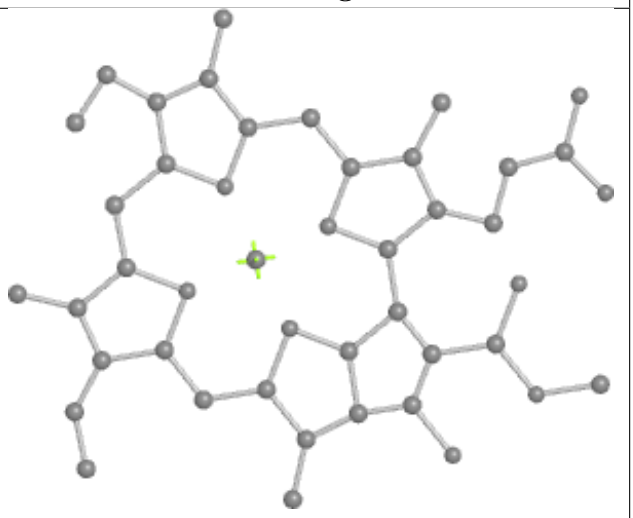
Bond lengths



Bond angles

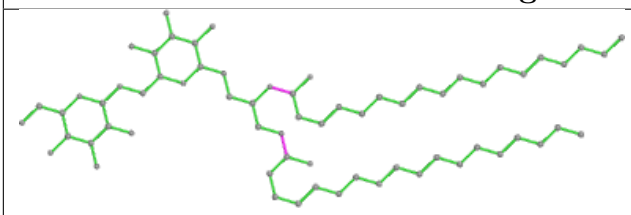


Torsions

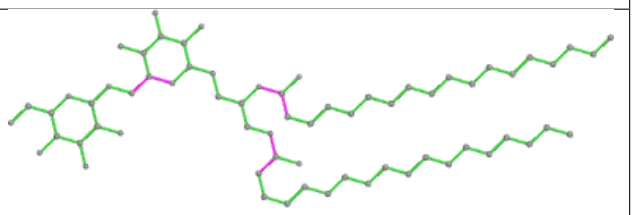


Rings

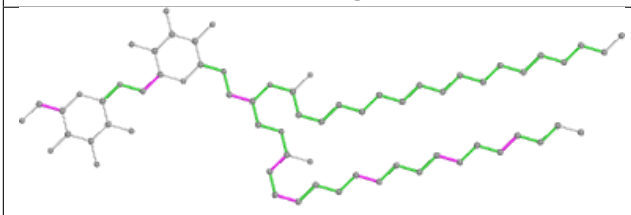
Ligand DGD Y 301



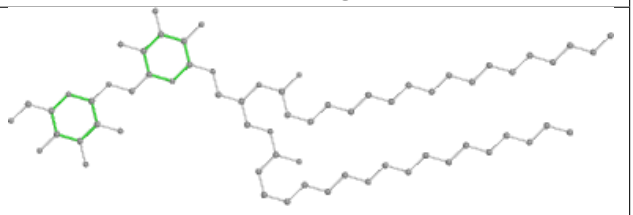
Bond lengths



Bond angles

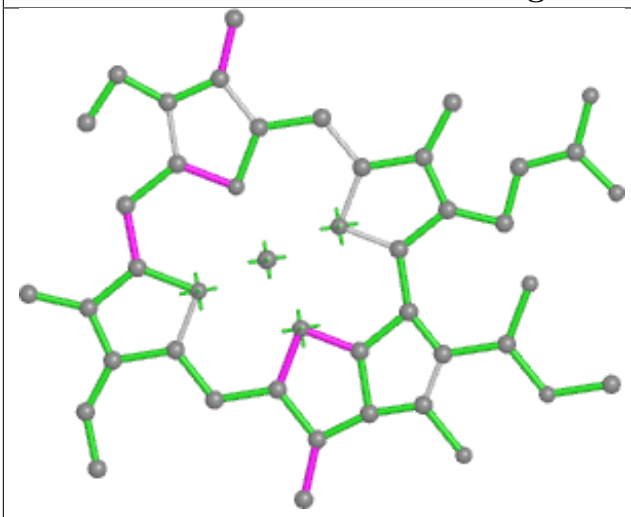


Torsions

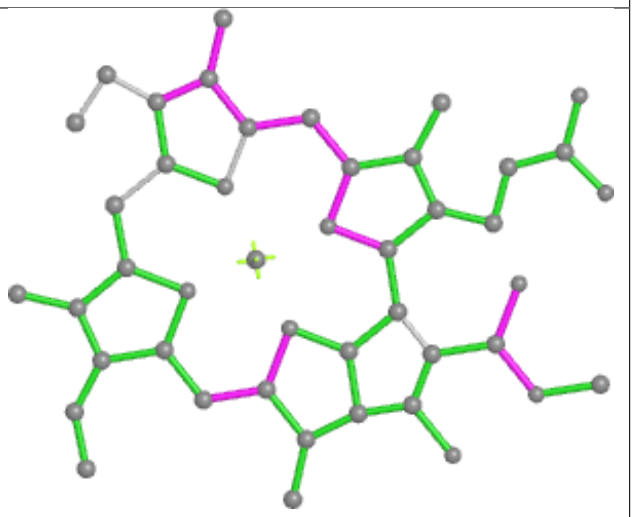


Rings

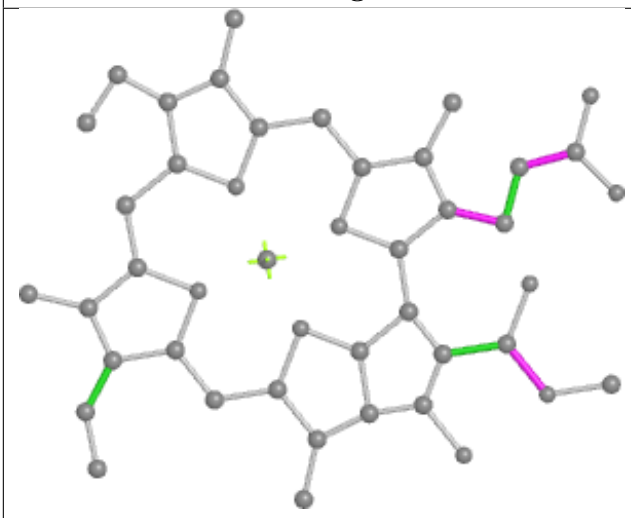
Ligand CLA b 514



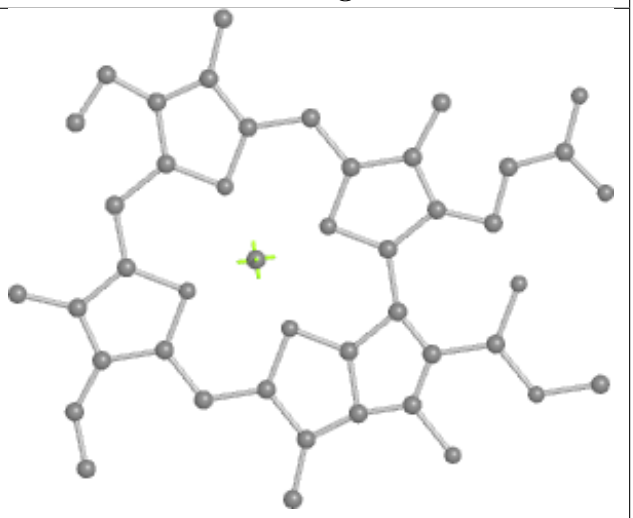
Bond lengths



Bond angles

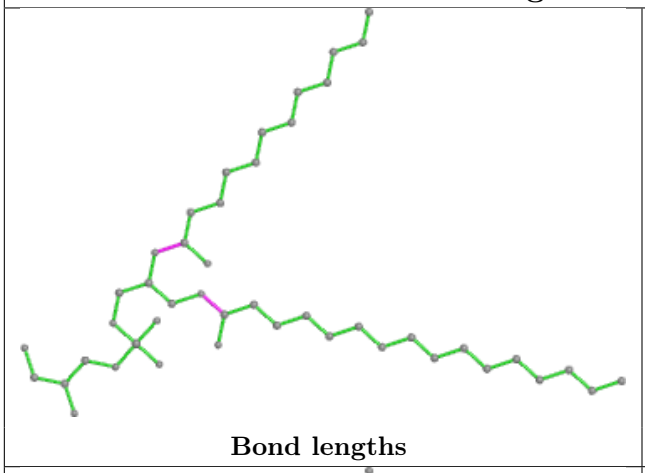


Torsions

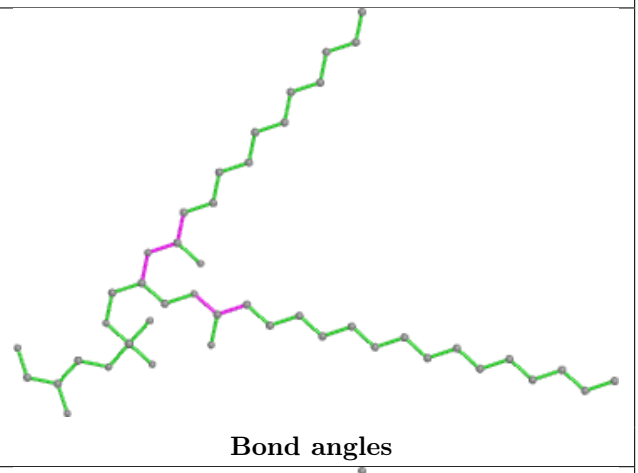


Rings

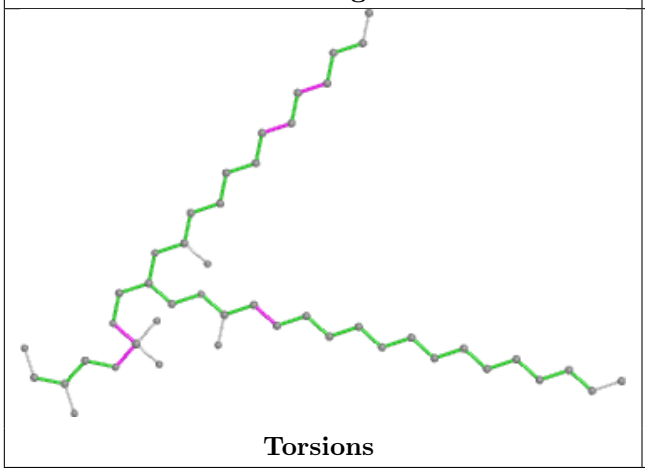
Ligand LHG S 618



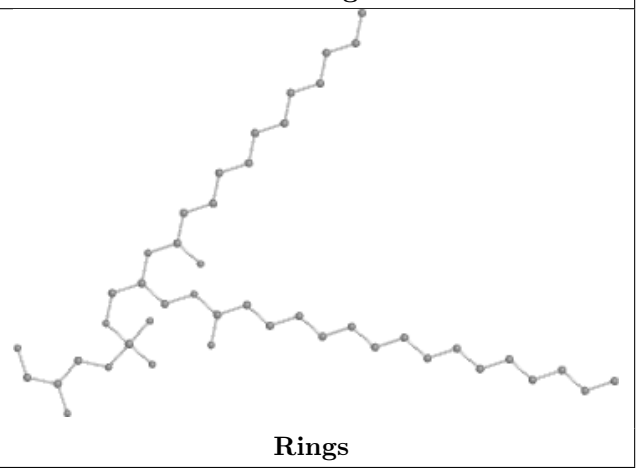
Bond lengths



Bond angles

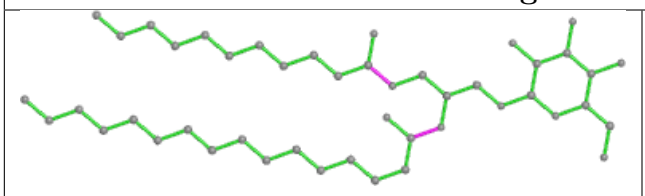


Torsions

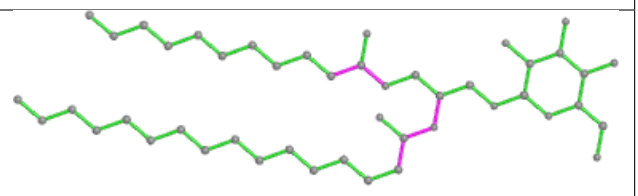


Rings

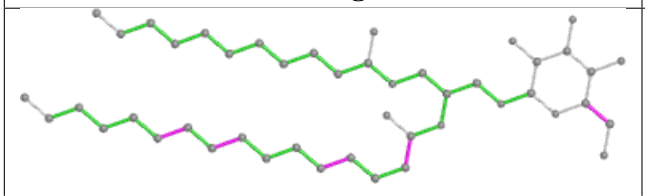
Ligand LMG D 410



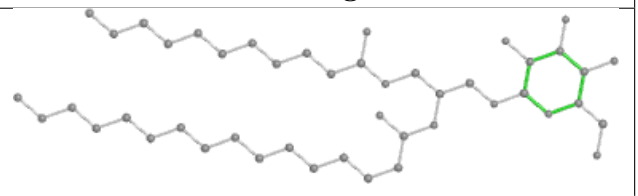
Bond lengths



Bond angles

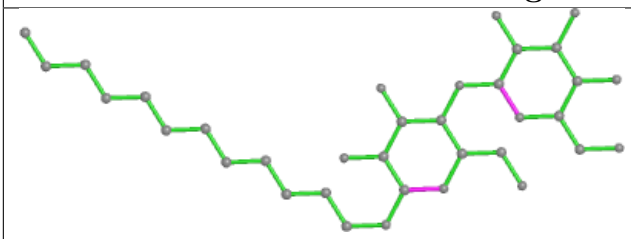


Torsions

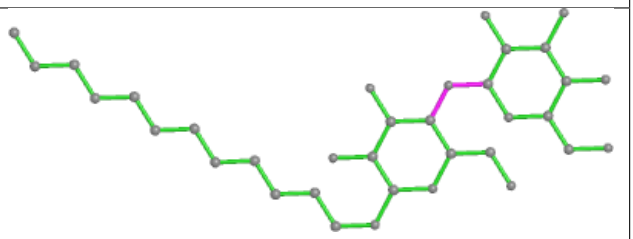


Rings

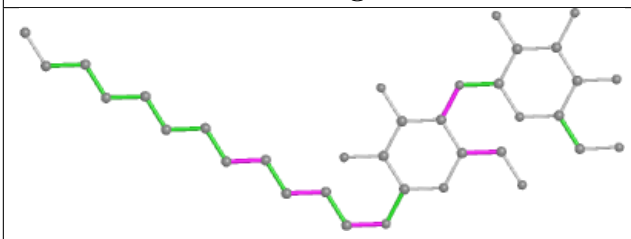
Ligand LMU c 519



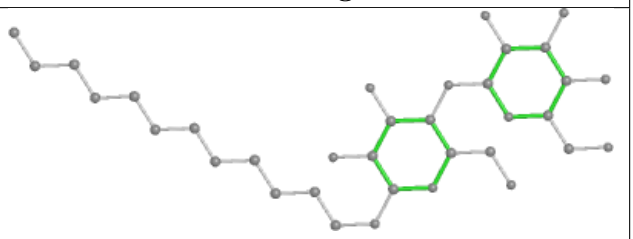
Bond lengths



Bond angles

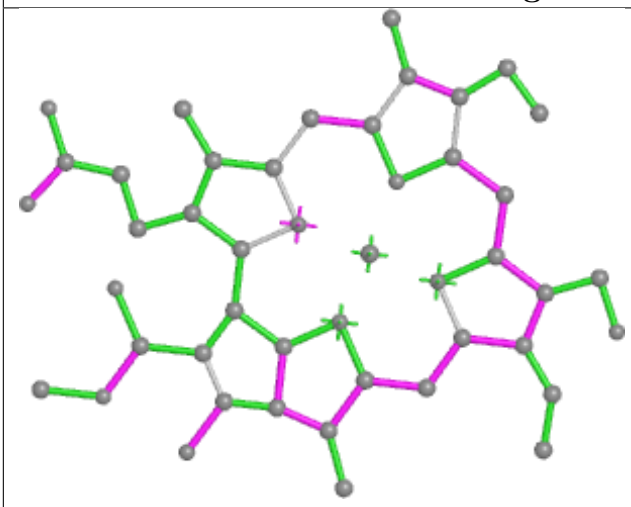


Torsions

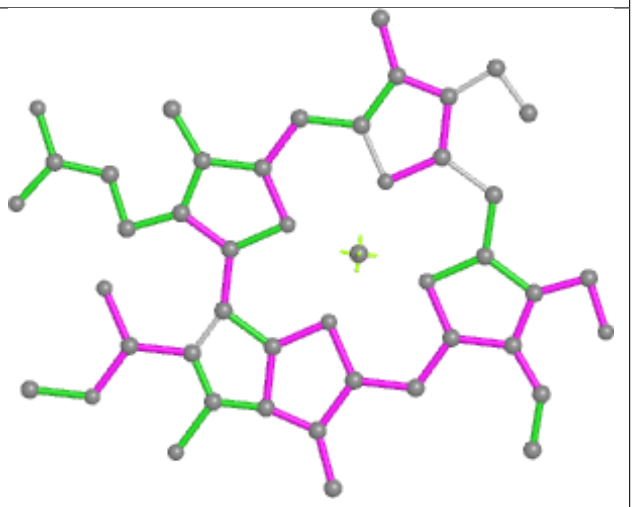


Rings

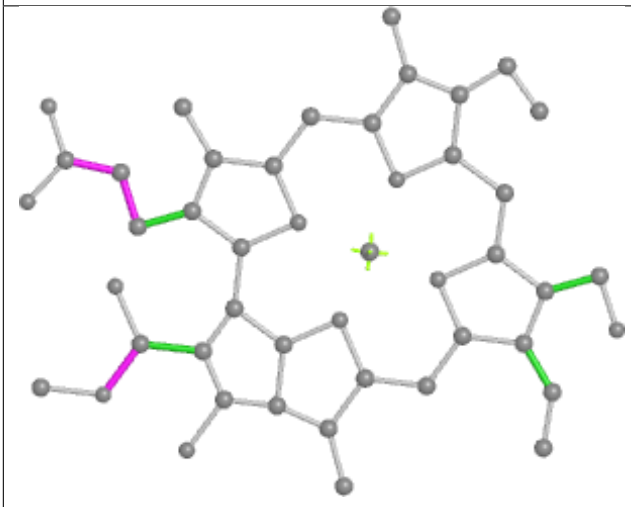
Ligand CHL Y 308



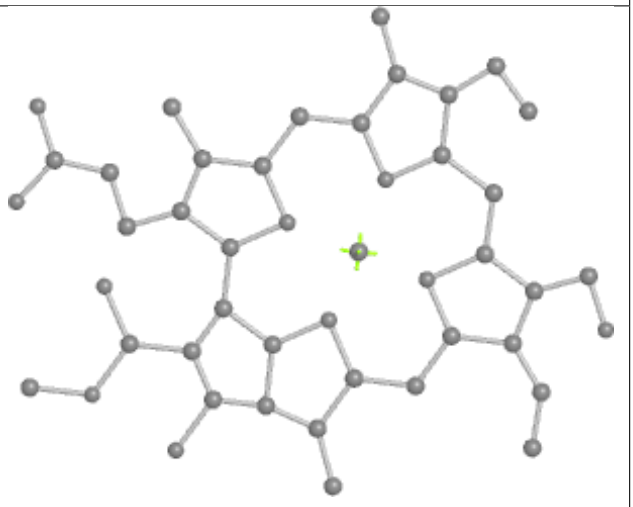
Bond lengths



Bond angles

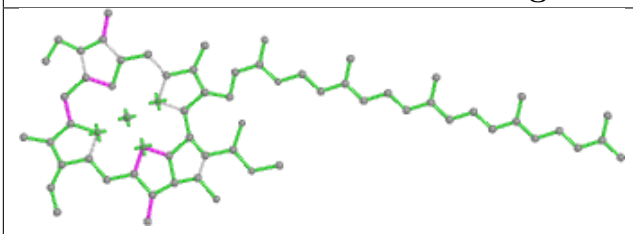


Torsions

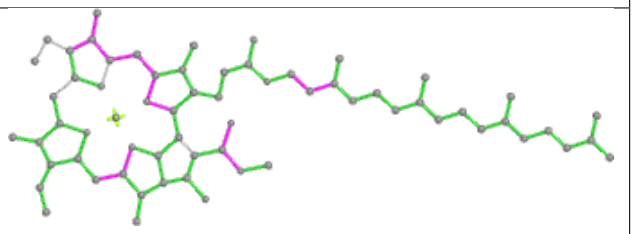


Rings

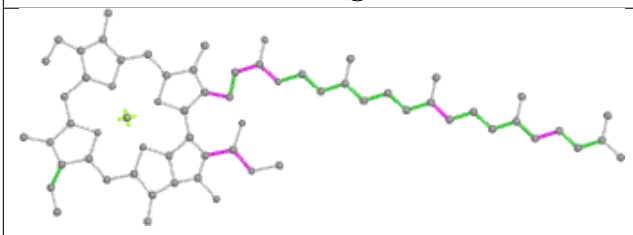
Ligand CLA c 503



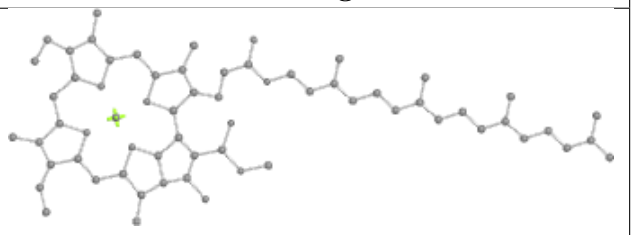
Bond lengths



Bond angles

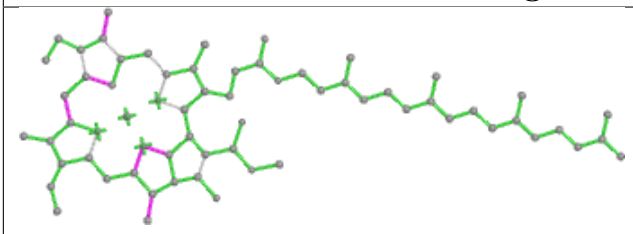


Torsions

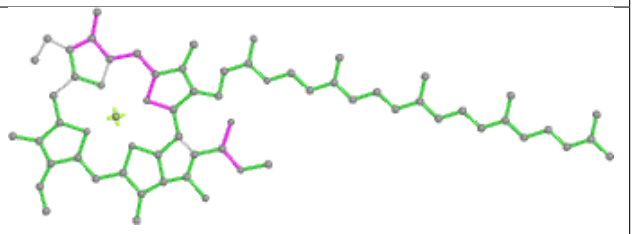


Rings

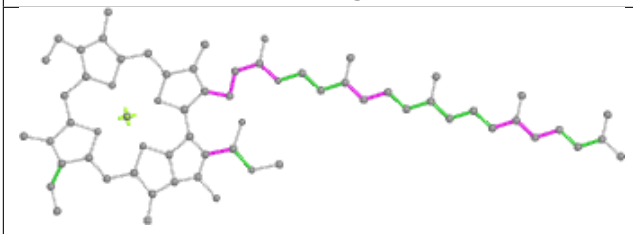
Ligand CLA Y 305



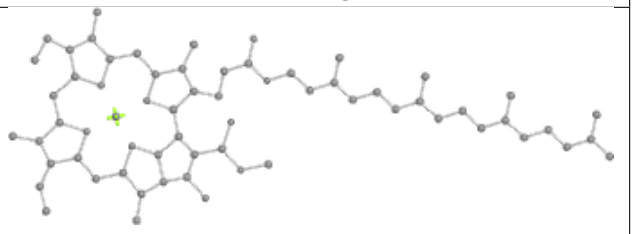
Bond lengths



Bond angles

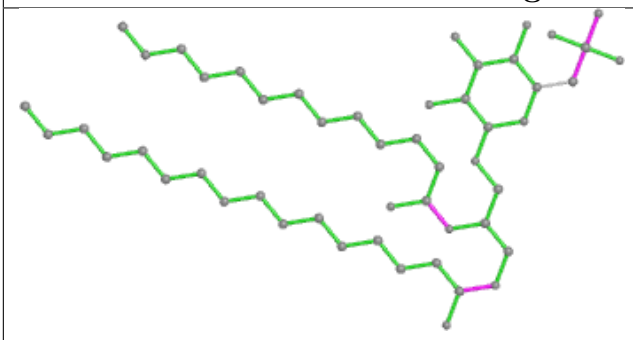


Torsions

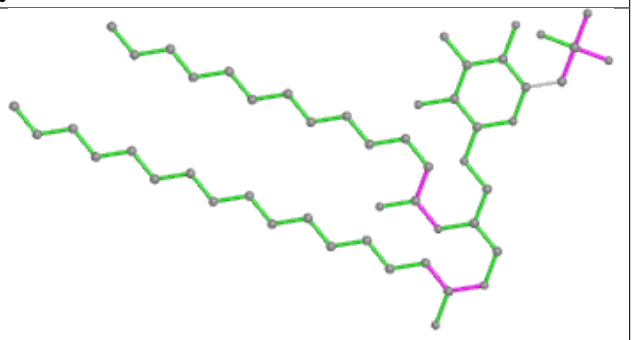


Rings

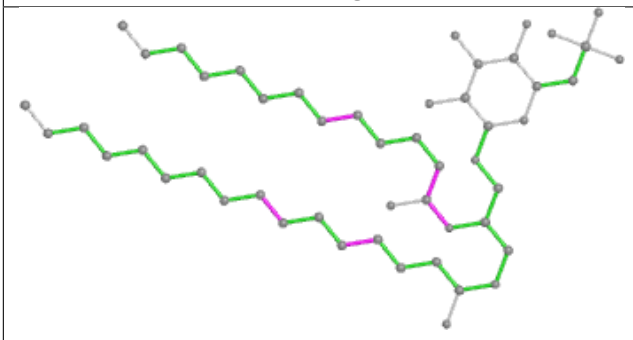
Ligand SQD A 407



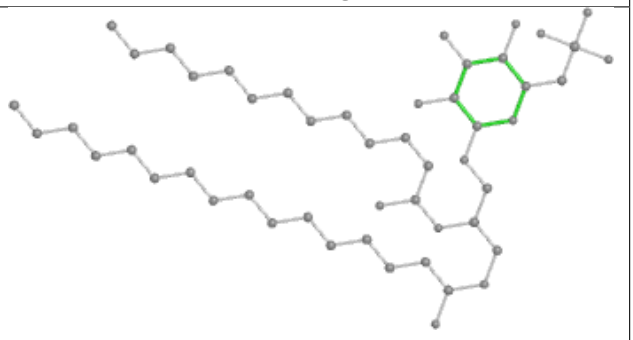
Bond lengths



Bond angles

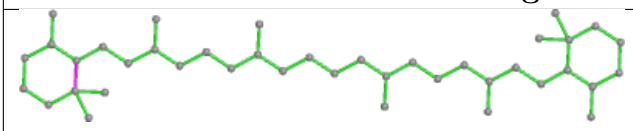


Torsions

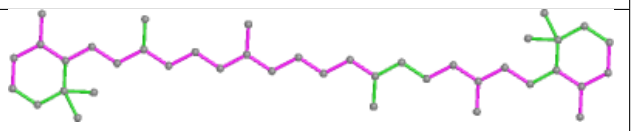


Rings

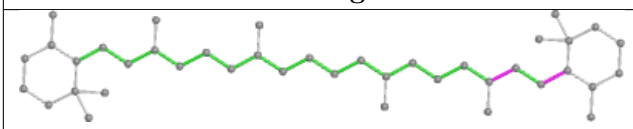
Ligand BCR V 101



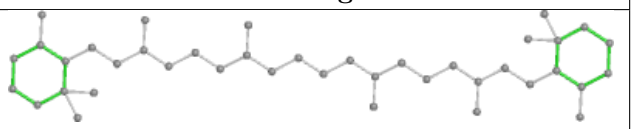
Bond lengths



Bond angles

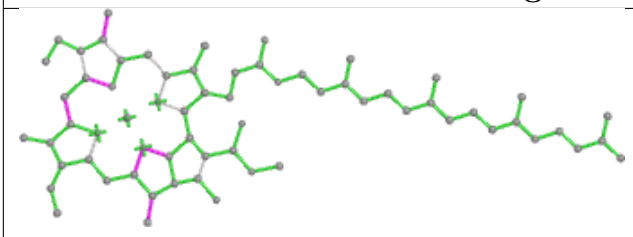


Torsions

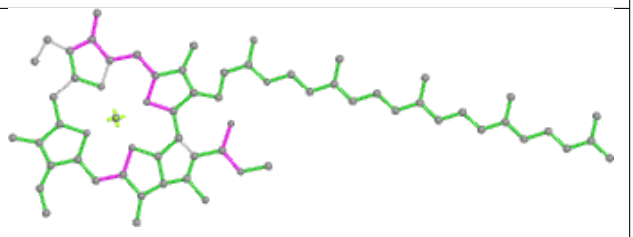


Rings

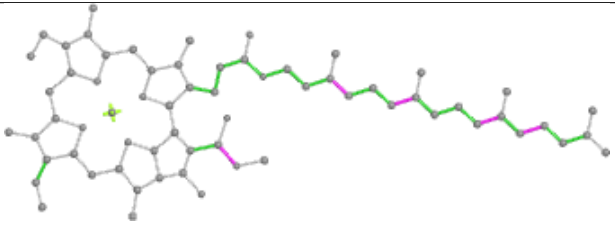
Ligand CLA B 505



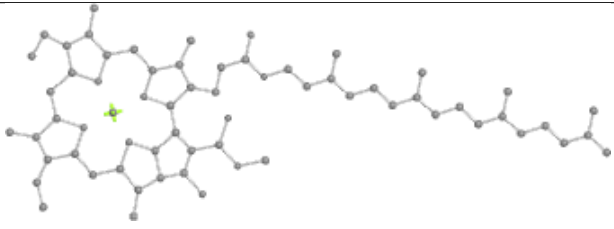
Bond lengths



Bond angles

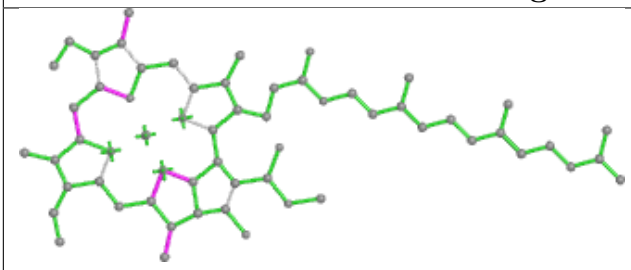


Torsions

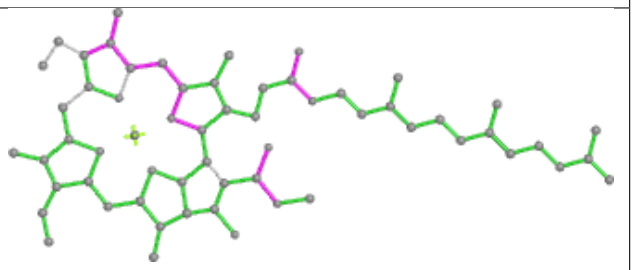


Rings

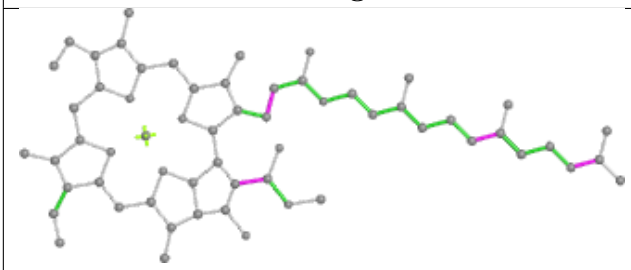
Ligand CLA r 301



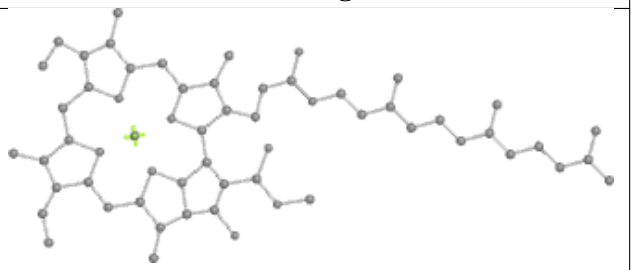
Bond lengths



Bond angles

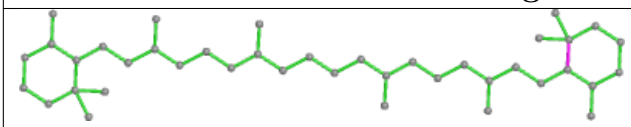


Torsions

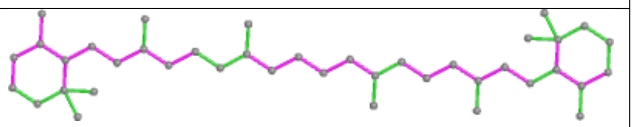


Rings

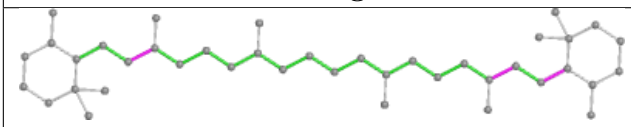
Ligand BCR C 515



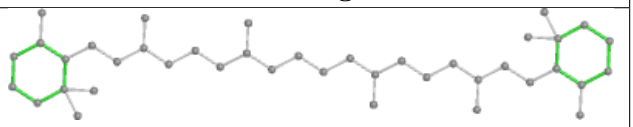
Bond lengths



Bond angles

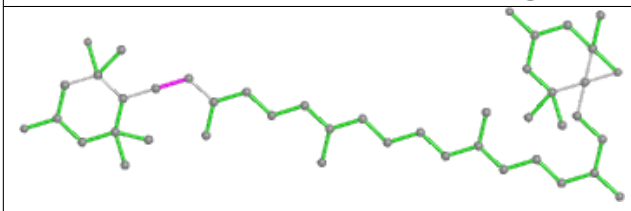


Torsions

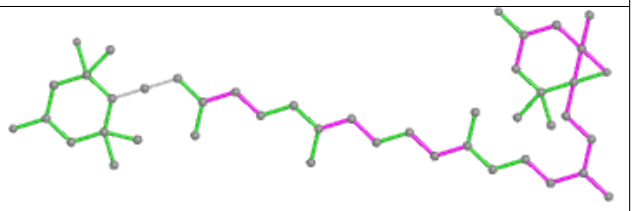


Rings

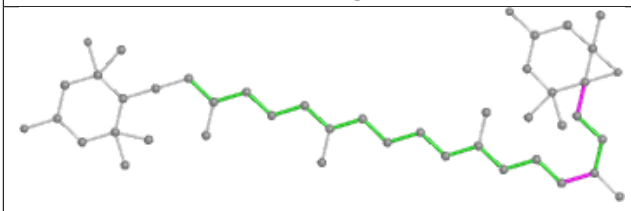
Ligand NEX Y 318



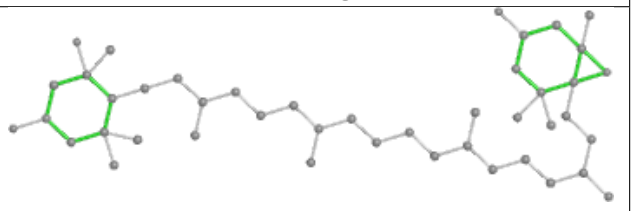
Bond lengths



Bond angles

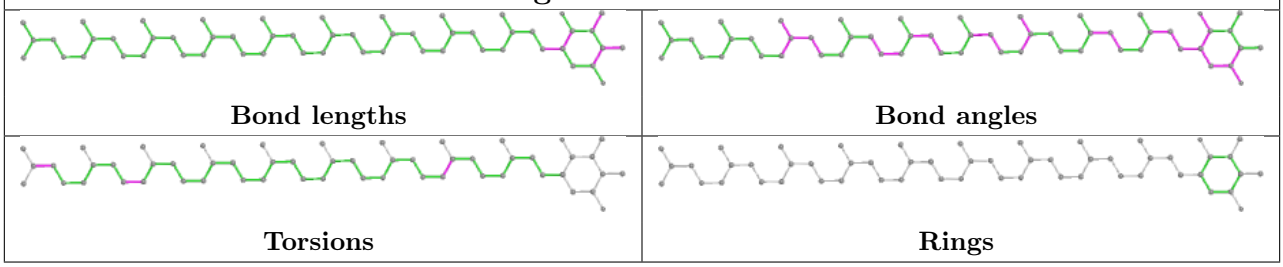


Torsions

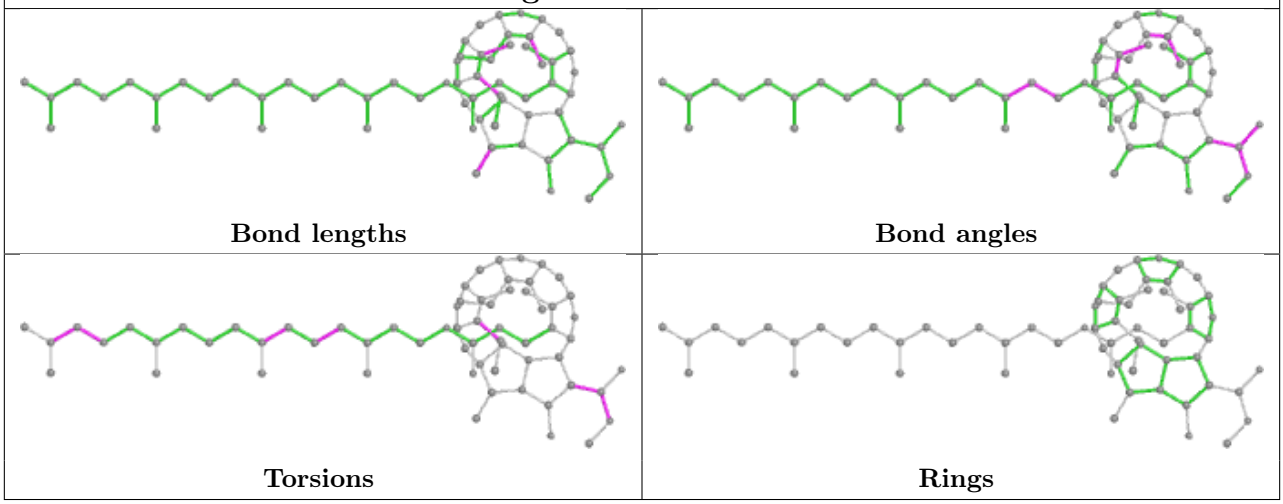


Rings

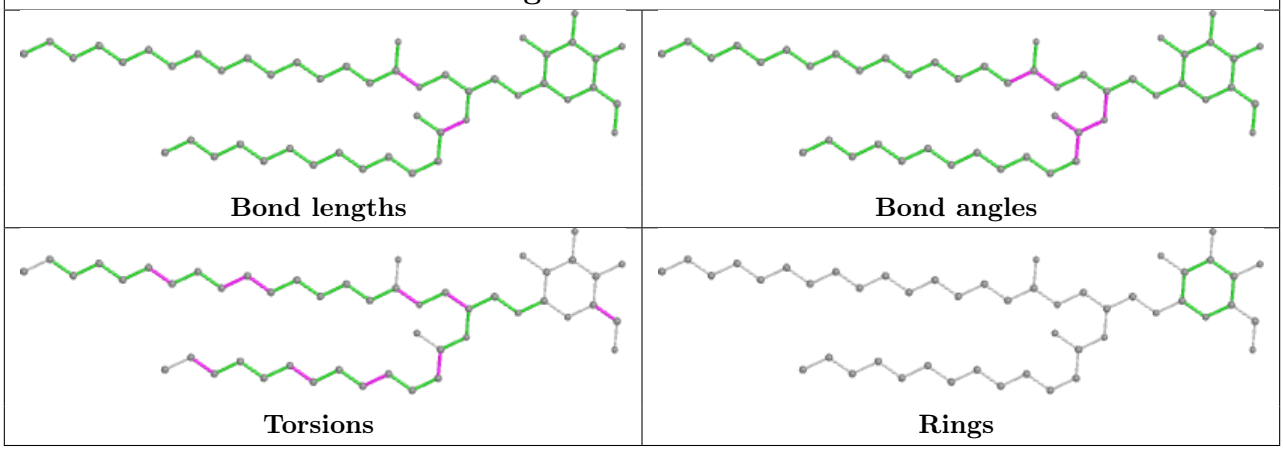
Ligand PL9 d 406



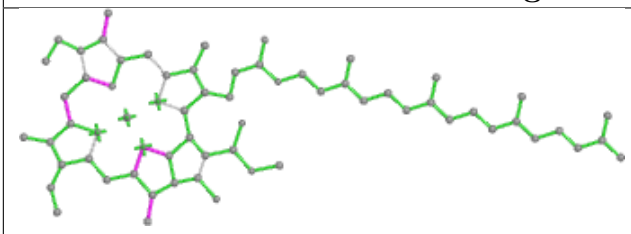
Ligand PHO D 402



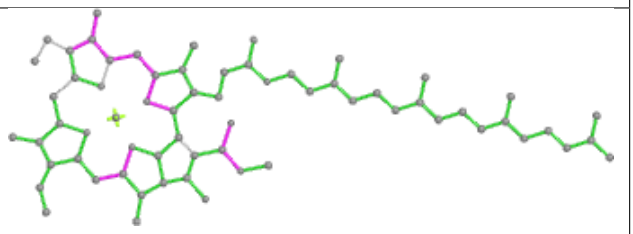
Ligand LMG d 410



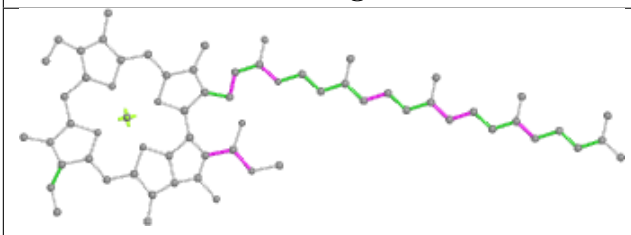
Ligand CLA Y 314



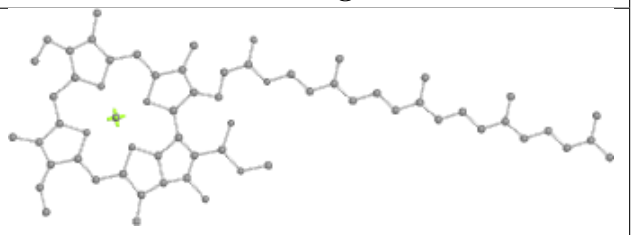
Bond lengths



Bond angles

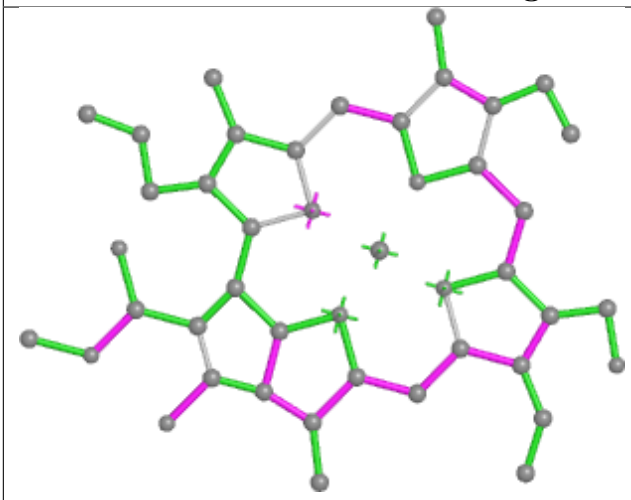


Torsions

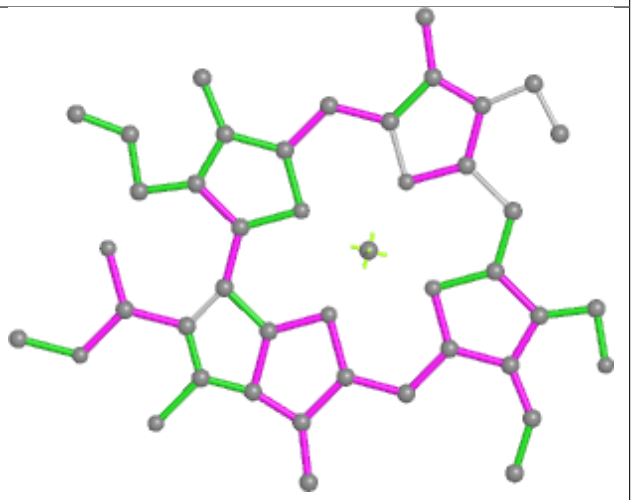


Rings

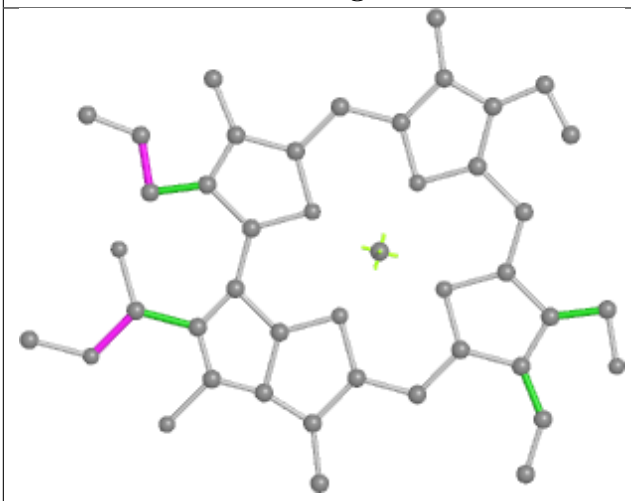
Ligand CHL G 608



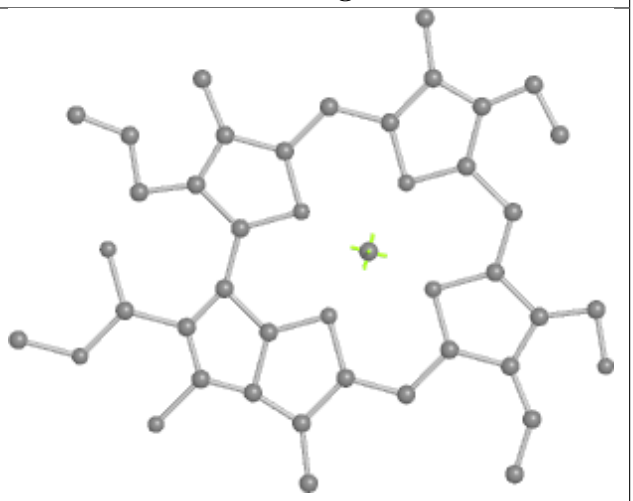
Bond lengths



Bond angles

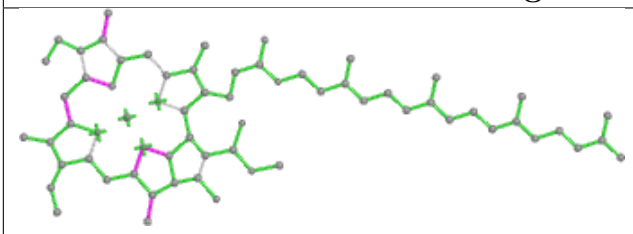


Torsions

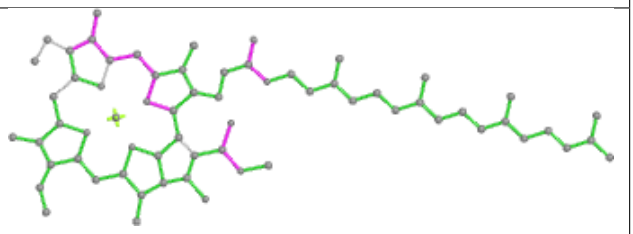


Rings

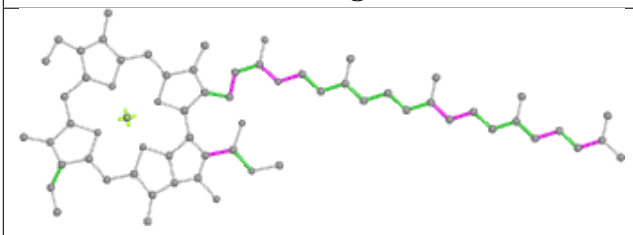
Ligand CLA C 505



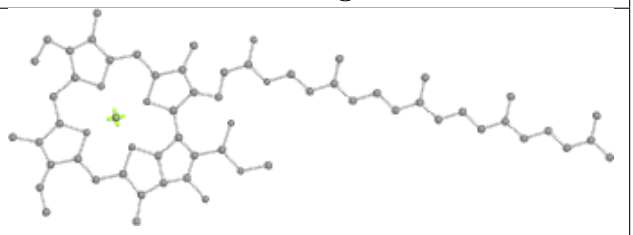
Bond lengths



Bond angles

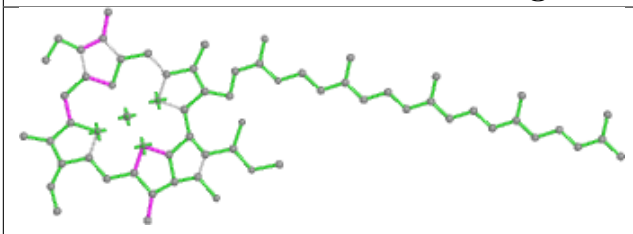


Torsions

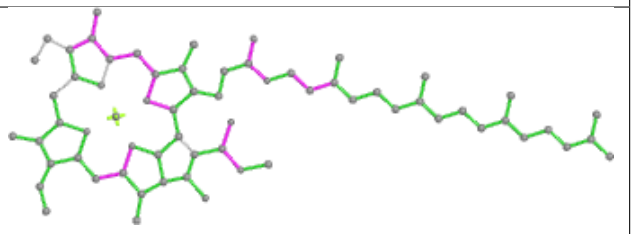


Rings

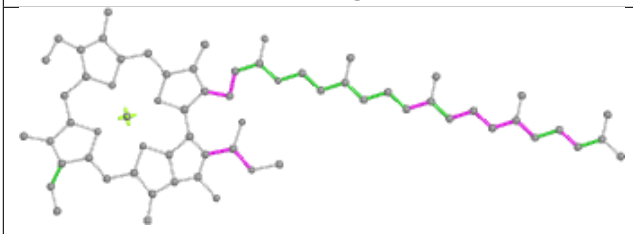
Ligand CLA c 501



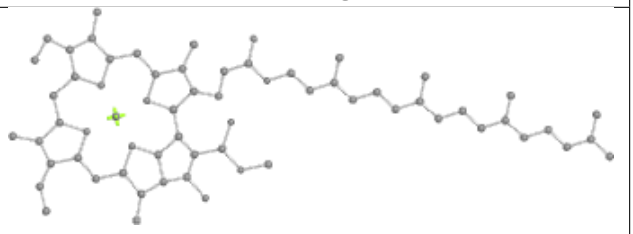
Bond lengths



Bond angles

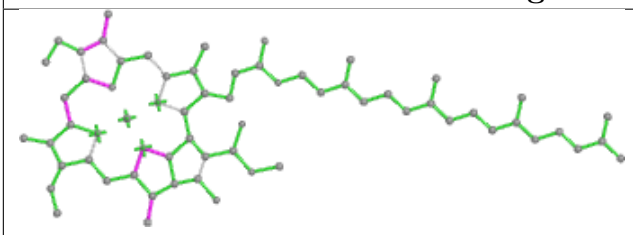


Torsions

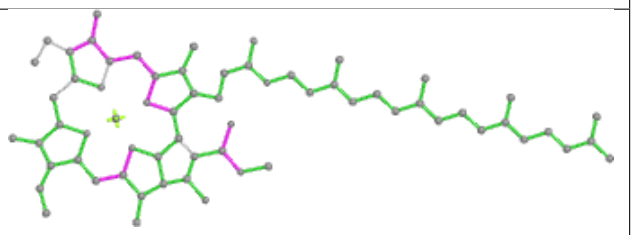


Rings

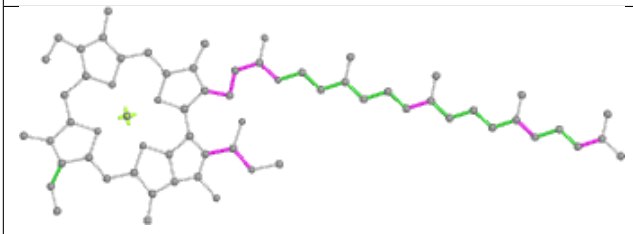
Ligand CLA b 501



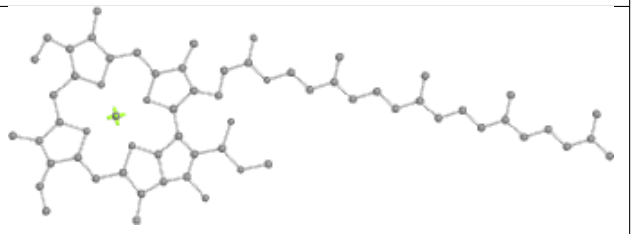
Bond lengths



Bond angles

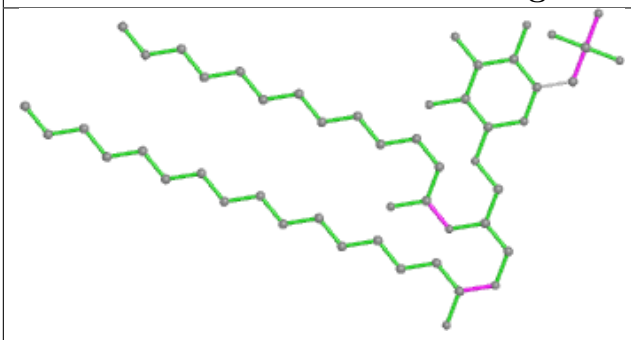


Torsions

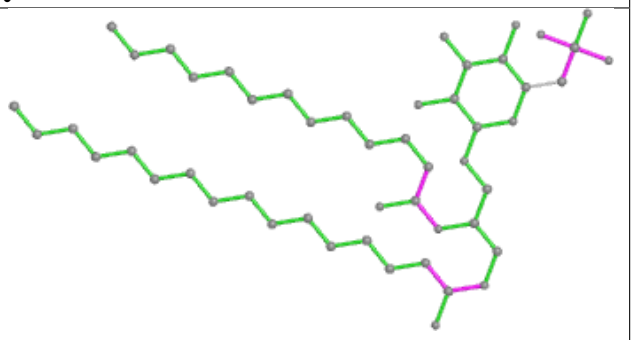


Rings

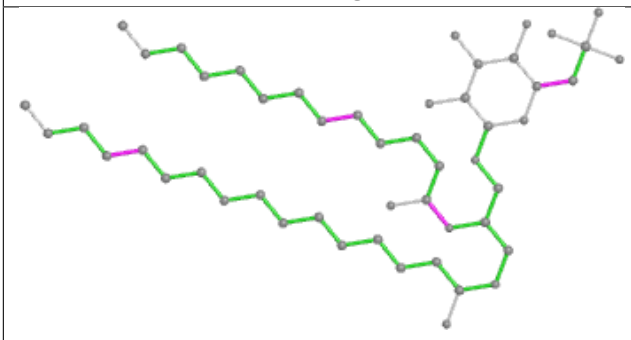
Ligand SQD a 407



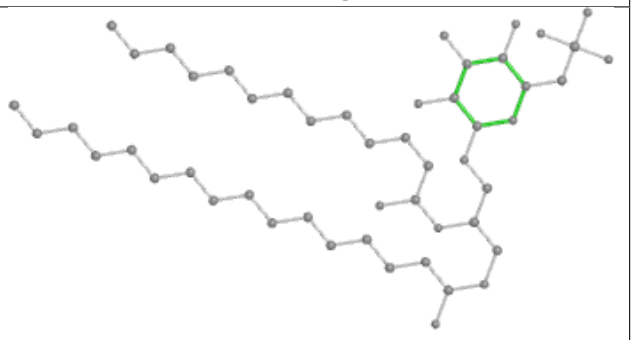
Bond lengths



Bond angles

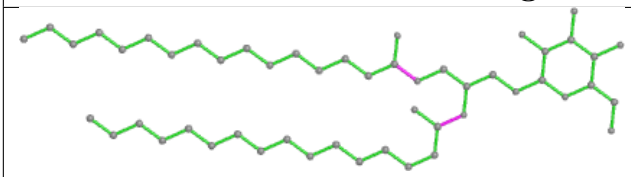


Torsions

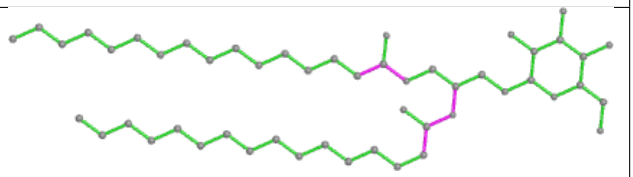


Rings

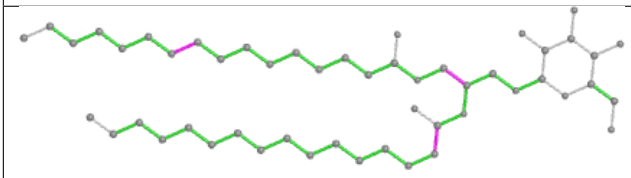
Ligand LMG C 520



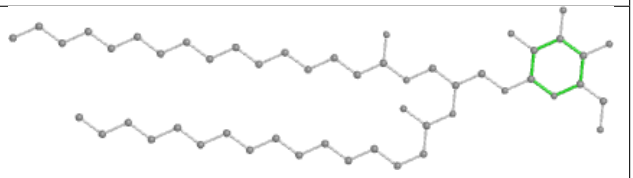
Bond lengths



Bond angles

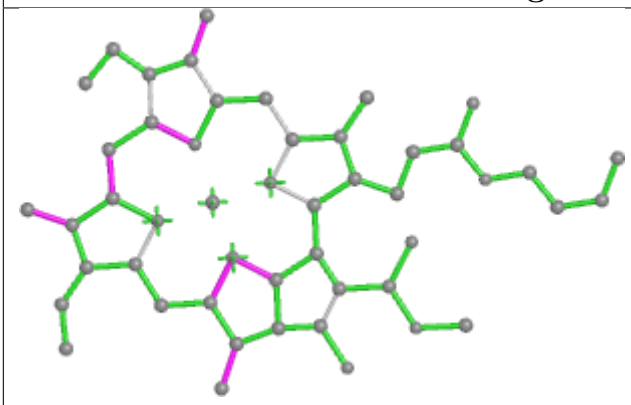


Torsions

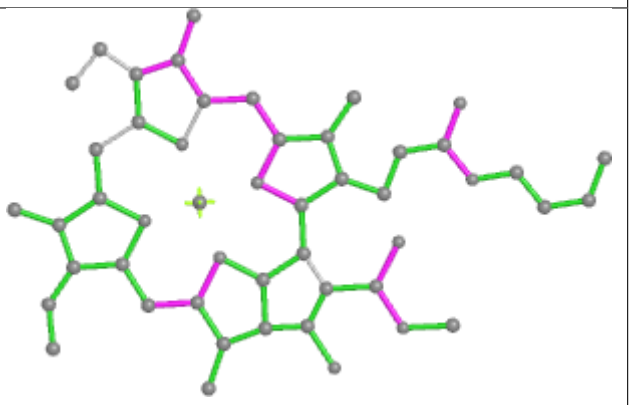


Rings

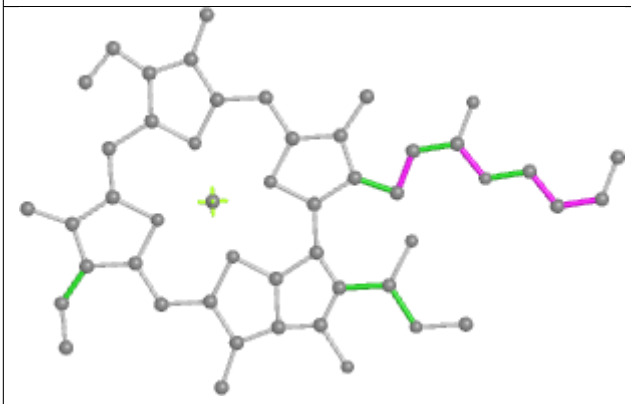
Ligand CLA S 610



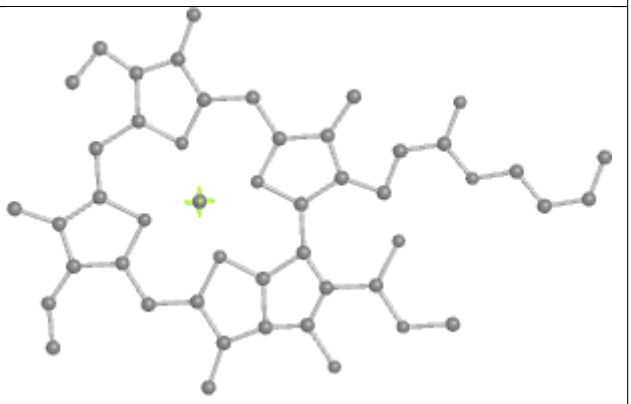
Bond lengths



Bond angles

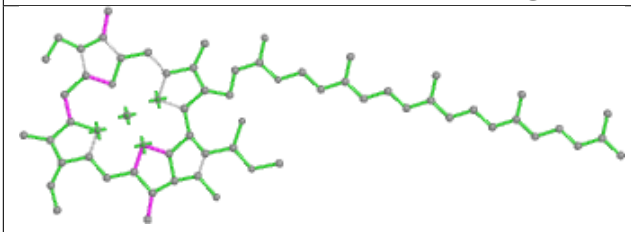


Torsions

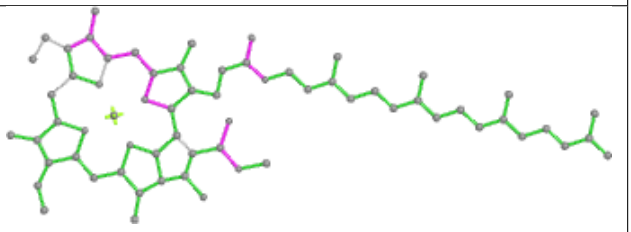


Rings

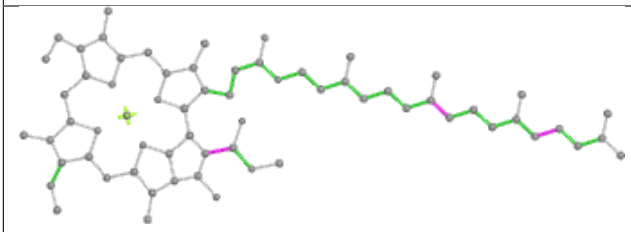
Ligand CLA C 507



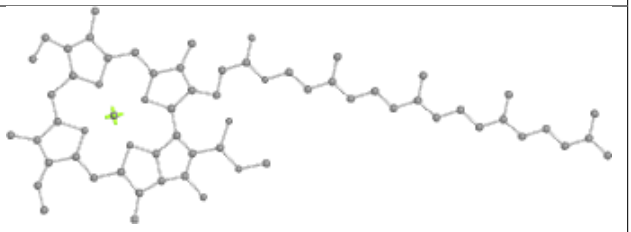
Bond lengths



Bond angles

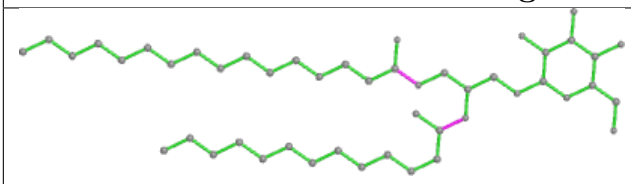


Torsions

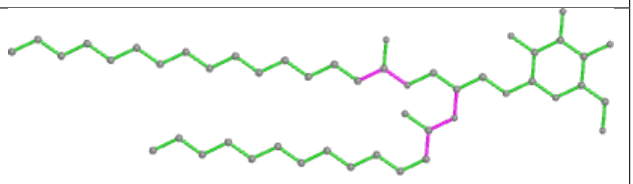


Rings

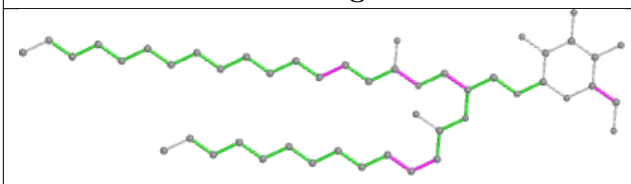
Ligand LMG H 102



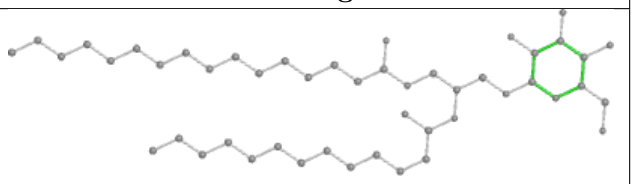
Bond lengths



Bond angles

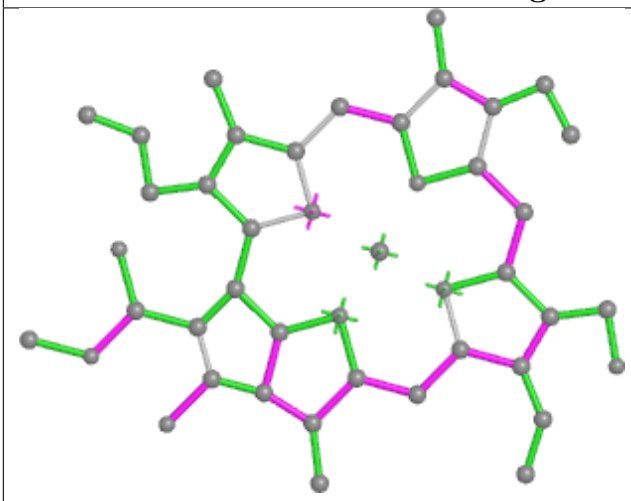


Torsions

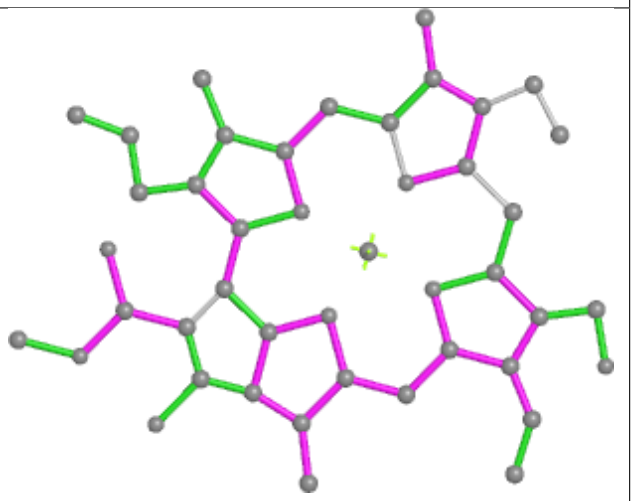


Rings

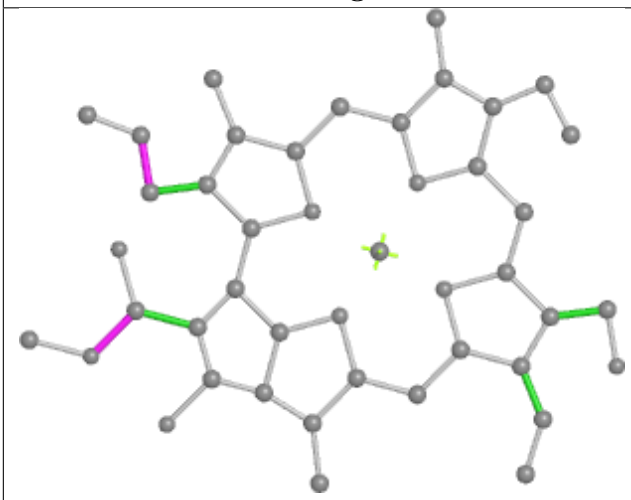
Ligand CHL r 304



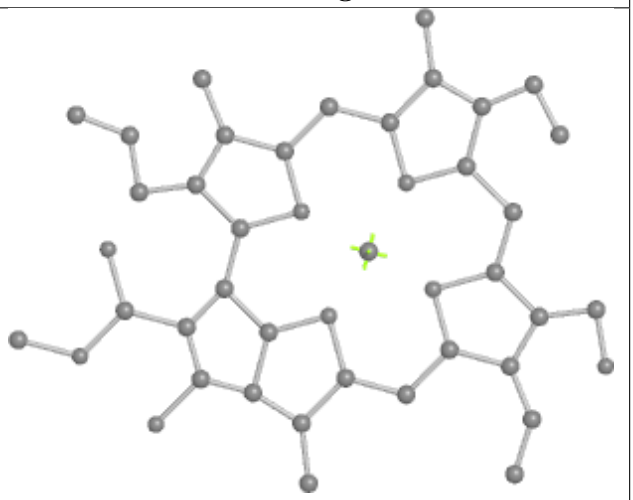
Bond lengths



Bond angles

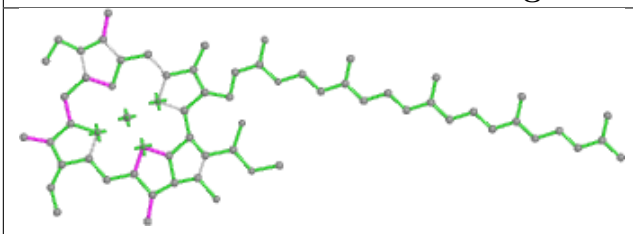


Torsions

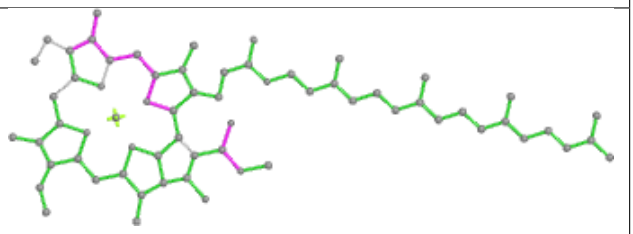


Rings

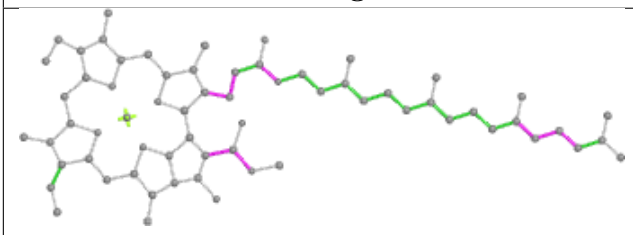
Ligand CLA A 402



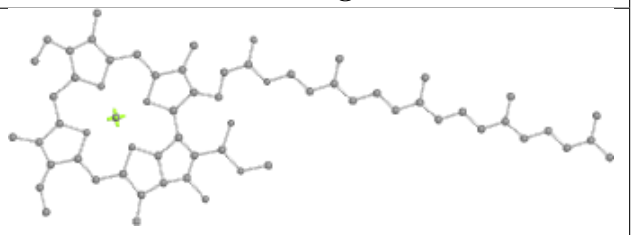
Bond lengths



Bond angles

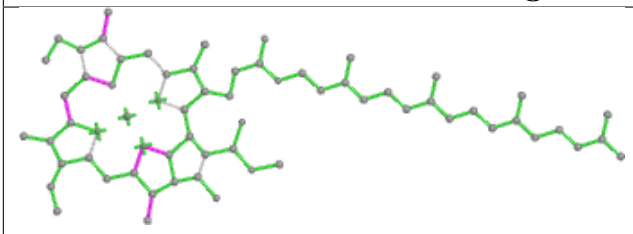


Torsions

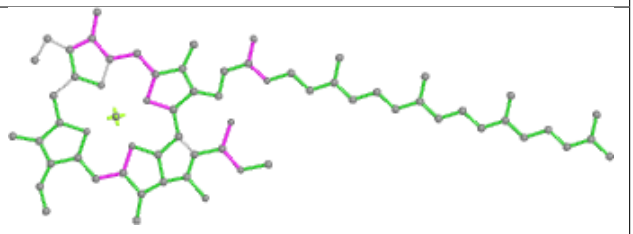


Rings

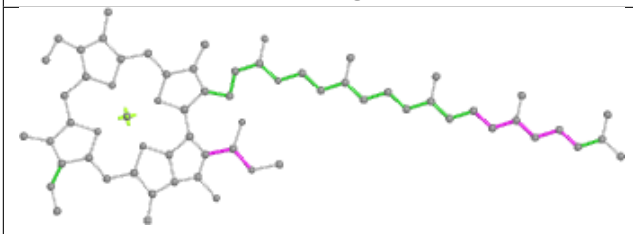
Ligand CLA C 504



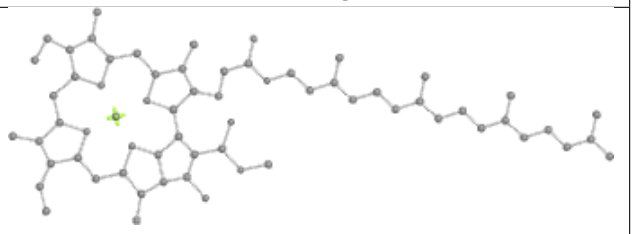
Bond lengths



Bond angles

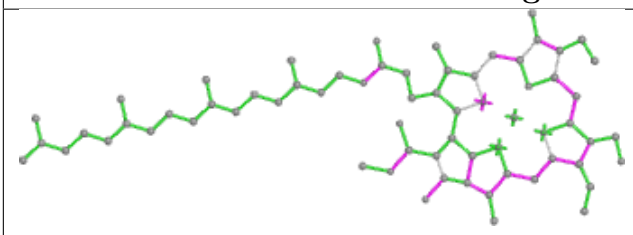


Torsions

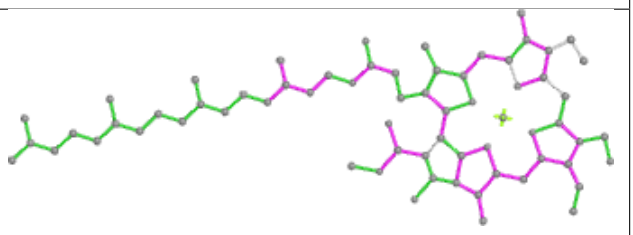


Rings

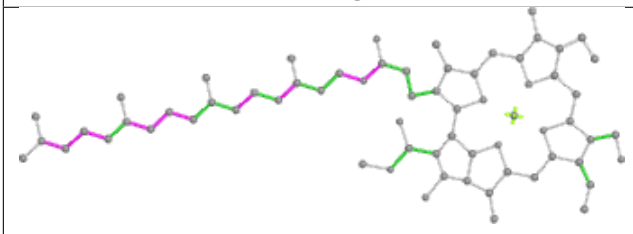
Ligand CHL N 310



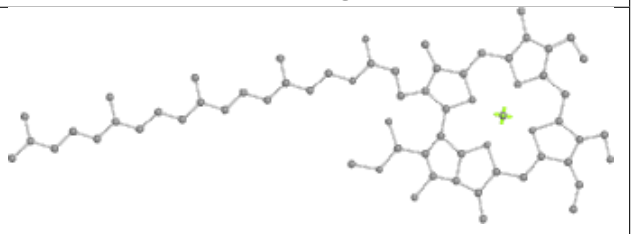
Bond lengths



Bond angles

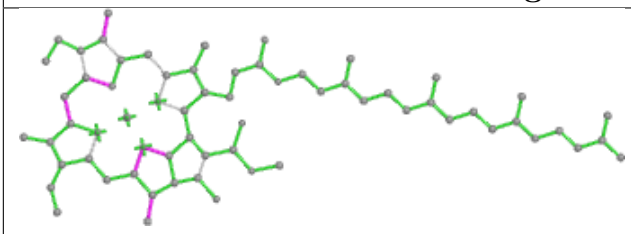


Torsions

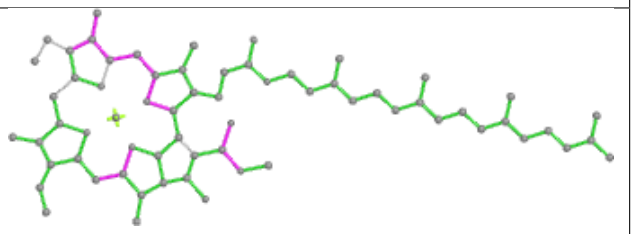


Rings

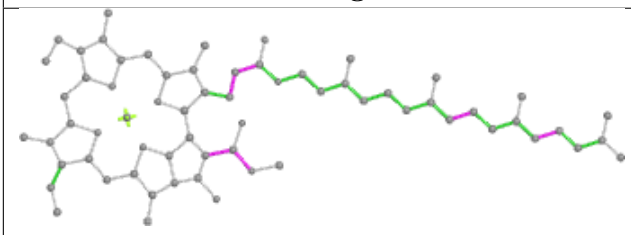
Ligand CLA B 501



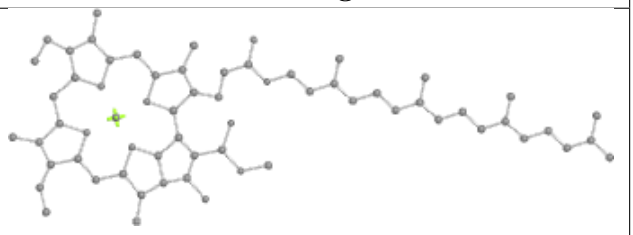
Bond lengths



Bond angles

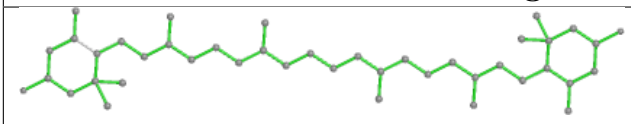


Torsions

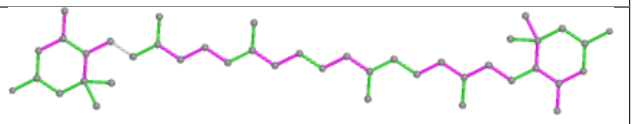


Rings

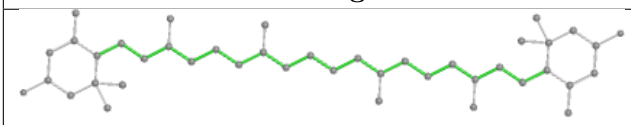
Ligand LUT Y 317



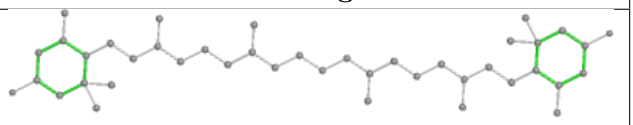
Bond lengths



Bond angles

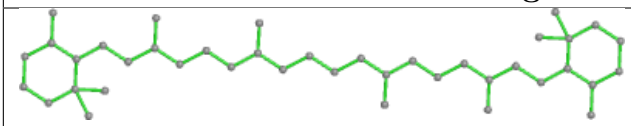


Torsions

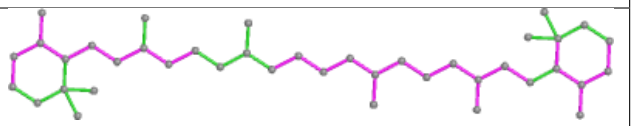


Rings

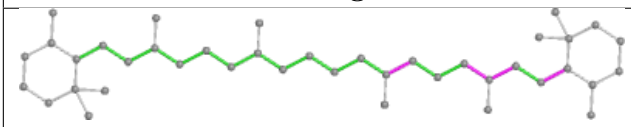
Ligand BCR B 517



Bond lengths



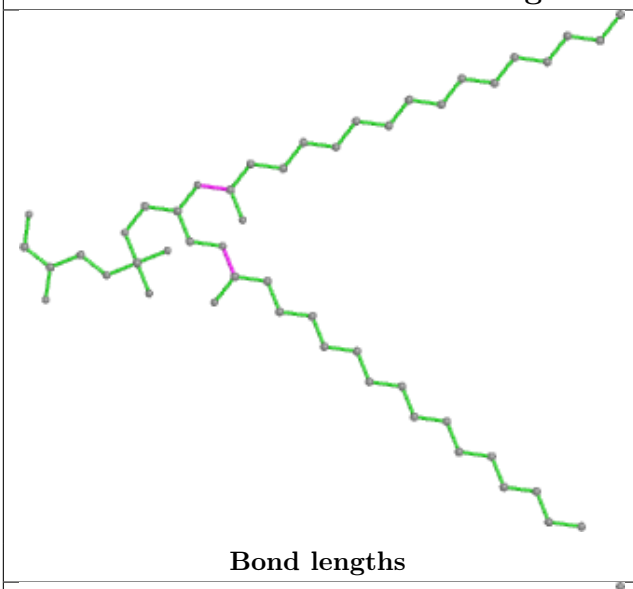
Bond angles



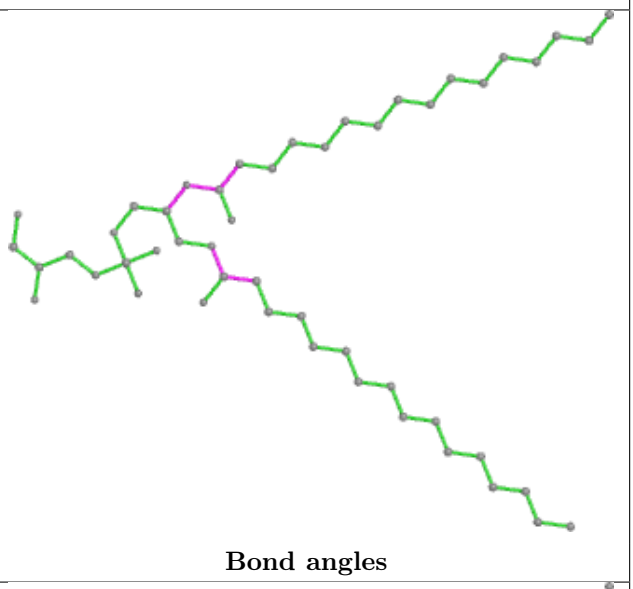
Torsions

Rings

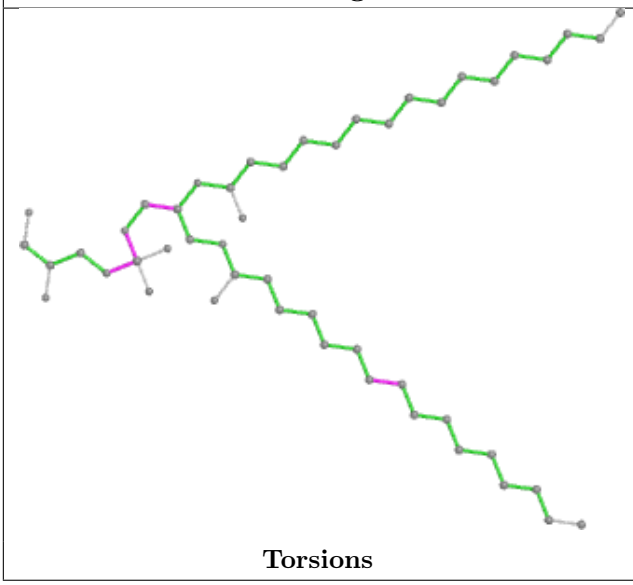
Ligand LHG L 101



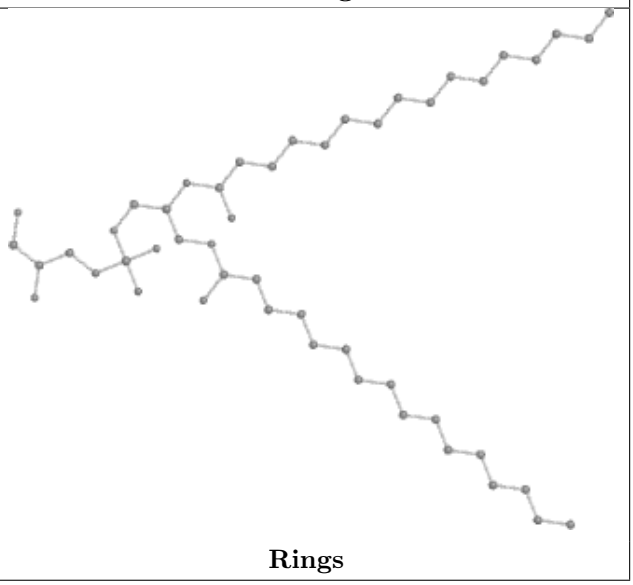
Bond lengths



Bond angles

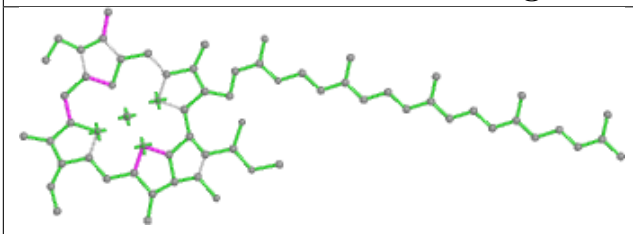


Torsions

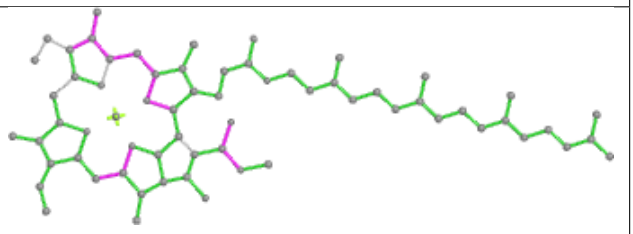


Rings

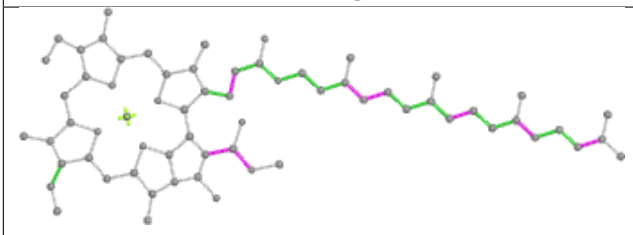
Ligand CLA G 613



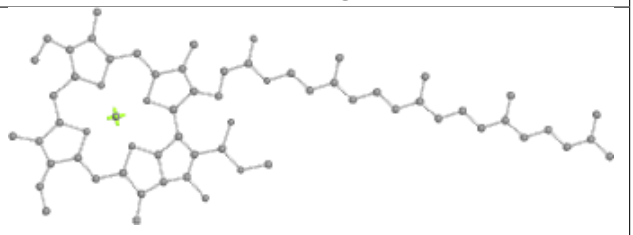
Bond lengths



Bond angles

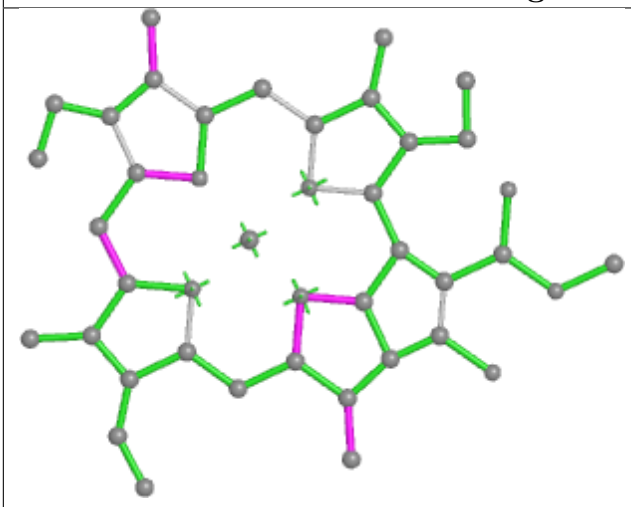


Torsions

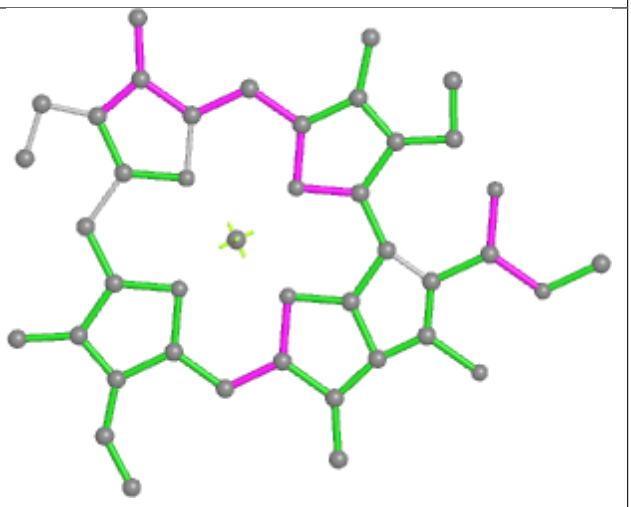


Rings

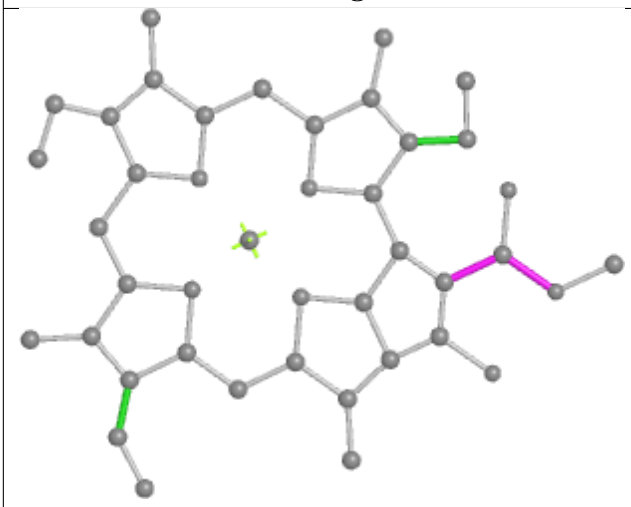
Ligand CLA d 404



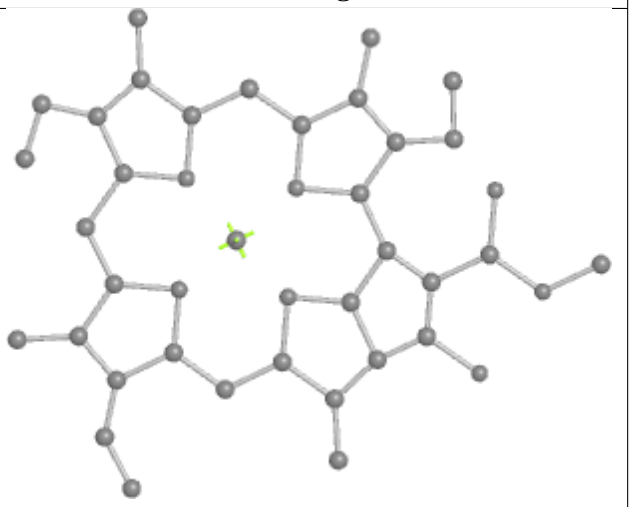
Bond lengths



Bond angles

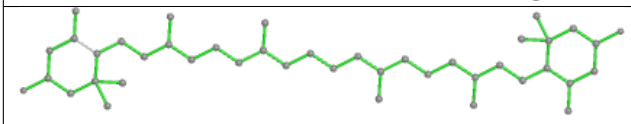


Torsions

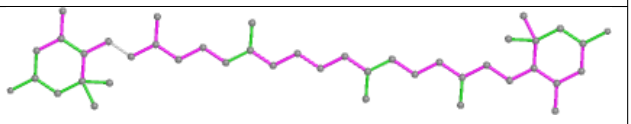


Rings

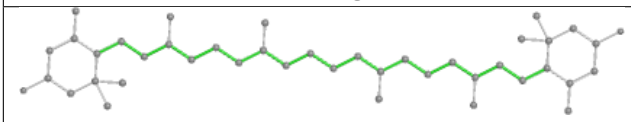
Ligand LUT S 616



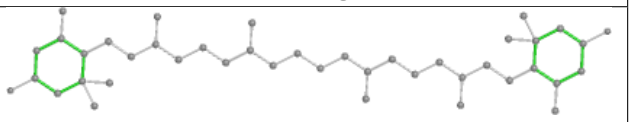
Bond lengths



Bond angles

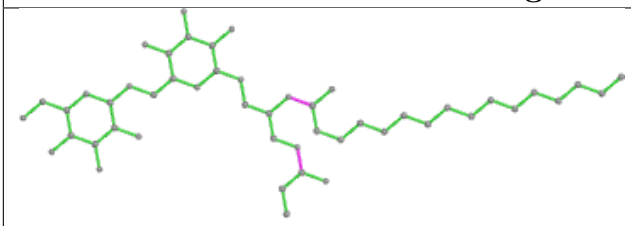


Torsions

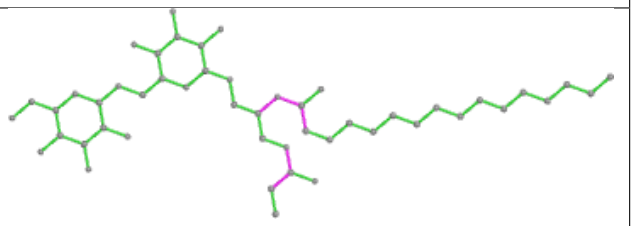


Rings

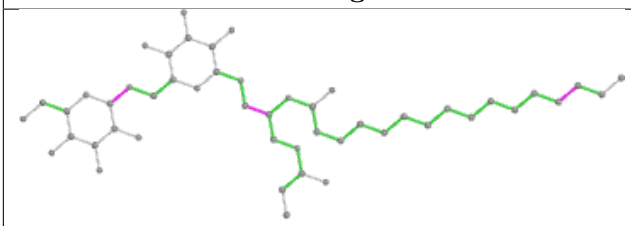
Ligand DGD c 516



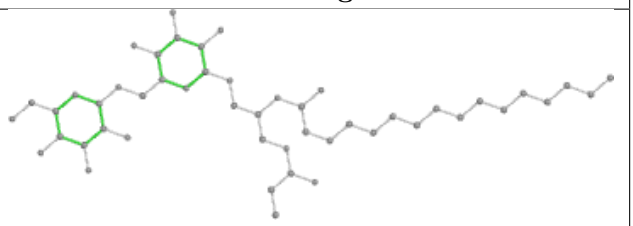
Bond lengths



Bond angles

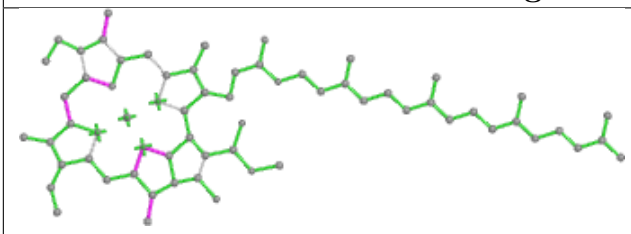


Torsions

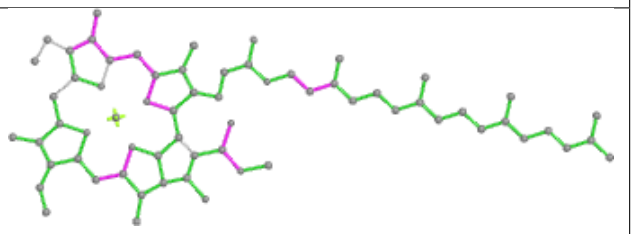


Rings

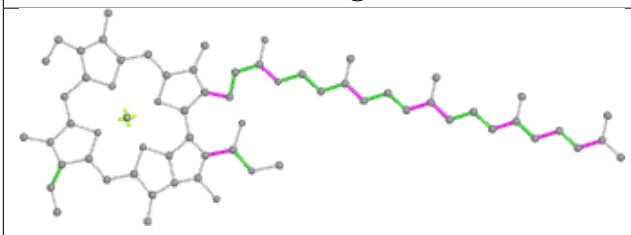
Ligand CLA C 513



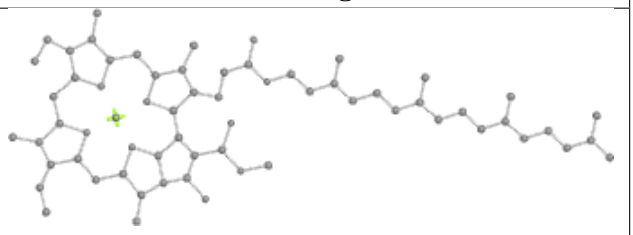
Bond lengths



Bond angles

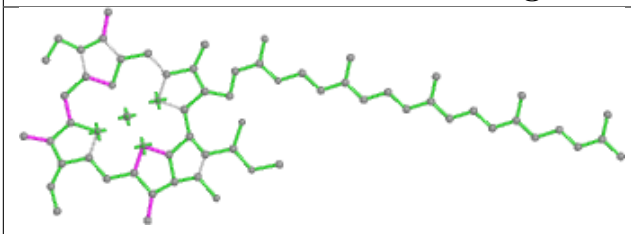


Torsions

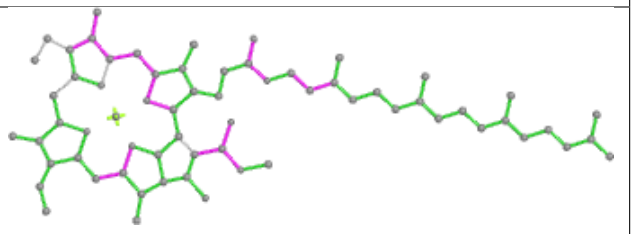


Rings

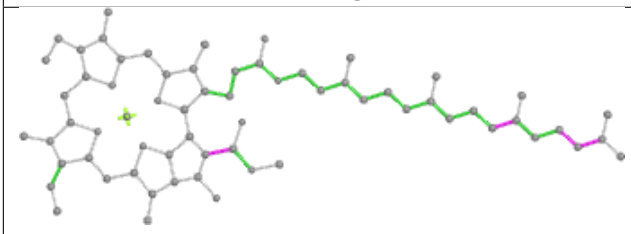
Ligand CLA D 401



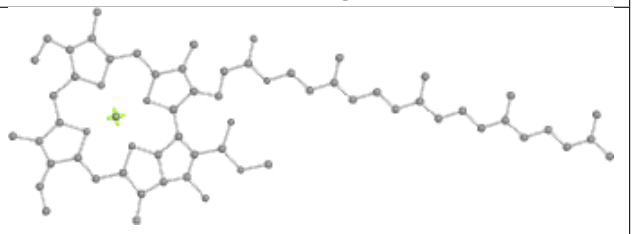
Bond lengths



Bond angles

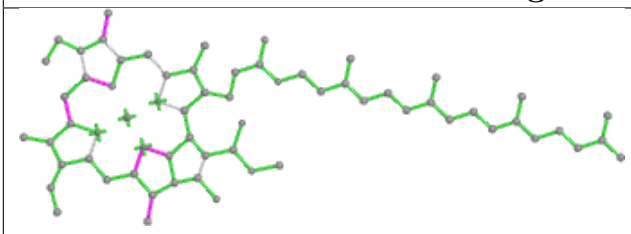


Torsions

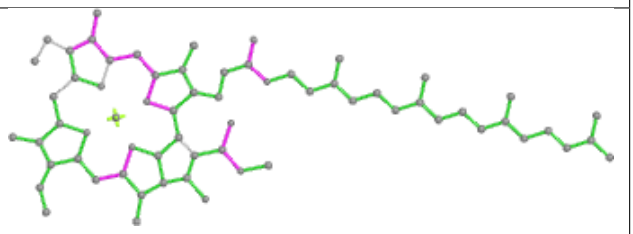


Rings

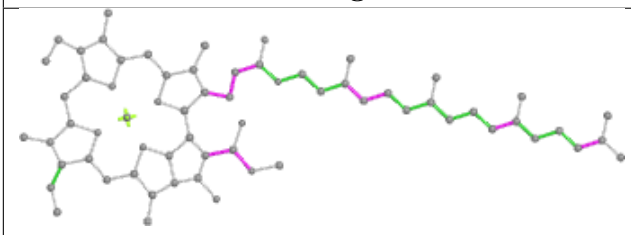
Ligand CLA b 507



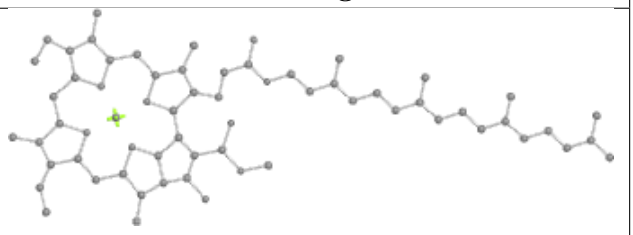
Bond lengths



Bond angles

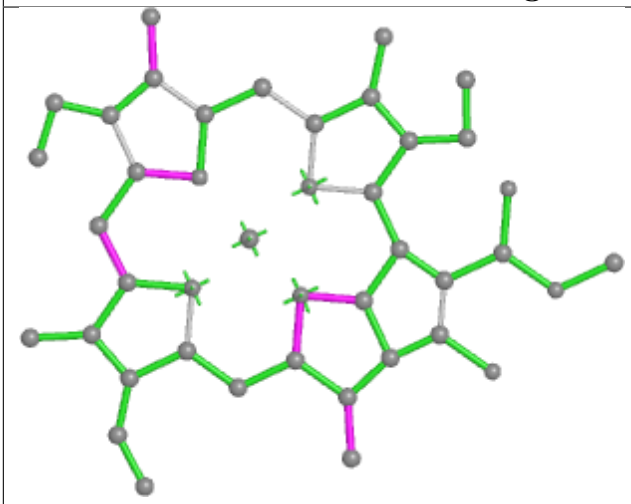


Torsions

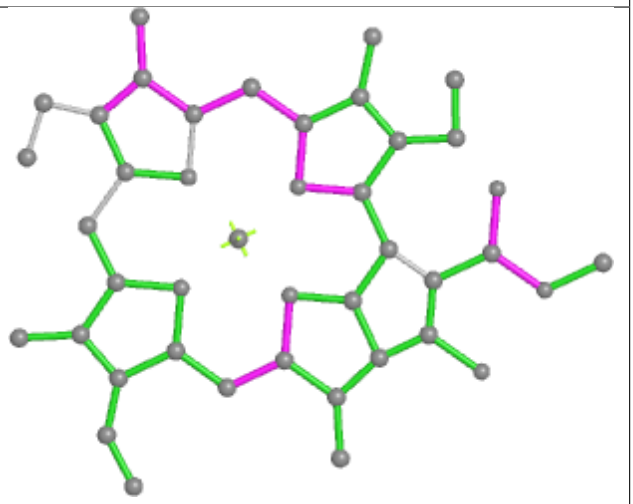


Rings

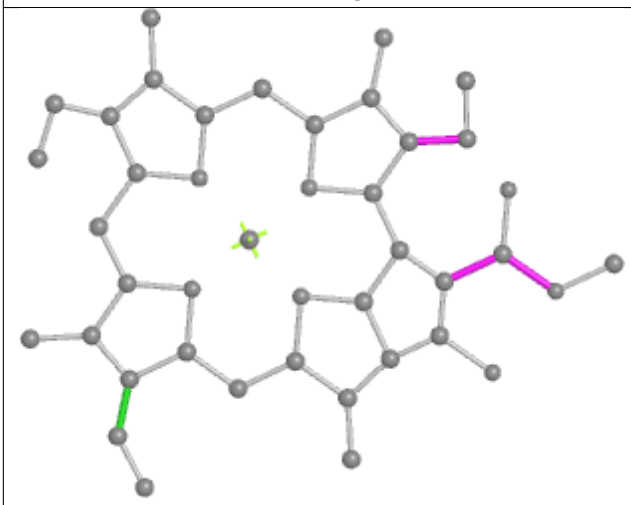
Ligand CLA N 315



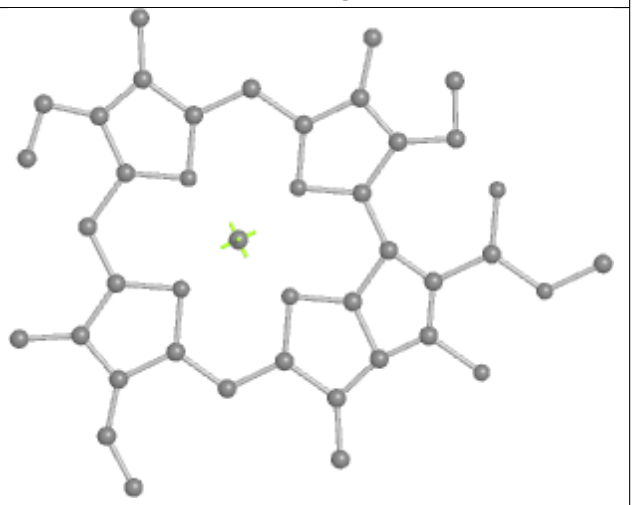
Bond lengths



Bond angles

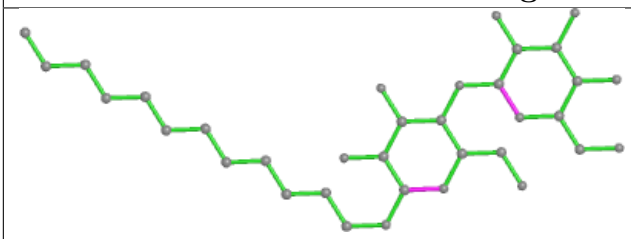


Torsions

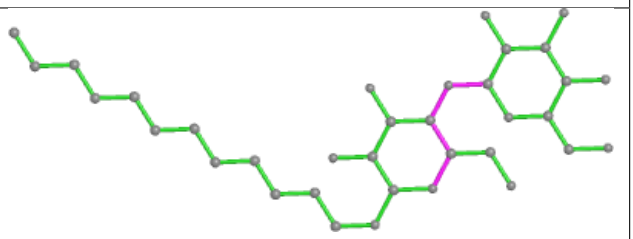


Rings

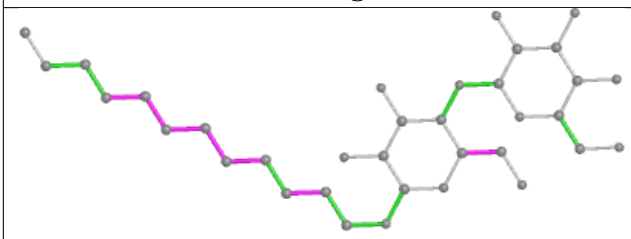
Ligand LMU C 523



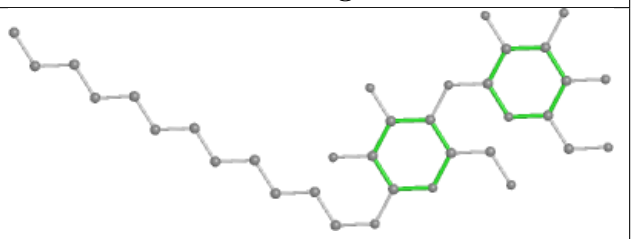
Bond lengths



Bond angles

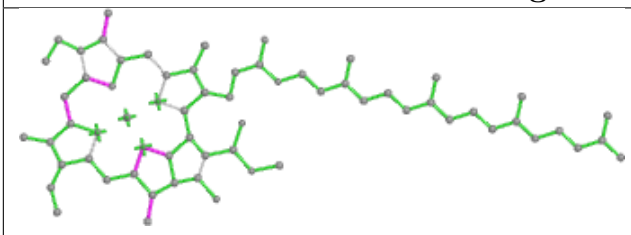


Torsions

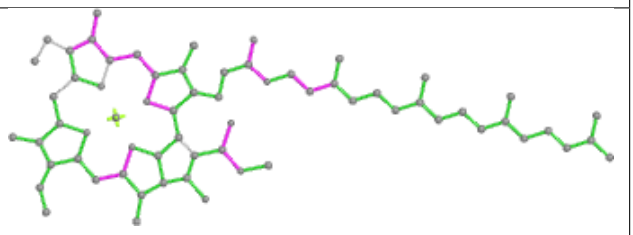


Rings

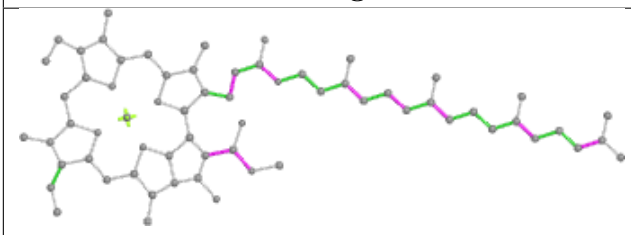
Ligand CLA c 502



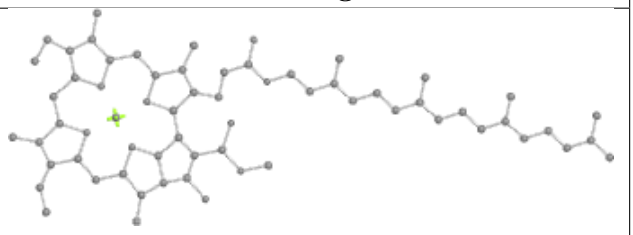
Bond lengths



Bond angles

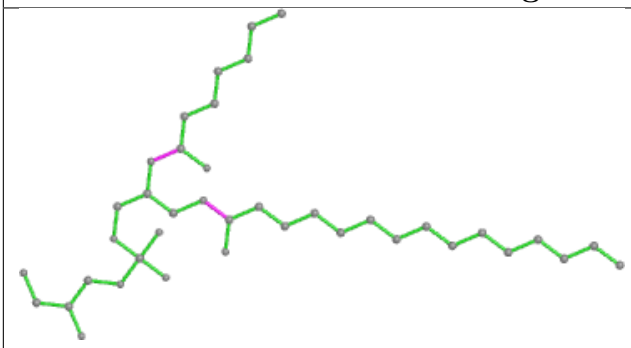


Torsions

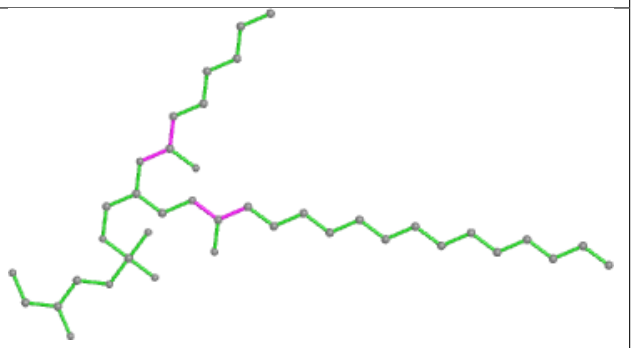


Rings

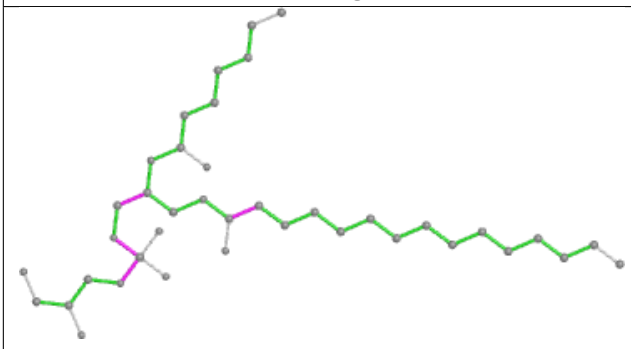
Ligand LHG D 409



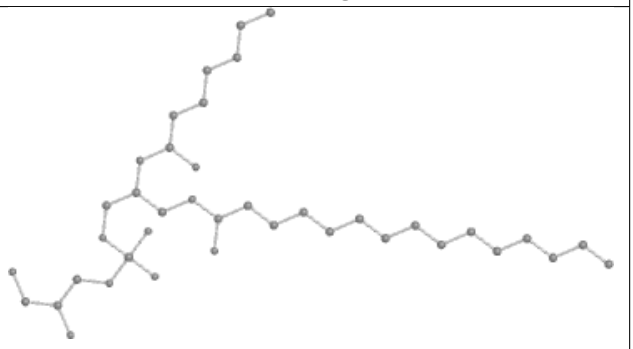
Bond lengths



Bond angles

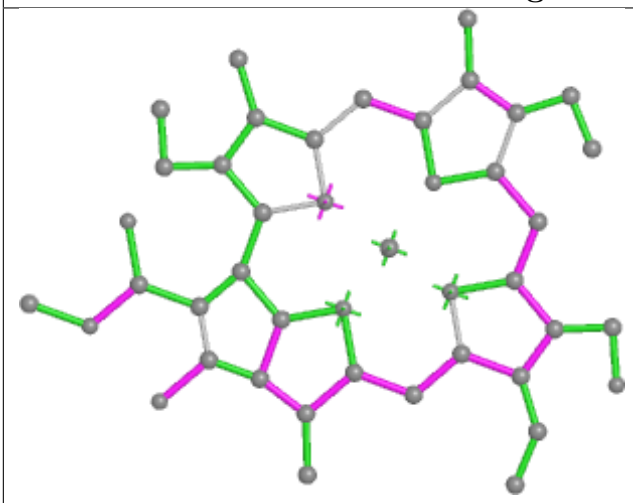


Torsions

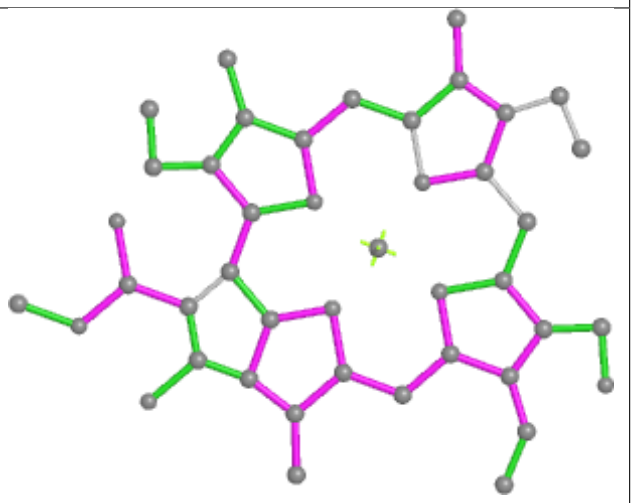


Rings

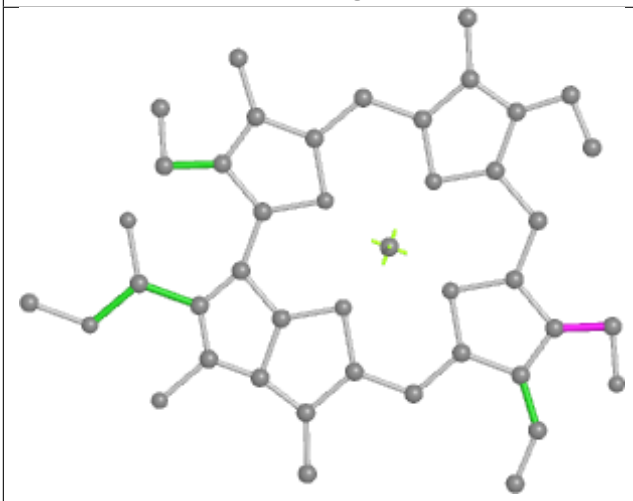
Ligand CHL S 607



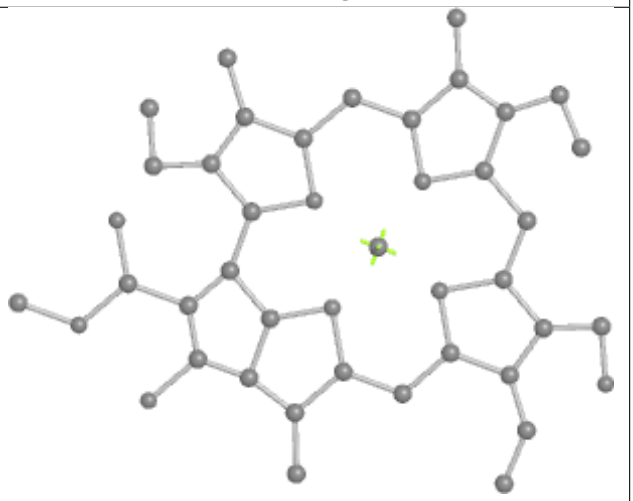
Bond lengths



Bond angles

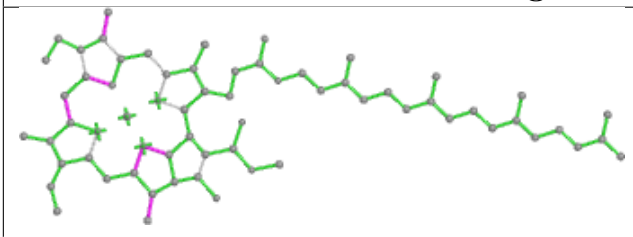


Torsions

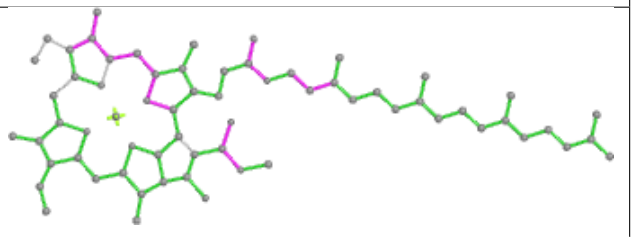


Rings

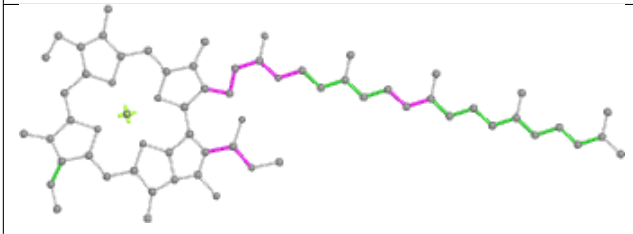
Ligand CLA b 509



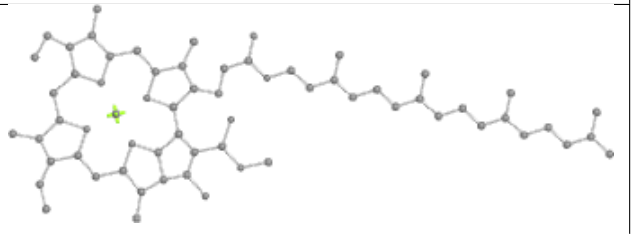
Bond lengths



Bond angles

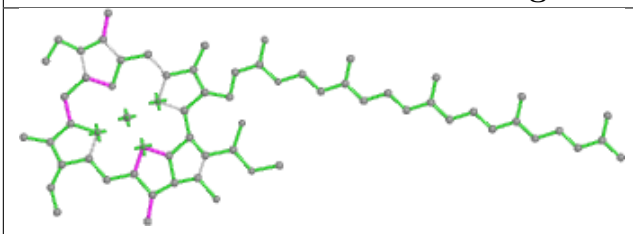


Torsions

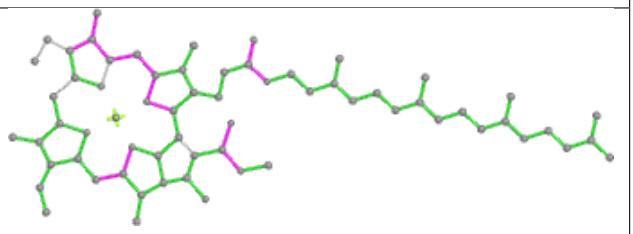


Rings

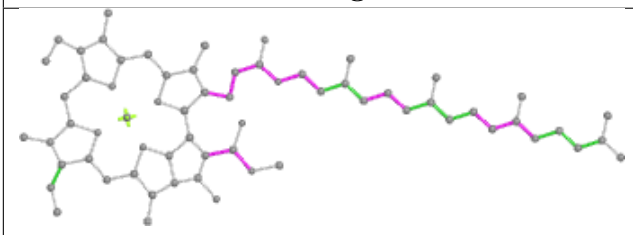
Ligand CLA c 506



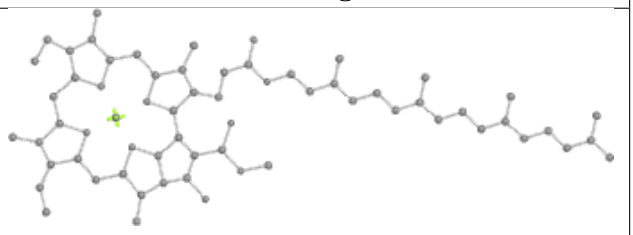
Bond lengths



Bond angles

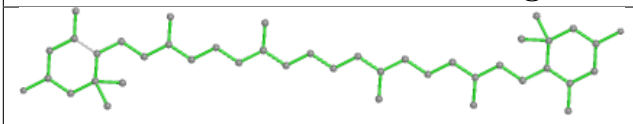


Torsions

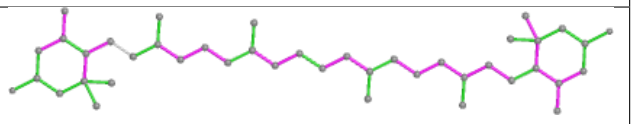


Rings

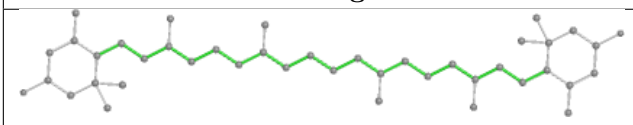
Ligand LUT G 616



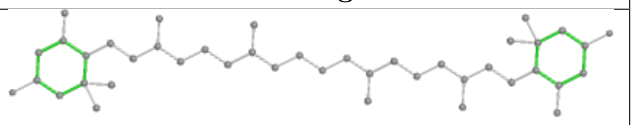
Bond lengths



Bond angles

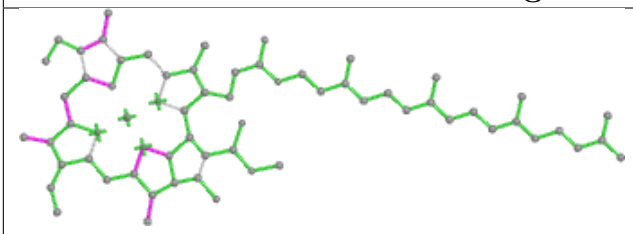


Torsions

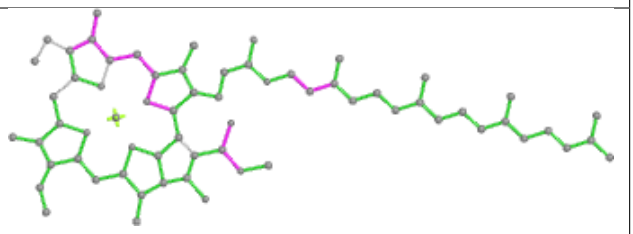


Rings

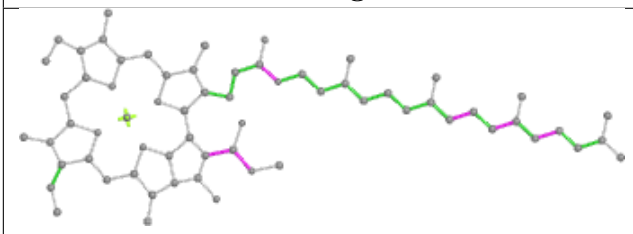
Ligand CLA C 502



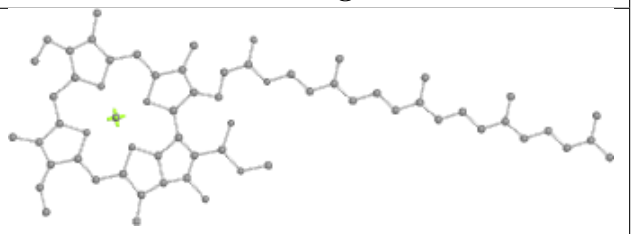
Bond lengths



Bond angles

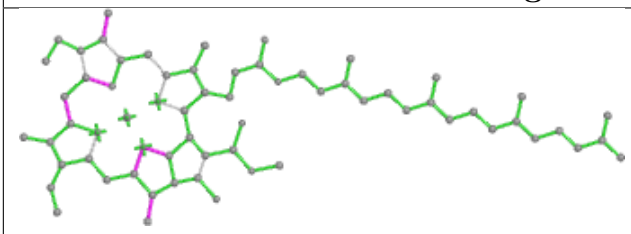


Torsions

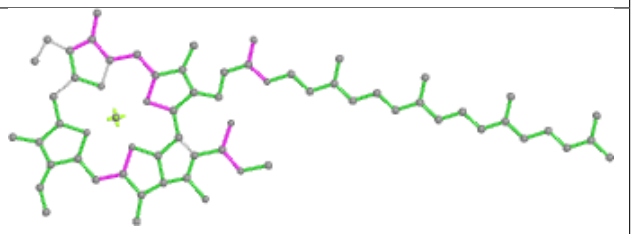


Rings

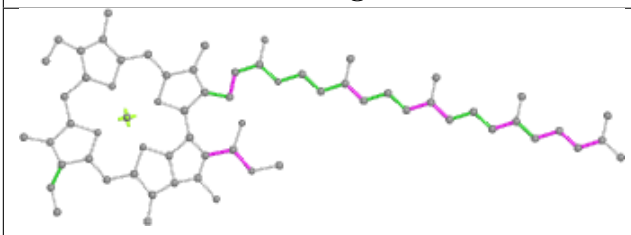
Ligand CLA B 508



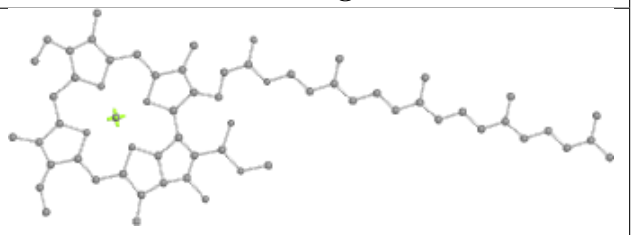
Bond lengths



Bond angles

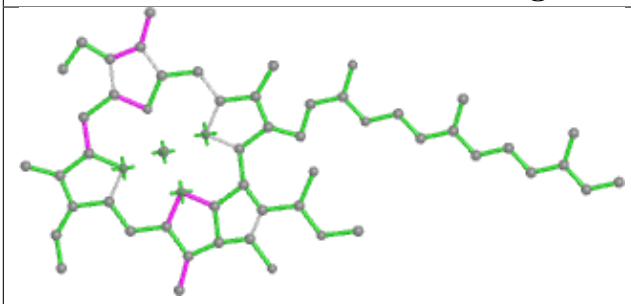


Torsions

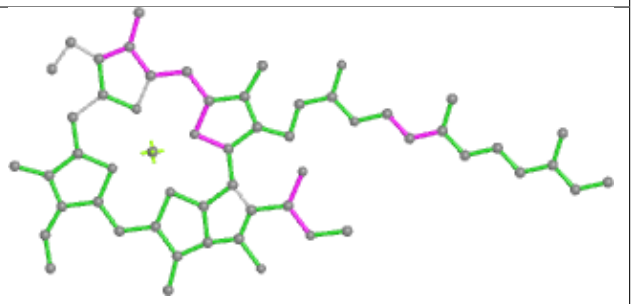


Rings

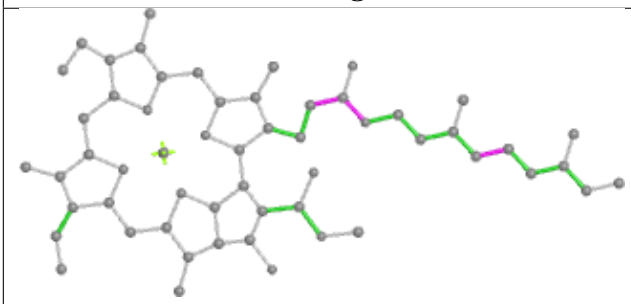
Ligand CLA c 512



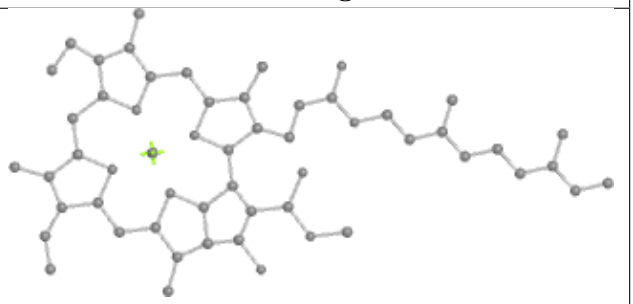
Bond lengths



Bond angles

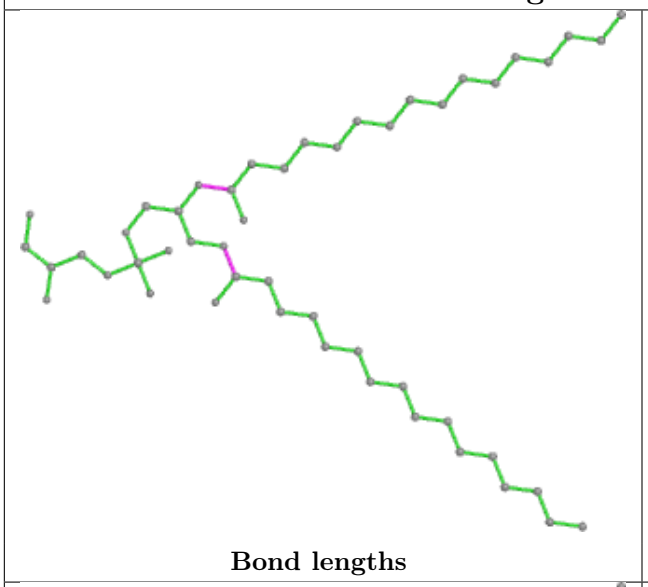


Torsions

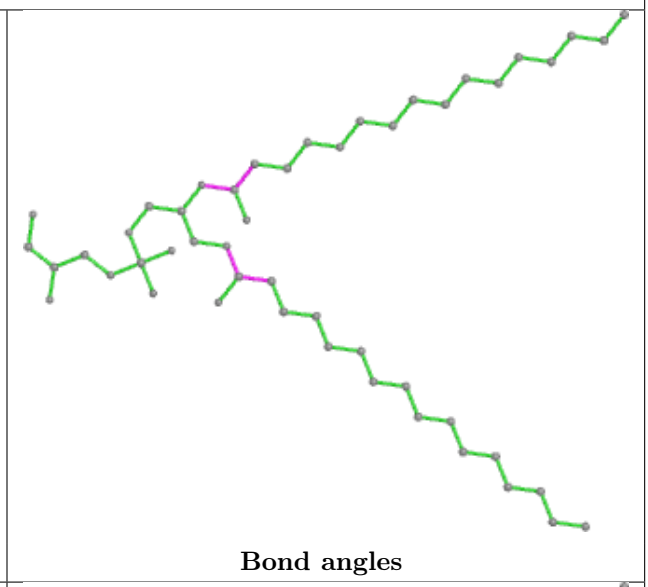


Rings

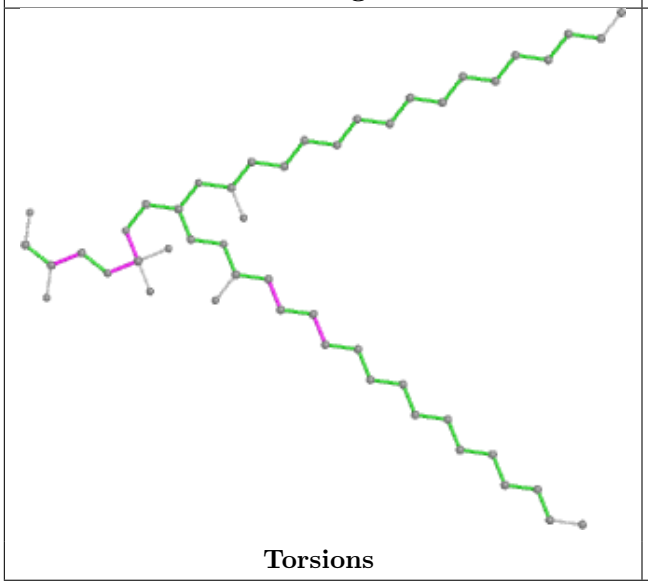
Ligand LHG b 521



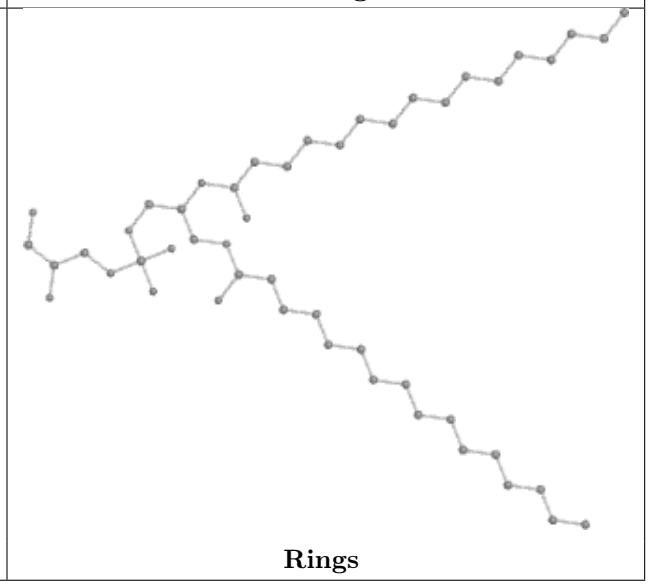
Bond lengths



Bond angles

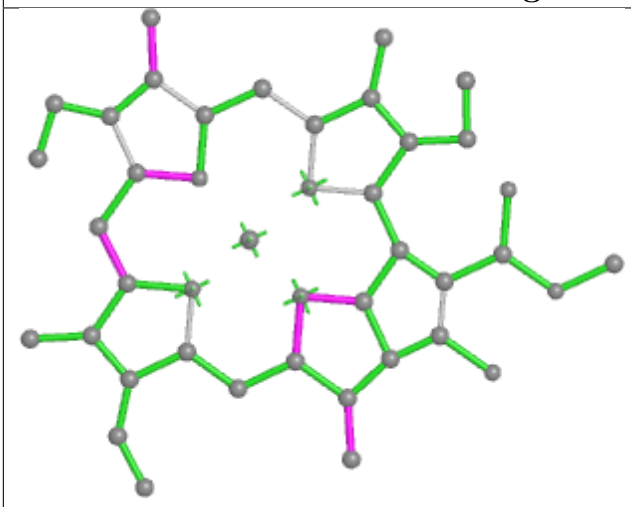


Torsions

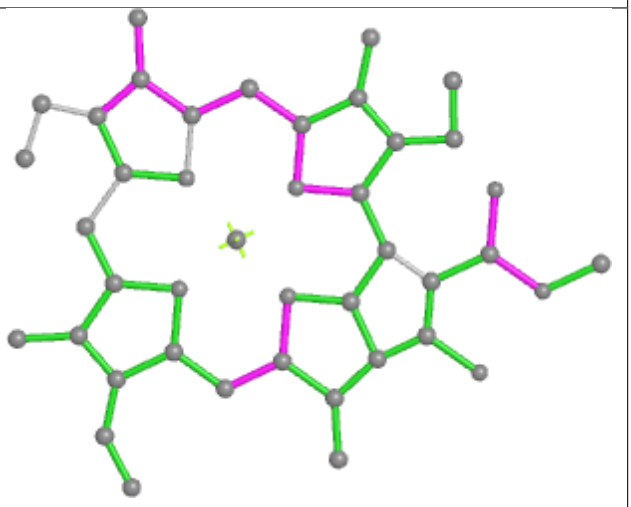


Rings

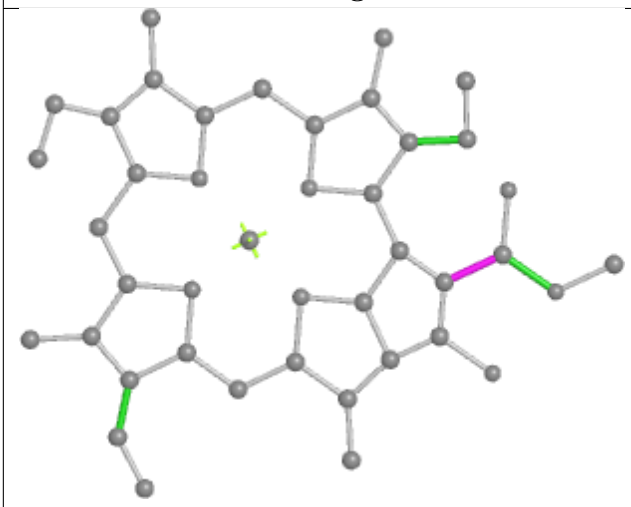
Ligand CLA G 614



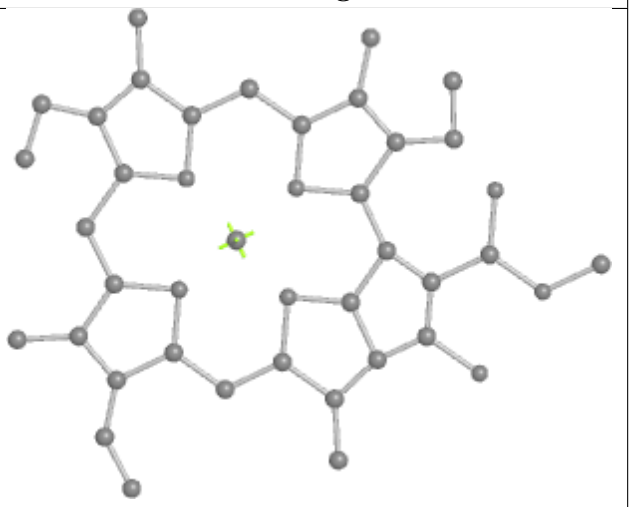
Bond lengths



Bond angles

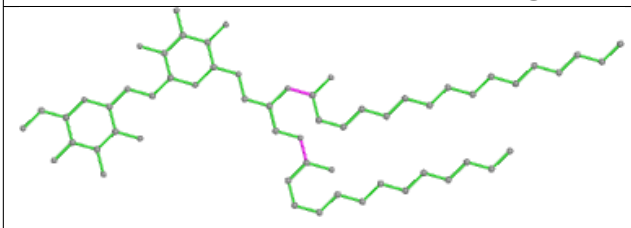


Torsions

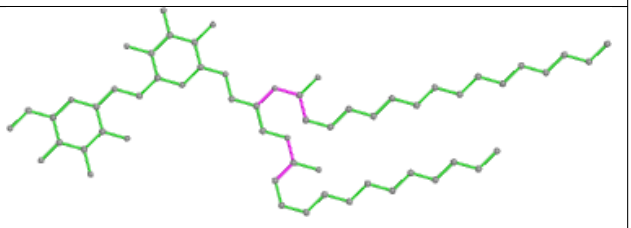


Rings

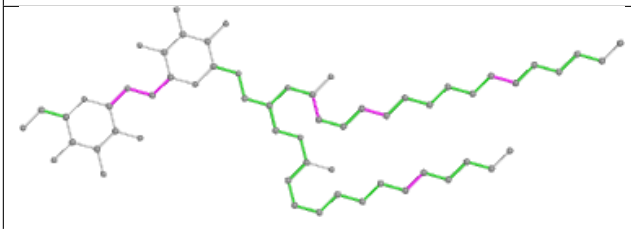
Ligand DGD c 517



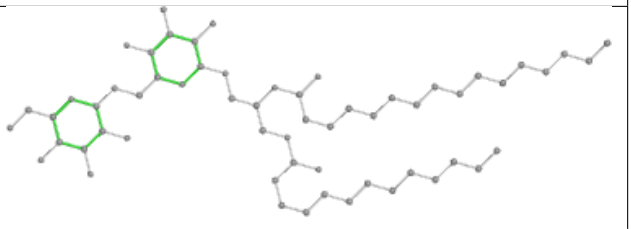
Bond lengths



Bond angles

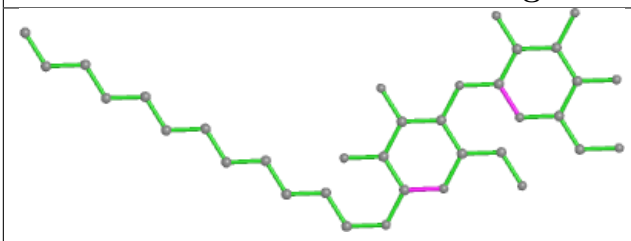


Torsions

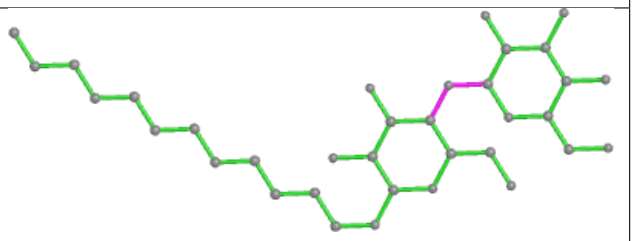


Rings

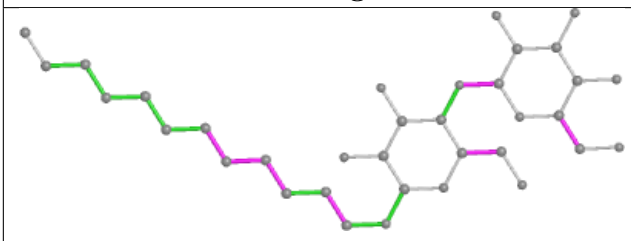
Ligand LMU S 619



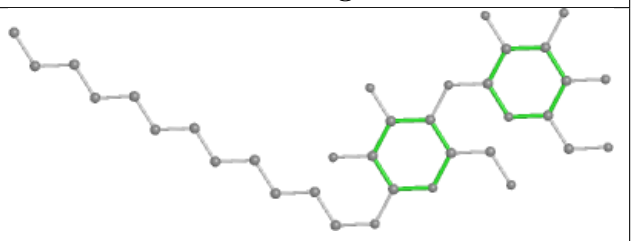
Bond lengths



Bond angles

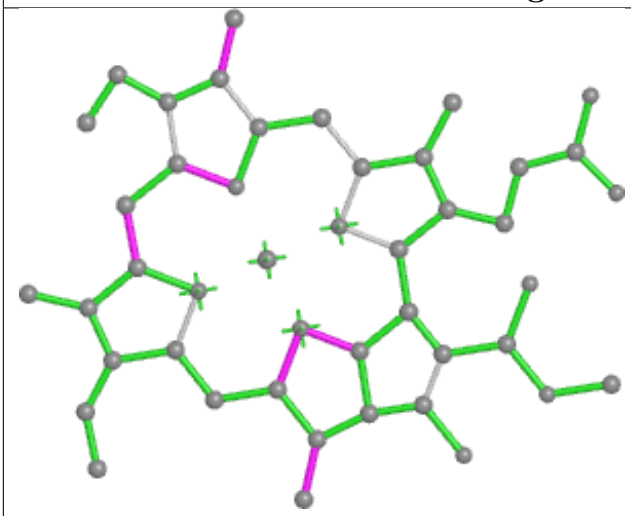


Torsions

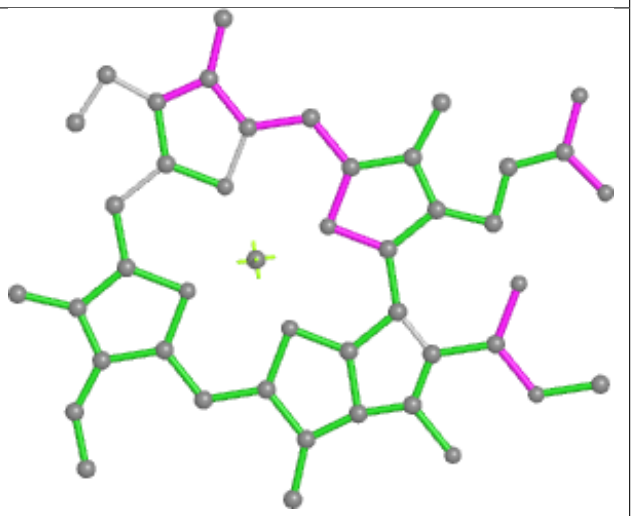


Rings

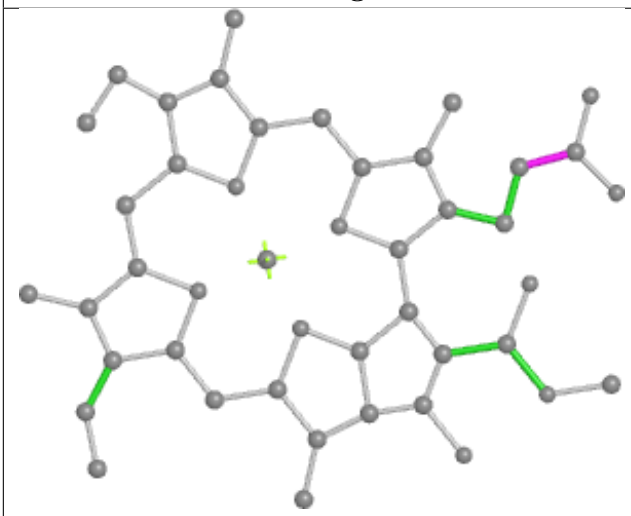
Ligand CLA S 612



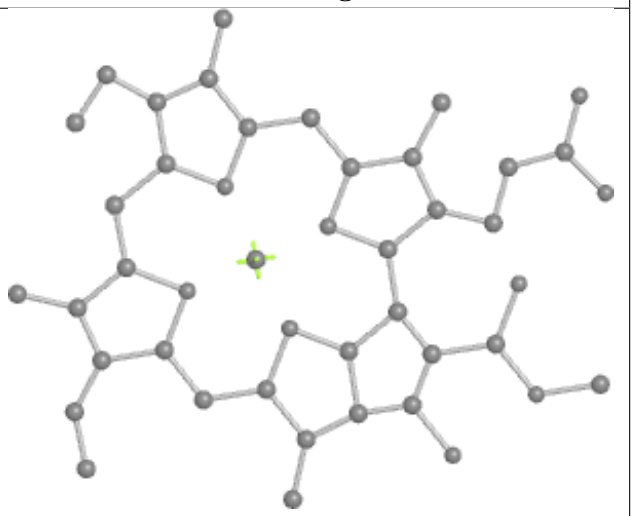
Bond lengths



Bond angles

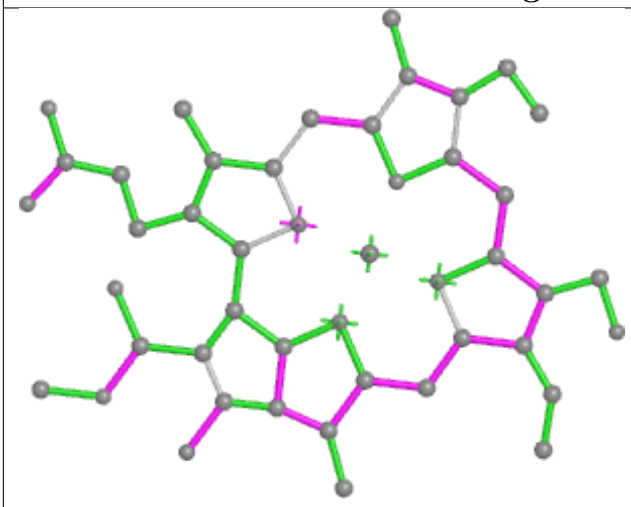


Torsions

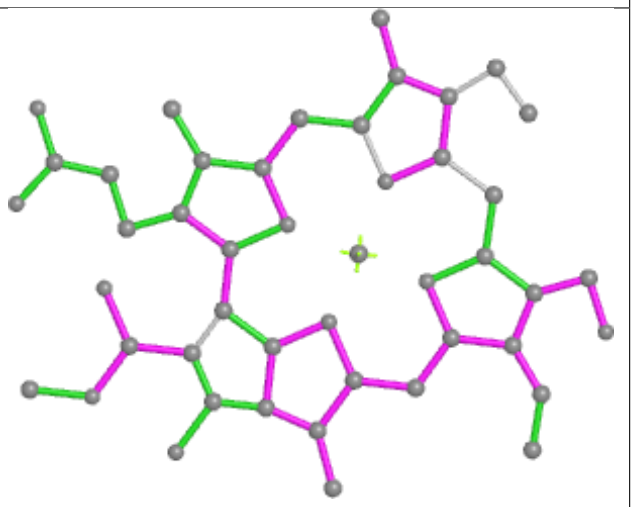


Rings

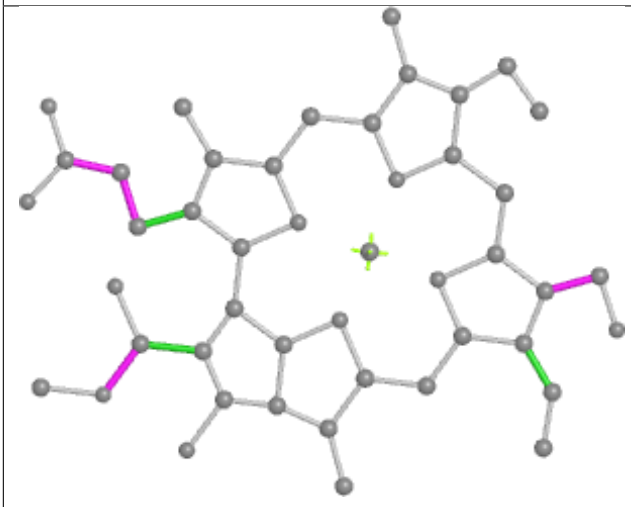
Ligand CHL N 307



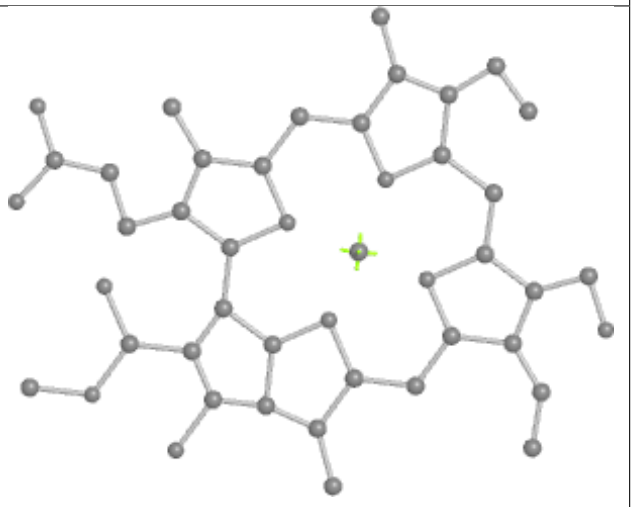
Bond lengths



Bond angles

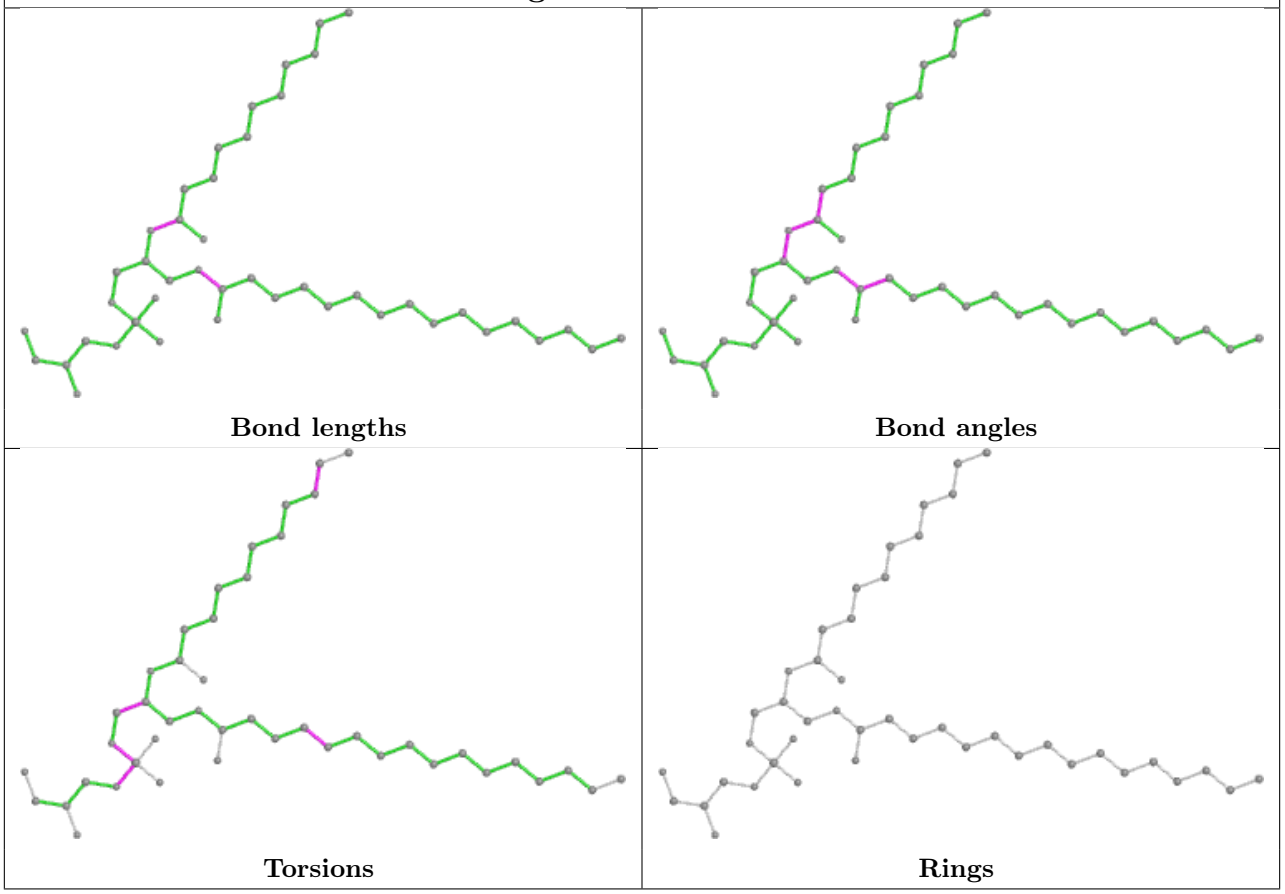


Torsions

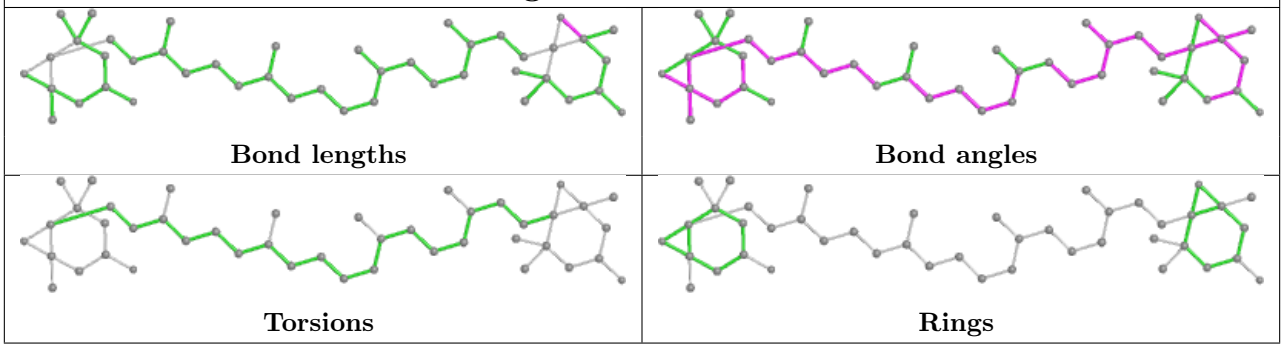


Rings

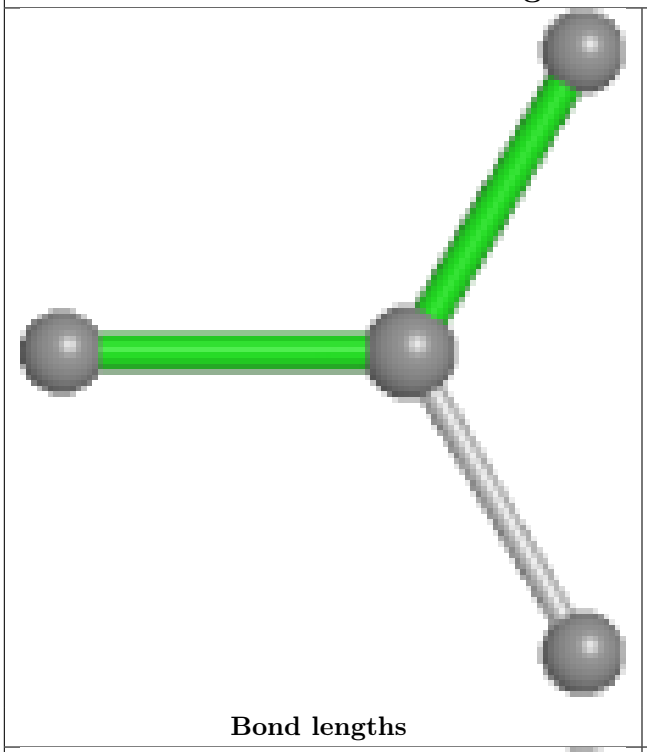
Ligand LHG a 411



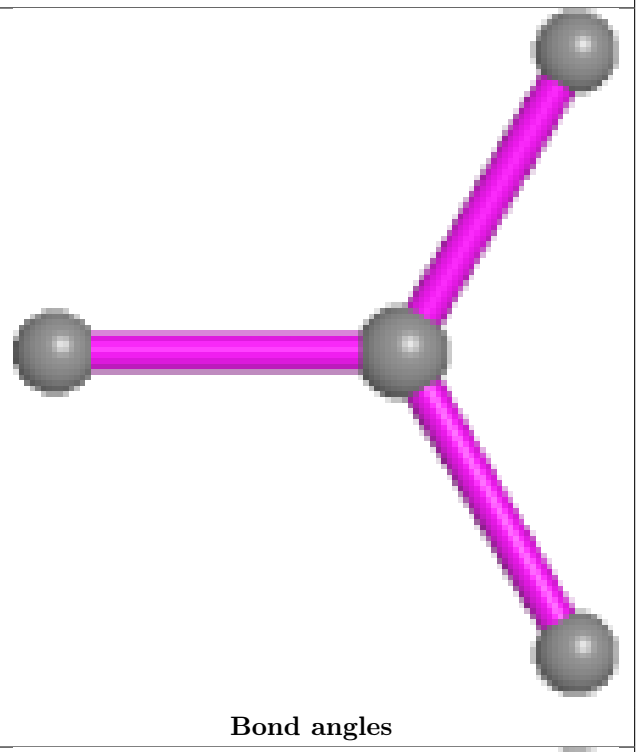
Ligand XAT N 301



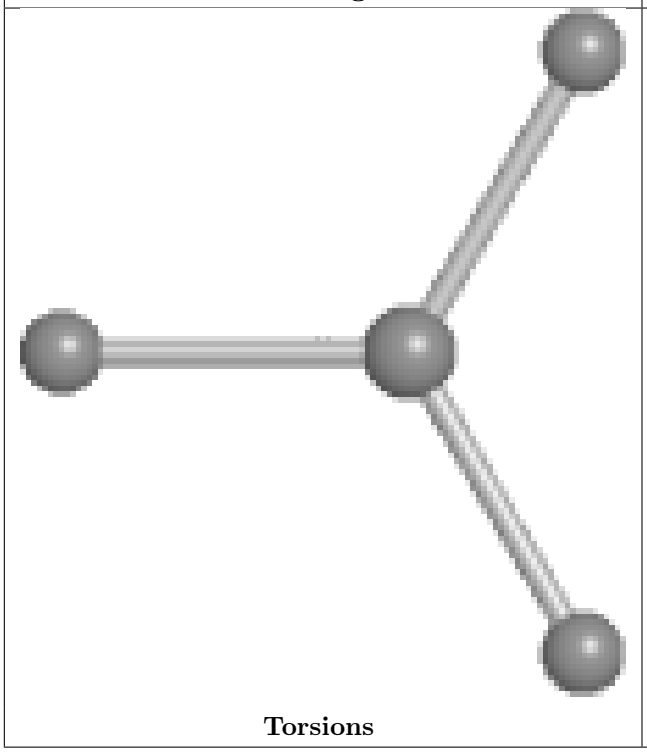
Ligand BCT D 403



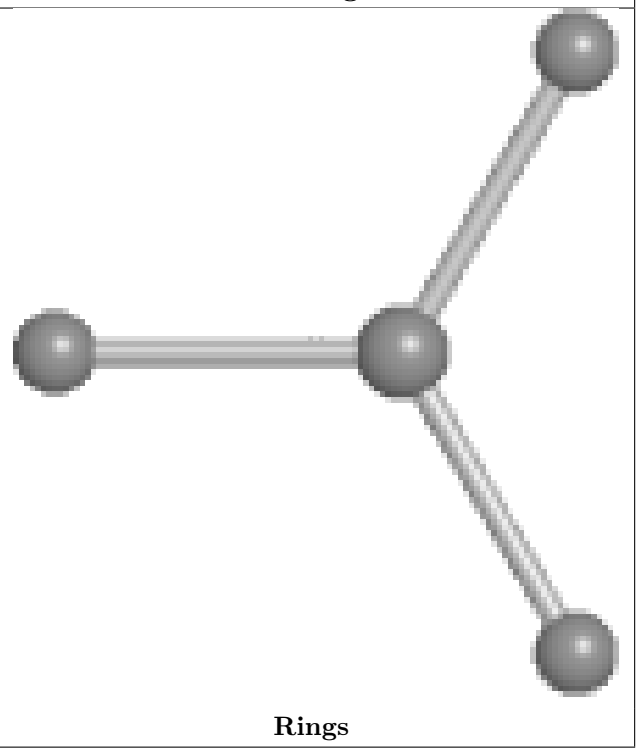
Bond lengths



Bond angles

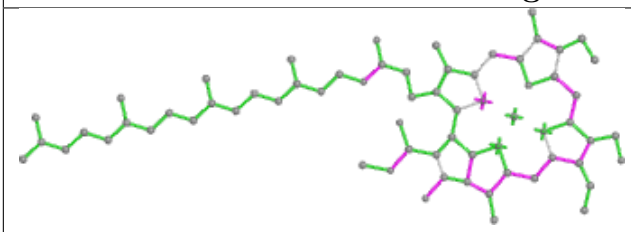


Torsions

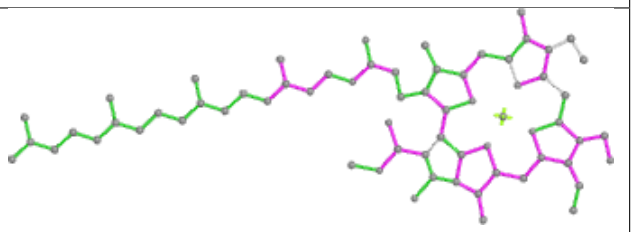


Rings

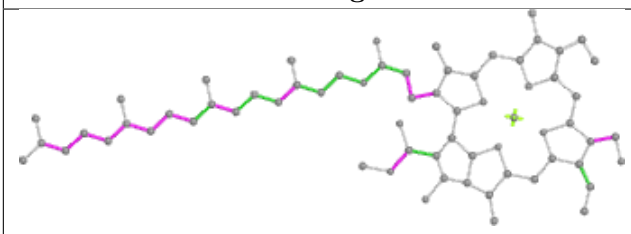
Ligand CHL G 619



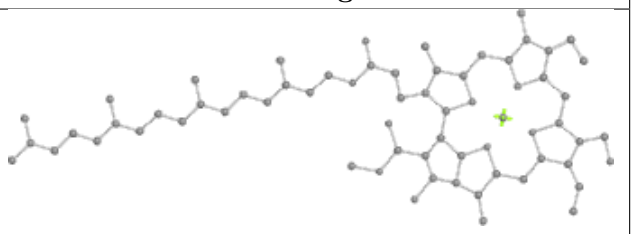
Bond lengths



Bond angles

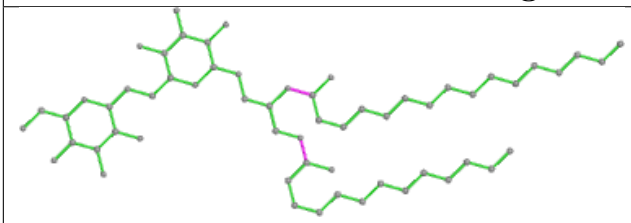


Torsions

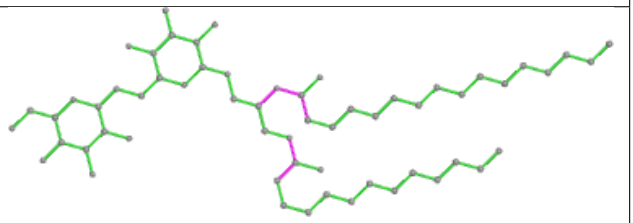


Rings

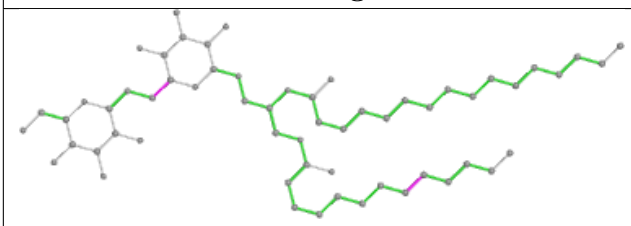
Ligand DGD C 519



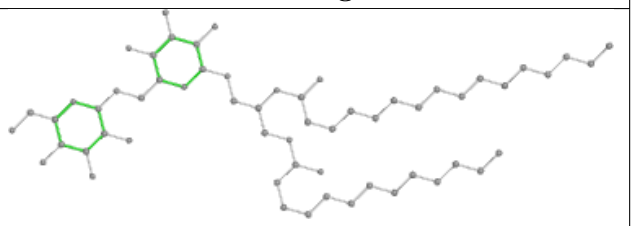
Bond lengths



Bond angles

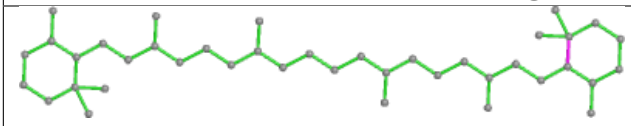


Torsions

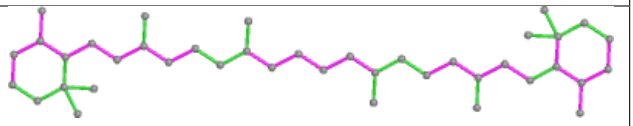


Rings

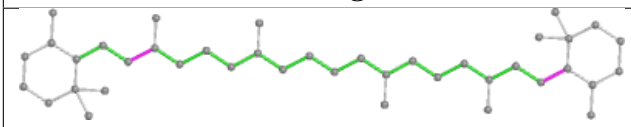
Ligand BCR b 517



Bond lengths



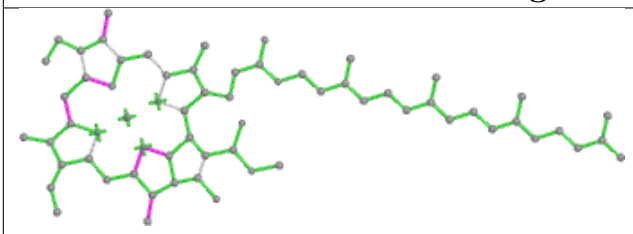
Bond angles



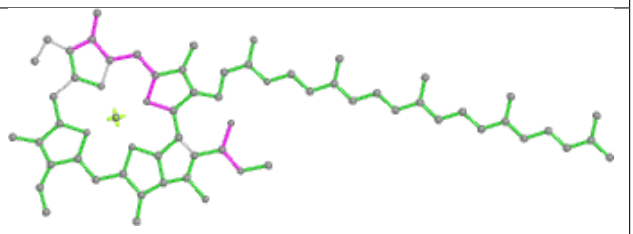
Torsions

Rings

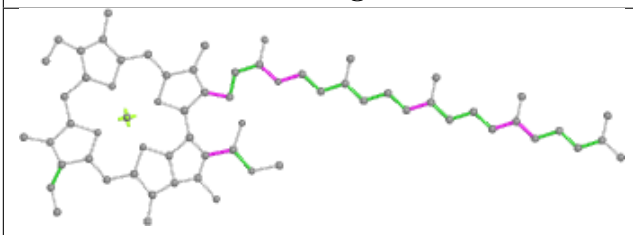
Ligand CLA c 507



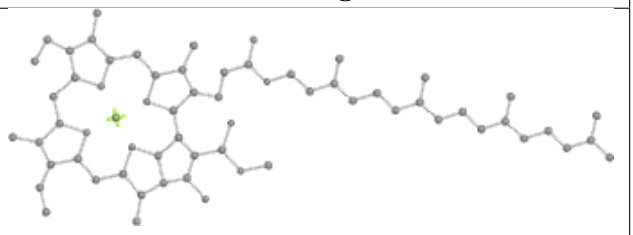
Bond lengths



Bond angles

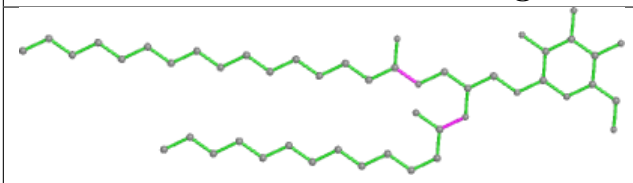


Torsions

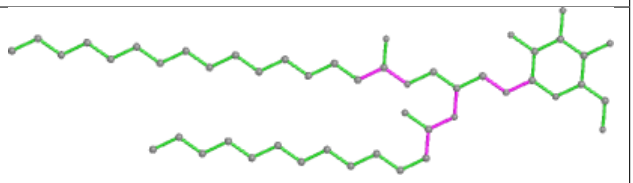


Rings

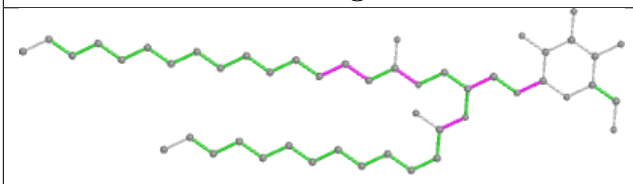
Ligand LMG W 201



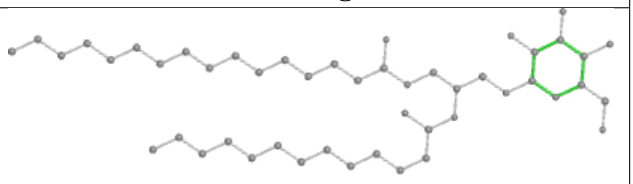
Bond lengths



Bond angles

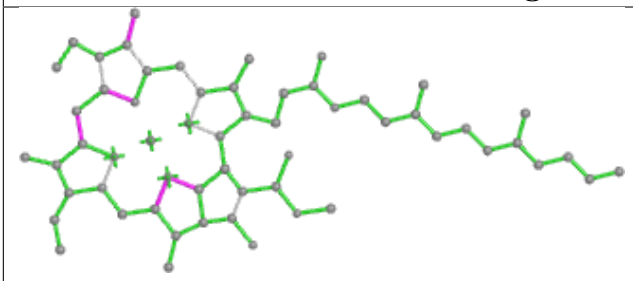


Torsions

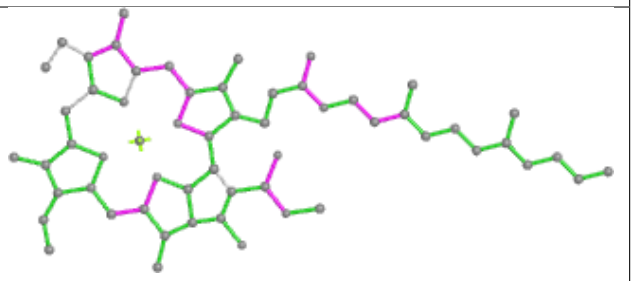


Rings

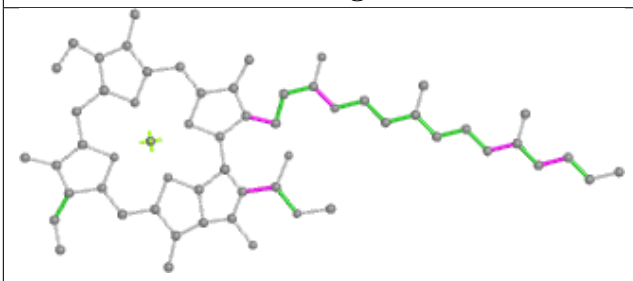
Ligand CLA Y 306



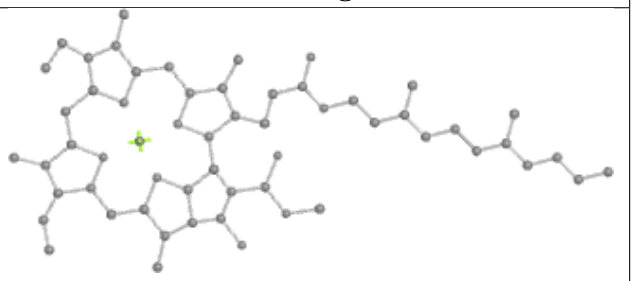
Bond lengths



Bond angles

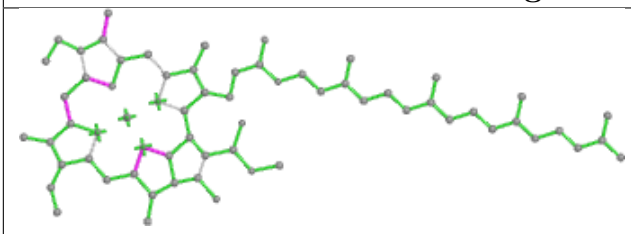


Torsions

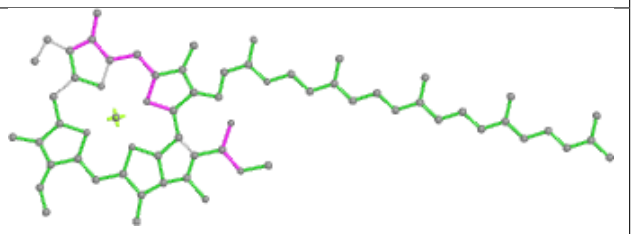


Rings

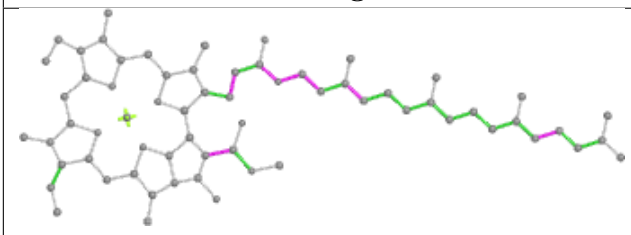
Ligand CLA C 509



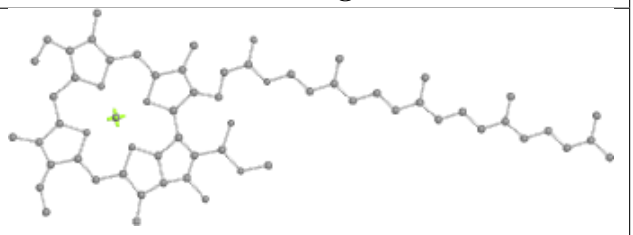
Bond lengths



Bond angles

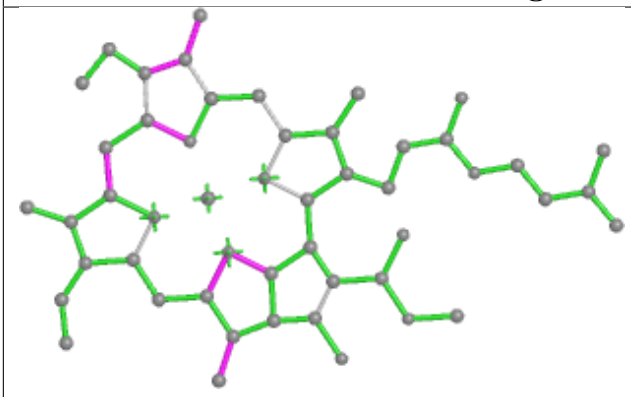


Torsions

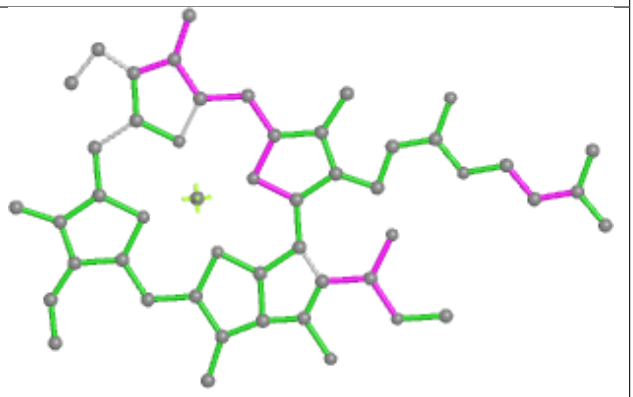


Rings

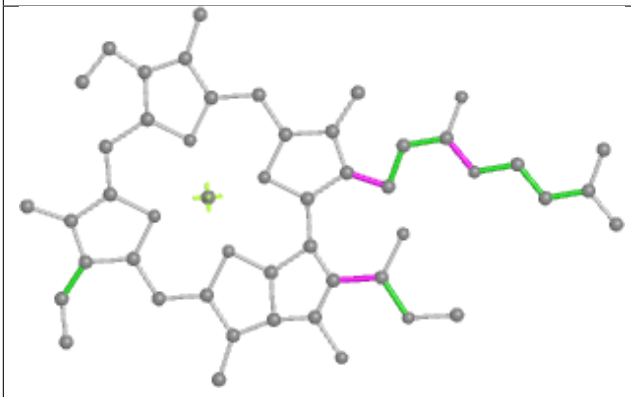
Ligand CLA S 605



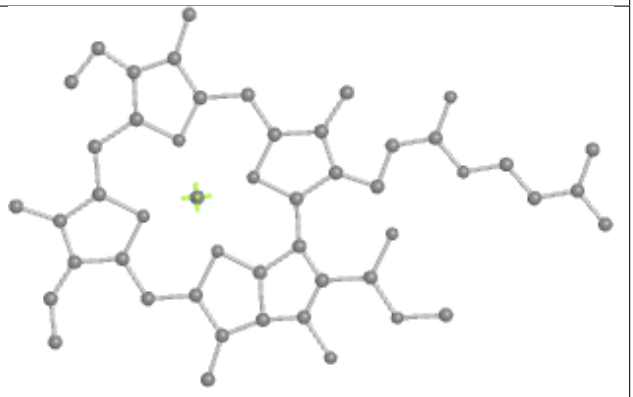
Bond lengths



Bond angles

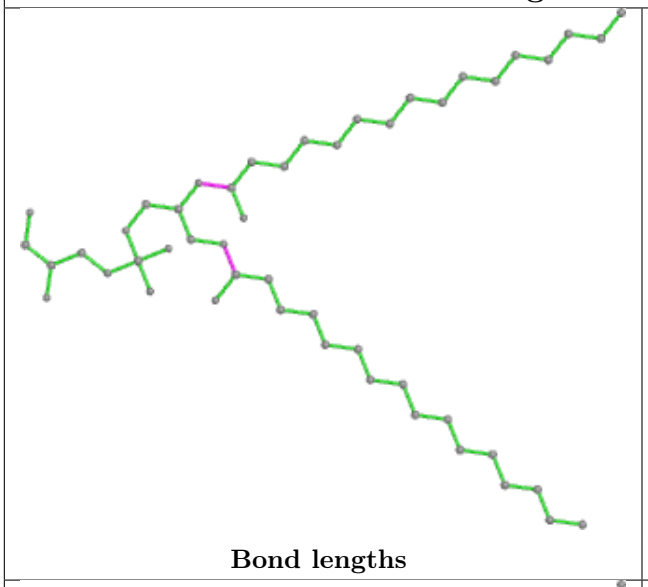


Torsions

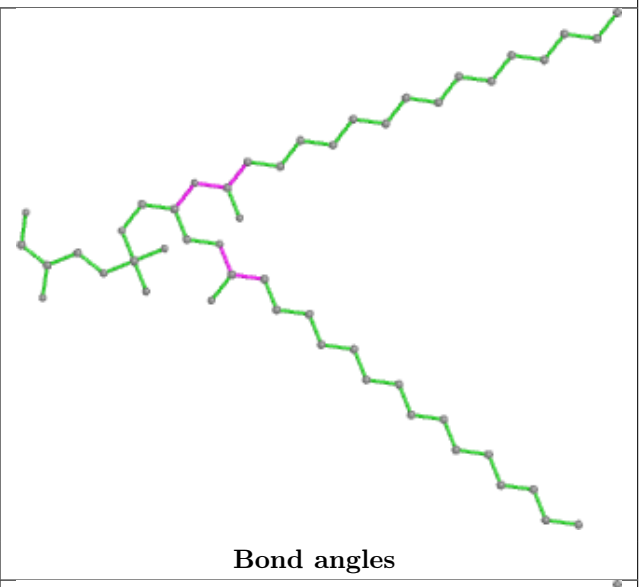


Rings

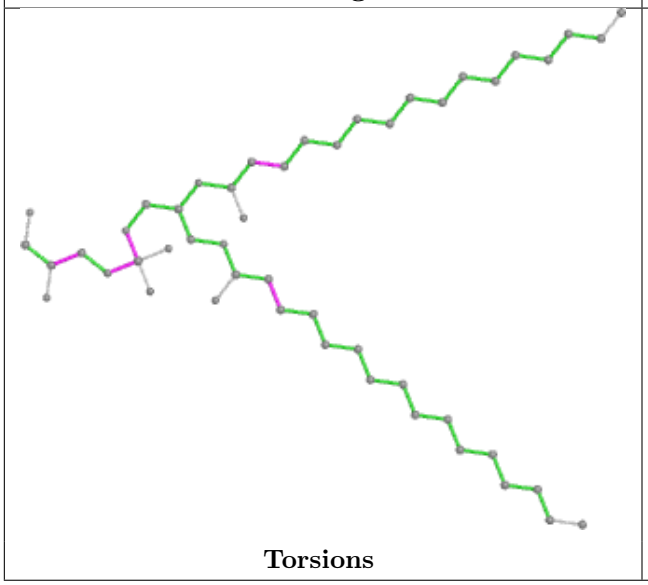
Ligand LHG d 408



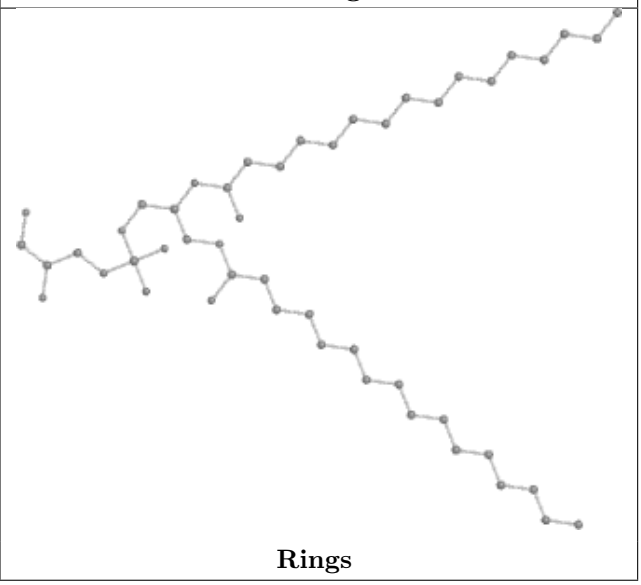
Bond lengths



Bond angles

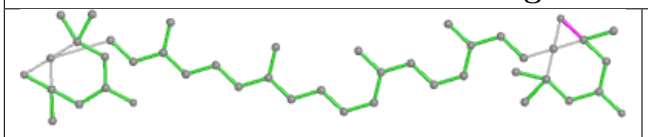


Torsions

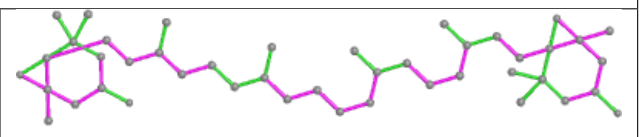


Rings

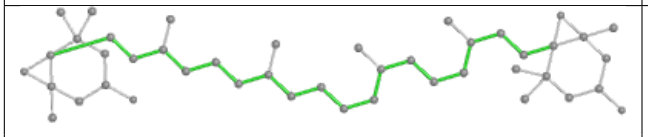
Ligand XAT Y 302



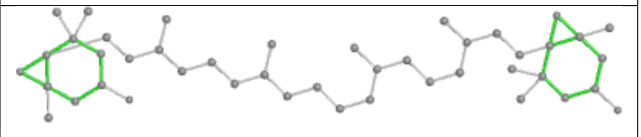
Bond lengths



Bond angles

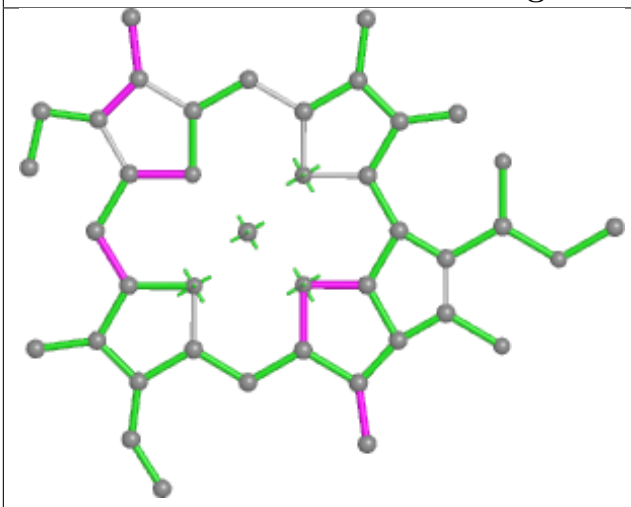


Torsions

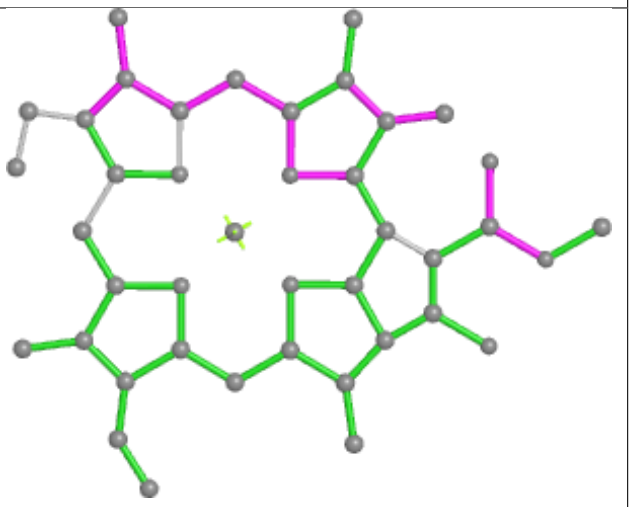


Rings

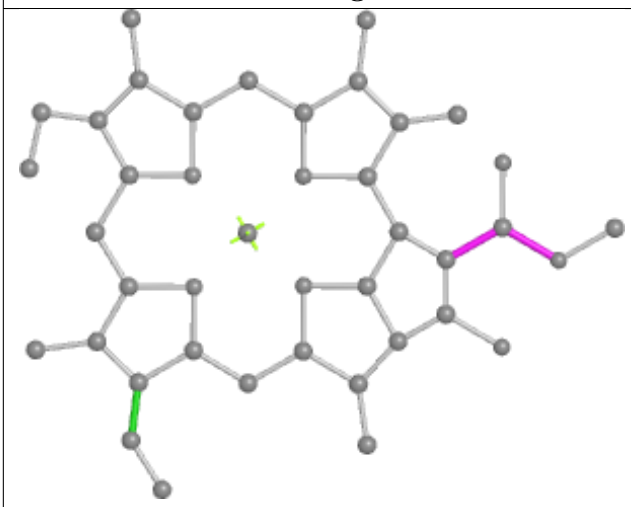
Ligand CLA S 609



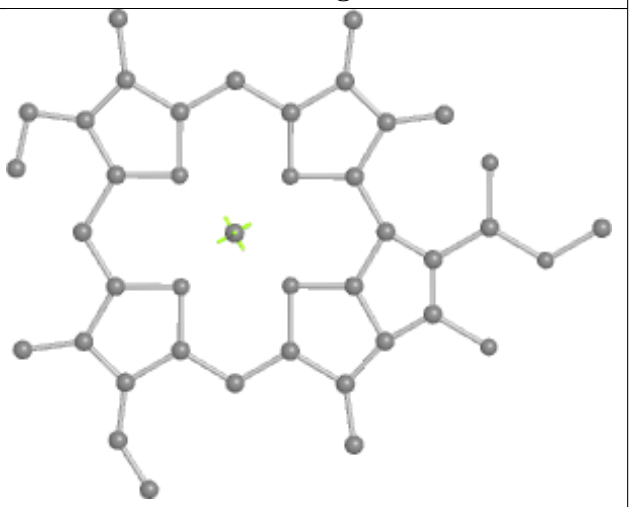
Bond lengths



Bond angles

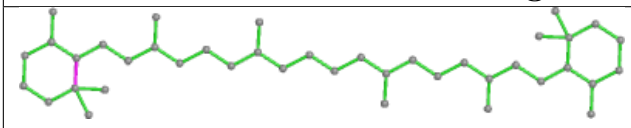


Torsions

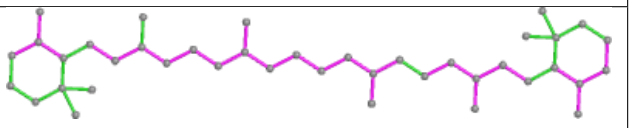


Rings

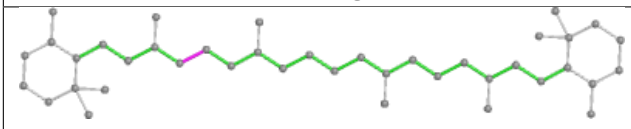
Ligand BCR k 101



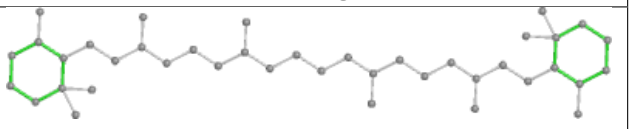
Bond lengths



Bond angles

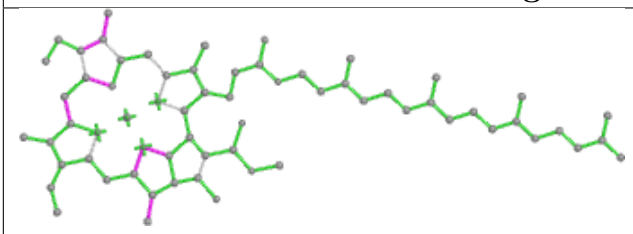


Torsions

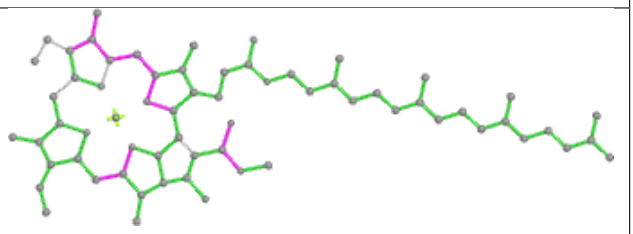


Rings

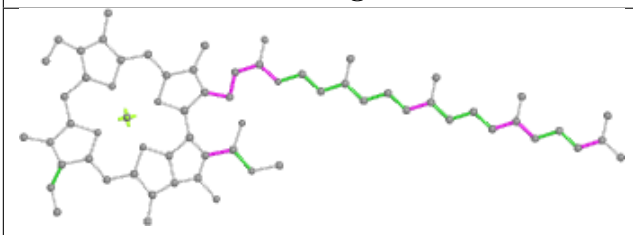
Ligand CLA G 603



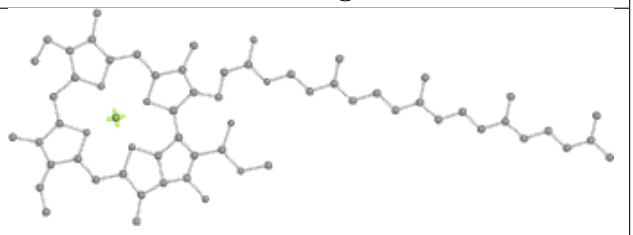
Bond lengths



Bond angles

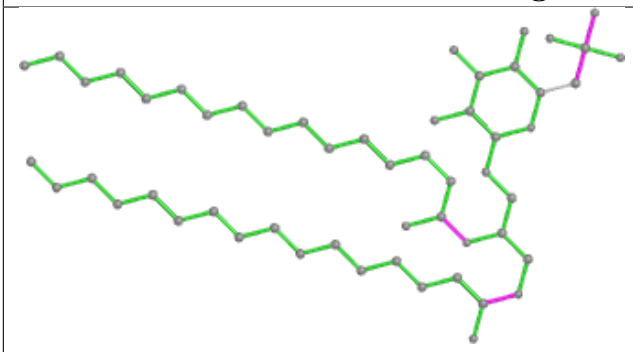


Torsions

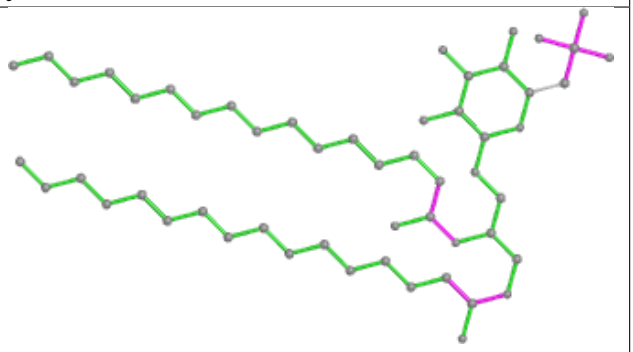


Rings

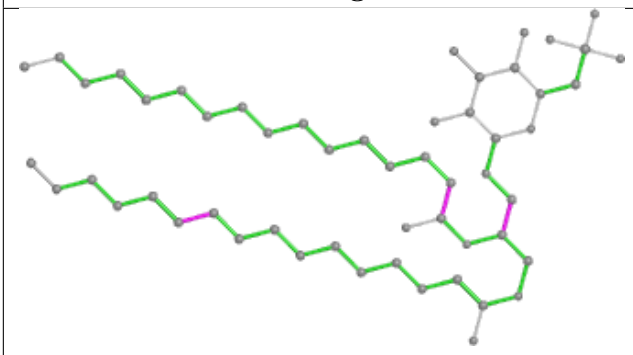
Ligand SQD t 102



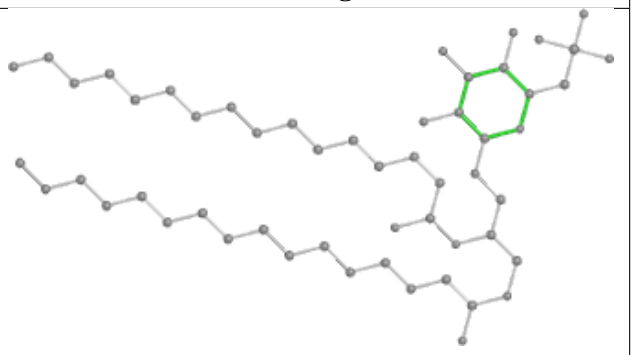
Bond lengths



Bond angles

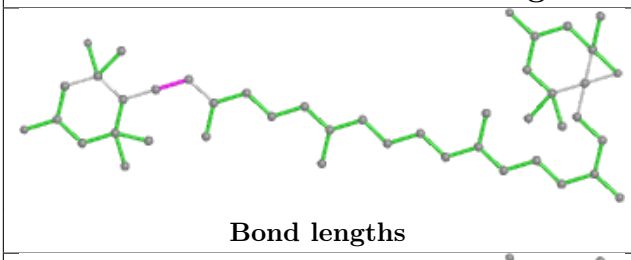


Torsions

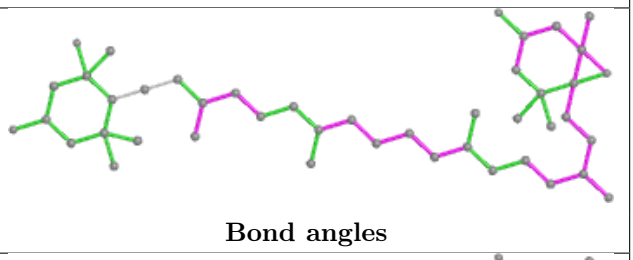


Rings

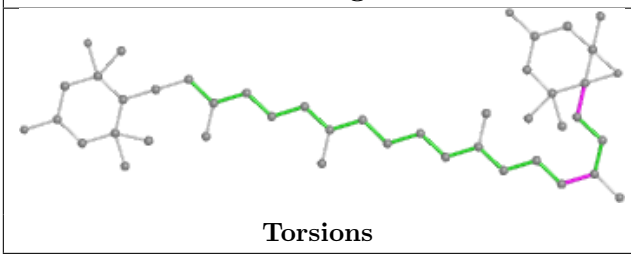
Ligand NEX r 310



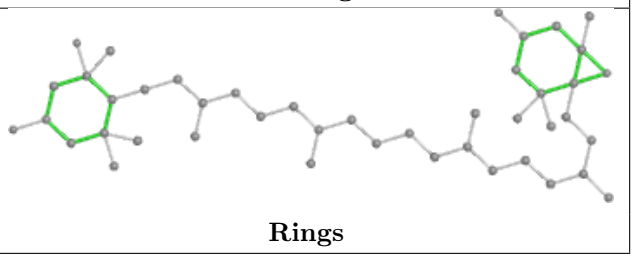
Bond lengths



Bond angles

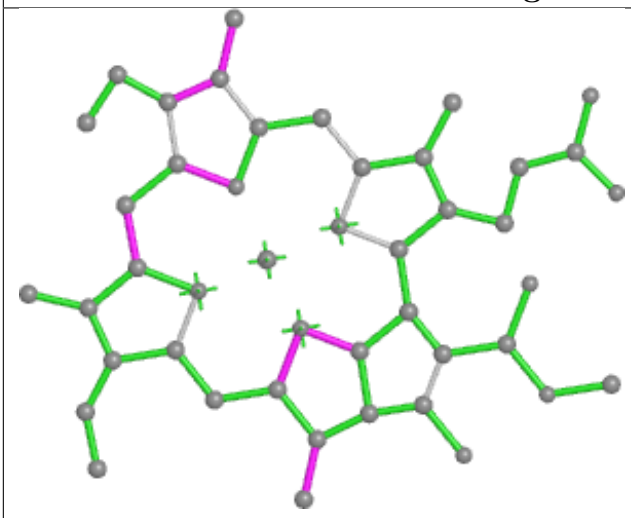


Torsions

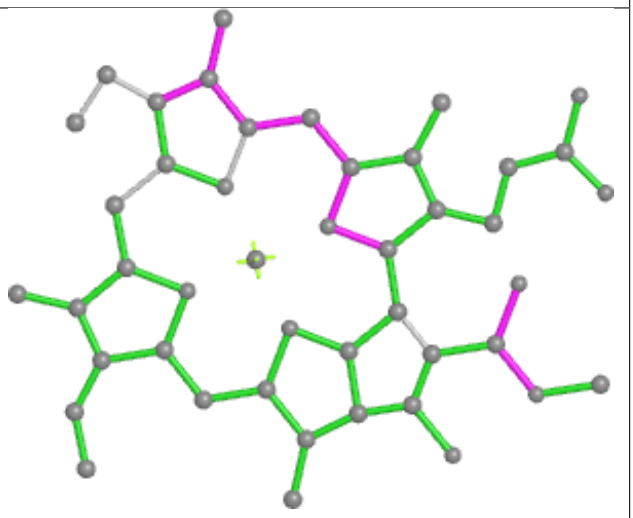


Rings

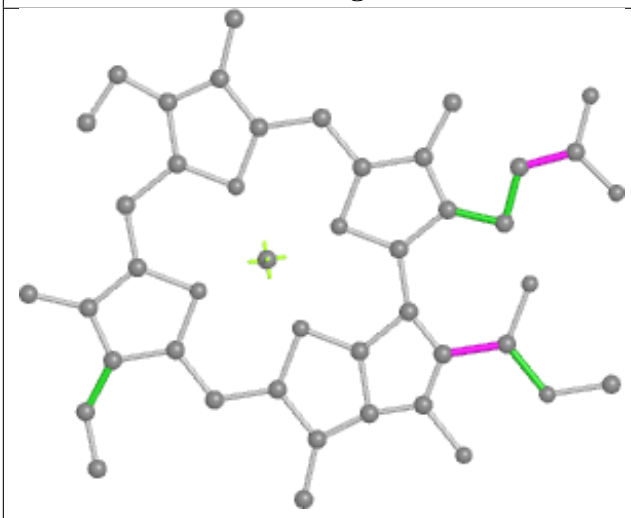
Ligand CLA N 313



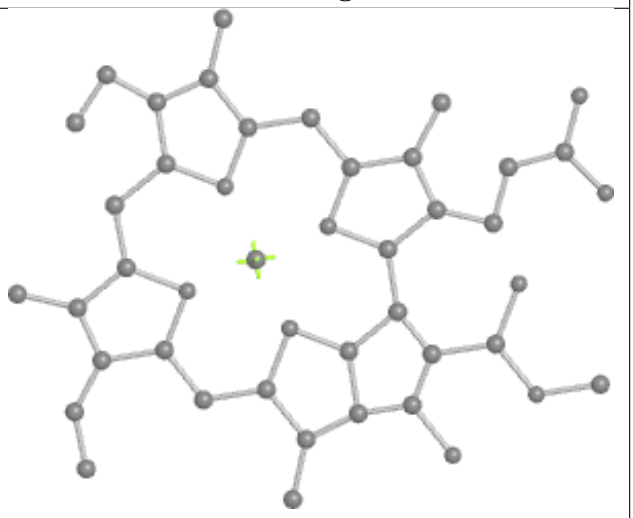
Bond lengths



Bond angles

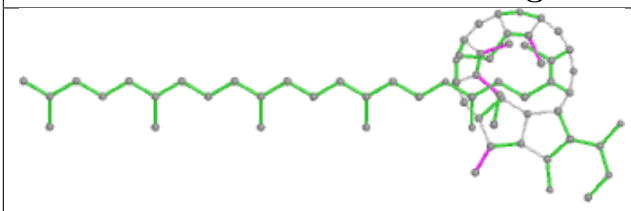


Torsions

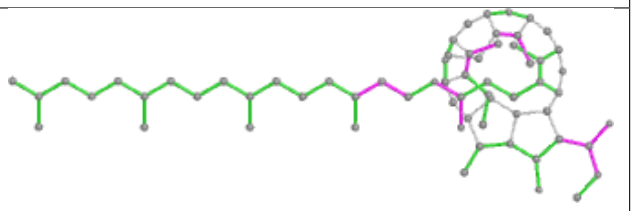


Rings

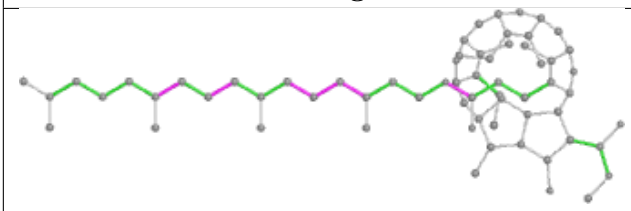
Ligand PHO a 404



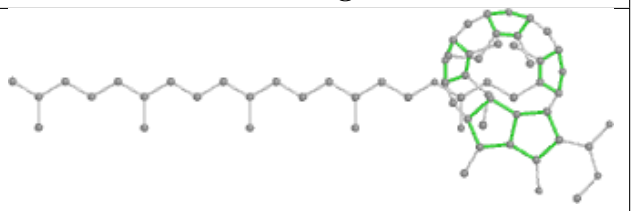
Bond lengths



Bond angles

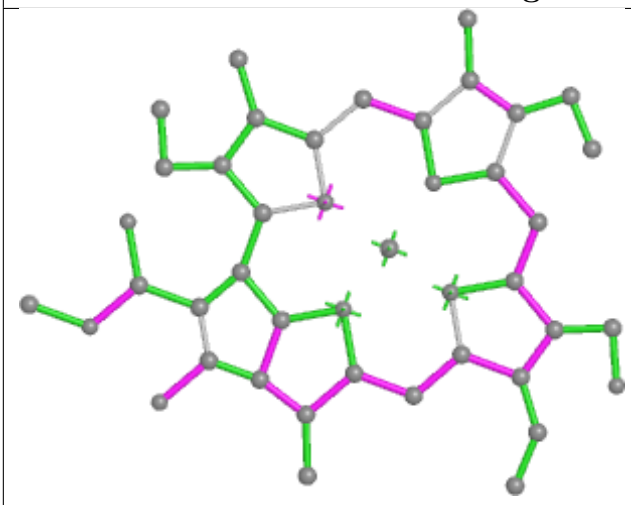


Torsions

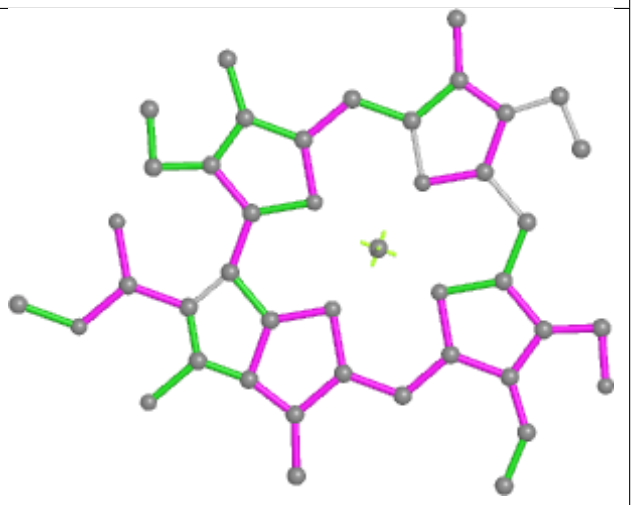


Rings

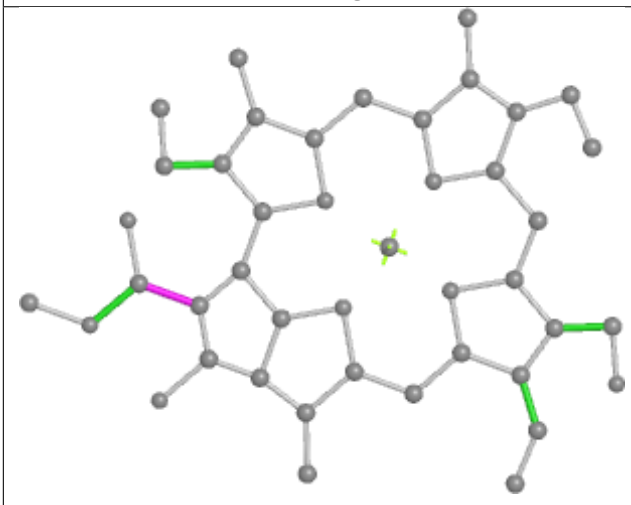
Ligand CHL G 606



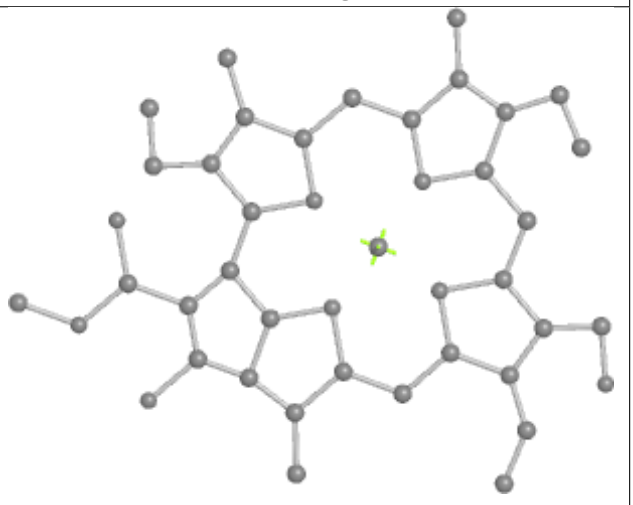
Bond lengths



Bond angles

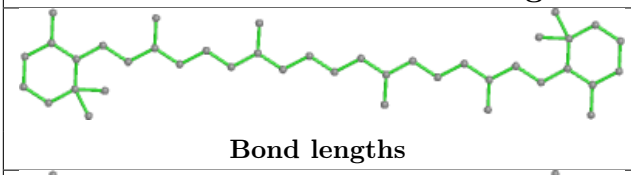


Torsions

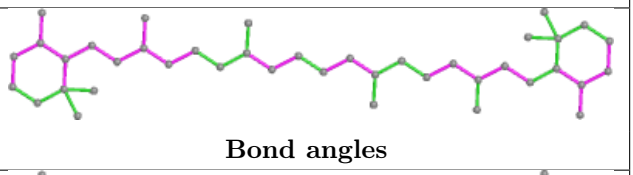


Rings

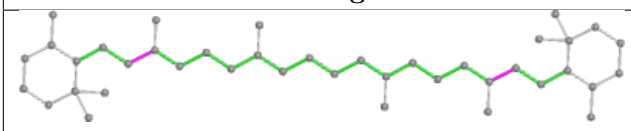
Ligand BCR b 519



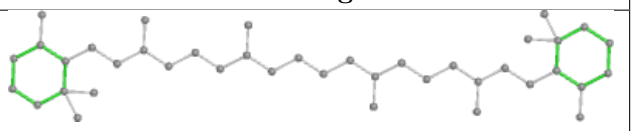
Bond lengths



Bond angles

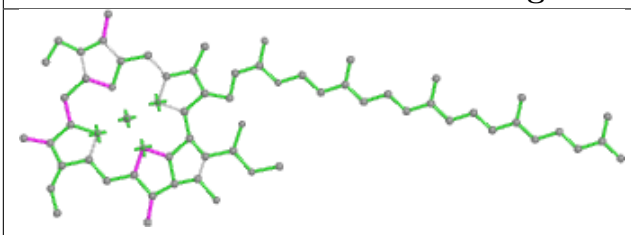


Torsions

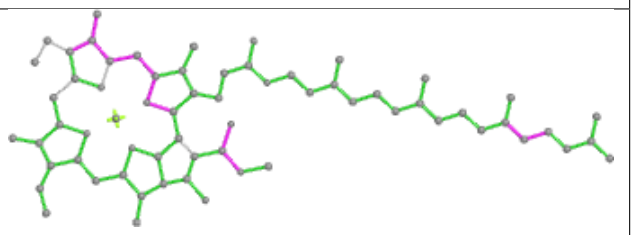


Rings

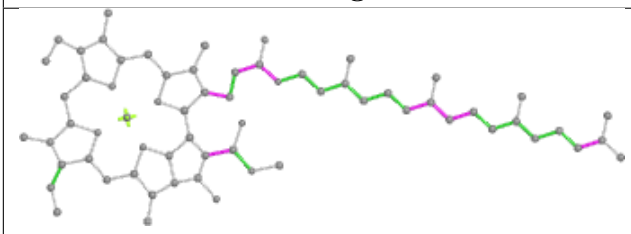
Ligand CLA b 512



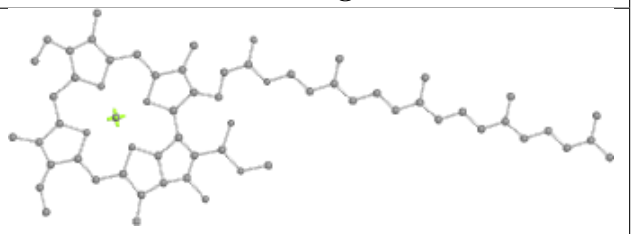
Bond lengths



Bond angles

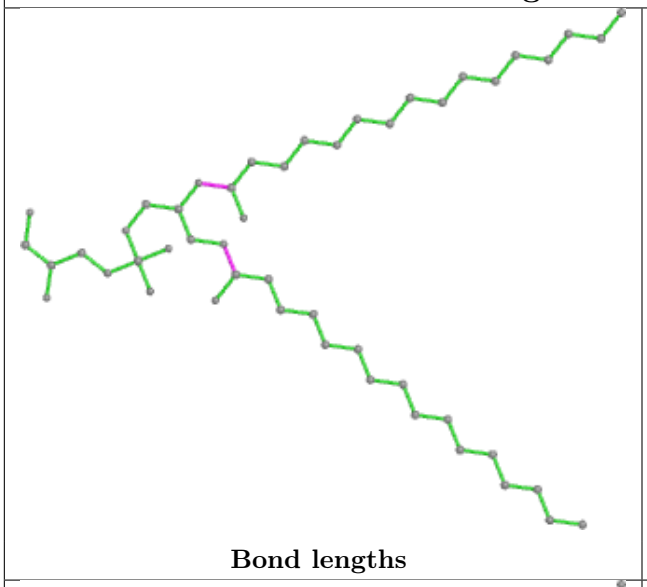


Torsions

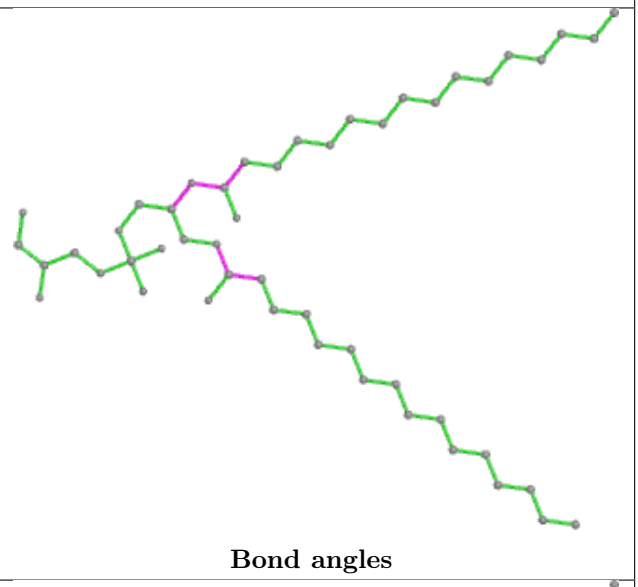


Rings

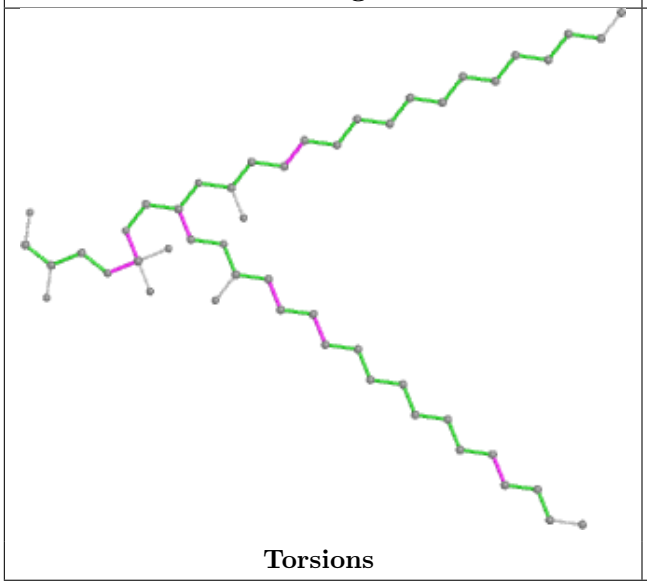
Ligand LHG N 319



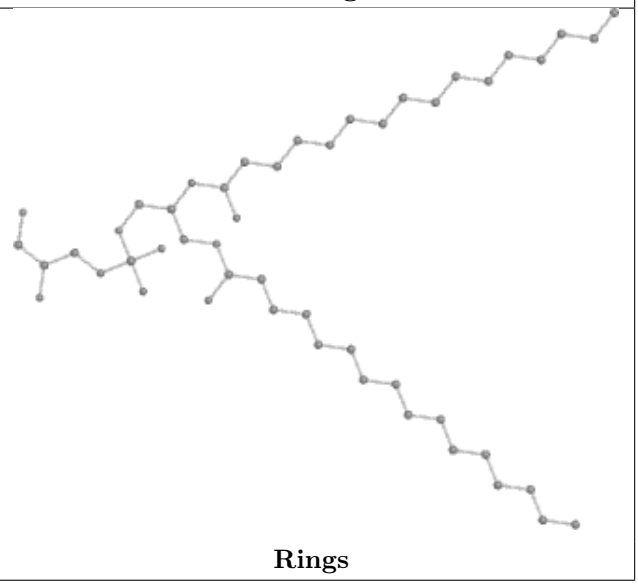
Bond lengths



Bond angles

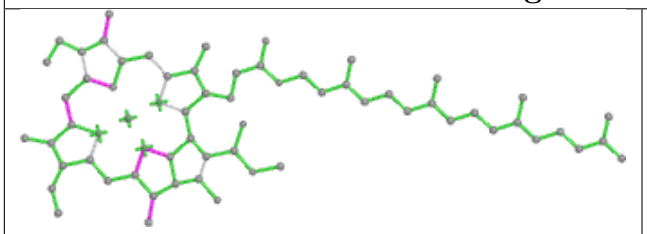


Torsions

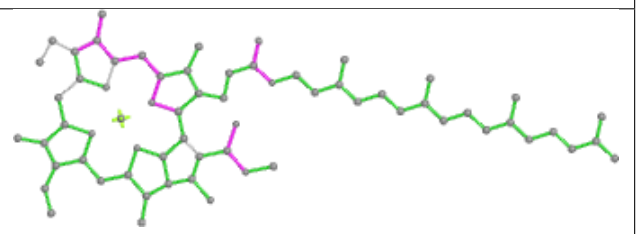


Rings

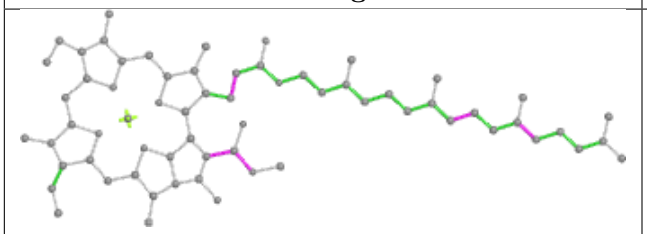
Ligand CLA N 311



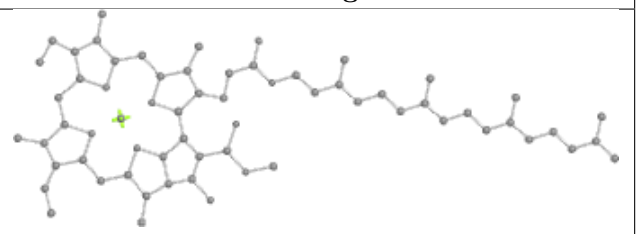
Bond lengths



Bond angles

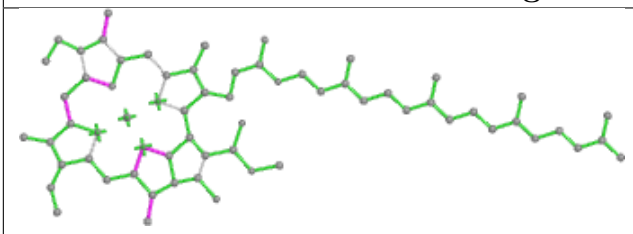


Torsions

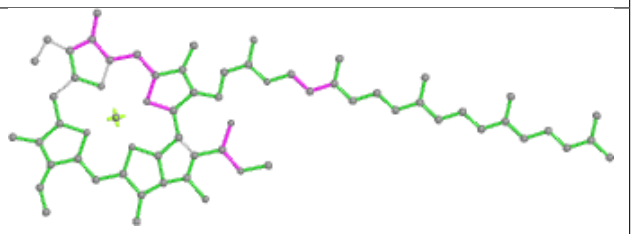


Rings

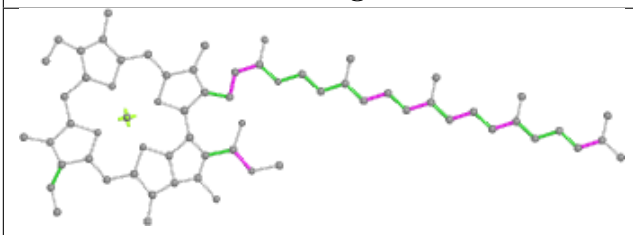
Ligand CLA G 602



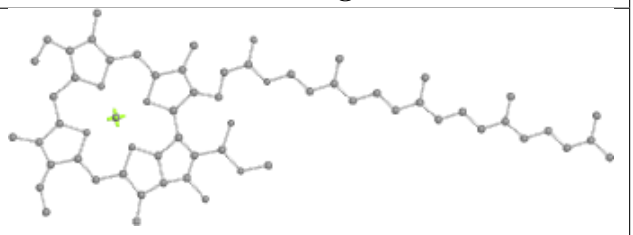
Bond lengths



Bond angles

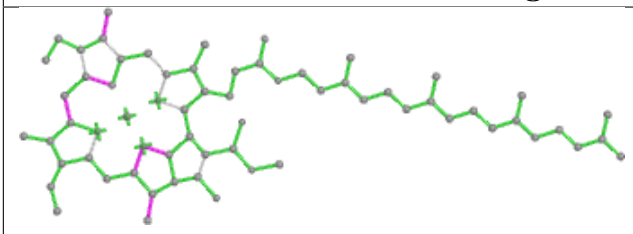


Torsions

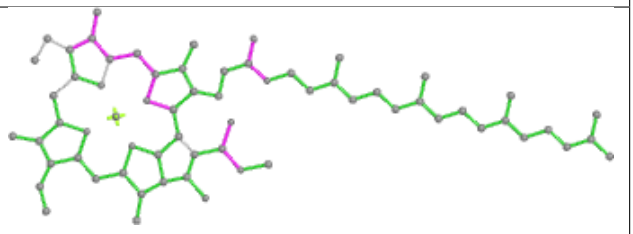


Rings

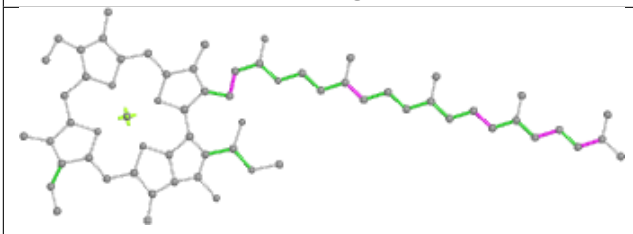
Ligand CLA B 503



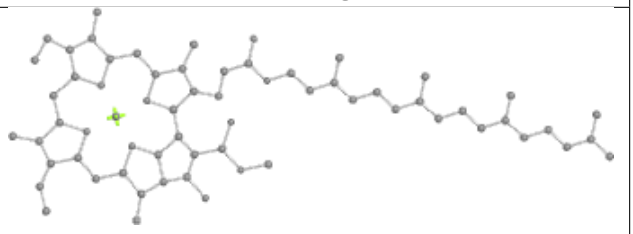
Bond lengths



Bond angles

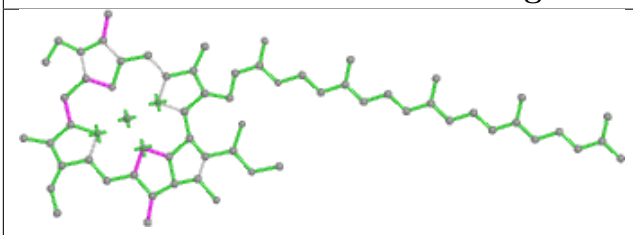


Torsions

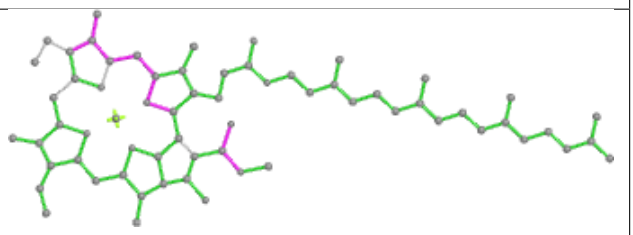


Rings

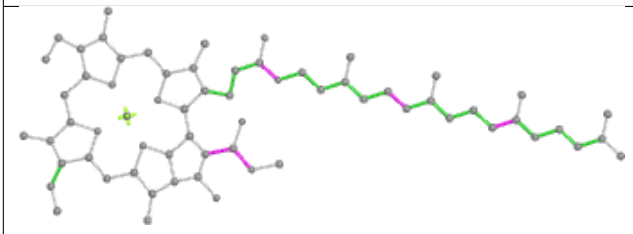
Ligand CLA B 507



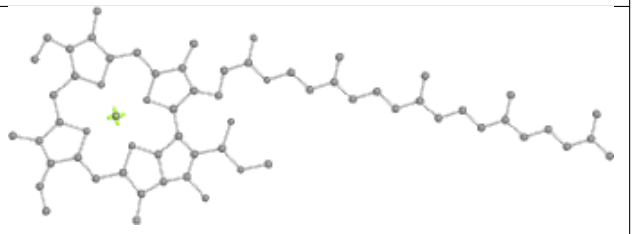
Bond lengths



Bond angles

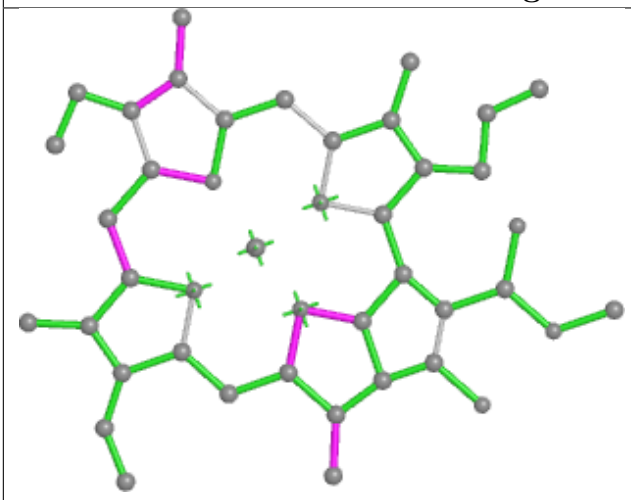


Torsions

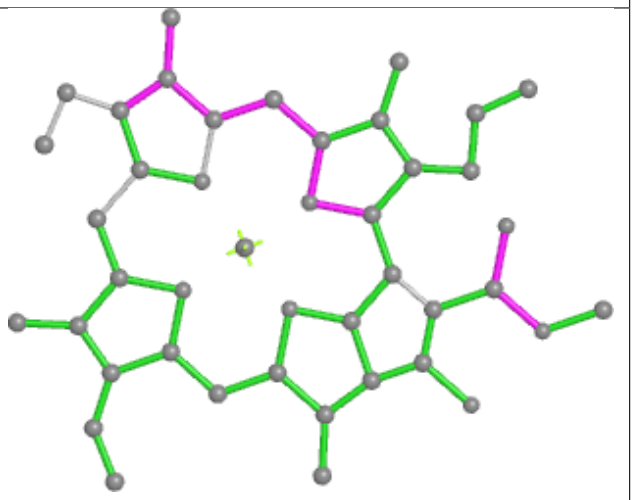


Rings

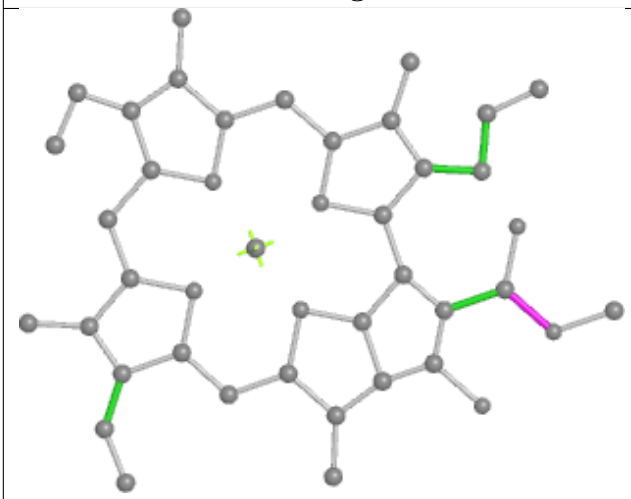
Ligand CLA G 612



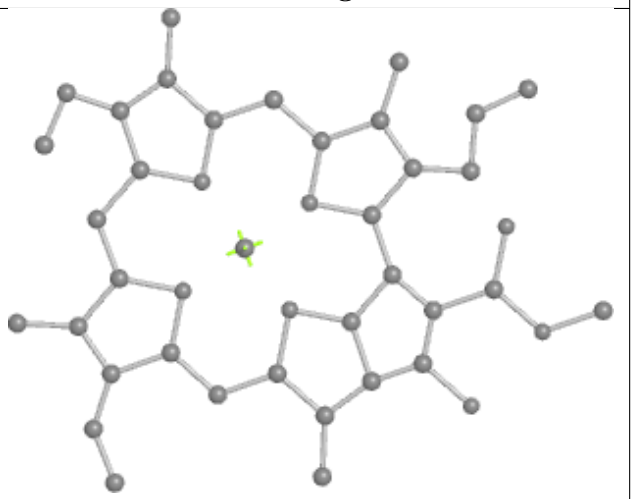
Bond lengths



Bond angles

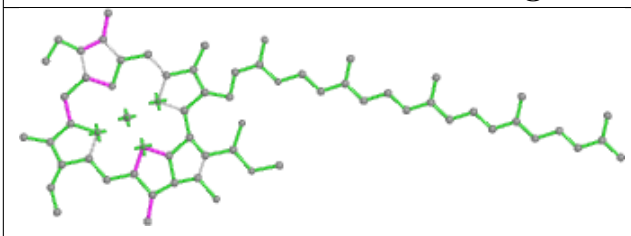


Torsions

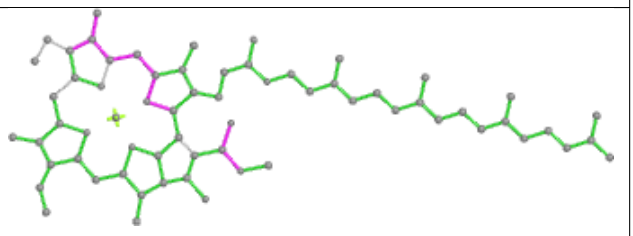


Rings

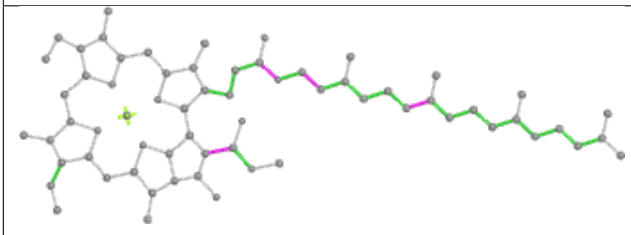
Ligand CLA C 512



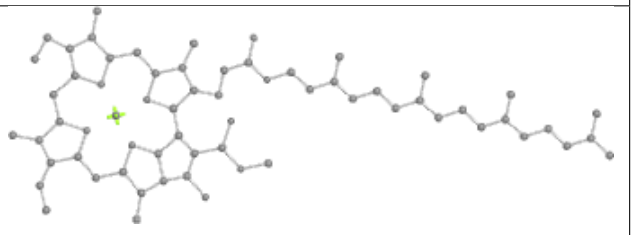
Bond lengths



Bond angles

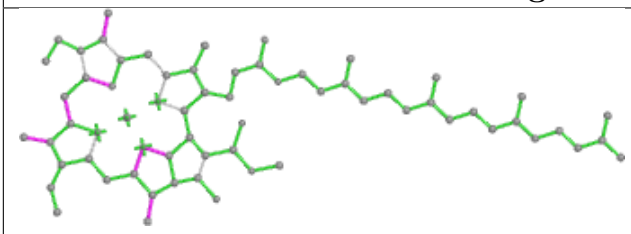


Torsions

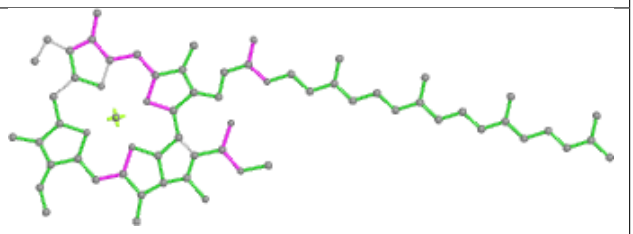


Rings

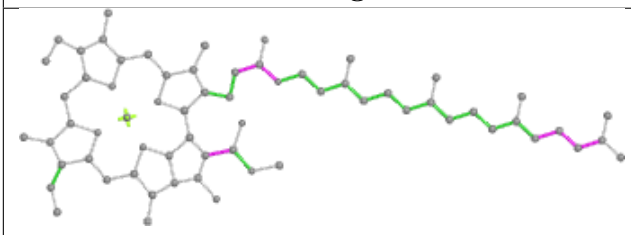
Ligand CLA a 402



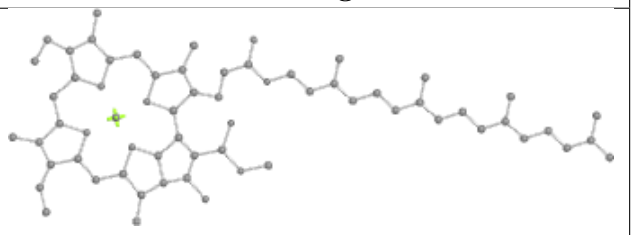
Bond lengths



Bond angles

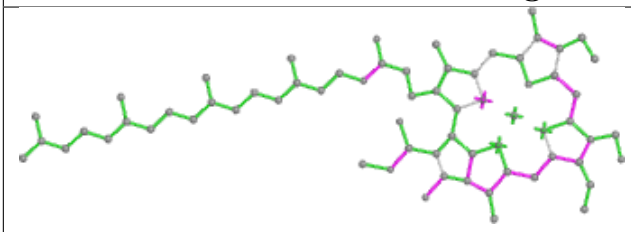


Torsions

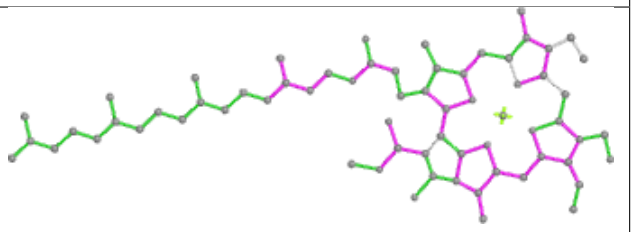


Rings

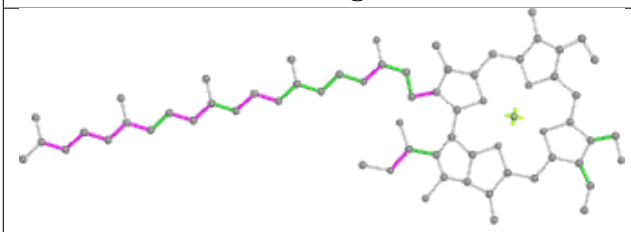
Ligand CHL Y 303



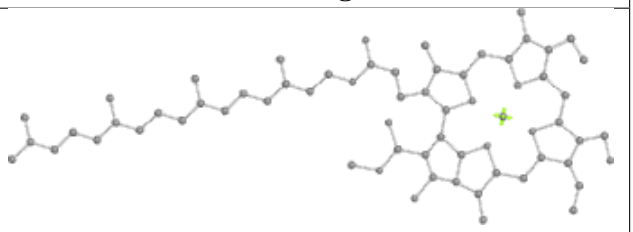
Bond lengths



Bond angles

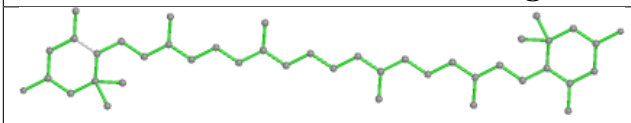


Torsions

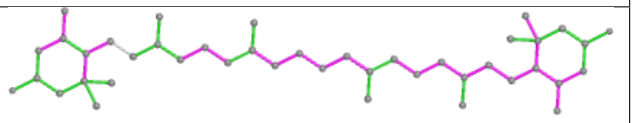


Rings

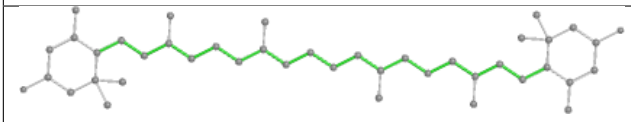
Ligand LUT Y 316



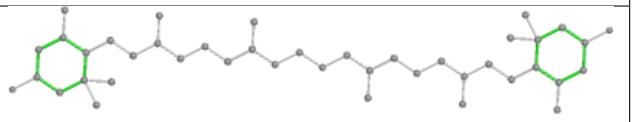
Bond lengths



Bond angles

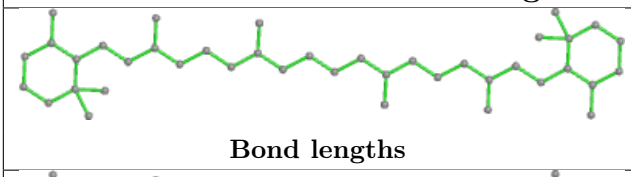


Torsions

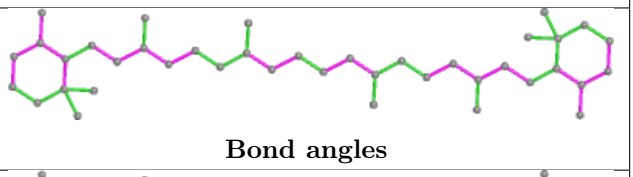


Rings

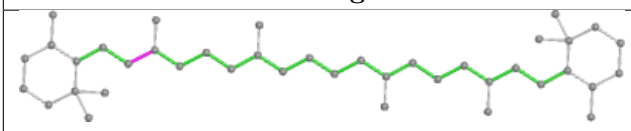
Ligand BCR B 518



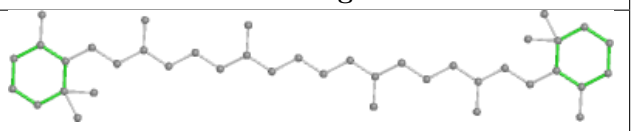
Bond lengths



Bond angles

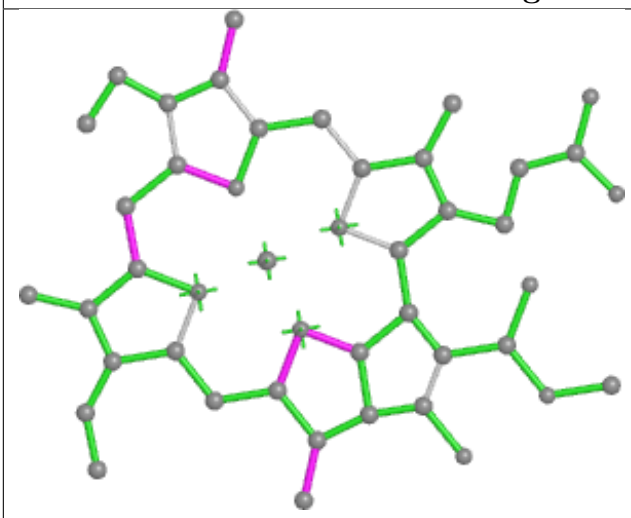


Torsions

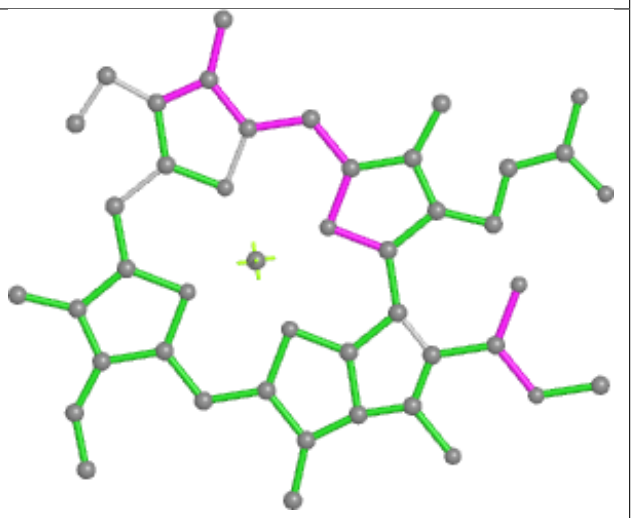


Rings

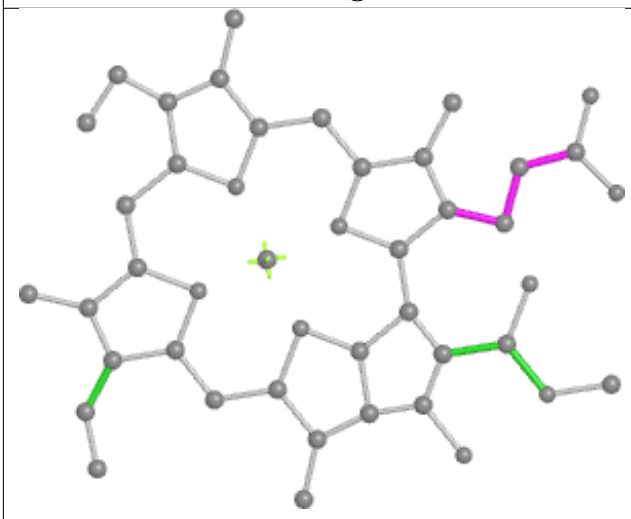
Ligand CLA G 611



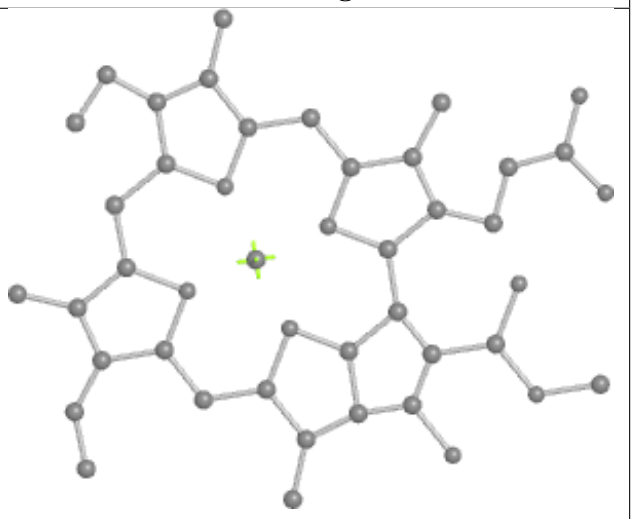
Bond lengths



Bond angles

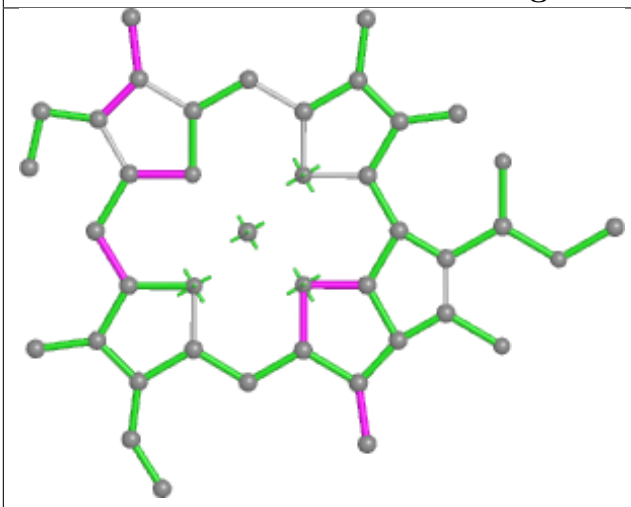


Torsions

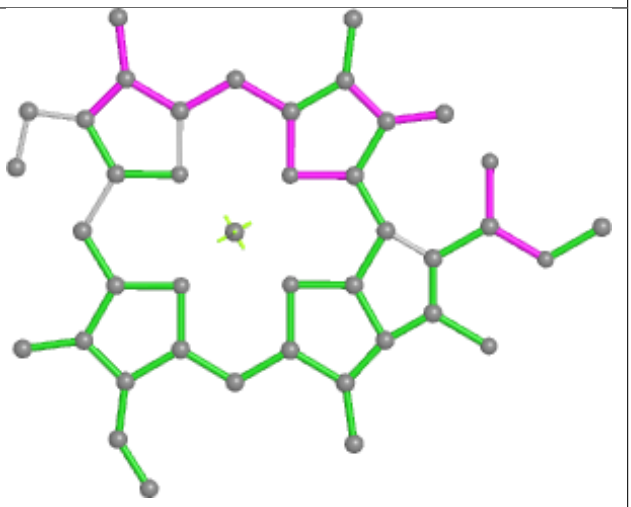


Rings

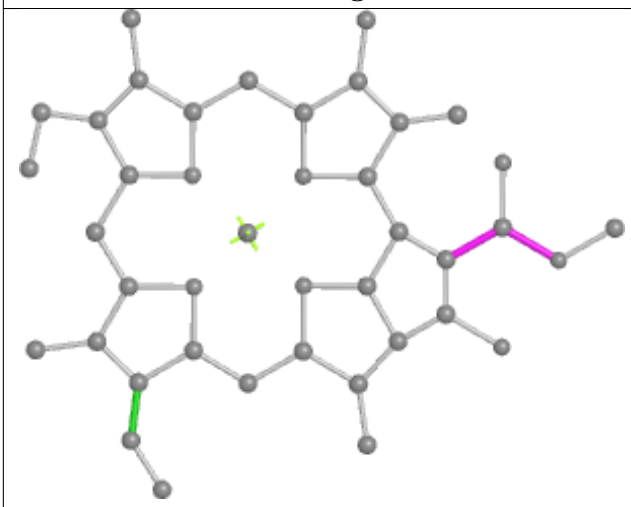
Ligand CLA r 308



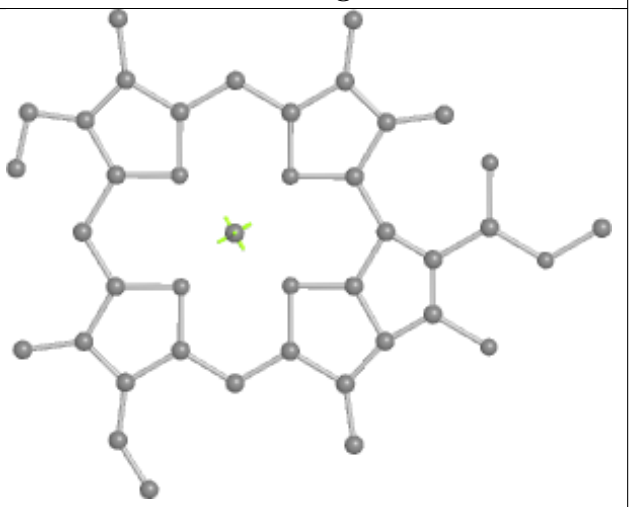
Bond lengths



Bond angles

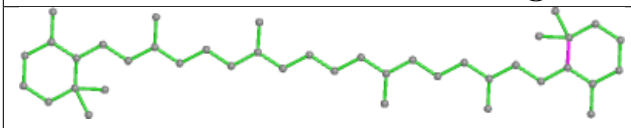


Torsions

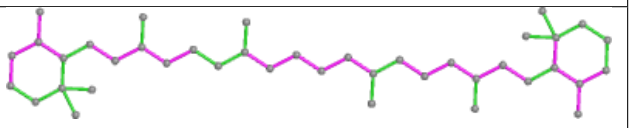


Rings

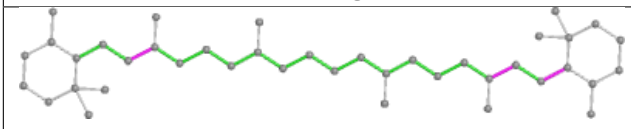
Ligand BCR c 514



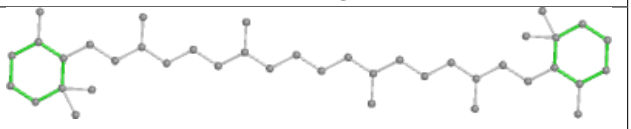
Bond lengths



Bond angles

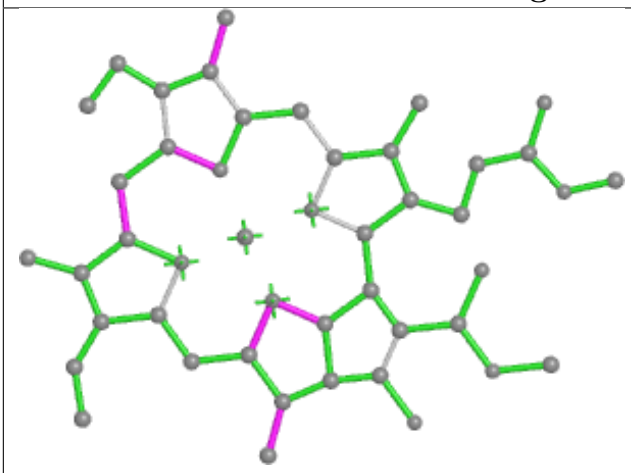


Torsions

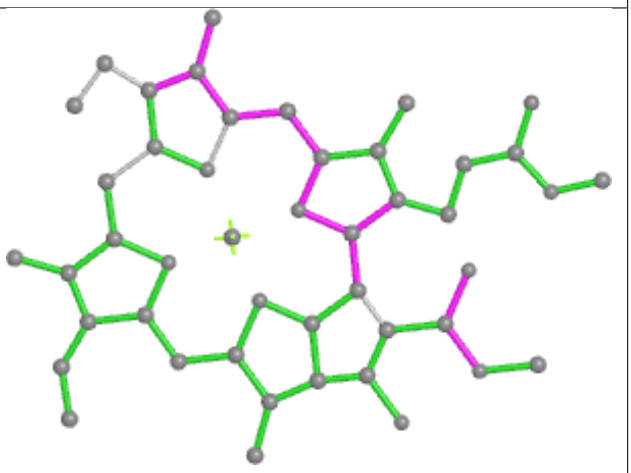


Rings

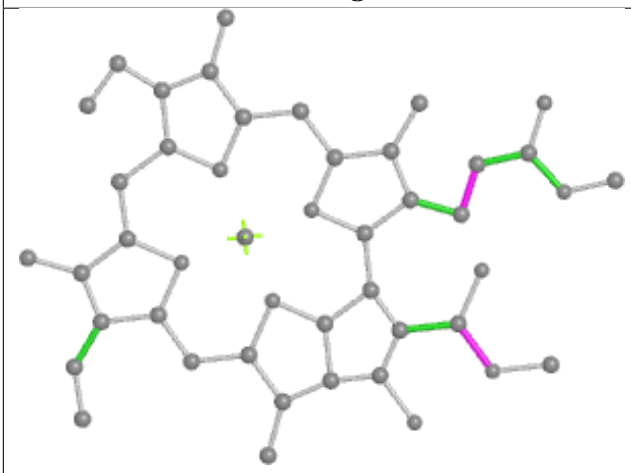
Ligand CLA r 302



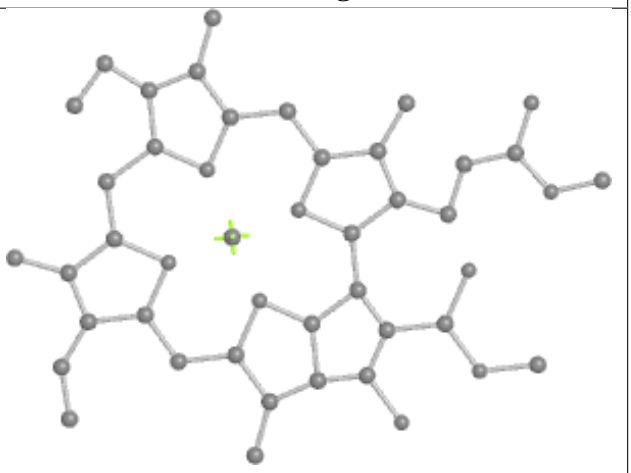
Bond lengths



Bond angles

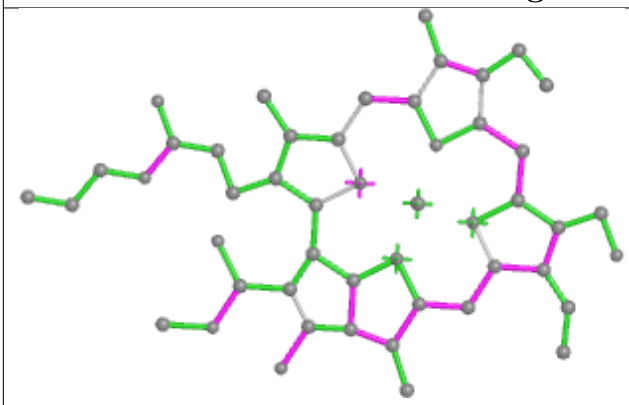


Torsions

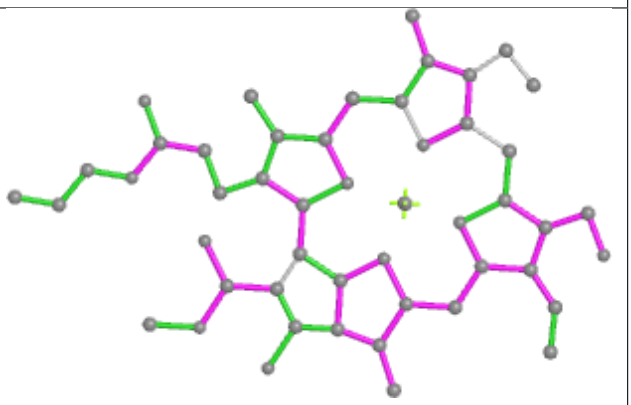


Rings

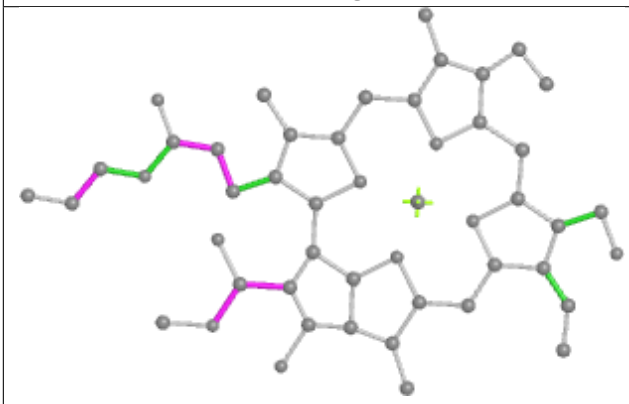
Ligand CHL S 608



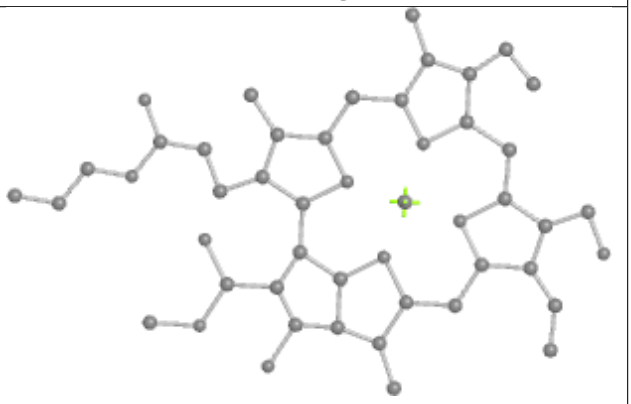
Bond lengths



Bond angles

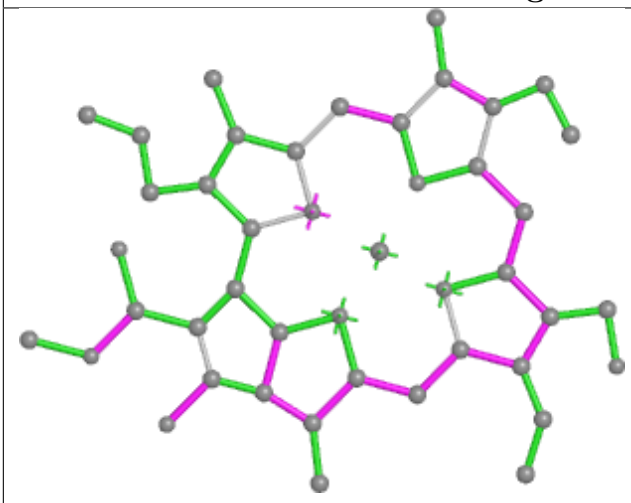


Torsions

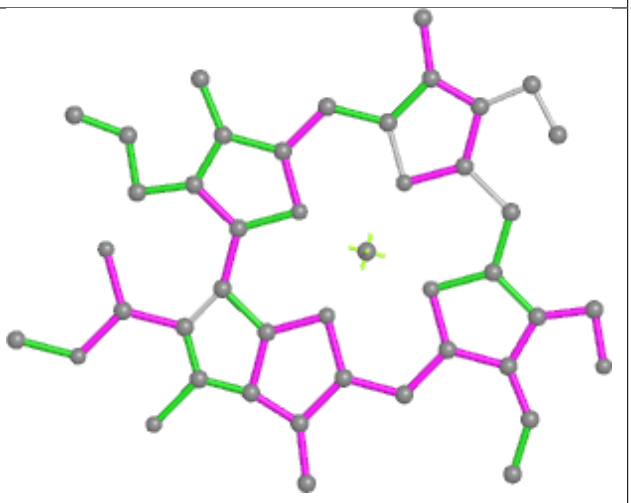


Rings

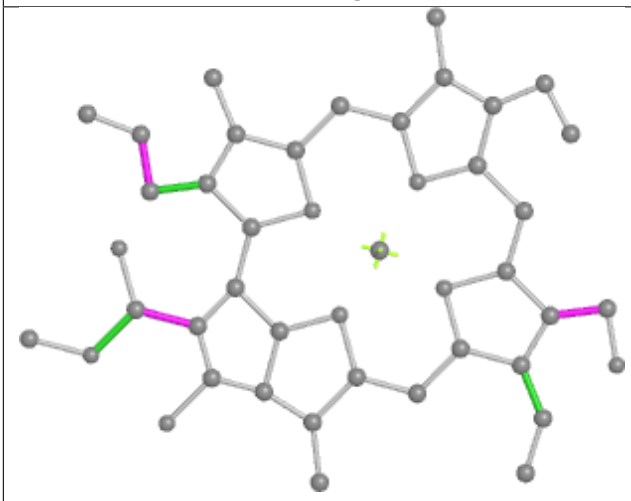
Ligand CHL S 606



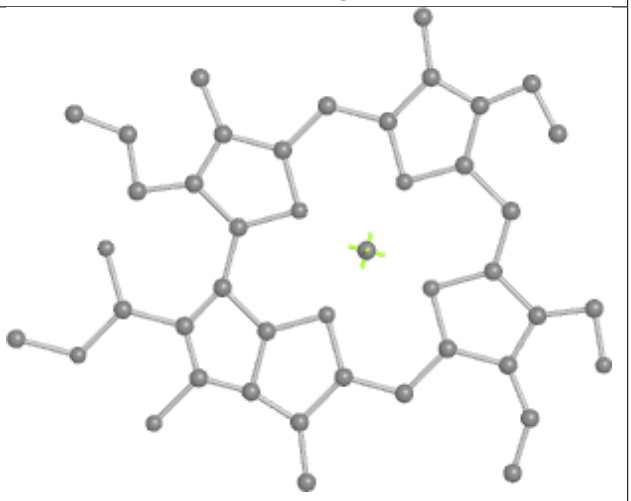
Bond lengths



Bond angles

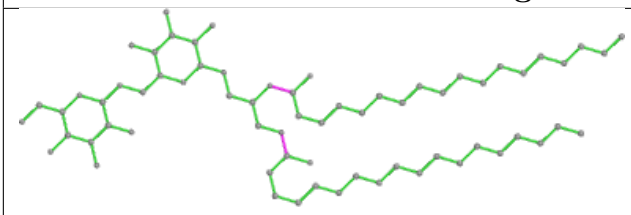


Torsions

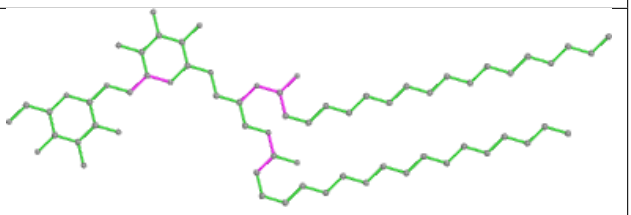


Rings

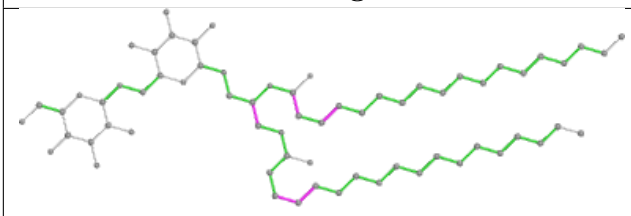
Ligand DGD W 202



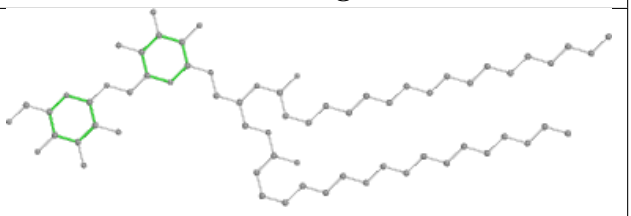
Bond lengths



Bond angles

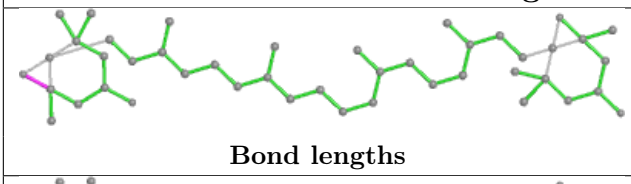


Torsions

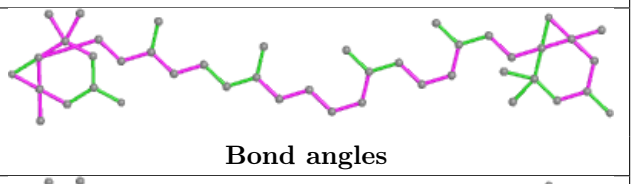


Rings

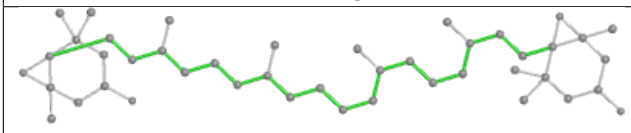
Ligand XAT G 620



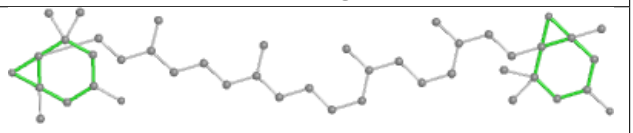
Bond lengths



Bond angles

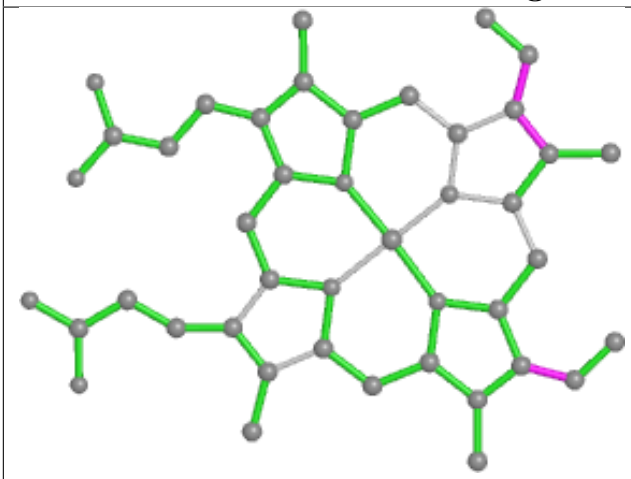


Torsions

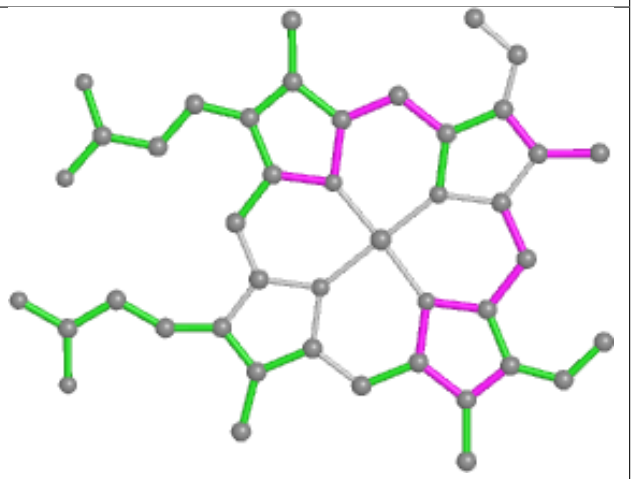


Rings

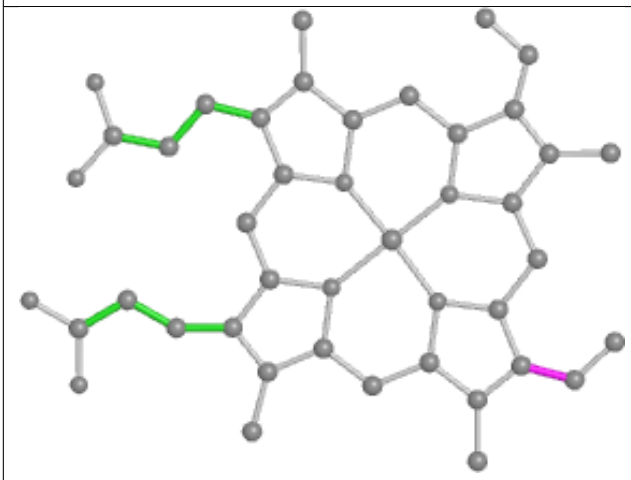
Ligand HEM f 101



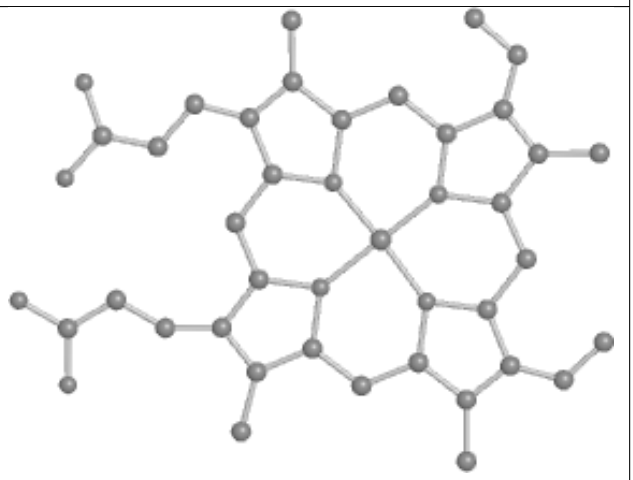
Bond lengths



Bond angles

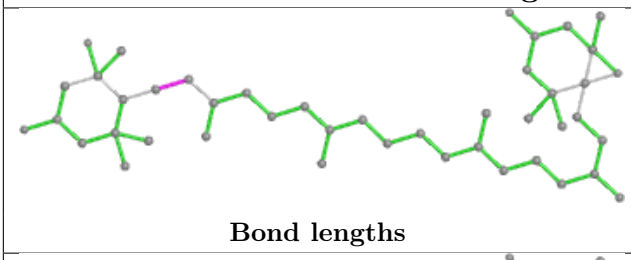


Torsions

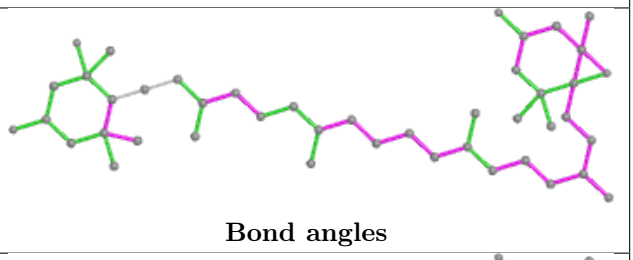


Rings

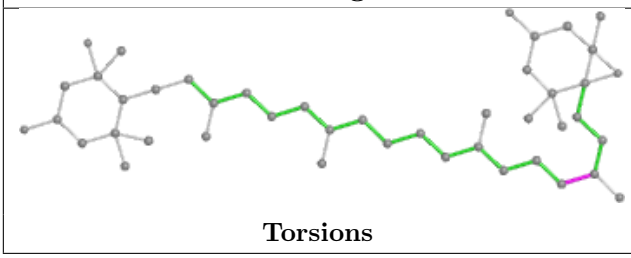
Ligand NEX G 617



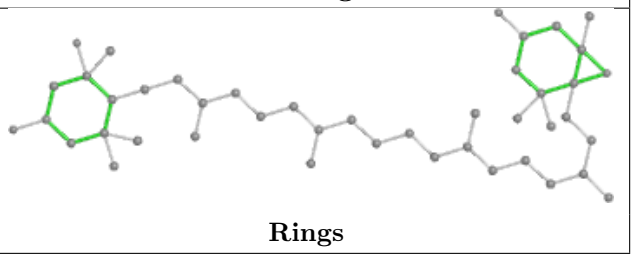
Bond lengths



Bond angles

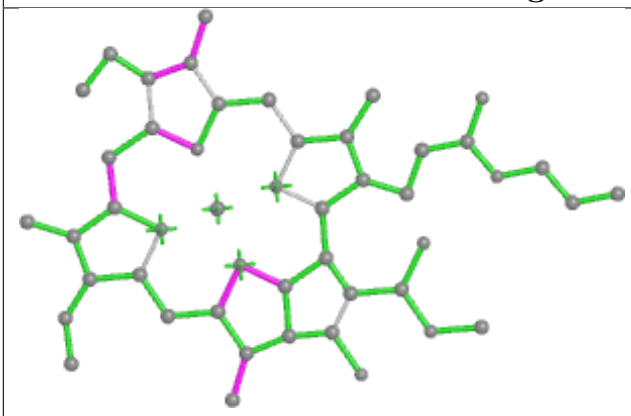


Torsions

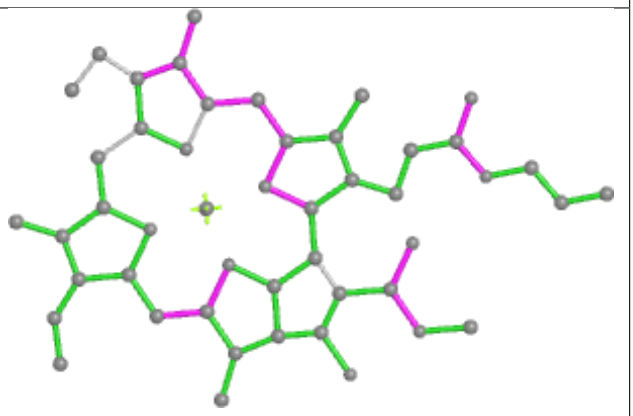


Rings

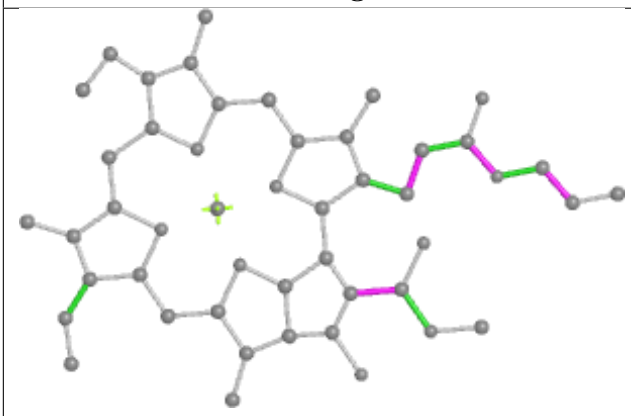
Ligand CLA S 614



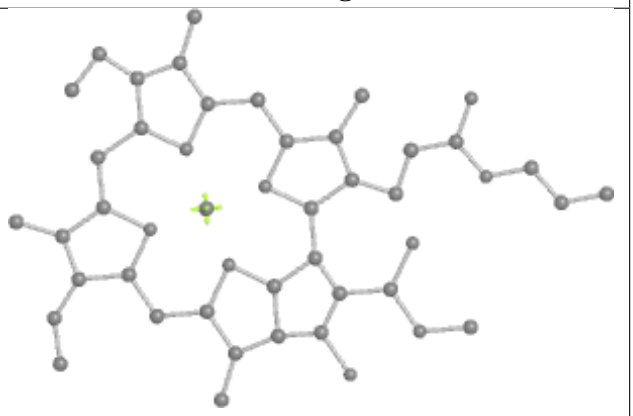
Bond lengths



Bond angles

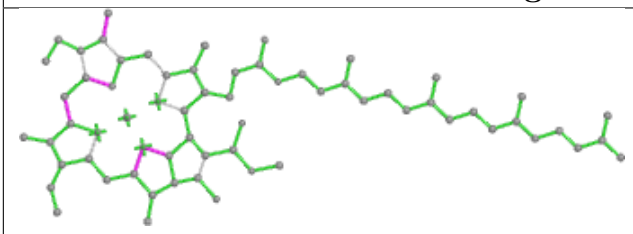


Torsions

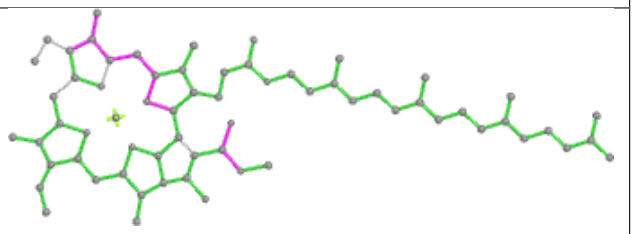


Rings

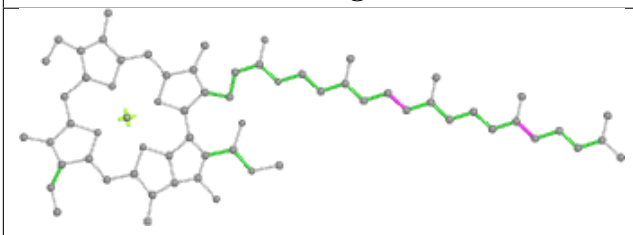
Ligand CLA B 515



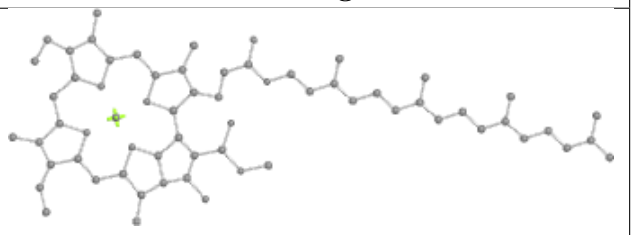
Bond lengths



Bond angles

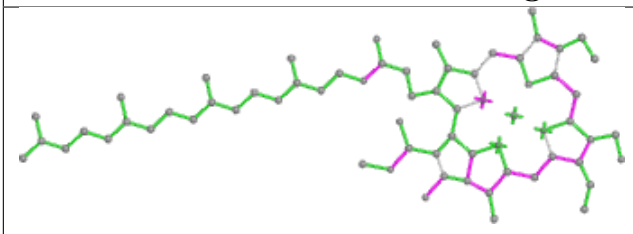


Torsions

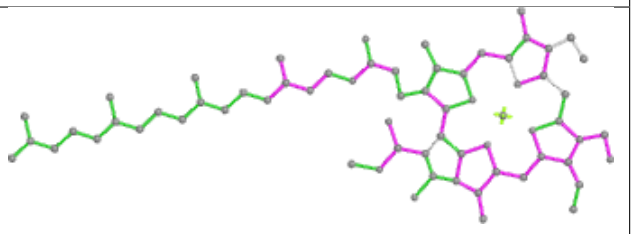


Rings

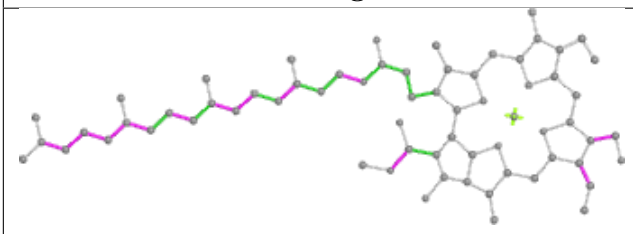
Ligand CHL Y 310



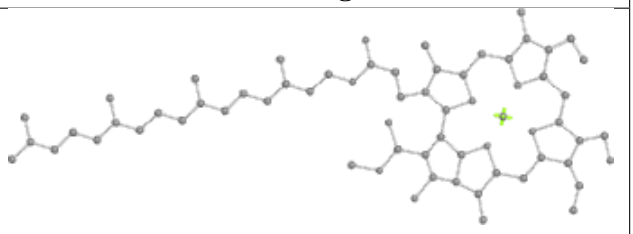
Bond lengths



Bond angles

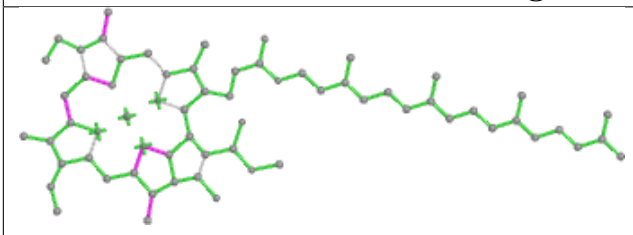


Torsions

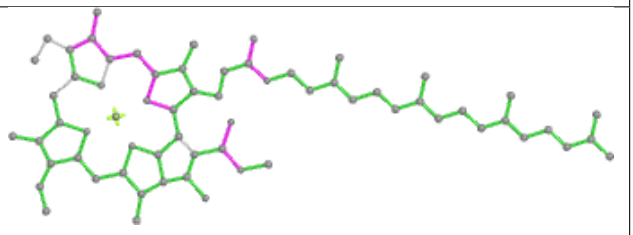


Rings

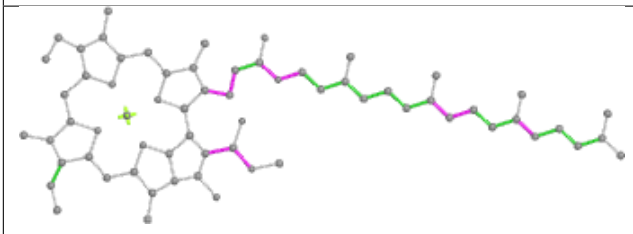
Ligand CLA b 506



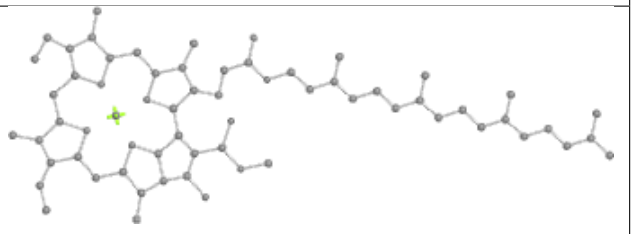
Bond lengths



Bond angles

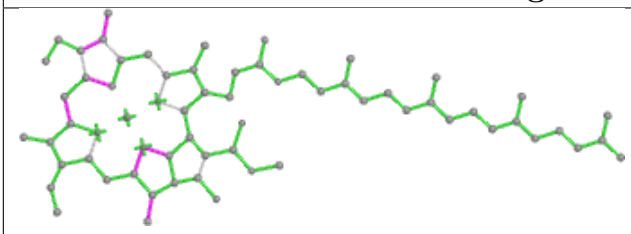


Torsions

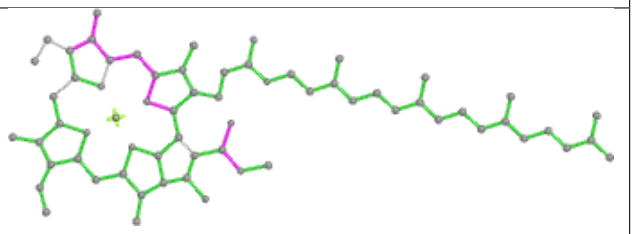


Rings

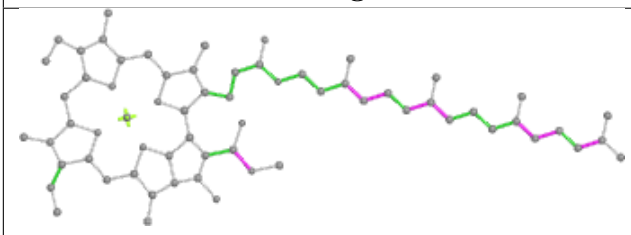
Ligand CLA b 515



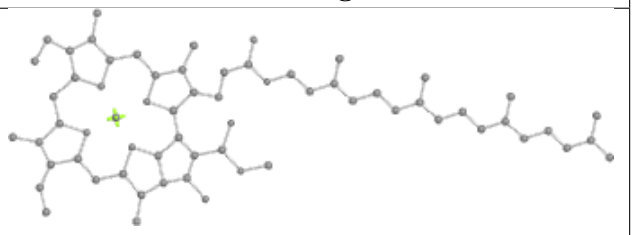
Bond lengths



Bond angles

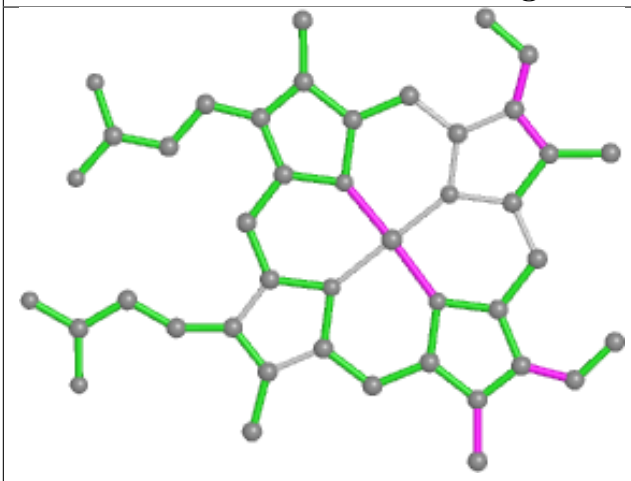


Torsions

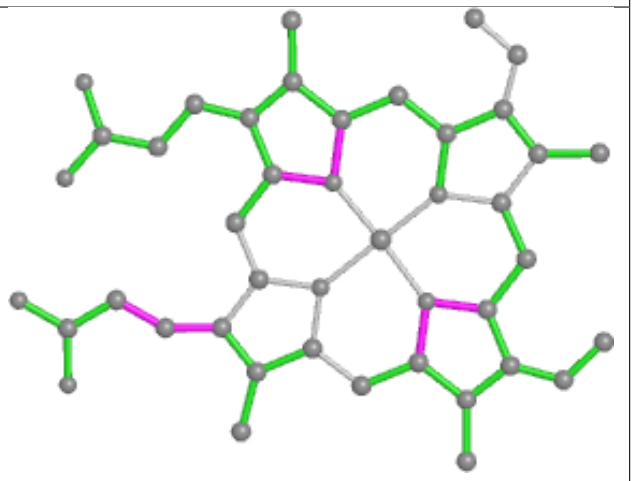


Rings

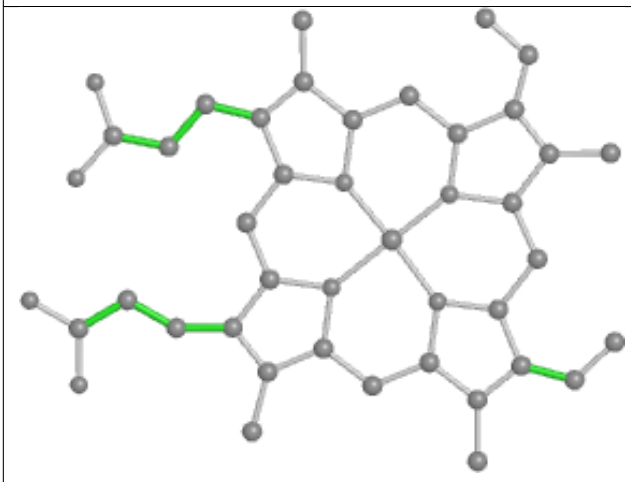
Ligand HEM F 101



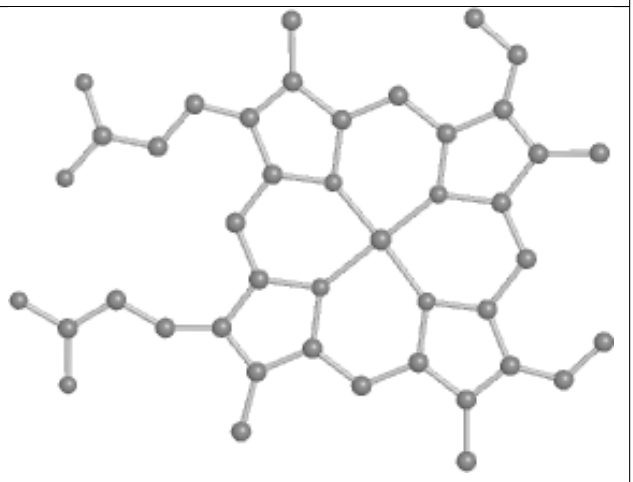
Bond lengths



Bond angles

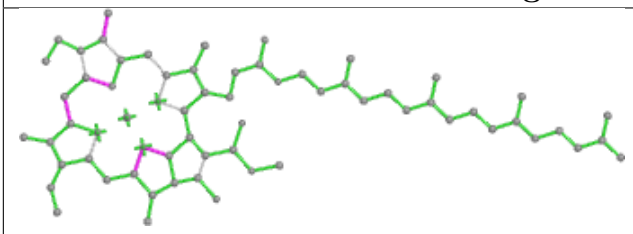


Torsions

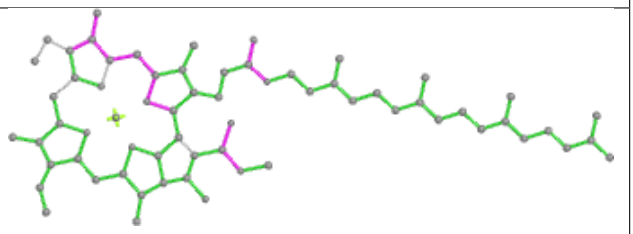


Rings

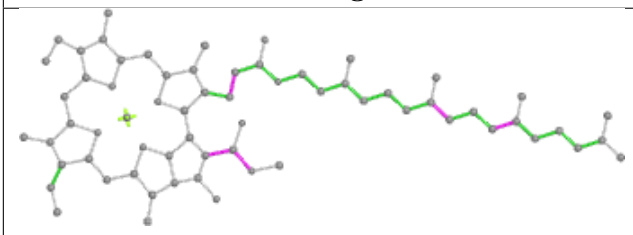
Ligand CLA G 610



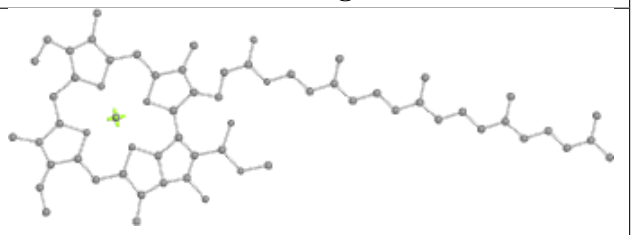
Bond lengths



Bond angles

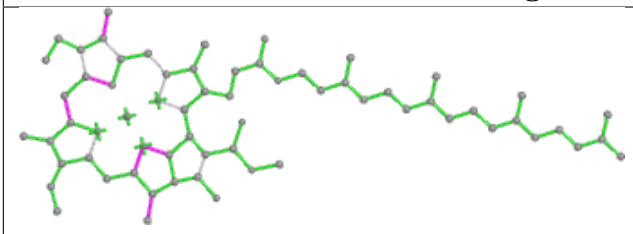


Torsions

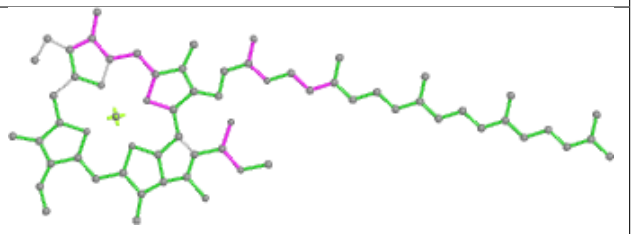


Rings

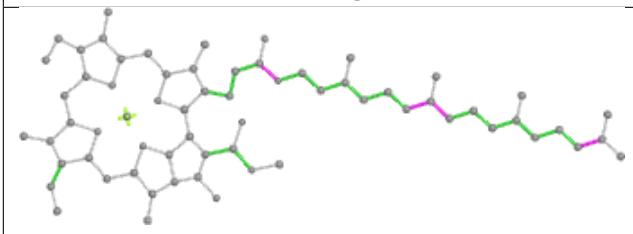
Ligand CLA Y 312



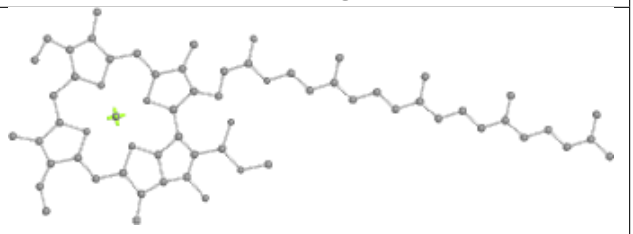
Bond lengths



Bond angles

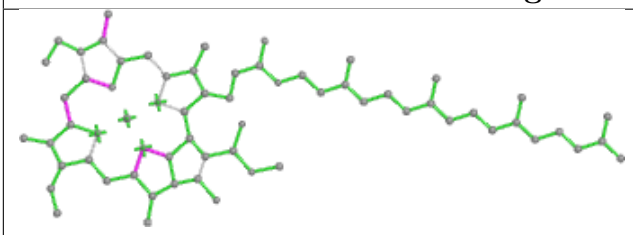


Torsions

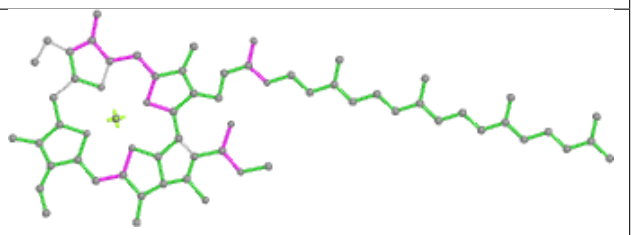


Rings

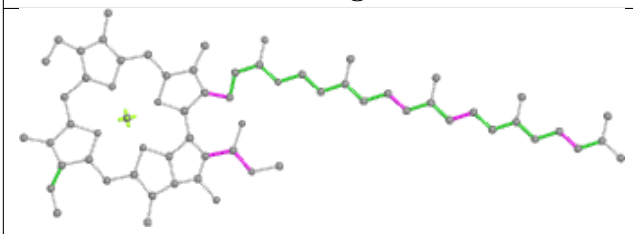
Ligand CLA C 503



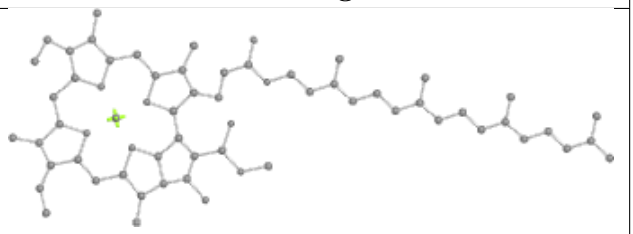
Bond lengths



Bond angles

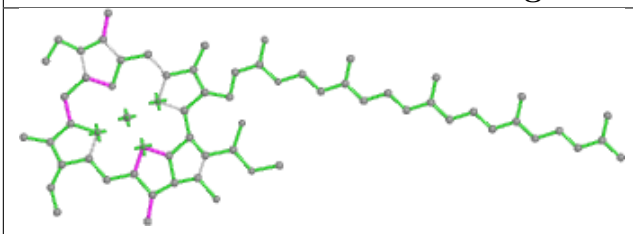


Torsions

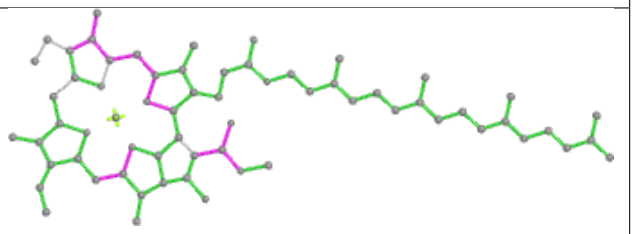


Rings

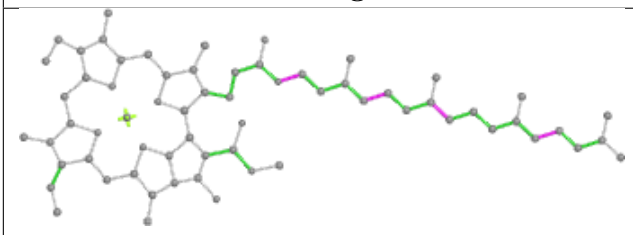
Ligand CLA B 502



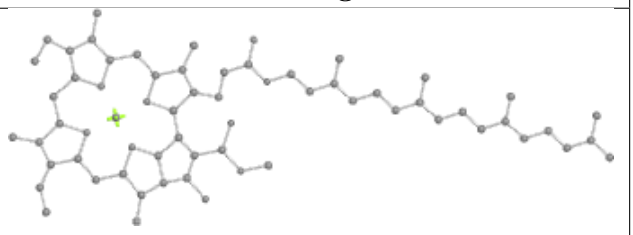
Bond lengths



Bond angles

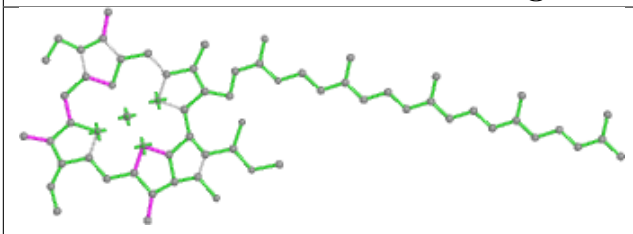


Torsions

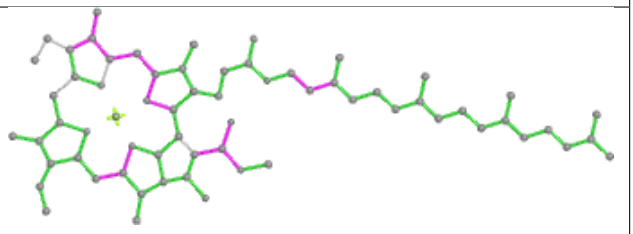


Rings

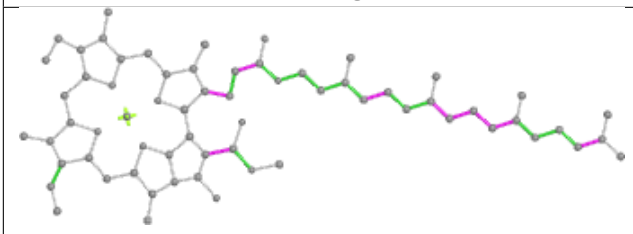
Ligand CLA d 403



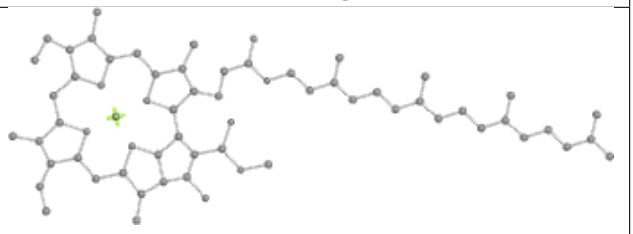
Bond lengths



Bond angles

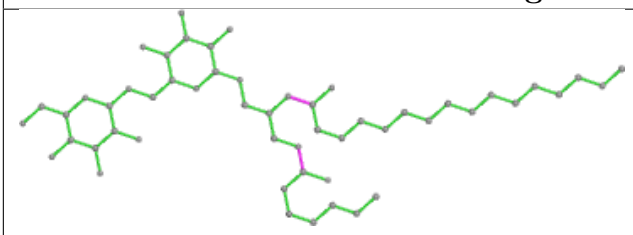


Torsions

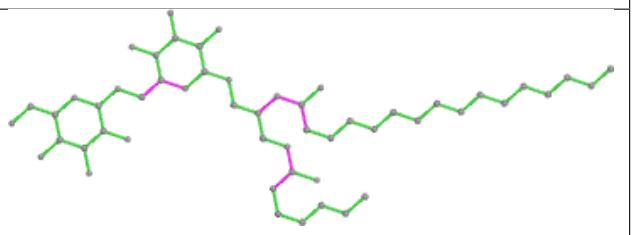


Rings

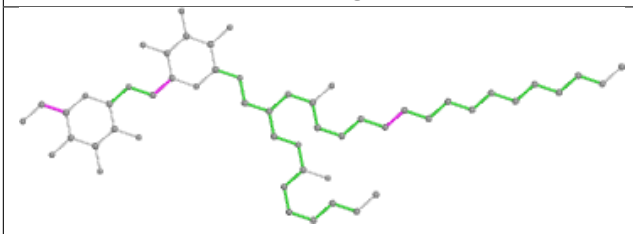
Ligand DGD c 515



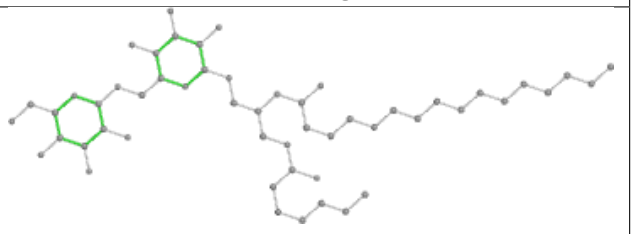
Bond lengths



Bond angles

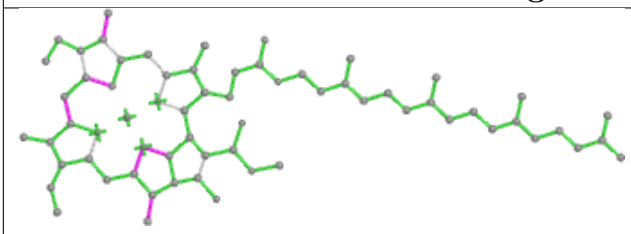


Torsions

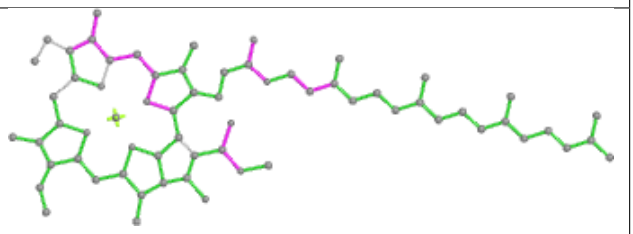


Rings

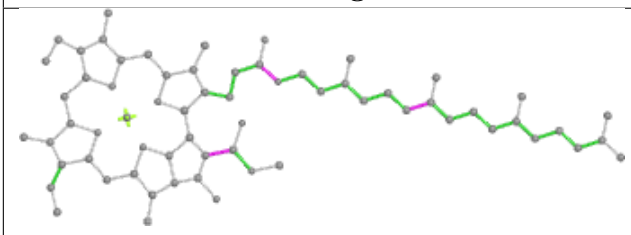
Ligand CLA b 513



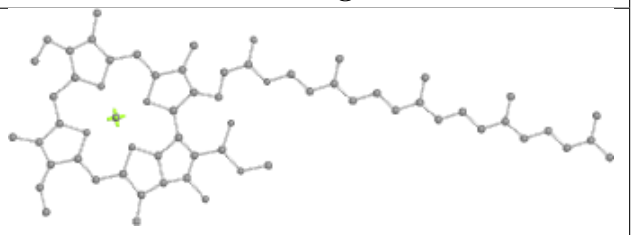
Bond lengths



Bond angles

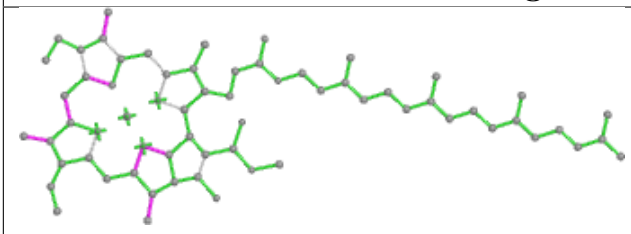


Torsions

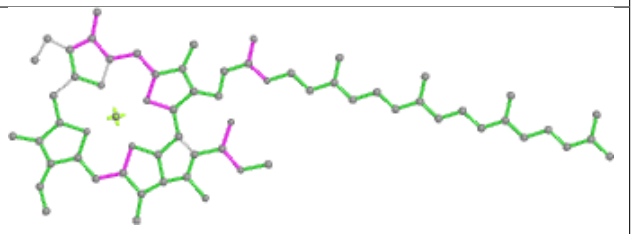


Rings

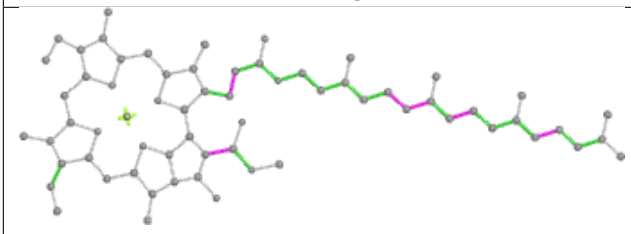
Ligand CLA B 506



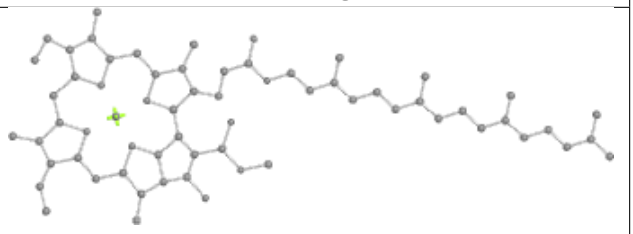
Bond lengths



Bond angles

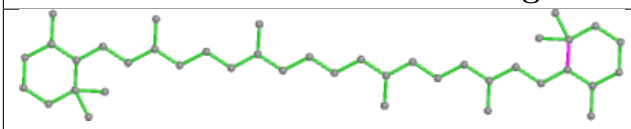


Torsions

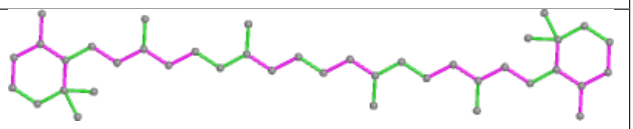


Rings

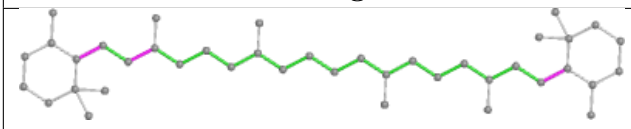
Ligand BCR C 514



Bond lengths



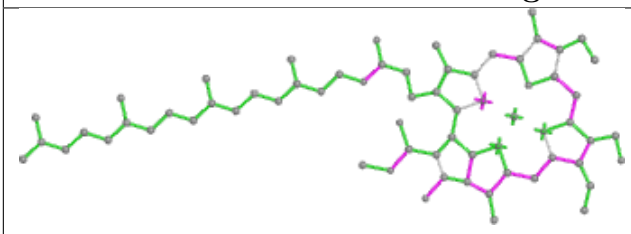
Bond angles

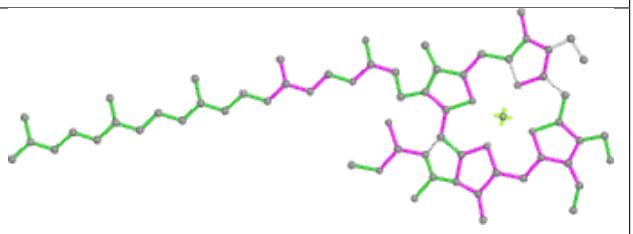


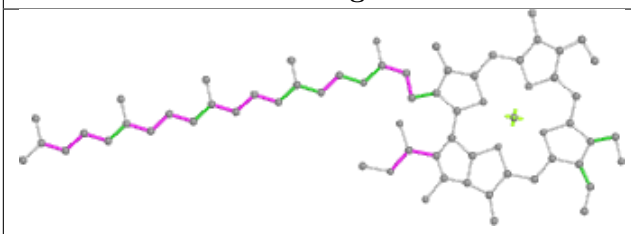
Torsions

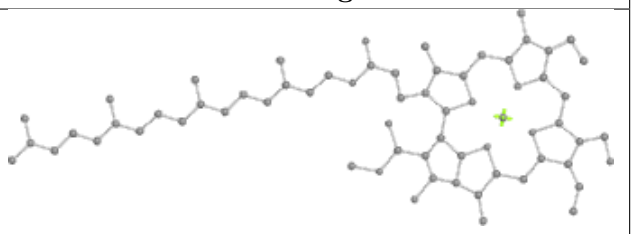
Rings

Ligand CHL N 306

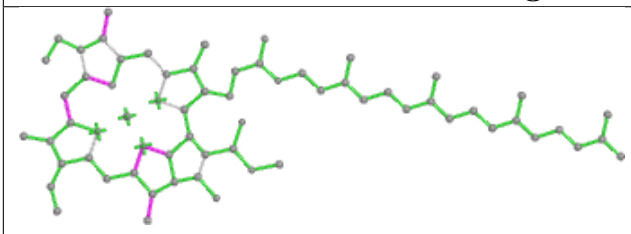

Bond lengths

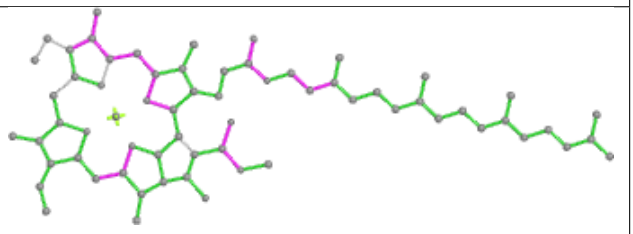

Bond angles

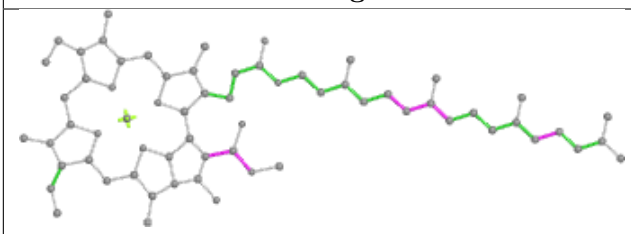

Torsions

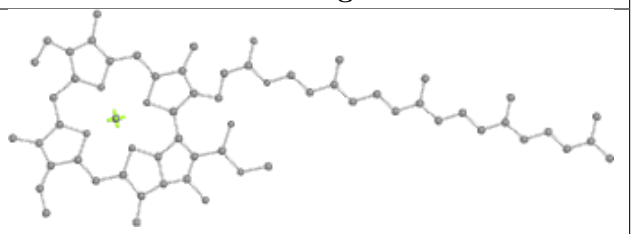

Rings

Ligand CLA C 506

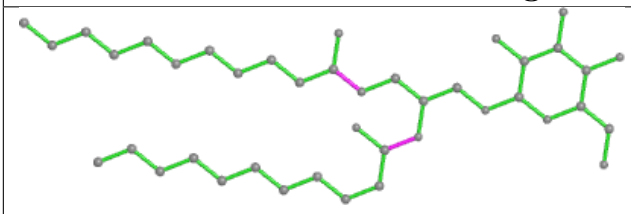

Bond lengths

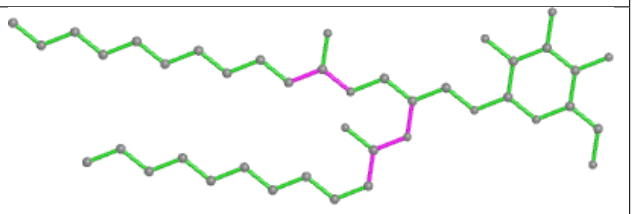

Bond angles

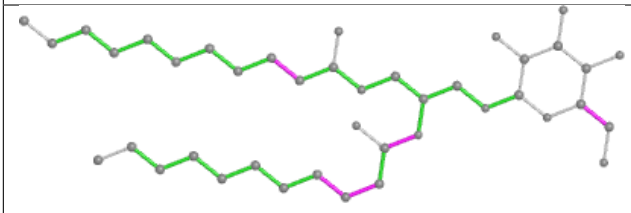

Torsions

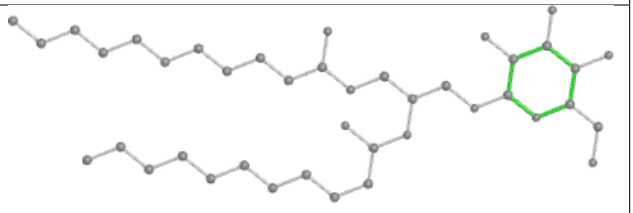

Rings

Ligand LMG d 409

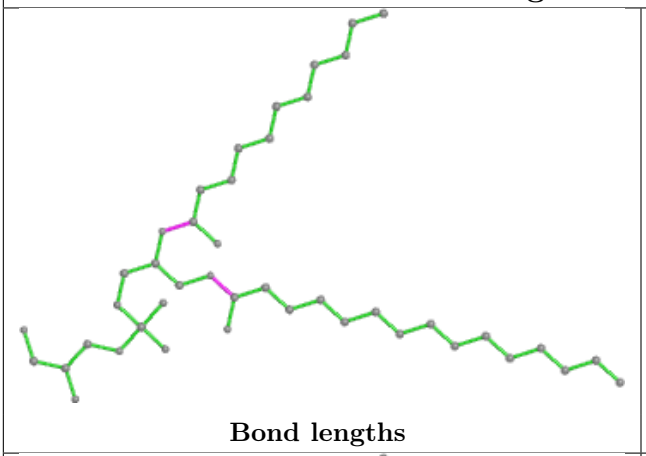

Bond lengths


Bond angles

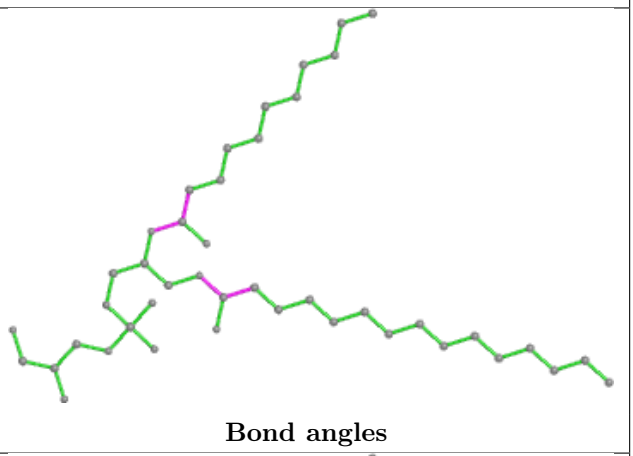

Torsions


Rings

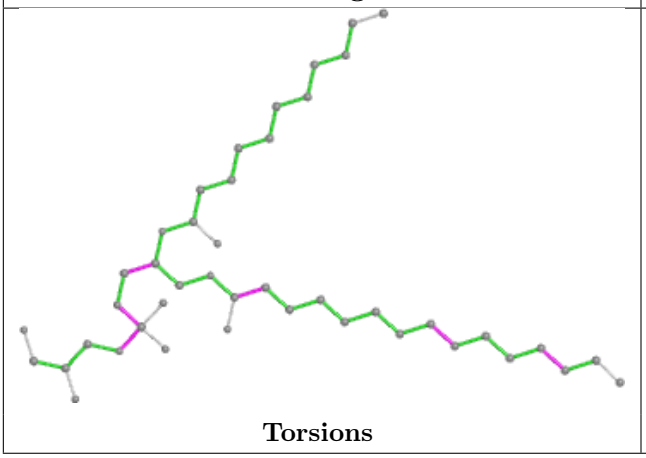
Ligand LHG a 410



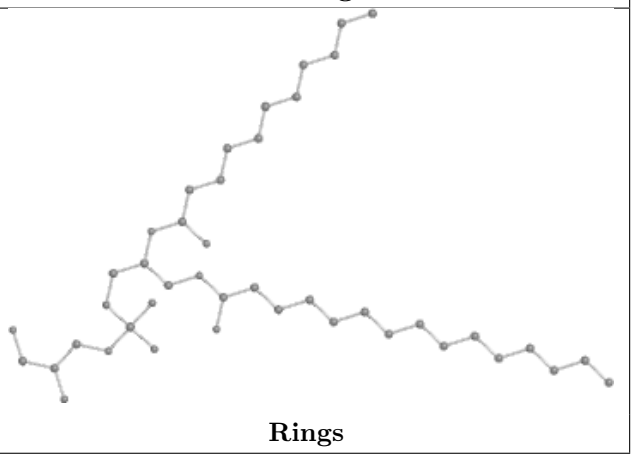
Bond lengths



Bond angles

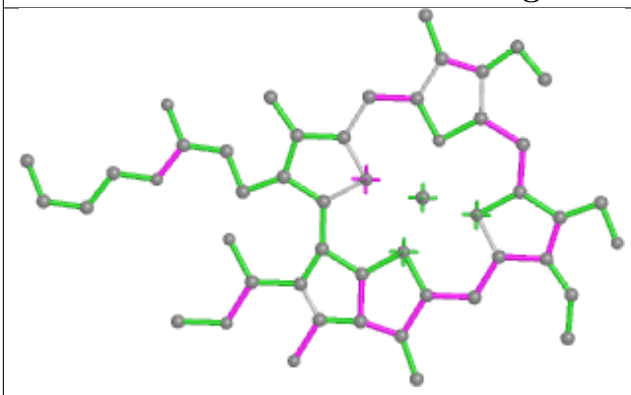


Torsions

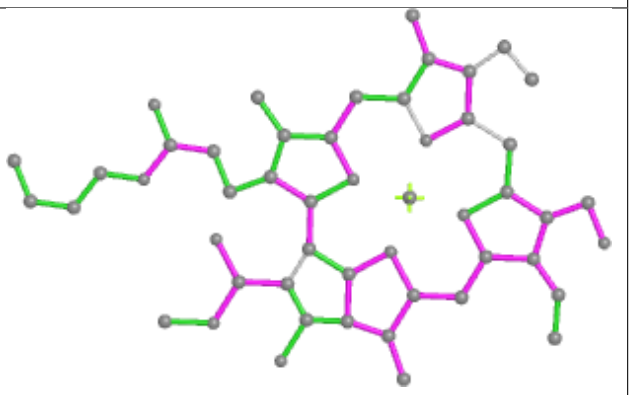


Rings

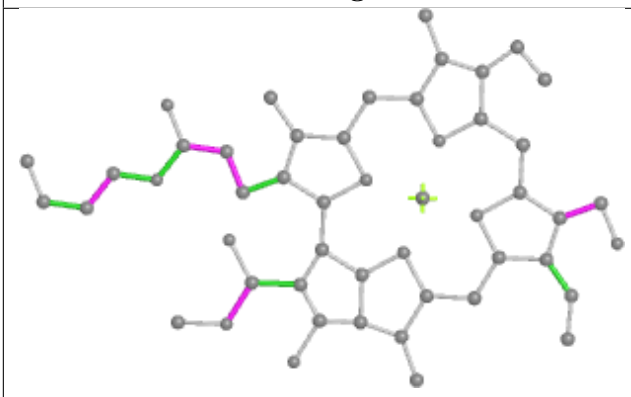
Ligand CHL G 607



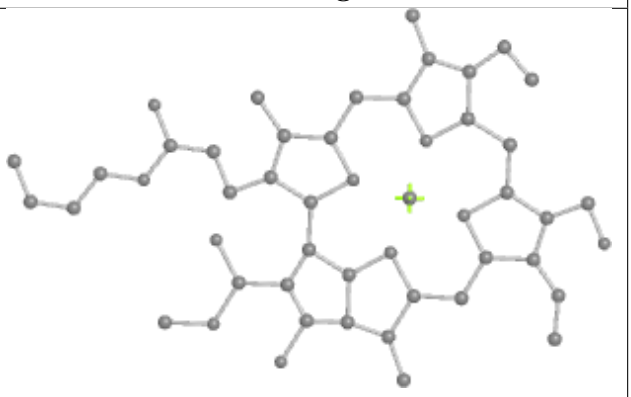
Bond lengths



Bond angles

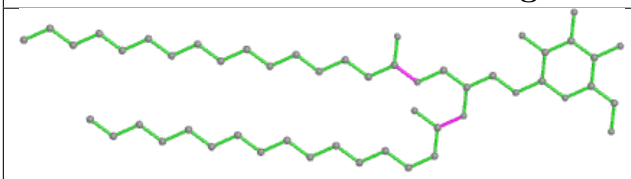


Torsions

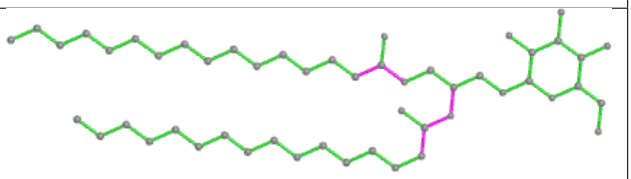


Rings

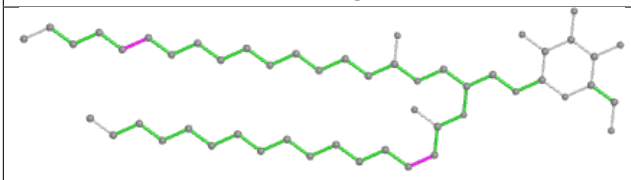
Ligand LMG B 519



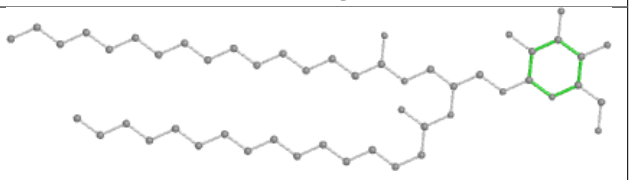
Bond lengths



Bond angles

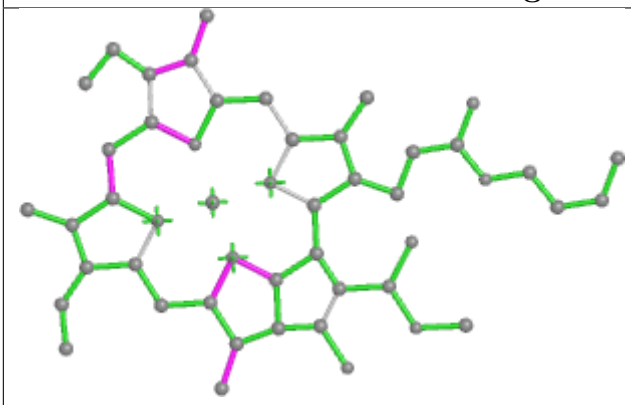


Torsions

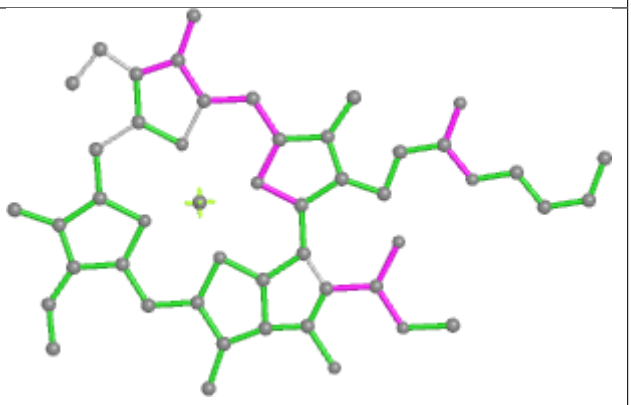


Rings

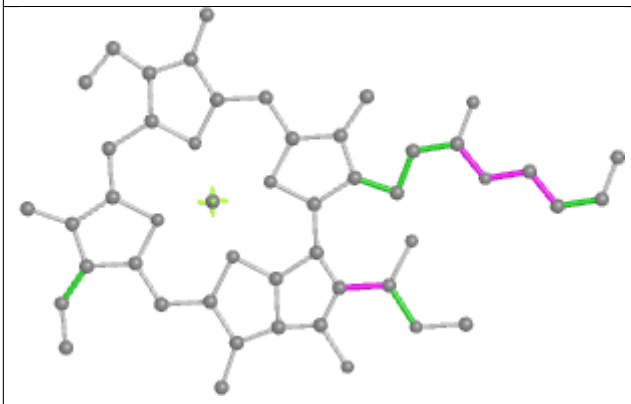
Ligand CLA A 403



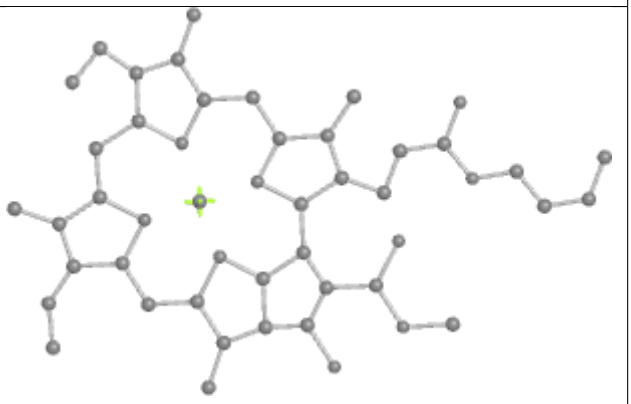
Bond lengths



Bond angles

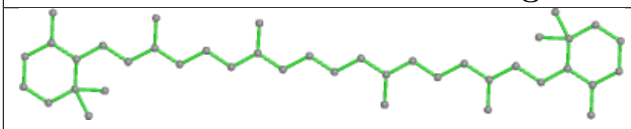


Torsions

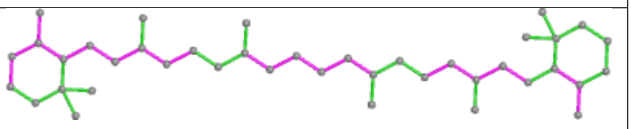


Rings

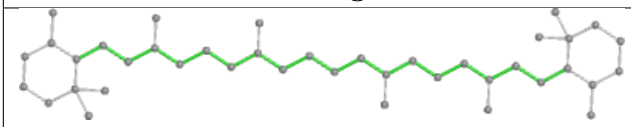
Ligand BCR A 406



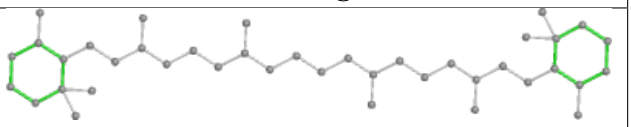
Bond lengths



Bond angles

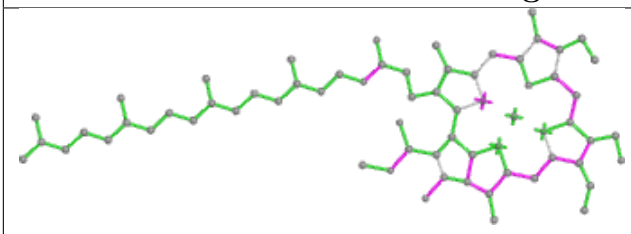


Torsions

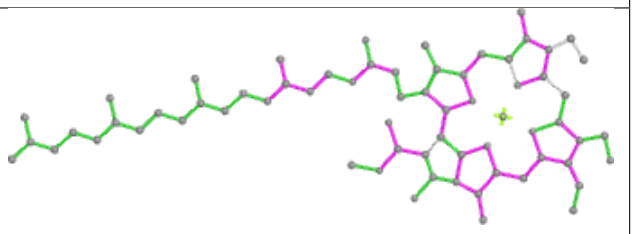


Rings

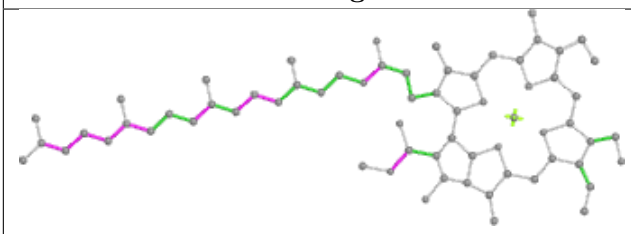
Ligand CHL N 302



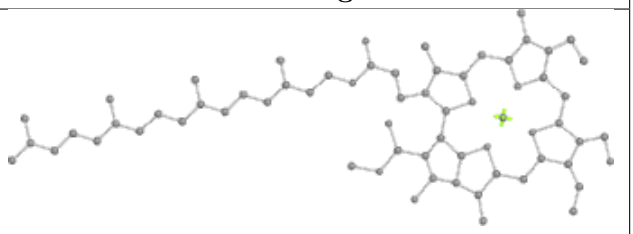
Bond lengths



Bond angles

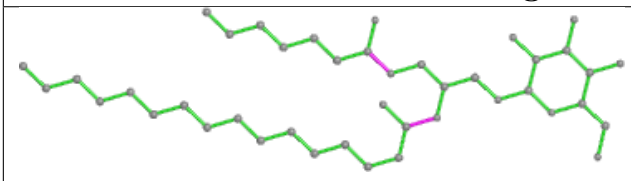


Torsions

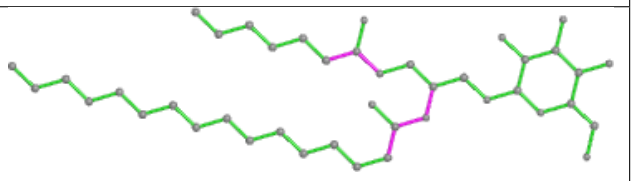


Rings

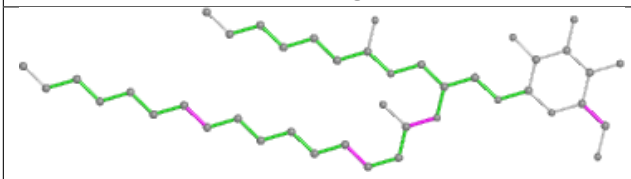
Ligand LMG b 520



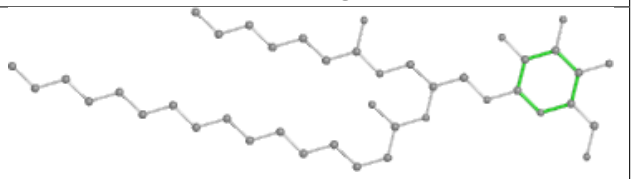
Bond lengths



Bond angles

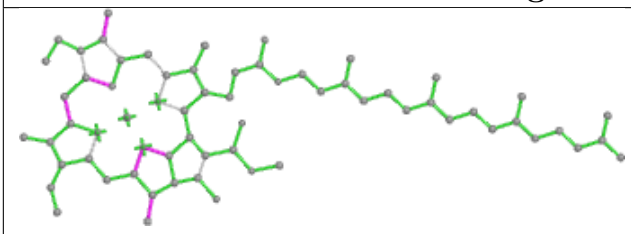


Torsions

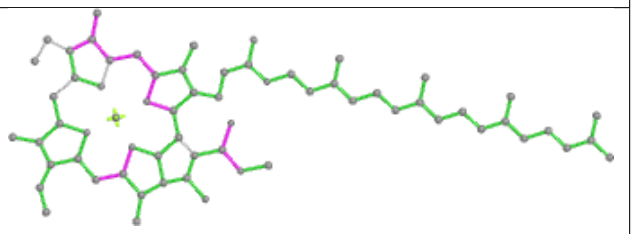


Rings

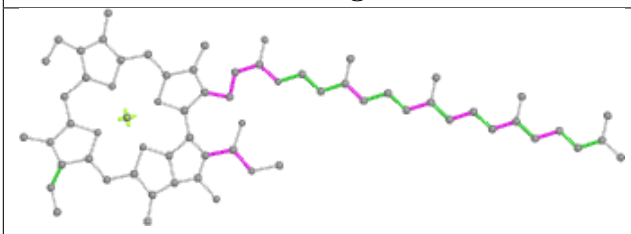
Ligand CLA b 505



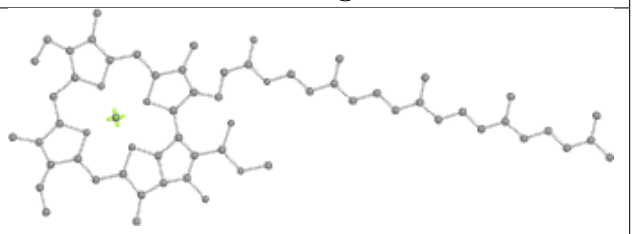
Bond lengths



Bond angles

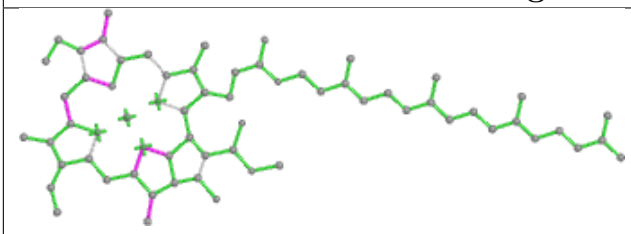


Torsions

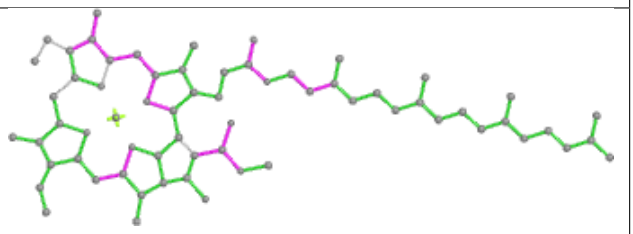


Rings

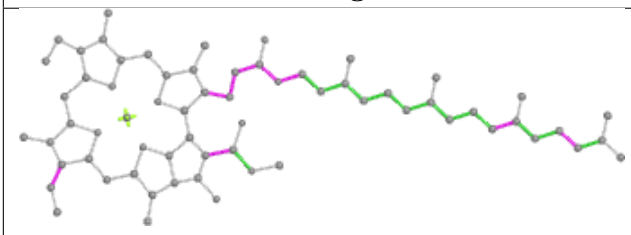
Ligand CLA d 401



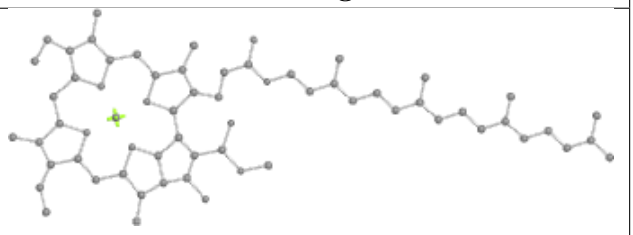
Bond lengths



Bond angles

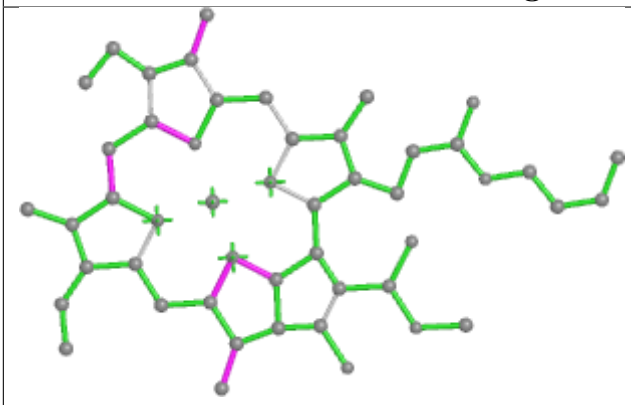


Torsions

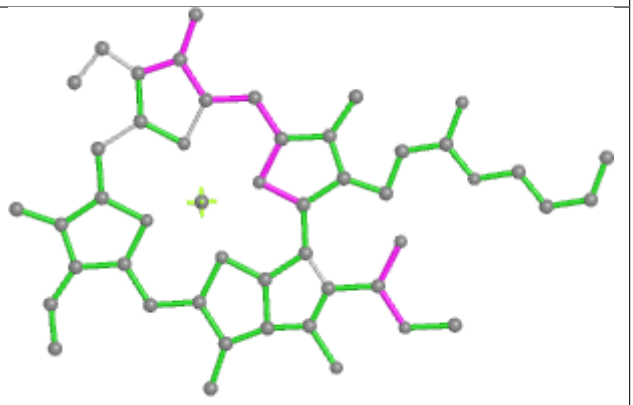


Rings

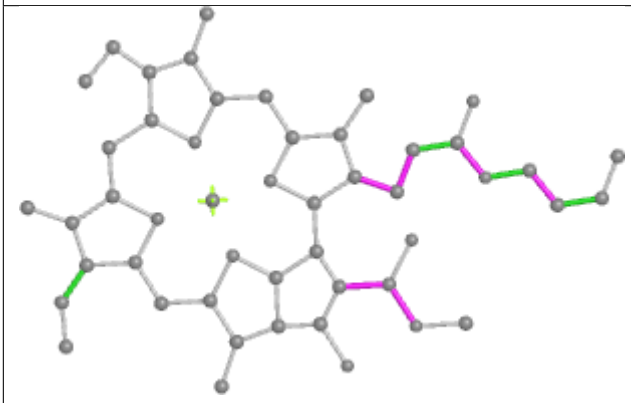
Ligand CLA N 312



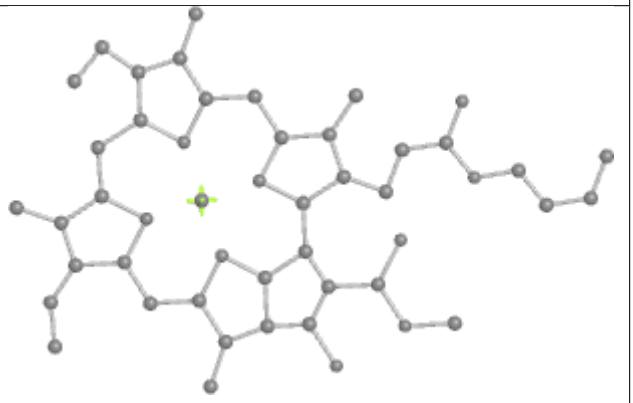
Bond lengths



Bond angles

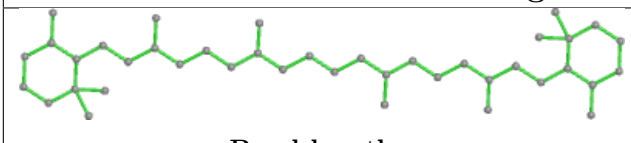


Torsions

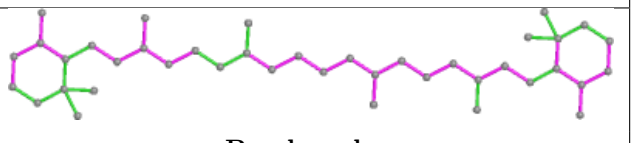


Rings

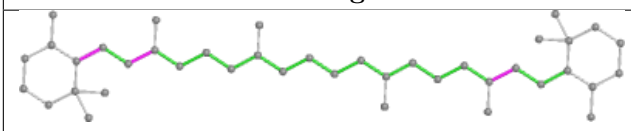
Ligand BCR z 101



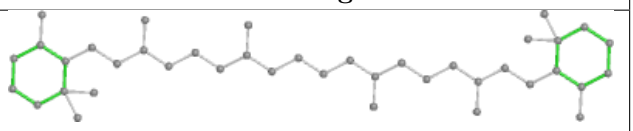
Bond lengths



Bond angles

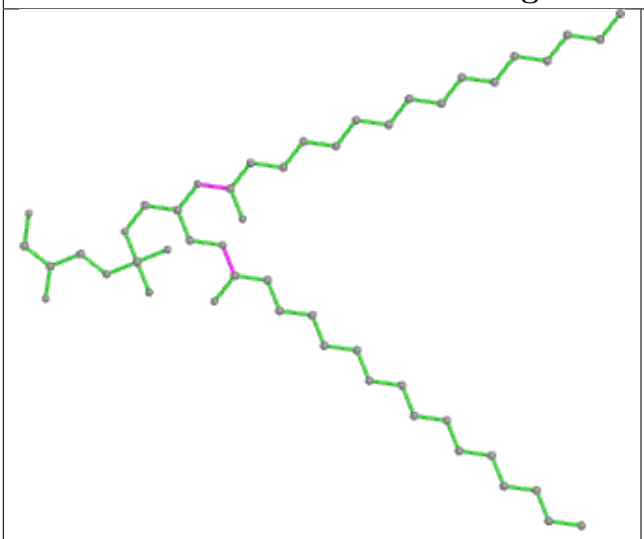


Torsions

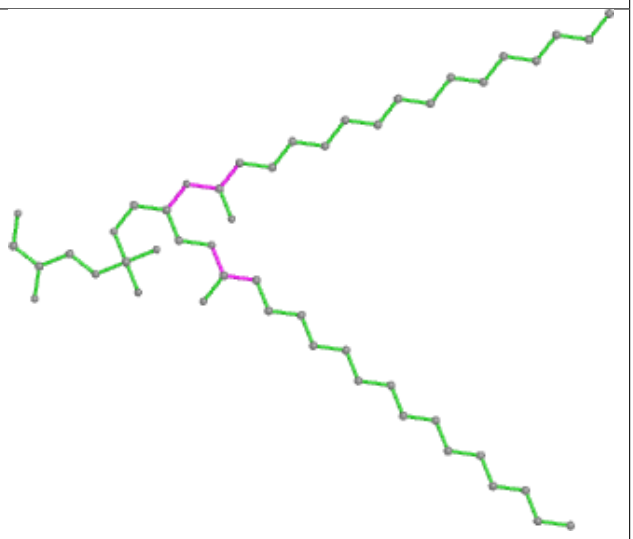


Rings

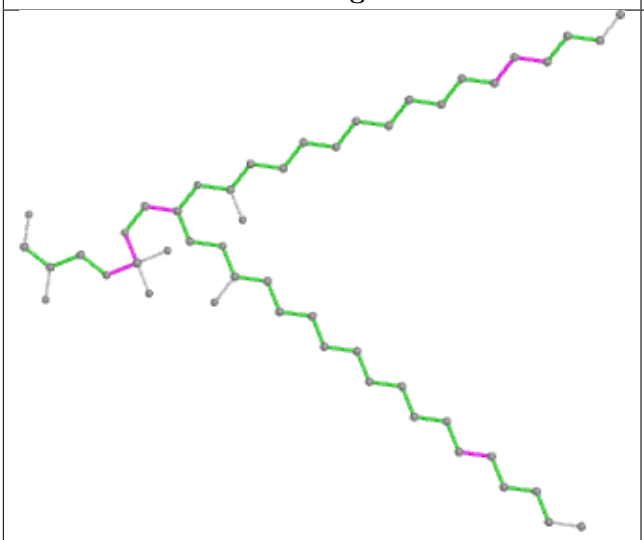
Ligand LHG G 618



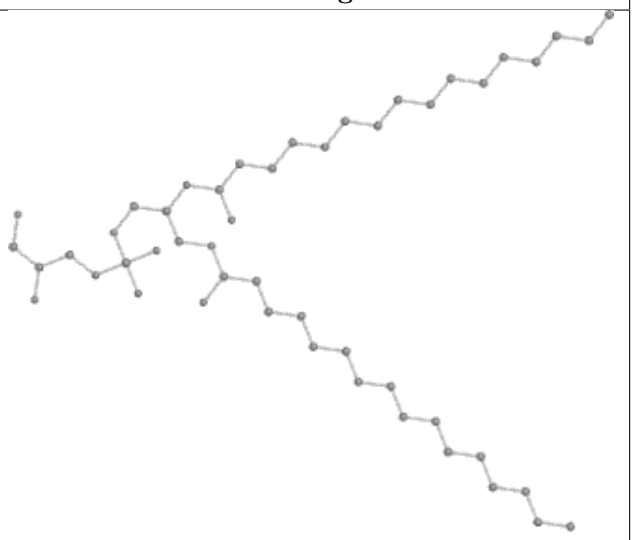
Bond lengths



Bond angles

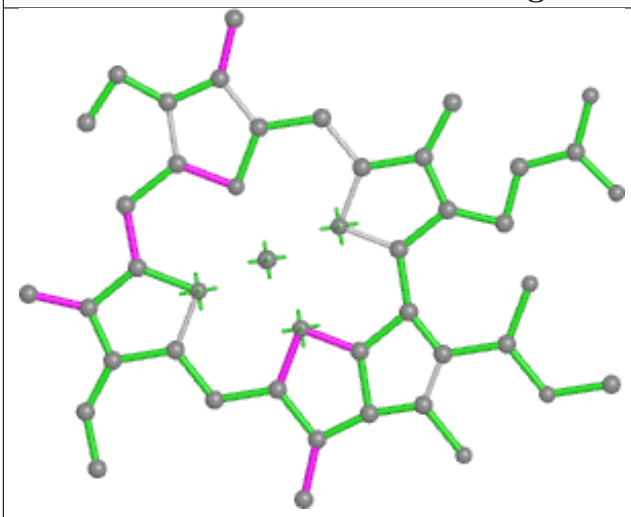


Torsions

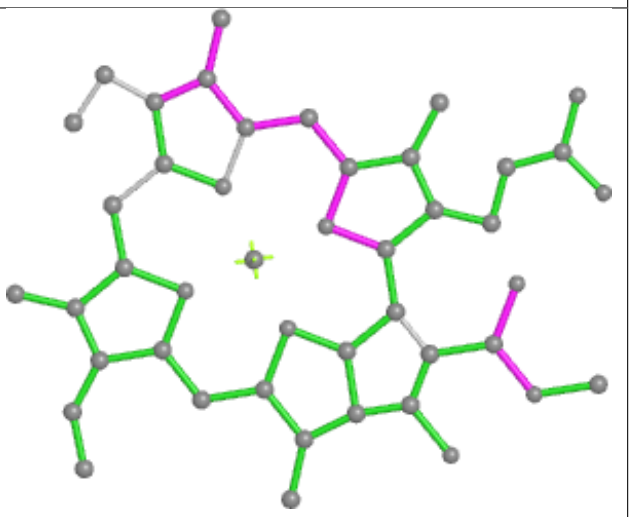


Rings

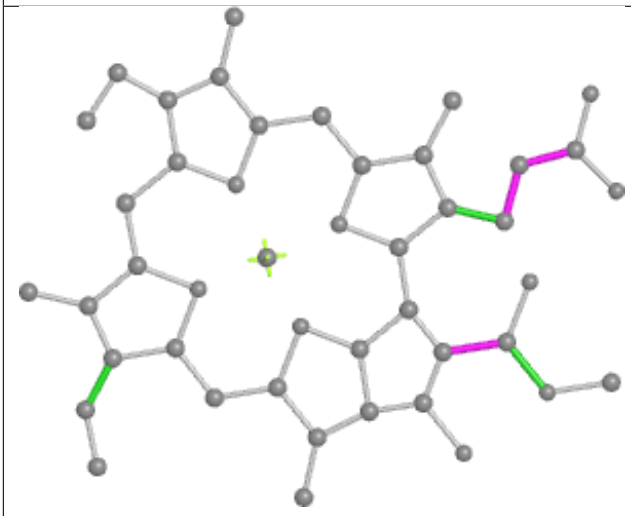
Ligand CLA b 516



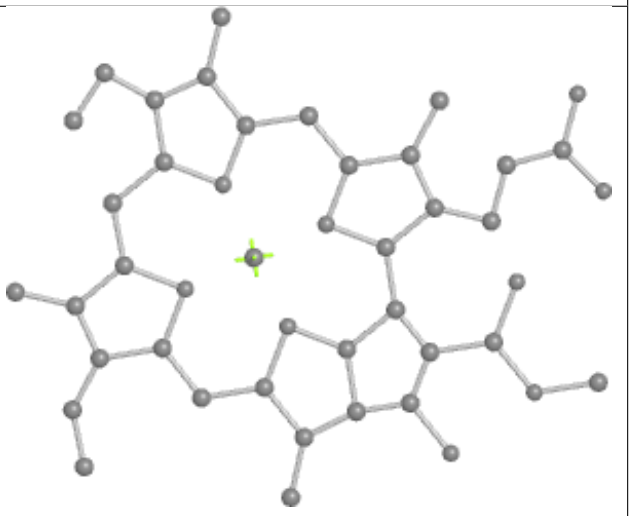
Bond lengths



Bond angles

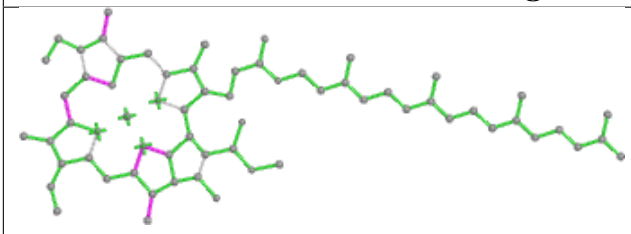


Torsions

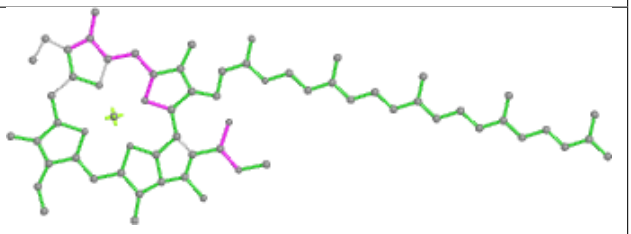


Rings

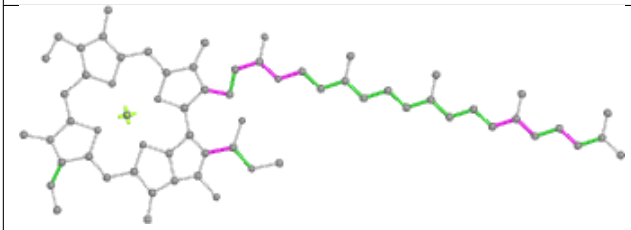
Ligand CLA B 510



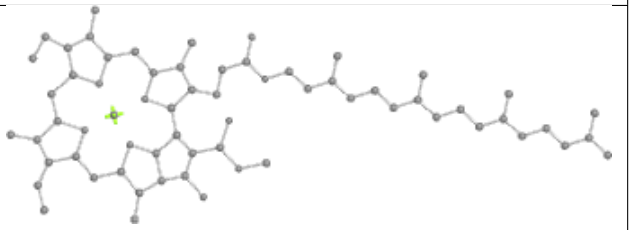
Bond lengths



Bond angles

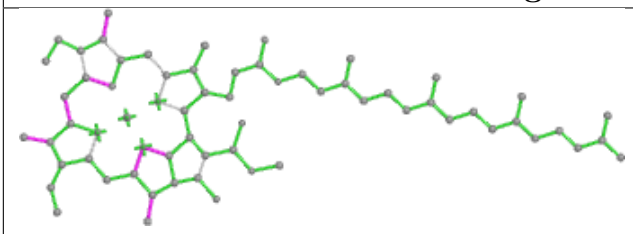


Torsions

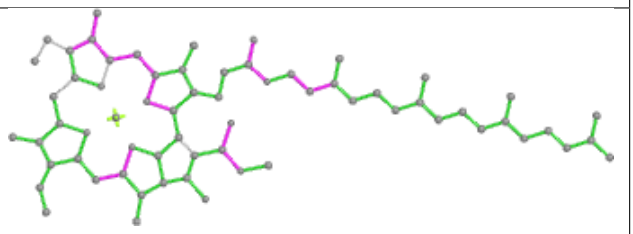


Rings

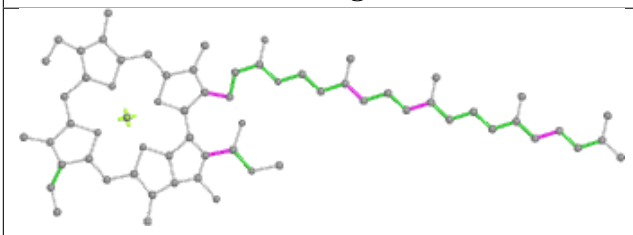
Ligand CLA B 511



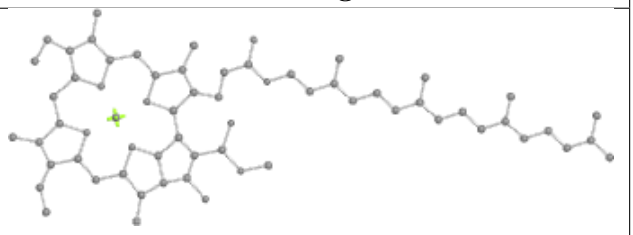
Bond lengths



Bond angles

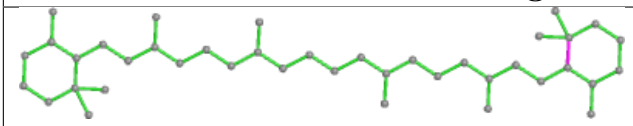


Torsions

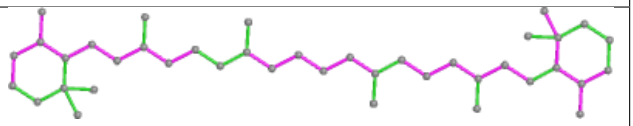


Rings

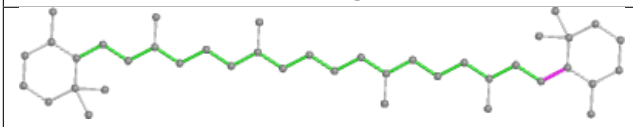
Ligand BCR a 406



Bond lengths



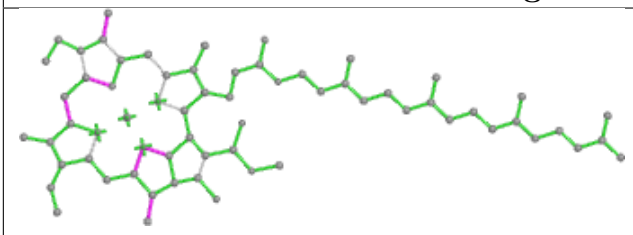
Bond angles



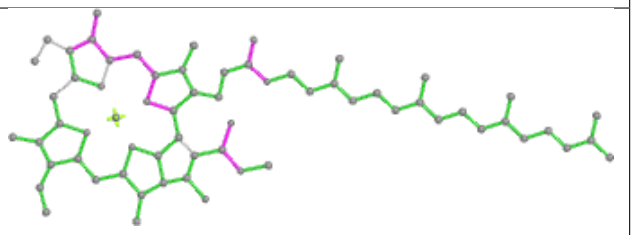
Torsions

Rings

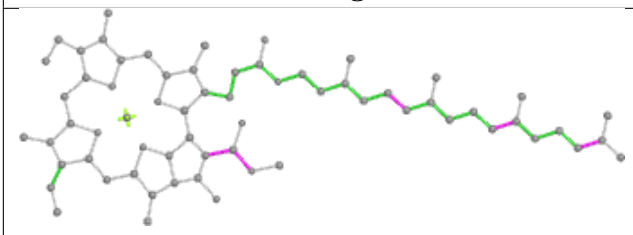
Ligand CLA Y 311



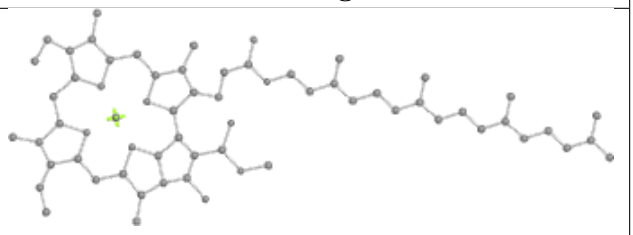
Bond lengths



Bond angles

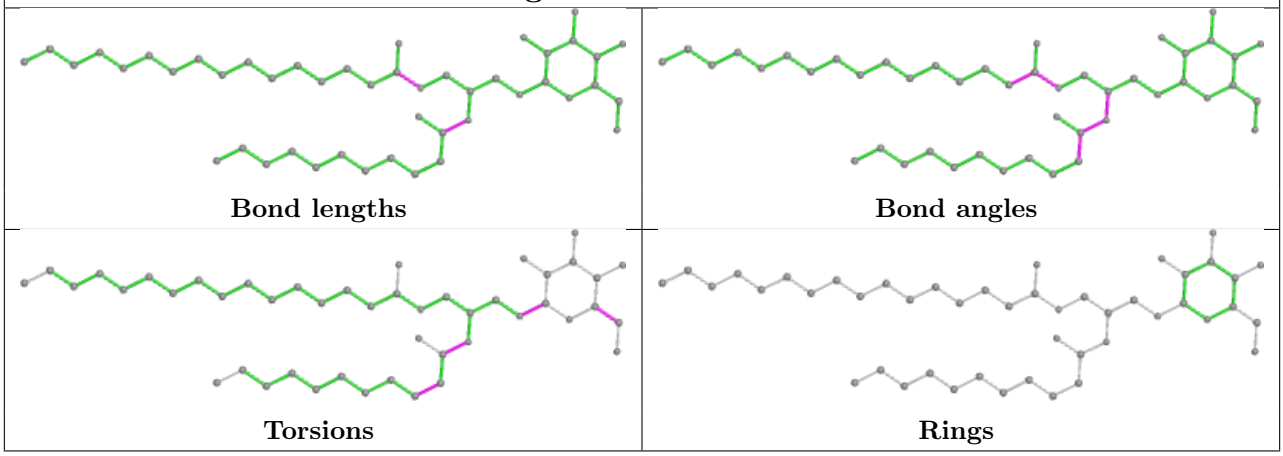


Torsions

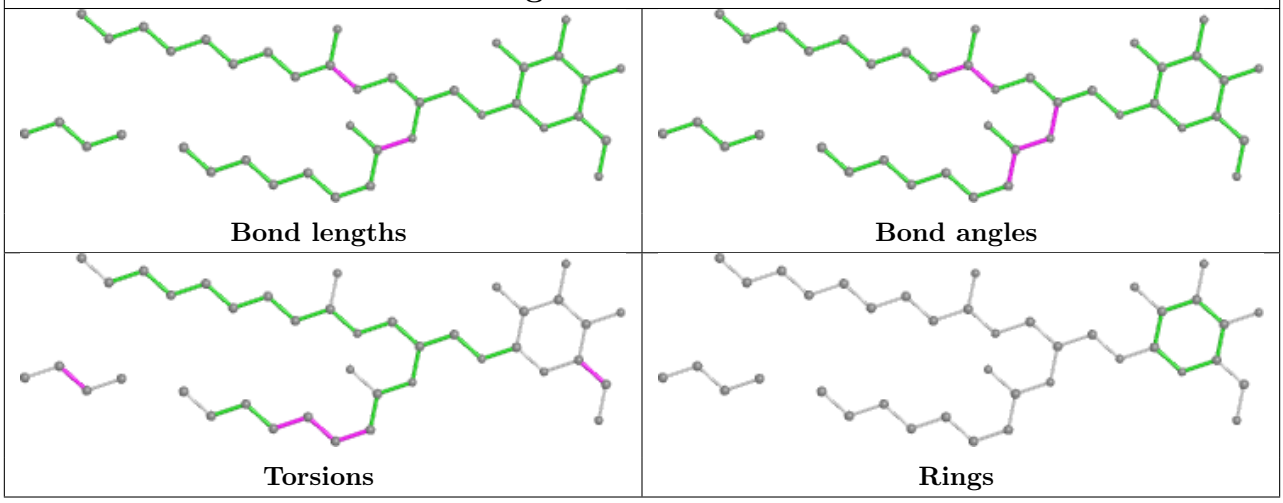


Rings

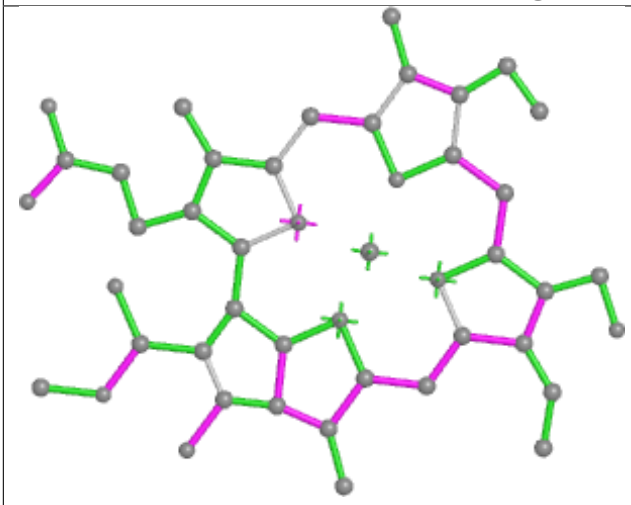
Ligand LMG a 408



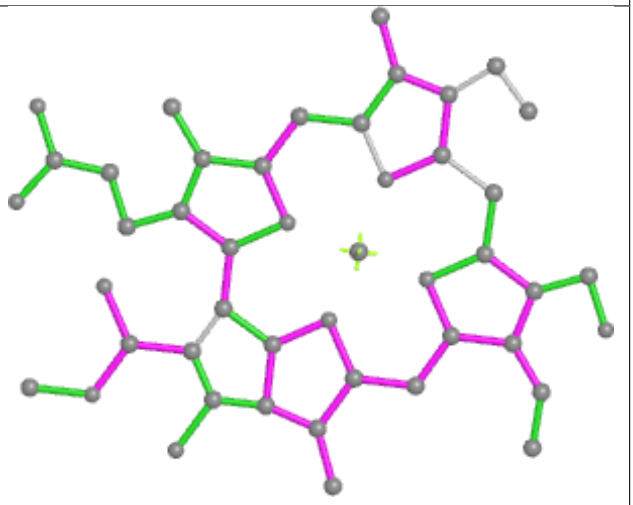
Ligand LMG c 518



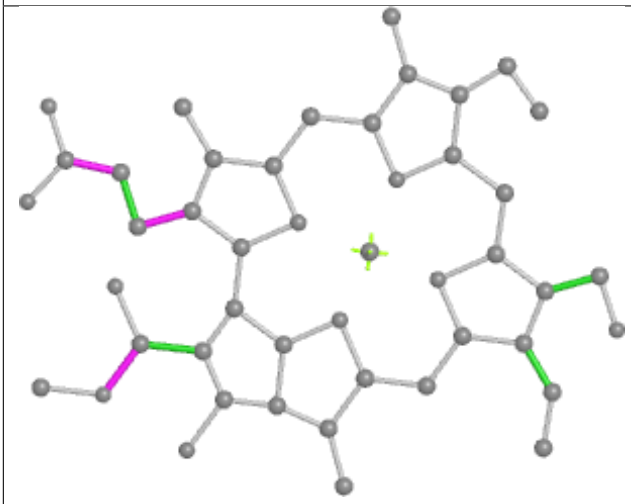
Ligand CHL r 306



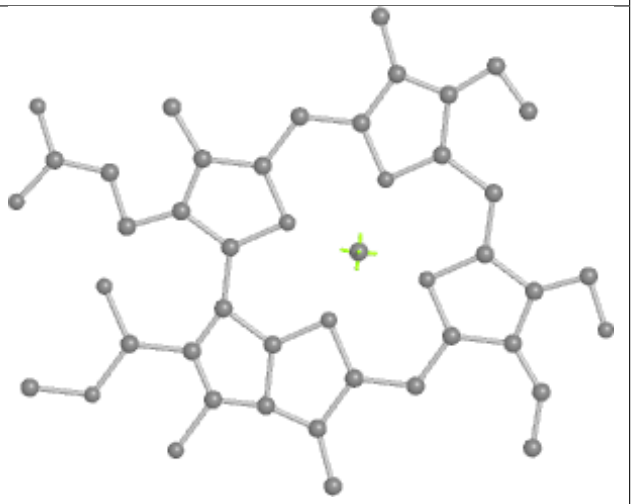
Bond lengths



Bond angles

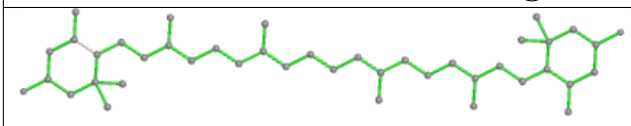


Torsions

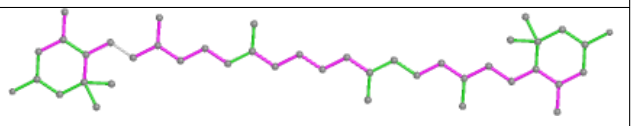


Rings

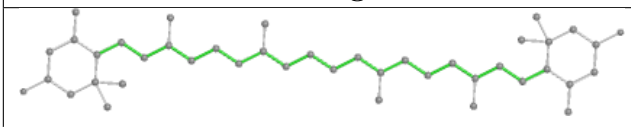
Ligand LUT G 615



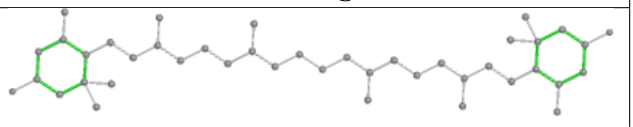
Bond lengths



Bond angles

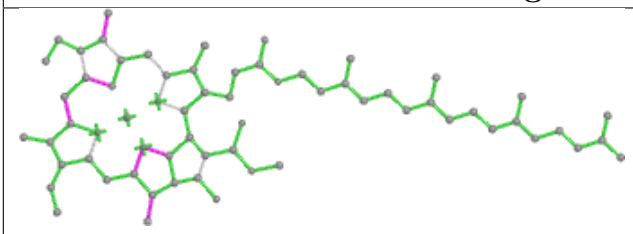


Torsions

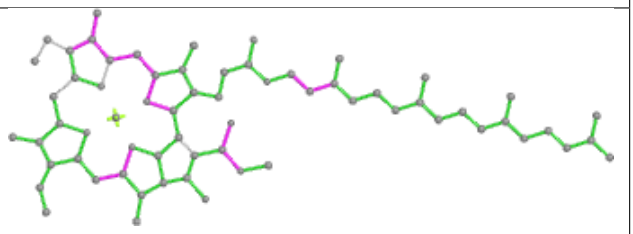


Rings

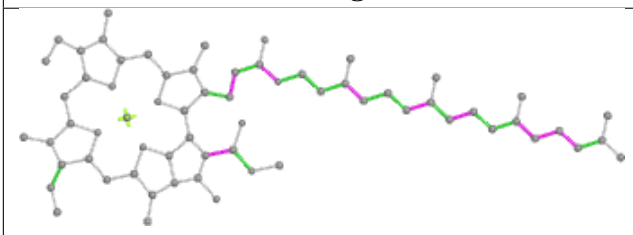
Ligand CLA C 510



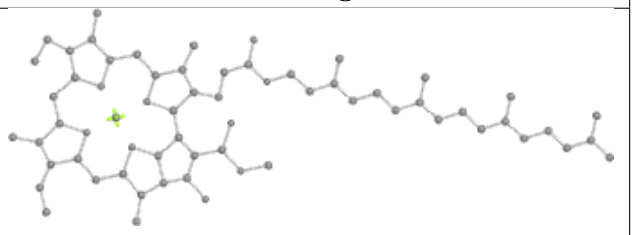
Bond lengths



Bond angles

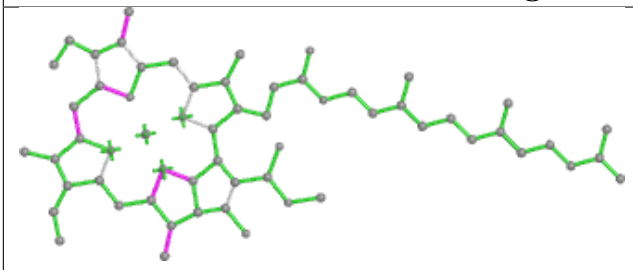


Torsions

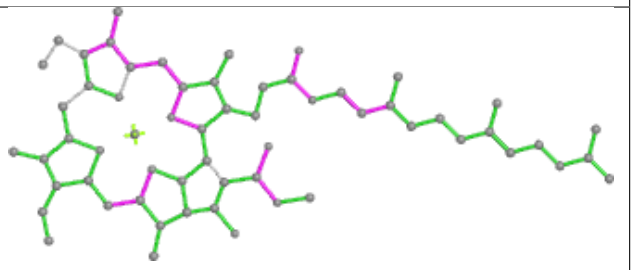


Rings

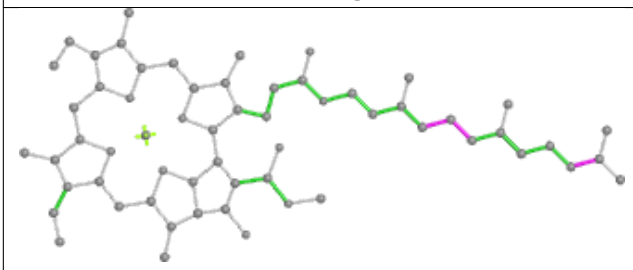
Ligand CLA A 405



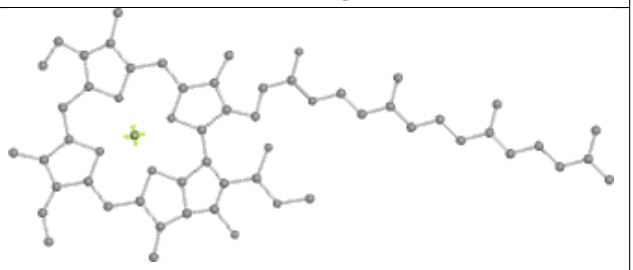
Bond lengths



Bond angles

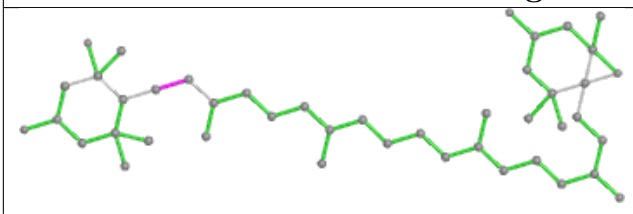


Torsions

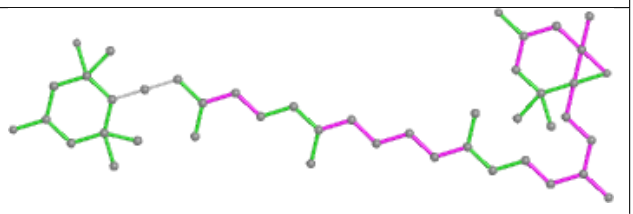


Rings

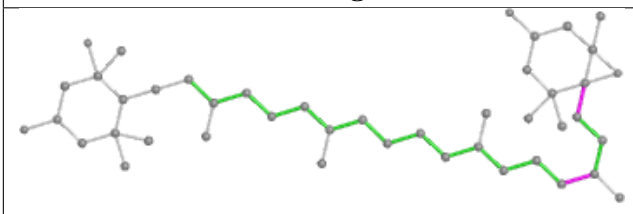
Ligand NEX S 617



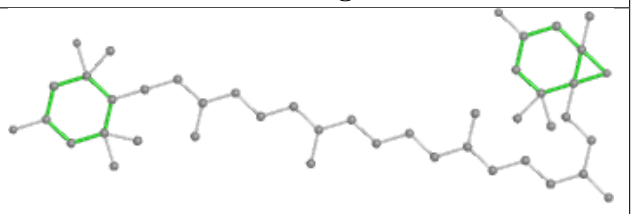
Bond lengths



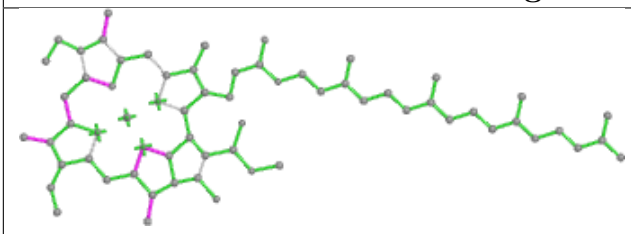
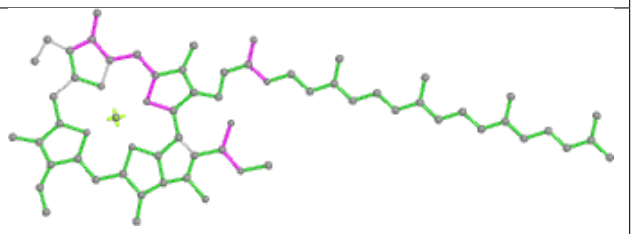
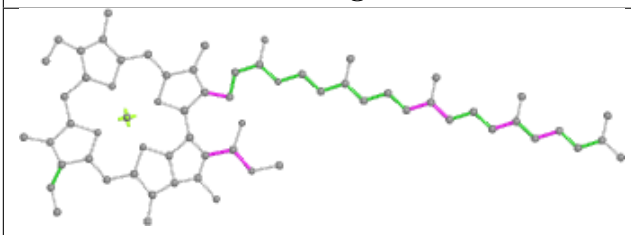
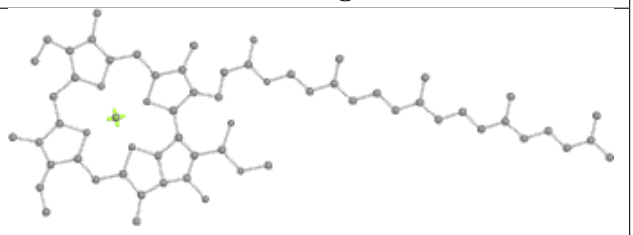
Bond angles

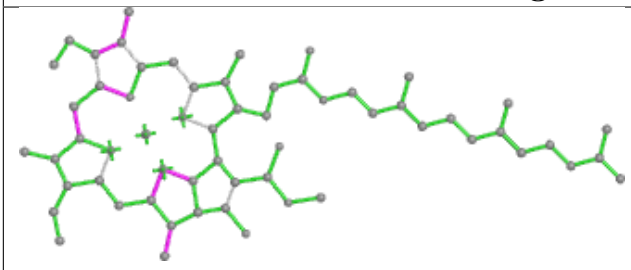
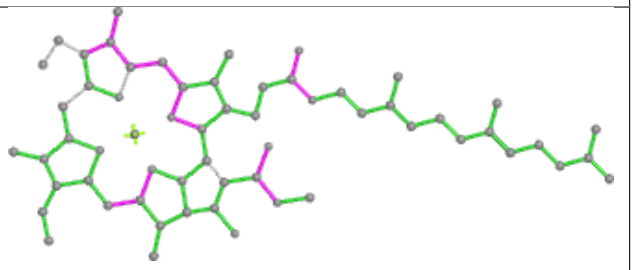
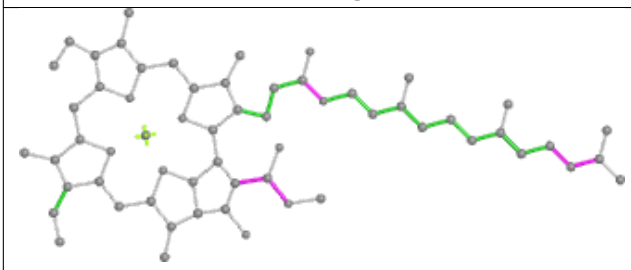
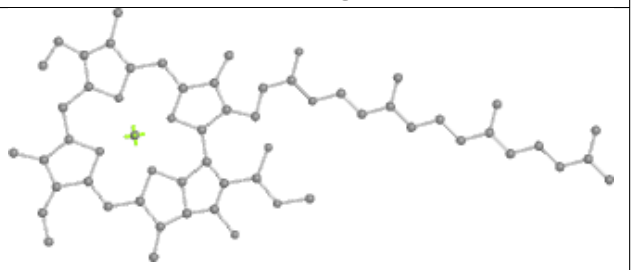


Torsions

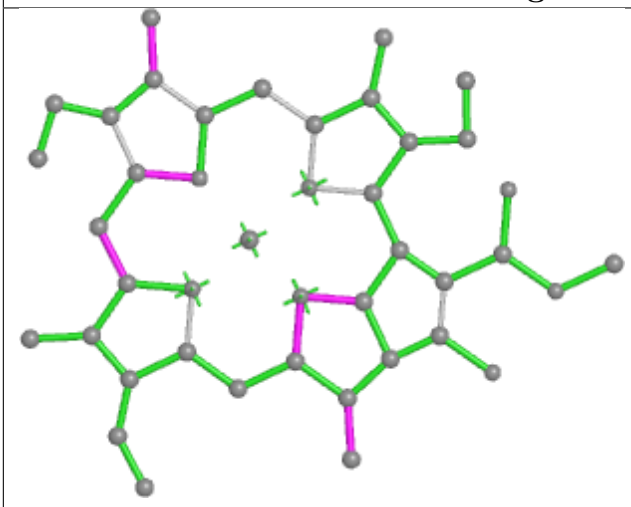


Rings

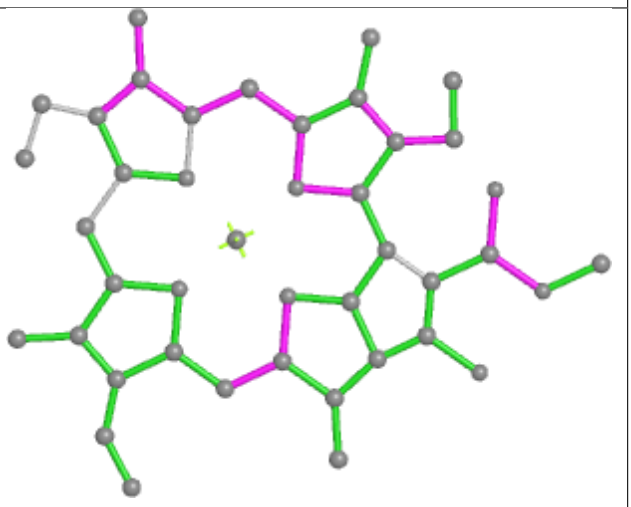
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

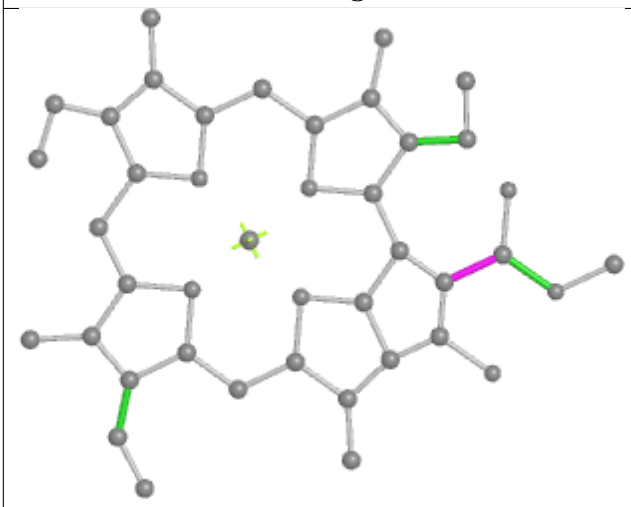
Ligand CLA S 603



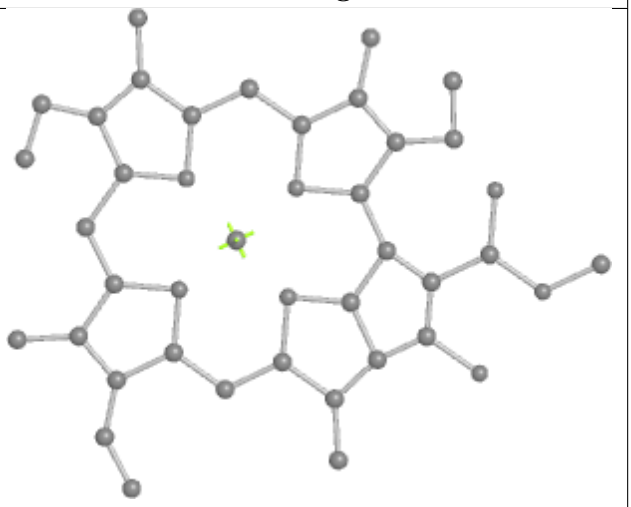
Bond lengths



Bond angles

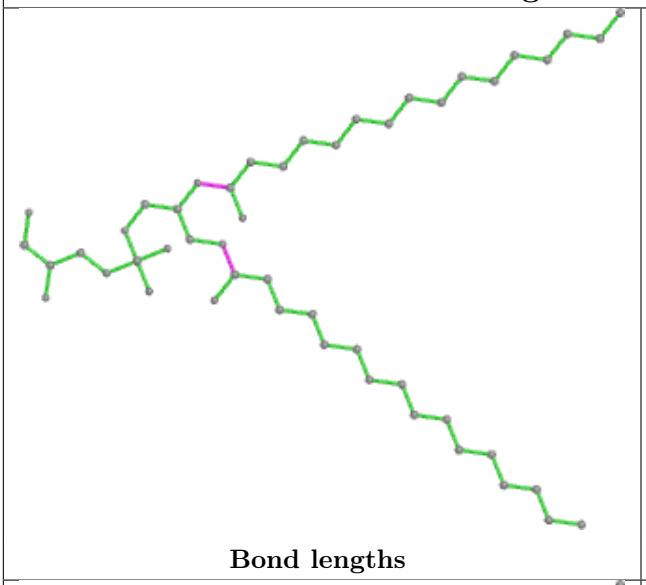


Torsions

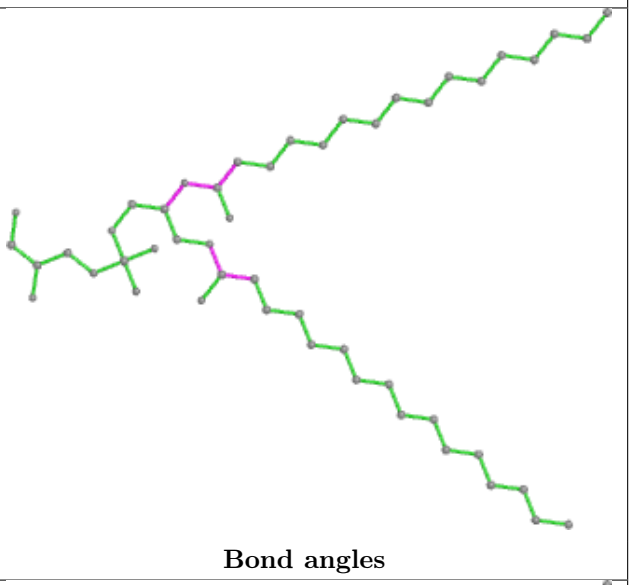


Rings

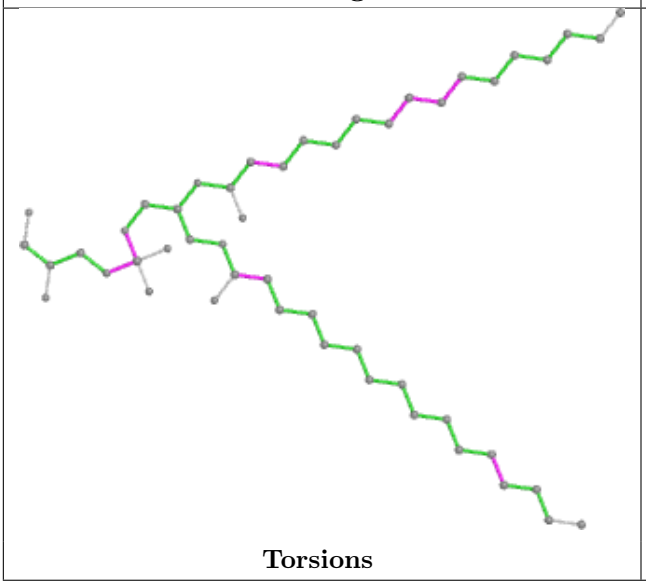
Ligand LHG D 408



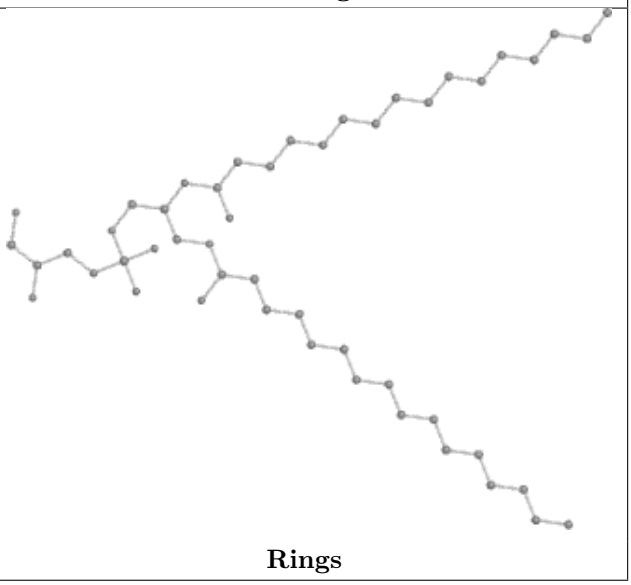
Bond lengths



Bond angles

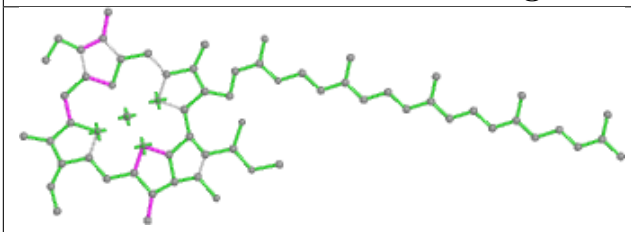


Torsions

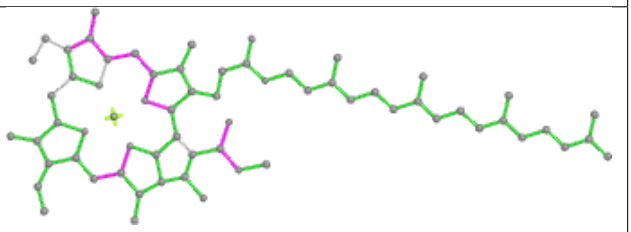


Rings

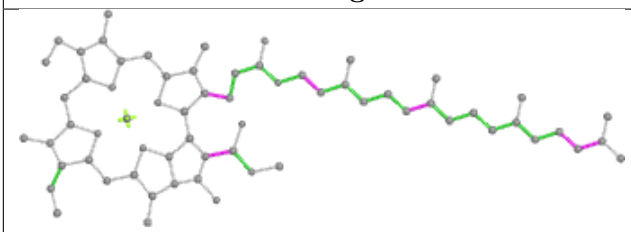
Ligand CLA N 304



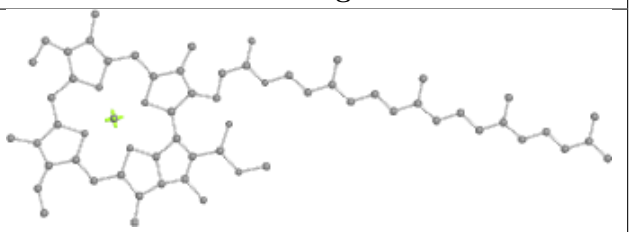
Bond lengths



Bond angles

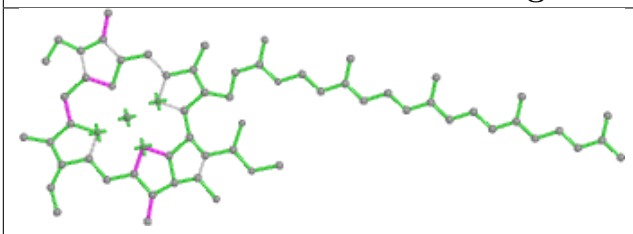


Torsions

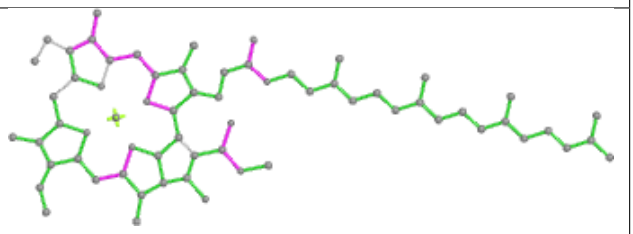


Rings

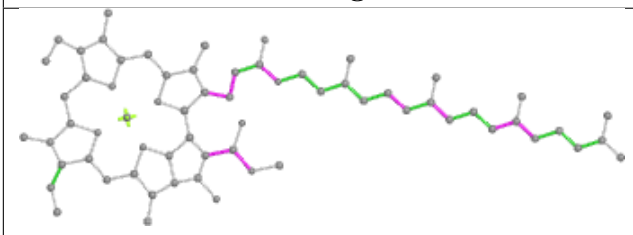
Ligand CLA b 504



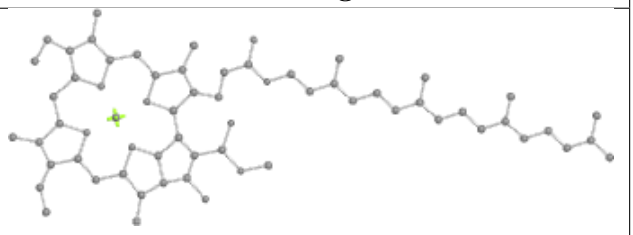
Bond lengths



Bond angles

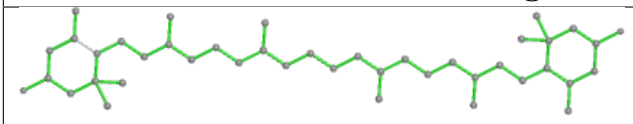


Torsions

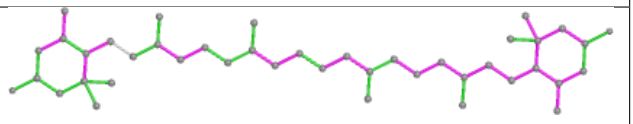


Rings

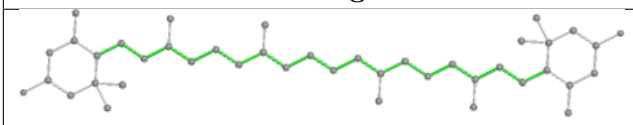
Ligand LUT N 317



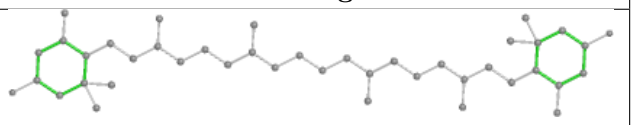
Bond lengths



Bond angles

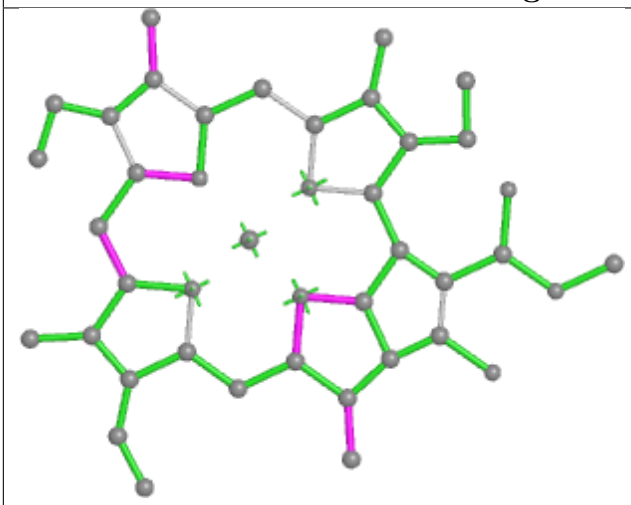


Torsions

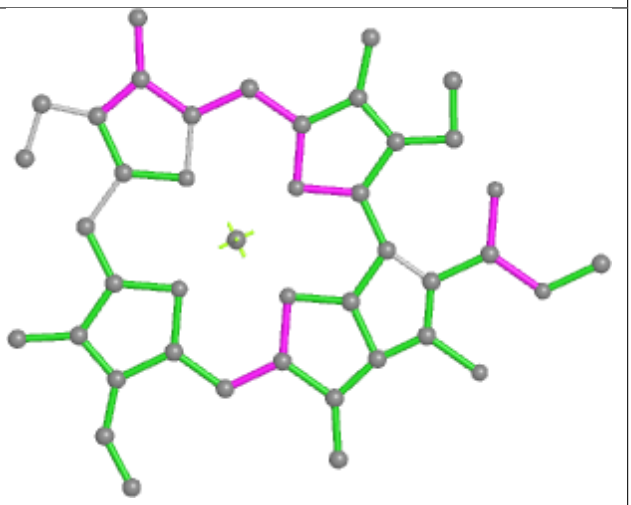


Rings

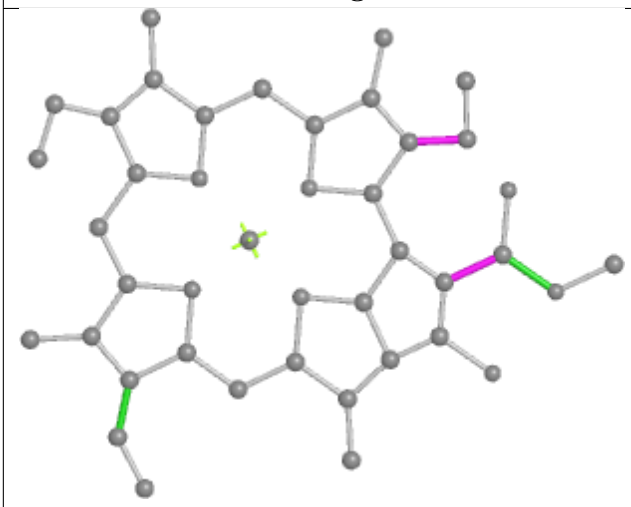
Ligand CLA G 604



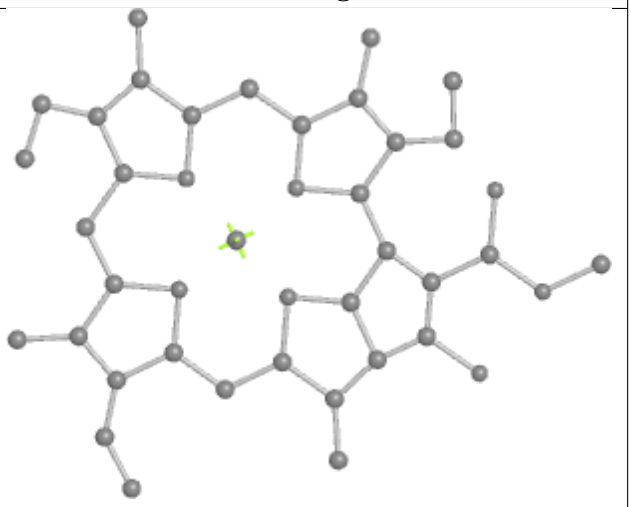
Bond lengths



Bond angles

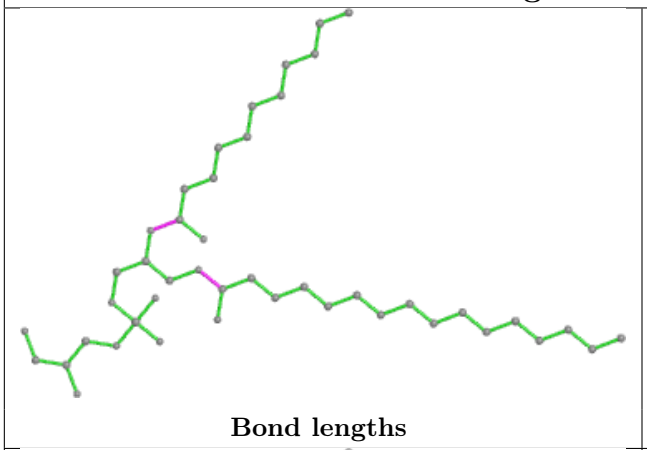


Torsions

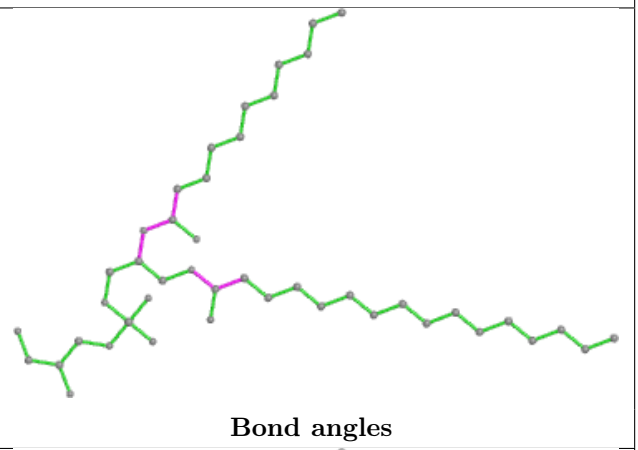


Rings

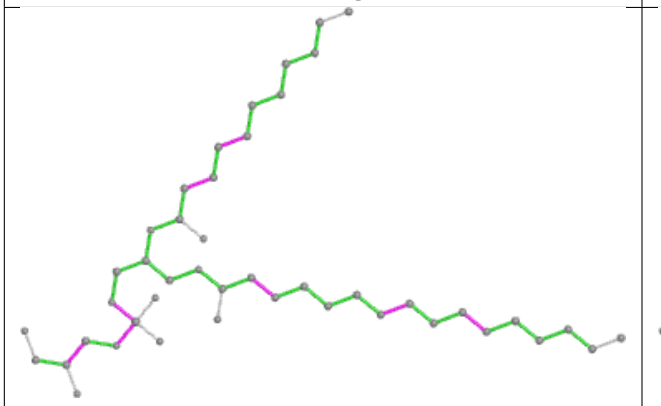
Ligand LHG B 520



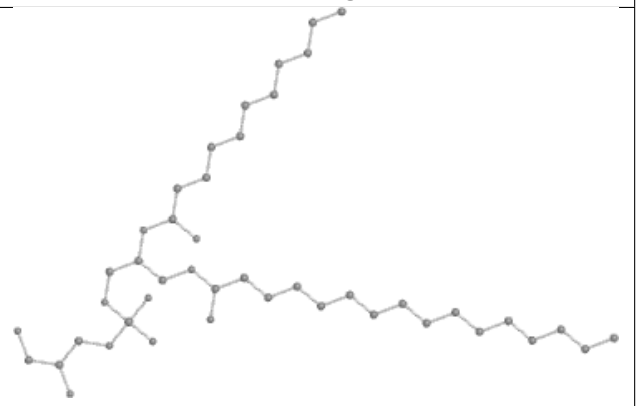
Bond lengths



Bond angles

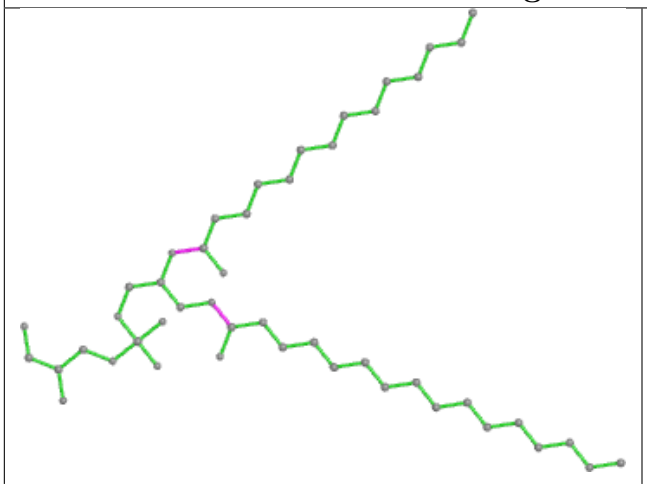


Torsions

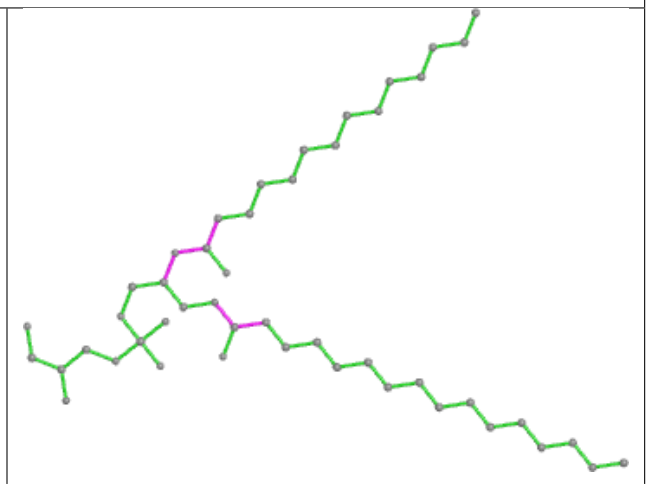


Rings

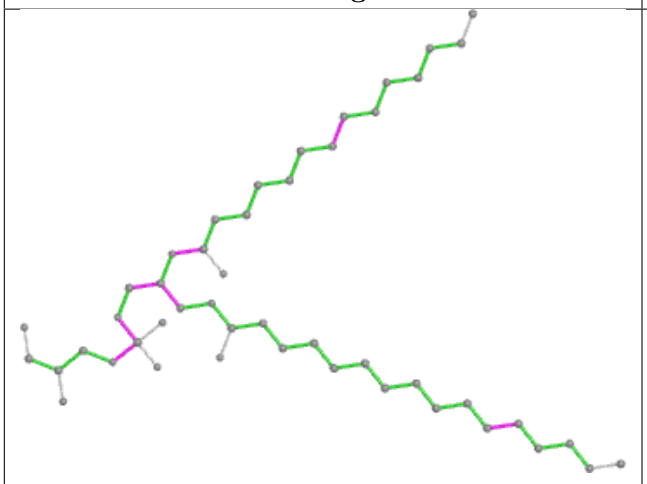
Ligand LHG C 521



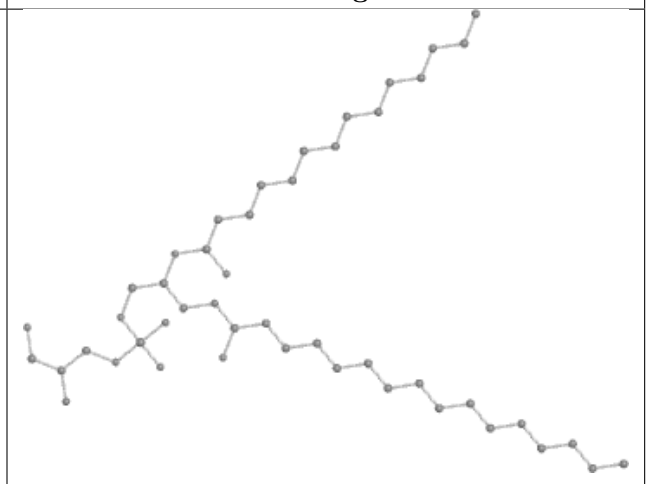
Bond lengths



Bond angles

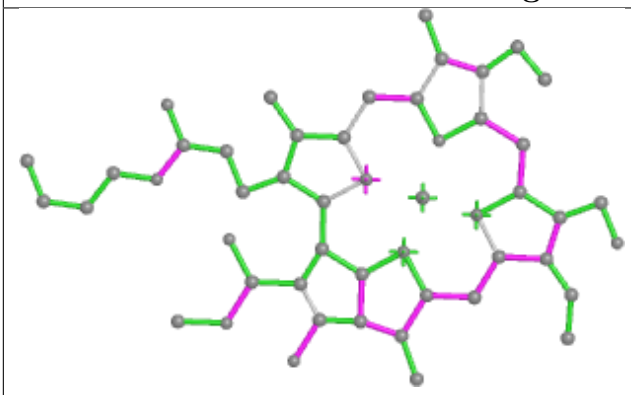


Torsions

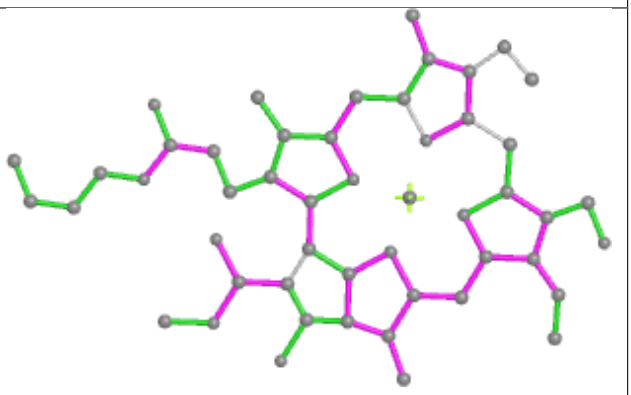


Rings

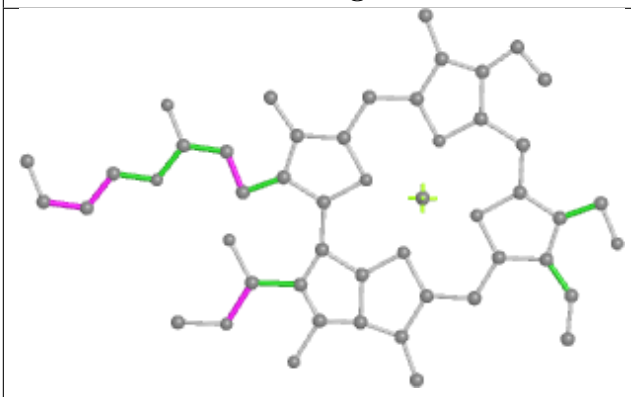
Ligand CHL N 309



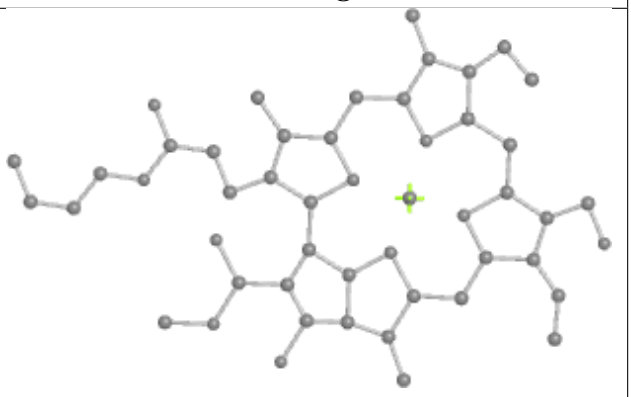
Bond lengths



Bond angles

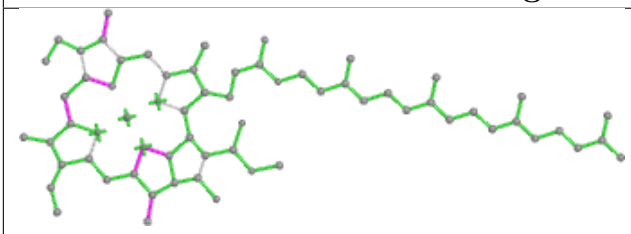


Torsions

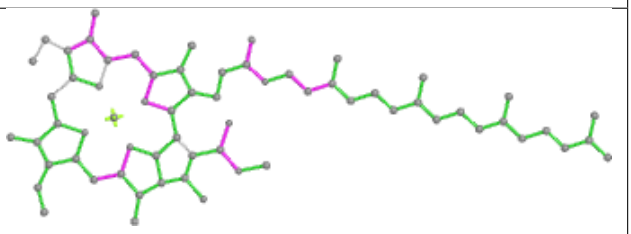


Rings

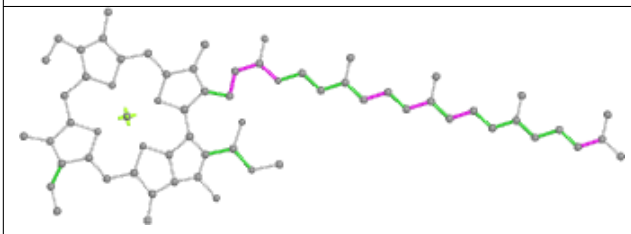
Ligand CLA N 303



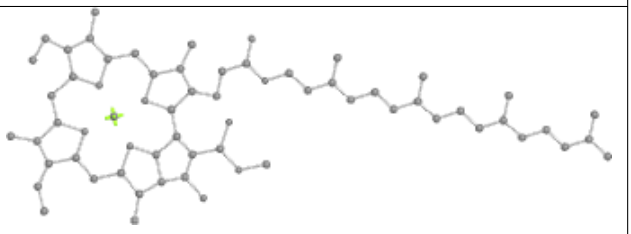
Bond lengths



Bond angles

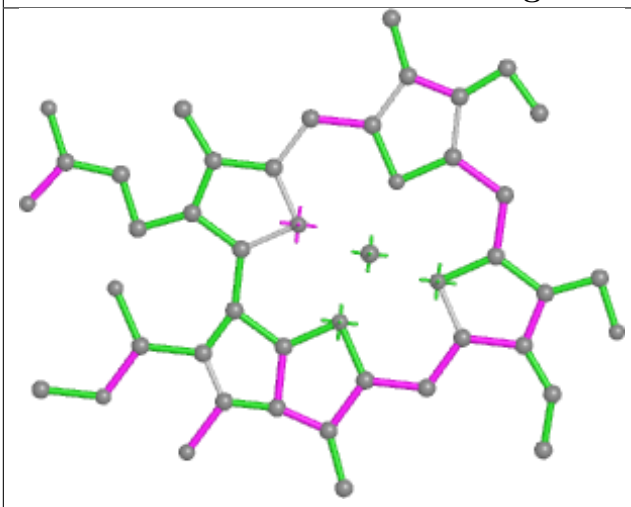


Torsions

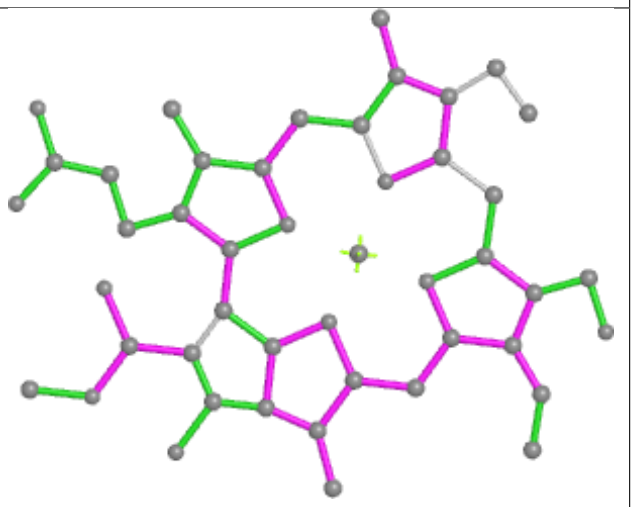


Rings

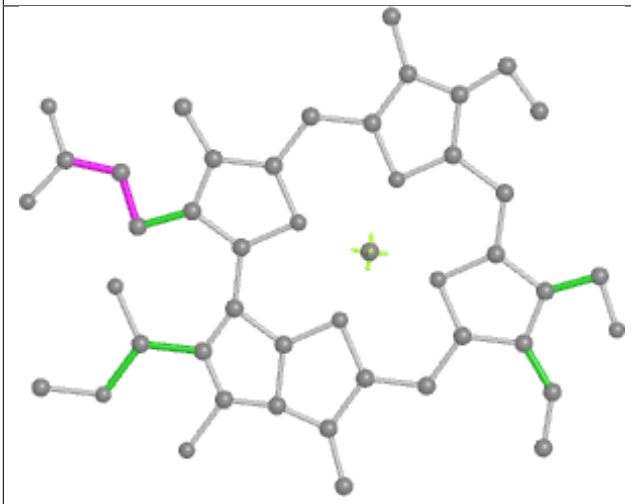
Ligand CHL Y 307



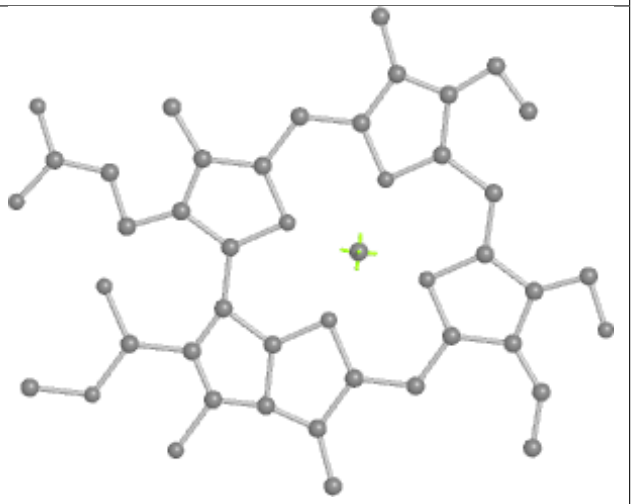
Bond lengths



Bond angles

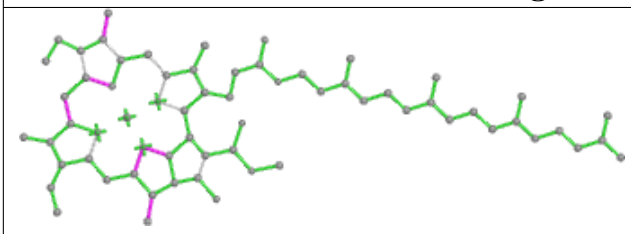


Torsions

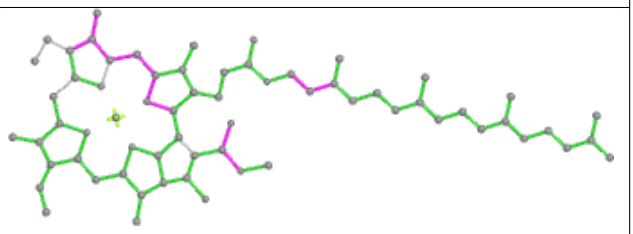


Rings

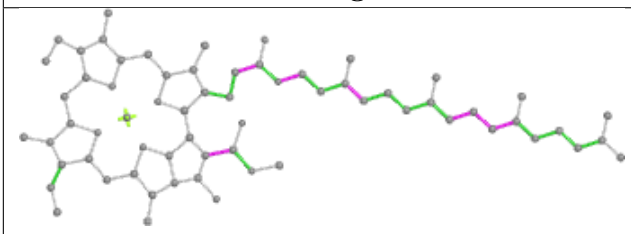
Ligand CLA c 510



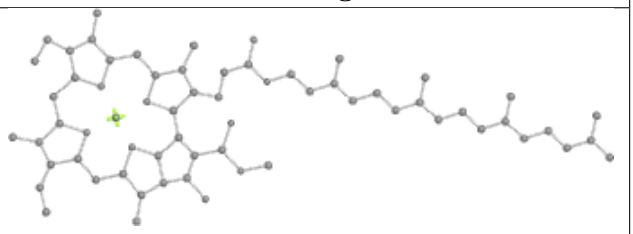
Bond lengths



Bond angles

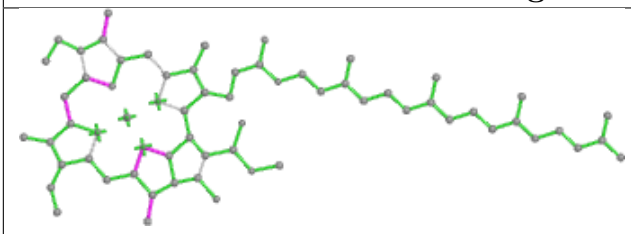


Torsions

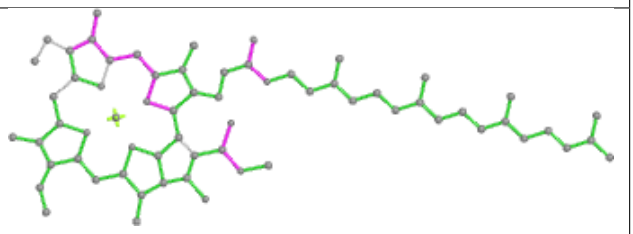


Rings

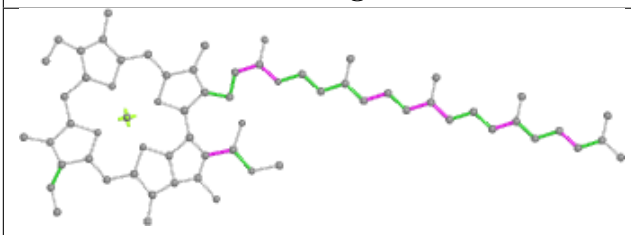
Ligand CLA b 510



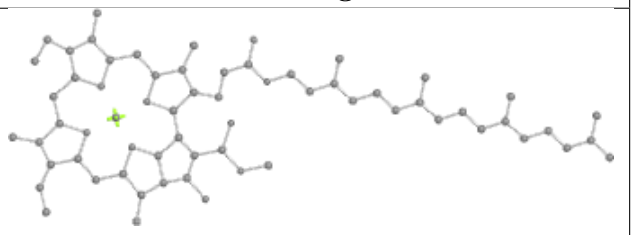
Bond lengths



Bond angles

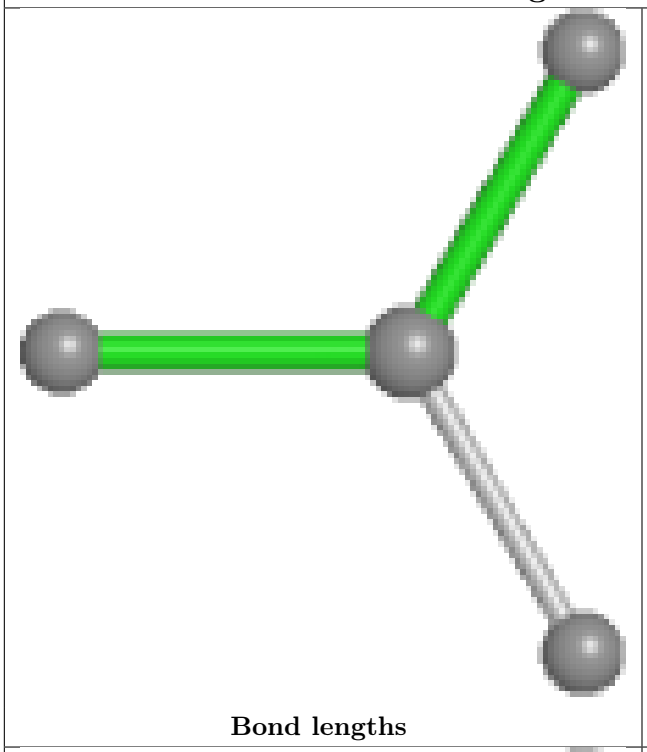


Torsions

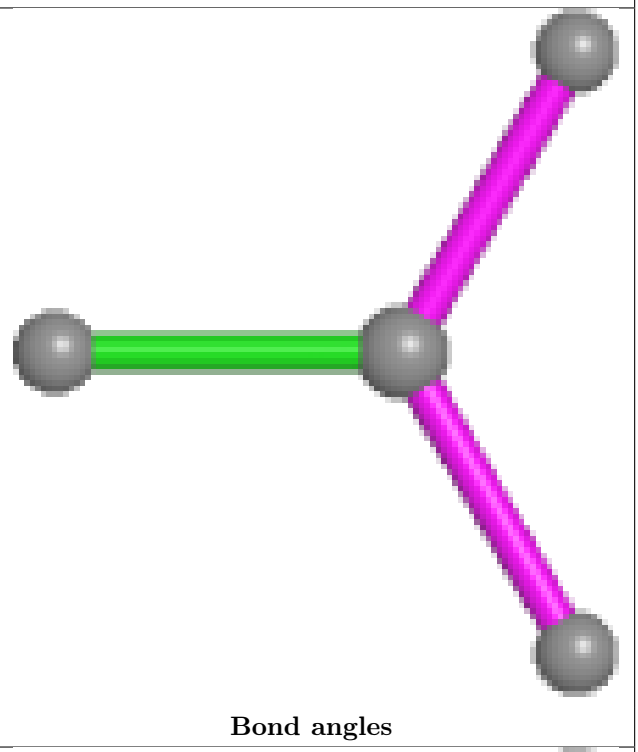


Rings

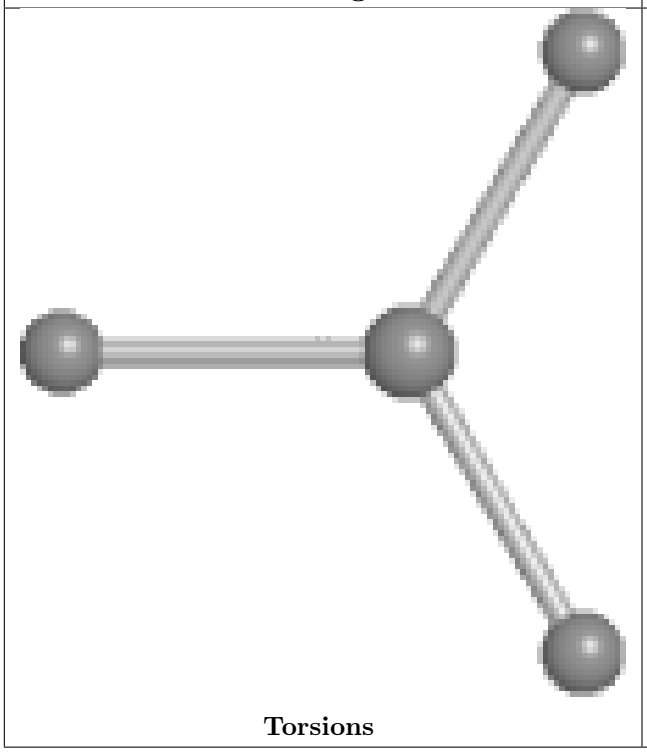
Ligand BCT a 409



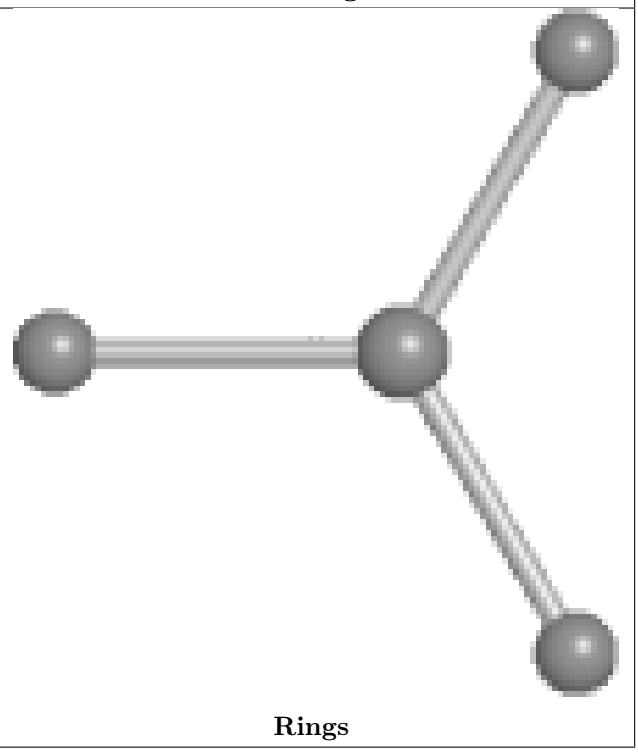
Bond lengths



Bond angles

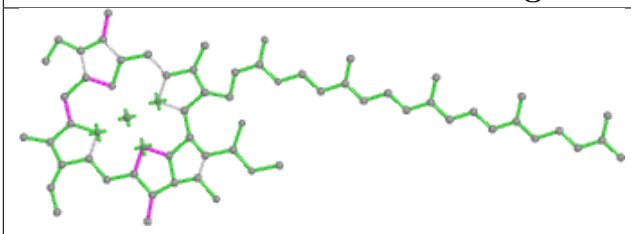


Torsions

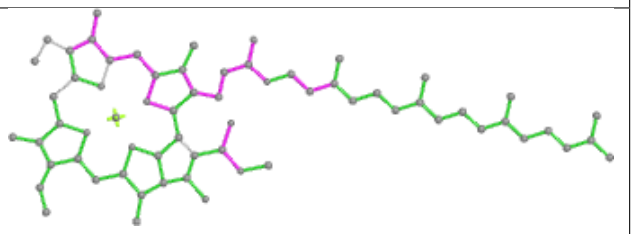


Rings

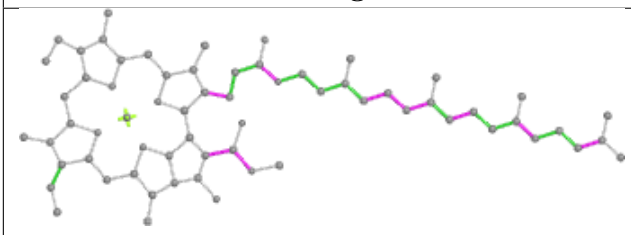
Ligand CLA B 504



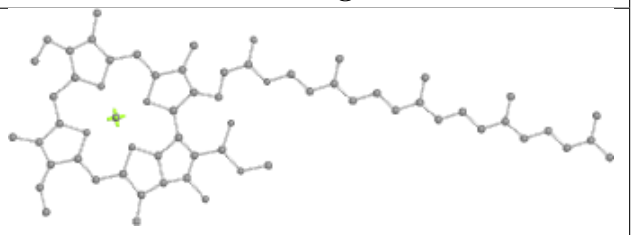
Bond lengths



Bond angles

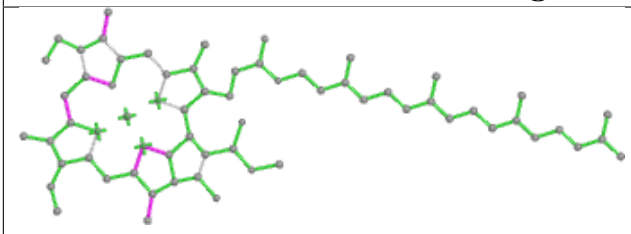


Torsions

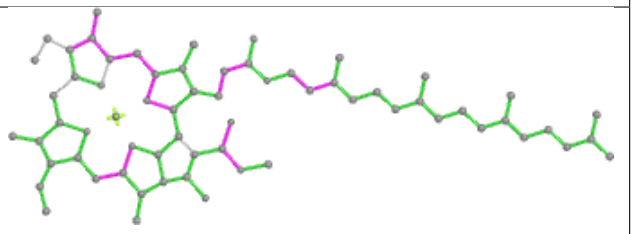


Rings

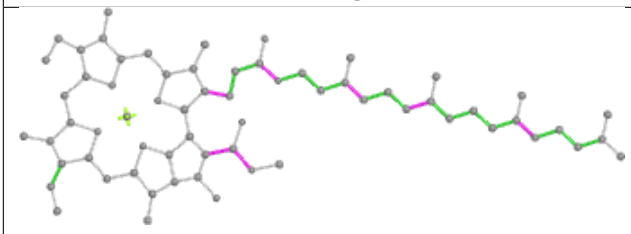
Ligand CLA c 511



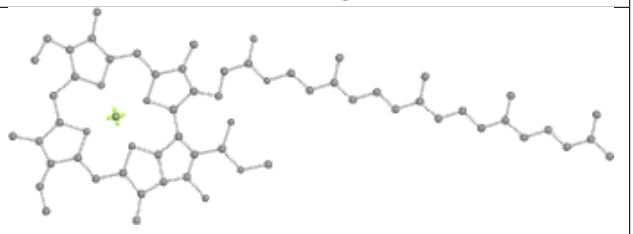
Bond lengths



Bond angles

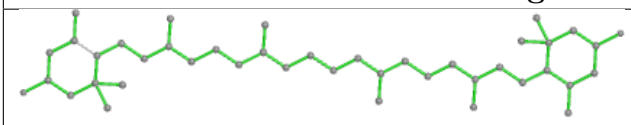


Torsions

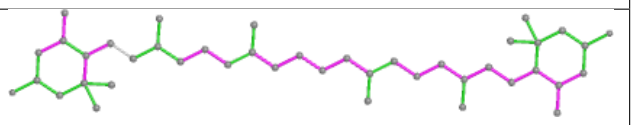


Rings

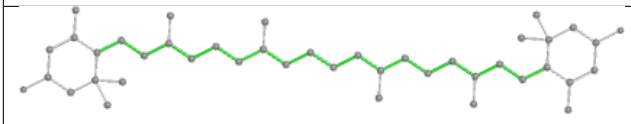
Ligand LUT S 615



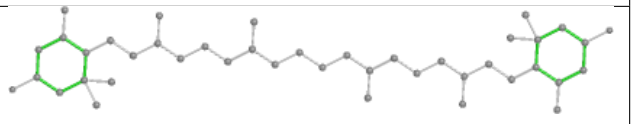
Bond lengths



Bond angles

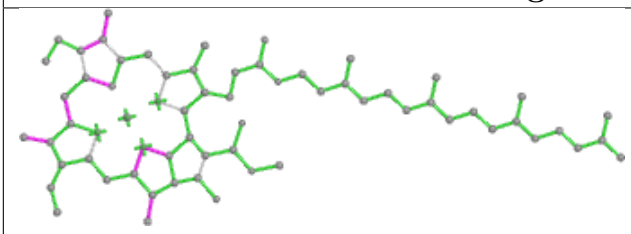


Torsions

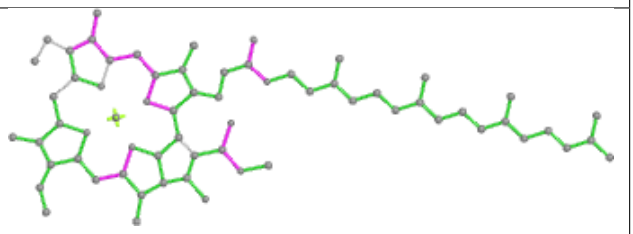


Rings

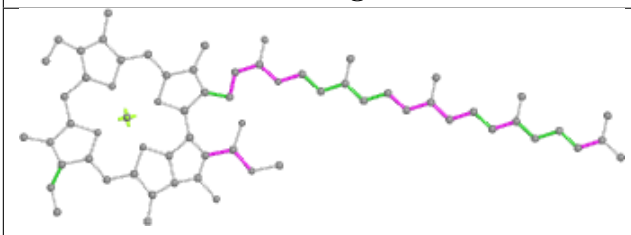
Ligand CLA b 511



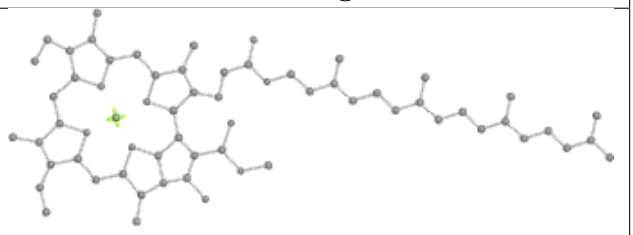
Bond lengths



Bond angles

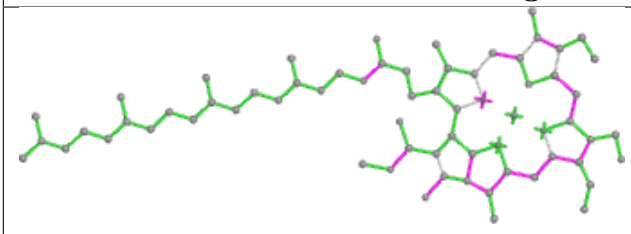


Torsions

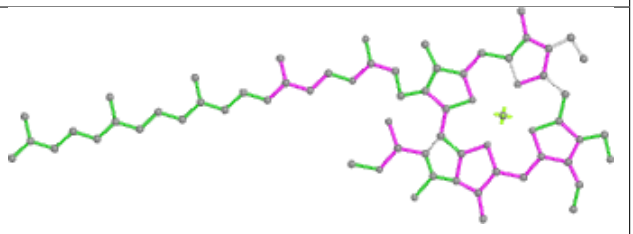


Rings

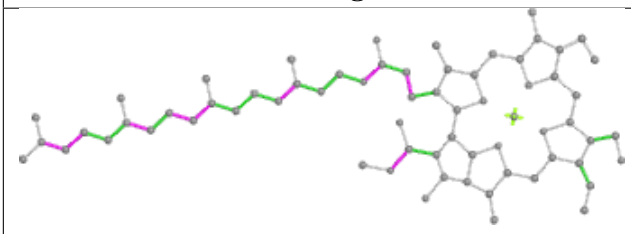
Ligand CHL G 601



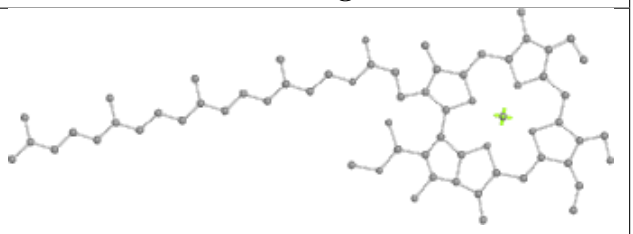
Bond lengths



Bond angles

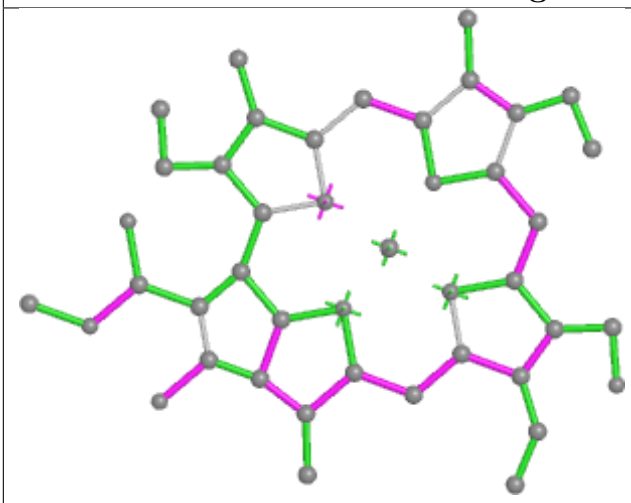


Torsions

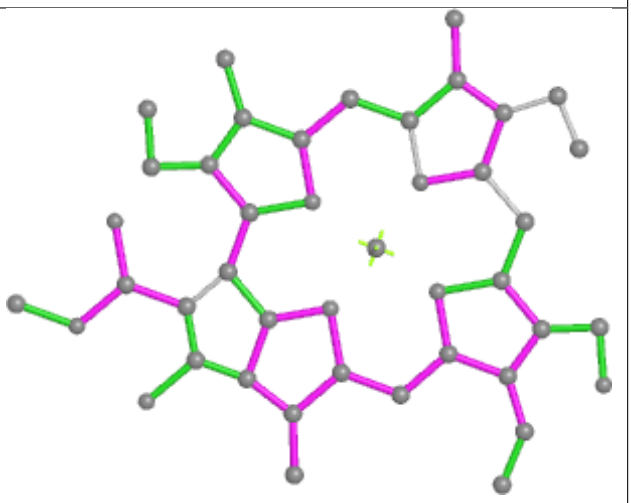


Rings

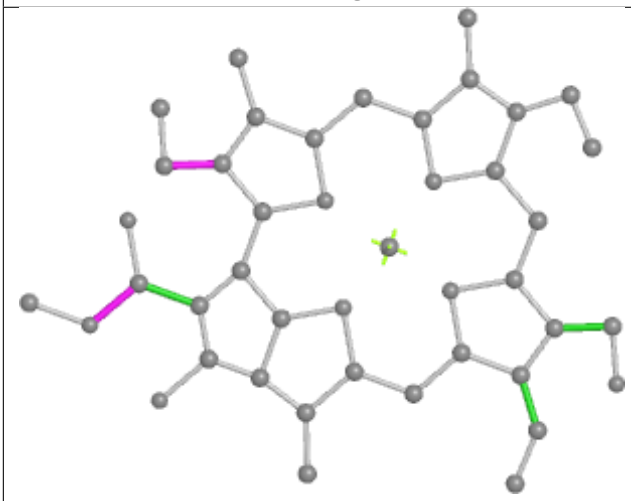
Ligand CHL r 305



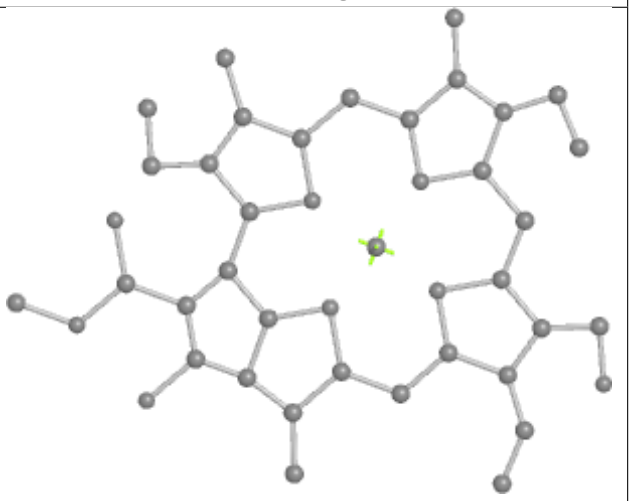
Bond lengths



Bond angles

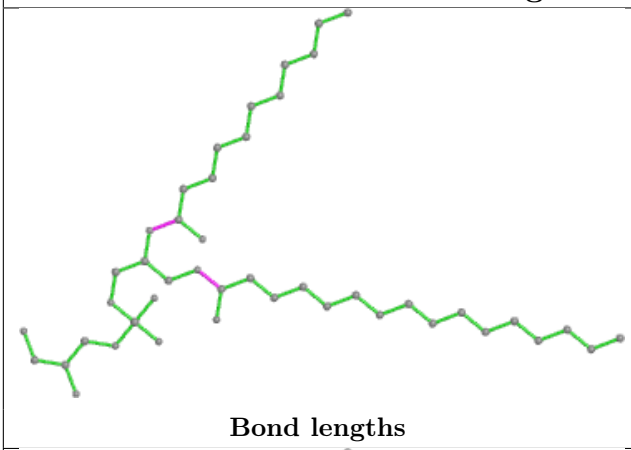


Torsions

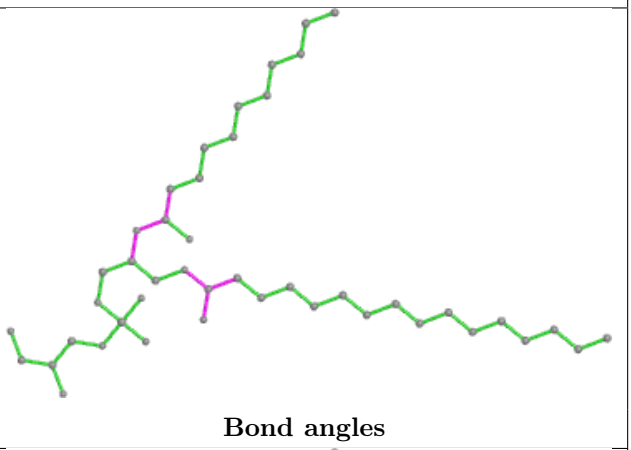


Rings

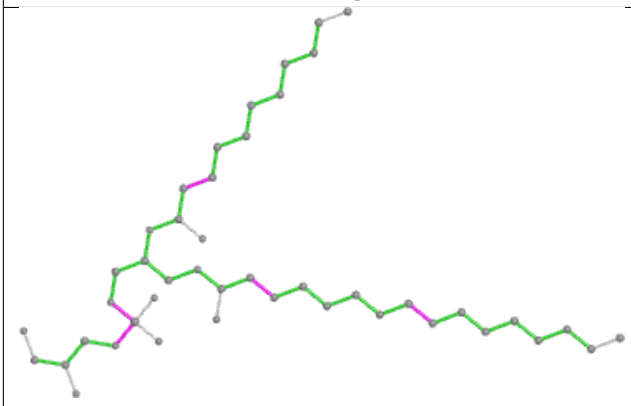
Ligand LHG d 407



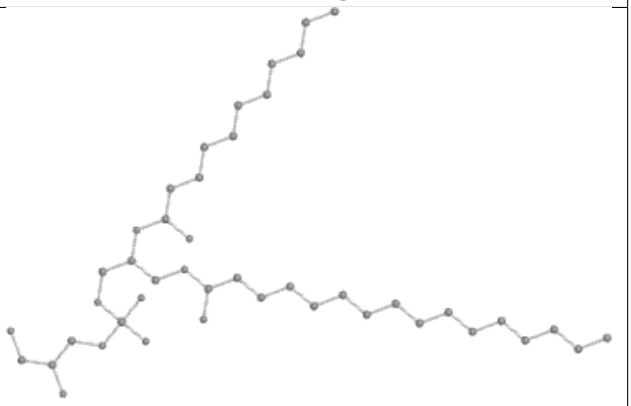
Bond lengths



Bond angles

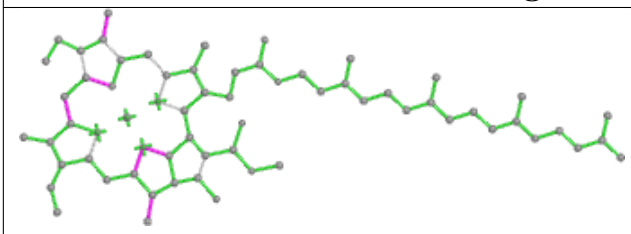


Torsions

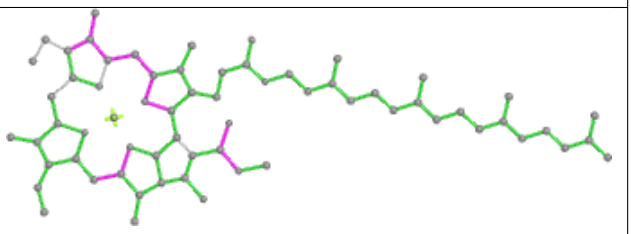


Rings

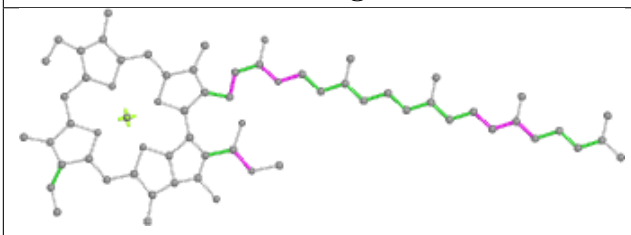
Ligand CLA N 314



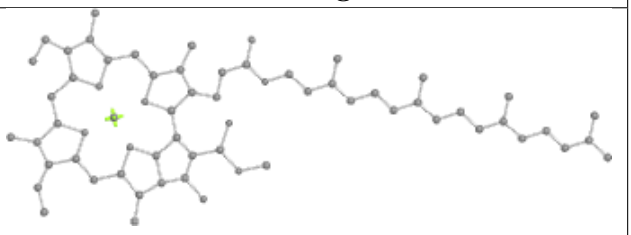
Bond lengths



Bond angles

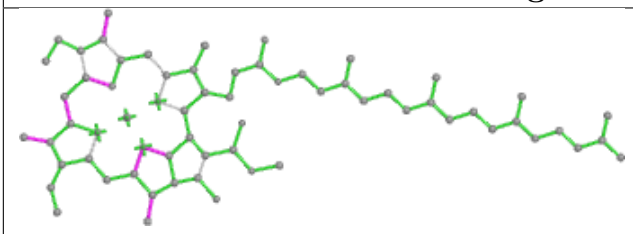


Torsions

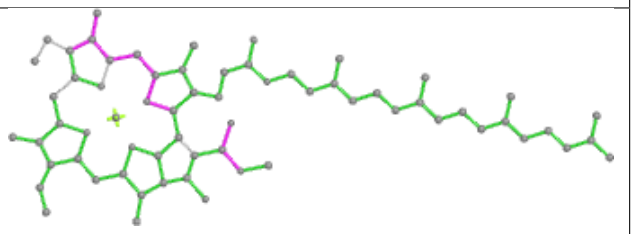


Rings

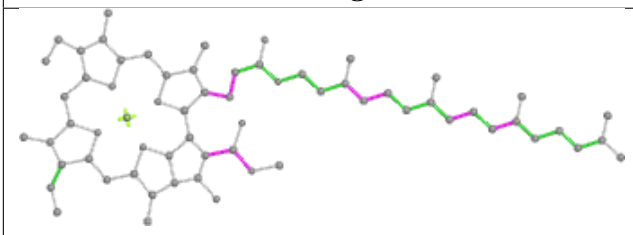
Ligand CLA b 503



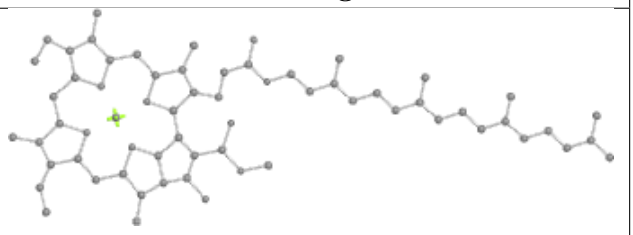
Bond lengths



Bond angles

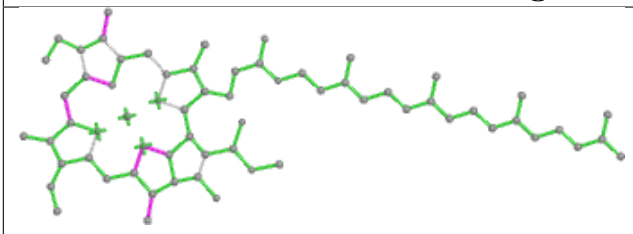


Torsions

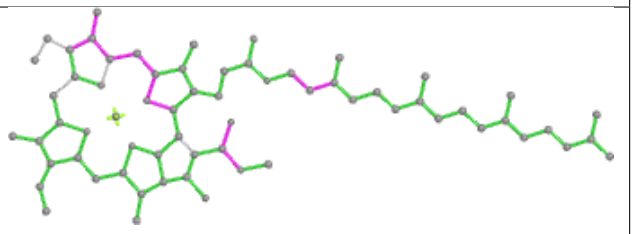


Rings

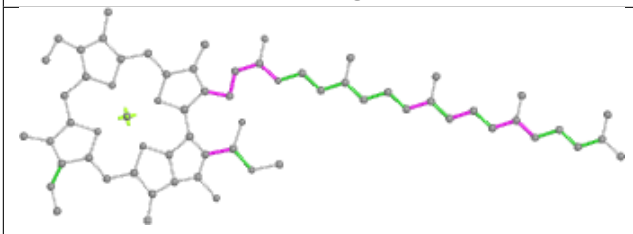
Ligand CLA c 509



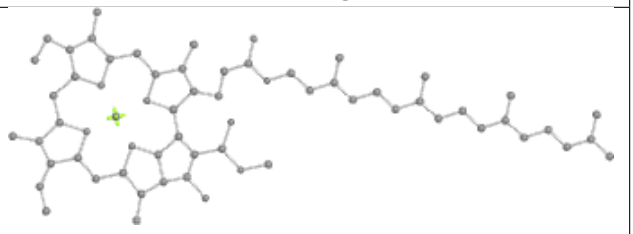
Bond lengths



Bond angles

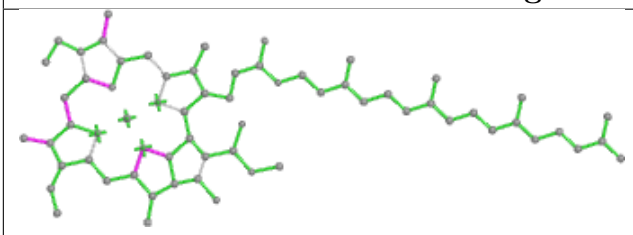


Torsions

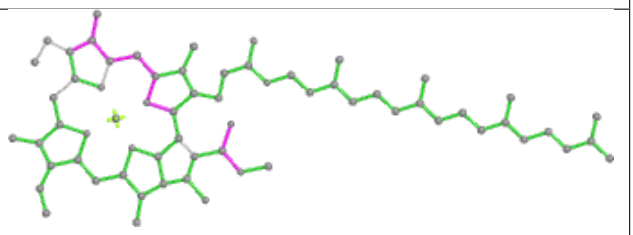


Rings

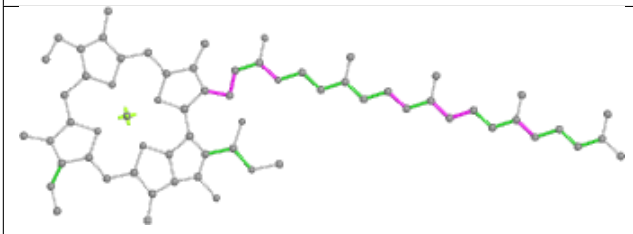
Ligand CLA B 516



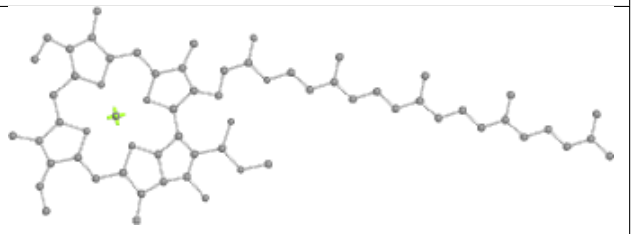
Bond lengths



Bond angles

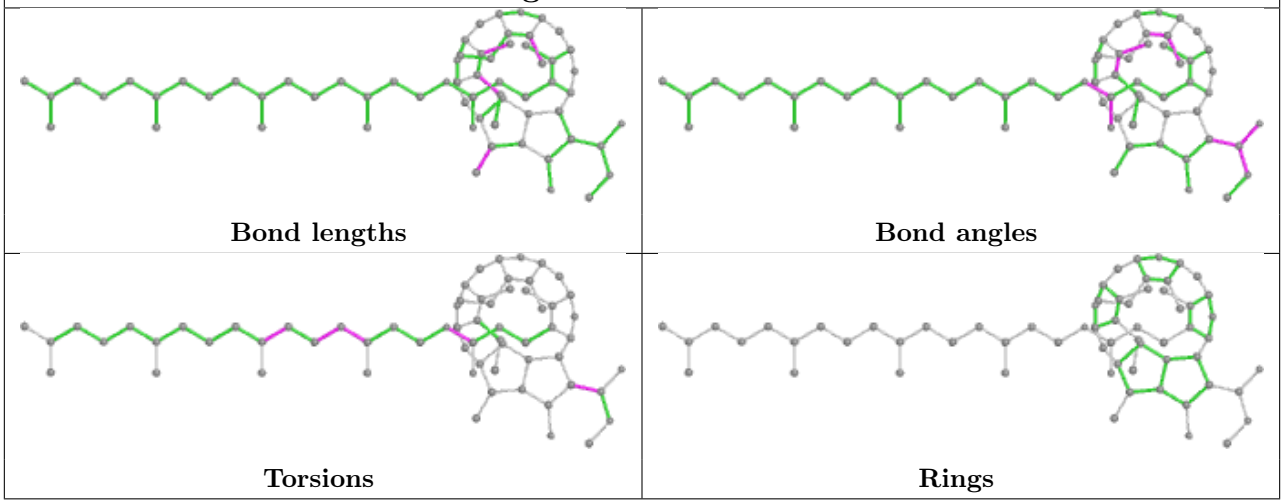


Torsions

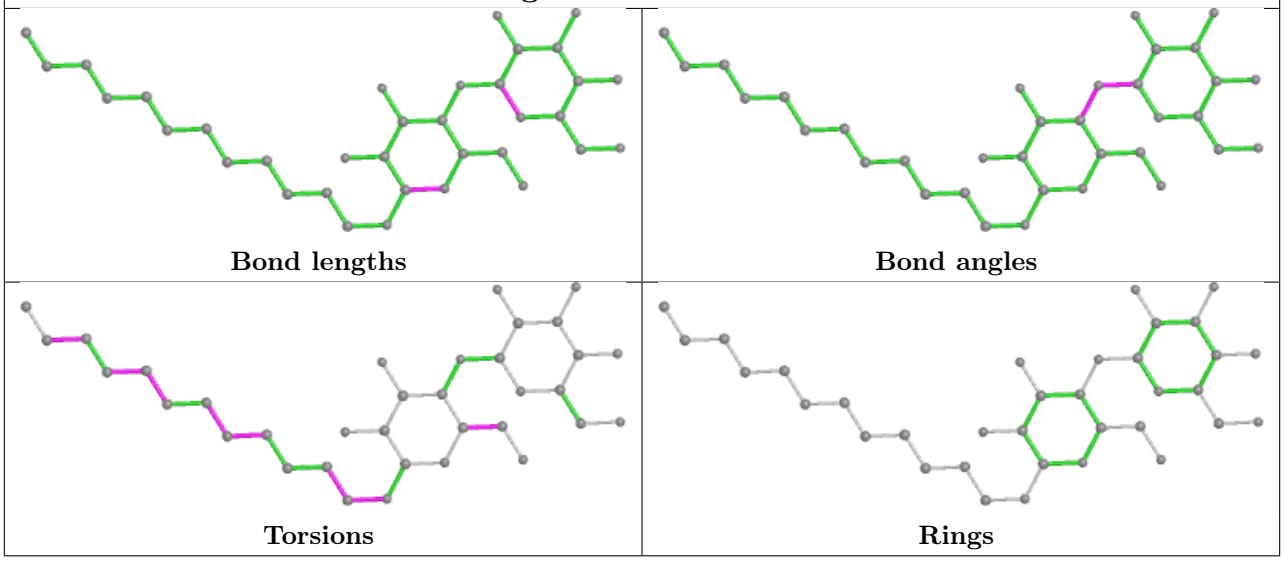


Rings

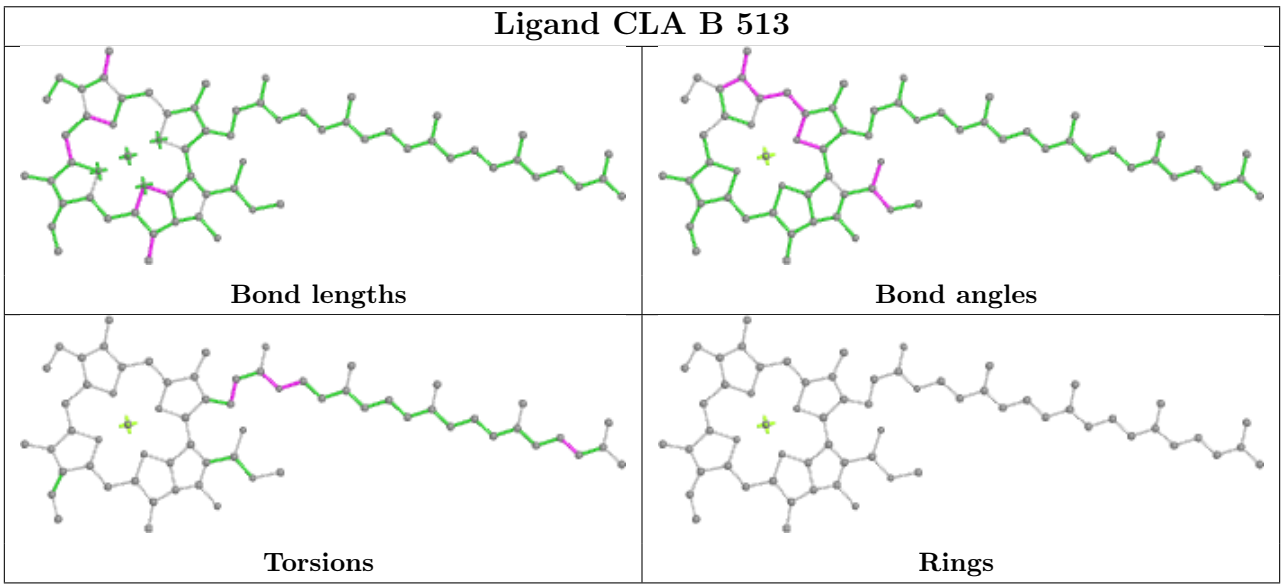
Ligand PHO A 404



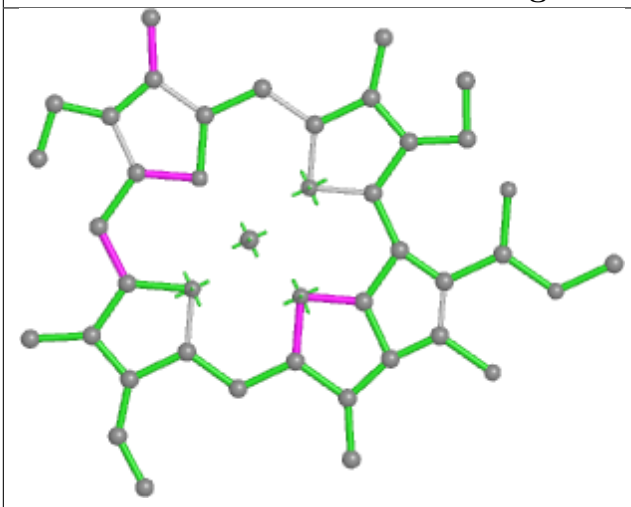
Ligand LMU C 522



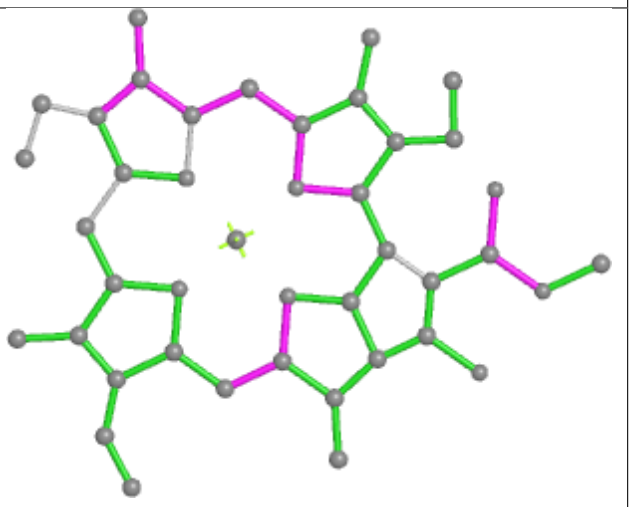
Ligand CLA B 513



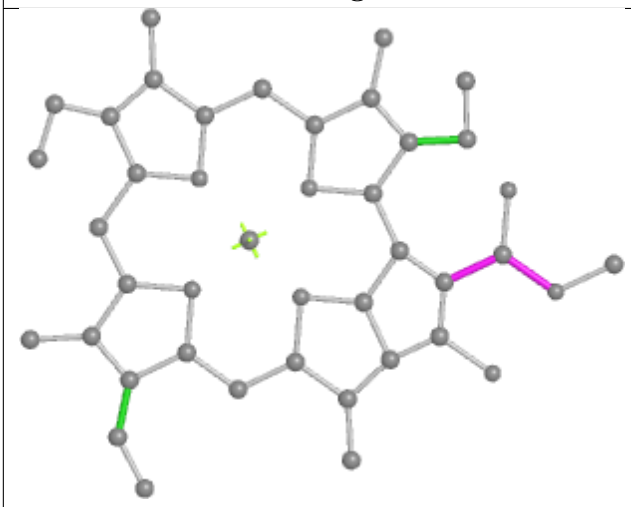
Ligand CLA c 513



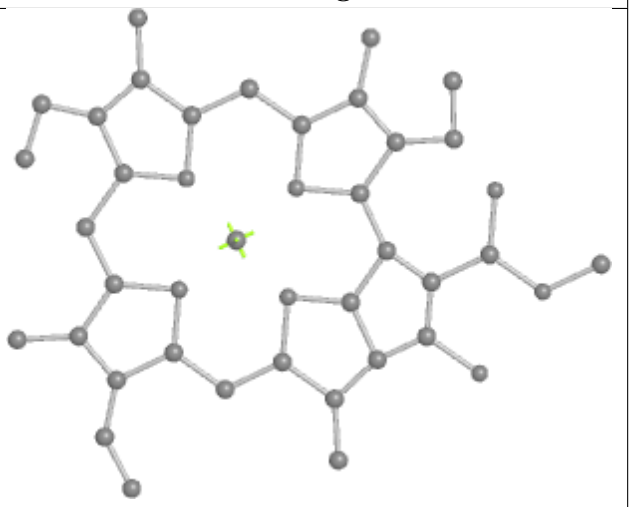
Bond lengths



Bond angles

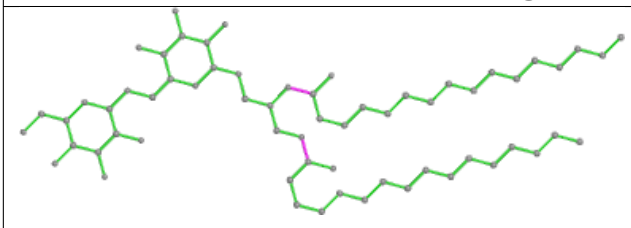


Torsions

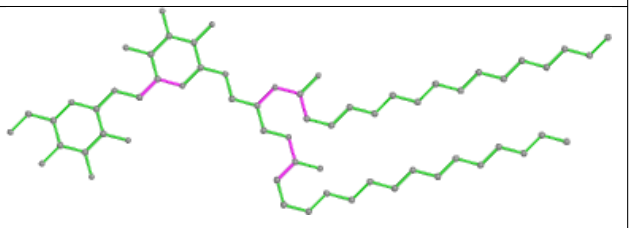


Rings

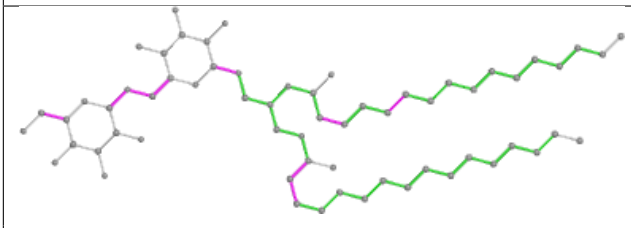
Ligand DGD C 518



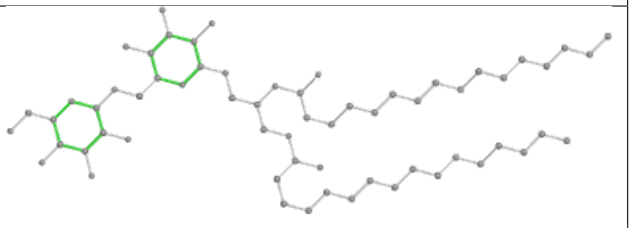
Bond lengths



Bond angles

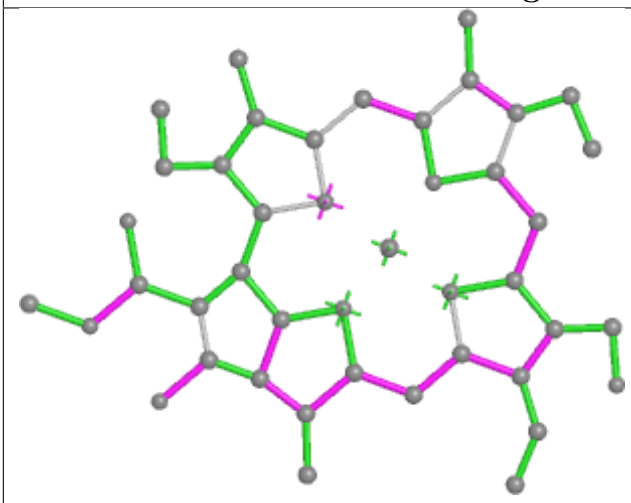


Torsions

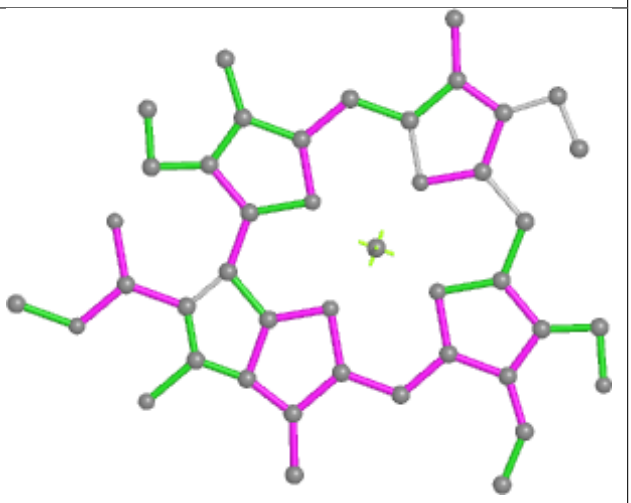


Rings

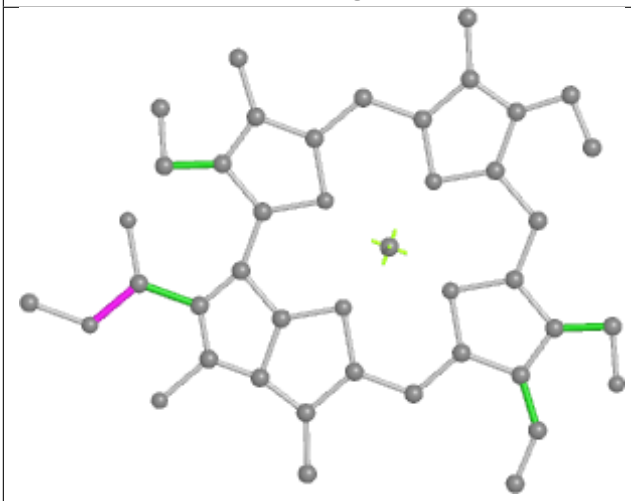
Ligand CHL G 605



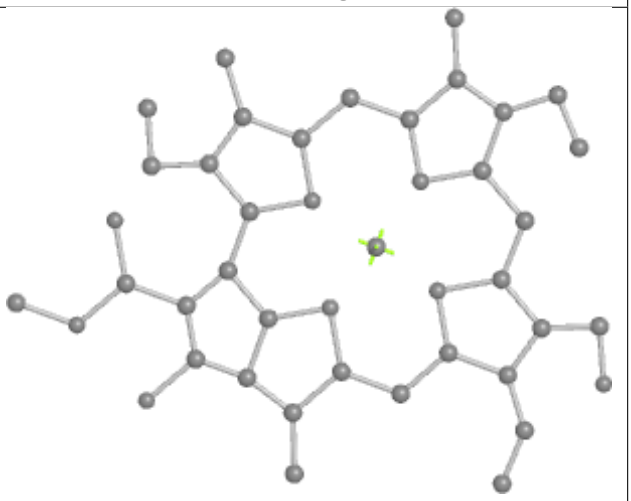
Bond lengths



Bond angles

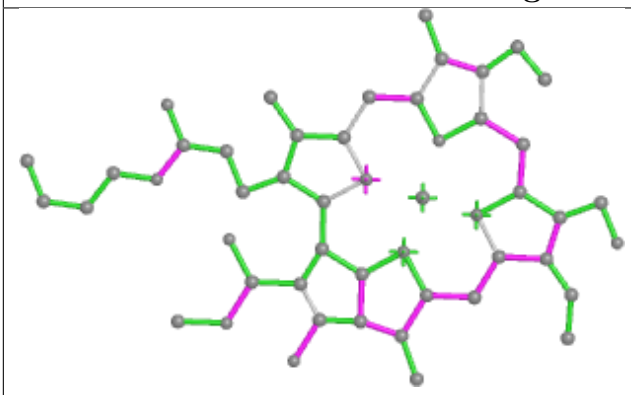


Torsions

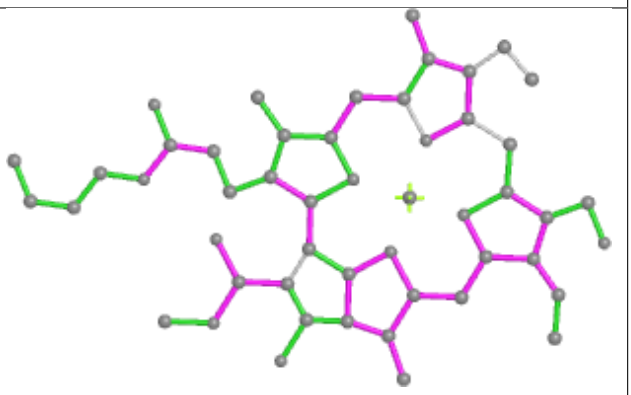


Rings

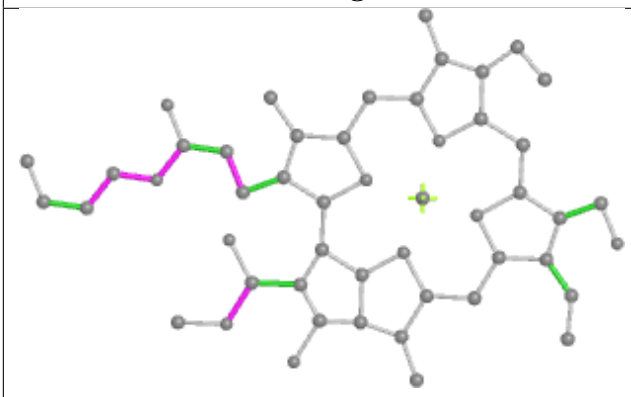
Ligand CHL Y 309



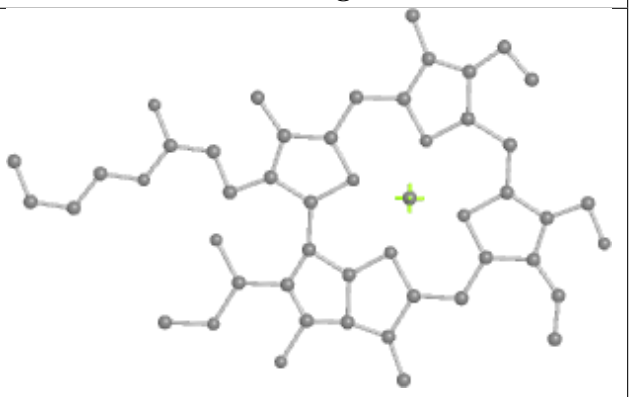
Bond lengths



Bond angles

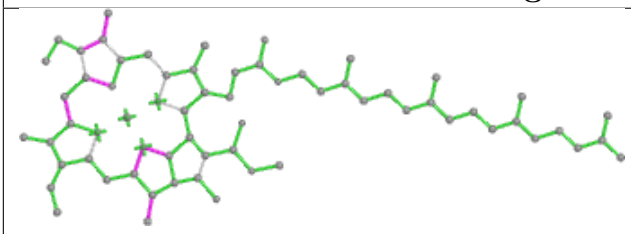


Torsions

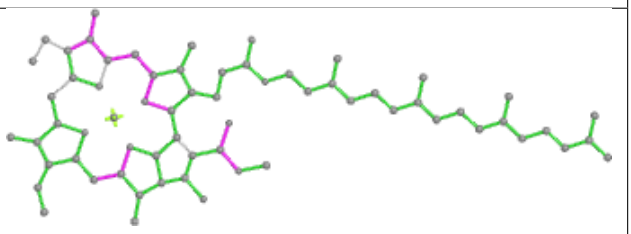


Rings

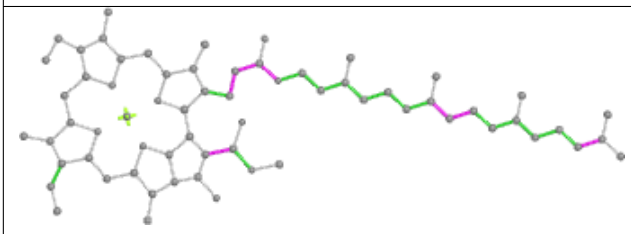
Ligand CLA C 501



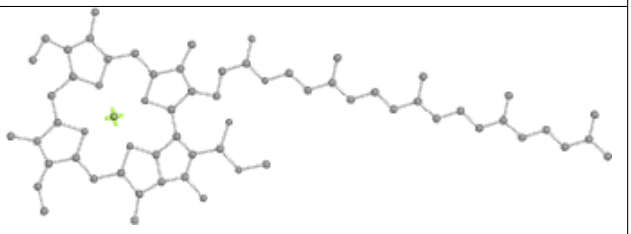
Bond lengths



Bond angles

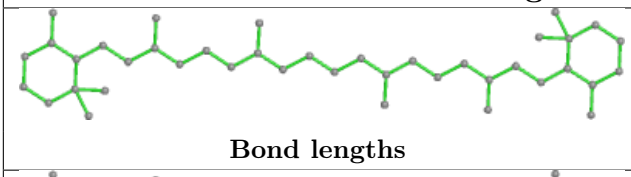


Torsions

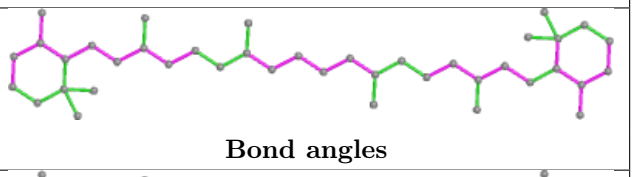


Rings

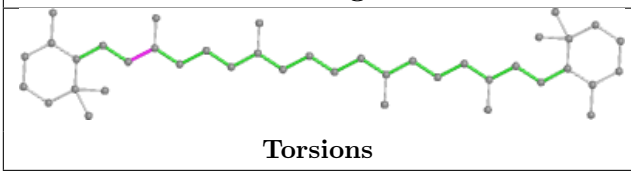
Ligand BCR b 518



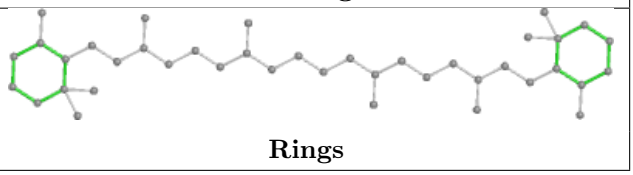
Bond lengths



Bond angles

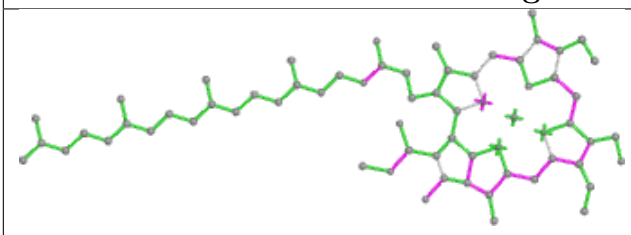


Torsions

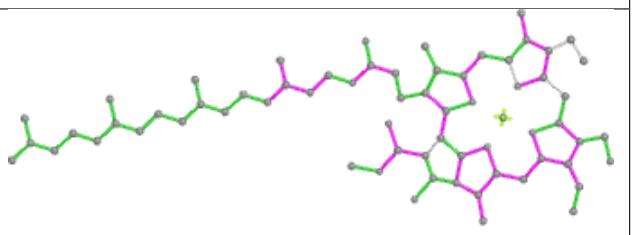


Rings

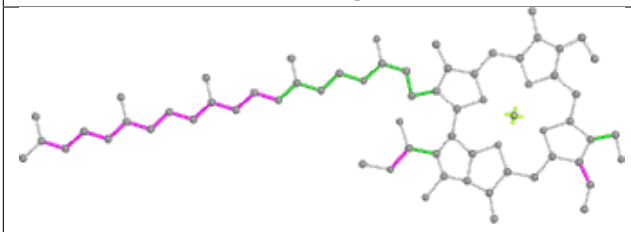
Ligand CHL G 609



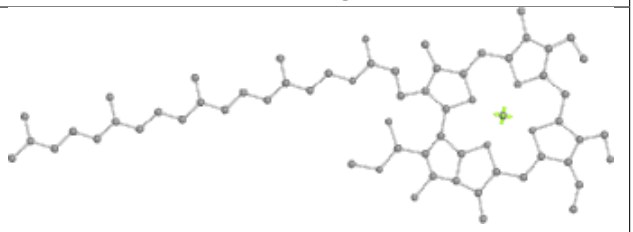
Bond lengths



Bond angles

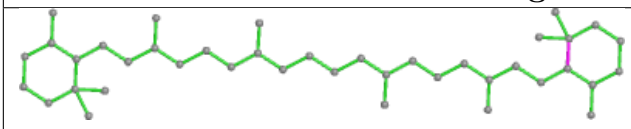


Torsions

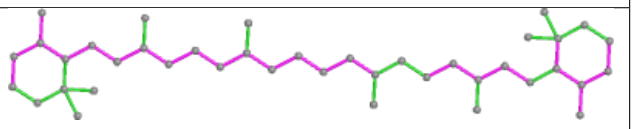


Rings

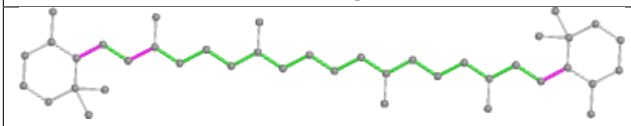
Ligand BCR t 101



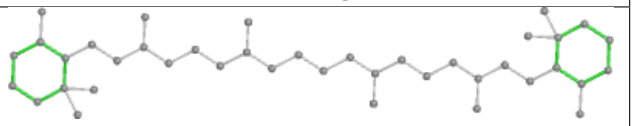
Bond lengths



Bond angles

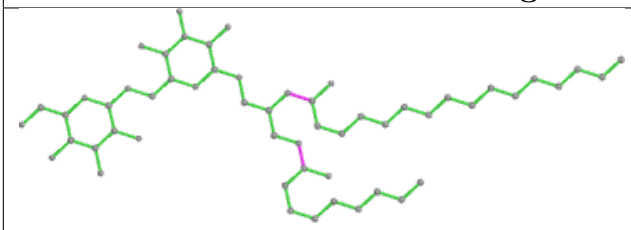


Torsions

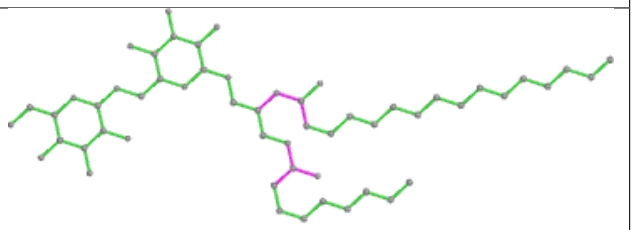


Rings

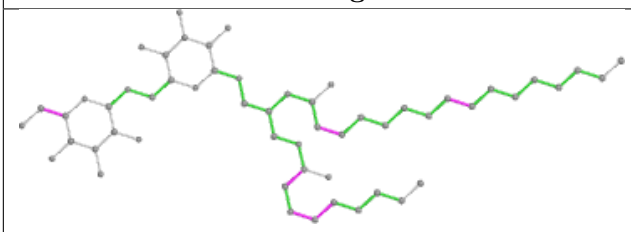
Ligand DGD C 517



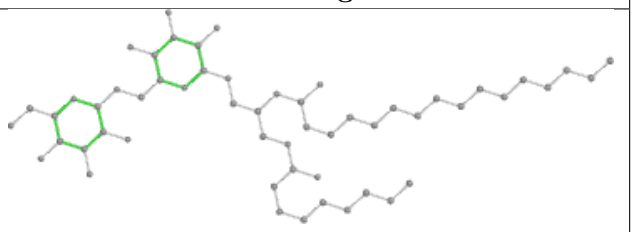
Bond lengths



Bond angles

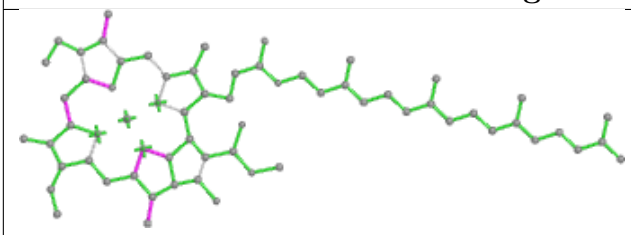


Torsions

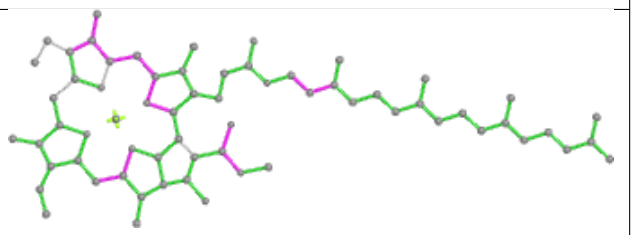


Rings

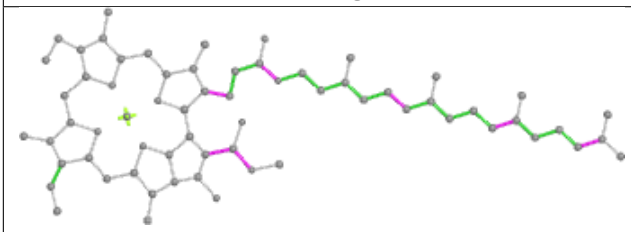
Ligand CLA N 305



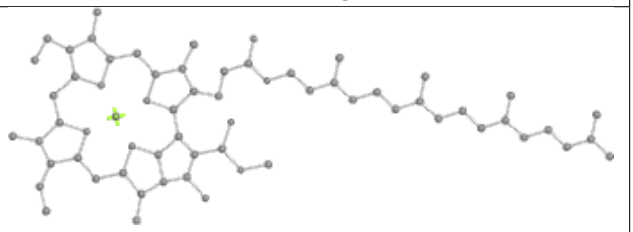
Bond lengths



Bond angles

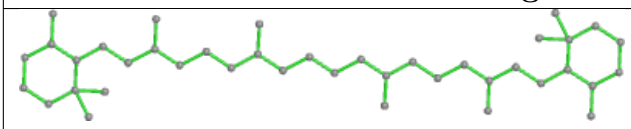


Torsions

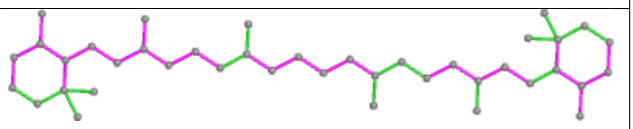


Rings

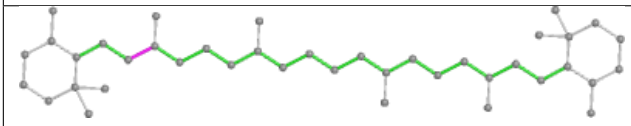
Ligand BCR D 406



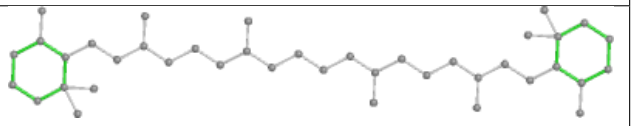
Bond lengths



Bond angles

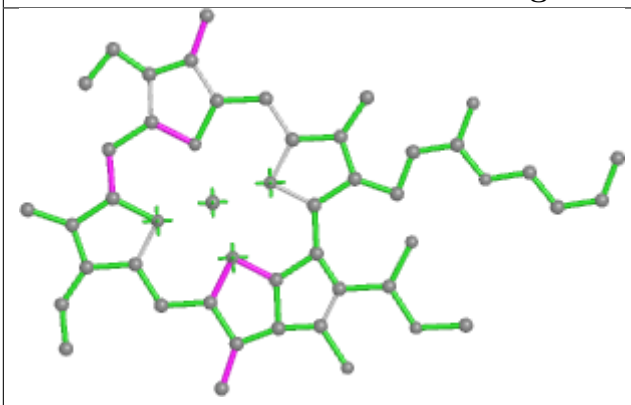


Torsions

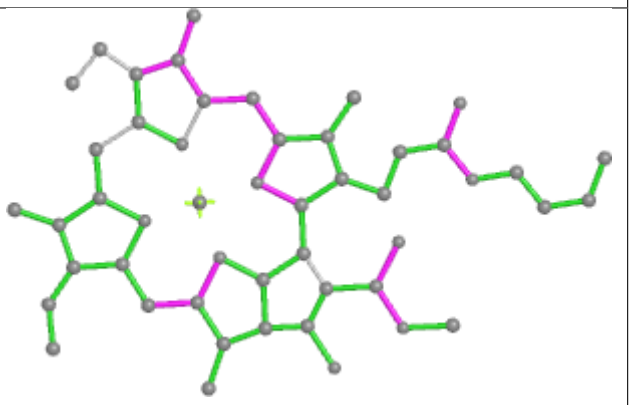


Rings

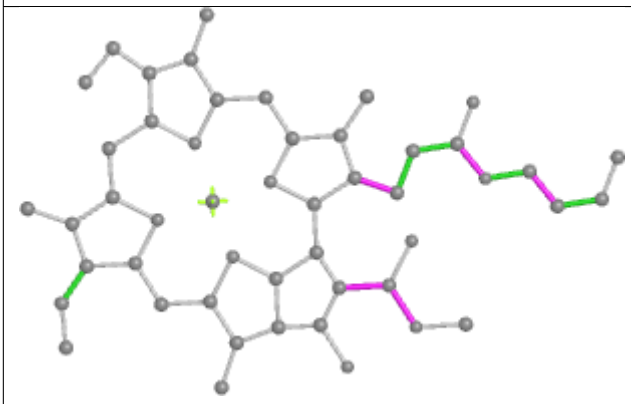
Ligand CLA r 303



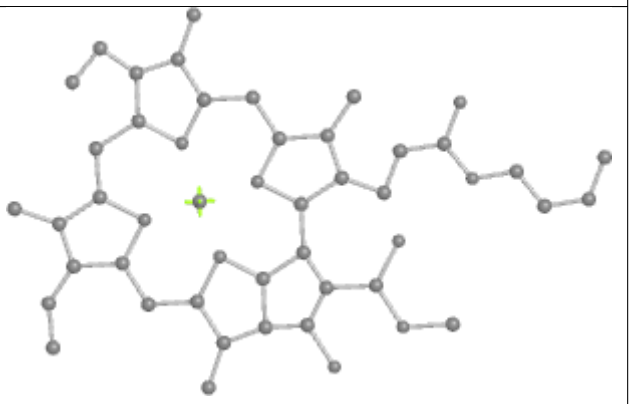
Bond lengths



Bond angles

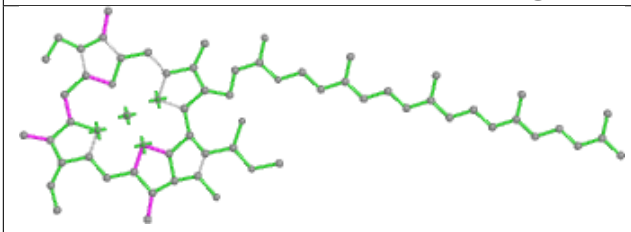


Torsions

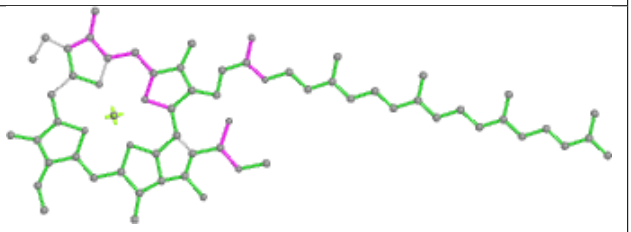


Rings

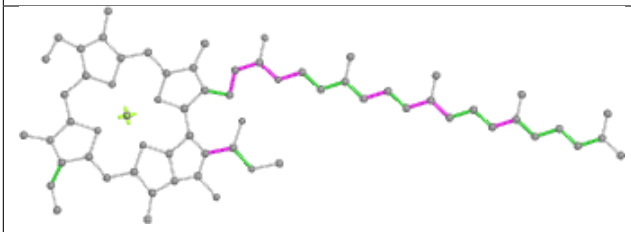
Ligand CLA c 508



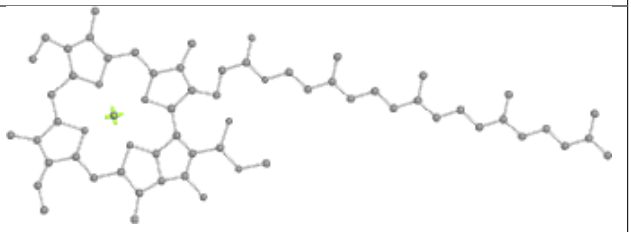
Bond lengths



Bond angles

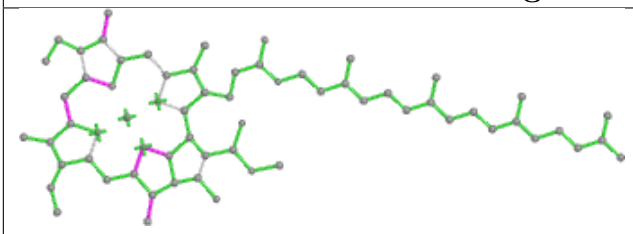


Torsions

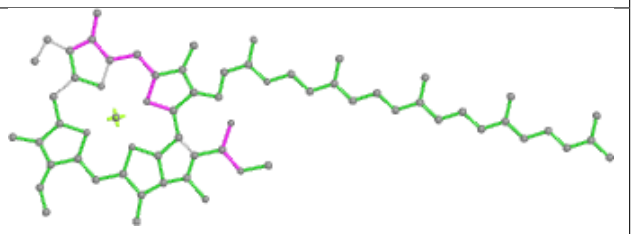


Rings

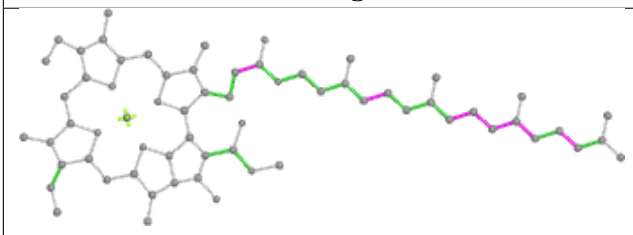
Ligand CLA Y 313



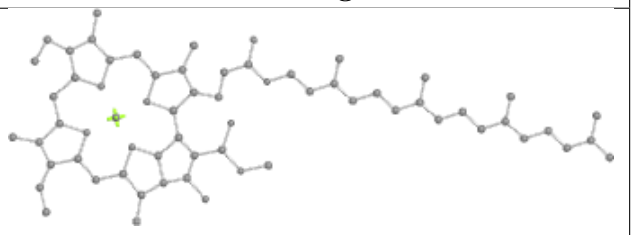
Bond lengths



Bond angles

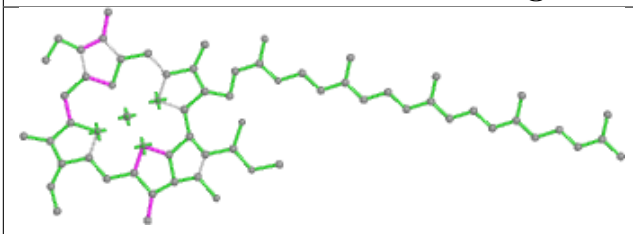


Torsions

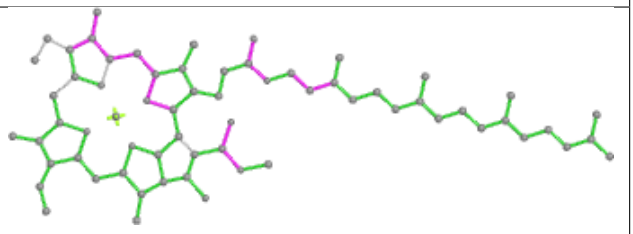


Rings

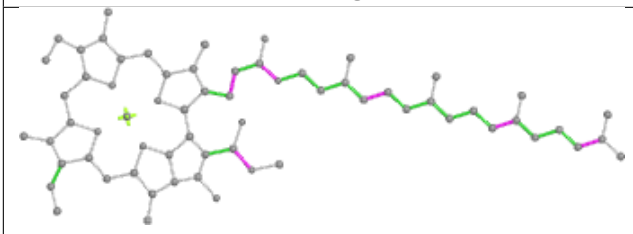
Ligand CLA b 508



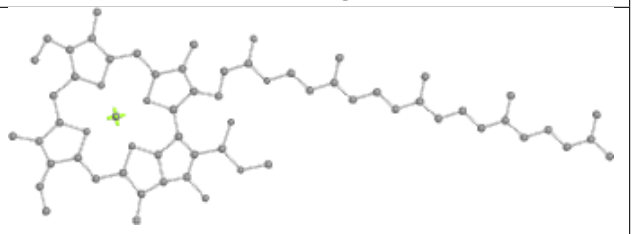
Bond lengths



Bond angles

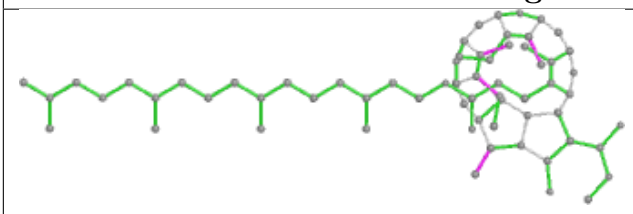


Torsions

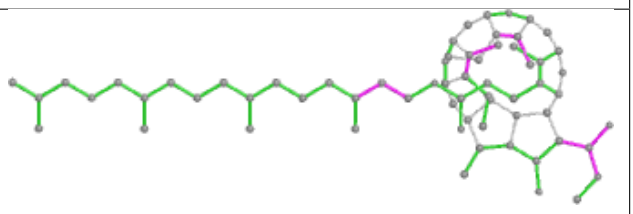


Rings

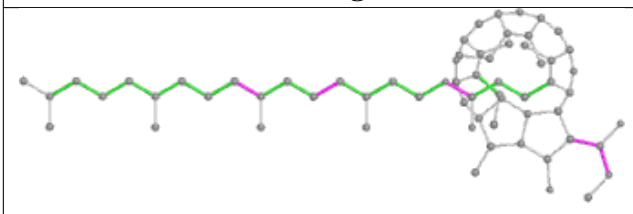
Ligand PHO d 402



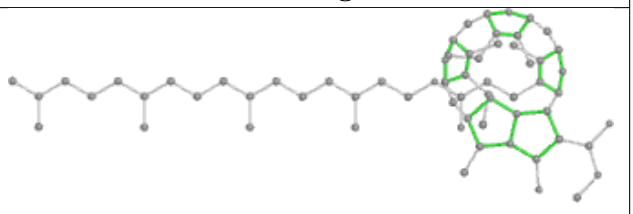
Bond lengths



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.

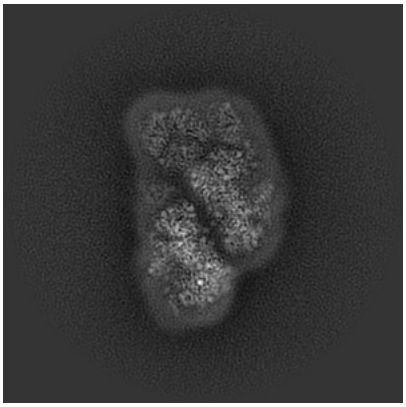
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60830. These allow visual inspection of the internal detail of the map and identification of artifacts.

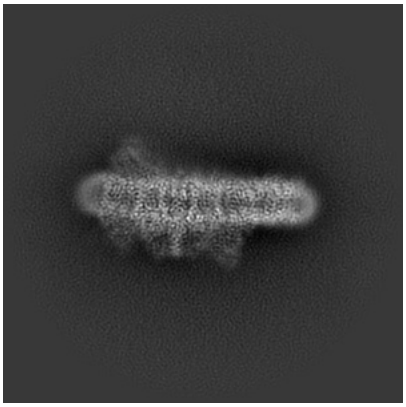
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

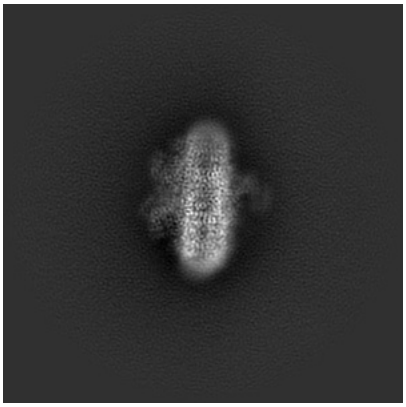
6.1.1 Primary map



X



Y

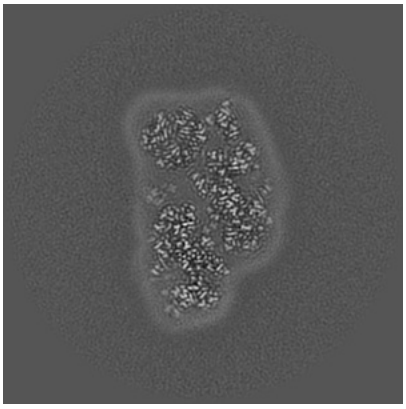


Z

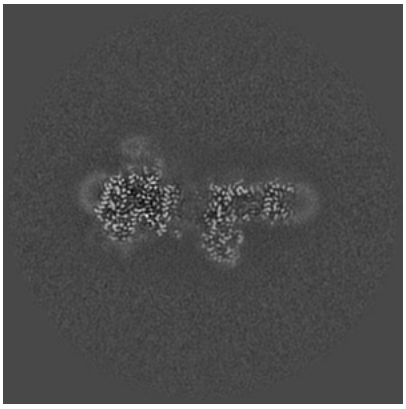
The images above show the map projected in three orthogonal directions.

6.2 Central slices

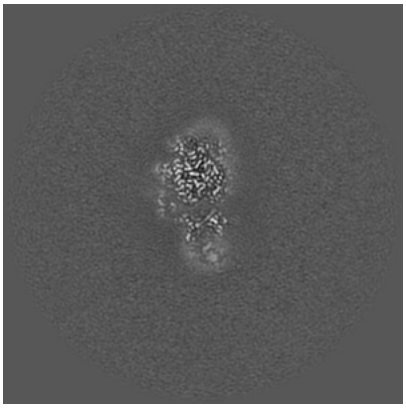
6.2.1 Primary map



X Index: 200



Y Index: 200

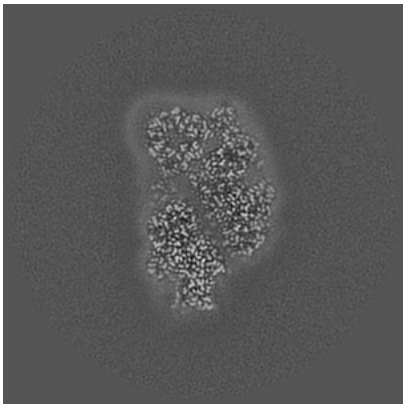


Z Index: 200

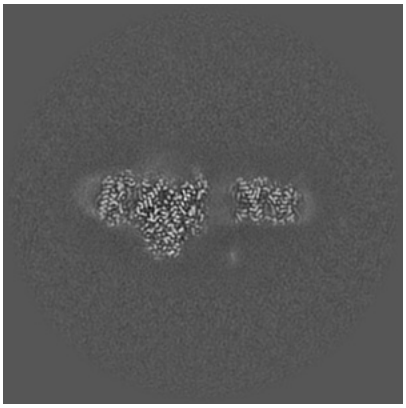
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

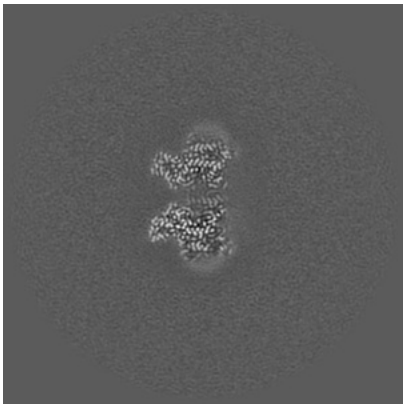
6.3.1 Primary map



X Index: 188



Y Index: 181

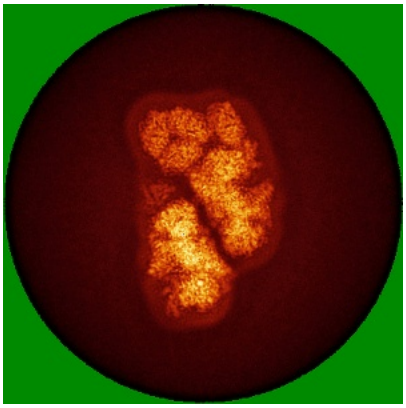


Z Index: 174

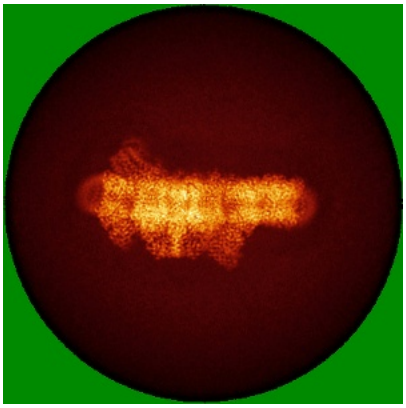
The images above show the largest variance slices of the map in three orthogonal directions.

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

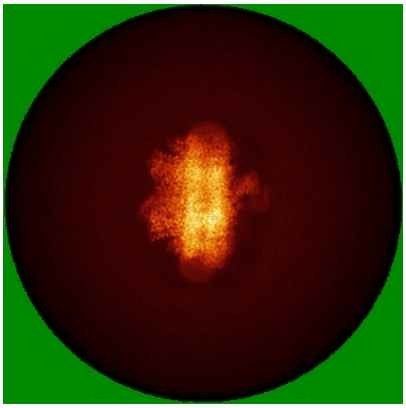
6.4.1 Primary map



X



Y

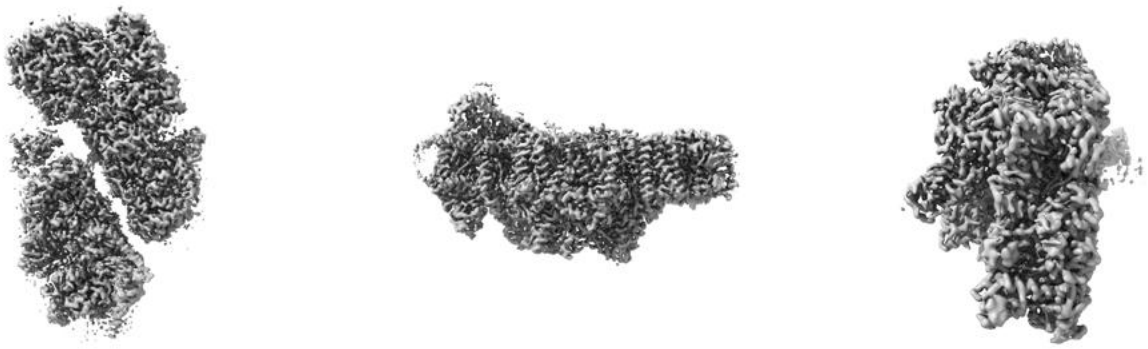


Z

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 6.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

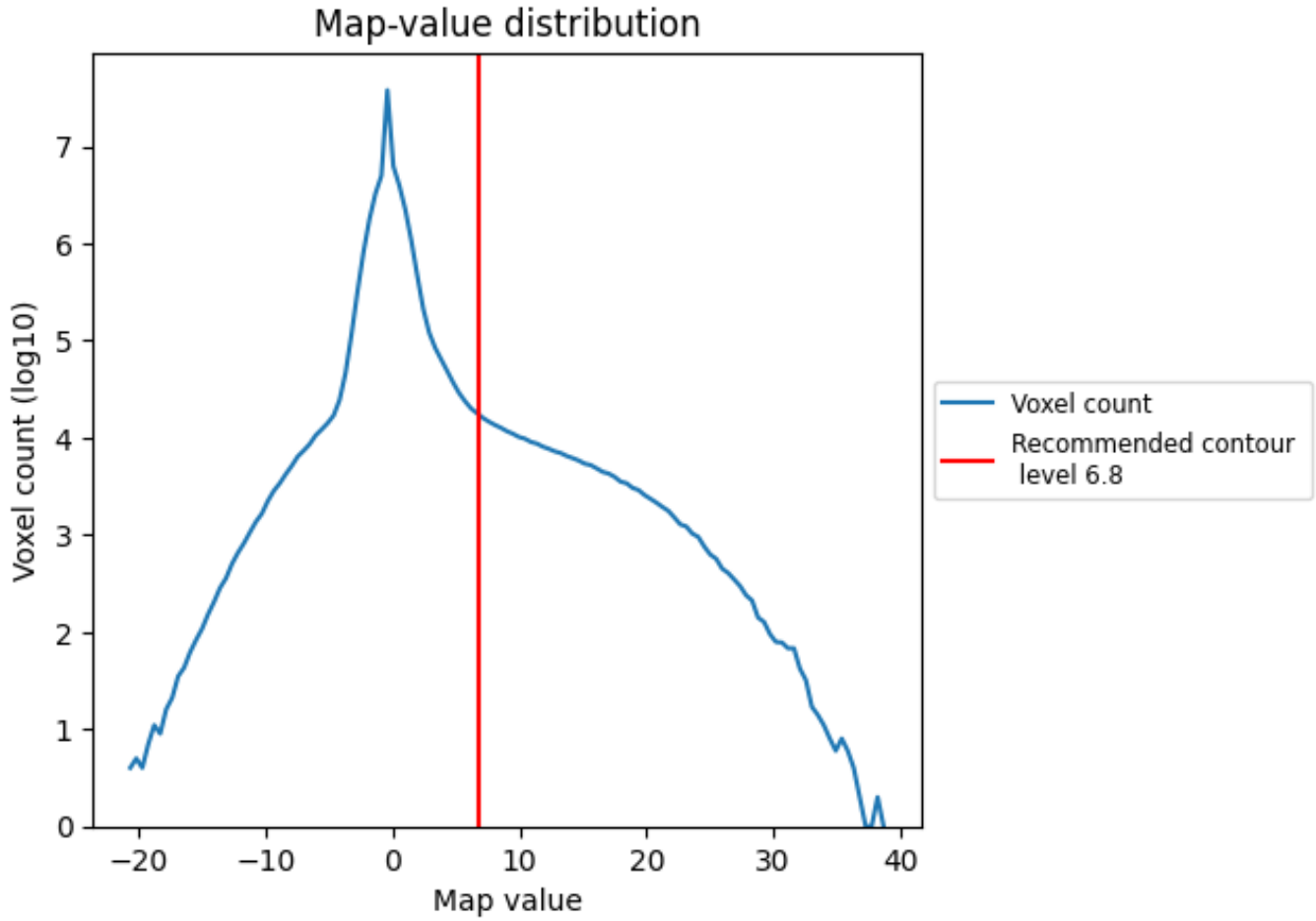
6.6 Mask visualisation (i)

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

7 Map analysis

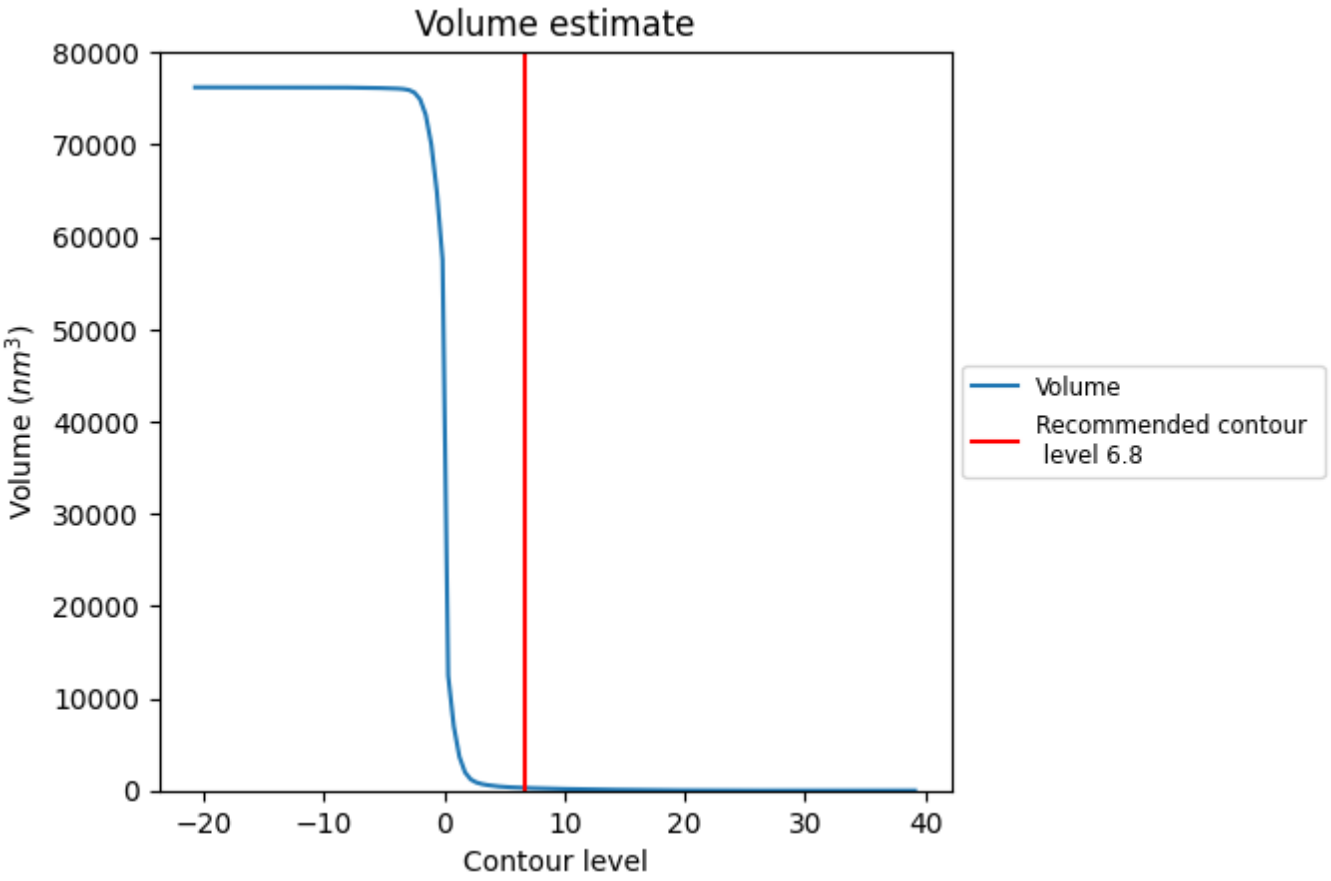
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

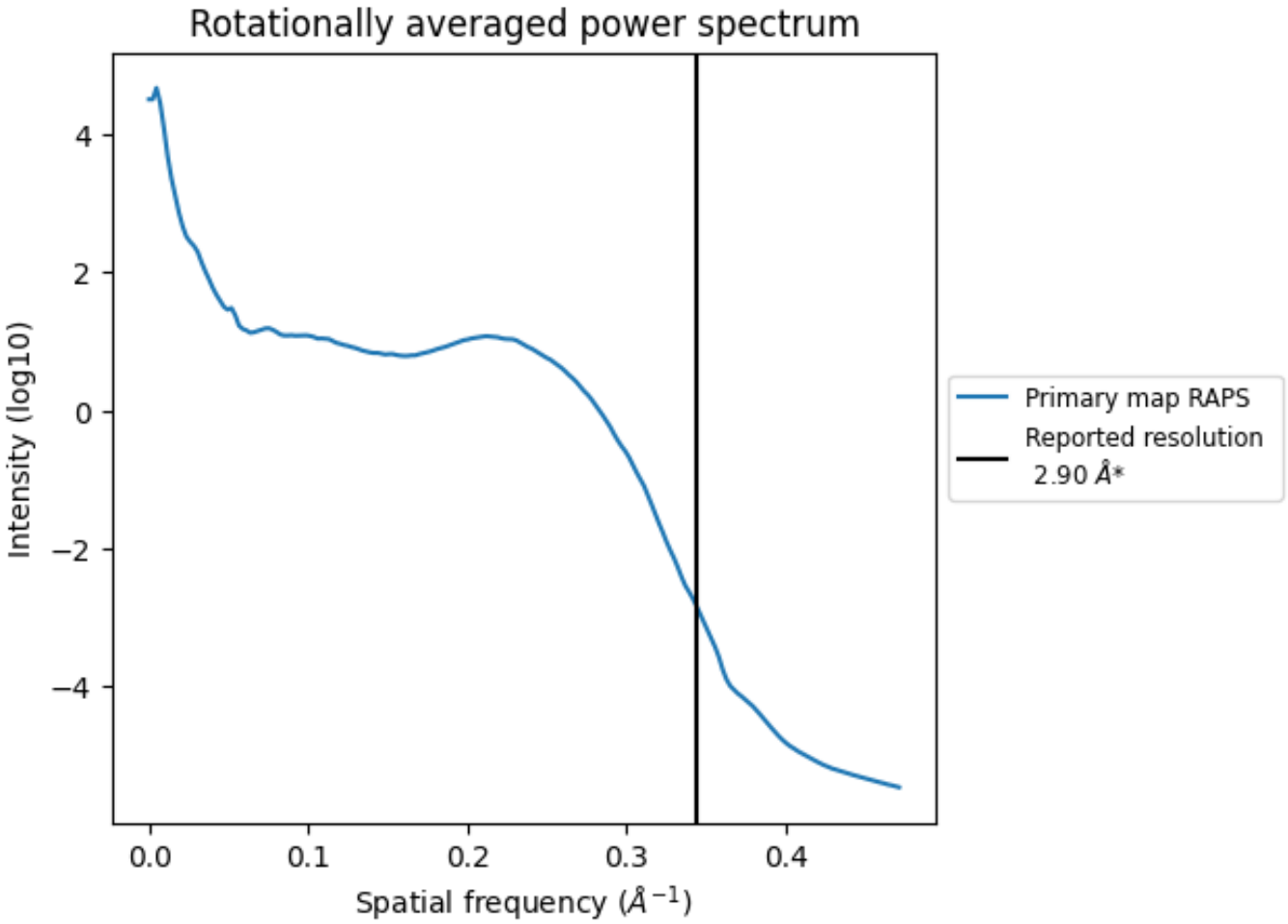
7.2 Volume estimate



The volume at the recommended contour level is 285 nm^3; this corresponds to an approximate mass of 258 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 0.345 Å^{-1}

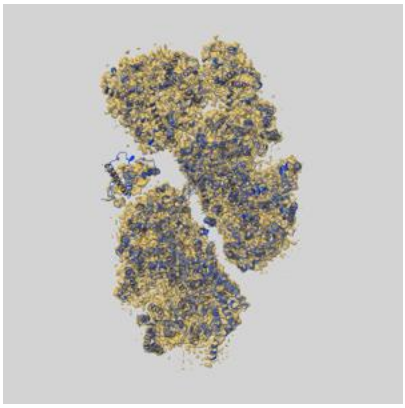
8 Fourier-Shell correlation (i)

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

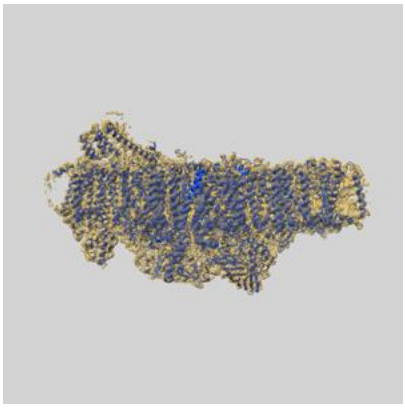
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60830 and PDB model 9IS4. Per-residue inclusion information can be found in section 3 on page 31.

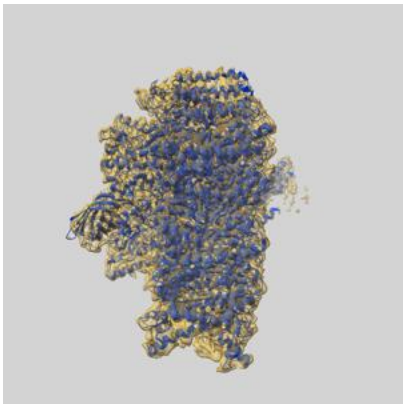
9.1 Map-model overlay



X



Y



Z

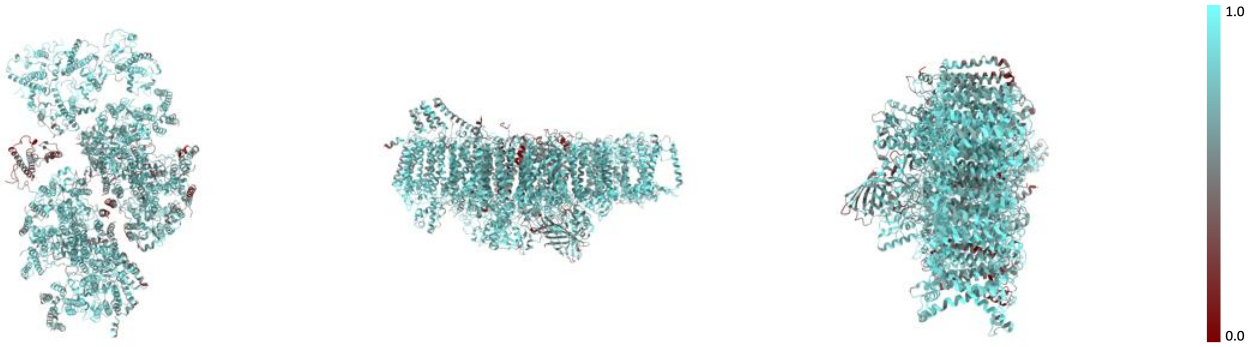
The images above show the 3D surface view of the map at the recommended contour level 6.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

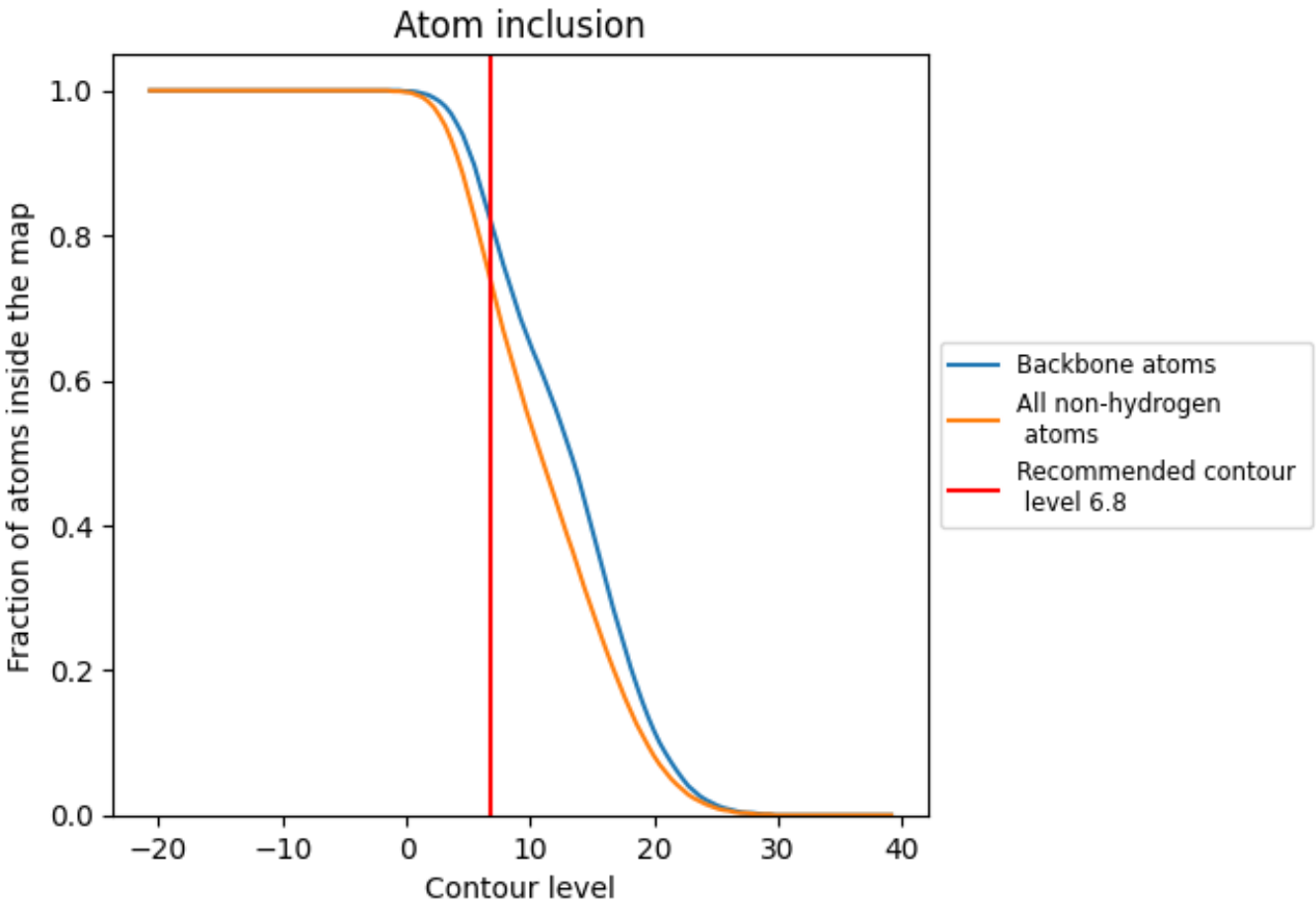
9.3 Atom inclusion mapped to coordinate model (i)



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 (6.8).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (6.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7390	0.5410
1	0.6550	0.4420
A	0.7560	0.5570
B	0.7390	0.5550
C	0.7710	0.5630
D	0.7740	0.5590
E	0.5850	0.4840
F	0.6420	0.4700
G	0.7610	0.5440
H	0.6610	0.5350
I	0.7790	0.5600
K	0.7990	0.5520
L	0.6360	0.5600
M	0.3420	0.4950
N	0.7790	0.5590
O	0.5660	0.5080
S	0.7790	0.5390
T	0.5450	0.5260
V	0.5990	0.4990
W	0.6120	0.5410
X	0.3970	0.4580
Y	0.7480	0.5640
Z	0.7150	0.5180
a	0.7870	0.5550
b	0.8230	0.5630
c	0.8060	0.5390
d	0.8450	0.5650
e	0.7830	0.4830
f	0.7330	0.4730
h	0.7960	0.5390
i	0.7130	0.5000
k	0.7500	0.5230
l	0.7300	0.5610
m	0.3480	0.5110
r	0.3650	0.4400

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
t	0.4210	0.5210
v	0.5080	0.4330
x	0.6220	0.4900
z	0.5690	0.4530