Full wwPDB EM Validation Report ⓘ

Sep 29, 2026 – 06:52 PM JST

PDB ID	:	9VJS / pdb_00009vjs
EMDB ID	:	EMD-65121
Title	:	Cryo-EM structure of Euglenophyte photosystem I
Authors	:	Zhao, L.S.; Qin, B.Y.; Li, K.; Liu, L.N.; Zhang, Y.Z.
Deposited on	:	2025-06-21
Resolution	:	2.72 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:

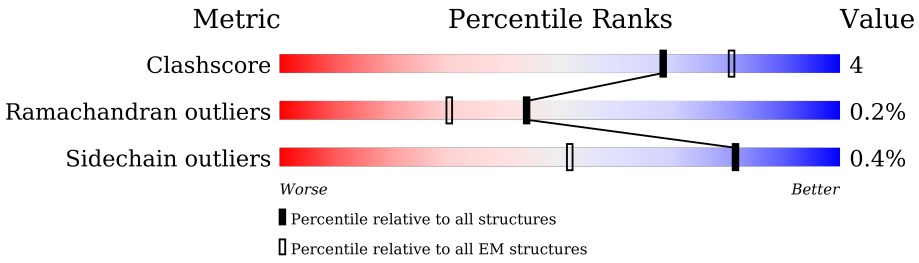
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

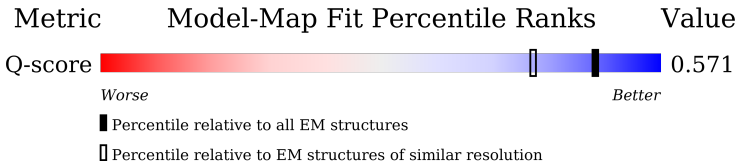
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.72 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10355 (2.22 - 3.22)

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	A	751	95%
2	B	733	94% 5%
3	C	81	89% 10%
4	D	203	89% 8%

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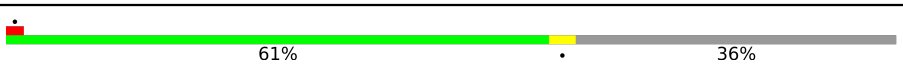
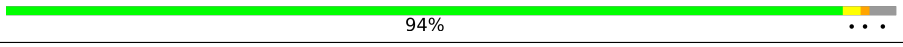
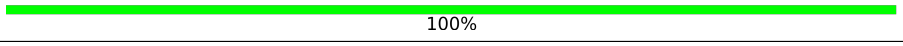
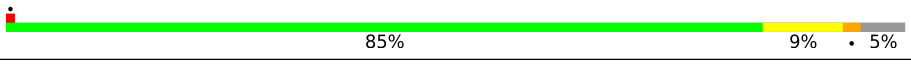
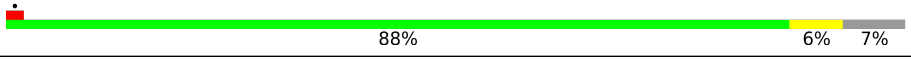
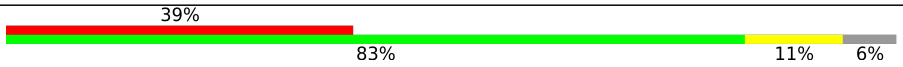
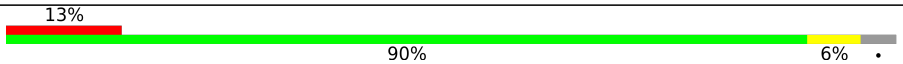
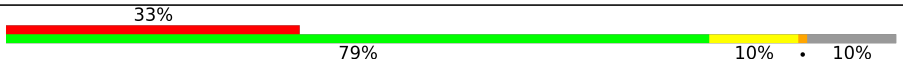
Mol	Chain	Length	Quality of chain
5	E	99	
6	F	172	
7	J	37	
8	M	31	
9	a	209	
10	b	225	
11	c	230	
12	d	184	
13	e	177	
14	f	185	
15	g	191	
15	j	191	
16	h	188	
16	o	188	
17	i	185	
18	k	174	
18	l	174	
18	m	174	
18	n	174	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 54391 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	740	5871	3854	992	1004	21	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	SER	THR	conflict	UNP P19430

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	730	5856	3853	983	1005	15	0	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	595	363	104	117	11	0	0

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	187	1462	935	248	277	2	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	63	510	324	86	100	0	0

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	166	Total	C	N	O	S	0	0
			1267	813	213	239	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			304	209	43	51	1		

- Molecule 8 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	31	Total	C	N	O	S	0	0
			242	162	37	42	1		

- Molecule 9 is a protein called LHC-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	199	Total	C	N	O	S	0	0
			1514	977	258	273	6		

- Molecule 10 is a protein called Light harvesting chlorophyll a /b binding protein of PSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	219	Total	C	N	O	S	0	0
			1665	1086	274	301	4		

- Molecule 11 is a protein called LHC-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	222	Total	C	N	O	S	0	0
			1683	1090	283	305	5		

- Molecule 12 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	172	Total	C	N	O	S	0	0
			1327	858	219	246	4		

- Molecule 13 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	166	Total	C	N	O	S	0	0
			1274	819	220	228	7		

- Molecule 14 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	172	Total	C	N	O	S	0	0
			1338	860	232	241	5		

- Molecule 15 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	182	Total	C	N	O	S	0	0
			1441	939	245	251	6		
15	j	180	Total	C	N	O	S	0	0
			1420	924	242	248	6		

- Molecule 16 is a protein called LHC-10, 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	178	Total	C	N	O	S	0	0
			1361	870	243	244	4		
16	o	177	Total	C	N	O	S	0	0
			1356	867	242	243	4		

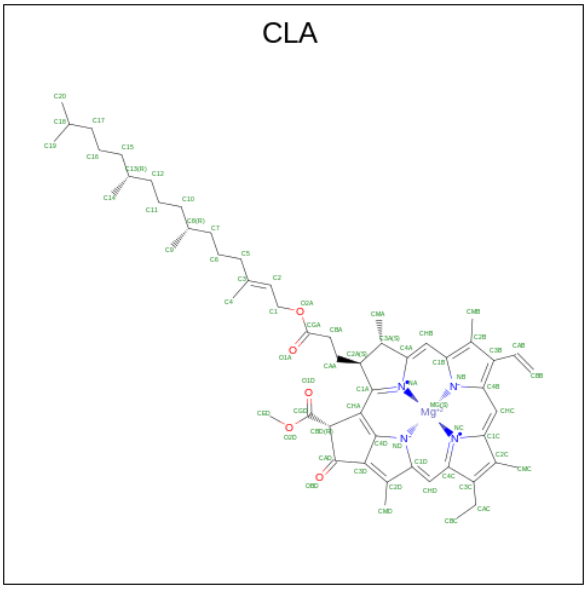
- Molecule 17 is a protein called LHC-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	172	Total	C	N	O	S	0	0
			1342	861	231	245	5		

- Molecule 18 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	168	Total	C	N	O	S	0	0
			1260	813	215	228	4		
18	l	167	Total	C	N	O	S	0	0
			1253	808	214	227	4		
18	m	168	Total	C	N	O	S	0	0
			1260	813	215	228	4		
18	n	156	Total	C	N	O	S	0	0
			1170	754	199	213	4		

- Molecule 19 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
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	e	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	e	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	g	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	h	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	h	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	i	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	m	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	m	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	n	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	o	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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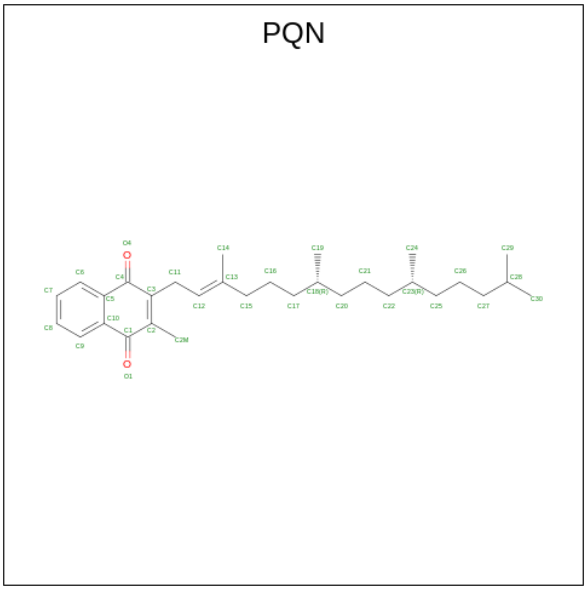
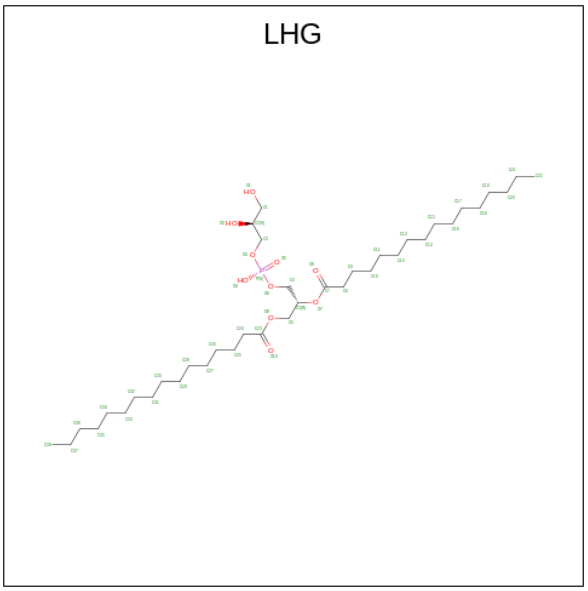
Mol	Chain	Residues	Atoms					AltConf
19	o	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



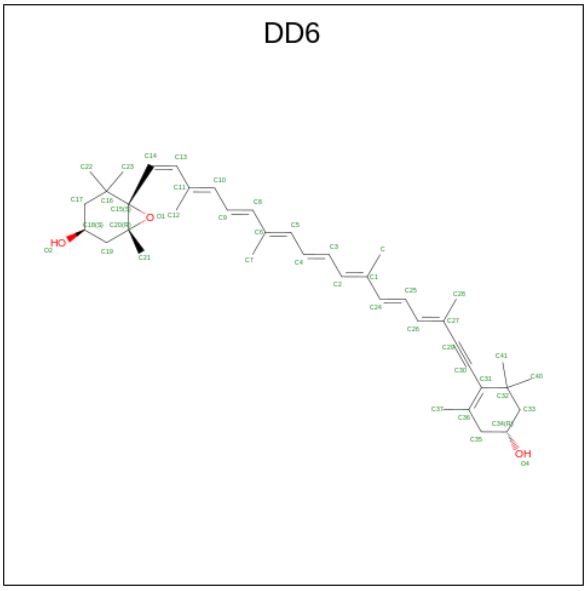
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 22 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			43	40	3	
22	A	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
22	F	1	Total	C	O	0
			43	40	3	
22	J	1	Total	C	O	0
			43	40	3	
22	J	1	Total	C	O	0
			43	40	3	
22	a	1	Total	C	O	0
			43	40	3	
22	a	1	Total	C	O	0
			43	40	3	
22	b	1	Total	C	O	0
			43	40	3	
22	b	1	Total	C	O	0
			43	40	3	
22	b	1	Total	C	O	0
			43	40	3	
22	c	1	Total	C	O	0
			43	40	3	
22	c	1	Total	C	O	0
			43	40	3	
22	c	1	Total	C	O	0
			43	40	3	
22	d	1	Total	C	O	0
			43	40	3	
22	d	1	Total	C	O	0
			43	40	3	
22	e	1	Total	C	O	0
			43	40	3	
22	e	1	Total	C	O	0
			43	40	3	
22	f	1	Total	C	O	0
			43	40	3	
22	f	1	Total	C	O	0
			43	40	3	
22	g	1	Total	C	O	0
			43	40	3	
22	g	1	Total	C	O	0
			43	40	3	
22	h	1	Total	C	O	0
			43	40	3	
22	h	1	Total	C	O	0
			43	40	3	

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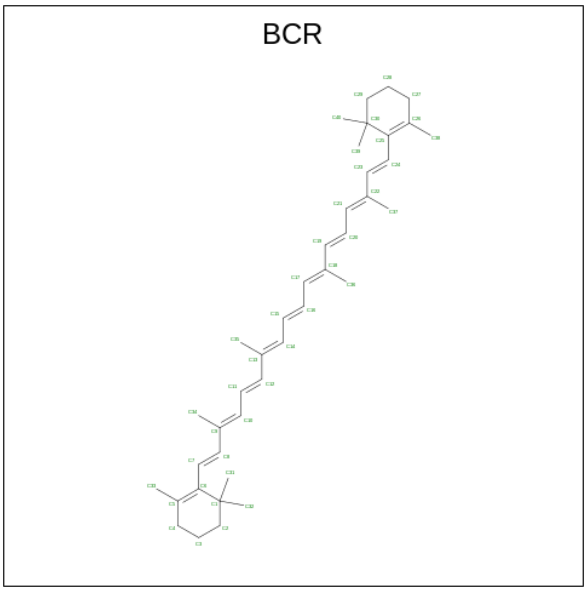
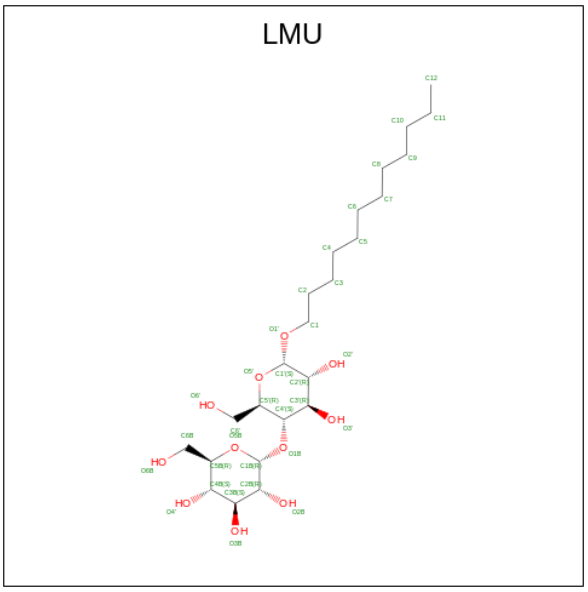
Mol	Chain	Residues	Atoms	AltConf
22	i	1	Total C O 43 40 3	0
22	i	1	Total C O 43 40 3	0
22	j	1	Total C O 43 40 3	0
22	j	1	Total C O 43 40 3	0
22	k	1	Total C O 43 40 3	0
22	k	1	Total C O 43 40 3	0
22	l	1	Total C O 43 40 3	0
22	l	1	Total C O 43 40 3	0
22	m	1	Total C O 43 40 3	0
22	m	1	Total C O 43 40 3	0
22	n	1	Total C O 43 40 3	0
22	n	1	Total C O 43 40 3	0
22	o	1	Total C O 43 40 3	0
22	o	1	Total C O 43 40 3	0

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



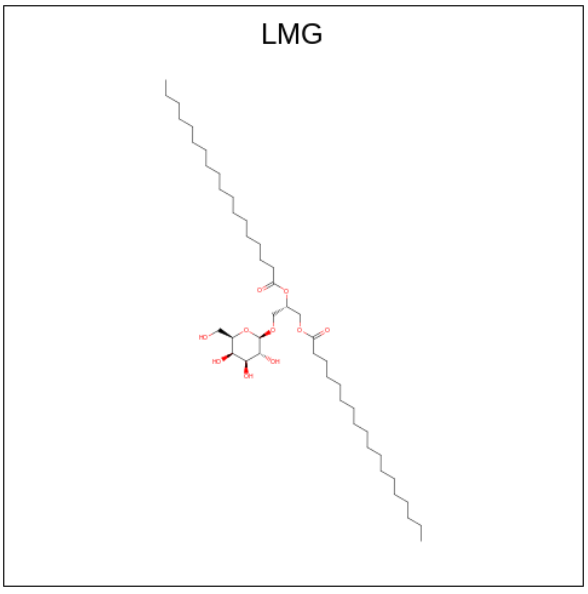
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 39 39	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	M	1	Total C 40 40	0

- Molecule 24 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



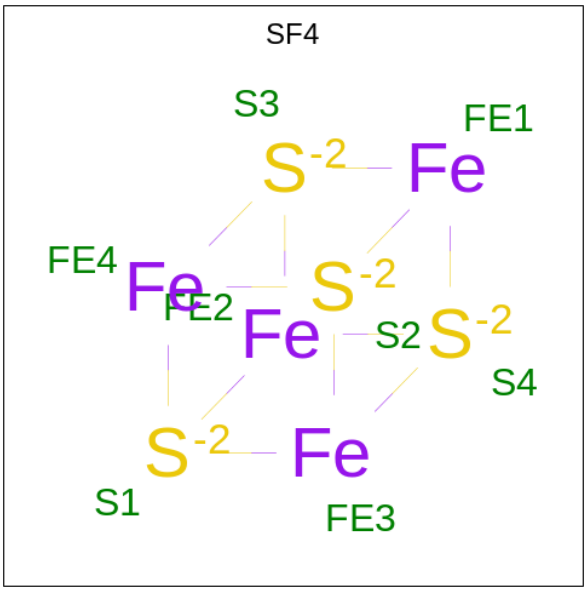
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			34	24	10	
24	a	1	Total	C	O	0
			34	24	10	
24	c	1	Total	C	O	0
			34	24	10	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



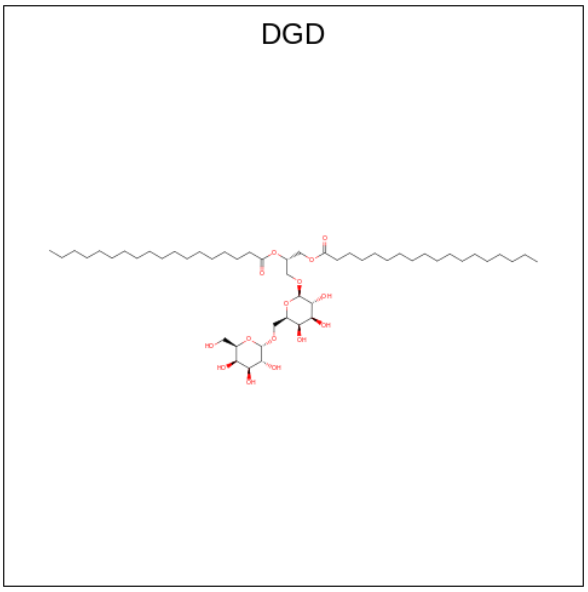
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C O 34 24 10	0
25	a	1	Total C O 40 30 10	0
25	a	1	Total C O 27 17 10	0
25	a	1	Total C O 40 30 10	0
25	b	1	Total C O 42 32 10	0
25	c	1	Total C O 38 28 10	0
25	d	1	Total C O 31 21 10	0
25	e	1	Total C O 44 34 10	0
25	f	1	Total C O 26 16 10	0
25	g	1	Total C O 37 27 10	0
25	g	1	Total C O 33 23 10	0
25	g	1	Total C O 44 34 10	0
25	h	1	Total C O 35 25 10	0
25	i	1	Total C O 41 31 10	0
25	j	1	Total C O 37 27 10	0
25	k	1	Total C O 37 27 10	0

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



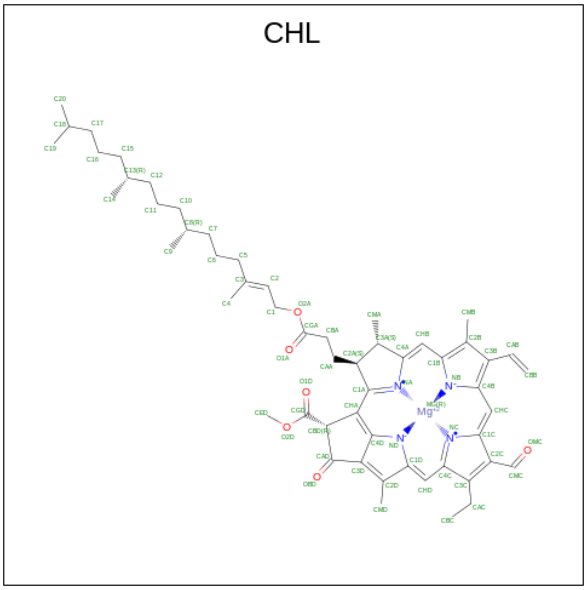
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total Fe S 8 4 4	0
26	C	1	Total Fe S 8 4 4	0
26	C	1	Total Fe S 8 4 4	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			62	47	15	

- Molecule 28 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
28	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	b	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	b	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	b	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	b	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
28	b	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
28	c	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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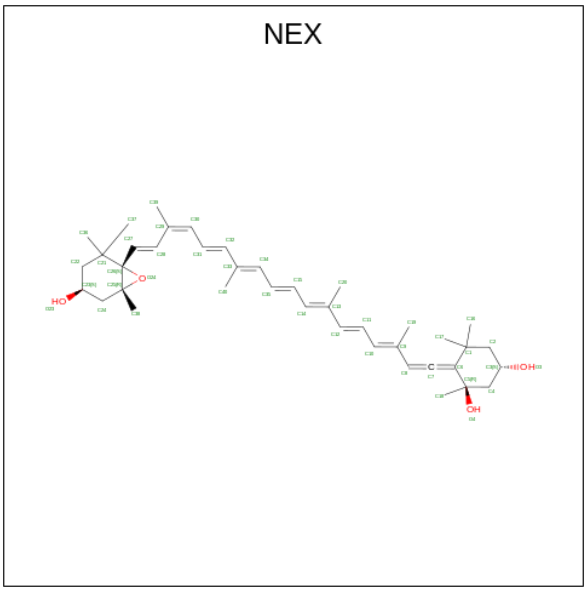
Mol	Chain	Residues	Atoms					AltConf
28	c	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	c	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	d	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	d	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	e	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
28	e	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
28	f	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	f	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	g	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	g	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
28	h	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	i	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	i	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
28	k	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	m	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
28	o	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 29 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).



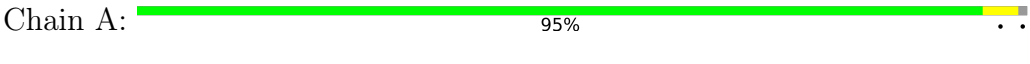
Mol	Chain	Residues	Atoms			AltConf
29	a	1	Total	C	O	0
			44	40	4	

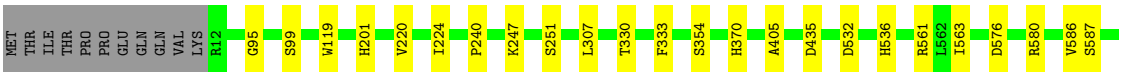
3 Residue-property plots (i)

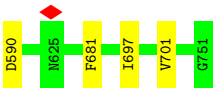
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:

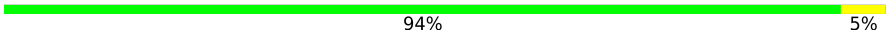


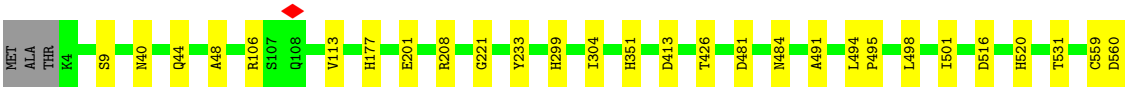




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



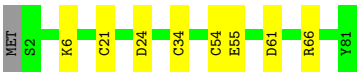




• Molecule 3: Photosystem I iron-sulfur center

Chain C:

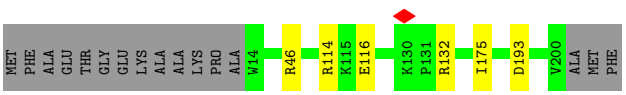




• Molecule 4: PsaD

Chain D:

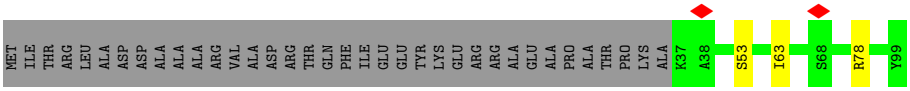




• Molecule 5: PsaE

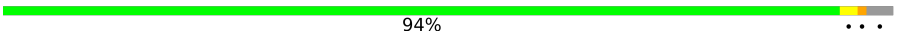
Chain E:

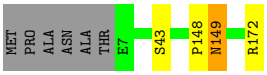




• Molecule 6: PsaF

Chain F:





• Molecule 7: Photosystem I reaction center subunit IX

Chain J:

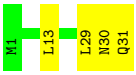


There are no outlier residues recorded for this chain.

• Molecule 8: Photosystem I reaction center subunit XII

Chain M:





• Molecule 9: LHC-1

Chain a:





• Molecule 10: Light harvesting chlorophyll a /b binding protein of PSII

Chain b:





• Molecule 11: LHC-3

Chain c:

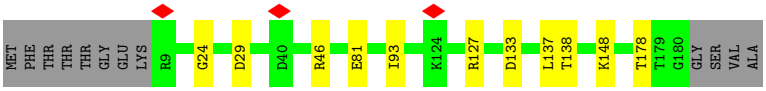




• Molecule 12: Chloroplast light-harvesting complex I protein

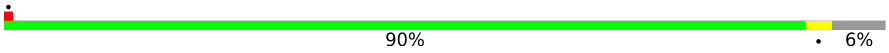
Chain d:

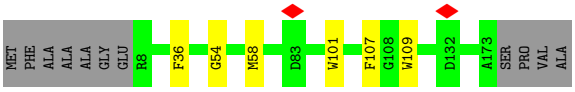




• Molecule 13: Chloroplast light-harvesting complex I protein

Chain e:

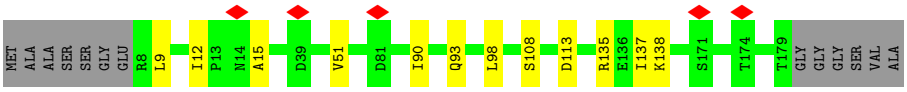




• Molecule 14: Chloroplast light-harvesting complex I protein

Chain f:





• Molecule 15: Chloroplast light-harvesting complex I protein

Chain g:

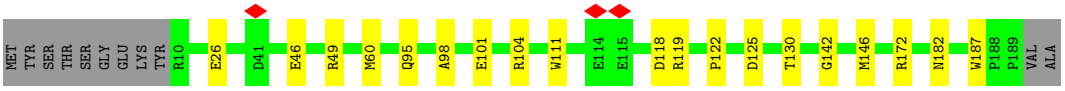




• Molecule 15: Chloroplast light-harvesting complex I protein

Chain j:





• Molecule 16: LHC-10, 15

Chain h:

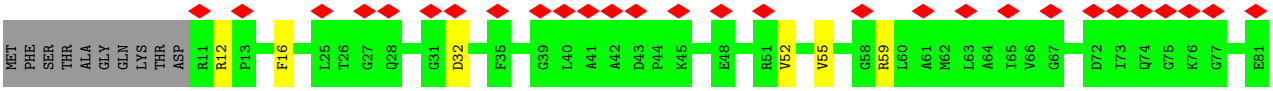


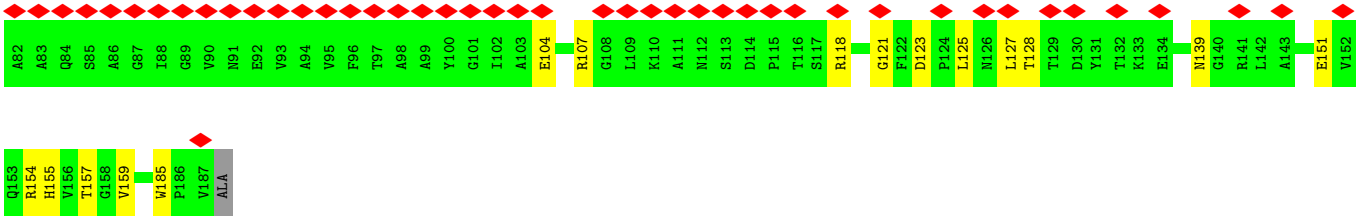


• Molecule 16: LHC-10, 15

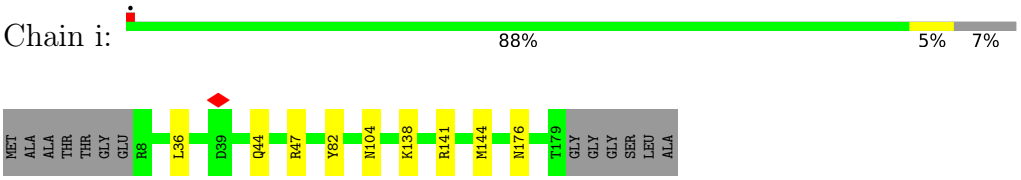
Chain o:



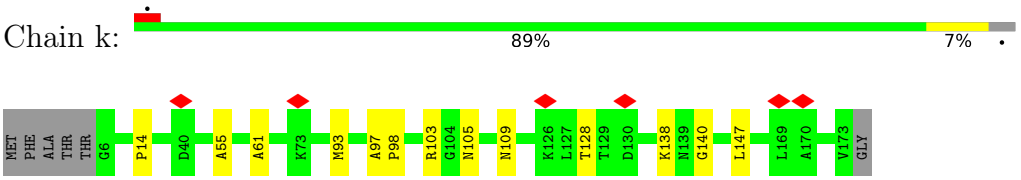




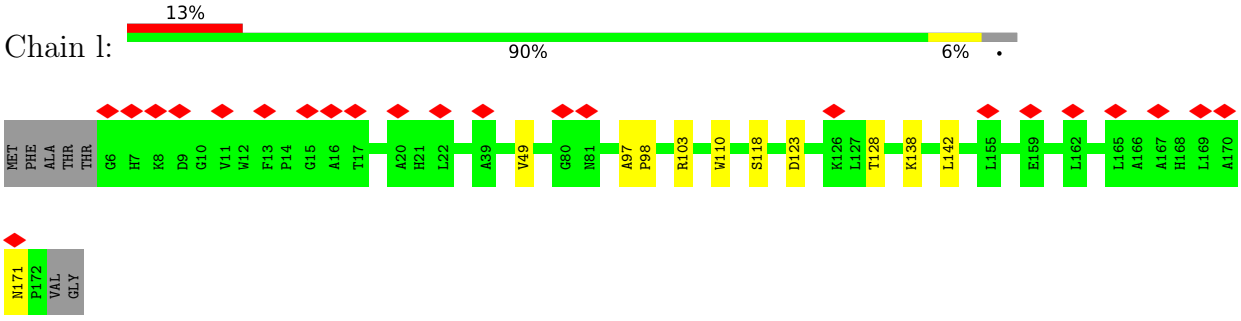
• Molecule 17: LHC-11



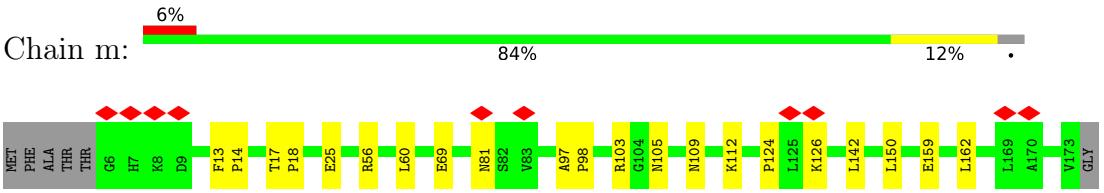
• Molecule 18: Chloroplast light-harvesting complex I protein



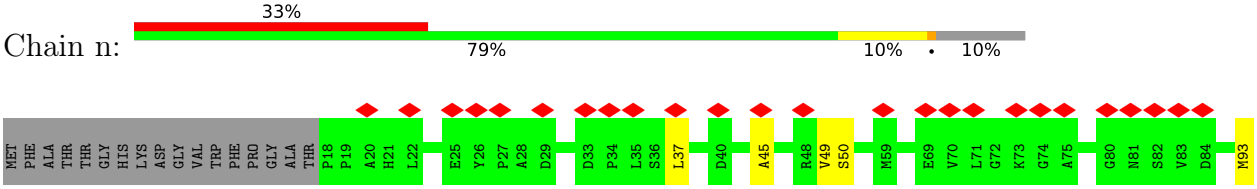
• Molecule 18: Chloroplast light-harvesting complex I protein

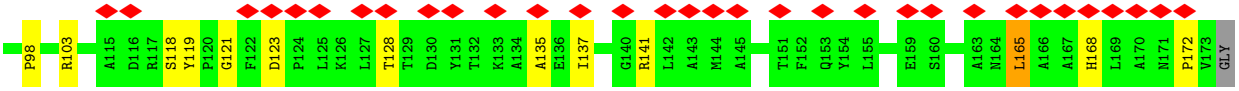


• Molecule 18: Chloroplast light-harvesting complex I protein



• Molecule 18: Chloroplast light-harvesting complex I protein




P98
R103
A115
D116
R117
S118
Y119
P120
G121
F122
D123
P124
L125
K126
L127
T128
T129
D130
Y131
T132
K133
A134
A135
E136
I137
G140
R141
L142
A143
M144
A145
T151
F152
Q153
Y154
L155
E159
S160
A163
N164
L165
A166
A167
H168
L169
A170
N171
P172
V173
GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.443	Depositor
Minimum map value	-0.463	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	417.2, 417.2, 417.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8344, 0.8344, 0.8344	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NEX, CHL, BCR, LMG, PQN, DD6, DGD, CLA, LMU, LHG, SF4

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	A	0.16	0/6071	0.33	0/8276
2	B	0.17	0/6066	0.36	0/8272
3	C	0.48	0/605	0.47	0/819
4	D	0.18	0/1498	0.38	0/2030
5	E	0.18	0/522	0.38	0/707
6	F	0.24	0/1293	0.39	0/1751
7	J	0.18	0/313	0.34	0/429
8	M	0.32	0/246	0.42	0/332
9	a	0.45	0/1562	0.55	1/2135 (0.0%)
10	b	0.28	1/1715 (0.1%)	0.38	0/2338
11	c	0.20	0/1725	0.33	0/2341
12	d	0.17	0/1370	0.37	0/1865
13	e	0.19	0/1311	0.40	0/1772
14	f	0.21	0/1377	0.42	0/1871
15	g	0.17	0/1490	0.36	0/2033
15	j	0.20	0/1468	0.39	0/2004
16	h	0.17	0/1399	0.35	0/1907
16	o	0.23	0/1394	0.47	0/1900
17	i	0.19	0/1380	0.41	0/1876
18	k	0.21	0/1297	0.41	0/1768
18	l	0.22	0/1290	0.41	0/1758
18	m	0.26	0/1297	0.44	0/1768
18	n	0.21	0/1202	0.46	0/1637
All	All	0.22	1/37891 (0.0%)	0.39	1/51589 (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
2	B	0	1
16	h	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	135	THR	CA-C	-5.67	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	126	ARG	N-CA-C	-5.73	105.12	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	667	TRP	Peptide
16	h	185	TRP	Peptide

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	A	5871	0	5731	19	0
2	B	5856	0	5659	30	0
3	C	595	0	579	5	0
4	D	1462	0	1450	5	0
5	E	510	0	489	3	0
6	F	1267	0	1299	3	0
7	J	304	0	317	0	0
8	M	242	0	258	6	0
9	a	1514	0	1466	13	0
10	b	1665	0	1645	13	0
11	c	1683	0	1680	9	0
12	d	1327	0	1271	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	e	1274	0	1233	4	0
14	f	1338	0	1313	10	0
15	g	1441	0	1393	7	0
15	j	1420	0	1371	14	0
16	h	1361	0	1339	9	0
16	o	1356	0	1334	17	0
17	i	1342	0	1316	6	0
18	k	1260	0	1234	9	0
18	l	1253	0	1225	10	0
18	m	1260	0	1234	13	0
18	n	1170	0	1155	16	0
19	A	2506	0	2465	17	0
19	B	2277	0	2172	19	0
19	D	52	0	43	1	0
19	F	229	0	219	2	0
19	J	47	0	35	1	0
19	a	529	0	454	7	0
19	b	528	0	452	10	0
19	c	634	0	547	1	0
19	d	523	0	446	7	0
19	e	480	0	415	4	0
19	f	565	0	468	4	0
19	g	419	0	355	2	0
19	h	634	0	545	4	0
19	i	559	0	458	2	0
19	j	687	0	589	22	0
19	k	529	0	456	4	0
19	l	458	0	379	11	0
19	m	507	0	416	4	0
19	n	458	0	379	24	0
19	o	555	0	451	18	0
20	A	33	0	46	0	0
20	B	33	0	46	0	0
21	A	49	0	74	0	0
22	A	86	0	0	0	0
22	F	43	0	0	0	0
22	J	86	0	0	1	0
22	a	86	0	0	5	0
22	b	129	0	0	2	0
22	c	129	0	0	2	0
22	d	86	0	0	0	0
22	e	86	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	f	86	0	0	2	0
22	g	86	0	0	5	0
22	h	86	0	0	0	0
22	i	86	0	0	1	0
22	j	86	0	0	11	0
22	k	86	0	0	0	0
22	l	86	0	0	5	0
22	m	86	0	0	1	0
22	n	86	0	0	10	0
22	o	86	0	0	6	0
23	A	159	0	221	3	0
23	B	280	0	392	6	0
23	J	40	0	56	6	0
23	M	40	0	56	7	0
24	A	34	0	44	1	0
24	a	34	0	44	0	0
24	c	34	0	44	3	0
25	A	34	0	38	0	0
25	a	107	0	124	6	0
25	b	42	0	54	2	0
25	c	38	0	46	6	0
25	d	31	0	32	1	0
25	e	44	0	61	0	0
25	f	26	0	22	1	0
25	g	114	0	141	1	0
25	h	35	0	40	2	0
25	i	41	0	52	7	0
25	j	37	0	44	0	0
25	k	37	0	44	2	0
26	B	8	0	0	0	0
26	C	16	0	0	0	0
27	B	62	0	85	2	0
28	a	192	0	132	11	0
28	b	257	0	193	10	0
28	c	173	0	151	12	0
28	d	104	0	80	5	0
28	e	112	0	94	12	0
28	f	104	0	80	5	0
28	g	163	0	131	8	0
28	h	48	0	33	2	0
28	i	104	0	80	2	0
28	k	48	0	33	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	m	48	0	33	2	0
28	o	48	0	33	2	0
29	a	44	0	56	0	0
All	All	54391	0	50670	391	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 4.

All (391) 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)
19:j:306:CLA:HBB1	22:j:316:DD6:C1	1.69	1.22
28:e:304:CHL:H93	22:e:313:DD6:C10	1.72	1.19
19:n:206:CLA:HMB1	22:n:210:DD6:C23	1.95	0.95
19:n:206:CLA:CMB	22:n:210:DD6:C23	2.45	0.94
19:l:201:CLA:CBB	22:l:210:DD6:C10	2.49	0.89
19:l:201:CLA:HBB1	22:l:210:DD6:C10	2.04	0.87
19:n:206:CLA:HBB2	22:n:210:DD6:C12	2.06	0.85
19:j:306:CLA:HBB1	22:j:316:DD6:C	2.07	0.85
19:n:206:CLA:C3B	22:n:210:DD6:C21	2.58	0.82
19:j:306:CLA:CBB	22:j:316:DD6:C1	2.57	0.81
19:n:206:CLA:CAB	22:n:210:DD6:C21	2.58	0.80
17:i:138:LYS:NZ	25:i:316:LMG:O9	2.15	0.80
19:j:306:CLA:HBB1	22:j:316:DD6:C2	2.12	0.79
19:n:206:CLA:CBB	22:n:210:DD6:C14	2.62	0.77
18:l:138:LYS:HG2	19:l:201:CLA:H12	1.67	0.77
28:i:304:CHL:H61	22:i:314:DD6:C10	2.14	0.77
28:g:310:CHL:H2	22:g:314:DD6:C40	2.15	0.77
28:e:304:CHL:H12	22:e:313:DD6:C22	2.14	0.77
28:e:304:CHL:C9	22:e:313:DD6:C10	2.58	0.77
19:b:309:CLA:HMA2	28:b:310:CHL:HBC3	1.66	0.76
28:c:305:CHL:HMC	22:c:318:DD6:C9	2.16	0.76
16:h:56:TYR:HH	16:h:100:TYR:HH	1.31	0.75
19:l:201:CLA:CBB	22:l:210:DD6:C9	2.64	0.75
19:j:306:CLA:CBB	22:j:316:DD6:C	2.65	0.74
19:n:206:CLA:HMB3	22:n:210:DD6:C23	2.15	0.74
19:l:201:CLA:HBB1	22:l:210:DD6:C9	2.18	0.73
28:d:202:CHL:H2A	28:d:202:CHL:HED2	1.70	0.73
10:b:38:TYR:OH	25:b:316:LMG:O2	2.07	0.72
2:B:627:ASN:OD1	2:B:732:LYS:NZ	2.23	0.72
15:j:46:GLU:OE2	15:j:49:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:123:ASP:OD2	16:h:128:THR:OG1	2.09	0.71
15:j:98:ALA:HA	19:j:305:CLA:HAB	1.73	0.71
28:e:304:CHL:C9	22:e:313:DD6:C8	2.68	0.70
19:n:206:CLA:HAB	22:n:210:DD6:C21	2.20	0.70
28:c:305:CHL:HMC	22:c:318:DD6:C8	2.21	0.70
2:B:221:GLY:O	2:B:233:TYR:OH	2.09	0.70
25:i:316:LMG:H171	25:i:316:LMG:H291	1.73	0.70
16:h:33:ARG:NH2	16:h:134:GLU:OE2	2.25	0.69
17:i:82:TYR:OH	19:i:309:CLA:O1D	2.10	0.69
19:b:306:CLA:HBA2	19:b:306:CLA:HBD	1.74	0.69
1:A:95:GLY:O	1:A:99:SER:OG	2.09	0.69
18:n:103:ARG:NH2	19:n:203:CLA:O1D	2.26	0.69
18:l:103:ARG:NH2	19:l:203:CLA:O1D	2.26	0.69
28:e:304:CHL:H93	22:e:313:DD6:C9	2.23	0.68
3:C:61:ASP:OD2	5:E:53:SER:OG	2.09	0.68
18:m:103:ARG:NH2	19:m:305:CLA:O1D	2.27	0.68
28:e:304:CHL:C9	22:e:313:DD6:C9	2.72	0.67
19:j:306:CLA:CBB	22:j:316:DD6:C2	2.72	0.67
16:h:114:ASP:OD2	16:h:116:THR:OG1	2.12	0.67
18:n:172:PRO:HG3	19:n:209:CLA:HMA3	1.76	0.67
25:i:316:LMG:O5	25:i:316:LMG:O4	2.09	0.66
28:e:304:CHL:H91	22:e:313:DD6:C8	2.26	0.66
19:o:303:CLA:HAB	22:o:313:DD6:C3	2.26	0.65
2:B:516:ASP:OD2	2:B:593:TYR:OH	2.13	0.65
2:B:201:GLU:OE2	2:B:208:ARG:NH1	2.30	0.65
2:B:9:SER:HG	27:B:829:DGD:HO4E	1.43	0.65
25:g:312:LMG:O4	25:g:312:LMG:O5	2.07	0.65
11:c:50:GLN:OE1	11:c:53:ARG:NH1	2.30	0.64
19:A:853:CLA:HHC	19:A:853:CLA:HBB1	1.79	0.64
18:k:103:ARG:NH2	19:k:305:CLA:O1D	2.30	0.64
18:n:165:LEU:HD13	19:n:206:CLA:HMA1	1.80	0.63
14:f:12:ILE:CG2	14:f:15:ALA:HB2	2.29	0.63
25:b:316:LMG:O5	25:b:316:LMG:O4	2.09	0.62
9:a:120:GLY:HA2	19:a:306:CLA:HAB	1.81	0.62
12:d:148:LYS:NZ	19:d:203:CLA:O1D	2.31	0.61
25:c:320:LMG:O5	25:c:320:LMG:O4	2.12	0.61
19:o:303:CLA:HAB	22:o:313:DD6:C4	2.31	0.61
19:o:303:CLA:HAB	22:o:313:DD6:C5	2.31	0.61
19:B:845:CLA:HBA1	19:B:849:CLA:HBC2	1.82	0.61
18:k:105:ASN:ND2	18:k:109:ASN:O	2.33	0.61
18:m:105:ASN:ND2	18:m:109:ASN:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:122:PRO:HB3	28:g:310:CHL:HBC2	1.83	0.60
19:j:305:CLA:H42	18:n:98:PRO:HB3	1.83	0.60
1:A:370:HIS:ND1	19:A:816:CLA:OBD	2.35	0.60
28:a:312:CHL:HBB1	22:a:321:DD6:C29	2.32	0.60
28:g:310:CHL:C2	22:g:314:DD6:C40	2.79	0.60
28:e:304:CHL:C1	22:e:313:DD6:C22	2.81	0.59
18:l:138:LYS:HG2	19:l:201:CLA:C1	2.33	0.59
18:l:142:LEU:HD21	19:l:201:CLA:HMB2	1.84	0.59
18:n:37:LEU:HD13	19:n:205:CLA:H42	1.83	0.59
28:e:304:CHL:C2	22:e:313:DD6:C22	2.80	0.58
19:n:206:CLA:CAB	22:n:210:DD6:C14	2.81	0.58
18:n:135:ALA:HA	19:n:201:CLA:HED3	1.84	0.58
16:o:55:VAL:HG12	16:o:59:ARG:HE	1.67	0.58
19:A:810:CLA:HMB3	23:J:804:BCR:H373	1.86	0.58
12:d:133:ASP:OD2	12:d:138:THR:OG1	2.11	0.58
28:g:310:CHL:C5	22:g:314:DD6:C40	2.81	0.58
28:b:310:CHL:HHC	28:b:310:CHL:HBB1	1.85	0.57
19:d:208:CLA:HBB1	19:d:208:CLA:H51	1.86	0.57
1:A:580:ARG:NH1	4:D:116:GLU:OE2	2.37	0.57
2:B:559:CYS:SG	2:B:561:GLY:N	2.78	0.57
28:f:304:CHL:HBA2	22:f:315:DD6:C33	2.34	0.57
16:h:56:TYR:OH	16:h:100:TYR:OH	2.12	0.56
19:a:302:CLA:HAA1	25:a:316:LMG:HC5	1.86	0.56
19:A:810:CLA:CMB	23:J:804:BCR:H373	2.35	0.56
18:m:13:PHE:O	18:m:14:PRO:C	2.46	0.56
3:C:6:LYS:NZ	4:D:193:ASP:OD1	2.28	0.56
28:b:311:CHL:HMC	28:b:311:CHL:HBC2	1.86	0.56
19:B:807:CLA:H93	23:M:801:BCR:H362	1.86	0.56
28:a:312:CHL:CBB	22:a:321:DD6:C27	2.84	0.56
4:D:114:ARG:NH2	4:D:116:GLU:OE1	2.39	0.56
10:b:178:LYS:NZ	19:b:302:CLA:O1D	2.36	0.56
17:i:44:GLN:OE1	17:i:47:ARG:NH1	2.38	0.56
15:j:26:GLU:N	15:j:26:GLU:OE1	2.39	0.55
11:c:93:VAL:O	11:c:97:THR:OG1	2.20	0.55
28:g:310:CHL:C3	22:g:314:DD6:C40	2.84	0.55
19:j:306:CLA:HMC3	22:j:316:DD6:C9	2.36	0.55
4:D:46:ARG:NH1	19:D:301:CLA:O1D	2.40	0.55
18:n:50:SER:OG	19:n:203:CLA:O2D	2.24	0.55
13:e:101:TRP:CE3	19:e:310:CLA:HAB	2.42	0.55
28:k:301:CHL:H2A	28:k:301:CHL:HED3	1.89	0.55
1:A:587:SER:OG	1:A:590:ASP:OD2	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:104:ARG:NH2	19:g:304:CLA:O1D	2.40	0.54
15:g:130:THR:HG21	28:g:303:CHL:HED3	1.89	0.54
25:i:316:LMG:HC8	25:i:316:LMG:H121	1.89	0.54
19:n:205:CLA:H41	19:n:205:CLA:H71	1.88	0.54
19:B:833:CLA:O1A	8:M:30:ASN:HB2	2.07	0.54
18:m:17:THR:O	18:m:18:PRO:C	2.51	0.54
15:j:187:TRP:HZ2	19:j:310:CLA:HED3	1.72	0.54
18:n:49:VAL:HG22	18:n:118:SER:OG	2.08	0.54
19:j:306:CLA:HMC1	22:j:316:DD6:C6	2.37	0.54
17:i:104:ASN:OD1	18:m:112:LYS:NZ	2.27	0.54
2:B:9:SER:OG	27:B:829:DGD:O4E	2.13	0.53
16:o:16:PHE:HE1	28:o:301:CHL:HAB	1.73	0.53
12:d:81:GLU:OE2	12:d:81:GLU:N	2.42	0.53
28:f:304:CHL:HBA1	22:f:315:DD6:C41	2.38	0.53
16:o:55:VAL:HG12	16:o:59:ARG:NE	2.23	0.53
6:F:148:PRO:HG2	19:b:305:CLA:H12	1.90	0.53
28:b:312:CHL:HHC	28:b:312:CHL:HBB1	1.91	0.53
2:B:351:HIS:ND1	19:B:814:CLA:OBD	2.40	0.53
14:f:90:ILE:HG23	19:f:314:CLA:HMD1	1.91	0.53
16:o:12:ARG:NH1	16:o:32:ASP:OD1	2.40	0.53
25:a:301:LMG:H112	19:a:306:CLA:HBA1	1.92	0.52
25:c:320:LMG:HC61	12:d:137:LEU:HD22	1.90	0.52
19:j:313:CLA:OBD	16:o:185:TRP:NE1	2.42	0.52
12:d:148:LYS:NZ	25:d:213:LMG:O2	2.25	0.52
9:a:120:GLY:HA2	19:a:306:CLA:CAB	2.40	0.52
2:B:40:ASN:OD1	2:B:44:GLN:NE2	2.41	0.52
14:f:135:ARG:NH1	19:f:303:CLA:O2D	2.42	0.52
28:g:306:CHL:HMC	22:g:315:DD6:C25	2.40	0.52
18:m:124:PRO:O	18:m:126:LYS:NZ	2.36	0.52
1:A:333:PHE:CE2	19:A:853:CLA:HED2	2.44	0.51
10:b:65:TRP:CD1	19:b:305:CLA:HMD3	2.45	0.51
8:M:13:LEU:CD2	23:M:801:BCR:H312	2.40	0.51
10:b:65:TRP:HD1	19:b:305:CLA:HMD3	1.76	0.51
28:d:202:CHL:H2A	28:d:202:CHL:CED	2.41	0.51
28:k:301:CHL:HBA2	25:k:312:LMG:HC1	1.91	0.51
10:b:23:GLY:O	11:c:141:SER:OG	2.10	0.51
12:d:127:ARG:NH1	13:e:109:TRP:O	2.44	0.51
18:l:171:ASN:OD1	18:l:171:ASN:N	2.43	0.51
16:o:151:GLU:OE2	16:o:154:ARG:NH2	2.44	0.51
19:B:833:CLA:C1B	23:M:801:BCR:H282	2.41	0.51
9:a:128:ASN:OD1	9:a:128:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:318:LMG:O5	25:a:318:LMG:O4	2.26	0.51
14:f:98:LEU:HD23	19:f:311:CLA:HMA1	1.92	0.50
15:j:118:ASP:OD1	15:j:119:ARG:N	2.43	0.50
28:a:312:CHL:CBB	22:a:321:DD6:C26	2.90	0.50
28:e:304:CHL:HBB1	28:e:304:CHL:H92	1.92	0.50
1:A:576:ASP:OD2	1:A:580:ARG:NH2	2.45	0.50
19:A:808:CLA:OBD	24:c:301:LMU:O2'	2.29	0.50
14:f:51:VAL:HG22	14:f:137:ILE:HD11	1.92	0.50
16:o:155:HIS:ND1	19:o:310:CLA:O1D	2.43	0.50
15:j:125:ASP:OD2	15:j:130:THR:OG1	2.23	0.50
18:k:128:THR:HG21	19:k:304:CLA:HED3	1.94	0.50
28:a:312:CHL:HBA1	25:a:318:LMG:HC2	1.94	0.49
19:B:832:CLA:H43	16:h:166:VAL:HG22	1.95	0.49
18:l:123:ASP:OD2	18:l:128:THR:OG1	2.29	0.49
19:n:203:CLA:HBC2	19:n:204:CLA:HBC1	1.94	0.49
28:a:315:CHL:HHC	28:a:315:CHL:HBB1	1.94	0.49
18:n:45:ALA:O	18:n:49:VAL:HG23	2.12	0.49
16:o:104:GLU:OE1	16:o:107:ARG:NH2	2.45	0.49
2:B:177:HIS:HE1	19:B:837:CLA:NB	2.10	0.49
19:B:849:CLA:HBA1	19:B:849:CLA:HBD	1.94	0.49
19:B:848:CLA:H3A	19:B:848:CLA:HBA2	1.56	0.49
19:o:303:CLA:HMC2	22:o:313:DD6:C9	2.43	0.49
10:b:95:THR:O	10:b:98:THR:OG1	2.30	0.48
19:h:203:CLA:C2B	25:h:216:LMG:HC62	2.43	0.48
1:A:532:ASP:O	1:A:536:HIS:ND1	2.45	0.48
2:B:494:LEU:O	2:B:495:PRO:C	2.57	0.48
2:B:494:LEU:HB2	2:B:495:PRO:HD3	1.95	0.48
28:a:311:CHL:HHC	28:a:311:CHL:HBB1	1.95	0.48
18:k:61:ALA:HB3	18:k:147:LEU:HD11	1.95	0.48
18:l:128:THR:HG21	19:l:202:CLA:HED3	1.95	0.48
25:i:316:LMG:HO4	25:i:316:LMG:HO5	1.62	0.48
19:n:206:CLA:HED3	19:n:206:CLA:H2A	1.95	0.48
3:C:21:CYS:SG	3:C:24:ASP:N	2.87	0.48
19:o:302:CLA:H2	19:o:303:CLA:HMD2	1.94	0.48
8:M:13:LEU:HD21	23:M:801:BCR:HC32	1.96	0.48
18:m:56:ARG:O	18:m:60:LEU:HD12	2.14	0.48
18:m:142:LEU:HD21	19:m:303:CLA:HBC2	1.94	0.48
28:i:301:CHL:HBD	25:i:316:LMG:HC1	1.95	0.48
15:j:182:ASN:ND2	19:j:308:CLA:OBD	2.45	0.48
19:g:301:CLA:H2A	19:g:301:CLA:HED3	1.96	0.48
18:k:138:LYS:NZ	19:k:302:CLA:O1D	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:HIS:HB3	2:B:304:ILE:HD11	1.96	0.48
28:m:301:CHL:HHC	28:m:301:CHL:HBB1	1.96	0.48
1:A:307:LEU:O	19:A:845:CLA:HBC1	2.14	0.47
9:a:104:HIS:HB3	28:a:315:CHL:HMA3	1.96	0.47
19:J:803:CLA:OBD	24:c:301:LMU:H5B	2.13	0.47
1:A:354:SER:OG	1:A:405:ALA:O	2.25	0.47
23:J:804:BCR:H331	23:J:804:BCR:C8	2.44	0.47
17:i:36:LEU:HD13	19:i:307:CLA:H42	1.97	0.47
2:B:413:ASP:O	6:F:172:ARG:NH2	2.48	0.47
6:F:149:ASN:HD22	6:F:149:ASN:C	2.22	0.47
9:a:9:ARG:NH2	9:a:22:LEU:O	2.47	0.47
19:m:302:CLA:H3A	19:m:302:CLA:HBA2	1.49	0.47
18:n:123:ASP:OD2	18:n:128:THR:OG1	2.32	0.47
19:A:804:CLA:H93	19:A:809:CLA:H172	1.97	0.47
1:A:435:ASP:OD2	1:A:561:ARG:NH1	2.48	0.47
2:B:560:ASP:HB3	2:B:567:THR:HG21	1.96	0.47
19:e:308:CLA:H61	19:e:308:CLA:H41	1.75	0.47
19:j:306:CLA:CMC	22:j:316:DD6:C8	2.93	0.47
18:n:168:HIS:CE1	19:n:206:CLA:HAA2	2.50	0.47
19:a:314:CLA:H11	19:a:314:CLA:HBA1	1.47	0.47
15:g:92:ILE:HG23	19:h:201:CLA:HMD1	1.97	0.47
28:h:202:CHL:HBD	25:h:216:LMG:HC1	1.96	0.47
16:o:123:ASP:OD2	16:o:128:THR:OG1	2.27	0.47
2:B:481:ASP:OD1	2:B:481:ASP:N	2.48	0.47
19:a:306:CLA:H41	19:a:306:CLA:H62	1.55	0.47
5:E:63:ILE:HD11	5:E:78:ARG:CB	2.45	0.47
19:b:306:CLA:H62	19:b:306:CLA:H41	1.53	0.47
18:k:97:ALA:HB3	18:k:98:PRO:HD3	1.96	0.46
19:o:309:CLA:H12	19:o:309:CLA:HBA2	1.47	0.46
9:a:63:VAL:O	9:a:67:VAL:HG23	2.15	0.46
9:a:127:TRP:O	9:a:128:ASN:C	2.56	0.46
28:a:312:CHL:HBB2	22:a:321:DD6:C26	2.46	0.46
12:d:46:ARG:NH1	19:d:207:CLA:O1A	2.45	0.46
19:o:304:CLA:H3A	19:o:304:CLA:HBA2	1.52	0.46
10:b:217:TRP:HH2	28:c:312:CHL:H52	1.80	0.46
11:c:158:PHE:HA	28:c:313:CHL:H51	1.97	0.46
2:B:491:ALA:HB1	2:B:494:LEU:HG	1.98	0.46
10:b:58:ALA:CB	19:b:306:CLA:HBA1	2.46	0.46
1:A:220:VAL:O	1:A:224:ILE:HD12	2.16	0.45
11:c:112:ASN:OD1	11:c:114:SER:OG	2.23	0.45
14:f:9:LEU:HB3	28:f:301:CHL:HED2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:m:97:ALA:HB3	18:m:98:PRO:HD3	1.97	0.45
18:n:137:ILE:HD11	18:n:141:ARG:NH2	2.31	0.45
16:o:121:GLY:HA2	19:o:304:CLA:HED3	1.97	0.45
19:A:822:CLA:H203	23:J:804:BCR:H17C	1.97	0.45
2:B:560:ASP:CB	2:B:567:THR:HG21	2.46	0.45
28:d:205:CHL:H92	28:d:205:CHL:H61	1.69	0.45
3:C:54:CYS:SG	3:C:55:GLU:N	2.88	0.45
14:f:138:LYS:HB3	19:f:302:CLA:HMD2	1.96	0.45
28:h:202:CHL:H2A	28:h:202:CHL:HED3	1.98	0.45
23:B:850:BCR:H353	19:F:201:CLA:CGA	2.46	0.45
10:b:153:PRO:CG	28:b:312:CHL:HMD2	2.45	0.45
19:j:306:CLA:HMC1	22:j:316:DD6:C8	2.46	0.45
19:B:838:CLA:O1D	15:j:172:ARG:NH1	2.49	0.45
9:a:106:SER:O	9:a:107:ASN:CB	2.64	0.45
15:g:174:PRO:O	15:g:178:ASN:ND2	2.45	0.45
16:o:52:VAL:HG22	16:o:118:ARG:CD	2.47	0.45
1:A:681:PHE:HZ	19:A:829:CLA:HBC2	1.81	0.45
19:l:201:CLA:HBB1	22:l:210:DD6:C11	2.45	0.45
5:E:63:ILE:HD11	5:E:78:ARG:HB3	1.99	0.45
2:B:48:ALA:HB3	8:M:29:LEU:HD21	1.97	0.45
28:b:301:CHL:HBA1	28:b:301:CHL:H3A	1.59	0.45
19:A:842:CLA:H91	19:A:842:CLA:H111	1.86	0.44
9:a:135:ALA:N	25:a:301:LMG:O3	2.50	0.44
28:b:301:CHL:H92	28:c:312:CHL:H8	1.98	0.44
19:m:307:CLA:H61	19:m:307:CLA:H41	1.80	0.44
28:c:312:CHL:CHA	28:c:312:CHL:HBA1	2.48	0.44
14:f:138:LYS:HZ3	25:f:313:LMG:C2	2.30	0.44
16:h:134:GLU:OE2	16:h:138:LYS:NZ	2.50	0.44
28:c:313:CHL:HBB1	28:c:313:CHL:HHC	1.99	0.44
28:m:301:CHL:H11	28:m:301:CHL:H2A	2.00	0.44
19:o:303:CLA:CAB	22:o:313:DD6:C4	2.95	0.44
23:B:831:BCR:H382	23:B:831:BCR:H23C	1.99	0.44
15:g:101:GLU:OE1	15:g:104:ARG:NH1	2.50	0.44
16:h:138:LYS:HB3	19:h:203:CLA:HMD2	2.00	0.44
16:o:52:VAL:HG22	16:o:118:ARG:HD2	1.99	0.44
16:o:139:ASN:ND2	19:o:302:CLA:OBD	2.51	0.44
19:o:304:CLA:HBD	19:o:304:CLA:HED2	1.71	0.44
19:n:206:CLA:C4B	22:n:210:DD6:C21	2.95	0.44
10:b:149:ASP:OD1	10:b:150:LYS:N	2.51	0.43
28:f:304:CHL:H92	28:f:304:CHL:H61	1.79	0.43
19:o:303:CLA:CAB	22:o:313:DD6:C5	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:ARG:NH1	2:B:113:VAL:O	2.51	0.43
25:a:301:LMG:O5	25:a:301:LMG:O4	2.18	0.43
11:c:219:ILE:HG22	11:c:223:GLN:HE21	1.83	0.43
13:e:54:GLY:O	13:e:58:MET:HG3	2.18	0.43
2:B:559:CYS:SG	2:B:560:ASP:N	2.91	0.43
28:b:312:CHL:HBC3	28:b:312:CHL:HHD	2.00	0.43
11:c:179:LYS:NZ	19:c:303:CLA:O1D	2.45	0.43
25:c:320:LMG:HC2	25:c:320:LMG:HC71	1.56	0.43
28:e:304:CHL:HMC	22:e:313:DD6:C8	2.49	0.43
14:f:108:SER:OG	14:f:113:ASP:OD1	2.36	0.43
23:M:801:BCR:H20C	23:M:801:BCR:H361	1.92	0.43
28:d:205:CHL:HBA2	28:d:205:CHL:H3A	1.27	0.43
28:e:304:CHL:HBA2	28:e:304:CHL:H3A	1.40	0.43
18:n:119:TYR:HB3	19:n:202:CLA:HED3	2.00	0.43
1:A:119:TRP:CD2	19:A:810:CLA:HED3	2.54	0.43
2:B:652:PHE:O	2:B:656:VAL:HG23	2.19	0.43
9:a:120:GLY:CA	19:a:306:CLA:HAB	2.49	0.43
12:d:24:GLY:N	12:d:29:ASP:OD2	2.49	0.43
19:B:801:CLA:H61	19:B:801:CLA:H41	1.91	0.43
23:J:804:BCR:H24C	23:J:804:BCR:H371	1.80	0.43
9:a:119:MET:HA	9:a:122:VAL:HG22	2.00	0.43
19:j:306:CLA:HED2	19:j:306:CLA:H11	2.01	0.43
16:o:127:LEU:HD23	16:o:127:LEU:H	1.84	0.43
1:A:330:THR:O	19:A:853:CLA:HAC2	2.19	0.43
2:B:516:ASP:O	2:B:520:HIS:ND1	2.45	0.43
2:B:656:VAL:HG22	19:B:843:CLA:HMB3	2.00	0.43
25:c:320:LMG:H182	25:c:320:LMG:O10	2.19	0.43
15:j:60:MET:HE3	19:j:304:CLA:HMC3	2.01	0.43
18:m:150:LEU:HD21	22:m:313:DD6:C23	2.49	0.43
8:M:13:LEU:HD21	23:M:801:BCR:H312	1.99	0.43
11:c:174:LYS:O	11:c:178:VAL:HG23	2.20	0.42
28:c:313:CHL:H92	28:c:313:CHL:H62	1.90	0.42
18:n:128:THR:CG2	19:n:202:CLA:HED1	2.49	0.42
19:B:840:CLA:CHD	19:B:841:CLA:HAB	2.49	0.42
10:b:211:ASN:O	10:b:214:VAL:HG22	2.19	0.42
15:j:101:GLU:HG2	15:j:104:ARG:HE	1.83	0.42
1:A:247:LYS:O	1:A:251:SER:OG	2.32	0.42
24:A:838:LMU:O5B	24:A:838:LMU:O3'	2.26	0.42
2:B:629:SER:O	2:B:633:ASN:ND2	2.49	0.42
3:C:66:ARG:HG3	4:D:175:ILE:HD12	2.01	0.42
19:F:204:CLA:O1D	22:J:802:DD6:O4	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:m:69:GLU:OE2	18:m:162:LEU:HD12	2.19	0.42
14:f:93:GLN:HG2	18:k:93:MET:HE2	2.02	0.42
17:i:141:ARG:HA	17:i:144:MET:HE3	2.02	0.42
19:k:302:CLA:C2C	25:k:312:LMG:HC71	2.49	0.42
18:l:49:VAL:HG22	18:l:118:SER:OG	2.20	0.42
19:o:304:CLA:CHB	19:o:304:CLA:H12	2.49	0.42
19:B:812:CLA:H2	23:B:826:BCR:H362	2.00	0.42
28:a:315:CHL:H3A	28:a:315:CHL:HBA2	1.26	0.42
19:o:302:CLA:H2	19:o:303:CLA:CMD	2.50	0.42
28:b:310:CHL:HMC	22:b:318:DD6:C22	2.50	0.42
19:b:315:CLA:HMC2	28:c:312:CHL:H3A	2.01	0.42
13:e:107:PHE:HZ	19:e:310:CLA:HBB2	1.84	0.42
2:B:498:LEU:HA	2:B:501:ILE:HG22	2.01	0.42
19:B:837:CLA:HBA2	19:B:837:CLA:H3A	1.44	0.42
18:m:81:ASN:OD1	18:m:81:ASN:N	2.51	0.42
2:B:531:THR:HG21	19:B:823:CLA:HMB3	2.02	0.42
25:c:320:LMG:H122	25:c:320:LMG:H152	1.66	0.42
19:d:208:CLA:H93	19:d:208:CLA:H112	1.90	0.42
18:k:55:ALA:HB1	18:k:140:GLY:HA3	2.01	0.42
18:n:121:GLY:N	19:n:202:CLA:O1D	2.48	0.42
2:B:623:TYR:O	2:B:627:ASN:ND2	2.53	0.42
9:a:201:HIS:O	9:a:206:ASN:ND2	2.49	0.42
12:d:178:THR:HG21	19:d:209:CLA:HAA2	2.02	0.42
1:A:201:HIS:ND1	19:A:819:CLA:OBD	2.53	0.42
19:d:208:CLA:H61	19:d:208:CLA:H41	1.80	0.42
23:B:826:BCR:H343	19:B:838:CLA:H3A	2.02	0.41
10:b:137:ARG:HA	28:b:312:CHL:HBC2	2.02	0.41
19:b:306:CLA:HBB1	22:b:318:DD6:C3	2.50	0.41
12:d:93:ILE:HD11	19:d:210:CLA:H43	2.02	0.41
15:j:146:MET:HE1	19:j:307:CLA:HAB	2.01	0.41
19:j:306:CLA:CBB	22:j:316:DD6:C3	2.98	0.41
19:A:841:CLA:H121	19:A:842:CLA:H72	2.02	0.41
28:c:305:CHL:H92	28:c:305:CHL:H61	1.84	0.41
19:n:203:CLA:C9	19:n:204:CLA:H91	2.51	0.41
15:j:95:GLN:HG3	18:n:93:MET:HE3	2.02	0.41
25:i:316:LMG:H121	25:i:316:LMG:H151	1.85	0.41
15:j:125:ASP:HB2	19:j:304:CLA:HED3	2.02	0.41
1:A:697:ILE:O	1:A:701:VAL:HG23	2.21	0.41
23:J:804:BCR:HC42	24:c:301:LMU:H112	2.01	0.41
16:o:185:TRP:HZ3	19:o:310:CLA:HED1	1.86	0.41
28:o:301:CHL:HMD2	19:o:307:CLA:CMD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:o:304:CLA:H62	19:o:304:CLA:H41	1.70	0.41
19:B:801:CLA:OBD	19:B:803:CLA:HMB3	2.20	0.41
23:B:826:BCR:H24C	23:B:826:BCR:H371	1.94	0.41
23:B:850:BCR:H392	23:B:850:BCR:H23C	2.01	0.41
28:d:205:CHL:H62	28:d:205:CHL:H41	1.89	0.41
28:f:301:CHL:HBA2	28:f:301:CHL:H3A	1.56	0.41
19:A:803:CLA:HBA1	2:B:426:THR:HG22	2.02	0.41
9:a:111:ILE:HG13	28:a:315:CHL:HMC	2.03	0.41
11:c:186:LEU:HD12	25:c:320:LMG:H151	2.03	0.41
1:A:563:ILE:HD12	1:A:586:VAL:HG21	2.02	0.41
23:A:835:BCR:H20C	23:A:835:BCR:H361	1.95	0.41
10:b:217:TRP:HH2	28:c:312:CHL:C5	2.34	0.41
15:g:119:ARG:NH2	18:l:110:TRP:O	2.46	0.41
19:h:201:CLA:C7	19:h:201:CLA:H41	2.50	0.41
18:l:97:ALA:HB3	18:l:98:PRO:HD3	2.01	0.41
16:o:157:THR:HG22	16:o:159:VAL:HG22	2.03	0.41
28:c:305:CHL:H62	28:c:305:CHL:H41	1.80	0.41
16:o:125:LEU:HB2	16:o:127:LEU:HD22	2.02	0.41
2:B:567:THR:HG23	2:B:570:ILE:HD12	2.03	0.40
19:A:802:CLA:H2	23:A:837:BCR:H362	2.02	0.40
19:e:310:CLA:HBA1	19:e:310:CLA:H3A	1.90	0.40
28:g:310:CHL:HBD	28:g:310:CHL:HAA1	2.03	0.40
19:j:305:CLA:H3A	19:j:305:CLA:HBA2	1.46	0.40
1:A:220:VAL:HG13	1:A:240:PRO:HB3	2.02	0.40
23:A:836:BCR:H403	23:A:836:BCR:H23C	2.03	0.40
19:B:844:CLA:CGA	19:j:302:CLA:H43	2.51	0.40
18:k:14:PRO:HD3	28:k:301:CHL:HMA1	2.03	0.40
18:m:159:GLU:OE2	18:m:159:GLU:N	2.54	0.40
8:M:13:LEU:HD23	23:M:801:BCR:H312	2.02	0.40
28:a:312:CHL:HBB1	22:a:321:DD6:C27	2.50	0.40
16:h:102:ILE:H	16:h:102:ILE:HD12	1.86	0.40
15:j:142:GLY:O	15:j:146:MET:HG3	2.22	0.40
19:l:201:CLA:O2A	19:l:201:CLA:H2A	2.22	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	A	738/751 (98%)	718 (97%)	20 (3%)	0	100	100
2	B	728/733 (99%)	709 (97%)	19 (3%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	185/203 (91%)	175 (95%)	9 (5%)	1 (0%)	24	46
5	E	61/99 (62%)	56 (92%)	5 (8%)	0	100	100
6	F	164/172 (95%)	158 (96%)	5 (3%)	1 (1%)	21	42
7	J	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	M	29/31 (94%)	29 (100%)	0	0	100	100
9	a	197/209 (94%)	189 (96%)	5 (2%)	3 (2%)	8	20
10	b	217/225 (96%)	211 (97%)	6 (3%)	0	100	100
11	c	220/230 (96%)	213 (97%)	5 (2%)	2 (1%)	14	33
12	d	170/184 (92%)	160 (94%)	10 (6%)	0	100	100
13	e	164/177 (93%)	155 (94%)	9 (6%)	0	100	100
14	f	170/185 (92%)	166 (98%)	4 (2%)	0	100	100
15	g	180/191 (94%)	179 (99%)	1 (1%)	0	100	100
15	j	178/191 (93%)	168 (94%)	9 (5%)	1 (1%)	21	42
16	h	176/188 (94%)	171 (97%)	5 (3%)	0	100	100
16	o	175/188 (93%)	168 (96%)	7 (4%)	0	100	100
17	i	170/185 (92%)	164 (96%)	6 (4%)	0	100	100
18	k	166/174 (95%)	158 (95%)	8 (5%)	0	100	100
18	l	165/174 (95%)	158 (96%)	7 (4%)	0	100	100
18	m	166/174 (95%)	158 (95%)	7 (4%)	1 (1%)	21	42
18	n	154/174 (88%)	145 (94%)	9 (6%)	0	100	100
All	All	4686/4956 (95%)	4516 (96%)	161 (3%)	9 (0%)	44	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	a	136	LYS
9	a	107	ASN
11	c	30	GLU
18	m	25	GLU
6	F	43	SER
4	D	132	ARG
15	j	122	PRO
11	c	116	ILE
9	a	103	ILE

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	A	620/632 (98%)	620 (100%)	0	100	100
2	B	607/609 (100%)	606 (100%)	1 (0%)	87	95
3	C	69/70 (99%)	68 (99%)	1 (1%)	59	80
4	D	154/164 (94%)	154 (100%)	0	100	100
5	E	54/81 (67%)	54 (100%)	0	100	100
6	F	132/136 (97%)	131 (99%)	1 (1%)	73	87
7	J	34/34 (100%)	34 (100%)	0	100	100
8	M	26/26 (100%)	25 (96%)	1 (4%)	29	56
9	a	152/159 (96%)	146 (96%)	6 (4%)	28	56
10	b	167/170 (98%)	166 (99%)	1 (1%)	78	90
11	c	172/178 (97%)	172 (100%)	0	100	100
12	d	133/142 (94%)	133 (100%)	0	100	100
13	e	125/131 (95%)	124 (99%)	1 (1%)	73	87
14	f	141/147 (96%)	141 (100%)	0	100	100
15	g	144/151 (95%)	144 (100%)	0	100	100
15	j	142/151 (94%)	141 (99%)	1 (1%)	76	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	h	137/145 (94%)	136 (99%)	1 (1%)	76 89
16	o	137/145 (94%)	137 (100%)	0	100 100
17	i	142/148 (96%)	141 (99%)	1 (1%)	76 89
18	k	122/126 (97%)	122 (100%)	0	100 100
18	l	121/126 (96%)	121 (100%)	0	100 100
18	m	122/126 (97%)	122 (100%)	0	100 100
18	n	114/126 (90%)	113 (99%)	1 (1%)	70 86
All	All	3767/3923 (96%)	3751 (100%)	16 (0%)	81 92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	484	ASN
3	C	34	CYS
6	F	149	ASN
8	M	31	GLN
9	a	109	SER
9	a	111	ILE
9	a	117	LEU
9	a	119	MET
9	a	128	ASN
9	a	131	LEU
10	b	28	GLU
13	e	36	PHE
16	h	127	LEU
17	i	176	ASN
15	j	111	TRP
18	n	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	124	GLN
1	A	268	HIS
2	B	177	HIS
2	B	331	HIS
2	B	484	ASN

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Mol	Chain	Res	Type
2	B	490	GLN
6	F	149	ASN
9	a	107	ASN
10	b	62	ASN
11	c	180	ASN
11	c	223	GLN
12	d	83	GLN
13	e	155	GLN
15	g	170	HIS
16	h	57	HIS
17	i	129	ASN
17	i	153	GLN
15	j	82	ASN
15	j	155	GLN
15	j	157	HIS
18	l	105	ASN
18	l	168	HIS
18	n	54	HIS
18	n	105	ASN
18	n	153	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

348 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
22	DD6	f	316	-	39,45,45	0.16	0	52,67,67	0.59	1 (1%)
23	BCR	B	831	-	41,41,41	0.23	0	56,56,56	0.33	0
19	CLA	g	305	15	51,55,73	2.05	9 (17%)	61,91,113	1.67	11 (18%)
19	CLA	h	213	-	51,55,73	2.06	9 (17%)	61,91,113	1.67	8 (13%)
28	CHL	e	301	13	55,59,74	1.41	7 (12%)	62,96,114	2.10	12 (19%)
19	CLA	J	803	-	51,55,73	2.02	9 (17%)	61,91,113	1.55	6 (9%)
19	CLA	B	804	-	69,73,73	1.78	9 (13%)	83,113,113	1.35	9 (10%)
19	CLA	n	207	-	51,55,73	2.05	9 (17%)	61,91,113	1.67	7 (11%)
19	CLA	B	816	-	53,57,73	2.01	9 (16%)	62,93,113	1.66	7 (11%)
26	SF4	B	802	-	0,12,12	-	-	-		
19	CLA	B	805	2	69,73,73	1.76	9 (13%)	83,113,113	1.45	9 (10%)
19	CLA	n	208	-	51,55,73	2.03	9 (17%)	61,91,113	1.63	10 (16%)
19	CLA	a	308	9	64,68,73	1.85	9 (14%)	77,107,113	1.54	8 (10%)
19	CLA	B	815	-	64,68,73	1.79	9 (14%)	77,107,113	1.50	10 (12%)
19	CLA	A	801	-	69,73,73	1.71	8 (11%)	83,113,113	1.34	9 (10%)
19	CLA	B	848	-	51,55,73	2.07	9 (17%)	61,91,113	1.66	9 (14%)
25	LMG	c	320	-	38,38,55	0.88	0	46,46,63	1.24	2 (4%)
19	CLA	k	305	18	64,68,73	1.81	9 (14%)	77,107,113	1.39	7 (9%)
19	CLA	f	306	14	51,55,73	2.06	9 (17%)	61,91,113	1.56	6 (9%)
19	CLA	B	806	-	69,73,73	1.74	9 (13%)	83,113,113	1.35	7 (8%)
19	CLA	b	302	25	59,63,73	1.93	9 (15%)	71,101,113	1.49	7 (9%)
19	CLA	j	305	15	54,58,73	1.89	9 (16%)	65,95,113	1.58	10 (15%)
22	DD6	m	313	-	39,45,45	0.15	0	52,67,67	0.76	3 (5%)
19	CLA	n	202	18	51,55,73	2.12	9 (17%)	61,91,113	1.96	15 (24%)
19	CLA	k	307	18	64,68,73	1.84	9 (14%)	77,107,113	1.47	6 (7%)
19	CLA	B	838	-	54,58,73	2.05	9 (16%)	65,95,113	1.67	9 (13%)
28	CHL	b	301	10	60,64,74	1.39	7 (11%)	68,102,114	1.87	17 (25%)
19	CLA	h	208	-	64,68,73	1.85	9 (14%)	77,107,113	1.49	7 (9%)
19	CLA	B	835	-	60,64,73	1.90	9 (15%)	72,102,113	1.55	9 (12%)
28	CHL	i	304	17	60,64,74	1.39	7 (11%)	68,102,114	2.08	14 (20%)
19	CLA	i	312	17	51,55,73	2.04	9 (17%)	61,91,113	1.62	6 (9%)
25	LMG	i	316	-	41,41,55	0.91	2 (4%)	49,49,63	1.20	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CHL	b	311	-	52,56,74	1.43	7 (13%)	58,92,114	2.13	15 (25%)
19	CLA	l	207	-	51,55,73	2.04	9 (17%)	61,91,113	1.63	7 (11%)
25	LMG	a	316	-	27,27,55	0.96	1 (3%)	35,35,63	1.22	6 (17%)
22	DD6	e	313	-	39,45,45	0.20	0	52,67,67	0.97	3 (5%)
19	CLA	A	849	1	51,55,73	2.06	9 (17%)	61,91,113	1.59	6 (9%)
19	CLA	A	823	-	69,73,73	1.71	9 (13%)	83,113,113	1.36	9 (10%)
19	CLA	i	306	17	51,55,73	2.06	9 (17%)	61,91,113	1.61	7 (11%)
19	CLA	B	814	-	63,67,73	1.85	9 (14%)	75,105,113	1.51	7 (9%)
19	CLA	l	208	-	51,55,73	2.06	9 (17%)	61,91,113	1.59	6 (9%)
19	CLA	j	303	15	56,60,73	1.93	9 (16%)	67,97,113	1.49	8 (11%)
19	CLA	D	301	15	56,60,73	1.96	9 (16%)	67,97,113	1.49	7 (10%)
19	CLA	F	204	-	51,55,73	2.03	9 (17%)	61,91,113	1.53	7 (11%)
19	CLA	B	841	-	51,55,73	2.01	9 (17%)	61,91,113	1.60	8 (13%)
19	CLA	c	304	11	56,60,73	1.93	9 (16%)	67,97,113	1.46	7 (10%)
22	DD6	b	317	-	39,45,45	0.21	0	52,67,67	1.22	3 (5%)
19	CLA	A	809	-	69,73,73	1.76	9 (13%)	83,113,113	1.35	6 (7%)
19	CLA	A	843	-	69,73,73	1.84	9 (13%)	83,113,113	1.64	10 (12%)
19	CLA	n	205	18	64,68,73	1.87	9 (14%)	77,107,113	1.51	8 (10%)
19	CLA	l	205	-	64,68,73	1.84	9 (14%)	77,107,113	1.46	7 (9%)
20	PQN	A	830	-	34,34,34	0.39	0	42,45,45	0.71	1 (2%)
19	CLA	k	310	-	59,63,73	1.90	9 (15%)	71,101,113	1.46	6 (8%)
19	CLA	d	212	-	51,55,73	2.02	9 (17%)	61,91,113	1.51	6 (9%)
19	CLA	B	819	-	69,73,73	1.76	9 (13%)	83,113,113	1.37	6 (7%)
19	CLA	l	202	-	51,55,73	2.12	9 (17%)	61,91,113	1.77	9 (14%)
23	BCR	B	850	-	41,41,41	0.32	0	56,56,56	0.62	1 (1%)
19	CLA	B	818	-	69,73,73	1.74	9 (13%)	83,113,113	1.42	9 (10%)
19	CLA	A	802	-	69,73,73	1.72	10 (14%)	83,113,113	1.39	9 (10%)
19	CLA	B	836	-	68,72,73	1.75	9 (13%)	81,111,113	1.31	8 (9%)
19	CLA	A	807	1	69,73,73	1.75	9 (13%)	83,113,113	1.39	7 (8%)
19	CLA	B	847	-	69,73,73	1.81	9 (13%)	83,113,113	1.53	8 (9%)
19	CLA	A	825	-	54,58,73	2.01	9 (16%)	65,95,113	1.66	8 (12%)
19	CLA	A	829	-	69,73,73	1.76	9 (13%)	83,113,113	1.37	7 (8%)
19	CLA	n	209	-	51,55,73	2.12	9 (17%)	61,91,113	1.61	11 (18%)
22	DD6	A	832	-	39,45,45	0.23	0	52,67,67	1.02	3 (5%)
19	CLA	d	211	-	64,68,73	1.80	9 (14%)	77,107,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	g	302	-	59,63,73	1.91	9 (15%)	71,101,113	1.44	6 (8%)
22	DD6	n	211	-	39,45,45	0.13	0	52,67,67	0.66	1 (1%)
19	CLA	f	308	14	55,59,73	1.96	9 (16%)	66,96,113	1.51	6 (9%)
19	CLA	B	837	-	54,58,73	1.99	9 (16%)	65,95,113	1.59	10 (15%)
19	CLA	c	311	-	51,55,73	2.04	9 (17%)	61,91,113	1.58	6 (9%)
19	CLA	a	310	-	54,58,73	1.96	9 (16%)	65,95,113	1.53	7 (10%)
19	CLA	b	309	-	54,58,73	1.96	9 (16%)	65,95,113	1.50	6 (9%)
19	CLA	A	841	1	69,73,73	1.76	9 (13%)	83,113,113	1.37	5 (6%)
22	DD6	g	315	-	39,45,45	0.18	0	52,67,67	0.89	2 (3%)
19	CLA	h	211	-	55,59,73	1.96	9 (16%)	66,96,113	1.53	8 (12%)
19	CLA	j	310	-	51,55,73	2.00	9 (17%)	61,91,113	1.56	8 (13%)
29	NEX	a	317	-	38,46,46	0.37	1 (2%)	50,70,70	1.16	2 (4%)
23	BCR	M	801	-	41,41,41	0.13	0	56,56,56	0.35	0
19	CLA	a	304	-	51,55,73	2.05	9 (17%)	61,91,113	1.59	7 (11%)
19	CLA	B	846	2	51,55,73	1.99	9 (17%)	61,91,113	1.44	9 (14%)
28	CHL	i	301	17	52,56,74	1.40	5 (9%)	58,92,114	1.94	13 (22%)
19	CLA	i	305	-	51,55,73	2.09	9 (17%)	61,91,113	1.66	8 (13%)
19	CLA	B	812	2	68,72,73	1.77	9 (13%)	81,111,113	1.38	7 (8%)
19	CLA	l	203	18	64,68,73	1.86	9 (14%)	77,107,113	1.52	8 (10%)
19	CLA	l	209	-	51,55,73	2.07	9 (17%)	61,91,113	1.77	11 (18%)
28	CHL	d	202	12	52,56,74	1.43	5 (9%)	58,92,114	1.98	12 (20%)
19	CLA	m	303	-	51,55,73	2.07	9 (17%)	61,91,113	1.68	6 (9%)
19	CLA	A	844	-	69,73,73	1.74	9 (13%)	83,113,113	1.39	8 (9%)
19	CLA	f	309	-	64,68,73	1.86	9 (14%)	77,107,113	1.52	8 (10%)
28	CHL	m	301	18	52,56,74	1.46	6 (11%)	58,92,114	1.80	11 (18%)
19	CLA	o	311	-	54,58,73	1.97	8 (14%)	65,95,113	1.47	8 (12%)
19	CLA	c	302	11	51,55,73	2.03	9 (17%)	61,91,113	1.63	10 (16%)
19	CLA	i	303	-	51,55,73	2.05	9 (17%)	61,91,113	1.57	7 (11%)
19	CLA	A	814	-	51,55,73	2.03	9 (17%)	61,91,113	1.56	7 (11%)
22	DD6	i	314	-	39,45,45	0.19	0	52,67,67	0.74	1 (1%)
25	LMG	j	314	-	37,37,55	0.99	1 (2%)	45,45,63	1.49	5 (11%)
19	CLA	k	311	-	51,55,73	2.07	9 (17%)	61,91,113	1.64	7 (11%)
22	DD6	c	319	-	39,45,45	0.20	0	52,67,67	0.86	2 (3%)
19	CLA	k	308	18	54,58,73	2.00	9 (16%)	65,95,113	1.56	7 (10%)
19	CLA	n	206	18	51,55,73	2.18	9 (17%)	61,91,113	1.63	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A	822	-	69,73,73	1.71	9 (13%)	83,113,113	1.36	10 (12%)
25	LMG	d	213	-	31,31,55	1.16	1 (3%)	39,39,63	1.28	5 (12%)
23	BCR	B	825	-	41,41,41	0.20	0	56,56,56	0.37	0
26	SF4	C	801	-	0,12,12	-	-	-		
25	LMG	g	313	-	33,33,55	0.98	1 (3%)	41,41,63	1.21	6 (14%)
19	CLA	A	820	-	59,63,73	1.94	9 (15%)	71,101,113	1.55	6 (8%)
19	CLA	m	306	18	51,55,73	2.07	9 (17%)	61,91,113	1.70	7 (11%)
19	CLA	o	302	-	59,63,73	2.01	9 (15%)	71,101,113	1.74	11 (15%)
28	CHL	a	315	9	52,56,74	1.42	6 (11%)	58,92,114	1.91	10 (17%)
19	CLA	g	309	-	60,64,73	1.87	9 (15%)	72,102,113	1.45	5 (6%)
25	LMG	h	216	-	35,35,55	0.97	0	43,43,63	1.26	3 (6%)
19	CLA	e	309	-	51,55,73	2.06	9 (17%)	61,91,113	1.64	7 (11%)
19	CLA	A	847	1	51,55,73	2.06	9 (17%)	61,91,113	1.64	7 (11%)
28	CHL	b	310	-	52,56,74	1.44	6 (11%)	58,92,114	2.08	10 (17%)
22	DD6	b	319	-	39,45,45	0.17	0	52,67,67	0.68	2 (3%)
19	CLA	B	842	-	51,55,73	2.05	9 (17%)	61,91,113	1.61	10 (16%)
19	CLA	h	205	16	64,68,73	1.85	9 (14%)	77,107,113	1.47	10 (12%)
19	CLA	c	315	11	51,55,73	2.04	9 (17%)	61,91,113	1.58	8 (13%)
19	CLA	j	301	-	51,55,73	2.07	9 (17%)	61,91,113	1.70	8 (13%)
22	DD6	J	801	-	39,45,45	0.29	0	52,67,67	0.99	1 (1%)
19	CLA	m	302	-	51,55,73	2.02	9 (17%)	61,91,113	1.68	9 (14%)
23	BCR	B	828	-	41,41,41	0.16	0	56,56,56	0.46	0
19	CLA	F	202	-	61,65,73	1.87	9 (14%)	73,103,113	1.40	7 (9%)
19	CLA	f	310	-	51,55,73	2.04	9 (17%)	61,91,113	1.58	7 (11%)
19	CLA	d	207	-	51,55,73	2.07	9 (17%)	61,91,113	1.64	6 (9%)
19	CLA	i	307	17	58,62,73	1.93	9 (15%)	69,99,113	1.52	7 (10%)
19	CLA	n	203	18	64,68,73	1.85	9 (14%)	77,107,113	1.62	9 (11%)
19	CLA	f	307	14	58,62,73	1.95	10 (17%)	69,99,113	1.61	9 (13%)
19	CLA	B	823	-	51,55,73	2.03	9 (17%)	61,91,113	1.70	8 (13%)
19	CLA	B	833	2	60,64,73	1.90	9 (15%)	72,102,113	1.50	7 (9%)
28	CHL	h	202	16	52,56,74	1.38	7 (13%)	58,92,114	2.11	13 (22%)
23	BCR	A	837	-	41,41,41	0.22	0	56,56,56	0.51	0
19	CLA	g	307	15	64,68,73	1.82	9 (14%)	77,107,113	1.38	6 (7%)
19	CLA	A	848	1	54,58,73	1.96	9 (16%)	65,95,113	1.54	7 (10%)
19	CLA	b	303	-	55,59,73	1.96	9 (16%)	66,96,113	1.51	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	DD6	j	316	-	39,45,45	0.19	0	52,67,67	0.99	3 (5%)
19	CLA	B	843	-	51,55,73	2.05	9 (17%)	61,91,113	1.64	6 (9%)
25	LMG	a	318	-	40,40,55	0.82	1 (2%)	48,48,63	1.29	6 (12%)
19	CLA	o	309	-	51,55,73	2.07	9 (17%)	61,91,113	1.63	9 (14%)
19	CLA	d	209	12	60,64,73	1.86	9 (15%)	72,102,113	1.44	6 (8%)
22	DD6	l	211	-	39,45,45	0.17	0	52,67,67	0.79	1 (1%)
19	CLA	A	811	19	65,69,73	1.82	9 (13%)	78,108,113	1.44	7 (8%)
19	CLA	f	312	-	51,55,73	2.07	9 (17%)	61,91,113	1.60	5 (8%)
19	CLA	B	803	-	69,73,73	1.71	9 (13%)	83,113,113	1.33	8 (9%)
28	CHL	b	314	-	56,60,74	1.38	6 (10%)	63,97,114	2.03	13 (20%)
28	CHL	a	311	-	52,56,74	1.42	7 (13%)	58,92,114	1.84	12 (20%)
19	CLA	c	310	-	54,58,73	1.98	9 (16%)	65,95,113	1.48	5 (7%)
19	CLA	d	201	-	51,55,73	2.03	9 (17%)	61,91,113	1.58	7 (11%)
19	CLA	A	852	-	59,63,73	1.90	9 (15%)	71,101,113	1.44	6 (8%)
19	CLA	j	308	15	64,68,73	1.83	9 (14%)	77,107,113	1.44	7 (9%)
19	CLA	B	830	2	62,66,73	1.87	9 (14%)	74,104,113	1.46	9 (12%)
19	CLA	f	314	14	59,63,73	1.95	9 (15%)	71,101,113	1.67	9 (12%)
19	CLA	h	209	16	64,68,73	1.84	9 (14%)	77,107,113	1.42	7 (9%)
19	CLA	h	201	-	60,64,73	1.89	9 (15%)	72,102,113	1.47	7 (9%)
19	CLA	c	306	11	60,64,73	1.94	8 (13%)	72,102,113	1.53	6 (8%)
19	CLA	c	309	11	60,64,73	1.88	9 (15%)	72,102,113	1.45	6 (8%)
19	CLA	e	306	13	59,63,73	1.91	9 (15%)	71,101,113	1.50	7 (9%)
19	CLA	b	306	10	64,68,73	1.82	9 (14%)	77,107,113	1.51	9 (11%)
22	DD6	a	321	-	39,45,45	0.22	0	52,67,67	0.83	3 (5%)
28	CHL	d	205	12	60,64,74	1.36	7 (11%)	68,102,114	1.98	14 (20%)
19	CLA	h	212	-	60,64,73	1.87	9 (15%)	72,102,113	1.45	8 (11%)
19	CLA	A	808	1	54,58,73	1.99	9 (16%)	65,95,113	1.57	7 (10%)
19	CLA	m	310	-	59,63,73	1.91	9 (15%)	71,101,113	1.45	7 (9%)
19	CLA	a	305	9	64,68,73	1.84	10 (15%)	77,107,113	1.42	9 (11%)
19	CLA	B	807	2	69,73,73	1.72	9 (13%)	83,113,113	1.41	7 (8%)
19	CLA	e	302	-	59,63,73	1.91	9 (15%)	71,101,113	1.47	6 (8%)
19	CLA	B	811	2	62,66,73	1.85	9 (14%)	74,104,113	1.47	7 (9%)
19	CLA	A	839	-	52,56,73	2.00	9 (17%)	62,92,113	1.52	7 (11%)
25	LMG	a	301	-	40,40,55	0.88	3 (7%)	48,48,63	1.27	6 (12%)
28	CHL	g	303	15	60,64,74	1.34	6 (10%)	68,102,114	2.12	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	c	316	11	69,73,73	1.75	9 (13%)	83,113,113	1.33	7 (8%)
19	CLA	A	846	1	51,55,73	2.00	9 (17%)	61,91,113	1.60	8 (13%)
19	CLA	o	307	-	64,68,73	1.90	9 (14%)	77,107,113	1.75	13 (16%)
19	CLA	B	844	2	51,55,73	2.06	9 (17%)	61,91,113	1.66	8 (13%)
19	CLA	A	828	-	69,73,73	1.76	9 (13%)	83,113,113	1.40	8 (9%)
19	CLA	F	203	-	69,73,73	1.76	9 (13%)	83,113,113	1.43	7 (8%)
19	CLA	c	308	-	61,65,73	1.88	9 (14%)	73,103,113	1.51	6 (8%)
19	CLA	i	309	-	64,68,73	1.82	9 (14%)	77,107,113	1.36	8 (10%)
19	CLA	i	313	17	56,60,73	2.01	9 (16%)	67,97,113	1.72	9 (13%)
19	CLA	a	306	9	56,60,73	1.92	9 (16%)	67,97,113	1.59	9 (13%)
23	BCR	A	836	-	41,41,41	0.15	0	56,56,56	0.47	0
19	CLA	B	817	-	66,70,73	1.77	9 (13%)	79,109,113	1.45	10 (12%)
19	CLA	m	304	-	51,55,73	2.18	9 (17%)	61,91,113	2.07	13 (21%)
19	CLA	j	312	-	51,55,73	2.10	9 (17%)	61,91,113	1.75	9 (14%)
19	CLA	g	308	-	60,64,73	1.90	9 (15%)	72,102,113	1.51	7 (9%)
19	CLA	m	309	-	51,55,73	2.01	9 (17%)	61,91,113	1.67	9 (14%)
19	CLA	o	312	16	51,55,73	2.09	9 (17%)	61,91,113	1.68	6 (9%)
19	CLA	e	310	-	59,63,73	1.88	9 (15%)	71,101,113	1.59	9 (12%)
19	CLA	h	204	16	52,56,73	2.04	9 (17%)	62,92,113	1.59	6 (9%)
19	CLA	B	820	2	65,69,73	1.81	9 (13%)	78,108,113	1.45	7 (8%)
19	CLA	o	306	-	51,55,73	2.07	9 (17%)	61,91,113	1.63	7 (11%)
23	BCR	J	804	-	41,41,41	0.17	0	56,56,56	0.36	0
24	LMU	A	838	-	35,35,36	0.38	0	43,45,47	0.85	0
19	CLA	o	305	-	51,55,73	2.06	9 (17%)	61,91,113	1.64	11 (18%)
28	CHL	g	306	15	60,64,74	1.36	6 (10%)	68,102,114	2.09	17 (25%)
19	CLA	A	842	1	69,73,73	1.72	9 (13%)	83,113,113	1.41	11 (13%)
19	CLA	A	803	-	69,73,73	1.81	10 (14%)	83,113,113	1.44	9 (10%)
19	CLA	n	204	-	60,64,73	1.97	9 (15%)	72,102,113	1.58	8 (11%)
19	CLA	e	308	13	60,64,73	2.00	9 (15%)	72,102,113	1.73	12 (16%)
19	CLA	A	840	1	69,73,73	1.75	9 (13%)	83,113,113	1.38	6 (7%)
19	CLA	A	821	1	67,71,73	1.78	9 (13%)	80,110,113	1.38	7 (8%)
19	CLA	g	304	15	54,58,73	1.90	9 (16%)	65,95,113	1.53	11 (16%)
19	CLA	f	311	-	56,60,73	2.00	9 (16%)	67,97,113	1.73	9 (13%)
22	DD6	F	205	-	39,45,45	0.19	0	52,67,67	1.00	5 (9%)
24	LMU	c	301	-	34,35,36	0.43	0	42,45,47	0.85	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	DD6	i	315	-	39,45,45	0.17	0	52,67,67	0.95	3 (5%)
19	CLA	m	308	18	54,58,73	2.02	9 (16%)	65,95,113	1.53	8 (12%)
20	PQN	B	824	-	34,34,34	0.39	0	42,45,45	0.67	1 (2%)
19	CLA	A	853	-	51,55,73	2.06	9 (17%)	61,91,113	1.67	9 (14%)
19	CLA	m	307	18	64,68,73	1.84	9 (14%)	77,107,113	1.46	6 (7%)
22	DD6	d	215	-	39,45,45	0.25	0	52,67,67	0.85	2 (3%)
19	CLA	o	308	-	57,61,73	1.95	9 (15%)	68,98,113	1.53	7 (10%)
19	CLA	A	804	1	69,73,73	1.76	9 (13%)	83,113,113	1.40	8 (9%)
19	CLA	A	845	1	51,55,73	2.09	9 (17%)	61,91,113	1.60	7 (11%)
19	CLA	b	308	10	60,64,73	1.89	9 (15%)	72,102,113	1.45	6 (8%)
19	CLA	i	308	17	55,59,73	1.98	9 (16%)	66,96,113	1.52	6 (9%)
19	CLA	B	810	-	56,61,73	1.99	9 (16%)	70,99,113	1.54	7 (10%)
22	DD6	g	314	-	39,45,45	0.18	0	52,67,67	0.96	1 (1%)
19	CLA	l	204	18	60,64,73	1.90	9 (15%)	72,102,113	1.46	7 (9%)
19	CLA	l	206	-	51,55,73	2.18	9 (17%)	61,91,113	1.69	10 (16%)
23	BCR	B	834	-	41,41,41	0.18	0	56,56,56	0.37	0
28	CHL	k	301	18	52,56,74	1.41	7 (13%)	58,92,114	2.01	13 (22%)
19	CLA	A	850	1	69,73,73	1.79	9 (13%)	83,113,113	1.38	7 (8%)
19	CLA	j	304	15	64,68,73	1.82	9 (14%)	77,107,113	1.47	11 (14%)
19	CLA	a	302	9	51,55,73	2.03	9 (17%)	61,91,113	1.72	10 (16%)
22	DD6	k	313	-	39,45,45	0.18	0	52,67,67	0.88	2 (3%)
26	SF4	C	802	-	0,12,12	-	-	-		
19	CLA	A	813	-	64,68,73	1.86	9 (14%)	77,107,113	1.49	8 (10%)
19	CLA	B	840	2	51,55,73	2.13	9 (17%)	61,91,113	1.78	9 (14%)
22	DD6	d	214	-	39,45,45	0.18	0	52,67,67	0.84	2 (3%)
19	CLA	g	311	-	51,55,73	2.11	9 (17%)	61,91,113	1.71	8 (13%)
28	CHL	c	313	-	60,64,74	1.35	7 (11%)	68,102,114	1.93	15 (22%)
22	DD6	e	314	-	39,45,45	0.16	0	52,67,67	0.53	1 (1%)
19	CLA	e	311	13	59,63,73	1.92	9 (15%)	71,101,113	1.47	7 (9%)
19	CLA	j	306	15	51,55,73	2.14	9 (17%)	61,91,113	1.70	10 (16%)
19	CLA	h	207	-	51,55,73	2.05	9 (17%)	61,91,113	1.57	7 (11%)
19	CLA	d	210	-	64,68,73	1.86	9 (14%)	77,107,113	1.46	7 (9%)
28	CHL	o	301	16	52,56,74	1.46	6 (11%)	58,92,114	2.12	12 (20%)
19	CLA	d	208	-	64,68,73	1.77	9 (14%)	77,107,113	1.51	9 (11%)
22	DD6	j	315	-	39,45,45	0.20	0	52,67,67	0.90	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LMU	a	319	-	35,35,36	0.42	0	43,45,47	0.72	1 (2%)
19	CLA	k	303	-	51,55,73	2.07	9 (17%)	61,91,113	1.59	8 (13%)
19	CLA	c	307	-	59,63,73	1.91	9 (15%)	71,101,113	1.45	7 (9%)
19	CLA	e	307	13	64,68,73	1.84	9 (14%)	77,107,113	1.53	8 (10%)
19	CLA	b	307	10	64,68,73	1.83	9 (14%)	77,107,113	1.45	7 (9%)
19	CLA	h	210	-	51,55,73	2.07	9 (17%)	61,91,113	1.59	7 (11%)
22	DD6	h	214	-	39,45,45	0.16	0	52,67,67	0.92	2 (3%)
19	CLA	i	302	-	59,63,73	1.93	9 (15%)	71,101,113	1.50	7 (9%)
19	CLA	B	845	2	51,55,73	2.05	9 (17%)	61,91,113	1.61	8 (13%)
19	CLA	k	304	-	64,68,73	1.87	9 (14%)	77,107,113	1.50	9 (11%)
19	CLA	A	812	1	60,64,73	1.89	9 (15%)	72,102,113	1.43	7 (9%)
19	CLA	A	826	1	54,58,73	1.97	9 (16%)	65,95,113	1.50	7 (10%)
19	CLA	o	304	16	58,62,73	1.92	9 (15%)	69,99,113	1.64	11 (15%)
22	DD6	h	215	-	39,45,45	0.23	0	52,67,67	0.70	1 (1%)
22	DD6	J	802	-	39,45,45	0.22	0	52,67,67	0.96	4 (7%)
19	CLA	j	302	-	59,63,73	1.93	9 (15%)	71,101,113	1.49	8 (11%)
19	CLA	A	818	-	68,72,73	1.78	9 (13%)	81,111,113	1.41	7 (8%)
19	CLA	B	832	2	54,58,73	1.93	9 (16%)	65,95,113	1.66	9 (13%)
23	BCR	A	835	-	40,40,41	0.21	0	54,54,56	0.53	1 (1%)
19	CLA	A	815	-	55,59,73	1.98	9 (16%)	66,96,113	1.51	7 (10%)
19	CLA	A	805	19,1	56,60,73	1.94	9 (16%)	67,97,113	1.63	9 (13%)
19	CLA	a	307	9	59,63,73	1.93	9 (15%)	71,101,113	1.55	7 (9%)
19	CLA	B	849	-	65,69,73	1.81	9 (13%)	78,108,113	1.51	10 (12%)
19	CLA	j	311	-	54,58,73	1.96	9 (16%)	65,95,113	1.54	13 (20%)
19	CLA	o	303	16	52,56,73	2.05	9 (17%)	62,92,113	1.70	8 (12%)
22	DD6	o	314	-	39,45,45	0.15	0	52,67,67	0.90	3 (5%)
25	LMG	f	313	-	26,26,55	0.96	0	34,34,63	1.22	3 (8%)
19	CLA	f	302	-	59,63,73	1.92	9 (15%)	71,101,113	1.46	6 (8%)
19	CLA	A	819	-	68,72,73	1.78	9 (13%)	81,111,113	1.38	10 (12%)
25	LMG	g	312	-	37,37,55	0.92	1 (2%)	45,45,63	1.27	5 (11%)
25	LMG	e	312	-	44,44,55	0.84	1 (2%)	52,52,63	1.14	3 (5%)
22	DD6	k	314	-	39,45,45	0.19	0	52,67,67	1.42	3 (5%)
19	CLA	j	307	15	64,68,73	1.85	9 (14%)	77,107,113	1.56	8 (10%)
22	DD6	c	317	-	39,45,45	0.14	0	52,67,67	0.83	2 (3%)
19	CLA	A	824	-	69,73,73	1.75	9 (13%)	83,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	i	310	17	51,55,73	1.99	9 (17%)	61,91,113	1.59	9 (14%)
19	CLA	f	305	-	54,58,73	2.02	9 (16%)	65,95,113	1.68	8 (12%)
22	DD6	f	315	-	39,45,45	0.18	0	52,67,67	0.91	3 (5%)
19	CLA	k	306	18	51,55,73	2.03	9 (17%)	61,91,113	1.63	9 (14%)
28	CHL	e	304	13	65,69,74	1.32	8 (12%)	74,108,114	1.92	14 (18%)
28	CHL	c	312	-	60,64,74	1.38	7 (11%)	68,102,114	1.91	16 (23%)
19	CLA	B	839	2	69,73,73	1.75	9 (13%)	83,113,113	1.34	7 (8%)
19	CLA	c	314	-	51,55,73	2.06	9 (17%)	61,91,113	1.66	7 (11%)
19	CLA	j	313	15	60,64,73	1.91	9 (15%)	72,102,113	1.52	8 (11%)
27	DGD	B	829	-	63,63,67	0.92	1 (1%)	77,77,81	1.29	5 (6%)
19	CLA	A	817	-	69,73,73	1.77	9 (13%)	83,113,113	1.57	11 (13%)
19	CLA	b	315	-	51,55,73	2.12	9 (17%)	61,91,113	1.82	11 (18%)
19	CLA	A	827	1	55,59,73	1.99	9 (16%)	66,96,113	1.57	6 (9%)
19	CLA	n	201	-	51,55,73	2.03	9 (17%)	61,91,113	1.50	7 (11%)
23	BCR	B	826	-	41,41,41	0.22	0	56,56,56	0.47	0
19	CLA	e	305	13	54,58,73	2.02	9 (16%)	65,95,113	1.63	8 (12%)
19	CLA	b	305	10	51,55,73	1.98	9 (17%)	61,91,113	1.55	10 (16%)
25	LMG	g	316	-	44,44,55	0.76	0	52,52,63	1.29	6 (11%)
19	CLA	g	301	15	52,56,73	1.94	9 (17%)	62,92,113	1.56	9 (14%)
19	CLA	F	201	-	64,68,73	1.79	9 (14%)	77,107,113	1.40	7 (9%)
23	BCR	B	827	-	41,41,41	0.17	0	56,56,56	0.44	0
19	CLA	A	810	1	54,58,73	1.98	9 (16%)	65,95,113	1.52	7 (10%)
19	CLA	k	302	25	60,64,73	1.88	9 (15%)	72,102,113	1.53	9 (12%)
22	DD6	n	210	-	39,45,45	0.18	0	52,67,67	1.41	4 (7%)
21	LHG	A	831	-	48,48,48	0.63	0	51,54,54	1.19	5 (9%)
22	DD6	o	313	-	39,45,45	0.20	0	52,67,67	0.77	2 (3%)
19	CLA	b	313	-	51,55,73	2.07	9 (17%)	61,91,113	1.69	12 (19%)
25	LMG	b	316	19	42,42,55	0.86	0	50,50,63	1.24	5 (10%)
22	DD6	m	312	-	39,45,45	0.20	0	52,67,67	0.95	3 (5%)
19	CLA	b	304	-	59,63,73	1.82	9 (15%)	71,101,113	1.53	10 (14%)
25	LMG	k	312	19	37,37,55	0.92	0	45,45,63	1.12	4 (8%)
19	CLA	h	203	-	59,63,73	1.91	9 (15%)	71,101,113	1.47	6 (8%)
22	DD6	c	318	-	39,45,45	0.19	0	52,67,67	0.73	3 (5%)
25	LMG	A	851	-	34,34,55	0.83	1 (2%)	42,42,63	1.28	6 (14%)
19	CLA	d	204	-	56,60,73	1.98	9 (16%)	67,97,113	1.58	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CHL	a	313	-	52,56,74	1.43	6 (11%)	58,92,114	2.01	14 (24%)
28	CHL	b	312	-	57,61,74	1.43	8 (14%)	64,98,114	2.08	15 (23%)
19	CLA	k	309	-	51,55,73	2.12	9 (17%)	61,91,113	1.72	9 (14%)
19	CLA	l	201	-	51,55,73	2.01	9 (17%)	61,91,113	1.52	10 (16%)
19	CLA	a	309	-	60,64,73	1.90	9 (15%)	72,102,113	1.44	7 (9%)
28	CHL	a	312	-	52,56,74	1.42	6 (11%)	58,92,114	2.02	13 (22%)
23	BCR	A	834	-	41,41,41	0.13	0	56,56,56	0.37	0
19	CLA	a	314	-	51,55,73	2.06	9 (17%)	61,91,113	1.74	9 (14%)
19	CLA	d	206	-	51,55,73	2.01	9 (17%)	61,91,113	1.54	7 (11%)
19	CLA	j	309	-	60,64,73	1.89	9 (15%)	72,102,113	1.41	6 (8%)
19	CLA	o	310	-	51,55,73	2.07	9 (17%)	61,91,113	1.61	8 (13%)
22	DD6	a	320	-	39,45,45	0.21	0	52,67,67	0.95	2 (3%)
22	DD6	b	318	-	39,45,45	0.20	0	52,67,67	0.77	1 (1%)
28	CHL	f	301	14	52,56,74	1.41	7 (13%)	58,92,114	2.00	14 (24%)
22	DD6	A	833	-	39,45,45	0.18	0	52,67,67	0.89	3 (5%)
22	DD6	l	210	-	39,45,45	0.23	0	52,67,67	0.76	1 (1%)
19	CLA	i	311	-	56,60,73	2.00	9 (16%)	67,97,113	1.72	10 (14%)
28	CHL	g	310	-	55,59,74	1.45	7 (12%)	62,96,114	1.82	15 (24%)
19	CLA	m	305	18	64,68,73	1.79	9 (14%)	77,107,113	1.48	8 (10%)
19	CLA	B	822	-	69,73,73	1.76	9 (13%)	83,113,113	1.41	7 (8%)
19	CLA	B	821	-	60,64,73	1.91	9 (15%)	72,102,113	1.49	6 (8%)
19	CLA	h	206	16	51,55,73	2.05	9 (17%)	61,91,113	1.62	7 (11%)
19	CLA	a	303	-	59,63,73	1.92	9 (15%)	71,101,113	1.58	10 (14%)
19	CLA	B	809	2	58,62,73	1.90	9 (15%)	69,99,113	1.45	6 (8%)
19	CLA	B	808	-	69,73,73	1.74	9 (13%)	83,113,113	1.43	8 (9%)
19	CLA	m	311	-	51,55,73	2.06	9 (17%)	61,91,113	1.64	7 (11%)
28	CHL	c	305	11	65,69,74	1.33	7 (10%)	74,108,114	2.05	14 (18%)
19	CLA	B	801	-	68,72,73	1.73	9 (13%)	81,111,113	1.44	8 (9%)
19	CLA	B	813	-	58,62,73	1.95	9 (15%)	69,99,113	1.49	6 (8%)
19	CLA	c	303	-	59,63,73	1.93	9 (15%)	71,101,113	1.49	7 (9%)
19	CLA	e	303	-	51,55,73	2.02	9 (17%)	61,91,113	1.56	9 (14%)
19	CLA	f	303	14	51,55,73	2.04	9 (17%)	61,91,113	1.57	8 (13%)
19	CLA	A	806	1	69,73,73	1.78	9 (13%)	83,113,113	1.51	8 (9%)
19	CLA	d	203	-	51,55,73	2.08	9 (17%)	61,91,113	1.66	9 (14%)
19	CLA	A	816	-	63,67,73	1.80	9 (14%)	75,105,113	1.47	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CHL	f	304	14	60,64,74	1.33	7 (11%)	68,102,114	2.20	16 (23%)

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
22	DD6	f	316	-	-	1/26/80/80	0/3/3/3
23	BCR	B	831	-	-	6/29/63/63	0/2/2/2
19	CLA	g	305	15	-	7/18/94/115	-
19	CLA	h	213	-	-	4/18/94/115	-
28	CHL	e	301	13	-	11/23/99/117	-
19	CLA	J	803	-	-	2/18/94/115	-
19	CLA	B	804	-	-	8/39/115/115	-
19	CLA	n	207	-	-	2/18/94/115	-
19	CLA	B	816	-	-	3/20/96/115	-
26	SF4	B	802	-	-	-	0/6/5/5
19	CLA	B	805	2	-	11/39/115/115	-
19	CLA	n	208	-	-	13/18/94/115	-
19	CLA	a	308	9	-	3/33/109/115	-
19	CLA	B	815	-	-	8/33/109/115	-
19	CLA	A	801	-	-	9/39/115/115	-
19	CLA	B	848	-	-	6/18/94/115	-
25	LMG	c	320	-	-	19/33/53/70	0/1/1/1
19	CLA	k	305	18	-	6/33/109/115	-
19	CLA	f	306	14	-	4/18/94/115	-
19	CLA	B	806	-	-	12/39/115/115	-
19	CLA	b	302	25	-	7/27/103/115	-
19	CLA	j	305	15	-	12/21/97/115	-
22	DD6	m	313	-	-	0/26/80/80	0/3/3/3
19	CLA	n	202	18	-	7/18/94/115	-
19	CLA	k	307	18	-	1/33/109/115	-
19	CLA	B	838	-	-	5/21/97/115	-
28	CHL	b	301	10	-	17/29/105/117	-
19	CLA	h	208	-	-	2/33/109/115	-
19	CLA	B	835	-	-	10/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CHL	i	304	17	-	10/29/105/117	-
19	CLA	i	312	17	-	1/18/94/115	-
25	LMG	i	316	-	-	21/36/56/70	0/1/1/1
28	CHL	b	311	-	-	8/20/96/117	-
19	CLA	l	207	-	-	3/18/94/115	-
25	LMG	a	316	-	-	9/21/41/70	0/1/1/1
22	DD6	e	313	-	-	1/26/80/80	0/3/3/3
19	CLA	A	849	1	-	3/18/94/115	-
19	CLA	A	823	-	-	4/39/115/115	-
19	CLA	i	306	17	-	4/18/94/115	-
19	CLA	B	814	-	-	7/32/108/115	-
19	CLA	l	208	-	-	5/18/94/115	-
19	CLA	j	303	15	-	3/24/100/115	-
19	CLA	D	301	15	-	4/24/100/115	-
19	CLA	F	204	-	-	2/18/94/115	-
19	CLA	B	841	-	-	6/18/94/115	-
19	CLA	c	304	11	-	6/24/100/115	-
22	DD6	b	317	-	-	2/26/80/80	0/3/3/3
19	CLA	A	809	-	-	5/39/115/115	-
19	CLA	A	843	-	-	11/39/115/115	-
19	CLA	n	205	18	-	9/33/109/115	-
19	CLA	l	205	-	-	1/33/109/115	-
20	PQN	A	830	-	-	13/23/43/43	0/2/2/2
19	CLA	k	310	-	-	6/27/103/115	-
19	CLA	d	212	-	-	2/18/94/115	-
19	CLA	B	819	-	-	3/39/115/115	-
19	CLA	l	202	-	-	2/18/94/115	-
23	BCR	B	850	-	-	5/29/63/63	0/2/2/2
19	CLA	B	818	-	-	9/39/115/115	-
19	CLA	A	802	-	-	12/39/115/115	-
19	CLA	B	836	-	-	5/38/114/115	-
19	CLA	A	807	1	-	10/39/115/115	-
19	CLA	B	847	-	-	9/39/115/115	-
19	CLA	A	825	-	-	3/21/97/115	-
19	CLA	A	829	-	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	n	209	-	-	9/18/94/115	-
22	DD6	A	832	-	-	2/26/80/80	0/3/3/3
19	CLA	d	211	-	-	5/33/109/115	-
19	CLA	g	302	-	-	5/27/103/115	-
22	DD6	n	211	-	-	0/26/80/80	0/3/3/3
19	CLA	f	308	14	-	4/23/99/115	-
19	CLA	B	837	-	-	11/21/97/115	-
19	CLA	c	311	-	-	5/18/94/115	-
19	CLA	a	310	-	-	1/21/97/115	-
19	CLA	b	309	-	-	0/21/97/115	-
19	CLA	A	841	1	-	9/39/115/115	-
22	DD6	g	315	-	-	0/26/80/80	0/3/3/3
19	CLA	h	211	-	-	6/23/99/115	-
19	CLA	j	310	-	-	8/18/94/115	-
29	NEX	a	317	-	-	6/27/83/83	0/3/3/3
23	BCR	M	801	-	-	3/29/63/63	0/2/2/2
19	CLA	a	304	-	-	6/18/94/115	-
19	CLA	B	846	2	-	6/18/94/115	-
28	CHL	i	301	17	-	11/20/96/117	-
19	CLA	i	305	-	-	2/18/94/115	-
19	CLA	B	812	2	-	5/38/114/115	-
19	CLA	l	203	18	-	11/33/109/115	-
19	CLA	l	209	-	-	4/18/94/115	-
28	CHL	d	202	12	-	14/20/96/117	-
19	CLA	m	303	-	-	4/18/94/115	-
19	CLA	A	844	-	-	7/39/115/115	-
19	CLA	f	309	-	-	8/33/109/115	-
28	CHL	m	301	18	-	11/20/96/117	-
19	CLA	o	311	-	-	8/21/97/115	-
19	CLA	c	302	11	-	5/18/94/115	-
19	CLA	i	303	-	-	5/18/94/115	-
19	CLA	A	814	-	-	3/18/94/115	-
22	DD6	i	314	-	-	0/26/80/80	0/3/3/3
25	LMG	j	314	-	-	12/32/52/70	0/1/1/1
19	CLA	k	311	-	-	4/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DD6	c	319	-	-	0/26/80/80	0/3/3/3
19	CLA	k	308	18	-	2/21/97/115	-
19	CLA	n	206	18	-	6/18/94/115	-
19	CLA	A	822	-	-	12/39/115/115	-
25	LMG	d	213	-	-	9/26/46/70	0/1/1/1
23	BCR	B	825	-	-	0/29/63/63	0/2/2/2
26	SF4	C	801	-	-	-	0/6/5/5
25	LMG	g	313	-	-	11/28/48/70	0/1/1/1
19	CLA	A	820	-	-	8/27/103/115	-
19	CLA	m	306	18	-	2/18/94/115	-
19	CLA	o	302	-	-	17/27/103/115	-
28	CHL	a	315	9	-	11/20/96/117	-
19	CLA	g	309	-	-	5/29/105/115	-
25	LMG	h	216	-	-	10/30/50/70	0/1/1/1
19	CLA	e	309	-	-	2/18/94/115	-
19	CLA	A	847	1	-	7/18/94/115	-
28	CHL	b	310	-	-	5/20/96/117	-
22	DD6	b	319	-	-	0/26/80/80	0/3/3/3
19	CLA	B	842	-	-	5/18/94/115	-
19	CLA	h	205	16	-	2/33/109/115	-
19	CLA	c	315	11	-	4/18/94/115	-
19	CLA	j	301	-	-	2/18/94/115	-
22	DD6	J	801	-	-	2/26/80/80	0/3/3/3
19	CLA	m	302	-	-	11/18/94/115	-
23	BCR	B	828	-	-	0/29/63/63	0/2/2/2
19	CLA	F	202	-	-	8/30/106/115	-
19	CLA	f	310	-	-	3/18/94/115	-
19	CLA	d	207	-	-	3/18/94/115	-
19	CLA	i	307	17	-	5/26/102/115	-
19	CLA	n	203	18	-	13/33/109/115	-
19	CLA	f	307	14	-	3/26/102/115	-
19	CLA	B	823	-	-	3/18/94/115	-
19	CLA	B	833	2	-	8/29/105/115	-
28	CHL	h	202	16	-	11/20/96/117	-
23	BCR	A	837	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	g	307	15	-	4/33/109/115	-
19	CLA	A	848	1	-	8/21/97/115	-
19	CLA	b	303	-	-	7/23/99/115	-
22	DD6	j	316	-	-	0/26/80/80	0/3/3/3
19	CLA	B	843	-	-	3/18/94/115	-
25	LMG	a	318	-	-	20/35/55/70	0/1/1/1
19	CLA	o	309	-	-	7/18/94/115	-
19	CLA	d	209	12	-	6/29/105/115	-
22	DD6	l	211	-	-	0/26/80/80	0/3/3/3
19	CLA	A	811	19	-	7/35/111/115	-
19	CLA	f	312	-	-	6/18/94/115	-
19	CLA	B	803	-	-	9/39/115/115	-
28	CHL	b	314	-	-	13/25/101/117	-
28	CHL	a	311	-	-	5/20/96/117	-
19	CLA	c	310	-	-	3/21/97/115	-
19	CLA	d	201	-	-	1/18/94/115	-
19	CLA	A	852	-	-	6/27/103/115	-
19	CLA	j	308	15	-	9/33/109/115	-
19	CLA	B	830	2	-	11/31/107/115	-
19	CLA	f	314	14	-	9/27/103/115	-
19	CLA	h	209	16	-	9/33/109/115	-
19	CLA	h	201	-	-	6/29/105/115	-
19	CLA	c	306	11	-	10/29/105/115	-
19	CLA	c	309	11	-	5/29/105/115	-
19	CLA	e	306	13	-	6/27/103/115	-
19	CLA	b	306	10	-	18/33/109/115	-
22	DD6	a	321	-	-	0/26/80/80	0/3/3/3
28	CHL	d	205	12	-	18/29/105/117	-
19	CLA	h	212	-	-	7/29/105/115	-
19	CLA	A	808	1	-	1/21/97/115	-
19	CLA	m	310	-	-	8/27/103/115	-
19	CLA	a	305	9	-	9/33/109/115	-
19	CLA	B	807	2	-	14/39/115/115	-
19	CLA	e	302	-	-	6/27/103/115	-
19	CLA	B	811	2	-	13/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	839	-	-	4/19/95/115	-
25	LMG	a	301	-	-	18/35/55/70	0/1/1/1
28	CHL	g	303	15	-	10/29/105/117	-
19	CLA	c	316	11	-	8/39/115/115	-
19	CLA	A	846	1	-	5/18/94/115	-
19	CLA	o	307	-	-	12/33/109/115	-
19	CLA	B	844	2	-	4/18/94/115	-
19	CLA	A	828	-	-	9/39/115/115	-
19	CLA	F	203	-	-	24/39/115/115	-
19	CLA	c	308	-	-	2/30/106/115	-
19	CLA	i	309	-	-	14/33/109/115	-
19	CLA	i	313	17	-	8/24/100/115	-
19	CLA	a	306	9	-	11/24/100/115	-
23	BCR	A	836	-	-	2/29/63/63	0/2/2/2
19	CLA	B	817	-	-	12/36/112/115	-
19	CLA	m	304	-	-	5/18/94/115	-
19	CLA	j	312	-	-	4/18/94/115	-
19	CLA	g	308	-	-	4/29/105/115	-
19	CLA	m	309	-	-	10/18/94/115	-
19	CLA	o	312	16	-	3/18/94/115	-
19	CLA	e	310	-	-	11/27/103/115	-
19	CLA	h	204	16	-	3/19/95/115	-
19	CLA	B	820	2	-	8/35/111/115	-
19	CLA	o	306	-	-	7/18/94/115	-
23	BCR	J	804	-	-	0/29/63/63	0/2/2/2
24	LMU	A	838	-	-	6/21/57/61	0/2/2/2
19	CLA	o	305	-	-	7/18/94/115	-
28	CHL	g	306	15	-	9/29/105/117	-
19	CLA	A	842	1	-	20/39/115/115	-
19	CLA	A	803	-	-	5/39/115/115	-
19	CLA	n	204	-	-	7/29/105/115	-
19	CLA	e	308	13	-	7/29/105/115	-
19	CLA	A	840	1	-	9/39/115/115	-
19	CLA	A	821	1	-	5/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	g	304	15	-	6/21/97/115	-
19	CLA	f	311	-	-	5/24/100/115	-
22	DD6	F	205	-	-	2/26/80/80	0/3/3/3
24	LMU	c	301	-	-	3/21/57/61	0/2/2/2
22	DD6	i	315	-	-	1/26/80/80	0/3/3/3
19	CLA	m	308	18	-	7/21/97/115	-
20	PQN	B	824	-	-	5/23/43/43	0/2/2/2
19	CLA	A	853	-	-	8/18/94/115	-
19	CLA	m	307	18	-	7/33/109/115	-
22	DD6	d	215	-	-	0/26/80/80	0/3/3/3
19	CLA	o	308	-	-	4/25/101/115	-
19	CLA	A	804	1	-	8/39/115/115	-
19	CLA	A	845	1	-	0/18/94/115	-
19	CLA	b	308	10	-	4/29/105/115	-
19	CLA	i	308	17	-	8/23/99/115	-
19	CLA	B	810	-	-	8/23/99/115	-
22	DD6	g	314	-	-	1/26/80/80	0/3/3/3
19	CLA	l	204	18	-	6/29/105/115	-
19	CLA	l	206	-	-	7/18/94/115	-
23	BCR	B	834	-	-	4/29/63/63	0/2/2/2
28	CHL	k	301	18	-	15/20/96/117	-
19	CLA	A	850	1	-	9/39/115/115	-
19	CLA	j	304	15	-	14/33/109/115	-
19	CLA	a	302	9	-	11/18/94/115	-
22	DD6	k	313	-	-	1/26/80/80	0/3/3/3
26	SF4	C	802	-	-	-	0/6/5/5
19	CLA	A	813	-	-	5/33/109/115	-
19	CLA	B	840	2	-	7/18/94/115	-
22	DD6	d	214	-	-	0/26/80/80	0/3/3/3
19	CLA	g	311	-	-	5/18/94/115	-
28	CHL	c	313	-	-	9/29/105/117	-
22	DD6	e	314	-	-	0/26/80/80	0/3/3/3
19	CLA	e	311	13	-	5/27/103/115	-
19	CLA	j	306	15	-	7/18/94/115	-
19	CLA	h	207	-	-	3/18/94/115	-
19	CLA	d	210	-	-	6/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CHL	o	301	16	-	9/20/96/117	-
19	CLA	d	208	-	-	11/33/109/115	-
22	DD6	j	315	-	-	0/26/80/80	0/3/3/3
24	LMU	a	319	-	-	10/21/57/61	1/2/2/2
19	CLA	k	303	-	-	3/18/94/115	-
19	CLA	c	307	-	-	10/27/103/115	-
19	CLA	e	307	13	-	5/33/109/115	-
19	CLA	b	307	10	-	2/33/109/115	-
19	CLA	h	210	-	-	0/18/94/115	-
22	DD6	h	214	-	-	0/26/80/80	0/3/3/3
19	CLA	i	302	-	-	7/27/103/115	-
19	CLA	B	845	2	-	4/18/94/115	-
19	CLA	k	304	-	-	10/33/109/115	-
19	CLA	A	812	1	-	3/29/105/115	-
19	CLA	A	826	1	-	3/21/97/115	-
19	CLA	o	304	16	-	16/26/102/115	-
22	DD6	h	215	-	-	1/26/80/80	0/3/3/3
22	DD6	J	802	-	-	3/26/80/80	0/3/3/3
19	CLA	j	302	-	-	7/27/103/115	-
19	CLA	A	818	-	-	4/38/114/115	-
19	CLA	B	832	2	-	7/21/97/115	-
23	BCR	A	835	-	-	5/27/61/63	0/2/2/2
19	CLA	A	815	-	-	4/23/99/115	-
19	CLA	A	805	19,1	-	3/24/100/115	-
19	CLA	a	307	9	-	4/27/103/115	-
19	CLA	B	849	-	-	16/35/111/115	-
19	CLA	j	311	-	-	5/21/97/115	-
19	CLA	o	303	16	-	11/19/95/115	-
22	DD6	o	314	-	-	1/26/80/80	0/3/3/3
25	LMG	f	313	-	-	10/20/40/70	0/1/1/1
19	CLA	f	302	-	-	4/27/103/115	-
19	CLA	A	819	-	-	5/37/113/115	-
25	LMG	g	312	-	-	13/32/52/70	0/1/1/1
25	LMG	e	312	-	-	18/39/59/70	0/1/1/1
22	DD6	k	314	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	j	307	15	-	7/33/109/115	-
22	DD6	c	317	-	-	1/26/80/80	0/3/3/3
19	CLA	A	824	-	-	7/39/115/115	-
19	CLA	i	310	17	-	12/18/94/115	-
19	CLA	f	305	-	-	2/21/97/115	-
22	DD6	f	315	-	-	0/26/80/80	0/3/3/3
19	CLA	k	306	18	-	4/18/94/115	-
28	CHL	e	304	13	-	18/35/111/117	-
28	CHL	c	312	-	-	19/29/105/117	-
19	CLA	B	839	2	-	10/39/115/115	-
19	CLA	c	314	-	-	6/18/94/115	-
19	CLA	j	313	15	-	4/29/105/115	-
27	DGD	B	829	-	-	25/51/91/95	0/2/2/2
19	CLA	A	817	-	-	7/39/115/115	-
19	CLA	b	315	-	-	10/18/94/115	-
19	CLA	A	827	1	-	6/23/99/115	-
19	CLA	n	201	-	-	6/18/94/115	-
23	BCR	B	826	-	-	8/29/63/63	0/2/2/2
19	CLA	e	305	13	-	1/21/97/115	-
19	CLA	b	305	10	-	3/18/94/115	-
25	LMG	g	316	-	-	30/39/59/70	0/1/1/1
19	CLA	g	301	15	-	3/19/95/115	-
19	CLA	F	201	-	-	6/33/109/115	-
23	BCR	B	827	-	-	2/29/63/63	0/2/2/2
19	CLA	A	810	1	-	5/21/97/115	-
19	CLA	k	302	25	-	12/29/105/115	-
22	DD6	n	210	-	-	2/26/80/80	0/3/3/3
21	LHG	A	831	-	-	19/53/53/53	-
22	DD6	o	313	-	-	0/26/80/80	0/3/3/3
19	CLA	b	313	-	-	8/18/94/115	-
25	LMG	b	316	19	-	13/37/57/70	0/1/1/1
22	DD6	m	312	-	-	1/26/80/80	0/3/3/3
19	CLA	b	304	-	-	8/27/103/115	-
25	LMG	k	312	19	-	10/32/52/70	0/1/1/1
19	CLA	h	203	-	-	2/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DD6	c	318	-	-	1/26/80/80	0/3/3/3
25	LMG	A	851	-	-	13/29/49/70	0/1/1/1
19	CLA	d	204	-	-	5/24/100/115	-
28	CHL	a	313	-	-	9/20/96/117	-
28	CHL	b	312	-	-	12/26/102/117	-
19	CLA	k	309	-	-	3/18/94/115	-
19	CLA	l	201	-	-	5/18/94/115	-
19	CLA	a	309	-	-	2/29/105/115	-
28	CHL	a	312	-	-	8/20/96/117	-
23	BCR	A	834	-	-	0/29/63/63	0/2/2/2
19	CLA	a	314	-	-	8/18/94/115	-
19	CLA	d	206	-	-	3/18/94/115	-
19	CLA	j	309	-	-	6/29/105/115	-
19	CLA	o	310	-	-	4/18/94/115	-
22	DD6	a	320	-	-	0/26/80/80	0/3/3/3
22	DD6	b	318	-	-	0/26/80/80	0/3/3/3
28	CHL	f	301	14	-	11/20/96/117	-
22	DD6	A	833	-	-	1/26/80/80	0/3/3/3
22	DD6	l	210	-	-	1/26/80/80	0/3/3/3
19	CLA	i	311	-	-	6/24/100/115	-
28	CHL	g	310	-	-	13/23/99/117	-
19	CLA	m	305	18	-	7/33/109/115	-
19	CLA	B	822	-	-	10/39/115/115	-
19	CLA	B	821	-	-	7/29/105/115	-
19	CLA	h	206	16	-	2/18/94/115	-
19	CLA	a	303	-	-	12/27/103/115	-
19	CLA	B	809	2	-	4/26/102/115	-
19	CLA	B	808	-	-	8/39/115/115	-
19	CLA	m	311	-	-	7/18/94/115	-
28	CHL	c	305	11	-	13/35/111/117	-
19	CLA	B	801	-	-	11/38/114/115	-
19	CLA	B	813	-	-	5/25/101/115	-
19	CLA	c	303	-	-	6/27/103/115	-
19	CLA	e	303	-	-	2/18/94/115	-
19	CLA	f	303	14	-	3/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	806	1	-	16/39/115/115	-
19	CLA	d	203	-	-	4/18/94/115	-
19	CLA	A	816	-	-	7/32/108/115	-
28	CHL	f	304	14	-	11/29/105/117	-

All (2390) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	o	311	CLA	C1D-ND	7.75	1.47	1.37
19	A	819	CLA	C1D-ND	7.71	1.47	1.37
19	k	311	CLA	C1D-ND	7.67	1.47	1.37
19	B	842	CLA	C1D-ND	7.64	1.47	1.37
19	B	830	CLA	C1D-ND	7.61	1.47	1.37
19	c	316	CLA	C1D-ND	7.60	1.47	1.37
19	B	836	CLA	C1D-ND	7.60	1.47	1.37
19	A	853	CLA	C1D-ND	7.58	1.47	1.37
19	n	201	CLA	C1D-ND	7.58	1.47	1.37
19	A	826	CLA	C1D-ND	7.57	1.47	1.37
19	i	309	CLA	C1D-ND	7.56	1.47	1.37
19	c	304	CLA	C1D-ND	7.56	1.47	1.37
19	b	303	CLA	C1D-ND	7.55	1.47	1.37
19	c	306	CLA	C1D-ND	7.53	1.47	1.37
19	e	303	CLA	C1D-ND	7.51	1.47	1.37
19	c	315	CLA	C1D-ND	7.51	1.47	1.37
19	b	308	CLA	C1D-ND	7.51	1.47	1.37
19	e	311	CLA	C1D-ND	7.49	1.47	1.37
19	j	311	CLA	C1D-ND	7.49	1.47	1.37
19	F	204	CLA	C1D-ND	7.49	1.47	1.37
19	f	303	CLA	C1D-ND	7.49	1.47	1.37
19	m	306	CLA	C1D-ND	7.48	1.47	1.37
19	D	301	CLA	C1D-ND	7.48	1.47	1.37
19	i	303	CLA	C1D-ND	7.48	1.47	1.37
19	h	204	CLA	C1D-ND	7.46	1.47	1.37
19	a	303	CLA	C1D-ND	7.46	1.47	1.37
19	h	210	CLA	C1D-ND	7.45	1.46	1.37
19	d	204	CLA	C1D-ND	7.45	1.46	1.37
19	k	303	CLA	C1D-ND	7.44	1.46	1.37
19	i	306	CLA	C1D-ND	7.44	1.46	1.37
19	a	309	CLA	C1D-ND	7.43	1.46	1.37
19	d	203	CLA	C1D-ND	7.42	1.46	1.37
19	B	835	CLA	C1D-ND	7.41	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	839	CLA	C1D-ND	7.40	1.46	1.37
19	e	306	CLA	C1D-ND	7.39	1.46	1.37
19	A	839	CLA	C1D-ND	7.39	1.46	1.37
19	l	208	CLA	C1D-ND	7.39	1.46	1.37
19	d	201	CLA	C1D-ND	7.39	1.46	1.37
19	A	810	CLA	C1D-ND	7.38	1.46	1.37
19	h	212	CLA	C1D-ND	7.38	1.46	1.37
19	b	302	CLA	C1D-ND	7.37	1.46	1.37
19	g	302	CLA	C1D-ND	7.37	1.46	1.37
19	g	307	CLA	C1D-ND	7.36	1.46	1.37
19	d	209	CLA	C1D-ND	7.36	1.46	1.37
19	j	302	CLA	C1D-ND	7.35	1.46	1.37
19	j	306	CLA	C1D-ND	7.35	1.46	1.37
19	d	211	CLA	C1D-ND	7.35	1.46	1.37
19	j	309	CLA	C1D-ND	7.35	1.46	1.37
19	A	812	CLA	C1D-ND	7.34	1.46	1.37
19	m	303	CLA	C1D-ND	7.34	1.46	1.37
19	o	310	CLA	C1D-ND	7.34	1.46	1.37
19	A	821	CLA	C1D-ND	7.34	1.46	1.37
19	B	810	CLA	C1D-ND	7.33	1.46	1.37
19	B	805	CLA	C1D-ND	7.33	1.46	1.37
19	g	305	CLA	C1D-ND	7.33	1.46	1.37
19	g	308	CLA	C1D-ND	7.33	1.46	1.37
19	c	307	CLA	C1D-ND	7.32	1.46	1.37
19	k	306	CLA	C1D-ND	7.32	1.46	1.37
19	i	308	CLA	C1D-ND	7.32	1.46	1.37
19	A	845	CLA	C1D-ND	7.31	1.46	1.37
19	d	212	CLA	C1D-ND	7.31	1.46	1.37
19	h	211	CLA	C1D-ND	7.31	1.46	1.37
19	j	313	CLA	C1D-ND	7.31	1.46	1.37
19	l	204	CLA	C1D-ND	7.31	1.46	1.37
19	B	833	CLA	C1D-ND	7.31	1.46	1.37
19	o	308	CLA	C1D-ND	7.30	1.46	1.37
19	d	210	CLA	C1D-ND	7.30	1.46	1.37
19	A	808	CLA	C1D-ND	7.30	1.46	1.37
19	A	806	CLA	C1D-ND	7.30	1.46	1.37
19	a	304	CLA	C1D-ND	7.30	1.46	1.37
19	A	849	CLA	C1D-ND	7.30	1.46	1.37
19	j	303	CLA	C1D-ND	7.30	1.46	1.37
19	B	819	CLA	C1D-ND	7.30	1.46	1.37
19	h	209	CLA	C1D-ND	7.29	1.46	1.37
19	a	307	CLA	C1D-ND	7.29	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	841	CLA	C1D-ND	7.29	1.46	1.37
19	b	313	CLA	C1D-ND	7.29	1.46	1.37
19	A	816	CLA	C1D-ND	7.29	1.46	1.37
19	k	308	CLA	C1D-ND	7.28	1.46	1.37
19	b	306	CLA	C1D-ND	7.28	1.46	1.37
19	A	844	CLA	C1D-ND	7.28	1.46	1.37
19	o	312	CLA	C1D-ND	7.28	1.46	1.37
19	f	310	CLA	C1D-ND	7.27	1.46	1.37
19	B	841	CLA	C1D-ND	7.26	1.46	1.37
19	B	806	CLA	C1D-ND	7.26	1.46	1.37
19	A	804	CLA	C1D-ND	7.26	1.46	1.37
19	B	811	CLA	C1D-ND	7.26	1.46	1.37
19	B	844	CLA	C1D-ND	7.26	1.46	1.37
19	a	310	CLA	C1D-ND	7.25	1.46	1.37
19	d	207	CLA	C1D-ND	7.25	1.46	1.37
19	i	307	CLA	C1D-ND	7.25	1.46	1.37
19	n	205	CLA	C1D-ND	7.25	1.46	1.37
19	e	309	CLA	C1D-ND	7.24	1.46	1.37
19	k	310	CLA	C1D-ND	7.23	1.46	1.37
19	f	308	CLA	C1D-ND	7.23	1.46	1.37
19	i	302	CLA	C1D-ND	7.23	1.46	1.37
19	A	824	CLA	C1D-ND	7.22	1.46	1.37
19	g	311	CLA	C1D-ND	7.22	1.46	1.37
19	m	310	CLA	C1D-ND	7.22	1.46	1.37
19	c	303	CLA	C1D-ND	7.22	1.46	1.37
19	l	206	CLA	C1D-ND	7.21	1.46	1.37
19	j	308	CLA	C1D-ND	7.21	1.46	1.37
19	k	309	CLA	C1D-ND	7.21	1.46	1.37
19	A	814	CLA	C1D-ND	7.21	1.46	1.37
19	f	302	CLA	C1D-ND	7.20	1.46	1.37
19	g	309	CLA	C1D-ND	7.20	1.46	1.37
19	B	849	CLA	C1D-ND	7.20	1.46	1.37
19	B	818	CLA	C1D-ND	7.20	1.46	1.37
19	B	814	CLA	C1D-ND	7.19	1.46	1.37
19	c	302	CLA	C1D-ND	7.19	1.46	1.37
19	c	310	CLA	C1D-ND	7.19	1.46	1.37
19	h	207	CLA	C1D-ND	7.19	1.46	1.37
19	A	818	CLA	C1D-ND	7.18	1.46	1.37
19	B	813	CLA	C1D-ND	7.18	1.46	1.37
19	B	848	CLA	C1D-ND	7.17	1.46	1.37
19	f	306	CLA	C1D-ND	7.17	1.46	1.37
19	c	309	CLA	C1D-ND	7.17	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	l	205	CLA	C1D-ND	7.16	1.46	1.37
19	f	312	CLA	C1D-ND	7.16	1.46	1.37
19	A	850	CLA	C1D-ND	7.16	1.46	1.37
19	A	815	CLA	C1D-ND	7.16	1.46	1.37
19	o	305	CLA	C1D-ND	7.16	1.46	1.37
19	A	852	CLA	C1D-ND	7.16	1.46	1.37
19	c	308	CLA	C1D-ND	7.15	1.46	1.37
19	A	813	CLA	C1D-ND	7.15	1.46	1.37
19	h	203	CLA	C1D-ND	7.15	1.46	1.37
19	B	809	CLA	C1D-ND	7.15	1.46	1.37
19	h	201	CLA	C1D-ND	7.14	1.46	1.37
19	B	847	CLA	C1D-ND	7.14	1.46	1.37
19	l	207	CLA	C1D-ND	7.14	1.46	1.37
19	c	314	CLA	C1D-ND	7.14	1.46	1.37
19	e	302	CLA	C1D-ND	7.14	1.46	1.37
19	o	306	CLA	C1D-ND	7.14	1.46	1.37
19	e	305	CLA	C1D-ND	7.13	1.46	1.37
19	l	201	CLA	C1D-ND	7.12	1.46	1.37
19	b	307	CLA	C1D-ND	7.11	1.46	1.37
19	m	307	CLA	C1D-ND	7.11	1.46	1.37
19	A	807	CLA	C1D-ND	7.10	1.46	1.37
19	l	209	CLA	C1D-ND	7.10	1.46	1.37
19	m	308	CLA	C1D-ND	7.10	1.46	1.37
19	B	821	CLA	C1D-ND	7.10	1.46	1.37
19	B	843	CLA	C1D-ND	7.10	1.46	1.37
19	F	203	CLA	C1D-ND	7.10	1.46	1.37
19	i	312	CLA	C1D-ND	7.10	1.46	1.37
19	m	311	CLA	C1D-ND	7.10	1.46	1.37
19	B	807	CLA	C1D-ND	7.09	1.46	1.37
19	A	829	CLA	C1D-ND	7.09	1.46	1.37
19	F	202	CLA	C1D-ND	7.08	1.46	1.37
19	A	809	CLA	C1D-ND	7.08	1.46	1.37
19	f	309	CLA	C1D-ND	7.07	1.46	1.37
19	e	307	CLA	C1D-ND	7.07	1.46	1.37
19	n	204	CLA	C1D-ND	7.07	1.46	1.37
19	B	812	CLA	C1D-ND	7.06	1.46	1.37
19	A	827	CLA	C1D-ND	7.06	1.46	1.37
19	n	207	CLA	C1D-ND	7.05	1.46	1.37
19	k	305	CLA	C1D-ND	7.05	1.46	1.37
19	B	837	CLA	C1D-ND	7.04	1.46	1.37
19	A	840	CLA	C1D-ND	7.04	1.46	1.37
19	A	847	CLA	C1D-ND	7.04	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	311	CLA	C1D-ND	7.04	1.46	1.37
19	B	822	CLA	C1D-ND	7.04	1.46	1.37
19	b	309	CLA	C1D-ND	7.03	1.46	1.37
19	e	308	CLA	C1D-ND	7.03	1.46	1.37
19	B	845	CLA	C1D-ND	7.01	1.46	1.37
19	A	848	CLA	C1D-ND	7.01	1.46	1.37
19	h	208	CLA	C1D-ND	7.00	1.46	1.37
19	m	305	CLA	C1D-ND	7.00	1.46	1.37
19	a	305	CLA	C1D-ND	6.99	1.46	1.37
19	d	206	CLA	C1D-ND	6.99	1.46	1.37
19	l	202	CLA	C1D-ND	6.98	1.46	1.37
19	o	304	CLA	C1D-ND	6.98	1.46	1.37
19	B	840	CLA	C1D-ND	6.97	1.46	1.37
19	n	202	CLA	C1D-ND	6.96	1.46	1.37
19	A	843	CLA	C1D-ND	6.96	1.46	1.37
19	f	307	CLA	C1D-ND	6.95	1.46	1.37
19	a	308	CLA	C1D-ND	6.94	1.46	1.37
19	a	306	CLA	C1D-ND	6.94	1.46	1.37
19	A	846	CLA	C1D-ND	6.94	1.46	1.37
19	B	820	CLA	C1D-ND	6.94	1.46	1.37
19	J	803	CLA	C1D-ND	6.93	1.46	1.37
19	i	311	CLA	C1D-ND	6.93	1.46	1.37
19	A	823	CLA	C1D-ND	6.93	1.46	1.37
19	k	304	CLA	C1D-ND	6.92	1.46	1.37
19	A	805	CLA	C1D-ND	6.92	1.46	1.37
19	A	817	CLA	C1D-ND	6.91	1.46	1.37
19	B	838	CLA	C1D-ND	6.91	1.46	1.37
19	A	825	CLA	C1D-ND	6.91	1.46	1.37
19	B	817	CLA	C1D-ND	6.91	1.46	1.37
19	n	209	CLA	C1D-ND	6.91	1.46	1.37
19	A	828	CLA	C1D-ND	6.90	1.46	1.37
19	j	312	CLA	C1D-ND	6.90	1.46	1.37
19	B	823	CLA	C1D-ND	6.90	1.46	1.37
19	k	307	CLA	C1D-ND	6.90	1.46	1.37
19	o	307	CLA	C1D-ND	6.89	1.46	1.37
19	a	314	CLA	C1D-ND	6.89	1.46	1.37
19	h	213	CLA	C1D-ND	6.88	1.46	1.37
19	f	305	CLA	C1D-ND	6.87	1.46	1.37
19	A	820	CLA	C1D-ND	6.87	1.46	1.37
19	j	301	CLA	C1D-ND	6.87	1.46	1.37
19	A	811	CLA	C1D-ND	6.86	1.46	1.37
19	B	815	CLA	C1D-ND	6.85	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	o	309	CLA	C1D-ND	6.85	1.46	1.37
19	n	206	CLA	MG-NB	-6.85	1.92	2.05
19	o	303	CLA	C1D-ND	6.85	1.46	1.37
19	d	208	CLA	C1D-ND	6.82	1.46	1.37
19	h	206	CLA	C1D-ND	6.82	1.46	1.37
19	f	311	CLA	C1D-ND	6.82	1.46	1.37
19	o	302	CLA	C1D-ND	6.80	1.46	1.37
19	B	816	CLA	C1D-ND	6.79	1.46	1.37
19	j	304	CLA	C1D-ND	6.79	1.46	1.37
19	i	313	CLA	C1D-ND	6.79	1.46	1.37
19	F	201	CLA	C1D-ND	6.78	1.46	1.37
19	a	302	CLA	C1D-ND	6.77	1.46	1.37
19	l	203	CLA	C1D-ND	6.77	1.46	1.37
19	i	305	CLA	C1D-ND	6.75	1.46	1.37
19	B	804	CLA	C1D-ND	6.74	1.46	1.37
19	b	305	CLA	C1D-ND	6.73	1.46	1.37
19	e	310	CLA	C1D-ND	6.72	1.46	1.37
19	f	314	CLA	C1D-ND	6.72	1.46	1.37
19	h	205	CLA	C1D-ND	6.70	1.46	1.37
19	m	309	CLA	C1D-ND	6.69	1.46	1.37
19	j	310	CLA	C1D-ND	6.67	1.46	1.37
19	A	822	CLA	C1D-ND	6.64	1.45	1.37
19	b	315	CLA	C1D-ND	6.64	1.45	1.37
19	B	803	CLA	C1D-ND	6.63	1.45	1.37
19	j	307	CLA	C1D-ND	6.59	1.45	1.37
19	n	208	CLA	MG-ND	-6.59	1.92	2.05
19	m	302	CLA	C1D-ND	6.57	1.45	1.37
19	n	203	CLA	C1D-ND	6.56	1.45	1.37
19	B	846	CLA	MG-ND	-6.54	1.92	2.05
19	k	302	CLA	C1D-ND	6.54	1.45	1.37
19	B	832	CLA	C1D-ND	6.53	1.45	1.37
19	B	846	CLA	MG-NB	-6.53	1.92	2.05
19	m	304	CLA	MG-NA	-6.52	1.90	2.06
19	i	310	CLA	C1D-ND	6.52	1.45	1.37
19	j	305	CLA	C1D-ND	6.50	1.45	1.37
19	A	803	CLA	C1D-ND	6.47	1.45	1.37
19	B	801	CLA	C1D-ND	6.44	1.45	1.37
19	A	842	CLA	C1D-ND	6.44	1.45	1.37
19	B	808	CLA	C1D-ND	6.44	1.45	1.37
19	n	206	CLA	MG-NA	-6.42	1.91	2.06
19	m	304	CLA	C1D-ND	6.39	1.45	1.37
19	n	206	CLA	C1D-ND	6.36	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	l	206	CLA	MG-NB	-6.31	1.93	2.05
19	m	304	CLA	MG-ND	-6.30	1.93	2.05
19	A	802	CLA	C1D-ND	6.29	1.45	1.37
19	n	206	CLA	MG-ND	-6.28	1.93	2.05
19	A	801	CLA	MG-ND	-6.21	1.93	2.05
19	A	802	CLA	MG-ND	-6.20	1.93	2.05
19	o	302	CLA	MG-NA	-6.18	1.91	2.06
19	n	208	CLA	C1D-ND	6.15	1.45	1.37
19	j	306	CLA	MG-ND	-6.12	1.93	2.05
19	B	801	CLA	MG-ND	-6.10	1.93	2.05
19	g	301	CLA	C1D-ND	6.06	1.45	1.37
19	B	804	CLA	MG-ND	-6.05	1.93	2.05
19	b	315	CLA	MG-NB	-6.04	1.93	2.05
19	l	206	CLA	MG-ND	-6.04	1.93	2.05
19	A	803	CLA	MG-ND	-6.03	1.93	2.05
19	o	312	CLA	C1B-NB	6.03	1.45	1.37
19	e	308	CLA	MG-NB	-6.03	1.93	2.05
19	e	305	CLA	C1B-NB	6.02	1.45	1.37
19	o	309	CLA	MG-ND	-6.02	1.93	2.05
19	g	304	CLA	C1D-ND	6.02	1.45	1.37
19	m	302	CLA	MG-NB	-6.01	1.93	2.05
19	n	209	CLA	MG-ND	-6.01	1.93	2.05
19	b	315	CLA	MG-NA	-6.00	1.92	2.06
19	e	308	CLA	MG-NA	-5.96	1.92	2.06
19	A	843	CLA	C1B-NB	5.96	1.45	1.37
19	o	302	CLA	MG-ND	-5.96	1.94	2.05
19	A	843	CLA	MG-NA	-5.95	1.92	2.06
19	A	801	CLA	C1D-ND	5.95	1.45	1.37
19	k	309	CLA	C1B-NB	5.93	1.45	1.37
19	h	205	CLA	MG-ND	-5.93	1.94	2.05
19	d	203	CLA	C1B-NB	5.93	1.45	1.37
19	B	847	CLA	C1B-NB	5.93	1.45	1.37
19	b	304	CLA	C1D-ND	5.93	1.45	1.37
19	m	303	CLA	C1B-NB	5.93	1.45	1.37
19	b	302	CLA	C1B-NB	5.91	1.45	1.37
19	j	304	CLA	MG-ND	-5.91	1.94	2.05
19	o	307	CLA	C1B-NB	5.90	1.45	1.37
19	B	803	CLA	MG-ND	-5.89	1.94	2.05
19	l	202	CLA	C1B-NB	5.89	1.45	1.37
19	A	804	CLA	C1B-NB	5.89	1.45	1.37
19	n	207	CLA	C1B-NB	5.89	1.45	1.37
19	n	203	CLA	MG-ND	-5.88	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	822	CLA	MG-ND	-5.88	1.94	2.05
19	n	205	CLA	C1B-NB	5.87	1.45	1.37
19	a	308	CLA	C1B-NB	5.87	1.45	1.37
19	f	302	CLA	C1B-NB	5.87	1.45	1.37
19	B	840	CLA	MG-ND	-5.87	1.94	2.05
19	f	309	CLA	C1B-NB	5.86	1.45	1.37
19	m	304	CLA	MG-NB	-5.86	1.94	2.05
19	f	307	CLA	C1B-NB	5.86	1.45	1.37
19	c	314	CLA	C1B-NB	5.85	1.45	1.37
19	e	309	CLA	C1B-NB	5.84	1.45	1.37
19	j	310	CLA	MG-ND	-5.84	1.94	2.05
19	g	308	CLA	C1B-NB	5.84	1.45	1.37
19	i	312	CLA	C1B-NB	5.84	1.45	1.37
19	o	308	CLA	C1B-NB	5.84	1.45	1.37
19	l	203	CLA	MG-ND	-5.83	1.94	2.05
19	c	315	CLA	C1B-NB	5.83	1.44	1.37
19	b	304	CLA	MG-ND	-5.82	1.94	2.05
19	o	307	CLA	MG-NA	-5.82	1.92	2.06
19	j	313	CLA	C1B-NB	5.81	1.44	1.37
19	j	302	CLA	C1B-NB	5.81	1.44	1.37
19	g	311	CLA	C1B-NB	5.81	1.44	1.37
19	f	311	CLA	C1B-NB	5.81	1.44	1.37
19	l	209	CLA	C1B-NB	5.81	1.44	1.37
19	k	302	CLA	MG-NB	-5.81	1.94	2.05
19	m	311	CLA	C1B-NB	5.81	1.44	1.37
19	B	840	CLA	C1B-NB	5.79	1.44	1.37
19	o	310	CLA	C1B-NB	5.79	1.44	1.37
19	g	305	CLA	MG-ND	-5.79	1.94	2.05
19	f	314	CLA	C1B-NB	5.79	1.44	1.37
19	l	205	CLA	C1B-NB	5.79	1.44	1.37
19	l	208	CLA	C1B-NB	5.79	1.44	1.37
19	e	308	CLA	C1B-NB	5.79	1.44	1.37
19	k	311	CLA	C1B-NB	5.78	1.44	1.37
19	l	202	CLA	MG-NA	-5.78	1.92	2.06
19	d	204	CLA	C1B-NB	5.78	1.44	1.37
19	l	206	CLA	MG-NA	-5.77	1.92	2.06
19	h	208	CLA	C1B-NB	5.77	1.44	1.37
19	i	310	CLA	MG-ND	-5.77	1.94	2.05
19	A	849	CLA	C1B-NB	5.77	1.44	1.37
19	o	302	CLA	MG-NB	-5.77	1.94	2.05
19	A	850	CLA	C1B-NB	5.77	1.44	1.37
19	k	304	CLA	C1B-NB	5.77	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	f	312	CLA	C1B-NB	5.76	1.44	1.37
19	i	307	CLA	C1B-NB	5.76	1.44	1.37
19	A	842	CLA	MG-ND	-5.76	1.94	2.05
19	o	306	CLA	C1B-NB	5.76	1.44	1.37
19	i	313	CLA	MG-ND	-5.76	1.94	2.05
19	i	313	CLA	C1B-NB	5.76	1.44	1.37
19	k	302	CLA	MG-ND	-5.76	1.94	2.05
19	m	306	CLA	C1B-NB	5.76	1.44	1.37
19	A	827	CLA	C1B-NB	5.75	1.44	1.37
19	B	823	CLA	C1B-NB	5.75	1.44	1.37
19	h	204	CLA	C1B-NB	5.75	1.44	1.37
19	i	311	CLA	C1B-NB	5.75	1.44	1.37
19	m	310	CLA	C1B-NB	5.75	1.44	1.37
19	m	308	CLA	C1B-NB	5.74	1.44	1.37
19	a	309	CLA	C1B-NB	5.74	1.44	1.37
19	k	307	CLA	C1B-NB	5.74	1.44	1.37
19	n	202	CLA	MG-NA	-5.74	1.92	2.06
19	h	203	CLA	C1B-NB	5.74	1.44	1.37
19	B	811	CLA	C1B-NB	5.74	1.44	1.37
19	k	308	CLA	C1B-NB	5.74	1.44	1.37
19	g	304	CLA	MG-ND	-5.74	1.94	2.05
19	a	307	CLA	C1B-NB	5.74	1.44	1.37
19	A	820	CLA	C1B-NB	5.73	1.44	1.37
19	k	303	CLA	C1B-NB	5.73	1.44	1.37
19	n	204	CLA	C1B-NB	5.73	1.44	1.37
19	k	304	CLA	MG-ND	-5.73	1.94	2.05
19	d	210	CLA	C1B-NB	5.73	1.44	1.37
19	c	308	CLA	C1B-NB	5.73	1.44	1.37
19	e	303	CLA	C1B-NB	5.73	1.44	1.37
19	d	206	CLA	MG-ND	-5.72	1.94	2.05
19	o	309	CLA	MG-NB	-5.72	1.94	2.05
19	B	833	CLA	C1B-NB	5.72	1.44	1.37
19	A	808	CLA	C1B-NB	5.72	1.44	1.37
19	h	206	CLA	C1B-NB	5.72	1.44	1.37
19	n	202	CLA	C1B-NB	5.72	1.44	1.37
19	A	813	CLA	C1B-NB	5.72	1.44	1.37
19	B	838	CLA	C1B-NB	5.72	1.44	1.37
19	j	312	CLA	C1B-NB	5.71	1.44	1.37
19	b	315	CLA	MG-ND	-5.71	1.94	2.05
19	B	810	CLA	C1B-NB	5.71	1.44	1.37
19	B	838	CLA	MG-ND	-5.70	1.94	2.05
19	h	210	CLA	C1B-NB	5.70	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	304	CLA	C1B-NB	5.70	1.44	1.37
19	o	307	CLA	MG-ND	-5.70	1.94	2.05
19	a	314	CLA	MG-ND	-5.70	1.94	2.05
19	j	312	CLA	MG-ND	-5.70	1.94	2.05
19	i	303	CLA	C1B-NB	5.69	1.44	1.37
19	f	308	CLA	C1B-NB	5.69	1.44	1.37
19	l	204	CLA	C1B-NB	5.69	1.44	1.37
19	A	852	CLA	C1B-NB	5.69	1.44	1.37
19	B	844	CLA	C1B-NB	5.69	1.44	1.37
19	c	309	CLA	C1B-NB	5.69	1.44	1.37
19	A	844	CLA	C1B-NB	5.68	1.44	1.37
19	b	307	CLA	C1B-NB	5.68	1.44	1.37
19	A	828	CLA	C1B-NB	5.68	1.44	1.37
19	A	829	CLA	C1B-NB	5.68	1.44	1.37
19	i	305	CLA	MG-ND	-5.68	1.94	2.05
19	l	201	CLA	MG-ND	-5.68	1.94	2.05
19	A	815	CLA	C1B-NB	5.68	1.44	1.37
19	c	306	CLA	C1B-NB	5.68	1.44	1.37
19	b	308	CLA	C1B-NB	5.68	1.44	1.37
19	B	821	CLA	C1B-NB	5.68	1.44	1.37
19	A	839	CLA	MG-ND	-5.68	1.94	2.05
19	f	311	CLA	MG-ND	-5.68	1.94	2.05
19	A	805	CLA	C1B-NB	5.68	1.44	1.37
19	e	307	CLA	C1B-NB	5.68	1.44	1.37
19	l	207	CLA	C1B-NB	5.68	1.44	1.37
19	j	308	CLA	C1B-NB	5.67	1.44	1.37
19	n	202	CLA	MG-ND	-5.67	1.94	2.05
19	B	822	CLA	C1B-NB	5.67	1.44	1.37
19	b	313	CLA	C1B-NB	5.67	1.44	1.37
19	o	305	CLA	C1B-NB	5.67	1.44	1.37
19	F	203	CLA	MG-ND	-5.67	1.94	2.05
19	n	209	CLA	MG-NB	-5.67	1.94	2.05
19	g	307	CLA	C1B-NB	5.66	1.44	1.37
19	B	811	CLA	MG-ND	-5.66	1.94	2.05
19	f	305	CLA	C1B-NB	5.66	1.44	1.37
19	i	302	CLA	C1B-NB	5.66	1.44	1.37
19	A	809	CLA	MG-ND	-5.66	1.94	2.05
19	A	840	CLA	C1B-NB	5.66	1.44	1.37
19	J	803	CLA	C1B-NB	5.66	1.44	1.37
19	m	302	CLA	MG-ND	-5.66	1.94	2.05
19	h	209	CLA	C1B-NB	5.66	1.44	1.37
19	B	812	CLA	C1B-NB	5.66	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	i	313	CLA	MG-NB	-5.65	1.94	2.05
19	o	304	CLA	MG-ND	-5.65	1.94	2.05
19	A	841	CLA	C1B-NB	5.65	1.44	1.37
19	h	206	CLA	MG-ND	-5.64	1.94	2.05
19	B	820	CLA	MG-ND	-5.64	1.94	2.05
19	A	853	CLA	C1B-NB	5.64	1.44	1.37
19	D	301	CLA	C1B-NB	5.64	1.44	1.37
19	A	803	CLA	MG-NB	-5.64	1.94	2.05
19	c	311	CLA	MG-ND	-5.64	1.94	2.05
19	e	310	CLA	MG-ND	-5.64	1.94	2.05
19	B	819	CLA	C1B-NB	5.64	1.44	1.37
19	A	820	CLA	MG-ND	-5.64	1.94	2.05
19	g	302	CLA	C1B-NB	5.64	1.44	1.37
19	A	811	CLA	MG-ND	-5.64	1.94	2.05
19	i	308	CLA	C1B-NB	5.64	1.44	1.37
19	A	806	CLA	C1B-NB	5.64	1.44	1.37
19	B	805	CLA	C1B-NB	5.63	1.44	1.37
19	B	830	CLA	C1B-NB	5.63	1.44	1.37
19	e	302	CLA	C1B-NB	5.63	1.44	1.37
19	n	204	CLA	MG-ND	-5.63	1.94	2.05
19	c	311	CLA	C1B-NB	5.63	1.44	1.37
19	m	305	CLA	MG-ND	-5.63	1.94	2.05
19	m	309	CLA	MG-ND	-5.63	1.94	2.05
19	B	814	CLA	C1B-NB	5.63	1.44	1.37
19	k	310	CLA	C1B-NB	5.62	1.44	1.37
19	f	314	CLA	MG-ND	-5.62	1.94	2.05
19	A	818	CLA	C1B-NB	5.62	1.44	1.37
19	e	311	CLA	C1B-NB	5.62	1.44	1.37
19	j	307	CLA	MG-ND	-5.62	1.94	2.05
19	c	302	CLA	C1B-NB	5.61	1.44	1.37
19	f	305	CLA	MG-ND	-5.61	1.94	2.05
19	c	307	CLA	C1B-NB	5.61	1.44	1.37
19	l	203	CLA	C1B-NB	5.61	1.44	1.37
19	A	813	CLA	MG-ND	-5.61	1.94	2.05
19	m	304	CLA	C1B-NB	5.61	1.44	1.37
19	k	306	CLA	C1B-NB	5.61	1.44	1.37
19	A	821	CLA	MG-ND	-5.61	1.94	2.05
19	A	817	CLA	C1B-NB	5.60	1.44	1.37
19	B	845	CLA	C1B-NB	5.60	1.44	1.37
19	B	837	CLA	MG-NB	-5.60	1.94	2.05
19	f	310	CLA	C1B-NB	5.60	1.44	1.37
19	f	314	CLA	MG-NA	-5.60	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	840	CLA	MG-NA	-5.60	1.93	2.06
19	i	313	CLA	MG-NA	-5.59	1.93	2.06
19	c	310	CLA	C1B-NB	5.59	1.44	1.37
19	f	303	CLA	C1B-NB	5.59	1.44	1.37
19	f	306	CLA	C1B-NB	5.59	1.44	1.37
19	j	301	CLA	MG-ND	-5.59	1.94	2.05
19	j	304	CLA	MG-NB	-5.59	1.94	2.05
19	j	301	CLA	C1B-NB	5.59	1.44	1.37
19	n	204	CLA	MG-NB	-5.59	1.94	2.05
19	j	306	CLA	MG-NB	-5.59	1.94	2.05
19	i	305	CLA	C1B-NB	5.59	1.44	1.37
19	B	838	CLA	MG-NB	-5.59	1.94	2.05
19	B	840	CLA	MG-NB	-5.59	1.94	2.05
19	B	817	CLA	C1B-NB	5.58	1.44	1.37
19	h	213	CLA	MG-ND	-5.58	1.94	2.05
19	j	303	CLA	MG-ND	-5.58	1.94	2.05
19	A	820	CLA	MG-NB	-5.58	1.94	2.05
19	B	816	CLA	MG-ND	-5.58	1.94	2.05
19	A	812	CLA	C1B-NB	5.58	1.44	1.37
19	B	813	CLA	C1B-NB	5.58	1.44	1.37
19	B	843	CLA	C1B-NB	5.58	1.44	1.37
19	F	203	CLA	C1B-NB	5.58	1.44	1.37
19	a	308	CLA	MG-ND	-5.58	1.94	2.05
19	j	309	CLA	MG-ND	-5.57	1.94	2.05
19	A	847	CLA	MG-ND	-5.57	1.94	2.05
19	o	303	CLA	MG-ND	-5.57	1.94	2.05
19	k	305	CLA	MG-ND	-5.57	1.94	2.05
19	j	311	CLA	MG-ND	-5.57	1.94	2.05
19	n	203	CLA	MG-NA	-5.57	1.93	2.06
19	d	209	CLA	C1B-NB	5.57	1.44	1.37
19	A	846	CLA	MG-ND	-5.57	1.94	2.05
19	B	806	CLA	MG-ND	-5.56	1.94	2.05
19	k	310	CLA	MG-ND	-5.56	1.94	2.05
19	A	803	CLA	C1B-NB	5.56	1.44	1.37
19	b	309	CLA	MG-ND	-5.56	1.94	2.05
19	i	311	CLA	MG-ND	-5.56	1.94	2.05
19	c	303	CLA	C1B-NB	5.56	1.44	1.37
19	A	812	CLA	MG-ND	-5.56	1.94	2.05
19	a	305	CLA	C1B-NB	5.56	1.44	1.37
19	B	835	CLA	C1B-NB	5.55	1.44	1.37
19	h	213	CLA	C1B-NB	5.55	1.44	1.37
19	l	203	CLA	MG-NB	-5.55	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	821	CLA	C1B-NB	5.55	1.44	1.37
19	A	823	CLA	MG-ND	-5.55	1.94	2.05
19	m	310	CLA	MG-ND	-5.55	1.94	2.05
19	n	201	CLA	C1B-NB	5.55	1.44	1.37
19	n	203	CLA	C1B-NB	5.55	1.44	1.37
19	B	809	CLA	MG-ND	-5.55	1.94	2.05
19	B	812	CLA	MG-ND	-5.54	1.94	2.05
19	c	307	CLA	MG-ND	-5.54	1.94	2.05
19	d	207	CLA	C1B-NB	5.54	1.44	1.37
19	B	845	CLA	MG-ND	-5.54	1.94	2.05
19	e	308	CLA	MG-ND	-5.54	1.94	2.05
19	i	306	CLA	C1B-NB	5.54	1.44	1.37
19	B	832	CLA	MG-ND	-5.54	1.94	2.05
19	F	202	CLA	MG-ND	-5.54	1.94	2.05
19	f	314	CLA	MG-NB	-5.54	1.94	2.05
19	k	305	CLA	C1B-NB	5.54	1.44	1.37
19	a	303	CLA	C1B-NB	5.53	1.44	1.37
19	b	306	CLA	MG-ND	-5.53	1.94	2.05
19	k	309	CLA	MG-NA	-5.53	1.93	2.06
19	j	307	CLA	C1B-NB	5.53	1.44	1.37
19	A	845	CLA	MG-NB	-5.53	1.94	2.05
19	g	311	CLA	MG-ND	-5.53	1.94	2.05
19	c	304	CLA	MG-ND	-5.53	1.94	2.05
19	k	306	CLA	MG-ND	-5.53	1.94	2.05
19	A	847	CLA	C1B-NB	5.53	1.44	1.37
19	k	303	CLA	MG-ND	-5.53	1.94	2.05
19	B	842	CLA	C1B-NB	5.53	1.44	1.37
19	d	211	CLA	C1B-NB	5.53	1.44	1.37
19	h	205	CLA	MG-NB	-5.53	1.94	2.05
19	B	836	CLA	MG-ND	-5.52	1.94	2.05
19	A	842	CLA	MG-NA	-5.52	1.93	2.06
19	B	839	CLA	C1B-NB	5.52	1.44	1.37
19	b	309	CLA	C1B-NB	5.52	1.44	1.37
19	h	212	CLA	MG-ND	-5.52	1.94	2.05
19	A	825	CLA	C1B-NB	5.52	1.44	1.37
19	F	201	CLA	C1B-NB	5.52	1.44	1.37
19	a	305	CLA	MG-ND	-5.52	1.94	2.05
19	h	211	CLA	MG-ND	-5.52	1.94	2.05
19	A	814	CLA	C1B-NB	5.52	1.44	1.37
19	o	305	CLA	MG-ND	-5.52	1.94	2.05
19	b	303	CLA	C1B-NB	5.52	1.44	1.37
19	B	839	CLA	MG-ND	-5.52	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	838	CLA	MG-NA	-5.52	1.93	2.06
19	k	309	CLA	MG-NB	-5.51	1.94	2.05
19	e	307	CLA	MG-ND	-5.51	1.94	2.05
19	F	202	CLA	C1B-NB	5.51	1.44	1.37
19	j	312	CLA	MG-NB	-5.51	1.94	2.05
19	A	826	CLA	C1B-NB	5.51	1.44	1.37
19	A	845	CLA	C1B-NB	5.51	1.44	1.37
19	l	209	CLA	MG-ND	-5.51	1.94	2.05
19	e	306	CLA	C1B-NB	5.51	1.44	1.37
19	B	809	CLA	C1B-NB	5.51	1.44	1.37
19	h	207	CLA	MG-ND	-5.51	1.94	2.05
19	h	213	CLA	MG-NB	-5.50	1.94	2.05
19	B	815	CLA	C1B-NB	5.50	1.44	1.37
19	A	810	CLA	MG-NB	-5.50	1.94	2.05
19	l	203	CLA	MG-NA	-5.50	1.93	2.06
19	g	309	CLA	C1B-NB	5.50	1.44	1.37
19	A	825	CLA	MG-ND	-5.50	1.94	2.05
19	n	209	CLA	MG-NA	-5.50	1.93	2.06
19	n	208	CLA	MG-NA	-5.50	1.93	2.06
19	b	303	CLA	MG-ND	-5.49	1.94	2.05
19	d	212	CLA	MG-ND	-5.49	1.94	2.05
19	g	301	CLA	MG-ND	-5.49	1.94	2.05
19	c	310	CLA	MG-ND	-5.49	1.94	2.05
19	m	307	CLA	MG-ND	-5.49	1.94	2.05
19	j	304	CLA	MG-NA	-5.49	1.93	2.06
19	o	310	CLA	MG-ND	-5.49	1.94	2.05
19	A	816	CLA	C1B-NB	5.49	1.44	1.37
19	l	202	CLA	MG-ND	-5.49	1.94	2.05
19	A	825	CLA	MG-NB	-5.49	1.94	2.05
19	A	843	CLA	MG-ND	-5.49	1.94	2.05
19	F	204	CLA	C1B-NB	5.49	1.44	1.37
19	A	811	CLA	MG-NB	-5.49	1.94	2.05
19	i	309	CLA	MG-ND	-5.48	1.94	2.05
19	j	309	CLA	C1B-NB	5.48	1.44	1.37
19	f	306	CLA	MG-ND	-5.48	1.94	2.05
19	i	302	CLA	MG-ND	-5.48	1.94	2.05
19	g	301	CLA	MG-NA	-5.48	1.93	2.06
19	f	311	CLA	MG-NB	-5.48	1.94	2.05
19	o	306	CLA	MG-ND	-5.48	1.94	2.05
19	m	308	CLA	MG-ND	-5.47	1.94	2.05
19	A	803	CLA	MG-NA	-5.47	1.93	2.06
19	d	201	CLA	C1B-NB	5.47	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	h	212	CLA	C1B-NB	5.47	1.44	1.37
19	m	307	CLA	C1B-NB	5.47	1.44	1.37
19	d	201	CLA	MG-ND	-5.46	1.95	2.05
19	d	206	CLA	C1B-NB	5.46	1.44	1.37
19	j	312	CLA	MG-NA	-5.46	1.93	2.06
19	B	808	CLA	MG-ND	-5.46	1.95	2.05
19	B	844	CLA	MG-ND	-5.46	1.95	2.05
19	f	309	CLA	MG-ND	-5.46	1.95	2.05
19	A	842	CLA	MG-NB	-5.45	1.95	2.05
19	B	816	CLA	C1B-NB	5.45	1.44	1.37
19	A	850	CLA	MG-ND	-5.45	1.95	2.05
19	h	211	CLA	C1B-NB	5.45	1.44	1.37
19	n	203	CLA	MG-NB	-5.45	1.95	2.05
19	A	810	CLA	MG-ND	-5.45	1.95	2.05
19	n	204	CLA	MG-NA	-5.45	1.93	2.06
19	B	804	CLA	MG-NB	-5.45	1.95	2.05
19	B	821	CLA	MG-ND	-5.45	1.95	2.05
19	A	807	CLA	C1B-NB	5.45	1.44	1.37
19	A	807	CLA	MG-ND	-5.44	1.95	2.05
19	A	848	CLA	C1B-NB	5.44	1.44	1.37
19	h	207	CLA	C1B-NB	5.44	1.44	1.37
19	j	313	CLA	MG-ND	-5.44	1.95	2.05
19	k	304	CLA	MG-NB	-5.44	1.95	2.05
19	a	302	CLA	MG-NA	-5.44	1.93	2.06
19	l	208	CLA	MG-ND	-5.44	1.95	2.05
19	n	207	CLA	MG-ND	-5.44	1.95	2.05
19	d	203	CLA	MG-ND	-5.44	1.95	2.05
19	F	204	CLA	MG-ND	-5.44	1.95	2.05
19	A	809	CLA	C1B-NB	5.44	1.44	1.37
19	f	305	CLA	MG-NA	-5.44	1.93	2.06
19	l	205	CLA	MG-ND	-5.43	1.95	2.05
19	c	303	CLA	MG-NB	-5.43	1.95	2.05
19	o	311	CLA	MG-ND	-5.43	1.95	2.05
19	B	811	CLA	MG-NB	-5.43	1.95	2.05
19	b	307	CLA	MG-ND	-5.43	1.95	2.05
19	B	807	CLA	C1B-NB	5.43	1.44	1.37
19	a	307	CLA	MG-ND	-5.43	1.95	2.05
19	D	301	CLA	MG-ND	-5.43	1.95	2.05
19	l	202	CLA	MG-NB	-5.43	1.95	2.05
19	A	819	CLA	MG-ND	-5.43	1.95	2.05
19	B	837	CLA	MG-ND	-5.43	1.95	2.05
19	g	311	CLA	MG-NB	-5.43	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	309	CLA	MG-ND	-5.43	1.95	2.05
19	A	843	CLA	MG-NB	-5.42	1.95	2.05
19	B	807	CLA	MG-ND	-5.42	1.95	2.05
19	B	820	CLA	C1B-NB	5.42	1.44	1.37
19	A	848	CLA	MG-ND	-5.42	1.95	2.05
19	o	307	CLA	MG-NB	-5.42	1.95	2.05
19	f	311	CLA	MG-NA	-5.42	1.93	2.06
19	h	201	CLA	C1B-NB	5.42	1.44	1.37
19	a	314	CLA	MG-NA	-5.42	1.93	2.06
19	h	201	CLA	MG-ND	-5.41	1.95	2.05
19	B	847	CLA	MG-NA	-5.41	1.93	2.06
19	i	310	CLA	MG-NB	-5.41	1.95	2.05
19	j	302	CLA	MG-ND	-5.41	1.95	2.05
19	a	308	CLA	MG-NB	-5.41	1.95	2.05
19	i	309	CLA	C1B-NB	5.41	1.44	1.37
19	g	309	CLA	MG-ND	-5.41	1.95	2.05
19	d	207	CLA	MG-ND	-5.41	1.95	2.05
19	i	303	CLA	MG-ND	-5.41	1.95	2.05
19	f	307	CLA	MG-ND	-5.41	1.95	2.05
19	d	212	CLA	C1B-NB	5.41	1.44	1.37
19	i	310	CLA	MG-NA	-5.41	1.93	2.06
19	a	310	CLA	C1B-NB	5.40	1.44	1.37
19	B	808	CLA	MG-NB	-5.40	1.95	2.05
19	B	814	CLA	MG-ND	-5.40	1.95	2.05
19	o	308	CLA	MG-ND	-5.40	1.95	2.05
19	B	818	CLA	MG-ND	-5.40	1.95	2.05
19	c	316	CLA	C1B-NB	5.40	1.44	1.37
19	i	311	CLA	MG-NB	-5.40	1.95	2.05
19	B	808	CLA	MG-NA	-5.40	1.93	2.06
19	A	829	CLA	MG-ND	-5.40	1.95	2.05
19	A	839	CLA	C1B-NB	5.40	1.44	1.37
19	A	818	CLA	MG-ND	-5.39	1.95	2.05
19	a	314	CLA	MG-NB	-5.39	1.95	2.05
19	f	312	CLA	MG-ND	-5.39	1.95	2.05
19	h	208	CLA	MG-ND	-5.39	1.95	2.05
19	a	306	CLA	MG-ND	-5.39	1.95	2.05
19	c	314	CLA	MG-ND	-5.39	1.95	2.05
19	a	310	CLA	MG-ND	-5.39	1.95	2.05
19	B	804	CLA	C1B-NB	5.39	1.44	1.37
19	m	311	CLA	MG-ND	-5.39	1.95	2.05
19	c	306	CLA	MG-NB	-5.39	1.95	2.05
19	B	813	CLA	MG-NB	-5.38	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	304	CLA	MG-NA	-5.38	1.93	2.06
19	f	303	CLA	MG-ND	-5.38	1.95	2.05
19	c	316	CLA	MG-ND	-5.38	1.95	2.05
19	A	826	CLA	MG-ND	-5.38	1.95	2.05
19	d	207	CLA	MG-NB	-5.38	1.95	2.05
19	h	205	CLA	MG-NA	-5.38	1.93	2.06
19	B	843	CLA	MG-ND	-5.38	1.95	2.05
19	A	840	CLA	MG-ND	-5.38	1.95	2.05
19	a	302	CLA	MG-ND	-5.38	1.95	2.05
19	c	304	CLA	C1B-NB	5.37	1.44	1.37
19	B	822	CLA	MG-ND	-5.37	1.95	2.05
19	e	306	CLA	MG-ND	-5.37	1.95	2.05
19	e	303	CLA	MG-ND	-5.37	1.95	2.05
19	B	801	CLA	MG-NB	-5.37	1.95	2.05
19	F	201	CLA	MG-ND	-5.37	1.95	2.05
19	A	815	CLA	MG-ND	-5.37	1.95	2.05
19	B	823	CLA	MG-ND	-5.37	1.95	2.05
19	a	303	CLA	MG-ND	-5.37	1.95	2.05
19	j	306	CLA	MG-NA	-5.36	1.93	2.06
19	A	802	CLA	MG-NB	-5.36	1.95	2.05
19	j	307	CLA	MG-NB	-5.36	1.95	2.05
19	f	310	CLA	MG-ND	-5.36	1.95	2.05
19	A	817	CLA	MG-NA	-5.36	1.93	2.06
19	m	309	CLA	MG-NA	-5.36	1.93	2.06
19	d	208	CLA	MG-ND	-5.36	1.95	2.05
19	A	825	CLA	MG-NA	-5.36	1.93	2.06
19	m	309	CLA	MG-NB	-5.36	1.95	2.05
19	m	305	CLA	C1B-NB	5.36	1.44	1.37
19	A	827	CLA	MG-ND	-5.36	1.95	2.05
19	B	835	CLA	MG-ND	-5.36	1.95	2.05
19	A	852	CLA	MG-ND	-5.36	1.95	2.05
19	l	204	CLA	MG-ND	-5.36	1.95	2.05
19	m	303	CLA	MG-ND	-5.36	1.95	2.05
19	g	311	CLA	MG-NA	-5.36	1.93	2.06
19	B	808	CLA	C1B-NB	5.36	1.44	1.37
19	B	815	CLA	MG-ND	-5.36	1.95	2.05
19	B	817	CLA	MG-ND	-5.36	1.95	2.05
19	B	848	CLA	MG-NB	-5.36	1.95	2.05
19	n	205	CLA	MG-NB	-5.36	1.95	2.05
19	o	304	CLA	MG-NA	-5.35	1.93	2.06
19	h	204	CLA	MG-ND	-5.35	1.95	2.05
19	i	307	CLA	MG-ND	-5.35	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	816	CLA	MG-NA	-5.35	1.93	2.06
19	o	312	CLA	MG-ND	-5.35	1.95	2.05
19	B	818	CLA	C1B-NB	5.35	1.44	1.37
19	A	828	CLA	MG-ND	-5.35	1.95	2.05
19	c	302	CLA	MG-ND	-5.35	1.95	2.05
19	B	847	CLA	MG-ND	-5.35	1.95	2.05
19	B	848	CLA	MG-ND	-5.35	1.95	2.05
19	j	301	CLA	MG-NB	-5.35	1.95	2.05
19	A	814	CLA	MG-ND	-5.35	1.95	2.05
19	d	211	CLA	MG-ND	-5.35	1.95	2.05
19	b	308	CLA	MG-ND	-5.35	1.95	2.05
19	o	303	CLA	C1B-NB	5.35	1.44	1.37
19	A	805	CLA	MG-ND	-5.34	1.95	2.05
19	g	302	CLA	MG-ND	-5.34	1.95	2.05
19	A	811	CLA	C1B-NB	5.34	1.44	1.37
19	n	201	CLA	MG-ND	-5.34	1.95	2.05
19	e	310	CLA	MG-NA	-5.34	1.93	2.06
19	B	849	CLA	MG-ND	-5.34	1.95	2.05
19	B	837	CLA	MG-NA	-5.34	1.93	2.06
19	o	304	CLA	MG-NB	-5.34	1.95	2.05
19	A	801	CLA	MG-NB	-5.34	1.95	2.05
19	h	205	CLA	C1B-NB	5.34	1.44	1.37
19	f	302	CLA	MG-ND	-5.34	1.95	2.05
19	m	307	CLA	MG-NB	-5.34	1.95	2.05
19	f	308	CLA	MG-ND	-5.34	1.95	2.05
19	d	209	CLA	MG-ND	-5.34	1.95	2.05
19	j	303	CLA	C1B-NB	5.34	1.44	1.37
19	a	304	CLA	MG-ND	-5.33	1.95	2.05
19	a	302	CLA	MG-NB	-5.33	1.95	2.05
19	c	306	CLA	MG-ND	-5.33	1.95	2.05
19	i	305	CLA	MG-NB	-5.33	1.95	2.05
19	l	207	CLA	MG-ND	-5.33	1.95	2.05
19	A	849	CLA	MG-ND	-5.33	1.95	2.05
19	d	204	CLA	MG-ND	-5.33	1.95	2.05
19	i	305	CLA	MG-NA	-5.33	1.93	2.06
19	B	841	CLA	MG-ND	-5.33	1.95	2.05
19	n	205	CLA	MG-ND	-5.33	1.95	2.05
28	b	310	CHL	CMC-C2C	5.33	1.56	1.45
19	i	306	CLA	MG-ND	-5.33	1.95	2.05
19	i	311	CLA	MG-NA	-5.33	1.93	2.06
19	c	308	CLA	MG-ND	-5.32	1.95	2.05
19	f	305	CLA	MG-NB	-5.32	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	803	CLA	MG-ND	-5.32	1.95	2.05
19	b	305	CLA	MG-ND	-5.32	1.95	2.05
19	k	308	CLA	MG-ND	-5.31	1.95	2.05
19	l	209	CLA	MG-NA	-5.31	1.93	2.06
19	B	848	CLA	C1B-NB	5.31	1.44	1.37
19	B	810	CLA	MG-ND	-5.31	1.95	2.05
19	m	306	CLA	MG-ND	-5.31	1.95	2.05
19	e	302	CLA	MG-ND	-5.31	1.95	2.05
19	o	311	CLA	C1B-NB	5.31	1.44	1.37
19	e	311	CLA	MG-ND	-5.31	1.95	2.05
19	e	305	CLA	MG-ND	-5.31	1.95	2.05
19	i	308	CLA	MG-ND	-5.31	1.95	2.05
19	A	806	CLA	MG-NB	-5.30	1.95	2.05
19	h	210	CLA	MG-ND	-5.30	1.95	2.05
19	b	313	CLA	MG-ND	-5.30	1.95	2.05
19	k	307	CLA	MG-ND	-5.30	1.95	2.05
19	B	842	CLA	MG-ND	-5.30	1.95	2.05
19	g	307	CLA	MG-ND	-5.30	1.95	2.05
19	d	210	CLA	MG-NB	-5.30	1.95	2.05
19	h	201	CLA	MG-NB	-5.30	1.95	2.05
19	A	824	CLA	C1B-NB	5.30	1.44	1.37
19	j	301	CLA	MG-NA	-5.30	1.93	2.06
19	k	311	CLA	MG-ND	-5.30	1.95	2.05
19	g	301	CLA	MG-NB	-5.30	1.95	2.05
19	A	819	CLA	MG-NB	-5.30	1.95	2.05
19	A	850	CLA	MG-NB	-5.29	1.95	2.05
19	A	812	CLA	MG-NB	-5.29	1.95	2.05
19	d	210	CLA	MG-ND	-5.29	1.95	2.05
28	d	202	CHL	CMC-C2C	5.29	1.56	1.45
19	B	844	CLA	MG-NB	-5.29	1.95	2.05
19	j	305	CLA	MG-ND	-5.28	1.95	2.05
19	h	203	CLA	MG-ND	-5.28	1.95	2.05
19	j	311	CLA	C1B-NB	5.28	1.44	1.37
19	j	308	CLA	MG-ND	-5.28	1.95	2.05
19	A	813	CLA	MG-NB	-5.27	1.95	2.05
28	o	301	CHL	CMC-C2C	5.27	1.56	1.45
19	B	830	CLA	MG-ND	-5.27	1.95	2.05
19	n	202	CLA	MG-NB	-5.27	1.95	2.05
19	A	815	CLA	MG-NB	-5.27	1.95	2.05
19	A	847	CLA	MG-NB	-5.27	1.95	2.05
19	h	208	CLA	MG-NB	-5.27	1.95	2.05
19	A	816	CLA	MG-ND	-5.27	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	o	302	CLA	C1B-NB	5.27	1.44	1.37
19	A	824	CLA	MG-ND	-5.26	1.95	2.05
19	m	308	CLA	MG-NA	-5.26	1.93	2.06
19	h	206	CLA	MG-NB	-5.26	1.95	2.05
19	k	307	CLA	MG-NB	-5.26	1.95	2.05
28	a	315	CHL	CMC-C2C	5.26	1.56	1.45
19	A	845	CLA	MG-ND	-5.26	1.95	2.05
19	e	309	CLA	MG-ND	-5.26	1.95	2.05
19	B	821	CLA	MG-NB	-5.26	1.95	2.05
19	B	833	CLA	MG-ND	-5.26	1.95	2.05
19	A	820	CLA	MG-NA	-5.25	1.93	2.06
19	A	806	CLA	MG-ND	-5.25	1.95	2.05
28	e	301	CHL	CMC-C2C	5.25	1.56	1.45
19	e	311	CLA	MG-NB	-5.24	1.95	2.05
19	c	309	CLA	MG-ND	-5.24	1.95	2.05
19	A	852	CLA	MG-NB	-5.24	1.95	2.05
19	f	306	CLA	MG-NB	-5.24	1.95	2.05
19	i	312	CLA	MG-ND	-5.24	1.95	2.05
19	o	310	CLA	MG-NB	-5.24	1.95	2.05
19	a	303	CLA	MG-NB	-5.24	1.95	2.05
19	B	813	CLA	MG-ND	-5.24	1.95	2.05
28	a	313	CHL	CMC-C2C	5.23	1.56	1.45
19	c	303	CLA	MG-ND	-5.23	1.95	2.05
19	A	845	CLA	MG-NA	-5.23	1.93	2.06
19	B	819	CLA	MG-ND	-5.23	1.95	2.05
19	A	844	CLA	MG-ND	-5.23	1.95	2.05
19	A	827	CLA	MG-NA	-5.23	1.93	2.06
19	B	843	CLA	MG-NA	-5.23	1.93	2.06
19	F	201	CLA	MG-NB	-5.23	1.95	2.05
19	A	853	CLA	MG-ND	-5.23	1.95	2.05
19	j	307	CLA	MG-NA	-5.23	1.93	2.06
19	f	309	CLA	MG-NB	-5.23	1.95	2.05
19	j	302	CLA	MG-NB	-5.23	1.95	2.05
19	h	209	CLA	MG-ND	-5.22	1.95	2.05
19	b	306	CLA	MG-NB	-5.22	1.95	2.05
19	a	307	CLA	MG-NB	-5.22	1.95	2.05
19	b	305	CLA	MG-NA	-5.22	1.93	2.06
19	B	847	CLA	MG-NB	-5.22	1.95	2.05
19	B	806	CLA	C1B-NB	5.22	1.44	1.37
19	A	813	CLA	MG-NA	-5.21	1.93	2.06
19	A	847	CLA	MG-NA	-5.21	1.93	2.06
19	B	849	CLA	MG-NA	-5.21	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	841	CLA	MG-ND	-5.21	1.95	2.05
19	b	302	CLA	MG-ND	-5.21	1.95	2.05
19	B	804	CLA	MG-NA	-5.21	1.93	2.06
28	k	301	CHL	CMC-C2C	5.21	1.56	1.45
19	F	202	CLA	MG-NB	-5.21	1.95	2.05
19	A	811	CLA	MG-NA	-5.21	1.93	2.06
19	b	313	CLA	MG-NB	-5.20	1.95	2.05
19	k	308	CLA	MG-NB	-5.20	1.95	2.05
19	g	308	CLA	MG-ND	-5.20	1.95	2.05
19	a	309	CLA	MG-ND	-5.20	1.95	2.05
19	B	805	CLA	MG-ND	-5.20	1.95	2.05
19	B	848	CLA	MG-NA	-5.20	1.93	2.06
19	c	308	CLA	MG-NB	-5.20	1.95	2.05
19	l	205	CLA	MG-NB	-5.20	1.95	2.05
19	B	820	CLA	MG-NB	-5.19	1.95	2.05
19	B	843	CLA	MG-NB	-5.19	1.95	2.05
19	A	839	CLA	MG-NB	-5.19	1.95	2.05
19	A	828	CLA	MG-NA	-5.19	1.93	2.06
19	B	849	CLA	C1B-NB	5.19	1.44	1.37
19	A	827	CLA	MG-NB	-5.19	1.95	2.05
19	A	817	CLA	MG-ND	-5.19	1.95	2.05
19	m	302	CLA	MG-NA	-5.19	1.94	2.06
19	A	818	CLA	MG-NB	-5.18	1.95	2.05
19	b	308	CLA	MG-NB	-5.18	1.95	2.05
19	A	810	CLA	C1B-NB	5.18	1.44	1.37
19	B	842	CLA	MG-NB	-5.18	1.95	2.05
19	i	302	CLA	MG-NB	-5.18	1.95	2.05
28	g	310	CHL	CMC-C2C	5.18	1.56	1.45
19	i	308	CLA	MG-NB	-5.18	1.95	2.05
19	c	314	CLA	MG-NB	-5.18	1.95	2.05
28	b	301	CHL	CMC-C2C	5.18	1.56	1.45
19	o	303	CLA	MG-NB	-5.18	1.95	2.05
19	o	306	CLA	MG-NA	-5.18	1.94	2.06
19	a	305	CLA	MG-NB	-5.17	1.95	2.05
19	f	307	CLA	MG-NB	-5.17	1.95	2.05
19	d	203	CLA	MG-NB	-5.17	1.95	2.05
19	A	840	CLA	MG-NB	-5.17	1.95	2.05
19	F	203	CLA	MG-NB	-5.17	1.95	2.05
19	l	204	CLA	MG-NB	-5.17	1.95	2.05
19	A	808	CLA	MG-ND	-5.17	1.95	2.05
19	B	832	CLA	MG-NB	-5.17	1.95	2.05
19	j	310	CLA	MG-NA	-5.17	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	l	209	CLA	MG-NB	-5.17	1.95	2.05
19	A	804	CLA	MG-ND	-5.16	1.95	2.05
19	A	841	CLA	MG-NB	-5.16	1.95	2.05
28	a	312	CHL	CMC-C2C	5.16	1.56	1.45
19	A	824	CLA	MG-NB	-5.16	1.95	2.05
19	B	836	CLA	MG-NB	-5.16	1.95	2.05
19	e	305	CLA	MG-NA	-5.16	1.94	2.06
19	A	809	CLA	MG-NB	-5.15	1.95	2.05
19	d	204	CLA	MG-NB	-5.15	1.95	2.05
19	n	209	CLA	C1B-NB	5.15	1.44	1.37
19	h	211	CLA	MG-NB	-5.15	1.95	2.05
19	j	309	CLA	MG-NB	-5.15	1.95	2.05
19	h	206	CLA	MG-NA	-5.15	1.94	2.06
19	m	310	CLA	MG-NB	-5.15	1.95	2.05
19	e	307	CLA	MG-NB	-5.15	1.95	2.05
19	A	817	CLA	MG-NB	-5.15	1.95	2.05
19	c	303	CLA	MG-NA	-5.14	1.94	2.06
19	a	307	CLA	MG-NA	-5.14	1.94	2.06
19	o	303	CLA	MG-NA	-5.14	1.94	2.06
19	A	846	CLA	MG-NB	-5.14	1.95	2.05
19	e	310	CLA	MG-NB	-5.14	1.95	2.05
19	B	836	CLA	C1B-NB	5.14	1.44	1.37
19	h	203	CLA	MG-NB	-5.14	1.95	2.05
19	m	308	CLA	MG-NB	-5.13	1.95	2.05
19	o	312	CLA	MG-NB	-5.13	1.95	2.05
19	b	313	CLA	MG-NA	-5.13	1.94	2.06
19	h	207	CLA	MG-NB	-5.13	1.95	2.05
19	o	312	CLA	MG-NA	-5.13	1.94	2.06
28	b	314	CHL	CMC-C2C	5.13	1.56	1.45
19	f	307	CLA	MG-NA	-5.13	1.94	2.06
19	B	835	CLA	MG-NB	-5.12	1.95	2.05
19	A	829	CLA	MG-NB	-5.12	1.95	2.05
19	h	208	CLA	MG-NA	-5.12	1.94	2.06
28	f	301	CHL	CMC-C2C	5.12	1.56	1.45
19	B	803	CLA	C1B-NB	5.12	1.44	1.37
19	B	841	CLA	C1B-NB	5.12	1.44	1.37
19	b	302	CLA	MG-NB	-5.12	1.95	2.05
19	n	207	CLA	MG-NB	-5.12	1.95	2.05
19	A	819	CLA	C1B-NB	5.11	1.44	1.37
19	c	314	CLA	MG-NA	-5.11	1.94	2.06
19	B	821	CLA	MG-NA	-5.11	1.94	2.06
19	d	206	CLA	MG-NB	-5.11	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	305	CLA	MG-NB	-5.11	1.95	2.05
19	A	848	CLA	MG-NB	-5.11	1.95	2.05
19	e	306	CLA	MG-NB	-5.11	1.95	2.05
19	f	309	CLA	MG-NA	-5.11	1.94	2.06
19	B	816	CLA	MG-NB	-5.10	1.95	2.05
19	B	845	CLA	MG-NA	-5.10	1.94	2.06
19	h	210	CLA	MG-NB	-5.10	1.95	2.05
19	B	814	CLA	MG-NA	-5.10	1.94	2.06
19	b	307	CLA	MG-NB	-5.10	1.95	2.05
19	c	306	CLA	MG-NA	-5.10	1.94	2.06
28	b	311	CHL	CMC-C2C	5.10	1.55	1.45
19	b	304	CLA	MG-NA	-5.10	1.94	2.06
19	k	302	CLA	MG-NA	-5.09	1.94	2.06
19	B	845	CLA	MG-NB	-5.09	1.95	2.05
19	m	306	CLA	MG-NB	-5.09	1.95	2.05
28	m	301	CHL	CMC-C2C	5.09	1.55	1.45
19	f	302	CLA	MG-NB	-5.09	1.95	2.05
19	e	302	CLA	MG-NB	-5.09	1.95	2.05
19	B	803	CLA	MG-NB	-5.09	1.95	2.05
19	d	210	CLA	MG-NA	-5.09	1.94	2.06
19	f	312	CLA	MG-NA	-5.09	1.94	2.06
19	A	805	CLA	MG-NA	-5.09	1.94	2.06
19	B	819	CLA	MG-NB	-5.08	1.95	2.05
28	d	205	CHL	CMC-C2C	5.08	1.55	1.45
19	c	302	CLA	MG-NB	-5.08	1.95	2.05
19	m	305	CLA	MG-NB	-5.08	1.95	2.05
19	k	307	CLA	MG-NA	-5.08	1.94	2.06
19	A	801	CLA	C1B-NB	5.08	1.44	1.37
28	i	301	CHL	CMC-C2C	5.08	1.55	1.45
19	n	201	CLA	MG-NB	-5.08	1.95	2.05
19	a	306	CLA	C1B-NB	5.08	1.44	1.37
19	m	311	CLA	MG-NB	-5.07	1.95	2.05
19	j	305	CLA	MG-NA	-5.07	1.94	2.06
19	c	310	CLA	MG-NB	-5.07	1.95	2.05
19	B	805	CLA	MG-NB	-5.07	1.95	2.05
19	f	310	CLA	MG-NB	-5.07	1.95	2.05
19	k	310	CLA	MG-NB	-5.07	1.95	2.05
19	A	846	CLA	C1B-NB	5.07	1.44	1.37
19	i	309	CLA	MG-NB	-5.07	1.95	2.05
19	B	810	CLA	MG-NB	-5.07	1.95	2.05
19	j	308	CLA	MG-NB	-5.06	1.95	2.05
19	j	313	CLA	MG-NB	-5.06	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	306	CLA	MG-NB	-5.06	1.95	2.05
19	m	311	CLA	MG-NA	-5.06	1.94	2.06
19	b	302	CLA	MG-NA	-5.06	1.94	2.06
19	j	303	CLA	MG-NB	-5.06	1.95	2.05
19	A	806	CLA	MG-NA	-5.06	1.94	2.06
19	B	844	CLA	MG-NA	-5.06	1.94	2.06
19	B	832	CLA	MG-NA	-5.06	1.94	2.06
19	j	305	CLA	MG-NB	-5.05	1.95	2.05
19	n	207	CLA	MG-NA	-5.05	1.94	2.06
19	A	849	CLA	MG-NB	-5.05	1.95	2.05
19	B	814	CLA	MG-NB	-5.05	1.95	2.05
19	o	305	CLA	MG-NB	-5.05	1.95	2.05
19	o	306	CLA	MG-NB	-5.05	1.95	2.05
19	o	308	CLA	MG-NB	-5.05	1.95	2.05
19	B	833	CLA	MG-NB	-5.05	1.95	2.05
19	B	809	CLA	MG-NB	-5.05	1.95	2.05
19	A	815	CLA	MG-NA	-5.05	1.94	2.06
19	d	208	CLA	MG-NA	-5.05	1.94	2.06
19	B	822	CLA	MG-NA	-5.05	1.94	2.06
19	o	309	CLA	MG-NA	-5.05	1.94	2.06
19	A	809	CLA	MG-NA	-5.04	1.94	2.06
19	f	308	CLA	MG-NB	-5.04	1.95	2.05
19	o	305	CLA	MG-NA	-5.04	1.94	2.06
28	i	304	CHL	CMC-C2C	5.04	1.55	1.45
19	m	303	CLA	MG-NB	-5.04	1.95	2.05
19	A	850	CLA	MG-NA	-5.04	1.94	2.06
19	k	303	CLA	MG-NB	-5.04	1.95	2.05
19	g	302	CLA	MG-NB	-5.03	1.95	2.05
19	c	315	CLA	MG-NA	-5.03	1.94	2.06
19	h	204	CLA	MG-NB	-5.03	1.95	2.05
19	A	844	CLA	MG-NB	-5.03	1.95	2.05
19	i	307	CLA	MG-NB	-5.03	1.95	2.05
19	j	310	CLA	MG-NB	-5.03	1.95	2.05
19	c	311	CLA	MG-NB	-5.03	1.95	2.05
19	h	213	CLA	MG-NA	-5.03	1.94	2.06
19	f	312	CLA	MG-NB	-5.03	1.95	2.05
19	i	312	CLA	MG-NB	-5.03	1.95	2.05
19	B	849	CLA	MG-NB	-5.02	1.95	2.05
19	B	833	CLA	MG-NA	-5.02	1.94	2.06
19	A	808	CLA	MG-NB	-5.02	1.95	2.05
28	a	311	CHL	CMC-C2C	5.02	1.55	1.45
19	c	307	CLA	MG-NB	-5.02	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	306	CLA	MG-NA	-5.02	1.94	2.06
19	a	314	CLA	C1B-NB	5.02	1.44	1.37
19	i	303	CLA	MG-NB	-5.01	1.95	2.05
19	B	813	CLA	MG-NA	-5.01	1.94	2.06
19	b	309	CLA	MG-NB	-5.01	1.95	2.05
19	B	830	CLA	MG-NB	-5.01	1.95	2.05
19	d	207	CLA	MG-NA	-5.01	1.94	2.06
19	A	807	CLA	MG-NB	-5.01	1.95	2.05
19	h	209	CLA	MG-NB	-5.01	1.95	2.05
19	k	311	CLA	MG-NB	-5.01	1.95	2.05
19	b	306	CLA	C1B-NB	5.01	1.43	1.37
28	b	312	CHL	CMC-C2C	5.01	1.55	1.45
19	d	201	CLA	MG-NB	-5.00	1.95	2.05
28	c	305	CHL	CMC-C2C	5.00	1.55	1.45
19	i	306	CLA	MG-NB	-5.00	1.95	2.05
19	l	208	CLA	MG-NB	-5.00	1.95	2.05
19	a	310	CLA	MG-NB	-5.00	1.95	2.05
19	a	306	CLA	MG-NB	-5.00	1.95	2.05
19	A	823	CLA	C1B-NB	5.00	1.43	1.37
19	c	308	CLA	MG-NA	-5.00	1.94	2.06
19	B	818	CLA	MG-NA	-4.99	1.94	2.06
19	B	807	CLA	MG-NB	-4.99	1.95	2.05
19	j	306	CLA	C1B-NB	4.99	1.43	1.37
19	b	305	CLA	MG-NB	-4.99	1.95	2.05
19	l	207	CLA	MG-NB	-4.99	1.95	2.05
19	A	818	CLA	MG-NA	-4.99	1.94	2.06
19	d	212	CLA	MG-NB	-4.99	1.95	2.05
19	a	309	CLA	MG-NB	-4.99	1.95	2.05
19	l	201	CLA	MG-NA	-4.99	1.94	2.06
19	A	822	CLA	C1B-NB	4.98	1.43	1.37
19	D	301	CLA	MG-NB	-4.98	1.95	2.05
19	l	206	CLA	C1B-NB	4.98	1.43	1.37
19	f	302	CLA	MG-NA	-4.98	1.94	2.06
19	h	203	CLA	MG-NA	-4.98	1.94	2.06
19	A	804	CLA	MG-NA	-4.98	1.94	2.06
19	e	307	CLA	MG-NA	-4.98	1.94	2.06
19	B	817	CLA	MG-NA	-4.98	1.94	2.06
19	g	307	CLA	MG-NB	-4.98	1.95	2.05
19	A	822	CLA	MG-NB	-4.98	1.95	2.05
19	g	309	CLA	MG-NB	-4.98	1.95	2.05
19	F	203	CLA	MG-NA	-4.98	1.94	2.06
19	B	806	CLA	MG-NB	-4.98	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	g	305	CLA	MG-NA	-4.97	1.94	2.06
19	m	306	CLA	MG-NA	-4.97	1.94	2.06
19	i	302	CLA	MG-NA	-4.97	1.94	2.06
19	g	308	CLA	MG-NB	-4.97	1.95	2.05
19	n	205	CLA	MG-NA	-4.97	1.94	2.06
19	B	818	CLA	MG-NB	-4.97	1.95	2.05
19	B	812	CLA	MG-NB	-4.97	1.95	2.05
19	B	815	CLA	MG-NB	-4.97	1.95	2.05
19	A	828	CLA	MG-NB	-4.96	1.96	2.05
19	i	308	CLA	MG-NA	-4.96	1.94	2.06
19	F	204	CLA	MG-NB	-4.96	1.96	2.05
19	c	309	CLA	MG-NB	-4.96	1.96	2.05
19	B	839	CLA	MG-NB	-4.96	1.96	2.05
19	A	823	CLA	MG-NB	-4.96	1.96	2.05
19	o	304	CLA	C1B-NB	4.95	1.43	1.37
19	A	805	CLA	MG-NB	-4.95	1.96	2.05
19	e	309	CLA	MG-NB	-4.95	1.96	2.05
19	A	814	CLA	MG-NB	-4.94	1.96	2.05
19	e	302	CLA	MG-NA	-4.94	1.94	2.06
19	B	822	CLA	MG-NB	-4.94	1.96	2.05
19	m	303	CLA	MG-NA	-4.94	1.94	2.06
19	g	304	CLA	MG-NA	-4.93	1.94	2.06
19	a	305	CLA	MG-NA	-4.93	1.94	2.06
19	i	312	CLA	MG-NA	-4.93	1.94	2.06
19	B	805	CLA	MG-NA	-4.93	1.94	2.06
19	A	829	CLA	MG-NA	-4.93	1.94	2.06
19	A	808	CLA	MG-NA	-4.93	1.94	2.06
19	a	302	CLA	C1B-NB	4.93	1.43	1.37
19	d	211	CLA	MG-NB	-4.92	1.96	2.05
19	A	840	CLA	MG-NA	-4.92	1.94	2.06
28	c	312	CHL	CMC-C2C	4.91	1.55	1.45
19	B	841	CLA	MG-NB	-4.91	1.96	2.05
19	c	304	CLA	MG-NB	-4.91	1.96	2.05
19	J	803	CLA	MG-NB	-4.90	1.96	2.05
19	l	207	CLA	MG-NA	-4.90	1.94	2.06
19	m	307	CLA	MG-NA	-4.90	1.94	2.06
19	B	801	CLA	C1B-NB	4.90	1.43	1.37
19	A	804	CLA	MG-NB	-4.90	1.96	2.05
19	h	212	CLA	MG-NB	-4.90	1.96	2.05
19	B	810	CLA	MG-NA	-4.90	1.94	2.06
19	c	316	CLA	MG-NB	-4.90	1.96	2.05
19	h	207	CLA	MG-NA	-4.90	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	o	311	CLA	MG-NB	-4.89	1.96	2.05
19	g	305	CLA	C1B-NB	4.89	1.43	1.37
19	A	821	CLA	MG-NB	-4.89	1.96	2.05
19	j	311	CLA	MG-NB	-4.89	1.96	2.05
19	c	309	CLA	MG-NA	-4.88	1.94	2.06
19	A	802	CLA	C1B-NB	4.88	1.43	1.37
19	c	315	CLA	MG-ND	-4.88	1.96	2.05
19	d	208	CLA	MG-NB	-4.88	1.96	2.05
19	d	209	CLA	MG-NB	-4.88	1.96	2.05
19	k	308	CLA	MG-NA	-4.88	1.94	2.06
19	m	305	CLA	MG-NA	-4.87	1.94	2.06
19	j	308	CLA	MG-NA	-4.87	1.94	2.06
19	A	807	CLA	MG-NA	-4.87	1.94	2.06
19	A	824	CLA	MG-NA	-4.87	1.94	2.06
19	h	201	CLA	MG-NA	-4.87	1.94	2.06
19	a	308	CLA	MG-NA	-4.86	1.94	2.06
19	d	208	CLA	C1B-NB	4.86	1.43	1.37
19	B	823	CLA	MG-NB	-4.86	1.96	2.05
19	o	309	CLA	C1B-NB	4.86	1.43	1.37
19	o	308	CLA	MG-NA	-4.85	1.94	2.06
19	e	309	CLA	MG-NA	-4.85	1.94	2.06
19	A	849	CLA	MG-NA	-4.85	1.94	2.06
19	i	306	CLA	MG-NA	-4.85	1.94	2.06
19	b	315	CLA	C1B-NB	4.85	1.43	1.37
19	d	203	CLA	MG-NA	-4.85	1.94	2.06
19	f	306	CLA	MG-NA	-4.85	1.94	2.06
19	B	837	CLA	C1B-NB	4.84	1.43	1.37
19	f	303	CLA	MG-NB	-4.84	1.96	2.05
19	a	304	CLA	MG-NB	-4.84	1.96	2.05
19	e	310	CLA	C1B-NB	4.84	1.43	1.37
19	b	304	CLA	MG-NB	-4.83	1.96	2.05
19	J	803	CLA	MG-NA	-4.83	1.94	2.06
19	A	801	CLA	MG-NA	-4.83	1.94	2.06
19	c	311	CLA	MG-NA	-4.83	1.94	2.06
28	e	304	CHL	CMC-C2C	4.83	1.55	1.45
19	g	305	CLA	MG-NB	-4.83	1.96	2.05
28	g	303	CHL	CMC-C2C	4.83	1.55	1.45
19	B	815	CLA	MG-NA	-4.82	1.94	2.06
19	B	817	CLA	MG-NB	-4.82	1.96	2.05
19	B	820	CLA	MG-NA	-4.82	1.94	2.06
19	B	812	CLA	MG-NA	-4.82	1.94	2.06
19	l	205	CLA	MG-NA	-4.82	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	e	311	CLA	MG-NA	-4.82	1.94	2.06
19	a	310	CLA	MG-NA	-4.81	1.94	2.06
19	g	302	CLA	MG-NA	-4.81	1.94	2.06
19	e	305	CLA	MG-NB	-4.81	1.96	2.05
19	F	201	CLA	MG-NA	-4.81	1.94	2.06
19	k	305	CLA	MG-NA	-4.81	1.94	2.06
19	B	841	CLA	MG-NA	-4.81	1.94	2.06
28	g	306	CHL	CMC-C2C	4.80	1.55	1.45
19	h	209	CLA	MG-NA	-4.80	1.94	2.06
19	B	832	CLA	C1B-NB	4.80	1.43	1.37
19	i	307	CLA	MG-NA	-4.79	1.94	2.06
19	b	303	CLA	MG-NB	-4.79	1.96	2.05
19	A	823	CLA	MG-NA	-4.79	1.94	2.06
19	A	802	CLA	MG-NA	-4.79	1.94	2.06
19	A	814	CLA	MG-NA	-4.79	1.94	2.06
19	B	823	CLA	MG-NA	-4.79	1.94	2.06
19	B	835	CLA	MG-NA	-4.79	1.94	2.06
19	l	204	CLA	MG-NA	-4.78	1.94	2.06
19	A	846	CLA	MG-NA	-4.78	1.94	2.06
19	A	826	CLA	MG-NB	-4.78	1.96	2.05
19	F	202	CLA	MG-NA	-4.78	1.94	2.06
19	A	848	CLA	MG-NA	-4.78	1.94	2.06
19	A	841	CLA	MG-NA	-4.78	1.94	2.06
28	h	202	CHL	CMC-C2C	4.77	1.55	1.45
19	A	852	CLA	MG-NA	-4.77	1.94	2.06
19	A	853	CLA	MG-NA	-4.77	1.94	2.06
19	B	801	CLA	MG-NA	-4.77	1.94	2.06
19	B	846	CLA	MG-NA	-4.77	1.94	2.06
19	k	311	CLA	MG-NA	-4.77	1.94	2.06
19	g	304	CLA	C1B-NB	4.76	1.43	1.37
19	B	846	CLA	C1B-NB	4.76	1.43	1.37
19	B	819	CLA	MG-NA	-4.76	1.95	2.06
19	g	304	CLA	MG-NB	-4.76	1.96	2.05
19	e	306	CLA	MG-NA	-4.76	1.95	2.06
19	g	309	CLA	MG-NA	-4.75	1.95	2.06
19	g	308	CLA	MG-NA	-4.75	1.95	2.06
19	B	803	CLA	MG-NA	-4.75	1.95	2.06
19	l	208	CLA	MG-NA	-4.74	1.95	2.06
19	f	310	CLA	MG-NA	-4.73	1.95	2.06
19	b	307	CLA	MG-NA	-4.73	1.95	2.06
19	B	846	CLA	C1D-ND	4.73	1.43	1.37
19	b	309	CLA	MG-NA	-4.72	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	809	CLA	MG-NA	-4.72	1.95	2.06
19	j	302	CLA	MG-NA	-4.72	1.95	2.06
19	a	303	CLA	MG-NA	-4.72	1.95	2.06
19	d	206	CLA	MG-NA	-4.71	1.95	2.06
19	j	313	CLA	MG-NA	-4.71	1.95	2.06
19	h	210	CLA	MG-NA	-4.70	1.95	2.06
19	k	306	CLA	MG-NA	-4.70	1.95	2.06
19	k	310	CLA	MG-NA	-4.70	1.95	2.06
28	f	304	CHL	CMC-C2C	4.70	1.55	1.45
19	f	308	CLA	MG-NA	-4.70	1.95	2.06
19	b	304	CLA	C1B-NB	4.70	1.43	1.37
19	l	201	CLA	MG-NB	-4.69	1.96	2.05
19	A	822	CLA	MG-NA	-4.69	1.95	2.06
19	a	309	CLA	MG-NA	-4.69	1.95	2.06
19	l	201	CLA	C1B-NB	4.68	1.43	1.37
19	A	816	CLA	MG-NB	-4.68	1.96	2.05
19	c	315	CLA	MG-NB	-4.68	1.96	2.05
19	g	307	CLA	MG-NA	-4.68	1.95	2.06
19	d	204	CLA	MG-NA	-4.67	1.95	2.06
19	B	807	CLA	MG-NA	-4.67	1.95	2.06
19	c	310	CLA	MG-NA	-4.66	1.95	2.06
19	A	816	CLA	MG-NA	-4.65	1.95	2.06
19	c	307	CLA	MG-NA	-4.64	1.95	2.06
19	h	204	CLA	MG-NA	-4.64	1.95	2.06
19	b	305	CLA	C1B-NB	4.63	1.43	1.37
19	n	208	CLA	MG-NB	-4.63	1.96	2.05
19	m	310	CLA	MG-NA	-4.63	1.95	2.06
19	A	853	CLA	MG-NB	-4.62	1.96	2.05
19	B	842	CLA	MG-NA	-4.61	1.95	2.06
19	e	303	CLA	MG-NB	-4.61	1.96	2.05
19	a	304	CLA	MG-NA	-4.61	1.95	2.06
19	o	310	CLA	MG-NA	-4.61	1.95	2.06
28	c	313	CHL	CMC-C2C	4.61	1.54	1.45
19	b	306	CLA	MG-NA	-4.60	1.95	2.06
19	k	302	CLA	C1B-NB	4.60	1.43	1.37
19	B	830	CLA	MG-NA	-4.59	1.95	2.06
19	h	212	CLA	MG-NA	-4.59	1.95	2.06
19	d	212	CLA	MG-NA	-4.58	1.95	2.06
19	j	309	CLA	MG-NA	-4.58	1.95	2.06
19	c	302	CLA	MG-NA	-4.56	1.95	2.06
19	n	206	CLA	MG-NC	-4.56	1.95	2.06
19	A	812	CLA	MG-NA	-4.56	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	821	CLA	MG-NA	-4.55	1.95	2.06
19	d	201	CLA	MG-NA	-4.54	1.95	2.06
19	A	844	CLA	MG-NA	-4.54	1.95	2.06
19	i	303	CLA	MG-NA	-4.53	1.95	2.06
19	n	208	CLA	C1B-NB	4.52	1.43	1.37
19	B	811	CLA	MG-NA	-4.51	1.95	2.06
19	B	806	CLA	MG-NA	-4.51	1.95	2.06
19	A	826	CLA	MG-NA	-4.51	1.95	2.06
19	h	211	CLA	MG-NA	-4.50	1.95	2.06
19	D	301	CLA	MG-NA	-4.50	1.95	2.06
19	k	303	CLA	MG-NA	-4.47	1.95	2.06
19	A	810	CLA	MG-NA	-4.47	1.95	2.06
19	B	839	CLA	MG-NA	-4.47	1.95	2.06
19	d	209	CLA	MG-NA	-4.46	1.95	2.06
19	F	204	CLA	MG-NA	-4.46	1.95	2.06
19	j	310	CLA	C1B-NB	4.45	1.43	1.37
19	c	316	CLA	MG-NA	-4.44	1.95	2.06
19	b	308	CLA	MG-NA	-4.44	1.95	2.06
19	B	830	CLA	C4B-NB	4.43	1.43	1.37
19	m	302	CLA	C1B-NB	4.42	1.43	1.37
19	a	304	CLA	C4B-NB	4.40	1.43	1.37
19	h	209	CLA	C4B-NB	4.40	1.43	1.37
19	j	304	CLA	C1B-NB	4.38	1.43	1.37
19	a	309	CLA	C4B-NB	4.38	1.43	1.37
19	m	309	CLA	C1B-NB	4.36	1.43	1.37
19	f	303	CLA	MG-NA	-4.35	1.95	2.06
19	k	303	CLA	C4B-NB	4.34	1.43	1.37
19	i	306	CLA	C4B-NB	4.34	1.43	1.37
19	b	303	CLA	MG-NA	-4.33	1.96	2.06
19	e	305	CLA	C4B-NB	4.32	1.43	1.37
19	o	311	CLA	MG-NA	-4.32	1.96	2.06
19	m	304	CLA	MG-NC	-4.31	1.96	2.06
19	i	302	CLA	C4B-NB	4.30	1.43	1.37
19	e	303	CLA	C4B-NB	4.30	1.43	1.37
19	d	211	CLA	C4B-NB	4.30	1.43	1.37
19	e	303	CLA	MG-NA	-4.30	1.96	2.06
19	j	305	CLA	C1B-NB	4.29	1.43	1.37
19	h	207	CLA	C4B-NB	4.29	1.43	1.37
19	i	309	CLA	MG-NA	-4.29	1.96	2.06
19	c	309	CLA	C4B-NB	4.29	1.43	1.37
19	f	308	CLA	C4B-NB	4.28	1.43	1.37
19	g	307	CLA	C4B-NB	4.28	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	853	CLA	C4B-NB	4.27	1.43	1.37
19	c	307	CLA	C4B-NB	4.27	1.43	1.37
19	A	839	CLA	MG-NA	-4.27	1.96	2.06
19	h	210	CLA	C4B-NB	4.27	1.43	1.37
19	j	303	CLA	MG-NA	-4.27	1.96	2.06
19	o	302	CLA	MG-NC	-4.27	1.96	2.06
19	e	309	CLA	C4B-NB	4.26	1.43	1.37
19	e	302	CLA	C4B-NB	4.26	1.43	1.37
19	b	308	CLA	C4B-NB	4.26	1.43	1.37
19	n	206	CLA	C1B-NB	4.25	1.43	1.37
19	i	305	CLA	C4B-NB	4.25	1.43	1.37
19	o	311	CLA	C4B-NB	4.25	1.43	1.37
19	l	206	CLA	MG-NC	-4.25	1.96	2.06
19	b	315	CLA	MG-NC	-4.25	1.96	2.06
19	g	308	CLA	C4B-NB	4.24	1.43	1.37
19	h	204	CLA	C4B-NB	4.24	1.43	1.37
19	d	209	CLA	C4B-NB	4.23	1.43	1.37
19	i	303	CLA	C4B-NB	4.23	1.43	1.37
19	n	201	CLA	C4B-NB	4.23	1.43	1.37
19	f	303	CLA	C4B-NB	4.23	1.43	1.37
19	m	311	CLA	C4B-NB	4.22	1.43	1.37
19	A	819	CLA	MG-NA	-4.22	1.96	2.06
19	c	311	CLA	C4B-NB	4.21	1.43	1.37
19	d	211	CLA	MG-NA	-4.21	1.96	2.06
19	f	310	CLA	C4B-NB	4.21	1.43	1.37
19	n	201	CLA	MG-NA	-4.21	1.96	2.06
19	h	212	CLA	C4B-NB	4.20	1.43	1.37
19	B	842	CLA	C4B-NB	4.19	1.42	1.37
19	f	312	CLA	C4B-NB	4.19	1.42	1.37
19	B	819	CLA	C4B-NB	4.19	1.42	1.37
19	c	315	CLA	C4B-NB	4.19	1.42	1.37
19	F	204	CLA	C4B-NB	4.19	1.42	1.37
19	h	203	CLA	C4B-NB	4.19	1.42	1.37
19	i	309	CLA	C4B-NB	4.19	1.42	1.37
19	m	310	CLA	C4B-NB	4.18	1.42	1.37
19	d	203	CLA	C4B-NB	4.18	1.42	1.37
19	A	824	CLA	C4B-NB	4.18	1.42	1.37
19	j	302	CLA	C4B-NB	4.17	1.42	1.37
19	A	805	CLA	C4B-NB	4.17	1.42	1.37
19	A	826	CLA	C4B-NB	4.17	1.42	1.37
19	B	823	CLA	C4B-NB	4.17	1.42	1.37
19	b	303	CLA	C4B-NB	4.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	o	310	CLA	C4B-NB	4.16	1.42	1.37
19	B	810	CLA	C4B-NB	4.16	1.42	1.37
19	k	311	CLA	C4B-NB	4.16	1.42	1.37
19	A	819	CLA	C4B-NB	4.16	1.42	1.37
19	F	202	CLA	C4B-NB	4.16	1.42	1.37
19	l	208	CLA	C4B-NB	4.16	1.42	1.37
19	o	305	CLA	C4B-NB	4.16	1.42	1.37
19	f	302	CLA	C4B-NB	4.16	1.42	1.37
19	A	817	CLA	C4B-NB	4.16	1.42	1.37
19	l	207	CLA	C4B-NB	4.15	1.42	1.37
19	A	844	CLA	C4B-NB	4.15	1.42	1.37
19	B	812	CLA	C4B-NB	4.15	1.42	1.37
19	o	306	CLA	C4B-NB	4.15	1.42	1.37
19	l	204	CLA	C4B-NB	4.15	1.42	1.37
19	A	808	CLA	C4B-NB	4.15	1.42	1.37
19	m	306	CLA	C4B-NB	4.15	1.42	1.37
19	a	303	CLA	C4B-NB	4.15	1.42	1.37
19	k	308	CLA	C4B-NB	4.14	1.42	1.37
19	J	803	CLA	C4B-NB	4.14	1.42	1.37
19	h	211	CLA	C4B-NB	4.14	1.42	1.37
19	b	302	CLA	C4B-NB	4.14	1.42	1.37
19	g	302	CLA	C4B-NB	4.14	1.42	1.37
19	A	804	CLA	C4B-NB	4.14	1.42	1.37
19	B	806	CLA	C4B-NB	4.13	1.42	1.37
19	i	308	CLA	C4B-NB	4.13	1.42	1.37
19	j	303	CLA	C4B-NB	4.13	1.42	1.37
19	o	308	CLA	C4B-NB	4.13	1.42	1.37
19	j	311	CLA	MG-NA	-4.12	1.96	2.06
19	n	209	CLA	MG-NC	-4.12	1.96	2.06
19	D	301	CLA	C4B-NB	4.12	1.42	1.37
19	i	312	CLA	C4B-NB	4.12	1.42	1.37
19	m	303	CLA	C4B-NB	4.12	1.42	1.37
19	A	845	CLA	C4B-NB	4.12	1.42	1.37
19	A	849	CLA	C4B-NB	4.11	1.42	1.37
19	n	205	CLA	C4B-NB	4.11	1.42	1.37
19	A	842	CLA	C1B-NB	4.11	1.42	1.37
19	b	309	CLA	C4B-NB	4.11	1.42	1.37
19	f	309	CLA	C4B-NB	4.11	1.42	1.37
19	c	310	CLA	C4B-NB	4.11	1.42	1.37
19	e	311	CLA	C4B-NB	4.11	1.42	1.37
19	c	316	CLA	C4B-NB	4.10	1.42	1.37
19	m	308	CLA	C4B-NB	4.10	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	303	CLA	C4B-NB	4.10	1.42	1.37
19	k	310	CLA	C4B-NB	4.10	1.42	1.37
19	A	821	CLA	C4B-NB	4.10	1.42	1.37
19	j	308	CLA	C4B-NB	4.10	1.42	1.37
19	c	302	CLA	C4B-NB	4.10	1.42	1.37
19	A	848	CLA	C4B-NB	4.10	1.42	1.37
19	B	836	CLA	MG-NA	-4.09	1.96	2.06
19	B	805	CLA	C4B-NB	4.09	1.42	1.37
19	B	835	CLA	C4B-NB	4.09	1.42	1.37
19	d	204	CLA	C4B-NB	4.09	1.42	1.37
19	o	312	CLA	C4B-NB	4.09	1.42	1.37
19	B	836	CLA	C4B-NB	4.09	1.42	1.37
19	A	841	CLA	C4B-NB	4.09	1.42	1.37
19	i	307	CLA	C4B-NB	4.08	1.42	1.37
19	c	304	CLA	C4B-NB	4.08	1.42	1.37
19	e	306	CLA	C4B-NB	4.08	1.42	1.37
19	j	309	CLA	C4B-NB	4.08	1.42	1.37
19	B	821	CLA	C4B-NB	4.08	1.42	1.37
19	e	307	CLA	C4B-NB	4.07	1.42	1.37
19	c	304	CLA	MG-NA	-4.07	1.96	2.06
19	d	207	CLA	C4B-NB	4.07	1.42	1.37
19	B	815	CLA	C4B-NB	4.07	1.42	1.37
19	b	307	CLA	C4B-NB	4.06	1.42	1.37
19	c	314	CLA	C4B-NB	4.06	1.42	1.37
19	B	839	CLA	C4B-NB	4.06	1.42	1.37
19	A	807	CLA	C4B-NB	4.05	1.42	1.37
19	a	310	CLA	C4B-NB	4.05	1.42	1.37
19	j	311	CLA	C4B-NB	4.05	1.42	1.37
19	A	829	CLA	C4B-NB	4.05	1.42	1.37
19	d	201	CLA	C4B-NB	4.05	1.42	1.37
19	n	204	CLA	C4B-NB	4.05	1.42	1.37
19	c	306	CLA	C4B-NB	4.04	1.42	1.37
19	A	852	CLA	C4B-NB	4.04	1.42	1.37
19	b	313	CLA	C4B-NB	4.04	1.42	1.37
19	o	307	CLA	C4B-NB	4.04	1.42	1.37
19	A	828	CLA	C4B-NB	4.03	1.42	1.37
19	f	306	CLA	C4B-NB	4.03	1.42	1.37
19	h	201	CLA	C4B-NB	4.03	1.42	1.37
19	h	208	CLA	C4B-NB	4.03	1.42	1.37
19	B	847	CLA	C4B-NB	4.03	1.42	1.37
19	A	816	CLA	C4B-NB	4.03	1.42	1.37
19	A	815	CLA	C4B-NB	4.03	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	818	CLA	C4B-NB	4.02	1.42	1.37
19	A	850	CLA	C4B-NB	4.02	1.42	1.37
19	g	311	CLA	C4B-NB	4.01	1.42	1.37
19	l	205	CLA	C4B-NB	4.01	1.42	1.37
19	d	212	CLA	C4B-NB	4.01	1.42	1.37
19	B	813	CLA	C4B-NB	4.01	1.42	1.37
19	B	820	CLA	C4B-NB	4.01	1.42	1.37
19	f	307	CLA	C4B-NB	4.01	1.42	1.37
19	n	207	CLA	C4B-NB	4.01	1.42	1.37
19	k	307	CLA	C4B-NB	4.01	1.42	1.37
19	h	213	CLA	C4B-NB	4.00	1.42	1.37
19	A	840	CLA	C4B-NB	4.00	1.42	1.37
19	l	209	CLA	C4B-NB	4.00	1.42	1.37
19	g	301	CLA	C1B-NB	4.00	1.42	1.37
19	g	309	CLA	C4B-NB	3.99	1.42	1.37
19	B	837	CLA	MG-NC	-3.99	1.96	2.06
19	A	806	CLA	C4B-NB	3.99	1.42	1.37
19	j	307	CLA	C4B-NB	3.99	1.42	1.37
19	f	311	CLA	C4B-NB	3.98	1.42	1.37
19	A	810	CLA	C4B-NB	3.98	1.42	1.37
19	k	306	CLA	C4B-NB	3.98	1.42	1.37
19	B	833	CLA	C4B-NB	3.97	1.42	1.37
19	n	202	CLA	C4B-NB	3.96	1.42	1.37
19	a	305	CLA	C4B-NB	3.96	1.42	1.37
19	a	307	CLA	C4B-NB	3.96	1.42	1.37
19	k	309	CLA	C4B-NB	3.96	1.42	1.37
19	A	822	CLA	C4B-NB	3.96	1.42	1.37
19	k	305	CLA	C4B-NB	3.96	1.42	1.37
19	A	814	CLA	C4B-NB	3.95	1.42	1.37
19	n	209	CLA	C4B-NB	3.95	1.42	1.37
19	A	846	CLA	C4B-NB	3.95	1.42	1.37
19	h	206	CLA	C4B-NB	3.95	1.42	1.37
19	A	839	CLA	C4B-NB	3.95	1.42	1.37
19	j	306	CLA	MG-NC	-3.94	1.96	2.06
19	A	843	CLA	C4B-NB	3.94	1.42	1.37
19	f	305	CLA	C4B-NB	3.94	1.42	1.37
19	B	841	CLA	C4B-NB	3.94	1.42	1.37
19	a	308	CLA	C4B-NB	3.94	1.42	1.37
19	o	304	CLA	MG-NC	-3.93	1.96	2.06
19	c	308	CLA	C4B-NB	3.93	1.42	1.37
19	m	307	CLA	C4B-NB	3.93	1.42	1.37
19	B	848	CLA	MG-NC	-3.93	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	814	CLA	C4B-NB	3.92	1.42	1.37
19	B	807	CLA	C4B-NB	3.92	1.42	1.37
19	B	849	CLA	C4B-NB	3.91	1.42	1.37
19	A	813	CLA	C4B-NB	3.91	1.42	1.37
19	k	302	CLA	MG-NC	-3.91	1.97	2.06
19	o	303	CLA	C4B-NB	3.91	1.42	1.37
19	B	816	CLA	C4B-NB	3.91	1.42	1.37
19	F	203	CLA	C4B-NB	3.91	1.42	1.37
19	A	811	CLA	C4B-NB	3.91	1.42	1.37
19	g	301	CLA	MG-NC	-3.90	1.97	2.06
19	A	809	CLA	C4B-NB	3.90	1.42	1.37
19	B	822	CLA	C4B-NB	3.90	1.42	1.37
19	d	210	CLA	C4B-NB	3.90	1.42	1.37
19	B	844	CLA	C4B-NB	3.90	1.42	1.37
19	l	202	CLA	C4B-NB	3.89	1.42	1.37
19	f	314	CLA	C4B-NB	3.88	1.42	1.37
19	A	842	CLA	MG-NC	-3.88	1.97	2.06
19	e	308	CLA	C4B-NB	3.88	1.42	1.37
19	j	312	CLA	C4B-NB	3.88	1.42	1.37
19	A	843	CLA	MG-NC	-3.88	1.97	2.06
19	g	305	CLA	MG-NC	-3.88	1.97	2.06
19	B	817	CLA	C4B-NB	3.87	1.42	1.37
19	A	812	CLA	C4B-NB	3.87	1.42	1.37
19	j	313	CLA	C4B-NB	3.87	1.42	1.37
19	n	208	CLA	MG-NC	-3.87	1.97	2.06
19	i	311	CLA	C4B-NB	3.86	1.42	1.37
19	A	847	CLA	C4B-NB	3.86	1.42	1.37
19	F	201	CLA	C4B-NB	3.86	1.42	1.37
19	A	801	CLA	C4B-NB	3.86	1.42	1.37
19	B	840	CLA	C4B-NB	3.86	1.42	1.37
19	e	308	CLA	MG-NC	-3.86	1.97	2.06
19	j	301	CLA	C4B-NB	3.85	1.42	1.37
19	d	208	CLA	MG-NC	-3.85	1.97	2.06
19	j	304	CLA	MG-NC	-3.84	1.97	2.06
19	o	303	CLA	MG-NC	-3.84	1.97	2.06
19	d	206	CLA	C4B-NB	3.84	1.42	1.37
19	b	304	CLA	MG-NC	-3.84	1.97	2.06
19	B	818	CLA	C4B-NB	3.84	1.42	1.37
19	B	838	CLA	C4B-NB	3.83	1.42	1.37
19	a	302	CLA	C4B-NB	3.83	1.42	1.37
19	A	827	CLA	C4B-NB	3.83	1.42	1.37
19	B	845	CLA	C4B-NB	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	809	CLA	C4B-NB	3.82	1.42	1.37
19	B	843	CLA	C4B-NB	3.82	1.42	1.37
19	g	304	CLA	C4B-NB	3.81	1.42	1.37
19	l	203	CLA	C4B-NB	3.81	1.42	1.37
19	B	848	CLA	C4B-NB	3.81	1.42	1.37
19	o	309	CLA	MG-NC	-3.81	1.97	2.06
19	b	304	CLA	C4B-NB	3.80	1.42	1.37
19	m	302	CLA	MG-NC	-3.80	1.97	2.06
19	B	804	CLA	C4B-NB	3.78	1.42	1.37
19	i	310	CLA	C1B-NB	3.78	1.42	1.37
19	a	302	CLA	MG-NC	-3.77	1.97	2.06
19	A	803	CLA	C4B-NB	3.77	1.42	1.37
19	l	201	CLA	C4B-NB	3.76	1.42	1.37
19	B	849	CLA	MG-NC	-3.76	1.97	2.06
19	B	811	CLA	C4B-NB	3.75	1.42	1.37
19	a	306	CLA	C4B-NB	3.75	1.42	1.37
19	A	825	CLA	C4B-NB	3.74	1.42	1.37
19	b	306	CLA	C4B-NB	3.74	1.42	1.37
19	a	314	CLA	MG-NC	-3.74	1.97	2.06
19	a	314	CLA	C4B-NB	3.74	1.42	1.37
25	d	213	LMG	C4-C5	3.73	1.60	1.53
19	n	203	CLA	C4B-NB	3.73	1.42	1.37
19	j	305	CLA	MG-NC	-3.73	1.97	2.06
19	e	310	CLA	MG-NC	-3.72	1.97	2.06
19	B	803	CLA	C4B-NB	3.72	1.42	1.37
19	o	302	CLA	C4B-NB	3.72	1.42	1.37
19	A	820	CLA	C4B-NB	3.71	1.42	1.37
19	k	304	CLA	C4B-NB	3.69	1.42	1.37
19	j	306	CLA	C4B-NB	3.69	1.42	1.37
19	A	823	CLA	C4B-NB	3.69	1.42	1.37
19	l	202	CLA	MG-NC	-3.67	1.97	2.06
19	B	832	CLA	MG-NC	-3.66	1.97	2.06
19	d	208	CLA	C4B-NB	3.66	1.42	1.37
19	B	840	CLA	MG-NC	-3.66	1.97	2.06
19	o	309	CLA	C4B-NB	3.65	1.42	1.37
19	o	307	CLA	MG-NC	-3.65	1.97	2.06
19	i	313	CLA	C4B-NB	3.65	1.42	1.37
19	j	310	CLA	C4B-NB	3.65	1.42	1.37
19	m	305	CLA	C4B-NB	3.64	1.42	1.37
19	B	808	CLA	C4B-NB	3.64	1.42	1.37
19	g	304	CLA	MG-NC	-3.62	1.97	2.06
19	a	306	CLA	MG-NC	-3.59	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	f	314	CLA	MG-NC	-3.59	1.97	2.06
19	m	309	CLA	MG-NC	-3.59	1.97	2.06
19	h	205	CLA	C4B-NB	3.57	1.42	1.37
19	B	838	CLA	MG-NC	-3.57	1.97	2.06
19	B	846	CLA	C4B-NB	3.56	1.42	1.37
19	B	847	CLA	MG-NC	-3.56	1.97	2.06
19	i	310	CLA	MG-NC	-3.55	1.97	2.06
19	n	204	CLA	MG-NC	-3.55	1.97	2.06
19	A	845	CLA	MG-NC	-3.54	1.97	2.06
19	b	306	CLA	MG-NC	-3.54	1.97	2.06
19	l	201	CLA	MG-NC	-3.53	1.97	2.06
19	i	305	CLA	MG-NC	-3.53	1.97	2.06
19	b	305	CLA	C4B-NB	3.53	1.42	1.37
19	B	846	CLA	MG-NC	-3.53	1.97	2.06
19	A	817	CLA	MG-NC	-3.52	1.97	2.06
19	j	310	CLA	MG-NC	-3.52	1.97	2.06
19	B	804	CLA	MG-NC	-3.52	1.97	2.06
19	i	313	CLA	MG-NC	-3.52	1.97	2.06
19	b	305	CLA	MG-NC	-3.52	1.97	2.06
19	n	202	CLA	MG-NC	-3.50	1.97	2.06
19	k	304	CLA	MG-NC	-3.50	1.97	2.06
19	l	206	CLA	C4B-NB	3.50	1.42	1.37
19	A	853	CLA	MG-NC	-3.50	1.98	2.06
19	h	205	CLA	MG-NC	-3.49	1.98	2.06
19	j	312	CLA	MG-NC	-3.49	1.98	2.06
19	B	832	CLA	C4B-NB	3.48	1.42	1.37
19	j	307	CLA	MG-NC	-3.47	1.98	2.06
19	j	301	CLA	MG-NC	-3.47	1.98	2.06
19	f	305	CLA	MG-NC	-3.47	1.98	2.06
19	B	841	CLA	MG-NC	-3.47	1.98	2.06
19	g	305	CLA	C4B-NB	3.47	1.42	1.37
19	A	803	CLA	MG-NC	-3.45	1.98	2.06
19	A	801	CLA	MG-NC	-3.45	1.98	2.06
19	i	311	CLA	MG-NC	-3.45	1.98	2.06
19	b	315	CLA	C4B-NB	3.44	1.42	1.37
19	n	203	CLA	MG-NC	-3.44	1.98	2.06
19	k	309	CLA	MG-NC	-3.44	1.98	2.06
19	e	310	CLA	C4B-NB	3.43	1.42	1.37
19	c	303	CLA	MG-NC	-3.43	1.98	2.06
19	g	311	CLA	MG-NC	-3.42	1.98	2.06
19	l	203	CLA	MG-NC	-3.42	1.98	2.06
19	f	311	CLA	MG-NC	-3.41	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	i	310	CLA	C4B-NB	3.41	1.42	1.37
19	d	210	CLA	MG-NC	-3.40	1.98	2.06
19	m	308	CLA	MG-NC	-3.39	1.98	2.06
19	A	827	CLA	MG-NC	-3.39	1.98	2.06
28	o	301	CHL	O2D-CGD	3.39	1.41	1.33
19	B	816	CLA	MG-NC	-3.38	1.98	2.06
19	m	304	CLA	C4B-NB	3.38	1.41	1.37
19	c	306	CLA	MG-NC	-3.38	1.98	2.06
19	o	306	CLA	MG-NC	-3.38	1.98	2.06
19	h	206	CLA	MG-NC	-3.37	1.98	2.06
19	a	307	CLA	MG-NC	-3.37	1.98	2.06
19	m	306	CLA	MG-NC	-3.37	1.98	2.06
19	A	806	CLA	MG-NC	-3.35	1.98	2.06
28	m	301	CHL	O2D-CGD	3.35	1.41	1.33
19	h	201	CLA	MG-NC	-3.34	1.98	2.06
19	A	825	CLA	MG-NC	-3.34	1.98	2.06
19	h	213	CLA	MG-NC	-3.33	1.98	2.06
19	B	822	CLA	MG-NC	-3.33	1.98	2.06
19	e	305	CLA	MG-NC	-3.33	1.98	2.06
19	B	808	CLA	MG-NC	-3.32	1.98	2.06
28	d	202	CHL	O2D-CGD	3.32	1.41	1.33
19	j	304	CLA	C4B-NB	3.32	1.41	1.37
19	b	313	CLA	MG-NC	-3.32	1.98	2.06
19	o	305	CLA	MG-NC	-3.31	1.98	2.06
19	A	847	CLA	MG-NC	-3.31	1.98	2.06
28	g	306	CHL	O2D-CGD	3.31	1.41	1.33
19	d	207	CLA	MG-NC	-3.31	1.98	2.06
28	b	314	CHL	O2D-CGD	3.31	1.41	1.33
19	A	813	CLA	MG-NC	-3.30	1.98	2.06
19	B	843	CLA	MG-NC	-3.30	1.98	2.06
19	b	302	CLA	MG-NC	-3.30	1.98	2.06
19	o	304	CLA	C4B-NB	3.30	1.41	1.37
19	i	302	CLA	MG-NC	-3.29	1.98	2.06
19	o	312	CLA	MG-NC	-3.29	1.98	2.06
28	b	301	CHL	O2D-CGD	3.29	1.41	1.33
19	B	813	CLA	MG-NC	-3.29	1.98	2.06
19	A	811	CLA	MG-NC	-3.29	1.98	2.06
19	A	805	CLA	MG-NC	-3.29	1.98	2.06
19	l	209	CLA	MG-NC	-3.29	1.98	2.06
19	B	812	CLA	MG-NC	-3.28	1.98	2.06
28	a	315	CHL	O2D-CGD	3.28	1.41	1.33
28	a	312	CHL	O2D-CGD	3.27	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	837	CLA	C4B-NB	3.27	1.41	1.37
19	A	820	CLA	MG-NC	-3.27	1.98	2.06
19	B	821	CLA	MG-NC	-3.27	1.98	2.06
19	f	312	CLA	MG-NC	-3.26	1.98	2.06
28	c	312	CHL	O2D-CGD	3.26	1.41	1.33
19	c	315	CLA	MG-NC	-3.26	1.98	2.06
19	A	815	CLA	MG-NC	-3.26	1.98	2.06
19	f	307	CLA	MG-NC	-3.26	1.98	2.06
19	B	801	CLA	C4B-NB	3.25	1.41	1.37
19	B	805	CLA	MG-NC	-3.25	1.98	2.06
19	n	208	CLA	C4B-NB	3.25	1.41	1.37
28	g	310	CHL	O2D-CGD	3.25	1.41	1.33
28	k	301	CHL	O2D-CGD	3.25	1.41	1.33
19	f	309	CLA	MG-NC	-3.24	1.98	2.06
28	b	310	CHL	O2D-CGD	3.23	1.41	1.33
19	A	818	CLA	MG-NC	-3.23	1.98	2.06
19	l	204	CLA	MG-NC	-3.23	1.98	2.06
19	c	314	CLA	MG-NC	-3.23	1.98	2.06
28	c	305	CHL	O2D-CGD	3.23	1.41	1.33
19	k	302	CLA	C4B-NB	3.23	1.41	1.37
19	B	845	CLA	MG-NC	-3.22	1.98	2.06
28	a	313	CHL	O2D-CGD	3.22	1.41	1.33
19	A	804	CLA	MG-NC	-3.22	1.98	2.06
19	A	850	CLA	MG-NC	-3.22	1.98	2.06
19	m	309	CLA	C4B-NB	3.22	1.41	1.37
19	A	829	CLA	MG-NC	-3.21	1.98	2.06
19	k	308	CLA	MG-NC	-3.21	1.98	2.06
19	e	307	CLA	MG-NC	-3.21	1.98	2.06
28	c	313	CHL	O2D-CGD	3.21	1.41	1.33
19	A	824	CLA	MG-NC	-3.20	1.98	2.06
19	g	301	CLA	C4B-NB	3.20	1.41	1.37
19	B	820	CLA	MG-NC	-3.20	1.98	2.06
28	f	301	CHL	O2D-CGD	3.20	1.41	1.33
19	c	309	CLA	MG-NC	-3.20	1.98	2.06
19	m	311	CLA	MG-NC	-3.20	1.98	2.06
28	a	311	CHL	O2D-CGD	3.19	1.41	1.33
19	A	809	CLA	MG-NC	-3.19	1.98	2.06
19	h	209	CLA	MG-NC	-3.19	1.98	2.06
19	e	302	CLA	MG-NC	-3.19	1.98	2.06
19	B	814	CLA	MG-NC	-3.19	1.98	2.06
19	a	303	CLA	MG-NC	-3.19	1.98	2.06
19	B	833	CLA	MG-NC	-3.19	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	h	207	CLA	MG-NC	-3.19	1.98	2.06
19	h	208	CLA	MG-NC	-3.19	1.98	2.06
19	A	840	CLA	MG-NC	-3.18	1.98	2.06
19	B	835	CLA	MG-NC	-3.18	1.98	2.06
19	e	309	CLA	MG-NC	-3.18	1.98	2.06
19	i	306	CLA	MG-NC	-3.18	1.98	2.06
19	l	207	CLA	MG-NC	-3.17	1.98	2.06
19	B	818	CLA	MG-NC	-3.17	1.98	2.06
19	i	308	CLA	MG-NC	-3.17	1.98	2.06
19	A	807	CLA	MG-NC	-3.17	1.98	2.06
28	b	311	CHL	O2D-CGD	3.16	1.40	1.33
19	A	846	CLA	MG-NC	-3.16	1.98	2.06
28	b	312	CHL	O2D-CGD	3.16	1.40	1.33
19	A	849	CLA	MG-NC	-3.16	1.98	2.06
19	j	313	CLA	MG-NC	-3.16	1.98	2.06
19	j	305	CLA	C4B-NB	3.15	1.41	1.37
19	n	205	CLA	MG-NC	-3.15	1.98	2.06
19	B	810	CLA	MG-NC	-3.14	1.98	2.06
28	i	304	CHL	O2D-CGD	3.14	1.40	1.33
19	g	308	CLA	MG-NC	-3.14	1.98	2.06
19	B	844	CLA	MG-NC	-3.14	1.98	2.06
19	h	210	CLA	MG-NC	-3.14	1.98	2.06
19	A	802	CLA	C4B-NB	3.13	1.41	1.37
19	e	306	CLA	MG-NC	-3.13	1.98	2.06
19	m	303	CLA	MG-NC	-3.13	1.98	2.06
19	f	302	CLA	MG-NC	-3.13	1.98	2.06
19	k	307	CLA	MG-NC	-3.13	1.98	2.06
19	n	207	CLA	MG-NC	-3.13	1.98	2.06
19	n	206	CLA	C4B-NB	3.13	1.41	1.37
19	i	312	CLA	MG-NC	-3.13	1.98	2.06
19	a	305	CLA	MG-NC	-3.12	1.98	2.06
19	A	828	CLA	MG-NC	-3.12	1.98	2.06
19	B	817	CLA	MG-NC	-3.12	1.98	2.06
19	o	310	CLA	MG-NC	-3.12	1.98	2.06
19	c	308	CLA	MG-NC	-3.12	1.98	2.06
19	j	308	CLA	MG-NC	-3.12	1.98	2.06
19	a	308	CLA	MG-NC	-3.12	1.98	2.06
19	d	204	CLA	MG-NC	-3.12	1.98	2.06
19	e	311	CLA	MG-NC	-3.12	1.98	2.06
19	h	203	CLA	MG-NC	-3.12	1.98	2.06
19	m	307	CLA	MG-NC	-3.12	1.98	2.06
28	i	301	CHL	O2D-CGD	3.11	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	e	304	CHL	O2D-CGD	3.11	1.40	1.33
19	F	201	CLA	MG-NC	-3.11	1.98	2.06
19	g	302	CLA	MG-NC	-3.10	1.98	2.06
19	F	203	CLA	MG-NC	-3.10	1.98	2.06
19	f	306	CLA	MG-NC	-3.10	1.98	2.06
19	B	801	CLA	MG-NC	-3.10	1.98	2.06
19	B	803	CLA	MG-NC	-3.10	1.98	2.06
19	B	823	CLA	MG-NC	-3.10	1.98	2.06
19	B	842	CLA	MG-NC	-3.09	1.98	2.06
19	l	208	CLA	MG-NC	-3.09	1.98	2.06
19	F	202	CLA	MG-NC	-3.09	1.98	2.06
28	d	205	CHL	O2D-CGD	3.09	1.40	1.33
19	d	203	CLA	MG-NC	-3.08	1.99	2.06
19	A	848	CLA	MG-NC	-3.08	1.99	2.06
19	o	308	CLA	MG-NC	-3.08	1.99	2.06
19	A	808	CLA	MG-NC	-3.08	1.99	2.06
19	k	311	CLA	MG-NC	-3.07	1.99	2.06
19	B	815	CLA	MG-NC	-3.07	1.99	2.06
19	J	803	CLA	MG-NC	-3.07	1.99	2.06
19	m	305	CLA	MG-NC	-3.06	1.99	2.06
19	c	307	CLA	MG-NC	-3.06	1.99	2.06
19	A	814	CLA	MG-NC	-3.06	1.99	2.06
19	g	309	CLA	MG-NC	-3.05	1.99	2.06
28	g	303	CHL	O2D-CGD	3.05	1.40	1.33
19	B	806	CLA	MG-NC	-3.05	1.99	2.06
19	k	306	CLA	MG-NC	-3.04	1.99	2.06
19	j	302	CLA	MG-NC	-3.04	1.99	2.06
19	A	810	CLA	MG-NC	-3.04	1.99	2.06
19	A	822	CLA	MG-NC	-3.04	1.99	2.06
19	k	305	CLA	MG-NC	-3.04	1.99	2.06
19	a	309	CLA	MG-NC	-3.04	1.99	2.06
28	f	304	CHL	O2D-CGD	3.04	1.40	1.33
19	c	311	CLA	MG-NC	-3.04	1.99	2.06
19	f	310	CLA	MG-NC	-3.04	1.99	2.06
19	B	819	CLA	MG-NC	-3.04	1.99	2.06
19	A	802	CLA	MG-NC	-3.03	1.99	2.06
19	A	823	CLA	MG-NC	-3.03	1.99	2.06
19	l	205	CLA	MG-NC	-3.02	1.99	2.06
28	h	202	CHL	O2D-CGD	3.02	1.40	1.33
19	f	308	CLA	MG-NC	-3.01	1.99	2.06
19	k	303	CLA	MG-NC	-3.01	1.99	2.06
19	i	307	CLA	MG-NC	-3.01	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	852	CLA	MG-NC	-3.01	1.99	2.06
19	a	304	CLA	MG-NC	-3.01	1.99	2.06
19	b	309	CLA	MG-NC	-3.00	1.99	2.06
28	a	312	CHL	MG-NA	3.00	2.13	2.06
19	i	303	CLA	MG-NC	-3.00	1.99	2.06
19	B	809	CLA	MG-NC	-3.00	1.99	2.06
19	k	310	CLA	MG-NC	-2.98	1.99	2.06
19	b	307	CLA	MG-NC	-2.97	1.99	2.06
28	o	301	CHL	O2A-CGA	2.97	1.42	1.33
19	g	307	CLA	MG-NC	-2.96	1.99	2.06
19	B	807	CLA	MG-NC	-2.96	1.99	2.06
28	b	311	CHL	O2A-CGA	2.96	1.42	1.33
19	A	816	CLA	MG-NC	-2.96	1.99	2.06
19	A	819	CLA	MG-NC	-2.95	1.99	2.06
28	a	312	CHL	O2A-CGA	2.95	1.42	1.33
28	c	312	CHL	O2A-CGA	2.95	1.42	1.33
19	c	316	CLA	MG-NC	-2.95	1.99	2.06
19	h	212	CLA	MG-NC	-2.95	1.99	2.06
19	f	303	CLA	MG-NC	-2.95	1.99	2.06
28	o	301	CHL	MG-NA	2.94	2.13	2.06
19	m	310	CLA	MG-NC	-2.94	1.99	2.06
19	d	206	CLA	MG-NC	-2.94	1.99	2.06
19	A	821	CLA	MG-NC	-2.94	1.99	2.06
19	B	830	CLA	MG-NC	-2.94	1.99	2.06
19	i	309	CLA	MG-NC	-2.94	1.99	2.06
28	a	315	CHL	O2A-CGA	2.93	1.41	1.33
19	A	841	CLA	MG-NC	-2.93	1.99	2.06
19	h	204	CLA	MG-NC	-2.93	1.99	2.06
28	e	301	CHL	O2D-CGD	2.93	1.40	1.33
19	a	310	CLA	MG-NC	-2.93	1.99	2.06
28	i	301	CHL	O2A-CGA	2.93	1.41	1.33
19	c	302	CLA	MG-NC	-2.93	1.99	2.06
28	m	301	CHL	O2A-CGA	2.92	1.41	1.33
28	a	313	CHL	O2A-CGA	2.92	1.41	1.33
19	A	842	CLA	C4B-NB	2.92	1.41	1.37
19	h	211	CLA	MG-NC	-2.92	1.99	2.06
19	b	308	CLA	MG-NC	-2.92	1.99	2.06
19	j	309	CLA	MG-NC	-2.91	1.99	2.06
19	d	201	CLA	MG-NC	-2.91	1.99	2.06
19	F	204	CLA	MG-NC	-2.91	1.99	2.06
19	D	301	CLA	MG-NC	-2.91	1.99	2.06
28	g	310	CHL	O2A-CGA	2.91	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	312	CHL	MG-NA	2.90	2.13	2.06
19	A	812	CLA	MG-NC	-2.90	1.99	2.06
19	o	311	CLA	MG-NC	-2.90	1.99	2.06
19	A	844	CLA	MG-NC	-2.90	1.99	2.06
28	g	310	CHL	MG-NA	2.90	2.13	2.06
19	c	310	CLA	MG-NC	-2.89	1.99	2.06
28	d	205	CHL	MG-NA	2.89	2.13	2.06
28	d	202	CHL	O2A-CGA	2.88	1.41	1.33
28	b	301	CHL	MG-NA	2.87	2.13	2.06
19	m	302	CLA	C4B-NB	2.87	1.41	1.37
28	c	305	CHL	O2A-CGA	2.87	1.41	1.33
28	e	304	CHL	O2A-CGA	2.86	1.41	1.33
28	i	304	CHL	O2A-CGA	2.85	1.41	1.33
19	b	303	CLA	MG-NC	-2.85	1.99	2.06
28	a	311	CHL	O2A-CGA	2.85	1.41	1.33
28	b	310	CHL	MG-NA	2.85	2.13	2.06
19	d	212	CLA	MG-NC	-2.84	1.99	2.06
19	A	826	CLA	MG-NC	-2.84	1.99	2.06
28	b	312	CHL	O2A-CGA	2.83	1.41	1.33
28	d	202	CHL	MG-NA	2.83	2.13	2.06
28	b	301	CHL	O2A-CGA	2.82	1.41	1.33
28	b	312	CHL	MG-NA	2.82	2.13	2.06
19	B	839	CLA	MG-NC	-2.82	1.99	2.06
28	a	313	CHL	MG-NA	2.82	2.13	2.06
19	n	201	CLA	MG-NC	-2.81	1.99	2.06
28	c	313	CHL	O2A-CGA	2.81	1.41	1.33
19	j	303	CLA	MG-NC	-2.81	1.99	2.06
28	b	311	CHL	MG-NA	2.80	2.12	2.06
28	a	311	CHL	MG-NA	2.80	2.12	2.06
28	a	315	CHL	MG-NA	2.80	2.12	2.06
28	f	301	CHL	O2A-CGA	2.80	1.41	1.33
19	e	303	CLA	MG-NC	-2.79	1.99	2.06
19	d	209	CLA	MG-NC	-2.79	1.99	2.06
28	h	202	CHL	O2A-CGA	2.78	1.41	1.33
28	f	301	CHL	MG-NA	2.77	2.12	2.06
28	m	301	CHL	MG-NA	2.77	2.12	2.06
28	b	314	CHL	O2A-CGA	2.75	1.41	1.33
28	k	301	CHL	O2A-CGA	2.74	1.41	1.33
19	c	304	CLA	MG-NC	-2.74	1.99	2.06
28	b	310	CHL	O2A-CGA	2.74	1.41	1.33
19	B	836	CLA	MG-NC	-2.74	1.99	2.06
28	e	301	CHL	O2A-CGA	2.74	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	205	CHL	O2A-CGA	2.73	1.41	1.33
28	f	304	CHL	O2A-CGA	2.73	1.41	1.33
28	c	305	CHL	MG-NA	2.72	2.12	2.06
28	g	303	CHL	MG-NA	2.72	2.12	2.06
19	d	211	CLA	MG-NC	-2.71	1.99	2.06
28	h	202	CHL	MG-NA	2.70	2.12	2.06
19	B	811	CLA	MG-NC	-2.69	1.99	2.06
28	g	303	CHL	O2A-CGA	2.67	1.41	1.33
19	B	846	CLA	C1D-C2D	-2.66	1.40	1.45
28	i	301	CHL	MG-NA	2.66	2.12	2.06
28	k	301	CHL	MG-NA	2.65	2.12	2.06
28	g	306	CHL	MG-NA	2.62	2.12	2.06
19	A	839	CLA	MG-NC	-2.60	2.00	2.06
28	c	313	CHL	MG-NA	2.59	2.12	2.06
28	e	301	CHL	MG-NA	2.58	2.12	2.06
28	e	304	CHL	MG-NA	2.58	2.12	2.06
28	g	306	CHL	O2A-CGA	2.57	1.40	1.33
19	j	311	CLA	MG-NC	-2.57	2.00	2.06
19	k	302	CLA	C1D-C2D	-2.55	1.40	1.45
25	i	316	LMG	O7-C8	-2.55	1.40	1.46
28	c	312	CHL	C2-C3	2.54	1.39	1.33
19	b	305	CLA	C1D-C2D	-2.54	1.40	1.45
19	i	310	CLA	C1D-C2D	-2.53	1.40	1.45
28	i	304	CHL	MG-NA	2.53	2.12	2.06
19	g	304	CLA	C1D-C2D	-2.51	1.40	1.45
25	j	314	LMG	O1-C1	2.51	1.44	1.40
28	c	313	CHL	C2-C3	2.51	1.39	1.33
28	m	301	CHL	MG-ND	-2.50	2.00	2.05
28	b	312	CHL	C2-C3	2.50	1.39	1.33
28	b	314	CHL	MG-NA	2.49	2.12	2.06
19	g	304	CLA	C3D-C4D	-2.49	1.38	1.44
19	b	306	CLA	C1D-C2D	-2.48	1.40	1.45
19	A	842	CLA	C3D-C4D	-2.47	1.38	1.44
25	a	301	LMG	C7-C8	2.47	1.58	1.50
19	m	309	CLA	C3D-C4D	-2.46	1.38	1.44
19	A	842	CLA	C1D-C2D	-2.45	1.40	1.45
19	g	301	CLA	C3D-C4D	-2.45	1.38	1.44
19	o	309	CLA	C1D-C2D	-2.44	1.40	1.45
19	j	305	CLA	C1D-C2D	-2.44	1.40	1.45
19	m	302	CLA	C3D-C4D	-2.43	1.38	1.44
28	b	301	CHL	C2-C3	2.43	1.38	1.33
28	d	205	CHL	MG-NB	2.43	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	i	304	CHL	MG-NB	2.42	2.10	2.05
19	l	201	CLA	C1D-C2D	-2.42	1.40	1.45
19	m	302	CLA	C1D-C2D	-2.41	1.40	1.45
19	b	306	CLA	C3D-C4D	-2.41	1.38	1.44
28	d	202	CHL	MG-NB	2.41	2.10	2.05
19	j	305	CLA	C3D-C4D	-2.40	1.38	1.44
19	g	301	CLA	C1D-C2D	-2.40	1.40	1.45
19	l	206	CLA	C1D-C2D	-2.40	1.40	1.45
19	m	309	CLA	C1D-C2D	-2.40	1.40	1.45
28	a	312	CHL	MG-NB	2.40	2.10	2.05
19	o	302	CLA	C3D-C4D	-2.40	1.38	1.44
19	j	304	CLA	C1D-C2D	-2.40	1.40	1.45
25	g	312	LMG	O3-C3	-2.39	1.37	1.43
19	n	208	CLA	C1D-C2D	-2.39	1.40	1.45
19	j	311	CLA	C1D-C2D	-2.39	1.40	1.45
28	f	304	CHL	MG-NA	2.39	2.11	2.06
19	g	305	CLA	C1D-C2D	-2.38	1.40	1.45
19	b	315	CLA	C3D-C4D	-2.38	1.38	1.44
19	A	802	CLA	C3D-C4D	-2.38	1.38	1.44
28	g	306	CHL	MG-NB	2.38	2.10	2.05
28	g	310	CHL	MG-NB	2.37	2.10	2.05
28	c	305	CHL	C2-C3	2.37	1.38	1.33
19	e	310	CLA	C3D-C4D	-2.36	1.38	1.44
19	B	801	CLA	C3D-C4D	-2.36	1.38	1.44
19	B	836	CLA	C1D-C2D	-2.36	1.40	1.45
28	b	310	CHL	MG-NB	2.35	2.10	2.05
19	n	208	CLA	C3D-C4D	-2.35	1.38	1.44
19	B	832	CLA	C3D-C4D	-2.35	1.38	1.44
19	j	310	CLA	C1D-C2D	-2.35	1.40	1.45
28	b	314	CHL	C2-C3	2.35	1.38	1.33
19	l	206	CLA	C3D-C4D	-2.35	1.38	1.44
19	n	206	CLA	C3D-C4D	-2.35	1.38	1.44
19	F	202	CLA	C1D-C2D	-2.34	1.40	1.45
28	e	304	CHL	C2-C3	2.34	1.38	1.33
19	i	305	CLA	C1D-C2D	-2.34	1.40	1.45
28	b	312	CHL	MG-NB	2.34	2.10	2.05
19	j	303	CLA	C1D-C2D	-2.33	1.40	1.45
19	c	307	CLA	C1D-C2D	-2.33	1.40	1.45
19	i	309	CLA	C1D-C2D	-2.32	1.40	1.45
28	o	301	CHL	MG-NB	2.32	2.10	2.05
19	B	837	CLA	C3D-C4D	-2.32	1.38	1.44
19	c	304	CLA	C1D-C2D	-2.32	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	k	301	CHL	C4D-ND	-2.32	1.34	1.37
19	B	806	CLA	C1D-C2D	-2.32	1.40	1.45
19	A	812	CLA	C1D-C2D	-2.32	1.40	1.45
19	g	305	CLA	C3D-C4D	-2.32	1.38	1.44
19	A	826	CLA	C1D-C2D	-2.31	1.40	1.45
19	o	303	CLA	C3D-C4D	-2.31	1.39	1.44
19	A	803	CLA	C1D-C2D	-2.31	1.40	1.45
19	b	304	CLA	C1D-C2D	-2.31	1.40	1.45
19	F	204	CLA	C1D-C2D	-2.31	1.40	1.45
19	i	310	CLA	C3D-C4D	-2.31	1.39	1.44
19	B	808	CLA	C1D-C2D	-2.30	1.40	1.45
19	f	303	CLA	C1D-C2D	-2.30	1.40	1.45
19	o	303	CLA	C1D-C2D	-2.30	1.40	1.45
19	A	821	CLA	C1D-C2D	-2.29	1.40	1.45
19	n	209	CLA	C1D-C2D	-2.29	1.40	1.45
19	b	304	CLA	C3D-C4D	-2.29	1.39	1.44
19	a	306	CLA	C1D-C2D	-2.29	1.40	1.45
28	m	301	CHL	C4D-ND	-2.29	1.34	1.37
19	k	302	CLA	C3D-C4D	-2.29	1.39	1.44
19	o	304	CLA	C3D-C4D	-2.29	1.39	1.44
19	A	801	CLA	C1D-C2D	-2.29	1.40	1.45
19	n	206	CLA	C1D-C2D	-2.29	1.40	1.45
19	o	309	CLA	C3D-C4D	-2.29	1.39	1.44
19	a	314	CLA	C3D-C4D	-2.28	1.39	1.44
19	o	311	CLA	C1D-C2D	-2.28	1.40	1.45
19	b	303	CLA	C1D-C2D	-2.28	1.40	1.45
19	B	837	CLA	C1D-C2D	-2.28	1.40	1.45
19	j	306	CLA	C1D-C2D	-2.28	1.40	1.45
19	e	303	CLA	C1D-C2D	-2.28	1.40	1.45
19	a	302	CLA	C1D-C2D	-2.27	1.40	1.45
19	B	839	CLA	C1D-C2D	-2.27	1.40	1.45
28	b	311	CHL	MG-NB	2.27	2.10	2.05
19	g	307	CLA	C1D-C2D	-2.27	1.40	1.45
19	c	316	CLA	C1D-C2D	-2.27	1.40	1.45
19	a	304	CLA	C1D-C2D	-2.27	1.40	1.45
19	a	314	CLA	C1D-C2D	-2.27	1.40	1.45
19	d	212	CLA	C1D-C2D	-2.27	1.40	1.45
19	A	819	CLA	C1D-C2D	-2.27	1.40	1.45
19	o	304	CLA	C1D-C2D	-2.27	1.40	1.45
19	B	848	CLA	C3D-C4D	-2.27	1.39	1.44
19	B	823	CLA	C3D-C4D	-2.27	1.39	1.44
28	b	314	CHL	MG-NB	2.26	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	309	CLA	C1D-C2D	-2.26	1.40	1.45
19	o	302	CLA	C1D-C2D	-2.26	1.40	1.45
28	g	310	CHL	C2-C3	2.26	1.38	1.32
19	k	303	CLA	C1D-C2D	-2.26	1.40	1.45
19	b	315	CLA	C1D-C2D	-2.26	1.40	1.45
19	A	820	CLA	C3D-C4D	-2.26	1.39	1.44
19	D	301	CLA	C1D-C2D	-2.26	1.40	1.45
19	e	305	CLA	C1D-C2D	-2.26	1.40	1.45
28	e	304	CHL	MG-NB	2.26	2.10	2.05
19	B	832	CLA	C1D-C2D	-2.26	1.40	1.45
19	B	830	CLA	C1D-C2D	-2.26	1.40	1.45
19	d	211	CLA	C1D-C2D	-2.26	1.40	1.45
19	j	307	CLA	C3D-C4D	-2.26	1.39	1.44
19	B	841	CLA	C1D-C2D	-2.26	1.40	1.45
19	B	816	CLA	C1D-C2D	-2.26	1.40	1.45
19	B	803	CLA	C1D-C2D	-2.26	1.40	1.45
19	c	310	CLA	C1D-C2D	-2.26	1.40	1.45
28	b	301	CHL	MG-NB	2.25	2.10	2.05
19	A	822	CLA	C1D-C2D	-2.25	1.40	1.45
19	B	820	CLA	C3D-C4D	-2.25	1.39	1.44
19	h	213	CLA	C1D-C2D	-2.25	1.40	1.45
19	j	309	CLA	C1D-C2D	-2.25	1.40	1.45
19	j	313	CLA	C1D-C2D	-2.25	1.40	1.45
19	i	305	CLA	C3D-C4D	-2.25	1.39	1.44
19	B	804	CLA	C1D-C2D	-2.25	1.40	1.45
19	B	811	CLA	C1D-C2D	-2.25	1.40	1.45
19	B	819	CLA	C1D-C2D	-2.25	1.40	1.45
19	a	310	CLA	C1D-C2D	-2.25	1.40	1.45
28	i	304	CHL	C2-C3	2.25	1.38	1.33
19	j	304	CLA	C3D-C4D	-2.25	1.39	1.44
19	j	310	CLA	C3D-C4D	-2.25	1.39	1.44
19	h	212	CLA	C1D-C2D	-2.24	1.40	1.45
19	m	310	CLA	C1D-C2D	-2.24	1.40	1.45
28	d	205	CHL	C2-C3	2.24	1.38	1.33
19	d	208	CLA	C3D-C4D	-2.24	1.39	1.44
19	i	313	CLA	C1D-C2D	-2.24	1.40	1.45
19	J	803	CLA	C1D-C2D	-2.24	1.40	1.45
19	j	308	CLA	C1D-C2D	-2.24	1.40	1.45
19	A	815	CLA	C1D-C2D	-2.24	1.40	1.45
19	A	824	CLA	C1D-C2D	-2.24	1.40	1.45
19	e	309	CLA	C3D-C4D	-2.24	1.39	1.44
19	e	310	CLA	C1D-C2D	-2.24	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	i	303	CLA	C1D-C2D	-2.24	1.40	1.45
19	A	809	CLA	C1D-C2D	-2.23	1.40	1.45
19	k	307	CLA	C3D-C4D	-2.23	1.39	1.44
28	i	301	CHL	MG-NB	2.23	2.10	2.05
19	c	302	CLA	C1D-C2D	-2.23	1.40	1.45
19	B	822	CLA	C3D-C4D	-2.23	1.39	1.44
19	A	828	CLA	C1D-C2D	-2.23	1.40	1.45
19	B	808	CLA	C3D-C4D	-2.23	1.39	1.44
19	a	306	CLA	C3D-C4D	-2.23	1.39	1.44
19	a	309	CLA	C1D-C2D	-2.23	1.40	1.45
19	j	301	CLA	C1D-C2D	-2.23	1.40	1.45
19	a	302	CLA	C3D-C4D	-2.23	1.39	1.44
19	g	309	CLA	C1D-C2D	-2.23	1.40	1.45
19	A	823	CLA	C1D-C2D	-2.22	1.40	1.45
19	A	827	CLA	C3D-C4D	-2.22	1.39	1.44
19	h	203	CLA	C1D-C2D	-2.22	1.40	1.45
19	f	302	CLA	C1D-C2D	-2.22	1.40	1.45
19	A	852	CLA	C1D-C2D	-2.22	1.40	1.45
19	d	201	CLA	C1D-C2D	-2.22	1.40	1.45
19	A	810	CLA	C1D-C2D	-2.22	1.40	1.45
19	A	816	CLA	C1D-C2D	-2.22	1.40	1.45
19	a	303	CLA	C1D-C2D	-2.22	1.40	1.45
19	A	825	CLA	C3D-C4D	-2.22	1.39	1.44
19	A	839	CLA	C1D-C2D	-2.22	1.40	1.45
19	B	809	CLA	C1D-C2D	-2.22	1.40	1.45
19	h	210	CLA	C1D-C2D	-2.22	1.40	1.45
19	j	307	CLA	C1D-C2D	-2.22	1.40	1.45
19	f	309	CLA	C3D-C4D	-2.22	1.39	1.44
19	c	311	CLA	C3D-C4D	-2.22	1.39	1.44
19	A	812	CLA	C3D-C4D	-2.22	1.39	1.44
19	A	813	CLA	C1D-C2D	-2.22	1.41	1.45
19	B	817	CLA	C1D-C2D	-2.21	1.41	1.45
19	n	201	CLA	C1D-C2D	-2.21	1.41	1.45
19	a	305	CLA	C1D-C2D	-2.21	1.41	1.45
28	e	301	CHL	C2-C3	2.21	1.38	1.32
19	j	302	CLA	C1D-C2D	-2.21	1.41	1.45
19	B	821	CLA	C1D-C2D	-2.21	1.41	1.45
19	g	302	CLA	C1D-C2D	-2.21	1.41	1.45
19	A	818	CLA	C3D-C4D	-2.21	1.39	1.44
19	A	807	CLA	C1D-C2D	-2.21	1.41	1.45
19	B	849	CLA	C1D-C2D	-2.21	1.41	1.45
19	F	201	CLA	C3D-C4D	-2.21	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	f	308	CLA	C1D-C2D	-2.21	1.41	1.45
19	i	312	CLA	C1D-C2D	-2.21	1.41	1.45
19	A	808	CLA	C3D-C4D	-2.21	1.39	1.44
19	l	205	CLA	C1D-C2D	-2.21	1.41	1.45
19	j	306	CLA	C3D-C4D	-2.21	1.39	1.44
19	h	207	CLA	C1D-C2D	-2.21	1.41	1.45
19	k	310	CLA	C1D-C2D	-2.21	1.41	1.45
19	A	844	CLA	C1D-C2D	-2.21	1.41	1.45
19	A	802	CLA	C1D-C2D	-2.21	1.41	1.45
19	B	840	CLA	C3D-C4D	-2.21	1.39	1.44
19	h	208	CLA	C3D-C4D	-2.21	1.39	1.44
19	k	303	CLA	C3D-C4D	-2.20	1.39	1.44
19	B	845	CLA	C1D-C2D	-2.20	1.41	1.45
19	b	307	CLA	C1D-C2D	-2.20	1.41	1.45
19	h	213	CLA	C3D-C4D	-2.20	1.39	1.44
19	m	305	CLA	C3D-C4D	-2.20	1.39	1.44
19	h	204	CLA	C1D-C2D	-2.20	1.41	1.45
19	B	847	CLA	C3D-C4D	-2.20	1.39	1.44
19	A	829	CLA	C3D-C4D	-2.20	1.39	1.44
19	A	850	CLA	C1D-C2D	-2.20	1.41	1.45
19	e	307	CLA	C1D-C2D	-2.20	1.41	1.45
19	j	313	CLA	C3D-C4D	-2.20	1.39	1.44
19	b	305	CLA	C3D-C4D	-2.20	1.39	1.44
19	A	829	CLA	C1D-C2D	-2.20	1.41	1.45
19	h	211	CLA	C1D-C2D	-2.20	1.41	1.45
19	k	307	CLA	C1D-C2D	-2.20	1.41	1.45
19	A	803	CLA	C1C-C2C	2.20	1.48	1.44
19	d	204	CLA	C1D-C2D	-2.20	1.41	1.45
19	f	306	CLA	C1D-C2D	-2.20	1.41	1.45
19	B	817	CLA	C3D-C4D	-2.20	1.39	1.44
19	B	838	CLA	C1D-C2D	-2.20	1.41	1.45
28	c	313	CHL	MG-NB	2.20	2.10	2.05
19	F	203	CLA	C1D-C2D	-2.20	1.41	1.45
19	A	820	CLA	C1D-C2D	-2.20	1.41	1.45
19	b	308	CLA	C1D-C2D	-2.20	1.41	1.45
19	B	841	CLA	C3D-C4D	-2.19	1.39	1.44
19	f	310	CLA	C1D-C2D	-2.19	1.41	1.45
19	d	209	CLA	C1D-C2D	-2.19	1.41	1.45
19	n	203	CLA	C1D-C2D	-2.19	1.41	1.45
19	d	206	CLA	C1D-C2D	-2.19	1.41	1.45
19	g	311	CLA	C1D-C2D	-2.19	1.41	1.45
19	A	846	CLA	C3D-C4D	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	e	311	CLA	C1D-C2D	-2.19	1.41	1.45
19	f	312	CLA	C1D-C2D	-2.19	1.41	1.45
19	i	307	CLA	C3D-C4D	-2.19	1.39	1.44
19	o	307	CLA	C3D-C4D	-2.19	1.39	1.44
19	a	307	CLA	C1D-C2D	-2.19	1.41	1.45
19	e	302	CLA	C1D-C2D	-2.19	1.41	1.45
28	e	301	CHL	MG-NB	2.19	2.10	2.05
19	B	811	CLA	C3D-C4D	-2.19	1.39	1.44
19	B	807	CLA	C1D-C2D	-2.19	1.41	1.45
19	h	208	CLA	C1D-C2D	-2.19	1.41	1.45
19	i	307	CLA	C1D-C2D	-2.19	1.41	1.45
28	a	313	CHL	MG-NB	2.19	2.10	2.05
19	A	805	CLA	C3D-C4D	-2.19	1.39	1.44
19	i	311	CLA	C3D-C4D	-2.19	1.39	1.44
19	A	843	CLA	C3D-C4D	-2.19	1.39	1.44
19	B	849	CLA	C3D-C4D	-2.19	1.39	1.44
19	h	201	CLA	C1D-C2D	-2.19	1.41	1.45
28	f	301	CHL	MG-NB	2.19	2.10	2.05
19	A	853	CLA	C1D-C2D	-2.19	1.41	1.45
19	f	311	CLA	C1D-C2D	-2.19	1.41	1.45
19	B	833	CLA	C3D-C4D	-2.18	1.39	1.44
19	A	847	CLA	C1D-C2D	-2.18	1.41	1.45
19	B	813	CLA	C1D-C2D	-2.18	1.41	1.45
19	B	844	CLA	C1D-C2D	-2.18	1.41	1.45
19	f	309	CLA	C1D-C2D	-2.18	1.41	1.45
19	b	302	CLA	C1D-C2D	-2.18	1.41	1.45
19	i	308	CLA	C1D-C2D	-2.18	1.41	1.45
19	A	823	CLA	C3D-C4D	-2.18	1.39	1.44
19	l	203	CLA	C1D-C2D	-2.18	1.41	1.45
28	b	311	CHL	MG-NC	2.18	2.11	2.06
19	B	823	CLA	C1D-C2D	-2.18	1.41	1.45
19	A	841	CLA	C1D-C2D	-2.18	1.41	1.45
19	B	815	CLA	C3D-C4D	-2.18	1.39	1.44
19	B	848	CLA	C1D-C2D	-2.18	1.41	1.45
19	o	305	CLA	C1D-C2D	-2.18	1.41	1.45
19	A	845	CLA	C1D-C2D	-2.18	1.41	1.45
19	i	313	CLA	C3D-C4D	-2.18	1.39	1.44
28	k	301	CHL	MG-ND	-2.18	2.01	2.05
19	B	815	CLA	C1D-C2D	-2.18	1.41	1.45
19	B	819	CLA	C3D-C4D	-2.17	1.39	1.44
19	A	848	CLA	C1D-C2D	-2.17	1.41	1.45
19	e	307	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	810	CLA	C1D-C2D	-2.17	1.41	1.45
19	j	312	CLA	C1D-C2D	-2.17	1.41	1.45
19	k	305	CLA	C1D-C2D	-2.17	1.41	1.45
19	j	302	CLA	C3D-C4D	-2.17	1.39	1.44
19	f	305	CLA	C3D-C4D	-2.17	1.39	1.44
28	c	312	CHL	MG-NB	2.17	2.10	2.05
19	i	306	CLA	C1D-C2D	-2.17	1.41	1.45
19	d	207	CLA	C3D-C4D	-2.17	1.39	1.44
19	g	308	CLA	C3D-C4D	-2.17	1.39	1.44
28	a	315	CHL	MG-ND	-2.17	2.01	2.05
19	B	833	CLA	C1D-C2D	-2.17	1.41	1.45
19	A	850	CLA	C3D-C4D	-2.17	1.39	1.44
19	c	306	CLA	C3D-C4D	-2.17	1.39	1.44
19	A	811	CLA	C3D-C4D	-2.17	1.39	1.44
19	A	807	CLA	C3D-C4D	-2.17	1.39	1.44
19	A	815	CLA	C3D-C4D	-2.17	1.39	1.44
19	A	846	CLA	C1D-C2D	-2.17	1.41	1.45
19	d	210	CLA	C1D-C2D	-2.17	1.41	1.45
19	c	311	CLA	C1D-C2D	-2.17	1.41	1.45
19	A	822	CLA	C3D-C4D	-2.17	1.39	1.44
19	c	309	CLA	C1D-C2D	-2.17	1.41	1.45
19	m	311	CLA	C1D-C2D	-2.17	1.41	1.45
19	o	312	CLA	C1D-C2D	-2.17	1.41	1.45
19	l	207	CLA	C3D-C4D	-2.17	1.39	1.44
19	o	308	CLA	C3D-C4D	-2.17	1.39	1.44
25	e	312	LMG	C7-C8	2.17	1.57	1.50
19	n	203	CLA	C3D-C4D	-2.17	1.39	1.44
19	F	201	CLA	C1D-C2D	-2.17	1.41	1.45
19	h	205	CLA	C1D-C2D	-2.17	1.41	1.45
19	A	814	CLA	C1D-C2D	-2.17	1.41	1.45
19	A	839	CLA	C3D-C4D	-2.17	1.39	1.44
19	B	814	CLA	C1D-C2D	-2.16	1.41	1.45
19	a	308	CLA	C3D-C4D	-2.16	1.39	1.44
19	f	305	CLA	C1D-C2D	-2.16	1.41	1.45
19	o	310	CLA	C1D-C2D	-2.16	1.41	1.45
19	A	827	CLA	C1D-C2D	-2.16	1.41	1.45
19	b	313	CLA	C1D-C2D	-2.16	1.41	1.45
19	h	209	CLA	C1D-C2D	-2.16	1.41	1.45
19	A	804	CLA	C1D-C2D	-2.16	1.41	1.45
19	d	203	CLA	C1D-C2D	-2.16	1.41	1.45
19	l	207	CLA	C1D-C2D	-2.16	1.41	1.45
19	m	308	CLA	C1D-C2D	-2.16	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	838	CLA	C3D-C4D	-2.16	1.39	1.44
19	m	303	CLA	C1D-C2D	-2.16	1.41	1.45
19	A	811	CLA	C1D-C2D	-2.16	1.41	1.45
19	d	207	CLA	C1D-C2D	-2.16	1.41	1.45
19	e	306	CLA	C1D-C2D	-2.16	1.41	1.45
19	n	204	CLA	C1D-C2D	-2.16	1.41	1.45
19	a	307	CLA	C3D-C4D	-2.16	1.39	1.44
19	f	307	CLA	C3D-C4D	-2.16	1.39	1.44
19	B	822	CLA	C1D-C2D	-2.16	1.41	1.45
19	h	201	CLA	C3D-C4D	-2.16	1.39	1.44
19	f	307	CLA	C1D-C2D	-2.16	1.41	1.45
19	j	308	CLA	C3D-C4D	-2.16	1.39	1.44
19	B	812	CLA	C1D-C2D	-2.16	1.41	1.45
28	h	202	CHL	MG-NB	2.15	2.10	2.05
28	c	313	CHL	MG-ND	-2.15	2.01	2.05
19	B	810	CLA	C3D-C4D	-2.15	1.39	1.44
19	h	206	CLA	C3D-C4D	-2.15	1.39	1.44
19	A	813	CLA	C3D-C4D	-2.15	1.39	1.44
19	B	816	CLA	C3D-C4D	-2.15	1.39	1.44
19	F	203	CLA	C3D-C4D	-2.15	1.39	1.44
28	g	306	CHL	C2-C3	2.15	1.38	1.33
19	m	307	CLA	C3D-C4D	-2.15	1.39	1.44
19	f	311	CLA	C3D-C4D	-2.15	1.39	1.44
28	h	202	CHL	C4D-ND	-2.15	1.34	1.37
19	l	202	CLA	C1D-C2D	-2.15	1.41	1.45
19	A	804	CLA	C3D-C4D	-2.15	1.39	1.44
19	b	302	CLA	C3D-C4D	-2.15	1.39	1.44
19	A	840	CLA	C1D-C2D	-2.15	1.41	1.45
19	B	807	CLA	C3D-C4D	-2.15	1.39	1.44
19	c	303	CLA	C3D-C4D	-2.15	1.39	1.44
19	A	847	CLA	C3D-C4D	-2.15	1.39	1.44
19	b	307	CLA	C3D-C4D	-2.15	1.39	1.44
19	B	820	CLA	C1D-C2D	-2.15	1.41	1.45
19	n	207	CLA	C3D-C4D	-2.15	1.39	1.44
19	e	305	CLA	C3D-C4D	-2.15	1.39	1.44
19	B	842	CLA	C3D-C4D	-2.15	1.39	1.44
19	A	825	CLA	C1D-C2D	-2.15	1.41	1.45
19	f	314	CLA	C1D-C2D	-2.15	1.41	1.45
28	c	305	CHL	MG-NB	2.15	2.10	2.05
19	h	204	CLA	C3D-C4D	-2.15	1.39	1.44
19	l	204	CLA	C1D-C2D	-2.15	1.41	1.45
19	c	314	CLA	C3D-C4D	-2.14	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	n	204	CLA	C3D-C4D	-2.14	1.39	1.44
19	c	308	CLA	C3D-C4D	-2.14	1.39	1.44
19	j	301	CLA	C3D-C4D	-2.14	1.39	1.44
19	A	818	CLA	C1D-C2D	-2.14	1.41	1.45
19	A	840	CLA	C3D-C4D	-2.14	1.39	1.44
19	l	209	CLA	C3D-C4D	-2.14	1.39	1.44
19	A	809	CLA	C3D-C4D	-2.14	1.39	1.44
19	A	852	CLA	C3D-C4D	-2.14	1.39	1.44
19	d	210	CLA	C3D-C4D	-2.14	1.39	1.44
19	A	817	CLA	C3D-C4D	-2.14	1.39	1.44
19	B	845	CLA	C3D-C4D	-2.14	1.39	1.44
19	B	805	CLA	C1D-C2D	-2.14	1.41	1.45
19	A	828	CLA	C3D-C4D	-2.14	1.39	1.44
19	d	208	CLA	C1D-C2D	-2.14	1.41	1.45
28	c	312	CHL	MG-NC	2.14	2.11	2.06
25	A	851	LMG	O7-C8	-2.14	1.41	1.46
19	A	848	CLA	C3D-C4D	-2.14	1.39	1.44
19	k	304	CLA	C1D-C2D	-2.14	1.41	1.45
19	f	314	CLA	C3D-C4D	-2.14	1.39	1.44
25	g	313	LMG	O6-C5	-2.14	1.39	1.44
19	m	307	CLA	C1D-C2D	-2.14	1.41	1.45
19	h	203	CLA	C3D-C4D	-2.14	1.39	1.44
19	m	311	CLA	C3D-C4D	-2.14	1.39	1.44
19	n	205	CLA	C3D-C4D	-2.14	1.39	1.44
19	B	812	CLA	C3D-C4D	-2.14	1.39	1.44
19	o	306	CLA	C3D-C4D	-2.14	1.39	1.44
19	B	843	CLA	C3D-C4D	-2.14	1.39	1.44
19	B	801	CLA	C1D-C2D	-2.14	1.41	1.45
19	e	302	CLA	C3D-C4D	-2.14	1.39	1.44
19	m	303	CLA	C3D-C4D	-2.14	1.39	1.44
19	a	303	CLA	C3D-C4D	-2.13	1.39	1.44
19	B	843	CLA	C1D-C2D	-2.13	1.41	1.45
19	c	315	CLA	C1D-C2D	-2.13	1.41	1.45
19	b	308	CLA	C3D-C4D	-2.13	1.39	1.44
19	l	203	CLA	C3D-C4D	-2.13	1.39	1.44
19	o	307	CLA	C1D-C2D	-2.13	1.41	1.45
19	B	805	CLA	C3D-C4D	-2.13	1.39	1.44
19	i	311	CLA	C1D-C2D	-2.13	1.41	1.45
19	A	814	CLA	C3D-C4D	-2.13	1.39	1.44
19	f	306	CLA	C3D-C4D	-2.13	1.39	1.44
19	k	311	CLA	C3D-C4D	-2.13	1.39	1.44
19	A	810	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	813	CLA	C3D-C4D	-2.13	1.39	1.44
19	d	206	CLA	C3D-C4D	-2.13	1.39	1.44
19	o	308	CLA	C1D-C2D	-2.13	1.41	1.45
19	B	806	CLA	C3D-C4D	-2.13	1.39	1.44
19	k	306	CLA	C3D-C4D	-2.13	1.39	1.44
19	l	202	CLA	C3D-C4D	-2.13	1.39	1.44
19	k	310	CLA	C3D-C4D	-2.13	1.39	1.44
19	m	306	CLA	C3D-C4D	-2.13	1.39	1.44
19	A	817	CLA	C1D-C2D	-2.13	1.41	1.45
19	A	845	CLA	C3D-C4D	-2.13	1.39	1.44
28	b	312	CHL	MG-NC	2.13	2.11	2.06
19	A	844	CLA	C3D-C4D	-2.13	1.39	1.44
19	B	844	CLA	C3D-C4D	-2.13	1.39	1.44
19	h	209	CLA	C3D-C4D	-2.13	1.39	1.44
19	a	308	CLA	C1D-C2D	-2.13	1.41	1.45
19	i	306	CLA	C3D-C4D	-2.13	1.39	1.44
19	A	849	CLA	C1D-C2D	-2.13	1.41	1.45
19	e	309	CLA	C1D-C2D	-2.13	1.41	1.45
19	n	202	CLA	C1D-C2D	-2.13	1.41	1.45
19	B	814	CLA	C3D-C4D	-2.13	1.39	1.44
19	B	835	CLA	C3D-C4D	-2.13	1.39	1.44
28	o	301	CHL	MG-NC	2.13	2.11	2.06
28	f	304	CHL	MG-NB	2.13	2.10	2.05
19	o	306	CLA	C1D-C2D	-2.13	1.41	1.45
19	b	313	CLA	C3D-C4D	-2.13	1.39	1.44
19	A	843	CLA	C1D-C2D	-2.12	1.41	1.45
19	A	806	CLA	C1D-C2D	-2.12	1.41	1.45
19	i	302	CLA	C1D-C2D	-2.12	1.41	1.45
19	k	308	CLA	C3D-C4D	-2.12	1.39	1.44
19	B	842	CLA	C1D-C2D	-2.12	1.41	1.45
19	g	309	CLA	C3D-C4D	-2.12	1.39	1.44
19	m	310	CLA	C3D-C4D	-2.12	1.39	1.44
19	c	308	CLA	C1D-C2D	-2.12	1.41	1.45
19	c	314	CLA	C1D-C2D	-2.12	1.41	1.45
19	k	308	CLA	C1D-C2D	-2.12	1.41	1.45
19	m	304	CLA	C3D-C4D	-2.12	1.39	1.44
19	A	841	CLA	C3D-C4D	-2.12	1.39	1.44
19	d	212	CLA	C3D-C4D	-2.12	1.39	1.44
19	j	312	CLA	C3D-C4D	-2.12	1.39	1.44
19	h	210	CLA	C3D-C4D	-2.12	1.39	1.44
19	A	849	CLA	C3D-C4D	-2.12	1.39	1.44
19	n	209	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	301	CLA	C3D-C4D	-2.12	1.39	1.44
19	l	208	CLA	C1D-C2D	-2.12	1.41	1.45
19	g	311	CLA	C3D-C4D	-2.12	1.39	1.44
19	i	312	CLA	C3D-C4D	-2.12	1.39	1.44
19	B	821	CLA	C3D-C4D	-2.12	1.39	1.44
19	h	205	CLA	C3D-C4D	-2.12	1.39	1.44
19	k	305	CLA	C3D-C4D	-2.12	1.39	1.44
19	b	309	CLA	C3D-C4D	-2.12	1.39	1.44
19	n	202	CLA	C3D-C4D	-2.12	1.39	1.44
19	A	806	CLA	C3D-C4D	-2.12	1.39	1.44
19	c	309	CLA	C3D-C4D	-2.12	1.39	1.44
19	h	206	CLA	C1D-C2D	-2.12	1.41	1.45
19	A	803	CLA	C3D-C4D	-2.11	1.39	1.44
19	j	309	CLA	C3D-C4D	-2.11	1.39	1.44
19	B	839	CLA	C3D-C4D	-2.11	1.39	1.44
19	n	205	CLA	C1D-C2D	-2.11	1.41	1.45
19	k	306	CLA	C1D-C2D	-2.11	1.41	1.45
19	d	201	CLA	C3D-C4D	-2.11	1.39	1.44
19	e	308	CLA	C3D-C4D	-2.11	1.39	1.44
19	o	312	CLA	C3D-C4D	-2.11	1.39	1.44
28	f	304	CHL	C2-C3	2.11	1.38	1.33
19	A	805	CLA	C1D-C2D	-2.11	1.41	1.45
19	B	809	CLA	C3D-C4D	-2.11	1.39	1.44
19	c	307	CLA	C3D-C4D	-2.11	1.39	1.44
19	c	303	CLA	C1D-C2D	-2.11	1.41	1.45
19	i	302	CLA	C3D-C4D	-2.11	1.39	1.44
19	A	824	CLA	C3D-C4D	-2.11	1.39	1.44
19	c	304	CLA	C3D-C4D	-2.11	1.39	1.44
19	B	840	CLA	C1D-C2D	-2.11	1.41	1.45
19	B	818	CLA	C3D-C4D	-2.11	1.39	1.44
19	d	203	CLA	C3D-C4D	-2.11	1.39	1.44
19	e	308	CLA	C1D-C2D	-2.11	1.41	1.45
19	l	205	CLA	C3D-C4D	-2.11	1.39	1.44
19	B	835	CLA	C1D-C2D	-2.10	1.41	1.45
19	i	303	CLA	C3D-C4D	-2.10	1.39	1.44
19	J	803	CLA	C3D-C4D	-2.10	1.39	1.44
19	g	302	CLA	C3D-C4D	-2.10	1.39	1.44
19	e	311	CLA	C3D-C4D	-2.10	1.39	1.44
28	e	304	CHL	C4D-ND	-2.10	1.34	1.37
19	e	306	CLA	C3D-C4D	-2.10	1.39	1.44
19	c	302	CLA	C3D-C4D	-2.10	1.39	1.44
19	m	304	CLA	C1D-C2D	-2.10	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	l	208	CLA	C3D-C4D	-2.10	1.39	1.44
19	i	308	CLA	C3D-C4D	-2.10	1.39	1.44
19	k	304	CLA	C3D-C4D	-2.10	1.39	1.44
19	A	816	CLA	C3D-C4D	-2.10	1.39	1.44
19	n	207	CLA	C1D-C2D	-2.09	1.41	1.45
19	A	808	CLA	C1D-C2D	-2.09	1.41	1.45
19	g	307	CLA	C3D-C4D	-2.09	1.39	1.44
19	g	308	CLA	C1D-C2D	-2.09	1.41	1.45
19	o	310	CLA	C3D-C4D	-2.09	1.39	1.44
19	a	310	CLA	C3D-C4D	-2.09	1.39	1.44
19	d	204	CLA	C3D-C4D	-2.09	1.39	1.44
19	f	312	CLA	C3D-C4D	-2.09	1.39	1.44
19	a	305	CLA	C3D-C4D	-2.09	1.39	1.44
19	f	308	CLA	C3D-C4D	-2.09	1.39	1.44
19	b	303	CLA	C3D-C4D	-2.09	1.39	1.44
19	B	846	CLA	C3D-C4D	-2.08	1.39	1.44
19	f	302	CLA	C3D-C4D	-2.08	1.39	1.44
28	b	311	CHL	C4D-ND	-2.08	1.34	1.37
19	F	204	CLA	C3D-C4D	-2.08	1.39	1.44
19	a	304	CLA	C3D-C4D	-2.08	1.39	1.44
19	c	315	CLA	C3D-C4D	-2.08	1.39	1.44
19	h	207	CLA	C3D-C4D	-2.08	1.39	1.44
19	f	310	CLA	C3D-C4D	-2.08	1.39	1.44
19	d	209	CLA	C3D-C4D	-2.08	1.39	1.44
19	A	821	CLA	C3D-C4D	-2.08	1.39	1.44
27	B	829	DGD	O2G-C2G	-2.08	1.41	1.46
19	B	804	CLA	C3D-C4D	-2.08	1.39	1.44
19	B	830	CLA	C3D-C4D	-2.08	1.39	1.44
19	k	309	CLA	C1D-C2D	-2.08	1.41	1.45
19	k	309	CLA	C3D-C4D	-2.08	1.39	1.44
19	l	204	CLA	C3D-C4D	-2.08	1.39	1.44
19	A	853	CLA	C3D-C4D	-2.07	1.39	1.44
19	a	309	CLA	C3D-C4D	-2.07	1.39	1.44
25	i	316	LMG	C7-C8	2.07	1.57	1.50
19	f	303	CLA	C3D-C4D	-2.07	1.39	1.44
19	F	202	CLA	C3D-C4D	-2.07	1.39	1.44
25	a	301	LMG	O8-C9	-2.07	1.40	1.45
19	o	305	CLA	C3D-C4D	-2.07	1.39	1.44
28	a	312	CHL	MG-NC	2.07	2.11	2.06
19	l	209	CLA	C1D-C2D	-2.07	1.41	1.45
19	A	826	CLA	C3D-C4D	-2.07	1.39	1.44
28	a	311	CHL	C4D-ND	-2.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	310	CLA	C3D-C4D	-2.07	1.39	1.44
19	A	802	CLA	C1C-C2C	2.07	1.48	1.44
19	B	818	CLA	C1D-C2D	-2.07	1.41	1.45
19	B	803	CLA	C3D-C4D	-2.07	1.39	1.44
19	m	308	CLA	C3D-C4D	-2.07	1.39	1.44
19	j	303	CLA	C3D-C4D	-2.07	1.39	1.44
25	a	318	LMG	C7-C8	2.06	1.57	1.50
19	h	212	CLA	C3D-C4D	-2.06	1.39	1.44
28	g	303	CHL	C2-C3	2.06	1.37	1.33
19	f	307	CLA	C1C-C2C	2.06	1.48	1.44
28	e	301	CHL	MG-ND	-2.06	2.01	2.05
28	g	303	CHL	C4D-ND	-2.06	1.34	1.37
19	e	303	CLA	C3D-C4D	-2.06	1.39	1.44
28	a	313	CHL	MG-NC	2.06	2.11	2.06
19	c	316	CLA	C3D-C4D	-2.05	1.39	1.44
19	m	305	CLA	C1D-C2D	-2.05	1.41	1.45
19	a	305	CLA	C1C-C2C	2.05	1.48	1.44
19	l	201	CLA	C3D-C4D	-2.05	1.39	1.44
28	f	301	CHL	MG-NC	2.05	2.11	2.06
28	a	311	CHL	MG-NB	2.05	2.09	2.05
19	B	847	CLA	C1D-C2D	-2.05	1.41	1.45
19	d	211	CLA	C3D-C4D	-2.05	1.39	1.44
19	h	211	CLA	C3D-C4D	-2.05	1.39	1.44
19	B	836	CLA	C3D-C4D	-2.05	1.39	1.44
28	b	310	CHL	MG-NC	2.05	2.11	2.06
28	k	301	CHL	MG-NB	2.04	2.09	2.05
19	i	309	CLA	C3D-C4D	-2.04	1.39	1.44
28	f	301	CHL	MG-ND	-2.03	2.01	2.05
25	a	301	LMG	C9-C8	2.03	1.56	1.50
19	A	819	CLA	C3D-C4D	-2.03	1.39	1.44
28	i	304	CHL	MG-NC	2.03	2.11	2.06
19	k	311	CLA	C1D-C2D	-2.03	1.41	1.45
28	a	315	CHL	MG-NC	2.03	2.11	2.06
28	e	304	CHL	MG-ND	-2.02	2.01	2.05
19	n	201	CLA	C3D-C4D	-2.02	1.39	1.44
19	m	306	CLA	C1D-C2D	-2.02	1.41	1.45
19	j	311	CLA	C3D-C4D	-2.02	1.39	1.44
28	c	305	CHL	MG-ND	-2.02	2.01	2.05
25	a	316	LMG	C7-C8	2.02	1.56	1.50
28	f	304	CHL	C4D-ND	-2.02	1.34	1.37
28	d	205	CHL	MG-NC	2.02	2.11	2.06
28	b	301	CHL	C4D-ND	-2.01	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	g	310	CHL	MG-NC	2.01	2.11	2.06
29	a	317	NEX	C1-C6	-2.01	1.51	1.54
28	b	312	CHL	C4D-ND	-2.01	1.34	1.37
28	h	202	CHL	C4C-C3C	-2.00	1.41	1.45
28	a	311	CHL	MG-ND	-2.00	2.01	2.05

All (2476) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f	304	CHL	C4A-NA-C1A	12.59	112.36	106.71
28	i	304	CHL	C4A-NA-C1A	11.73	111.98	106.71
28	c	305	CHL	C4A-NA-C1A	11.73	111.98	106.71
28	g	303	CHL	C4A-NA-C1A	11.58	111.91	106.71
28	e	301	CHL	C4A-NA-C1A	11.34	111.80	106.71
28	g	306	CHL	C4A-NA-C1A	11.29	111.78	106.71
28	b	311	CHL	C4A-NA-C1A	11.25	111.76	106.71
28	o	301	CHL	C4A-NA-C1A	11.21	111.74	106.71
28	b	312	CHL	C4A-NA-C1A	11.01	111.66	106.71
28	b	310	CHL	C4A-NA-C1A	10.85	111.58	106.71
28	h	202	CHL	C4A-NA-C1A	10.68	111.51	106.71
28	d	205	CHL	C4A-NA-C1A	10.58	111.46	106.71
28	b	314	CHL	C4A-NA-C1A	10.57	111.46	106.71
28	e	304	CHL	C4A-NA-C1A	10.38	111.37	106.71
28	c	313	CHL	C4A-NA-C1A	10.21	111.30	106.71
28	a	312	CHL	C4A-NA-C1A	9.92	111.17	106.71
28	f	301	CHL	C4A-NA-C1A	9.87	111.14	106.71
28	a	313	CHL	C4A-NA-C1A	9.79	111.11	106.71
28	k	301	CHL	C4A-NA-C1A	9.70	111.07	106.71
28	i	301	CHL	C4A-NA-C1A	9.37	110.92	106.71
28	c	312	CHL	C4A-NA-C1A	9.18	110.83	106.71
28	d	202	CHL	C4A-NA-C1A	9.18	110.83	106.71
28	a	315	CHL	C4A-NA-C1A	9.07	110.78	106.71
28	b	301	CHL	C4A-NA-C1A	8.60	110.57	106.71
19	m	304	CLA	C4A-NA-C1A	-8.22	103.01	106.71
19	i	313	CLA	C4A-NA-C1A	-8.19	103.02	106.71
19	o	307	CLA	C4A-NA-C1A	-8.11	103.06	106.71
22	k	314	DD6	O1-C20-C19	-8.06	107.33	113.38
19	o	302	CLA	C4A-NA-C1A	-8.01	103.11	106.71
19	e	308	CLA	C4A-NA-C1A	-7.97	103.12	106.71
28	m	301	CHL	C4A-NA-C1A	7.97	110.29	106.71
19	f	314	CLA	C4A-NA-C1A	-7.92	103.14	106.71
19	n	202	CLA	C4A-NA-C1A	-7.80	103.20	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	315	CLA	C4A-NA-C1A	-7.76	103.22	106.71
19	n	203	CLA	C4A-NA-C1A	-7.73	103.23	106.71
19	i	311	CLA	C4A-NA-C1A	-7.72	103.23	106.71
19	j	312	CLA	C4A-NA-C1A	-7.70	103.24	106.71
19	B	840	CLA	C4A-NA-C1A	-7.69	103.25	106.71
19	f	311	CLA	C4A-NA-C1A	-7.62	103.28	106.71
19	A	843	CLA	C4A-NA-C1A	-7.61	103.28	106.71
28	g	310	CHL	C4A-NA-C1A	7.52	110.09	106.71
19	g	311	CLA	C4A-NA-C1A	-7.41	103.38	106.71
19	k	309	CLA	C4A-NA-C1A	-7.31	103.42	106.71
28	a	311	CHL	C4A-NA-C1A	7.30	109.99	106.71
19	j	301	CLA	C4A-NA-C1A	-7.27	103.44	106.71
19	a	308	CLA	C4A-NA-C1A	-7.24	103.45	106.71
19	B	838	CLA	C4A-NA-C1A	-7.23	103.45	106.71
19	e	307	CLA	C4A-NA-C1A	-7.21	103.47	106.71
19	l	202	CLA	C4A-NA-C1A	-7.17	103.48	106.71
19	A	806	CLA	C4A-NA-C1A	-7.16	103.49	106.71
19	l	209	CLA	C4A-NA-C1A	-7.13	103.50	106.71
19	A	825	CLA	C4A-NA-C1A	-7.09	103.52	106.71
19	B	847	CLA	C4A-NA-C1A	-7.08	103.52	106.71
19	f	307	CLA	C4A-NA-C1A	-7.08	103.52	106.71
19	A	820	CLA	C4A-NA-C1A	-7.06	103.53	106.71
19	n	204	CLA	C4A-NA-C1A	-7.06	103.53	106.71
19	A	817	CLA	C4A-NA-C1A	-7.03	103.55	106.71
19	f	305	CLA	C4A-NA-C1A	-6.97	103.57	106.71
19	o	304	CLA	C4A-NA-C1A	-6.96	103.58	106.71
19	j	307	CLA	C4A-NA-C1A	-6.94	103.59	106.71
19	a	314	CLA	C4A-NA-C1A	-6.90	103.60	106.71
19	h	213	CLA	C4A-NA-C1A	-6.90	103.61	106.71
19	l	203	CLA	C4A-NA-C1A	-6.88	103.61	106.71
19	m	303	CLA	C4A-NA-C1A	-6.83	103.64	106.71
19	f	309	CLA	C4A-NA-C1A	-6.79	103.65	106.71
19	B	814	CLA	C4A-NA-C1A	-6.78	103.66	106.71
19	c	314	CLA	C4A-NA-C1A	-6.72	103.68	106.71
19	B	823	CLA	C4A-NA-C1A	-6.70	103.69	106.71
19	a	302	CLA	C4A-NA-C1A	-6.69	103.70	106.71
19	A	813	CLA	C4A-NA-C1A	-6.68	103.70	106.71
19	m	311	CLA	C4A-NA-C1A	-6.65	103.72	106.71
19	A	847	CLA	C4A-NA-C1A	-6.64	103.72	106.71
19	k	304	CLA	C4A-NA-C1A	-6.64	103.72	106.71
19	j	313	CLA	C4A-NA-C1A	-6.62	103.73	106.71
19	B	816	CLA	C4A-NA-C1A	-6.60	103.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	803	CLA	C4A-NA-C1A	-6.59	103.74	106.71
19	n	207	CLA	C4A-NA-C1A	-6.53	103.77	106.71
19	l	205	CLA	C4A-NA-C1A	-6.52	103.78	106.71
19	B	845	CLA	C4A-NA-C1A	-6.51	103.78	106.71
19	c	308	CLA	C4A-NA-C1A	-6.47	103.80	106.71
19	a	307	CLA	C4A-NA-C1A	-6.47	103.80	106.71
19	h	208	CLA	C4A-NA-C1A	-6.42	103.82	106.71
19	B	844	CLA	C4A-NA-C1A	-6.41	103.83	106.71
19	i	305	CLA	C4A-NA-C1A	-6.37	103.84	106.71
19	o	312	CLA	C4A-NA-C1A	-6.37	103.84	106.71
19	e	309	CLA	C1D-ND-C4D	-6.36	101.82	106.33
19	A	811	CLA	C4A-NA-C1A	-6.36	103.85	106.71
19	m	306	CLA	C4A-NA-C1A	-6.35	103.85	106.71
19	i	307	CLA	C1D-ND-C4D	-6.32	101.84	106.33
19	h	205	CLA	C4A-NA-C1A	-6.32	103.86	106.71
19	k	307	CLA	C1D-ND-C4D	-6.32	101.85	106.33
19	B	843	CLA	C4A-NA-C1A	-6.31	103.87	106.71
19	d	203	CLA	C4A-NA-C1A	-6.30	103.87	106.71
19	d	207	CLA	C4A-NA-C1A	-6.30	103.87	106.71
19	d	204	CLA	C1D-ND-C4D	-6.30	101.86	106.33
19	c	315	CLA	C1D-ND-C4D	-6.29	101.87	106.33
19	A	827	CLA	C1D-ND-C4D	-6.29	101.87	106.33
19	B	801	CLA	C4A-NA-C1A	-6.27	103.89	106.71
19	a	308	CLA	C1D-ND-C4D	-6.27	101.88	106.33
19	n	205	CLA	C4A-NA-C1A	-6.27	103.89	106.71
19	B	822	CLA	C4A-NA-C1A	-6.27	103.89	106.71
19	k	302	CLA	C4A-NA-C1A	-6.26	103.89	106.71
19	l	207	CLA	C1D-ND-C4D	-6.26	101.89	106.33
19	h	210	CLA	C1D-ND-C4D	-6.25	101.89	106.33
19	b	302	CLA	C1D-ND-C4D	-6.25	101.90	106.33
19	a	307	CLA	C1D-ND-C4D	-6.24	101.90	106.33
19	a	314	CLA	C1D-ND-C4D	-6.24	101.90	106.33
19	F	203	CLA	C4A-NA-C1A	-6.24	103.90	106.71
19	n	205	CLA	C1D-ND-C4D	-6.23	101.91	106.33
19	A	808	CLA	C1D-ND-C4D	-6.23	101.91	106.33
19	A	804	CLA	C1D-ND-C4D	-6.22	101.91	106.33
19	o	306	CLA	C4A-NA-C1A	-6.22	103.91	106.71
19	B	848	CLA	C1D-ND-C4D	-6.22	101.92	106.33
19	A	805	CLA	C4A-NA-C1A	-6.22	103.91	106.71
19	h	208	CLA	C1D-ND-C4D	-6.21	101.92	106.33
19	o	312	CLA	C1D-ND-C4D	-6.21	101.92	106.33
19	A	846	CLA	C4A-NA-C1A	-6.21	103.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	k	311	CLA	C1D-ND-C4D	-6.21	101.92	106.33
19	n	207	CLA	C1D-ND-C4D	-6.21	101.92	106.33
19	B	823	CLA	C1D-ND-C4D	-6.21	101.92	106.33
19	b	306	CLA	C1D-ND-C4D	-6.21	101.93	106.33
19	d	210	CLA	C1D-ND-C4D	-6.20	101.93	106.33
19	g	308	CLA	C1D-ND-C4D	-6.20	101.93	106.33
19	m	306	CLA	C1D-ND-C4D	-6.20	101.93	106.33
19	o	303	CLA	C4A-NA-C1A	-6.20	103.92	106.71
19	k	303	CLA	C1D-ND-C4D	-6.20	101.93	106.33
19	B	842	CLA	C1D-ND-C4D	-6.19	101.94	106.33
19	B	813	CLA	C1D-ND-C4D	-6.18	101.94	106.33
19	B	805	CLA	C4A-NA-C1A	-6.18	103.93	106.71
19	B	847	CLA	C1D-ND-C4D	-6.18	101.95	106.33
19	b	313	CLA	C1D-ND-C4D	-6.18	101.95	106.33
19	h	204	CLA	C1D-ND-C4D	-6.18	101.95	106.33
19	k	306	CLA	C4A-NA-C1A	-6.17	103.93	106.71
19	k	308	CLA	C1D-ND-C4D	-6.17	101.95	106.33
19	o	310	CLA	C1D-ND-C4D	-6.17	101.95	106.33
19	j	308	CLA	C1D-ND-C4D	-6.17	101.95	106.33
19	B	833	CLA	C1D-ND-C4D	-6.16	101.96	106.33
19	m	303	CLA	C1D-ND-C4D	-6.16	101.96	106.33
19	l	206	CLA	C1D-ND-C4D	-6.15	101.96	106.33
19	A	807	CLA	C4A-NA-C1A	-6.15	103.94	106.71
19	B	822	CLA	C1D-ND-C4D	-6.15	101.97	106.33
19	d	208	CLA	C1D-ND-C4D	-6.15	101.97	106.33
19	B	819	CLA	C1D-ND-C4D	-6.15	101.97	106.33
19	j	302	CLA	C1D-ND-C4D	-6.14	101.97	106.33
19	A	825	CLA	C1D-ND-C4D	-6.14	101.98	106.33
19	c	303	CLA	C1D-ND-C4D	-6.14	101.98	106.33
19	i	303	CLA	C1D-ND-C4D	-6.13	101.98	106.33
19	g	305	CLA	C1D-ND-C4D	-6.13	101.98	106.33
19	A	848	CLA	C1D-ND-C4D	-6.13	101.98	106.33
19	g	308	CLA	C4A-NA-C1A	-6.13	103.95	106.71
19	h	206	CLA	C4A-NA-C1A	-6.13	103.95	106.71
19	f	309	CLA	C1D-ND-C4D	-6.12	101.98	106.33
19	d	207	CLA	C1D-ND-C4D	-6.12	101.98	106.33
19	a	304	CLA	C1D-ND-C4D	-6.12	101.99	106.33
19	a	303	CLA	C1D-ND-C4D	-6.12	101.99	106.33
19	i	312	CLA	C1D-ND-C4D	-6.12	101.99	106.33
19	c	308	CLA	C1D-ND-C4D	-6.11	101.99	106.33
19	B	820	CLA	C4A-NA-C1A	-6.11	103.96	106.71
19	B	810	CLA	C1D-ND-C4D	-6.11	101.99	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	845	CLA	C1D-ND-C4D	-6.11	102.00	106.33
19	e	307	CLA	C1D-ND-C4D	-6.11	102.00	106.33
19	A	829	CLA	C1D-ND-C4D	-6.11	102.00	106.33
19	c	309	CLA	C1D-ND-C4D	-6.10	102.00	106.33
19	m	307	CLA	C1D-ND-C4D	-6.10	102.00	106.33
19	o	310	CLA	C4A-NA-C1A	-6.10	103.96	106.71
19	j	306	CLA	C4A-NA-C1A	-6.10	103.97	106.71
19	d	203	CLA	C1D-ND-C4D	-6.10	102.00	106.33
19	i	308	CLA	C1D-ND-C4D	-6.10	102.00	106.33
19	a	309	CLA	C1D-ND-C4D	-6.10	102.00	106.33
19	f	302	CLA	C1D-ND-C4D	-6.10	102.00	106.33
19	B	808	CLA	C4A-NA-C1A	-6.09	103.97	106.71
19	A	850	CLA	C4A-NA-C1A	-6.09	103.97	106.71
19	B	805	CLA	C1D-ND-C4D	-6.09	102.01	106.33
19	o	303	CLA	C1D-ND-C4D	-6.08	102.01	106.33
19	l	207	CLA	C4A-NA-C1A	-6.08	103.97	106.71
19	A	810	CLA	C1D-ND-C4D	-6.08	102.02	106.33
19	A	840	CLA	C1D-ND-C4D	-6.08	102.02	106.33
19	c	306	CLA	C1D-ND-C4D	-6.08	102.02	106.33
19	B	815	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	B	830	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	f	307	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	h	209	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	A	818	CLA	C4A-NA-C1A	-6.07	103.98	106.71
19	c	314	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	h	203	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	A	853	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	h	201	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	B	807	CLA	C1D-ND-C4D	-6.07	102.02	106.33
19	j	307	CLA	C1D-ND-C4D	-6.07	102.03	106.33
19	e	310	CLA	C4A-NA-C1A	-6.07	103.98	106.71
19	A	816	CLA	C1D-ND-C4D	-6.06	102.03	106.33
19	B	849	CLA	C1D-ND-C4D	-6.06	102.03	106.33
19	h	213	CLA	C1D-ND-C4D	-6.06	102.03	106.33
19	m	309	CLA	C1D-ND-C4D	-6.06	102.03	106.33
19	k	307	CLA	C4A-NA-C1A	-6.06	103.98	106.71
19	h	204	CLA	C4A-NA-C1A	-6.06	103.98	106.71
19	A	841	CLA	C1D-ND-C4D	-6.06	102.03	106.33
19	d	204	CLA	C4A-NA-C1A	-6.06	103.98	106.71
19	o	308	CLA	C1D-ND-C4D	-6.05	102.03	106.33
19	A	849	CLA	C1D-ND-C4D	-6.05	102.03	106.33
19	g	307	CLA	C1D-ND-C4D	-6.05	102.03	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	806	CLA	C1D-ND-C4D	-6.05	102.04	106.33
19	k	311	CLA	C4A-NA-C1A	-6.05	103.99	106.71
19	i	312	CLA	C4A-NA-C1A	-6.05	103.99	106.71
19	m	302	CLA	C1D-ND-C4D	-6.04	102.04	106.33
19	o	306	CLA	C1D-ND-C4D	-6.04	102.04	106.33
19	B	821	CLA	C1D-ND-C4D	-6.04	102.04	106.33
19	b	308	CLA	C1D-ND-C4D	-6.04	102.04	106.33
19	A	814	CLA	C1D-ND-C4D	-6.04	102.04	106.33
19	A	818	CLA	C1D-ND-C4D	-6.04	102.05	106.33
19	e	311	CLA	C1D-ND-C4D	-6.04	102.05	106.33
19	A	828	CLA	C1D-ND-C4D	-6.03	102.05	106.33
19	b	307	CLA	C1D-ND-C4D	-6.03	102.05	106.33
19	b	307	CLA	C4A-NA-C1A	-6.03	103.99	106.71
19	B	811	CLA	C4A-NA-C1A	-6.03	103.99	106.71
19	l	205	CLA	C1D-ND-C4D	-6.03	102.05	106.33
19	A	815	CLA	C1D-ND-C4D	-6.03	102.05	106.33
19	B	843	CLA	C1D-ND-C4D	-6.03	102.05	106.33
19	j	304	CLA	C4A-NA-C1A	-6.02	104.00	106.71
19	k	309	CLA	C1D-ND-C4D	-6.02	102.06	106.33
19	A	844	CLA	C1D-ND-C4D	-6.01	102.06	106.33
19	B	832	CLA	C4A-NA-C1A	-6.01	104.00	106.71
19	A	850	CLA	C1D-ND-C4D	-6.01	102.06	106.33
19	B	844	CLA	C1D-ND-C4D	-6.01	102.06	106.33
19	l	208	CLA	C1D-ND-C4D	-6.01	102.06	106.33
19	i	306	CLA	C1D-ND-C4D	-6.01	102.07	106.33
19	A	852	CLA	C1D-ND-C4D	-6.01	102.07	106.33
19	A	805	CLA	C1D-ND-C4D	-6.01	102.07	106.33
19	A	820	CLA	C1D-ND-C4D	-6.01	102.07	106.33
19	j	306	CLA	C1D-ND-C4D	-6.01	102.07	106.33
19	B	820	CLA	C1D-ND-C4D	-6.01	102.07	106.33
19	d	201	CLA	C1D-ND-C4D	-6.00	102.07	106.33
19	k	306	CLA	C1D-ND-C4D	-6.00	102.07	106.33
19	d	210	CLA	C4A-NA-C1A	-5.99	104.01	106.71
19	m	311	CLA	C1D-ND-C4D	-5.99	102.08	106.33
19	e	302	CLA	C1D-ND-C4D	-5.99	102.08	106.33
19	i	302	CLA	C1D-ND-C4D	-5.99	102.08	106.33
19	B	835	CLA	C1D-ND-C4D	-5.99	102.08	106.33
19	f	308	CLA	C1D-ND-C4D	-5.99	102.08	106.33
19	B	837	CLA	C1D-ND-C4D	-5.99	102.08	106.33
19	A	812	CLA	C1D-ND-C4D	-5.99	102.08	106.33
19	k	310	CLA	C1D-ND-C4D	-5.99	102.08	106.33
19	f	303	CLA	C1D-ND-C4D	-5.98	102.08	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	l	209	CLA	C1D-ND-C4D	-5.98	102.08	106.33
19	A	817	CLA	C1D-ND-C4D	-5.98	102.09	106.33
19	e	305	CLA	C1D-ND-C4D	-5.97	102.09	106.33
19	B	841	CLA	C1D-ND-C4D	-5.97	102.09	106.33
19	j	313	CLA	C1D-ND-C4D	-5.97	102.09	106.33
22	n	210	DD6	O1-C20-C19	-5.97	108.90	113.38
19	e	310	CLA	C1D-ND-C4D	-5.97	102.10	106.33
19	f	310	CLA	C4A-NA-C1A	-5.97	104.02	106.71
19	e	305	CLA	C4A-NA-C1A	-5.96	104.03	106.71
19	B	812	CLA	C1D-ND-C4D	-5.96	102.10	106.33
19	c	316	CLA	C1D-ND-C4D	-5.96	102.10	106.33
19	l	204	CLA	C1D-ND-C4D	-5.96	102.10	106.33
19	B	817	CLA	C1D-ND-C4D	-5.96	102.10	106.33
19	c	307	CLA	C1D-ND-C4D	-5.95	102.11	106.33
19	o	309	CLA	C1D-ND-C4D	-5.95	102.11	106.33
19	e	306	CLA	C1D-ND-C4D	-5.95	102.11	106.33
19	m	307	CLA	C4A-NA-C1A	-5.95	104.03	106.71
19	f	310	CLA	C1D-ND-C4D	-5.94	102.11	106.33
19	F	201	CLA	C1D-ND-C4D	-5.94	102.11	106.33
19	c	311	CLA	C1D-ND-C4D	-5.94	102.11	106.33
19	h	206	CLA	C1D-ND-C4D	-5.94	102.11	106.33
19	A	846	CLA	C1D-ND-C4D	-5.94	102.12	106.33
19	n	204	CLA	C1D-ND-C4D	-5.94	102.12	106.33
19	j	309	CLA	C1D-ND-C4D	-5.93	102.12	106.33
19	a	306	CLA	C1D-ND-C4D	-5.92	102.13	106.33
19	B	821	CLA	C4A-NA-C1A	-5.92	104.04	106.71
19	B	810	CLA	C4A-NA-C1A	-5.92	104.04	106.71
19	B	811	CLA	C1D-ND-C4D	-5.92	102.13	106.33
19	e	308	CLA	C1D-ND-C4D	-5.92	102.13	106.33
19	A	824	CLA	C1D-ND-C4D	-5.92	102.13	106.33
19	f	311	CLA	C1D-ND-C4D	-5.92	102.13	106.33
19	o	302	CLA	C1D-ND-C4D	-5.91	102.13	106.33
19	A	839	CLA	C1D-ND-C4D	-5.91	102.14	106.33
19	e	309	CLA	C4A-NA-C1A	-5.91	104.05	106.71
19	g	309	CLA	C1D-ND-C4D	-5.91	102.14	106.33
19	m	305	CLA	C1D-ND-C4D	-5.91	102.14	106.33
19	l	202	CLA	C1D-ND-C4D	-5.91	102.14	106.33
19	g	311	CLA	C1D-ND-C4D	-5.91	102.14	106.33
19	B	814	CLA	C1D-ND-C4D	-5.90	102.14	106.33
19	o	311	CLA	C1D-ND-C4D	-5.90	102.14	106.33
19	A	843	CLA	C1D-ND-C4D	-5.90	102.15	106.33
19	g	302	CLA	C1D-ND-C4D	-5.89	102.15	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	c	302	CLA	C1D-ND-C4D	-5.89	102.15	106.33
19	B	836	CLA	C1D-ND-C4D	-5.89	102.15	106.33
19	d	201	CLA	C4A-NA-C1A	-5.89	104.06	106.71
19	B	832	CLA	C1D-ND-C4D	-5.88	102.16	106.33
19	d	209	CLA	C1D-ND-C4D	-5.88	102.16	106.33
19	e	303	CLA	C1D-ND-C4D	-5.88	102.16	106.33
19	n	201	CLA	C1D-ND-C4D	-5.88	102.16	106.33
19	A	807	CLA	C1D-ND-C4D	-5.88	102.16	106.33
19	B	839	CLA	C1D-ND-C4D	-5.87	102.16	106.33
19	a	302	CLA	C1D-ND-C4D	-5.87	102.16	106.33
19	o	304	CLA	C1D-ND-C4D	-5.87	102.16	106.33
19	A	819	CLA	C1D-ND-C4D	-5.87	102.17	106.33
19	m	305	CLA	C4A-NA-C1A	-5.87	104.07	106.71
19	b	303	CLA	C1D-ND-C4D	-5.87	102.17	106.33
19	B	849	CLA	C4A-NA-C1A	-5.86	104.07	106.71
19	i	306	CLA	C4A-NA-C1A	-5.86	104.07	106.71
19	D	301	CLA	C1D-ND-C4D	-5.86	102.17	106.33
19	f	312	CLA	C4A-NA-C1A	-5.86	104.07	106.71
19	A	826	CLA	C1D-ND-C4D	-5.86	102.17	106.33
19	j	301	CLA	C1D-ND-C4D	-5.86	102.17	106.33
19	d	211	CLA	C1D-ND-C4D	-5.85	102.18	106.33
19	A	842	CLA	C4A-NA-C1A	-5.85	104.07	106.71
19	a	310	CLA	C1D-ND-C4D	-5.85	102.18	106.33
19	f	312	CLA	C1D-ND-C4D	-5.85	102.18	106.33
19	i	311	CLA	C1D-ND-C4D	-5.85	102.18	106.33
22	J	801	DD6	C14-C13-C11	5.85	134.61	125.53
19	f	306	CLA	C1D-ND-C4D	-5.85	102.18	106.33
19	a	304	CLA	C4A-NA-C1A	-5.85	104.08	106.71
19	d	212	CLA	C1D-ND-C4D	-5.85	102.18	106.33
19	o	307	CLA	C1D-ND-C4D	-5.85	102.18	106.33
19	c	304	CLA	C1D-ND-C4D	-5.85	102.18	106.33
19	B	845	CLA	C1D-ND-C4D	-5.84	102.18	106.33
19	A	847	CLA	C1D-ND-C4D	-5.84	102.19	106.33
19	F	204	CLA	C1D-ND-C4D	-5.84	102.19	106.33
19	m	310	CLA	C1D-ND-C4D	-5.84	102.19	106.33
19	i	313	CLA	C1D-ND-C4D	-5.84	102.19	106.33
19	A	813	CLA	C1D-ND-C4D	-5.84	102.19	106.33
19	A	827	CLA	C4A-NA-C1A	-5.83	104.08	106.71
19	i	309	CLA	C1D-ND-C4D	-5.83	102.19	106.33
19	m	309	CLA	C4A-NA-C1A	-5.83	104.08	106.71
19	j	312	CLA	C1D-ND-C4D	-5.83	102.19	106.33
19	m	302	CLA	C4A-NA-C1A	-5.83	104.09	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	840	CLA	C1D-ND-C4D	-5.81	102.21	106.33
19	d	208	CLA	C4A-NA-C1A	-5.81	104.09	106.71
19	j	303	CLA	C1D-ND-C4D	-5.78	102.23	106.33
19	l	206	CLA	C4A-NA-C1A	-5.78	104.11	106.71
19	B	801	CLA	C1D-ND-C4D	-5.77	102.23	106.33
19	o	305	CLA	C1D-ND-C4D	-5.77	102.24	106.33
19	h	211	CLA	C1D-ND-C4D	-5.77	102.24	106.33
19	J	803	CLA	C1D-ND-C4D	-5.77	102.24	106.33
19	D	301	CLA	C4A-NA-C1A	-5.76	104.11	106.71
19	h	212	CLA	C1D-ND-C4D	-5.76	102.24	106.33
19	h	207	CLA	C1D-ND-C4D	-5.76	102.24	106.33
19	A	821	CLA	C4A-NA-C1A	-5.76	104.12	106.71
19	f	314	CLA	C1D-ND-C4D	-5.76	102.25	106.33
19	n	203	CLA	C1D-ND-C4D	-5.75	102.25	106.33
19	c	306	CLA	C4A-NA-C1A	-5.75	104.12	106.71
19	b	309	CLA	C1D-ND-C4D	-5.75	102.25	106.33
19	i	305	CLA	C1D-ND-C4D	-5.75	102.25	106.33
19	o	308	CLA	C4A-NA-C1A	-5.75	104.12	106.71
19	b	313	CLA	C4A-NA-C1A	-5.75	104.12	106.71
19	f	303	CLA	C4A-NA-C1A	-5.75	104.12	106.71
19	A	823	CLA	C1D-ND-C4D	-5.75	102.25	106.33
19	B	838	CLA	C1D-ND-C4D	-5.74	102.25	106.33
19	m	308	CLA	C1D-ND-C4D	-5.74	102.26	106.33
19	h	201	CLA	C4A-NA-C1A	-5.74	104.13	106.71
19	A	811	CLA	C1D-ND-C4D	-5.73	102.26	106.33
19	i	310	CLA	C1D-ND-C4D	-5.73	102.27	106.33
19	A	849	CLA	C4A-NA-C1A	-5.72	104.14	106.71
19	A	821	CLA	C1D-ND-C4D	-5.72	102.27	106.33
19	B	808	CLA	C1D-ND-C4D	-5.72	102.28	106.33
19	A	809	CLA	C1D-ND-C4D	-5.71	102.28	106.33
19	B	818	CLA	C4A-NA-C1A	-5.70	104.14	106.71
19	b	315	CLA	C1D-ND-C4D	-5.70	102.28	106.33
19	f	305	CLA	C1D-ND-C4D	-5.70	102.29	106.33
19	k	303	CLA	C4A-NA-C1A	-5.70	104.14	106.71
19	A	842	CLA	C1D-ND-C4D	-5.69	102.29	106.33
19	a	305	CLA	C1D-ND-C4D	-5.69	102.29	106.33
19	B	818	CLA	C1D-ND-C4D	-5.69	102.29	106.33
19	F	203	CLA	C1D-ND-C4D	-5.68	102.30	106.33
19	B	809	CLA	C4A-NA-C1A	-5.68	104.15	106.71
19	g	309	CLA	C4A-NA-C1A	-5.67	104.16	106.71
19	c	310	CLA	C1D-ND-C4D	-5.67	102.31	106.33
19	j	305	CLA	C1D-ND-C4D	-5.67	102.31	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	809	CLA	C1D-ND-C4D	-5.66	102.31	106.33
19	k	302	CLA	C1D-ND-C4D	-5.66	102.31	106.33
19	A	853	CLA	C4A-NA-C1A	-5.66	104.16	106.71
19	A	802	CLA	C1D-ND-C4D	-5.66	102.31	106.33
19	B	806	CLA	C1D-ND-C4D	-5.65	102.32	106.33
19	g	301	CLA	C1D-ND-C4D	-5.65	102.32	106.33
19	F	202	CLA	C1D-ND-C4D	-5.65	102.32	106.33
19	B	816	CLA	C1D-ND-C4D	-5.65	102.32	106.33
19	A	823	CLA	C4A-NA-C1A	-5.65	104.17	106.71
19	n	209	CLA	C1D-ND-C4D	-5.65	102.32	106.33
19	B	833	CLA	C4A-NA-C1A	-5.65	104.17	106.71
19	B	807	CLA	C4A-NA-C1A	-5.64	104.17	106.71
19	h	211	CLA	C4A-NA-C1A	-5.64	104.17	106.71
19	d	206	CLA	C1D-ND-C4D	-5.64	102.33	106.33
19	A	809	CLA	C4A-NA-C1A	-5.64	104.17	106.71
19	k	305	CLA	C1D-ND-C4D	-5.64	102.33	106.33
19	A	802	CLA	C4A-NA-C1A	-5.63	104.17	106.71
19	c	302	CLA	C4A-NA-C1A	-5.63	104.17	106.71
19	i	307	CLA	C4A-NA-C1A	-5.63	104.18	106.71
19	h	203	CLA	C4A-NA-C1A	-5.62	104.18	106.71
19	A	829	CLA	C4A-NA-C1A	-5.61	104.19	106.71
19	j	311	CLA	C1D-ND-C4D	-5.58	102.37	106.33
19	k	304	CLA	C1D-ND-C4D	-5.58	102.37	106.33
19	j	302	CLA	C4A-NA-C1A	-5.58	104.20	106.71
19	h	210	CLA	C4A-NA-C1A	-5.57	104.20	106.71
19	k	310	CLA	C4A-NA-C1A	-5.57	104.20	106.71
19	l	208	CLA	C4A-NA-C1A	-5.57	104.20	106.71
19	B	817	CLA	C4A-NA-C1A	-5.57	104.20	106.71
19	F	201	CLA	C4A-NA-C1A	-5.57	104.20	106.71
19	k	308	CLA	C4A-NA-C1A	-5.56	104.21	106.71
19	B	804	CLA	C4A-NA-C1A	-5.56	104.21	106.71
19	o	305	CLA	C4A-NA-C1A	-5.56	104.21	106.71
19	n	206	CLA	C1D-ND-C4D	-5.56	102.39	106.33
19	A	814	CLA	C4A-NA-C1A	-5.55	104.21	106.71
19	b	304	CLA	C4A-NA-C1A	-5.55	104.21	106.71
19	j	308	CLA	C4A-NA-C1A	-5.53	104.22	106.71
19	A	812	CLA	C4A-NA-C1A	-5.53	104.22	106.71
19	c	307	CLA	C4A-NA-C1A	-5.53	104.22	106.71
19	i	303	CLA	C4A-NA-C1A	-5.53	104.22	106.71
19	o	309	CLA	C4A-NA-C1A	-5.52	104.23	106.71
19	n	208	CLA	C4A-NA-C1A	-5.51	104.23	106.71
19	f	306	CLA	C4A-NA-C1A	-5.50	104.23	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	848	CLA	C4A-NA-C1A	-5.50	104.23	106.71
19	A	808	CLA	C4A-NA-C1A	-5.49	104.24	106.71
19	l	203	CLA	C1D-ND-C4D	-5.48	102.44	106.33
19	A	841	CLA	C4A-NA-C1A	-5.48	104.24	106.71
19	b	302	CLA	C4A-NA-C1A	-5.48	104.24	106.71
19	b	304	CLA	C1D-ND-C4D	-5.48	102.44	106.33
19	n	202	CLA	C1D-ND-C4D	-5.48	102.44	106.33
19	A	804	CLA	C4A-NA-C1A	-5.48	104.24	106.71
19	j	310	CLA	C1D-ND-C4D	-5.48	102.44	106.33
19	B	835	CLA	C4A-NA-C1A	-5.47	104.25	106.71
19	b	303	CLA	C4A-NA-C1A	-5.47	104.25	106.71
19	d	206	CLA	C4A-NA-C1A	-5.46	104.25	106.71
19	B	839	CLA	C4A-NA-C1A	-5.46	104.25	106.71
19	l	204	CLA	C4A-NA-C1A	-5.46	104.25	106.71
19	n	206	CLA	CHD-C1D-ND	-5.45	119.45	124.45
19	f	302	CLA	C4A-NA-C1A	-5.44	104.26	106.71
19	g	302	CLA	C4A-NA-C1A	-5.43	104.26	106.71
19	A	848	CLA	C4A-NA-C1A	-5.43	104.27	106.71
19	d	209	CLA	C4A-NA-C1A	-5.43	104.27	106.71
19	e	306	CLA	C4A-NA-C1A	-5.42	104.27	106.71
19	A	815	CLA	C4A-NA-C1A	-5.42	104.27	106.71
19	j	303	CLA	C4A-NA-C1A	-5.42	104.27	106.71
19	A	852	CLA	C4A-NA-C1A	-5.42	104.27	106.71
19	B	815	CLA	C4A-NA-C1A	-5.42	104.27	106.71
19	b	306	CLA	C4A-NA-C1A	-5.42	104.27	106.71
19	A	822	CLA	C1D-ND-C4D	-5.41	102.49	106.33
19	b	309	CLA	C4A-NA-C1A	-5.41	104.27	106.71
19	a	305	CLA	C4A-NA-C1A	-5.41	104.28	106.71
19	j	304	CLA	C1D-ND-C4D	-5.41	102.49	106.33
19	h	205	CLA	C1D-ND-C4D	-5.38	102.52	106.33
19	h	209	CLA	C4A-NA-C1A	-5.37	104.29	106.71
19	m	310	CLA	C4A-NA-C1A	-5.37	104.29	106.71
19	B	806	CLA	C4A-NA-C1A	-5.37	104.29	106.71
19	b	305	CLA	C1D-ND-C4D	-5.36	102.52	106.33
19	e	302	CLA	C4A-NA-C1A	-5.36	104.30	106.71
19	B	813	CLA	C4A-NA-C1A	-5.35	104.30	106.71
19	e	303	CLA	C4A-NA-C1A	-5.35	104.30	106.71
19	f	308	CLA	C4A-NA-C1A	-5.35	104.30	106.71
19	c	306	CLA	CHD-C1D-ND	-5.34	119.55	124.45
19	B	819	CLA	C4A-NA-C1A	-5.33	104.31	106.71
19	c	304	CLA	C4A-NA-C1A	-5.33	104.31	106.71
19	h	207	CLA	C4A-NA-C1A	-5.31	104.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	J	803	CLA	C4A-NA-C1A	-5.27	104.33	106.71
19	A	839	CLA	C4A-NA-C1A	-5.25	104.34	106.71
19	h	212	CLA	C4A-NA-C1A	-5.25	104.35	106.71
22	b	317	DD6	C14-C13-C11	5.25	133.67	125.53
19	A	828	CLA	C4A-NA-C1A	-5.24	104.35	106.71
19	A	844	CLA	C4A-NA-C1A	-5.24	104.35	106.71
19	A	845	CLA	C4A-NA-C1A	-5.24	104.35	106.71
19	b	308	CLA	C4A-NA-C1A	-5.24	104.35	106.71
19	g	304	CLA	C1D-ND-C4D	-5.23	102.62	106.33
19	B	818	CLA	CHD-C1D-ND	-5.23	119.65	124.45
19	A	840	CLA	C4A-NA-C1A	-5.23	104.36	106.71
19	F	202	CLA	C4A-NA-C1A	-5.23	104.36	106.71
19	m	304	CLA	CHD-C1D-ND	-5.22	119.66	124.45
19	c	310	CLA	C4A-NA-C1A	-5.21	104.36	106.71
19	b	315	CLA	CHD-C1D-ND	-5.21	119.66	124.45
19	c	303	CLA	C4A-NA-C1A	-5.21	104.36	106.71
19	F	204	CLA	C4A-NA-C1A	-5.20	104.37	106.71
29	a	317	NEX	C5-C6-C1	5.20	124.85	119.70
19	a	306	CLA	C4A-NA-C1A	-5.20	104.37	106.71
19	B	847	CLA	CHD-C1D-ND	-5.19	119.68	124.45
19	m	305	CLA	CHD-C1D-ND	-5.19	119.68	124.45
19	B	803	CLA	C4A-NA-C1A	-5.19	104.37	106.71
22	n	210	DD6	C14-C13-C11	5.17	133.56	125.53
19	B	812	CLA	C4A-NA-C1A	-5.16	104.38	106.71
19	A	803	CLA	C1D-ND-C4D	-5.15	102.67	106.33
19	A	801	CLA	CHD-C1D-ND	-5.14	119.73	124.45
19	B	803	CLA	C1D-ND-C4D	-5.14	102.69	106.33
19	m	308	CLA	C4A-NA-C1A	-5.13	104.40	106.71
19	d	208	CLA	CHD-C1D-ND	-5.13	119.74	124.45
19	c	311	CLA	C4A-NA-C1A	-5.12	104.40	106.71
19	A	819	CLA	C4A-NA-C1A	-5.12	104.41	106.71
19	o	302	CLA	CHD-C1D-ND	-5.11	119.75	124.45
19	B	830	CLA	C4A-NA-C1A	-5.11	104.41	106.71
19	a	309	CLA	C4A-NA-C1A	-5.11	104.41	106.71
19	k	311	CLA	CHD-C1D-ND	-5.11	119.76	124.45
19	B	849	CLA	CHD-C1D-ND	-5.09	119.78	124.45
19	k	305	CLA	C4A-NA-C1A	-5.09	104.42	106.71
19	B	837	CLA	CHD-C1D-ND	-5.08	119.78	124.45
19	B	804	CLA	C1D-ND-C4D	-5.08	102.73	106.33
19	o	303	CLA	CHD-C1D-ND	-5.08	119.79	124.45
19	g	305	CLA	C4A-NA-C1A	-5.08	104.42	106.71
19	g	305	CLA	CHD-C1D-ND	-5.07	119.79	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	c	303	CLA	CHD-C1D-ND	-5.07	119.80	124.45
19	e	311	CLA	C4A-NA-C1A	-5.06	104.43	106.71
19	m	306	CLA	CHD-C1D-ND	-5.06	119.80	124.45
19	B	848	CLA	CHD-C1D-ND	-5.05	119.81	124.45
19	c	309	CLA	C4A-NA-C1A	-5.05	104.43	106.71
19	g	307	CLA	C4A-NA-C1A	-5.05	104.44	106.71
19	i	302	CLA	C4A-NA-C1A	-5.04	104.44	106.71
19	A	845	CLA	CHD-C1D-ND	-5.03	119.83	124.45
19	A	806	CLA	CHD-C1D-ND	-5.02	119.84	124.45
19	A	816	CLA	C4A-NA-C1A	-5.02	104.45	106.71
19	B	837	CLA	C4A-NA-C1A	-5.01	104.45	106.71
19	B	832	CLA	CHD-C1D-ND	-5.01	119.85	124.45
19	e	310	CLA	CHD-C1D-ND	-5.01	119.85	124.45
19	B	840	CLA	CHD-C1D-ND	-5.01	119.85	124.45
19	A	810	CLA	C4A-NA-C1A	-5.00	104.46	106.71
19	b	304	CLA	CHD-C1D-ND	-5.00	119.86	124.45
19	a	306	CLA	CHD-C1D-ND	-4.99	119.87	124.45
22	b	317	DD6	O1-C20-C19	-4.99	109.63	113.38
19	B	835	CLA	CHD-C1D-ND	-4.98	119.87	124.45
19	a	302	CLA	CHD-C1D-ND	-4.98	119.87	124.45
19	l	201	CLA	C1D-ND-C4D	-4.98	102.80	106.33
19	B	841	CLA	CHD-C1D-ND	-4.98	119.88	124.45
19	i	302	CLA	CHD-C1D-ND	-4.98	119.88	124.45
19	n	209	CLA	CHD-C1D-ND	-4.98	119.88	124.45
19	n	208	CLA	CHD-C1D-ND	-4.97	119.88	124.45
19	m	304	CLA	C3A-C2A-C1A	-4.97	93.90	101.34
19	j	306	CLA	CHD-C1D-ND	-4.96	119.89	124.45
19	B	801	CLA	CHD-C1D-ND	-4.96	119.89	124.45
19	j	309	CLA	C4A-NA-C1A	-4.96	104.48	106.71
19	a	314	CLA	CHD-C1D-ND	-4.96	119.90	124.45
19	m	304	CLA	C1D-ND-C4D	-4.95	102.82	106.33
19	o	304	CLA	CHD-C1D-ND	-4.95	119.91	124.45
19	l	202	CLA	CHD-C1D-ND	-4.95	119.91	124.45
19	i	311	CLA	CHD-C1D-ND	-4.94	119.91	124.45
19	n	204	CLA	CHD-C1D-ND	-4.94	119.92	124.45
19	m	309	CLA	CHD-C1D-ND	-4.93	119.92	124.45
19	B	805	CLA	CHD-C1D-ND	-4.93	119.92	124.45
19	j	313	CLA	CHD-C1D-ND	-4.93	119.92	124.45
19	A	822	CLA	C4A-NA-C1A	-4.92	104.49	106.71
19	i	308	CLA	C4A-NA-C1A	-4.92	104.49	106.71
19	B	841	CLA	C4A-NA-C1A	-4.91	104.50	106.71
19	B	842	CLA	C4A-NA-C1A	-4.90	104.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	804	CLA	CHD-C1D-ND	-4.90	119.95	124.45
19	n	208	CLA	C1D-ND-C4D	-4.90	102.86	106.33
19	a	303	CLA	C4A-NA-C1A	-4.89	104.51	106.71
19	i	310	CLA	C4A-NA-C1A	-4.89	104.51	106.71
19	A	853	CLA	CHD-C1D-ND	-4.88	119.97	124.45
19	j	310	CLA	C4A-NA-C1A	-4.88	104.51	106.71
19	e	308	CLA	CHD-C1D-ND	-4.88	119.97	124.45
19	h	201	CLA	CHD-C1D-ND	-4.87	119.97	124.45
19	a	310	CLA	C4A-NA-C1A	-4.87	104.52	106.71
19	j	312	CLA	CHD-C1D-ND	-4.87	119.98	124.45
19	g	301	CLA	CHD-C1D-ND	-4.87	119.98	124.45
19	l	208	CLA	CHD-C1D-ND	-4.86	119.98	124.45
19	i	308	CLA	CHD-C1D-ND	-4.86	119.99	124.45
25	j	314	LMG	C7-O1-C1	4.86	123.22	113.74
19	b	305	CLA	CHD-C1D-ND	-4.85	120.00	124.45
19	A	843	CLA	CHD-C1D-ND	-4.84	120.01	124.45
19	n	201	CLA	C4A-NA-C1A	-4.84	104.53	106.71
19	j	304	CLA	CHD-C1D-ND	-4.83	120.01	124.45
19	c	316	CLA	C4A-NA-C1A	-4.83	104.53	106.71
19	i	306	CLA	CHD-C1D-ND	-4.83	120.02	124.45
19	h	205	CLA	CHD-C1D-ND	-4.83	120.02	124.45
19	A	825	CLA	CHD-C1D-ND	-4.83	120.02	124.45
19	n	202	CLA	CHD-C1D-ND	-4.83	120.02	124.45
19	l	206	CLA	CHD-C1D-ND	-4.82	120.02	124.45
19	m	304	CLA	C2A-C3A-C4A	-4.82	94.08	101.87
19	B	820	CLA	CHD-C1D-ND	-4.82	120.02	124.45
19	f	305	CLA	CHD-C1D-ND	-4.82	120.02	124.45
19	A	811	CLA	CHD-C1D-ND	-4.81	120.03	124.45
19	d	207	CLA	CHD-C1D-ND	-4.81	120.03	124.45
19	a	308	CLA	CHD-C1D-ND	-4.81	120.04	124.45
19	A	827	CLA	CHD-C1D-ND	-4.80	120.04	124.45
19	f	314	CLA	CHD-C1D-ND	-4.80	120.04	124.45
19	A	808	CLA	CHD-C1D-ND	-4.80	120.04	124.45
19	B	838	CLA	CHD-C1D-ND	-4.80	120.05	124.45
19	o	308	CLA	CHD-C1D-ND	-4.79	120.05	124.45
19	A	824	CLA	C4A-NA-C1A	-4.78	104.56	106.71
19	B	833	CLA	CHD-C1D-ND	-4.78	120.06	124.45
19	g	308	CLA	CHD-C1D-ND	-4.78	120.06	124.45
19	m	302	CLA	CHD-C1D-ND	-4.78	120.06	124.45
19	g	304	CLA	CHD-C1D-ND	-4.78	120.06	124.45
19	B	842	CLA	CHD-C1D-ND	-4.77	120.07	124.45
19	o	307	CLA	CHD-C1D-ND	-4.77	120.07	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	e	309	CLA	CHD-C1D-ND	-4.77	120.07	124.45
19	c	311	CLA	CHD-C1D-ND	-4.76	120.08	124.45
19	o	306	CLA	CHD-C1D-ND	-4.76	120.08	124.45
19	A	828	CLA	CHD-C1D-ND	-4.76	120.08	124.45
19	c	314	CLA	CHD-C1D-ND	-4.75	120.09	124.45
19	d	212	CLA	C4A-NA-C1A	-4.75	104.57	106.71
19	B	812	CLA	CHD-C1D-ND	-4.75	120.09	124.45
28	g	310	CHL	O2D-CGD-CBD	4.75	119.71	111.27
19	c	308	CLA	CHD-C1D-ND	-4.75	120.09	124.45
19	A	823	CLA	CHD-C1D-ND	-4.74	120.09	124.45
19	k	304	CLA	CHD-C1D-ND	-4.74	120.10	124.45
19	A	802	CLA	CHD-C1D-ND	-4.74	120.10	124.45
19	a	305	CLA	CHD-C1D-ND	-4.73	120.10	124.45
19	A	840	CLA	CHD-C1D-ND	-4.73	120.11	124.45
19	f	311	CLA	CHD-C1D-ND	-4.73	120.11	124.45
19	d	210	CLA	CHD-C1D-ND	-4.72	120.11	124.45
19	d	204	CLA	CHD-C1D-ND	-4.72	120.11	124.45
19	h	208	CLA	CHD-C1D-ND	-4.72	120.12	124.45
19	A	817	CLA	CHD-C1D-ND	-4.72	120.12	124.45
19	A	849	CLA	CHD-C1D-ND	-4.72	120.12	124.45
19	e	307	CLA	CHD-C1D-ND	-4.72	120.12	124.45
19	A	805	CLA	CHD-C1D-ND	-4.71	120.13	124.45
19	B	844	CLA	CHD-C1D-ND	-4.71	120.13	124.45
19	l	207	CLA	CHD-C1D-ND	-4.71	120.13	124.45
19	a	307	CLA	CHD-C1D-ND	-4.71	120.13	124.45
19	h	209	CLA	CHD-C1D-ND	-4.70	120.13	124.45
19	f	309	CLA	CHD-C1D-ND	-4.70	120.13	124.45
19	j	305	CLA	CHD-C1D-ND	-4.70	120.14	124.45
19	h	206	CLA	CHD-C1D-ND	-4.69	120.14	124.45
19	n	209	CLA	C4A-NA-C1A	-4.69	104.60	106.71
19	c	315	CLA	CHD-C1D-ND	-4.69	120.14	124.45
19	B	810	CLA	CHD-C1D-ND	-4.69	120.14	124.45
19	o	312	CLA	CHD-C1D-ND	-4.69	120.14	124.45
19	i	307	CLA	CHD-C1D-ND	-4.69	120.14	124.45
19	A	848	CLA	CHD-C1D-ND	-4.69	120.14	124.45
19	b	305	CLA	C4A-NA-C1A	-4.69	104.60	106.71
19	j	305	CLA	C4A-NA-C1A	-4.69	104.60	106.71
19	k	305	CLA	CHD-C1D-ND	-4.69	120.15	124.45
19	B	843	CLA	CHD-C1D-ND	-4.69	120.15	124.45
19	b	302	CLA	CHD-C1D-ND	-4.69	120.15	124.45
19	A	829	CLA	CHD-C1D-ND	-4.68	120.15	124.45
19	l	204	CLA	CHD-C1D-ND	-4.68	120.15	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	m	311	CLA	CHD-C1D-ND	-4.68	120.15	124.45
19	B	822	CLA	CHD-C1D-ND	-4.68	120.15	124.45
19	A	842	CLA	CHD-C1D-ND	-4.68	120.16	124.45
19	g	311	CLA	CHD-C1D-ND	-4.68	120.16	124.45
19	k	309	CLA	CHD-C1D-ND	-4.67	120.16	124.45
19	l	203	CLA	CHD-C1D-ND	-4.67	120.16	124.45
19	A	803	CLA	CHD-C1D-ND	-4.67	120.17	124.45
19	B	823	CLA	CHD-C1D-ND	-4.66	120.17	124.45
19	B	814	CLA	CHD-C1D-ND	-4.66	120.17	124.45
19	f	307	CLA	CHD-C1D-ND	-4.66	120.17	124.45
19	i	313	CLA	CHD-C1D-ND	-4.66	120.17	124.45
19	i	310	CLA	CHD-C1D-ND	-4.66	120.17	124.45
19	i	312	CLA	CHD-C1D-ND	-4.66	120.17	124.45
19	o	310	CLA	CHD-C1D-ND	-4.66	120.17	124.45
28	g	306	CHL	O2D-CGD-CBD	4.66	119.54	111.27
19	j	301	CLA	CHD-C1D-ND	-4.65	120.18	124.45
19	j	310	CLA	CHD-C1D-ND	-4.65	120.18	124.45
19	g	301	CLA	C4A-NA-C1A	-4.65	104.61	106.71
19	d	211	CLA	C4A-NA-C1A	-4.65	104.62	106.71
19	n	205	CLA	CHD-C1D-ND	-4.64	120.19	124.45
19	A	813	CLA	CHD-C1D-ND	-4.64	120.19	124.45
19	f	306	CLA	CHD-C1D-ND	-4.64	120.19	124.45
19	i	305	CLA	CHD-C1D-ND	-4.64	120.19	124.45
19	B	815	CLA	CHD-C1D-ND	-4.63	120.19	124.45
19	a	303	CLA	CHD-C1D-ND	-4.63	120.19	124.45
29	a	317	NEX	C2-C1-C6	4.63	113.72	109.21
19	A	815	CLA	CHD-C1D-ND	-4.63	120.20	124.45
19	e	306	CLA	CHD-C1D-ND	-4.63	120.20	124.45
19	j	308	CLA	CHD-C1D-ND	-4.63	120.20	124.45
19	b	313	CLA	CHD-C1D-ND	-4.62	120.20	124.45
19	m	307	CLA	CHD-C1D-ND	-4.62	120.20	124.45
19	d	203	CLA	CHD-C1D-ND	-4.62	120.21	124.45
19	A	847	CLA	CHD-C1D-ND	-4.62	120.21	124.45
19	l	209	CLA	CHD-C1D-ND	-4.62	120.21	124.45
19	o	305	CLA	CHD-C1D-ND	-4.61	120.21	124.45
19	j	307	CLA	CHD-C1D-ND	-4.61	120.22	124.45
19	c	309	CLA	CHD-C1D-ND	-4.61	120.22	124.45
19	m	308	CLA	CHD-C1D-ND	-4.61	120.22	124.45
19	k	307	CLA	CHD-C1D-ND	-4.61	120.22	124.45
19	A	818	CLA	CHD-C1D-ND	-4.60	120.22	124.45
19	B	816	CLA	CHD-C1D-ND	-4.60	120.22	124.45
19	n	206	CLA	CHB-C1B-NB	-4.60	119.38	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	816	CLA	CHD-C1D-ND	-4.60	120.23	124.45
19	B	807	CLA	CHD-C1D-ND	-4.60	120.23	124.45
19	A	826	CLA	C4A-NA-C1A	-4.60	104.64	106.71
19	A	846	CLA	CHD-C1D-ND	-4.60	120.23	124.45
19	B	803	CLA	CHD-C1D-ND	-4.59	120.23	124.45
19	d	206	CLA	CHD-C1D-ND	-4.59	120.23	124.45
19	n	207	CLA	CHD-C1D-ND	-4.59	120.23	124.45
19	n	203	CLA	CHD-C1D-ND	-4.59	120.24	124.45
22	a	320	DD6	C14-C13-C11	4.59	132.65	125.53
19	e	302	CLA	CHD-C1D-ND	-4.59	120.24	124.45
19	k	308	CLA	CHD-C1D-ND	-4.59	120.24	124.45
19	A	814	CLA	CHD-C1D-ND	-4.59	120.24	124.45
19	m	303	CLA	CHD-C1D-ND	-4.59	120.24	124.45
19	A	820	CLA	CHD-C1D-ND	-4.58	120.24	124.45
19	A	807	CLA	CHD-C1D-ND	-4.58	120.25	124.45
19	A	850	CLA	CHD-C1D-ND	-4.58	120.25	124.45
19	h	210	CLA	CHD-C1D-ND	-4.58	120.25	124.45
19	B	817	CLA	CHD-C1D-ND	-4.58	120.25	124.45
19	B	819	CLA	CHD-C1D-ND	-4.58	120.25	124.45
19	B	821	CLA	CHD-C1D-ND	-4.58	120.25	124.45
19	f	308	CLA	CHD-C1D-ND	-4.57	120.25	124.45
19	B	813	CLA	CHD-C1D-ND	-4.57	120.25	124.45
19	b	307	CLA	CHD-C1D-ND	-4.57	120.25	124.45
19	B	845	CLA	CHD-C1D-ND	-4.57	120.26	124.45
19	A	822	CLA	CHD-C1D-ND	-4.56	120.26	124.45
19	l	205	CLA	CHD-C1D-ND	-4.56	120.26	124.45
19	c	315	CLA	C4A-NA-C1A	-4.56	104.66	106.71
28	c	305	CHL	O2D-CGD-CBD	4.56	119.37	111.27
19	A	844	CLA	CHD-C1D-ND	-4.56	120.26	124.45
19	g	309	CLA	CHD-C1D-ND	-4.56	120.27	124.45
19	h	213	CLA	CHD-C1D-ND	-4.56	120.27	124.45
19	F	201	CLA	CHD-C1D-ND	-4.55	120.27	124.45
19	k	306	CLA	CHD-C1D-ND	-4.55	120.27	124.45
19	A	804	CLA	CHD-C1D-ND	-4.55	120.28	124.45
19	g	307	CLA	CHD-C1D-ND	-4.55	120.28	124.45
19	e	305	CLA	CHD-C1D-ND	-4.54	120.28	124.45
19	c	310	CLA	CHD-C1D-ND	-4.54	120.28	124.45
19	A	841	CLA	CHD-C1D-ND	-4.54	120.29	124.45
19	f	312	CLA	CHD-C1D-ND	-4.54	120.29	124.45
19	g	302	CLA	CHD-C1D-ND	-4.53	120.29	124.45
19	B	846	CLA	CHD-C1D-ND	-4.53	120.29	124.45
19	i	309	CLA	C4A-NA-C1A	-4.53	104.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	810	CLA	CHD-C1D-ND	-4.53	120.30	124.45
19	h	207	CLA	CHD-C1D-ND	-4.53	120.30	124.45
22	g	314	DD6	C14-C13-C11	4.52	132.55	125.53
19	d	201	CLA	CHD-C1D-ND	-4.52	120.30	124.45
19	h	203	CLA	CHD-C1D-ND	-4.52	120.30	124.45
19	j	302	CLA	CHD-C1D-ND	-4.52	120.30	124.45
19	A	824	CLA	CHD-C1D-ND	-4.52	120.30	124.45
19	c	302	CLA	CHD-C1D-ND	-4.52	120.30	124.45
19	a	310	CLA	CHD-C1D-ND	-4.51	120.31	124.45
19	l	201	CLA	CHD-C1D-ND	-4.51	120.31	124.45
22	m	312	DD6	C14-C13-C11	4.51	132.52	125.53
19	f	302	CLA	CHD-C1D-ND	-4.50	120.32	124.45
19	b	306	CLA	CHD-C1D-ND	-4.50	120.32	124.45
19	A	801	CLA	CHB-C1B-NB	-4.49	119.50	124.26
19	B	809	CLA	CHD-C1D-ND	-4.49	120.33	124.45
19	A	809	CLA	CHD-C1D-ND	-4.49	120.33	124.45
19	A	801	CLA	C4A-NA-C1A	-4.48	104.69	106.71
19	A	819	CLA	CHD-C1D-ND	-4.47	120.34	124.45
19	e	311	CLA	CHD-C1D-ND	-4.47	120.34	124.45
19	A	801	CLA	C1D-ND-C4D	-4.47	103.16	106.33
19	F	202	CLA	CHD-C1D-ND	-4.47	120.35	124.45
19	j	309	CLA	CHD-C1D-ND	-4.47	120.35	124.45
19	F	203	CLA	CHD-C1D-ND	-4.46	120.36	124.45
19	k	303	CLA	CHD-C1D-ND	-4.46	120.36	124.45
19	g	304	CLA	C4A-NA-C1A	-4.46	104.70	106.71
19	a	309	CLA	CHD-C1D-ND	-4.45	120.36	124.45
19	m	310	CLA	CHD-C1D-ND	-4.45	120.37	124.45
22	h	214	DD6	C14-C13-C11	4.45	132.43	125.53
22	j	315	DD6	C14-C13-C11	4.44	132.43	125.53
19	k	310	CLA	CHD-C1D-ND	-4.44	120.37	124.45
19	A	852	CLA	CHD-C1D-ND	-4.44	120.38	124.45
19	b	309	CLA	CHD-C1D-ND	-4.43	120.38	124.45
19	o	309	CLA	CHD-C1D-ND	-4.43	120.38	124.45
19	k	302	CLA	CHD-C1D-ND	-4.42	120.39	124.45
19	d	209	CLA	CHD-C1D-ND	-4.41	120.40	124.45
19	B	803	CLA	CHB-C1B-NB	-4.41	119.59	124.26
19	b	308	CLA	CHD-C1D-ND	-4.41	120.41	124.45
19	B	806	CLA	CHD-C1D-ND	-4.40	120.41	124.45
19	h	204	CLA	CHD-C1D-ND	-4.40	120.41	124.45
19	f	310	CLA	CHD-C1D-ND	-4.39	120.42	124.45
19	A	802	CLA	CHB-C1B-NB	-4.39	119.61	124.26
19	B	839	CLA	CHD-C1D-ND	-4.38	120.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	d	212	CLA	CHD-C1D-ND	-4.38	120.43	124.45
19	h	212	CLA	CHD-C1D-ND	-4.37	120.43	124.45
19	i	303	CLA	CHD-C1D-ND	-4.37	120.44	124.45
19	A	821	CLA	CHD-C1D-ND	-4.37	120.44	124.45
19	J	803	CLA	CHD-C1D-ND	-4.37	120.44	124.45
19	c	316	CLA	CHD-C1D-ND	-4.37	120.44	124.45
22	A	832	DD6	C14-C13-C11	4.36	132.30	125.53
19	f	303	CLA	CHD-C1D-ND	-4.36	120.45	124.45
19	d	211	CLA	CHD-C1D-ND	-4.35	120.45	124.45
19	h	211	CLA	CHD-C1D-ND	-4.35	120.46	124.45
19	B	830	CLA	CHD-C1D-ND	-4.35	120.46	124.45
19	A	826	CLA	CHD-C1D-ND	-4.33	120.47	124.45
19	e	303	CLA	CHD-C1D-ND	-4.33	120.47	124.45
19	A	812	CLA	CHD-C1D-ND	-4.33	120.48	124.45
28	b	310	CHL	O2D-CGD-CBD	4.33	118.96	111.27
19	b	303	CLA	CHD-C1D-ND	-4.32	120.48	124.45
19	A	828	CLA	CHB-C1B-NB	-4.31	119.69	124.26
28	d	202	CHL	O2D-CGD-CBD	4.31	118.93	111.27
19	D	301	CLA	CHD-C1D-ND	-4.31	120.50	124.45
19	A	839	CLA	CHD-C1D-ND	-4.30	120.51	124.45
19	F	204	CLA	CHD-C1D-ND	-4.30	120.51	124.45
22	g	315	DD6	C14-C13-C11	4.29	132.19	125.53
19	i	309	CLA	CHD-C1D-ND	-4.28	120.52	124.45
19	n	201	CLA	CHD-C1D-ND	-4.28	120.53	124.45
19	c	307	CLA	CHD-C1D-ND	-4.27	120.53	124.45
19	o	311	CLA	CHD-C1D-ND	-4.27	120.53	124.45
19	a	304	CLA	CHD-C1D-ND	-4.26	120.54	124.45
19	c	304	CLA	CHD-C1D-ND	-4.26	120.54	124.45
19	j	303	CLA	CHD-C1D-ND	-4.26	120.54	124.45
19	B	808	CLA	CHD-C1D-ND	-4.24	120.55	124.45
28	h	202	CHL	O2D-CGD-CBD	4.23	118.79	111.27
22	l	211	DD6	C14-C13-C11	4.23	132.09	125.53
28	d	205	CHL	O2D-CGD-CBD	4.23	118.78	111.27
28	e	304	CHL	O2D-CGD-CBD	4.22	118.78	111.27
22	k	313	DD6	C14-C13-C11	4.22	132.09	125.53
21	A	831	LHG	O4-P-O5	4.22	133.09	112.24
19	B	823	CLA	CHB-C1B-NB	-4.22	119.79	124.26
19	B	811	CLA	CHD-C1D-ND	-4.21	120.58	124.45
19	B	801	CLA	CHB-C1B-NB	-4.20	119.81	124.26
22	k	314	DD6	C21-C20-C19	4.20	119.00	114.28
19	n	206	CLA	C4A-NA-C1A	-4.19	104.82	106.71
19	B	816	CLA	CHB-C1B-NB	-4.18	119.83	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	e	313	DD6	C14-C13-C11	4.16	131.98	125.53
19	B	846	CLA	C1D-ND-C4D	-4.16	103.38	106.33
22	f	315	DD6	C14-C13-C11	4.15	131.97	125.53
22	J	802	DD6	O1-C20-C19	-4.14	110.27	113.38
19	B	836	CLA	CHD-C1D-ND	-4.13	120.66	124.45
22	o	314	DD6	O1-C20-C19	-4.12	110.29	113.38
19	o	311	CLA	C4A-NA-C1A	-4.11	104.86	106.71
19	A	822	CLA	CHB-C1B-NB	-4.11	119.90	124.26
28	c	313	CHL	O2D-CGD-CBD	4.11	118.58	111.27
19	j	311	CLA	CHD-C1D-ND	-4.11	120.68	124.45
22	d	214	DD6	C14-C13-C11	4.11	131.90	125.53
19	A	808	CLA	CHB-C1B-NB	-4.07	119.95	124.26
19	o	307	CLA	CHB-C1B-NB	-4.07	119.95	124.26
22	F	205	DD6	O1-C20-C19	-4.07	110.33	113.38
22	i	315	DD6	C14-C13-C11	4.06	131.83	125.53
19	n	209	CLA	CHB-C1B-NB	-4.05	119.97	124.26
19	e	305	CLA	CHB-C1B-NB	-4.05	119.97	124.26
22	j	316	DD6	C14-C13-C11	4.05	131.81	125.53
19	B	830	CLA	CHB-C1B-NB	-4.04	119.97	124.26
19	l	201	CLA	CHB-C1B-NB	-4.04	119.98	124.26
19	B	836	CLA	C4A-NA-C1A	-4.03	104.89	106.71
28	a	311	CHL	O2D-CGD-CBD	4.03	118.43	111.27
19	i	310	CLA	CHB-C1B-NB	-4.02	120.00	124.26
19	o	312	CLA	CHB-C1B-NB	-4.02	120.00	124.26
19	c	311	CLA	CHB-C1B-NB	-4.01	120.01	124.26
28	b	314	CHL	O2D-CGD-CBD	4.01	118.40	111.27
19	n	202	CLA	CHB-C1B-NB	-3.99	120.03	124.26
19	F	203	CLA	CHB-C1B-NB	-3.98	120.04	124.26
19	a	302	CLA	CHB-C1B-NB	-3.98	120.04	124.26
19	j	305	CLA	CHB-C1B-NB	-3.97	120.06	124.26
28	c	312	CHL	CAA-C2A-C3A	-3.96	101.92	112.78
19	B	843	CLA	CHB-C1B-NB	-3.95	120.08	124.26
28	o	301	CHL	O2D-CGD-CBD	3.94	118.27	111.27
19	e	310	CLA	CHB-C1B-NB	-3.94	120.08	124.26
19	m	304	CLA	CHB-C1B-NB	-3.93	120.09	124.26
19	A	809	CLA	CHB-C1B-NB	-3.93	120.10	124.26
22	c	317	DD6	C14-C13-C11	3.92	131.61	125.53
19	g	304	CLA	CHB-C1B-NB	-3.91	120.11	124.26
19	j	310	CLA	CHB-C1B-NB	-3.91	120.12	124.26
19	B	846	CLA	CHB-C1B-NB	-3.90	120.12	124.26
19	c	315	CLA	CHB-C1B-NB	-3.89	120.14	124.26
19	e	306	CLA	CHB-C1B-NB	-3.89	120.14	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	312	CHL	O2D-CGD-CBD	3.89	118.18	111.27
19	A	823	CLA	CHB-C1B-NB	-3.88	120.15	124.26
22	d	215	DD6	O1-C20-C19	-3.88	110.47	113.38
19	a	310	CLA	CHB-C1B-NB	-3.86	120.17	124.26
19	b	304	CLA	CHB-C1B-NB	-3.85	120.18	124.26
19	b	306	CLA	CHB-C1B-NB	-3.85	120.18	124.26
19	A	816	CLA	CHB-C1B-NB	-3.83	120.20	124.26
28	a	311	CHL	C3B-C4B-NB	-3.82	106.97	110.52
22	c	319	DD6	C14-C13-C11	3.82	131.46	125.53
19	A	804	CLA	CHB-C1B-NB	-3.82	120.22	124.26
19	B	821	CLA	CHB-C1B-NB	-3.82	120.22	124.26
19	l	206	CLA	CHB-C1B-NB	-3.81	120.22	124.26
28	m	301	CHL	O2D-CGD-CBD	3.81	118.03	111.27
28	g	303	CHL	C3B-C4B-NB	-3.81	106.98	110.52
19	d	208	CLA	CHB-C1B-NB	-3.80	120.23	124.26
19	B	849	CLA	CHB-C1B-NB	-3.80	120.23	124.26
28	g	303	CHL	O2D-CGD-CBD	3.80	118.02	111.27
19	o	302	CLA	CHB-C1B-NB	-3.79	120.24	124.26
19	o	309	CLA	CHB-C1B-NB	-3.79	120.24	124.26
19	k	302	CLA	CHB-C1B-NB	-3.79	120.25	124.26
19	o	303	CLA	CHB-C1B-NB	-3.79	120.25	124.26
19	B	841	CLA	CHB-C1B-NB	-3.78	120.25	124.26
19	A	803	CLA	CHB-C1B-NB	-3.78	120.26	124.26
19	A	826	CLA	CHB-C1B-NB	-3.78	120.26	124.26
19	d	212	CLA	CHB-C1B-NB	-3.77	120.26	124.26
28	i	304	CHL	O2D-CGD-CBD	3.77	117.96	111.27
19	f	305	CLA	CHB-C1B-NB	-3.76	120.27	124.26
19	i	312	CLA	CHB-C1B-NB	-3.76	120.27	124.26
28	m	301	CHL	C3B-C4B-NB	-3.76	107.03	110.52
19	A	842	CLA	CHB-C1B-NB	-3.75	120.28	124.26
19	B	832	CLA	CHB-C1B-NB	-3.75	120.29	124.26
19	f	307	CLA	CHB-C1B-NB	-3.75	120.29	124.26
19	n	203	CLA	CHB-C1B-NB	-3.75	120.29	124.26
19	m	308	CLA	CHB-C1B-NB	-3.75	120.29	124.26
19	n	207	CLA	CHB-C1B-NB	-3.75	120.29	124.26
19	A	821	CLA	CHB-C1B-NB	-3.74	120.30	124.26
19	A	819	CLA	CHB-C1B-NB	-3.74	120.30	124.26
19	g	307	CLA	CHB-C1B-NB	-3.74	120.30	124.26
19	j	304	CLA	CHB-C1B-NB	-3.73	120.31	124.26
19	b	305	CLA	CHB-C1B-NB	-3.73	120.31	124.26
19	n	208	CLA	CHB-C1B-NB	-3.73	120.31	124.26
19	A	845	CLA	CHB-C1B-NB	-3.72	120.31	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	312	CHL	O2D-CGD-CBD	3.72	117.89	111.27
19	l	209	CLA	CHB-C1B-NB	-3.72	120.31	124.26
19	l	204	CLA	CHB-C1B-NB	-3.72	120.32	124.26
19	g	301	CLA	CHB-C1B-NB	-3.72	120.32	124.26
28	f	304	CHL	C3B-C4B-NB	-3.72	107.07	110.52
19	j	306	CLA	CHB-C1B-NB	-3.72	120.32	124.26
19	o	307	CLA	C3A-C2A-C1A	-3.72	95.77	101.34
19	B	809	CLA	CHB-C1B-NB	-3.72	120.32	124.26
19	m	302	CLA	CHB-C1B-NB	-3.71	120.33	124.26
19	A	811	CLA	CHB-C1B-NB	-3.71	120.33	124.26
19	B	806	CLA	CHB-C1B-NB	-3.71	120.33	124.26
19	B	804	CLA	CHB-C1B-NB	-3.71	120.33	124.26
19	f	311	CLA	CHB-C1B-NB	-3.71	120.33	124.26
19	B	817	CLA	CHB-C1B-NB	-3.71	120.33	124.26
19	b	313	CLA	CHB-C1B-NB	-3.71	120.33	124.26
19	m	305	CLA	CHB-C1B-NB	-3.71	120.33	124.26
28	a	315	CHL	O2D-CGD-CBD	3.71	117.85	111.27
19	B	818	CLA	CHB-C1B-NB	-3.70	120.34	124.26
28	k	301	CHL	O2D-CGD-CBD	3.70	117.84	111.27
19	B	807	CLA	CHB-C1B-NB	-3.70	120.34	124.26
19	B	819	CLA	CHB-C1B-NB	-3.70	120.34	124.26
19	B	805	CLA	CHB-C1B-NB	-3.69	120.35	124.26
19	h	208	CLA	CHB-C1B-NB	-3.69	120.35	124.26
28	i	304	CHL	C3B-C4B-NB	-3.69	107.09	110.52
19	e	308	CLA	CHB-C1B-NB	-3.69	120.36	124.26
19	A	807	CLA	CHB-C1B-NB	-3.68	120.36	124.26
19	A	824	CLA	CHB-C1B-NB	-3.68	120.36	124.26
19	g	305	CLA	CHB-C1B-NB	-3.68	120.36	124.26
19	m	309	CLA	CHB-C1B-NB	-3.67	120.37	124.26
19	o	308	CLA	CHB-C1B-NB	-3.67	120.37	124.26
19	f	312	CLA	CHB-C1B-NB	-3.67	120.37	124.26
28	a	312	CHL	CAA-C2A-C3A	-3.67	102.72	112.78
19	m	311	CLA	CHB-C1B-NB	-3.67	120.37	124.26
19	k	311	CLA	CHB-C1B-NB	-3.67	120.38	124.26
19	j	311	CLA	C4A-NA-C1A	-3.67	105.06	106.71
19	n	206	CLA	CHC-C4B-NB	-3.66	120.38	124.26
19	f	314	CLA	CHB-C1B-NB	-3.66	120.38	124.26
19	e	307	CLA	CHB-C1B-NB	-3.65	120.39	124.26
19	a	306	CLA	CHB-C1B-NB	-3.65	120.39	124.26
19	c	314	CLA	CHB-C1B-NB	-3.65	120.39	124.26
19	A	849	CLA	CHB-C1B-NB	-3.65	120.39	124.26
19	F	202	CLA	CHB-C1B-NB	-3.65	120.40	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	n	202	CLA	C3A-C2A-C1A	-3.65	95.88	101.34
19	e	302	CLA	CHB-C1B-NB	-3.64	120.40	124.26
19	j	311	CLA	CHB-C1B-NB	-3.64	120.40	124.26
19	m	310	CLA	CHB-C1B-NB	-3.64	120.40	124.26
19	e	309	CLA	CHB-C1B-NB	-3.64	120.40	124.26
19	F	201	CLA	CHB-C1B-NB	-3.64	120.40	124.26
19	h	205	CLA	CHB-C1B-NB	-3.64	120.40	124.26
19	k	305	CLA	CHB-C1B-NB	-3.64	120.41	124.26
19	J	803	CLA	CHB-C1B-NB	-3.64	120.41	124.26
25	j	314	LMG	O6-C1-O1	-3.63	101.37	109.97
28	i	301	CHL	CAA-C2A-C3A	-3.63	102.83	112.78
19	o	306	CLA	CHB-C1B-NB	-3.63	120.41	124.26
19	n	204	CLA	CHB-C1B-NB	-3.63	120.42	124.26
19	b	315	CLA	CHB-C1B-NB	-3.62	120.42	124.26
19	B	812	CLA	CHB-C1B-NB	-3.62	120.43	124.26
22	l	210	DD6	C14-C13-C11	3.62	131.14	125.53
19	f	306	CLA	CHB-C1B-NB	-3.62	120.43	124.26
19	h	211	CLA	CHB-C1B-NB	-3.62	120.43	124.26
19	B	815	CLA	CHB-C1B-NB	-3.62	120.43	124.26
19	a	303	CLA	CHB-C1B-NB	-3.62	120.43	124.26
19	k	307	CLA	CHB-C1B-NB	-3.61	120.43	124.26
19	l	202	CLA	CHB-C1B-NB	-3.61	120.43	124.26
22	b	318	DD6	C14-C13-C11	3.61	131.14	125.53
19	B	848	CLA	CHB-C1B-NB	-3.61	120.43	124.26
19	c	303	CLA	CHB-C1B-NB	-3.61	120.43	124.26
19	o	305	CLA	CHB-C1B-NB	-3.61	120.43	124.26
19	a	307	CLA	CHB-C1B-NB	-3.61	120.44	124.26
19	l	203	CLA	CHB-C1B-NB	-3.61	120.44	124.26
19	b	309	CLA	CHB-C1B-NB	-3.61	120.44	124.26
19	k	304	CLA	CHB-C1B-NB	-3.61	120.44	124.26
19	f	309	CLA	CHB-C1B-NB	-3.60	120.45	124.26
19	c	310	CLA	CHB-C1B-NB	-3.60	120.45	124.26
19	j	313	CLA	CHB-C1B-NB	-3.60	120.45	124.26
19	b	307	CLA	CHB-C1B-NB	-3.60	120.45	124.26
19	c	309	CLA	CHB-C1B-NB	-3.60	120.45	124.26
19	A	827	CLA	CHB-C1B-NB	-3.59	120.45	124.26
22	e	313	DD6	O1-C20-C19	-3.59	110.68	113.38
19	A	813	CLA	CHB-C1B-NB	-3.59	120.45	124.26
19	d	206	CLA	CHB-C1B-NB	-3.59	120.46	124.26
19	A	843	CLA	CHB-C1B-NB	-3.59	120.46	124.26
19	A	848	CLA	CHB-C1B-NB	-3.58	120.46	124.26
19	e	311	CLA	CHB-C1B-NB	-3.58	120.46	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	839	CLA	CHB-C1B-NB	-3.58	120.46	124.26
19	k	306	CLA	CHB-C1B-NB	-3.58	120.46	124.26
19	h	204	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	A	829	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	B	811	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	h	212	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	o	311	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	A	850	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	B	814	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	k	308	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	c	308	CLA	CHB-C1B-NB	-3.58	120.47	124.26
19	A	852	CLA	CHB-C1B-NB	-3.57	120.47	124.26
28	f	304	CHL	O2D-CGD-CBD	3.57	117.62	111.27
19	i	313	CLA	CHB-C1B-NB	-3.57	120.48	124.26
19	e	303	CLA	CHB-C1B-NB	-3.57	120.48	124.26
19	b	302	CLA	CHB-C1B-NB	-3.57	120.48	124.26
19	f	308	CLA	CHB-C1B-NB	-3.57	120.48	124.26
19	a	305	CLA	CHB-C1B-NB	-3.57	120.48	124.26
19	A	847	CLA	CHB-C1B-NB	-3.56	120.48	124.26
19	B	845	CLA	CHB-C1B-NB	-3.56	120.49	124.26
19	A	814	CLA	CHB-C1B-NB	-3.56	120.49	124.26
19	A	840	CLA	CHB-C1B-NB	-3.56	120.49	124.26
19	c	316	CLA	CHB-C1B-NB	-3.56	120.49	124.26
19	h	203	CLA	CHB-C1B-NB	-3.56	120.49	124.26
19	B	844	CLA	CHB-C1B-NB	-3.56	120.49	124.26
19	l	208	CLA	CHB-C1B-NB	-3.55	120.49	124.26
28	a	312	CHL	O2D-CGD-CBD	3.55	117.58	111.27
19	a	309	CLA	CHB-C1B-NB	-3.55	120.50	124.26
19	m	303	CLA	CHB-C1B-NB	-3.55	120.50	124.26
19	o	304	CLA	CHB-C1B-NB	-3.55	120.50	124.26
19	B	810	CLA	CHB-C1B-NB	-3.55	120.50	124.26
19	d	207	CLA	CHB-C1B-NB	-3.55	120.50	124.26
19	B	833	CLA	CHB-C1B-NB	-3.55	120.50	124.26
19	i	308	CLA	CHB-C1B-NB	-3.55	120.50	124.26
19	a	314	CLA	CHB-C1B-NB	-3.54	120.51	124.26
19	c	306	CLA	CHB-C1B-NB	-3.54	120.51	124.26
19	c	307	CLA	CHB-C1B-NB	-3.54	120.51	124.26
19	i	305	CLA	CHB-C1B-NB	-3.54	120.51	124.26
19	i	306	CLA	CHB-C1B-NB	-3.54	120.51	124.26
19	B	836	CLA	CHB-C1B-NB	-3.54	120.51	124.26
19	A	805	CLA	CHB-C1B-NB	-3.54	120.51	124.26
28	a	313	CHL	O2D-CGD-CBD	3.54	117.55	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	810	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	b	303	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	l	207	CLA	CHB-C1B-NB	-3.53	120.52	124.26
22	o	313	DD6	C14-C13-C11	3.53	131.01	125.53
19	B	813	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	A	812	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	B	808	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	i	302	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	d	209	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	i	303	CLA	CHB-C1B-NB	-3.53	120.52	124.26
19	i	311	CLA	CHB-C1B-NB	-3.53	120.53	124.26
19	B	838	CLA	CHB-C1B-NB	-3.52	120.53	124.26
19	D	301	CLA	CHB-C1B-NB	-3.52	120.53	124.26
19	h	207	CLA	CHB-C1B-NB	-3.51	120.54	124.26
19	h	206	CLA	CHB-C1B-NB	-3.51	120.54	124.26
19	m	307	CLA	CHB-C1B-NB	-3.51	120.54	124.26
19	B	842	CLA	CHB-C1B-NB	-3.51	120.54	124.26
19	a	304	CLA	CHB-C1B-NB	-3.51	120.54	124.26
19	A	815	CLA	CHB-C1B-NB	-3.51	120.54	124.26
19	g	311	CLA	CHB-C1B-NB	-3.51	120.55	124.26
19	A	846	CLA	CHB-C1B-NB	-3.50	120.55	124.26
19	f	302	CLA	CHB-C1B-NB	-3.50	120.55	124.26
19	i	307	CLA	CHB-C1B-NB	-3.50	120.55	124.26
19	d	211	CLA	CHB-C1B-NB	-3.50	120.55	124.26
19	k	310	CLA	CHB-C1B-NB	-3.50	120.55	124.26
19	b	308	CLA	CHB-C1B-NB	-3.50	120.55	124.26
19	f	310	CLA	CHB-C1B-NB	-3.50	120.55	124.26
19	c	302	CLA	CHB-C1B-NB	-3.50	120.56	124.26
19	k	303	CLA	CHB-C1B-NB	-3.50	120.56	124.26
19	F	204	CLA	CHB-C1B-NB	-3.50	120.56	124.26
28	b	310	CHL	C3B-C4B-NB	-3.49	107.28	110.52
19	d	210	CLA	CHB-C1B-NB	-3.49	120.56	124.26
28	c	305	CHL	CHD-C1D-ND	-3.49	121.25	124.45
19	i	309	CLA	CHB-C1B-NB	-3.49	120.56	124.26
19	j	302	CLA	CHB-C1B-NB	-3.49	120.57	124.26
19	g	309	CLA	CHB-C1B-NB	-3.48	120.57	124.26
19	B	840	CLA	CHB-C1B-NB	-3.48	120.57	124.26
28	e	304	CHL	C3B-C4B-NB	-3.48	107.29	110.52
28	e	301	CHL	O2D-CGD-O1D	-3.48	117.04	123.84
19	n	205	CLA	CHB-C1B-NB	-3.48	120.58	124.26
28	b	311	CHL	O2D-CGD-CBD	3.48	117.44	111.27
28	c	305	CHL	C3B-C4B-NB	-3.47	107.29	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	837	CLA	CHB-C1B-NB	-3.47	120.58	124.26
19	B	822	CLA	CHB-C1B-NB	-3.47	120.58	124.26
19	h	210	CLA	CHB-C1B-NB	-3.47	120.58	124.26
19	A	844	CLA	CHB-C1B-NB	-3.46	120.59	124.26
19	j	312	CLA	CHB-C1B-NB	-3.46	120.59	124.26
19	j	309	CLA	CHB-C1B-NB	-3.46	120.59	124.26
19	m	306	CLA	CHB-C1B-NB	-3.46	120.59	124.26
19	o	310	CLA	CHB-C1B-NB	-3.46	120.59	124.26
19	A	806	CLA	CHB-C1B-NB	-3.46	120.60	124.26
19	A	841	CLA	CHB-C1B-NB	-3.46	120.60	124.26
19	g	302	CLA	CHB-C1B-NB	-3.46	120.60	124.26
22	a	321	DD6	O1-C20-C19	-3.45	110.79	113.38
19	l	201	CLA	C4A-NA-C1A	-3.45	105.16	106.71
19	A	853	CLA	CHB-C1B-NB	-3.45	120.61	124.26
19	B	847	CLA	CHB-C1B-NB	-3.45	120.61	124.26
19	j	308	CLA	CHB-C1B-NB	-3.45	120.61	124.26
19	A	843	CLA	CHC-C4B-NB	-3.44	120.62	124.26
19	n	201	CLA	CHB-C1B-NB	-3.44	120.62	124.26
19	d	203	CLA	CHB-C1B-NB	-3.44	120.62	124.26
19	f	303	CLA	CHB-C1B-NB	-3.44	120.62	124.26
28	a	311	CHL	CAA-C2A-C3A	-3.44	103.36	112.78
19	m	304	CLA	C2A-C1A-CHA	3.43	129.87	123.86
19	A	817	CLA	CHB-C1B-NB	-3.43	120.62	124.26
19	l	205	CLA	CHB-C1B-NB	-3.43	120.62	124.26
19	A	820	CLA	CHB-C1B-NB	-3.42	120.63	124.26
19	d	201	CLA	CHB-C1B-NB	-3.42	120.64	124.26
28	b	310	CHL	CHD-C1D-ND	-3.42	121.31	124.45
28	b	311	CHL	CAA-C2A-C3A	-3.42	103.42	112.78
19	h	209	CLA	CHB-C1B-NB	-3.41	120.64	124.26
19	a	308	CLA	CHB-C1B-NB	-3.41	120.65	124.26
22	i	315	DD6	C33-C34-C35	3.41	114.97	110.30
19	g	308	CLA	CHB-C1B-NB	-3.41	120.65	124.26
19	j	307	CLA	CHB-C1B-NB	-3.41	120.65	124.26
19	j	303	CLA	CHB-C1B-NB	-3.41	120.65	124.26
28	d	205	CHL	CHD-C1D-ND	-3.40	121.33	124.45
19	j	301	CLA	CHB-C1B-NB	-3.40	120.66	124.26
19	A	825	CLA	CHB-C1B-NB	-3.39	120.66	124.26
28	k	301	CHL	CAA-C2A-C3A	-3.39	103.49	112.78
22	m	313	DD6	C14-C13-C11	3.39	130.78	125.53
28	b	301	CHL	C3B-C4B-NB	-3.37	107.39	110.52
19	l	201	CLA	C2C-C1C-NC	3.37	113.13	109.97
28	b	314	CHL	CAA-C2A-C3A	-3.36	103.56	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	306	CHL	C3B-C4B-NB	-3.36	107.40	110.52
28	b	312	CHL	C3B-C4B-NB	-3.36	107.40	110.52
28	o	301	CHL	C3B-C4B-NB	-3.36	107.40	110.52
28	f	301	CHL	C3B-C4B-NB	-3.35	107.41	110.52
19	d	204	CLA	CHB-C1B-NB	-3.35	120.71	124.26
19	a	303	CLA	CBA-CAA-C2A	3.35	123.74	113.86
19	c	304	CLA	CHB-C1B-NB	-3.35	120.72	124.26
28	o	301	CHL	CAA-C2A-C3A	-3.32	103.69	112.78
19	b	306	CLA	C2C-C1C-NC	3.31	113.07	109.97
28	c	313	CHL	C1-C2-C3	3.31	131.76	126.04
28	c	312	CHL	C3B-C4B-NB	-3.31	107.45	110.52
19	h	201	CLA	CHB-C1B-NB	-3.30	120.76	124.26
22	A	832	DD6	O1-C20-C19	-3.30	110.91	113.38
28	a	313	CHL	C3B-C4B-NB	-3.29	107.46	110.52
19	f	311	CLA	C1-C2-C3	-3.29	120.35	126.04
27	B	829	DGD	O6D-C1D-O3G	-3.29	102.19	109.97
19	A	839	CLA	CHB-C1B-NB	-3.29	120.78	124.26
28	a	315	CHL	C3B-C4B-NB	-3.28	107.47	110.52
22	h	215	DD6	C14-C13-C11	3.28	130.62	125.53
28	h	202	CHL	C3B-C4B-NB	-3.28	107.47	110.52
19	k	309	CLA	CHB-C1B-NB	-3.27	120.80	124.26
28	g	306	CHL	CHD-C1D-ND	-3.27	121.45	124.45
19	B	835	CLA	CHB-C1B-NB	-3.26	120.80	124.26
22	j	316	DD6	C33-C34-C35	3.26	114.77	110.30
28	i	301	CHL	C3B-C4B-NB	-3.26	107.49	110.52
28	c	312	CHL	C1-C2-C3	3.26	131.68	126.04
19	a	303	CLA	CAA-C2A-C3A	3.25	121.69	112.78
22	c	318	DD6	C14-C13-C11	3.25	130.57	125.53
19	B	820	CLA	CHB-C1B-NB	-3.25	120.82	124.26
19	A	853	CLA	CHC-C4B-NB	-3.25	120.82	124.26
28	f	304	CHL	OMC-CMC-C2C	-3.25	118.34	125.69
28	g	306	CHL	C1-C2-C3	3.24	131.65	126.04
19	A	818	CLA	CHB-C1B-NB	-3.24	120.83	124.26
28	d	202	CHL	C3B-C4B-NB	-3.23	107.52	110.52
27	B	829	DGD	O3G-C3G-C2G	-3.22	103.12	110.90
19	h	213	CLA	CHB-C1B-NB	-3.22	120.85	124.26
28	b	301	CHL	CHD-C1D-ND	-3.22	121.50	124.45
22	i	314	DD6	C14-C13-C11	3.21	130.51	125.53
22	A	833	DD6	C32-C31-C36	-3.21	118.11	122.63
25	j	314	LMG	O1-C1-C2	3.20	113.30	108.30
28	e	301	CHL	C3B-C4B-NB	-3.19	107.55	110.52
28	h	202	CHL	CAA-C2A-C3A	-3.19	104.04	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	310	CHL	CAA-C2A-C3A	-3.19	104.06	112.78
19	a	314	CLA	C3D-C4D-ND	3.18	115.38	110.24
28	b	312	CHL	CHD-C1D-ND	-3.17	121.54	124.45
19	o	309	CLA	C2C-C1C-NC	3.16	112.94	109.97
28	g	303	CHL	CHD-C1D-ND	-3.16	121.55	124.45
28	k	301	CHL	C4D-CHA-C1A	3.16	125.09	121.25
19	e	309	CLA	C3D-C4D-ND	3.15	115.34	110.24
19	n	202	CLA	C2A-C3A-C4A	-3.15	96.78	101.87
28	a	312	CHL	CHD-C1D-ND	-3.14	121.57	124.45
19	A	844	CLA	C1-C2-C3	-3.13	120.62	126.04
28	b	301	CHL	C1-C2-C3	3.12	131.44	126.04
28	c	305	CHL	C1-C2-C3	3.12	131.44	126.04
28	b	312	CHL	C1-C2-C3	3.12	131.44	126.04
22	b	317	DD6	C32-C31-C36	-3.12	118.23	122.63
28	b	301	CHL	O2D-CGD-CBD	3.12	116.81	111.27
19	m	302	CLA	C2C-C1C-NC	3.11	112.89	109.97
28	f	301	CHL	CAA-C2A-C3A	-3.11	104.27	112.78
19	B	823	CLA	C3D-C4D-ND	3.11	115.27	110.24
28	e	301	CHL	CAA-C2A-C3A	-3.11	104.27	112.78
19	o	302	CLA	C3A-C2A-C1A	-3.11	96.69	101.34
28	a	315	CHL	CAA-C2A-C3A	-3.10	104.28	112.78
28	e	304	CHL	O1D-CGD-CBD	-3.10	118.15	124.48
19	B	832	CLA	C1-C2-C3	-3.09	121.75	126.75
28	i	304	CHL	O2A-CGA-CBA	3.09	121.61	111.91
19	A	827	CLA	C3D-C4D-ND	3.09	115.23	110.24
19	m	302	CLA	C3D-C4D-ND	3.08	115.23	110.24
19	B	808	CLA	C1-C2-C3	-3.08	120.72	126.04
28	c	312	CHL	O2A-CGA-CBA	3.08	121.56	111.91
25	e	312	LMG	O6-C1-O1	-3.08	102.69	109.97
22	A	832	DD6	C32-C31-C36	-3.07	118.30	122.63
19	A	843	CLA	C3A-C2A-C1A	-3.07	96.74	101.34
22	n	211	DD6	C14-C13-C11	3.06	130.28	125.53
25	d	213	LMG	O1-C1-C2	-3.06	103.52	108.30
19	l	207	CLA	C3D-C4D-ND	3.06	115.19	110.24
19	e	310	CLA	C2C-C1C-NC	3.06	112.84	109.97
19	i	310	CLA	C2C-C1C-NC	3.06	112.83	109.97
28	h	202	CHL	OMC-CMC-C2C	-3.05	118.79	125.69
28	g	303	CHL	CAA-C2A-C3A	-3.05	104.43	112.78
28	c	305	CHL	C2B-C1B-NB	-3.05	108.19	110.23
28	d	202	CHL	CAA-C2A-C3A	-3.05	104.43	112.78
28	m	301	CHL	CAA-C2A-C3A	-3.04	104.44	112.78
19	d	208	CLA	C3D-C4D-ND	3.04	115.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	311	CHL	O2A-CGA-CBA	3.04	121.46	111.91
19	a	308	CLA	C3D-C4D-ND	3.04	115.16	110.24
28	g	310	CHL	C3B-C4B-NB	-3.04	107.69	110.52
28	c	313	CHL	O2A-CGA-CBA	3.04	121.44	111.91
28	a	313	CHL	CAA-C2A-C3A	-3.04	104.46	112.78
19	A	825	CLA	C3D-C4D-ND	3.03	115.14	110.24
28	f	301	CHL	O2D-CGD-CBD	3.03	116.65	111.27
19	n	207	CLA	C3D-C4D-ND	3.03	115.13	110.24
19	k	307	CLA	C3D-C4D-ND	3.02	115.13	110.24
19	B	801	CLA	C3D-C4D-ND	3.02	115.12	110.24
19	i	305	CLA	CHC-C4B-NB	-3.02	121.06	124.26
19	j	306	CLA	C2C-C1C-NC	3.02	112.80	109.97
19	e	305	CLA	CHC-C4B-NB	-3.01	121.07	124.26
19	B	848	CLA	C3D-C4D-ND	3.01	115.11	110.24
19	B	815	CLA	C3D-C4D-ND	3.01	115.11	110.24
28	b	311	CHL	C3B-C4B-NB	-3.01	107.73	110.52
28	e	301	CHL	C1-C2-C3	3.00	131.61	126.75
28	g	310	CHL	C1-C2-C3	3.00	131.61	126.75
28	c	313	CHL	C3B-C4B-NB	-3.00	107.73	110.52
19	B	820	CLA	C3D-C4D-ND	3.00	115.09	110.24
19	n	205	CLA	C3D-C4D-ND	3.00	115.09	110.24
28	f	304	CHL	O2A-CGA-O1A	-2.99	116.03	123.59
28	c	305	CHL	O2A-CGA-CBA	2.99	121.30	111.91
19	o	312	CLA	C3D-C4D-ND	2.99	115.08	110.24
28	i	304	CHL	CHD-C1D-ND	-2.99	121.70	124.45
19	A	817	CLA	C3D-C4D-ND	2.99	115.07	110.24
22	A	833	DD6	C14-C13-C11	2.99	130.16	125.53
19	A	804	CLA	C3D-C4D-ND	2.98	115.06	110.24
19	B	813	CLA	C3D-C4D-ND	2.98	115.06	110.24
19	b	302	CLA	C3D-C4D-ND	2.98	115.06	110.24
19	o	303	CLA	C3D-C4D-ND	2.98	115.06	110.24
19	j	307	CLA	C3D-C4D-ND	2.98	115.06	110.24
19	A	845	CLA	C3D-C4D-ND	2.98	115.06	110.24
19	c	308	CLA	C3D-C4D-ND	2.98	115.06	110.24
19	e	310	CLA	C3D-C4D-ND	2.98	115.06	110.24
19	h	208	CLA	C3D-C4D-ND	2.98	115.06	110.24
28	b	301	CHL	CAA-C2A-C3A	-2.98	104.62	112.78
19	B	822	CLA	C3D-C4D-ND	2.98	115.05	110.24
28	e	301	CHL	O2A-CGA-CBA	2.97	121.24	111.91
19	c	303	CLA	C3D-C4D-ND	2.97	115.04	110.24
19	c	315	CLA	C3D-C4D-ND	2.97	115.04	110.24
19	B	849	CLA	C3D-C4D-ND	2.97	115.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	f	309	CLA	C3D-C4D-ND	2.97	115.04	110.24
28	b	312	CHL	O2A-CGA-CBA	2.97	121.22	111.91
19	k	308	CLA	C3D-C4D-ND	2.96	115.03	110.24
28	d	205	CHL	C3B-C4B-NB	-2.96	107.77	110.52
22	f	316	DD6	C14-C13-C11	2.96	130.13	125.53
22	o	314	DD6	C14-C13-C11	2.96	130.13	125.53
19	g	308	CLA	C3D-C4D-ND	2.96	115.03	110.24
19	m	309	CLA	C3D-C4D-ND	2.96	115.03	110.24
19	B	847	CLA	C3D-C4D-ND	2.96	115.02	110.24
28	e	304	CHL	CHD-C1D-ND	-2.96	121.73	124.45
28	c	312	CHL	C2A-C1A-CHA	2.96	129.03	123.86
19	A	817	CLA	CHC-C4B-NB	-2.96	121.13	124.26
28	d	205	CHL	O2A-CGA-CBA	2.96	121.18	111.91
28	g	303	CHL	O2A-CGA-O1A	-2.95	116.14	123.59
19	b	313	CLA	C3D-C4D-ND	2.95	115.02	110.24
19	k	309	CLA	C3D-C4D-ND	2.95	115.01	110.24
19	d	203	CLA	C3D-C4D-ND	2.95	115.01	110.24
19	A	829	CLA	C3D-C4D-ND	2.95	115.01	110.24
19	A	818	CLA	C3D-C4D-ND	2.95	115.01	110.24
28	e	304	CHL	OMC-CMC-C2C	-2.95	119.02	125.69
19	a	307	CLA	C3D-C4D-ND	2.95	115.01	110.24
19	i	307	CLA	C3D-C4D-ND	2.95	115.01	110.24
28	m	301	CHL	C2B-C1B-NB	-2.95	108.26	110.23
19	A	848	CLA	C3D-C4D-ND	2.95	115.00	110.24
25	A	851	LMG	O1-C1-C2	-2.95	103.70	108.30
19	h	207	CLA	CHC-C4B-NB	-2.95	121.14	124.26
19	h	213	CLA	C3D-C4D-ND	2.95	115.00	110.24
19	a	314	CLA	C2C-C1C-NC	2.95	112.73	109.97
28	g	306	CHL	O2A-CGA-O1A	-2.94	116.16	123.59
19	A	808	CLA	C3D-C4D-ND	2.94	115.00	110.24
19	o	310	CLA	C3D-C4D-ND	2.94	115.00	110.24
19	d	210	CLA	C3D-C4D-ND	2.94	115.00	110.24
19	h	201	CLA	C3D-C4D-ND	2.94	114.99	110.24
19	i	313	CLA	C3D-C4D-ND	2.94	114.99	110.24
28	b	312	CHL	O1D-CGD-CBD	-2.94	118.47	124.48
19	h	206	CLA	C3D-C4D-ND	2.94	114.99	110.24
19	A	820	CLA	C3D-C4D-ND	2.94	114.99	110.24
28	b	314	CHL	CHD-C1D-ND	-2.93	121.76	124.45
28	f	304	CHL	CHD-C1D-ND	-2.93	121.76	124.45
19	A	805	CLA	C3D-C4D-ND	2.93	114.98	110.24
19	B	832	CLA	C3D-C4D-ND	2.93	114.98	110.24
19	n	202	CLA	CBA-CAA-C2A	2.93	122.51	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	c	314	CLA	C3D-C4D-ND	2.93	114.97	110.24
19	o	307	CLA	C3D-C4D-ND	2.93	114.97	110.24
28	g	310	CHL	CAA-C2A-C3A	-2.93	104.76	112.78
19	f	307	CLA	C3D-C4D-ND	2.92	114.97	110.24
19	h	203	CLA	C3D-C4D-ND	2.92	114.97	110.24
28	k	301	CHL	C3B-C4B-NB	-2.92	107.80	110.52
19	d	207	CLA	C3D-C4D-ND	2.92	114.97	110.24
19	d	204	CLA	C3D-C4D-ND	2.92	114.96	110.24
19	f	302	CLA	C3D-C4D-ND	2.92	114.96	110.24
19	f	311	CLA	C3D-C4D-ND	2.92	114.96	110.24
19	F	201	CLA	C3D-C4D-ND	2.92	114.96	110.24
28	b	311	CHL	O2A-CGA-CBA	2.92	121.06	111.91
19	l	209	CLA	C3D-C4D-ND	2.92	114.96	110.24
19	e	308	CLA	C3D-C4D-ND	2.91	114.95	110.24
19	c	306	CLA	C3D-C4D-ND	2.91	114.95	110.24
19	i	312	CLA	C3D-C4D-ND	2.91	114.95	110.24
19	A	802	CLA	C3D-C4D-ND	2.91	114.95	110.24
19	B	821	CLA	C3D-C4D-ND	2.91	114.95	110.24
19	o	306	CLA	C3D-C4D-ND	2.91	114.94	110.24
28	a	313	CHL	O2A-CGA-CBA	2.91	121.03	111.91
19	B	810	CLA	C3D-C4D-ND	2.91	114.94	110.24
19	B	843	CLA	C3D-C4D-ND	2.90	114.94	110.24
19	a	302	CLA	C3D-C4D-ND	2.90	114.93	110.24
19	m	306	CLA	C3D-C4D-ND	2.90	114.93	110.24
28	e	304	CHL	C1-C2-C3	2.90	131.06	126.04
19	o	304	CLA	C3D-C4D-ND	2.90	114.93	110.24
19	m	311	CLA	C3D-C4D-ND	2.90	114.92	110.24
19	j	302	CLA	C3D-C4D-ND	2.90	114.92	110.24
19	n	202	CLA	C2A-C1A-CHA	2.89	128.92	123.86
19	A	843	CLA	C3D-C4D-ND	2.89	114.91	110.24
19	l	205	CLA	C3D-C4D-ND	2.89	114.91	110.24
19	l	206	CLA	C3D-C4D-ND	2.89	114.91	110.24
28	i	304	CHL	C1-C2-C3	2.89	131.04	126.04
19	e	307	CLA	C3D-C4D-ND	2.88	114.90	110.24
19	k	311	CLA	C3D-C4D-ND	2.88	114.90	110.24
19	c	309	CLA	C3D-C4D-ND	2.88	114.90	110.24
19	B	846	CLA	C4A-NA-C1A	-2.88	105.41	106.71
19	B	812	CLA	C3D-C4D-ND	2.88	114.90	110.24
19	B	833	CLA	C3D-C4D-ND	2.88	114.89	110.24
19	A	840	CLA	C3D-C4D-ND	2.88	114.89	110.24
19	h	210	CLA	C3D-C4D-ND	2.88	114.89	110.24
19	n	203	CLA	C3D-C4D-ND	2.88	114.89	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	815	CLA	C3D-C4D-ND	2.87	114.89	110.24
19	a	303	CLA	C3D-C4D-ND	2.87	114.89	110.24
19	B	807	CLA	C3D-C4D-ND	2.87	114.89	110.24
19	m	305	CLA	C3D-C4D-ND	2.87	114.89	110.24
19	k	303	CLA	C3D-C4D-ND	2.87	114.88	110.24
19	m	304	CLA	CHC-C4B-NB	-2.87	121.22	124.26
19	A	806	CLA	C3D-C4D-ND	2.87	114.88	110.24
25	g	312	LMG	O3-C3-C2	-2.87	103.72	110.35
19	B	841	CLA	C3D-C4D-ND	2.87	114.88	110.24
19	B	846	CLA	C4D-CHA-C1A	-2.87	117.76	121.25
19	e	308	CLA	C3A-C2A-C1A	-2.87	97.05	101.34
19	A	849	CLA	C3D-C4D-ND	2.86	114.87	110.24
19	A	841	CLA	C3D-C4D-ND	2.86	114.87	110.24
19	j	308	CLA	C3D-C4D-ND	2.86	114.87	110.24
19	b	307	CLA	C3D-C4D-ND	2.86	114.87	110.24
19	A	814	CLA	C3D-C4D-ND	2.86	114.87	110.24
19	B	835	CLA	C3D-C4D-ND	2.86	114.87	110.24
19	m	303	CLA	C3D-C4D-ND	2.86	114.87	110.24
19	m	307	CLA	C3D-C4D-ND	2.86	114.86	110.24
19	B	842	CLA	C3D-C4D-ND	2.86	114.86	110.24
19	A	828	CLA	C3D-C4D-ND	2.86	114.86	110.24
19	i	311	CLA	C3D-C4D-ND	2.86	114.86	110.24
28	b	310	CHL	O2A-CGA-CBA	2.86	120.88	111.91
19	A	816	CLA	C3D-C4D-ND	2.86	114.86	110.24
19	B	837	CLA	C3D-C4D-ND	2.86	114.86	110.24
19	l	202	CLA	C3D-C4D-ND	2.86	114.86	110.24
19	A	846	CLA	C3D-C4D-ND	2.86	114.86	110.24
19	B	819	CLA	C3D-C4D-ND	2.86	114.86	110.24
19	a	306	CLA	C2C-C1C-NC	2.86	112.65	109.97
19	A	850	CLA	C3D-C4D-ND	2.85	114.86	110.24
28	b	314	CHL	C1-C2-C3	2.85	130.98	126.04
19	B	817	CLA	C3D-C4D-ND	2.85	114.85	110.24
19	n	208	CLA	C2C-C1C-NC	2.85	112.64	109.97
19	e	302	CLA	C3D-C4D-ND	2.85	114.85	110.24
19	f	314	CLA	C3D-C4D-ND	2.85	114.85	110.24
19	j	311	CLA	CBA-CAA-C2A	2.85	122.28	113.86
19	B	832	CLA	C2C-C1C-NC	2.85	112.64	109.97
19	A	853	CLA	C3D-C4D-ND	2.85	114.84	110.24
19	k	306	CLA	C3D-C4D-ND	2.85	114.84	110.24
28	i	301	CHL	O2A-CGA-CBA	2.85	120.84	111.91
19	B	814	CLA	C3D-C4D-ND	2.84	114.83	110.24
28	b	312	CHL	CAA-C2A-C3A	-2.84	105.00	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	822	CLA	CHC-C4B-NB	-2.84	121.25	124.26
28	a	312	CHL	C3B-C4B-NB	-2.84	107.88	110.52
19	a	306	CLA	C3D-C4D-ND	2.84	114.83	110.24
19	B	805	CLA	C3D-C4D-ND	2.84	114.82	110.24
19	a	309	CLA	C3D-C4D-ND	2.84	114.82	110.24
19	B	844	CLA	C3D-C4D-ND	2.83	114.82	110.24
19	B	840	CLA	C3D-C4D-ND	2.83	114.82	110.24
19	j	313	CLA	C3D-C4D-ND	2.83	114.82	110.24
28	b	312	CHL	C2A-C3A-C4A	2.83	106.44	101.87
19	h	209	CLA	C3D-C4D-ND	2.83	114.81	110.24
22	a	320	DD6	O1-C20-C15	-2.83	56.62	58.96
22	F	205	DD6	C21-C20-C19	2.83	117.46	114.28
19	c	311	CLA	C3D-C4D-ND	2.83	114.81	110.24
28	f	304	CHL	CAA-C2A-C3A	-2.83	105.04	112.78
19	b	315	CLA	C3D-C4D-ND	2.83	114.81	110.24
19	j	305	CLA	C2C-C1C-NC	2.83	112.62	109.97
19	j	301	CLA	C3D-C4D-ND	2.82	114.81	110.24
19	A	852	CLA	C3D-C4D-ND	2.82	114.81	110.24
19	B	808	CLA	C3D-C4D-ND	2.82	114.80	110.24
19	A	844	CLA	C3D-C4D-ND	2.82	114.80	110.24
19	j	312	CLA	C3D-C4D-ND	2.82	114.80	110.24
19	e	305	CLA	C3D-C4D-ND	2.82	114.80	110.24
19	i	303	CLA	C3D-C4D-ND	2.82	114.80	110.24
28	g	303	CHL	C2B-C1B-NB	-2.82	108.34	110.23
19	l	208	CLA	C3D-C4D-ND	2.82	114.80	110.24
19	k	310	CLA	C3D-C4D-ND	2.82	114.79	110.24
19	B	838	CLA	C3D-C4D-ND	2.81	114.78	110.24
19	n	204	CLA	C3D-C4D-ND	2.81	114.78	110.24
19	n	206	CLA	C3D-C4D-ND	2.81	114.78	110.24
19	j	307	CLA	CHC-C4B-NB	-2.81	121.29	124.26
19	o	302	CLA	C3D-C4D-ND	2.81	114.78	110.24
19	i	311	CLA	C1-C2-C3	-2.80	121.20	126.04
19	A	847	CLA	C3D-C4D-ND	2.80	114.77	110.24
19	e	311	CLA	C3D-C4D-ND	2.80	114.77	110.24
19	i	302	CLA	C3D-C4D-ND	2.80	114.77	110.24
19	g	301	CLA	C2C-C1C-NC	2.80	112.59	109.97
19	o	303	CLA	C2C-C1C-NC	2.80	112.59	109.97
21	A	831	LHG	O8-C23-C24	2.80	120.69	111.91
19	g	301	CLA	C3D-C4D-ND	2.80	114.76	110.24
19	B	845	CLA	C3D-C4D-ND	2.80	114.76	110.24
19	f	310	CLA	C3D-C4D-ND	2.80	114.76	110.24
19	i	306	CLA	C3D-C4D-ND	2.80	114.76	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g	303	CHL	OMC-CMC-C2C	-2.79	119.37	125.69
19	g	305	CLA	C3D-C4D-ND	2.79	114.75	110.24
28	d	202	CHL	C2B-C1B-NB	-2.79	108.36	110.23
28	f	301	CHL	C2B-C1B-NB	-2.79	108.36	110.23
19	h	204	CLA	C3D-C4D-ND	2.79	114.75	110.24
19	o	308	CLA	C3D-C4D-ND	2.79	114.75	110.24
19	A	810	CLA	C3D-C4D-ND	2.79	114.75	110.24
19	f	308	CLA	C3D-C4D-ND	2.79	114.75	110.24
28	g	310	CHL	O2A-CGA-CBA	2.79	120.65	111.91
28	f	304	CHL	C2B-C1B-NB	-2.78	108.37	110.23
28	i	304	CHL	C2B-C1B-NB	-2.78	108.37	110.23
19	g	311	CLA	C3D-C4D-ND	2.78	114.74	110.24
19	a	304	CLA	C3D-C4D-ND	2.78	114.74	110.24
19	f	312	CLA	C3D-C4D-ND	2.78	114.74	110.24
19	i	308	CLA	C3D-C4D-ND	2.78	114.73	110.24
28	e	301	CHL	O2D-CGD-CBD	2.78	116.20	111.27
19	g	307	CLA	C3D-C4D-ND	2.77	114.72	110.24
19	A	813	CLA	C3D-C4D-ND	2.77	114.72	110.24
19	l	204	CLA	C3D-C4D-ND	2.77	114.72	110.24
19	b	308	CLA	C3D-C4D-ND	2.77	114.72	110.24
19	f	305	CLA	C3D-C4D-ND	2.77	114.72	110.24
19	k	302	CLA	C3D-C4D-ND	2.77	114.72	110.24
28	a	315	CHL	C2B-C1B-NB	-2.77	108.38	110.23
19	o	309	CLA	C3D-C4D-ND	2.77	114.71	110.24
24	c	301	LMU	C1B-O1B-C4'	-2.76	111.12	117.96
28	f	304	CHL	O2A-CGA-CBA	2.76	120.57	111.91
19	A	842	CLA	C3D-C4D-ND	2.76	114.70	110.24
19	d	201	CLA	C3D-C4D-ND	2.76	114.70	110.24
19	g	309	CLA	C3D-C4D-ND	2.76	114.70	110.24
28	b	314	CHL	C3B-C4B-NB	-2.76	107.96	110.52
19	f	314	CLA	C3A-C2A-C1A	-2.76	97.21	101.34
19	d	209	CLA	C3D-C4D-ND	2.76	114.69	110.24
22	F	205	DD6	C33-C34-C35	2.75	114.08	110.30
19	J	803	CLA	C3D-C4D-ND	2.75	114.69	110.24
19	c	302	CLA	C3D-C4D-ND	2.75	114.69	110.24
25	g	313	LMG	O6-C1-O1	-2.75	103.46	109.97
19	b	304	CLA	C3D-C4D-ND	2.75	114.68	110.24
19	i	305	CLA	C3D-C4D-ND	2.75	114.68	110.24
28	e	301	CHL	O2A-CGA-O1A	-2.75	116.66	123.59
19	A	807	CLA	C3D-C4D-ND	2.75	114.68	110.24
19	A	839	CLA	C3D-C4D-ND	2.74	114.68	110.24
19	j	306	CLA	C3D-C4D-ND	2.74	114.68	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f	304	CHL	C1-C2-C3	2.74	130.78	126.04
28	c	305	CHL	CAA-C2A-C3A	-2.74	105.27	112.78
19	g	302	CLA	C3D-C4D-ND	2.74	114.67	110.24
19	c	307	CLA	C3D-C4D-ND	2.74	114.66	110.24
28	d	205	CHL	CAA-C2A-C3A	-2.73	105.29	112.78
19	o	305	CLA	C3D-C4D-ND	2.73	114.66	110.24
19	a	310	CLA	C1-C2-C3	-2.73	122.33	126.75
19	n	209	CLA	C2C-C1C-NC	2.73	112.53	109.97
19	e	306	CLA	C3D-C4D-ND	2.73	114.65	110.24
28	g	306	CHL	O2A-CGA-CBA	2.73	120.46	111.91
19	B	830	CLA	C3D-C4D-ND	2.73	114.65	110.24
19	f	306	CLA	C3D-C4D-ND	2.73	114.65	110.24
19	A	801	CLA	CHA-C1A-NA	-2.72	120.16	126.40
19	k	304	CLA	C3D-C4D-ND	2.72	114.64	110.24
25	b	316	LMG	O1-C7-C8	-2.72	104.33	110.90
19	A	811	CLA	C3D-C4D-ND	2.72	114.64	110.24
19	b	306	CLA	C3D-C4D-ND	2.72	114.64	110.24
28	a	313	CHL	CHD-C1D-ND	-2.72	121.96	124.45
19	j	309	CLA	C3D-C4D-ND	2.72	114.63	110.24
19	A	823	CLA	C3D-C4D-ND	2.72	114.63	110.24
19	l	203	CLA	C3D-C4D-ND	2.72	114.63	110.24
28	g	310	CHL	CHD-C1D-ND	-2.72	121.96	124.45
28	b	301	CHL	O1D-CGD-CBD	-2.72	118.93	124.48
25	g	316	LMG	O6-C1-O1	-2.71	103.55	109.97
25	c	320	LMG	O6-C1-O1	-2.71	103.55	109.97
19	a	310	CLA	C3D-C4D-ND	2.71	114.62	110.24
19	j	305	CLA	C3D-C4D-ND	2.71	114.62	110.24
19	c	309	CLA	CHC-C4B-NB	-2.71	121.39	124.26
19	A	824	CLA	C3D-C4D-ND	2.71	114.62	110.24
19	A	810	CLA	CMA-C3A-C4A	2.71	119.05	111.77
28	c	313	CHL	CAA-C2A-C3A	-2.71	105.36	112.78
28	b	314	CHL	O2A-CGA-CBA	2.71	120.41	111.91
19	m	306	CLA	CHC-C4B-NB	-2.71	121.39	124.26
28	k	301	CHL	CHD-C1D-ND	-2.70	121.97	124.45
19	B	816	CLA	C3D-C4D-ND	2.70	114.61	110.24
19	m	308	CLA	C3D-C4D-ND	2.70	114.61	110.24
28	b	301	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
28	c	312	CHL	OMC-CMC-C2C	-2.70	119.58	125.69
19	d	208	CLA	C2C-C1C-NC	2.70	112.50	109.97
28	d	202	CHL	C2A-C1A-CHA	2.70	128.57	123.86
28	m	301	CHL	OMC-CMC-C2C	-2.70	119.59	125.69
28	c	312	CHL	C2B-C1B-NB	-2.69	108.43	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	d	206	CLA	C3D-C4D-ND	2.69	114.59	110.24
19	d	212	CLA	C3D-C4D-ND	2.69	114.59	110.24
19	b	315	CLA	C3A-C2A-C1A	-2.69	97.31	101.34
19	F	203	CLA	C3D-C4D-ND	2.69	114.59	110.24
19	A	809	CLA	C3D-C4D-ND	2.69	114.59	110.24
28	g	303	CHL	O2A-CGA-CBA	2.69	120.34	111.91
19	b	309	CLA	C3D-C4D-ND	2.69	114.58	110.24
19	b	313	CLA	CAA-C2A-C3A	2.69	120.13	112.78
19	A	817	CLA	CAA-C2A-C1A	-2.68	103.18	111.97
19	h	211	CLA	C1-C2-C3	-2.68	121.41	126.04
19	B	835	CLA	C1-C2-C3	-2.68	121.41	126.04
19	B	839	CLA	C3D-C4D-ND	2.68	114.57	110.24
19	m	310	CLA	C3D-C4D-ND	2.68	114.57	110.24
22	d	214	DD6	O1-C20-C15	-2.68	56.74	58.96
19	B	811	CLA	C3D-C4D-ND	2.68	114.56	110.24
19	m	309	CLA	C2C-C1C-NC	2.68	112.48	109.97
19	d	211	CLA	C3D-C4D-ND	2.67	114.56	110.24
19	g	305	CLA	C2C-C1C-NC	2.67	112.47	109.97
19	B	809	CLA	C3D-C4D-ND	2.67	114.56	110.24
19	B	849	CLA	C1-C2-C3	-2.66	121.44	126.04
19	o	307	CLA	CAA-C2A-C1A	-2.66	103.25	111.97
28	a	311	CHL	C2B-C1B-NB	-2.66	108.45	110.23
25	a	301	LMG	O7-C10-O9	-2.66	117.27	123.70
28	b	311	CHL	CHD-C1D-ND	-2.66	122.01	124.45
28	b	311	CHL	C2B-C1B-NB	-2.66	108.45	110.23
28	a	311	CHL	CHD-C1D-ND	-2.66	122.01	124.45
19	f	303	CLA	C3D-C4D-ND	2.66	114.53	110.24
19	h	211	CLA	C3D-C4D-ND	2.65	114.53	110.24
28	h	202	CHL	CHD-C1D-ND	-2.65	122.02	124.45
22	m	313	DD6	O1-C20-C19	-2.65	111.39	113.38
22	c	317	DD6	C32-C31-C36	-2.65	118.89	122.63
23	A	835	BCR	C12-C13-C14	-2.65	118.91	124.81
28	b	314	CHL	OMC-CMC-C2C	-2.65	119.70	125.69
19	k	305	CLA	C3D-C4D-ND	2.65	114.52	110.24
19	A	812	CLA	C3D-C4D-ND	2.64	114.51	110.24
19	h	207	CLA	C3D-C4D-ND	2.64	114.51	110.24
19	B	848	CLA	C2C-C1C-NC	2.64	112.44	109.97
19	B	818	CLA	C3D-C4D-ND	2.64	114.51	110.24
19	B	841	CLA	C2C-C1C-NC	2.64	112.44	109.97
19	A	826	CLA	C3D-C4D-ND	2.64	114.51	110.24
28	o	301	CHL	O2A-CGA-CBA	2.63	120.17	111.91
19	n	202	CLA	CAA-C2A-C1A	-2.63	103.35	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	n	201	CLA	C3D-C4D-ND	2.63	114.49	110.24
19	a	305	CLA	C3D-C4D-ND	2.63	114.49	110.24
19	j	310	CLA	C2C-C1C-NC	2.63	112.43	109.97
28	e	304	CHL	O2A-CGA-CBA	2.63	120.15	111.91
28	d	202	CHL	CHD-C1D-ND	-2.62	122.04	124.45
28	h	202	CHL	O2A-CGA-CBA	2.62	120.14	111.91
19	c	316	CLA	C3D-C4D-ND	2.62	114.47	110.24
28	a	311	CHL	O1D-CGD-CBD	-2.62	119.13	124.48
22	k	314	DD6	C14-C13-C11	2.62	129.59	125.53
19	l	201	CLA	CHC-C1C-C2C	-2.62	119.46	126.73
28	a	315	CHL	O2A-CGA-CBA	2.62	120.12	111.91
19	F	202	CLA	C3D-C4D-ND	2.62	114.47	110.24
28	e	301	CHL	CHD-C1D-ND	-2.61	122.05	124.45
19	B	815	CLA	CAA-C2A-C3A	2.61	119.93	112.78
28	e	304	CHL	C2B-C1B-NB	-2.61	108.48	110.23
28	i	304	CHL	O2A-CGA-O1A	-2.61	117.00	123.59
19	A	822	CLA	C3D-C4D-ND	2.61	114.46	110.24
19	D	301	CLA	C3D-C4D-ND	2.61	114.45	110.24
22	a	321	DD6	C21-C20-C19	2.61	117.21	114.28
28	m	301	CHL	CHD-C1D-ND	-2.61	122.06	124.45
19	b	303	CLA	C3D-C4D-ND	2.60	114.45	110.24
19	c	310	CLA	C3D-C4D-ND	2.60	114.45	110.24
19	h	205	CLA	C3D-C4D-ND	2.60	114.45	110.24
22	n	210	DD6	C33-C34-C35	2.60	113.86	110.30
22	b	319	DD6	C14-C13-C11	2.60	129.56	125.53
19	m	304	CLA	C4D-CHA-C1A	-2.60	118.09	121.25
28	a	315	CHL	CHD-C1D-ND	-2.60	122.07	124.45
19	c	302	CLA	CAA-C2A-C1A	-2.59	103.47	111.97
28	i	304	CHL	CAA-C2A-C3A	-2.59	105.68	112.78
19	e	303	CLA	C3D-C4D-ND	2.59	114.43	110.24
23	B	850	BCR	C24-C23-C22	2.59	130.15	126.23
19	B	846	CLA	CMC-C2C-C1C	2.59	128.98	125.04
19	h	212	CLA	C3D-C4D-ND	2.58	114.42	110.24
25	d	213	LMG	O2-C2-C1	-2.58	103.77	110.05
25	d	213	LMG	O7-C10-O9	-2.58	117.46	123.70
25	g	312	LMG	C7-O1-C1	2.58	118.77	113.74
19	i	310	CLA	C3D-C4D-ND	2.58	114.41	110.24
19	m	304	CLA	C3D-C4D-ND	2.57	114.40	110.24
19	A	801	CLA	C4D-CHA-C1A	-2.57	118.12	121.25
22	J	802	DD6	C21-C20-C19	2.57	117.17	114.28
19	g	304	CLA	C3D-C4D-ND	2.57	114.39	110.24
19	o	304	CLA	C2C-C1C-NC	2.57	112.38	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	F	203	CLA	CBA-CAA-C2A	2.57	121.44	113.86
28	b	301	CHL	O2A-CGA-CBA	2.56	119.95	111.91
19	F	204	CLA	C3D-C4D-ND	2.56	114.38	110.24
28	b	314	CHL	O1D-CGD-CBD	-2.56	119.25	124.48
19	f	309	CLA	CAA-C2A-C1A	-2.56	103.60	111.97
28	b	312	CHL	OMC-CMC-C2C	-2.55	119.91	125.69
19	n	209	CLA	C3D-C4D-ND	2.55	114.37	110.24
19	B	847	CLA	CAA-C2A-C1A	-2.55	103.61	111.97
19	A	821	CLA	C3D-C4D-ND	2.55	114.36	110.24
28	k	301	CHL	OMC-CMC-C2C	-2.55	119.93	125.69
19	B	842	CLA	CBA-CAA-C2A	2.55	121.38	113.86
28	b	311	CHL	CAC-C3C-C4C	-2.55	121.51	124.81
19	A	819	CLA	C3D-C4D-ND	2.55	114.36	110.24
20	B	824	PQN	C11-C3-C4	-2.54	115.78	118.50
28	d	202	CHL	O2A-CGA-CBA	2.54	119.89	111.91
28	g	306	CHL	O1D-CGD-CBD	-2.54	119.29	124.48
19	g	304	CLA	C2C-C1C-NC	2.54	112.35	109.97
19	a	306	CLA	C1-C2-C3	-2.54	121.66	126.04
19	b	306	CLA	CHC-C1C-C2C	-2.54	119.69	126.73
25	g	312	LMG	O6-C1-O1	-2.54	103.97	109.97
19	c	304	CLA	C3D-C4D-ND	2.53	114.33	110.24
28	f	304	CHL	O1D-CGD-CBD	-2.53	119.31	124.48
19	n	202	CLA	C3D-C4D-ND	2.53	114.33	110.24
19	b	304	CLA	CHC-C4B-NB	-2.53	121.58	124.26
28	g	306	CHL	CMA-C3A-C4A	-2.52	104.99	111.77
28	g	303	CHL	CHB-C1B-NB	2.52	126.93	124.26
28	i	301	CHL	O2D-CGD-CBD	2.52	115.75	111.27
19	B	835	CLA	O2A-C1-C2	2.52	115.26	108.64
19	o	311	CLA	C3D-C4D-ND	2.52	114.32	110.24
19	j	311	CLA	CHA-C1A-NA	-2.52	120.63	126.40
19	i	302	CLA	CHC-C4B-NB	-2.52	121.59	124.26
19	B	836	CLA	C3D-C4D-ND	2.52	114.31	110.24
28	c	305	CHL	O2A-CGA-O1A	-2.52	117.24	123.59
25	a	318	LMG	O1-C1-C2	-2.52	104.38	108.30
25	d	213	LMG	O3-C3-C2	-2.51	104.54	110.35
28	a	312	CHL	C2A-C3A-C4A	2.51	105.93	101.87
25	i	316	LMG	O7-C10-O9	-2.51	117.63	123.70
25	b	316	LMG	O6-C1-O1	-2.51	104.03	109.97
19	j	303	CLA	C3D-C4D-ND	2.51	114.30	110.24
19	i	309	CLA	C3D-C4D-ND	2.51	114.30	110.24
19	A	803	CLA	C3D-C4D-ND	2.51	114.29	110.24
19	h	209	CLA	CHC-C4B-NB	-2.51	121.61	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	849	CLA	C2C-C1C-NC	2.50	112.31	109.97
19	B	840	CLA	CHC-C4B-NB	-2.50	121.61	124.26
25	i	316	LMG	O6-C1-O1	-2.50	104.05	109.97
28	b	312	CHL	C2B-C1B-NB	-2.50	108.56	110.23
28	i	301	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
25	b	316	LMG	O3-C3-C2	-2.50	104.57	110.35
19	A	842	CLA	C2C-C1C-NC	2.50	112.31	109.97
28	f	301	CHL	O1D-CGD-CBD	-2.50	119.38	124.48
19	g	304	CLA	CHC-C4B-NB	-2.49	121.62	124.26
19	A	817	CLA	CAA-C2A-C3A	2.49	119.61	112.78
28	i	304	CHL	O1D-CGD-CBD	-2.49	119.38	124.48
28	d	205	CHL	C2A-C3A-C4A	2.49	105.89	101.87
19	j	306	CLA	CHC-C1C-C2C	-2.49	119.81	126.73
19	j	305	CLA	C1-C2-C3	-2.49	122.72	126.75
25	a	301	LMG	O1-C7-C8	-2.49	104.89	110.90
19	o	309	CLA	CHC-C1C-C2C	-2.49	119.82	126.73
19	A	805	CLA	CHC-C4B-NB	-2.48	121.63	124.26
19	o	307	CLA	CBA-CAA-C2A	2.48	121.19	113.86
19	B	806	CLA	C3D-C4D-ND	2.48	114.25	110.24
28	f	301	CHL	O2A-CGA-CBA	2.48	119.69	111.91
19	n	202	CLA	C4D-CHA-C1A	-2.48	118.23	121.25
19	b	305	CLA	C3D-C4D-ND	2.48	114.25	110.24
19	g	304	CLA	C1-C2-C3	-2.48	122.74	126.75
22	A	833	DD6	O1-C20-C15	-2.48	56.91	58.96
19	A	842	CLA	C1-C2-C3	-2.48	121.76	126.04
19	e	310	CLA	CHC-C1C-C2C	-2.48	119.85	126.73
28	k	301	CHL	C2B-C1B-NB	-2.47	108.57	110.23
28	d	202	CHL	OMC-CMC-C2C	-2.47	120.10	125.69
28	g	303	CHL	C1-C2-C3	2.47	130.32	126.04
19	h	206	CLA	CHC-C4B-NB	-2.47	121.64	124.26
19	l	202	CLA	CAA-C2A-C1A	-2.47	103.89	111.97
28	c	313	CHL	CHD-C1D-ND	-2.47	122.19	124.45
28	a	313	CHL	CHB-C1B-NB	2.47	126.87	124.26
25	h	216	LMG	O6-C1-O1	-2.46	104.14	109.97
28	m	301	CHL	O2A-CGA-CBA	2.46	119.64	111.91
28	k	301	CHL	O2A-CGA-CBA	2.46	119.63	111.91
19	B	803	CLA	C3D-C4D-ND	2.46	114.22	110.24
28	c	312	CHL	CHD-C1D-ND	-2.46	122.19	124.45
28	i	301	CHL	CHD-C1D-ND	-2.46	122.19	124.45
19	A	843	CLA	C1-C2-C3	-2.46	121.79	126.04
19	d	204	CLA	C1-C2-C3	2.46	130.29	126.04
28	a	312	CHL	O2A-CGA-CBA	2.45	119.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	830	PQN	C11-C3-C4	-2.45	115.88	118.50
19	m	304	CLA	CHA-C1A-NA	-2.45	120.78	126.40
25	j	314	LMG	O3-C3-C2	-2.45	104.68	110.35
19	n	202	CLA	CAA-C2A-C3A	2.45	119.49	112.78
19	B	837	CLA	CHC-C4B-NB	-2.45	121.67	124.26
19	i	311	CLA	CHC-C4B-NB	-2.45	121.67	124.26
22	e	314	DD6	C14-C13-C11	2.45	129.33	125.53
19	h	205	CLA	CHC-C4B-NB	-2.44	121.67	124.26
19	o	304	CLA	CHC-C4B-NB	-2.44	121.67	124.26
19	B	804	CLA	C3D-C4D-ND	2.44	114.19	110.24
19	B	846	CLA	CHA-C1A-NA	-2.44	120.80	126.40
28	b	301	CHL	C2C-C3C-C4C	2.44	108.23	106.49
25	h	216	LMG	C1-O6-C5	-2.44	108.90	113.69
28	c	313	CHL	C2B-C1B-NB	-2.43	108.60	110.23
19	a	314	CLA	CHC-C1C-C2C	-2.43	119.97	126.73
22	F	205	DD6	C32-C31-C36	-2.43	119.20	122.63
19	c	304	CLA	CHA-C1A-NA	-2.43	120.83	126.40
22	o	314	DD6	C32-C31-C36	-2.43	119.20	122.63
19	j	304	CLA	C3D-C4D-ND	2.43	114.17	110.24
25	g	312	LMG	O2-C2-C1	-2.43	104.15	110.05
28	f	304	CHL	O2D-CGD-O1D	-2.43	119.09	123.84
19	b	315	CLA	CHC-C4B-NB	-2.42	121.69	124.26
19	B	804	CLA	CHC-C4B-NB	-2.42	121.69	124.26
19	o	303	CLA	CHC-C1C-C2C	-2.42	120.00	126.73
19	o	302	CLA	CHC-C4B-NB	-2.42	121.69	124.26
22	j	315	DD6	C32-C31-C36	-2.42	119.22	122.63
25	d	213	LMG	O6-C1-O1	-2.42	104.25	109.97
25	a	301	LMG	O6-C1-O1	-2.42	104.25	109.97
28	g	303	CHL	CHA-C1A-NA	-2.42	120.86	126.40
28	f	301	CHL	C2A-C3A-C4A	2.42	105.77	101.87
28	b	301	CHL	C4D-CHA-C1A	2.42	124.19	121.25
19	A	803	CLA	C3A-C2A-C1A	-2.42	97.72	101.34
28	o	301	CHL	C2B-C1B-NB	-2.42	108.61	110.23
28	i	304	CHL	C2A-C3A-C4A	2.41	105.77	101.87
28	d	202	CHL	O1D-CGD-CBD	-2.41	119.55	124.48
28	g	306	CHL	C2B-C1B-NB	-2.41	108.61	110.23
19	a	306	CLA	CHC-C1C-C2C	-2.41	120.03	126.73
28	g	306	CHL	C3C-C4C-NC	-2.41	107.87	110.57
22	n	210	DD6	C21-C20-C19	2.41	116.99	114.28
28	i	301	CHL	OMC-CMC-C2C	-2.41	120.24	125.69
25	A	851	LMG	O6-C1-O1	-2.41	104.27	109.97
19	A	819	CLA	CHA-C1A-NA	-2.41	120.88	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	e	308	CLA	C4D-CHA-C1A	-2.41	118.32	121.25
28	g	310	CHL	CBC-CAC-C3C	-2.41	105.80	112.43
19	g	301	CLA	CHC-C1C-C2C	-2.41	120.05	126.73
19	o	307	CLA	CHA-C1A-NA	-2.40	120.89	126.40
22	J	802	DD6	C14-C13-C11	2.40	129.26	125.53
19	a	304	CLA	CHC-C4B-NB	-2.40	121.72	124.26
19	o	306	CLA	CHC-C4B-NB	-2.40	121.72	124.26
28	o	301	CHL	C2A-C3A-C4A	2.40	105.75	101.87
19	l	206	CLA	C2C-C1C-NC	2.40	112.22	109.97
19	B	847	CLA	CHC-C4B-NB	-2.40	121.72	124.26
28	a	311	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
28	b	301	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
19	A	802	CLA	CHC-C4B-NB	-2.40	121.72	124.26
28	d	205	CHL	C1-C2-C3	2.40	130.19	126.04
19	b	315	CLA	C2C-C1C-NC	2.39	112.22	109.97
19	n	208	CLA	CHC-C1C-C2C	-2.39	120.08	126.73
19	B	837	CLA	C2C-C1C-NC	2.39	112.21	109.97
19	a	302	CLA	C2C-C1C-NC	2.39	112.21	109.97
28	b	311	CHL	C4D-CHA-C1A	2.39	124.16	121.25
28	i	301	CHL	O1D-CGD-CBD	-2.39	119.59	124.48
19	m	302	CLA	CHC-C1C-C2C	-2.39	120.09	126.73
19	d	211	CLA	CBA-CAA-C2A	2.39	120.91	113.86
28	b	310	CHL	O2A-CGA-O1A	-2.39	117.57	123.59
25	a	316	LMG	O1-C1-C2	-2.39	104.58	108.30
19	i	310	CLA	CHC-C1C-C2C	-2.39	120.10	126.73
19	j	305	CLA	CHC-C1C-C2C	-2.39	120.10	126.73
19	A	805	CLA	CAA-C2A-C3A	2.39	119.31	112.78
28	e	304	CHL	CAA-C2A-C3A	-2.38	106.25	112.78
19	j	310	CLA	C3D-C4D-ND	2.38	114.09	110.24
28	f	304	CHL	CHB-C1B-NB	2.38	126.78	124.26
28	f	304	CHL	CMA-C3A-C4A	-2.38	105.38	111.77
19	k	309	CLA	CHC-C4B-NB	-2.38	121.74	124.26
19	e	308	CLA	C2A-C1A-CHA	2.38	128.02	123.86
25	k	312	LMG	O3-C3-C2	-2.38	104.85	110.35
19	g	304	CLA	CHC-C1C-C2C	-2.38	120.13	126.73
28	a	315	CHL	O1D-CGD-CBD	-2.38	119.62	124.48
19	o	305	CLA	CAA-C2A-C3A	2.38	119.28	112.78
25	a	318	LMG	O6-C1-O1	-2.37	104.35	109.97
19	k	302	CLA	C2C-C1C-NC	2.37	112.20	109.97
19	b	313	CLA	CAA-C2A-C1A	-2.37	104.20	111.97
28	g	306	CHL	CAA-C2A-C3A	-2.37	106.28	112.78
19	a	310	CLA	C2C-C1C-NC	2.37	112.19	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	n	209	CLA	CHC-C1C-C2C	-2.37	120.15	126.73
19	d	208	CLA	CHC-C1C-C2C	-2.37	120.15	126.73
19	c	306	CLA	CHD-C1D-C2D	2.37	130.44	125.48
28	c	312	CHL	O1D-CGD-CBD	-2.37	119.64	124.48
28	a	313	CHL	C2B-C1B-NB	-2.37	108.65	110.23
28	e	304	CHL	O2A-CGA-O1A	-2.37	117.62	123.59
19	o	304	CLA	CHC-C1C-C2C	-2.36	120.16	126.73
19	A	805	CLA	CAA-C2A-C1A	-2.36	104.23	111.97
28	a	312	CHL	O1D-CGD-CBD	-2.36	119.65	124.48
19	g	305	CLA	CHC-C1C-C2C	-2.36	120.17	126.73
28	a	313	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
19	l	206	CLA	CHC-C4B-NB	-2.36	121.76	124.26
19	B	836	CLA	CMA-C3A-C4A	2.36	118.11	111.77
28	g	306	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
19	b	307	CLA	C1-C2-C3	-2.35	121.97	126.04
28	f	301	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
19	A	802	CLA	CHA-C1A-NA	-2.35	121.01	126.40
28	d	202	CHL	C2C-C3C-C4C	2.35	108.16	106.49
28	b	312	CHL	O2A-CGA-O1A	-2.35	117.66	123.59
19	m	304	CLA	CHD-C1D-C2D	2.35	130.41	125.48
25	A	851	LMG	O1-C7-C8	-2.35	105.24	110.90
22	J	802	DD6	C32-C31-C36	-2.35	119.32	122.63
19	l	201	CLA	CHB-C4A-NA	2.35	127.75	124.51
28	a	313	CHL	O1D-CGD-CBD	-2.34	119.69	124.48
19	j	307	CLA	CBA-CAA-C2A	2.34	120.78	113.86
19	B	836	CLA	CHA-C1A-NA	-2.34	121.03	126.40
19	A	824	CLA	CHC-C4B-NB	-2.34	121.78	124.26
19	B	822	CLA	CHC-C4B-NB	-2.34	121.78	124.26
28	b	312	CHL	CMD-C2D-C1D	2.34	128.84	124.71
19	B	804	CLA	CHA-C1A-NA	-2.34	121.05	126.40
19	b	304	CLA	C1-C2-C3	-2.34	122.00	126.04
19	B	817	CLA	CAA-C2A-C1A	-2.34	104.32	111.97
19	i	313	CLA	CHA-C1A-NA	-2.33	121.05	126.40
19	b	313	CLA	CBA-CAA-C2A	2.33	120.75	113.86
19	l	206	CLA	CHA-C1A-NA	-2.33	121.06	126.40
19	B	815	CLA	O2A-C1-C2	2.33	114.76	108.64
28	g	303	CHL	C2A-C3A-C4A	2.33	105.63	101.87
19	B	807	CLA	O2A-C1-C2	2.33	114.76	108.64
25	g	313	LMG	O3-C3-C2	-2.33	104.97	110.35
28	a	312	CHL	CHB-C1B-NB	2.33	126.72	124.26
28	b	311	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
19	B	830	CLA	O2A-C1-C2	2.33	114.75	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	k	301	CHL	C2C-C3C-C4C	2.32	108.15	106.49
19	B	838	CLA	C3A-C2A-C1A	-2.32	97.86	101.34
28	b	311	CHL	OMC-CMC-C2C	-2.32	120.43	125.69
19	c	307	CLA	C2C-C1C-NC	2.32	112.15	109.97
28	o	301	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
28	c	305	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
19	b	315	CLA	CHD-C1D-C2D	2.32	130.35	125.48
19	A	828	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	j	303	CLA	C1-C2-C3	-2.32	122.03	126.04
28	i	301	CHL	CHB-C1B-NB	2.32	126.71	124.26
19	A	853	CLA	C2C-C1C-NC	2.32	112.14	109.97
19	A	817	CLA	CBA-CAA-C2A	2.32	120.70	113.86
19	j	312	CLA	CHC-C4B-NB	-2.32	121.81	124.26
19	k	308	CLA	C1-C2-C3	-2.31	123.01	126.75
19	A	839	CLA	C2C-C1C-NC	2.31	112.14	109.97
25	k	312	LMG	O2-C2-C1	-2.31	104.44	110.05
28	a	315	CHL	OMC-CMC-C2C	-2.31	120.47	125.69
19	B	832	CLA	CHC-C1C-C2C	-2.31	120.32	126.73
19	e	308	CLA	CHC-C4B-NB	-2.31	121.81	124.26
28	b	301	CHL	C2B-C1B-NB	-2.31	108.69	110.23
19	c	315	CLA	CHC-C4B-NB	-2.31	121.81	124.26
19	m	305	CLA	CHD-C1D-C2D	2.31	130.32	125.48
19	n	206	CLA	CHD-C1D-C2D	2.31	130.32	125.48
25	a	318	LMG	O3-C3-C2	-2.31	105.02	110.35
28	g	310	CHL	C2C-C3C-C4C	2.30	108.13	106.49
19	B	815	CLA	CBA-CAA-C2A	2.30	120.66	113.86
19	h	205	CLA	CHA-C1A-NA	-2.30	121.12	126.40
19	j	303	CLA	CHA-C1A-NA	-2.30	121.12	126.40
28	f	301	CHL	CHD-C1D-ND	-2.30	122.34	124.45
19	A	816	CLA	CAA-C2A-C3A	2.30	119.08	112.78
19	g	308	CLA	CHC-C4B-NB	-2.30	121.82	124.26
19	B	848	CLA	CHC-C1C-C2C	-2.30	120.34	126.73
28	b	314	CHL	C4-C3-C5	-2.30	113.35	115.98
19	j	304	CLA	C2C-C1C-NC	2.30	112.13	109.97
19	m	309	CLA	CHC-C1C-C2C	-2.30	120.34	126.73
19	k	311	CLA	CHD-C1D-C2D	2.30	130.30	125.48
19	f	314	CLA	CHA-C1A-NA	-2.30	121.13	126.40
19	A	825	CLA	CHC-C4B-NB	-2.30	121.83	124.26
19	B	818	CLA	CHD-C1D-C2D	2.30	130.30	125.48
19	o	311	CLA	C2C-C1C-NC	2.30	112.12	109.97
19	B	808	CLA	CBA-CAA-C2A	2.29	120.64	113.86
19	j	308	CLA	C1-C2-C3	-2.29	122.07	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	e	304	CHL	C2A-C3A-C4A	2.29	105.58	101.87
19	e	305	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	j	304	CLA	C1-C2-C3	-2.29	122.08	126.04
19	A	803	CLA	CHC-C4B-NB	-2.29	121.83	124.26
28	m	301	CHL	C2C-C3C-C4C	2.29	108.12	106.49
19	e	308	CLA	CHA-C1A-NA	-2.29	121.15	126.40
19	A	819	CLA	CBA-CAA-C2A	2.29	118.40	114.28
22	c	319	DD6	O1-C20-C15	-2.29	57.06	58.96
28	c	305	CHL	C3C-C4C-NC	-2.29	108.00	110.57
28	g	306	CHL	C2A-C3A-C4A	2.29	105.56	101.87
19	j	312	CLA	CHA-C1A-NA	-2.29	121.16	126.40
28	m	301	CHL	C4D-CHA-C1A	2.29	124.03	121.25
28	i	301	CHL	CHA-C1A-NA	-2.29	121.17	126.40
25	a	318	LMG	O2-C2-C1	-2.28	104.50	110.05
19	b	305	CLA	CHC-C4B-NB	-2.28	121.84	124.26
22	k	313	DD6	O1-C20-C19	-2.28	111.67	113.38
19	b	305	CLA	C2C-C1C-NC	2.28	112.11	109.97
28	a	313	CHL	O2A-CGA-O1A	-2.28	117.83	123.59
28	d	205	CHL	OMC-CMC-C2C	-2.28	120.53	125.69
19	B	803	CLA	CHA-C1A-NA	-2.28	121.18	126.40
19	m	309	CLA	CHC-C4B-NB	-2.28	121.84	124.26
19	B	847	CLA	CHD-C1D-C2D	2.28	130.26	125.48
19	B	849	CLA	CHC-C1C-C2C	-2.28	120.40	126.73
28	c	305	CHL	C2A-C3A-C4A	2.28	105.55	101.87
28	e	301	CHL	O1D-CGD-CBD	-2.28	119.83	124.48
19	o	307	CLA	CHC-C4B-NB	-2.28	121.85	124.26
19	B	819	CLA	CHC-C4B-NB	-2.27	121.85	124.26
19	j	310	CLA	CHC-C1C-C2C	-2.27	120.41	126.73
19	i	309	CLA	CHA-C1A-NA	-2.27	121.19	126.40
19	j	304	CLA	CHA-C1A-NA	-2.27	121.19	126.40
19	f	303	CLA	CHC-C4B-NB	-2.27	121.85	124.26
28	c	313	CHL	C2A-C3A-C4A	2.27	105.54	101.87
19	c	302	CLA	CBA-CAA-C2A	2.27	120.57	113.86
19	c	304	CLA	C2C-C1C-NC	2.27	112.10	109.97
19	b	315	CLA	CHC-C1C-C2C	-2.27	120.42	126.73
19	B	830	CLA	CHA-C1A-NA	-2.27	121.20	126.40
19	D	301	CLA	C2C-C1C-NC	2.27	112.10	109.97
25	i	316	LMG	O2-C2-C1	-2.27	104.53	110.05
19	j	301	CLA	CHC-C4B-NB	-2.27	121.85	124.26
19	B	838	CLA	CHA-C1A-NA	-2.27	121.20	126.40
19	l	209	CLA	CAA-C2A-C1A	-2.27	104.55	111.97
19	b	315	CLA	CHA-C1A-NA	-2.27	121.21	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	e	309	CLA	CHC-C4B-NB	-2.26	121.86	124.26
28	a	313	CHL	C2A-C3A-C4A	2.26	105.52	101.87
19	B	841	CLA	CHC-C1C-C2C	-2.26	120.45	126.73
19	B	845	CLA	CHC-C4B-NB	-2.26	121.86	124.26
19	j	311	CLA	C2A-C1A-CHA	2.26	127.81	123.86
19	n	208	CLA	CHB-C4A-NA	2.26	127.64	124.51
19	f	314	CLA	CHC-C4B-NB	-2.26	121.87	124.26
28	e	301	CHL	C2B-C1B-NB	-2.26	108.72	110.23
19	A	806	CLA	CHC-C4B-NB	-2.26	121.87	124.26
19	n	202	CLA	CHC-C4B-NB	-2.26	121.87	124.26
25	g	316	LMG	O3-C3-C2	-2.26	105.13	110.35
25	f	313	LMG	O6-C1-O1	-2.26	104.63	109.97
19	B	849	CLA	CHD-C1D-C2D	2.26	130.21	125.48
19	n	201	CLA	CHA-C1A-NA	-2.26	121.23	126.40
19	j	311	CLA	C3D-C4D-ND	2.25	113.88	110.24
19	A	801	CLA	CHC-C4B-NB	-2.25	121.87	124.26
19	B	840	CLA	C3A-C2A-C1A	-2.25	97.96	101.34
19	h	205	CLA	CBA-CAA-C2A	2.25	120.51	113.86
19	l	209	CLA	C3A-C2A-C1A	-2.25	97.97	101.34
25	f	313	LMG	O2-C2-C1	-2.25	104.58	110.05
19	A	816	CLA	CHC-C4B-NB	-2.25	121.88	124.26
19	n	203	CLA	C3A-C2A-C1A	-2.25	97.97	101.34
19	h	211	CLA	CHA-C1A-NA	-2.25	121.25	126.40
19	d	208	CLA	CHD-C1D-C2D	2.25	130.19	125.48
28	a	311	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
19	B	801	CLA	CHC-C4B-NB	-2.25	121.88	124.26
19	A	803	CLA	CHA-C1A-NA	-2.24	121.26	126.40
19	k	304	CLA	CHA-C1A-NA	-2.24	121.26	126.40
19	J	803	CLA	CHC-C4B-NB	-2.24	121.88	124.26
19	A	801	CLA	CHD-C1D-C2D	2.24	130.19	125.48
19	k	302	CLA	CHA-C1A-NA	-2.24	121.26	126.40
19	o	302	CLA	CHD-C1D-C2D	2.24	130.19	125.48
19	k	309	CLA	C3A-C2A-C1A	-2.24	97.98	101.34
28	d	202	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
28	i	304	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
22	d	215	DD6	C33-C34-C35	2.24	113.37	110.30
19	g	311	CLA	CHA-C1A-NA	-2.24	121.27	126.40
19	h	212	CLA	CHA-C1A-NA	-2.24	121.27	126.40
19	j	311	CLA	C1-C2-C3	-2.24	123.13	126.75
28	o	301	CHL	O2A-CGA-O1A	-2.24	117.95	123.59
28	b	301	CHL	O2A-CGA-O1A	-2.24	117.95	123.59
28	f	304	CHL	CHA-C1A-NA	-2.24	121.28	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	308	CLA	CHC-C4B-NB	-2.24	121.89	124.26
28	b	312	CHL	CHB-C1B-NB	2.23	126.62	124.26
19	c	303	CLA	CHD-C1D-C2D	2.23	130.16	125.48
19	o	310	CLA	CHA-C1A-NA	-2.23	121.28	126.40
19	A	846	CLA	CHC-C4B-NB	-2.23	121.89	124.26
19	i	313	CLA	C3A-C2A-C1A	-2.23	98.00	101.34
19	a	308	CLA	CHA-C1A-NA	-2.23	121.29	126.40
19	f	305	CLA	C1-C2-C3	-2.23	123.15	126.75
19	o	302	CLA	C2C-C1C-NC	2.23	112.06	109.97
22	h	214	DD6	O1-C20-C15	-2.23	57.12	58.96
19	A	828	CLA	CMC-C2C-C1C	2.23	128.43	125.04
19	l	203	CLA	CAA-C2A-C1A	-2.23	104.68	111.97
19	o	305	CLA	CAA-C2A-C1A	-2.23	104.68	111.97
19	o	307	CLA	CAA-C2A-C3A	2.23	118.87	112.78
19	e	310	CLA	CHD-C1D-C2D	2.23	130.15	125.48
19	B	840	CLA	CHA-C1A-NA	-2.23	121.30	126.40
19	c	316	CLA	CHA-C1A-NA	-2.23	121.30	126.40
28	m	301	CHL	C3C-C4C-NC	-2.23	108.08	110.57
19	d	203	CLA	CBA-CAA-C2A	2.22	120.43	113.86
19	B	801	CLA	CHD-C1D-C2D	2.22	130.15	125.48
19	b	306	CLA	CHD-C4C-C3C	-2.22	121.57	124.84
19	k	304	CLA	CHC-C4B-NB	-2.22	121.90	124.26
25	k	312	LMG	C1-O6-C5	-2.22	109.33	113.69
19	j	311	CLA	C2C-C1C-NC	2.22	112.05	109.97
28	d	205	CHL	O2A-CGA-O1A	-2.22	117.98	123.59
27	B	829	DGD	O5D-C6D-C5D	-2.22	104.94	109.05
19	A	819	CLA	C2C-C1C-NC	2.22	112.05	109.97
19	a	303	CLA	CHA-C1A-NA	-2.22	121.32	126.40
28	g	310	CHL	O2A-CGA-O1A	-2.22	117.99	123.59
19	o	302	CLA	CHA-C1A-NA	-2.22	121.32	126.40
22	o	313	DD6	C32-C31-C36	-2.22	119.50	122.63
19	B	848	CLA	CHD-C1D-C2D	2.22	130.13	125.48
25	a	301	LMG	C1-C2-C3	-2.22	105.38	110.00
19	F	204	CLA	CHA-C1A-NA	-2.22	121.32	126.40
19	e	306	CLA	C1-C2-C3	2.22	129.88	126.04
19	B	812	CLA	CHC-C4B-NB	-2.22	121.91	124.26
19	B	837	CLA	C1-C2-C3	-2.22	123.17	126.75
19	B	840	CLA	CHD-C1D-C2D	2.21	130.12	125.48
28	f	301	CHL	CHB-C1B-NB	2.21	126.60	124.26
19	o	303	CLA	CHD-C1D-C2D	2.21	130.12	125.48
19	i	302	CLA	CHD-C1D-C2D	2.21	130.12	125.48
28	g	310	CHL	OMC-CMC-C2C	-2.21	120.69	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	312	LMG	C1-O6-C5	-2.21	109.35	113.69
28	k	301	CHL	O2A-CGA-O1A	-2.21	118.02	123.59
19	B	837	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
19	A	818	CLA	CHC-C4B-NB	-2.21	121.92	124.26
19	n	202	CLA	CHA-C1A-NA	-2.21	121.34	126.40
22	m	313	DD6	O1-C20-C15	-2.21	57.13	58.96
19	e	310	CLA	C1-C2-C3	-2.21	122.23	126.04
19	B	839	CLA	CHA-C1A-NA	-2.20	121.35	126.40
28	f	301	CHL	C2A-C1A-CHA	2.20	127.71	123.86
19	A	806	CLA	CHD-C1D-C2D	2.20	130.10	125.48
19	n	204	CLA	CHA-C1A-NA	-2.20	121.35	126.40
19	f	303	CLA	CHA-C1A-NA	-2.20	121.35	126.40
19	B	842	CLA	CAA-C2A-C3A	2.20	118.81	112.78
19	o	305	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	A	806	CLA	C1-C2-C3	-2.20	122.24	126.04
19	A	842	CLA	CHC-C4B-NB	-2.20	121.93	124.26
28	c	313	CHL	C4D-CHA-C1A	2.20	123.93	121.25
25	k	312	LMG	O6-C1-O1	-2.20	104.77	109.97
22	e	313	DD6	C32-C31-C36	2.20	125.74	122.63
19	A	807	CLA	CHC-C4B-NB	-2.20	121.93	124.26
28	h	202	CHL	C2B-C1B-NB	-2.20	108.76	110.23
19	B	832	CLA	CHD-C1D-C2D	2.20	130.09	125.48
25	e	312	LMG	O3-C3-C2	-2.20	105.27	110.35
19	A	826	CLA	C2C-C1C-NC	2.20	112.03	109.97
19	j	309	CLA	C2C-C1C-NC	2.20	112.03	109.97
19	B	811	CLA	CAC-C3C-C4C	2.20	127.66	124.81
25	j	314	LMG	O2-C2-C1	-2.20	104.71	110.05
19	B	811	CLA	CHA-C1A-NA	-2.20	121.37	126.40
25	a	316	LMG	C1-O6-C5	-2.20	109.38	113.69
19	b	303	CLA	CHA-C1A-NA	-2.19	121.37	126.40
19	n	209	CLA	CHD-C1D-C2D	2.19	130.08	125.48
22	c	318	DD6	C32-C31-C36	2.19	125.73	122.63
19	b	308	CLA	C2C-C1C-NC	2.19	112.03	109.97
19	n	201	CLA	C2C-C1C-NC	2.19	112.03	109.97
28	o	301	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
19	a	302	CLA	CHC-C1C-C2C	-2.19	120.64	126.73
19	n	204	CLA	CHC-C4B-NB	-2.19	121.94	124.26
28	e	304	CHL	CMA-C3A-C4A	-2.19	105.88	111.77
19	o	304	CLA	CHD-C1D-C2D	2.19	130.08	125.48
19	B	839	CLA	C2C-C1C-NC	2.19	112.03	109.97
19	i	309	CLA	C2C-C1C-NC	2.19	112.03	109.97
19	j	304	CLA	CHC-C4B-NB	-2.19	121.94	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	l	202	CLA	CHC-C4B-NB	-2.19	121.94	124.26
28	c	313	CHL	OMC-CMC-C2C	-2.19	120.73	125.69
28	b	311	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
19	B	835	CLA	CHD-C1D-C2D	2.19	130.07	125.48
19	j	304	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
19	B	830	CLA	C2C-C1C-NC	2.19	112.02	109.97
28	f	301	CHL	O2A-CGA-O1A	-2.19	118.07	123.59
19	k	302	CLA	C1-C2-C3	-2.19	122.26	126.04
25	g	316	LMG	O7-C10-O9	-2.19	118.42	123.70
19	a	302	CLA	CHD-C1D-C2D	2.19	130.07	125.48
19	b	304	CLA	C2C-C1C-NC	2.19	112.02	109.97
19	j	311	CLA	CAA-C2A-C1A	2.19	119.14	111.97
28	o	301	CHL	CHD-C1D-ND	-2.19	122.44	124.45
25	A	851	LMG	O3-C3-C2	-2.19	105.30	110.35
19	g	305	CLA	CHD-C1D-C2D	2.19	130.06	125.48
19	B	841	CLA	CHD-C1D-C2D	2.19	130.06	125.48
19	i	311	CLA	CHD-C1D-C2D	2.19	130.06	125.48
19	l	202	CLA	C3A-C2A-C1A	-2.19	98.07	101.34
19	d	201	CLA	C2C-C1C-NC	2.18	112.02	109.97
19	j	301	CLA	CHA-C1A-NA	-2.18	121.40	126.40
19	a	306	CLA	CHD-C1D-C2D	2.18	130.06	125.48
19	B	838	CLA	CHC-C4B-NB	-2.18	121.95	124.26
19	m	309	CLA	CHD-C1D-C2D	2.18	130.06	125.48
28	h	202	CHL	CHB-C1B-NB	2.18	126.57	124.26
28	i	304	CHL	CHB-C1B-NB	2.18	126.56	124.26
19	A	825	CLA	CAA-C2A-C1A	-2.18	104.83	111.97
19	j	312	CLA	C3A-C2A-C1A	-2.18	98.08	101.34
19	j	303	CLA	C2C-C1C-NC	2.18	112.01	109.97
28	k	301	CHL	C3C-C4C-NC	-2.18	108.13	110.57
19	l	209	CLA	CHC-C4B-NB	-2.18	121.95	124.26
19	B	817	CLA	CHB-C4A-NA	2.18	127.52	124.51
19	m	306	CLA	CHD-C1D-C2D	2.18	130.04	125.48
25	g	316	LMG	O1-C7-C8	-2.17	105.65	110.90
19	c	315	CLA	CHB-C4A-NA	2.17	127.52	124.51
25	b	316	LMG	O2-C2-C1	-2.17	104.77	110.05
19	A	804	CLA	C16-C15-C13	2.17	122.94	115.92
19	j	306	CLA	CHD-C1D-C2D	2.17	130.03	125.48
19	a	314	CLA	CHD-C1D-C2D	2.17	130.03	125.48
19	e	307	CLA	CHC-C4B-NB	-2.17	121.96	124.26
19	A	853	CLA	CHC-C1C-C2C	-2.17	120.70	126.73
25	g	313	LMG	C1-O6-C5	-2.17	109.43	113.69
19	l	206	CLA	CHC-C1C-C2C	-2.17	120.70	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	o	305	CLA	CHA-C1A-NA	-2.17	121.43	126.40
19	n	203	CLA	CHC-C4B-NB	-2.17	121.96	124.26
25	h	216	LMG	C3-C4-C5	-2.17	106.37	110.24
28	i	304	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
19	A	801	CLA	C3D-C4D-ND	2.17	113.74	110.24
19	c	302	CLA	CAA-C2A-C3A	2.17	118.71	112.78
22	f	315	DD6	O1-C20-C15	-2.16	57.17	58.96
22	a	321	DD6	C32-C31-C36	-2.16	119.58	122.63
19	l	201	CLA	CHD-C4C-C3C	-2.16	121.66	124.84
19	A	840	CLA	O2A-C1-C2	2.16	114.32	108.64
28	a	312	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
19	A	817	CLA	O2A-C1-C2	2.16	114.32	108.64
19	B	801	CLA	CHA-C1A-NA	-2.16	121.44	126.40
19	B	804	CLA	CHD-C1D-C2D	2.16	130.02	125.48
19	B	836	CLA	C2C-C1C-NC	2.16	112.00	109.97
19	d	212	CLA	C2C-C1C-NC	2.16	112.00	109.97
28	b	301	CHL	C4-C3-C5	-2.16	111.64	115.27
19	B	833	CLA	CHC-C4B-NB	-2.16	121.97	124.26
19	f	303	CLA	C2C-C1C-NC	2.16	112.00	109.97
19	B	805	CLA	CHD-C1D-C2D	2.16	130.01	125.48
25	c	320	LMG	O3-C3-C2	-2.16	105.36	110.35
19	A	845	CLA	CHD-C1D-C2D	2.16	130.01	125.48
28	b	311	CHL	CHB-C1B-NB	2.16	126.54	124.26
19	B	837	CLA	CHD-C1D-C2D	2.16	130.00	125.48
19	n	208	CLA	CBA-CAA-C2A	2.16	120.23	113.86
19	A	813	CLA	CHC-C4B-NB	-2.16	121.97	124.26
19	i	309	CLA	CHC-C4B-NB	-2.16	121.97	124.26
19	o	311	CLA	CHA-C1A-NA	-2.16	121.46	126.40
19	c	314	CLA	CHC-C4B-NB	-2.16	121.97	124.26
25	g	313	LMG	O1-C7-C8	-2.15	105.70	110.90
19	j	304	CLA	CHD-C1D-C2D	2.15	130.00	125.48
28	c	312	CHL	C4D-CHA-C1A	2.15	123.87	121.25
28	g	303	CHL	O1D-CGD-CBD	-2.15	120.08	124.48
19	b	304	CLA	CHD-C1D-C2D	2.15	130.00	125.48
19	e	307	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	i	315	DD6	O1-C20-C15	-2.15	57.18	58.96
19	d	210	CLA	CHC-C4B-NB	-2.15	121.98	124.26
19	n	208	CLA	CHD-C1D-C2D	2.15	129.99	125.48
19	k	302	CLA	CHC-C1C-C2C	-2.15	120.75	126.73
24	a	319	LMU	C1'-O5'-C5'	2.15	116.38	113.03
19	B	823	CLA	CHC-C4B-NB	-2.15	121.98	124.26
19	m	303	CLA	CHC-C4B-NB	-2.15	121.98	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	313	CHL	CHC-C1C-NC	2.15	127.47	124.20
19	A	802	CLA	CHB-C4A-NA	2.15	127.49	124.51
19	A	842	CLA	CHC-C1C-C2C	-2.15	120.76	126.73
28	c	312	CHL	CHA-C1A-NA	-2.15	121.47	126.40
28	b	310	CHL	C4D-CHA-C1A	2.15	123.87	121.25
19	A	825	CLA	CHD-C1D-C2D	2.15	129.99	125.48
19	j	312	CLA	CHD-C1D-C2D	2.15	129.99	125.48
22	j	316	DD6	C32-C31-C36	-2.15	119.60	122.63
19	f	309	CLA	CHC-C4B-NB	-2.15	121.98	124.26
19	o	305	CLA	CHC-C4B-NB	-2.15	121.98	124.26
19	B	842	CLA	CHA-C1A-NA	-2.15	121.48	126.40
25	e	312	LMG	C1-C2-C3	-2.15	105.53	110.00
19	k	305	CLA	C2C-C1C-NC	2.15	111.98	109.97
19	B	805	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
19	f	314	CLA	CHD-C1D-C2D	2.15	129.98	125.48
28	d	205	CHL	C2C-C3C-C4C	2.15	108.02	106.49
19	A	819	CLA	CHC-C4B-NB	-2.15	121.98	124.26
19	f	307	CLA	CMC-C2C-C1C	2.15	128.31	125.04
25	a	318	LMG	O7-C10-O9	-2.15	118.52	123.70
19	A	822	CLA	CHA-C1A-NA	-2.15	121.48	126.40
28	d	205	CHL	O1D-CGD-CBD	-2.15	120.09	124.48
28	b	314	CHL	C2C-C3C-C4C	2.14	108.02	106.49
19	f	305	CLA	CHD-C1D-C2D	2.14	129.98	125.48
28	c	313	CHL	CHB-C1B-NB	2.14	126.53	124.26
28	b	311	CHL	C2A-C3A-C4A	2.14	105.33	101.87
28	g	306	CHL	CHA-C1A-NA	-2.14	121.49	126.40
19	o	302	CLA	CHC-C1C-C2C	-2.14	120.78	126.73
21	A	831	LHG	C20-C19-C18	-2.14	103.55	114.42
25	f	313	LMG	O3-C3-C2	-2.14	105.40	110.35
19	d	201	CLA	CHC-C4B-NB	-2.14	121.99	124.26
19	k	306	CLA	CHC-C4B-NB	-2.14	121.99	124.26
19	A	821	CLA	CHA-C1A-NA	-2.14	121.49	126.40
28	h	202	CHL	O2A-CGA-O1A	-2.14	118.19	123.59
19	j	313	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	b	303	CLA	C2C-C1C-NC	2.14	111.98	109.97
19	c	316	CLA	C2C-C1C-NC	2.14	111.98	109.97
19	A	853	CLA	CHD-C1D-C2D	2.14	129.97	125.48
28	i	301	CHL	C2C-C3C-C4C	2.14	108.01	106.49
19	b	306	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	h	212	CLA	CHB-C4A-NA	2.14	127.47	124.51
19	j	305	CLA	CHC-C4B-NB	-2.14	121.99	124.26
21	A	831	LHG	C18-C17-C16	-2.14	103.58	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	h	213	CLA	CHC-C4B-NB	-2.14	122.00	124.26
19	d	211	CLA	C2C-C1C-NC	2.14	111.97	109.97
19	A	843	CLA	CHD-C1D-C2D	2.14	129.96	125.48
28	k	301	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
19	e	303	CLA	C2C-C1C-NC	2.13	111.97	109.97
19	e	303	CLA	CHC-C4B-NB	-2.13	122.00	124.26
25	a	316	LMG	O2-C2-C1	-2.13	104.86	110.05
28	a	311	CHL	C2A-C3A-C4A	2.13	105.32	101.87
19	B	842	CLA	CHD-C1D-C2D	2.13	129.95	125.48
19	h	211	CLA	C2C-C1C-NC	2.13	111.97	109.97
19	l	208	CLA	CHD-C1D-C2D	2.13	129.95	125.48
19	n	206	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	e	301	CHL	CHB-C1B-NB	2.13	126.51	124.26
19	o	307	CLA	C1-C2-C3	-2.13	122.36	126.04
19	o	308	CLA	CHD-C1D-C2D	2.13	129.94	125.48
19	h	205	CLA	CHD-C1D-C2D	2.13	129.94	125.48
19	B	820	CLA	CHD-C1D-C2D	2.13	129.94	125.48
28	a	315	CHL	C2A-C3A-C4A	2.13	105.30	101.87
28	a	313	CHL	C2C-C3C-C4C	2.13	108.00	106.49
19	b	304	CLA	CHC-C1C-C2C	-2.12	120.83	126.73
19	F	202	CLA	CHC-C4B-NB	-2.12	122.01	124.26
25	g	313	LMG	O7-C10-O9	-2.12	118.57	123.70
19	g	307	CLA	C2C-C1C-NC	2.12	111.96	109.97
19	e	308	CLA	CHD-C1D-C2D	2.12	129.94	125.48
19	l	202	CLA	CHD-C1D-C2D	2.12	129.94	125.48
19	B	849	CLA	CHC-C4B-NB	-2.12	122.01	124.26
19	i	311	CLA	C3A-C2A-C1A	-2.12	98.16	101.34
19	i	303	CLA	C2C-C1C-NC	2.12	111.96	109.97
19	e	303	CLA	CHA-C1A-NA	-2.12	121.54	126.40
19	e	311	CLA	C1-C2-C3	2.12	129.71	126.04
19	i	306	CLA	CHD-C1D-C2D	2.12	129.93	125.48
19	b	305	CLA	CHC-C1C-C2C	-2.12	120.84	126.73
25	a	316	LMG	C3-C4-C5	-2.12	106.46	110.24
19	B	848	CLA	CHC-C4B-NB	-2.12	122.01	124.26
19	n	202	CLA	CHD-C1D-C2D	2.12	129.93	125.48
19	h	201	CLA	CHD-C1D-C2D	2.12	129.93	125.48
28	b	310	CHL	C2A-C1A-CHA	2.12	127.56	123.86
19	c	302	CLA	C2C-C1C-NC	2.12	111.96	109.97
19	B	813	CLA	CHC-C4B-NB	-2.12	122.02	124.26
19	h	207	CLA	CHA-C1A-NA	-2.12	121.55	126.40
19	e	308	CLA	C2A-C3A-C4A	-2.12	98.45	101.87
19	n	204	CLA	CHD-C1D-C2D	2.12	129.92	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	g	304	CLA	CHD-C1D-C2D	2.11	129.92	125.48
19	k	306	CLA	CHA-C1A-NA	-2.11	121.56	126.40
28	g	306	CHL	CHB-C1B-NB	2.11	126.50	124.26
19	A	842	CLA	CHA-C1A-NA	-2.11	121.56	126.40
19	g	301	CLA	CHD-C1D-C2D	2.11	129.91	125.48
28	c	313	CHL	O2A-CGA-O1A	-2.11	118.26	123.59
19	h	213	CLA	CHA-C1A-NA	-2.11	121.56	126.40
19	B	820	CLA	CHC-C4B-NB	-2.11	122.02	124.26
19	B	846	CLA	CHC-C4B-NB	-2.11	122.02	124.26
19	B	844	CLA	CBA-CAA-C2A	2.11	120.10	113.86
28	h	202	CHL	O1D-CGD-CBD	-2.11	120.16	124.48
28	g	306	CHL	OMC-CMC-C2C	-2.11	120.91	125.69
28	f	301	CHL	O2D-CGD-O1D	-2.11	119.71	123.84
19	l	209	CLA	CAA-C2A-C3A	2.11	118.55	112.78
19	A	812	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	n	209	CLA	CHC-C4B-NB	-2.11	122.02	124.26
27	B	829	DGD	O2D-C2D-C1D	-2.11	104.92	110.05
19	g	311	CLA	CHC-C4B-NB	-2.11	122.03	124.26
19	i	313	CLA	CHC-C4B-NB	-2.11	122.03	124.26
19	B	838	CLA	CHD-C1D-C2D	2.11	129.90	125.48
19	A	808	CLA	CHD-C1D-C2D	2.11	129.90	125.48
19	B	806	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	A	824	CLA	C2C-C1C-NC	2.11	111.95	109.97
19	d	207	CLA	CHD-C1D-C2D	2.11	129.90	125.48
22	b	319	DD6	C32-C31-C36	2.11	125.61	122.63
19	B	803	CLA	CHC-C4B-NB	-2.11	122.03	124.26
19	f	307	CLA	CHC-C4B-NB	-2.11	122.03	124.26
28	b	301	CHL	C2A-C3A-C4A	2.11	105.27	101.87
19	j	313	CLA	CHD-C1D-C2D	2.11	129.90	125.48
19	l	205	CLA	CHA-C1A-NA	-2.11	121.58	126.40
19	A	823	CLA	CHC-C4B-NB	-2.11	122.03	124.26
19	l	205	CLA	CHC-C4B-NB	-2.11	122.03	124.26
19	j	311	CLA	CMC-C2C-C1C	2.11	128.25	125.04
25	A	851	LMG	C3-C4-C5	-2.11	106.48	110.24
19	i	308	CLA	CHD-C1D-C2D	2.10	129.90	125.48
19	j	306	CLA	CHC-C4B-NB	-2.10	122.03	124.26
19	m	302	CLA	CHD-C1D-C2D	2.10	129.89	125.48
19	a	305	CLA	CHB-C4A-NA	2.10	127.42	124.51
19	m	311	CLA	CHC-C4B-NB	-2.10	122.03	124.26
19	o	307	CLA	CHD-C1D-C2D	2.10	129.89	125.48
27	B	829	DGD	CBB-CAB-C9B	-2.10	103.75	114.42
19	A	811	CLA	CHD-C1D-C2D	2.10	129.89	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	316	LMG	C1-O6-C5	-2.10	109.56	113.69
22	g	315	DD6	O1-C20-C15	-2.10	57.22	58.96
19	A	839	CLA	CHA-C1A-NA	-2.10	121.59	126.40
28	g	310	CHL	O2D-CGD-O1D	-2.10	119.74	123.84
19	a	308	CLA	CHD-C1D-C2D	2.10	129.88	125.48
25	a	316	LMG	O3-C3-C2	-2.10	105.50	110.35
19	f	305	CLA	CAA-C2A-C1A	-2.10	105.10	111.97
19	k	304	CLA	CBA-CAA-C2A	2.10	120.05	113.86
19	c	314	CLA	CHD-C1D-C2D	2.10	129.88	125.48
19	B	817	CLA	CAA-C2A-C3A	2.10	118.52	112.78
28	h	202	CHL	C2A-C3A-C4A	2.10	105.25	101.87
19	B	833	CLA	CHD-C1D-C2D	2.10	129.88	125.48
19	A	826	CLA	CHA-C1A-NA	-2.10	121.60	126.40
19	d	209	CLA	C2C-C1C-NC	2.09	111.93	109.97
19	A	829	CLA	CHC-C4B-NB	-2.09	122.04	124.26
19	i	310	CLA	CHD-C4C-C3C	-2.09	121.76	124.84
19	l	203	CLA	CHD-C1D-C2D	2.09	129.87	125.48
28	a	312	CHL	OMC-CMC-C2C	-2.09	120.95	125.69
19	e	309	CLA	CHD-C1D-C2D	2.09	129.87	125.48
19	o	309	CLA	CHA-C1A-NA	-2.09	121.60	126.40
19	A	814	CLA	C2C-C1C-NC	2.09	111.93	109.97
19	a	305	CLA	CHC-C4B-NB	-2.09	122.04	124.26
28	c	312	CHL	CHB-C1B-NB	2.09	126.47	124.26
19	m	308	CLA	CHB-C4A-NA	2.09	127.41	124.51
28	a	313	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
19	B	812	CLA	CHD-C1D-C2D	2.09	129.87	125.48
19	A	849	CLA	CHD-C1D-C2D	2.09	129.87	125.48
19	c	311	CLA	CHD-C1D-C2D	2.09	129.87	125.48
19	k	304	CLA	CHD-C1D-C2D	2.09	129.87	125.48
19	A	843	CLA	C10-C8-C7	2.09	123.12	112.13
19	B	808	CLA	CHC-C4B-NB	-2.09	122.05	124.26
25	a	301	LMG	O3-C3-C2	-2.09	105.52	110.35
19	e	307	CLA	CHD-C1D-C2D	2.09	129.86	125.48
19	g	308	CLA	CHD-C1D-C2D	2.09	129.86	125.48
19	o	306	CLA	CHD-C1D-C2D	2.09	129.86	125.48
19	i	307	CLA	CMC-C2C-C1C	2.09	128.22	125.04
19	l	209	CLA	CHA-C1A-NA	-2.09	121.62	126.40
19	A	827	CLA	CHD-C1D-C2D	2.09	129.86	125.48
19	h	205	CLA	CHB-C4A-NA	2.09	127.40	124.51
19	B	818	CLA	CHB-C4A-NA	2.09	127.40	124.51
19	m	305	CLA	C2C-C1C-NC	2.09	111.93	109.97
19	A	813	CLA	CHA-C1A-NA	-2.09	121.62	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	851	LMG	O2-C2-C1	-2.09	104.98	110.05
19	A	804	CLA	CHC-C4B-NB	-2.09	122.05	124.26
19	f	311	CLA	CHC-C4B-NB	-2.09	122.05	124.26
19	j	311	CLA	CMA-C3A-C4A	2.09	117.38	111.77
28	b	314	CHL	O2A-CGA-O1A	-2.08	118.33	123.59
19	n	209	CLA	CHA-C1A-NA	-2.08	121.62	126.40
19	A	822	CLA	C2C-C1C-NC	2.08	111.92	109.97
19	A	846	CLA	CHA-C1A-NA	-2.08	121.63	126.40
19	B	818	CLA	C16-C15-C13	2.08	122.65	115.92
19	c	308	CLA	CHD-C1D-C2D	2.08	129.85	125.48
19	i	305	CLA	CAA-C2A-C1A	-2.08	105.15	111.97
28	b	301	CHL	C3C-C4C-NC	-2.08	108.24	110.57
19	k	303	CLA	CHC-C4B-NB	-2.08	122.05	124.26
19	n	205	CLA	C6-C7-C8	2.08	122.65	115.92
19	A	802	CLA	CHD-C1D-C2D	2.08	129.85	125.48
19	i	311	CLA	CHA-C1A-NA	-2.08	121.63	126.40
25	g	316	LMG	O1-C1-C2	-2.08	105.05	108.30
19	d	203	CLA	CHC-C4B-NB	-2.08	122.05	124.26
19	A	805	CLA	CHD-C1D-C2D	2.08	129.84	125.48
22	F	205	DD6	C14-C13-C11	2.08	128.76	125.53
22	f	315	DD6	C33-C34-C35	2.08	113.15	110.30
19	k	305	CLA	CHD-C1D-C2D	2.08	129.84	125.48
19	h	204	CLA	C2C-C1C-NC	2.08	111.92	109.97
19	l	203	CLA	C2C-C1C-NC	2.08	111.92	109.97
19	l	206	CLA	CHD-C1D-C2D	2.08	129.84	125.48
19	e	303	CLA	CHC-C1C-C2C	-2.08	120.96	126.73
19	f	309	CLA	CHD-C1D-C2D	2.08	129.84	125.48
19	A	844	CLA	CBA-CAA-C2A	2.08	119.99	113.86
19	o	311	CLA	CHC-C1C-C2C	-2.08	120.96	126.73
19	l	207	CLA	CHC-C4B-NB	-2.08	122.06	124.26
19	B	823	CLA	C2C-C1C-NC	2.08	111.92	109.97
19	m	308	CLA	CHC-C4B-NB	-2.07	122.06	124.26
19	i	303	CLA	CHA-C1A-NA	-2.07	121.65	126.40
19	a	303	CLA	CHC-C4B-NB	-2.07	122.06	124.26
19	k	308	CLA	CHC-C4B-NB	-2.07	122.06	124.26
19	B	805	CLA	CHC-C4B-NB	-2.07	122.06	124.26
19	B	842	CLA	CHC-C4B-NB	-2.07	122.06	124.26
19	b	302	CLA	CHC-C4B-NB	-2.07	122.06	124.26
19	n	203	CLA	CHA-C1A-NA	-2.07	121.65	126.40
19	g	301	CLA	CHC-C1C-NC	2.07	127.35	124.20
19	b	305	CLA	CHD-C1D-C2D	2.07	129.82	125.48
19	j	305	CLA	CHD-C1D-C2D	2.07	129.82	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	k	309	CLA	CHA-C1A-NA	-2.07	121.65	126.40
19	o	304	CLA	CHA-C1A-NA	-2.07	121.65	126.40
28	e	304	CHL	CHA-C1A-NA	-2.07	121.66	126.40
19	g	302	CLA	C2C-C1C-NC	2.07	111.91	109.97
19	h	206	CLA	CHD-C1D-C2D	2.07	129.82	125.48
19	b	309	CLA	CHC-C4B-NB	-2.07	122.07	124.26
19	i	306	CLA	CHC-C4B-NB	-2.07	122.07	124.26
19	A	823	CLA	CHD-C1D-C2D	2.07	129.82	125.48
19	j	306	CLA	CHA-C1A-NA	-2.07	121.66	126.40
19	A	823	CLA	C2C-C1C-NC	2.07	111.91	109.97
19	A	811	CLA	CHC-C4B-NB	-2.07	122.07	124.26
19	d	210	CLA	CHD-C1D-C2D	2.07	129.82	125.48
19	f	311	CLA	CHA-C1A-NA	-2.07	121.66	126.40
19	d	206	CLA	CHD-C1D-C2D	2.07	129.82	125.48
25	g	313	LMG	O2-C2-C1	-2.07	105.03	110.05
19	n	208	CLA	C3D-C4D-ND	2.07	113.58	110.24
19	A	817	CLA	CHD-C1D-C2D	2.07	129.81	125.48
19	h	208	CLA	CHD-C1D-C2D	2.07	129.81	125.48
28	a	312	CHL	C4D-CHA-C1A	2.07	123.76	121.25
28	g	303	CHL	C4D-CHA-C1A	2.07	123.76	121.25
19	j	302	CLA	O2A-C1-C2	2.07	114.06	108.64
19	B	807	CLA	C2C-C1C-NC	2.07	111.91	109.97
28	c	305	CHL	C2C-C3C-C4C	2.06	107.96	106.49
19	B	843	CLA	CHD-C1D-C2D	2.06	129.81	125.48
19	B	809	CLA	CHA-C1A-NA	-2.06	121.67	126.40
19	i	307	CLA	CHD-C1D-C2D	2.06	129.81	125.48
19	l	201	CLA	C3D-C4D-ND	2.06	113.58	110.24
19	f	310	CLA	C2C-C1C-NC	2.06	111.91	109.97
19	a	302	CLA	CHA-C1A-NA	-2.06	121.67	126.40
19	j	301	CLA	CHD-C1D-C2D	2.06	129.81	125.48
19	g	311	CLA	CHD-C1D-C2D	2.06	129.80	125.48
19	k	311	CLA	C2C-C1C-NC	2.06	111.90	109.97
19	B	803	CLA	CHD-C1D-C2D	2.06	129.80	125.48
19	A	823	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	h	203	CLA	CHC-C4B-NB	-2.06	122.08	124.26
19	A	809	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	B	805	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	j	307	CLA	CHD-C1D-C2D	2.06	129.80	125.48
19	m	311	CLA	CHD-C1D-C2D	2.06	129.80	125.48
28	b	314	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
19	F	202	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	a	307	CLA	CHD-C1D-C2D	2.06	129.80	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	810	CLA	CHD-C1D-C2D	2.06	129.79	125.48
19	B	822	CLA	CHD-C1D-C2D	2.06	129.79	125.48
19	e	311	CLA	CHC-C4B-NB	-2.06	122.08	124.26
19	A	803	CLA	CHD-C1D-C2D	2.06	129.79	125.48
19	m	302	CLA	CHA-C1A-NA	-2.06	121.69	126.40
19	A	848	CLA	C2C-C1C-NC	2.05	111.90	109.97
19	A	847	CLA	CHA-C1A-NA	-2.05	121.69	126.40
19	B	835	CLA	CHC-C4B-NB	-2.05	122.08	124.26
28	b	311	CHL	CHA-C1A-NA	-2.05	121.70	126.40
19	d	204	CLA	CHD-C1D-C2D	2.05	129.79	125.48
19	f	311	CLA	CHD-C1D-C2D	2.05	129.79	125.48
19	A	821	CLA	C2C-C1C-NC	2.05	111.89	109.97
19	h	210	CLA	C2C-C1C-NC	2.05	111.89	109.97
19	A	816	CLA	CBA-CAA-C2A	2.05	119.92	113.86
19	n	205	CLA	CHC-C4B-NB	-2.05	122.08	124.26
19	f	307	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	a	305	CLA	CBA-CAA-C2A	2.05	119.92	113.86
19	i	305	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	b	313	CLA	CHB-C4A-NA	2.05	127.35	124.51
19	D	301	CLA	CHA-C1A-NA	-2.05	121.70	126.40
28	g	310	CHL	CMA-C3A-C4A	-2.05	106.26	111.77
19	i	313	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	a	305	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	l	204	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	l	209	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	B	814	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	o	312	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	h	201	CLA	CHC-C4B-NB	-2.05	122.09	124.26
19	j	302	CLA	CHC-C4B-NB	-2.05	122.09	124.26
19	k	309	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	o	305	CLA	CHD-C1D-C2D	2.05	129.78	125.48
25	g	316	LMG	O2-C2-C1	-2.05	105.07	110.05
19	B	823	CLA	CHD-C1D-C2D	2.05	129.77	125.48
19	j	310	CLA	CHD-C1D-C2D	2.05	129.77	125.48
19	A	822	CLA	O2A-C1-C2	2.05	114.01	108.64
28	b	310	CHL	C2B-C1B-NB	-2.05	108.86	110.23
19	A	813	CLA	CHD-C1D-C2D	2.05	129.77	125.48
19	i	312	CLA	CHD-C1D-C2D	2.05	129.77	125.48
19	j	313	CLA	CHC-C4B-NB	-2.05	122.09	124.26
19	f	310	CLA	CHA-C1A-NA	-2.05	121.71	126.40
28	h	202	CHL	CHD-C4C-NC	2.05	127.43	124.20
19	A	829	CLA	CHD-C1D-C2D	2.05	129.77	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	302	CLA	CHC-C4B-NB	-2.04	122.09	124.26
19	b	313	CLA	CHC-C4B-NB	-2.04	122.09	124.26
19	f	302	CLA	CHC-C4B-NB	-2.04	122.09	124.26
19	n	209	CLA	CHC-C1C-NC	2.04	127.30	124.20
19	c	315	CLA	CHD-C1D-C2D	2.04	129.76	125.48
28	i	301	CHL	CMA-C3A-C4A	-2.04	106.28	111.77
19	f	308	CLA	CHC-C4B-NB	-2.04	122.10	124.26
19	n	203	CLA	CHD-C1D-C2D	2.04	129.76	125.48
28	d	205	CHL	C2B-C1B-NB	-2.04	108.86	110.23
28	c	312	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
28	g	310	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
19	B	810	CLA	CHC-C4B-NB	-2.04	122.10	124.26
19	f	307	CLA	CHA-C1A-NA	-2.04	121.73	126.40
19	m	310	CLA	CHA-C1A-NA	-2.04	121.73	126.40
19	A	818	CLA	CHD-C1D-C2D	2.04	129.76	125.48
19	A	847	CLA	CHD-C1D-C2D	2.04	129.76	125.48
19	A	850	CLA	CHC-C4B-NB	-2.04	122.10	124.26
19	d	203	CLA	CHD-C1D-C2D	2.04	129.75	125.48
19	h	209	CLA	CHD-C1D-C2D	2.04	129.75	125.48
19	o	310	CLA	C2C-C1C-NC	2.04	111.88	109.97
19	A	848	CLA	CHD-C1D-C2D	2.04	129.75	125.48
28	b	312	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
19	h	210	CLA	CHC-C4B-NB	-2.04	122.10	124.26
19	b	302	CLA	CHD-C1D-C2D	2.04	129.75	125.48
19	b	313	CLA	CHD-C1D-C2D	2.04	129.75	125.48
28	a	312	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
19	a	309	CLA	CHC-C4B-NB	-2.04	122.10	124.26
28	o	301	CHL	C2C-C3C-C4C	2.04	107.94	106.49
19	d	208	CLA	CHC-C1C-NC	2.03	127.29	124.20
19	a	303	CLA	CHD-C1D-C2D	2.03	129.75	125.48
19	k	306	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
19	m	305	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
19	A	852	CLA	C2C-C1C-NC	2.03	111.88	109.97
19	l	207	CLA	CHD-C1D-C2D	2.03	129.74	125.48
19	B	816	CLA	CHC-C4B-NB	-2.03	122.11	124.26
19	k	307	CLA	CHD-C1D-C2D	2.03	129.74	125.48
25	a	316	LMG	O6-C1-O1	-2.03	105.17	109.97
19	n	207	CLA	CHC-C4B-NB	-2.03	122.11	124.26
19	g	305	CLA	CHD-C4C-C3C	-2.03	121.86	124.84
19	a	304	CLA	C2C-C1C-NC	2.03	111.87	109.97
19	m	310	CLA	C2C-C1C-NC	2.03	111.87	109.97
19	o	308	CLA	C2C-C1C-NC	2.03	111.87	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	m	307	CLA	CHD-C1D-C2D	2.03	129.74	125.48
28	d	205	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
19	A	828	CLA	CHD-C1D-C2D	2.03	129.73	125.48
19	o	310	CLA	CHD-C1D-C2D	2.03	129.73	125.48
19	A	815	CLA	CHD-C1D-C2D	2.03	129.73	125.48
25	a	301	LMG	O2-C2-C1	-2.03	105.12	110.05
19	c	302	CLA	CHA-C1A-NA	-2.03	121.76	126.40
19	B	846	CLA	CHD-C1D-C2D	2.03	129.73	125.48
19	e	306	CLA	CHD-C1D-C2D	2.03	129.73	125.48
19	A	807	CLA	CHD-C1D-C2D	2.03	129.73	125.48
28	c	312	CHL	O2A-CGA-O1A	-2.03	118.48	123.59
19	h	212	CLA	C2C-C1C-NC	2.02	111.87	109.97
19	A	822	CLA	CHD-C1D-C2D	2.02	129.73	125.48
19	A	812	CLA	CHC-C4B-NB	-2.02	122.11	124.26
19	a	307	CLA	CHA-C1A-NA	-2.02	121.76	126.40
19	c	307	CLA	CHA-C1A-NA	-2.02	121.76	126.40
19	a	314	CLA	CHA-C1A-NA	-2.02	121.77	126.40
19	B	815	CLA	CHD-C1D-C2D	2.02	129.72	125.48
19	A	845	CLA	CHC-C4B-NB	-2.02	122.12	124.26
19	B	815	CLA	CHC-C4B-NB	-2.02	122.12	124.26
19	B	804	CLA	C1-C2-C3	-2.02	122.55	126.04
28	g	310	CHL	C2A-C3A-C4A	2.02	105.14	101.87
19	B	806	CLA	C2C-C1C-NC	2.02	111.87	109.97
22	m	312	DD6	O1-C20-C15	-2.02	57.29	58.96
19	d	211	CLA	CHA-C1A-NA	-2.02	121.77	126.40
19	l	201	CLA	CHA-C1A-NA	-2.02	121.77	126.40
28	a	311	CHL	O2A-CGA-O1A	-2.02	118.49	123.59
19	A	846	CLA	CHD-C1D-C2D	2.02	129.72	125.48
19	A	816	CLA	CHD-C1D-C2D	2.02	129.72	125.48
19	A	810	CLA	CHA-C1A-NA	-2.02	121.77	126.40
19	B	816	CLA	CHD-C1D-C2D	2.02	129.71	125.48
19	A	844	CLA	C2C-C1C-NC	2.02	111.86	109.97
19	j	302	CLA	CHA-C1A-NA	-2.02	121.78	126.40
19	A	815	CLA	CHC-C4B-NB	-2.02	122.12	124.26
19	A	842	CLA	CHD-C1D-C2D	2.02	129.71	125.48
22	m	312	DD6	C32-C31-C36	-2.02	119.79	122.63
19	A	850	CLA	CHD-C1D-C2D	2.02	129.71	125.48
19	j	308	CLA	CHD-C1D-C2D	2.02	129.71	125.48
19	e	305	CLA	C1-C2-C3	-2.02	123.49	126.75
19	A	814	CLA	CHD-C1D-C2D	2.02	129.71	125.48
19	a	309	CLA	C2C-C1C-NC	2.02	111.86	109.97
19	F	203	CLA	CHA-C1A-NA	-2.02	121.78	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	h	208	CLA	CHC-C4B-NB	-2.01	122.12	124.26
19	F	201	CLA	C2C-C1C-NC	2.01	111.86	109.97
19	B	814	CLA	CAA-C2A-C1A	-2.01	105.38	111.97
19	A	816	CLA	CHA-C1A-NA	-2.01	121.79	126.40
19	B	817	CLA	CHD-C1D-C2D	2.01	129.70	125.48
19	b	307	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	A	831	LHG	C11-C10-C9	-2.01	104.21	114.42
19	k	303	CLA	C2C-C1C-NC	2.01	111.86	109.97
19	n	207	CLA	CHD-C1D-C2D	2.01	129.70	125.48
19	A	820	CLA	CHD-C1D-C2D	2.01	129.70	125.48
19	h	213	CLA	CHD-C1D-C2D	2.01	129.70	125.48
19	i	310	CLA	CHD-C1D-C2D	2.01	129.70	125.48
19	d	206	CLA	CHA-C1A-NA	-2.01	121.79	126.40
19	A	808	CLA	CHC-C4B-NB	-2.01	122.13	124.26
19	g	305	CLA	CHC-C1C-NC	2.01	127.25	124.20
19	d	203	CLA	CHA-C1A-NA	-2.01	121.79	126.40
28	c	313	CHL	C3C-C4C-NC	-2.01	108.32	110.57
22	c	318	DD6	O1-C20-C15	-2.01	57.29	58.96
19	B	821	CLA	CHC-C4B-NB	-2.01	122.13	124.26
19	e	302	CLA	CHD-C1D-C2D	2.01	129.70	125.48
25	a	318	LMG	C6-C5-C4	-2.01	108.30	113.00
19	B	844	CLA	CHA-C1A-NA	-2.01	121.80	126.40
19	c	303	CLA	CHC-C4B-NB	-2.01	122.13	124.26
28	f	304	CHL	C3C-C4C-NC	-2.01	108.32	110.57
19	A	804	CLA	CHB-C4A-NA	2.01	127.29	124.51
19	f	306	CLA	CHD-C1D-C2D	2.01	129.69	125.48
19	n	205	CLA	CHD-C1D-C2D	2.01	129.69	125.48
19	k	310	CLA	CHA-C1A-NA	-2.01	121.80	126.40
19	g	305	CLA	CHC-C4B-NB	-2.01	122.13	124.26
19	m	304	CLA	CBA-CAA-C2A	2.01	119.78	113.86
19	F	204	CLA	CHC-C1C-C2C	-2.01	121.16	126.73
19	m	308	CLA	CHD-C1D-C2D	2.00	129.69	125.48
19	l	204	CLA	C2C-C1C-NC	2.00	111.85	109.97
19	k	303	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	b	313	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	F	201	CLA	CHD-C1D-C2D	2.00	129.68	125.48
19	k	306	CLA	CHD-C1D-C2D	2.00	129.68	125.48
19	B	845	CLA	CHB-C4A-NA	2.00	127.28	124.51
19	o	304	CLA	CHC-C1C-NC	2.00	127.24	124.20
19	B	830	CLA	CHC-C4B-NB	-2.00	122.14	124.26
19	B	845	CLA	CHD-C1D-C2D	2.00	129.68	125.48
19	b	305	CLA	CHB-C4A-NA	2.00	127.28	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	844	CLA	CHD-C1D-C2D	2.00	129.68	125.48
19	A	819	CLA	CHC-C1C-C2C	-2.00	121.17	126.73
19	B	818	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	g	304	CLA	CHC-C1C-NC	2.00	127.24	124.20
28	c	305	CHL	O1D-CGD-CBD	-2.00	120.39	124.48
19	B	817	CLA	CHC-C4B-NB	-2.00	122.14	124.26
19	o	309	CLA	CHD-C4C-C3C	-2.00	121.90	124.84

There are no chirality outliers.

All (2268) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	804	CLA	CHA-CBD-CGD-O2D
19	A	804	CLA	C14-C13-C15-C16
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	CHA-CBD-CGD-O1D
19	A	810	CLA	C4B-C3B-CAB-CBB
19	A	811	CLA	C1A-C2A-CAA-CBA
19	A	811	CLA	C3A-C2A-CAA-CBA
19	A	811	CLA	C2B-C3B-CAB-CBB
19	A	811	CLA	C4B-C3B-CAB-CBB
19	A	813	CLA	C1A-C2A-CAA-CBA
19	A	816	CLA	C1A-C2A-CAA-CBA
19	A	816	CLA	C3A-C2A-CAA-CBA
19	A	817	CLA	C3A-C2A-CAA-CBA
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	823	CLA	C2A-CAA-CBA-CGA
19	A	825	CLA	C2B-C3B-CAB-CBB
19	A	825	CLA	C4B-C3B-CAB-CBB
19	A	827	CLA	C2-C3-C5-C6
19	A	828	CLA	CHA-CBD-CGD-O1D
19	A	828	CLA	CHA-CBD-CGD-O2D
19	A	839	CLA	CHA-CBD-CGD-O1D
19	A	839	CLA	CHA-CBD-CGD-O2D
19	A	840	CLA	O2A-C1-C2-C3
19	A	842	CLA	C1A-C2A-CAA-CBA
19	A	842	CLA	CBD-CGD-O2D-CED
19	A	842	CLA	C11-C10-C8-C9
19	A	843	CLA	C11-C10-C8-C9
19	A	846	CLA	CHA-CBD-CGD-O1D
19	A	847	CLA	C1A-C2A-CAA-CBA
19	A	847	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A	847	CLA	C4B-C3B-CAB-CBB
19	A	848	CLA	C2B-C3B-CAB-CBB
19	A	848	CLA	C4B-C3B-CAB-CBB
19	A	848	CLA	CHA-CBD-CGD-O1D
19	A	848	CLA	CHA-CBD-CGD-O2D
19	A	849	CLA	C2B-C3B-CAB-CBB
19	A	849	CLA	C4B-C3B-CAB-CBB
19	A	852	CLA	C2B-C3B-CAB-CBB
19	A	853	CLA	CHA-CBD-CGD-O1D
19	A	853	CLA	CHA-CBD-CGD-O2D
19	A	853	CLA	CAD-CBD-CGD-O1D
19	B	801	CLA	C2B-C3B-CAB-CBB
19	B	801	CLA	C2-C3-C5-C6
19	B	801	CLA	C4-C3-C5-C6
19	B	803	CLA	CHA-CBD-CGD-O1D
19	B	803	CLA	CHA-CBD-CGD-O2D
19	B	807	CLA	C2B-C3B-CAB-CBB
19	B	807	CLA	C4B-C3B-CAB-CBB
19	B	808	CLA	C2B-C3B-CAB-CBB
19	B	808	CLA	C4B-C3B-CAB-CBB
19	B	808	CLA	CHA-CBD-CGD-O1D
19	B	808	CLA	CHA-CBD-CGD-O2D
19	B	809	CLA	C1A-C2A-CAA-CBA
19	B	811	CLA	C2B-C3B-CAB-CBB
19	B	811	CLA	C4B-C3B-CAB-CBB
19	B	814	CLA	C2B-C3B-CAB-CBB
19	B	814	CLA	C4B-C3B-CAB-CBB
19	B	815	CLA	C3A-C2A-CAA-CBA
19	B	816	CLA	CHA-CBD-CGD-O1D
19	B	816	CLA	CHA-CBD-CGD-O2D
19	B	817	CLA	C1A-C2A-CAA-CBA
19	B	817	CLA	C2B-C3B-CAB-CBB
19	B	817	CLA	C4B-C3B-CAB-CBB
19	B	818	CLA	CHA-CBD-CGD-O1D
19	B	818	CLA	CHA-CBD-CGD-O2D
19	B	820	CLA	C2-C3-C5-C6
19	B	821	CLA	C2B-C3B-CAB-CBB
19	B	821	CLA	C4B-C3B-CAB-CBB
19	B	830	CLA	C1A-C2A-CAA-CBA
19	B	832	CLA	C2B-C3B-CAB-CBB
19	B	832	CLA	C4B-C3B-CAB-CBB
19	B	833	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B	833	CLA	CHA-CBD-CGD-O2D
19	B	837	CLA	C3A-C2A-CAA-CBA
19	B	838	CLA	C2B-C3B-CAB-CBB
19	B	838	CLA	C4B-C3B-CAB-CBB
19	B	839	CLA	C1A-C2A-CAA-CBA
19	B	840	CLA	C1A-C2A-CAA-CBA
19	B	841	CLA	C2B-C3B-CAB-CBB
19	B	841	CLA	C4B-C3B-CAB-CBB
19	B	842	CLA	C1A-C2A-CAA-CBA
19	B	842	CLA	C3A-C2A-CAA-CBA
19	B	844	CLA	C1A-C2A-CAA-CBA
19	B	845	CLA	CHA-CBD-CGD-O1D
19	B	845	CLA	CHA-CBD-CGD-O2D
19	B	847	CLA	CHA-CBD-CGD-O1D
19	B	847	CLA	CHA-CBD-CGD-O2D
19	B	848	CLA	C1A-C2A-CAA-CBA
19	B	848	CLA	C3A-C2A-CAA-CBA
19	B	849	CLA	C1A-C2A-CAA-CBA
19	B	849	CLA	CBD-CGD-O2D-CED
19	B	849	CLA	C2-C3-C5-C6
19	B	849	CLA	C4-C3-C5-C6
19	D	301	CLA	C4-C3-C5-C6
19	F	203	CLA	C1A-C2A-CAA-CBA
19	F	203	CLA	C3A-C2A-CAA-CBA
19	F	203	CLA	C2B-C3B-CAB-CBB
19	F	203	CLA	C4B-C3B-CAB-CBB
19	F	203	CLA	CHA-CBD-CGD-O1D
19	F	203	CLA	CHA-CBD-CGD-O2D
19	F	203	CLA	CAD-CBD-CGD-O1D
19	F	203	CLA	C2-C3-C5-C6
19	F	203	CLA	C4-C3-C5-C6
19	F	204	CLA	C4B-C3B-CAB-CBB
19	a	302	CLA	C1A-C2A-CAA-CBA
19	a	302	CLA	C3A-C2A-CAA-CBA
19	a	302	CLA	CHA-CBD-CGD-O1D
19	a	302	CLA	CHA-CBD-CGD-O2D
19	a	303	CLA	C3A-C2A-CAA-CBA
19	a	305	CLA	C2B-C3B-CAB-CBB
19	a	305	CLA	C4B-C3B-CAB-CBB
19	a	306	CLA	C1A-C2A-CAA-CBA
19	a	306	CLA	C3A-C2A-CAA-CBA
19	a	306	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	a	306	CLA	C4B-C3B-CAB-CBB
19	a	306	CLA	C2-C3-C5-C6
19	a	306	CLA	C4-C3-C5-C6
19	a	308	CLA	CHA-CBD-CGD-O1D
19	a	308	CLA	CHA-CBD-CGD-O2D
19	a	314	CLA	C1A-C2A-CAA-CBA
19	a	314	CLA	CBA-CGA-O2A-C1
19	a	314	CLA	O1A-CGA-O2A-C1
19	a	314	CLA	CBD-CGD-O2D-CED
19	b	304	CLA	CBD-CGD-O2D-CED
19	b	304	CLA	C2-C3-C5-C6
19	b	304	CLA	C4-C3-C5-C6
19	b	305	CLA	C2B-C3B-CAB-CBB
19	b	305	CLA	C4B-C3B-CAB-CBB
19	b	306	CLA	C1A-C2A-CAA-CBA
19	b	306	CLA	CHA-CBD-CGD-O1D
19	b	306	CLA	CHA-CBD-CGD-O2D
19	b	306	CLA	C2-C3-C5-C6
19	b	306	CLA	C4-C3-C5-C6
19	b	313	CLA	C3A-C2A-CAA-CBA
19	b	315	CLA	C1A-C2A-CAA-CBA
19	c	302	CLA	C1A-C2A-CAA-CBA
19	c	303	CLA	C2B-C3B-CAB-CBB
19	c	303	CLA	C4B-C3B-CAB-CBB
19	c	306	CLA	C2-C3-C5-C6
19	c	306	CLA	C4-C3-C5-C6
19	c	307	CLA	C1A-C2A-CAA-CBA
19	c	307	CLA	C3A-C2A-CAA-CBA
19	c	309	CLA	CHA-CBD-CGD-O1D
19	c	309	CLA	CHA-CBD-CGD-O2D
19	c	310	CLA	CHA-CBD-CGD-O1D
19	c	310	CLA	CHA-CBD-CGD-O2D
19	c	311	CLA	CHA-CBD-CGD-O1D
19	c	314	CLA	C1A-C2A-CAA-CBA
19	c	316	CLA	C2A-CAA-CBA-CGA
19	d	203	CLA	C1A-C2A-CAA-CBA
19	d	203	CLA	C3A-C2A-CAA-CBA
19	d	206	CLA	C2B-C3B-CAB-CBB
19	d	206	CLA	C4B-C3B-CAB-CBB
19	d	208	CLA	C6-C7-C8-C9
19	d	210	CLA	C2B-C3B-CAB-CBB
19	d	210	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	d	210	CLA	C2-C3-C5-C6
19	d	210	CLA	C4-C3-C5-C6
19	e	302	CLA	CHA-CBD-CGD-O1D
19	e	302	CLA	CHA-CBD-CGD-O2D
19	e	308	CLA	C2-C3-C5-C6
19	e	308	CLA	C4-C3-C5-C6
19	e	310	CLA	C2B-C3B-CAB-CBB
19	e	310	CLA	C4B-C3B-CAB-CBB
19	f	308	CLA	C2-C3-C5-C6
19	f	308	CLA	C4-C3-C5-C6
19	f	311	CLA	C1A-C2A-CAA-CBA
19	f	314	CLA	C1A-C2A-CAA-CBA
19	f	314	CLA	C4-C3-C5-C6
19	g	301	CLA	CBD-CGD-O2D-CED
19	g	302	CLA	C2B-C3B-CAB-CBB
19	g	302	CLA	C4B-C3B-CAB-CBB
19	g	304	CLA	CHA-CBD-CGD-O1D
19	h	203	CLA	C4B-C3B-CAB-CBB
19	h	207	CLA	C3A-C2A-CAA-CBA
19	h	213	CLA	C1A-C2A-CAA-CBA
19	i	303	CLA	C2B-C3B-CAB-CBB
19	i	303	CLA	C4B-C3B-CAB-CBB
19	i	307	CLA	C2B-C3B-CAB-CBB
19	i	307	CLA	C4B-C3B-CAB-CBB
19	i	308	CLA	CHA-CBD-CGD-O1D
19	i	308	CLA	CHA-CBD-CGD-O2D
19	i	308	CLA	CAD-CBD-CGD-O1D
19	i	308	CLA	C4-C3-C5-C6
19	i	310	CLA	C1A-C2A-CAA-CBA
19	i	310	CLA	C2B-C3B-CAB-CBB
19	i	310	CLA	C4B-C3B-CAB-CBB
19	i	313	CLA	C1A-C2A-CAA-CBA
19	i	313	CLA	C2-C3-C5-C6
19	i	313	CLA	C4-C3-C5-C6
19	j	303	CLA	C4B-C3B-CAB-CBB
19	j	304	CLA	CBD-CGD-O2D-CED
19	j	304	CLA	C11-C10-C8-C9
19	j	305	CLA	C3A-C2A-CAA-CBA
19	j	310	CLA	C2B-C3B-CAB-CBB
19	j	310	CLA	C4B-C3B-CAB-CBB
19	j	311	CLA	C1A-C2A-CAA-CBA
19	j	313	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	k	302	CLA	C1A-C2A-CAA-CBA
19	k	302	CLA	C2B-C3B-CAB-CBB
19	k	302	CLA	C4B-C3B-CAB-CBB
19	k	310	CLA	O2A-C1-C2-C3
19	l	203	CLA	C2B-C3B-CAB-CBB
19	l	203	CLA	C4B-C3B-CAB-CBB
19	l	206	CLA	C2B-C3B-CAB-CBB
19	l	206	CLA	C4B-C3B-CAB-CBB
19	l	206	CLA	CBD-CGD-O2D-CED
19	l	209	CLA	C1A-C2A-CAA-CBA
19	l	209	CLA	C3A-C2A-CAA-CBA
19	m	302	CLA	C1A-C2A-CAA-CBA
19	m	302	CLA	C3A-C2A-CAA-CBA
19	m	302	CLA	C2B-C3B-CAB-CBB
19	m	302	CLA	C4B-C3B-CAB-CBB
19	m	302	CLA	CHA-CBD-CGD-O1D
19	m	302	CLA	CHA-CBD-CGD-O2D
19	m	304	CLA	C1A-C2A-CAA-CBA
19	m	304	CLA	C4B-C3B-CAB-CBB
19	m	305	CLA	C2B-C3B-CAB-CBB
19	m	305	CLA	C4B-C3B-CAB-CBB
19	m	307	CLA	C2-C3-C5-C6
19	m	307	CLA	C4-C3-C5-C6
19	m	308	CLA	C2B-C3B-CAB-CBB
19	m	308	CLA	C4B-C3B-CAB-CBB
19	m	308	CLA	CHA-CBD-CGD-O1D
19	m	308	CLA	CHA-CBD-CGD-O2D
19	m	309	CLA	C1A-C2A-CAA-CBA
19	m	309	CLA	C3A-C2A-CAA-CBA
19	m	309	CLA	CBD-CGD-O2D-CED
19	m	311	CLA	C2A-CAA-CBA-CGA
19	n	201	CLA	CHA-CBD-CGD-O2D
19	n	202	CLA	C3A-C2A-CAA-CBA
19	n	202	CLA	C2A-CAA-CBA-CGA
19	n	204	CLA	C1A-C2A-CAA-CBA
19	n	205	CLA	C2-C3-C5-C6
19	n	205	CLA	C4-C3-C5-C6
19	n	208	CLA	C2B-C3B-CAB-CBB
19	n	208	CLA	C4B-C3B-CAB-CBB
19	n	208	CLA	CHA-CBD-CGD-O1D
19	n	208	CLA	CAD-CBD-CGD-O1D
19	n	208	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	n	208	CLA	CBD-CGD-O2D-CED
19	n	209	CLA	C1A-C2A-CAA-CBA
19	n	209	CLA	C3A-C2A-CAA-CBA
19	n	209	CLA	C2B-C3B-CAB-CBB
19	n	209	CLA	C4B-C3B-CAB-CBB
19	o	302	CLA	C1A-C2A-CAA-CBA
19	o	302	CLA	C3A-C2A-CAA-CBA
19	o	302	CLA	C2B-C3B-CAB-CBB
19	o	302	CLA	C4B-C3B-CAB-CBB
19	o	302	CLA	C2-C3-C5-C6
19	o	302	CLA	C4-C3-C5-C6
19	o	303	CLA	C2B-C3B-CAB-CBB
19	o	303	CLA	C4B-C3B-CAB-CBB
19	o	304	CLA	C3A-C2A-CAA-CBA
19	o	304	CLA	C2B-C3B-CAB-CBB
19	o	304	CLA	C4B-C3B-CAB-CBB
19	o	304	CLA	CHA-CBD-CGD-O1D
19	o	304	CLA	CHA-CBD-CGD-O2D
19	o	304	CLA	CBD-CGD-O2D-CED
19	o	304	CLA	C2-C3-C5-C6
19	o	304	CLA	C4-C3-C5-C6
19	o	305	CLA	C1A-C2A-CAA-CBA
19	o	305	CLA	C3A-C2A-CAA-CBA
19	o	305	CLA	C2B-C3B-CAB-CBB
19	o	305	CLA	C4B-C3B-CAB-CBB
19	o	306	CLA	C1A-C2A-CAA-CBA
19	o	308	CLA	C2B-C3B-CAB-CBB
19	o	308	CLA	C4B-C3B-CAB-CBB
19	o	309	CLA	CBA-CGA-O2A-C1
19	o	309	CLA	O1A-CGA-O2A-C1
19	o	309	CLA	CBD-CGD-O2D-CED
19	o	310	CLA	C2B-C3B-CAB-CBB
19	o	310	CLA	C4B-C3B-CAB-CBB
19	o	312	CLA	C1A-C2A-CAA-CBA
21	A	831	LHG	C4-O6-P-O4
22	J	801	DD6	C10-C11-C13-C14
22	J	801	DD6	C12-C11-C13-C14
22	i	315	DD6	C27-C29-C30-C31
22	l	210	DD6	C13-C14-C15-O1
22	n	210	DD6	C12-C11-C13-C14
23	A	835	BCR	C23-C24-C25-C30
23	A	836	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	A	836	BCR	C23-C24-C25-C30
23	A	837	BCR	C7-C8-C9-C10
23	A	837	BCR	C7-C8-C9-C34
23	B	826	BCR	C5-C6-C7-C8
23	B	831	BCR	C21-C22-C23-C24
23	B	831	BCR	C37-C22-C23-C24
23	B	850	BCR	C23-C24-C25-C26
23	B	850	BCR	C23-C24-C25-C30
23	M	801	BCR	C7-C8-C9-C10
23	M	801	BCR	C7-C8-C9-C34
25	A	851	LMG	C2-C1-O1-C7
25	A	851	LMG	O6-C1-O1-C7
25	a	318	LMG	C11-C10-O7-C8
25	c	320	LMG	C2-C1-O1-C7
25	c	320	LMG	O6-C1-O1-C7
25	d	213	LMG	O9-C10-O7-C8
25	e	312	LMG	C2-C1-O1-C7
25	e	312	LMG	O6-C1-O1-C7
25	g	312	LMG	O6-C1-O1-C7
25	g	312	LMG	C8-C7-O1-C1
25	g	316	LMG	C9-C8-O7-C10
25	h	216	LMG	C2-C1-O1-C7
25	h	216	LMG	C11-C10-O7-C8
25	i	316	LMG	O9-C10-O7-C8
25	i	316	LMG	C11-C10-O7-C8
25	j	314	LMG	O6-C1-O1-C7
25	j	314	LMG	C8-C7-O1-C1
27	B	829	DGD	C2B-C1B-O2G-C2G
28	a	311	CHL	C1C-C2C-CMC-OMC
28	a	312	CHL	C2B-C3B-CAB-CBB
28	a	312	CHL	C4B-C3B-CAB-CBB
28	a	312	CHL	C1C-C2C-CMC-OMC
28	a	312	CHL	CHA-CBD-CGD-O2D
28	a	313	CHL	C1C-C2C-CMC-OMC
28	a	313	CHL	C3C-C2C-CMC-OMC
28	a	315	CHL	C1A-C2A-CAA-CBA
28	a	315	CHL	C3A-C2A-CAA-CBA
28	a	315	CHL	C1C-C2C-CMC-OMC
28	a	315	CHL	C3C-C2C-CMC-OMC
28	a	315	CHL	CHA-CBD-CGD-O1D
28	a	315	CHL	CBD-CGD-O2D-CED
28	b	301	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
28	b	301	CHL	C3C-C2C-CMC-OMC
28	b	301	CHL	O2A-C1-C2-C3
28	b	301	CHL	C1-C2-C3-C4
28	b	301	CHL	C4-C3-C5-C6
28	b	310	CHL	C1C-C2C-CMC-OMC
28	b	312	CHL	C2A-CAA-CBA-CGA
28	b	312	CHL	C3C-C2C-CMC-OMC
28	b	312	CHL	C3-C5-C6-C7
28	b	314	CHL	C1C-C2C-CMC-OMC
28	b	314	CHL	C3C-C2C-CMC-OMC
28	b	314	CHL	C2-C3-C5-C6
28	c	305	CHL	C1C-C2C-CMC-OMC
28	c	305	CHL	C2-C3-C5-C6
28	c	305	CHL	C4-C3-C5-C6
28	c	312	CHL	C1C-C2C-CMC-OMC
28	c	312	CHL	C3C-C2C-CMC-OMC
28	c	312	CHL	C1-C2-C3-C4
28	c	312	CHL	C4-C3-C5-C6
28	c	313	CHL	C1C-C2C-CMC-OMC
28	c	313	CHL	O2A-C1-C2-C3
28	d	202	CHL	C1A-C2A-CAA-CBA
28	d	202	CHL	C1C-C2C-CMC-OMC
28	d	202	CHL	C3C-C2C-CMC-OMC
28	d	202	CHL	CBD-CGD-O2D-CED
28	d	205	CHL	C3A-C2A-CAA-CBA
28	d	205	CHL	C1C-C2C-CMC-OMC
28	d	205	CHL	C3C-C2C-CMC-OMC
28	d	205	CHL	C1-C2-C3-C4
28	d	205	CHL	C4-C3-C5-C6
28	e	301	CHL	C1A-C2A-CAA-CBA
28	e	301	CHL	C2B-C3B-CAB-CBB
28	e	301	CHL	C4B-C3B-CAB-CBB
28	e	301	CHL	CHA-CBD-CGD-O1D
28	e	301	CHL	O2A-C1-C2-C3
28	e	301	CHL	C1-C2-C3-C4
28	e	301	CHL	C1-C2-C3-C5
28	e	304	CHL	C1A-C2A-CAA-CBA
28	e	304	CHL	C3A-C2A-CAA-CBA
28	e	304	CHL	C1C-C2C-CMC-OMC
28	e	304	CHL	C1-C2-C3-C4
28	e	304	CHL	C1-C2-C3-C5
28	f	301	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
28	f	301	CHL	C3C-C2C-CMC-OMC
28	f	304	CHL	C1C-C2C-CMC-OMC
28	f	304	CHL	C4-C3-C5-C6
28	g	303	CHL	C2B-C3B-CAB-CBB
28	g	303	CHL	C4B-C3B-CAB-CBB
28	g	303	CHL	C1C-C2C-CMC-OMC
28	g	303	CHL	C3C-C2C-CMC-OMC
28	g	303	CHL	C1-C2-C3-C4
28	g	306	CHL	O1A-CGA-O2A-C1
28	g	306	CHL	C1C-C2C-CMC-OMC
28	g	306	CHL	C3C-C2C-CMC-OMC
28	g	306	CHL	C1-C2-C3-C4
28	g	310	CHL	C1A-C2A-CAA-CBA
28	g	310	CHL	C3A-C2A-CAA-CBA
28	g	310	CHL	C1C-C2C-CMC-OMC
28	g	310	CHL	C3C-C2C-CMC-OMC
28	g	310	CHL	O2A-C1-C2-C3
28	g	310	CHL	C1-C2-C3-C4
28	g	310	CHL	C1-C2-C3-C5
28	h	202	CHL	C1A-C2A-CAA-CBA
28	h	202	CHL	C2B-C3B-CAB-CBB
28	h	202	CHL	C4B-C3B-CAB-CBB
28	h	202	CHL	C1C-C2C-CMC-OMC
28	h	202	CHL	C3C-C2C-CMC-OMC
28	h	202	CHL	CBD-CGD-O2D-CED
28	i	301	CHL	C1A-C2A-CAA-CBA
28	i	301	CHL	C1C-C2C-CMC-OMC
28	i	301	CHL	C3C-C2C-CMC-OMC
28	i	301	CHL	CHA-CBD-CGD-O1D
28	i	304	CHL	C1C-C2C-CMC-OMC
28	i	304	CHL	C3C-C2C-CMC-OMC
28	k	301	CHL	C1A-C2A-CAA-CBA
28	k	301	CHL	C3A-C2A-CAA-CBA
28	k	301	CHL	C1C-C2C-CMC-OMC
28	k	301	CHL	C3C-C2C-CMC-OMC
28	m	301	CHL	C1A-C2A-CAA-CBA
28	m	301	CHL	C1C-C2C-CMC-OMC
28	m	301	CHL	C3C-C2C-CMC-OMC
28	m	301	CHL	CHA-CBD-CGD-O1D
28	m	301	CHL	CHA-CBD-CGD-O2D
28	m	301	CHL	CBD-CGD-O2D-CED
28	o	301	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	o	301	CHL	C2B-C3B-CAB-CBB
28	o	301	CHL	C4B-C3B-CAB-CBB
28	o	301	CHL	C1C-C2C-CMC-OMC
28	o	301	CHL	C3C-C2C-CMC-OMC
28	o	301	CHL	CHA-CBD-CGD-O1D
28	o	301	CHL	CBD-CGD-O2D-CED
29	a	317	NEX	C9-C10-C11-C12
29	a	317	NEX	C11-C12-C13-C14
19	j	304	CLA	O1D-CGD-O2D-CED
19	o	304	CLA	O1D-CGD-O2D-CED
28	k	301	CHL	O1D-CGD-O2D-CED
24	A	838	LMU	C3'-C4'-O1B-C1B
19	B	849	CLA	O1D-CGD-O2D-CED
19	n	206	CLA	O1D-CGD-O2D-CED
28	m	301	CHL	O1D-CGD-O2D-CED
19	B	841	CLA	CBD-CGD-O2D-CED
19	i	310	CLA	CBD-CGD-O2D-CED
19	l	201	CLA	CBD-CGD-O2D-CED
19	m	302	CLA	CBD-CGD-O2D-CED
19	n	206	CLA	CBD-CGD-O2D-CED
28	a	312	CHL	CBD-CGD-O2D-CED
28	b	311	CHL	CBD-CGD-O2D-CED
28	b	312	CHL	CBD-CGD-O2D-CED
28	k	301	CHL	CBD-CGD-O2D-CED
25	A	851	LMG	O10-C28-O8-C9
25	h	216	LMG	O10-C28-O8-C9
19	b	304	CLA	O1D-CGD-O2D-CED
19	a	314	CLA	O1D-CGD-O2D-CED
19	g	301	CLA	O1D-CGD-O2D-CED
19	l	206	CLA	O1D-CGD-O2D-CED
19	m	309	CLA	O1D-CGD-O2D-CED
19	o	309	CLA	O1D-CGD-O2D-CED
28	d	202	CHL	O1D-CGD-O2D-CED
28	g	306	CHL	CBA-CGA-O2A-C1
19	a	302	CLA	CBD-CGD-O2D-CED
19	e	310	CLA	CBD-CGD-O2D-CED
19	n	202	CLA	CBD-CGD-O2D-CED
19	n	209	CLA	CBD-CGD-O2D-CED
28	b	301	CHL	CBD-CGD-O2D-CED
28	c	313	CHL	CBD-CGD-O2D-CED
28	f	301	CHL	CBD-CGD-O2D-CED
19	a	302	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	i	310	CLA	O1A-CGA-O2A-C1
25	a	301	LMG	O10-C28-O8-C9
25	a	318	LMG	O10-C28-O8-C9
25	c	320	LMG	O10-C28-O8-C9
25	e	312	LMG	O10-C28-O8-C9
25	g	312	LMG	O10-C28-O8-C9
28	b	301	CHL	O1A-CGA-O2A-C1
19	A	842	CLA	O1D-CGD-O2D-CED
28	a	312	CHL	O1D-CGD-O2D-CED
28	b	311	CHL	C4C-C3C-CAC-CBC
19	n	208	CLA	O1D-CGD-O2D-CED
28	a	313	CHL	O1D-CGD-O2D-CED
28	f	304	CHL	O1D-CGD-O2D-CED
19	j	305	CLA	CBD-CGD-O2D-CED
19	k	304	CLA	CBD-CGD-O2D-CED
28	b	311	CHL	O1D-CGD-O2D-CED
25	a	301	LMG	O9-C10-O7-C8
25	a	318	LMG	O9-C10-O7-C8
25	g	313	LMG	O9-C10-O7-C8
25	g	316	LMG	O9-C10-O7-C8
25	h	216	LMG	O9-C10-O7-C8
27	B	829	DGD	O1B-C1B-O2G-C2G
28	m	301	CHL	O1A-CGA-O2A-C1
28	b	311	CHL	C2C-C3C-CAC-CBC
19	A	817	CLA	C3-C5-C6-C7
19	B	807	CLA	C3-C5-C6-C7
19	B	815	CLA	C3-C5-C6-C7
19	B	833	CLA	C3-C5-C6-C7
19	a	307	CLA	C3-C5-C6-C7
19	c	307	CLA	C3-C5-C6-C7
19	e	306	CLA	C3-C5-C6-C7
19	l	203	CLA	C3-C5-C6-C7
19	l	204	CLA	C3-C5-C6-C7
19	o	302	CLA	C3-C5-C6-C7
19	a	302	CLA	CBA-CGA-O2A-C1
19	i	310	CLA	CBA-CGA-O2A-C1
19	j	304	CLA	CBA-CGA-O2A-C1
25	a	301	LMG	C29-C28-O8-C9
25	e	312	LMG	C29-C28-O8-C9
25	h	216	LMG	C29-C28-O8-C9
28	b	301	CHL	CBA-CGA-O2A-C1
28	c	312	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	f	301	CHL	CBA-CGA-O2A-C1
25	a	316	LMG	C29-C28-O8-C9
25	d	213	LMG	C11-C10-O7-C8
19	m	302	CLA	O1D-CGD-O2D-CED
19	a	306	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	C4-C3-C5-C6
19	B	835	CLA	C4-C3-C5-C6
19	e	311	CLA	C4-C3-C5-C6
19	h	201	CLA	C4-C3-C5-C6
28	i	304	CHL	C4-C3-C5-C6
19	f	314	CLA	C2-C3-C5-C6
19	h	201	CLA	C2-C3-C5-C6
28	c	312	CHL	C2-C3-C5-C6
28	a	313	CHL	CBD-CGD-O2D-CED
19	a	303	CLA	C2A-CAA-CBA-CGA
19	e	311	CLA	C2A-CAA-CBA-CGA
19	g	305	CLA	C2A-CAA-CBA-CGA
19	i	302	CLA	C2A-CAA-CBA-CGA
19	j	306	CLA	C2A-CAA-CBA-CGA
19	o	306	CLA	C2A-CAA-CBA-CGA
28	b	310	CHL	C2A-CAA-CBA-CGA
28	k	301	CHL	C2A-CAA-CBA-CGA
28	f	301	CHL	O1A-CGA-O2A-C1
19	B	810	CLA	C3-C5-C6-C7
19	F	202	CLA	C3-C5-C6-C7
19	b	306	CLA	C3-C5-C6-C7
28	i	304	CHL	C3-C5-C6-C7
19	B	835	CLA	CBA-CGA-O2A-C1
19	n	206	CLA	CBA-CGA-O2A-C1
25	A	851	LMG	C29-C28-O8-C9
25	a	318	LMG	C29-C28-O8-C9
25	c	320	LMG	C29-C28-O8-C9
25	g	312	LMG	C29-C28-O8-C9
25	g	313	LMG	C29-C28-O8-C9
25	j	314	LMG	C29-C28-O8-C9
28	a	315	CHL	CBA-CGA-O2A-C1
28	m	301	CHL	CBA-CGA-O2A-C1
25	A	851	LMG	O6-C5-C6-O5
25	d	213	LMG	O6-C5-C6-O5
25	a	301	LMG	C4-C5-C6-O5
28	h	202	CHL	O1D-CGD-O2D-CED
28	c	312	CHL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
19	B	841	CLA	O1D-CGD-O2D-CED
19	i	310	CLA	O1D-CGD-O2D-CED
19	j	304	CLA	O1A-CGA-O2A-C1
19	n	206	CLA	O1A-CGA-O2A-C1
25	g	316	LMG	O10-C28-O8-C9
28	a	315	CHL	O1A-CGA-O2A-C1
28	c	312	CHL	O1A-CGA-O2A-C1
25	a	316	LMG	O6-C5-C6-O5
19	b	315	CLA	CBD-CGD-O2D-CED
19	d	208	CLA	CBD-CGD-O2D-CED
19	o	305	CLA	CBD-CGD-O2D-CED
28	f	304	CHL	CBD-CGD-O2D-CED
28	g	306	CHL	CBD-CGD-O2D-CED
19	a	309	CLA	C3-C5-C6-C7
19	j	302	CLA	C3-C5-C6-C7
19	j	304	CLA	C3-C5-C6-C7
19	k	304	CLA	C3-C5-C6-C7
19	o	304	CLA	C3-C5-C6-C7
28	c	312	CHL	C3-C5-C6-C7
21	A	831	LHG	C24-C23-O8-C6
25	g	316	LMG	C29-C28-O8-C9
19	n	208	CLA	O1A-CGA-O2A-C1
25	g	313	LMG	O10-C28-O8-C9
27	B	829	DGD	C4E-C5E-C6E-O5E
28	o	301	CHL	O1D-CGD-O2D-CED
25	a	301	LMG	C11-C10-O7-C8
25	a	301	LMG	O6-C5-C6-O5
25	A	851	LMG	C4-C5-C6-O5
19	A	806	CLA	C3-C5-C6-C7
19	A	813	CLA	C3-C5-C6-C7
19	A	816	CLA	C3-C5-C6-C7
19	B	820	CLA	C3-C5-C6-C7
19	B	839	CLA	C3-C5-C6-C7
28	b	301	CHL	C3-C5-C6-C7
19	n	208	CLA	CBA-CGA-O2A-C1
28	a	313	CHL	CBA-CGA-O2A-C1
19	l	201	CLA	O1D-CGD-O2D-CED
27	B	829	DGD	O6E-C5E-C6E-O5E
25	d	213	LMG	C4-C5-C6-O5
19	a	306	CLA	C3-C5-C6-C7
19	B	821	CLA	C4-C3-C5-C6
19	B	821	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	D	301	CLA	C2-C3-C5-C6
19	o	302	CLA	CBD-CGD-O2D-CED
19	j	305	CLA	C2A-CAA-CBA-CGA
19	o	304	CLA	C2A-CAA-CBA-CGA
28	c	312	CHL	C2A-CAA-CBA-CGA
28	d	205	CHL	C2A-CAA-CBA-CGA
25	b	316	LMG	O6-C1-O1-C7
19	a	302	CLA	O1D-CGD-O2D-CED
28	c	313	CHL	O1D-CGD-O2D-CED
28	i	301	CHL	O1D-CGD-O2D-CED
28	b	314	CHL	CBD-CGD-O2D-CED
25	g	316	LMG	O6-C5-C6-O5
19	B	835	CLA	O1A-CGA-O2A-C1
19	i	309	CLA	C3-C5-C6-C7
19	k	305	CLA	C3-C5-C6-C7
19	n	209	CLA	O1D-CGD-O2D-CED
28	a	315	CHL	O1D-CGD-O2D-CED
19	A	822	CLA	CBA-CGA-O2A-C1
19	B	807	CLA	CBA-CGA-O2A-C1
19	B	837	CLA	CBA-CGA-O2A-C1
19	B	849	CLA	CBA-CGA-O2A-C1
19	o	304	CLA	CBA-CGA-O2A-C1
28	a	311	CHL	CBA-CGA-O2A-C1
28	d	202	CHL	CBA-CGA-O2A-C1
28	g	310	CHL	CBA-CGA-O2A-C1
28	k	301	CHL	CBA-CGA-O2A-C1
19	A	816	CLA	C8-C10-C11-C12
19	o	302	CLA	C5-C6-C7-C8
24	c	301	LMU	C3'-C4'-O1B-C1B
19	d	204	CLA	C3-C5-C6-C7
25	b	316	LMG	C2-C1-O1-C7
25	j	314	LMG	C2-C1-O1-C7
25	a	316	LMG	O10-C28-O8-C9
25	g	316	LMG	C4-C5-C6-O5
19	B	835	CLA	C2-C3-C5-C6
19	e	311	CLA	C2-C3-C5-C6
19	A	807	CLA	C11-C10-C8-C9
19	A	813	CLA	C11-C10-C8-C9
19	B	808	CLA	C14-C13-C15-C16
19	B	818	CLA	C14-C13-C15-C16
19	B	833	CLA	C6-C7-C8-C9
19	B	849	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	d	211	CLA	C11-C10-C8-C9
19	e	307	CLA	C6-C7-C8-C9
19	j	304	CLA	C6-C7-C8-C9
19	l	203	CLA	C11-C10-C8-C9
20	A	830	PQN	C19-C18-C20-C21
28	c	305	CHL	C6-C7-C8-C9
19	A	819	CLA	C5-C6-C7-C8
19	A	842	CLA	C5-C6-C7-C8
19	l	201	CLA	C2A-CAA-CBA-CGA
19	m	310	CLA	C2A-CAA-CBA-CGA
28	f	304	CHL	C2A-CAA-CBA-CGA
22	A	832	DD6	C12-C11-C13-C14
22	J	802	DD6	C7-C6-C8-C9
22	b	317	DD6	C12-C11-C13-C14
23	B	826	BCR	C7-C8-C9-C34
23	B	831	BCR	C7-C8-C9-C34
23	B	850	BCR	C37-C22-C23-C24
29	a	317	NEX	C11-C12-C13-C20
22	A	832	DD6	C10-C11-C13-C14
22	b	317	DD6	C10-C11-C13-C14
23	B	850	BCR	C21-C22-C23-C24
25	a	318	LMG	C10-C11-C12-C13
19	o	304	CLA	O1A-CGA-O2A-C1
21	A	831	LHG	O10-C23-O8-C6
25	j	314	LMG	O10-C28-O8-C9
28	d	205	CHL	O1A-CGA-O2A-C1
19	A	824	CLA	C8-C10-C11-C12
19	A	840	CLA	C10-C11-C12-C13
19	B	805	CLA	C15-C16-C17-C18
19	e	307	CLA	C8-C10-C11-C12
19	f	307	CLA	C3-C5-C6-C7
19	m	309	CLA	CBA-CGA-O2A-C1
19	A	803	CLA	C5-C6-C7-C8
19	B	822	CLA	C15-C16-C17-C18
19	e	310	CLA	C5-C6-C7-C8
19	h	201	CLA	C5-C6-C7-C8
19	j	313	CLA	C5-C6-C7-C8
19	n	205	CLA	C10-C11-C12-C13
19	B	837	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	C15-C16-C17-C18
19	A	850	CLA	C15-C16-C17-C18
19	B	801	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	B	839	CLA	C8-C10-C11-C12
19	d	208	CLA	C10-C11-C12-C13
19	d	210	CLA	C8-C10-C11-C12
20	A	830	PQN	C23-C25-C26-C27
28	b	301	CHL	C5-C6-C7-C8
28	d	205	CHL	C5-C6-C7-C8
25	g	316	LMG	C28-C29-C30-C31
19	A	840	CLA	C15-C16-C17-C18
19	j	304	CLA	C8-C10-C11-C12
19	j	304	CLA	C10-C11-C12-C13
19	e	310	CLA	O1D-CGD-O2D-CED
25	a	318	LMG	O6-C5-C6-O5
19	A	842	CLA	C10-C11-C12-C13
28	e	304	CHL	C10-C11-C12-C13
25	A	851	LMG	C28-C29-C30-C31
25	g	313	LMG	C10-C11-C12-C13
25	h	216	LMG	C28-C29-C30-C31
27	B	829	DGD	C1A-C2A-C3A-C4A
19	g	304	CLA	CBD-CGD-O2D-CED
25	a	316	LMG	C4-C5-C6-O5
28	g	303	CHL	C5-C6-C7-C8
19	A	824	CLA	C12-C13-C15-C16
19	A	843	CLA	C6-C7-C8-C10
19	B	811	CLA	C11-C10-C8-C7
19	b	306	CLA	C11-C10-C8-C7
19	j	307	CLA	C11-C10-C8-C7
19	A	841	CLA	C3-C5-C6-C7
19	B	806	CLA	C3-C5-C6-C7
19	d	209	CLA	C3-C5-C6-C7
19	m	305	CLA	C3-C5-C6-C7
19	A	828	CLA	C2A-CAA-CBA-CGA
19	B	801	CLA	C2A-CAA-CBA-CGA
19	g	311	CLA	C2A-CAA-CBA-CGA
19	j	302	CLA	C2A-CAA-CBA-CGA
19	o	309	CLA	C2A-CAA-CBA-CGA
28	d	202	CHL	C2A-CAA-CBA-CGA
28	e	304	CHL	C2A-CAA-CBA-CGA
28	m	301	CHL	C2A-CAA-CBA-CGA
19	j	305	CLA	O1D-CGD-O2D-CED
28	e	304	CHL	C8-C10-C11-C12
19	A	822	CLA	O1A-CGA-O2A-C1
19	B	849	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	a	318	LMG	O6-C1-O1-C7
25	h	216	LMG	O6-C1-O1-C7
19	A	807	CLA	C5-C6-C7-C8
24	a	319	LMU	O1'-C1-C2-C3
25	g	316	LMG	C10-C11-C12-C13
19	A	841	CLA	C5-C6-C7-C8
19	B	822	CLA	C10-C11-C12-C13
19	F	203	CLA	C10-C11-C12-C13
19	b	306	CLA	C5-C6-C7-C8
28	f	304	CHL	C5-C6-C7-C8
25	a	301	LMG	C28-C29-C30-C31
25	k	312	LMG	C10-C11-C12-C13
19	A	822	CLA	C5-C6-C7-C8
19	d	208	CLA	C8-C10-C11-C12
19	j	307	CLA	C5-C6-C7-C8
19	a	306	CLA	O1D-CGD-O2D-CED
19	c	316	CLA	C8-C10-C11-C12
28	c	305	CHL	C5-C6-C7-C8
28	c	312	CHL	C5-C6-C7-C8
21	A	831	LHG	C3-O3-P-O6
21	A	831	LHG	C4-O6-P-O3
19	e	307	CLA	C3-C5-C6-C7
20	B	824	PQN	C13-C15-C16-C17
19	c	306	CLA	CBA-CGA-O2A-C1
28	d	205	CHL	CBA-CGA-O2A-C1
19	B	801	CLA	C5-C6-C7-C8
28	c	305	CHL	C10-C11-C12-C13
25	e	312	LMG	C28-C29-C30-C31
19	n	202	CLA	O1D-CGD-O2D-CED
25	A	851	LMG	O9-C10-O7-C8
19	A	807	CLA	C4-C3-C5-C6
24	c	301	LMU	C5'-C4'-O1B-C1B
19	A	852	CLA	C2A-CAA-CBA-CGA
19	B	830	CLA	C2A-CAA-CBA-CGA
19	B	837	CLA	C2A-CAA-CBA-CGA
19	k	310	CLA	C2A-CAA-CBA-CGA
28	a	315	CHL	C2A-CAA-CBA-CGA
19	c	316	CLA	C16-C17-C18-C20
19	j	313	CLA	C3-C5-C6-C7
19	A	852	CLA	CBA-CGA-O2A-C1
19	o	302	CLA	CBA-CGA-O2A-C1
19	o	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	842	CLA	C15-C16-C17-C18
25	g	313	LMG	C29-C30-C31-C32
19	o	304	CLA	C5-C6-C7-C8
25	e	312	LMG	C20-C21-C22-C23
25	g	312	LMG	C30-C31-C32-C33
25	g	316	LMG	C30-C31-C32-C33
27	B	829	DGD	CEB-CFB-CGB-CHB
19	m	309	CLA	O1A-CGA-O2A-C1
28	a	311	CHL	O1D-CGD-O2D-CED
19	g	305	CLA	CBA-CGA-O2A-C1
27	B	829	DGD	C3B-C4B-C5B-C6B
19	b	315	CLA	O1D-CGD-O2D-CED
25	c	320	LMG	C20-C21-C22-C23
27	B	829	DGD	C3A-C4A-C5A-C6A
19	k	304	CLA	O1D-CGD-O2D-CED
19	A	842	CLA	C8-C10-C11-C12
24	a	319	LMU	O5'-C1'-O1'-C1
25	a	318	LMG	C2-C1-O1-C7
25	i	316	LMG	C2-C1-O1-C7
19	B	815	CLA	CBA-CGA-O2A-C1
25	c	320	LMG	C11-C12-C13-C14
19	o	302	CLA	O1A-CGA-O2A-C1
28	a	311	CHL	O1A-CGA-O2A-C1
28	a	313	CHL	O1A-CGA-O2A-C1
19	f	314	CLA	C6-C7-C8-C10
19	a	303	CLA	C4-C3-C5-C6
21	A	831	LHG	C30-C31-C32-C33
25	b	316	LMG	C30-C31-C32-C33
19	A	807	CLA	C2-C3-C5-C6
19	k	304	CLA	C2-C3-C5-C6
19	B	805	CLA	C11-C12-C13-C14
19	B	806	CLA	C6-C7-C8-C9
20	A	830	PQN	C21-C22-C23-C24
20	B	824	PQN	C16-C17-C18-C19
25	A	851	LMG	C10-C11-C12-C13
25	a	318	LMG	C13-C14-C15-C16
19	A	821	CLA	C2A-CAA-CBA-CGA
19	B	807	CLA	O1A-CGA-O2A-C1
25	g	316	LMG	C14-C15-C16-C17
25	i	316	LMG	C16-C17-C18-C19
22	J	802	DD6	C5-C6-C8-C9
19	B	806	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	i	316	LMG	C17-C18-C19-C20
25	i	316	LMG	C4-C5-C6-O5
25	f	313	LMG	C10-C11-C12-C13
25	c	320	LMG	C15-C16-C17-C18
19	A	844	CLA	C4B-C3B-CAB-CBB
19	A	852	CLA	C4B-C3B-CAB-CBB
19	B	801	CLA	C4B-C3B-CAB-CBB
19	B	806	CLA	C4B-C3B-CAB-CBB
19	B	820	CLA	C4B-C3B-CAB-CBB
19	B	837	CLA	C4B-C3B-CAB-CBB
19	B	845	CLA	C4B-C3B-CAB-CBB
19	a	302	CLA	C4B-C3B-CAB-CBB
19	a	303	CLA	C4B-C3B-CAB-CBB
19	a	314	CLA	C4B-C3B-CAB-CBB
19	b	302	CLA	C4B-C3B-CAB-CBB
19	b	306	CLA	C4B-C3B-CAB-CBB
19	b	308	CLA	C4B-C3B-CAB-CBB
19	b	313	CLA	C4B-C3B-CAB-CBB
19	c	302	CLA	C4B-C3B-CAB-CBB
19	c	304	CLA	C4B-C3B-CAB-CBB
19	c	306	CLA	C4B-C3B-CAB-CBB
19	d	208	CLA	C4B-C3B-CAB-CBB
19	e	302	CLA	C4B-C3B-CAB-CBB
19	e	311	CLA	C4B-C3B-CAB-CBB
19	f	302	CLA	C4B-C3B-CAB-CBB
19	f	309	CLA	C4B-C3B-CAB-CBB
19	f	310	CLA	C4B-C3B-CAB-CBB
19	g	309	CLA	C4B-C3B-CAB-CBB
19	h	205	CLA	C4B-C3B-CAB-CBB
19	h	211	CLA	C4B-C3B-CAB-CBB
19	h	212	CLA	C4B-C3B-CAB-CBB
19	j	302	CLA	C4B-C3B-CAB-CBB
19	j	309	CLA	C4B-C3B-CAB-CBB
19	j	313	CLA	C4B-C3B-CAB-CBB
19	k	309	CLA	C4B-C3B-CAB-CBB
19	k	311	CLA	C4B-C3B-CAB-CBB
19	l	209	CLA	C4B-C3B-CAB-CBB
19	m	307	CLA	C4B-C3B-CAB-CBB
19	m	309	CLA	C4B-C3B-CAB-CBB
19	n	207	CLA	C4B-C3B-CAB-CBB
19	o	309	CLA	C4B-C3B-CAB-CBB
19	o	311	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	a	313	CHL	C4B-C3B-CAB-CBB
28	b	314	CHL	C4B-C3B-CAB-CBB
19	B	810	CLA	C6-C7-C8-C10
19	F	203	CLA	C16-C17-C18-C19
19	j	308	CLA	C11-C12-C13-C15
19	o	302	CLA	C6-C7-C8-C9
25	i	316	LMG	O6-C1-O1-C7
25	i	316	LMG	C15-C16-C17-C18
19	d	208	CLA	O1D-CGD-O2D-CED
25	k	312	LMG	C12-C13-C14-C15
19	B	807	CLA	C8-C10-C11-C12
27	B	829	DGD	C2A-C3A-C4A-C5A
27	B	829	DGD	C7A-C8A-C9A-CAA
25	g	312	LMG	O6-C5-C6-O5
19	j	302	CLA	CBA-CGA-O2A-C1
25	j	314	LMG	C30-C31-C32-C33
19	A	804	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	820	CLA	C3A-C2A-CAA-CBA
19	A	842	CLA	C3A-C2A-CAA-CBA
19	A	843	CLA	C3A-C2A-CAA-CBA
19	B	804	CLA	C3A-C2A-CAA-CBA
19	B	809	CLA	C3A-C2A-CAA-CBA
19	B	830	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	B	839	CLA	C3A-C2A-CAA-CBA
19	B	844	CLA	C3A-C2A-CAA-CBA
19	b	315	CLA	C3A-C2A-CAA-CBA
19	c	302	CLA	C3A-C2A-CAA-CBA
19	c	314	CLA	C3A-C2A-CAA-CBA
19	c	315	CLA	C3A-C2A-CAA-CBA
19	e	308	CLA	C3A-C2A-CAA-CBA
19	f	305	CLA	C3A-C2A-CAA-CBA
19	h	211	CLA	C3A-C2A-CAA-CBA
19	h	212	CLA	C3A-C2A-CAA-CBA
19	h	213	CLA	C3A-C2A-CAA-CBA
19	i	303	CLA	C3A-C2A-CAA-CBA
19	i	305	CLA	C3A-C2A-CAA-CBA
19	k	303	CLA	C3A-C2A-CAA-CBA
19	k	306	CLA	C3A-C2A-CAA-CBA
19	l	203	CLA	C3A-C2A-CAA-CBA
19	l	208	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	m	304	CLA	C3A-C2A-CAA-CBA
19	n	201	CLA	C3A-C2A-CAA-CBA
19	n	203	CLA	C3A-C2A-CAA-CBA
19	o	303	CLA	C3A-C2A-CAA-CBA
19	o	306	CLA	C3A-C2A-CAA-CBA
19	o	310	CLA	C3A-C2A-CAA-CBA
19	o	312	CLA	C3A-C2A-CAA-CBA
28	b	310	CHL	C3A-C2A-CAA-CBA
28	b	314	CHL	C3A-C2A-CAA-CBA
28	c	312	CHL	C3A-C2A-CAA-CBA
28	d	202	CHL	C3A-C2A-CAA-CBA
28	h	202	CHL	C3A-C2A-CAA-CBA
28	i	301	CHL	C3A-C2A-CAA-CBA
21	A	831	LHG	C25-C26-C27-C28
25	g	316	LMG	C21-C22-C23-C24
19	B	810	CLA	C6-C7-C8-C9
19	F	203	CLA	C16-C17-C18-C20
19	o	302	CLA	C6-C7-C8-C10
28	b	301	CHL	C6-C7-C8-C9
25	g	316	LMG	C19-C20-C21-C22
25	g	316	LMG	C23-C24-C25-C26
19	e	305	CLA	O2A-C1-C2-C3
19	m	310	CLA	O2A-C1-C2-C3
19	A	828	CLA	C5-C6-C7-C8
19	A	842	CLA	C4-C3-C5-C6
19	b	308	CLA	C4-C3-C5-C6
19	A	806	CLA	CBA-CGA-O2A-C1
19	b	306	CLA	CBA-CGA-O2A-C1
19	A	842	CLA	C2-C3-C5-C6
19	b	308	CLA	C2-C3-C5-C6
25	g	316	LMG	C11-C10-O7-C8
19	i	310	CLA	C2A-CAA-CBA-CGA
28	c	313	CHL	C2A-CAA-CBA-CGA
19	g	305	CLA	O1A-CGA-O2A-C1
19	A	810	CLA	C2B-C3B-CAB-CBB
19	A	827	CLA	C2B-C3B-CAB-CBB
19	A	839	CLA	C2B-C3B-CAB-CBB
19	A	844	CLA	C2B-C3B-CAB-CBB
19	B	806	CLA	C2B-C3B-CAB-CBB
19	B	820	CLA	C2B-C3B-CAB-CBB
19	B	822	CLA	C2B-C3B-CAB-CBB
19	B	837	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	F	204	CLA	C2B-C3B-CAB-CBB
19	a	302	CLA	C2B-C3B-CAB-CBB
19	a	303	CLA	C2B-C3B-CAB-CBB
19	a	314	CLA	C2B-C3B-CAB-CBB
19	b	302	CLA	C2B-C3B-CAB-CBB
19	b	303	CLA	C2B-C3B-CAB-CBB
19	b	306	CLA	C2B-C3B-CAB-CBB
19	b	308	CLA	C2B-C3B-CAB-CBB
19	b	313	CLA	C2B-C3B-CAB-CBB
19	c	302	CLA	C2B-C3B-CAB-CBB
19	c	304	CLA	C2B-C3B-CAB-CBB
19	c	314	CLA	C2B-C3B-CAB-CBB
19	d	208	CLA	C2B-C3B-CAB-CBB
19	d	212	CLA	C2B-C3B-CAB-CBB
19	e	302	CLA	C2B-C3B-CAB-CBB
19	e	311	CLA	C2B-C3B-CAB-CBB
19	f	302	CLA	C2B-C3B-CAB-CBB
19	f	309	CLA	C2B-C3B-CAB-CBB
19	f	310	CLA	C2B-C3B-CAB-CBB
19	f	312	CLA	C2B-C3B-CAB-CBB
19	g	309	CLA	C2B-C3B-CAB-CBB
19	h	201	CLA	C2B-C3B-CAB-CBB
19	h	203	CLA	C2B-C3B-CAB-CBB
19	h	205	CLA	C2B-C3B-CAB-CBB
19	h	211	CLA	C2B-C3B-CAB-CBB
19	h	212	CLA	C2B-C3B-CAB-CBB
19	j	302	CLA	C2B-C3B-CAB-CBB
19	j	303	CLA	C2B-C3B-CAB-CBB
19	j	309	CLA	C2B-C3B-CAB-CBB
19	k	309	CLA	C2B-C3B-CAB-CBB
19	k	311	CLA	C2B-C3B-CAB-CBB
19	l	209	CLA	C2B-C3B-CAB-CBB
19	m	304	CLA	C2B-C3B-CAB-CBB
19	m	307	CLA	C2B-C3B-CAB-CBB
19	m	309	CLA	C2B-C3B-CAB-CBB
19	m	311	CLA	C2B-C3B-CAB-CBB
19	n	201	CLA	C2B-C3B-CAB-CBB
19	n	202	CLA	C2B-C3B-CAB-CBB
19	n	207	CLA	C2B-C3B-CAB-CBB
19	o	309	CLA	C2B-C3B-CAB-CBB
19	o	311	CLA	C2B-C3B-CAB-CBB
28	a	313	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	b	314	CHL	C2B-C3B-CAB-CBB
28	f	304	CHL	C2B-C3B-CAB-CBB
19	g	307	CLA	C5-C6-C7-C8
19	A	828	CLA	C3-C5-C6-C7
19	c	306	CLA	C3-C5-C6-C7
19	d	211	CLA	C3-C5-C6-C7
20	A	830	PQN	C13-C15-C16-C17
19	g	304	CLA	CBA-CGA-O2A-C1
19	j	305	CLA	CBA-CGA-O2A-C1
28	b	312	CHL	O1A-CGA-O2A-C1
28	h	202	CHL	O1A-CGA-O2A-C1
25	a	316	LMG	O9-C10-O7-C8
25	f	313	LMG	O9-C10-O7-C8
25	k	312	LMG	O9-C10-O7-C8
25	g	313	LMG	C12-C13-C14-C15
23	A	835	BCR	C23-C24-C25-C26
23	B	826	BCR	C1-C6-C7-C8
23	B	831	BCR	C23-C24-C25-C26
23	B	831	BCR	C23-C24-C25-C30
19	i	302	CLA	CBA-CGA-O2A-C1
19	A	844	CLA	C13-C15-C16-C17
19	B	811	CLA	C5-C6-C7-C8
19	B	814	CLA	C5-C6-C7-C8
19	B	815	CLA	C8-C10-C11-C12
25	g	313	LMG	C11-C10-O7-C8
25	g	312	LMG	C15-C16-C17-C18
25	b	316	LMG	C28-C29-C30-C31
19	A	821	CLA	C5-C6-C7-C8
19	m	305	CLA	C5-C6-C7-C8
19	F	201	CLA	C4-C3-C5-C6
19	A	802	CLA	C2-C3-C5-C6
19	A	802	CLA	C6-C7-C8-C10
19	A	802	CLA	C12-C13-C15-C16
19	A	806	CLA	C12-C13-C15-C16
19	A	811	CLA	C11-C12-C13-C15
19	B	805	CLA	C11-C12-C13-C15
19	F	201	CLA	C2-C3-C5-C6
19	a	303	CLA	C2-C3-C5-C6
19	f	311	CLA	C2-C3-C5-C6
20	A	830	PQN	C17-C18-C20-C21
20	B	824	PQN	C16-C17-C18-C20
19	c	316	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	A	852	CLA	O1A-CGA-O2A-C1
19	c	306	CLA	O1A-CGA-O2A-C1
19	g	304	CLA	O1A-CGA-O2A-C1
19	j	305	CLA	O1A-CGA-O2A-C1
19	o	307	CLA	O1A-CGA-O2A-C1
28	g	310	CHL	O1A-CGA-O2A-C1
19	B	806	CLA	C13-C15-C16-C17
21	A	831	LHG	O9-C7-O7-C5
25	j	314	LMG	O9-C10-O7-C8
28	e	304	CHL	CBA-CGA-O2A-C1
19	A	802	CLA	C2A-CAA-CBA-CGA
19	F	203	CLA	C2A-CAA-CBA-CGA
19	b	303	CLA	C2A-CAA-CBA-CGA
19	b	315	CLA	C2A-CAA-CBA-CGA
28	g	310	CHL	C2A-CAA-CBA-CGA
19	i	307	CLA	C5-C6-C7-C8
28	c	313	CHL	C5-C6-C7-C8
27	B	829	DGD	CAA-CBA-CCA-CDA
27	B	829	DGD	C5B-C6B-C7B-C8B
19	b	306	CLA	O1A-CGA-O2A-C1
25	a	316	LMG	O6-C1-O1-C7
25	k	312	LMG	O6-C1-O1-C7
19	m	310	CLA	C5-C6-C7-C8
24	a	319	LMU	C1-C2-C3-C4
25	c	320	LMG	C17-C18-C19-C20
25	d	213	LMG	C10-C11-C12-C13
25	A	851	LMG	C11-C10-O7-C8
25	a	316	LMG	C11-C10-O7-C8
25	e	312	LMG	C11-C10-O7-C8
25	f	313	LMG	C11-C10-O7-C8
28	c	312	CHL	C2C-C3C-CAC-CBC
28	e	304	CHL	CBD-CGD-O2D-CED
21	A	831	LHG	C10-C11-C12-C13
25	a	301	LMG	C11-C12-C13-C14
25	h	216	LMG	C11-C12-C13-C14
25	g	312	LMG	C2-C1-O1-C7
27	B	829	DGD	O2G-C2G-C3G-O3G
19	f	314	CLA	C6-C7-C8-C9
21	A	831	LHG	C9-C10-C11-C12
24	a	319	LMU	O5B-C5B-C6B-O6B
19	f	311	CLA	C4-C3-C5-C6
22	f	316	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	g	314	DD6	C27-C29-C30-C31
22	h	215	DD6	C27-C29-C30-C31
22	k	313	DD6	C27-C29-C30-C31
22	o	314	DD6	C27-C29-C30-C31
19	A	802	CLA	C6-C7-C8-C9
19	A	802	CLA	C14-C13-C15-C16
19	A	806	CLA	C14-C13-C15-C16
19	A	824	CLA	C14-C13-C15-C16
19	A	828	CLA	C11-C10-C8-C9
19	A	841	CLA	C14-C13-C15-C16
19	B	849	CLA	C11-C12-C13-C14
28	e	301	CHL	O1D-CGD-O2D-CED
19	j	309	CLA	C3-C5-C6-C7
19	A	843	CLA	C2A-CAA-CBA-CGA
19	B	809	CLA	C2A-CAA-CBA-CGA
19	B	820	CLA	C2A-CAA-CBA-CGA
19	d	209	CLA	C2A-CAA-CBA-CGA
25	e	312	LMG	O6-C5-C6-O5
25	h	216	LMG	O6-C5-C6-O5
19	B	811	CLA	C2C-C3C-CAC-CBC
21	A	831	LHG	C33-C34-C35-C36
25	A	851	LMG	C11-C12-C13-C14
23	B	850	BCR	C17-C18-C19-C20
19	B	815	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	815	CLA	C1A-C2A-CAA-CBA
19	A	817	CLA	C1A-C2A-CAA-CBA
19	A	843	CLA	C1A-C2A-CAA-CBA
19	A	848	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	815	CLA	C1A-C2A-CAA-CBA
19	B	819	CLA	C1A-C2A-CAA-CBA
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	837	CLA	C1A-C2A-CAA-CBA
19	B	846	CLA	C1A-C2A-CAA-CBA
19	F	201	CLA	C1A-C2A-CAA-CBA
19	a	303	CLA	C1A-C2A-CAA-CBA
19	b	313	CLA	C1A-C2A-CAA-CBA
19	c	315	CLA	C1A-C2A-CAA-CBA
19	e	308	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	f	305	CLA	C1A-C2A-CAA-CBA
19	h	207	CLA	C1A-C2A-CAA-CBA
19	h	211	CLA	C1A-C2A-CAA-CBA
19	h	212	CLA	C1A-C2A-CAA-CBA
19	i	303	CLA	C1A-C2A-CAA-CBA
19	i	305	CLA	C1A-C2A-CAA-CBA
19	j	305	CLA	C1A-C2A-CAA-CBA
19	j	307	CLA	C1A-C2A-CAA-CBA
19	k	303	CLA	C1A-C2A-CAA-CBA
19	k	306	CLA	C1A-C2A-CAA-CBA
19	l	203	CLA	C1A-C2A-CAA-CBA
19	l	208	CLA	C1A-C2A-CAA-CBA
19	n	201	CLA	C1A-C2A-CAA-CBA
19	n	202	CLA	C1A-C2A-CAA-CBA
19	n	203	CLA	C1A-C2A-CAA-CBA
19	n	208	CLA	C1A-C2A-CAA-CBA
19	o	303	CLA	C1A-C2A-CAA-CBA
19	o	304	CLA	C1A-C2A-CAA-CBA
19	o	307	CLA	C1A-C2A-CAA-CBA
19	o	310	CLA	C1A-C2A-CAA-CBA
28	a	313	CHL	C1A-C2A-CAA-CBA
28	b	312	CHL	C1A-C2A-CAA-CBA
28	b	314	CHL	C1A-C2A-CAA-CBA
28	c	305	CHL	C1A-C2A-CAA-CBA
28	c	312	CHL	C1A-C2A-CAA-CBA
28	d	205	CHL	C1A-C2A-CAA-CBA
28	f	304	CHL	C1A-C2A-CAA-CBA
28	g	303	CHL	C1A-C2A-CAA-CBA
28	i	304	CHL	C1A-C2A-CAA-CBA
19	c	316	CLA	C16-C17-C18-C19
19	j	308	CLA	C11-C12-C13-C14
28	i	304	CHL	C6-C7-C8-C9
27	B	829	DGD	C9A-CAA-CBA-CCA
19	o	302	CLA	O1D-CGD-O2D-CED
19	k	305	CLA	C5-C6-C7-C8
20	A	830	PQN	C20-C21-C22-C23
25	a	318	LMG	C31-C32-C33-C34
19	A	807	CLA	C15-C16-C17-C18
19	B	817	CLA	C10-C11-C12-C13
19	A	848	CLA	CBA-CGA-O2A-C1
19	B	848	CLA	CBA-CGA-O2A-C1
25	b	316	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
28	b	314	CHL	O1A-CGA-O2A-C1
19	n	203	CLA	C2C-C3C-CAC-CBC
19	c	304	CLA	C4-C3-C5-C6
19	j	308	CLA	C4-C3-C5-C6
19	k	304	CLA	C4-C3-C5-C6
19	A	804	CLA	C15-C16-C17-C18
19	j	302	CLA	O1A-CGA-O2A-C1
28	k	301	CHL	O1A-CGA-O2A-C1
19	A	822	CLA	C16-C17-C18-C19
24	A	838	LMU	O5'-C5'-C6'-O6'
19	o	305	CLA	O1D-CGD-O2D-CED
25	a	318	LMG	O1-C7-C8-C9
25	c	320	LMG	C7-C8-C9-O8
25	e	312	LMG	O1-C7-C8-C9
25	g	313	LMG	C7-C8-C9-O8
25	g	316	LMG	O1-C7-C8-C9
25	i	316	LMG	C7-C8-C9-O8
25	k	312	LMG	O6-C5-C6-O5
25	g	316	LMG	C20-C21-C22-C23
25	a	316	LMG	C8-C7-O1-C1
25	a	318	LMG	C8-C7-O1-C1
25	d	213	LMG	C8-C7-O1-C1
25	k	312	LMG	C8-C7-O1-C1
19	F	202	CLA	CBD-CGD-O2D-CED
19	B	849	CLA	C8-C10-C11-C12
20	A	830	PQN	C18-C20-C21-C22
25	a	301	LMG	C33-C34-C35-C36
28	g	303	CHL	O1D-CGD-O2D-CED
25	c	320	LMG	C18-C19-C20-C21
24	c	301	LMU	O5B-C5B-C6B-O6B
25	c	320	LMG	O6-C5-C6-O5
24	a	319	LMU	C2'-C1'-O1'-C1
25	g	312	LMG	C11-C10-O7-C8
19	B	818	CLA	C13-C15-C16-C17
19	F	203	CLA	C13-C15-C16-C17
25	f	313	LMG	O6-C5-C6-O5
25	j	314	LMG	O6-C5-C6-O5
19	A	802	CLA	C4-C3-C5-C6
19	d	209	CLA	C4-C3-C5-C6
19	h	209	CLA	C4-C3-C5-C6
19	o	304	CLA	C6-C7-C8-C9
24	A	838	LMU	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	B	830	CLA	CBA-CGA-O2A-C1
19	f	309	CLA	CBA-CGA-O2A-C1
19	l	203	CLA	C10-C11-C12-C13
25	k	312	LMG	C17-C18-C19-C20
25	a	318	LMG	C9-C8-O7-C10
19	l	203	CLA	C5-C6-C7-C8
19	A	822	CLA	C2-C1-O2A-CGA
19	B	807	CLA	C2-C1-O2A-CGA
28	e	304	CHL	C5-C6-C7-C8
19	A	817	CLA	CBA-CGA-O2A-C1
19	b	302	CLA	CBA-CGA-O2A-C1
25	a	318	LMG	C14-C15-C16-C17
25	i	316	LMG	C28-C29-C30-C31
19	B	820	CLA	C10-C11-C12-C13
19	o	303	CLA	O2A-C1-C2-C3
19	A	806	CLA	O1A-CGA-O2A-C1
19	B	848	CLA	O1A-CGA-O2A-C1
19	o	307	CLA	C11-C12-C13-C14
25	d	213	LMG	C11-C12-C13-C14
25	g	316	LMG	C13-C14-C15-C16
19	e	307	CLA	C10-C11-C12-C13
19	A	801	CLA	C6-C7-C8-C10
19	A	803	CLA	C11-C10-C8-C7
19	A	809	CLA	C11-C12-C13-C15
19	A	828	CLA	C11-C10-C8-C7
19	A	841	CLA	C12-C13-C15-C16
19	A	842	CLA	C11-C10-C8-C7
19	B	806	CLA	C11-C12-C13-C15
19	B	808	CLA	C6-C7-C8-C10
19	B	817	CLA	C6-C7-C8-C10
19	B	822	CLA	C12-C13-C15-C16
19	B	849	CLA	C11-C10-C8-C7
19	F	201	CLA	C11-C10-C8-C7
19	c	304	CLA	C2-C3-C5-C6
19	d	209	CLA	C2-C3-C5-C6
19	h	209	CLA	C2-C3-C5-C6
19	j	304	CLA	C11-C10-C8-C7
20	A	830	PQN	C21-C22-C23-C25
19	B	817	CLA	CAA-CBA-CGA-O2A
19	i	302	CLA	O1A-CGA-O2A-C1
19	A	801	CLA	C6-C7-C8-C9
19	A	809	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	A	811	CLA	C11-C12-C13-C14
19	A	842	CLA	C14-C13-C15-C16
19	A	850	CLA	C14-C13-C15-C16
19	B	811	CLA	C11-C10-C8-C9
19	B	822	CLA	C11-C10-C8-C9
19	B	822	CLA	C14-C13-C15-C16
19	F	201	CLA	C11-C10-C8-C9
19	b	306	CLA	C11-C10-C8-C9
19	e	308	CLA	C6-C7-C8-C9
23	A	835	BCR	C12-C13-C14-C15
25	a	301	LMG	C32-C33-C34-C35
19	B	841	CLA	CBA-CGA-O2A-C1
28	b	311	CHL	C2A-CAA-CBA-CGA
19	j	307	CLA	C3-C5-C6-C7
25	k	312	LMG	C11-C10-O7-C8
25	h	216	LMG	C31-C32-C33-C34
19	a	305	CLA	C8-C10-C11-C12
19	b	306	CLA	CAA-CBA-CGA-O2A
19	A	802	CLA	C4B-C3B-CAB-CBB
19	A	815	CLA	C4B-C3B-CAB-CBB
19	A	818	CLA	C4B-C3B-CAB-CBB
19	A	827	CLA	C4B-C3B-CAB-CBB
19	A	829	CLA	C4B-C3B-CAB-CBB
19	A	839	CLA	C4B-C3B-CAB-CBB
19	A	842	CLA	C4B-C3B-CAB-CBB
19	B	822	CLA	C4B-C3B-CAB-CBB
19	B	835	CLA	C4B-C3B-CAB-CBB
19	B	843	CLA	C4B-C3B-CAB-CBB
19	b	303	CLA	C4B-C3B-CAB-CBB
19	c	314	CLA	C4B-C3B-CAB-CBB
19	d	203	CLA	C4B-C3B-CAB-CBB
19	d	207	CLA	C4B-C3B-CAB-CBB
19	d	209	CLA	C4B-C3B-CAB-CBB
19	d	212	CLA	C4B-C3B-CAB-CBB
19	f	308	CLA	C4B-C3B-CAB-CBB
19	f	312	CLA	C4B-C3B-CAB-CBB
19	h	201	CLA	C4B-C3B-CAB-CBB
19	h	213	CLA	C4B-C3B-CAB-CBB
19	i	308	CLA	C4B-C3B-CAB-CBB
19	j	306	CLA	C4B-C3B-CAB-CBB
19	j	308	CLA	C4B-C3B-CAB-CBB
19	j	311	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	j	312	CLA	C4B-C3B-CAB-CBB
19	k	308	CLA	C4B-C3B-CAB-CBB
19	l	207	CLA	C4B-C3B-CAB-CBB
19	m	311	CLA	C4B-C3B-CAB-CBB
19	n	201	CLA	C4B-C3B-CAB-CBB
19	n	202	CLA	C4B-C3B-CAB-CBB
28	d	205	CHL	C4B-C3B-CAB-CBB
28	f	304	CHL	C4B-C3B-CAB-CBB
19	n	205	CLA	C5-C6-C7-C8
25	a	301	LMG	C10-C11-C12-C13
25	i	316	LMG	O6-C5-C6-O5
19	A	801	CLA	C4-C3-C5-C6
19	B	819	CLA	C4-C3-C5-C6
19	A	801	CLA	C2-C3-C5-C6
19	i	311	CLA	C2-C3-C5-C6
19	j	308	CLA	C2-C3-C5-C6
28	b	312	CHL	O1D-CGD-O2D-CED
19	a	303	CLA	C6-C7-C8-C10
27	B	829	DGD	C9B-CAB-CBB-CCB
19	F	203	CLA	CBA-CGA-O2A-C1
19	j	310	CLA	CBA-CGA-O2A-C1
19	g	304	CLA	O1D-CGD-O2D-CED
19	A	813	CLA	C3A-C2A-CAA-CBA
19	B	817	CLA	C3A-C2A-CAA-CBA
28	f	301	CHL	C3A-C2A-CAA-CBA
25	e	312	LMG	C24-C25-C26-C27
24	a	319	LMU	C2-C1-O1'-C1'
19	g	307	CLA	C11-C12-C13-C15
28	d	205	CHL	C6-C7-C8-C9
19	o	311	CLA	CBA-CGA-O2A-C1
19	B	805	CLA	C8-C10-C11-C12
19	c	306	CLA	O2A-C1-C2-C3
19	A	807	CLA	C3-C5-C6-C7
19	h	201	CLA	C3-C5-C6-C7
19	i	311	CLA	C4-C3-C5-C6
19	B	819	CLA	C2-C3-C5-C6
21	A	831	LHG	C35-C36-C37-C38
28	a	311	CHL	C3C-C2C-CMC-OMC
28	a	312	CHL	C3C-C2C-CMC-OMC
28	b	310	CHL	C3C-C2C-CMC-OMC
28	c	305	CHL	C3C-C2C-CMC-OMC
28	c	313	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
28	e	301	CHL	C3C-C2C-CMC-OMC
28	e	304	CHL	C3C-C2C-CMC-OMC
28	f	304	CHL	C3C-C2C-CMC-OMC
19	m	310	CLA	C3-C5-C6-C7
25	b	316	LMG	C19-C20-C21-C22
19	g	302	CLA	CBA-CGA-O2A-C1
28	d	202	CHL	O1A-CGA-O2A-C1
25	g	316	LMG	C15-C16-C17-C18
19	A	818	CLA	C2B-C3B-CAB-CBB
19	A	842	CLA	C2B-C3B-CAB-CBB
19	B	813	CLA	C2B-C3B-CAB-CBB
19	B	835	CLA	C2B-C3B-CAB-CBB
19	B	843	CLA	C2B-C3B-CAB-CBB
19	B	845	CLA	C2B-C3B-CAB-CBB
19	b	315	CLA	C2B-C3B-CAB-CBB
19	c	306	CLA	C2B-C3B-CAB-CBB
19	d	203	CLA	C2B-C3B-CAB-CBB
19	d	209	CLA	C2B-C3B-CAB-CBB
19	i	308	CLA	C2B-C3B-CAB-CBB
19	j	306	CLA	C2B-C3B-CAB-CBB
19	j	308	CLA	C2B-C3B-CAB-CBB
19	k	305	CLA	C2B-C3B-CAB-CBB
28	d	205	CHL	C2B-C3B-CAB-CBB
19	A	844	CLA	C15-C16-C17-C18
19	B	841	CLA	O1A-CGA-O2A-C1
25	g	313	LMG	O7-C8-C9-O8
25	g	316	LMG	O7-C8-C9-O8
25	i	316	LMG	O1-C7-C8-O7
25	a	318	LMG	C33-C34-C35-C36
28	c	305	CHL	C8-C10-C11-C12
19	B	817	CLA	C4-C3-C5-C6
19	A	802	CLA	C2-C1-O2A-CGA
19	A	842	CLA	C2-C1-O2A-CGA
19	F	203	CLA	C2-C1-O2A-CGA
19	a	306	CLA	C2-C1-O2A-CGA
19	k	302	CLA	C2-C1-O2A-CGA
19	o	307	CLA	C2-C1-O2A-CGA
19	B	806	CLA	C11-C12-C13-C14
19	B	830	CLA	C6-C7-C8-C9
19	k	304	CLA	C11-C10-C8-C9
28	e	304	CHL	C6-C7-C8-C9
19	A	847	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	A	841	CLA	C10-C11-C12-C13
19	A	827	CLA	C4-C3-C5-C6
28	b	314	CHL	C4-C3-C5-C6
25	j	314	LMG	C31-C32-C33-C34
19	h	209	CLA	C11-C12-C13-C14
28	b	301	CHL	C6-C7-C8-C10
28	i	304	CHL	CBD-CGD-O2D-CED
23	A	835	BCR	C1-C6-C7-C8
23	A	835	BCR	C5-C6-C7-C8
23	B	834	BCR	C1-C6-C7-C8
23	B	834	BCR	C5-C6-C7-C8
25	e	312	LMG	C22-C23-C24-C25
28	c	312	CHL	C4C-C3C-CAC-CBC
22	n	210	DD6	C10-C11-C13-C14
23	B	826	BCR	C7-C8-C9-C10
23	B	831	BCR	C7-C8-C9-C10
25	e	312	LMG	O9-C10-O7-C8
25	g	316	LMG	C18-C19-C20-C21
19	A	822	CLA	C15-C16-C17-C18
25	e	312	LMG	C23-C24-C25-C26
19	A	822	CLA	C16-C17-C18-C20
28	i	304	CHL	C6-C7-C8-C10
25	g	312	LMG	C13-C14-C15-C16
25	b	316	LMG	C16-C17-C18-C19
19	A	804	CLA	C12-C13-C15-C16
19	A	807	CLA	C11-C10-C8-C7
19	A	842	CLA	C11-C12-C13-C15
19	A	842	CLA	C12-C13-C15-C16
19	A	850	CLA	C12-C13-C15-C16
19	B	804	CLA	C6-C7-C8-C10
19	B	818	CLA	C12-C13-C15-C16
19	B	822	CLA	C11-C10-C8-C7
19	B	830	CLA	C6-C7-C8-C10
19	B	833	CLA	C6-C7-C8-C10
19	B	835	CLA	C6-C7-C8-C10
19	F	203	CLA	C12-C13-C15-C16
19	d	208	CLA	C6-C7-C8-C10
19	e	308	CLA	C6-C7-C8-C10
19	k	305	CLA	C6-C7-C8-C10
28	e	304	CHL	C6-C7-C8-C10
25	d	213	LMG	C15-C16-C17-C18
19	m	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	d	205	CHL	C6-C7-C8-C10
19	l	203	CLA	CAA-CBA-CGA-O2A
19	B	821	CLA	C2A-CAA-CBA-CGA
19	B	805	CLA	C13-C15-C16-C17
19	A	843	CLA	C3-C5-C6-C7
19	f	302	CLA	CBA-CGA-O2A-C1
19	A	807	CLA	CAD-CBD-CGD-O2D
19	A	808	CLA	CAD-CBD-CGD-O2D
19	A	826	CLA	CAD-CBD-CGD-O2D
19	A	847	CLA	CAD-CBD-CGD-O2D
19	B	806	CLA	CAD-CBD-CGD-O2D
19	B	812	CLA	CAD-CBD-CGD-O2D
19	B	842	CLA	CAD-CBD-CGD-O2D
19	F	203	CLA	CAD-CBD-CGD-O2D
19	a	306	CLA	CAD-CBD-CGD-O2D
19	d	208	CLA	CAD-CBD-CGD-O2D
19	e	307	CLA	CAD-CBD-CGD-O2D
19	f	306	CLA	CAD-CBD-CGD-O2D
19	f	310	CLA	CAD-CBD-CGD-O2D
19	f	311	CLA	CAD-CBD-CGD-O2D
19	g	309	CLA	CAD-CBD-CGD-O2D
19	h	208	CLA	CAD-CBD-CGD-O2D
19	i	303	CLA	CAD-CBD-CGD-O2D
19	j	302	CLA	CAD-CBD-CGD-O2D
19	k	304	CLA	CAD-CBD-CGD-O2D
19	k	309	CLA	CAD-CBD-CGD-O2D
19	l	206	CLA	CAD-CBD-CGD-O2D
19	l	208	CLA	CAD-CBD-CGD-O2D
19	m	306	CLA	CAD-CBD-CGD-O2D
19	m	307	CLA	CAD-CBD-CGD-O2D
19	m	310	CLA	CAD-CBD-CGD-O2D
19	n	204	CLA	CAD-CBD-CGD-O2D
25	d	213	LMG	C9-C8-O7-C10
28	d	202	CHL	CAD-CBD-CGD-O2D
19	n	203	CLA	C4C-C3C-CAC-CBC
19	A	827	CLA	CBA-CGA-O2A-C1
19	o	303	CLA	CBA-CGA-O2A-C1
19	l	204	CLA	C4-C3-C5-C6
25	g	316	LMG	C11-C12-C13-C14
25	g	316	LMG	C7-C8-C9-O8
21	A	831	LHG	O6-C4-C5-O7
19	A	802	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	A	806	CLA	C8-C10-C11-C12
19	e	310	CLA	C6-C7-C8-C10
19	o	307	CLA	C11-C12-C13-C15
19	A	804	CLA	CHA-CBD-CGD-O1D
19	A	806	CLA	CHA-CBD-CGD-O2D
19	A	824	CLA	CHA-CBD-CGD-O1D
19	A	824	CLA	CHA-CBD-CGD-O2D
19	A	846	CLA	CHA-CBD-CGD-O2D
19	B	805	CLA	CHA-CBD-CGD-O1D
19	B	805	CLA	CHA-CBD-CGD-O2D
19	B	813	CLA	CHA-CBD-CGD-O1D
19	B	821	CLA	CHA-CBD-CGD-O1D
19	B	821	CLA	CHA-CBD-CGD-O2D
19	B	839	CLA	CHA-CBD-CGD-O1D
19	B	839	CLA	CHA-CBD-CGD-O2D
19	B	844	CLA	CHA-CBD-CGD-O1D
19	a	304	CLA	CHA-CBD-CGD-O1D
19	b	313	CLA	CHA-CBD-CGD-O1D
19	b	313	CLA	CHA-CBD-CGD-O2D
19	b	315	CLA	CHA-CBD-CGD-O1D
19	b	315	CLA	CHA-CBD-CGD-O2D
19	c	316	CLA	CHA-CBD-CGD-O1D
19	c	316	CLA	CHA-CBD-CGD-O2D
19	f	312	CLA	CHA-CBD-CGD-O1D
19	f	312	CLA	CHA-CBD-CGD-O2D
19	g	304	CLA	CHA-CBD-CGD-O2D
19	i	309	CLA	CHA-CBD-CGD-O1D
19	i	309	CLA	CHA-CBD-CGD-O2D
19	j	310	CLA	CHA-CBD-CGD-O1D
19	j	310	CLA	CHA-CBD-CGD-O2D
19	m	303	CLA	CHA-CBD-CGD-O1D
19	m	303	CLA	CHA-CBD-CGD-O2D
19	n	201	CLA	CHA-CBD-CGD-O1D
28	a	312	CHL	CHA-CBD-CGD-O1D
28	b	301	CHL	CHA-CBD-CGD-O1D
28	d	202	CHL	CHA-CBD-CGD-O1D
28	d	205	CHL	O1D-CGD-O2D-CED
19	A	817	CLA	O1A-CGA-O2A-C1
19	A	848	CLA	O1A-CGA-O2A-C1
19	f	309	CLA	O1A-CGA-O2A-C1
19	j	310	CLA	O1A-CGA-O2A-C1
19	B	811	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	n	203	CLA	C5-C6-C7-C8
25	a	301	LMG	C13-C14-C15-C16
25	g	316	LMG	C17-C18-C19-C20
25	e	312	LMG	O1-C7-C8-O7
25	g	316	LMG	O1-C7-C8-O7
19	B	847	CLA	C5-C6-C7-C8
19	e	310	CLA	C6-C7-C8-C9
19	B	803	CLA	C4-C3-C5-C6
24	A	838	LMU	O1'-C1-C2-C3
19	B	830	CLA	O1A-CGA-O2A-C1
19	b	302	CLA	O1A-CGA-O2A-C1
19	B	817	CLA	C2-C3-C5-C6
22	c	318	DD6	C27-C29-C30-C31
22	k	314	DD6	C27-C29-C30-C31
22	m	312	DD6	C27-C29-C30-C31
19	i	309	CLA	CBA-CGA-O2A-C1
25	b	316	LMG	O9-C10-O7-C8
19	A	841	CLA	C11-C10-C8-C9
19	A	842	CLA	C11-C12-C13-C14
19	j	307	CLA	C11-C10-C8-C9
24	a	319	LMU	C5-C6-C7-C8
25	j	314	LMG	C12-C13-C14-C15
19	B	812	CLA	C2A-CAA-CBA-CGA
19	l	202	CLA	C2A-CAA-CBA-CGA
28	b	312	CHL	CBA-CGA-O2A-C1
19	A	819	CLA	C13-C15-C16-C17
25	g	316	LMG	C31-C32-C33-C34
19	f	307	CLA	C5-C6-C7-C8
19	A	810	CLA	C1A-C2A-CAA-CBA
19	A	853	CLA	C1A-C2A-CAA-CBA
19	b	304	CLA	C1A-C2A-CAA-CBA
19	d	211	CLA	C1A-C2A-CAA-CBA
19	e	309	CLA	C1A-C2A-CAA-CBA
19	g	311	CLA	C1A-C2A-CAA-CBA
28	b	301	CHL	C1A-C2A-CAA-CBA
25	b	316	LMG	C10-C11-C12-C13
28	f	304	CHL	C6-C7-C8-C9
19	A	804	CLA	C13-C15-C16-C17
19	A	842	CLA	C13-C15-C16-C17
19	B	815	CLA	C2-C1-O2A-CGA
19	B	830	CLA	C2-C1-O2A-CGA
20	A	830	PQN	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	B	803	CLA	C3-C5-C6-C7
19	o	303	CLA	O1A-CGA-O2A-C1
19	A	816	CLA	C4B-C3B-CAB-CBB
19	A	846	CLA	C4B-C3B-CAB-CBB
19	A	850	CLA	C4B-C3B-CAB-CBB
19	B	813	CLA	C4B-C3B-CAB-CBB
19	B	840	CLA	C4B-C3B-CAB-CBB
19	B	842	CLA	C4B-C3B-CAB-CBB
19	B	846	CLA	C4B-C3B-CAB-CBB
19	B	847	CLA	C4B-C3B-CAB-CBB
19	F	202	CLA	C4B-C3B-CAB-CBB
19	b	304	CLA	C4B-C3B-CAB-CBB
19	b	315	CLA	C4B-C3B-CAB-CBB
19	c	307	CLA	C4B-C3B-CAB-CBB
19	e	306	CLA	C4B-C3B-CAB-CBB
19	f	303	CLA	C4B-C3B-CAB-CBB
19	f	314	CLA	C4B-C3B-CAB-CBB
19	g	308	CLA	C4B-C3B-CAB-CBB
19	h	206	CLA	C4B-C3B-CAB-CBB
19	i	302	CLA	C4B-C3B-CAB-CBB
19	i	309	CLA	C4B-C3B-CAB-CBB
19	i	311	CLA	C4B-C3B-CAB-CBB
19	i	313	CLA	C4B-C3B-CAB-CBB
19	k	305	CLA	C4B-C3B-CAB-CBB
19	k	306	CLA	C4B-C3B-CAB-CBB
19	m	306	CLA	C4B-C3B-CAB-CBB
19	n	204	CLA	C4B-C3B-CAB-CBB
21	A	831	LHG	C3-O3-P-O5
28	e	304	CHL	C4B-C3B-CAB-CBB
28	g	310	CHL	C4B-C3B-CAB-CBB
28	i	301	CHL	C4B-C3B-CAB-CBB
28	k	301	CHL	C4B-C3B-CAB-CBB
19	n	203	CLA	C11-C12-C13-C14
25	a	318	LMG	C18-C19-C20-C21
19	B	814	CLA	CBA-CGA-O2A-C1
21	A	831	LHG	O6-C4-C5-C6
19	o	311	CLA	O1A-CGA-O2A-C1
19	a	302	CLA	C2A-CAA-CBA-CGA
25	b	316	LMG	C14-C15-C16-C17
19	A	806	CLA	CAD-CBD-CGD-O1D
19	B	805	CLA	CAD-CBD-CGD-O1D
19	B	811	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B	818	CLA	CAD-CBD-CGD-O1D
19	B	839	CLA	CAD-CBD-CGD-O1D
19	a	304	CLA	CAD-CBD-CGD-O1D
19	b	315	CLA	CAD-CBD-CGD-O1D
19	c	310	CLA	CAD-CBD-CGD-O1D
19	c	316	CLA	CAD-CBD-CGD-O1D
19	f	312	CLA	CAD-CBD-CGD-O1D
19	i	308	CLA	C2-C3-C5-C6
19	i	309	CLA	CAD-CBD-CGD-O1D
19	j	310	CLA	CAD-CBD-CGD-O1D
19	m	308	CLA	CAD-CBD-CGD-O1D
28	b	301	CHL	CAD-CBD-CGD-O1D
28	e	301	CHL	CAD-CBD-CGD-O1D
19	d	206	CLA	CAA-CBA-CGA-O2A
19	A	802	CLA	C8-C10-C11-C12
19	F	203	CLA	O1A-CGA-O2A-C1
20	A	830	PQN	C25-C26-C27-C28
21	A	831	LHG	C18-C19-C20-C21
19	b	303	CLA	CBA-CGA-O2A-C1
19	A	821	CLA	C11-C12-C13-C15
19	A	843	CLA	C11-C12-C13-C15
19	B	801	CLA	C11-C10-C8-C7
19	B	808	CLA	C12-C13-C15-C16
19	B	840	CLA	C3A-C2A-CAA-CBA
19	F	202	CLA	C6-C7-C8-C10
19	b	306	CLA	C3A-C2A-CAA-CBA
19	i	310	CLA	C3A-C2A-CAA-CBA
19	l	203	CLA	C11-C10-C8-C7
19	m	307	CLA	C11-C10-C8-C7
20	A	830	PQN	C16-C17-C18-C20
28	c	305	CHL	C6-C7-C8-C10
19	B	806	CLA	C8-C10-C11-C12
19	i	309	CLA	C2A-CAA-CBA-CGA
19	o	307	CLA	C2A-CAA-CBA-CGA
28	f	301	CHL	C2A-CAA-CBA-CGA
27	B	829	DGD	C1G-C2G-C3G-O3G
28	b	312	CHL	C1C-C2C-CMC-OMC
25	c	320	LMG	O7-C8-C9-O8
27	B	829	DGD	O1G-C1G-C2G-O2G
25	a	318	LMG	C29-C30-C31-C32
25	f	313	LMG	C8-C7-O1-C1
19	g	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	a	303	CLA	C6-C7-C8-C9
19	A	803	CLA	C4-C3-C5-C6
19	B	812	CLA	C4-C3-C5-C6
19	k	302	CLA	C11-C10-C8-C9
25	i	316	LMG	C11-C12-C13-C14
19	a	303	CLA	C5-C6-C7-C8
19	A	803	CLA	C11-C10-C8-C9
19	A	824	CLA	C11-C10-C8-C9
19	A	850	CLA	C11-C10-C8-C9
19	B	804	CLA	C6-C7-C8-C9
19	B	815	CLA	C6-C7-C8-C9
19	F	203	CLA	C14-C13-C15-C16
25	e	312	LMG	C29-C30-C31-C32
19	B	832	CLA	C2A-CAA-CBA-CGA
28	e	304	CHL	C3-C5-C6-C7
19	F	201	CLA	CAA-CBA-CGA-O2A
19	A	801	CLA	C2B-C3B-CAB-CBB
19	A	802	CLA	C2B-C3B-CAB-CBB
19	A	814	CLA	C2B-C3B-CAB-CBB
19	A	815	CLA	C2B-C3B-CAB-CBB
19	A	829	CLA	C2B-C3B-CAB-CBB
19	A	846	CLA	C2B-C3B-CAB-CBB
19	B	833	CLA	C2B-C3B-CAB-CBB
19	b	304	CLA	C2B-C3B-CAB-CBB
19	d	207	CLA	C2B-C3B-CAB-CBB
19	e	306	CLA	C2B-C3B-CAB-CBB
19	f	308	CLA	C2B-C3B-CAB-CBB
19	f	314	CLA	C2B-C3B-CAB-CBB
19	g	311	CLA	C2B-C3B-CAB-CBB
19	h	213	CLA	C2B-C3B-CAB-CBB
19	i	311	CLA	C2B-C3B-CAB-CBB
19	i	313	CLA	C2B-C3B-CAB-CBB
19	j	304	CLA	C2B-C3B-CAB-CBB
19	j	305	CLA	C2B-C3B-CAB-CBB
19	j	311	CLA	C2B-C3B-CAB-CBB
19	j	312	CLA	C2B-C3B-CAB-CBB
19	k	304	CLA	C2B-C3B-CAB-CBB
19	k	308	CLA	C2B-C3B-CAB-CBB
19	l	207	CLA	C2B-C3B-CAB-CBB
19	n	204	CLA	C2B-C3B-CAB-CBB
28	e	304	CHL	C2B-C3B-CAB-CBB
25	i	316	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	B	829	DGD	C5A-C6A-C7A-C8A
19	c	307	CLA	C4-C3-C5-C6
27	B	829	DGD	CDB-CEB-CFB-CGB
19	l	204	CLA	C2-C3-C5-C6
19	g	307	CLA	C11-C12-C13-C14
19	h	209	CLA	C11-C12-C13-C15
19	B	816	CLA	C1-C2-C3-C4
25	g	313	LMG	C7-C8-O7-C10
19	A	822	CLA	C2A-CAA-CBA-CGA
19	A	841	CLA	C2A-CAA-CBA-CGA
19	b	304	CLA	C2A-CAA-CBA-CGA
19	b	313	CLA	C2A-CAA-CBA-CGA
19	h	212	CLA	C2A-CAA-CBA-CGA
19	m	302	CLA	C2A-CAA-CBA-CGA
19	n	209	CLA	C2A-CAA-CBA-CGA
28	g	306	CHL	C2A-CAA-CBA-CGA
27	B	829	DGD	C4A-C5A-C6A-C7A
19	b	306	CLA	C2-C1-O2A-CGA
19	c	306	CLA	C2-C1-O2A-CGA
19	f	309	CLA	C2-C1-O2A-CGA
19	g	309	CLA	C2-C1-O2A-CGA
19	i	309	CLA	C2-C1-O2A-CGA
19	j	305	CLA	C2-C1-O2A-CGA
28	b	301	CHL	C2-C1-O2A-CGA
28	d	205	CHL	C2-C1-O2A-CGA
19	o	307	CLA	C3-C5-C6-C7
25	g	312	LMG	C31-C32-C33-C34
19	A	823	CLA	C5-C6-C7-C8
19	A	827	CLA	O1A-CGA-O2A-C1
19	f	302	CLA	O1A-CGA-O2A-C1
19	g	302	CLA	O1A-CGA-O2A-C1
24	a	319	LMU	C3-C4-C5-C6
19	d	208	CLA	C4-C3-C5-C6
23	B	827	BCR	C23-C24-C25-C30
23	B	834	BCR	C23-C24-C25-C26
23	B	834	BCR	C23-C24-C25-C30
28	g	303	CHL	O1A-CGA-O2A-C1
19	B	837	CLA	O1D-CGD-O2D-CED
19	B	803	CLA	C5-C6-C7-C8
19	A	816	CLA	CAA-CBA-CGA-O2A
19	A	806	CLA	C10-C11-C12-C13
19	j	307	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	c	312	CHL	C6-C7-C8-C10
25	g	316	LMG	O6-C1-O1-C7
19	B	822	CLA	C5-C6-C7-C8
19	i	313	CLA	C2A-CAA-CBA-CGA
25	a	316	LMG	C2-C1-O1-C7
25	k	312	LMG	C2-C1-O1-C7
25	b	316	LMG	C21-C22-C23-C24
25	a	301	LMG	O7-C8-C9-O8
25	a	318	LMG	O1-C7-C8-O7
25	f	313	LMG	O1-C7-C8-O7
25	i	316	LMG	O7-C8-C9-O8
25	g	312	LMG	C11-C12-C13-C14
25	k	312	LMG	C28-C29-C30-C31
27	B	829	DGD	O1G-C1G-C2G-C3G
19	A	822	CLA	C4-C3-C5-C6
19	A	823	CLA	C4-C3-C5-C6
19	g	305	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	C2-C3-C5-C6
19	B	803	CLA	C2-C3-C5-C6
19	B	808	CLA	C6-C7-C8-C9
19	B	817	CLA	C6-C7-C8-C9
19	B	835	CLA	C6-C7-C8-C9
19	k	305	CLA	C6-C7-C8-C9
19	b	306	CLA	C11-C12-C13-C14
25	c	320	LMG	C16-C17-C18-C19
25	b	316	LMG	C12-C13-C14-C15
21	A	831	LHG	C7-C8-C9-C10
19	A	801	CLA	C16-C17-C18-C19
19	n	203	CLA	C11-C12-C13-C15
19	a	303	CLA	CBA-CGA-O2A-C1
19	B	836	CLA	C8-C10-C11-C12
19	k	302	CLA	C11-C10-C8-C7
19	B	839	CLA	CBA-CGA-O2A-C1
19	d	211	CLA	CBA-CGA-O2A-C1
19	e	303	CLA	CBA-CGA-O2A-C1
28	b	312	CHL	C2C-C3C-CAC-CBC
19	B	830	CLA	C5-C6-C7-C8
19	i	309	CLA	O1A-CGA-O2A-C1
19	A	814	CLA	C4B-C3B-CAB-CBB
19	B	818	CLA	C4B-C3B-CAB-CBB
19	B	833	CLA	C4B-C3B-CAB-CBB
19	B	836	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	a	304	CLA	C4B-C3B-CAB-CBB
19	a	310	CLA	C4B-C3B-CAB-CBB
19	g	311	CLA	C4B-C3B-CAB-CBB
19	j	301	CLA	C4B-C3B-CAB-CBB
19	j	304	CLA	C4B-C3B-CAB-CBB
19	j	305	CLA	C4B-C3B-CAB-CBB
19	k	304	CLA	C4B-C3B-CAB-CBB
19	j	312	CLA	C2A-CAA-CBA-CGA
19	n	206	CLA	C2A-CAA-CBA-CGA
19	A	813	CLA	C11-C12-C13-C15
19	A	811	CLA	C5-C6-C7-C8
25	c	320	LMG	C19-C20-C21-C22
19	B	836	CLA	C13-C15-C16-C17
19	g	301	CLA	C2-C1-O2A-CGA
19	o	311	CLA	C2-C1-O2A-CGA
19	A	829	CLA	C2A-CAA-CBA-CGA
19	B	805	CLA	C2A-CAA-CBA-CGA
19	B	817	CLA	C2A-CAA-CBA-CGA
19	e	306	CLA	C2A-CAA-CBA-CGA
19	o	305	CLA	C2A-CAA-CBA-CGA
19	A	847	CLA	C3A-C2A-CAA-CBA
19	B	810	CLA	C3A-C2A-CAA-CBA
19	B	811	CLA	C3A-C2A-CAA-CBA
19	B	835	CLA	C3A-C2A-CAA-CBA
19	B	849	CLA	C3A-C2A-CAA-CBA
19	i	309	CLA	C3A-C2A-CAA-CBA
19	j	311	CLA	C3A-C2A-CAA-CBA
19	j	312	CLA	C3A-C2A-CAA-CBA
19	l	206	CLA	C3A-C2A-CAA-CBA
19	n	204	CLA	C3A-C2A-CAA-CBA
28	b	301	CHL	C3A-C2A-CAA-CBA
28	m	301	CHL	C3A-C2A-CAA-CBA
19	b	303	CLA	O1A-CGA-O2A-C1
19	a	308	CLA	C8-C10-C11-C12
25	j	314	LMG	C14-C15-C16-C17
28	k	301	CHL	C2C-C3C-CAC-CBC
19	A	803	CLA	C2-C3-C5-C6
19	c	307	CLA	C2-C3-C5-C6
22	J	802	DD6	C27-C29-C30-C31
19	A	840	CLA	C6-C7-C8-C9
19	B	803	CLA	C11-C12-C13-C14
19	B	807	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	849	CLA	C6-C7-C8-C9
19	a	305	CLA	C6-C7-C8-C9
19	a	305	CLA	C11-C10-C8-C9
19	j	309	CLA	C6-C7-C8-C9
19	n	203	CLA	C6-C7-C8-C9
19	A	801	CLA	C16-C17-C18-C20
22	F	205	DD6	C4-C5-C6-C7
23	A	837	BCR	C11-C10-C9-C34
23	A	837	BCR	C16-C17-C18-C36
23	B	826	BCR	C11-C10-C9-C34
23	B	826	BCR	C20-C21-C22-C37
29	a	317	NEX	C39-C29-C30-C31
19	A	822	CLA	O2A-C1-C2-C3
19	A	841	CLA	O2A-C1-C2-C3
19	F	203	CLA	O2A-C1-C2-C3
19	b	303	CLA	O2A-C1-C2-C3
28	b	312	CHL	O2A-C1-C2-C3
27	B	829	DGD	CAB-CBB-CCB-CDB
25	a	301	LMG	C7-C8-O7-C10
19	A	826	CLA	C1A-C2A-CAA-CBA
19	A	846	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	C1A-C2A-CAA-CBA
19	B	805	CLA	C1A-C2A-CAA-CBA
19	B	811	CLA	C1A-C2A-CAA-CBA
19	j	304	CLA	C1A-C2A-CAA-CBA
28	b	310	CHL	C1A-C2A-CAA-CBA
28	b	311	CHL	C1A-C2A-CAA-CBA
28	f	301	CHL	C1A-C2A-CAA-CBA
19	A	822	CLA	C12-C13-C15-C16
19	F	203	CLA	C6-C7-C8-C10
19	m	305	CLA	C6-C7-C8-C10
20	B	824	PQN	C21-C22-C23-C25
25	e	312	LMG	C11-C12-C13-C14
19	A	840	CLA	C2A-CAA-CBA-CGA
28	c	305	CHL	C2A-CAA-CBA-CGA
28	g	303	CHL	C2A-CAA-CBA-CGA
19	A	809	CLA	C13-C15-C16-C17
20	B	824	PQN	C23-C25-C26-C27
19	B	847	CLA	C15-C16-C17-C18
19	B	847	CLA	C4-C3-C5-C6
19	B	814	CLA	C8-C10-C11-C12
19	A	816	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A	850	CLA	C2B-C3B-CAB-CBB
19	B	836	CLA	C2B-C3B-CAB-CBB
19	B	840	CLA	C2B-C3B-CAB-CBB
19	B	842	CLA	C2B-C3B-CAB-CBB
19	B	846	CLA	C2B-C3B-CAB-CBB
19	B	847	CLA	C2B-C3B-CAB-CBB
19	F	202	CLA	C2B-C3B-CAB-CBB
19	c	307	CLA	C2B-C3B-CAB-CBB
19	g	308	CLA	C2B-C3B-CAB-CBB
19	h	206	CLA	C2B-C3B-CAB-CBB
19	i	309	CLA	C2B-C3B-CAB-CBB
19	k	306	CLA	C2B-C3B-CAB-CBB
19	n	205	CLA	C2B-C3B-CAB-CBB
28	g	310	CHL	C2B-C3B-CAB-CBB
28	i	301	CHL	C2B-C3B-CAB-CBB
28	k	301	CHL	C2B-C3B-CAB-CBB
25	c	320	LMG	O9-C10-O7-C8
25	i	316	LMG	C29-C30-C31-C32
22	F	205	DD6	C4-C5-C6-C8
23	A	837	BCR	C11-C10-C9-C8
23	A	837	BCR	C16-C17-C18-C19
23	B	826	BCR	C11-C10-C9-C8
23	B	826	BCR	C20-C21-C22-C23
29	a	317	NEX	C28-C29-C30-C31
19	B	849	CLA	C5-C6-C7-C8
19	B	833	CLA	C2A-CAA-CBA-CGA
19	B	807	CLA	C4-C3-C5-C6
19	B	810	CLA	C4-C3-C5-C6
19	k	310	CLA	C4-C3-C5-C6
19	m	310	CLA	C4-C3-C5-C6
19	A	805	CLA	C2-C1-O2A-CGA
19	A	852	CLA	C2-C1-O2A-CGA
19	c	303	CLA	C2-C1-O2A-CGA
19	o	302	CLA	C2-C1-O2A-CGA
19	B	812	CLA	C2-C3-C5-C6
19	n	206	CLA	C2-C1-O2A-CGA
19	n	205	CLA	C6-C7-C8-C9
19	h	212	CLA	C3-C5-C6-C7
24	a	319	LMU	C9-C10-C11-C12
19	A	820	CLA	C5-C6-C7-C8
19	A	853	CLA	C2-C1-O2A-CGA
19	n	209	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
28	c	305	CHL	O1A-CGA-O2A-C1
23	B	827	BCR	C23-C24-C25-C26
23	M	801	BCR	C1-C6-C7-C8
19	A	847	CLA	CAA-CBA-CGA-O2A
19	i	312	CLA	CAA-CBA-CGA-O2A
19	j	309	CLA	C5-C6-C7-C8
19	B	814	CLA	O1A-CGA-O2A-C1
19	n	203	CLA	CBA-CGA-O2A-C1
19	A	817	CLA	C4-C3-C5-C6
19	A	850	CLA	C4-C3-C5-C6
19	B	818	CLA	C4-C3-C5-C6
19	e	310	CLA	C4-C3-C5-C6
19	g	302	CLA	C4-C3-C5-C6
20	A	830	PQN	C14-C13-C15-C16
22	c	317	DD6	C2-C1-C24-C25
19	A	823	CLA	C2-C3-C5-C6
19	b	306	CLA	CAA-CBA-CGA-O1A
25	e	312	LMG	C8-C7-O1-C1
19	c	311	CLA	CAA-CBA-CGA-O2A
25	c	320	LMG	C14-C15-C16-C17
19	B	837	CLA	CBD-CGD-O2D-CED
19	B	846	CLA	C2A-CAA-CBA-CGA
19	B	838	CLA	CBA-CGA-O2A-C1
19	A	820	CLA	C4B-C3B-CAB-CBB
19	A	828	CLA	C4B-C3B-CAB-CBB
19	A	840	CLA	C4B-C3B-CAB-CBB
19	d	204	CLA	C4B-C3B-CAB-CBB
19	h	209	CLA	C4B-C3B-CAB-CBB
19	i	306	CLA	C4B-C3B-CAB-CBB
19	n	205	CLA	C4B-C3B-CAB-CBB
19	o	312	CLA	C4B-C3B-CAB-CBB
28	i	304	CHL	C4B-C3B-CAB-CBB
25	g	316	LMG	C24-C25-C26-C27
19	n	204	CLA	CAA-CBA-CGA-O2A
19	a	305	CLA	C4-C3-C5-C6
24	A	838	LMU	C11-C10-C9-C8
25	a	301	LMG	C17-C18-C19-C20
19	B	803	CLA	C6-C7-C8-C10
19	a	305	CLA	C2-C3-C5-C6
19	a	305	CLA	C6-C7-C8-C10
19	e	310	CLA	C2-C3-C5-C6
19	k	302	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	n	203	CLA	C6-C7-C8-C10
19	A	841	CLA	C8-C10-C11-C12
28	b	314	CHL	C1-C2-C3-C4
28	c	305	CHL	C1-C2-C3-C4
28	c	313	CHL	C1-C2-C3-C4
19	f	306	CLA	CAA-CBA-CGA-O2A
25	g	312	LMG	O7-C10-C11-C12
19	h	211	CLA	C2A-CAA-CBA-CGA
21	A	831	LHG	C8-C7-O7-C5
19	A	815	CLA	CBA-CGA-O2A-C1
19	A	820	CLA	CBA-CGA-O2A-C1
19	A	807	CLA	CAA-CBA-CGA-O2A
19	B	801	CLA	CAA-CBA-CGA-O2A
19	f	303	CLA	CAA-CBA-CGA-O2A
19	i	310	CLA	CAA-CBA-CGA-O2A
25	a	318	LMG	O7-C10-C11-C12
19	A	819	CLA	C4-C3-C5-C6
19	g	309	CLA	C4-C3-C5-C6
19	m	311	CLA	CAA-CBA-CGA-O2A
19	A	843	CLA	C11-C12-C13-C14
19	B	807	CLA	C6-C7-C8-C9
19	B	812	CLA	C11-C12-C13-C14
19	B	820	CLA	C11-C10-C8-C9
19	F	202	CLA	C6-C7-C8-C9
19	f	309	CLA	C11-C10-C8-C9
19	m	307	CLA	C11-C10-C8-C9
19	A	818	CLA	C3A-C2A-CAA-CBA
19	B	805	CLA	C3A-C2A-CAA-CBA
19	b	302	CLA	C3A-C2A-CAA-CBA
19	f	311	CLA	C3A-C2A-CAA-CBA
19	k	302	CLA	C3A-C2A-CAA-CBA
19	m	311	CLA	C3A-C2A-CAA-CBA
19	o	307	CLA	C3A-C2A-CAA-CBA
28	e	301	CHL	C3A-C2A-CAA-CBA
19	d	211	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	CAA-CBA-CGA-O2A
19	B	840	CLA	CAA-CBA-CGA-O2A
19	b	313	CLA	CAA-CBA-CGA-O2A
19	A	820	CLA	CAD-CBD-CGD-O2D
19	A	821	CLA	CAD-CBD-CGD-O2D
19	A	829	CLA	CAD-CBD-CGD-O2D
19	A	844	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	853	CLA	CAD-CBD-CGD-O2D
19	B	814	CLA	CAD-CBD-CGD-O2D
19	B	823	CLA	CAD-CBD-CGD-O2D
19	B	832	CLA	CAD-CBD-CGD-O2D
19	B	836	CLA	CAD-CBD-CGD-O2D
19	B	837	CLA	CAD-CBD-CGD-O2D
19	B	840	CLA	CAD-CBD-CGD-O2D
19	B	843	CLA	CAD-CBD-CGD-O2D
19	b	303	CLA	CAD-CBD-CGD-O2D
19	c	302	CLA	CAD-CBD-CGD-O2D
19	c	306	CLA	CAD-CBD-CGD-O2D
19	c	307	CLA	CAD-CBD-CGD-O2D
19	c	315	CLA	CAD-CBD-CGD-O2D
19	d	210	CLA	CAD-CBD-CGD-O2D
19	i	308	CLA	CAD-CBD-CGD-O2D
19	i	310	CLA	CAD-CBD-CGD-O2D
19	k	302	CLA	CAD-CBD-CGD-O2D
19	k	303	CLA	CAD-CBD-CGD-O2D
19	k	310	CLA	CAD-CBD-CGD-O2D
19	k	311	CLA	CAD-CBD-CGD-O2D
19	n	205	CLA	CAD-CBD-CGD-O2D
19	n	209	CLA	CAD-CBD-CGD-O2D
19	o	307	CLA	CAD-CBD-CGD-O2D
19	o	311	CLA	CAD-CBD-CGD-O2D
25	i	316	LMG	C9-C8-O7-C10
28	g	310	CHL	CAD-CBD-CGD-O2D
19	m	305	CLA	C4C-C3C-CAC-CBC
28	k	301	CHL	C4C-C3C-CAC-CBC
19	j	305	CLA	CAA-CBA-CGA-O2A
19	j	306	CLA	CAA-CBA-CGA-O2A
28	d	205	CHL	CAA-CBA-CGA-O2A
19	n	203	CLA	C10-C11-C12-C13
28	e	304	CHL	C4-C3-C5-C6
19	A	819	CLA	C2-C3-C5-C6
19	a	304	CLA	CAA-CBA-CGA-O2A
19	d	204	CLA	CAA-CBA-CGA-O2A
19	i	306	CLA	CAA-CBA-CGA-O2A
19	m	309	CLA	CAA-CBA-CGA-O2A
19	o	303	CLA	CAA-CBA-CGA-O2A
25	c	320	LMG	O7-C10-C11-C12
28	b	311	CHL	CAA-CBA-CGA-O2A
28	b	312	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	i	301	CHL	CAA-CBA-CGA-O2A
24	A	838	LMU	O5B-C1B-O1B-C4'
19	B	849	CLA	C14-C13-C15-C16
22	A	833	DD6	C13-C14-C15-O1
22	e	313	DD6	C13-C14-C15-O1
25	i	316	LMG	O1-C7-C8-C9
19	A	843	CLA	CAA-CBA-CGA-O2A
19	B	804	CLA	CAA-CBA-CGA-O2A
19	B	830	CLA	CAA-CBA-CGA-O2A
19	B	838	CLA	CAA-CBA-CGA-O2A
19	c	307	CLA	CAA-CBA-CGA-O2A
19	i	313	CLA	CAA-CBA-CGA-O2A
19	o	311	CLA	CAA-CBA-CGA-O2A
19	B	817	CLA	CAA-CBA-CGA-O1A
19	A	818	CLA	O2A-C1-C2-C3
19	A	821	CLA	O2A-C1-C2-C3
19	B	804	CLA	O2A-C1-C2-C3
19	B	806	CLA	O2A-C1-C2-C3
19	B	837	CLA	O2A-C1-C2-C3
19	B	847	CLA	O2A-C1-C2-C3
19	j	311	CLA	O2A-C1-C2-C3
19	k	302	CLA	O2A-C1-C2-C3
19	l	204	CLA	O2A-C1-C2-C3
19	o	311	CLA	C2A-CAA-CBA-CGA
19	k	304	CLA	C5-C6-C7-C8
19	A	820	CLA	CAA-CBA-CGA-O2A
19	e	306	CLA	CAA-CBA-CGA-O2A
19	l	208	CLA	CAA-CBA-CGA-O2A
19	a	303	CLA	O1A-CGA-O2A-C1
19	j	307	CLA	C11-C12-C13-C15
27	B	829	DGD	CFB-CGB-CHB-CIB
19	A	809	CLA	CHA-CBD-CGD-O1D
19	A	809	CLA	CHA-CBD-CGD-O2D
19	A	814	CLA	CHA-CBD-CGD-O2D
19	A	840	CLA	CHA-CBD-CGD-O1D
19	A	849	CLA	CHA-CBD-CGD-O2D
19	B	804	CLA	CHA-CBD-CGD-O2D
19	B	807	CLA	CHA-CBD-CGD-O1D
19	B	807	CLA	CHA-CBD-CGD-O2D
19	B	811	CLA	CHA-CBD-CGD-O1D
19	B	813	CLA	CHA-CBD-CGD-O2D
19	B	844	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	848	CLA	CHA-CBD-CGD-O1D
19	B	848	CLA	CHA-CBD-CGD-O2D
19	D	301	CLA	CHA-CBD-CGD-O1D
19	D	301	CLA	CHA-CBD-CGD-O2D
19	J	803	CLA	CHA-CBD-CGD-O1D
19	a	304	CLA	CHA-CBD-CGD-O2D
19	b	307	CLA	CHA-CBD-CGD-O1D
19	b	307	CLA	CHA-CBD-CGD-O2D
19	c	303	CLA	CHA-CBD-CGD-O1D
19	c	303	CLA	CHA-CBD-CGD-O2D
19	c	304	CLA	CHA-CBD-CGD-O2D
19	c	308	CLA	CHA-CBD-CGD-O1D
19	c	311	CLA	CHA-CBD-CGD-O2D
19	e	303	CLA	CHA-CBD-CGD-O2D
19	f	307	CLA	CHA-CBD-CGD-O2D
19	g	305	CLA	CHA-CBD-CGD-O1D
19	g	305	CLA	CHA-CBD-CGD-O2D
19	h	207	CLA	CHA-CBD-CGD-O2D
19	h	209	CLA	CHA-CBD-CGD-O1D
19	h	209	CLA	CHA-CBD-CGD-O2D
19	i	302	CLA	CHA-CBD-CGD-O1D
19	i	302	CLA	CHA-CBD-CGD-O2D
19	i	307	CLA	CHA-CBD-CGD-O2D
19	j	306	CLA	CHA-CBD-CGD-O1D
19	j	306	CLA	CHA-CBD-CGD-O2D
19	j	308	CLA	CHA-CBD-CGD-O1D
19	j	308	CLA	CHA-CBD-CGD-O2D
19	k	307	CLA	CHA-CBD-CGD-O2D
19	l	201	CLA	CHA-CBD-CGD-O1D
19	l	201	CLA	CHA-CBD-CGD-O2D
19	l	205	CLA	CHA-CBD-CGD-O1D
19	n	208	CLA	CHA-CBD-CGD-O2D
19	o	303	CLA	CHA-CBD-CGD-O1D
19	o	303	CLA	CHA-CBD-CGD-O2D
19	o	306	CLA	CHA-CBD-CGD-O1D
19	o	306	CLA	CHA-CBD-CGD-O2D
28	f	301	CHL	CHA-CBD-CGD-O2D
28	g	306	CHL	CHA-CBD-CGD-O1D
28	h	202	CHL	CHA-CBD-CGD-O2D
28	i	301	CHL	CHA-CBD-CGD-O2D
28	k	301	CHL	CHA-CBD-CGD-O1D
28	o	301	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	b	302	CLA	CAA-CBA-CGA-O2A
19	A	817	CLA	C2-C3-C5-C6
19	B	818	CLA	C2-C3-C5-C6
19	h	204	CLA	O2A-C1-C2-C3
25	c	320	LMG	C12-C13-C14-C15
28	c	312	CHL	C6-C7-C8-C9
19	A	812	CLA	CAA-CBA-CGA-O2A
19	e	310	CLA	CAA-CBA-CGA-O2A
25	f	313	LMG	C11-C12-C13-C14
19	B	823	CLA	CAA-CBA-CGA-O2A
19	a	307	CLA	CAA-CBA-CGA-O2A
19	c	309	CLA	CAA-CBA-CGA-O2A
19	c	314	CLA	CAA-CBA-CGA-O2A
19	l	204	CLA	CAA-CBA-CGA-O2A
19	m	303	CLA	CAA-CBA-CGA-O2A
19	k	302	CLA	C5-C6-C7-C8
19	e	302	CLA	CAA-CBA-CGA-O2A
19	m	302	CLA	CAA-CBA-CGA-O2A
19	o	308	CLA	CAA-CBA-CGA-O2A
19	A	824	CLA	C11-C10-C8-C7
19	d	208	CLA	C2-C3-C5-C6
19	h	208	CLA	C6-C7-C8-C10
19	n	203	CLA	C11-C10-C8-C7
19	i	309	CLA	C11-C12-C13-C14
19	B	811	CLA	CAA-CBA-CGA-O2A
19	h	209	CLA	CAA-CBA-CGA-O2A
19	h	211	CLA	CAA-CBA-CGA-O2A
28	a	315	CHL	CAA-CBA-CGA-O2A
19	B	801	CLA	C11-C10-C8-C9
19	n	203	CLA	C11-C10-C8-C9
19	A	843	CLA	CAA-CBA-CGA-O1A
19	n	204	CLA	C5-C6-C7-C8
19	A	828	CLA	C2B-C3B-CAB-CBB
19	d	204	CLA	C2B-C3B-CAB-CBB
19	b	305	CLA	C2-C1-O2A-CGA
28	h	202	CHL	CBA-CGA-O2A-C1
19	A	810	CLA	CAA-CBA-CGA-O2A
28	i	304	CHL	C2A-CAA-CBA-CGA
19	m	309	CLA	CAA-CBA-CGA-O1A
19	m	310	CLA	CAA-CBA-CGA-O2A
25	i	316	LMG	O7-C10-C11-C12
19	A	807	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	B	801	CLA	CAA-CBA-CGA-O1A
19	B	830	CLA	CAA-CBA-CGA-O1A
19	m	311	CLA	CAA-CBA-CGA-O1A
19	A	850	CLA	C2-C3-C5-C6
19	B	810	CLA	C2-C3-C5-C6
24	a	319	LMU	C2B-C1B-O1B-C4'
25	g	316	LMG	C12-C13-C14-C15
28	i	301	CHL	CAA-CBA-CGA-O1A
19	A	819	CLA	C1A-C2A-CAA-CBA
19	B	810	CLA	C1A-C2A-CAA-CBA
19	B	835	CLA	C1A-C2A-CAA-CBA
19	F	202	CLA	C1A-C2A-CAA-CBA
19	a	305	CLA	C1A-C2A-CAA-CBA
19	c	311	CLA	C1A-C2A-CAA-CBA
19	i	309	CLA	C1A-C2A-CAA-CBA
19	i	311	CLA	C1A-C2A-CAA-CBA
19	l	202	CLA	C1A-C2A-CAA-CBA
19	m	311	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	CAA-CBA-CGA-O1A
19	c	307	CLA	CAA-CBA-CGA-O1A
19	f	306	CLA	CAA-CBA-CGA-O1A
19	i	310	CLA	CAA-CBA-CGA-O1A
25	i	316	LMG	O10-C28-C29-C30
19	d	204	CLA	CAA-CBA-CGA-O1A
19	i	306	CLA	CAA-CBA-CGA-O1A
19	j	305	CLA	CAA-CBA-CGA-O1A
19	l	203	CLA	CAA-CBA-CGA-O1A
28	c	312	CHL	CAA-CBA-CGA-O1A
27	B	829	DGD	C6A-C7A-C8A-C9A
25	a	301	LMG	C7-C8-C9-O8
25	f	313	LMG	O1-C7-C8-C9
19	B	846	CLA	CAA-CBA-CGA-O2A
19	j	304	CLA	C2A-CAA-CBA-CGA
19	B	823	CLA	CAA-CBA-CGA-O1A
19	B	840	CLA	CAA-CBA-CGA-O1A
19	j	306	CLA	CAA-CBA-CGA-O1A
19	l	208	CLA	CAA-CBA-CGA-O1A
27	B	829	DGD	CBB-CCB-CDB-CEB
19	k	302	CLA	C4-C3-C5-C6
25	g	316	LMG	O7-C10-C11-C12
19	g	308	CLA	C5-C6-C7-C8
19	e	302	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	f	303	CLA	CAA-CBA-CGA-O1A
19	m	303	CLA	CAA-CBA-CGA-O1A
28	c	313	CHL	CAA-CBA-CGA-O1A
19	B	847	CLA	C10-C11-C12-C13
19	A	801	CLA	C4B-C3B-CAB-CBB
19	a	309	CLA	C4B-C3B-CAB-CBB
19	c	308	CLA	C4B-C3B-CAB-CBB
19	d	201	CLA	C4B-C3B-CAB-CBB
28	d	202	CHL	C4B-C3B-CAB-CBB
28	f	301	CHL	C4B-C3B-CAB-CBB
19	A	806	CLA	CAA-CBA-CGA-O1A
19	a	304	CLA	CAA-CBA-CGA-O1A
19	e	306	CLA	CAA-CBA-CGA-O1A
28	b	311	CHL	CAA-CBA-CGA-O1A
19	A	840	CLA	CAA-CBA-CGA-O2A
19	A	812	CLA	CAA-CBA-CGA-O1A
19	B	838	CLA	CAA-CBA-CGA-O1A
19	i	313	CLA	CAA-CBA-CGA-O1A
19	m	302	CLA	CAA-CBA-CGA-O1A
19	o	303	CLA	CAA-CBA-CGA-O1A
25	g	313	LMG	O9-C10-C11-C12
19	f	314	CLA	CAA-CBA-CGA-O2A
19	A	820	CLA	CAA-CBA-CGA-O1A
19	B	811	CLA	CAA-CBA-CGA-O1A
19	B	832	CLA	CAA-CBA-CGA-O2A
19	g	311	CLA	CAA-CBA-CGA-O2A
19	o	307	CLA	CAA-CBA-CGA-O2A
25	f	313	LMG	O7-C10-C11-C12
25	b	316	LMG	C29-C30-C31-C32
19	b	302	CLA	CAA-CBA-CGA-O1A
25	a	301	LMG	C31-C32-C33-C34
19	A	812	CLA	CAD-CBD-CGD-O1D
19	A	825	CLA	CAD-CBD-CGD-O1D
19	A	843	CLA	CAD-CBD-CGD-O1D
19	A	850	CLA	CAD-CBD-CGD-O1D
19	B	807	CLA	CAD-CBD-CGD-O1D
19	J	803	CLA	CAD-CBD-CGD-O1D
19	a	307	CLA	CAD-CBD-CGD-O1D
19	c	303	CLA	CAD-CBD-CGD-O1D
19	g	308	CLA	CAD-CBD-CGD-O1D
19	i	302	CLA	CAD-CBD-CGD-O1D
19	i	306	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	l	206	CLA	CAD-CBD-CGD-O1D
19	l	207	CLA	CAD-CBD-CGD-O1D
25	a	301	LMG	C9-C8-O7-C10
25	i	316	LMG	C7-C8-O7-C10
28	g	306	CHL	CAD-CBD-CGD-O1D
28	k	301	CHL	CAD-CBD-CGD-O1D
29	a	317	NEX	C7-C8-C9-C10
28	d	202	CHL	CAA-CBA-CGA-O1A
19	A	801	CLA	CAA-CBA-CGA-O2A
19	c	315	CLA	CAA-CBA-CGA-O2A
19	d	207	CLA	CAA-CBA-CGA-O2A
19	o	306	CLA	CAA-CBA-CGA-O2A
25	A	851	LMG	O8-C28-C29-C30
19	B	806	CLA	C14-C13-C15-C16
19	m	305	CLA	C6-C7-C8-C9
20	A	830	PQN	C16-C17-C18-C19
19	A	840	CLA	C8-C10-C11-C12
19	i	307	CLA	CAA-CBA-CGA-O2A
19	k	310	CLA	CAA-CBA-CGA-O2A
28	c	312	CHL	CAA-CBA-CGA-O2A
28	d	202	CHL	CAA-CBA-CGA-O2A
25	g	316	LMG	O9-C10-C11-C12
19	f	306	CLA	C2C-C3C-CAC-CBC
19	j	303	CLA	C2A-CAA-CBA-CGA
19	A	844	CLA	CAA-CBA-CGA-O2A
19	A	848	CLA	CAA-CBA-CGA-O2A
19	F	203	CLA	CAA-CBA-CGA-O2A
19	h	204	CLA	CAA-CBA-CGA-O2A
25	j	314	LMG	O7-C10-C11-C12
25	e	312	LMG	C14-C15-C16-C17
19	B	846	CLA	CAA-CBA-CGA-O1A
19	c	309	CLA	CAA-CBA-CGA-O1A
19	h	209	CLA	CAA-CBA-CGA-O1A
19	o	308	CLA	CAA-CBA-CGA-O1A
25	f	313	LMG	O9-C10-C11-C12
25	A	851	LMG	C30-C31-C32-C33
19	A	826	CLA	C3A-C2A-CAA-CBA
19	B	803	CLA	C12-C13-C15-C16
19	B	807	CLA	C2-C3-C5-C6
19	B	849	CLA	C6-C7-C8-C10
19	F	202	CLA	C3A-C2A-CAA-CBA
19	a	314	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	c	311	CLA	C3A-C2A-CAA-CBA
19	f	309	CLA	C6-C7-C8-C10
19	i	311	CLA	C3A-C2A-CAA-CBA
19	j	309	CLA	C6-C7-C8-C10
19	n	205	CLA	C6-C7-C8-C10
19	k	310	CLA	CAA-CBA-CGA-O1A
19	o	302	CLA	CAA-CBA-CGA-O1A
25	a	318	LMG	O9-C10-C11-C12
25	c	320	LMG	O9-C10-C11-C12
19	A	829	CLA	CAA-CBA-CGA-O2A
19	A	853	CLA	CAA-CBA-CGA-O2A
19	e	308	CLA	CAA-CBA-CGA-O2A
19	f	309	CLA	CAA-CBA-CGA-O2A
19	f	312	CLA	CAA-CBA-CGA-O2A
19	h	212	CLA	CAA-CBA-CGA-O2A
19	n	208	CLA	CAA-CBA-CGA-O2A
19	o	302	CLA	CAA-CBA-CGA-O2A
28	f	301	CHL	CAA-CBA-CGA-O2A
19	j	310	CLA	C2-C1-O2A-CGA
19	c	309	CLA	C5-C6-C7-C8
19	l	204	CLA	CAA-CBA-CGA-O1A
19	m	310	CLA	CAA-CBA-CGA-O1A
19	n	208	CLA	CAA-CBA-CGA-O1A
28	d	205	CHL	CAA-CBA-CGA-O1A
19	e	309	CLA	CAA-CBA-CGA-O2A
19	j	301	CLA	CAA-CBA-CGA-O2A
19	j	308	CLA	CAA-CBA-CGA-O2A
19	m	308	CLA	CAA-CBA-CGA-O2A
19	A	806	CLA	C5-C6-C7-C8
19	B	839	CLA	O1A-CGA-O2A-C1
19	a	307	CLA	CAA-CBA-CGA-O1A
19	e	310	CLA	CAA-CBA-CGA-O1A
19	o	306	CLA	CAA-CBA-CGA-O1A
19	B	810	CLA	C5-C6-C7-C8
19	c	304	CLA	CAA-CBA-CGA-O2A
19	B	822	CLA	C13-C15-C16-C17
19	o	307	CLA	C8-C10-C11-C12
19	A	810	CLA	CAA-CBA-CGA-O1A
19	A	853	CLA	CAA-CBA-CGA-O1A
19	F	203	CLA	CAA-CBA-CGA-O1A
19	c	314	CLA	CAA-CBA-CGA-O1A
19	f	314	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	h	204	CLA	CAA-CBA-CGA-O1A
19	m	308	CLA	CAA-CBA-CGA-O1A
28	b	314	CHL	C2A-CAA-CBA-CGA
19	B	839	CLA	C10-C11-C12-C13
28	b	314	CHL	CBA-CGA-O2A-C1
19	A	829	CLA	CAA-CBA-CGA-O1A
19	A	844	CLA	CAA-CBA-CGA-O1A
19	B	809	CLA	CAA-CBA-CGA-O2A
19	g	307	CLA	CAA-CBA-CGA-O2A
19	i	309	CLA	CAA-CBA-CGA-O2A
19	k	311	CLA	CAA-CBA-CGA-O2A
21	A	831	LHG	O7-C7-C8-C9

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	a	319	LMU	C1'-C2'-C3'-C4'-C5'-O5'

152 monomers are involved in 270 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	831	BCR	1	0
19	J	803	CLA	1	0
19	B	848	CLA	1	0
25	c	320	LMG	6	0
19	k	305	CLA	1	0
19	b	302	CLA	1	0
19	j	305	CLA	3	0
22	m	313	DD6	1	0
19	n	202	CLA	3	0
19	B	838	CLA	2	0
28	b	301	CHL	2	0
28	i	304	CHL	1	0
25	i	316	LMG	7	0
28	b	311	CHL	1	0
25	a	316	LMG	1	0
22	e	313	DD6	10	0
19	B	814	CLA	1	0
19	D	301	CLA	1	0
19	F	204	CLA	1	0
19	B	841	CLA	1	0
19	A	809	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	n	205	CLA	2	0
19	l	202	CLA	1	0
23	B	850	BCR	2	0
19	A	802	CLA	1	0
19	A	829	CLA	1	0
19	n	209	CLA	1	0
19	B	837	CLA	2	0
19	b	309	CLA	1	0
19	A	841	CLA	1	0
22	g	315	DD6	1	0
19	j	310	CLA	1	0
23	M	801	BCR	7	0
28	i	301	CHL	1	0
19	B	812	CLA	1	0
19	l	203	CLA	1	0
28	d	202	CHL	2	0
19	m	303	CLA	1	0
28	m	301	CHL	2	0
22	i	314	DD6	1	0
19	n	206	CLA	13	0
19	A	822	CLA	1	0
25	d	213	LMG	1	0
19	o	302	CLA	3	0
28	a	315	CHL	4	0
25	h	216	LMG	2	0
28	b	310	CHL	3	0
19	m	302	CLA	1	0
19	d	207	CLA	1	0
19	i	307	CLA	1	0
19	n	203	CLA	4	0
19	B	823	CLA	1	0
19	B	833	CLA	2	0
28	h	202	CHL	2	0
23	A	837	BCR	1	0
22	j	316	DD6	11	0
19	B	843	CLA	1	0
25	a	318	LMG	2	0
19	o	309	CLA	1	0
19	d	209	CLA	1	0
19	B	803	CLA	1	0
28	a	311	CHL	1	0
19	j	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	f	314	CLA	1	0
19	h	201	CLA	2	0
19	b	306	CLA	4	0
22	a	321	DD6	5	0
28	d	205	CHL	3	0
19	A	808	CLA	1	0
19	B	807	CLA	1	0
25	a	301	LMG	3	0
28	g	303	CHL	1	0
19	o	307	CLA	1	0
19	B	844	CLA	1	0
19	i	309	CLA	1	0
19	a	306	CLA	5	0
23	A	836	BCR	1	0
19	e	310	CLA	3	0
23	J	804	BCR	6	0
24	A	838	LMU	1	0
28	g	306	CHL	1	0
19	A	842	CLA	2	0
19	A	803	CLA	1	0
19	n	204	CLA	2	0
19	e	308	CLA	1	0
19	g	304	CLA	1	0
19	f	311	CLA	1	0
24	c	301	LMU	3	0
19	A	853	CLA	3	0
19	m	307	CLA	1	0
19	A	804	CLA	1	0
19	A	845	CLA	1	0
22	g	314	DD6	4	0
28	k	301	CHL	3	0
19	j	304	CLA	2	0
19	a	302	CLA	1	0
19	B	840	CLA	1	0
28	c	313	CHL	3	0
19	j	306	CLA	12	0
19	d	210	CLA	1	0
28	o	301	CHL	2	0
19	d	208	CLA	3	0
19	B	845	CLA	1	0
19	k	304	CLA	1	0
19	o	304	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	J	802	DD6	1	0
19	j	302	CLA	1	0
19	B	832	CLA	1	0
23	A	835	BCR	1	0
19	B	849	CLA	2	0
19	o	303	CLA	8	0
25	f	313	LMG	1	0
19	f	302	CLA	1	0
19	A	819	CLA	1	0
25	g	312	LMG	1	0
19	j	307	CLA	1	0
22	f	315	DD6	2	0
28	e	304	CHL	12	0
28	c	312	CHL	5	0
19	j	313	CLA	1	0
27	B	829	DGD	2	0
19	b	315	CLA	1	0
19	n	201	CLA	1	0
23	B	826	BCR	3	0
19	b	305	CLA	3	0
19	g	301	CLA	1	0
19	F	201	CLA	1	0
19	A	810	CLA	3	0
19	k	302	CLA	2	0
22	n	210	DD6	10	0
22	o	313	DD6	6	0
25	b	316	LMG	2	0
25	k	312	LMG	2	0
19	h	203	CLA	2	0
22	c	318	DD6	2	0
28	b	312	CHL	4	0
19	l	201	CLA	9	0
28	a	312	CHL	6	0
19	a	314	CLA	1	0
19	o	310	CLA	2	0
22	b	318	DD6	2	0
28	f	301	CHL	2	0
22	l	210	DD6	5	0
28	g	310	CHL	6	0
19	m	305	CLA	1	0
28	c	305	CHL	4	0
19	B	801	CLA	2	0

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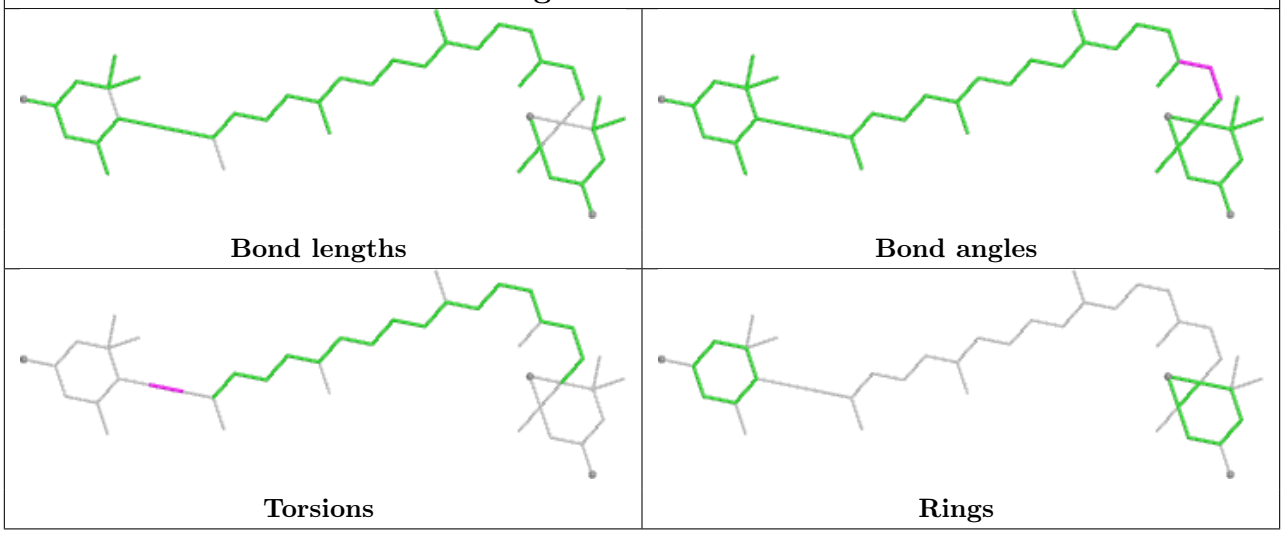
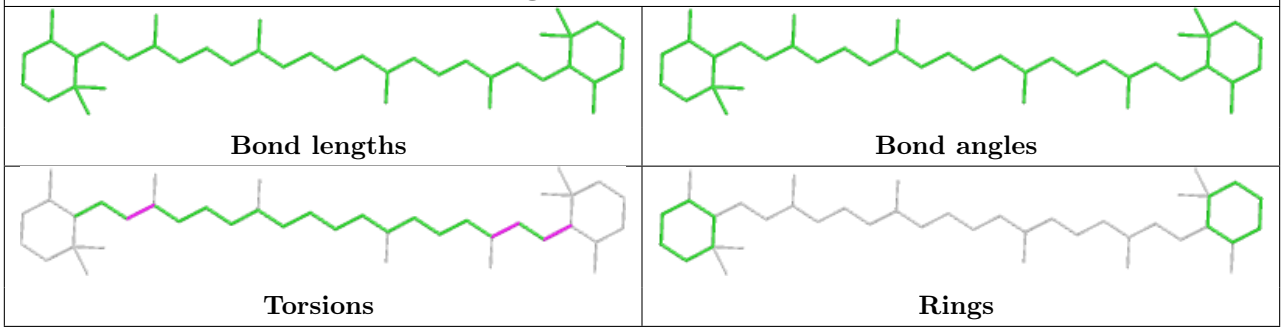
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	c	303	CLA	1	0
19	f	303	CLA	1	0
19	d	203	CLA	1	0
19	A	816	CLA	1	0
28	f	304	CHL	3	0

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.

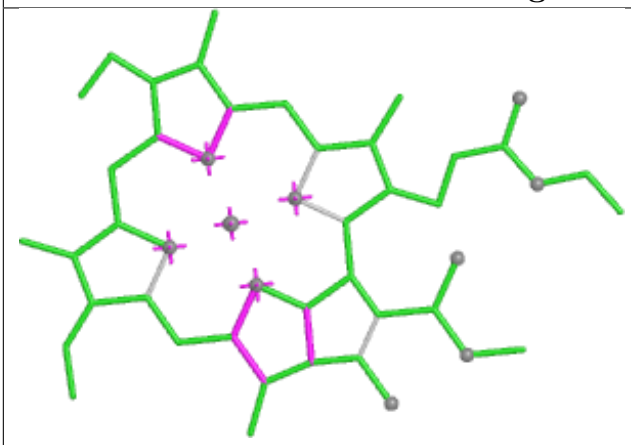
Ligand DD6 f 316



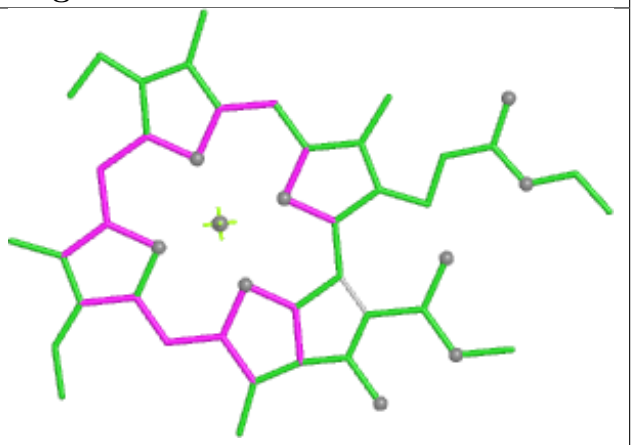
Ligand BCR B 831



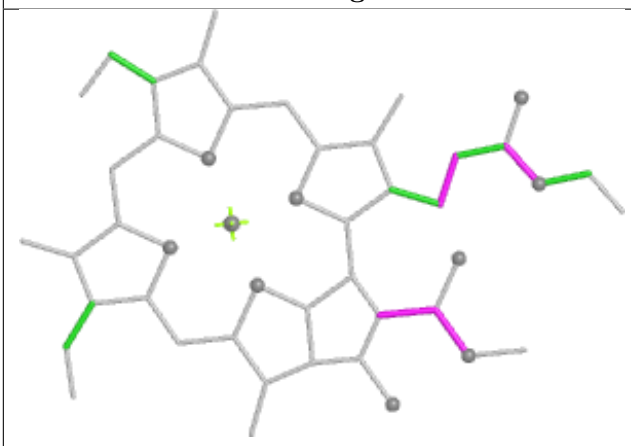
Ligand CLA g 305



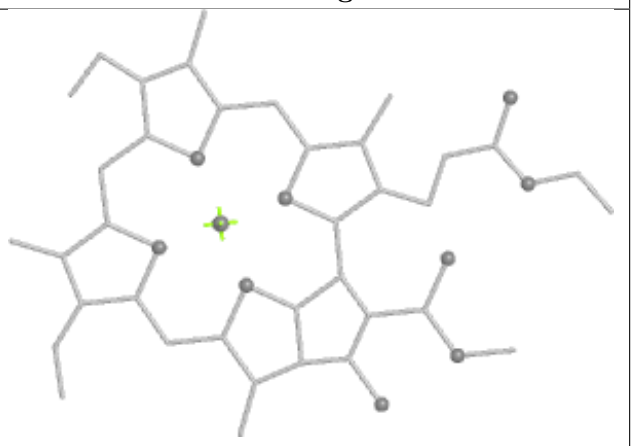
Bond lengths



Bond angles

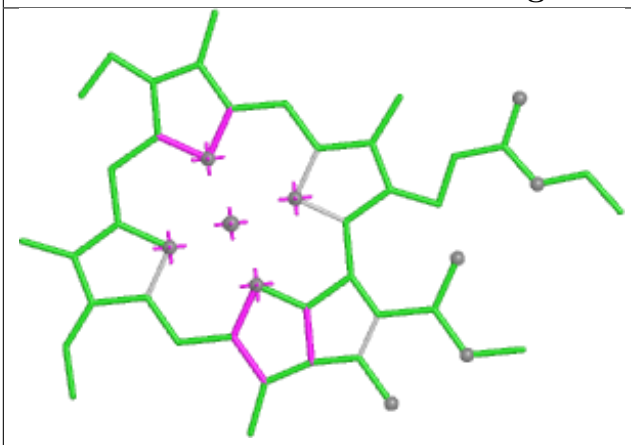


Torsions



Rings

Ligand CLA h 213



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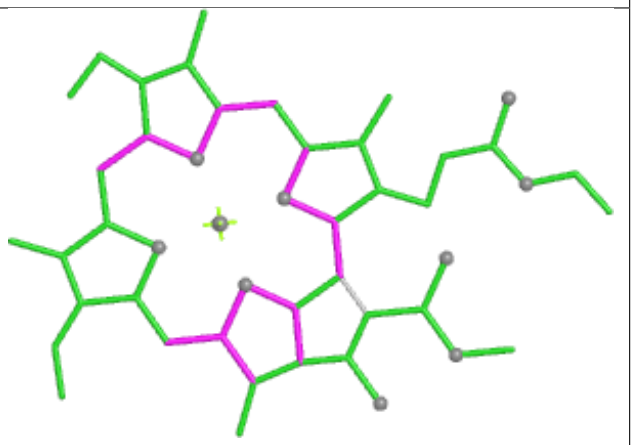

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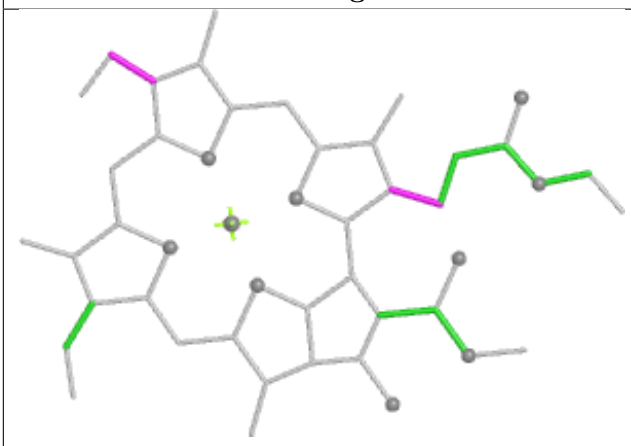

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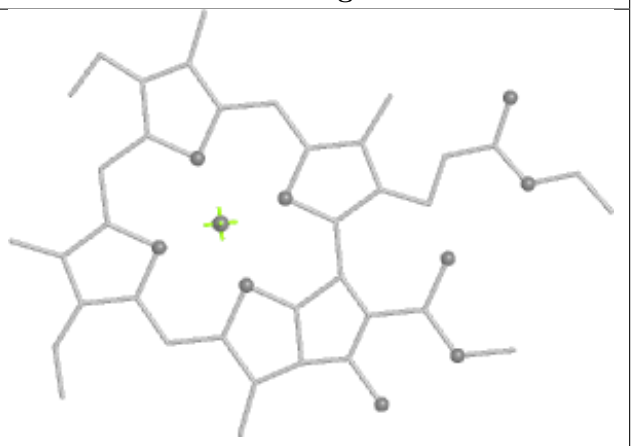
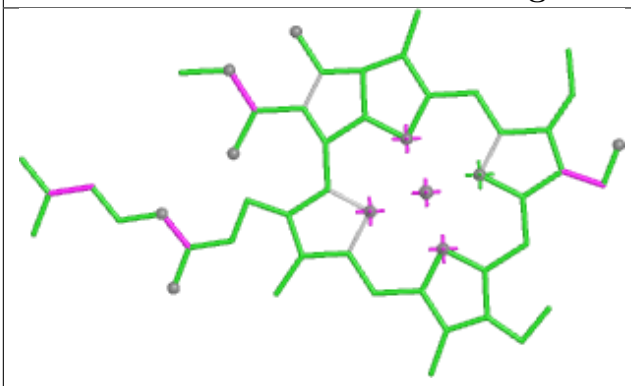


Rings

Ligand CHL e 301



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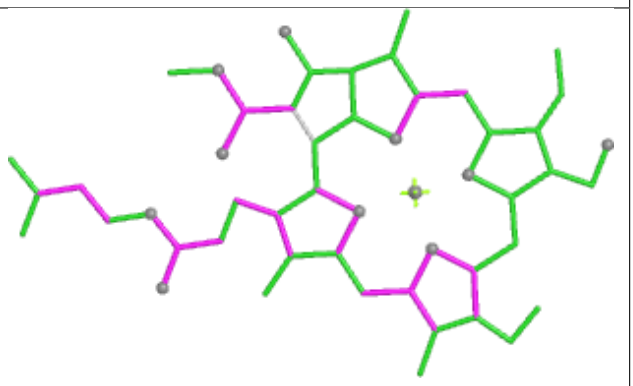

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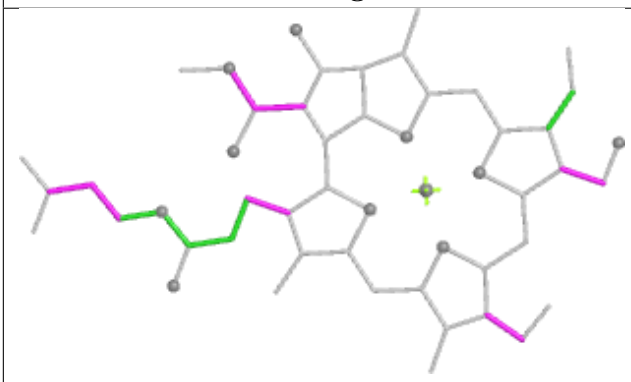

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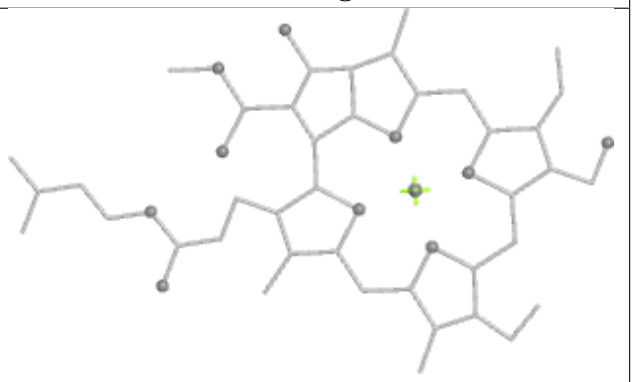
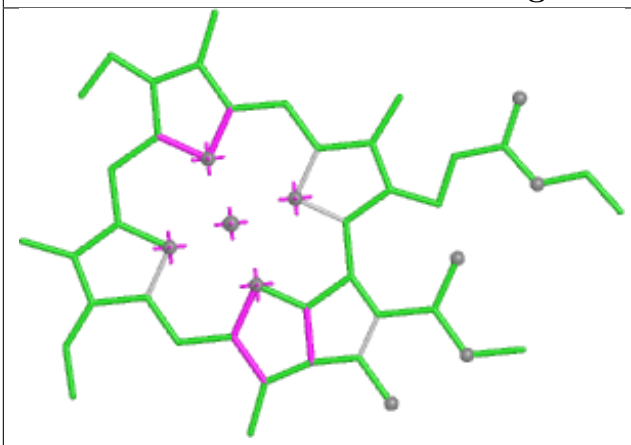


Rings

Ligand CLA J 803



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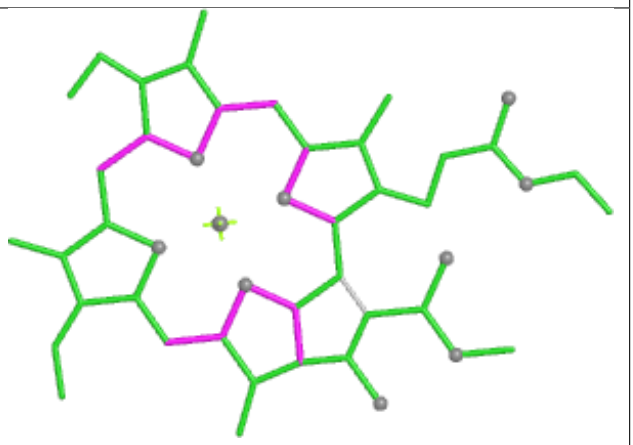
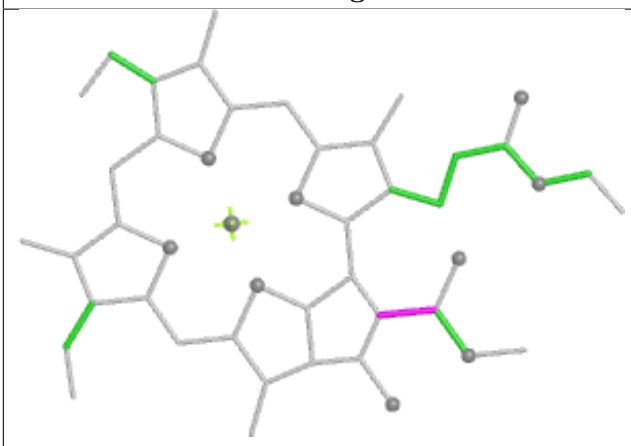


Bond angles



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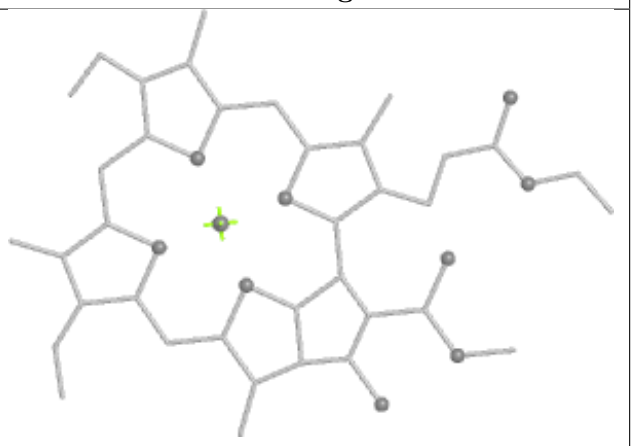
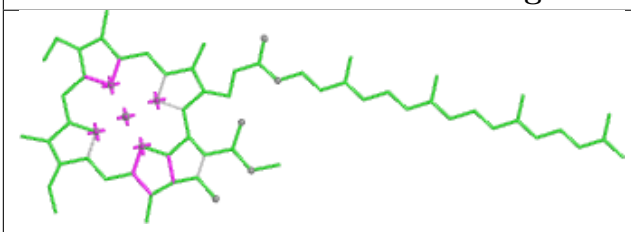


Rings

Ligand CLA B 804



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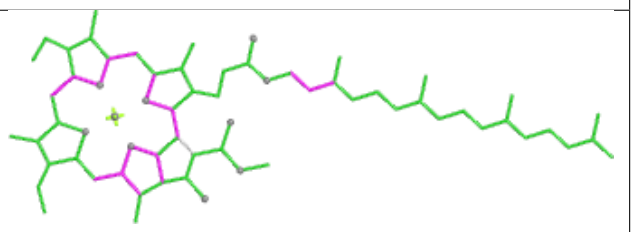

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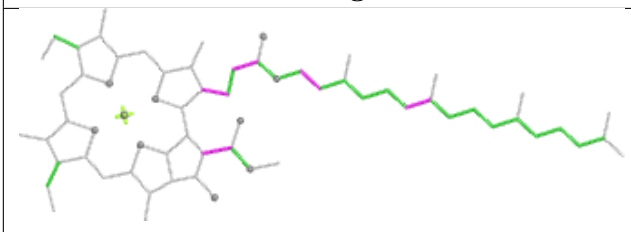

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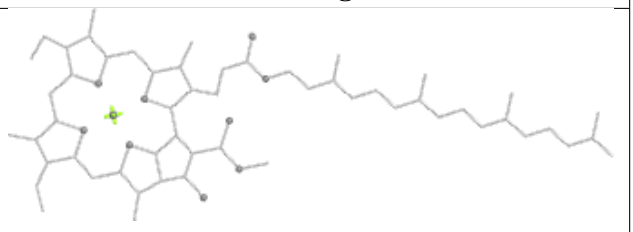
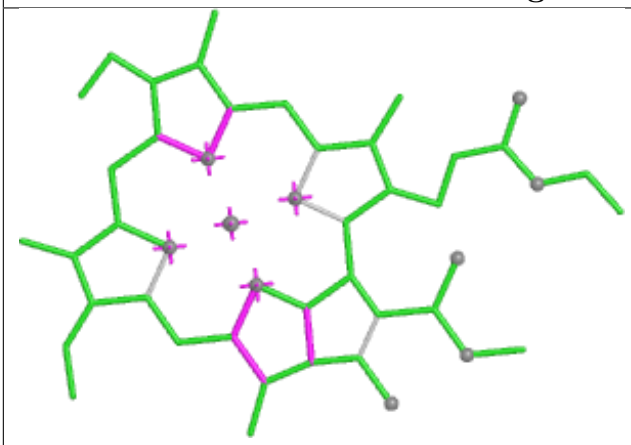


Rings

Ligand CLA n 207



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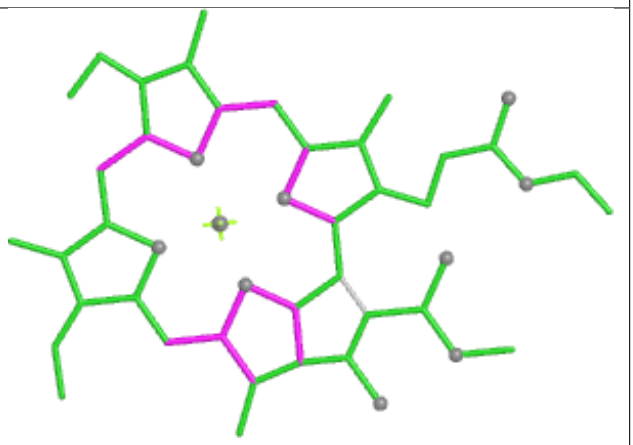

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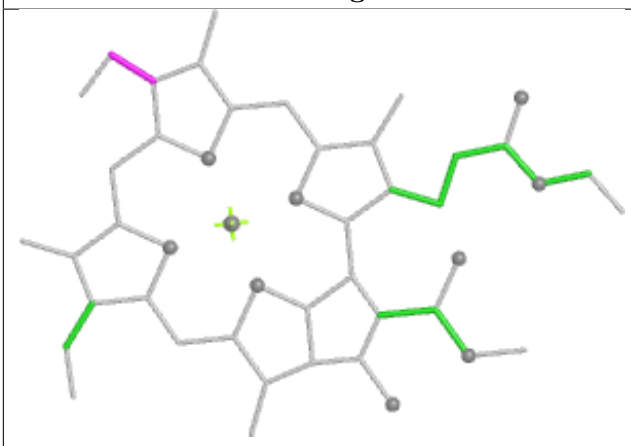

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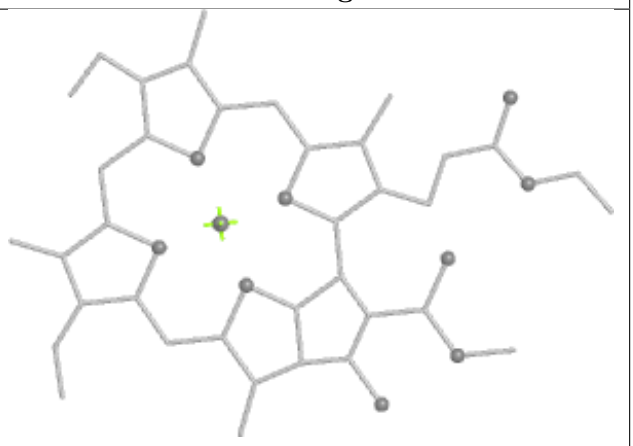
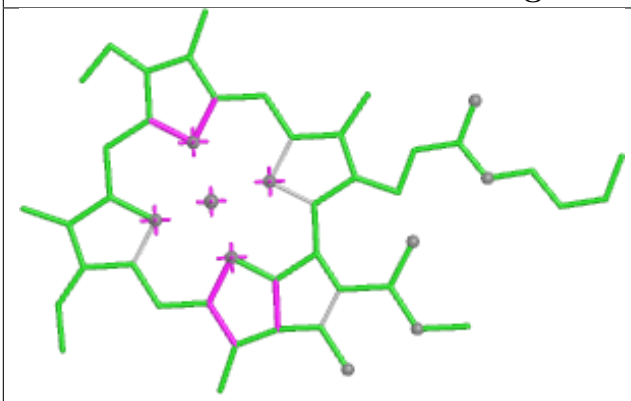


Rings

Ligand CLA B 816



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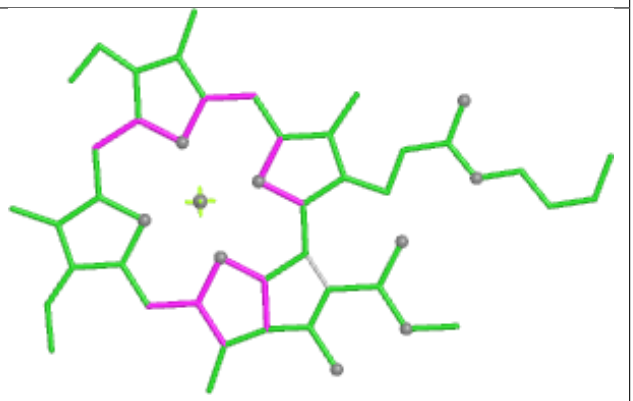

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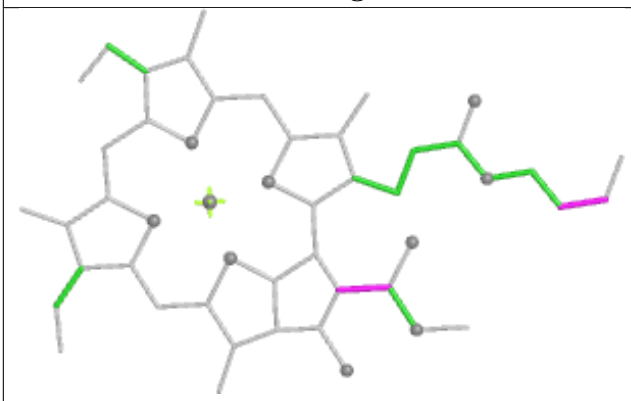

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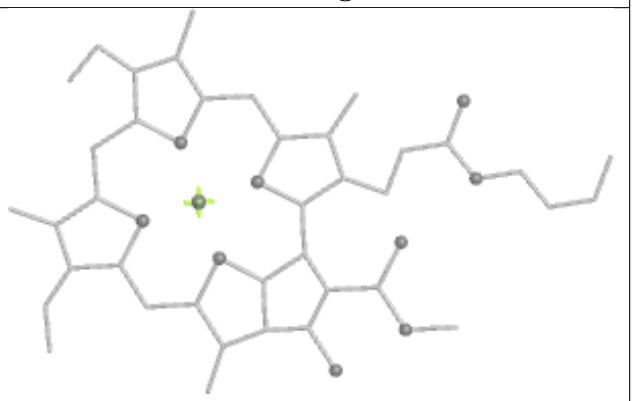
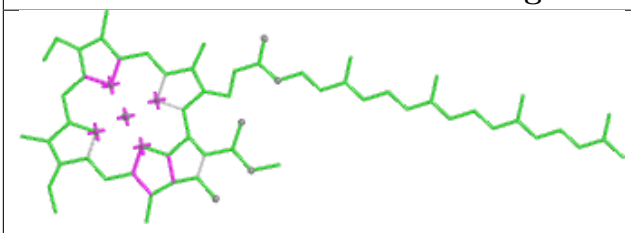


Rings

Ligand CLA B 805



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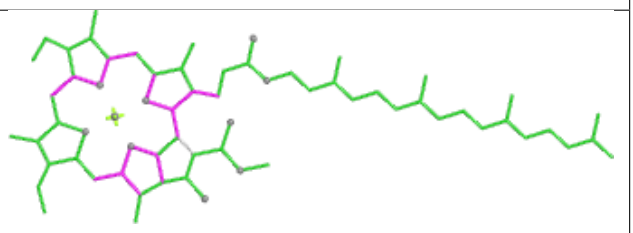

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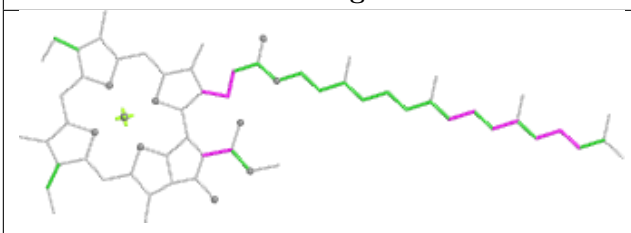

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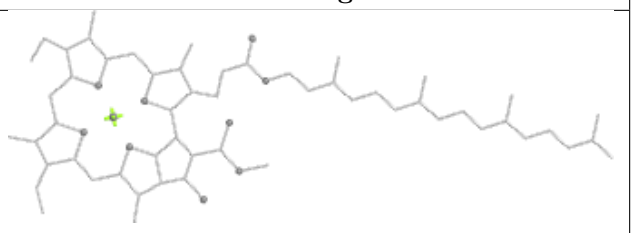
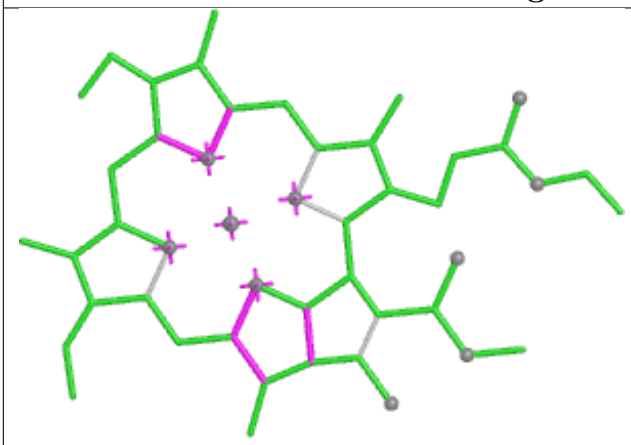


Rings

Ligand CLA n 208



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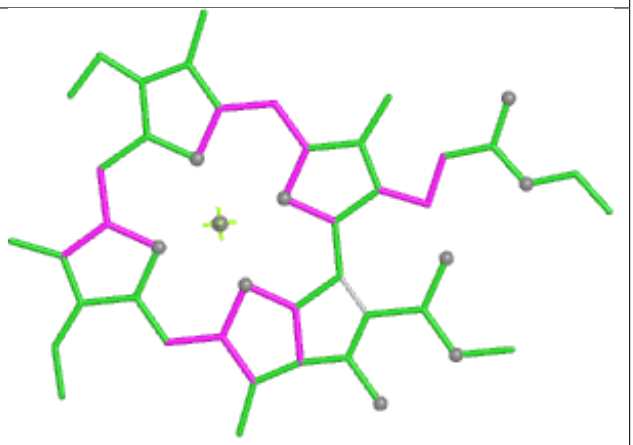

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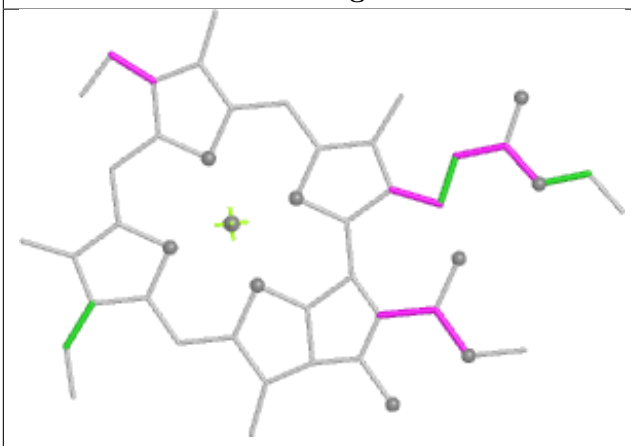

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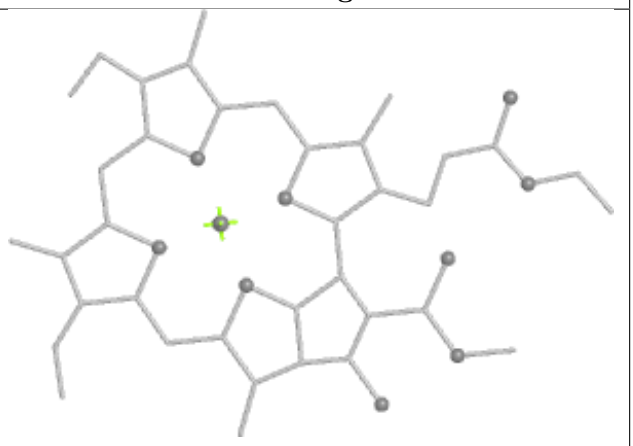
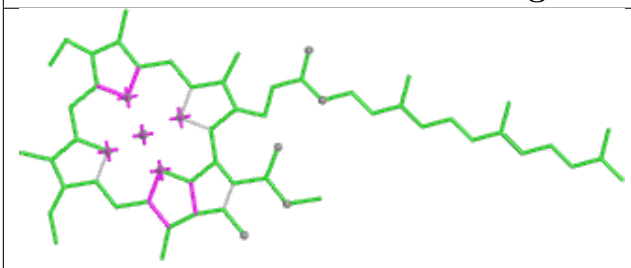


Rings

Ligand CLA a 308



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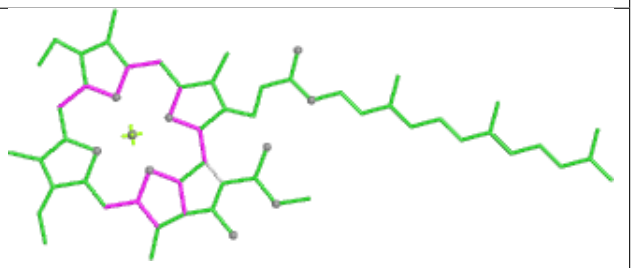

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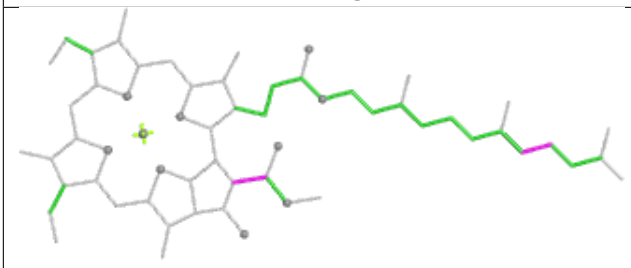

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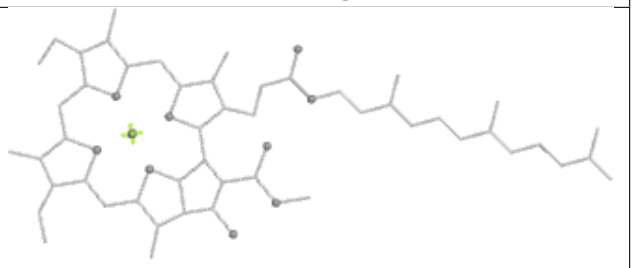
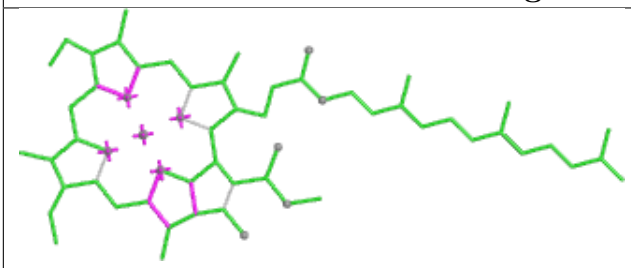
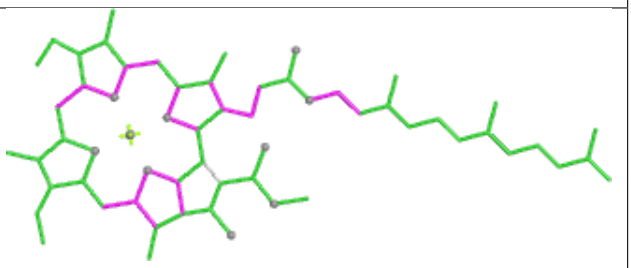
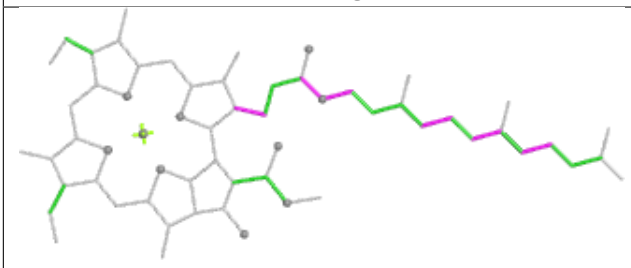
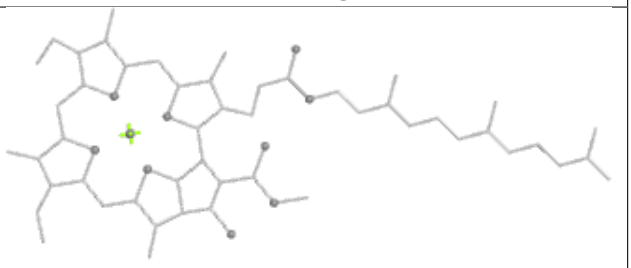
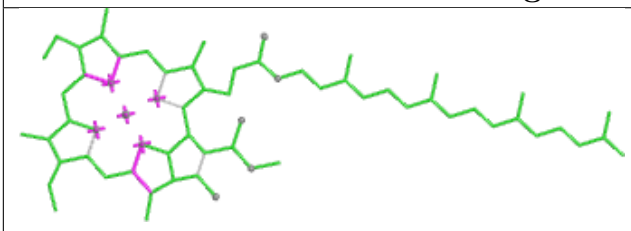
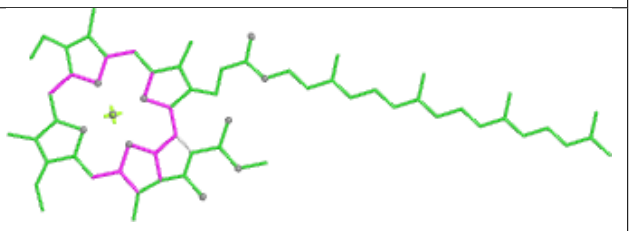


Rings

Ligand CLA B 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 801	
	
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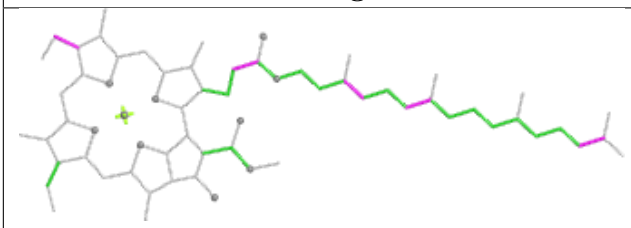
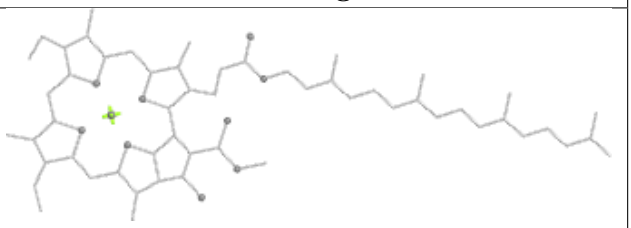
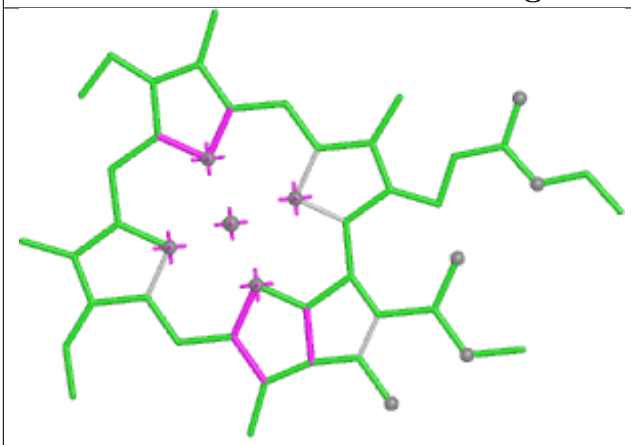
	
Torsions	Rings

Ligand CLA B 848



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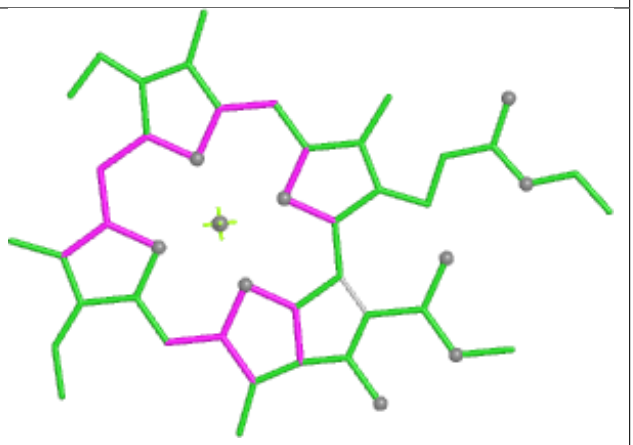
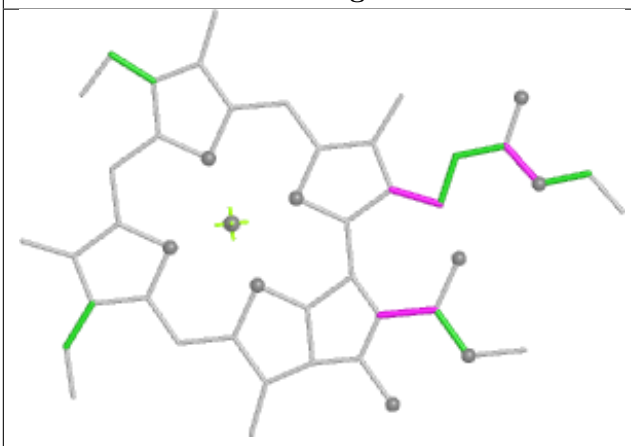


Bond angles



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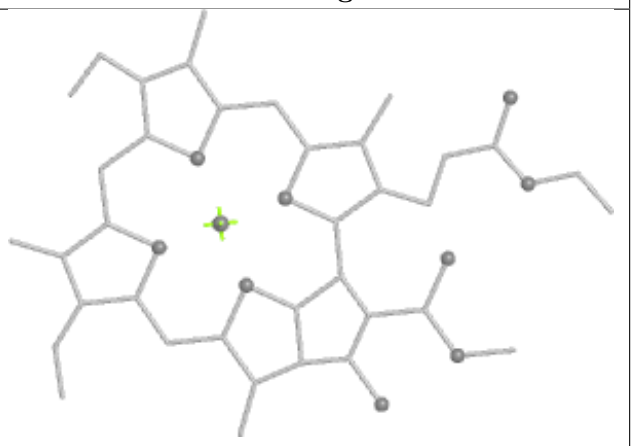
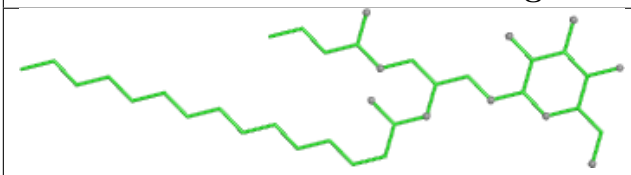


Rings

Ligand LMG c 320



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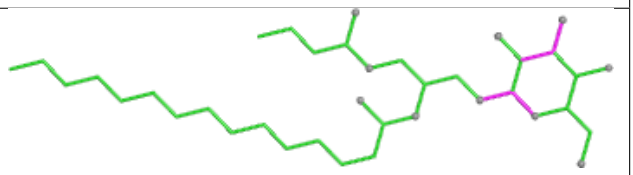
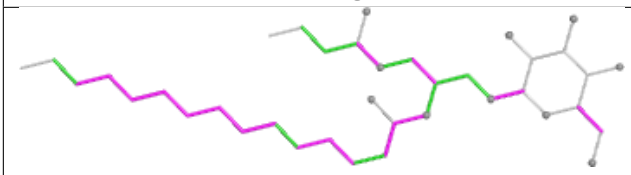


Bond angles



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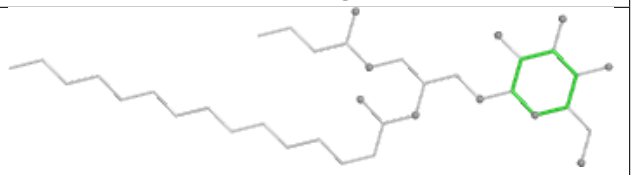
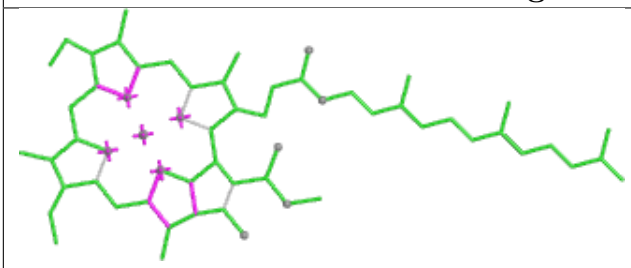
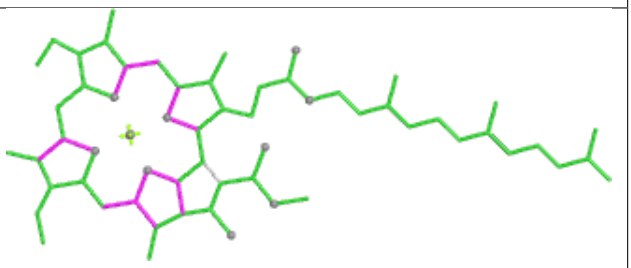
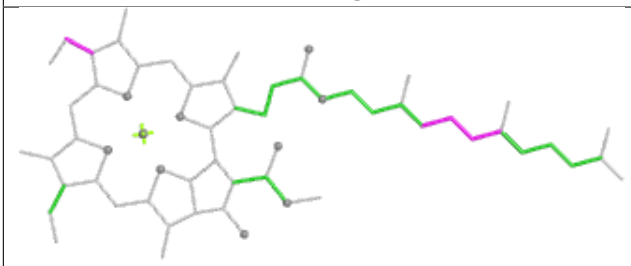
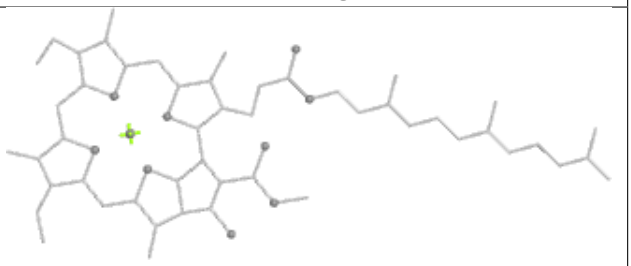
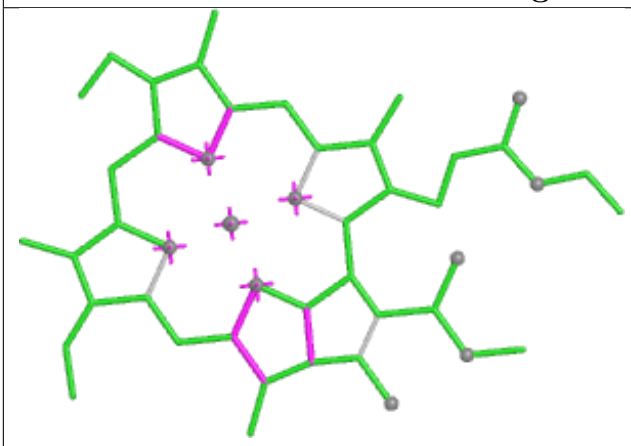
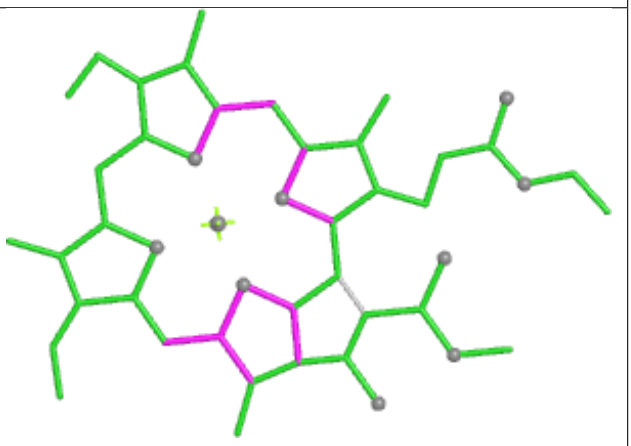
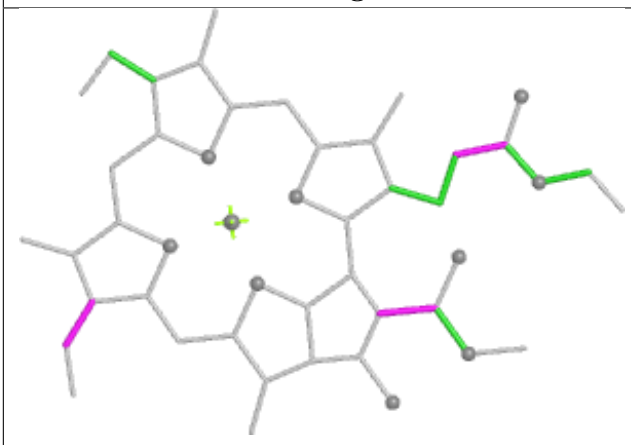
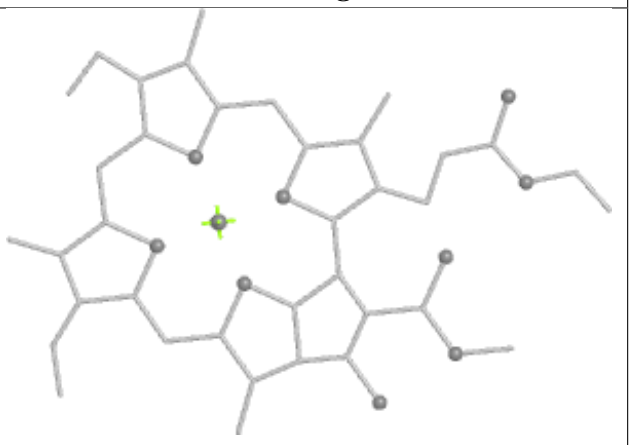
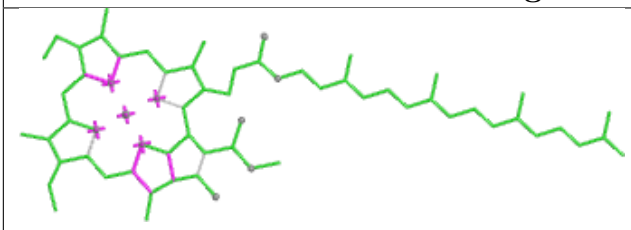


Rings

Ligand CLA k 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 806



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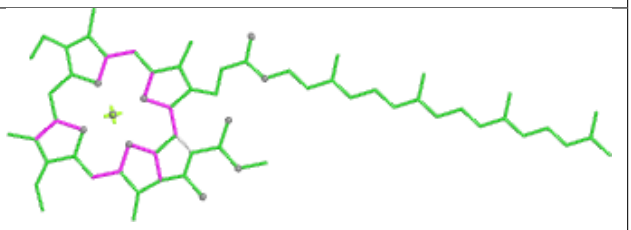

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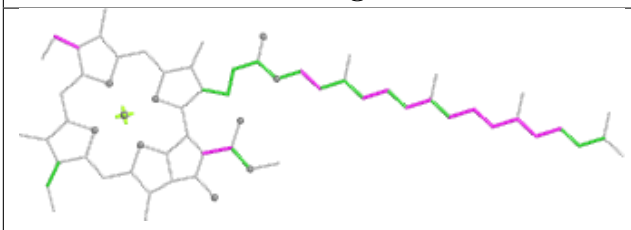

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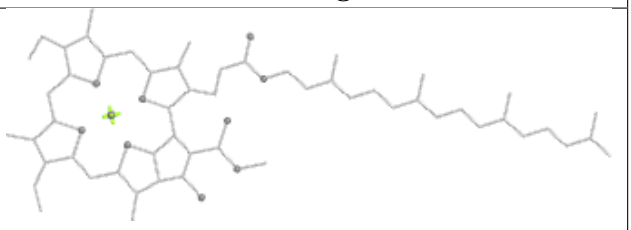
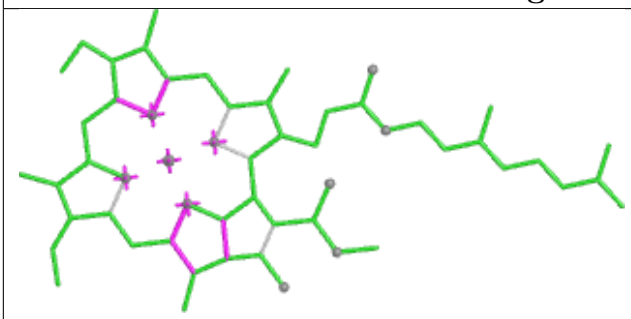


Rings

Ligand CLA b 302



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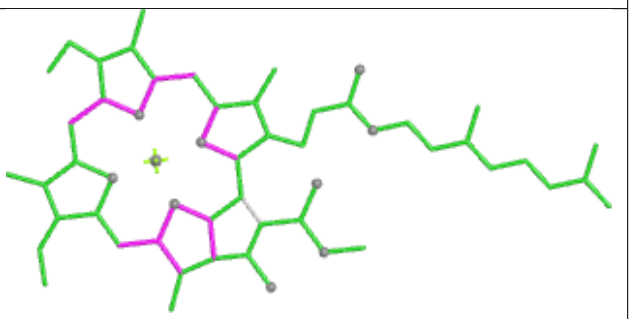

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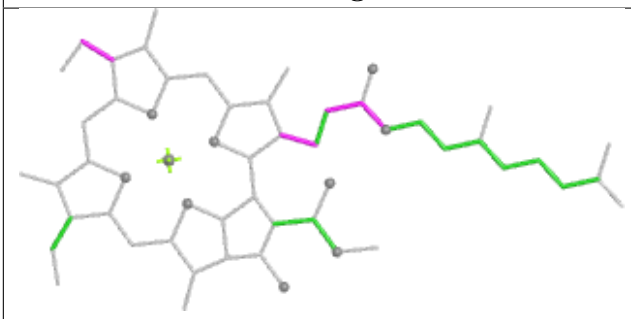

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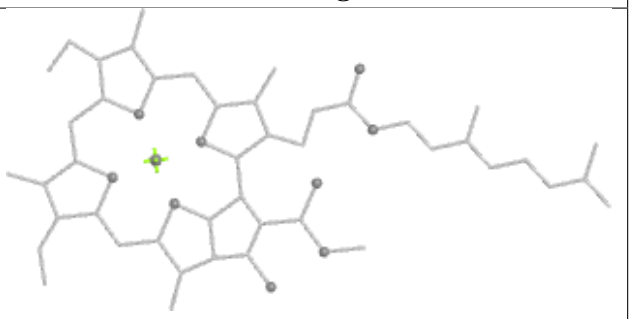
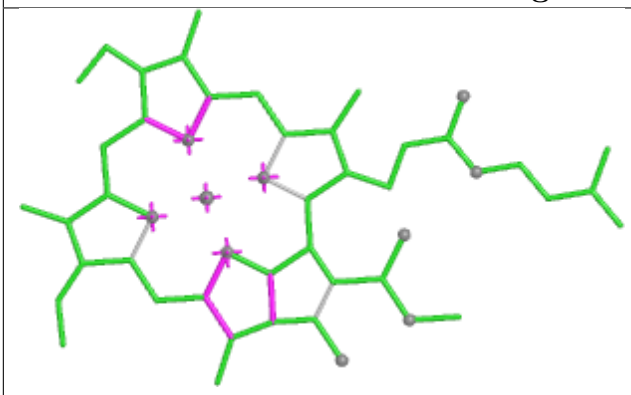


Rings

Ligand CLA j 305



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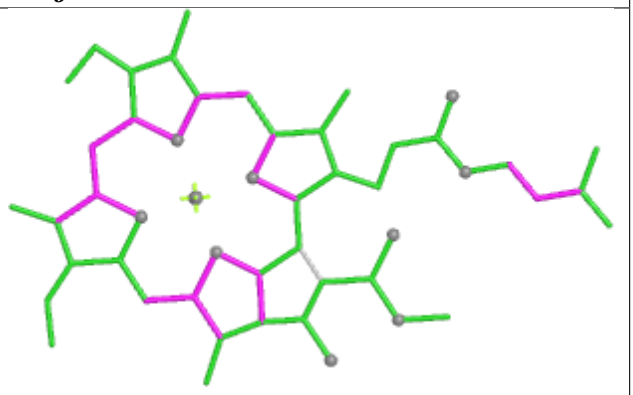

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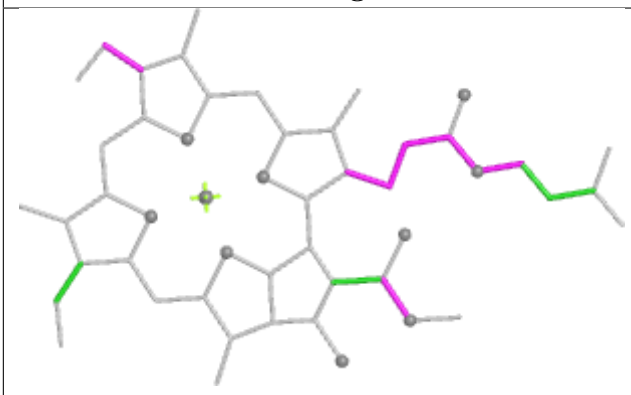

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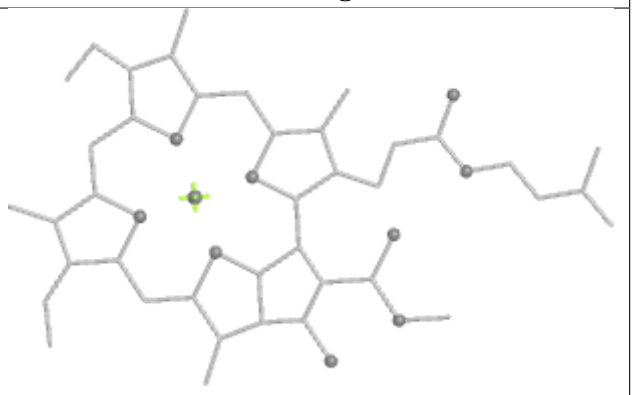
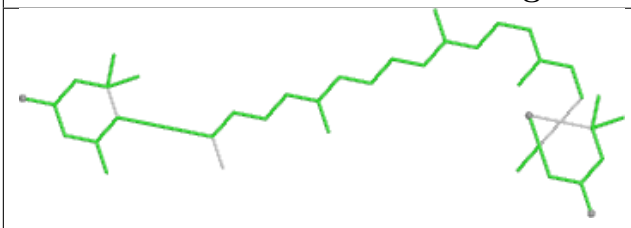


Rings

Ligand DD6 m 313



Bond lengths



Bond angles

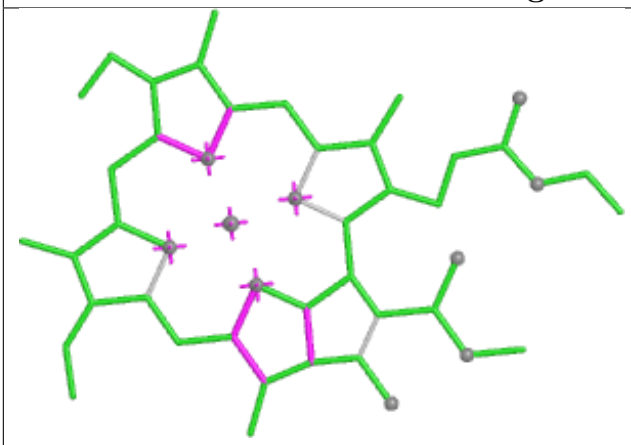


Torsions



Rings

Ligand CLA n 202



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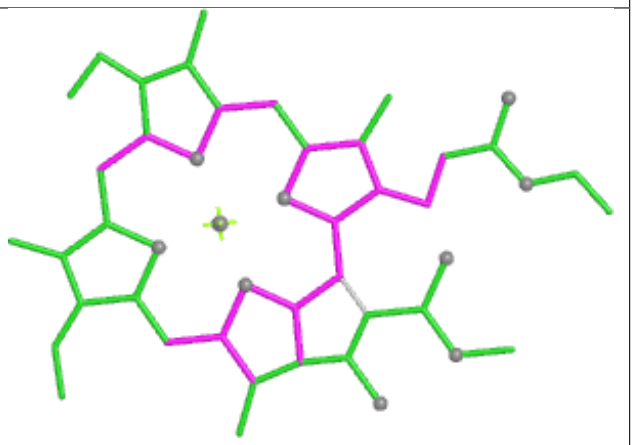

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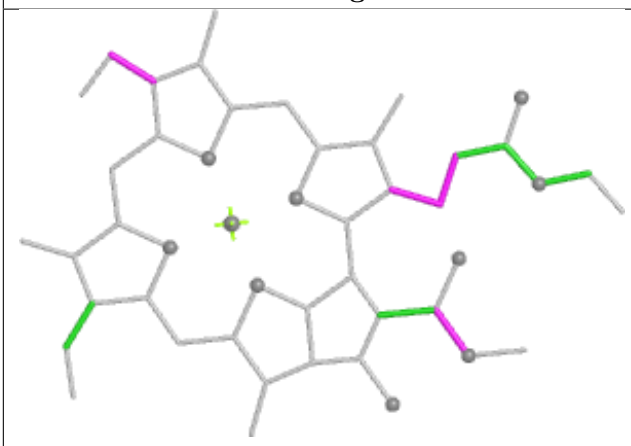

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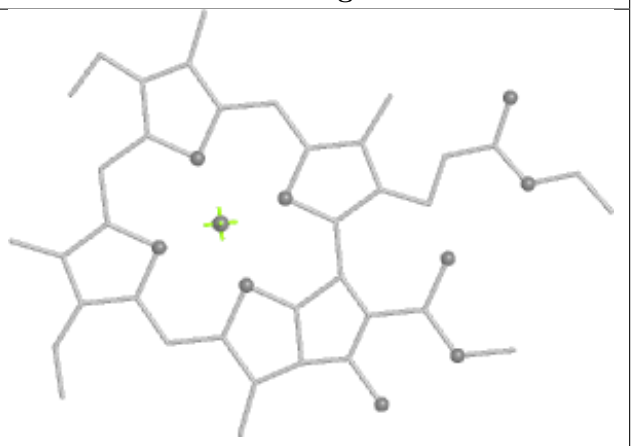
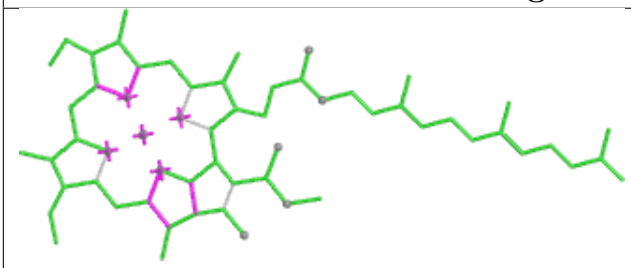


Rings

Ligand CLA k 307



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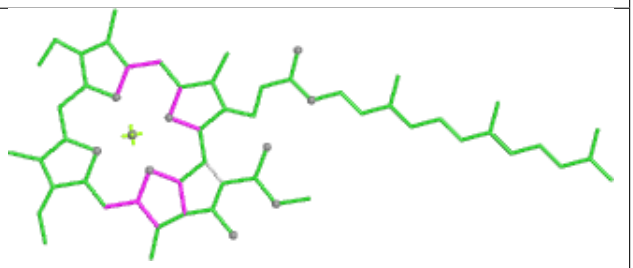

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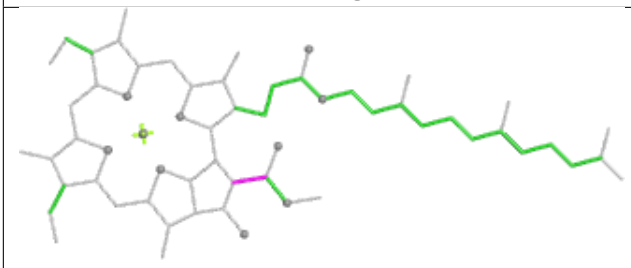

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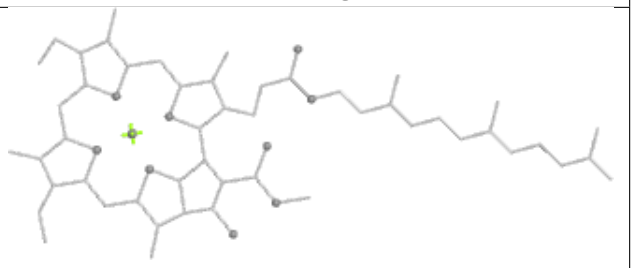
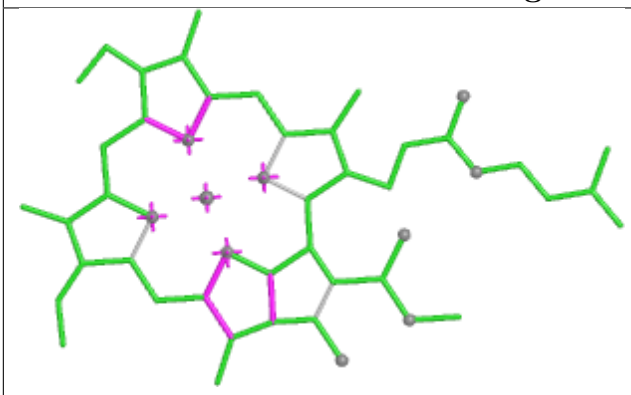


Rings

Ligand CLA B 838



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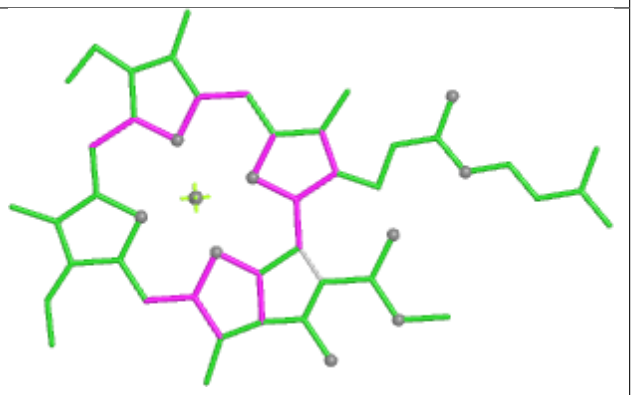

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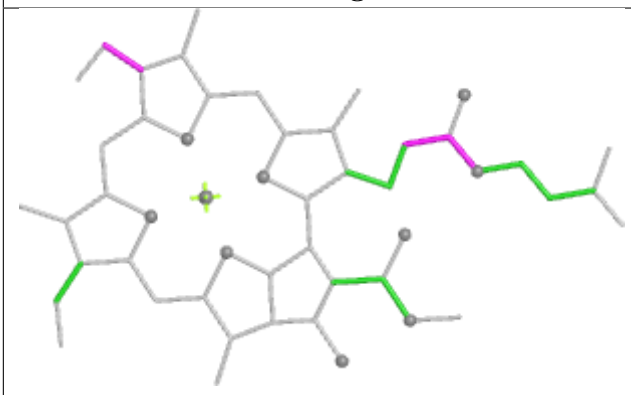

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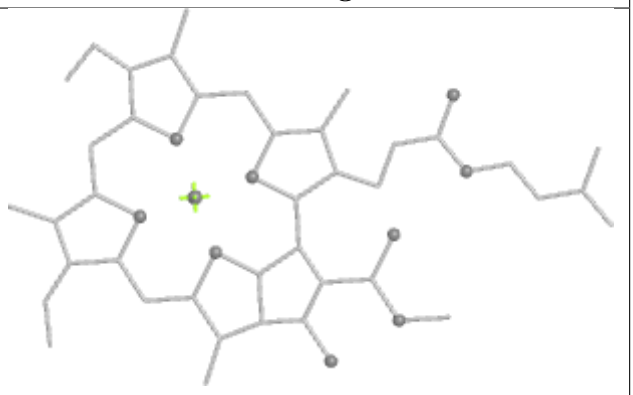
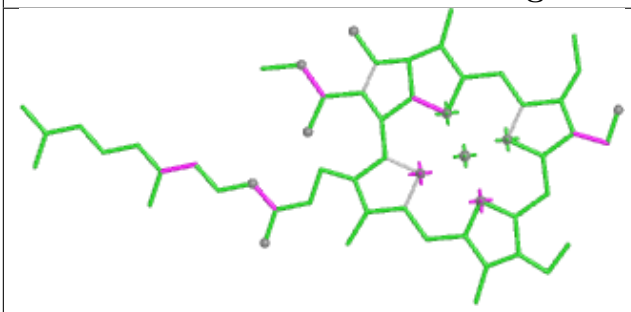


Rings

Ligand CHL b 301



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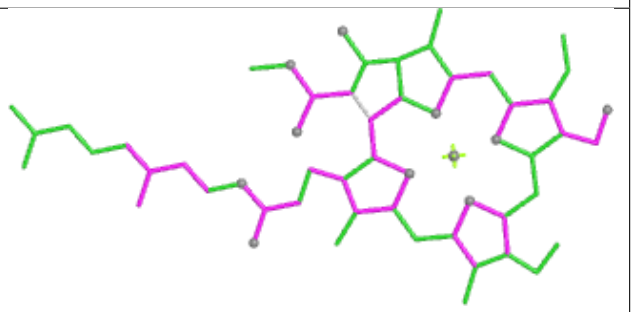

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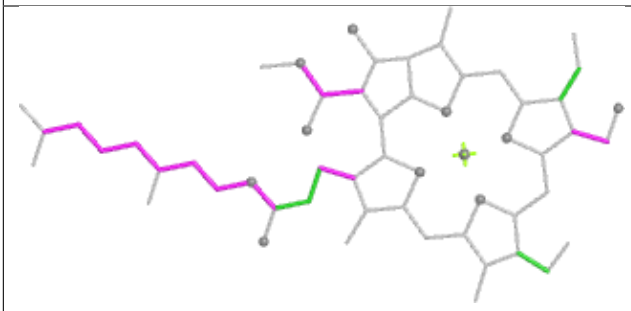

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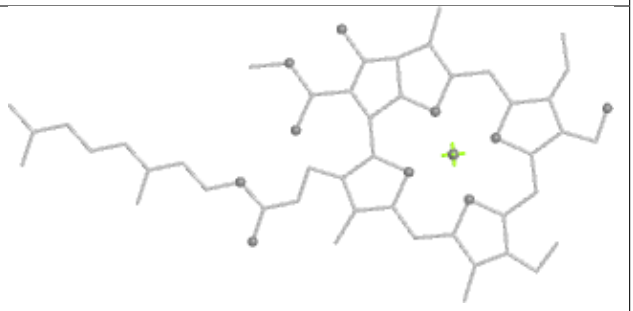
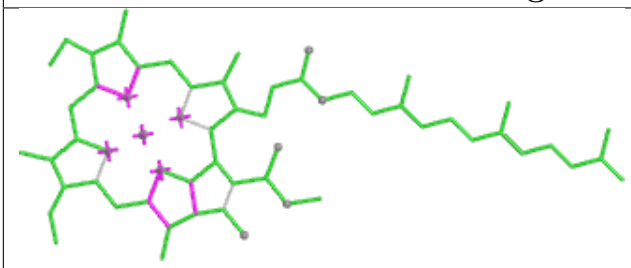
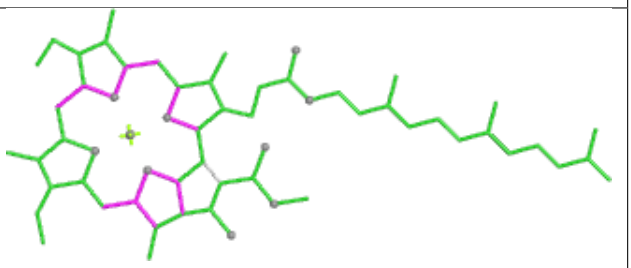
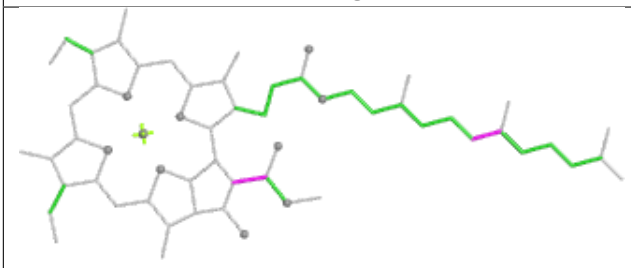
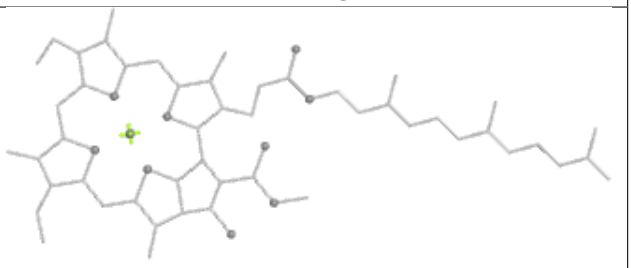
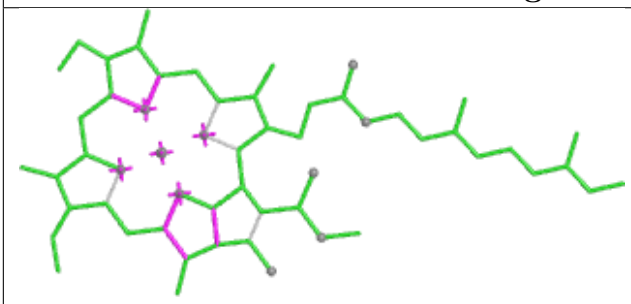
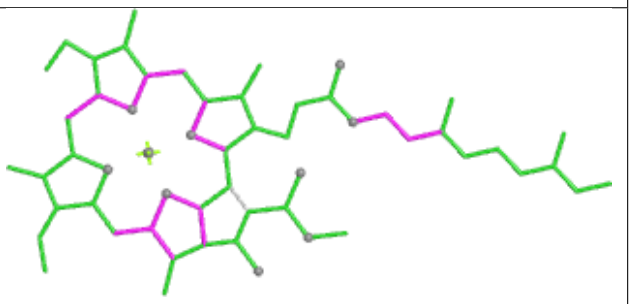


Rings

Ligand CLA h 208	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 835	
	
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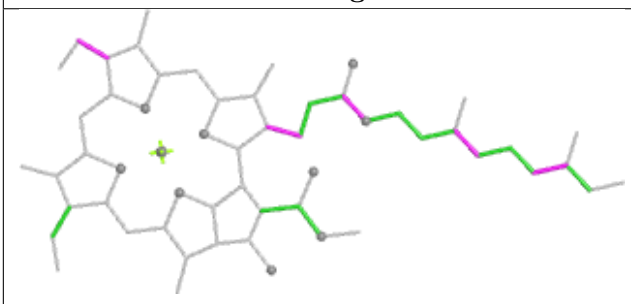
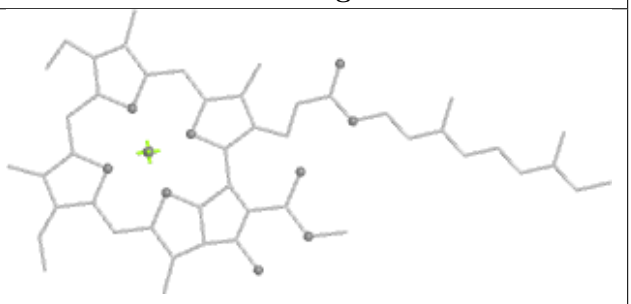
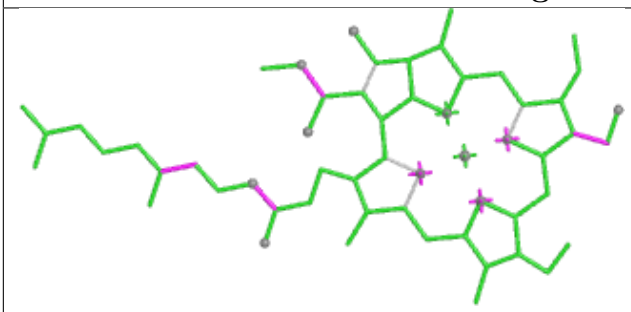
	
Torsions	Rings

Ligand CHL i 304



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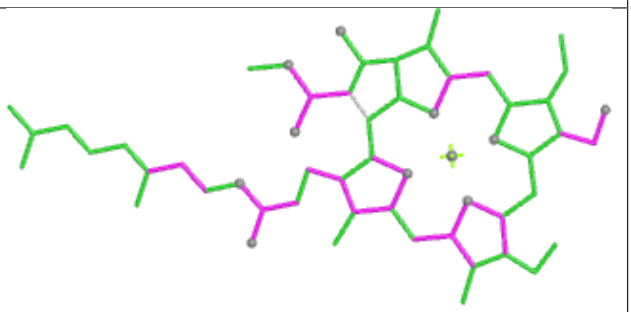
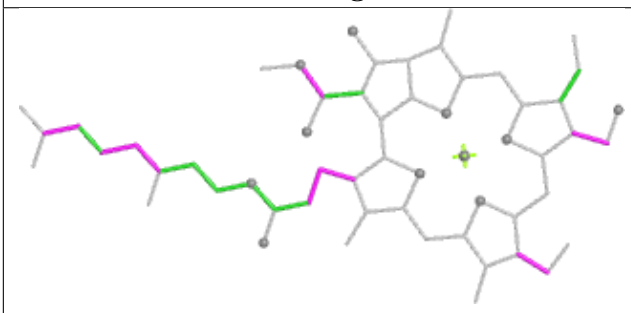


Bond angles



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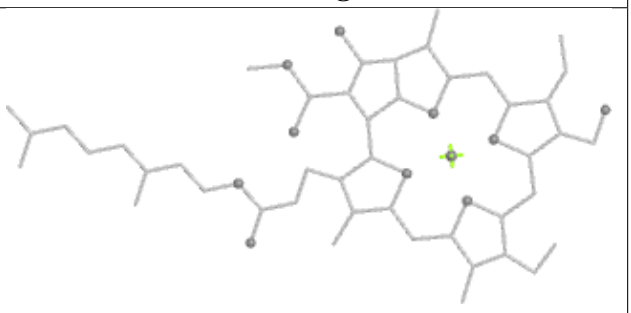
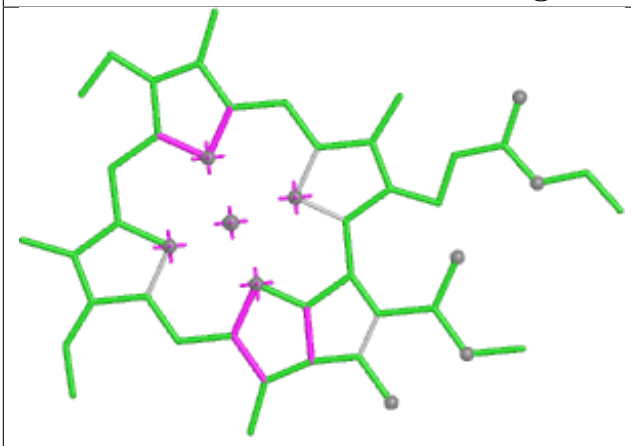


Rings

Ligand CLA i 312



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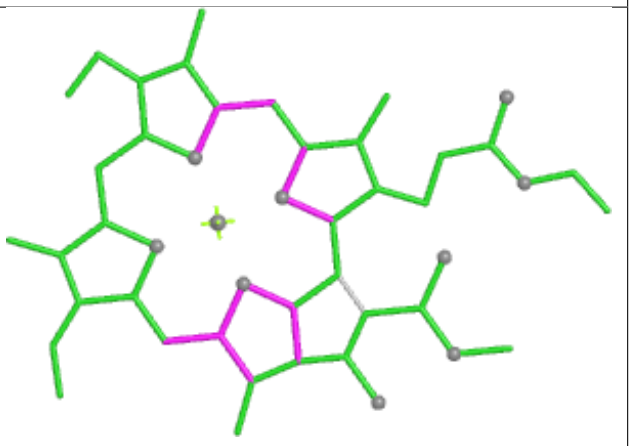

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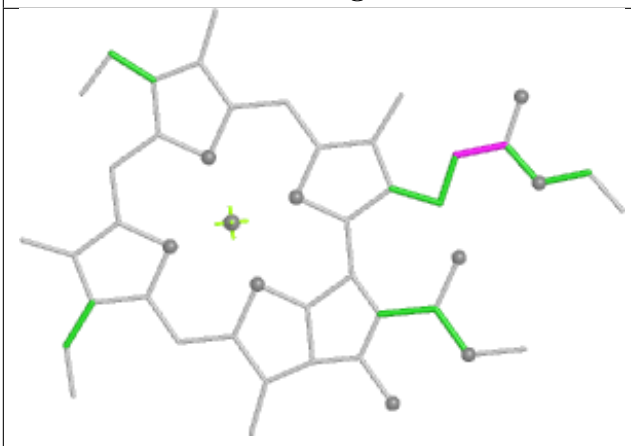

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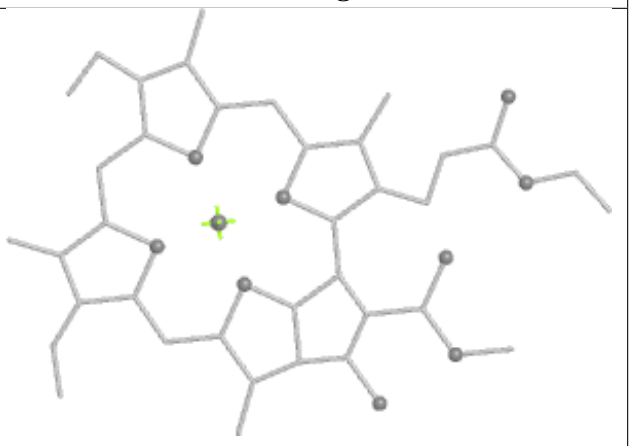
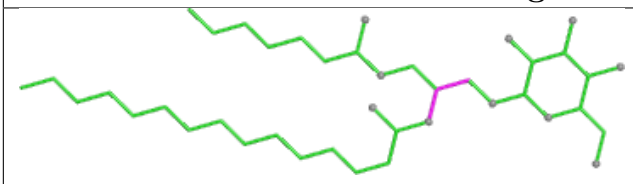


Rings

Ligand LMG i 316



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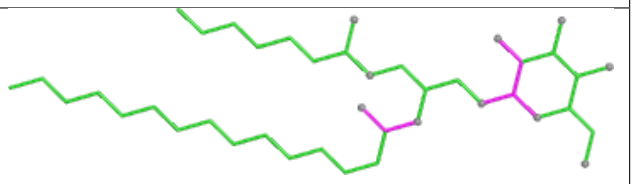
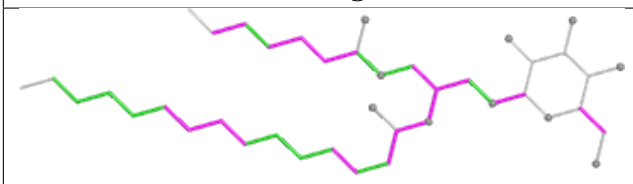


Bond angles



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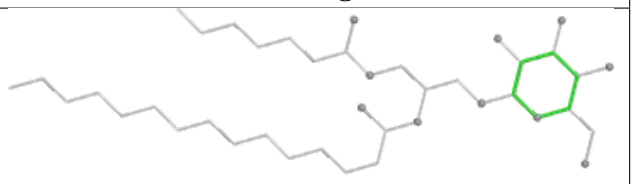
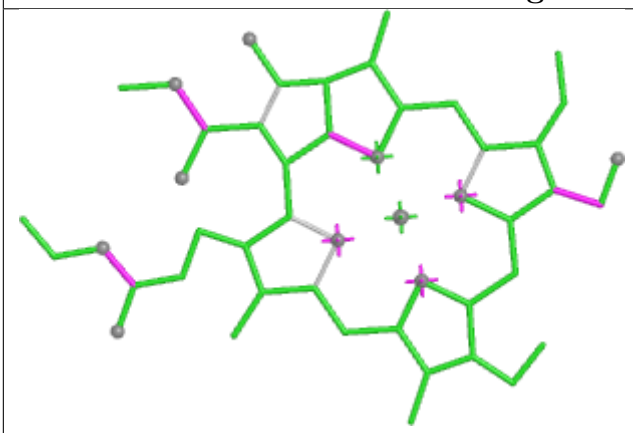
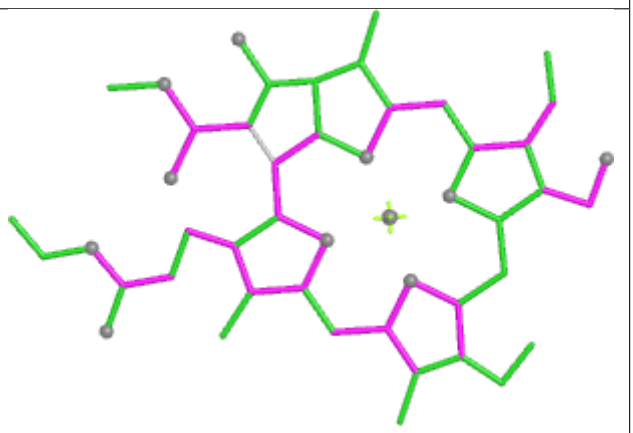


Rings

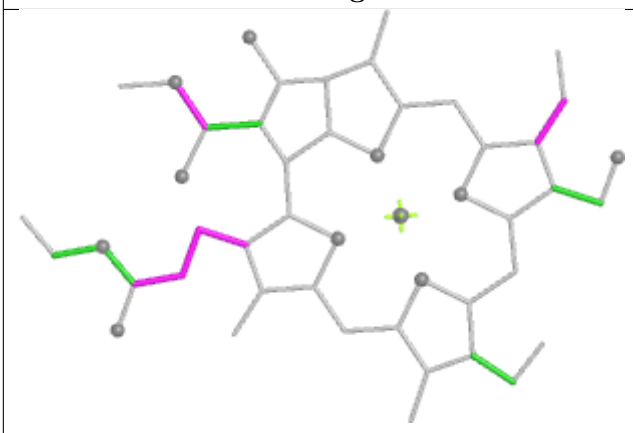
Ligand CHL b 311



Bond lengths



Bond angles



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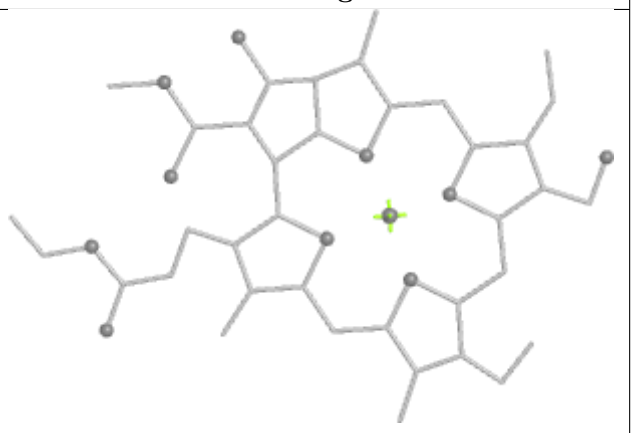
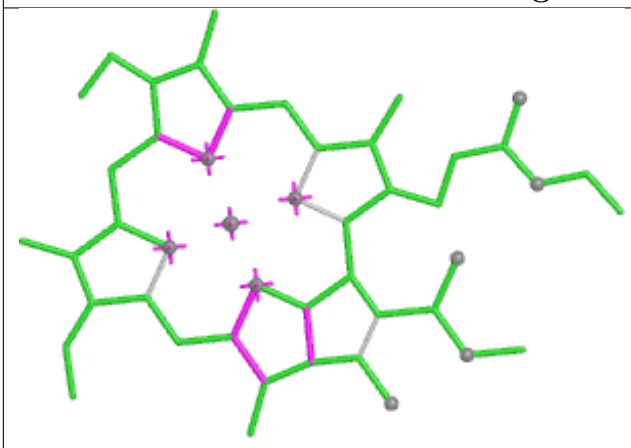


Rings

Ligand CLA l 207



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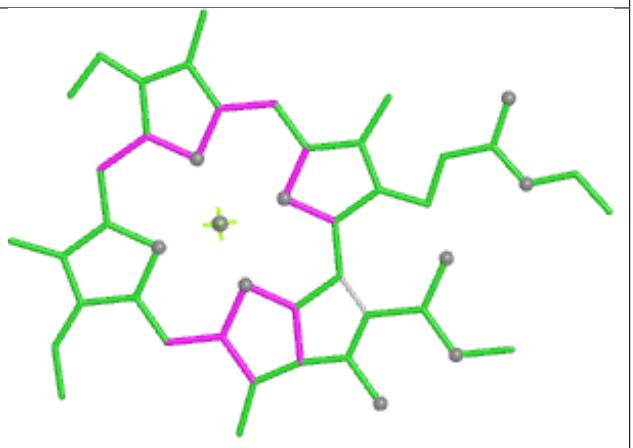

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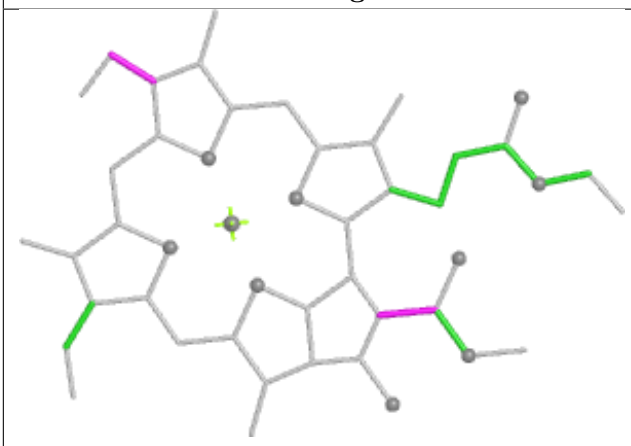
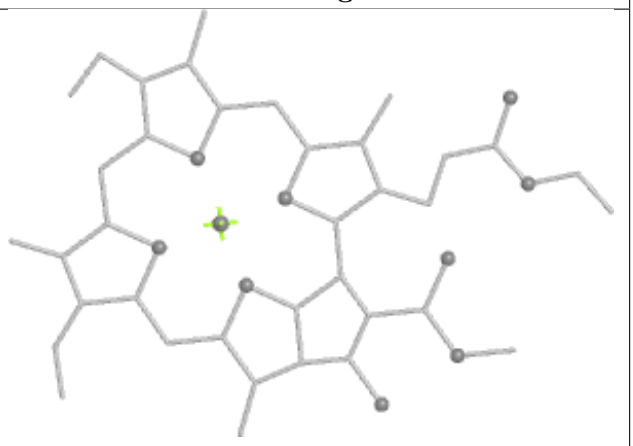
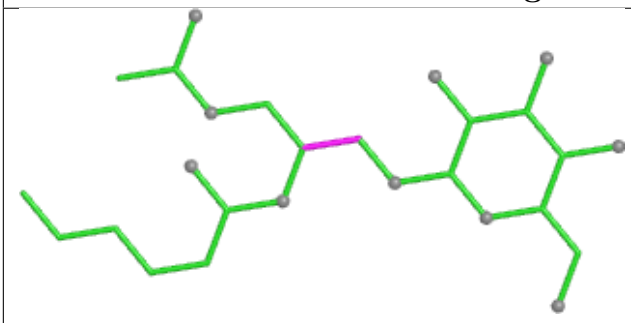


Torsions



Rings

Ligand LMG a 316



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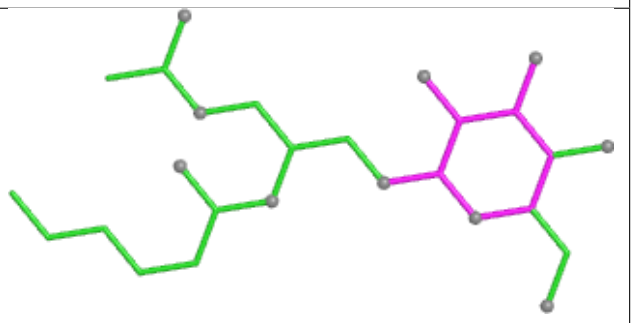

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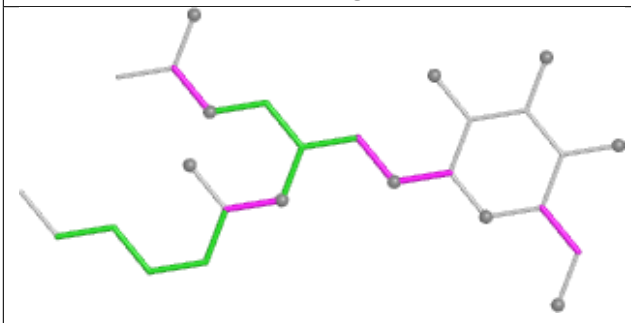

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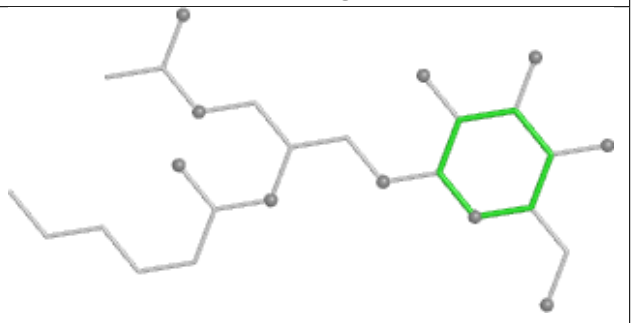
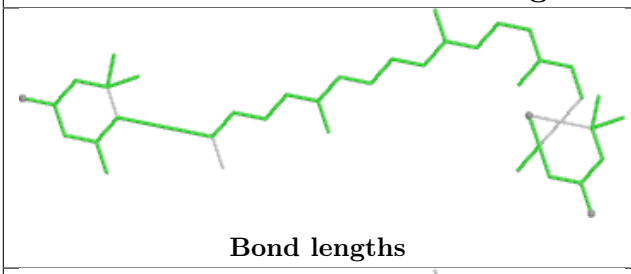


Rings

Ligand DD6 e 313



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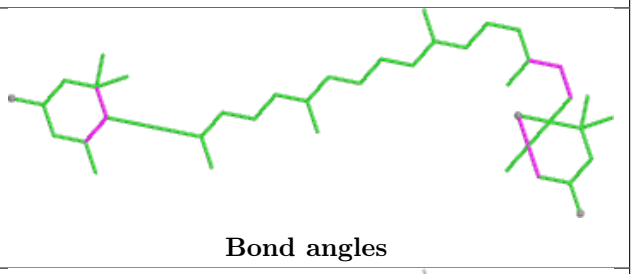

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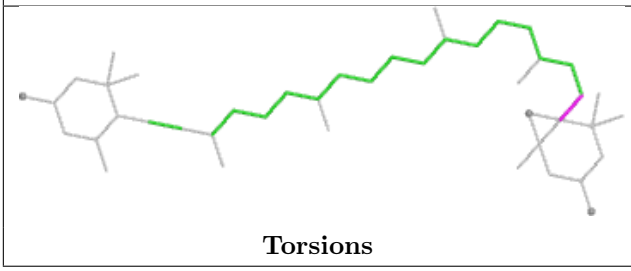

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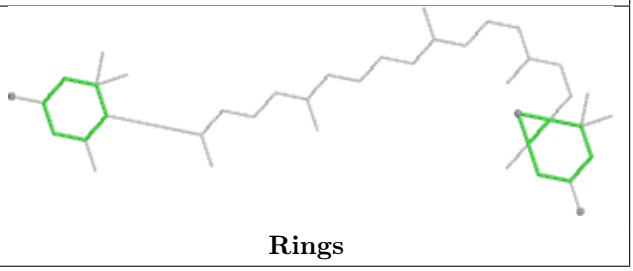
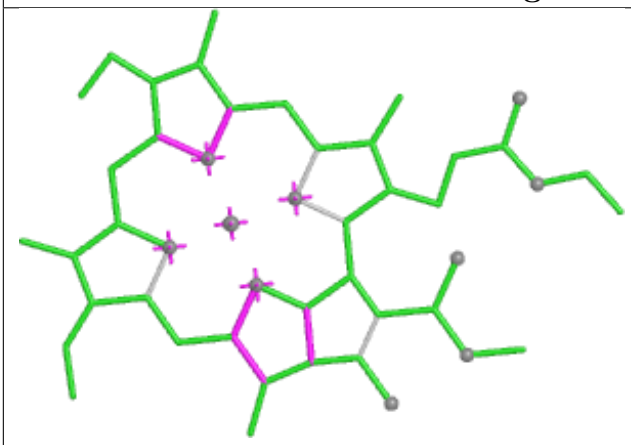


Rings

Ligand CLA A 849



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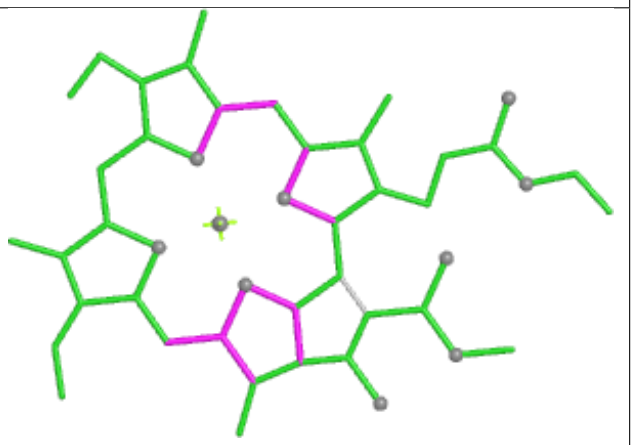
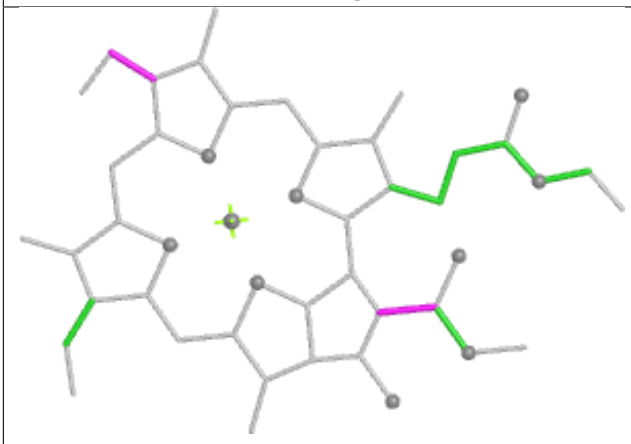


Bond angles



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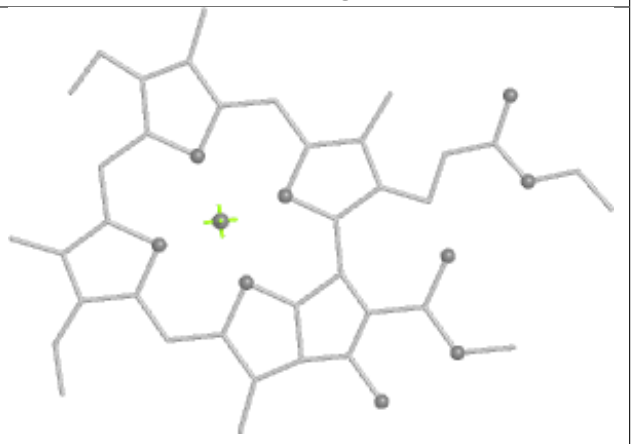
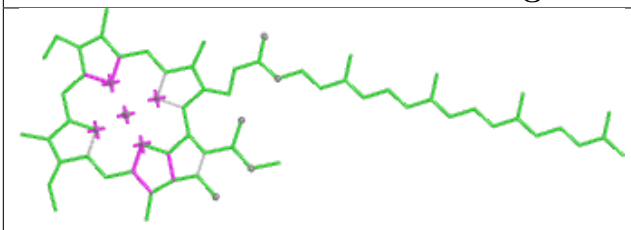


Rings

Ligand CLA A 823



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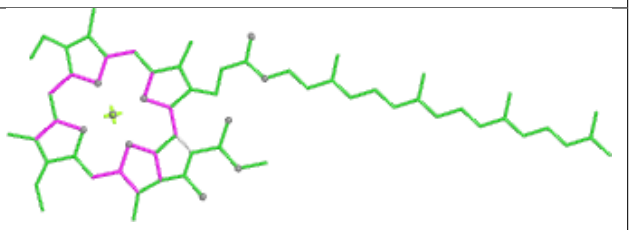

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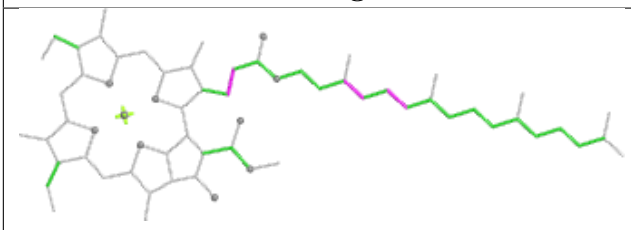

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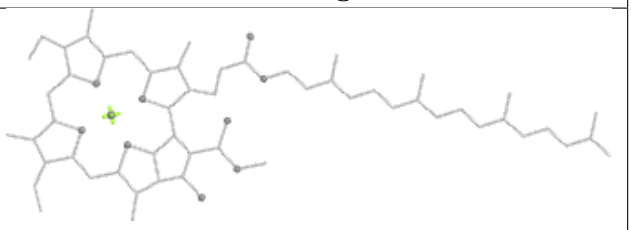
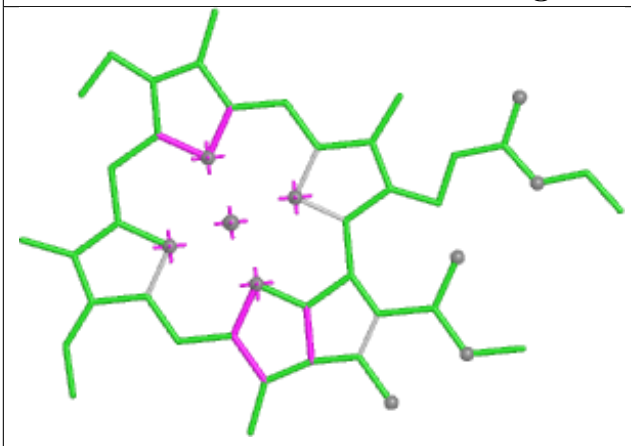


Rings

Ligand CLA i 306



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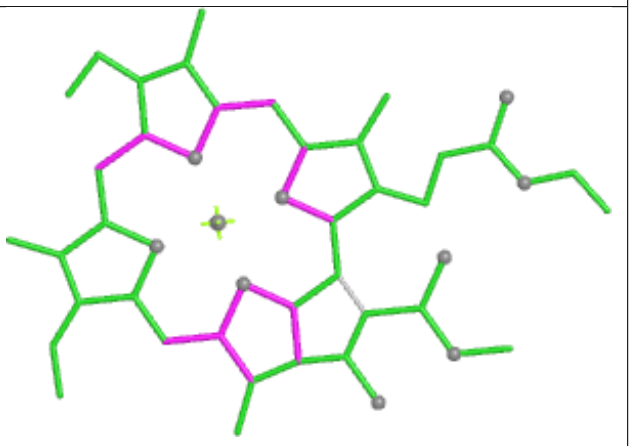

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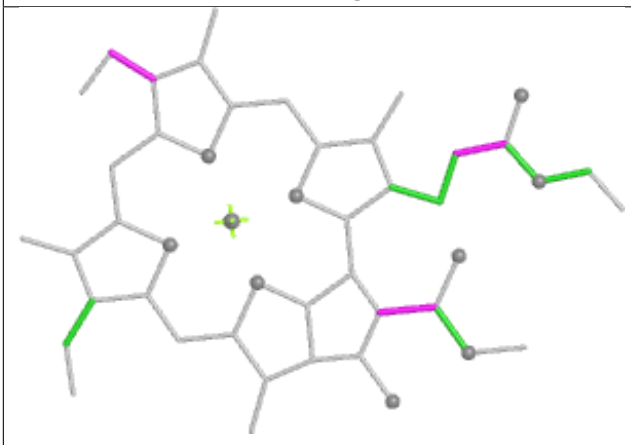

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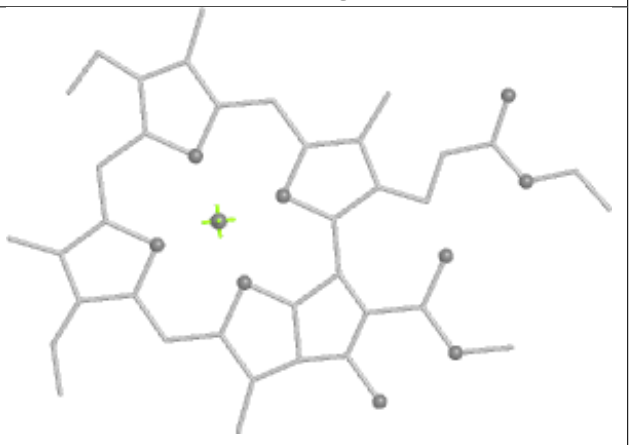
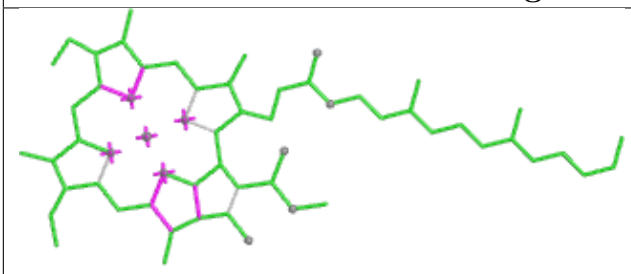
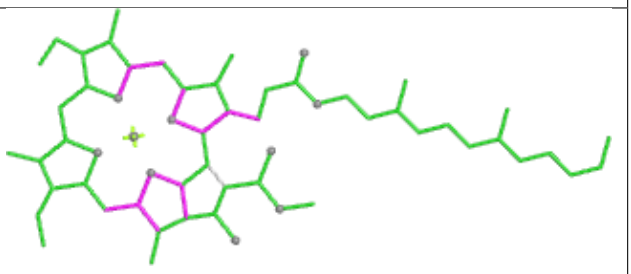
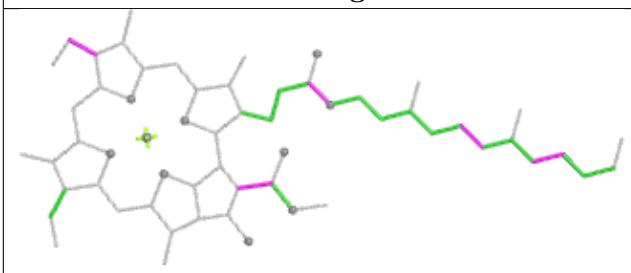
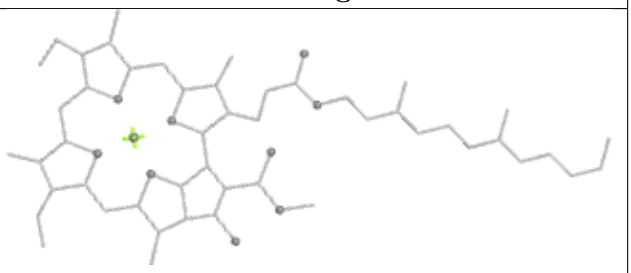


Rings

Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

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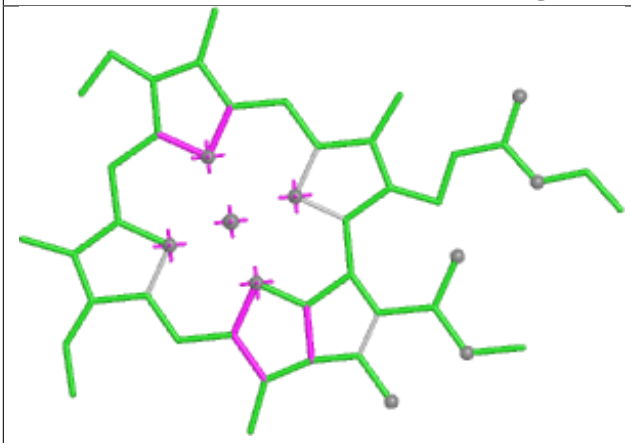
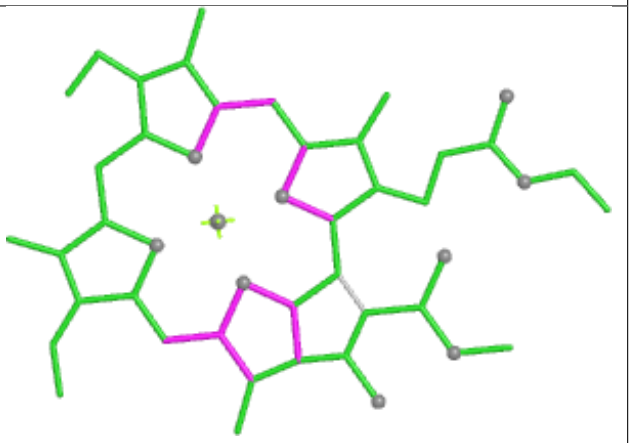
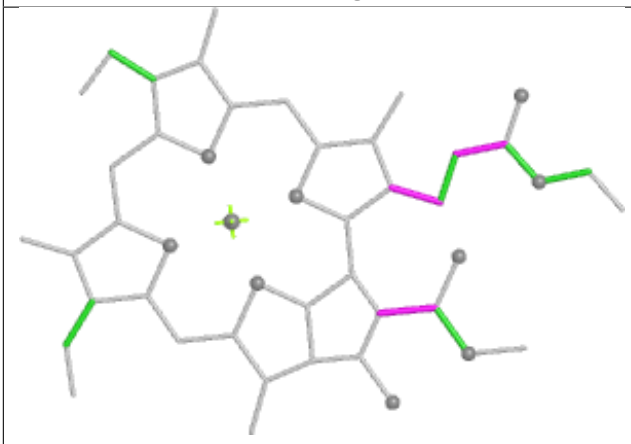
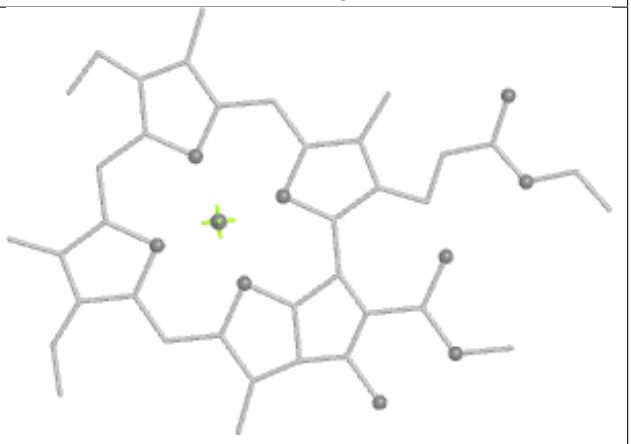
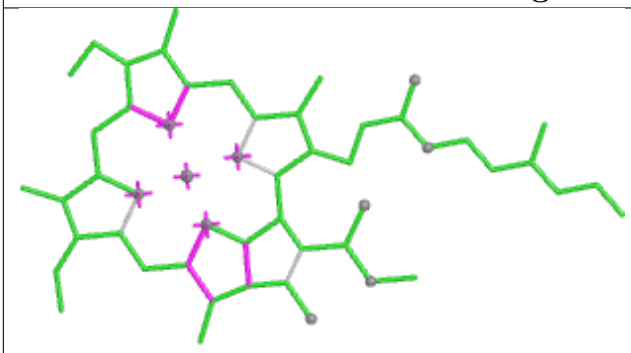
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 303



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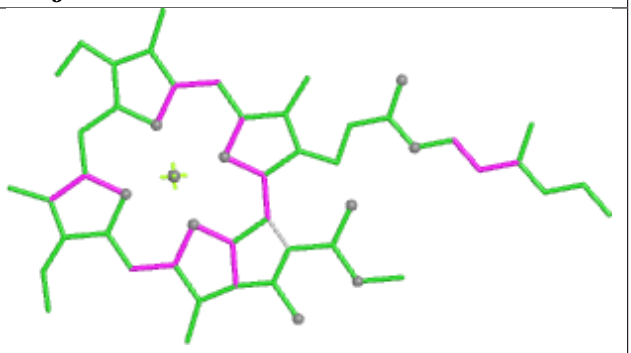
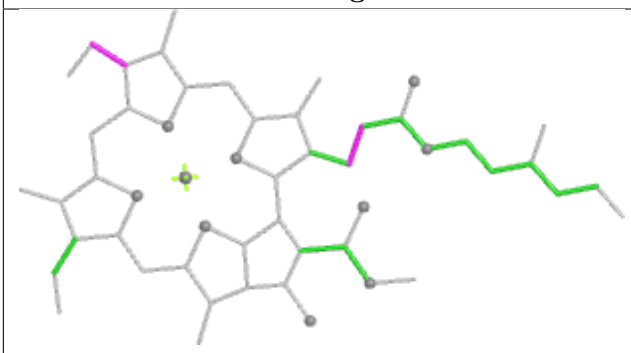


Bond angles



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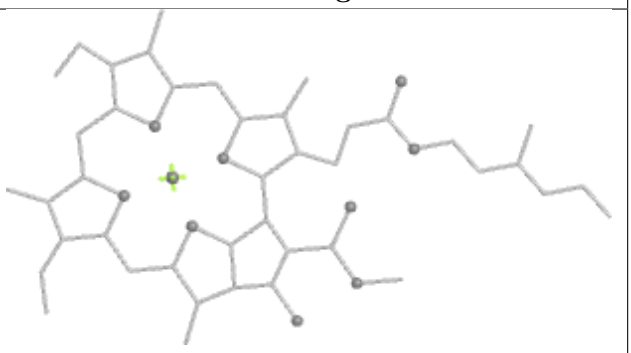
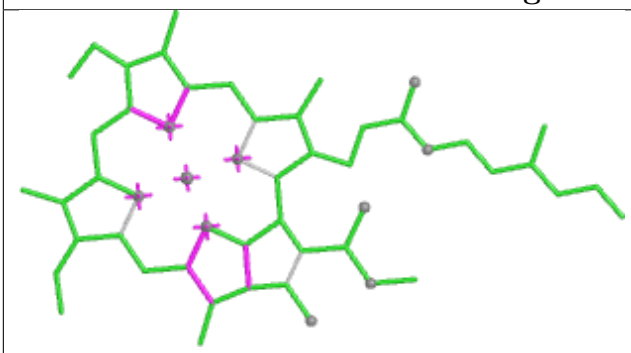


Rings

Ligand CLA D 301



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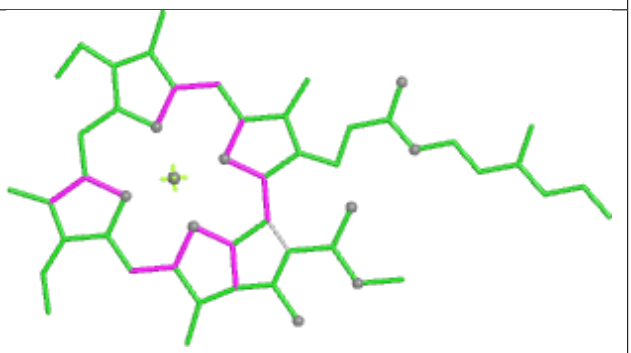

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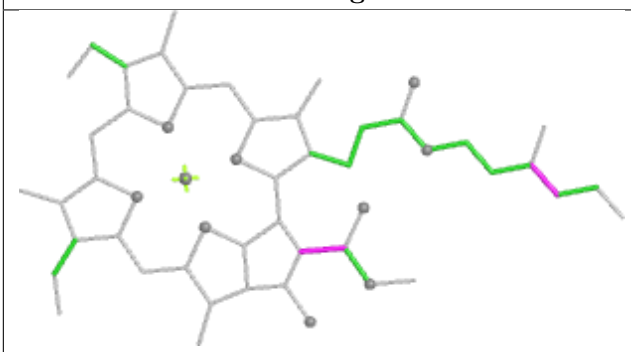

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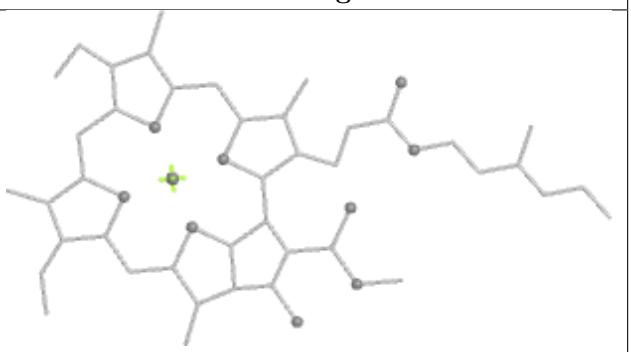
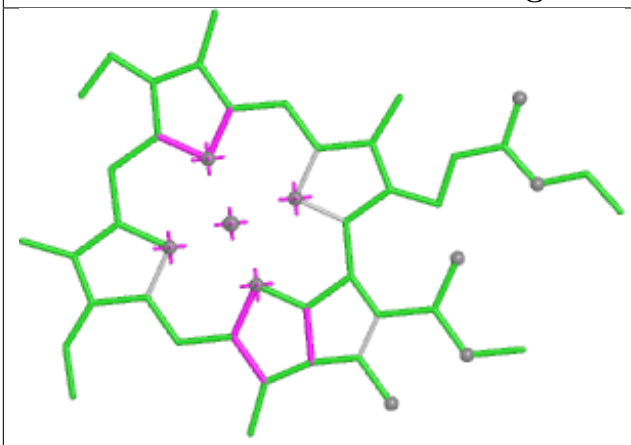


Rings

Ligand CLA F 204



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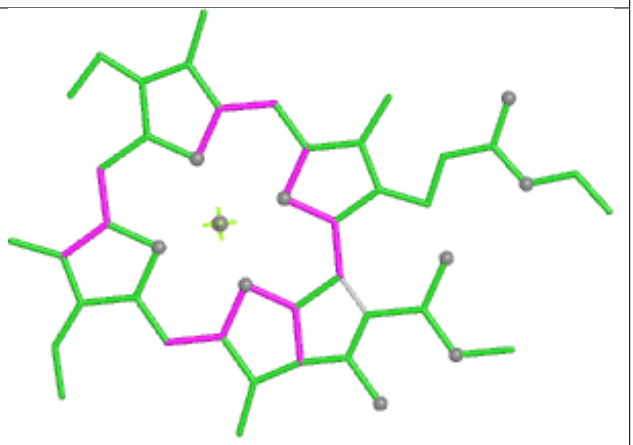

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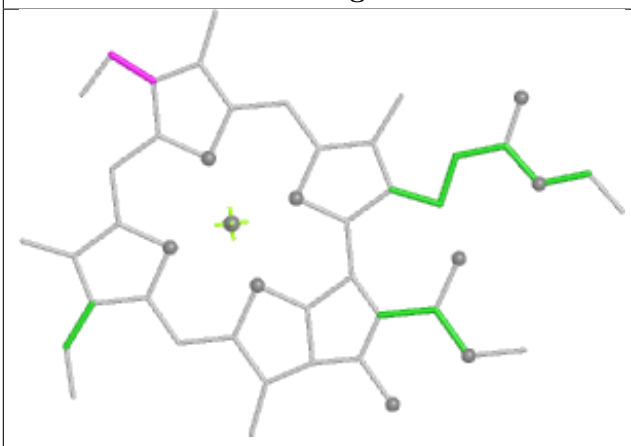

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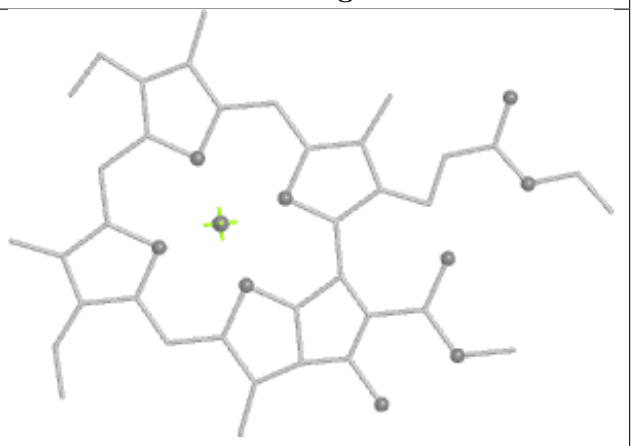
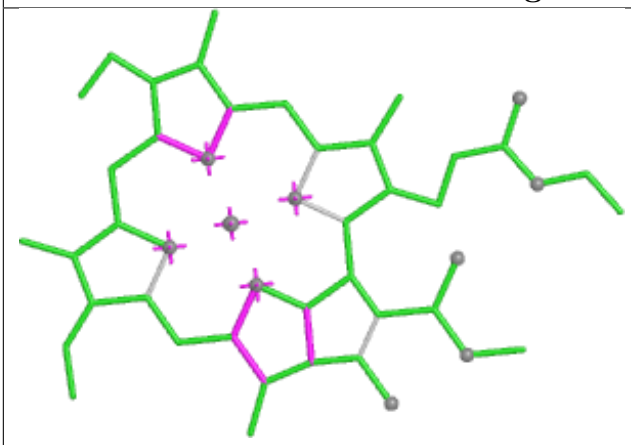


Rings

Ligand CLA B 841



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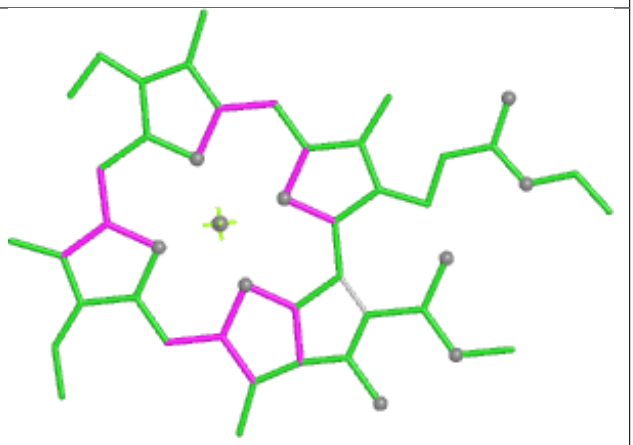

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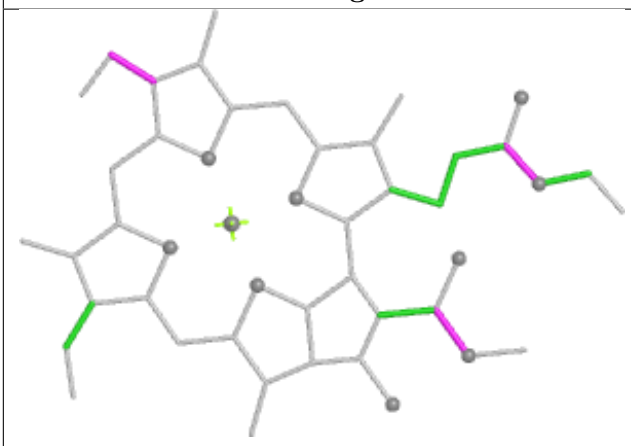

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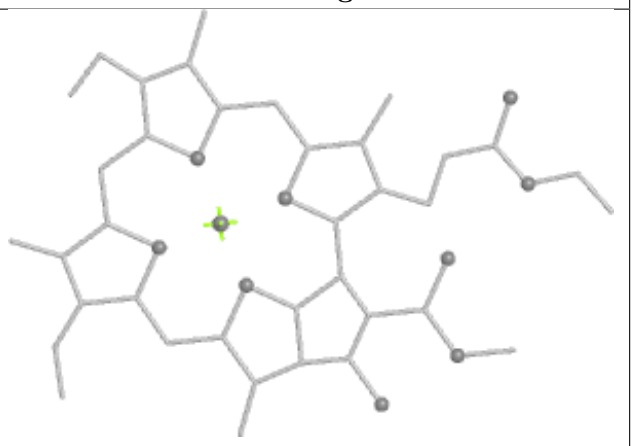
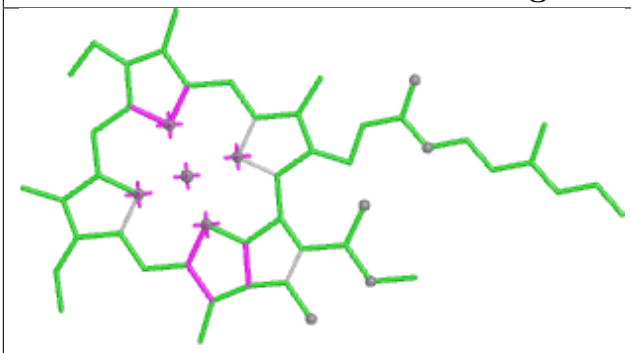


Rings

Ligand CLA c 304



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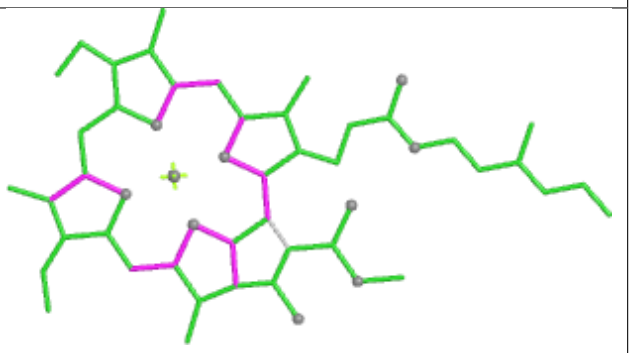
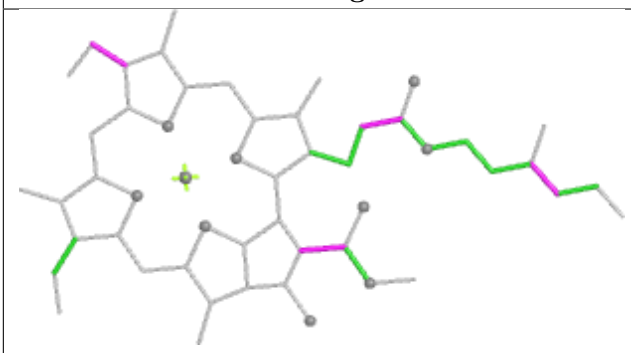


Bond angles



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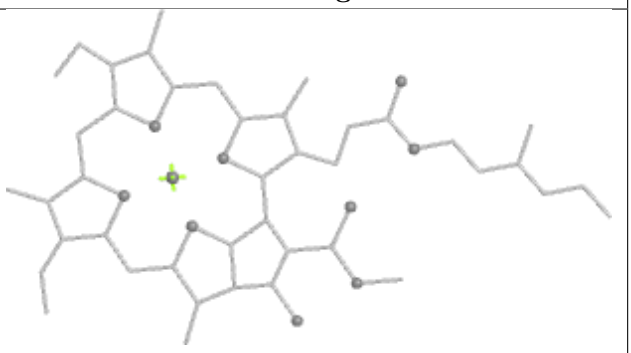
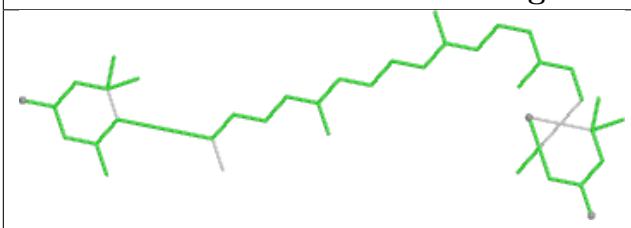


Rings

Ligand DD6 b 317



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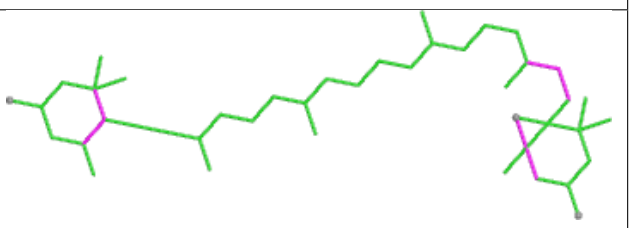
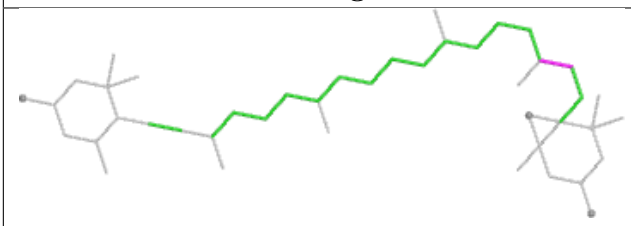


Bond angles



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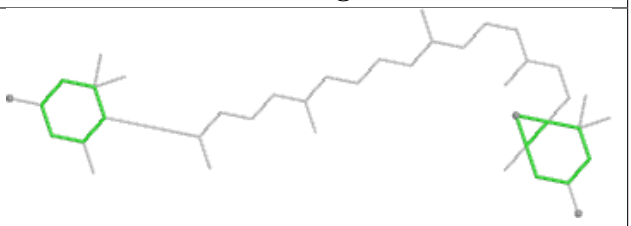
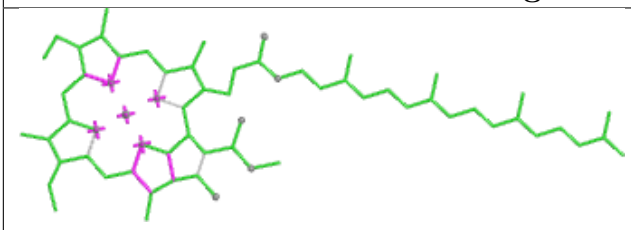


Rings

Ligand CLA A 809



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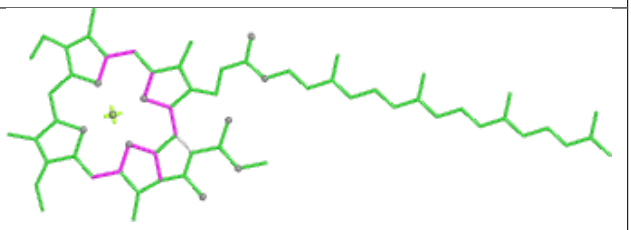
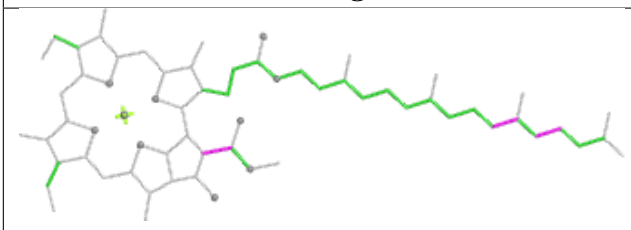


Bond angles



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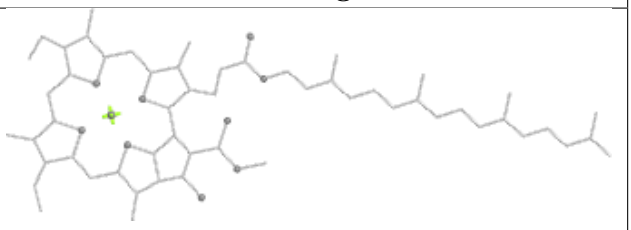
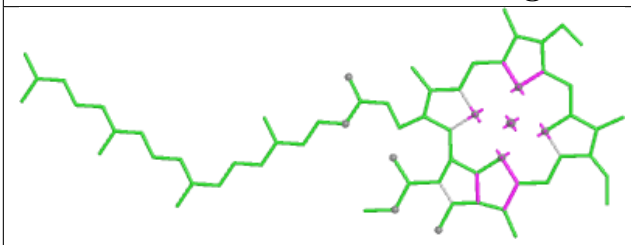
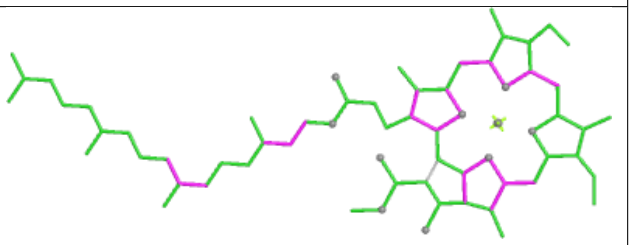


Rings

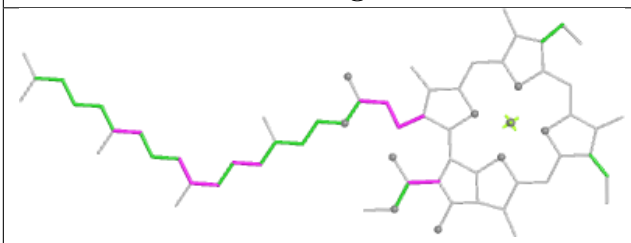
Ligand CLA A 843



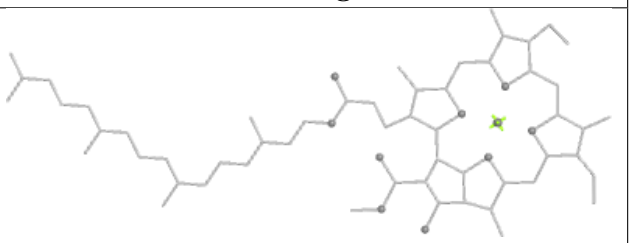
Bond lengths



Bond angles

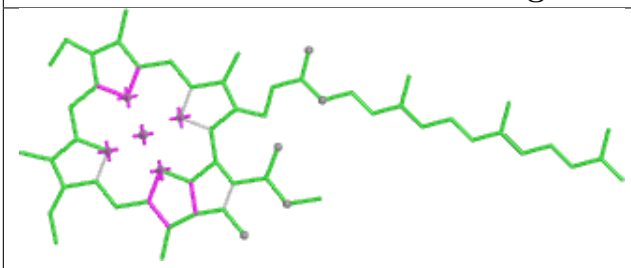


Torsions



Rings

Ligand CLA n 205



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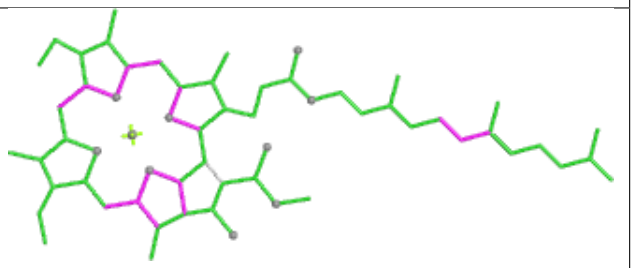

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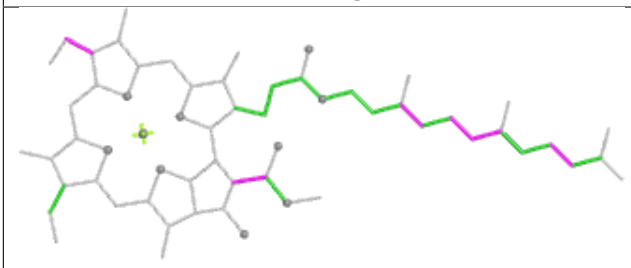

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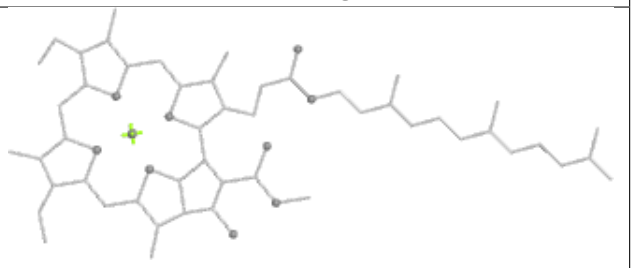
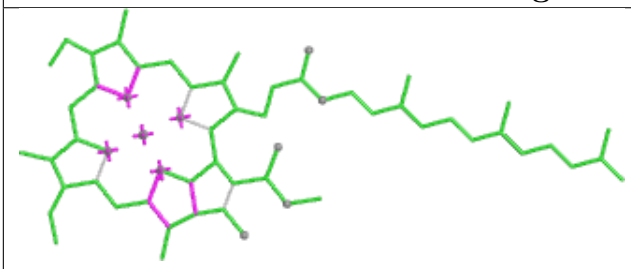


Rings

Ligand CLA l 205



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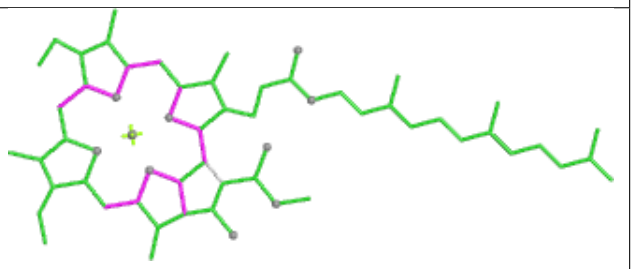

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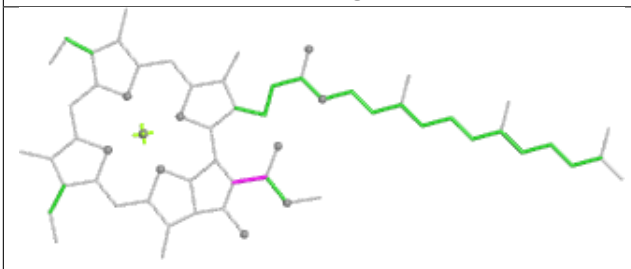

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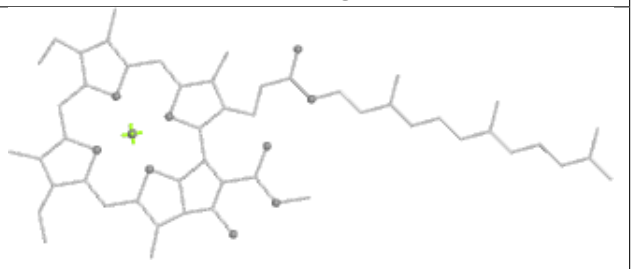
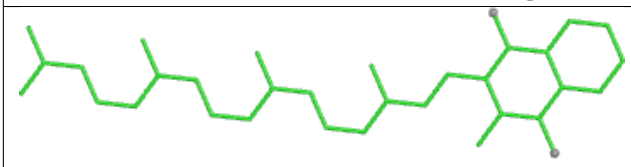


Rings

Ligand PQN A 830



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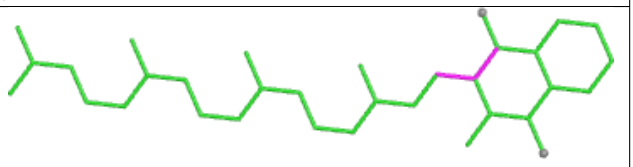
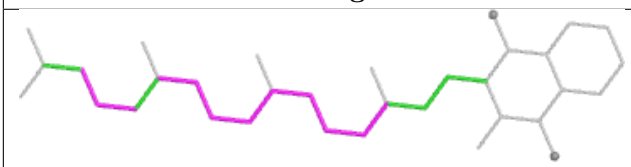


Bond angles



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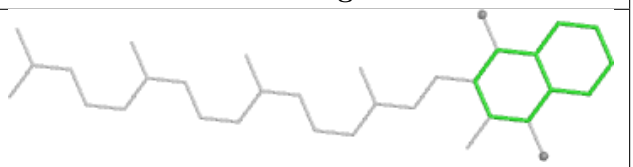
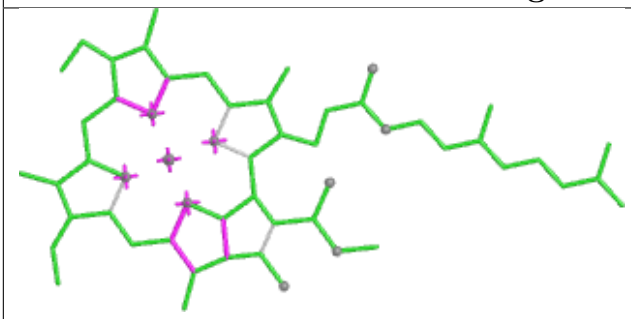


Rings

Ligand CLA k 310



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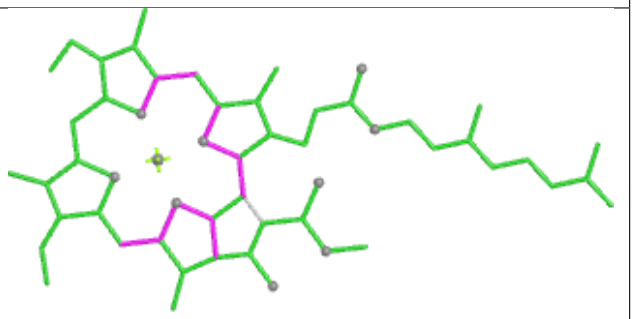

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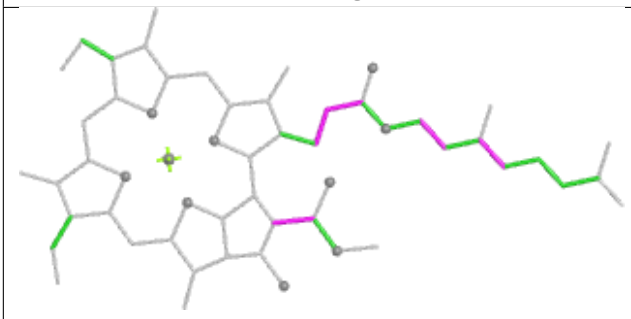

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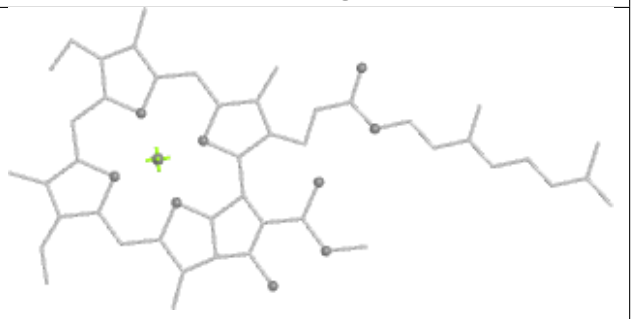
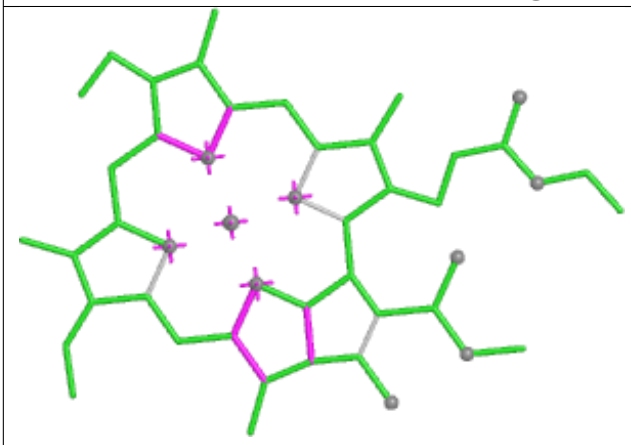


Rings

Ligand CLA d 212



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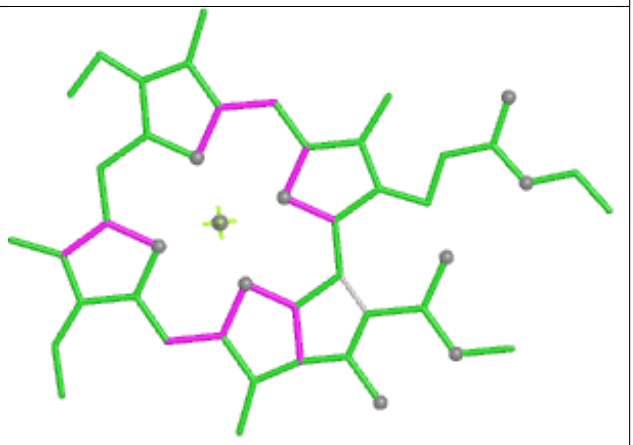

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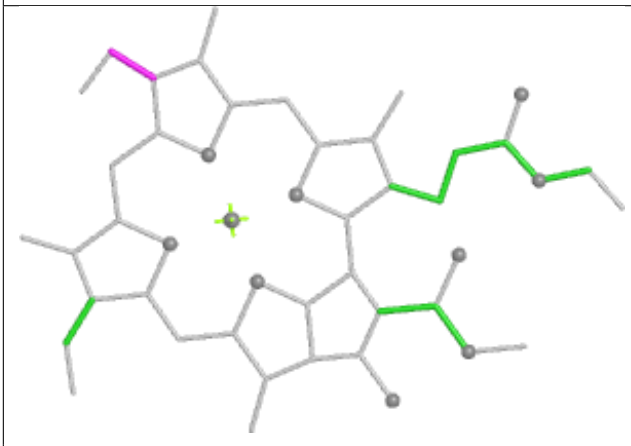

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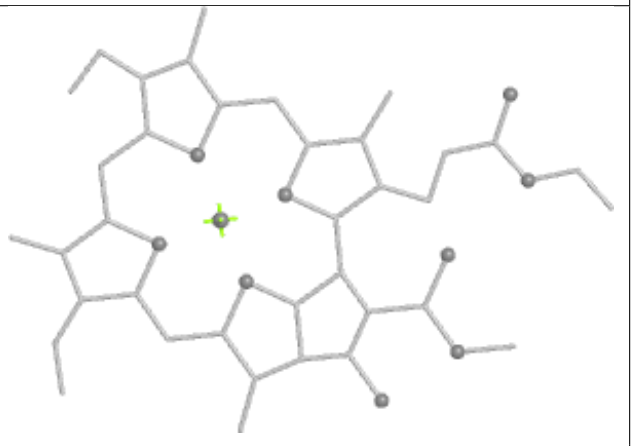
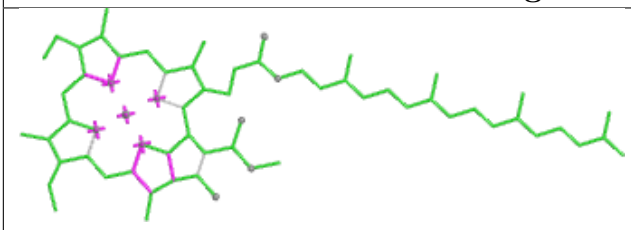


Rings

Ligand CLA B 819



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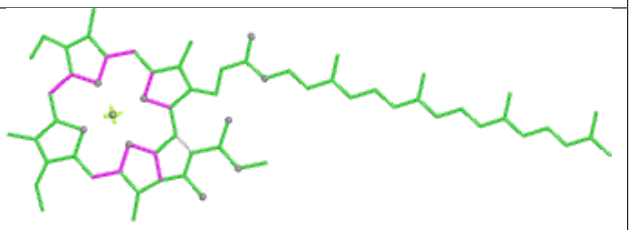
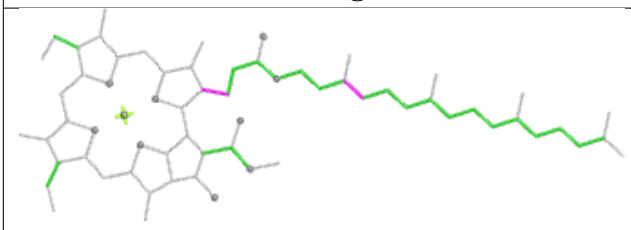


Bond angles



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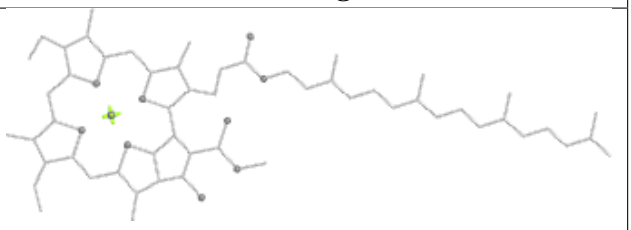
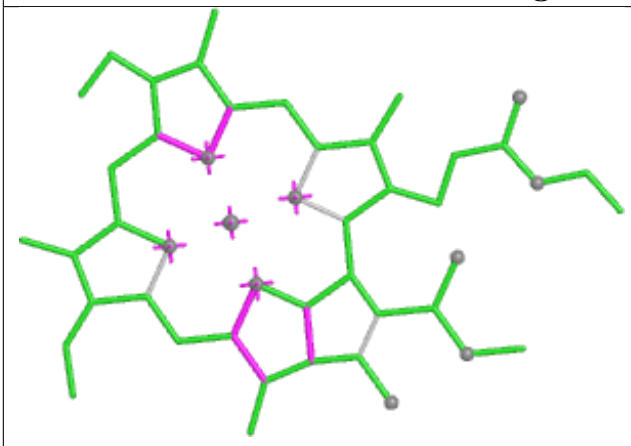


Rings

Ligand CLA l 202



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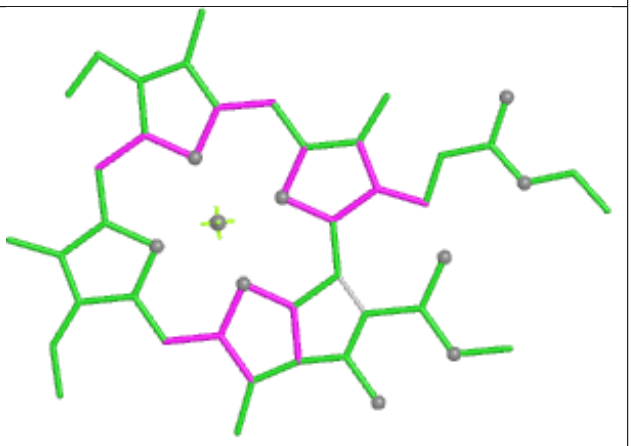
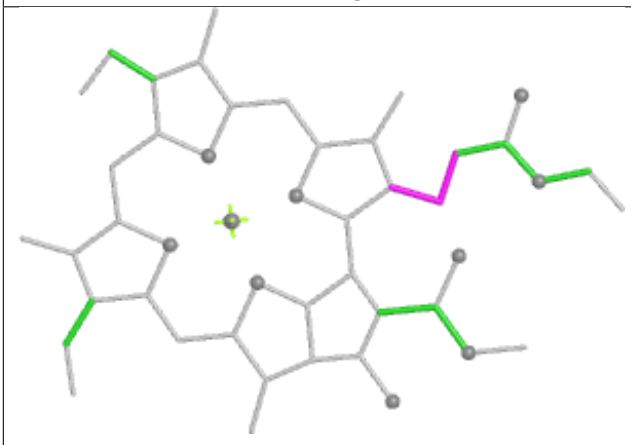


Bond angles



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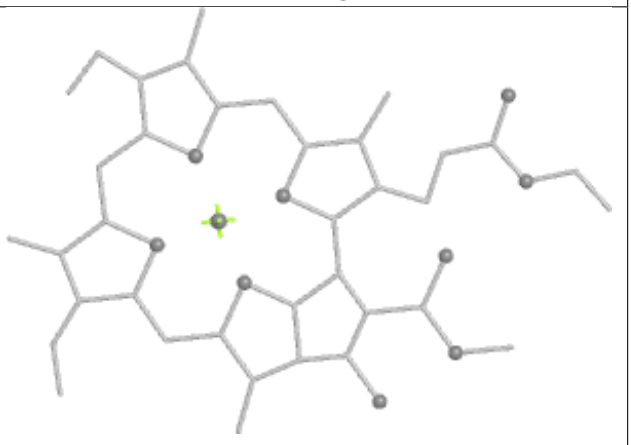
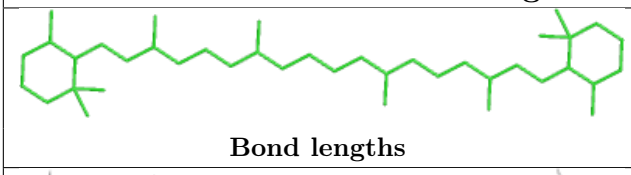


Rings

Ligand BCR B 850



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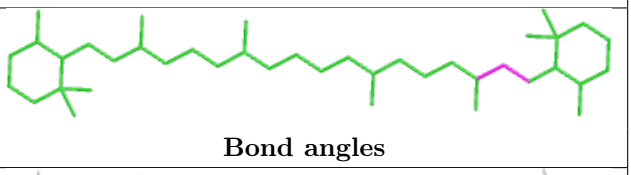
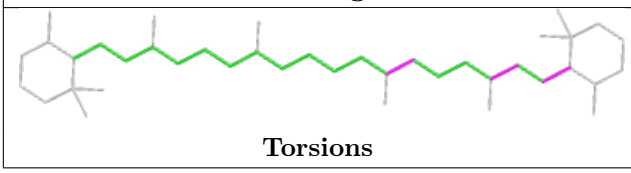


Bond angles



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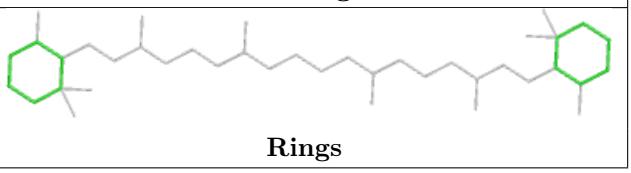
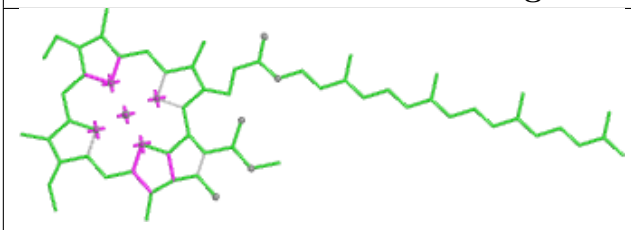


Rings

Ligand CLA B 818



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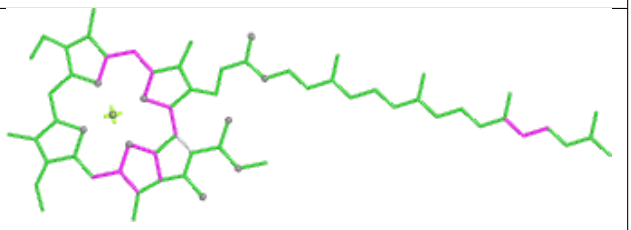
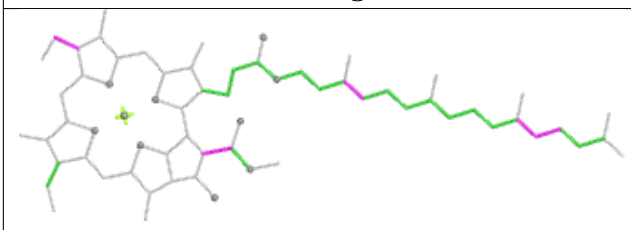


Bond angles



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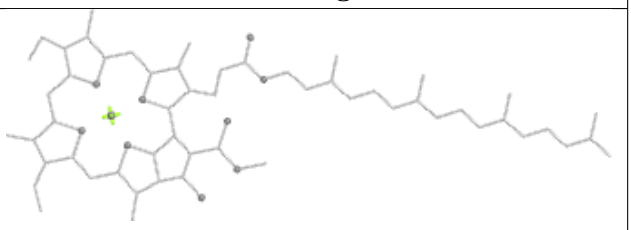
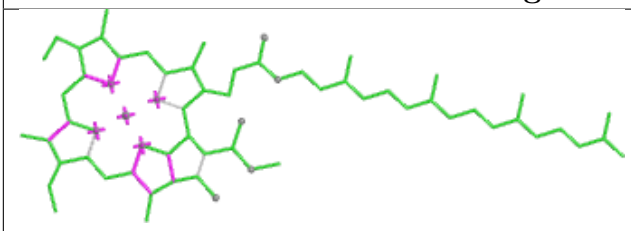


Rings

Ligand CLA A 802



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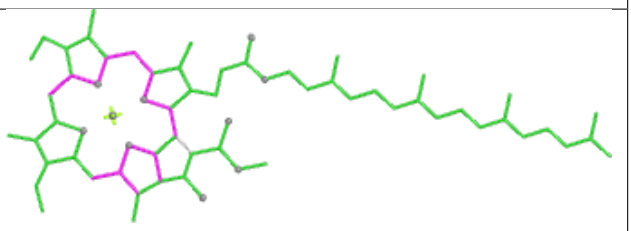

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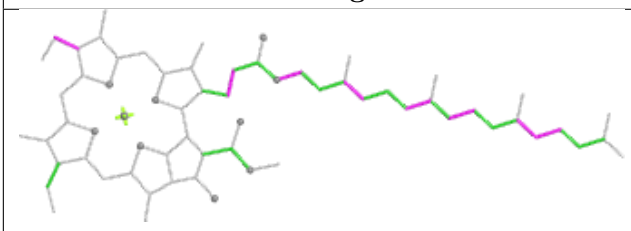

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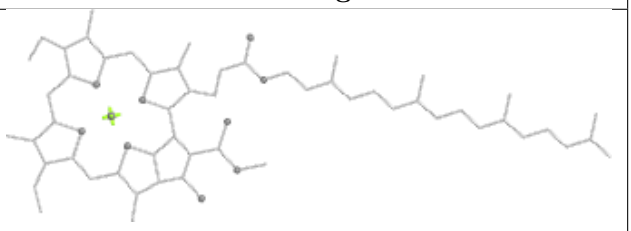
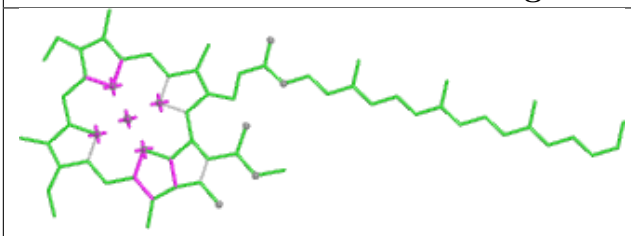


Rings

Ligand CLA B 836



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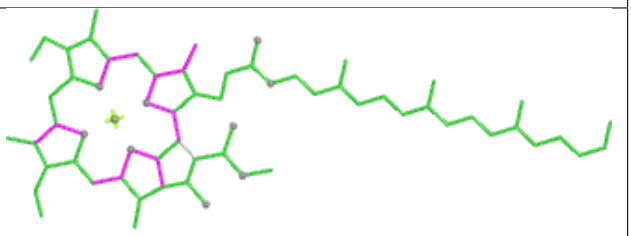
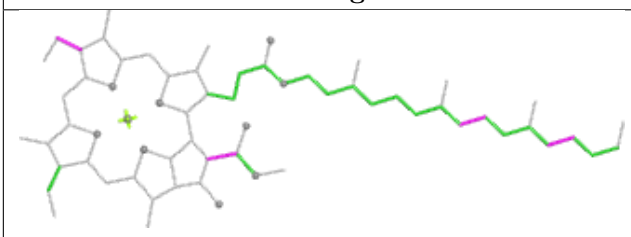


Bond angles



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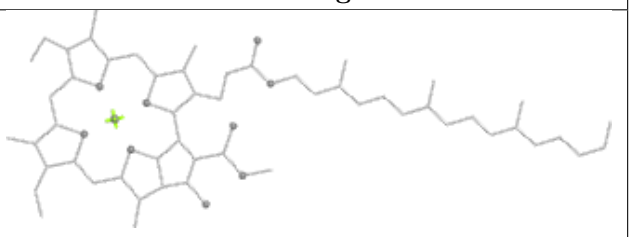
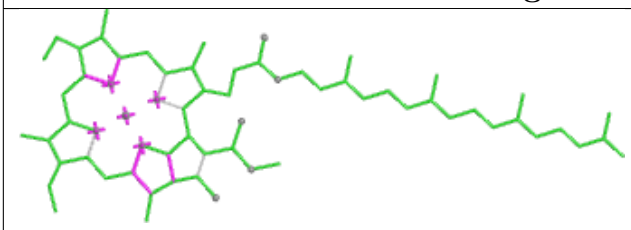
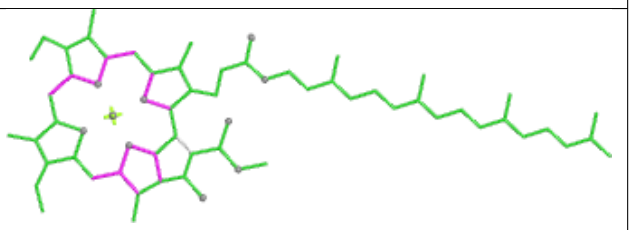


Rings

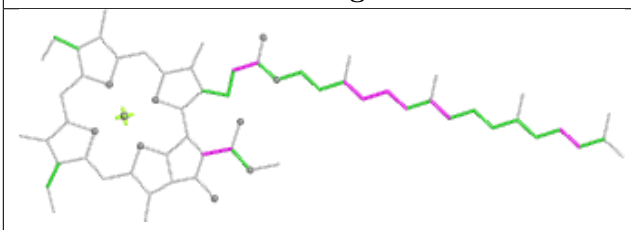
Ligand CLA A 807



Bond lengths



Bond angles



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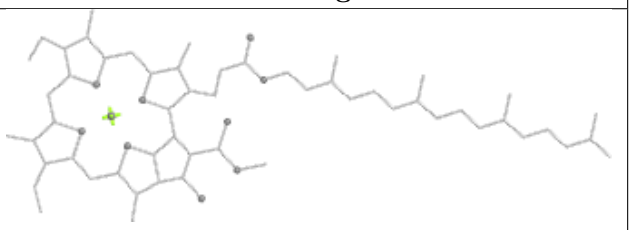
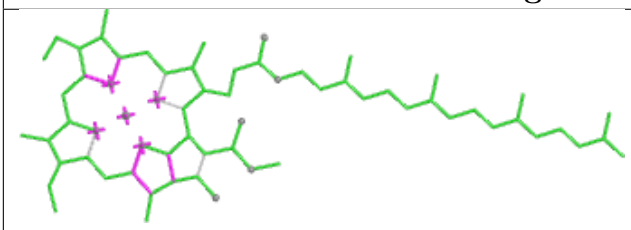
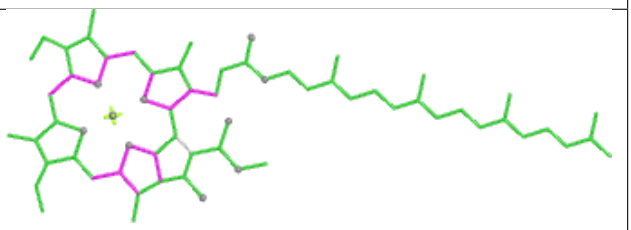


Rings

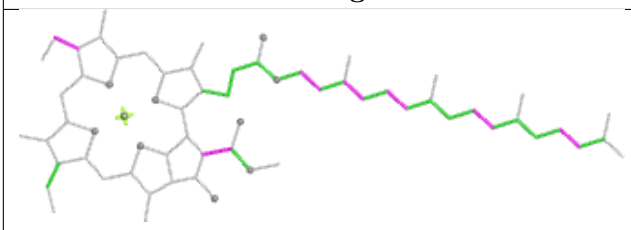
Ligand CLA B 847



Bond lengths



Bond angles



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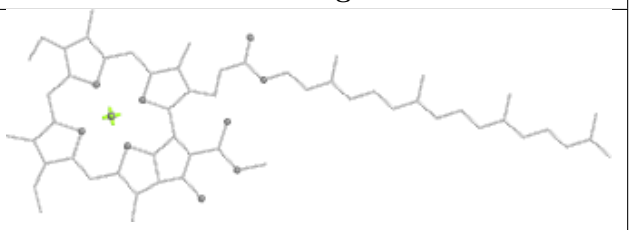
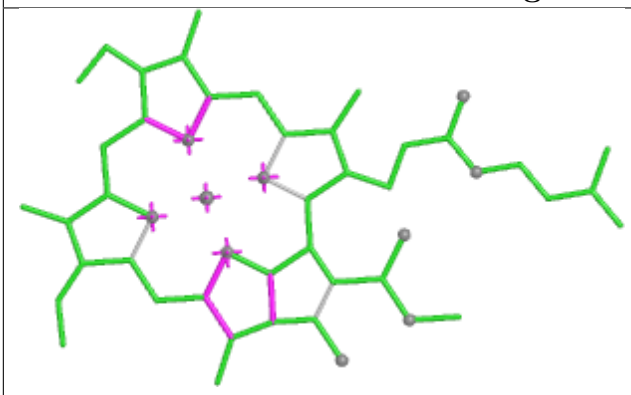
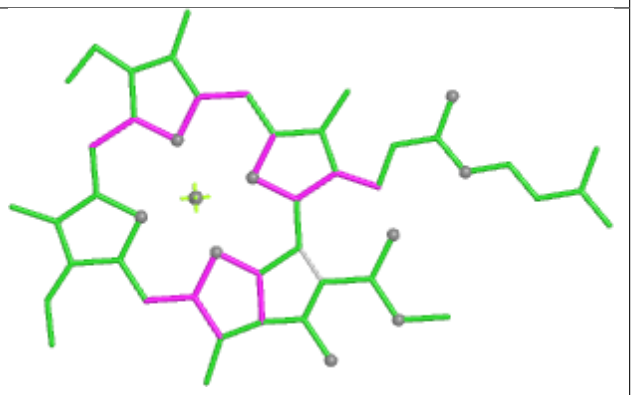


Rings

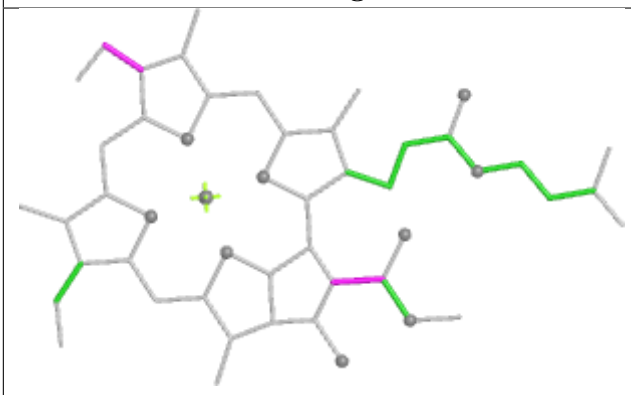
Ligand CLA A 825



Bond lengths



Bond angles



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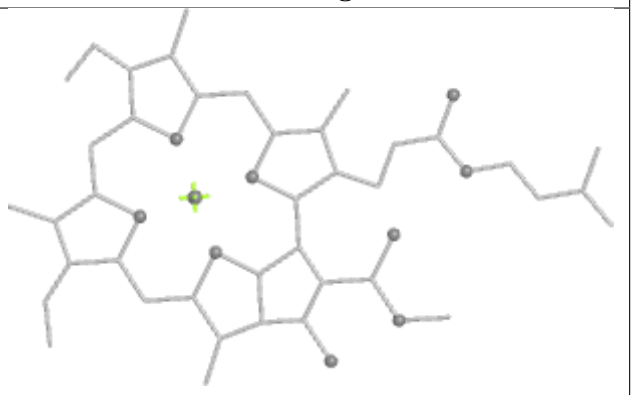
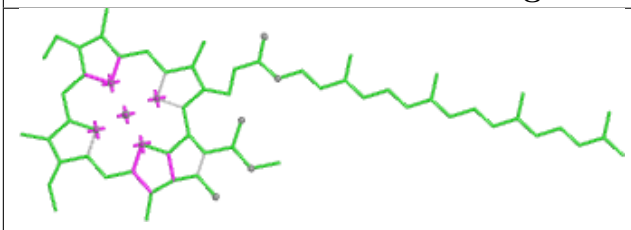
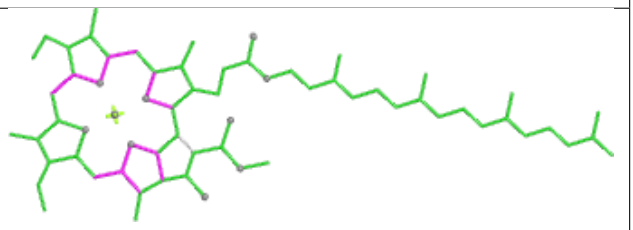


Rings

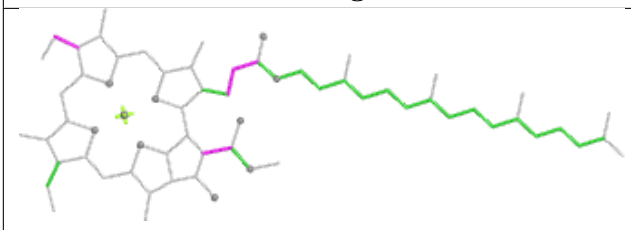
Ligand CLA A 829



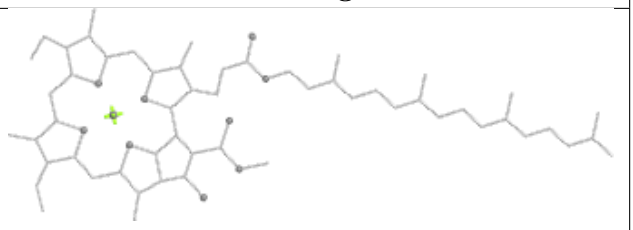
Bond lengths



Bond angles

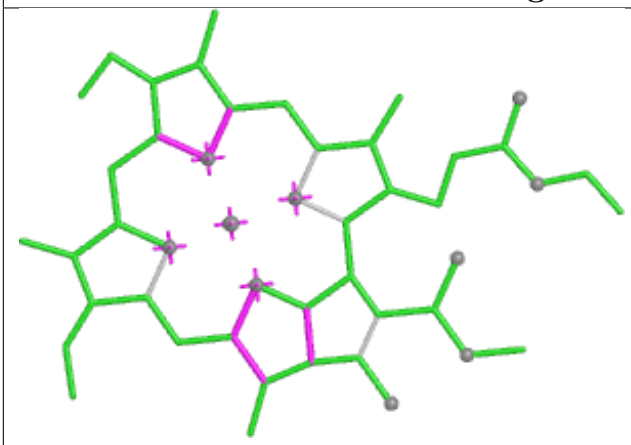


Torsions



Rings

Ligand CLA n 209



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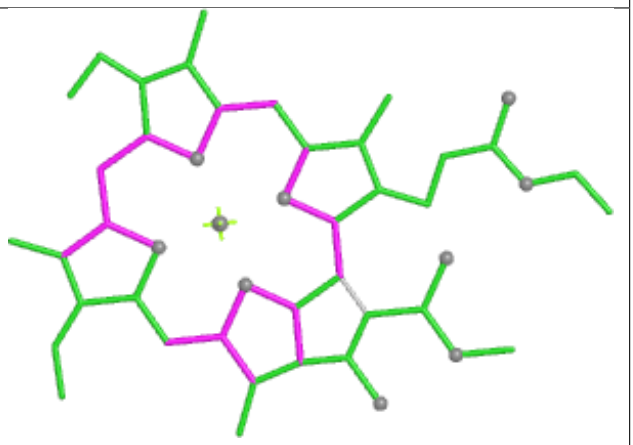
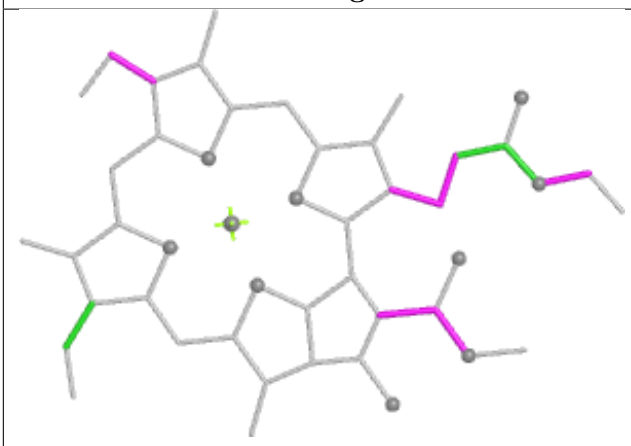


Bond angles



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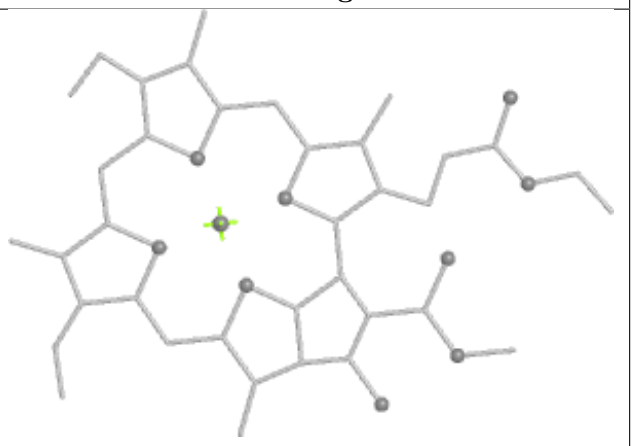
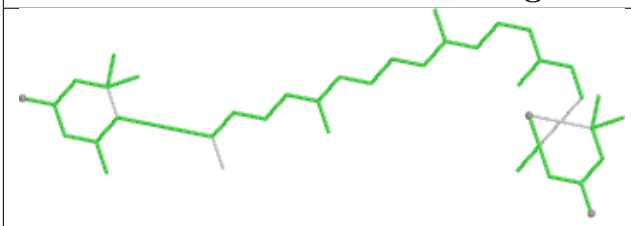


Rings

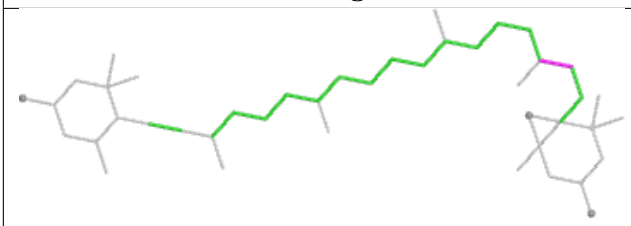
Ligand DD6 A 832



Bond lengths



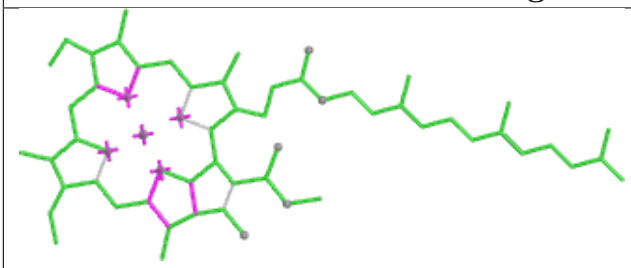
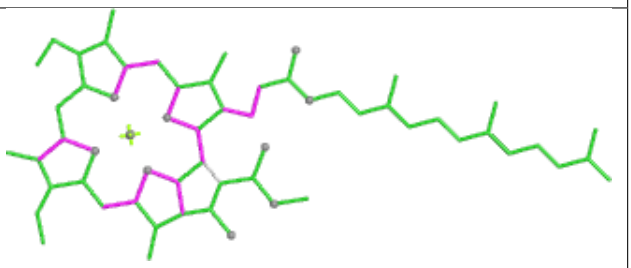
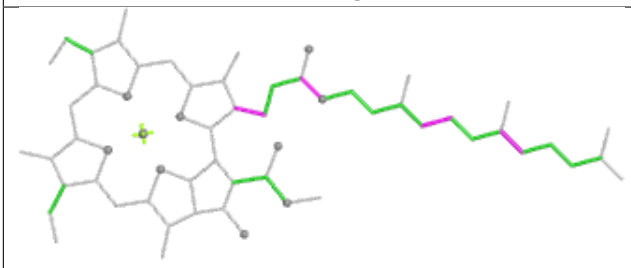
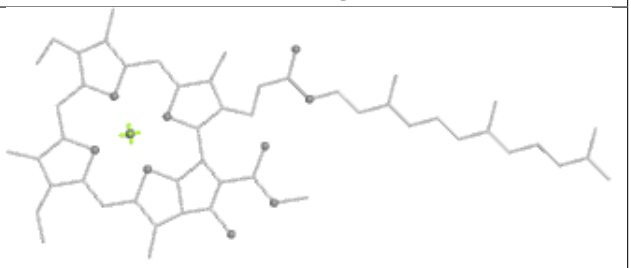
Bond angles

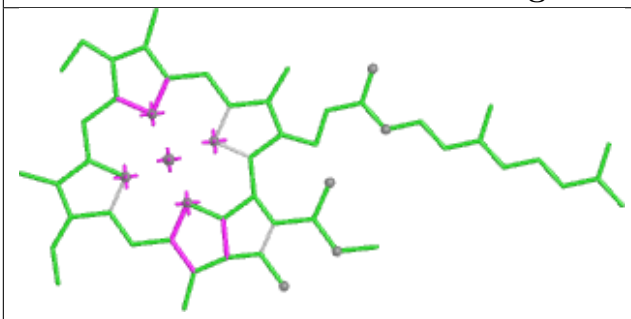
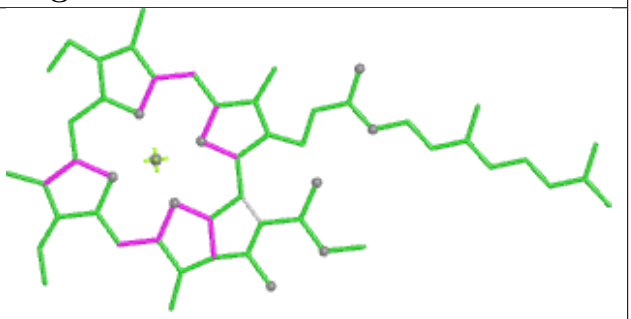
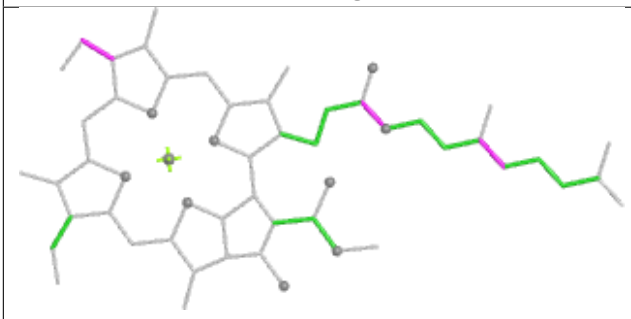
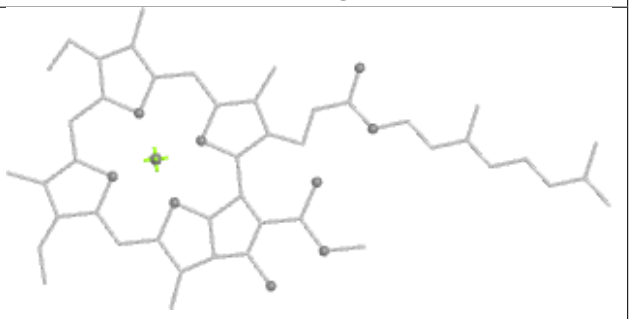


Torsions

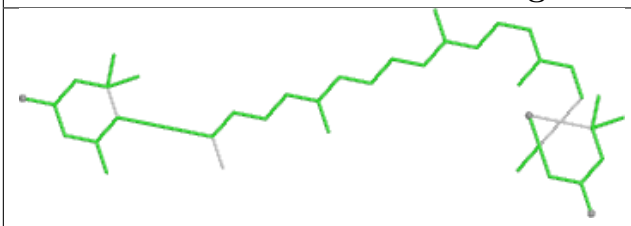


Rings

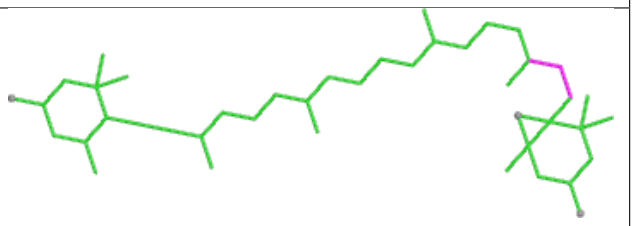
Ligand CLA d 211	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA g 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

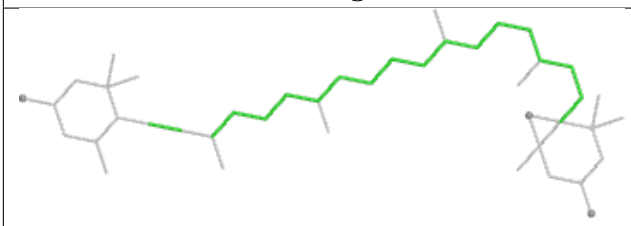
Ligand DD6 n 211



Bond lengths



Bond angles



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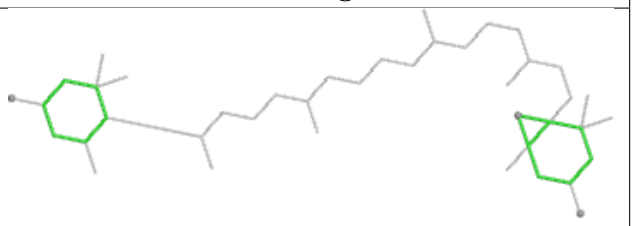
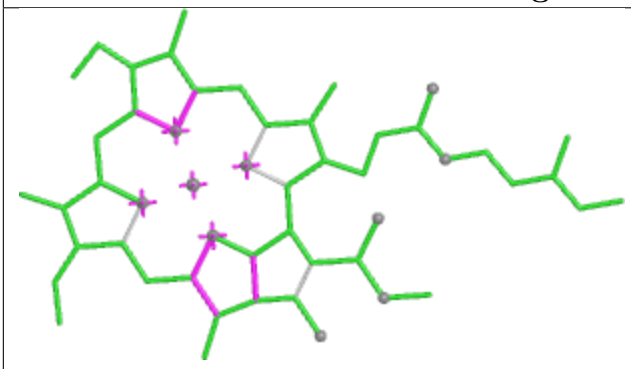


Rings

Ligand CLA f 308



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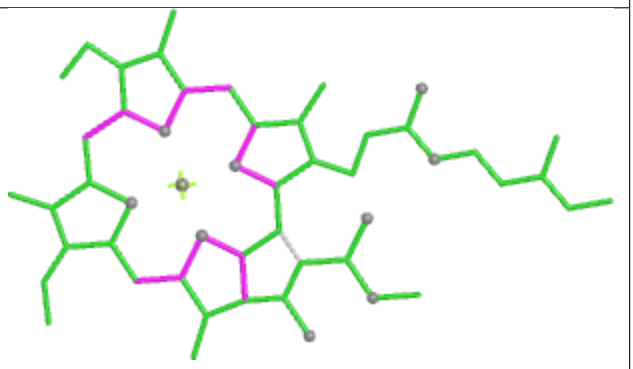
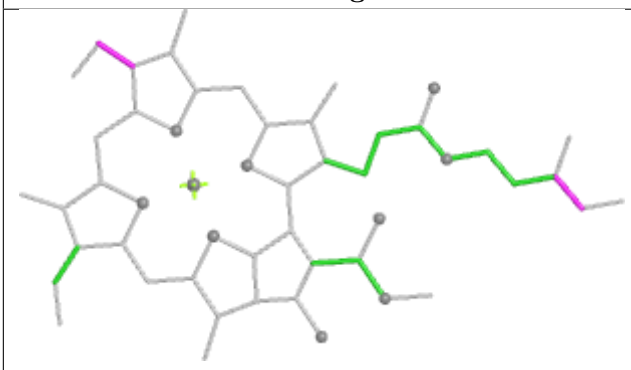


Bond angles



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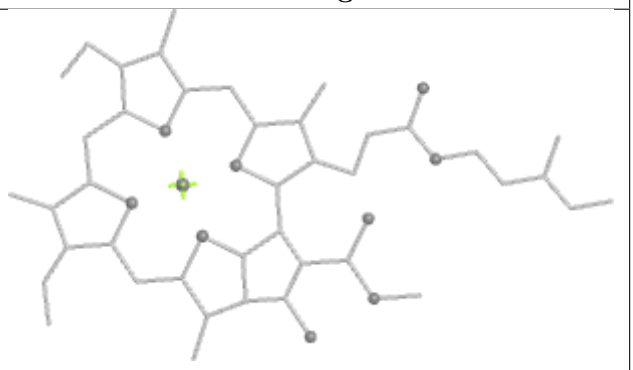
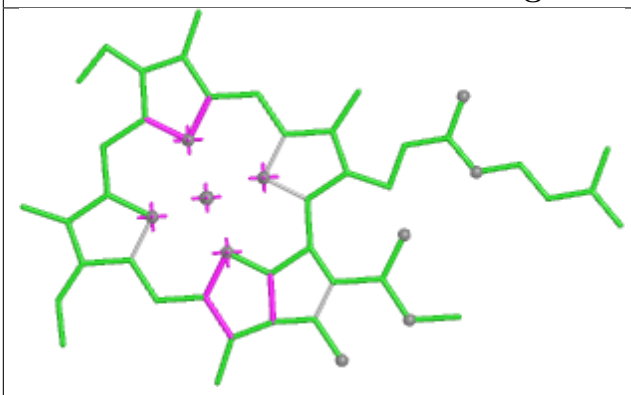


Rings

Ligand CLA B 837



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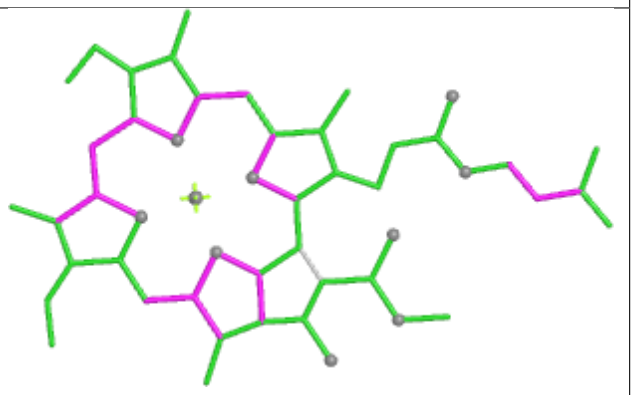
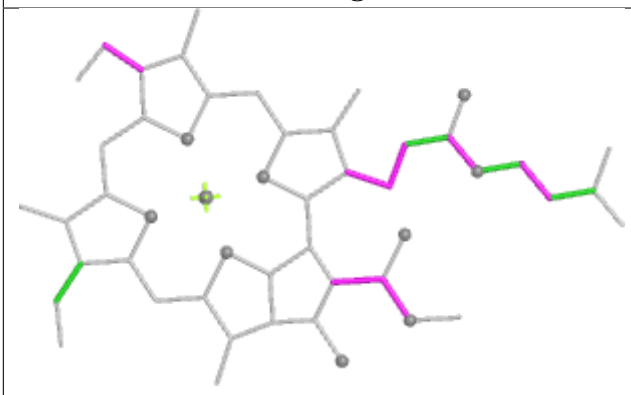


Bond angles



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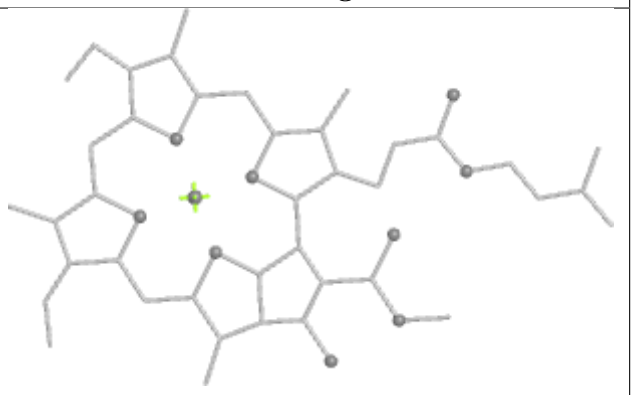
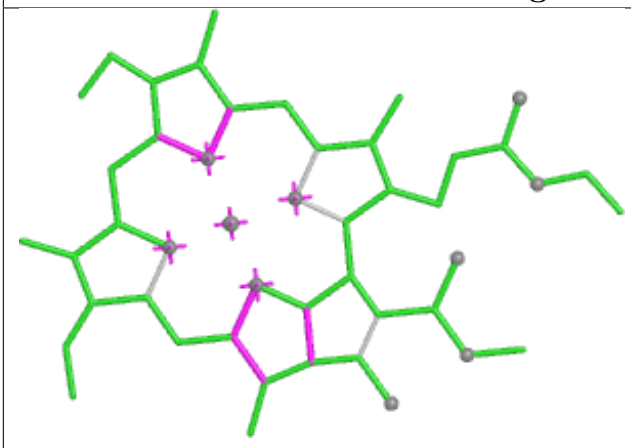


Rings

Ligand CLA c 311



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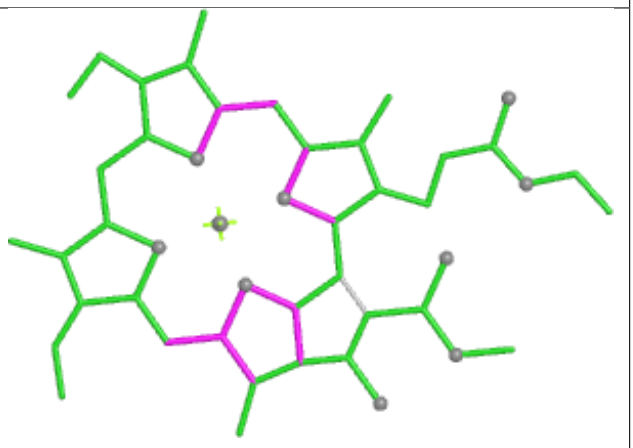
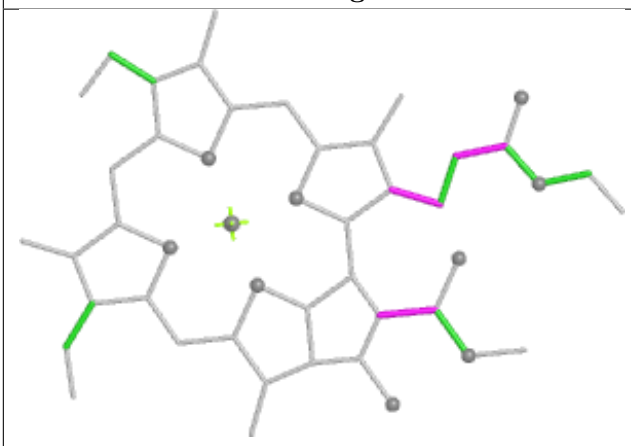


Bond angles



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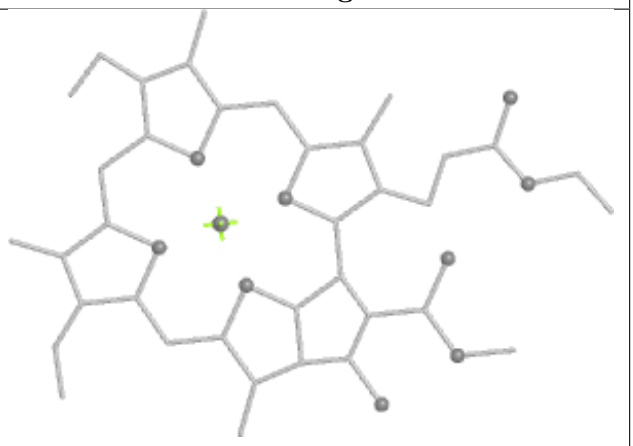
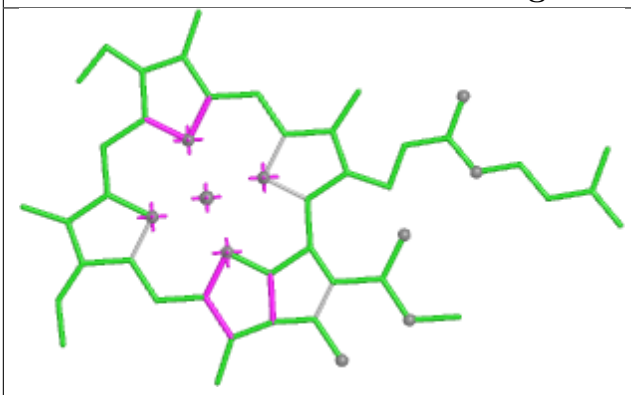


Rings

Ligand CLA a 310



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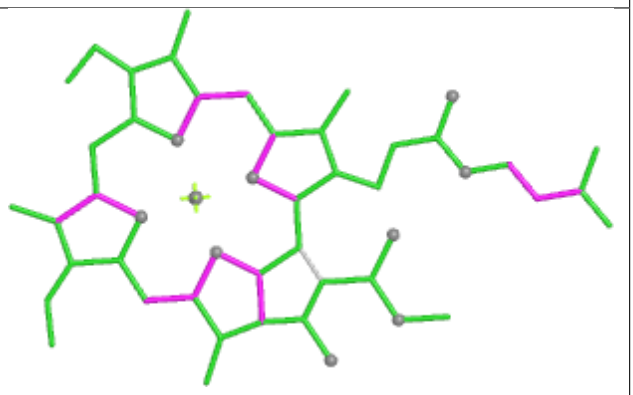
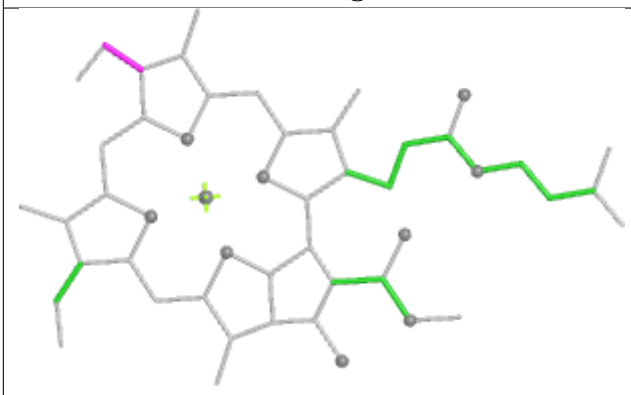


Bond angles



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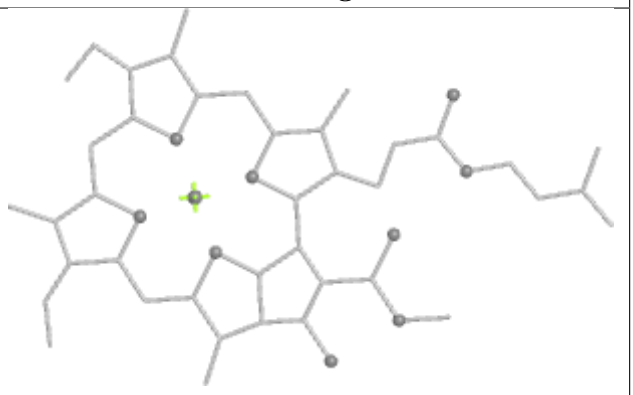
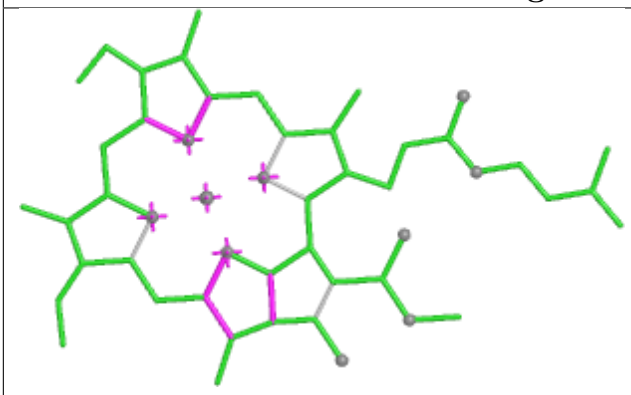


Rings

Ligand CLA b 309



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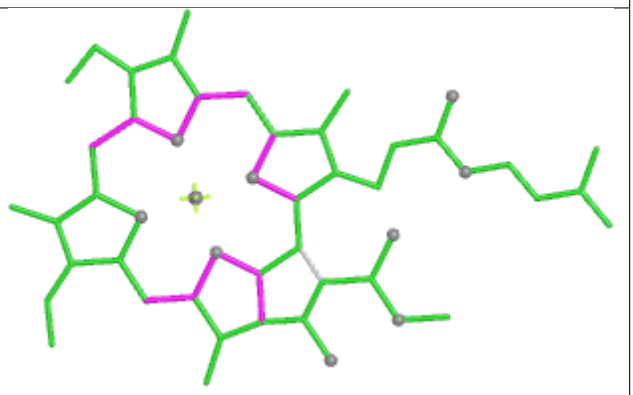
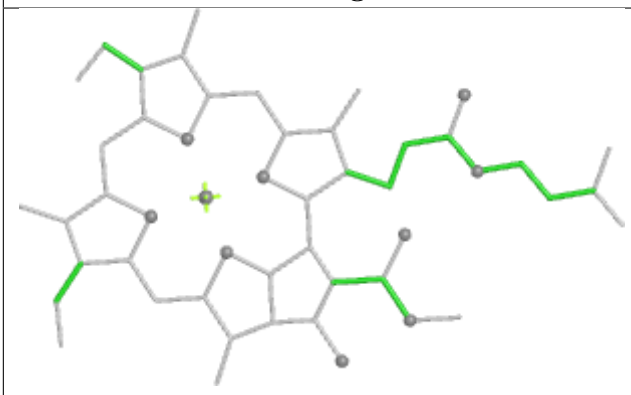


Bond angles



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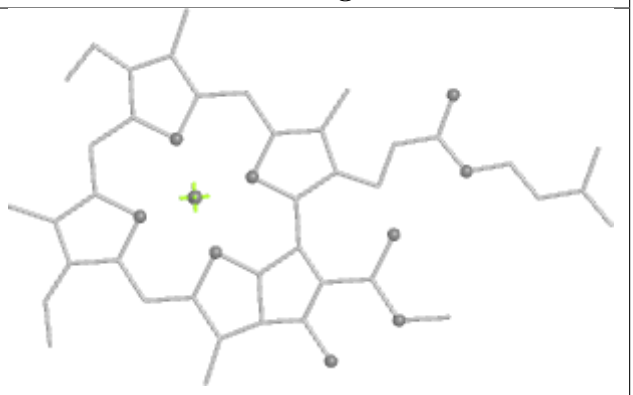
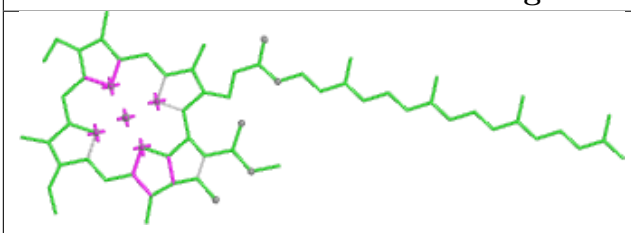


Rings

Ligand CLA A 841



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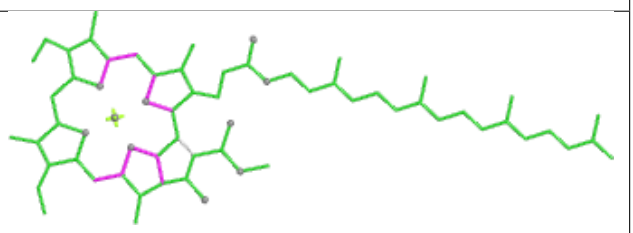
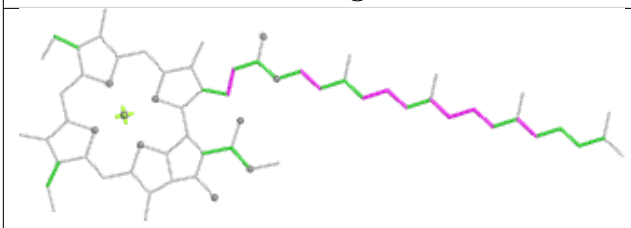


Bond angles



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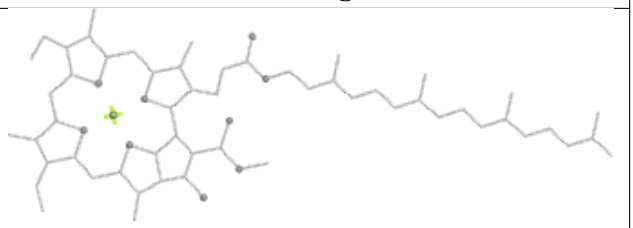
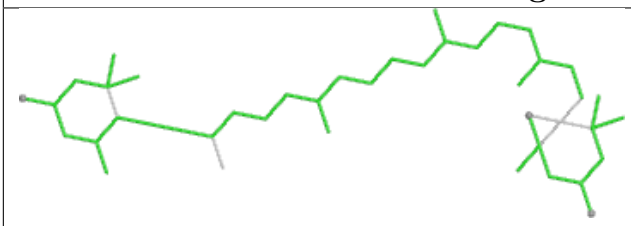
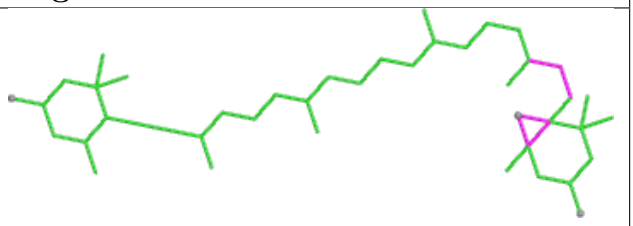


Rings

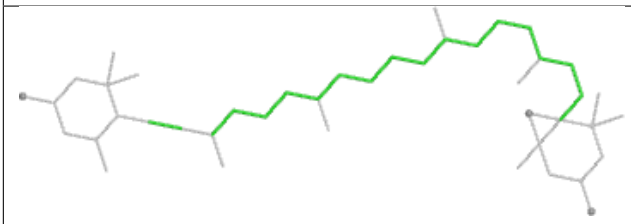
Ligand DD6 g 315



Bond lengths



Bond angles



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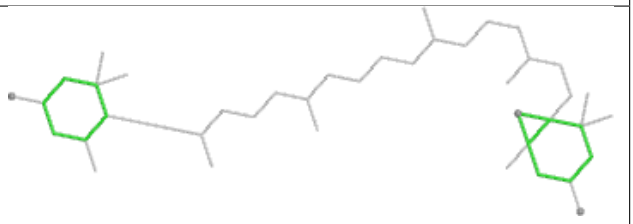
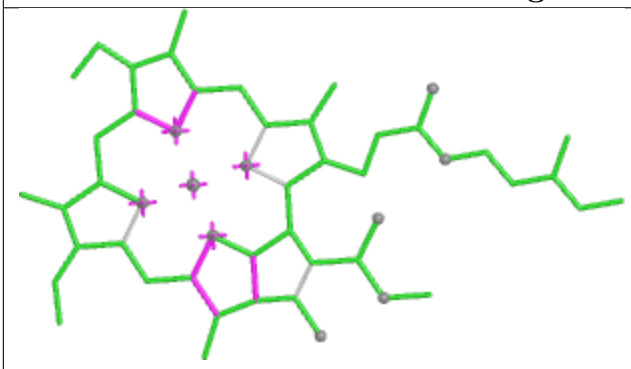


Rings

Ligand CLA h 211



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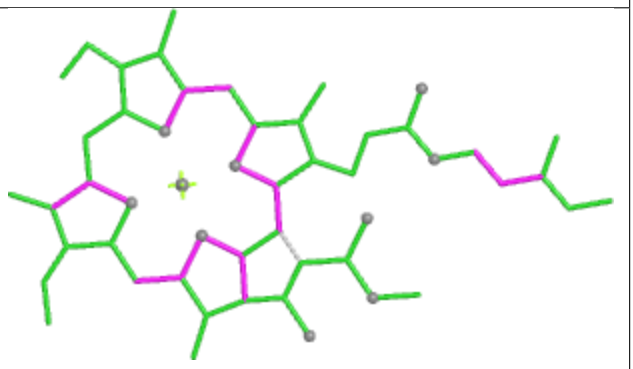
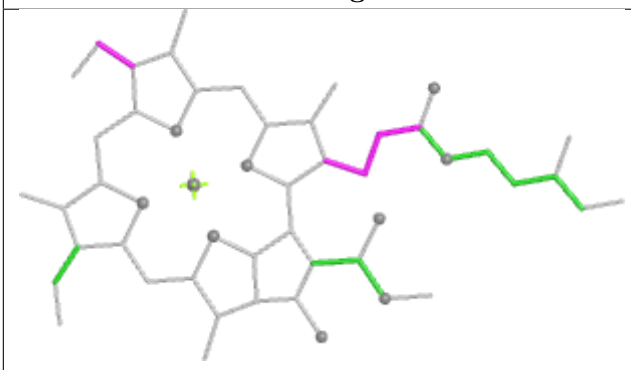


Bond angles



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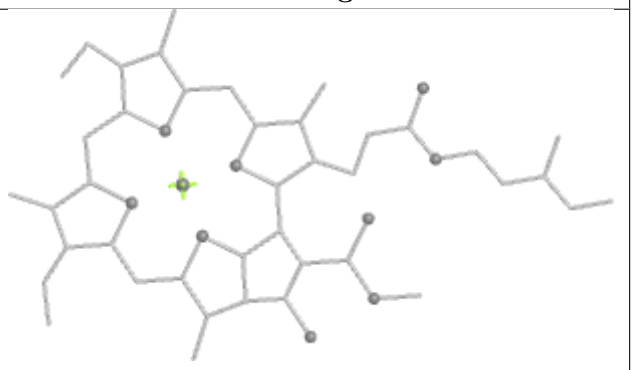
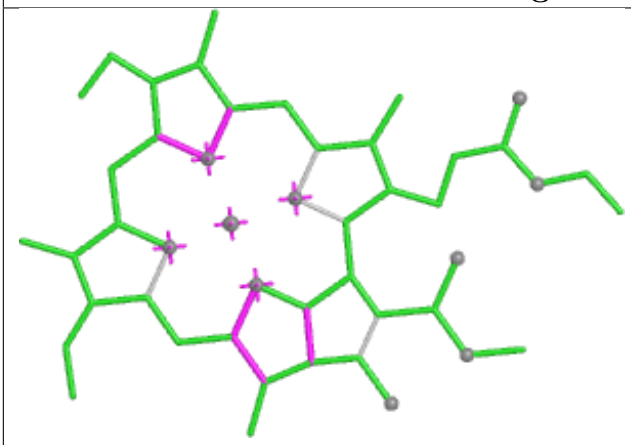


Rings

Ligand CLA j 310



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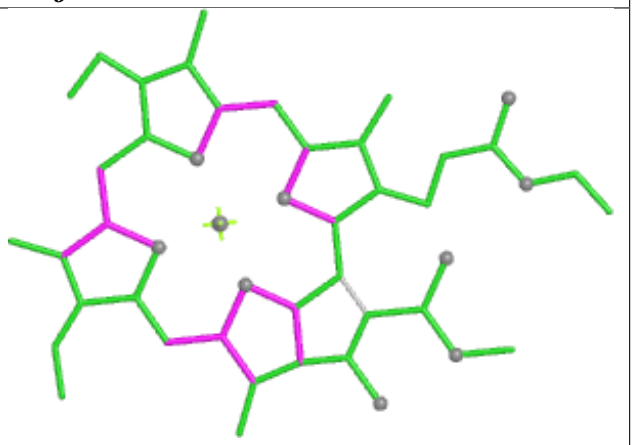
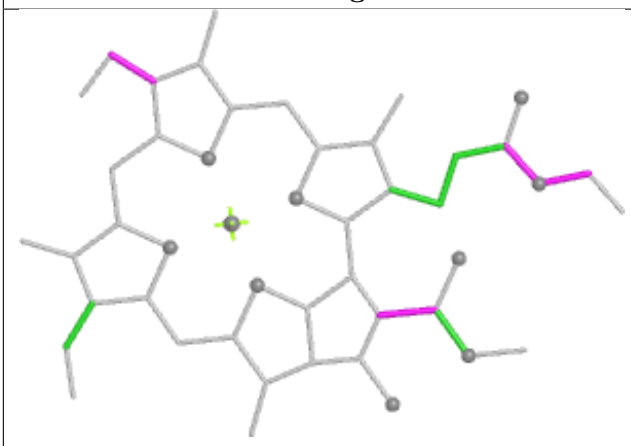


Bond angles



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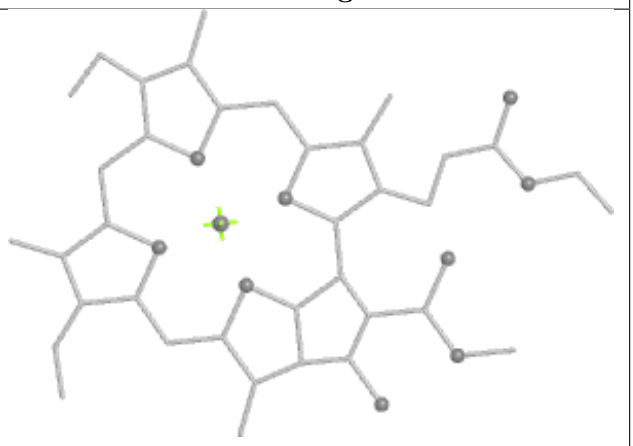
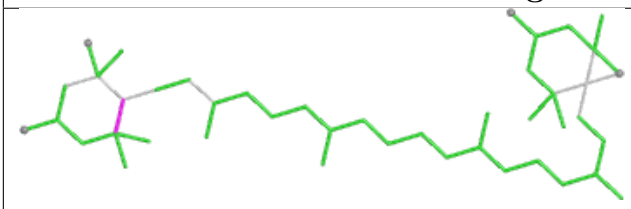


Rings

Ligand NEX a 317



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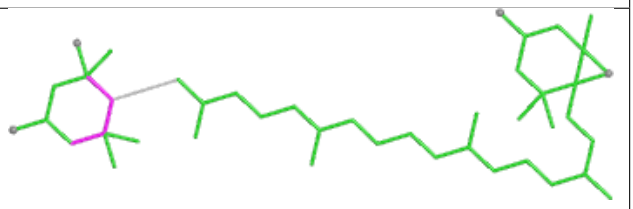
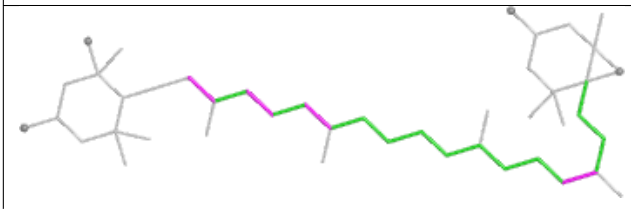
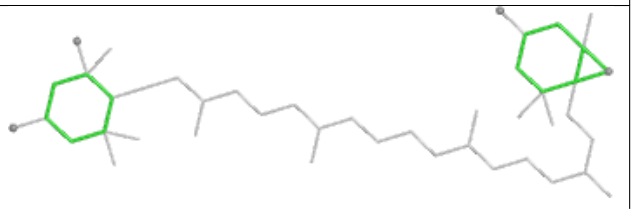


Bond angles

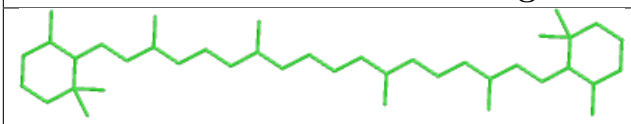


Torsions



Rings

Ligand BCR M 801



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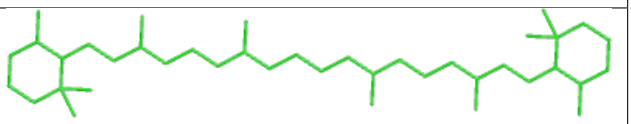

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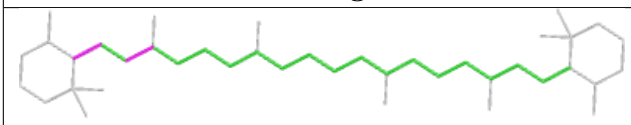

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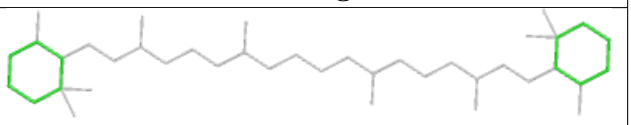
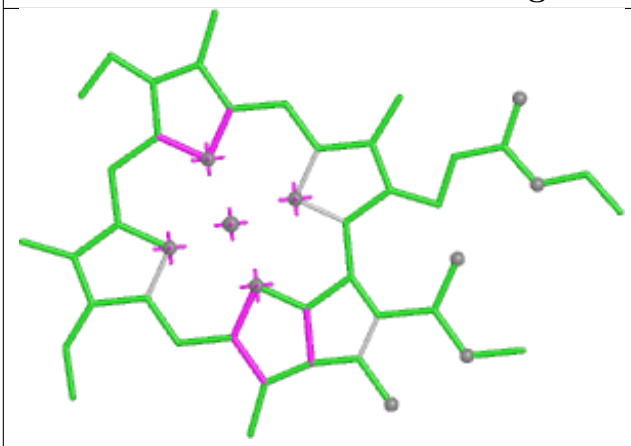


Rings

Ligand CLA a 304



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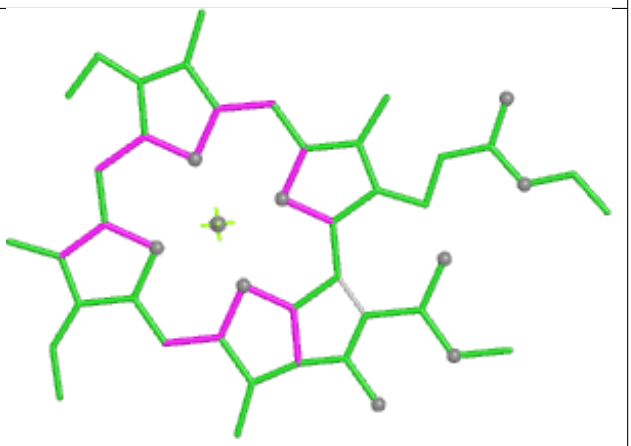

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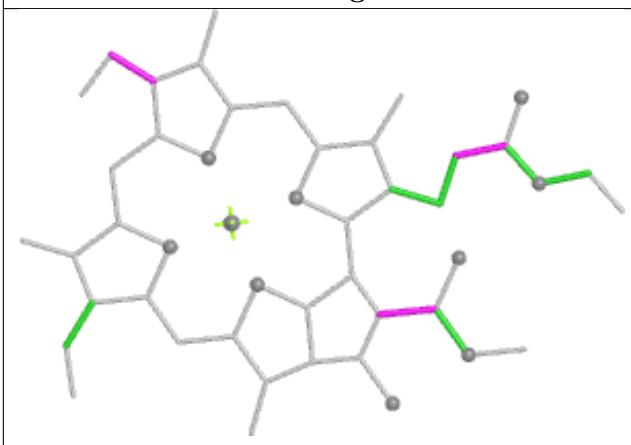

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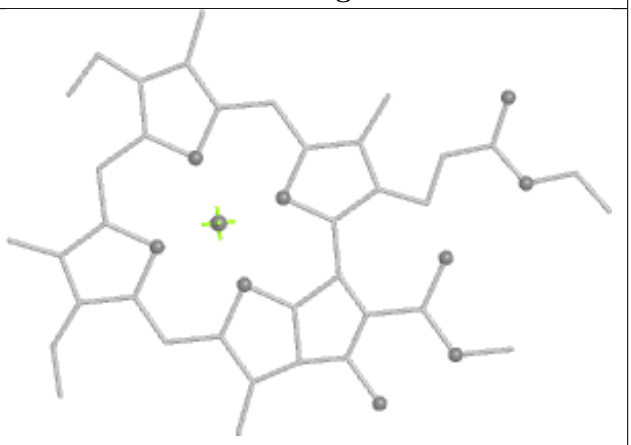
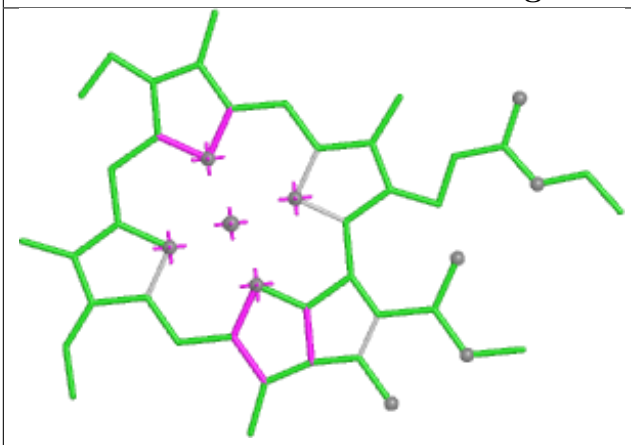


Rings

Ligand CLA B 846



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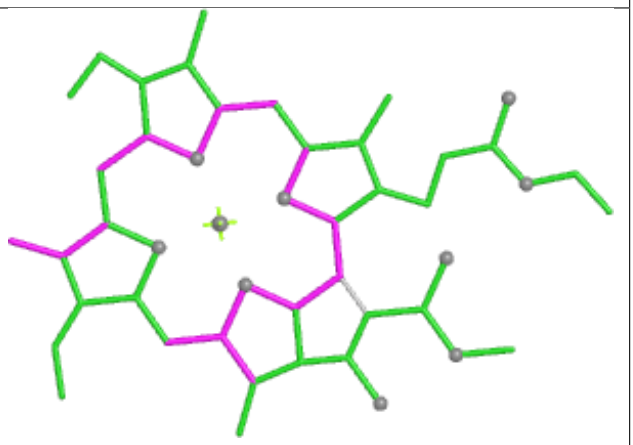

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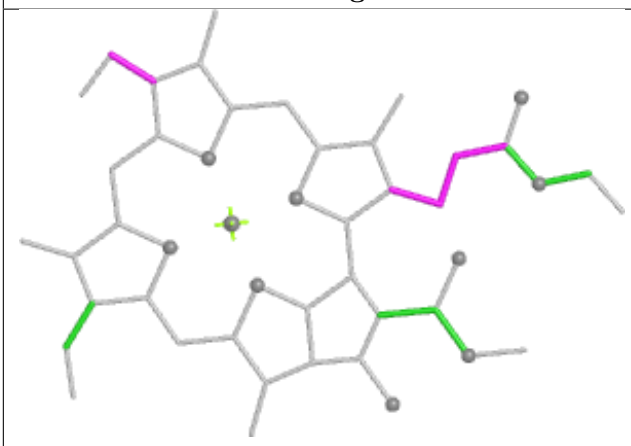

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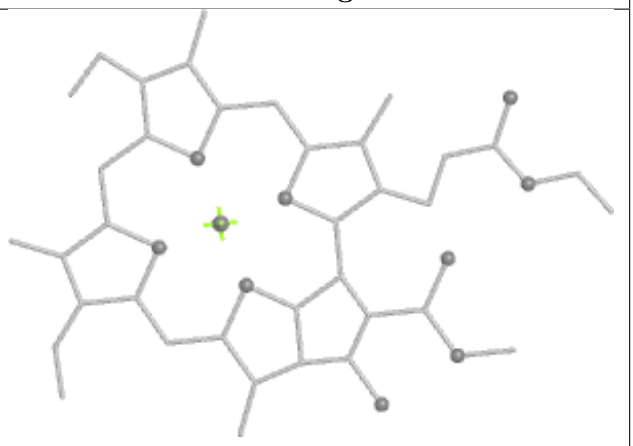
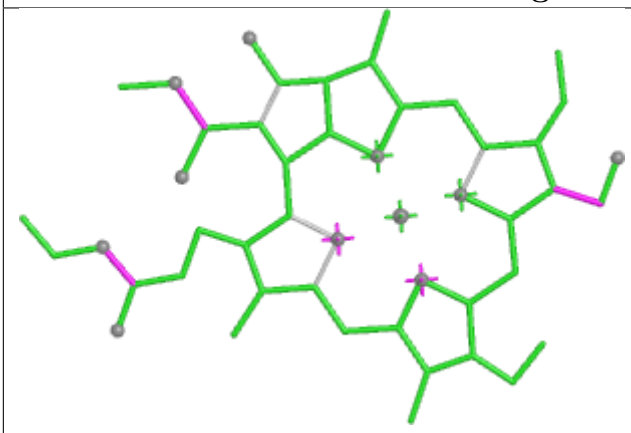


Rings

Ligand CHL i 301



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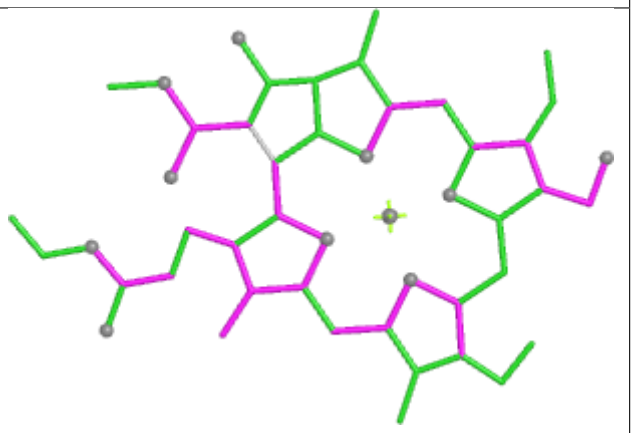

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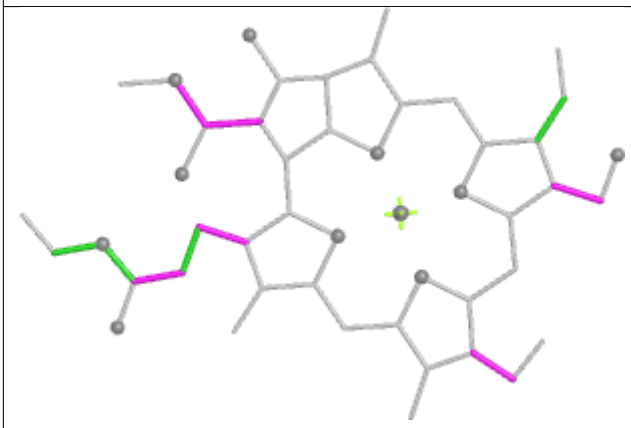

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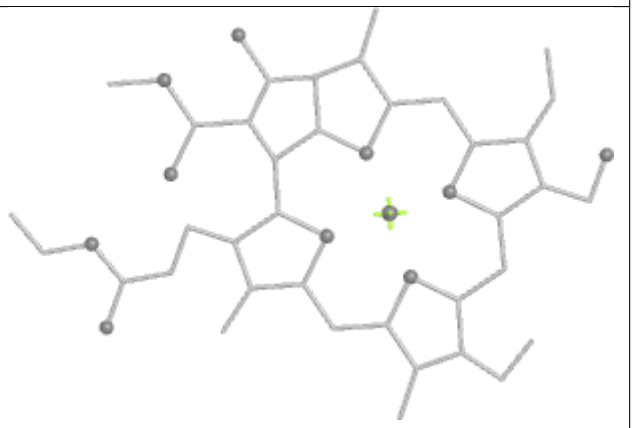
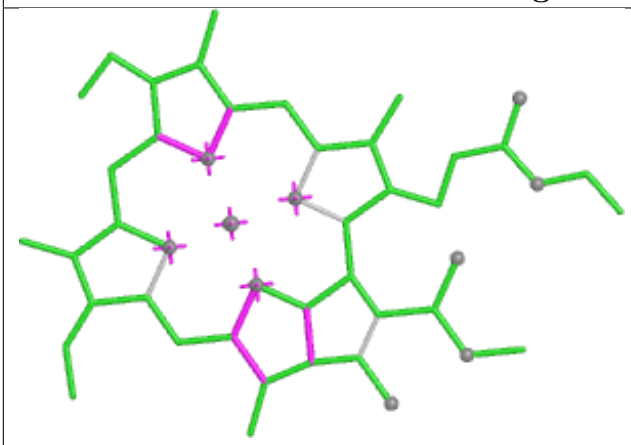


Rings

Ligand CLA i 305



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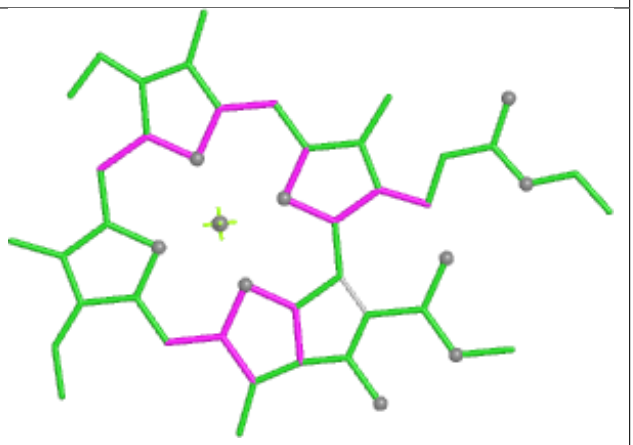

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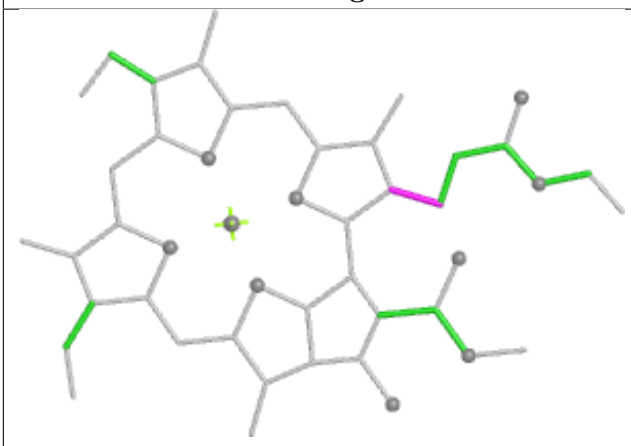

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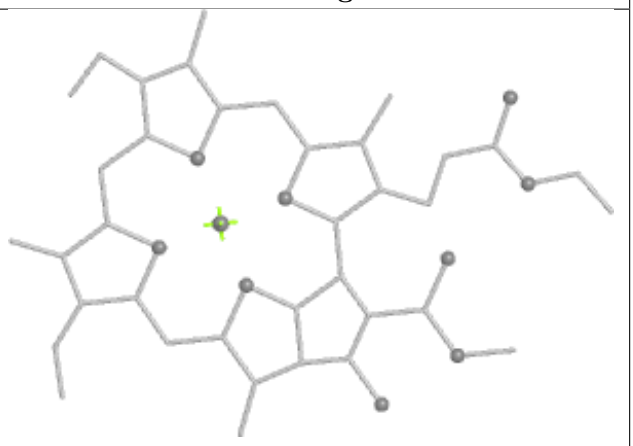
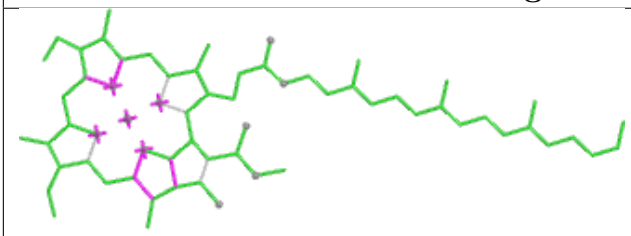


Rings

Ligand CLA B 812



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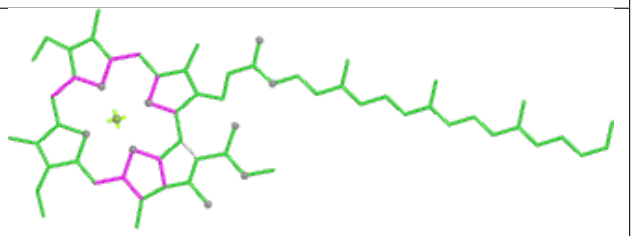
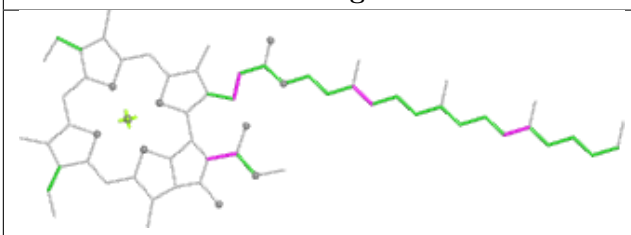


Bond angles



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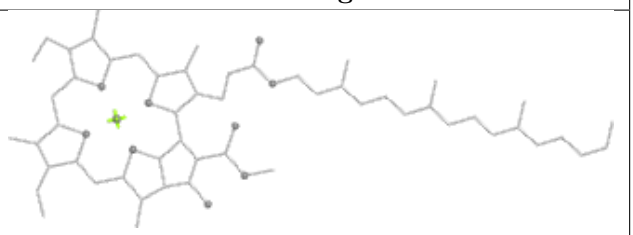
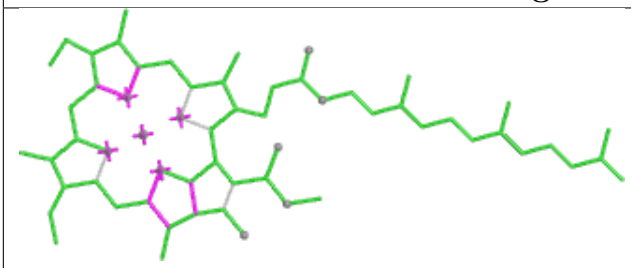


Rings

Ligand CLA l 203



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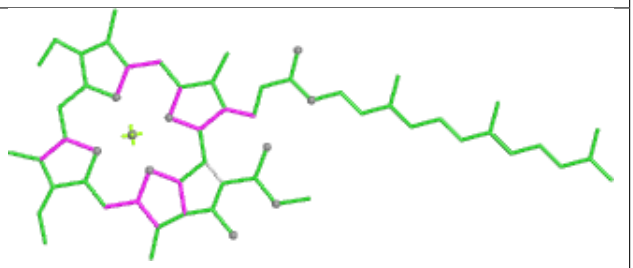
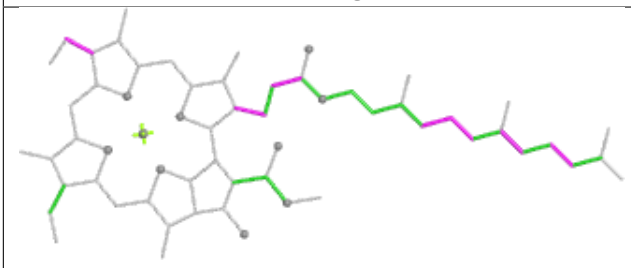


Bond angles



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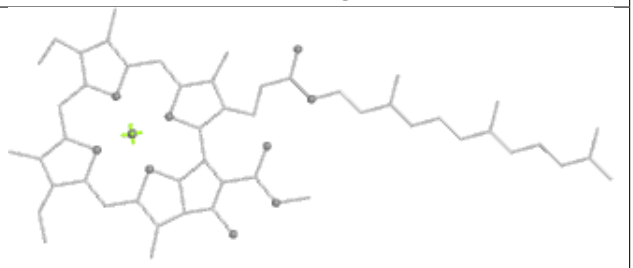
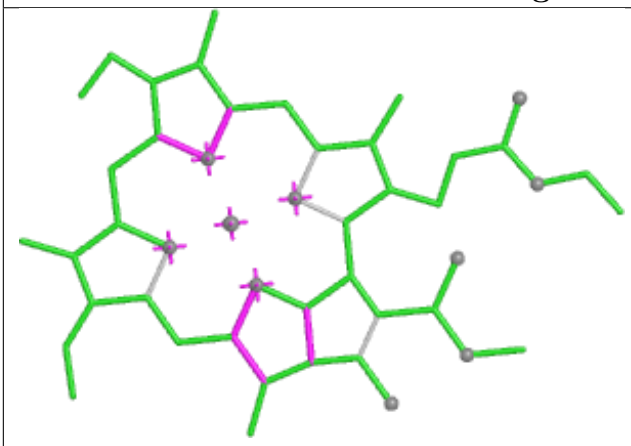


Rings

Ligand CLA l 209



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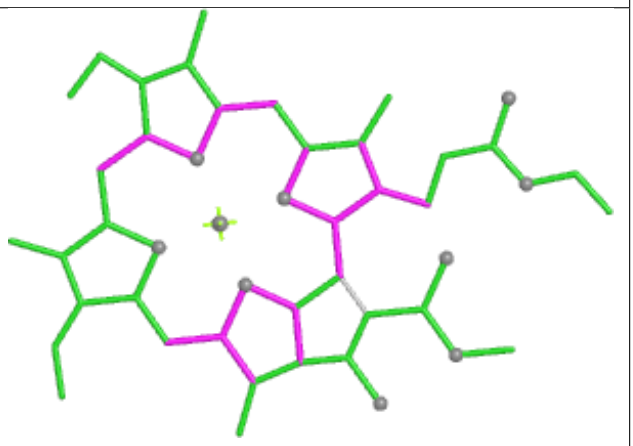
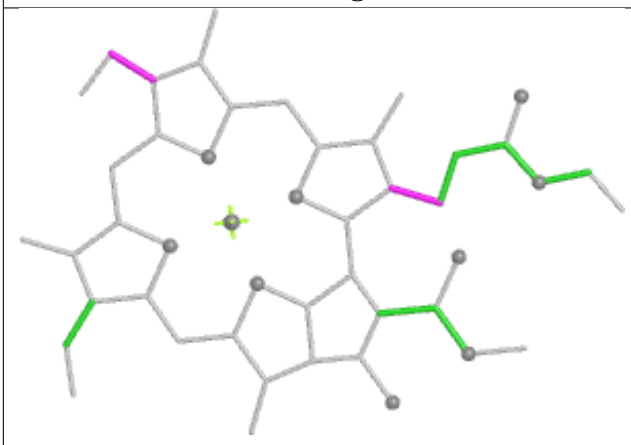


Bond angles



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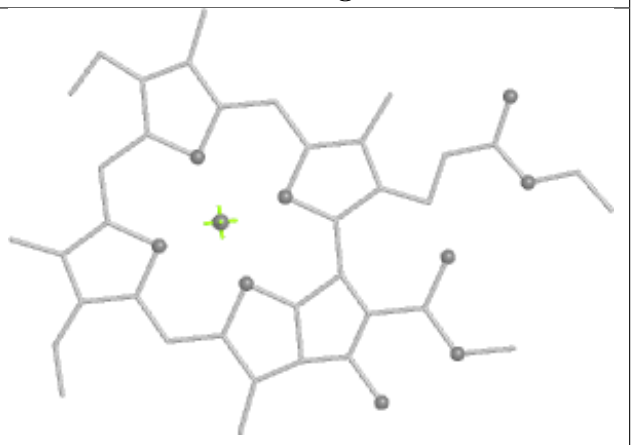
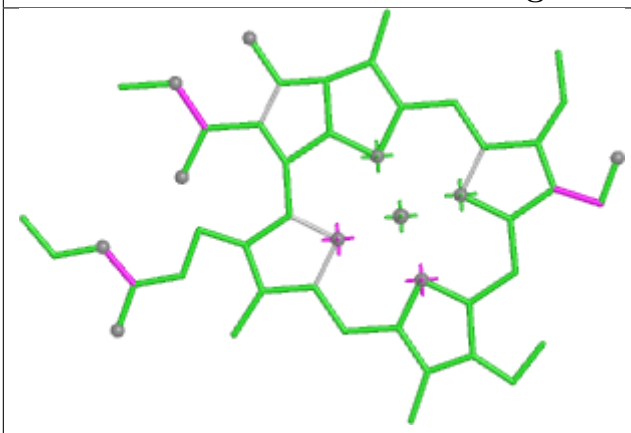


Rings

Ligand CHL d 202



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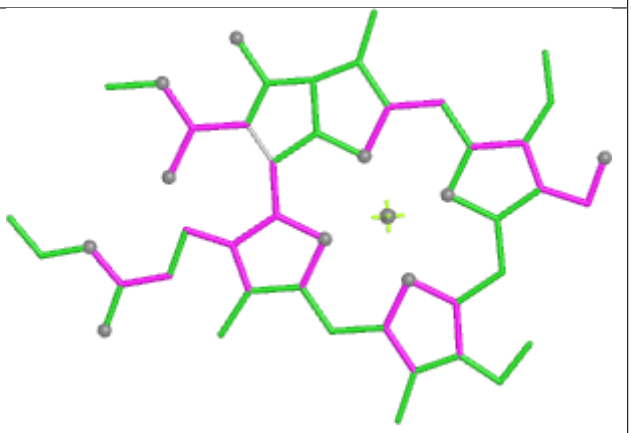
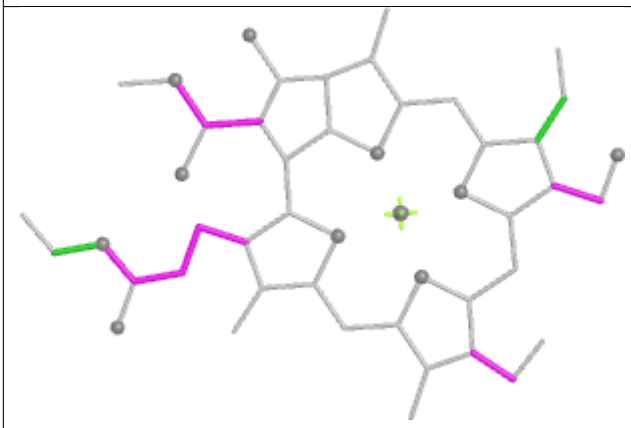


Bond angles



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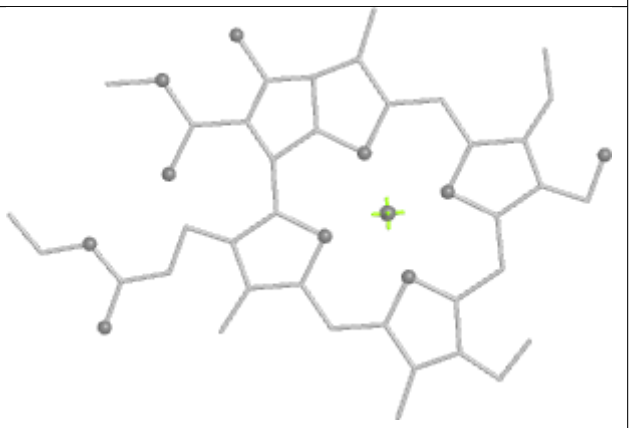
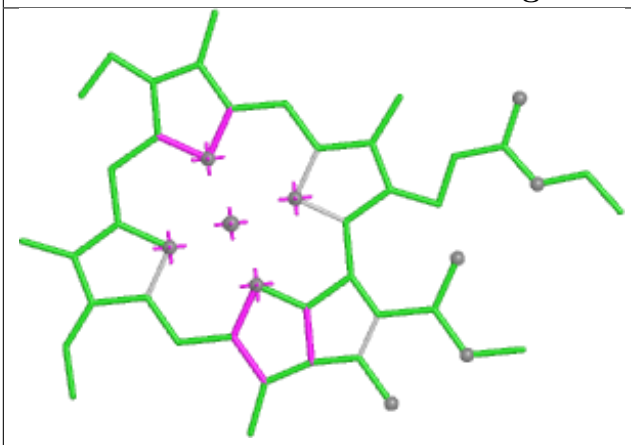


Rings

Ligand CLA m 303



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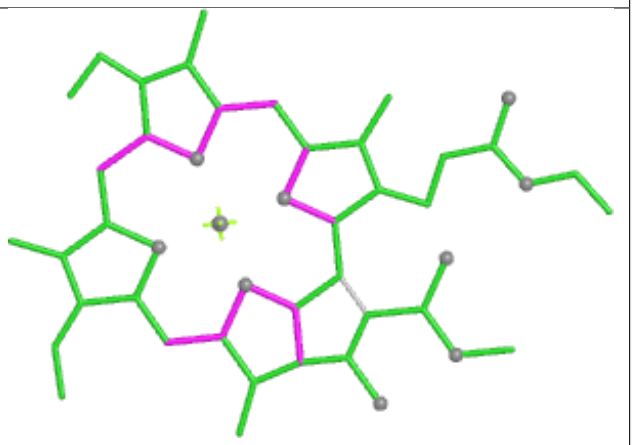
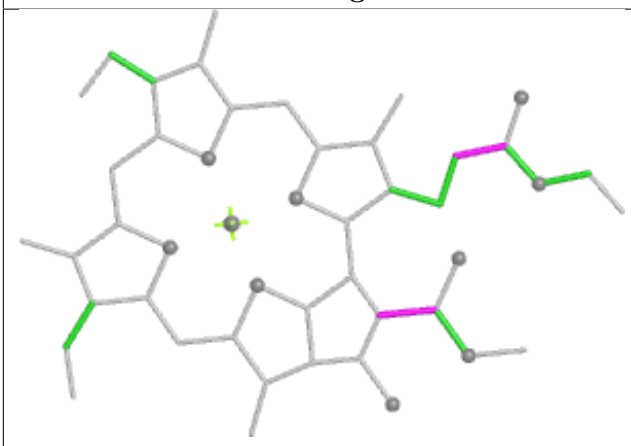


Bond angles



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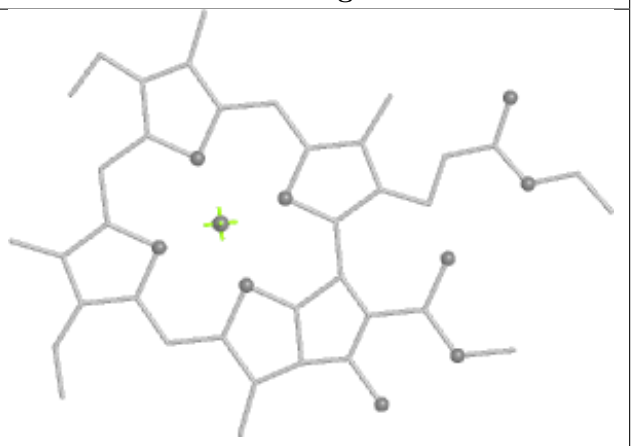
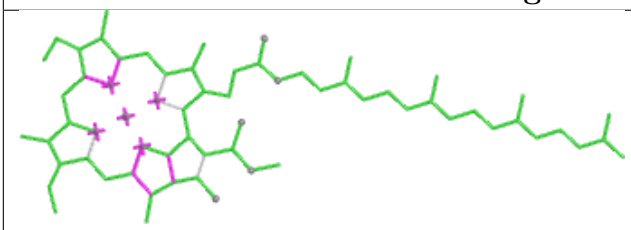


Rings

Ligand CLA A 844



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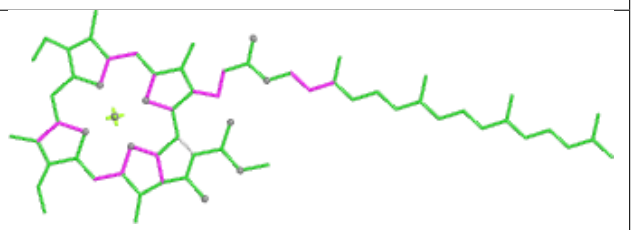

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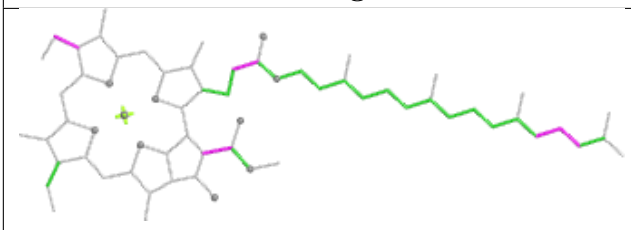

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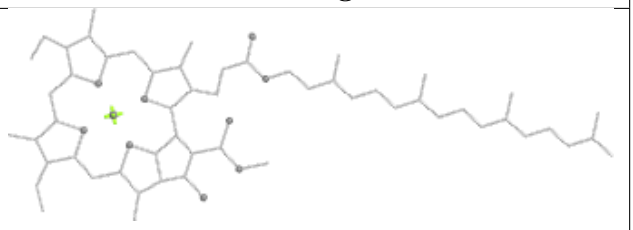
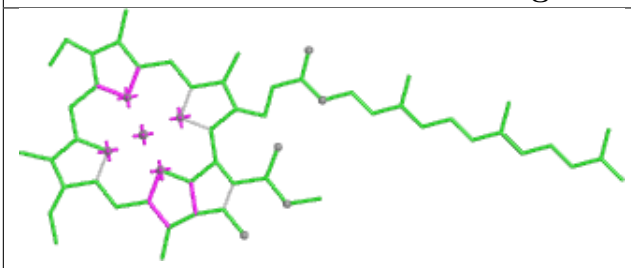


Rings

Ligand CLA f 309



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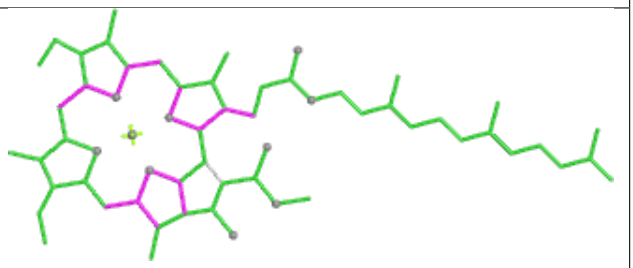
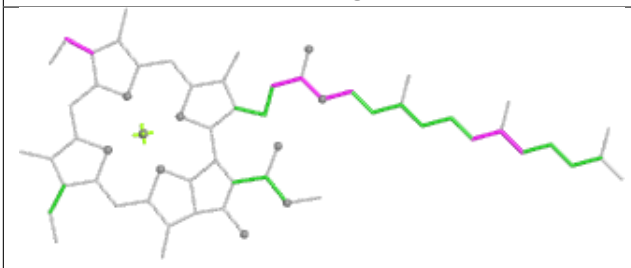


Bond angles



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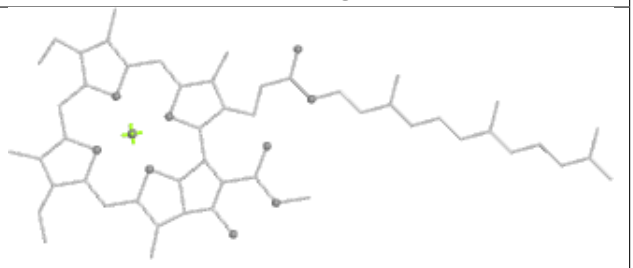
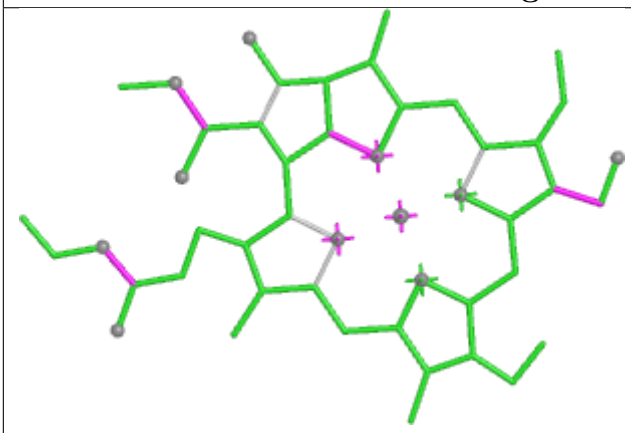


Rings

Ligand CHL m 301



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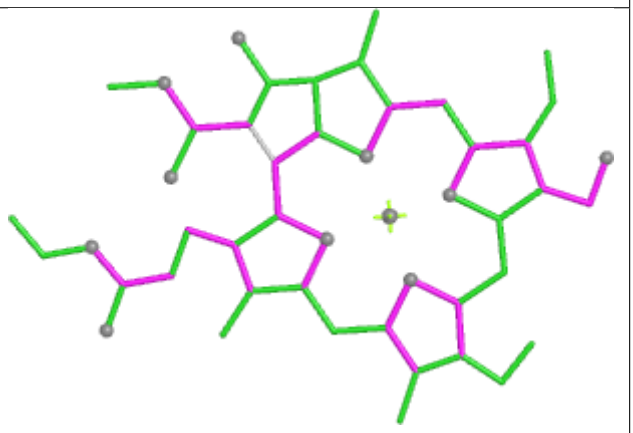
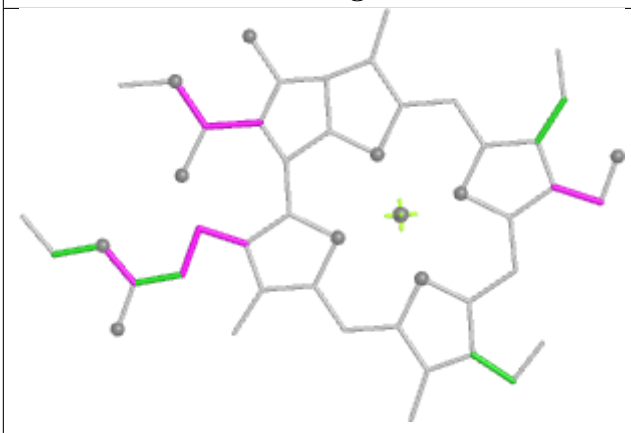


Bond angles

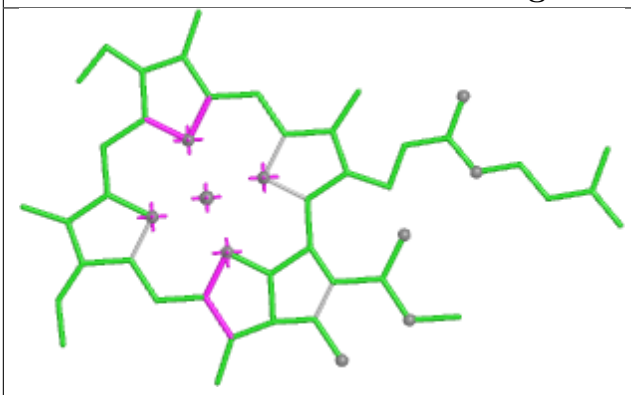


Torsions



Rings

Ligand CLA o 311



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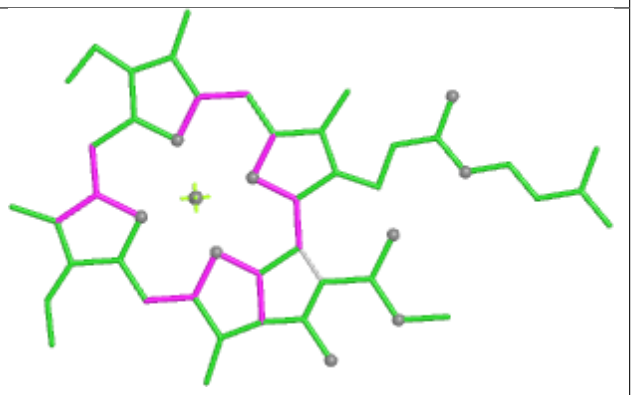
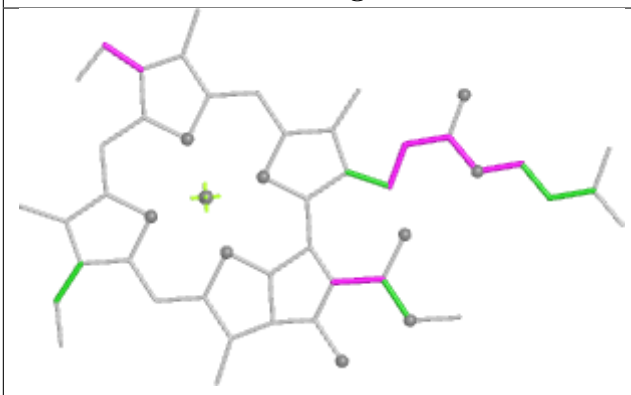


Bond angles



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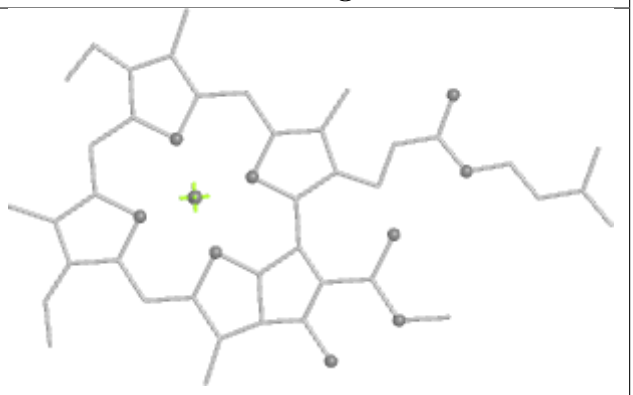
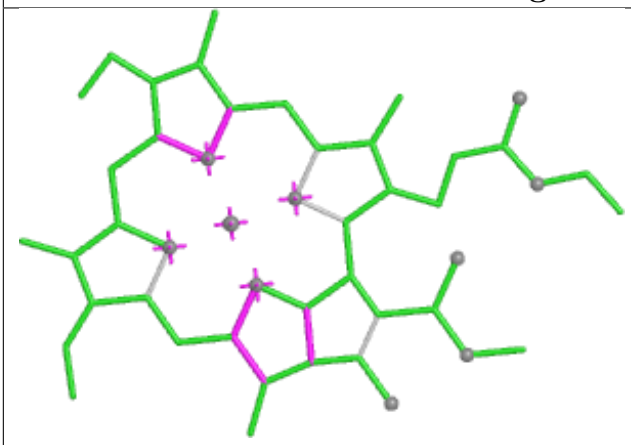
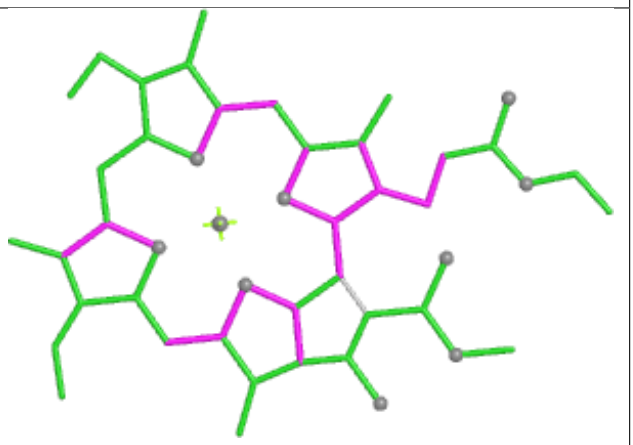


Rings

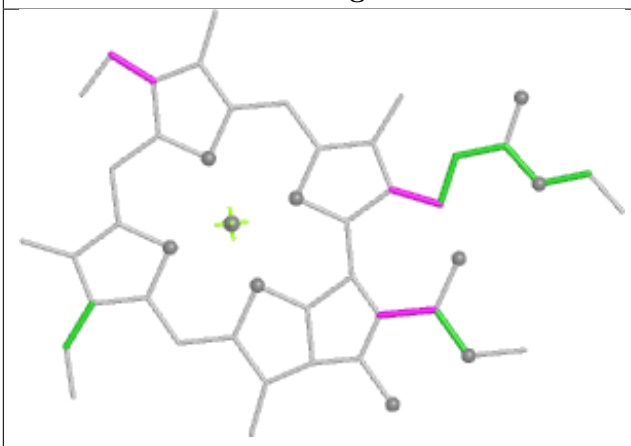
Ligand CLA c 302



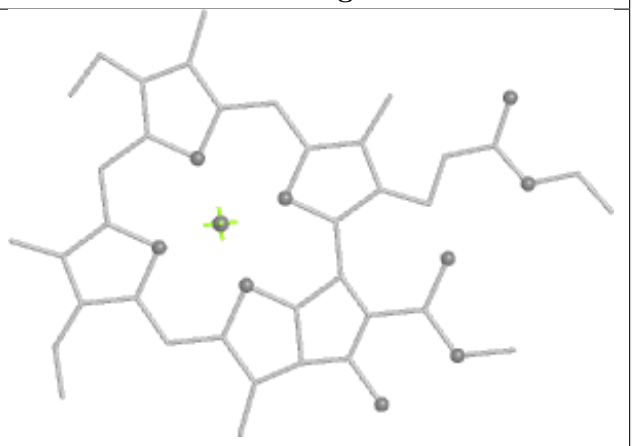
Bond lengths



Bond angles

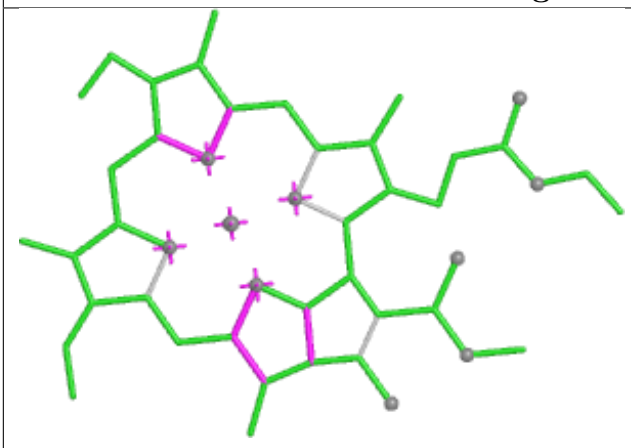


Torsions



Rings

Ligand CLA i 303



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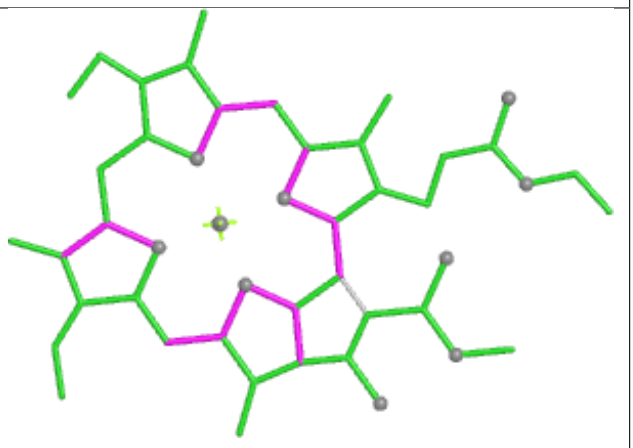

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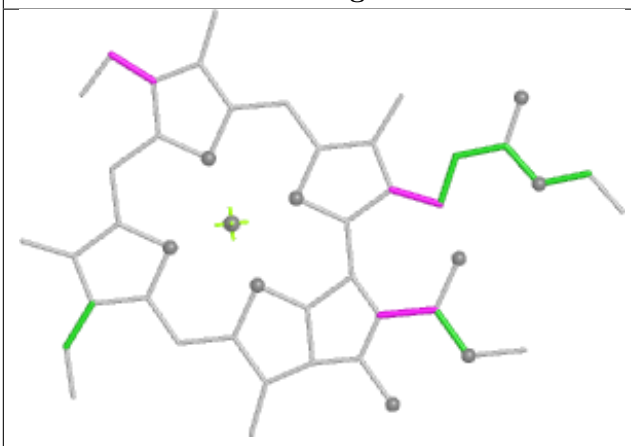

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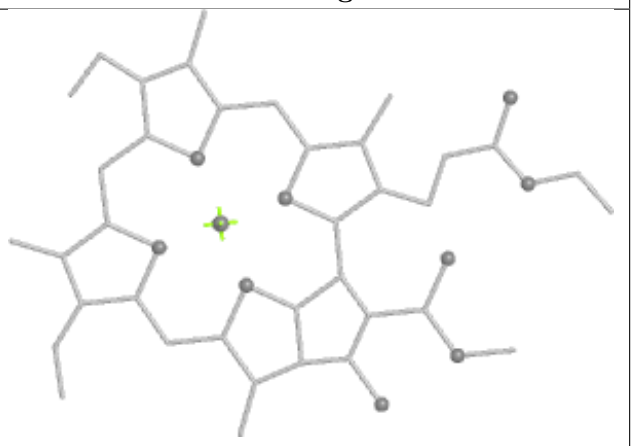
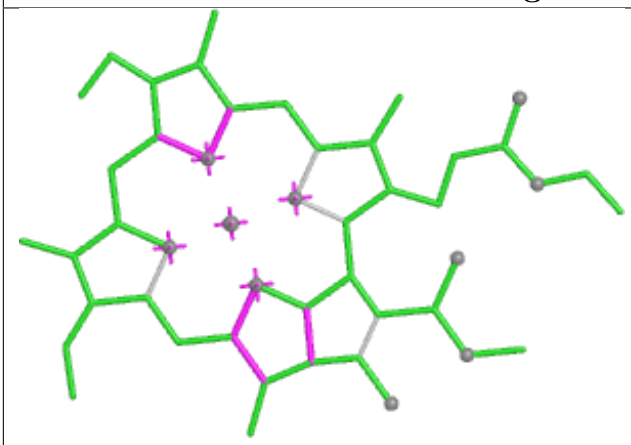


Rings

Ligand CLA A 814



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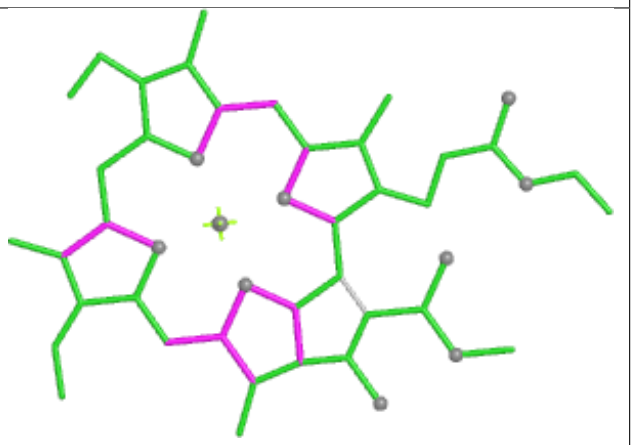

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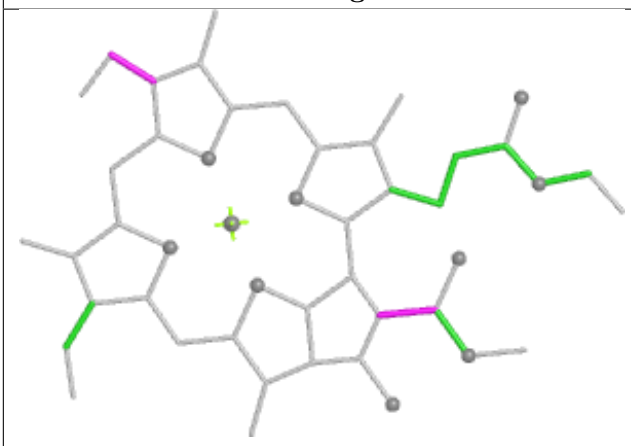

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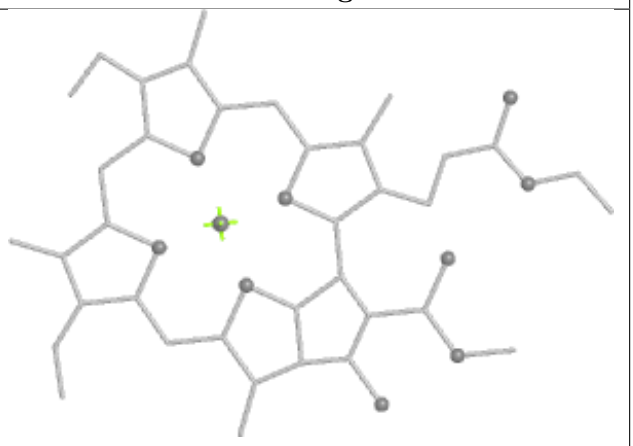
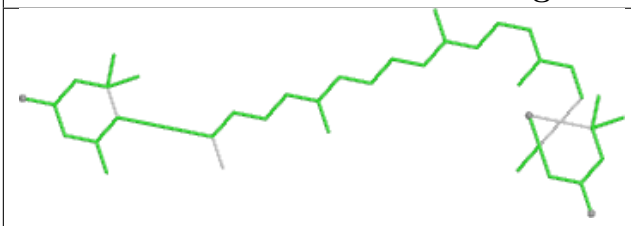


Rings

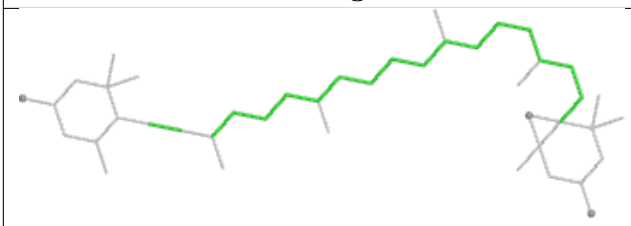
Ligand DD6 i 314



Bond lengths



Bond angles

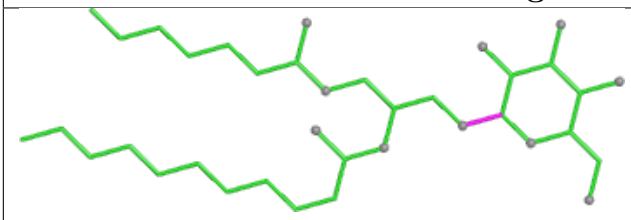


Torsions



Rings

Ligand LMG j 314



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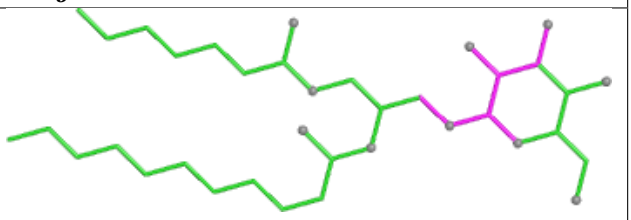

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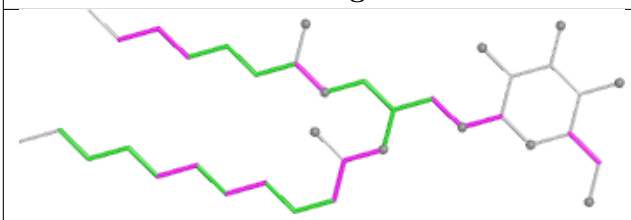

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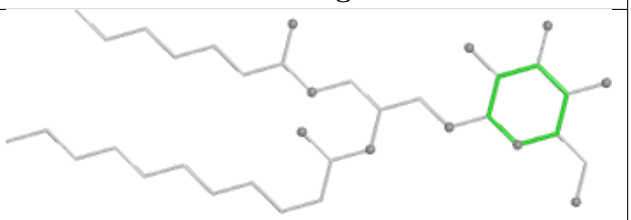
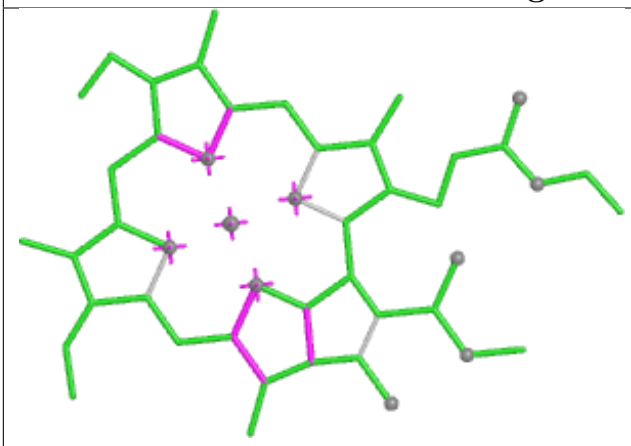


Rings

Ligand CLA k 311



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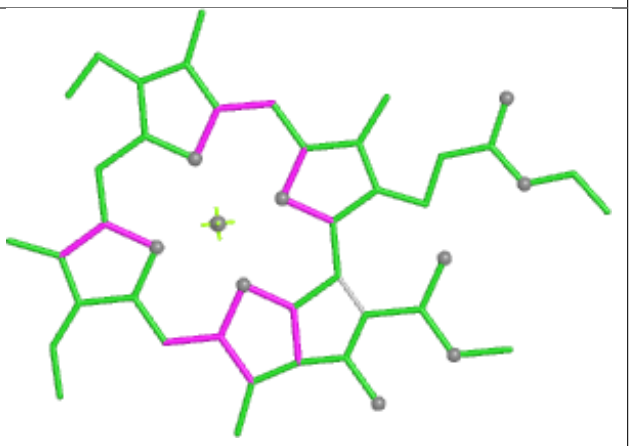
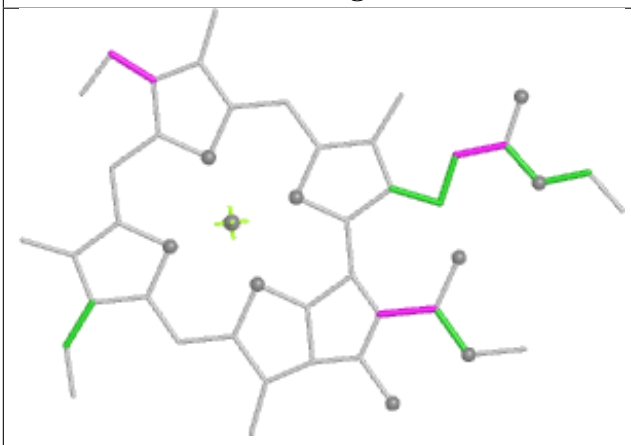


Bond angles



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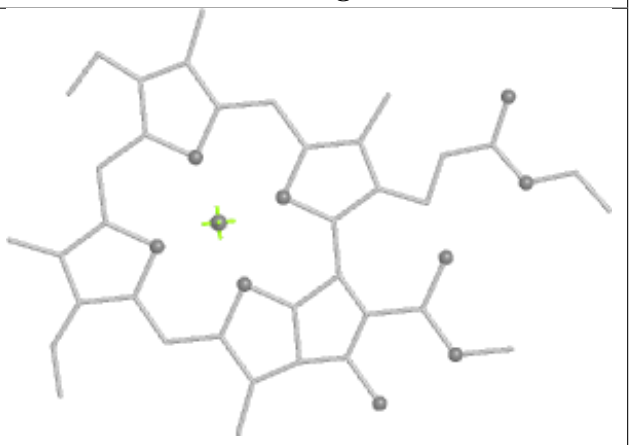
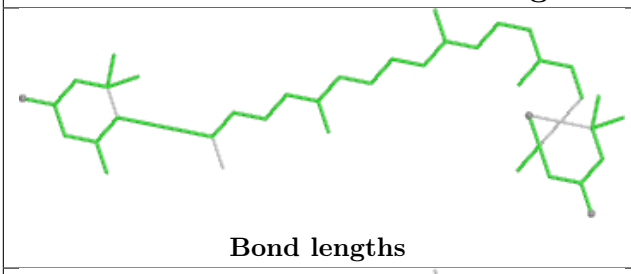


Rings

Ligand DD6 c 319



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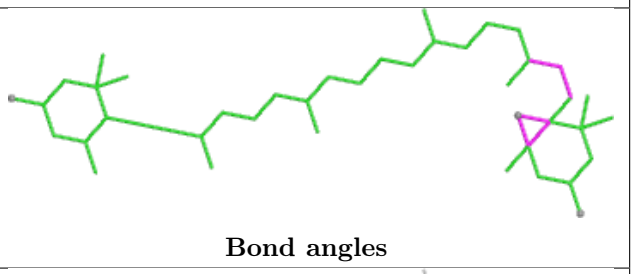
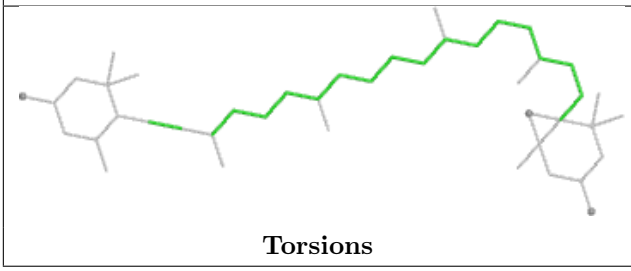


Bond angles



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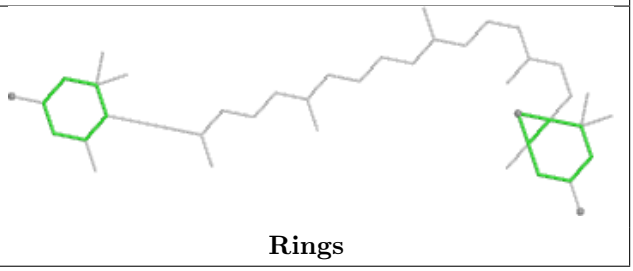
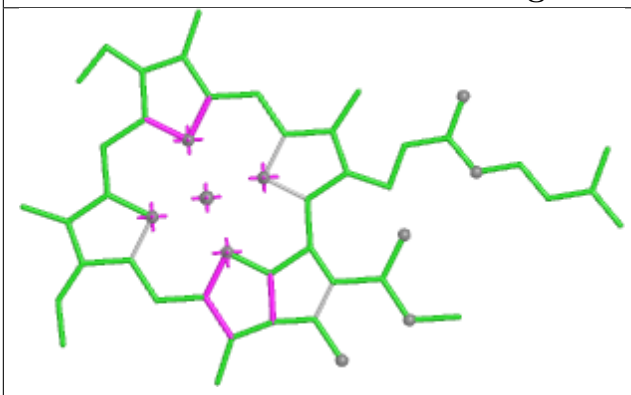


Rings

Ligand CLA k 308



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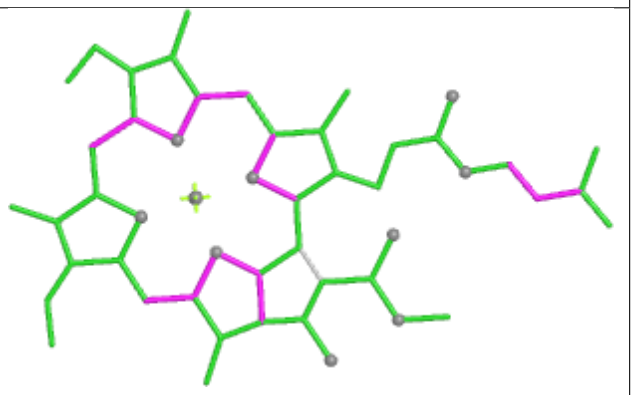
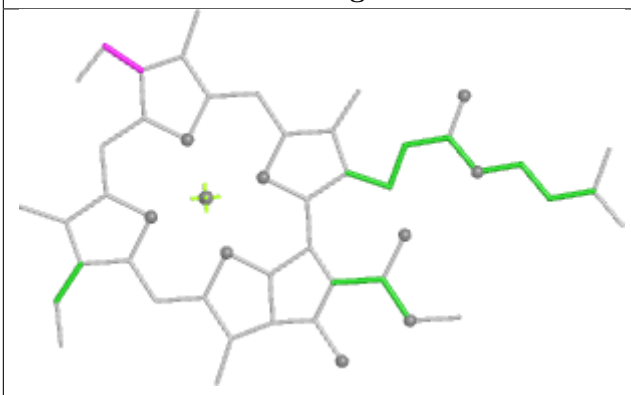


Bond angles



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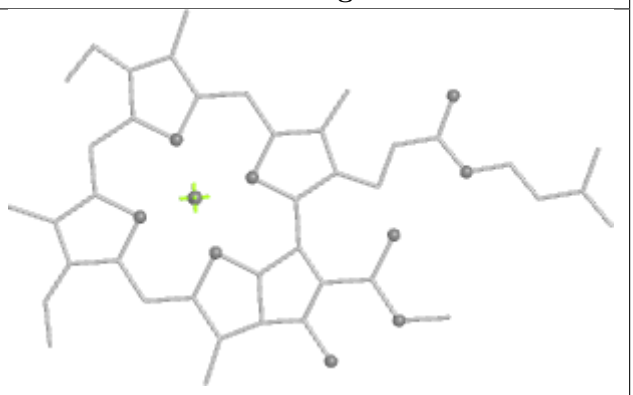
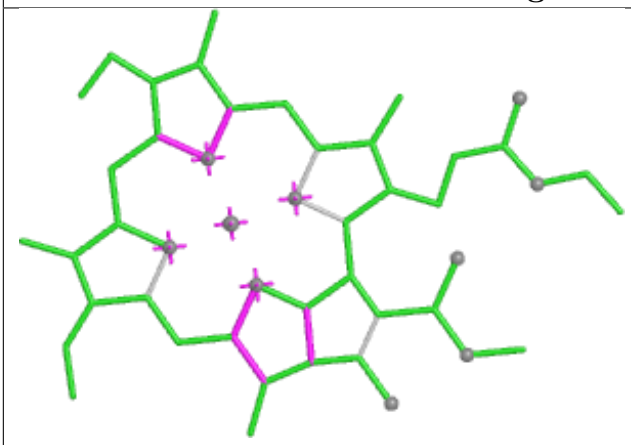


Rings

Ligand CLA n 206



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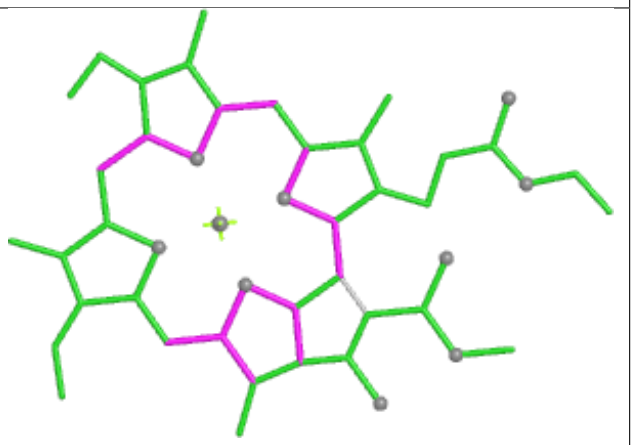
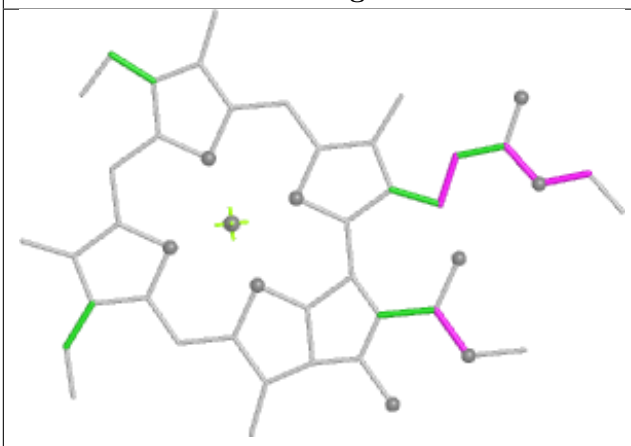


Bond angles



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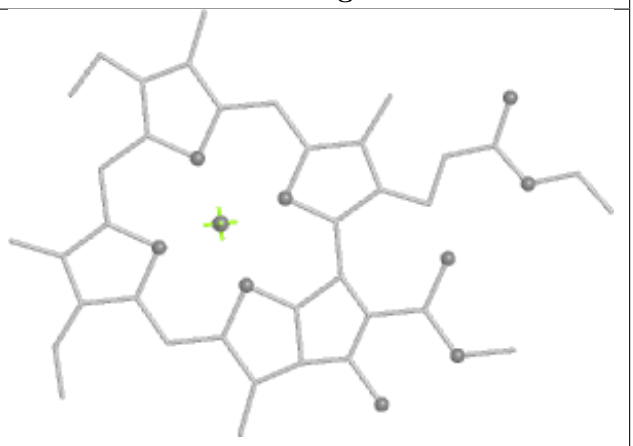
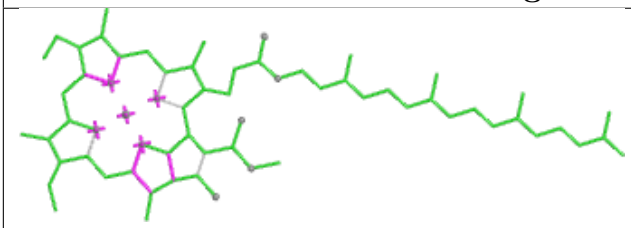


Rings

Ligand CLA A 822



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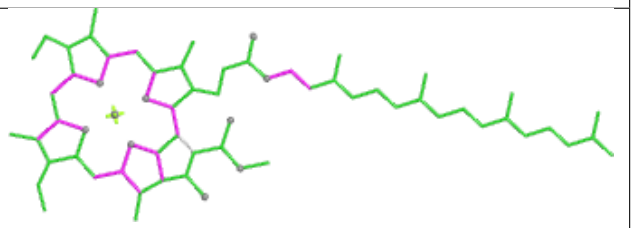
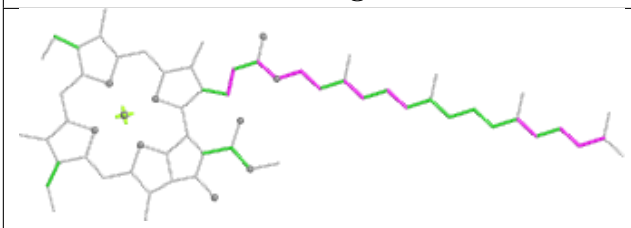


Bond angles



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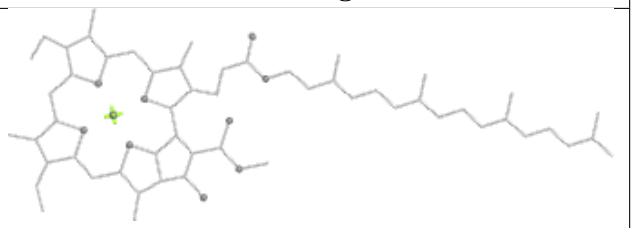
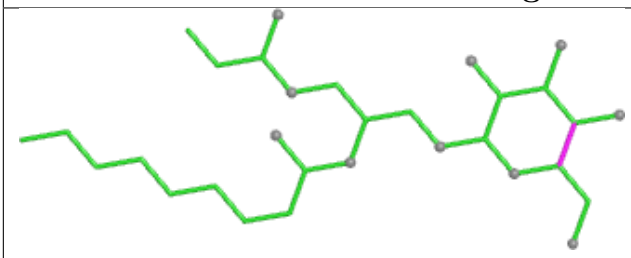


Rings

Ligand LMG d 213



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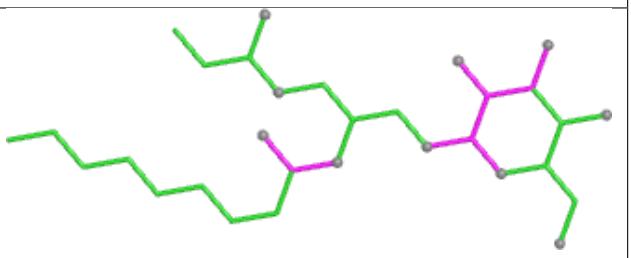
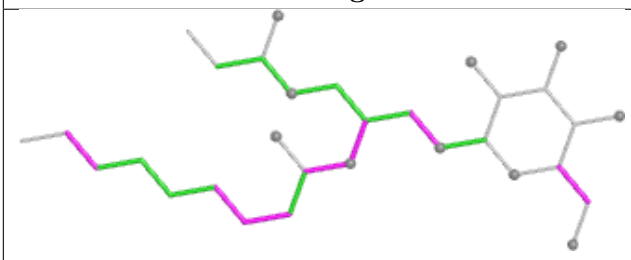


Bond angles



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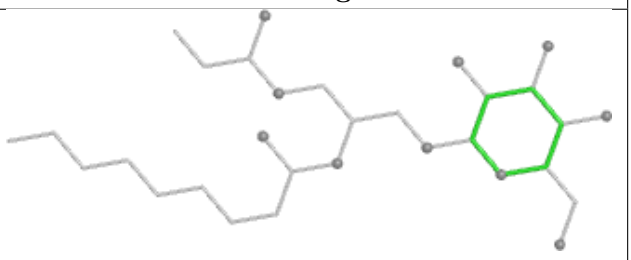
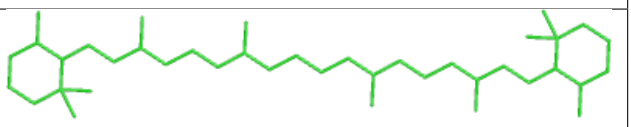


Rings

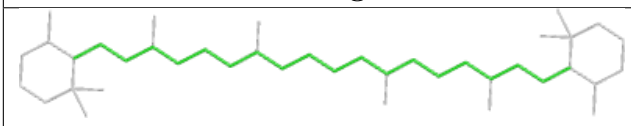
Ligand BCR B 825



Bond lengths



Bond angles



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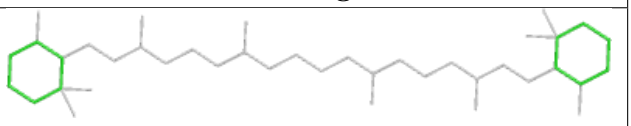
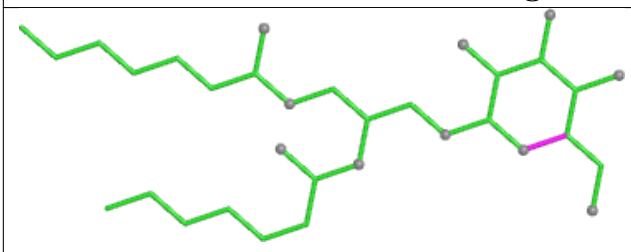


Rings

Ligand LMG g 313



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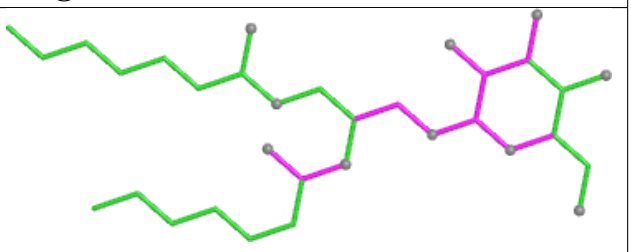
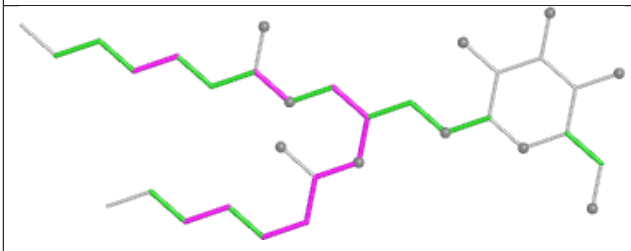


Bond angles



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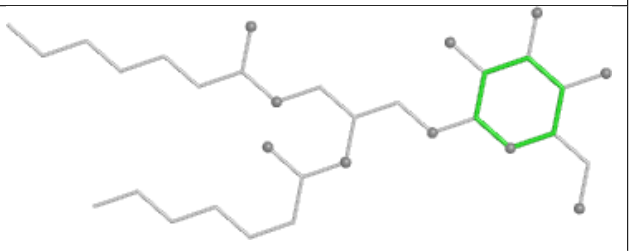
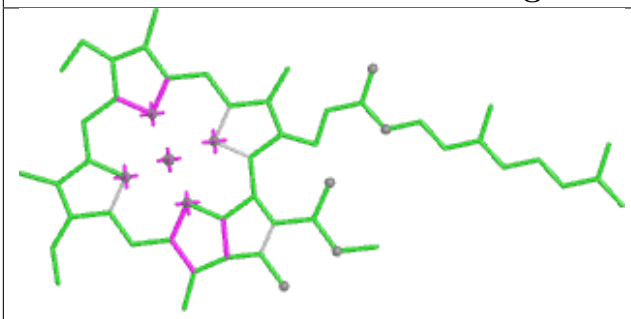


Rings

Ligand CLA A 820



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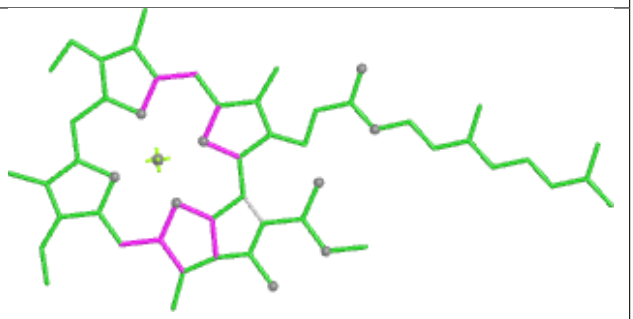
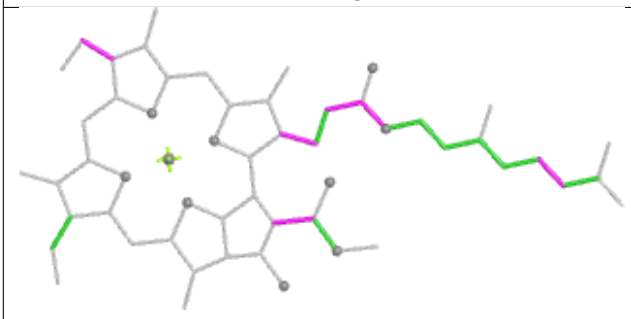


Bond angles



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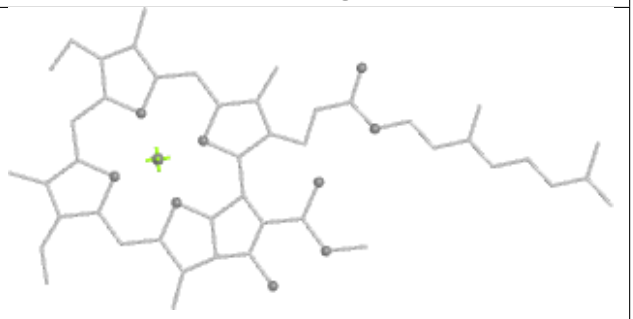
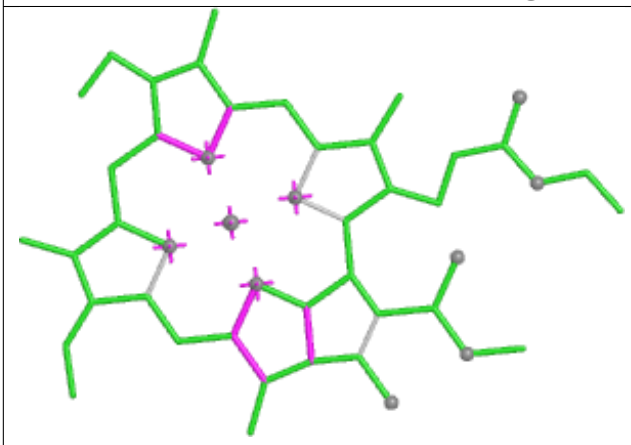


Rings

Ligand CLA m 306



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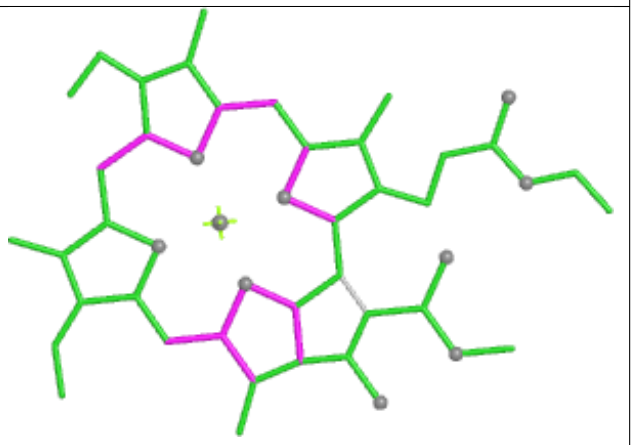
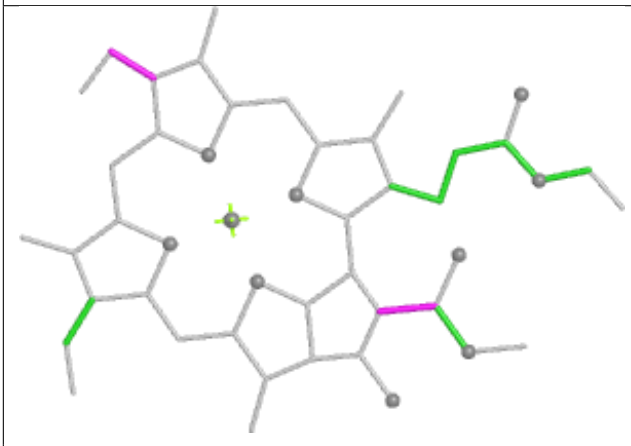


Bond angles



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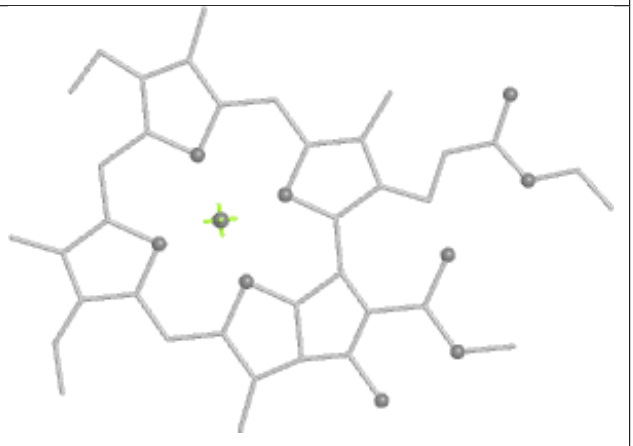
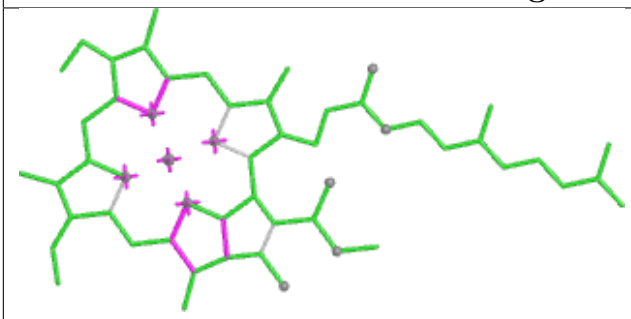


Rings

Ligand CLA o 302



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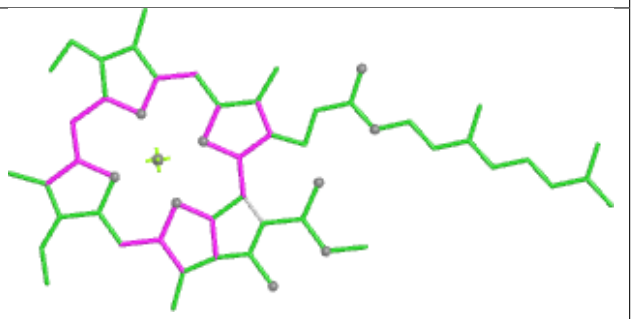
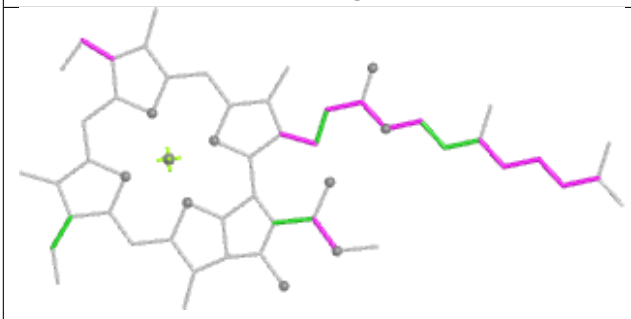
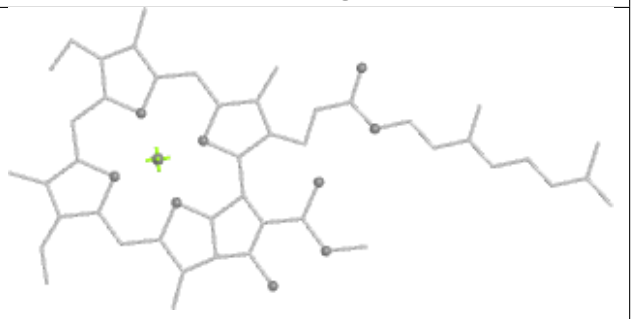


Bond angles

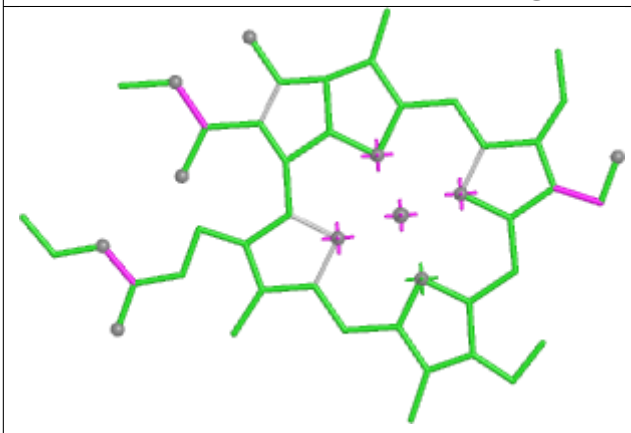


Torsions

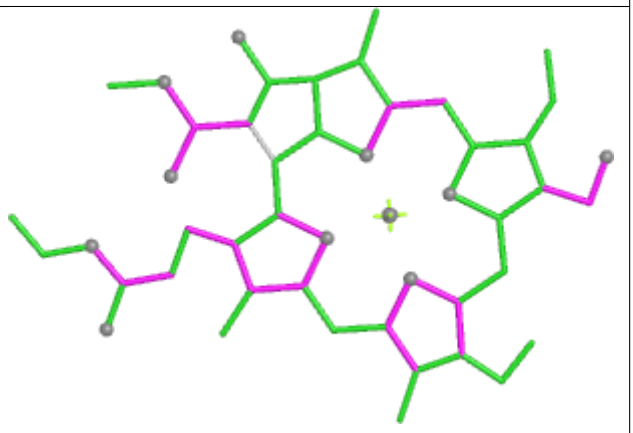


Rings

Ligand CHL a 315



Bond lengths



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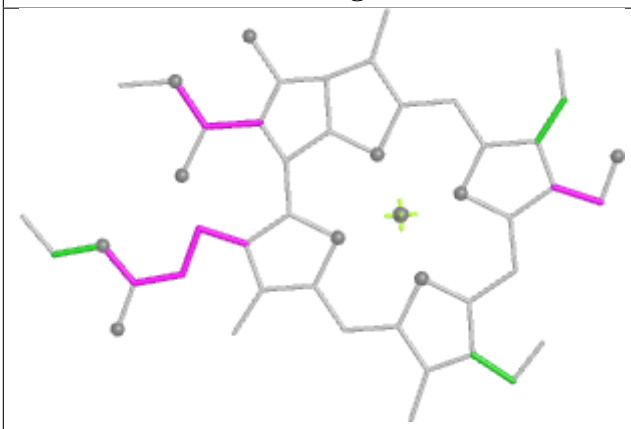
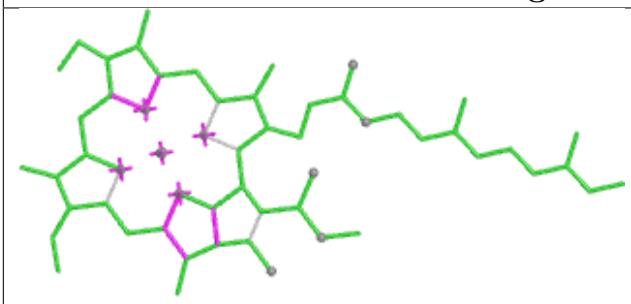


Torsions



Rings

Ligand CLA g 309



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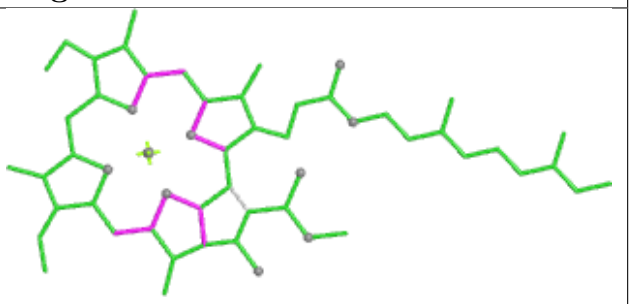
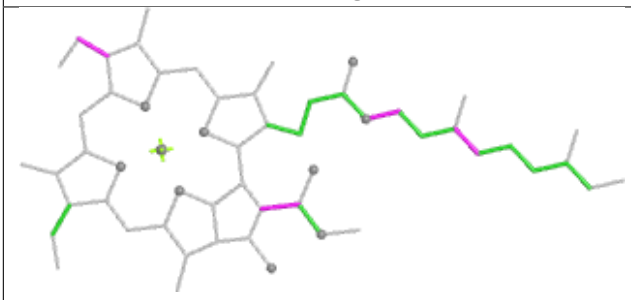


Bond angles



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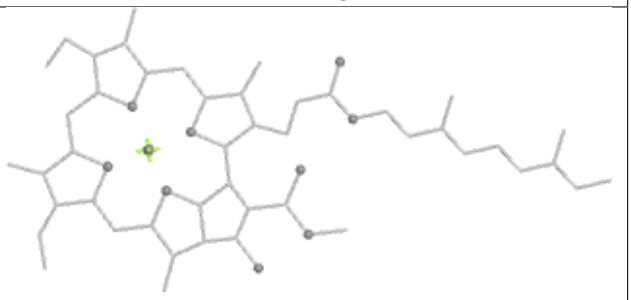
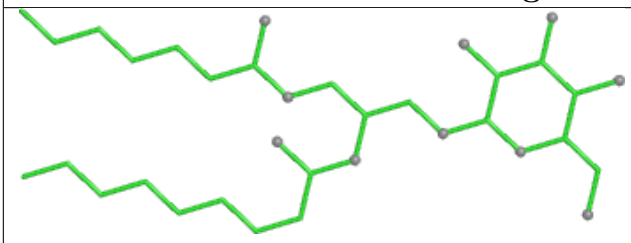


Rings

Ligand LMG h 216



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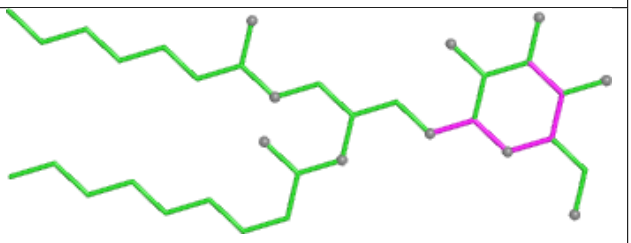

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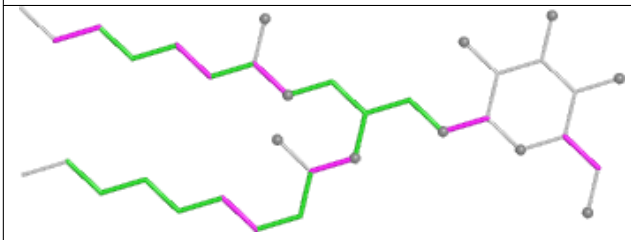

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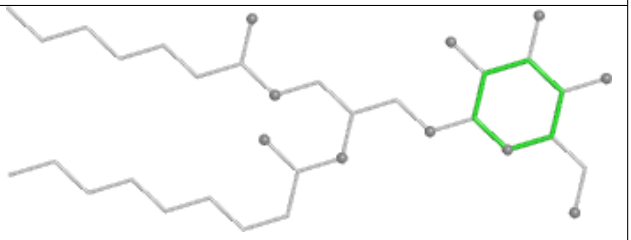
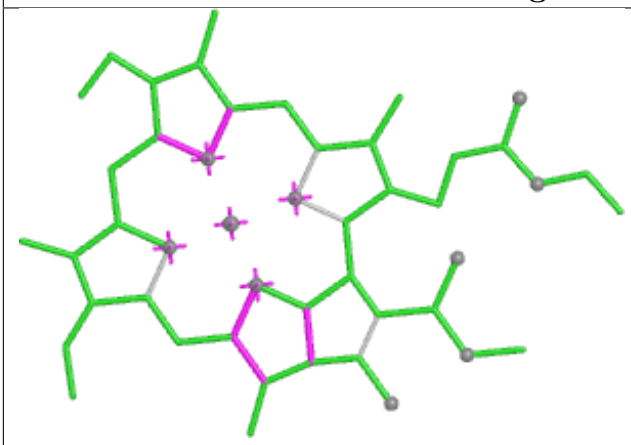


Rings

Ligand CLA e 309



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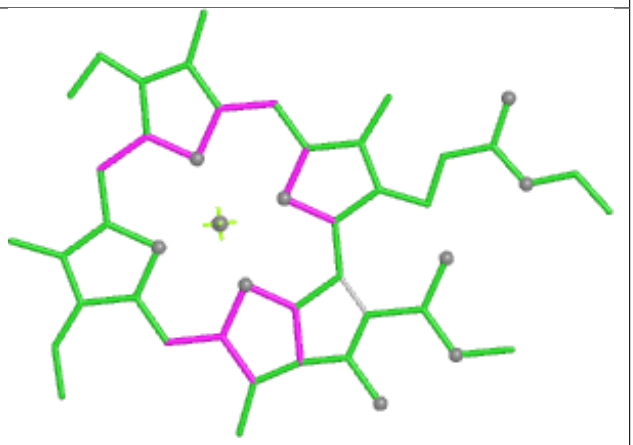
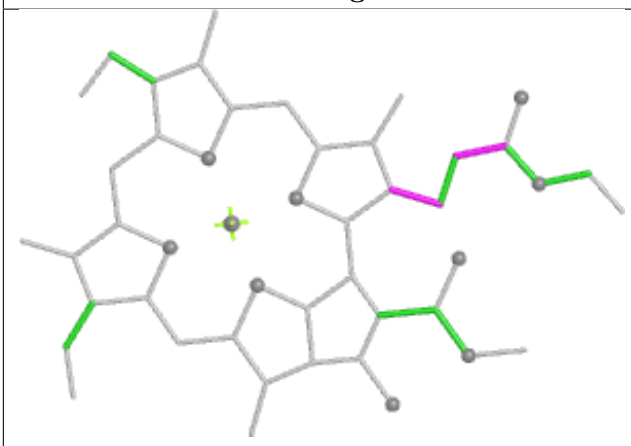


Bond angles



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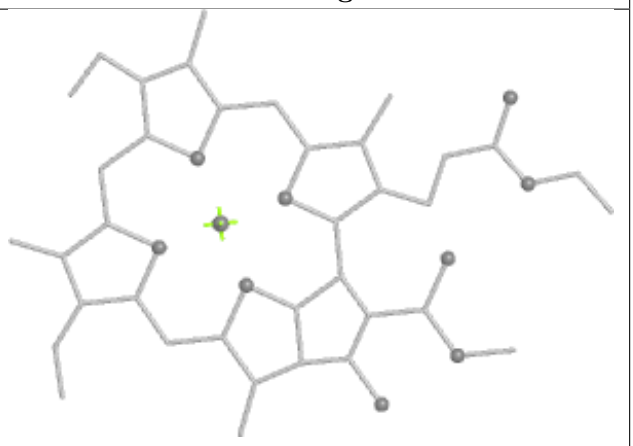
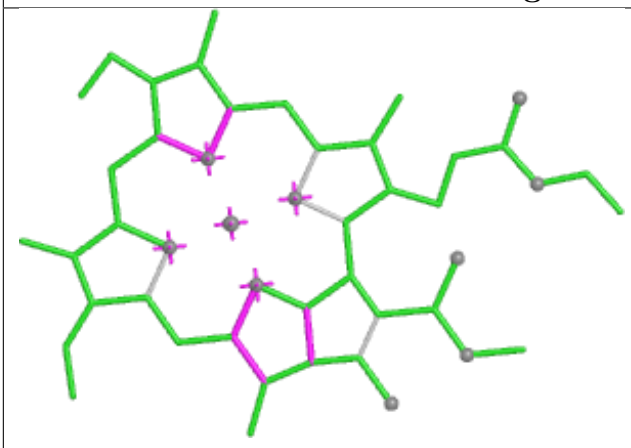


Rings

Ligand CLA A 847



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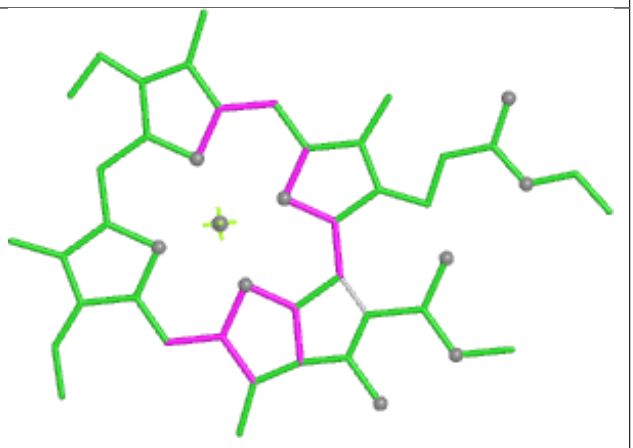
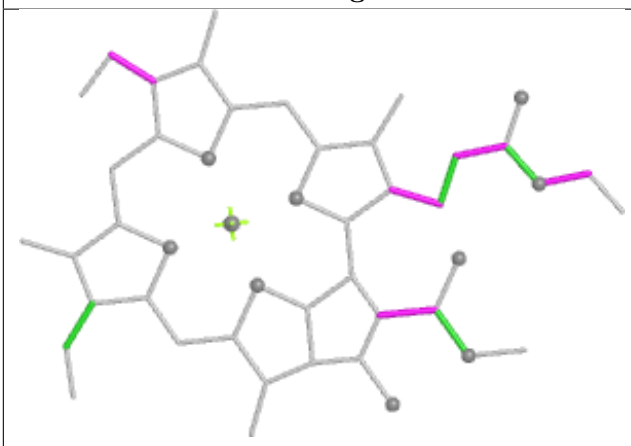


Bond angles



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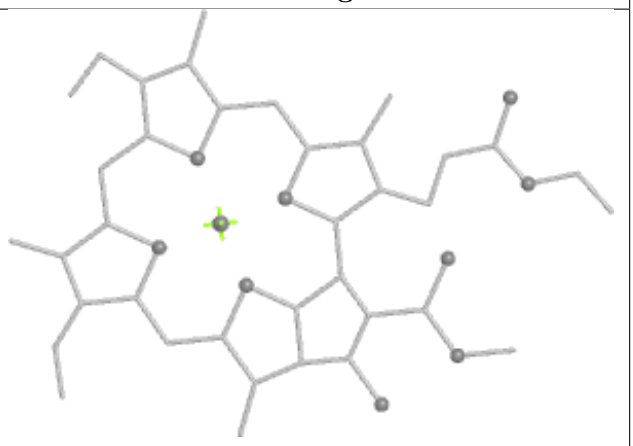
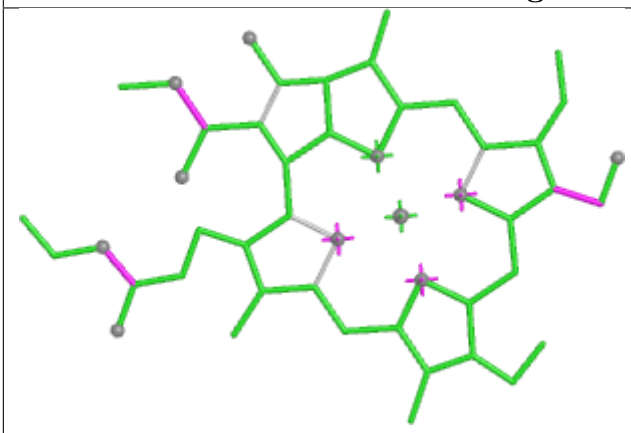


Rings

Ligand CHL b 310



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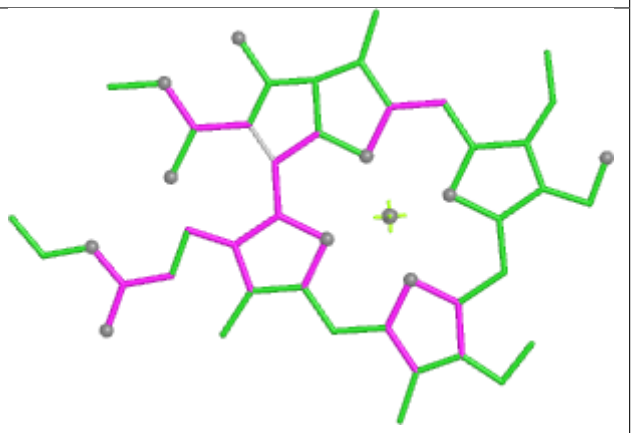
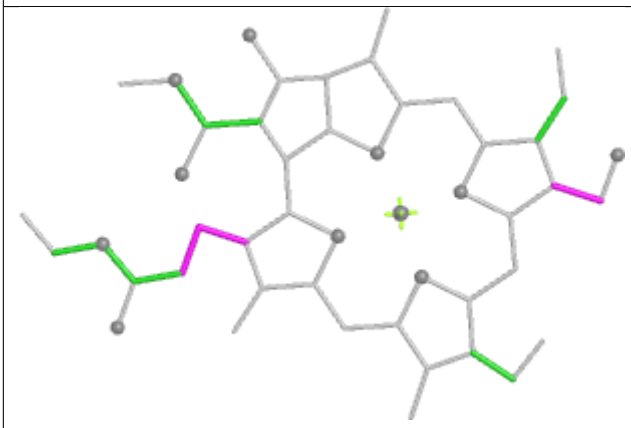


Bond angles



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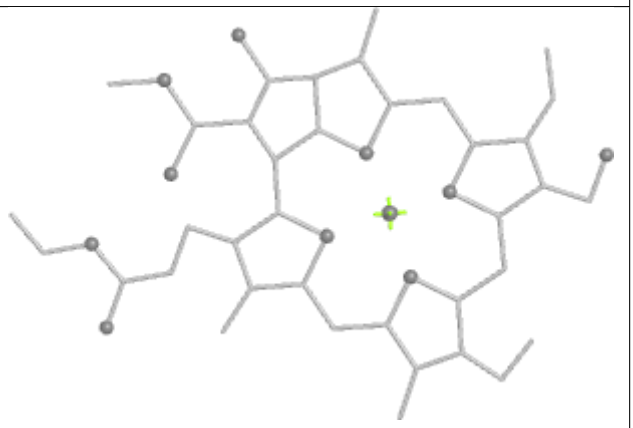
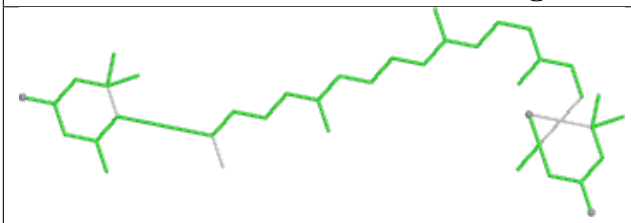


Rings

Ligand DD6 b 319



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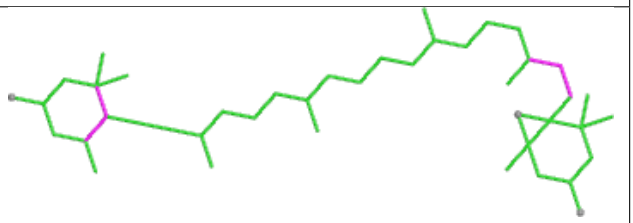
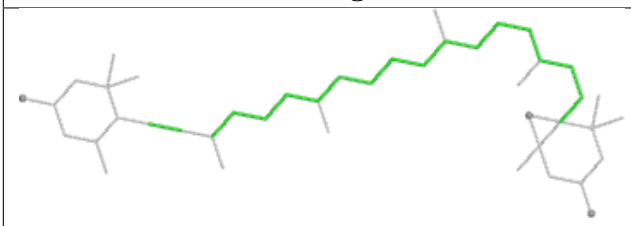


Bond angles



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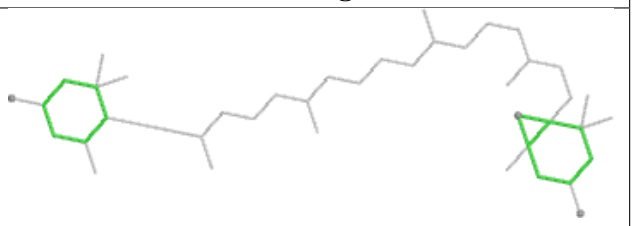
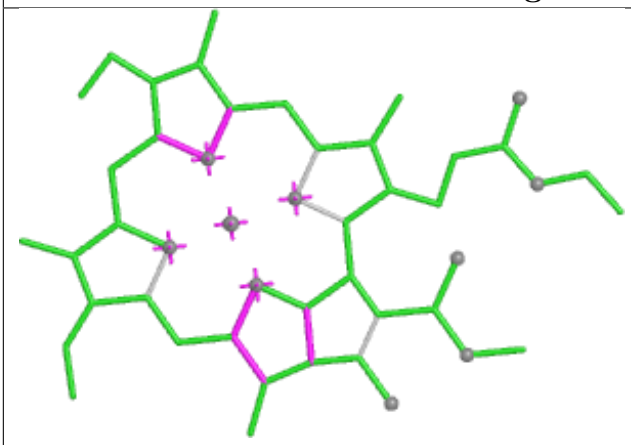


Rings

Ligand CLA B 842



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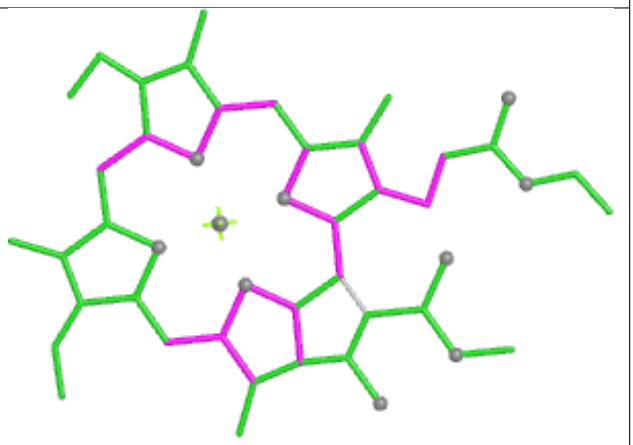
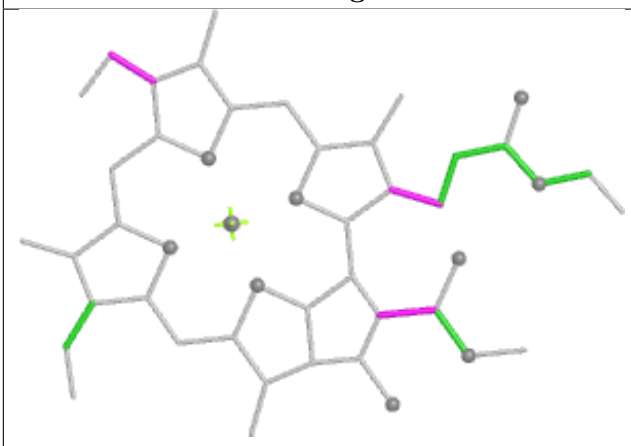


Bond angles



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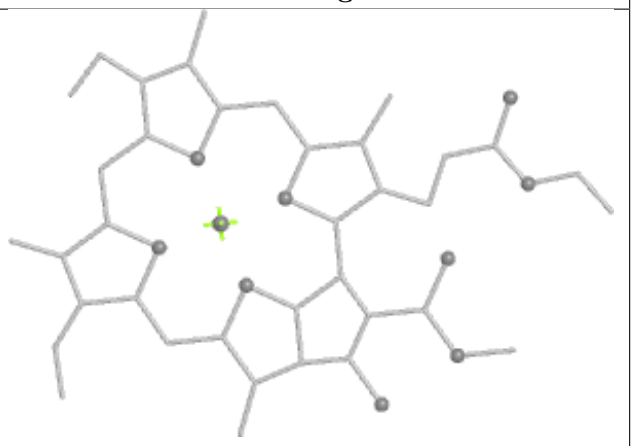
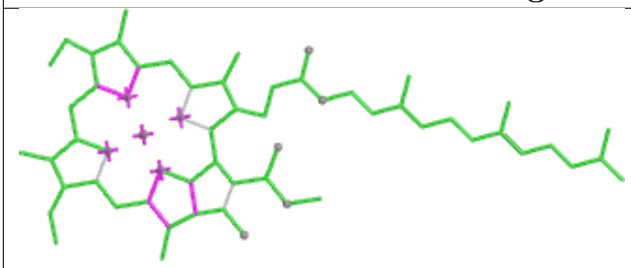


Rings

Ligand CLA h 205



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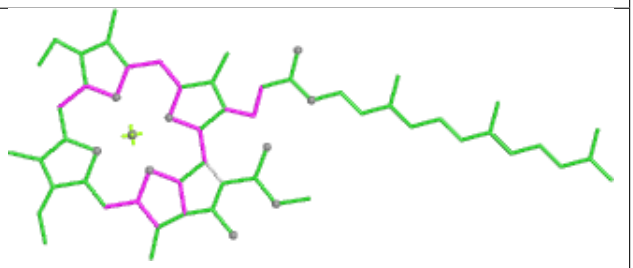
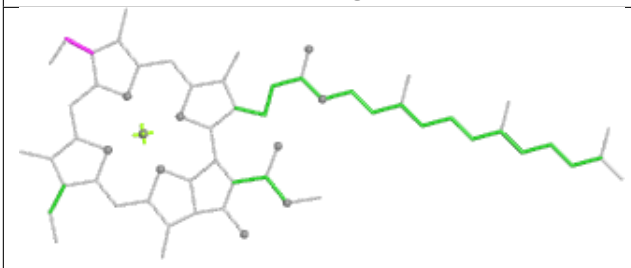


Bond angles



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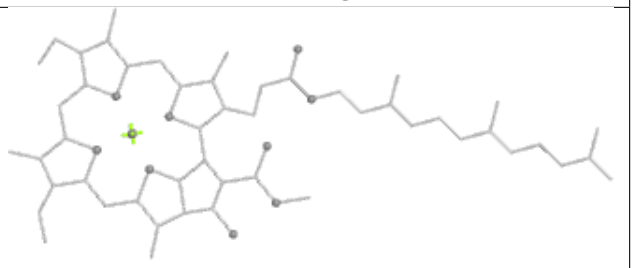
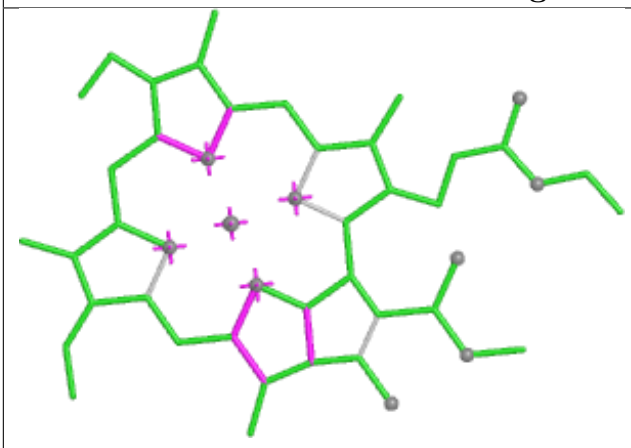


Rings

Ligand CLA c 315



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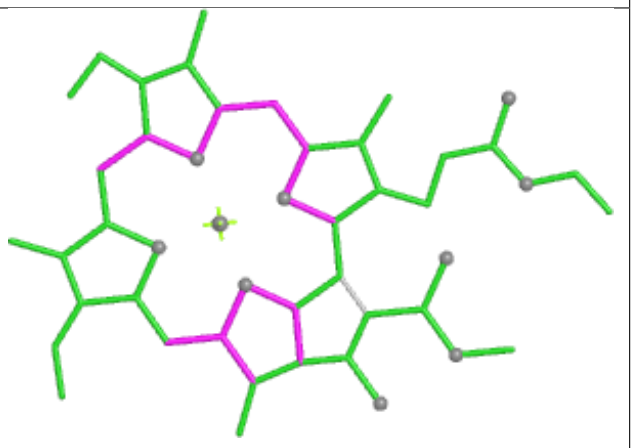
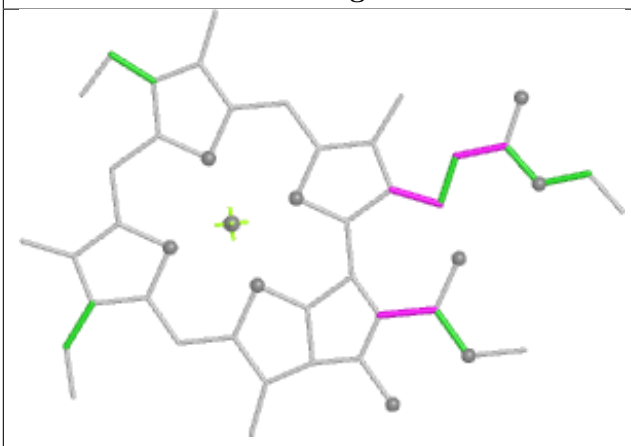


Bond angles



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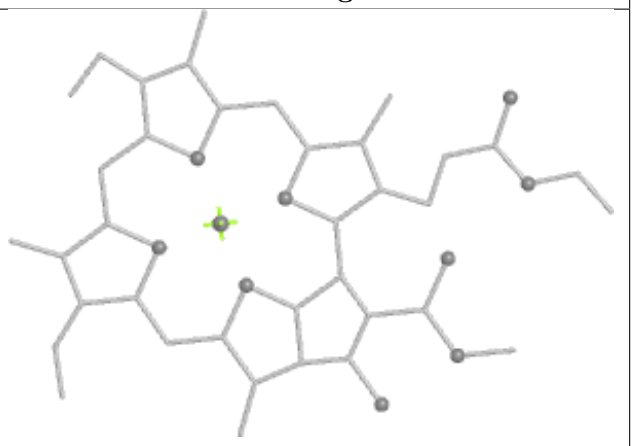
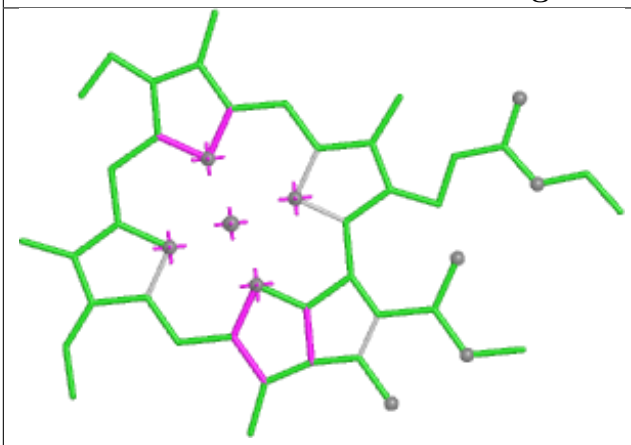


Rings

Ligand CLA j 301



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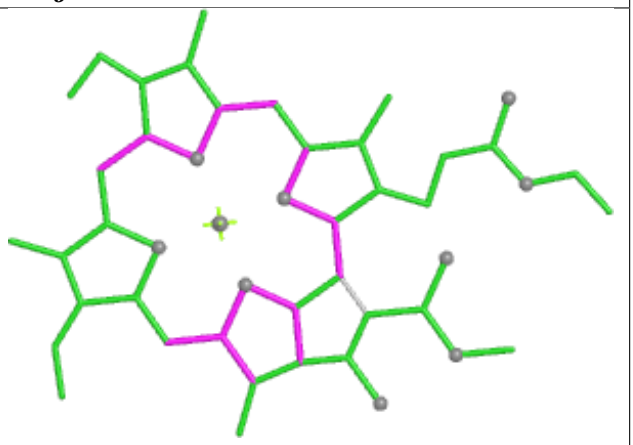
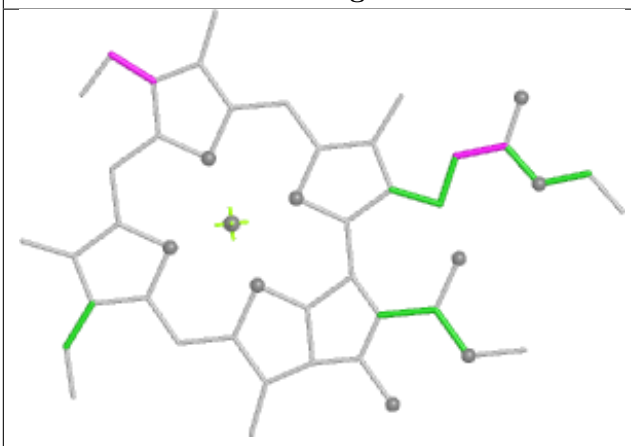


Bond angles



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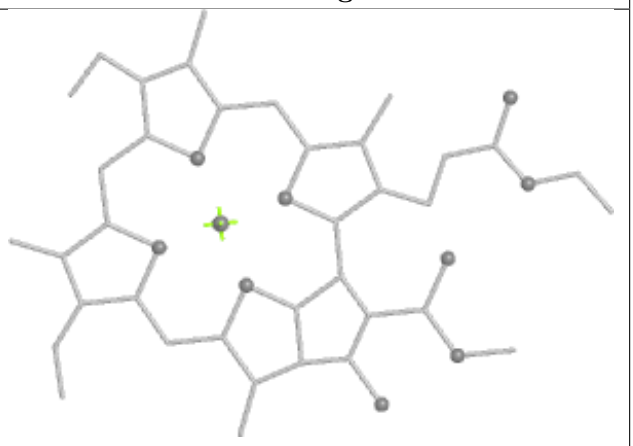
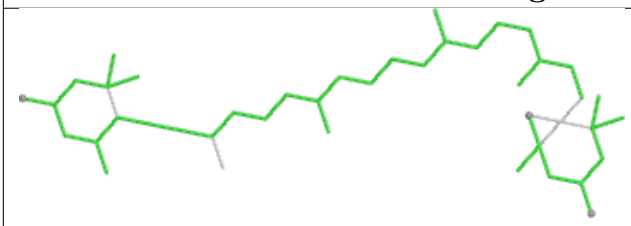


Rings

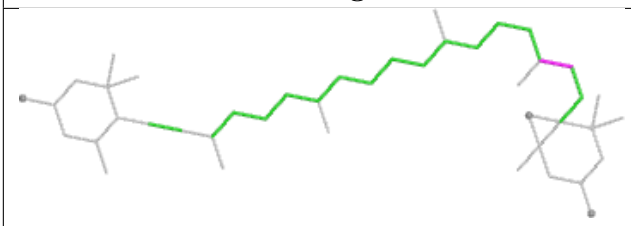
Ligand DD6 J 801



Bond lengths



Bond angles

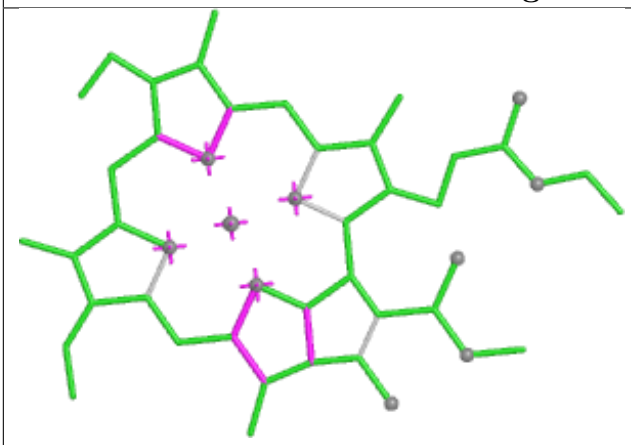


Torsions

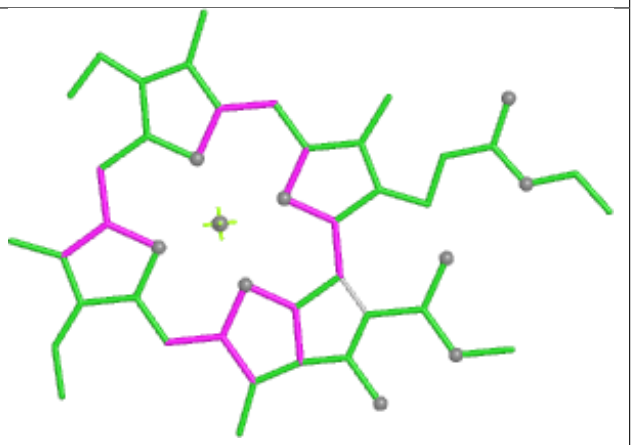


Rings

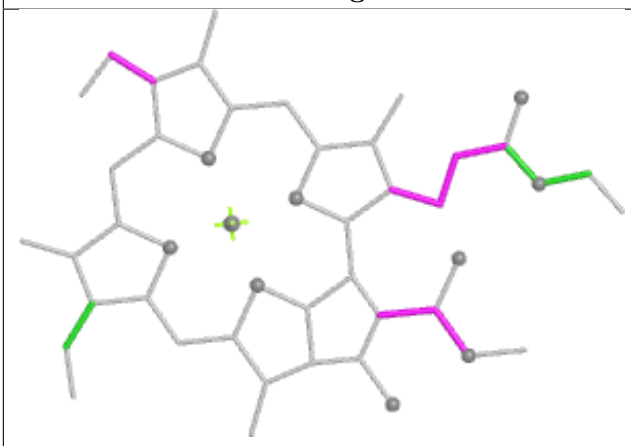
Ligand CLA m 302



Bond lengths



Bond angles



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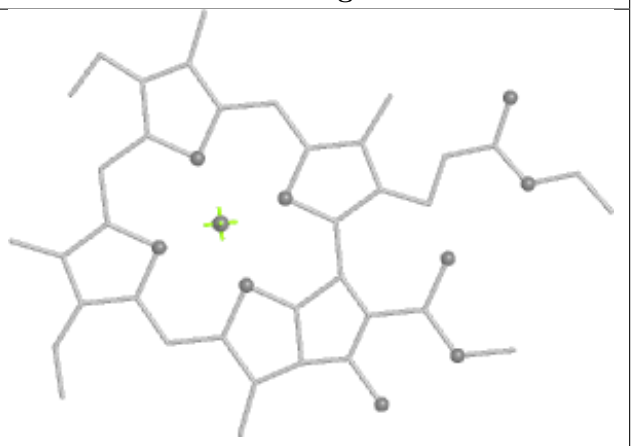


Rings

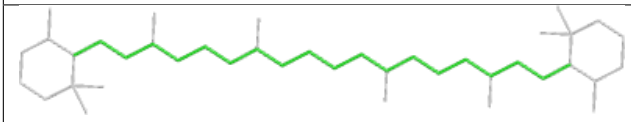
Ligand BCR B 828



Bond lengths



Bond angles



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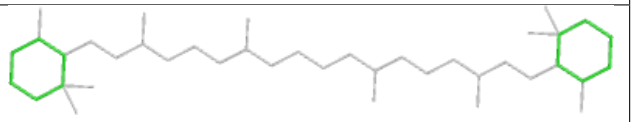
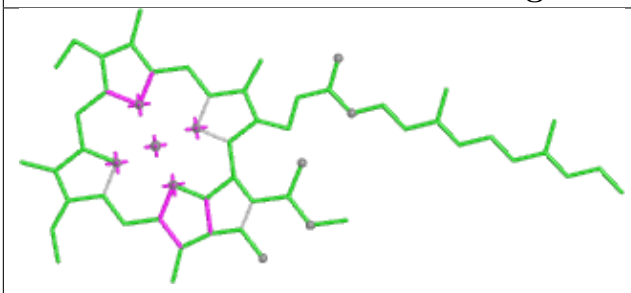
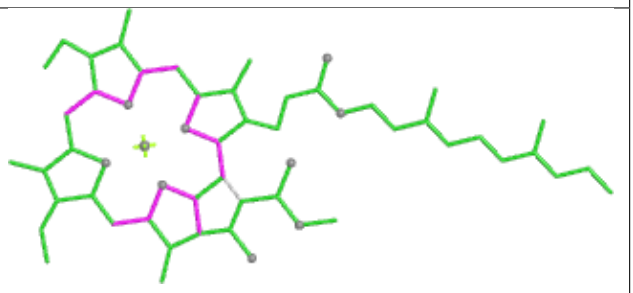


Rings

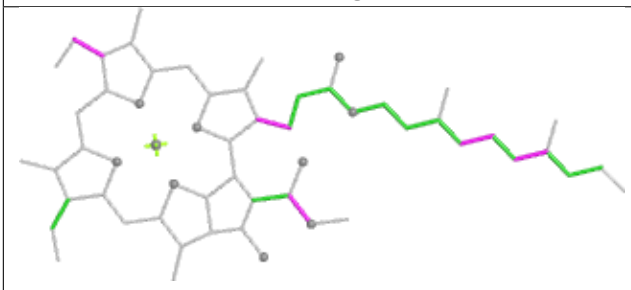
Ligand CLA F 202



Bond lengths



Bond angles



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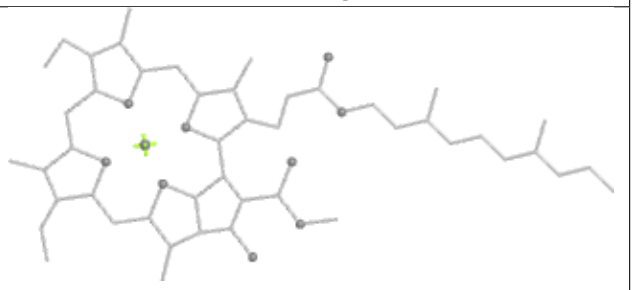
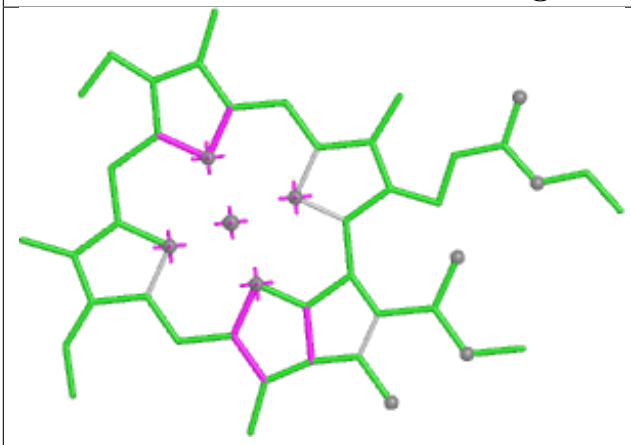
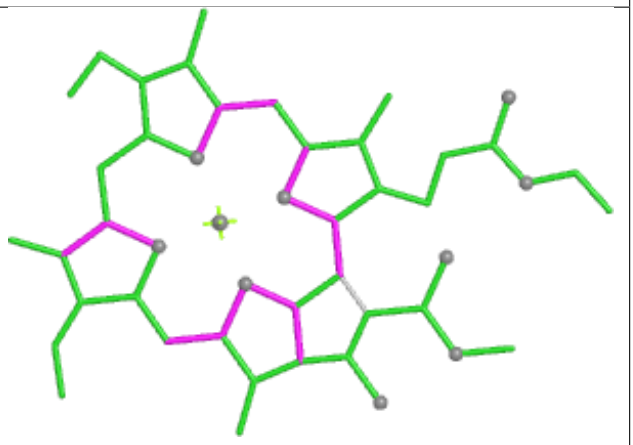


Rings

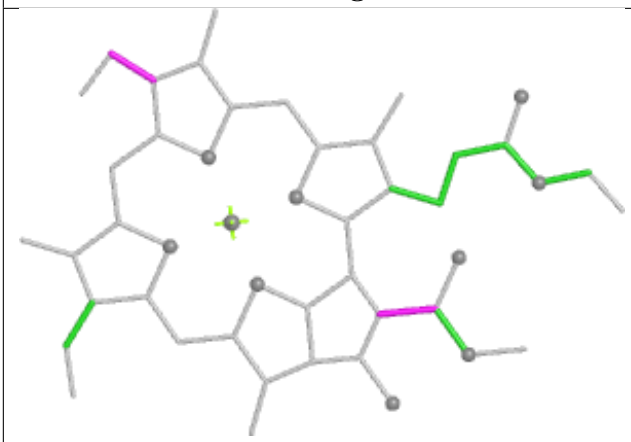
Ligand CLA f 310



Bond lengths



Bond angles



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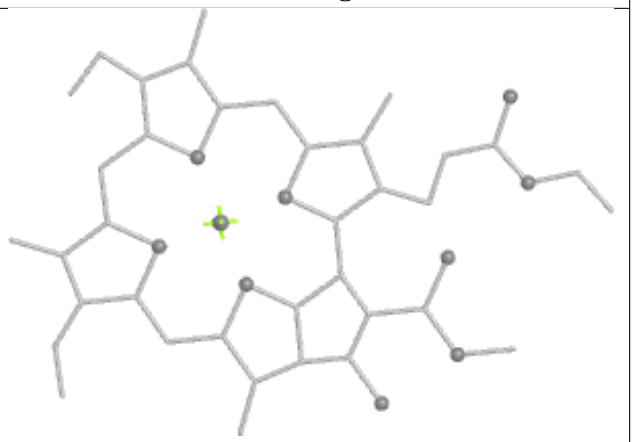
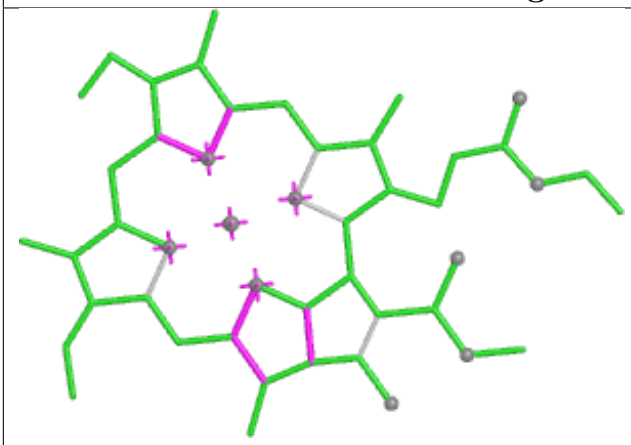


Rings

Ligand CLA d 207



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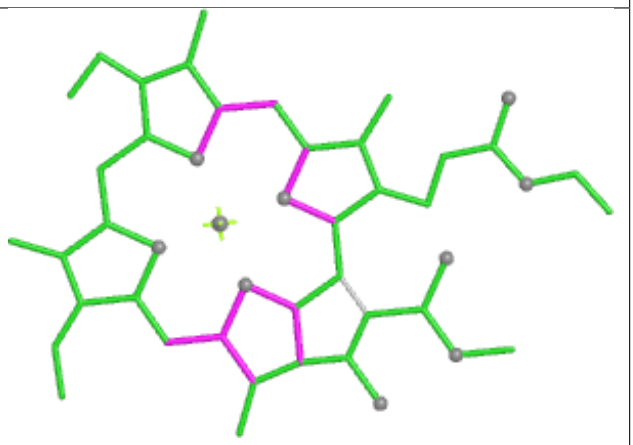

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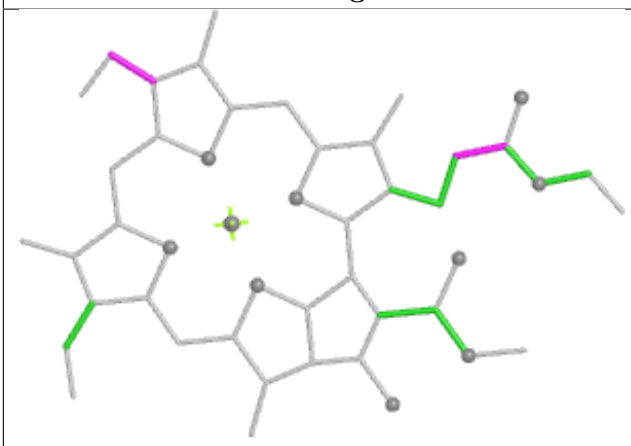

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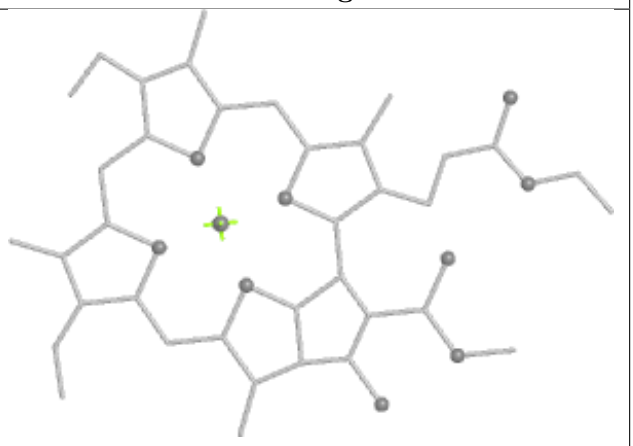
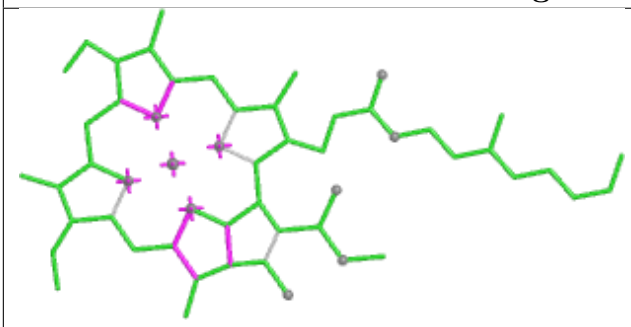


Rings

Ligand CLA i 307



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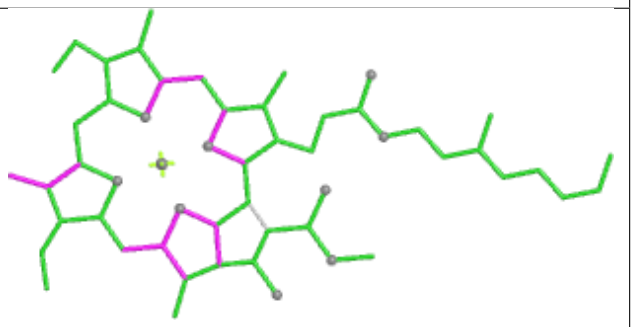

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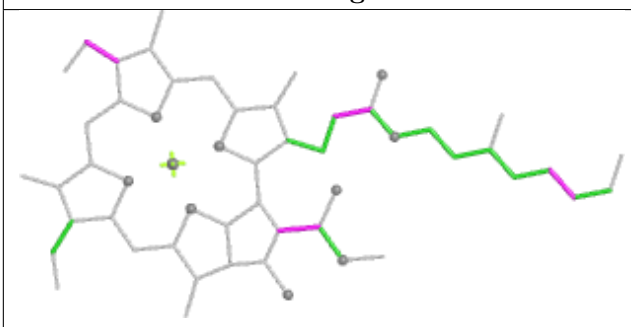

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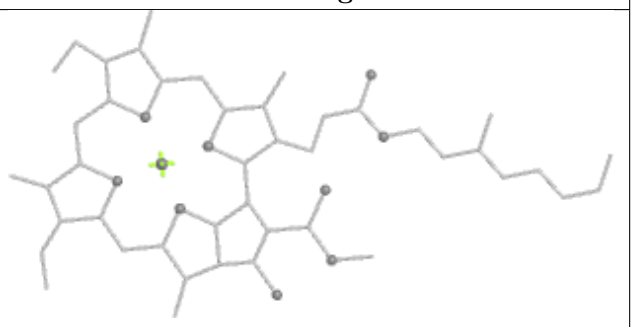
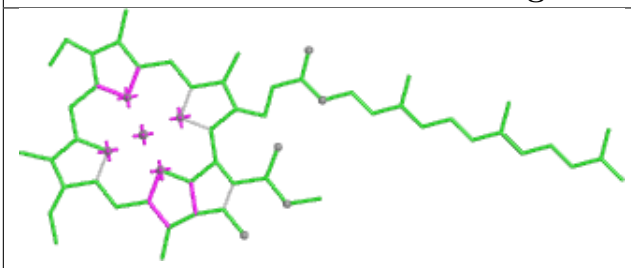
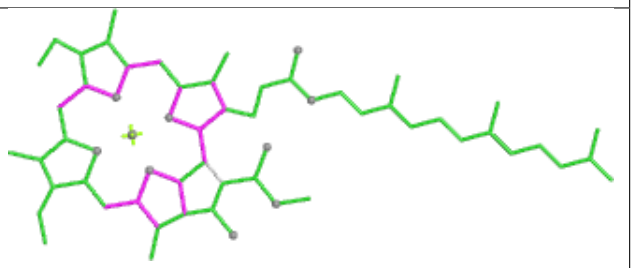
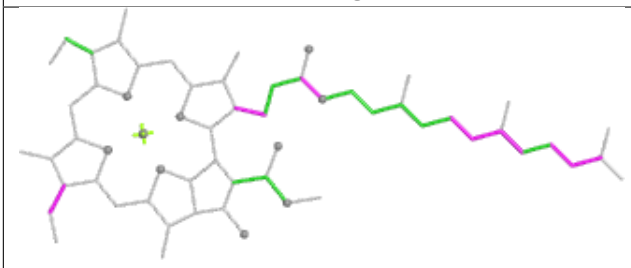
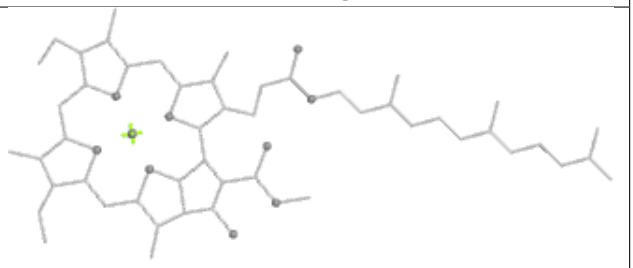
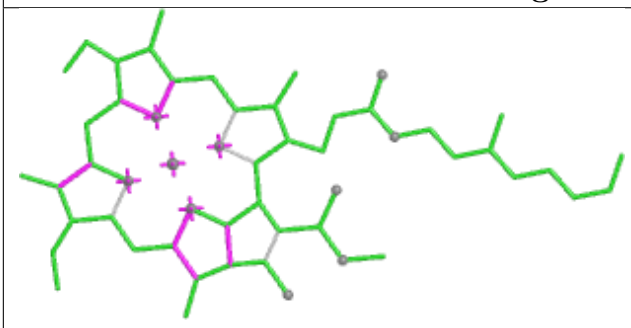
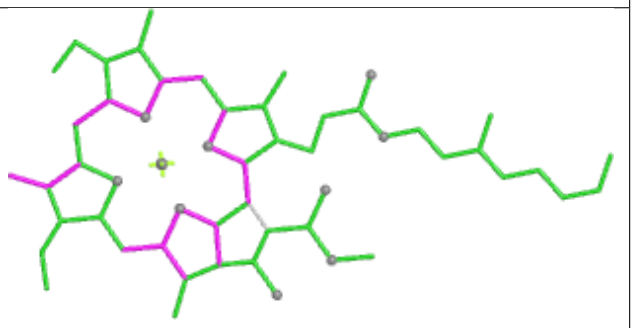
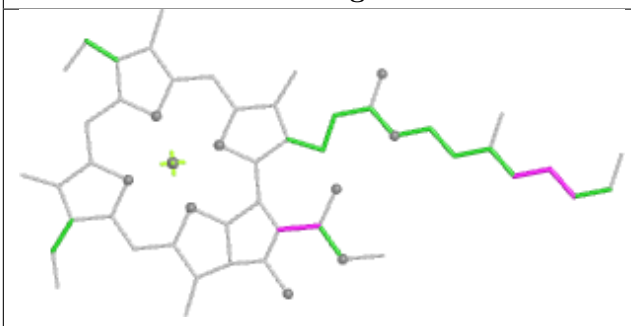
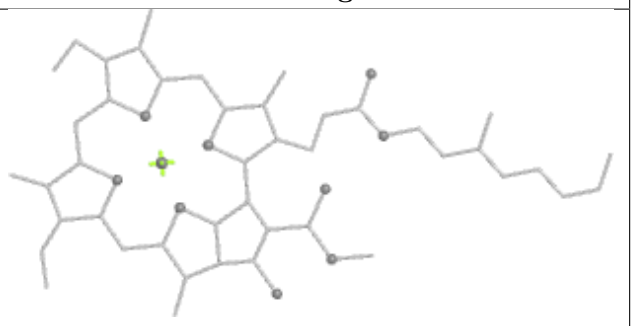
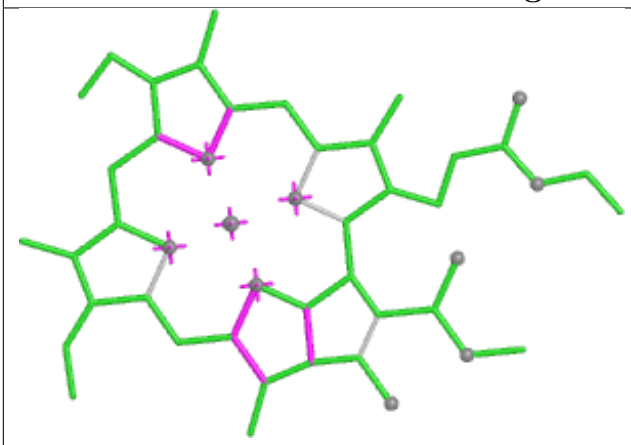


Rings

Ligand CLA n 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 823



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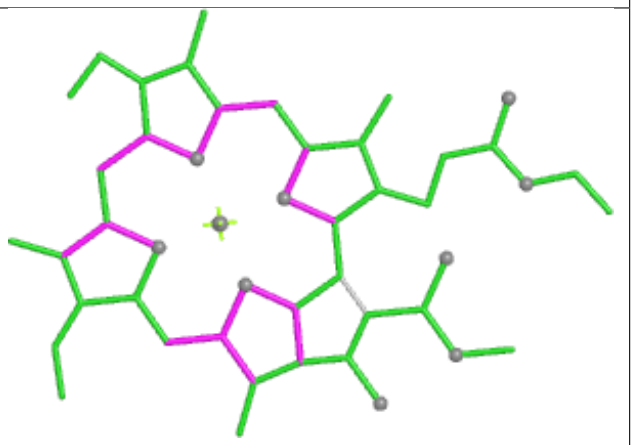
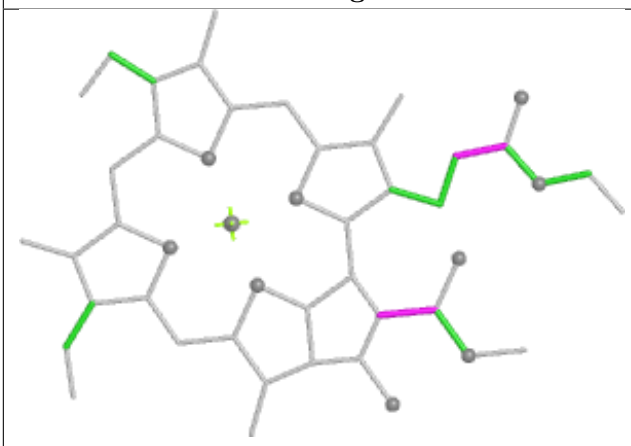


Bond angles



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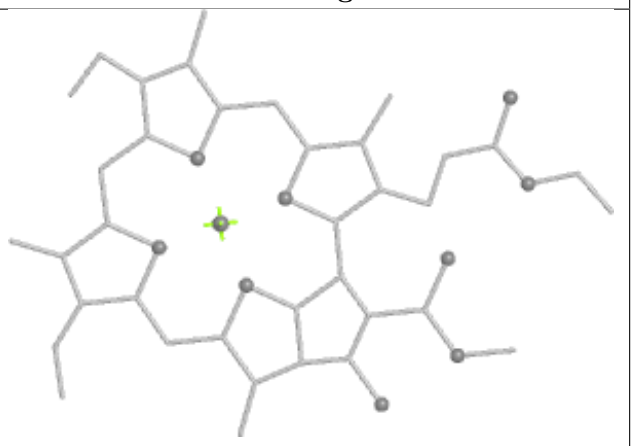
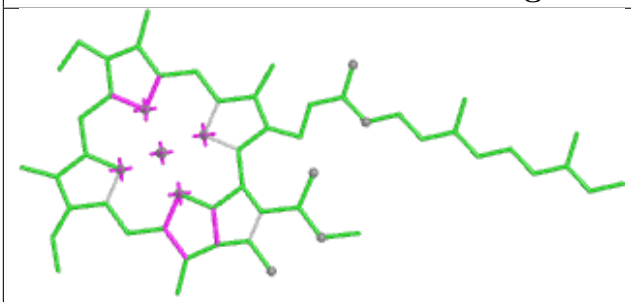


Rings

Ligand CLA B 833



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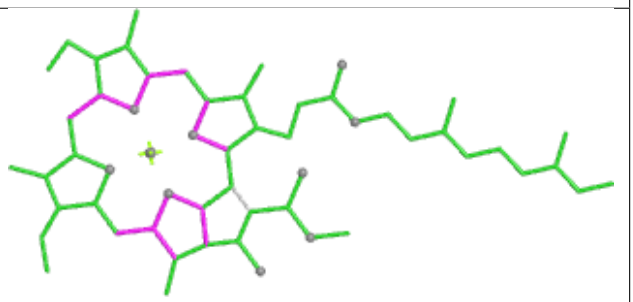
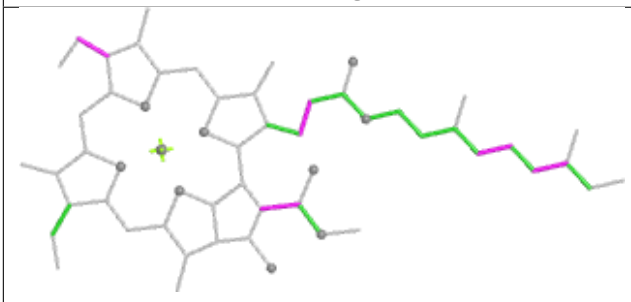


Bond angles



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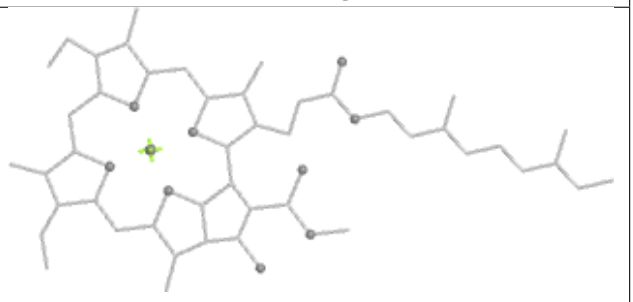
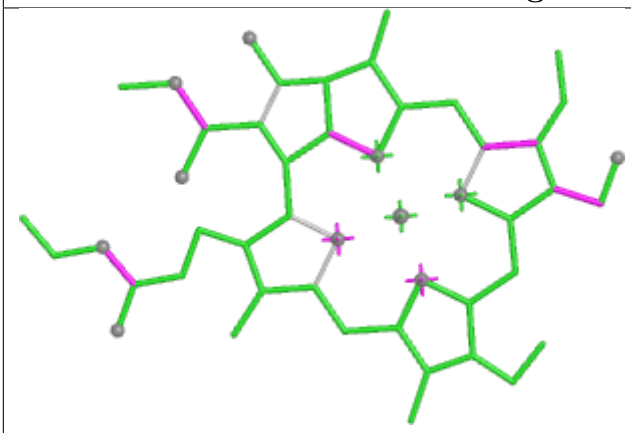


Rings

Ligand CHL h 202



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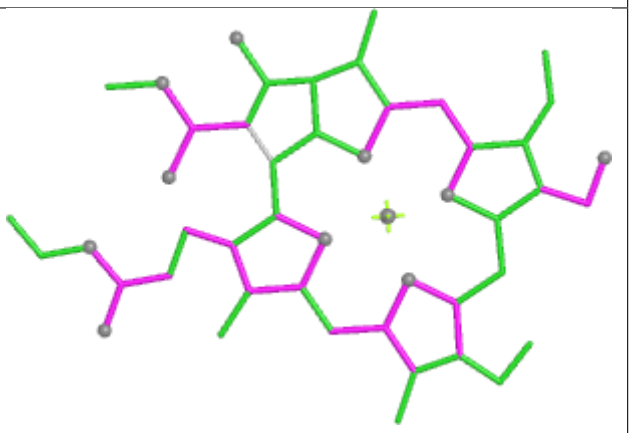
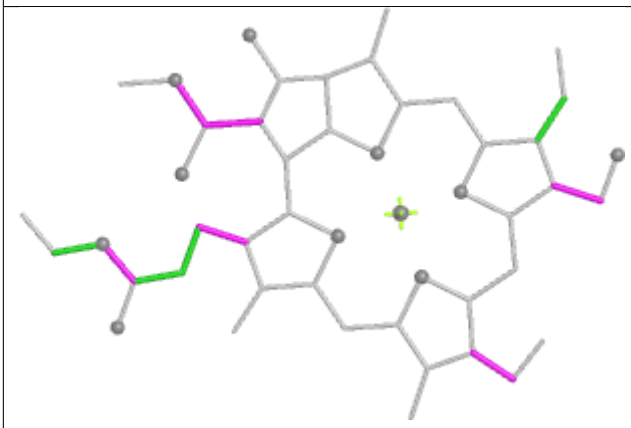


Bond angles



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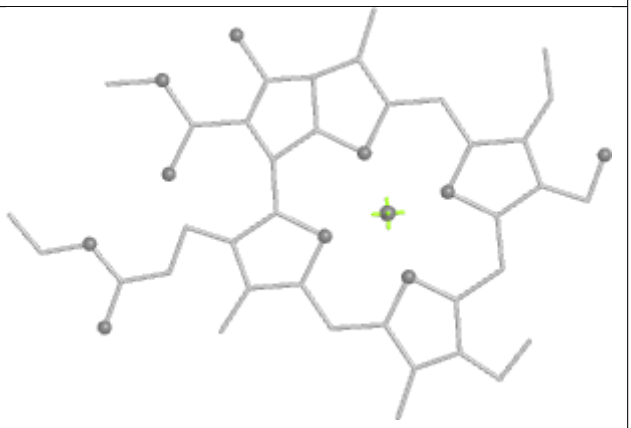
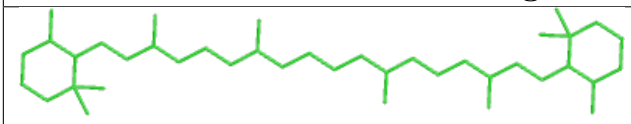


Rings

Ligand BCR A 837



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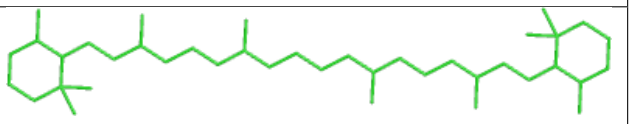
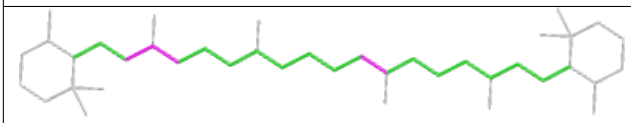


Bond angles



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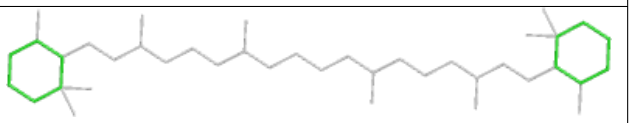
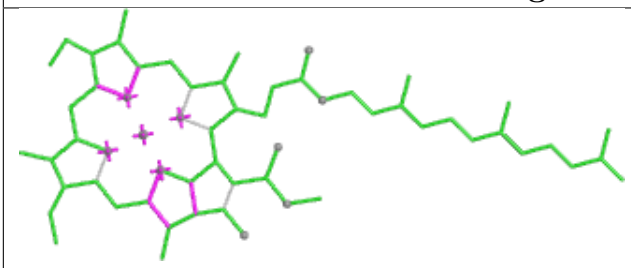


Rings

Ligand CLA g 307



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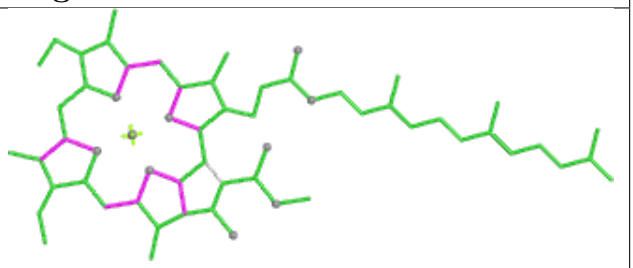

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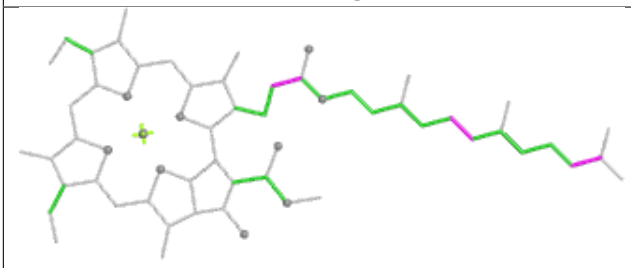

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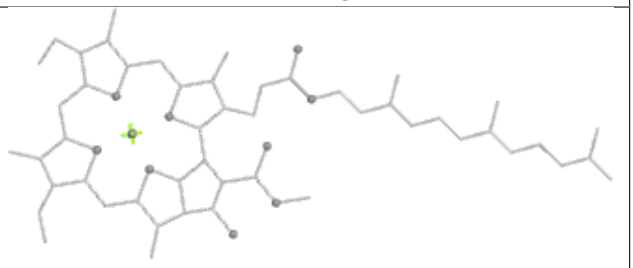
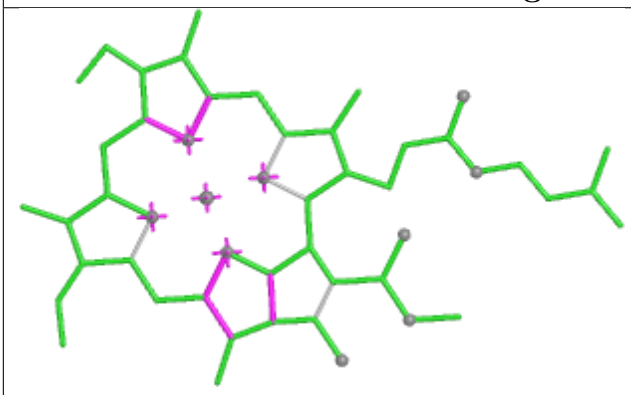


Rings

Ligand CLA A 848



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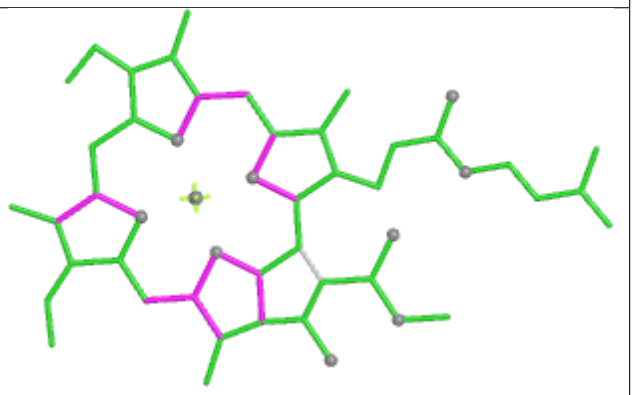
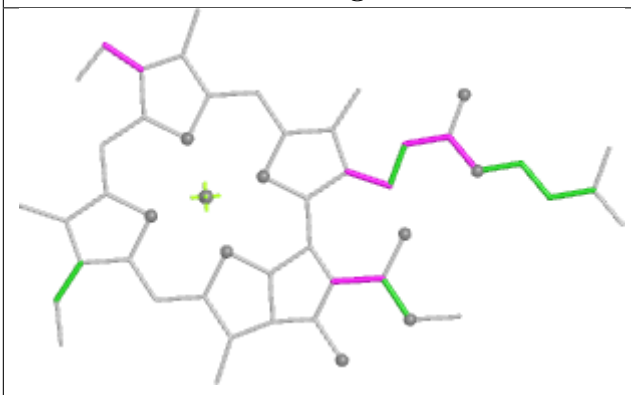


Bond angles



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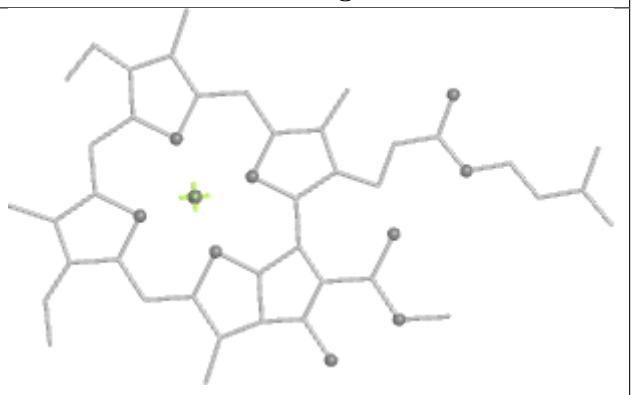
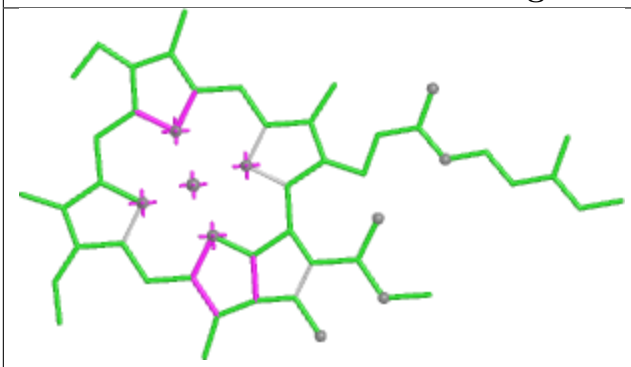


Rings

Ligand CLA b 303



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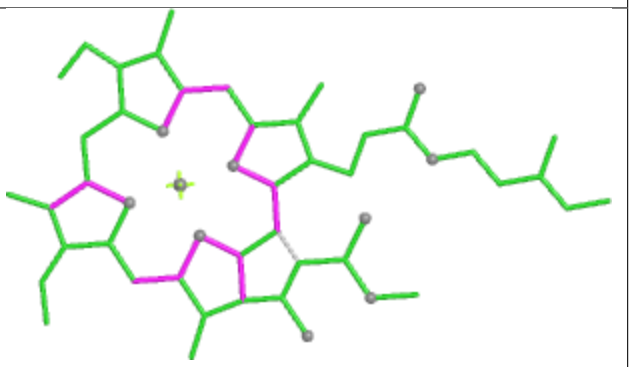
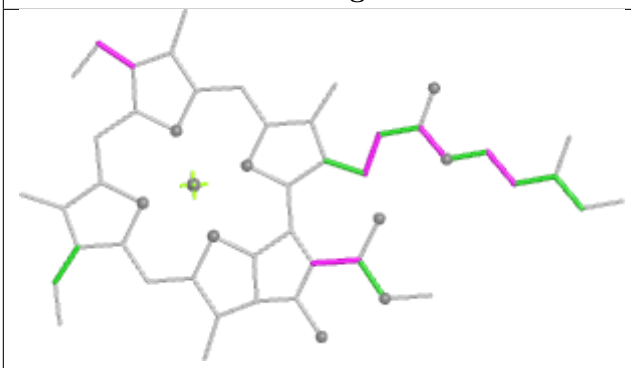


Bond angles



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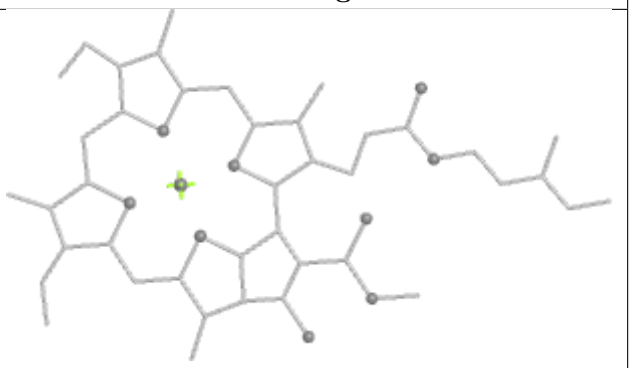
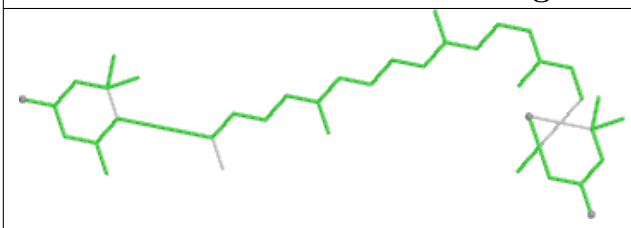


Rings

Ligand DD6 j 316



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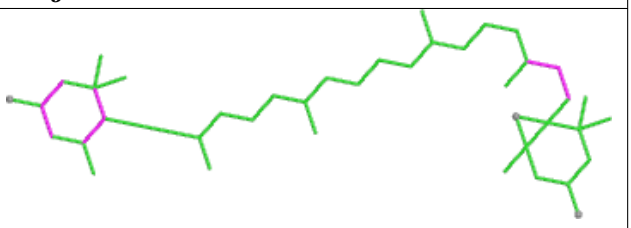
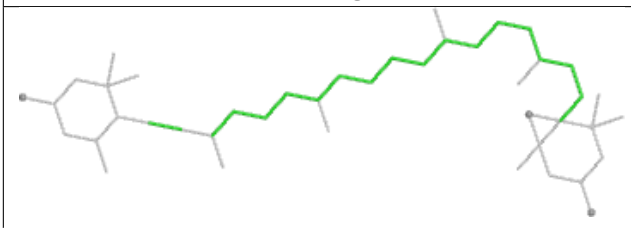


Bond angles



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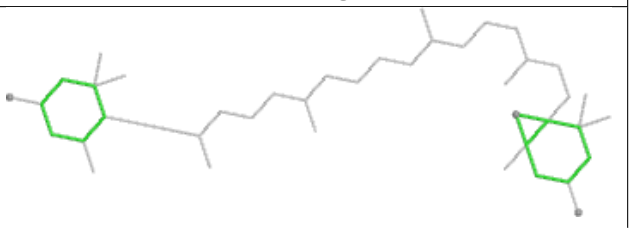
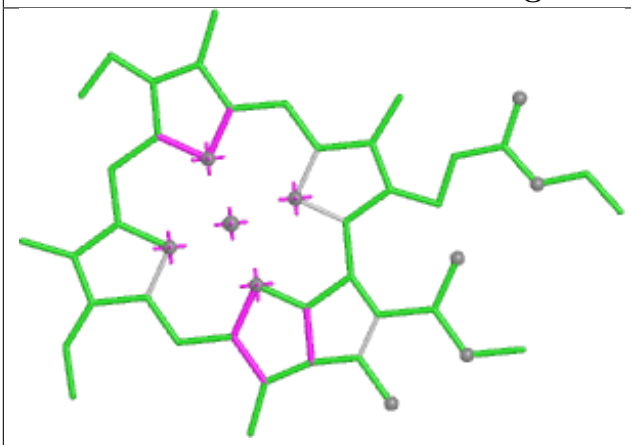
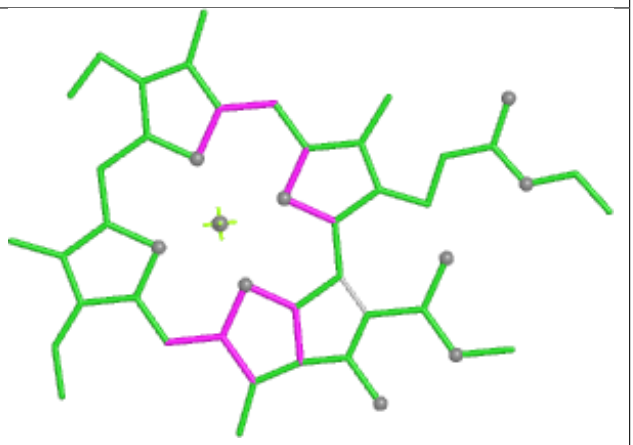


Rings

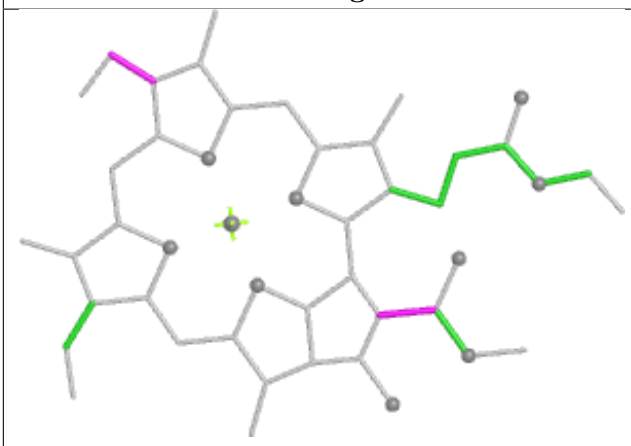
Ligand CLA B 843



Bond lengths



Bond angles



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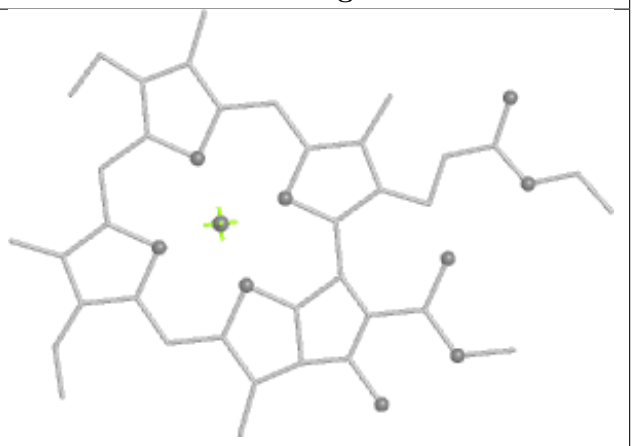
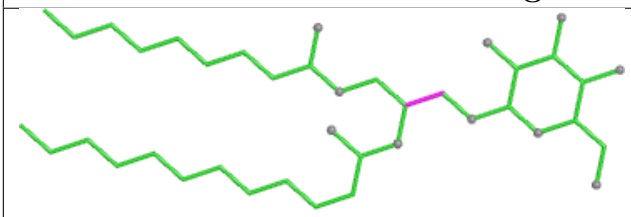


Rings

Ligand LMG a 318



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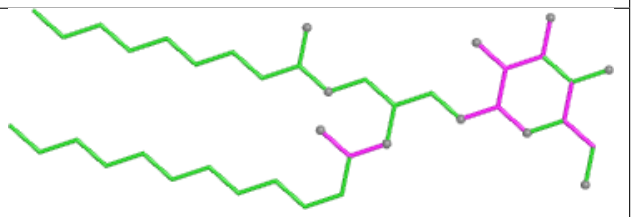
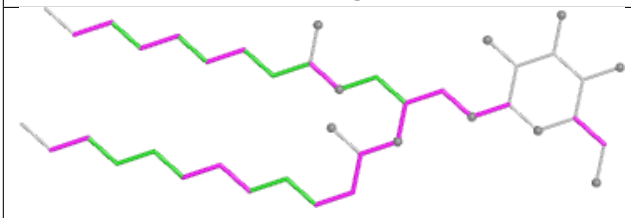


Bond angles



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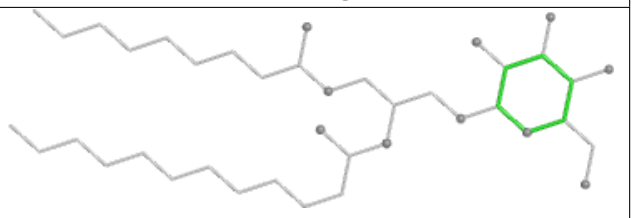
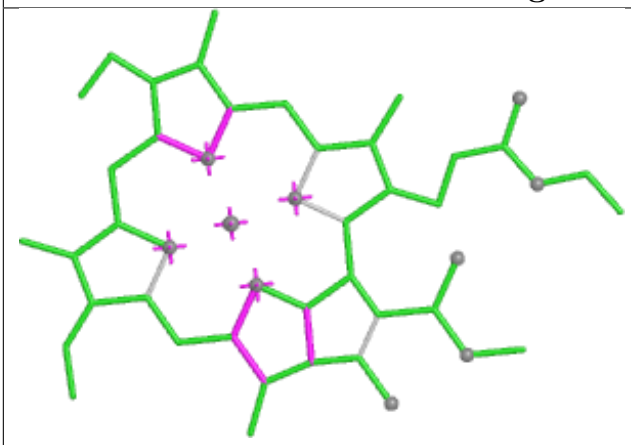


Rings

Ligand CLA o 309



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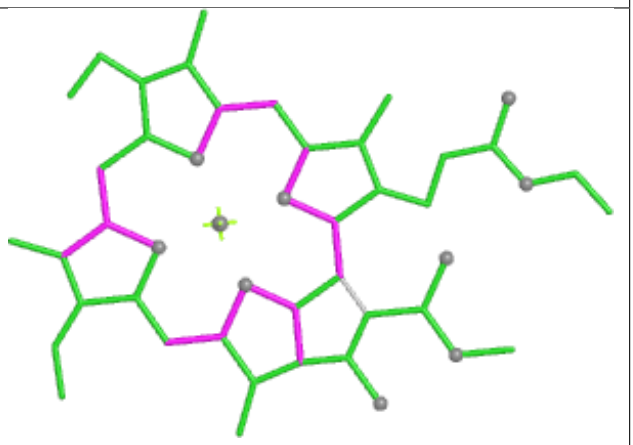
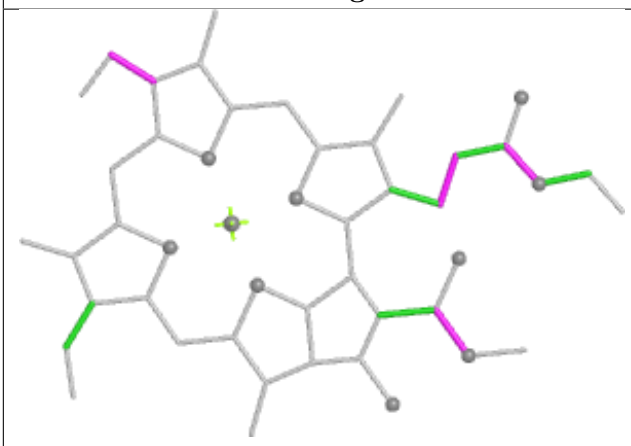


Bond angles



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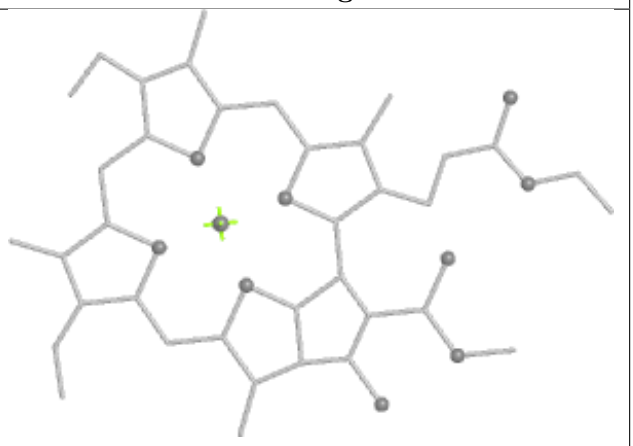
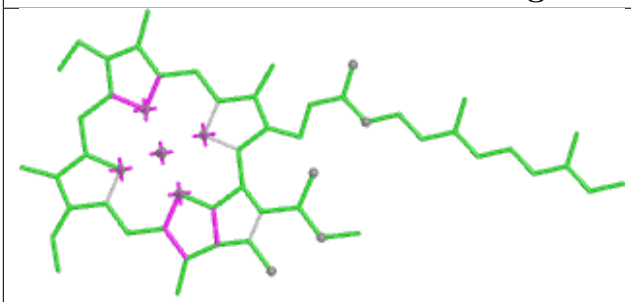


Rings

Ligand CLA d 209



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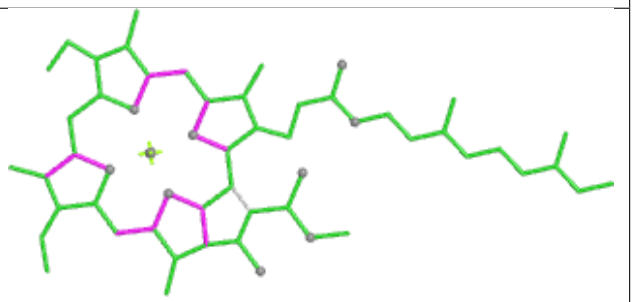

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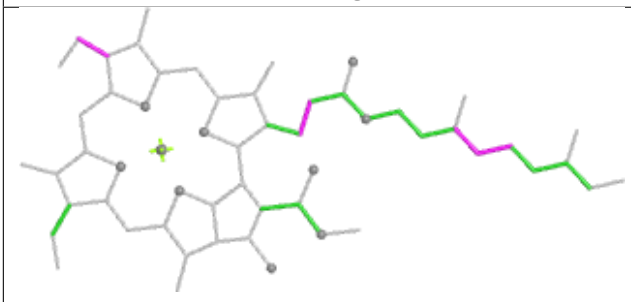

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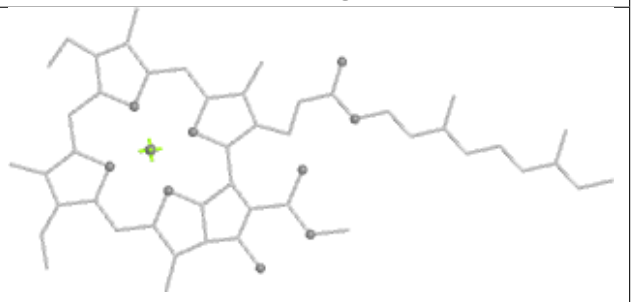

Rings

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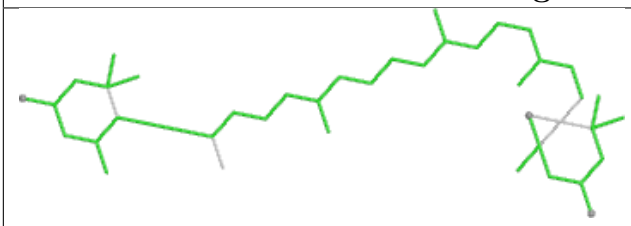

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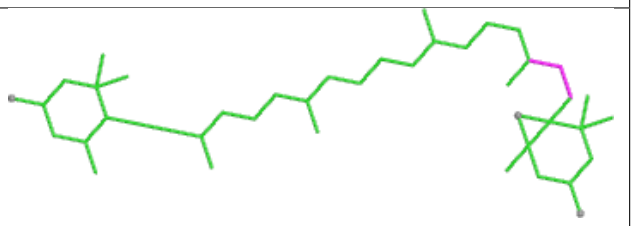

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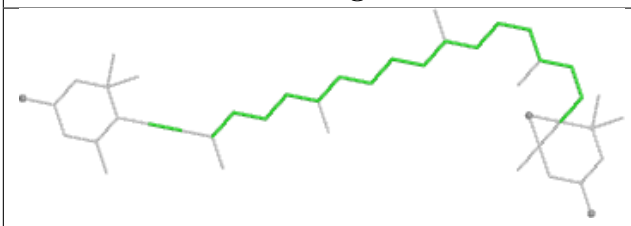

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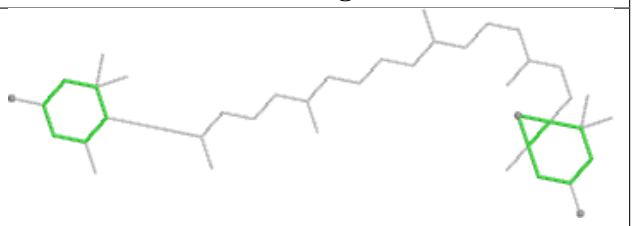
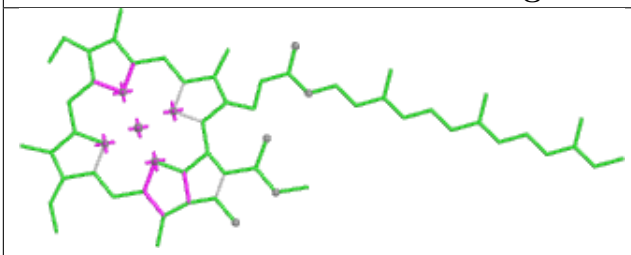


Rings

Ligand CLA A 811



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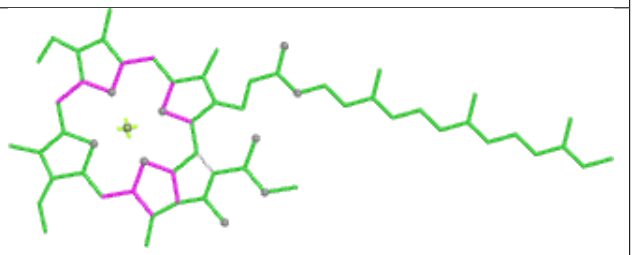

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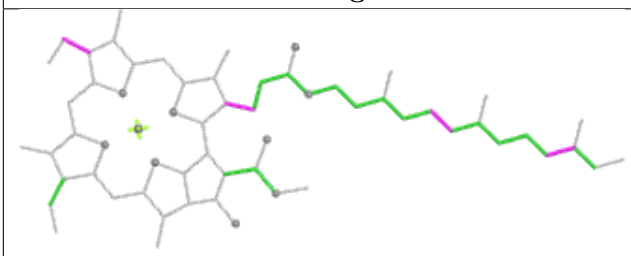

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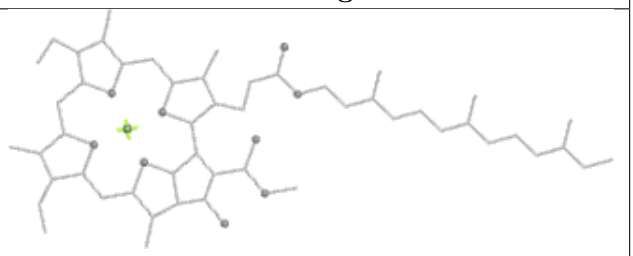
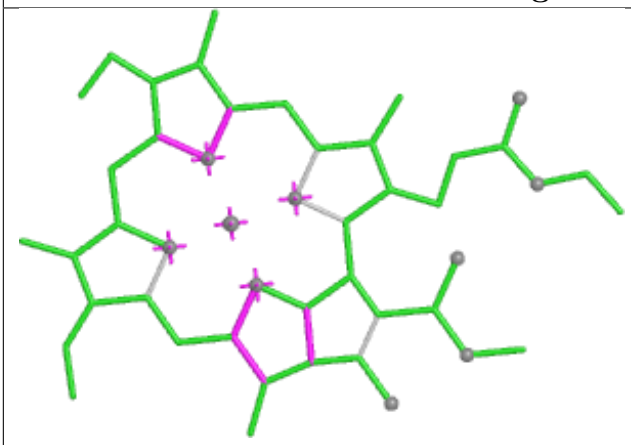


Rings

Ligand CLA f 312



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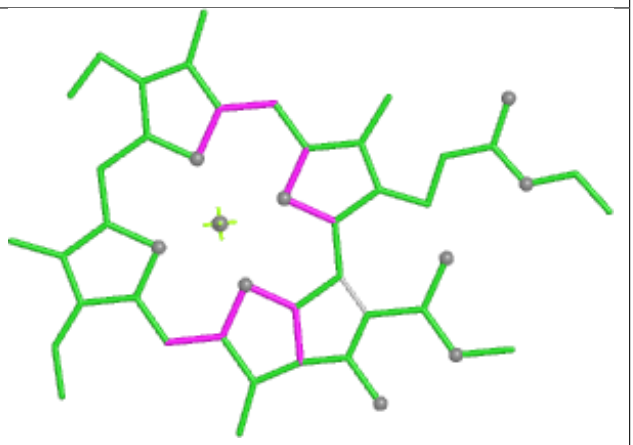

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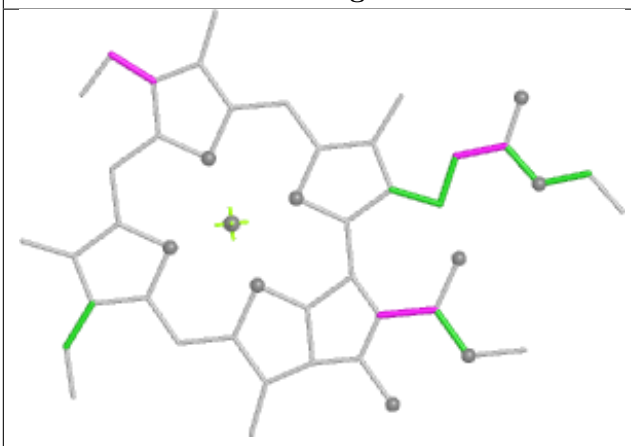

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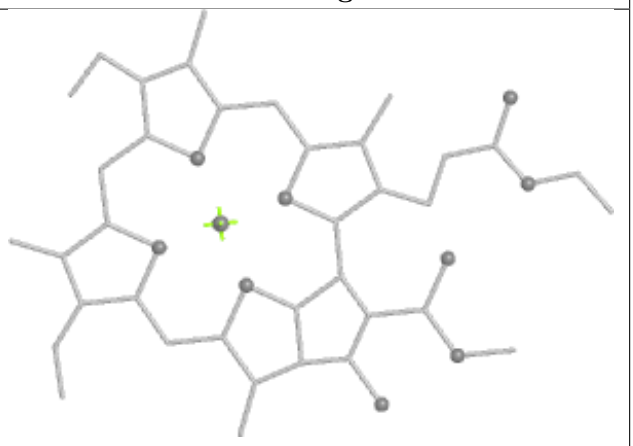

Rings

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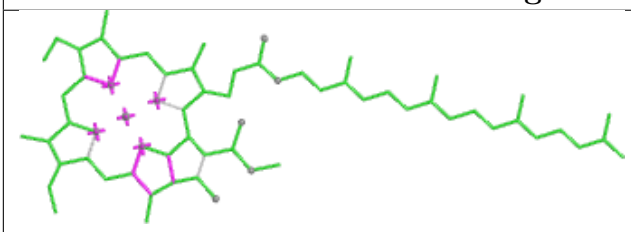

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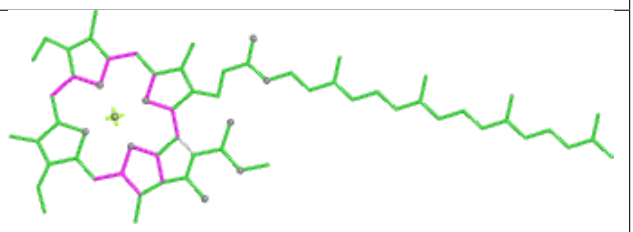

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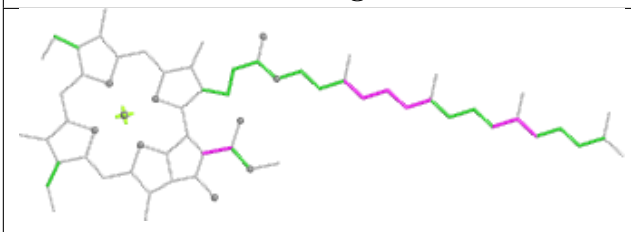

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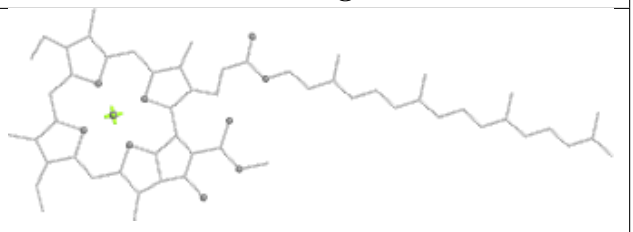
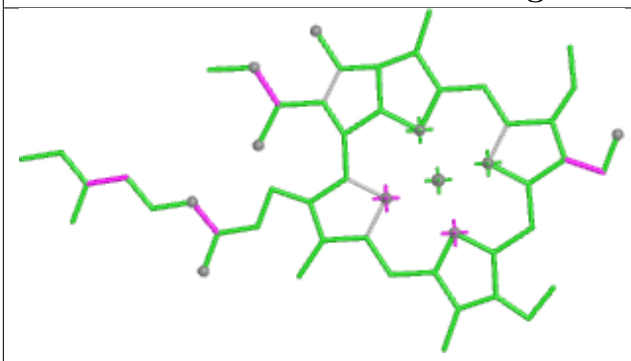


Rings

Ligand CHL b 314



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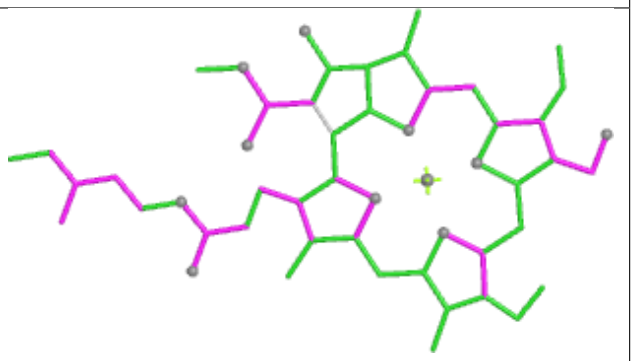

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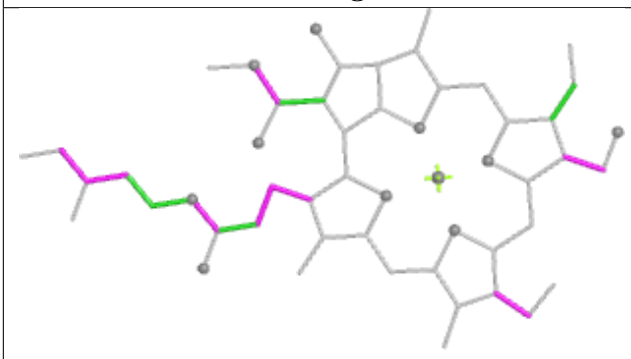

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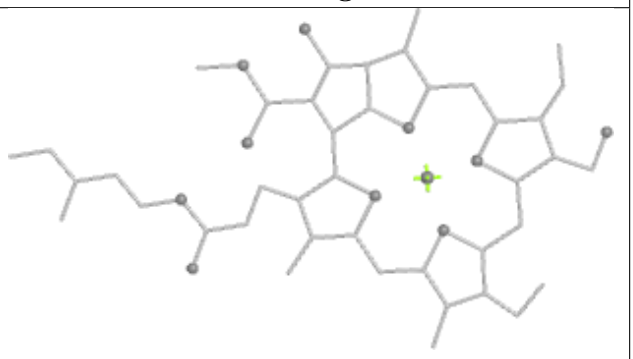

Rings

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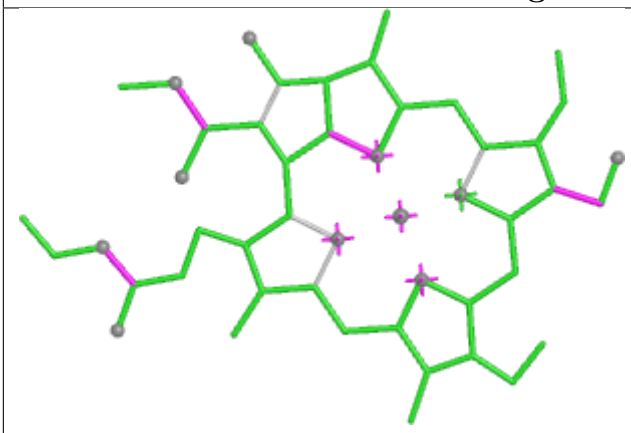

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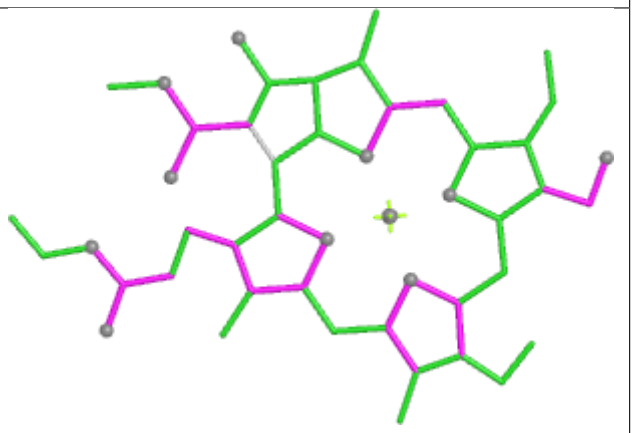

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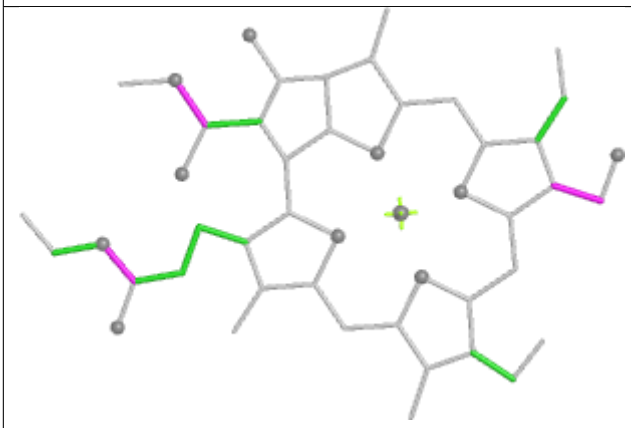

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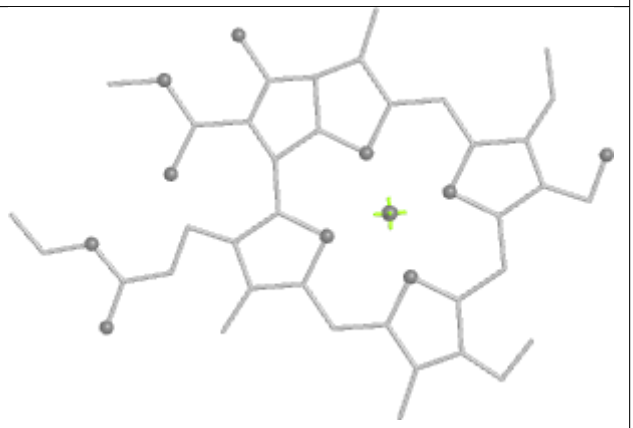
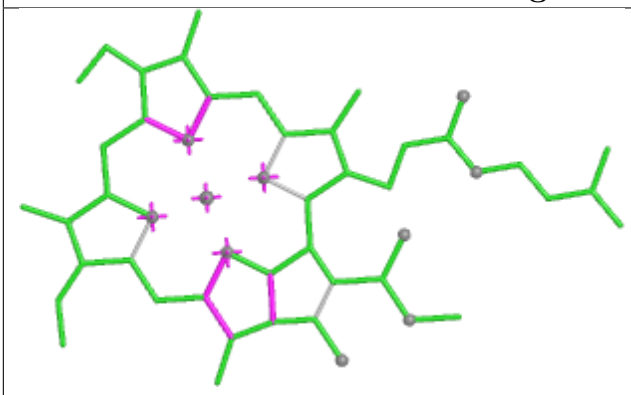


Rings

Ligand CLA c 310



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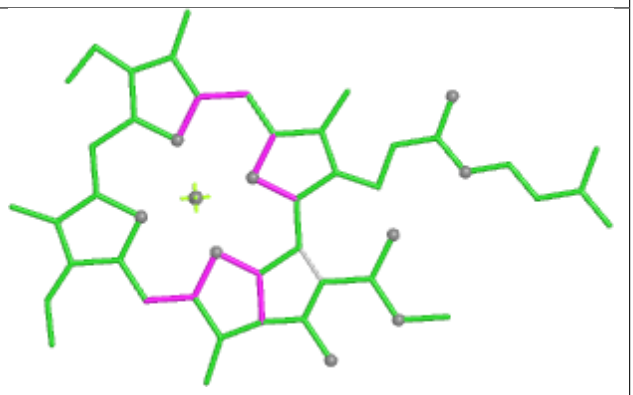
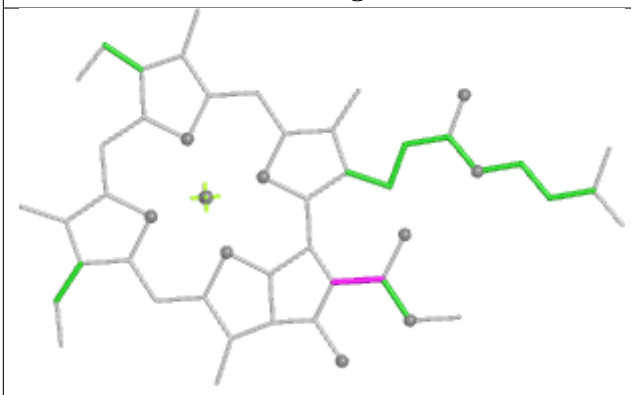


Bond angles



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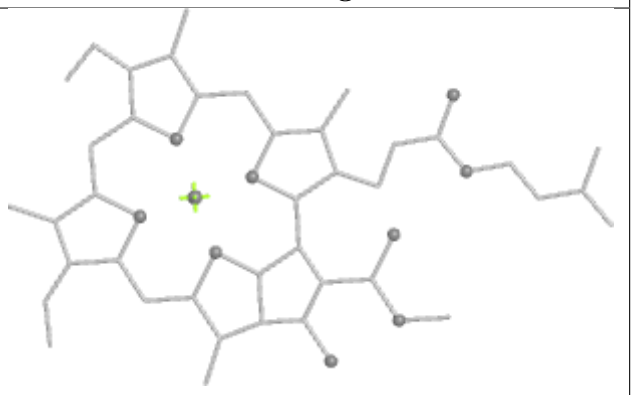
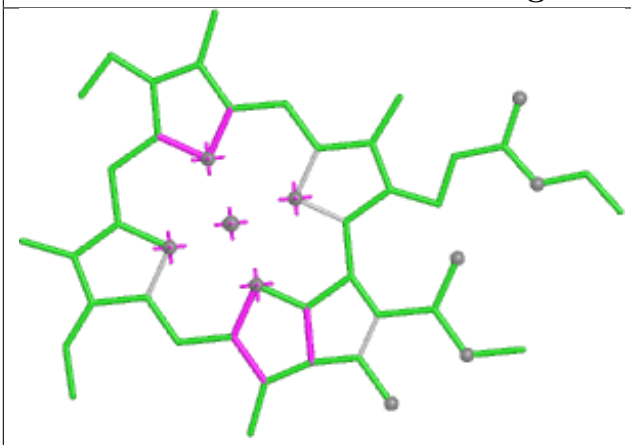


Rings

Ligand CLA d 201



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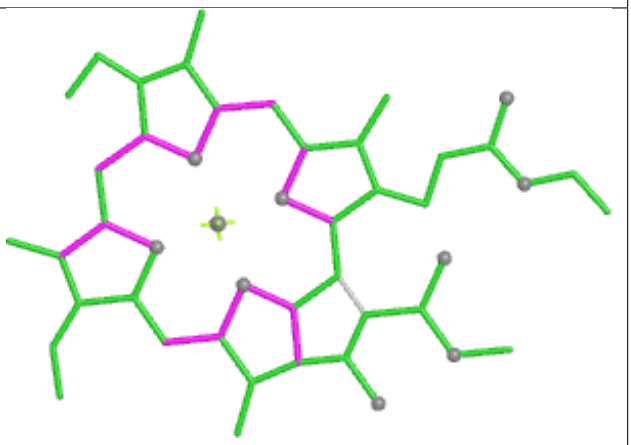

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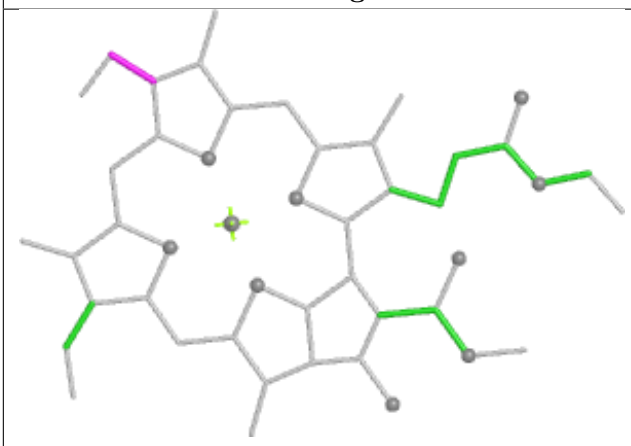

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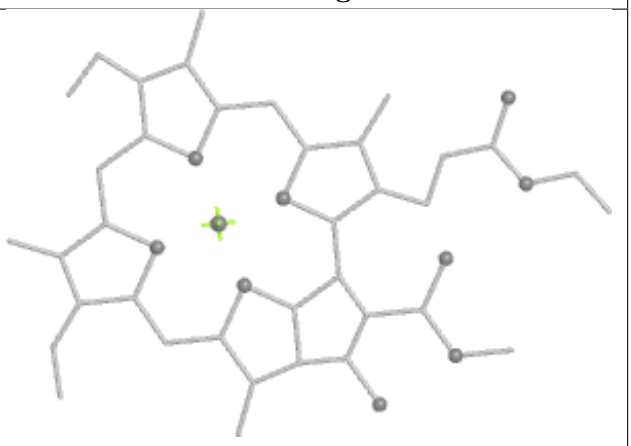
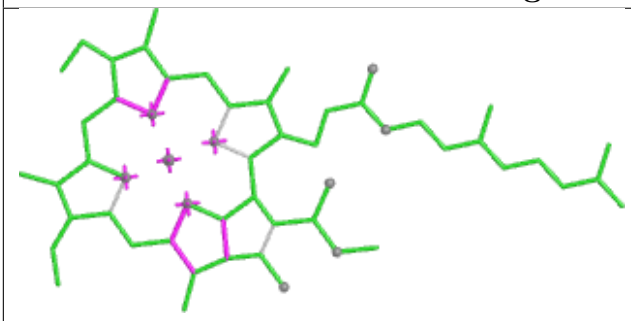


Rings

Ligand CLA A 852



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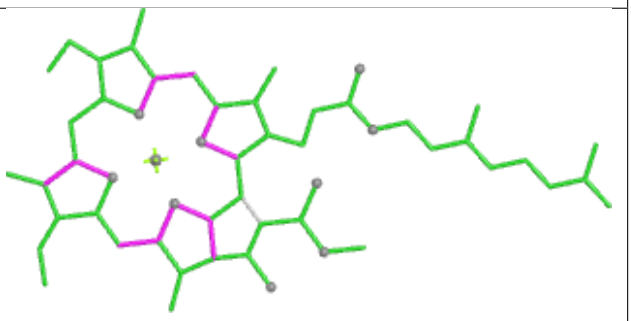
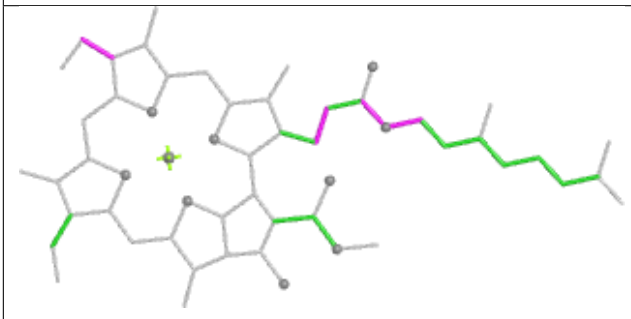


Bond angles



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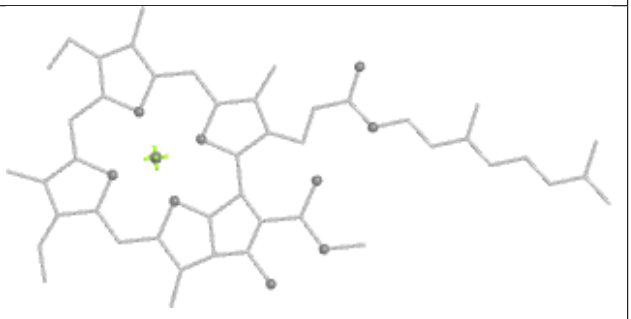
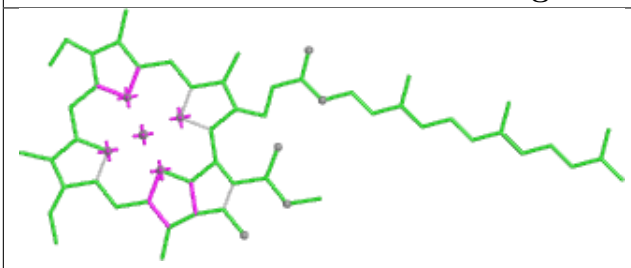
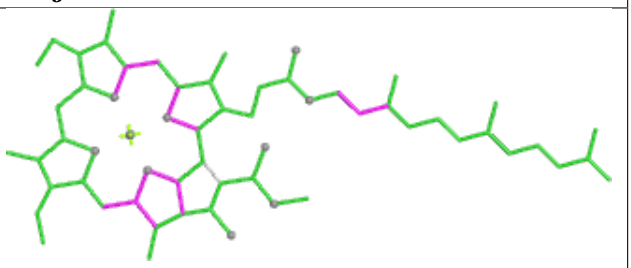
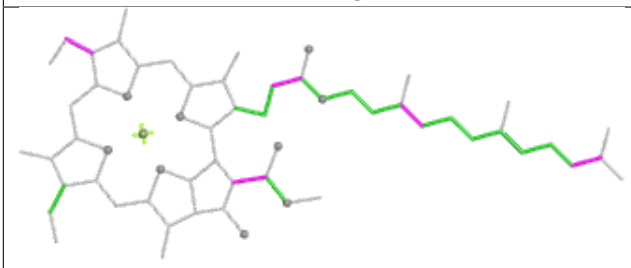
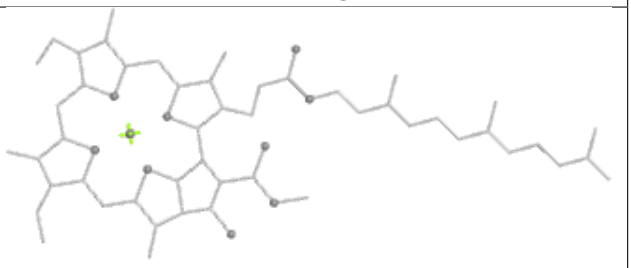


Rings

Ligand CLA j 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

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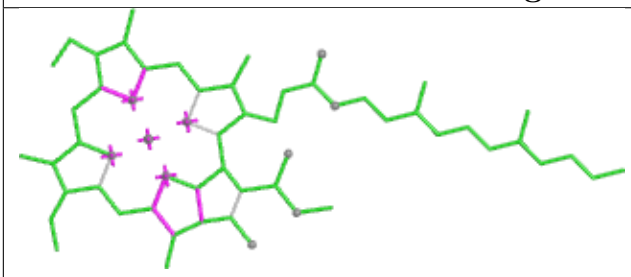	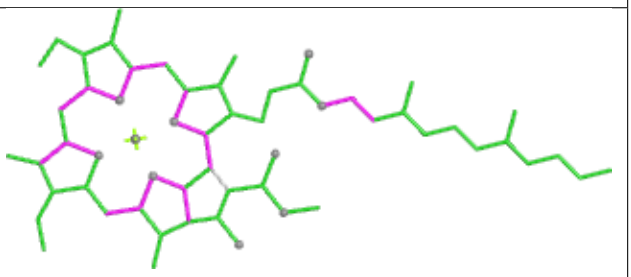
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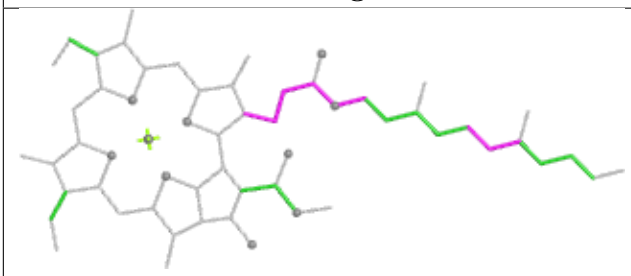
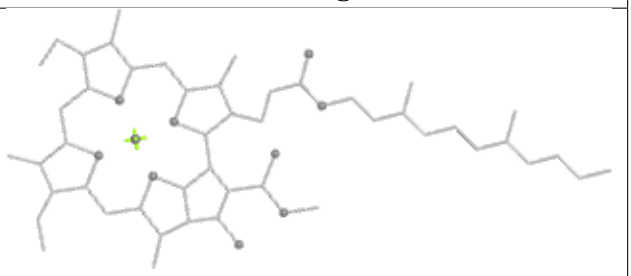
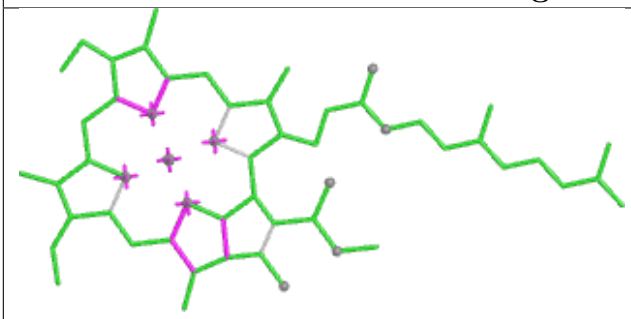
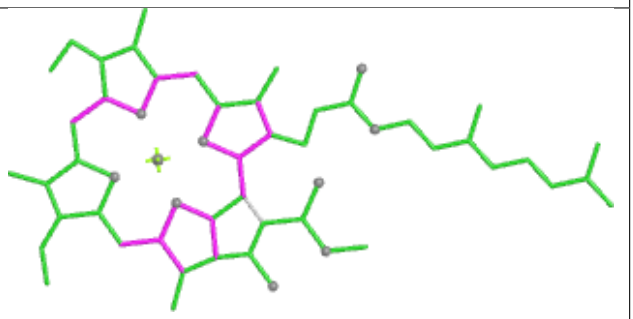
	
Torsions	Rings

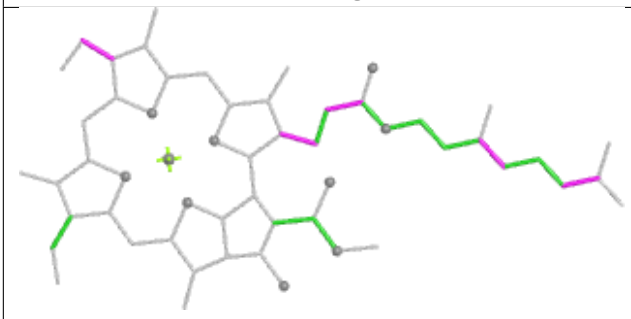
Ligand CLA f 314



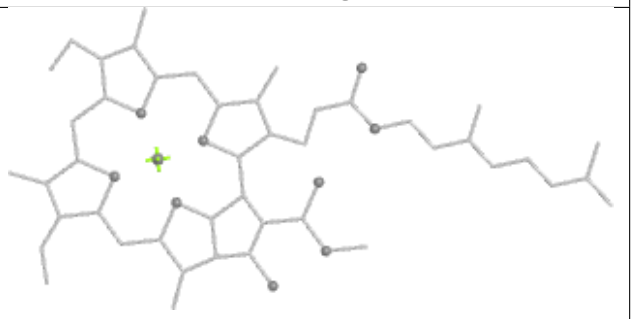
Bond lengths



Bond angles

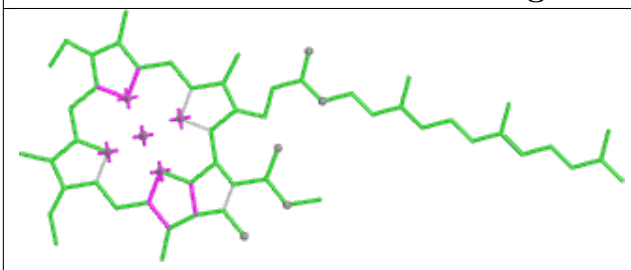


Torsions



Rings

Ligand CLA h 209



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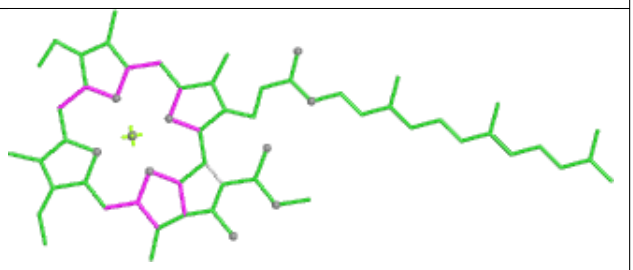
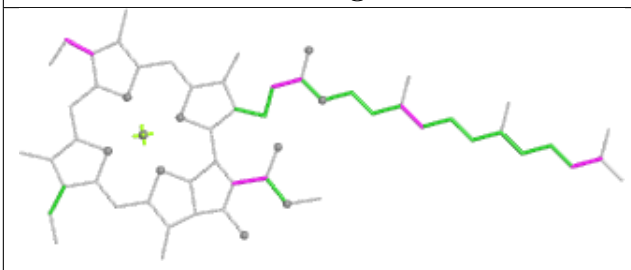
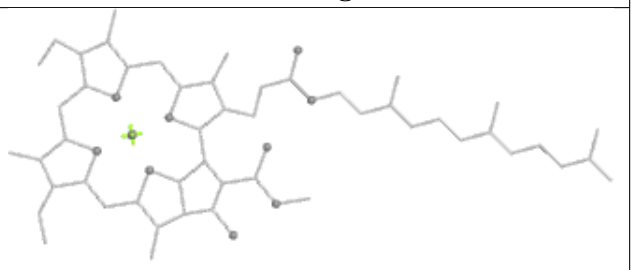


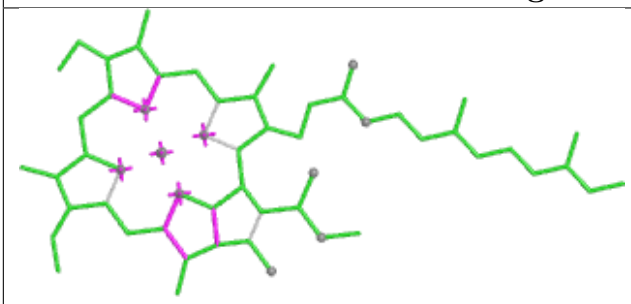
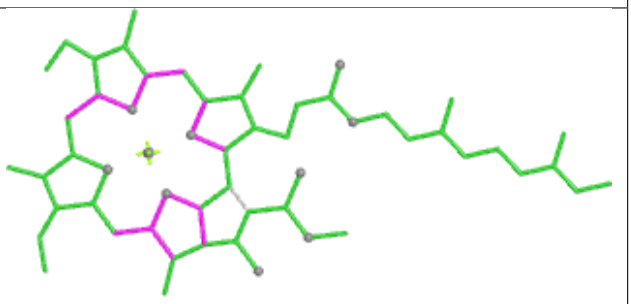
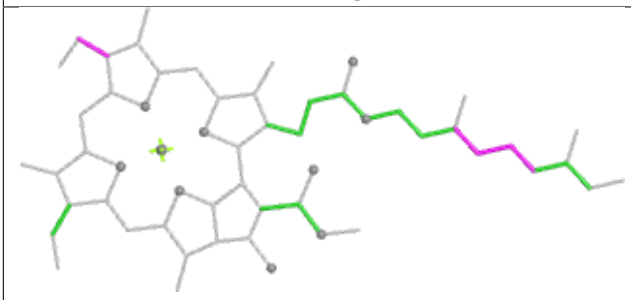
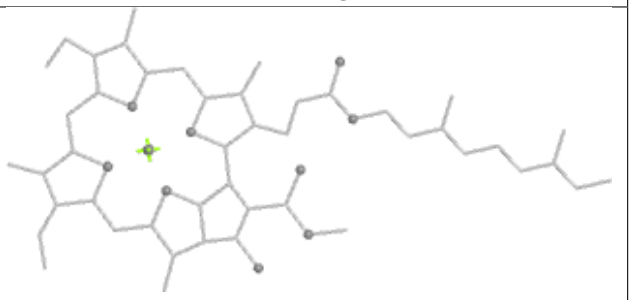
Bond angles



Torsions



Rings

Ligand CLA h 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

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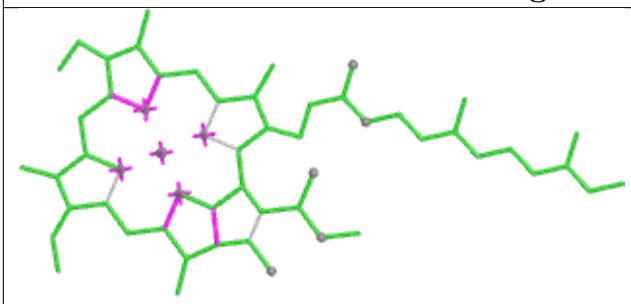
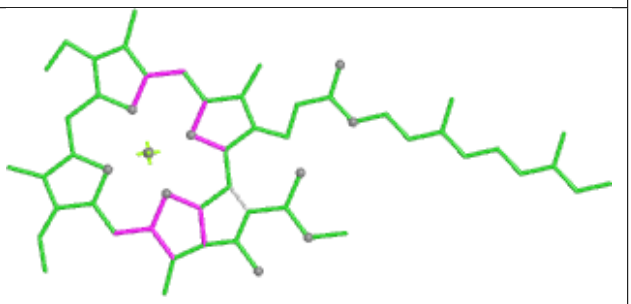
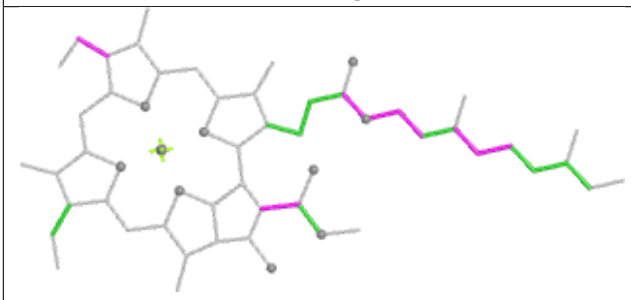
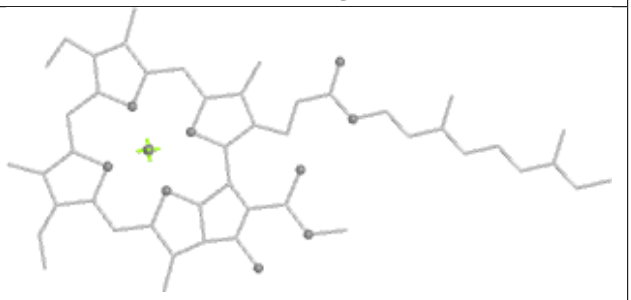
	
Bond lengths	Bond angles
	
Torsions	Rings

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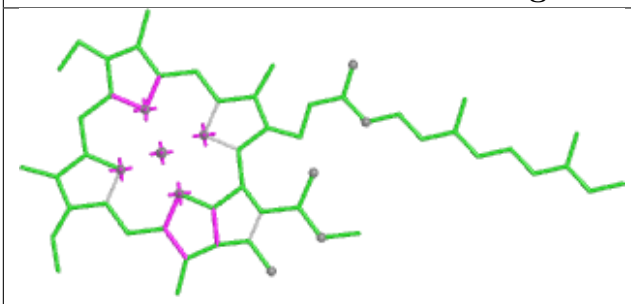
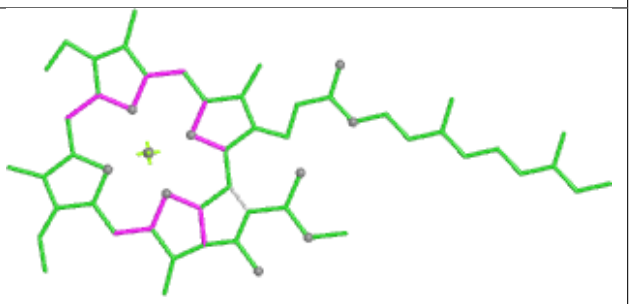
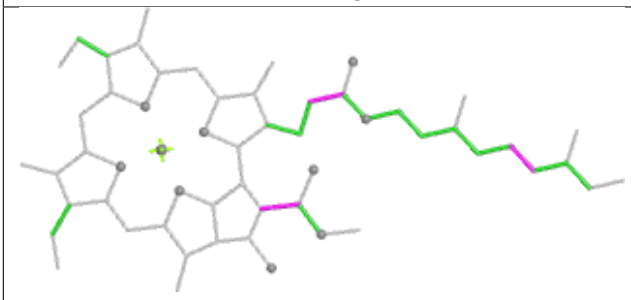
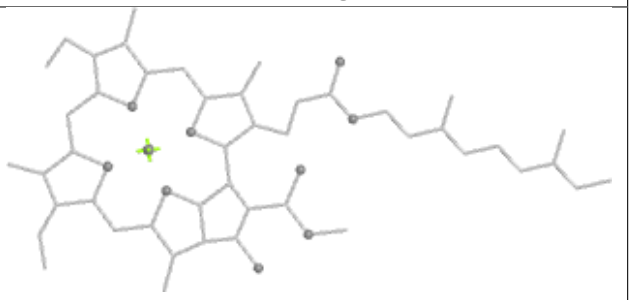
	
Bond lengths	Bond angles
	
Torsions	Rings

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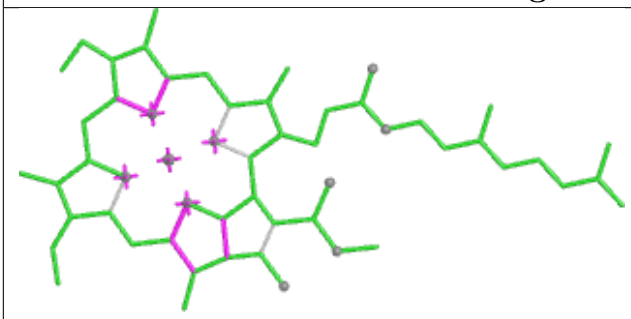
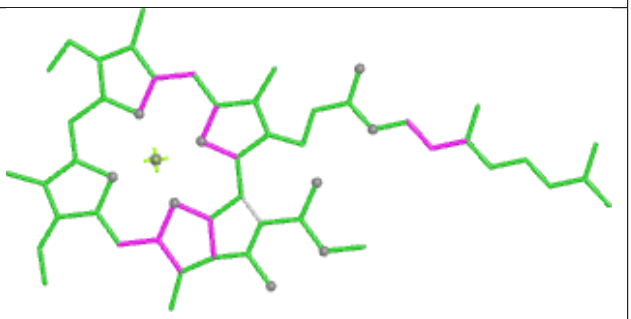
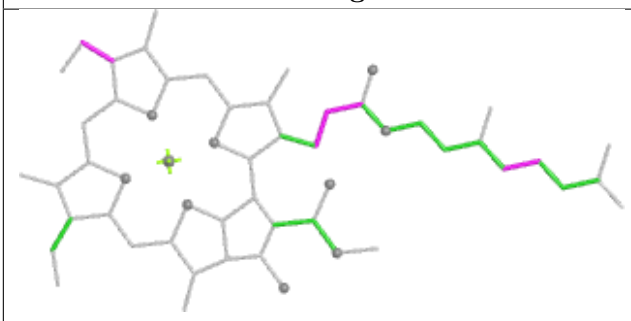
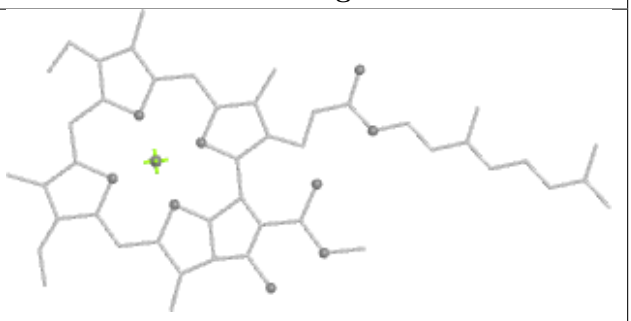
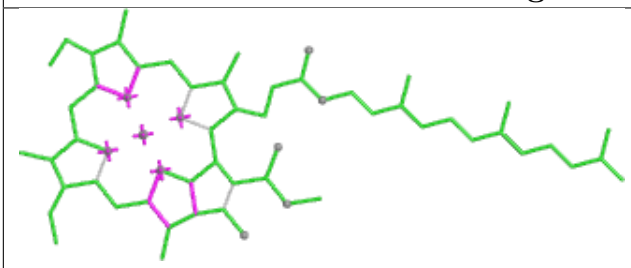
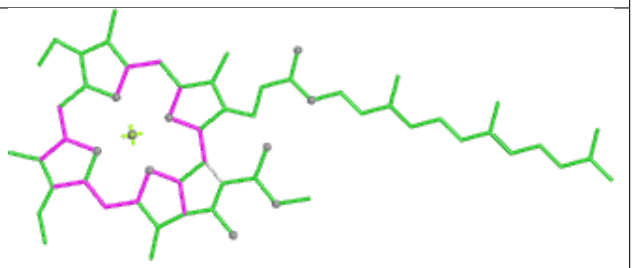
	
Bond lengths	Bond angles
	
Torsions	Rings

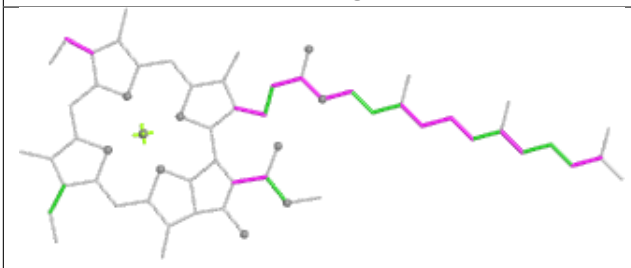
Ligand CLA b 306



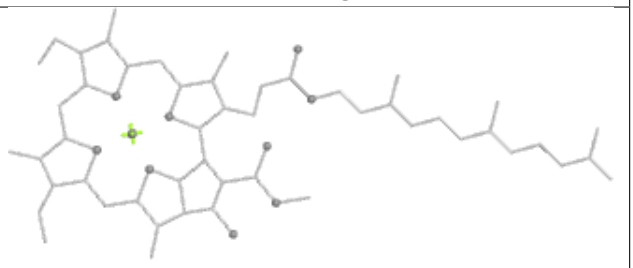
Bond lengths



Bond angles

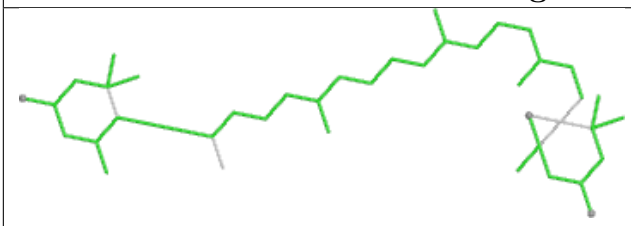


Torsions



Rings

Ligand DD6 a 321



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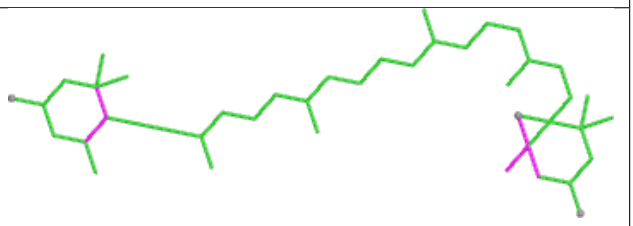
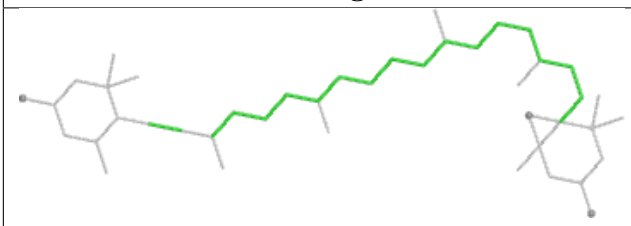


Bond angles



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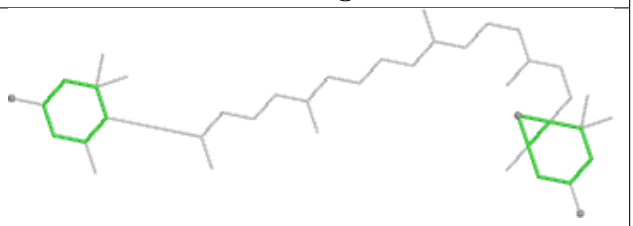
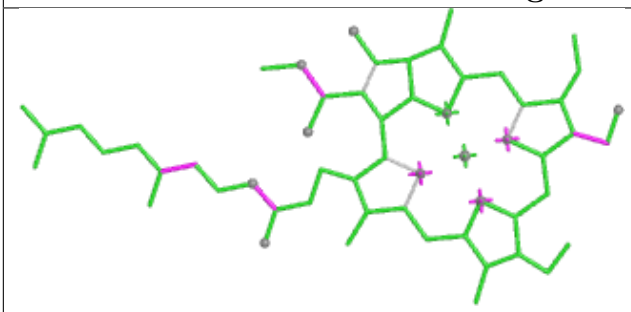


Rings

Ligand CHL d 205



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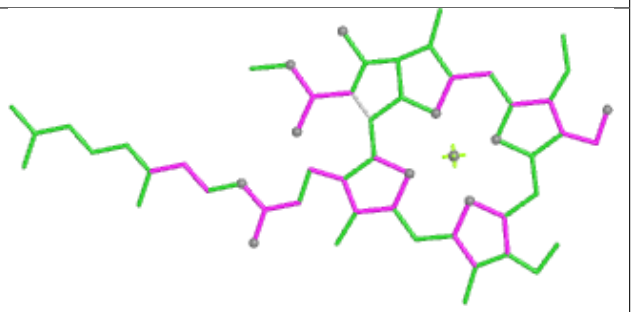
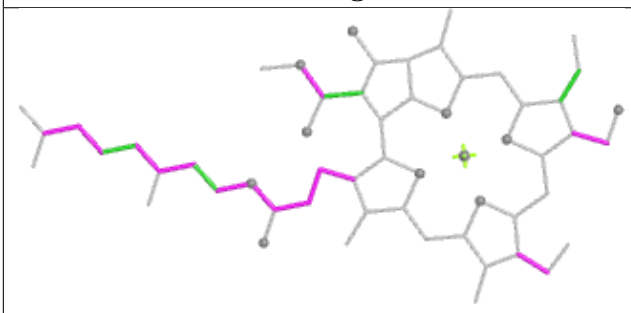


Bond angles



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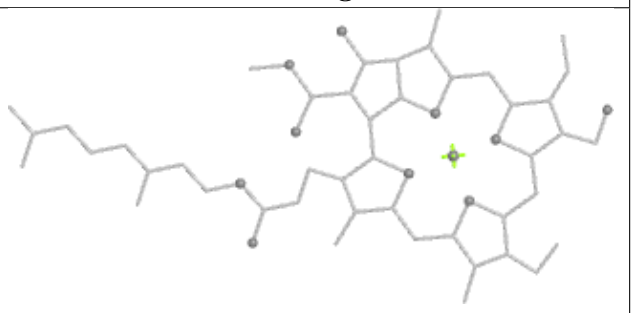
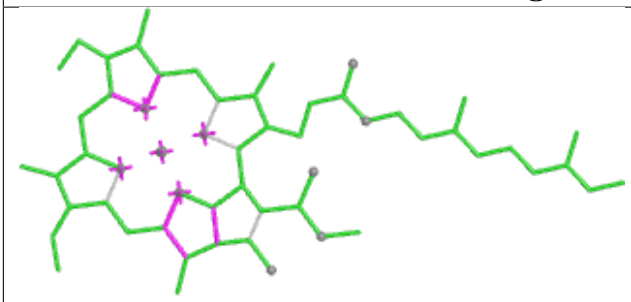


Rings

Ligand CLA h 212



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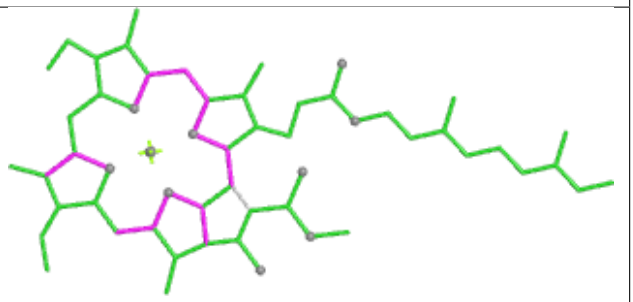
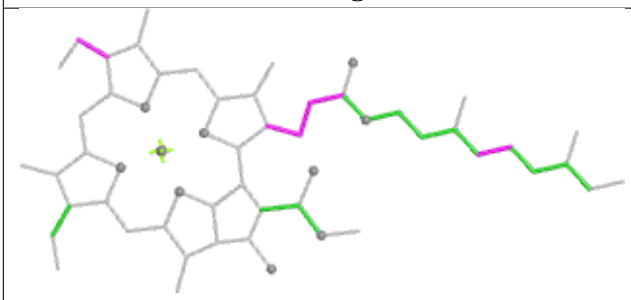


Bond angles



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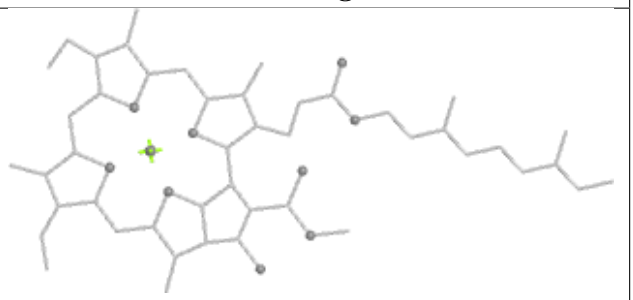
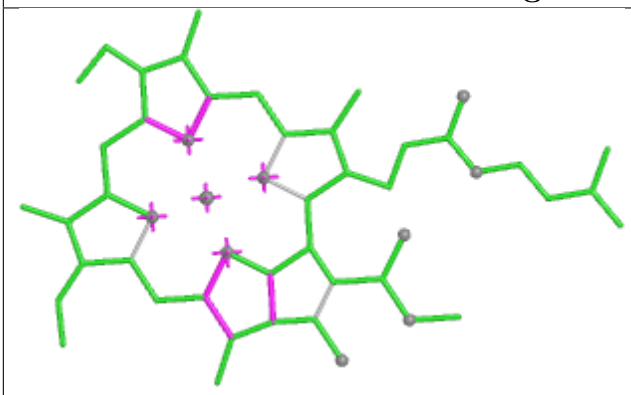


Rings

Ligand CLA A 808



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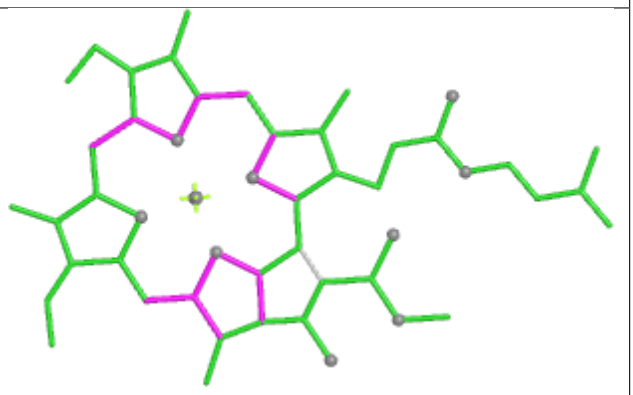
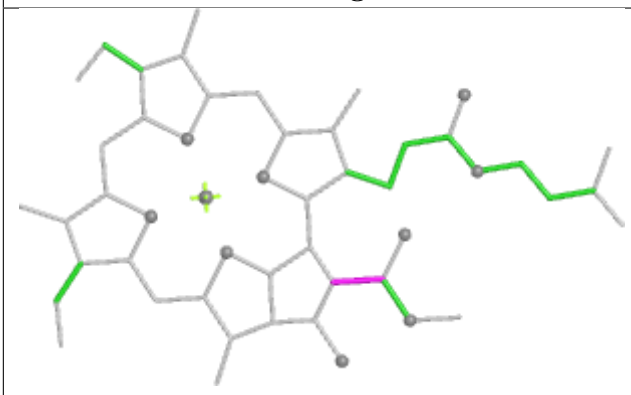


Bond angles



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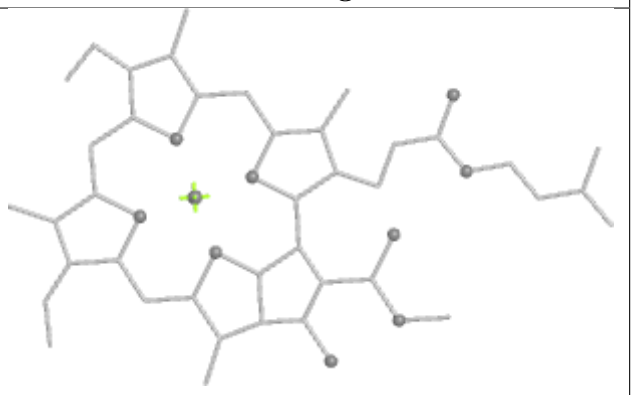
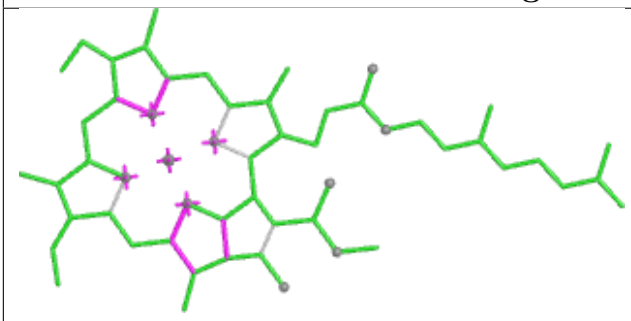


Rings

Ligand CLA m 310



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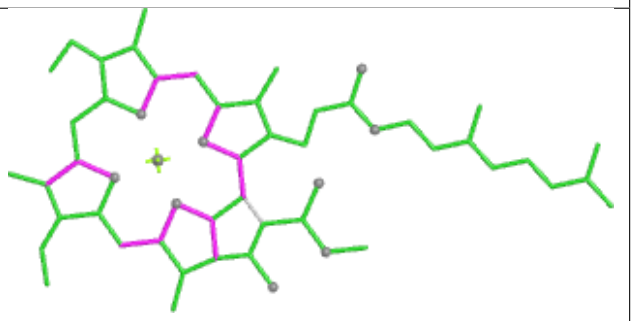
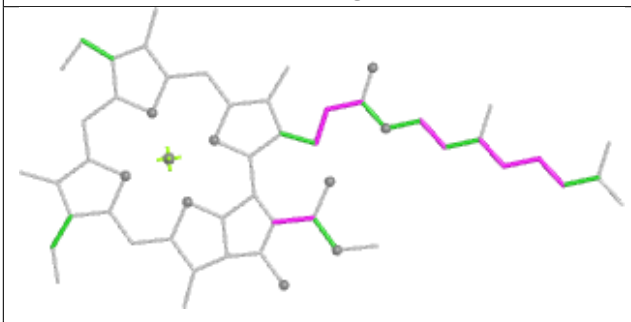


Bond angles



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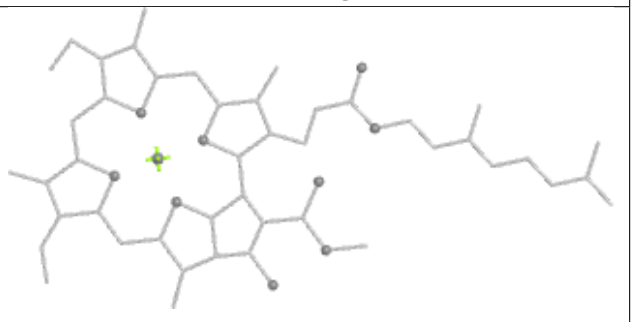
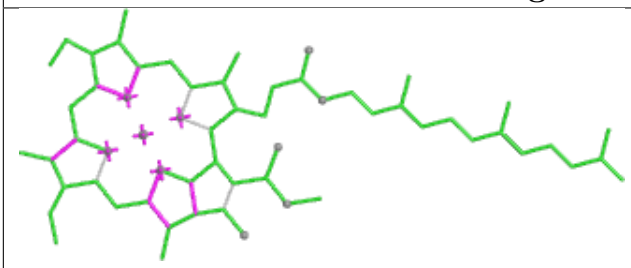
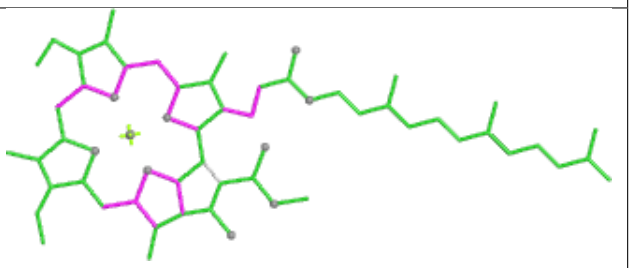
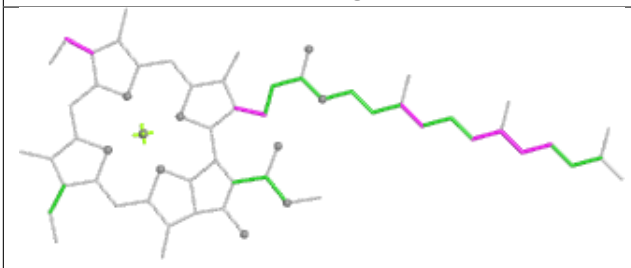
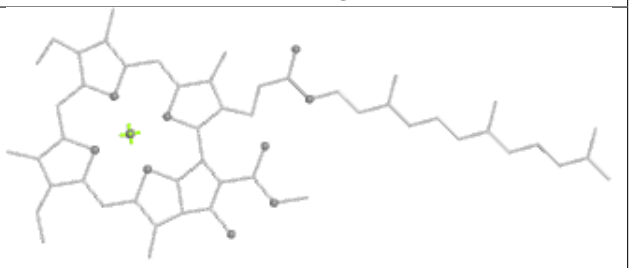
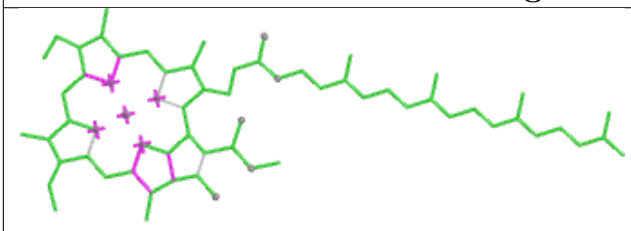
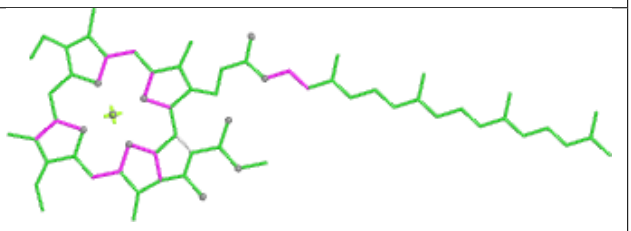
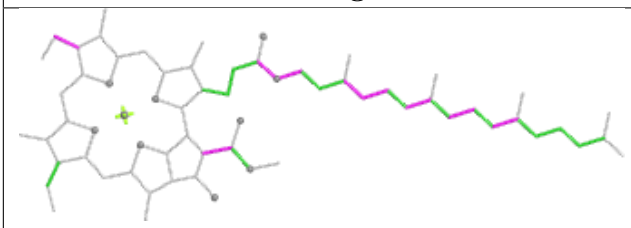
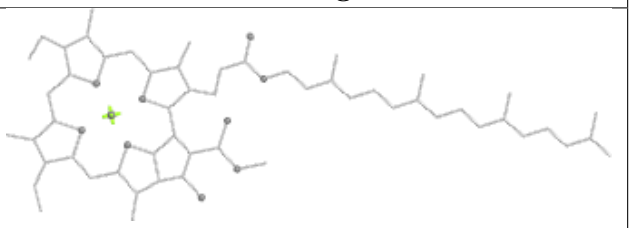
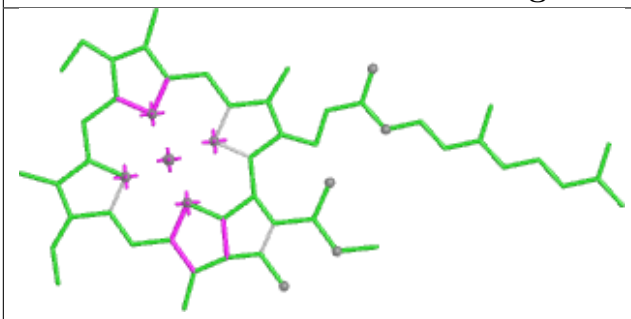


Rings

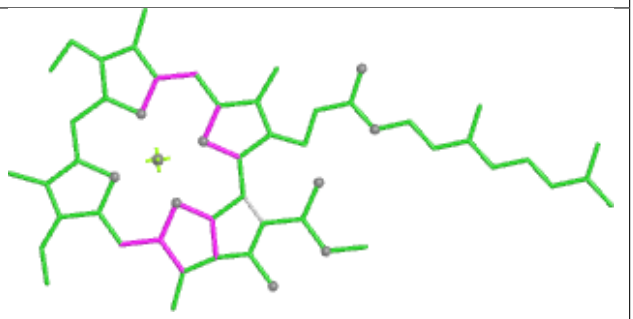
Ligand CLA a 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

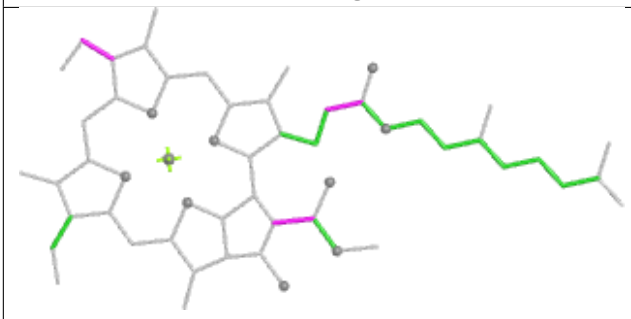
Ligand CLA e 302



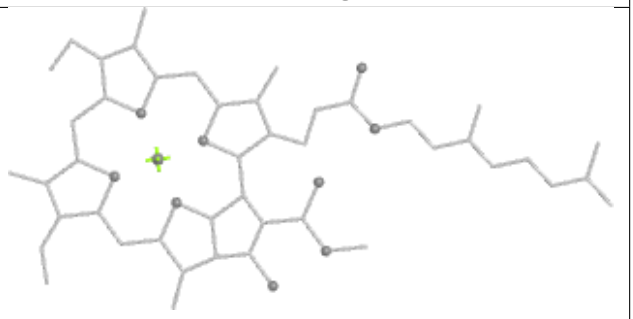
Bond lengths



Bond angles

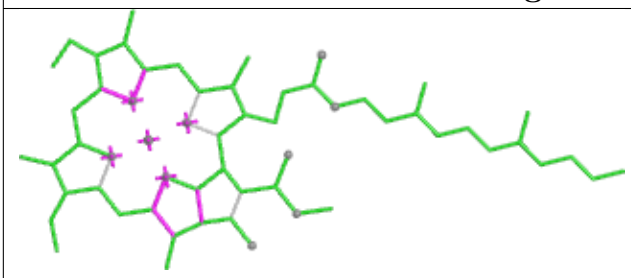


Torsions

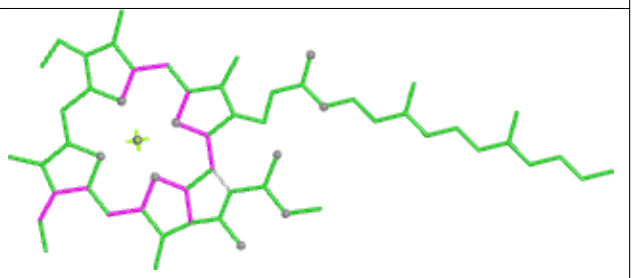


Rings

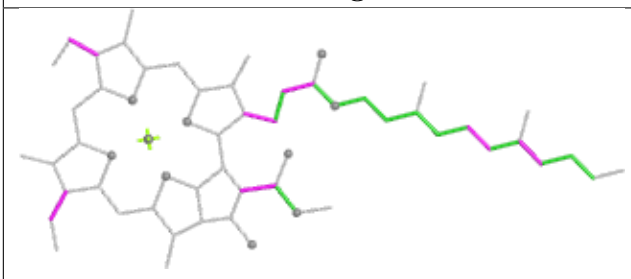
Ligand CLA B 811



Bond lengths



Bond angles



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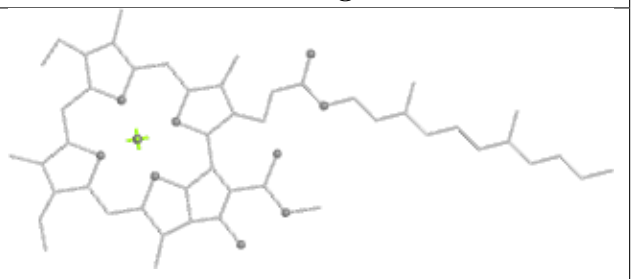
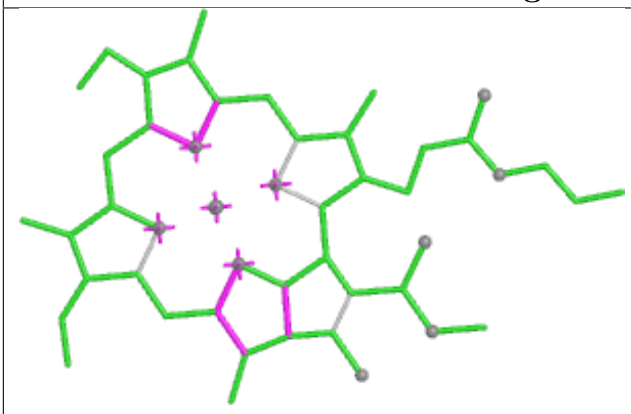
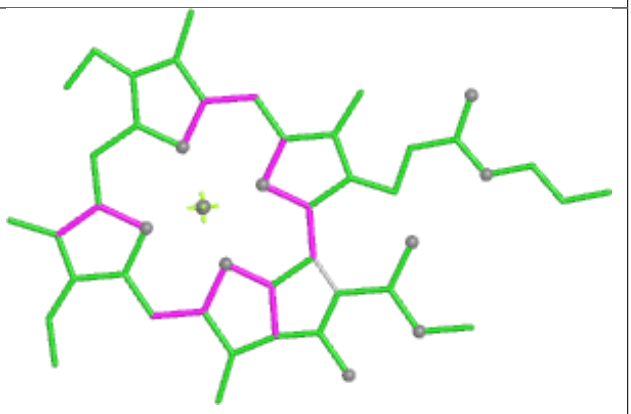


Rings

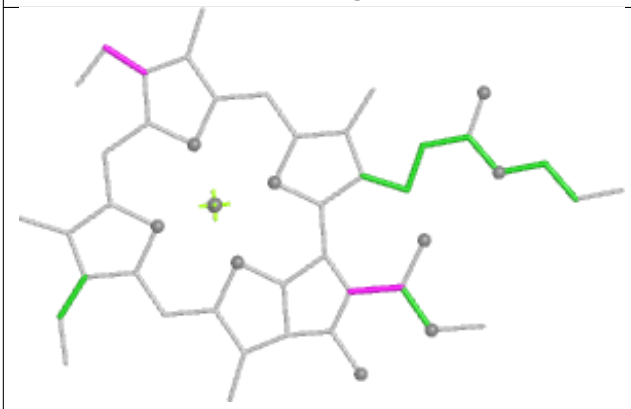
Ligand CLA A 839



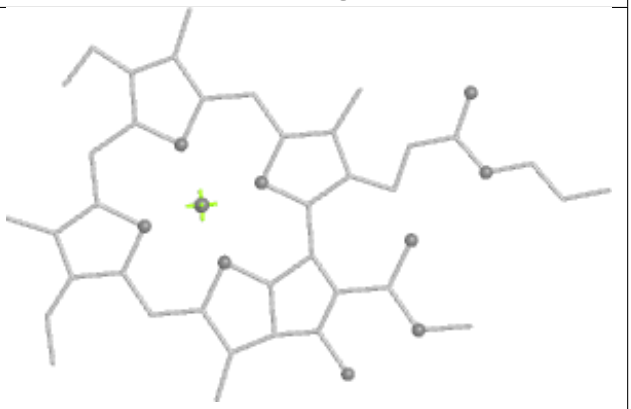
Bond lengths



Bond angles

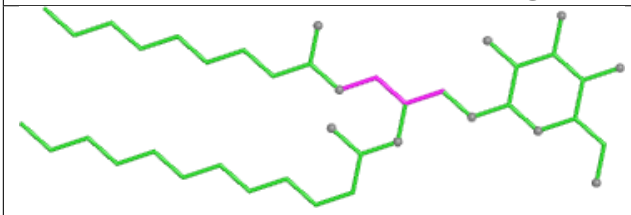


Torsions



Rings

Ligand LMG a 301



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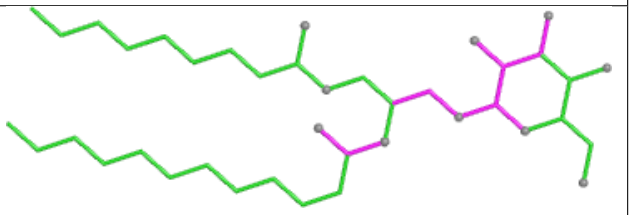
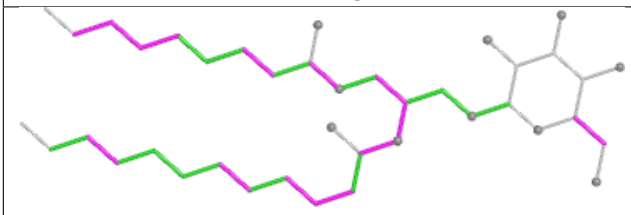


Bond angles



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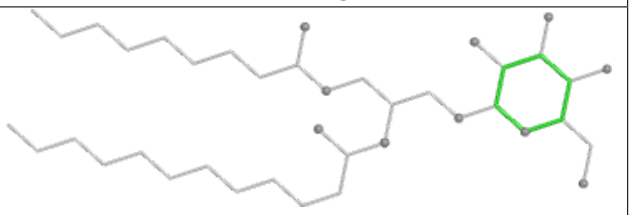
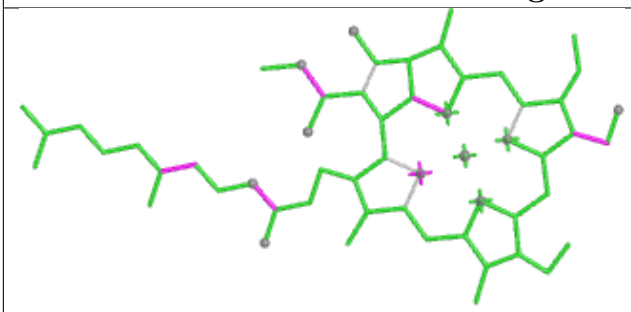


Rings

Ligand CHL g 303



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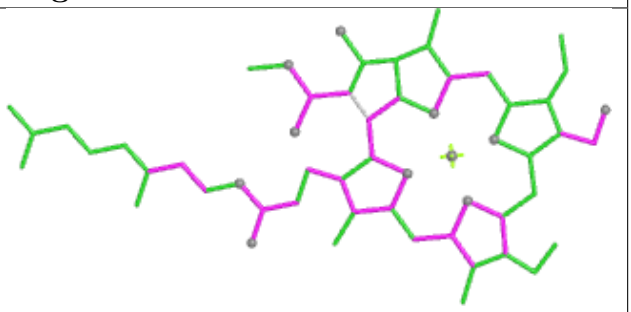
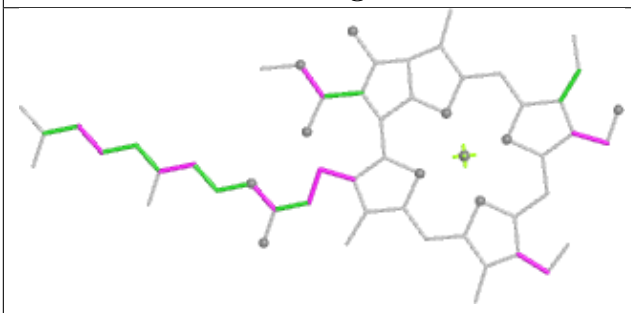


Bond angles



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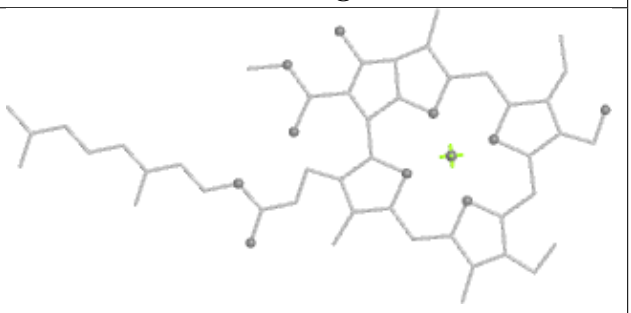
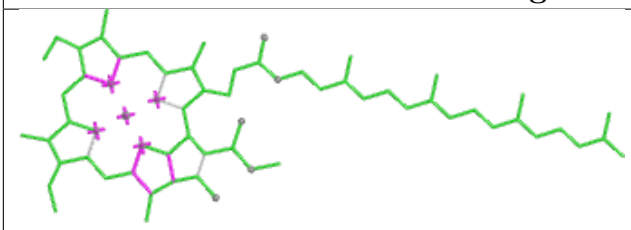


Rings

Ligand CLA c 316



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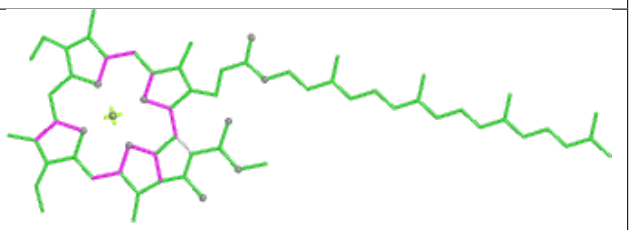
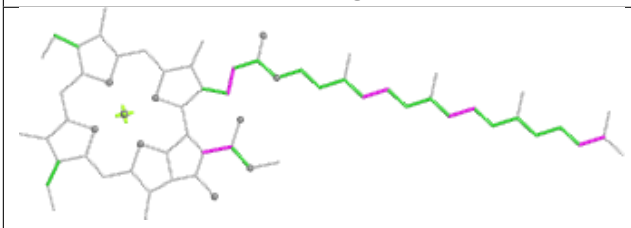


Bond angles



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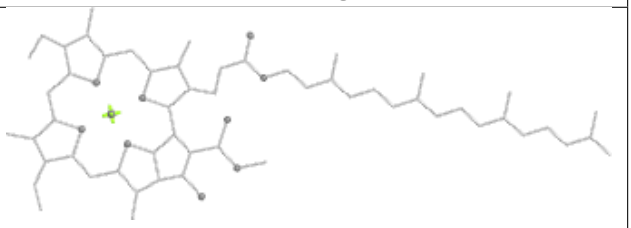
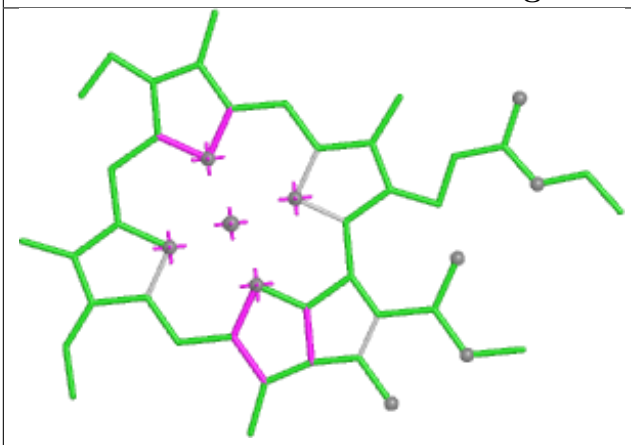


Rings

Ligand CLA A 846



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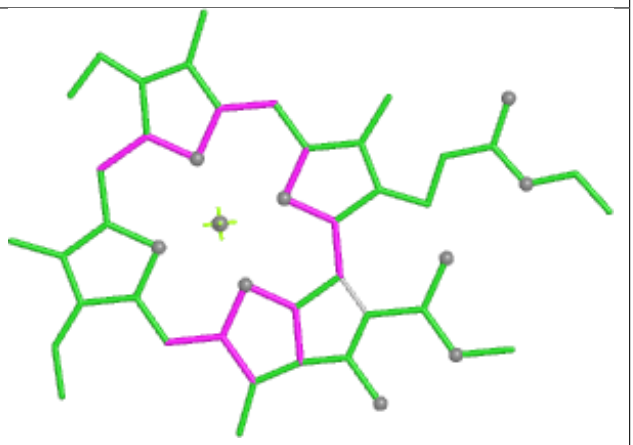
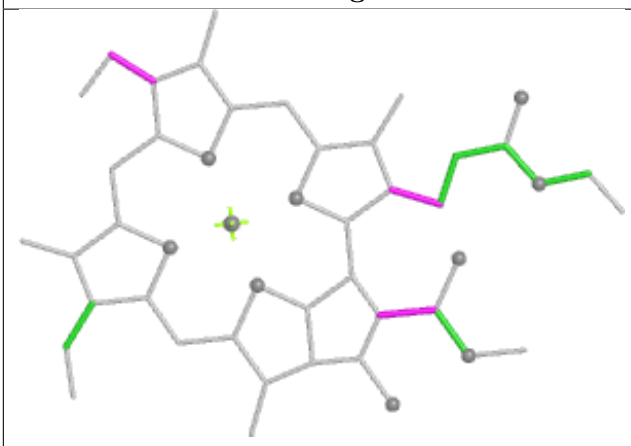


Bond angles



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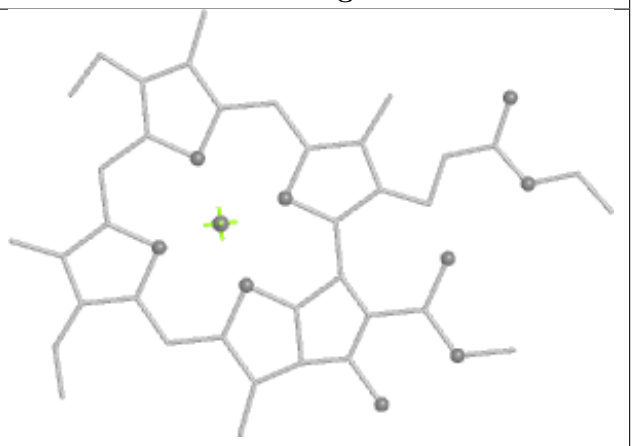
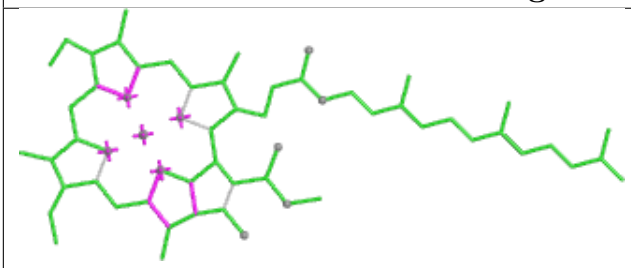


Rings

Ligand CLA o 307



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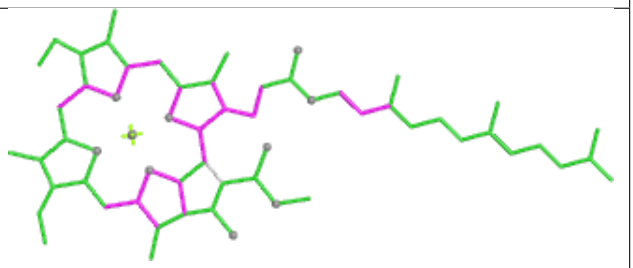
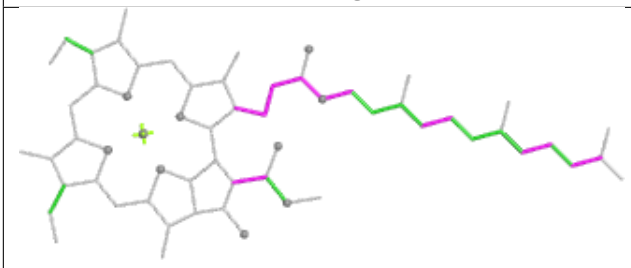


Bond angles



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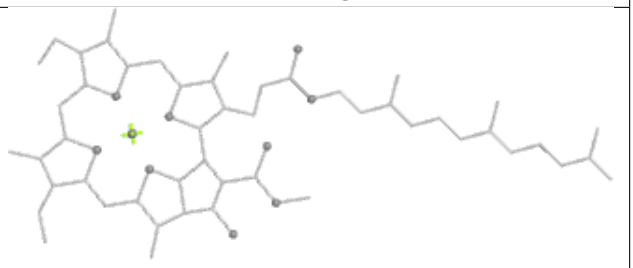
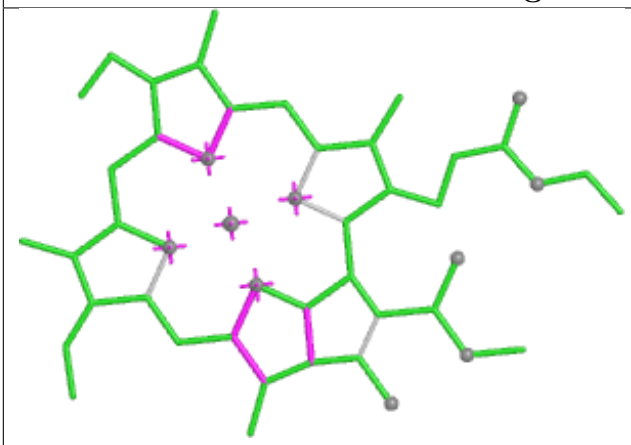


Rings

Ligand CLA B 844



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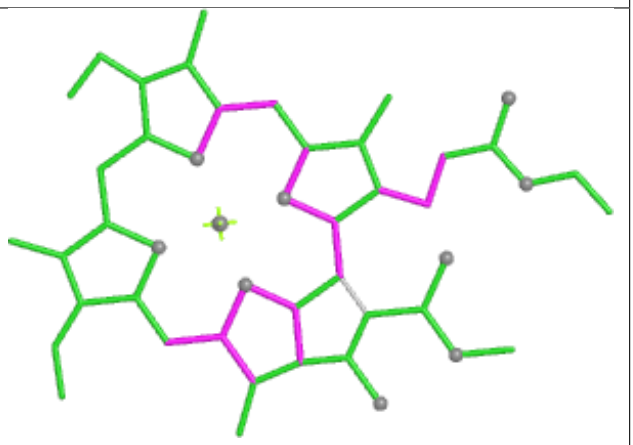
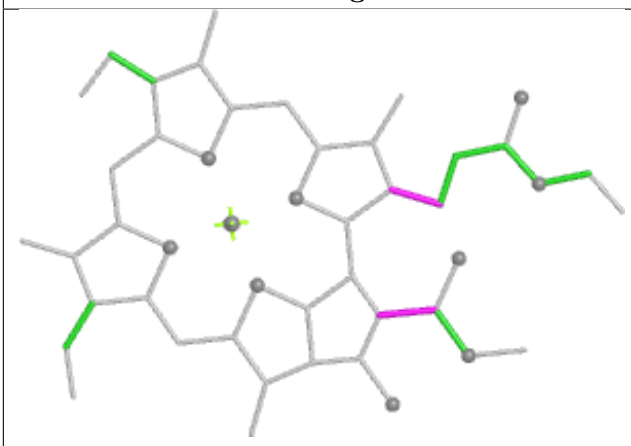


Bond angles



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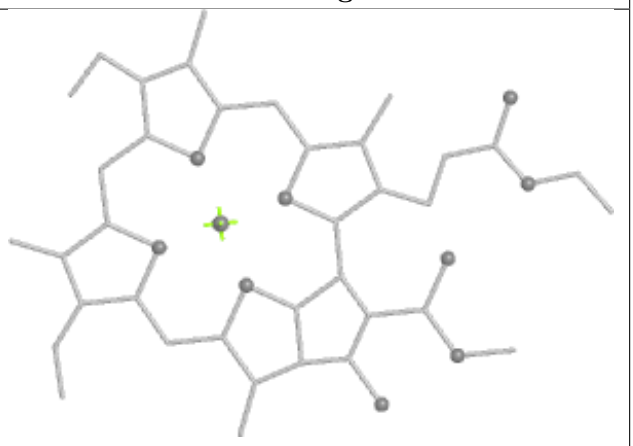
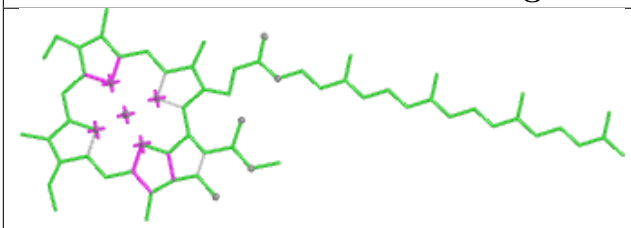


Rings

Ligand CLA A 828



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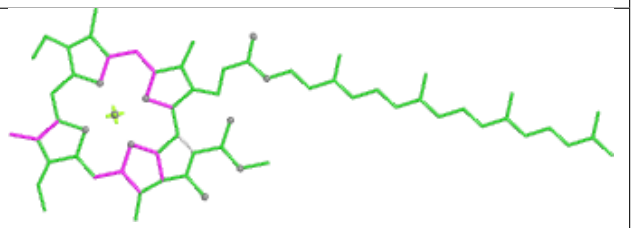
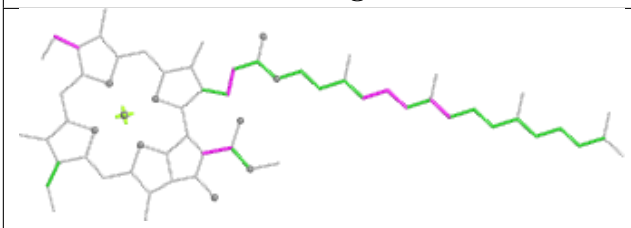


Bond angles



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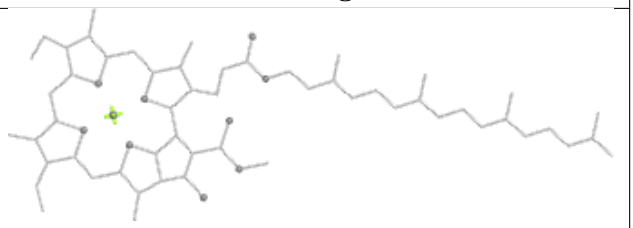
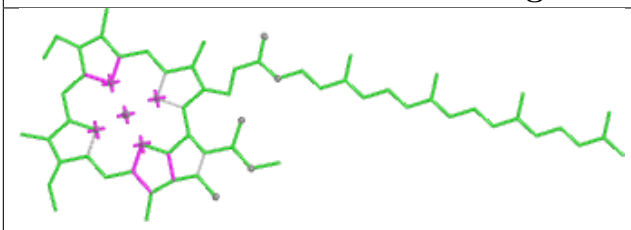
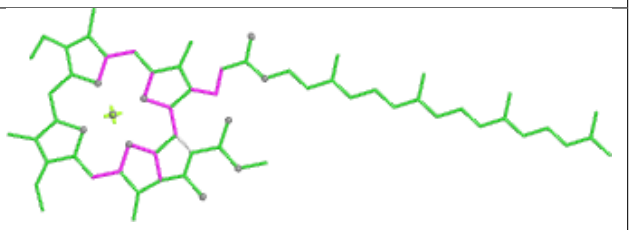
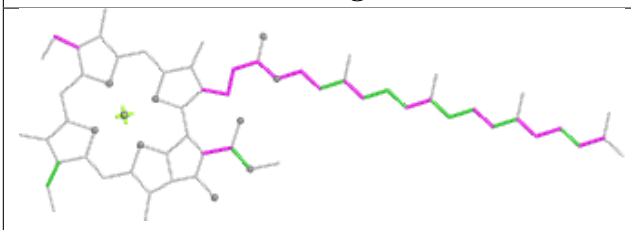
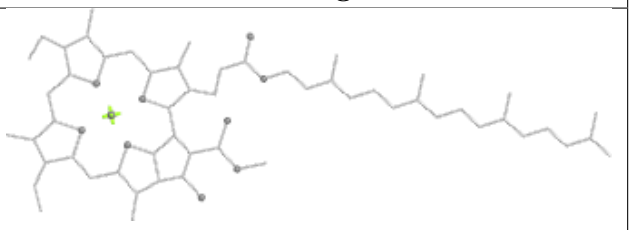
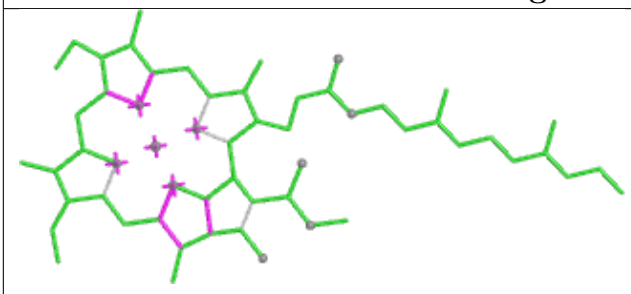
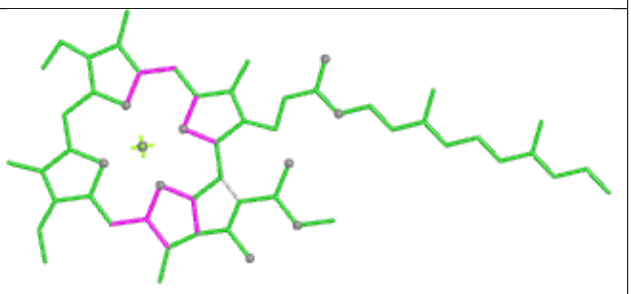
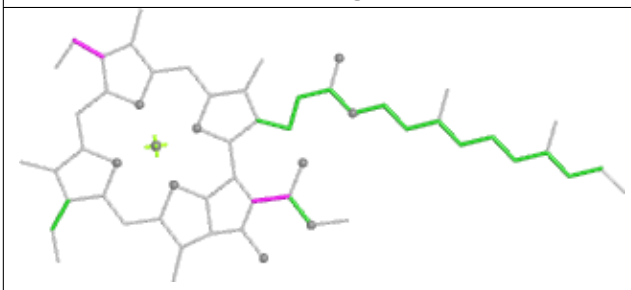
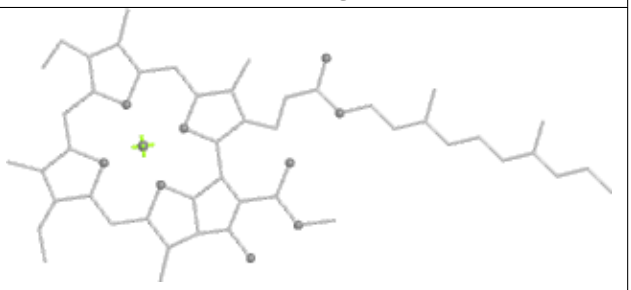
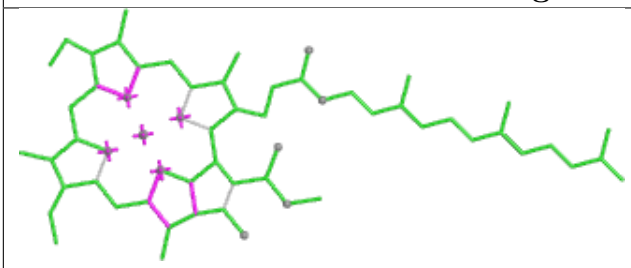
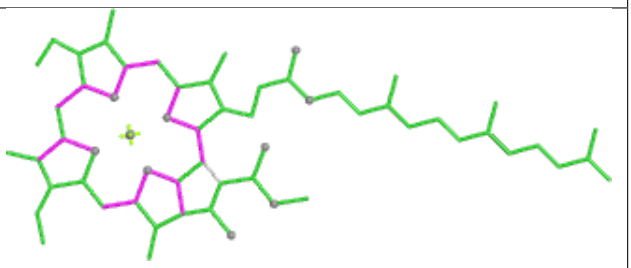
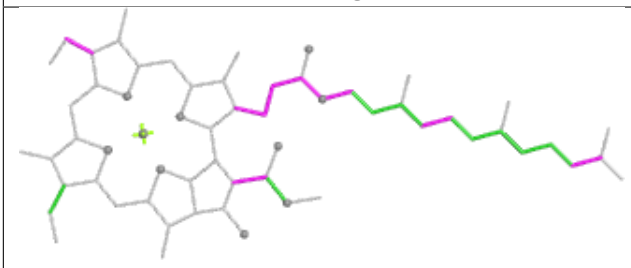
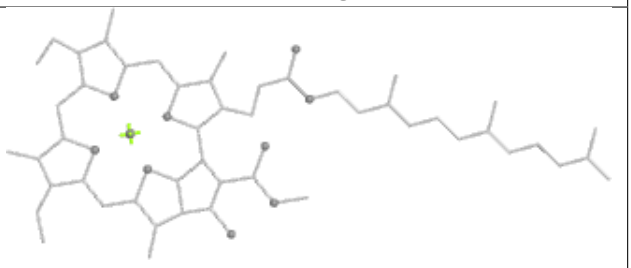
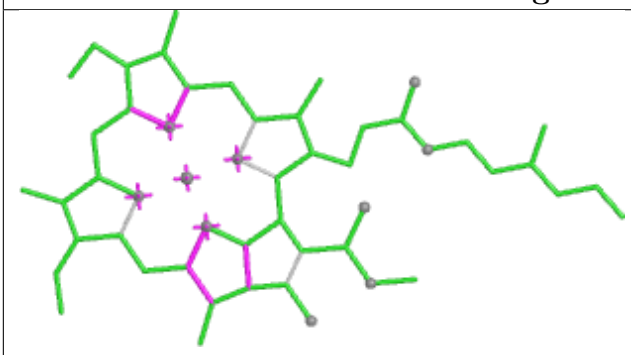
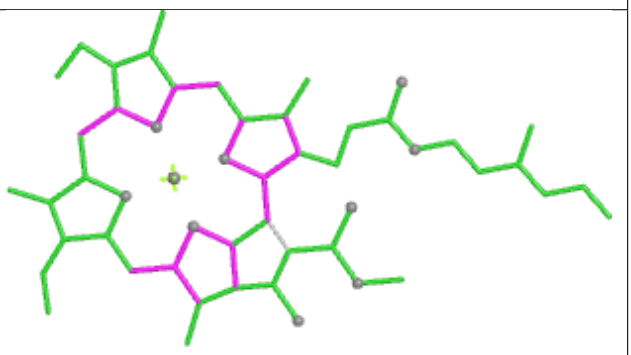
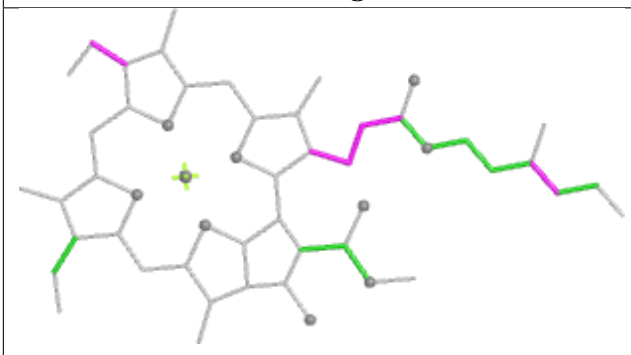
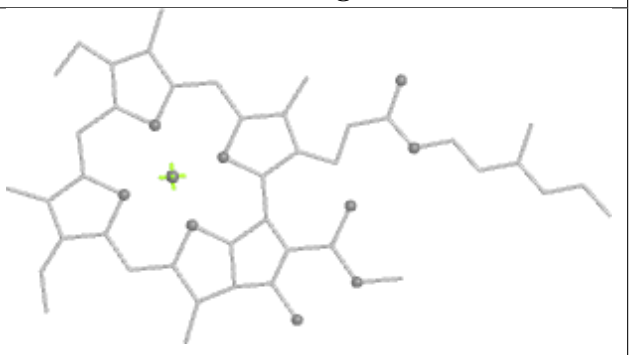


Rings

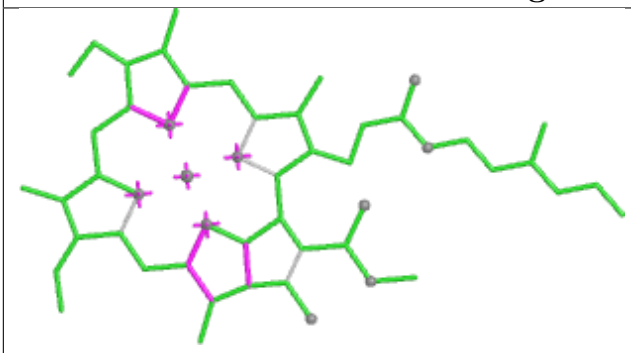
Ligand CLA F 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

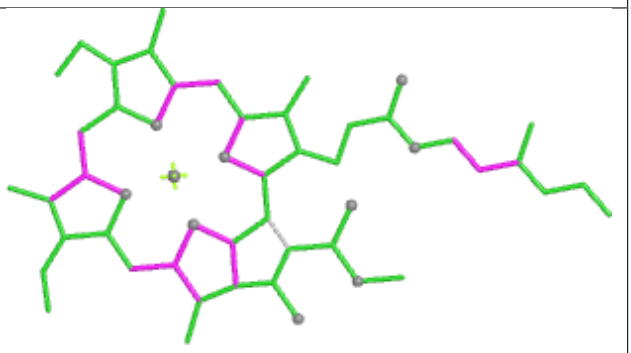
Ligand CLA i 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA i 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

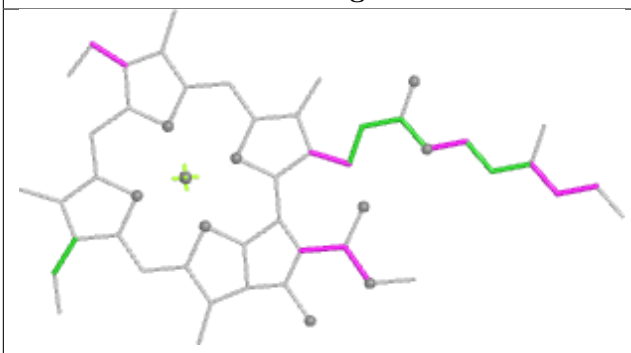
Ligand CLA a 306



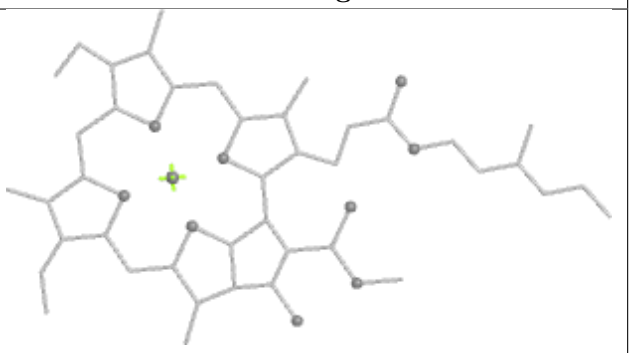
Bond lengths



Bond angles

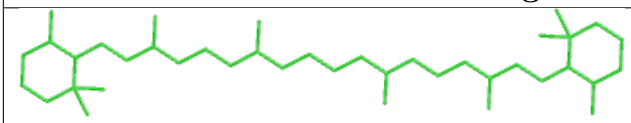


Torsions

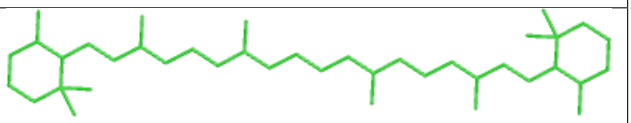


Rings

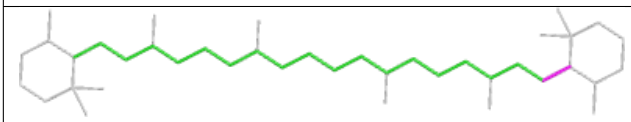
Ligand BCR A 836



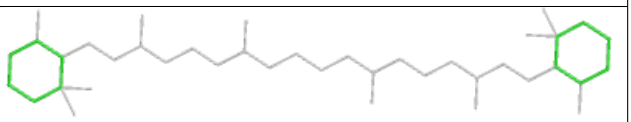
Bond lengths



Bond angles

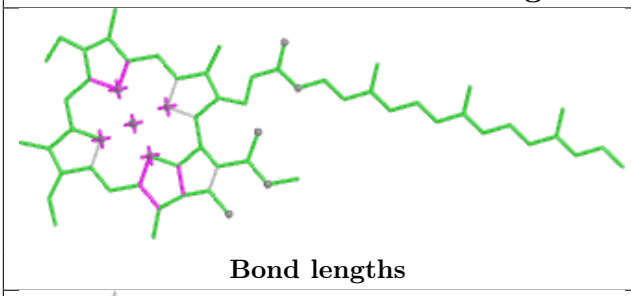


Torsions

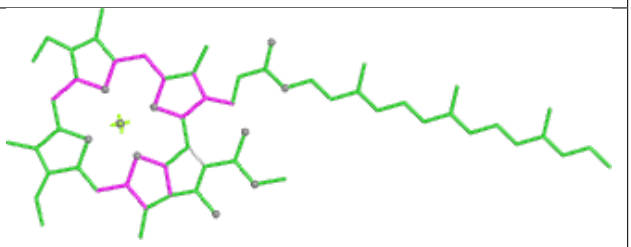


Rings

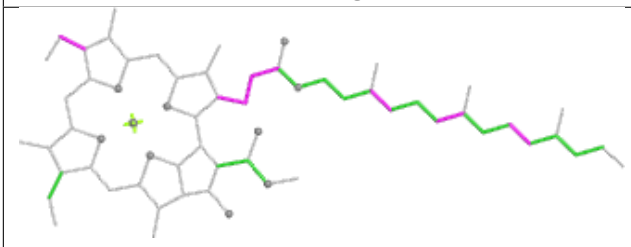
Ligand CLA B 817



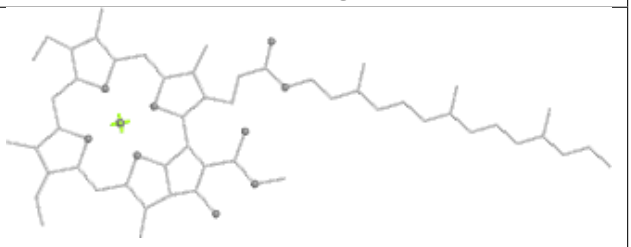
Bond lengths



Bond angles

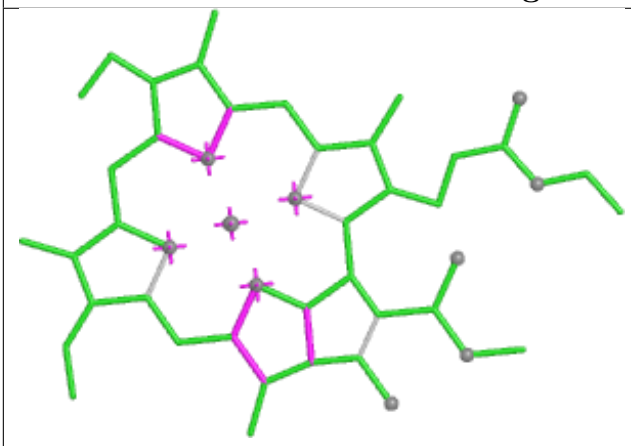


Torsions



Rings

Ligand CLA m 304



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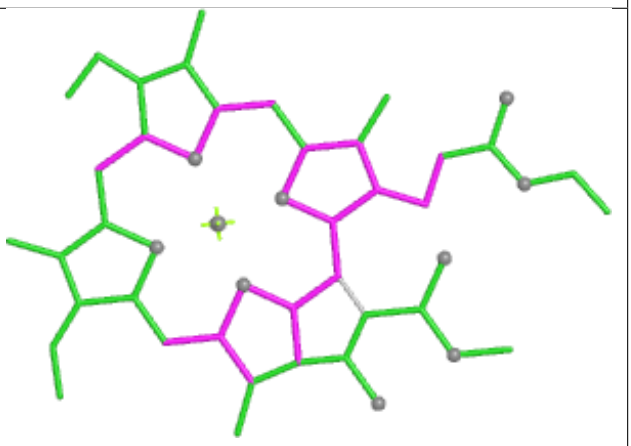

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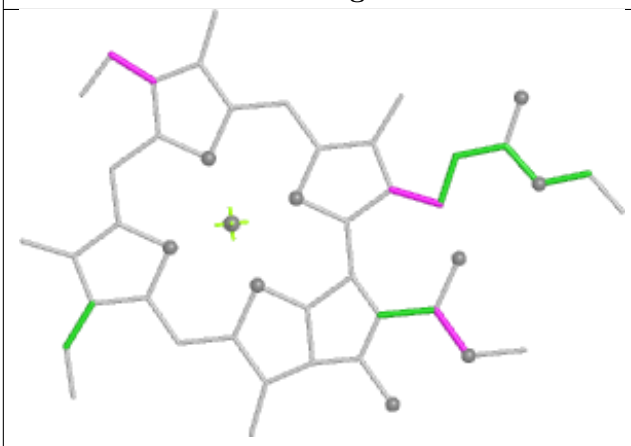
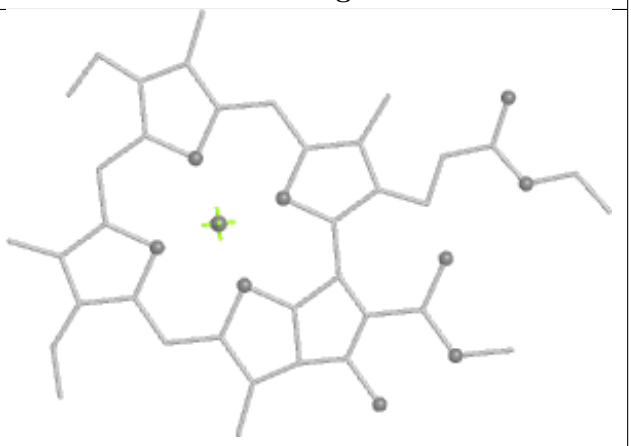
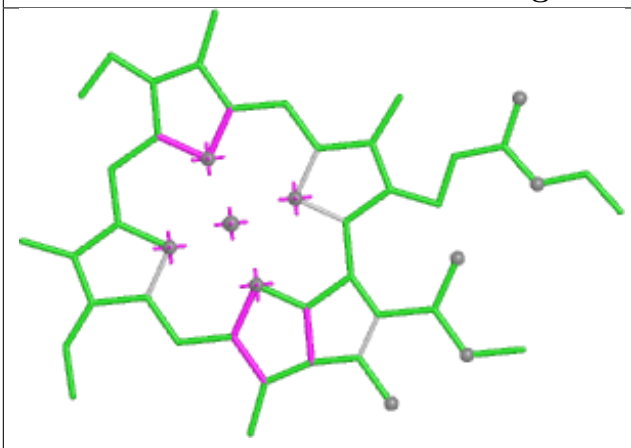


Torsions



Rings

Ligand CLA j 312



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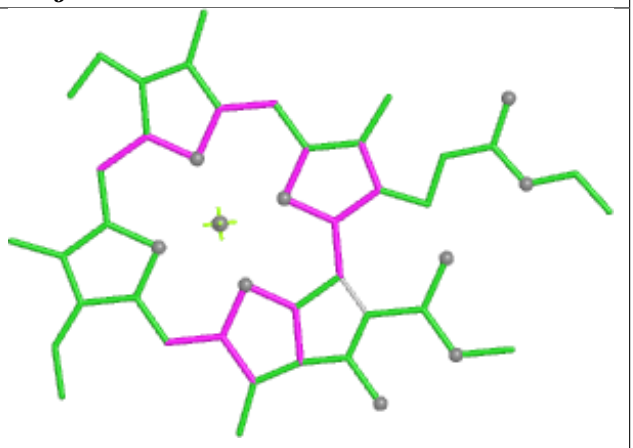

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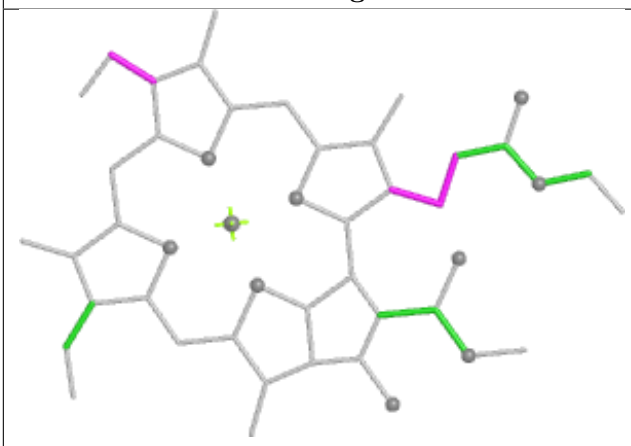

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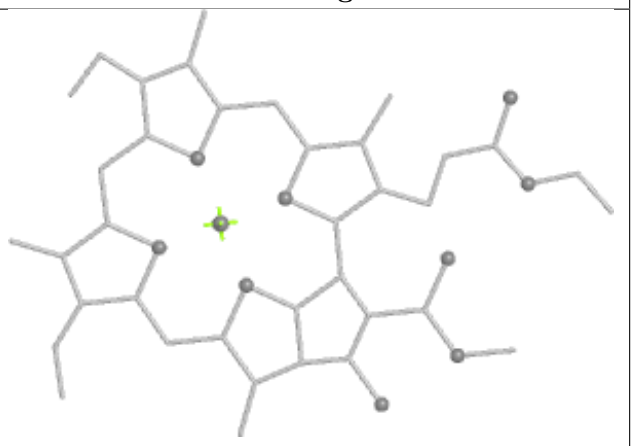
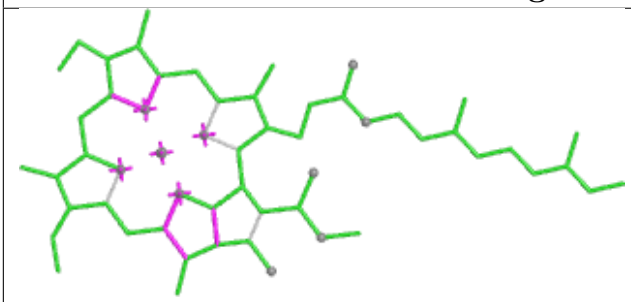


Rings

Ligand CLA g 308



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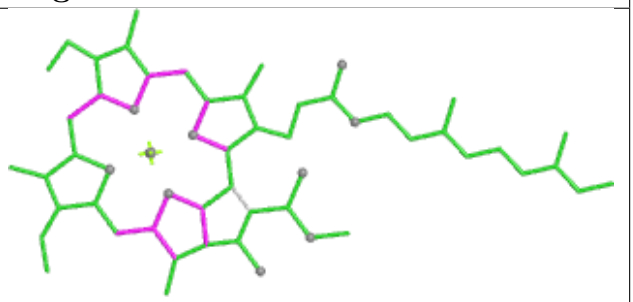

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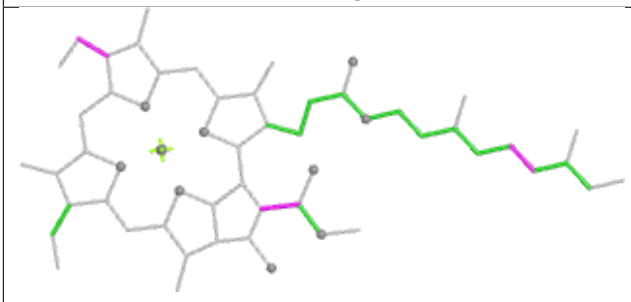

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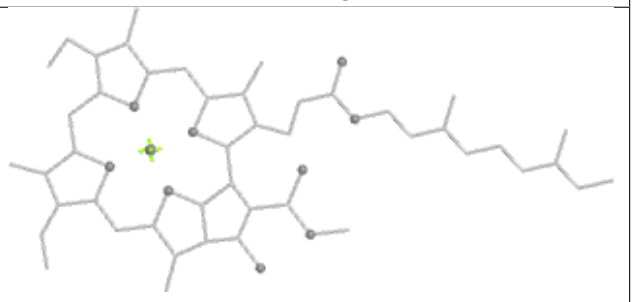
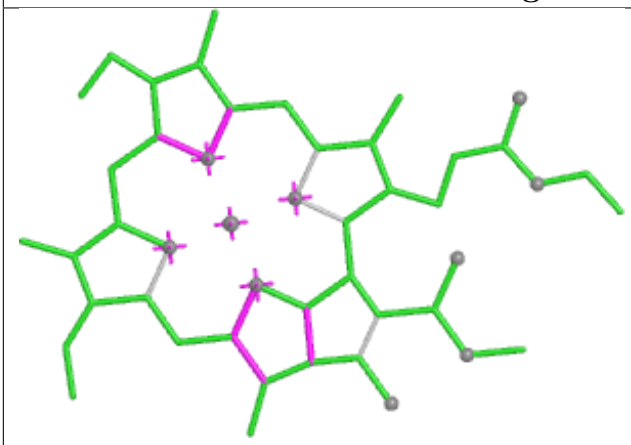


Rings

Ligand CLA m 309



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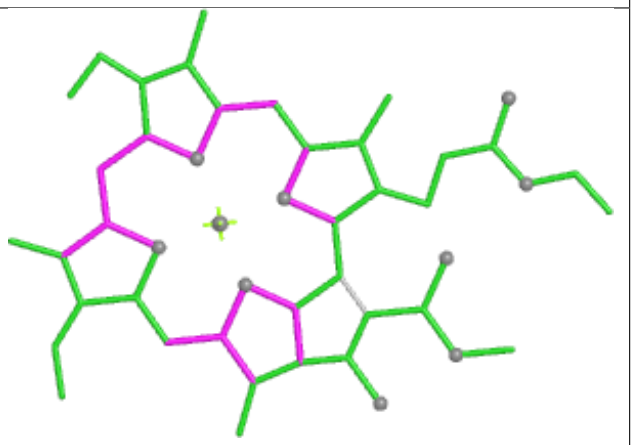

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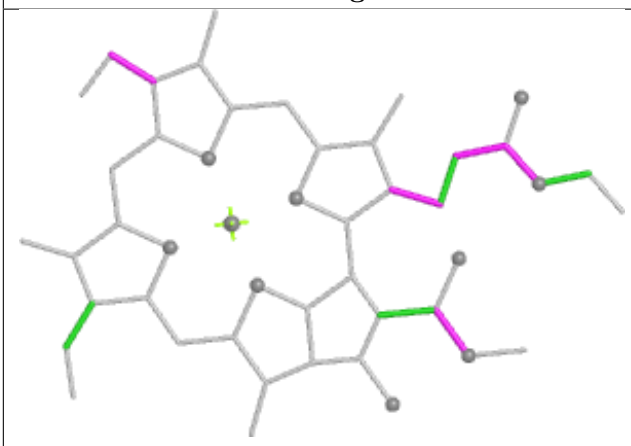

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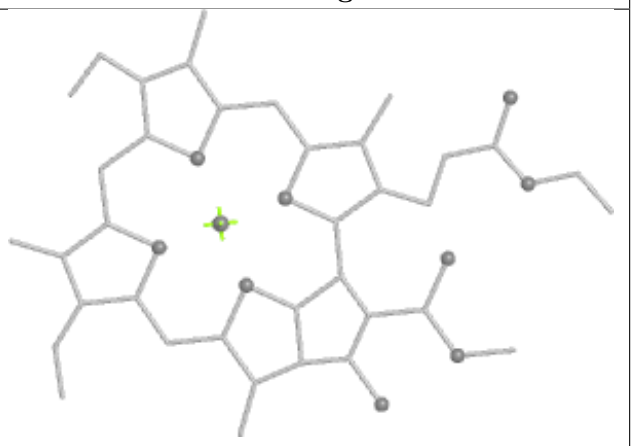
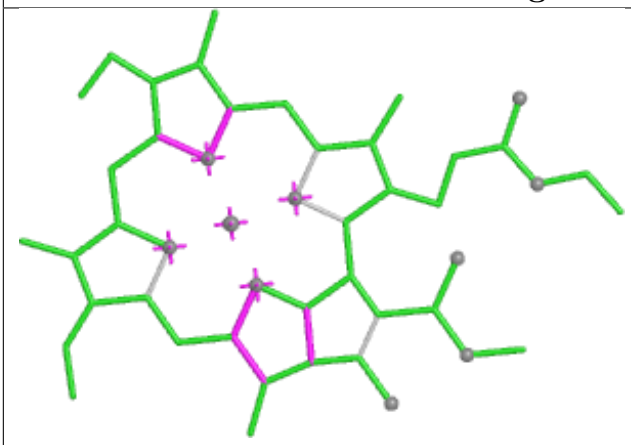


Rings

Ligand CLA o 312



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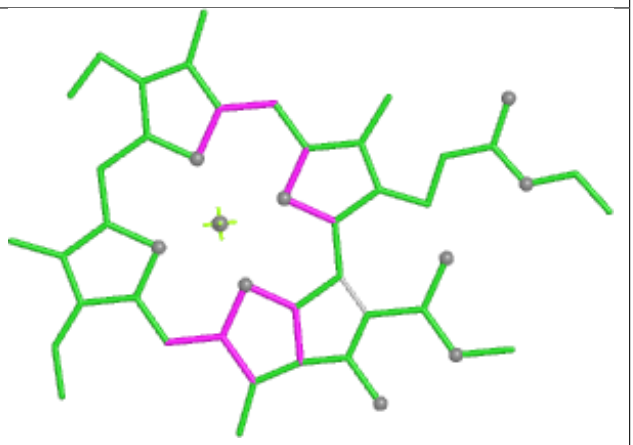

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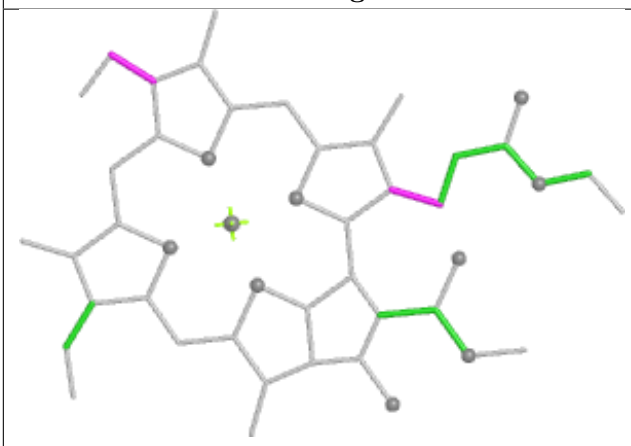

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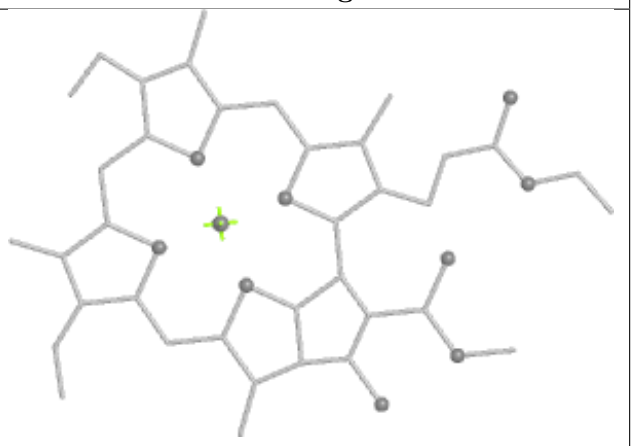
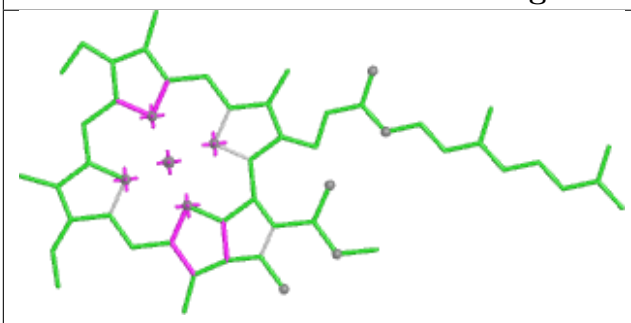


Rings

Ligand CLA e 310



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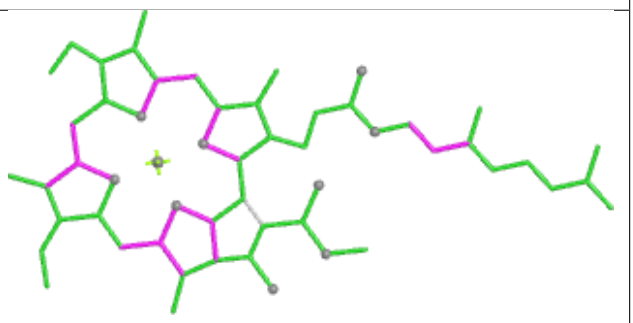

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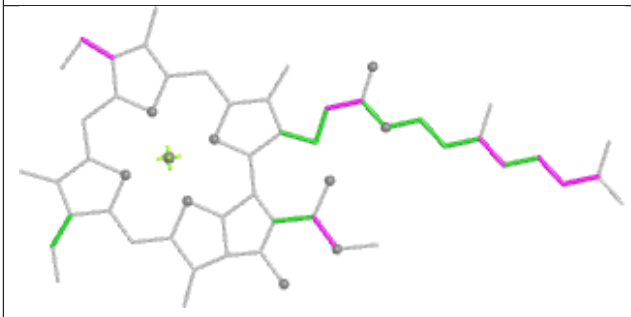

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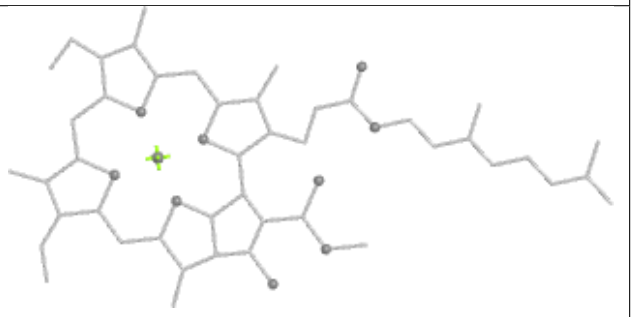
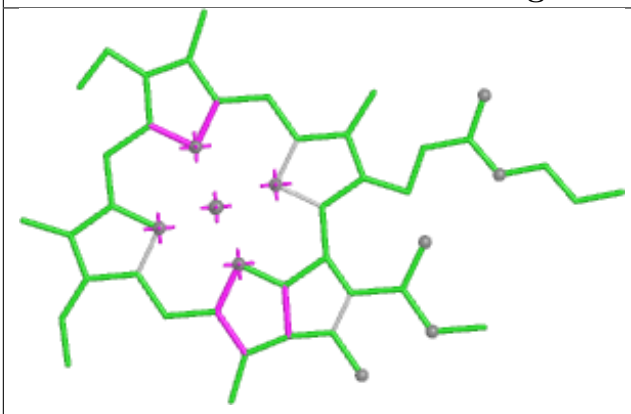


Rings

Ligand CLA h 204



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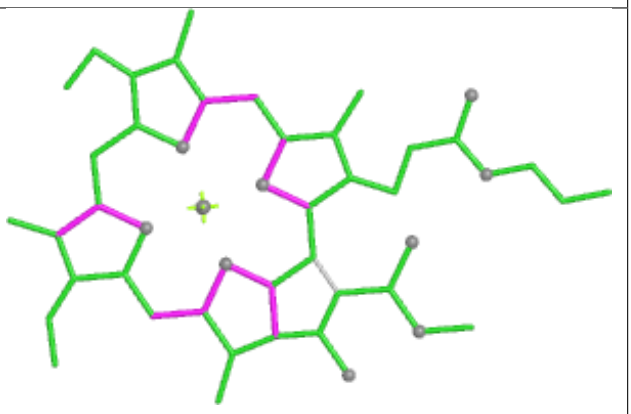

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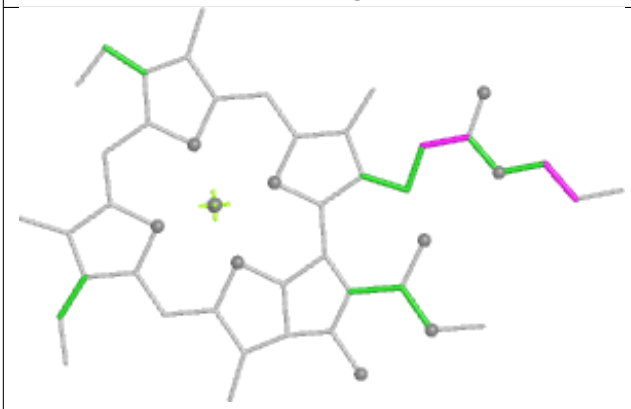

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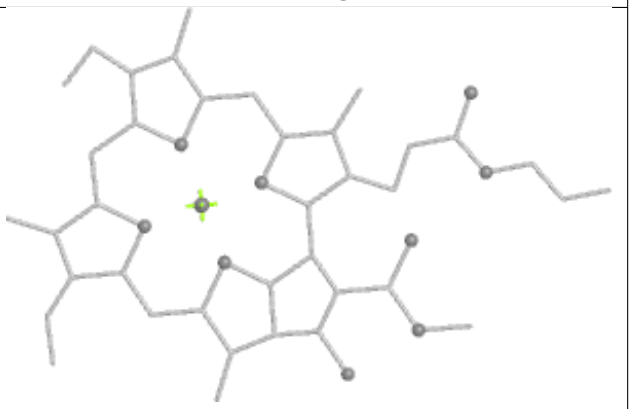
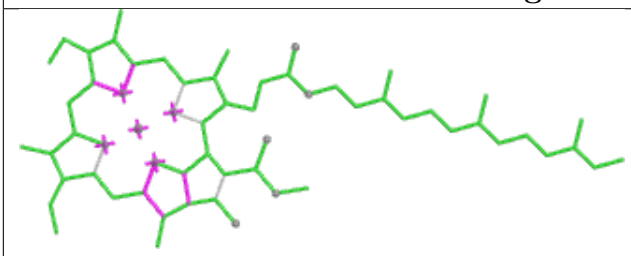


Rings

Ligand CLA B 820



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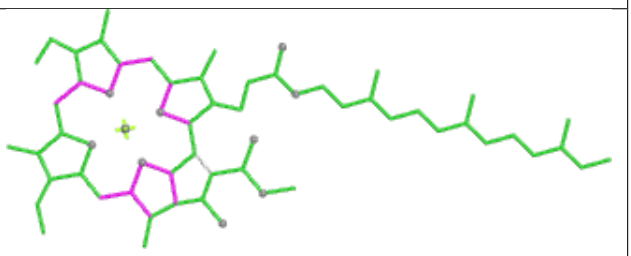

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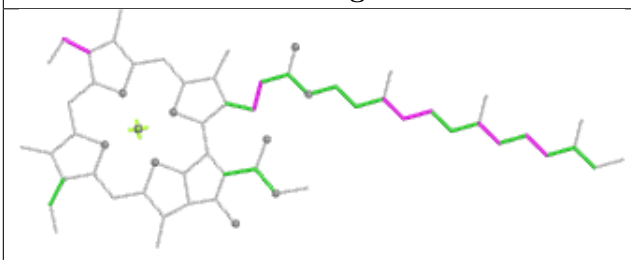

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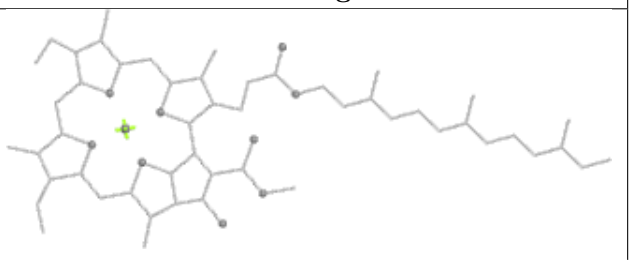
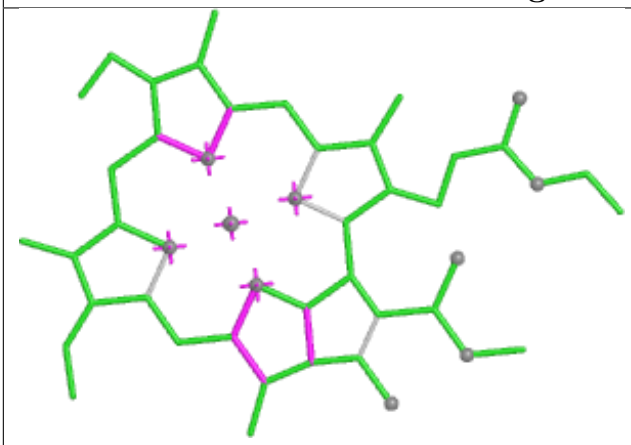


Rings

Ligand CLA o 306



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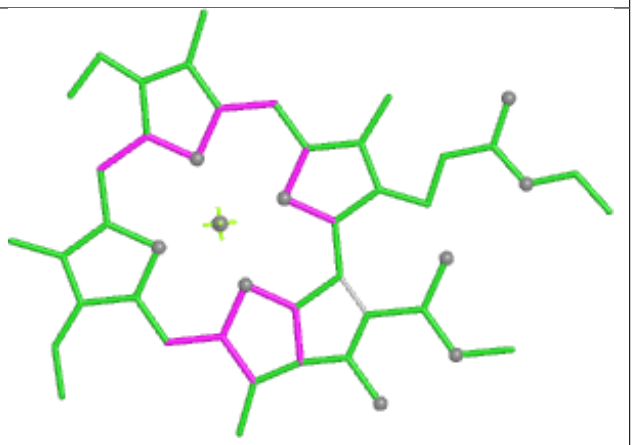
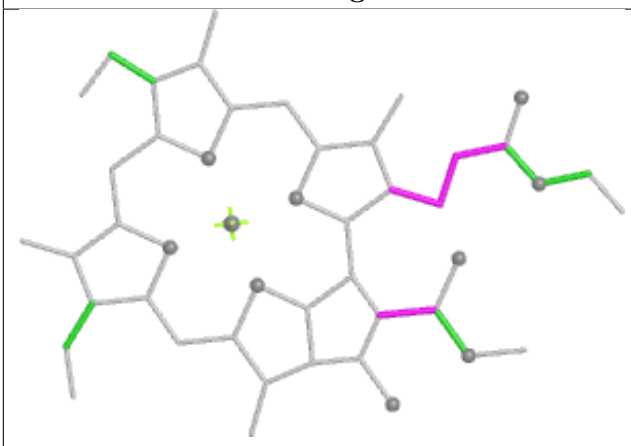


Bond angles



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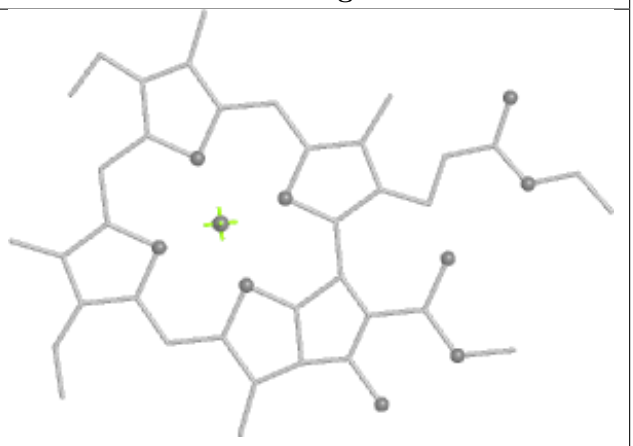


Rings

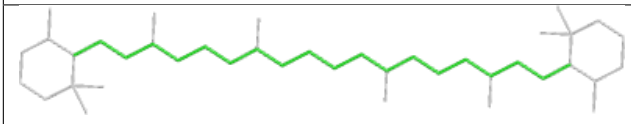
Ligand BCR J 804



Bond lengths



Bond angles



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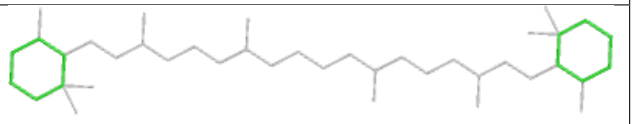
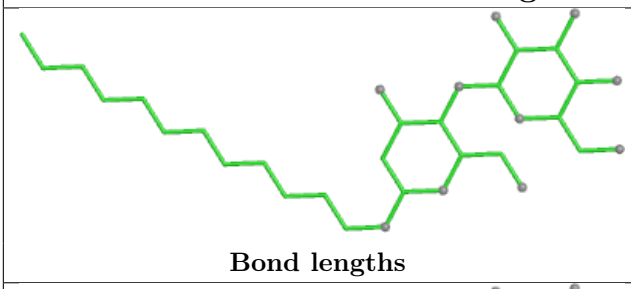


Rings

Ligand LMU A 838



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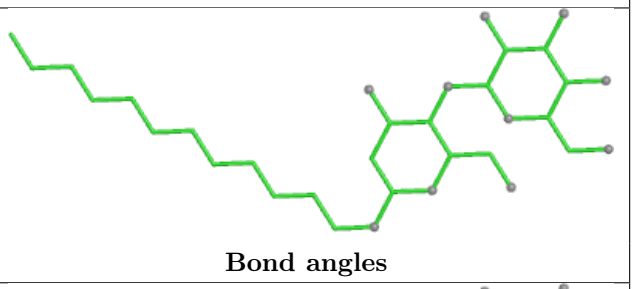
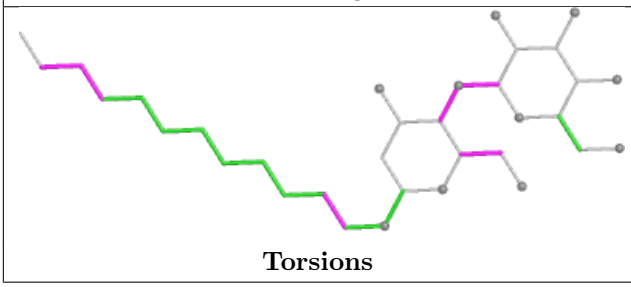


Bond angles



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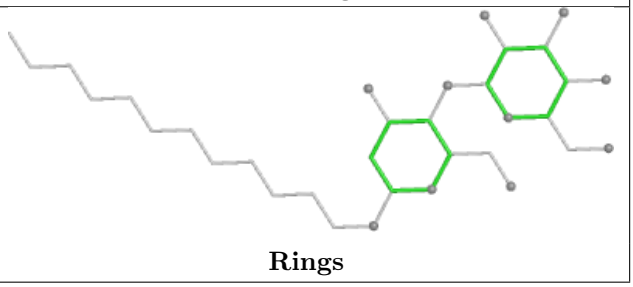
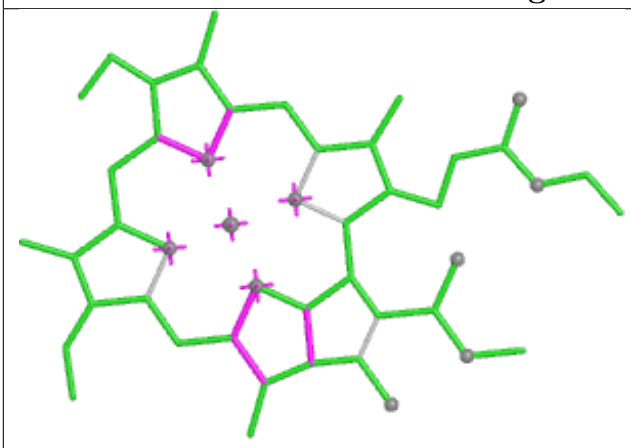


Rings

Ligand CLA o 305



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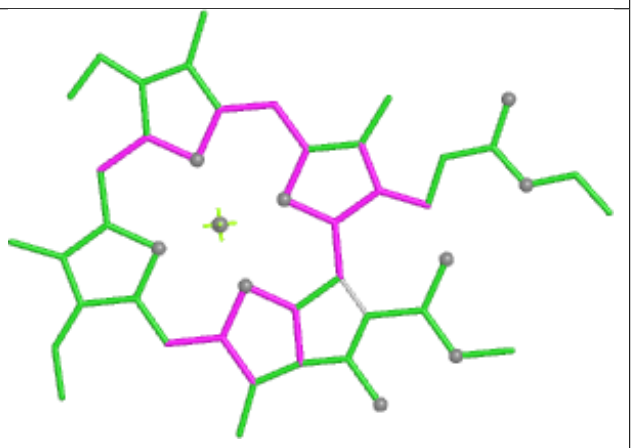

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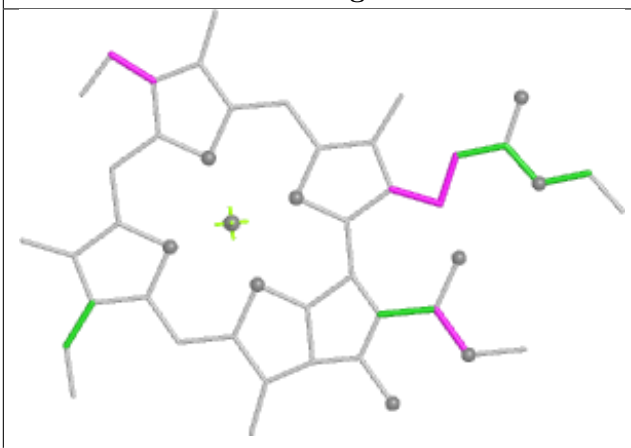

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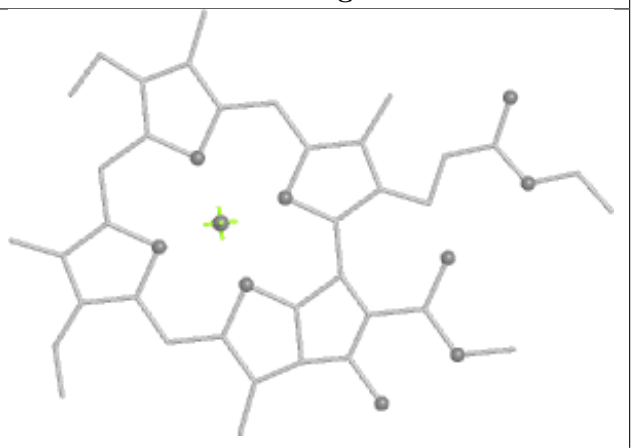
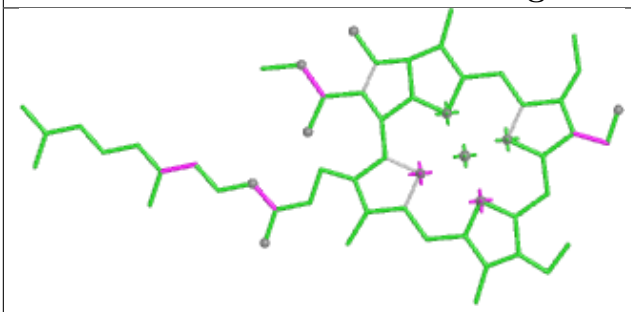


Rings

Ligand CHL g 306



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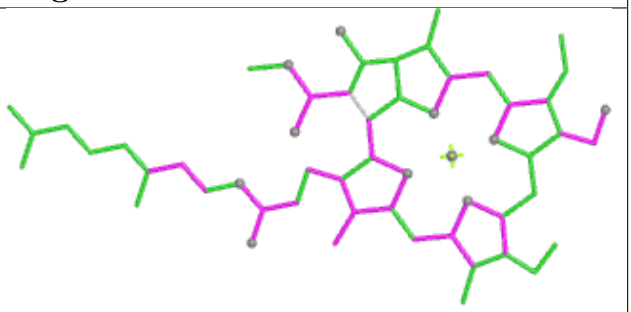
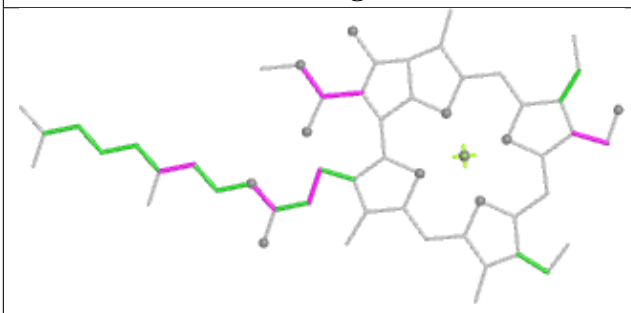


Bond angles



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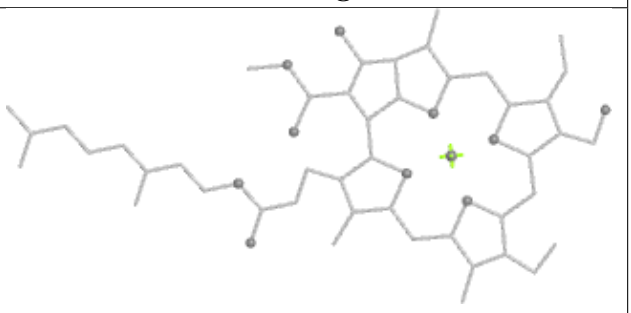
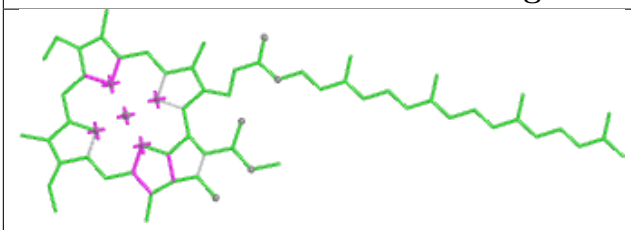


Rings

Ligand CLA A 842



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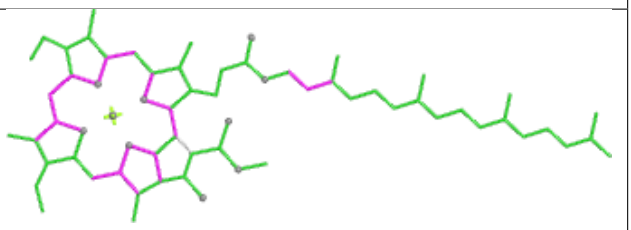
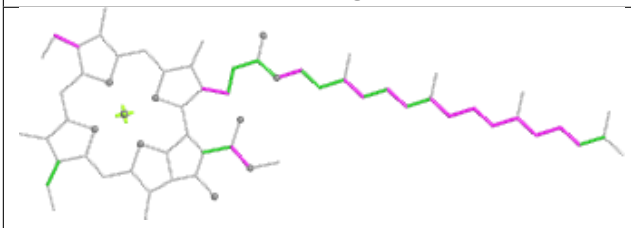


Bond angles



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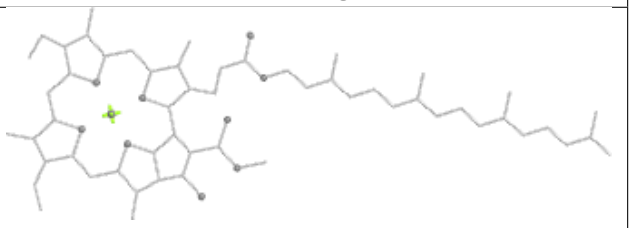
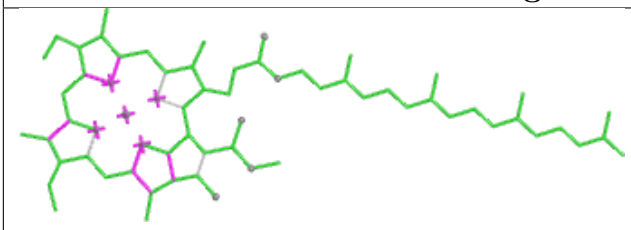
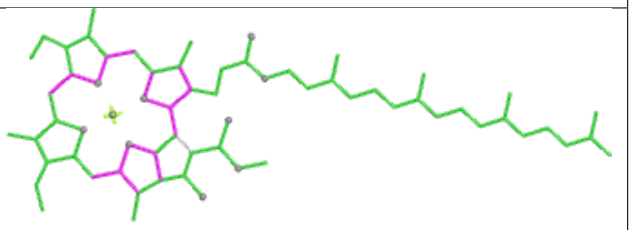
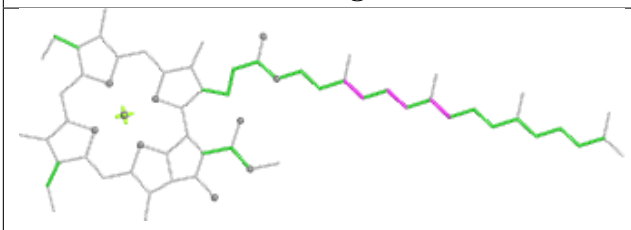
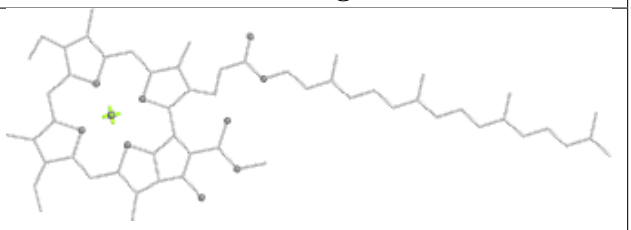
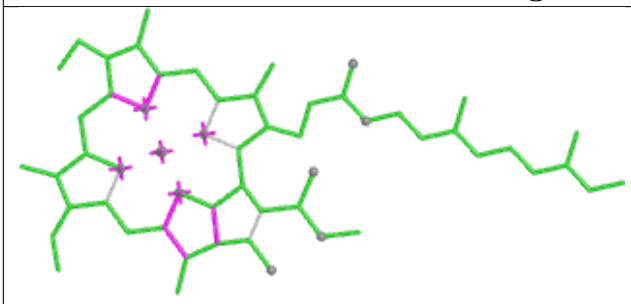
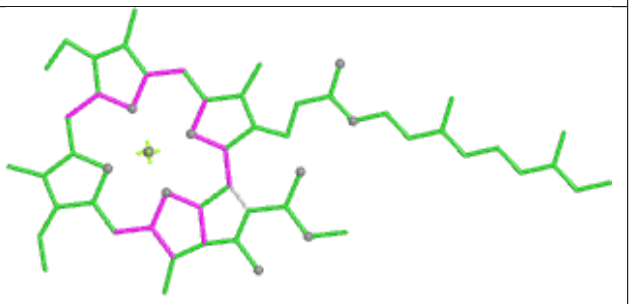
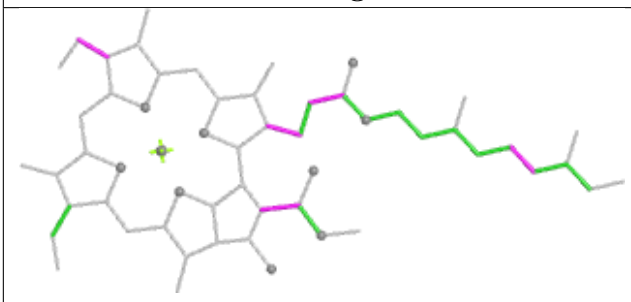
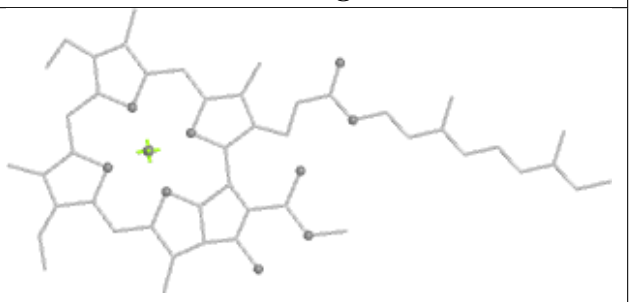


Rings

Ligand CLA A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

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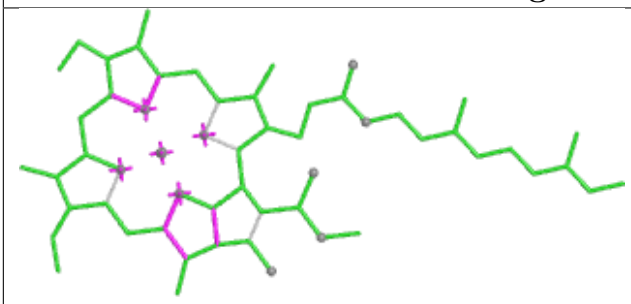	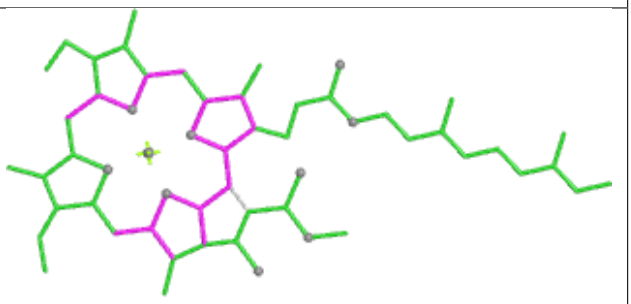
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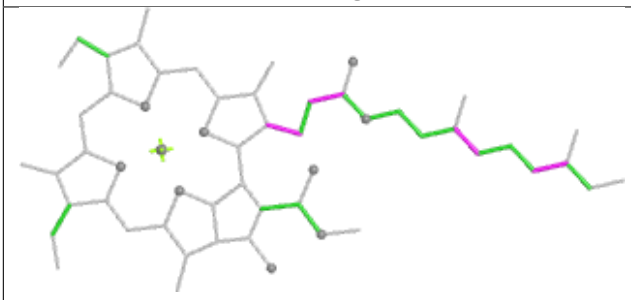	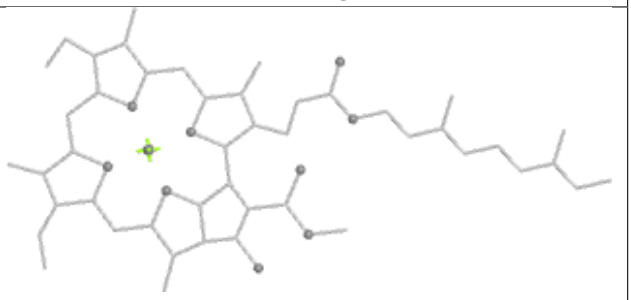
Torsions	Rings

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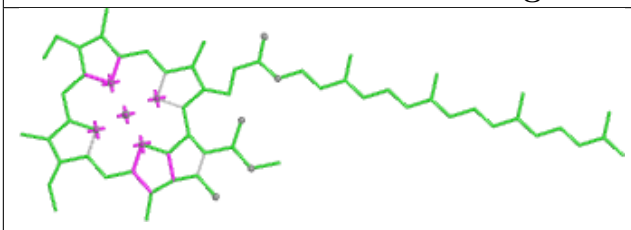	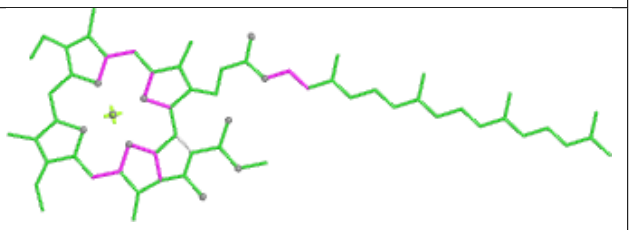
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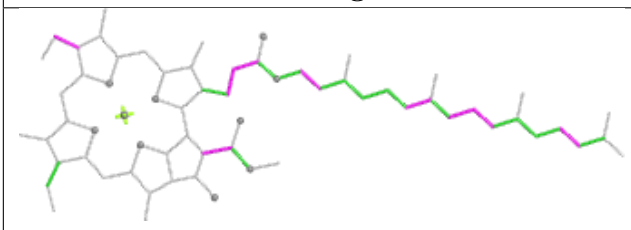	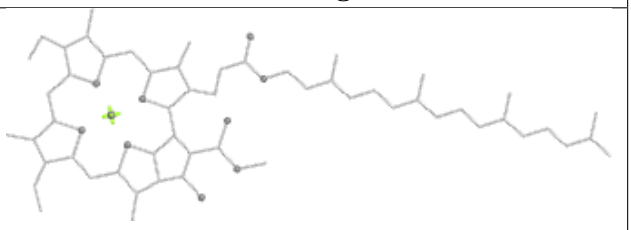
Torsions	Rings

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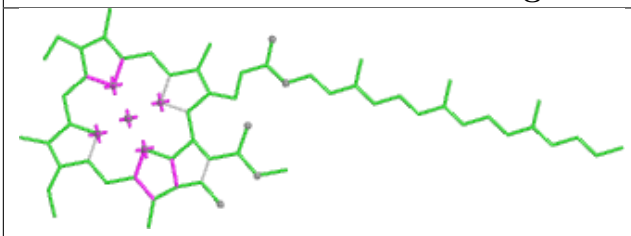

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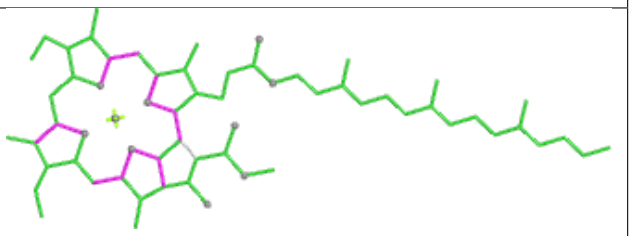

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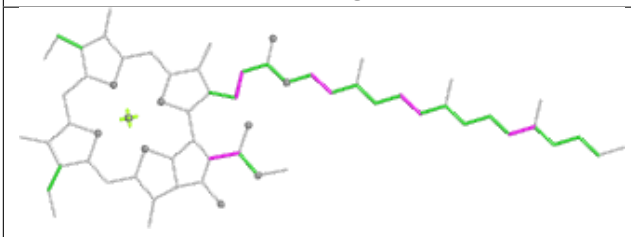

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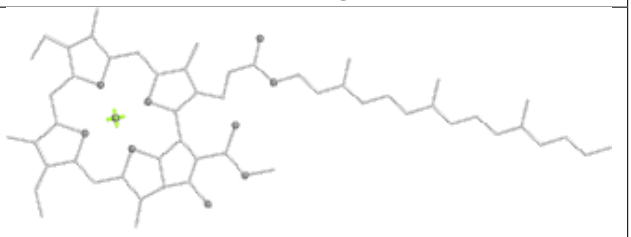

Rings

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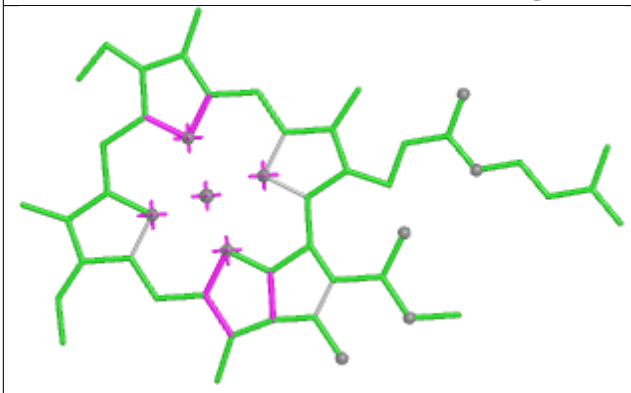

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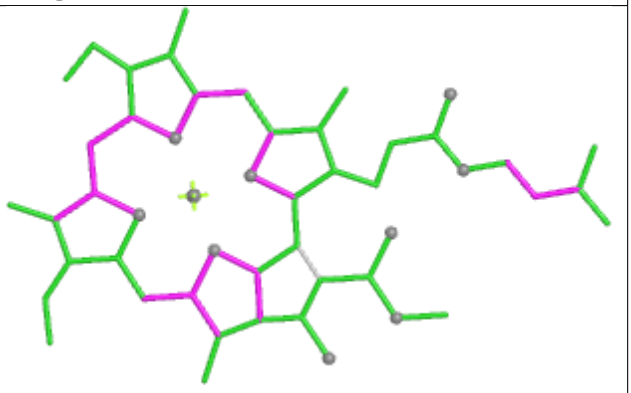

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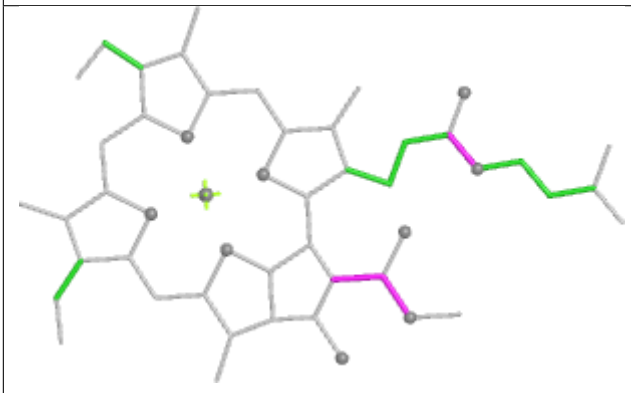

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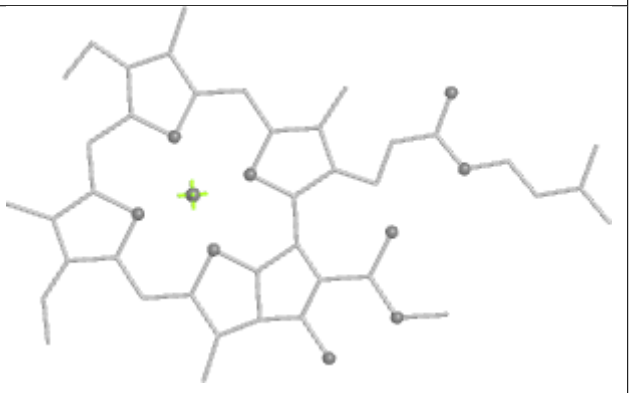

Rings

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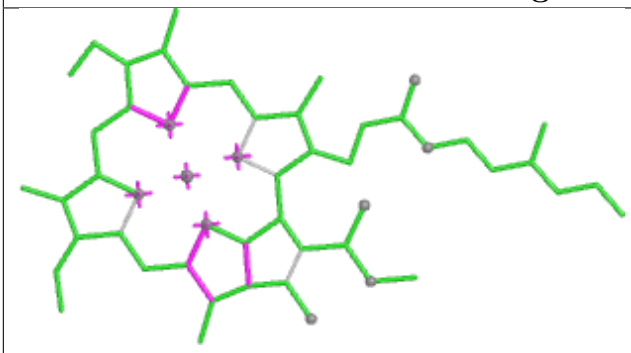

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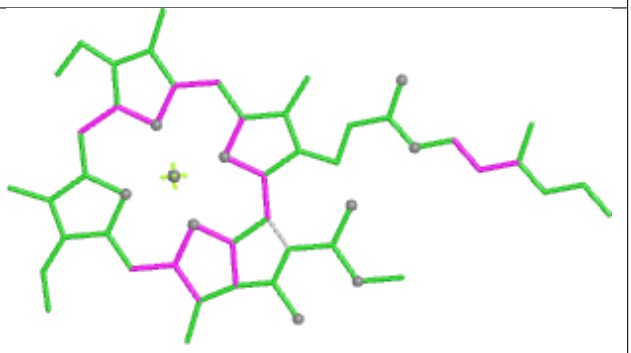

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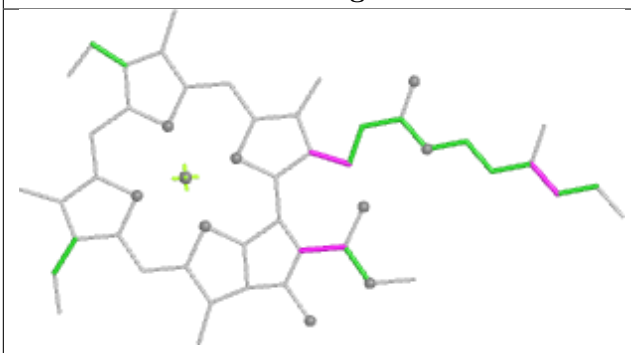

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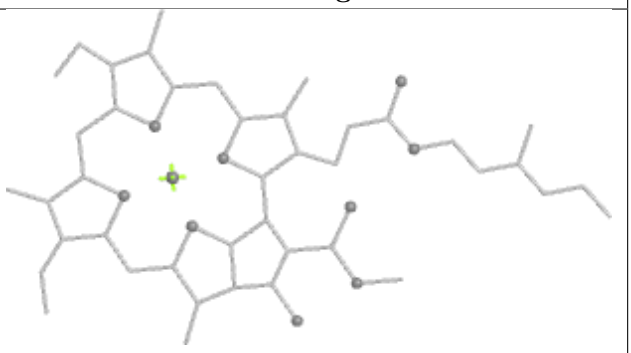

Rings

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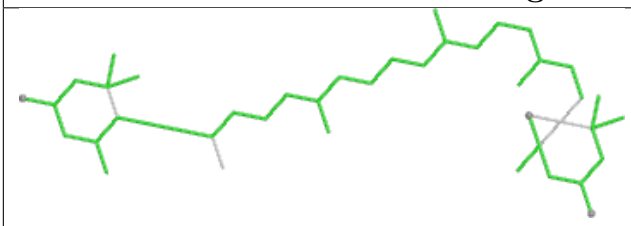

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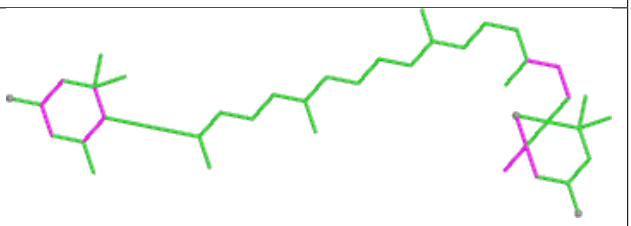

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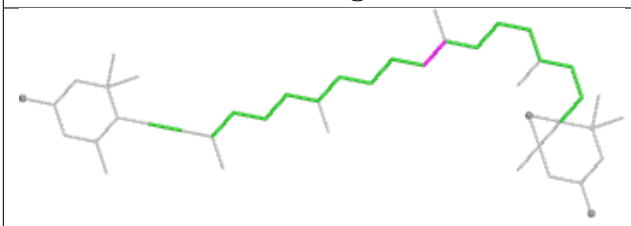

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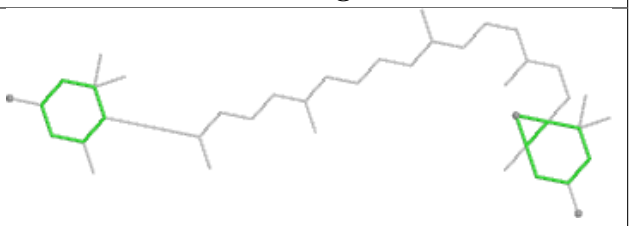

Rings

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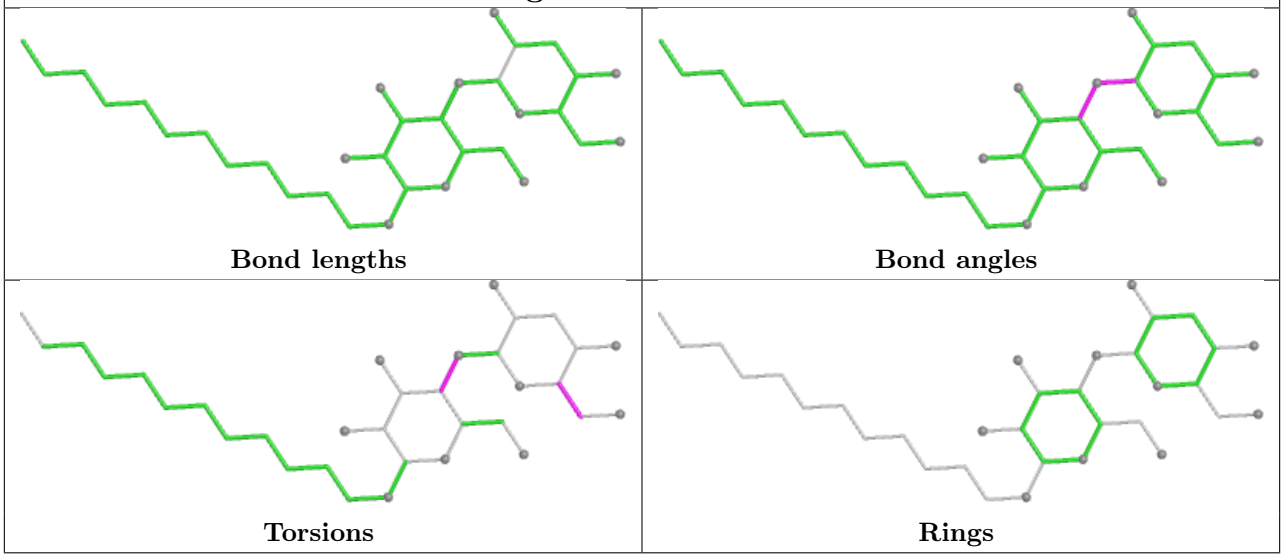

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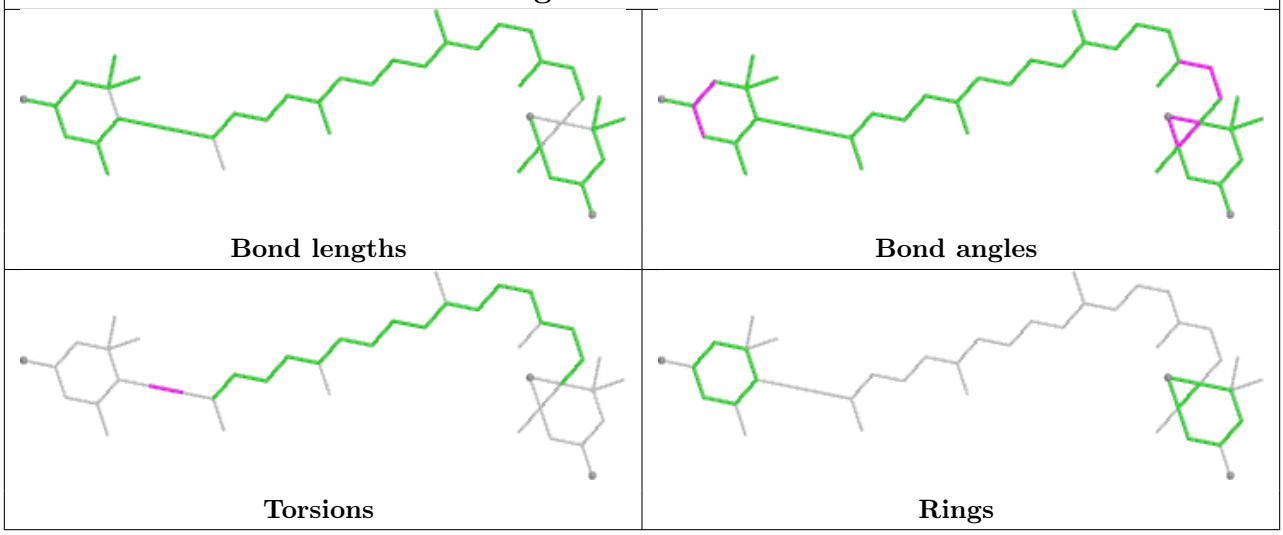

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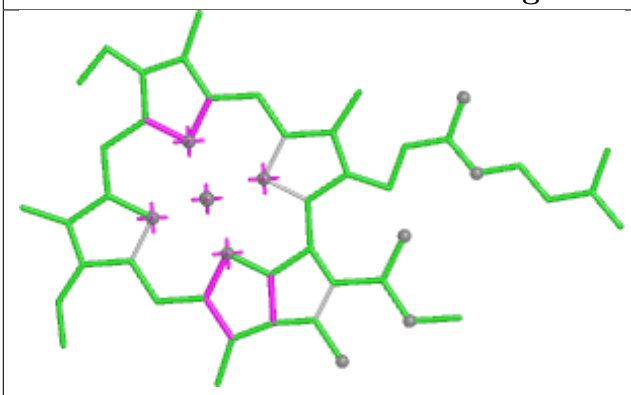

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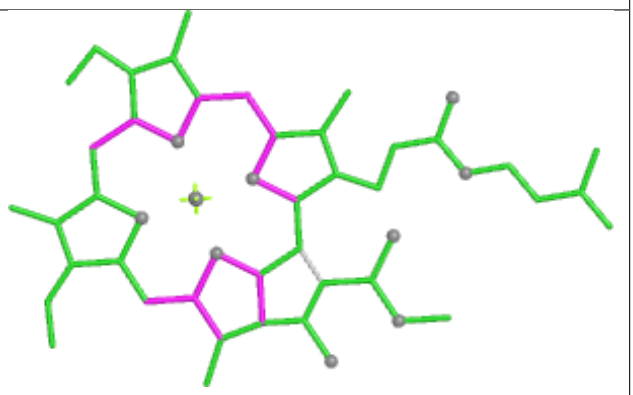

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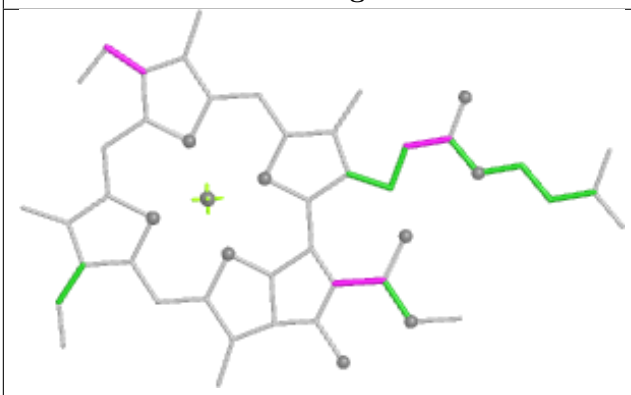

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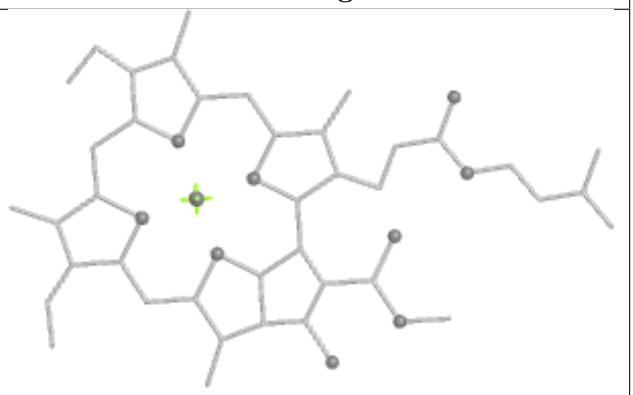

Rings

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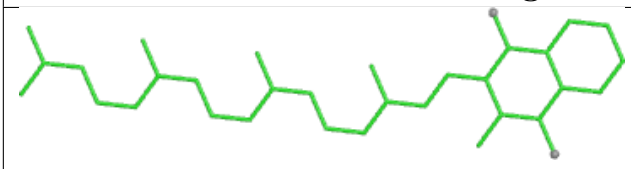

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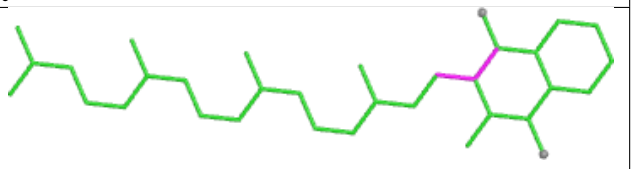

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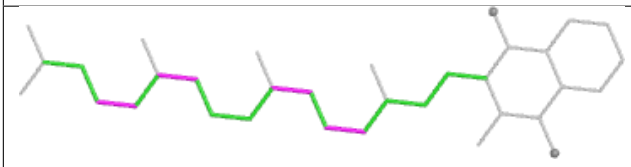

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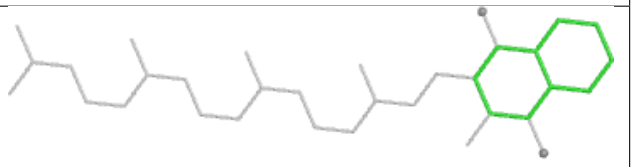

Rings

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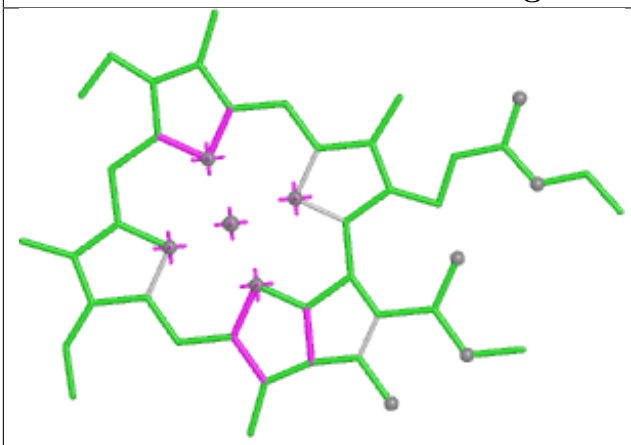

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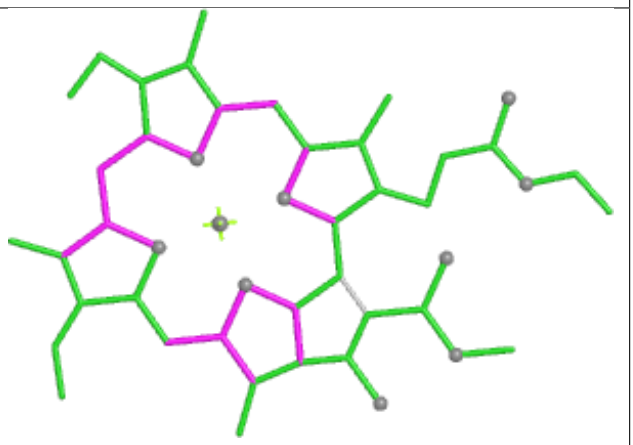

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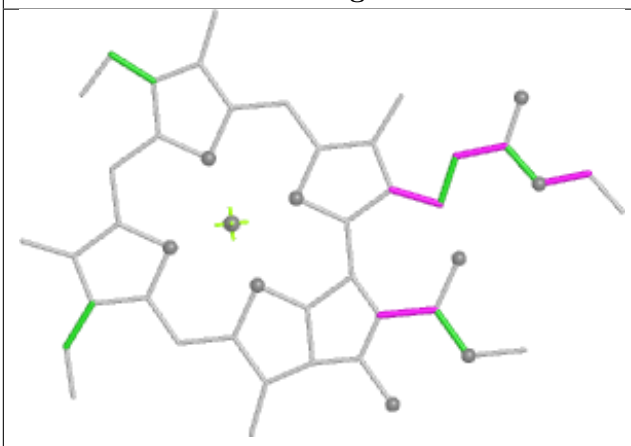

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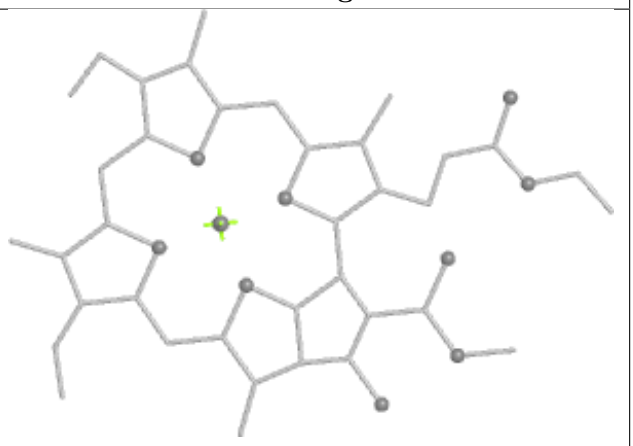

Rings

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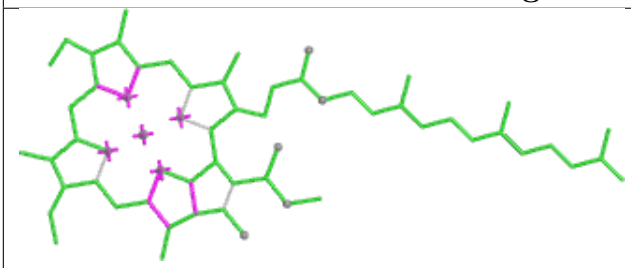

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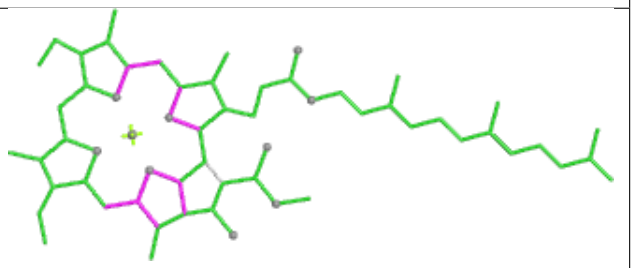

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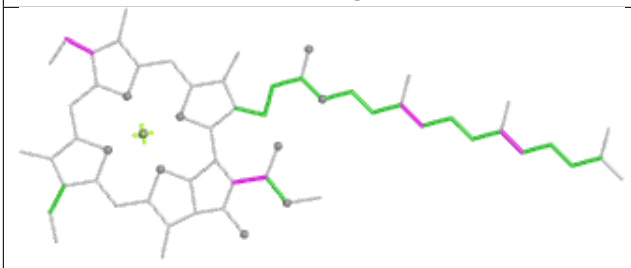

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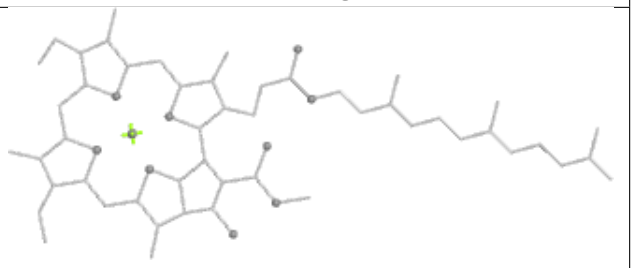
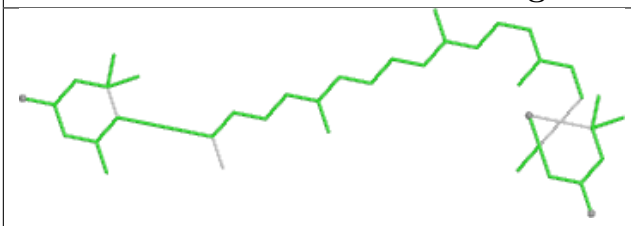


Rings

Ligand DD6 d 215



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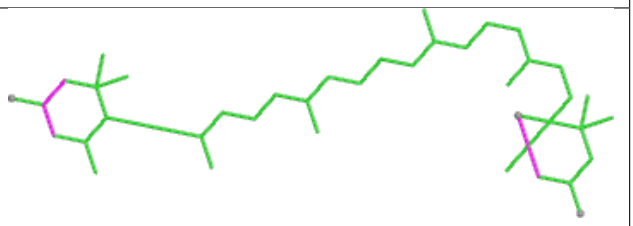

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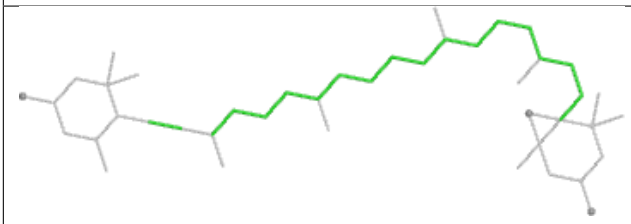

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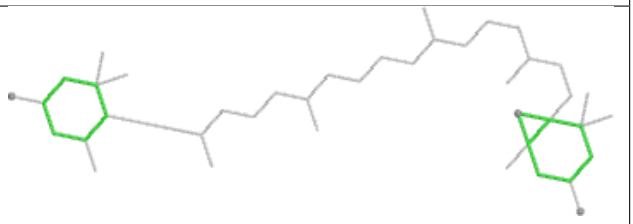
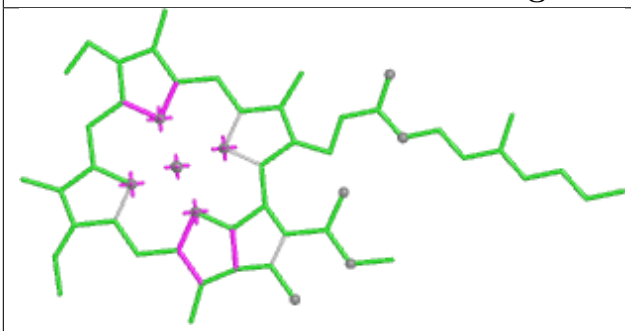


Rings

Ligand CLA o 308



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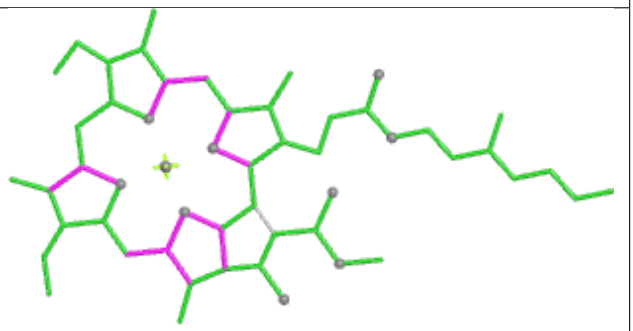

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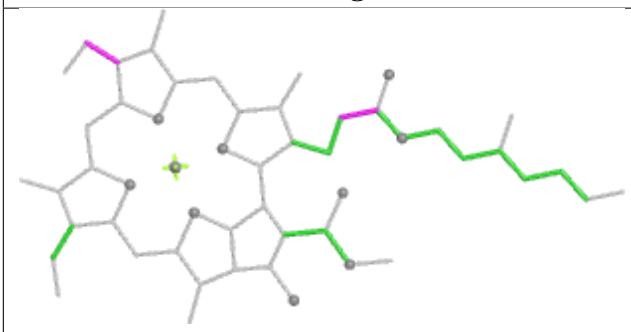

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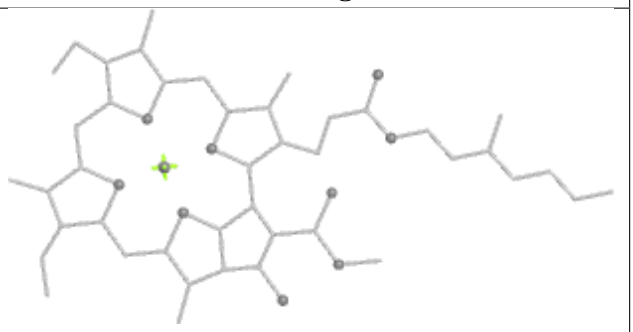
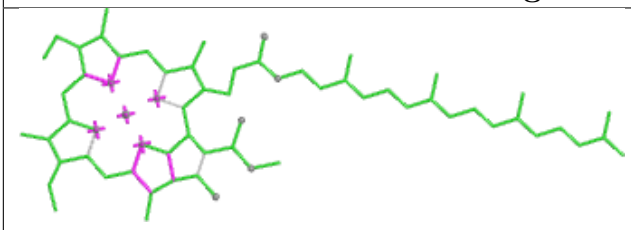


Rings

Ligand CLA A 804



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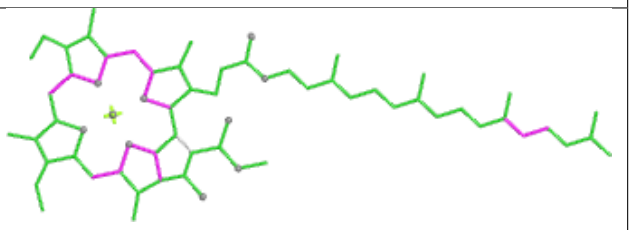

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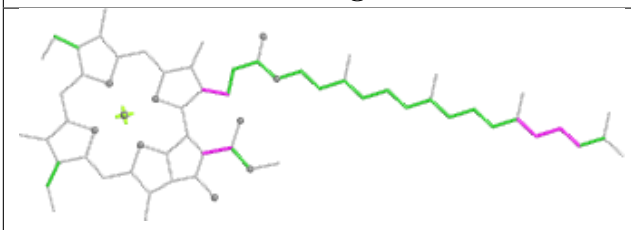

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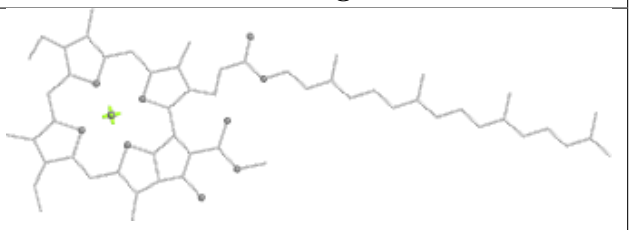
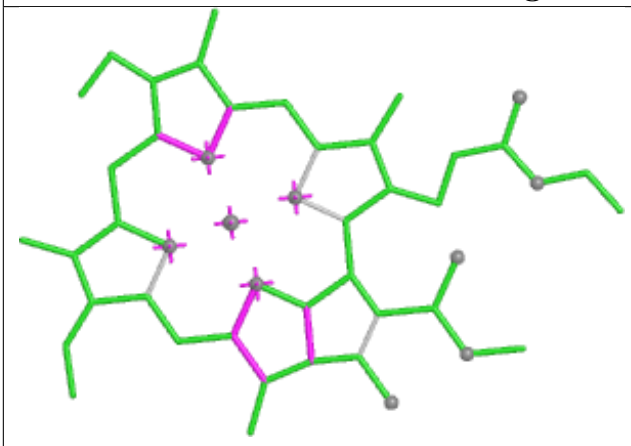
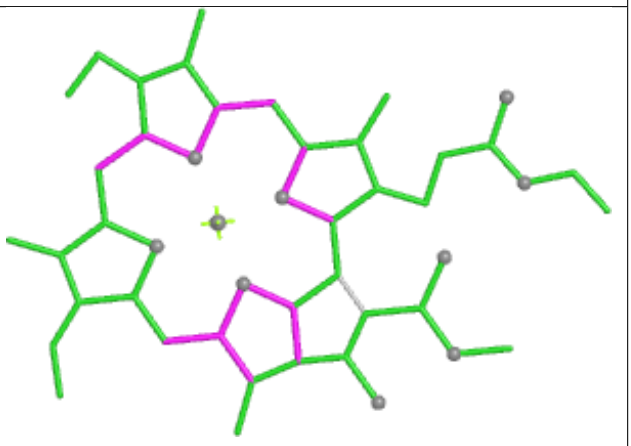


Rings

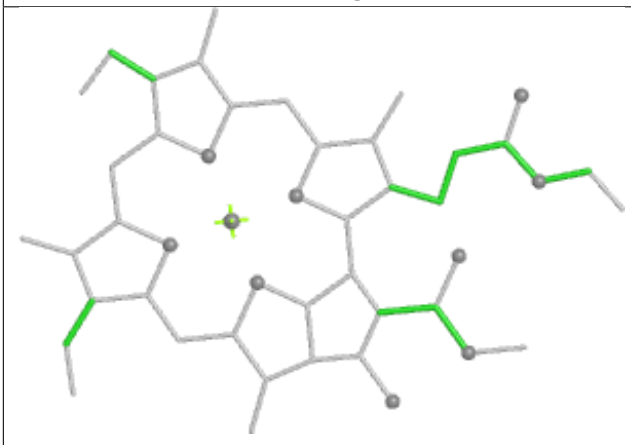
Ligand CLA A 845



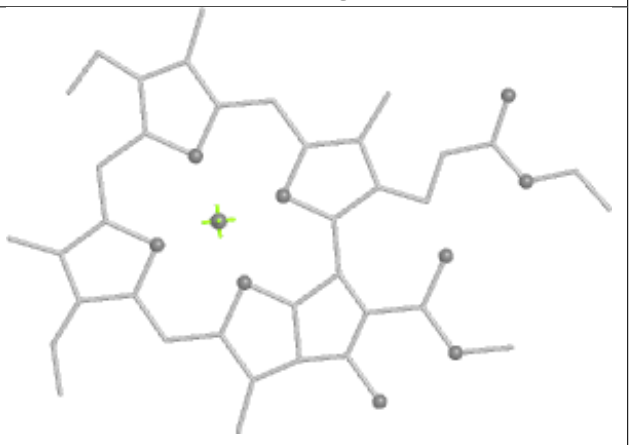
Bond lengths



Bond angles

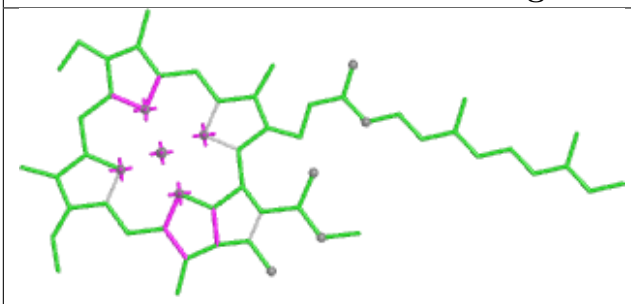


Torsions



Rings

Ligand CLA b 308



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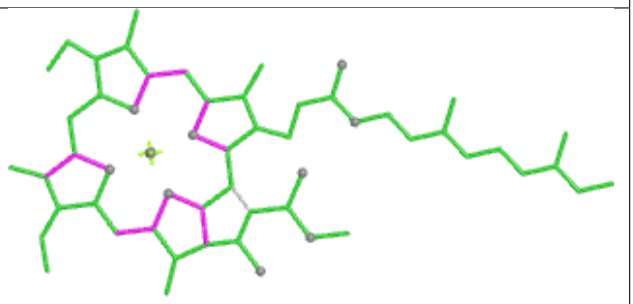

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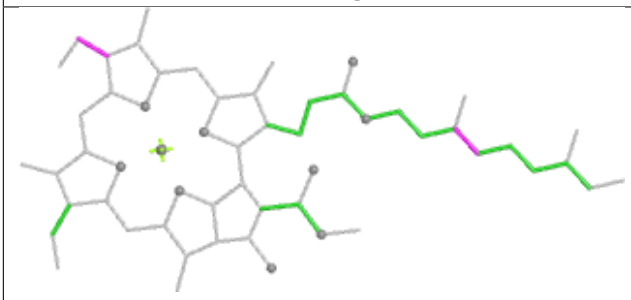

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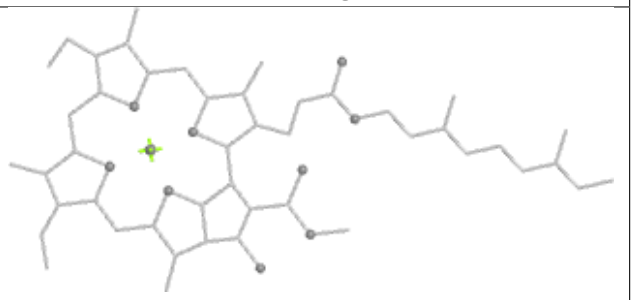
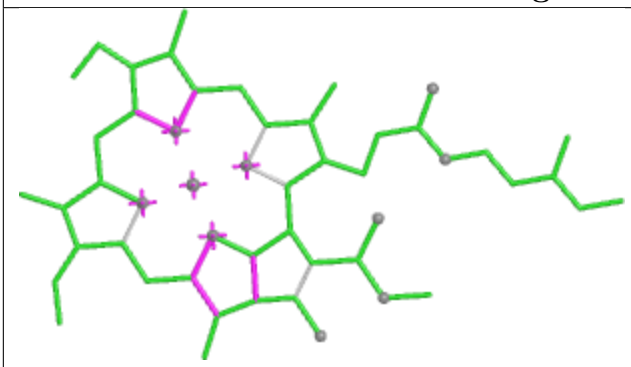


Rings

Ligand CLA i 308



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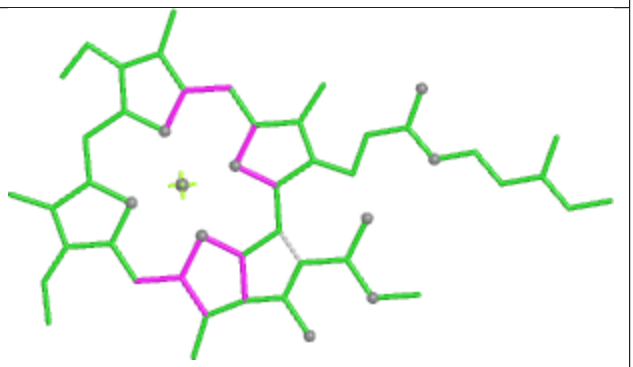
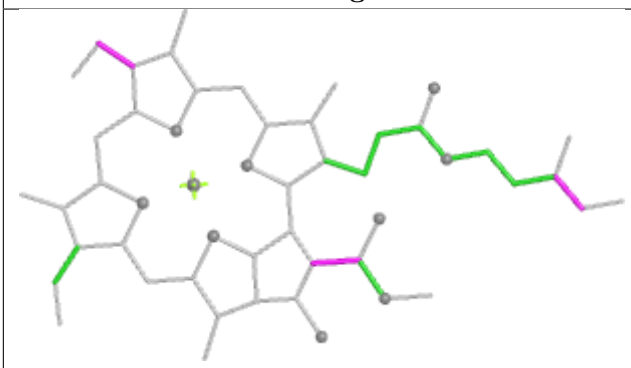


Bond angles



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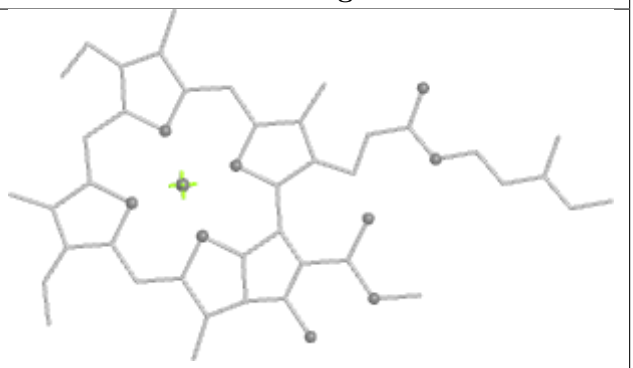
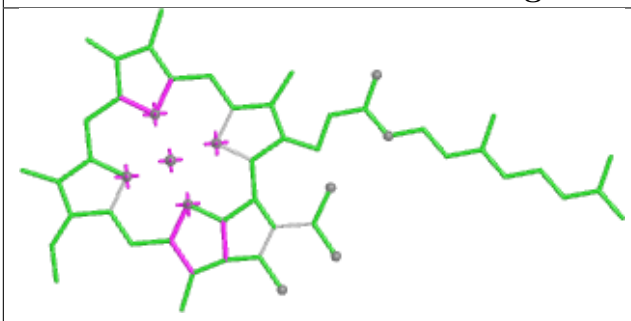


Rings

Ligand CLA B 810



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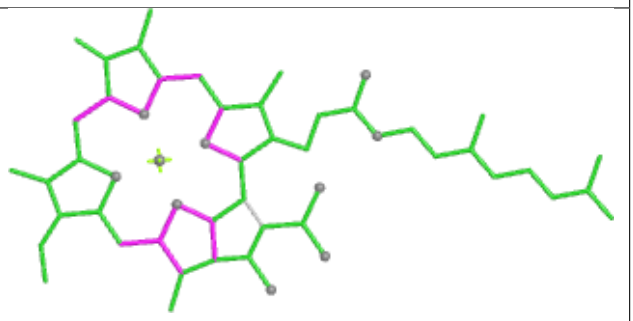

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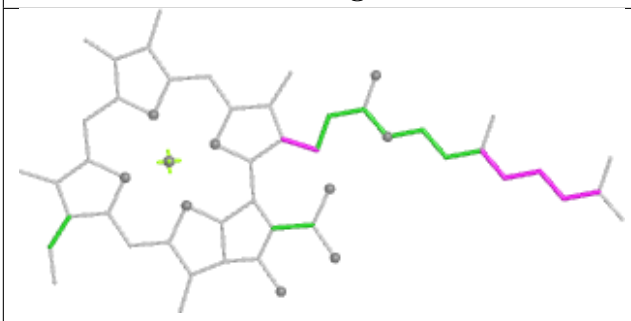

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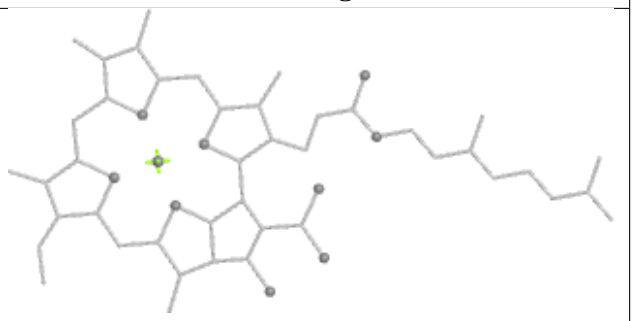
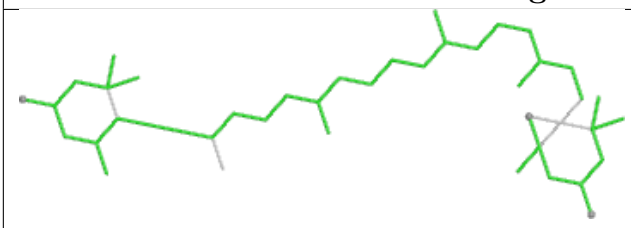


Rings

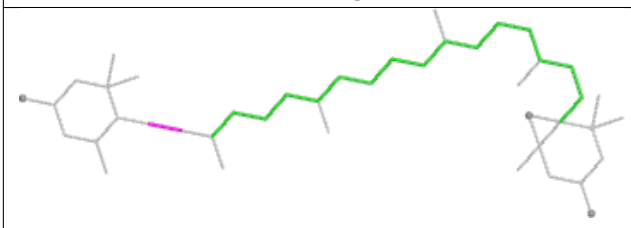
Ligand DD6 g 314



Bond lengths



Bond angles



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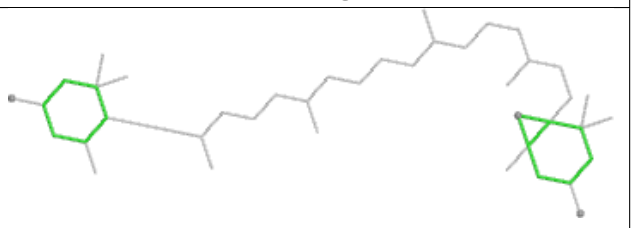
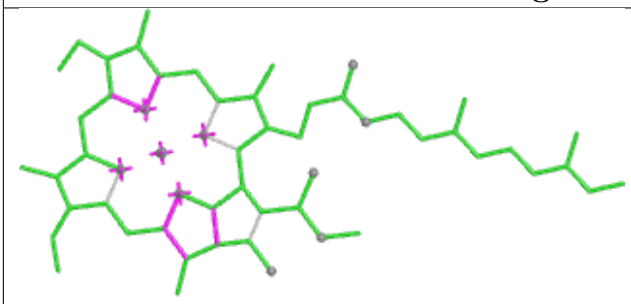
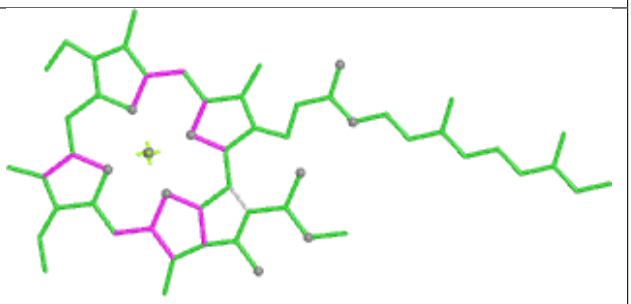
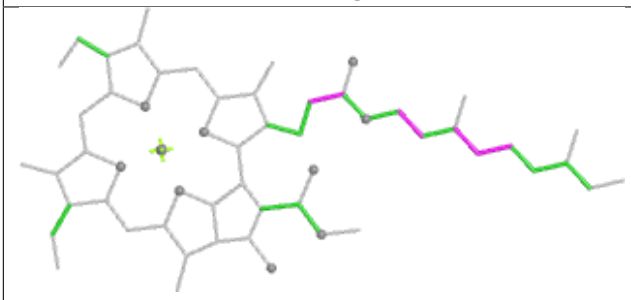
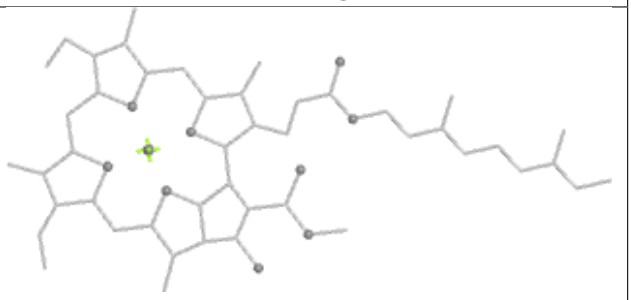


Rings

Ligand CLA l 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

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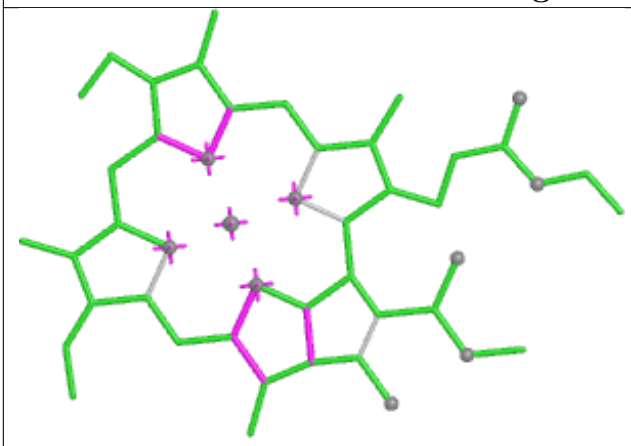
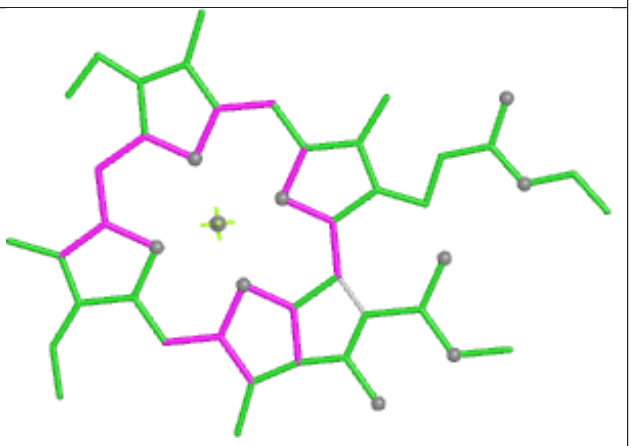
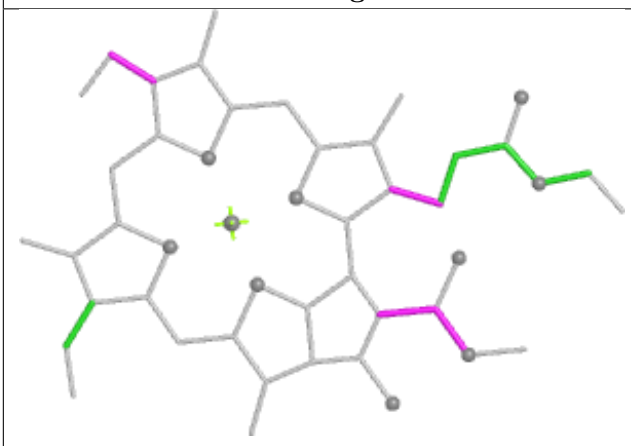
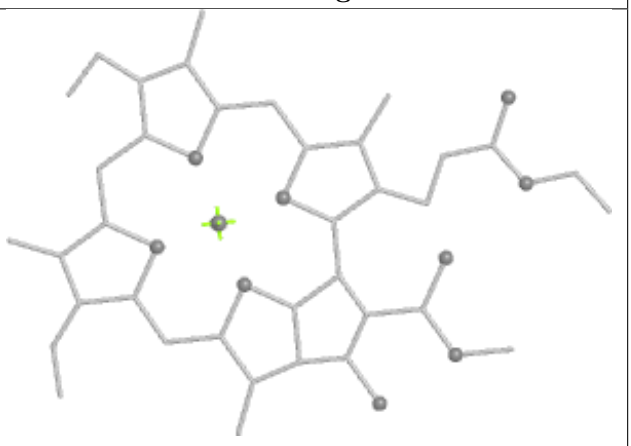
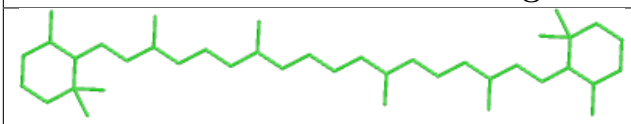
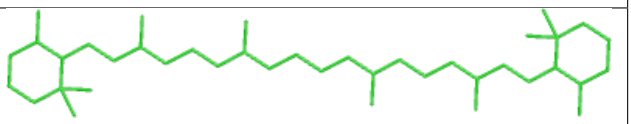
	
Bond lengths	Bond angles
	
Torsions	Rings

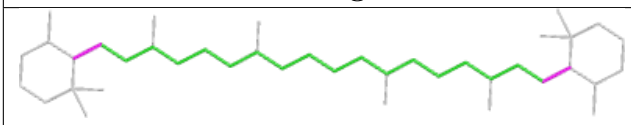
Ligand BCR B 834



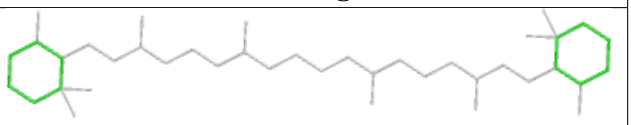
Bond lengths



Bond angles

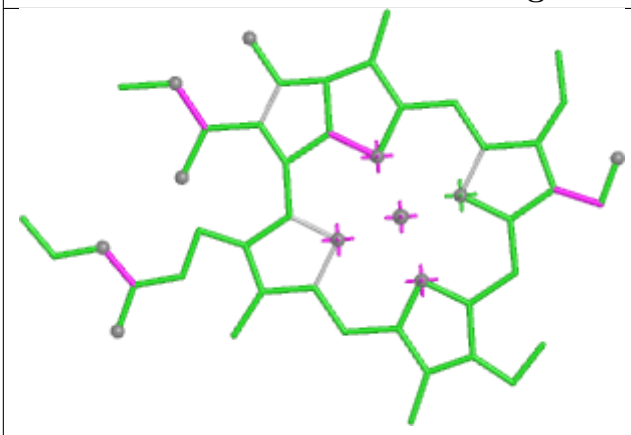


Torsions



Rings

Ligand CHL k 301



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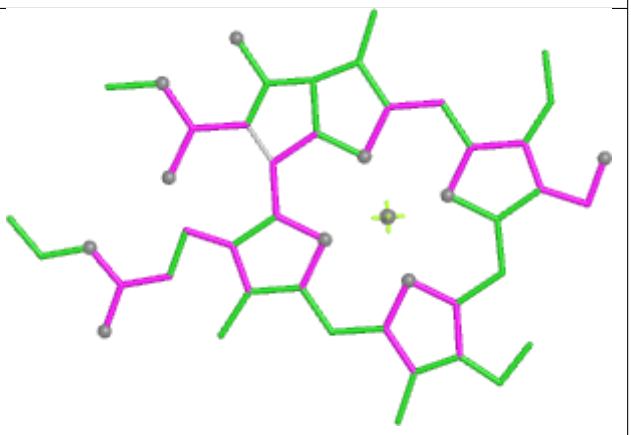
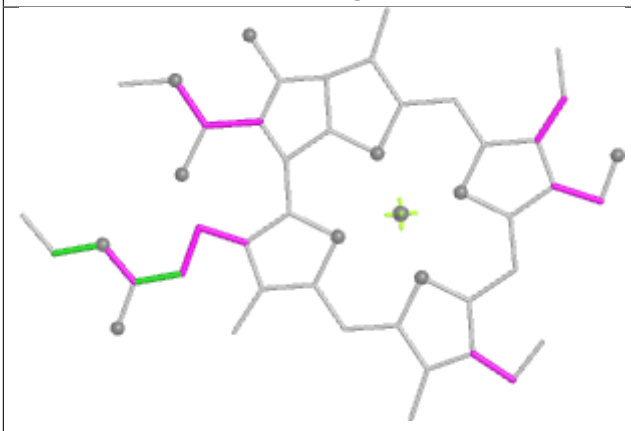


Bond angles



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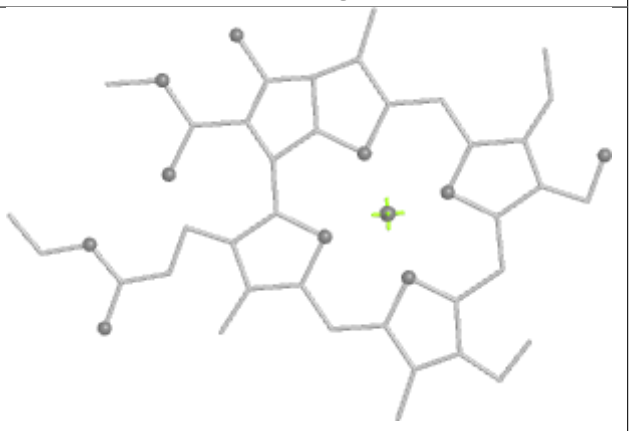
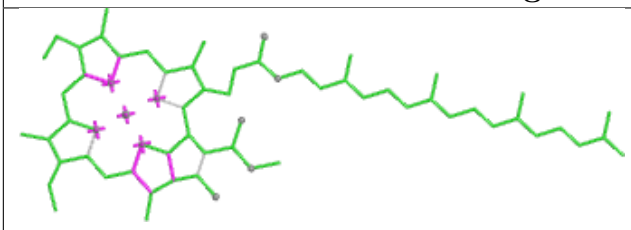
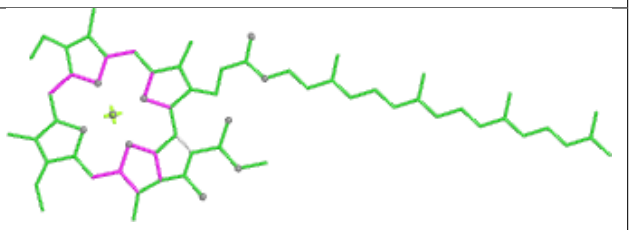
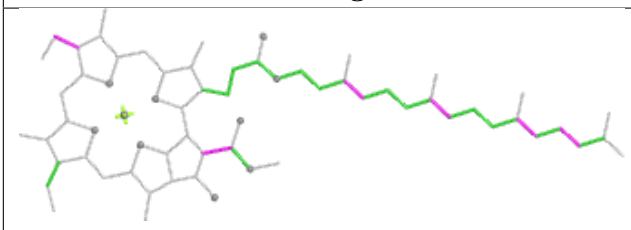
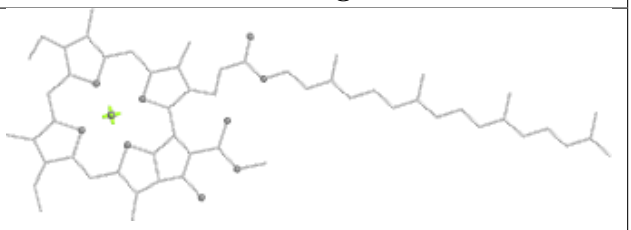
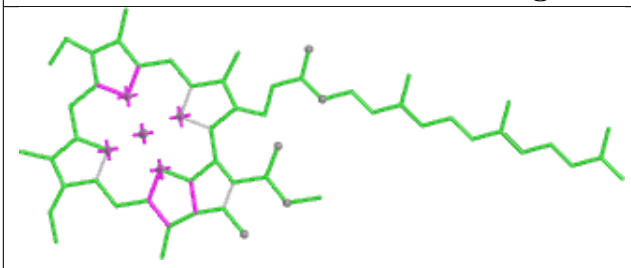
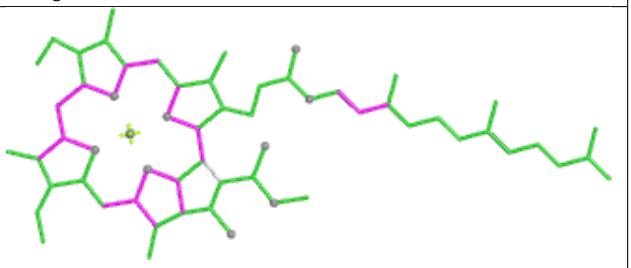
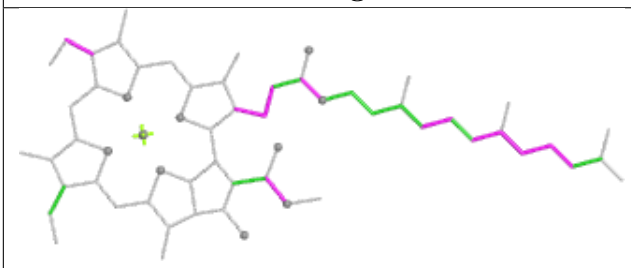
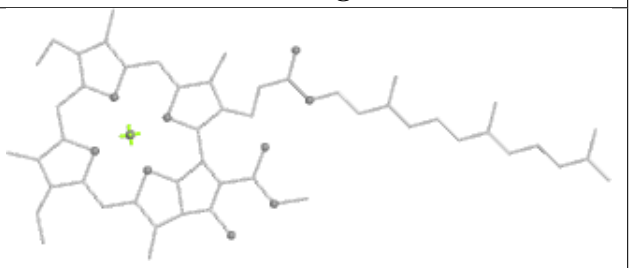
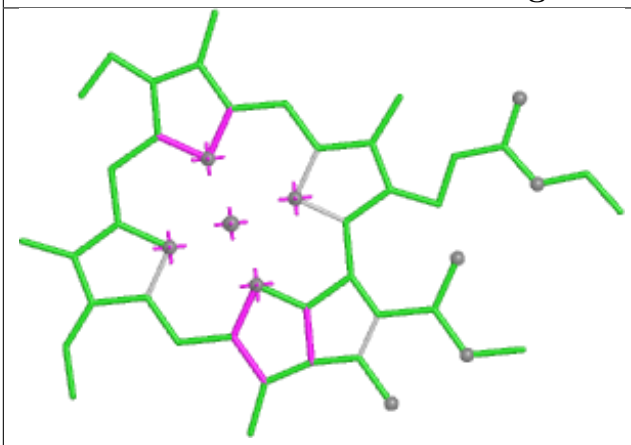


Rings

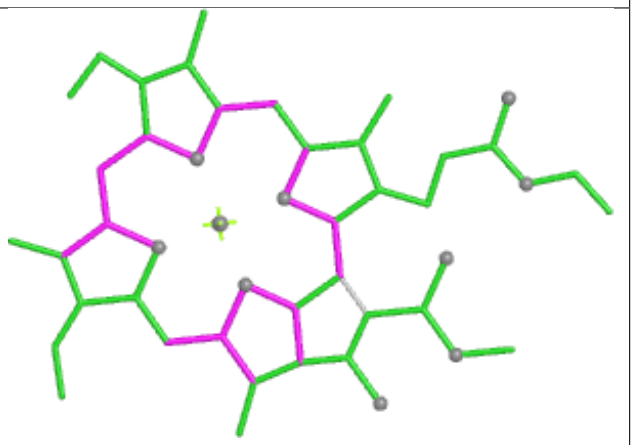
Ligand CLA A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA j 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

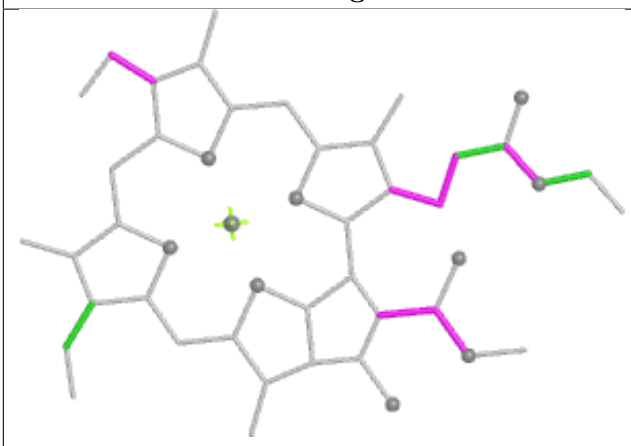
Ligand CLA a 302



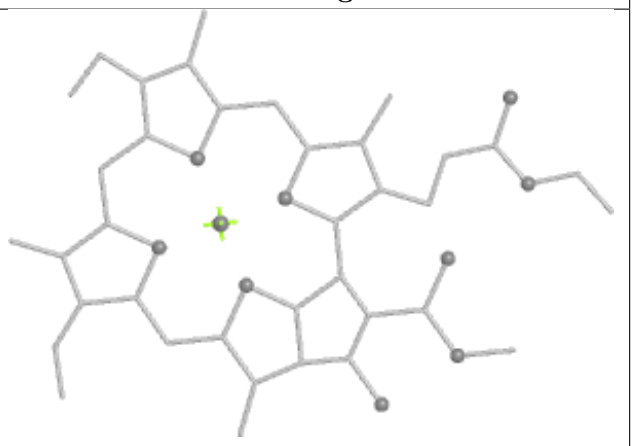
Bond lengths



Bond angles

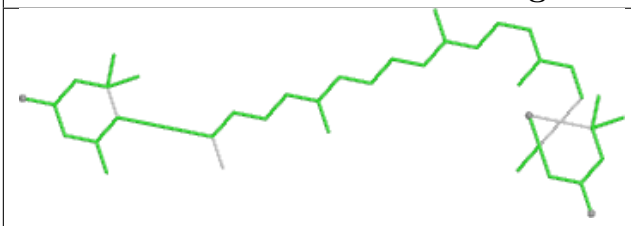


Torsions



Rings

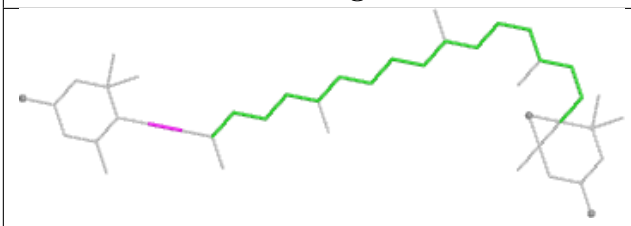
Ligand DD6 k 313



Bond lengths



Bond angles

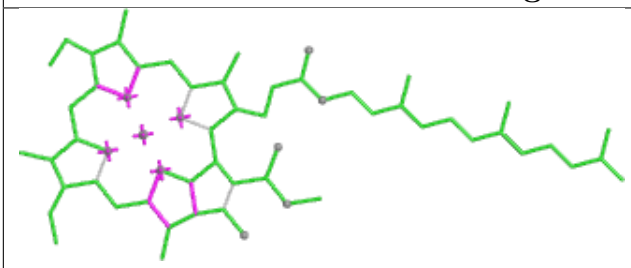


Torsions



Rings

Ligand CLA A 813



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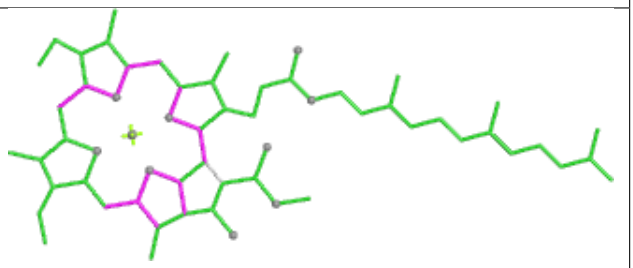
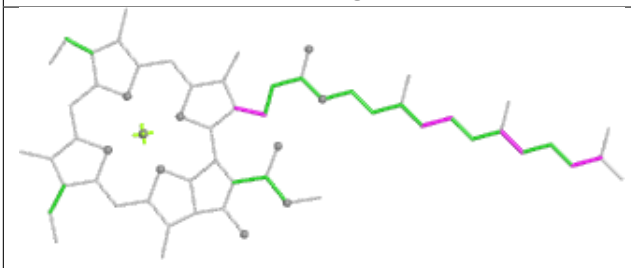


Bond angles



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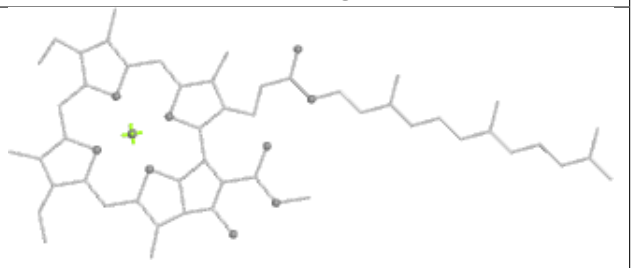
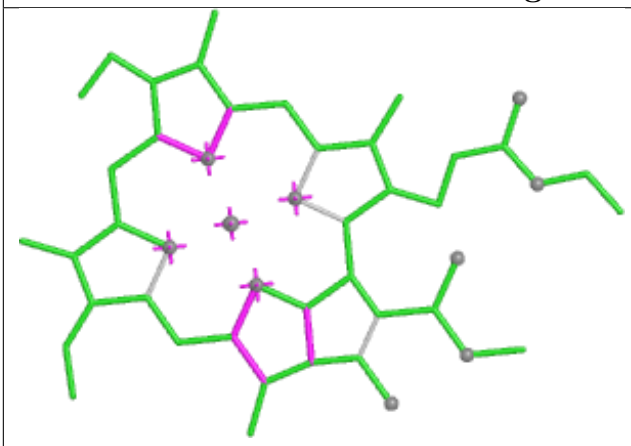
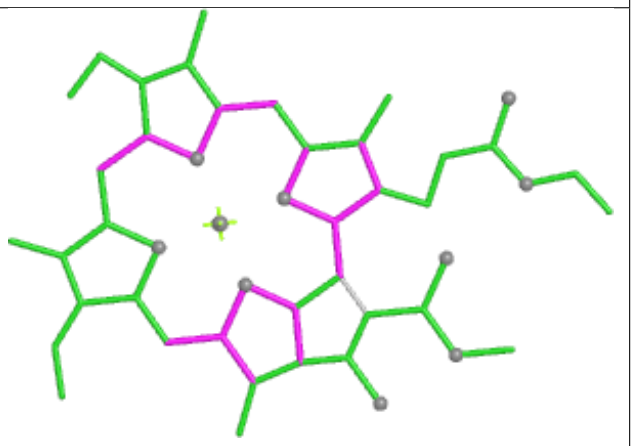


Rings

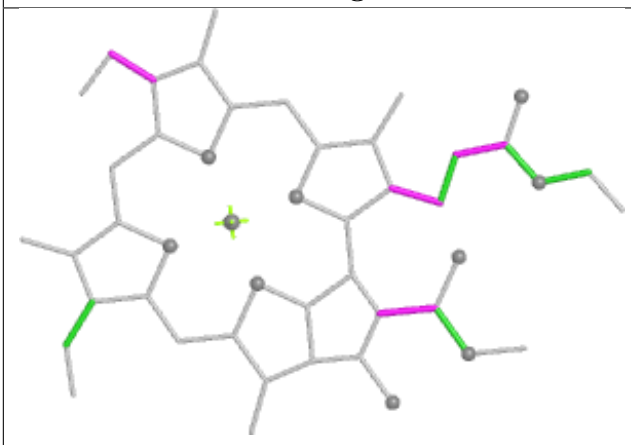
Ligand CLA B 840



Bond lengths



Bond angles



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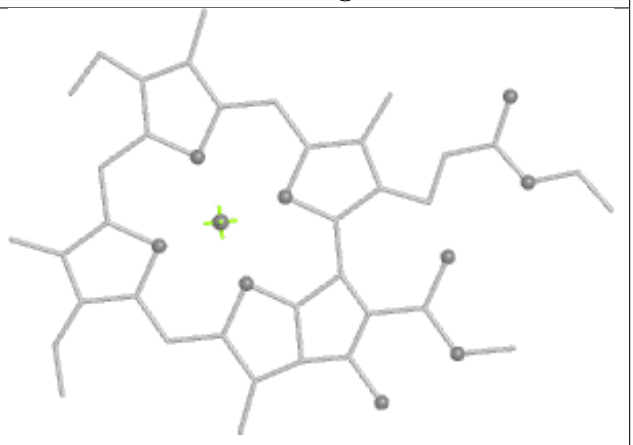
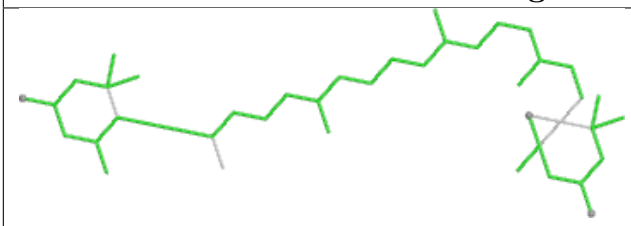
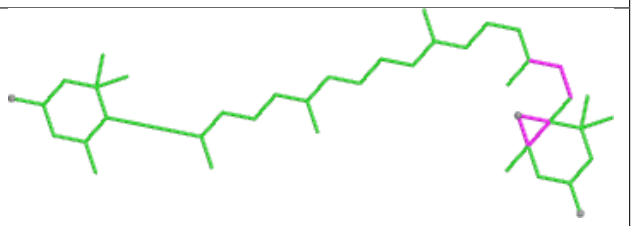


Rings

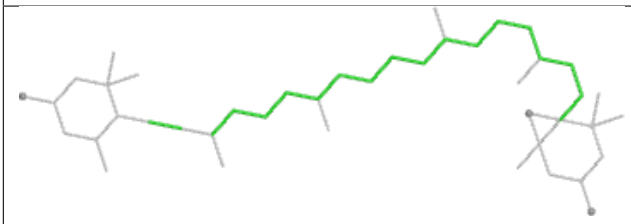
Ligand DD6 d 214



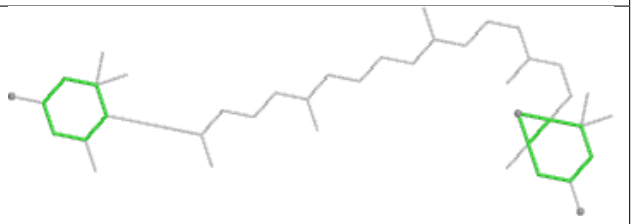
Bond lengths



Bond angles

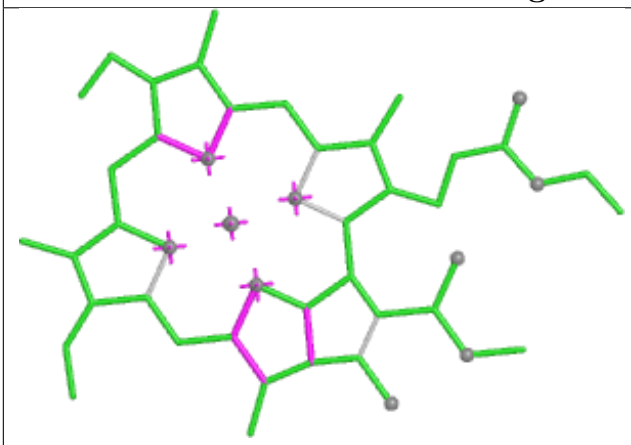


Torsions



Rings

Ligand CLA g 311



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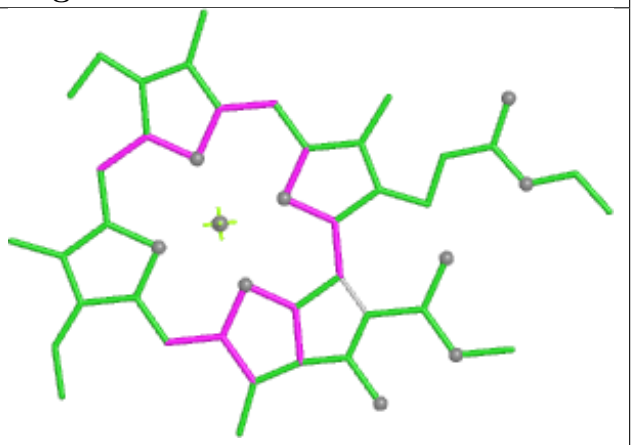

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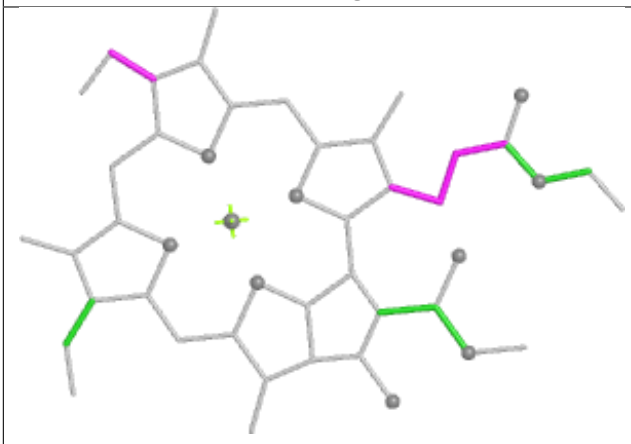

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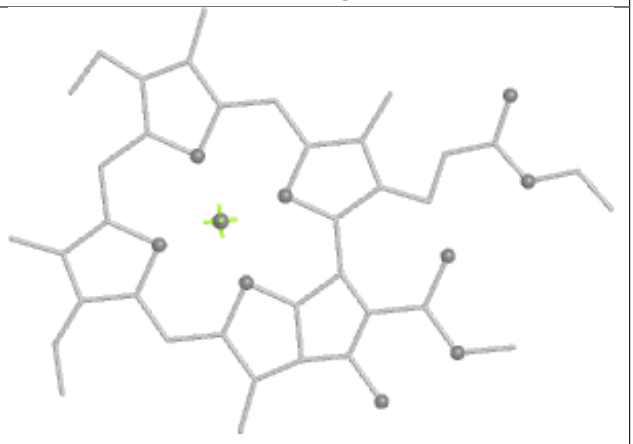

Rings

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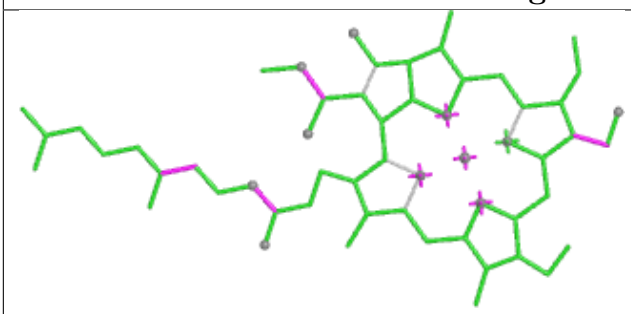

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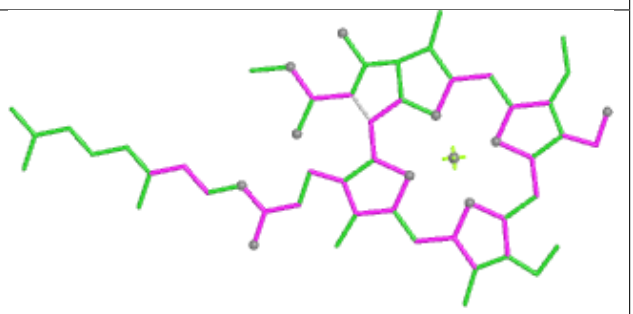

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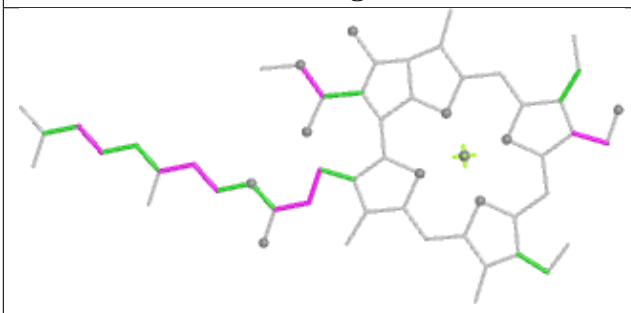

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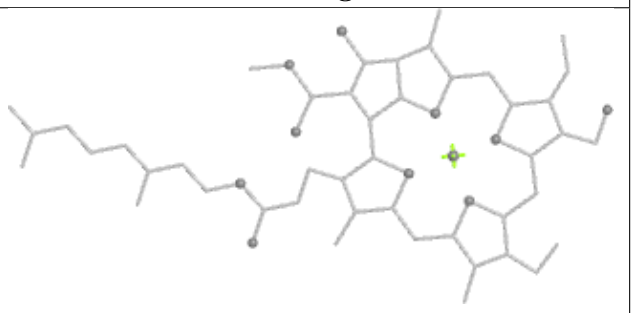

Rings

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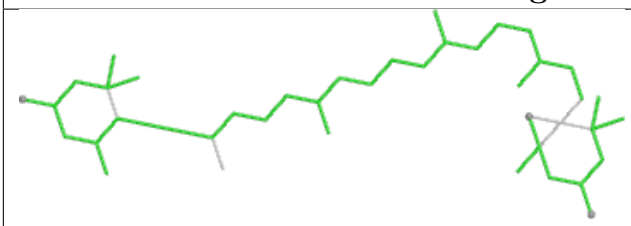

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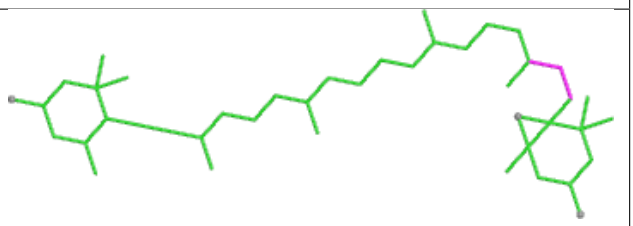

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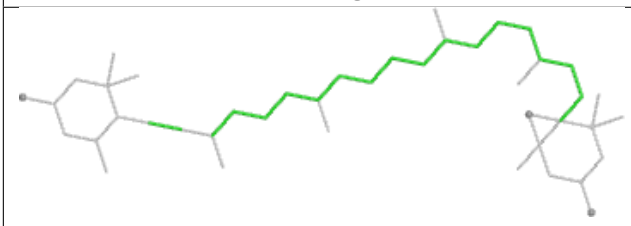
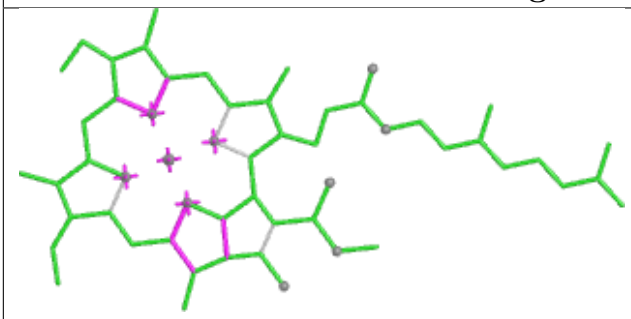


Torsions



Rings

Ligand CLA e 311



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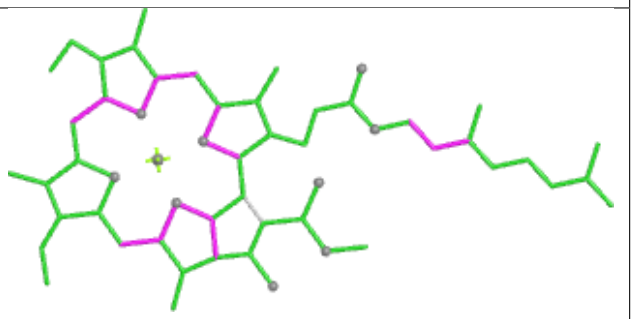

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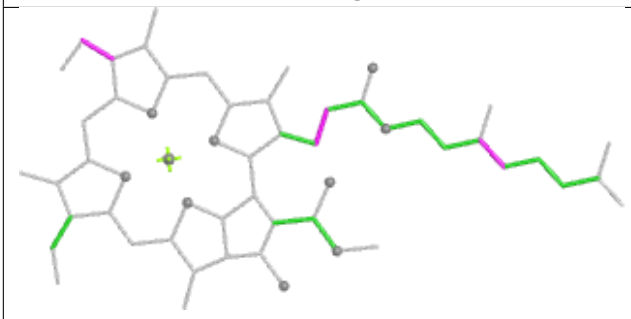

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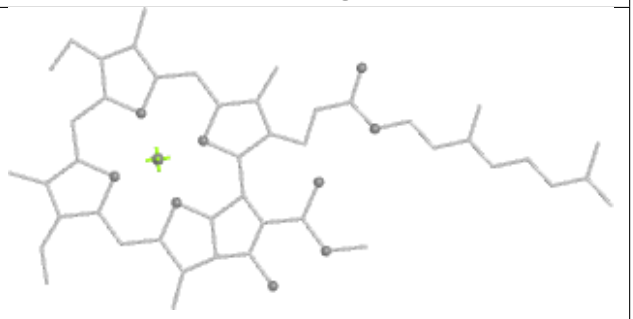

Rings

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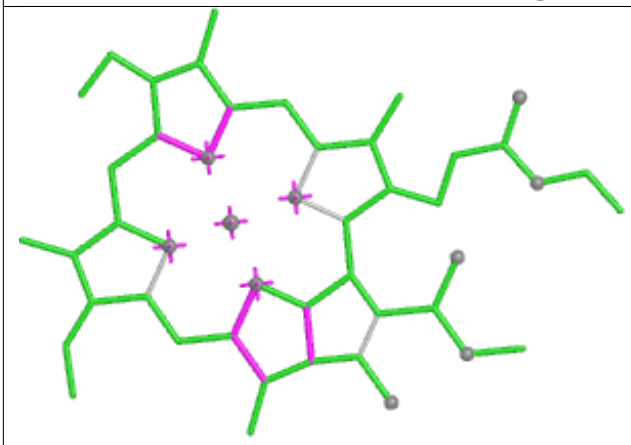

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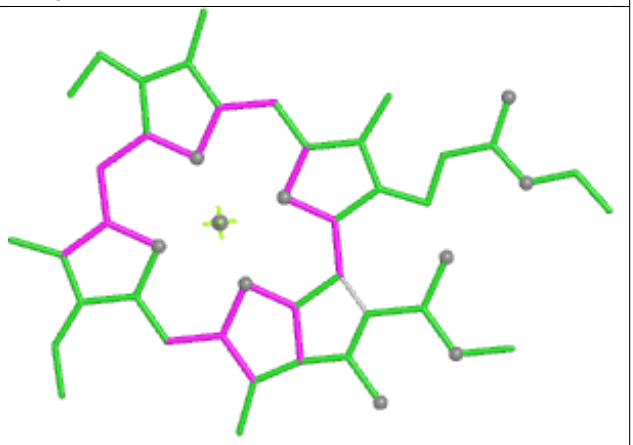

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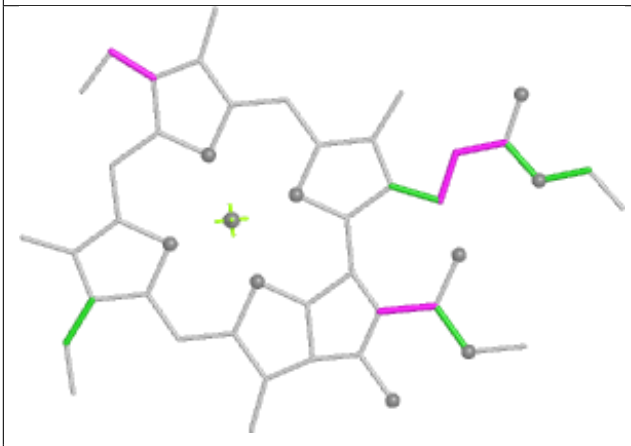

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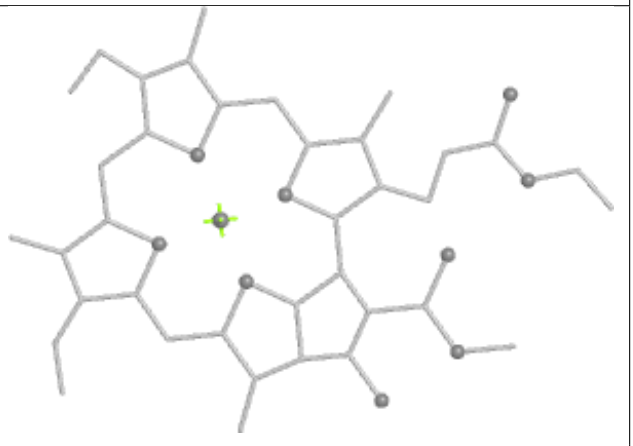

Rings

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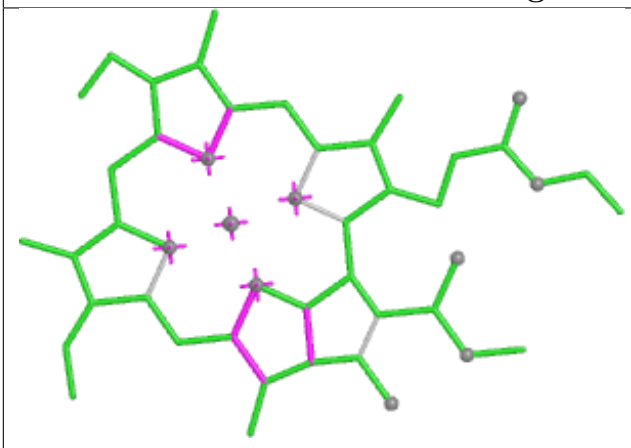

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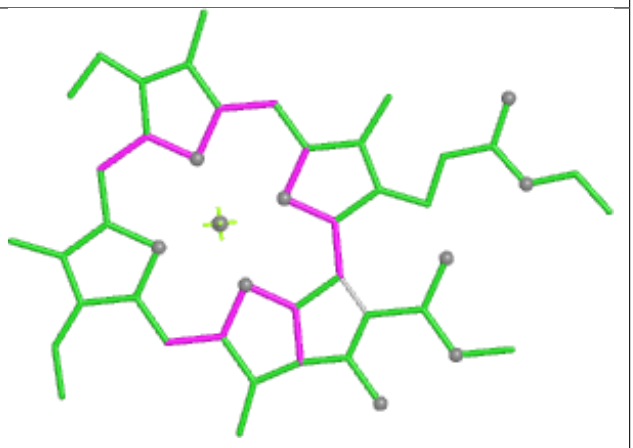
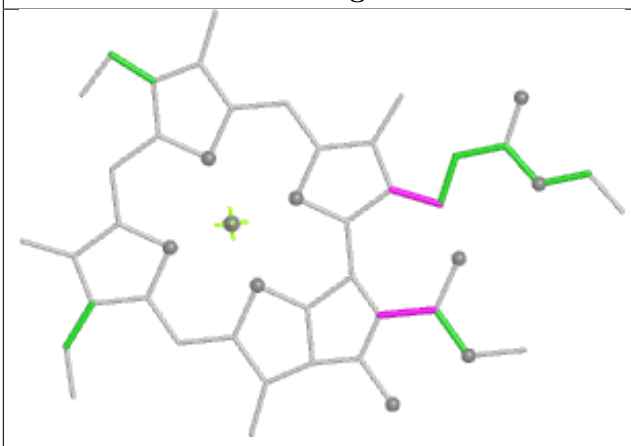


Bond angles



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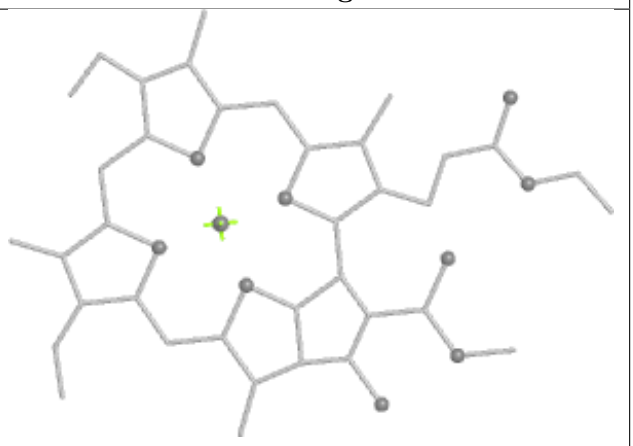

Rings

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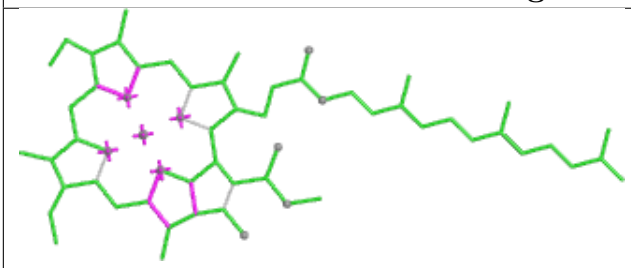

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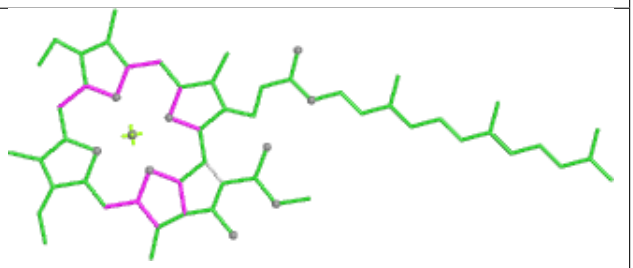

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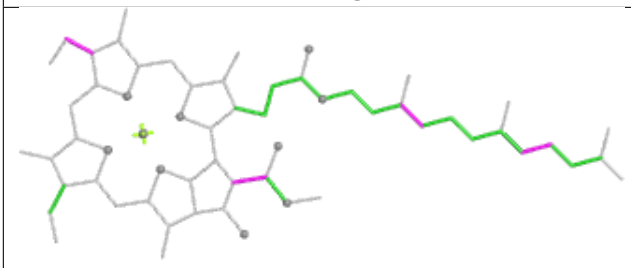

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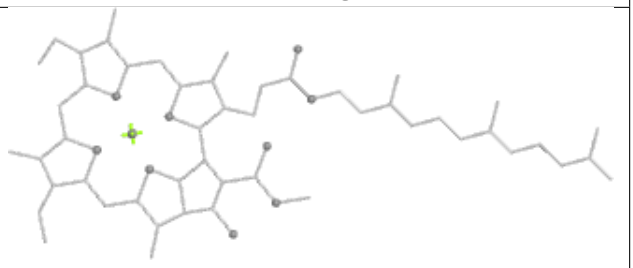
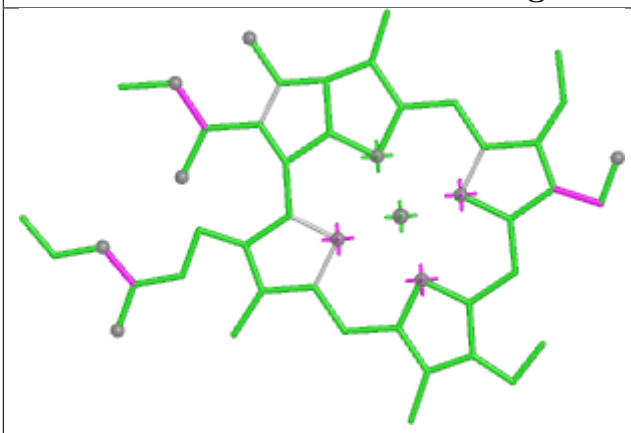


Rings

Ligand CHL o 301



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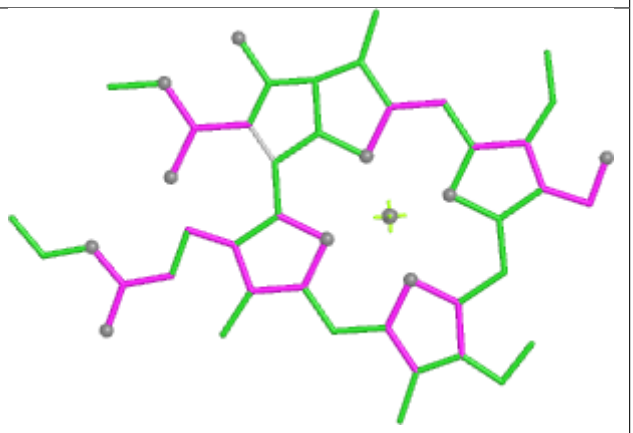
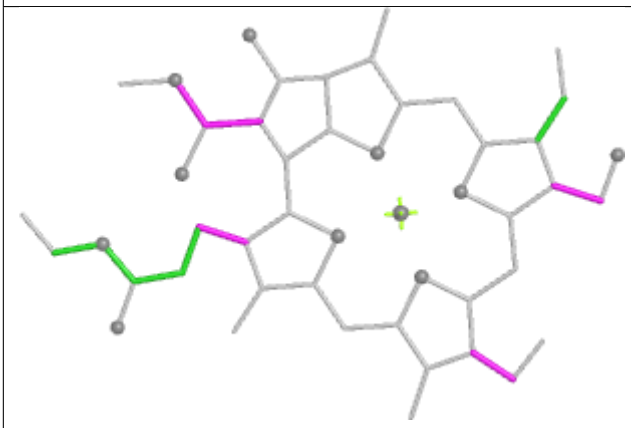


Bond angles



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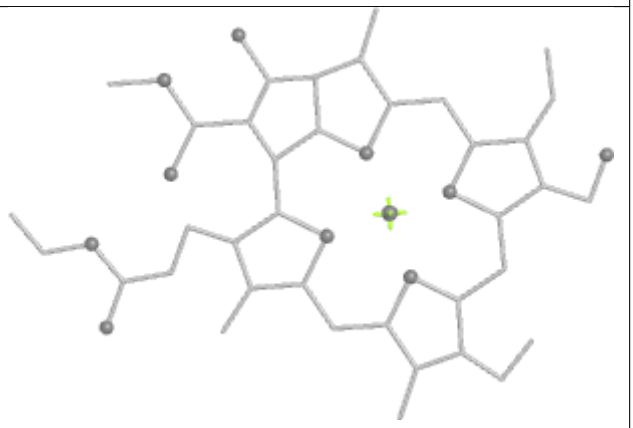
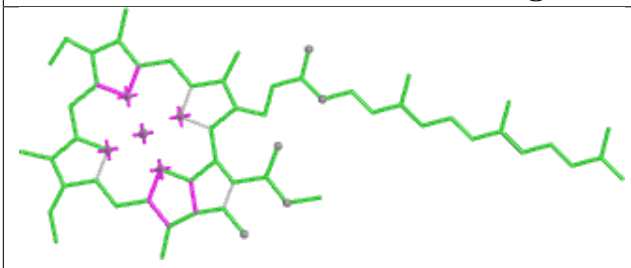


Rings

Ligand CLA d 208



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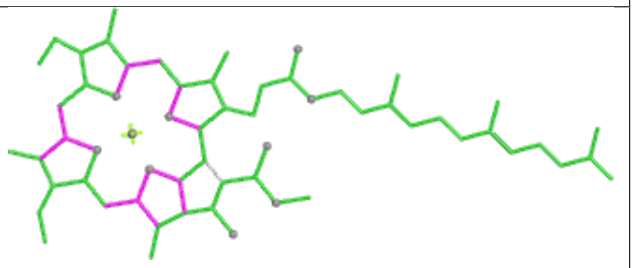
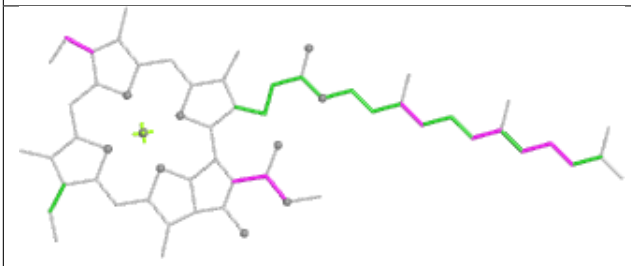


Bond angles



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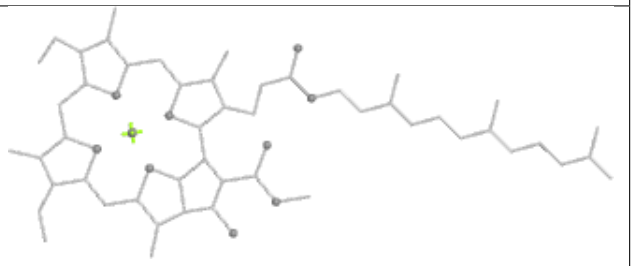

Rings

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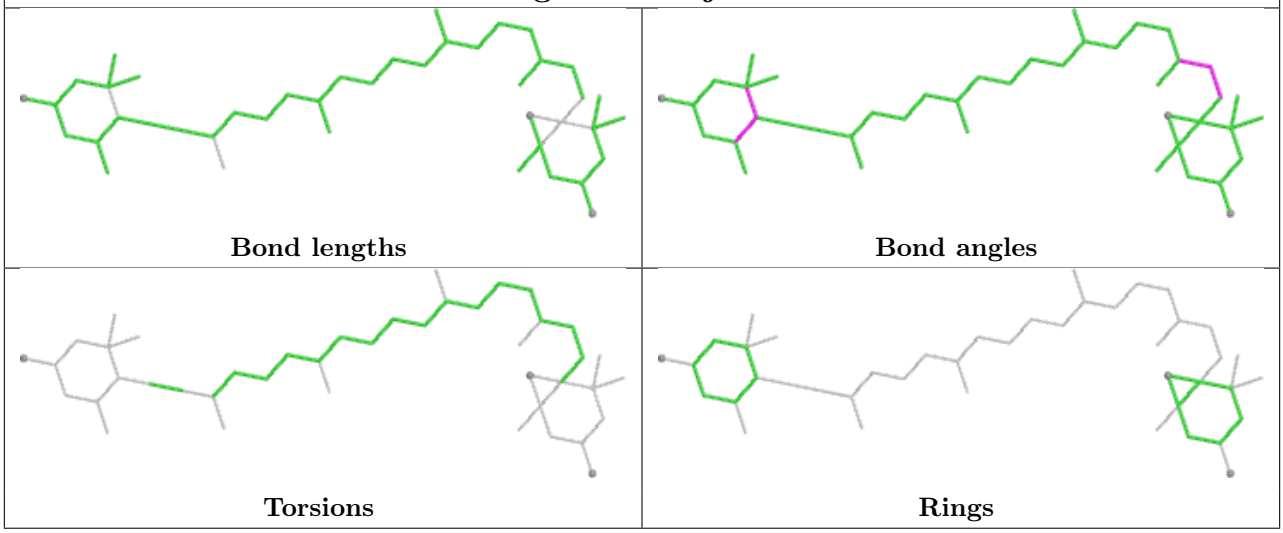

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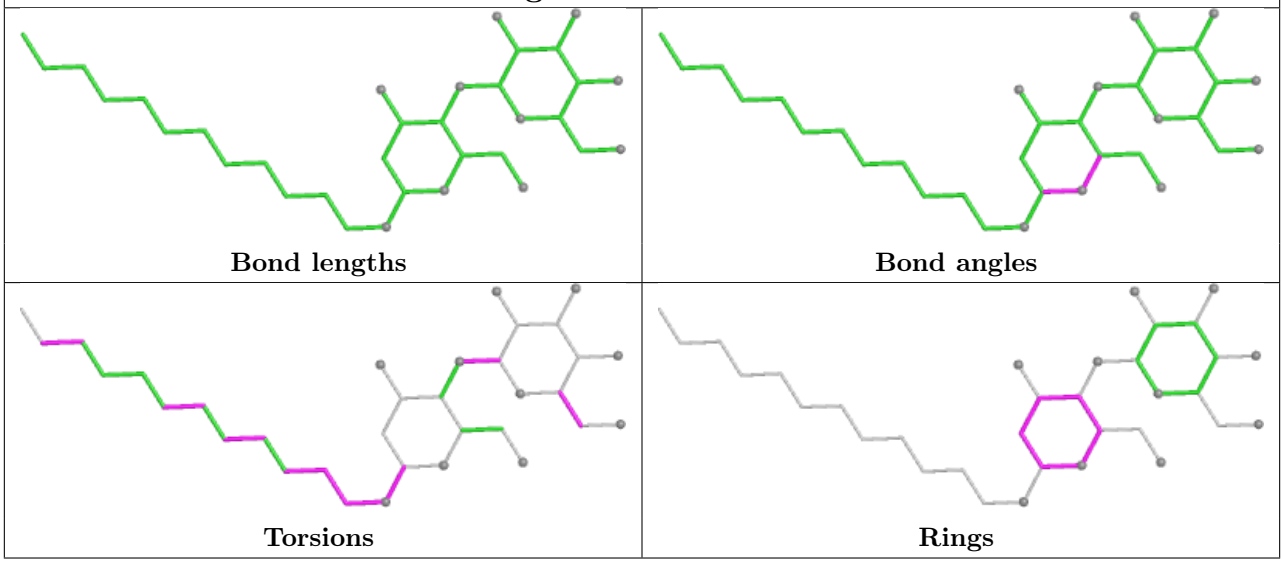

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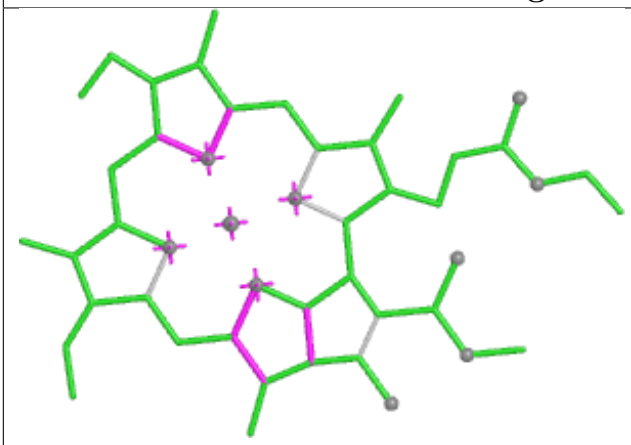

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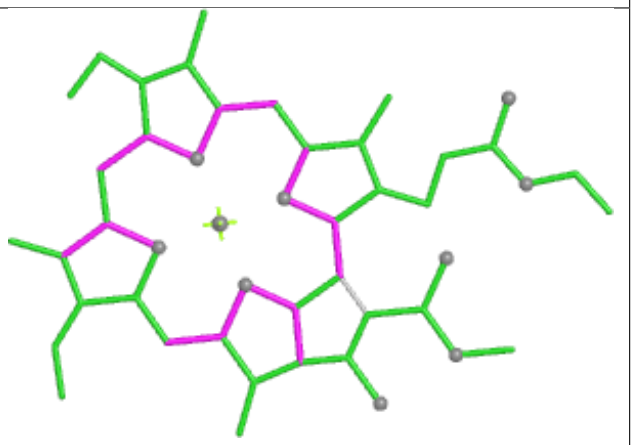
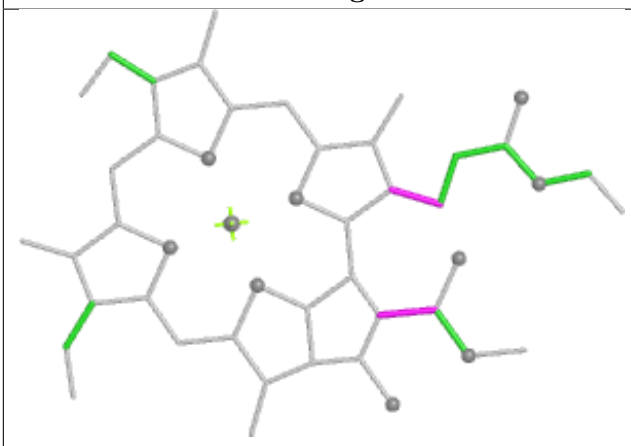


Bond angles



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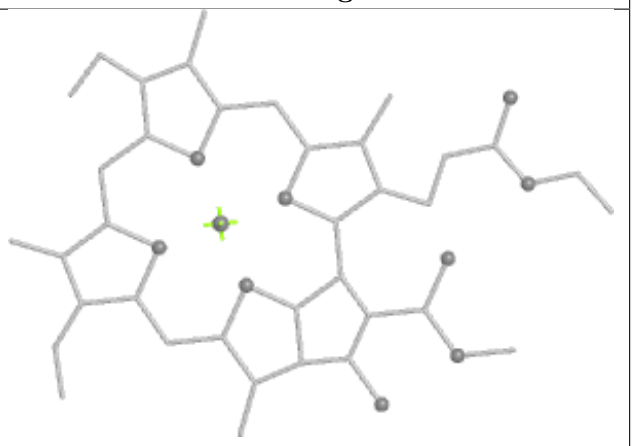

Rings

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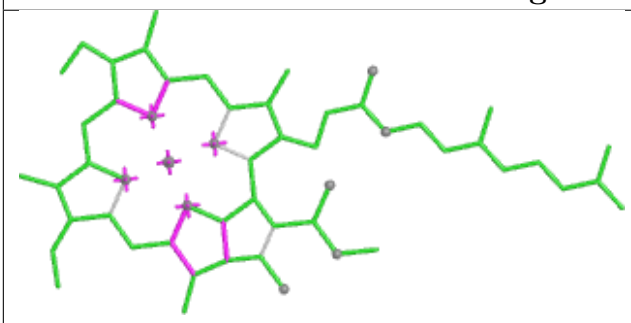

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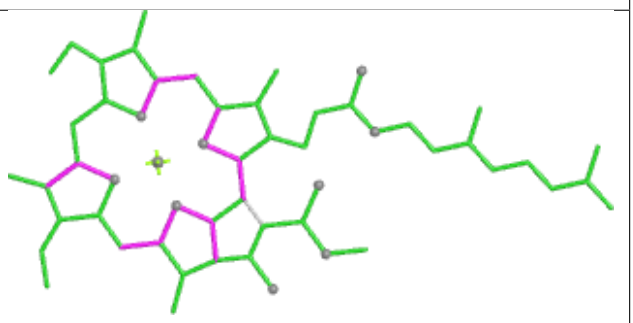
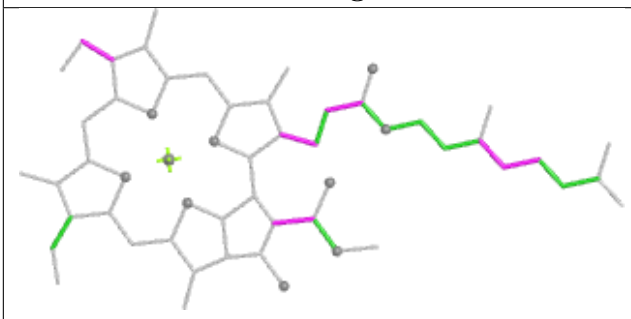


Bond angles



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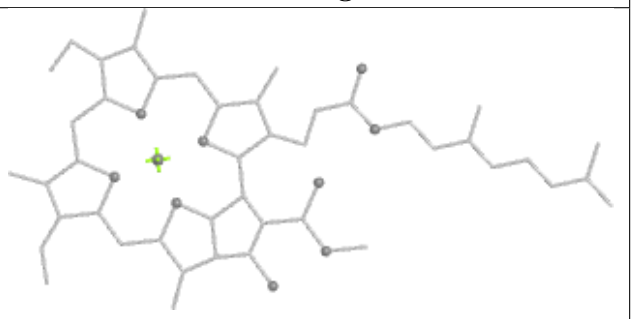

Rings

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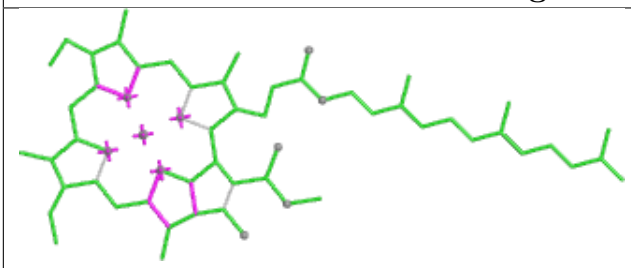
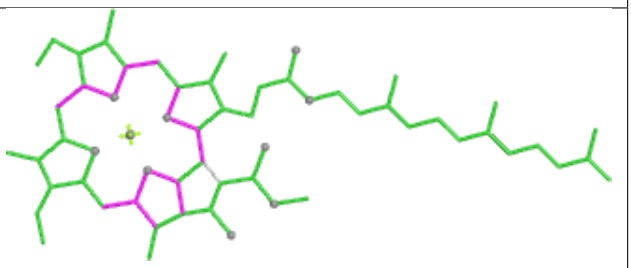
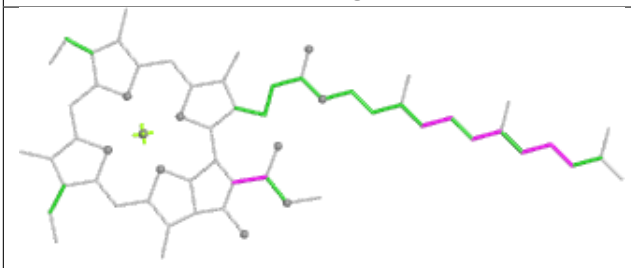
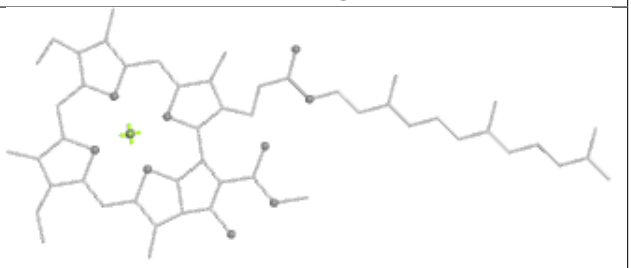
	
Bond lengths	Bond angles
	
Torsions	Rings

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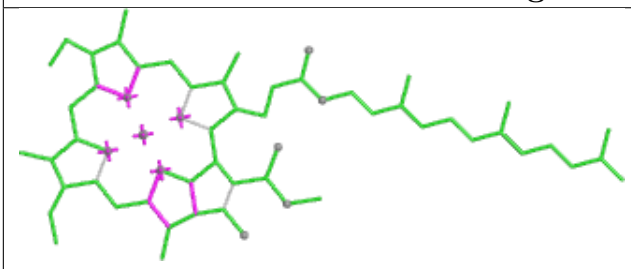
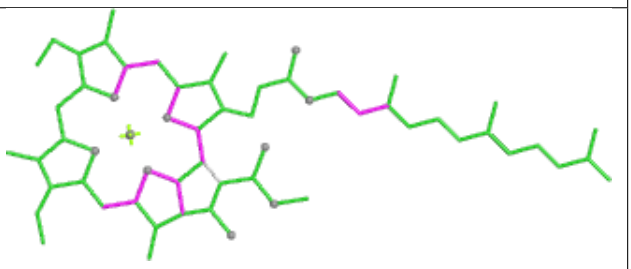
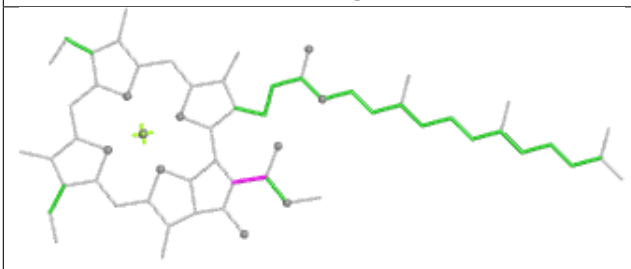
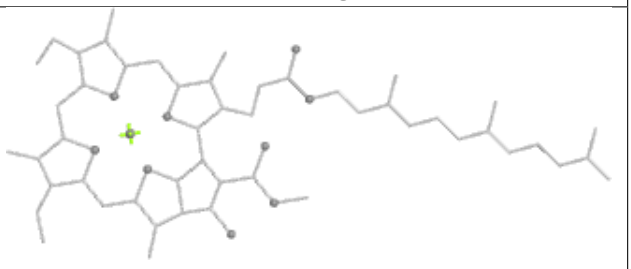
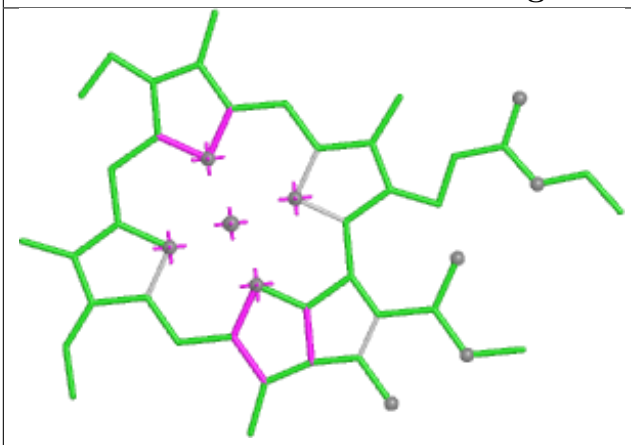
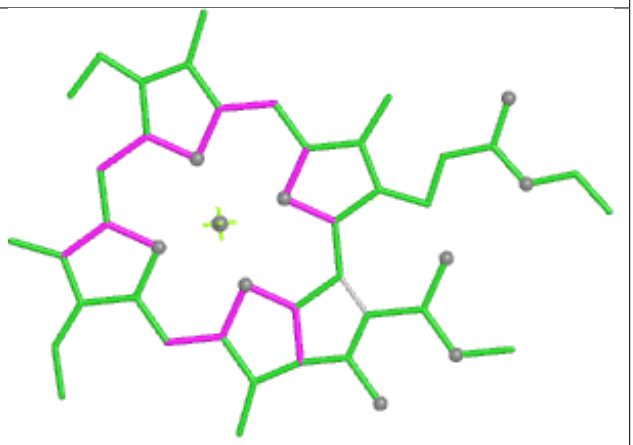
	
Bond lengths	Bond angles
	
Torsions	Rings

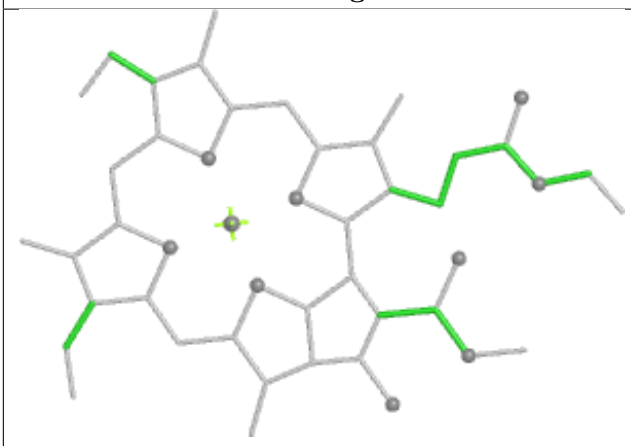
Ligand CLA h 210



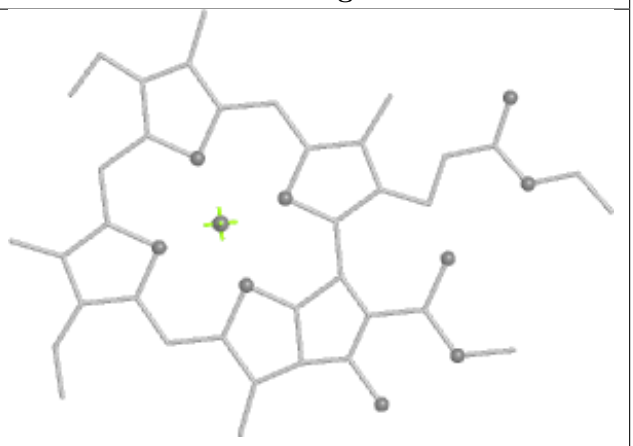
Bond lengths



Bond angles

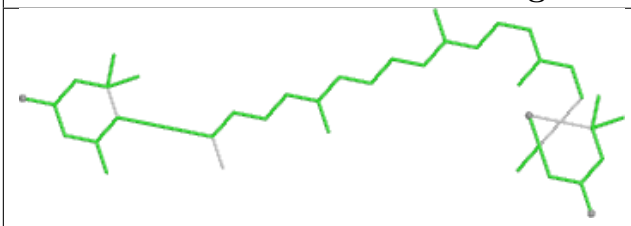


Torsions



Rings

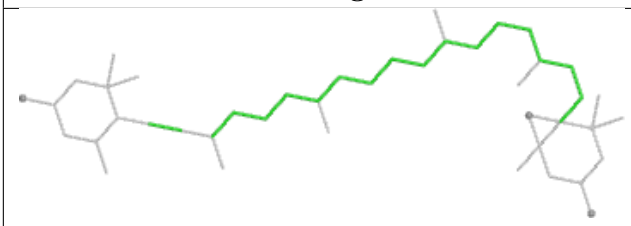
Ligand DD6 h 214



Bond lengths



Bond angles

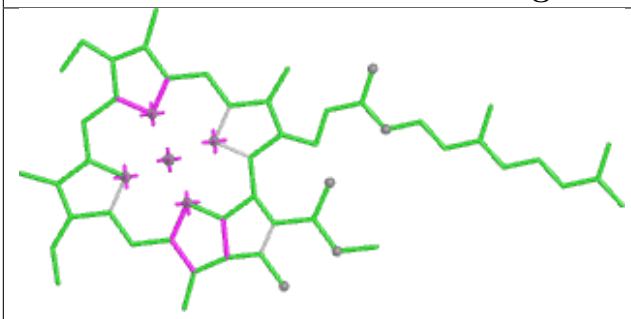


Torsions



Rings

Ligand CLA i 302



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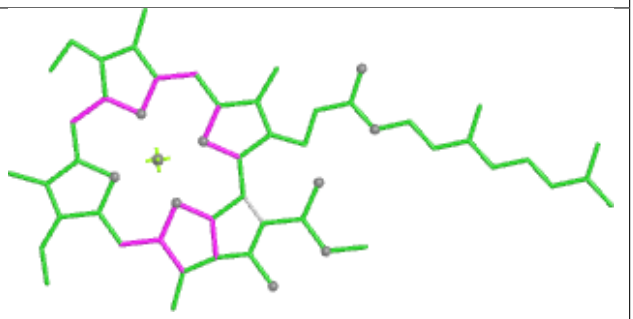
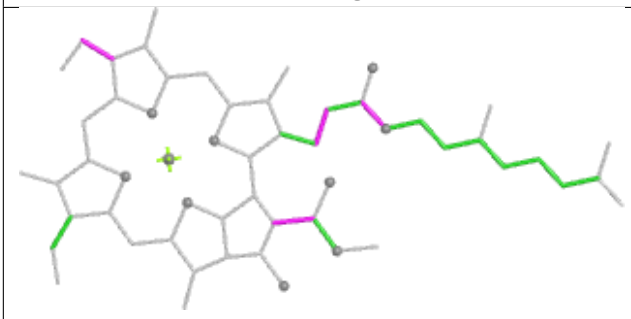
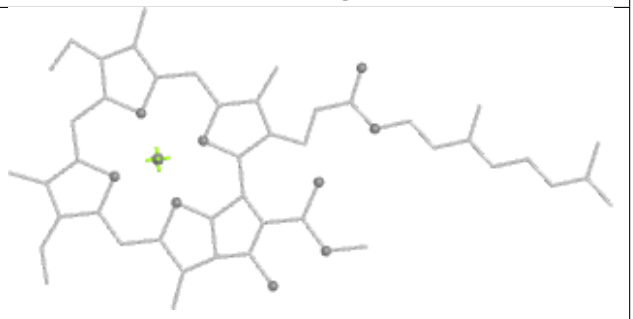


Bond angles

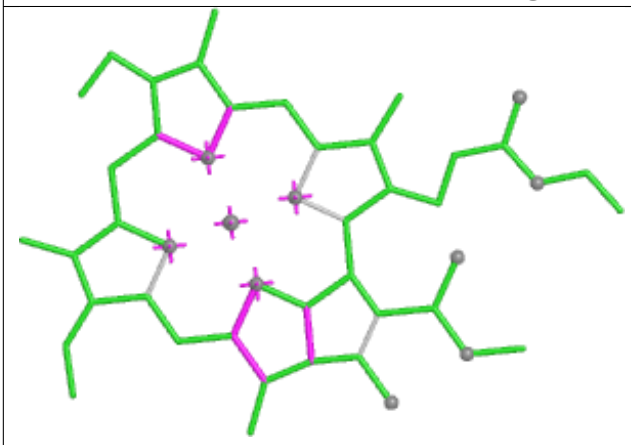


Torsions

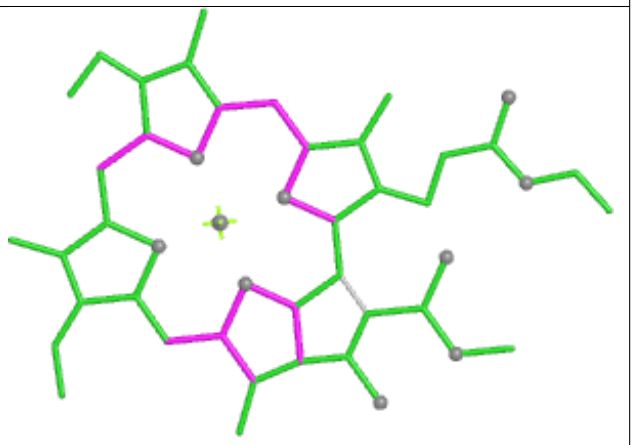


Rings

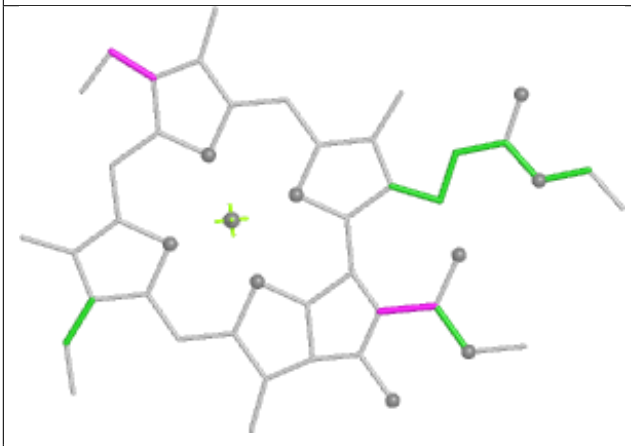
Ligand CLA B 845



Bond lengths



Bond angles



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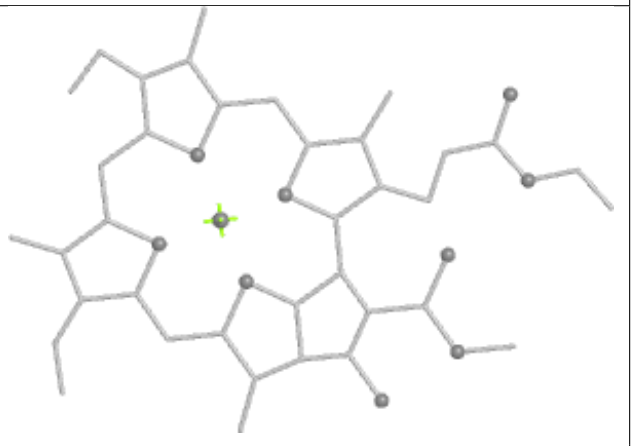
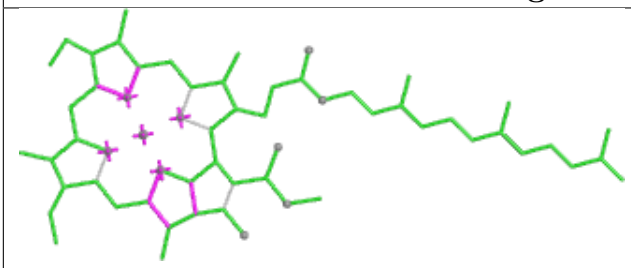
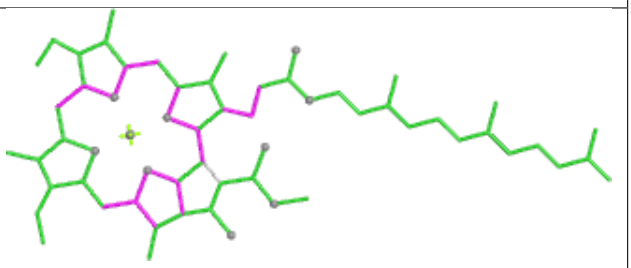
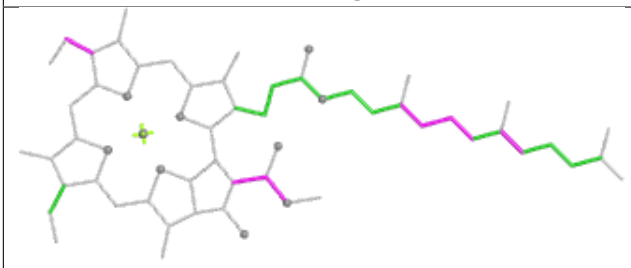
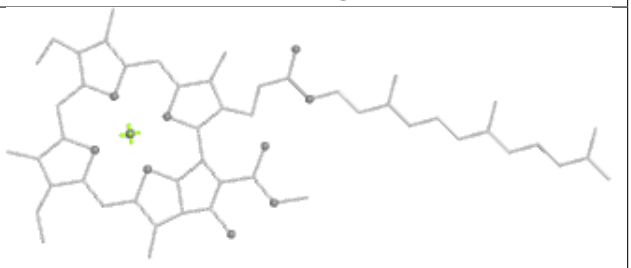
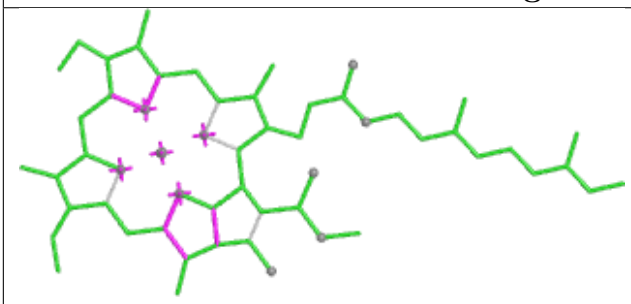
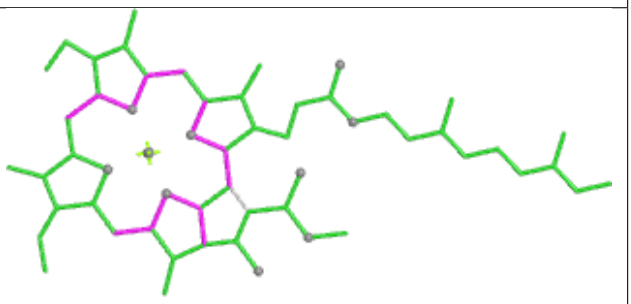
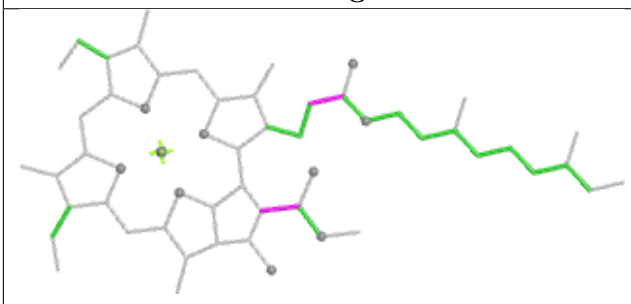
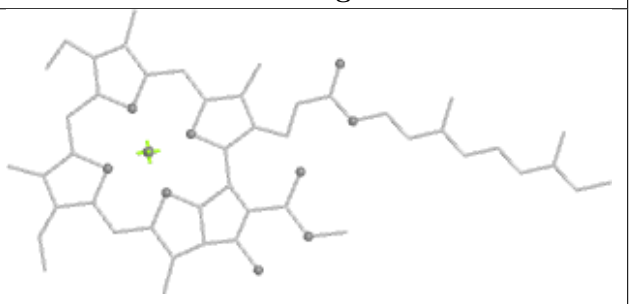
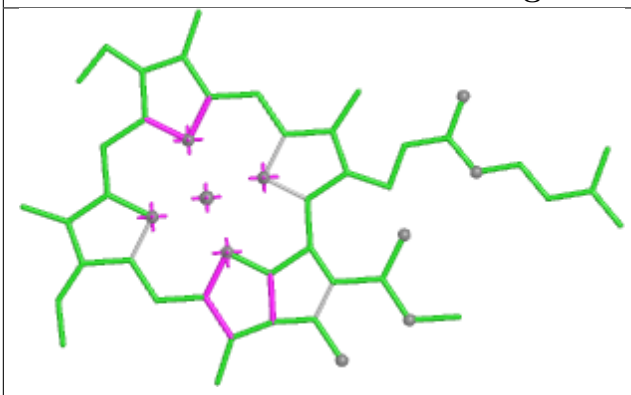


Rings

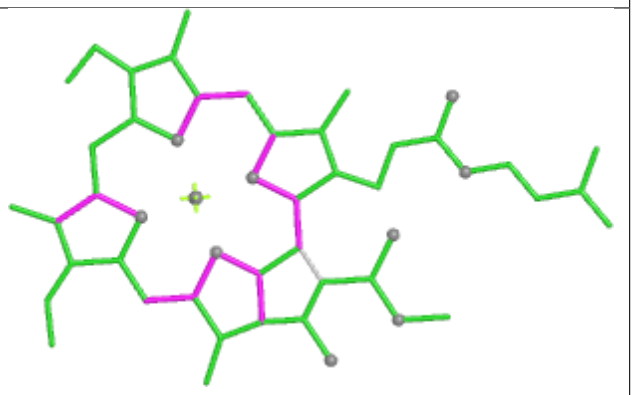
Ligand CLA k 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

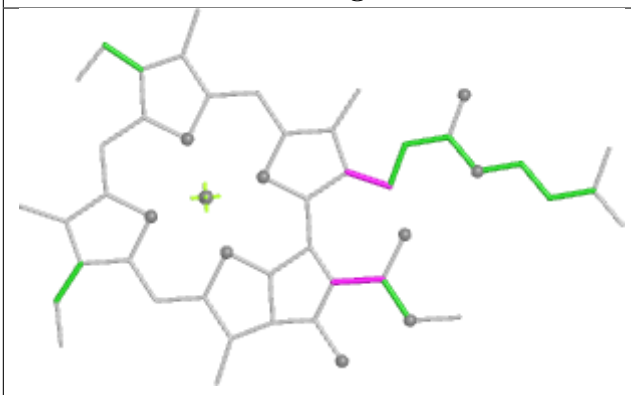
Ligand CLA A 826



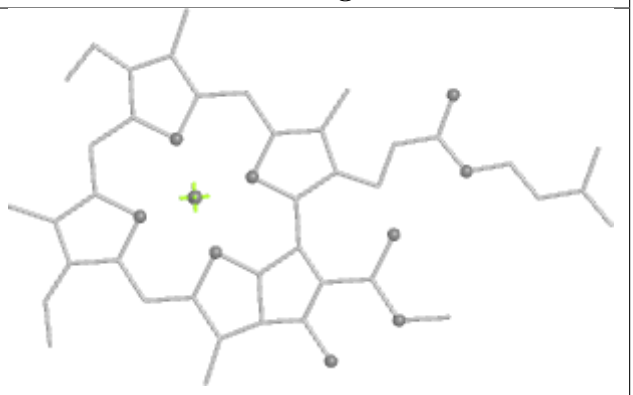
Bond lengths



Bond angles

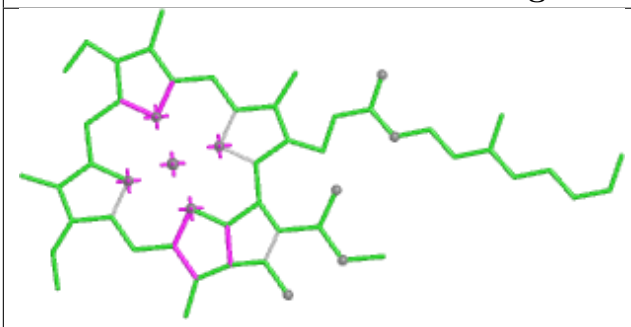


Torsions



Rings

Ligand CLA o 304



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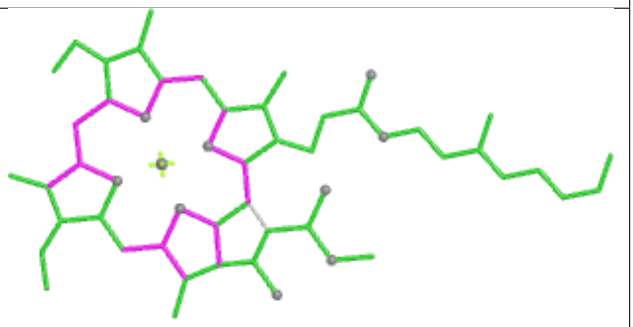
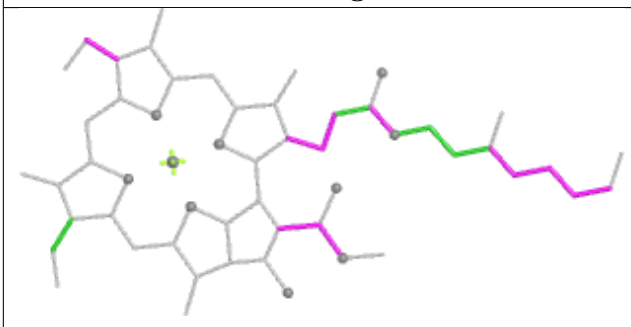


Bond angles



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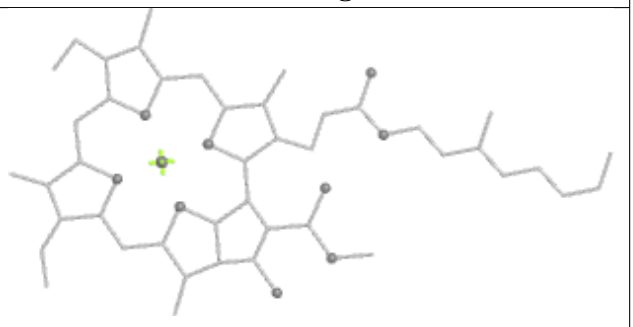
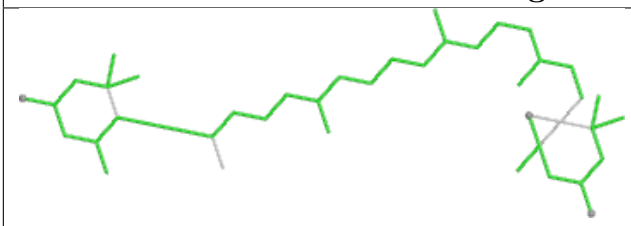


Rings

Ligand DD6 h 215



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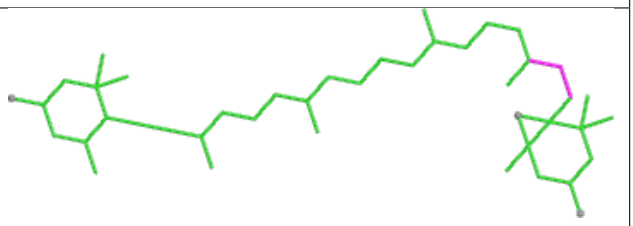
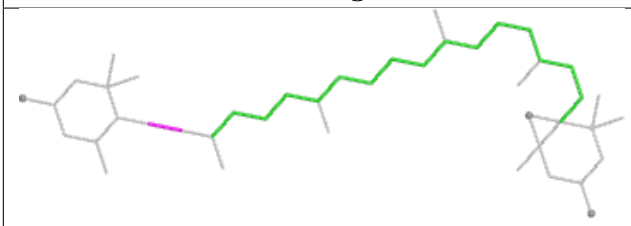


Bond angles



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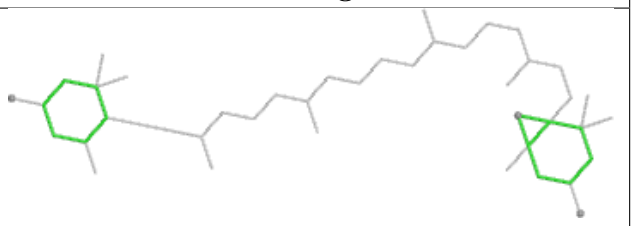
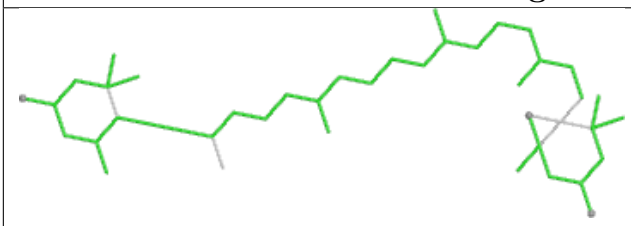


Rings

Ligand DD6 J 802



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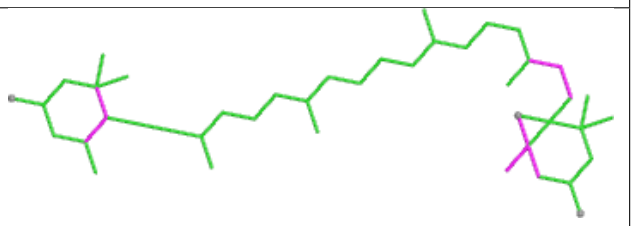
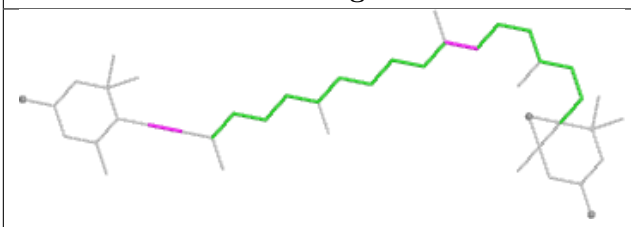
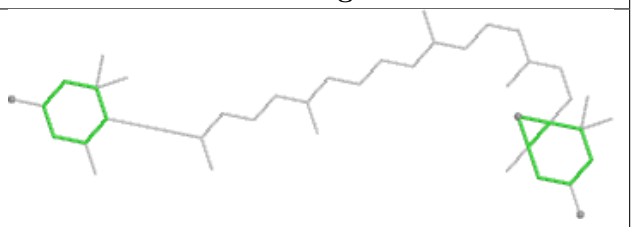


Bond angles

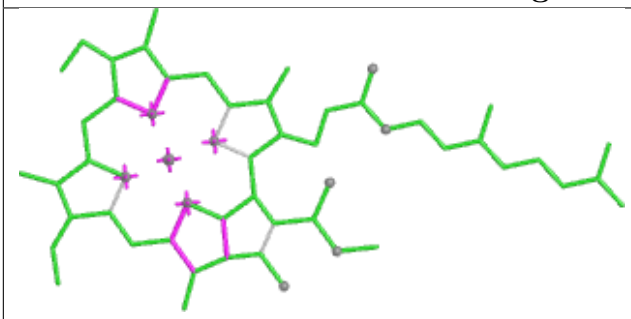


Torsions



Rings

Ligand CLA j 302



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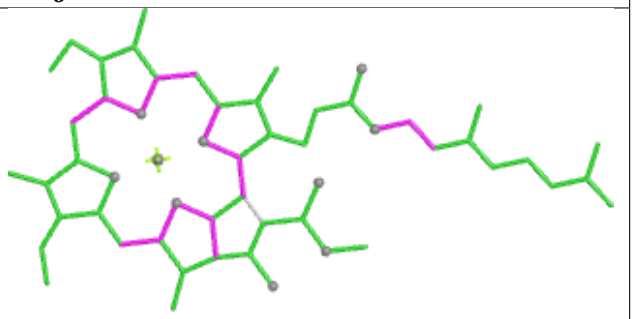
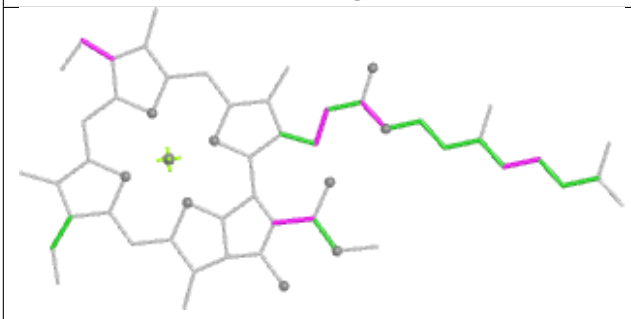


Bond angles



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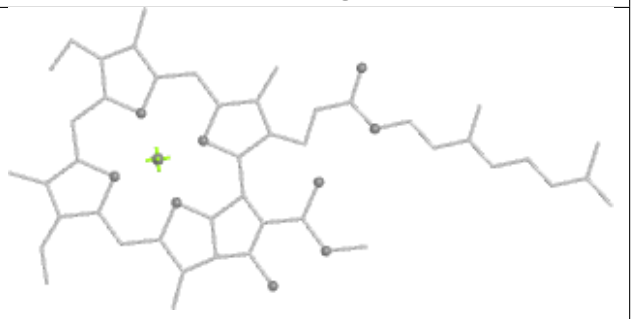
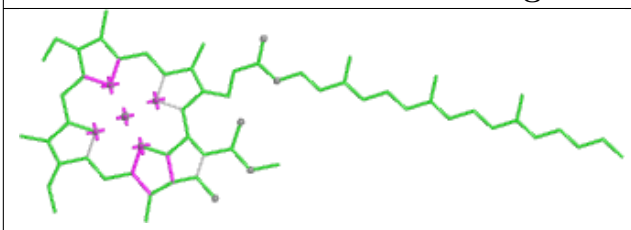


Rings

Ligand CLA A 818



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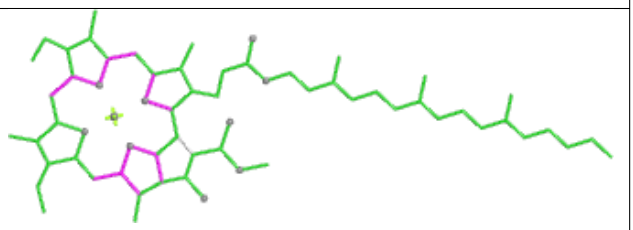
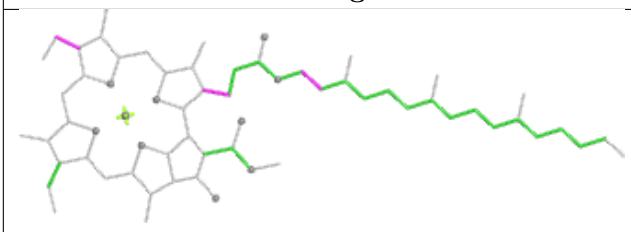


Bond angles



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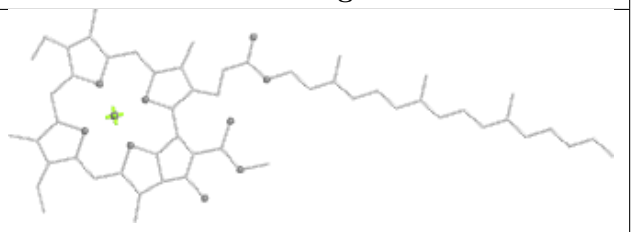
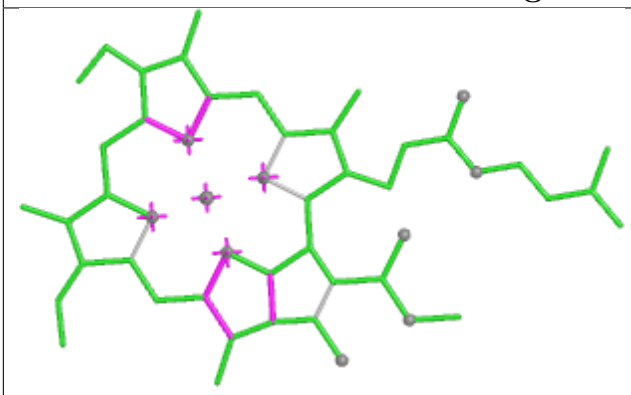


Rings

Ligand CLA B 832



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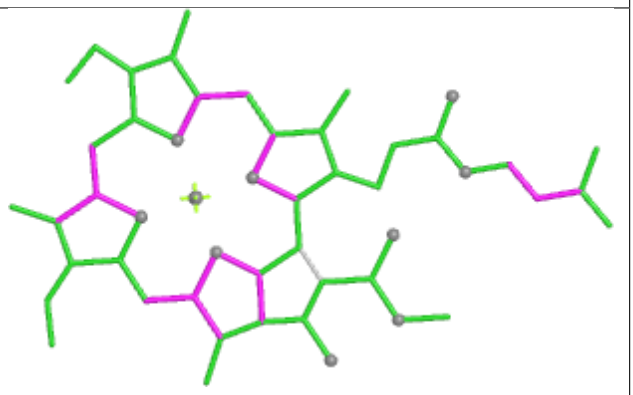
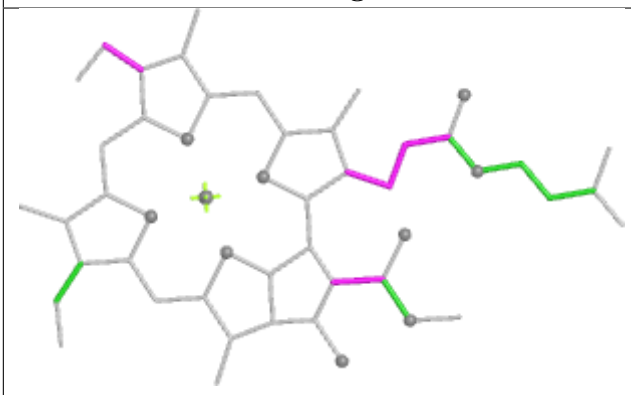
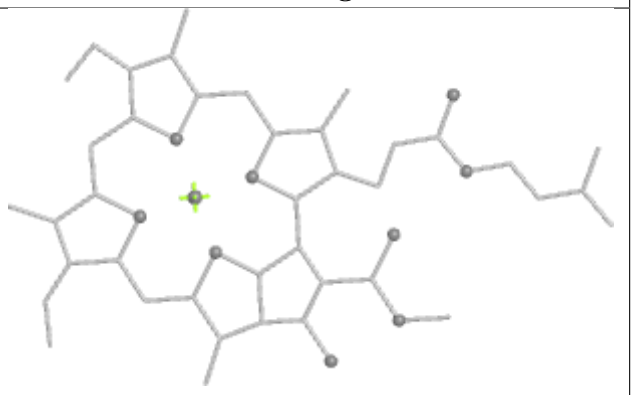


Bond angles

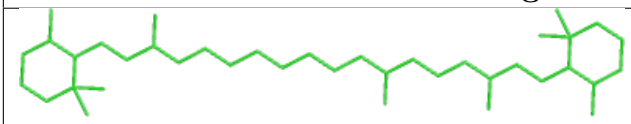


Torsions

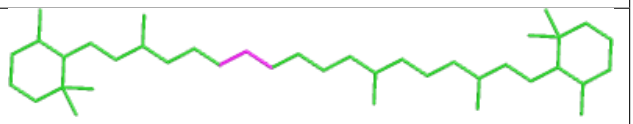


Rings

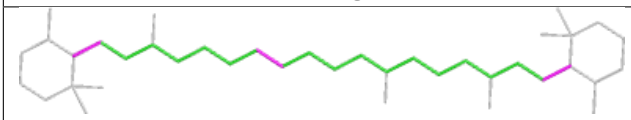
Ligand BCR A 835



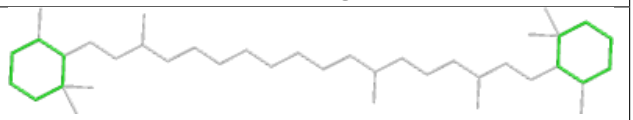
Bond lengths



Bond angles

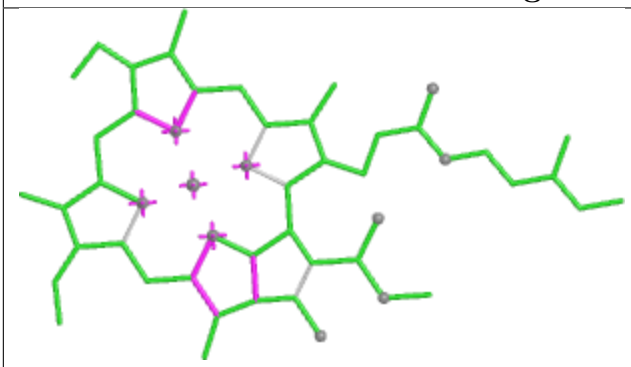


Torsions

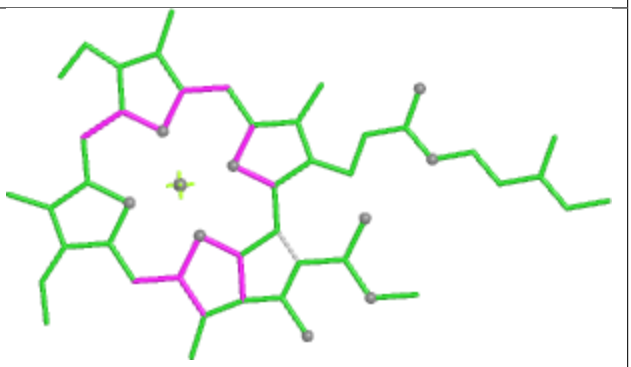


Rings

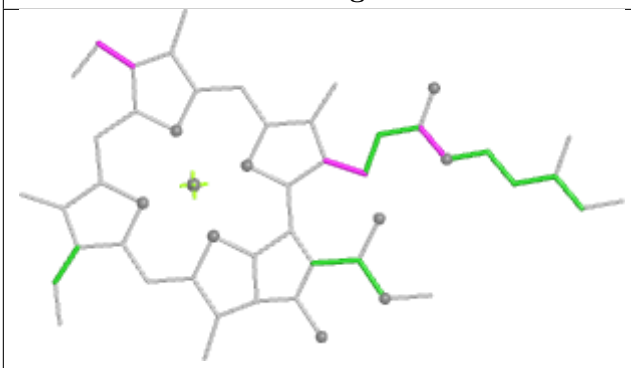
Ligand CLA A 815



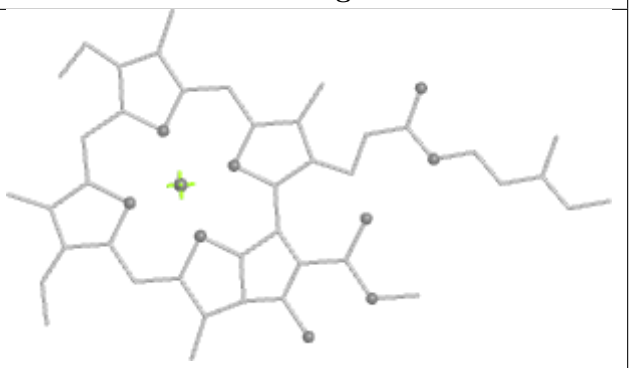
Bond lengths



Bond angles

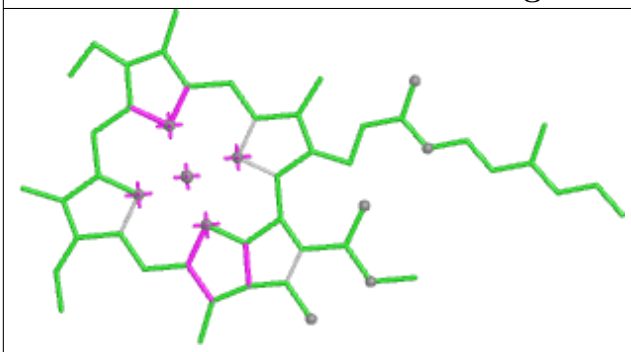


Torsions

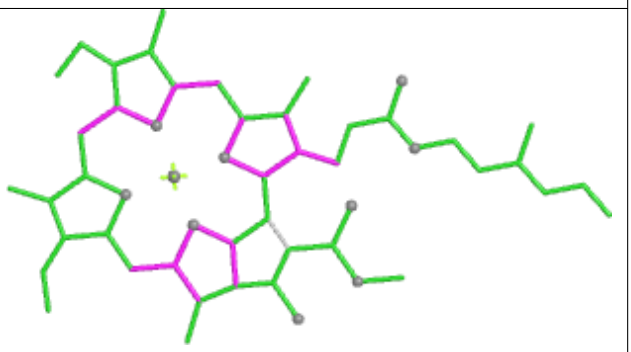


Rings

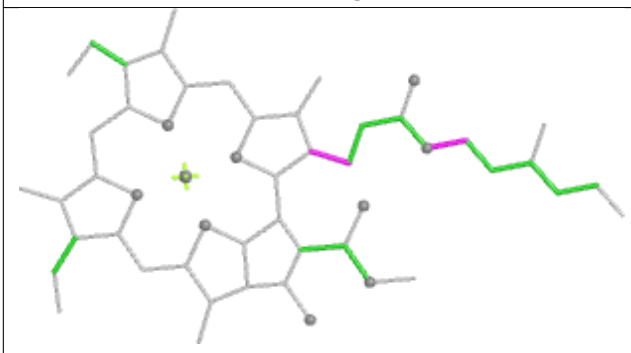
Ligand CLA A 805



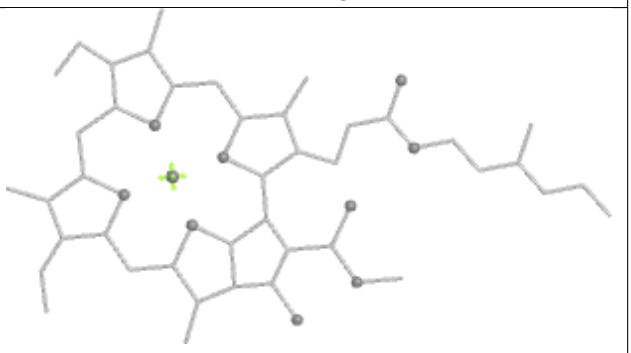
Bond lengths



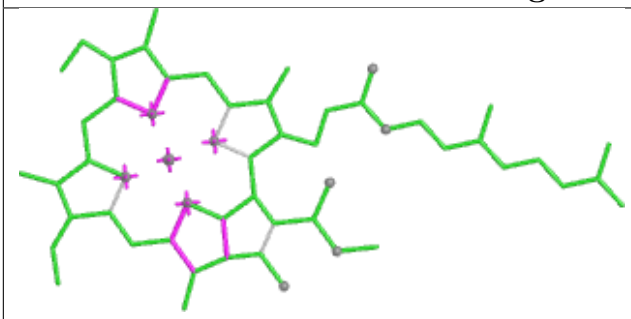
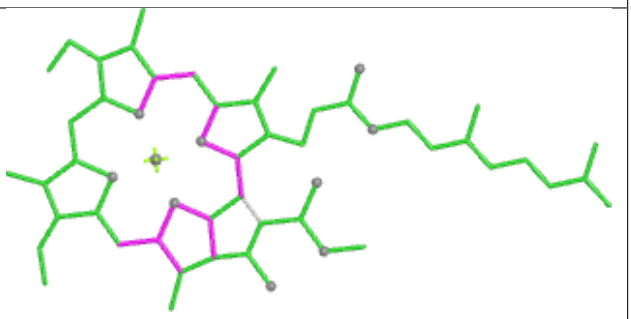
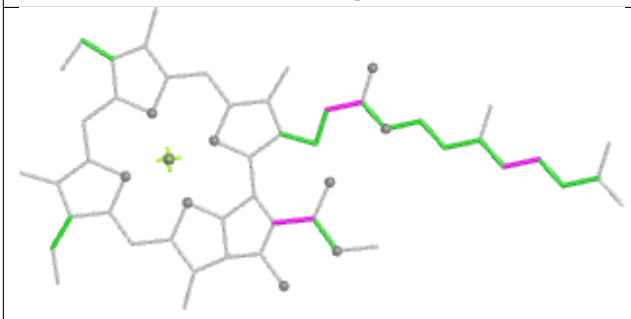
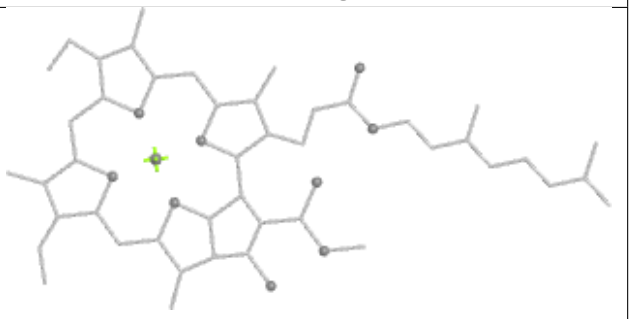
Bond angles



Torsions



Rings

Ligand CLA a 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

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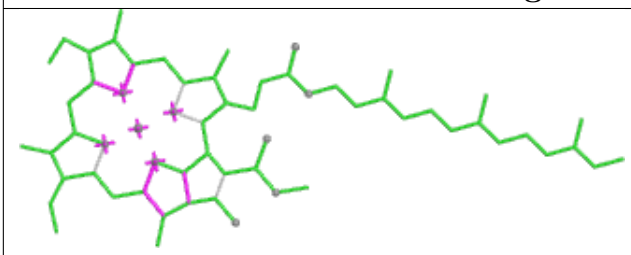
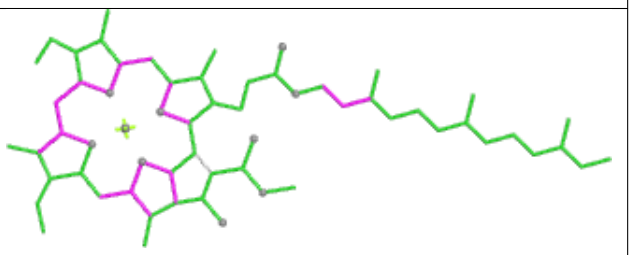
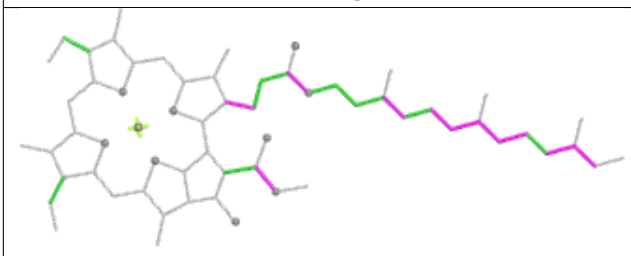
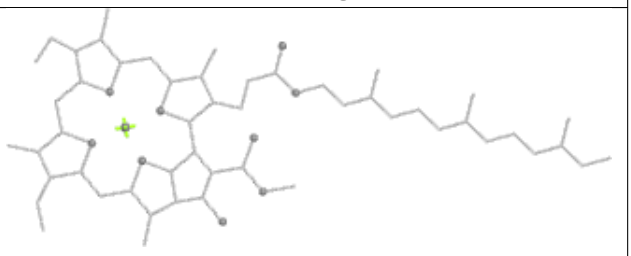
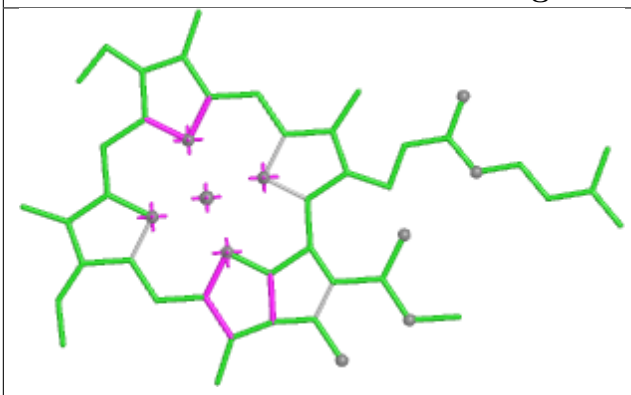
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 311



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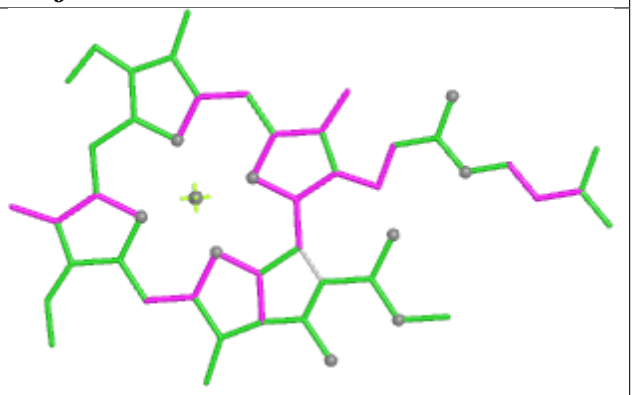

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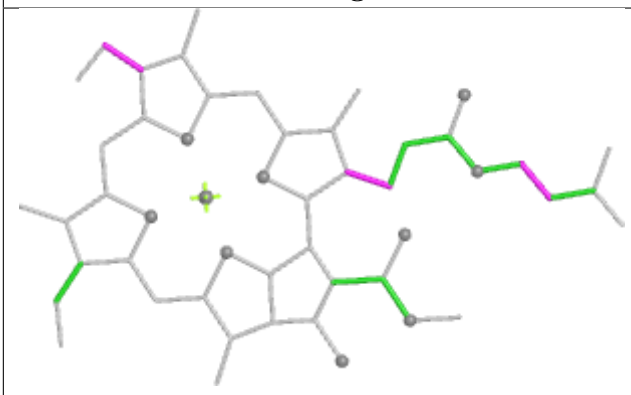

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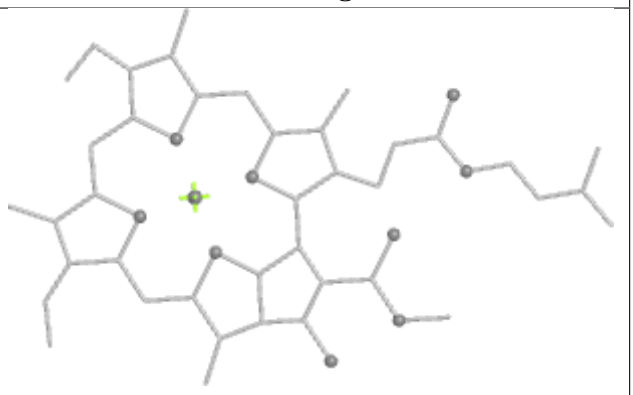
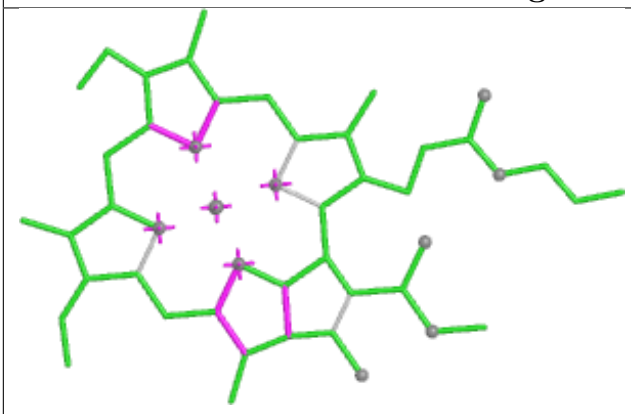


Rings

Ligand CLA o 303



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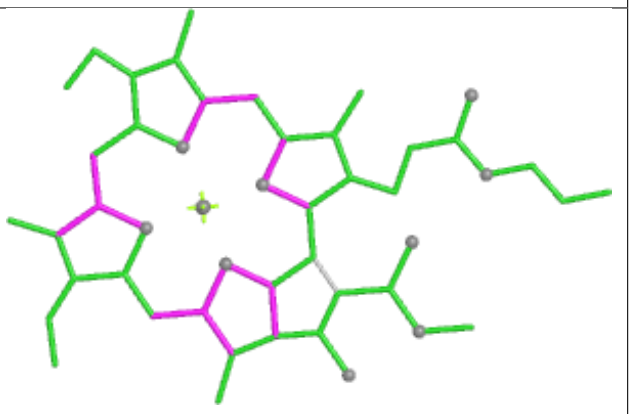
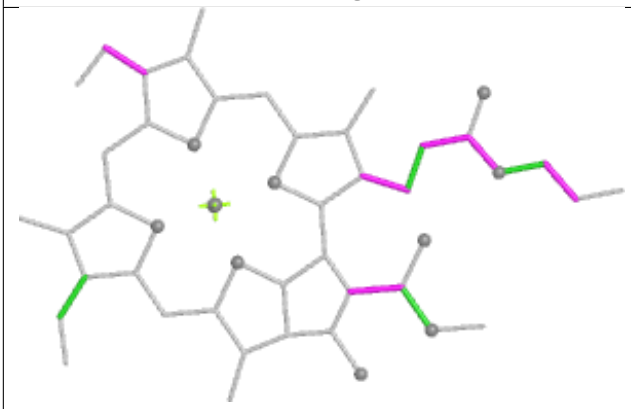


Bond angles



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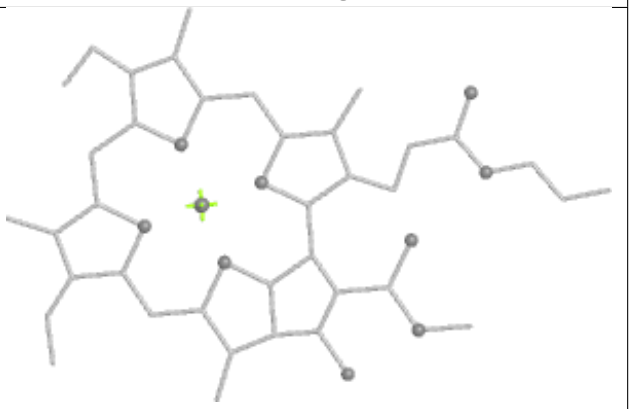
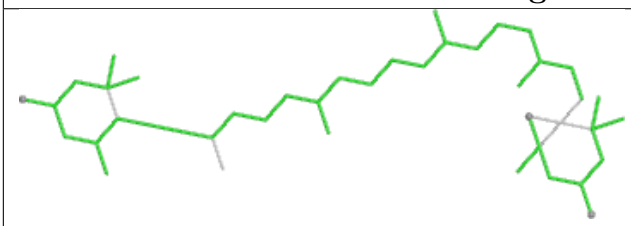


Rings

Ligand DD6 o 314



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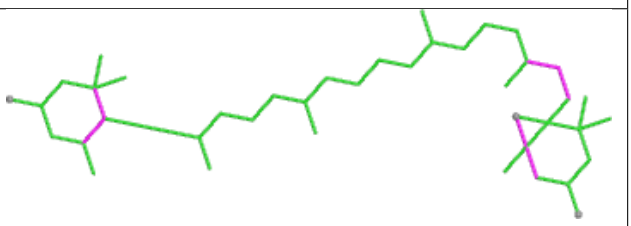

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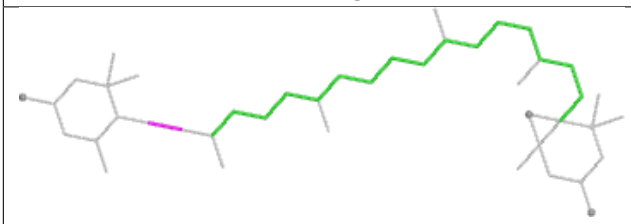
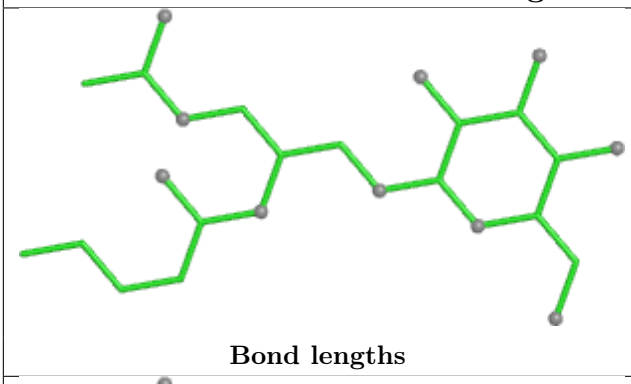


Torsions



Rings

Ligand LMG f 313



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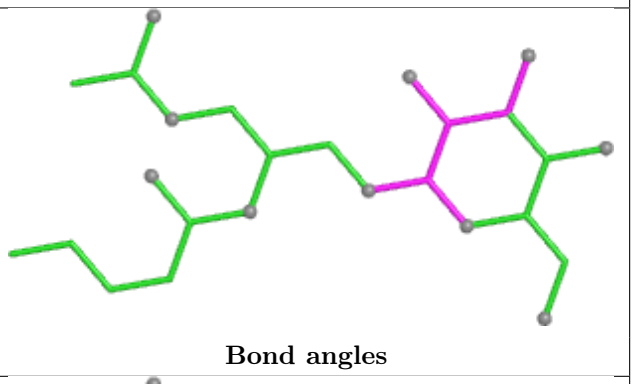
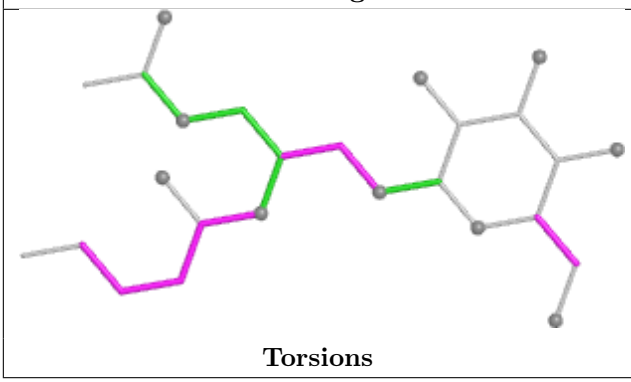


Bond angles



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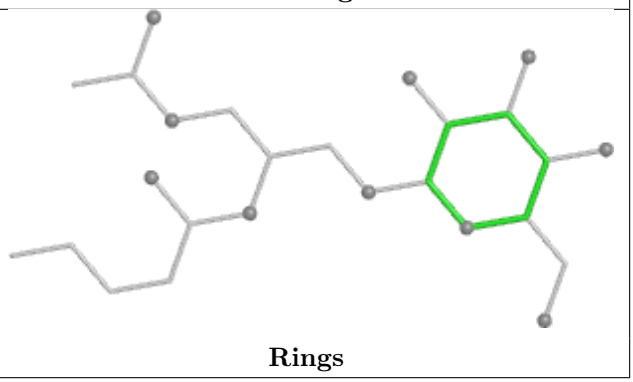
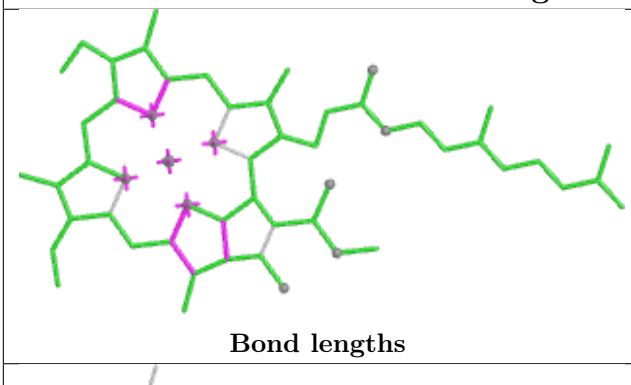


Rings

Ligand CLA f 302



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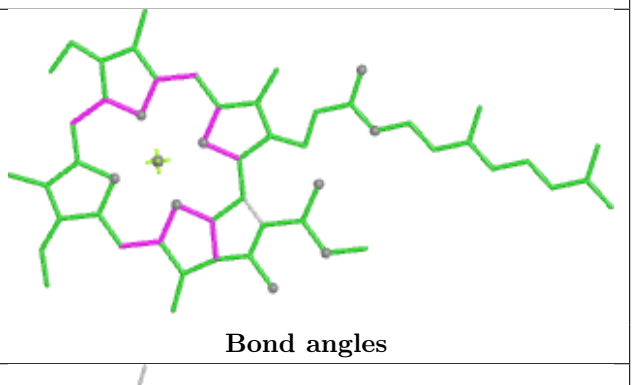
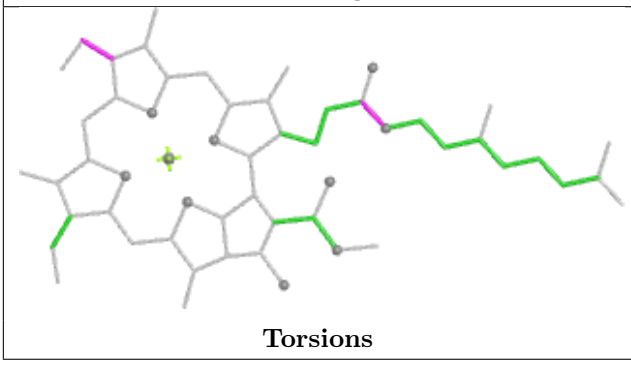


Bond angles



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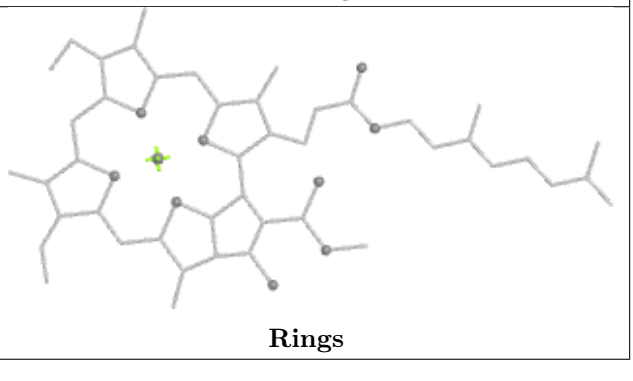
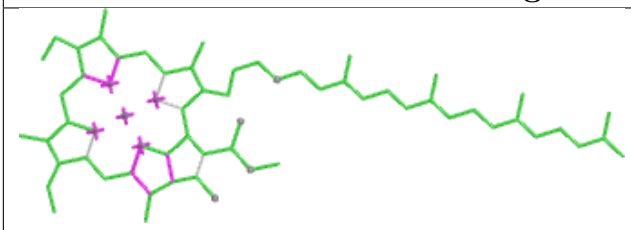


Rings

Ligand CLA A 819



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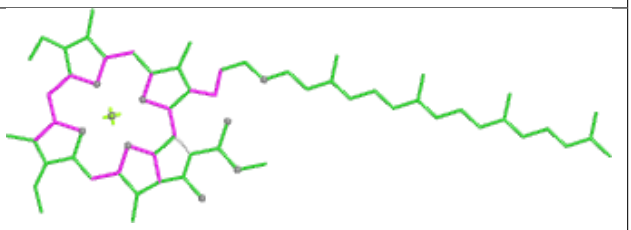
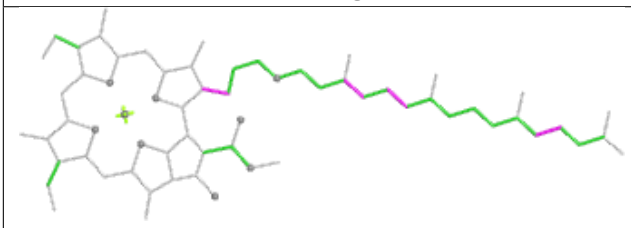


Bond angles



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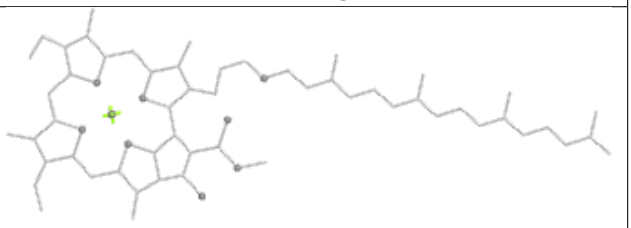
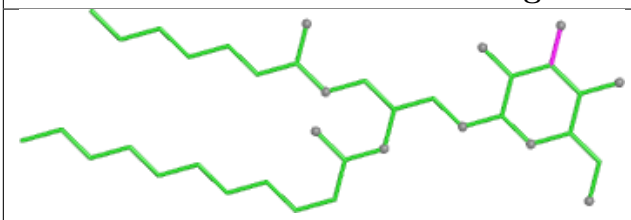


Rings

Ligand LMG g 312



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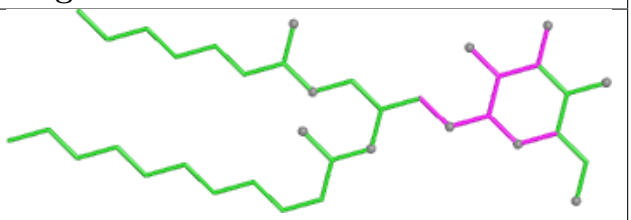
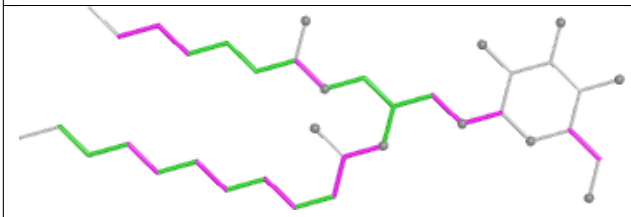


Bond angles



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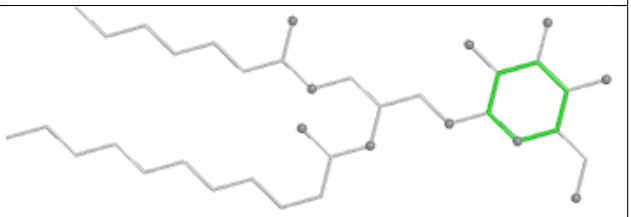
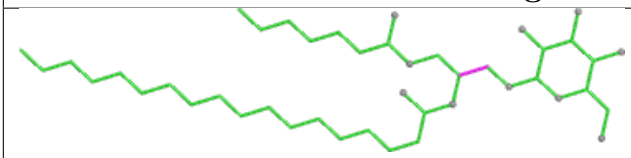


Rings

Ligand LMG e 312



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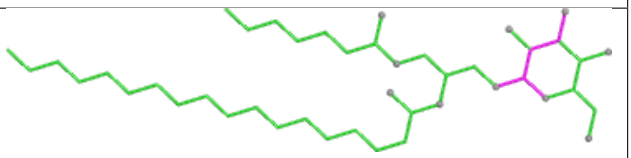

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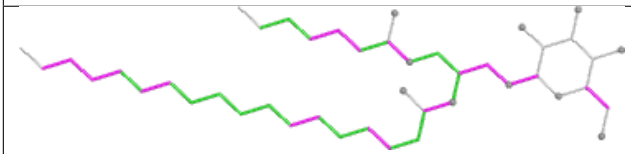
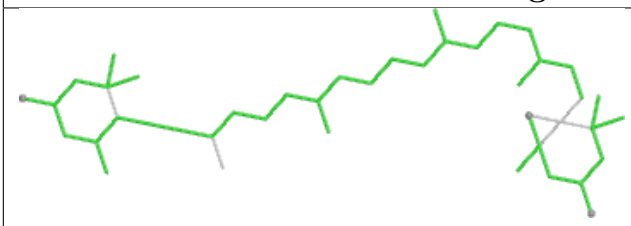


Torsions



Rings

Ligand DD6 k 314



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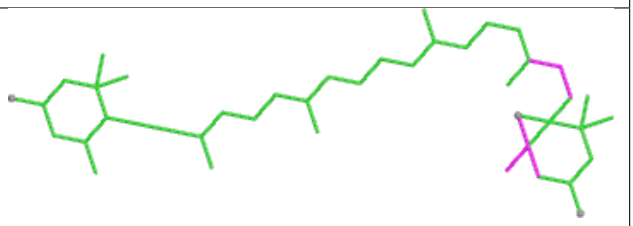
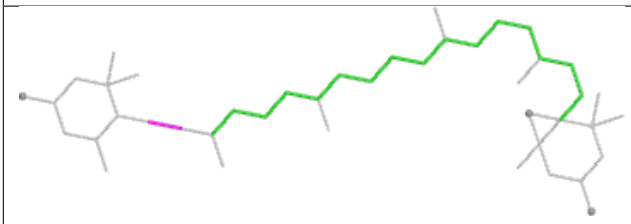


Bond angles



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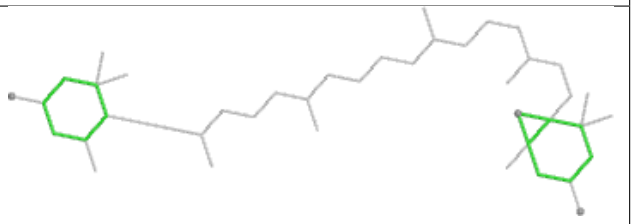
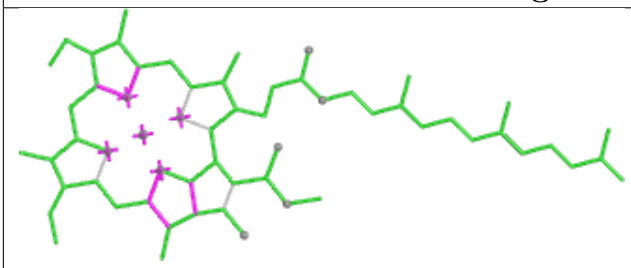


Rings

Ligand CLA j 307



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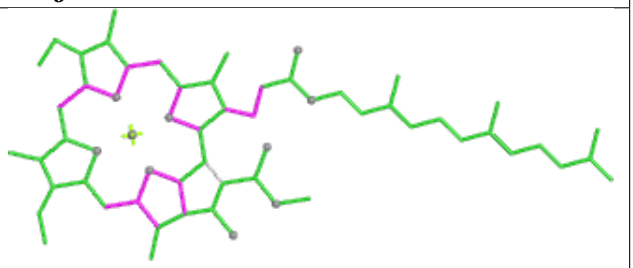
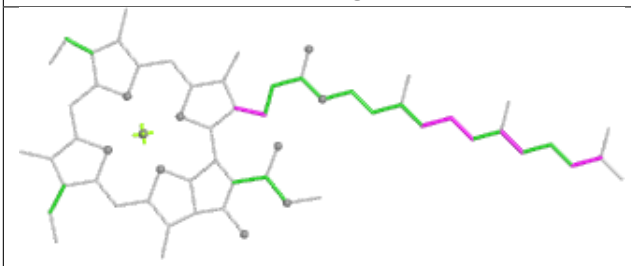


Bond angles



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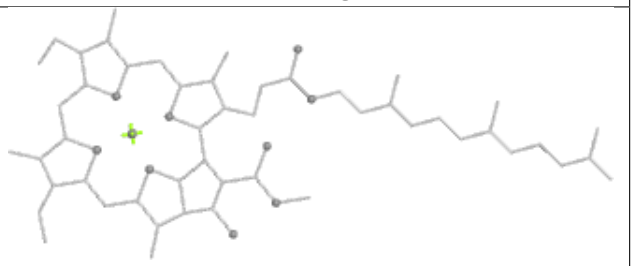
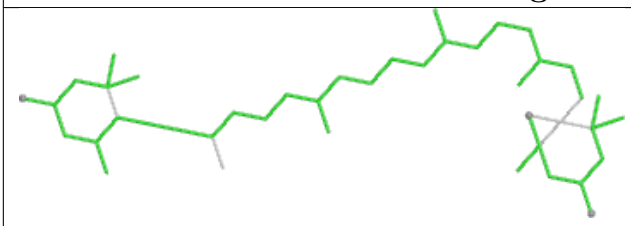


Rings

Ligand DD6 c 317



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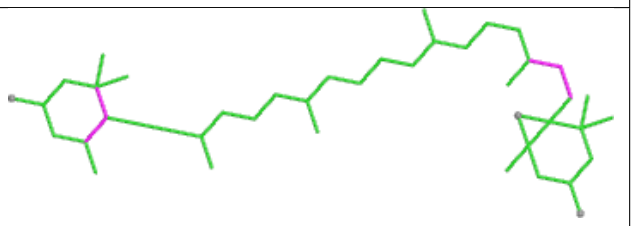
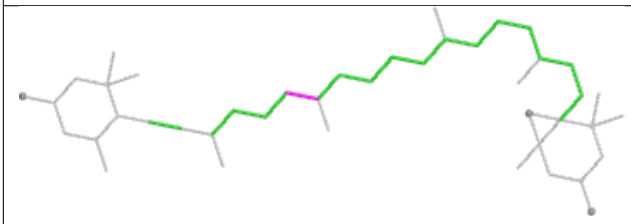


Bond angles



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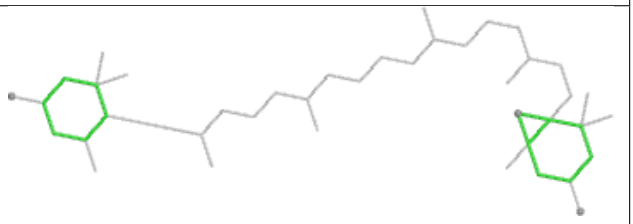
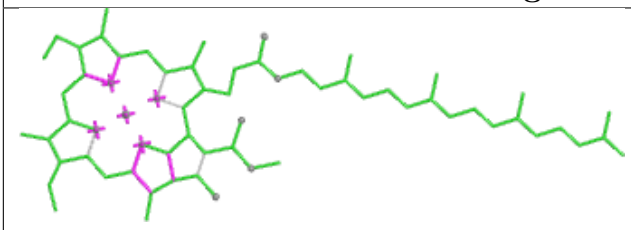


Rings

Ligand CLA A 824



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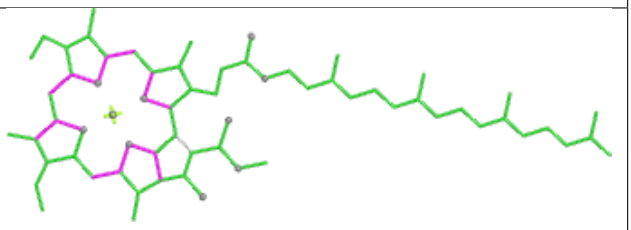
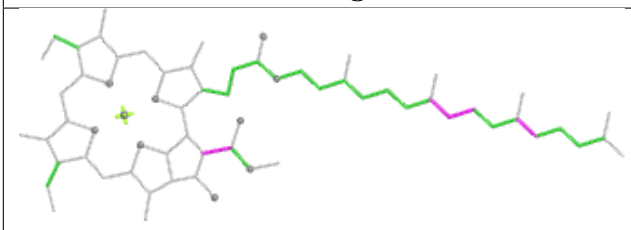


Bond angles



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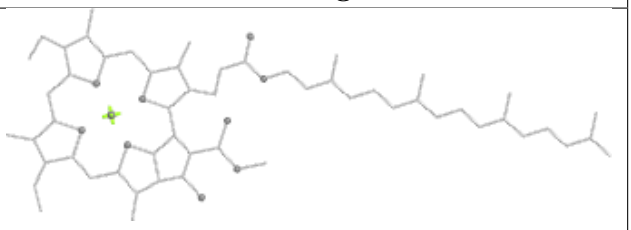
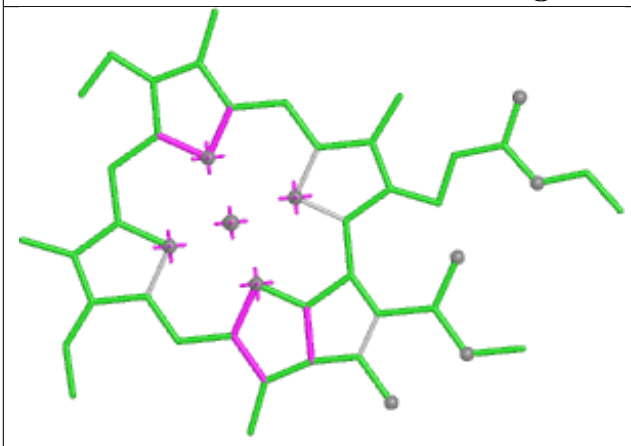
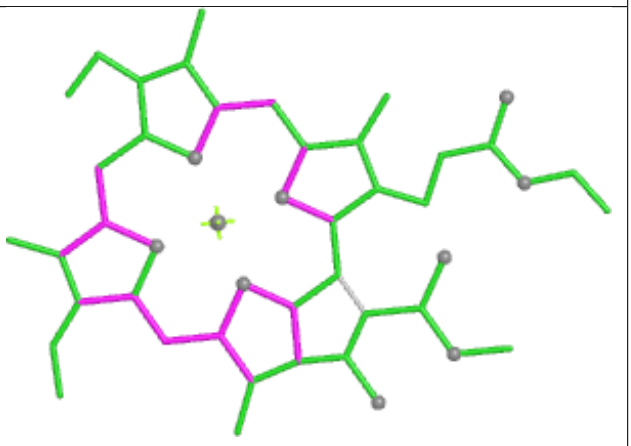


Rings

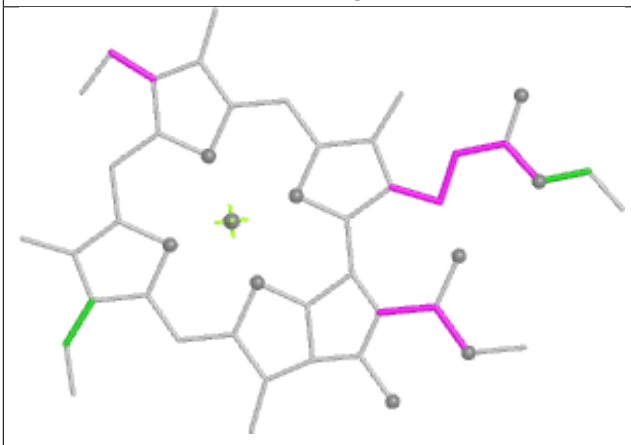
Ligand CLA i 310



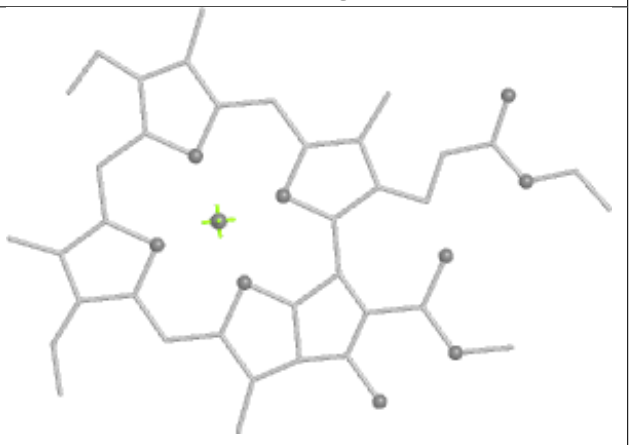
Bond lengths



Bond angles

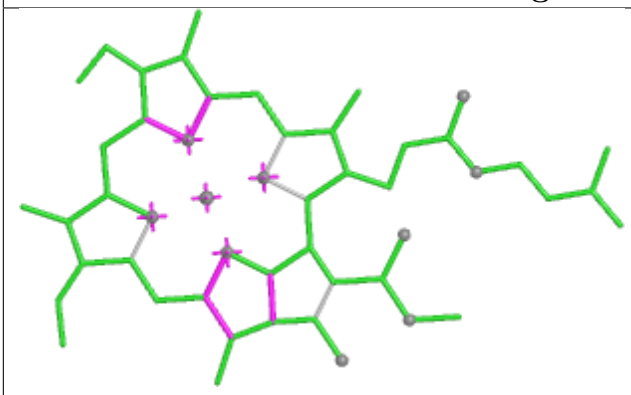


Torsions

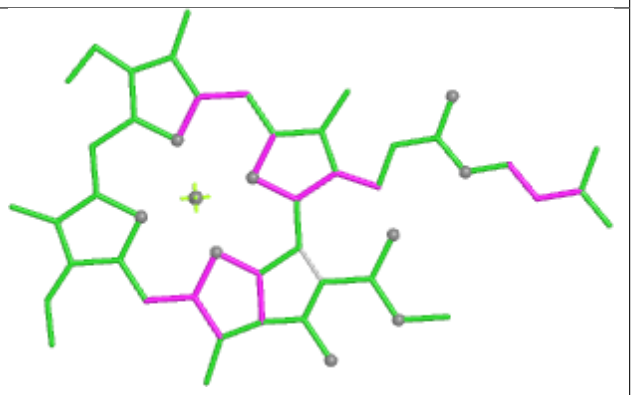


Rings

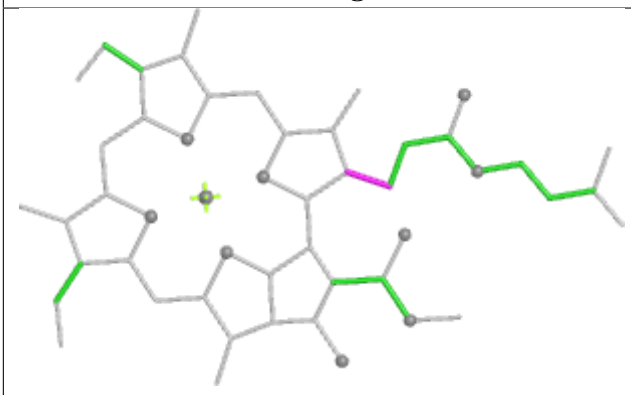
Ligand CLA f 305



Bond lengths



Bond angles



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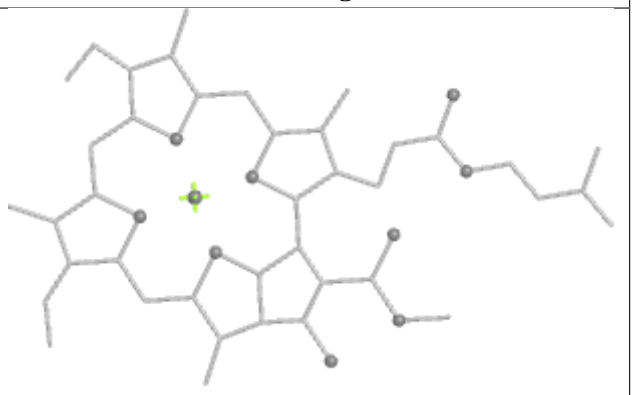
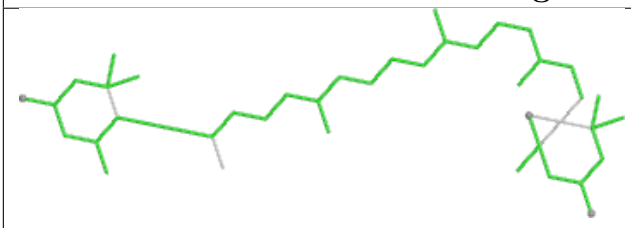


Rings

Ligand DD6 f 315



Bond lengths



Bond angles

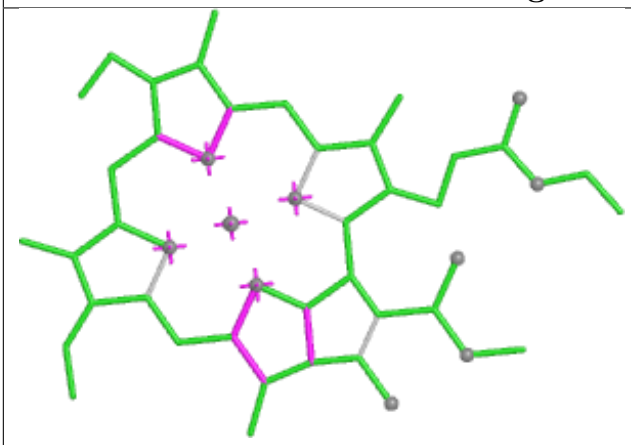


Torsions



Rings

Ligand CLA k 306



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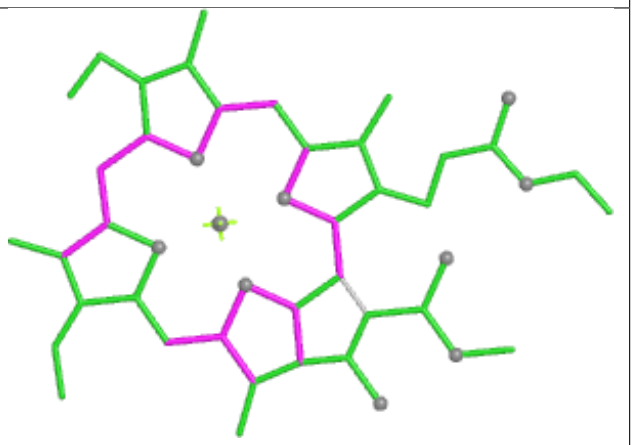
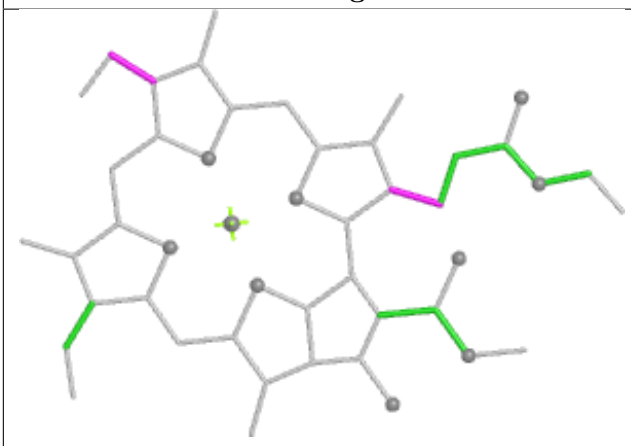


Bond angles



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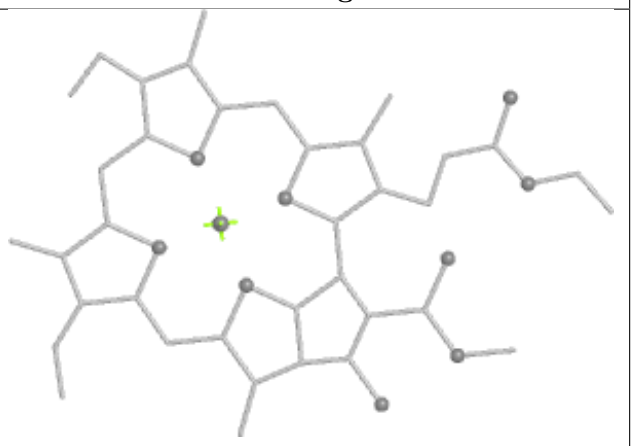
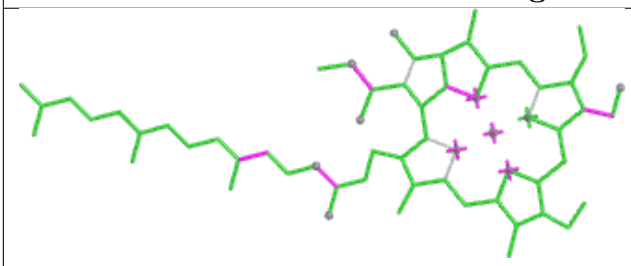


Rings

Ligand CHL e 304



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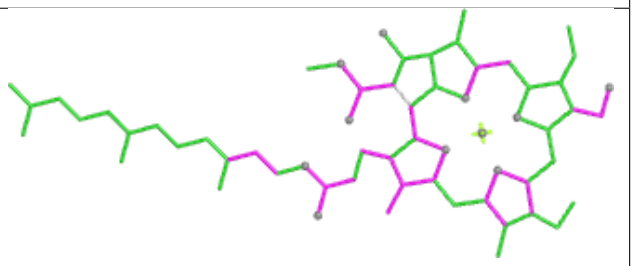
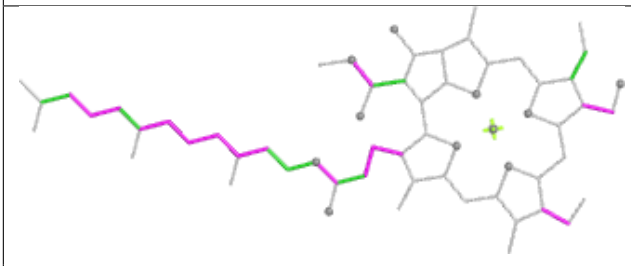


Bond angles



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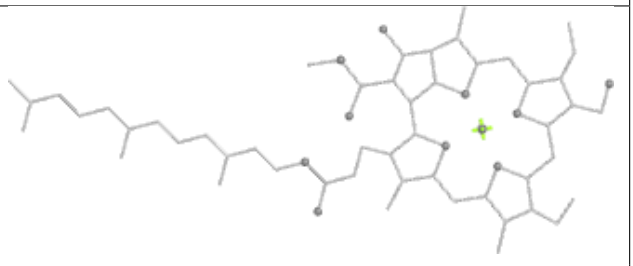
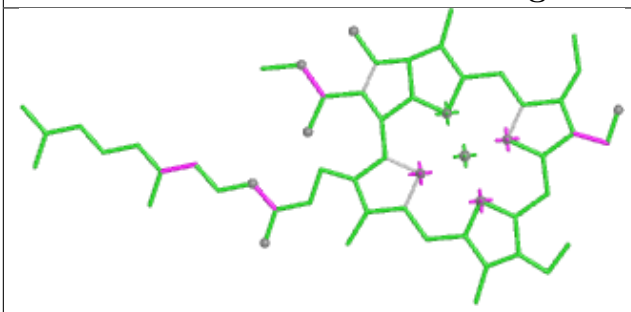


Rings

Ligand CHL c 312



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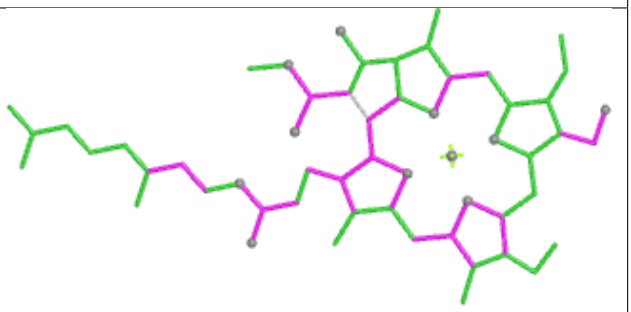
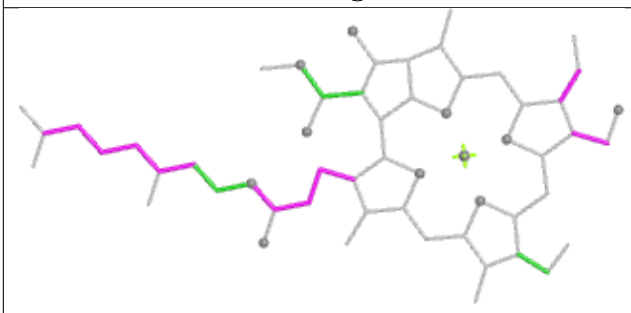


Bond angles



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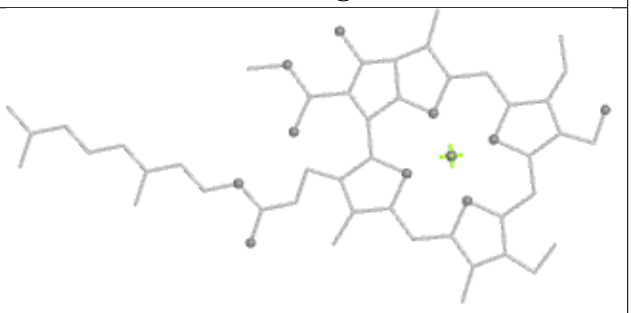
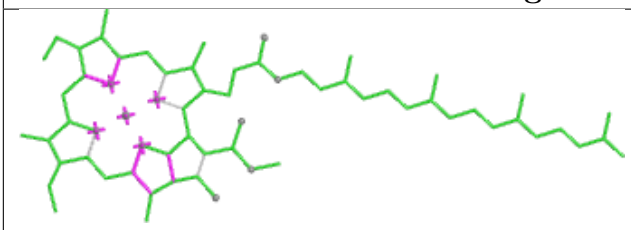


Rings

Ligand CLA B 839



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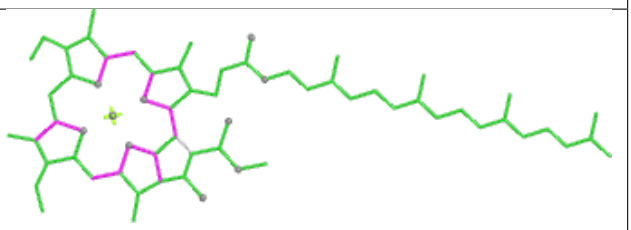
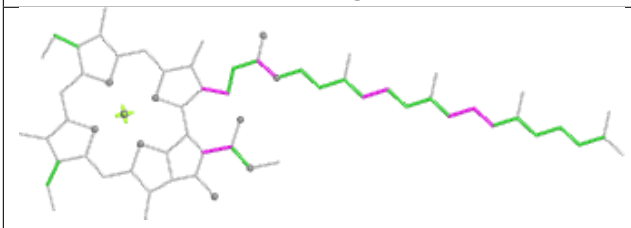


Bond angles



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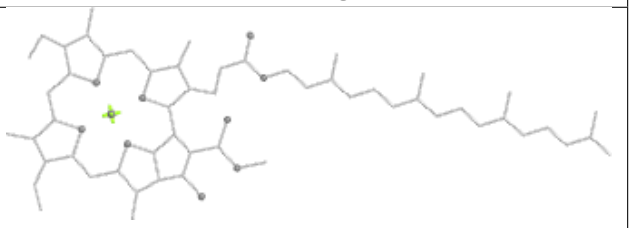
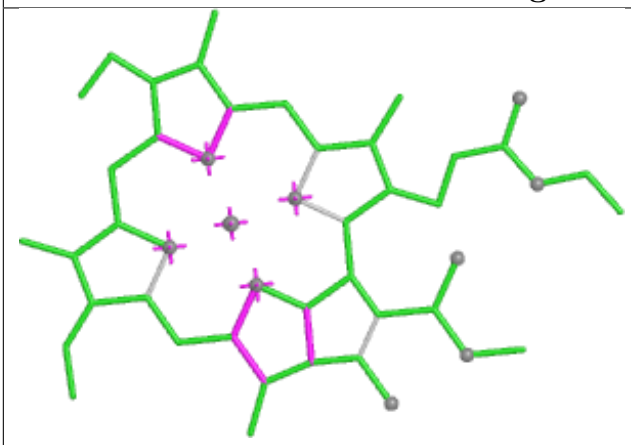


Rings

Ligand CLA c 314



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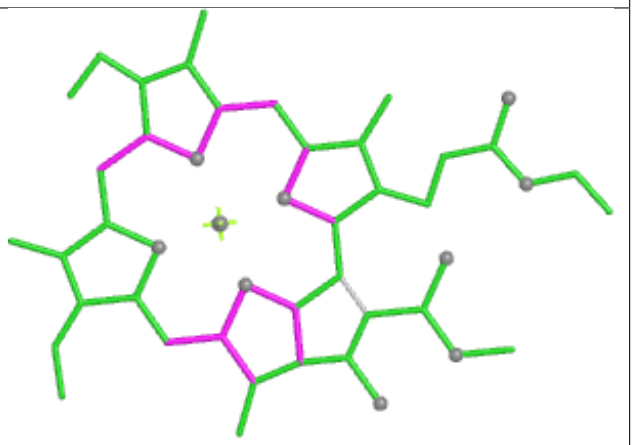
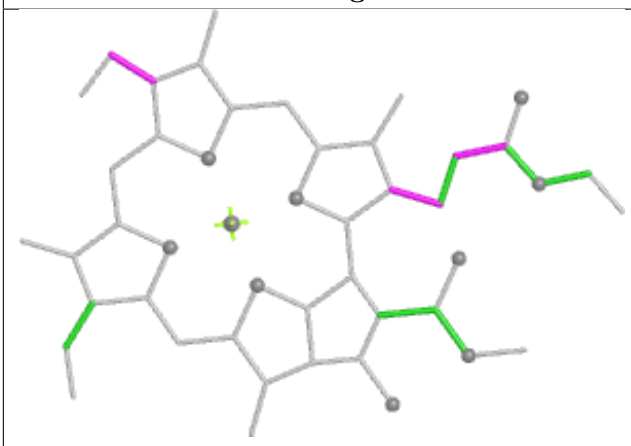


Bond angles



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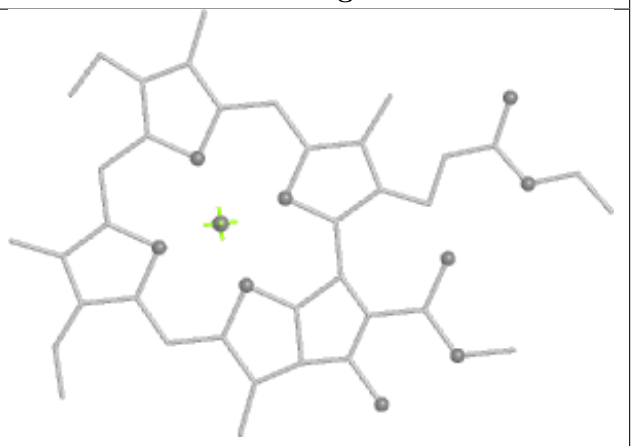
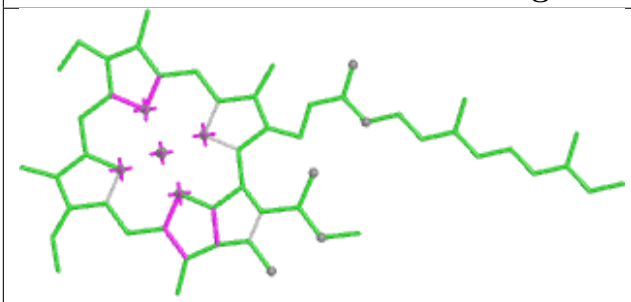


Rings

Ligand CLA j 313



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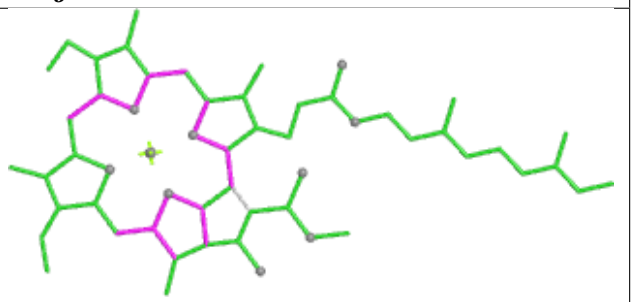

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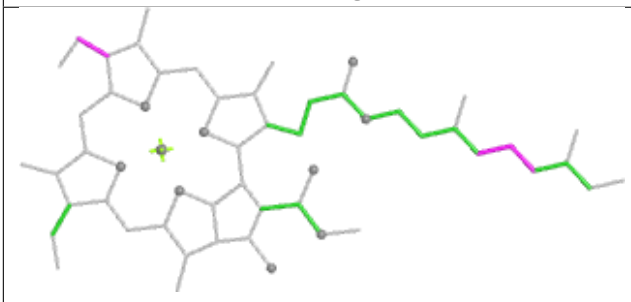

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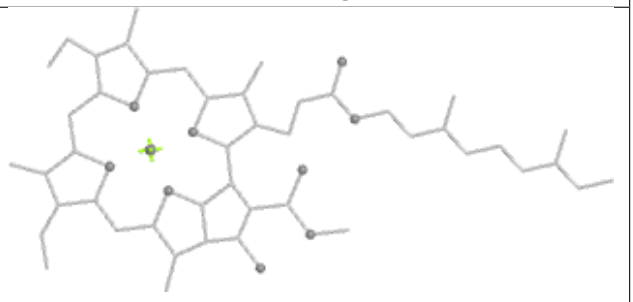
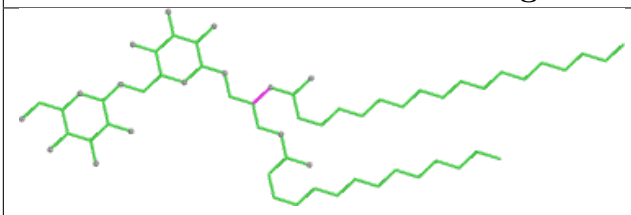


Rings

Ligand DGD B 829



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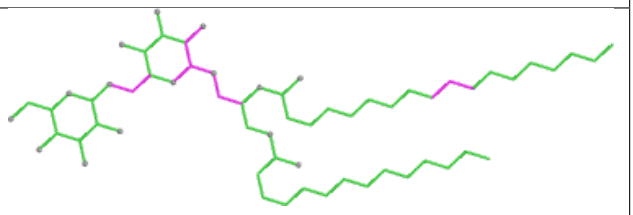
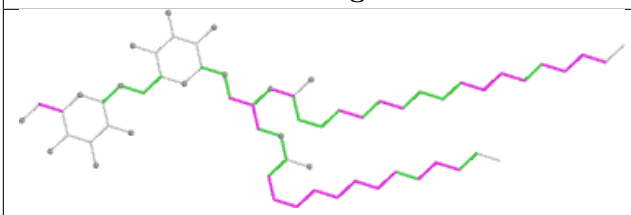


Bond angles



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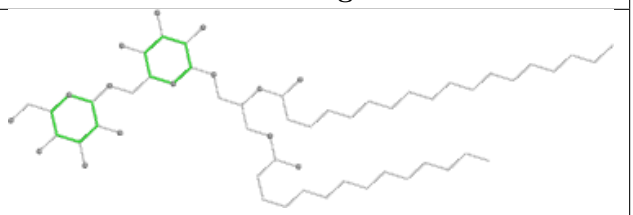
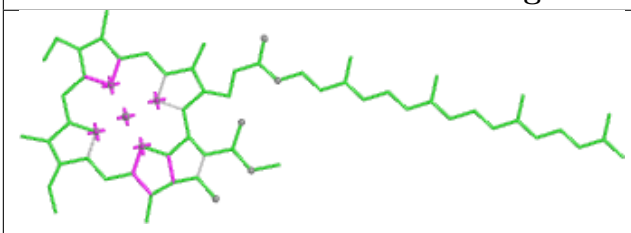


Rings

Ligand CLA A 817



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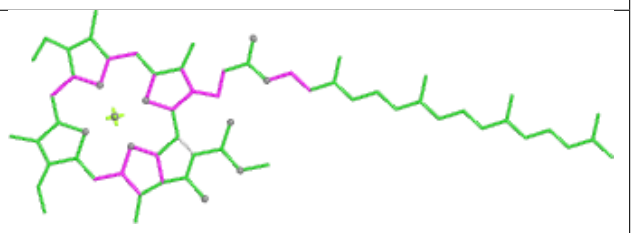

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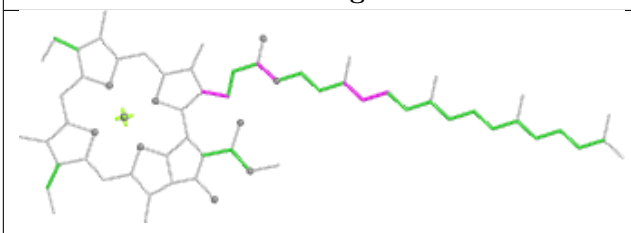

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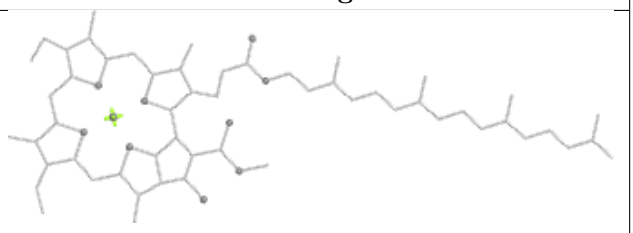
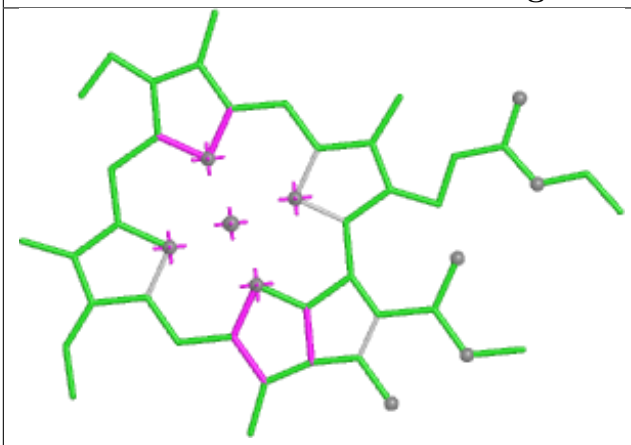


Rings

Ligand CLA b 315



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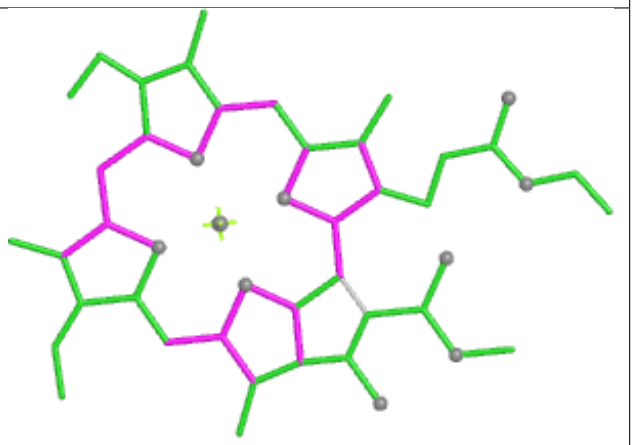
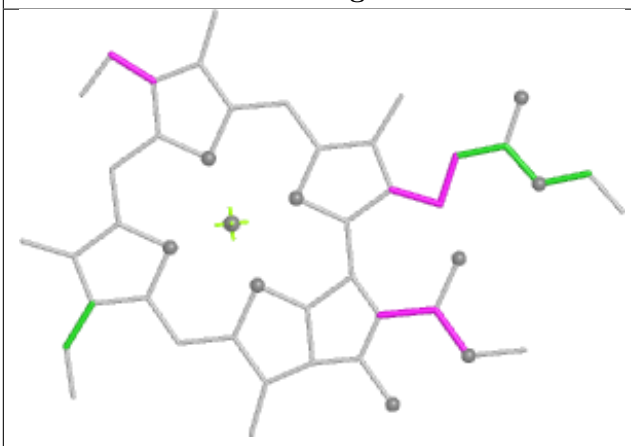


Bond angles



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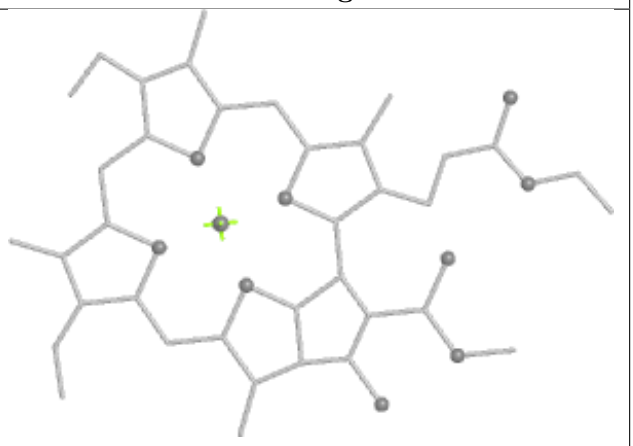
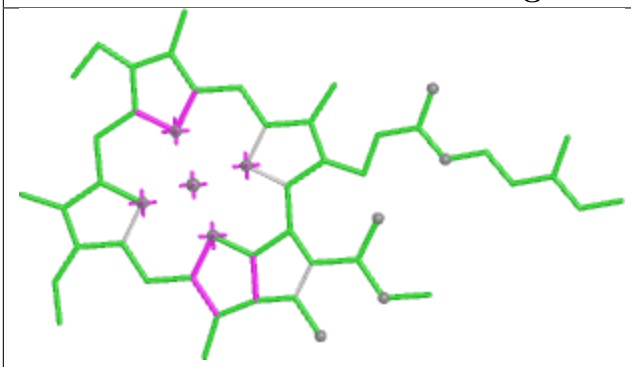


Rings

Ligand CLA A 827



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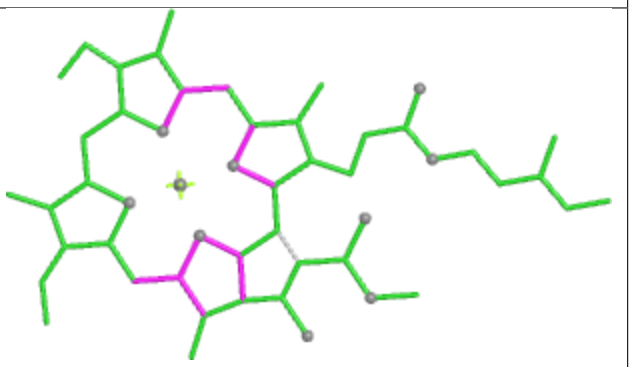
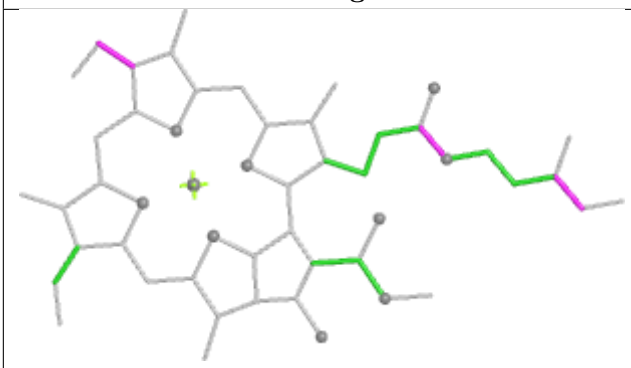


Bond angles



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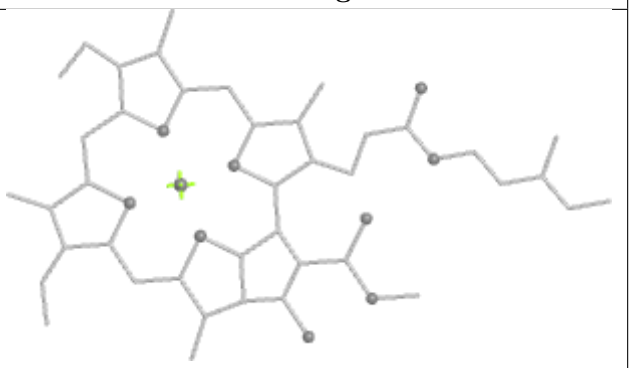
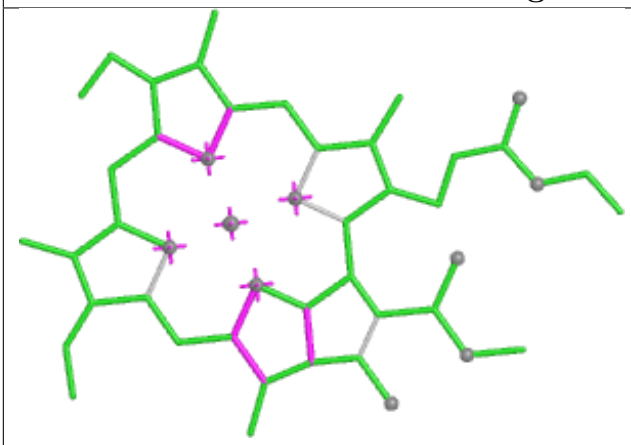
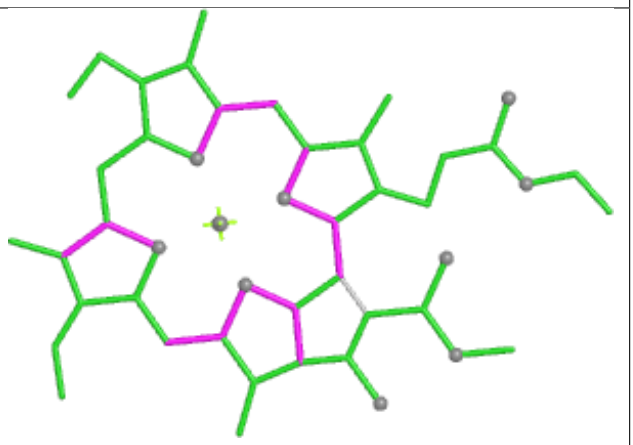


Rings

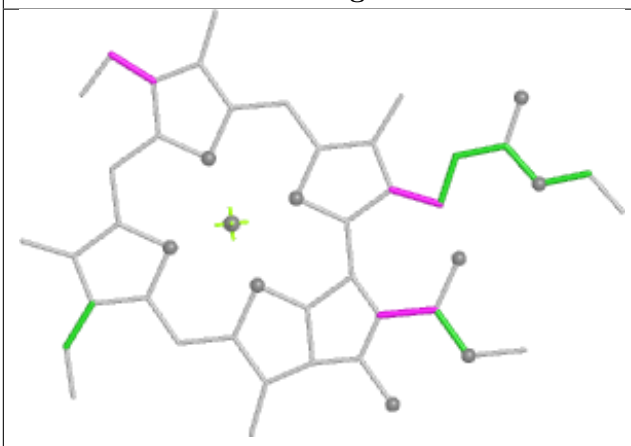
Ligand CLA n 201



Bond lengths



Bond angles



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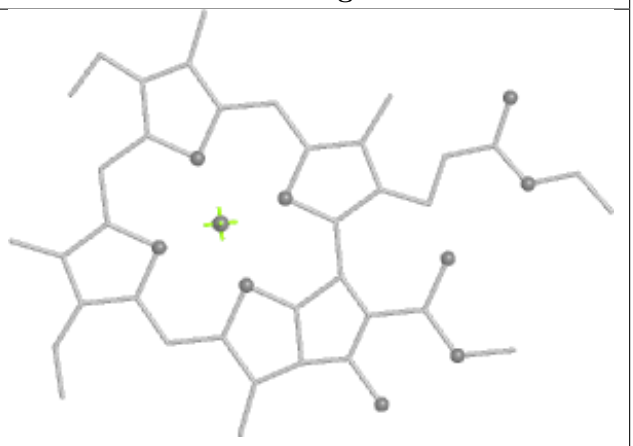


Rings

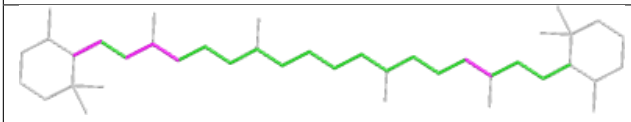
Ligand BCR B 826



Bond lengths



Bond angles



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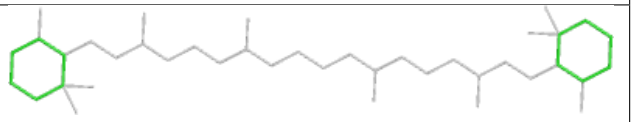
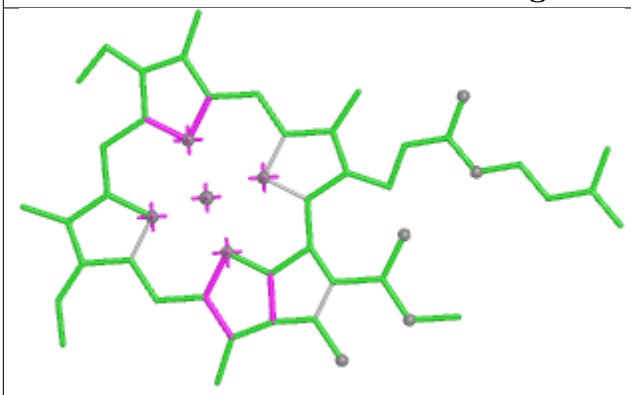
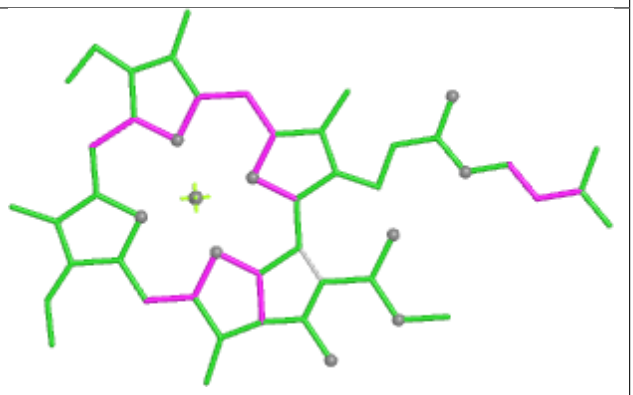


Rings

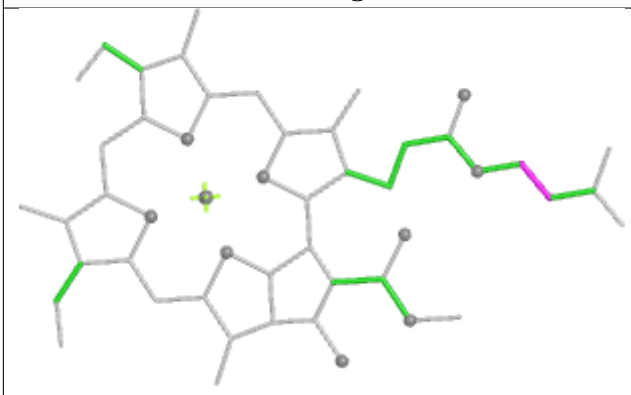
Ligand CLA e 305



Bond lengths



Bond angles



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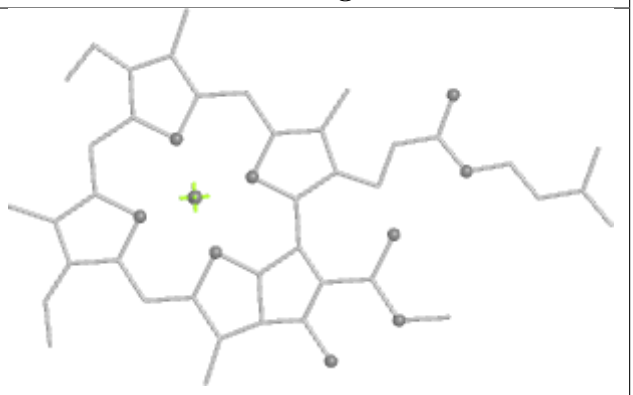
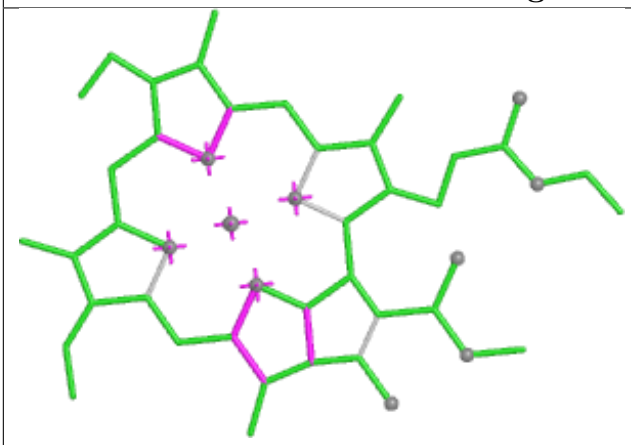


Rings

Ligand CLA b 305



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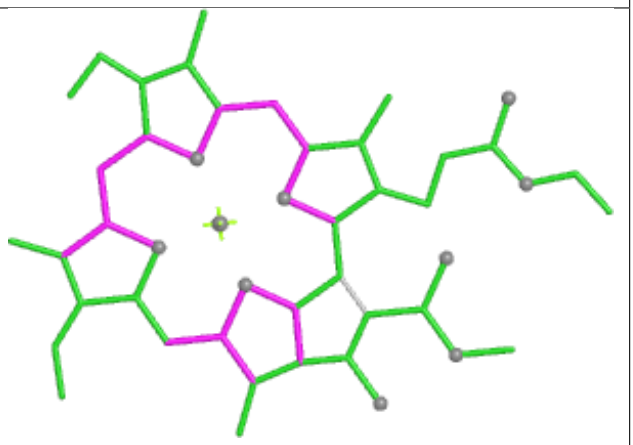
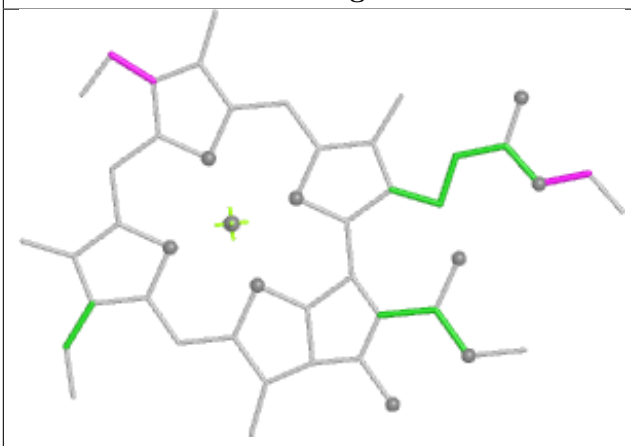
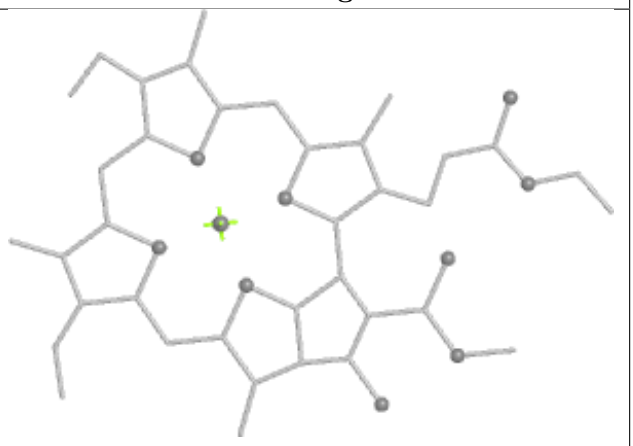


Bond angles

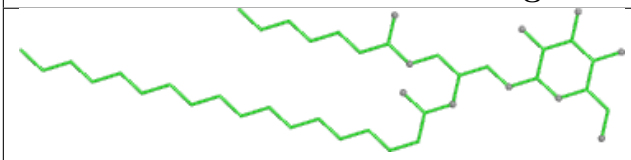


Torsions



Rings

Ligand LMG g 316



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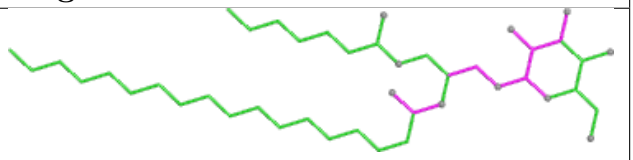
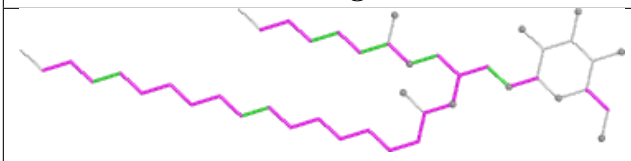


Bond angles



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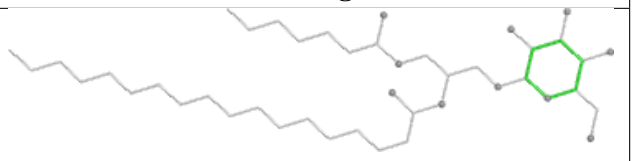
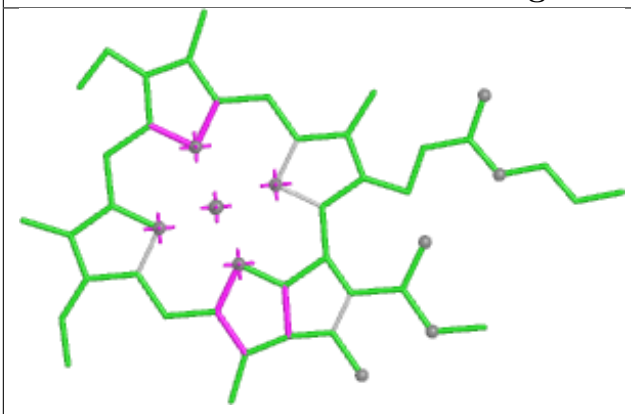


Rings

Ligand CLA g 301



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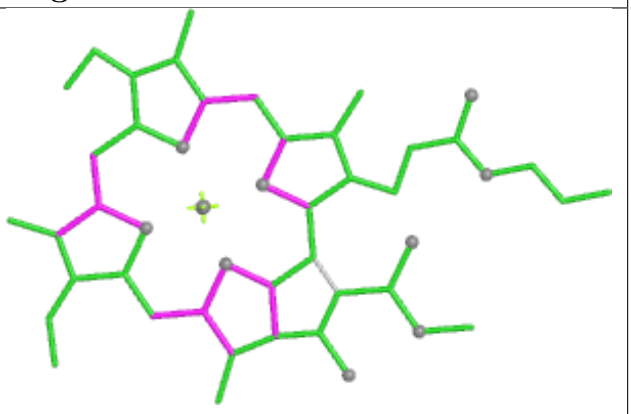

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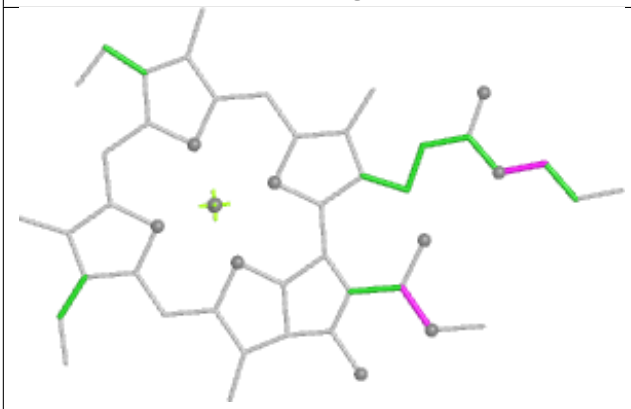

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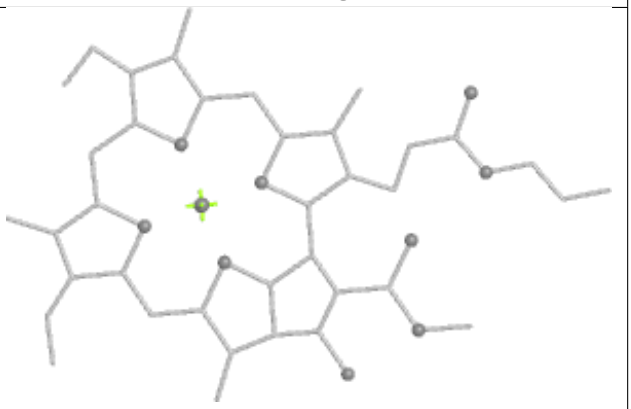
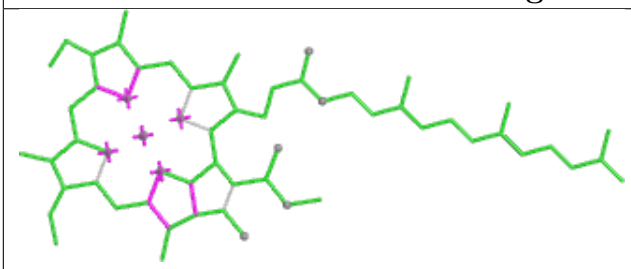


Rings

Ligand CLA F 201



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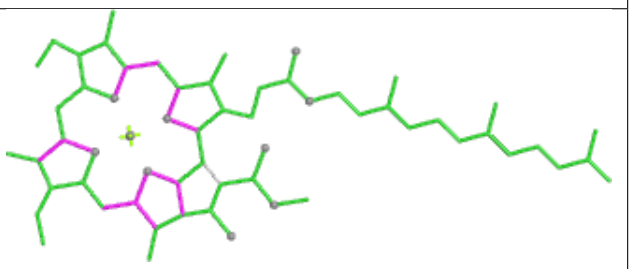
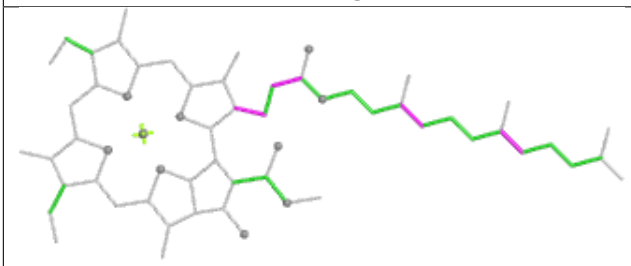


Bond angles



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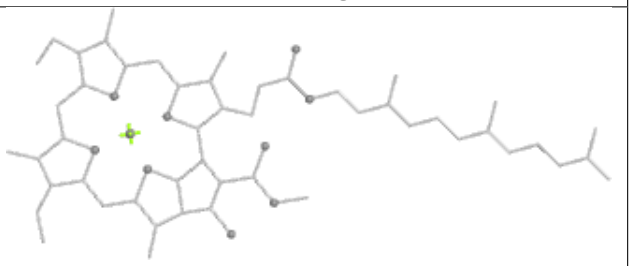
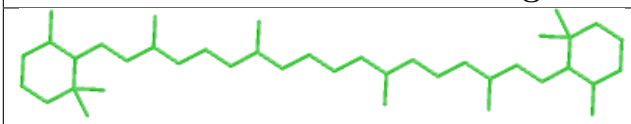


Rings

Ligand BCR B 827



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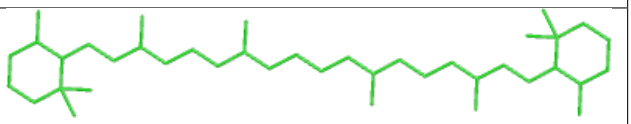
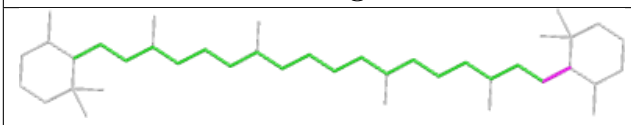


Bond angles



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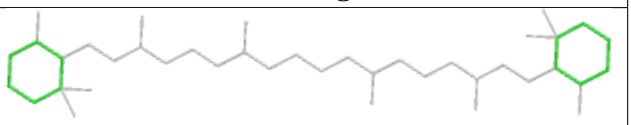
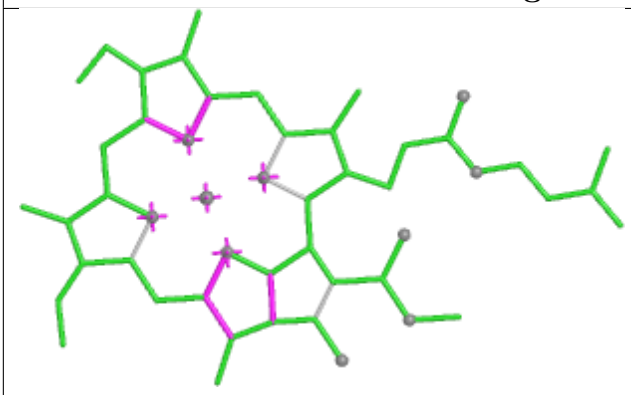


Rings

Ligand CLA A 810



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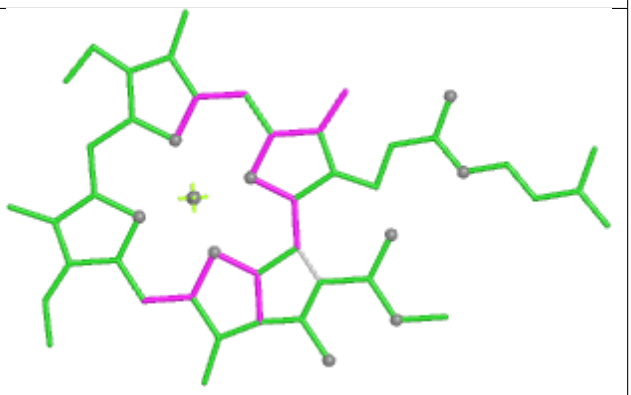

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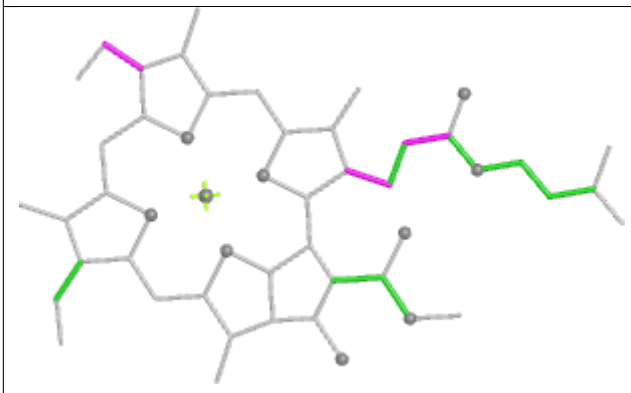

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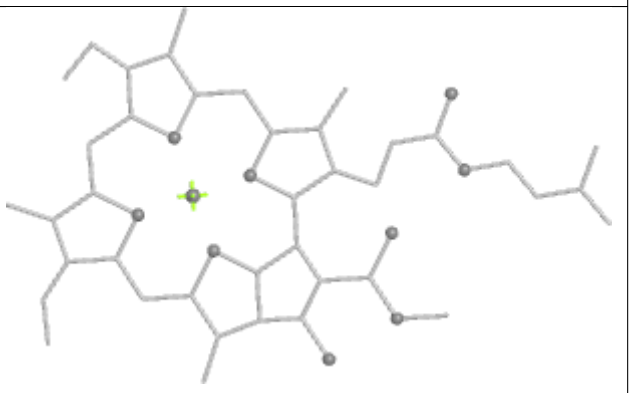
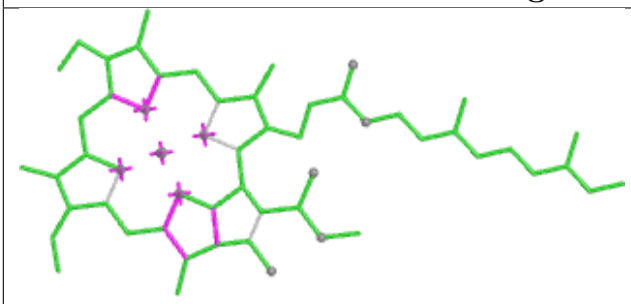


Rings

Ligand CLA k 302



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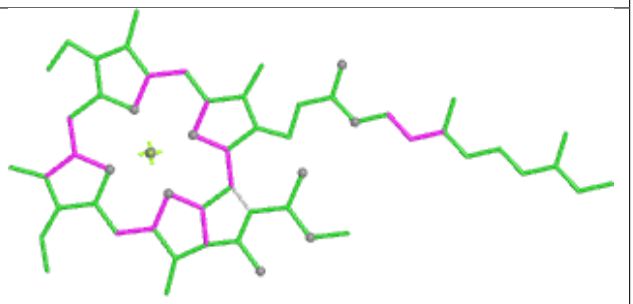
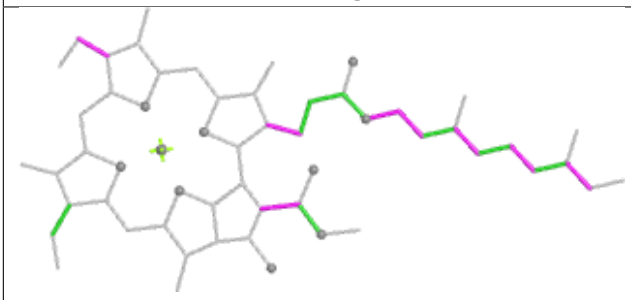


Bond angles



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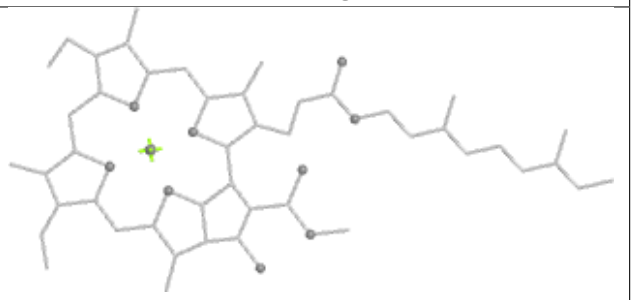
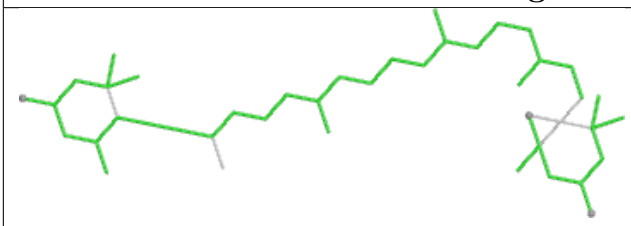


Rings

Ligand DD6 n 210



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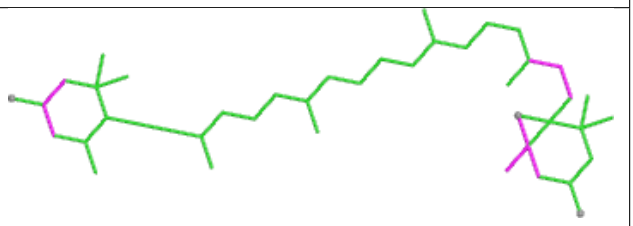
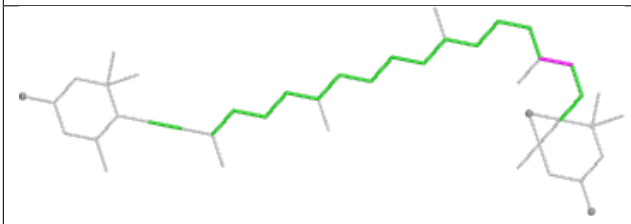


Bond angles

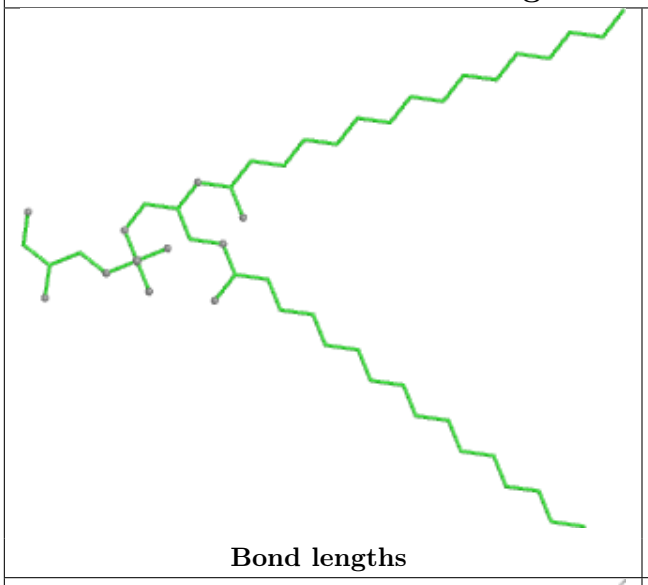


Torsions



Rings

Ligand LHG A 831



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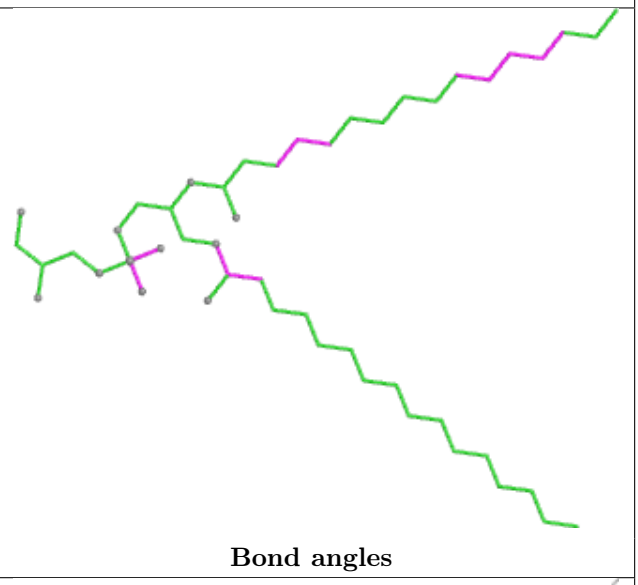
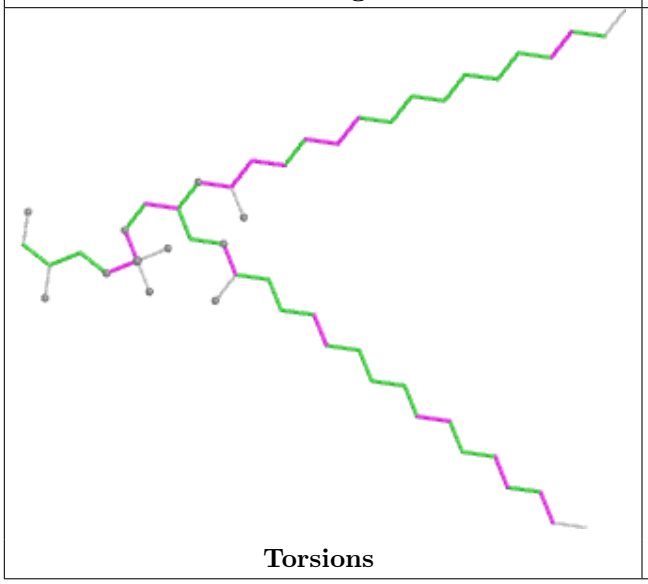


Bond angles



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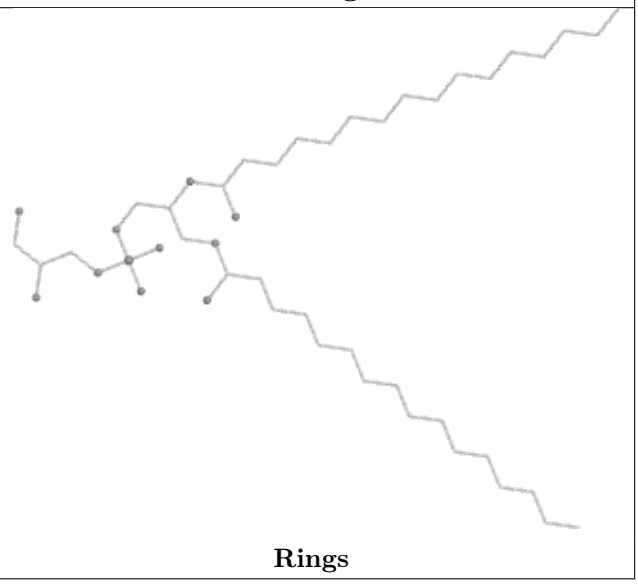
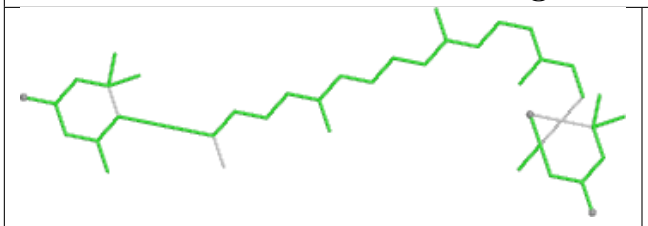


Rings

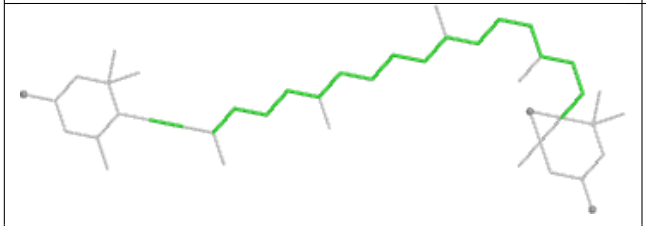
Ligand DD6 o 313



Bond lengths



Bond angles

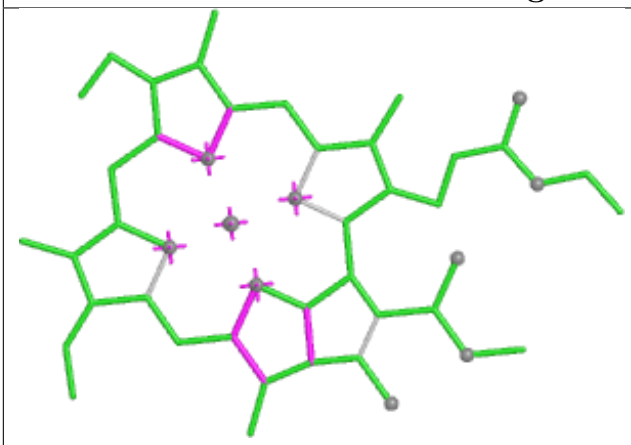


Torsions



Rings

Ligand CLA b 313



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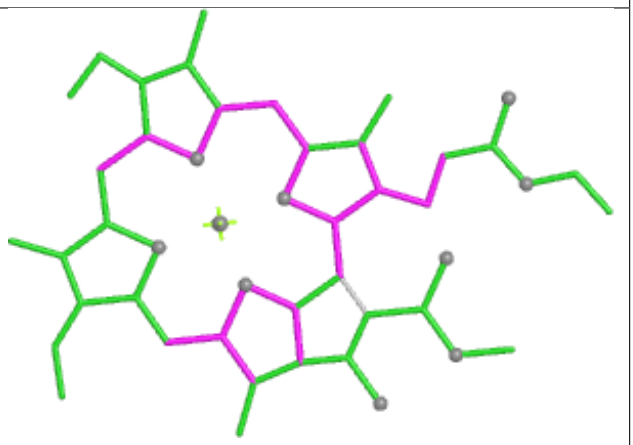
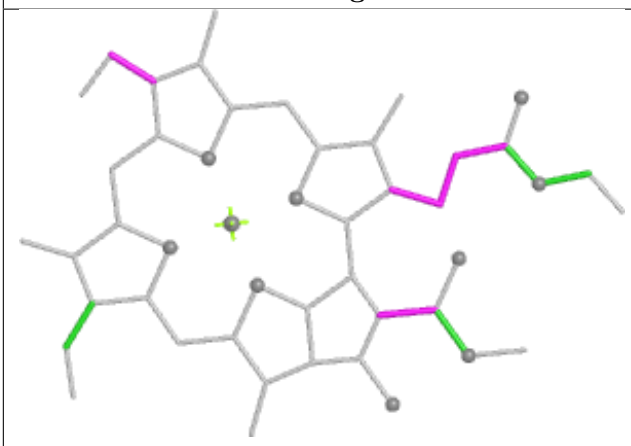


Bond angles



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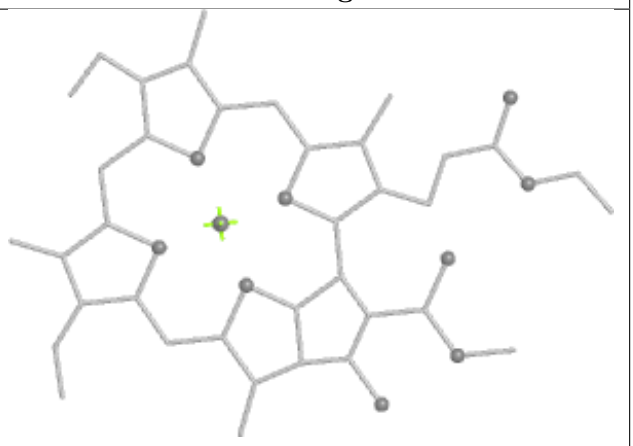
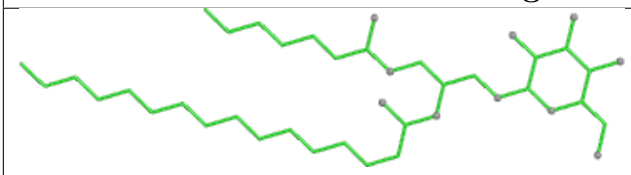


Rings

Ligand LMG b 316



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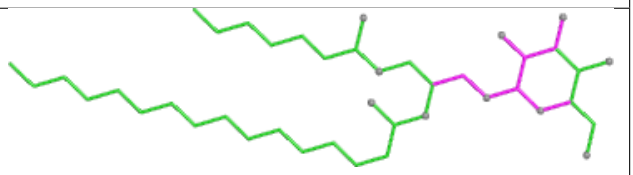
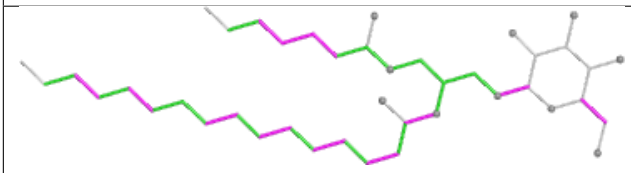


Bond angles



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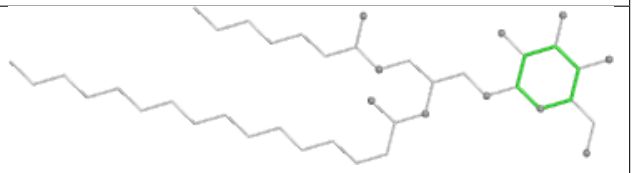
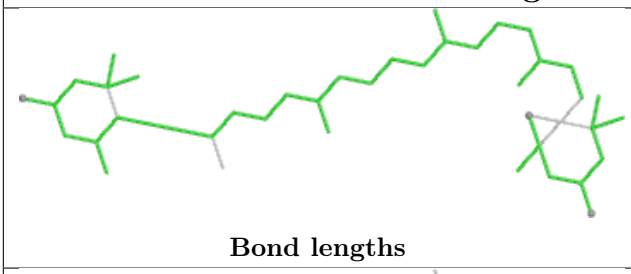


Rings

Ligand DD6 m 312



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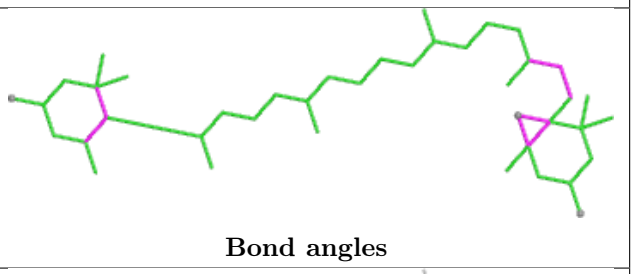
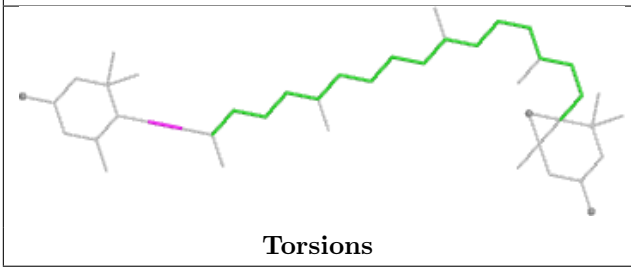


Bond angles



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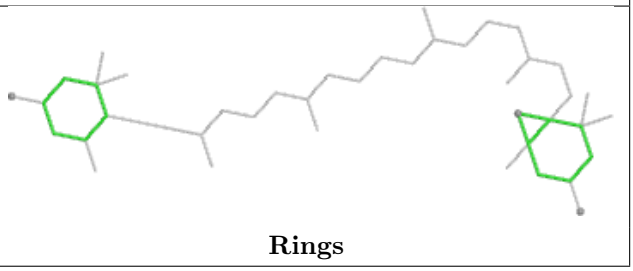
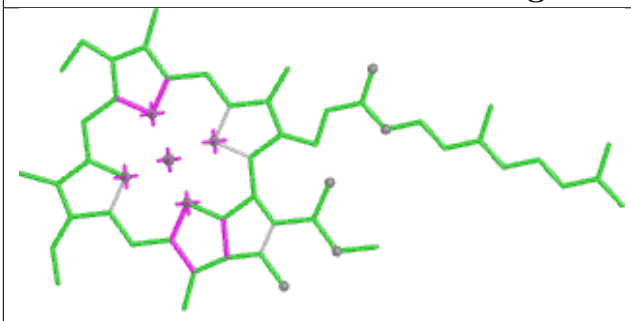


Rings

Ligand CLA b 304



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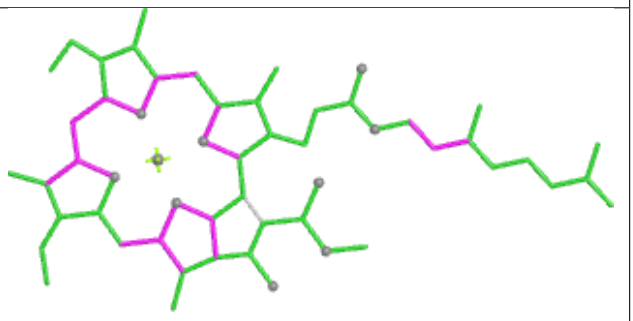
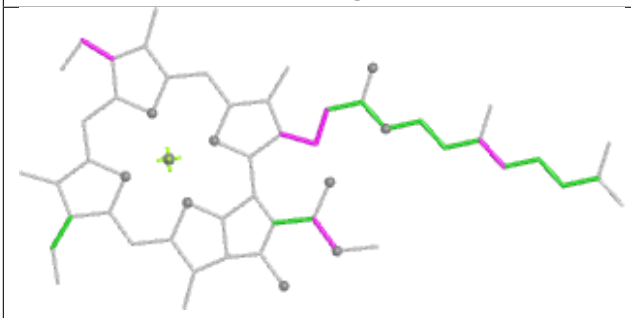


Bond angles



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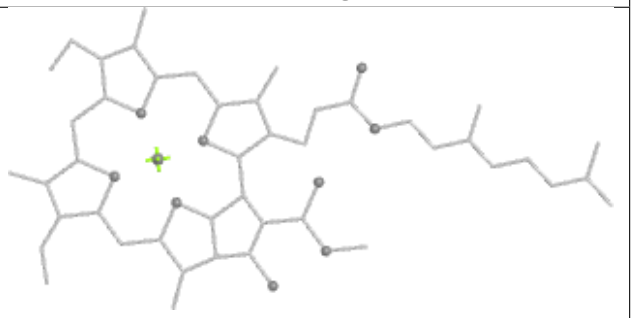
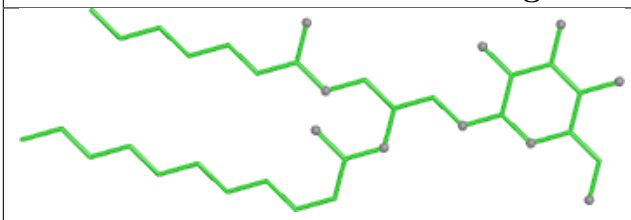


Rings

Ligand LMG k 312



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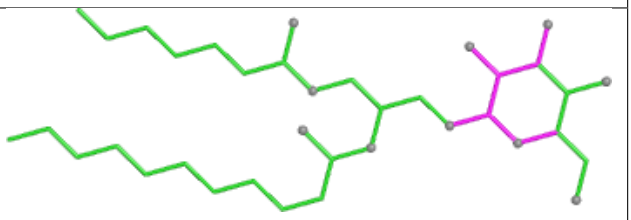
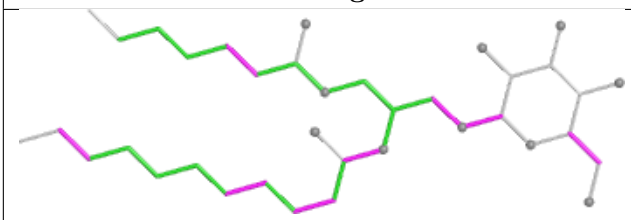


Bond angles



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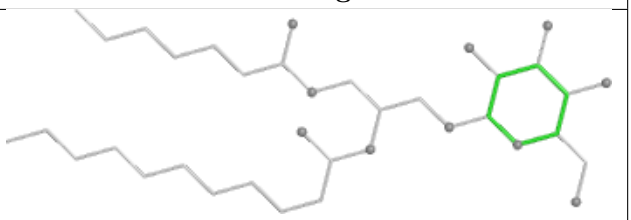
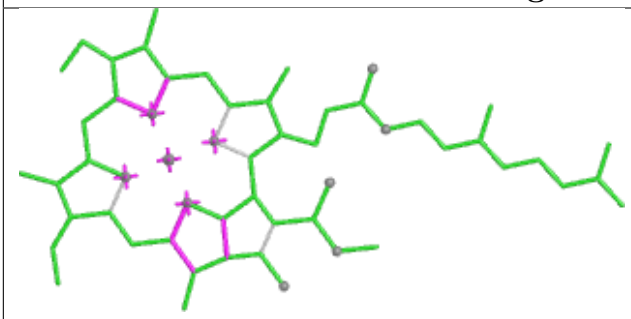
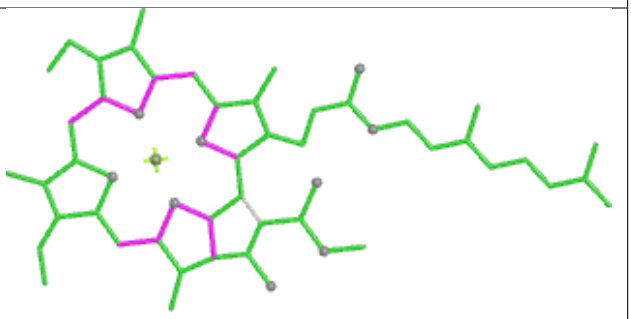


Rings

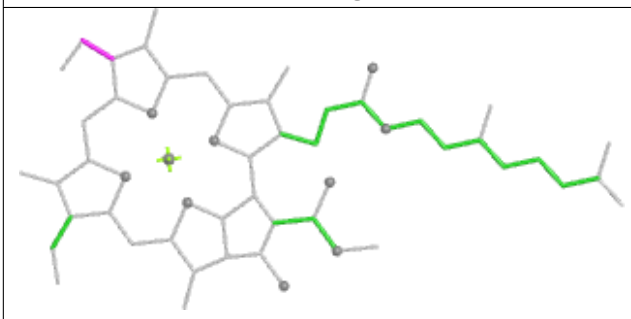
Ligand CLA h 203



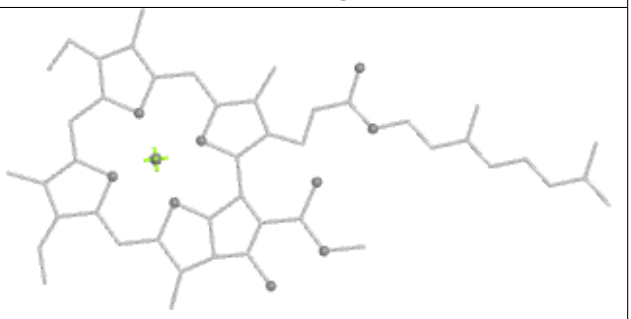
Bond lengths



Bond angles

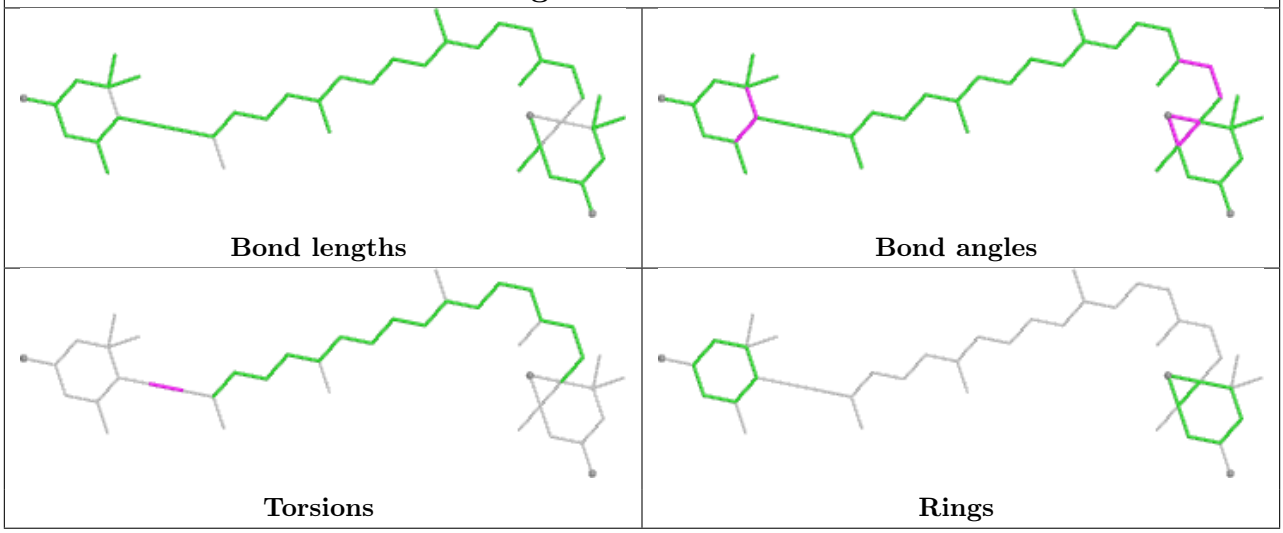


Torsions

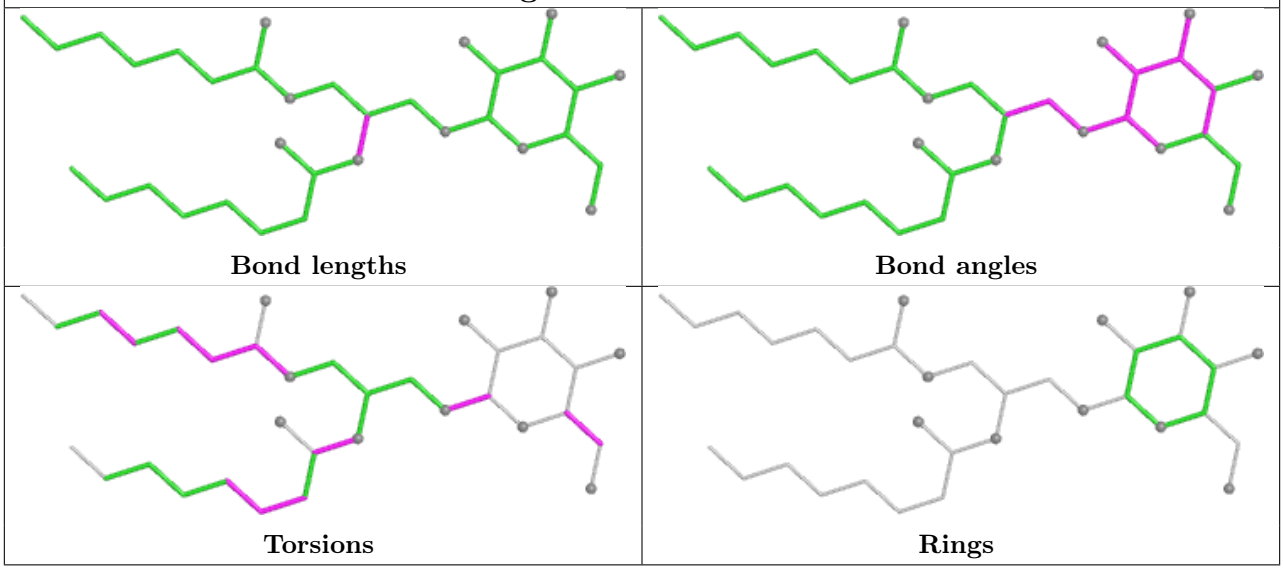


Rings

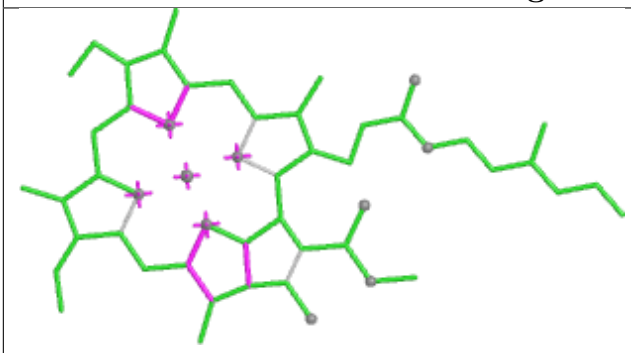
Ligand DD6 c 318



Ligand LMG A 851



Ligand CLA d 204



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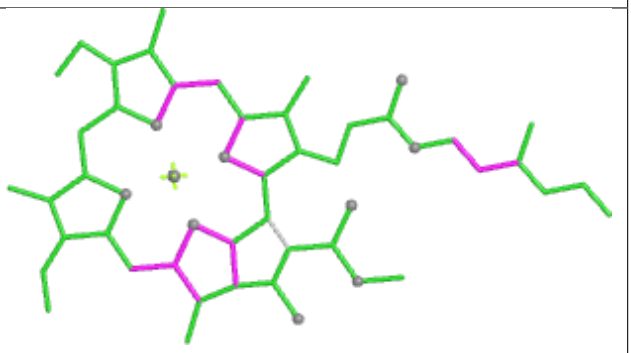
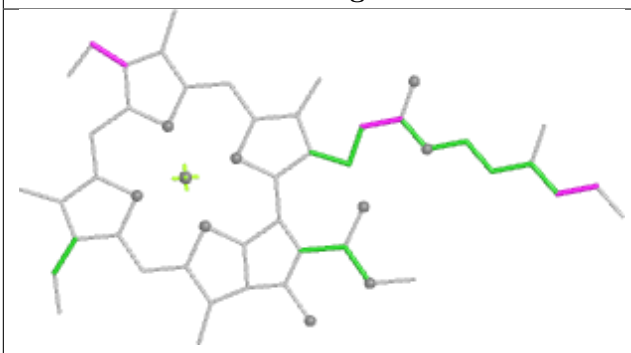


Bond angles



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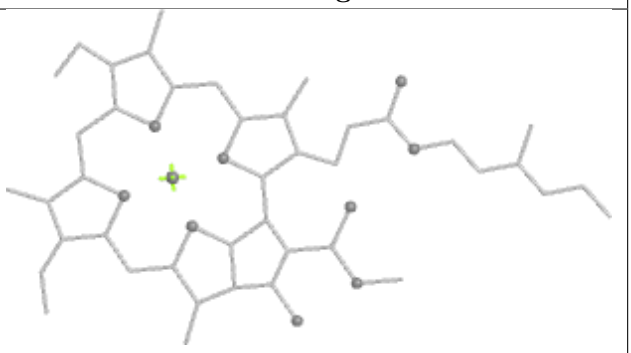
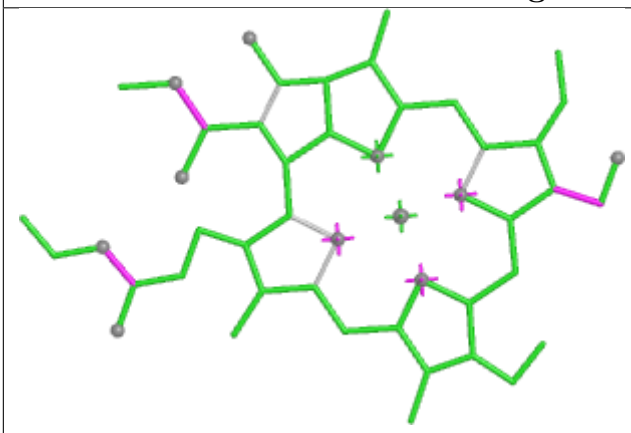


Rings

Ligand CHL a 313



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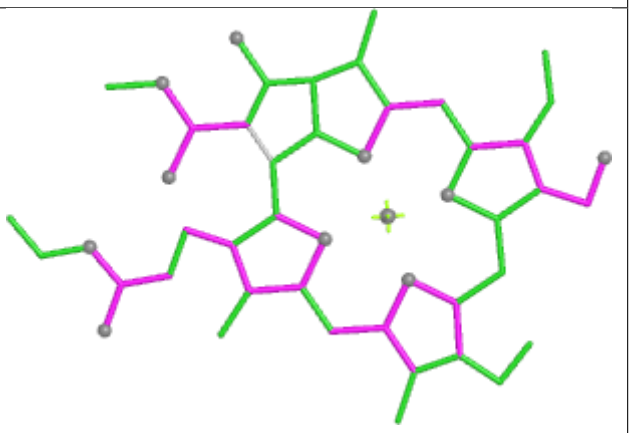

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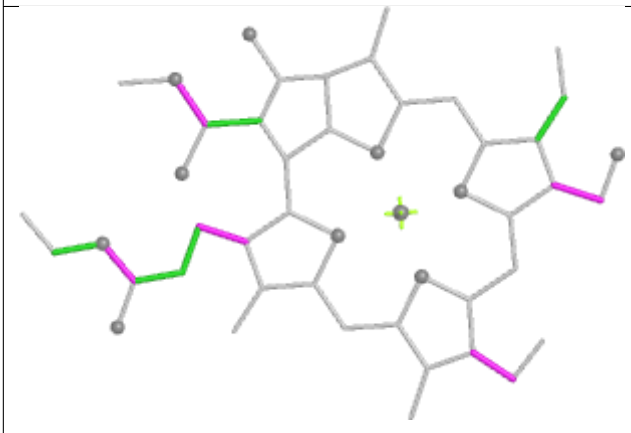

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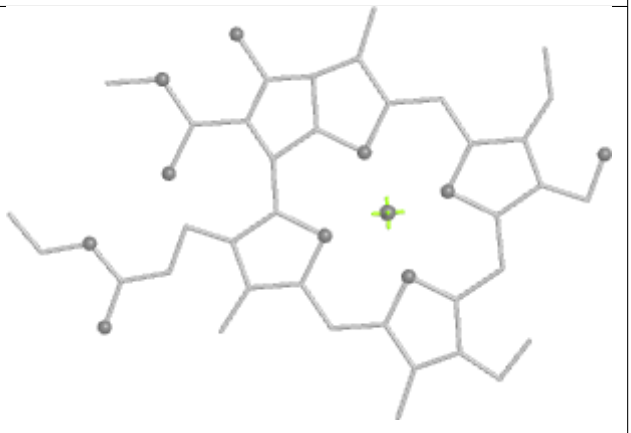
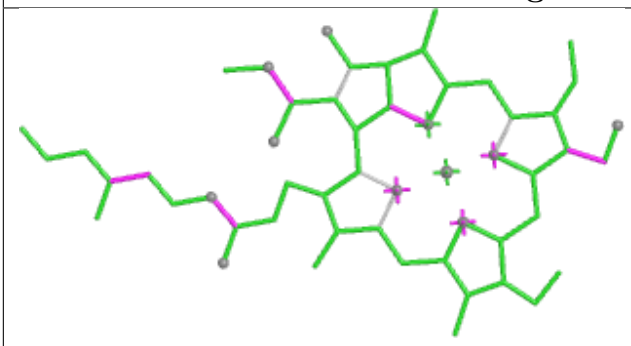


Rings

Ligand CHL b 312



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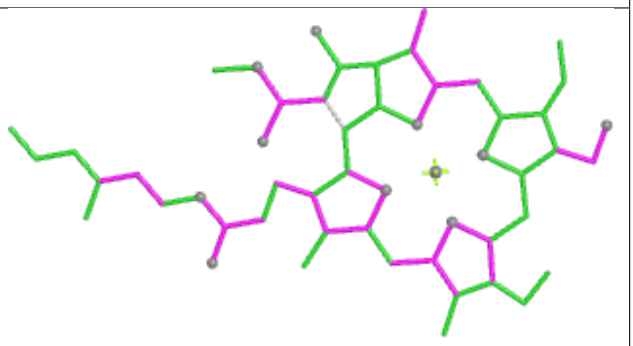
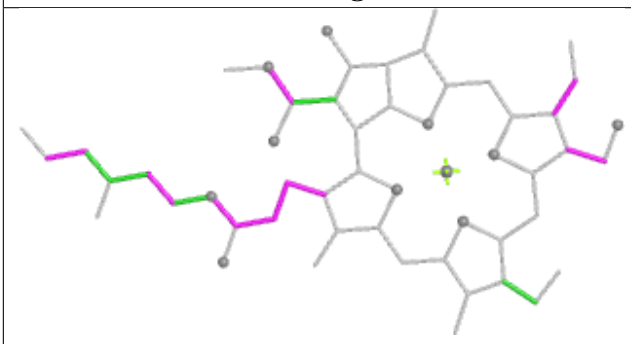


Bond angles



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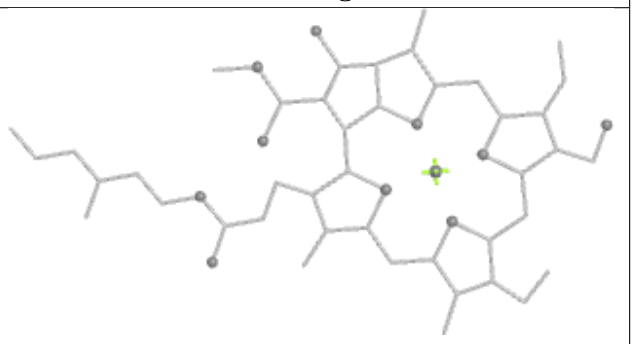
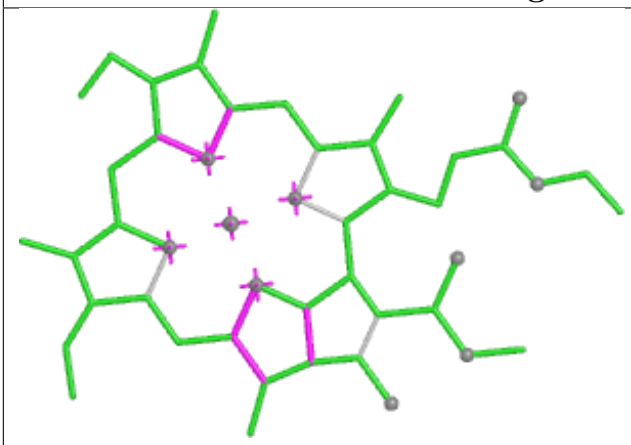


Rings

Ligand CLA k 309



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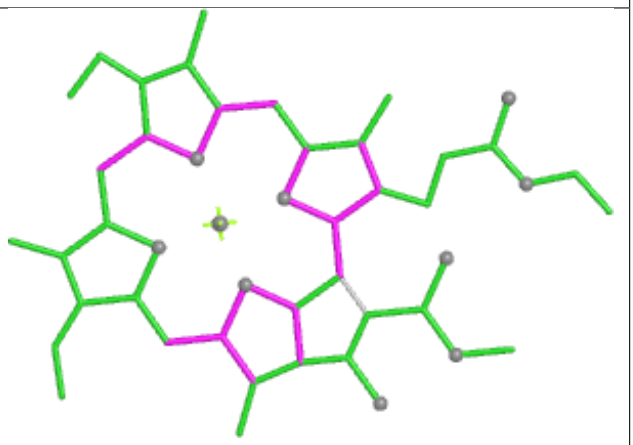
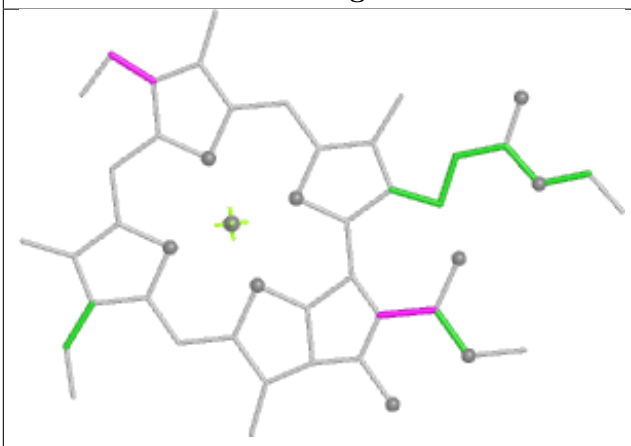


Bond angles



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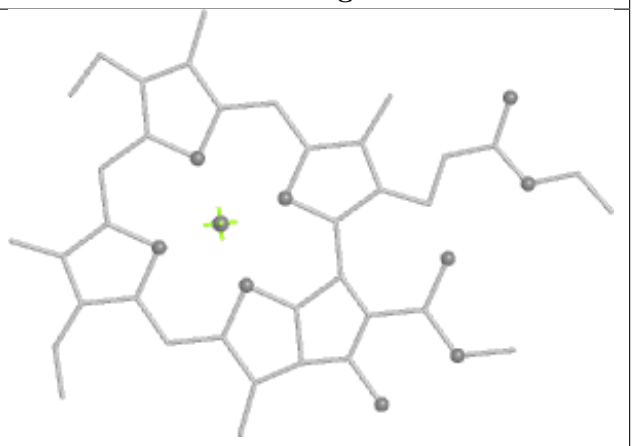
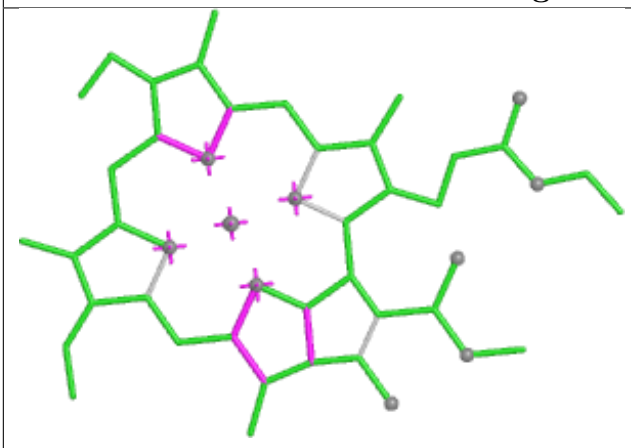


Rings

Ligand CLA l 201



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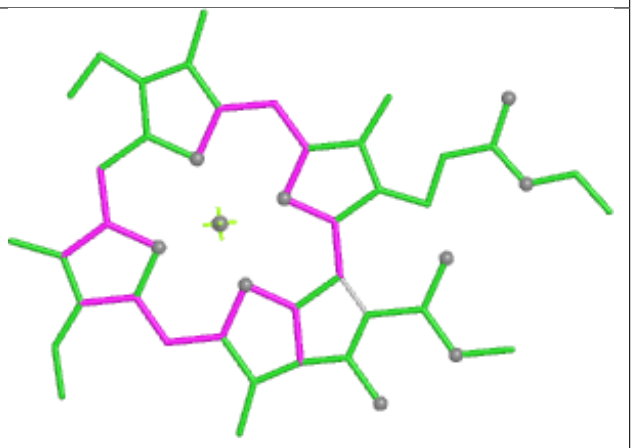
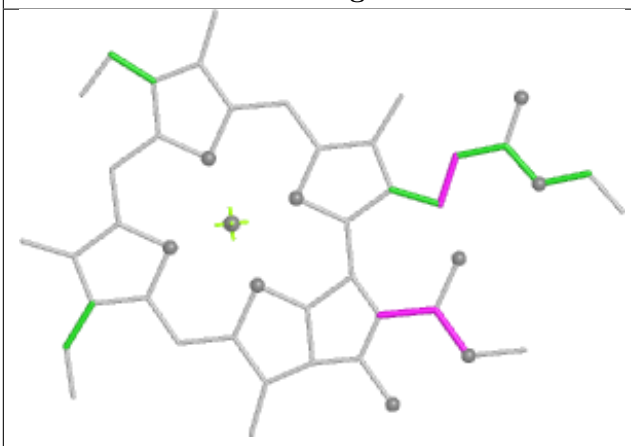


Bond angles



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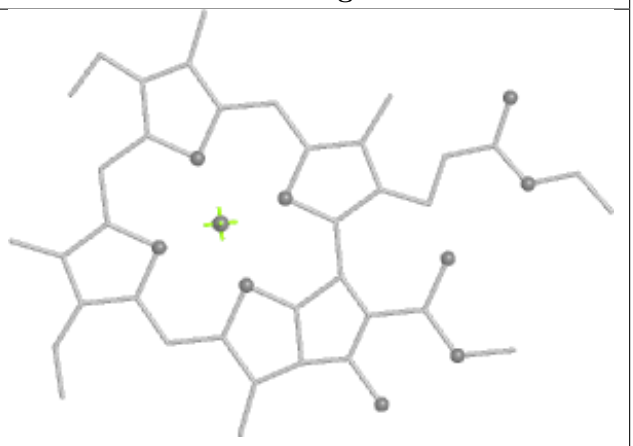
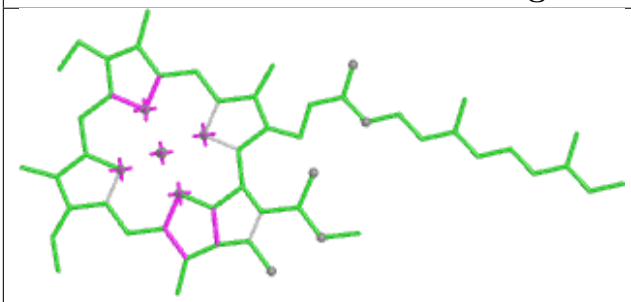


Rings

Ligand CLA a 309



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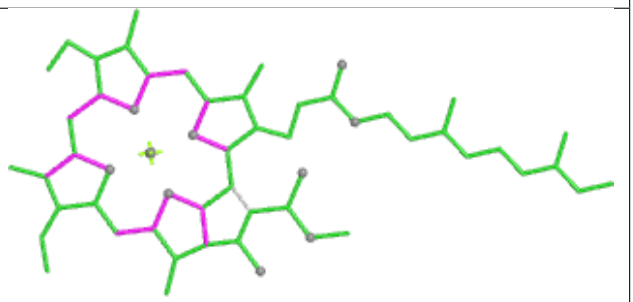
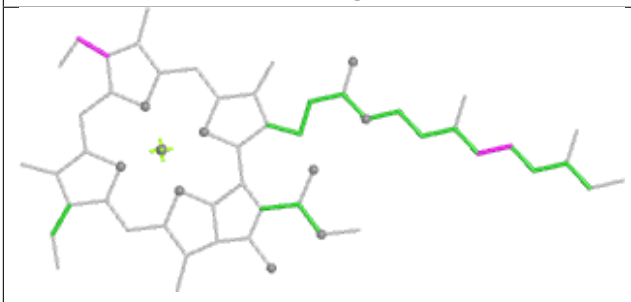


Bond angles



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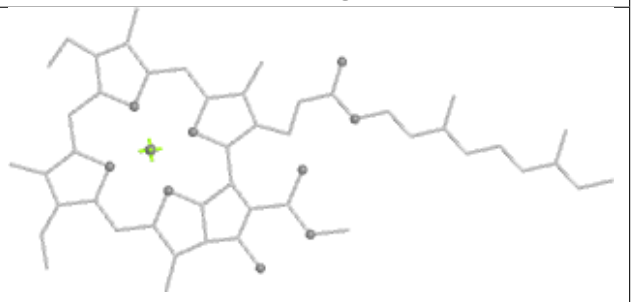
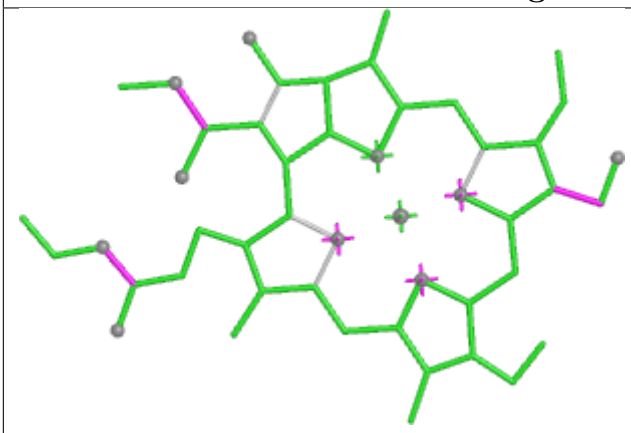


Rings

Ligand CHL a 312



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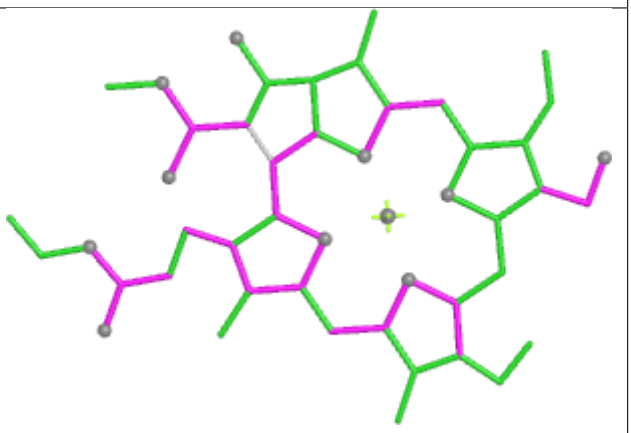

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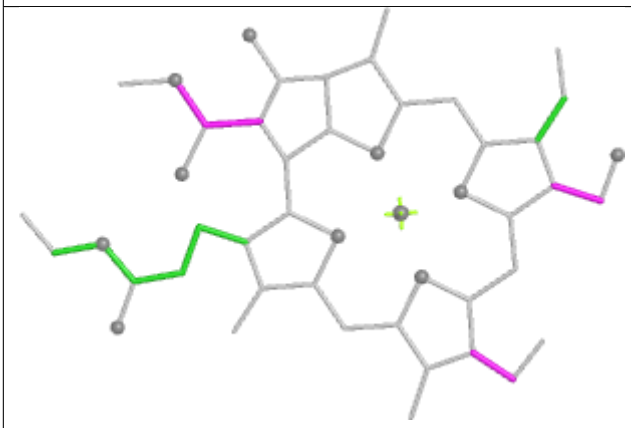

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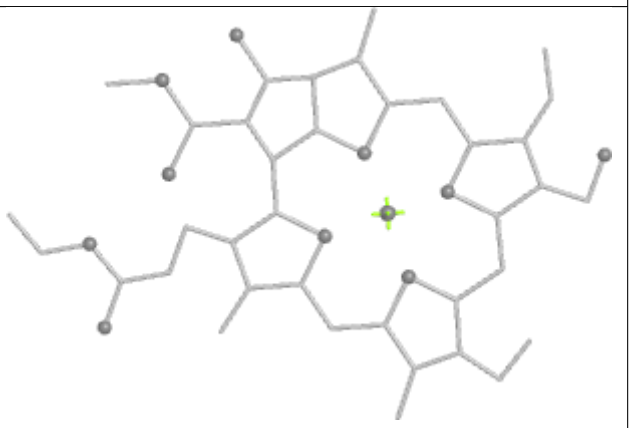
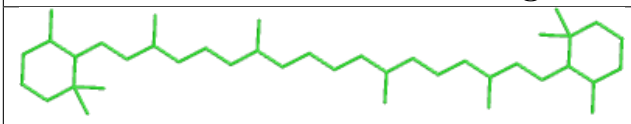


Rings

Ligand BCR A 834



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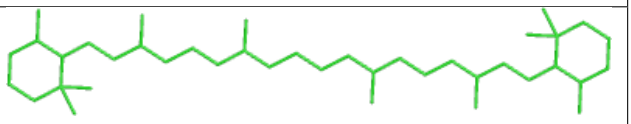
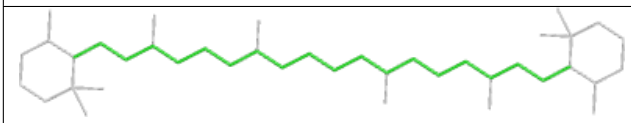


Bond angles



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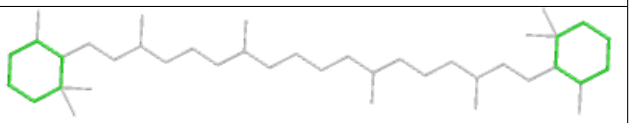
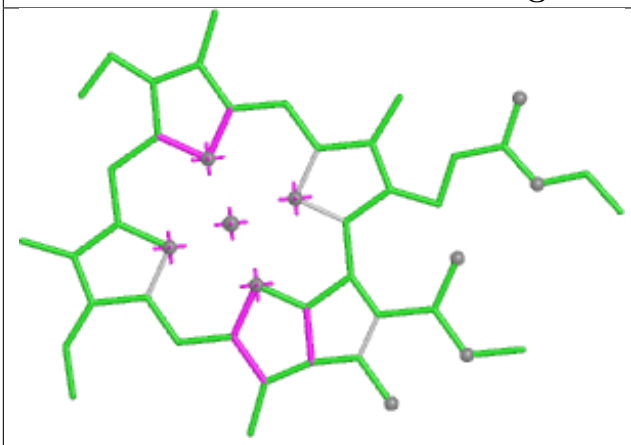


Rings

Ligand CLA a 314



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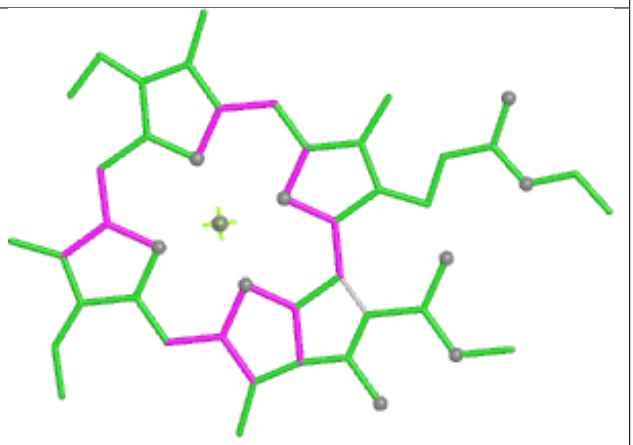

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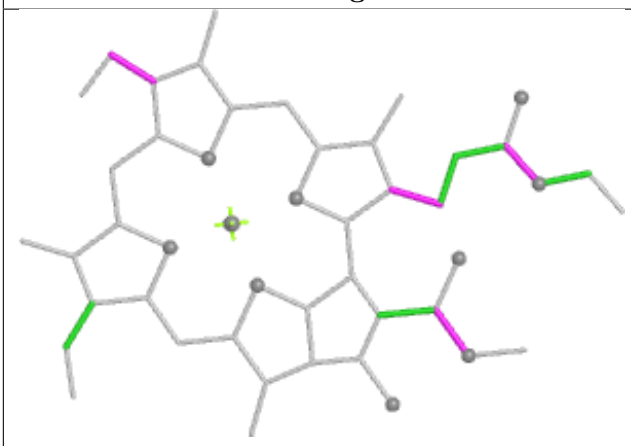

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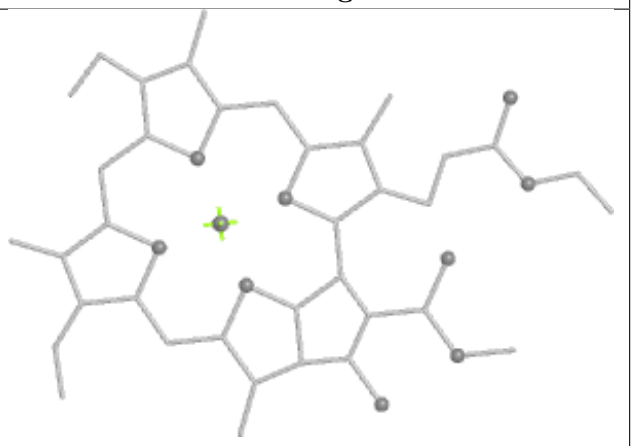
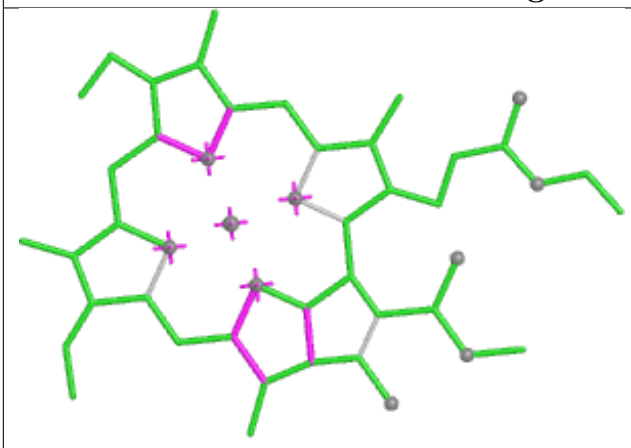


Rings

Ligand CLA d 206



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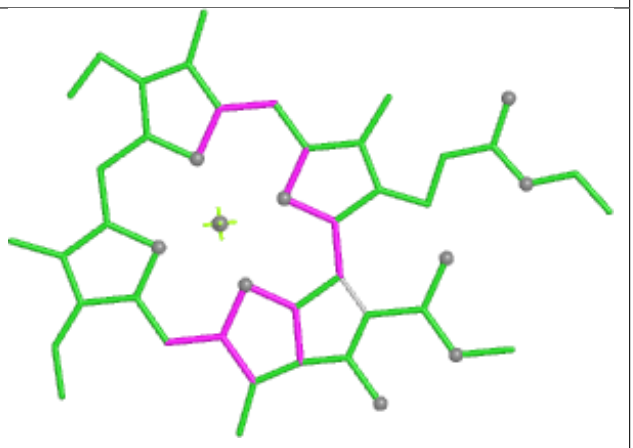

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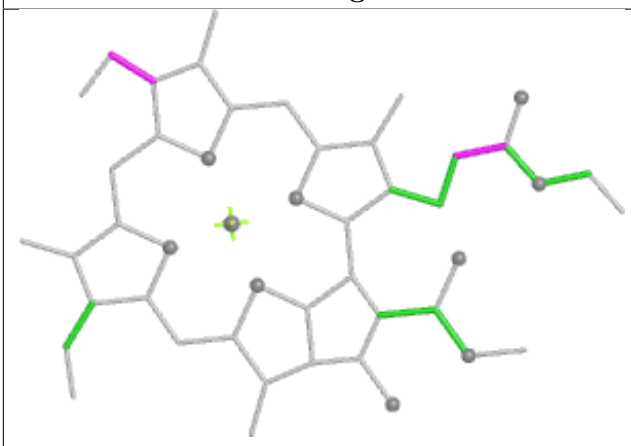

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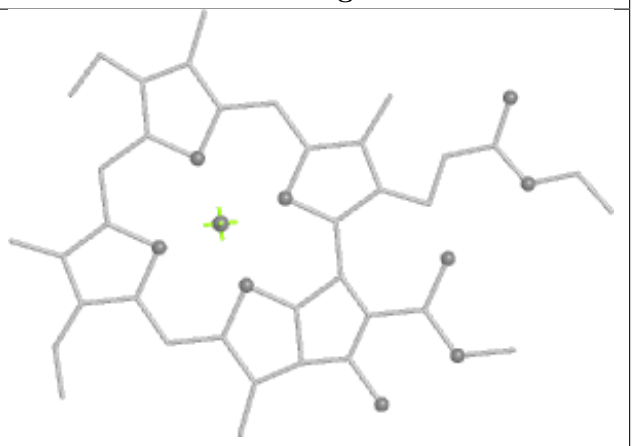
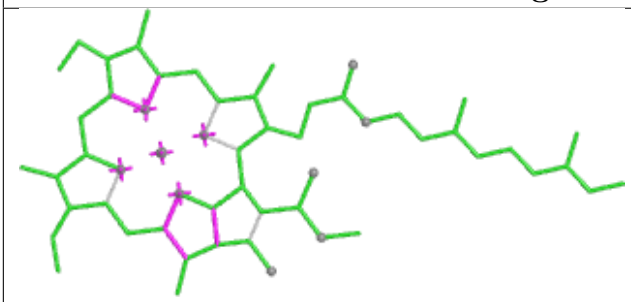


Rings

Ligand CLA j 309



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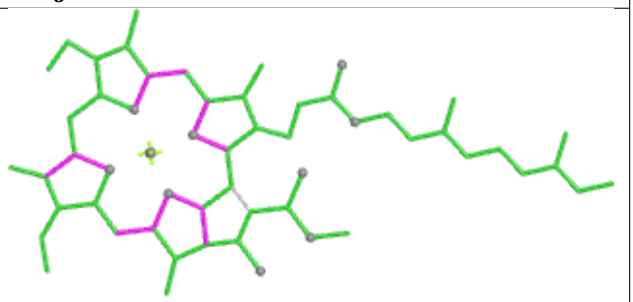

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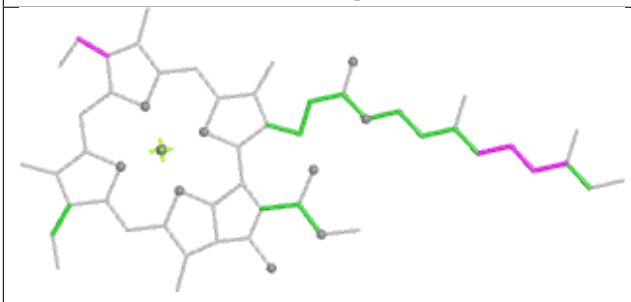

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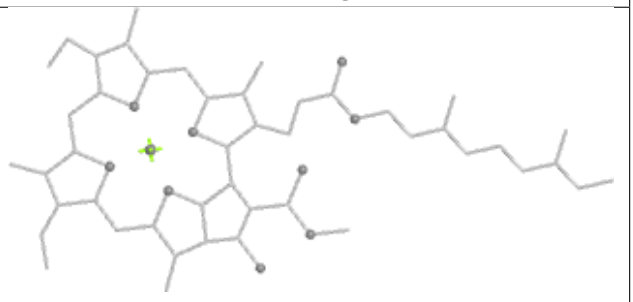
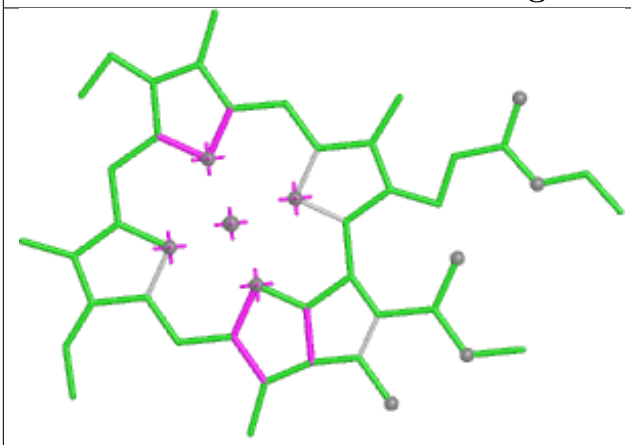


Rings

Ligand CLA o 310



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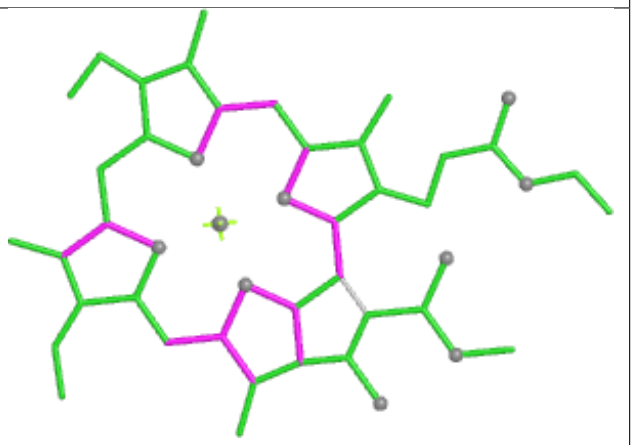
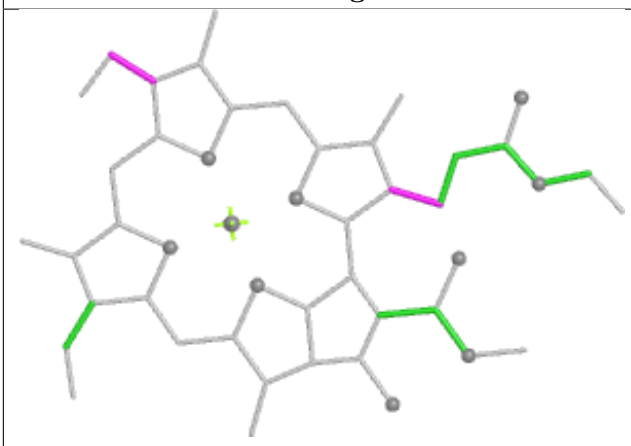


Bond angles



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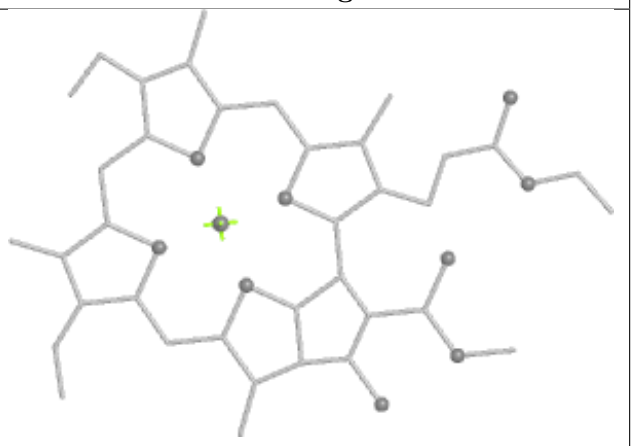
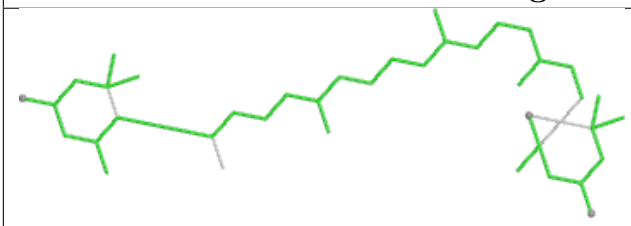


Rings

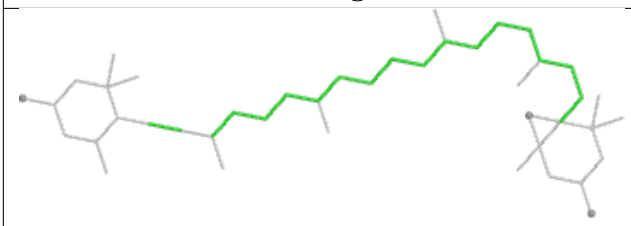
Ligand DD6 a 320



Bond lengths



Bond angles

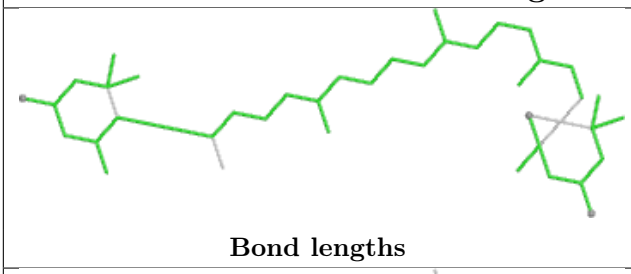


Torsions

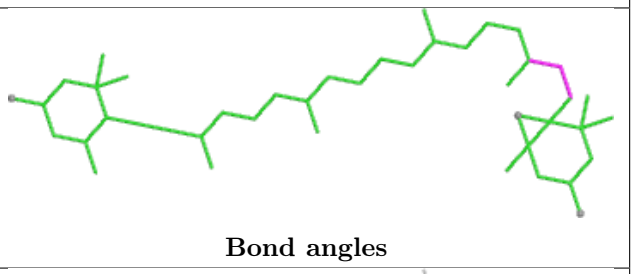


Rings

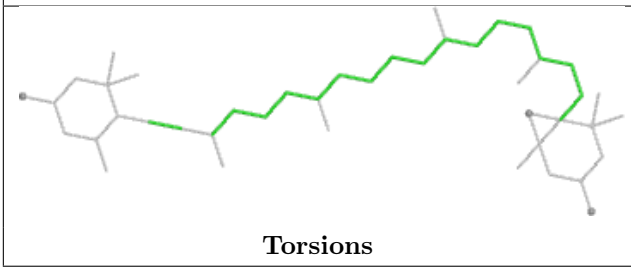
Ligand DD6 b 318



Bond lengths



Bond angles



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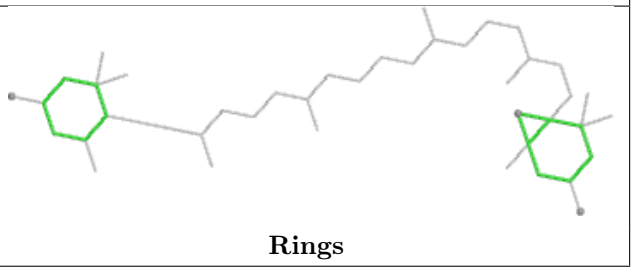
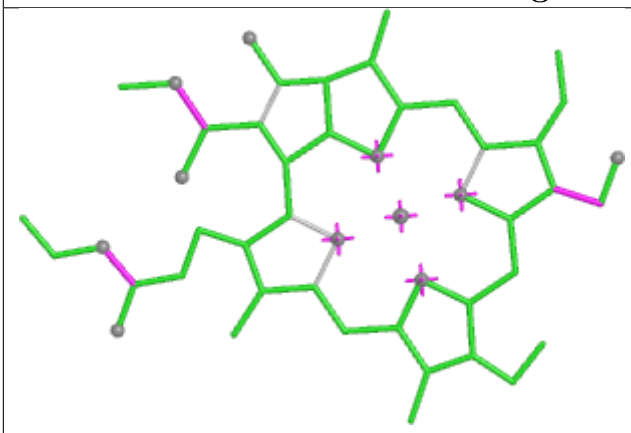
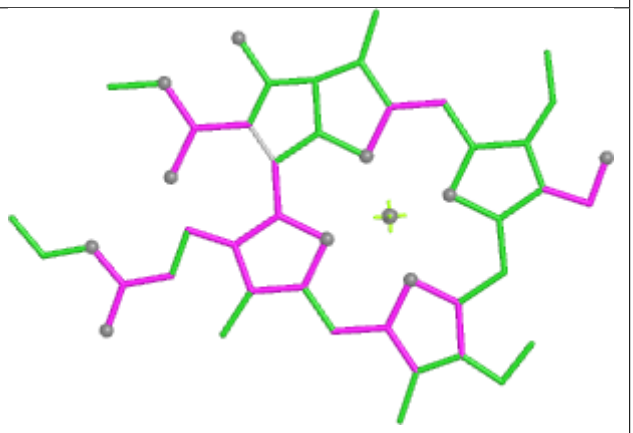


Rings

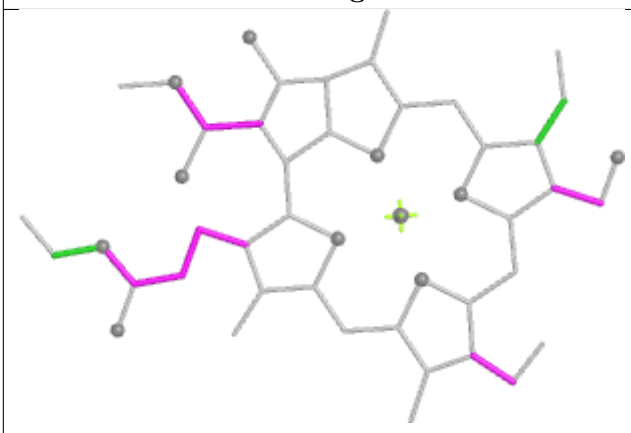
Ligand CHL f 301



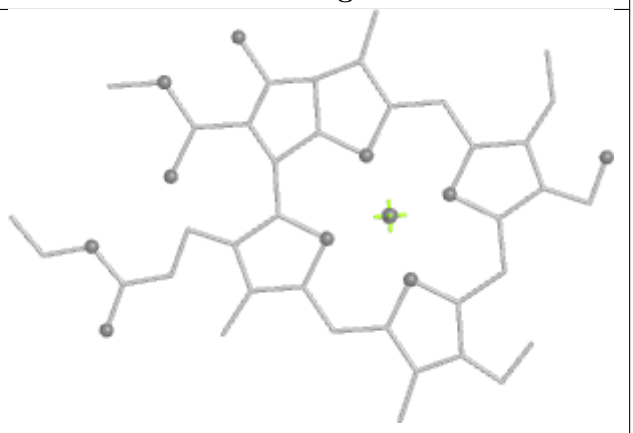
Bond lengths



Bond angles

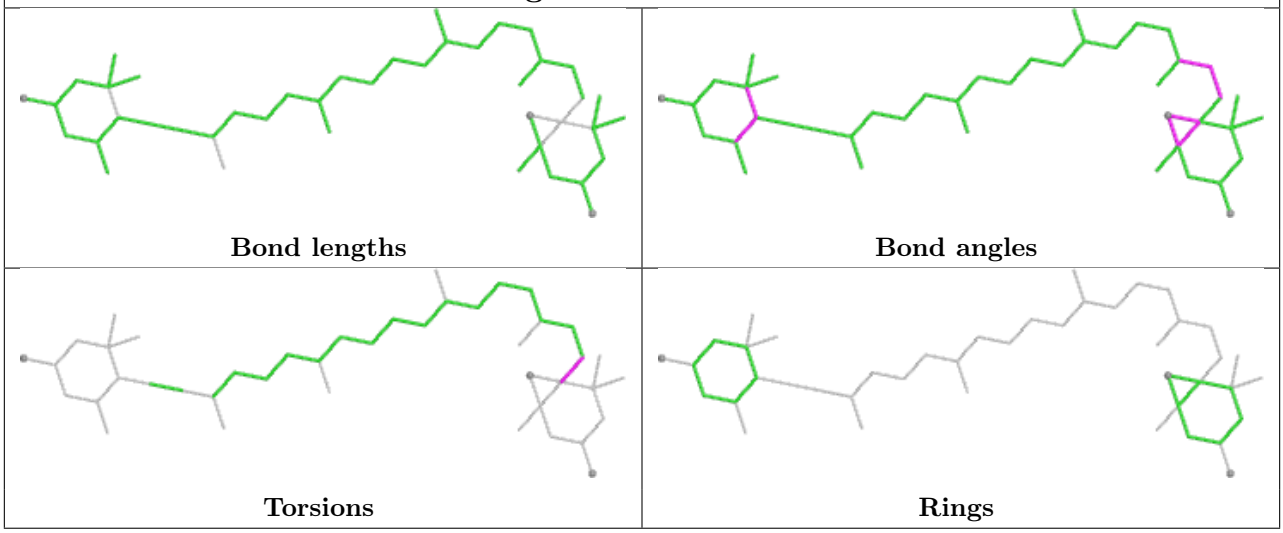


Torsions

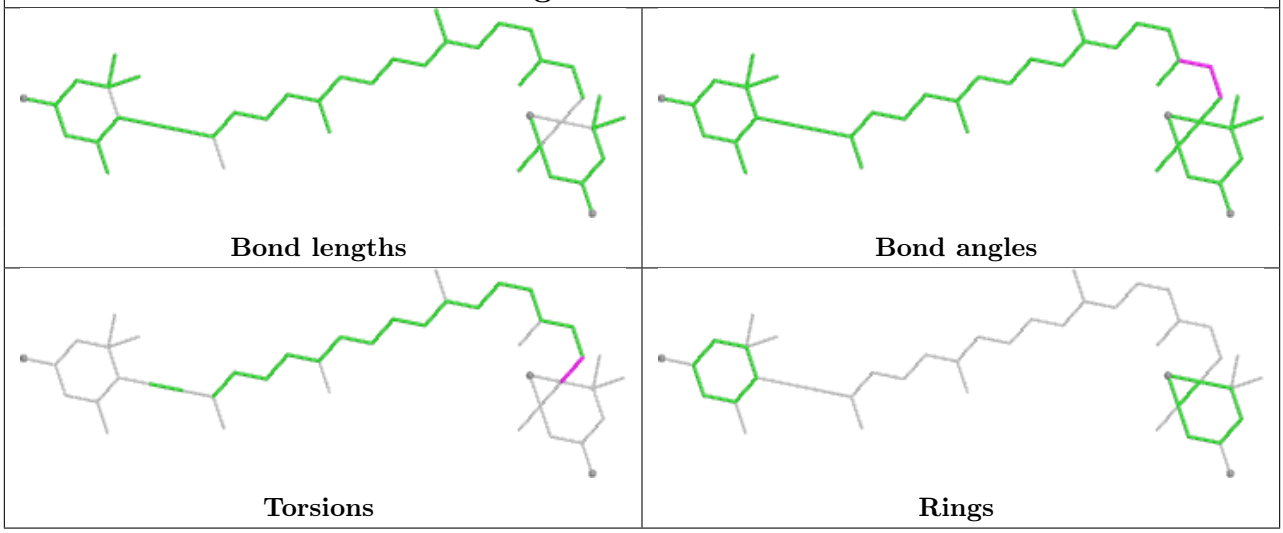


Rings

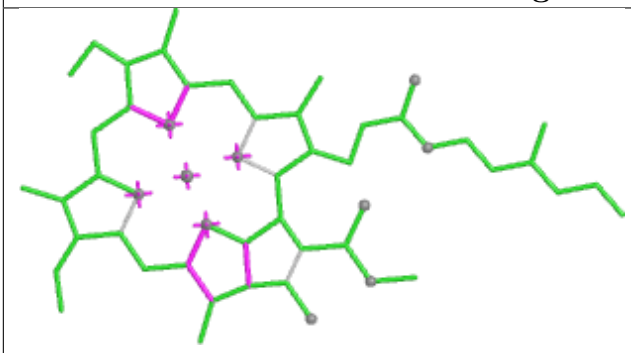
Ligand DD6 A 833



Ligand DD6 l 210



Ligand CLA i 311



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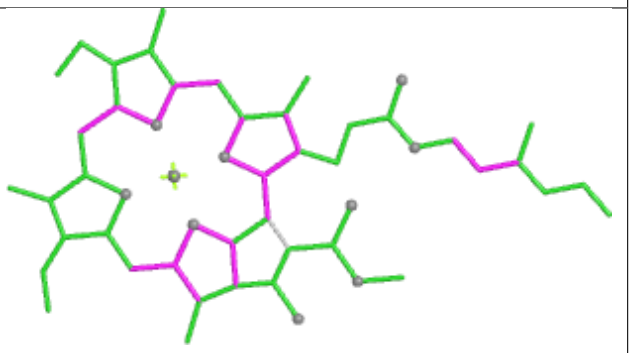

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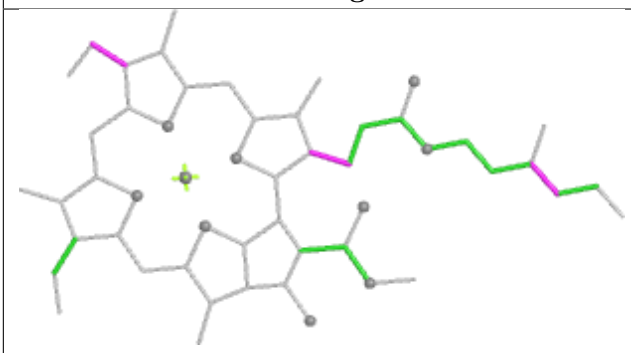

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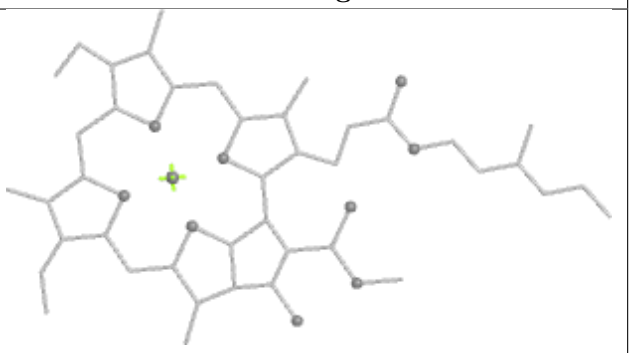
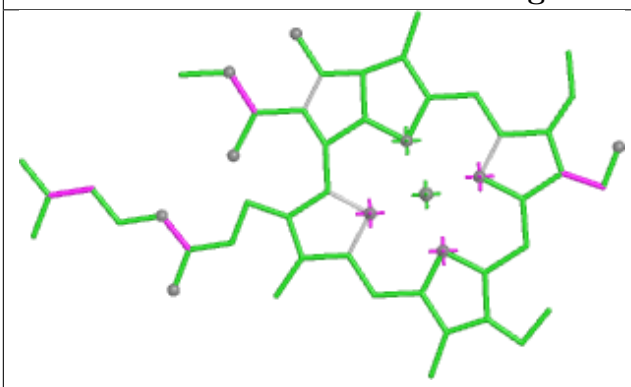


Rings

Ligand CHL g 310



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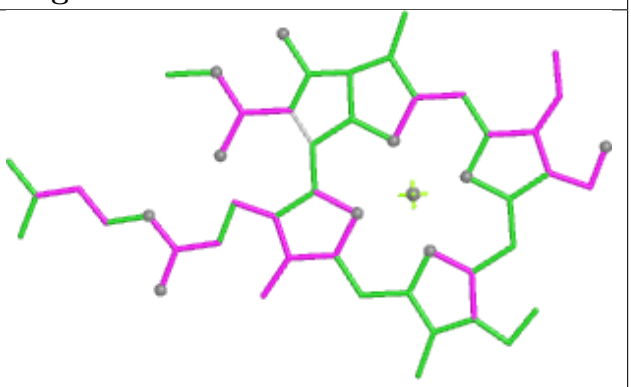
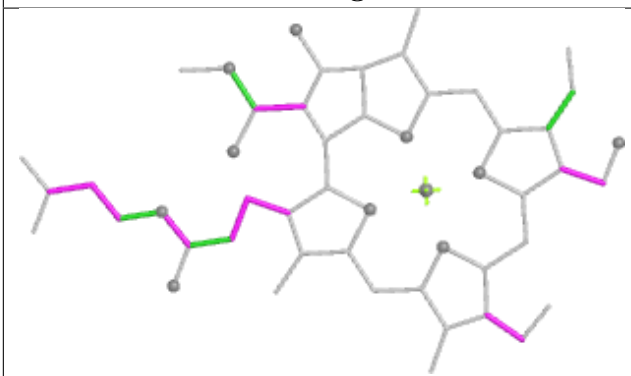


Bond angles



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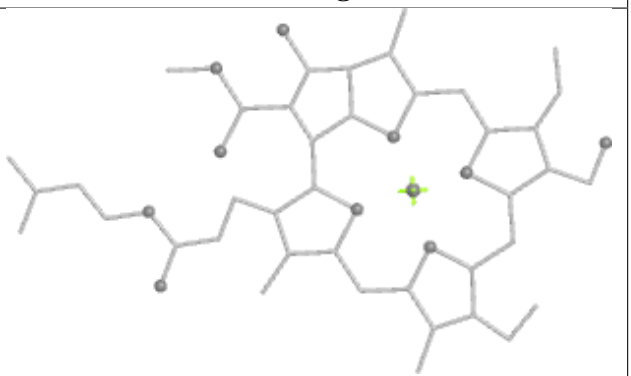
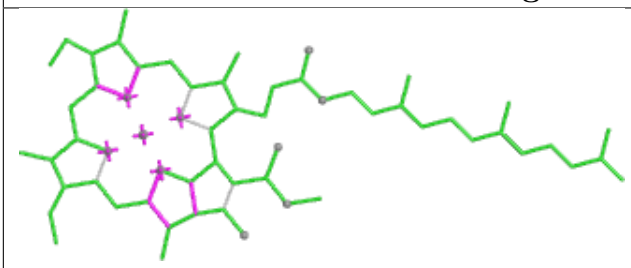
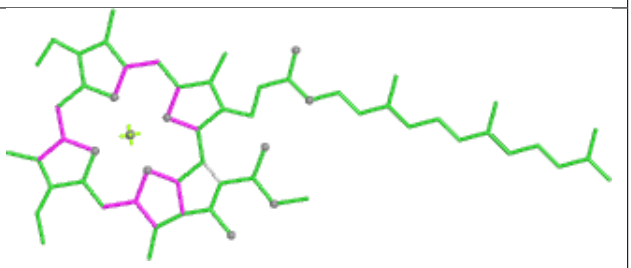
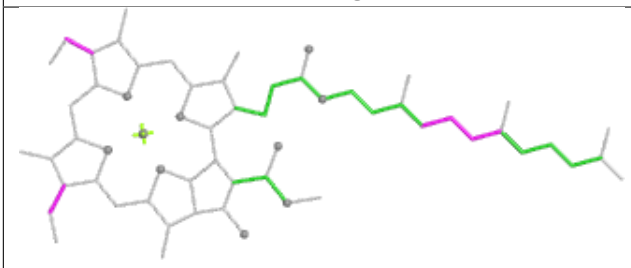
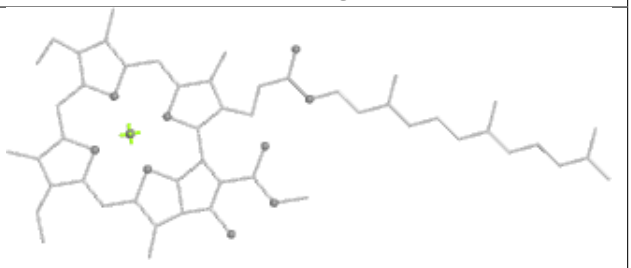


Rings

Ligand CLA m 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

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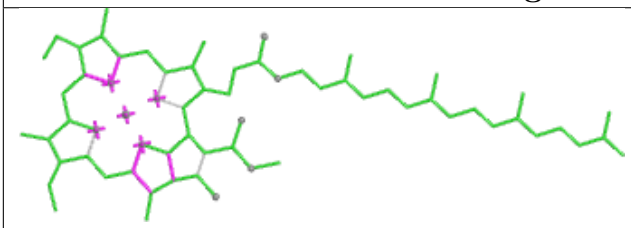
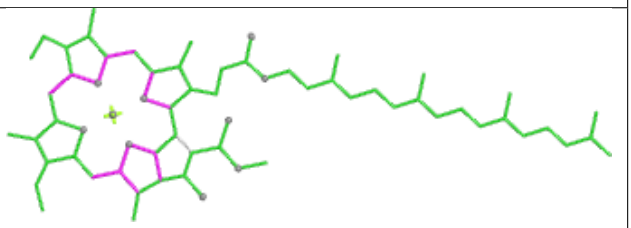
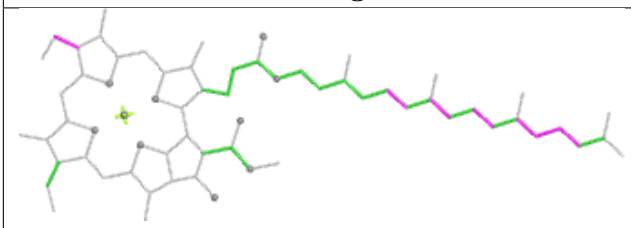
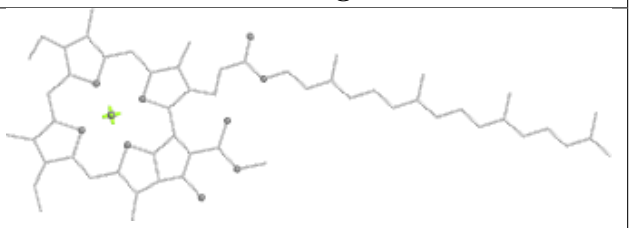
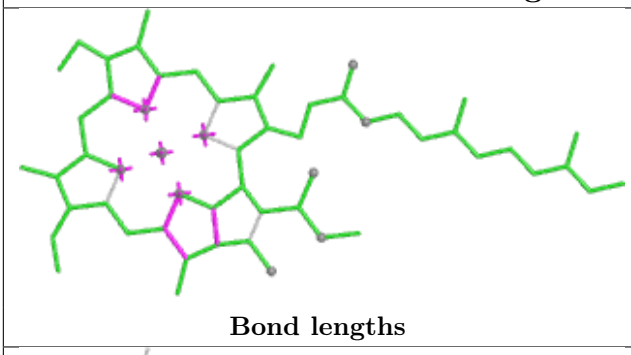
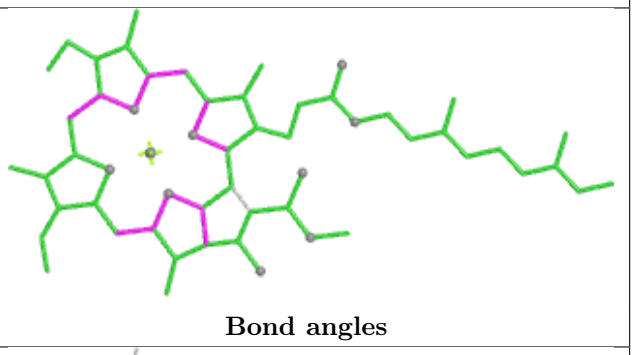
	
Bond lengths	Bond angles
	
Torsions	Rings

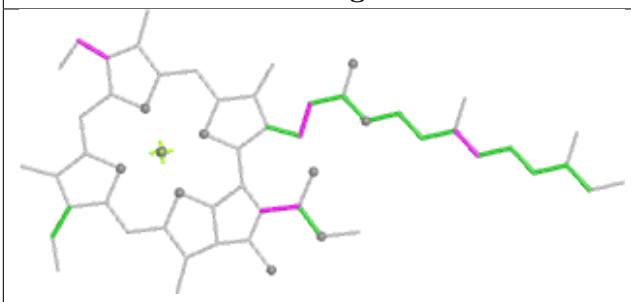
Ligand CLA B 821



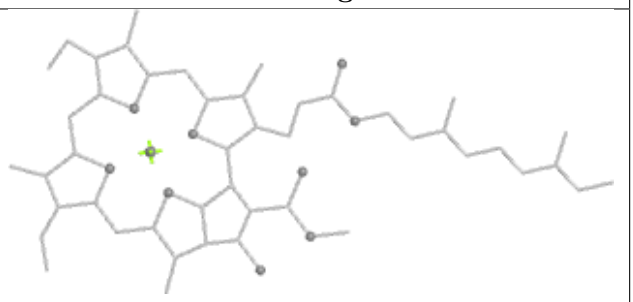
Bond lengths



Bond angles

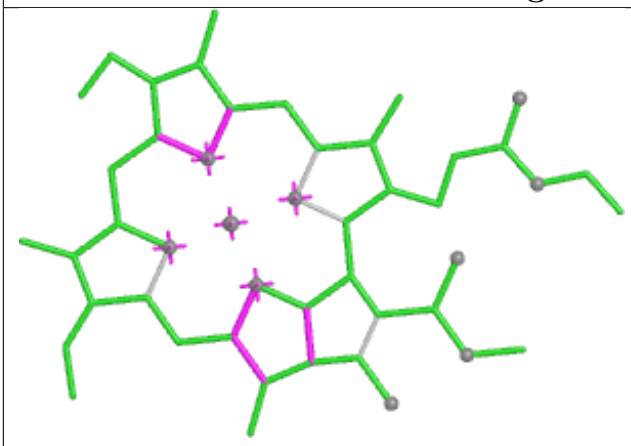


Torsions



Rings

Ligand CLA h 206



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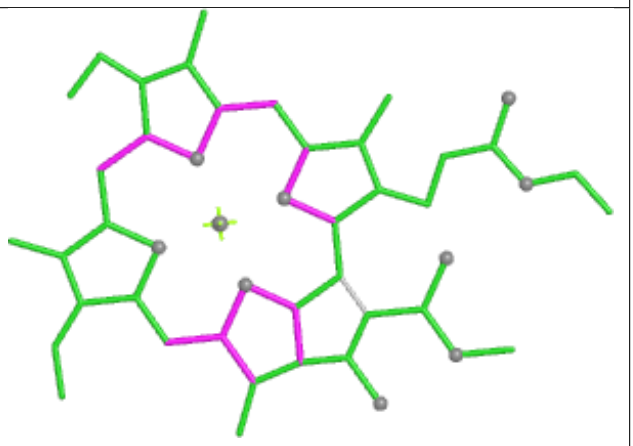
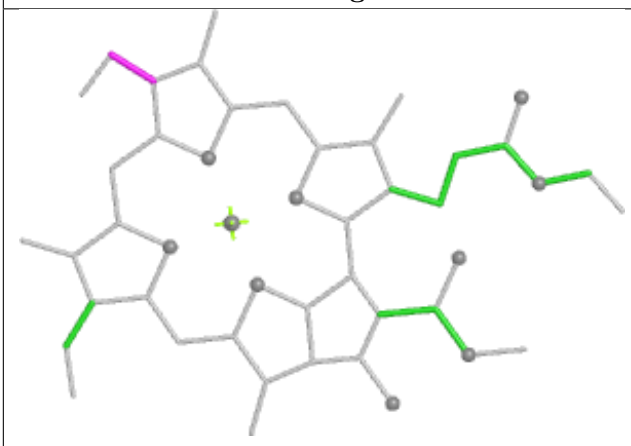


Bond angles



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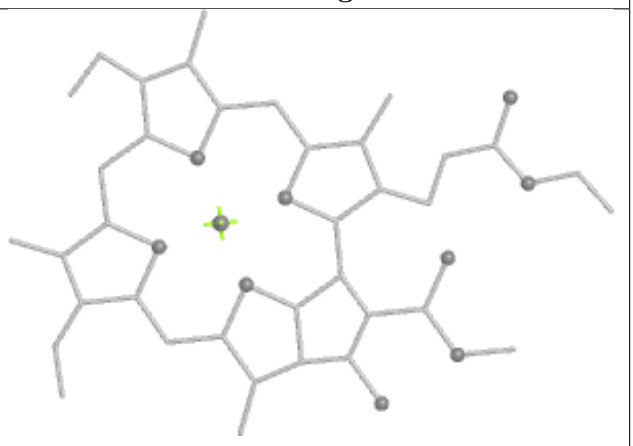
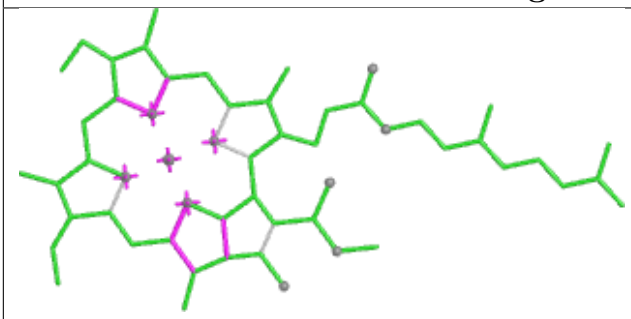


Rings

Ligand CLA a 303



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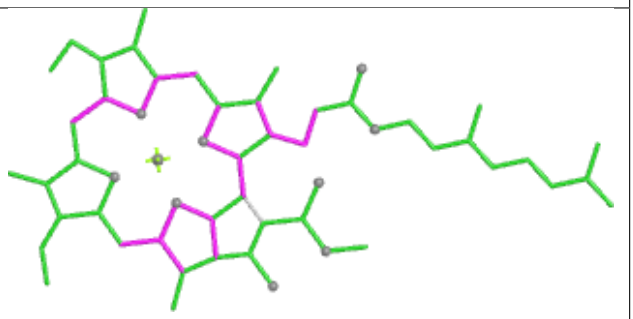
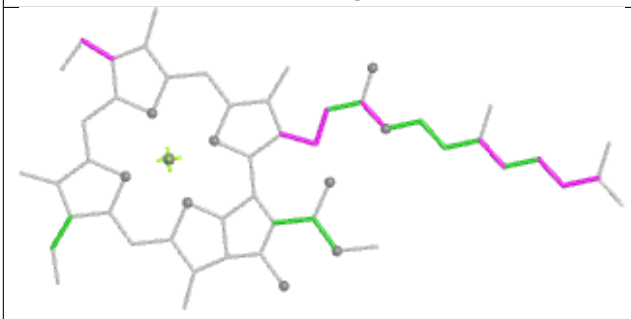


Bond angles



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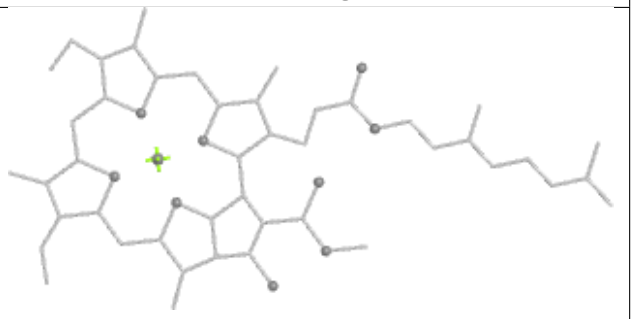
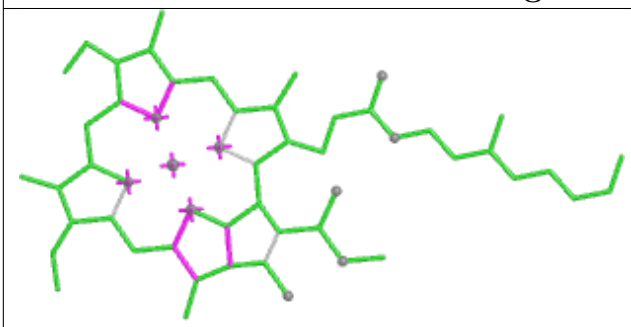


Rings

Ligand CLA B 809



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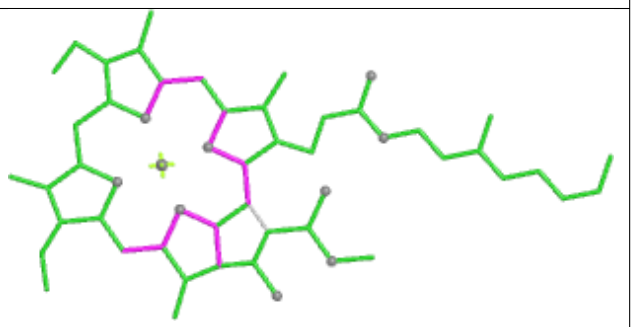
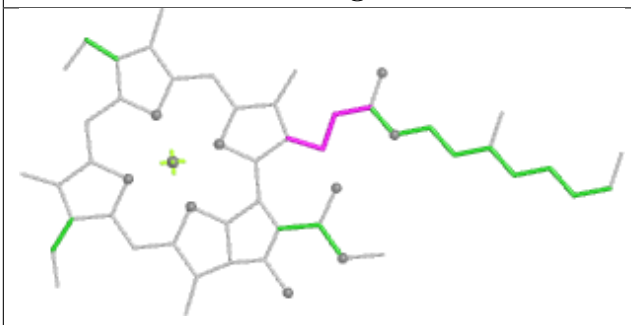


Bond angles



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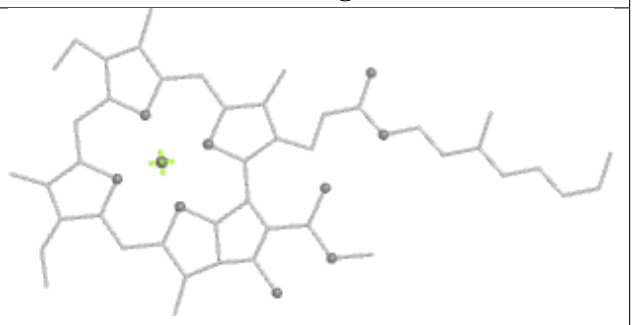
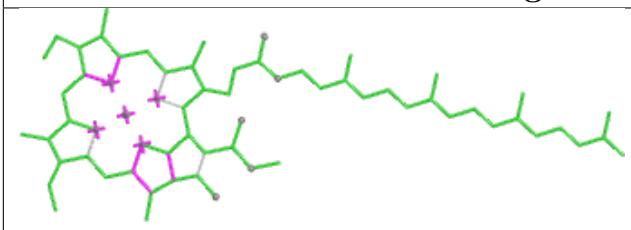


Rings

Ligand CLA B 808



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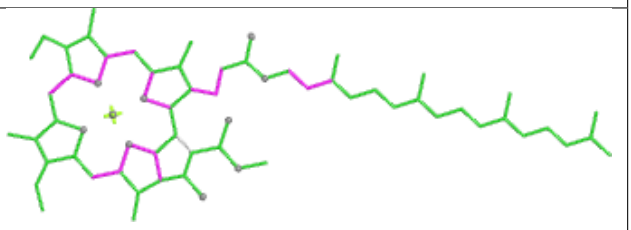
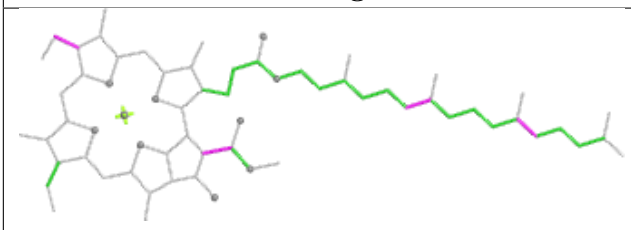


Bond angles



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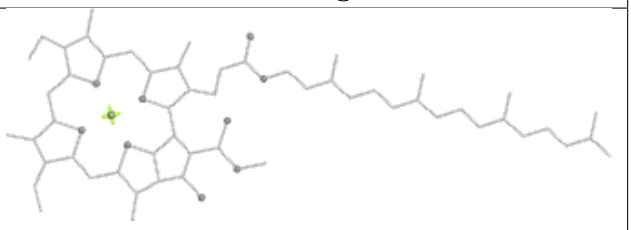
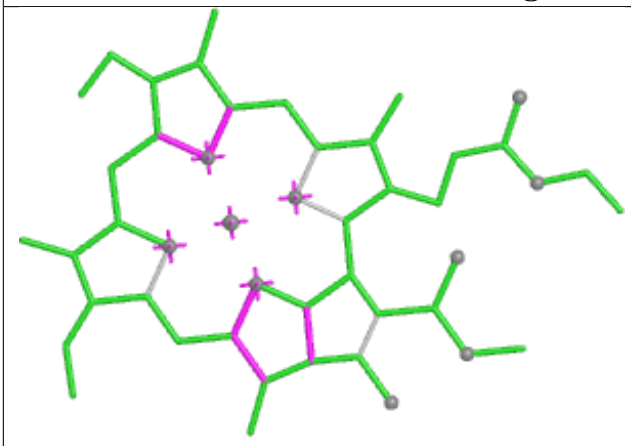


Rings

Ligand CLA m 311



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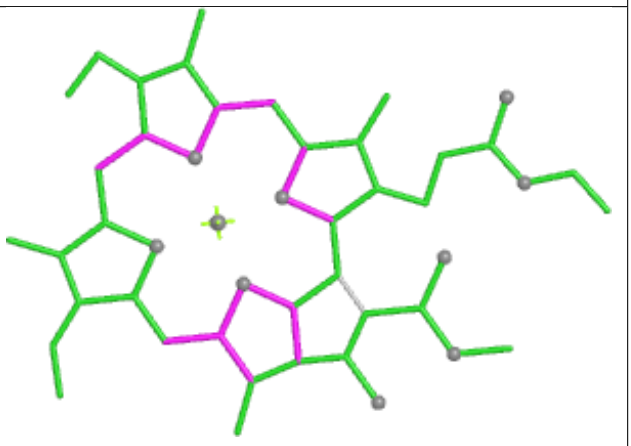
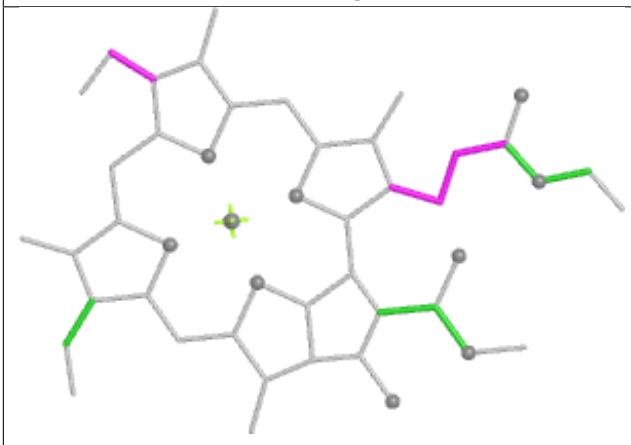


Bond angles



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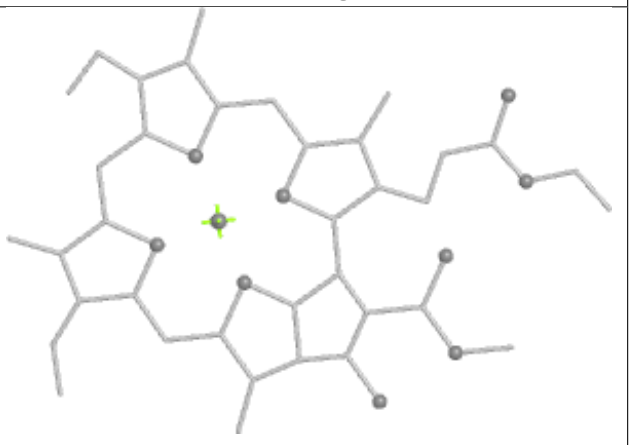
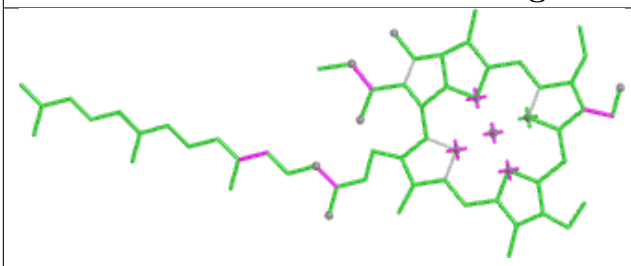


Rings

Ligand CHL c 305



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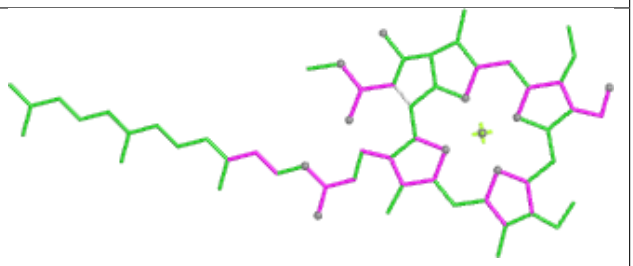
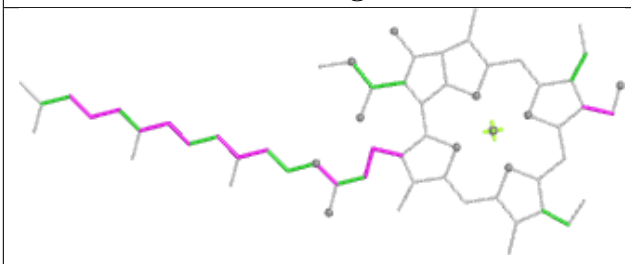


Bond angles



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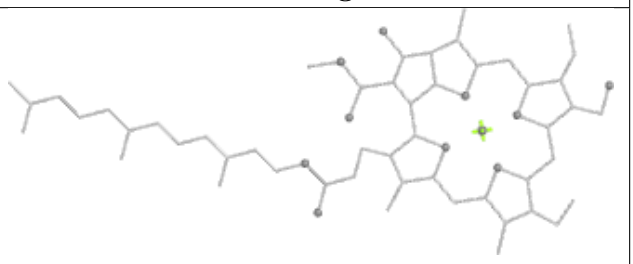
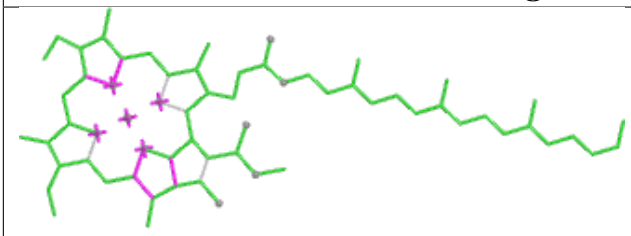


Rings

Ligand CLA B 801



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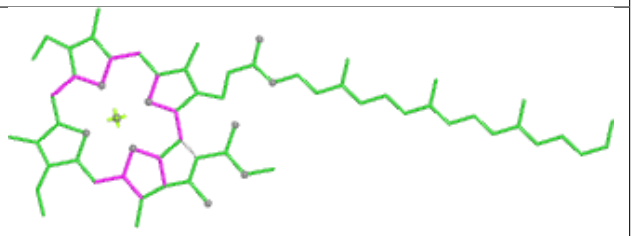
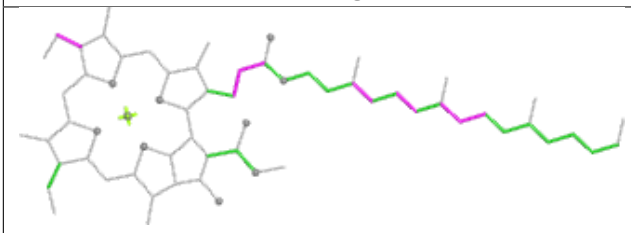


Bond angles



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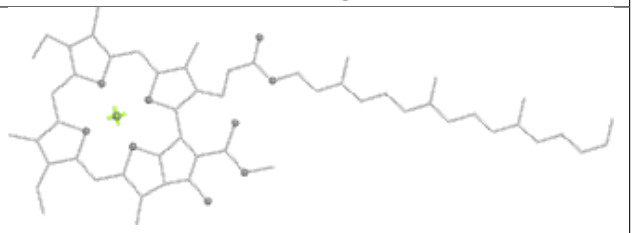
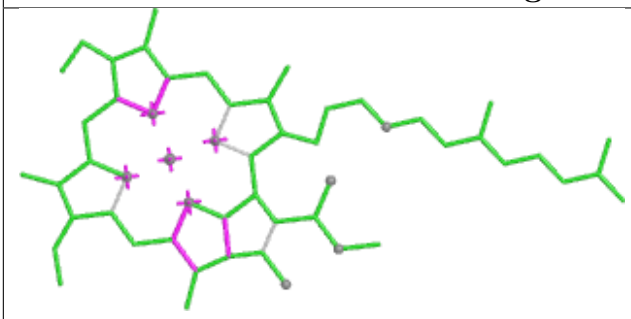
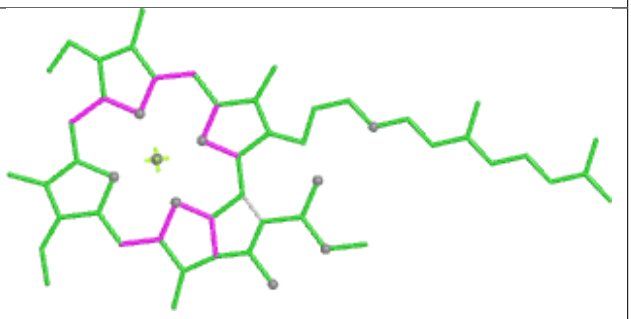


Rings

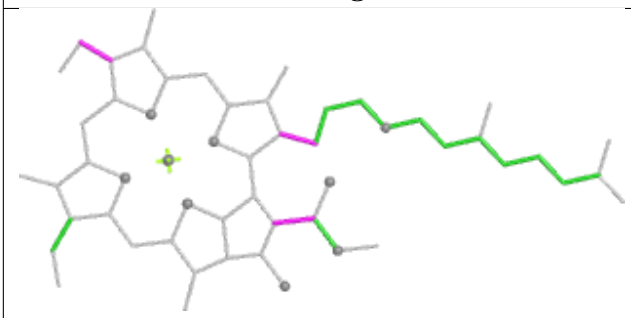
Ligand CLA B 813



Bond lengths



Bond angles



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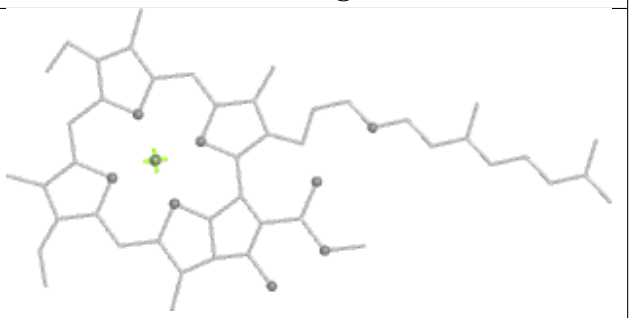
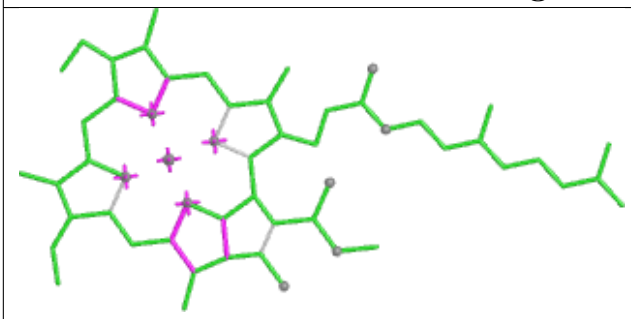
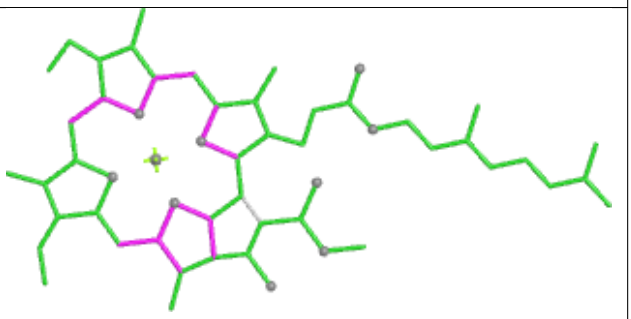


Rings

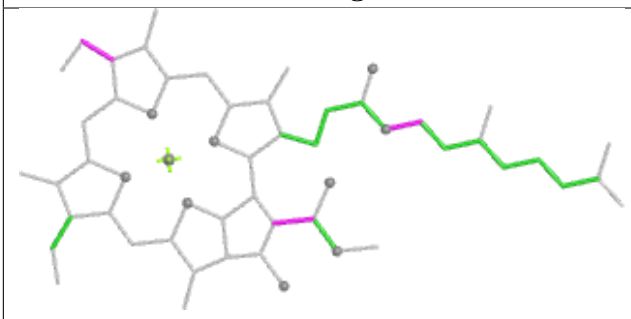
Ligand CLA c 303



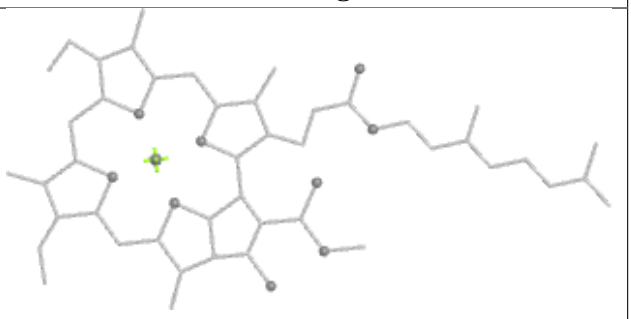
Bond lengths



Bond angles

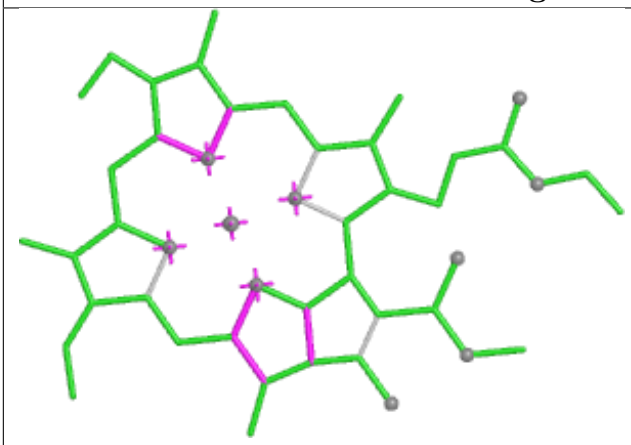


Torsions

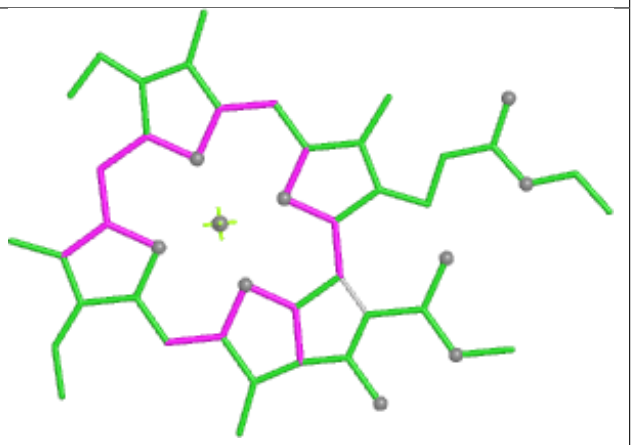


Rings

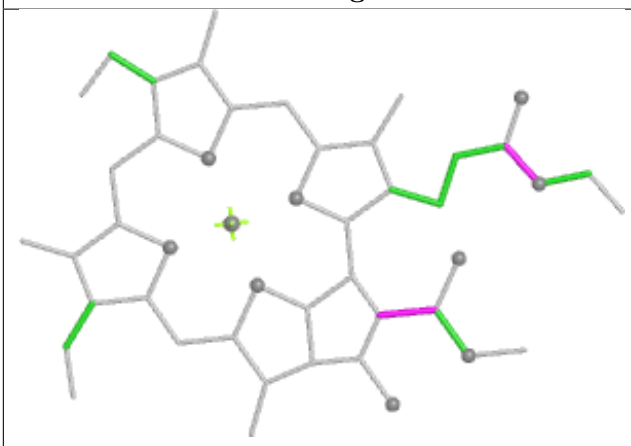
Ligand CLA e 303



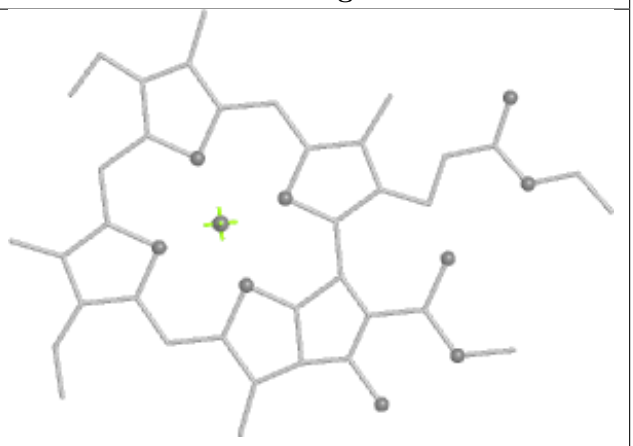
Bond lengths



Bond angles

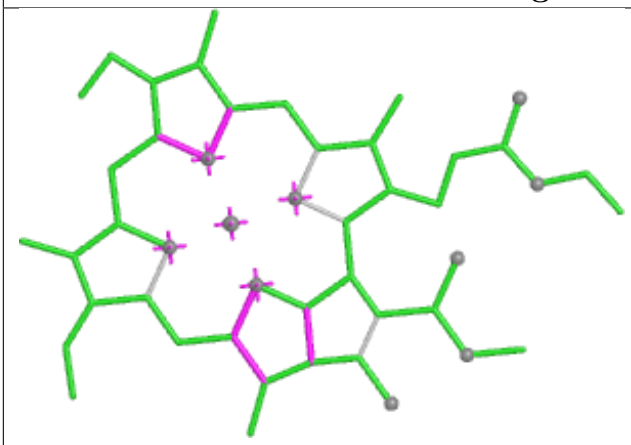


Torsions

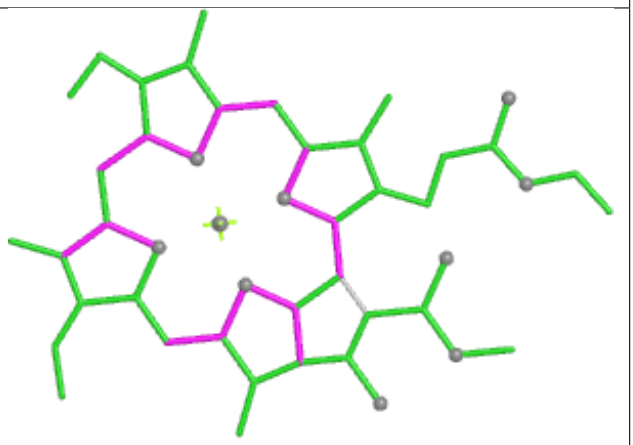


Rings

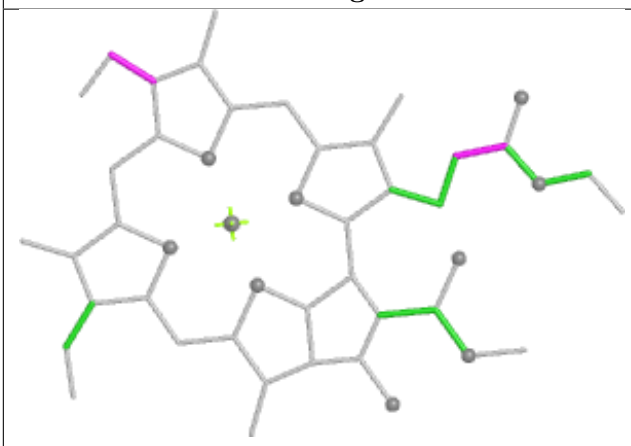
Ligand CLA f 303



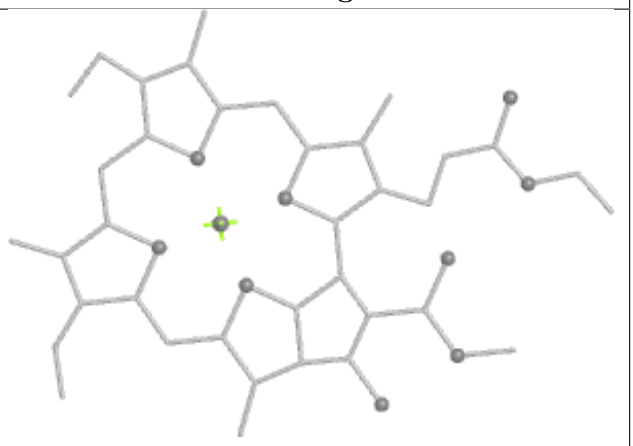
Bond lengths



Bond angles

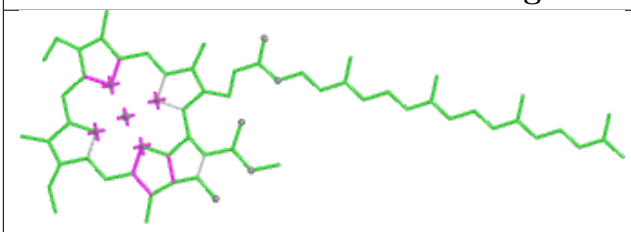


Torsions

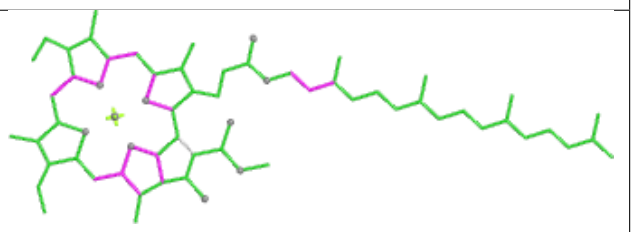


Rings

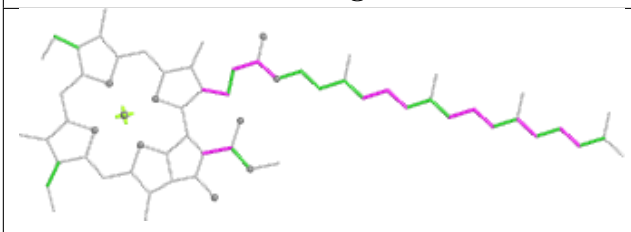
Ligand CLA A 806



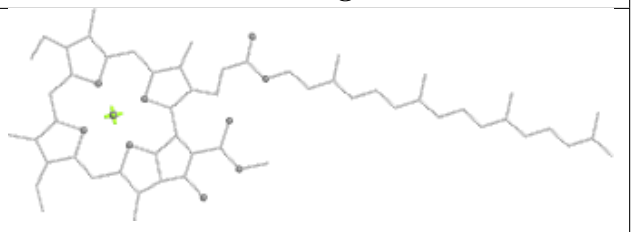
Bond lengths



Bond angles

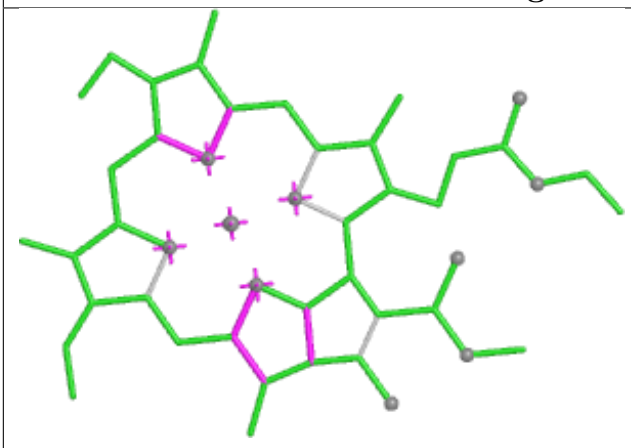


Torsions

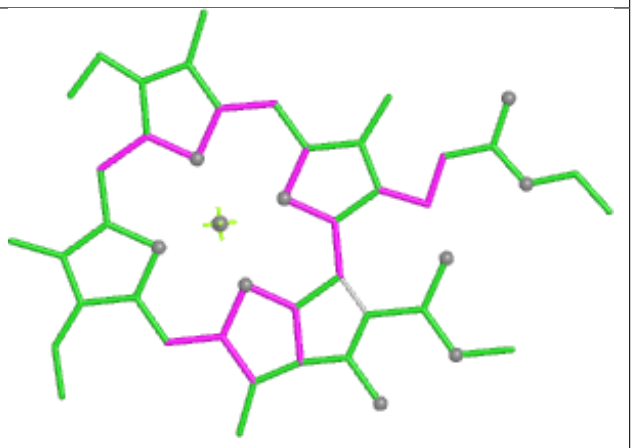


Rings

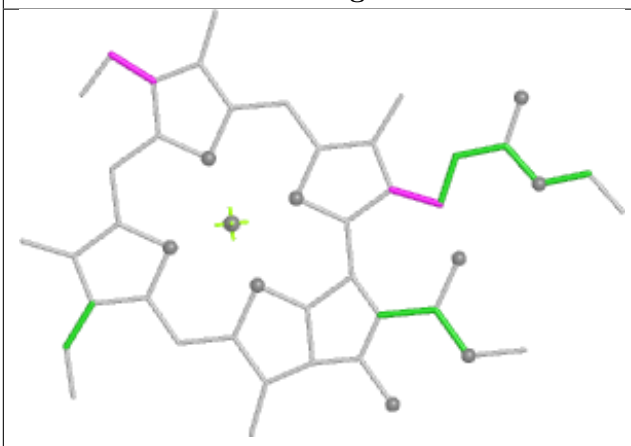
Ligand CLA d 203



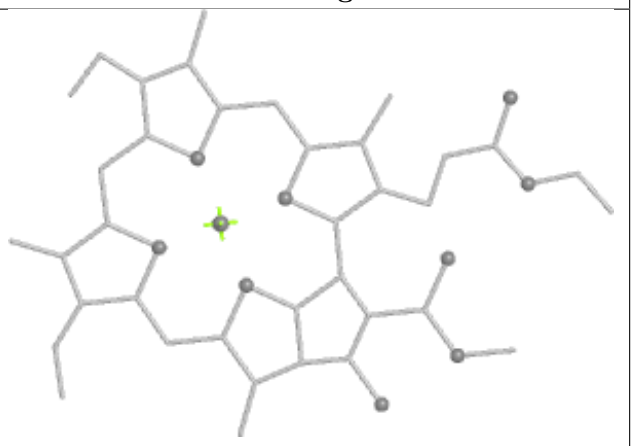
Bond lengths



Bond angles

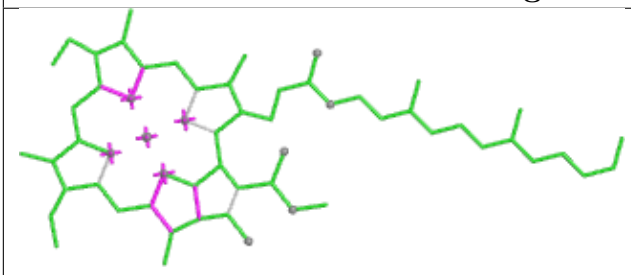


Torsions

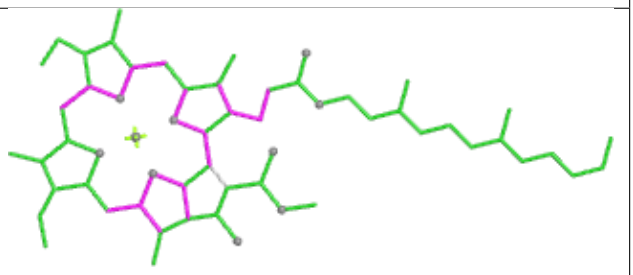


Rings

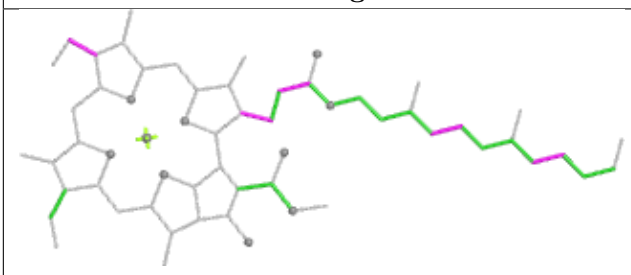
Ligand CLA A 816



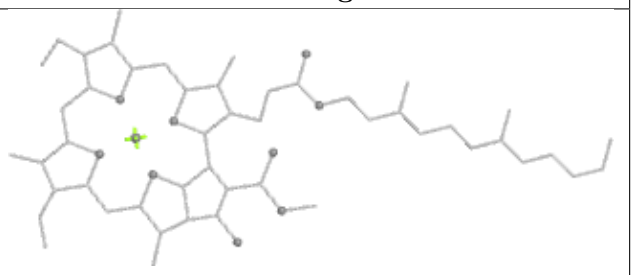
Bond lengths



Bond angles

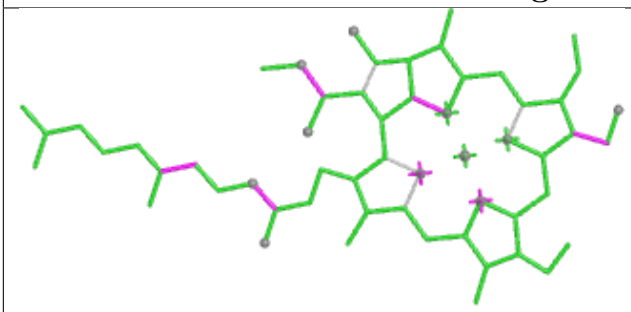


Torsions

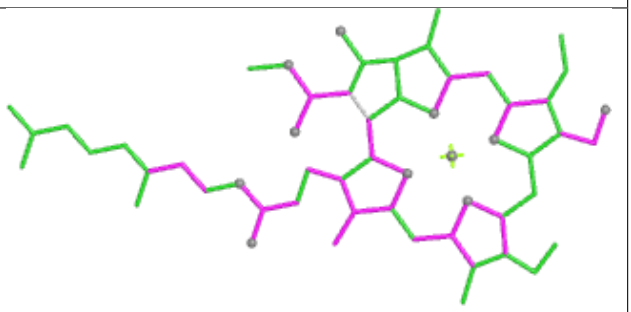


Rings

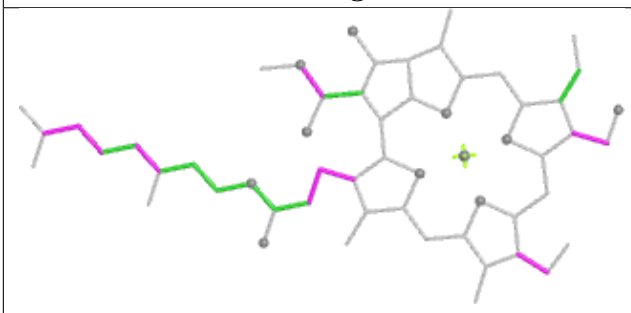
Ligand CHL f 304



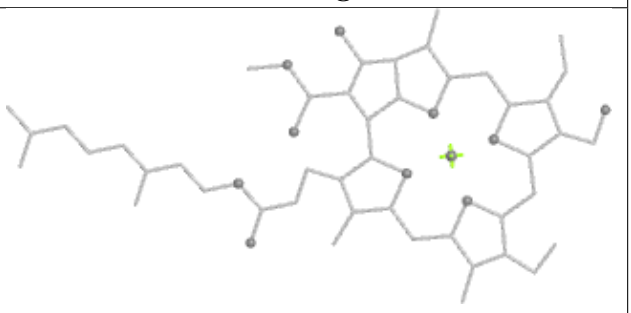
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

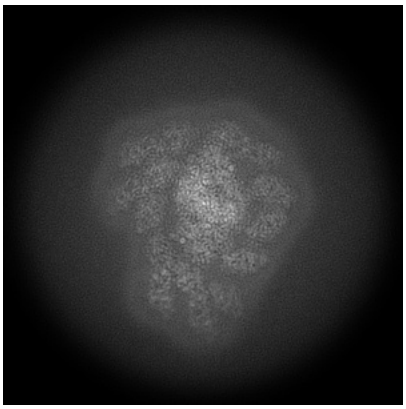
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-65121. These allow visual inspection of the internal detail of the map and identification of artifacts.

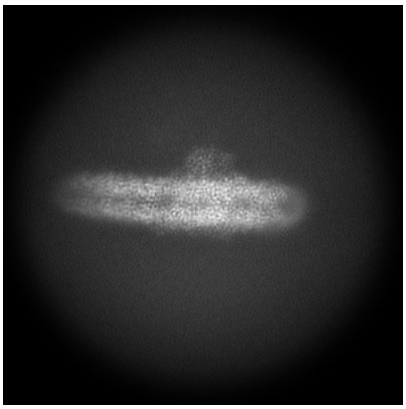
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

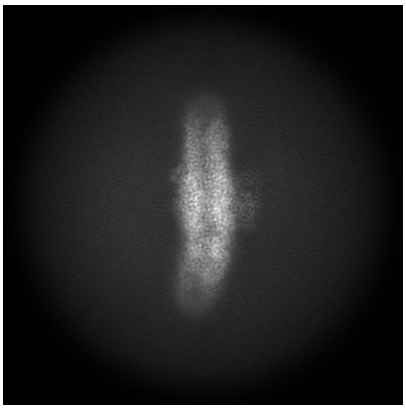
6.1.1 Primary map



X

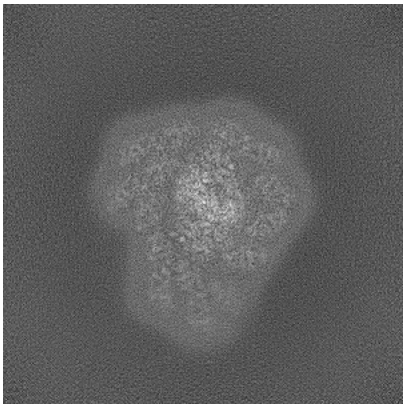


Y

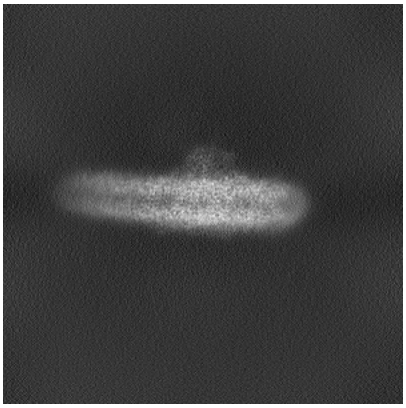


Z

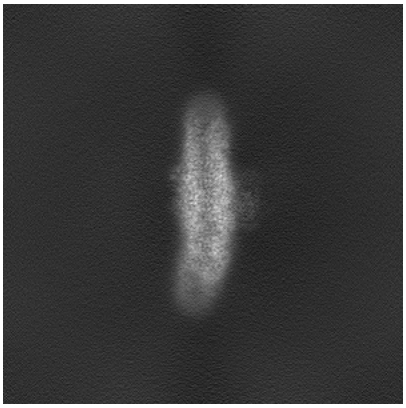
6.1.2 Raw map



X



Y

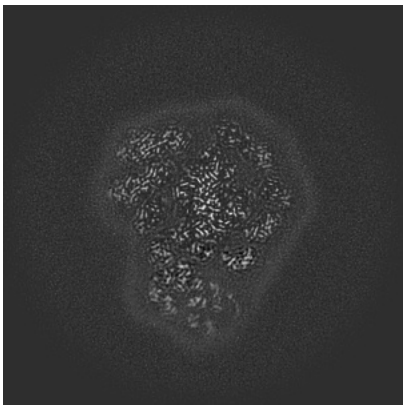


Z

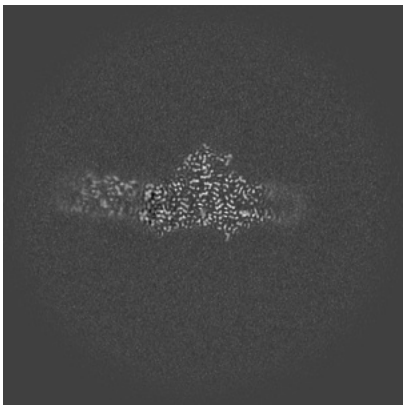
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

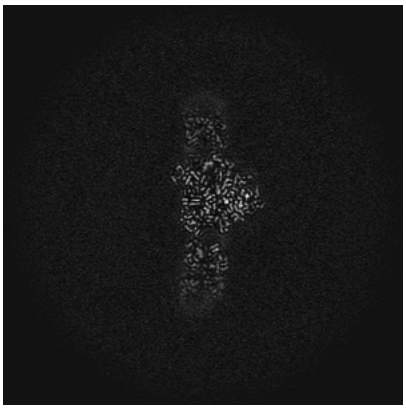
6.2.1 Primary map



X Index: 250

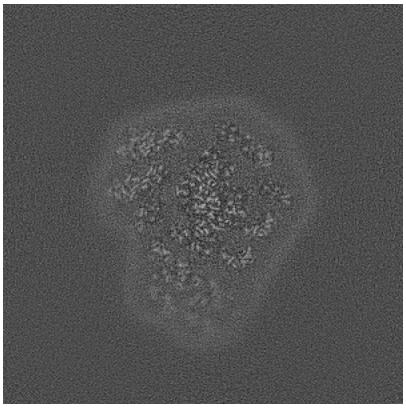


Y Index: 250

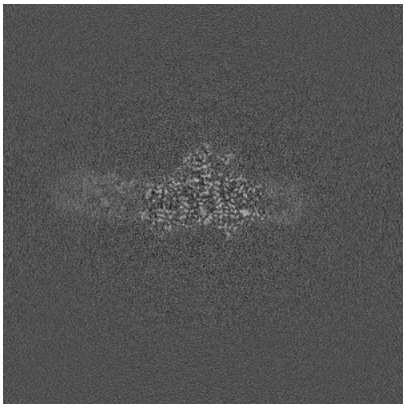


Z Index: 250

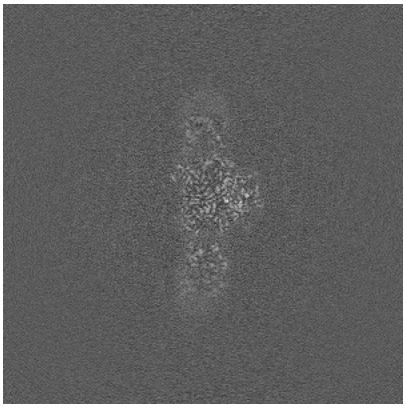
6.2.2 Raw map



X Index: 250



Y Index: 250

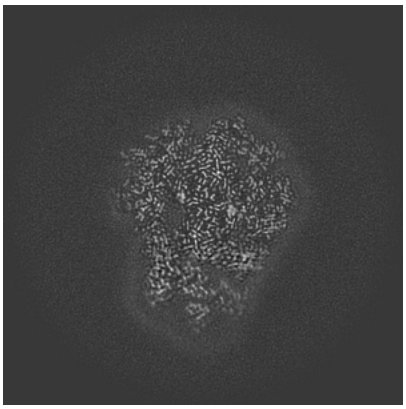


Z Index: 250

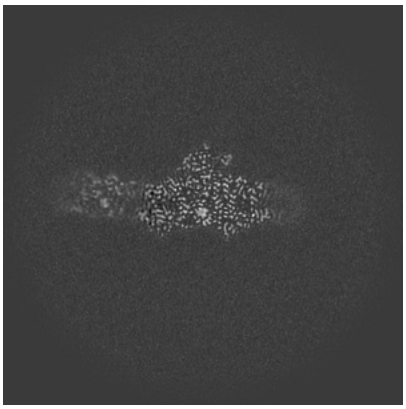
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

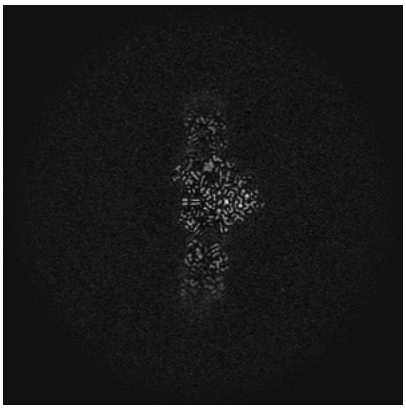
6.3.1 Primary map



X Index: 267

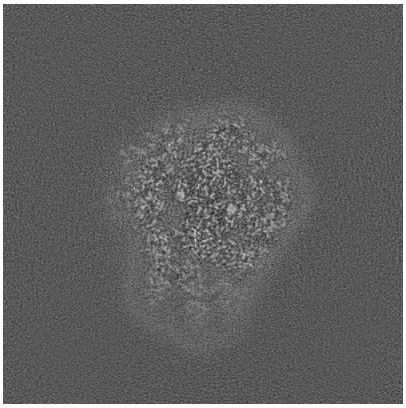


Y Index: 251

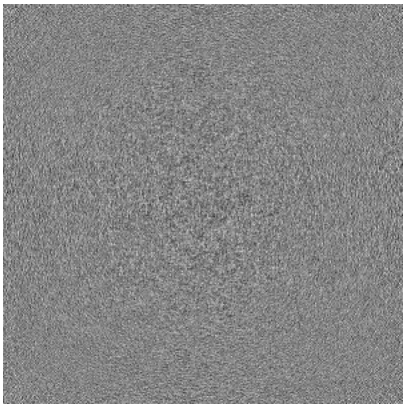


Z Index: 251

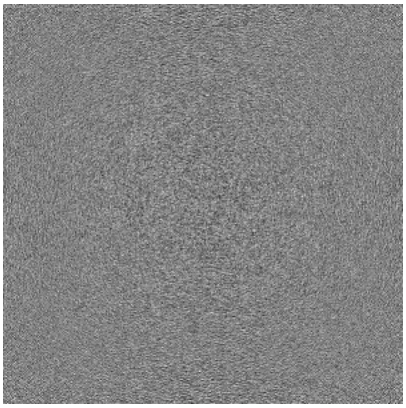
6.3.2 Raw map



X Index: 267



Y Index: 0

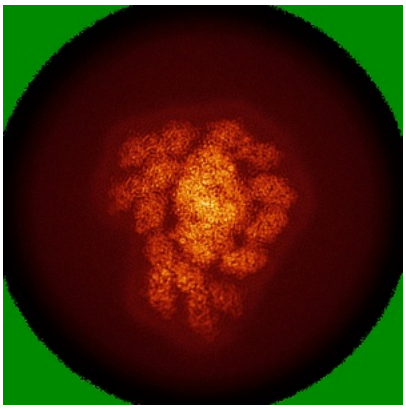


Z Index: 499

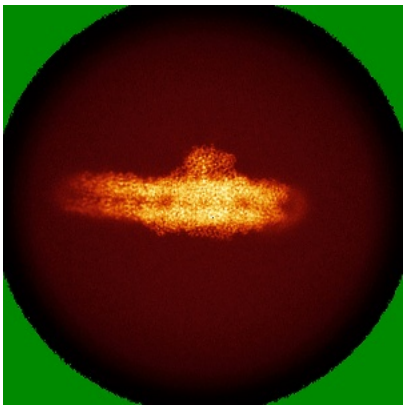
The images above show the largest variance slices of the map in three orthogonal directions.

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

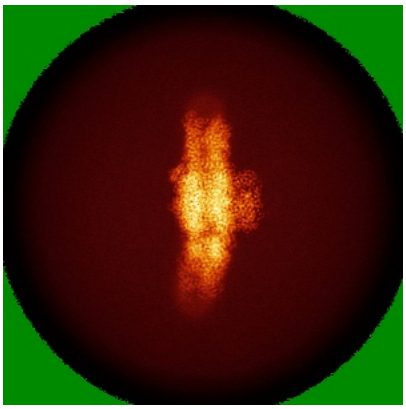
6.4.1 Primary map



X

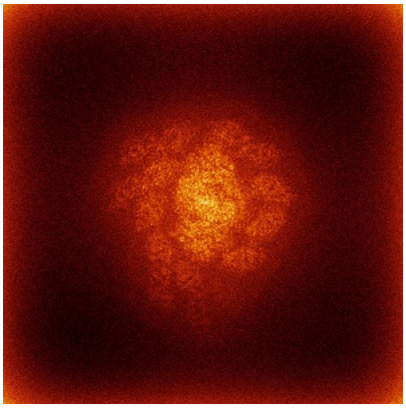


Y

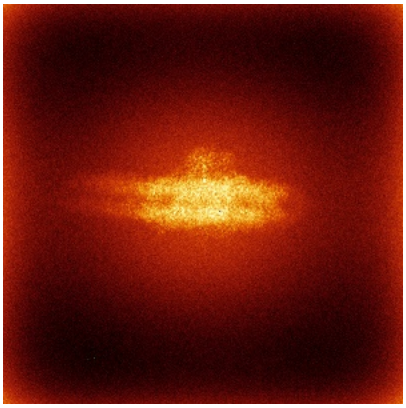


Z

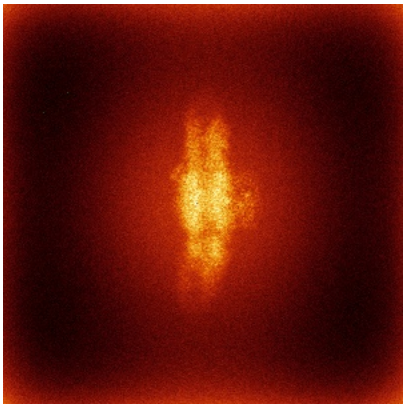
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

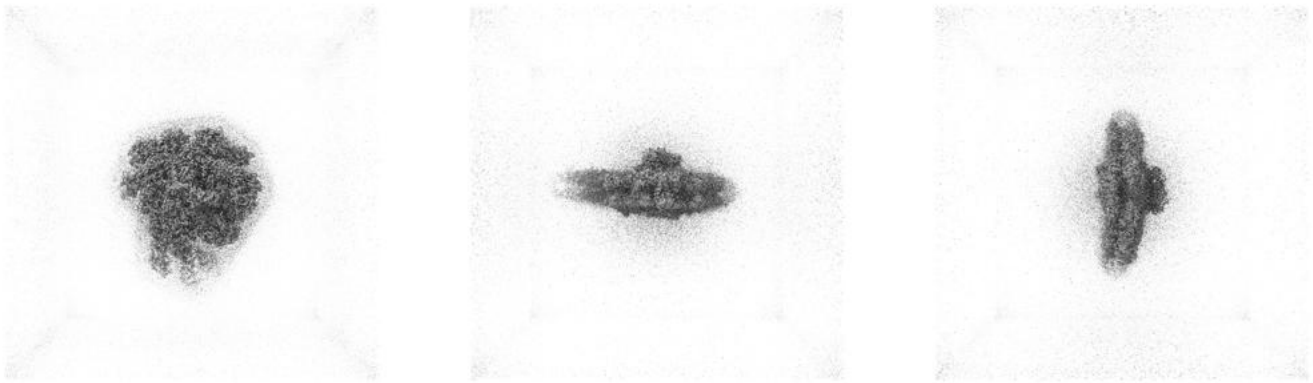
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

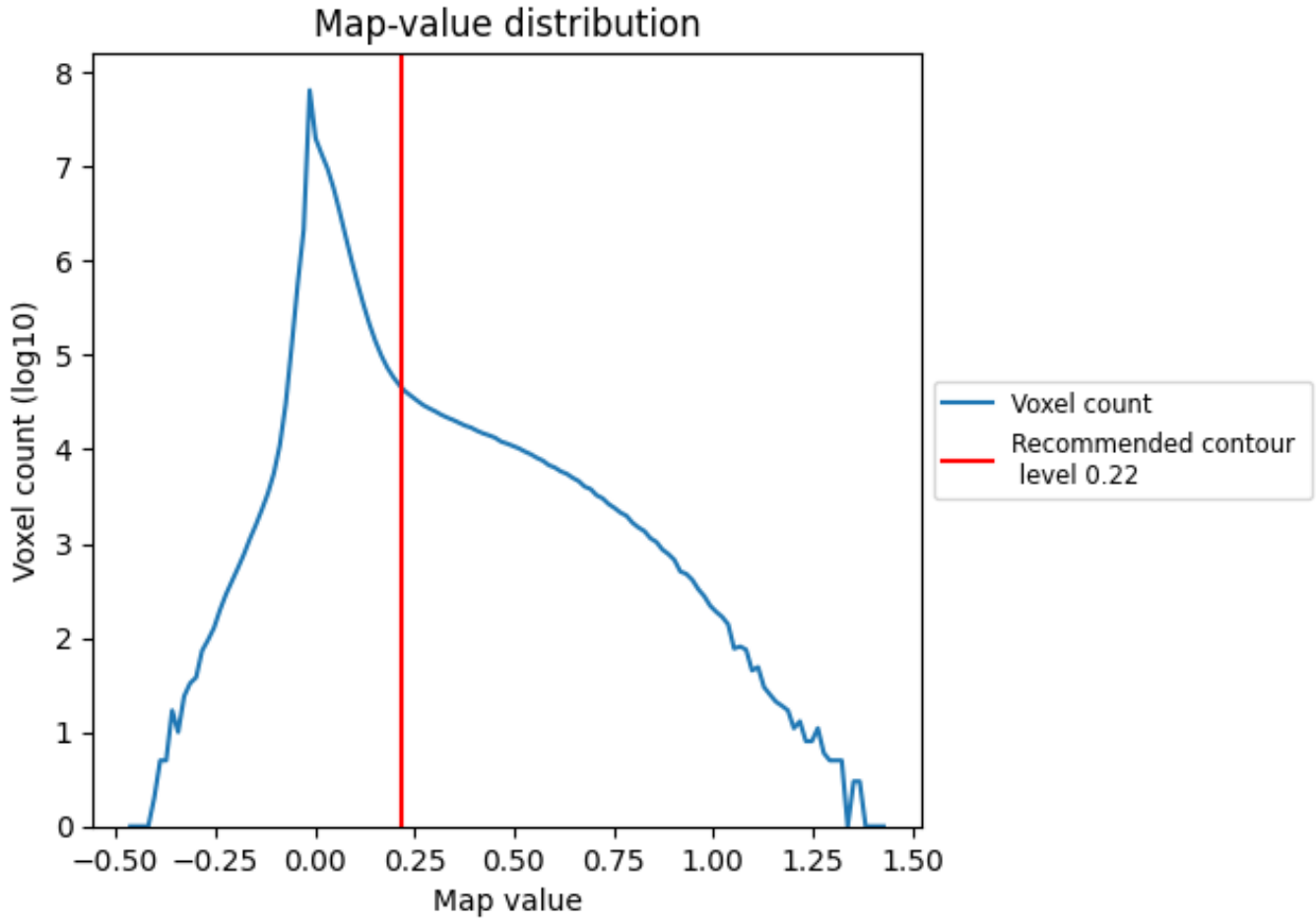
6.6 Mask visualisation (i)

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

7 Map analysis

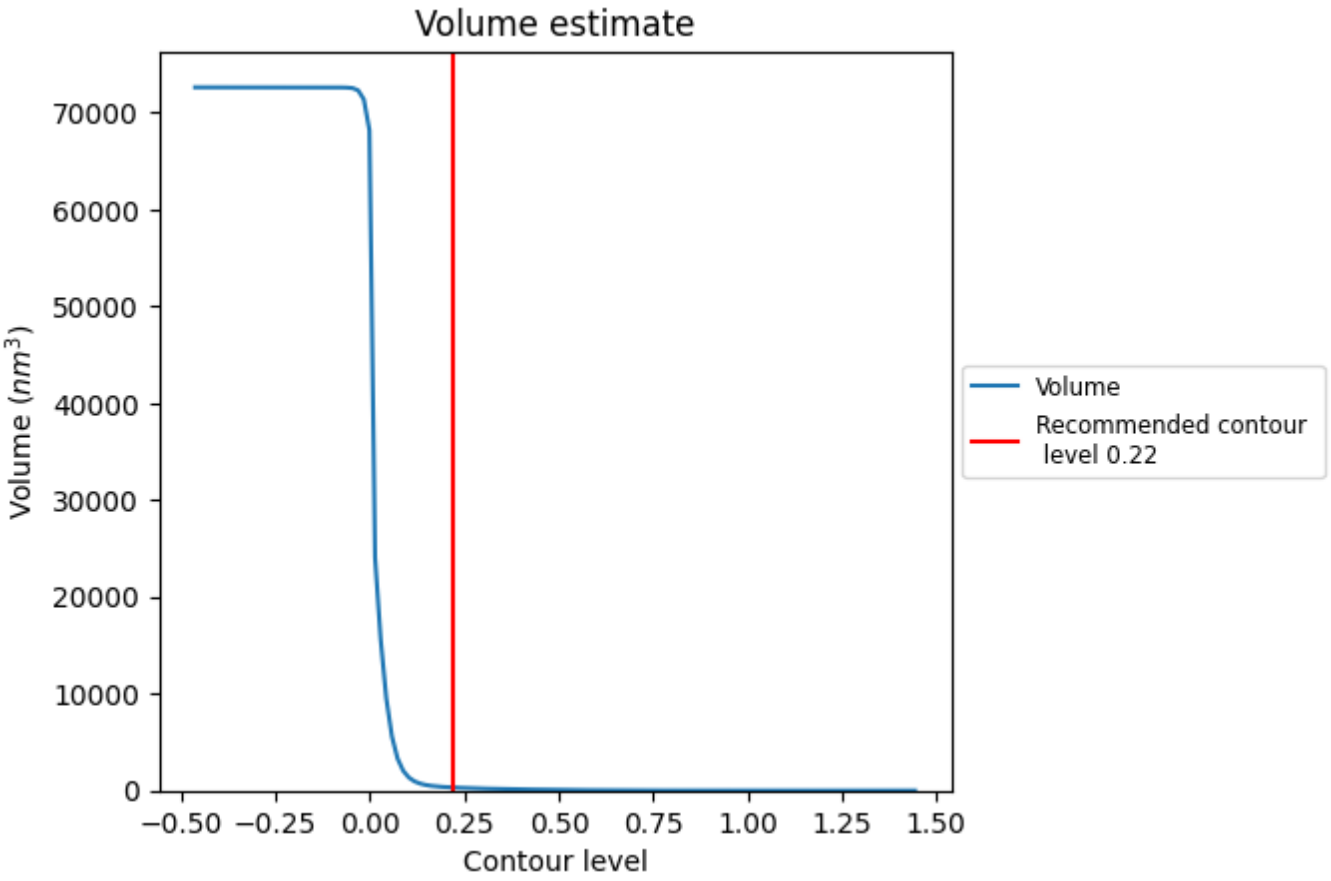
This section contains the results of statistical analysis of the map.

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.

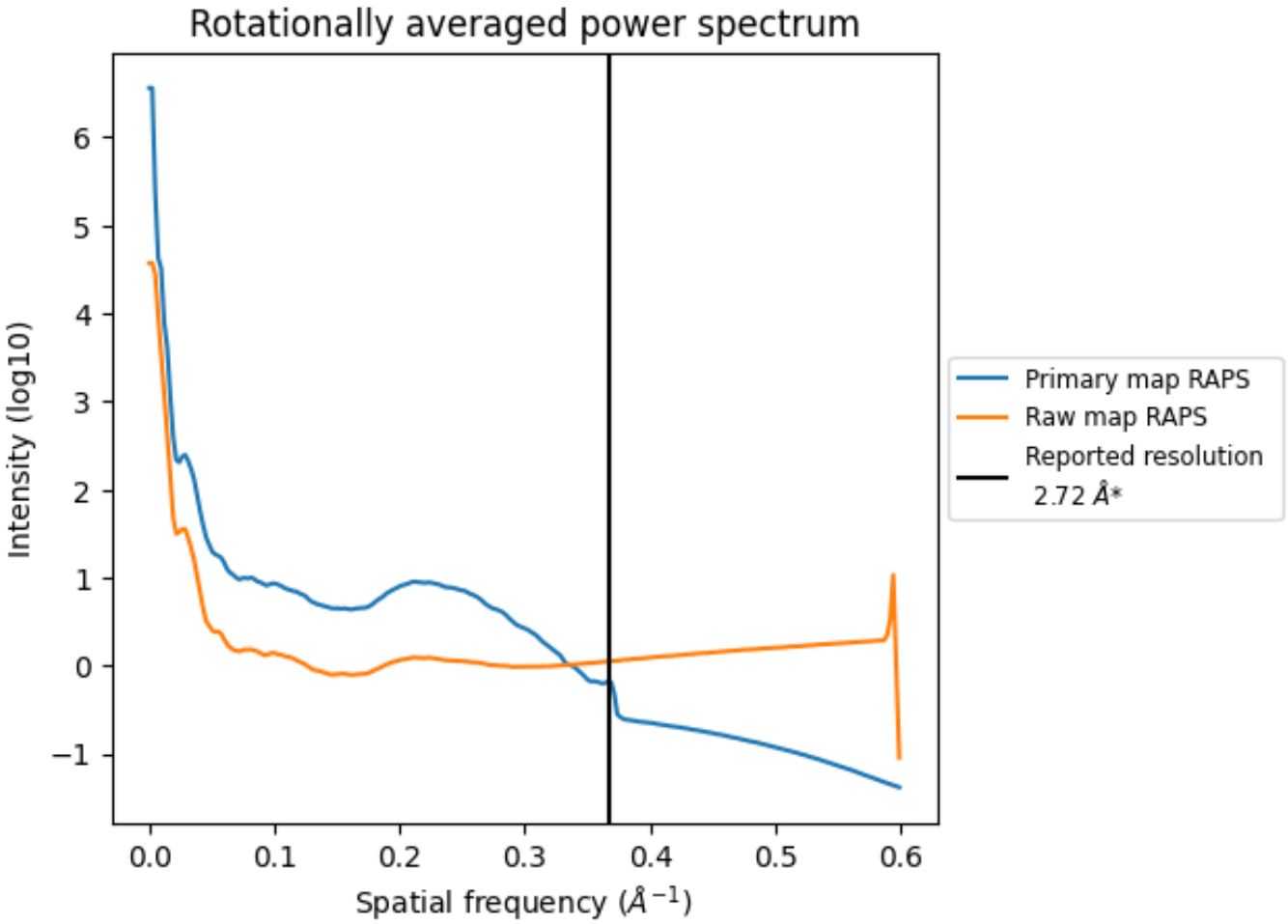
7.2 Volume estimate



The volume at the recommended contour level is 315 nm^3; this corresponds to an approximate mass of 285 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)

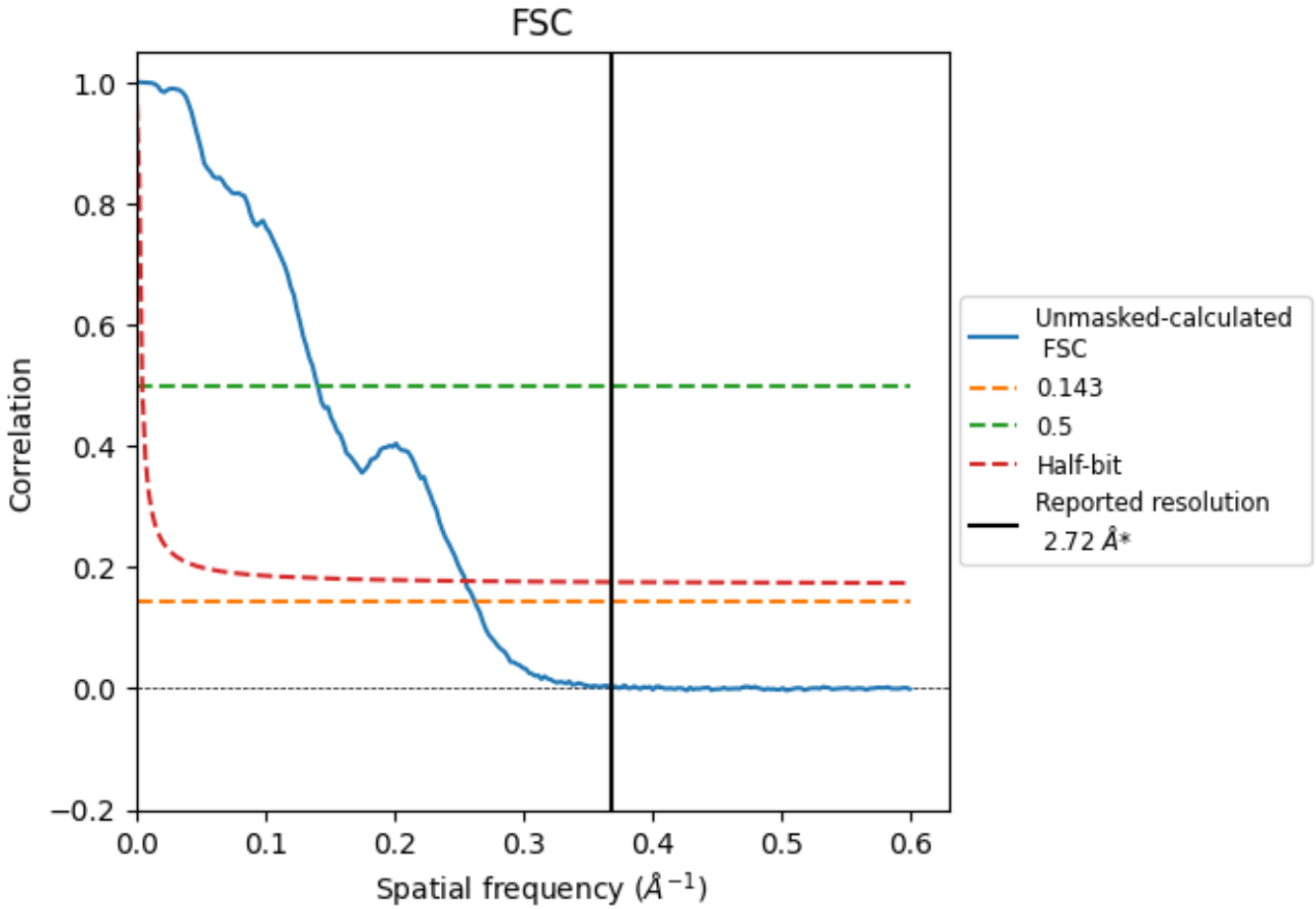


*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8.2 Resolution estimates (i)

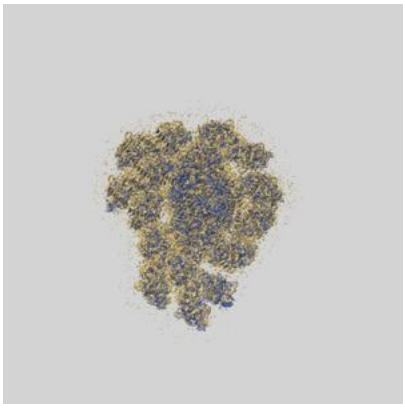
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	7.12	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.81 differs from the reported value 2.72 by more than 10 %

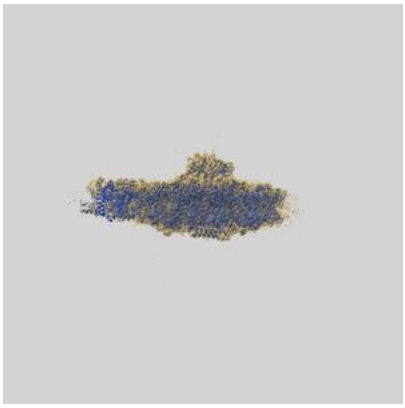
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-65121 and PDB model 9VJS. Per-residue inclusion information can be found in section 3 on page 30.

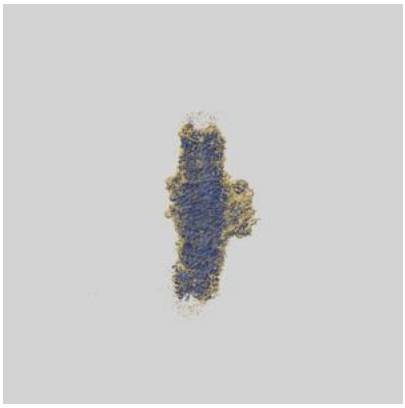
9.1 Map-model overlay



X



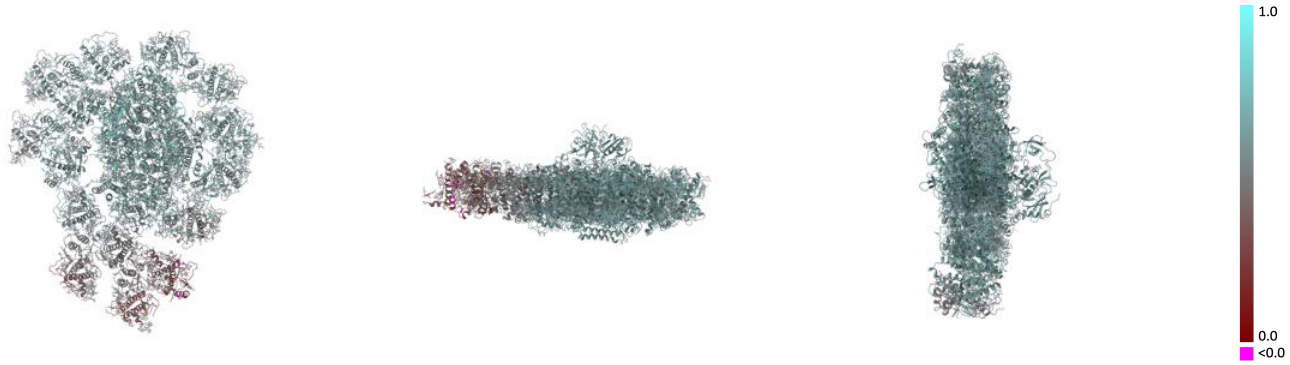
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.22 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.

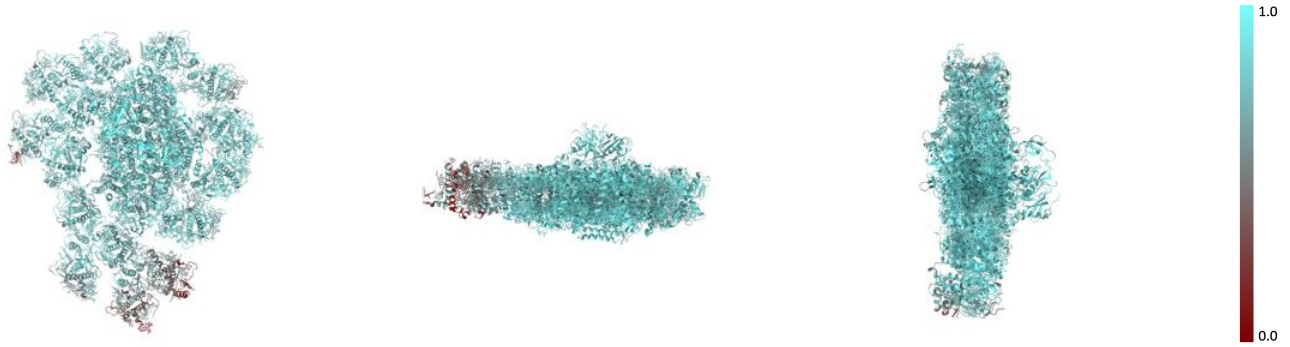
9.2 Q-score mapped to coordinate model



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.

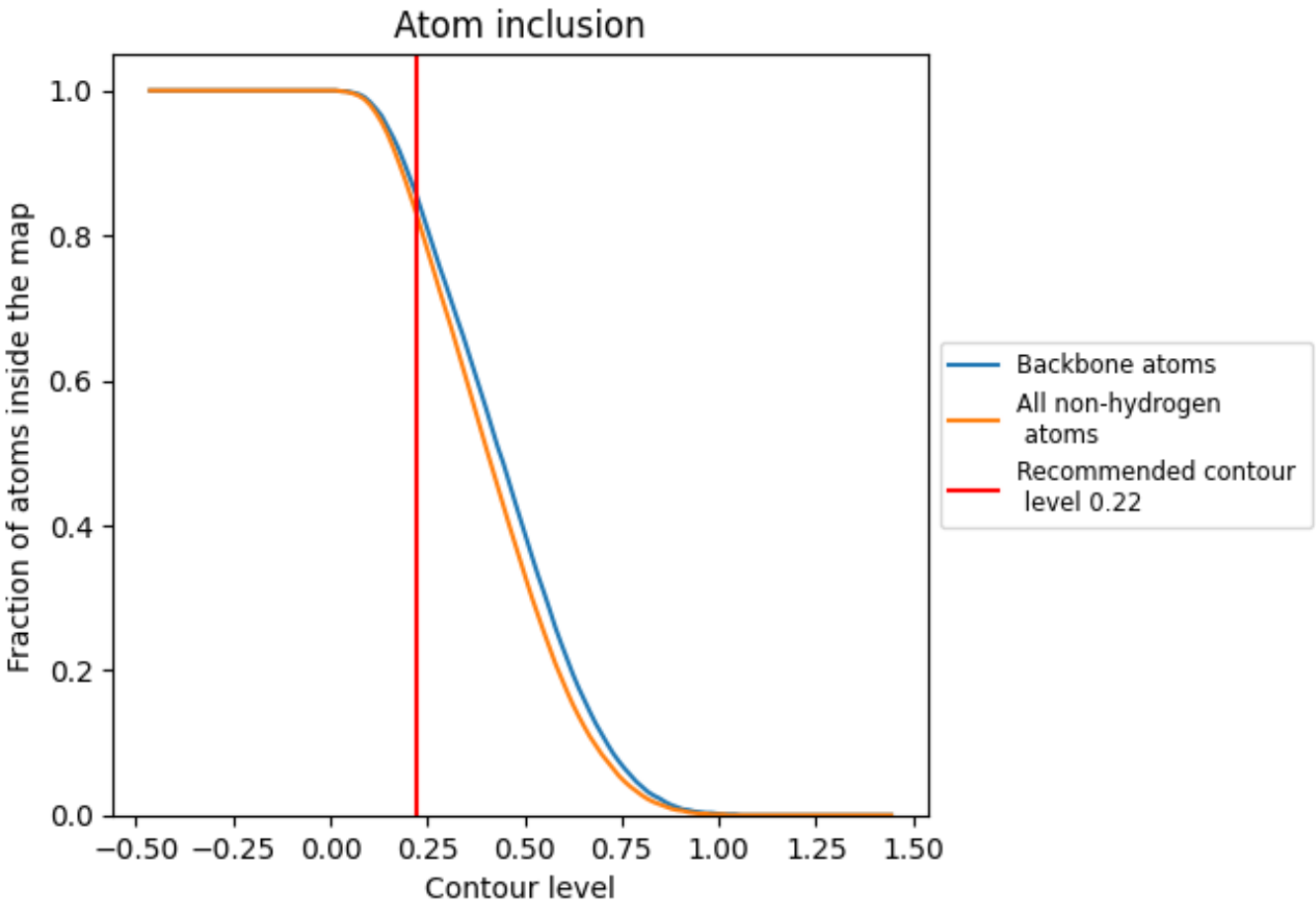
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.22).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.5710
A	0.9380	0.6360
B	0.9210	0.6160
C	0.9430	0.6200
D	0.8720	0.6140
E	0.8550	0.6040
F	0.8690	0.6070
J	0.8970	0.6150
M	0.8400	0.5830
a	0.8230	0.5250
b	0.8560	0.5880
c	0.8400	0.5980
d	0.7760	0.5790
e	0.8250	0.5930
f	0.8350	0.5860
g	0.9040	0.6140
h	0.8640	0.5950
i	0.8280	0.5570
j	0.7880	0.4850
k	0.7750	0.5630
l	0.6880	0.5250
m	0.7010	0.4350
n	0.4940	0.3690
o	0.4690	0.3550

