wwPDB EM Validation Summary Report

Sep 15, 2026 – 12:14 PM JST

PDB ID	:	9KQQ / pdb_00009kqq
EMDB ID	:	EMD-62512
Title	:	PSI-LHCI supercomplex binding with 8 Lhcas from C. subellipsoidea
Authors	:	Tsai, P.-C.; Kato, K.; Shen, J.-R.; Akita, F.
Deposited on	:	2024-11-26
Resolution	:	2.06 Å(reported)
Based on initial model	:	6zzx

This is a wwPDB EM Validation Summary 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:

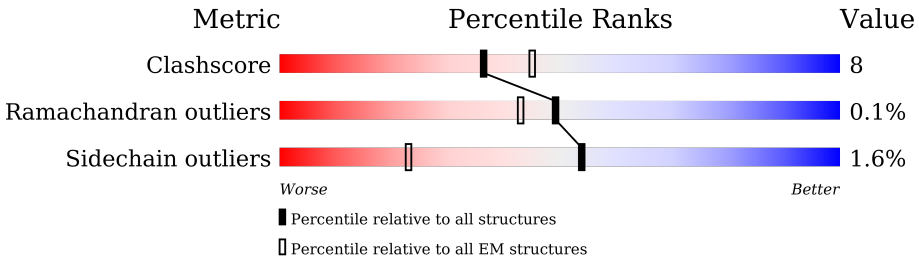
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

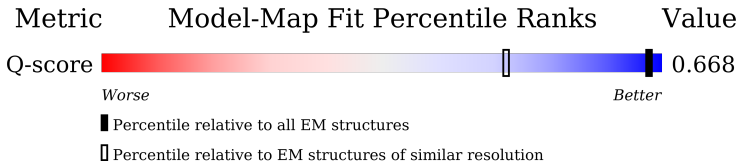
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.06 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	1895 (1.56 - 2.56)

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	90% 9%
2	B	734	90% 9%
3	C	81	93% 6%
4	D	192	66% 9% 26%

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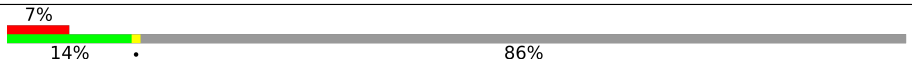
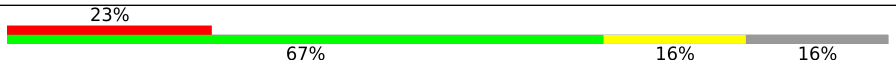
Mol	Chain	Length	Quality of chain
5	E	71	
6	F	245	
7	G	138	
8	I	36	
9	J	41	
10	K	131	
11	M	31	
12	a	229	
12	b	229	
13	3	246	
14	4	246	
15	5	274	
16	6	272	
17	7	259	
18	8	255	
19	L	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	b	308	-	-	X	-
29	LUT	4	301	-	X	-	-
29	LUT	4	302	-	X	-	-
29	LUT	5	303	-	X	-	-
29	LUT	6	303	-	X	-	-
29	LUT	F	303	-	X	-	-
29	LUT	J	103	-	X	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 46812 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	741	5823	3806	994	1005	18	0	0

- 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	732	5832	3829	989	1001	13	3	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	596	365	103	117	11	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1110	711	193	203	3	0	0

- Molecule 5 is a protein called Photosystem I reaction centre subunit IV/PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	60	490	316	83	90	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1264	805	223	234	2	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	20	Total	C	N	O	0	0
			159	107	23	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	33	Total	C	N	O	S	0	0
			248	171	34	41	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			336	232	48	55	1		

- Molecule 10 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	82	Total	C	N	O	S	0	0
			571	365	97	108	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			237	160	35	41	1		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	195	Total	C	N	O	S	0	0
			1458	944	245	267	2		
12	b	192	Total	C	N	O	S	0	0
			1441	933	242	264	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	220	Total	C	N	O	S	0	0
			1707	1117	275	312	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	207	Total	C	N	O	S	0	0
			1603	1045	264	290	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	231	Total	C	N	O	S	0	0
			1779	1160	306	309	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	234	Total	C	N	O	S	0	0
			1774	1159	296	311	8		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	7	216	Total	C	N	O	S	0	0
			1650	1070	280	298	2		

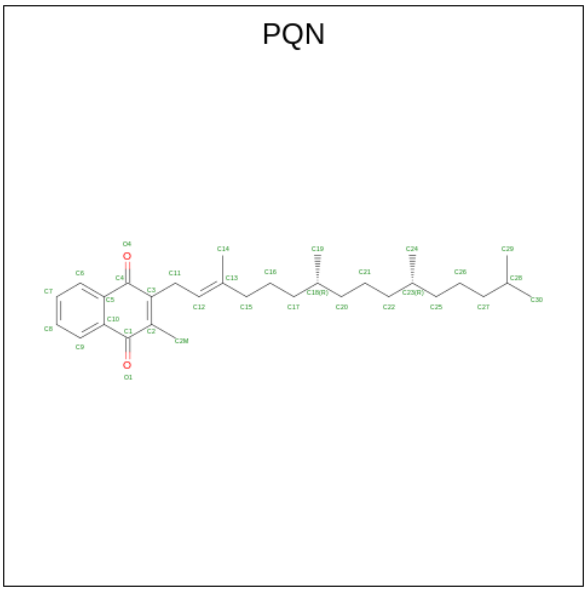
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	8	222	Total	C	N	O	S	0	0
			1701	1112	276	310	3		

- Molecule 19 is a protein called PSI subunit V.

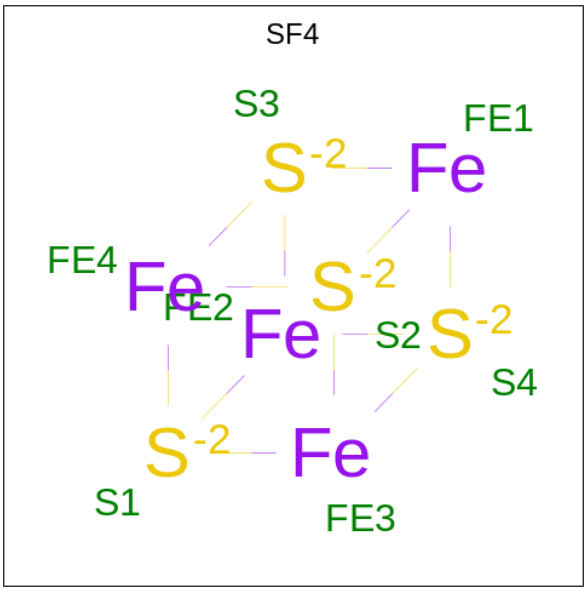
Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	122	Total	C	N	O	S	0	0
			890	585	148	155	2		

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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 IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	

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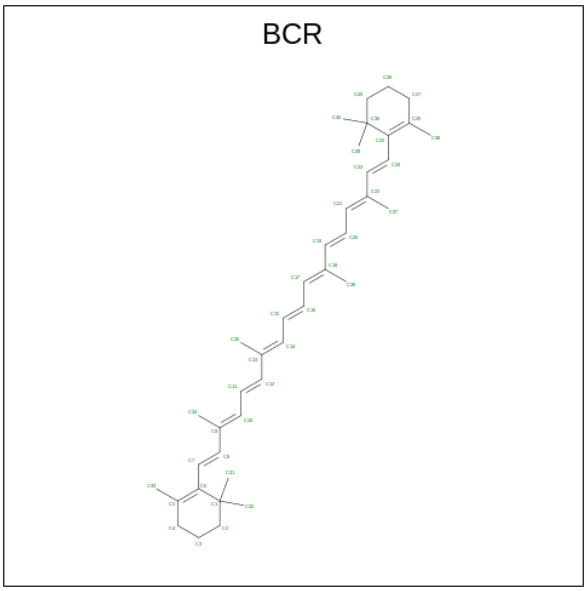
Mol	Chain	Residues	Atoms	AltConf
21	C	1	Total Fe S 8 4 4	0
21	C	1	Total Fe S 8 4 4	0

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0

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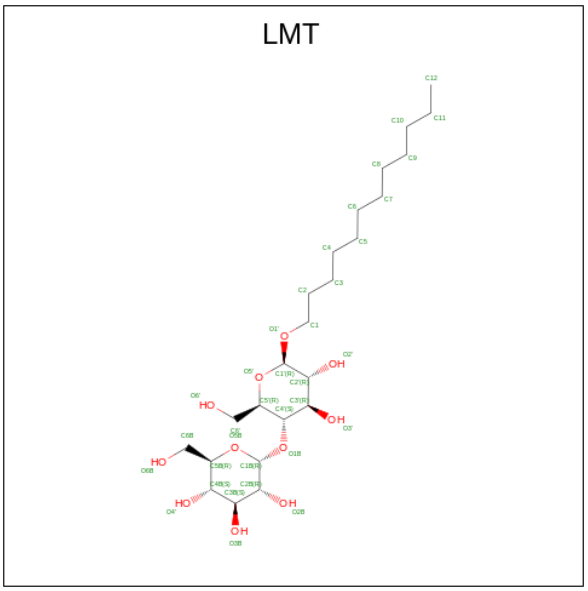
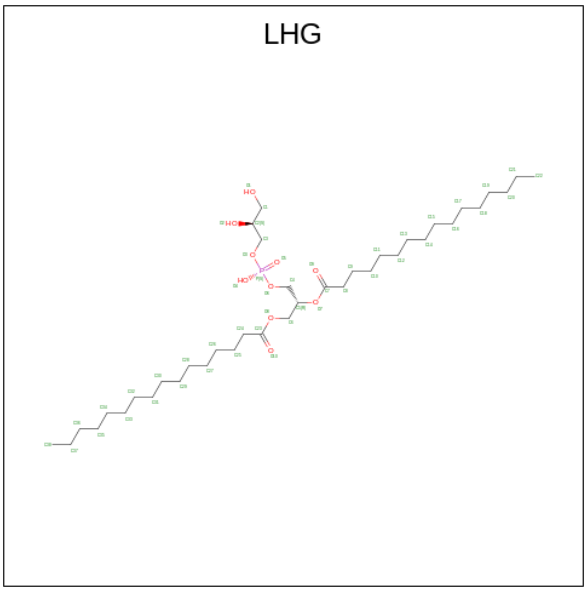
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	M	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	5	1	Total C 40 40	0
22	6	1	Total C 40 40	0
22	7	1	Total C 40 40	0
22	8	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O 35 24 11	0
23	A	1	Total C O 35 24 11	0
23	B	1	Total C O 35 24 11	0
23	F	1	Total C O 29 18 11	0
23	5	1	Total C O 30 19 11	0
23	5	1	Total C O 35 24 11	0
23	7	1	Total C O 35 24 11	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

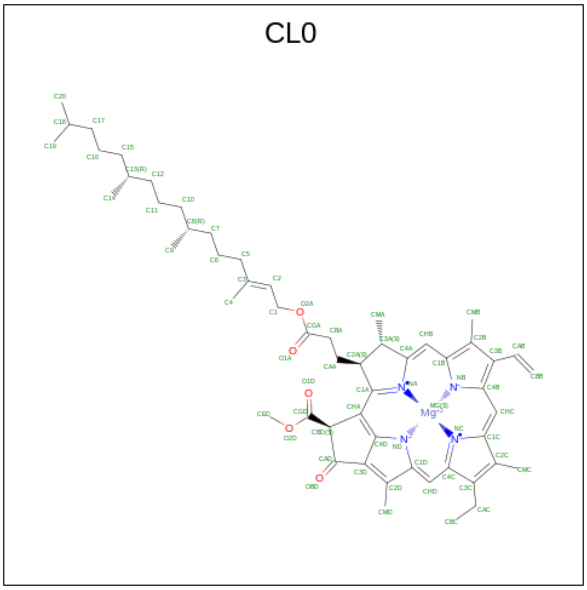


Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			42	31	10	1	
24	A	1	Total	C	O	P	0
			42	31	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	B	1	Total	C	O	P	0
			32	21	10	1	
24	a	1	Total	C	O	P	0
			49	38	10	1	
24	4	1	Total	C	O	P	0
			49	38	10	1	
24	5	1	Total	C	O	P	0
			35	24	10	1	
24	5	1	Total	C	O	P	0
			32	21	10	1	
24	7	1	Total	C	O	P	0
			49	38	10	1	
24	7	1	Total	C	O	P	0
			44	33	10	1	
24	8	1	Total	C	O	P	0
			49	38	10	1	
24	b	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 25 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

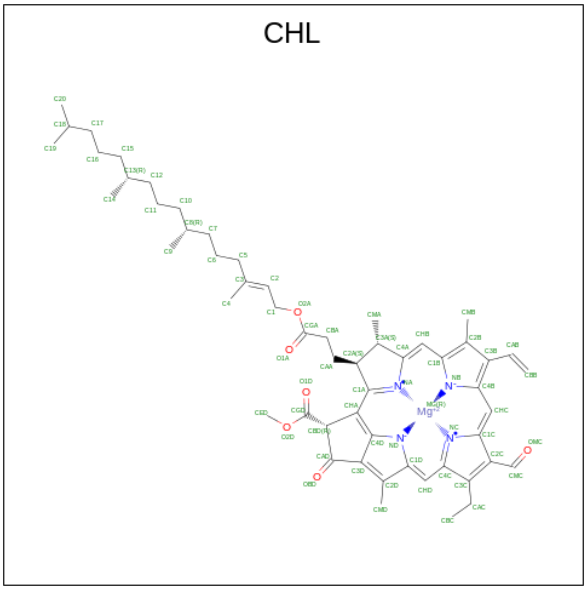
Mol	Chain	Residues	Atoms	AltConf
25	A	3	Total C 43 43	0
25	F	4	Total C 66 66	0
25	J	1	Total C 14 14	0
25	K	1	Total C 18 18	0
25	M	1	Total C 18 18	0
25	a	1	Total C 18 18	0
25	3	2	Total C 32 32	0
25	4	1	Total C 18 18	0
25	6	1	Total C 18 18	0
25	7	3	Total C 43 43	0
25	8	3	Total C 46 46	0

- Molecule 26 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 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
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
27	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
27	3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
27	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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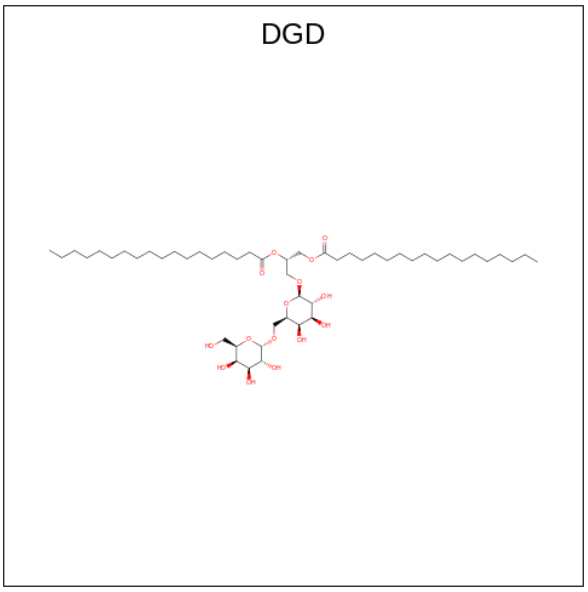
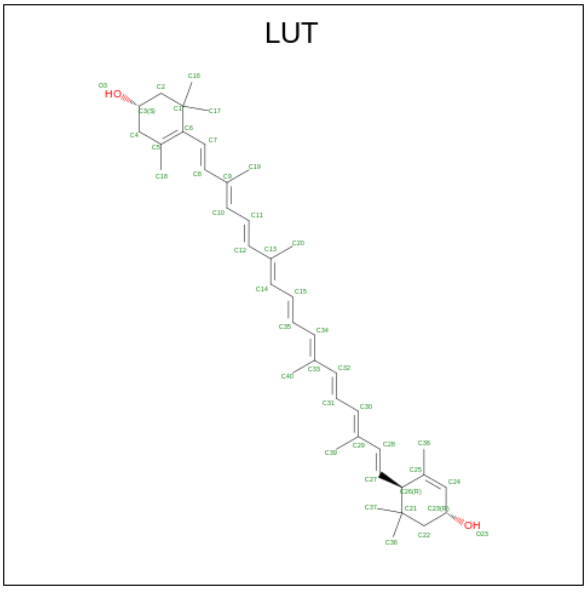
Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	b	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			61	46	15	
28	7	1	Total	C	O	0
			66	51	15	

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	F	1	Total	C	O	0
			42	40	2	

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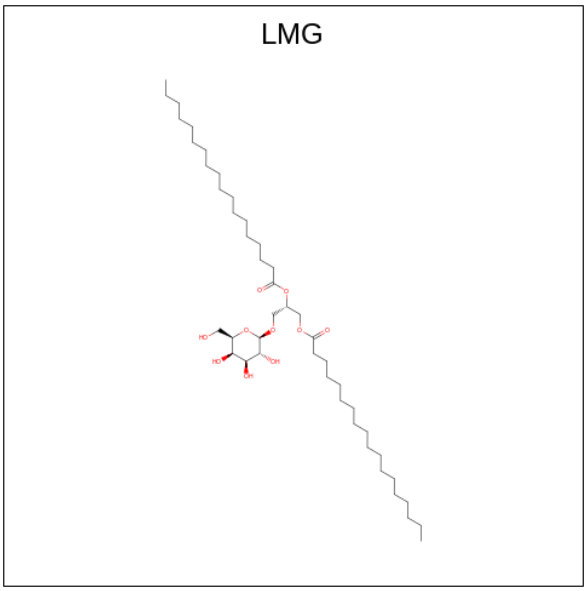
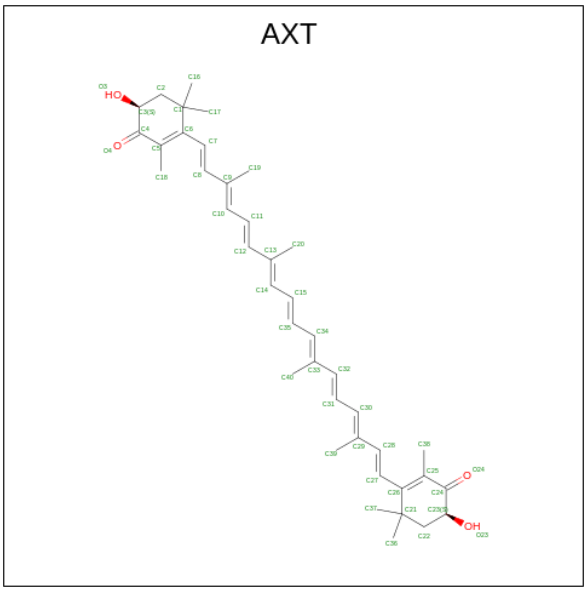
Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



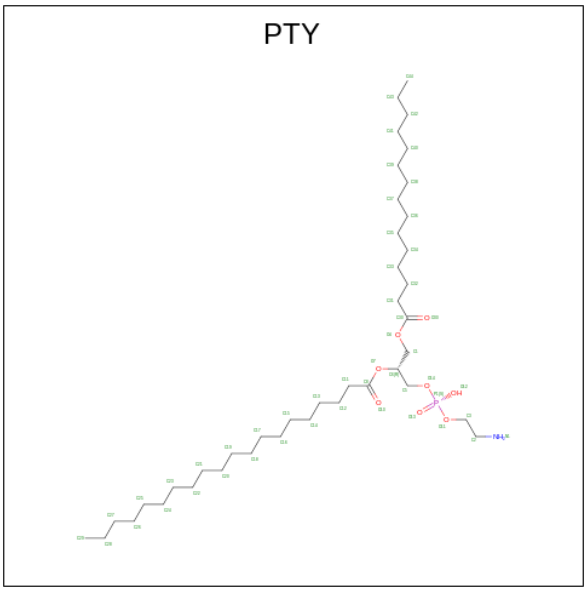
Mol	Chain	Residues	Atoms			AltConf
30	J	1	Total	C	O	0
			49	39	10	
30	J	1	Total	C	O	0
			29	19	10	
30	a	1	Total	C	O	0
			44	34	10	
30	7	1	Total	C	O	0
			41	31	10	
30	8	1	Total	C	O	0
			32	22	10	

- Molecule 31 is ASTAXANTHIN (CCD ID: AXT) (formula: $C_{40}H_{52}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	a	1	43	40	3	0

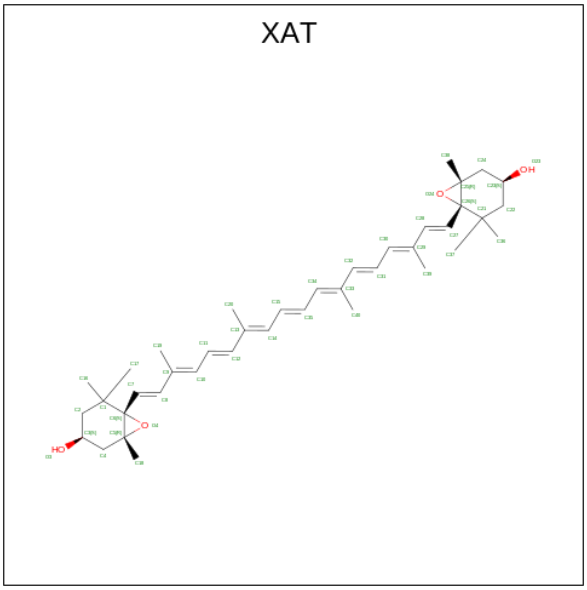
- Molecule 32 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
32	5	1	31	21	1	8	1	0

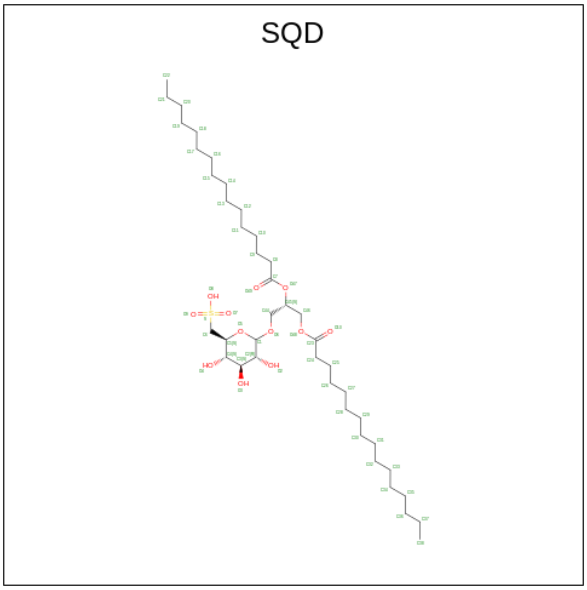
- Molecule 33 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand

of Interest" by depositor).



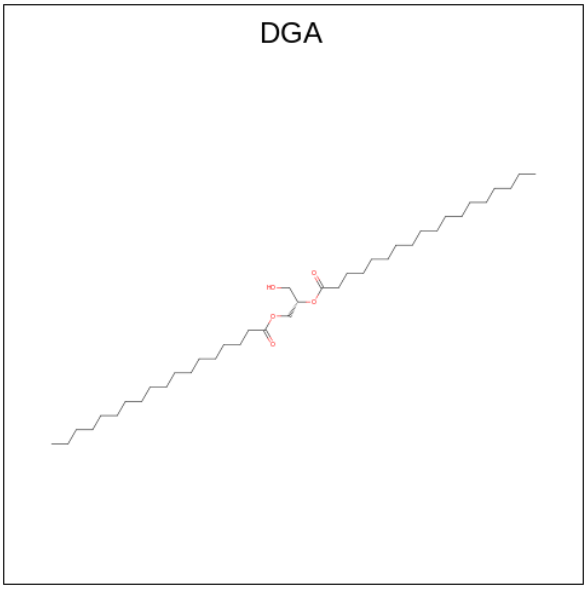
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	7	1	44	40	4	0

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
34	8	1	35	22	12	1	0

- Molecule 35 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
35	8	1	Total C O 28 23 5	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	A	189	Total O 189 189	0
36	B	174	Total O 174 174	0
36	C	37	Total O 37 37	0
36	D	26	Total O 26 26	0
36	E	9	Total O 9 9	0
36	F	30	Total O 30 30	0
36	I	1	Total O 1 1	0
36	J	5	Total O 5 5	0
36	K	2	Total O 2 2	0

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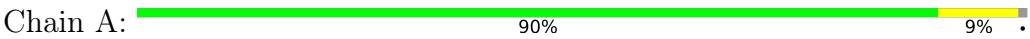
Mol	Chain	Residues	Atoms	AltConf
36	a	13	Total O 13 13	0
36	3	25	Total O 25 25	0
36	5	7	Total O 7 7	0
36	6	2	Total O 2 2	0
36	7	25	Total O 25 25	0
36	8	24	Total O 24 24	0
36	L	1	Total O 1 1	0

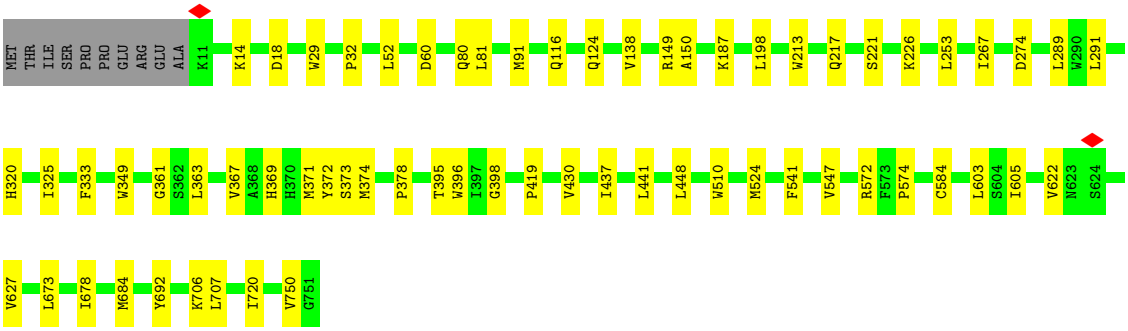
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

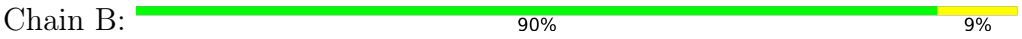
Chain A:

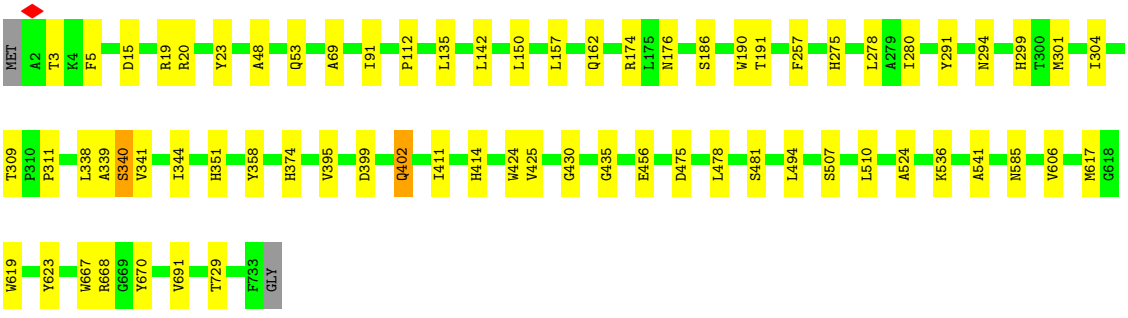




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

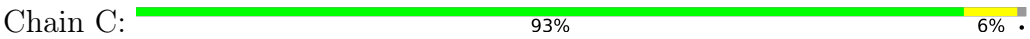
Chain B:

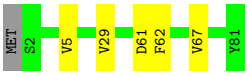




• Molecule 3: Photosystem I iron-sulfur center

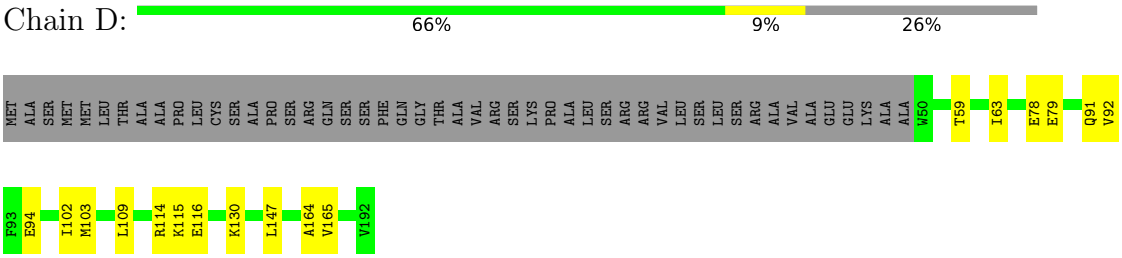
Chain C:





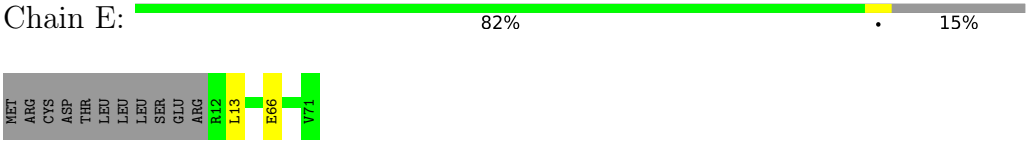
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



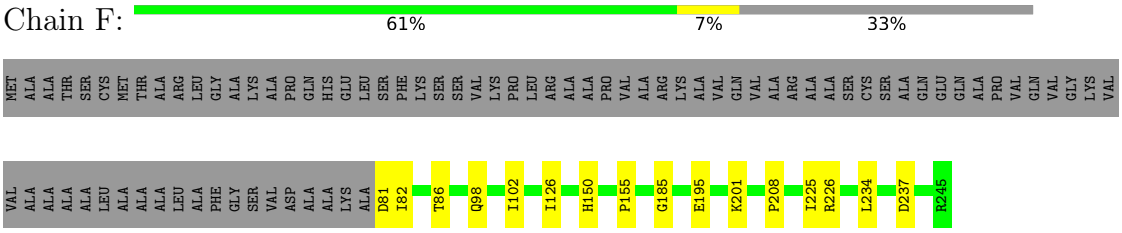
• Molecule 5: Photosystem I reaction centre subunit IV/PsaE

Chain E:



• Molecule 6: Photosystem I reaction center subunit III

Chain F:



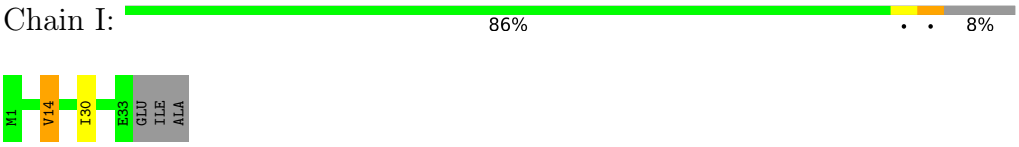
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:



• Molecule 9: Photosystem I reaction center subunit IX

Chain J:

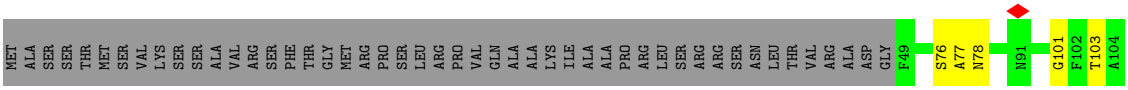




• Molecule 10: PSI-K

Chain K:



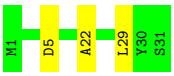




• Molecule 11: Photosystem I reaction center subunit XII

Chain M:

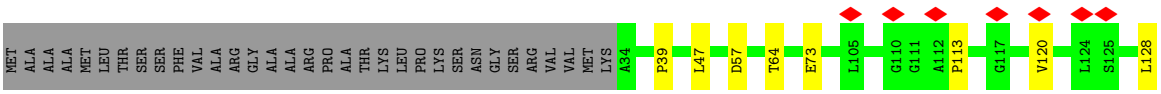




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain a:



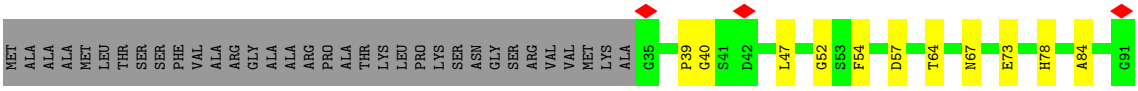


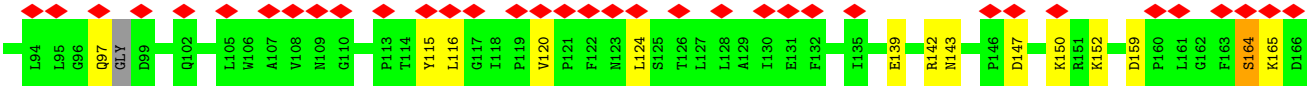


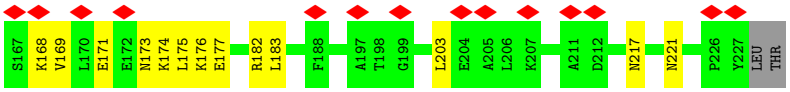
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain b:





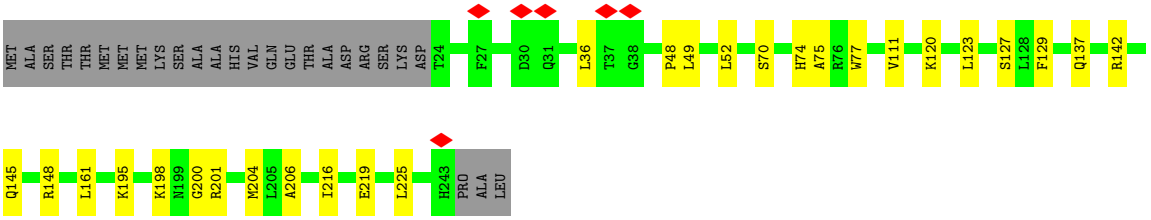




• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

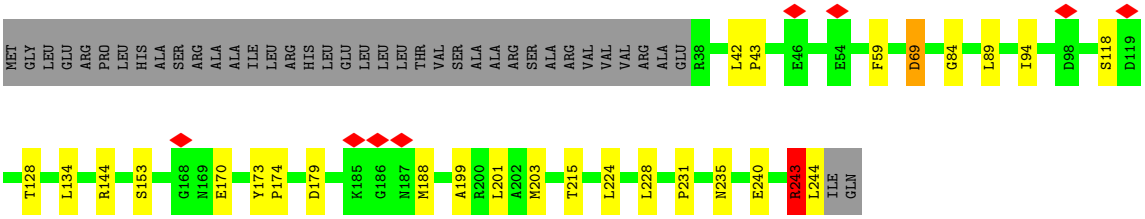




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

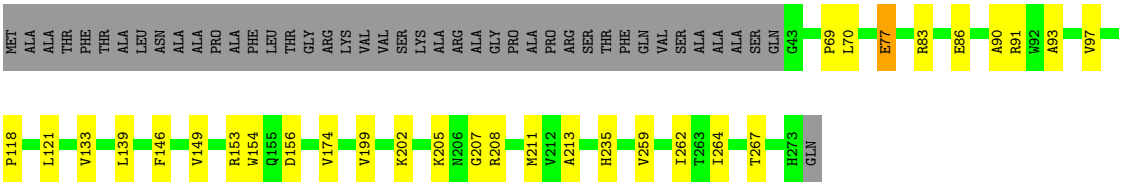




• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 5:

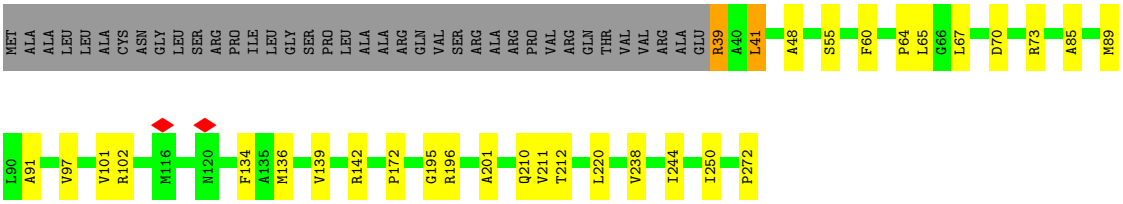




• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 6:

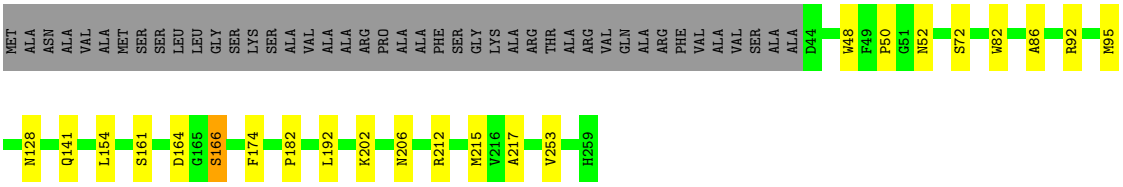




• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 7:

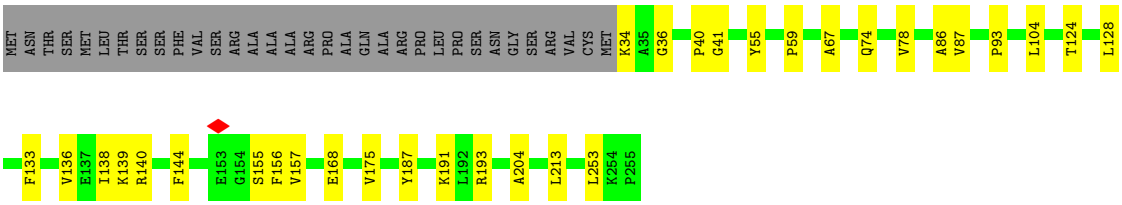




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 8:

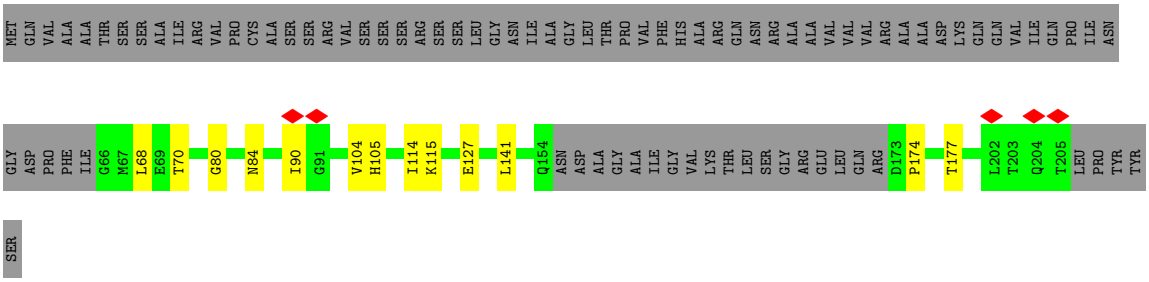




• Molecule 19: PSI subunit V

Chain L:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.519	Depositor
Minimum map value	-0.166	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, UNL, LHG, LMG, BCR, SF4, XAT, DGD, LMT, CHL, PQN, PTY, DGA, SQD, LUT, AXT

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	0.24	0/6021	0.42	0/8213
2	B	0.21	0/6041	0.41	1/8247 (0.0%)
3	C	0.28	0/606	0.47	0/822
4	D	0.16	0/1136	0.34	0/1537
5	E	0.17	0/502	0.31	0/686
6	F	0.19	0/1288	0.34	0/1737
7	G	0.10	0/165	0.24	0/226
8	I	0.25	0/254	0.52	0/347
9	J	0.18	0/348	0.35	0/476
10	K	0.16	0/580	0.37	0/789
11	M	0.17	0/240	0.42	0/325
12	a	0.16	0/1501	0.33	0/2045
12	b	0.22	0/1483	0.45	0/2019
13	3	0.23	0/1759	0.41	0/2394
14	4	0.22	0/1653	0.40	0/2250
15	5	0.18	0/1834	0.41	0/2496
16	6	0.19	0/1832	0.36	0/2501
17	7	0.18	0/1702	0.33	0/2323
18	8	0.19	0/1752	0.36	0/2379
19	L	0.18	0/912	0.34	0/1247
All	All	0.21	0/31609	0.39	1/43059 (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
14	4	0	1
16	6	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	668	ARG	N-CA-C	6.44	117.96	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	4	243	ARG	Sidechain
16	6	39	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5823	0	5662	52	0
2	B	5832	0	5609	45	0
3	C	596	0	573	3	0
4	D	1110	0	1131	10	0
5	E	490	0	482	2	0
6	F	1264	0	1300	11	0
7	G	159	0	152	0	0
8	I	248	0	269	2	0
9	J	336	0	340	8	0
10	K	571	0	592	4	0
11	M	237	0	260	3	0
12	a	1458	0	1423	12	0
12	b	1441	0	1403	46	0
13	3	1707	0	1667	25	0
14	4	1603	0	1572	25	0
15	5	1779	0	1763	25	0
16	6	1774	0	1758	26	0
17	7	1650	0	1595	18	0
18	8	1701	0	1683	24	0
19	L	890	0	917	9	0
20	A	33	0	46	0	0
20	B	33	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	8	0	0	0	0
21	C	16	0	0	0	0
22	3	120	0	168	9	0
22	5	40	0	56	8	0
22	6	40	0	56	1	0
22	7	40	0	56	3	0
22	8	40	0	56	5	0
22	A	200	0	280	11	0
22	B	240	0	336	13	0
22	F	40	0	56	1	0
22	I	40	0	56	2	0
22	J	40	0	56	6	0
22	K	80	0	112	9	0
22	L	80	0	112	2	0
22	M	40	0	56	0	0
23	5	65	0	77	2	0
23	7	35	0	45	1	0
23	A	70	0	87	2	0
23	B	35	0	45	4	0
23	F	29	0	30	1	0
24	4	49	0	74	7	0
24	5	67	0	74	4	0
24	7	93	0	135	7	0
24	8	49	0	74	0	0
24	A	133	0	188	7	0
24	B	32	0	34	0	0
24	a	49	0	74	12	0
24	b	35	0	40	2	0
25	3	32	0	0	0	0
25	4	18	0	0	0	0
25	6	18	0	0	0	0
25	7	43	0	0	0	0
25	8	46	0	0	0	0
25	A	43	0	0	0	0
25	F	66	0	0	0	0
25	J	14	0	0	3	0
25	K	18	0	0	0	0
25	M	18	0	0	0	0
25	a	18	0	0	0	0
26	A	65	0	72	2	0
27	3	818	0	759	22	0
27	4	829	0	606	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	5	956	0	783	41	0
27	6	819	0	643	35	0
27	7	768	0	648	33	0
27	8	897	0	797	24	0
27	A	2666	0	2592	120	0
27	B	2466	0	2374	66	0
27	F	96	0	66	0	0
27	J	42	0	28	2	0
27	K	189	0	126	3	0
27	L	105	0	86	3	0
27	a	758	0	634	23	0
27	b	677	0	479	62	0
28	7	66	0	96	5	0
28	B	61	0	83	1	0
29	3	84	0	110	10	0
29	4	84	0	110	8	0
29	5	84	0	110	8	0
29	6	84	0	110	4	0
29	7	42	0	55	3	0
29	8	84	0	112	8	0
29	F	42	0	55	4	0
29	J	42	0	54	1	0
29	a	84	0	108	2	0
29	b	84	0	112	10	0
30	7	41	0	52	1	0
30	8	32	0	34	3	0
30	J	78	0	99	5	0
30	a	44	0	58	2	0
31	a	43	0	52	0	0
32	5	31	0	35	1	0
33	7	44	0	56	0	0
34	8	35	0	34	1	0
35	8	28	0	38	3	0
36	3	25	0	0	1	0
36	5	7	0	0	0	0
36	6	2	0	0	1	0
36	7	25	0	0	0	0
36	8	24	0	0	0	0
36	A	189	0	0	2	0
36	B	174	0	0	1	0
36	C	37	0	0	0	0
36	D	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	E	9	0	0	0	0
36	F	30	0	0	1	0
36	I	1	0	0	0	0
36	J	5	0	0	0	0
36	K	2	0	0	0	0
36	L	1	0	0	0	0
36	a	13	0	0	0	0
All	All	46812	0	44942	705	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 8.

The worst 5 of 705 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)
12:b:84:ALA:CB	27:b:308:CHL:HBA2	1.55	1.36
27:b:308:CHL:CBB	27:b:317:CHL:HHD	1.55	1.34
27:b:308:CHL:CBB	27:b:317:CHL:HAC1	1.59	1.31
12:b:84:ALA:HB1	27:b:308:CHL:CBA	1.62	1.26
27:b:308:CHL:HBB1	27:b:317:CHL:CHD	1.74	1.17

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	739/751 (98%)	720 (97%)	19 (3%)	0	100	100
2	B	732/734 (100%)	719 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/192 (73%)	138 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
6	F	163/245 (66%)	161 (99%)	2 (1%)	0	100	100
7	G	18/138 (13%)	17 (94%)	1 (6%)	0	100	100
8	I	31/36 (86%)	31 (100%)	0	0	100	100
9	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
10	K	80/131 (61%)	80 (100%)	0	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
12	a	193/229 (84%)	188 (97%)	5 (3%)	0	100	100
12	b	188/229 (82%)	177 (94%)	9 (5%)	2 (1%)	11	4
13	3	218/246 (89%)	214 (98%)	4 (2%)	0	100	100
14	4	205/246 (83%)	198 (97%)	7 (3%)	0	100	100
15	5	229/274 (84%)	219 (96%)	10 (4%)	0	100	100
16	6	232/272 (85%)	227 (98%)	5 (2%)	0	100	100
17	7	214/259 (83%)	209 (98%)	5 (2%)	0	100	100
18	8	220/255 (86%)	217 (99%)	3 (1%)	0	100	100
19	L	118/210 (56%)	116 (98%)	2 (2%)	0	100	100
All	All	3925/4671 (84%)	3831 (98%)	92 (2%)	2 (0%)	49	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	b	165	LYS
12	b	164	SER

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	604/613 (98%)	599 (99%)	5 (1%)	73	77
2	B	594/593 (100%)	581 (98%)	13 (2%)	45	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	118/156 (76%)	117 (99%)	1 (1%)	73	77
5	E	56/67 (84%)	56 (100%)	0	100	100
6	F	131/183 (72%)	129 (98%)	2 (2%)	57	58
7	G	18/106 (17%)	17 (94%)	1 (6%)	19	12
8	I	26/28 (93%)	25 (96%)	1 (4%)	29	23
9	J	37/37 (100%)	36 (97%)	1 (3%)	39	35
10	K	60/100 (60%)	58 (97%)	2 (3%)	33	28
11	M	26/26 (100%)	26 (100%)	0	100	100
12	a	141/166 (85%)	141 (100%)	0	100	100
12	b	140/166 (84%)	138 (99%)	2 (1%)	59	60
13	3	176/197 (89%)	175 (99%)	1 (1%)	78	82
14	4	164/195 (84%)	158 (96%)	6 (4%)	30	24
15	5	179/208 (86%)	175 (98%)	4 (2%)	45	43
16	6	183/212 (86%)	180 (98%)	3 (2%)	55	55
17	7	168/195 (86%)	165 (98%)	3 (2%)	51	51
18	8	175/202 (87%)	172 (98%)	3 (2%)	53	53
19	L	91/161 (56%)	90 (99%)	1 (1%)	65	68
All	All	3155/3680 (86%)	3106 (98%)	49 (2%)	54	55

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	4	89	LEU
15	5	174	VAL
14	4	128	THR
14	4	244	LEU
16	6	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
15	5	165	GLN
17	7	127	GLN
15	5	172	ASN

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Mol	Chain	Res	Type
15	5	247	ASN
17	7	225	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 318 ligands modelled in this entry, 21 are unknown - leaving 297 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	CHL	A	845	1	69,73,74	2.75	22 (31%)	83,113,114	2.28	25 (30%)
27	CHL	b	317	-	52,56,74	3.16	19 (36%)	58,92,114	2.37	24 (41%)
27	CHL	8	315	18	69,73,74	2.30	22 (31%)	83,113,114	2.35	24 (28%)
27	CHL	L	303	-	64,68,74	2.04	20 (31%)	77,107,114	4.38	33 (42%)
27	CHL	a	310	12	69,73,74	2.93	21 (30%)	83,113,114	2.35	26 (31%)
27	CHL	A	819	1	59,63,74	2.63	21 (35%)	71,101,114	2.51	23 (32%)
27	CHL	a	316	36	52,56,74	2.42	19 (36%)	58,92,114	2.39	24 (41%)
27	CHL	B	831	2	50,54,74	2.73	21 (42%)	60,90,114	2.65	27 (45%)
27	CHL	B	847	36	69,73,74	2.89	23 (33%)	83,113,114	2.36	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CHL	a	319	36	54,58,74	2.86	23 (42%)	65,95,114	2.63	28 (43%)
27	CHL	7	311	17	64,68,74	2.41	21 (32%)	77,107,114	2.40	28 (36%)
29	LUT	8	304	-	42,43,43	5.52	19 (45%)	51,60,60	5.83	33 (64%)
23	LMT	A	808	-	36,36,36	1.24	6 (16%)	47,47,47	1.05	2 (4%)
27	CHL	B	816	2	65,69,74	2.59	21 (32%)	78,108,114	2.46	29 (37%)
27	CHL	A	855	1	69,73,74	2.62	23 (33%)	83,113,114	2.37	29 (34%)
27	CHL	a	320	12	50,54,74	3.25	22 (44%)	60,90,114	2.62	26 (43%)
32	PTY	5	305	-	30,30,49	0.56	0	33,35,54	0.55	1 (3%)
27	CHL	A	817	-	69,73,74	2.54	19 (27%)	83,113,114	2.31	24 (28%)
27	CHL	b	309	24	50,54,74	4.12	22 (44%)	60,90,114	2.66	25 (41%)
27	CHL	8	325	18	69,73,74	2.40	20 (28%)	83,113,114	2.31	25 (30%)
29	LUT	8	303	-	42,43,43	5.48	19 (45%)	51,60,60	5.73	33 (64%)
27	CHL	B	830	2	64,68,74	2.64	23 (35%)	77,107,114	2.41	26 (33%)
27	CHL	A	837	1	59,63,74	2.75	23 (38%)	71,101,114	2.59	25 (35%)
27	CHL	5	325	16	51,55,74	2.26	20 (39%)	57,91,114	2.42	24 (42%)
27	CHL	B	843	36	49,53,74	3.18	20 (40%)	59,89,114	2.66	21 (35%)
22	BCR	I	801	-	41,41,41	1.11	2 (4%)	56,56,56	1.15	4 (7%)
24	LHG	A	811	27	41,41,48	0.69	2 (4%)	44,47,54	1.18	4 (9%)
27	CHL	F	309	36	54,58,74	2.86	22 (40%)	65,95,114	2.62	26 (40%)
27	CHL	A	852	1	55,59,74	3.15	21 (38%)	66,96,114	2.78	28 (42%)
27	CHL	A	836	36	69,73,74	3.15	22 (31%)	83,113,114	2.28	25 (30%)
22	BCR	B	806	-	41,41,41	1.10	2 (4%)	56,56,56	1.36	5 (8%)
27	CHL	4	318	-	46,50,74	4.03	22 (47%)	55,85,114	2.70	24 (43%)
34	SQD	8	301	-	34,35,54	1.79	7 (20%)	43,46,65	1.51	6 (13%)
29	LUT	5	302	-	42,43,43	5.57	19 (45%)	51,60,60	5.71	33 (64%)
23	LMT	7	308	-	36,36,36	1.19	6 (16%)	47,47,47	0.89	0
27	CHL	6	305	16	50,54,74	2.69	22 (44%)	60,90,114	2.61	23 (38%)
24	LHG	A	812	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	6 (11%)
27	CHL	A	829	1	59,63,74	2.57	20 (33%)	71,101,114	2.55	22 (30%)
21	SF4	A	802	2,1	0,12,12	-	-	-		
22	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	5 (8%)
22	BCR	7	303	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	5 (8%)
27	CHL	a	312	36	54,58,74	3.83	21 (38%)	65,95,114	2.60	26 (40%)
27	CHL	A	825	1	69,73,74	2.96	23 (33%)	83,113,114	2.37	27 (32%)
27	CHL	6	317	-	51,55,74	2.91	19 (37%)	57,91,114	2.54	25 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CL0	A	815	1	69,73,73	1.81	16 (23%)	83,113,113	3.59	32 (38%)
27	CHL	B	844	2	69,73,74	2.38	21 (30%)	83,113,114	2.33	27 (32%)
27	CHL	a	313	24	59,63,74	2.54	22 (37%)	71,101,114	2.51	28 (39%)
27	CHL	4	312	14	52,56,74	2.14	18 (34%)	58,92,114	2.42	25 (43%)
27	CHL	7	313	17	69,73,74	2.66	22 (31%)	83,113,114	2.35	27 (32%)
27	CHL	7	321	17	51,55,74	2.59	20 (39%)	57,91,114	2.70	22 (38%)
27	CHL	8	313	18	54,58,74	3.11	22 (40%)	65,95,114	2.64	26 (40%)
27	CHL	B	822	2	69,73,74	2.56	20 (28%)	83,113,114	2.33	24 (28%)
27	CHL	6	309	16	51,55,74	3.13	22 (43%)	61,91,114	2.60	25 (40%)
23	LMT	B	810	-	36,36,36	1.20	5 (13%)	47,47,47	0.94	1 (2%)
24	LHG	5	324	27	31,31,48	0.79	1 (3%)	34,37,54	1.27	4 (11%)
27	CHL	b	305	-	50,54,74	3.89	22 (44%)	60,90,114	2.70	25 (41%)
27	CHL	a	311	12	64,68,74	2.71	21 (32%)	77,107,114	2.48	26 (33%)
27	CHL	6	308	16	70,74,74	1.86	19 (27%)	80,114,114	2.73	25 (31%)
27	CHL	A	858	1	69,73,74	2.67	22 (31%)	83,113,114	2.36	29 (34%)
27	CHL	B	829	2	59,63,74	2.56	21 (35%)	71,101,114	2.56	28 (39%)
27	CHL	5	323	15	60,64,74	3.15	20 (33%)	72,102,114	2.60	26 (36%)
27	CHL	5	315	15	69,73,74	3.00	22 (31%)	83,113,114	4.30	28 (33%)
27	CHL	B	837	2	69,73,74	2.69	22 (31%)	83,113,114	2.26	25 (30%)
28	DGD	7	307	27	67,67,67	0.91	2 (2%)	81,81,81	1.38	10 (12%)
27	CHL	B	827	2	64,68,74	2.37	19 (29%)	77,107,114	2.42	27 (35%)
27	CHL	5	309	15	64,68,74	2.49	22 (34%)	77,107,114	2.41	26 (33%)
29	LUT	b	303	-	42,43,43	1.65	8 (19%)	51,60,60	1.74	10 (19%)
27	CHL	8	322	36	54,58,74	2.59	19 (35%)	65,95,114	2.68	25 (38%)
27	CHL	A	847	1	60,64,74	2.81	20 (33%)	72,102,114	2.46	25 (34%)
27	CHL	4	309	-	51,55,74	2.50	18 (35%)	57,91,114	2.31	21 (36%)
27	CHL	b	311	12	51,55,74	2.69	21 (41%)	57,91,114	2.43	25 (43%)
27	CHL	a	318	36	52,56,74	3.29	20 (38%)	58,92,114	2.43	23 (39%)
27	CHL	3	312	13	69,73,74	2.94	24 (34%)	83,113,114	2.33	26 (31%)
27	CHL	5	316	36	70,74,74	1.81	18 (25%)	80,114,114	2.82	25 (31%)
27	CHL	7	312	17	48,52,74	3.01	20 (41%)	58,88,114	2.72	26 (44%)
27	CHL	b	310	12	50,54,74	3.93	23 (46%)	60,90,114	2.65	26 (43%)
27	CHL	5	307	15	59,63,74	3.39	21 (35%)	71,101,114	2.46	27 (38%)
22	BCR	B	802	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	7 (12%)
27	CHL	4	314	-	49,53,74	3.07	23 (46%)	59,89,114	2.71	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCR	B	803	-	41,41,41	1.15	2 (4%)	56,56,56	1.13	4 (7%)
27	CHL	B	825	2	64,68,74	2.66	22 (34%)	77,107,114	2.46	29 (37%)
27	CHL	8	319	36	59,63,74	2.71	23 (38%)	71,101,114	2.54	26 (36%)
24	LHG	a	305	27	48,48,48	0.28	0	51,54,54	0.30	0
27	CHL	B	841	2	59,63,74	2.52	21 (35%)	71,101,114	2.52	26 (36%)
27	CHL	4	306	14	60,64,74	2.63	21 (35%)	72,102,114	2.51	27 (37%)
27	CHL	4	315	14	51,55,74	2.75	22 (43%)	61,91,114	2.65	25 (40%)
27	CHL	5	319	-	51,55,74	3.61	20 (39%)	57,91,114	2.41	23 (40%)
27	CHL	A	842	1	70,74,74	2.10	18 (25%)	80,114,114	2.08	24 (30%)
27	CHL	4	319	14	49,53,74	3.11	24 (48%)	59,89,114	2.72	20 (33%)
29	LUT	a	304	-	42,43,43	5.54	19 (45%)	51,60,60	6.07	32 (62%)
27	CHL	6	319	16	47,51,74	2.38	19 (40%)	52,86,114	3.11	21 (40%)
27	CHL	B	815	2	69,73,74	2.52	23 (33%)	83,113,114	2.35	30 (36%)
23	LMT	F	302	-	30,30,36	1.33	6 (20%)	41,41,47	1.01	3 (7%)
27	CHL	B	850	2	54,58,74	3.04	25 (46%)	65,95,114	2.69	28 (43%)
27	CHL	3	311	13	64,68,74	2.51	21 (32%)	77,107,114	2.46	27 (35%)
27	CHL	6	314	24	50,54,74	3.15	21 (42%)	60,90,114	2.66	24 (40%)
27	CHL	4	311	14	51,55,74	3.71	22 (43%)	61,91,114	2.66	26 (42%)
29	LUT	7	304	-	42,43,43	5.54	21 (50%)	51,60,60	5.78	29 (56%)
27	CHL	b	307	12	59,63,74	2.54	20 (33%)	71,101,114	2.45	28 (39%)
27	CHL	A	832	1	64,68,74	2.77	22 (34%)	77,107,114	2.54	26 (33%)
21	SF4	C	101	3	0,12,12	-	-	-		
27	CHL	B	820	2	69,73,74	2.58	22 (31%)	83,113,114	2.32	26 (31%)
22	BCR	3	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	5 (8%)
27	CHL	8	312	18	69,73,74	2.82	21 (30%)	83,113,114	2.27	26 (31%)
24	LHG	B	808	27	31,31,48	0.78	1 (3%)	34,37,54	1.31	4 (11%)
27	CHL	A	844	1	69,73,74	2.65	24 (34%)	83,113,114	2.28	23 (27%)
27	CHL	A	849	1	69,73,74	2.78	23 (33%)	83,113,114	2.37	24 (28%)
27	CHL	B	813	2	59,63,74	2.72	22 (37%)	71,101,114	2.59	25 (35%)
27	CHL	A	824	1	64,68,74	2.42	20 (31%)	77,107,114	2.40	25 (32%)
27	CHL	A	820	1	69,73,74	2.50	22 (31%)	83,113,114	2.40	28 (33%)
27	CHL	6	306	16	61,65,74	4.49	22 (36%)	73,103,114	2.52	29 (39%)
27	CHL	6	315	16	54,58,74	3.43	23 (42%)	65,95,114	2.64	28 (43%)
27	CHL	7	323	36	56,60,74	2.95	21 (37%)	67,97,114	2.81	26 (38%)
27	CHL	b	313	12	50,54,74	3.67	22 (44%)	60,90,114	2.64	25 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CHL	5	312	36	54,58,74	3.81	22 (40%)	65,95,114	2.60	27 (41%)
27	CHL	A	854	1	60,64,74	2.86	24 (40%)	72,102,114	2.58	26 (36%)
27	CHL	A	823	1	69,73,74	2.25	20 (28%)	83,113,114	2.41	29 (34%)
27	CHL	4	305	14	49,53,74	3.09	21 (42%)	59,89,114	2.66	26 (44%)
27	CHL	4	320	14	54,58,74	2.87	23 (42%)	65,95,114	2.64	29 (44%)
27	CHL	7	314	17	66,70,74	3.38	22 (33%)	79,109,114	2.36	26 (32%)
27	CHL	4	308	14	64,68,74	2.79	22 (34%)	77,107,114	2.44	27 (35%)
27	CHL	6	318	-	51,55,74	3.29	19 (37%)	57,91,114	2.42	22 (38%)
27	CHL	A	826	1	66,70,74	2.79	22 (33%)	79,109,114	2.39	27 (34%)
27	CHL	B	839	2	64,68,74	2.56	24 (37%)	77,107,114	2.40	26 (33%)
27	CHL	A	857	24	50,54,74	2.87	22 (44%)	60,90,114	2.72	25 (41%)
20	PQN	A	801	-	34,34,34	0.37	0	42,45,45	0.56	0
23	LMT	A	809	-	36,36,36	1.21	5 (13%)	47,47,47	0.93	1 (2%)
27	CHL	A	850	1	69,73,74	2.39	20 (28%)	83,113,114	2.31	25 (30%)
30	LMG	7	301	-	41,41,55	0.87	1 (2%)	49,49,63	1.21	3 (6%)
27	CHL	B	832	36	69,73,74	2.36	22 (31%)	83,113,114	2.39	29 (34%)
27	CHL	B	838	2	69,73,74	2.59	22 (31%)	83,113,114	2.33	26 (31%)
27	CHL	K	207	10	51,55,74	3.44	21 (41%)	57,91,114	2.36	23 (40%)
22	BCR	B	804	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	3 (5%)
27	CHL	A	853	1	69,73,74	2.50	22 (31%)	83,113,114	2.34	26 (31%)
27	CHL	B	849	24	69,73,74	2.43	22 (31%)	83,113,114	2.28	25 (30%)
27	CHL	A	848	1	69,73,74	2.40	21 (30%)	83,113,114	2.38	27 (32%)
27	CHL	3	313	36	69,73,74	2.83	22 (31%)	83,113,114	2.29	26 (31%)
27	CHL	3	309	13	50,54,74	3.26	22 (44%)	60,90,114	2.72	23 (38%)
27	CHL	5	313	-	61,65,74	2.13	16 (26%)	73,103,114	4.59	39 (53%)
29	LUT	3	305	-	42,43,43	5.47	19 (45%)	51,60,60	5.84	33 (64%)
27	CHL	K	206	10	50,54,74	3.52	21 (42%)	60,90,114	2.62	23 (38%)
22	BCR	F	301	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	4 (7%)
27	CHL	b	306	12	50,54,74	4.39	22 (44%)	60,90,114	2.56	25 (41%)
27	CHL	A	840	36	69,73,74	2.69	23 (33%)	83,113,114	2.41	24 (28%)
35	DGA	8	306	-	27,27,43	0.22	0	29,29,45	0.17	0
22	BCR	K	202	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	6 (10%)
22	BCR	A	807	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
27	CHL	3	310	13	69,73,74	2.34	21 (30%)	83,113,114	2.34	26 (31%)
22	BCR	L	302	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CHL	A	834	1	69,73,74	2.34	22 (31%)	83,113,114	2.24	25 (30%)
27	CHL	5	310	15	69,73,74	3.32	22 (31%)	83,113,114	2.40	26 (31%)
27	CHL	A	818	1	69,73,74	2.30	24 (34%)	83,113,114	2.37	28 (33%)
27	CHL	J	106	9	46,50,74	3.82	21 (45%)	55,85,114	2.75	23 (41%)
27	CHL	a	317	12	69,73,74	2.39	22 (31%)	83,113,114	2.33	26 (31%)
27	CHL	3	321	13	49,53,74	3.16	21 (42%)	59,89,114	2.69	22 (37%)
33	XAT	7	305	-	39,47,47	1.64	8 (20%)	54,74,74	1.61	10 (18%)
27	CHL	B	842	2	69,73,74	3.05	22 (31%)	83,113,114	2.44	27 (32%)
27	CHL	8	318	24	50,54,74	3.50	21 (42%)	60,90,114	2.63	22 (36%)
27	CHL	A	827	1	58,62,74	2.80	24 (41%)	69,99,114	2.52	25 (36%)
24	LHG	b	302	27	34,34,48	0.74	1 (2%)	37,40,54	1.28	4 (10%)
22	BCR	6	301	-	41,41,41	1.68	8 (19%)	56,56,56	1.61	11 (19%)
22	BCR	A	806	-	41,41,41	1.15	2 (4%)	56,56,56	1.28	6 (10%)
29	LUT	F	303	-	42,43,43	5.51	19 (45%)	51,60,60	5.90	33 (64%)
27	CHL	A	835	1	51,55,74	3.12	22 (43%)	61,91,114	2.71	24 (39%)
27	CHL	3	319	13	59,63,74	2.94	21 (35%)	71,101,114	2.48	25 (35%)
27	CHL	7	319	17	70,74,74	1.79	18 (25%)	80,114,114	2.23	27 (33%)
27	CHL	a	308	12	49,53,74	3.05	22 (44%)	59,89,114	2.77	25 (42%)
27	CHL	5	318	15	69,73,74	2.76	22 (31%)	83,113,114	2.36	28 (33%)
27	CHL	B	819	2	69,73,74	2.61	23 (33%)	83,113,114	2.41	26 (31%)
27	CHL	4	307	14	64,68,74	2.55	22 (34%)	77,107,114	2.44	26 (33%)
29	LUT	4	301	-	42,43,43	5.61	20 (47%)	51,60,60	5.69	34 (66%)
22	BCR	5	301	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	4 (7%)
22	BCR	A	805	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	5 (8%)
27	CHL	6	312	16	50,54,74	3.28	22 (44%)	60,90,114	2.72	24 (40%)
27	CHL	A	831	-	59,63,74	2.14	15 (25%)	71,101,114	4.30	36 (50%)
22	BCR	K	203	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	6 (10%)
27	CHL	B	848	2	69,73,74	2.66	21 (30%)	83,113,114	2.30	25 (30%)
27	CHL	8	326	18	50,54,74	2.98	21 (42%)	60,90,114	2.76	26 (43%)
27	CHL	4	304	14	59,63,74	2.85	20 (33%)	71,101,114	2.49	26 (36%)
27	CHL	7	315	17	47,52,74	2.99	23 (48%)	56,88,114	2.63	21 (37%)
27	CHL	A	830	1	69,73,74	2.36	22 (31%)	83,113,114	2.43	25 (30%)
27	CHL	B	835	2	61,65,74	2.61	21 (34%)	73,103,114	2.53	25 (34%)
27	CHL	B	818	2	59,63,74	2.60	22 (37%)	71,101,114	2.54	24 (33%)
27	CHL	3	318	36	55,59,74	2.84	23 (41%)	66,96,114	2.65	27 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CHL	5	322	15	51,55,74	3.43	19 (37%)	57,91,114	2.45	23 (40%)
22	BCR	A	804	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	5 (8%)
30	LMG	8	307	-	32,32,55	0.27	0	40,40,63	0.33	0
27	CHL	A	839	1	69,73,74	2.44	22 (31%)	83,113,114	2.36	28 (33%)
27	CHL	A	859	36	69,73,74	2.77	21 (30%)	83,113,114	2.34	28 (33%)
24	LHG	5	304	-	34,34,48	0.36	0	37,40,54	0.44	0
27	CHL	B	814	2	69,73,74	2.51	24 (34%)	83,113,114	2.34	27 (32%)
27	CHL	4	316	-	50,54,74	3.73	19 (38%)	56,90,114	2.39	23 (41%)
27	CHL	B	812	-	69,73,74	2.45	21 (30%)	83,113,114	2.39	25 (30%)
27	CHL	A	838	1	64,68,74	2.69	22 (34%)	77,107,114	2.43	25 (32%)
30	LMG	J	101	-	49,49,55	0.81	1 (2%)	57,57,63	1.26	3 (5%)
27	CHL	3	320	13	65,69,74	2.29	22 (33%)	78,108,114	2.39	29 (37%)
27	CHL	7	320	36,28	51,55,74	2.17	20 (39%)	57,91,114	2.56	24 (42%)
30	LMG	a	301	-	44,44,55	0.87	2 (4%)	52,52,63	1.27	6 (11%)
27	CHL	6	307	-	69,73,74	2.01	19 (27%)	83,113,114	4.27	38 (45%)
22	BCR	3	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	7 (12%)
27	CHL	B	826	2	54,58,74	3.28	22 (40%)	65,95,114	2.65	25 (38%)
27	CHL	F	308	6	50,54,74	3.24	22 (44%)	60,90,114	2.69	24 (40%)
27	CHL	3	315	13	56,60,74	2.50	20 (35%)	67,97,114	2.58	26 (38%)
27	CHL	B	817	2	69,73,74	2.37	21 (30%)	83,113,114	2.47	27 (32%)
22	BCR	L	301	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	4 (7%)
27	CHL	K	204	36	54,58,74	4.04	23 (42%)	65,95,114	2.66	26 (40%)
27	CHL	a	309	36	64,68,74	3.76	22 (34%)	77,107,114	2.49	28 (36%)
27	CHL	4	317	14	49,53,74	2.99	21 (42%)	59,89,114	3.10	21 (35%)
22	BCR	A	803	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	3 (5%)
27	CHL	8	323	-	54,58,74	3.20	21 (38%)	65,95,114	2.72	24 (36%)
27	CHL	6	316	36	50,54,74	2.95	22 (44%)	56,90,114	2.52	23 (41%)
27	CHL	A	816	36	69,73,74	2.38	23 (33%)	83,113,114	2.36	26 (31%)
22	BCR	B	805	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	4 (7%)
28	DGD	B	809	-	62,62,67	0.98	2 (3%)	76,76,81	1.35	10 (13%)
27	CHL	a	314	12	49,53,74	2.90	21 (42%)	59,89,114	2.67	26 (44%)
29	LUT	3	304	-	42,43,43	5.53	19 (45%)	51,60,60	5.58	32 (62%)
27	CHL	A	851	1	50,54,74	2.72	21 (42%)	60,90,114	2.71	24 (40%)
24	LHG	8	305	27	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
27	CHL	b	304	12	50,54,74	3.58	22 (44%)	60,90,114	2.67	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCR	M	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	5 (8%)
29	LUT	J	103	-	42,43,43	5.59	20 (47%)	51,60,60	5.87	31 (60%)
27	CHL	a	315	12	65,69,74	2.55	21 (32%)	74,108,114	2.28	30 (40%)
27	CHL	B	840	2	69,73,74	2.60	21 (30%)	83,113,114	2.33	27 (32%)
27	CHL	b	312	-	50,54,74	3.02	20 (40%)	60,90,114	2.63	26 (43%)
27	CHL	b	314	12	50,54,74	2.94	22 (44%)	60,90,114	2.60	25 (41%)
27	CHL	A	822	1	59,63,74	2.89	24 (40%)	71,101,114	2.54	27 (38%)
27	CHL	K	205	10	50,54,74	3.06	22 (44%)	60,90,114	2.61	24 (40%)
27	CHL	B	833	36	59,63,74	2.77	23 (38%)	71,101,114	2.47	27 (38%)
27	CHL	A	821	1	69,73,74	2.54	23 (33%)	83,113,114	2.34	27 (32%)
27	CHL	B	834	2	69,73,74	2.97	21 (30%)	83,113,114	2.41	28 (33%)
27	CHL	B	836	2	69,73,74	2.59	22 (31%)	83,113,114	2.25	23 (27%)
27	CHL	8	320	18	56,60,74	2.81	21 (37%)	67,97,114	2.62	27 (40%)
27	CHL	8	311	18	50,54,74	2.98	22 (44%)	60,90,114	2.69	24 (40%)
27	CHL	A	856	36	69,73,74	2.36	22 (31%)	83,113,114	2.41	29 (34%)
27	CHL	8	314	18	70,74,74	1.99	18 (25%)	80,114,114	2.17	28 (35%)
29	LUT	b	301	-	42,43,43	5.62	19 (45%)	51,60,60	5.71	34 (66%)
30	LMG	J	104	-	29,29,55	0.99	1 (3%)	37,37,63	1.21	3 (8%)
27	CHL	3	308	13	69,73,74	2.95	21 (30%)	83,113,114	2.42	27 (32%)
27	CHL	5	311	15	50,54,74	2.94	21 (42%)	60,90,114	2.77	26 (43%)
22	BCR	3	301	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
27	CHL	5	320	15	50,54,74	2.93	24 (48%)	60,90,114	2.63	25 (41%)
29	LUT	6	302	-	42,43,43	5.56	19 (45%)	51,60,60	5.91	31 (60%)
27	CHL	B	851	2	66,70,74	2.63	22 (33%)	79,109,114	2.34	27 (34%)
27	CHL	A	828	1	69,73,74	2.56	23 (33%)	83,113,114	2.31	24 (28%)
27	CHL	b	316	-	52,56,74	2.83	19 (36%)	58,92,114	2.37	23 (39%)
27	CHL	6	311	16	69,73,74	2.73	22 (31%)	83,113,114	2.35	27 (32%)
27	CHL	L	304	-	49,53,74	2.80	22 (44%)	59,89,114	2.61	22 (37%)
27	CHL	B	846	36	69,73,74	2.34	21 (30%)	83,113,114	2.34	27 (32%)
27	CHL	4	310	24	50,54,74	3.81	23 (46%)	60,90,114	2.68	26 (43%)
29	LUT	a	302	-	42,43,43	5.58	19 (45%)	51,60,60	5.75	34 (66%)
27	CHL	5	317	36	51,55,74	2.23	18 (35%)	57,91,114	2.49	23 (40%)
27	CHL	5	308	15	50,54,74	2.97	20 (40%)	60,90,114	2.72	25 (41%)
27	CHL	B	821	2	62,66,74	2.57	23 (37%)	74,104,114	2.48	25 (33%)
27	CHL	6	310	16	59,63,74	2.83	24 (40%)	71,101,114	2.52	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CHL	b	315	12	69,73,74	3.62	23 (33%)	83,113,114	2.34	25 (30%)
21	SF4	C	102	3	0,12,12	-	-	-		
27	CHL	B	845	2	54,58,74	2.61	22 (40%)	65,95,114	2.72	27 (41%)
27	CHL	6	313	16	51,55,74	4.17	22 (43%)	61,91,114	2.68	26 (42%)
24	LHG	4	303	27	48,48,48	0.27	0	51,54,54	0.37	0
24	LHG	7	302	-	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
27	CHL	5	314	15	49,53,74	3.28	21 (42%)	59,89,114	2.64	22 (37%)
27	CHL	B	811	2	69,73,74	2.48	21 (30%)	83,113,114	2.46	29 (34%)
22	BCR	B	807	-	41,41,41	1.11	2 (4%)	56,56,56	1.09	3 (5%)
27	CHL	B	828	36	64,68,74	2.45	20 (31%)	77,107,114	2.33	27 (35%)
27	CHL	4	313	-	49,53,74	3.24	20 (40%)	59,89,114	3.10	22 (37%)
27	CHL	A	841	36	60,64,74	2.19	21 (35%)	68,102,114	2.57	26 (38%)
24	LHG	7	306	27	43,43,48	0.70	1 (2%)	46,49,54	1.22	4 (8%)
27	CHL	A	843	1	69,73,74	1.96	16 (23%)	83,113,114	4.75	39 (46%)
23	LMT	5	306	-	31,31,36	1.28	5 (16%)	42,42,47	0.96	3 (7%)
27	CHL	6	320	16	50,54,74	3.27	20 (40%)	60,90,114	2.63	26 (43%)
29	LUT	5	303	-	42,43,43	5.51	20 (47%)	51,60,60	5.89	32 (62%)
27	CHL	3	317	36	66,70,74	2.66	23 (34%)	79,109,114	2.46	26 (32%)
27	CHL	7	316	36	58,62,74	2.67	21 (36%)	70,100,114	2.47	27 (38%)
27	CHL	8	316	18	69,73,74	2.61	22 (31%)	83,113,114	2.33	26 (31%)
29	LUT	6	303	-	42,43,43	5.58	20 (47%)	51,60,60	5.63	32 (62%)
20	PQN	B	801	-	34,34,34	0.47	0	42,45,45	0.73	1 (2%)
27	CHL	A	833	1	65,69,74	2.11	20 (30%)	74,108,114	2.37	28 (37%)
27	CHL	8	321	36	70,74,74	2.19	19 (27%)	80,114,114	2.20	26 (32%)
27	CHL	7	318	17	59,63,74	2.73	22 (37%)	71,101,114	2.61	28 (39%)
27	CHL	b	308	-	50,54,74	4.06	23 (46%)	60,90,114	15.02	28 (46%)
22	BCR	8	302	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	8 (14%)
27	CHL	7	317	24	69,73,74	2.41	21 (30%)	83,113,114	2.40	27 (32%)
27	CHL	5	321	15	50,54,74	3.07	22 (44%)	60,90,114	2.63	25 (41%)
23	LMT	5	326	-	36,36,36	1.23	6 (16%)	47,47,47	0.94	2 (4%)
27	CHL	3	314	36	64,68,74	2.64	19 (29%)	77,107,114	2.45	27 (35%)
27	CHL	B	823	2	59,63,74	2.61	22 (37%)	71,101,114	2.56	28 (39%)
27	CHL	A	846	-	54,58,74	2.21	17 (31%)	65,95,114	4.49	33 (50%)
27	CHL	8	317	36	69,73,74	2.56	22 (31%)	83,113,114	2.32	26 (31%)
27	CHL	3	316	36	70,74,74	1.90	16 (22%)	80,114,114	2.26	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CHL	7	324	17	50,54,74	2.78	21 (42%)	60,90,114	2.57	23 (38%)
27	CHL	8	324	36	49,53,74	2.71	18 (36%)	53,88,114	2.55	24 (45%)
29	LUT	4	302	-	42,43,43	5.62	19 (45%)	51,60,60	5.60	31 (60%)
24	LHG	A	810	-	41,41,48	0.68	1 (2%)	44,47,54	1.32	6 (13%)
27	CHL	7	322	36	65,69,74	2.40	20 (30%)	74,108,114	2.28	27 (36%)
27	CHL	a	307	12	64,68,74	2.98	23 (35%)	77,107,114	2.40	26 (33%)
31	AXT	a	303	-	44,44,45	0.70	1 (2%)	55,62,64	0.99	1 (1%)
27	CHL	B	824	2	61,65,74	2.64	21 (34%)	73,103,114	2.50	27 (36%)

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
27	CHL	A	845	1	-	10/39/115/117	-
27	CHL	b	317	-	-	7/20/96/117	-
27	CHL	8	315	18	-	14/39/115/117	-
27	CHL	L	303	-	-	12/33/109/117	-
27	CHL	a	310	12	-	12/39/115/117	-
27	CHL	A	819	1	-	8/27/103/117	-
27	CHL	a	316	36	-	8/20/96/117	-
27	CHL	B	831	2	-	4/17/93/117	-
27	CHL	B	847	36	-	10/39/115/117	-
27	CHL	a	319	36	-	8/21/97/117	-
27	CHL	7	311	17	-	4/33/109/117	-
29	LUT	8	304	-	-	14/29/67/67	0/2/2/2
23	LMT	A	808	-	-	8/21/61/61	0/2/2/2
27	CHL	B	816	2	-	6/35/111/117	-
27	CHL	A	855	1	-	12/39/115/117	-
27	CHL	a	320	12	-	7/17/93/117	-
32	PTY	5	305	-	-	17/34/34/53	-
27	CHL	A	817	-	-	3/39/115/117	-
27	CHL	b	309	24	-	5/17/93/117	-
27	CHL	8	325	18	-	12/39/115/117	-
29	LUT	8	303	-	-	13/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	B	830	2	-	3/33/109/117	-
27	CHL	A	837	1	-	5/27/103/117	-
27	CHL	5	325	16	-	8/19/95/117	-
27	CHL	B	843	36	-	2/15/91/117	-
22	BCR	I	801	-	-	11/29/63/63	0/2/2/2
24	LHG	A	811	27	-	26/46/46/53	-
27	CHL	F	309	36	-	7/21/97/117	-
27	CHL	A	852	1	-	4/23/99/117	-
27	CHL	A	836	36	-	11/39/115/117	-
22	BCR	B	806	-	-	9/29/63/63	0/2/2/2
27	CHL	4	318	-	-	5/12/88/117	-
34	SQD	8	301	-	-	15/30/50/69	0/1/1/1
29	LUT	5	302	-	-	14/29/67/67	0/2/2/2
23	LMT	7	308	-	-	9/21/61/61	0/2/2/2
27	CHL	6	305	16	-	7/17/93/117	-
24	LHG	A	812	-	-	21/53/53/53	-
27	CHL	A	829	1	-	9/27/103/117	-
21	SF4	A	802	2,1	-	-	0/6/5/5
22	BCR	J	102	-	-	8/29/63/63	0/2/2/2
22	BCR	7	303	-	-	8/29/63/63	0/2/2/2
27	CHL	a	312	36	-	4/21/97/117	-
27	CHL	A	825	1	-	11/39/115/117	-
27	CHL	6	317	-	-	9/19/95/117	-
26	CL0	A	815	1	-	8/39/115/115	-
27	CHL	B	844	2	-	11/39/115/117	-
27	CHL	a	313	24	-	10/27/103/117	-
27	CHL	4	312	14	-	11/20/96/117	-
27	CHL	7	313	17	-	12/39/115/117	-
27	CHL	7	321	17	-	1/19/95/117	-
27	CHL	8	313	18	-	6/21/97/117	-
27	CHL	B	822	2	-	14/39/115/117	-
27	CHL	6	309	16	-	7/18/94/117	-
23	LMT	B	810	-	-	7/21/61/61	0/2/2/2
24	LHG	5	324	27	-	14/36/36/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	b	305	-	-	8/17/93/117	-
27	CHL	a	311	12	-	7/33/109/117	-
27	CHL	6	308	16	-	19/41/117/117	-
27	CHL	A	858	1	-	16/39/115/117	-
27	CHL	B	829	2	-	7/27/103/117	-
27	CHL	5	323	15	-	8/29/105/117	-
27	CHL	5	315	15	-	10/39/115/117	-
27	CHL	B	837	2	-	9/39/115/117	-
28	DGD	7	307	27	-	22/55/95/95	0/2/2/2
27	CHL	B	827	2	-	12/33/109/117	-
27	CHL	5	309	15	-	17/33/109/117	-
29	LUT	b	303	-	-	23/29/67/67	0/2/2/2
27	CHL	8	322	36	-	4/21/97/117	-
27	CHL	A	847	1	-	6/29/105/117	-
27	CHL	4	309	-	-	9/19/95/117	-
27	CHL	b	311	12	-	10/19/95/117	-
27	CHL	a	318	36	-	8/20/96/117	-
27	CHL	3	312	13	-	7/39/115/117	-
27	CHL	5	316	36	-	27/41/117/117	-
27	CHL	7	312	17	-	4/13/89/117	-
27	CHL	b	310	12	-	6/17/93/117	-
27	CHL	5	307	15	-	6/27/103/117	-
22	BCR	B	802	-	-	9/29/63/63	0/2/2/2
27	CHL	4	314	-	-	7/15/91/117	-
22	BCR	B	803	-	-	9/29/63/63	0/2/2/2
27	CHL	B	825	2	-	8/33/109/117	-
27	CHL	8	319	36	-	6/27/103/117	-
24	LHG	a	305	27	-	24/53/53/53	-
27	CHL	B	841	2	-	7/27/103/117	-
27	CHL	4	306	14	-	9/29/105/117	-
27	CHL	4	315	14	-	2/18/94/117	-
27	CHL	5	319	-	-	10/19/95/117	-
27	CHL	A	842	1	-	8/41/117/117	-
27	CHL	4	319	14	-	5/15/91/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LUT	a	304	-	-	14/29/67/67	0/2/2/2
27	CHL	6	319	16	-	8/14/90/117	-
27	CHL	B	815	2	-	14/39/115/117	-
23	LMT	F	302	-	-	5/15/55/61	0/2/2/2
27	CHL	B	850	2	-	3/21/97/117	-
27	CHL	3	311	13	-	15/33/109/117	-
27	CHL	6	314	24	-	5/17/93/117	-
27	CHL	4	311	14	-	7/18/94/117	-
29	LUT	7	304	-	-	17/29/67/67	0/2/2/2
27	CHL	b	307	12	-	8/27/103/117	-
27	CHL	A	832	1	-	13/33/109/117	-
21	SF4	C	101	3	-	-	0/6/5/5
27	CHL	B	820	2	-	10/39/115/117	-
22	BCR	3	302	-	-	11/29/63/63	0/2/2/2
27	CHL	8	312	18	-	14/39/115/117	-
24	LHG	B	808	27	-	6/36/36/53	-
27	CHL	A	844	1	-	6/39/115/117	-
27	CHL	A	849	1	-	7/39/115/117	-
27	CHL	B	813	2	-	9/27/103/117	-
27	CHL	A	824	1	-	9/33/109/117	-
27	CHL	A	820	1	-	7/39/115/117	-
27	CHL	6	306	16	-	12/30/106/117	-
27	CHL	6	315	16	-	4/21/97/117	-
27	CHL	7	323	36	-	10/24/100/117	-
27	CHL	b	313	12	-	9/17/93/117	-
27	CHL	5	312	36	-	6/21/97/117	-
27	CHL	A	854	1	-	3/29/105/117	-
27	CHL	A	823	1	-	13/39/115/117	-
27	CHL	4	305	14	-	6/15/91/117	-
27	CHL	4	320	14	-	9/21/97/117	-
27	CHL	7	314	17	-	9/36/112/117	-
27	CHL	4	308	14	-	11/33/109/117	-
27	CHL	6	318	-	-	9/19/95/117	-
27	CHL	A	826	1	-	11/36/112/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	B	839	2	-	6/33/109/117	-
27	CHL	A	857	24	-	5/17/93/117	-
20	PQN	A	801	-	-	3/23/43/43	0/2/2/2
23	LMT	A	809	-	-	6/21/61/61	0/2/2/2
27	CHL	A	850	1	-	10/39/115/117	-
30	LMG	7	301	-	-	18/36/56/70	0/1/1/1
27	CHL	B	832	36	-	7/39/115/117	-
27	CHL	B	838	2	-	11/39/115/117	-
27	CHL	K	207	10	-	8/19/95/117	-
22	BCR	B	804	-	-	10/29/63/63	0/2/2/2
27	CHL	A	853	1	-	10/39/115/117	-
27	CHL	B	849	24	-	6/39/115/117	-
27	CHL	A	848	1	-	6/39/115/117	-
27	CHL	3	313	36	-	7/39/115/117	-
27	CHL	3	309	13	-	2/17/93/117	-
27	CHL	5	313	-	-	10/30/106/117	-
29	LUT	3	305	-	-	12/29/67/67	0/2/2/2
27	CHL	K	206	10	-	4/17/93/117	-
22	BCR	F	301	-	-	10/29/63/63	0/2/2/2
27	CHL	b	306	12	-	5/17/93/117	-
27	CHL	A	840	36	-	8/39/115/117	-
35	DGA	8	306	-	-	5/29/29/45	-
22	BCR	K	202	-	-	9/29/63/63	0/2/2/2
22	BCR	A	807	-	-	11/29/63/63	0/2/2/2
27	CHL	3	310	13	-	13/39/115/117	-
22	BCR	L	302	-	-	8/29/63/63	0/2/2/2
27	CHL	A	834	1	-	6/39/115/117	-
27	CHL	5	310	15	-	5/39/115/117	-
27	CHL	A	818	1	-	7/39/115/117	-
27	CHL	J	106	9	-	6/12/88/117	-
27	CHL	a	317	12	-	9/39/115/117	-
27	CHL	3	321	13	-	7/15/91/117	-
33	XAT	7	305	-	-	7/31/93/93	0/4/4/4
27	CHL	B	842	2	-	7/39/115/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	8	318	24	-	8/17/93/117	-
27	CHL	A	827	1	-	7/26/102/117	-
24	LHG	b	302	27	-	17/39/39/53	-
22	BCR	6	301	-	-	23/29/63/63	0/2/2/2
22	BCR	A	806	-	-	9/29/63/63	0/2/2/2
29	LUT	F	303	-	-	18/29/67/67	0/2/2/2
27	CHL	A	835	1	-	8/18/94/117	-
27	CHL	3	319	13	-	11/27/103/117	-
27	CHL	7	319	17	-	19/41/117/117	-
27	CHL	a	308	12	-	7/15/91/117	-
27	CHL	5	318	15	-	9/39/115/117	-
27	CHL	B	819	2	-	11/39/115/117	-
27	CHL	4	307	14	-	7/33/109/117	-
29	LUT	4	301	-	-	15/29/67/67	0/2/2/2
22	BCR	5	301	-	-	13/29/63/63	0/2/2/2
22	BCR	A	805	-	-	4/29/63/63	0/2/2/2
27	CHL	6	312	16	-	7/17/93/117	-
27	CHL	A	831	-	-	12/27/103/117	-
22	BCR	K	203	-	-	5/29/63/63	0/2/2/2
27	CHL	B	848	2	-	9/39/115/117	-
27	CHL	8	326	18	-	3/17/93/117	-
27	CHL	4	304	14	-	4/27/103/117	-
27	CHL	7	315	17	-	3/13/89/117	-
27	CHL	A	830	1	-	7/39/115/117	-
27	CHL	B	835	2	-	11/30/106/117	-
27	CHL	B	818	2	-	6/27/103/117	-
27	CHL	3	318	36	-	7/23/99/117	-
27	CHL	5	322	15	-	3/19/95/117	-
22	BCR	A	804	-	-	6/29/63/63	0/2/2/2
30	LMG	8	307	-	-	13/27/47/70	0/1/1/1
27	CHL	A	839	1	-	15/39/115/117	-
27	CHL	A	859	36	-	7/39/115/117	-
24	LHG	5	304	-	-	21/39/39/53	-
27	CHL	B	814	2	-	15/39/115/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	4	316	-	-	10/17/93/117	-
27	CHL	B	812	-	-	6/39/115/117	-
27	CHL	A	838	1	-	8/33/109/117	-
30	LMG	J	101	-	-	26/44/64/70	0/1/1/1
27	CHL	3	320	13	-	6/35/111/117	-
27	CHL	7	320	36,28	-	10/19/95/117	-
30	LMG	a	301	-	-	16/39/59/70	0/1/1/1
27	CHL	6	307	-	-	16/39/115/117	-
22	BCR	3	303	-	-	10/29/63/63	0/2/2/2
27	CHL	B	826	2	-	7/21/97/117	-
27	CHL	F	308	6	-	8/17/93/117	-
27	CHL	3	315	13	-	10/24/100/117	-
27	CHL	B	817	2	-	11/39/115/117	-
22	BCR	L	301	-	-	10/29/63/63	0/2/2/2
27	CHL	K	204	36	-	6/21/97/117	-
27	CHL	a	309	36	-	9/33/109/117	-
27	CHL	4	317	14	-	8/15/91/117	-
22	BCR	A	803	-	-	7/29/63/63	0/2/2/2
27	CHL	8	323	-	-	4/21/97/117	-
27	CHL	6	316	36	-	11/17/93/117	-
27	CHL	A	816	36	-	6/39/115/117	-
22	BCR	B	805	-	-	8/29/63/63	0/2/2/2
28	DGD	B	809	-	-	22/50/90/95	0/2/2/2
27	CHL	a	314	12	-	10/15/91/117	-
29	LUT	3	304	-	-	15/29/67/67	0/2/2/2
27	CHL	A	851	1	-	6/17/93/117	-
24	LHG	8	305	27	-	16/53/53/53	-
27	CHL	b	304	12	-	6/17/93/117	-
22	BCR	M	102	-	-	9/29/63/63	0/2/2/2
29	LUT	J	103	-	-	18/29/67/67	0/2/2/2
27	CHL	a	315	12	-	12/35/111/117	-
27	CHL	B	840	2	-	10/39/115/117	-
27	CHL	b	312	-	-	4/17/93/117	-
27	CHL	b	314	12	-	6/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	A	822	1	-	5/27/103/117	-
27	CHL	K	205	10	-	3/17/93/117	-
27	CHL	B	833	36	-	7/27/103/117	-
27	CHL	A	821	1	-	13/39/115/117	-
27	CHL	B	834	2	-	6/39/115/117	-
27	CHL	B	836	2	-	5/39/115/117	-
27	CHL	8	320	18	-	8/24/100/117	-
27	CHL	8	311	18	-	2/17/93/117	-
27	CHL	A	856	36	-	4/39/115/117	-
27	CHL	8	314	18	-	10/41/117/117	-
29	LUT	b	301	-	-	15/29/67/67	0/2/2/2
30	LMG	J	104	-	-	7/24/44/70	0/1/1/1
27	CHL	3	308	13	-	6/39/115/117	-
27	CHL	5	311	15	-	5/17/93/117	-
22	BCR	3	301	-	-	8/29/63/63	0/2/2/2
27	CHL	5	320	15	-	3/17/93/117	-
29	LUT	6	302	-	-	16/29/67/67	0/2/2/2
27	CHL	B	851	2	-	9/36/112/117	-
27	CHL	A	828	1	-	12/39/115/117	-
27	CHL	b	316	-	-	6/20/96/117	-
27	CHL	6	311	16	-	9/39/115/117	-
27	CHL	L	304	-	-	2/15/91/117	-
27	CHL	B	846	36	-	15/39/115/117	-
27	CHL	4	310	24	-	8/17/93/117	-
29	LUT	a	302	-	-	15/29/67/67	0/2/2/2
27	CHL	5	317	36	-	5/19/95/117	-
27	CHL	5	308	15	-	5/17/93/117	-
27	CHL	B	821	2	-	9/31/107/117	-
27	CHL	6	310	16	-	12/27/103/117	-
27	CHL	b	315	12	-	14/39/115/117	-
21	SF4	C	102	3	-	-	0/6/5/5
27	CHL	B	845	2	-	2/21/97/117	-
27	CHL	6	313	16	-	8/18/94/117	-
24	LHG	4	303	27	-	30/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	7	302	-	-	32/53/53/53	-
27	CHL	5	314	15	-	6/15/91/117	-
27	CHL	B	811	2	-	9/39/115/117	-
22	BCR	B	807	-	-	6/29/63/63	0/2/2/2
27	CHL	B	828	36	-	4/33/109/117	-
27	CHL	4	313	-	-	8/15/91/117	-
27	CHL	A	841	36	-	10/29/105/117	-
27	CHL	A	843	1	-	13/39/115/117	-
24	LHG	7	306	27	-	20/48/48/53	-
23	LMT	5	306	-	-	6/16/56/61	0/2/2/2
27	CHL	6	320	16	-	6/17/93/117	-
29	LUT	5	303	-	-	19/29/67/67	0/2/2/2
27	CHL	3	317	36	-	9/36/112/117	-
27	CHL	7	316	36	-	9/25/101/117	-
27	CHL	8	316	18	-	11/39/115/117	-
29	LUT	6	303	-	-	18/29/67/67	0/2/2/2
20	PQN	B	801	-	-	3/23/43/43	0/2/2/2
27	CHL	A	833	1	-	13/35/111/117	-
27	CHL	8	321	36	-	17/41/117/117	-
27	CHL	7	318	17	-	9/27/103/117	-
27	CHL	b	308	-	-	5/17/93/117	-
22	BCR	8	302	-	-	7/29/63/63	0/2/2/2
27	CHL	7	317	24	-	13/39/115/117	-
27	CHL	5	321	15	-	5/17/93/117	-
23	LMT	5	326	-	-	9/21/61/61	0/2/2/2
27	CHL	3	314	36	-	12/33/109/117	-
27	CHL	B	823	2	-	8/27/103/117	-
27	CHL	A	846	-	-	3/21/97/117	-
27	CHL	8	317	36	-	12/39/115/117	-
27	CHL	3	316	36	-	8/41/117/117	-
27	CHL	7	324	17	-	8/17/93/117	-
27	CHL	8	324	36	-	2/15/92/117	-
29	LUT	4	302	-	-	19/29/67/67	0/2/2/2
24	LHG	A	810	-	-	21/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	7	322	36	-	10/35/111/117	-
27	CHL	a	307	12	-	4/33/109/117	-
31	AXT	a	303	-	-	1/29/71/75	0/2/2/2
27	CHL	B	824	2	-	6/30/106/117	-

The worst 5 of 5083 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	306	CHL	MG-NA	23.77	2.62	2.06
27	6	306	CHL	MG-NA	23.39	2.61	2.06
27	5	310	CHL	MG-NA	20.63	2.55	2.06
27	5	312	CHL	MG-NA	19.85	2.53	2.06
27	4	311	CHL	MG-NA	18.64	2.50	2.06

The worst 5 of 6430 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	308	CHL	C2B-C1B-NB	-110.37	36.24	110.23
27	b	308	CHL	CMB-C2B-C1B	-23.51	89.57	125.37
27	5	315	CHL	C4-C3-C5	-19.98	81.67	115.27
27	5	315	CHL	C5-C3-C2	19.36	160.28	121.12
27	5	313	CHL	C1D-ND-C4D	-17.88	93.63	106.33

There are no chirality outliers.

5 of 2766 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	804	BCR	C7-C8-C9-C10
22	A	804	BCR	C7-C8-C9-C34
22	A	805	BCR	C1-C6-C7-C8
22	A	806	BCR	C1-C6-C7-C8
22	A	806	BCR	C7-C8-C9-C34

There are no ring outliers.

240 monomers are involved in 573 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	845	CHL	3	0
27	b	317	CHL	15	0
27	L	303	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	310	CHL	2	0
27	a	316	CHL	6	0
27	B	831	CHL	2	0
27	B	847	CHL	1	0
27	a	319	CHL	1	0
27	7	311	CHL	1	0
29	8	304	LUT	2	0
23	A	808	LMT	2	0
27	B	816	CHL	4	0
27	A	855	CHL	4	0
27	a	320	CHL	1	0
32	5	305	PTY	1	0
27	A	817	CHL	5	0
27	b	309	CHL	3	0
29	8	303	LUT	6	0
27	B	830	CHL	3	0
27	A	837	CHL	2	0
27	5	325	CHL	4	0
22	I	801	BCR	2	0
24	A	811	LHG	3	0
27	A	852	CHL	2	0
27	A	836	CHL	2	0
22	B	806	BCR	4	0
34	8	301	SQD	1	0
29	5	302	LUT	3	0
23	7	308	LMT	1	0
27	6	305	CHL	1	0
24	A	812	LHG	3	0
27	A	829	CHL	1	0
22	J	102	BCR	6	0
22	7	303	BCR	3	0
27	A	825	CHL	2	0
27	6	317	CHL	4	0
26	A	815	CL0	2	0
27	B	844	CHL	5	0
27	a	313	CHL	1	0
27	4	312	CHL	4	0
27	7	313	CHL	3	0
27	7	321	CHL	3	0
27	B	822	CHL	4	0
23	B	810	LMT	4	0
24	5	324	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	305	CHL	1	0
27	a	311	CHL	2	0
27	6	308	CHL	12	0
27	A	858	CHL	4	0
27	B	829	CHL	2	0
27	5	323	CHL	3	0
27	5	315	CHL	3	0
27	B	837	CHL	4	0
28	7	307	DGD	5	0
27	B	827	CHL	1	0
27	5	309	CHL	4	0
29	b	303	LUT	7	0
27	A	847	CHL	1	0
27	4	309	CHL	3	0
27	b	311	CHL	6	0
27	a	318	CHL	5	0
27	5	316	CHL	8	0
27	b	310	CHL	1	0
27	5	307	CHL	1	0
22	B	802	BCR	3	0
27	4	314	CHL	2	0
24	a	305	LHG	12	0
27	B	841	CHL	5	0
27	4	306	CHL	6	0
27	4	315	CHL	2	0
27	5	319	CHL	3	0
27	A	842	CHL	7	0
27	4	319	CHL	1	0
27	6	319	CHL	3	0
27	B	815	CHL	2	0
23	F	302	LMT	1	0
27	3	311	CHL	1	0
27	4	311	CHL	1	0
29	7	304	LUT	3	0
27	b	307	CHL	1	0
27	A	832	CHL	3	0
27	B	820	CHL	6	0
22	3	302	BCR	5	0
27	8	312	CHL	4	0
27	A	844	CHL	1	0
27	A	824	CHL	3	0
27	A	820	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	306	CHL	3	0
27	7	323	CHL	4	0
27	b	313	CHL	1	0
27	A	854	CHL	1	0
27	A	823	CHL	3	0
27	4	320	CHL	2	0
27	6	318	CHL	3	0
27	A	826	CHL	3	0
27	B	839	CHL	3	0
27	A	857	CHL	1	0
27	A	850	CHL	2	0
30	7	301	LMG	1	0
27	B	832	CHL	1	0
27	B	838	CHL	1	0
27	K	207	CHL	1	0
22	B	804	BCR	1	0
27	A	853	CHL	4	0
27	B	849	CHL	2	0
27	A	848	CHL	2	0
27	3	313	CHL	1	0
27	3	309	CHL	1	0
27	5	313	CHL	3	0
29	3	305	LUT	6	0
22	F	301	BCR	1	0
27	b	306	CHL	5	0
27	A	840	CHL	3	0
35	8	306	DGA	3	0
22	K	202	BCR	4	0
22	A	807	BCR	3	0
27	3	310	CHL	4	0
22	L	302	BCR	1	0
27	A	834	CHL	5	0
27	5	310	CHL	1	0
27	A	818	CHL	2	0
27	J	106	CHL	2	0
27	a	317	CHL	1	0
27	B	842	CHL	1	0
27	8	318	CHL	1	0
27	A	827	CHL	1	0
24	b	302	LHG	2	0
22	6	301	BCR	1	0
29	F	303	LUT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	835	CHL	2	0
27	3	319	CHL	1	0
27	7	319	CHL	9	0
27	a	308	CHL	1	0
27	5	318	CHL	4	0
27	4	307	CHL	1	0
29	4	301	LUT	6	0
22	5	301	BCR	8	0
22	A	805	BCR	2	0
27	6	312	CHL	2	0
27	A	831	CHL	8	0
22	K	203	BCR	5	0
27	B	848	CHL	3	0
27	8	326	CHL	1	0
27	4	304	CHL	2	0
27	A	830	CHL	5	0
27	B	835	CHL	1	0
27	B	818	CHL	3	0
27	5	322	CHL	1	0
22	A	804	BCR	4	0
30	8	307	LMG	3	0
27	A	839	CHL	8	0
27	A	859	CHL	1	0
24	5	304	LHG	3	0
27	B	814	CHL	4	0
27	4	316	CHL	12	0
27	B	812	CHL	1	0
27	A	838	CHL	1	0
30	J	101	LMG	4	0
27	3	320	CHL	2	0
27	7	320	CHL	4	0
30	a	301	LMG	2	0
27	6	307	CHL	6	0
22	3	303	BCR	2	0
27	3	315	CHL	3	0
27	B	817	CHL	2	0
22	L	301	BCR	1	0
27	K	204	CHL	1	0
27	a	309	CHL	2	0
27	4	317	CHL	10	0
22	A	803	BCR	3	0
27	8	323	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	316	CHL	5	0
27	A	816	CHL	4	0
22	B	805	BCR	1	0
28	B	809	DGD	1	0
27	a	314	CHL	1	0
29	3	304	LUT	4	0
27	b	304	CHL	1	0
29	J	103	LUT	1	0
27	a	315	CHL	5	0
27	B	840	CHL	1	0
27	A	822	CHL	1	0
27	K	205	CHL	1	0
27	B	833	CHL	1	0
27	A	821	CHL	1	0
27	B	834	CHL	3	0
27	B	836	CHL	4	0
27	8	320	CHL	1	0
27	8	311	CHL	5	0
27	A	856	CHL	1	0
27	8	314	CHL	5	0
29	b	301	LUT	3	0
30	J	104	LMG	1	0
27	3	308	CHL	1	0
27	5	311	CHL	3	0
22	3	301	BCR	2	0
29	6	302	LUT	2	0
27	B	851	CHL	4	0
27	A	828	CHL	3	0
27	b	316	CHL	1	0
27	6	311	CHL	1	0
27	L	304	CHL	1	0
27	B	846	CHL	3	0
29	a	302	LUT	2	0
27	5	317	CHL	4	0
27	5	308	CHL	3	0
27	B	821	CHL	2	0
27	b	315	CHL	5	0
27	B	845	CHL	2	0
27	6	313	CHL	1	0
24	4	303	LHG	7	0
24	7	302	LHG	6	0
27	B	811	CHL	1	0

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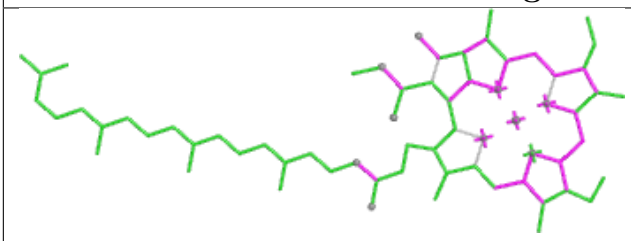
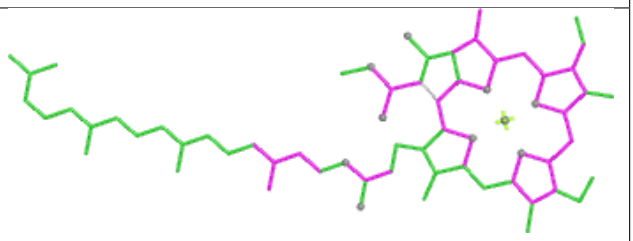
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	807	BCR	4	0
27	4	313	CHL	6	0
27	A	841	CHL	7	0
24	7	306	LHG	1	0
27	A	843	CHL	19	0
23	5	306	LMT	2	0
29	5	303	LUT	5	0
27	3	317	CHL	3	0
27	8	316	CHL	1	0
29	6	303	LUT	2	0
20	B	801	PQN	2	0
27	A	833	CHL	3	0
27	8	321	CHL	2	0
27	7	318	CHL	3	0
27	b	308	CHL	37	0
22	8	302	BCR	5	0
27	7	317	CHL	4	0
27	5	321	CHL	1	0
27	3	314	CHL	1	0
27	A	846	CHL	7	0
27	8	317	CHL	1	0
27	3	316	CHL	6	0
27	7	324	CHL	1	0
27	8	324	CHL	1	0
29	4	302	LUT	2	0
24	A	810	LHG	1	0
27	7	322	CHL	6	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.

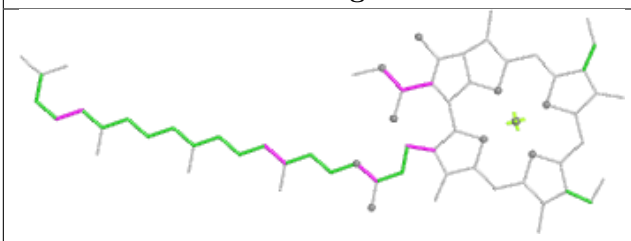
Ligand CHL A 845



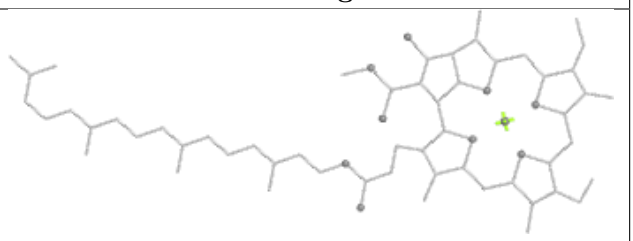
Bond lengths



Bond angles

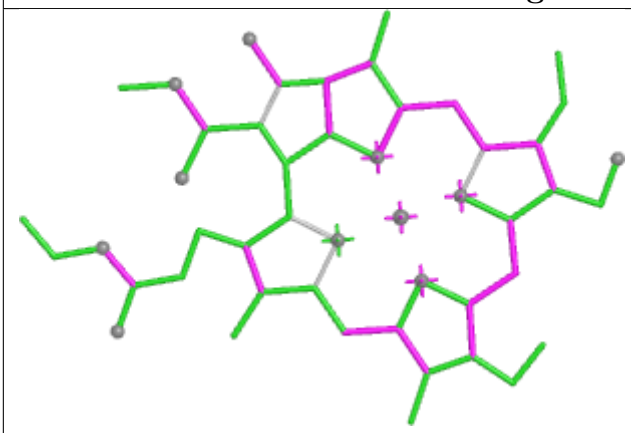


Torsions



Rings

Ligand CHL b 317



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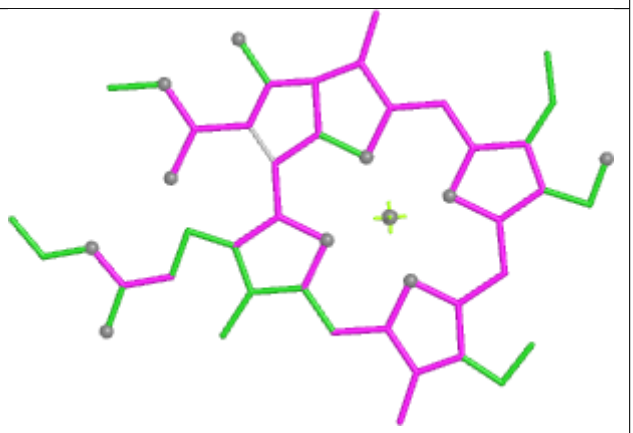

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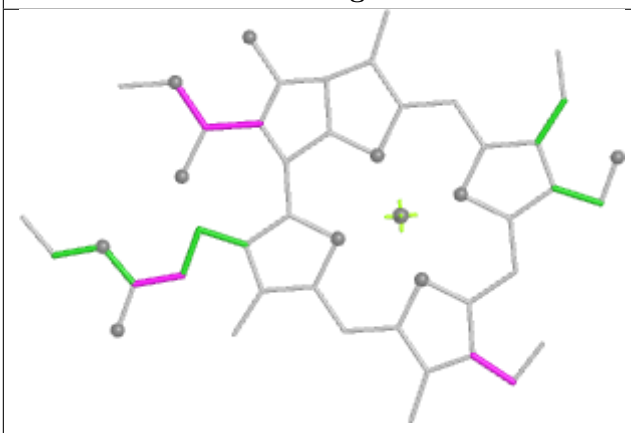

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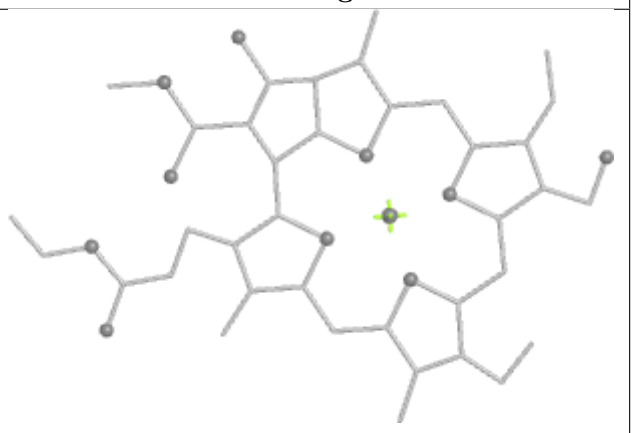
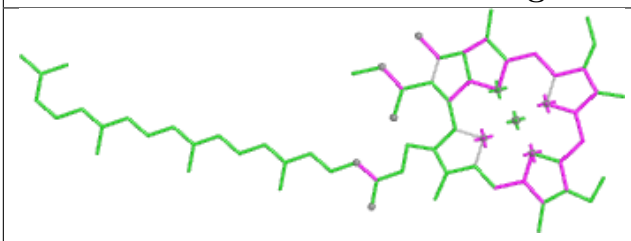


Rings

Ligand CHL 8 315



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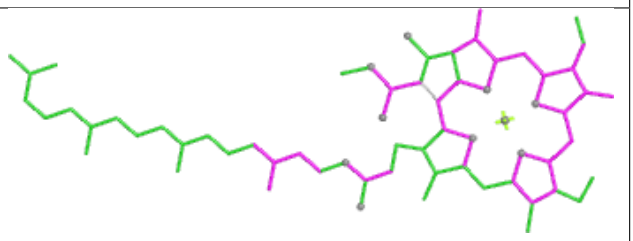
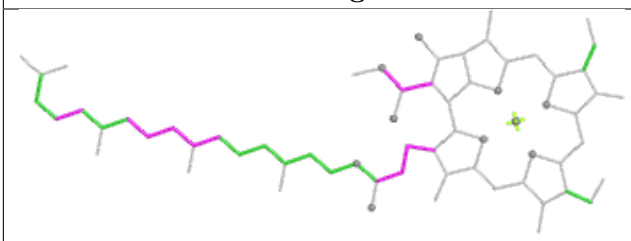
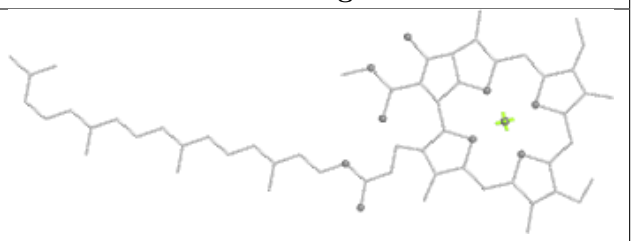


Bond angles

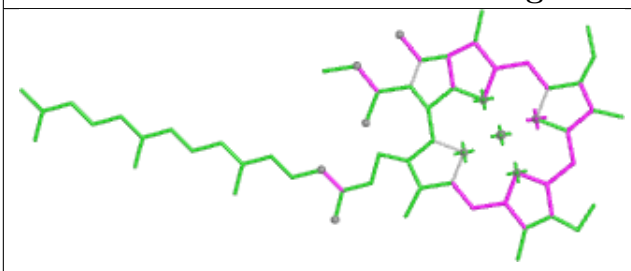


Torsions



Rings

Ligand CHL L 303



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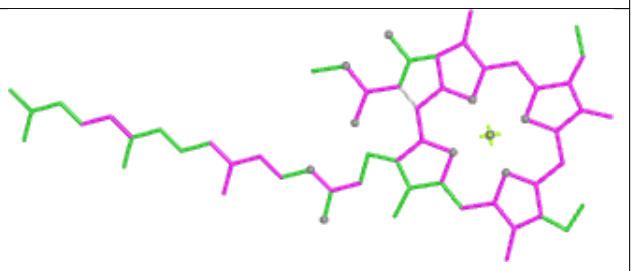
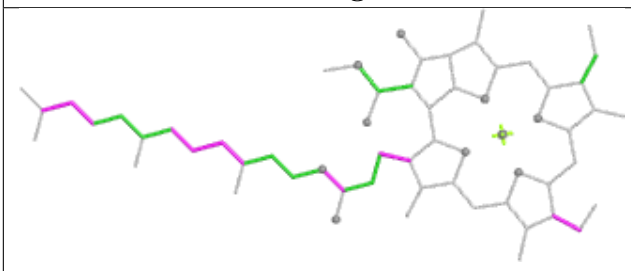
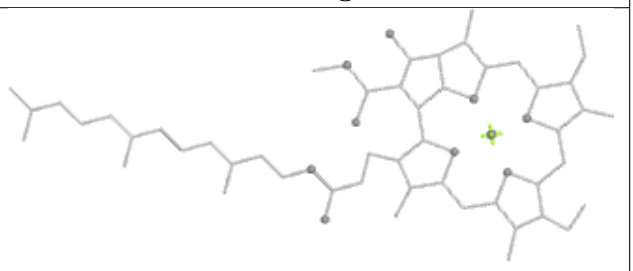


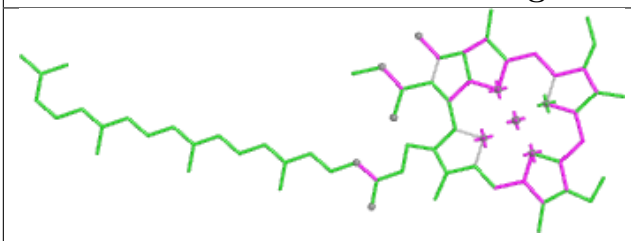
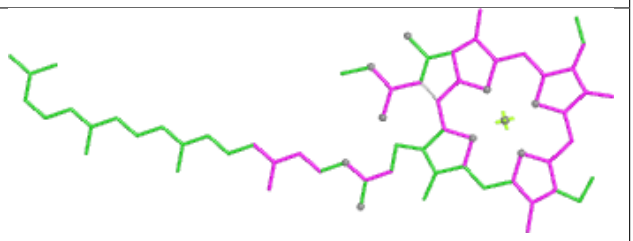
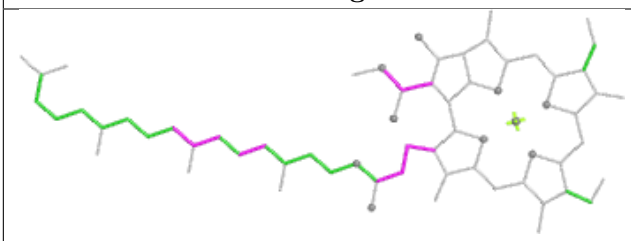
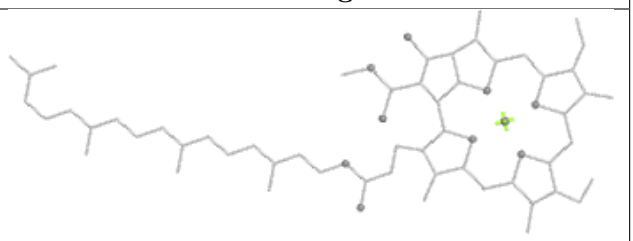
Bond angles

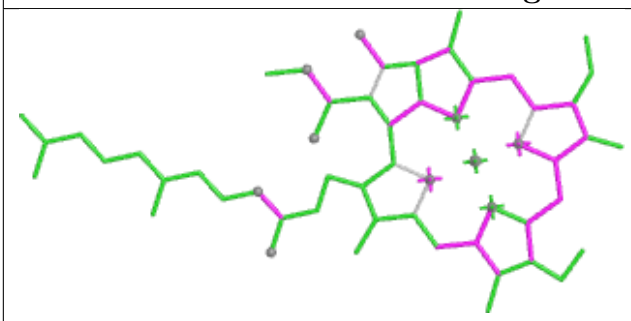
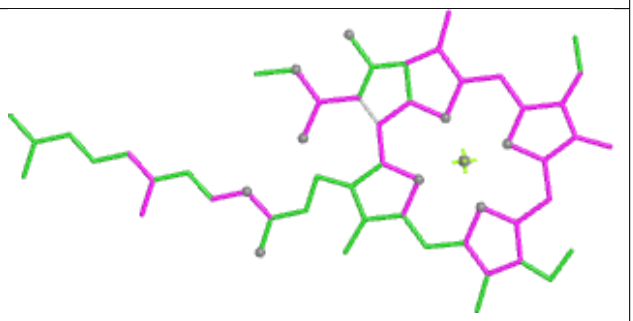


Torsions



Rings

Ligand CHL a 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL A 819	
	
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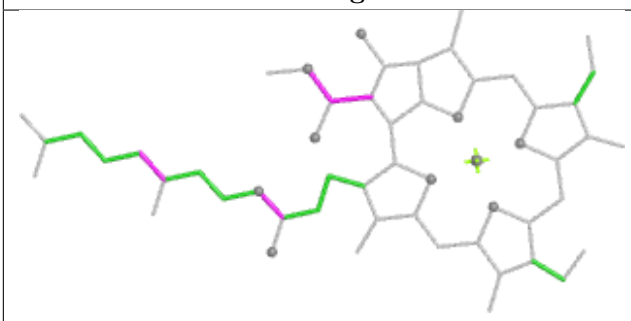
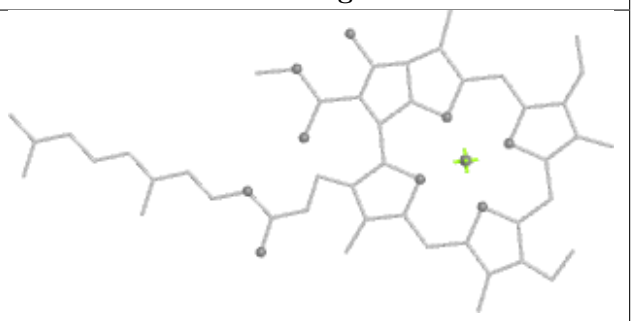
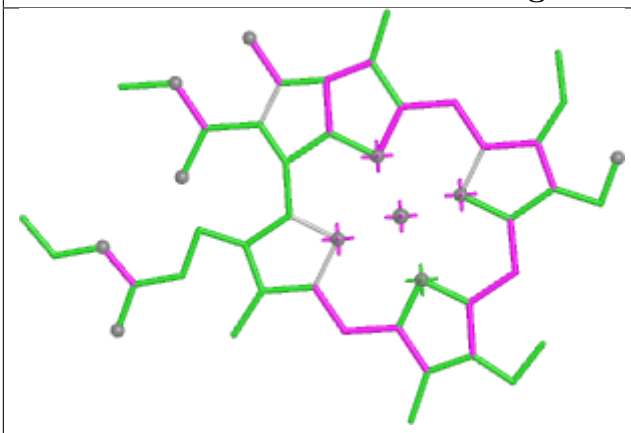
	
Torsions	Rings

Ligand CHL a 316



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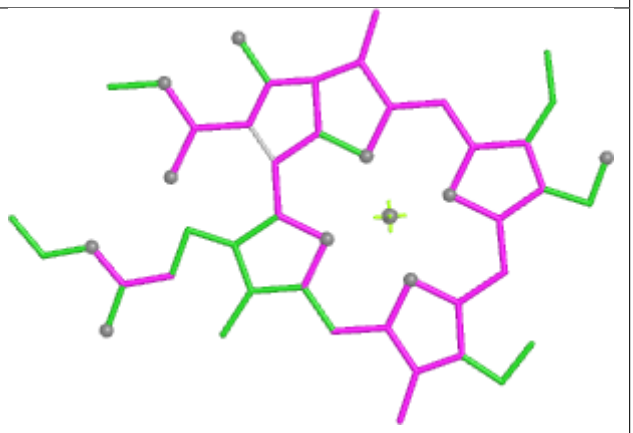

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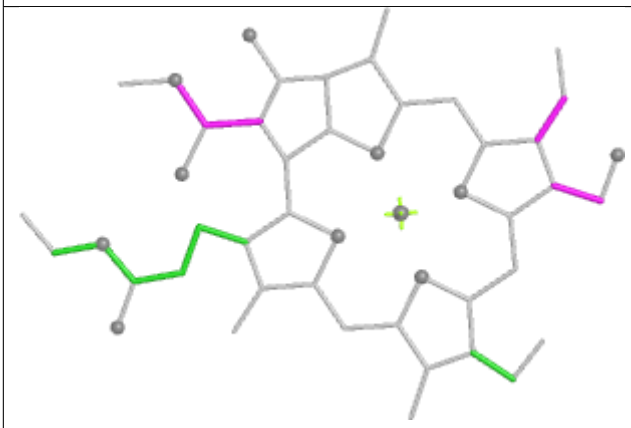

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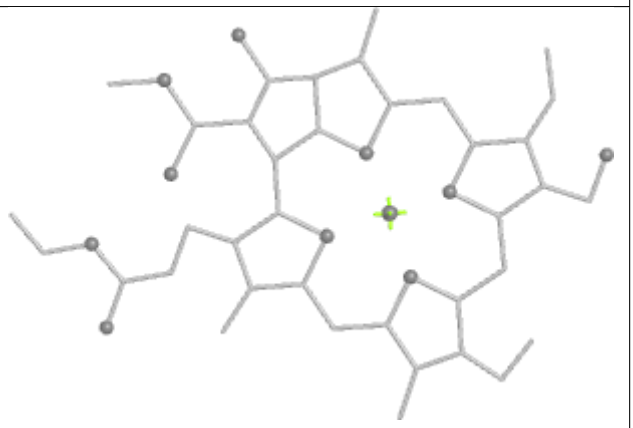
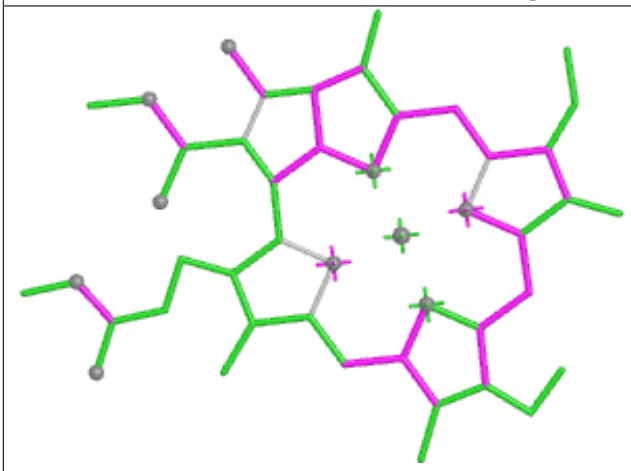


Rings

Ligand CHL B 831



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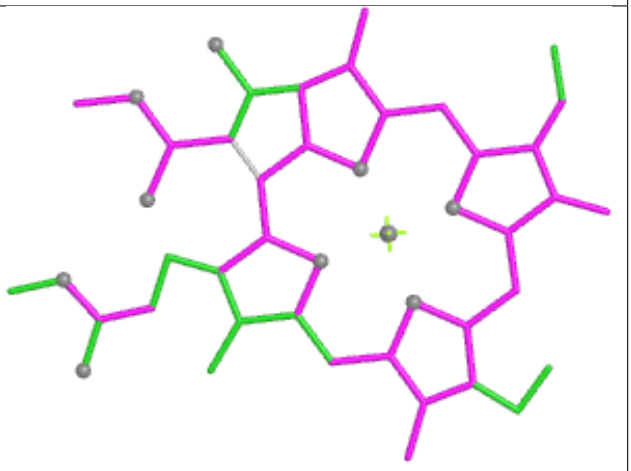

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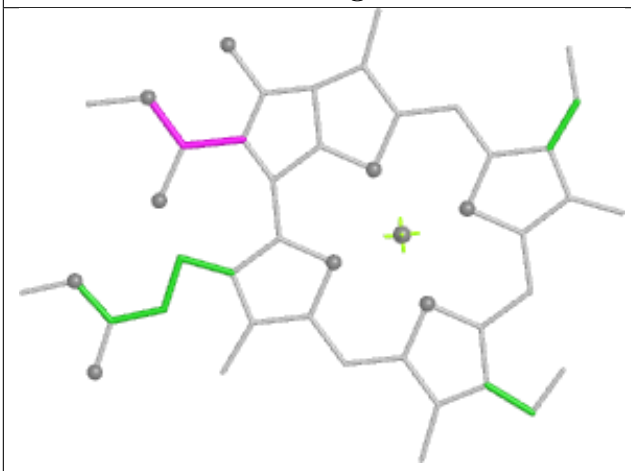

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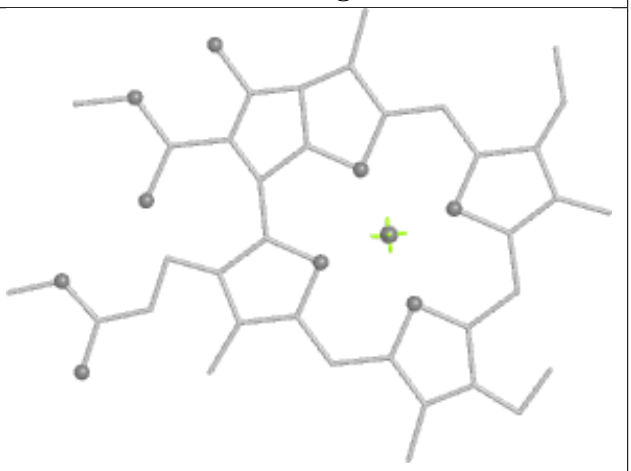
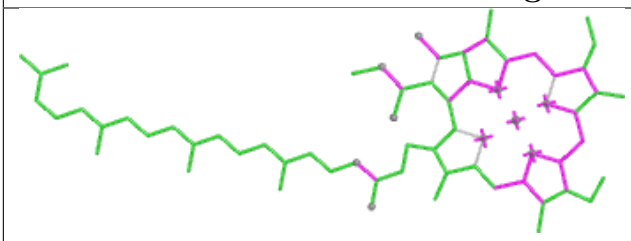


Rings

Ligand CHL B 847



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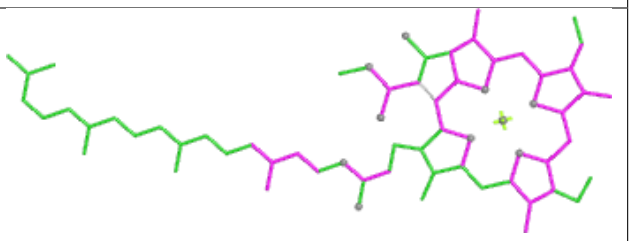

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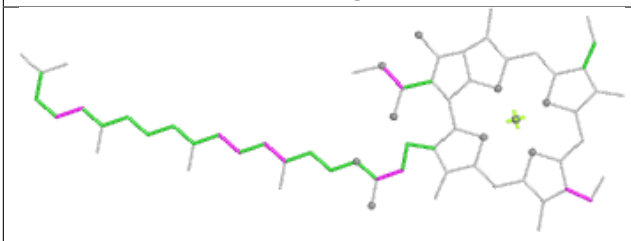

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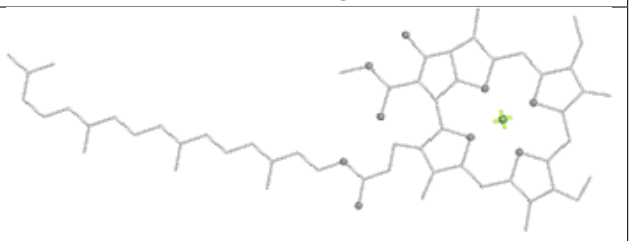
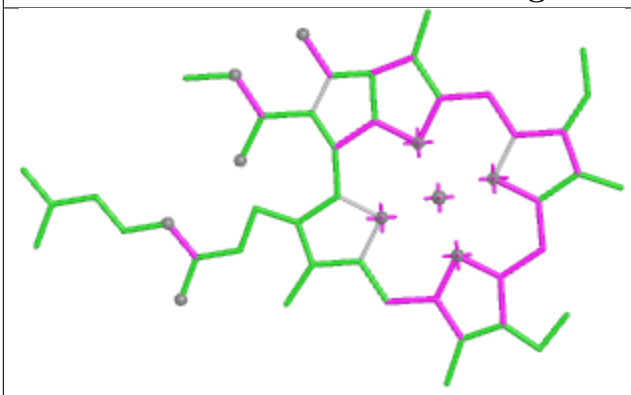


Rings

Ligand CHL a 319



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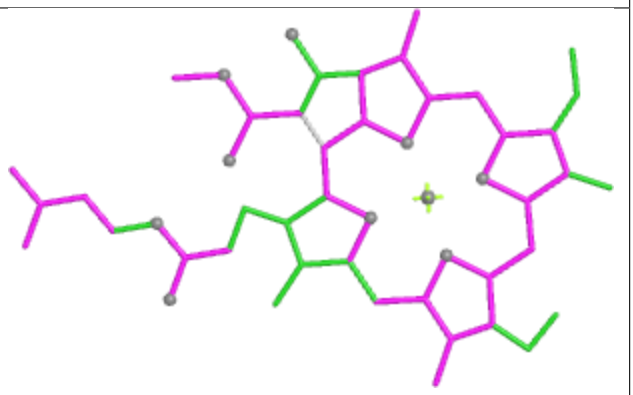

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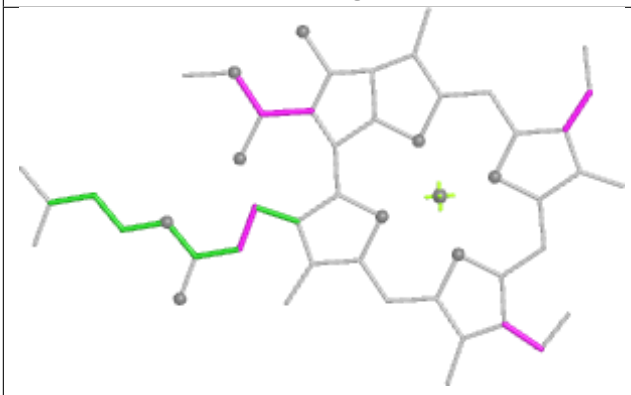

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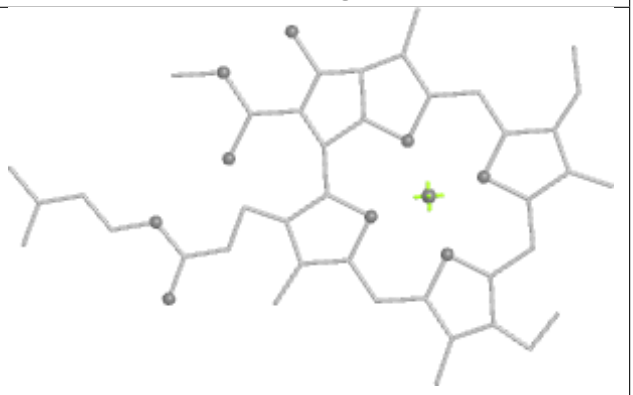
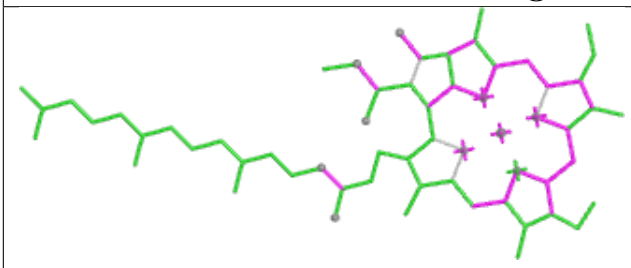


Rings

Ligand CHL 7 311



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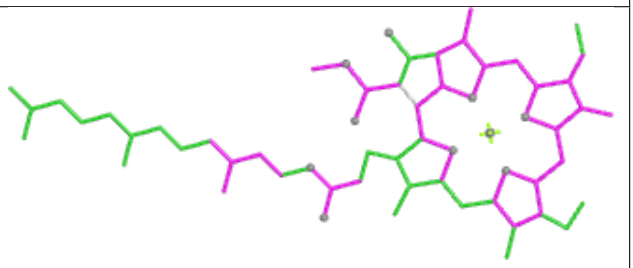

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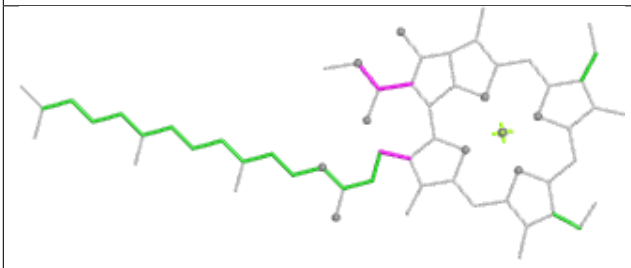

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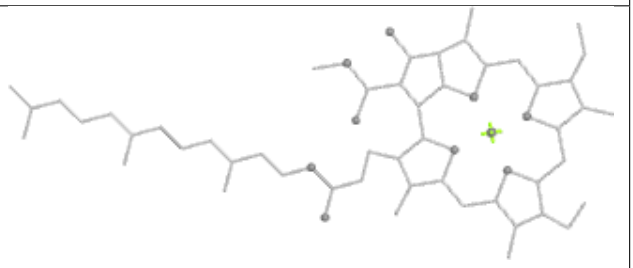
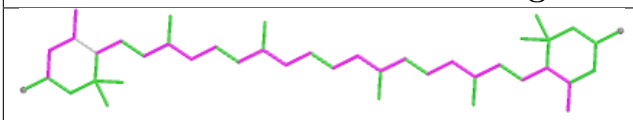
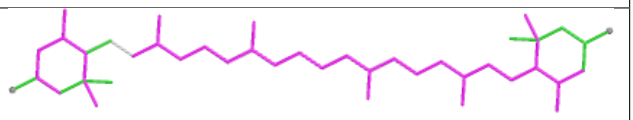


Rings

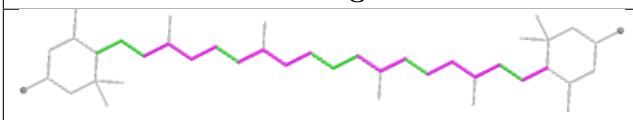
Ligand LUT 8 304



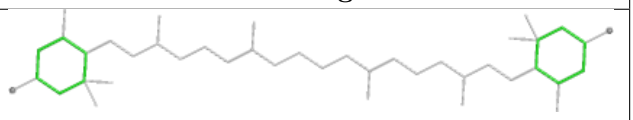
Bond lengths



Bond angles

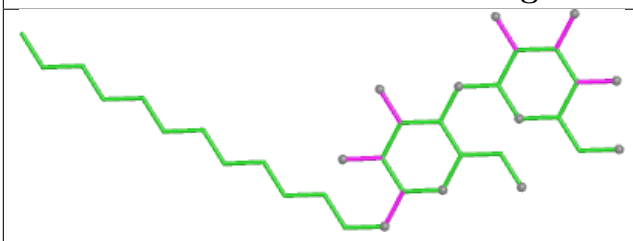


Torsions



Rings

Ligand LMT A 808



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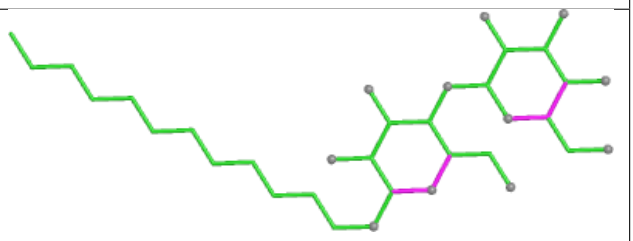
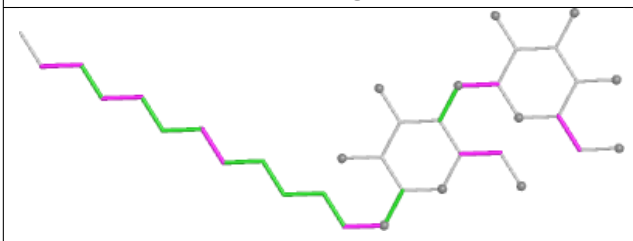


Bond angles



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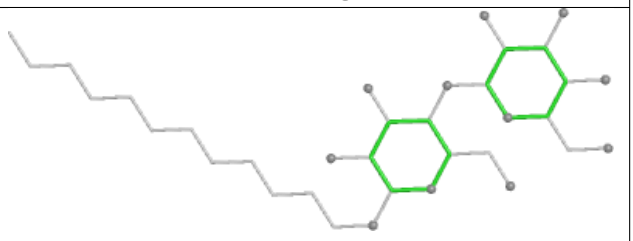
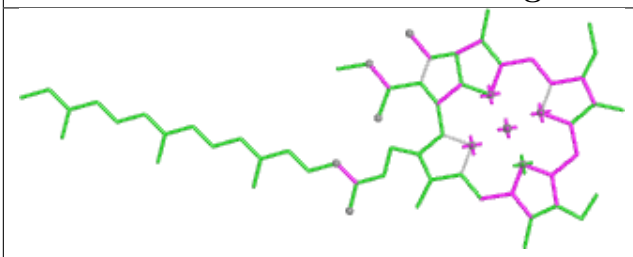


Rings

Ligand CHL B 816



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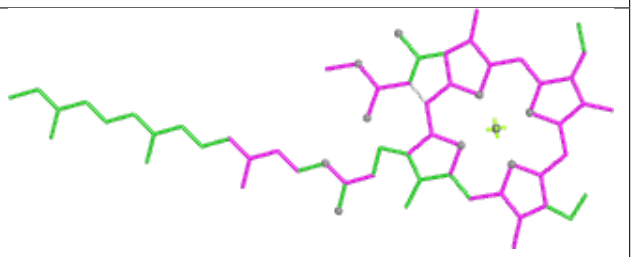

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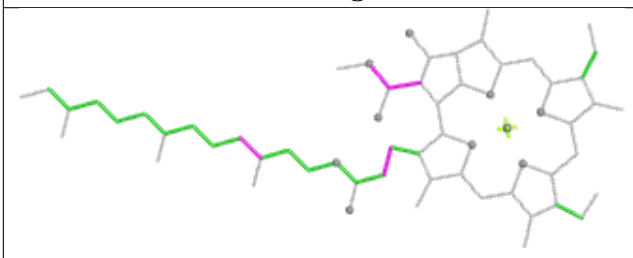

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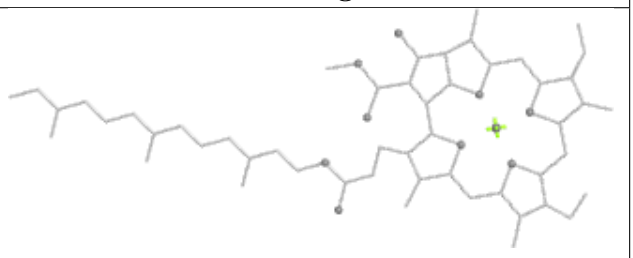
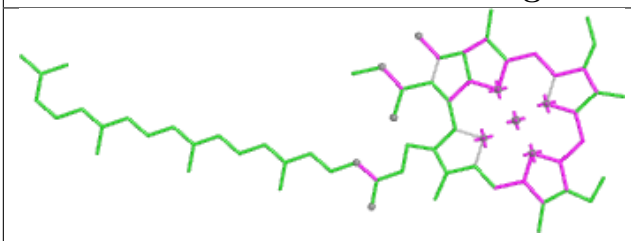


Rings

Ligand CHL A 855



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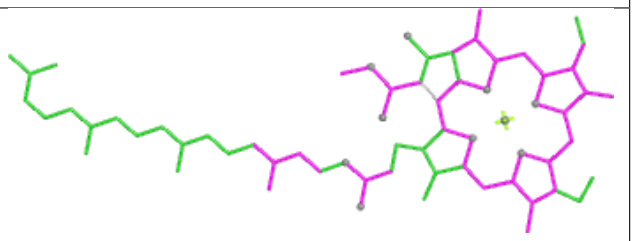
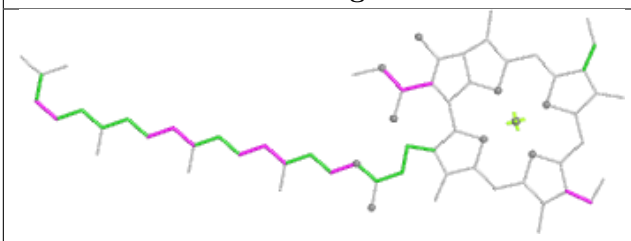


Bond angles



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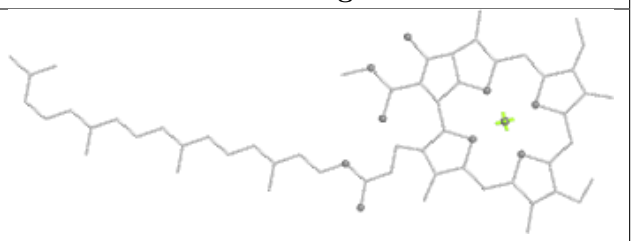
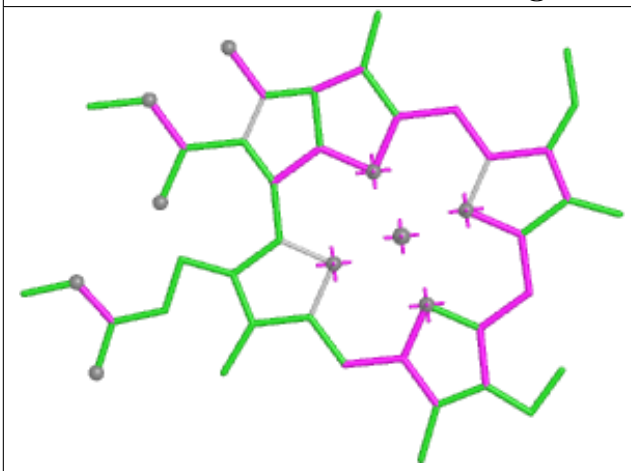


Rings

Ligand CHL a 320



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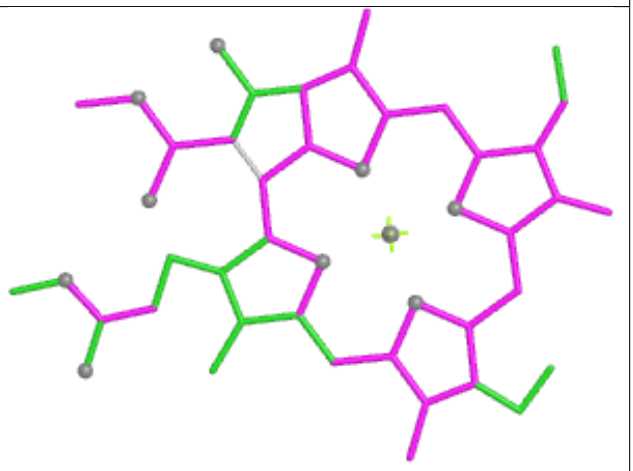
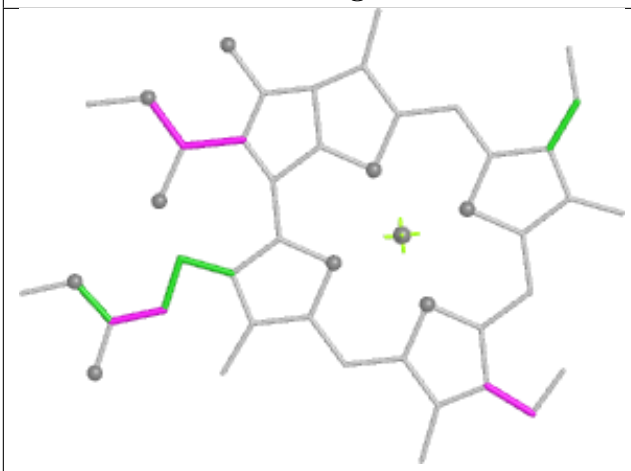


Bond angles

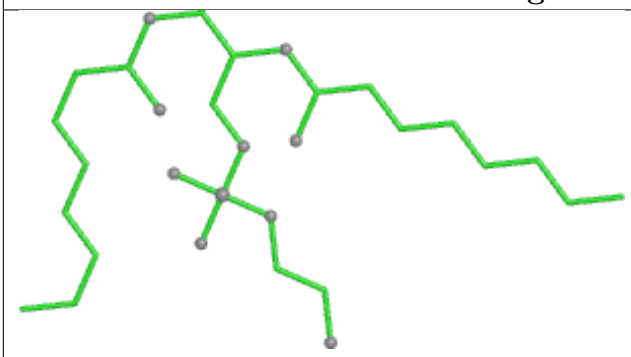


Torsions



Rings

Ligand PTY 5 305



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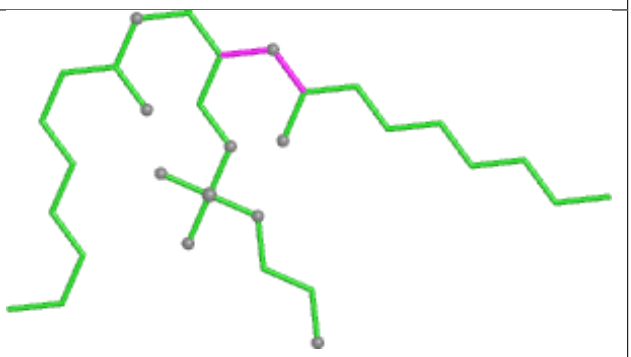
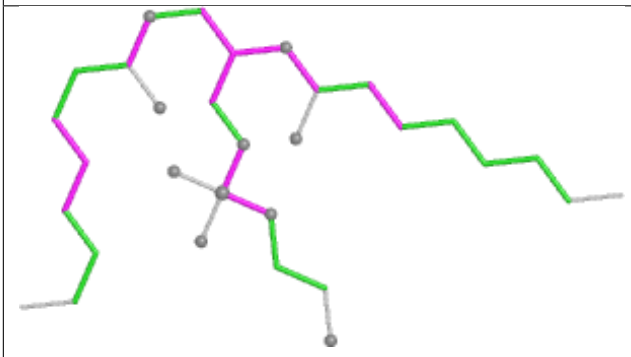


Bond angles



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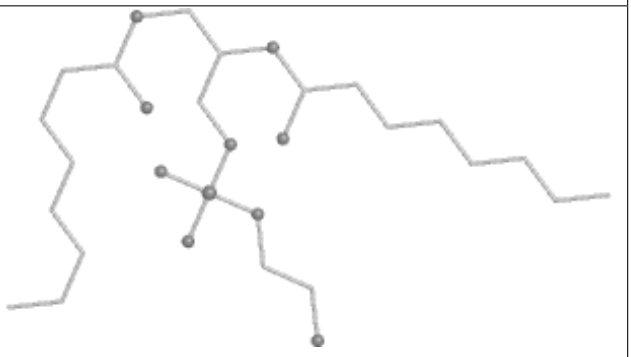
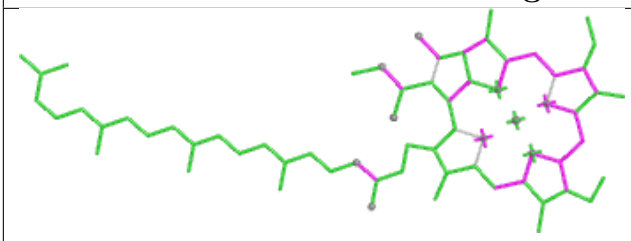


Rings

Ligand CHL A 817



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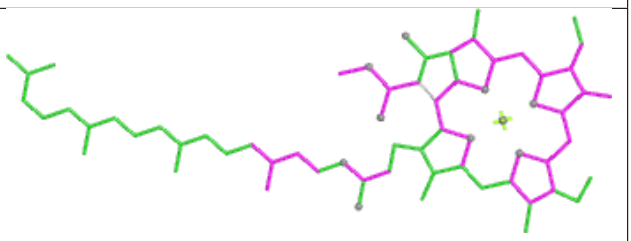
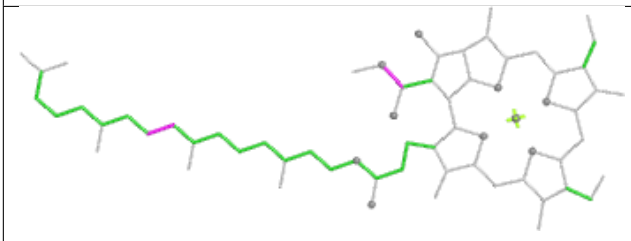


Bond angles



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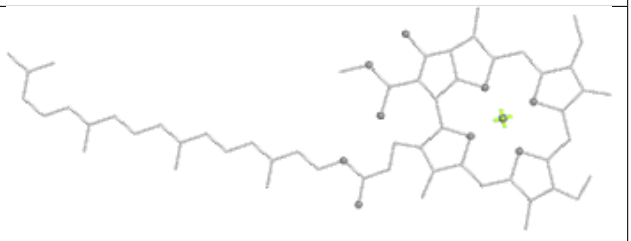
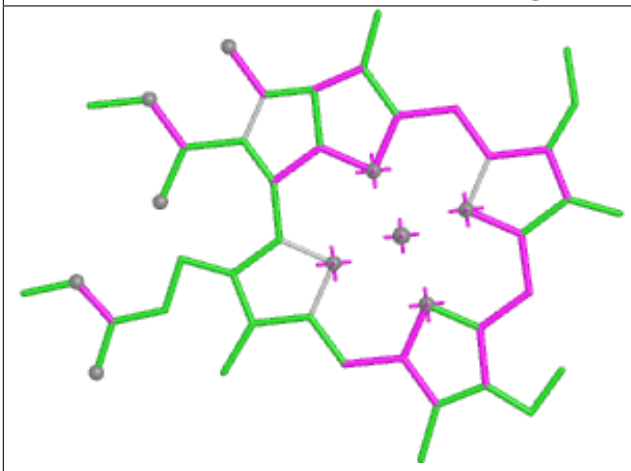


Rings

Ligand CHL b 309



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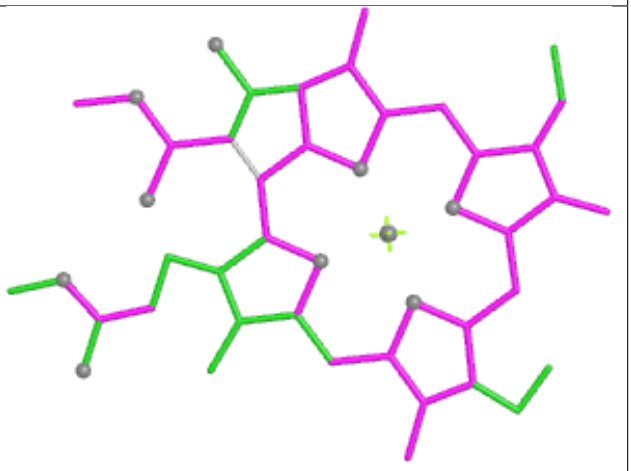
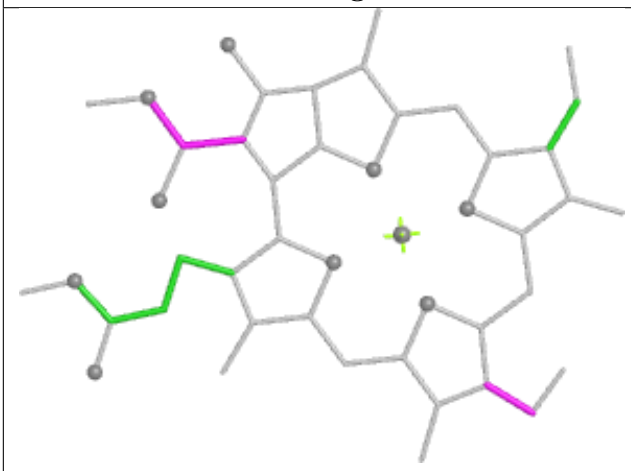


Bond angles



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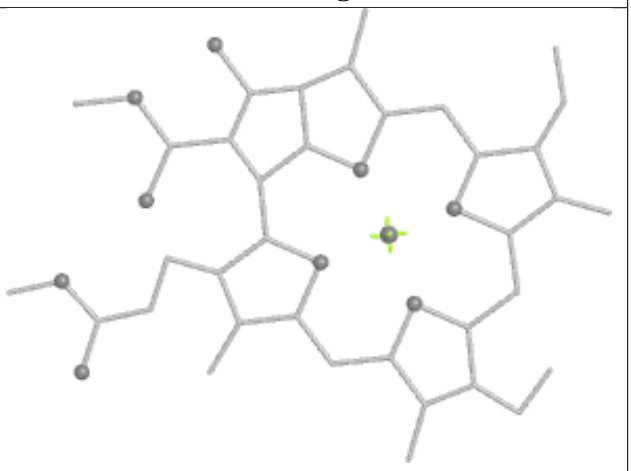
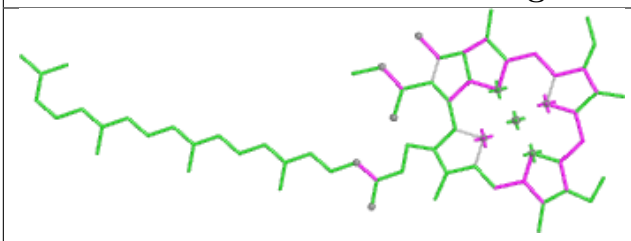


Rings

Ligand CHL 8 325



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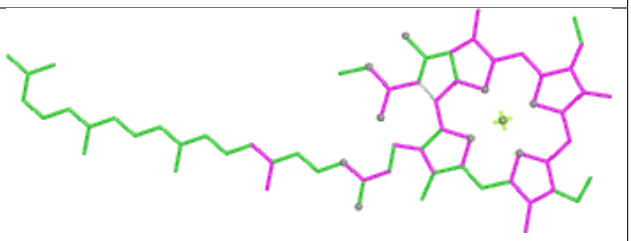
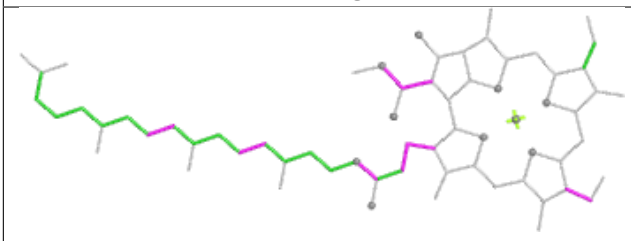


Bond angles



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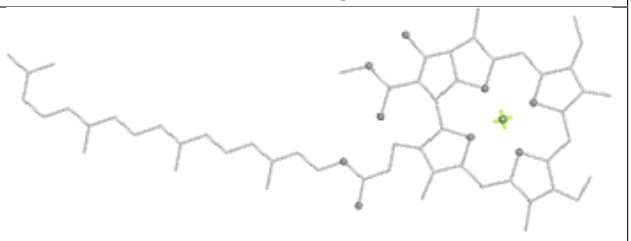
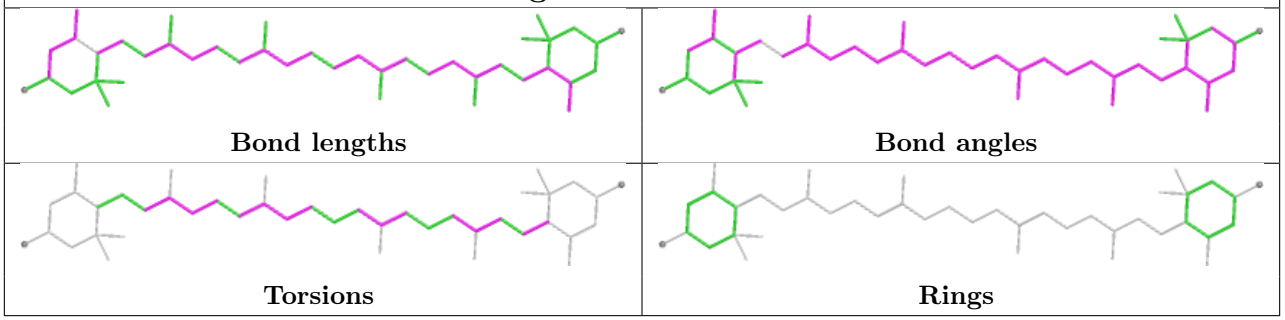
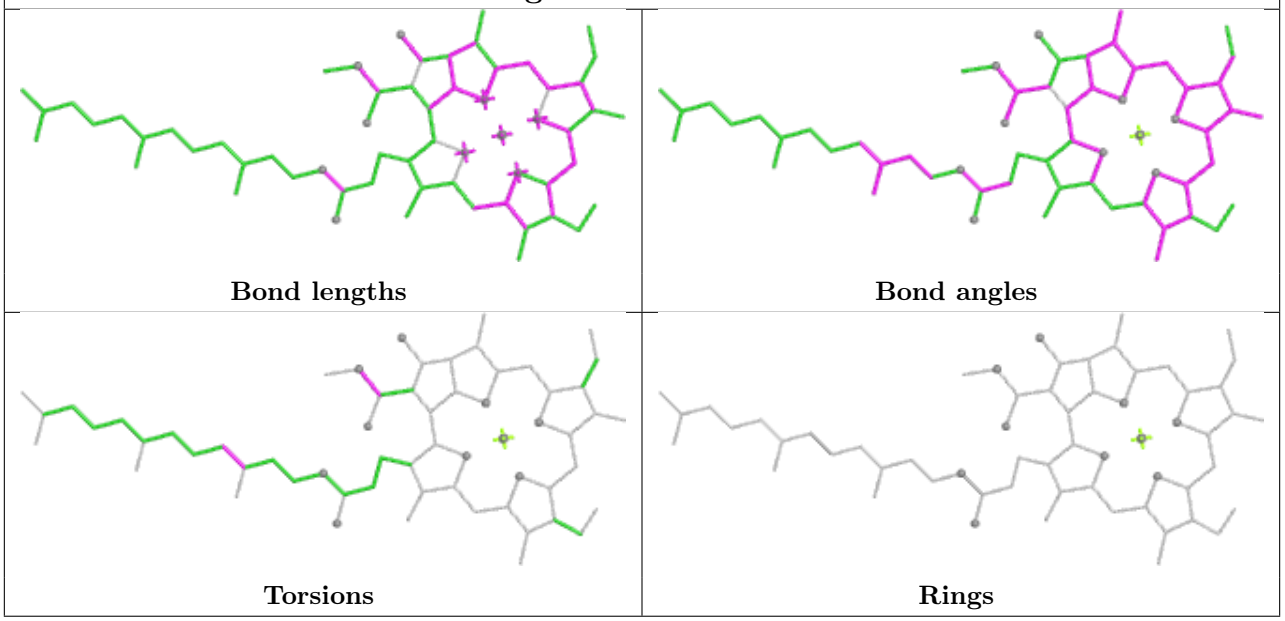


Rings

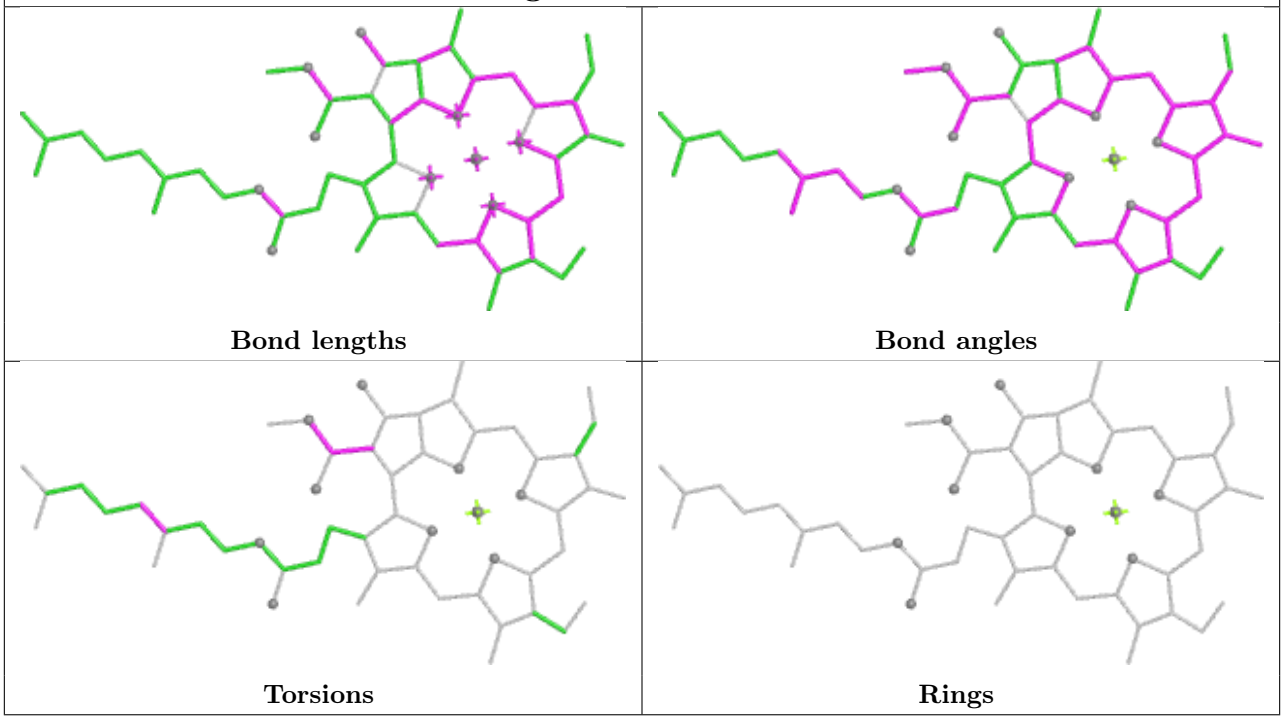
Ligand LUT 8 303



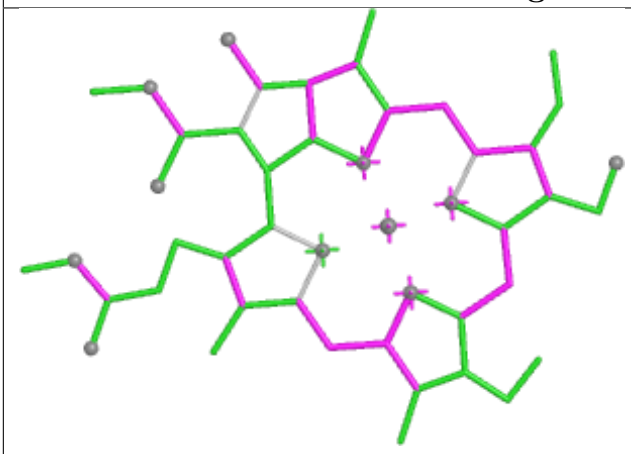
Ligand CHL B 830



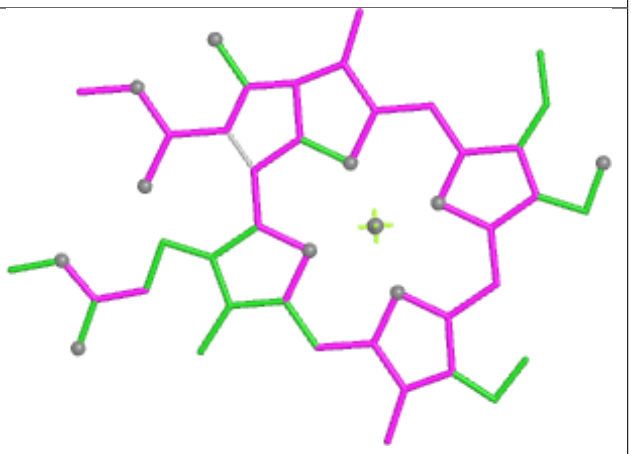
Ligand CHL A 837



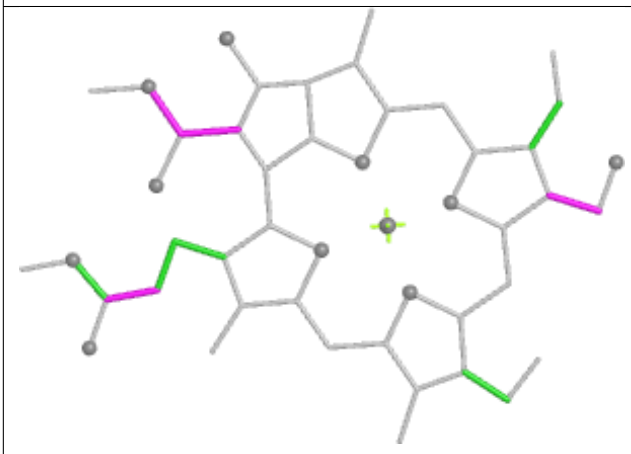
Ligand CHL 5 325



Bond lengths



Bond angles



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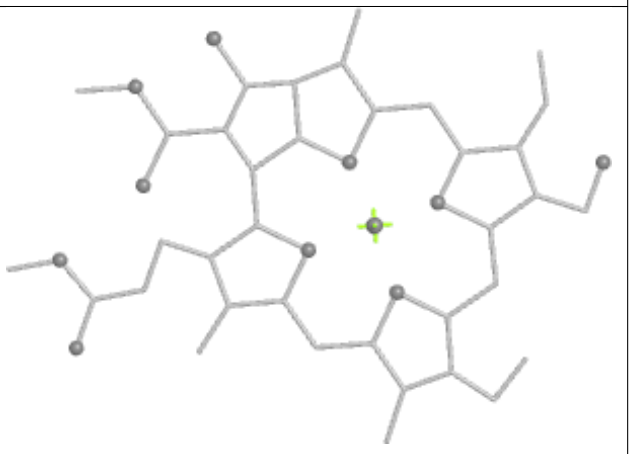
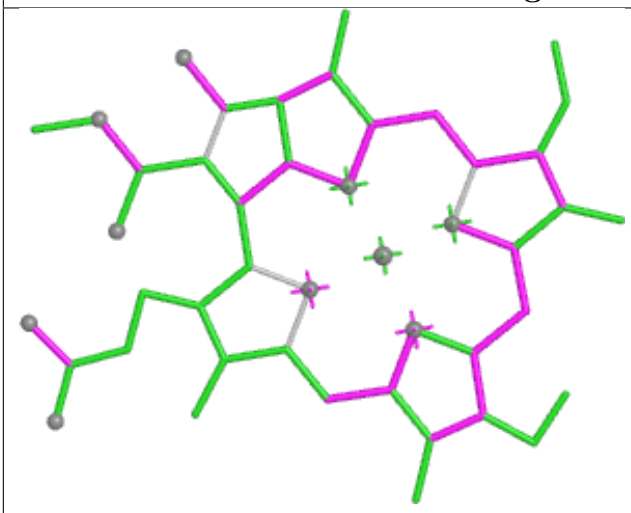


Rings

Ligand CHL B 843



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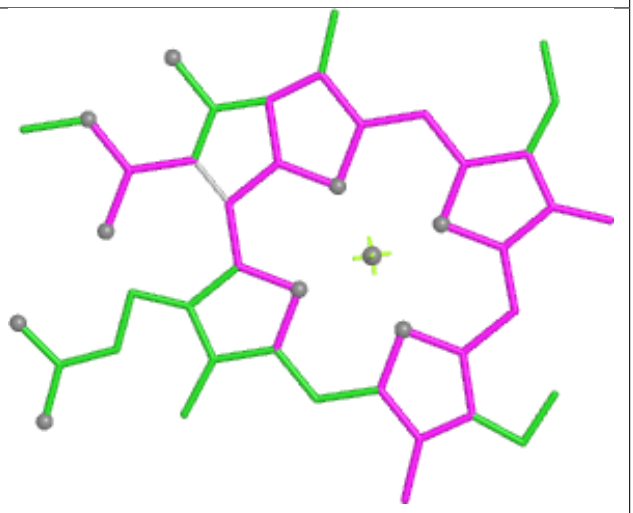
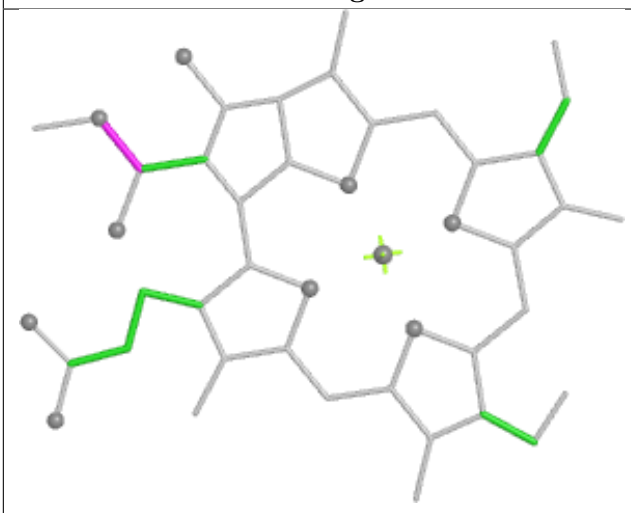


Bond angles



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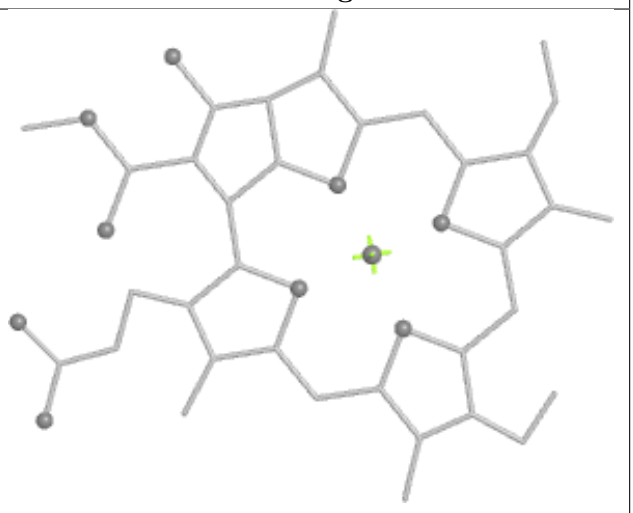
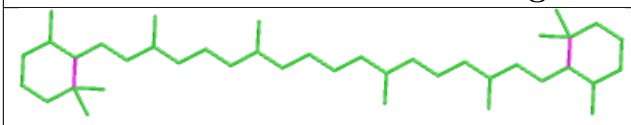


Rings

Ligand BCR I 801



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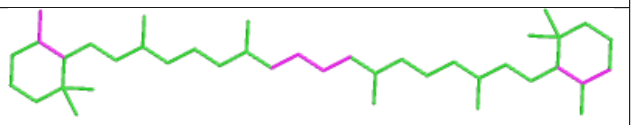
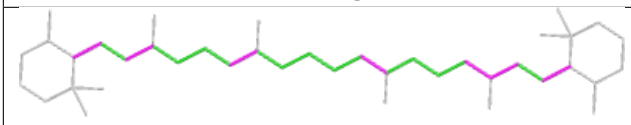


Bond angles



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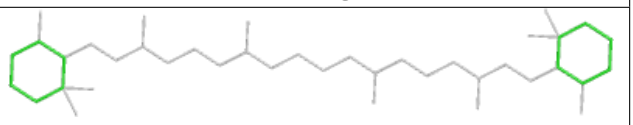
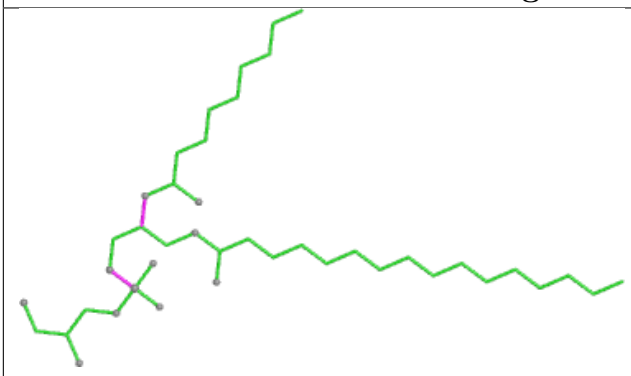
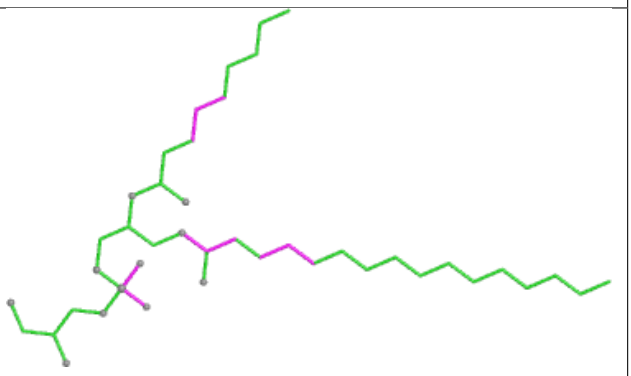


Rings

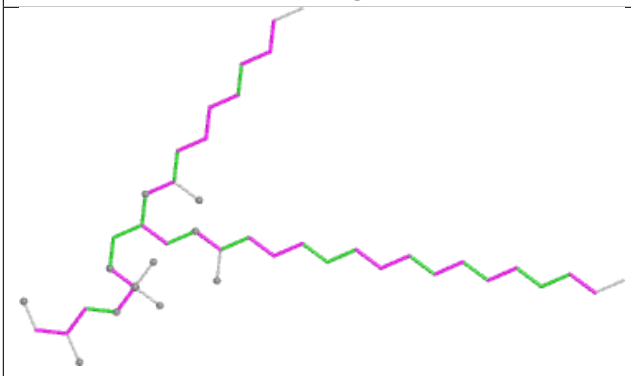
Ligand LHG A 811



Bond lengths



Bond angles



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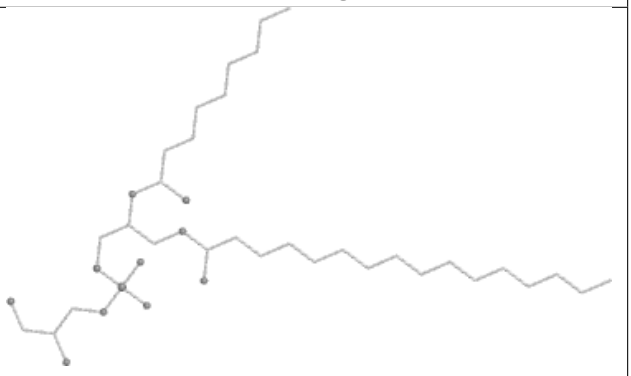
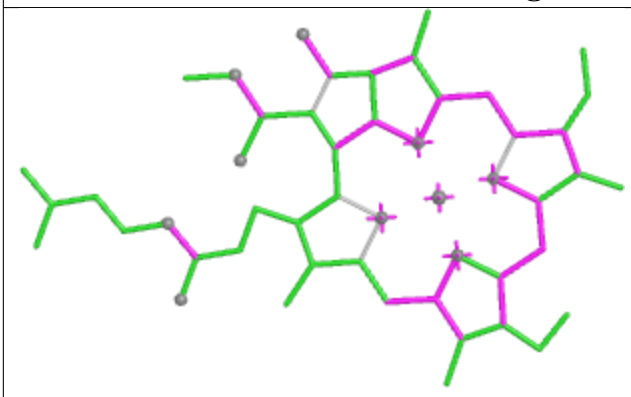


Rings

Ligand CHL F 309



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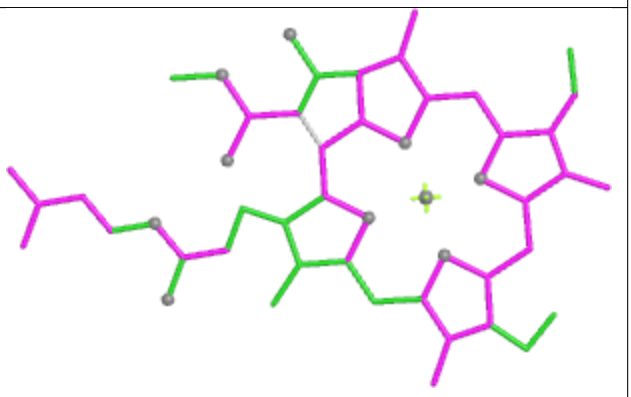
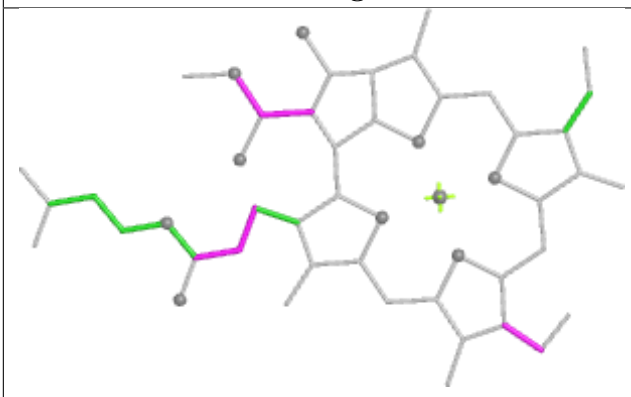


Bond angles



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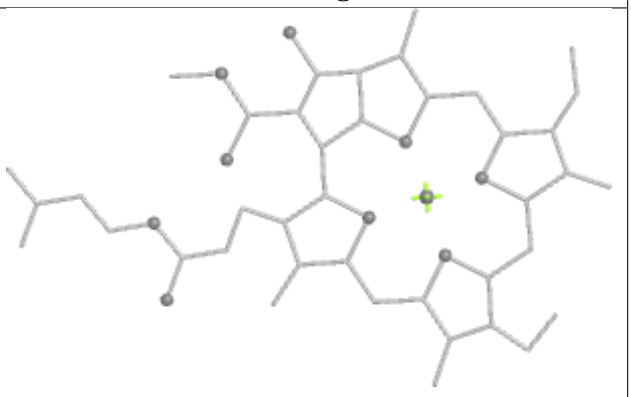
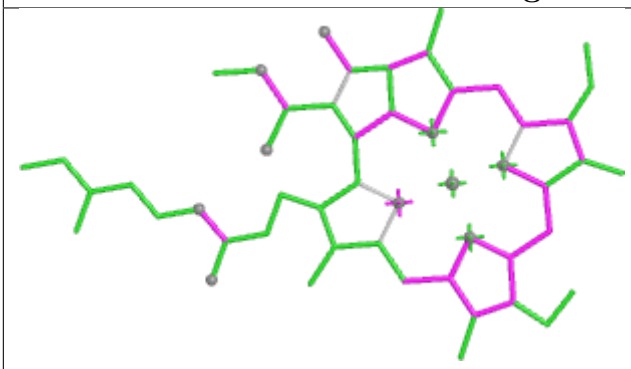
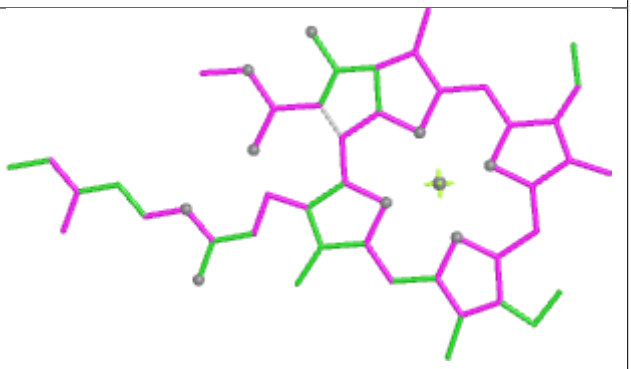
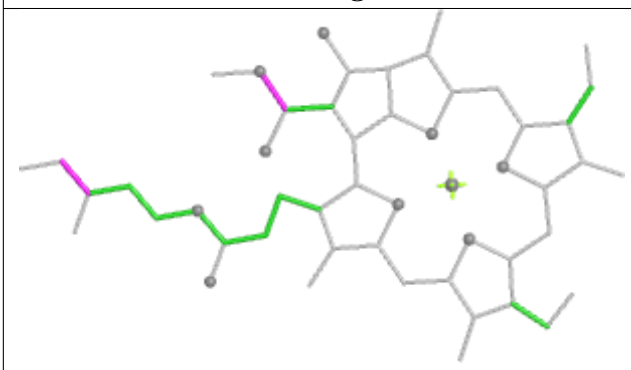
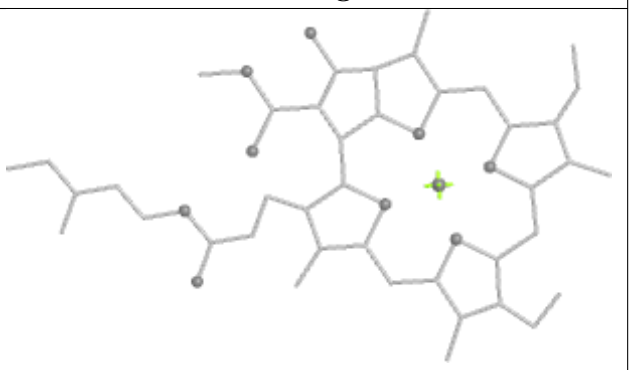


Rings

Ligand CHL A 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

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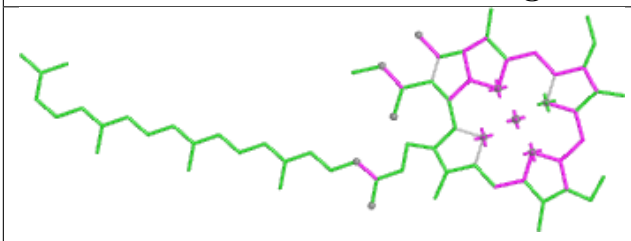
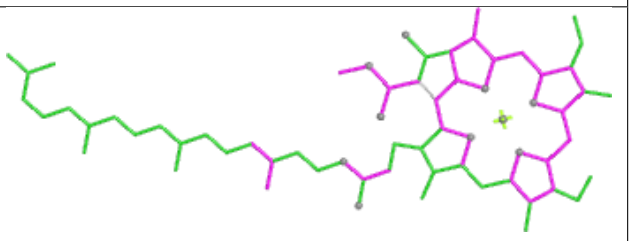
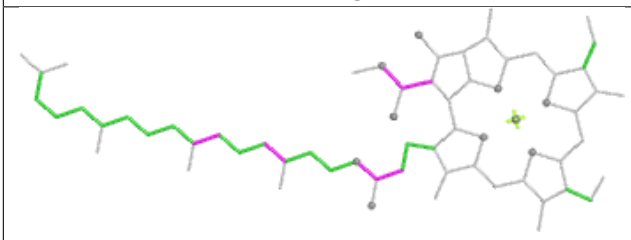
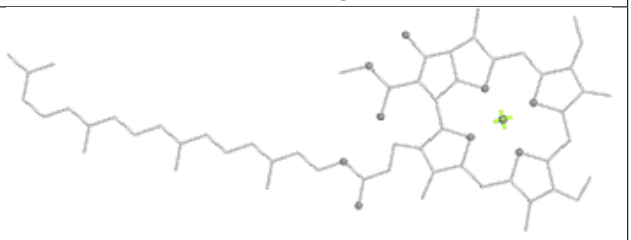
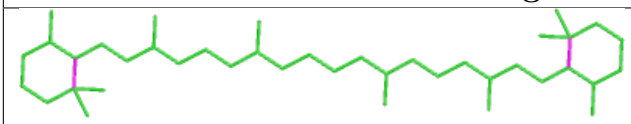
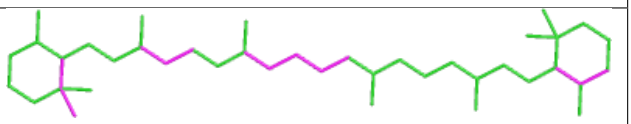
	
Bond lengths	Bond angles
	
Torsions	Rings

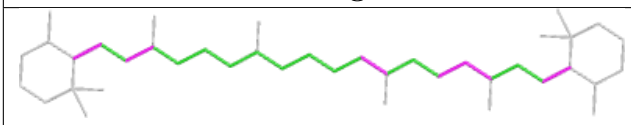
Ligand BCR B 806



Bond lengths



Bond angles



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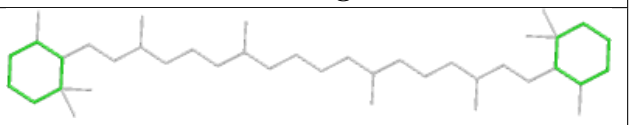
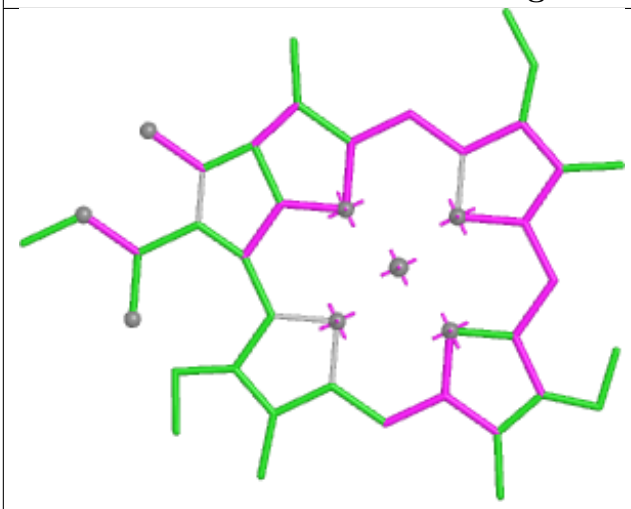


Rings

Ligand CHL 4 318



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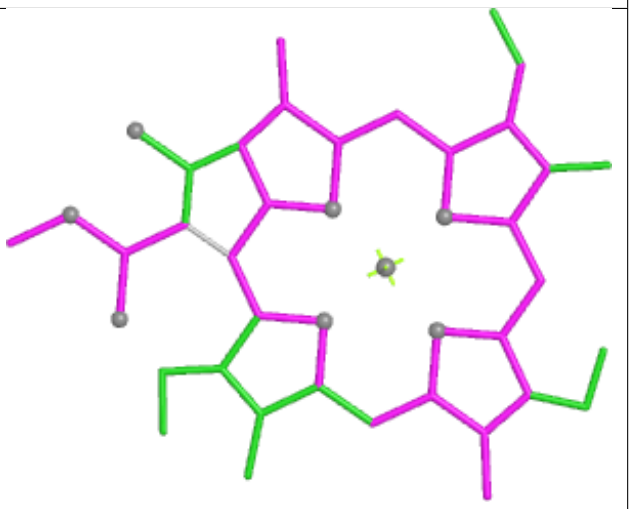
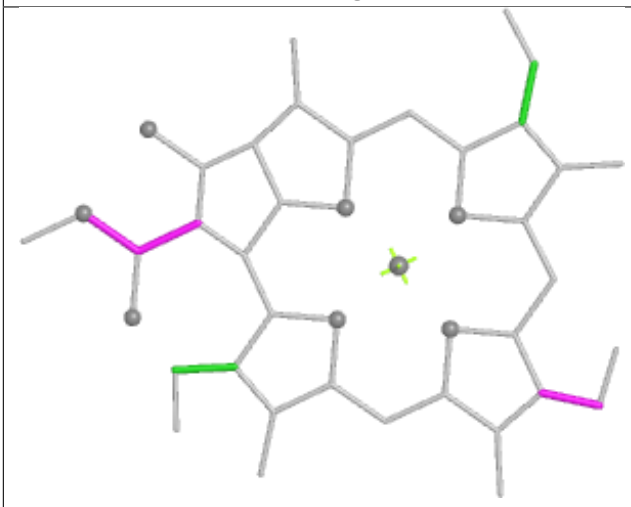


Bond angles

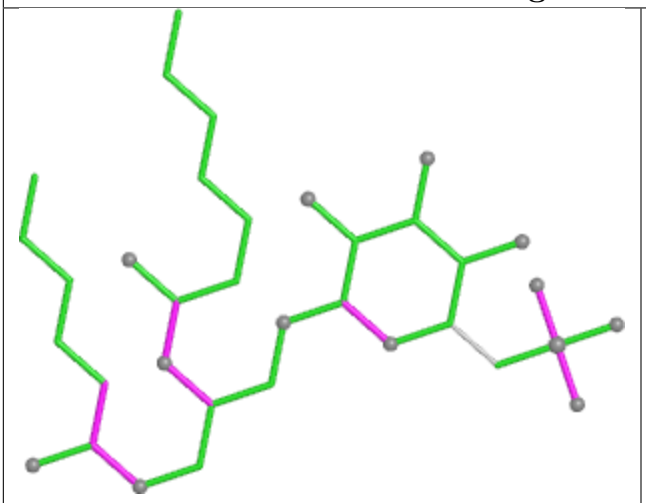


Torsions



Rings

Ligand SQD 8 301



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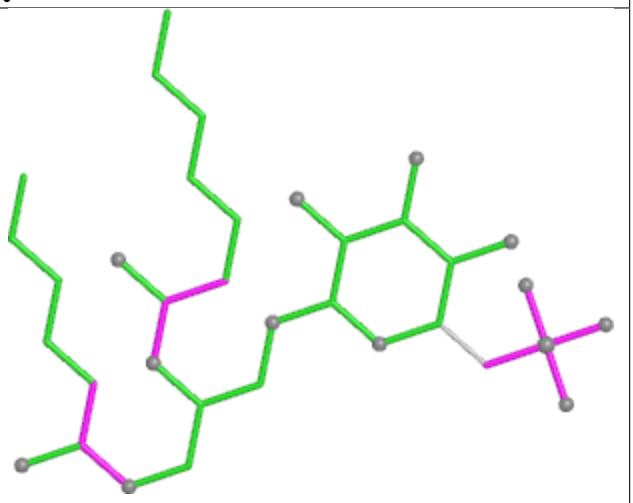
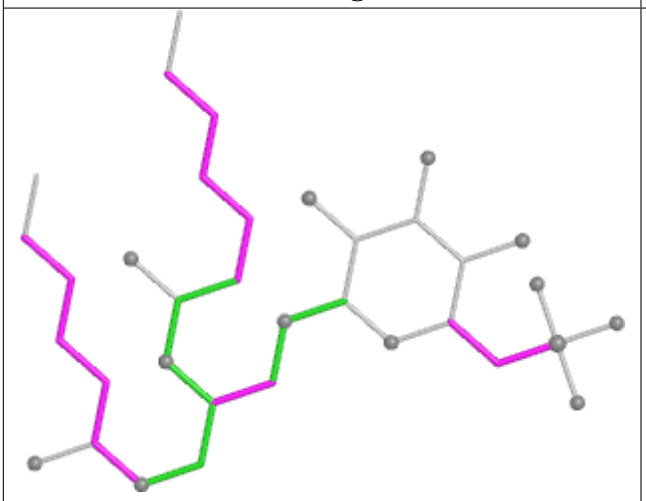


Bond angles



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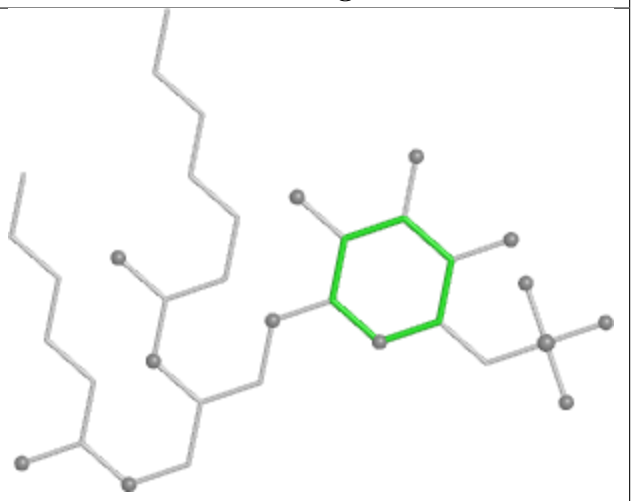
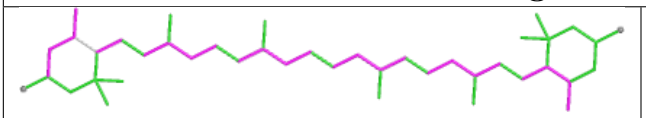


Rings

Ligand LUT 5 302



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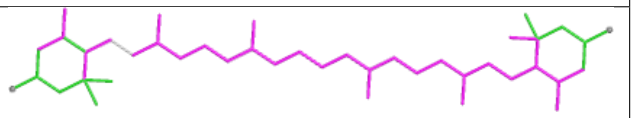
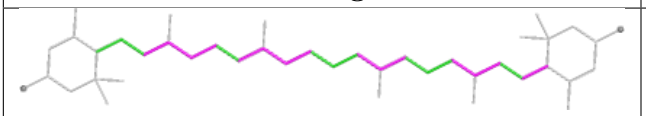


Bond angles



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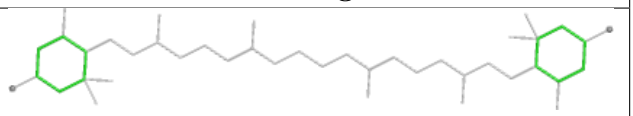
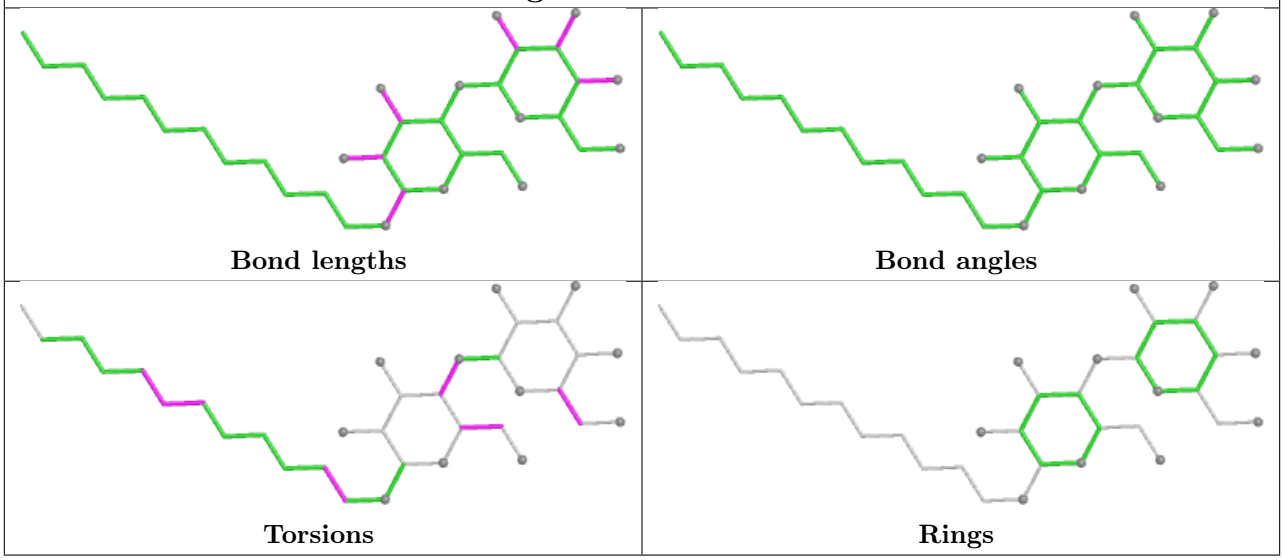
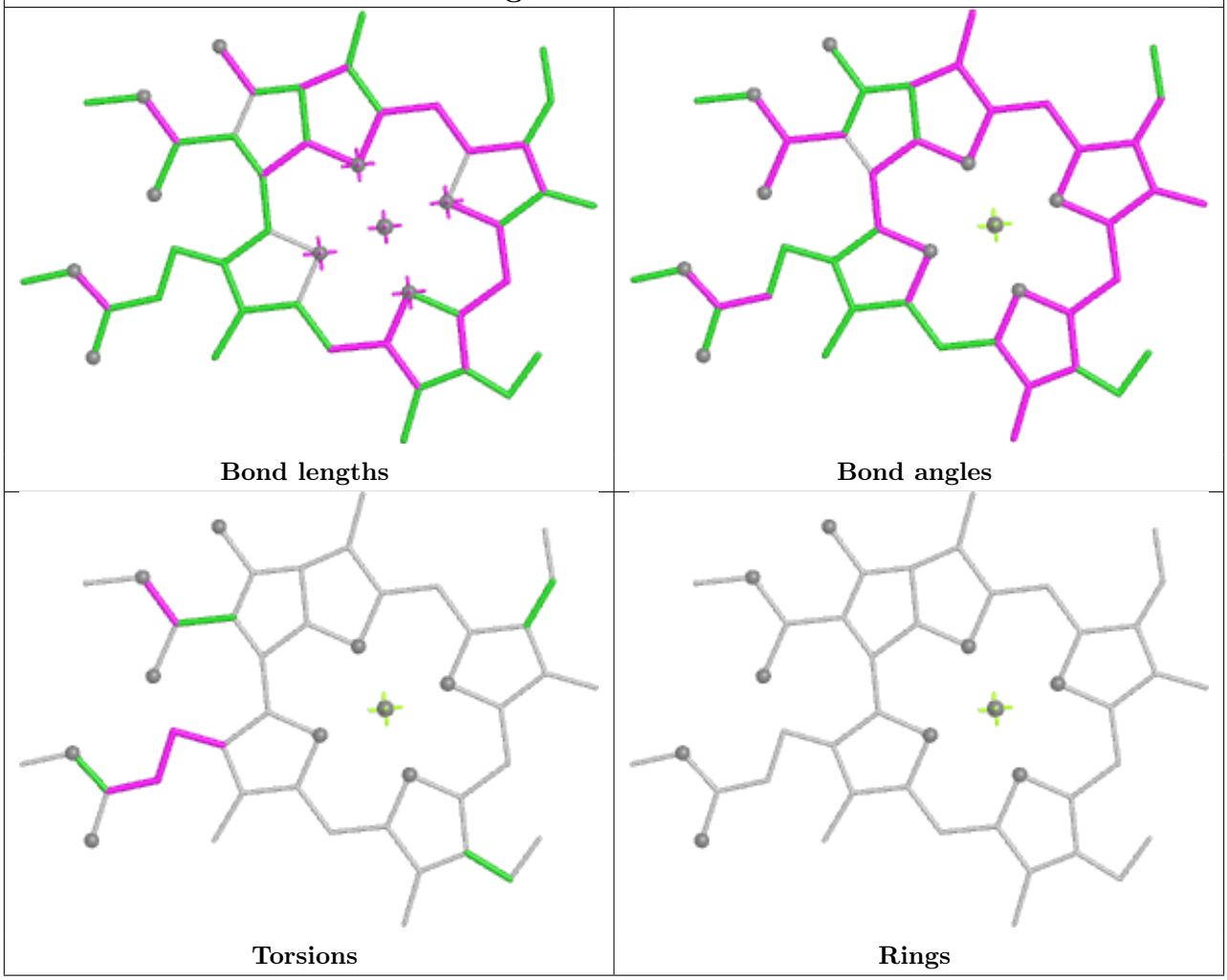


Rings

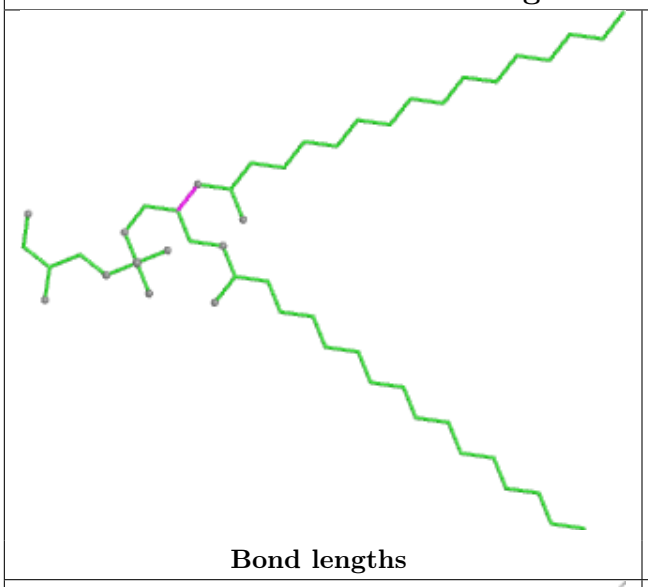
Ligand LMT 7 308



Ligand CHL 6 305



Ligand LHG A 812



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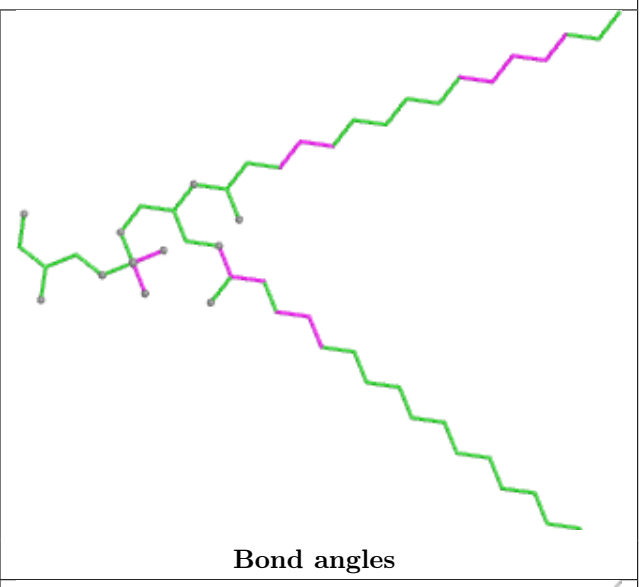
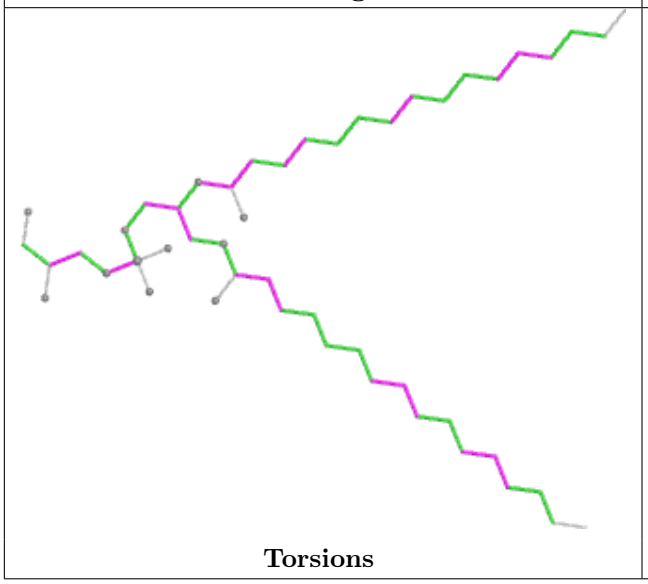


Bond angles



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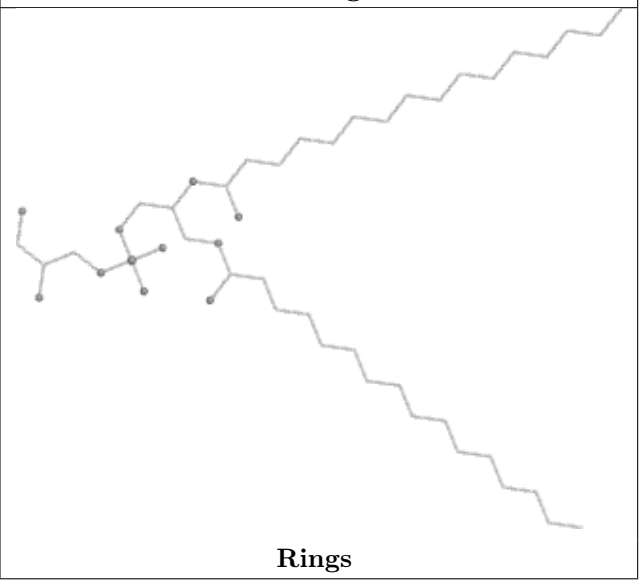
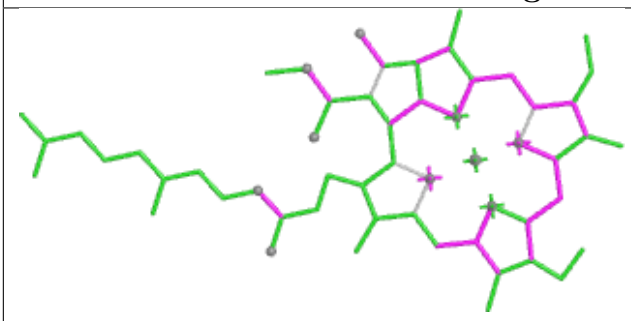


Rings

Ligand CHL A 829



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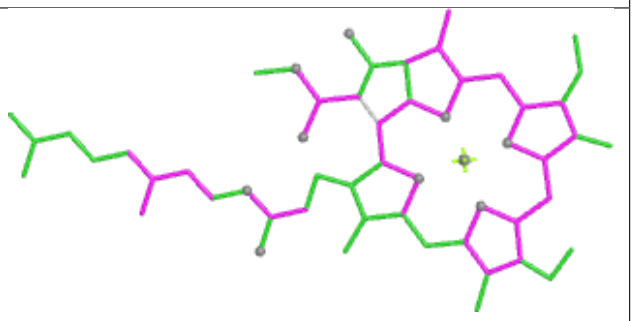
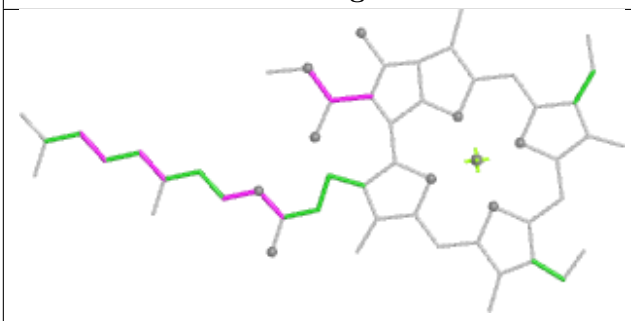


Bond angles



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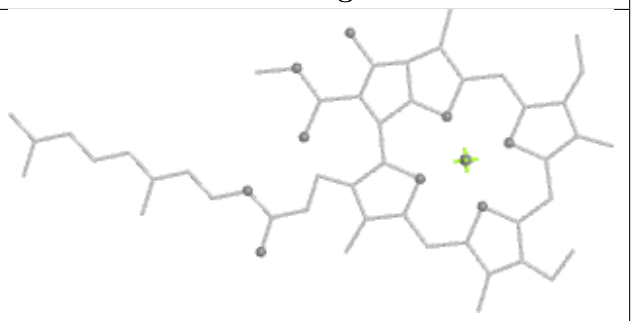
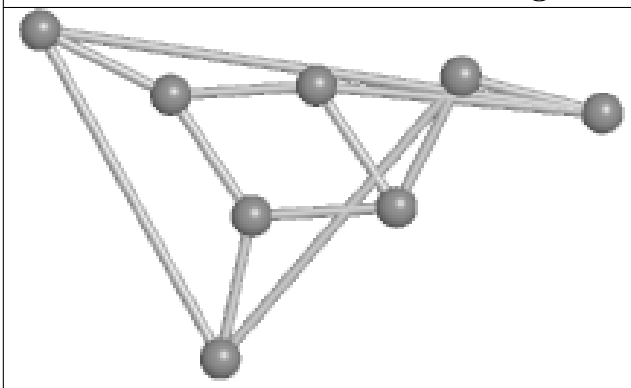


Rings

Ligand SF4 A 802



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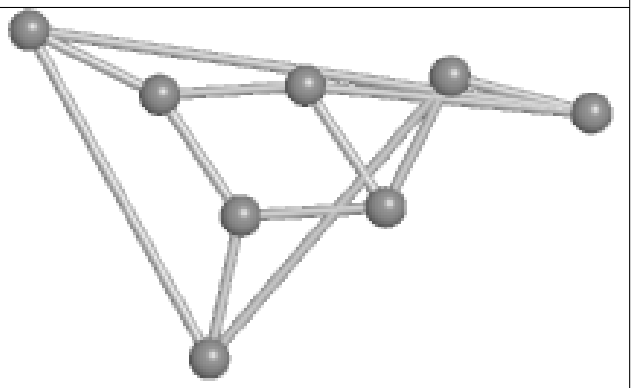
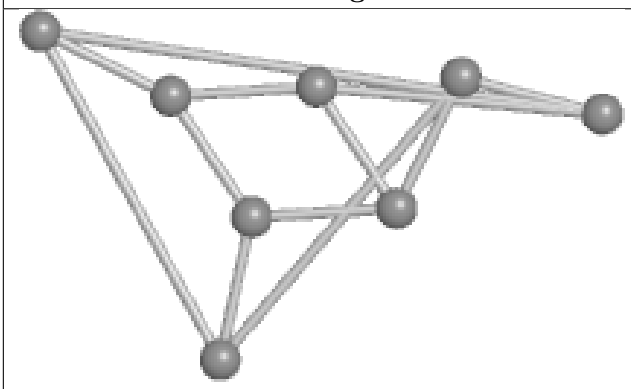


Bond angles



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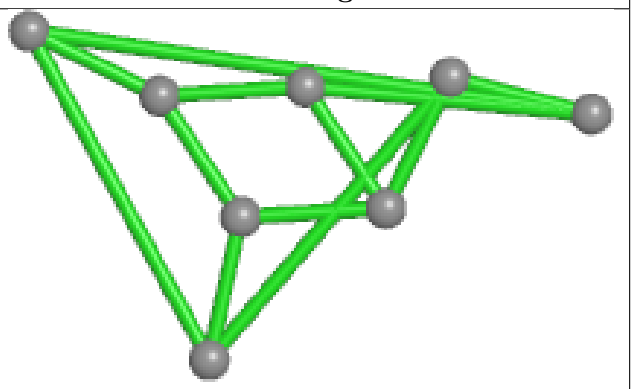
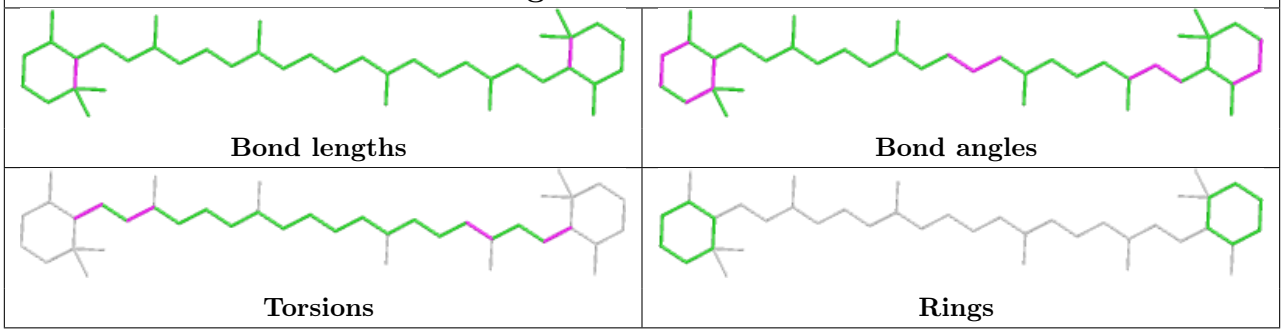


Rings

Ligand BCR J 102



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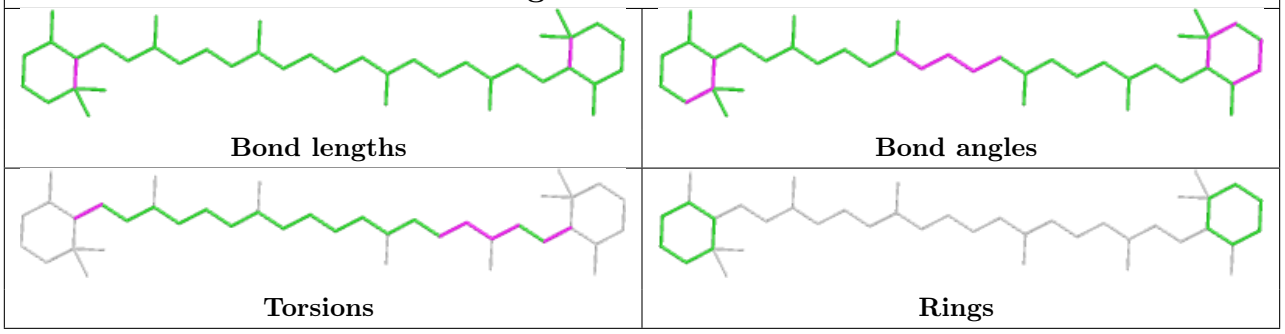
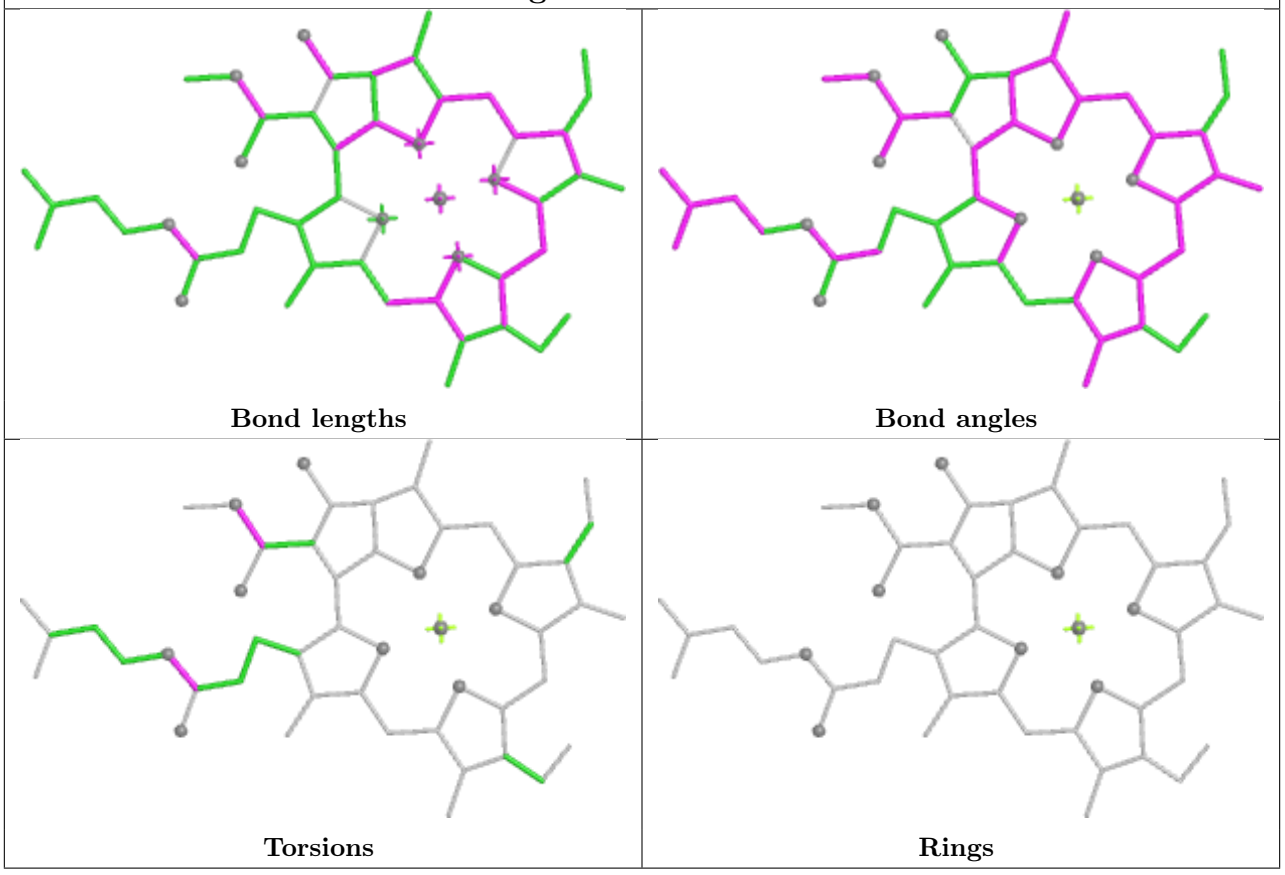
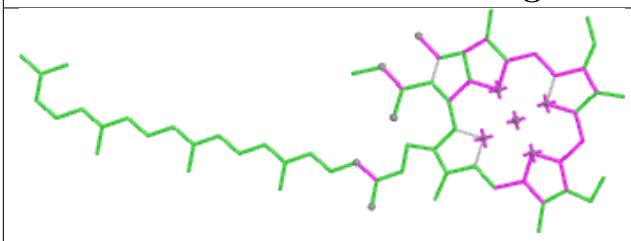


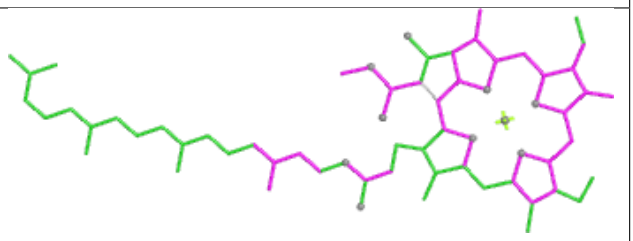
Ligand CHL a 312



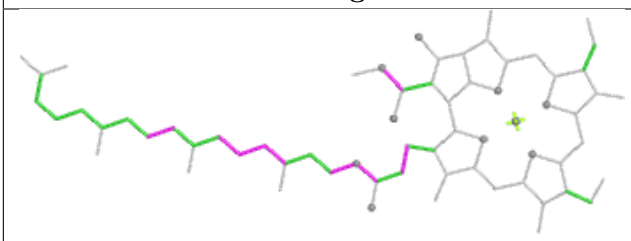
Ligand CHL A 825



Bond lengths



Bond angles



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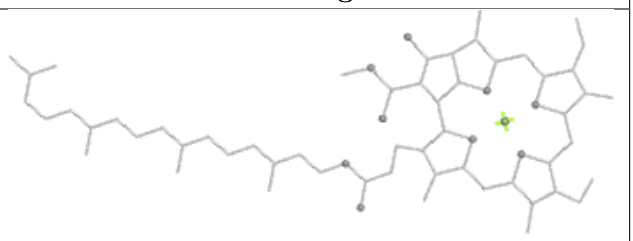
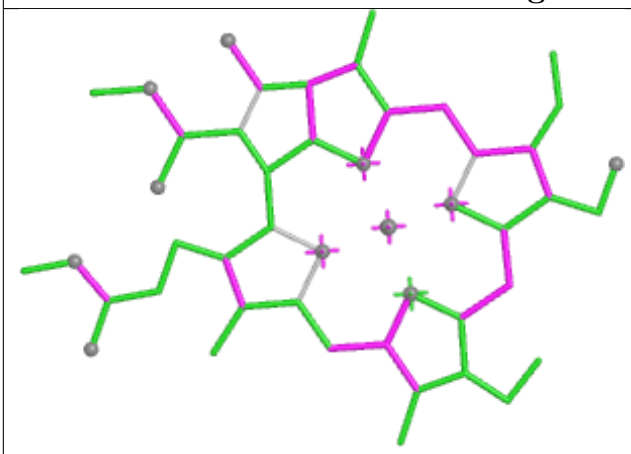


Rings

Ligand CHL 6 317



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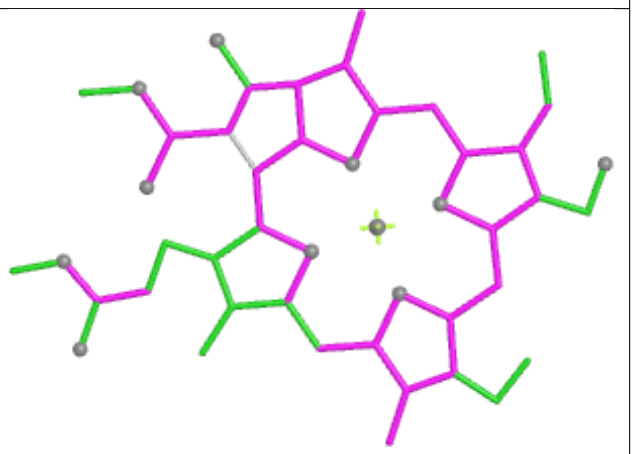
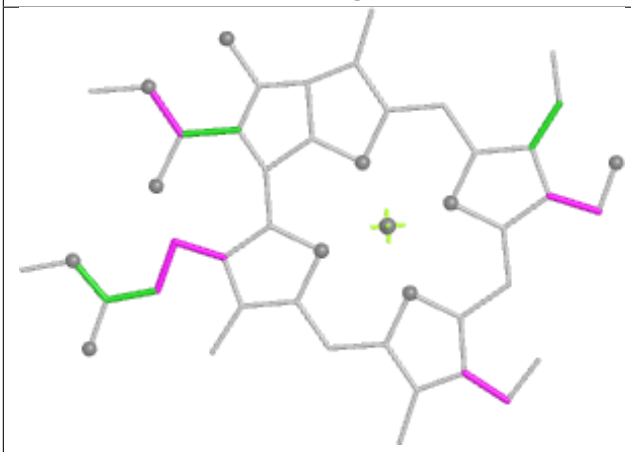


Bond angles



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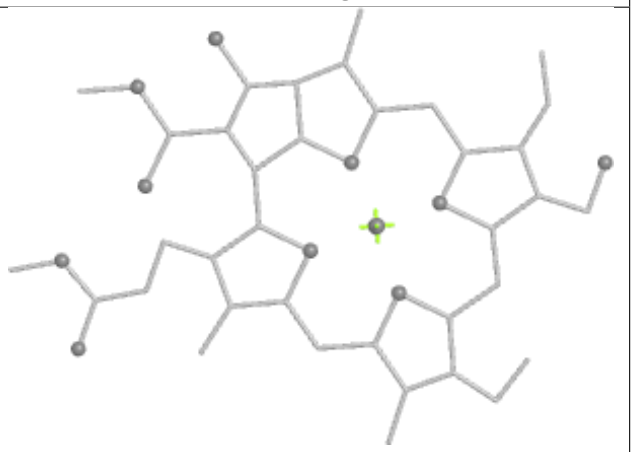
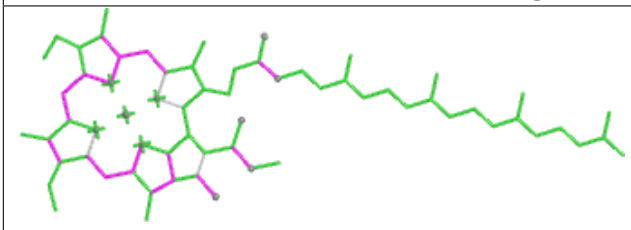


Rings

Ligand CL0 A 815



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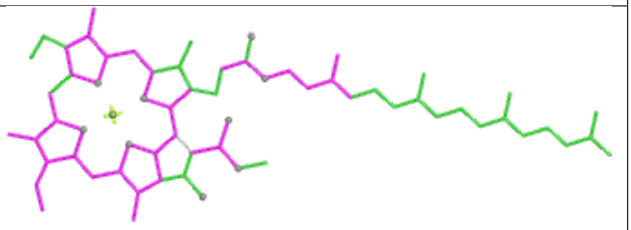
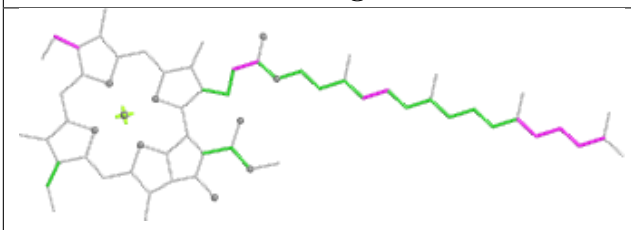


Bond angles



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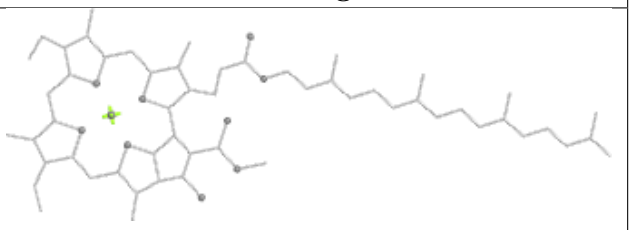
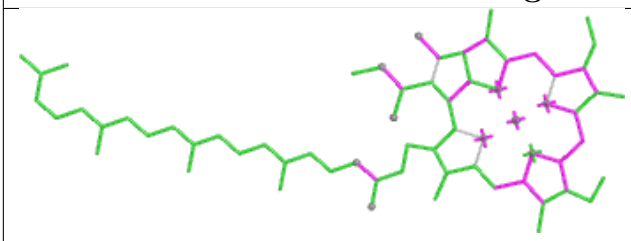
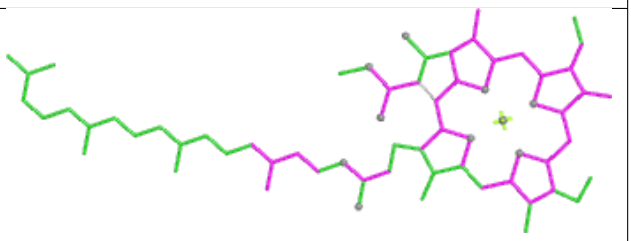


Rings

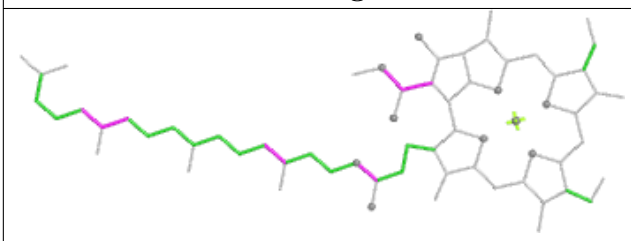
Ligand CHL B 844



Bond lengths



Bond angles



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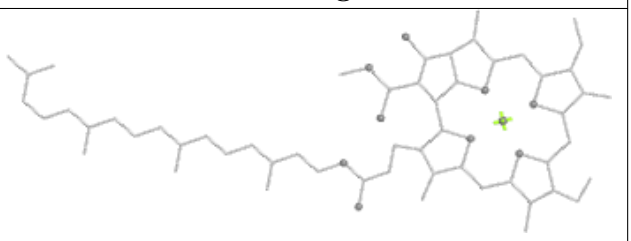
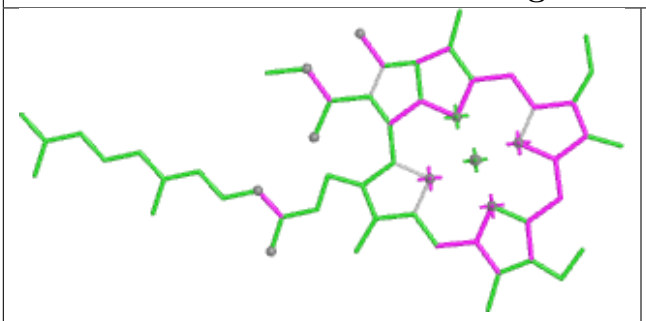
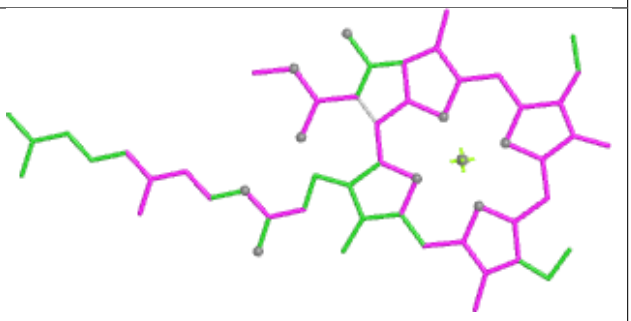


Rings

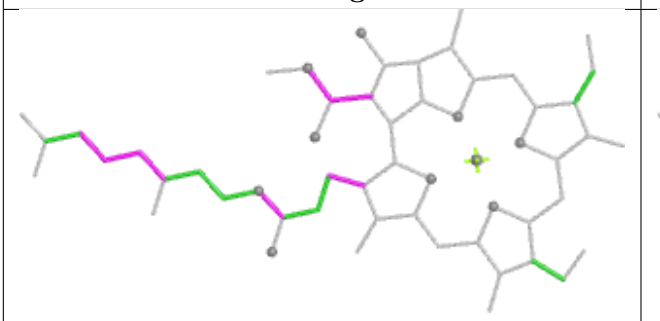
Ligand CHL a 313



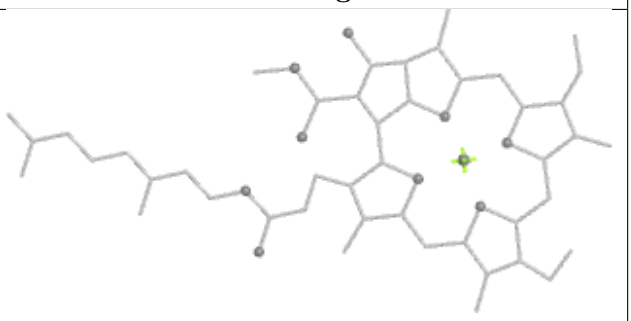
Bond lengths



Bond angles

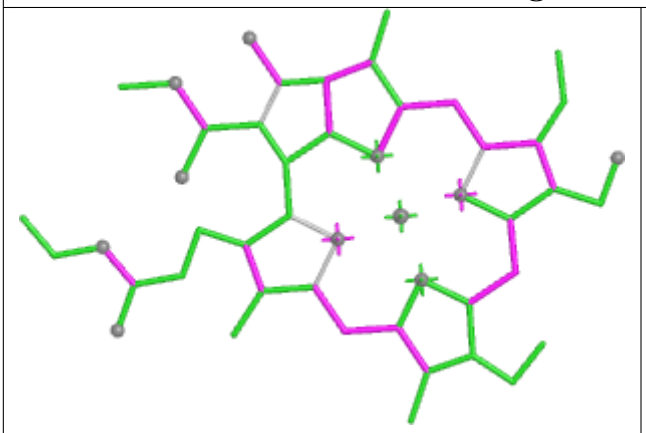


Torsions



Rings

Ligand CHL 4 312



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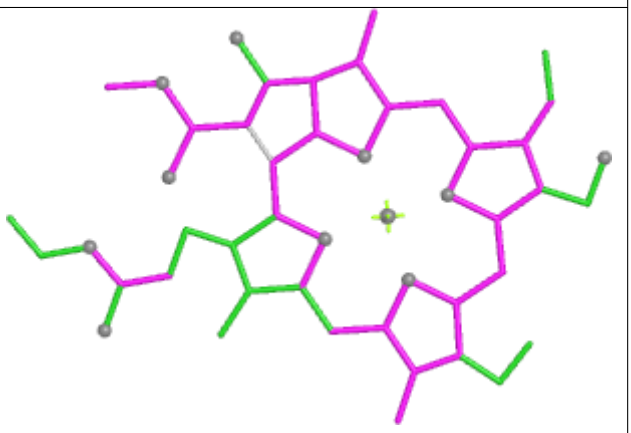
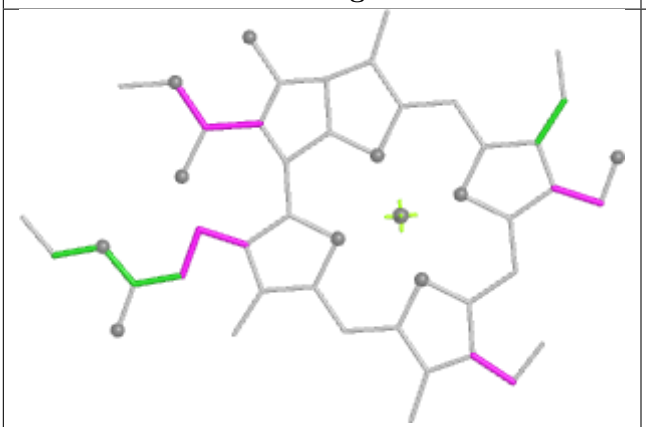


Bond angles

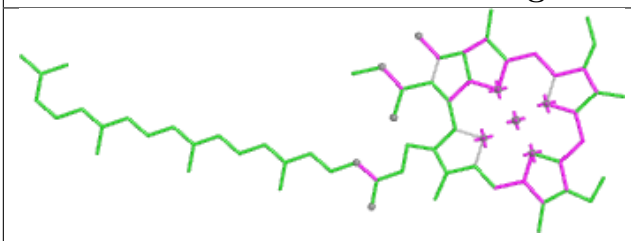


Torsions



Rings

Ligand CHL 7 313



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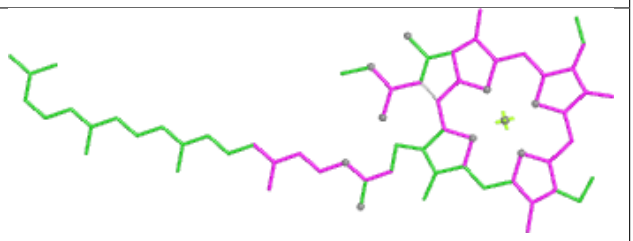

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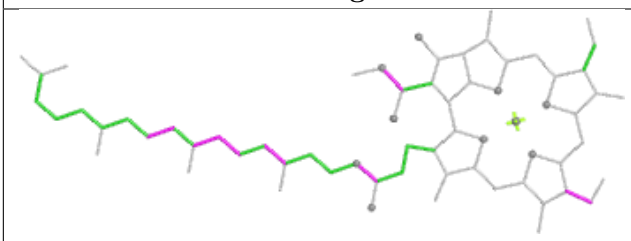

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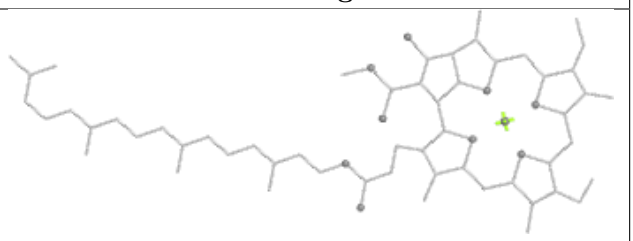
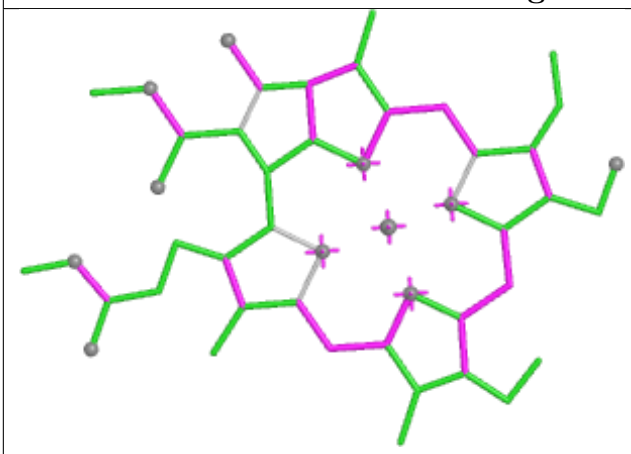


Rings

Ligand CHL 7 321



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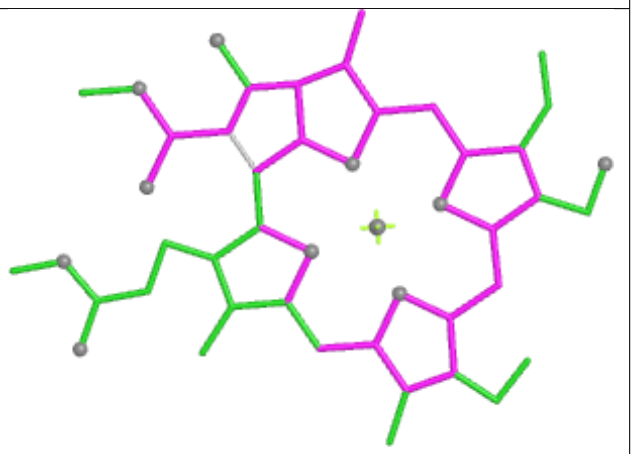

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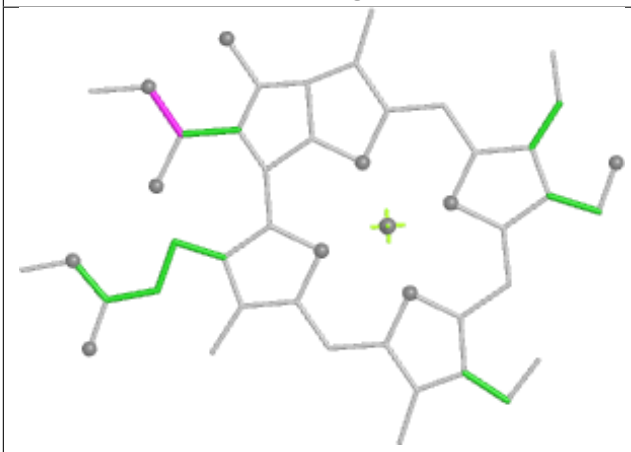

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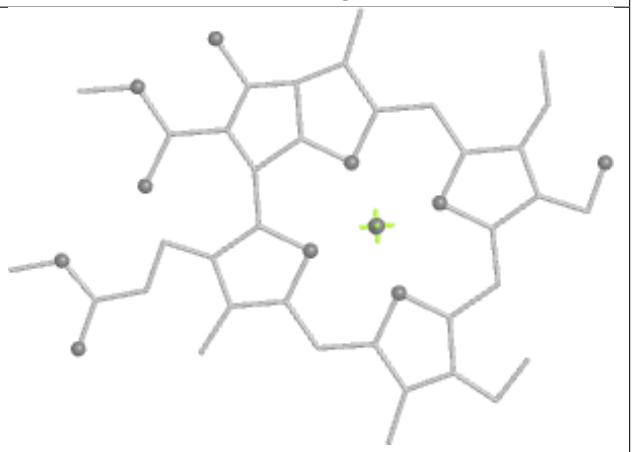

Rings

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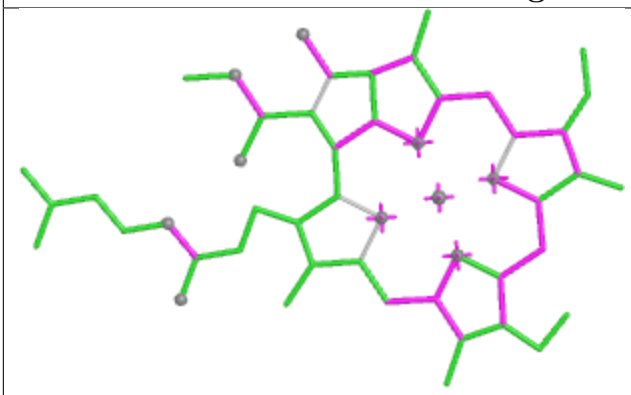

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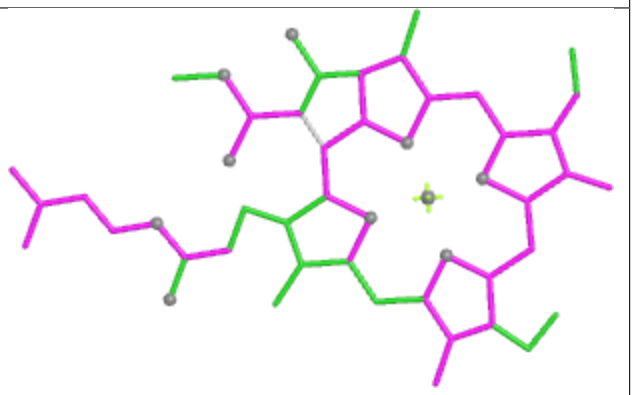

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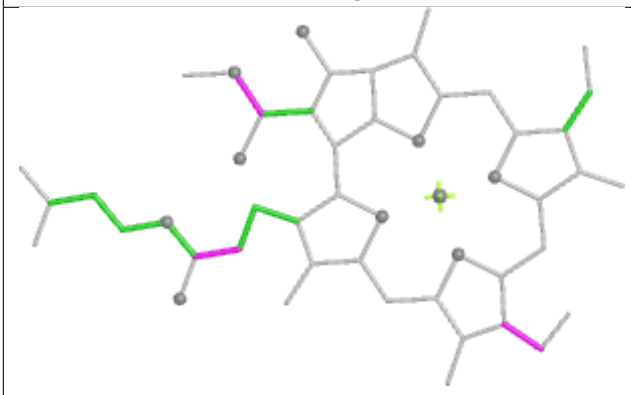

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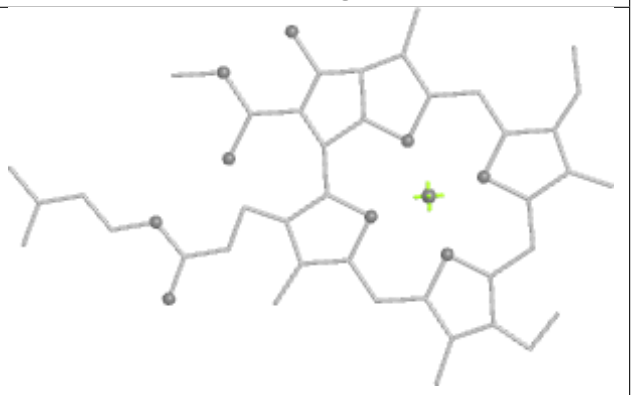
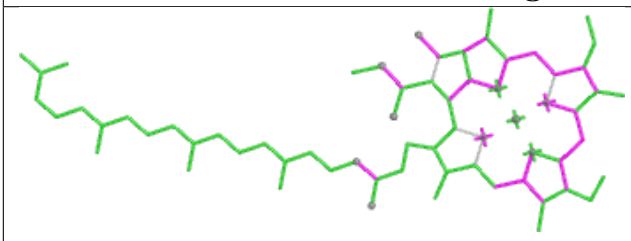


Rings

Ligand CHL B 822



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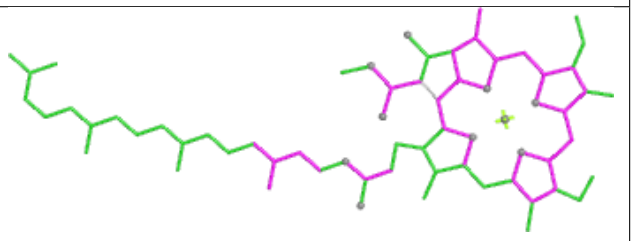
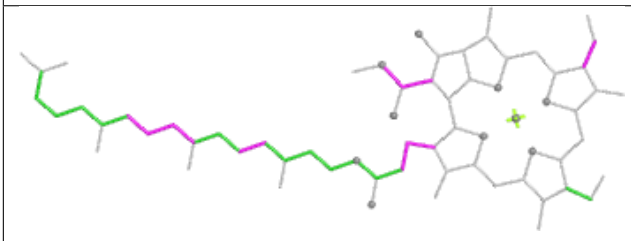


Bond angles



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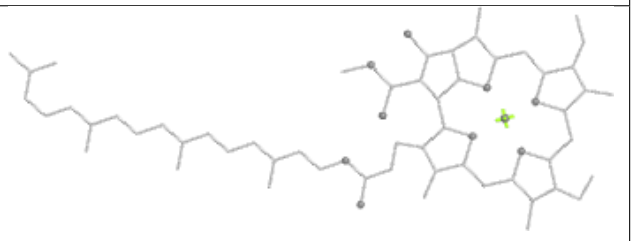
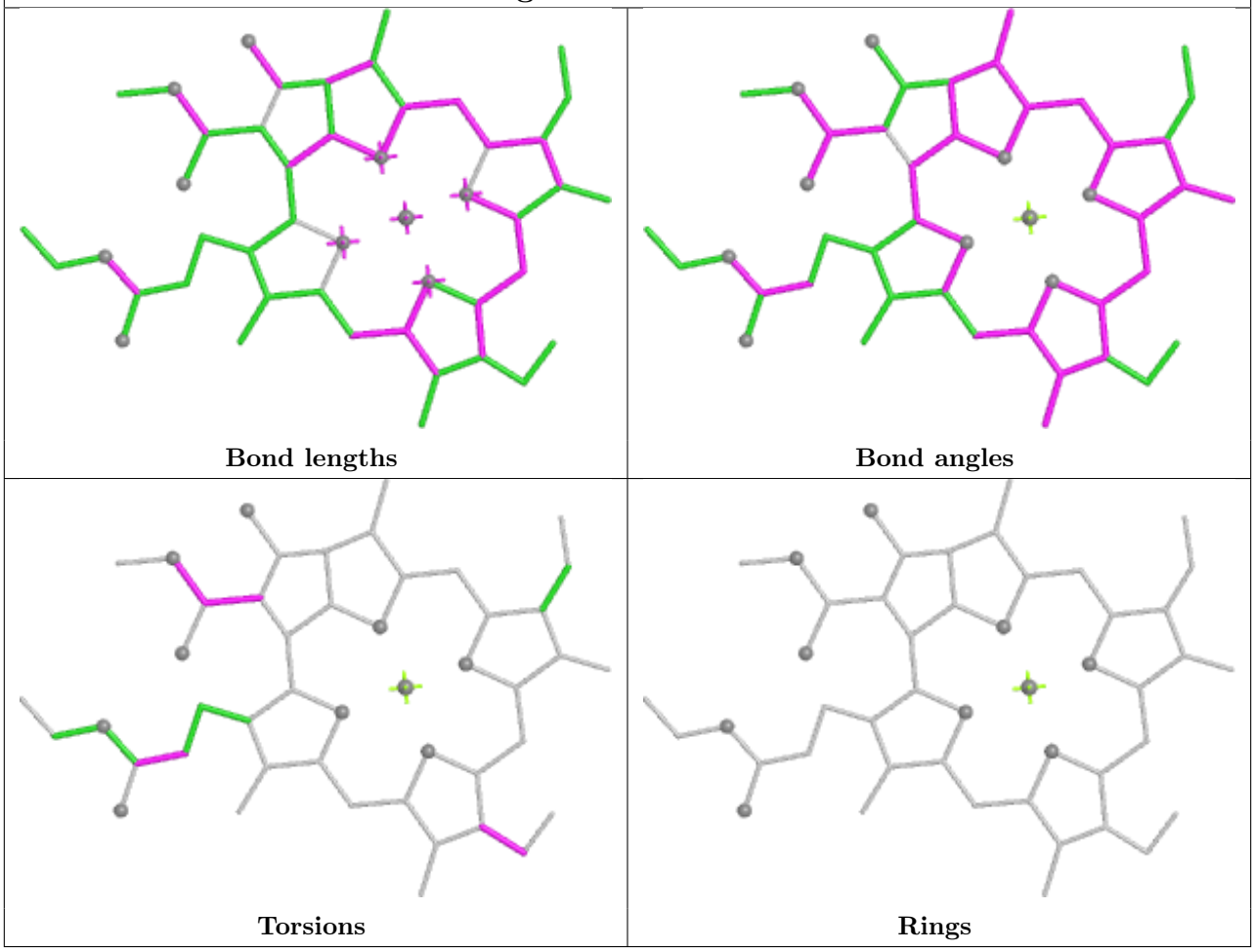


Rings

Ligand CHL 6 309



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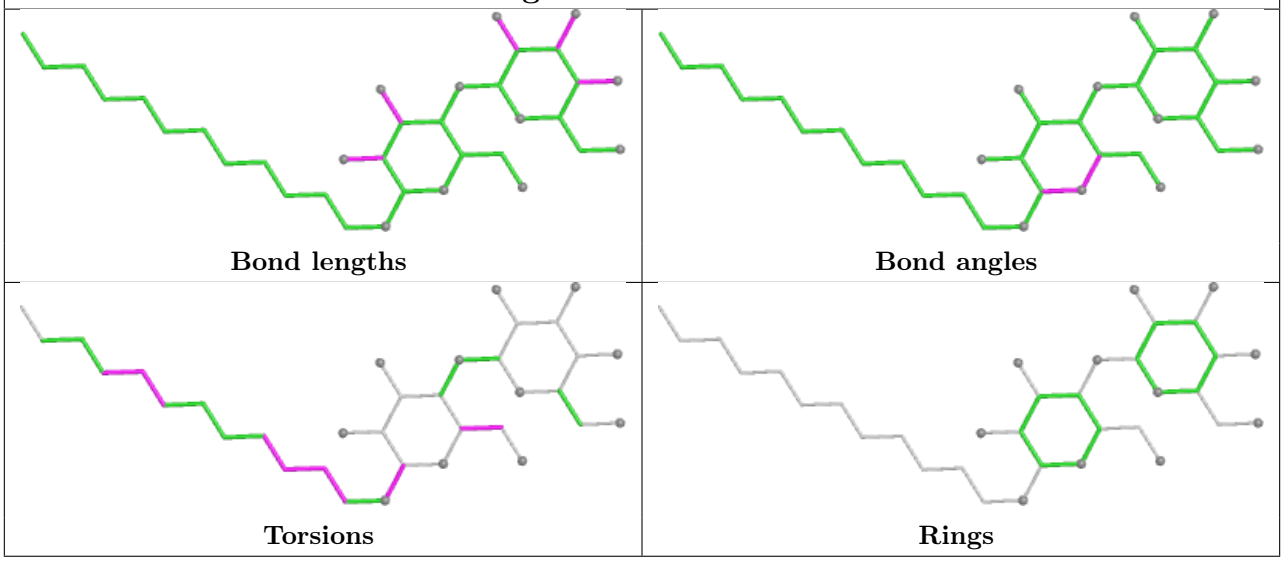

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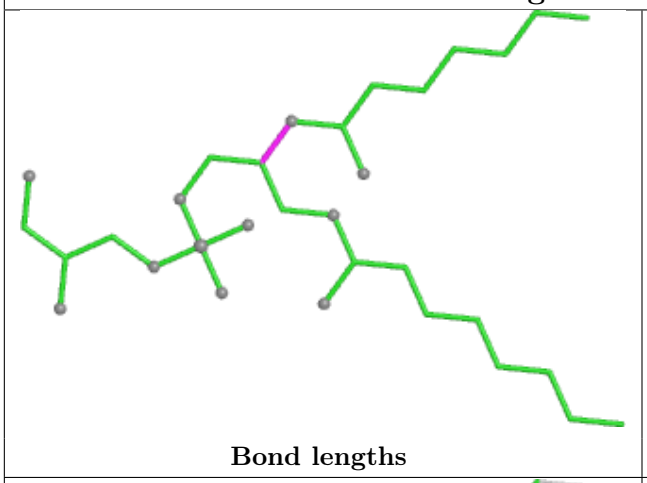

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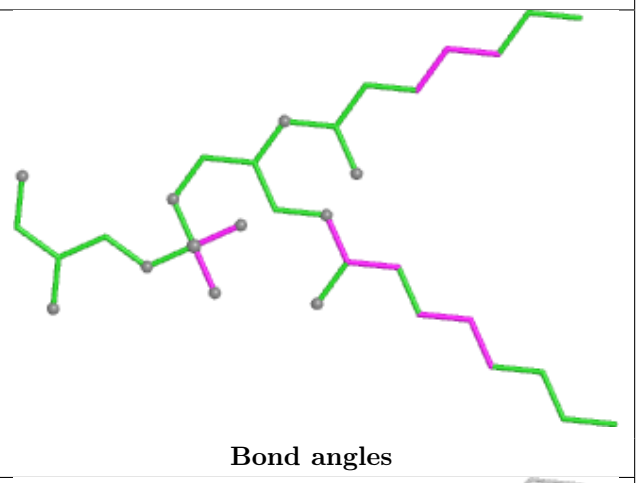

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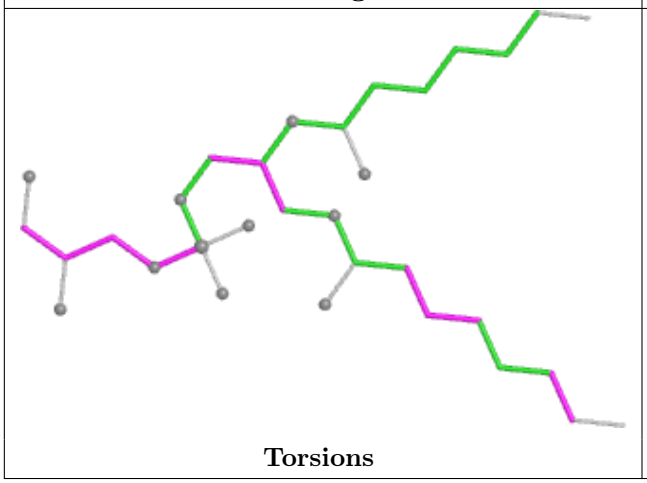

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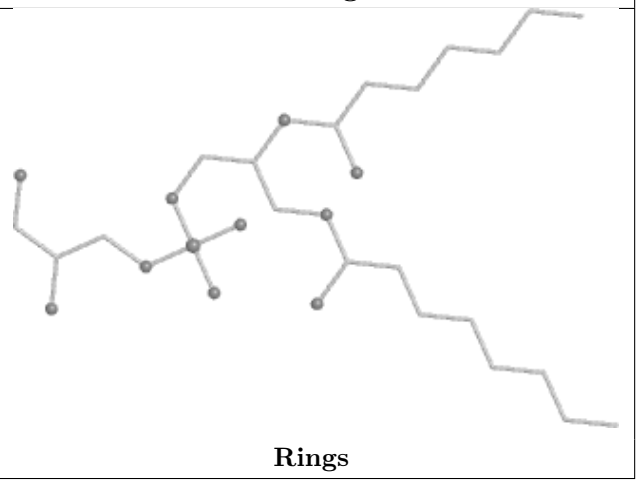

Rings

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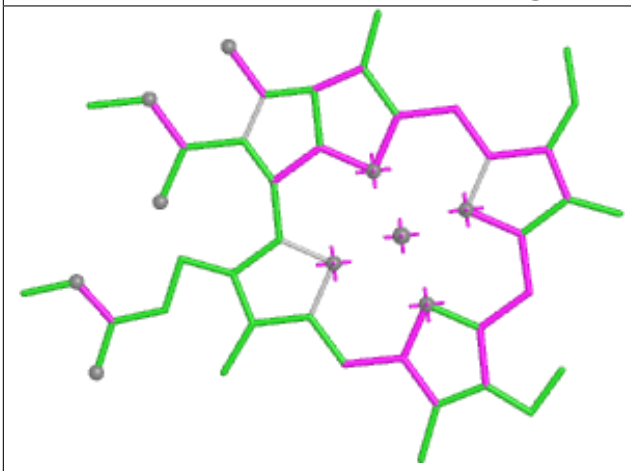

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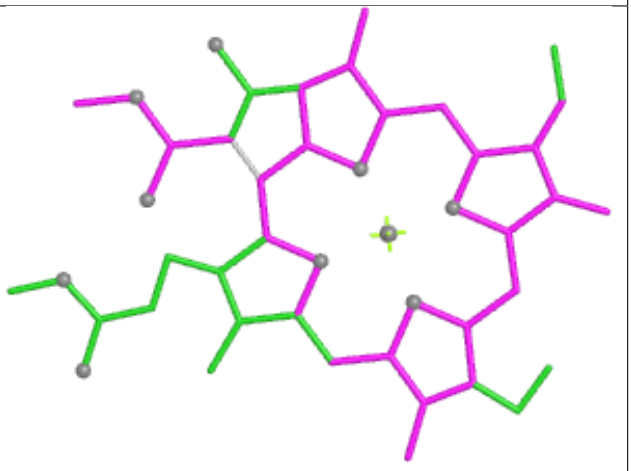
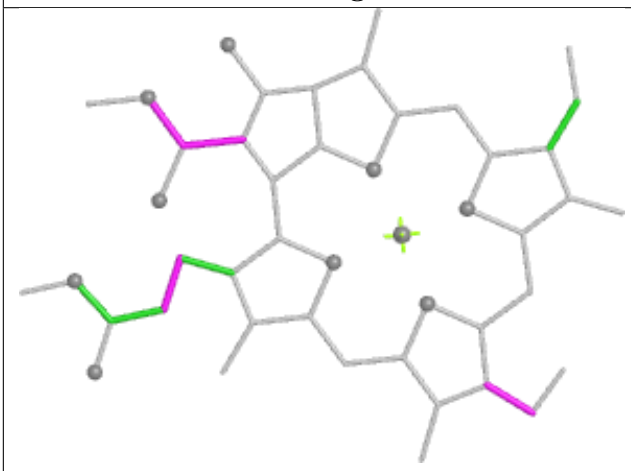


Bond angles



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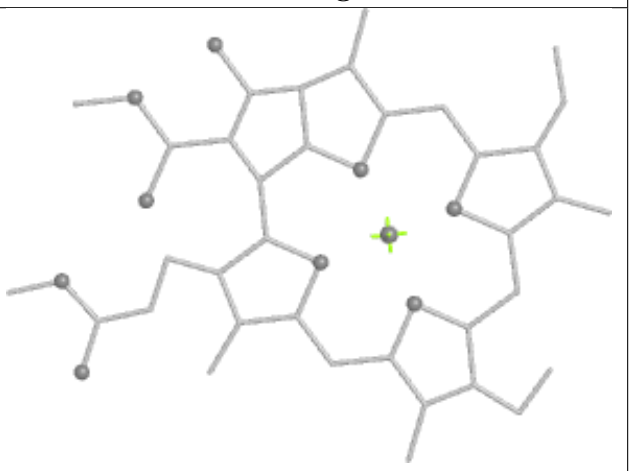
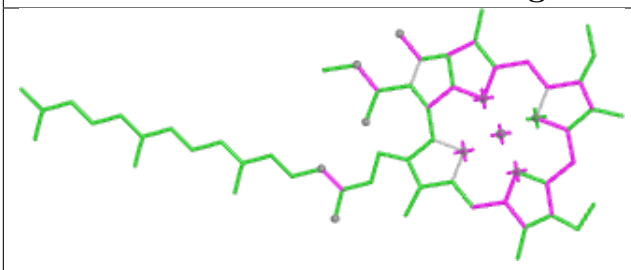


Rings

Ligand CHL a 311



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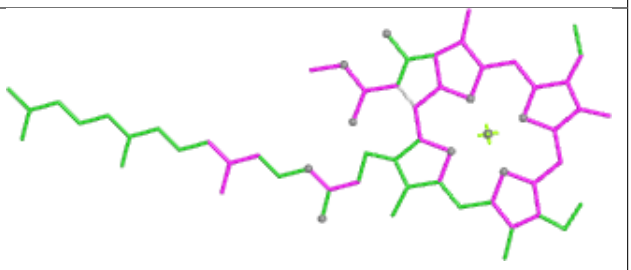
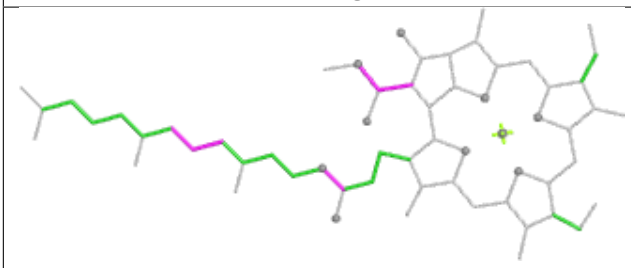


Bond angles



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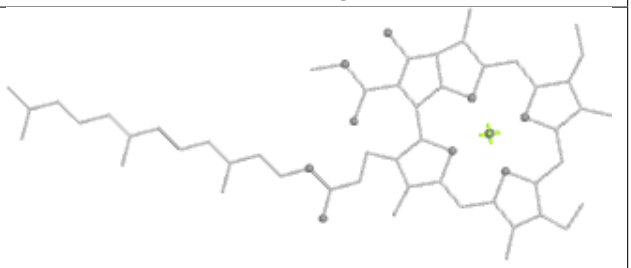
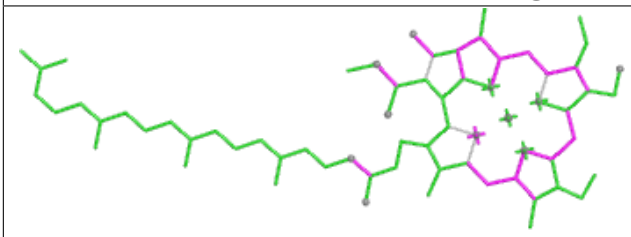
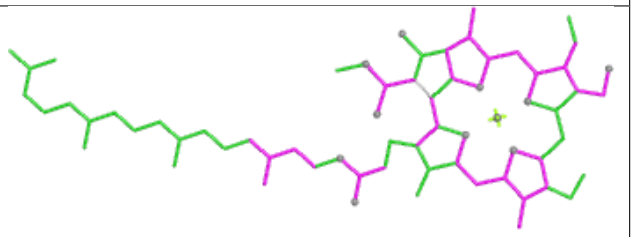
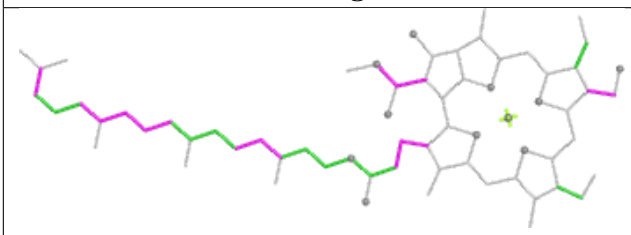
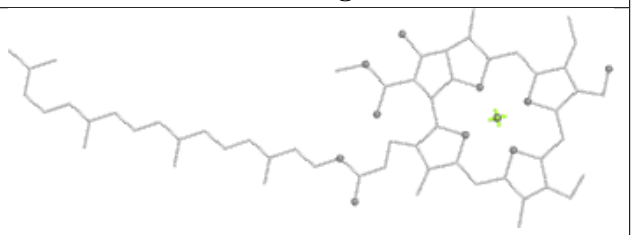


Rings

Ligand CHL 6 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

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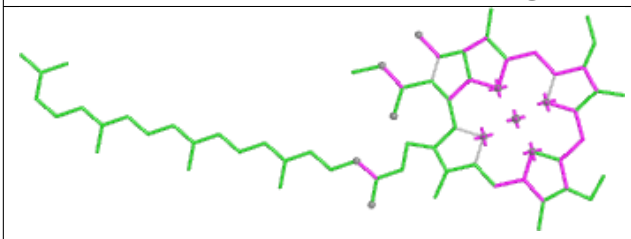
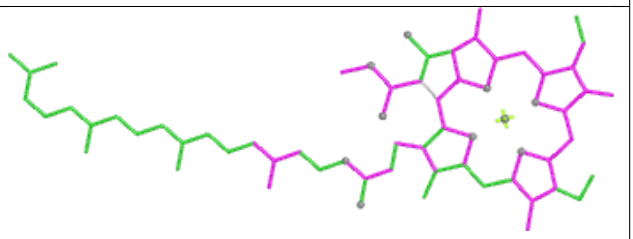
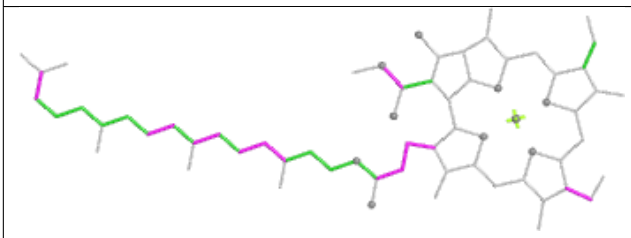
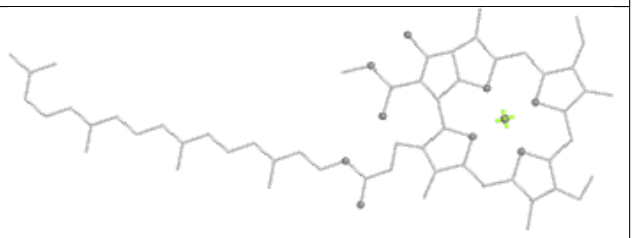
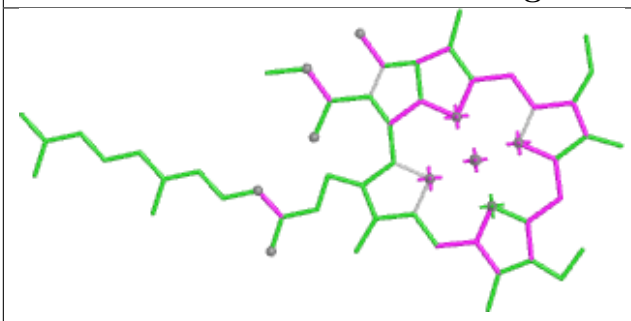
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL B 829



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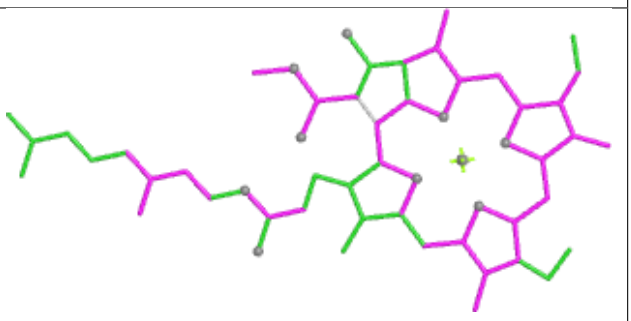
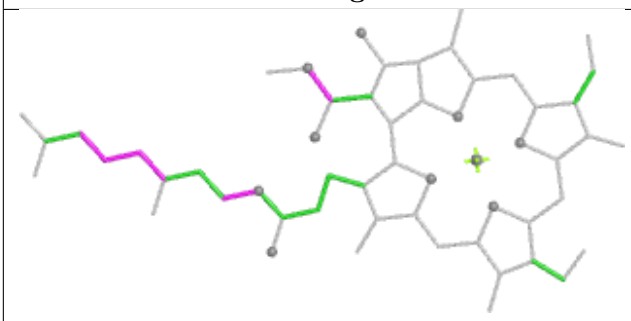
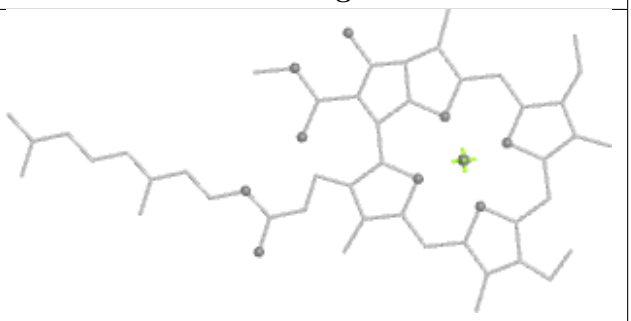


Bond angles

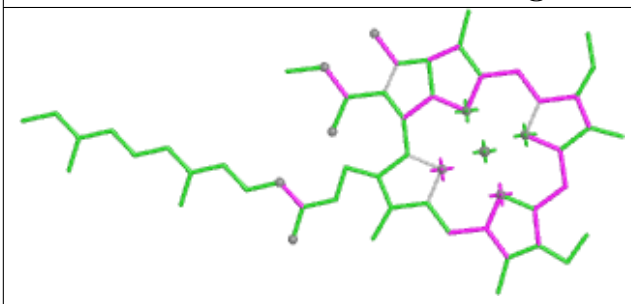


Torsions



Rings

Ligand CHL 5 323



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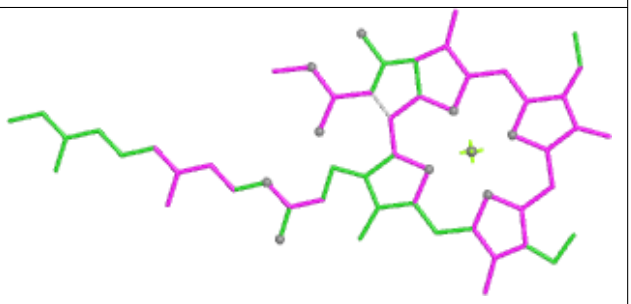
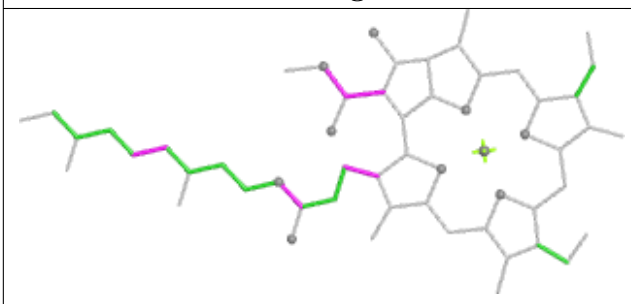


Bond angles



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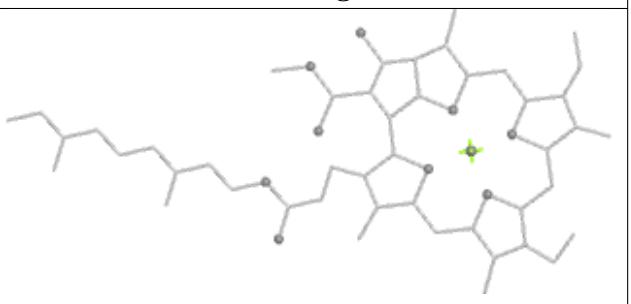
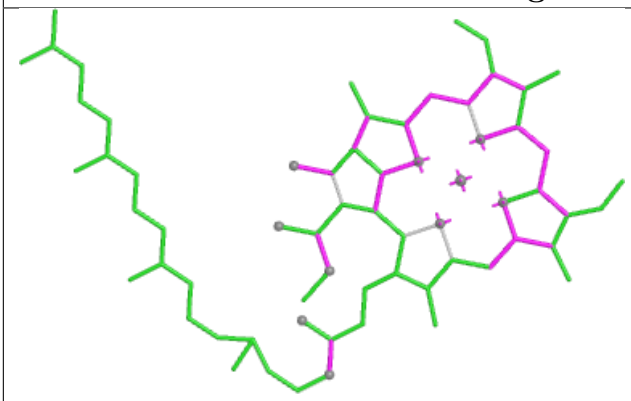


Rings

Ligand CHL 5 315



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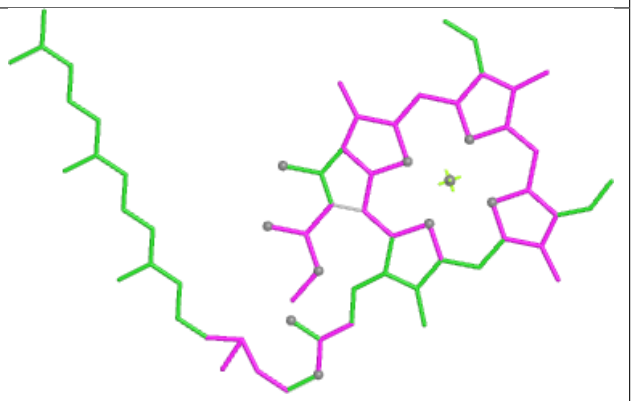
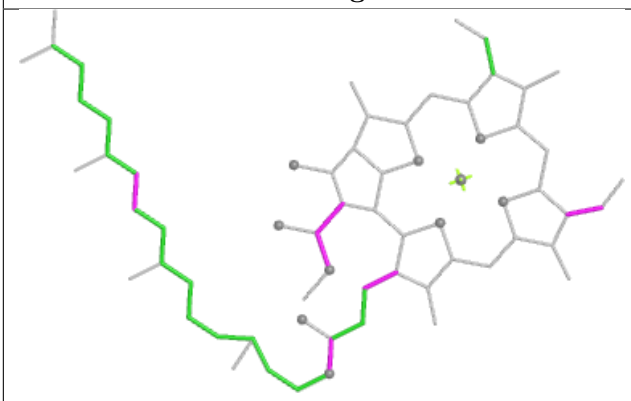


Bond angles



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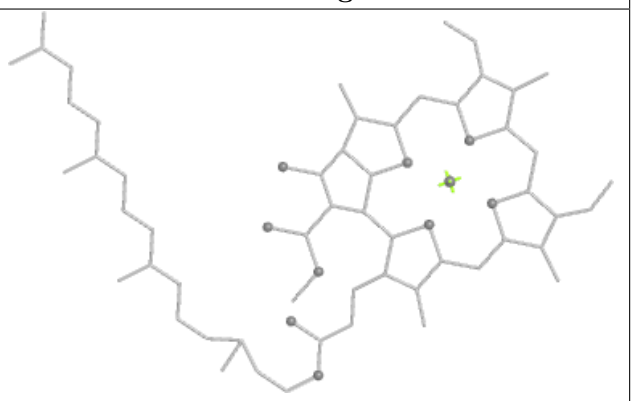
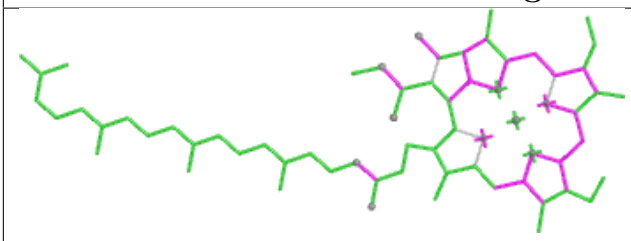


Rings

Ligand CHL B 837



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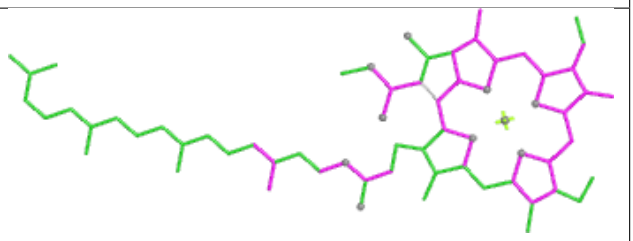
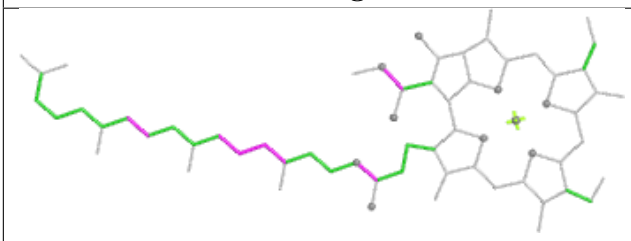


Bond angles



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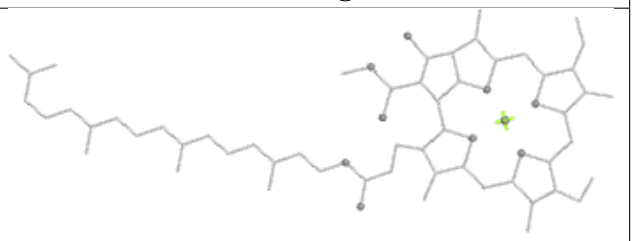
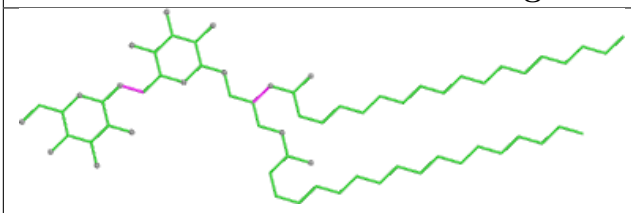
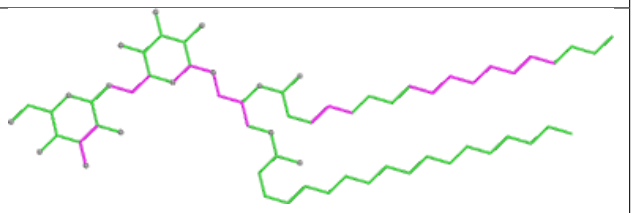


Rings

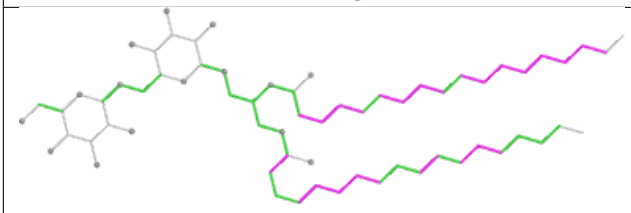
Ligand DGD 7 307



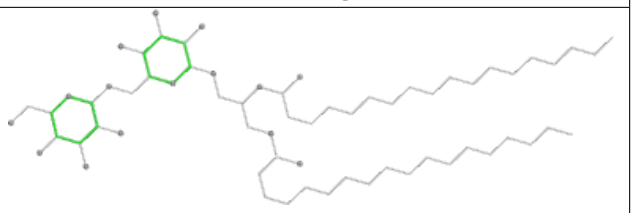
Bond lengths



Bond angles

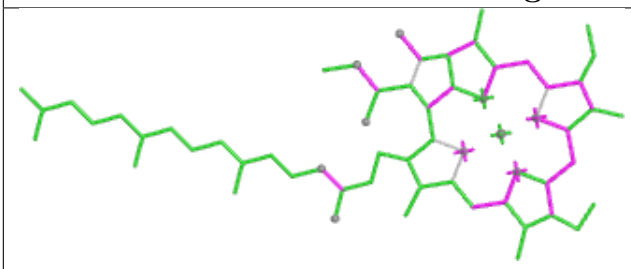


Torsions



Rings

Ligand CHL B 827



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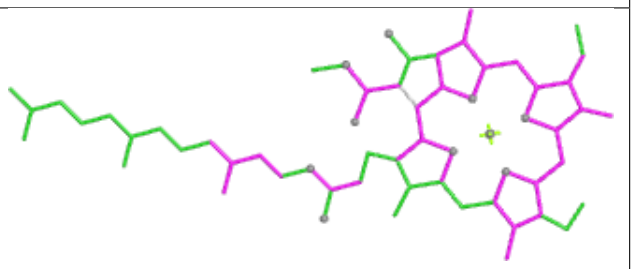

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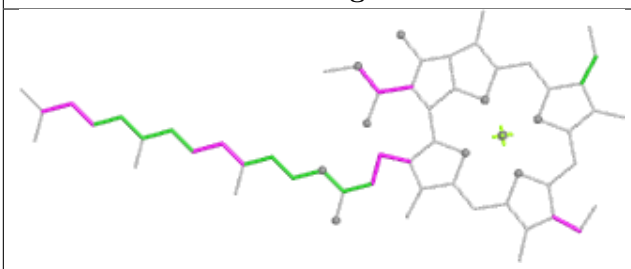

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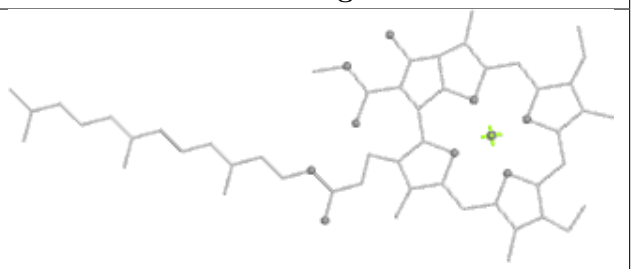
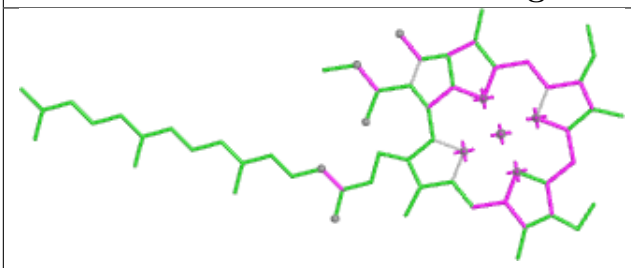


Rings

Ligand CHL 5 309



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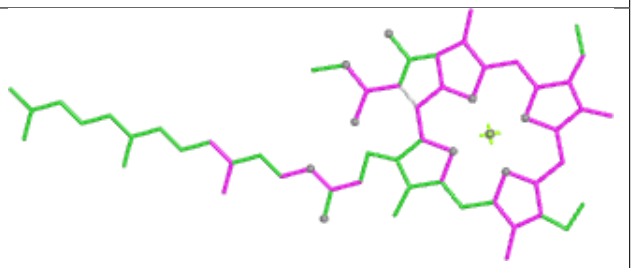

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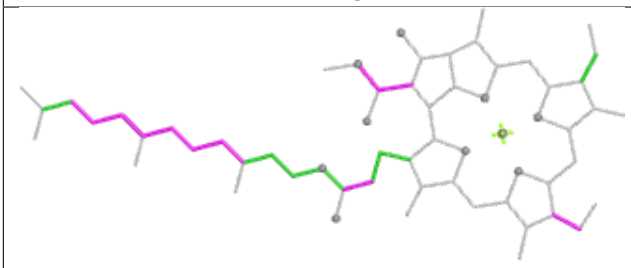

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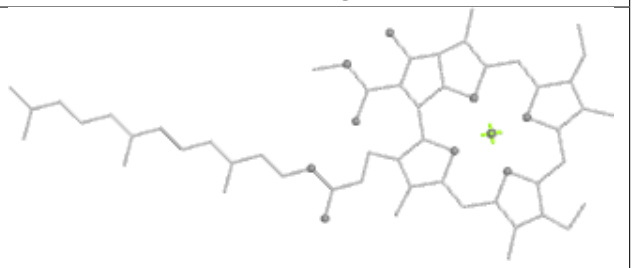
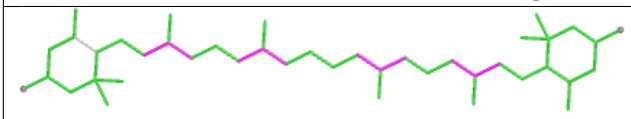


Rings

Ligand LUT b 303



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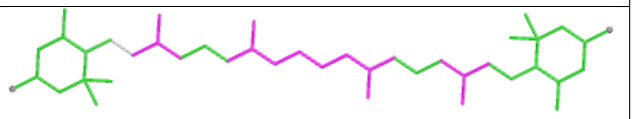

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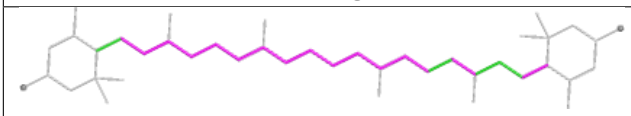

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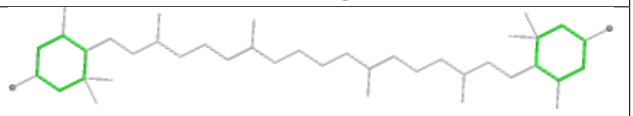
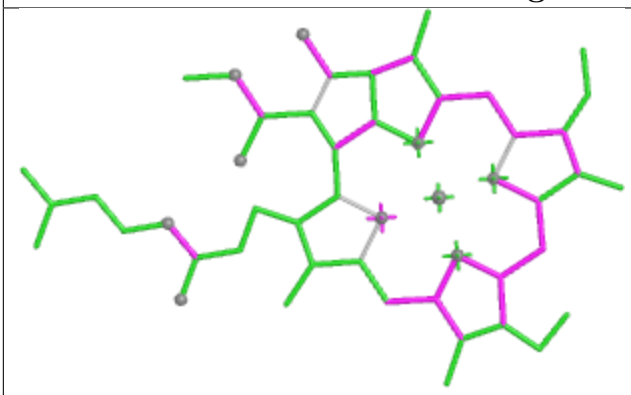


Rings

Ligand CHL 8 322



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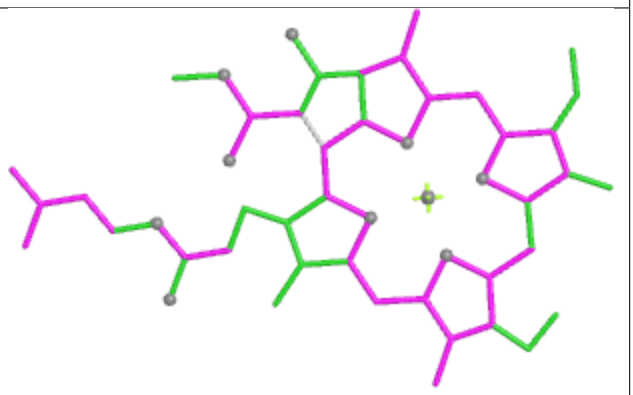

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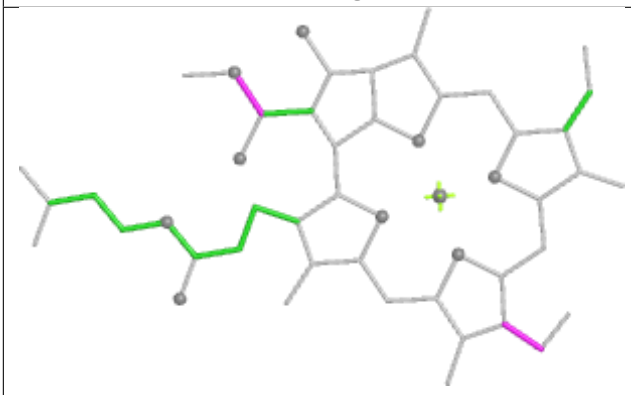

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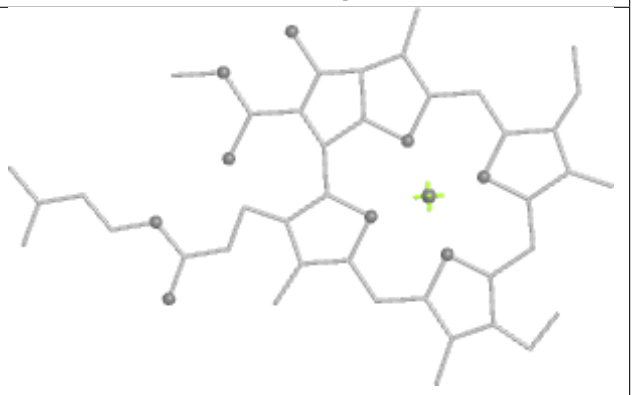
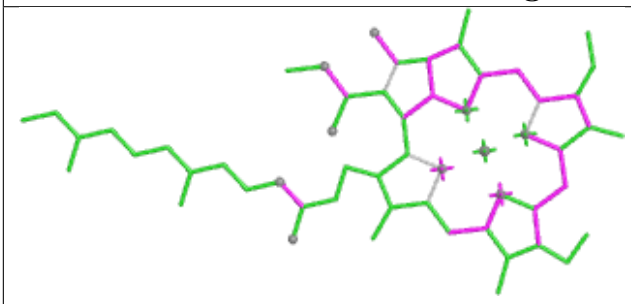


Rings

Ligand CHL A 847



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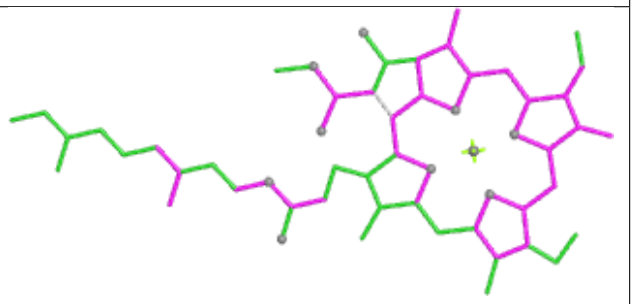

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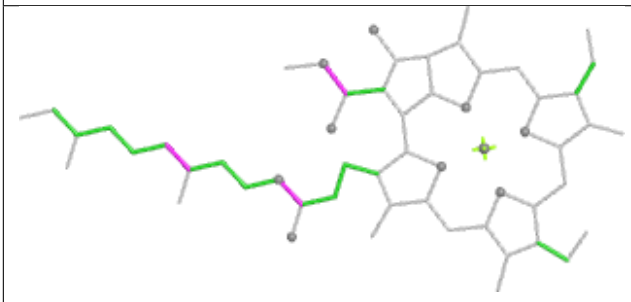

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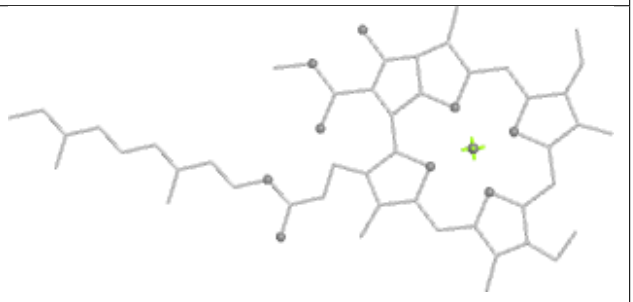
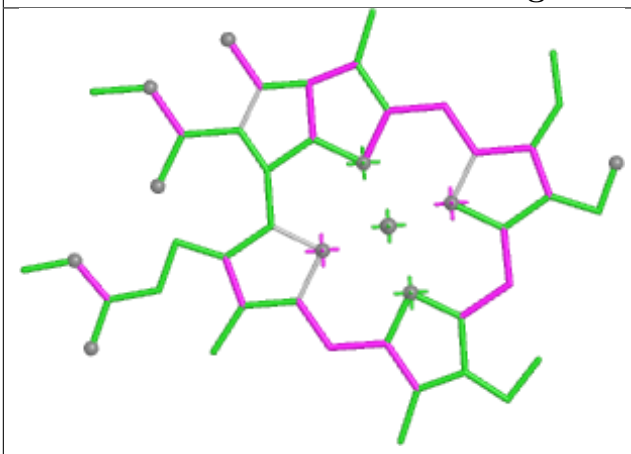


Rings

Ligand CHL 4 309



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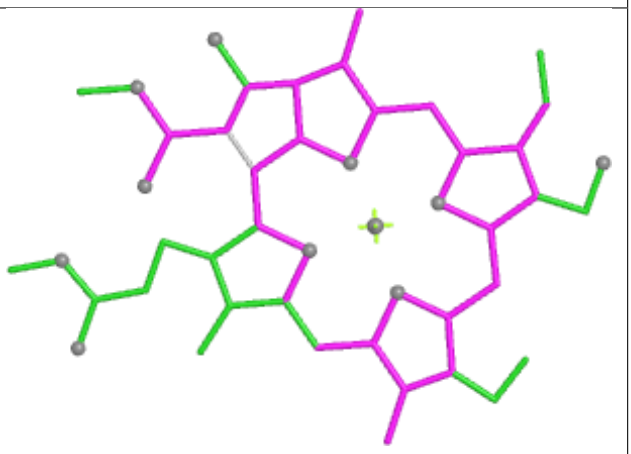

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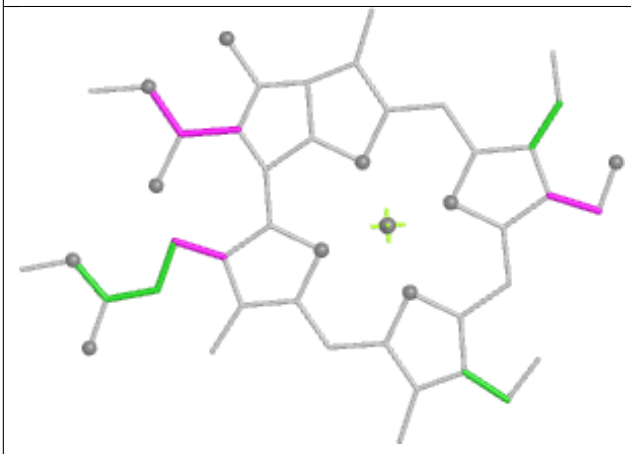

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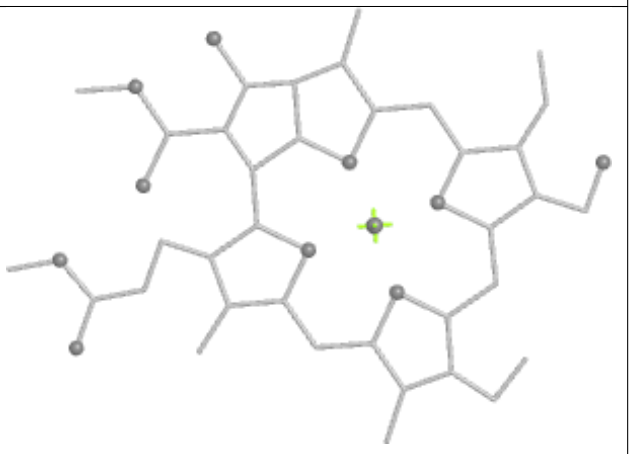
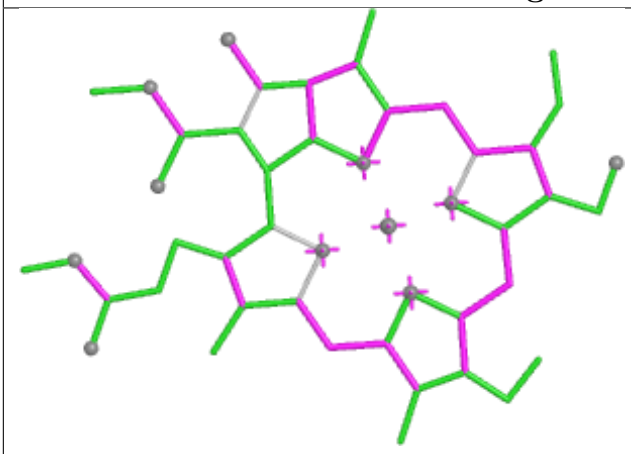


Rings

Ligand CHL b 311



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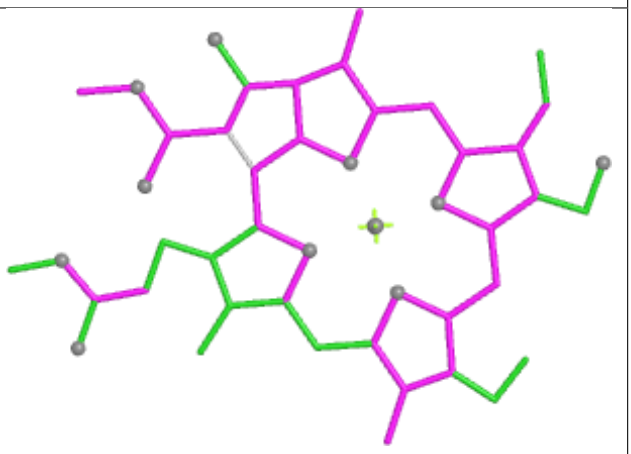

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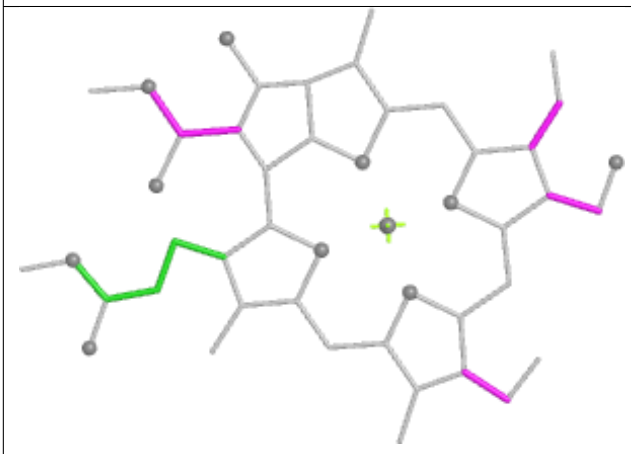

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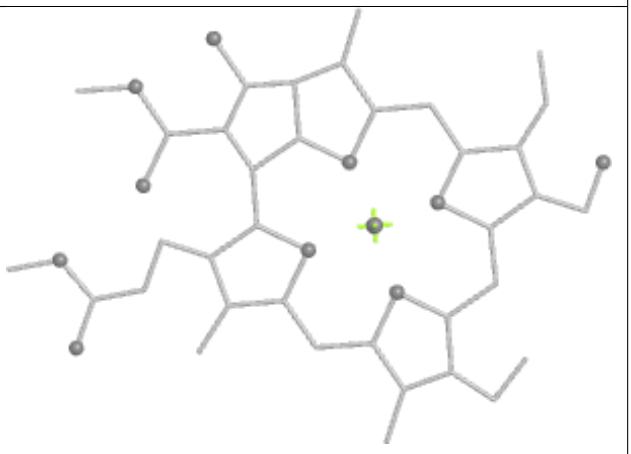
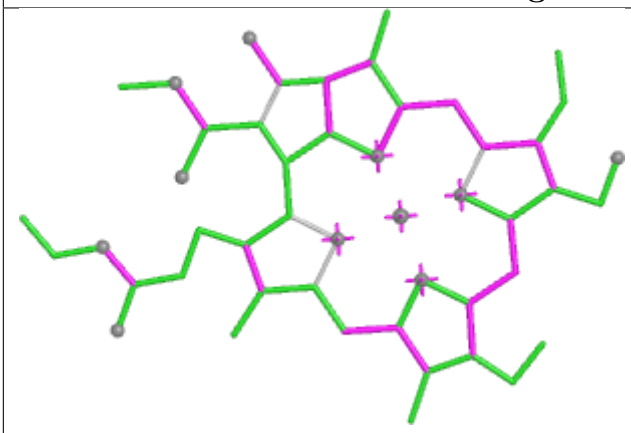


Rings

Ligand CHL a 318



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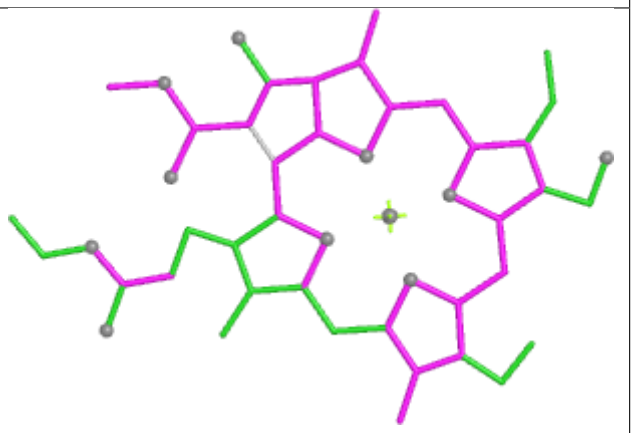

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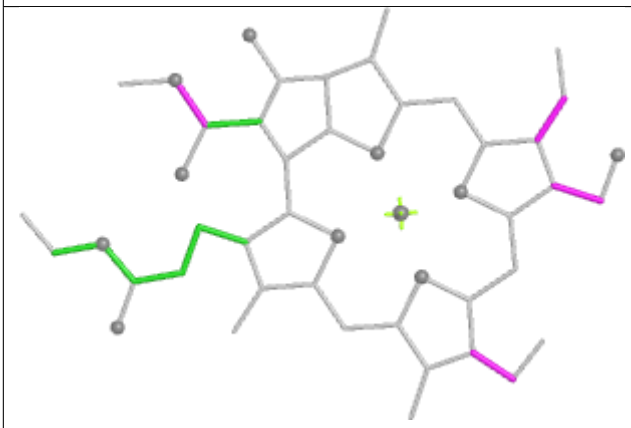

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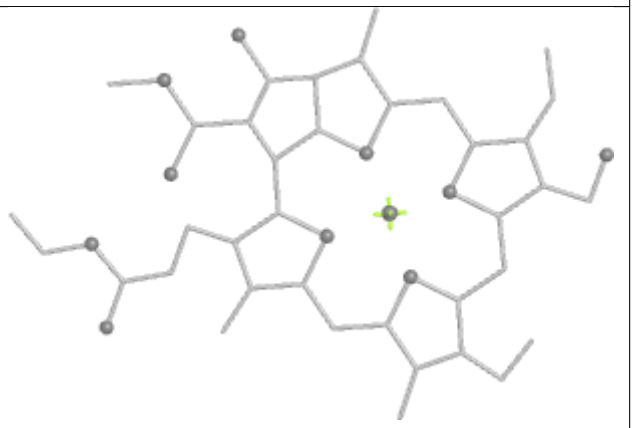
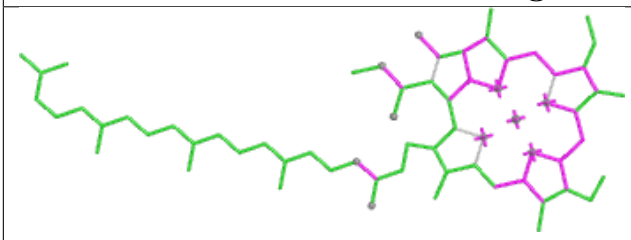


Rings

Ligand CHL 3 312



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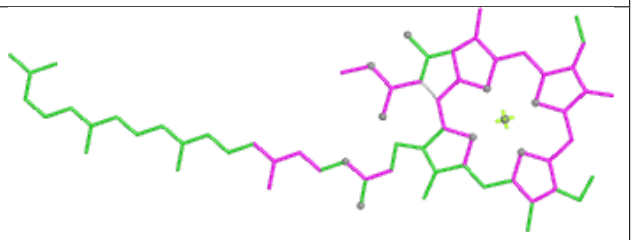

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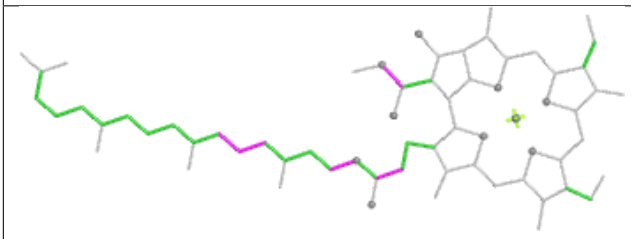

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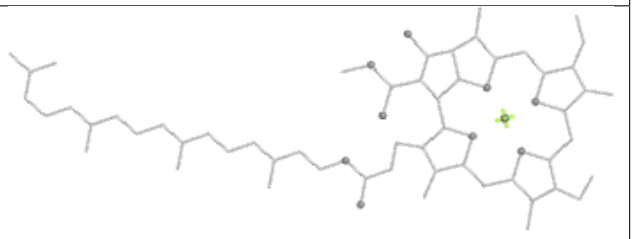
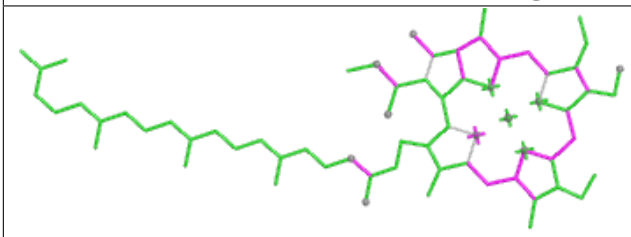


Rings

Ligand CHL 5 316



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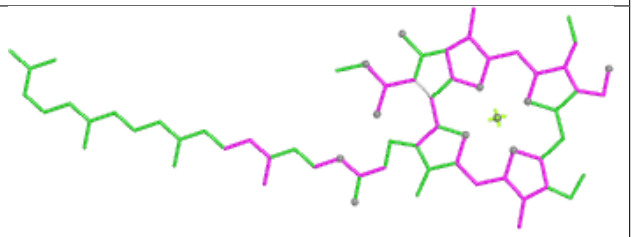

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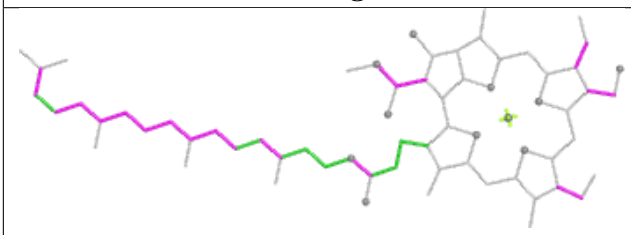

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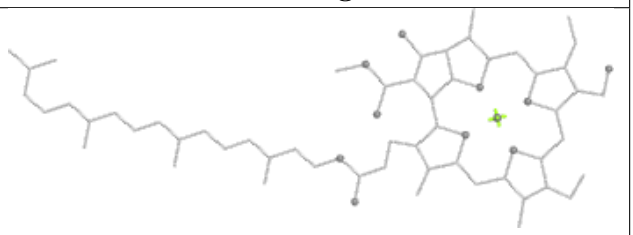
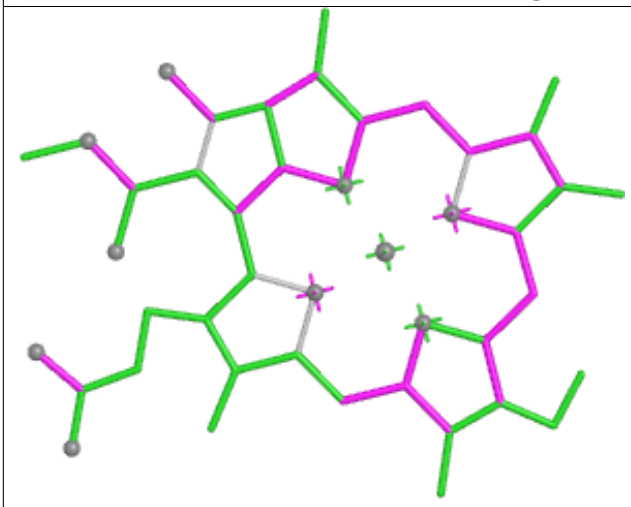


Rings

Ligand CHL 7 312



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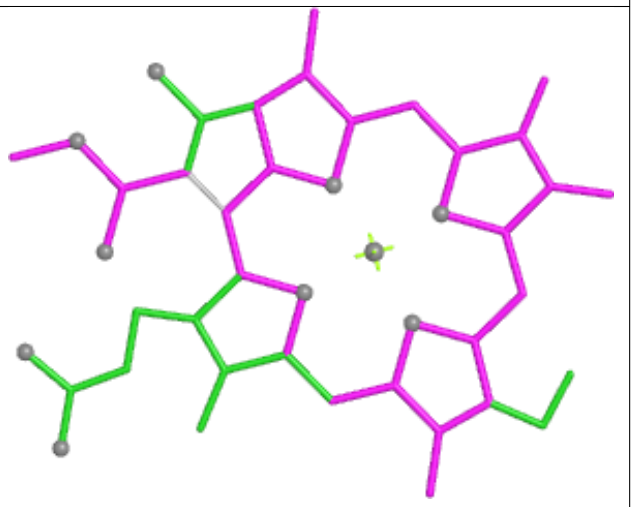

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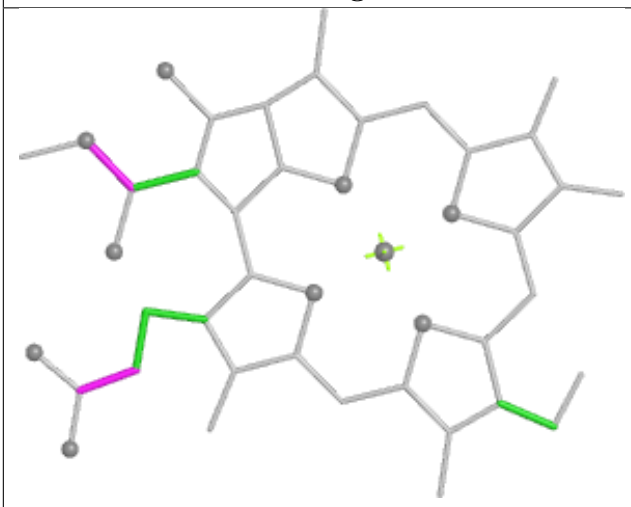

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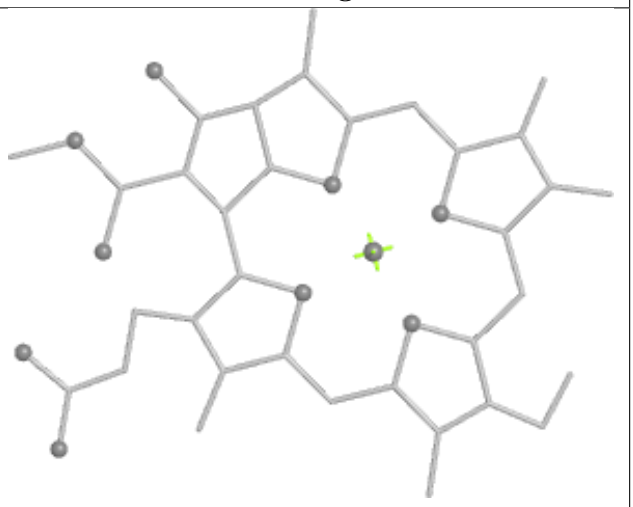
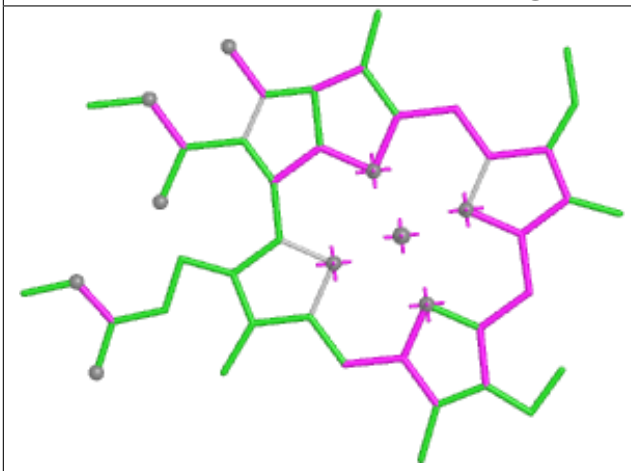


Rings

Ligand CHL b 310



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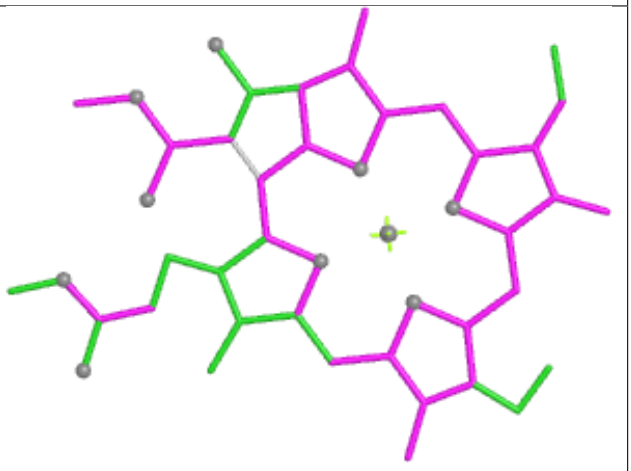
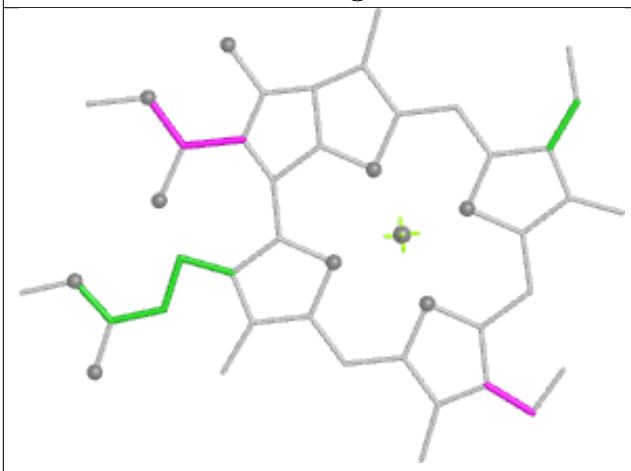


Bond angles



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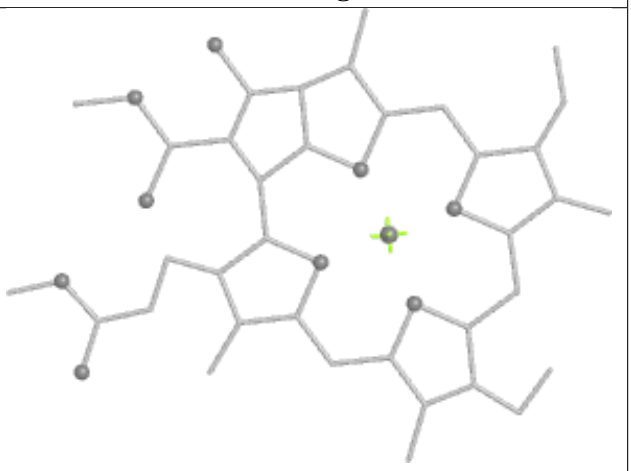
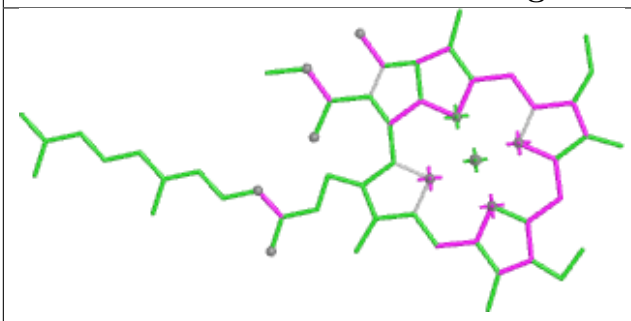


Rings

Ligand CHL 5 307



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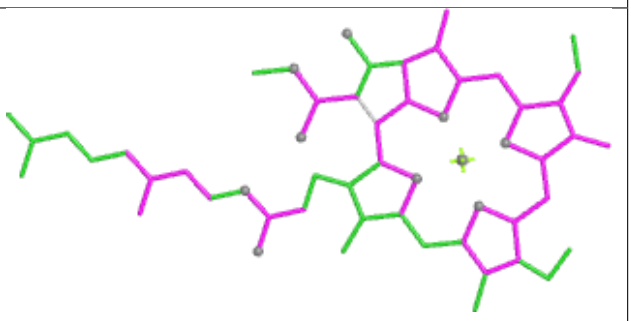
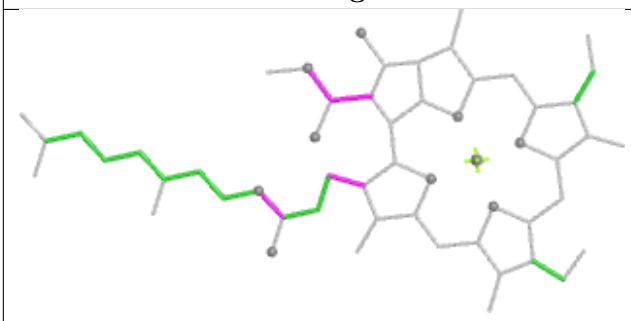


Bond angles



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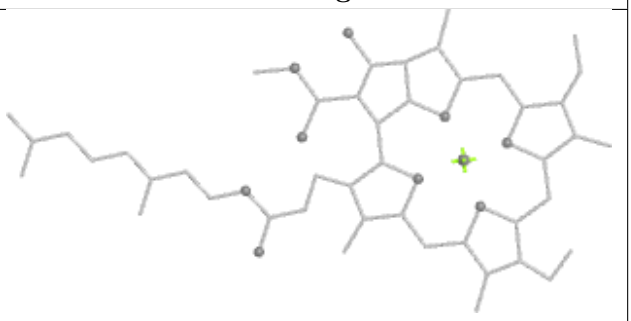
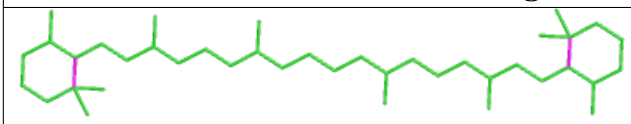


Rings

Ligand BCR B 802



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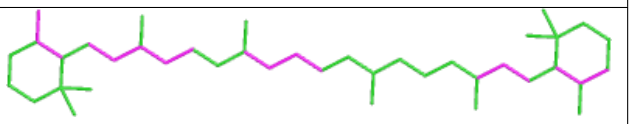
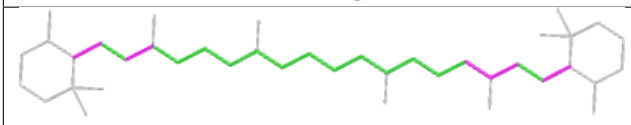


Bond angles



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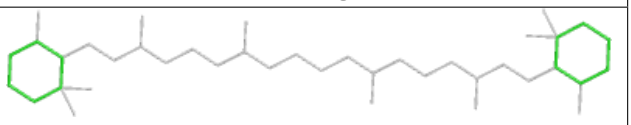
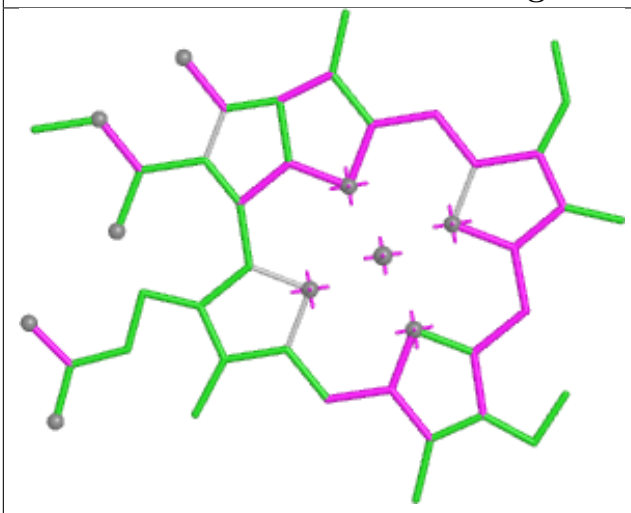
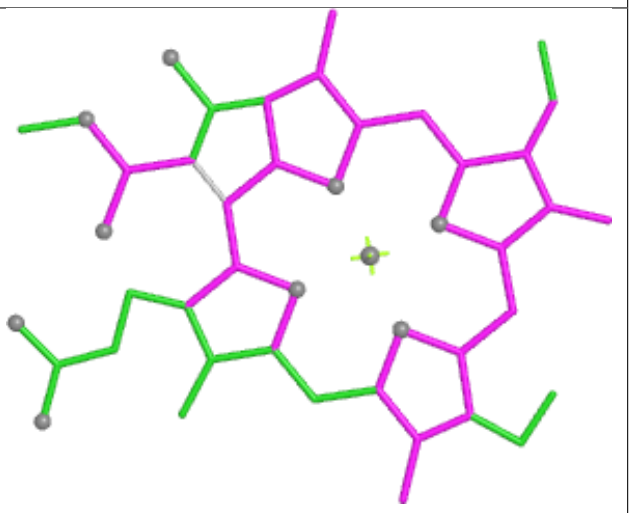


Rings

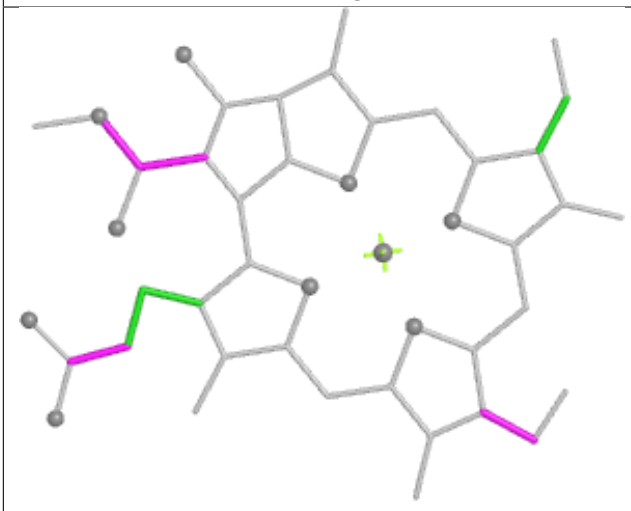
Ligand CHL 4 314



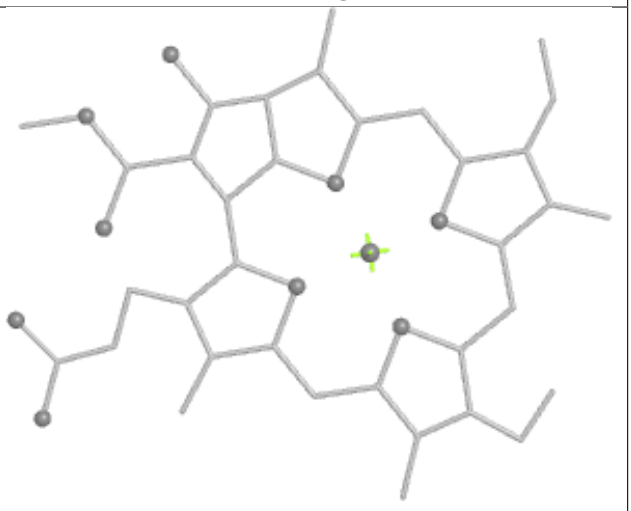
Bond lengths



Bond angles

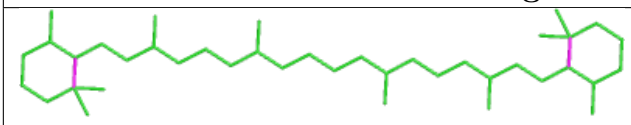


Torsions



Rings

Ligand BCR B 803



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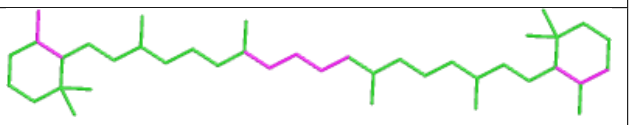
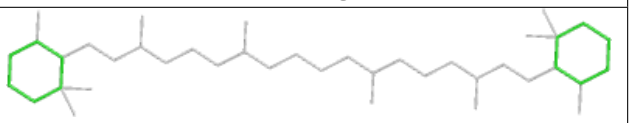


Bond angles

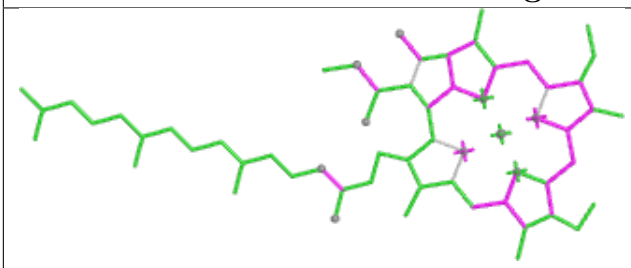


Torsions



Rings

Ligand CHL B 825



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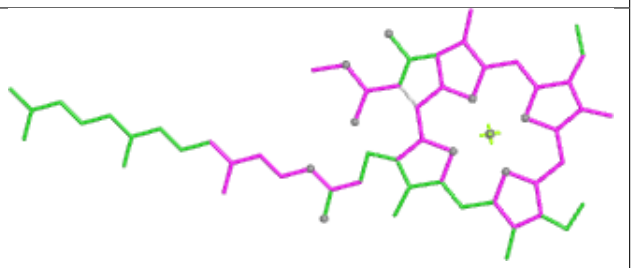
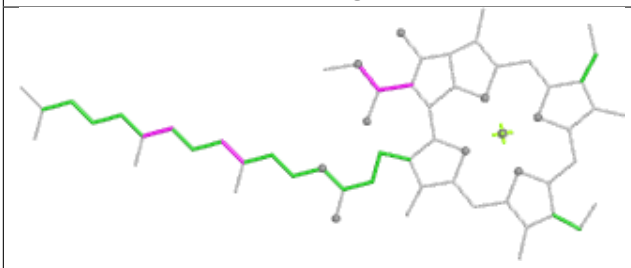


Bond angles



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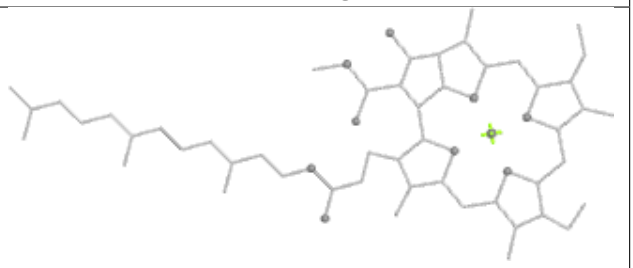
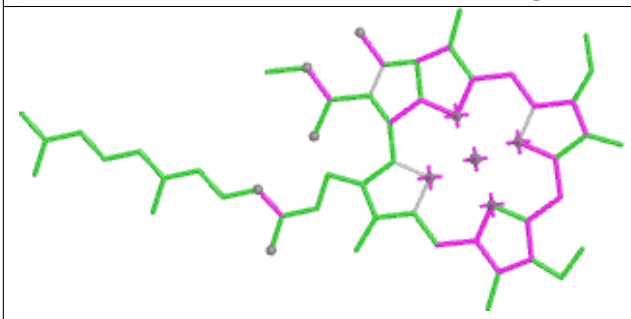


Rings

Ligand CHL 8 319



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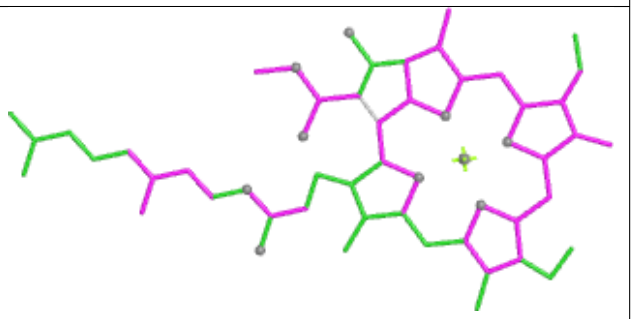
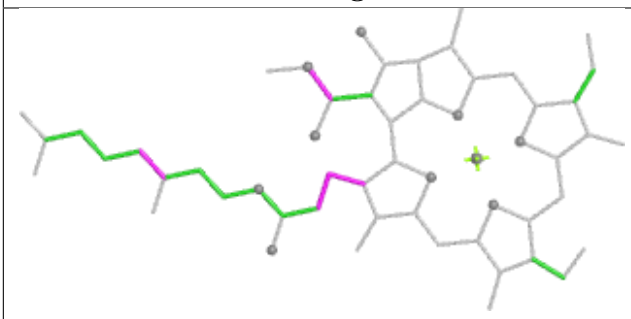


Bond angles



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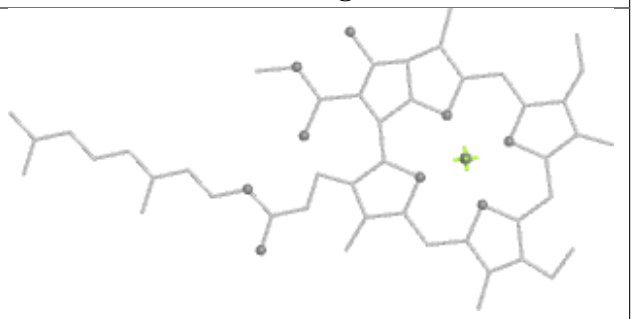
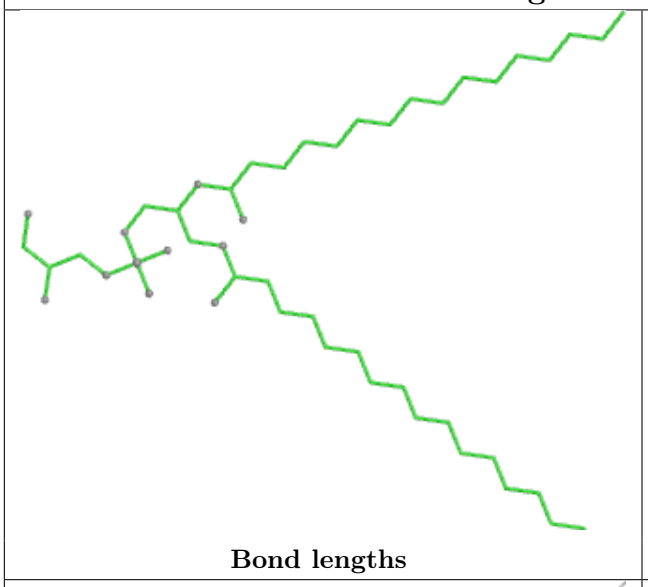


Rings

Ligand LHG a 305



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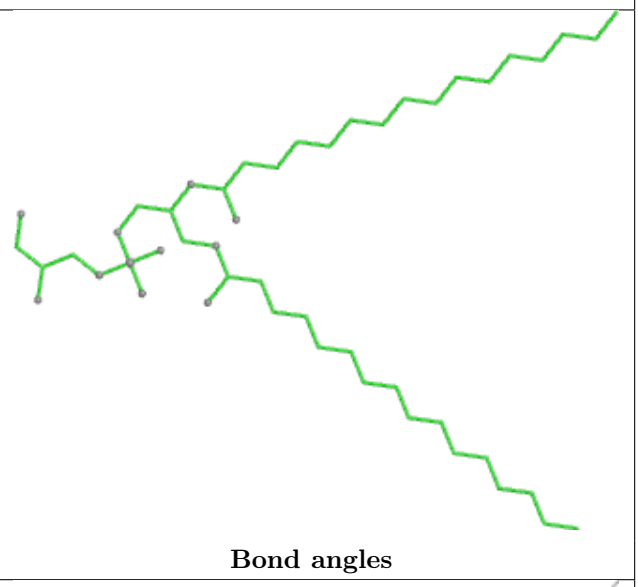
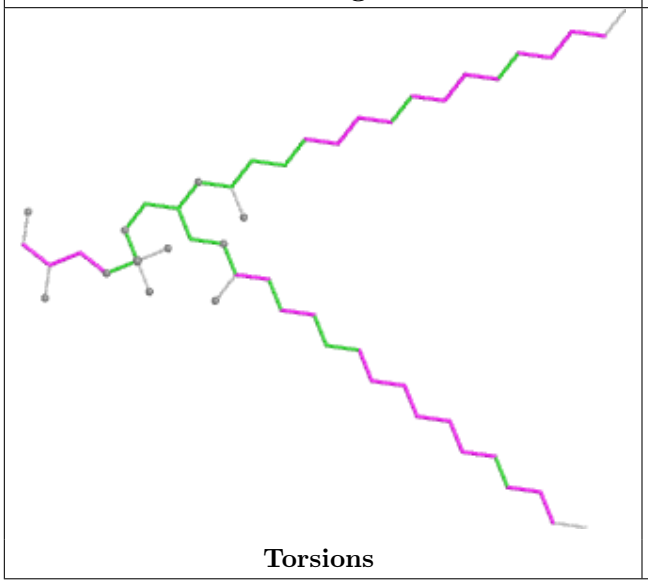


Bond angles



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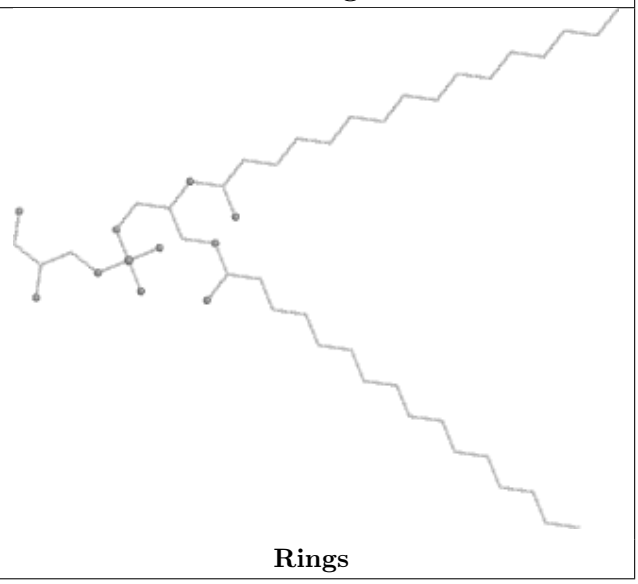
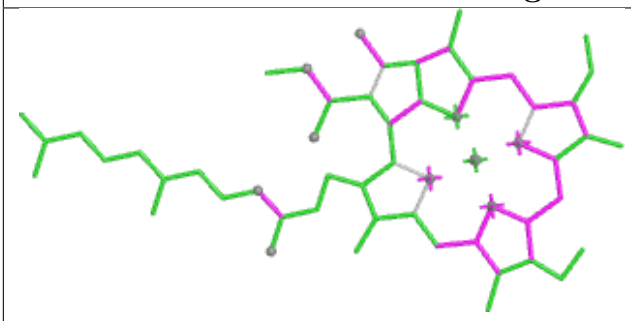


Rings

Ligand CHL B 841



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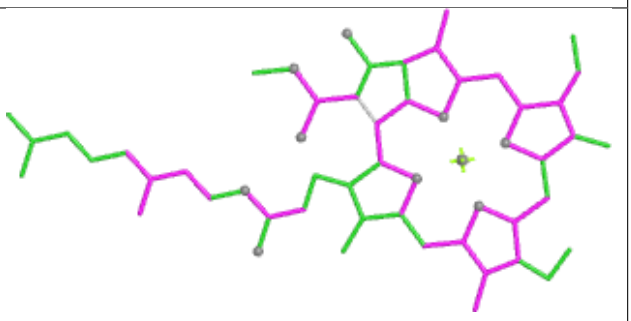
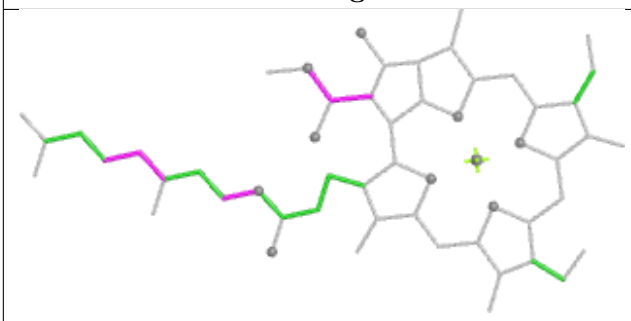


Bond angles



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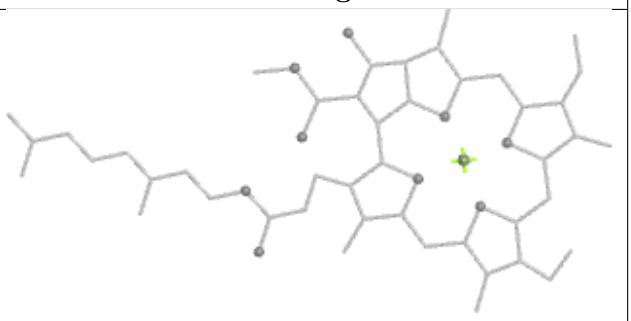
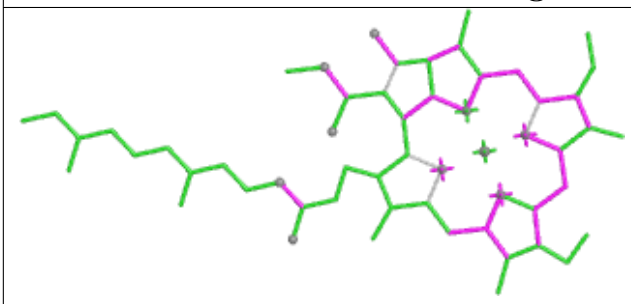


Rings

Ligand CHL 4 306



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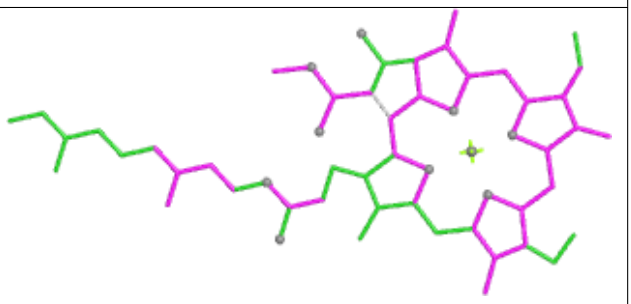
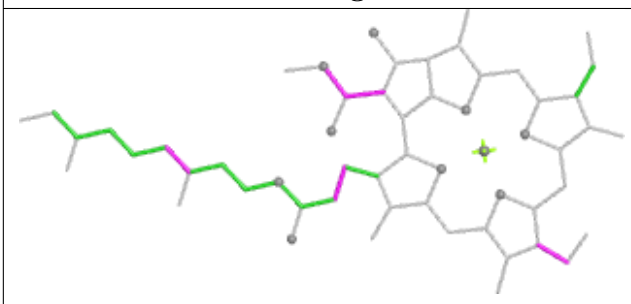


Bond angles



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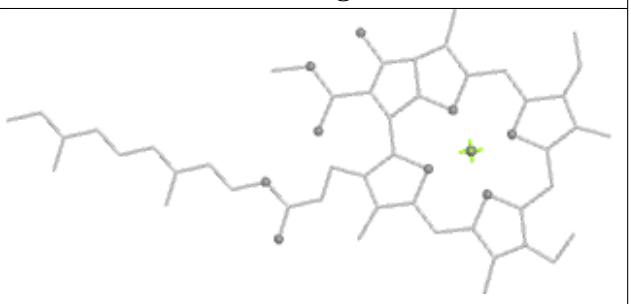
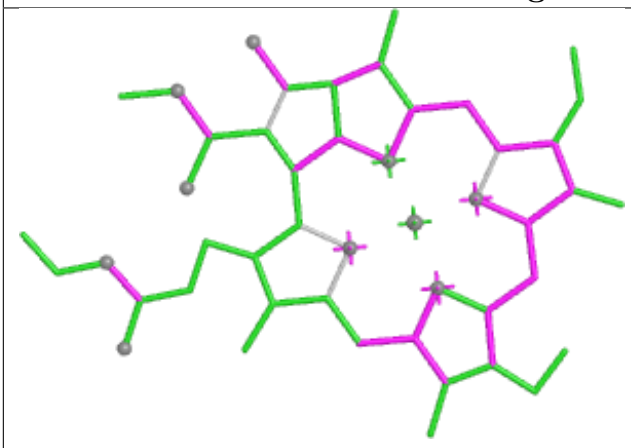


Rings

Ligand CHL 4 315



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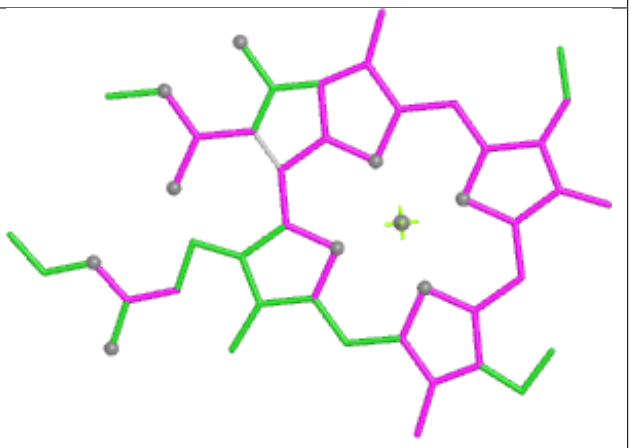
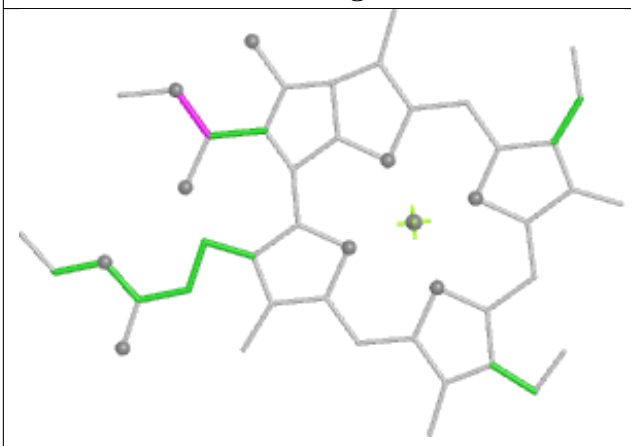


Bond angles



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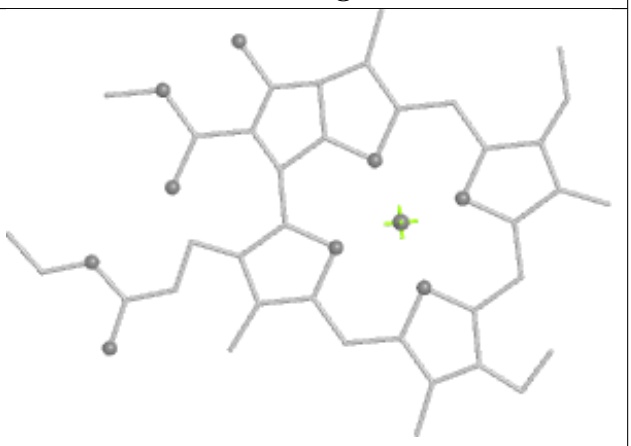
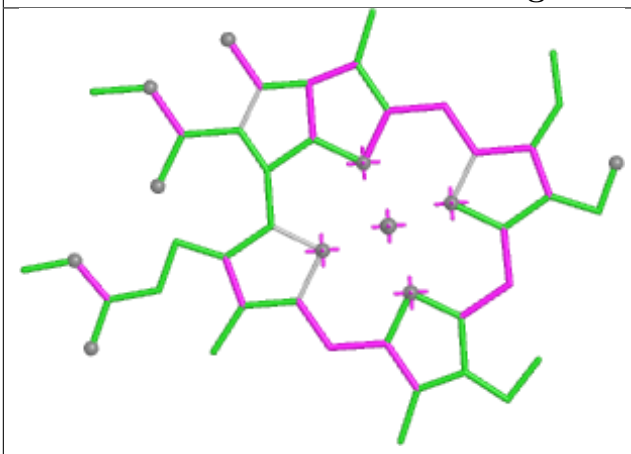


Rings

Ligand CHL 5 319



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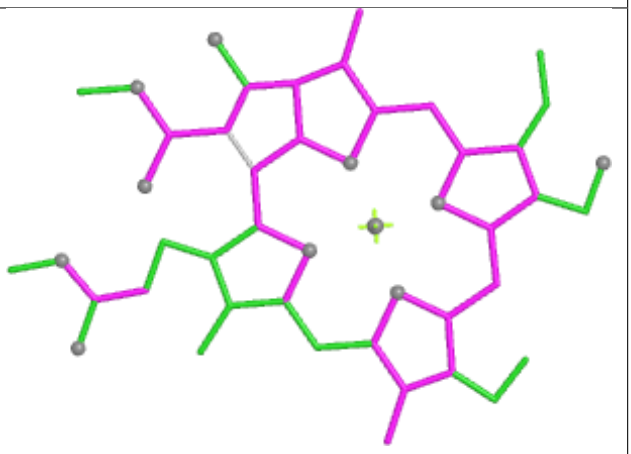
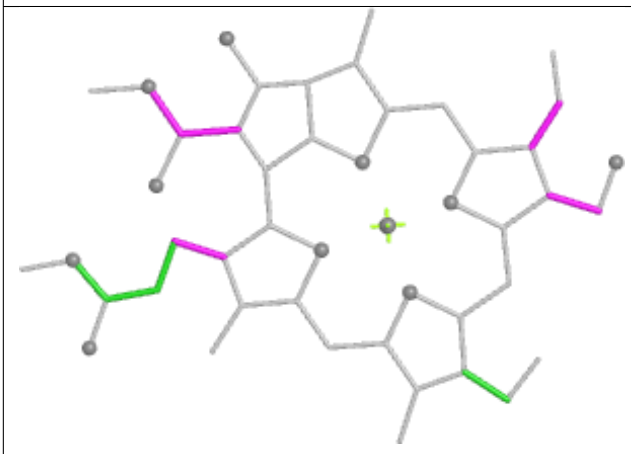


Bond angles



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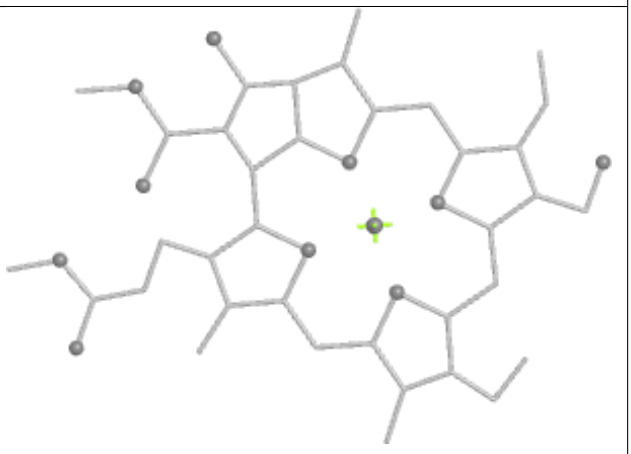
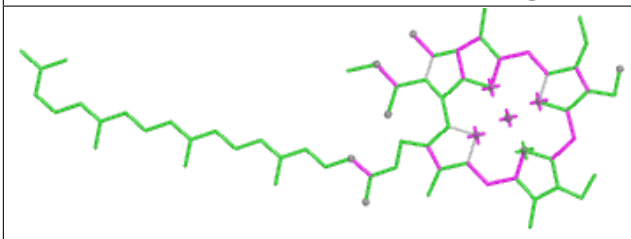


Rings

Ligand CHL A 842



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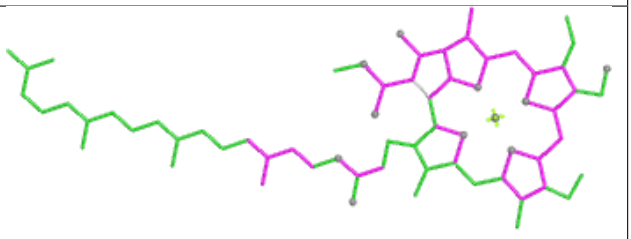

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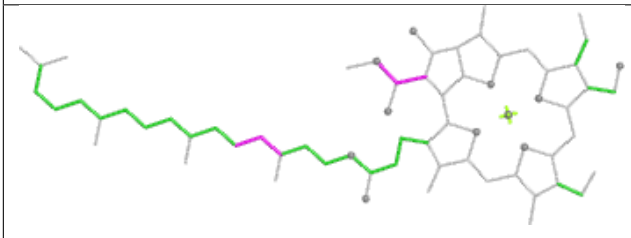

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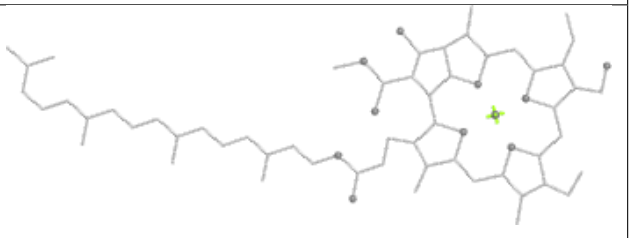
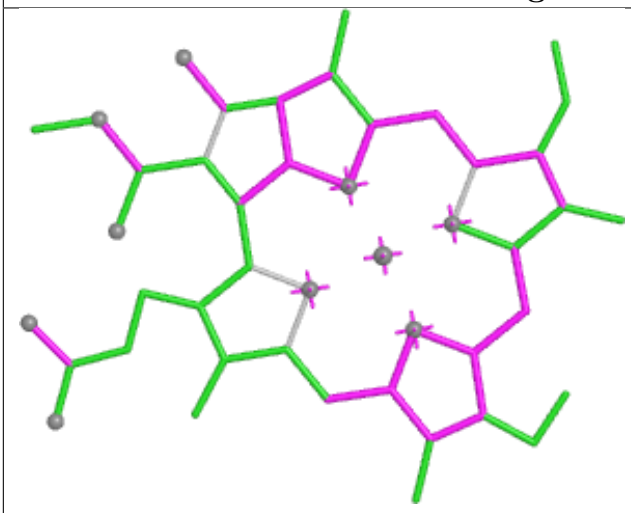


Rings

Ligand CHL 4 319



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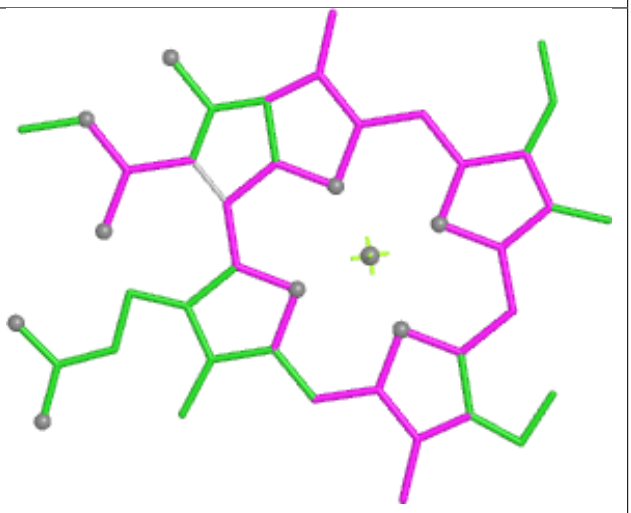
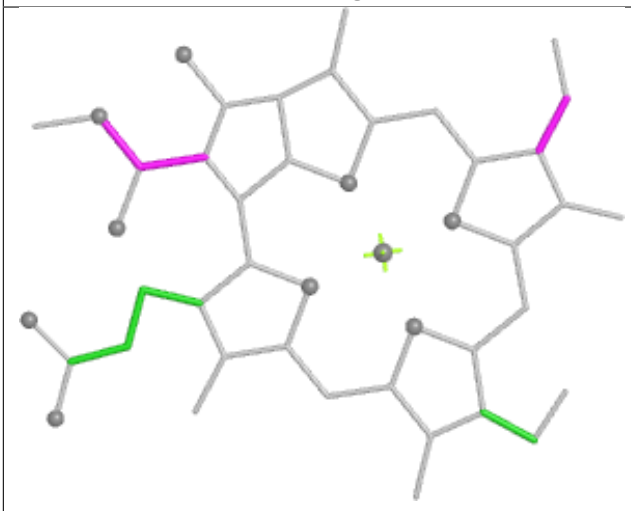


Bond angles



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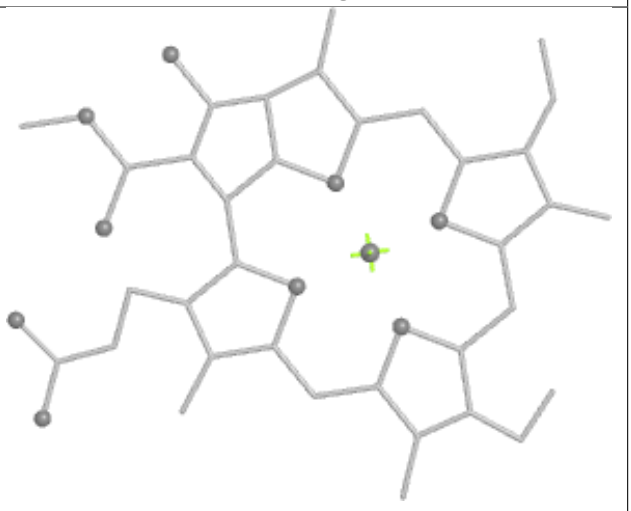
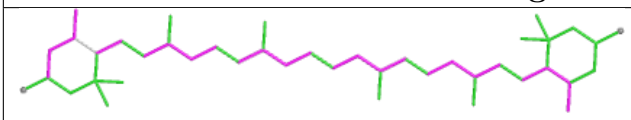


Rings

Ligand LUT a 304



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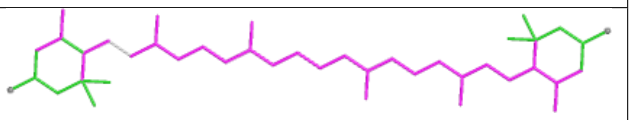
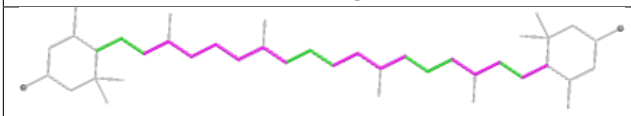


Bond angles



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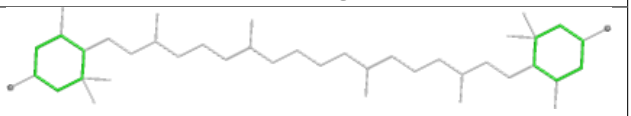
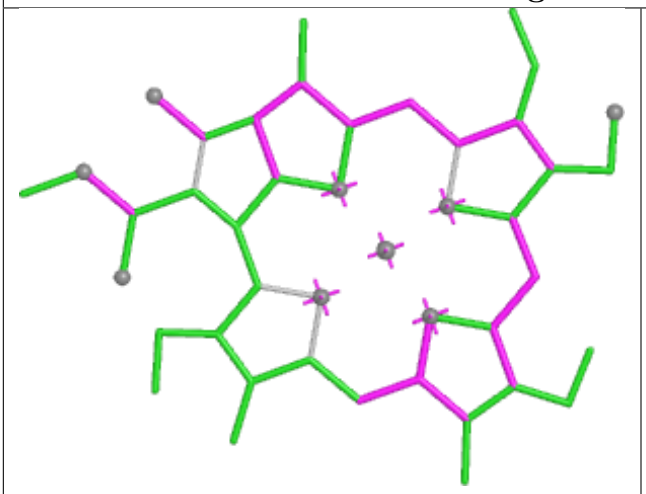


Rings

Ligand CHL 6 319



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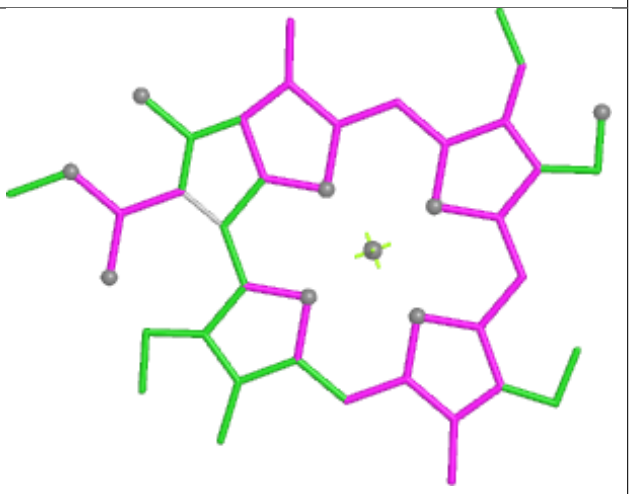


Bond angles

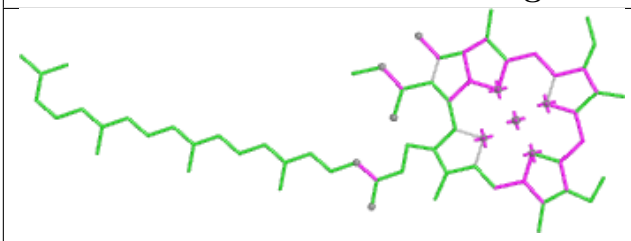


Torsions



Rings

Ligand CHL B 815



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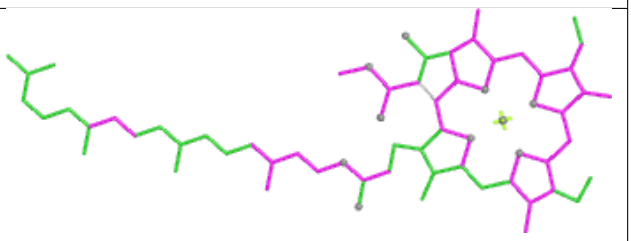
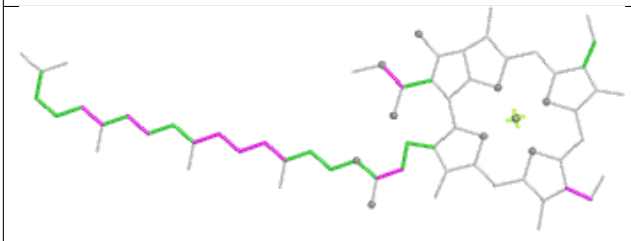


Bond angles



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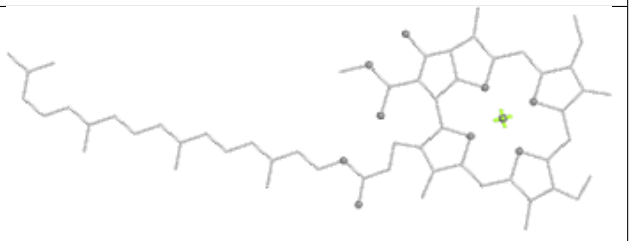
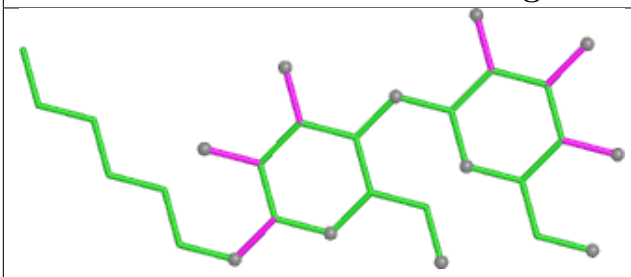
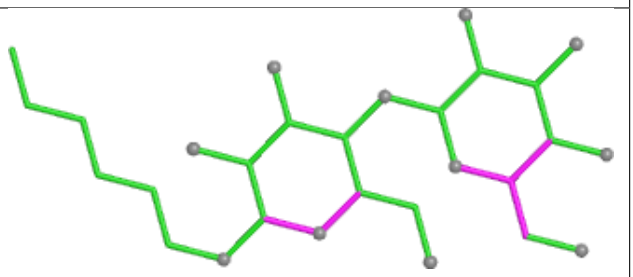


Rings

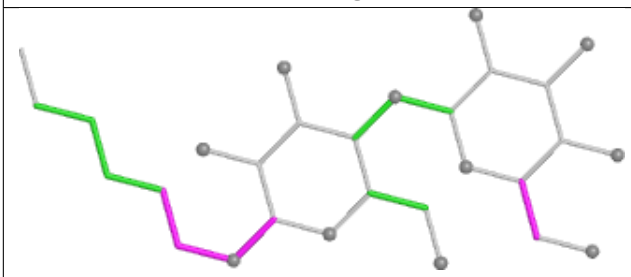
Ligand LMT F 302



Bond lengths



Bond angles



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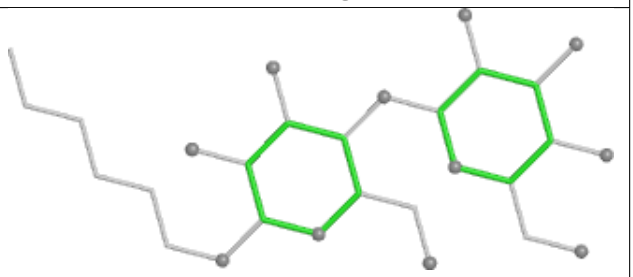
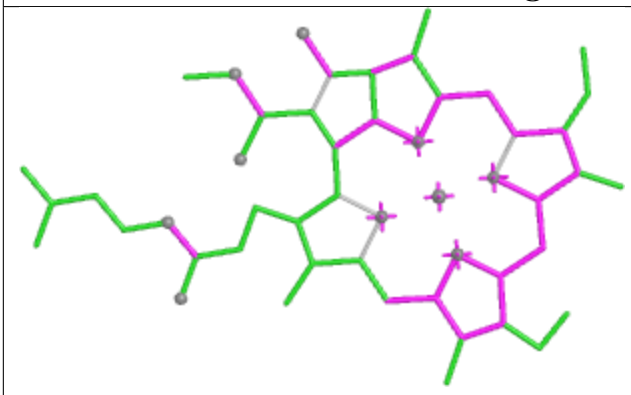
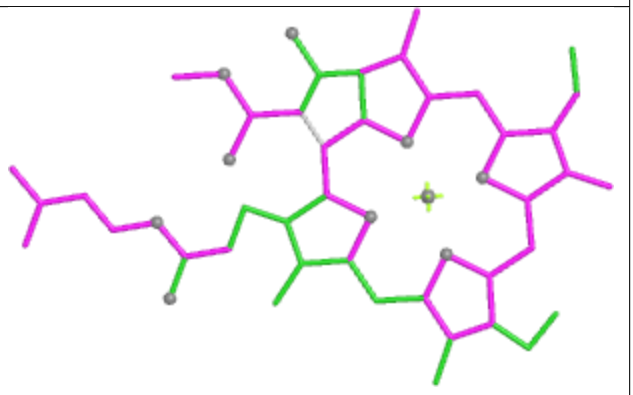


Rings

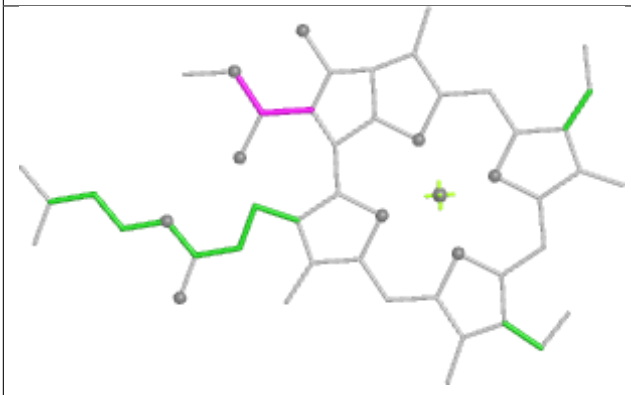
Ligand CHL B 850



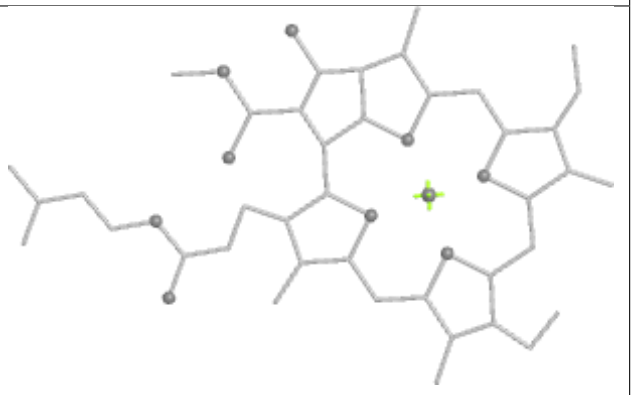
Bond lengths



Bond angles

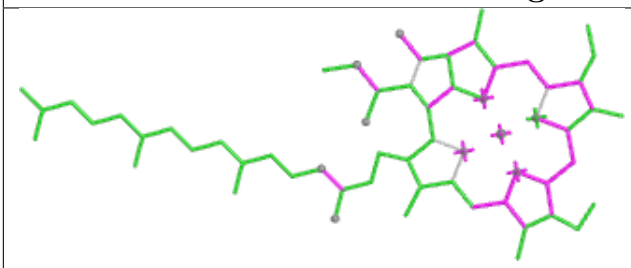


Torsions



Rings

Ligand CHL 3 311



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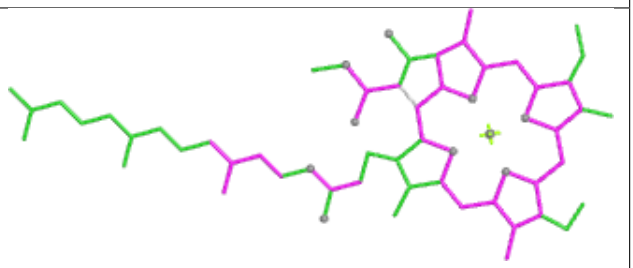

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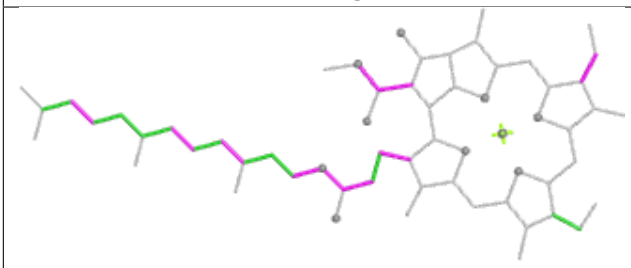

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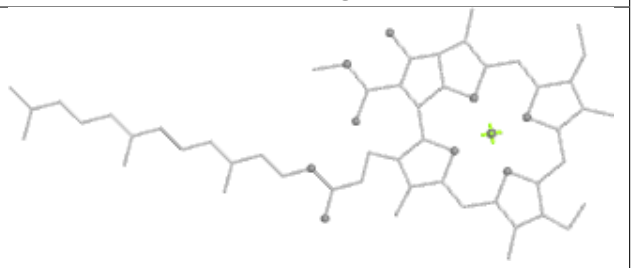
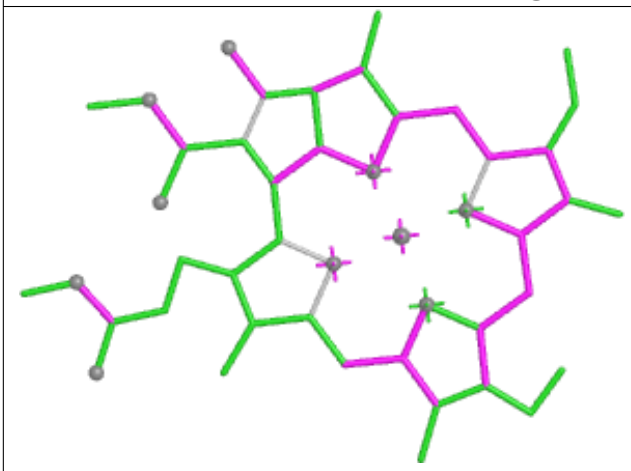


Rings

Ligand CHL 6 314



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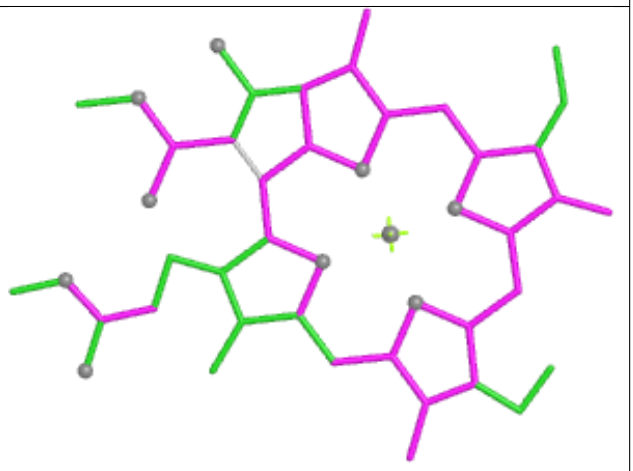

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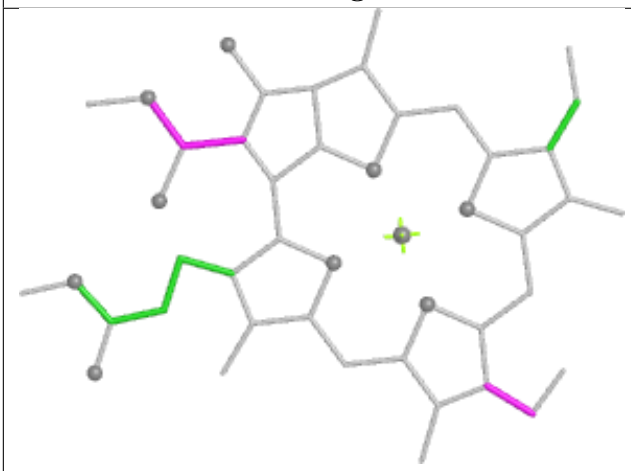
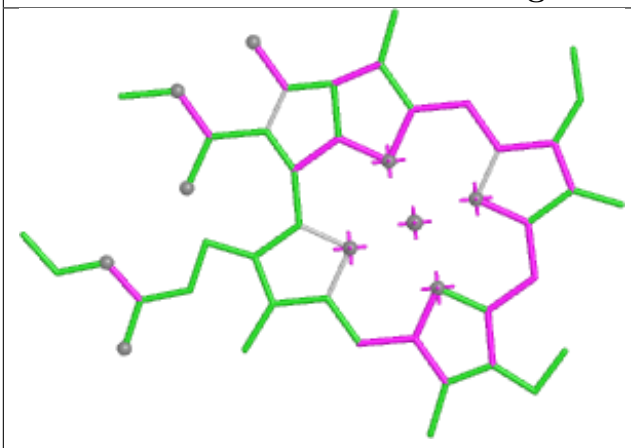


Torsions



Rings

Ligand CHL 4 311



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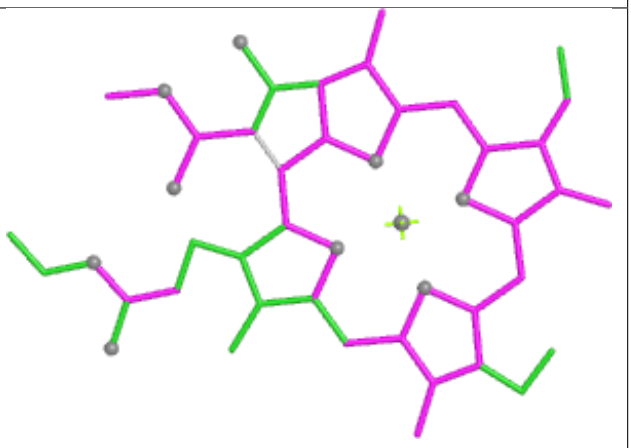
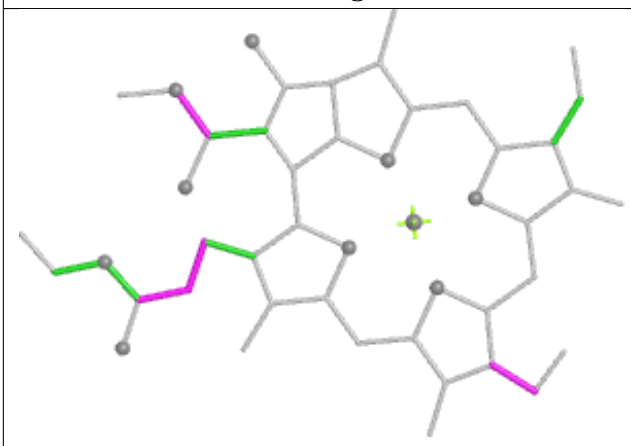


Bond angles



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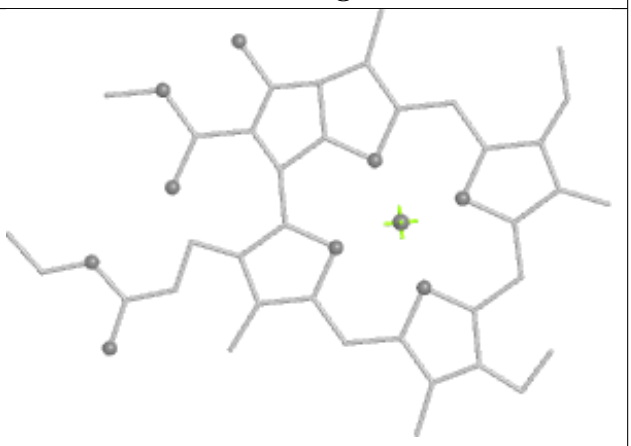
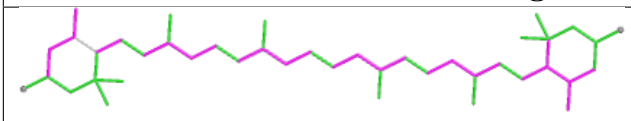


Rings

Ligand LUT 7 304



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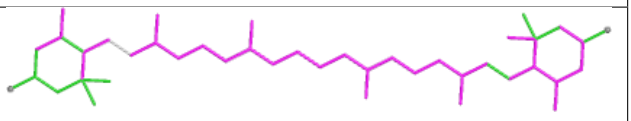
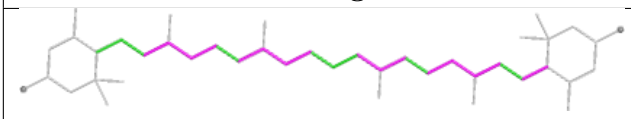


Bond angles



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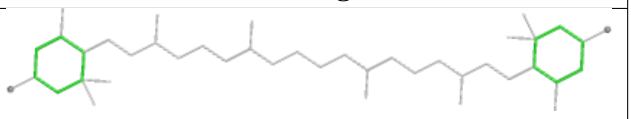
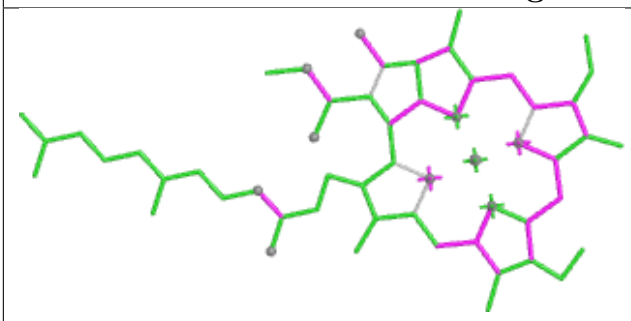


Rings

Ligand CHL b 307



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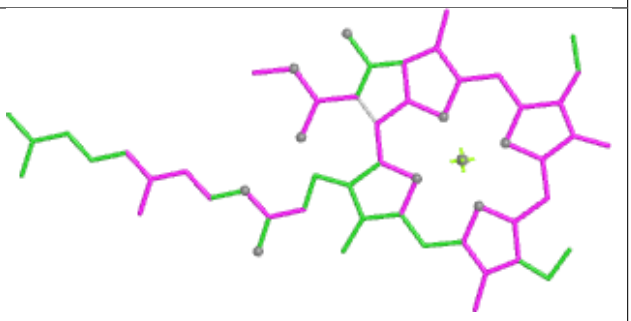

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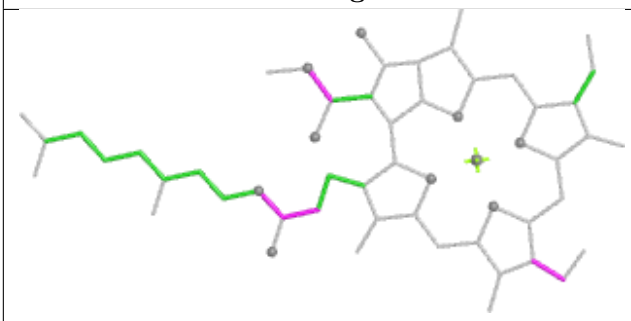

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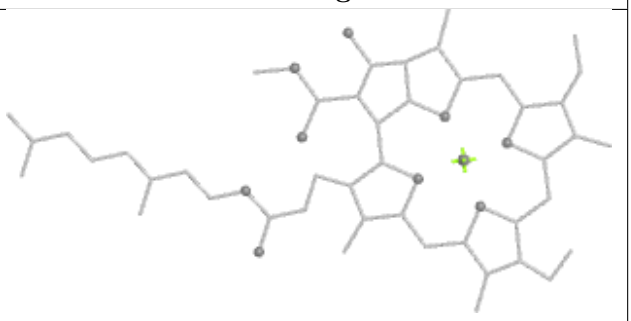
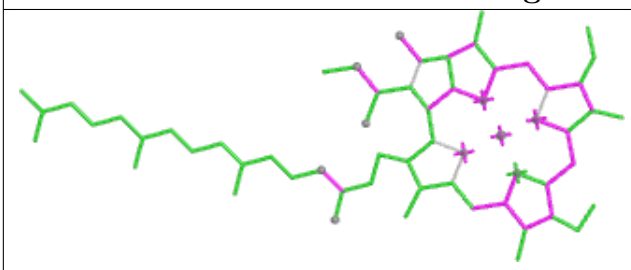


Rings

Ligand CHL A 832



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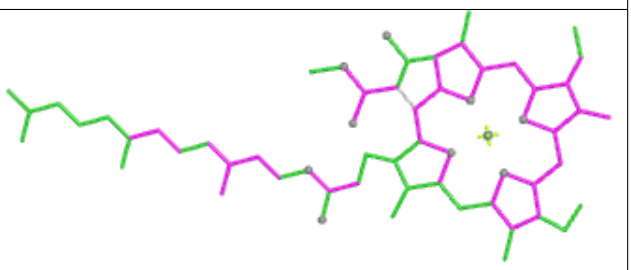
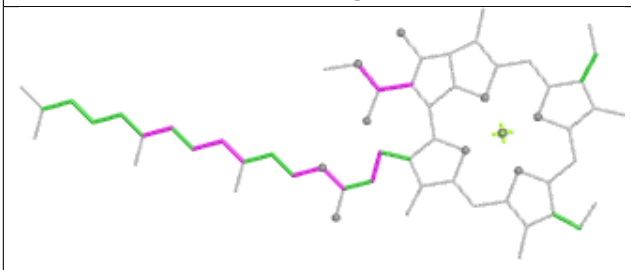


Bond angles



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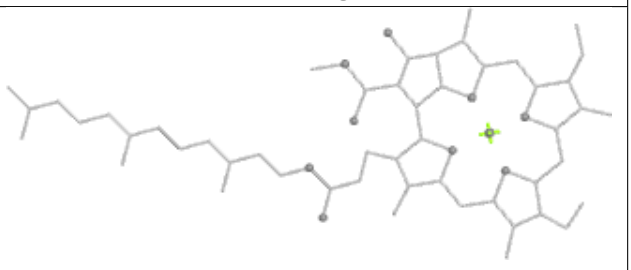
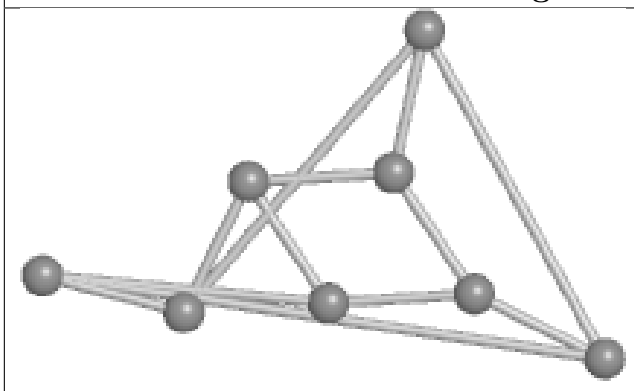


Rings

Ligand SF4 C 101



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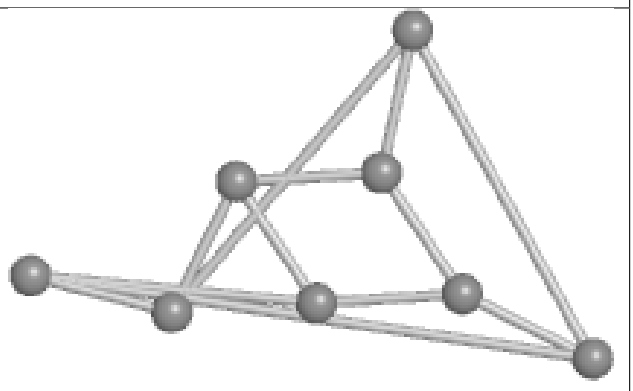
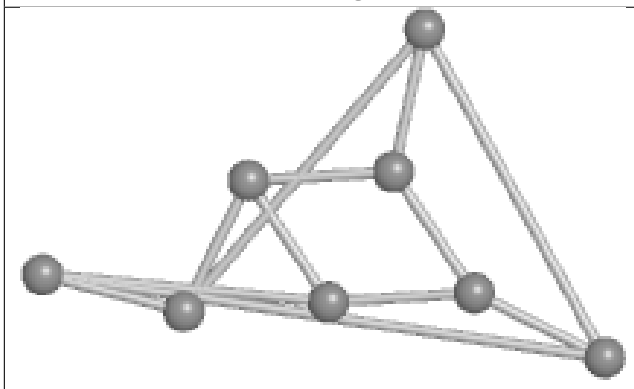


Bond angles



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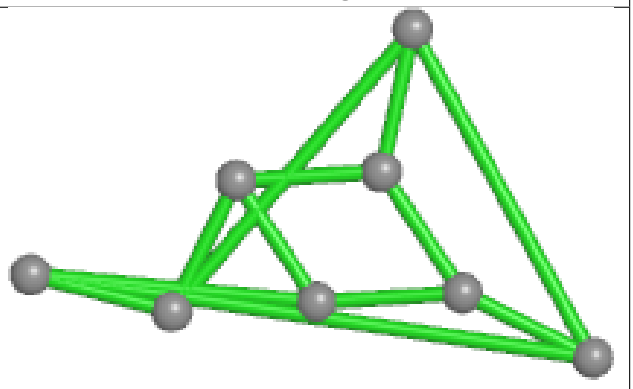
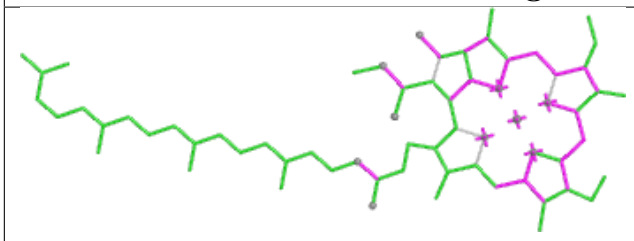


Rings

Ligand CHL B 820



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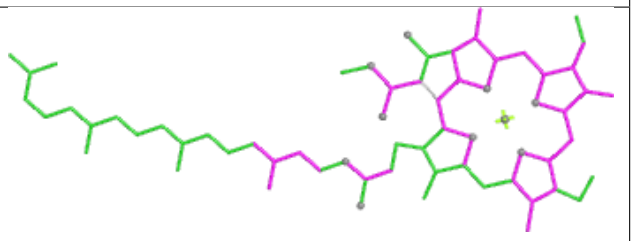
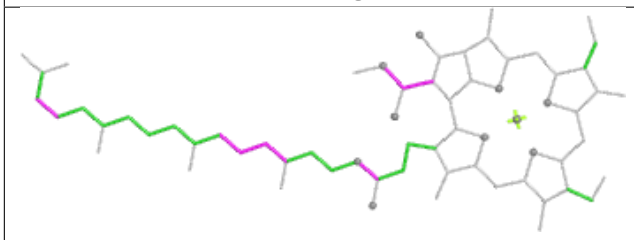


Bond angles



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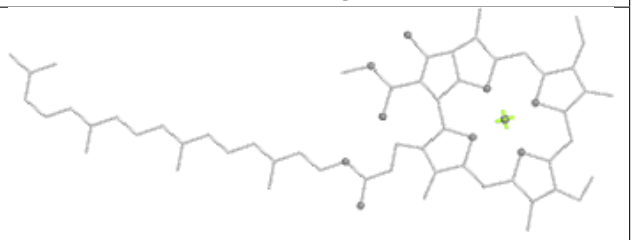
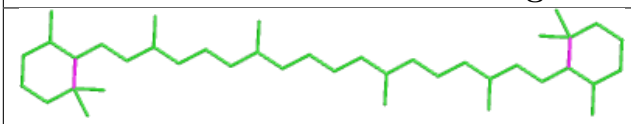


Rings

Ligand BCR 3 302



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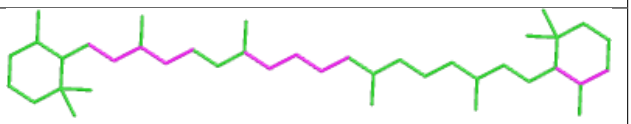
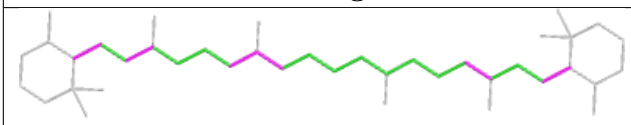


Bond angles



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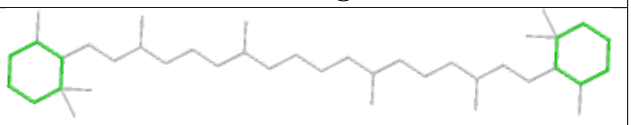
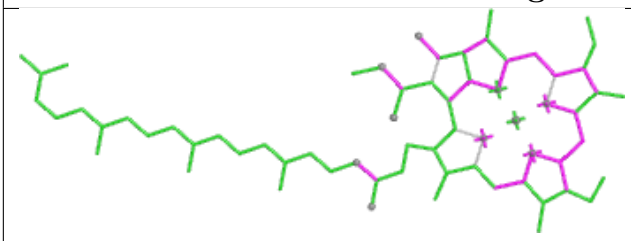


Rings

Ligand CHL 8 312



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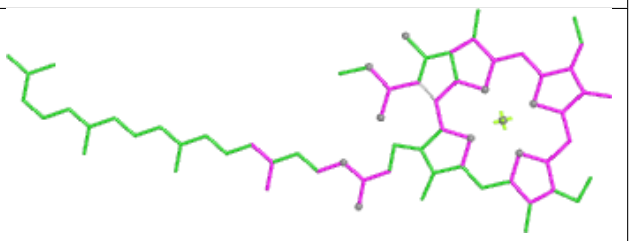
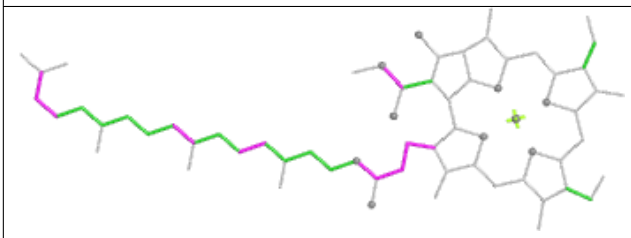


Bond angles



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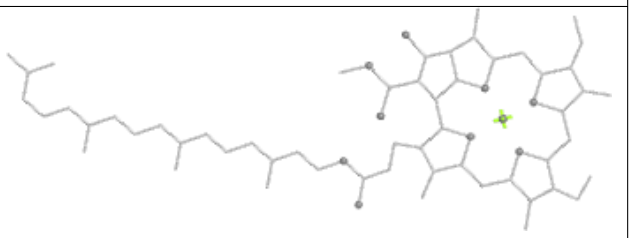
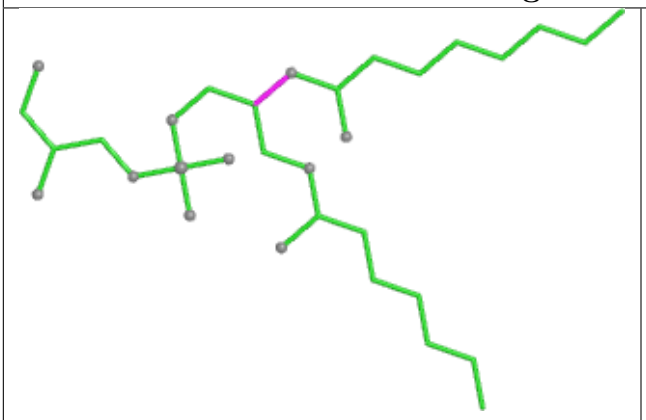


Rings

Ligand LHG B 808



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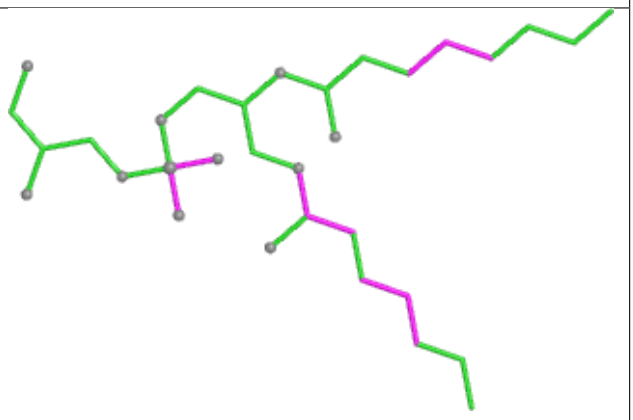

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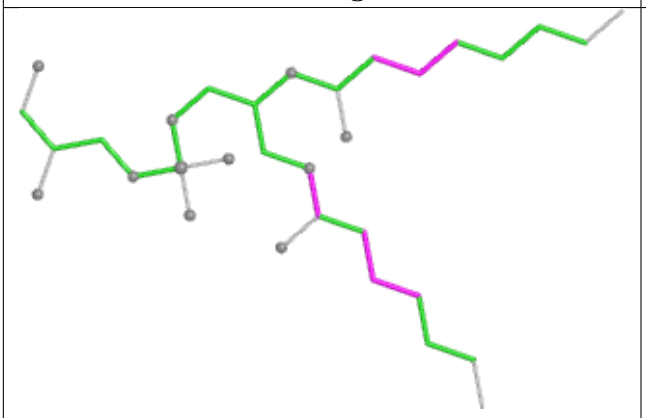

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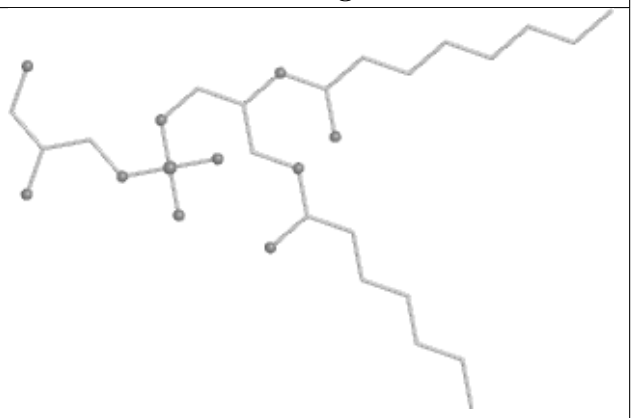
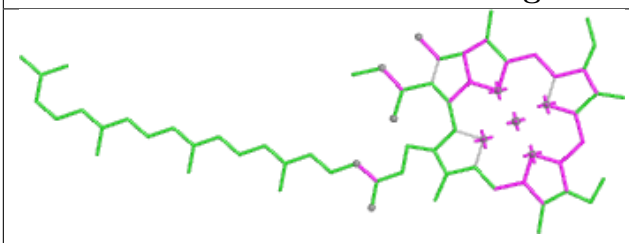


Rings

Ligand CHL A 844



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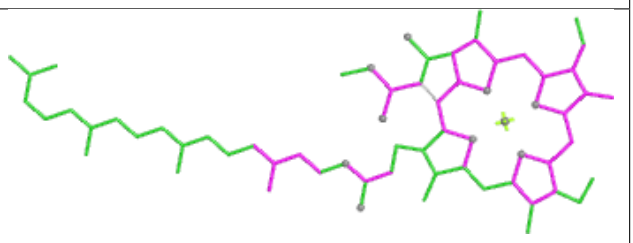
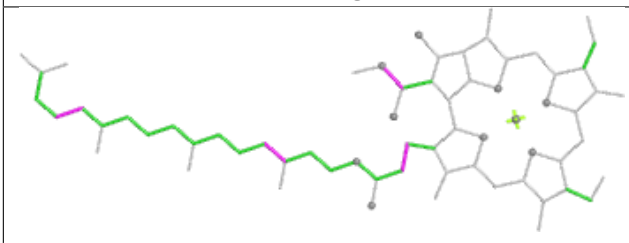


Bond angles



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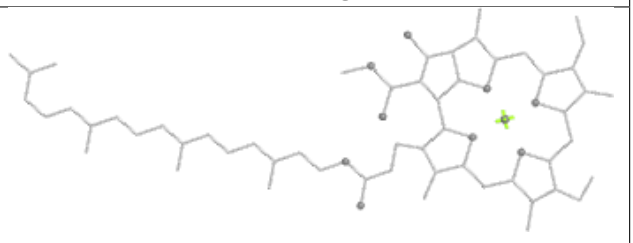
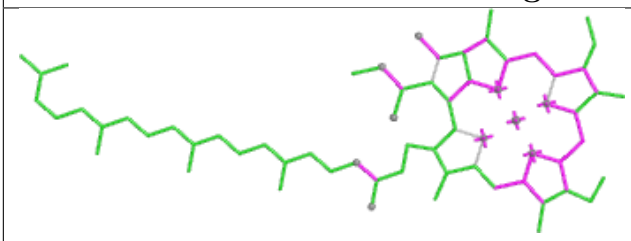
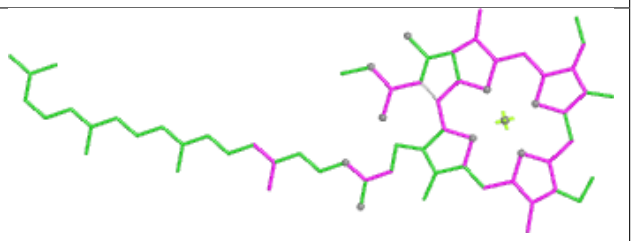
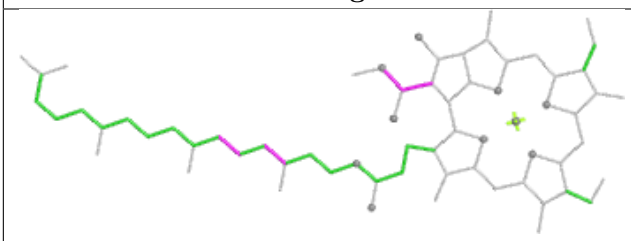
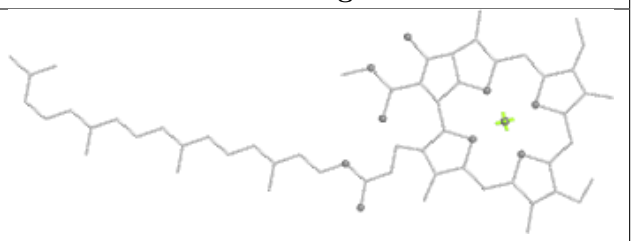


Rings

Ligand CHL A 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

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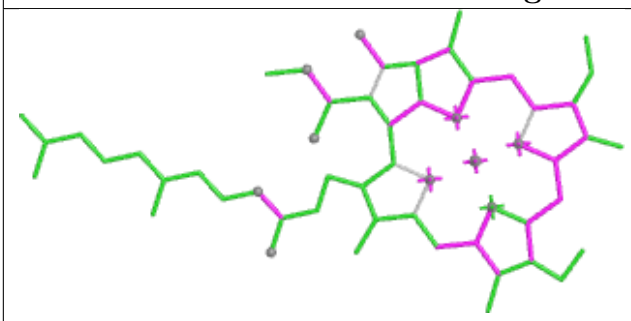
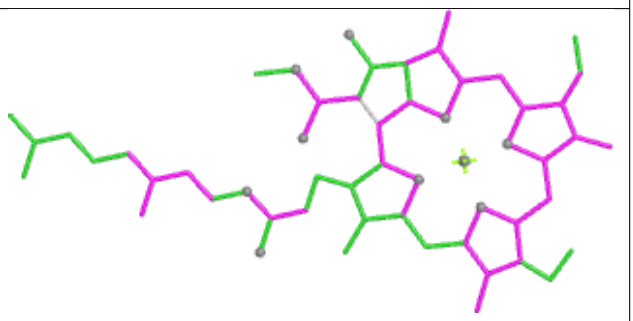
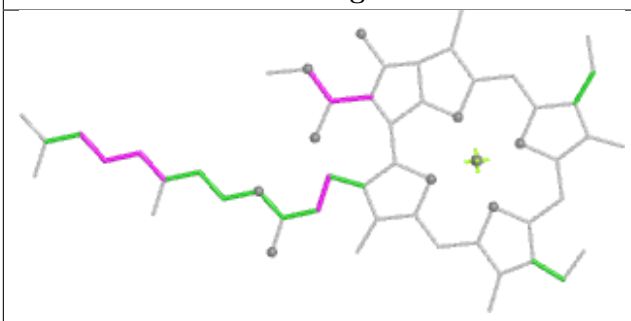
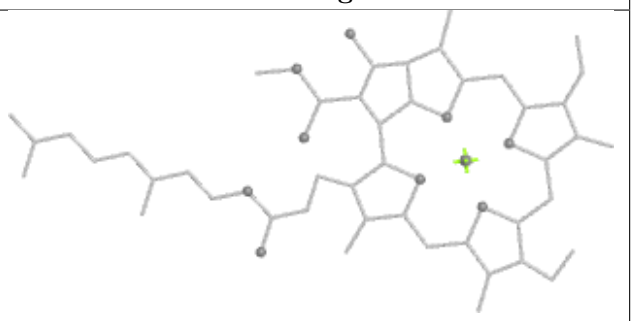
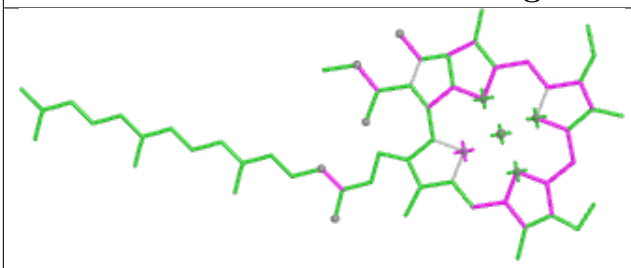
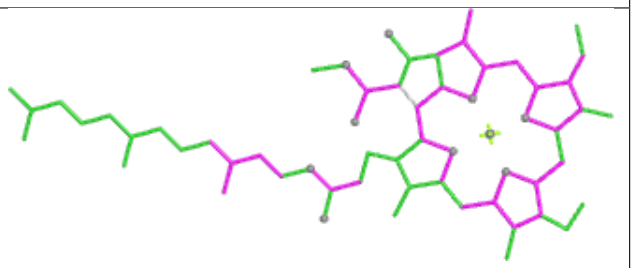
	
Bond lengths	Bond angles
	
Torsions	Rings

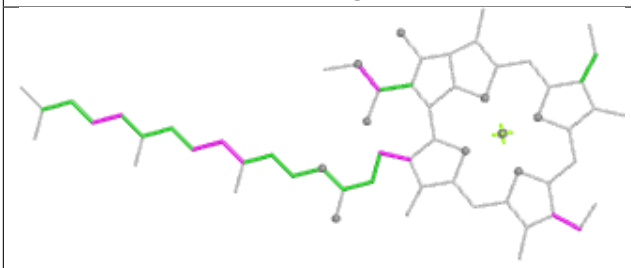
Ligand CHL A 824



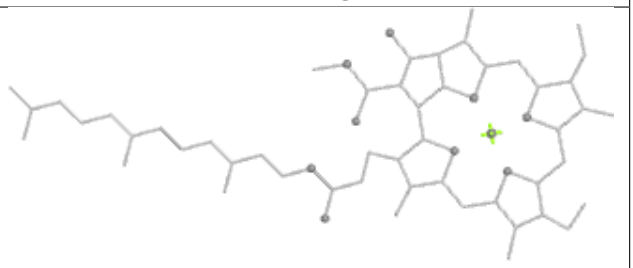
Bond lengths



Bond angles

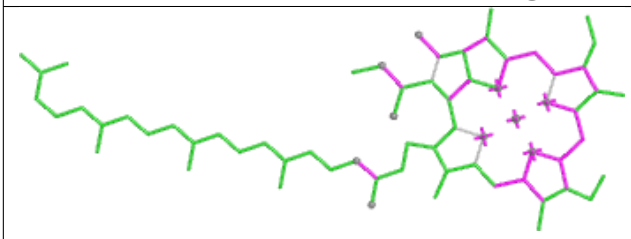


Torsions



Rings

Ligand CHL A 820



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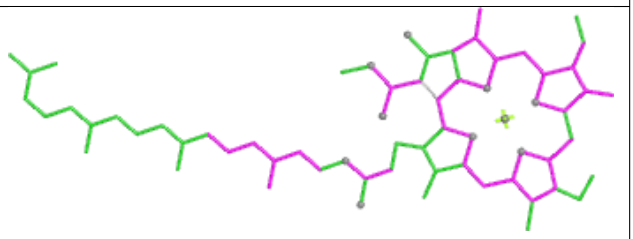

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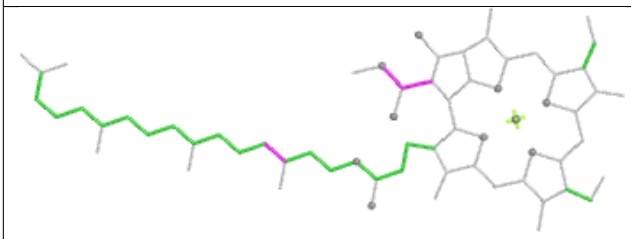

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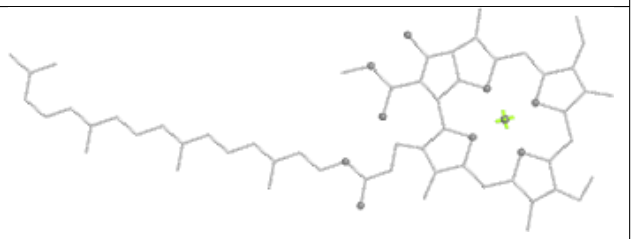
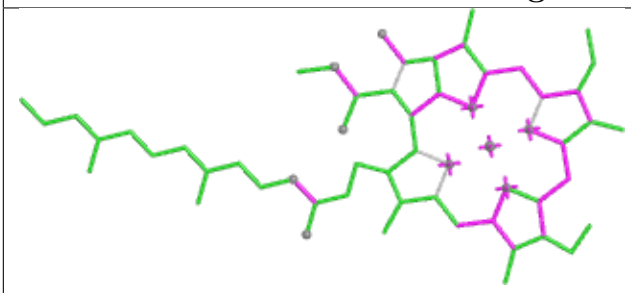


Rings

Ligand CHL 6 306



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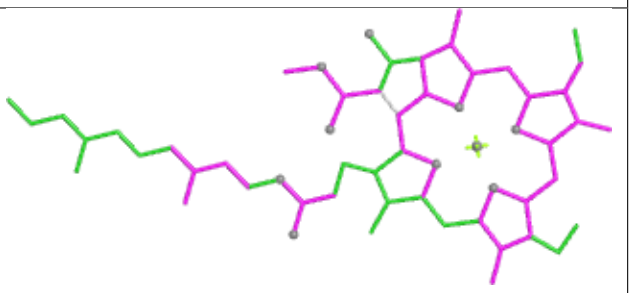

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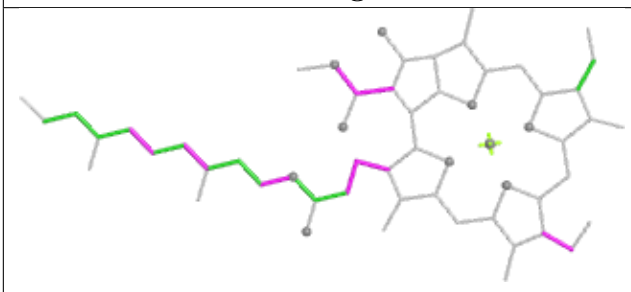

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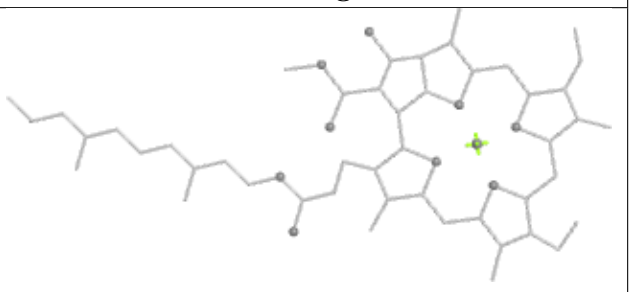
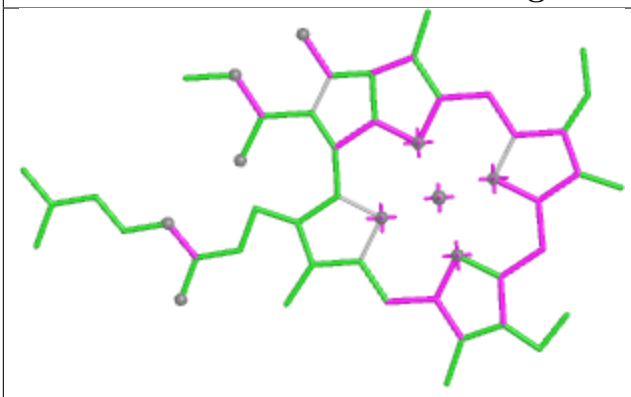


Rings

Ligand CHL 6 315



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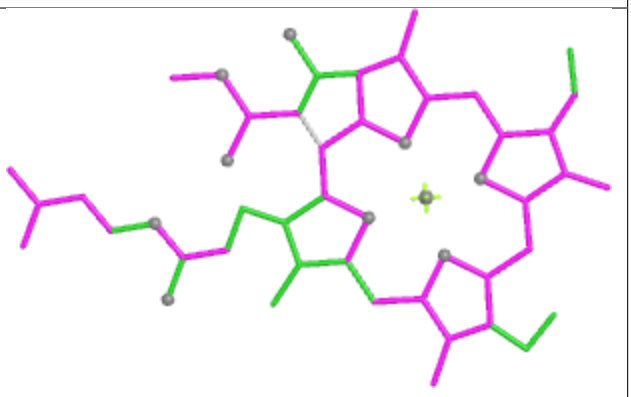
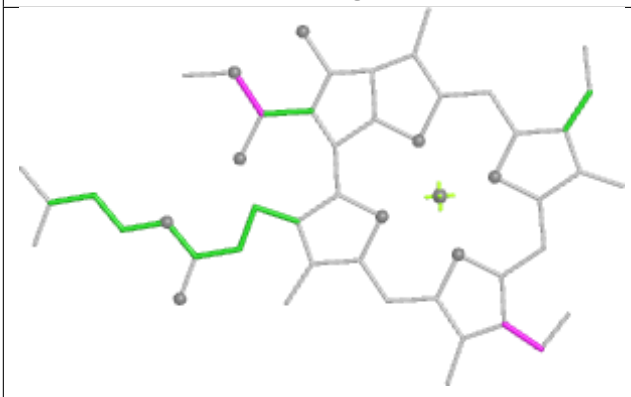


Bond angles



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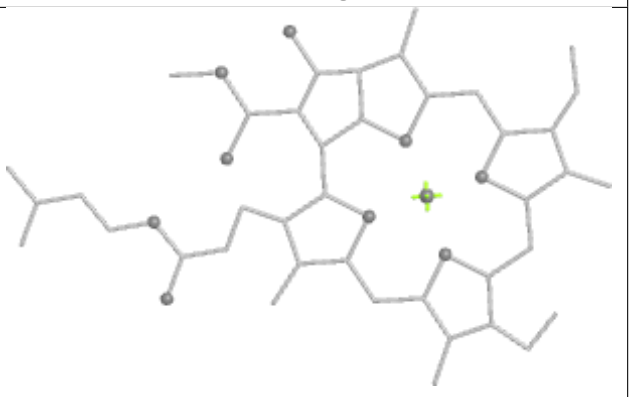
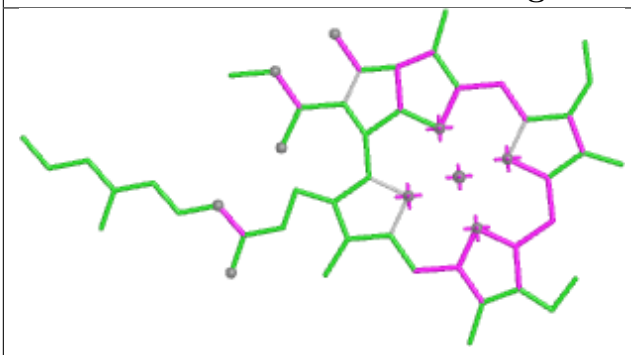


Rings

Ligand CHL 7 323



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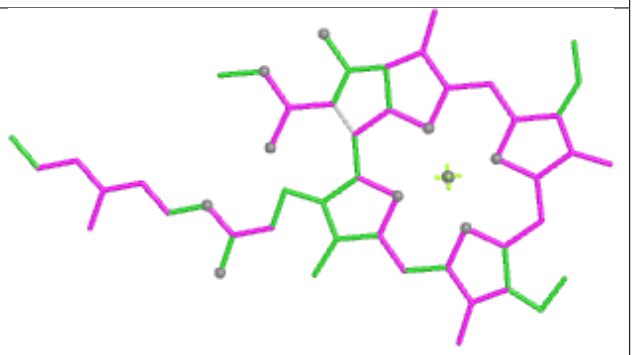
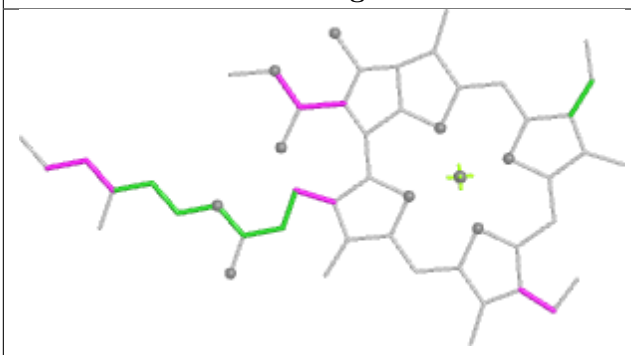


Bond angles



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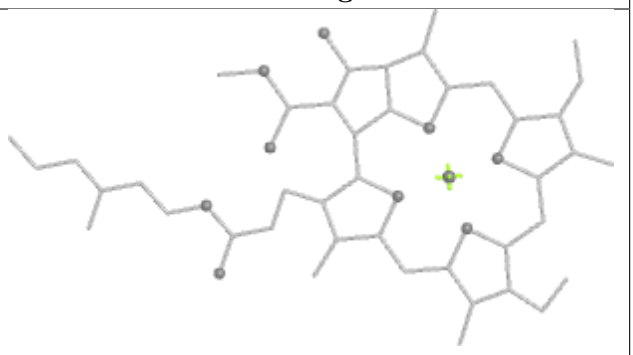
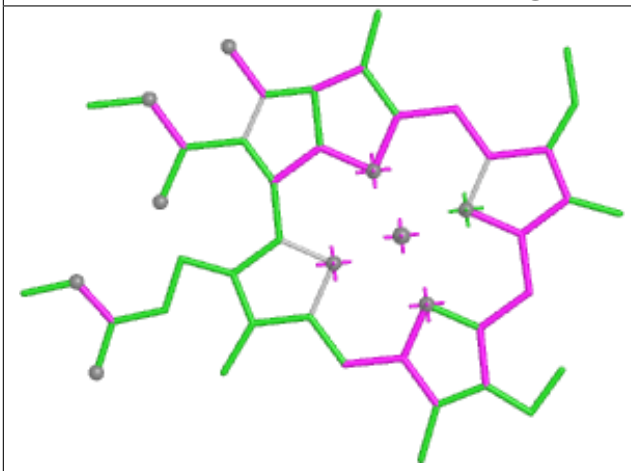


Rings

Ligand CHL b 313



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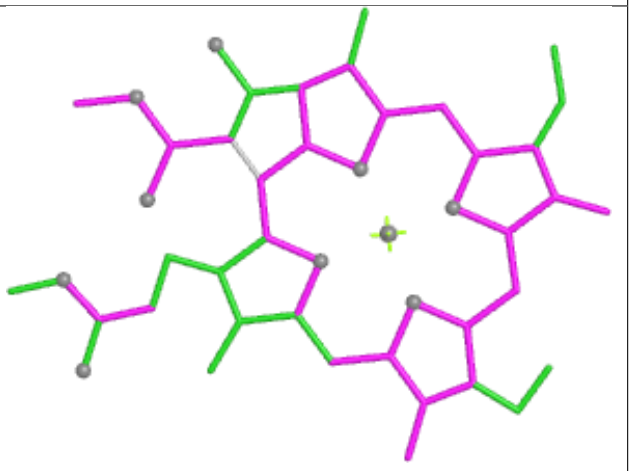

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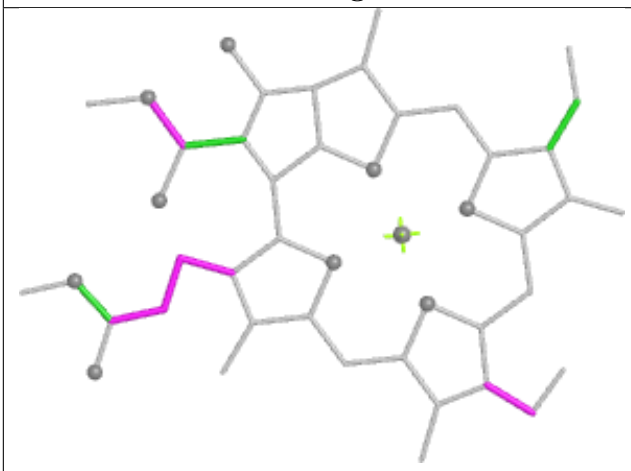

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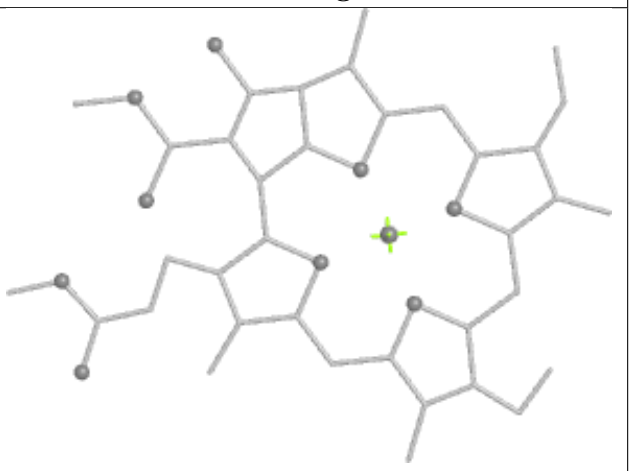
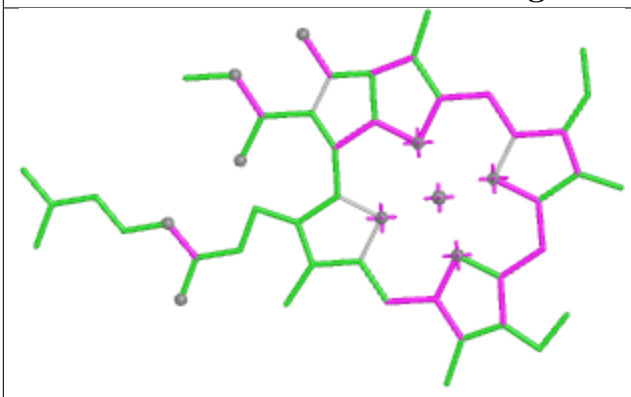


Rings

Ligand CHL 5 312



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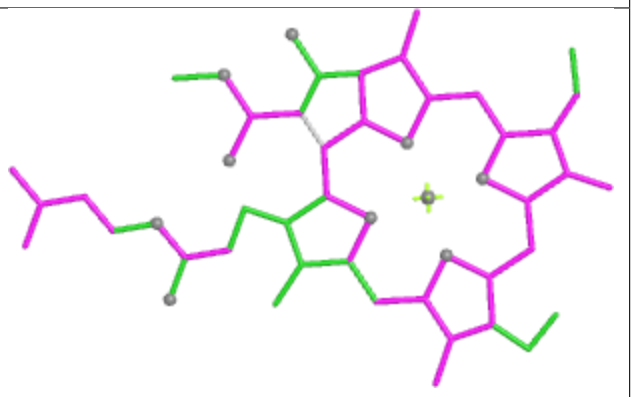
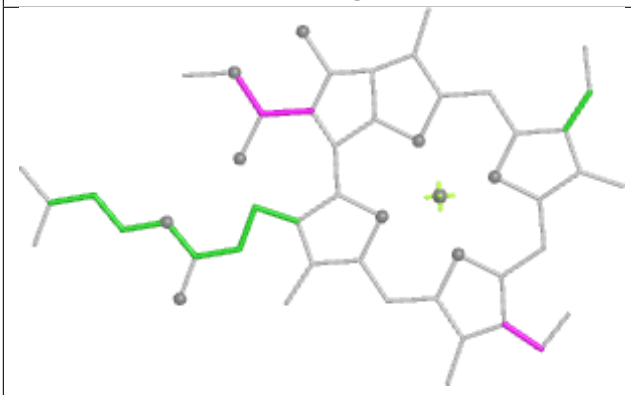


Bond angles



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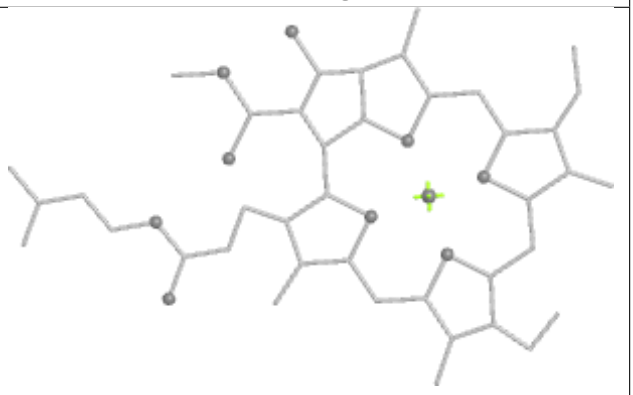
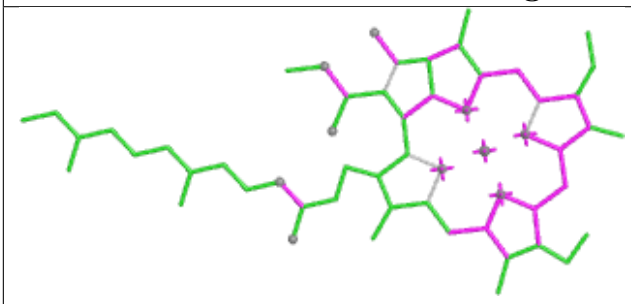


Rings

Ligand CHL A 854



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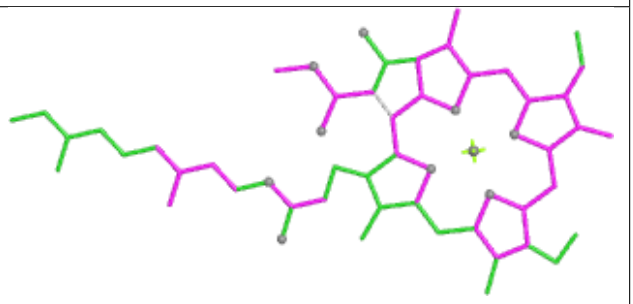

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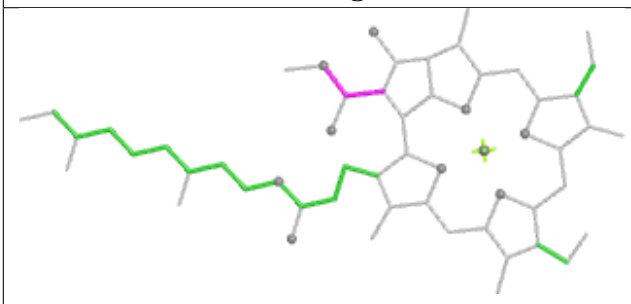

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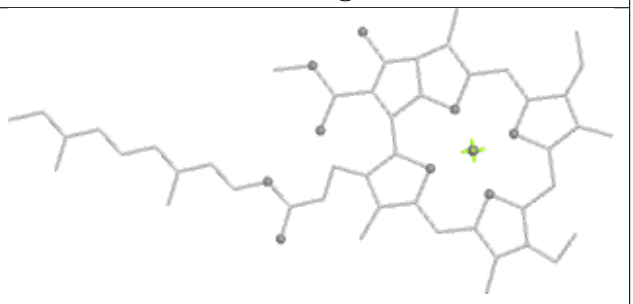
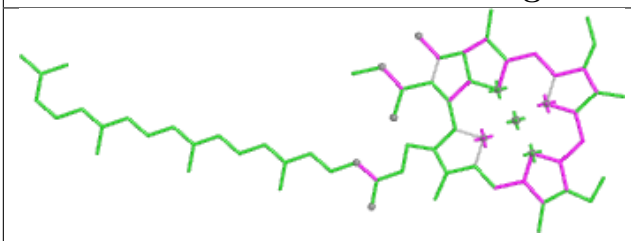


Rings

Ligand CHL A 823



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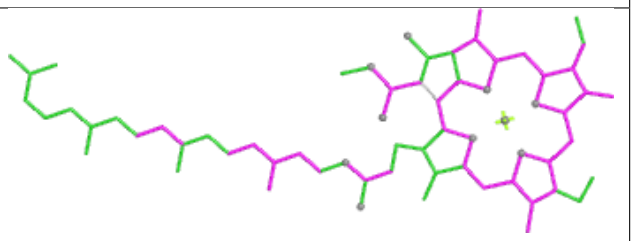
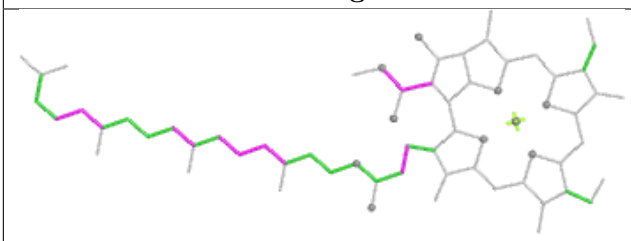


Bond angles



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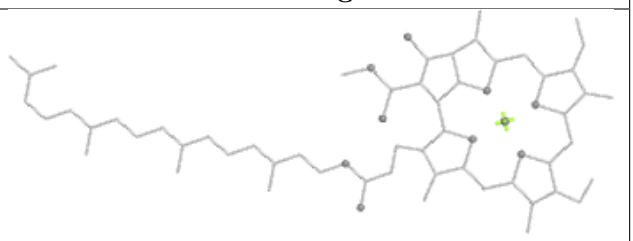
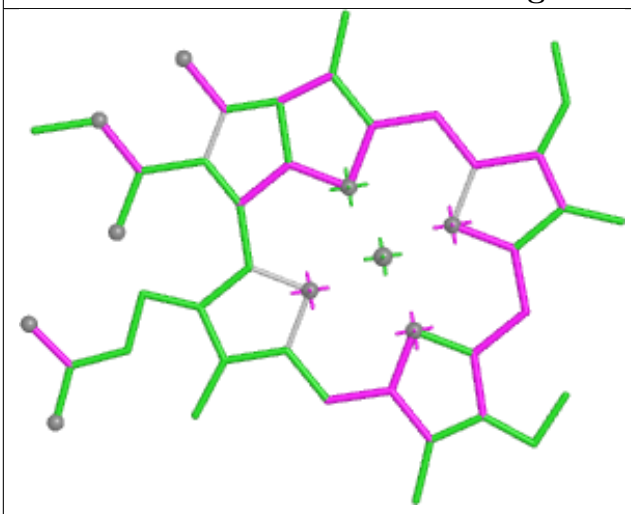


Rings

Ligand CHL 4 305



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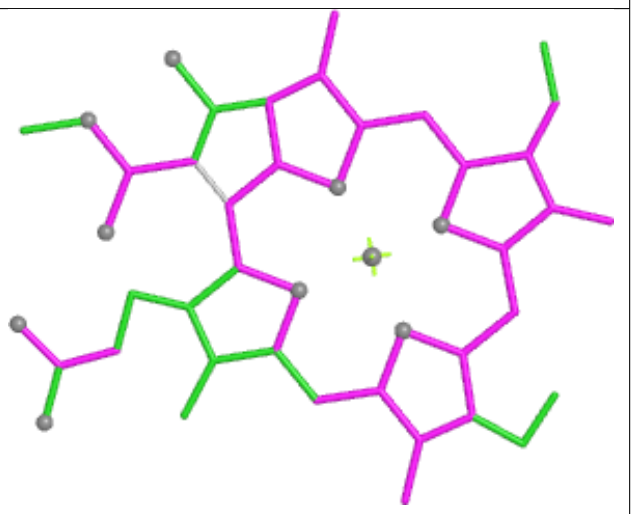

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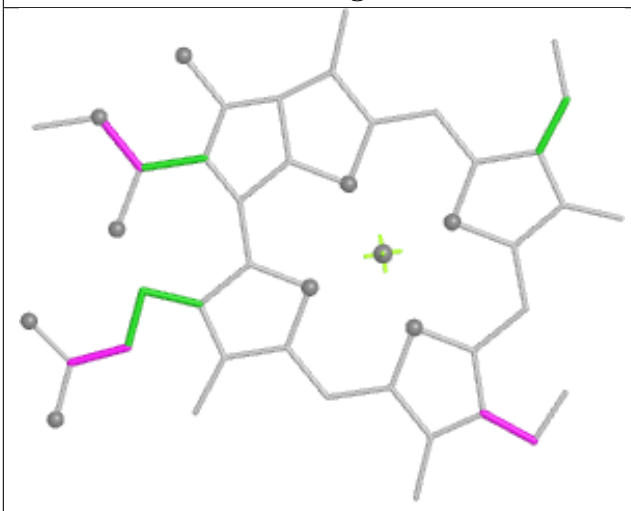

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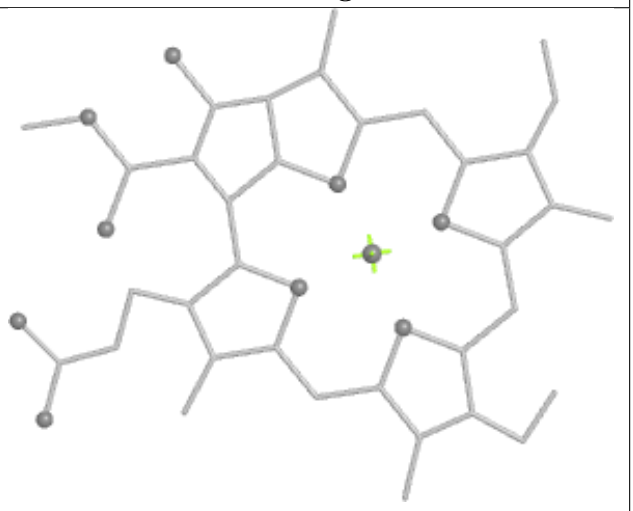
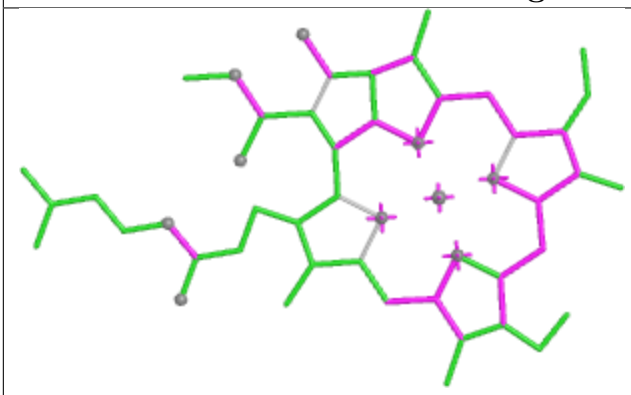


Rings

Ligand CHL 4 320



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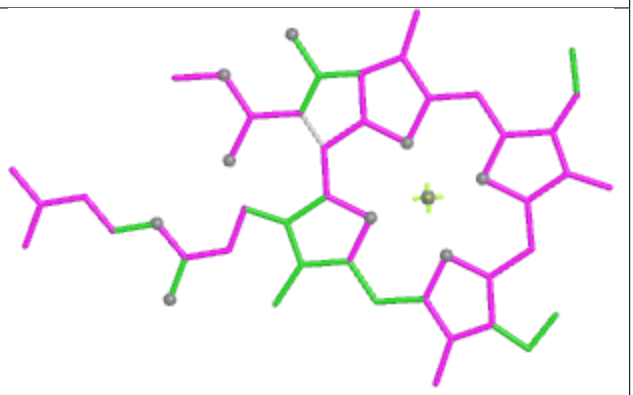
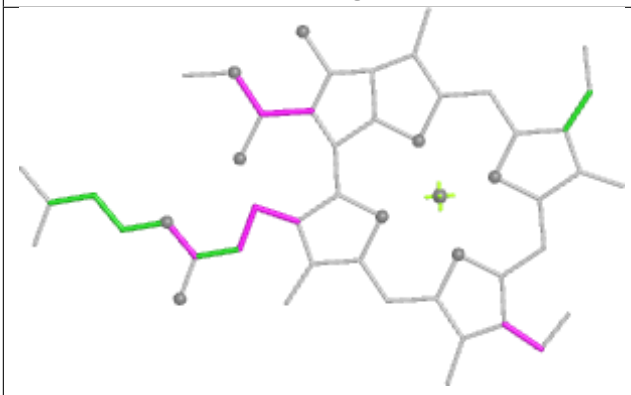


Bond angles



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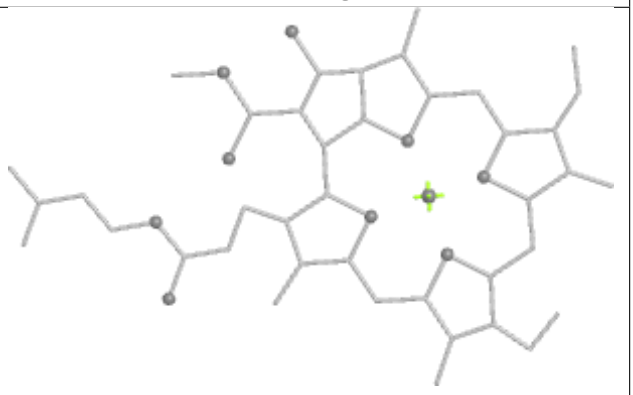
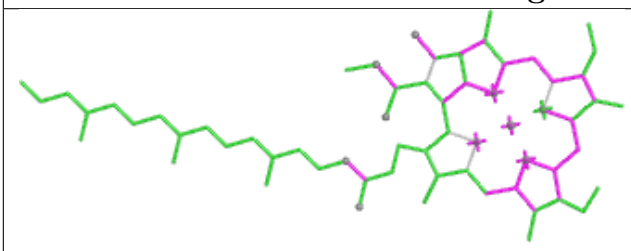


Rings

Ligand CHL 7 314



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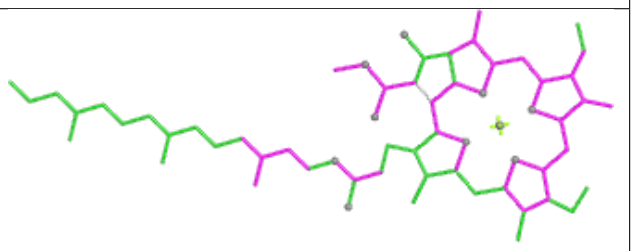
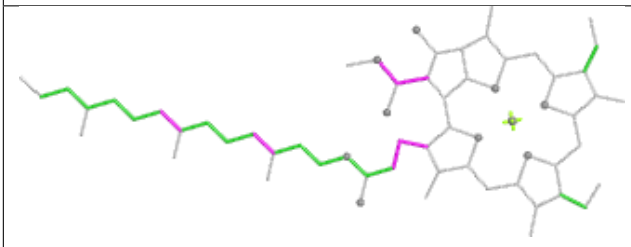


Bond angles



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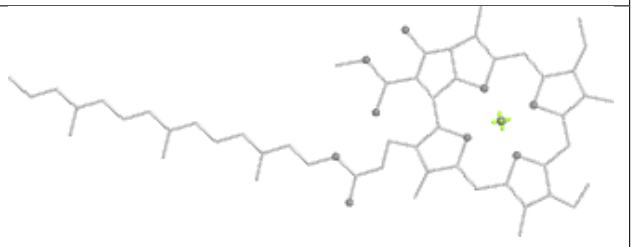
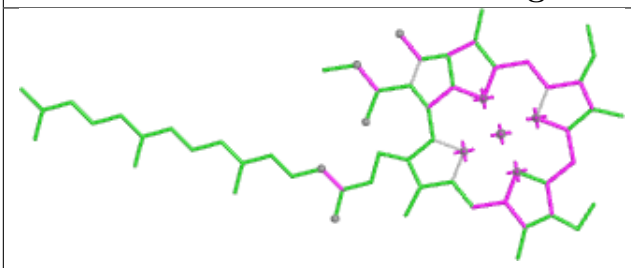
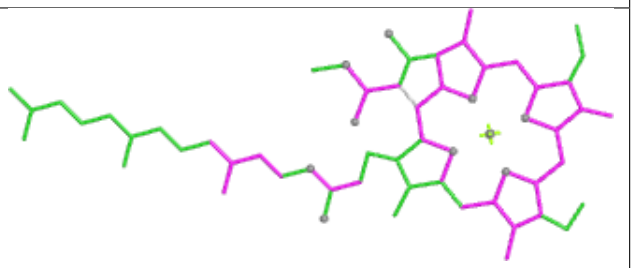


Rings

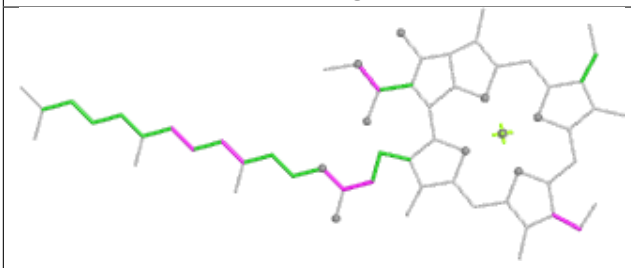
Ligand CHL 4 308



Bond lengths



Bond angles



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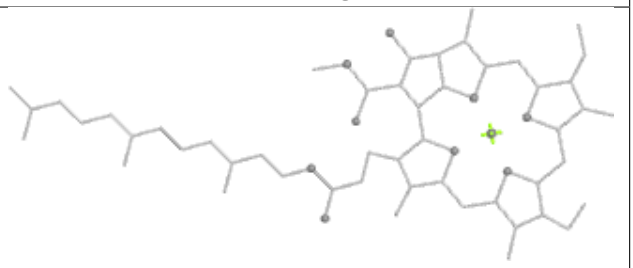
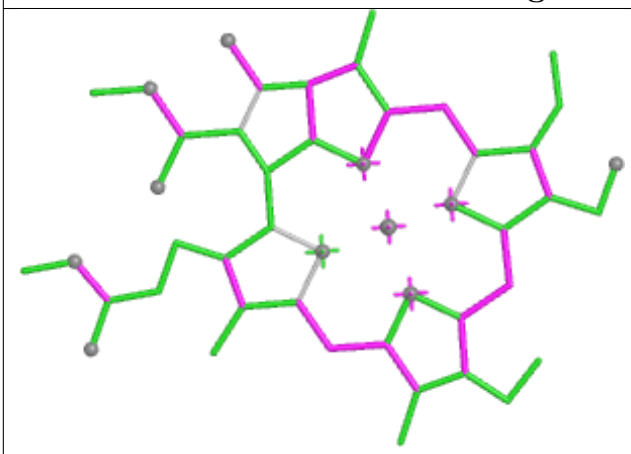


Rings

Ligand CHL 6 318



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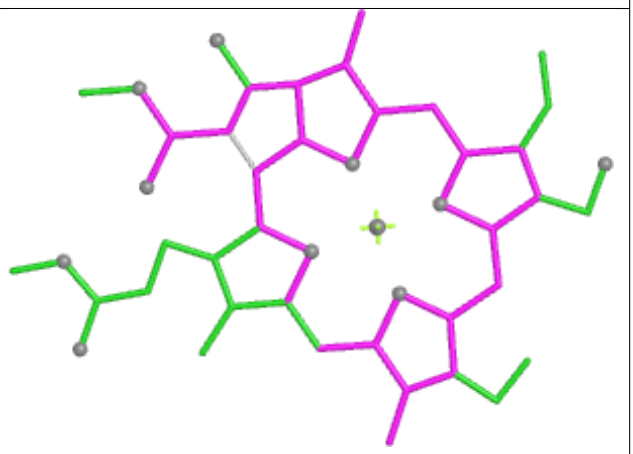
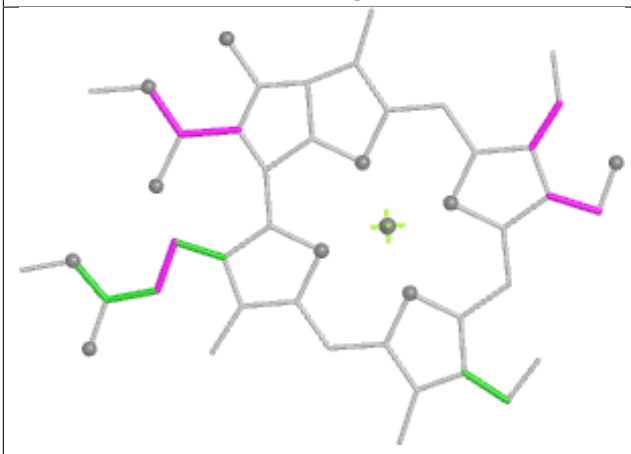


Bond angles



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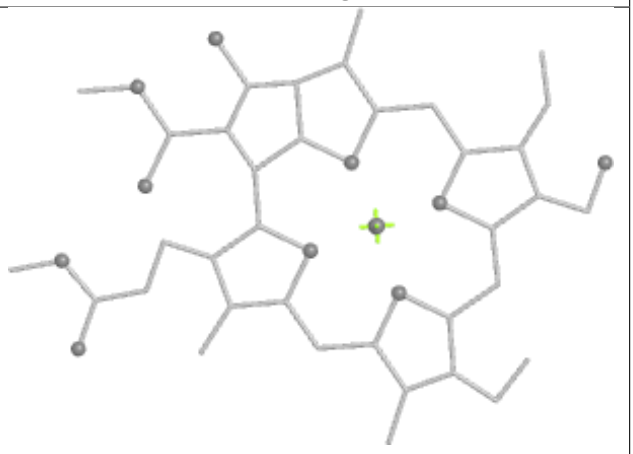
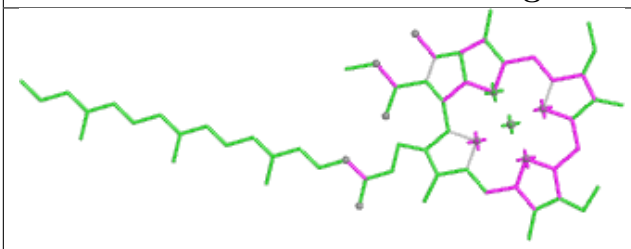
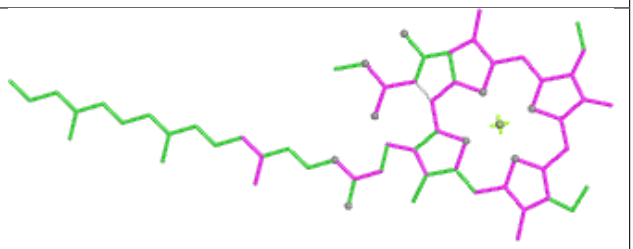


Rings

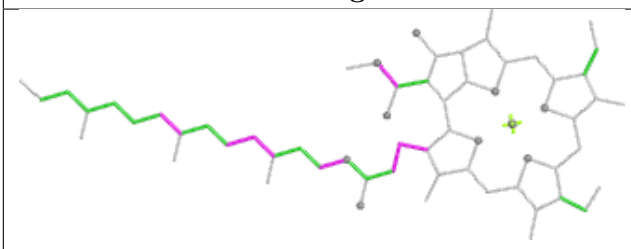
Ligand CHL A 826



Bond lengths



Bond angles



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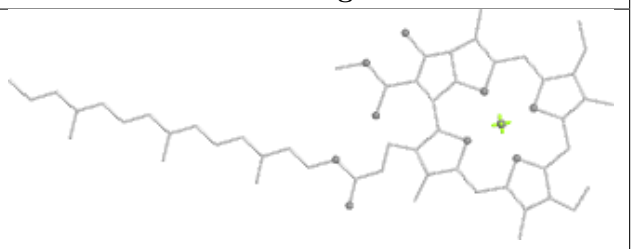
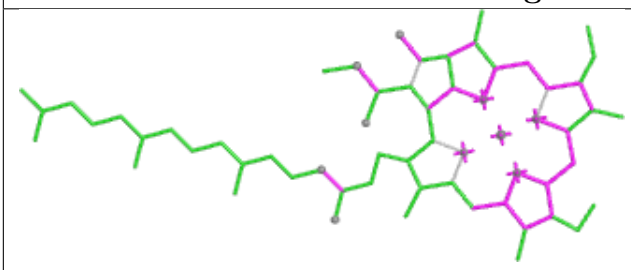
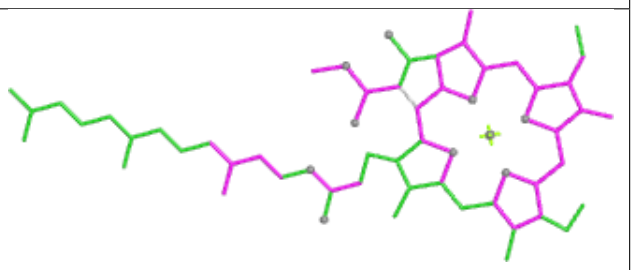


Rings

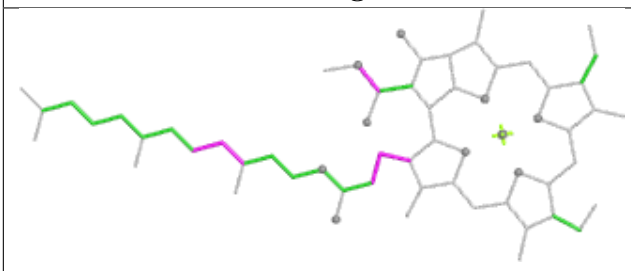
Ligand CHL B 839



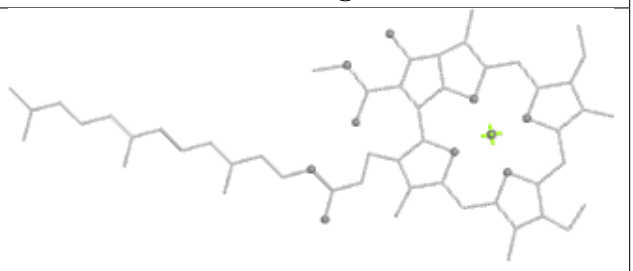
Bond lengths



Bond angles

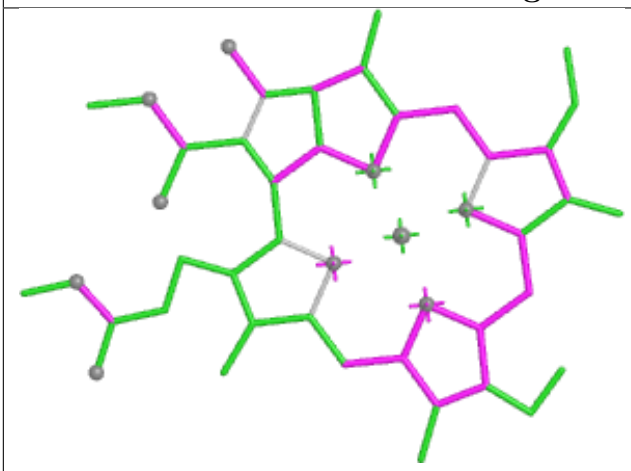


Torsions

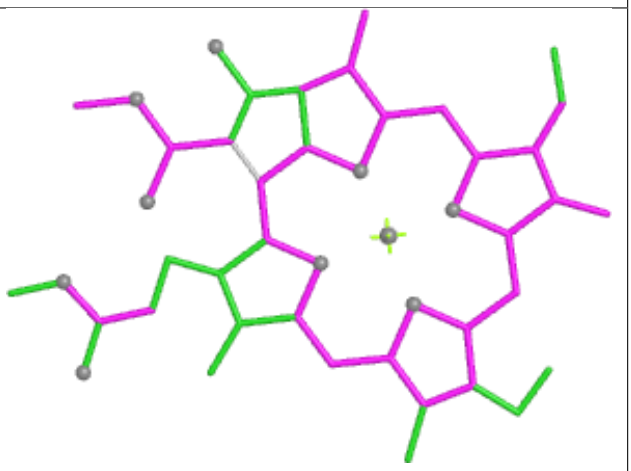


Rings

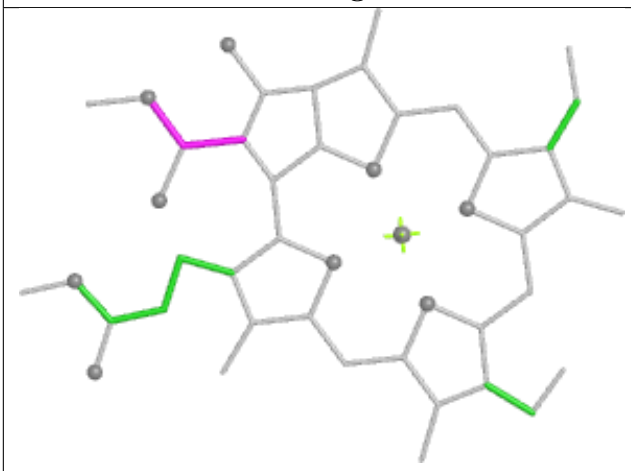
Ligand CHL A 857



Bond lengths



Bond angles



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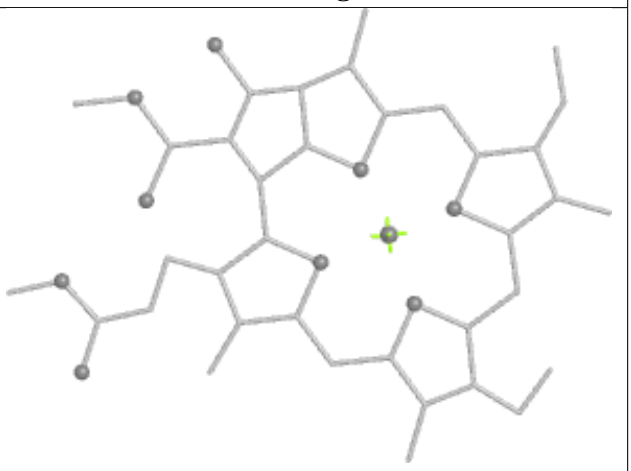
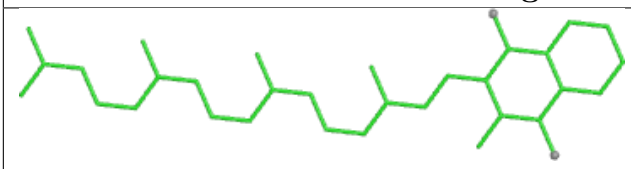
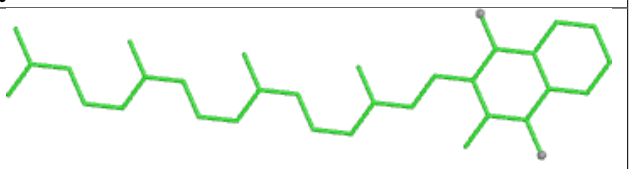


Rings

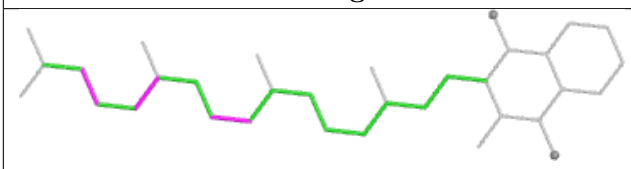
Ligand PQN A 801



Bond lengths



Bond angles



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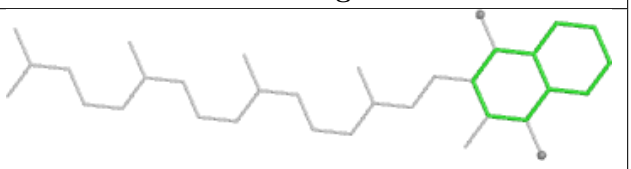
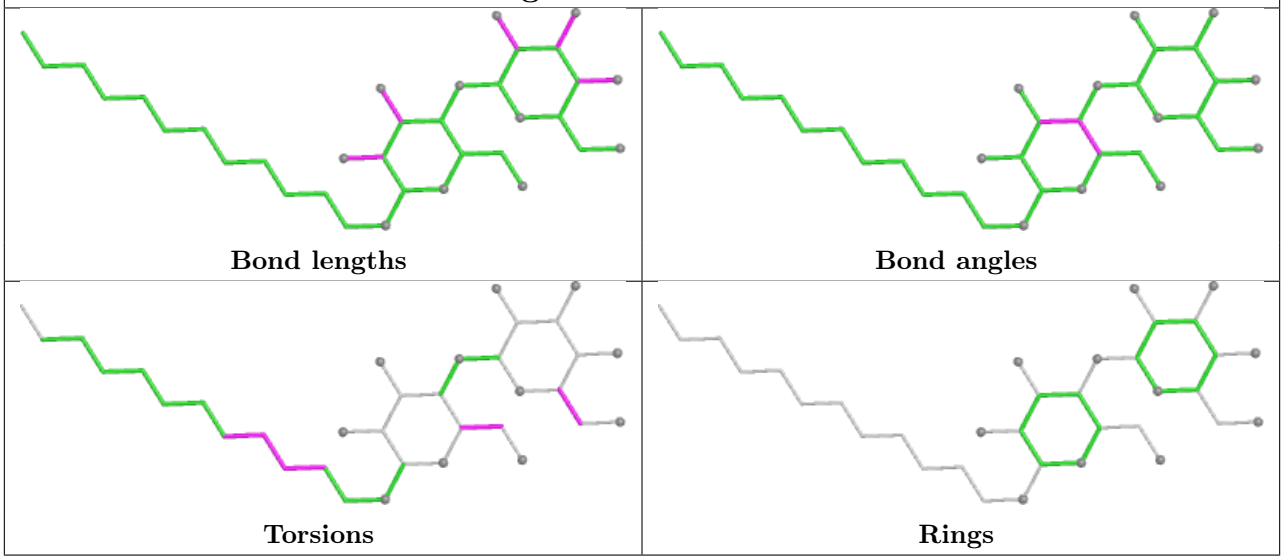
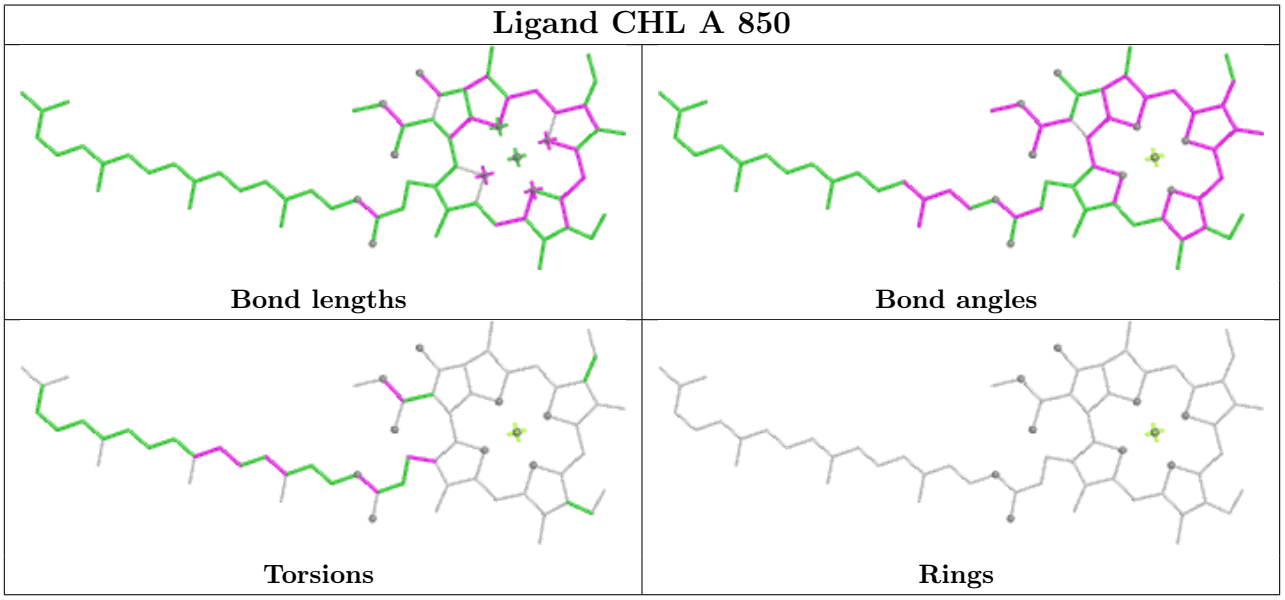


Rings

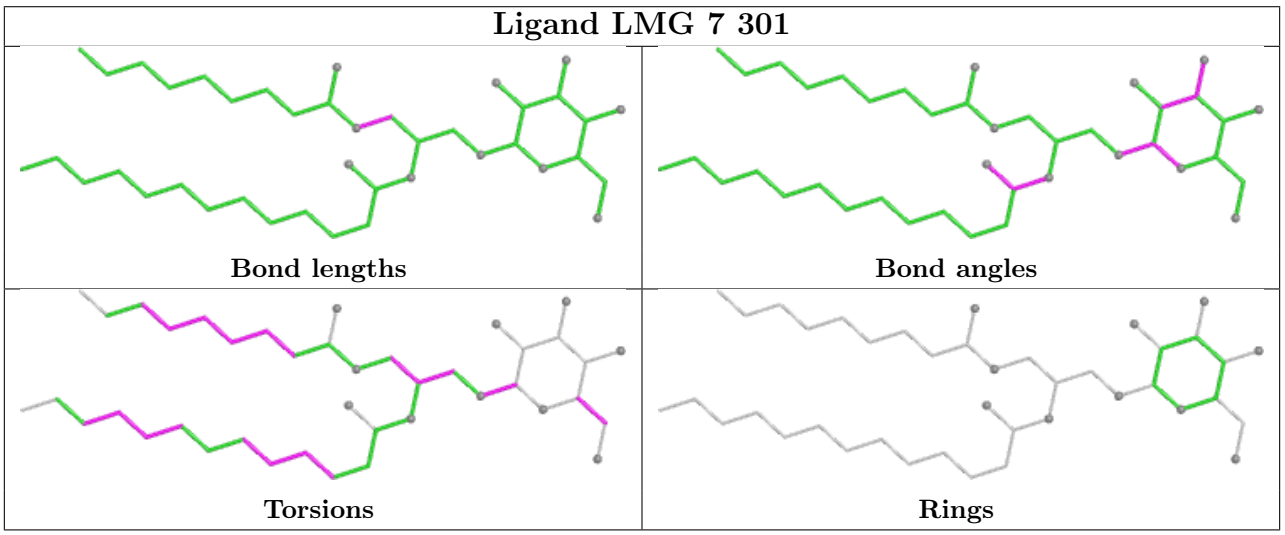
Ligand LMT A 809

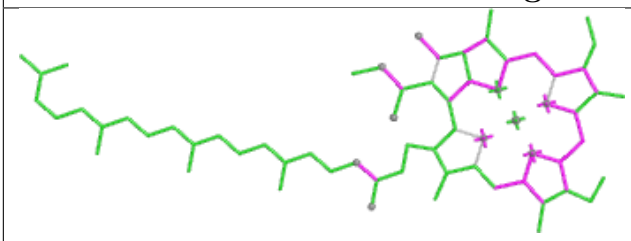
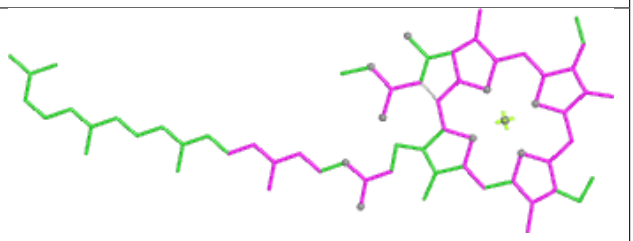
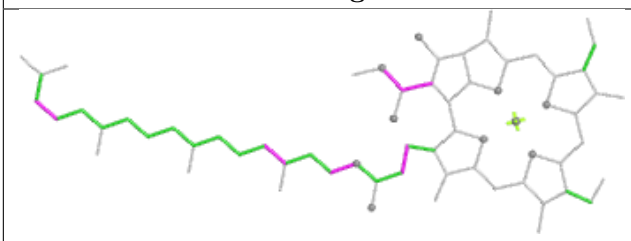
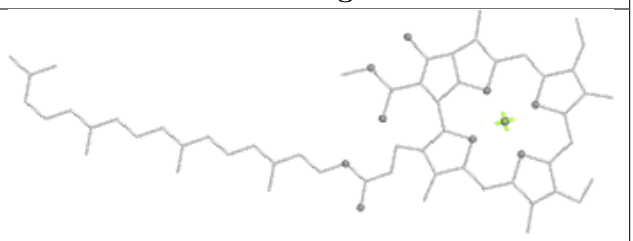


Ligand CHL A 850



Ligand LMG 7 301



Ligand CHL B 832	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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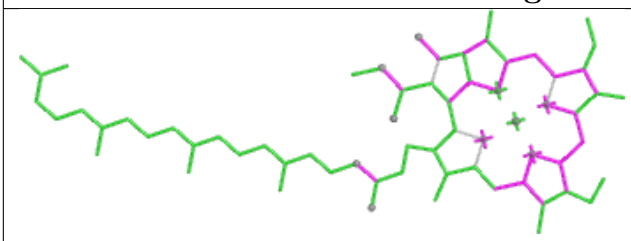
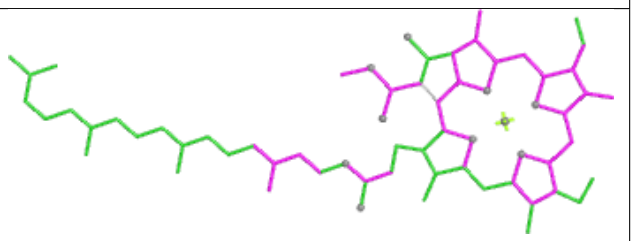
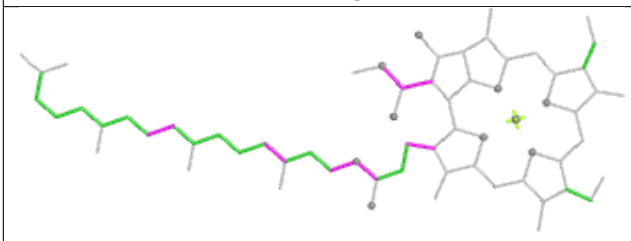
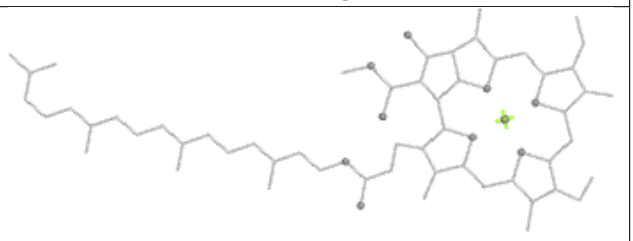
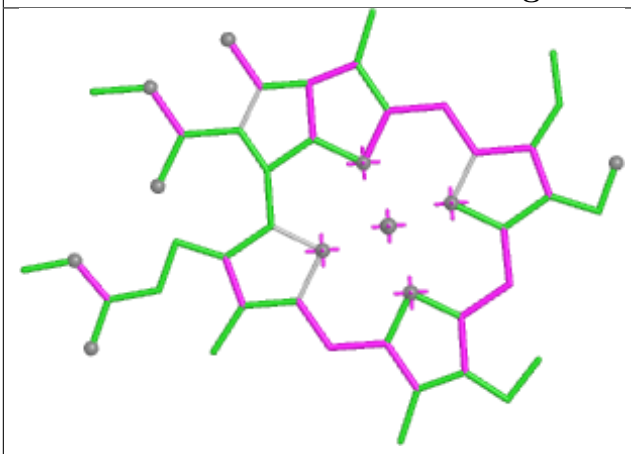
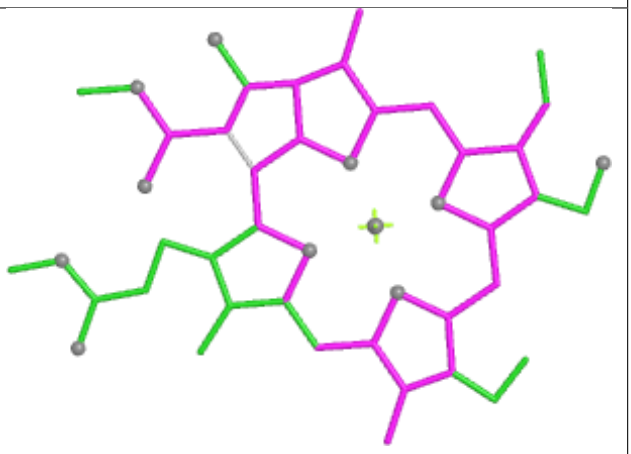
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

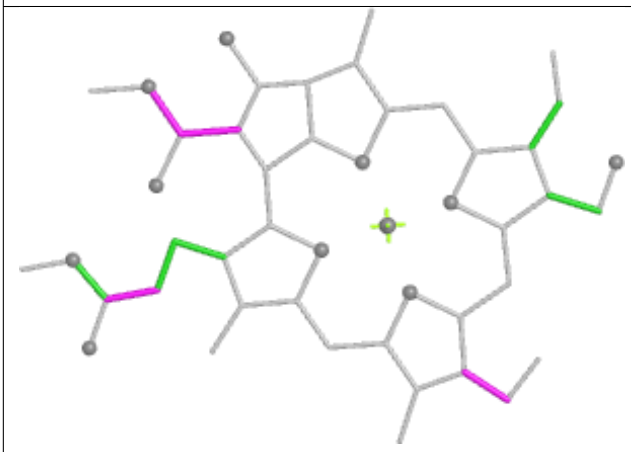
Ligand CHL K 207



Bond lengths



Bond angles



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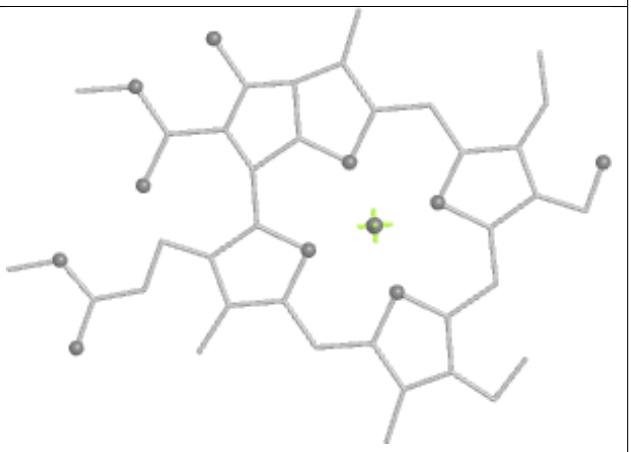
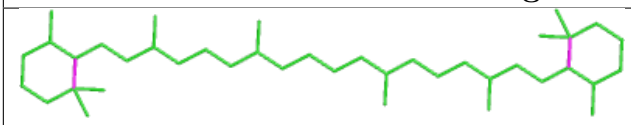


Rings

Ligand BCR B 804



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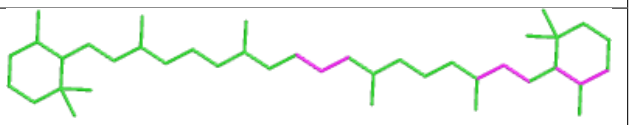
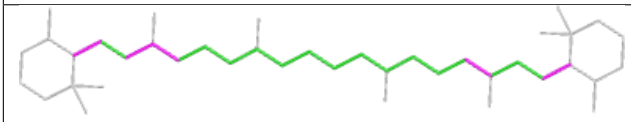


Bond angles



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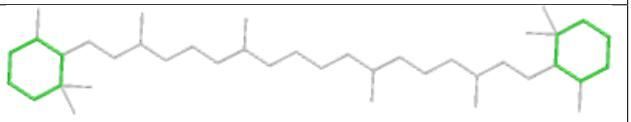
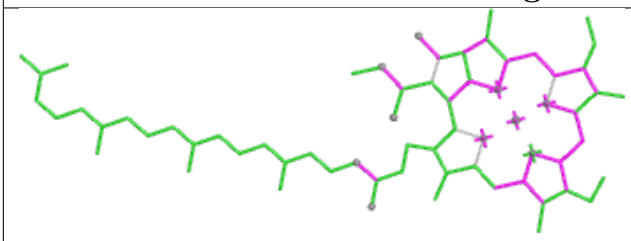
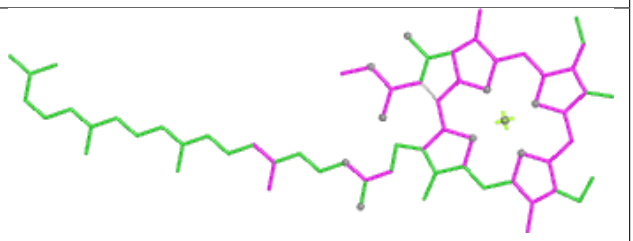
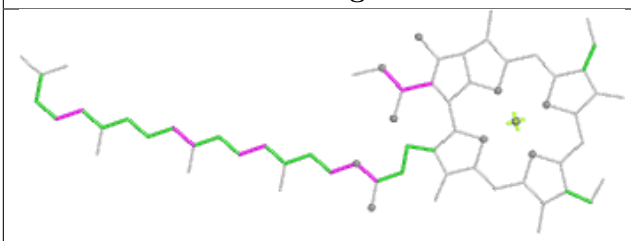
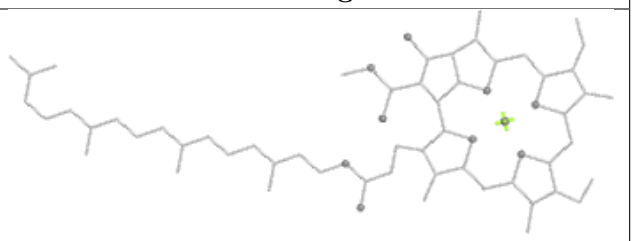


Rings

Ligand CHL A 853	
	
Bond lengths	Bond angles
	
Torsions	Rings

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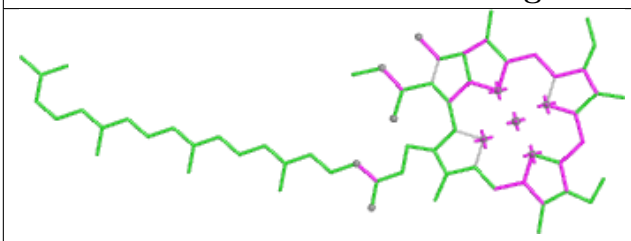
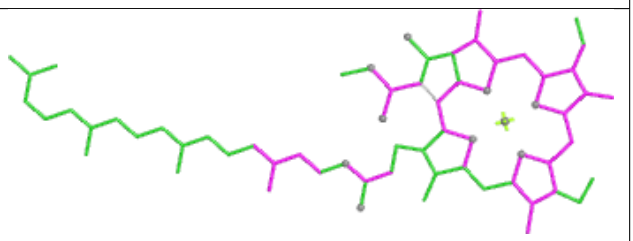
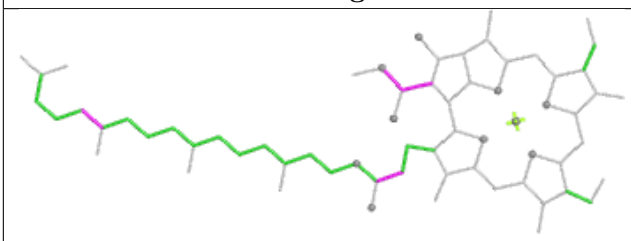
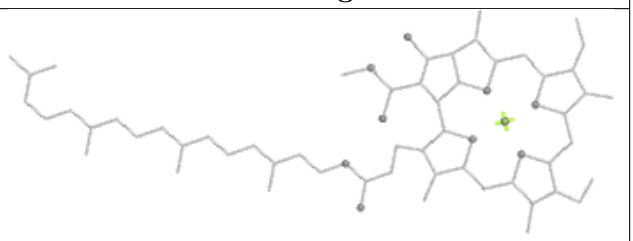
	
Bond lengths	Bond angles
	
Torsions	Rings

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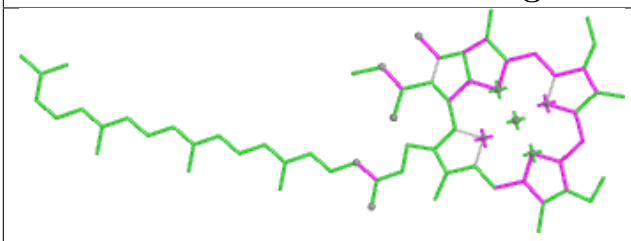
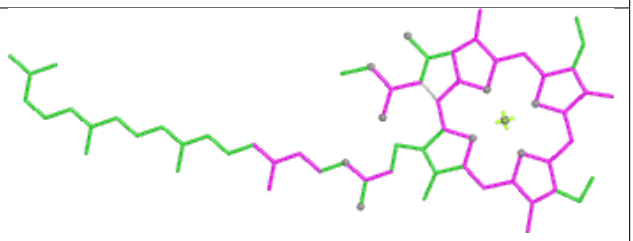
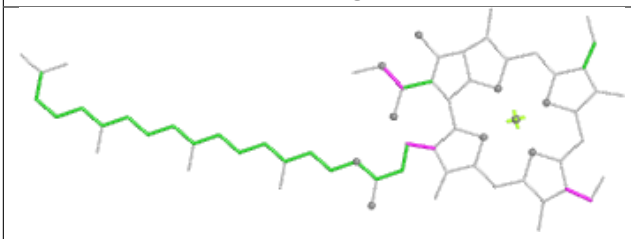
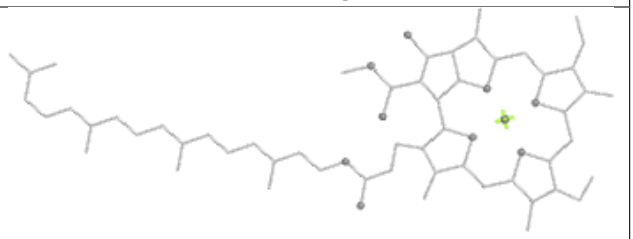
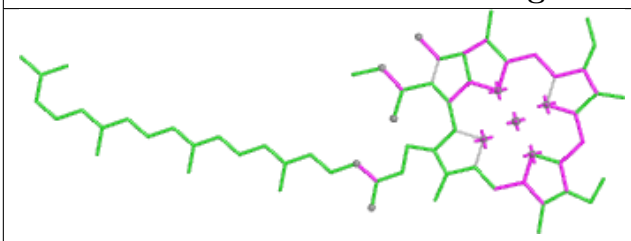
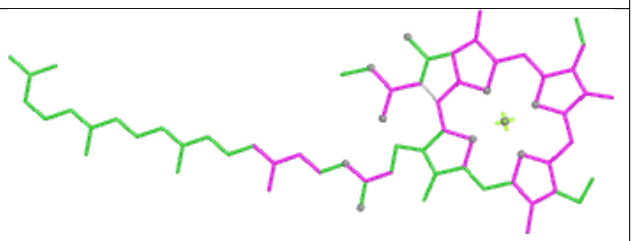
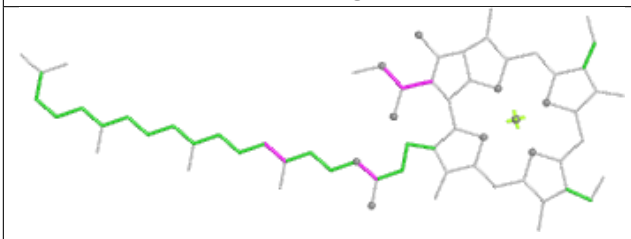
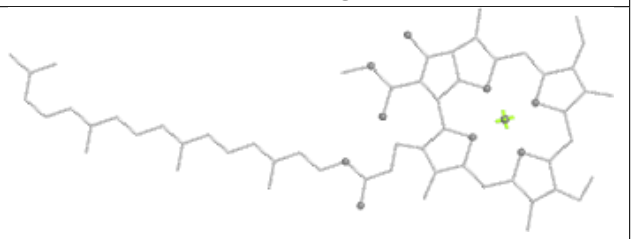
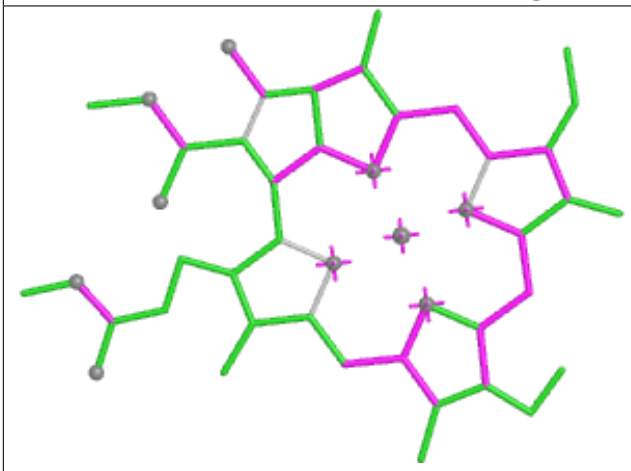
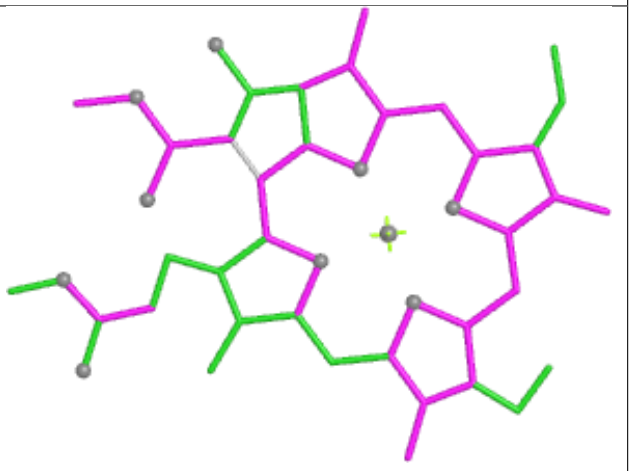
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 3 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

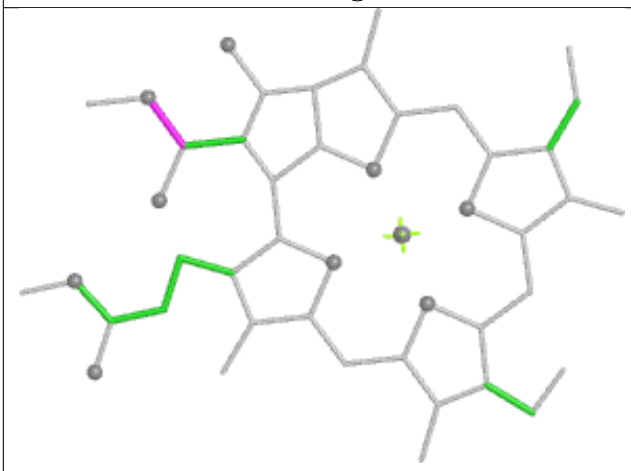
Ligand CHL 3 309



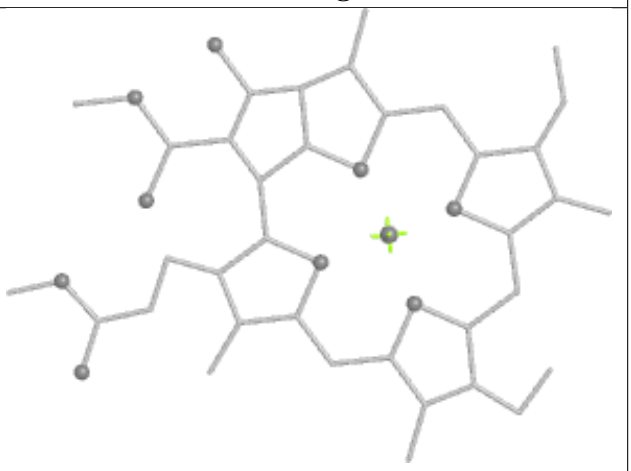
Bond lengths



Bond angles

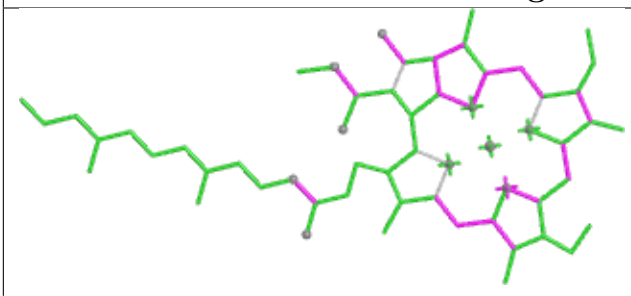


Torsions

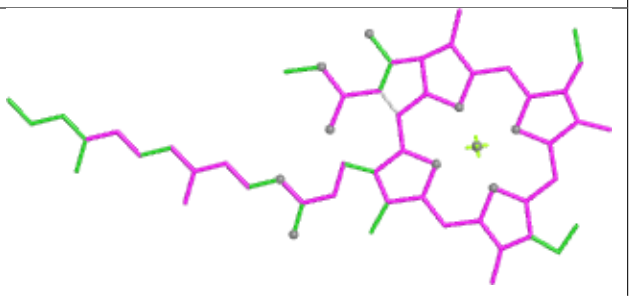


Rings

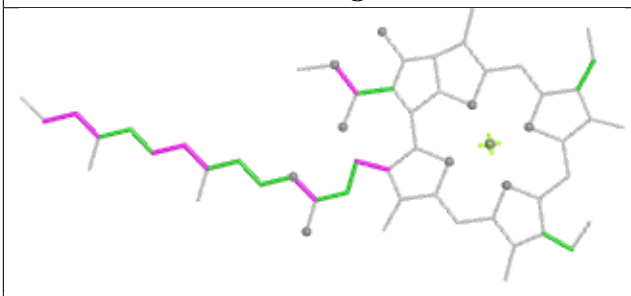
Ligand CHL 5 313



Bond lengths



Bond angles



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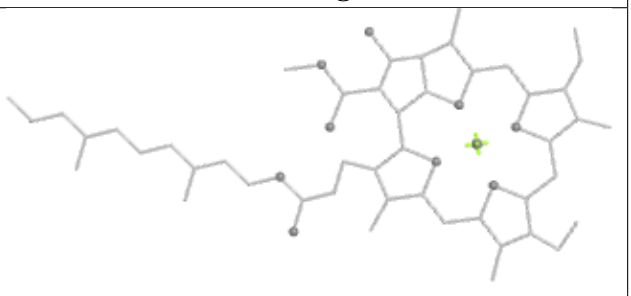
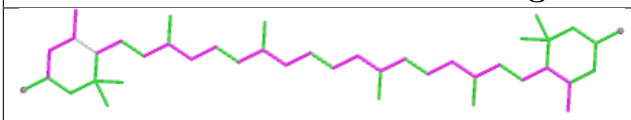
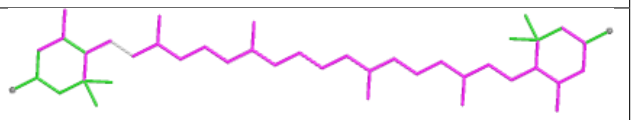


Rings

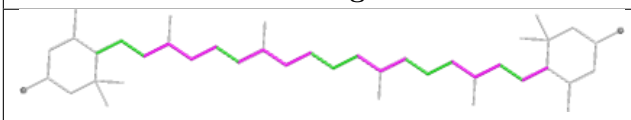
Ligand LUT 3 305



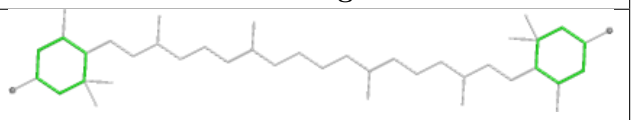
Bond lengths



Bond angles

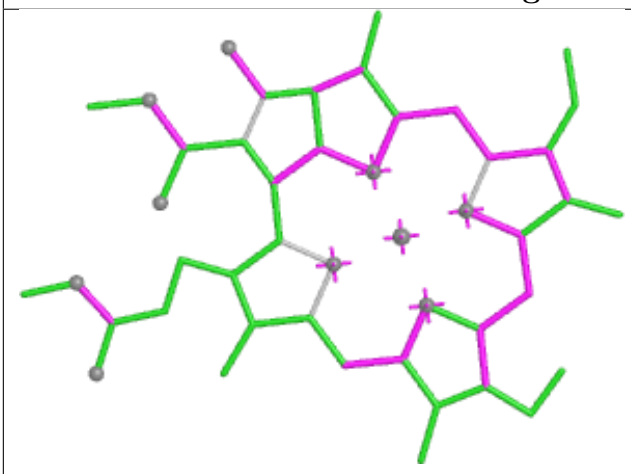


Torsions

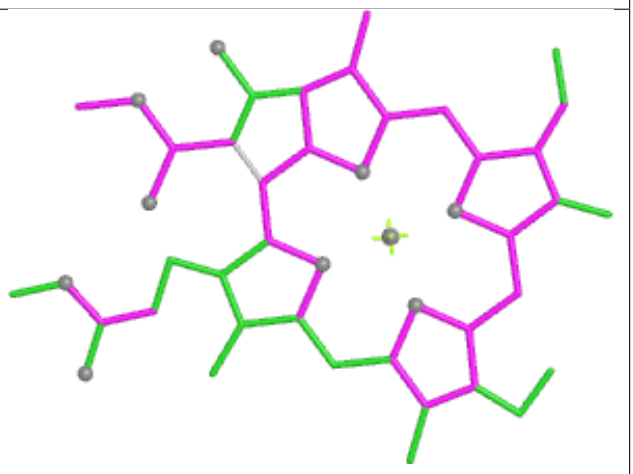


Rings

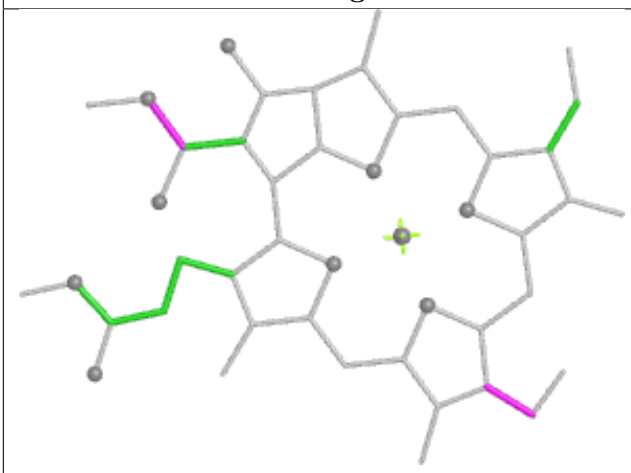
Ligand CHL K 206



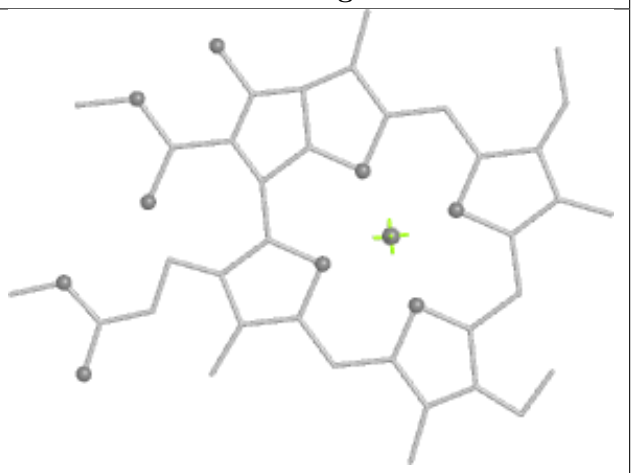
Bond lengths



Bond angles



Torsions

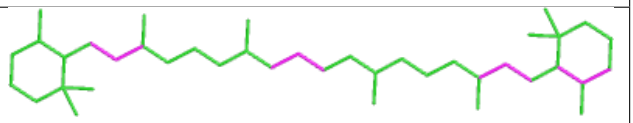


Rings

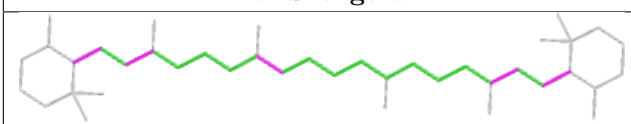
Ligand BCR F 301



Bond lengths



Bond angles



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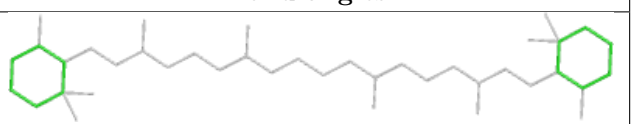
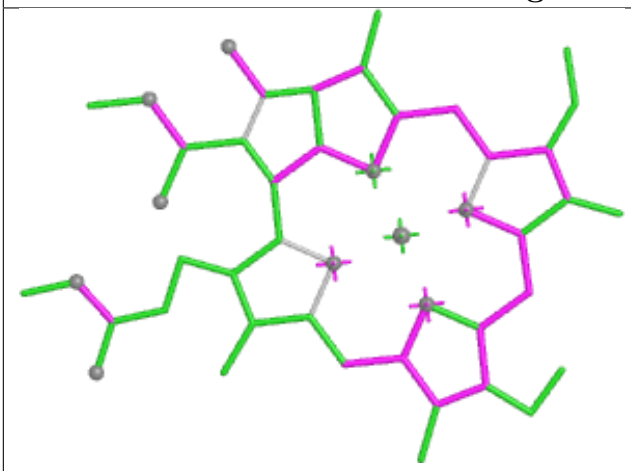
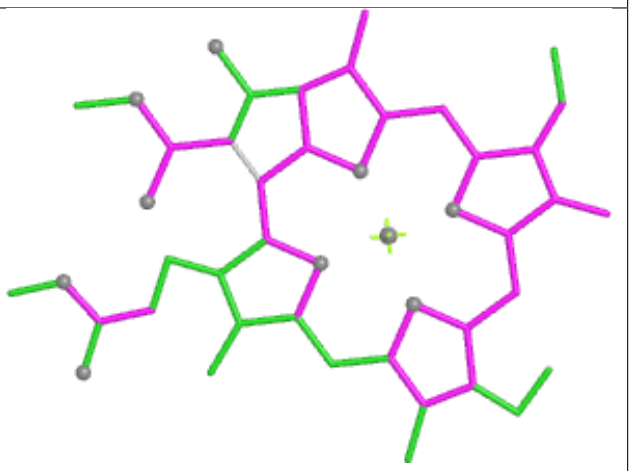


Rings

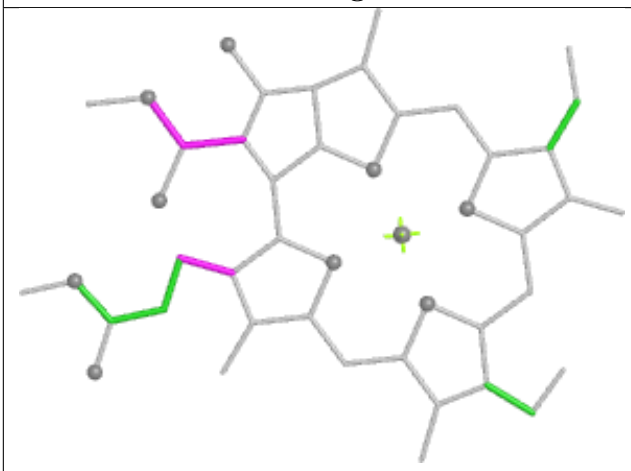
Ligand CHL b 306



Bond lengths



Bond angles



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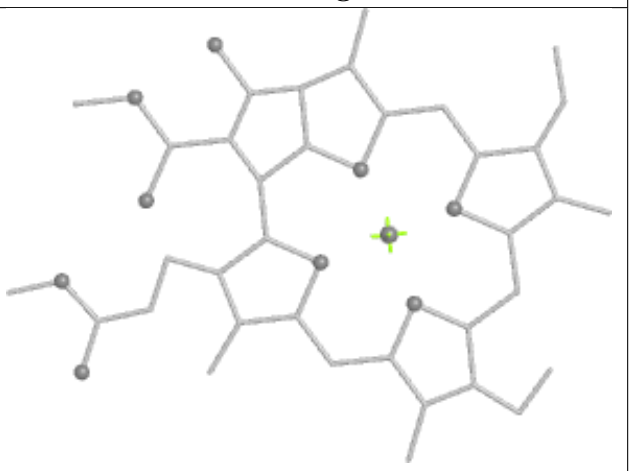
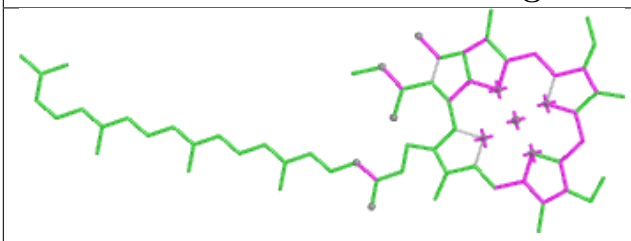
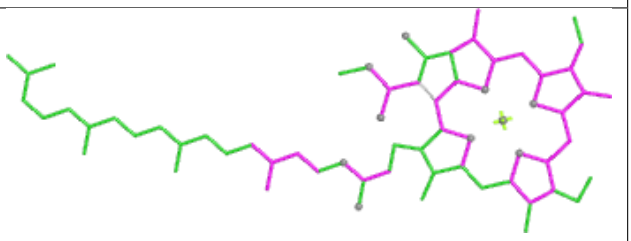


Rings

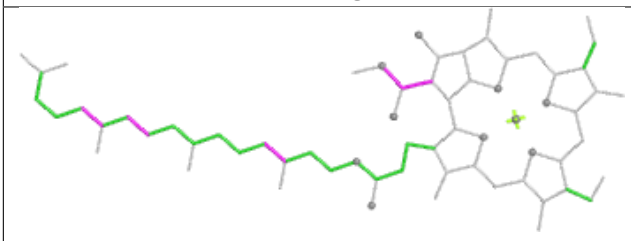
Ligand CHL A 840



Bond lengths



Bond angles



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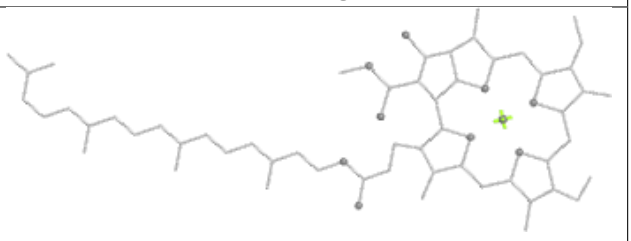
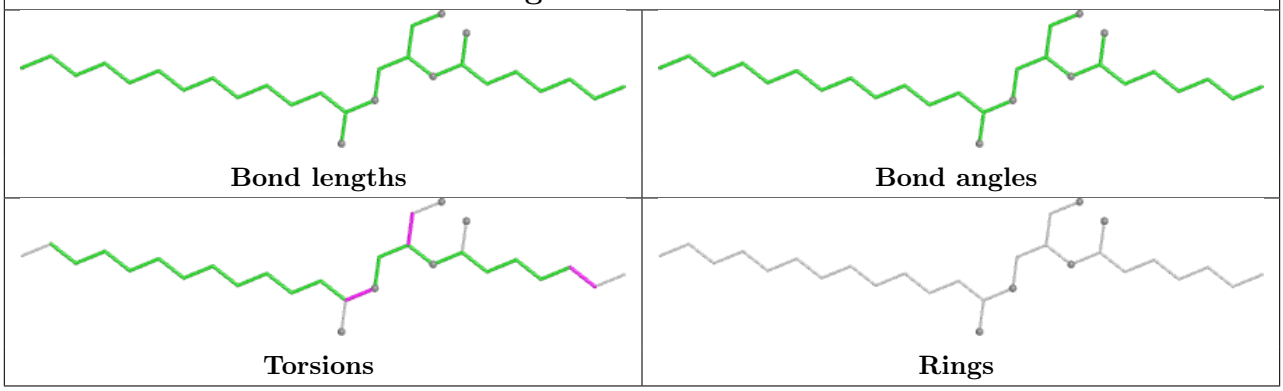
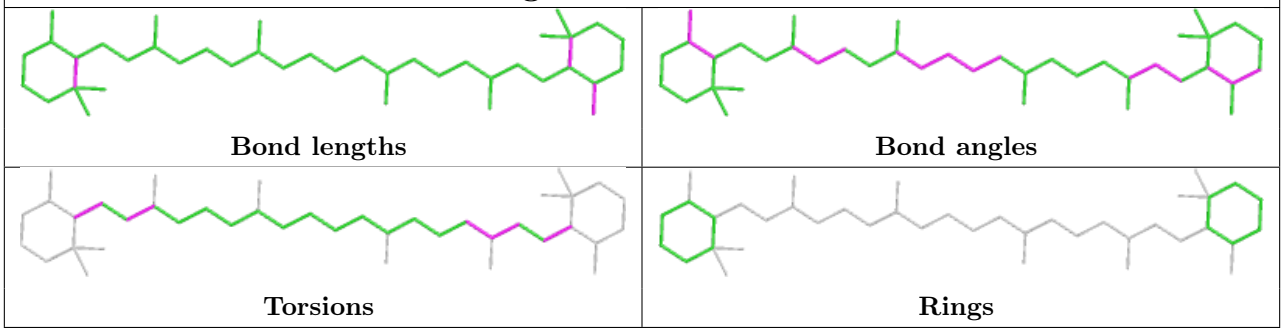


Rings

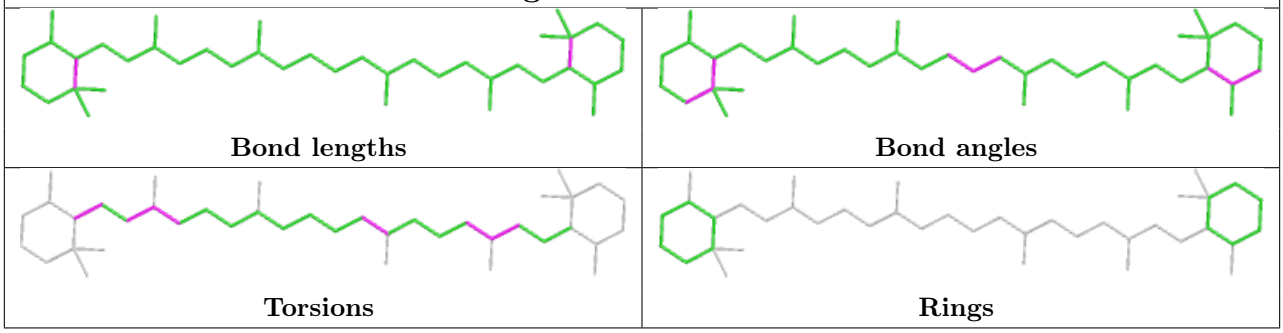
Ligand DGA 8 306



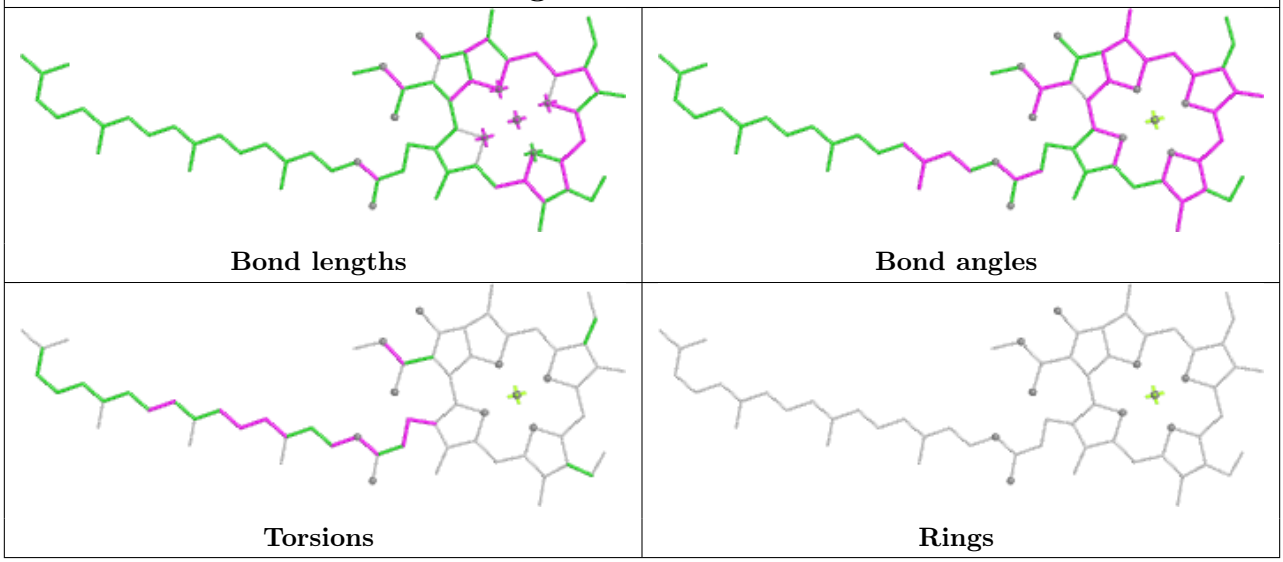
Ligand BCR K 202



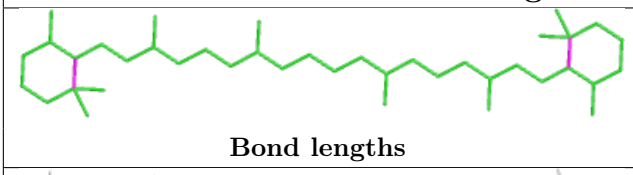
Ligand BCR A 807



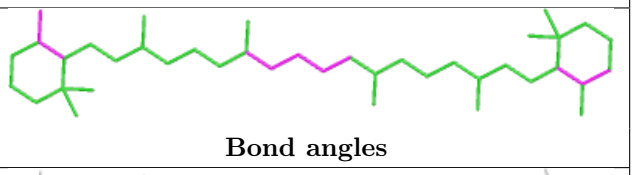
Ligand CHL 3 310



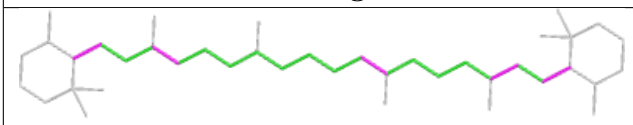
Ligand BCR L 302



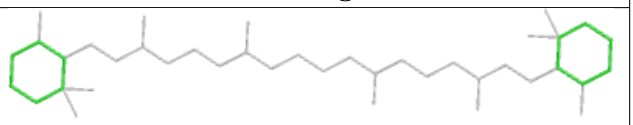
Bond lengths



Bond angles

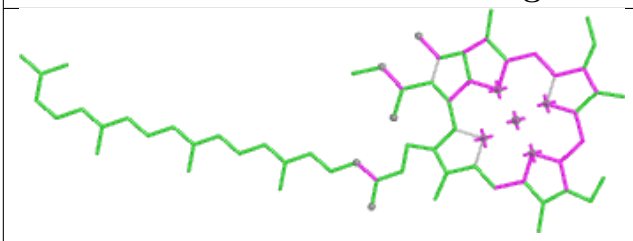


Torsions



Rings

Ligand CHL A 834



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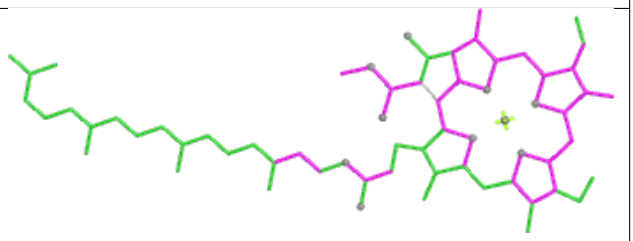
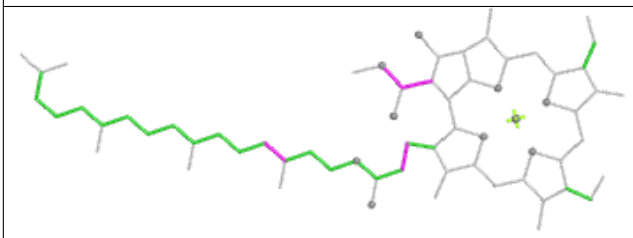


Bond angles



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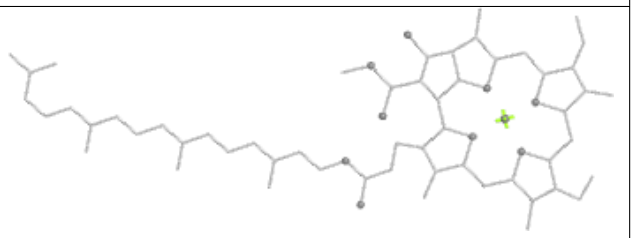
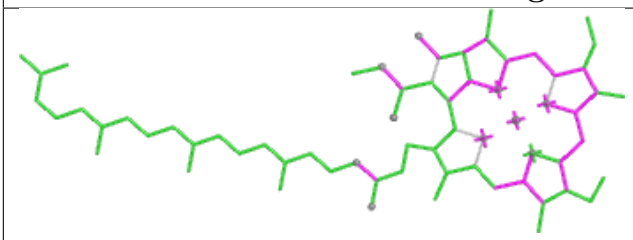


Rings

Ligand CHL 5 310



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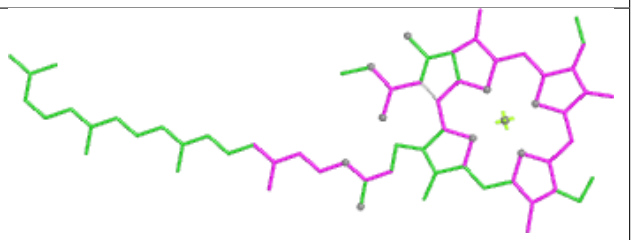

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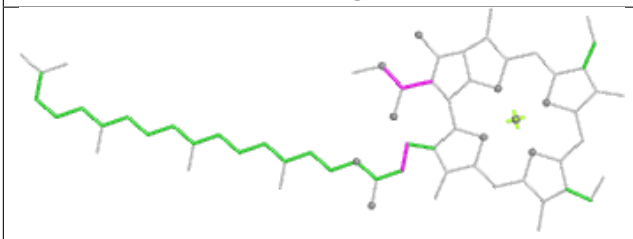

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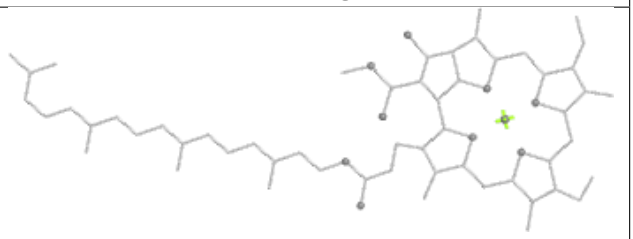
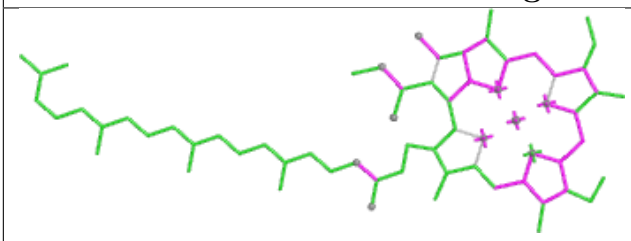


Rings

Ligand CHL A 818



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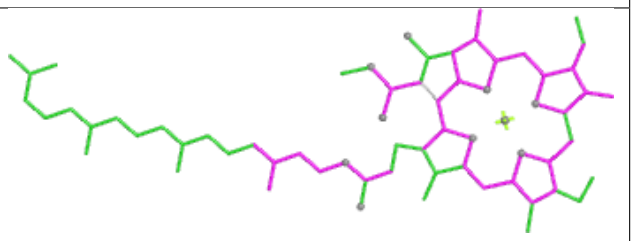
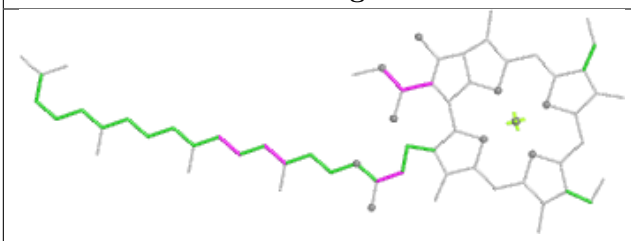


Bond angles



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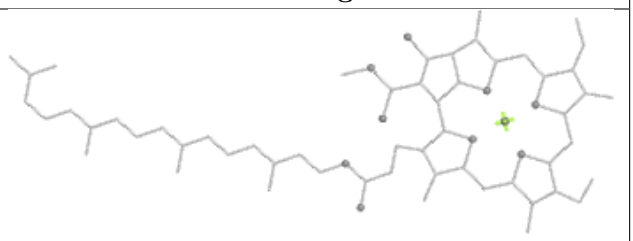
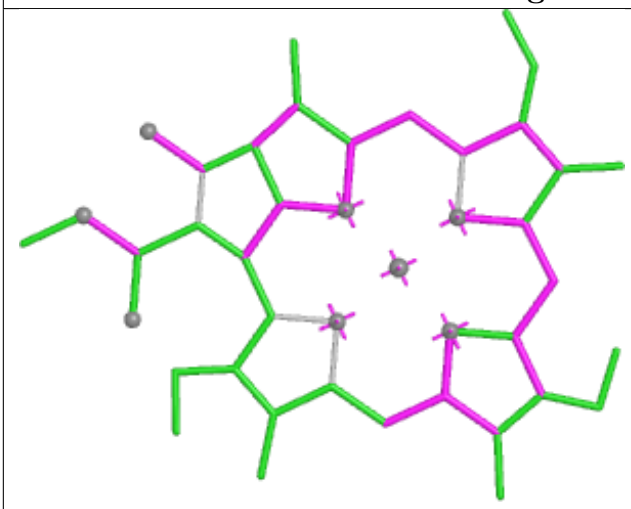


Rings

Ligand CHL J 106



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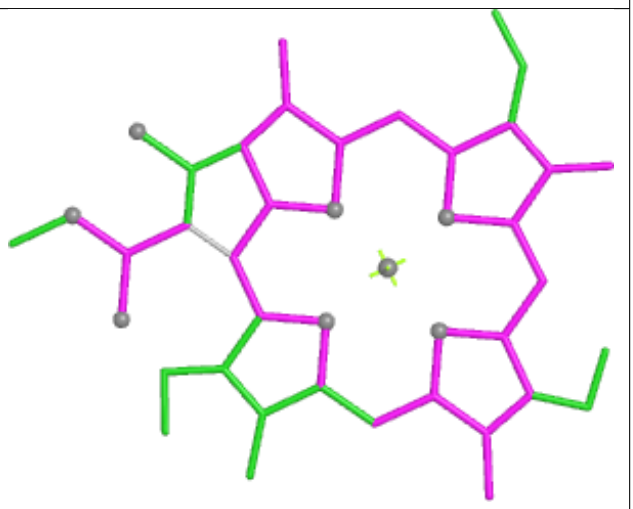
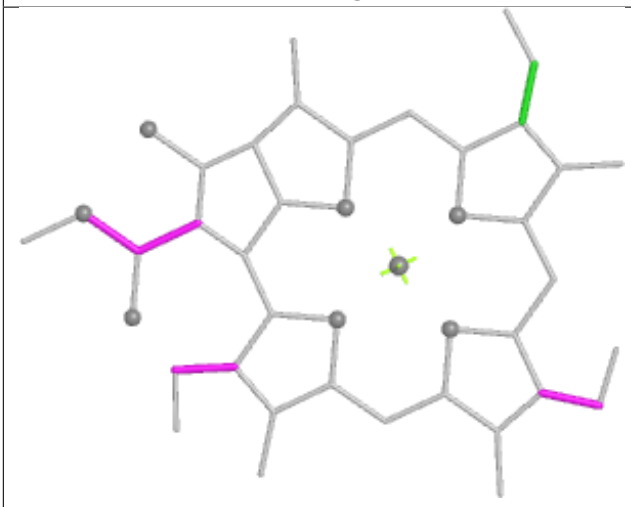


Bond angles

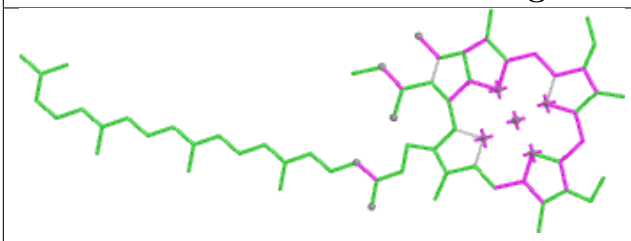


Torsions



Rings

Ligand CHL a 317



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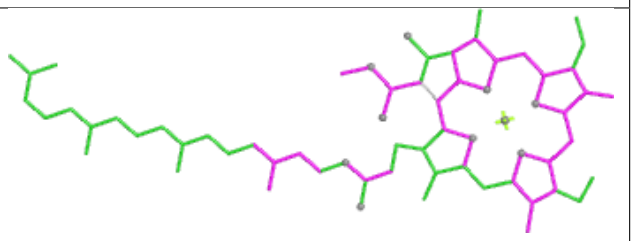
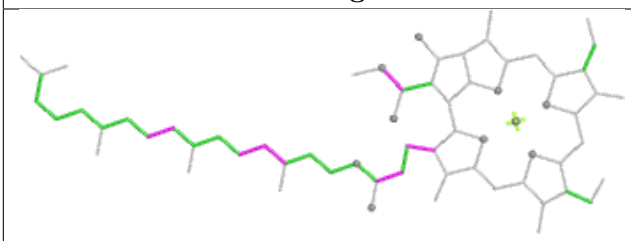


Bond angles



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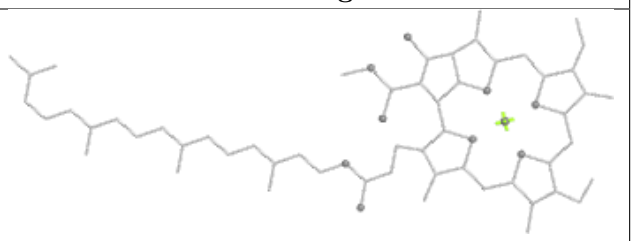
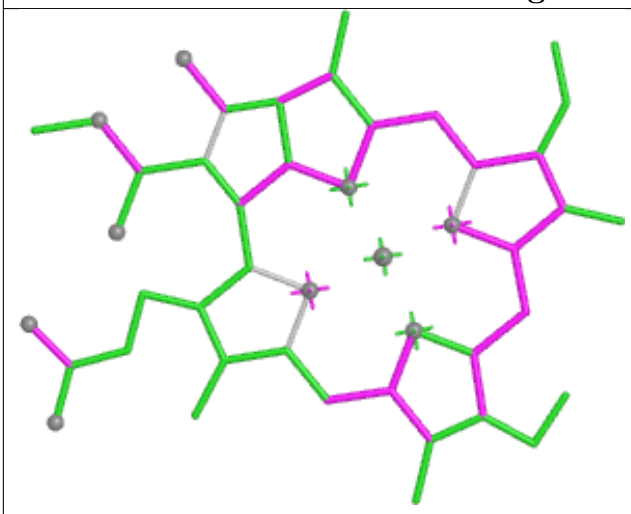


Rings

Ligand CHL 3 321



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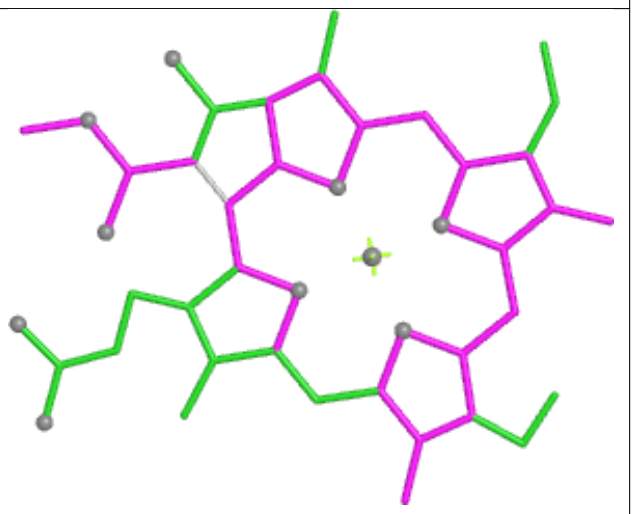
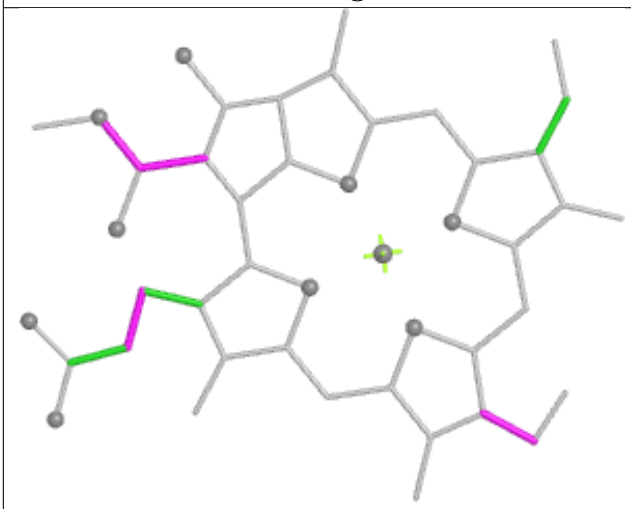


Bond angles



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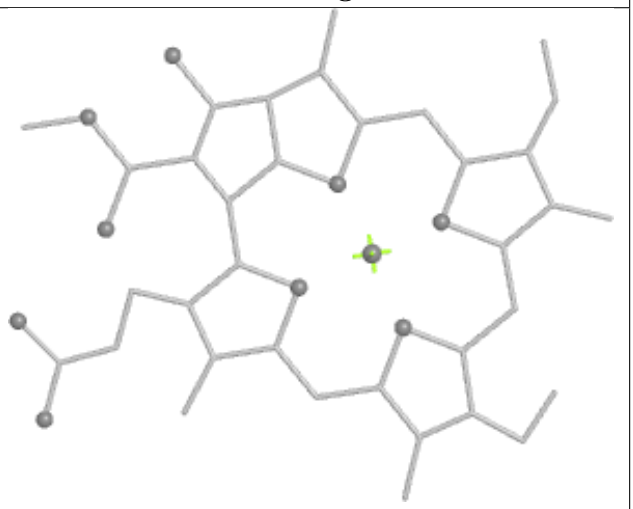
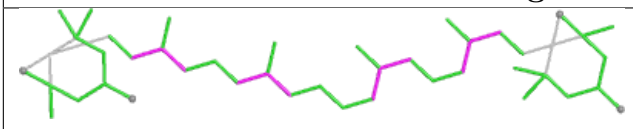


Rings

Ligand XAT 7 305



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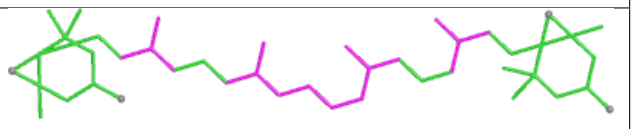
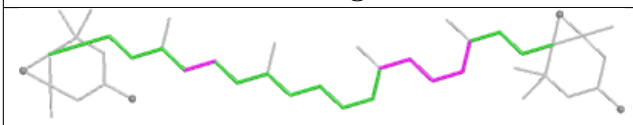


Bond angles



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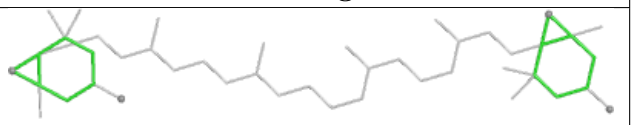
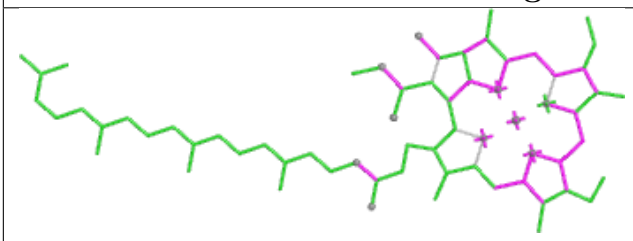


Rings

Ligand CHL B 842



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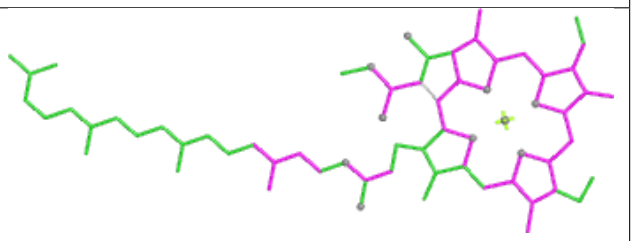
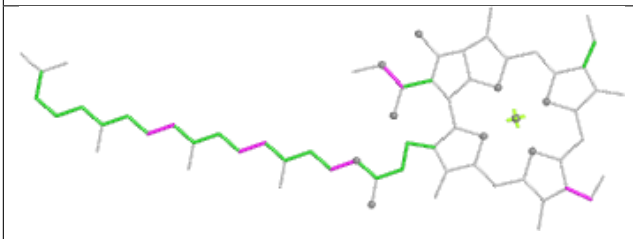


Bond angles



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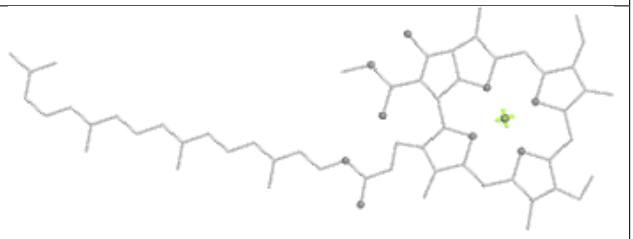
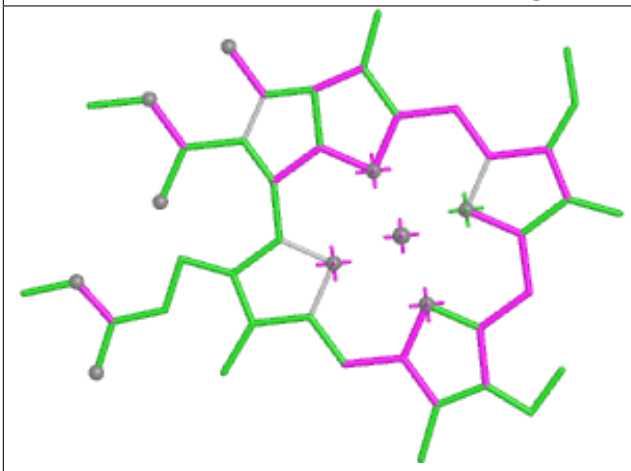


Rings

Ligand CHL 8 318



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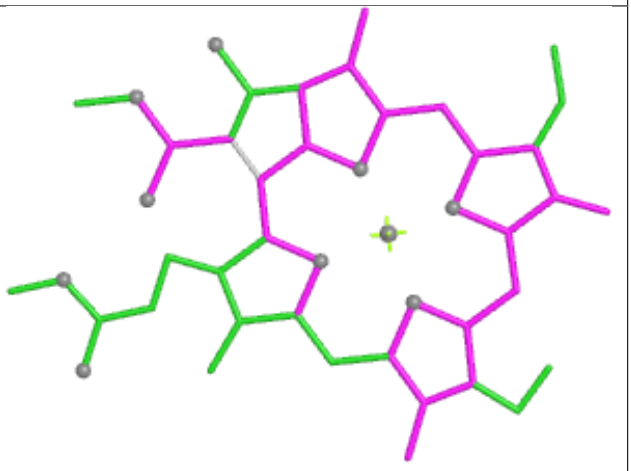
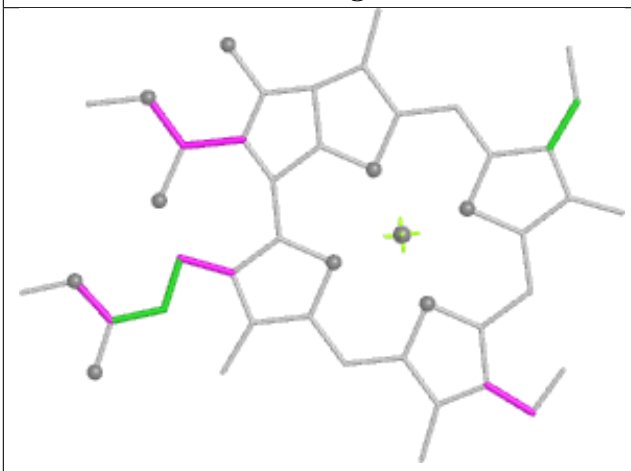


Bond angles



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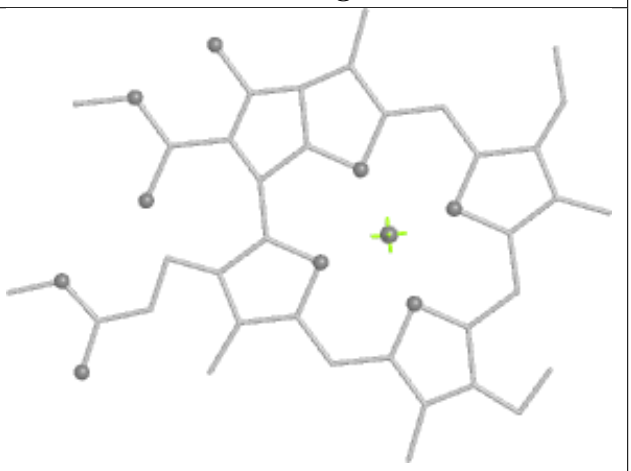
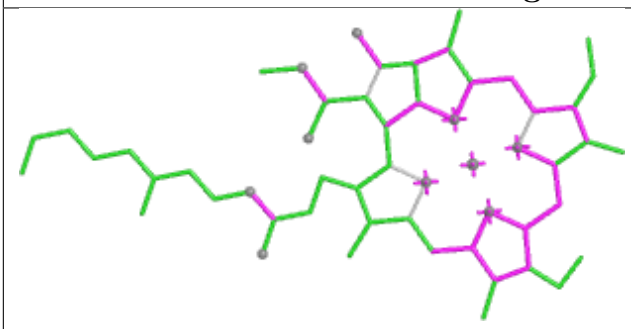
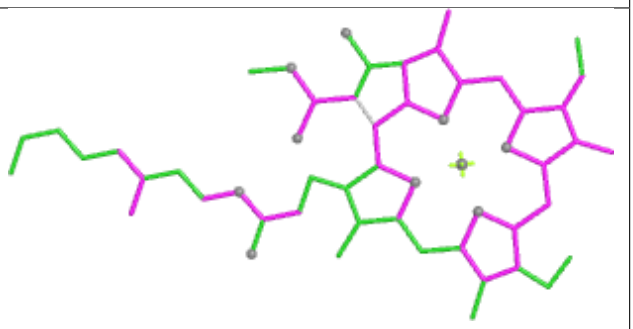


Rings

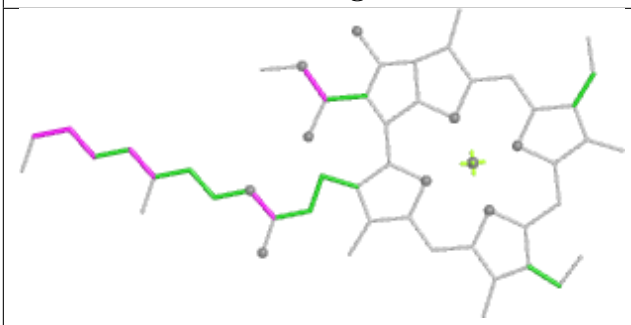
Ligand CHL A 827



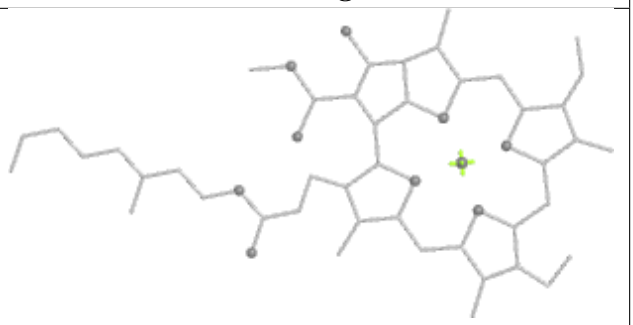
Bond lengths



Bond angles

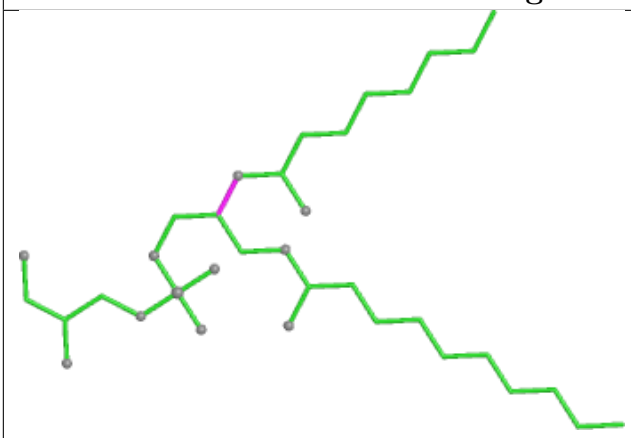


Torsions



Rings

Ligand LHG b 302



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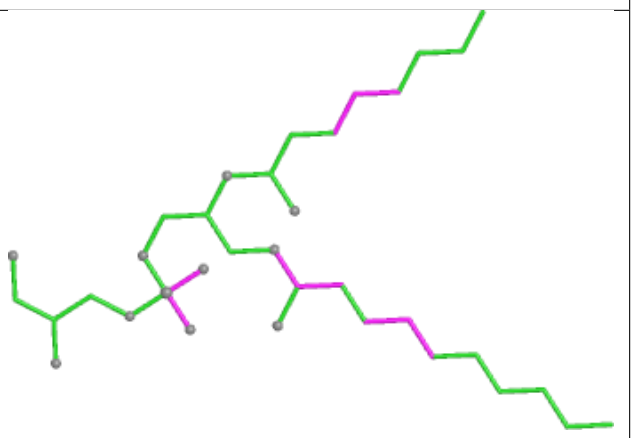
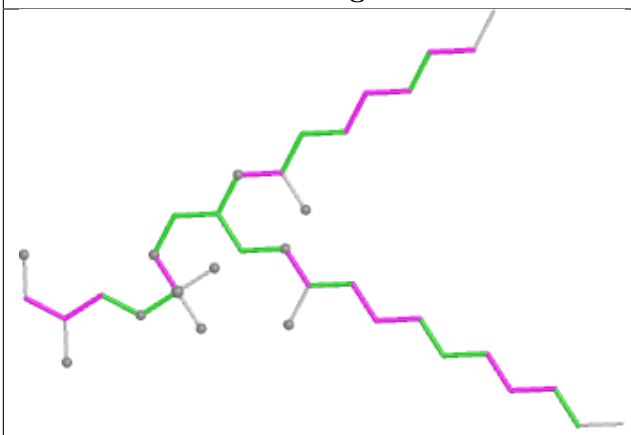


Bond angles



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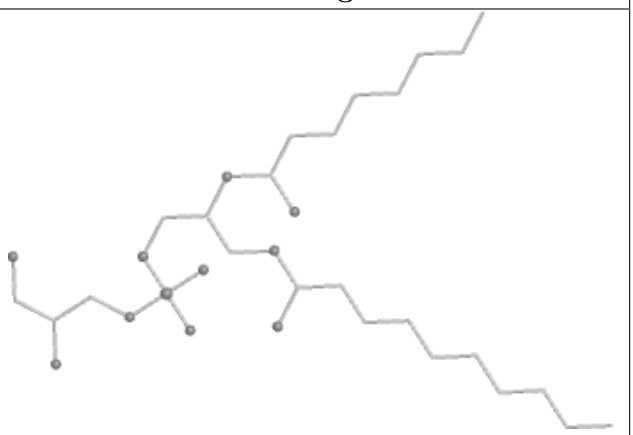
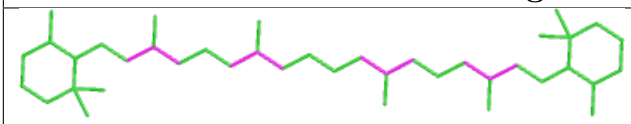
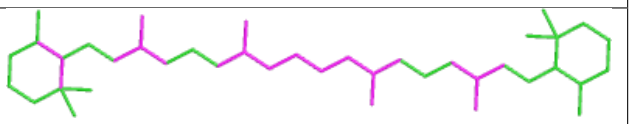
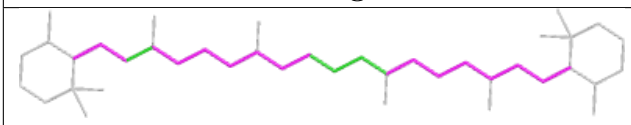
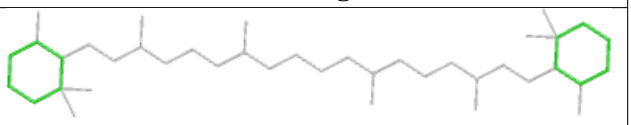
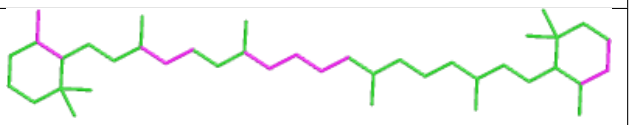
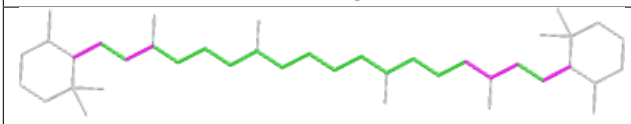
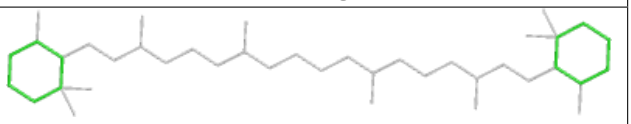
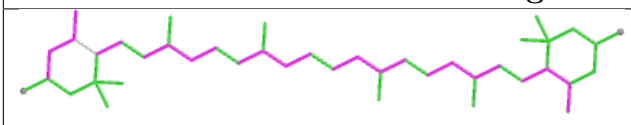
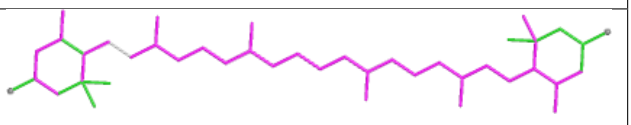
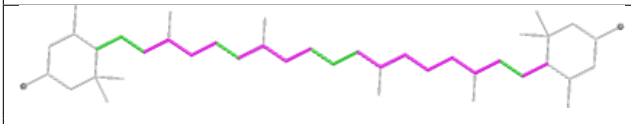
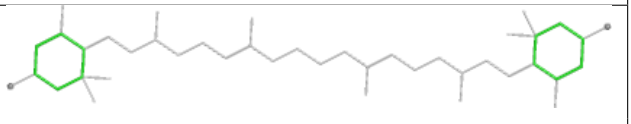


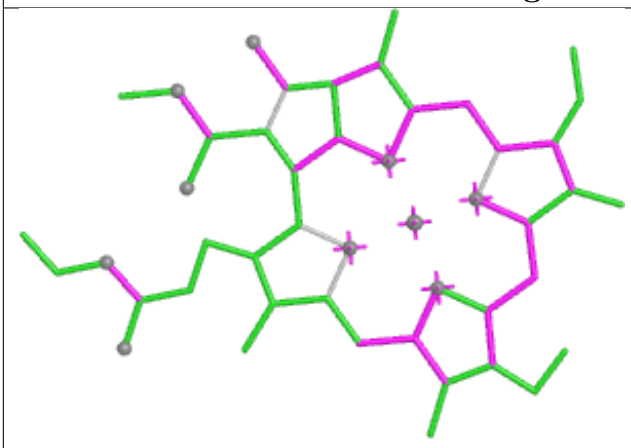
Rings

Ligand BCR 6 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

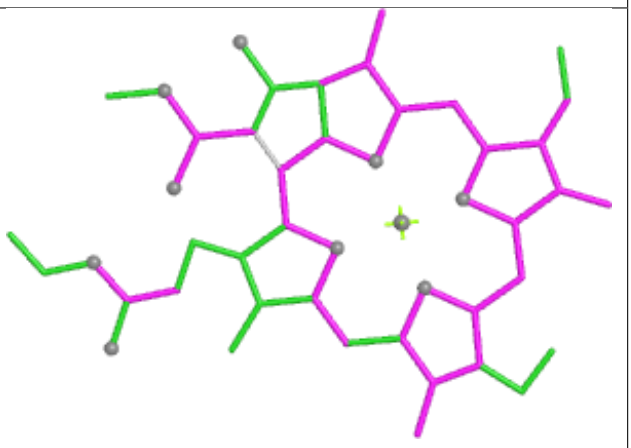
Ligand BCR A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT F 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

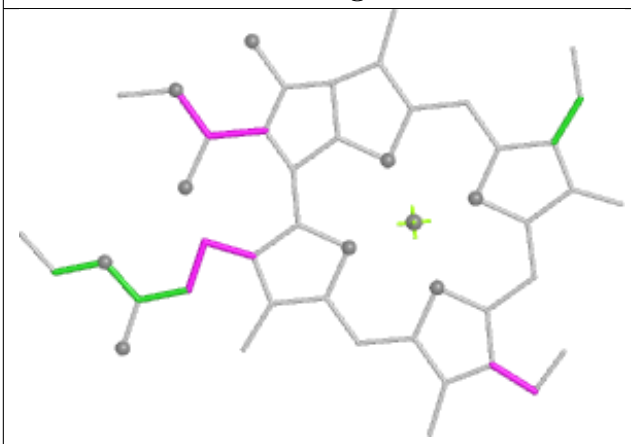
Ligand CHL A 835



Bond lengths



Bond angles



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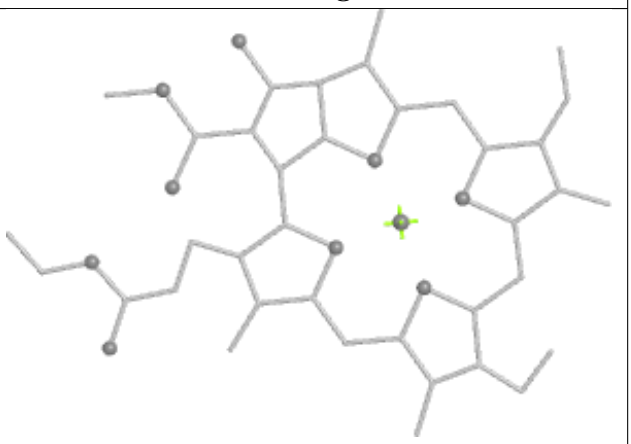
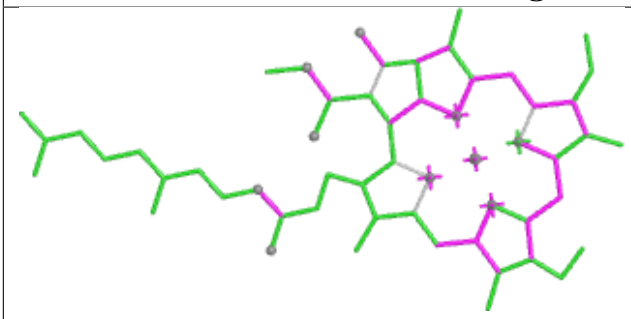


Rings

Ligand CHL 3 319



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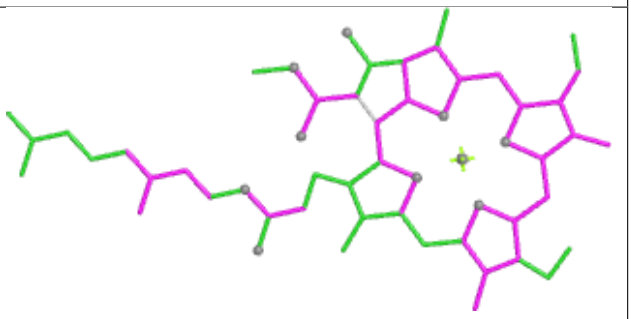

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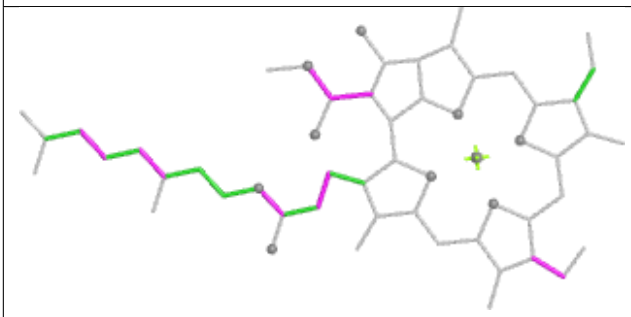

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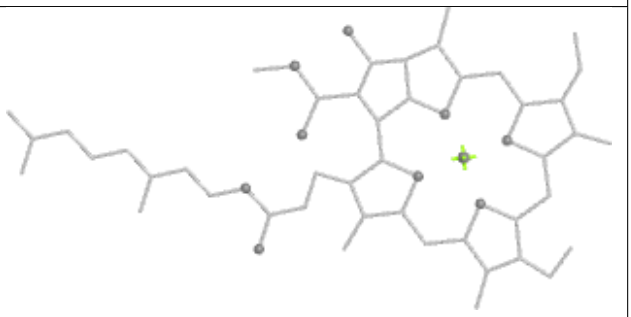
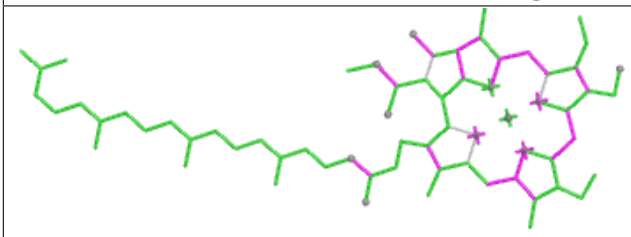


Rings

Ligand CHL 7 319



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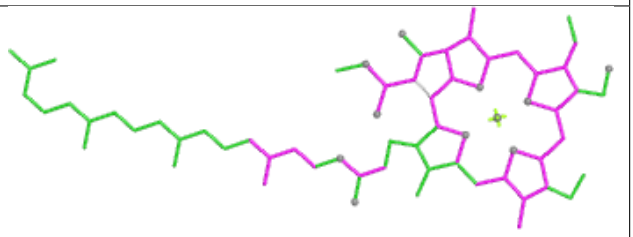
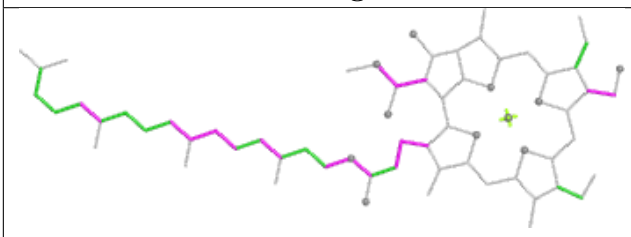


Bond angles



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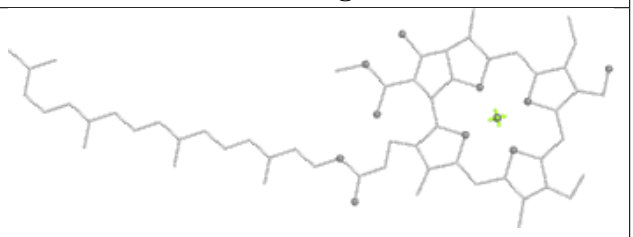
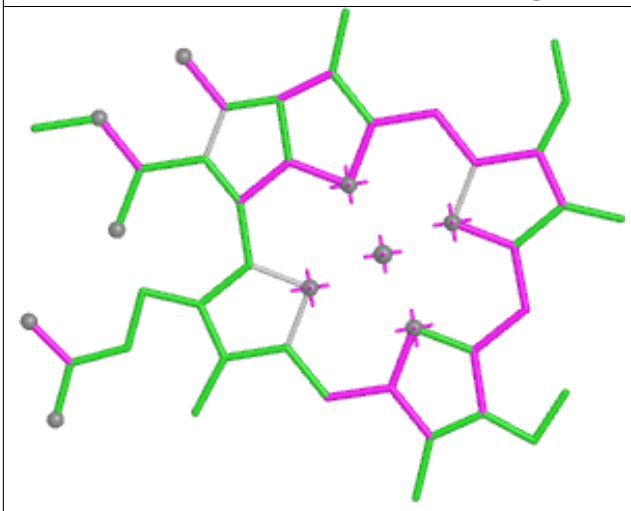


Rings

Ligand CHL a 308



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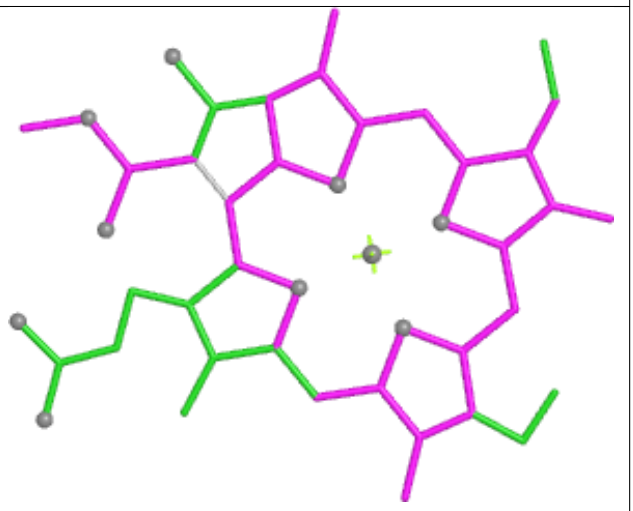

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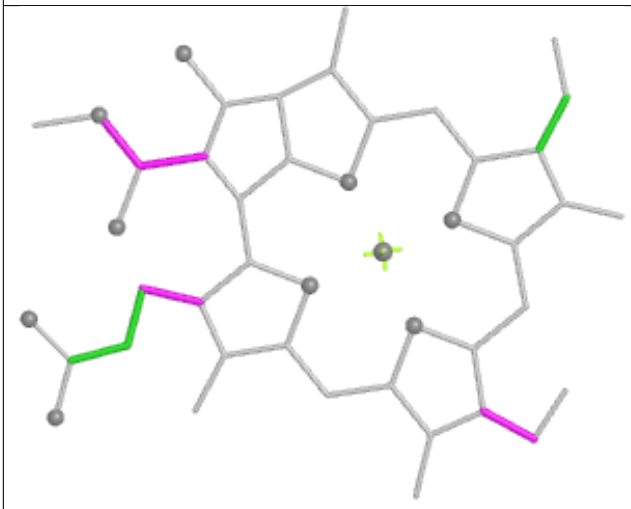

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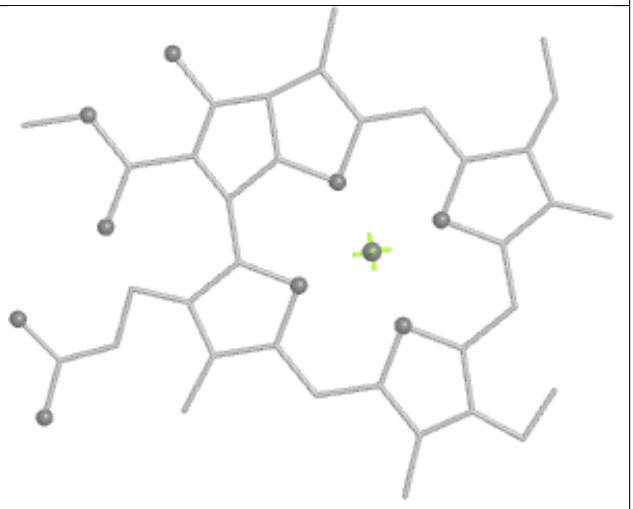
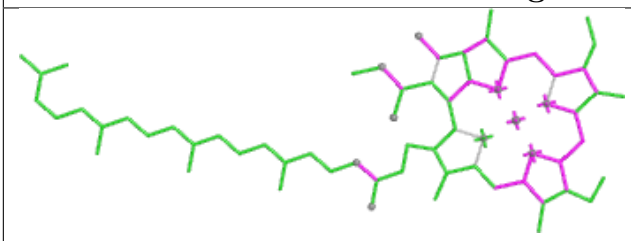
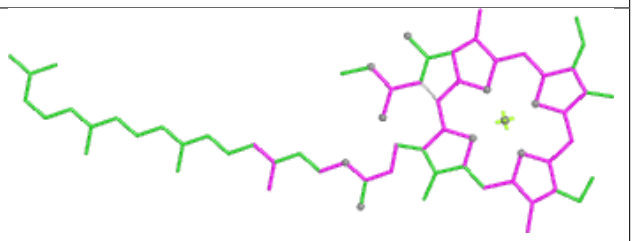
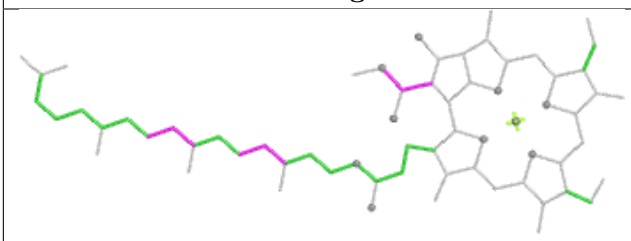
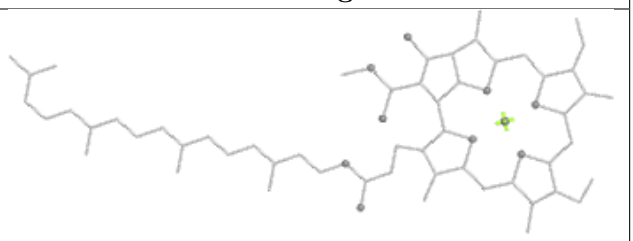
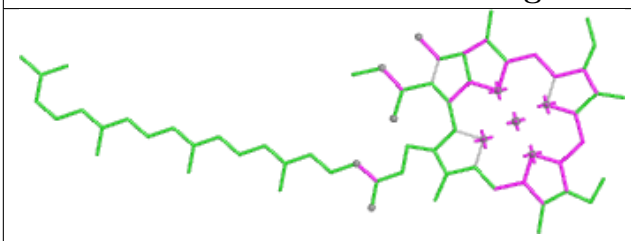
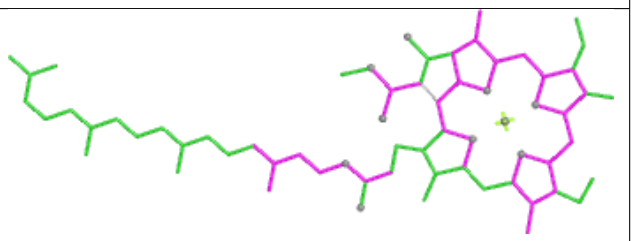


Rings

Ligand CHL 5 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL B 819	
	
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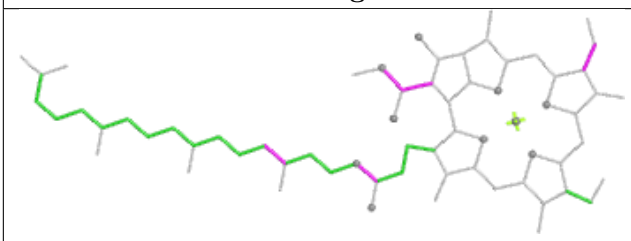
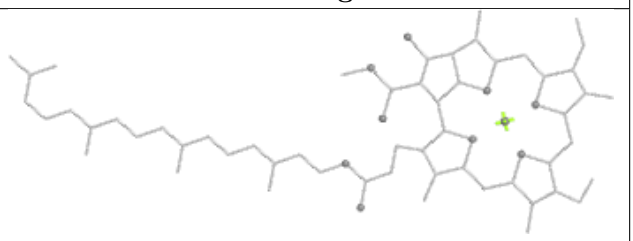
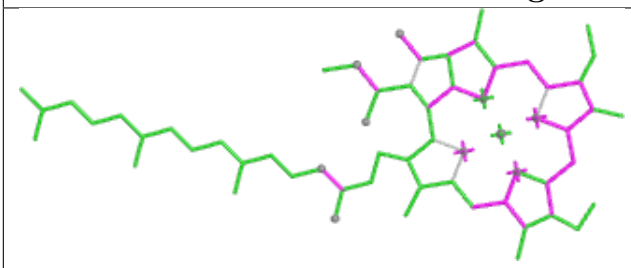
	
Torsions	Rings

Ligand CHL 4 307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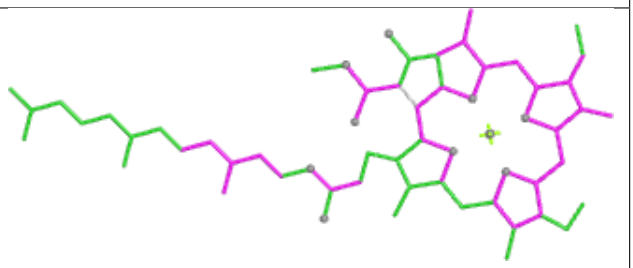
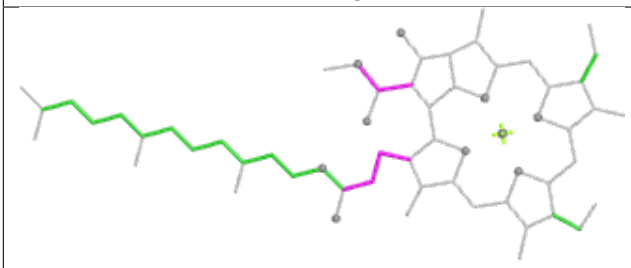

Bond angles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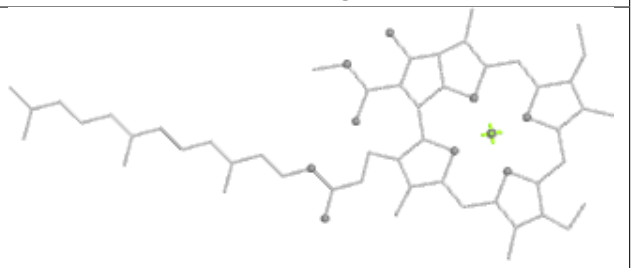
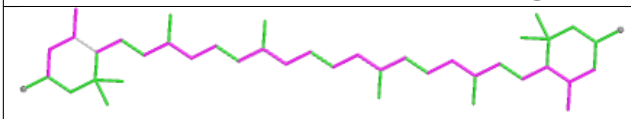

Rings

Ligand LUT 4 301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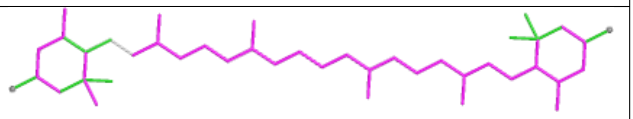
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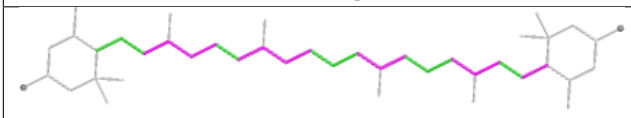
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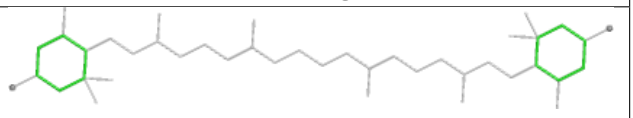
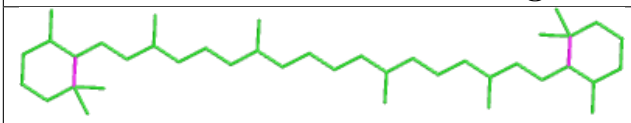

Rings

Ligand BCR 5 301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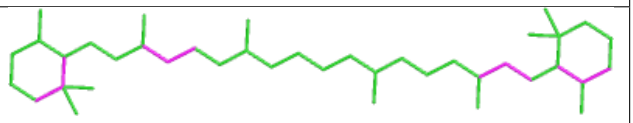
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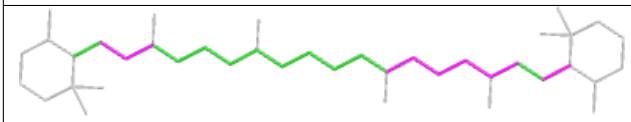
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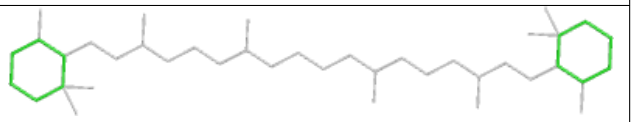
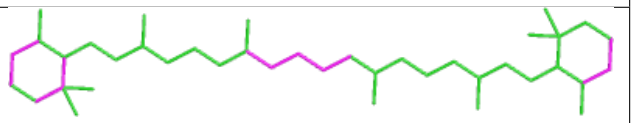
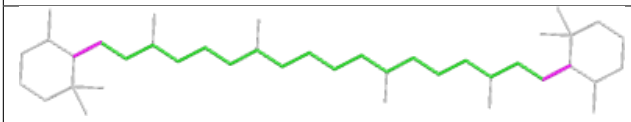

Rings

Ligand BCR A 805


Bond lengths


Bond angles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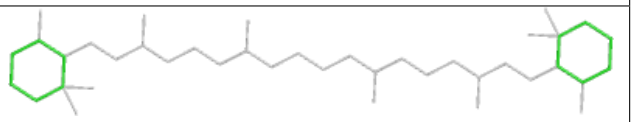
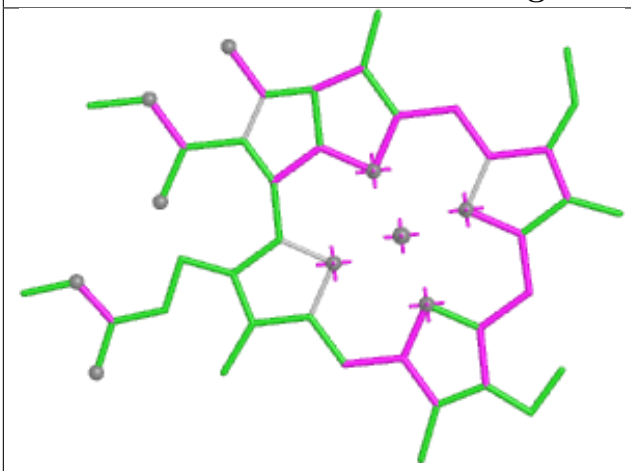
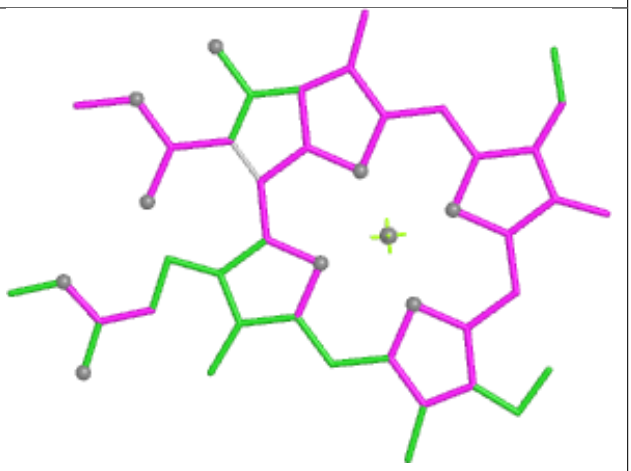

Rings

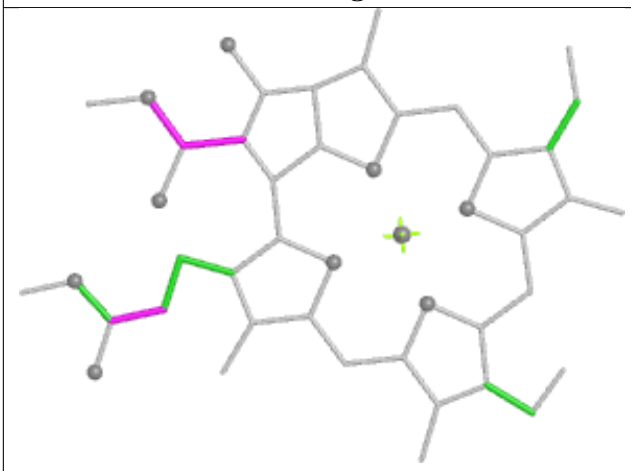
Ligand CHL 6 312



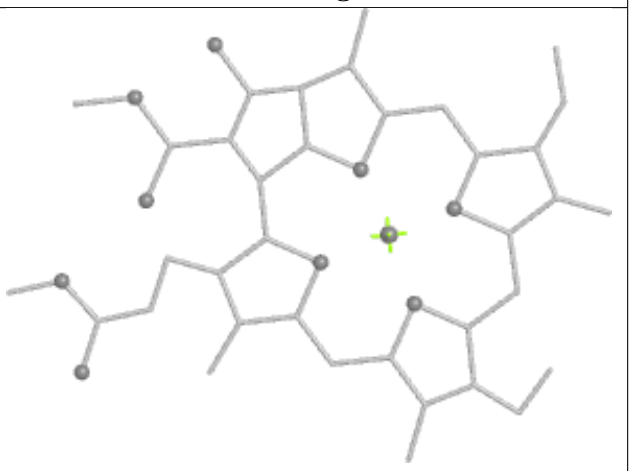
Bond lengths



Bond angles

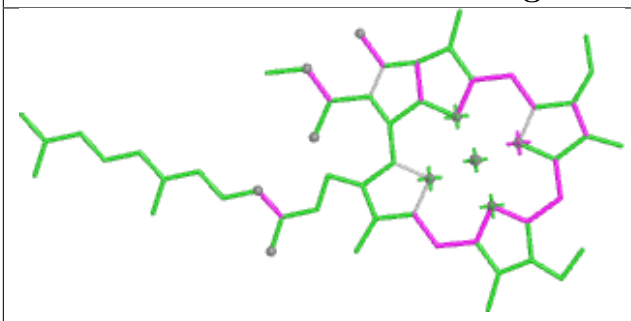


Torsions

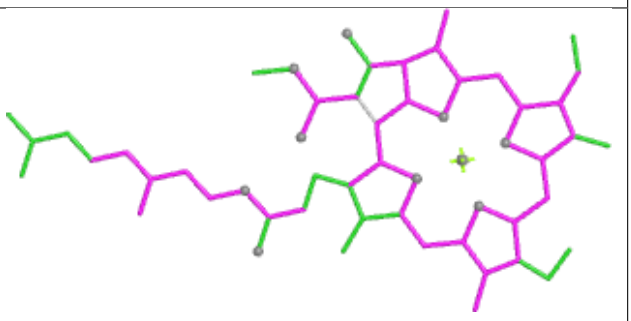


Rings

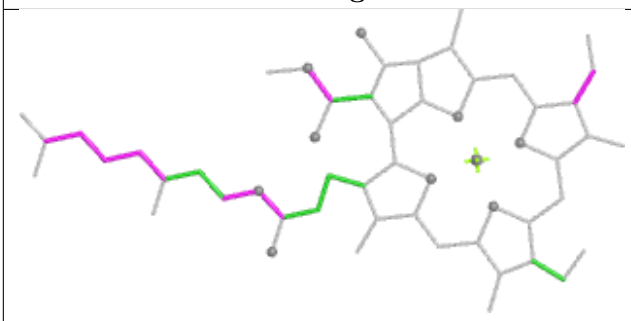
Ligand CHL A 831



Bond lengths



Bond angles



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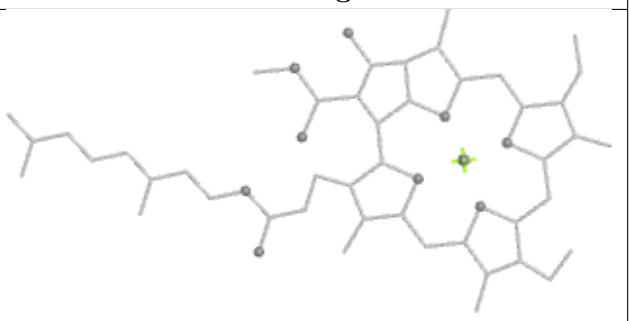
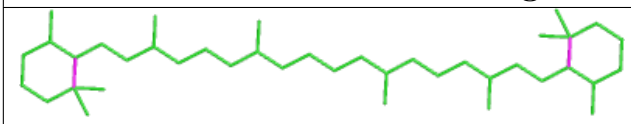


Rings

Ligand BCR K 203



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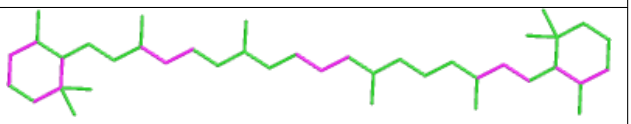
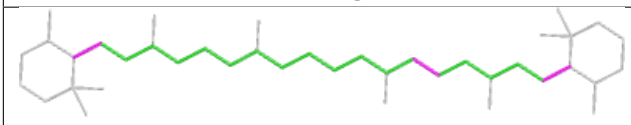


Bond angles



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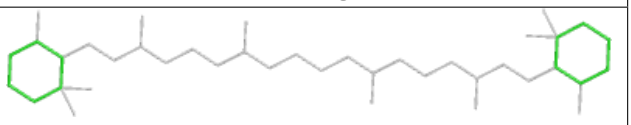
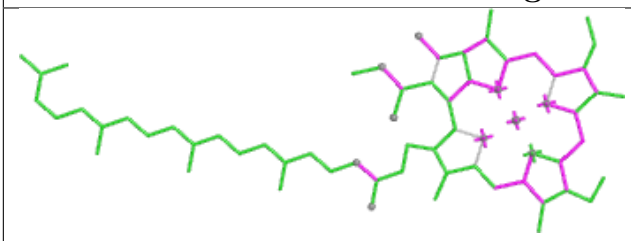


Rings

Ligand CHL B 848



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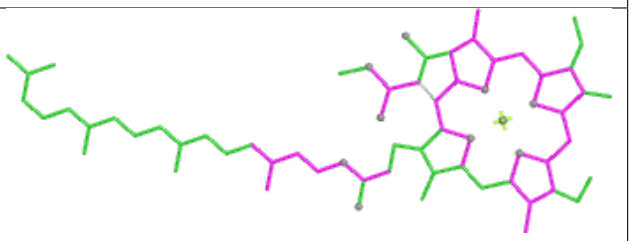

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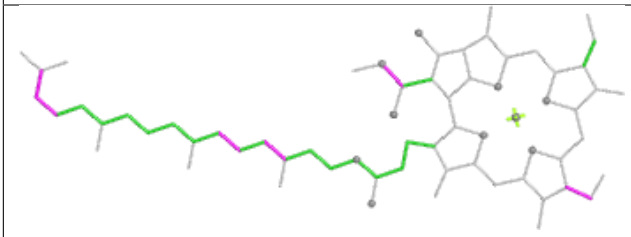

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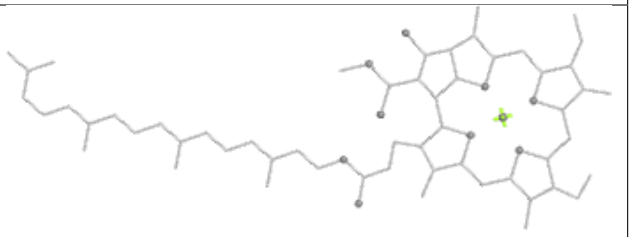
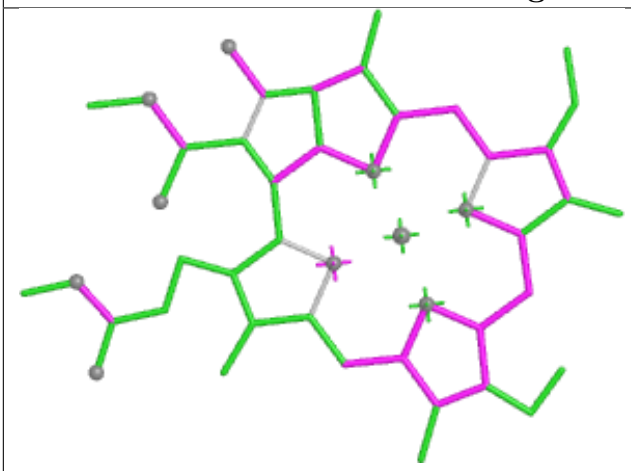


Rings

Ligand CHL 8 326



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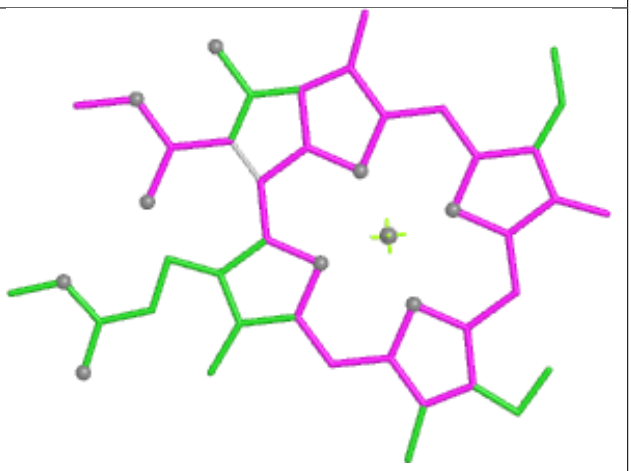
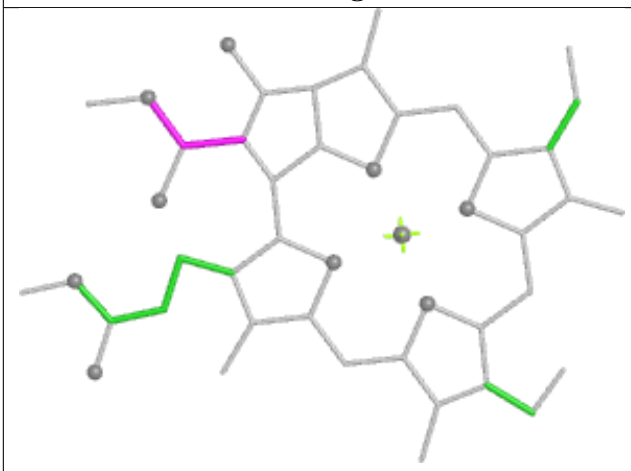


Bond angles



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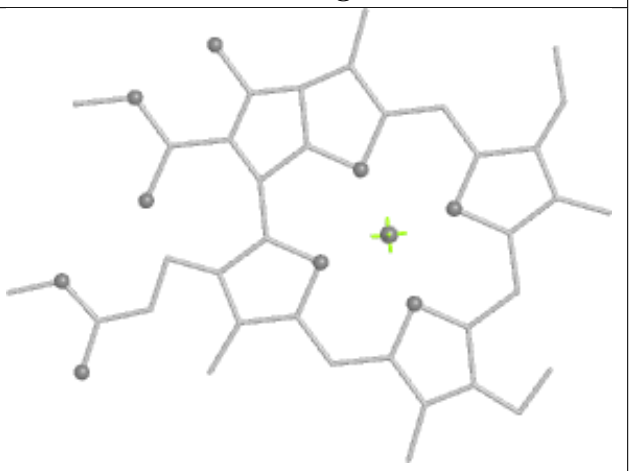
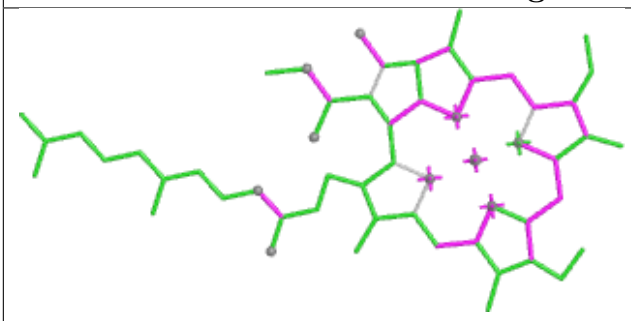


Rings

Ligand CHL 4 304



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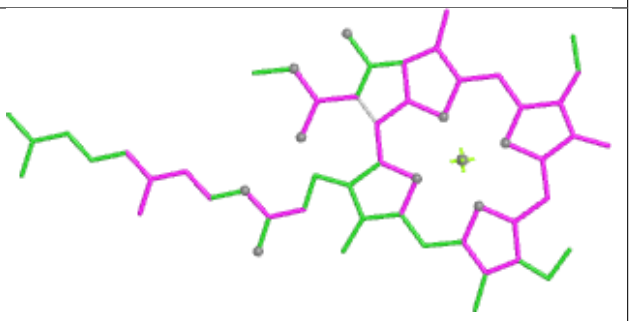
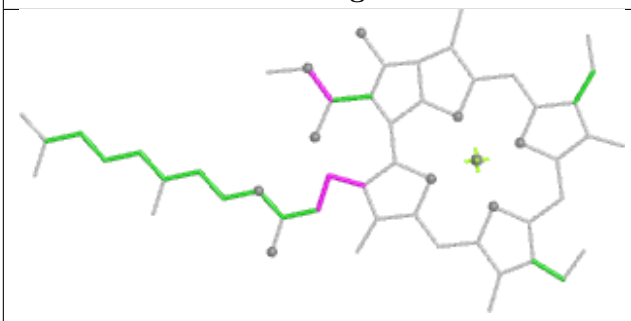


Bond angles



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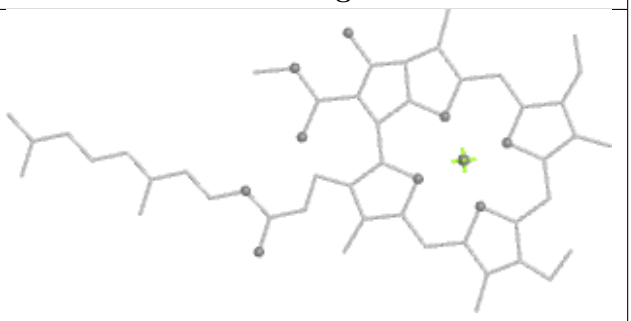
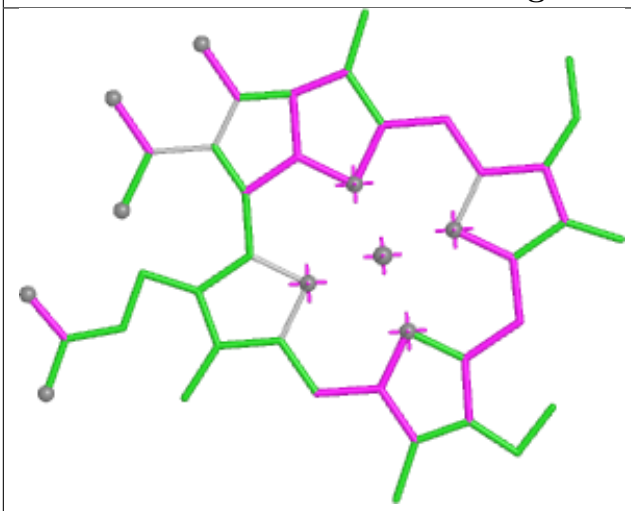


Rings

Ligand CHL 7 315



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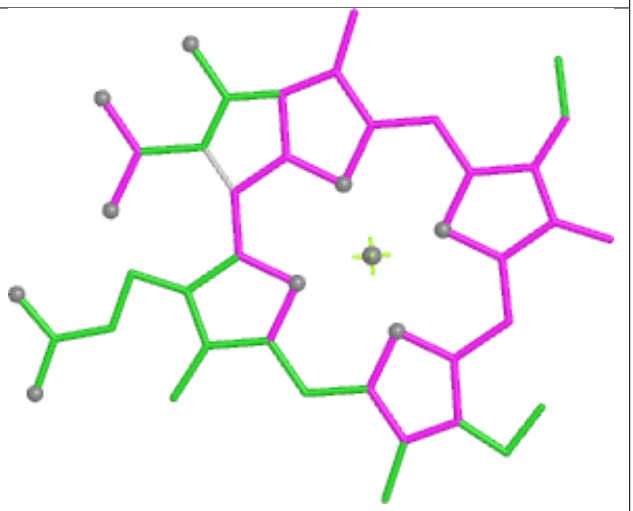
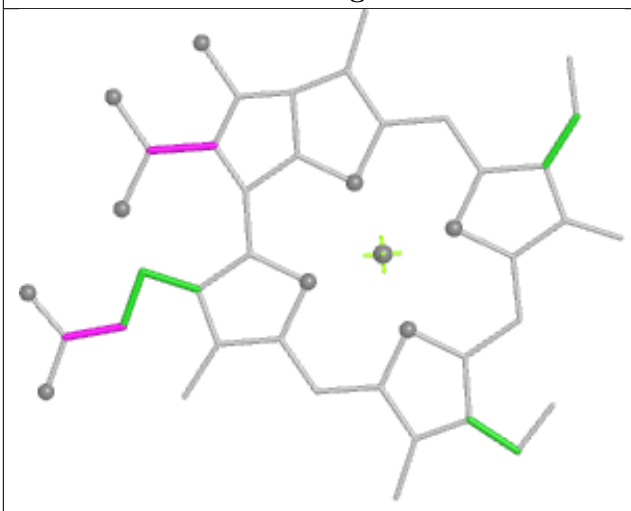


Bond angles



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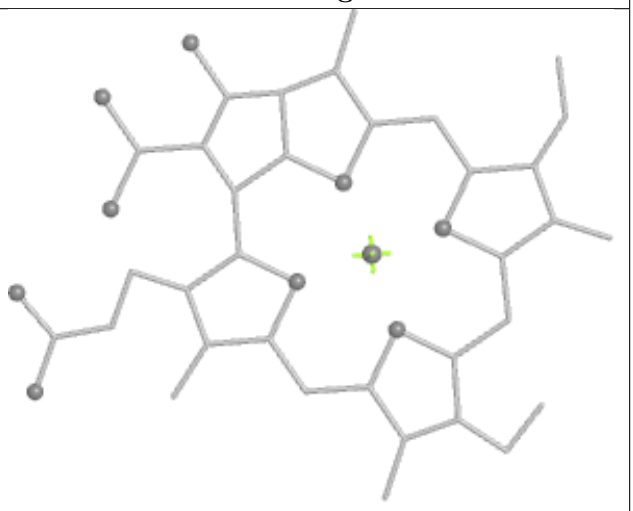
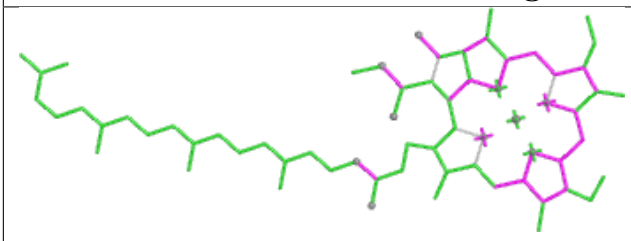


Rings

Ligand CHL A 830



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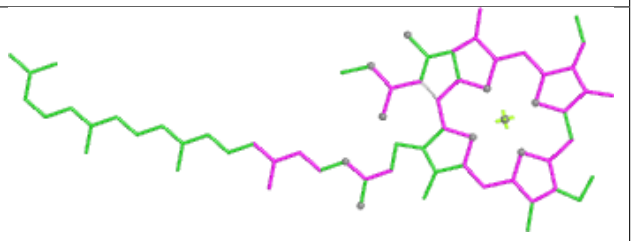

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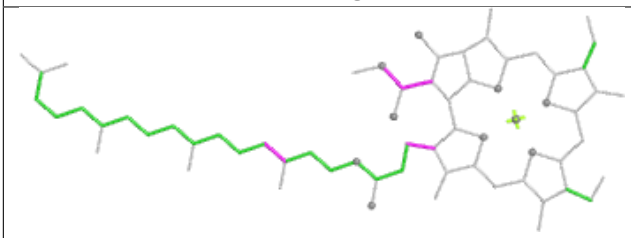

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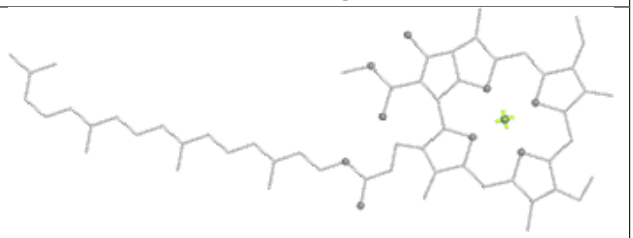
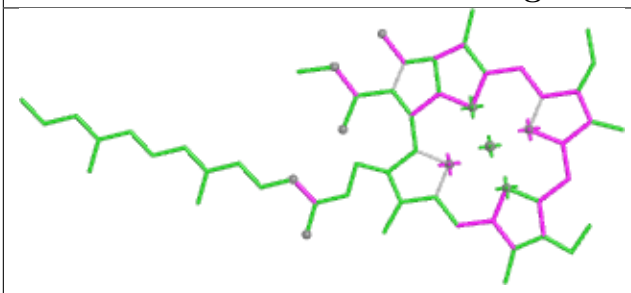


Rings

Ligand CHL B 835



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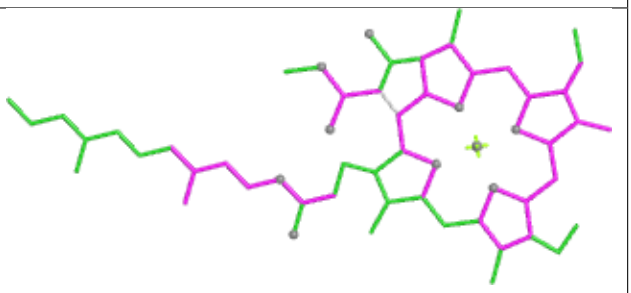
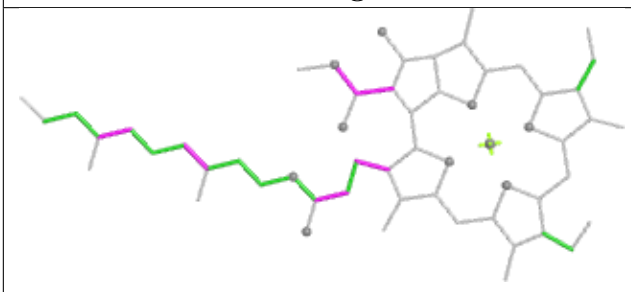


Bond angles



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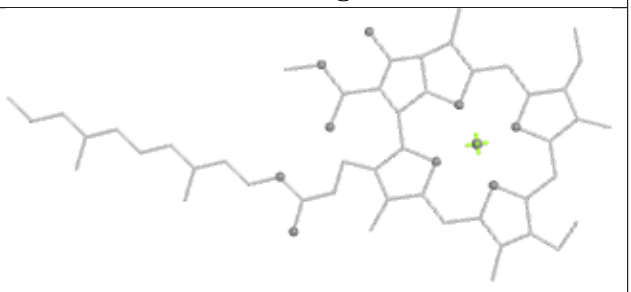
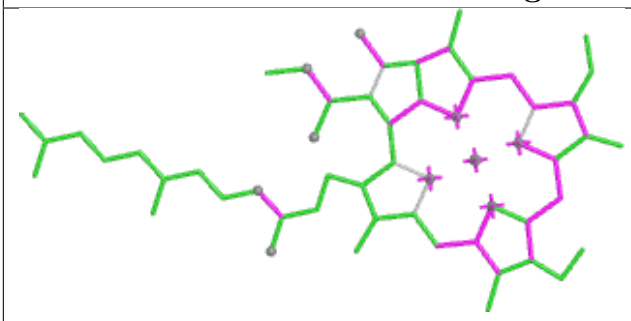


Rings

Ligand CHL B 818



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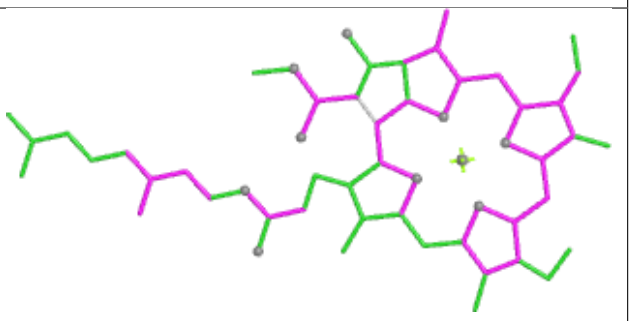
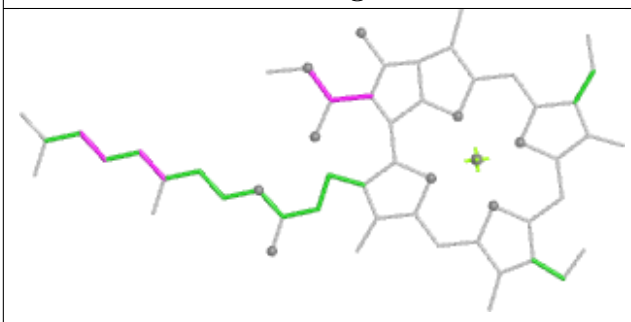


Bond angles



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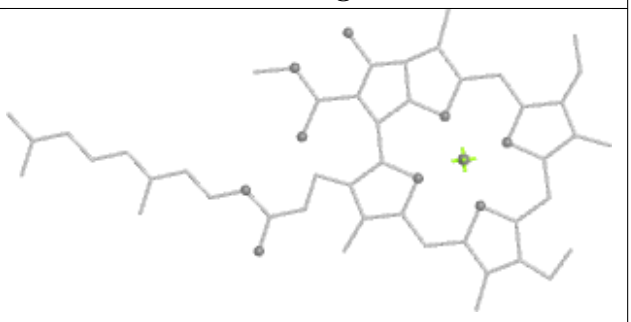
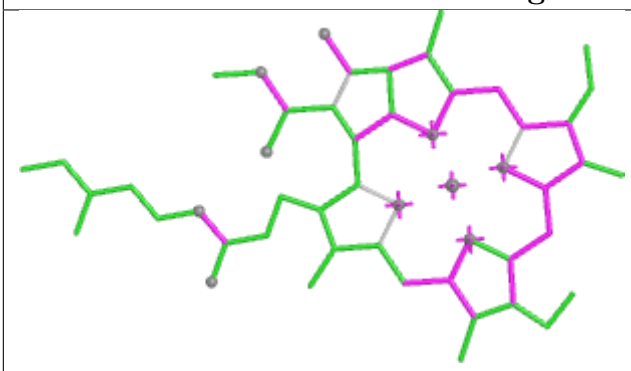


Rings

Ligand CHL 3 318



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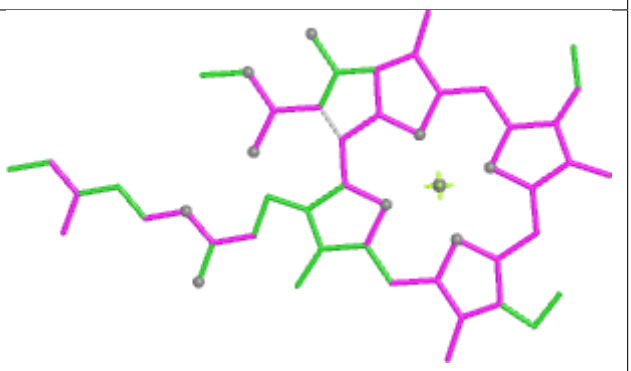
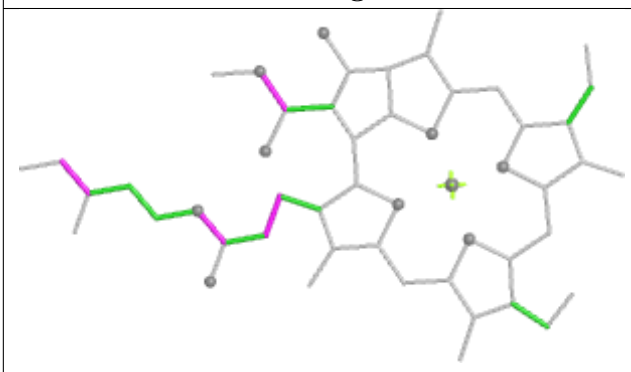


Bond angles



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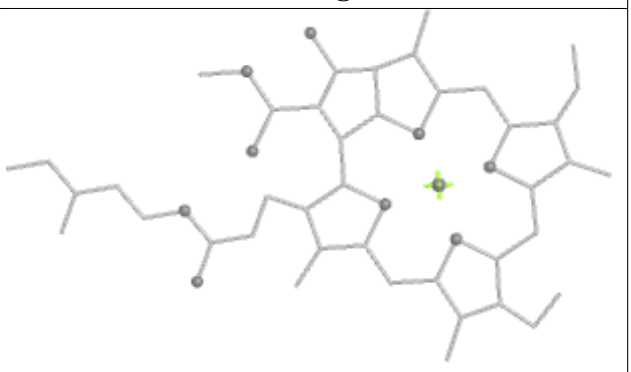
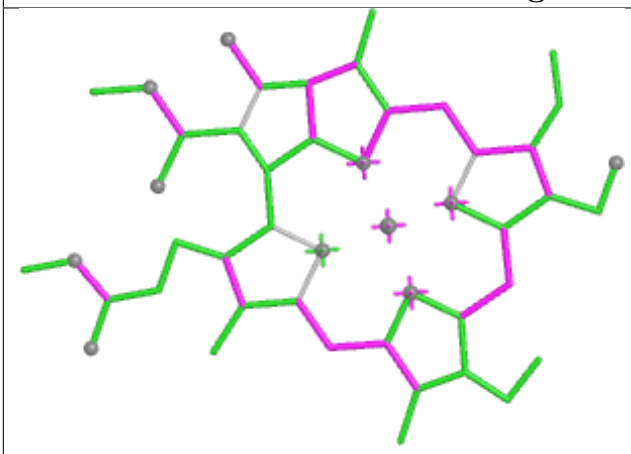


Rings

Ligand CHL 5 322



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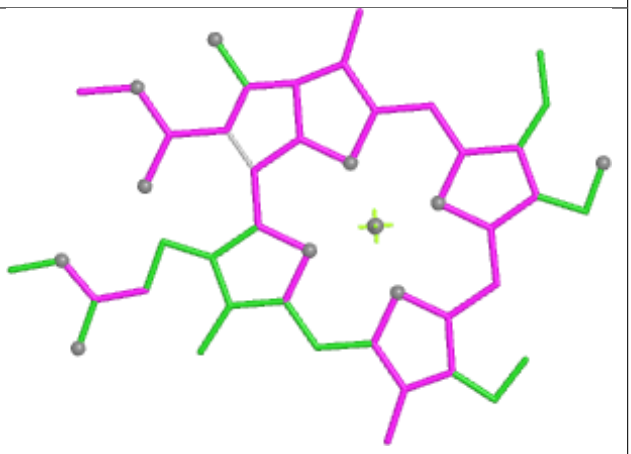
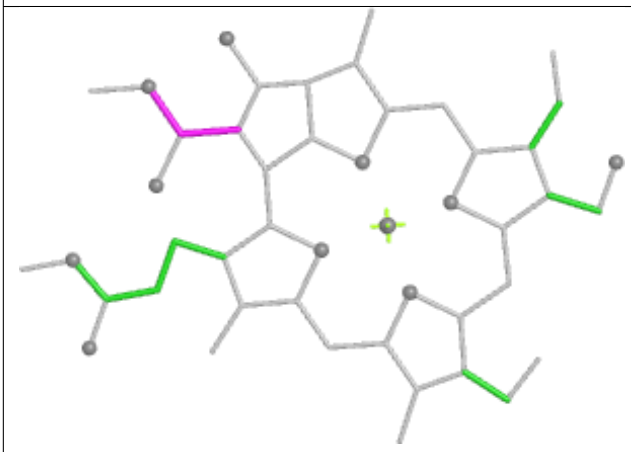


Bond angles



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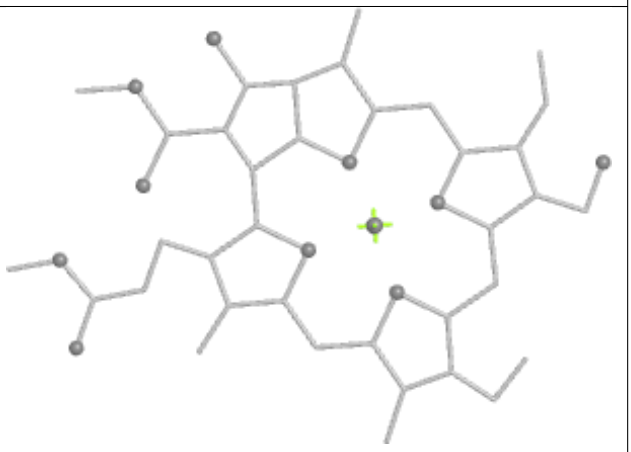
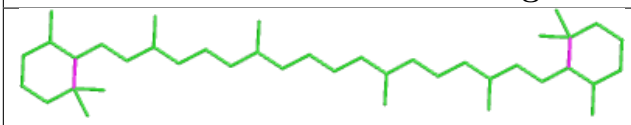


Rings

Ligand BCR A 804



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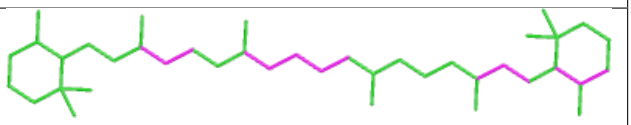
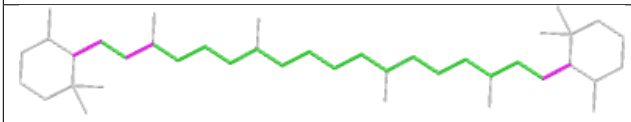


Bond angles



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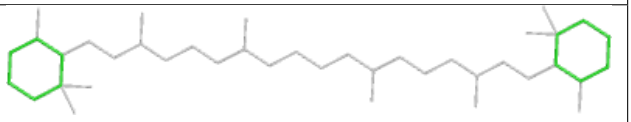
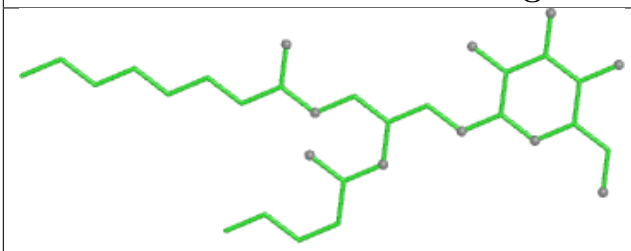


Rings

Ligand LMG 8 307



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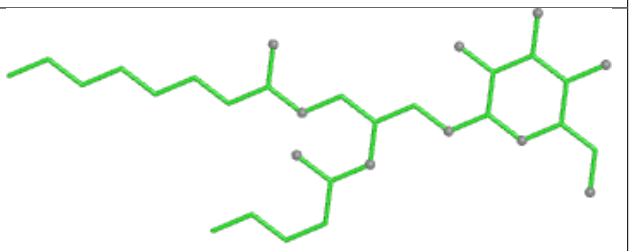
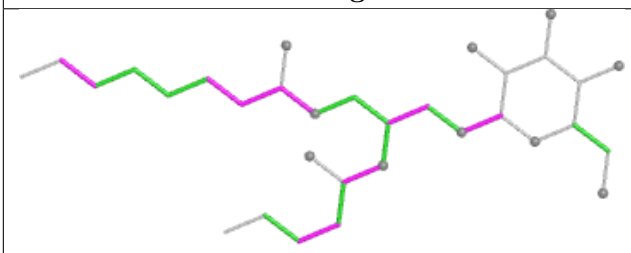


Bond angles



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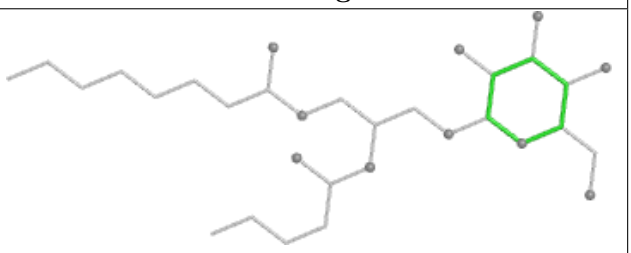
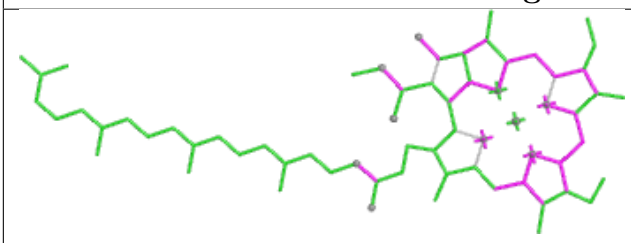
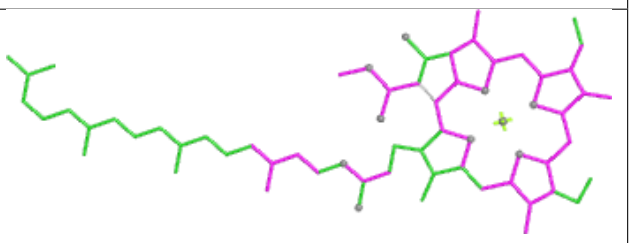


Rings

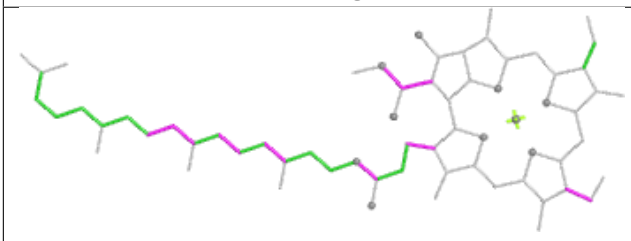
Ligand CHL A 839



Bond lengths



Bond angles



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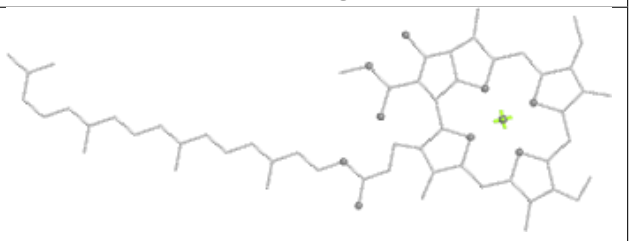
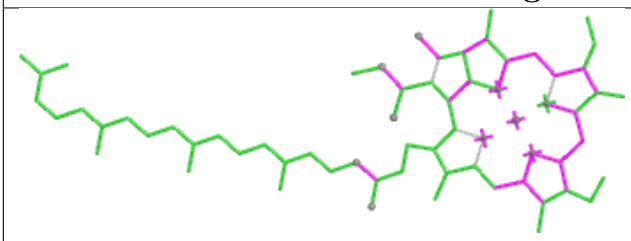


Rings

Ligand CHL A 859



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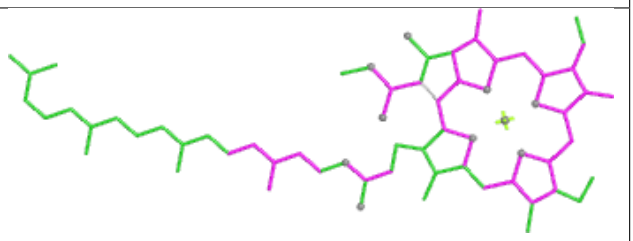
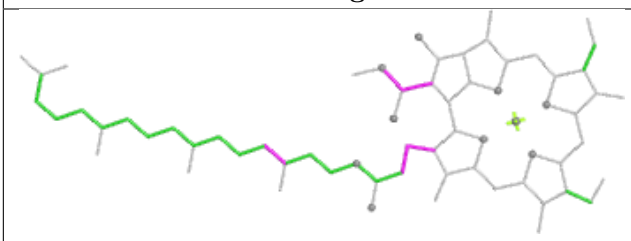
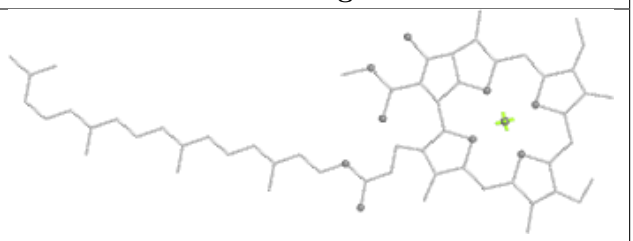


Bond angles

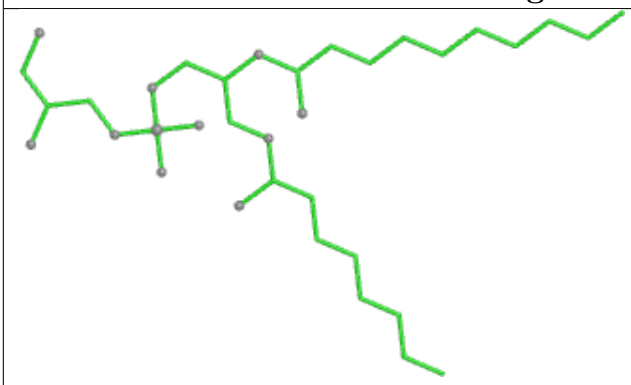


Torsions



Rings

Ligand LHG 5 304



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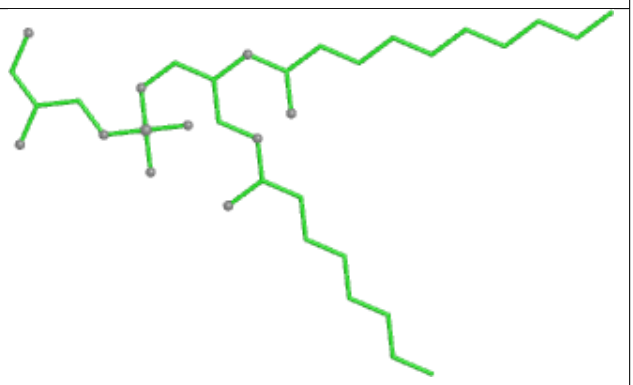

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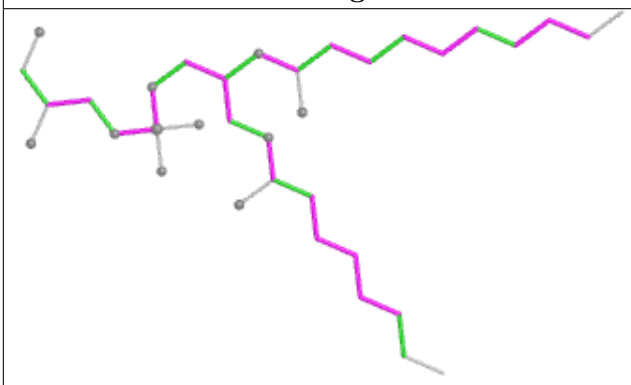

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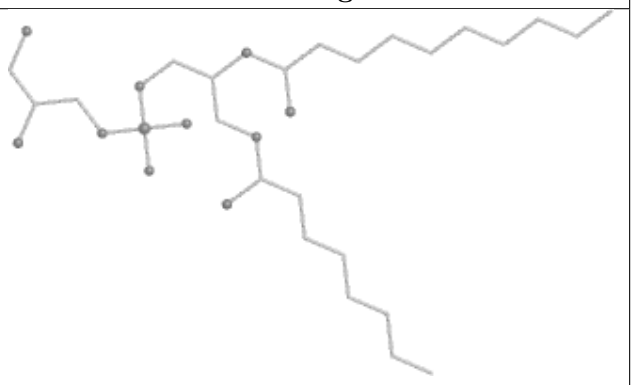
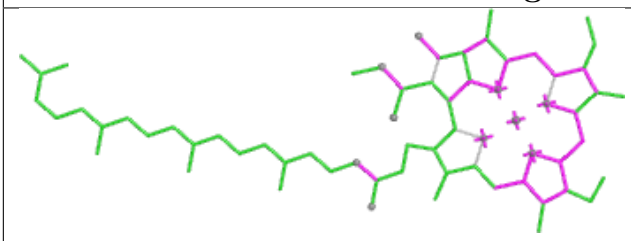


Rings

Ligand CHL B 814



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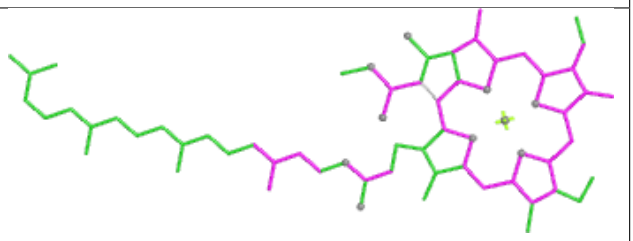

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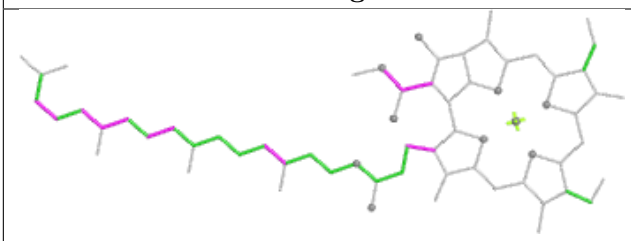

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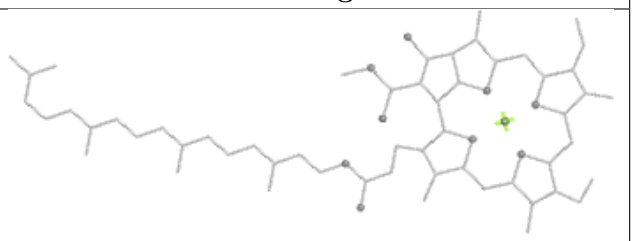
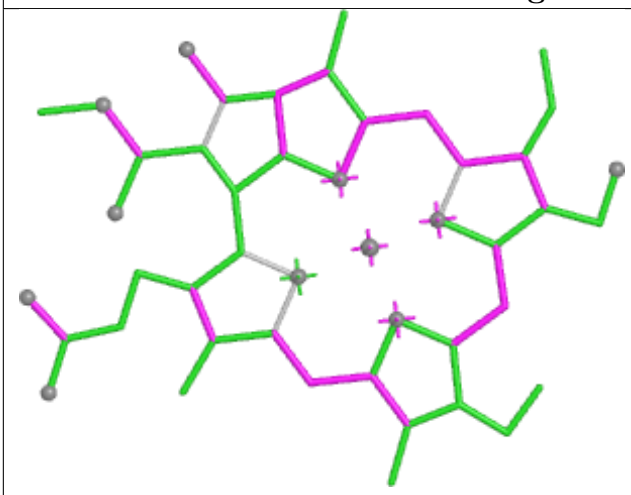


Rings

Ligand CHL 4 316



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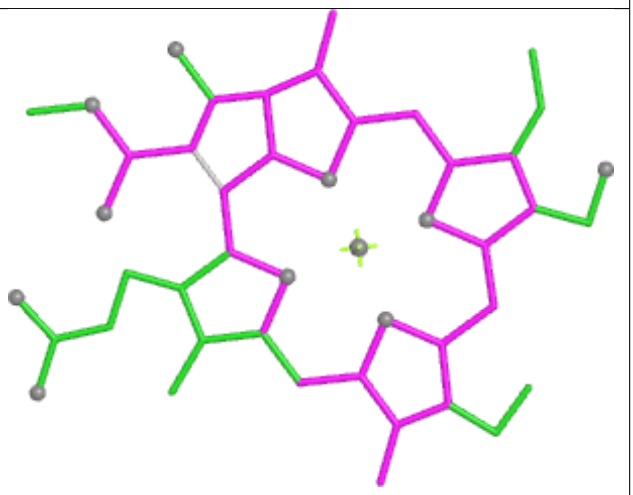

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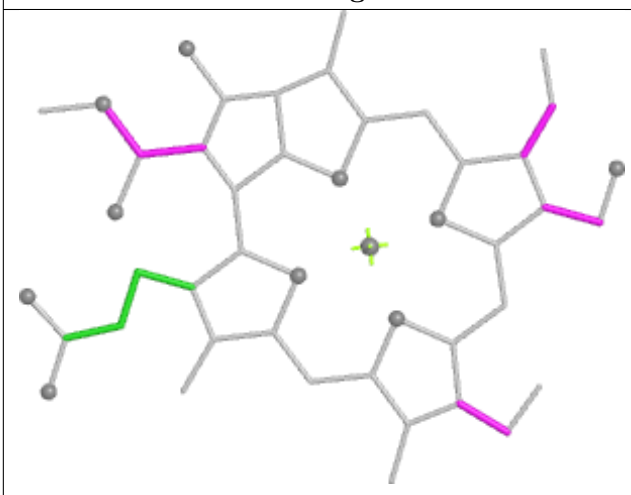

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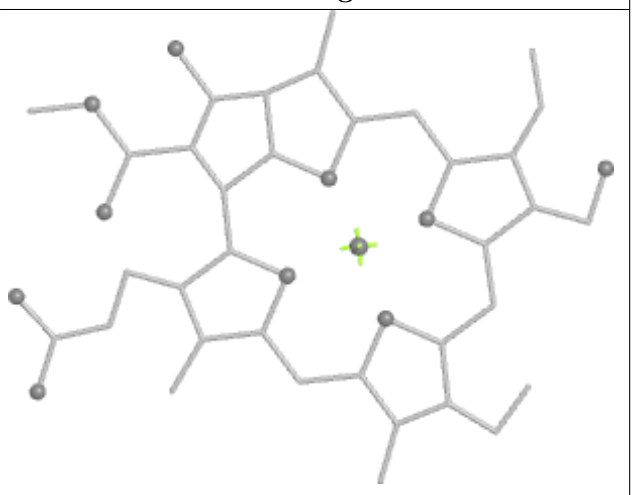
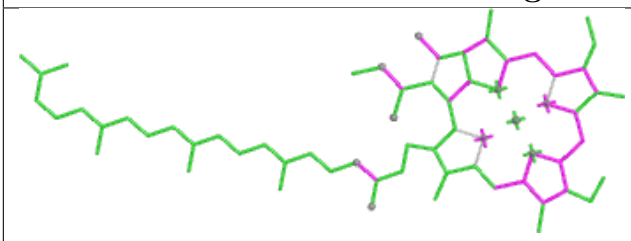


Rings

Ligand CHL B 812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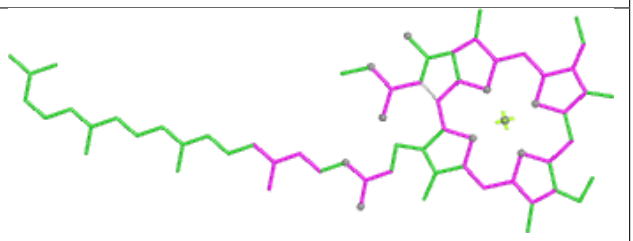
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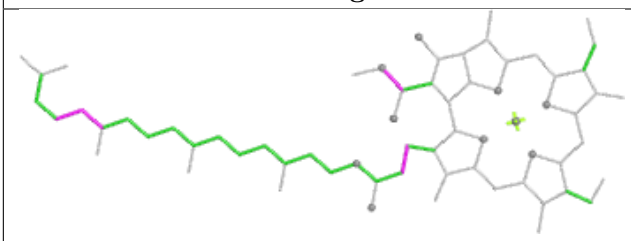
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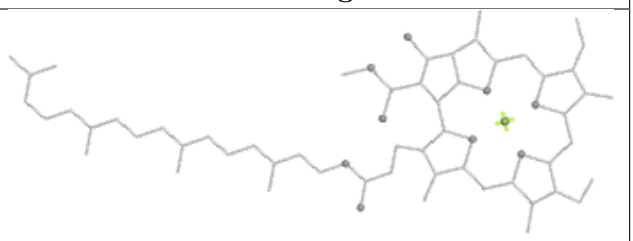
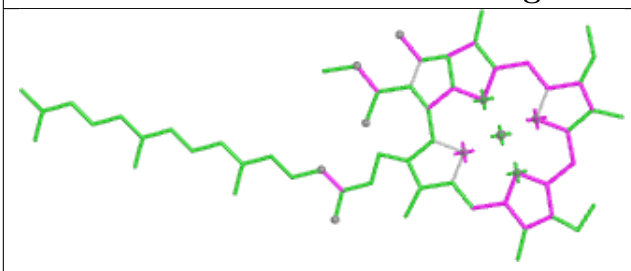

Rings

Ligand CHL A 838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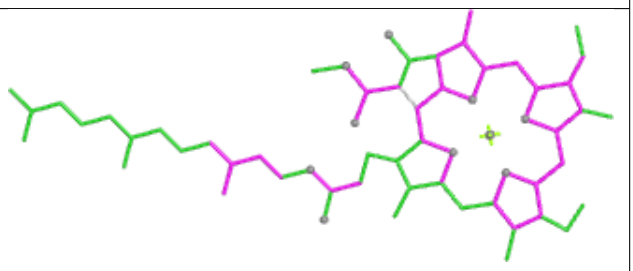
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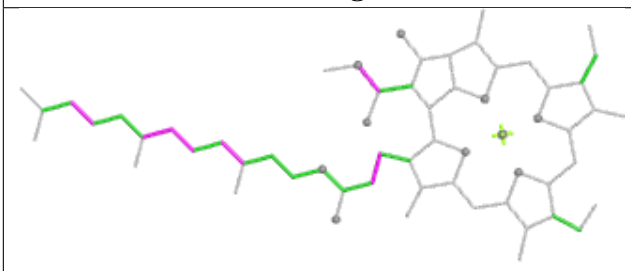
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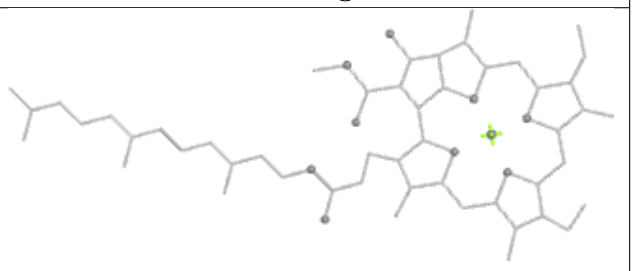
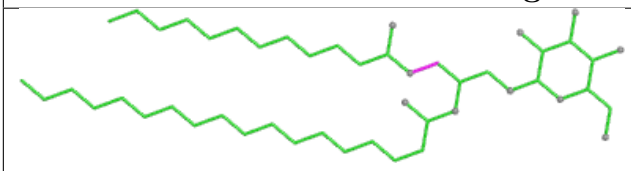

Rings

Ligand LMG J 101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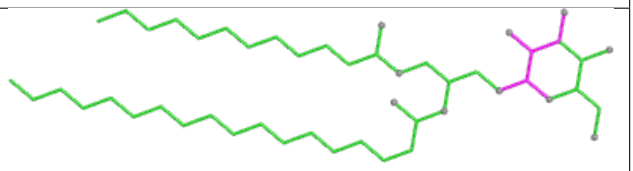
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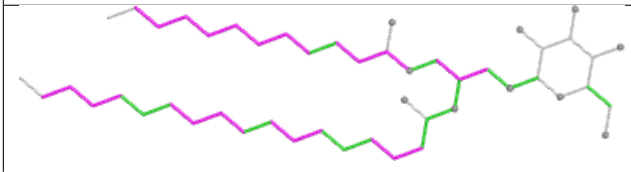
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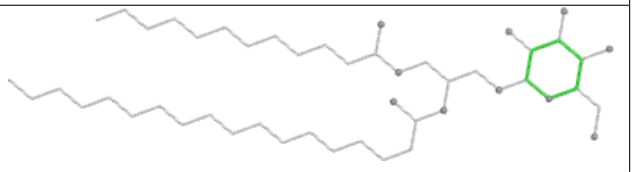
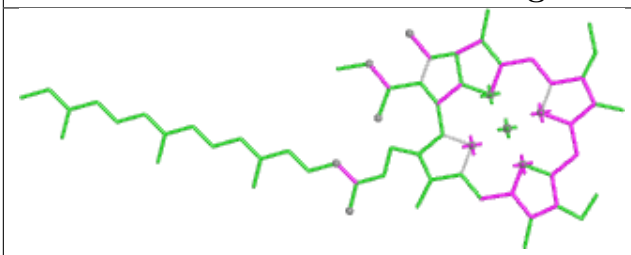

Rings

Ligand CHL 3 320



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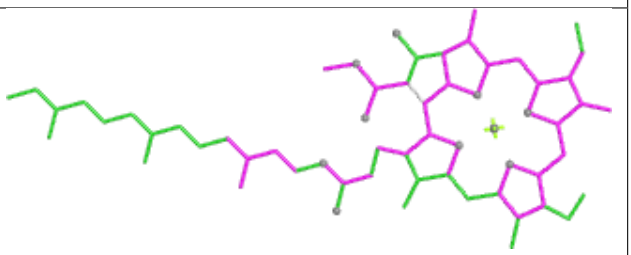

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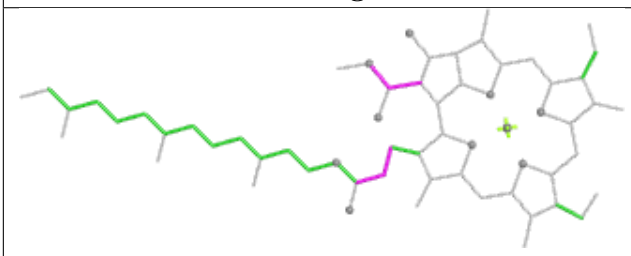

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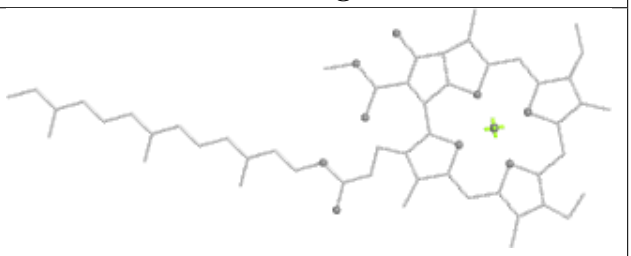
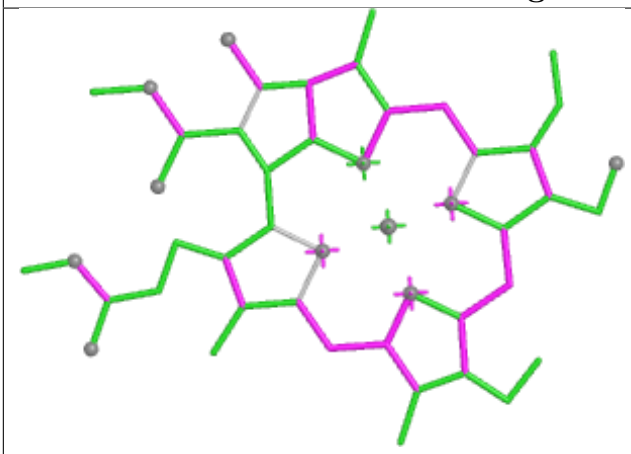


Rings

Ligand CHL 7 320



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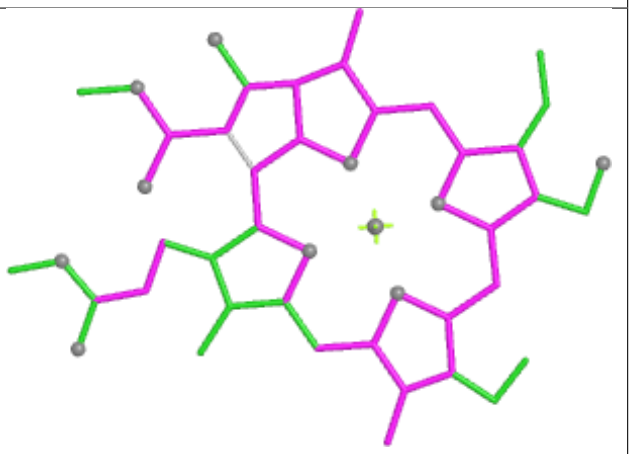

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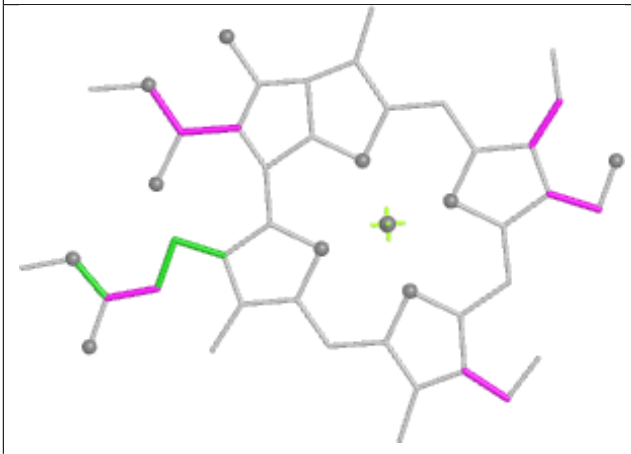

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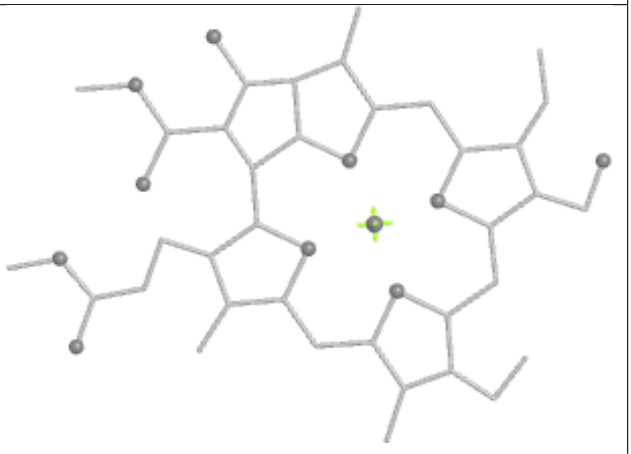
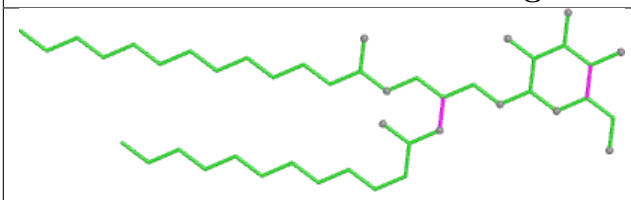


Rings

Ligand LMG a 301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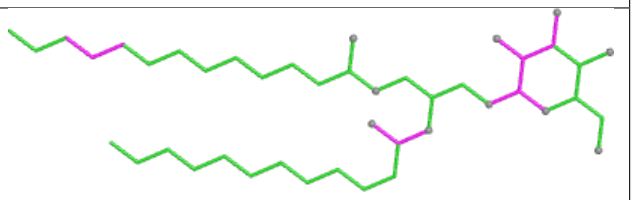
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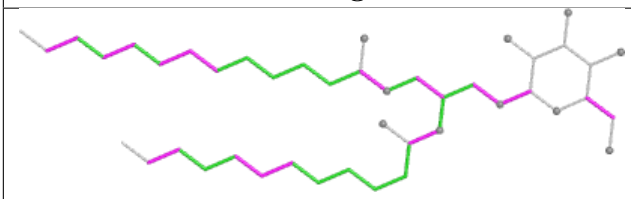
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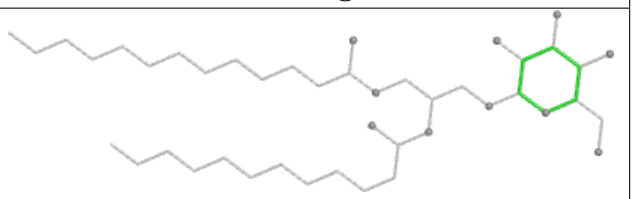
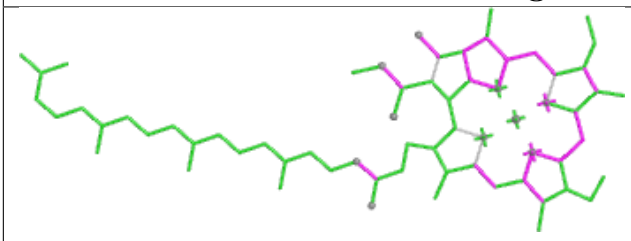

Rings

Ligand CHL 6 307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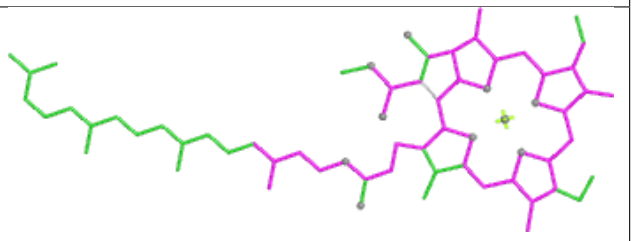
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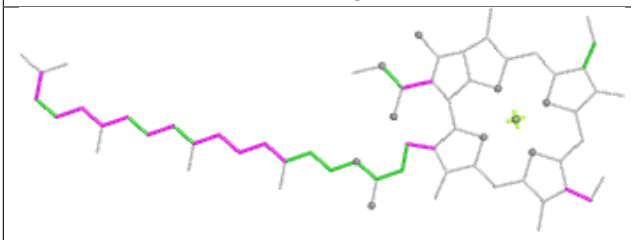
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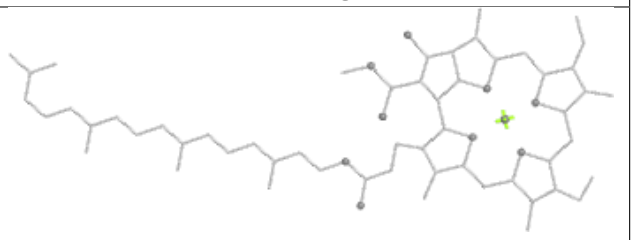
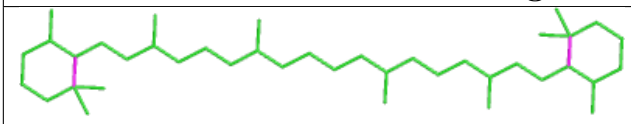

Rings

Ligand BCR 3 303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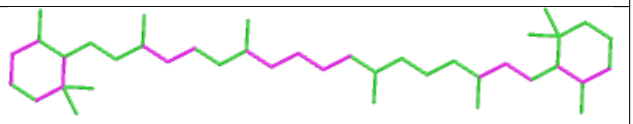
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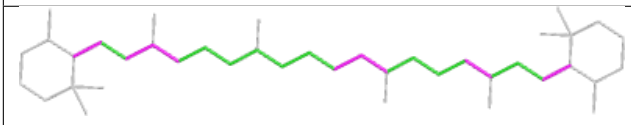
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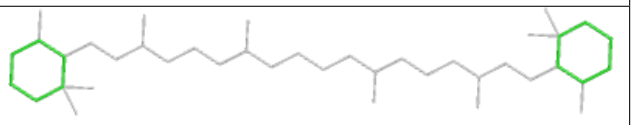
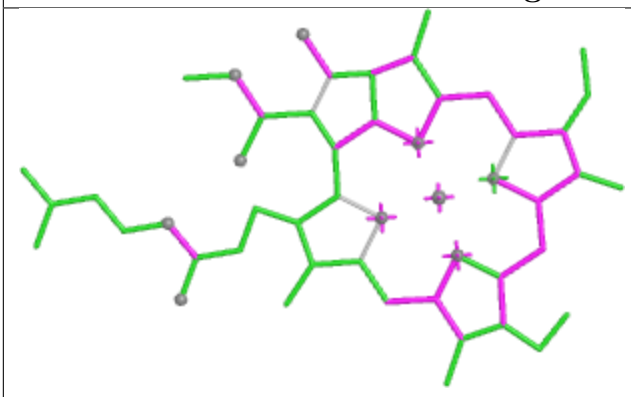

Rings

Ligand CHL B 826



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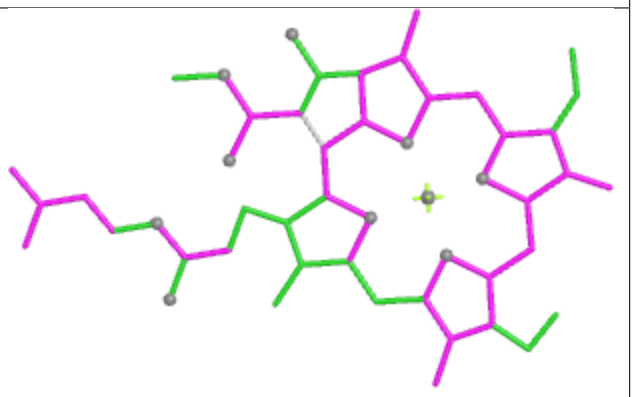
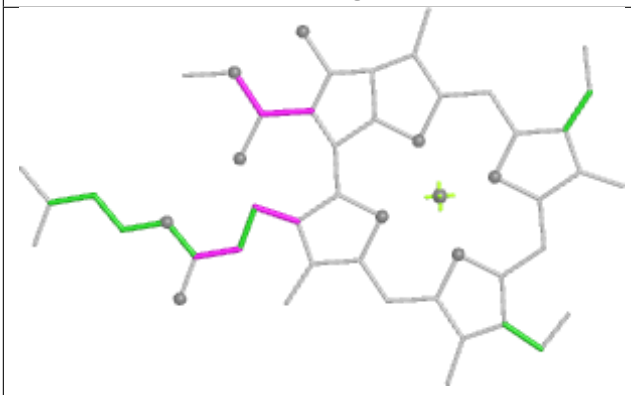


Bond angles



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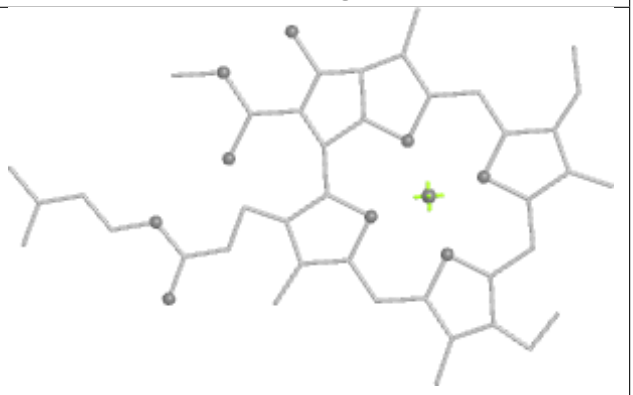
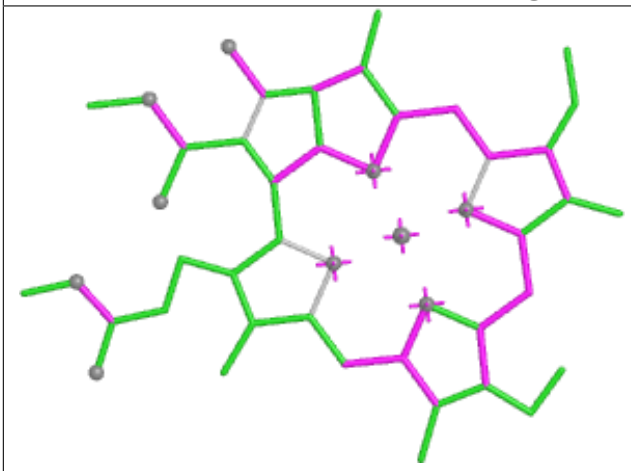


Rings

Ligand CHL F 308



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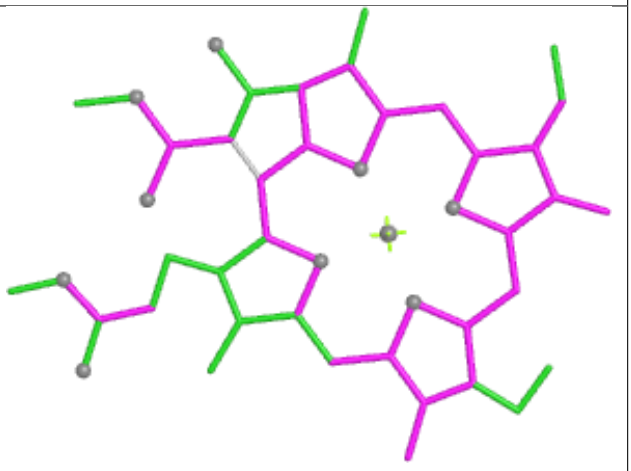
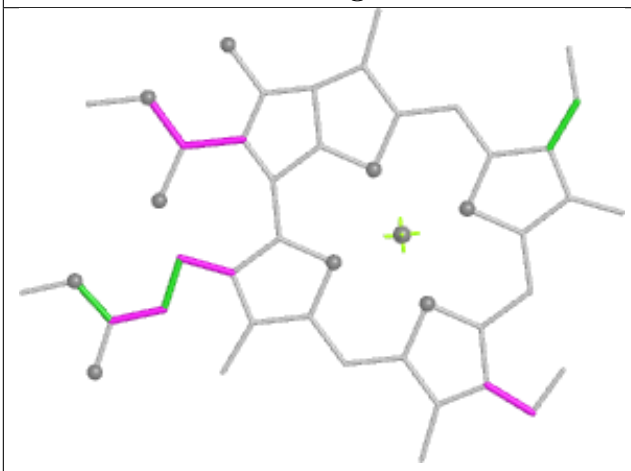


Bond angles



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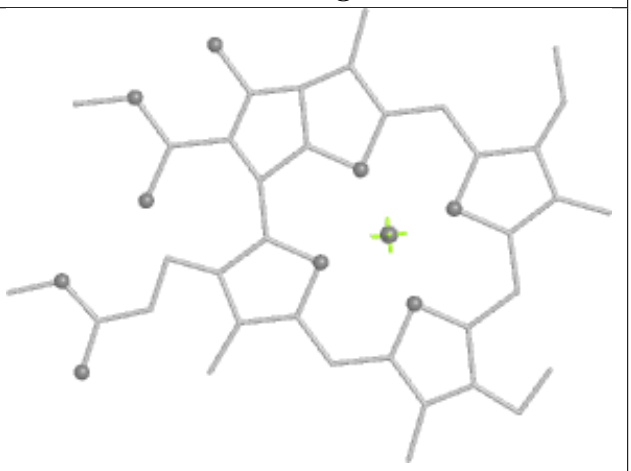
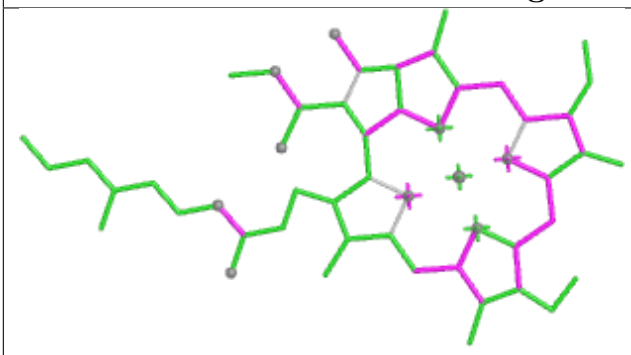
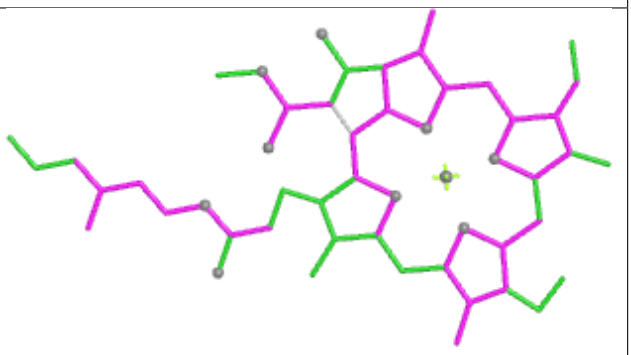


Rings

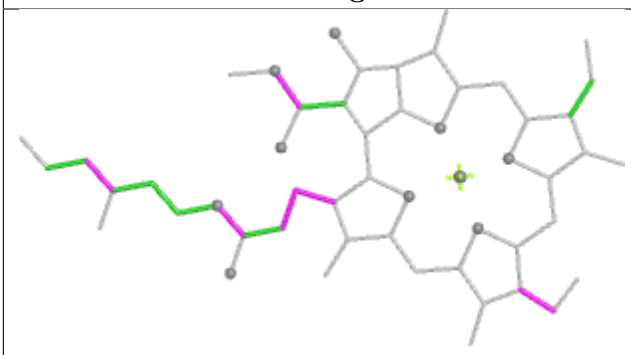
Ligand CHL 3 315



Bond lengths



Bond angles



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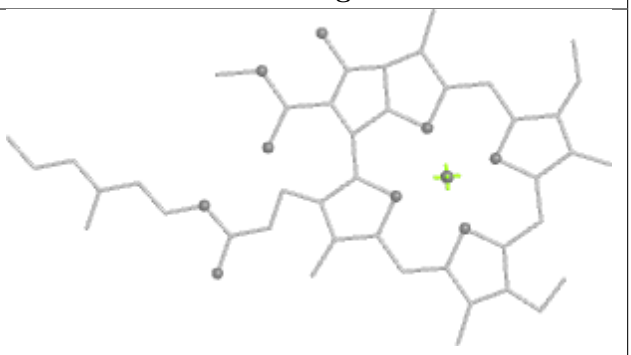
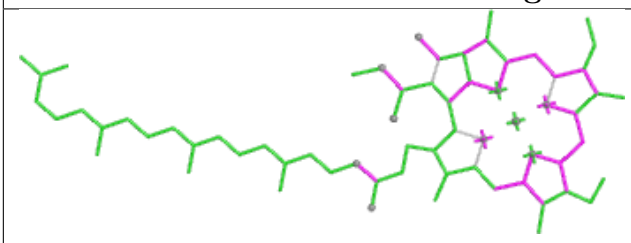
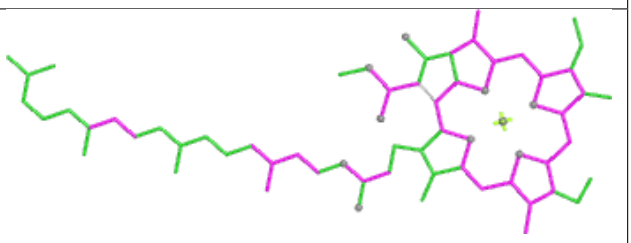


Rings

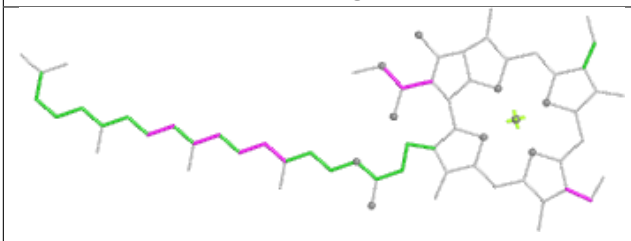
Ligand CHL B 817



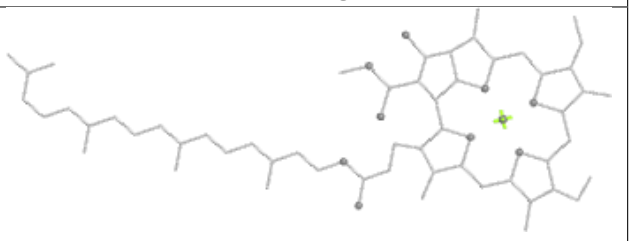
Bond lengths



Bond angles

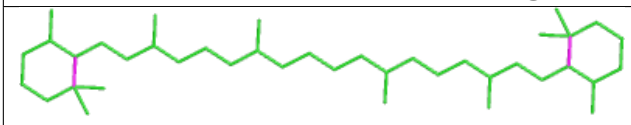


Torsions



Rings

Ligand BCR L 301



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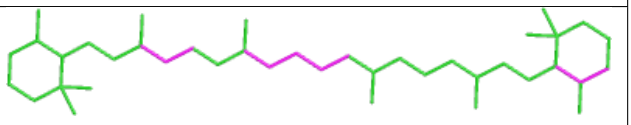

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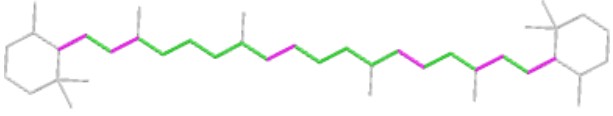

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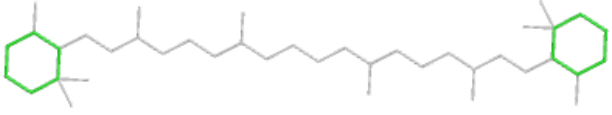
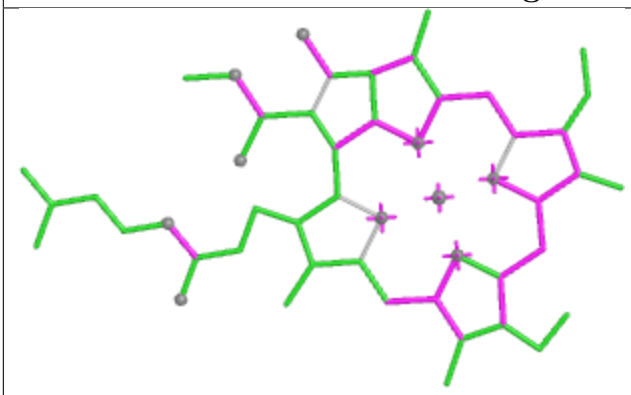


Rings

Ligand CHL K 204



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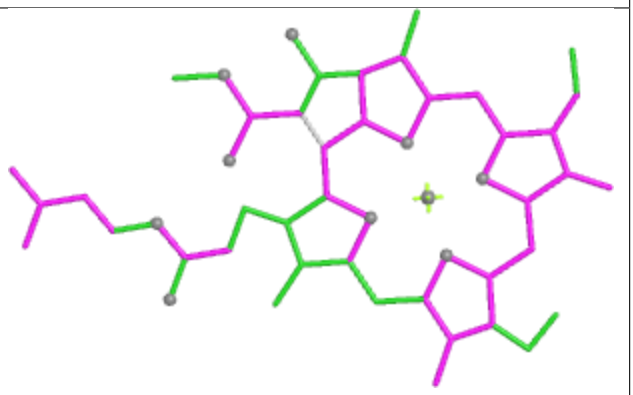

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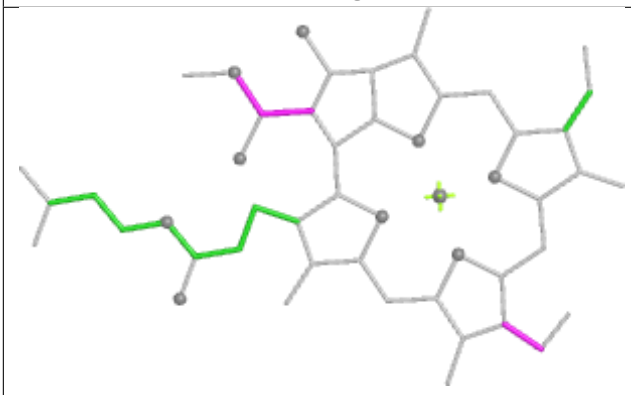

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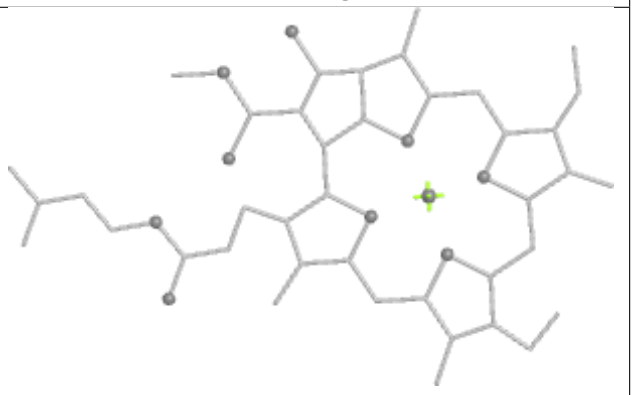
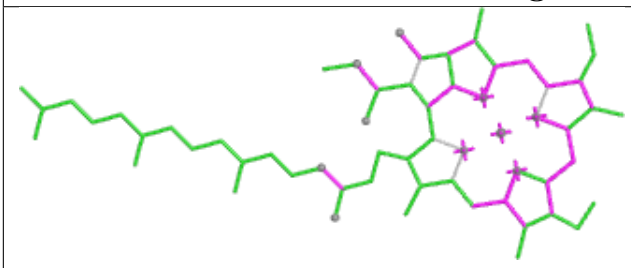


Rings

Ligand CHL a 309



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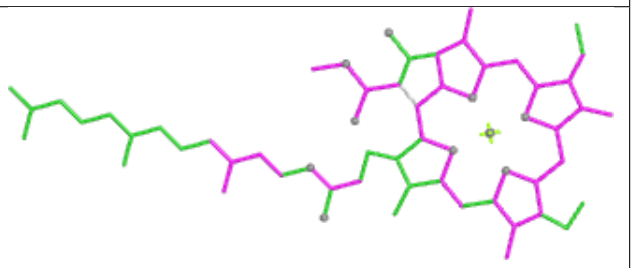
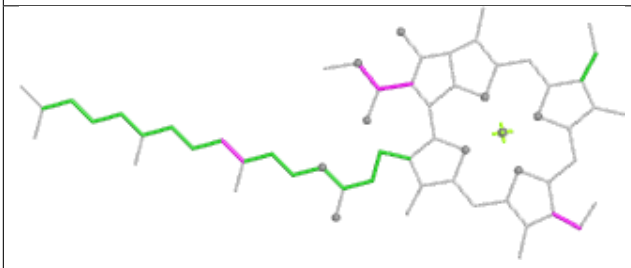


Bond angles



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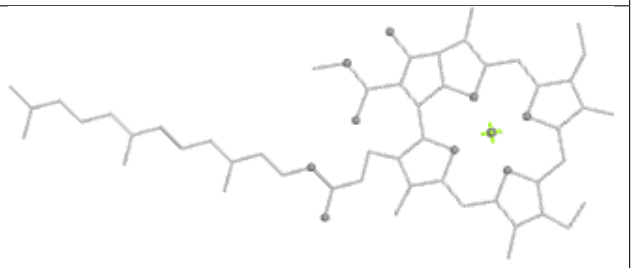
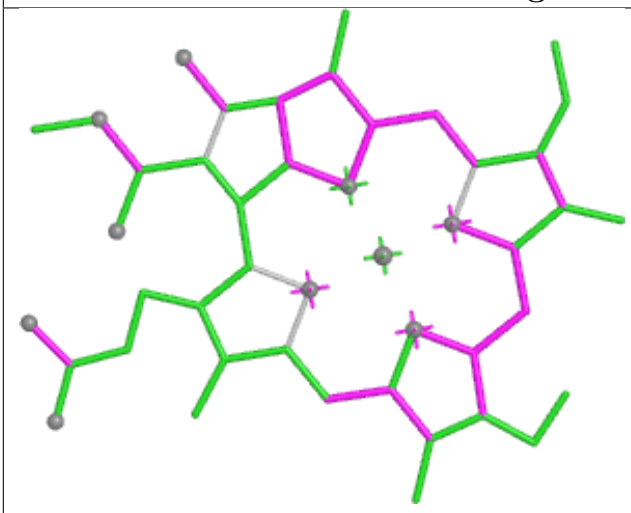


Rings

Ligand CHL 4 317



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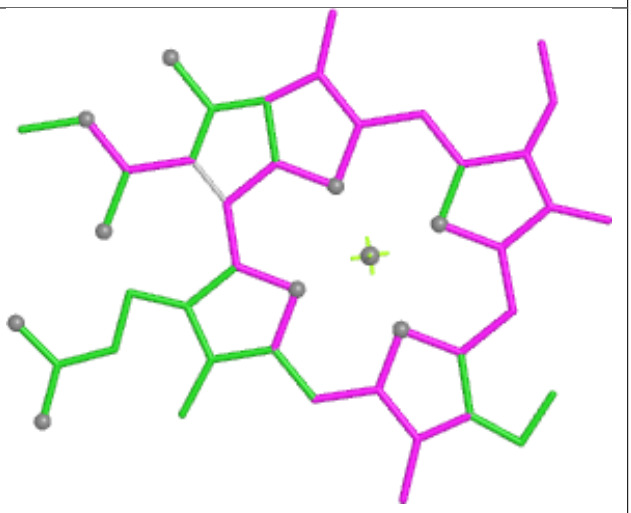

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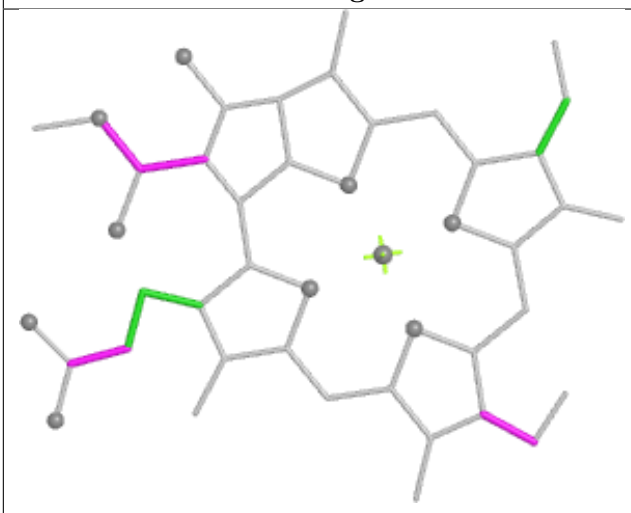

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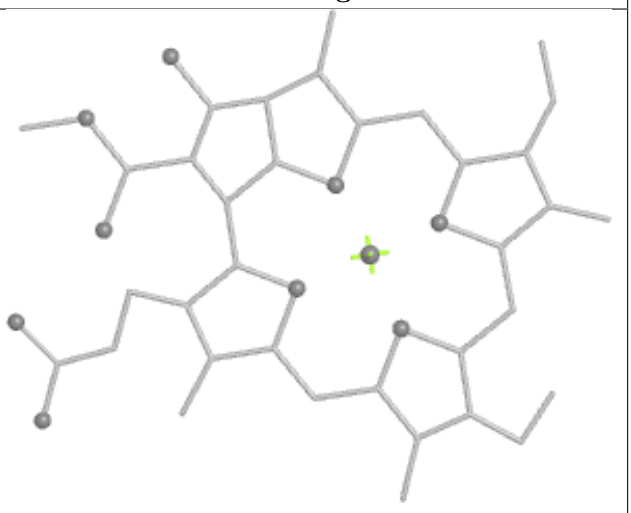
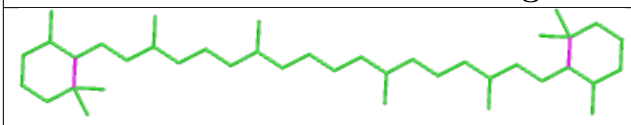


Rings

Ligand BCR A 803



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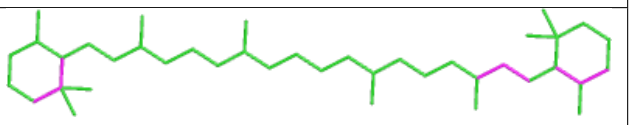

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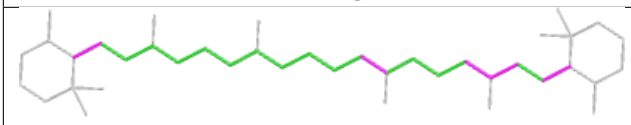

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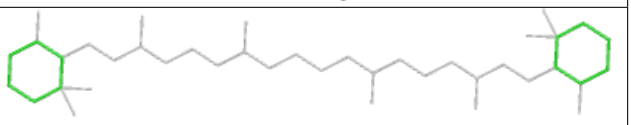
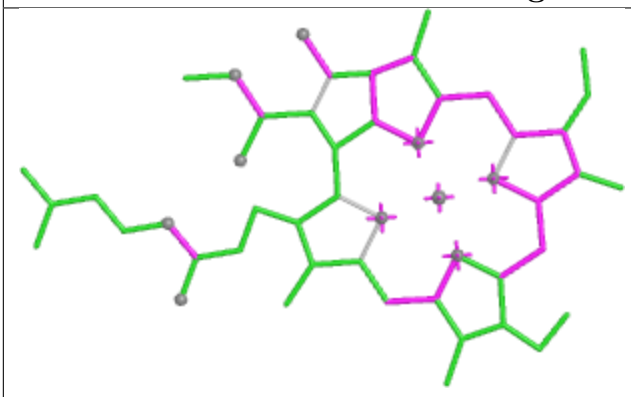


Rings

Ligand CHL 8 323



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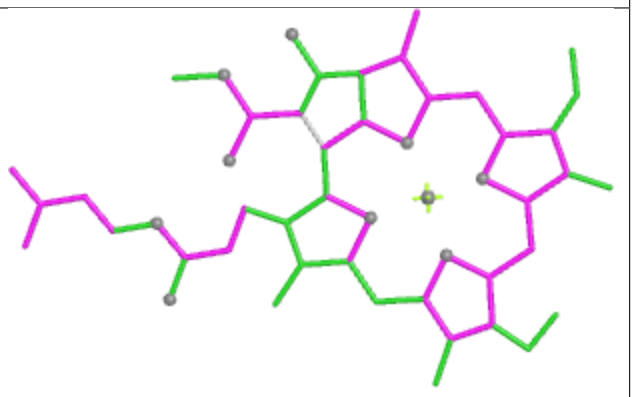

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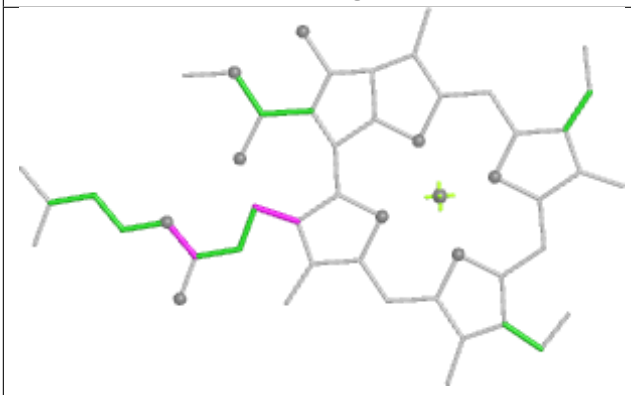

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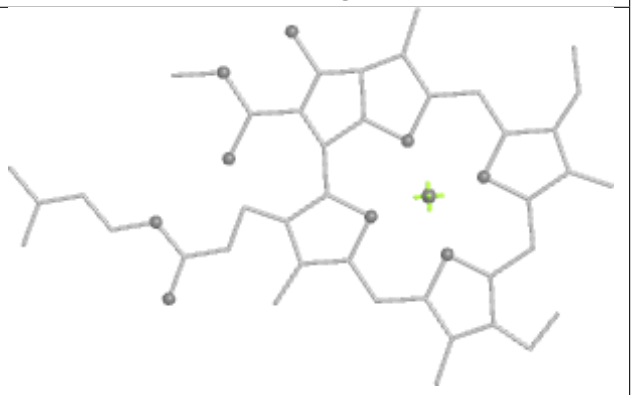
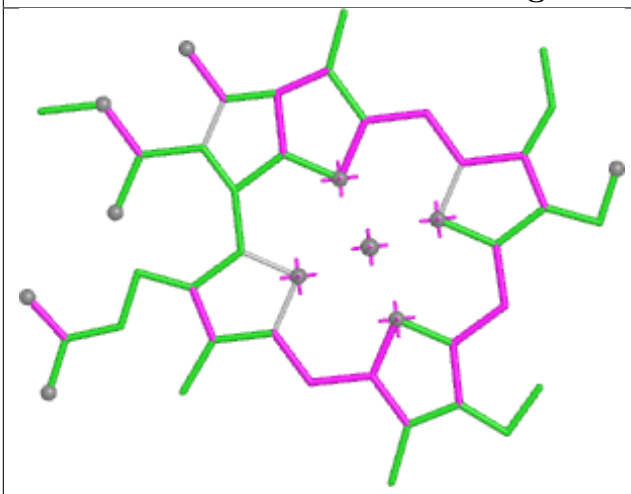


Rings

Ligand CHL 6 316



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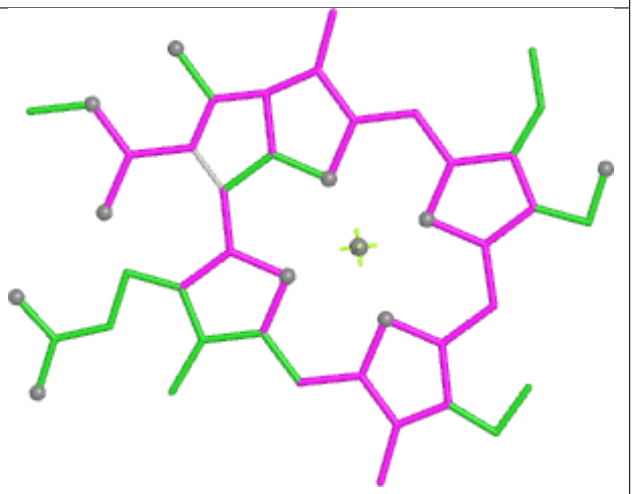
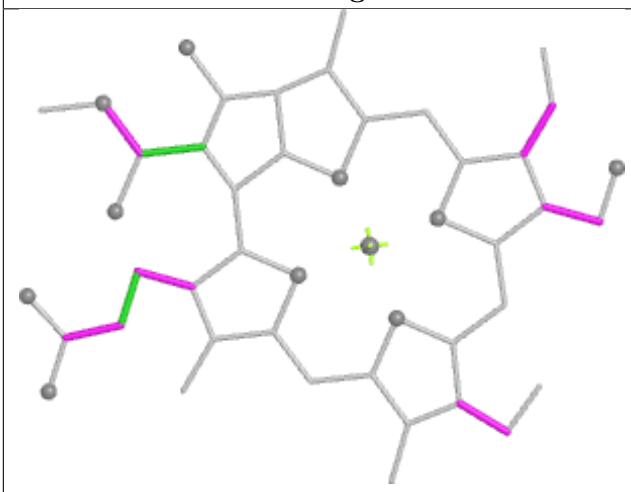


Bond angles



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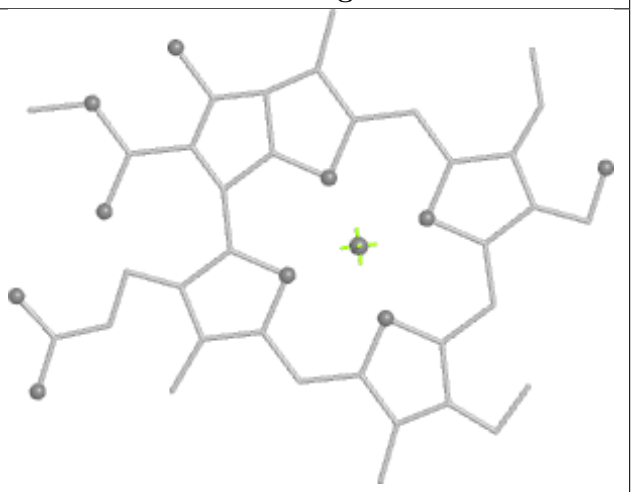
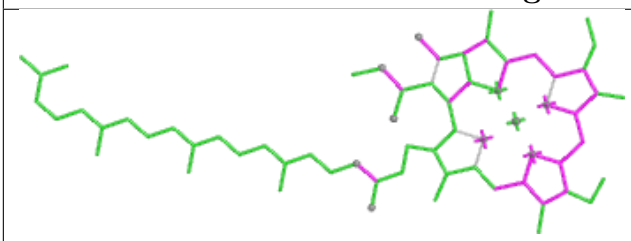


Rings

Ligand CHL A 816



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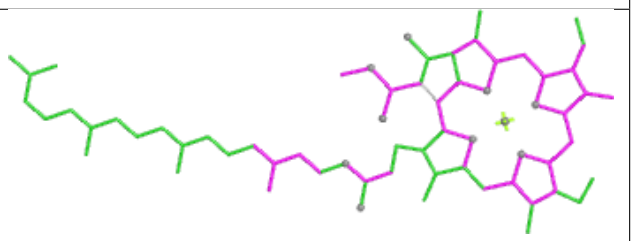
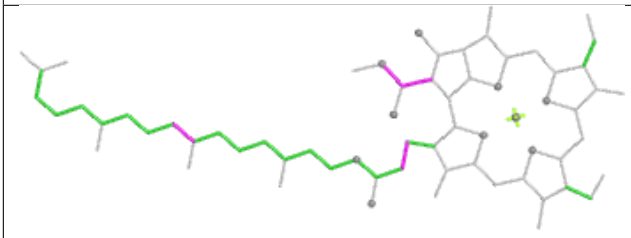


Bond angles



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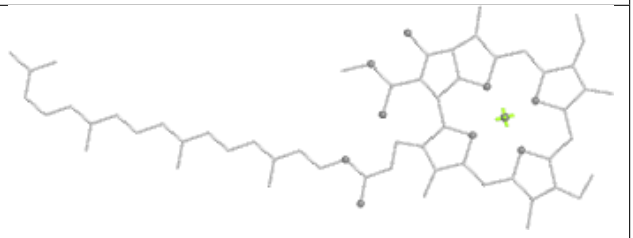
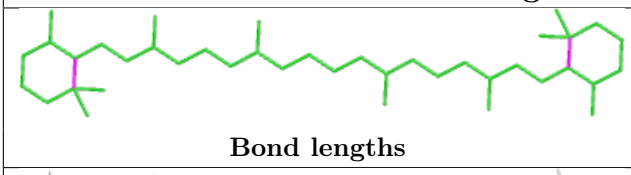


Rings

Ligand BCR B 805



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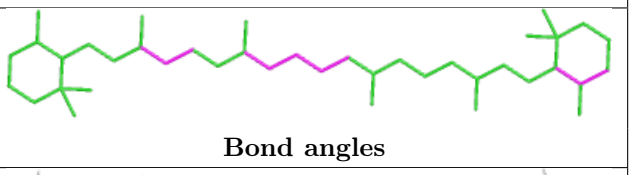
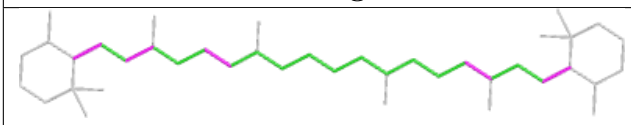


Bond angles



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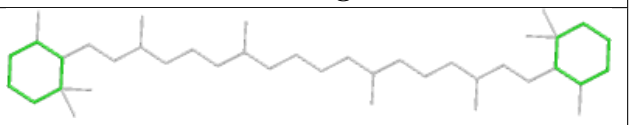
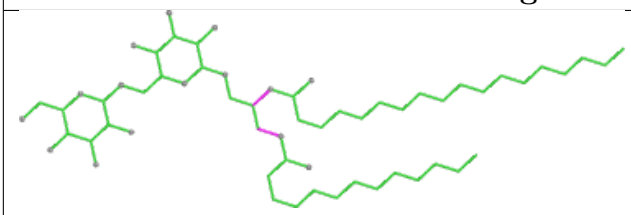


Rings

Ligand DGD B 809



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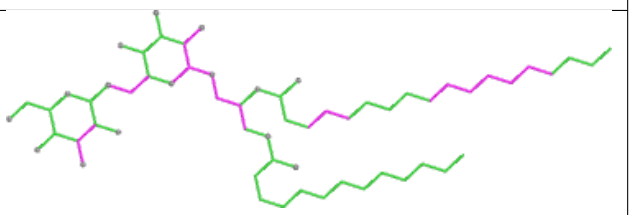
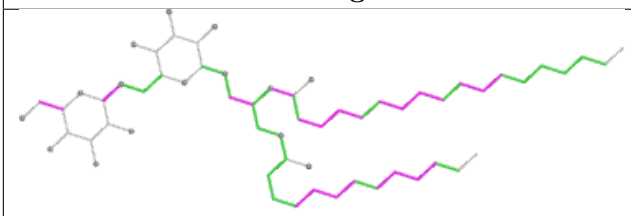


Bond angles



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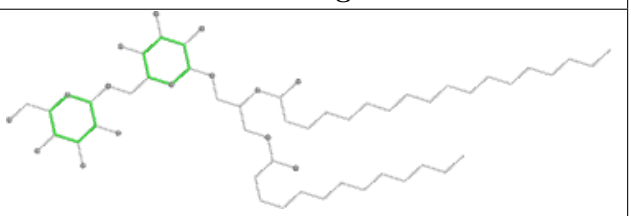
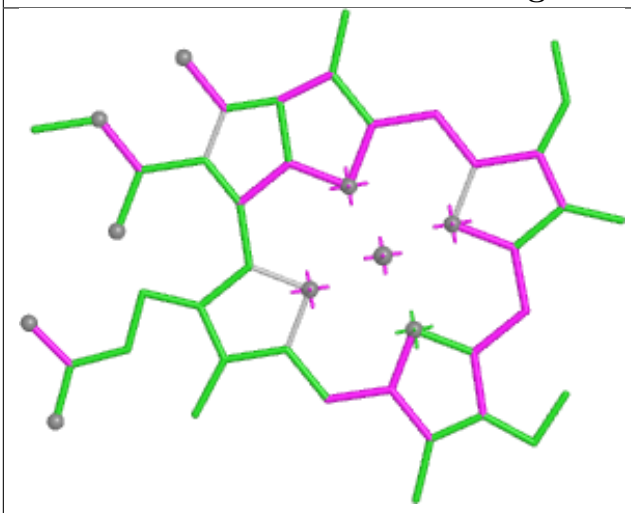


Rings

Ligand CHL a 314



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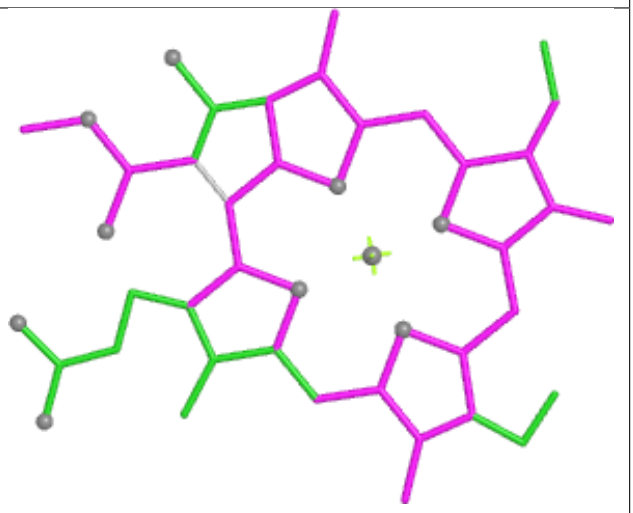
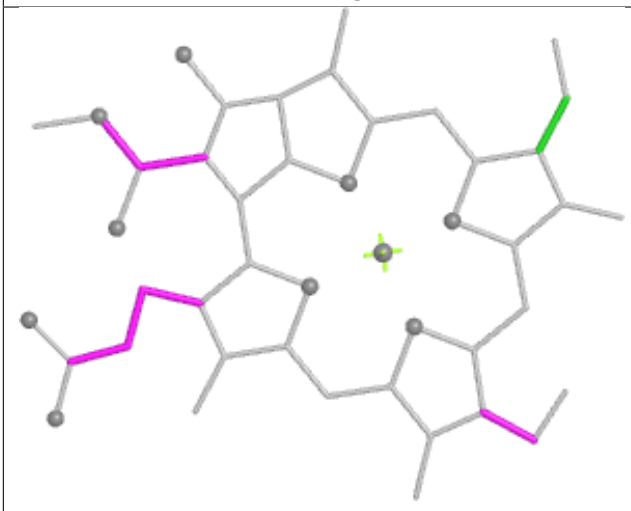


Bond angles



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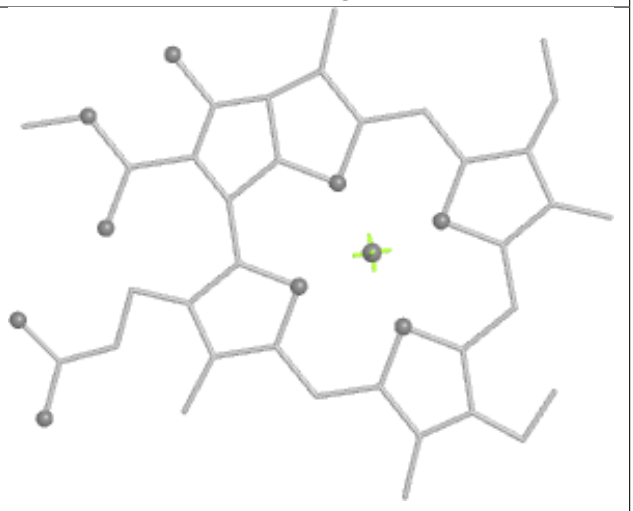
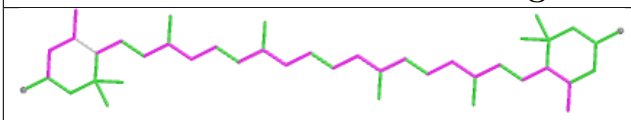


Rings

Ligand LUT 3 304



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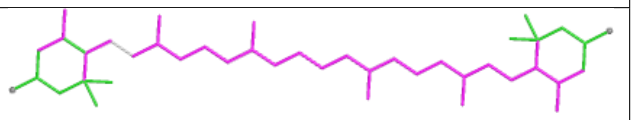
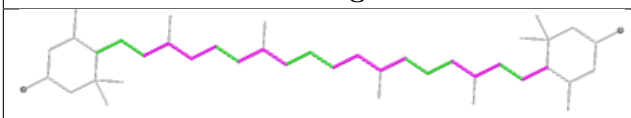


Bond angles



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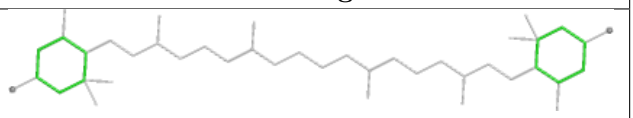
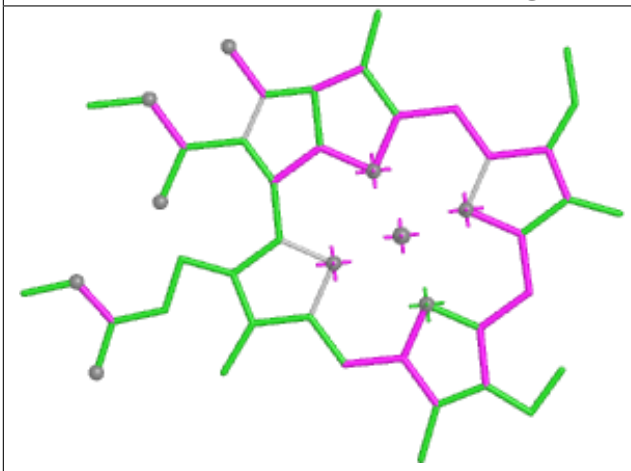
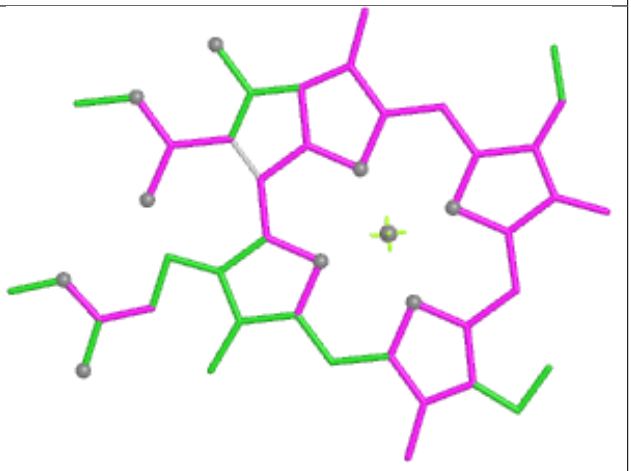


Rings

Ligand CHL A 851	
	
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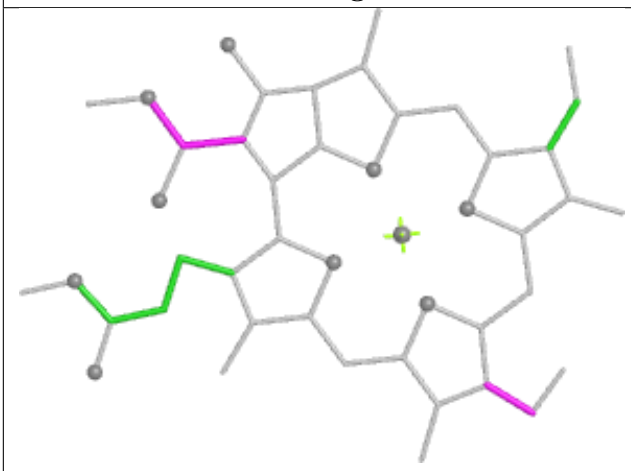
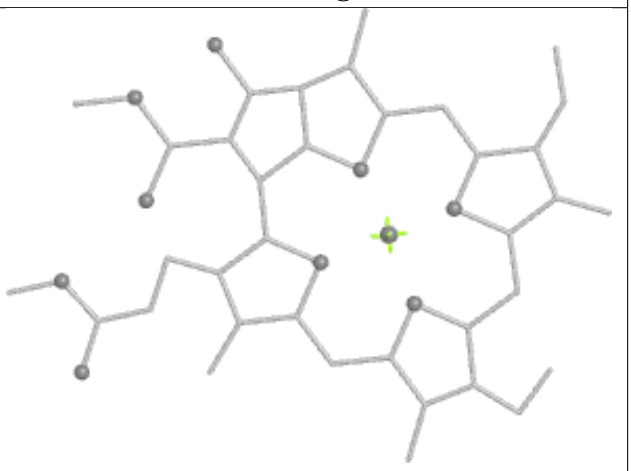
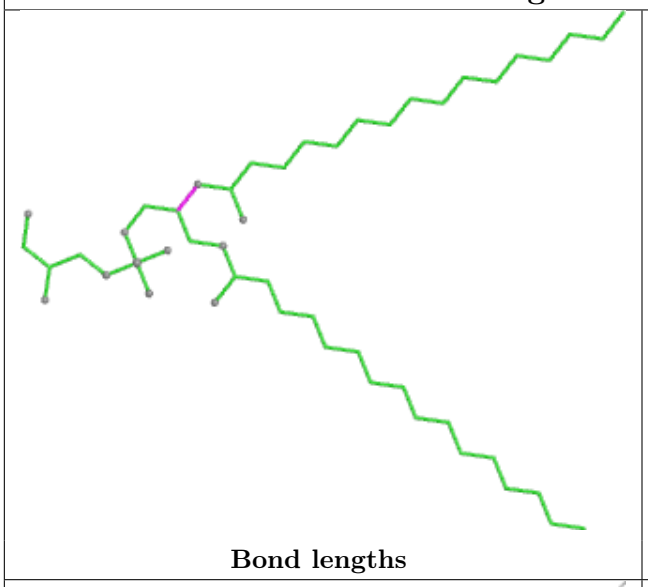
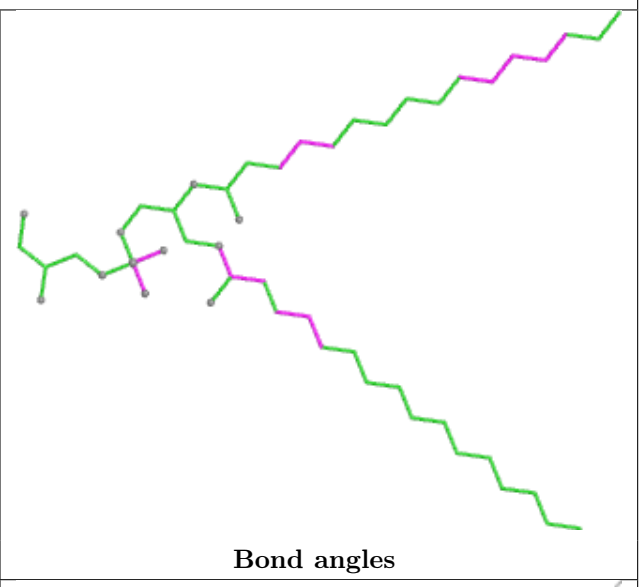
	
Torsions	**Rings**

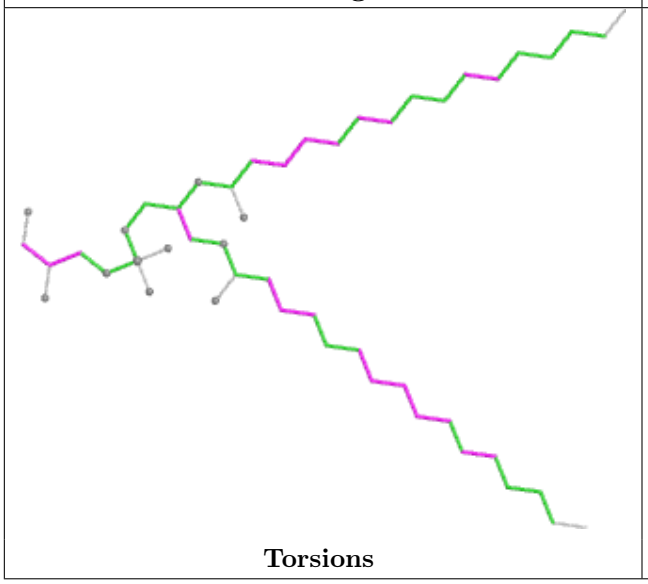
Ligand LHG 8 305



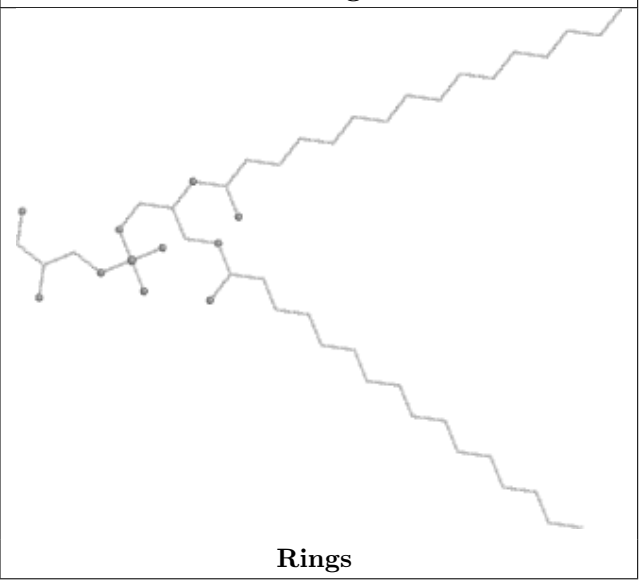
Bond lengths



Bond angles

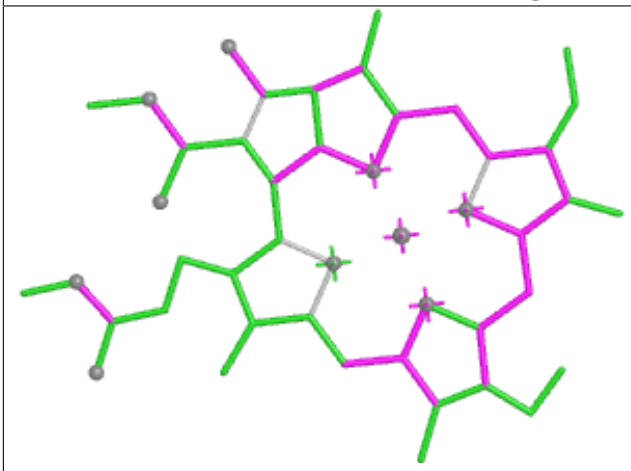


Torsions



Rings

Ligand CHL b 304



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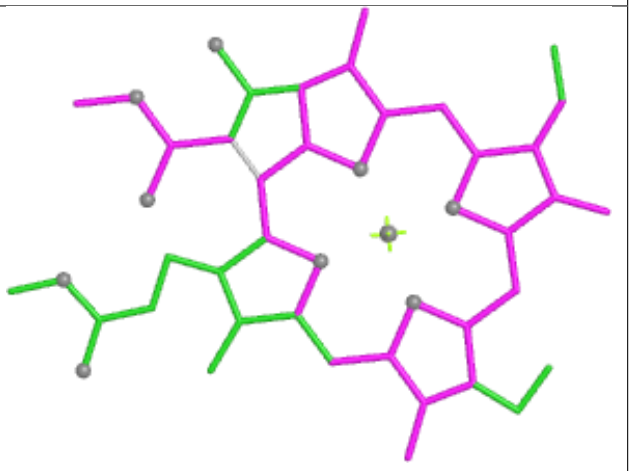
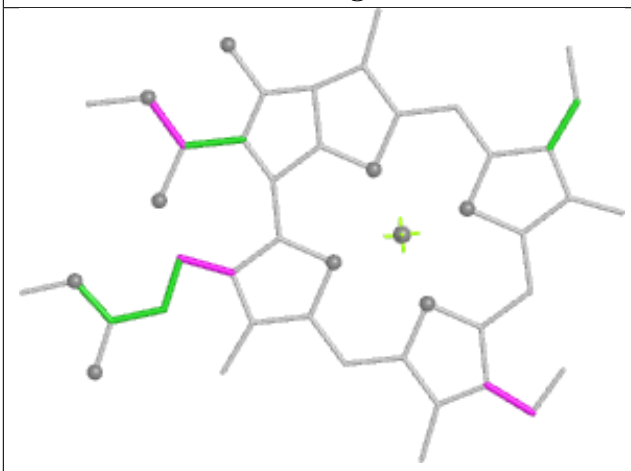


Bond angles



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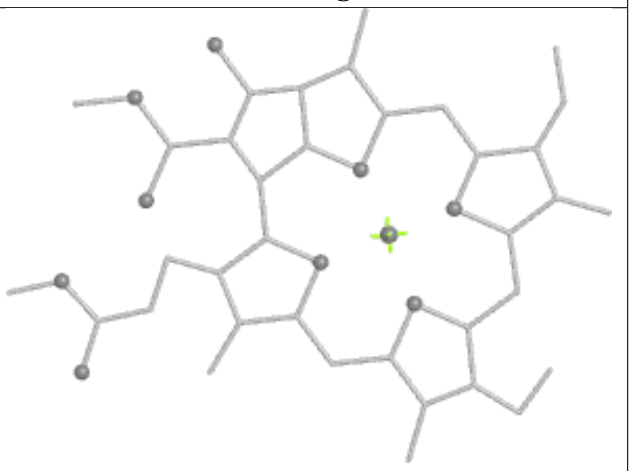
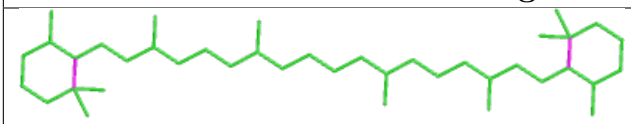


Rings

Ligand BCR M 102



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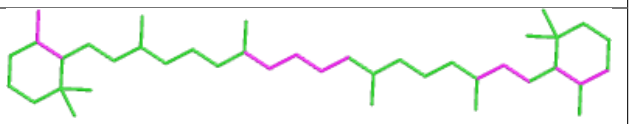
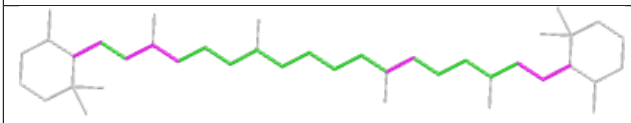


Bond angles



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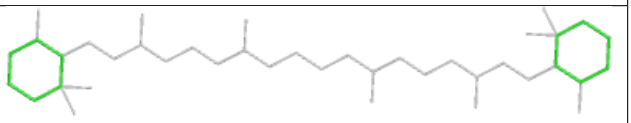
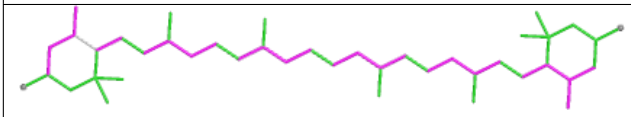


Rings

Ligand LUT J 103



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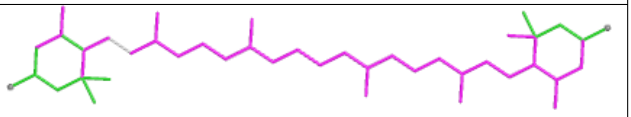

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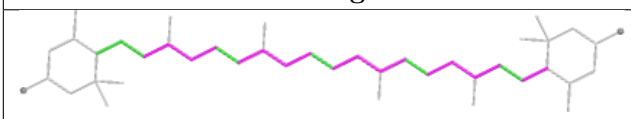

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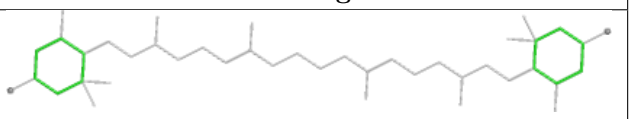
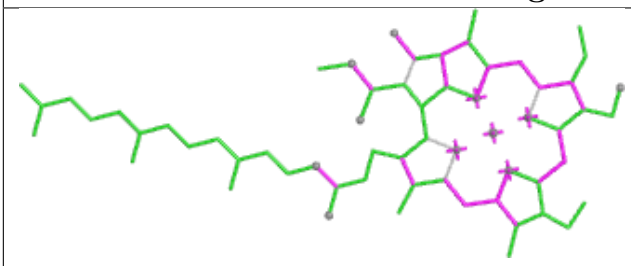


Rings

Ligand CHL a 315



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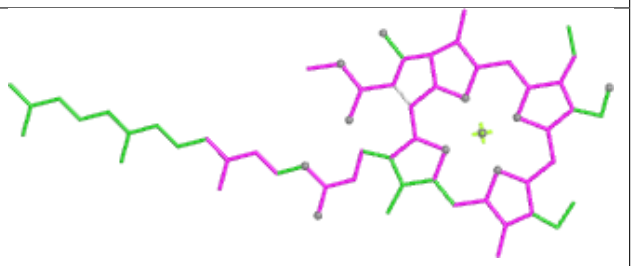
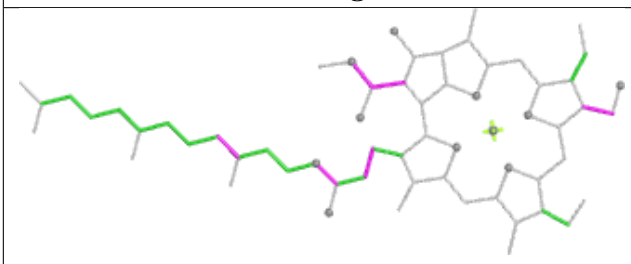


Bond angles



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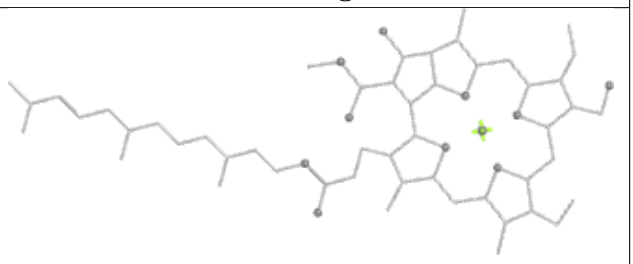
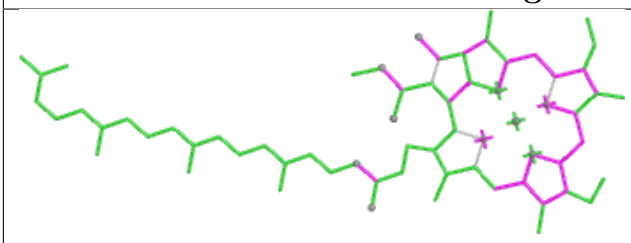


Rings

Ligand CHL B 840



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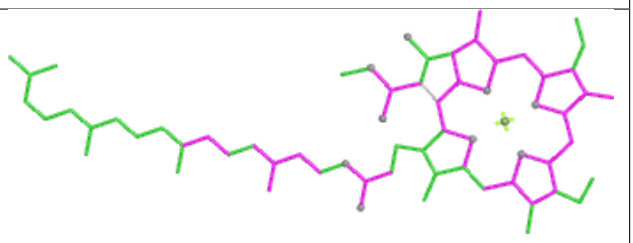

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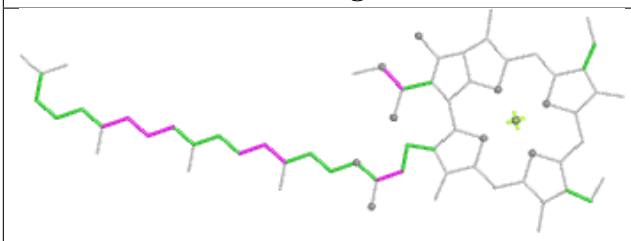

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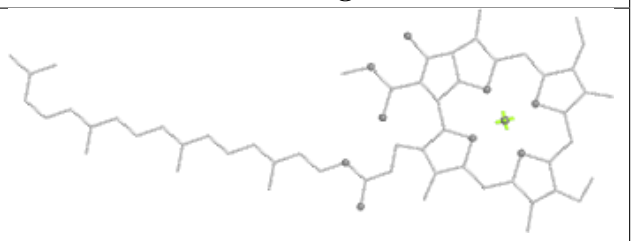
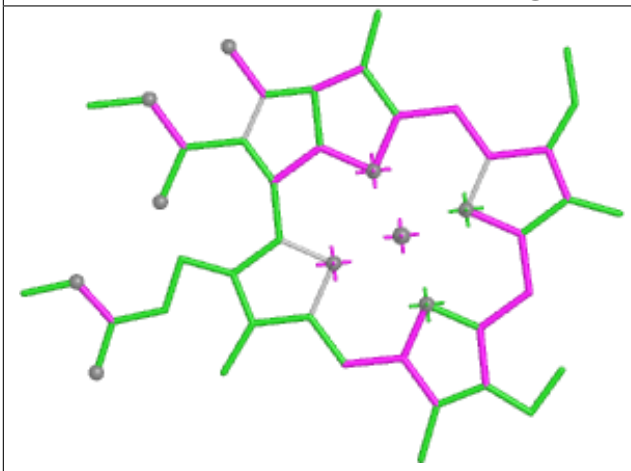


Rings

Ligand CHL b 312



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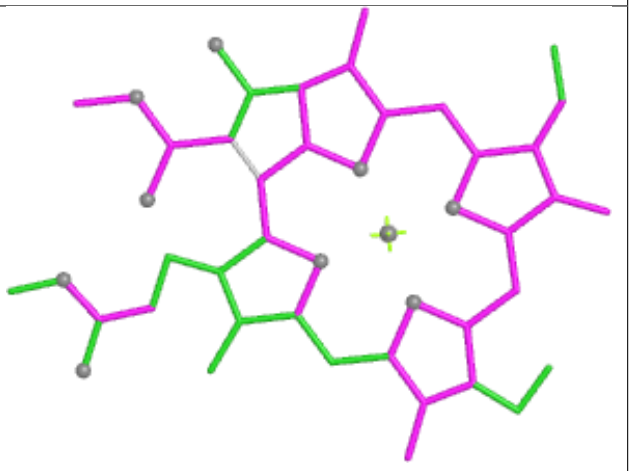
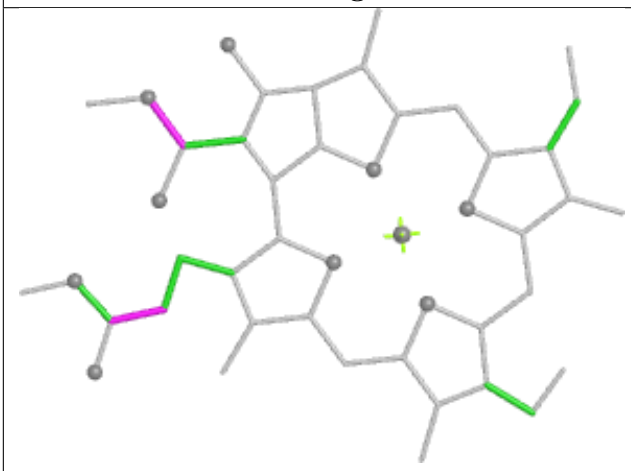


Bond angles



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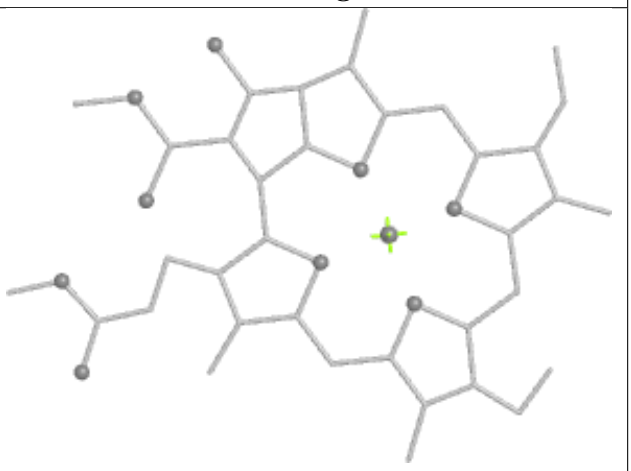
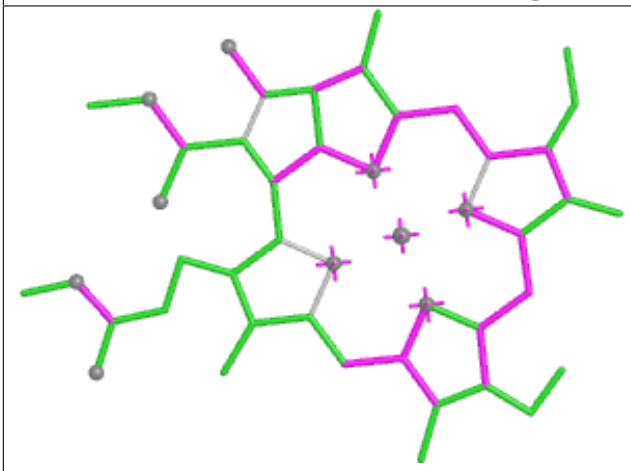


Rings

Ligand CHL b 314



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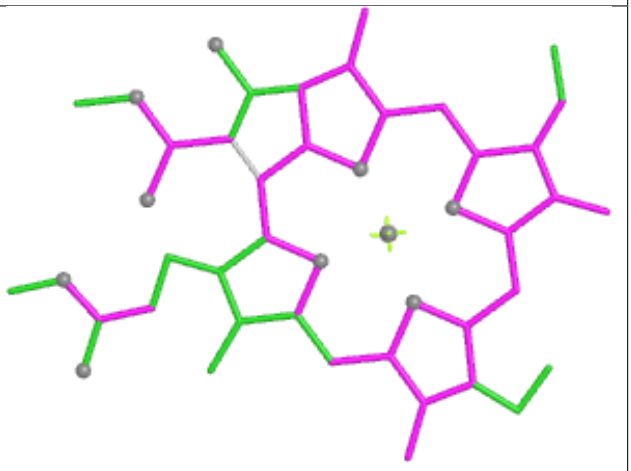
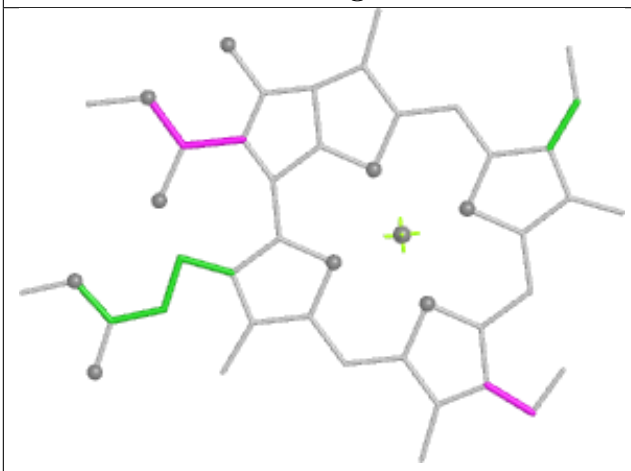


Bond angles



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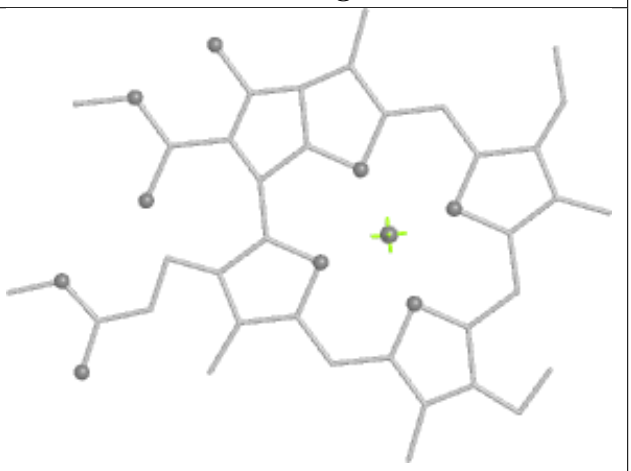
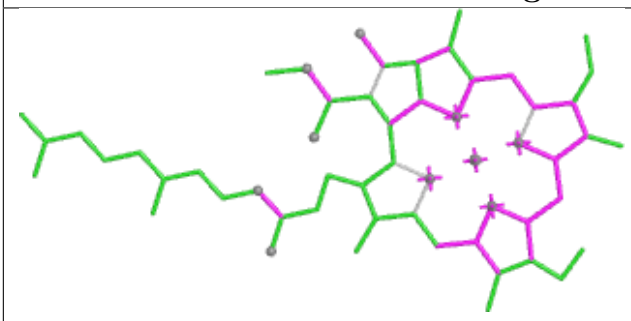


Rings

Ligand CHL A 822



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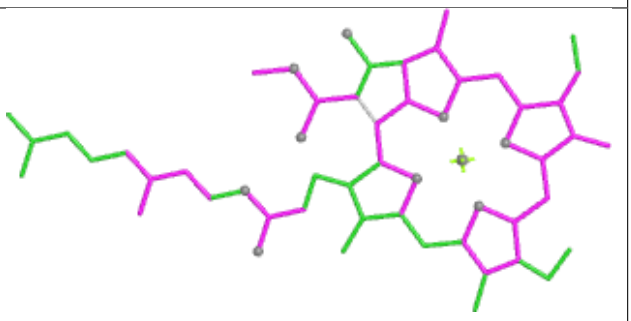
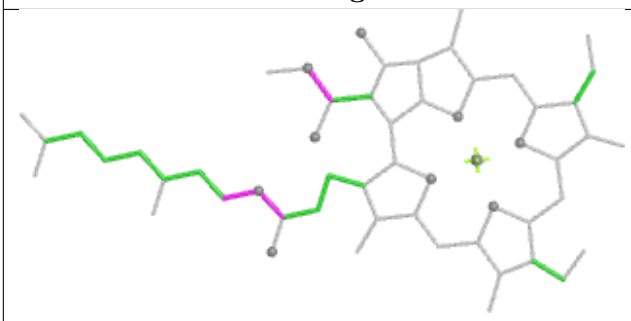


Bond angles



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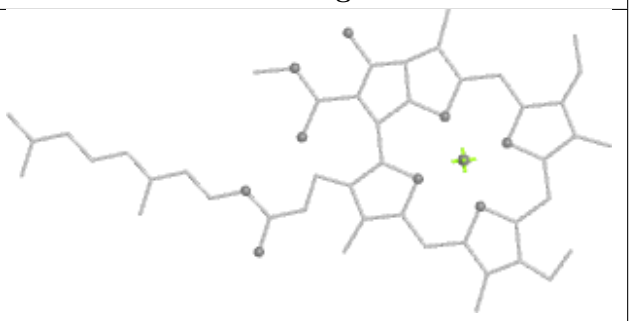
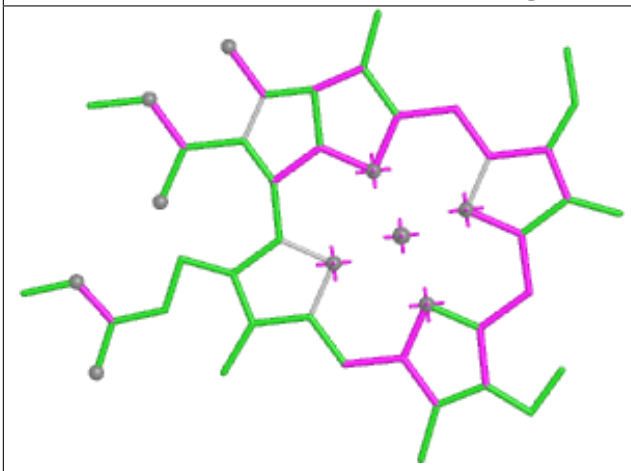


Rings

Ligand CHL K 205



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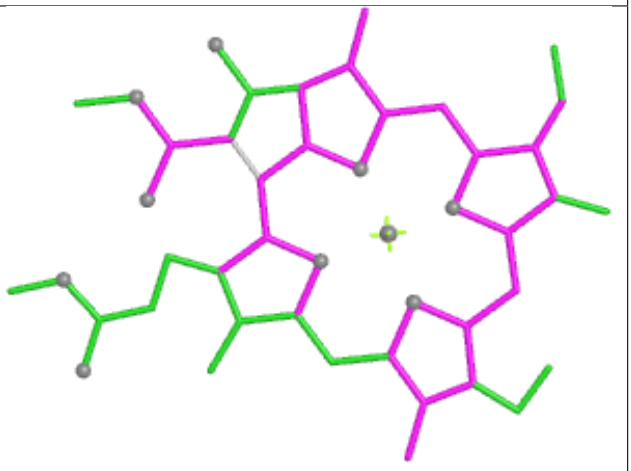
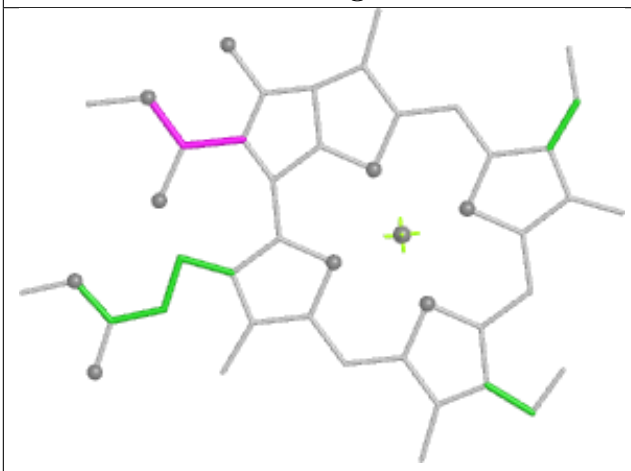


Bond angles



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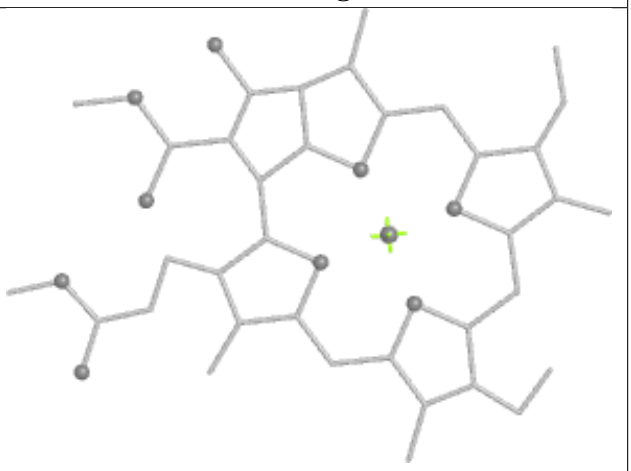
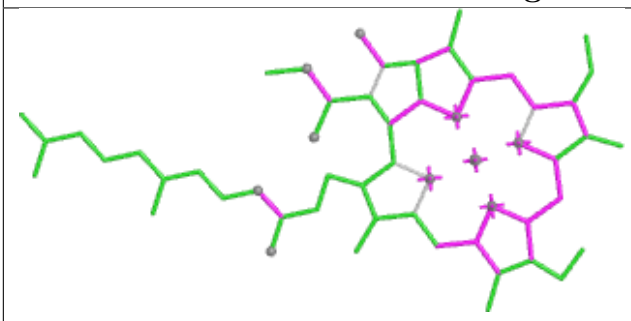


Rings

Ligand CHL B 833



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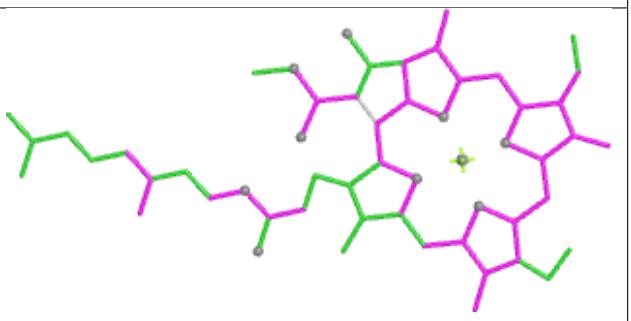
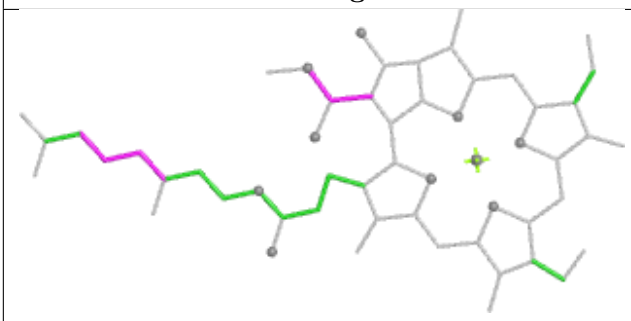


Bond angles



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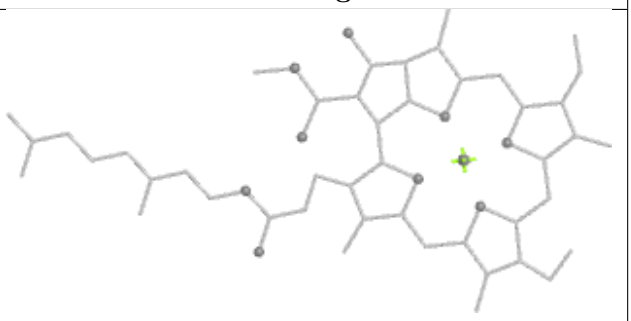
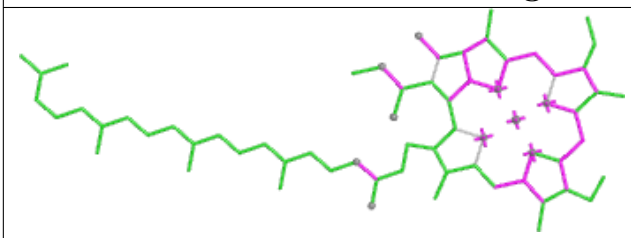


Rings

Ligand CHL A 821



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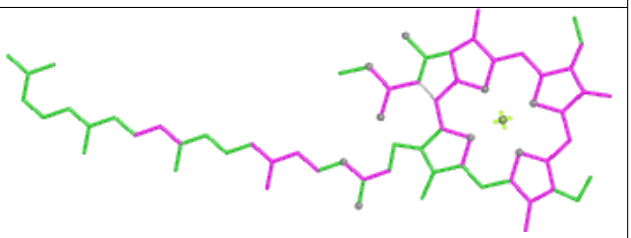
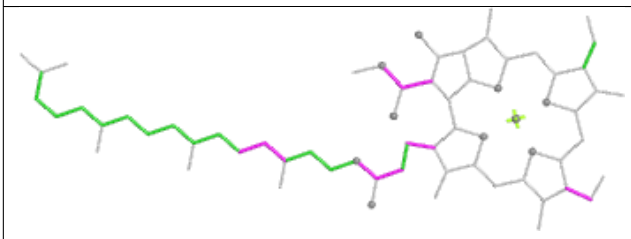


Bond angles



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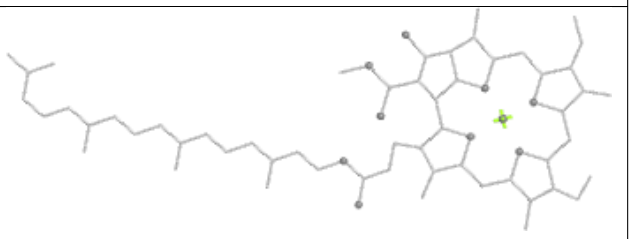
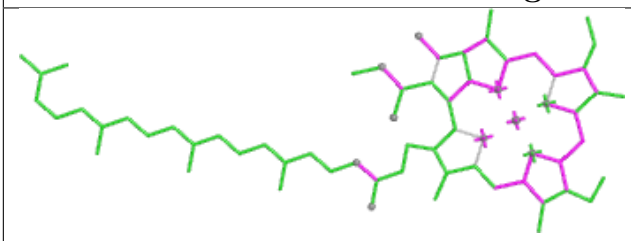
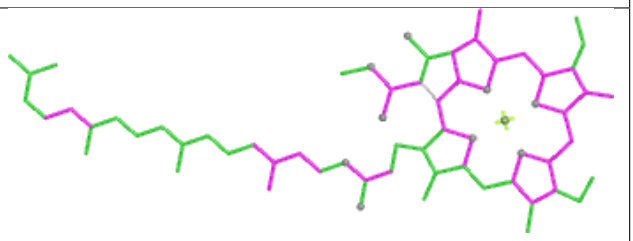
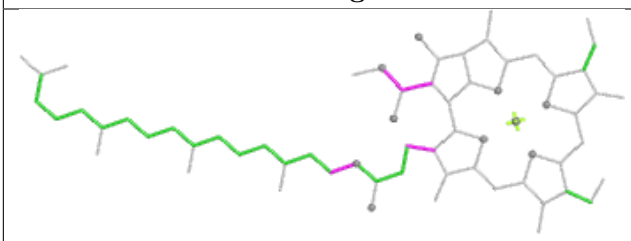
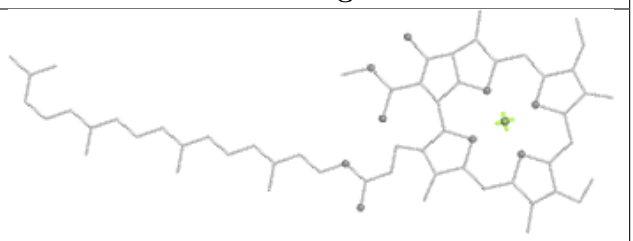


Rings

Ligand CHL B 834	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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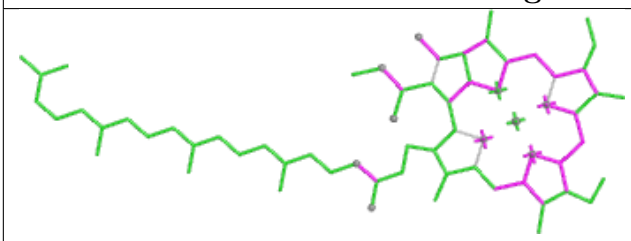
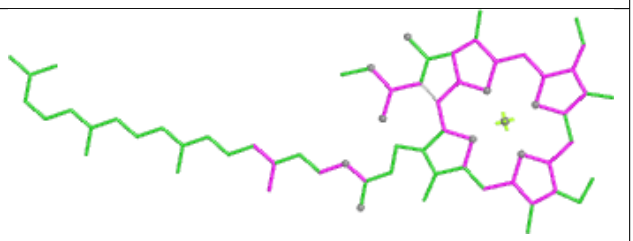
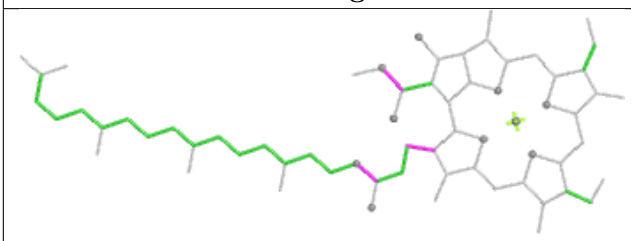
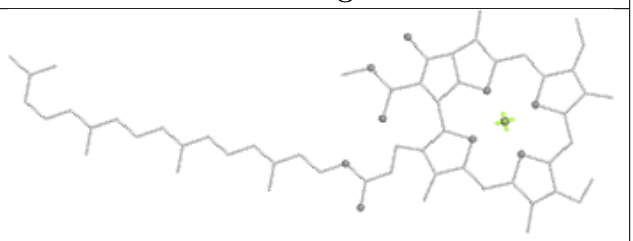
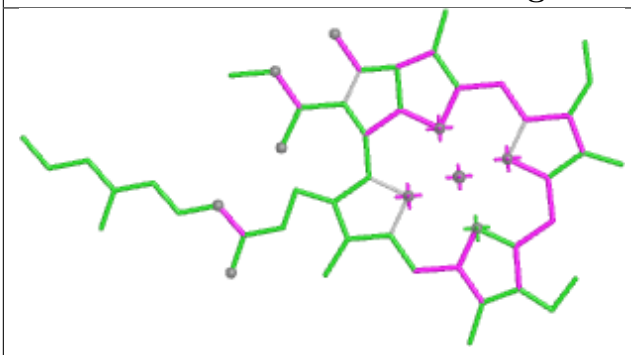
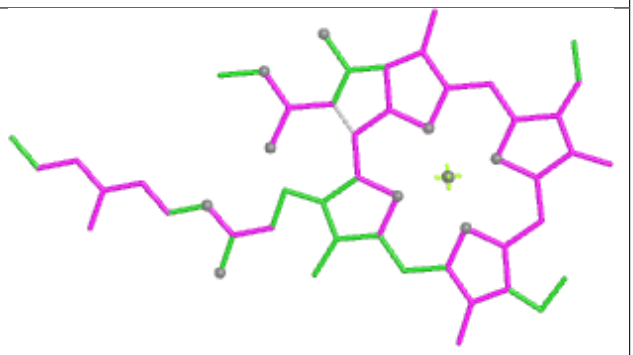
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

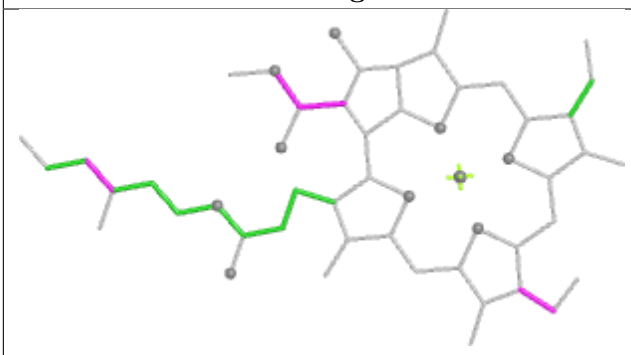
Ligand CHL 8 320



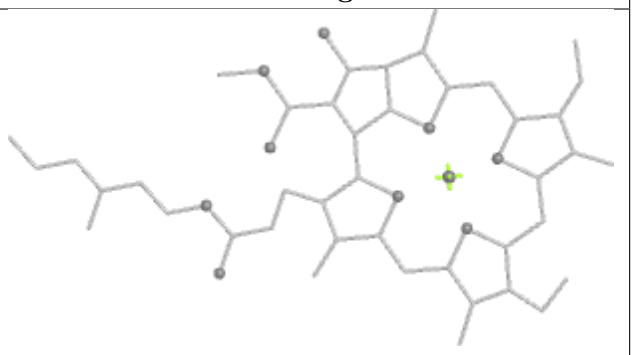
Bond lengths



Bond angles

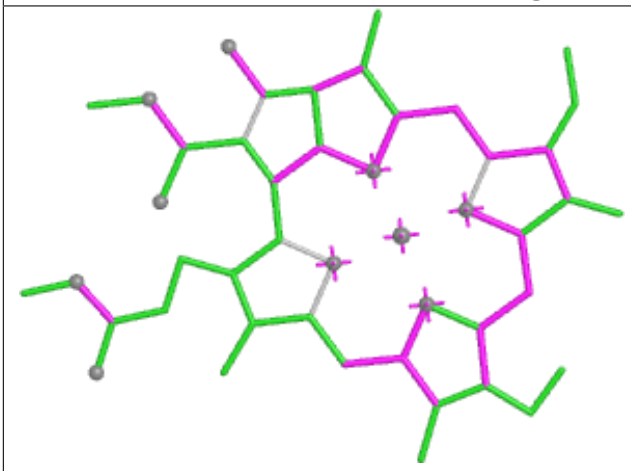


Torsions



Rings

Ligand CHL 8 311



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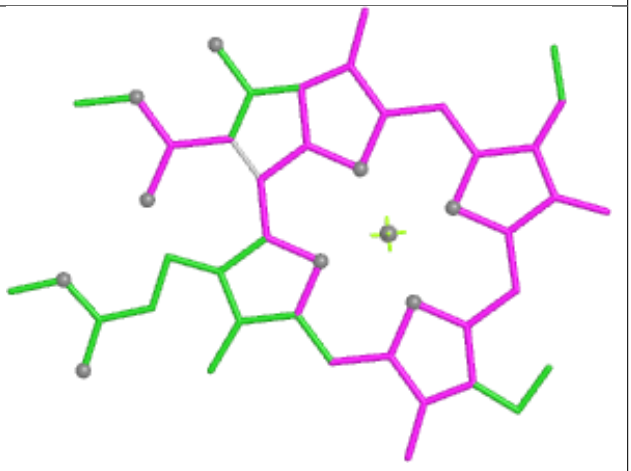
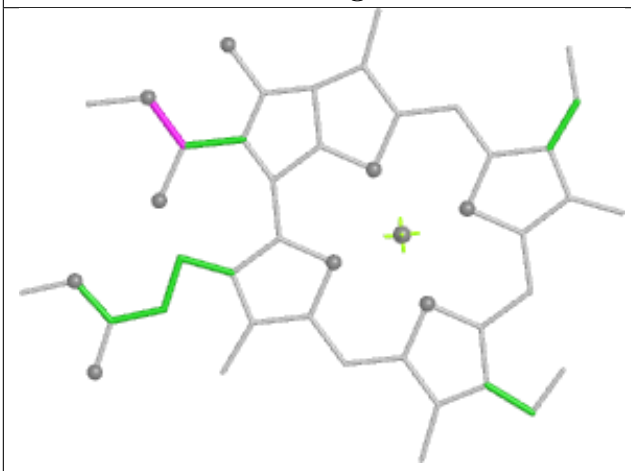
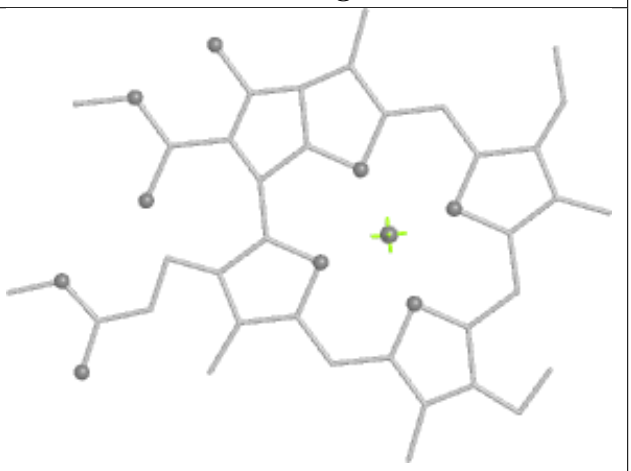


Bond angles

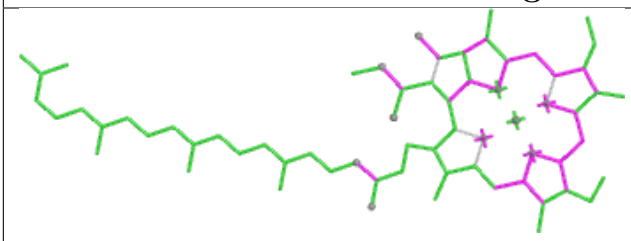


Torsions



Rings

Ligand CHL A 856



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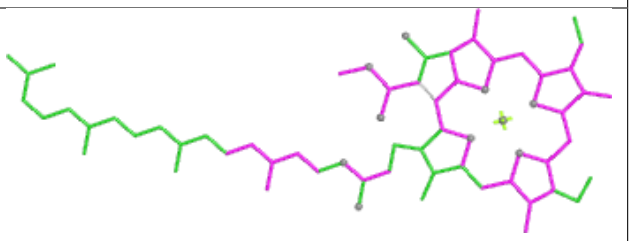

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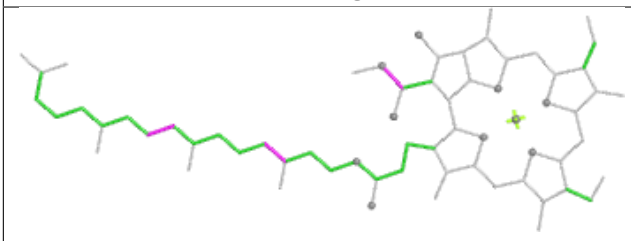

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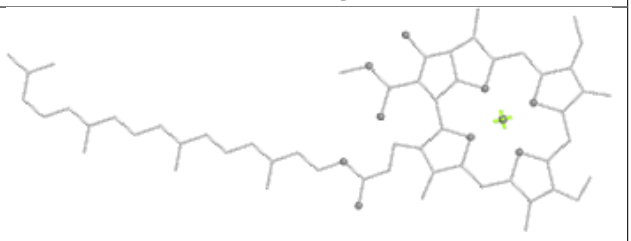
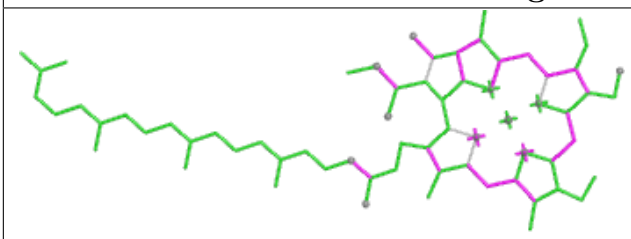


Rings

Ligand CHL 8 314



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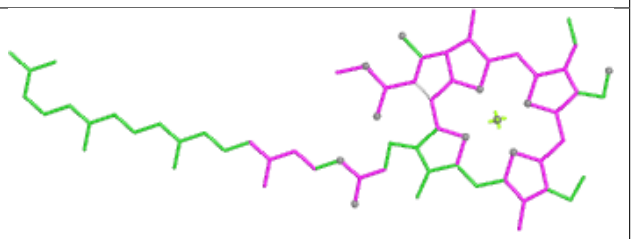

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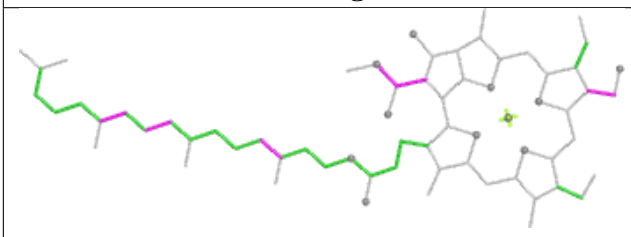

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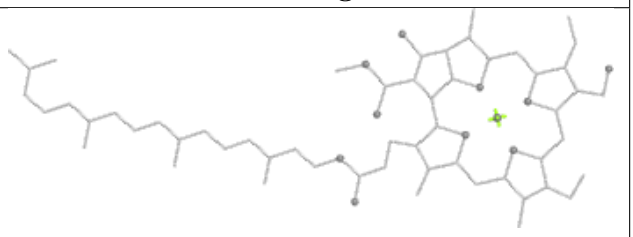
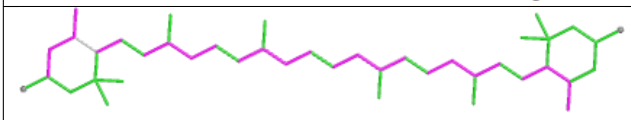


Rings

Ligand LUT b 301



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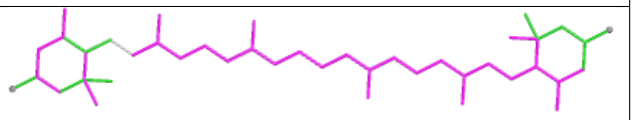

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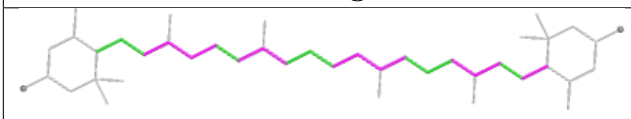

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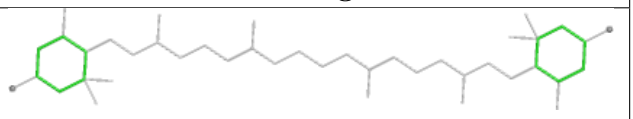
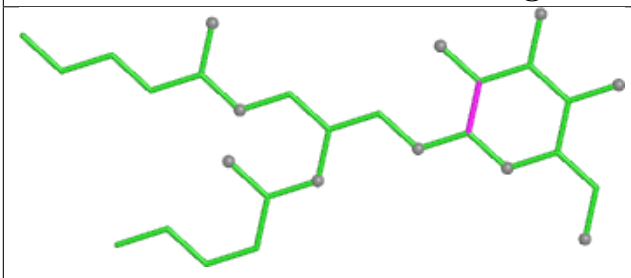


Rings

Ligand LMG J 104



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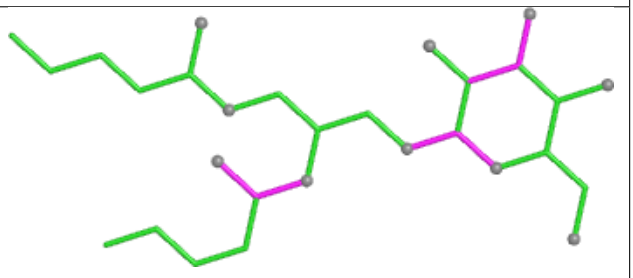

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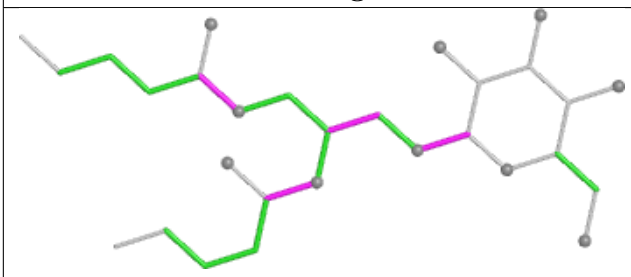

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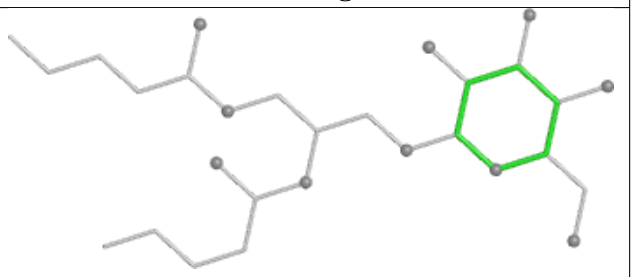
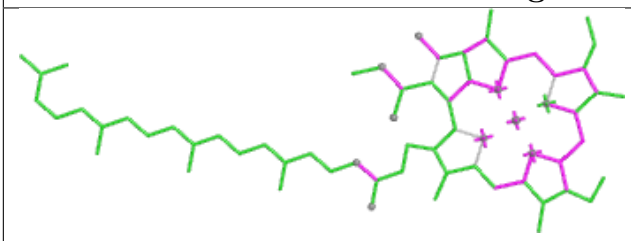


Rings

Ligand CHL 3 308



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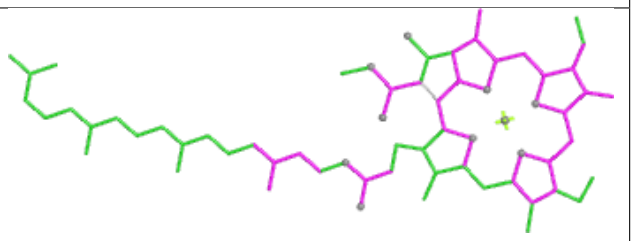

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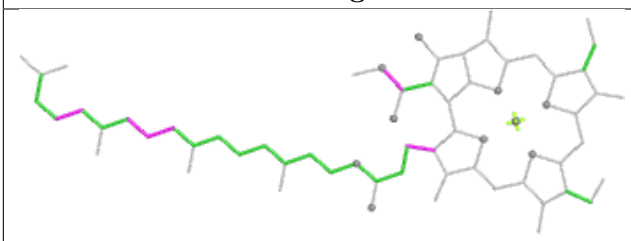

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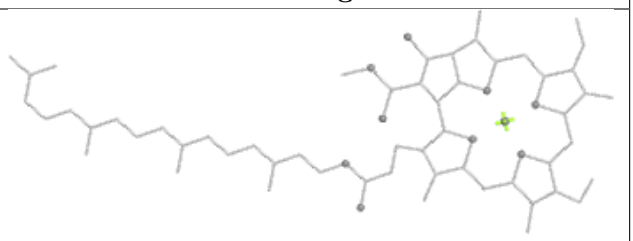
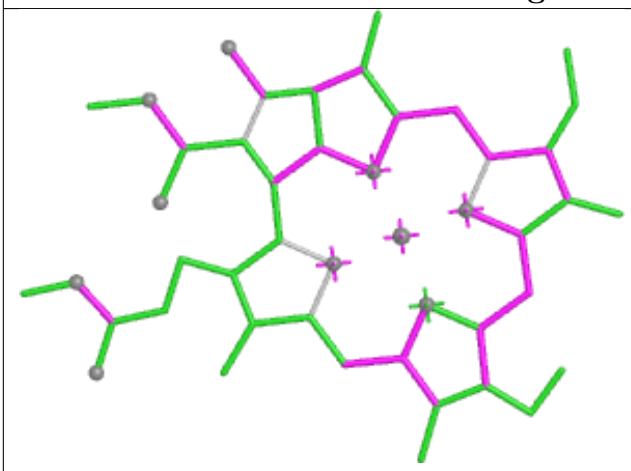


Rings

Ligand CHL 5 311



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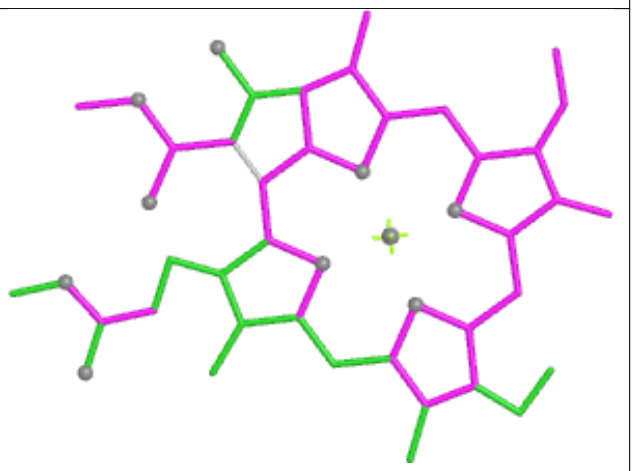

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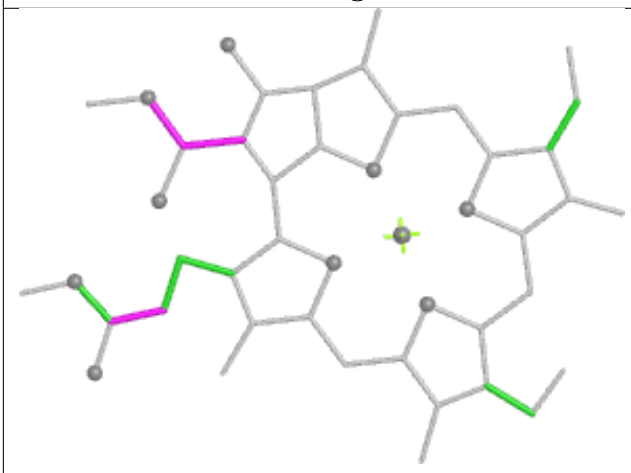
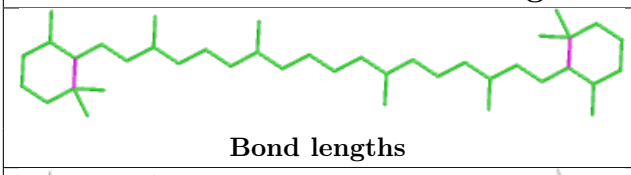


Torsions



Rings

Ligand BCR 3 301



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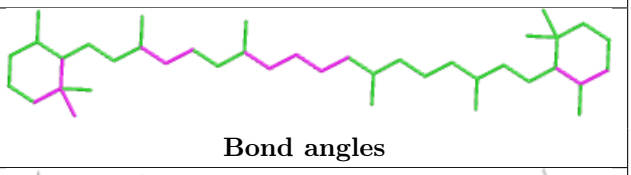

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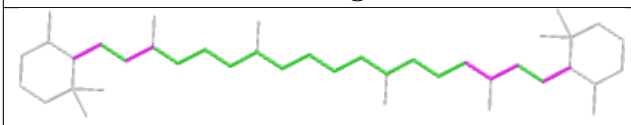

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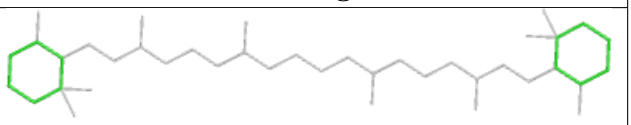
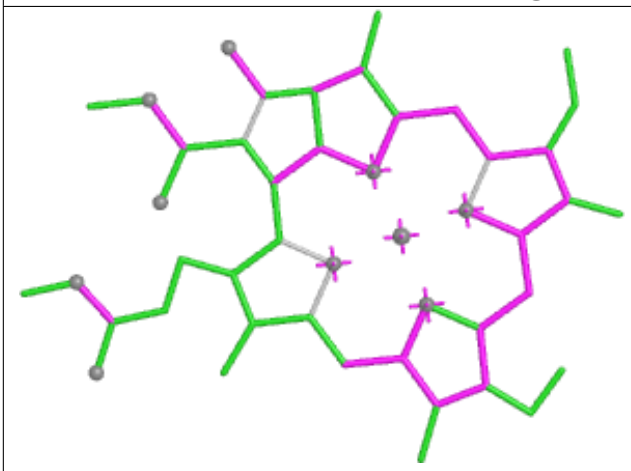


Rings

Ligand CHL 5 320



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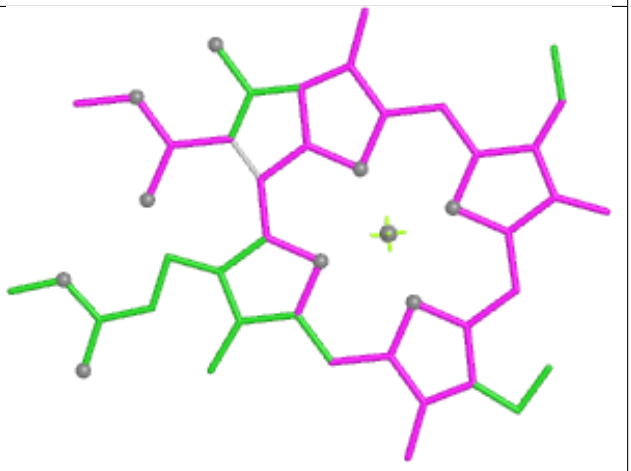
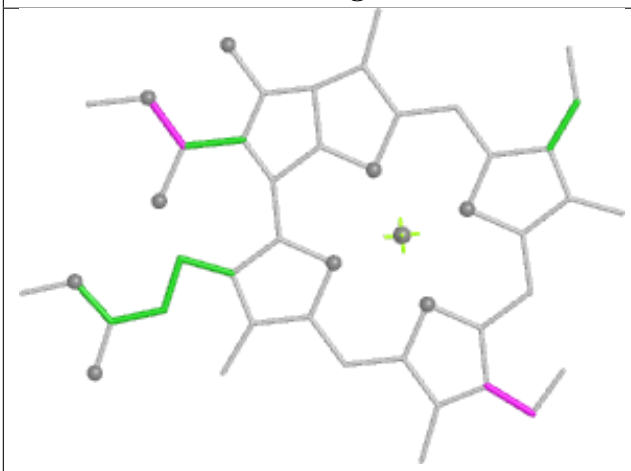


Bond angles



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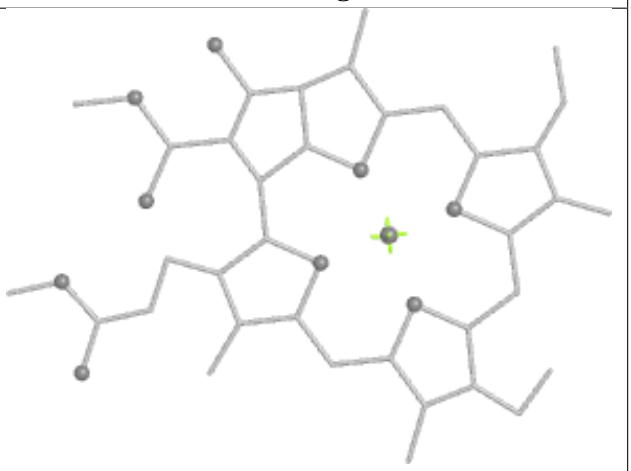
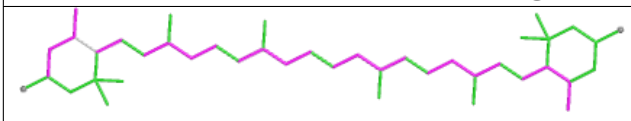


Rings

Ligand LUT 6 302



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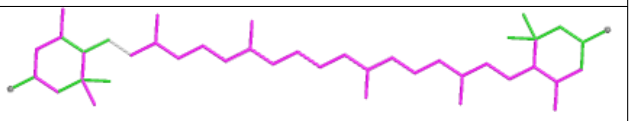

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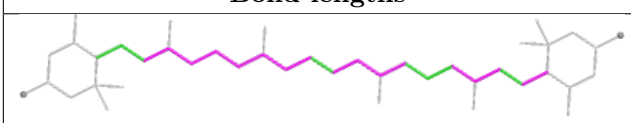

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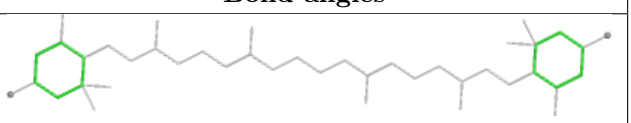
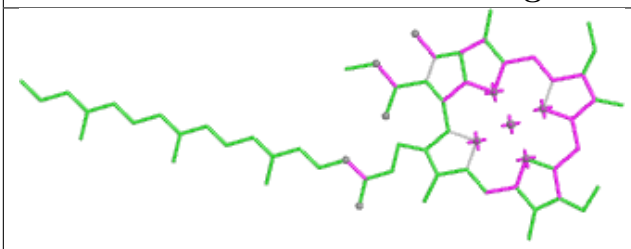


Rings

Ligand CHL B 851



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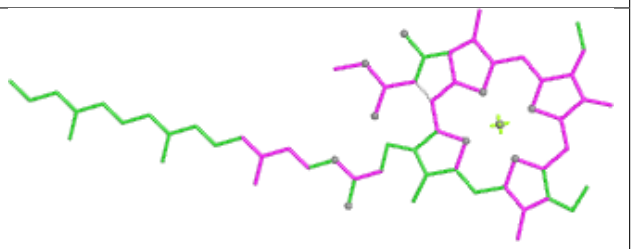
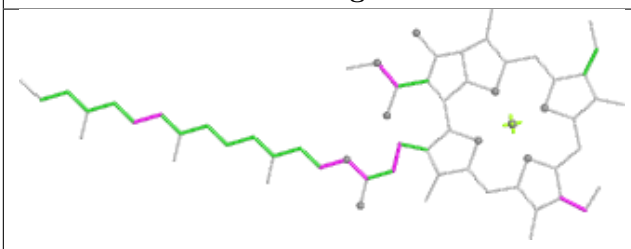


Bond angles



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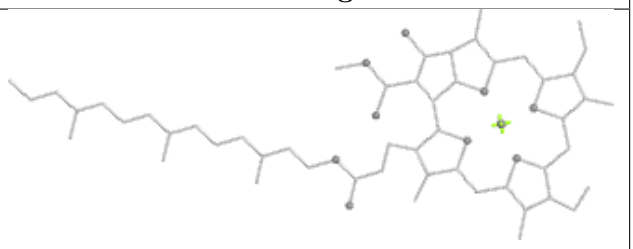
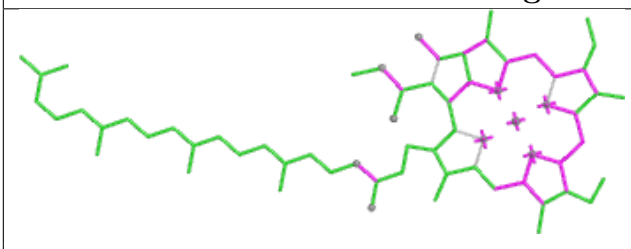


Rings

Ligand CHL A 828



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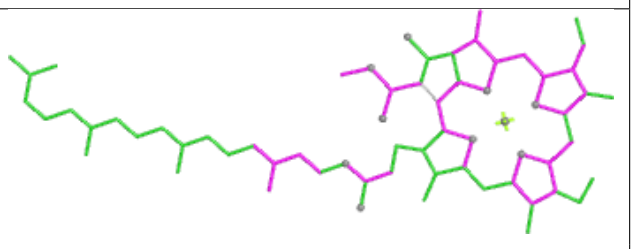
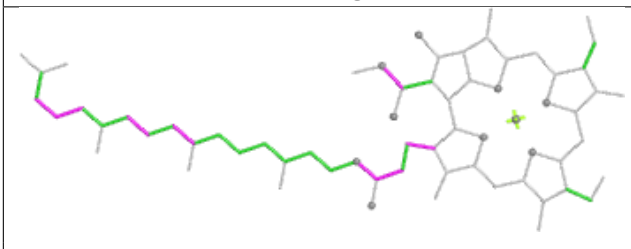


Bond angles



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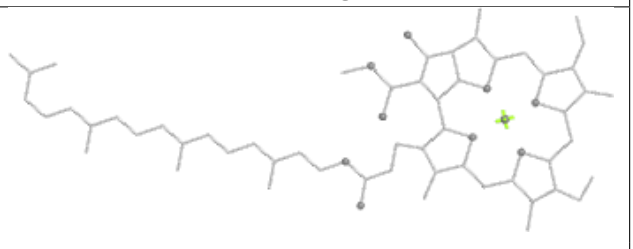
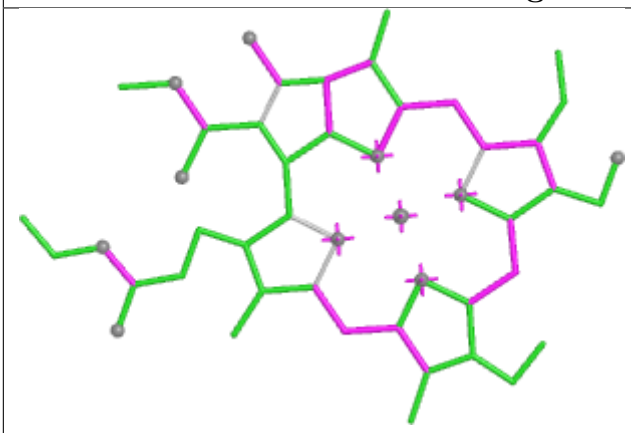


Rings

Ligand CHL b 316



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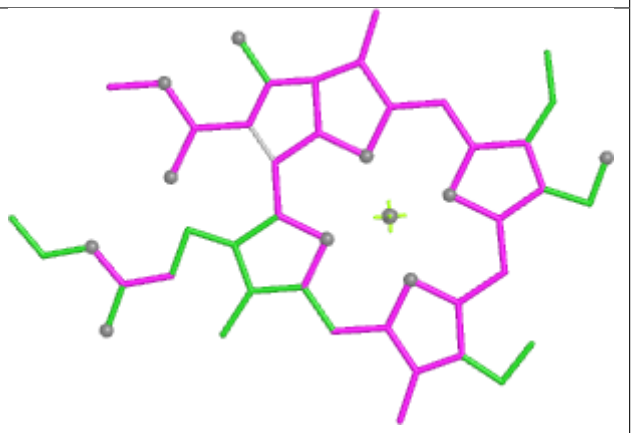
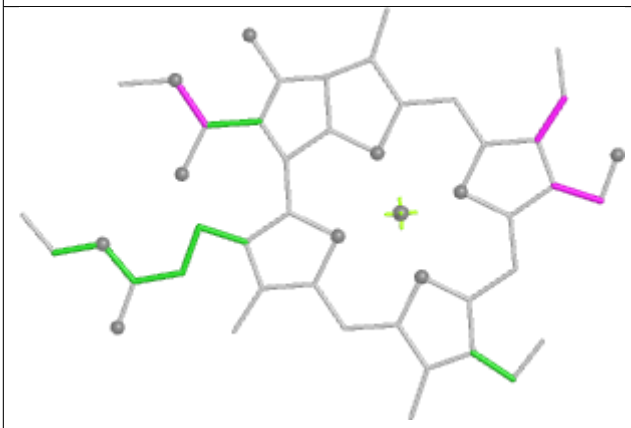


Bond angles



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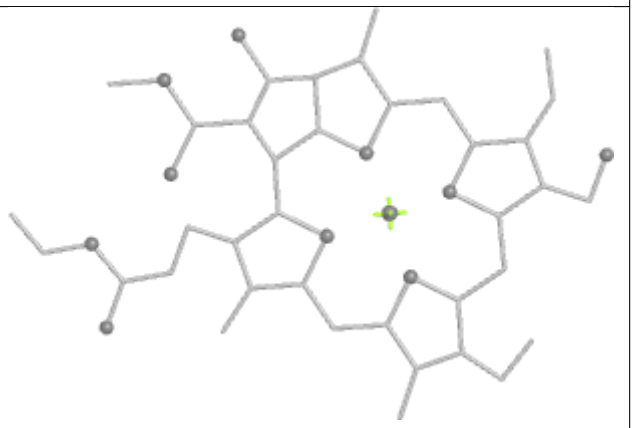
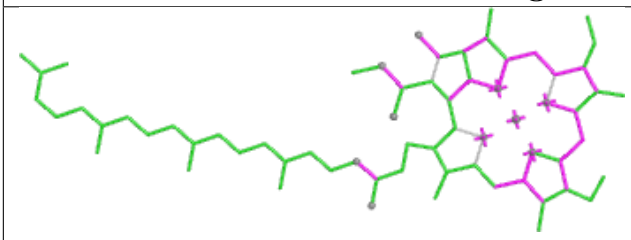


Rings

Ligand CHL 6 311



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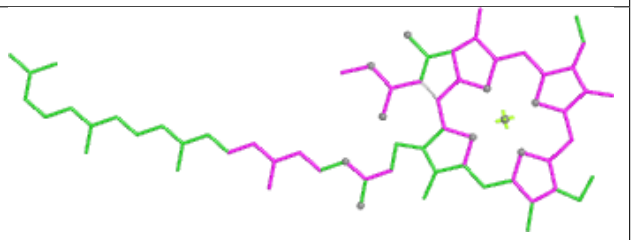
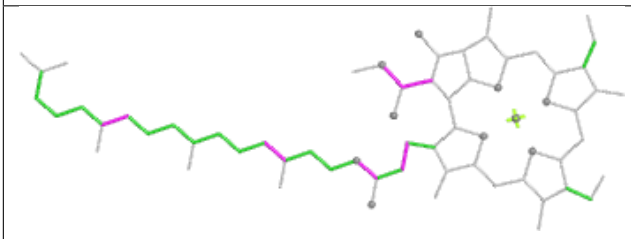


Bond angles



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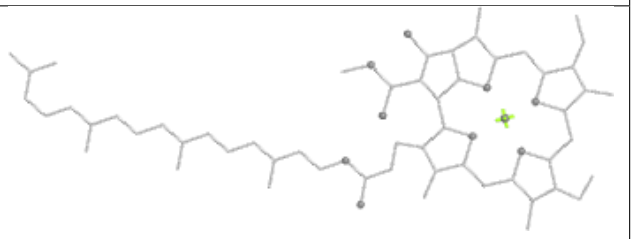
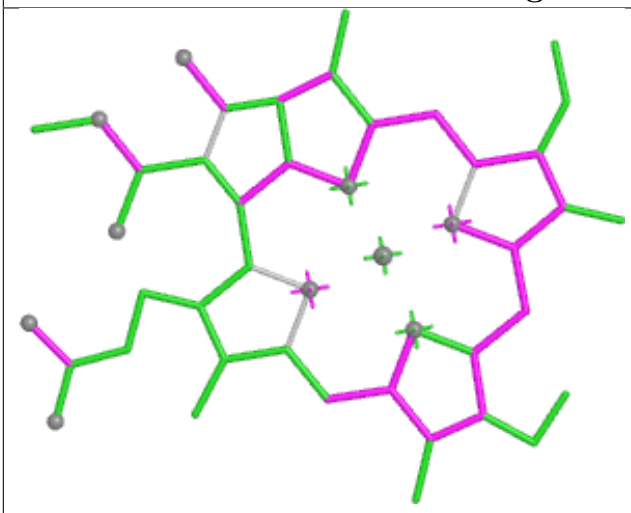
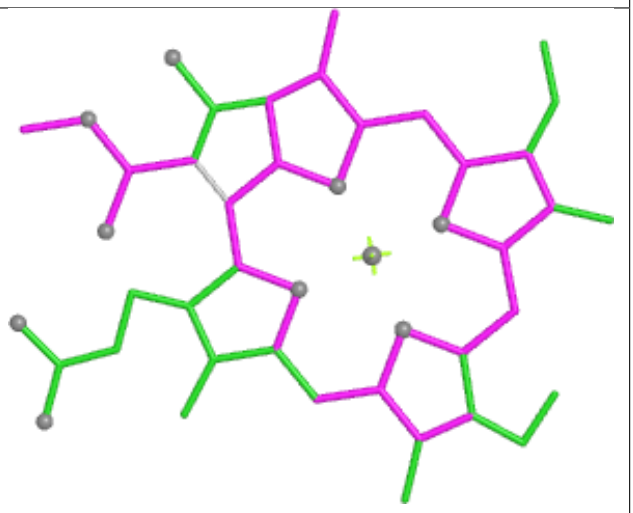


Rings

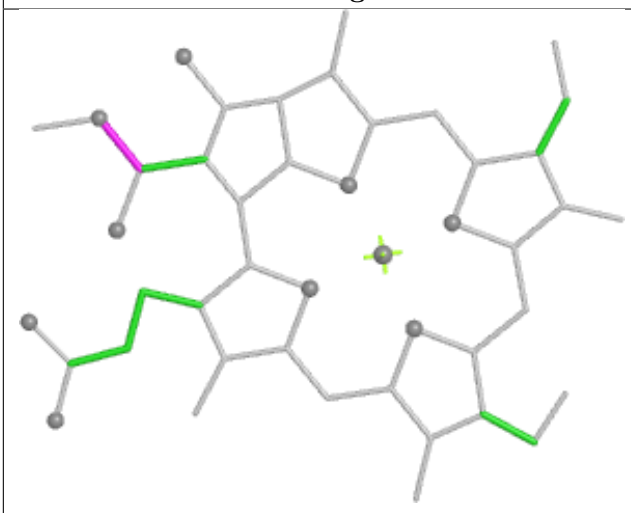
Ligand CHL L 304



Bond lengths



Bond angles



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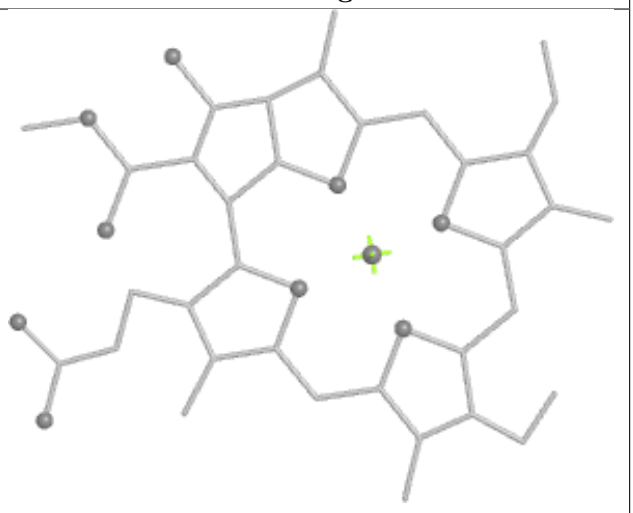
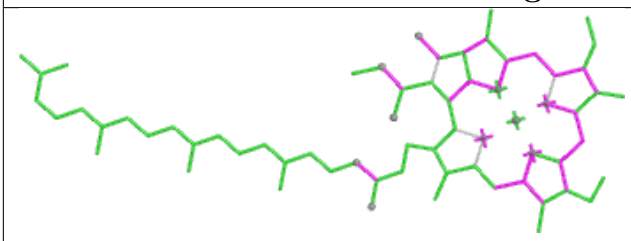
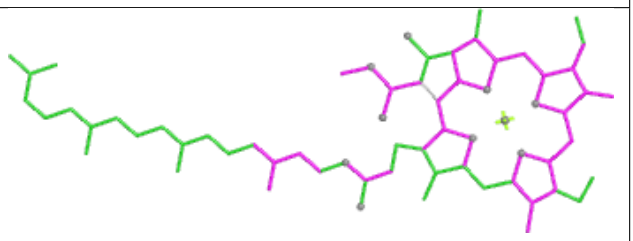


Rings

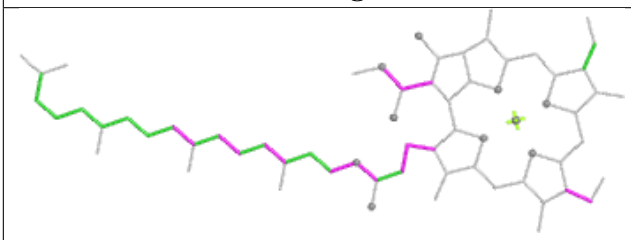
Ligand CHL B 846



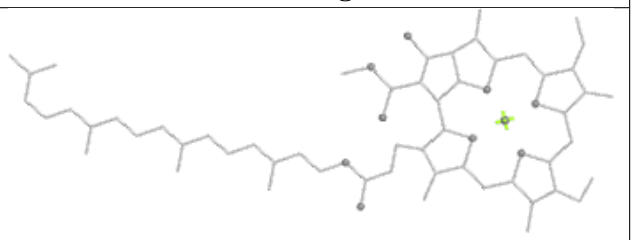
Bond lengths



Bond angles

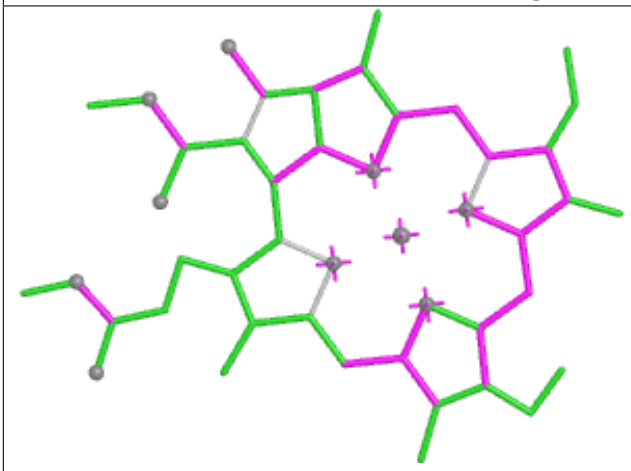


Torsions



Rings

Ligand CHL 4 310



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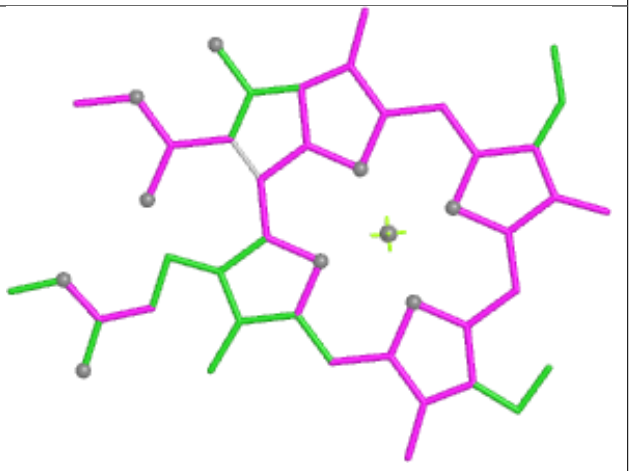

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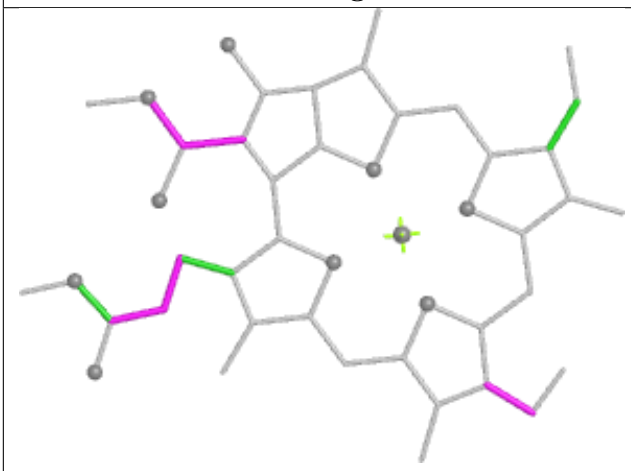

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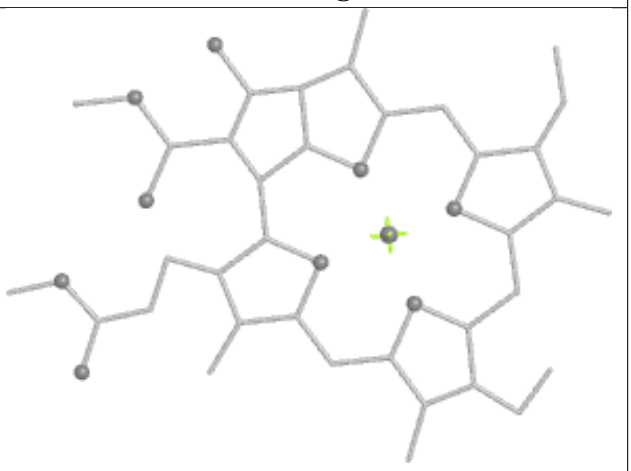
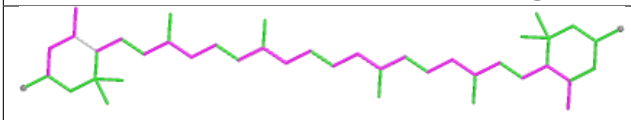


Rings

Ligand LUT a 302



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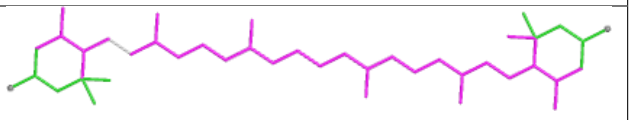

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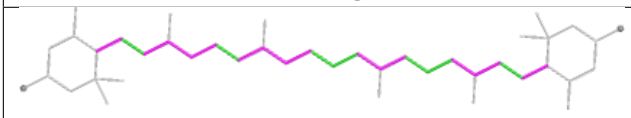

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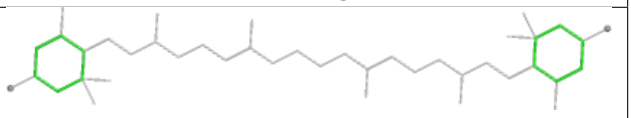
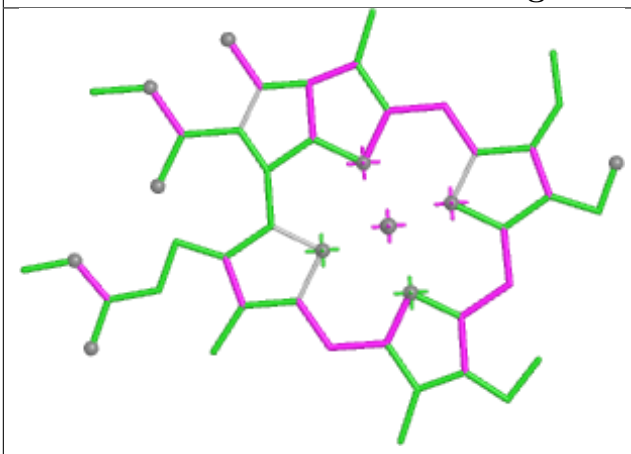


Rings

Ligand CHL 5 317



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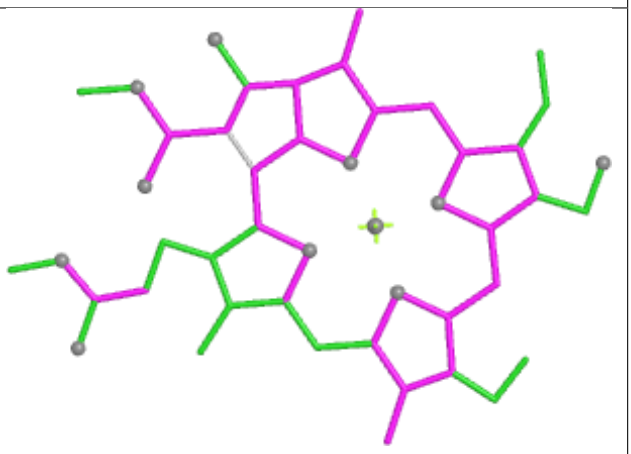

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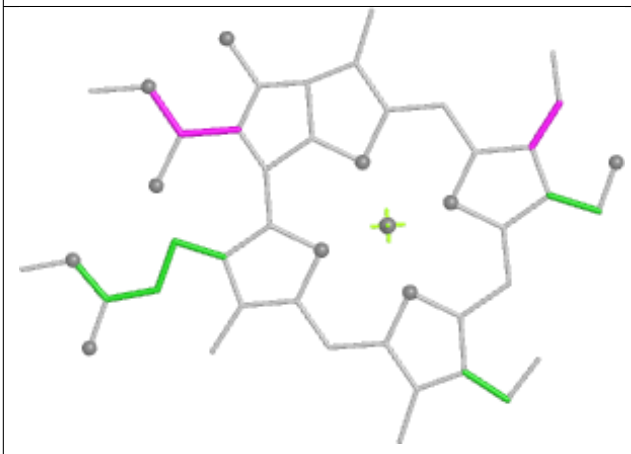

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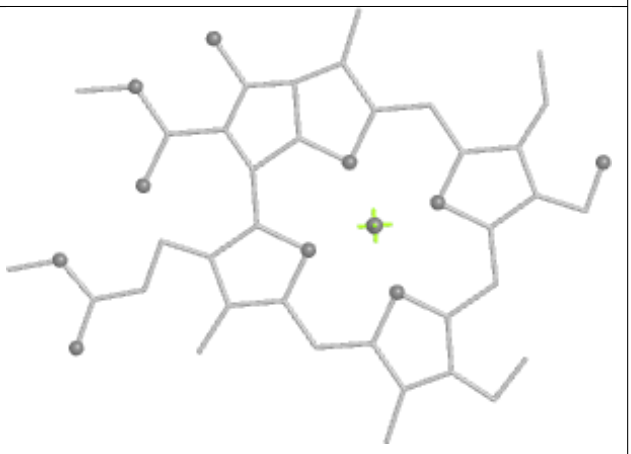
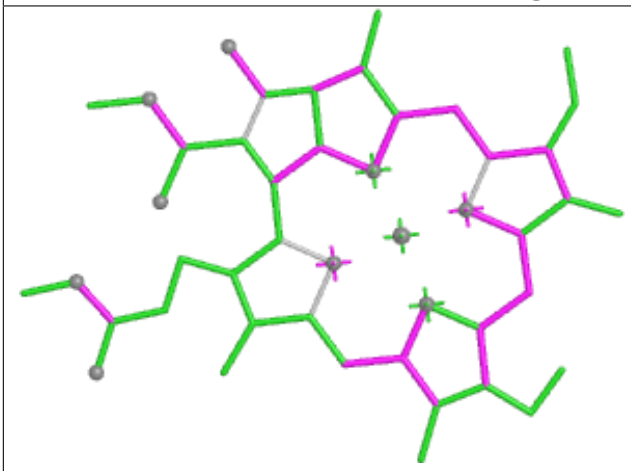


Rings

Ligand CHL 5 308



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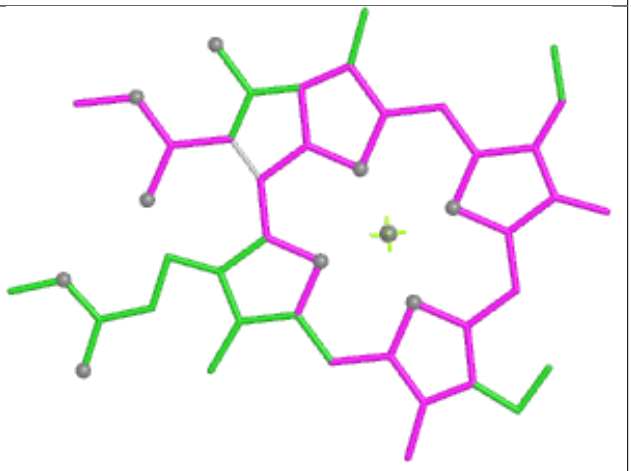

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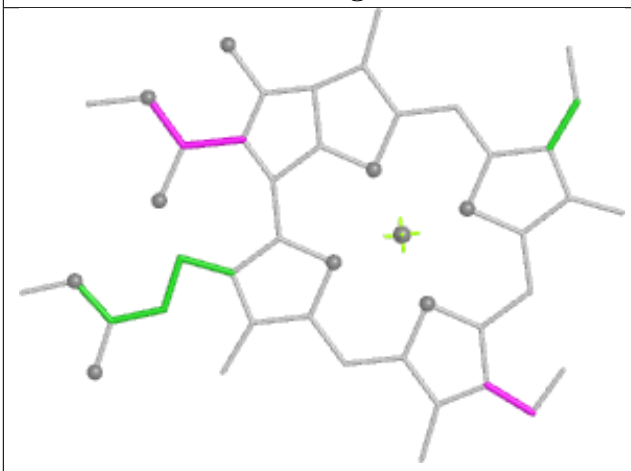

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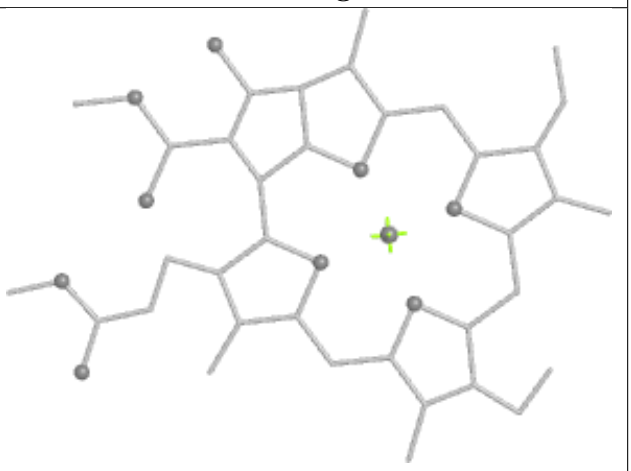
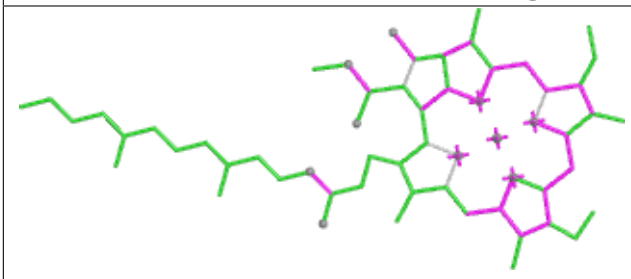


Rings

Ligand CHL B 821



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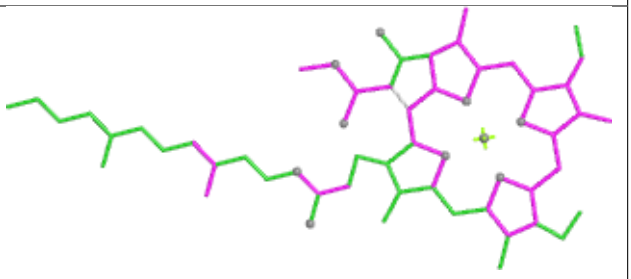

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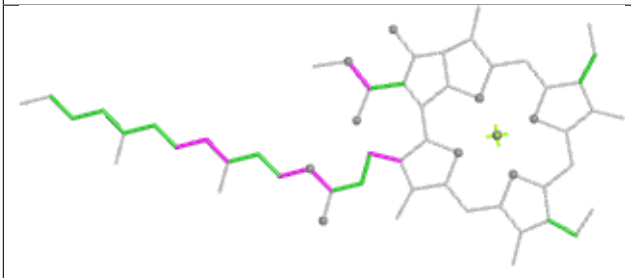

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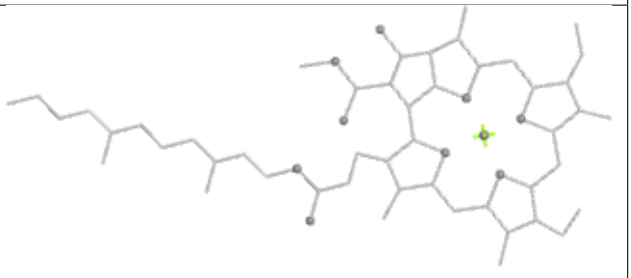
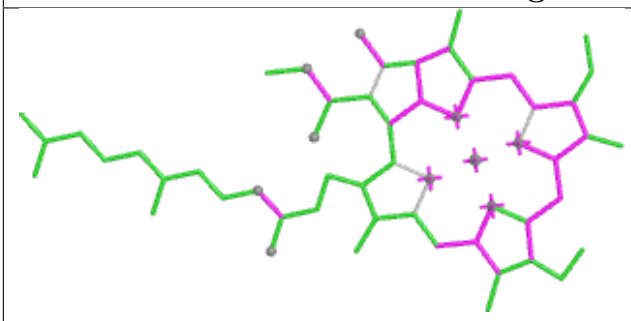
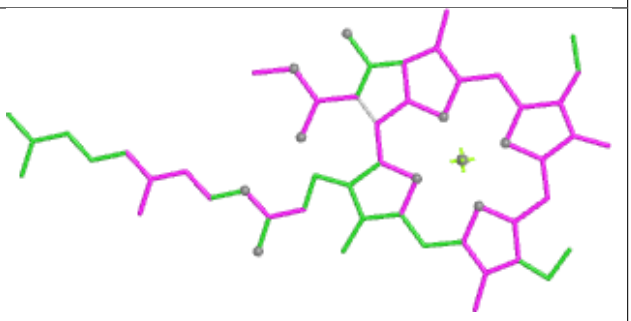
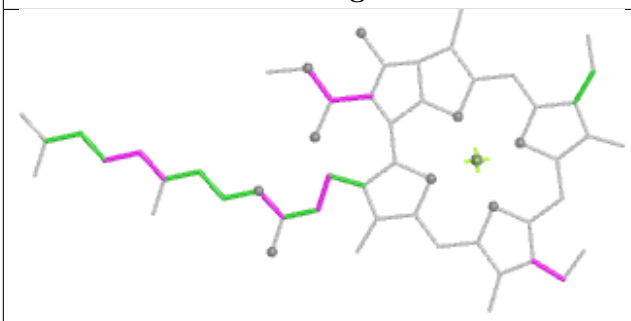
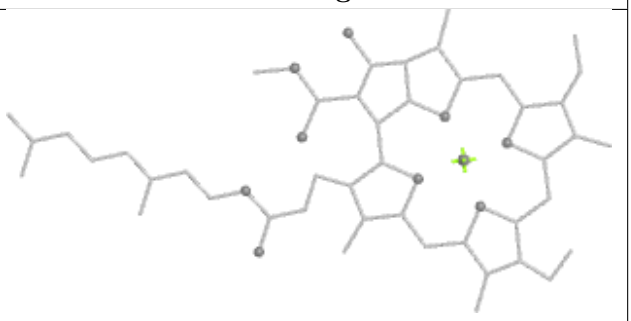
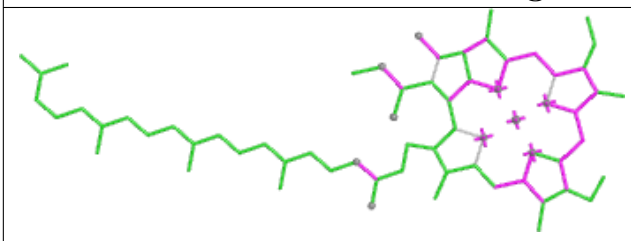
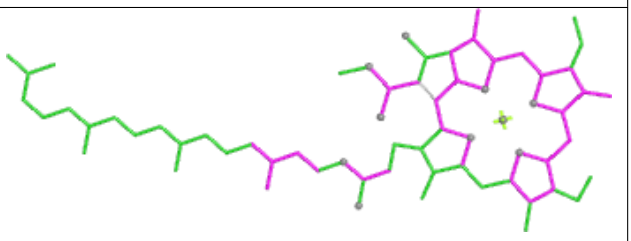


Rings

Ligand CHL 6 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL b 315	
	
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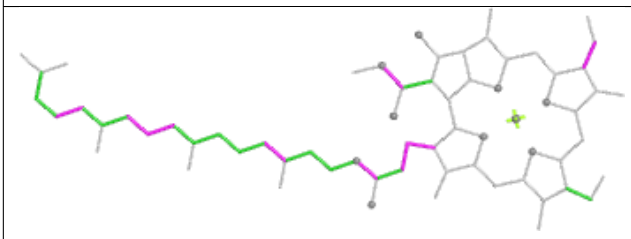
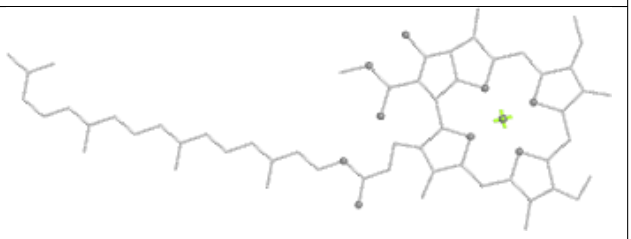
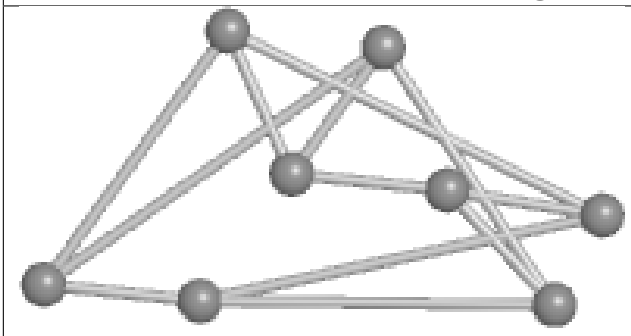
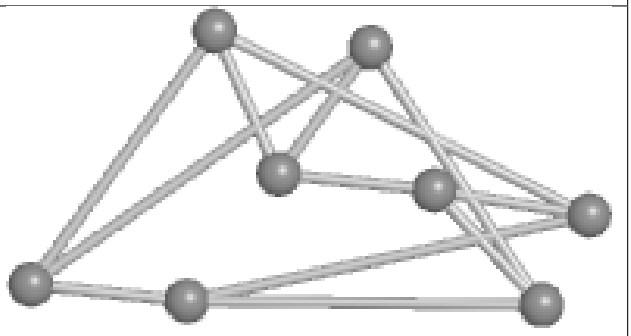
	
Torsions	Rings

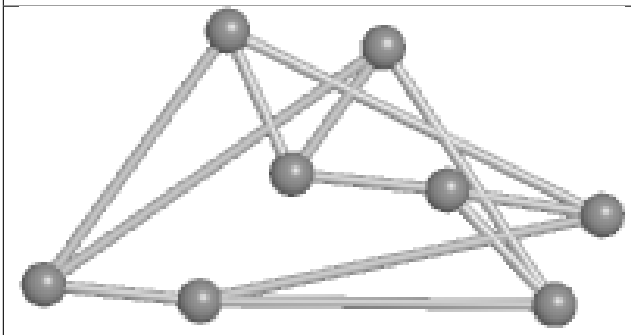
Ligand SF4 C 102



Bond lengths



Bond angles



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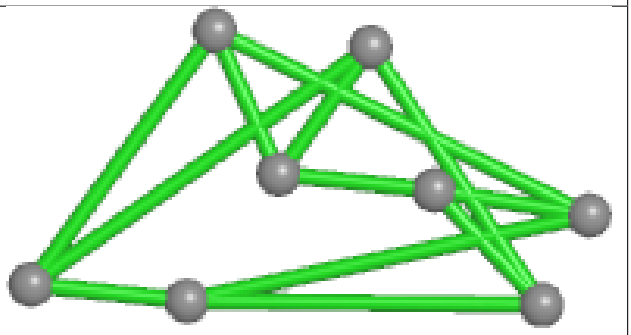
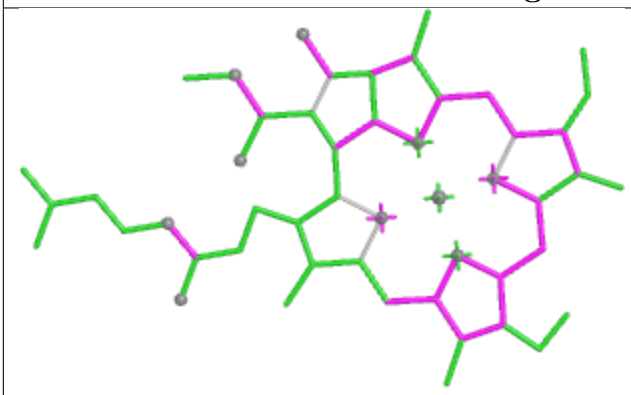


Rings

Ligand CHL B 845



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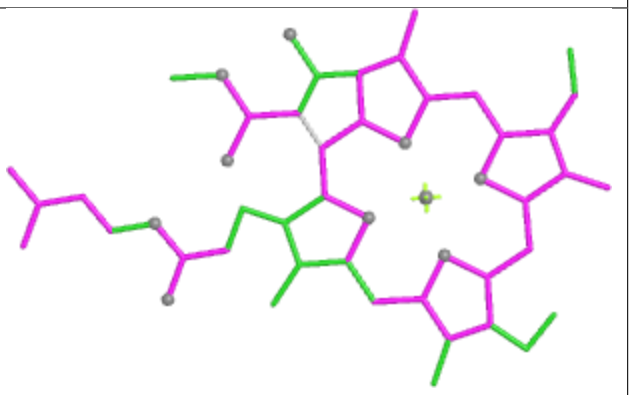
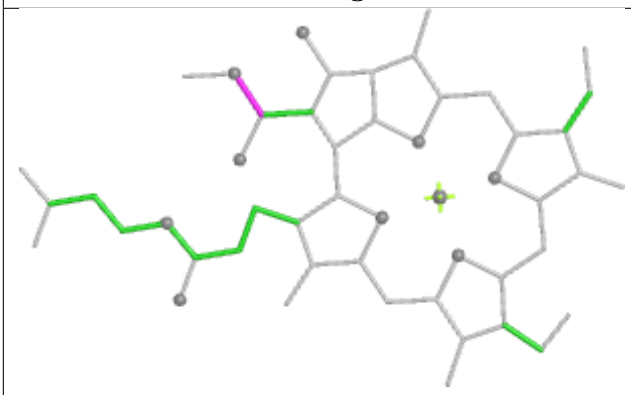


Bond angles



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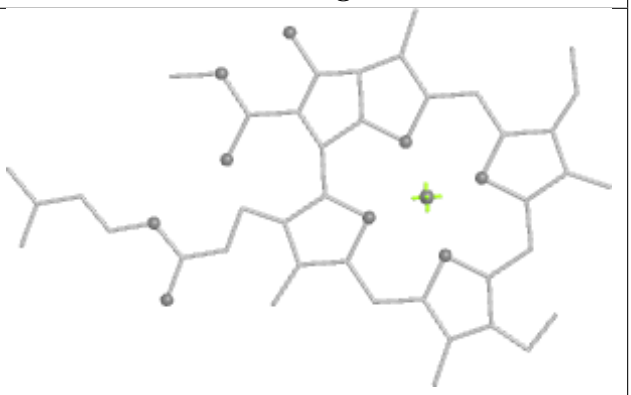
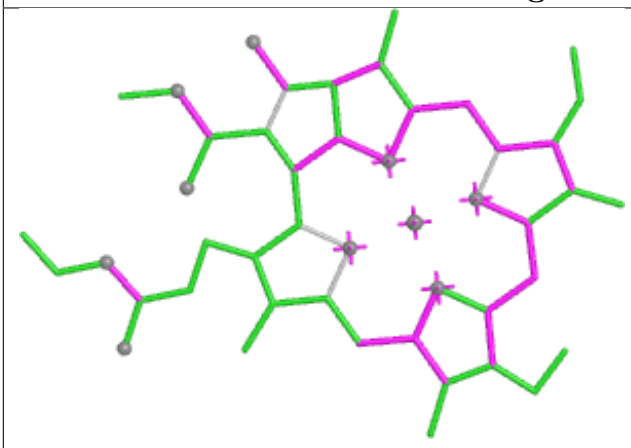


Rings

Ligand CHL 6 313



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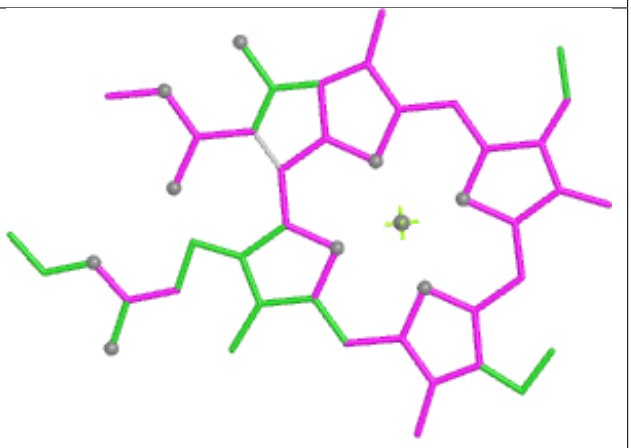
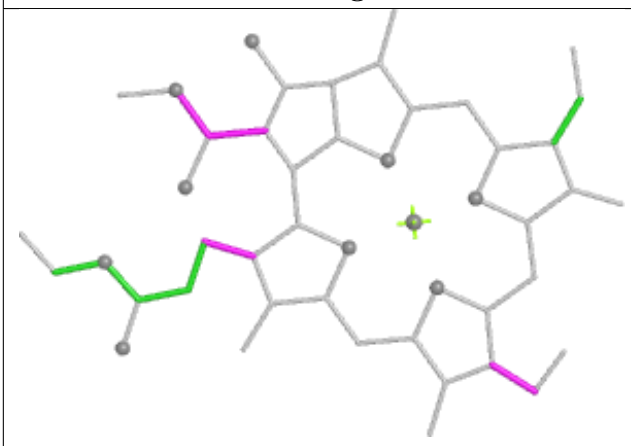


Bond angles



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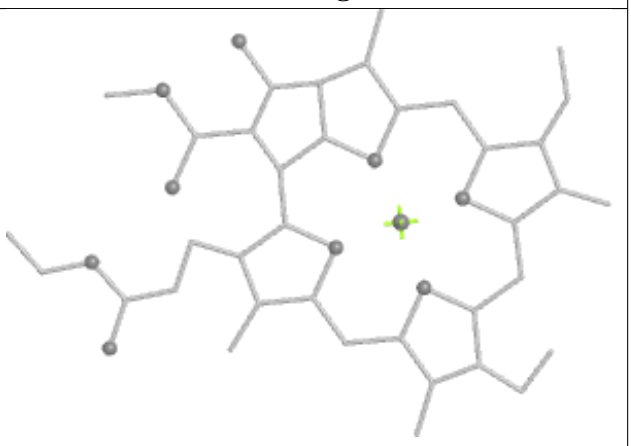
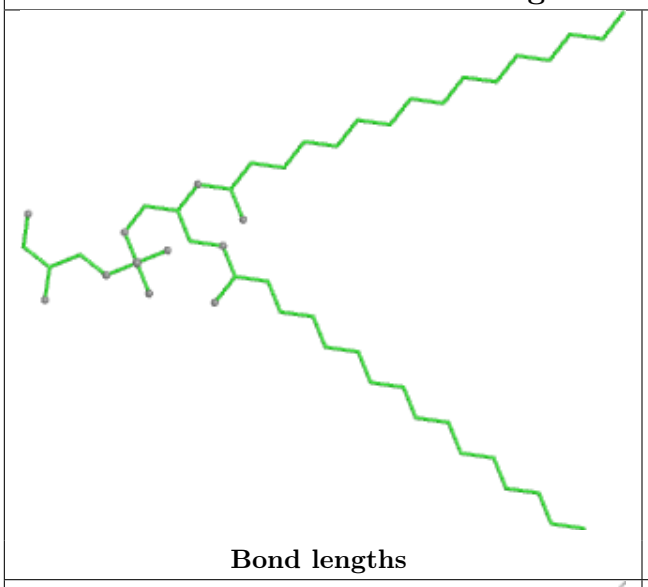


Rings

Ligand LHG 4 303



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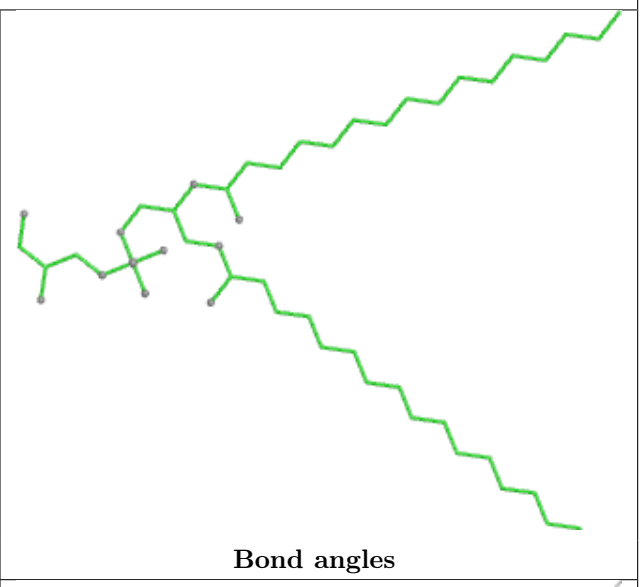

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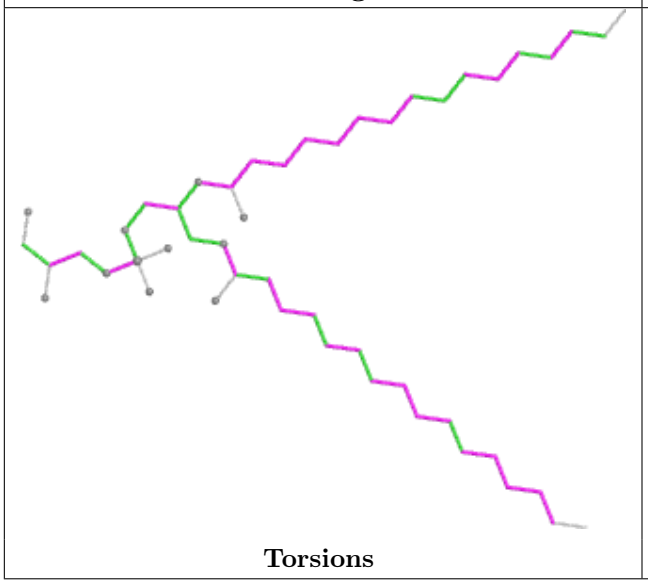

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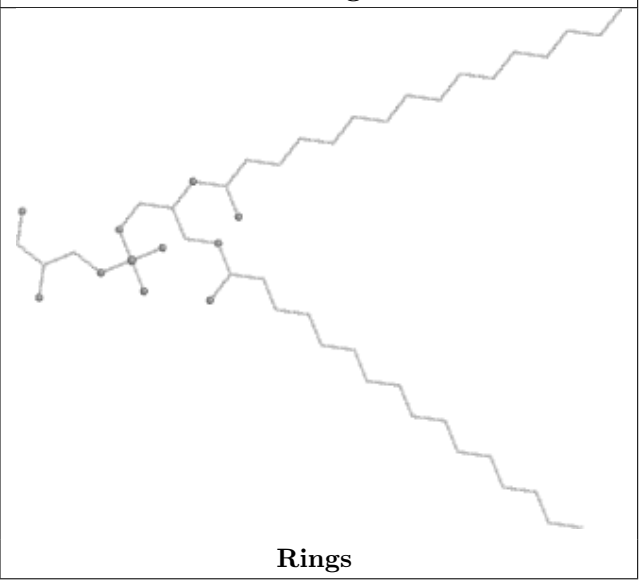
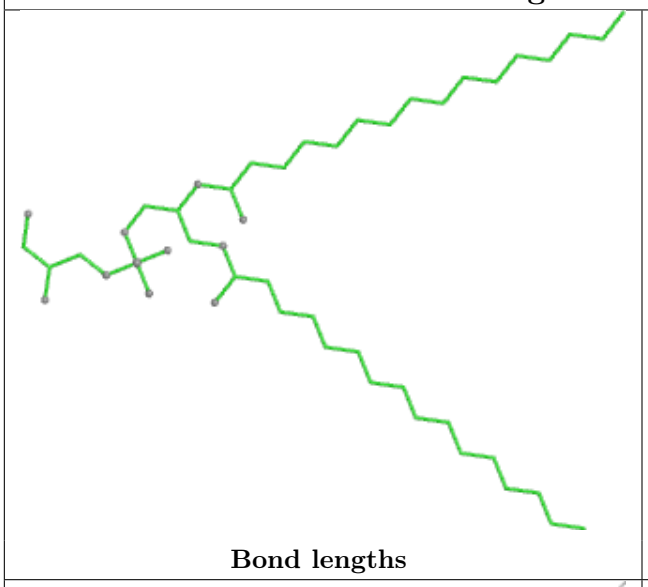


Rings

Ligand LHG 7 302



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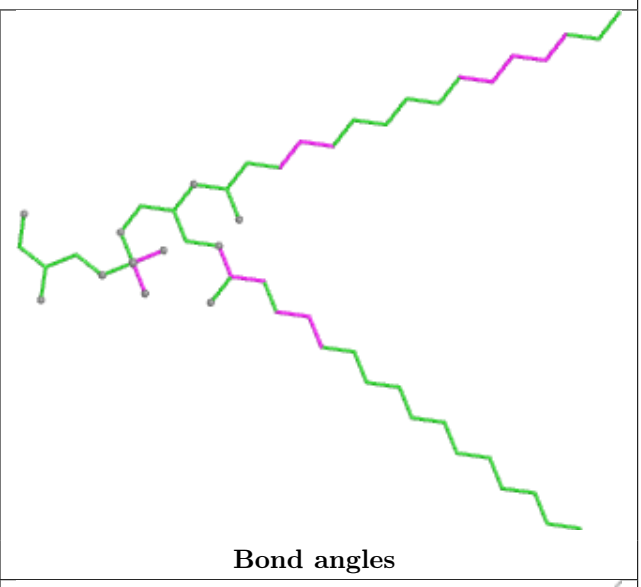
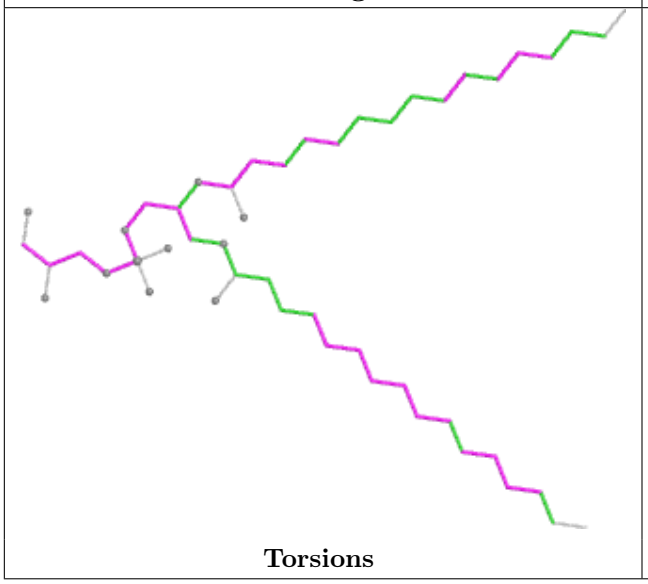


Bond angles



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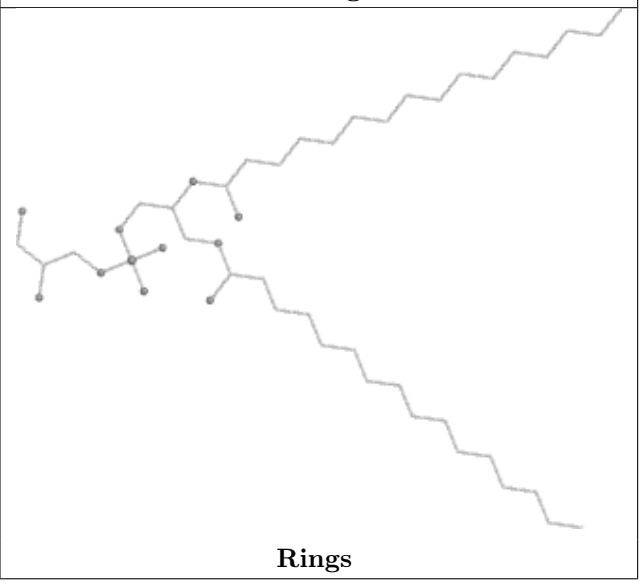
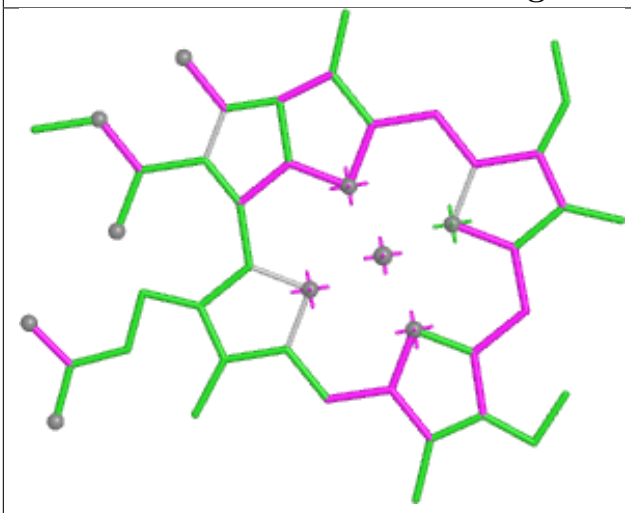


Rings

Ligand CHL 5 314



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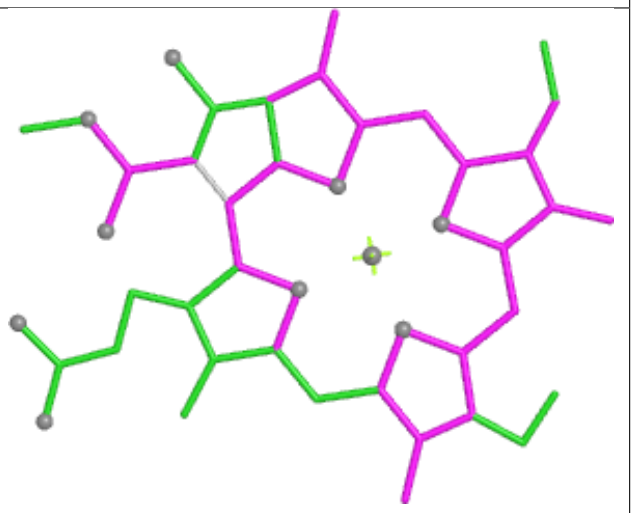
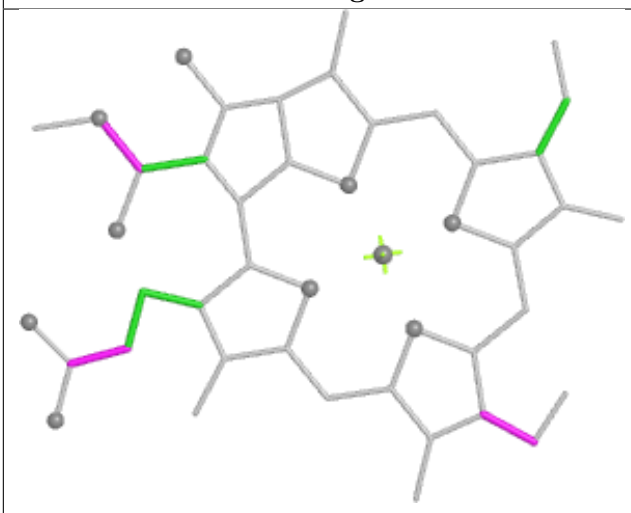


Bond angles



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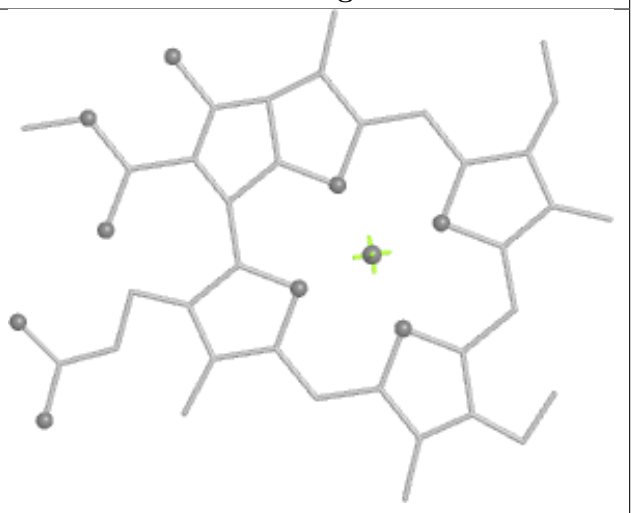
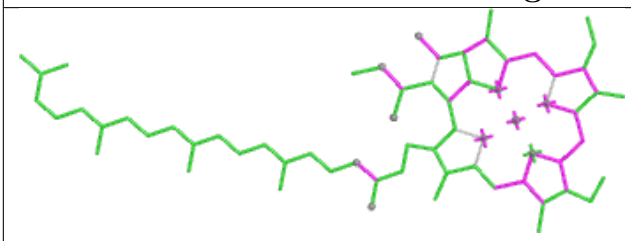
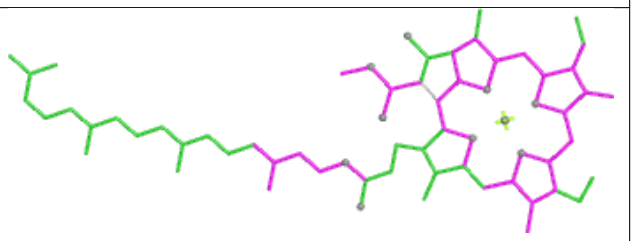


Rings

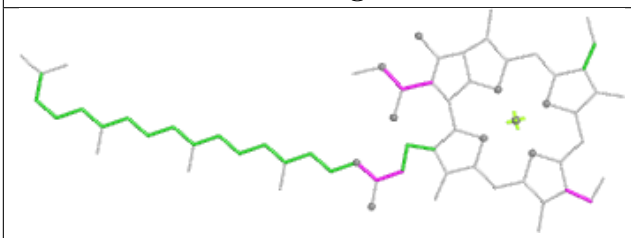
Ligand CHL B 811



Bond lengths



Bond angles



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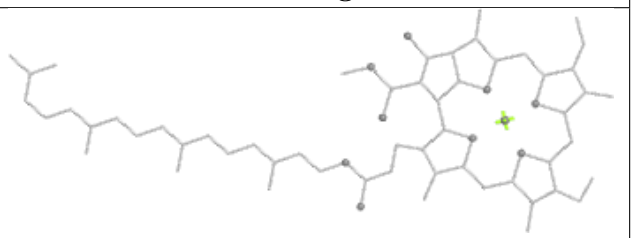
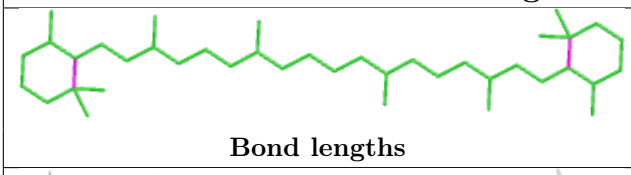
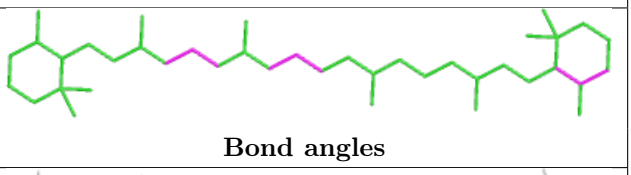


Rings

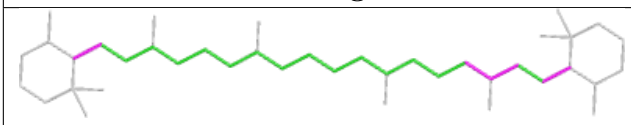
Ligand BCR B 807



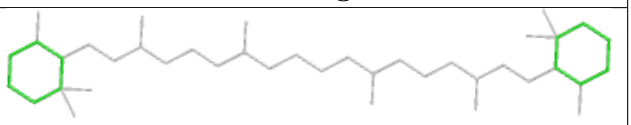
Bond lengths



Bond angles

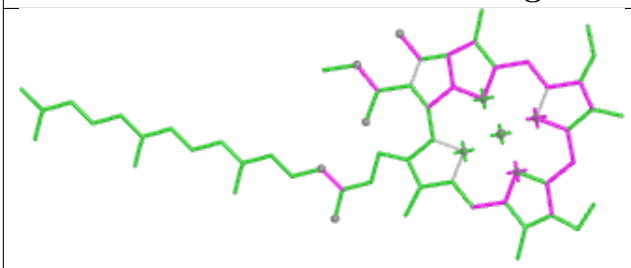


Torsions



Rings

Ligand CHL B 828



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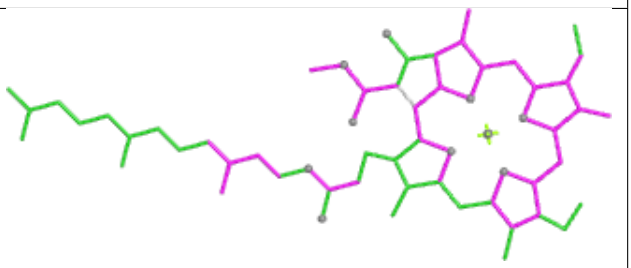

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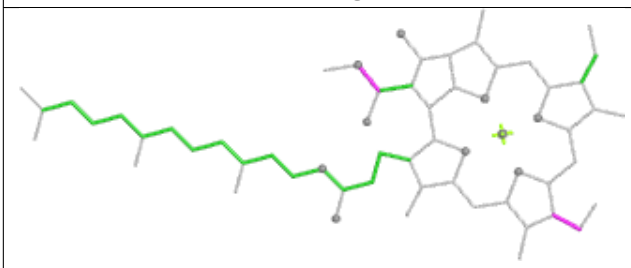

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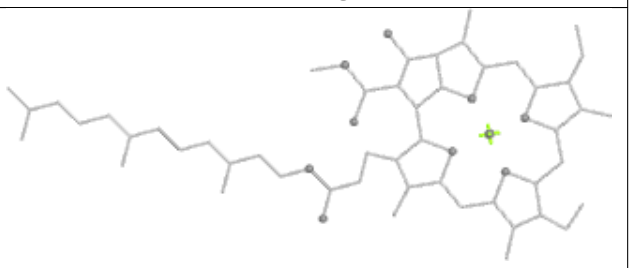
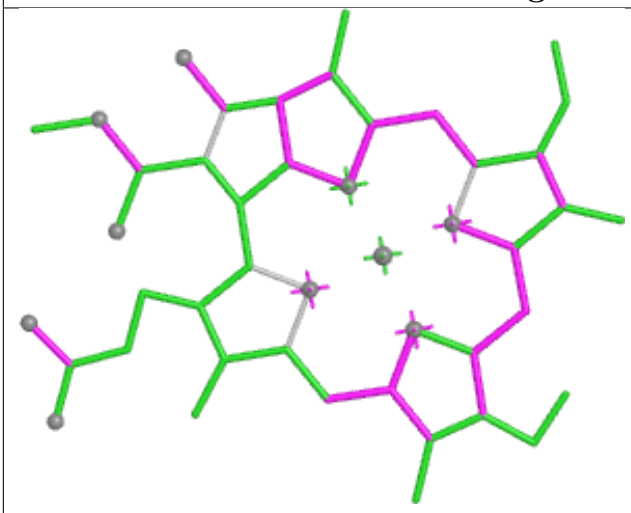


Rings

Ligand CHL 4 313



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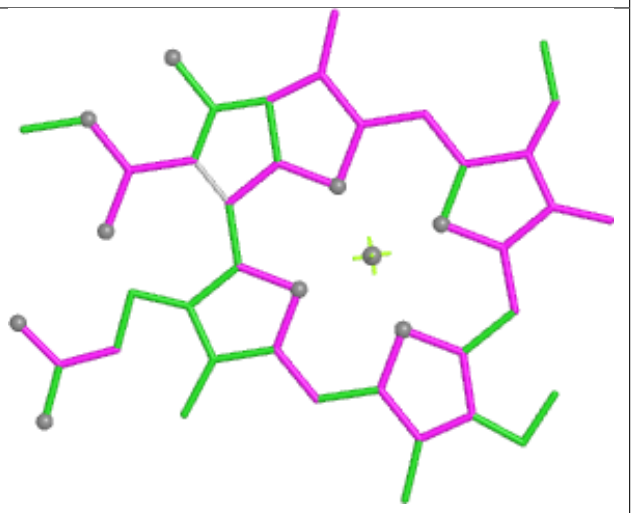
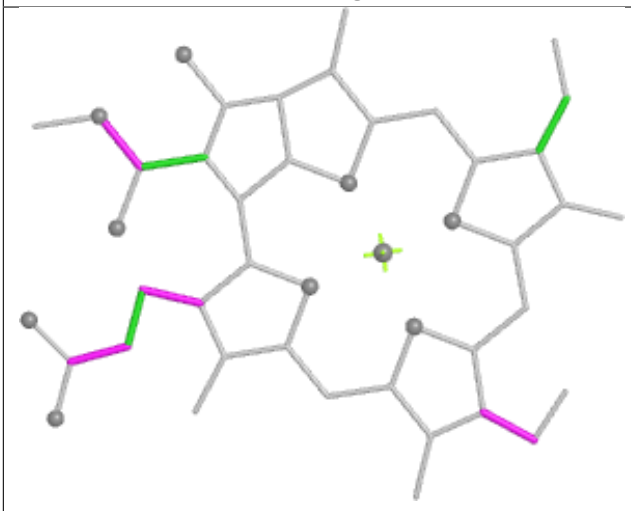


Bond angles



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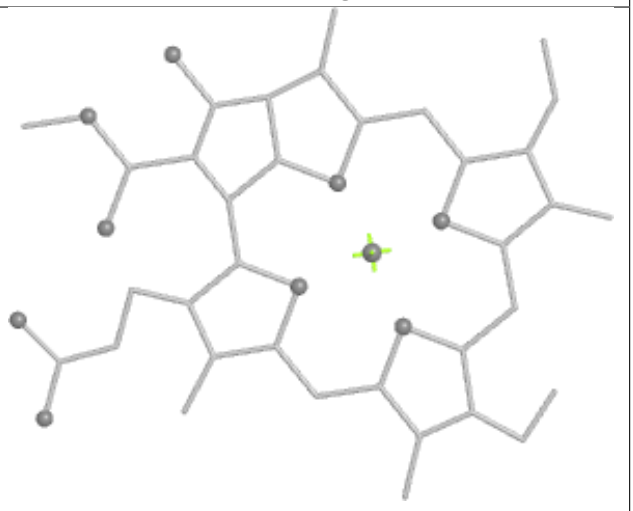
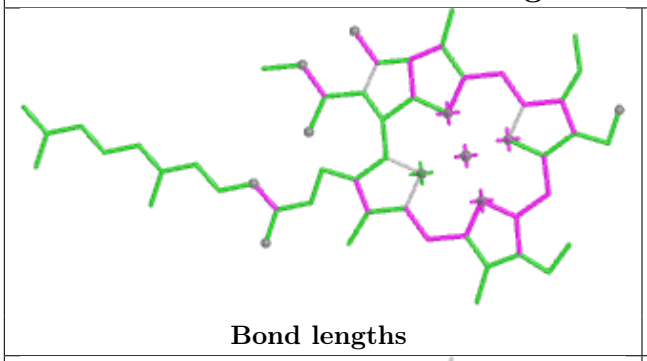


Rings

Ligand CHL A 841



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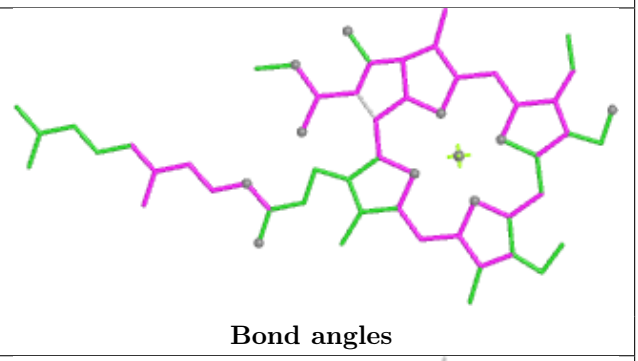

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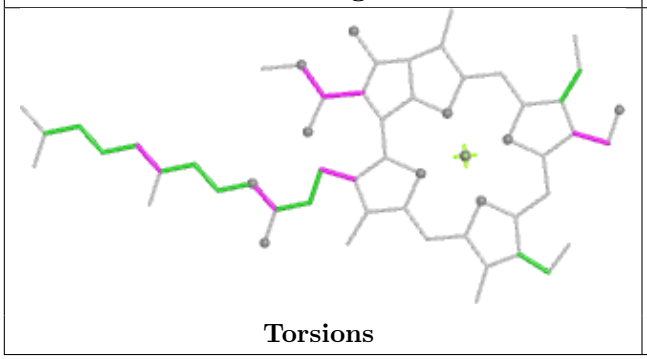

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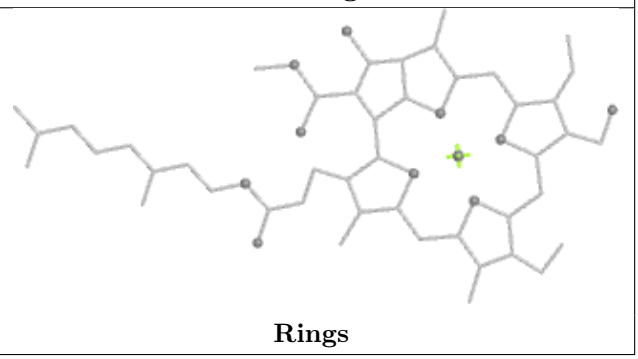
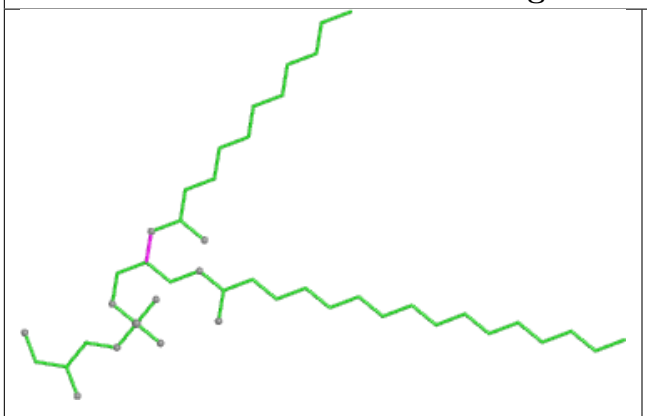


Rings

Ligand LHG 7 306



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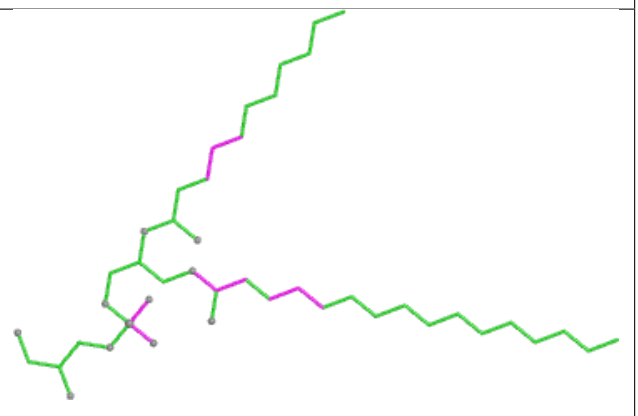

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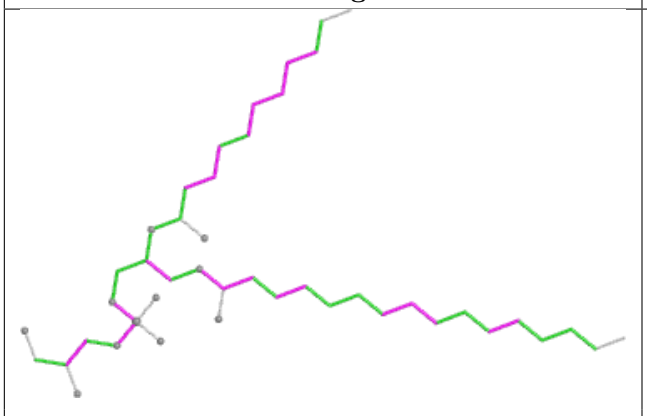

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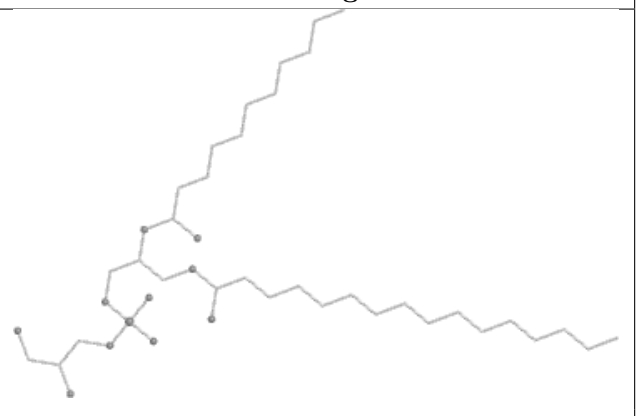
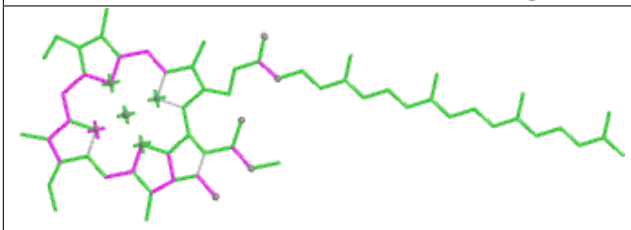


Rings

Ligand CHL A 843



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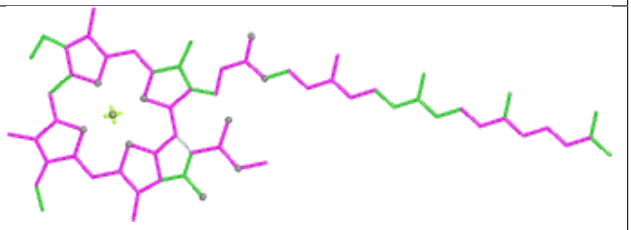

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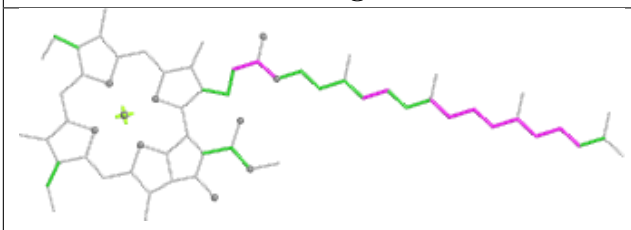

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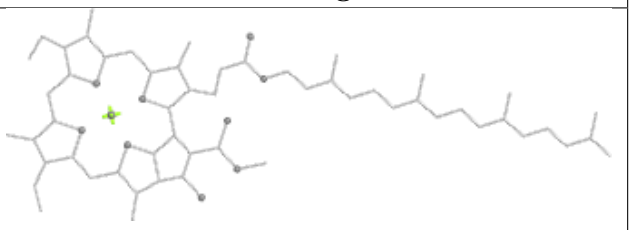
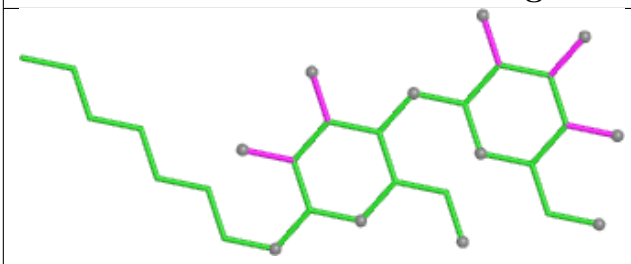


Rings

Ligand LMT 5 306



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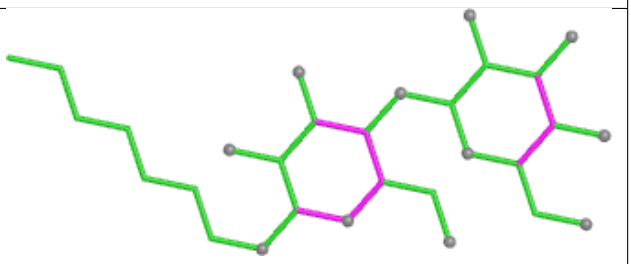

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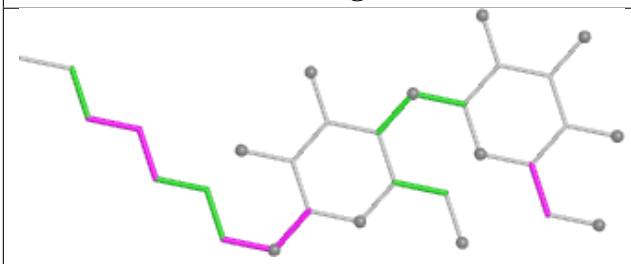

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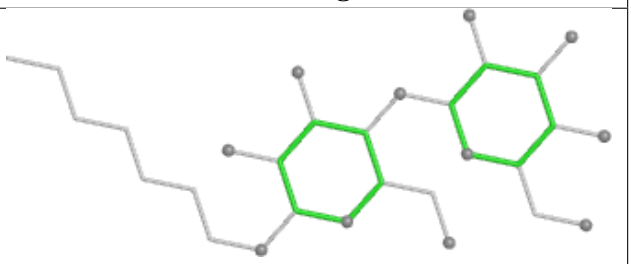

Rings

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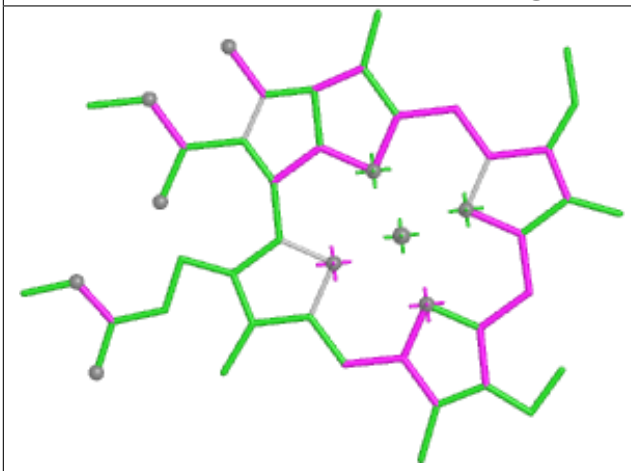

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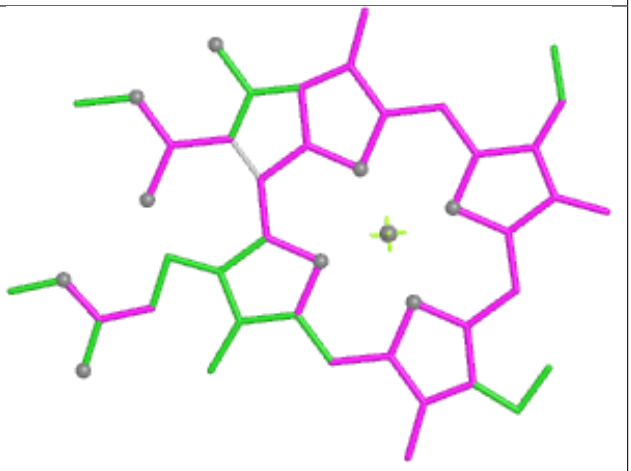

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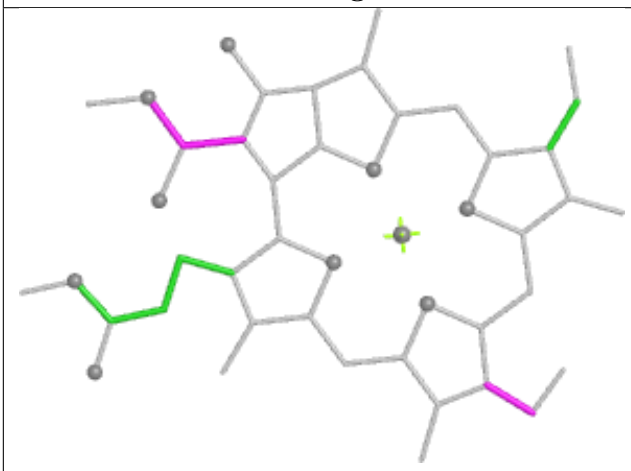

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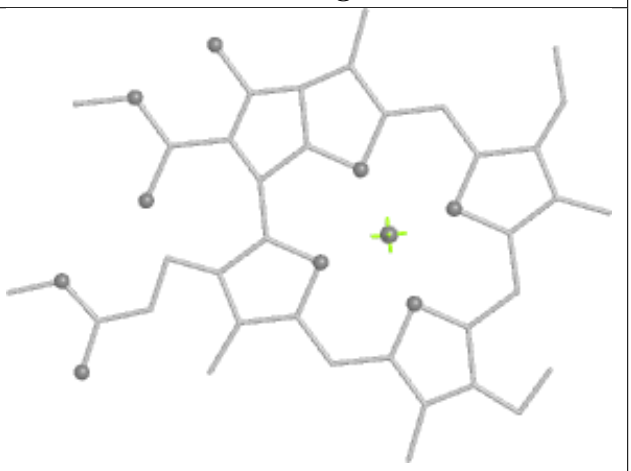
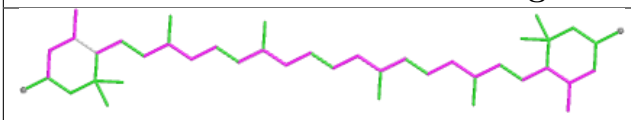


Rings

Ligand LUT 5 303



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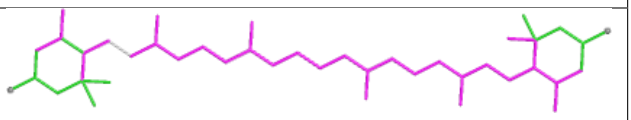

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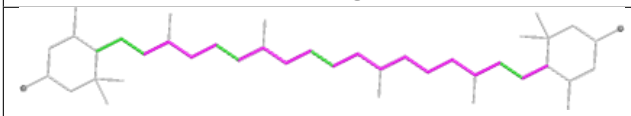

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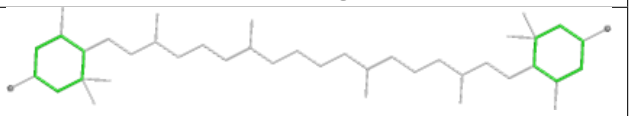
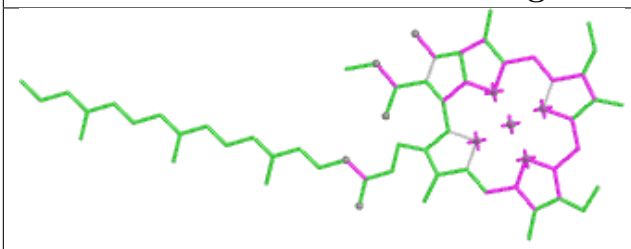


Rings

Ligand CHL 3 317



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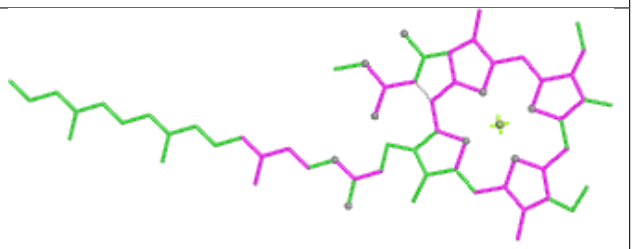

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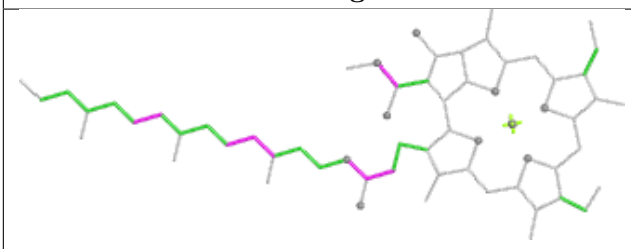

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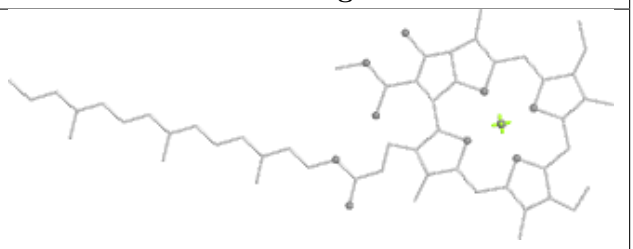
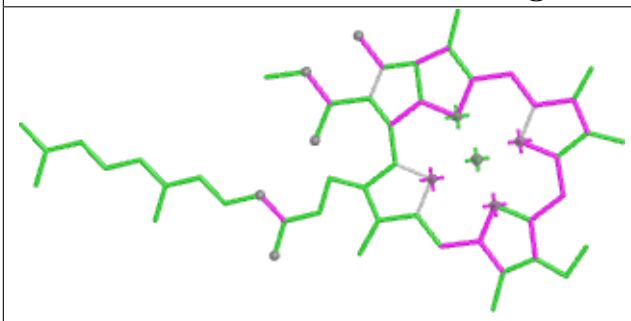


Rings

Ligand CHL 7 316



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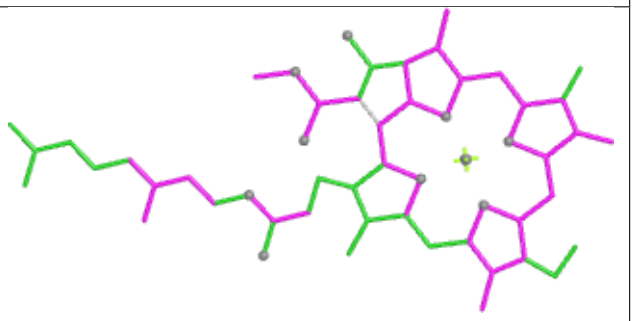

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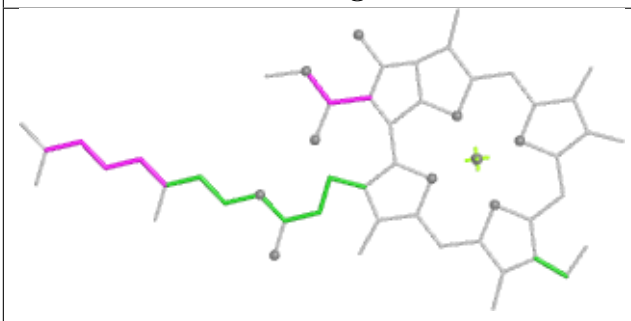

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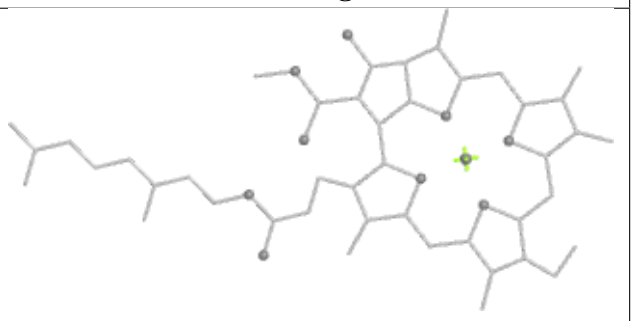
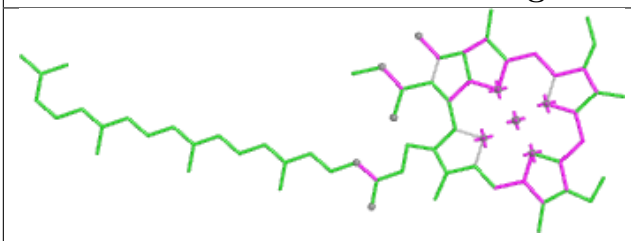


Rings

Ligand CHL 8 316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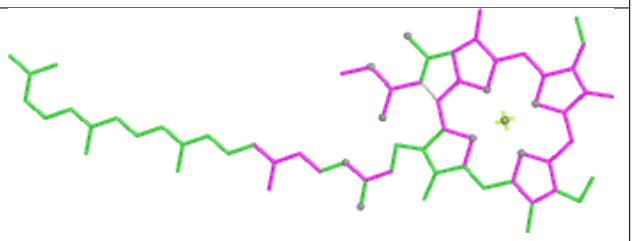
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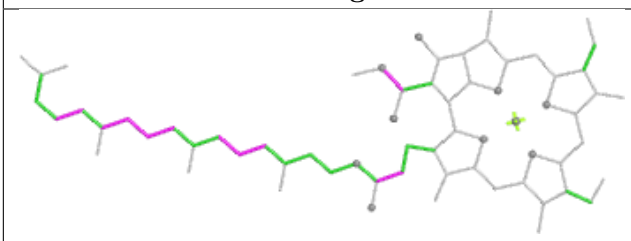
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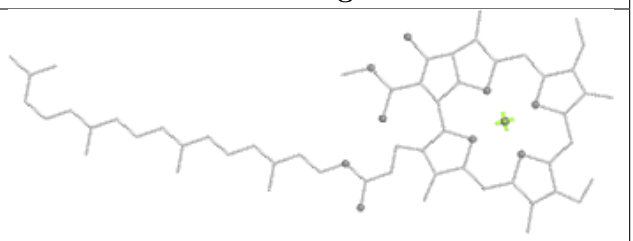
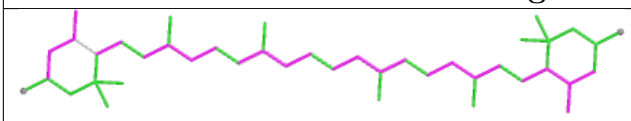

Rings

Ligand LUT 6 303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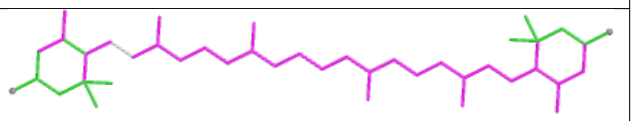
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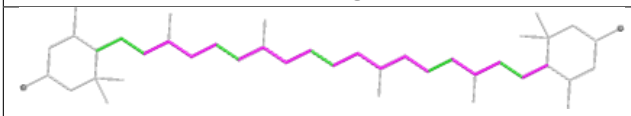
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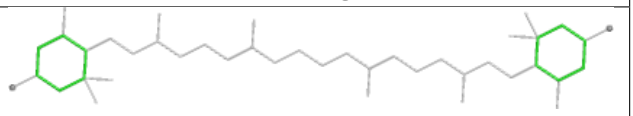
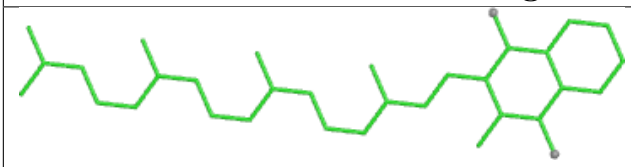

Rings

Ligand PQN B 801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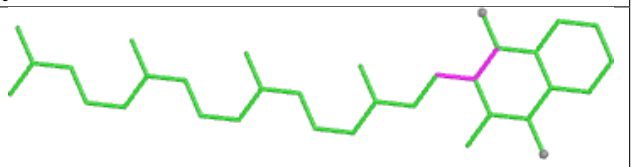
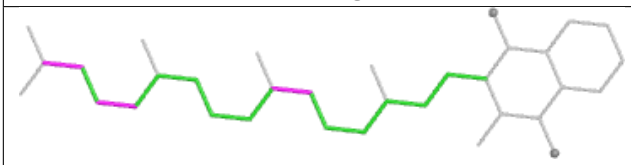

Bond angles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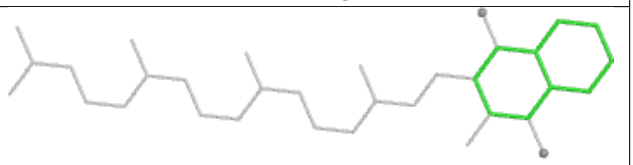
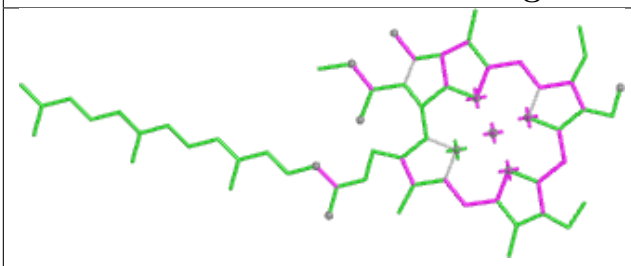
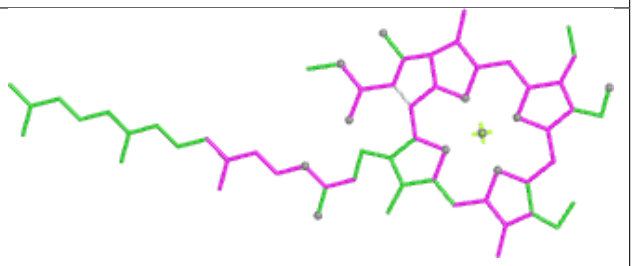

Rings

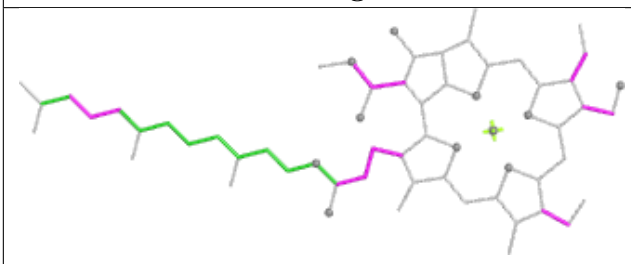
Ligand CHL A 833



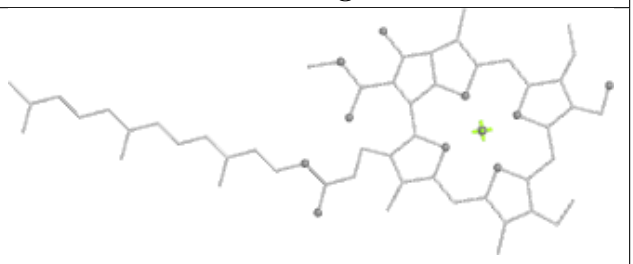
Bond lengths



Bond angles

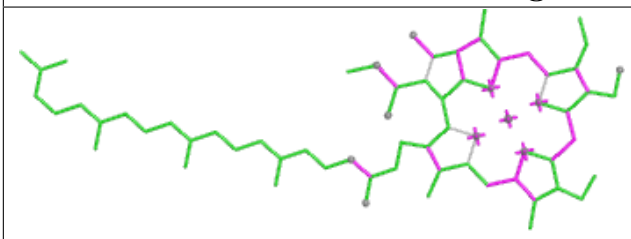


Torsions



Rings

Ligand CHL 8 321



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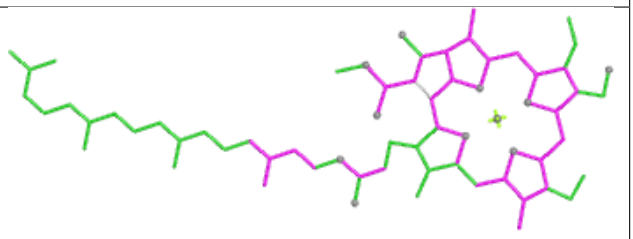

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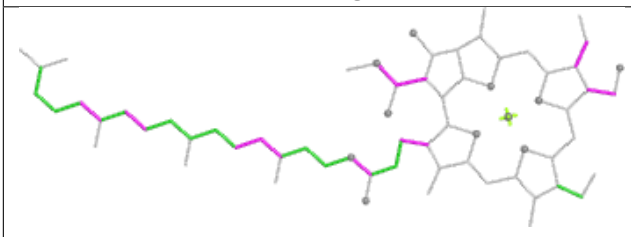

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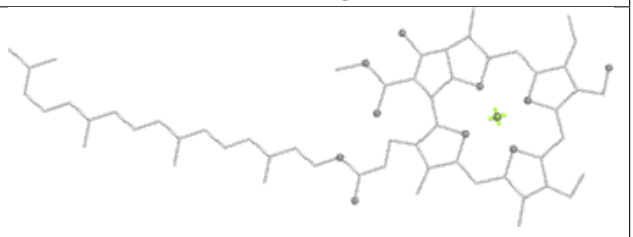
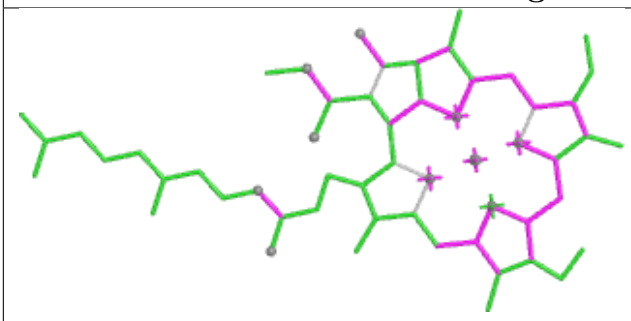


Rings

Ligand CHL 7 318



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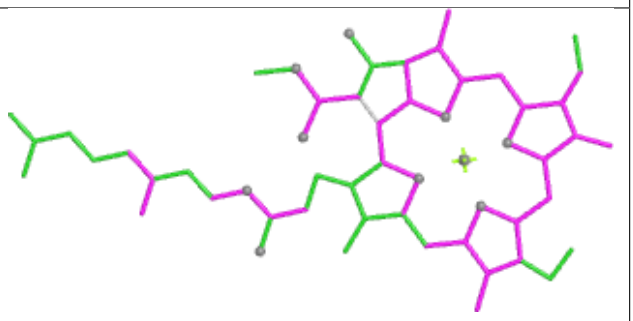

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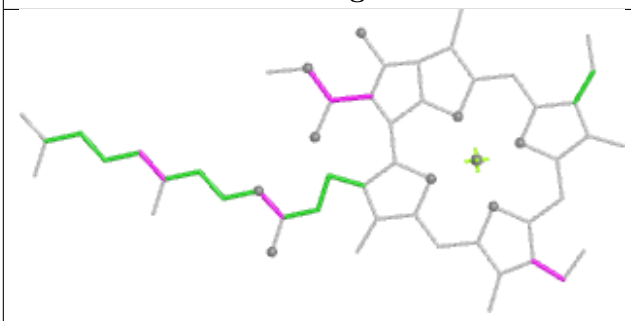

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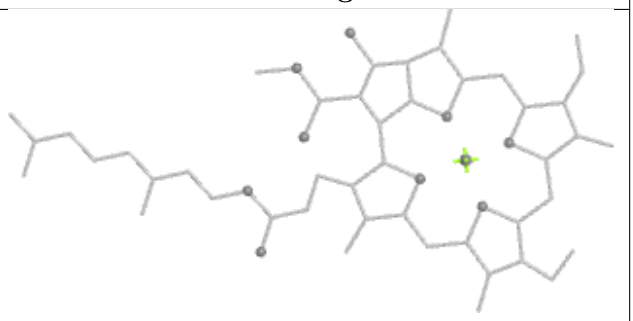
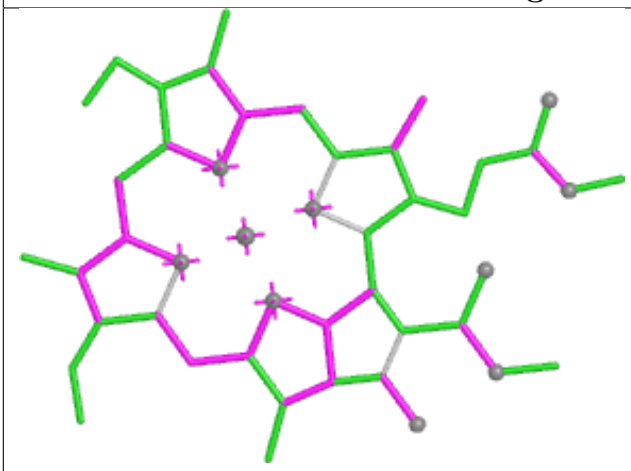


Rings

Ligand CHL b 308



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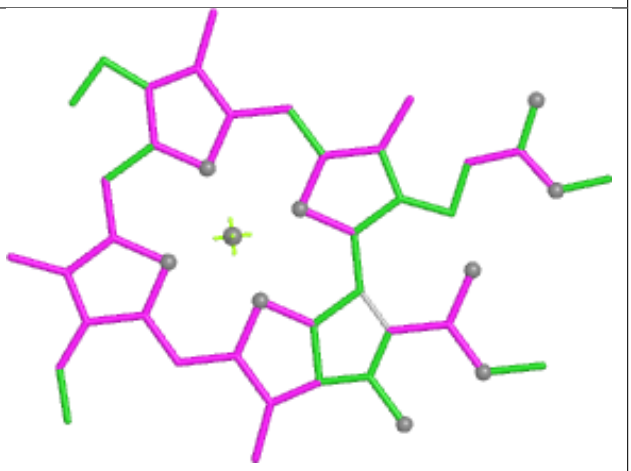

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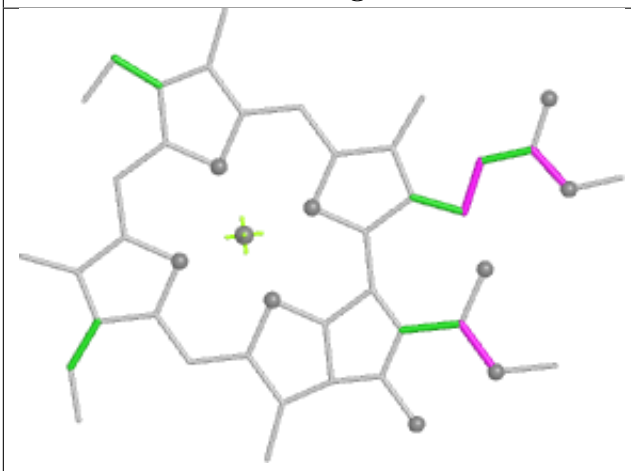

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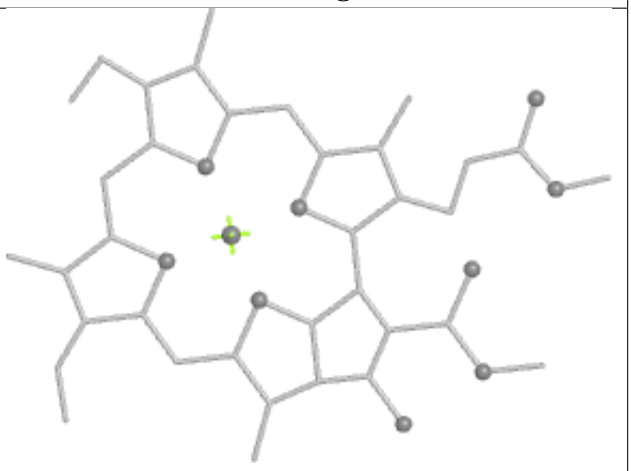
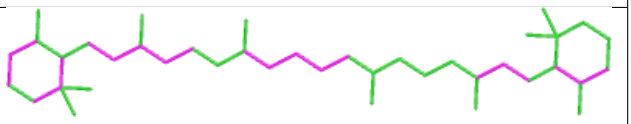


Rings

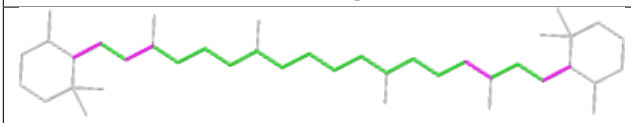
Ligand BCR 8 302



Bond lengths



Bond angles



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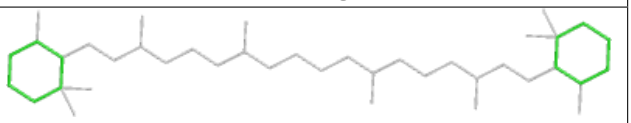
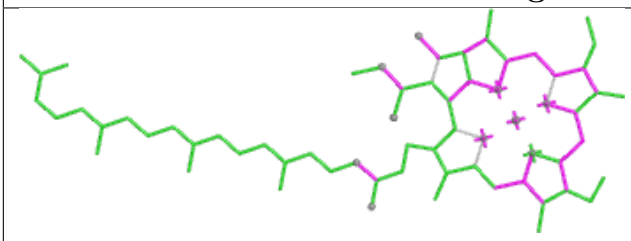


Rings

Ligand CHL 7 317



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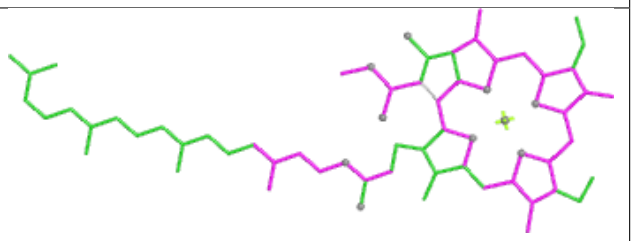
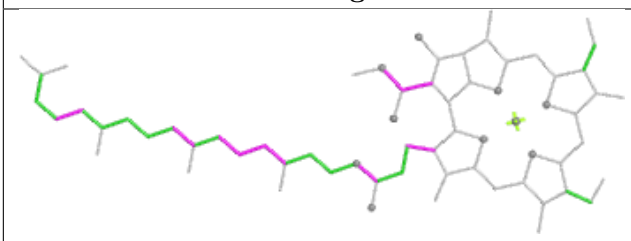


Bond angles



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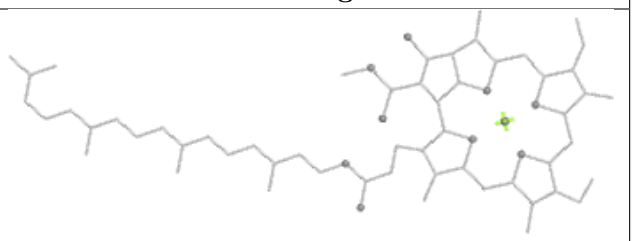
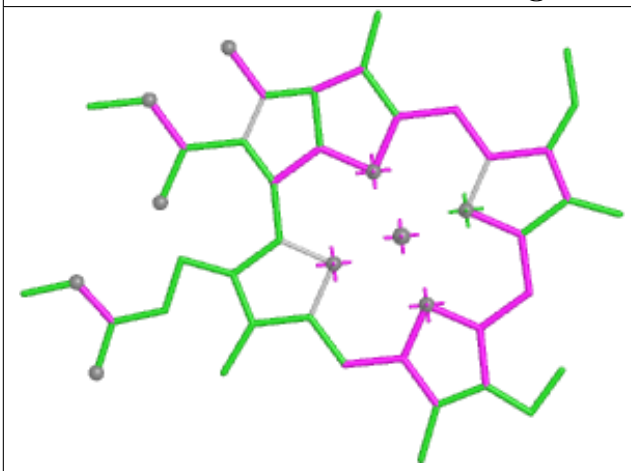


Rings

Ligand CHL 5 321



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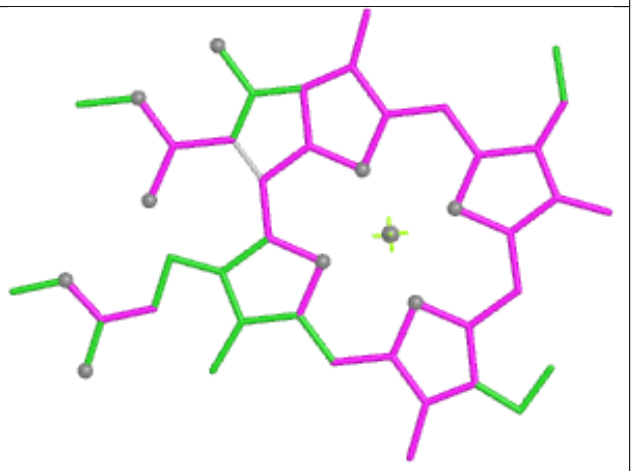
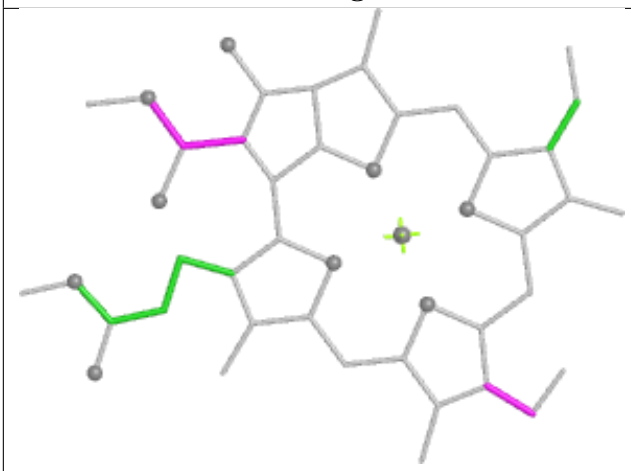


Bond angles

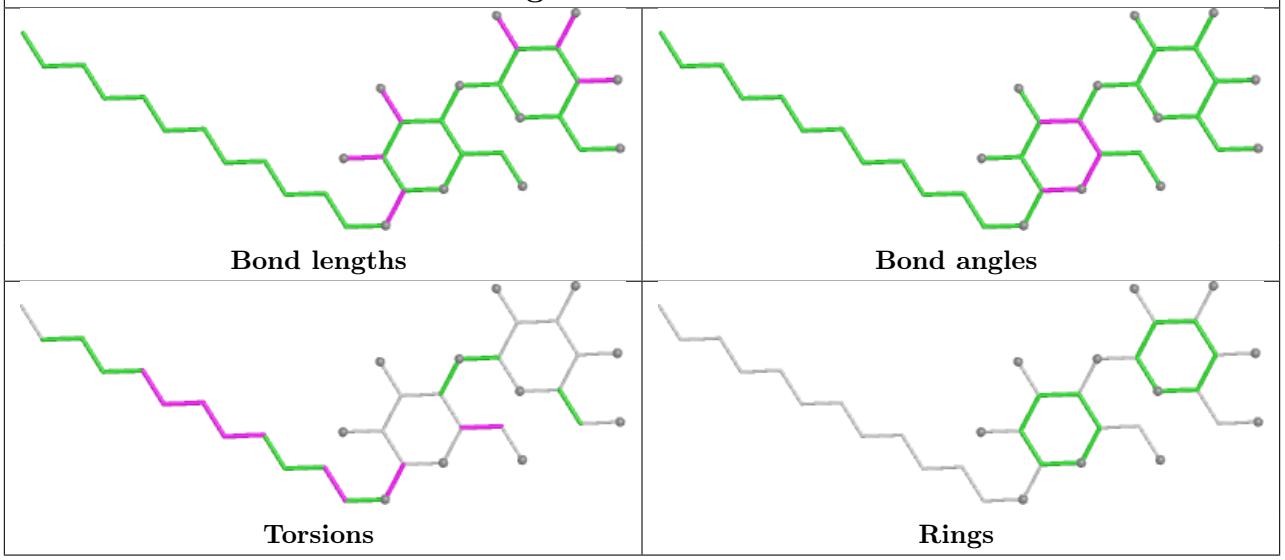


Torsions

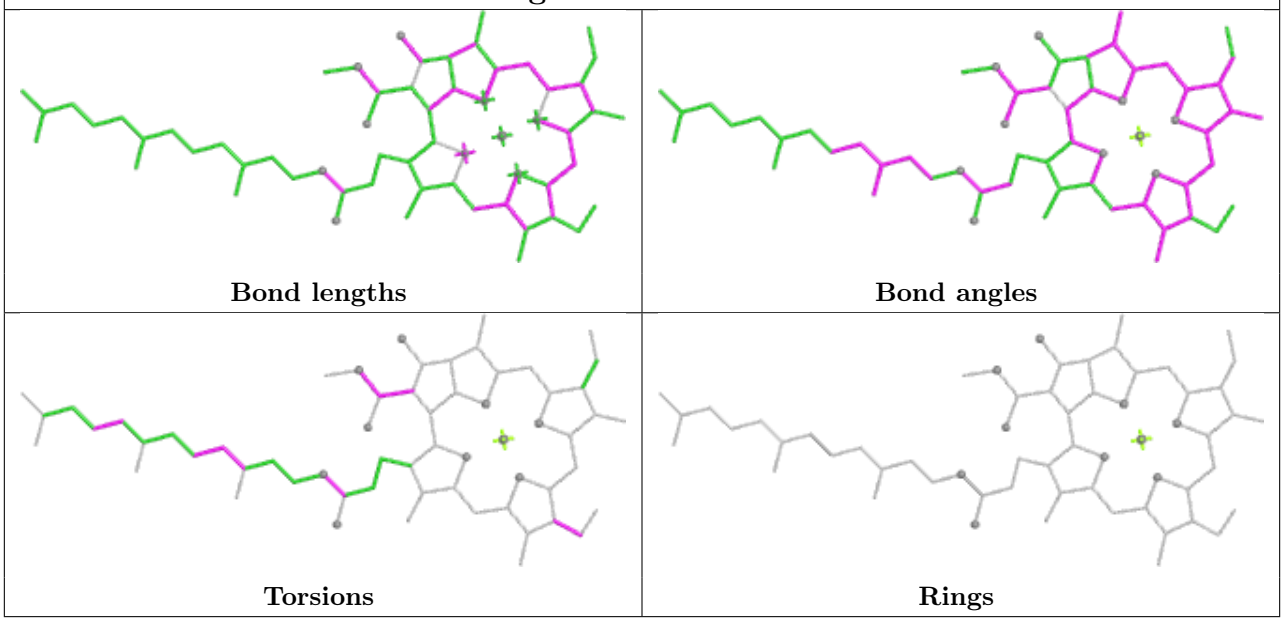


Rings

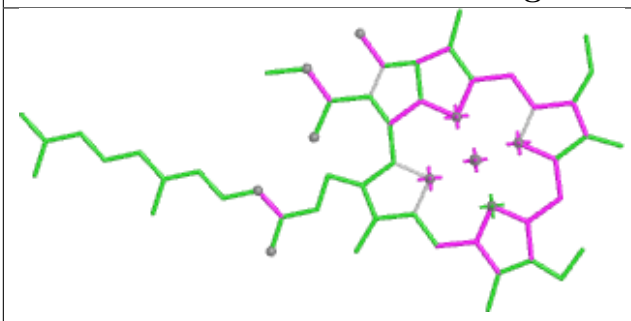
Ligand LMT 5 326



Ligand CHL 3 314



Ligand CHL B 823



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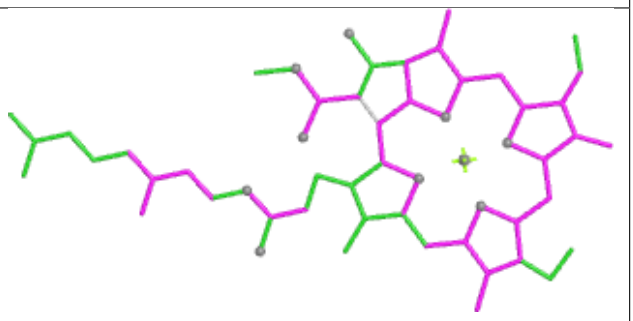
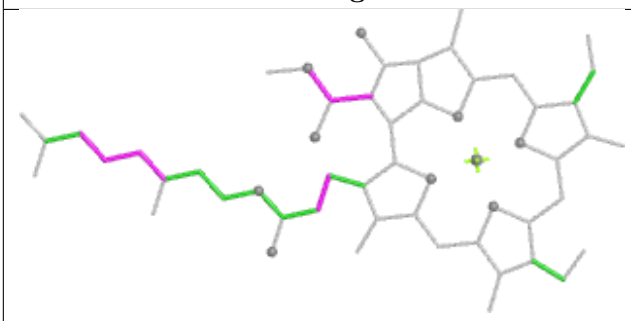


Bond angles



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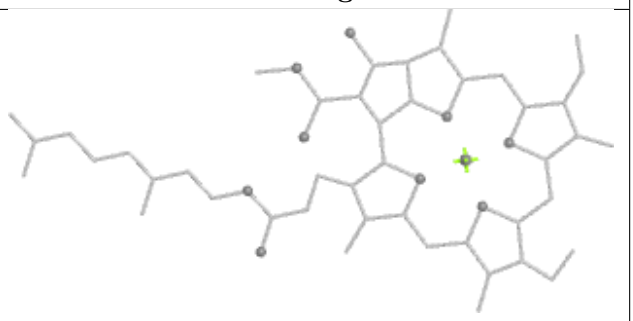
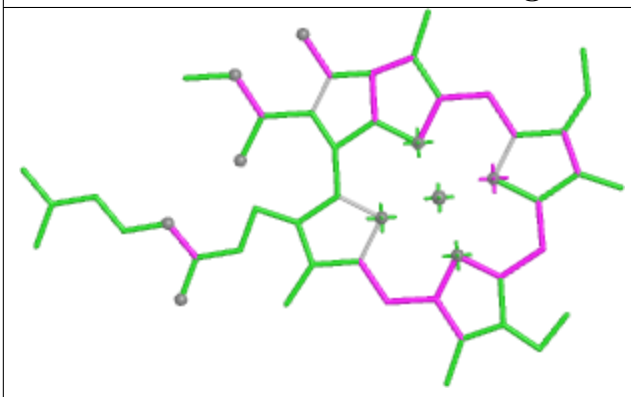


Rings

Ligand CHL A 846



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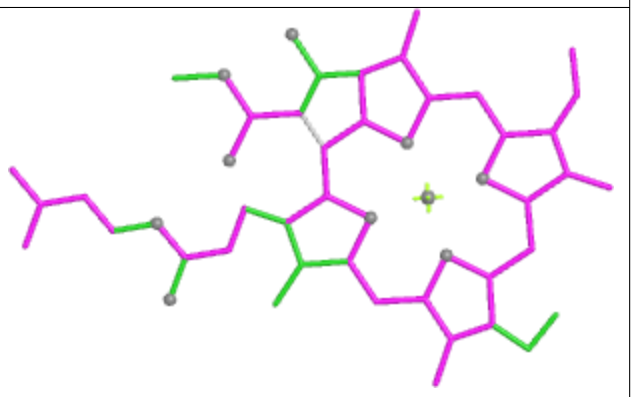
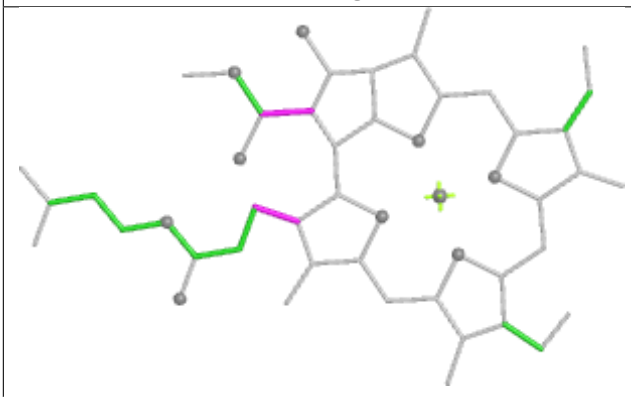


Bond angles



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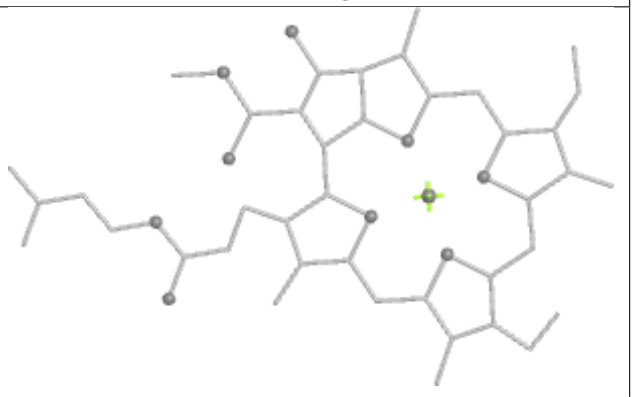
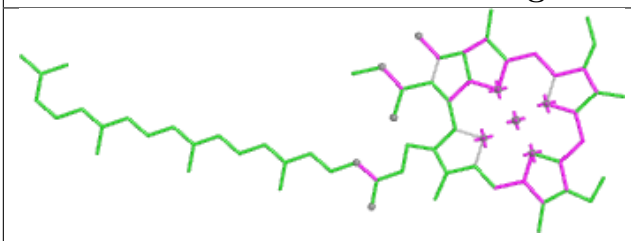


Rings

Ligand CHL 8 317



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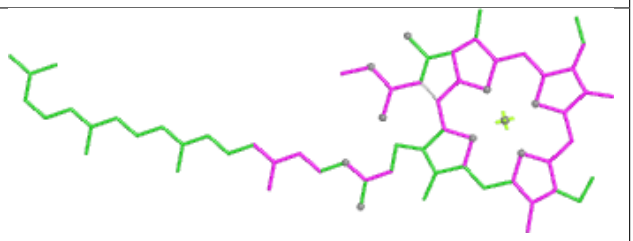
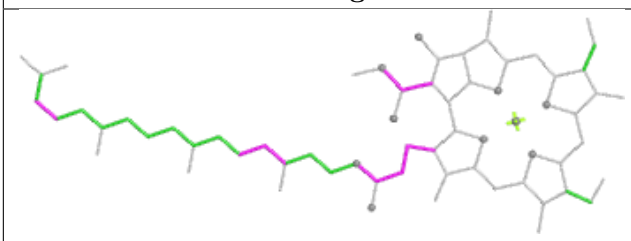


Bond angles



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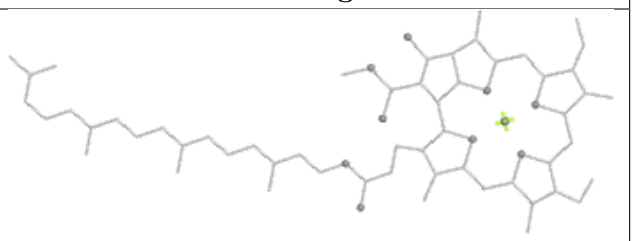
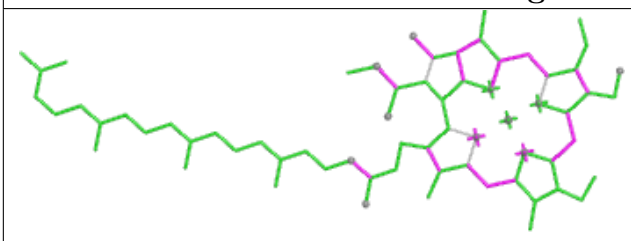


Rings

Ligand CHL 3 316



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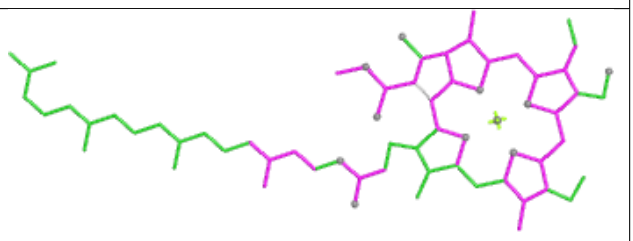
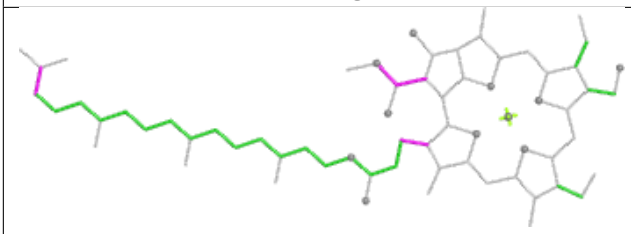


Bond angles



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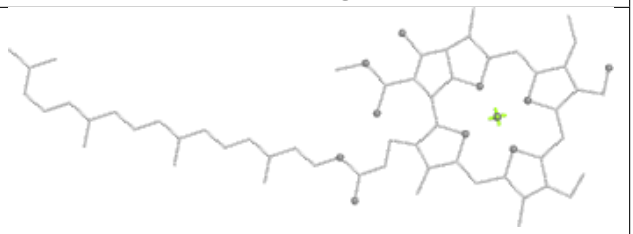
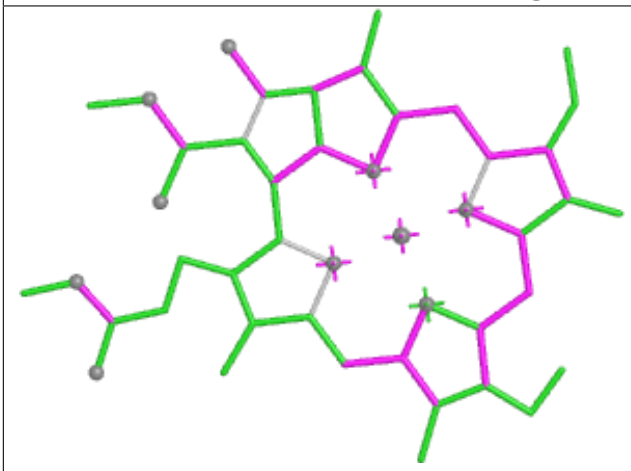


Rings

Ligand CHL 7 324



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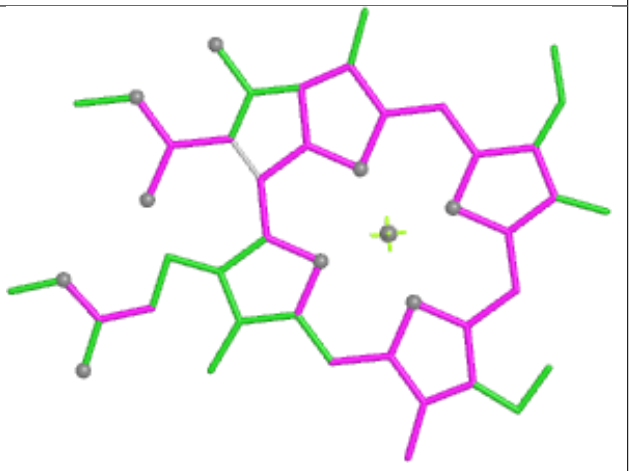

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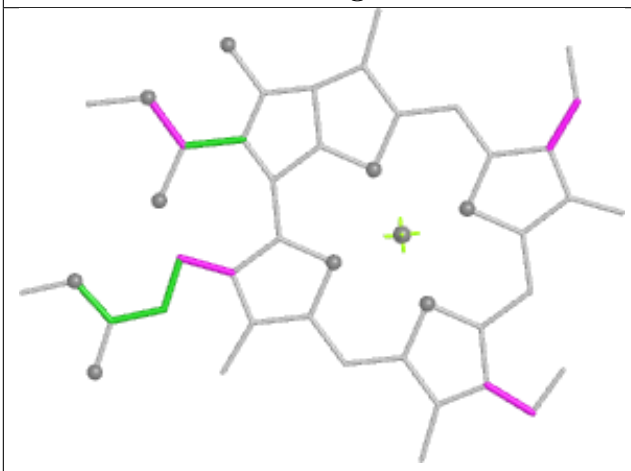

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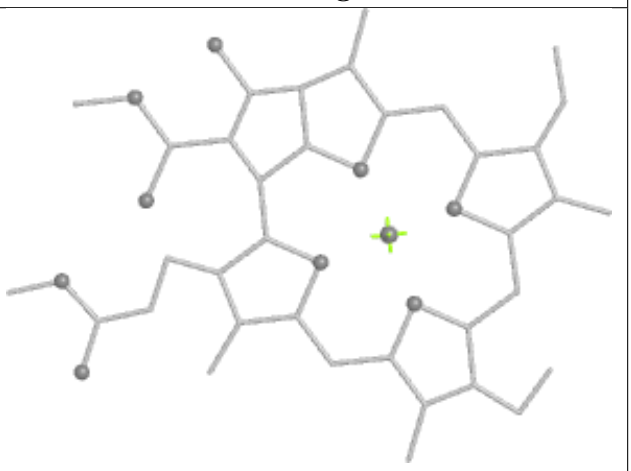
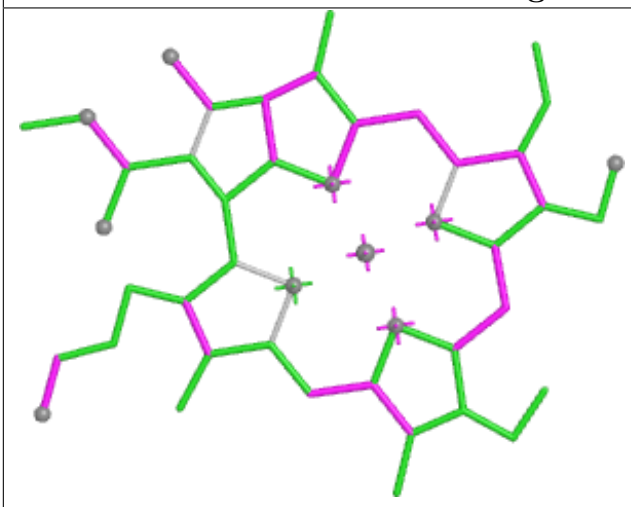


Rings

Ligand CHL 8 324



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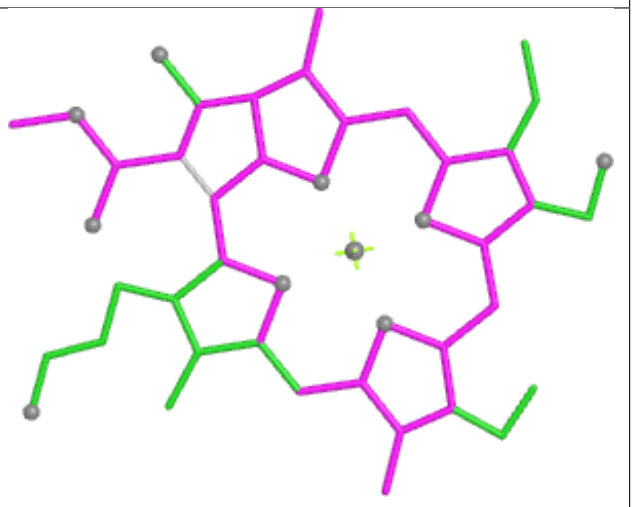
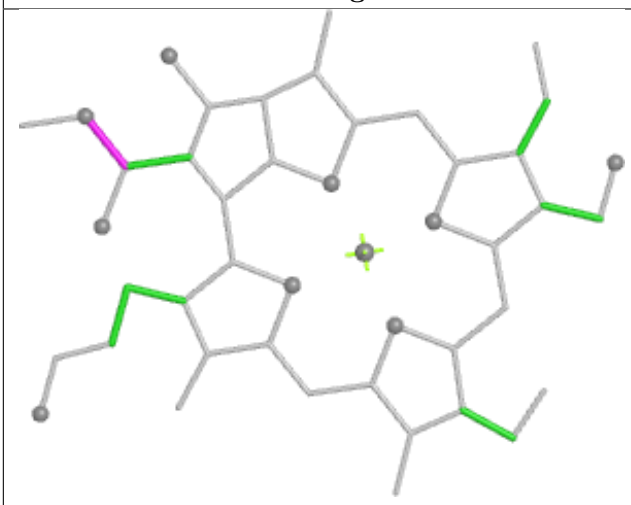


Bond angles



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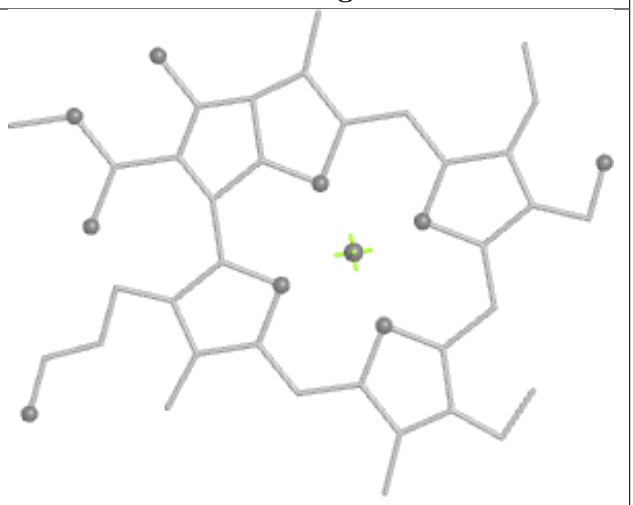
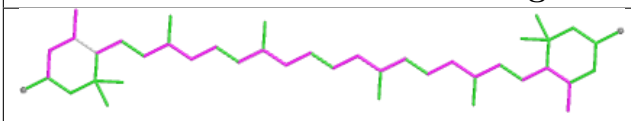


Rings

Ligand LUT 4 302



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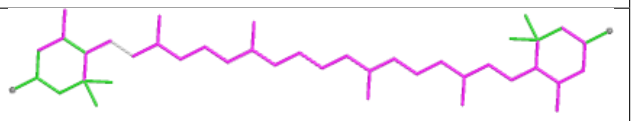
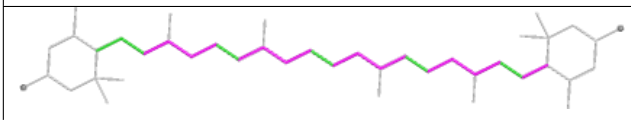


Bond angles



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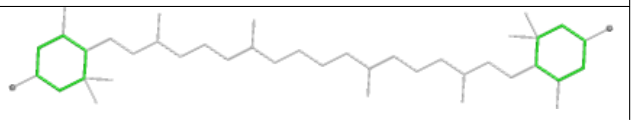
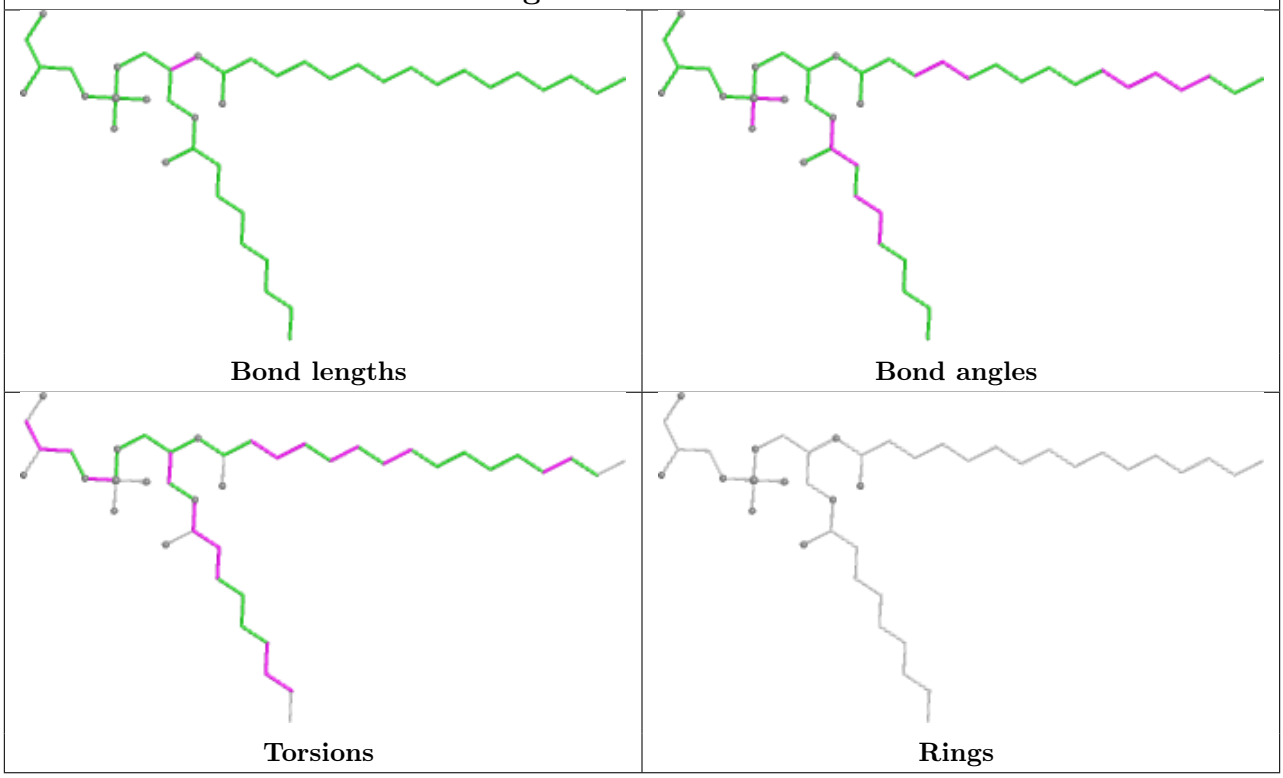
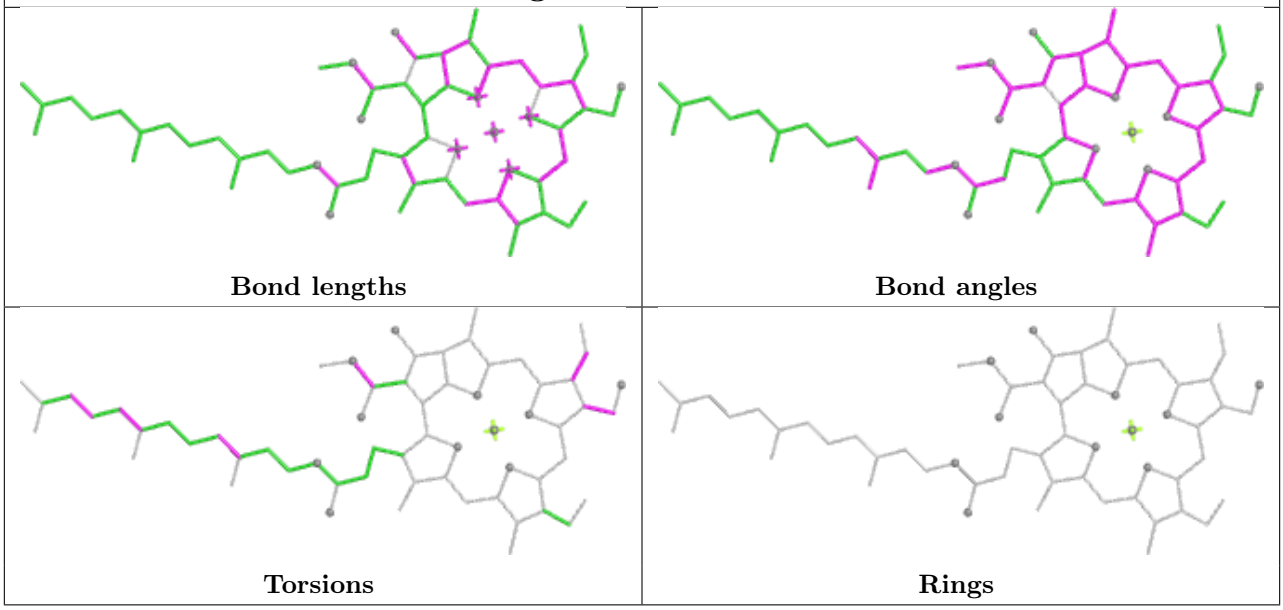


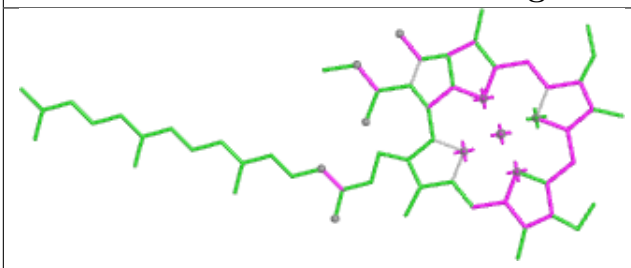
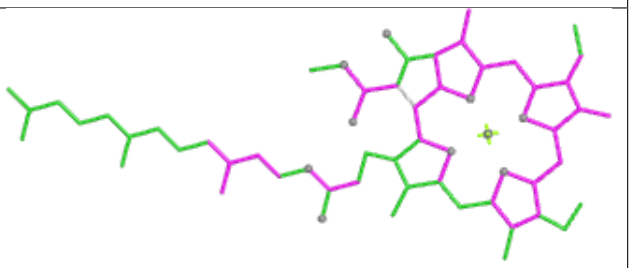
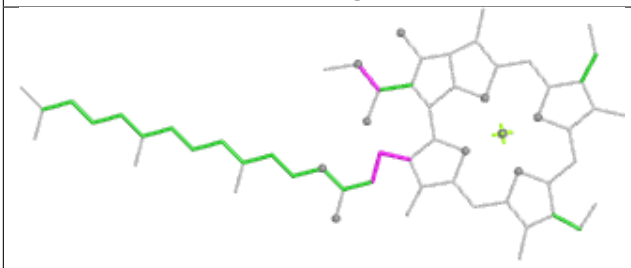
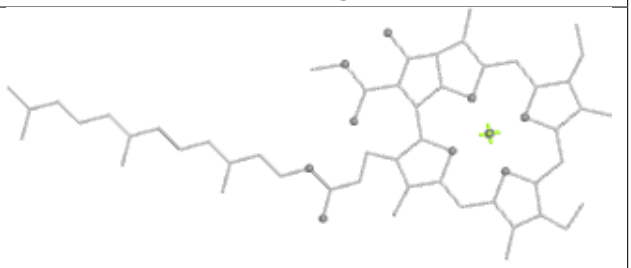
Rings

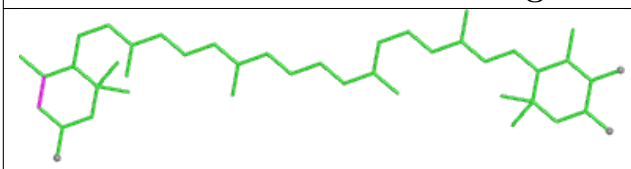
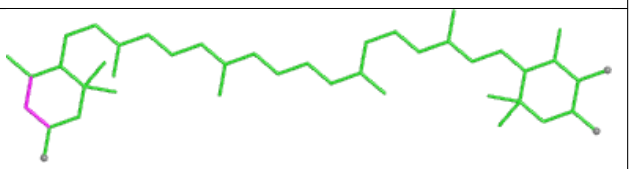
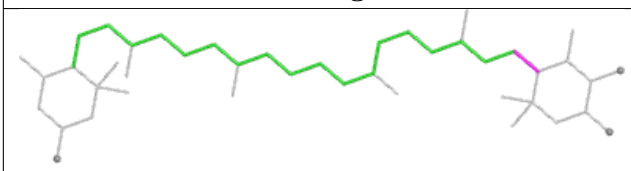
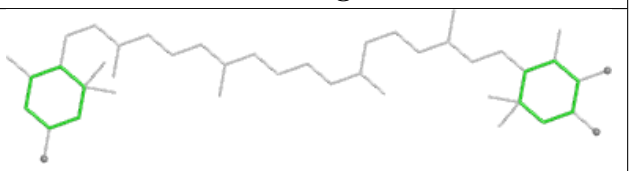
Ligand LHG A 810



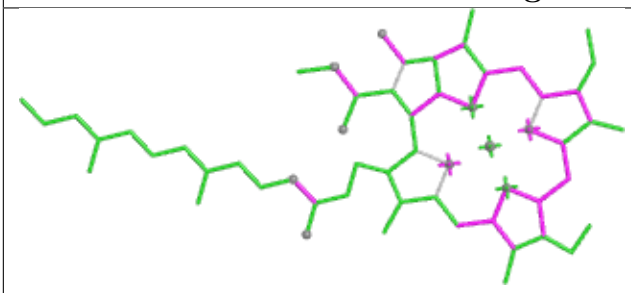
Ligand CHL 7 322



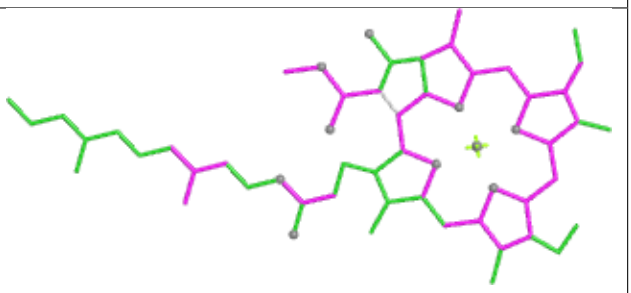
Ligand CHL a 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AXT a 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

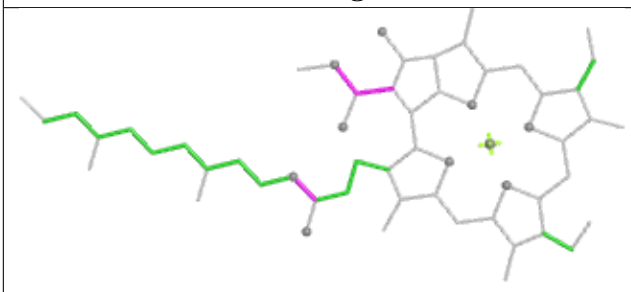
Ligand CHL B 824



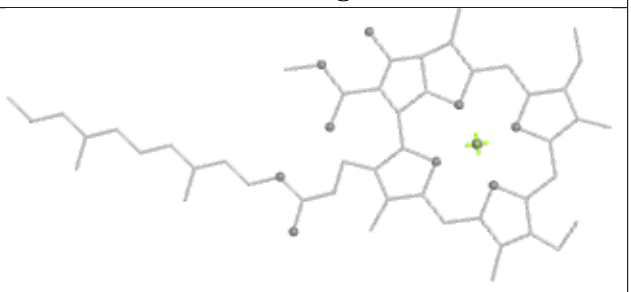
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

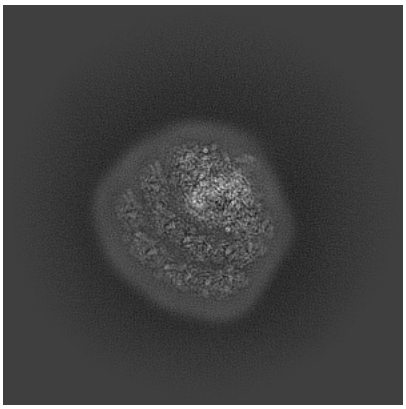
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62512. These allow visual inspection of the internal detail of the map and identification of artifacts.

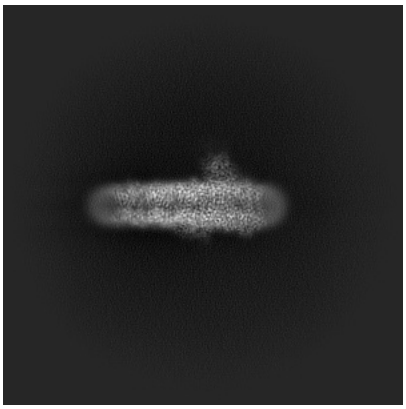
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

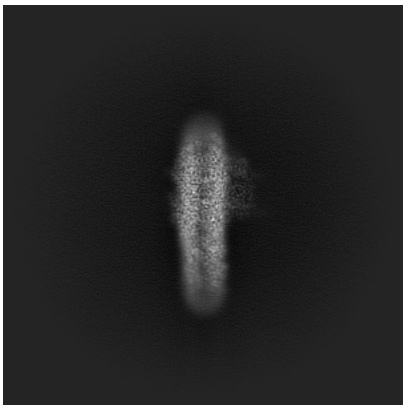
6.1.1 Primary map



X

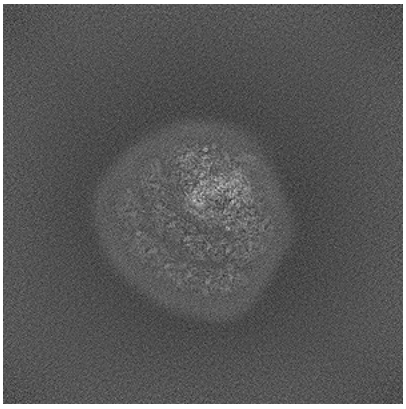


Y

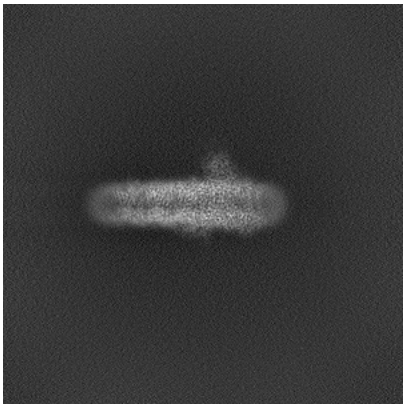


Z

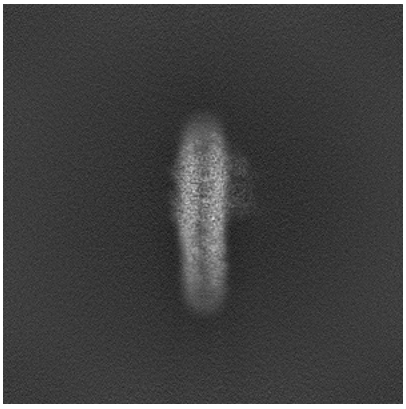
6.1.2 Raw map



X



Y

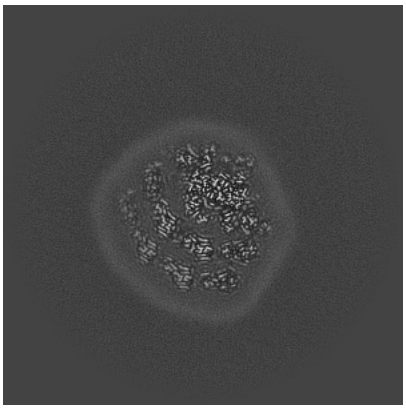


Z

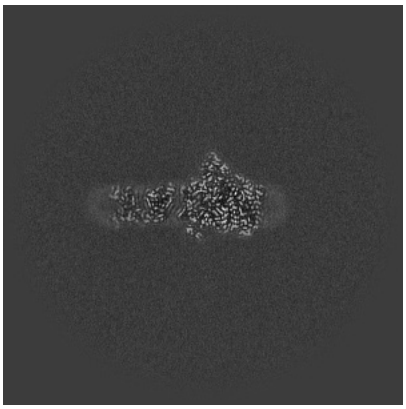
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 300

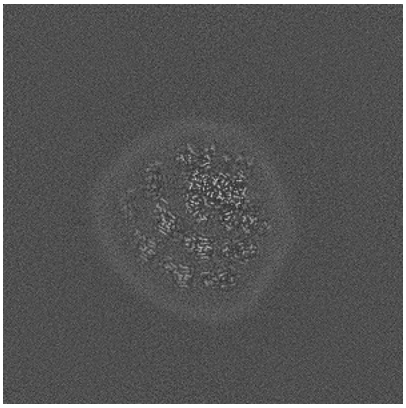


Y Index: 300

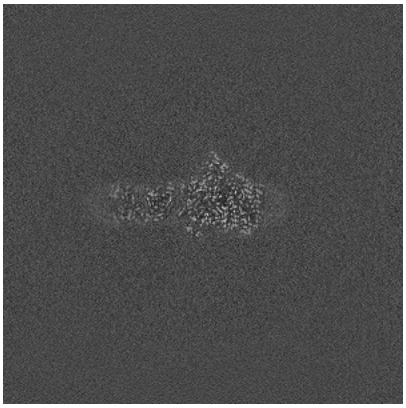


Z Index: 300

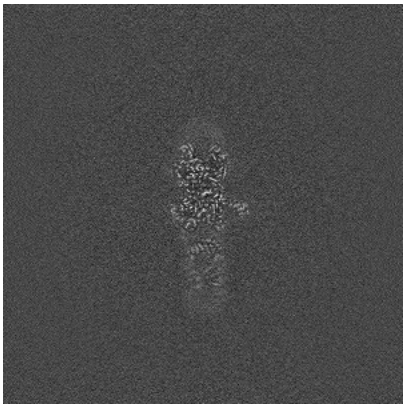
6.2.2 Raw map



X Index: 300



Y Index: 300

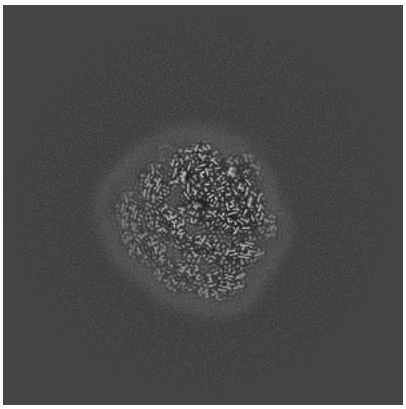


Z Index: 300

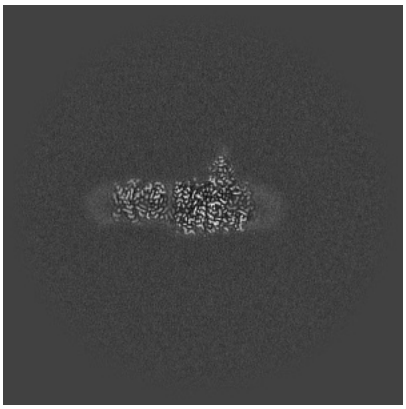
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

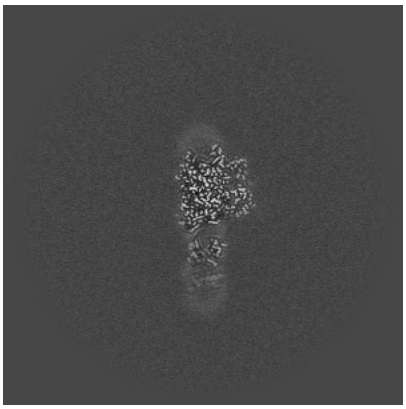
6.3.1 Primary map



X Index: 317

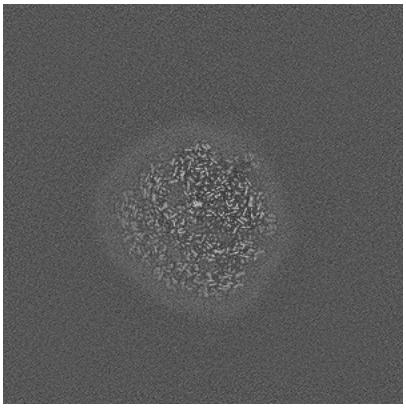


Y Index: 340

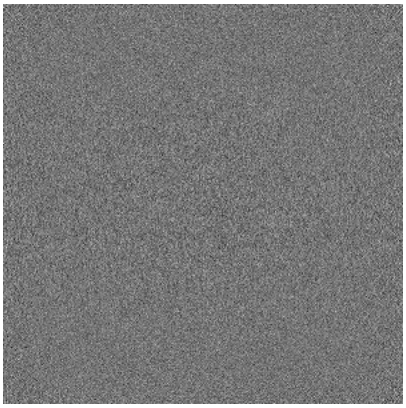


Z Index: 316

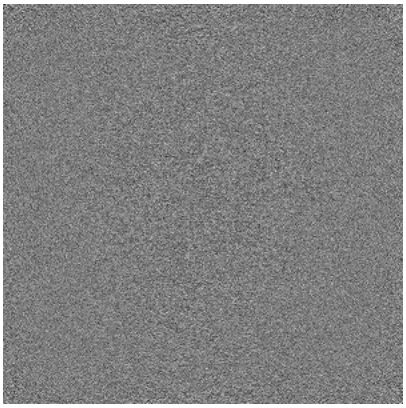
6.3.2 Raw map



X Index: 316



Y Index: 0

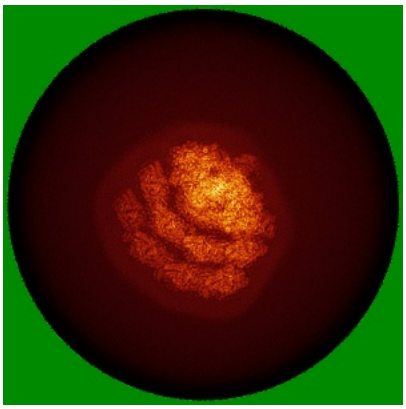


Z Index: 0

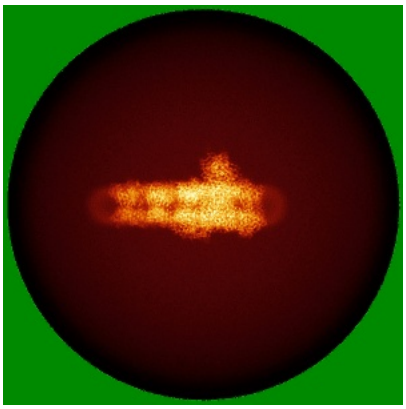
The images above show the largest variance slices of the map in three orthogonal directions.

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

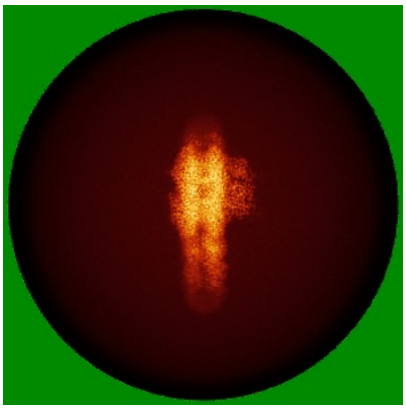
6.4.1 Primary map



X

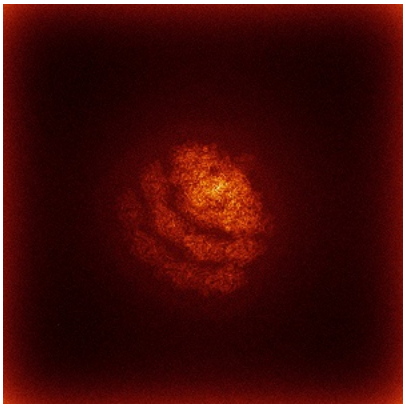


Y

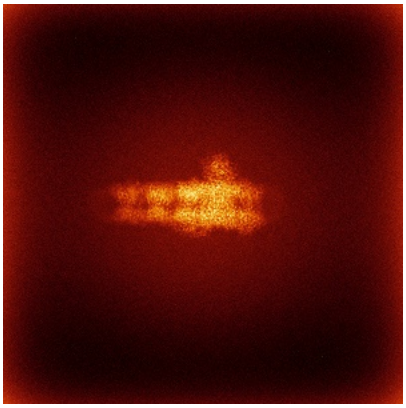


Z

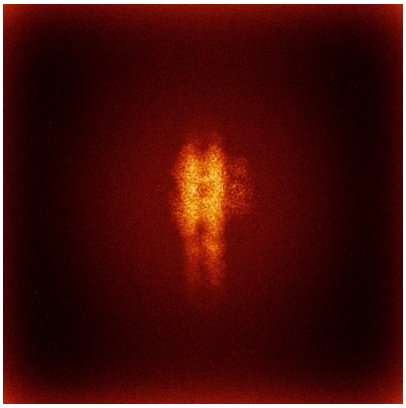
6.4.2 Raw map



X



Y

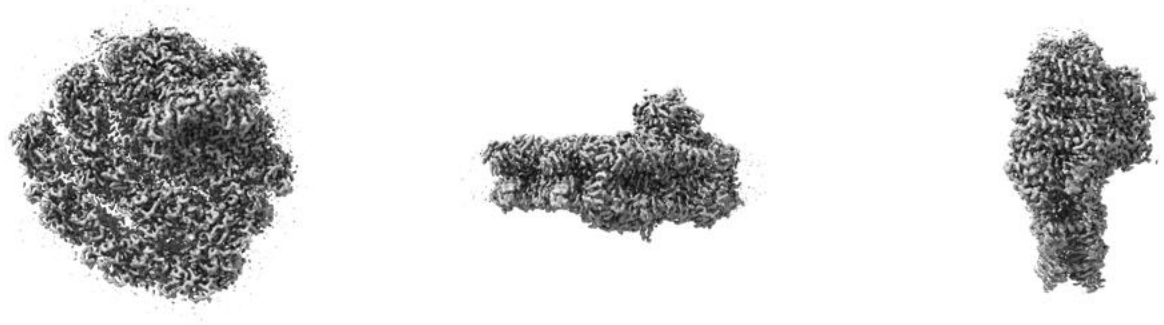


Z

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)

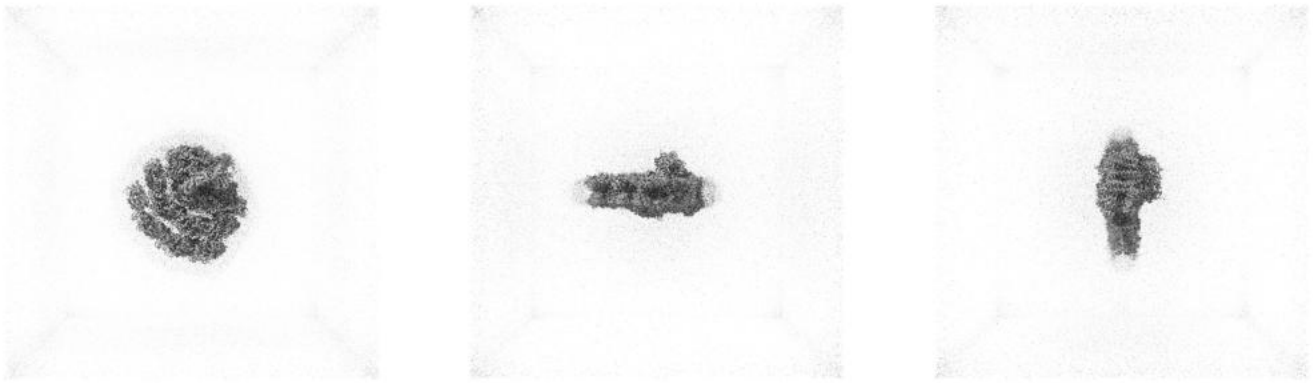
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

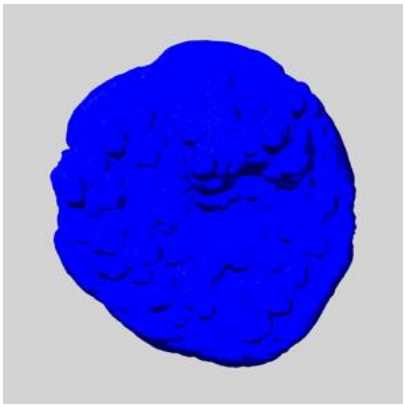
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

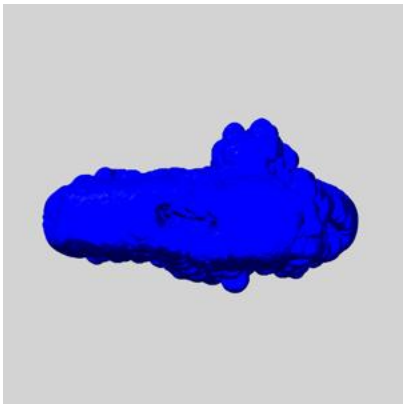
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

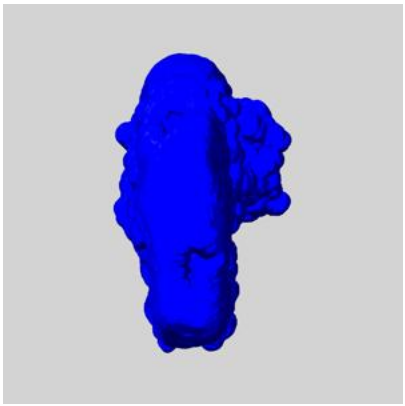
6.6.1 emd_62512_msk_1.map (i)



X



Y

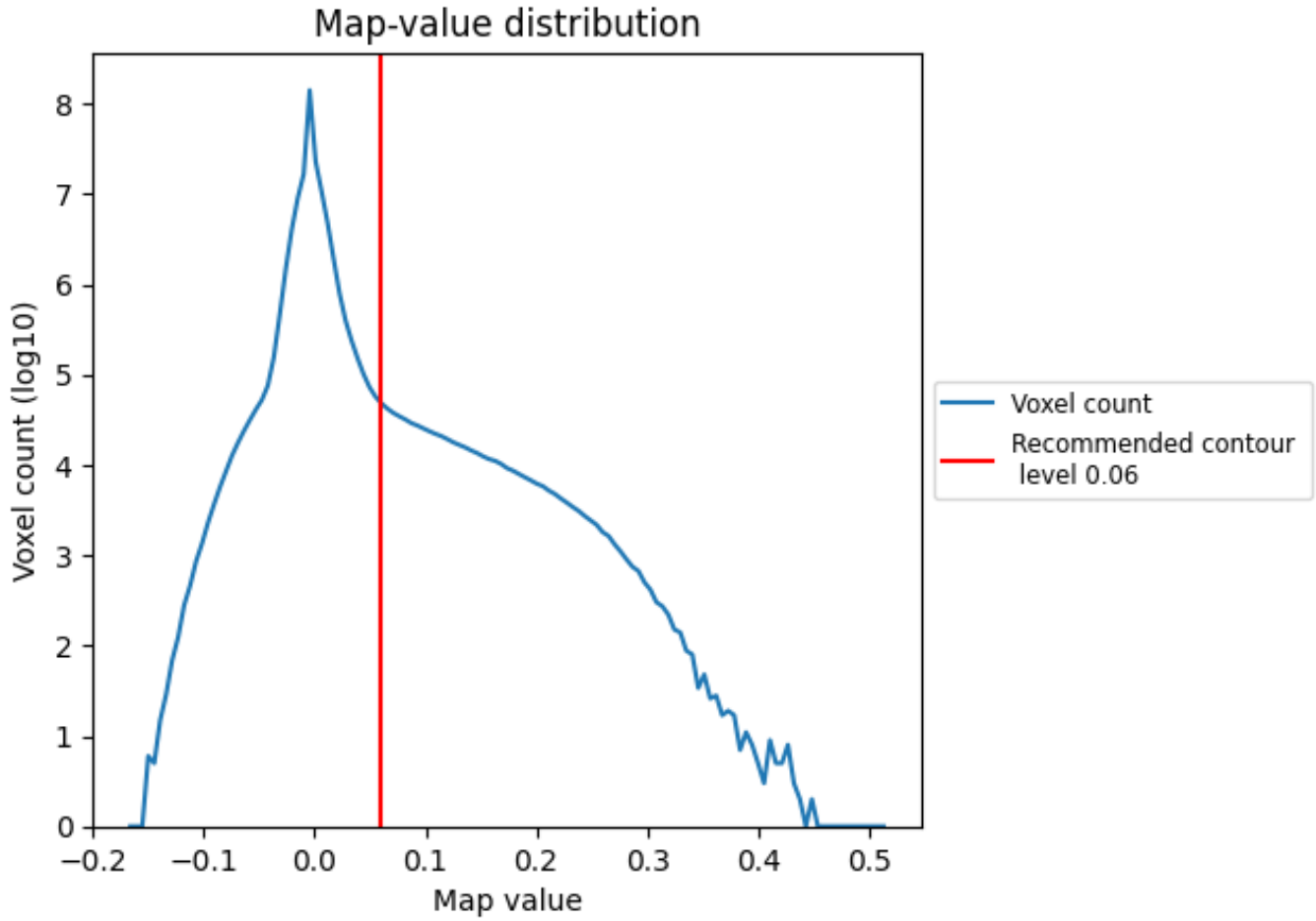


Z

7 Map analysis

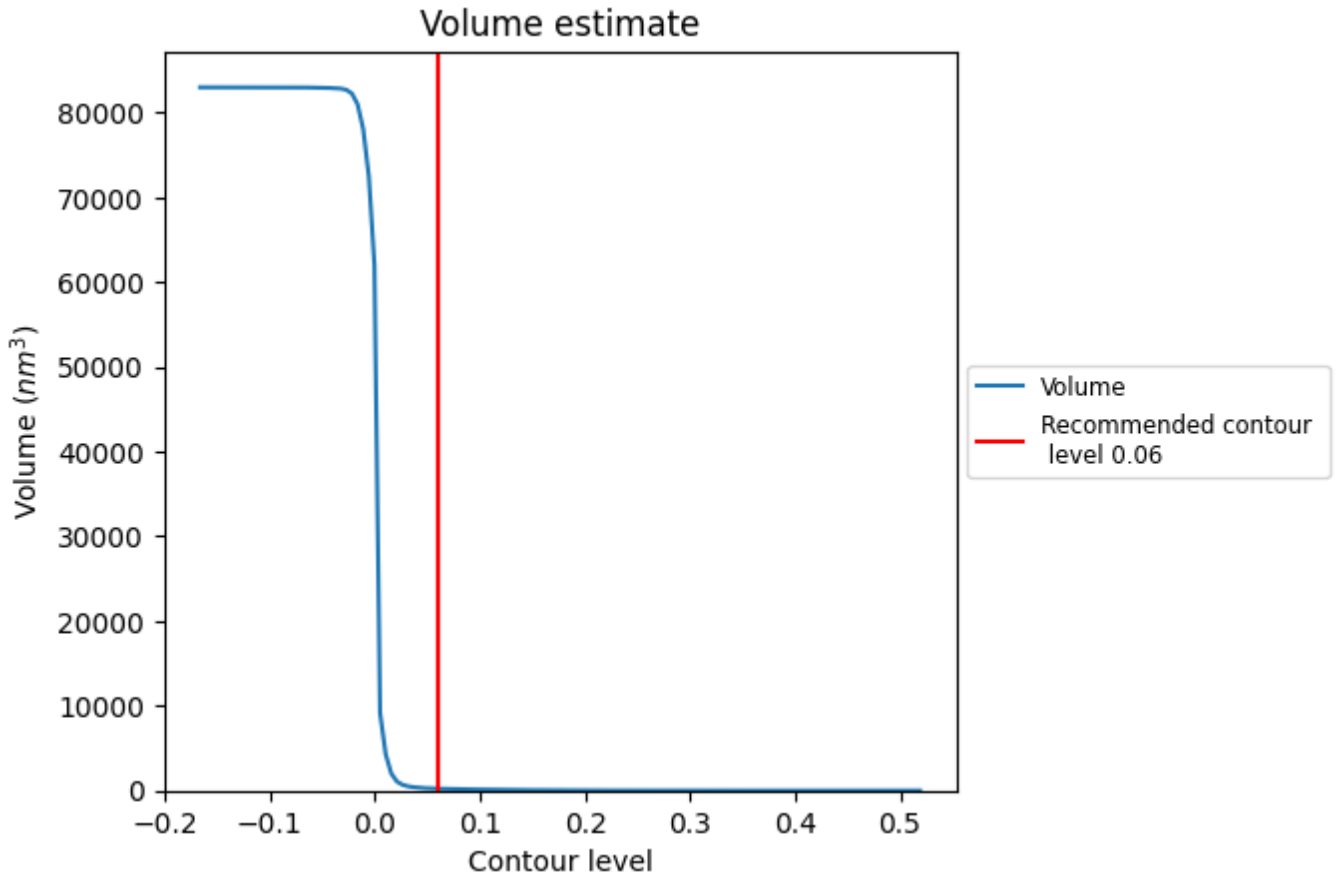
This section contains the results of statistical analysis of the map.

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.

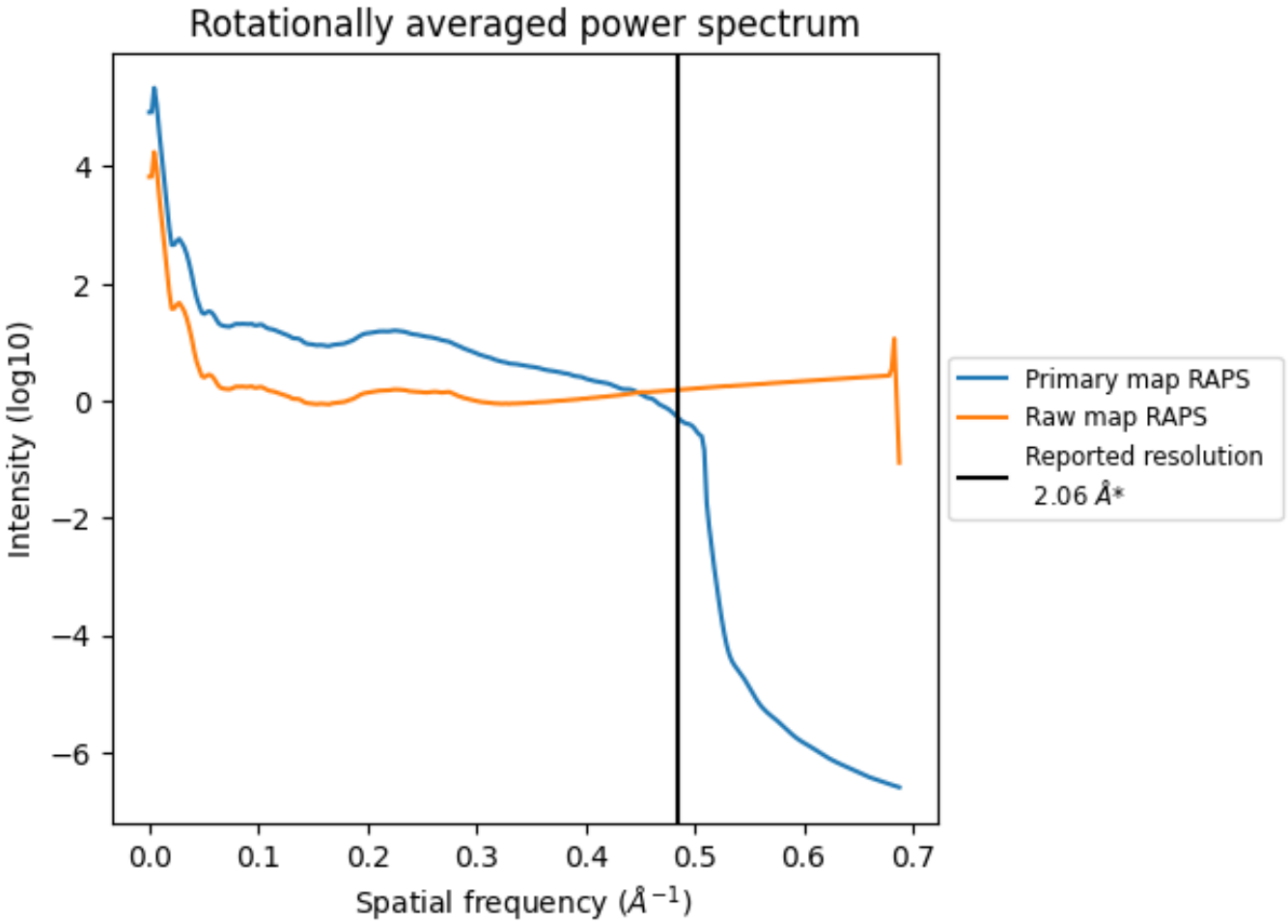
7.2 Volume estimate (i)



The volume at the recommended contour level is 225 nm^3; this corresponds to an approximate mass of 203 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)

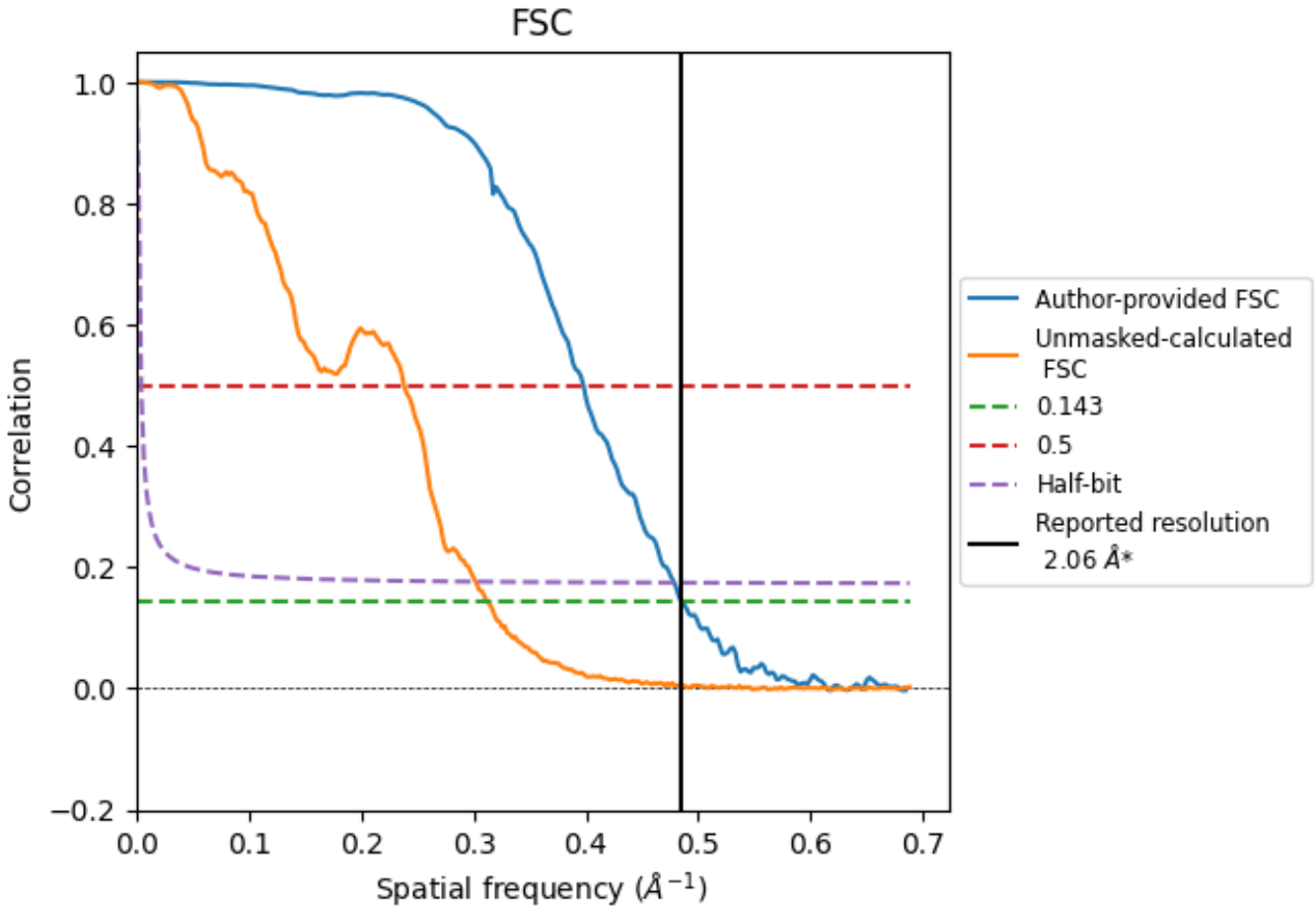


*Reported resolution corresponds to spatial frequency of 0.485 Å^{-1}

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 0.485 Å^{-1}

8.2 Resolution estimates (i)

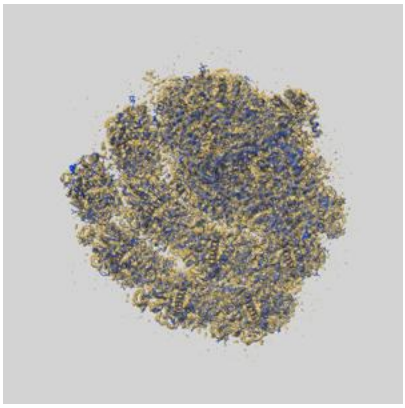
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.51	2.09
Unmasked-calculated*	3.20	4.20	3.31

*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 3.20 differs from the reported value 2.06 by more than 10 %

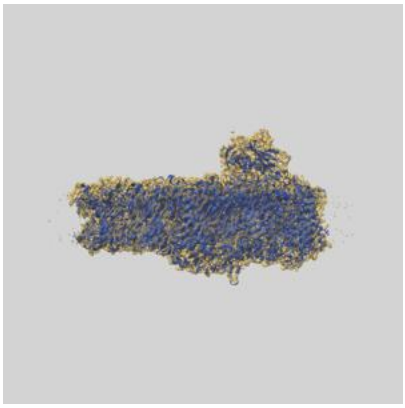
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62512 and PDB model 9KQQ. Per-residue inclusion information can be found in section 3 on page 31.

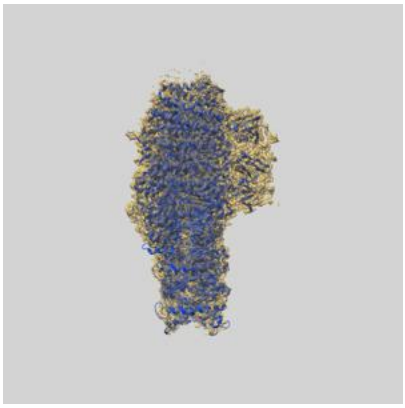
9.1 Map-model overlay



X



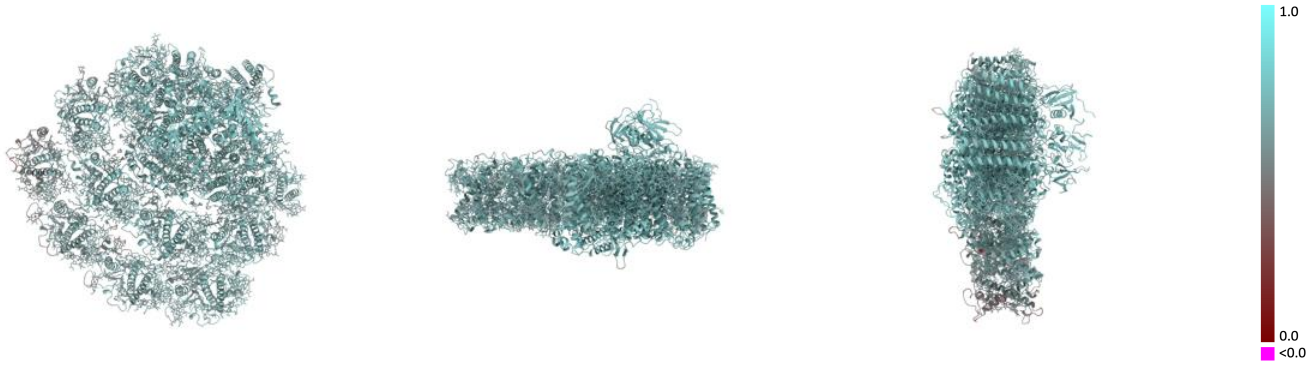
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

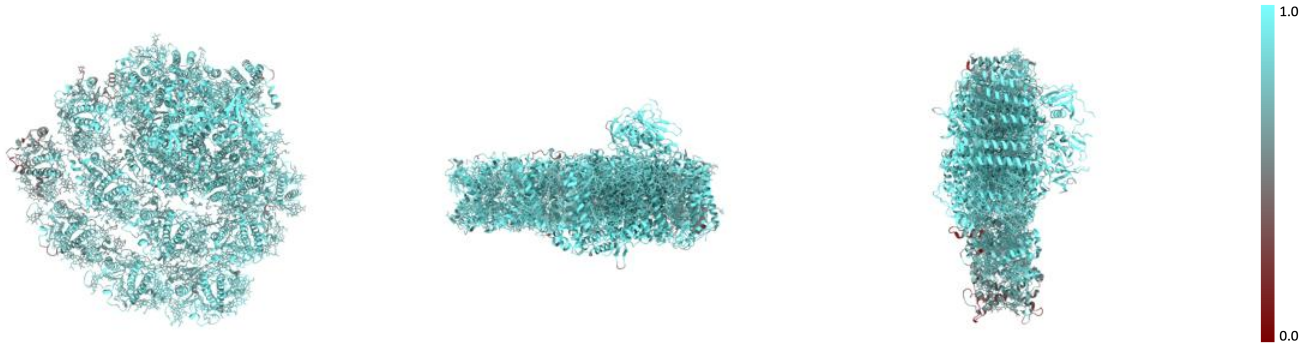
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

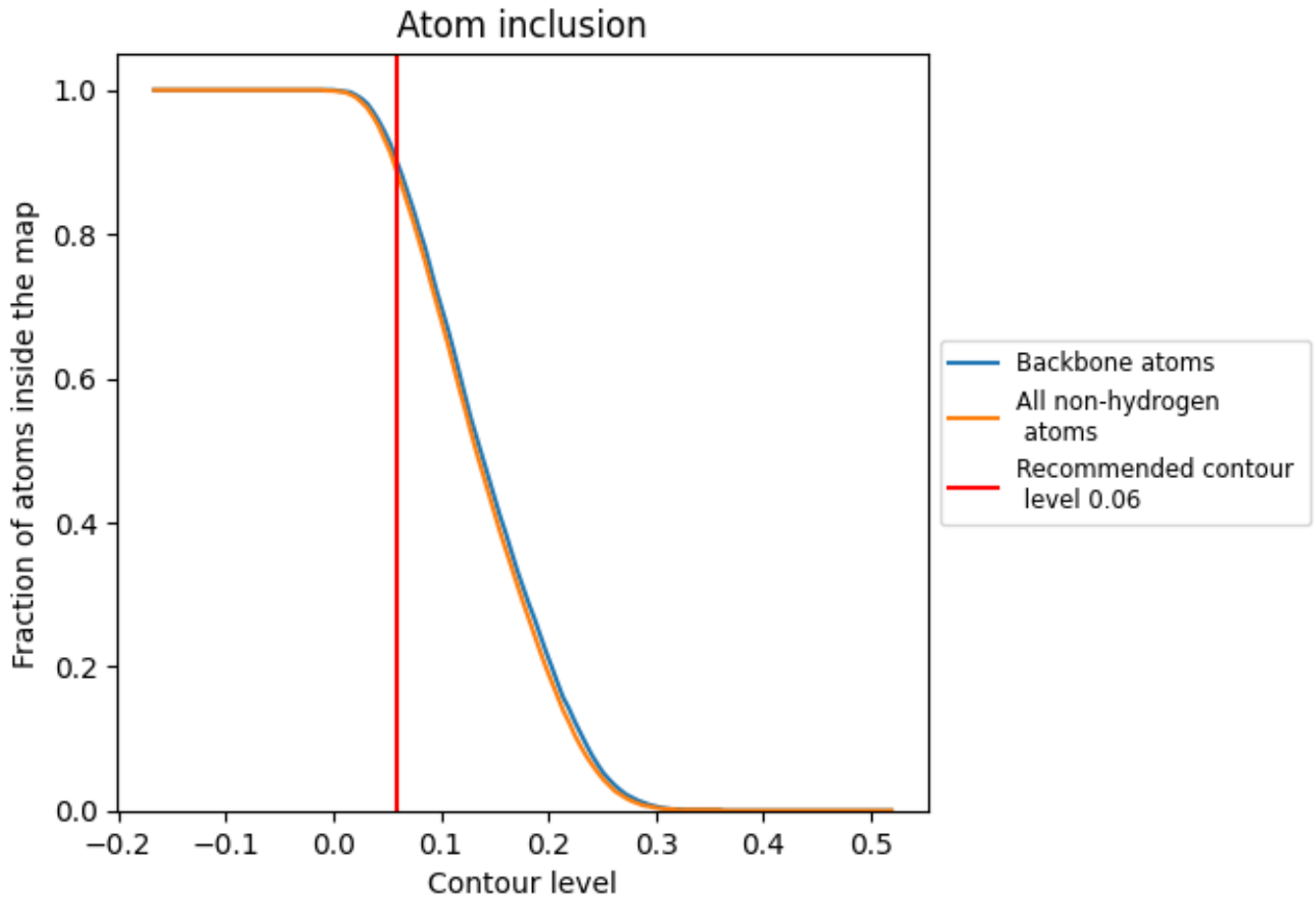
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.6680
3	0.8930	0.6640
4	0.7630	0.5820
5	0.8680	0.6390
6	0.8360	0.6240
7	0.9100	0.6740
8	0.8850	0.6680
A	0.9530	0.7160
B	0.9420	0.7060
C	0.9880	0.7270
D	0.9490	0.7040
E	0.9240	0.6890
F	0.9120	0.6940
G	0.4050	0.5050
I	0.9020	0.6870
J	0.9300	0.6950
K	0.8180	0.6410
L	0.8030	0.6480
M	0.8490	0.6630
a	0.8080	0.6200
b	0.6100	0.5250

