wwPDB EM Validation Summary Report (i)

Sep 11, 2026 – 05:49 am BST

PDB ID	:	9SE6 / pdb_00009se6
EMDB ID	:	EMD-54803
Title	:	Structure of Photosystem I from Chlamydomonas reinhardtii at 1.83 A resolution
Authors	:	Mahapatra, G.P.; Schuller, J.M.
Deposited on	:	2025-08-15
Resolution	:	1.83 Å(reported)
Based on initial model	:	7ZQC

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 (i) symbol.

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

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

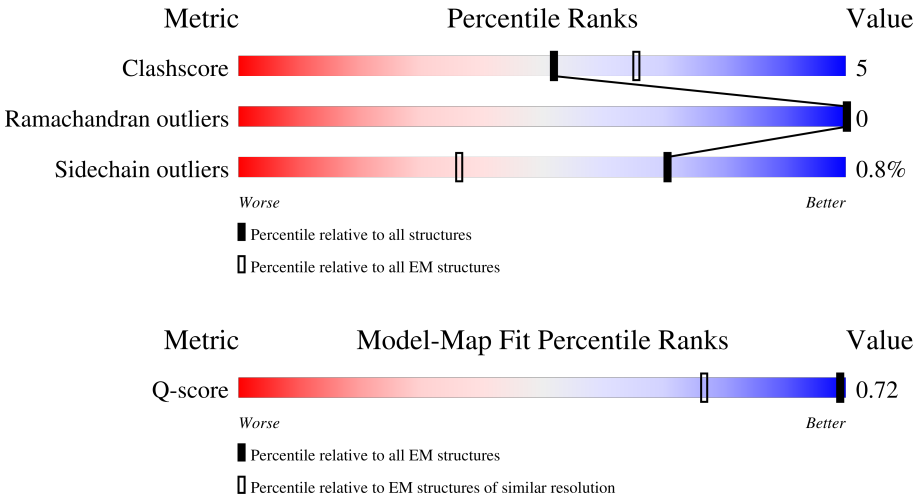
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 1.83 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	903 (1.33 - 2.33)

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	3	221	92% 8%
2	4	212	88% 12%
3	5	227	89% 10%
4	6	230	86% 14%

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Mol	Chain	Length	Quality of chain
5	7	213	90% 10%
6	8	217	87% 13%
7	A	742	94% 6%
8	B	733	93% 7%
9	C	80	94% 6%
10	D	144	94% 6%
11	E	64	95% 5%
12	I	37	5% 92% 8%
13	J	41	90% 10%
14	K	86	12% 90% 9%
15	1	194	5% 87% 13%
15	Z	194	90% 10%
16	F	165	92% 8%
17	G	95	60% 69% 26%
18	L	124	15% 92% 8%

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	NEX	5	323	X	-	-	-

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 48478 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 Light-harvesting chlorophyll-a/b protein of photosystem I, type III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3	221	1687	1100	273	306	8	0	0

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	212	1652	1083	269	295	5	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	5	227	1775	1154	297	316	8	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	230	1772	1167	293	306	6	0	0

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	7	213	1650	1072	274	298	6	0	0

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	8	217	1650	1073	280	293	4	0	0

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	742	Total	C	N	O	S	0	0
			5825	3808	994	1001	22		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	733	Total	C	N	O	S	0	0
			5824	3824	977	1005	18		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	80	Total	C	N	O	S	0	0
			601	369	103	117	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	144	Total	C	N	O	S	0	0
			1133	725	200	201	7		

- Molecule 11 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	E	64	Total	C	N	O	0	0
			506	322	89	95		

- Molecule 12 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	41	Total	C	N	O	S	0	0
			329	224	46	58	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ACE	-	acetylation	UNP P59777

- Molecule 14 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	86	Total	C	N	O	S	0	0
			583	370	100	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
15	1	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

- Molecule 16 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		

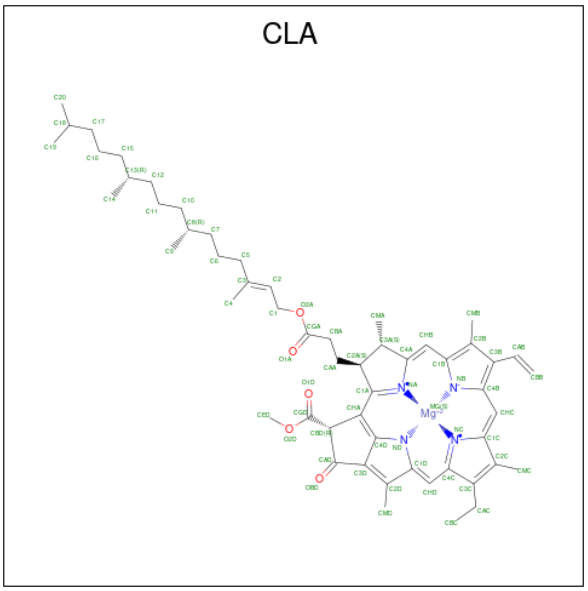
- Molecule 17 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	G	70	Total	C	N	O	0	0
			512	328	90	94		

- Molecule 18 is a protein called Chains: L.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	124	Total	C	N	O	S	0	0
			899	586	146	164	3		

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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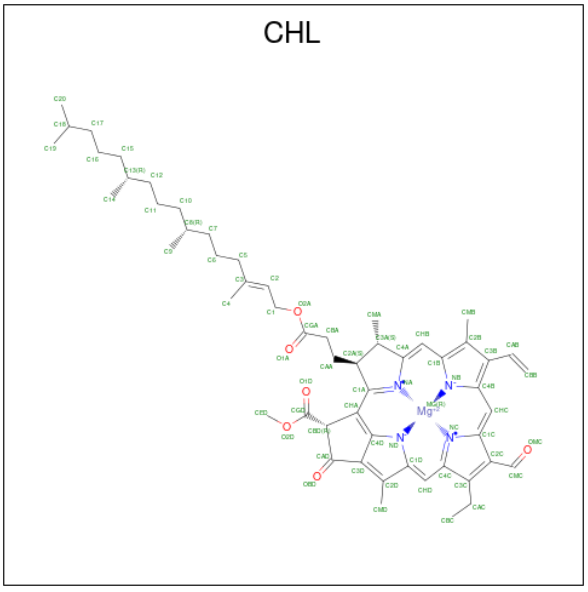
Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 20 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
20	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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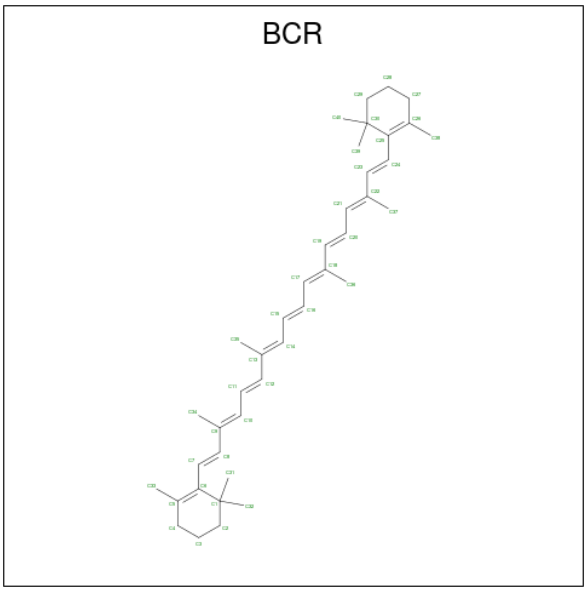
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	1	1	Total 46	C 35	Mg 1	N 4	O 6	0

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
21	3	1	Total 40	C 40	0
21	3	1	Total 40	C 40	0
21	3	1	Total 40	C 40	0
21	4	1	Total 40	C 40	0
21	5	1	Total 40	C 40	0
21	6	1	Total 40	C 40	0
21	7	1	Total 40	C 40	0
21	8	1	Total 40	C 40	0
21	A	1	Total 40	C 40	0

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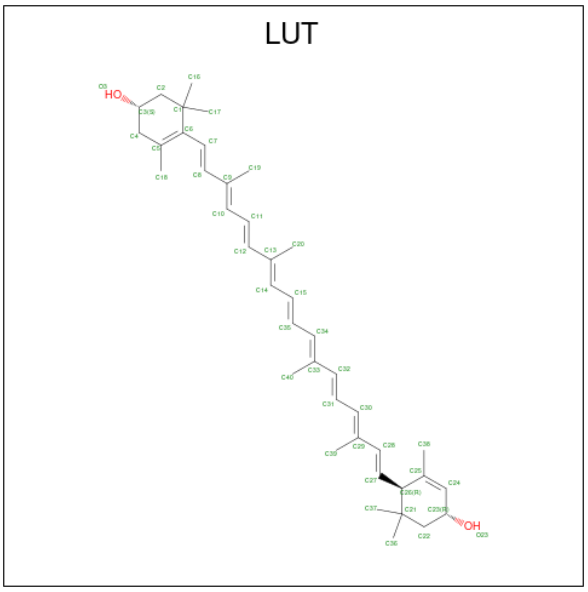
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0

- Molecule 22 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
22	3	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			20	19	1	
22	4	1	Total	C	O	0
			42	40	2	
22	5	1	Total	C	O	0
			42	40	2	
22	5	1	Total	C	O	0
			42	40	2	
22	6	1	Total	C	O	0
			42	40	2	
22	7	1	Total	C	O	0
			42	40	2	
22	8	1	Total	C	O	0
			42	40	2	
22	8	1	Total	C	O	0
			42	40	2	
22	J	1	Total	C	O	0
			42	40	2	
22	Z	1	Total	C	O	0
			42	40	2	
22	Z	1	Total	C	O	0
			26	25	1	
22	1	1	Total	C	O	0
			42	40	2	

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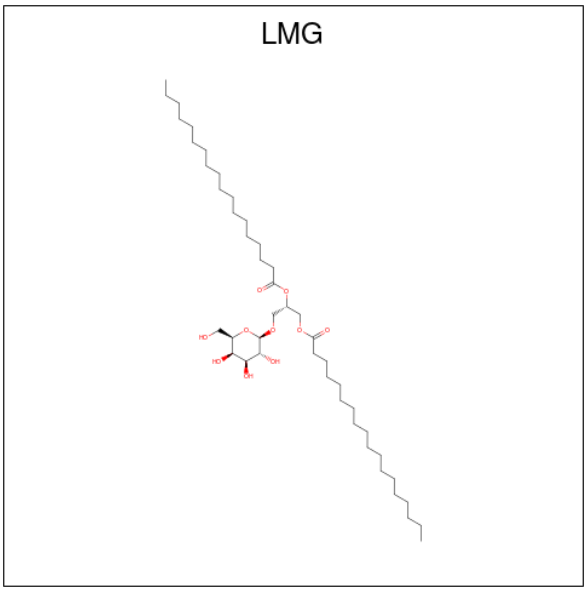
Mol	Chain	Residues	Atoms	AltConf
22	1	1	Total C O 42 40 2	0
22	F	1	Total C O 42 40 2	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
23	3	1	Total C O 37 27 10	0
23	4	1	Total C O 41 31 10	0
23	6	1	Total C O 27 22 5	0
23	6	1	Total C O 20 18 2	0
23	7	1	Total C O 32 22 10	0
23	8	1	Total C O 49 39 10	0
23	B	1	Total C O 43 33 10	0
23	J	1	Total C O 42 32 10	0
23	J	1	Total C O 35 25 10	0

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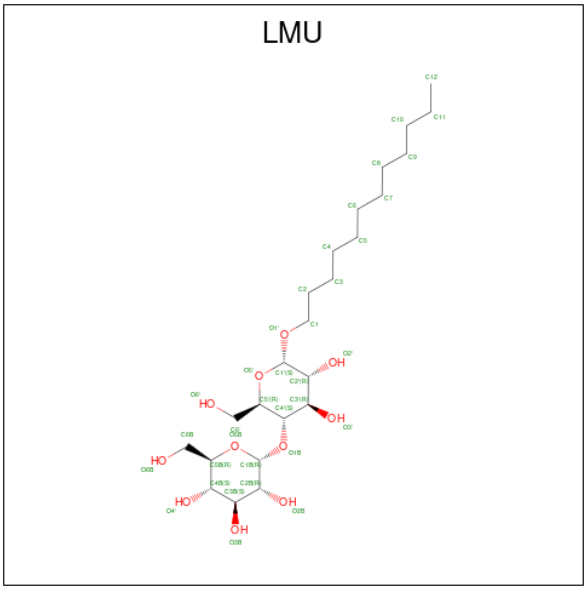
Mol	Chain	Residues	Atoms	AltConf
23	F	1	Total C O 32 22 10	0
23	G	1	Total C O 36 26 10	0
23	L	1	Total C O 40 30 10	0

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



Mol	Chain	Residues	Atoms	AltConf
24	3	1	Total C O 34 23 11	0
24	3	1	Total C O 24 18 6	0
24	3	1	Total C O 35 24 11	0
24	3	1	Total C O 24 18 6	0
24	4	1	Total C O 22 16 6	0
24	4	1	Total C O 20 14 6	0
24	4	1	Total C O 24 18 6	0
24	4	1	Total C O 22 16 6	0

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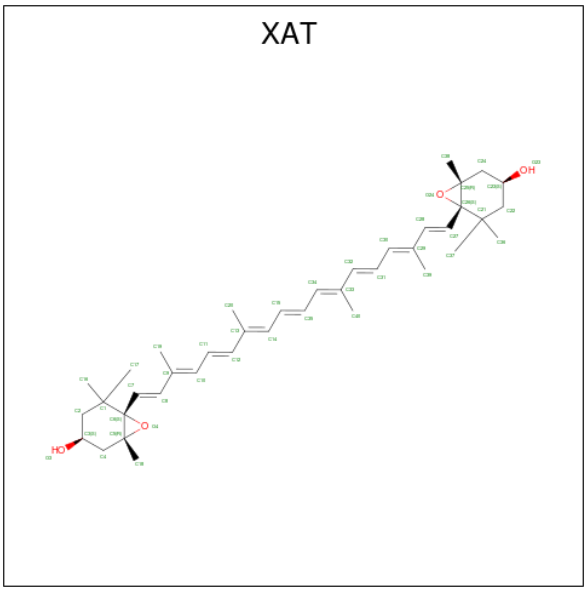
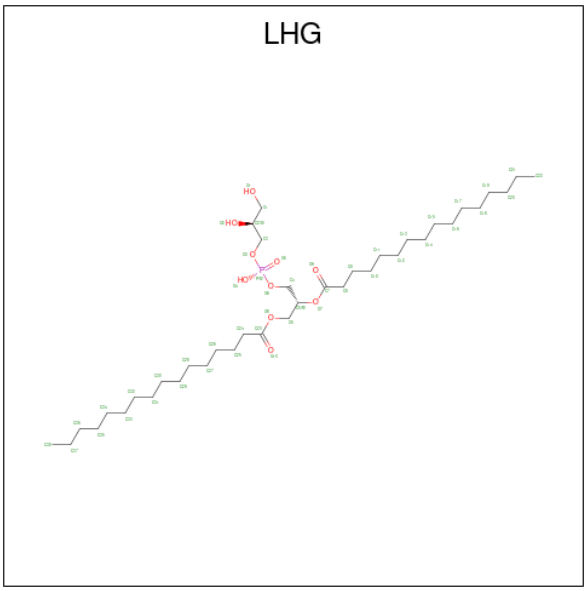
Mol	Chain	Residues	Atoms			AltConf
24	6	1	Total 24	C 18	O 6	0
24	6	1	Total 24	C 18	O 6	0
24	7	1	Total 21	C 15	O 6	0
24	7	1	Total 22	C 16	O 6	0
24	8	1	Total 24	C 18	O 6	0
24	A	1	Total 35	C 24	O 11	0
24	A	1	Total 20	C 14	O 6	0
24	A	1	Total 24	C 18	O 6	0
24	B	1	Total 35	C 24	O 11	0
24	K	1	Total 24	C 18	O 6	0
24	Z	1	Total 31	C 20	O 11	0
24	Z	1	Total 24	C 18	O 6	0
24	Z	1	Total 24	C 18	O 6	0
24	1	1	Total 35	C 24	O 11	0
24	1	1	Total 35	C 24	O 11	0
24	1	1	Total 19	C 13	O 6	0
24	1	1	Total 24	C 18	O 6	0
24	1	1	Total 22	C 16	O 6	0
24	F	1	Total 35	C 24	O 11	0

- Molecule 25 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).



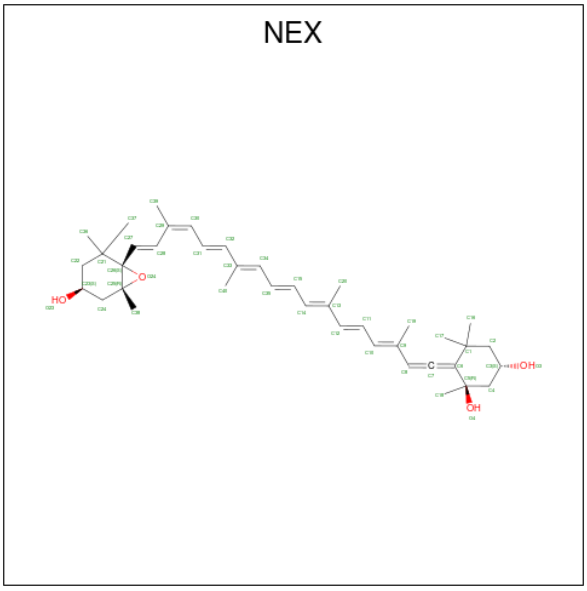
Mol	Chain	Residues	Atoms	AltConf
25	4	1	Total C O 44 40 4	0
25	5	1	Total C O 44 40 4	0
25	6	1	Total C O 44 40 4	0
25	7	1	Total C O 44 40 4	0
25	8	1	Total C O 44 40 4	0
25	Z	1	Total C O 44 40 4	0
25	1	1	Total C O 44 40 4	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



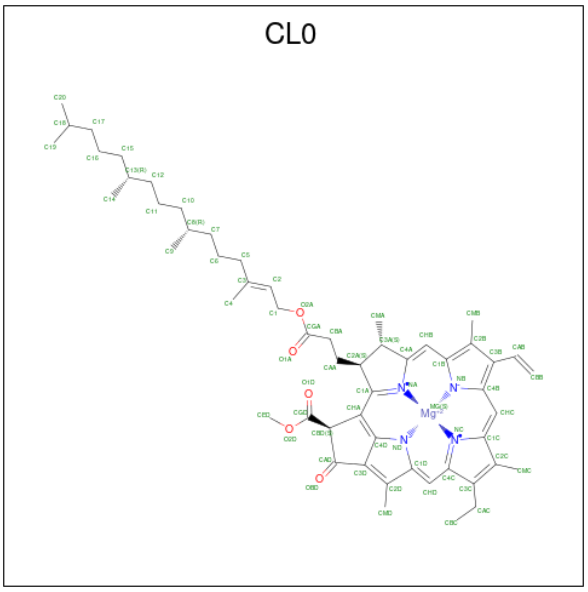
Mol	Chain	Residues	Atoms				AltConf
26	4	1	Total	C	O	P	0
			49	38	10	1	
26	4	1	Total	C	O	P	0
			38	27	10	1	
26	5	1	Total	C	O	P	0
			38	27	10	1	
26	5	1	Total	C	O	P	0
			37	26	10	1	
26	6	1	Total	C	O	P	0
			49	38	10	1	
26	6	1	Total	C	O	P	0
			36	25	10	1	
26	7	1	Total	C	O	P	0
			49	38	10	1	
26	8	1	Total	C	O	P	0
			44	33	10	1	
26	A	1	Total	C	O	P	0
			31	20	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	
26	A	1	Total	C	O	P	0
			38	27	10	1	
26	B	1	Total	C	O	P	0
			45	34	10	1	
26	Z	1	Total	C	O	P	0
			39	28	10	1	
26	1	1	Total	C	O	P	0
			44	33	10	1	

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



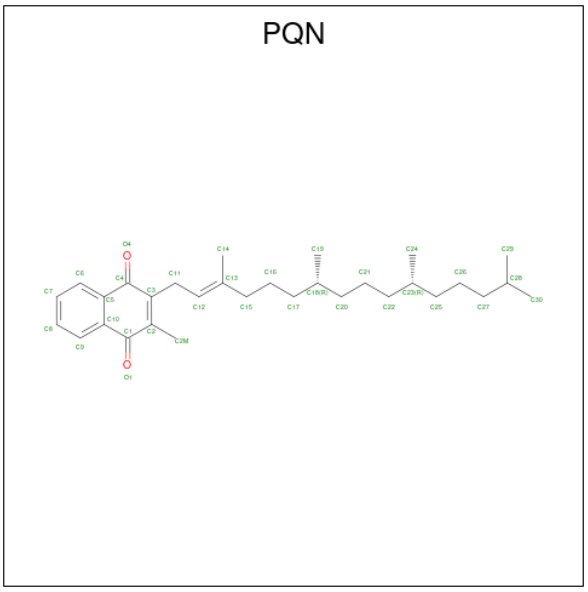
Mol	Chain	Residues	Atoms			AltConf
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	

- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



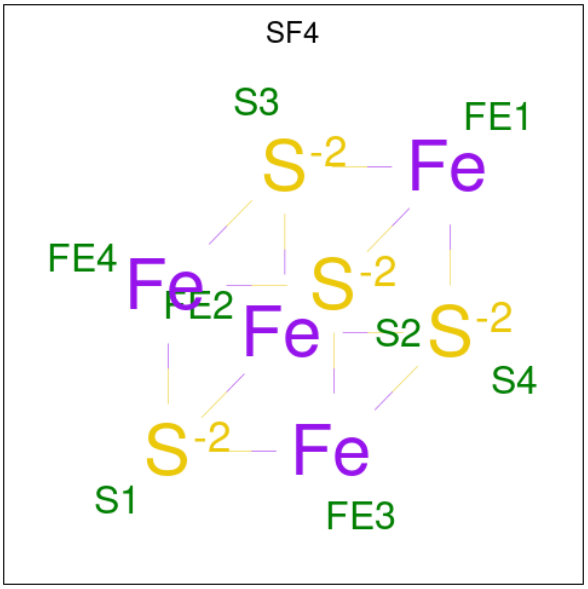
Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



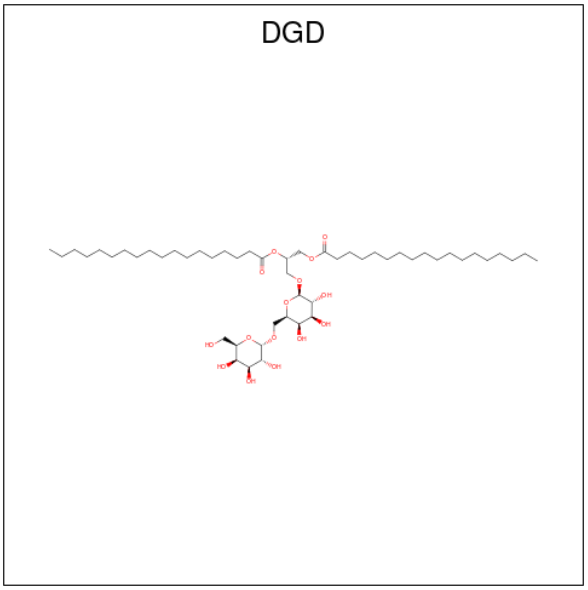
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	B	1	Total	C	O	0
			33	31	2	

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total 59	C 44	O 15	0

- Molecule 32 is water.

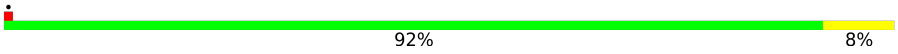
Mol	Chain	Residues	Atoms		AltConf
32	3	55	Total 55	O 55	0
32	4	17	Total 17	O 17	0
32	5	36	Total 36	O 36	0
32	6	21	Total 21	O 21	0
32	7	74	Total 74	O 74	0
32	8	61	Total 61	O 61	0
32	A	288	Total 288	O 288	0
32	B	237	Total 237	O 237	0
32	C	50	Total 50	O 50	0
32	D	49	Total 49	O 49	0
32	E	21	Total 21	O 21	0
32	I	2	Total 2	O 2	0
32	J	9	Total 9	O 9	0
32	K	3	Total 3	O 3	0
32	Z	11	Total 11	O 11	0
32	1	32	Total 32	O 32	0
32	F	47	Total 47	O 47	0
32	L	6	Total 6	O 6	0

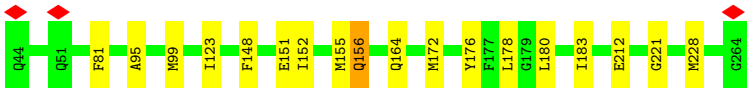
3 Residue-property plots (i)

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: Light-harvesting chlorophyll-a/b protein of photosystem I, type III

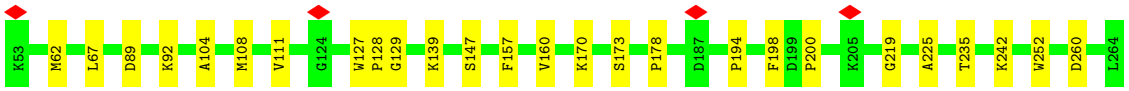
Chain 3:





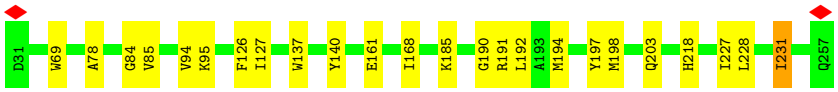
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



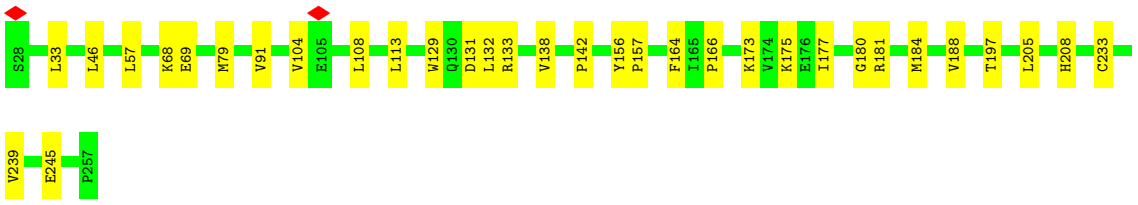
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

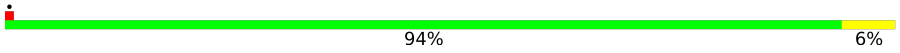
Chain 7:

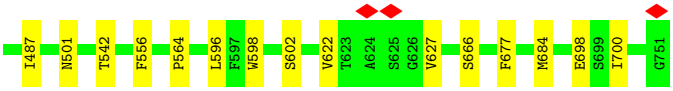
• Molecule 6: Chlorophyll a-b binding protein, chloroplastic

Chain 8:

• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

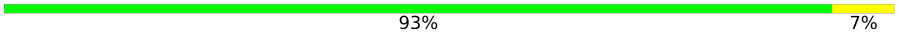
Chain A:

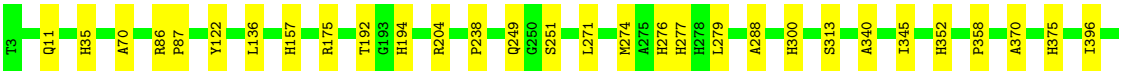


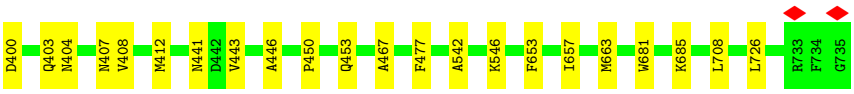


• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

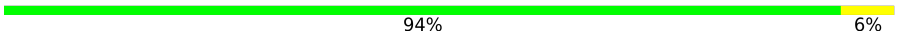


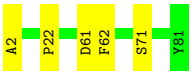




• Molecule 9: Photosystem I iron-sulfur center

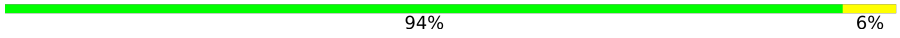
Chain C:





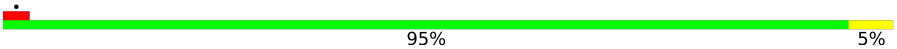
• Molecule 10: Photosystem I reaction center subunit II, chloroplastic

Chain D:



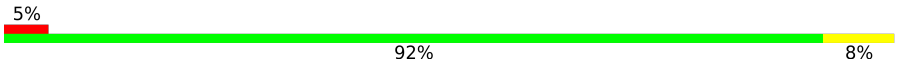
• Molecule 11: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



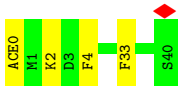
• Molecule 12: Photosystem I reaction center subunit VIII

Chain I:



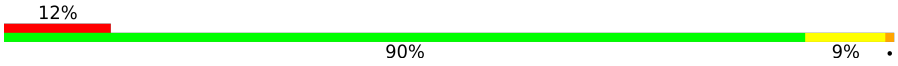
• Molecule 13: Photosystem I reaction center subunit IX

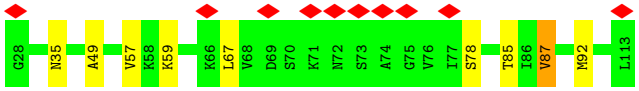
Chain J:



• Molecule 14: Photosystem I reaction center subunit psaK, chloroplastic

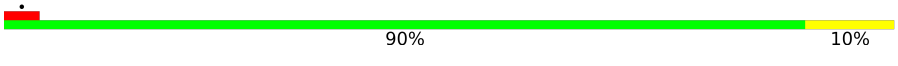
Chain K:

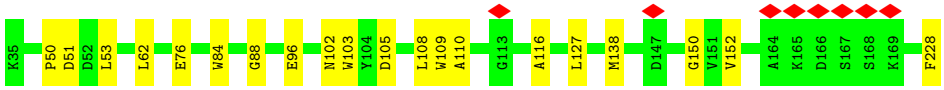




• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

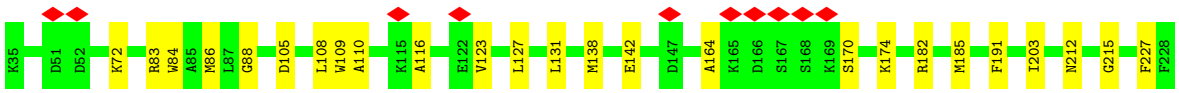
Chain Z:





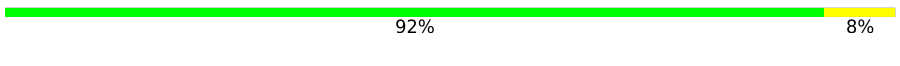
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



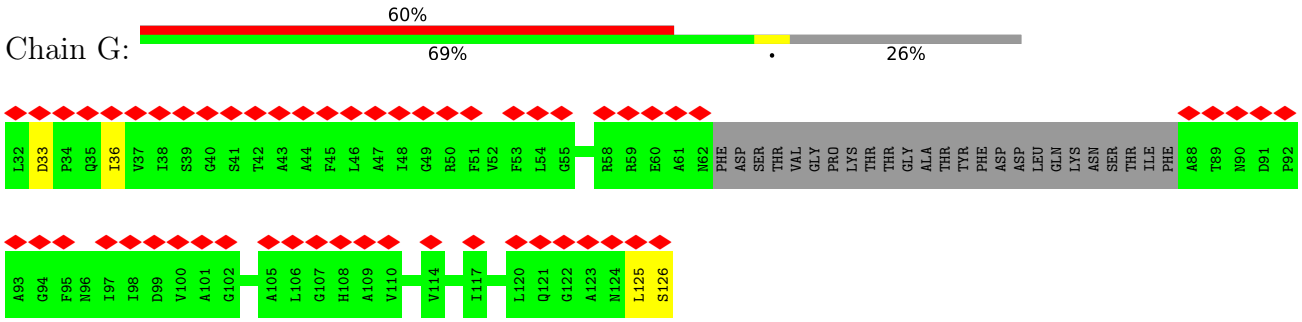
• Molecule 16: Photosystem I reaction center subunit III, chloroplastic

Chain F:



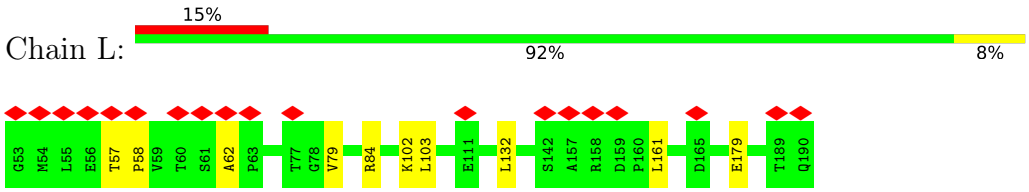
• Molecule 17: Photosystem I reaction center subunit V, chloroplastic

Chain G:



• Molecule 18: Chains: L

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246159	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	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, LMU, XAT, LUT, ACE, BCR, CLA, DGD, LHG, NEX, CHL, SF4, LMG, CL0

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	3	0.16	0/1735	0.39	1/2355 (0.0%)
2	4	0.13	0/1707	0.28	0/2325
3	5	0.14	0/1830	0.30	0/2492
4	6	0.13	0/1834	0.30	0/2505
5	7	0.14	0/1702	0.30	0/2310
6	8	0.14	0/1701	0.29	0/2315
7	A	0.15	0/6021	0.32	0/8208
8	B	0.15	0/6036	0.34	0/8240
9	C	0.12	0/611	0.34	0/826
10	D	0.12	0/1161	0.34	0/1567
11	E	0.11	0/516	0.29	0/700
12	I	0.13	0/293	0.29	0/406
13	J	0.17	0/338	0.33	0/464
14	K	0.12	0/588	0.26	0/795
15	1	0.15	0/1491	0.32	0/2028
15	Z	0.13	0/1491	0.27	0/2028
16	F	0.13	0/1292	0.31	0/1747
17	G	0.09	0/521	0.20	0/706
18	L	0.13	0/920	0.27	0/1257
All	All	0.14	0/31788	0.32	1/43274 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3	156	GLN	CA-CB-CG	7.14	128.39	114.10

There are no chirality outliers.

There are no planarity outliers.

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	3	1687	0	1646	16	0
2	4	1652	0	1613	19	0
3	5	1775	0	1746	19	0
4	6	1772	0	1770	29	0
5	7	1650	0	1589	16	0
6	8	1650	0	1629	19	0
7	A	5825	0	5675	40	0
8	B	5824	0	5577	41	0
9	C	601	0	581	3	0
10	D	1133	0	1150	6	0
11	E	506	0	504	2	0
12	I	281	0	292	2	0
13	J	329	0	328	3	0
14	K	583	0	620	7	0
15	1	1445	0	1396	20	0
15	Z	1445	0	1396	14	0
16	F	1266	0	1301	8	0
17	G	512	0	503	3	0
18	L	899	0	905	8	0
19	1	639	0	625	16	0
19	3	720	0	674	22	0
19	4	565	0	534	15	0
19	5	717	0	667	26	0
19	6	667	0	619	19	0
19	7	599	0	553	14	0
19	8	617	0	587	16	0
19	A	2653	0	2784	68	0
19	B	2528	0	2652	79	0
19	F	175	0	177	7	0
19	G	106	0	92	0	0
19	J	55	0	49	1	0
19	K	196	0	158	5	0
19	L	110	0	105	3	0
19	Z	637	0	616	10	0
20	1	92	0	62	2	0
20	3	66	0	70	0	0
20	4	287	0	270	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	5	206	0	167	5	0
20	6	338	0	307	15	0
20	7	224	0	202	3	0
20	8	198	0	210	5	0
20	Z	178	0	171	1	0
21	3	120	0	168	6	0
21	4	40	0	56	1	0
21	5	40	0	56	4	0
21	6	40	0	56	2	0
21	7	40	0	56	3	0
21	8	40	0	56	1	0
21	A	240	0	336	9	0
21	B	280	0	392	10	0
21	G	40	0	56	0	0
21	I	40	0	56	1	0
21	J	40	0	56	1	0
21	K	40	0	56	1	0
21	L	80	0	112	4	0
22	1	84	0	112	3	0
22	3	104	0	138	1	0
22	4	42	0	56	3	0
22	5	84	0	112	4	0
22	6	42	0	56	0	0
22	7	42	0	56	0	0
22	8	84	0	112	0	0
22	F	42	0	56	1	0
22	J	42	0	56	3	0
22	Z	68	0	89	1	0
23	3	37	0	44	4	0
23	4	41	0	55	0	0
23	6	47	0	68	3	0
23	7	32	0	34	0	0
23	8	49	0	71	1	0
23	B	43	0	56	1	0
23	F	32	0	34	1	0
23	G	36	0	42	0	0
23	J	77	0	97	4	0
23	L	40	0	50	2	0
24	1	135	0	177	5	0
24	3	117	0	157	3	0
24	4	88	0	115	2	0
24	6	48	0	70	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	7	43	0	54	1	0
24	8	24	0	35	1	0
24	A	79	0	105	1	0
24	B	35	0	46	2	0
24	F	35	0	46	2	0
24	K	24	0	35	0	0
24	Z	79	0	105	0	0
25	1	44	0	56	1	0
25	4	44	0	56	1	0
25	5	44	0	56	3	0
25	6	44	0	56	2	0
25	7	44	0	56	1	0
25	8	44	0	56	0	0
25	Z	44	0	56	2	0
26	1	44	0	58	0	0
26	4	87	0	123	5	0
26	5	75	0	90	2	0
26	6	85	0	116	7	0
26	7	49	0	74	1	0
26	8	44	0	61	3	0
26	A	118	0	155	3	0
26	B	45	0	63	6	0
26	Z	39	0	48	0	0
27	5	44	0	56	0	0
27	6	44	0	56	2	0
28	A	65	0	72	0	0
29	A	33	0	46	0	0
29	B	33	0	46	0	0
30	A	8	0	0	0	0
30	C	16	0	0	0	0
31	B	59	0	79	2	0
32	1	32	0	0	0	0
32	3	55	0	0	0	0
32	4	17	0	0	0	0
32	5	36	0	0	0	0
32	6	21	0	0	0	0
32	7	74	0	0	0	0
32	8	61	0	0	0	0
32	A	288	0	0	0	0
32	B	237	0	0	1	0
32	C	50	0	0	0	0
32	D	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	E	21	0	0	0	0
32	F	47	0	0	0	0
32	I	2	0	0	0	0
32	J	9	0	0	0	0
32	K	3	0	0	0	0
32	L	6	0	0	0	0
32	Z	11	0	0	0	0
All	All	48478	0	47958	518	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 5.

The worst 5 of 518 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:663:MET:HB2	19:B:804:CLA:C1C	2.07	0.83
20:5:308:CHL:HBB2	20:5:317:CHL:HHC	1.60	0.81
20:4:607:CHL:HBB2	20:4:615:CHL:HHC	1.65	0.77
21:5:320:BCR:HC42	26:6:318:LHG:H102	1.70	0.73
15:1:142:GLU:HG3	19:1:308:CLA:C4B	2.18	0.73

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	3	219/221 (99%)	216 (99%)	3 (1%)	0	100	100
2	4	210/212 (99%)	209 (100%)	1 (0%)	0	100	100
3	5	225/227 (99%)	222 (99%)	3 (1%)	0	100	100
4	6	228/230 (99%)	224 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	7	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
6	8	215/217 (99%)	214 (100%)	1 (0%)	0	100	100
7	A	740/742 (100%)	728 (98%)	12 (2%)	0	100	100
8	B	731/733 (100%)	714 (98%)	17 (2%)	0	100	100
9	C	78/80 (98%)	78 (100%)	0	0	100	100
10	D	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
11	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
12	I	35/37 (95%)	35 (100%)	0	0	100	100
13	J	39/41 (95%)	39 (100%)	0	0	100	100
14	K	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
15	1	192/194 (99%)	191 (100%)	1 (0%)	0	100	100
15	Z	192/194 (99%)	191 (100%)	1 (0%)	0	100	100
16	F	163/165 (99%)	161 (99%)	2 (1%)	0	100	100
17	G	66/95 (70%)	66 (100%)	0	0	100	100
18	L	120/124 (97%)	120 (100%)	0	0	100	100
All	All	3952/4019 (98%)	3897 (99%)	55 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	3	168/168 (100%)	168 (100%)	0	100	100
2	4	167/167 (100%)	165 (99%)	2 (1%)	63	51
3	5	184/184 (100%)	180 (98%)	4 (2%)	45	29
4	6	184/184 (100%)	182 (99%)	2 (1%)	65	54
5	7	164/164 (100%)	164 (100%)	0	100	100
6	8	163/163 (100%)	162 (99%)	1 (1%)	78	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	A	601/601 (100%)	600 (100%)	1 (0%)	87 84
8	B	596/596 (100%)	592 (99%)	4 (1%)	76 68
9	C	69/69 (100%)	69 (100%)	0	100 100
10	D	121/121 (100%)	117 (97%)	4 (3%)	33 15
11	E	55/55 (100%)	55 (100%)	0	100 100
12	I	31/31 (100%)	30 (97%)	1 (3%)	34 17
13	J	36/36 (100%)	36 (100%)	0	100 100
14	K	59/59 (100%)	58 (98%)	1 (2%)	53 37
15	1	137/137 (100%)	136 (99%)	1 (1%)	76 68
15	Z	137/137 (100%)	136 (99%)	1 (1%)	76 68
16	F	127/127 (100%)	125 (98%)	2 (2%)	55 39
17	G	49/71 (69%)	49 (100%)	0	100 100
18	L	90/90 (100%)	90 (100%)	0	100 100
All	All	3138/3160 (99%)	3114 (99%)	24 (1%)	70 65

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	D	57	THR
10	D	191	MET
10	D	175	ILE
12	I	102	GLU
4	6	233	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
7	A	387	GLN
15	1	212	ASN
8	B	84	HIS
15	1	128	ASN
8	B	77	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

328 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	SF4	C	101	9	0,12,12	-	-	-		
19	CLA	1	304	32	54,58,73	1.41	8 (14%)	65,95,113	1.42	8 (12%)
19	CLA	7	608	5	49,53,73	1.47	7 (14%)	59,89,113	1.49	5 (8%)
19	CLA	B	812	8	69,73,73	1.26	7 (10%)	83,113,113	1.24	7 (8%)
21	BCR	B	845	-	41,41,41	0.35	0	56,56,56	0.74	0
25	XAT	6	322	-	39,47,47	0.67	2 (5%)	54,74,74	0.82	0
19	CLA	7	603	5	56,60,73	1.39	7 (12%)	67,97,113	1.42	7 (10%)
19	CLA	B	826	32	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
19	CLA	A	838	7	61,65,73	1.34	7 (11%)	73,103,113	1.33	7 (9%)
24	LMU	3	322	-	35,35,36	0.48	0	46,46,47	0.64	0
19	CLA	F	303	32	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
19	CLA	A	805	7	69,73,73	1.25	8 (11%)	83,113,113	1.36	8 (9%)
25	XAT	Z	616	-	39,47,47	0.66	2 (5%)	54,74,74	0.82	0
19	CLA	8	309	6	69,73,73	1.24	6 (8%)	83,113,113	1.25	5 (6%)
19	CLA	6	305	4	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
20	CHL	5	317	3	47,51,74	1.11	5 (10%)	52,86,114	1.65	9 (17%)
21	BCR	G	204	-	41,41,41	0.34	0	56,56,56	0.59	0
19	CLA	B	820	32	64,68,73	1.33	7 (10%)	77,107,113	1.30	7 (9%)
19	CLA	A	839	7	55,59,73	1.41	7 (12%)	66,96,113	1.41	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	836	32	49,53,73	1.49	7 (14%)	59,89,113	1.47	7 (11%)
20	CHL	8	306	32	70,74,74	0.97	4 (5%)	80,114,114	1.33	10 (12%)
20	CHL	6	306	32	50,54,74	1.08	5 (10%)	56,90,114	1.31	8 (14%)
26	LHG	6	318	19	48,48,48	0.51	0	51,54,54	0.51	0
22	LUT	8	315	-	42,43,43	0.28	0	51,60,60	0.63	0
19	CLA	B	807	8	69,73,73	1.27	7 (10%)	83,113,113	1.27	7 (8%)
19	CLA	B	827	8	69,73,73	1.26	8 (11%)	83,113,113	1.28	8 (9%)
19	CLA	4	603	2	69,73,73	1.26	8 (11%)	83,113,113	1.26	4 (4%)
24	LMU	3	323	-	24,24,36	0.37	0	29,29,47	0.67	0
19	CLA	3	309	32	59,63,73	1.35	7 (11%)	71,101,113	1.39	6 (8%)
21	BCR	A	851	-	41,41,41	0.34	0	56,56,56	0.70	0
26	LHG	1	318	19	43,43,48	0.53	0	46,49,54	0.51	0
20	CHL	4	607	32	70,74,74	0.98	5 (7%)	80,114,114	1.17	8 (10%)
20	CHL	7	601	5	70,74,74	0.93	5 (7%)	80,114,114	1.18	10 (12%)
26	LHG	B	851	19	44,44,48	0.53	0	47,50,54	0.53	0
19	CLA	4	602	2	64,68,73	1.31	7 (10%)	77,107,113	1.30	7 (9%)
19	CLA	7	607	32	54,58,73	1.41	6 (11%)	65,95,113	1.47	8 (12%)
30	SF4	C	102	9	0,12,12	-	-	-		
19	CLA	8	308	6	49,53,73	1.47	7 (14%)	59,89,113	1.44	4 (6%)
19	CLA	B	816	8	69,73,73	1.25	8 (11%)	83,113,113	1.30	5 (6%)
22	LUT	5	318	-	42,43,43	0.30	0	51,60,60	0.74	0
19	CLA	G	202	17	64,68,73	1.31	7 (10%)	77,107,113	1.32	6 (7%)
19	CLA	5	302	3	69,73,73	1.26	7 (10%)	83,113,113	1.28	5 (6%)
19	CLA	8	314	6	49,53,73	1.49	7 (14%)	59,89,113	1.42	7 (11%)
20	CHL	4	606	32	47,51,74	1.11	5 (10%)	52,86,114	1.53	9 (17%)
20	CHL	7	605	32	50,54,74	1.10	5 (10%)	56,90,114	1.48	6 (10%)
25	XAT	4	617	-	39,47,47	0.65	2 (5%)	54,74,74	0.88	1 (1%)
19	CLA	B	803	8	69,73,73	1.25	7 (10%)	83,113,113	1.24	6 (7%)
24	LMU	4	625	-	22,22,36	0.39	0	27,27,47	0.60	0
20	CHL	1	305	32	50,54,74	1.03	4 (8%)	56,90,114	1.48	9 (16%)
30	SF4	A	854	7,8	0,12,12	-	-	-		
19	CLA	A	806	7,19	59,63,73	1.35	6 (10%)	71,101,113	1.35	5 (7%)
19	CLA	7	602	5	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
23	LMG	F	301	-	32,32,55	0.60	0	40,40,63	0.74	0
20	CHL	7	621	6	70,74,74	1.02	5 (7%)	80,114,114	1.29	7 (8%)
19	CLA	5	315	3	49,53,73	1.48	7 (14%)	59,89,113	1.42	6 (10%)
21	BCR	B	849	-	41,41,41	0.31	0	56,56,56	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	LHG	4	620	-	37,37,48	0.57	0	40,43,54	0.52	0
19	CLA	A	828	32	69,73,73	1.26	7 (10%)	83,113,113	1.31	6 (7%)
19	CLA	B	830	8	69,73,73	1.26	8 (11%)	83,113,113	1.23	8 (9%)
19	CLA	B	808	8	59,63,73	1.35	7 (11%)	71,101,113	1.35	6 (8%)
19	CLA	A	807	7	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	1	311	15	49,53,73	1.48	9 (18%)	59,89,113	1.44	4 (6%)
19	CLA	G	203	17	50,54,73	1.47	6 (12%)	60,90,113	1.42	4 (6%)
19	CLA	K	202	14	49,53,73	1.48	8 (16%)	59,89,113	1.53	6 (10%)
21	BCR	A	852	-	41,41,41	0.31	0	56,56,56	0.56	0
23	LMG	6	301	-	26,26,55	0.45	0	28,28,63	0.48	0
20	CHL	6	307	32	70,74,74	0.93	5 (7%)	80,114,114	1.16	9 (11%)
19	CLA	8	311	6	59,63,73	1.35	6 (10%)	71,101,113	1.35	4 (5%)
19	CLA	3	302	1	69,73,73	1.25	8 (11%)	83,113,113	1.34	6 (7%)
19	CLA	B	833	8	69,73,73	1.27	6 (8%)	83,113,113	1.31	7 (8%)
19	CLA	A	842	7	69,73,73	1.24	7 (10%)	83,113,113	1.28	7 (8%)
19	CLA	A	812	7	69,73,73	1.26	8 (11%)	83,113,113	1.25	7 (8%)
19	CLA	A	824	7	69,73,73	1.27	7 (10%)	83,113,113	1.29	7 (8%)
19	CLA	4	612	2	69,73,73	1.26	8 (11%)	83,113,113	1.41	7 (8%)
19	CLA	A	841	7	69,73,73	1.26	7 (10%)	83,113,113	1.31	8 (9%)
19	CLA	A	817	7	69,73,73	1.26	6 (8%)	83,113,113	1.28	6 (7%)
19	CLA	Z	612	32	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
19	CLA	6	320	32	59,63,73	1.35	7 (11%)	71,101,113	1.35	7 (9%)
24	LMU	4	622	-	22,22,36	0.41	0	27,27,47	0.70	0
26	LHG	A	847	-	48,48,48	0.51	0	51,54,54	0.47	0
19	CLA	1	302	15	64,68,73	1.31	7 (10%)	77,107,113	1.30	7 (9%)
21	BCR	I	201	-	41,41,41	0.35	0	56,56,56	0.76	0
19	CLA	A	809	7	54,58,73	1.41	8 (14%)	65,95,113	1.43	10 (15%)
19	CLA	A	823	32	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	LUT	6	319	-	42,43,43	0.30	0	51,60,60	0.68	0
24	LMU	A	855	-	36,36,36	0.45	0	47,47,47	1.08	2 (4%)
21	BCR	A	850	-	41,41,41	0.31	0	56,56,56	0.62	1 (1%)
19	CLA	B	819	8	69,73,73	1.26	9 (13%)	83,113,113	1.28	10 (12%)
19	CLA	6	316	4	49,53,73	1.49	8 (16%)	59,89,113	1.42	6 (10%)
19	CLA	F	304	16	69,73,73	1.25	8 (11%)	83,113,113	1.19	4 (4%)
19	CLA	4	610	26	64,68,73	1.31	6 (9%)	77,107,113	1.28	5 (6%)
19	CLA	B	821	8	60,64,73	1.35	7 (11%)	72,102,113	1.36	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	4	614	2	49,53,73	1.49	6 (12%)	59,89,113	1.44	4 (6%)
27	NEX	5	323	-	38,46,46	0.23	0	50,70,70	1.31	4 (8%)
19	CLA	B	822	8	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
23	LMG	4	621	-	41,41,55	0.54	0	49,49,63	0.69	0
20	CHL	6	308	32	55,59,74	1.04	5 (9%)	62,96,114	1.29	6 (9%)
19	CLA	B	811	8	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
26	LHG	A	801	-	30,30,48	0.61	0	33,36,54	0.60	0
25	XAT	7	616	-	39,47,47	0.66	2 (5%)	54,74,74	0.75	0
19	CLA	A	834	7	69,73,73	1.25	6 (8%)	83,113,113	1.31	5 (6%)
19	CLA	A	827	32	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
19	CLA	K	204	14	50,54,73	1.46	9 (18%)	60,90,113	1.43	5 (8%)
19	CLA	6	309	4	59,63,73	1.35	6 (10%)	71,101,113	1.33	7 (9%)
19	CLA	B	818	8	69,73,73	1.26	8 (11%)	83,113,113	1.26	7 (8%)
19	CLA	1	314	15	50,54,73	1.46	6 (12%)	60,90,113	1.44	5 (8%)
24	LMU	7	620	-	22,22,36	0.41	0	27,27,47	0.68	0
20	CHL	7	606	32	50,54,74	1.07	5 (10%)	56,90,114	1.50	9 (16%)
23	LMG	L	201	-	40,40,55	0.53	0	48,48,63	0.59	0
20	CHL	3	306	32	70,74,74	0.98	5 (7%)	80,114,114	1.19	7 (8%)
22	LUT	5	324	-	42,43,43	0.29	0	51,60,60	0.56	0
19	CLA	A	843	7	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)
19	CLA	7	609	5	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
21	BCR	B	847	-	41,41,41	0.31	0	56,56,56	0.58	0
19	CLA	3	307	1	65,69,73	1.28	8 (12%)	78,108,113	1.32	6 (7%)
24	LMU	A	857	-	24,24,36	0.37	0	29,29,47	0.61	0
29	PQN	A	845	-	34,34,34	0.34	0	42,45,45	0.52	1 (2%)
24	LMU	1	322	-	22,22,36	0.39	0	27,27,47	0.72	0
19	CLA	Z	610	26	64,68,73	1.29	7 (10%)	77,107,113	1.29	5 (6%)
24	LMU	6	328	-	24,24,36	0.38	0	29,29,47	0.64	0
19	CLA	5	316	3	69,73,73	1.25	9 (13%)	83,113,113	1.27	8 (9%)
22	LUT	7	615	-	42,43,43	0.28	0	51,60,60	0.61	0
19	CLA	B	837	8	64,68,73	1.32	9 (14%)	77,107,113	1.29	8 (10%)
20	CHL	6	317	4	47,51,74	1.11	5 (10%)	52,86,114	1.77	6 (11%)
19	CLA	L	204	32	49,53,73	1.50	6 (12%)	59,89,113	1.43	6 (10%)
19	CLA	8	312	6	69,73,73	1.27	8 (11%)	83,113,113	1.26	7 (8%)
19	CLA	8	303	6	69,73,73	1.26	8 (11%)	83,113,113	1.32	8 (9%)
19	CLA	A	816	7	59,63,73	1.37	7 (11%)	71,101,113	1.33	5 (7%)
19	CLA	1	312	32	69,73,73	1.25	6 (8%)	83,113,113	1.29	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LUT	F	305	-	42,43,43	0.28	0	51,60,60	0.78	1 (1%)
28	CL0	A	802	7	69,73,73	0.85	4 (5%)	83,113,113	1.11	5 (6%)
26	LHG	A	848	19	37,37,48	0.58	0	40,43,54	0.52	0
19	CLA	1	303	15	61,65,73	1.34	6 (9%)	73,103,113	1.37	7 (9%)
20	CHL	6	315	4	70,74,74	0.99	5 (7%)	80,114,114	1.25	6 (7%)
24	LMU	8	319	-	24,24,36	0.39	0	29,29,47	0.61	0
19	CLA	A	814	7	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
19	CLA	B	831	8	49,53,73	1.49	8 (16%)	59,89,113	1.48	5 (8%)
19	CLA	A	808	7	69,73,73	1.27	8 (11%)	83,113,113	1.28	6 (7%)
19	CLA	7	611	5	56,60,73	1.39	8 (14%)	67,97,113	1.39	5 (7%)
20	CHL	6	302	4	70,74,74	0.96	5 (7%)	80,114,114	1.29	8 (10%)
19	CLA	B	801	32	69,73,73	1.27	8 (11%)	83,113,113	1.21	6 (7%)
21	BCR	B	848	-	41,41,41	0.29	0	56,56,56	0.80	1 (1%)
19	CLA	8	307	32	54,58,73	1.42	7 (12%)	65,95,113	1.43	7 (10%)
26	LHG	5	321	19	36,36,48	0.58	0	39,42,54	0.54	0
19	CLA	8	313	6	61,65,73	1.33	8 (13%)	73,103,113	1.29	7 (9%)
19	CLA	A	819	7	69,73,73	1.24	7 (10%)	83,113,113	1.30	7 (8%)
20	CHL	4	601	2	70,74,74	0.97	5 (7%)	80,114,114	1.28	9 (11%)
19	CLA	B	825	32	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
24	LMU	7	619	-	21,21,36	0.40	0	26,26,47	0.71	0
19	CLA	1	310	26	65,69,73	1.28	7 (10%)	78,108,113	1.30	6 (7%)
26	LHG	6	325	-	35,35,48	0.56	0	38,41,54	0.73	1 (2%)
21	BCR	7	617	-	41,41,41	0.31	0	56,56,56	0.65	0
19	CLA	A	803	-	69,73,73	1.24	6 (8%)	83,113,113	1.22	8 (9%)
19	CLA	B	815	8	64,68,73	1.30	7 (10%)	77,107,113	1.31	6 (7%)
21	BCR	3	318	-	41,41,41	0.31	0	56,56,56	0.58	0
22	LUT	Z	615	-	42,43,43	0.30	0	51,60,60	0.70	0
19	CLA	5	304	3	54,58,73	1.41	8 (14%)	65,95,113	1.45	9 (13%)
19	CLA	A	837	7	69,73,73	1.26	8 (11%)	83,113,113	1.27	6 (7%)
24	LMU	B	853	-	36,36,36	0.46	0	47,47,47	0.66	0
21	BCR	L	205	-	41,41,41	0.35	0	56,56,56	0.56	0
19	CLA	A	810	7	69,73,73	1.25	7 (10%)	83,113,113	1.30	5 (6%)
21	BCR	3	319	-	41,41,41	0.30	0	56,56,56	0.61	0
21	BCR	B	844	-	41,41,41	0.36	0	56,56,56	0.89	4 (7%)
19	CLA	B	814	8	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
21	BCR	J	103	-	41,41,41	0.34	0	56,56,56	0.53	0
21	BCR	B	846	-	41,41,41	0.33	0	56,56,56	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	5	305	32	59,63,73	1.36	9 (15%)	71,101,113	1.35	5 (7%)
19	CLA	A	846	26	49,53,73	1.49	7 (14%)	59,89,113	1.45	6 (10%)
19	CLA	3	305	1	55,59,73	1.41	7 (12%)	66,96,113	1.38	7 (10%)
19	CLA	6	303	4	69,73,73	1.26	6 (8%)	83,113,113	1.28	6 (7%)
19	CLA	Z	614	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	8 (10%)
19	CLA	Z	607	32	54,58,73	1.42	9 (16%)	65,95,113	1.41	7 (10%)
19	CLA	B	817	8	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
19	CLA	7	612	5	69,73,73	1.26	7 (10%)	83,113,113	1.28	7 (8%)
24	LMU	3	325	-	24,24,36	0.37	0	29,29,47	0.65	0
22	LUT	3	320	-	19,20,43	0.45	0	20,28,60	0.49	0
19	CLA	4	609	2	64,68,73	1.29	7 (10%)	77,107,113	1.30	6 (7%)
19	CLA	5	311	26	59,63,73	1.35	6 (10%)	71,101,113	1.36	6 (8%)
19	CLA	A	836	7	69,73,73	1.25	8 (11%)	83,113,113	1.29	8 (9%)
19	CLA	Z	603	15	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
24	LMU	F	306	-	36,36,36	0.46	0	47,47,47	0.77	1 (2%)
19	CLA	Z	602	15	64,68,73	1.30	7 (10%)	77,107,113	1.33	6 (7%)
24	LMU	Z	619	-	32,32,36	0.47	0	43,43,47	0.85	1 (2%)
19	CLA	3	314	1	49,53,73	1.48	8 (16%)	59,89,113	1.40	6 (10%)
23	LMG	G	201	-	36,36,55	0.56	0	44,44,63	0.68	0
19	CLA	6	327	32	57,61,73	1.38	8 (14%)	68,98,113	1.37	6 (8%)
24	LMU	4	624	-	24,24,36	0.39	0	29,29,47	0.64	0
19	CLA	B	805	8	49,53,73	1.49	6 (12%)	59,89,113	1.45	7 (11%)
25	XAT	8	316	-	39,47,47	0.66	2 (5%)	54,74,74	0.72	0
19	CLA	B	824	8	69,73,73	1.25	8 (11%)	83,113,113	1.31	9 (10%)
19	CLA	5	313	3	60,64,73	1.33	8 (13%)	72,102,113	1.39	6 (8%)
19	CLA	5	312	3	49,53,73	1.48	7 (14%)	59,89,113	1.48	6 (10%)
20	CHL	4	605	32	70,74,74	0.90	5 (7%)	80,114,114	1.19	9 (11%)
19	CLA	8	310	26	49,53,73	1.48	7 (14%)	59,89,113	1.41	6 (10%)
20	CHL	Z	605	32	50,54,74	1.05	4 (8%)	56,90,114	1.55	10 (17%)
24	LMU	Z	620	-	24,24,36	0.40	0	29,29,47	0.60	0
20	CHL	Z	606	32	70,74,74	0.91	5 (7%)	80,114,114	1.35	7 (8%)
24	LMU	K	201	-	24,24,36	0.39	0	29,29,47	0.71	0
29	PQN	B	843	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)
19	CLA	A	833	7	59,63,73	1.36	7 (11%)	71,101,113	1.37	4 (5%)
19	CLA	B	828	8	69,73,73	1.25	7 (10%)	83,113,113	1.23	5 (6%)
23	LMG	8	321	-	49,49,55	0.52	0	57,57,63	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	3	313	32	64,68,73	1.29	7 (10%)	77,107,113	1.46	9 (11%)
22	LUT	4	616	-	42,43,43	0.29	0	51,60,60	0.70	0
19	CLA	J	102	13	59,63,73	1.35	8 (13%)	71,101,113	1.37	7 (9%)
19	CLA	3	303	32	69,73,73	1.25	8 (11%)	83,113,113	1.30	8 (9%)
19	CLA	B	835	8	64,68,73	1.30	8 (12%)	77,107,113	1.34	6 (7%)
24	LMU	3	324	-	36,36,36	0.45	0	47,47,47	1.06	4 (8%)
19	CLA	A	844	32	69,73,73	1.27	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	L	203	18	69,73,73	1.25	8 (11%)	83,113,113	1.32	9 (10%)
25	XAT	1	316	-	39,47,47	0.66	2 (5%)	54,74,74	0.83	0
22	LUT	3	317	-	42,43,43	0.26	0	51,60,60	0.60	0
19	CLA	8	304	32	64,68,73	1.30	7 (10%)	77,107,113	1.30	5 (6%)
19	CLA	A	830	7	69,73,73	1.26	7 (10%)	83,113,113	1.26	6 (7%)
19	CLA	B	813	8	69,73,73	1.26	7 (10%)	83,113,113	1.28	9 (10%)
20	CHL	5	306	32	50,54,74	1.13	5 (10%)	56,90,114	1.49	7 (12%)
19	CLA	A	831	7	69,73,73	1.27	7 (10%)	83,113,113	1.25	6 (7%)
21	BCR	8	317	-	41,41,41	0.31	0	56,56,56	0.53	0
19	CLA	Z	613	15	54,58,73	1.42	7 (12%)	65,95,113	1.42	6 (9%)
23	LMG	J	104	-	42,42,55	0.53	0	50,50,63	0.64	0
22	LUT	1	317	-	42,43,43	0.28	0	51,60,60	0.72	0
31	DGD	B	850	-	60,60,67	0.57	0	74,74,81	0.81	2 (2%)
19	CLA	3	308	1	69,73,73	1.24	7 (10%)	83,113,113	1.27	8 (9%)
21	BCR	6	321	-	41,41,41	0.31	0	56,56,56	0.56	0
19	CLA	Z	611	15	49,53,73	1.50	7 (14%)	59,89,113	1.41	5 (8%)
21	BCR	A	858	-	41,41,41	0.33	0	56,56,56	0.83	2 (3%)
26	LHG	5	301	-	37,37,48	0.57	0	40,43,54	0.56	0
19	CLA	B	823	8	63,67,73	1.32	9 (14%)	75,105,113	1.32	6 (8%)
19	CLA	5	309	3	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
19	CLA	B	840	32	69,73,73	1.26	8 (11%)	83,113,113	1.29	8 (9%)
26	LHG	Z	618	19	38,38,48	0.57	0	41,44,54	0.53	0
19	CLA	3	312	1	49,53,73	1.49	7 (14%)	59,89,113	1.41	5 (8%)
19	CLA	Z	604	32	61,65,73	1.33	8 (13%)	73,103,113	1.35	8 (10%)
19	CLA	A	811	7	69,73,73	1.25	7 (10%)	83,113,113	1.32	8 (9%)
20	CHL	4	615	2	50,54,74	1.05	4 (8%)	56,90,114	1.59	9 (16%)
19	CLA	B	832	8	59,63,73	1.35	8 (13%)	71,101,113	1.36	9 (12%)
19	CLA	B	842	26	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	Z	608	15	69,73,73	1.26	7 (10%)	83,113,113	1.24	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	5	314	3	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
19	CLA	3	310	1	50,54,73	1.46	8 (16%)	60,90,113	1.40	6 (10%)
22	LUT	Z	617	-	26,26,43	0.42	0	34,35,60	0.61	0
19	CLA	3	301	1	64,68,73	1.30	7 (10%)	77,107,113	1.34	9 (11%)
21	BCR	A	849	-	41,41,41	0.33	0	56,56,56	0.53	0
26	LHG	4	619	19	48,48,48	0.52	0	51,54,54	0.49	0
23	LMG	6	326	-	19,19,55	0.34	0	19,19,63	0.46	0
19	CLA	B	804	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	7 (8%)
19	CLA	4	604	32	54,58,73	1.41	8 (14%)	65,95,113	1.42	7 (10%)
19	CLA	B	829	8	69,73,73	1.24	7 (10%)	83,113,113	1.23	6 (7%)
19	CLA	K	205	14	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
20	CHL	5	307	32	70,74,74	0.97	5 (7%)	80,114,114	1.19	7 (8%)
19	CLA	B	841	8	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
19	CLA	6	304	4	55,59,73	1.41	6 (10%)	66,96,113	1.41	8 (12%)
21	BCR	3	315	-	41,41,41	0.31	0	56,56,56	0.55	0
19	CLA	B	806	8	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
19	CLA	B	838	8	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	LUT	1	315	-	42,43,43	0.30	0	51,60,60	0.68	0
20	CHL	1	306	32	50,54,74	1.08	4 (8%)	56,90,114	1.53	11 (19%)
19	CLA	A	826	7	59,63,73	1.37	7 (11%)	71,101,113	1.34	7 (9%)
23	LMG	7	622	-	32,32,55	0.57	0	40,40,63	0.73	0
21	BCR	B	802	-	41,41,41	0.36	0	56,56,56	1.07	4 (7%)
19	CLA	7	614	5	50,54,73	1.46	8 (16%)	60,90,113	1.41	4 (6%)
19	CLA	A	821	7	69,73,73	1.26	9 (13%)	83,113,113	1.27	10 (12%)
19	CLA	4	613	2	59,63,73	1.36	8 (13%)	71,101,113	1.34	6 (8%)
19	CLA	1	308	15	69,73,73	1.25	6 (8%)	83,113,113	1.27	4 (4%)
19	CLA	B	809	8	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
26	LHG	8	318	19	43,43,48	0.54	0	46,49,54	0.54	0
19	CLA	6	312	4	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
22	LUT	3	316	-	42,43,43	0.26	0	51,60,60	0.58	0
19	CLA	6	314	4	54,58,73	1.42	8 (14%)	65,95,113	1.39	7 (10%)
19	CLA	1	309	15	69,73,73	1.25	6 (8%)	83,113,113	1.27	7 (8%)
21	BCR	A	853	-	41,41,41	0.34	0	56,56,56	0.63	0
19	CLA	B	839	8	54,58,73	1.41	7 (12%)	65,95,113	1.46	8 (12%)
19	CLA	5	319	32	50,54,73	1.47	6 (12%)	60,90,113	1.50	5 (8%)
24	LMU	6	324	-	24,24,36	0.39	0	29,29,47	0.61	0
19	CLA	7	610	26	69,73,73	1.25	7 (10%)	83,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CHL	Z	601	15	70,74,74	0.96	5 (7%)	80,114,114	1.38	10 (12%)
19	CLA	A	813	7,19	69,73,73	1.23	7 (10%)	83,113,113	1.22	5 (6%)
19	CLA	A	815	7	69,73,73	1.27	7 (10%)	83,113,113	1.29	7 (8%)
19	CLA	4	608	2	64,68,73	1.29	6 (9%)	77,107,113	1.35	6 (7%)
19	CLA	B	834	8	62,66,73	1.31	7 (11%)	74,104,113	1.40	8 (10%)
19	CLA	1	307	32	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
19	CLA	A	822	7	59,63,73	1.34	7 (11%)	71,101,113	1.34	7 (9%)
19	CLA	A	825	7	49,53,73	1.49	8 (16%)	59,89,113	1.41	5 (8%)
24	LMU	4	623	-	20,20,36	0.40	0	25,25,47	0.78	0
19	CLA	5	310	3	64,68,73	1.29	7 (10%)	77,107,113	1.32	8 (10%)
19	CLA	K	203	32	64,68,73	1.31	7 (10%)	77,107,113	1.38	11 (14%)
19	CLA	A	835	7	69,73,73	1.27	9 (13%)	83,113,113	1.28	6 (7%)
23	LMG	J	105	-	35,35,55	0.60	0	43,43,63	0.72	0
19	CLA	A	832	7	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
21	BCR	L	202	-	41,41,41	0.34	0	56,56,56	0.53	0
21	BCR	5	320	-	41,41,41	0.29	0	56,56,56	0.60	0
24	LMU	1	321	-	24,24,36	0.38	0	29,29,47	0.63	0
19	CLA	1	313	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	9 (11%)
24	LMU	1	301	-	36,36,36	0.44	0	47,47,47	1.07	1 (2%)
19	CLA	3	304	32	46,50,73	1.51	7 (15%)	55,85,113	1.43	5 (9%)
22	LUT	8	301	-	42,43,43	0.30	0	51,60,60	0.62	1 (1%)
19	CLA	A	818	32	59,63,73	1.36	8 (13%)	71,101,113	1.38	6 (8%)
19	CLA	B	810	8	69,73,73	1.27	8 (11%)	83,113,113	1.30	5 (6%)
24	LMU	1	319	-	36,36,36	0.45	0	47,47,47	0.74	1 (2%)
26	LHG	7	618	19	48,48,48	0.51	0	51,54,54	0.49	0
25	XAT	5	322	-	39,47,47	0.66	2 (5%)	54,74,74	0.81	0
19	CLA	4	611	2	49,53,73	1.49	7 (14%)	59,89,113	1.46	5 (8%)
24	LMU	Z	621	-	24,24,36	0.39	0	29,29,47	0.60	0
19	CLA	6	313	32	69,73,73	1.26	8 (11%)	83,113,113	1.26	8 (9%)
19	CLA	A	840	7	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	Z	609	15	64,68,73	1.30	7 (10%)	77,107,113	1.31	8 (10%)
27	NEX	6	323	-	38,46,46	0.21	0	50,70,70	1.29	4 (8%)
19	CLA	F	302	32	69,73,73	1.27	7 (10%)	83,113,113	1.26	5 (6%)
21	BCR	4	618	-	41,41,41	0.31	0	56,56,56	0.58	0
19	CLA	3	311	1	64,68,73	1.31	6 (9%)	77,107,113	1.29	7 (9%)
23	LMG	3	321	-	37,37,55	0.57	0	45,45,63	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	6	310	4	64,68,73	1.31	8 (12%)	77,107,113	1.28	7 (9%)
19	CLA	A	804	32	69,73,73	1.26	8 (11%)	83,113,113	1.22	5 (6%)
19	CLA	A	829	7	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	LUT	J	101	-	42,43,43	0.30	0	51,60,60	0.77	1 (1%)
19	CLA	8	302	6	69,73,73	1.25	6 (8%)	83,113,113	1.30	8 (9%)
19	CLA	7	613	5	47,51,73	1.49	8 (17%)	56,86,113	1.45	6 (10%)
24	LMU	A	856	-	20,20,36	0.41	0	25,25,47	0.70	0
23	LMG	B	852	-	43,43,55	0.53	0	51,51,63	0.68	0
19	CLA	5	303	3	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
20	CHL	8	320	15	70,74,74	1.03	5 (7%)	80,114,114	1.27	7 (8%)
19	CLA	6	311	26	62,66,73	1.33	7 (11%)	74,104,113	1.29	5 (6%)
20	CHL	8	305	32	70,74,74	0.90	5 (7%)	80,114,114	1.24	7 (8%)
19	CLA	A	820	7	64,68,73	1.32	7 (10%)	77,107,113	1.27	6 (7%)
20	CHL	5	308	32	55,59,74	1.13	5 (9%)	62,96,114	1.45	8 (12%)
24	LMU	1	320	-	19,19,36	0.42	0	24,24,47	0.65	0
19	CLA	7	604	32	55,59,73	1.40	8 (14%)	66,96,113	1.40	5 (7%)
21	BCR	K	206	-	41,41,41	0.31	0	56,56,56	0.49	0

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
30	SF4	C	101	9	-	-	0/6/5/5
19	CLA	1	304	32	-	4/21/97/115	-
19	CLA	7	608	5	-	2/15/91/115	-
19	CLA	B	812	8	-	14/39/115/115	-
21	BCR	B	845	-	-	3/29/63/63	0/2/2/2
25	XAT	6	322	-	-	1/31/93/93	0/4/4/4
19	CLA	7	603	5	-	3/24/100/115	-
19	CLA	B	826	32	-	12/39/115/115	-
19	CLA	A	838	7	-	8/30/106/115	-
24	LMU	3	322	-	-	2/20/60/61	0/2/2/2
19	CLA	F	303	32	-	2/15/91/115	-
19	CLA	A	805	7	-	6/39/115/115	-
25	XAT	Z	616	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	8	309	6	-	6/39/115/115	-
19	CLA	6	305	4	-	17/39/115/115	-
20	CHL	5	317	3	-	3/14/90/117	-
21	BCR	G	204	-	-	0/29/63/63	0/2/2/2
19	CLA	B	820	32	-	10/33/109/115	-
19	CLA	A	839	7	-	2/23/99/115	-
19	CLA	B	836	32	-	5/15/91/115	-
20	CHL	8	306	32	-	12/41/117/117	-
20	CHL	6	306	32	-	6/17/93/117	-
26	LHG	6	318	19	-	15/53/53/53	-
22	LUT	8	315	-	-	2/29/67/67	0/2/2/2
19	CLA	B	807	8	-	2/39/115/115	-
19	CLA	B	827	8	-	4/39/115/115	-
19	CLA	4	603	2	-	12/39/115/115	-
24	LMU	3	323	-	-	5/15/35/61	0/1/1/2
19	CLA	3	309	32	-	5/27/103/115	-
21	BCR	A	851	-	-	4/29/63/63	0/2/2/2
26	LHG	1	318	19	-	11/48/48/53	-
20	CHL	4	607	32	-	21/41/117/117	-
20	CHL	7	601	5	-	13/41/117/117	-
26	LHG	B	851	19	-	13/49/49/53	-
19	CLA	4	602	2	-	3/33/109/115	-
19	CLA	7	607	32	-	1/21/97/115	-
30	SF4	C	102	9	-	-	0/6/5/5
19	CLA	8	308	6	-	4/15/91/115	-
19	CLA	B	816	8	-	13/39/115/115	-
22	LUT	5	318	-	-	4/29/67/67	0/2/2/2
19	CLA	G	202	17	-	9/33/109/115	-
19	CLA	5	302	3	-	8/39/115/115	-
19	CLA	8	314	6	-	1/15/91/115	-
20	CHL	4	606	32	-	4/14/90/117	-
20	CHL	7	605	32	-	0/17/93/117	-
25	XAT	4	617	-	-	0/31/93/93	0/4/4/4
19	CLA	B	803	8	-	8/39/115/115	-
24	LMU	4	625	-	-	0/13/33/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	1	305	32	-	2/17/93/117	-
30	SF4	A	854	7,8	-	-	0/6/5/5
19	CLA	A	806	7,19	-	2/27/103/115	-
19	CLA	7	602	5	-	1/39/115/115	-
23	LMG	F	301	-	-	11/27/47/70	0/1/1/1
20	CHL	7	621	6	-	12/41/117/117	-
19	CLA	5	315	3	-	4/15/91/115	-
21	BCR	B	849	-	-	2/29/63/63	0/2/2/2
26	LHG	4	620	-	-	12/42/42/53	-
19	CLA	A	828	32	-	12/39/115/115	-
19	CLA	B	830	8	-	11/39/115/115	-
19	CLA	B	808	8	-	5/27/103/115	-
19	CLA	A	807	7	-	18/39/115/115	-
19	CLA	1	311	15	-	5/15/91/115	-
19	CLA	G	203	17	-	2/17/93/115	-
19	CLA	K	202	14	-	4/15/91/115	-
21	BCR	A	852	-	-	5/29/63/63	0/2/2/2
23	LMG	6	301	-	-	7/28/28/70	-
20	CHL	6	307	32	-	14/41/117/117	-
19	CLA	8	311	6	-	6/27/103/115	-
19	CLA	3	302	1	-	12/39/115/115	-
19	CLA	B	833	8	-	7/39/115/115	-
19	CLA	A	842	7	-	9/39/115/115	-
19	CLA	A	812	7	-	12/39/115/115	-
19	CLA	A	824	7	-	22/39/115/115	-
19	CLA	4	612	2	-	14/39/115/115	-
19	CLA	A	841	7	-	5/39/115/115	-
19	CLA	A	817	7	-	7/39/115/115	-
19	CLA	Z	612	32	-	3/39/115/115	-
19	CLA	6	320	32	-	6/27/103/115	-
24	LMU	4	622	-	-	6/13/33/61	0/1/1/2
26	LHG	A	847	-	-	14/53/53/53	-
19	CLA	1	302	15	-	6/33/109/115	-
21	BCR	I	201	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	809	7	-	5/21/97/115	-
19	CLA	A	823	32	-	4/39/115/115	-
22	LUT	6	319	-	-	4/29/67/67	0/2/2/2
24	LMU	A	855	-	-	6/21/61/61	0/2/2/2
21	BCR	A	850	-	-	0/29/63/63	0/2/2/2
19	CLA	B	819	8	-	5/39/115/115	-
19	CLA	6	316	4	-	4/15/91/115	-
19	CLA	F	304	16	-	20/39/115/115	-
19	CLA	4	610	26	-	5/33/109/115	-
19	CLA	B	821	8	-	6/29/105/115	-
19	CLA	4	614	2	-	3/15/91/115	-
27	NEX	5	323	-	1/1/12/25	2/27/83/83	0/3/3/3
19	CLA	B	822	8	-	17/39/115/115	-
23	LMG	4	621	-	-	16/36/56/70	0/1/1/1
20	CHL	6	308	32	-	5/23/99/117	-
19	CLA	B	811	8	-	12/39/115/115	-
26	LHG	A	801	-	-	14/35/35/53	-
25	XAT	7	616	-	-	0/31/93/93	0/4/4/4
19	CLA	A	834	7	-	7/39/115/115	-
19	CLA	A	827	32	-	7/39/115/115	-
19	CLA	K	204	14	-	1/17/93/115	-
19	CLA	6	309	4	-	5/27/103/115	-
19	CLA	B	818	8	-	7/39/115/115	-
19	CLA	1	314	15	-	4/17/93/115	-
24	LMU	7	620	-	-	7/13/33/61	0/1/1/2
20	CHL	7	606	32	-	3/17/93/117	-
23	LMG	L	201	-	-	15/35/55/70	0/1/1/1
20	CHL	3	306	32	-	7/41/117/117	-
22	LUT	5	324	-	-	10/29/67/67	0/2/2/2
19	CLA	A	843	7	-	6/39/115/115	-
19	CLA	7	609	5	-	8/39/115/115	-
21	BCR	B	847	-	-	1/29/63/63	0/2/2/2
19	CLA	3	307	1	-	8/35/111/115	-
24	LMU	A	857	-	-	4/15/35/61	0/1/1/2
29	PQN	A	845	-	-	0/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMU	1	322	-	-	5/13/33/61	0/1/1/2
19	CLA	Z	610	26	-	7/33/109/115	-
24	LMU	6	328	-	-	7/15/35/61	0/1/1/2
19	CLA	5	316	3	-	16/39/115/115	-
22	LUT	7	615	-	-	2/29/67/67	0/2/2/2
19	CLA	B	837	8	-	6/33/109/115	-
20	CHL	6	317	4	-	0/14/90/117	-
19	CLA	L	204	32	-	3/15/91/115	-
19	CLA	8	312	6	-	5/39/115/115	-
19	CLA	8	303	6	-	18/39/115/115	-
19	CLA	A	816	7	-	6/27/103/115	-
19	CLA	1	312	32	-	10/39/115/115	-
22	LUT	F	305	-	-	10/29/67/67	0/2/2/2
28	CL0	A	802	7	-	3/39/115/115	-
26	LHG	A	848	19	-	11/42/42/53	-
19	CLA	1	303	15	-	8/30/106/115	-
20	CHL	6	315	4	-	17/41/117/117	-
24	LMU	8	319	-	-	6/15/35/61	0/1/1/2
19	CLA	A	814	7	-	8/39/115/115	-
19	CLA	B	831	8	-	0/15/91/115	-
19	CLA	A	808	7	-	10/39/115/115	-
19	CLA	7	611	5	-	5/24/100/115	-
20	CHL	6	302	4	-	14/41/117/117	-
19	CLA	B	801	32	-	11/39/115/115	-
21	BCR	B	848	-	-	2/29/63/63	0/2/2/2
19	CLA	8	307	32	-	2/21/97/115	-
26	LHG	5	321	19	-	14/41/41/53	-
19	CLA	8	313	6	-	8/30/106/115	-
19	CLA	A	819	7	-	7/39/115/115	-
20	CHL	4	601	2	-	4/41/117/117	-
19	CLA	B	825	32	-	9/39/115/115	-
24	LMU	7	619	-	-	4/12/32/61	0/1/1/2
19	CLA	1	310	26	-	13/35/111/115	-
26	LHG	6	325	-	-	14/40/40/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	7	617	-	-	4/29/63/63	0/2/2/2
19	CLA	A	803	-	-	1/39/115/115	-
19	CLA	B	815	8	-	6/33/109/115	-
21	BCR	3	318	-	-	4/29/63/63	0/2/2/2
22	LUT	Z	615	-	-	4/29/67/67	0/2/2/2
19	CLA	5	304	3	-	7/21/97/115	-
19	CLA	A	837	7	-	8/39/115/115	-
24	LMU	B	853	-	-	3/21/61/61	0/2/2/2
21	BCR	L	205	-	-	4/29/63/63	0/2/2/2
19	CLA	A	810	7	-	5/39/115/115	-
21	BCR	3	319	-	-	4/29/63/63	0/2/2/2
21	BCR	B	844	-	-	4/29/63/63	0/2/2/2
19	CLA	B	814	8	-	10/39/115/115	-
21	BCR	J	103	-	-	4/29/63/63	0/2/2/2
21	BCR	B	846	-	-	4/29/63/63	0/2/2/2
19	CLA	5	305	32	-	6/27/103/115	-
19	CLA	A	846	26	-	7/15/91/115	-
19	CLA	3	305	1	-	2/23/99/115	-
19	CLA	6	303	4	-	4/39/115/115	-
19	CLA	Z	614	15	-	10/33/109/115	-
19	CLA	Z	607	32	-	5/21/97/115	-
19	CLA	B	817	8	-	7/39/115/115	-
19	CLA	7	612	5	-	10/39/115/115	-
24	LMU	3	325	-	-	7/15/35/61	0/1/1/2
22	LUT	3	320	-	-	1/11/30/67	0/1/1/2
19	CLA	4	609	2	-	4/33/109/115	-
19	CLA	5	311	26	-	5/27/103/115	-
19	CLA	A	836	7	-	8/39/115/115	-
19	CLA	Z	603	15	-	9/39/115/115	-
24	LMU	F	306	-	-	8/21/61/61	0/2/2/2
19	CLA	Z	602	15	-	3/33/109/115	-
24	LMU	Z	619	-	-	5/17/57/61	0/2/2/2
19	CLA	3	314	1	-	0/15/91/115	-
23	LMG	G	201	-	-	6/31/51/70	0/1/1/1
19	CLA	6	327	32	-	5/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMU	4	624	-	-	6/15/35/61	0/1/1/2
19	CLA	B	805	8	-	5/15/91/115	-
25	XAT	8	316	-	-	0/31/93/93	0/4/4/4
19	CLA	B	824	8	-	12/39/115/115	-
19	CLA	5	313	3	-	6/29/105/115	-
19	CLA	5	312	3	-	4/15/91/115	-
20	CHL	4	605	32	-	11/41/117/117	-
19	CLA	8	310	26	-	4/15/91/115	-
20	CHL	Z	605	32	-	4/17/93/117	-
24	LMU	Z	620	-	-	2/15/35/61	0/1/1/2
20	CHL	Z	606	32	-	12/41/117/117	-
24	LMU	K	201	-	-	6/15/35/61	0/1/1/2
29	PQN	B	843	-	-	2/23/43/43	0/2/2/2
19	CLA	A	833	7	-	11/27/103/115	-
19	CLA	B	828	8	-	11/39/115/115	-
23	LMG	8	321	-	-	22/44/64/70	0/1/1/1
19	CLA	3	313	32	-	10/33/109/115	-
22	LUT	4	616	-	-	3/29/67/67	0/2/2/2
19	CLA	J	102	13	-	8/27/103/115	-
19	CLA	3	303	32	-	3/39/115/115	-
19	CLA	B	835	8	-	4/33/109/115	-
24	LMU	3	324	-	-	9/21/61/61	0/2/2/2
19	CLA	A	844	32	-	13/39/115/115	-
19	CLA	L	203	18	-	16/39/115/115	-
25	XAT	1	316	-	-	0/31/93/93	0/4/4/4
22	LUT	3	317	-	-	2/29/67/67	0/2/2/2
19	CLA	8	304	32	-	7/33/109/115	-
19	CLA	A	830	7	-	12/39/115/115	-
19	CLA	B	813	8	-	18/39/115/115	-
20	CHL	5	306	32	-	7/17/93/117	-
19	CLA	A	831	7	-	4/39/115/115	-
21	BCR	8	317	-	-	3/29/63/63	0/2/2/2
19	CLA	Z	613	15	-	2/21/97/115	-
23	LMG	J	104	-	-	9/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LUT	1	317	-	-	5/29/67/67	0/2/2/2
31	DGD	B	850	-	-	11/48/88/95	0/2/2/2
19	CLA	3	308	1	-	5/39/115/115	-
21	BCR	6	321	-	-	2/29/63/63	0/2/2/2
19	CLA	Z	611	15	-	5/15/91/115	-
21	BCR	A	858	-	-	5/29/63/63	0/2/2/2
26	LHG	5	301	-	-	12/42/42/53	-
19	CLA	B	823	8	-	5/32/108/115	-
19	CLA	5	309	3	-	12/39/115/115	-
19	CLA	B	840	32	-	11/39/115/115	-
26	LHG	Z	618	19	-	5/43/43/53	-
19	CLA	3	312	1	-	6/15/91/115	-
19	CLA	Z	604	32	-	11/30/106/115	-
19	CLA	A	811	7	-	13/39/115/115	-
20	CHL	4	615	2	-	6/17/93/117	-
19	CLA	B	832	8	-	2/27/103/115	-
19	CLA	B	842	26	-	8/39/115/115	-
19	CLA	Z	608	15	-	19/39/115/115	-
19	CLA	5	314	3	-	6/15/91/115	-
19	CLA	3	310	1	-	7/17/93/115	-
22	LUT	Z	617	-	-	3/18/37/67	0/1/1/2
19	CLA	3	301	1	-	3/33/109/115	-
21	BCR	A	849	-	-	2/29/63/63	0/2/2/2
26	LHG	4	619	19	-	11/53/53/53	-
23	LMG	6	326	-	-	6/17/17/70	-
19	CLA	B	804	-	-	15/39/115/115	-
19	CLA	4	604	32	-	4/21/97/115	-
19	CLA	B	829	8	-	6/39/115/115	-
19	CLA	K	205	14	-	2/15/91/115	-
20	CHL	5	307	32	-	11/41/117/117	-
19	CLA	B	841	8	-	12/39/115/115	-
19	CLA	6	304	4	-	10/23/99/115	-
21	BCR	3	315	-	-	7/29/63/63	0/2/2/2
19	CLA	B	806	8	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	838	8	-	3/39/115/115	-
22	LUT	1	315	-	-	4/29/67/67	0/2/2/2
20	CHL	1	306	32	-	6/17/93/117	-
19	CLA	A	826	7	-	4/27/103/115	-
23	LMG	7	622	-	-	9/27/47/70	0/1/1/1
21	BCR	B	802	-	-	7/29/63/63	0/2/2/2
19	CLA	7	614	5	-	6/17/93/115	-
19	CLA	A	821	7	-	3/39/115/115	-
19	CLA	4	613	2	-	6/27/103/115	-
19	CLA	1	308	15	-	16/39/115/115	-
19	CLA	B	809	8	-	10/39/115/115	-
26	LHG	8	318	19	-	16/48/48/53	-
19	CLA	6	312	4	-	2/15/91/115	-
22	LUT	3	316	-	-	3/29/67/67	0/2/2/2
19	CLA	6	314	4	-	7/21/97/115	-
19	CLA	1	309	15	-	3/39/115/115	-
21	BCR	A	853	-	-	4/29/63/63	0/2/2/2
19	CLA	B	839	8	-	1/21/97/115	-
19	CLA	5	319	32	-	12/17/93/115	-
24	LMU	6	324	-	-	6/15/35/61	0/1/1/2
19	CLA	7	610	26	-	7/39/115/115	-
20	CHL	Z	601	15	-	13/41/117/117	-
19	CLA	A	813	7,19	-	8/39/115/115	-
19	CLA	A	815	7	-	9/39/115/115	-
19	CLA	4	608	2	-	9/33/109/115	-
19	CLA	B	834	8	-	5/31/107/115	-
19	CLA	1	307	32	-	14/39/115/115	-
19	CLA	A	822	7	-	4/27/103/115	-
19	CLA	A	825	7	-	3/15/91/115	-
24	LMU	4	623	-	-	4/11/31/61	0/1/1/2
19	CLA	5	310	3	-	5/33/109/115	-
19	CLA	K	203	32	-	6/33/109/115	-
19	CLA	A	835	7	-	7/39/115/115	-
23	LMG	J	105	-	-	14/30/50/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	832	7	-	5/39/115/115	-
21	BCR	L	202	-	-	4/29/63/63	0/2/2/2
21	BCR	5	320	-	-	2/29/63/63	0/2/2/2
24	LMU	1	321	-	-	4/15/35/61	0/1/1/2
19	CLA	1	313	15	-	12/33/109/115	-
24	LMU	1	301	-	-	11/21/61/61	0/2/2/2
19	CLA	3	304	32	-	0/12/88/115	-
22	LUT	8	301	-	-	4/29/67/67	0/2/2/2
19	CLA	A	818	32	-	5/27/103/115	-
19	CLA	B	810	8	-	8/39/115/115	-
24	LMU	1	319	-	-	7/21/61/61	0/2/2/2
26	LHG	7	618	19	-	16/53/53/53	-
25	XAT	5	322	-	-	1/31/93/93	0/4/4/4
19	CLA	4	611	2	-	3/15/91/115	-
24	LMU	Z	621	-	-	3/15/35/61	0/1/1/2
19	CLA	6	313	32	-	4/39/115/115	-
19	CLA	A	840	7	-	8/39/115/115	-
19	CLA	Z	609	15	-	2/33/109/115	-
27	NEX	6	323	-	-	3/27/83/83	0/3/3/3
19	CLA	F	302	32	-	10/39/115/115	-
21	BCR	4	618	-	-	5/29/63/63	0/2/2/2
19	CLA	3	311	1	-	5/33/109/115	-
23	LMG	3	321	-	-	12/32/52/70	0/1/1/1
19	CLA	6	310	4	-	2/33/109/115	-
19	CLA	A	804	32	-	2/39/115/115	-
19	CLA	A	829	7	-	4/39/115/115	-
22	LUT	J	101	-	-	6/29/67/67	0/2/2/2
19	CLA	8	302	6	-	6/39/115/115	-
19	CLA	7	613	5	-	4/13/89/115	-
24	LMU	A	856	-	-	3/11/31/61	0/1/1/2
23	LMG	B	852	-	-	9/38/58/70	0/1/1/1
19	CLA	5	303	3	-	2/39/115/115	-
20	CHL	8	320	15	-	10/41/117/117	-
19	CLA	6	311	26	-	9/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	8	305	32	-	8/41/117/117	-
19	CLA	A	820	7	-	14/33/109/115	-
20	CHL	5	308	32	-	4/23/99/117	-
24	LMU	1	320	-	-	7/10/30/61	0/1/1/2
19	CLA	7	604	32	-	0/23/99/115	-
21	BCR	K	206	-	-	2/29/63/63	0/2/2/2

The worst 5 of 1538 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	601	CHL	MG-NA	4.83	2.17	2.06
20	6	302	CHL	MG-NA	4.81	2.17	2.06
20	7	621	CHL	MG-NA	4.71	2.17	2.06
20	8	320	CHL	MG-NA	4.37	2.16	2.06
20	5	317	CHL	C4D-ND	-4.28	1.31	1.37

The worst 5 of 1489 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	601	CHL	C4A-NA-C1A	8.19	110.39	106.71
19	K	202	CLA	C4A-NA-C1A	7.38	110.02	106.71
19	B	841	CLA	C4A-NA-C1A	7.37	110.02	106.71
20	6	317	CHL	C4A-NA-C1A	7.35	110.01	106.71
20	7	621	CHL	C4A-NA-C1A	7.33	110.00	106.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	5	323	NEX	C25

5 of 2193 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	3	302	CLA	C11-C12-C13-C14
19	3	305	CLA	C4-C3-C5-C6
19	3	309	CLA	CBD-CGD-O2D-CED
19	3	312	CLA	C2B-C3B-CAB-CBB
19	3	312	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

240 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	812	CLA	3	0
21	B	845	BCR	3	0
25	6	322	XAT	2	0
19	B	826	CLA	2	0
19	A	838	CLA	3	0
24	3	322	LMU	1	0
19	A	805	CLA	1	0
25	Z	616	XAT	2	0
19	8	309	CLA	3	0
19	6	305	CLA	4	0
20	5	317	CHL	1	0
19	B	820	CLA	1	0
19	A	839	CLA	1	0
20	8	306	CHL	2	0
20	6	306	CHL	2	0
26	6	318	LHG	6	0
19	B	807	CLA	1	0
19	B	827	CLA	1	0
19	4	603	CLA	4	0
19	3	309	CLA	3	0
21	A	851	BCR	1	0
20	4	607	CHL	5	0
26	B	851	LHG	6	0
19	4	602	CLA	1	0
22	5	318	LUT	2	0
19	5	302	CLA	2	0
20	4	606	CHL	1	0
20	7	605	CHL	1	0
25	4	617	XAT	1	0
19	B	803	CLA	1	0
20	1	305	CHL	2	0
19	7	602	CLA	2	0
23	F	301	LMG	1	0
20	7	621	CHL	2	0
26	4	620	LHG	2	0
19	B	830	CLA	2	0
19	A	807	CLA	2	0
19	1	311	CLA	3	0
21	A	852	BCR	1	0
23	6	301	LMG	1	0
20	6	307	CHL	8	0
19	8	311	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	302	CLA	3	0
19	B	833	CLA	1	0
19	A	842	CLA	3	0
19	A	812	CLA	1	0
19	A	824	CLA	2	0
19	4	612	CLA	3	0
19	A	841	CLA	1	0
19	A	817	CLA	1	0
19	Z	612	CLA	1	0
19	6	320	CLA	2	0
26	A	847	LHG	1	0
21	I	201	BCR	1	0
19	A	823	CLA	1	0
24	A	855	LMU	1	0
21	A	850	BCR	2	0
19	B	819	CLA	2	0
19	F	304	CLA	4	0
19	4	610	CLA	1	0
19	4	614	CLA	2	0
19	B	822	CLA	3	0
20	6	308	CHL	1	0
19	B	811	CLA	3	0
26	A	801	LHG	1	0
25	7	616	XAT	1	0
19	A	834	CLA	2	0
19	A	827	CLA	3	0
19	K	204	CLA	1	0
19	B	818	CLA	5	0
19	1	314	CLA	2	0
24	7	620	LMU	1	0
23	L	201	LMG	2	0
22	5	324	LUT	2	0
19	7	609	CLA	3	0
24	1	322	LMU	1	0
19	5	316	CLA	3	0
19	B	837	CLA	3	0
20	6	317	CHL	1	0
19	L	204	CLA	1	0
19	8	312	CLA	1	0
19	8	303	CLA	6	0
19	A	816	CLA	2	0
19	1	312	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	305	LUT	1	0
26	A	848	LHG	1	0
19	1	303	CLA	3	0
20	6	315	CHL	2	0
24	8	319	LMU	1	0
19	A	814	CLA	2	0
19	B	831	CLA	2	0
19	A	808	CLA	1	0
20	6	302	CHL	2	0
19	B	801	CLA	2	0
21	B	848	BCR	2	0
19	8	307	CLA	1	0
26	5	321	LHG	1	0
19	8	313	CLA	1	0
19	A	819	CLA	2	0
20	4	601	CHL	2	0
19	1	310	CLA	3	0
26	6	325	LHG	1	0
21	7	617	BCR	3	0
19	A	803	CLA	3	0
19	B	815	CLA	2	0
21	3	318	BCR	3	0
22	Z	615	LUT	1	0
19	5	304	CLA	4	0
19	A	837	CLA	5	0
24	B	853	LMU	2	0
21	L	205	BCR	2	0
19	A	810	CLA	3	0
21	3	319	BCR	1	0
21	B	844	BCR	2	0
19	B	814	CLA	4	0
21	J	103	BCR	1	0
21	B	846	BCR	1	0
19	5	305	CLA	2	0
19	A	846	CLA	1	0
19	3	305	CLA	2	0
19	6	303	CLA	4	0
19	Z	614	CLA	1	0
19	Z	607	CLA	1	0
19	B	817	CLA	5	0
19	7	612	CLA	5	0
19	4	609	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	5	311	CLA	1	0
19	A	836	CLA	1	0
19	Z	603	CLA	2	0
24	F	306	LMU	2	0
19	Z	602	CLA	1	0
19	3	314	CLA	4	0
19	6	327	CLA	1	0
19	B	805	CLA	3	0
19	B	824	CLA	6	0
19	5	313	CLA	3	0
19	5	312	CLA	4	0
20	4	605	CHL	3	0
20	Z	605	CHL	1	0
20	Z	606	CHL	1	0
19	A	833	CLA	2	0
19	B	828	CLA	3	0
23	8	321	LMG	1	0
19	3	313	CLA	3	0
22	4	616	LUT	3	0
19	J	102	CLA	1	0
19	3	303	CLA	3	0
19	B	835	CLA	1	0
24	3	324	LMU	2	0
19	A	844	CLA	1	0
19	L	203	CLA	2	0
25	1	316	XAT	1	0
22	3	317	LUT	1	0
19	8	304	CLA	3	0
19	A	830	CLA	2	0
19	B	813	CLA	3	0
20	5	306	CHL	2	0
19	A	831	CLA	1	0
21	8	317	BCR	1	0
23	J	104	LMG	1	0
22	1	317	LUT	1	0
31	B	850	DGD	2	0
19	3	308	CLA	3	0
21	6	321	BCR	2	0
19	Z	611	CLA	1	0
21	A	858	BCR	1	0
26	5	301	LHG	1	0
19	B	823	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	811	CLA	6	0
20	4	615	CHL	2	0
19	B	832	CLA	3	0
19	B	842	CLA	5	0
19	Z	608	CLA	5	0
19	3	310	CLA	1	0
21	A	849	BCR	2	0
26	4	619	LHG	3	0
23	6	326	LMG	2	0
19	B	804	CLA	10	0
19	4	604	CLA	1	0
19	B	829	CLA	1	0
20	5	307	CHL	3	0
19	B	841	CLA	2	0
19	6	304	CLA	1	0
21	3	315	BCR	2	0
19	B	806	CLA	2	0
19	B	838	CLA	3	0
22	1	315	LUT	2	0
20	1	306	CHL	1	0
19	A	826	CLA	1	0
21	B	802	BCR	2	0
19	A	821	CLA	3	0
19	4	613	CLA	1	0
19	1	308	CLA	2	0
19	B	809	CLA	3	0
26	8	318	LHG	3	0
19	6	312	CLA	2	0
19	6	314	CLA	2	0
19	1	309	CLA	2	0
21	A	853	BCR	3	0
19	B	839	CLA	1	0
19	5	319	CLA	6	0
19	7	610	CLA	4	0
19	A	813	CLA	3	0
19	A	815	CLA	4	0
19	4	608	CLA	1	0
19	B	834	CLA	2	0
19	1	307	CLA	3	0
24	4	623	LMU	2	0
19	5	310	CLA	1	0
19	K	203	CLA	4	0

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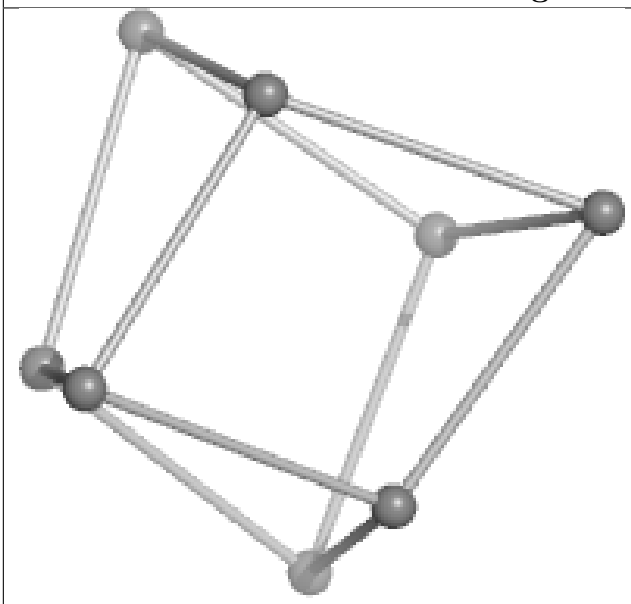
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J	105	LMG	3	0
19	A	832	CLA	3	0
21	L	202	BCR	2	0
21	5	320	BCR	4	0
24	1	321	LMU	1	0
24	1	301	LMU	2	0
19	A	818	CLA	1	0
19	B	810	CLA	1	0
24	1	319	LMU	1	0
26	7	618	LHG	1	0
25	5	322	XAT	3	0
19	6	313	CLA	2	0
19	A	840	CLA	2	0
19	Z	609	CLA	1	0
27	6	323	NEX	2	0
19	F	302	CLA	3	0
21	4	618	BCR	1	0
23	3	321	LMG	4	0
19	6	310	CLA	3	0
19	A	829	CLA	2	0
22	J	101	LUT	3	0
19	8	302	CLA	4	0
19	7	613	CLA	1	0
23	B	852	LMG	1	0
19	5	303	CLA	3	0
20	8	320	CHL	1	0
20	8	305	CHL	2	0
19	A	820	CLA	3	0
20	5	308	CHL	1	0
21	K	206	BCR	1	0

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

Ligand SF4 C 101



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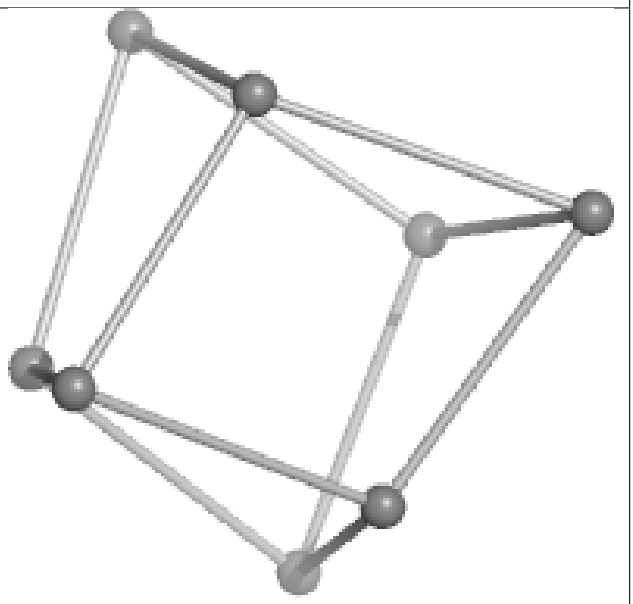
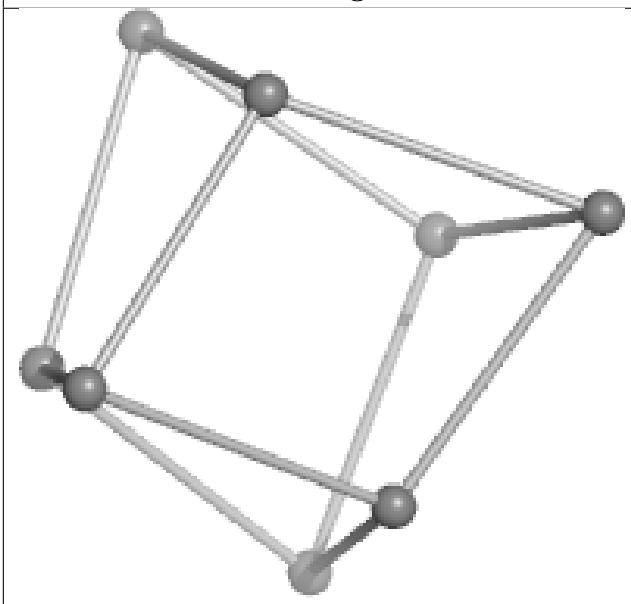
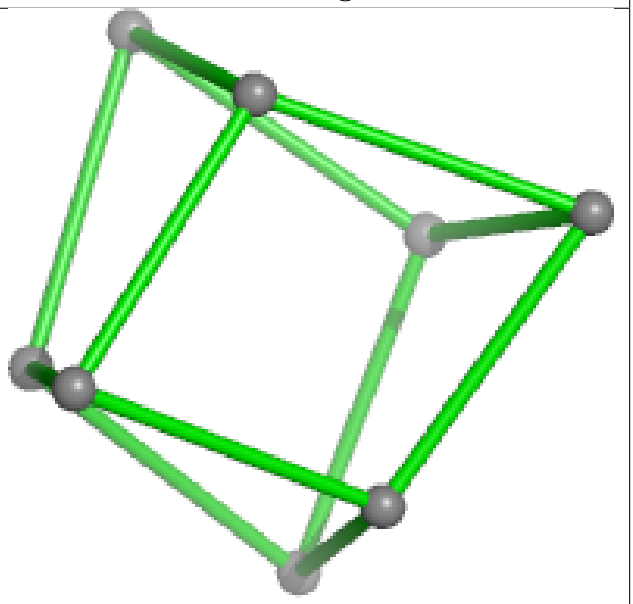


Bond angles

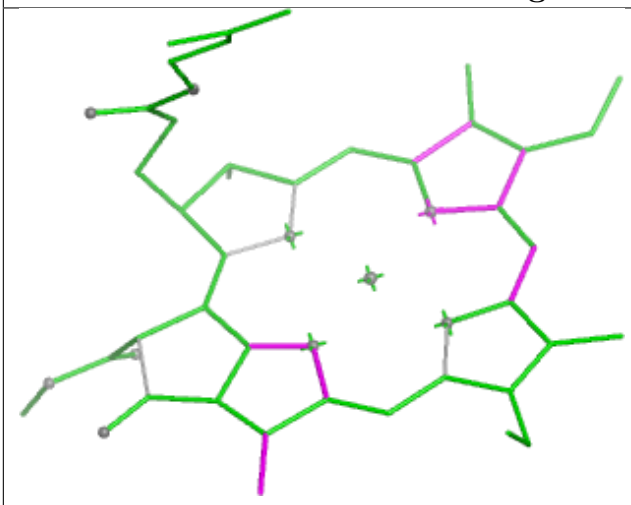


Torsions



Rings

Ligand CLA 1 304



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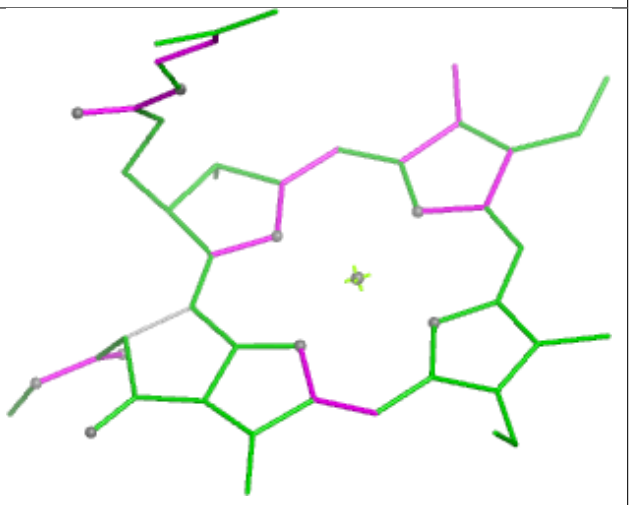

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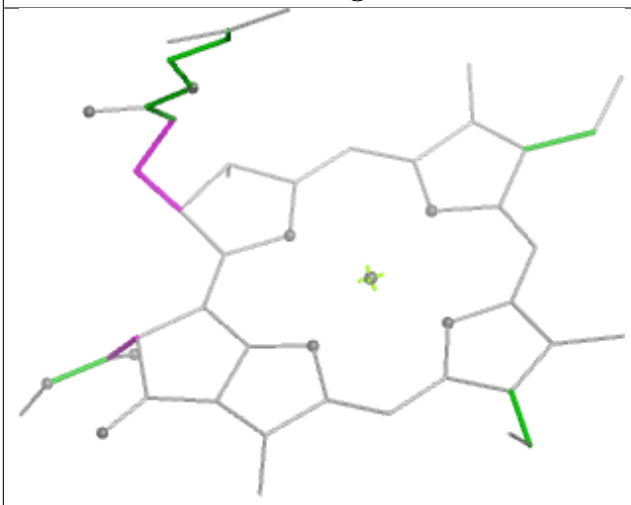

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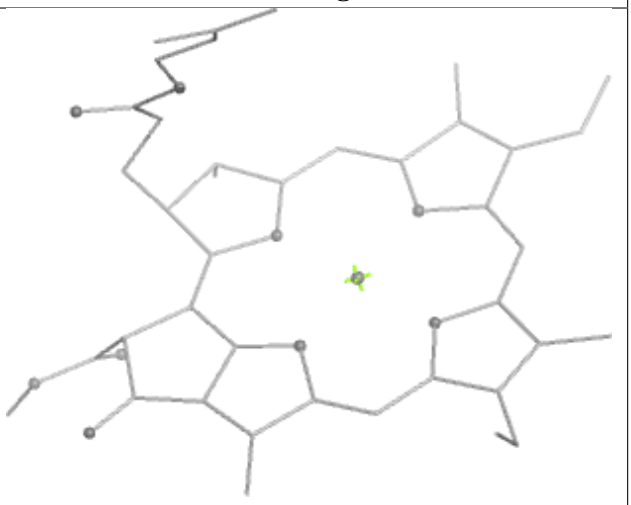
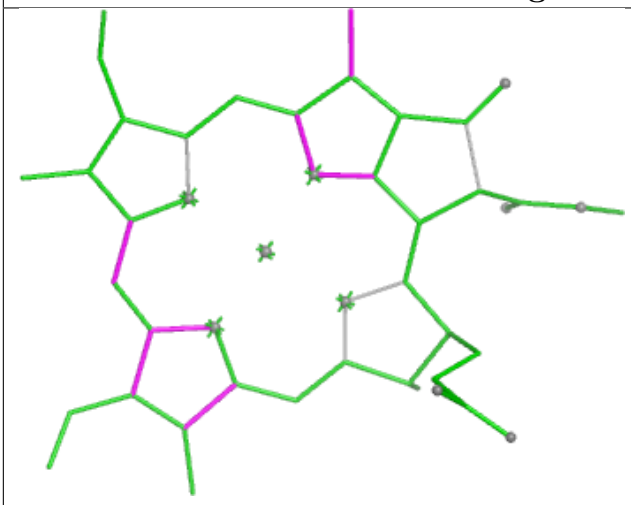
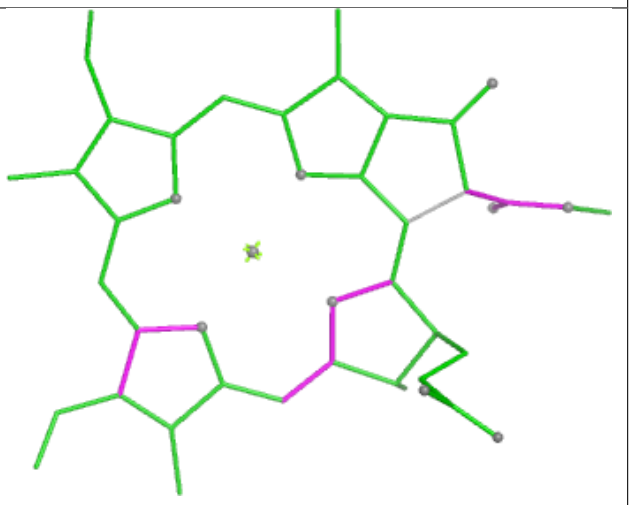


Rings

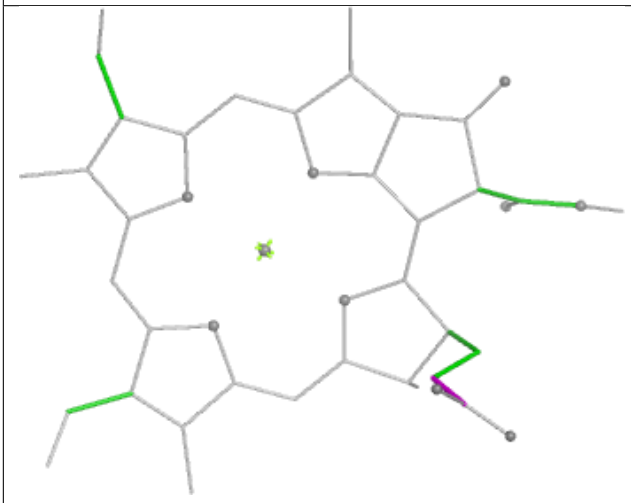
Ligand CLA 7 608



Bond lengths



Bond angles



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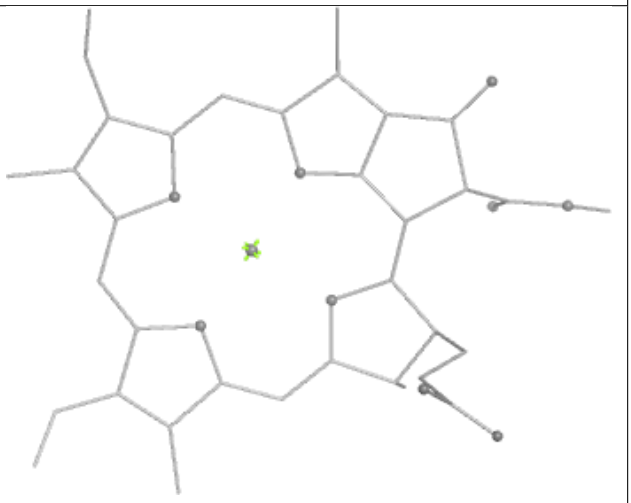

Rings

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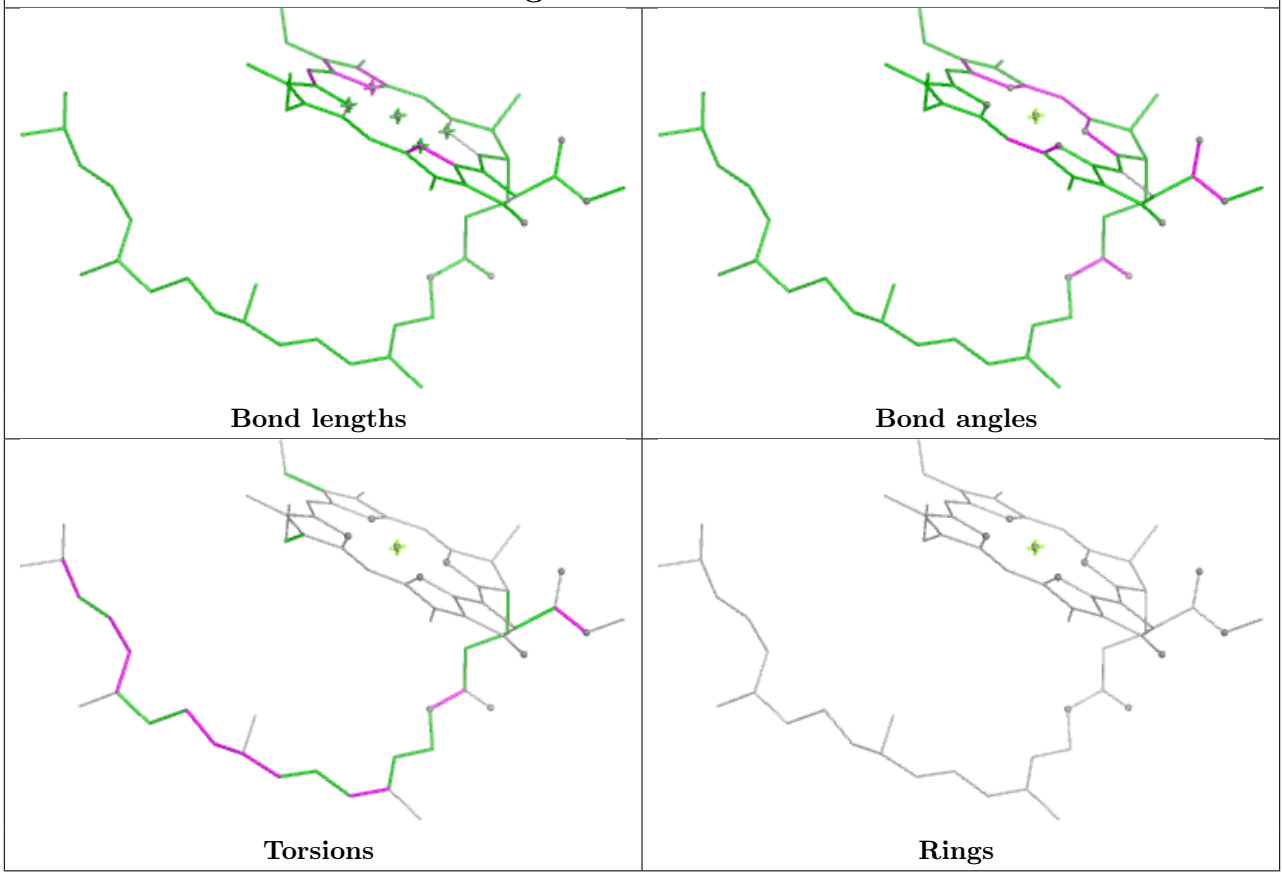

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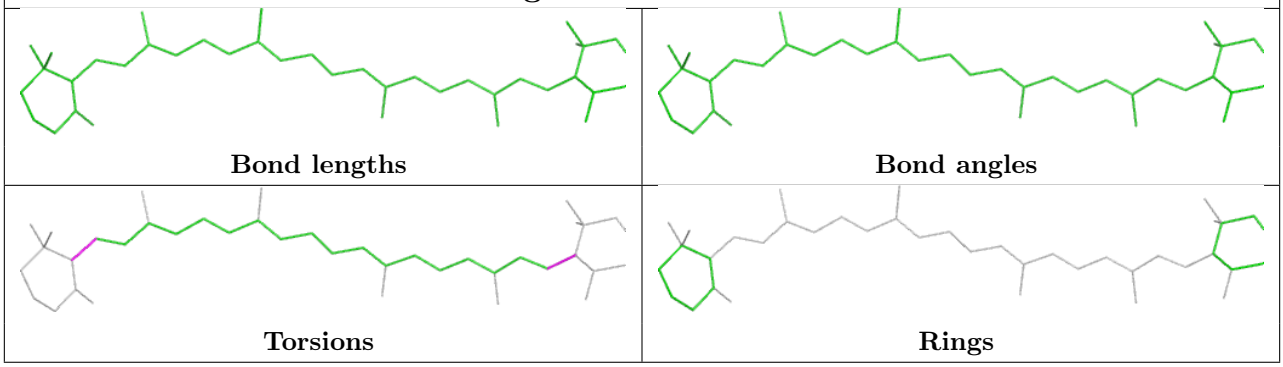
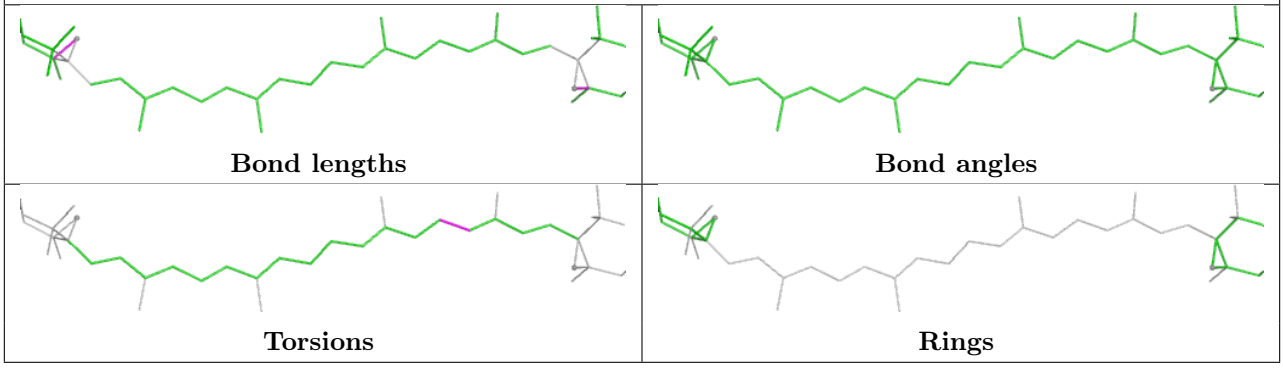


Ligand XAT 6 322



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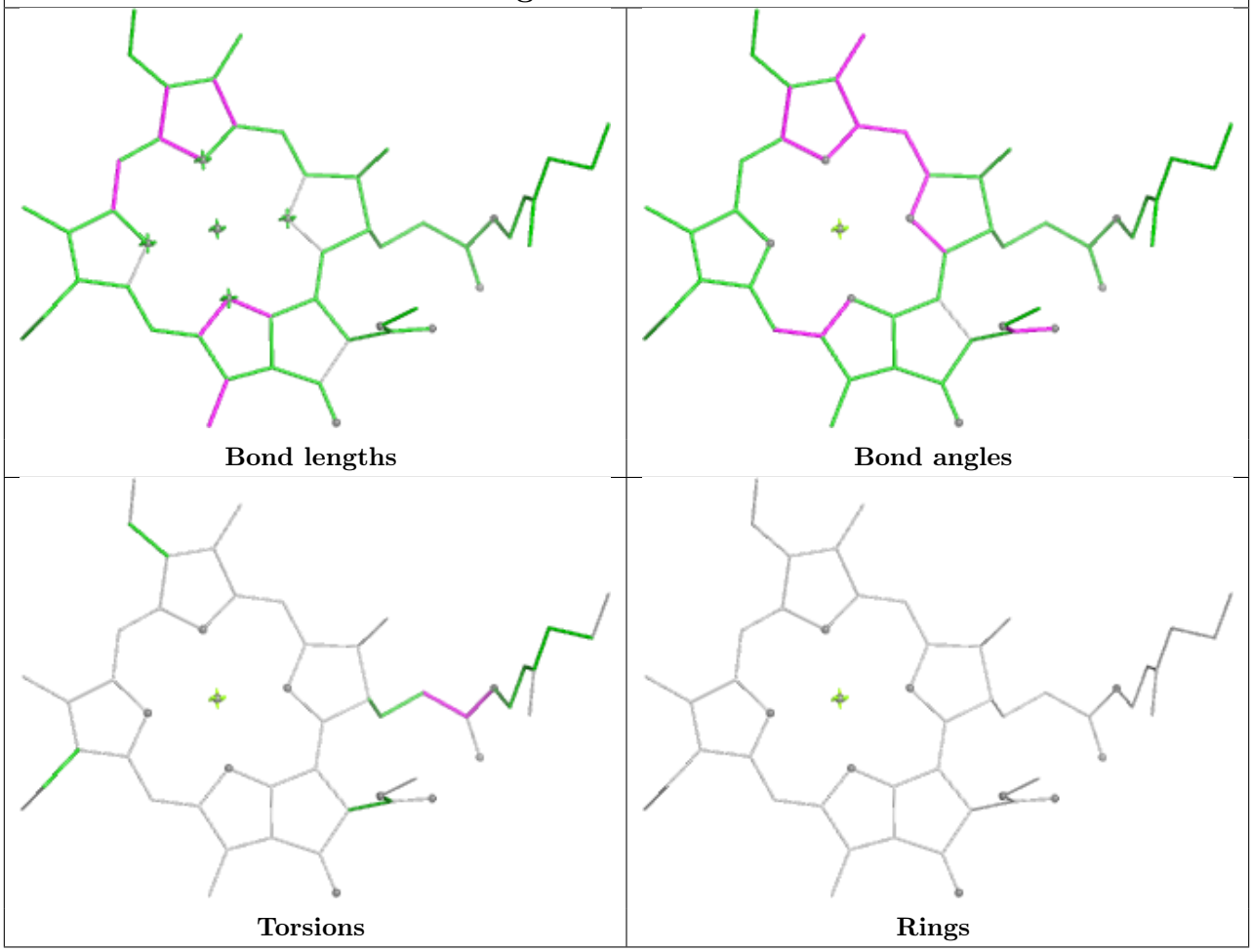

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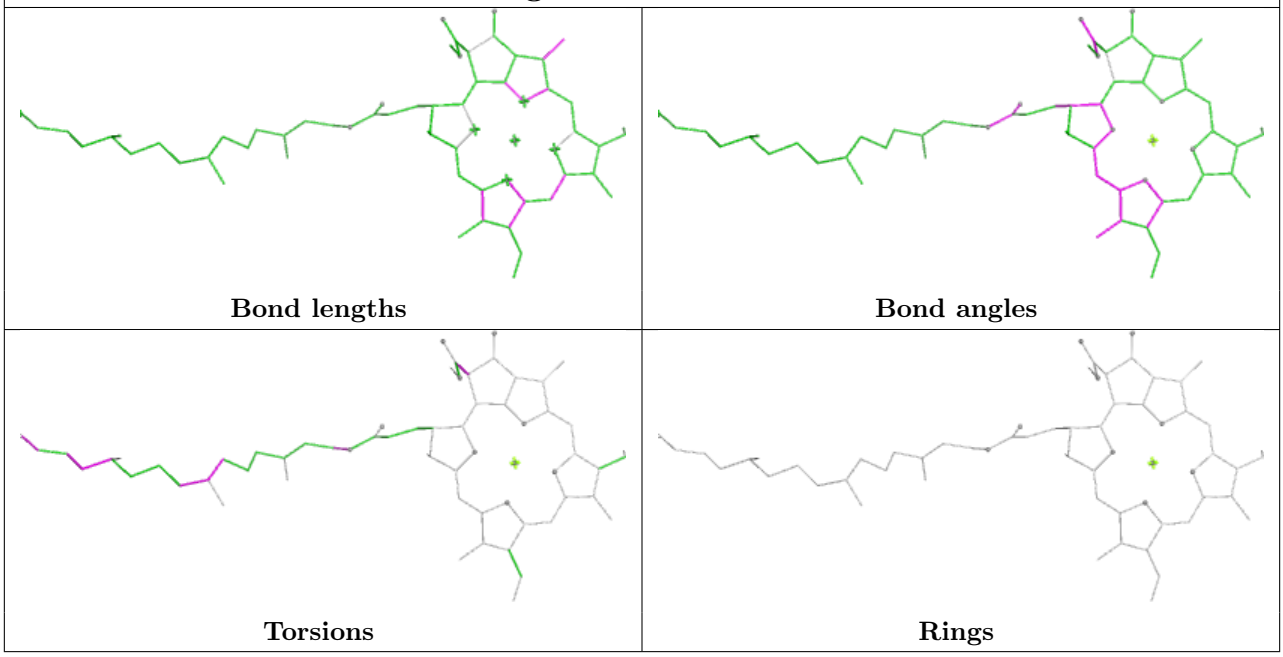
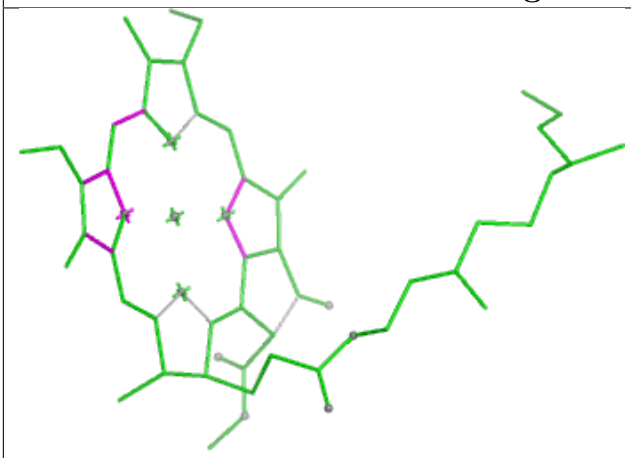
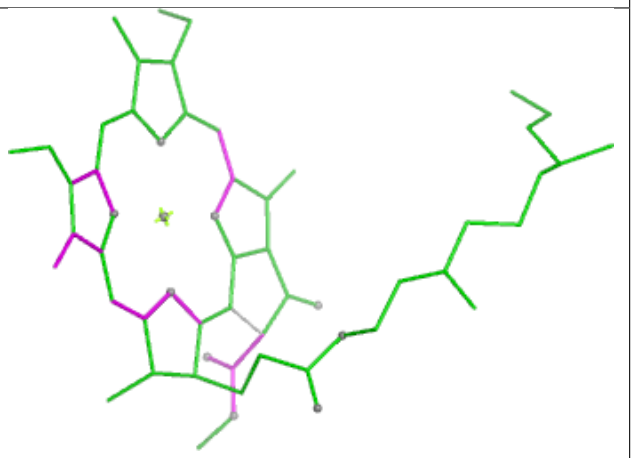


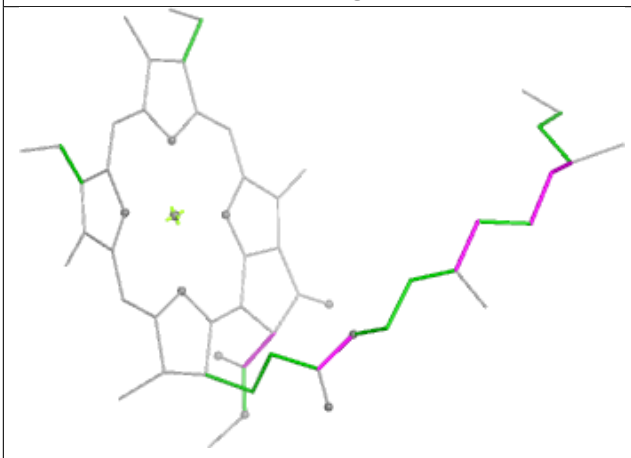
Ligand CLA A 838



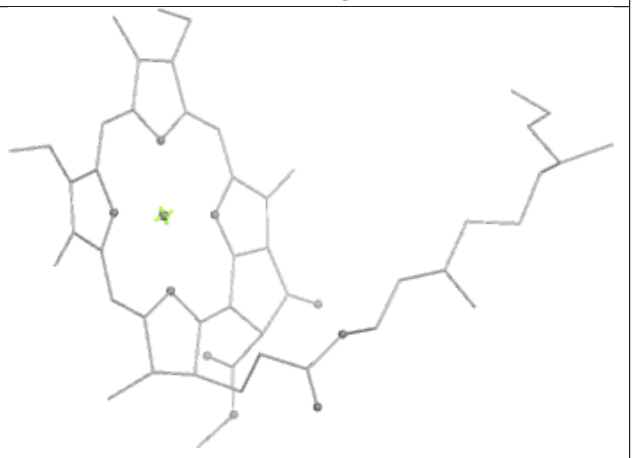
Bond lengths



Bond angles

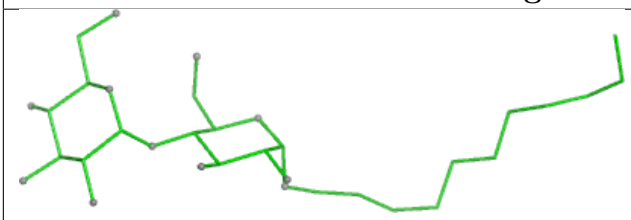


Torsions



Rings

Ligand LMU 3 322



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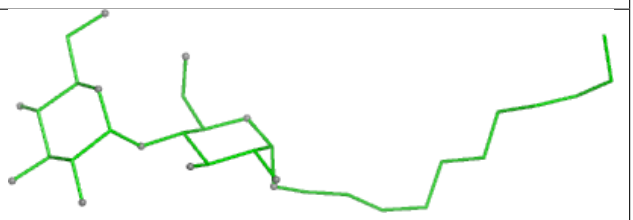

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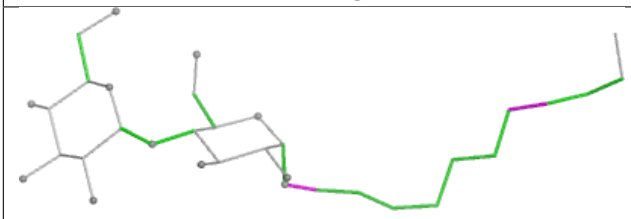

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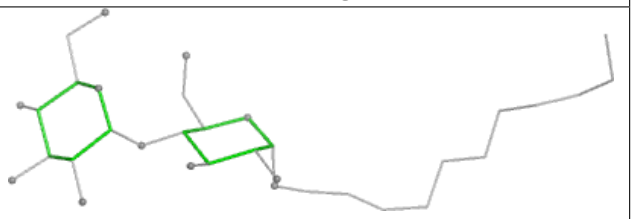
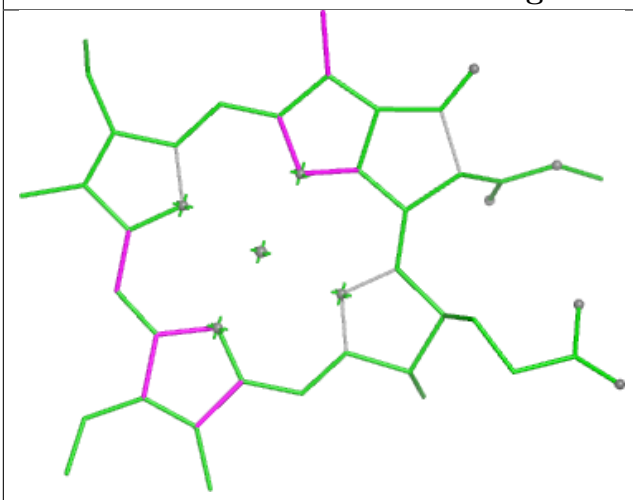


Rings

Ligand CLA F 303



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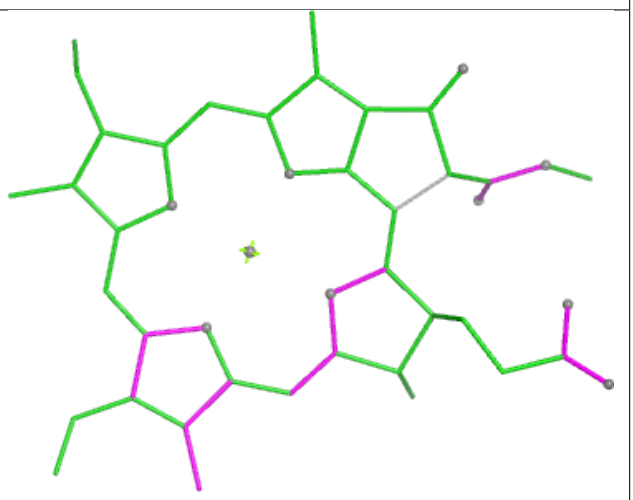
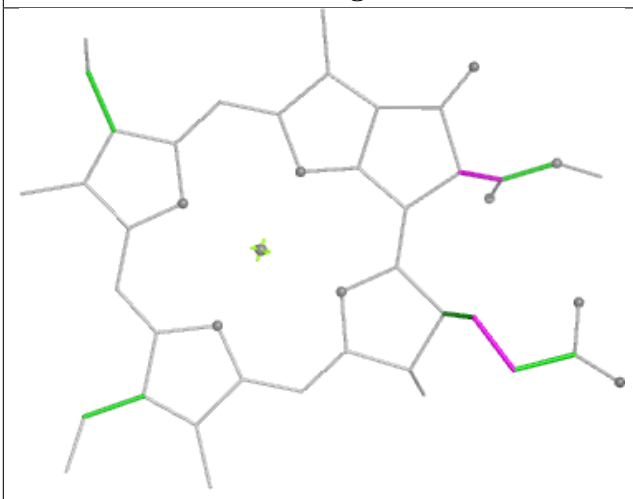


Bond angles



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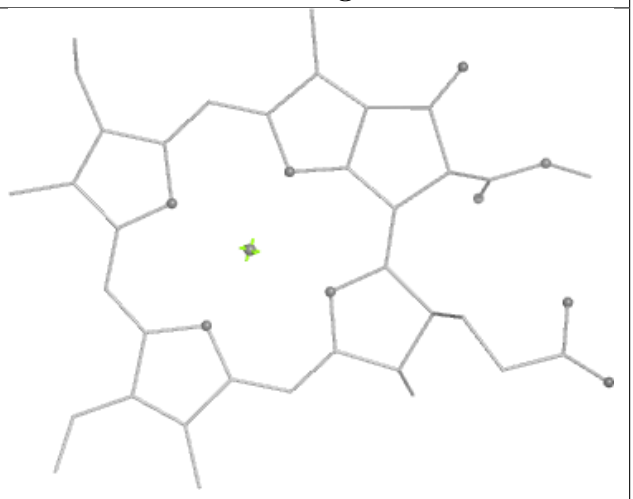
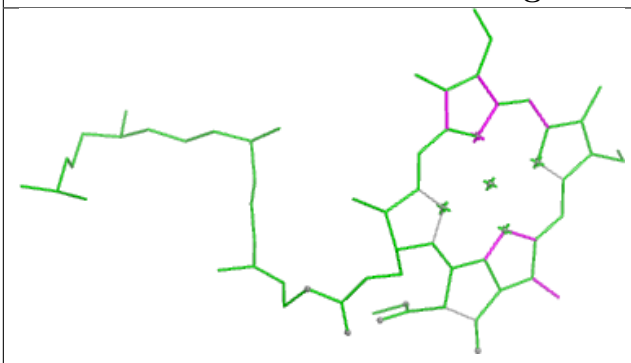


Rings

Ligand CLA A 805



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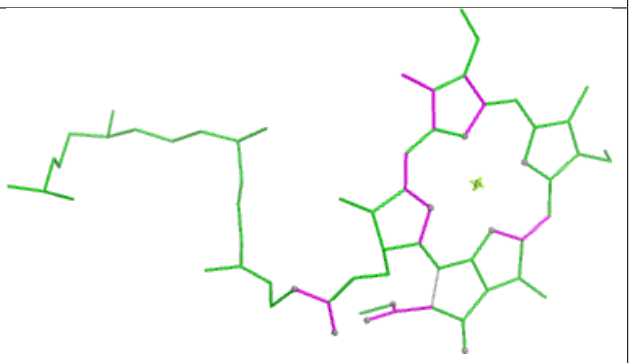

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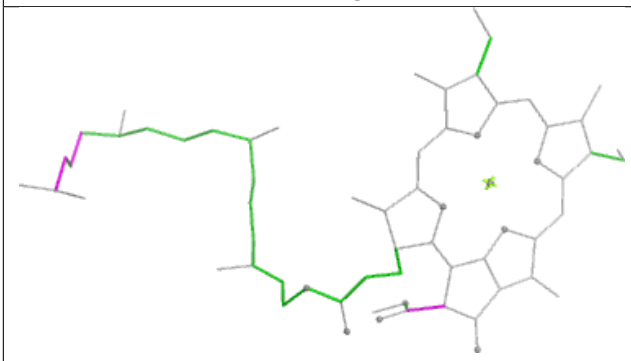

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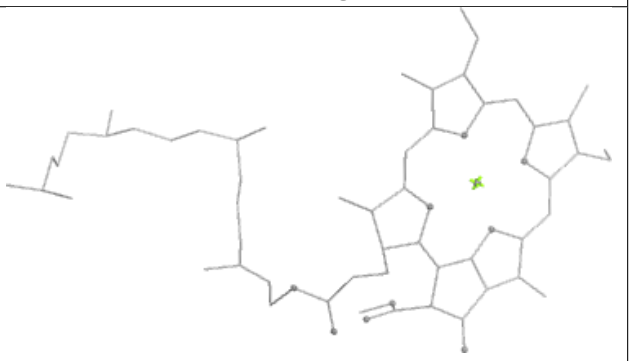
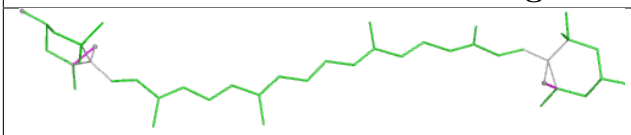


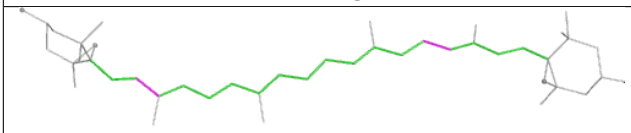
Rings

Ligand XAT Z 616



Bond lengths

Bond angles



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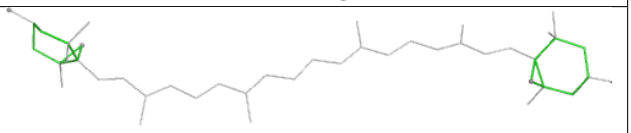
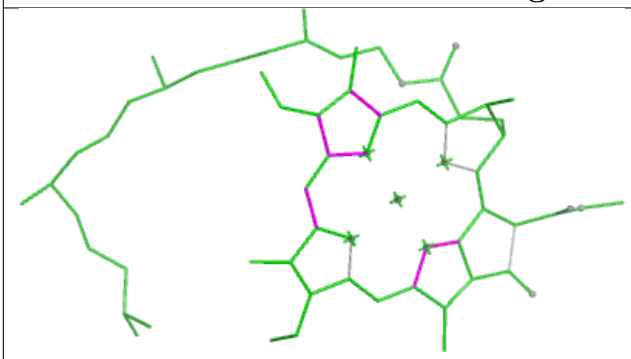


Rings

Ligand CLA 8 309



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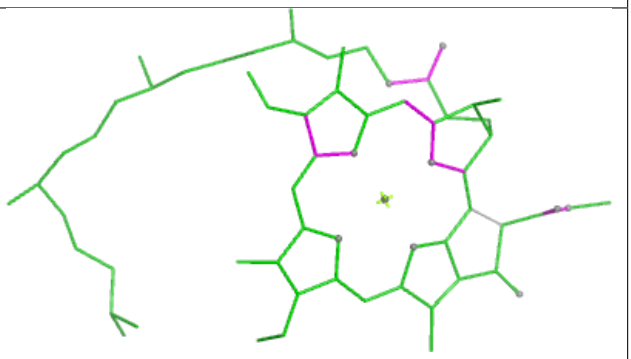

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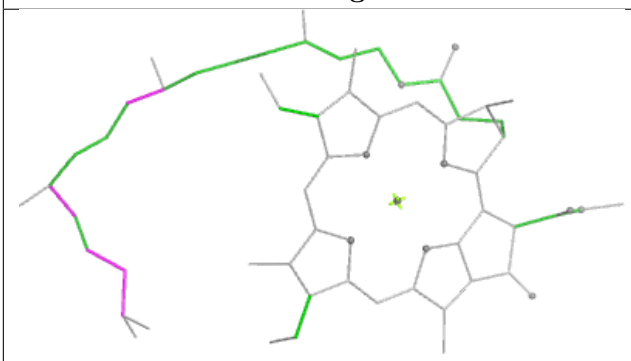
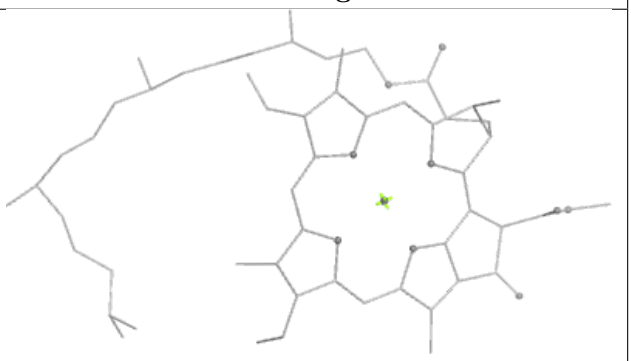
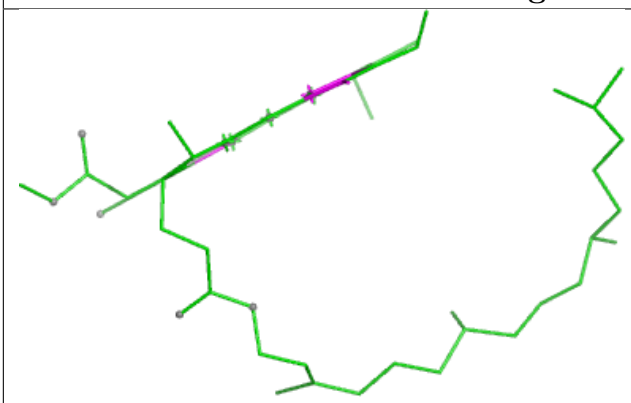


Torsions

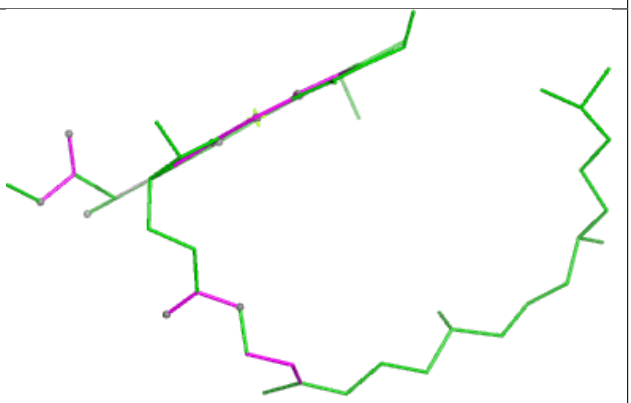


Rings

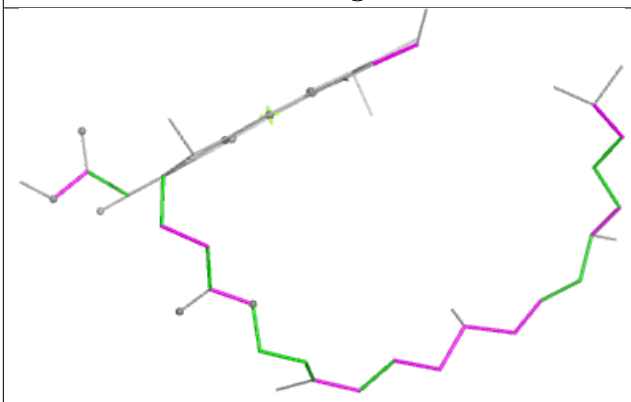
Ligand CLA 6 305



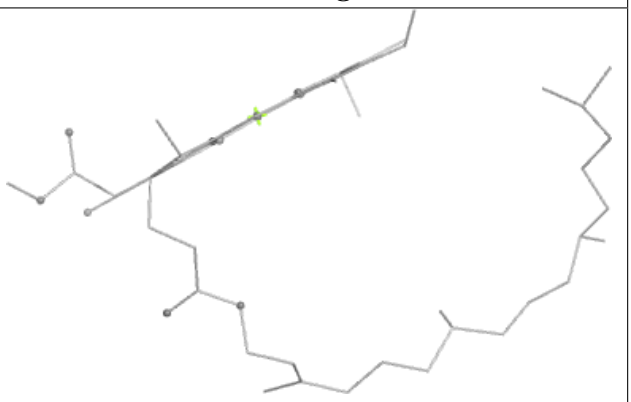
Bond lengths



Bond angles

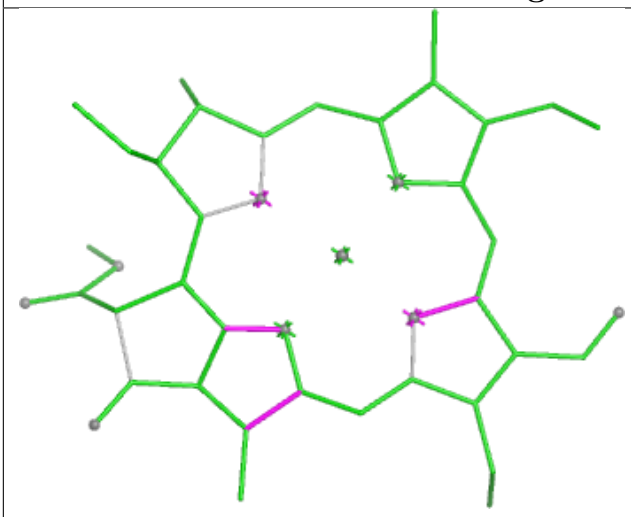


Torsions



Rings

Ligand CHL 5 317



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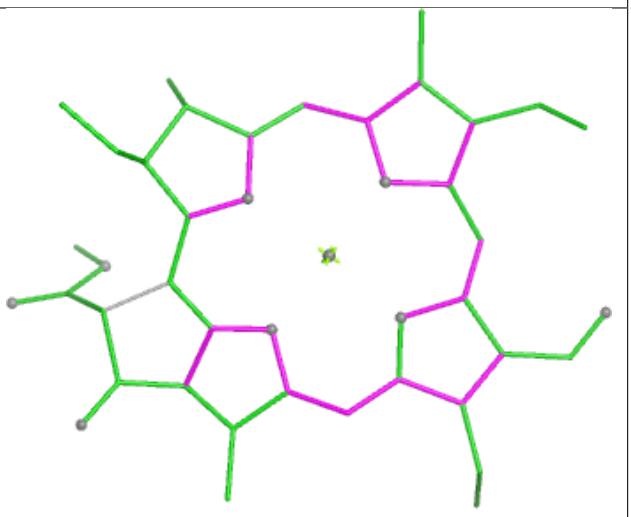

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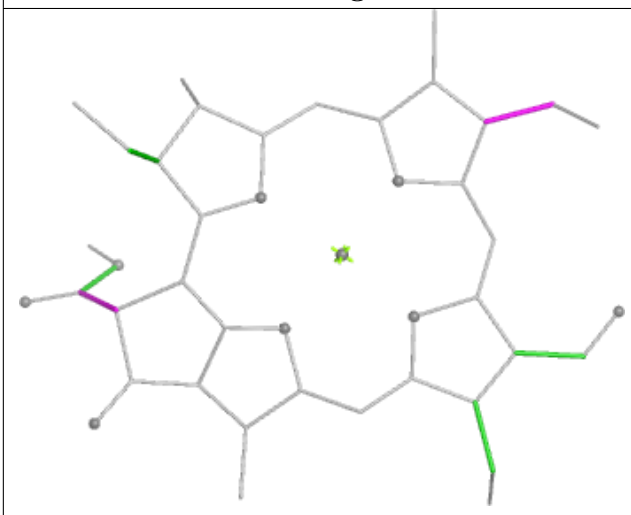

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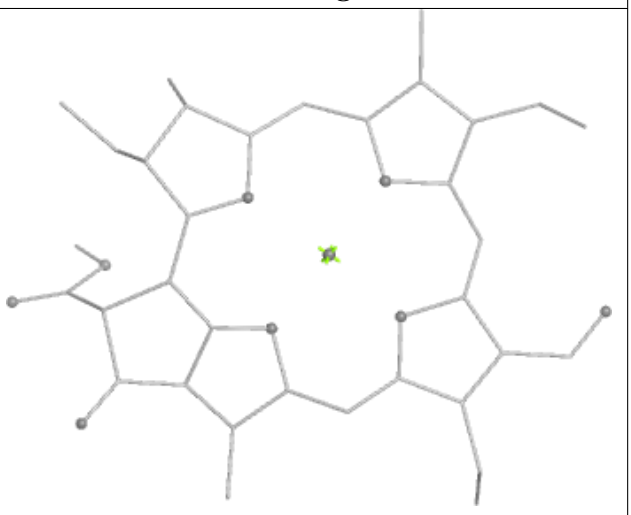
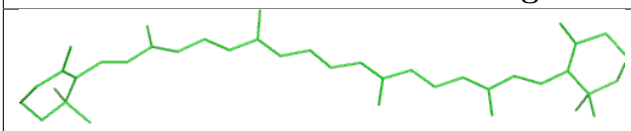


Rings

Ligand BCR G 204



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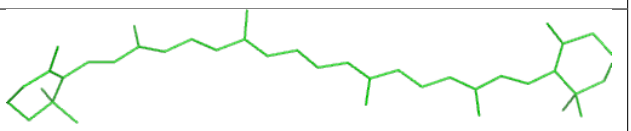

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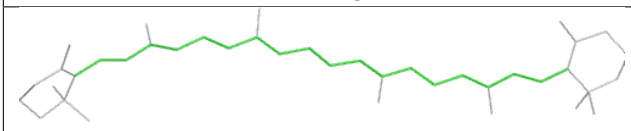

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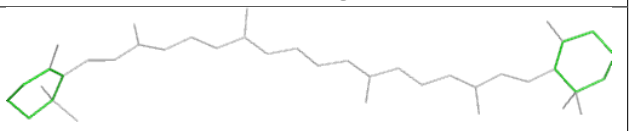
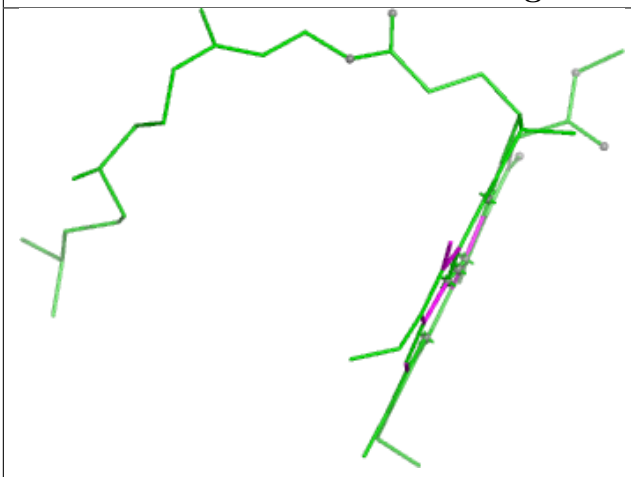


Rings

Ligand CLA B 820



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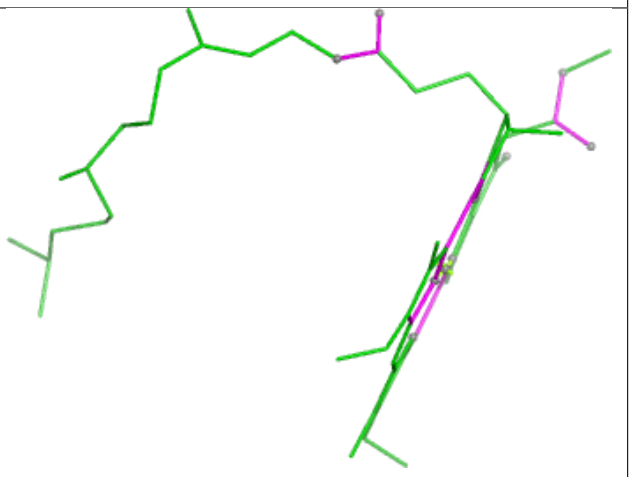

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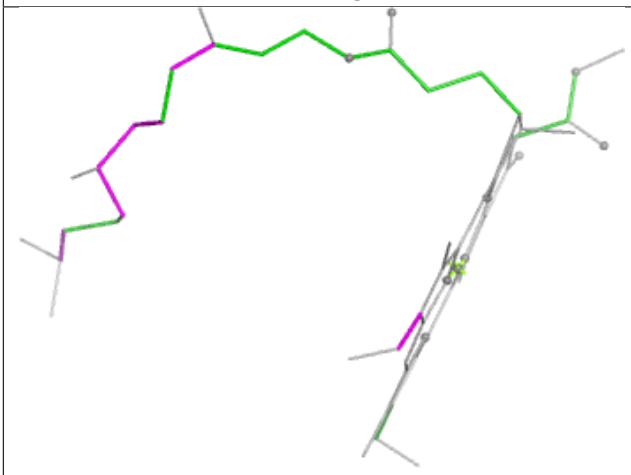
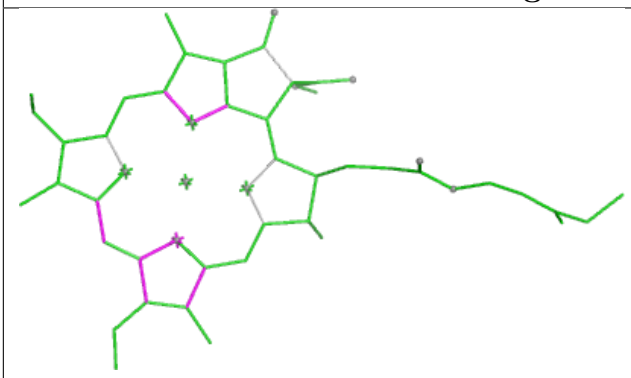


Torsions

Rings

Ligand CLA A 839



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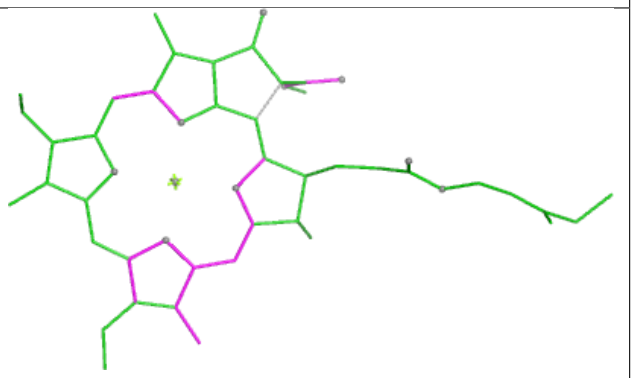

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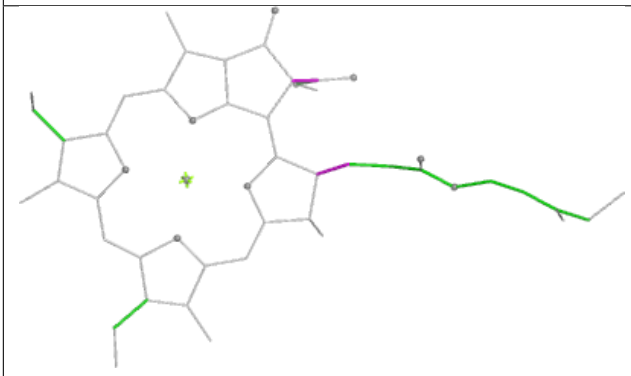

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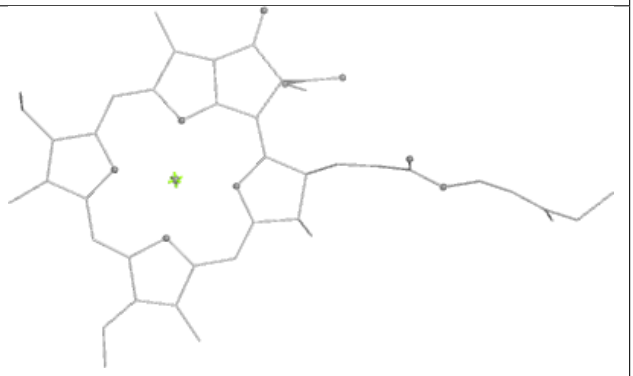
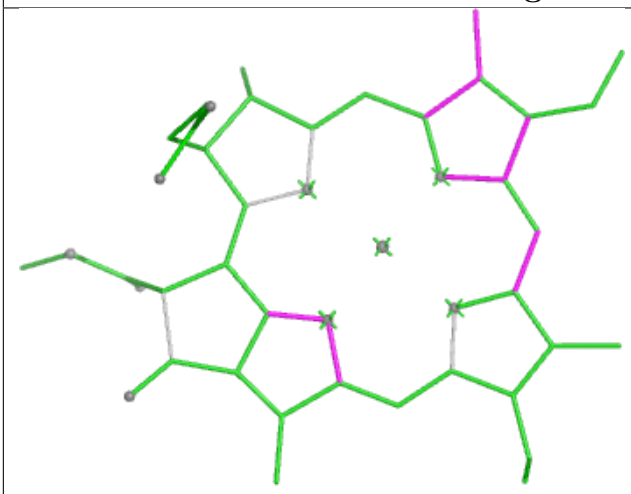


Rings

Ligand CLA B 836



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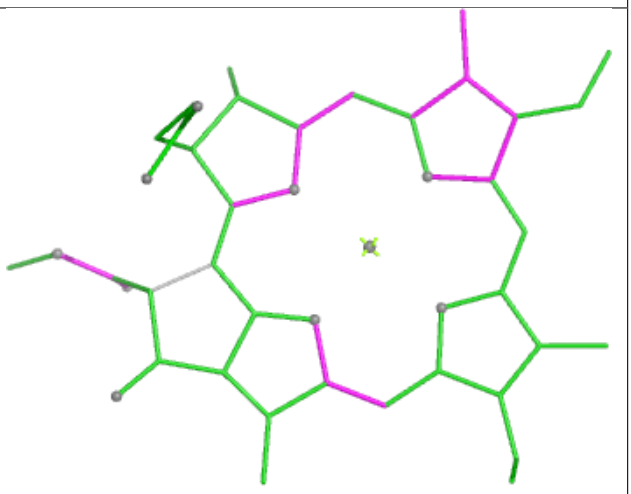
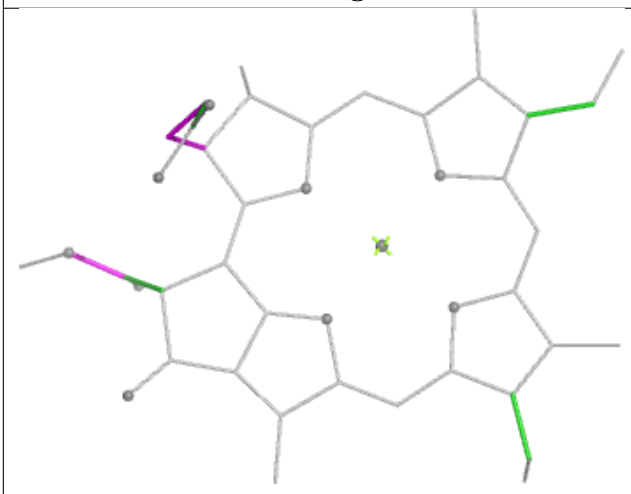


Bond angles



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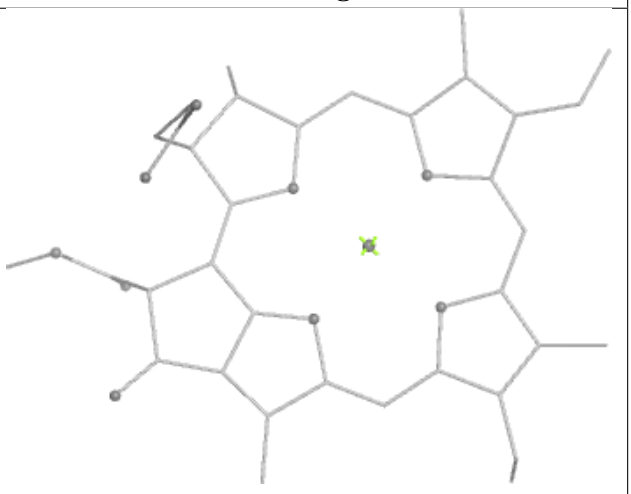
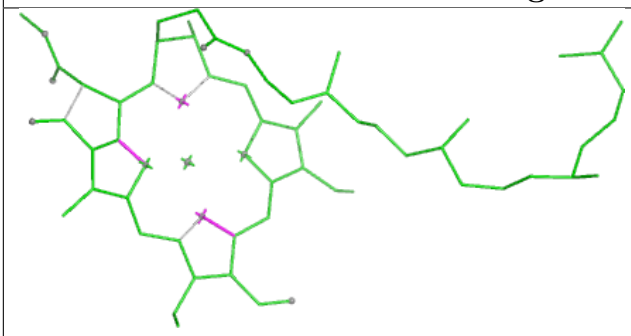


Rings

Ligand CHL 8 306



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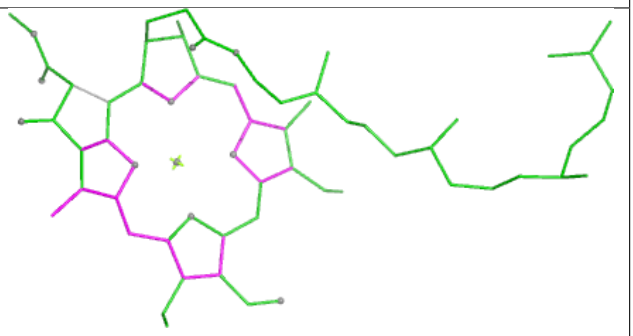

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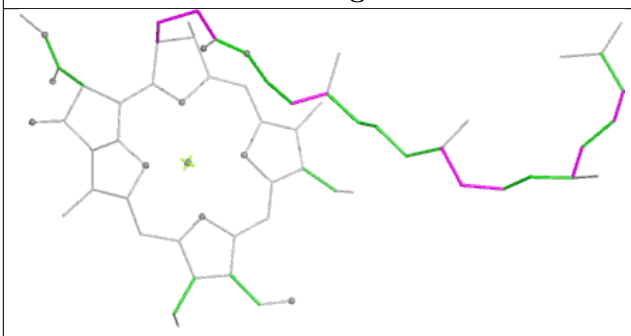

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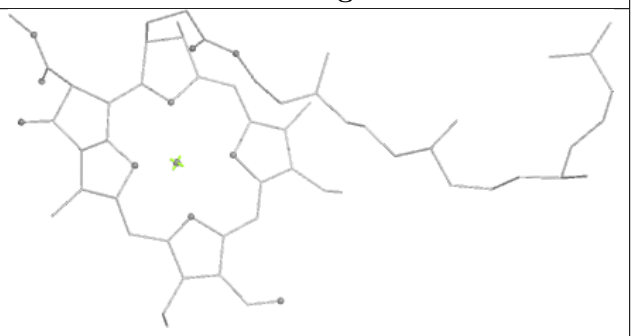
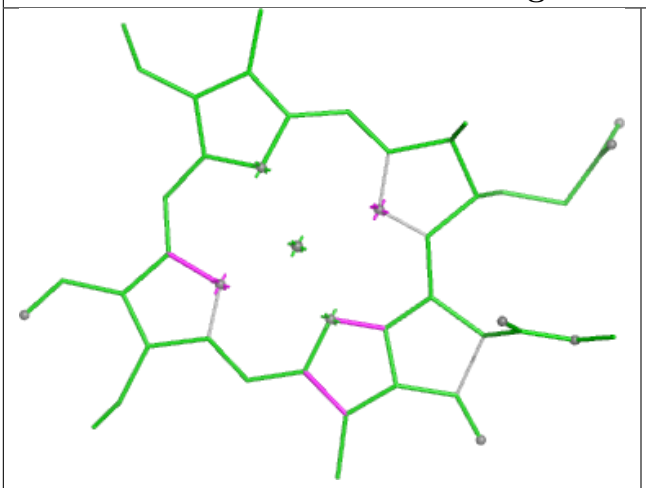


Rings

Ligand CHL 6 306



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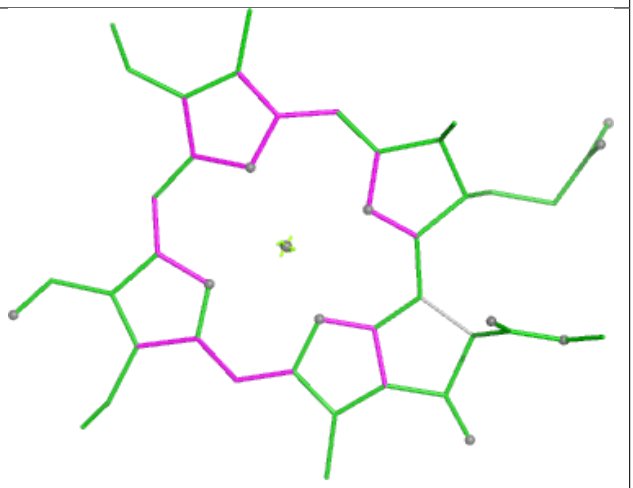

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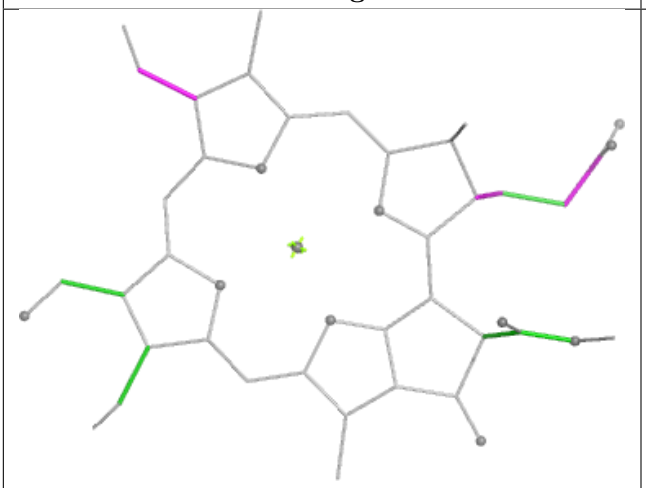

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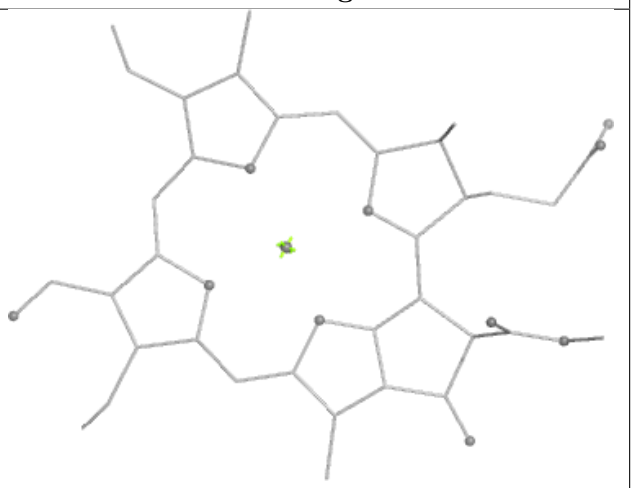
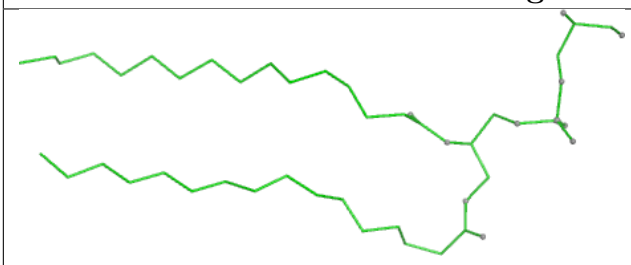


Rings

Ligand LHG 6 318



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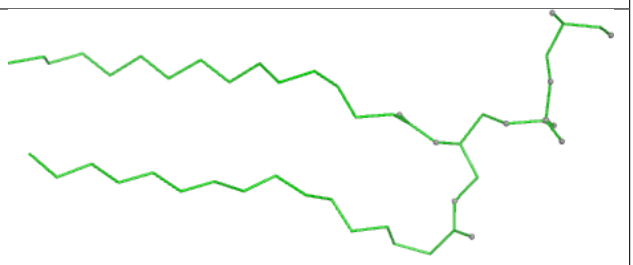
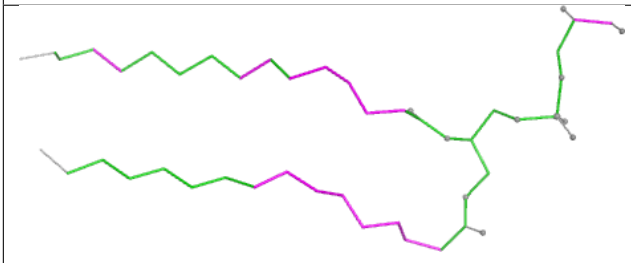


Bond angles



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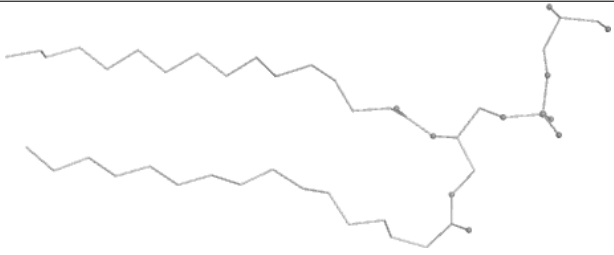
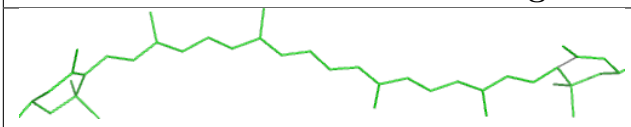
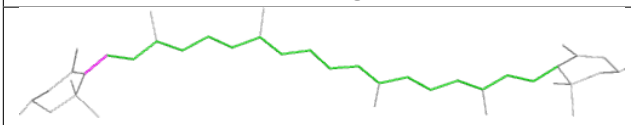
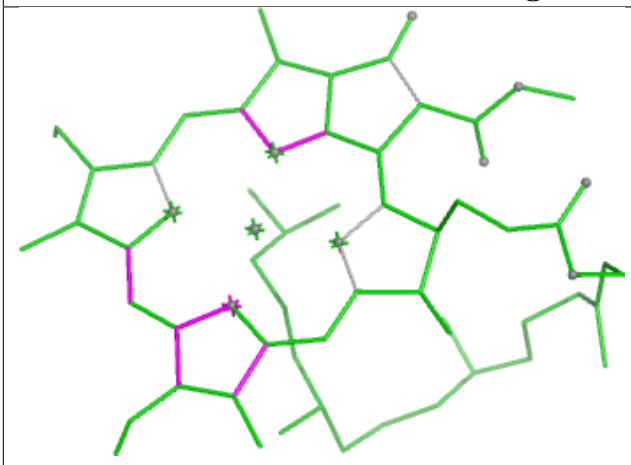
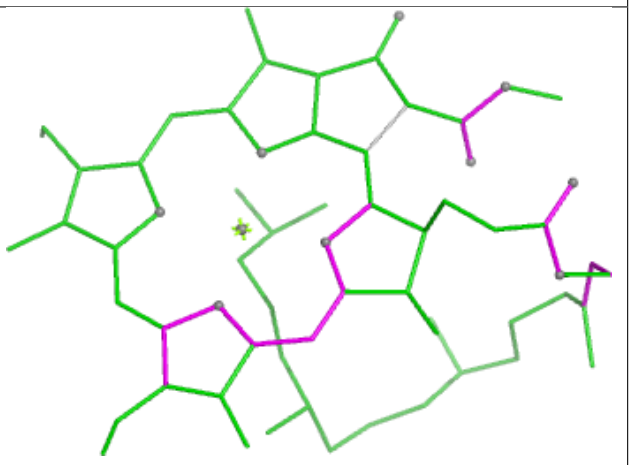
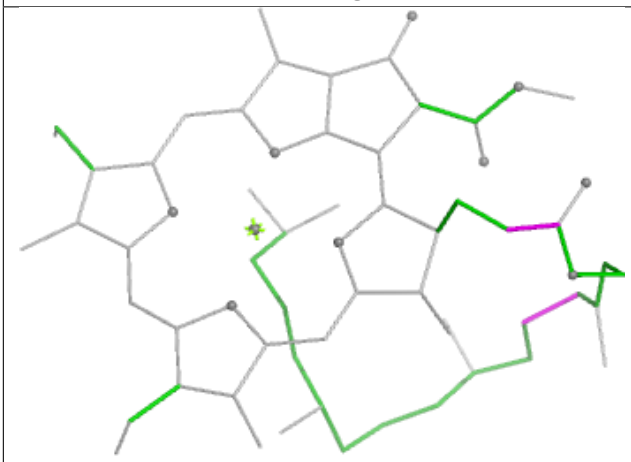
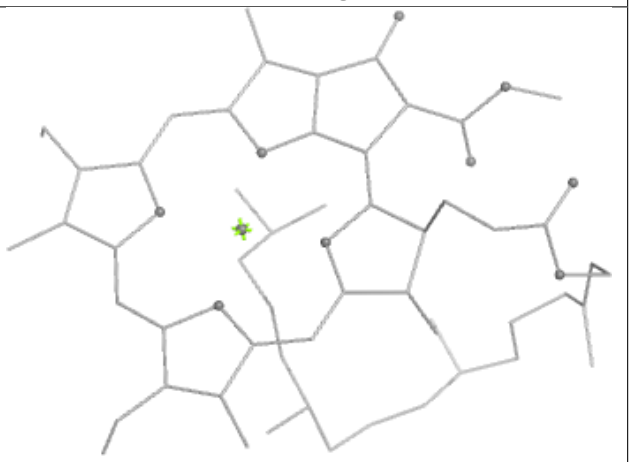
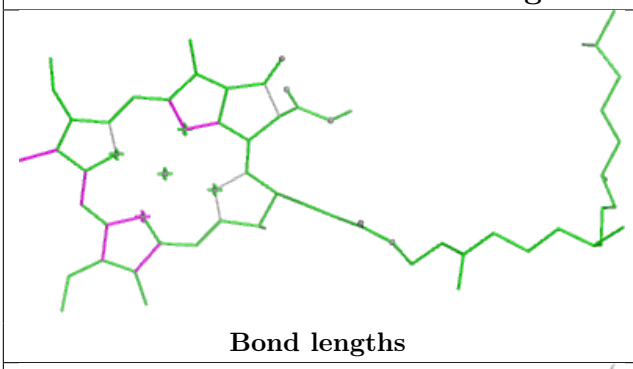


Rings

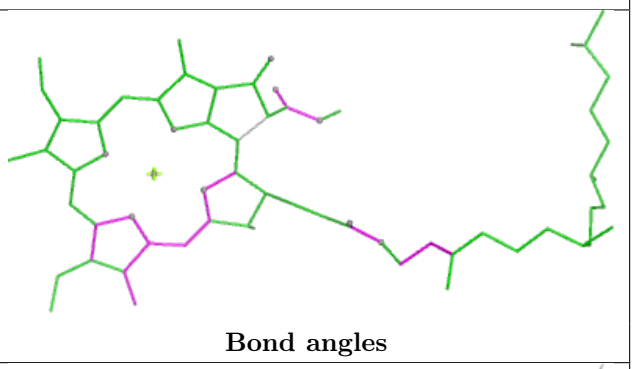
Ligand LUT 8 315	
 Bond lengths	Bond angles
 Torsions	Rings

Ligand CLA B 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

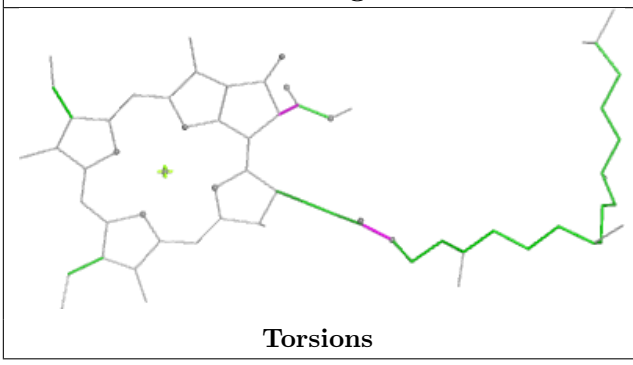
Ligand CLA B 827



Bond lengths



Bond angles



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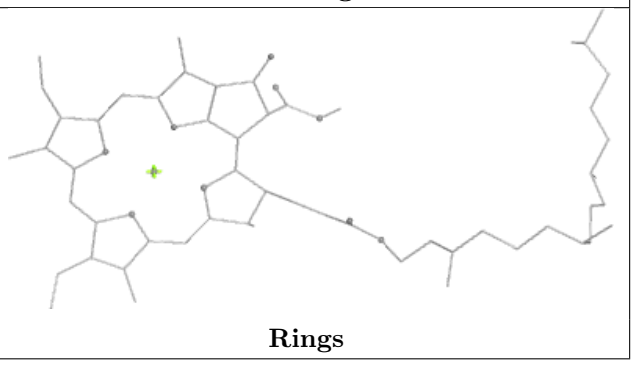
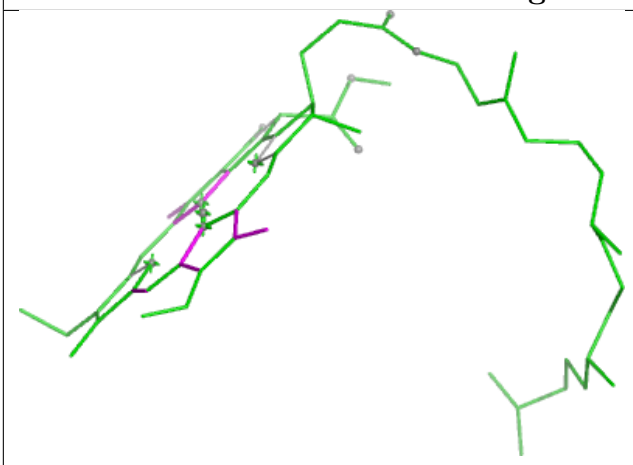


Rings

Ligand CLA 4 603



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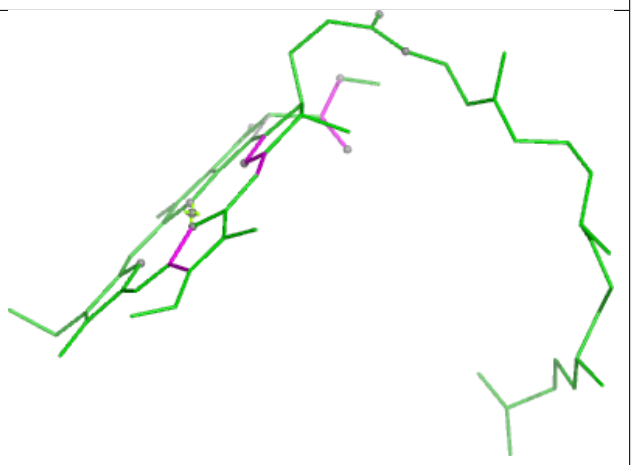
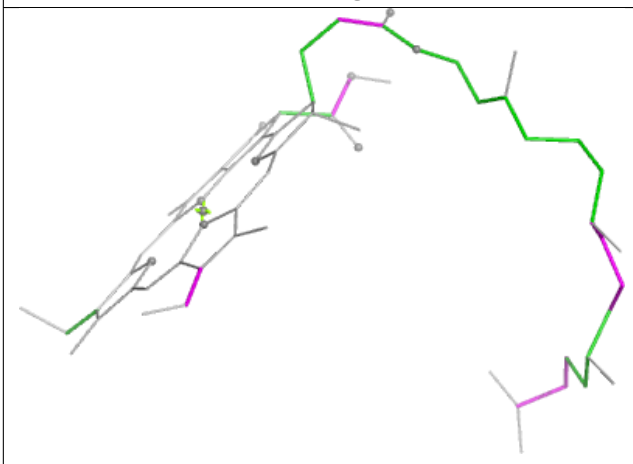


Bond angles



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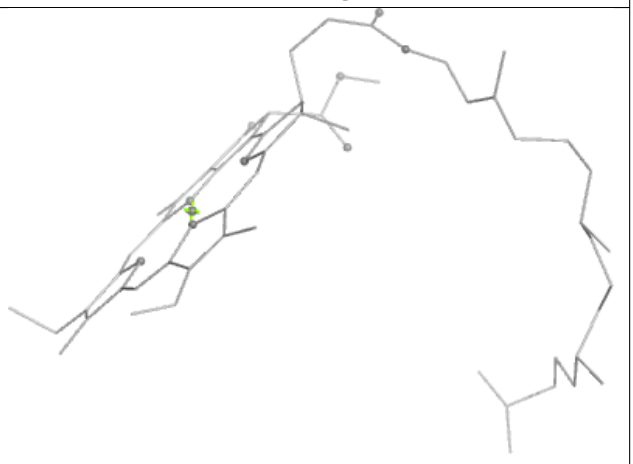
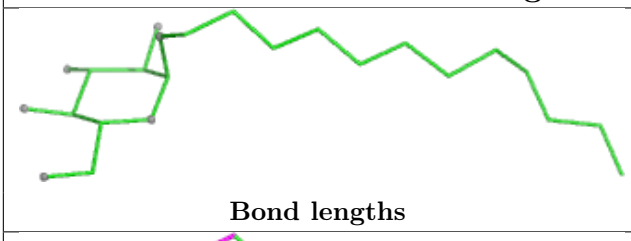


Rings

Ligand LMU 3 323



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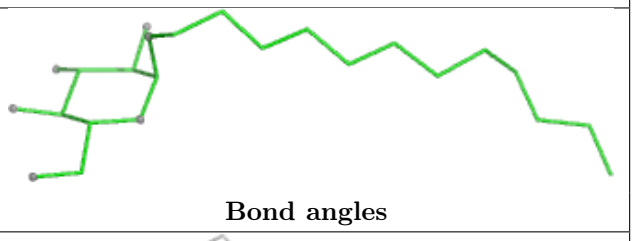
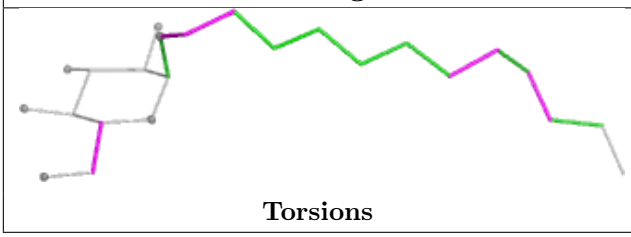


Bond angles



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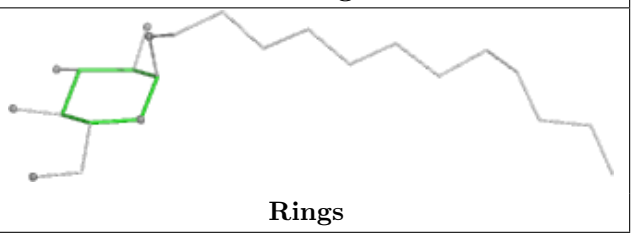
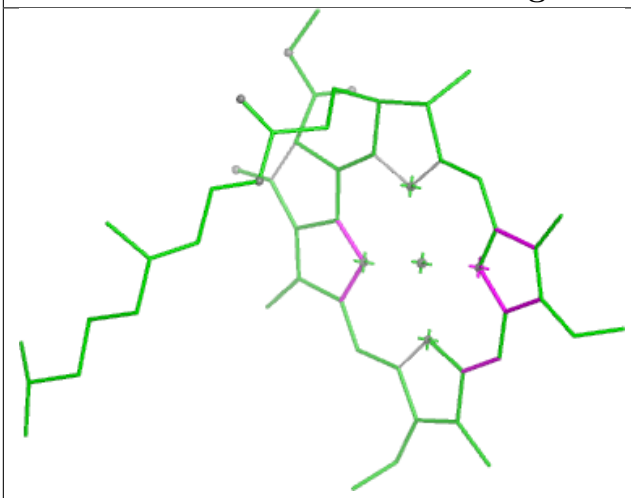


Rings

Ligand CLA 3 309



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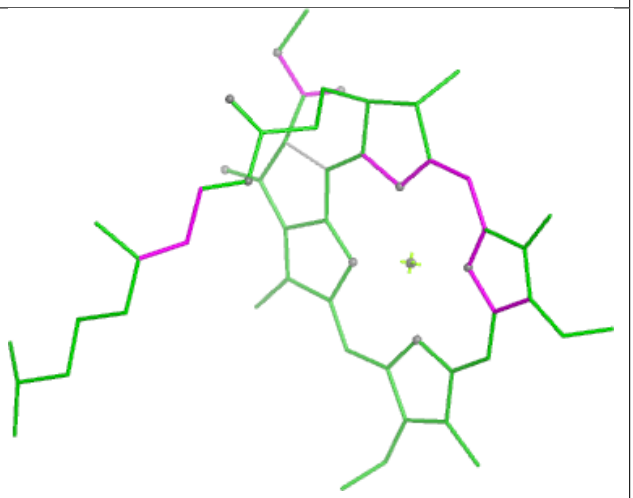
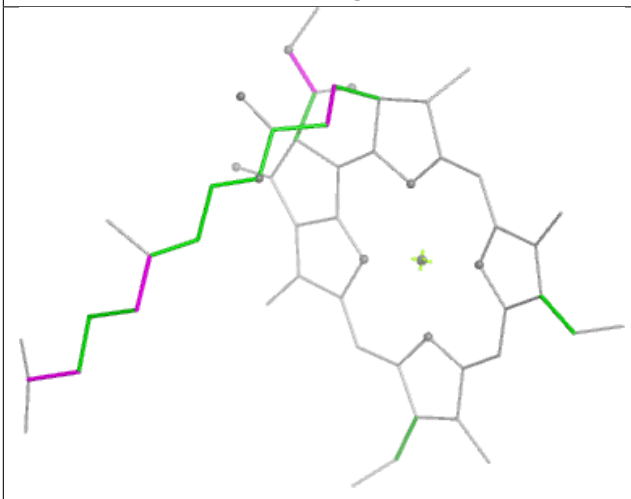


Bond angles



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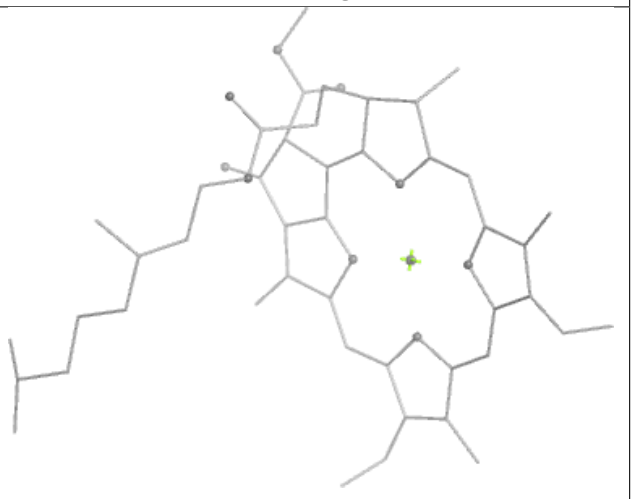
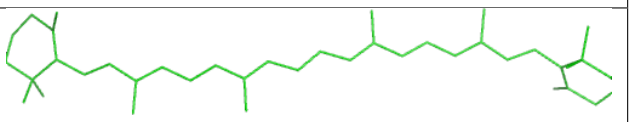
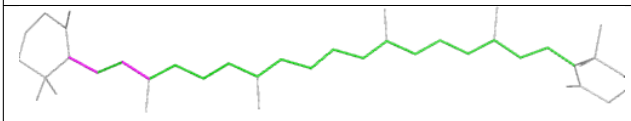
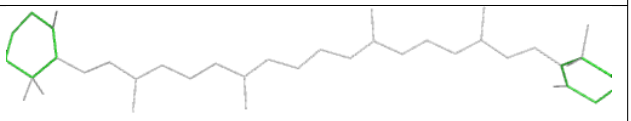
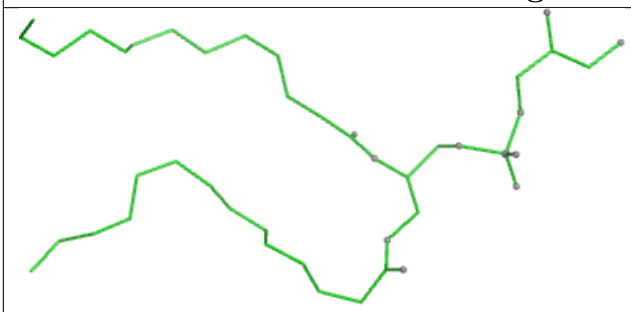
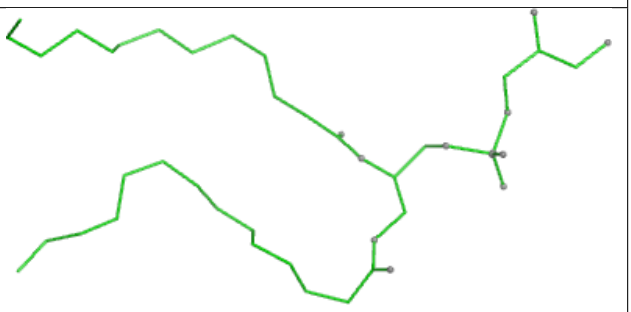
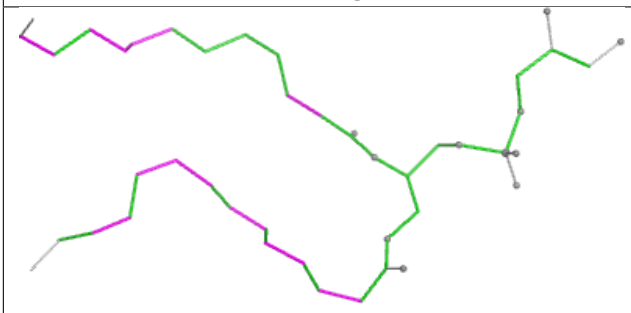
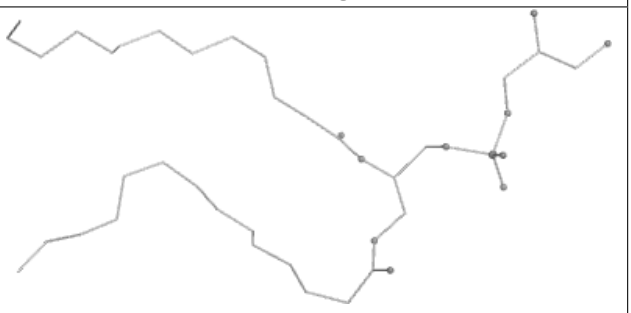
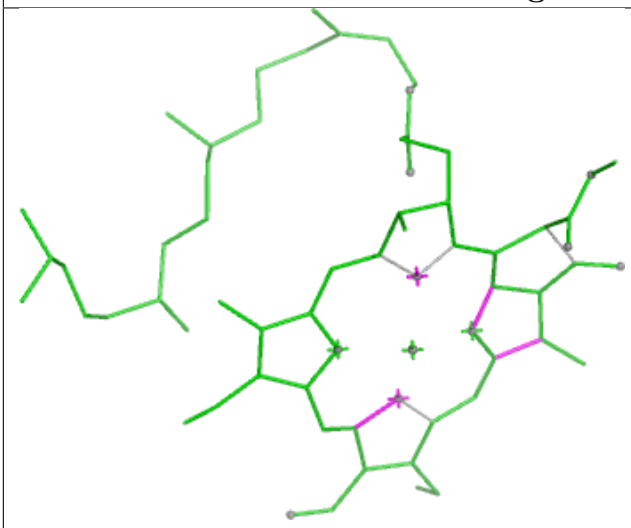


Rings

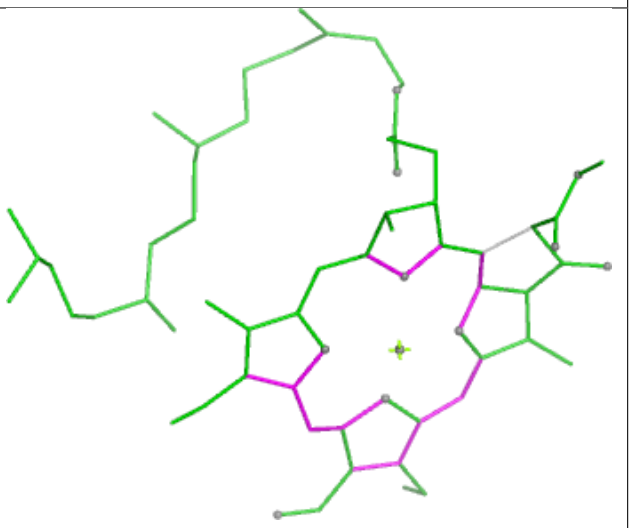
Ligand BCR A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG 1 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

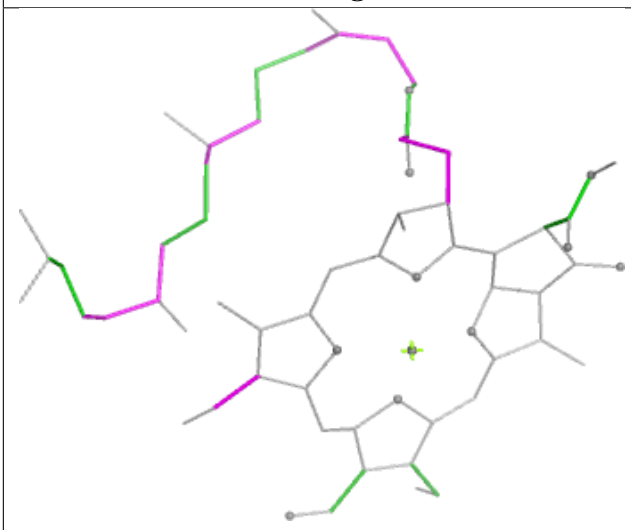
Ligand CHL 4 607



Bond lengths



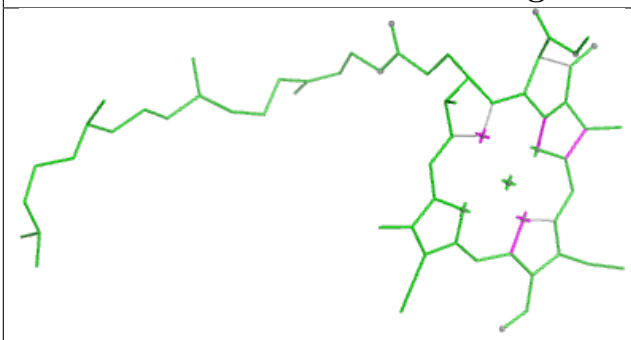
Bond angles



Torsions

Rings

Ligand CHL 7 601



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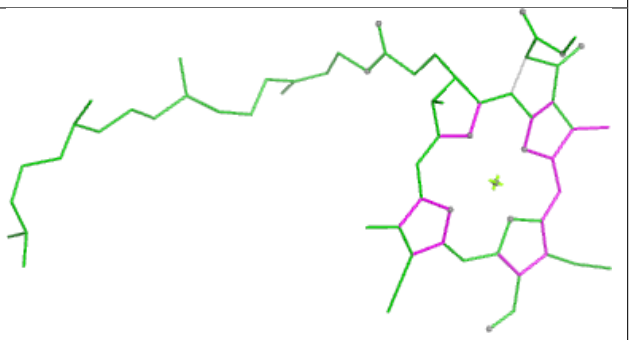
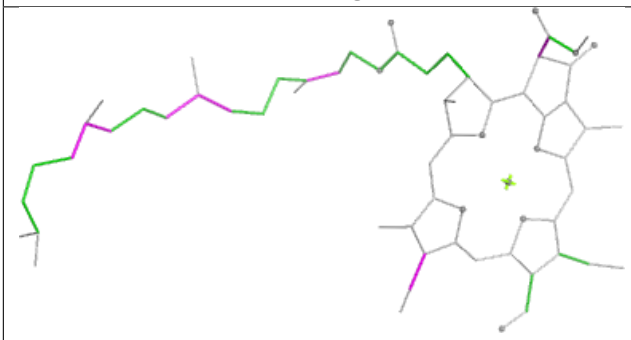
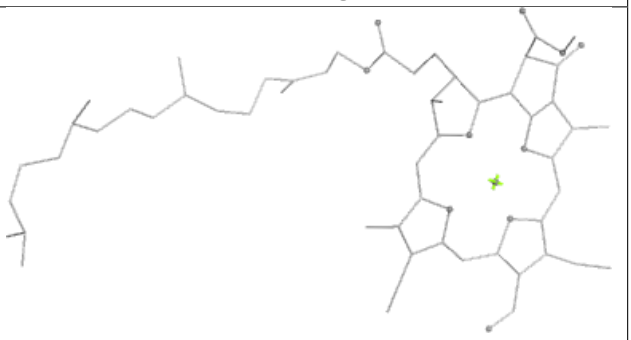


Bond angles

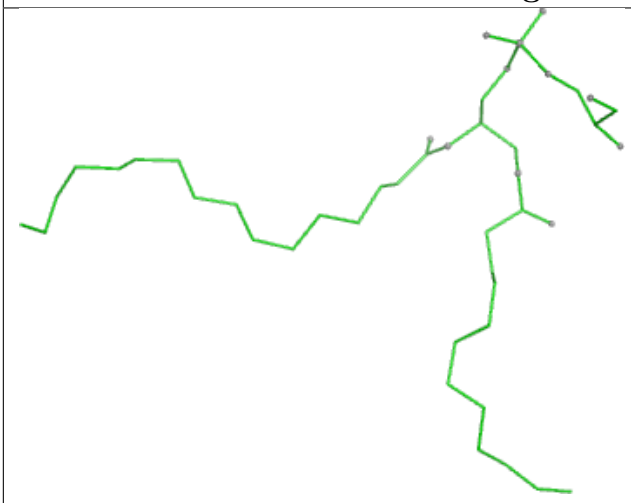


Torsions



Rings

Ligand LHG B 851



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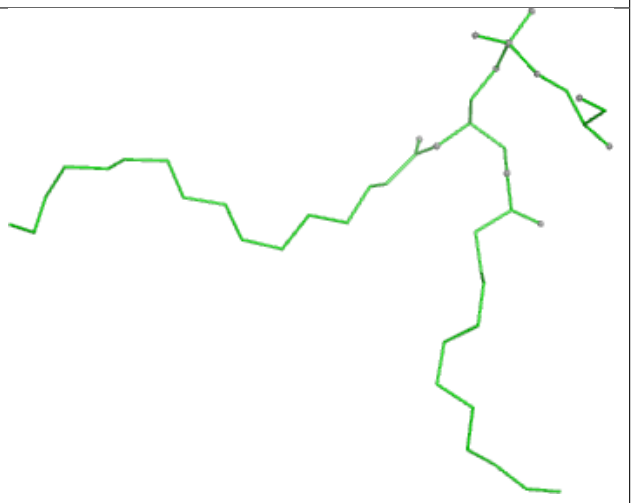

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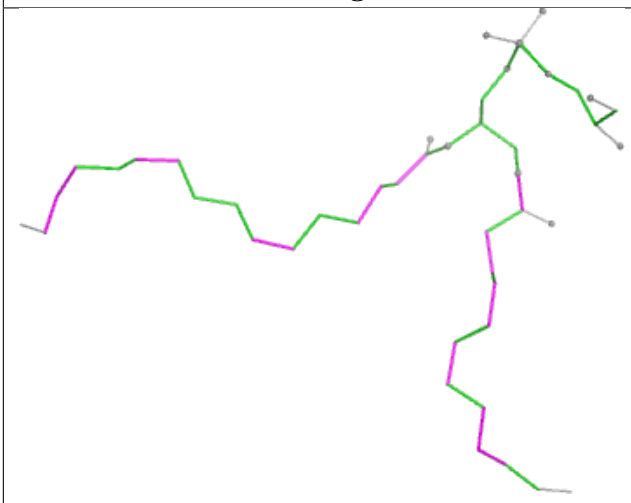
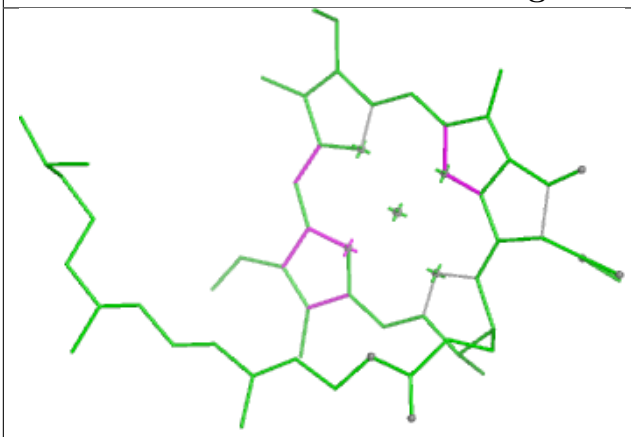


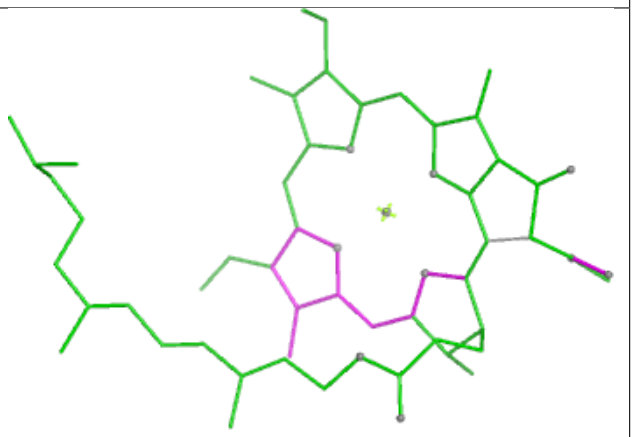
Torsions

Rings

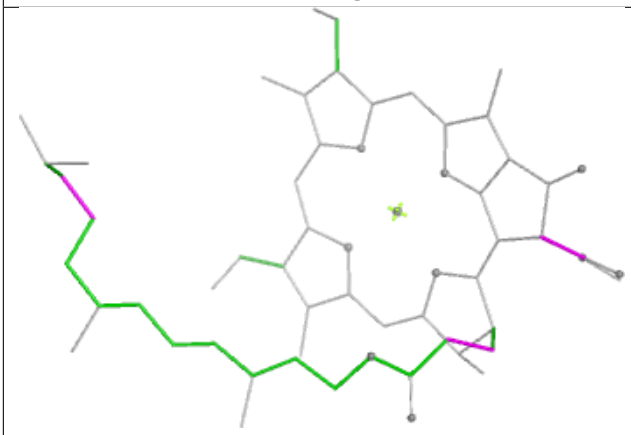
Ligand CLA 4 602



Bond lengths



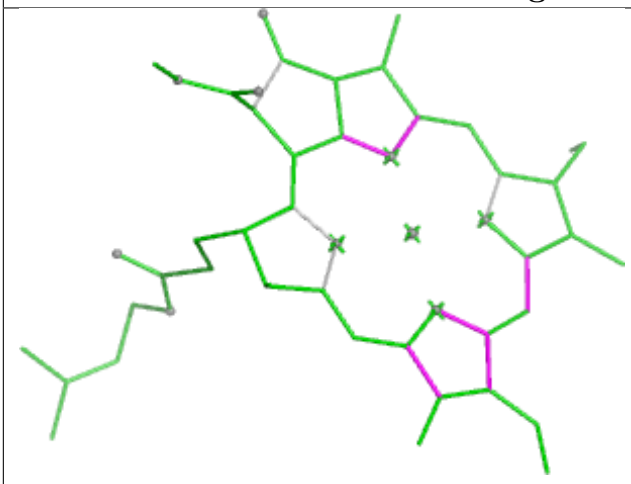
Bond angles



Torsions

Rings

Ligand CLA 7 607



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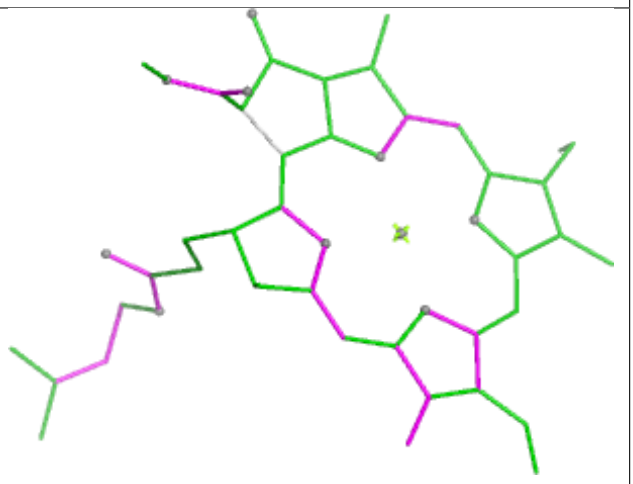
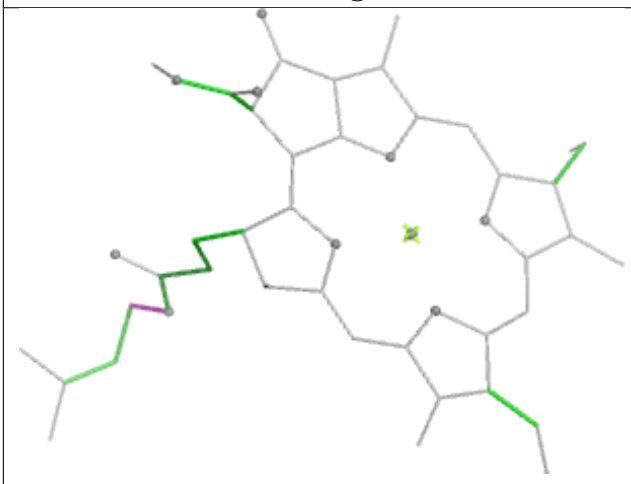


Bond angles



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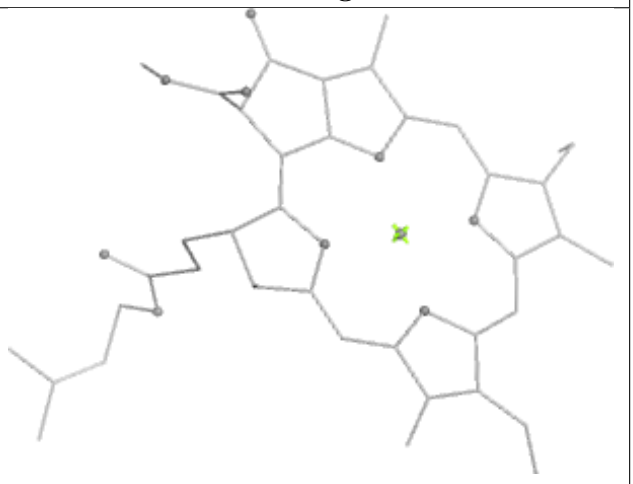
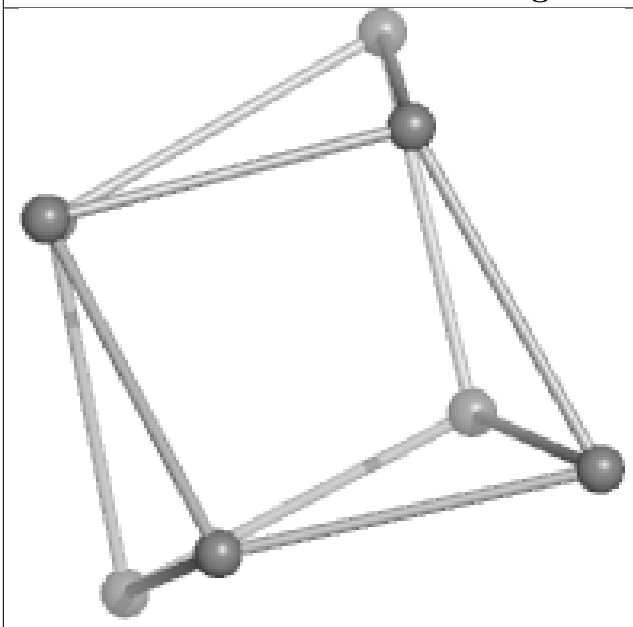


Rings

Ligand SF4 C 102



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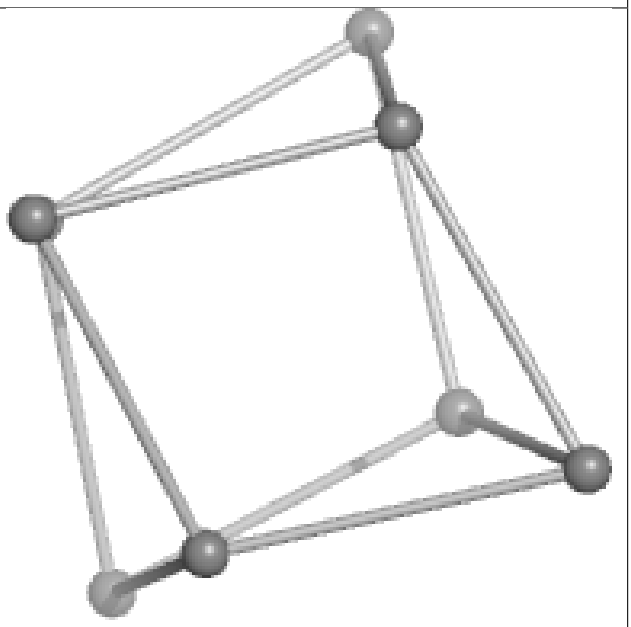
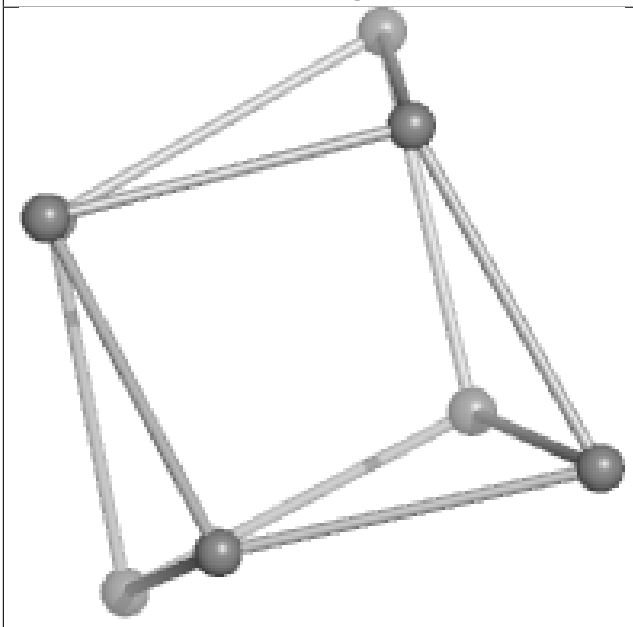


Bond angles



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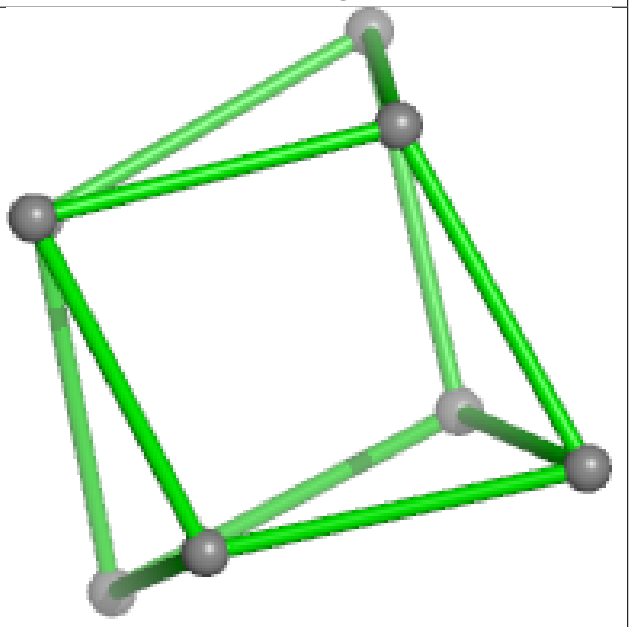
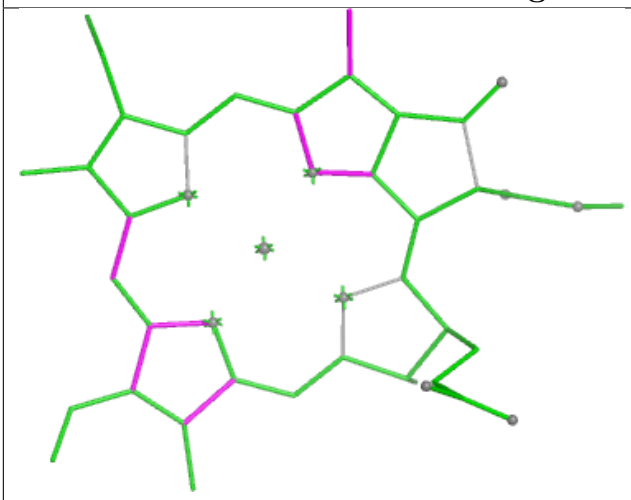


Rings

Ligand CLA 8 308



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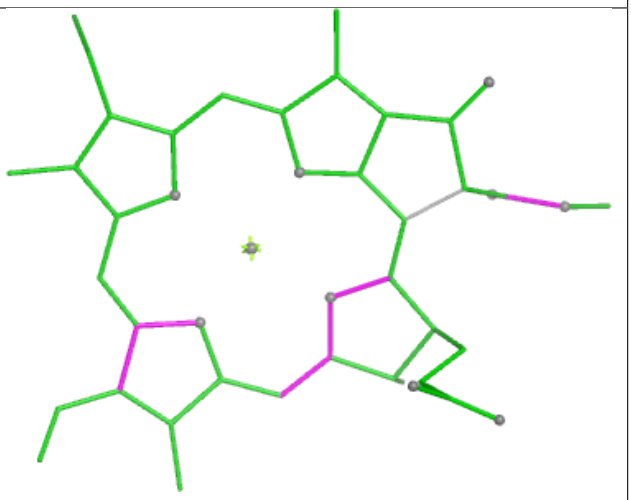
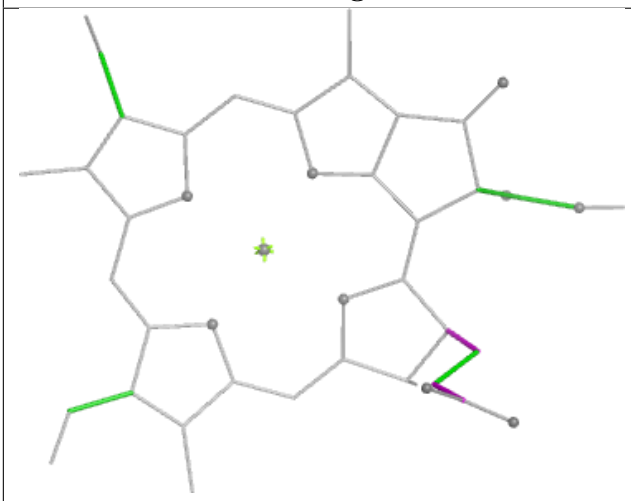


Bond angles



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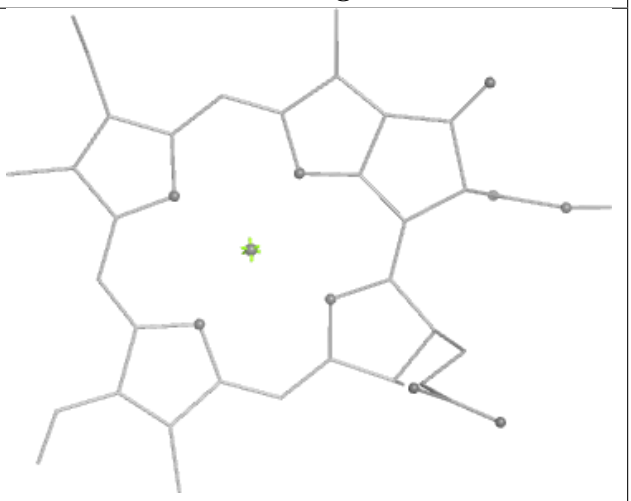
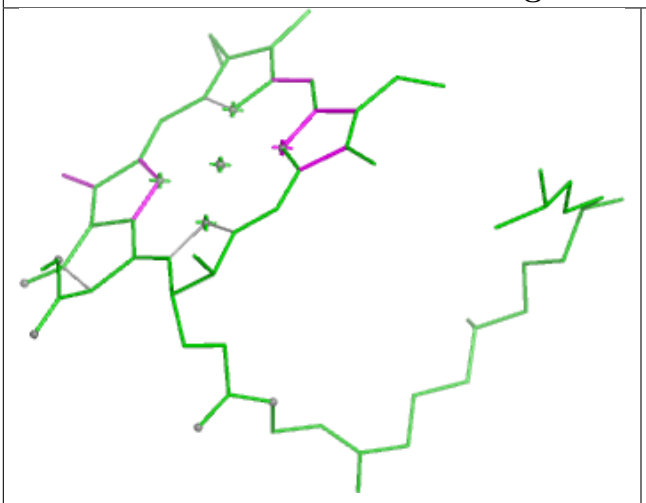


Rings

Ligand CLA B 816



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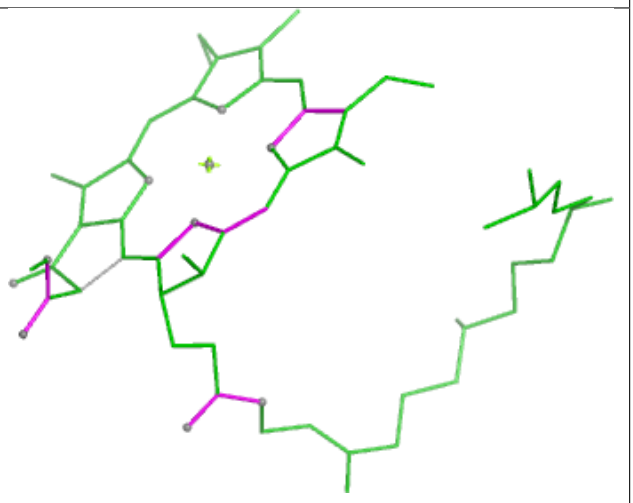
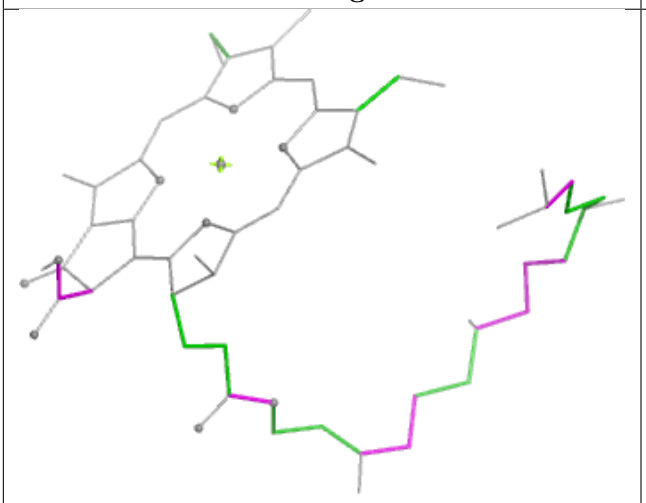


Bond angles



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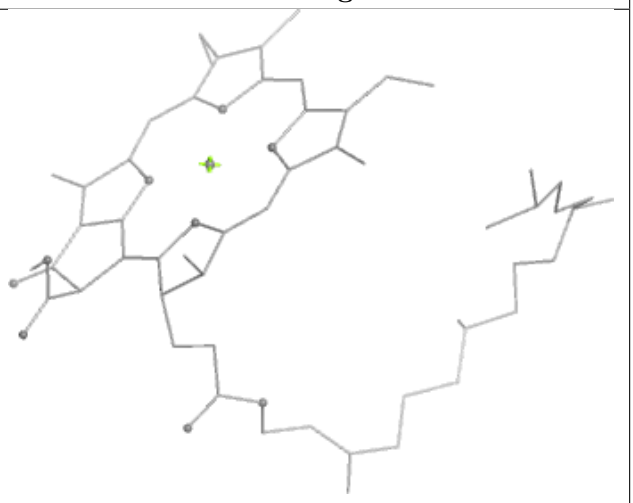
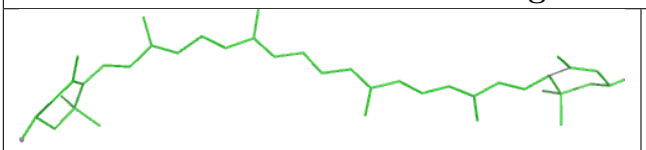


Rings

Ligand LUT 5 318



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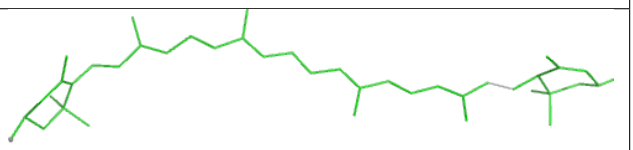

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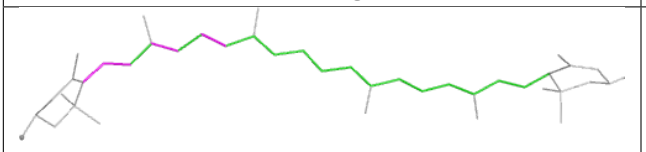
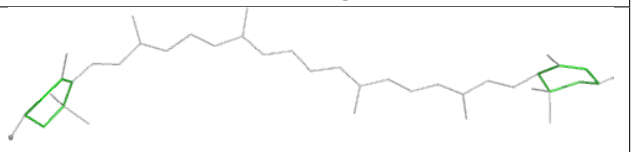
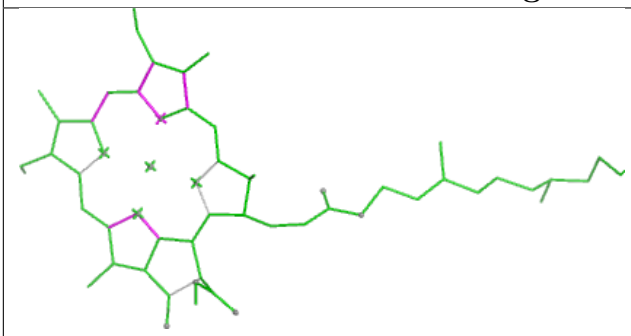


Torsions

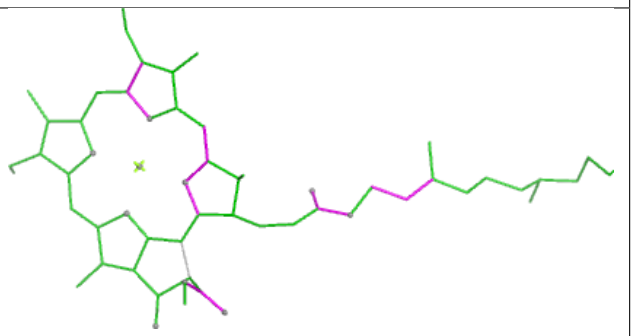


Rings

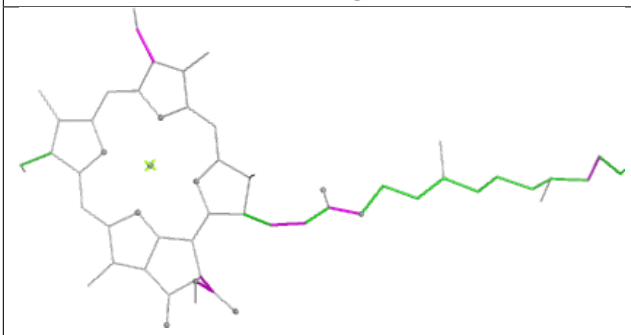
Ligand CLA G 202



Bond lengths



Bond angles



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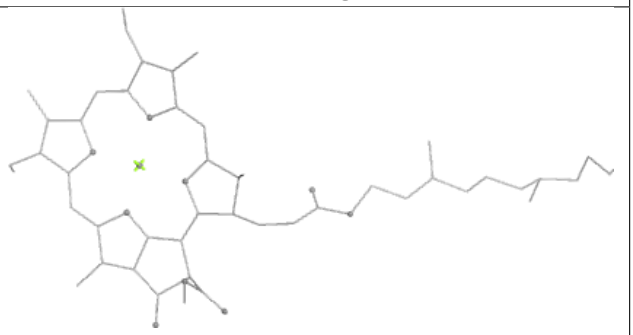
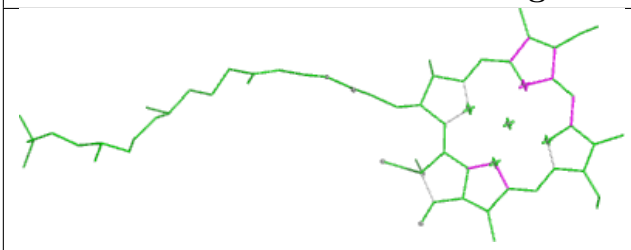


Rings

Ligand CLA 5 302



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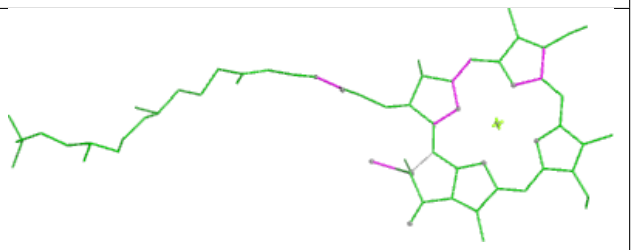
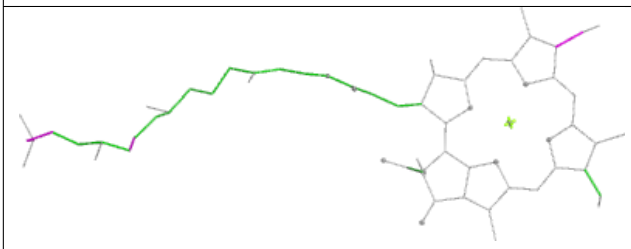


Bond angles



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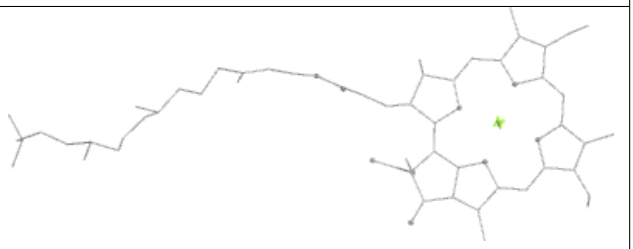
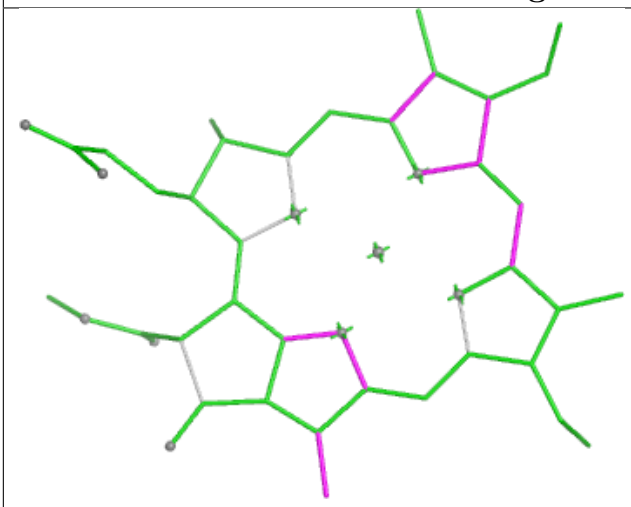


Rings

Ligand CLA 8 314



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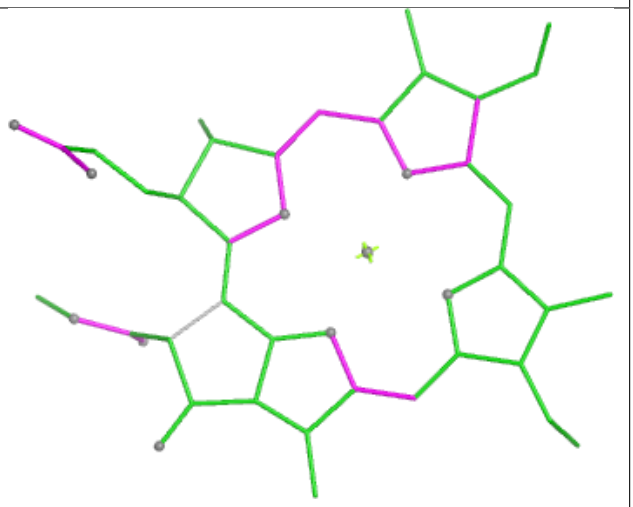
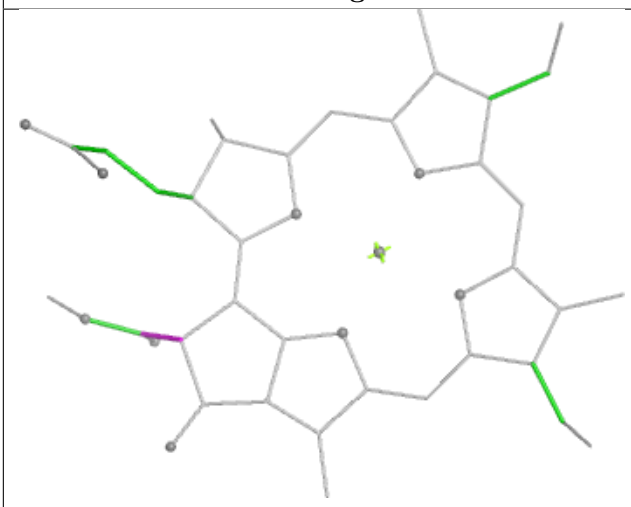
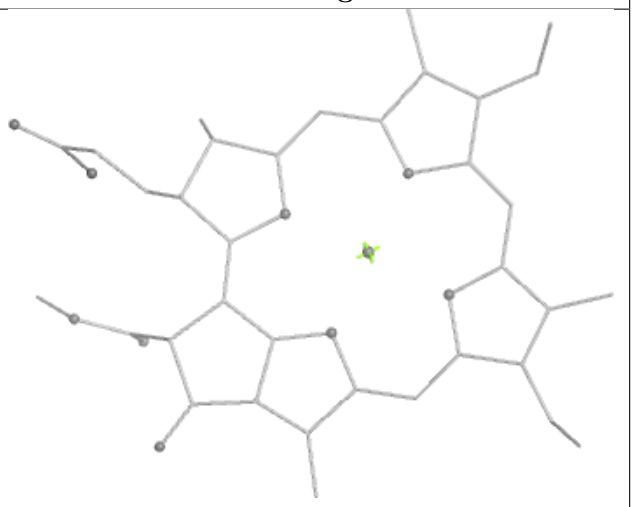


Bond angles

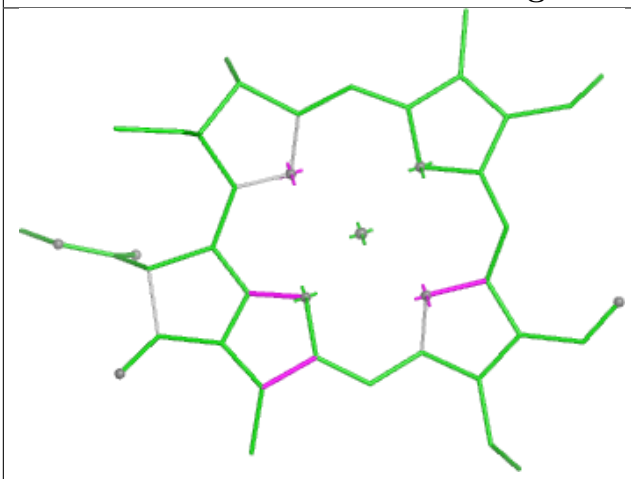


Torsions

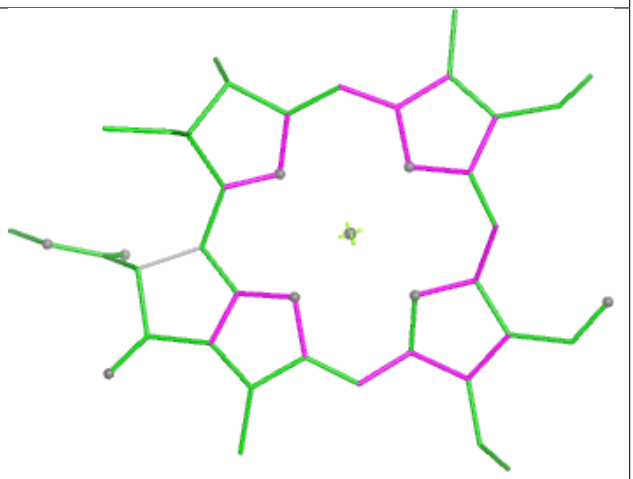


Rings

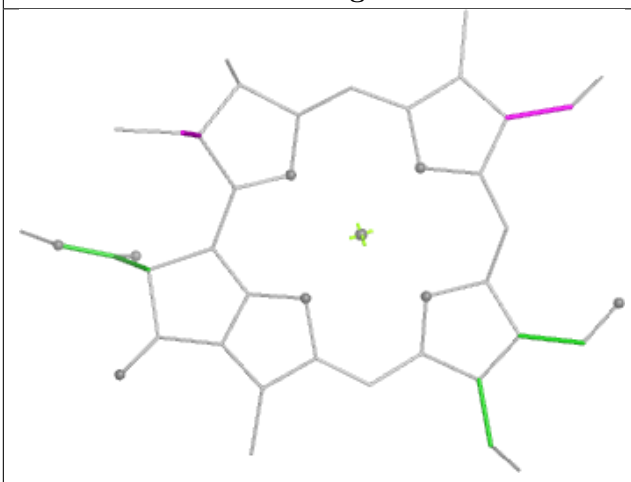
Ligand CHL 4 606



Bond lengths



Bond angles



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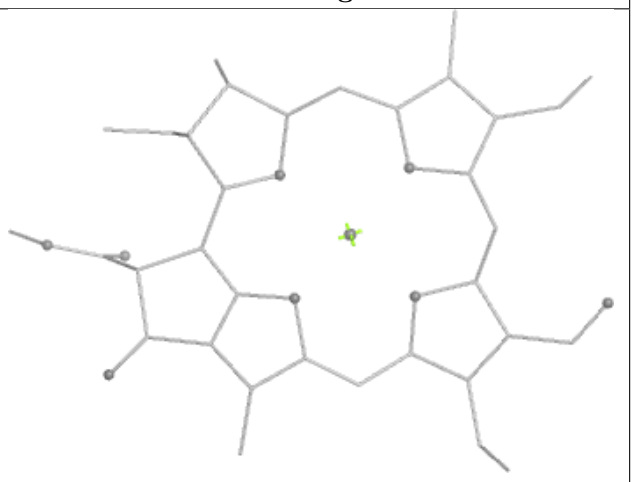
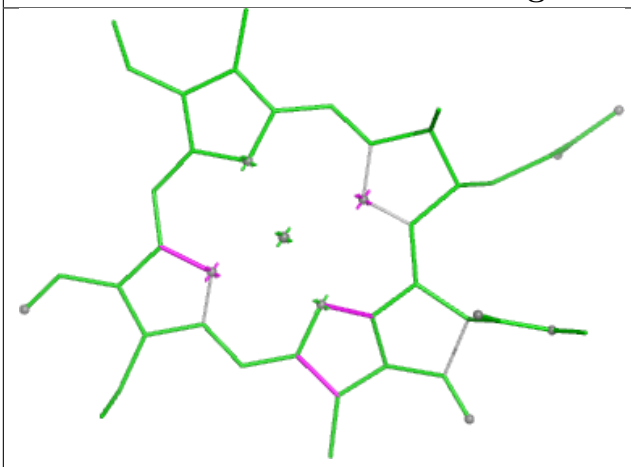


Rings

Ligand CHL 7 605



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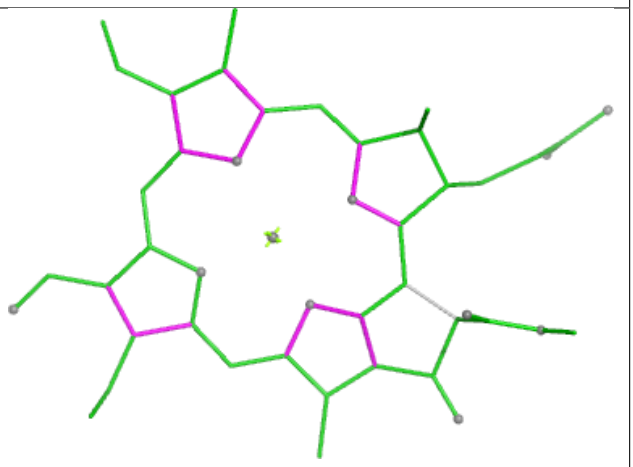
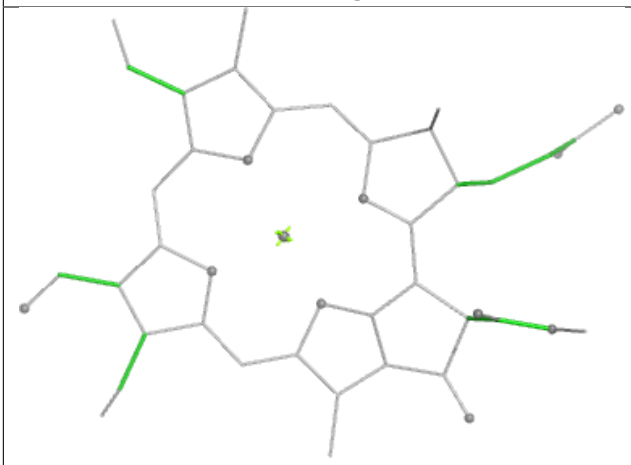
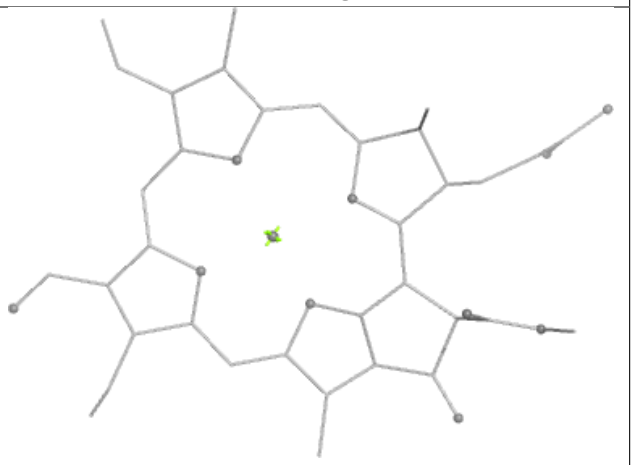


Bond angles

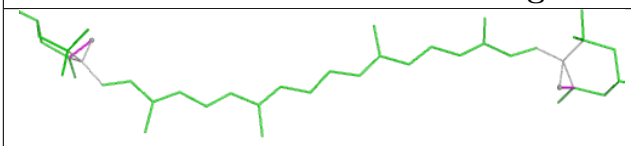


Torsions



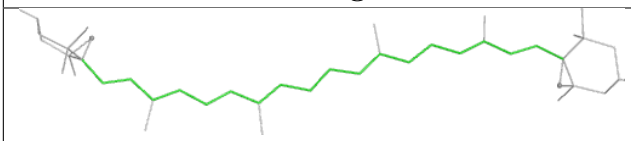
Rings

Ligand XAT 4 617



Bond lengths

Bond angles



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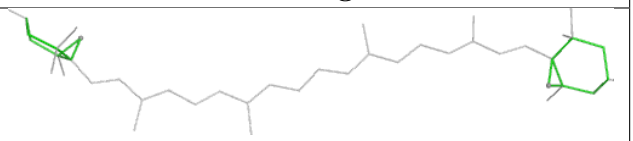
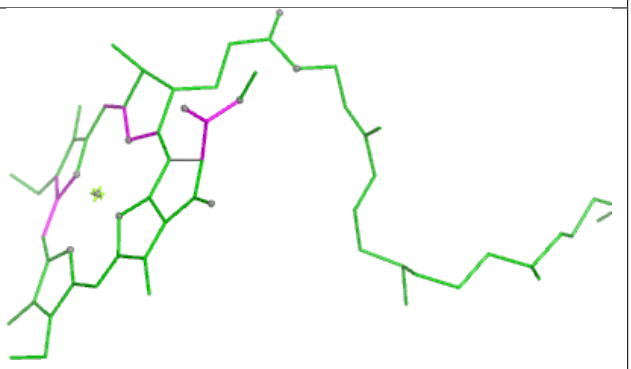


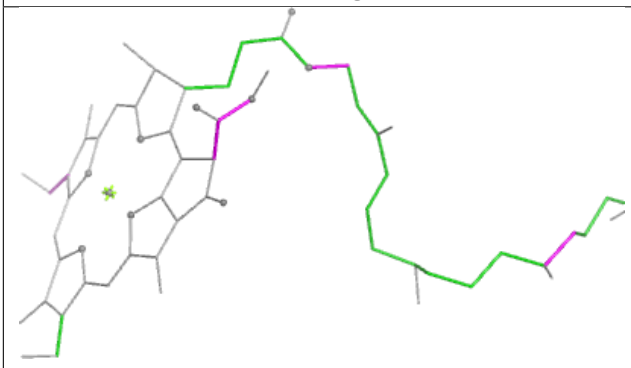
Rings

Ligand CLA B 803

Bond lengths



Bond angles



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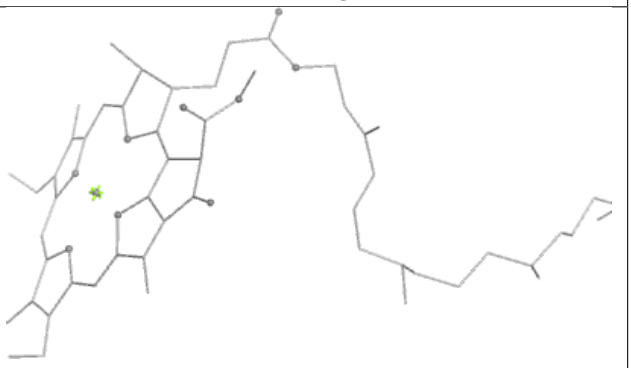
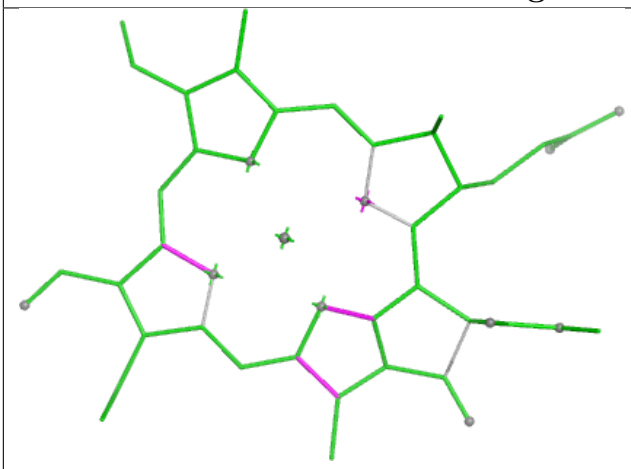


Rings

Ligand CHL 1 305



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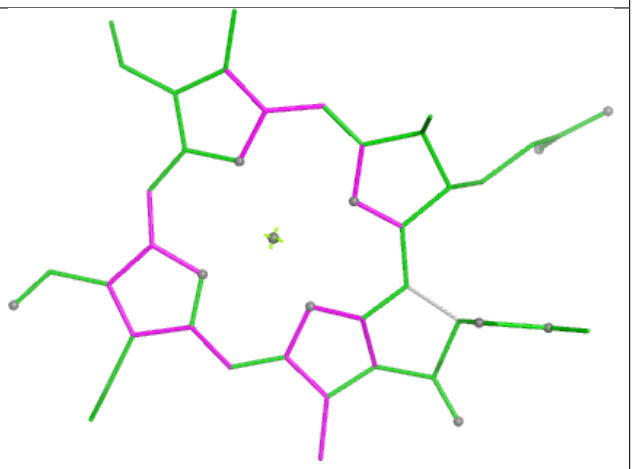
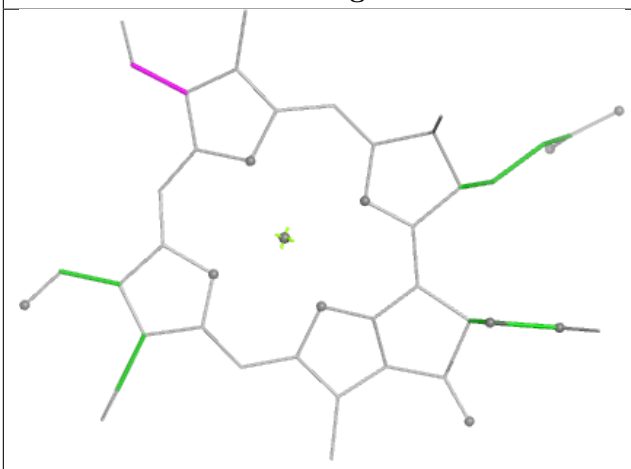


Bond angles



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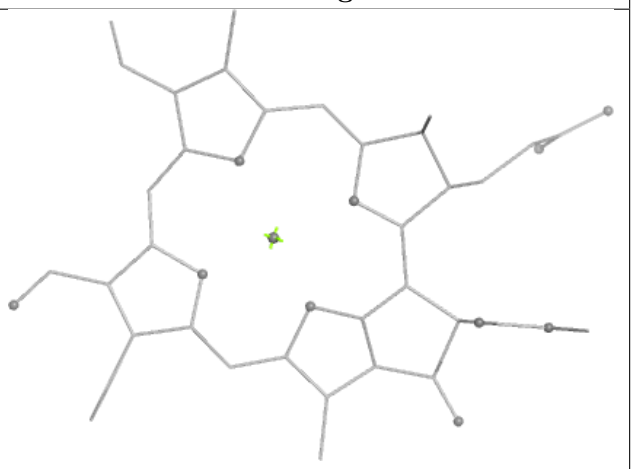
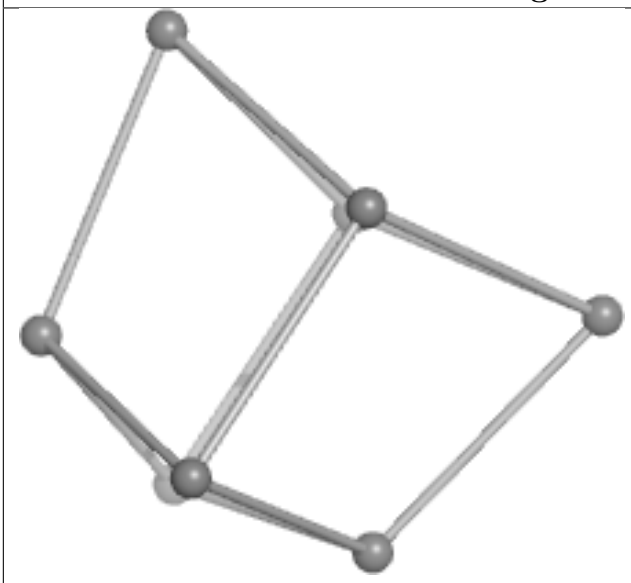


Rings

Ligand SF4 A 854



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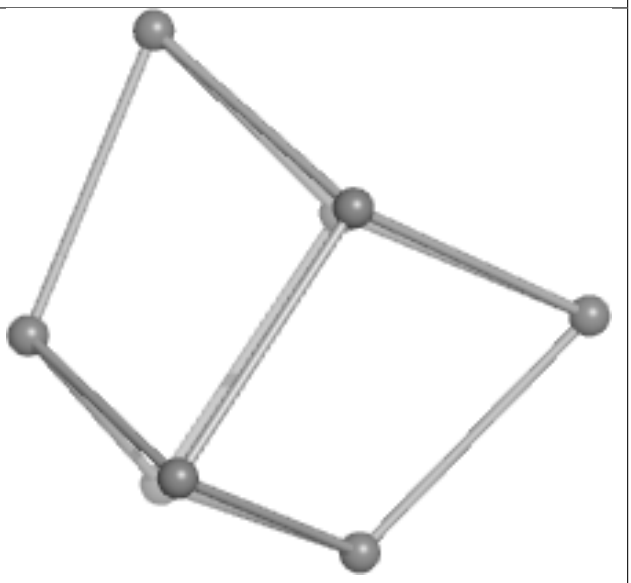
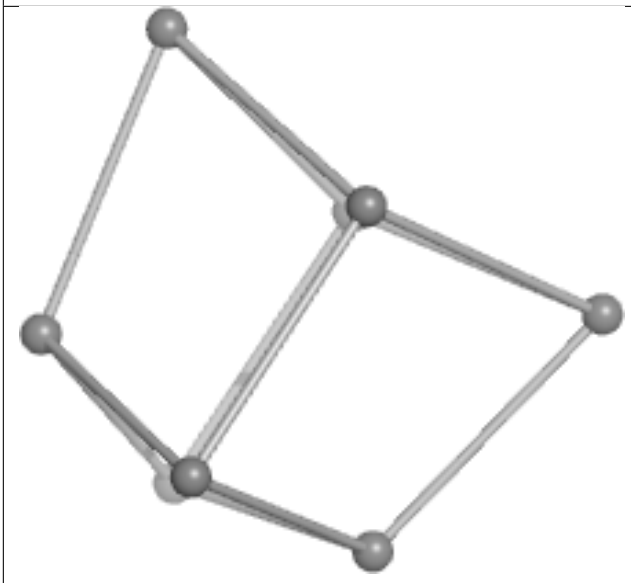


Bond angles



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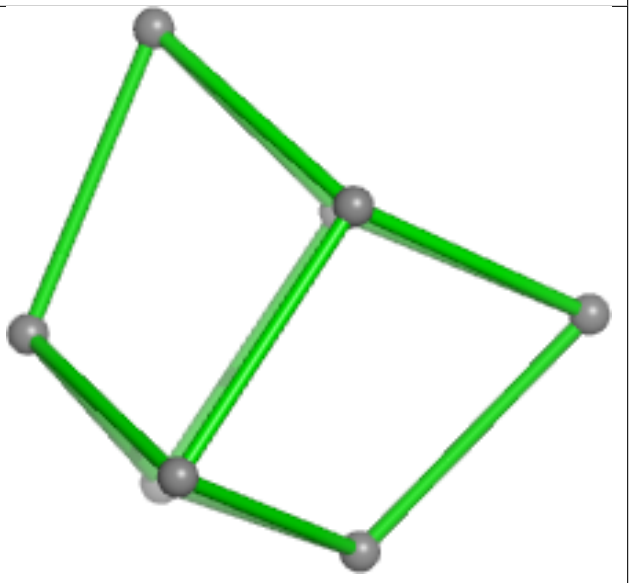
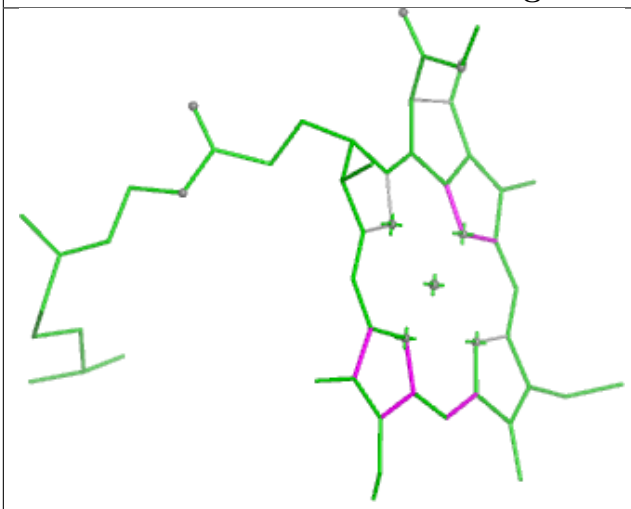


Rings

Ligand CLA A 806



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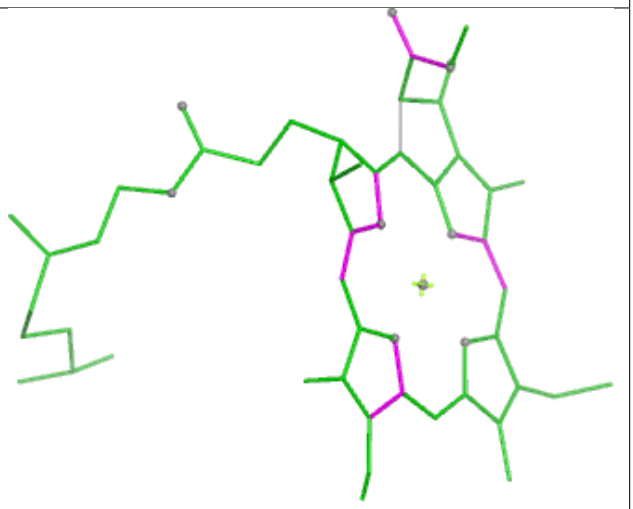
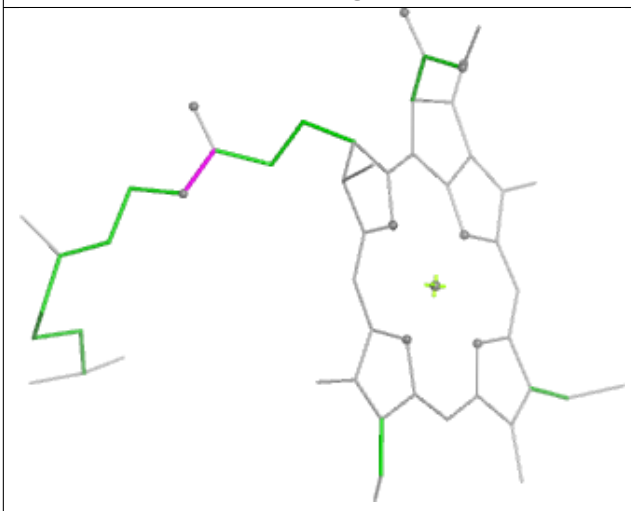


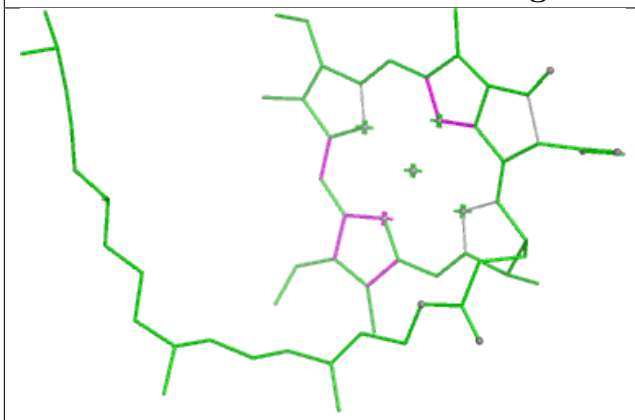
Bond angles



Torsions

Rings

Ligand CLA 7 602



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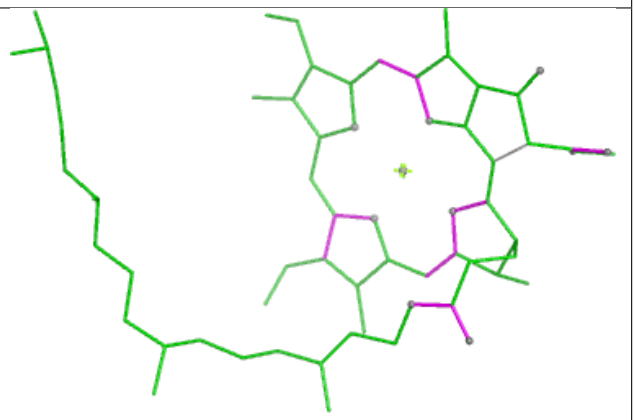
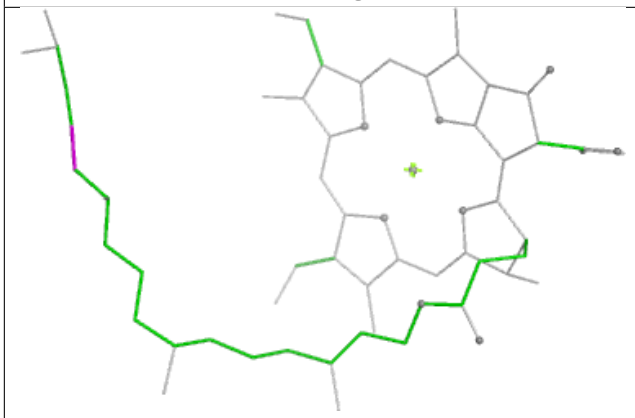


Bond angles



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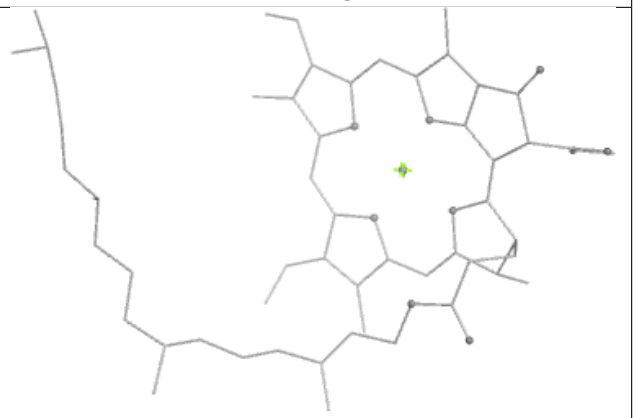
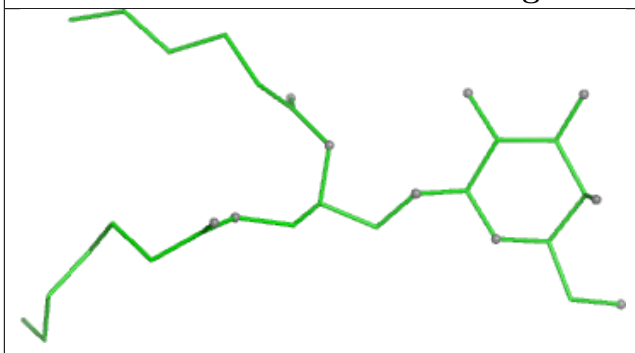


Rings

Ligand LMG F 301



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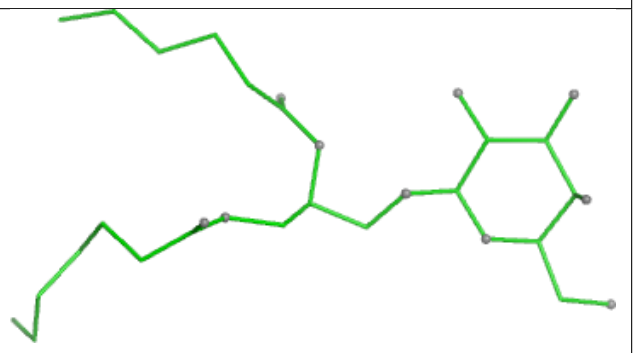
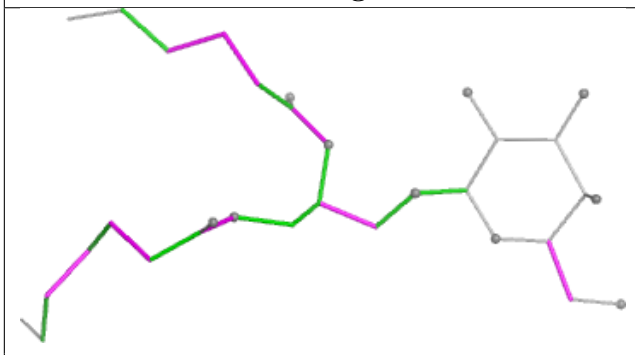


Bond angles



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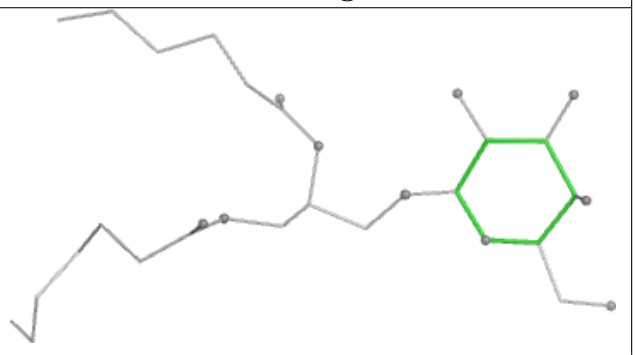
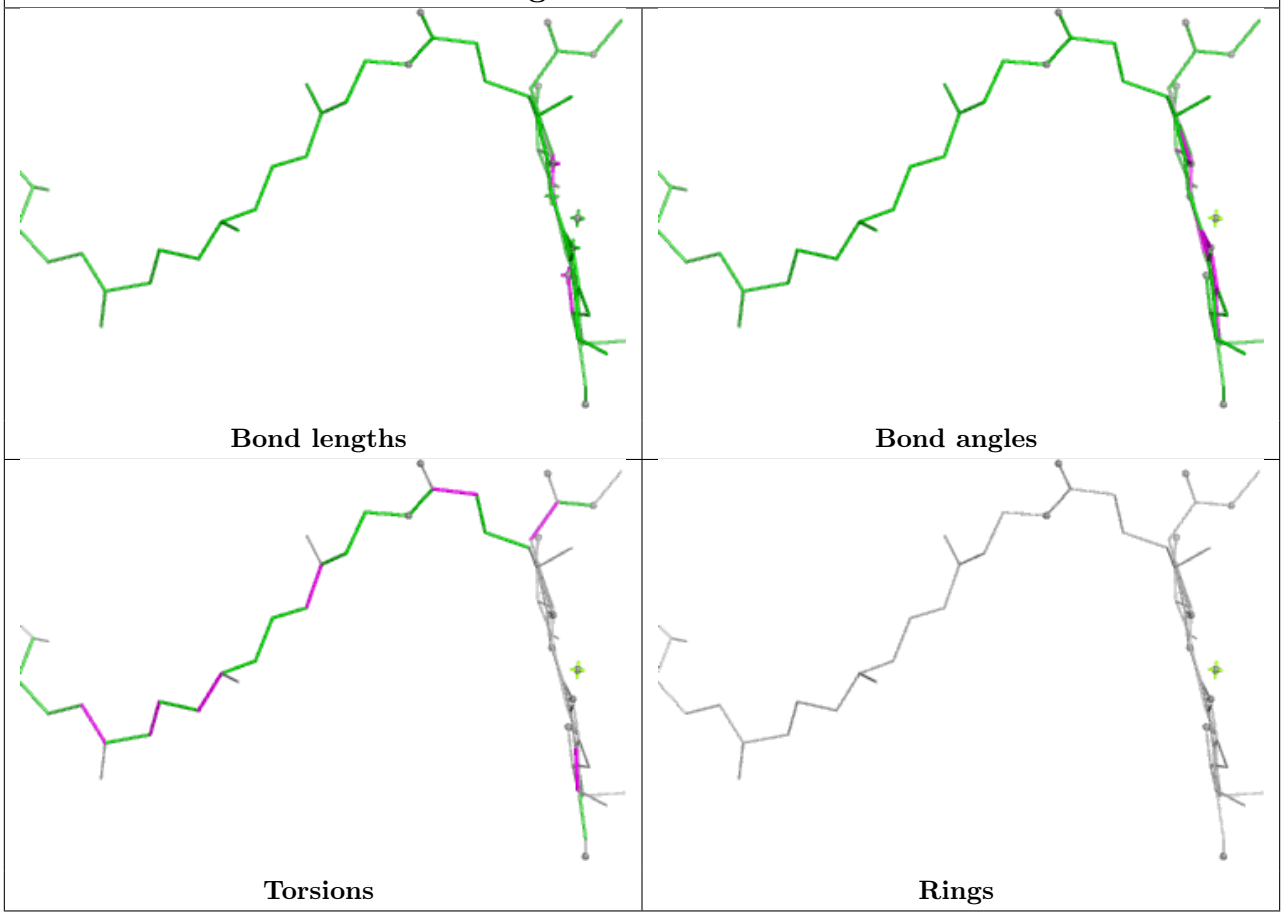
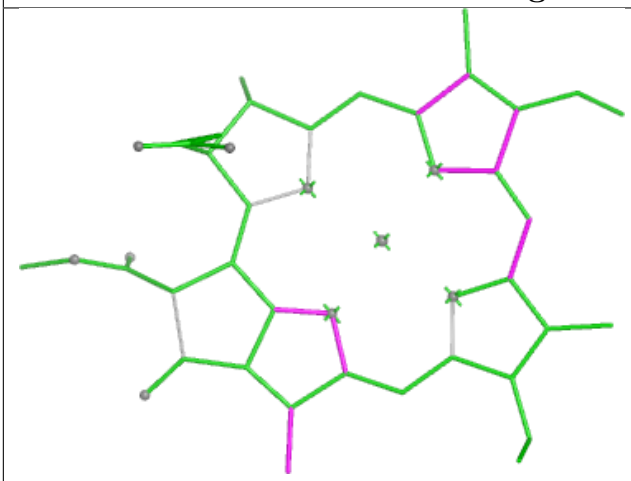


Rings

Ligand CHL 7 621



Ligand CLA 5 315



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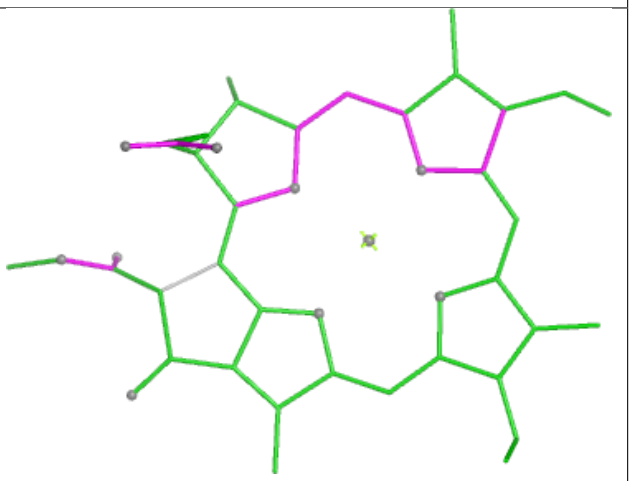
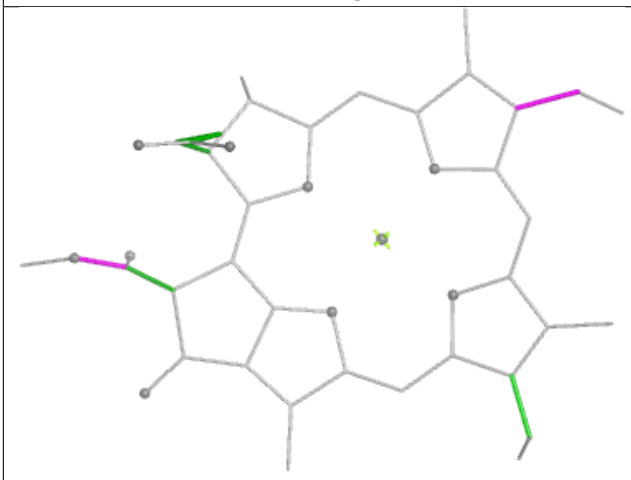


Bond angles



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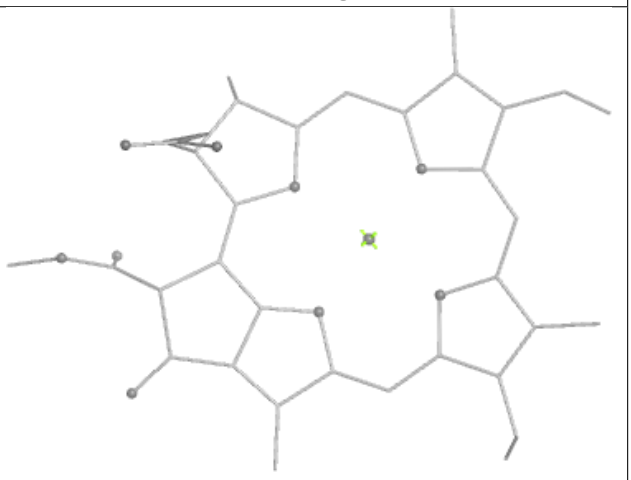
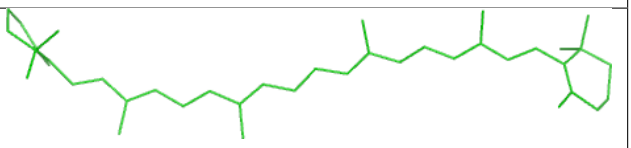


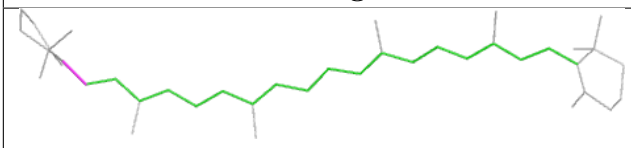
Rings

Ligand BCR B 849

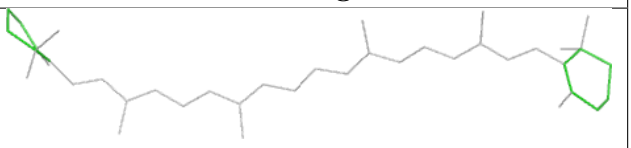
Bond lengths



Bond angles

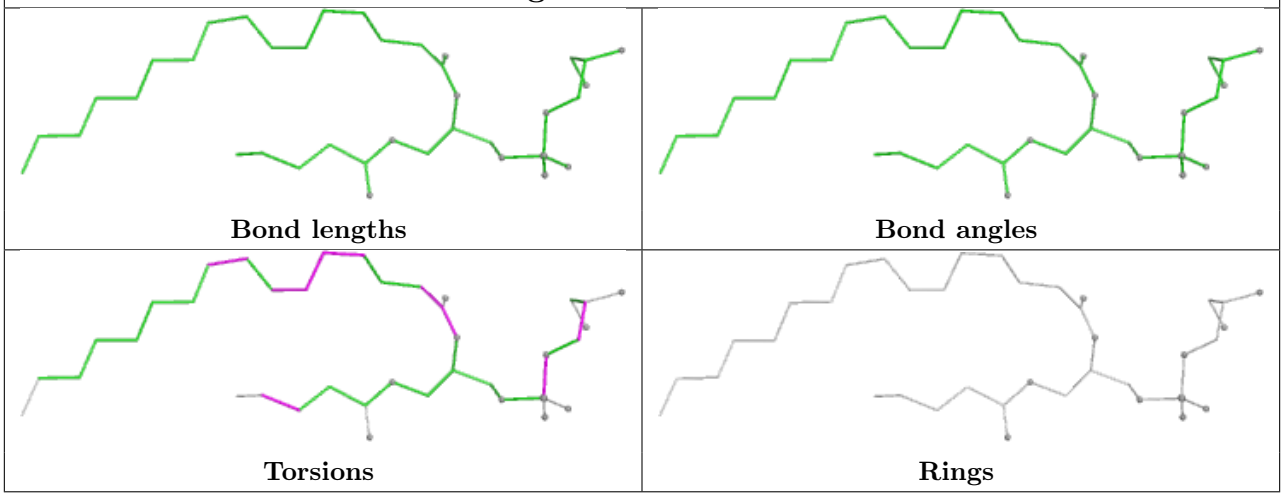


Torsions

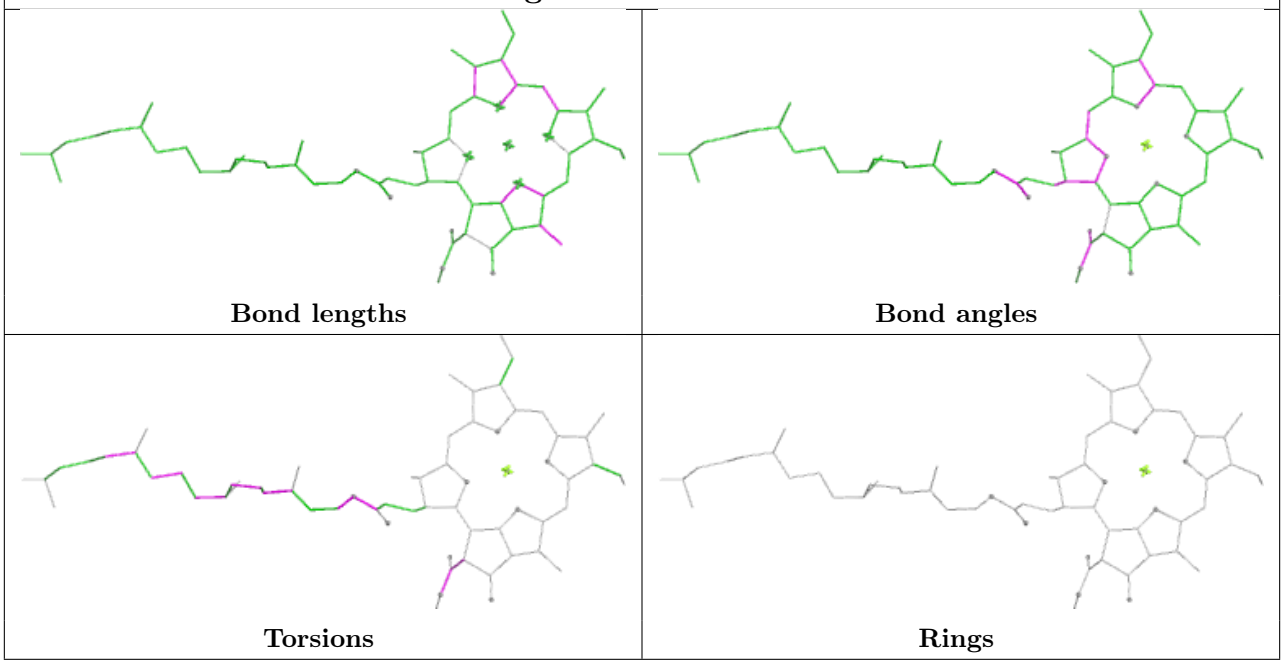


Rings

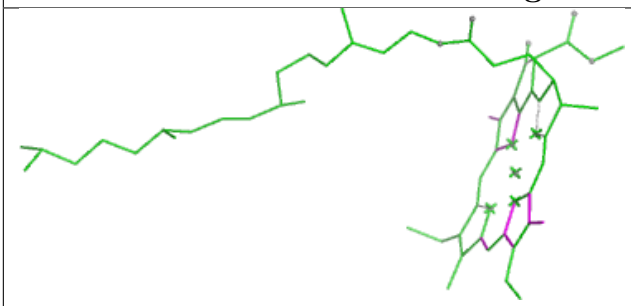
Ligand LHG 4 620



Ligand CLA A 828



Ligand CLA B 830



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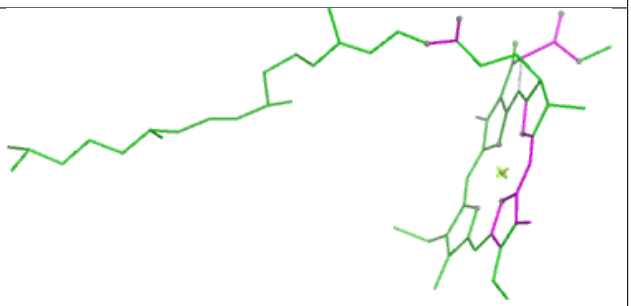
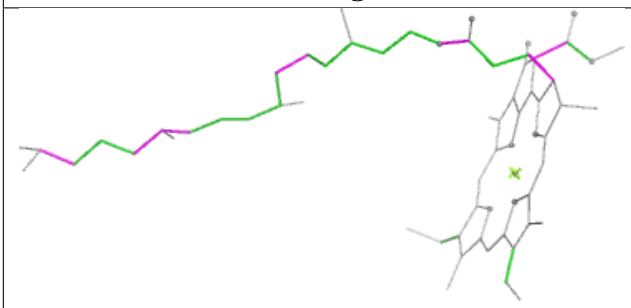


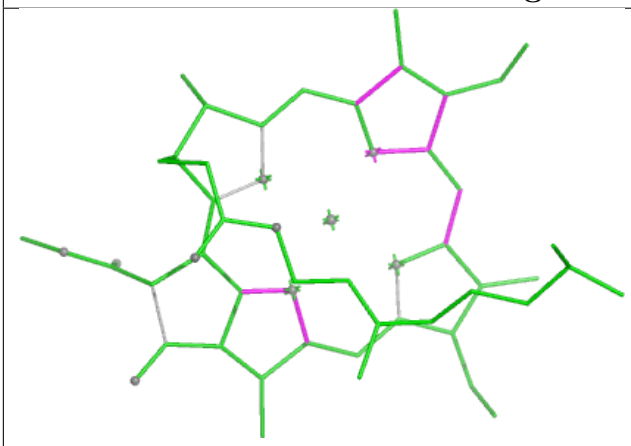
Bond angles



Torsions

Rings

Ligand CLA B 808



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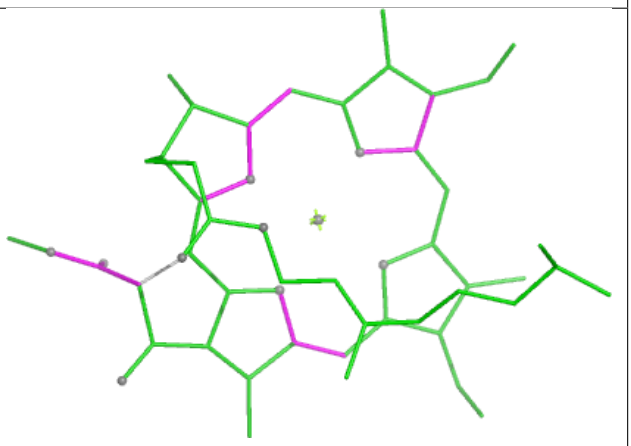
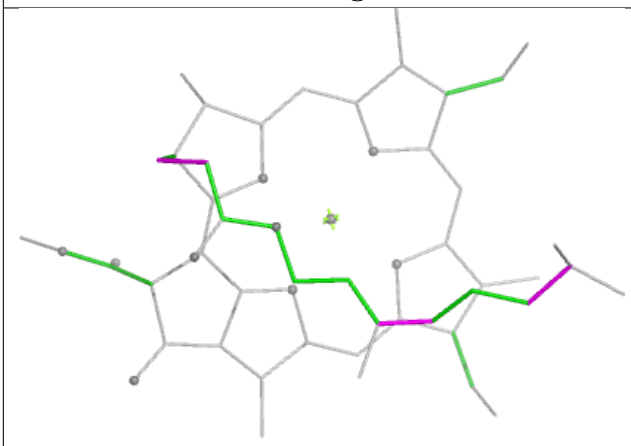


Bond angles



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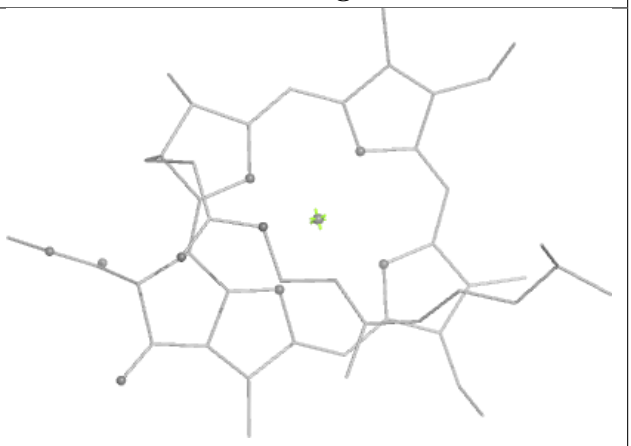
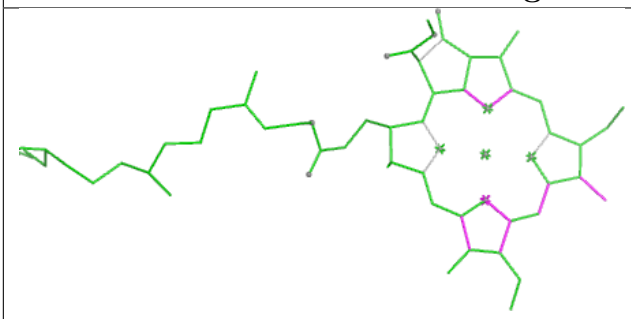


Rings

Ligand CLA A 807



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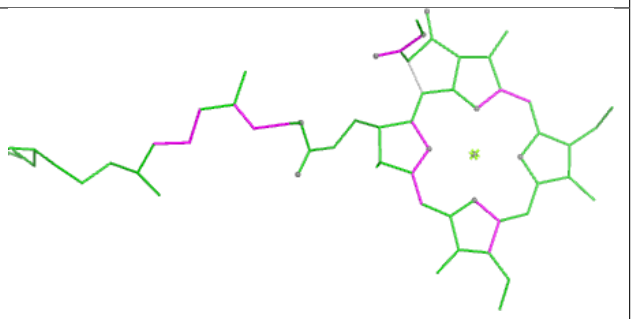
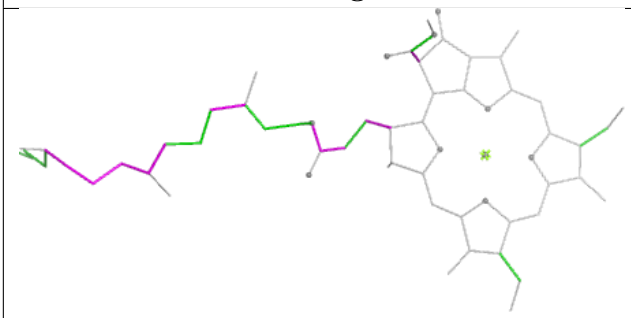


Bond angles



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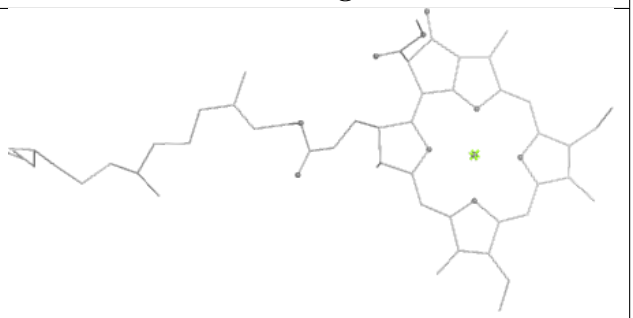
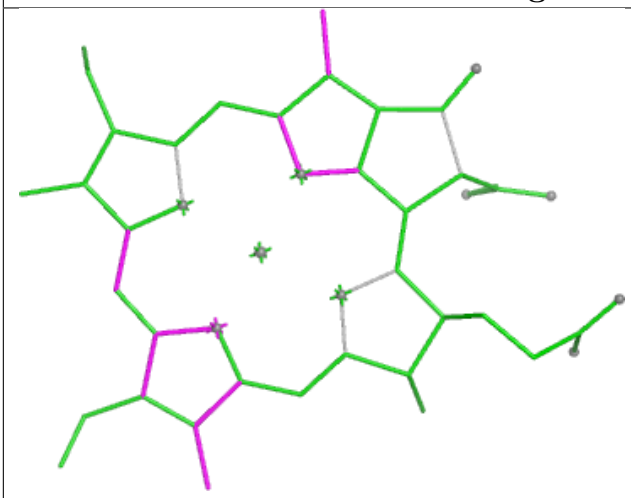
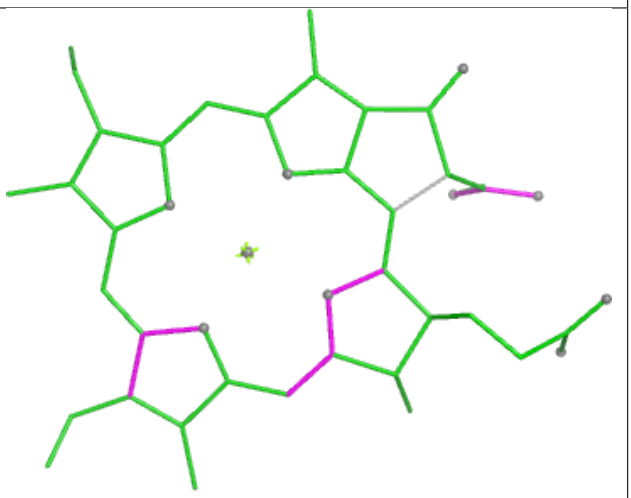


Rings

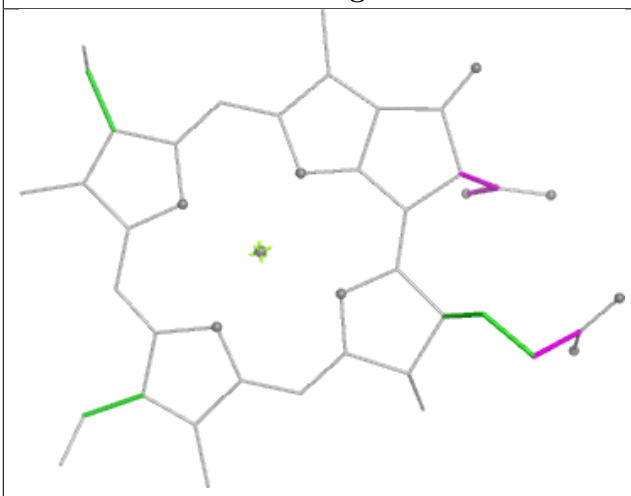
Ligand CLA 1 311



Bond lengths



Bond angles



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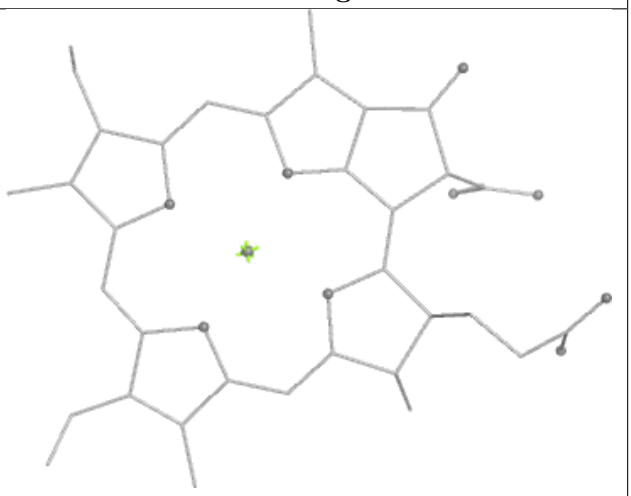
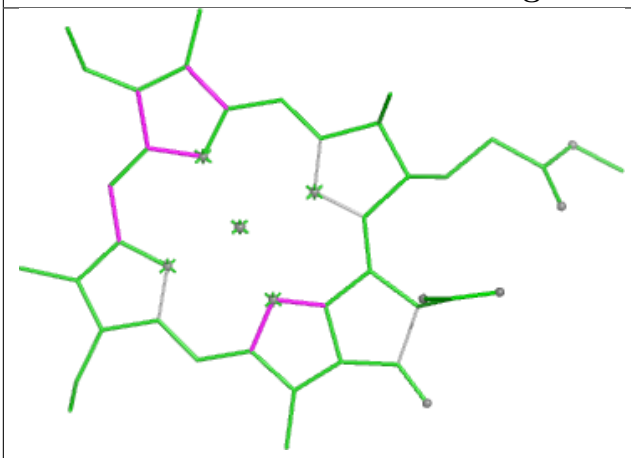


Rings

Ligand CLA G 203



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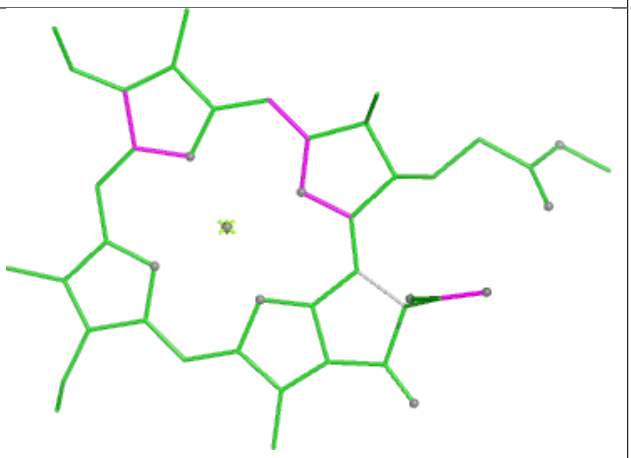
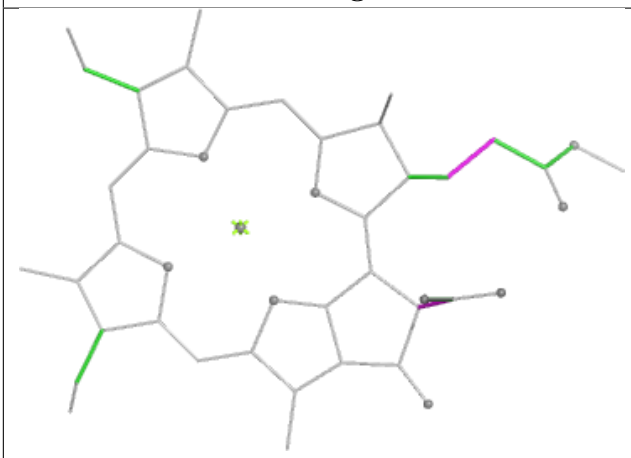


Bond angles



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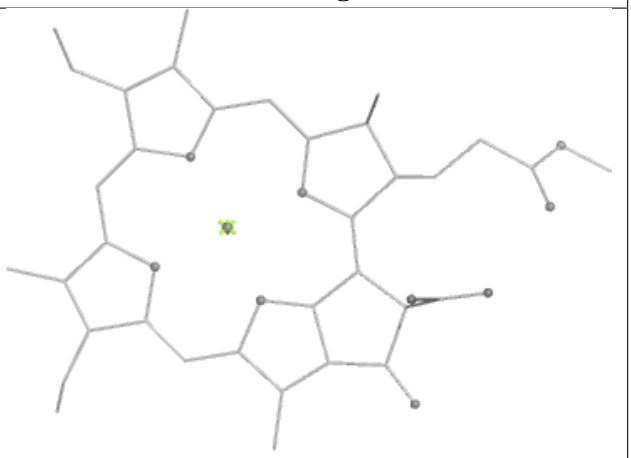
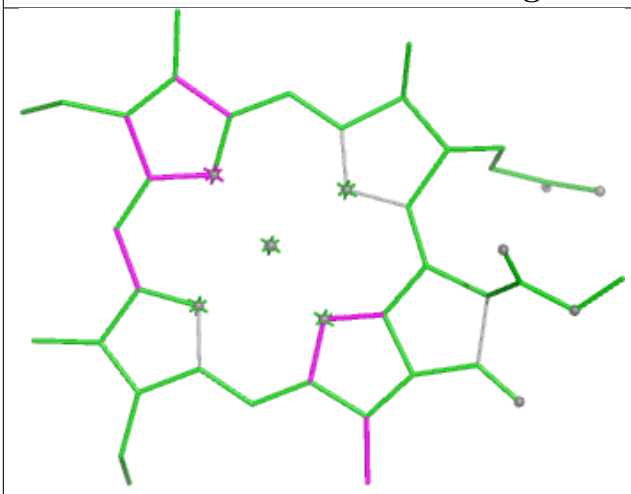
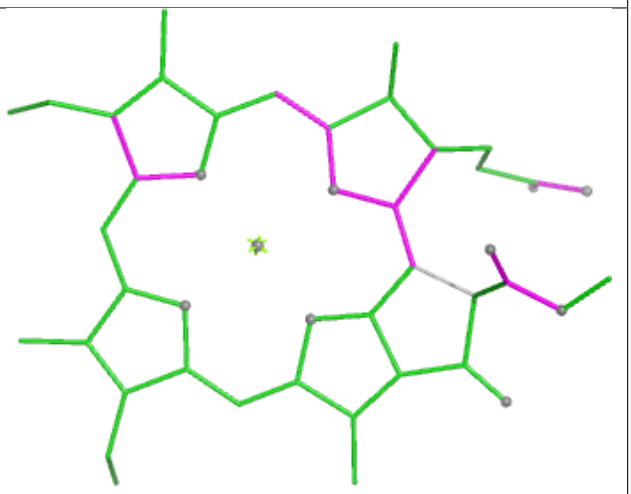


Rings

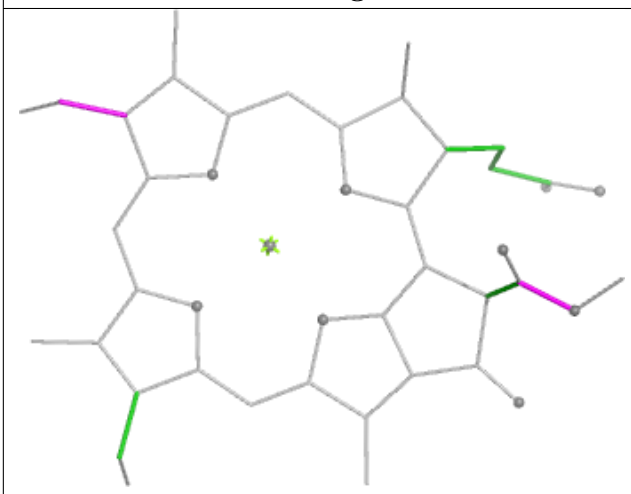
Ligand CLA K 202



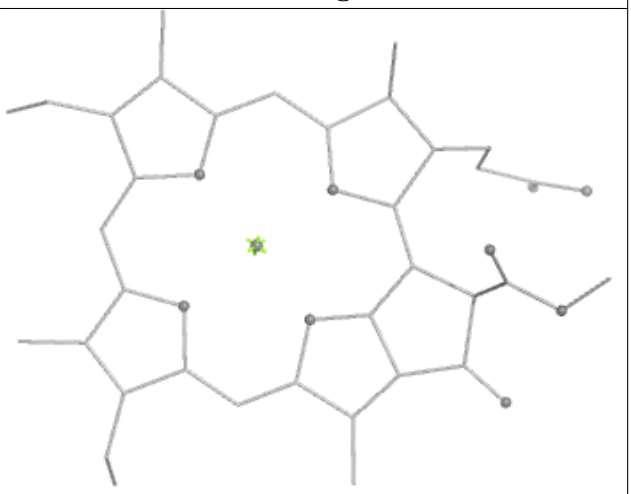
Bond lengths



Bond angles

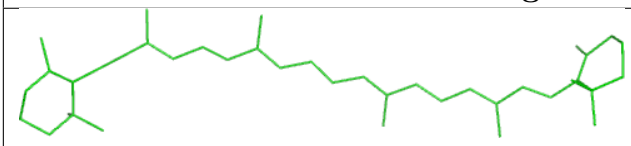


Torsions

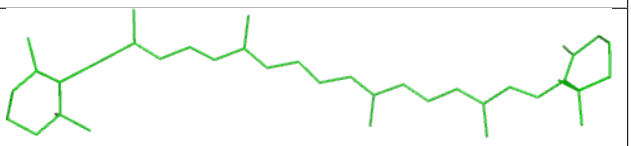


Rings

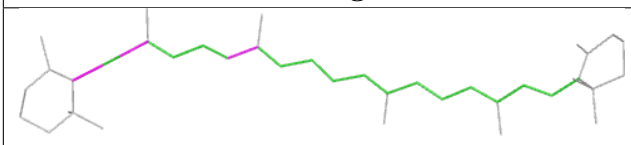
Ligand BCR A 852



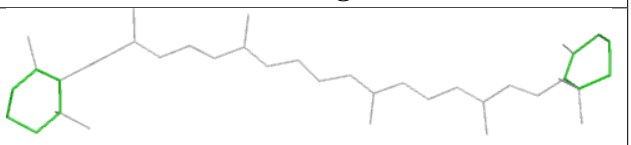
Bond lengths



Bond angles

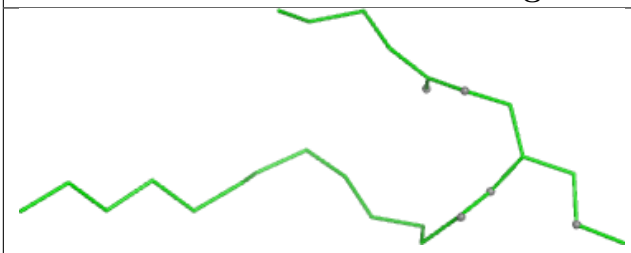


Torsions



Rings

Ligand LMG 6 301



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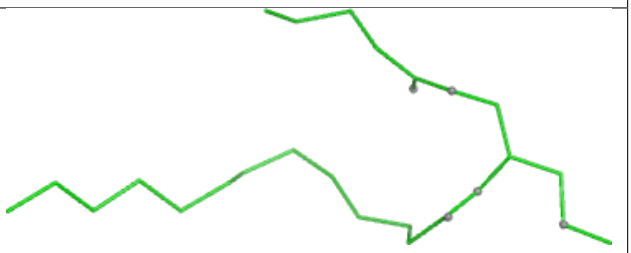

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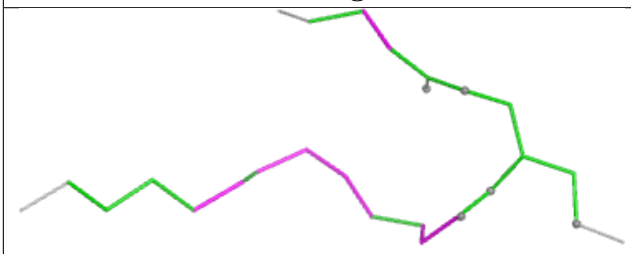

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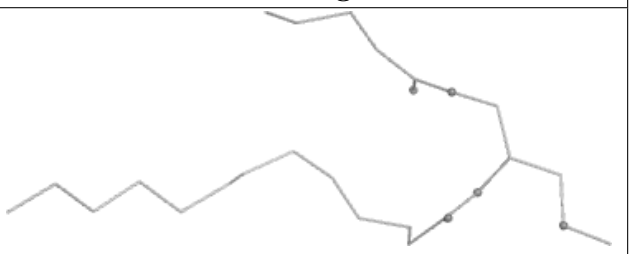

Rings

Ligand CHL 6 307

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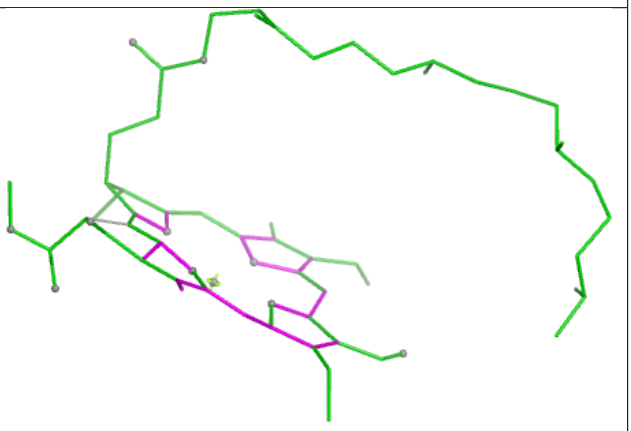

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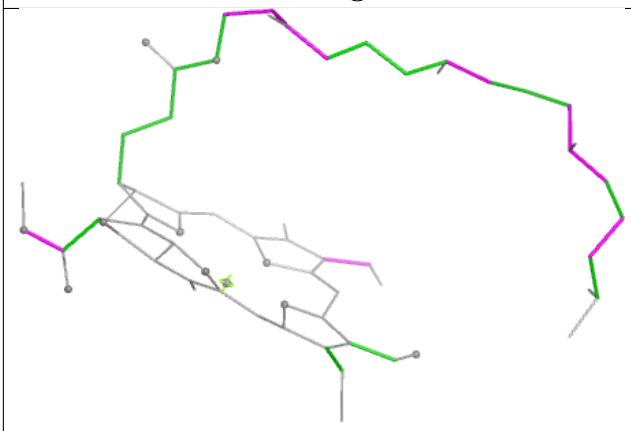

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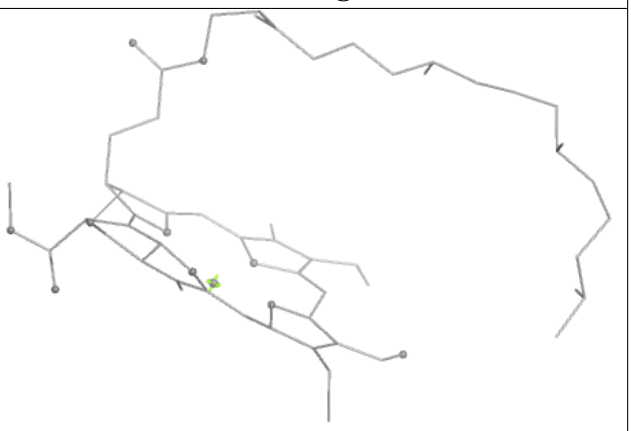
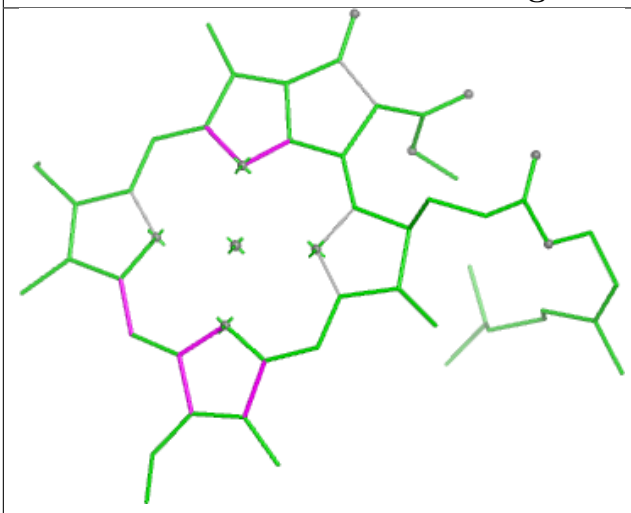


Rings

Ligand CLA 8 311



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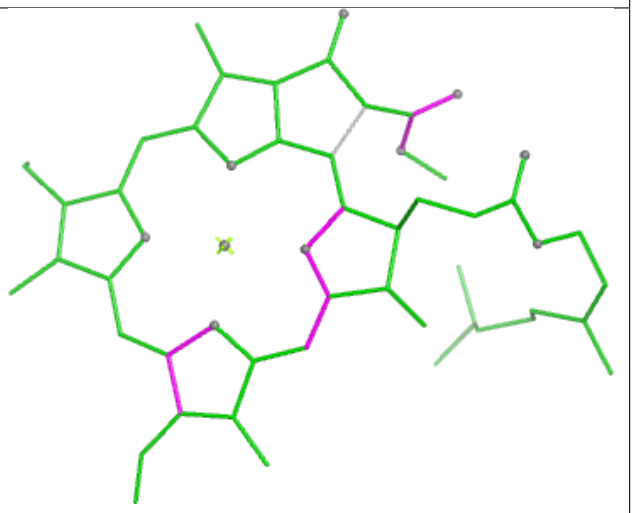
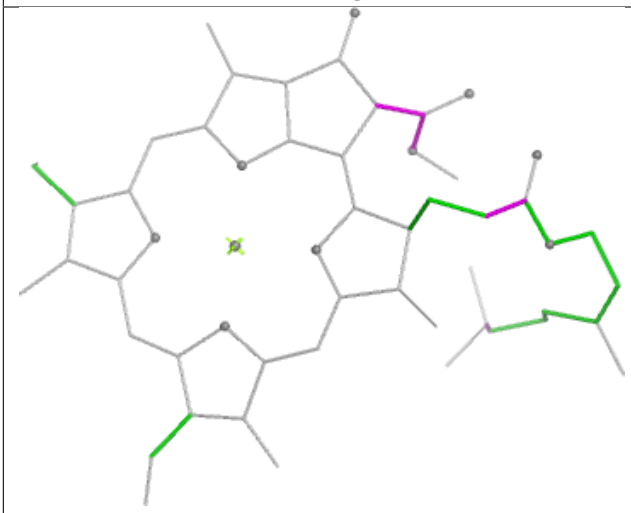


Bond angles



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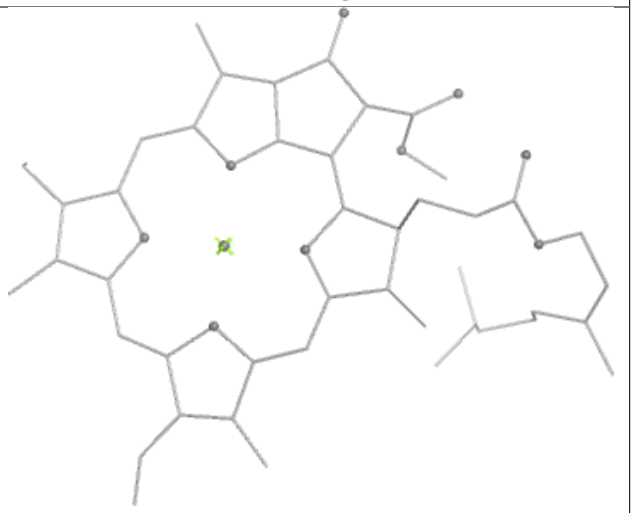
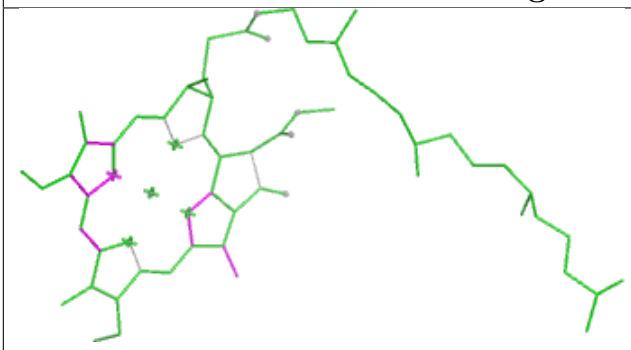


Rings

Ligand CLA 3 302



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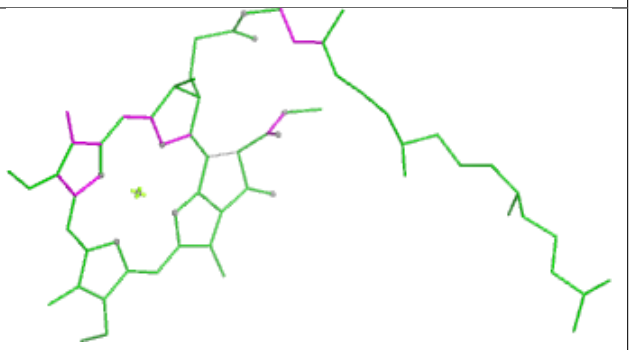
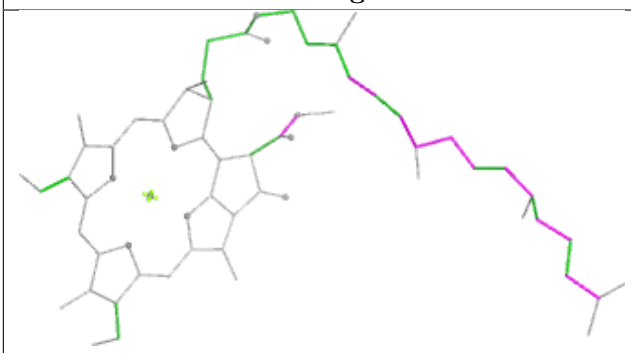


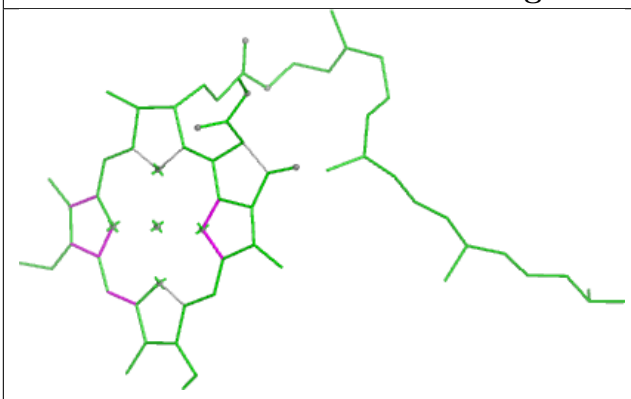
Bond angles



Torsions

Rings

Ligand CLA B 833



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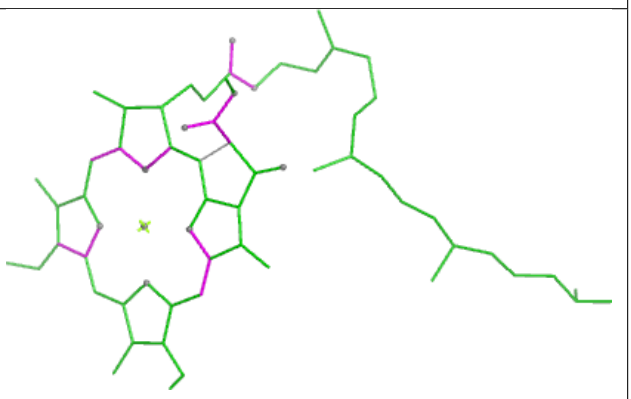

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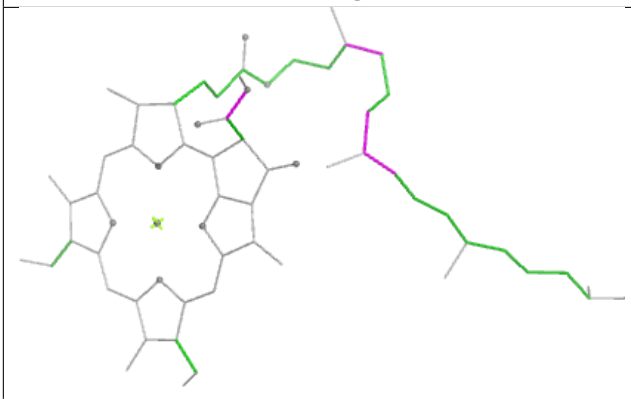
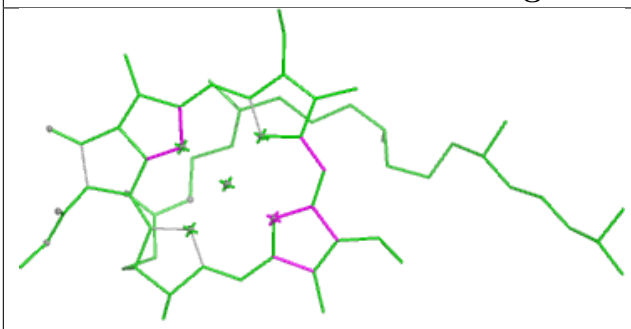


Torsions

Rings

Ligand CLA A 842



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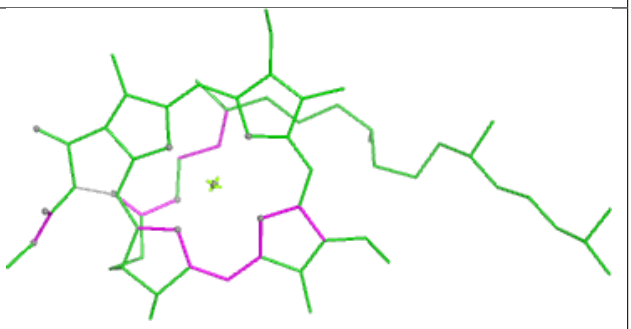
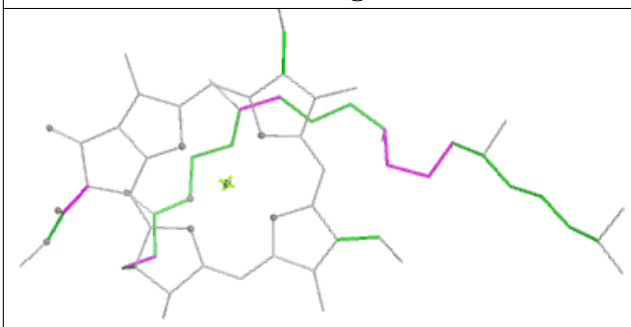


Bond angles



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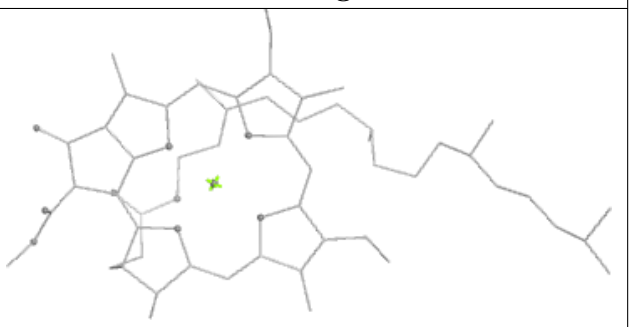
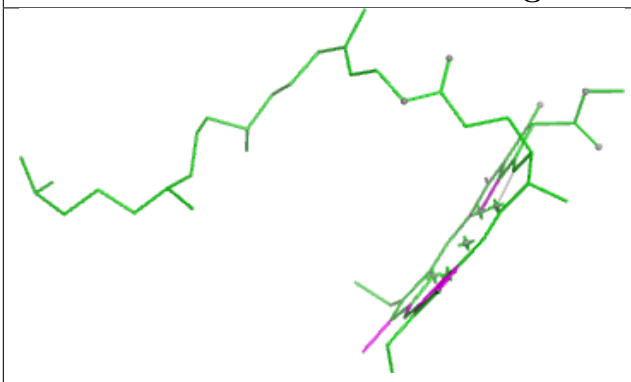


Rings

Ligand CLA A 812



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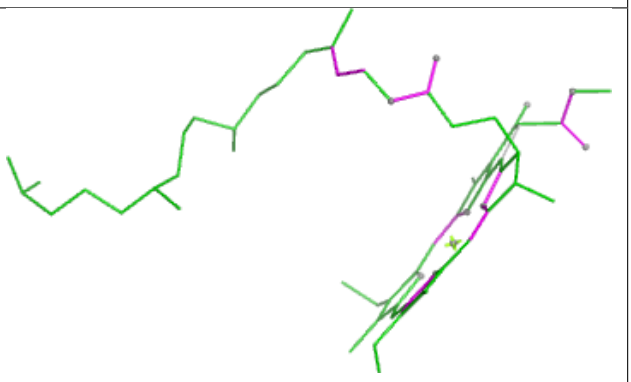

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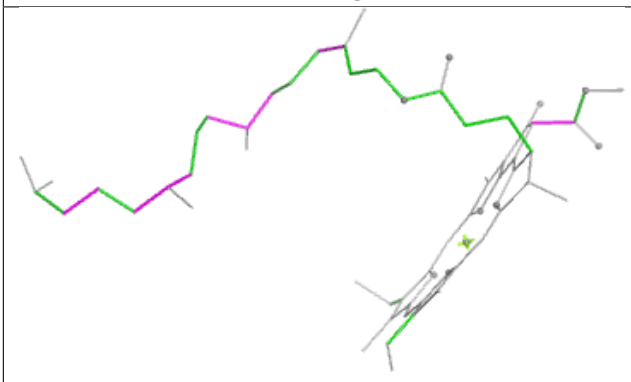

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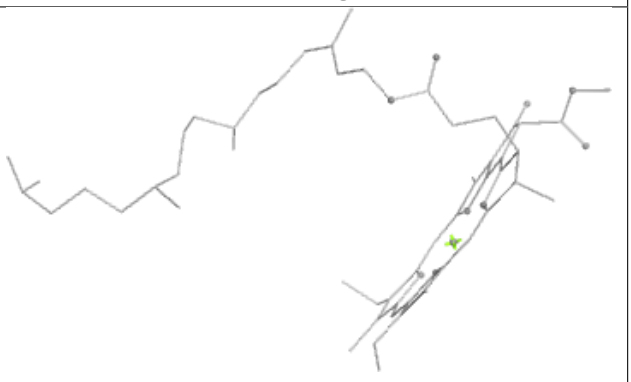
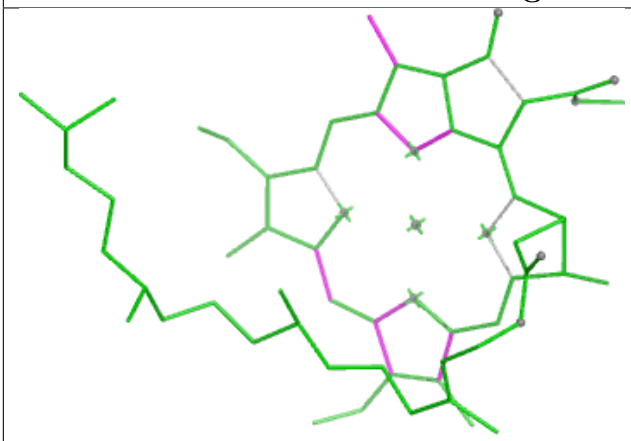


Rings

Ligand CLA A 824



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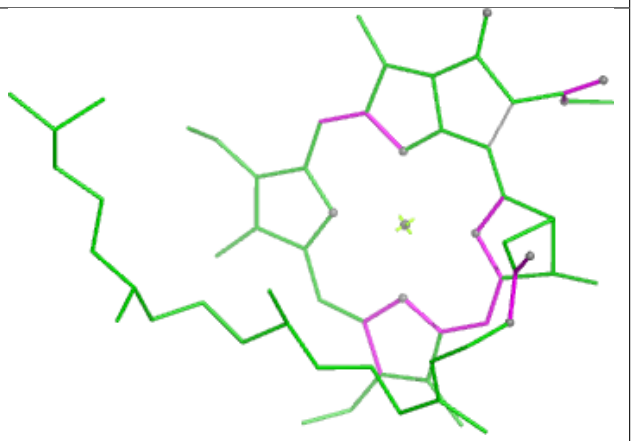
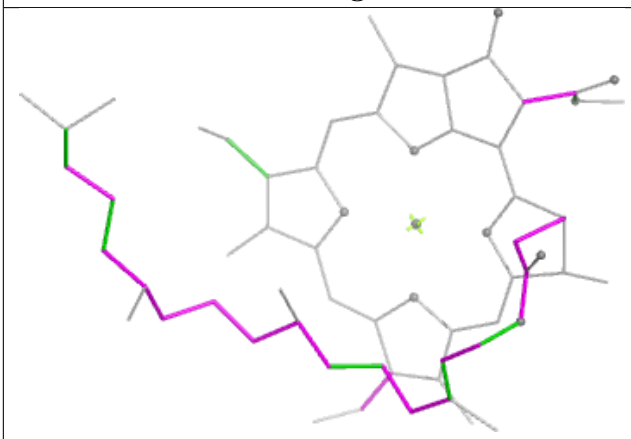
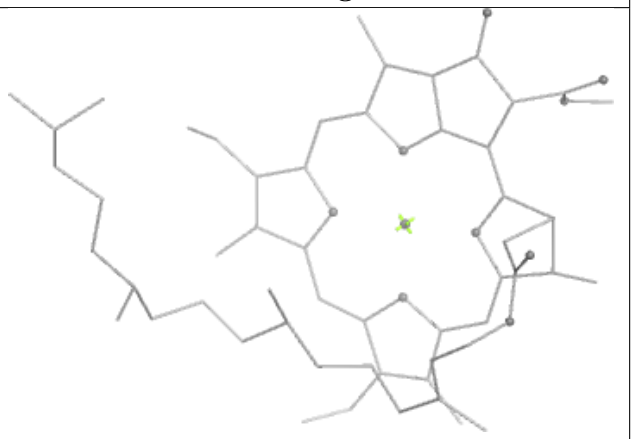


Bond angles

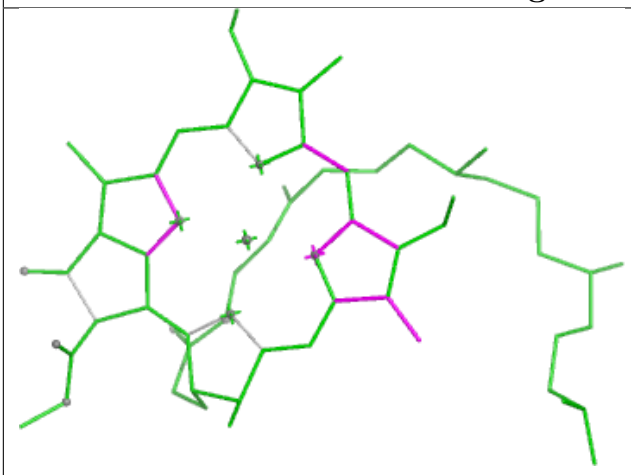


Torsions



Rings

Ligand CLA 4 612



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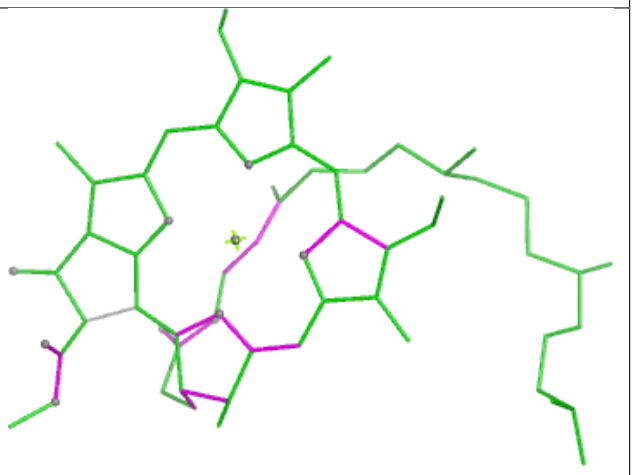

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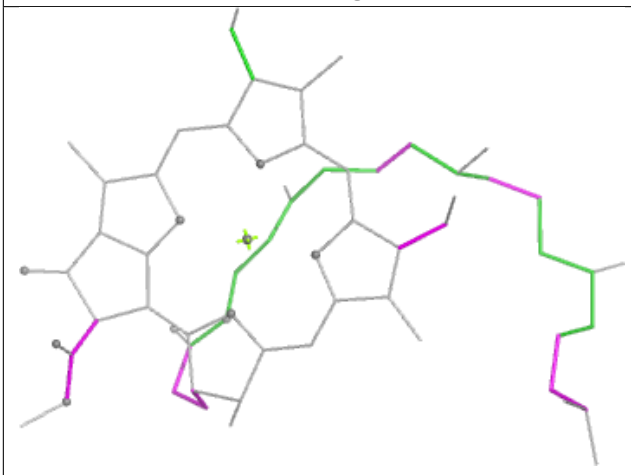

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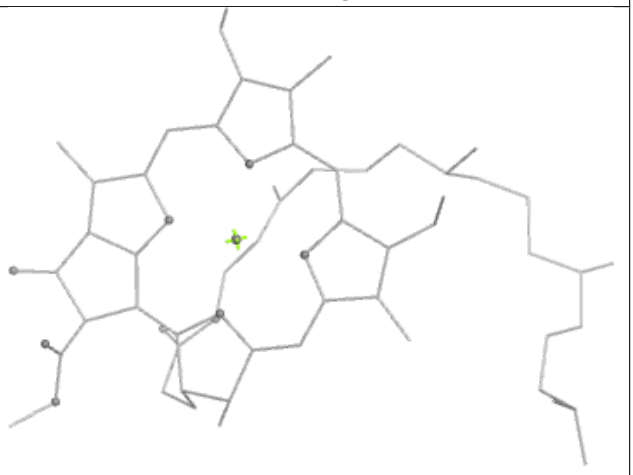
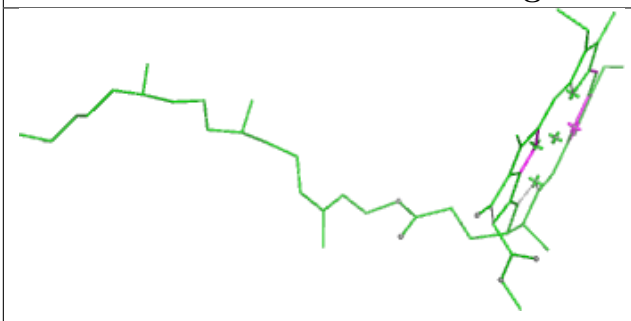


Rings

Ligand CLA A 841



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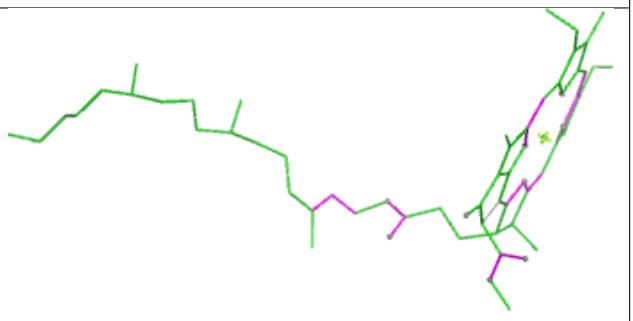

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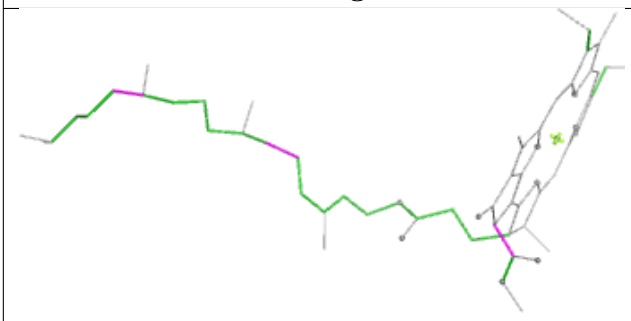
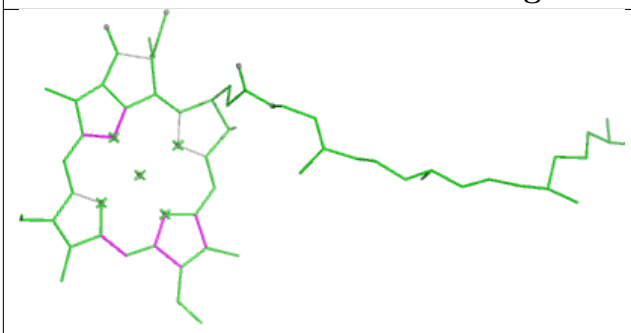


Torsions

Rings

Ligand CLA A 817



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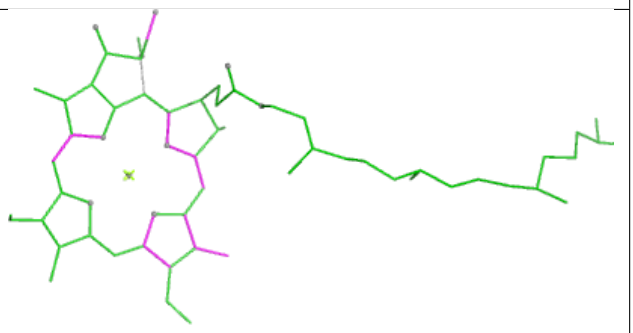

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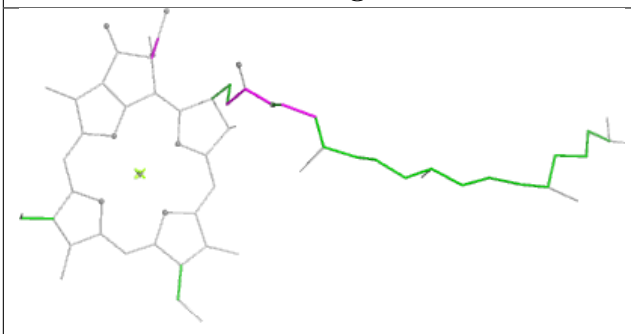

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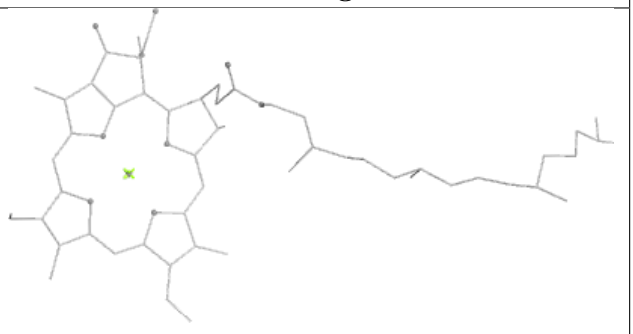
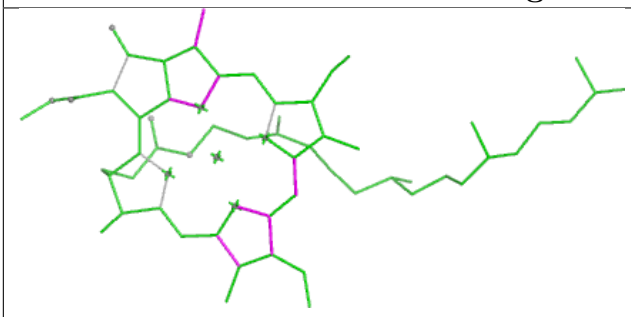


Rings

Ligand CLA Z 612



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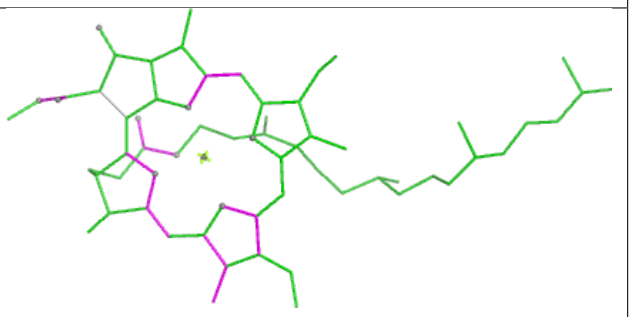

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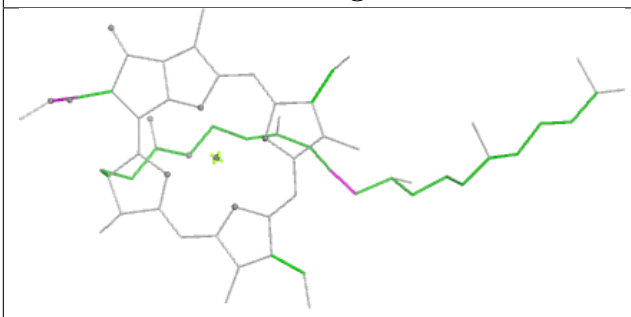

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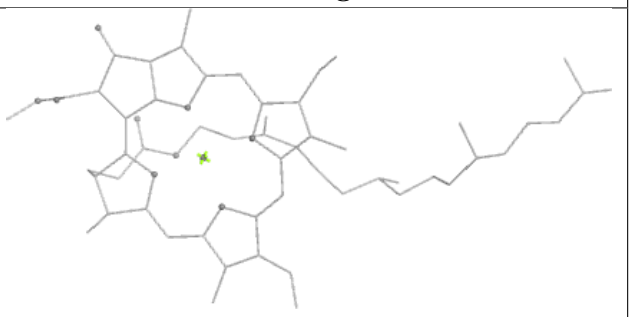
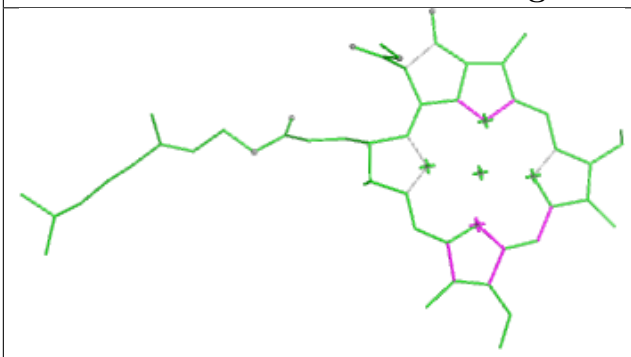


Rings

Ligand CLA 6 320



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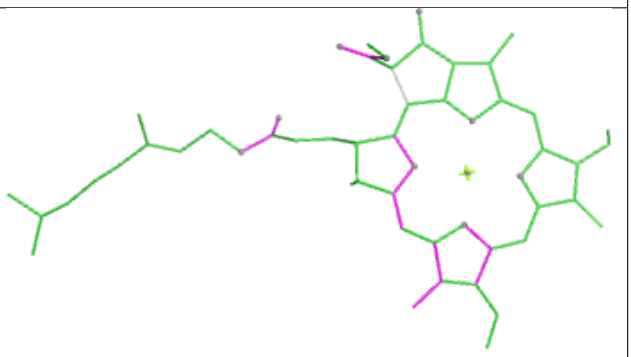
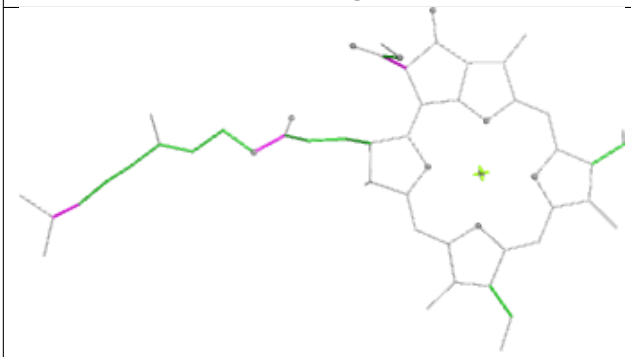


Bond angles



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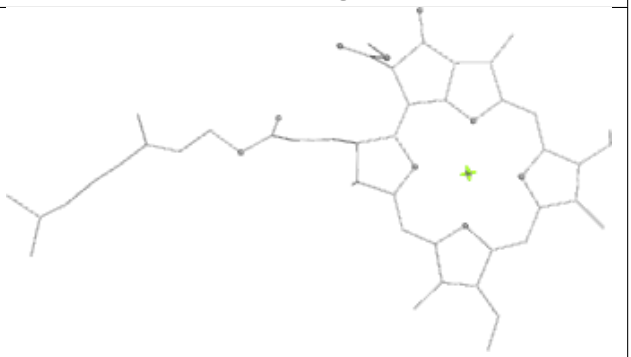
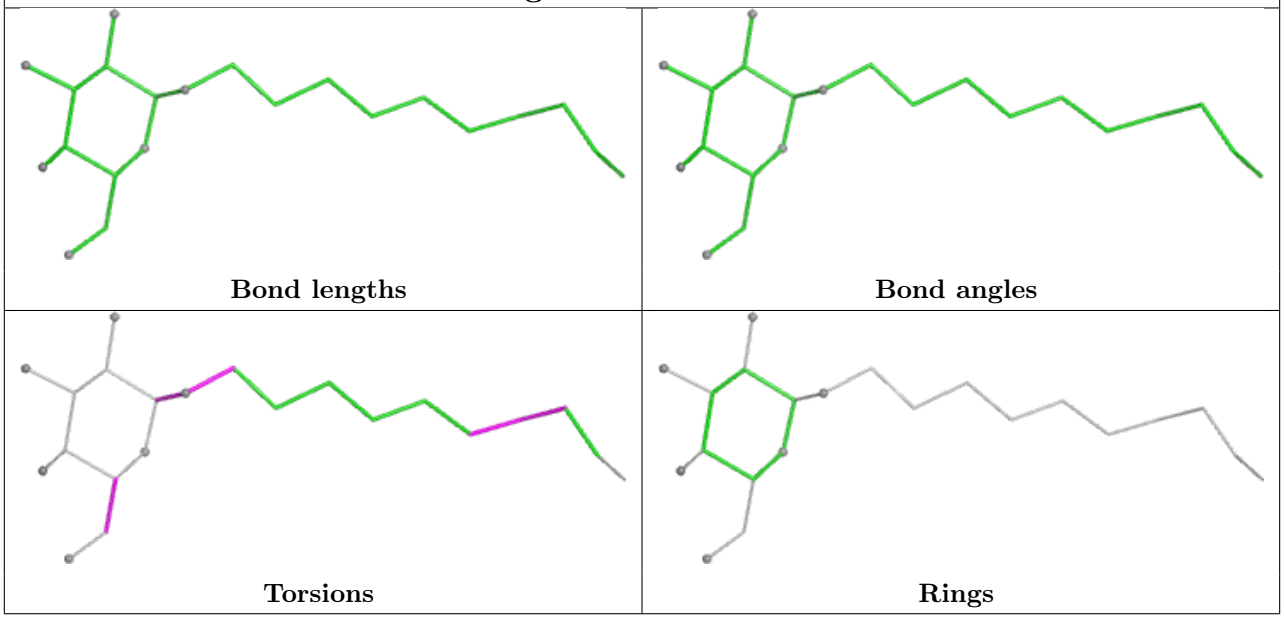
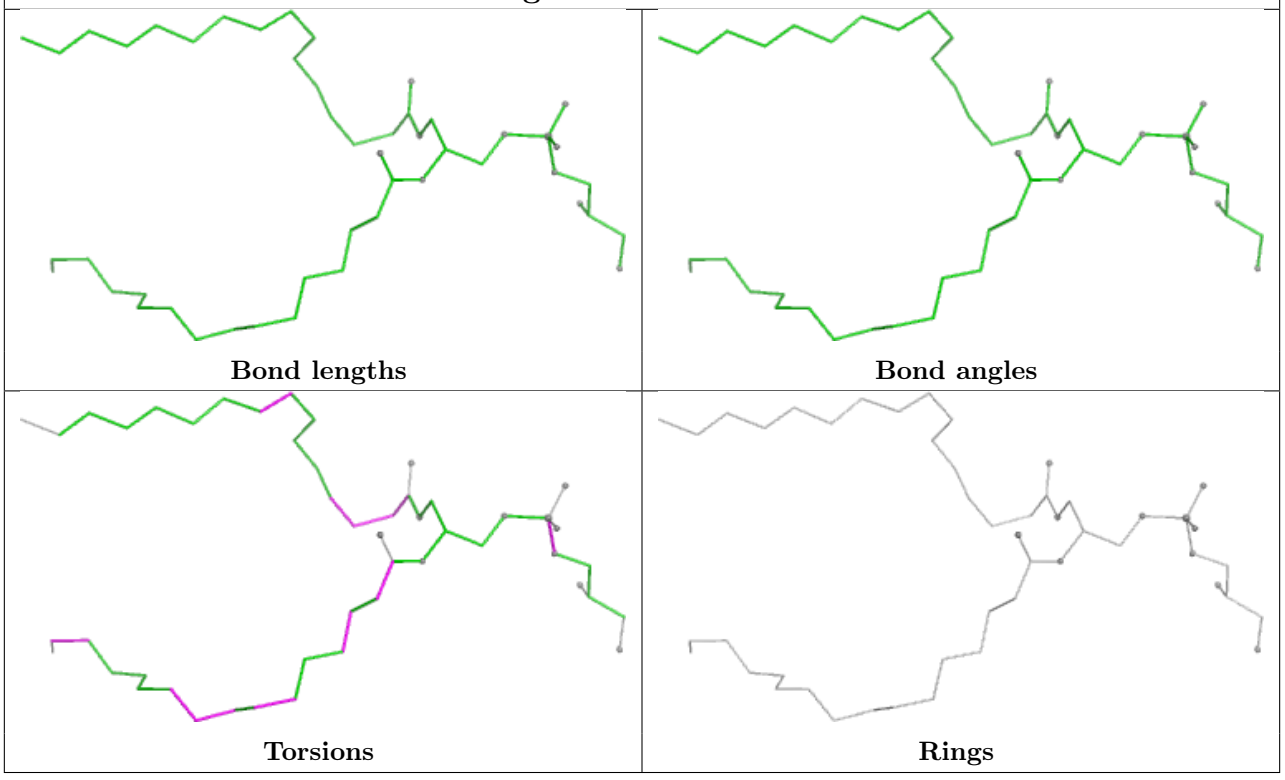


Rings

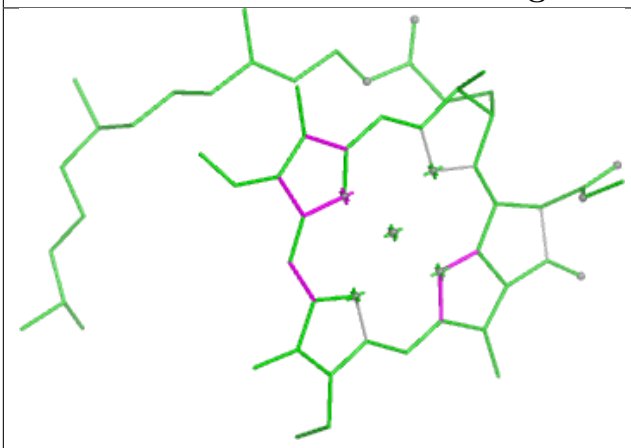
Ligand LMU 4 622



Ligand LHG A 847



Ligand CLA 1 302



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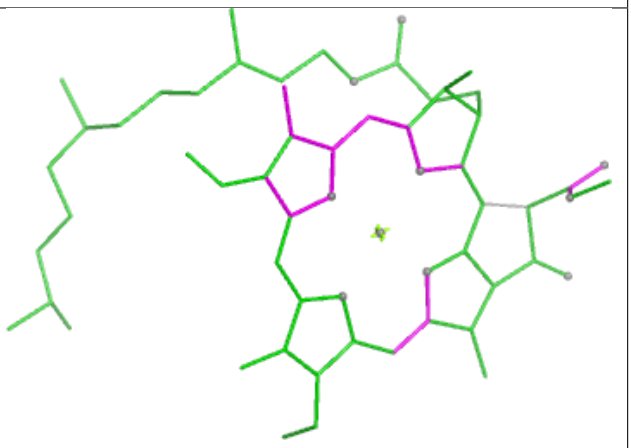
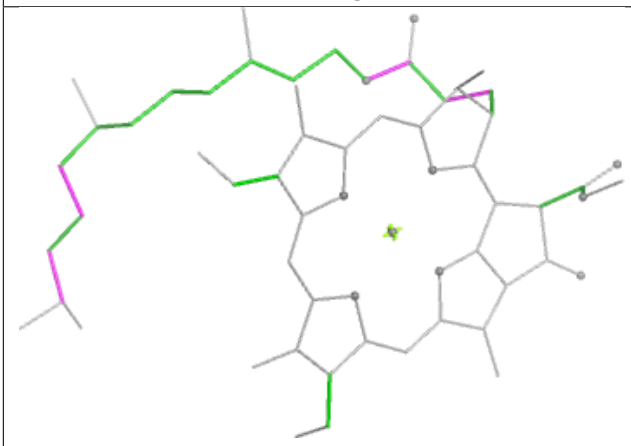
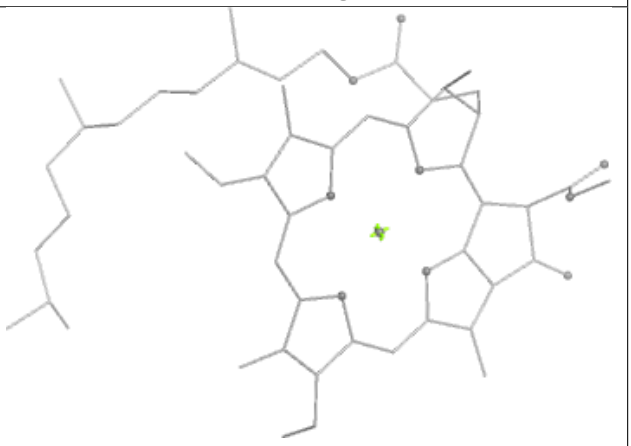


Bond angles

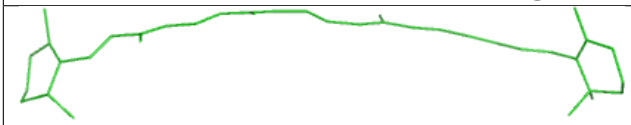


Torsions

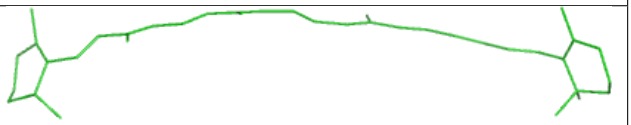


Rings

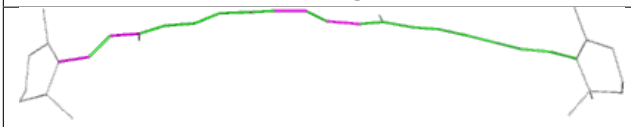
Ligand BCR I 201



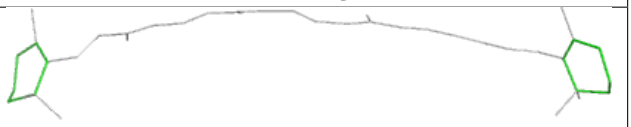
Bond lengths



Bond angles

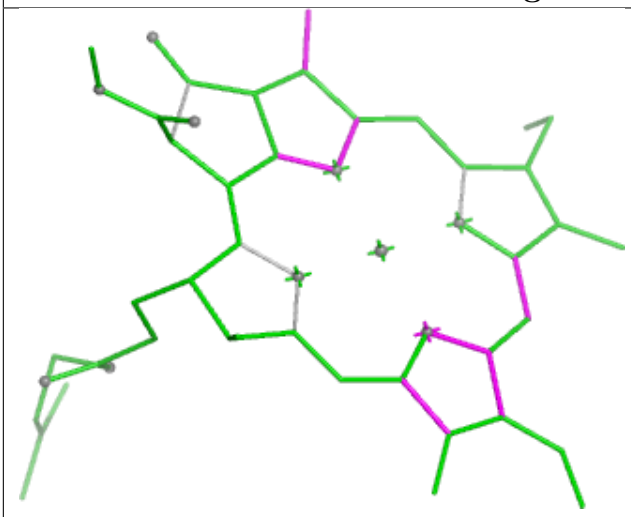


Torsions



Rings

Ligand CLA A 809



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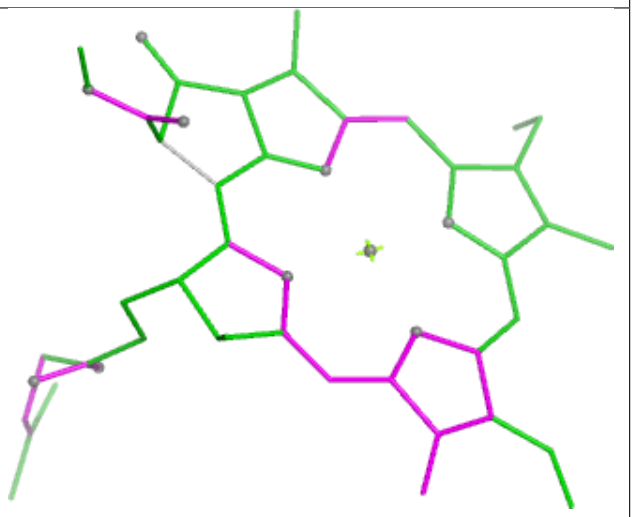

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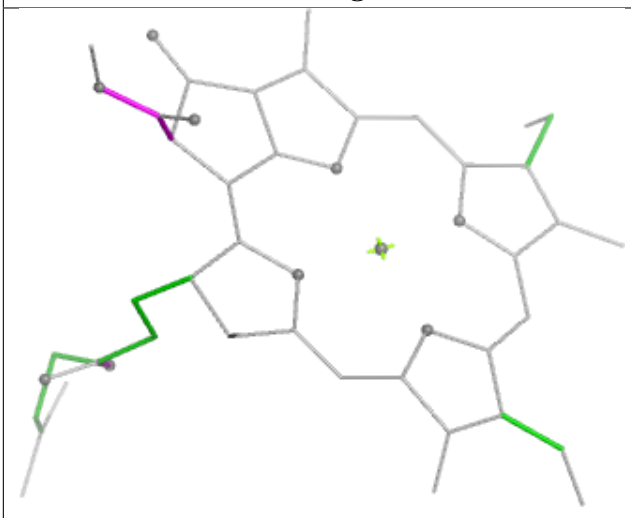

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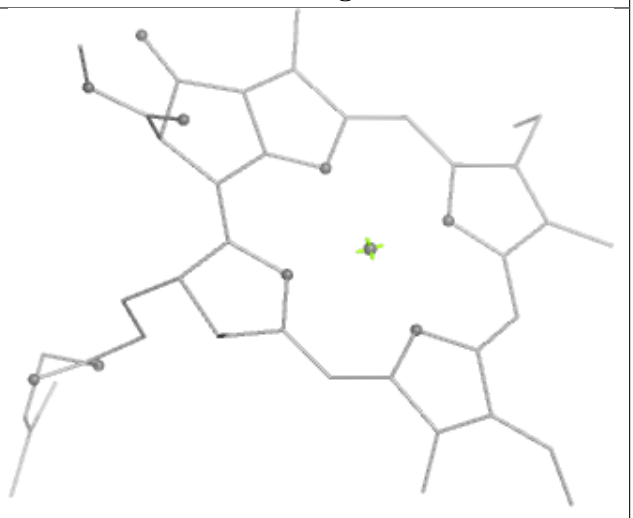
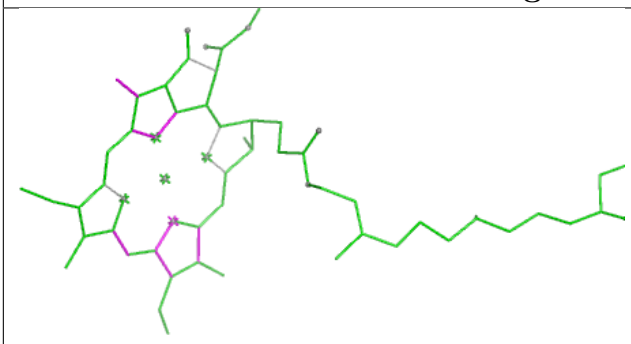


Rings

Ligand CLA A 823



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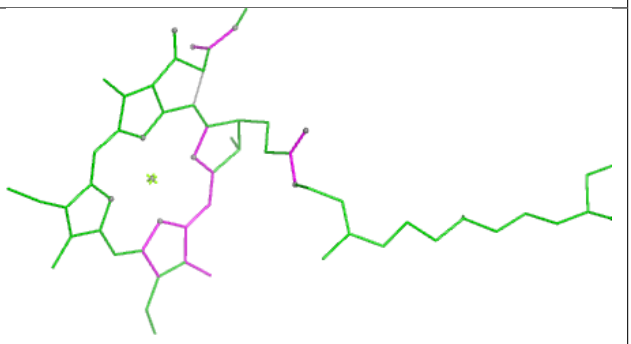
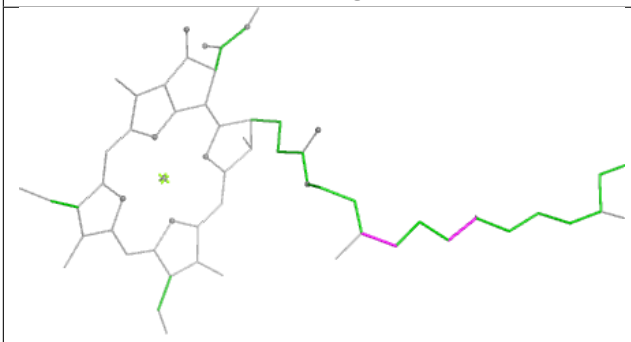


Bond angles



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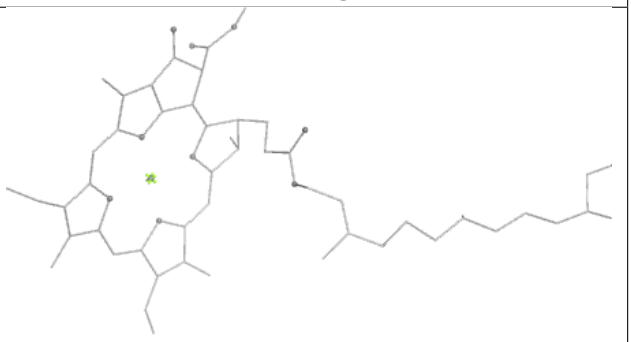
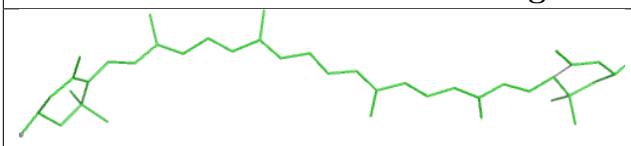


Rings

Ligand LUT 6 319



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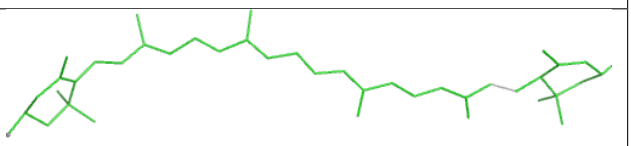
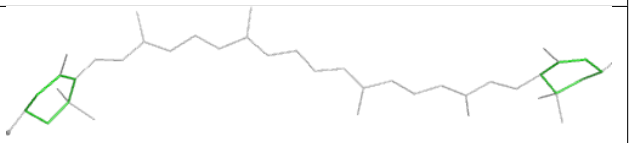


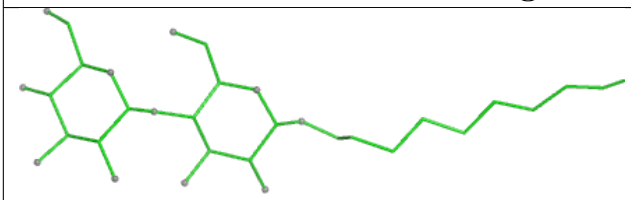
Bond angles

Torsions



Rings

Ligand LMU A 855



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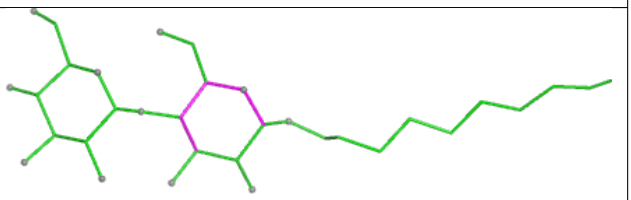
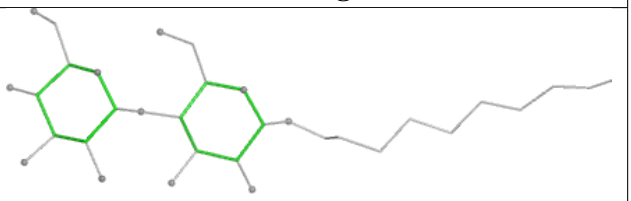


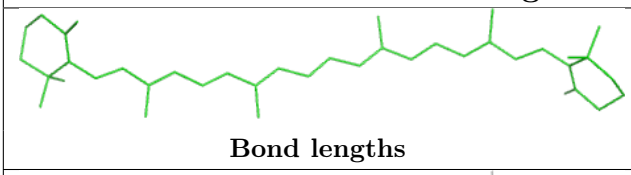
Bond angles

Torsions



Rings

Ligand BCR A 850



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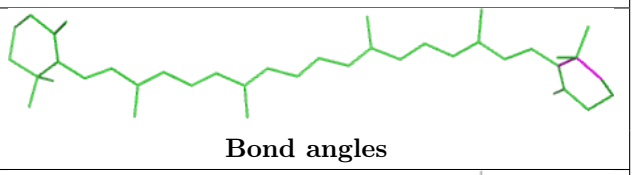

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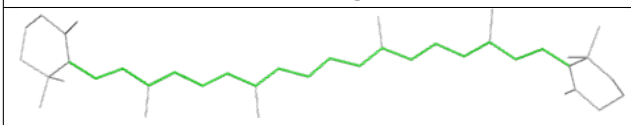

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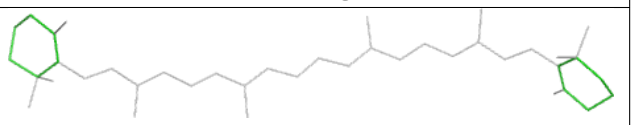
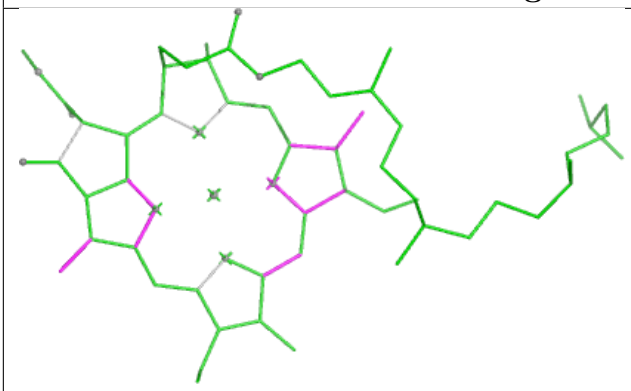


Rings

Ligand CLA B 819



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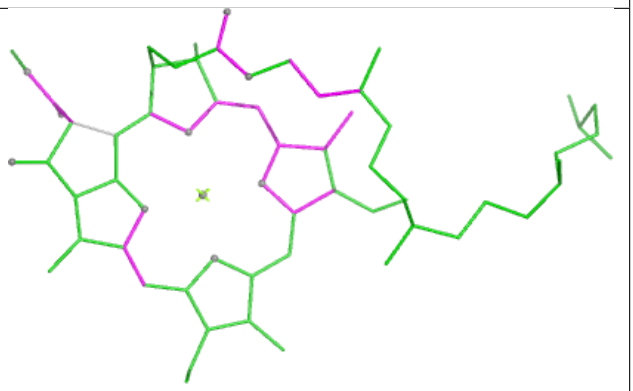
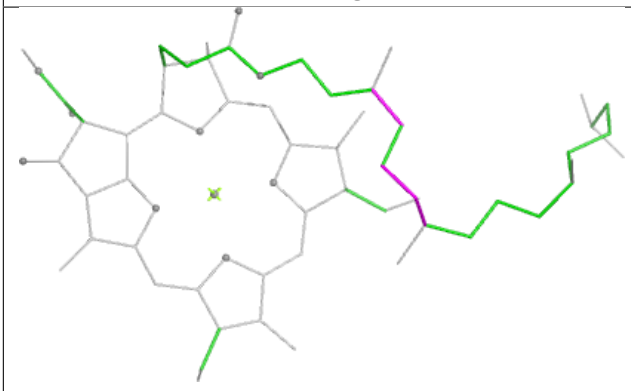


Bond angles



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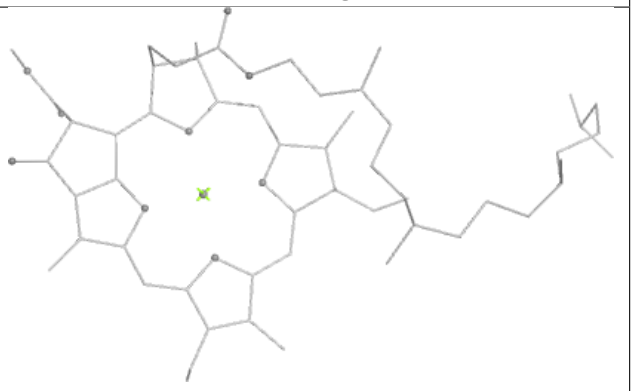
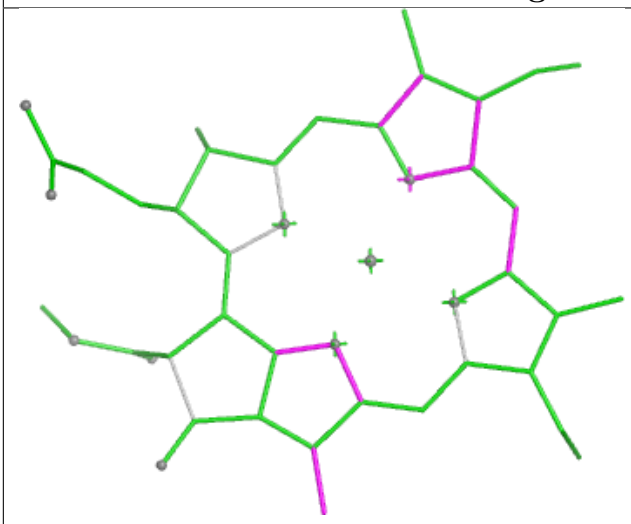


Rings

Ligand CLA 6 316



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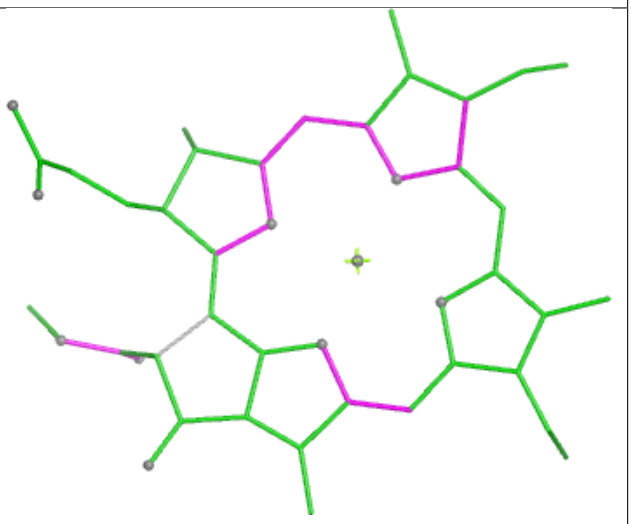

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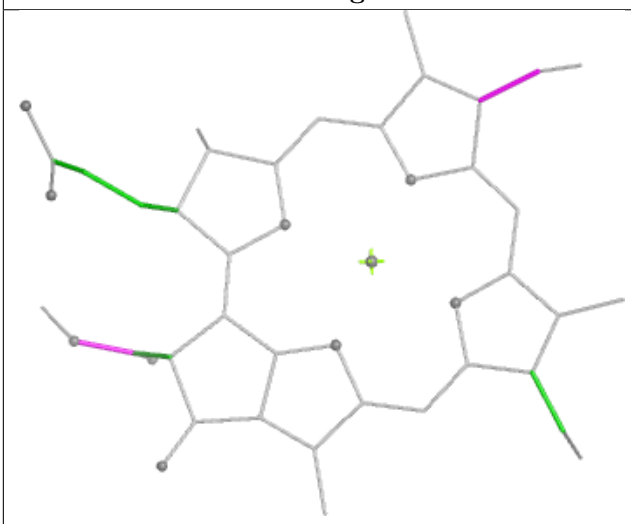

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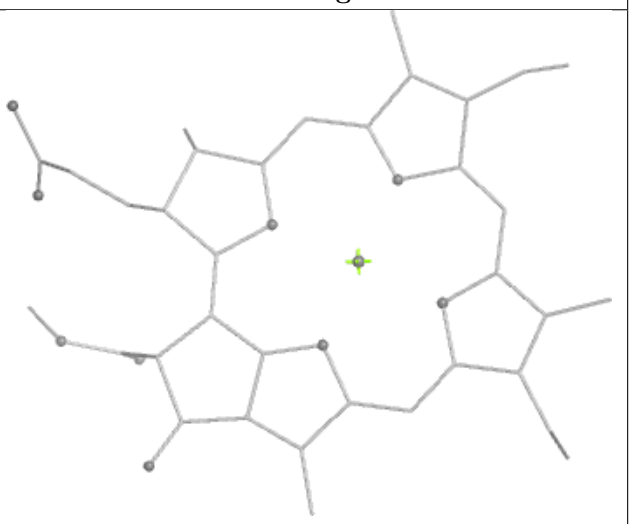
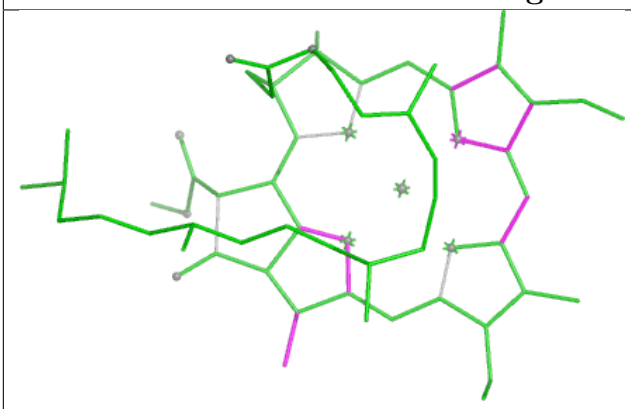


Rings

Ligand CLA F 304



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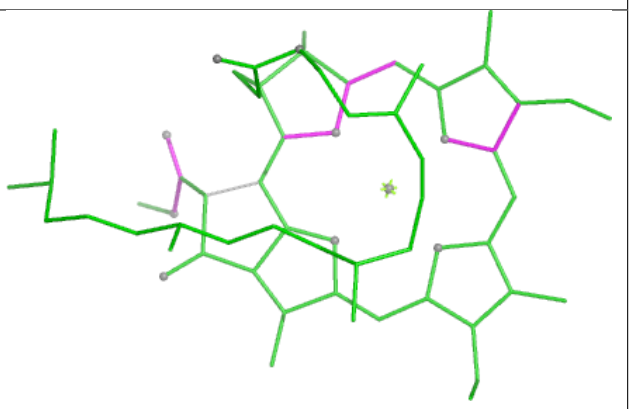

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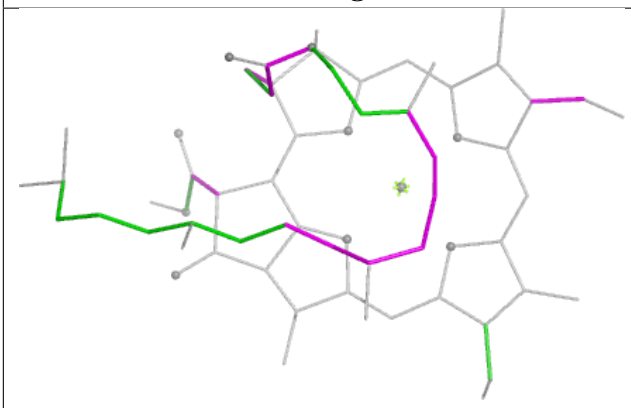

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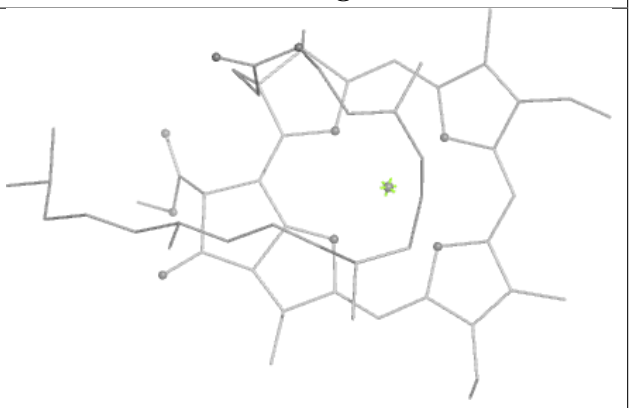
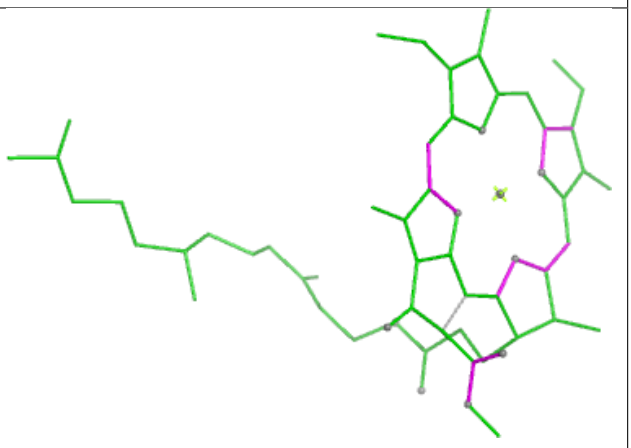


Rings

Ligand CLA 4 610

Bond lengths



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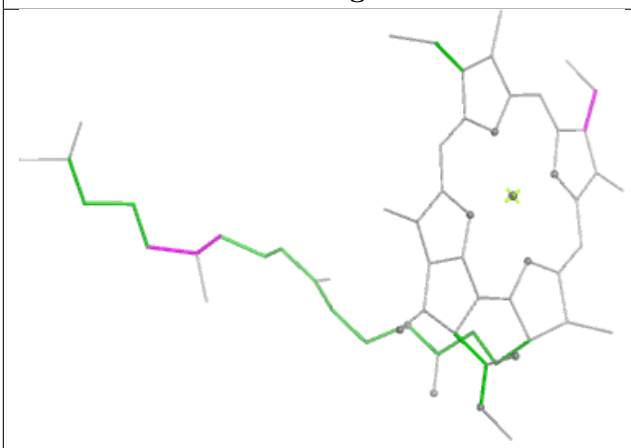

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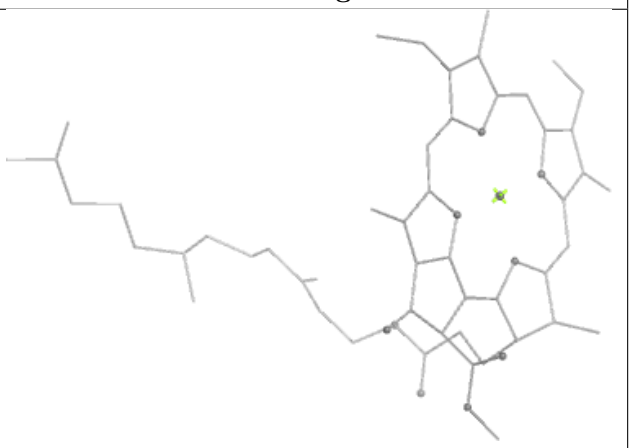
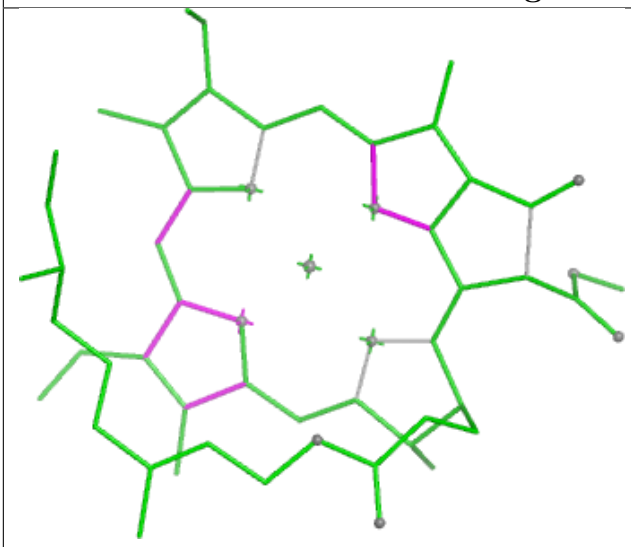


Rings

Ligand CLA B 821



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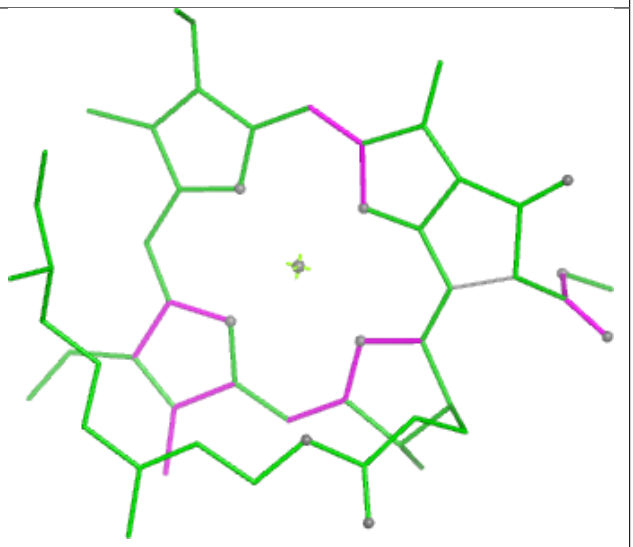
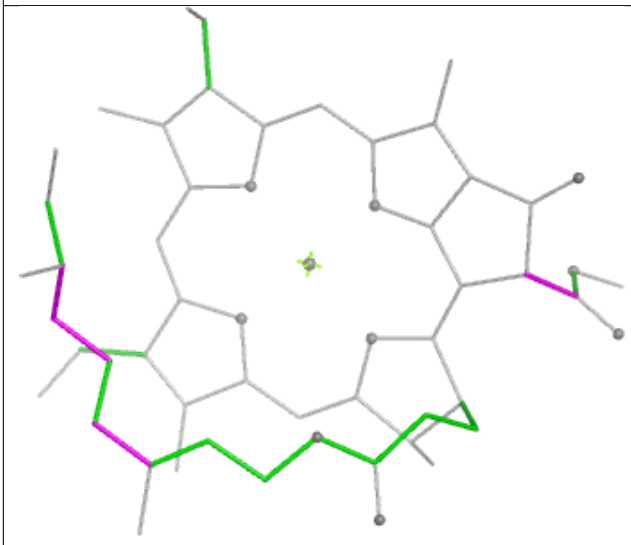


Bond angles



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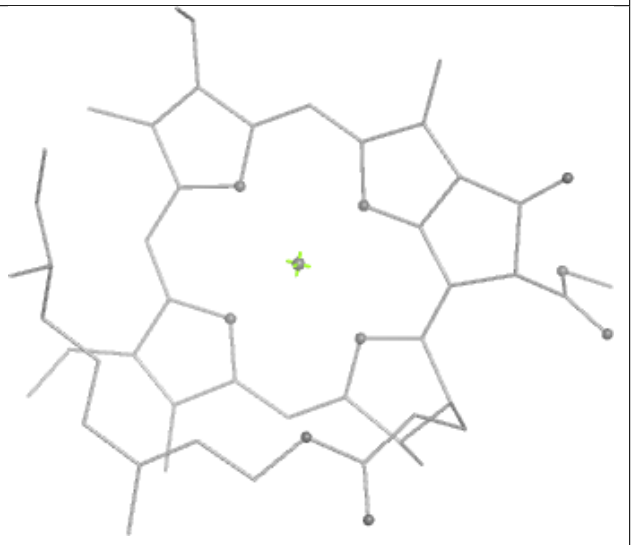
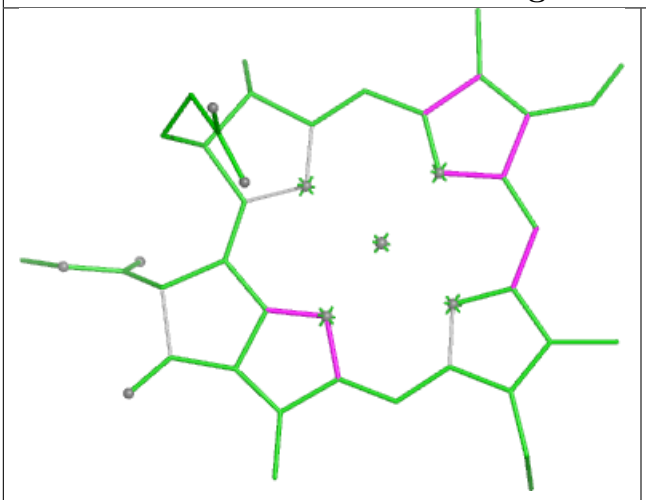


Rings

Ligand CLA 4 614



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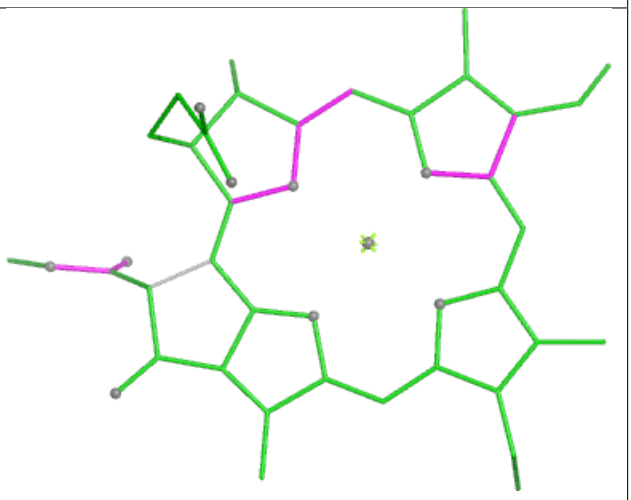
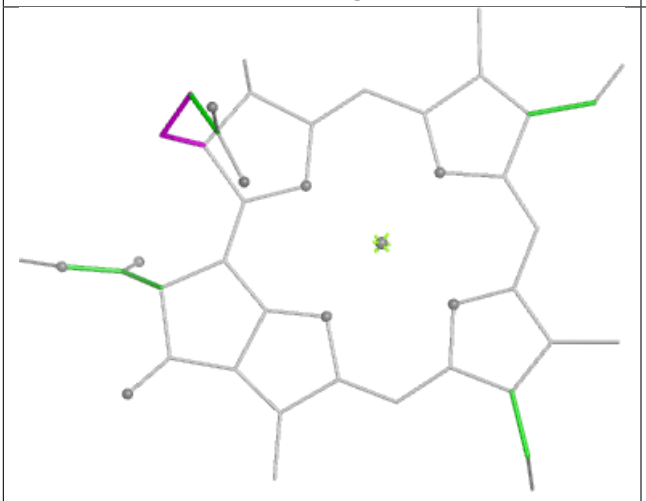


Bond angles



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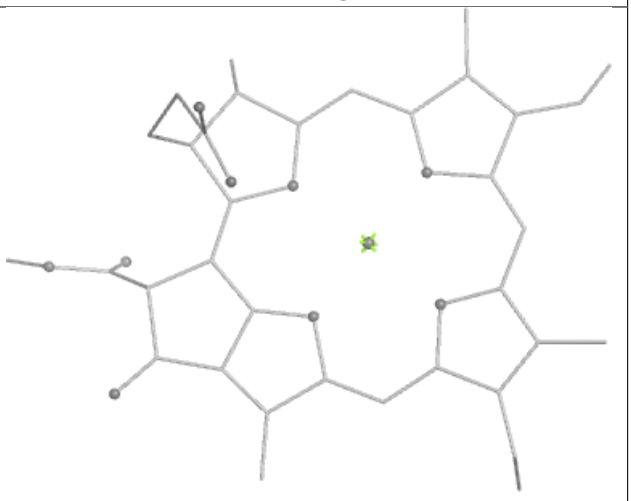
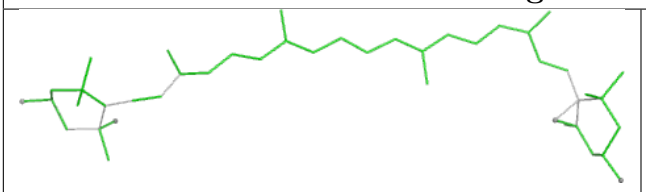


Rings

Ligand NEX 5 323



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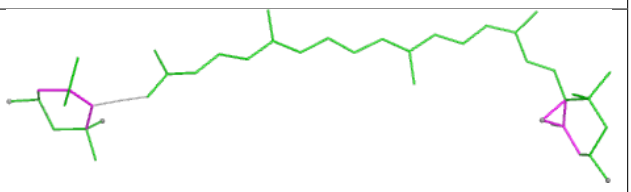
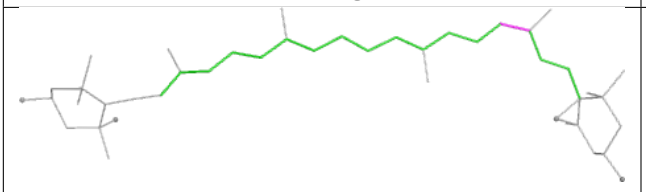


Bond angles



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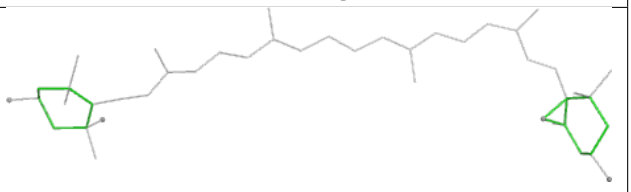
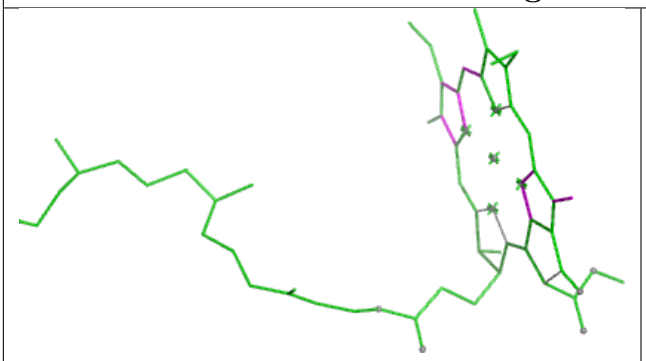


Rings

Ligand CLA B 822



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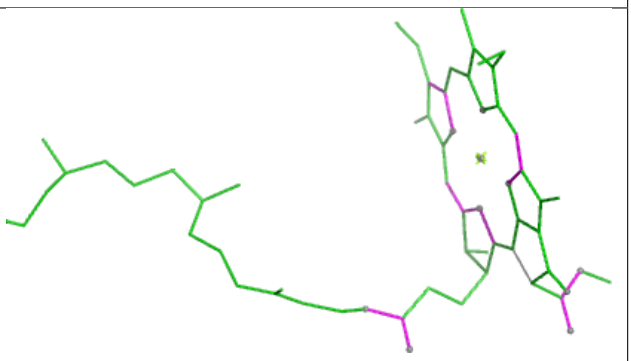
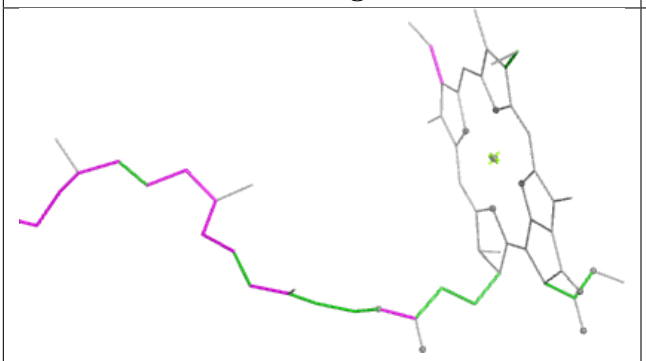


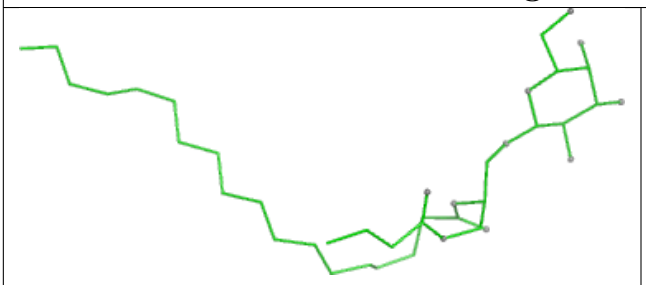
Bond angles



Torsions

Rings

Ligand LMG 4 621



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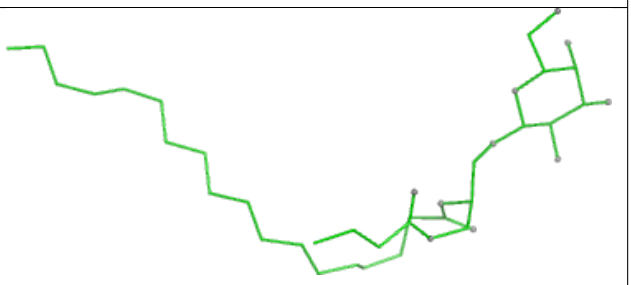
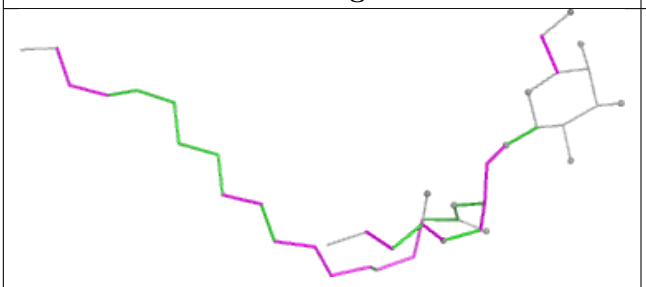


Bond angles



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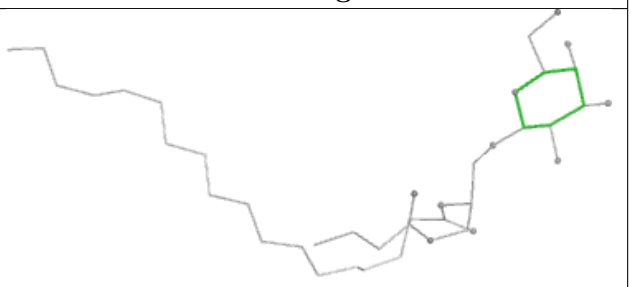
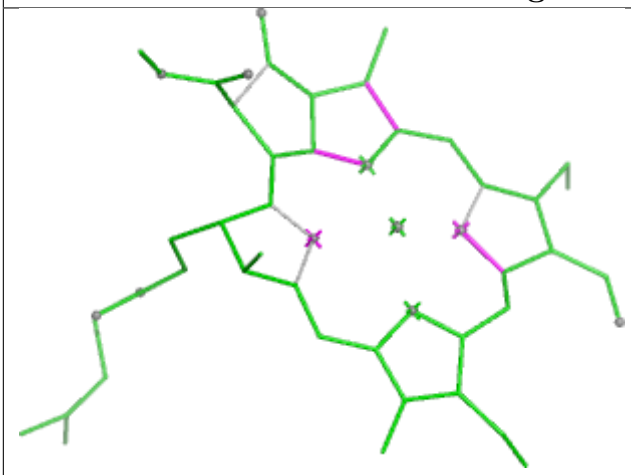
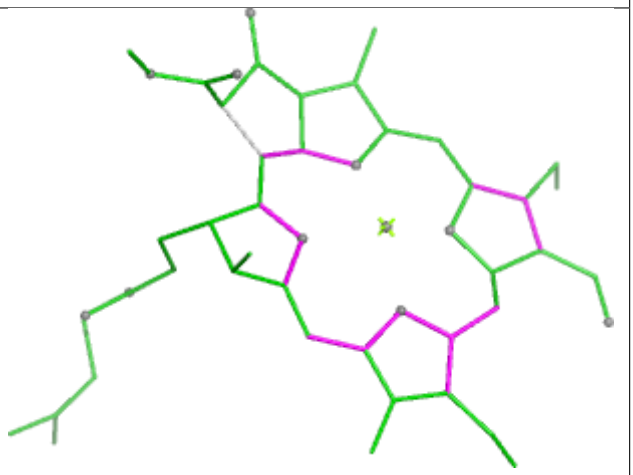


Rings

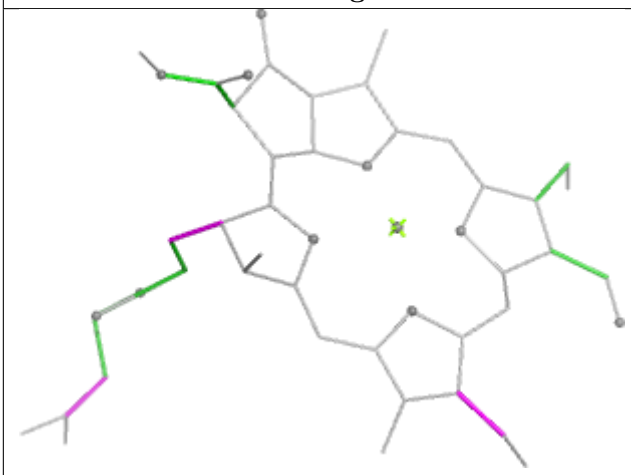
Ligand CHL 6 308



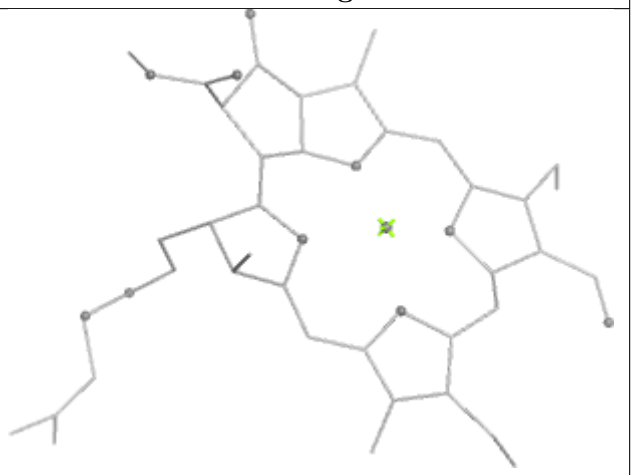
Bond lengths



Bond angles

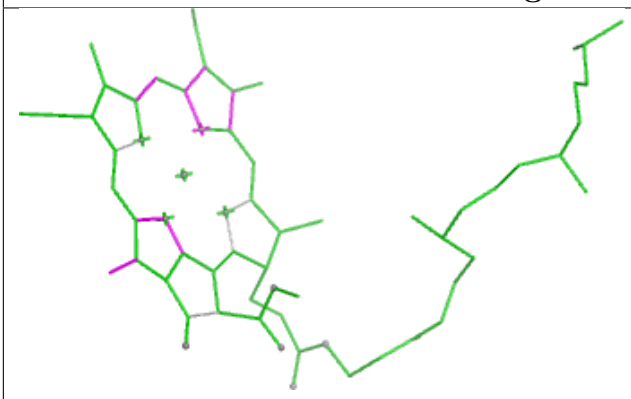


Torsions



Rings

Ligand CLA B 811



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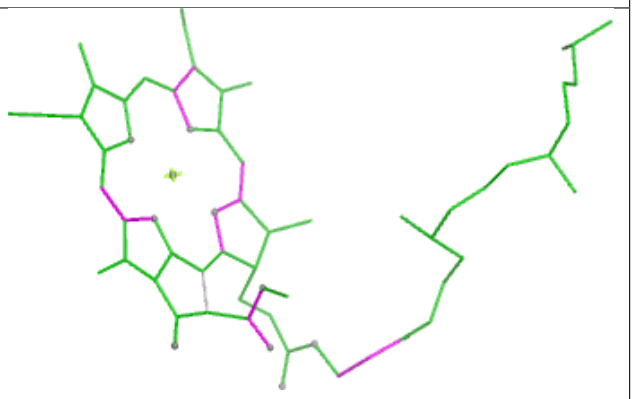
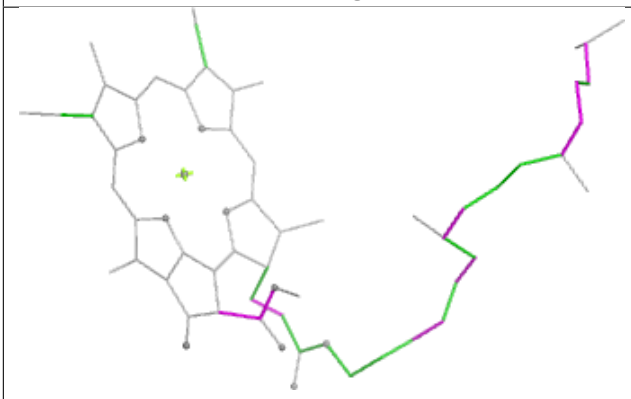


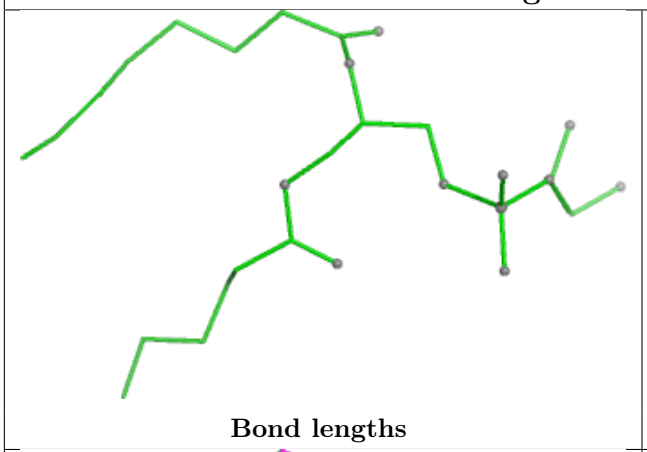
Bond angles



Torsions

Rings

Ligand LHG A 801



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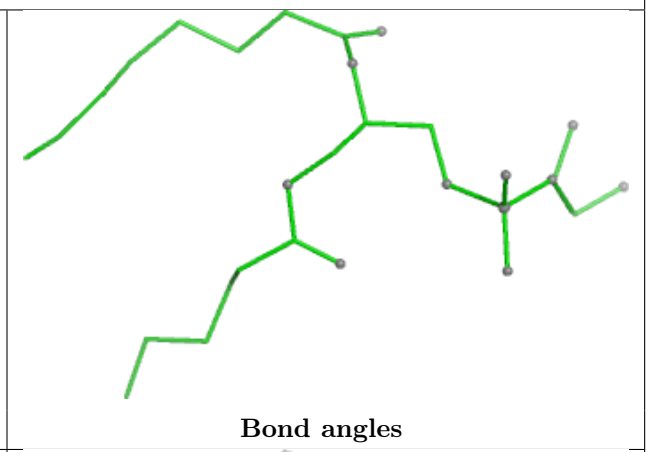
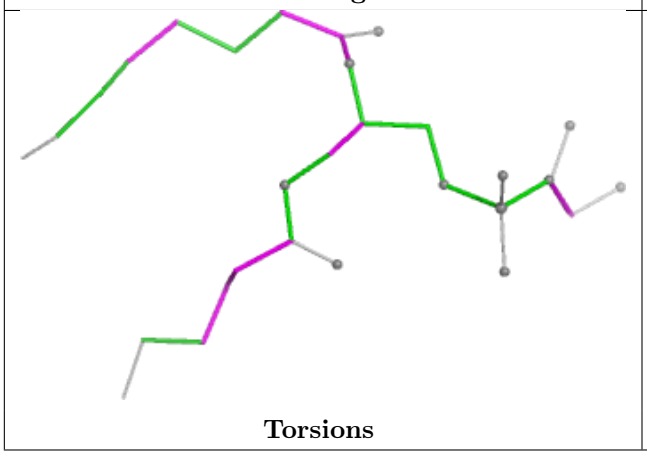


Bond angles



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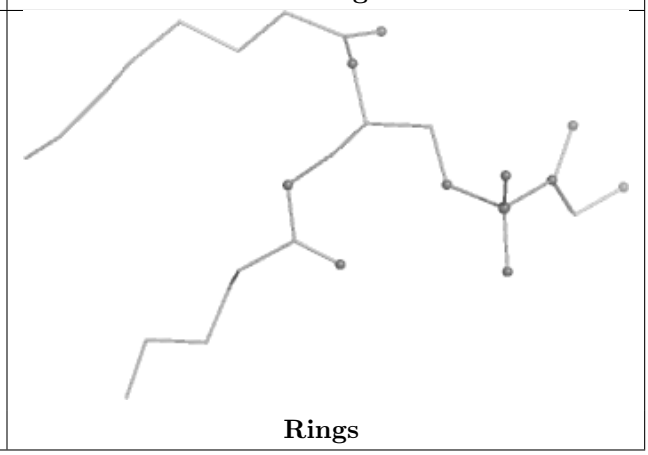
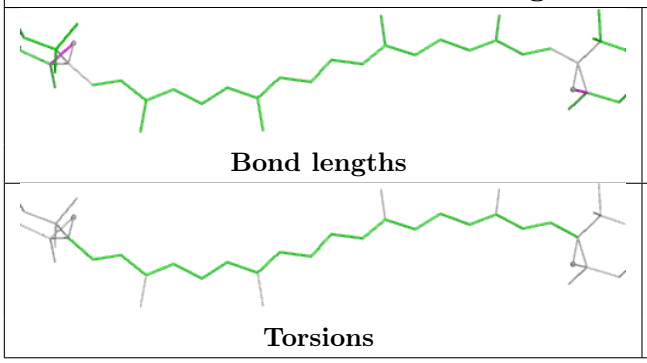


Rings

Ligand XAT 7 616



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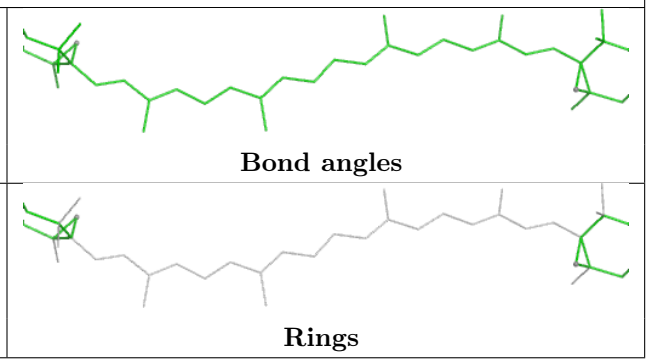

Bond angles

Torsions

Rings

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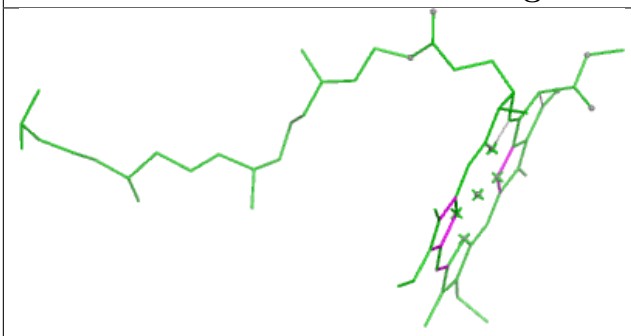

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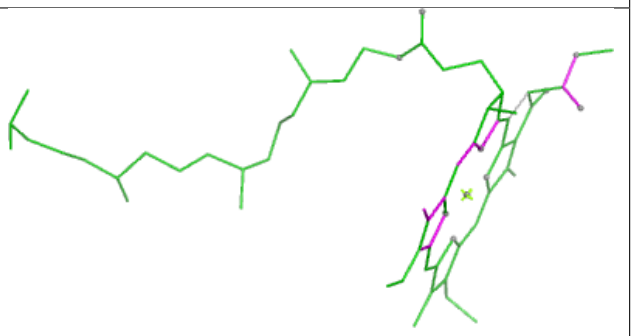
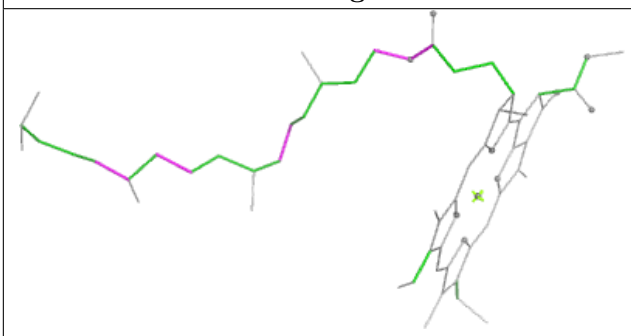


Bond angles



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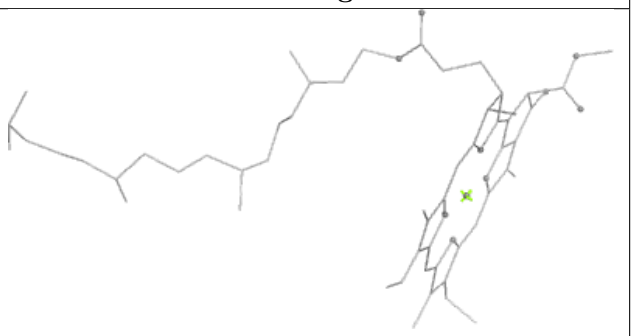
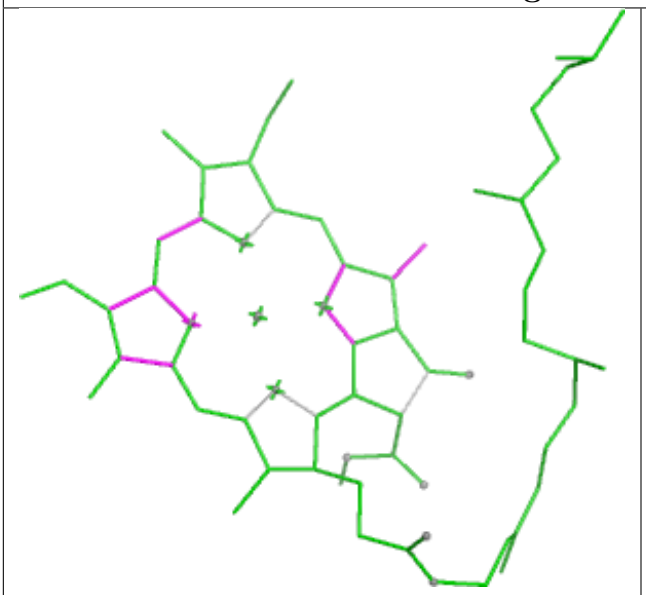


Rings

Ligand CLA A 827



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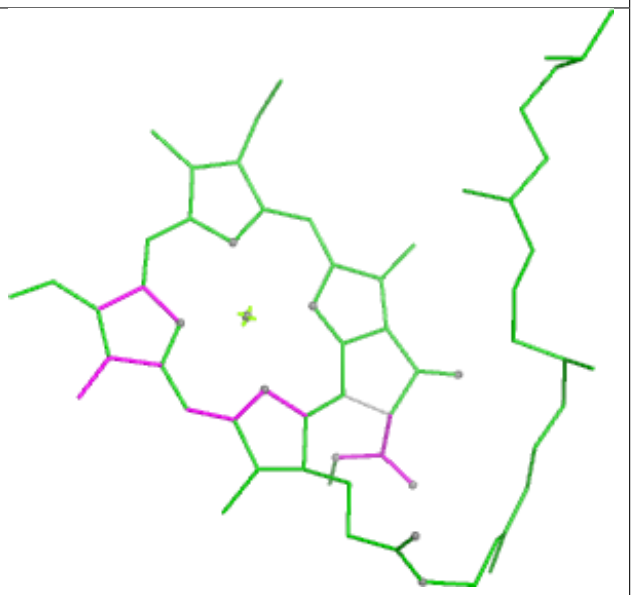
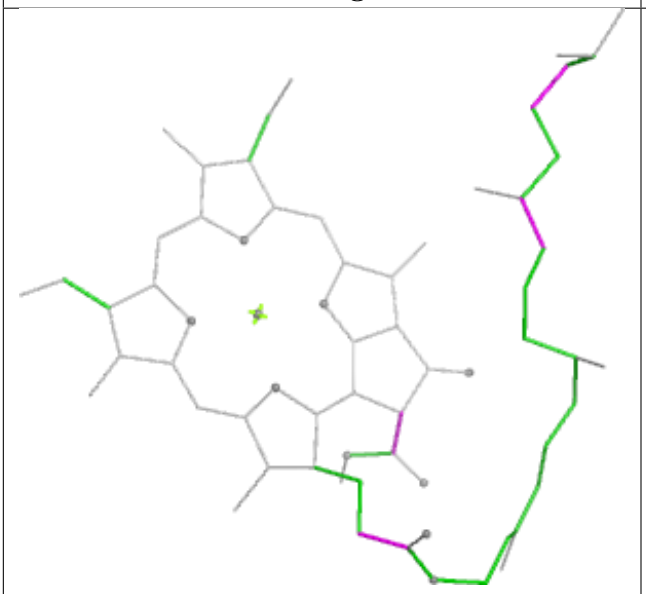


Bond angles



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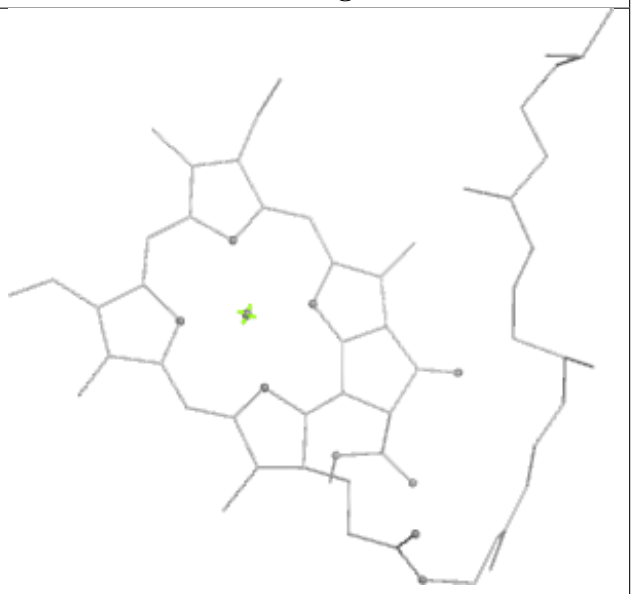
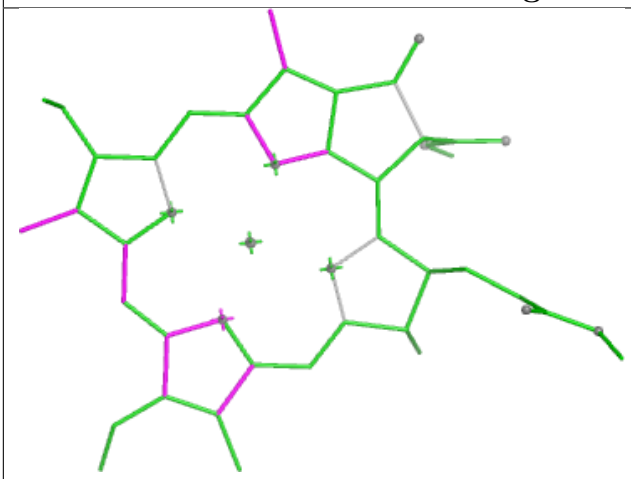


Rings

Ligand CLA K 204



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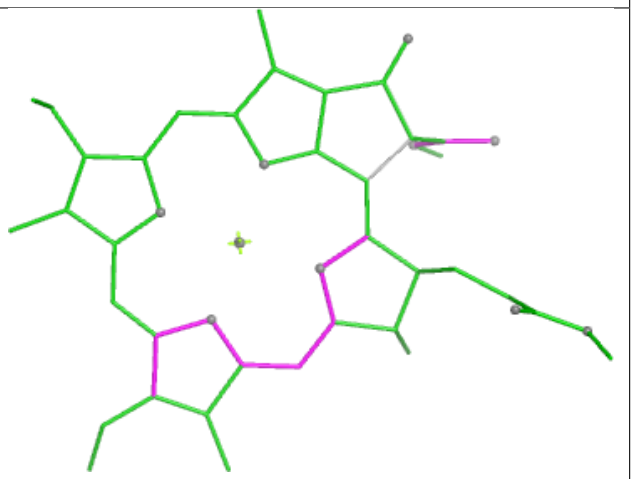
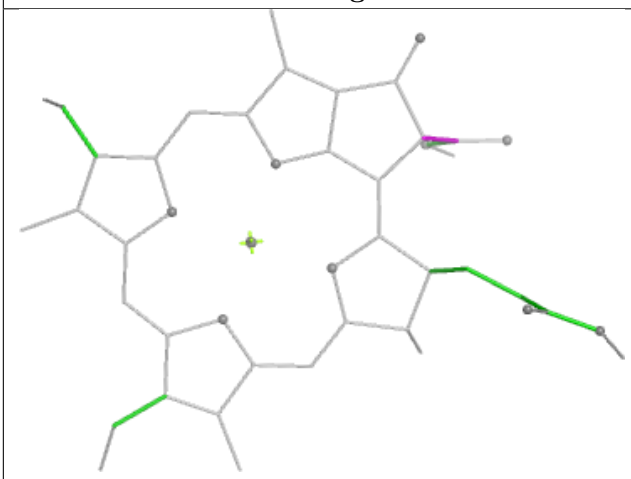


Bond angles



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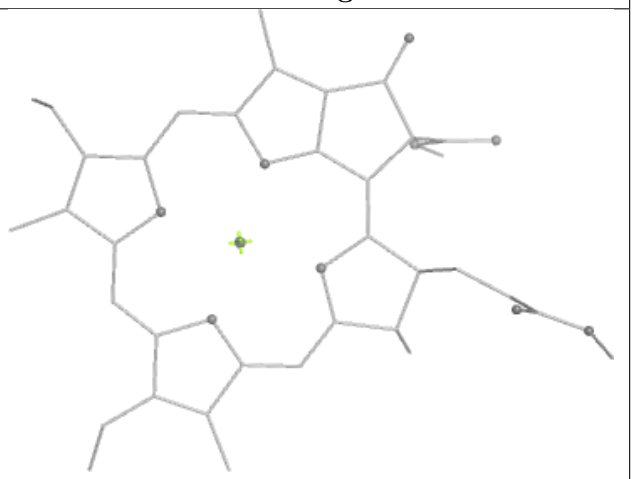
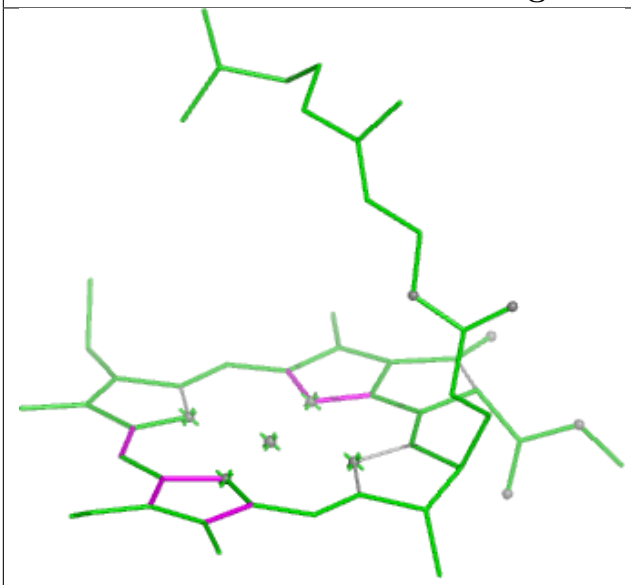


Rings

Ligand CLA 6 309



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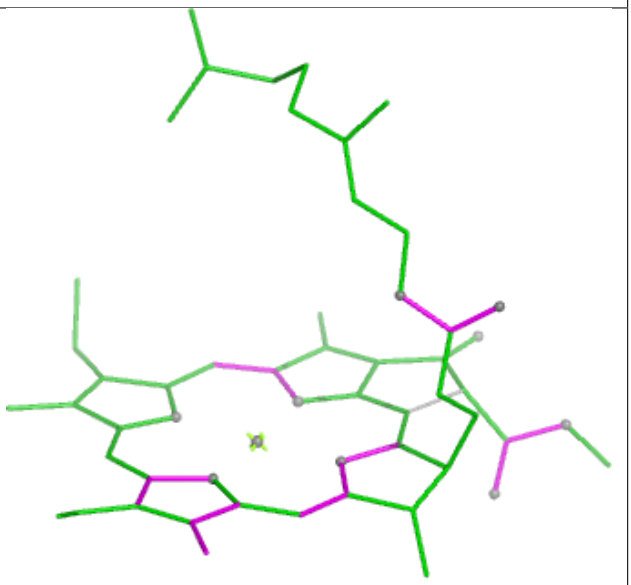

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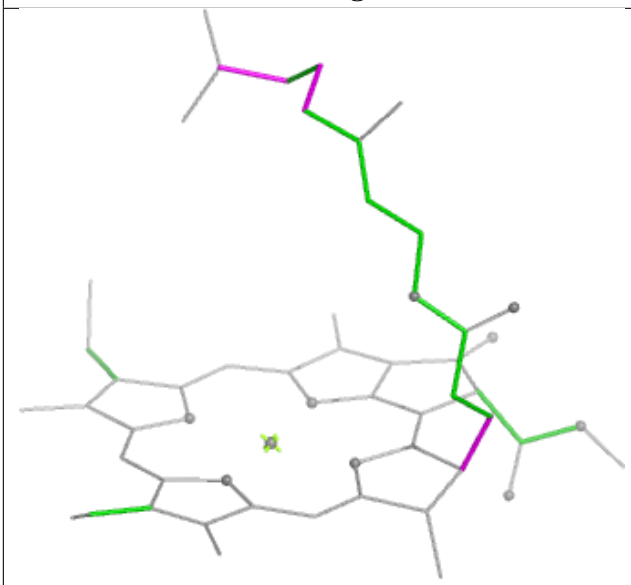

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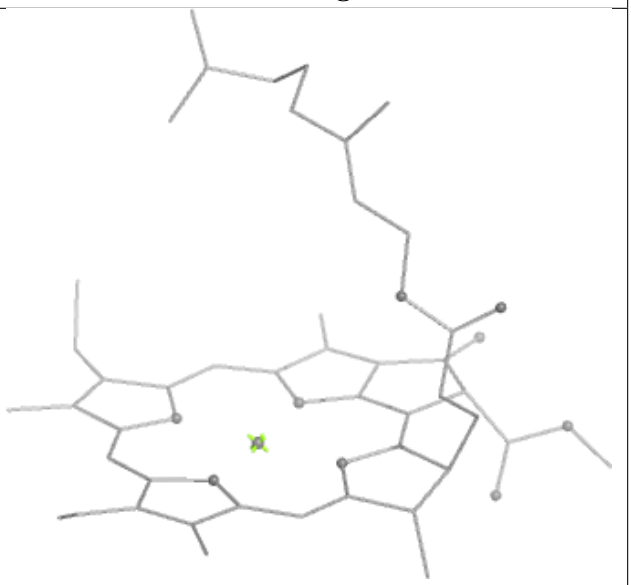
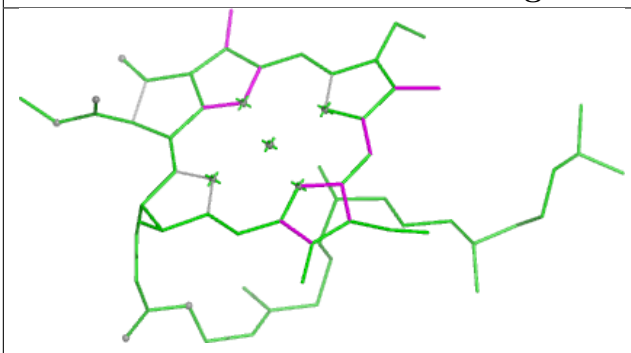
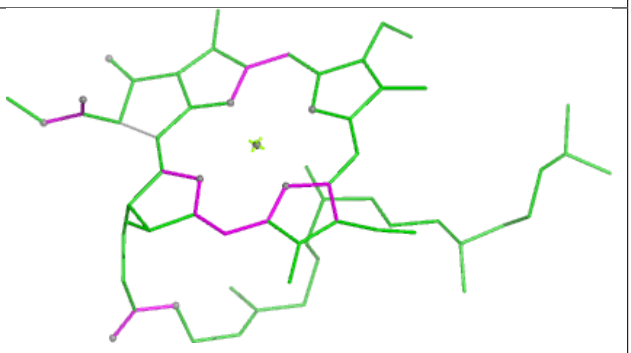
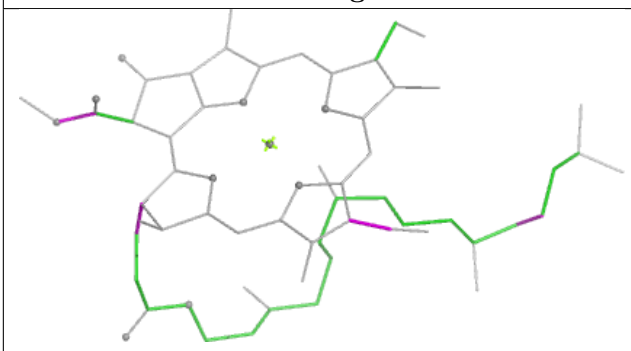
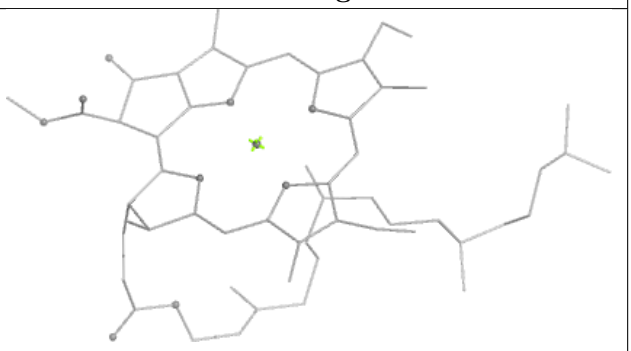
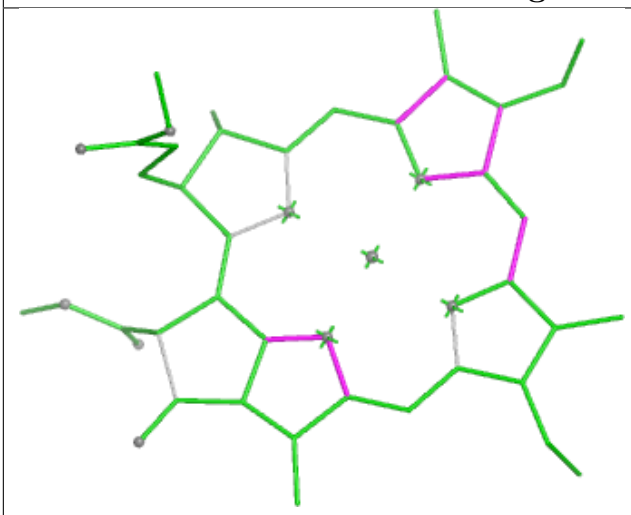


Rings

Ligand CLA B 818	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 1 314



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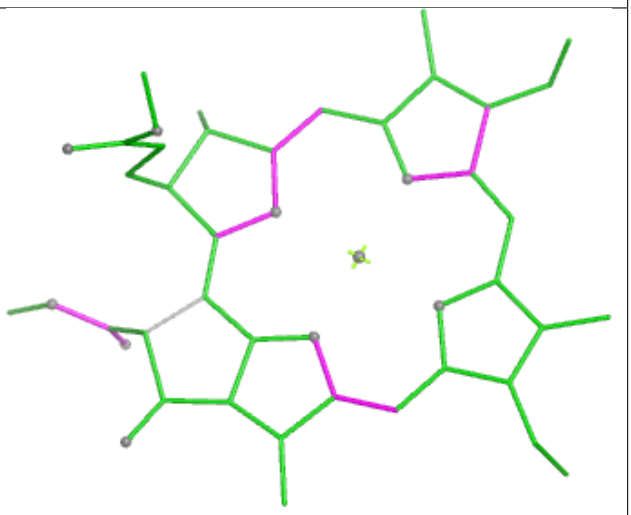
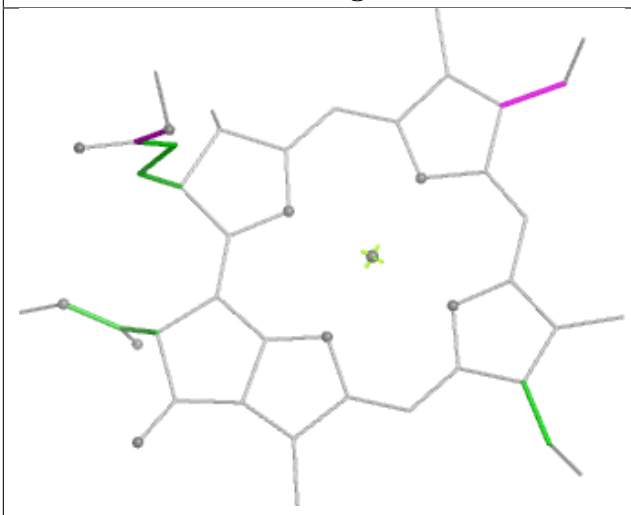


Bond angles



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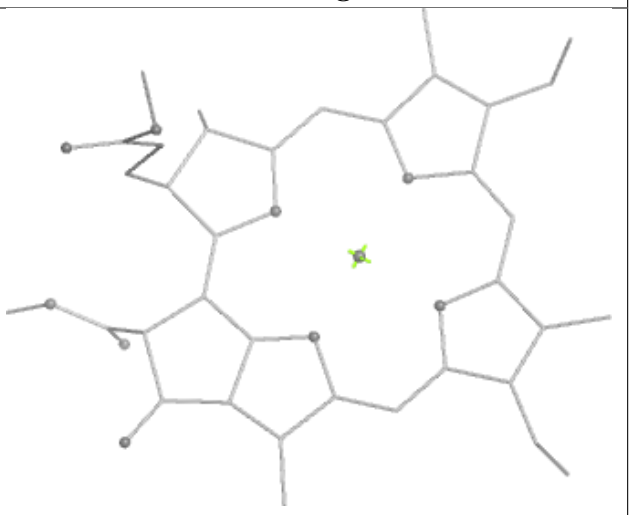
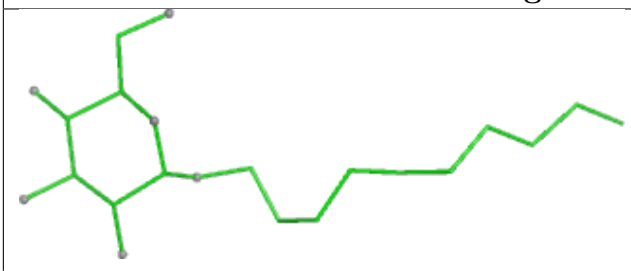


Rings

Ligand LMU 7 620



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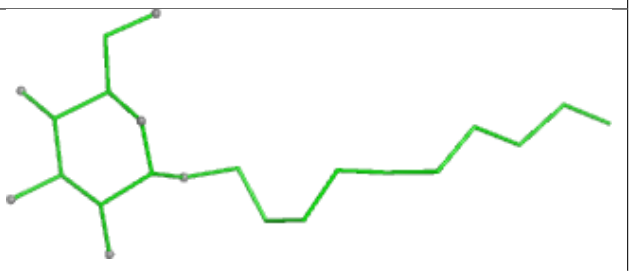

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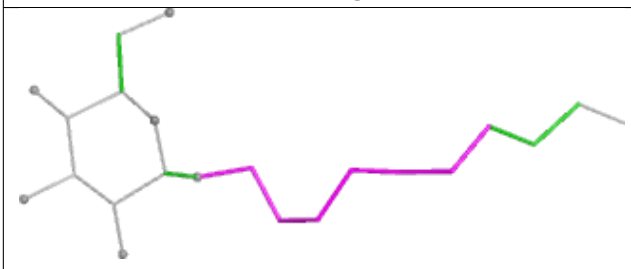

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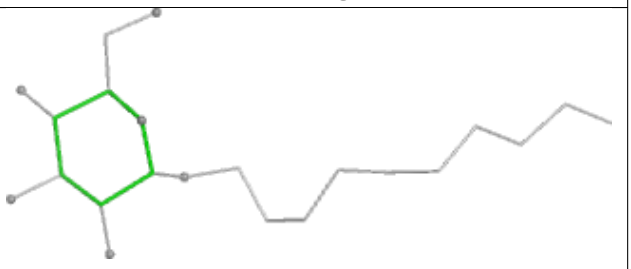
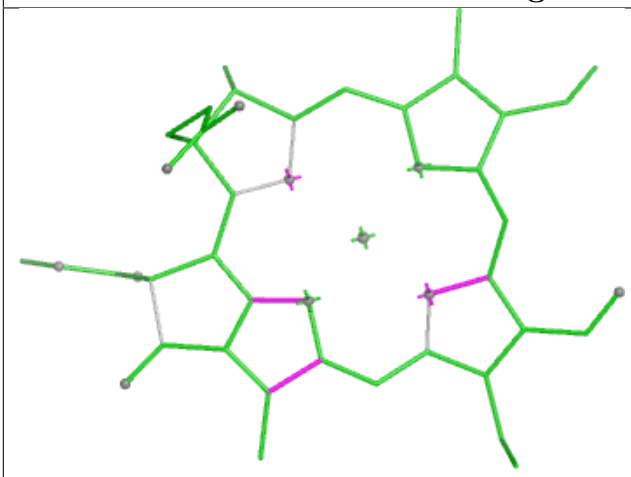


Rings

Ligand CHL 7 606



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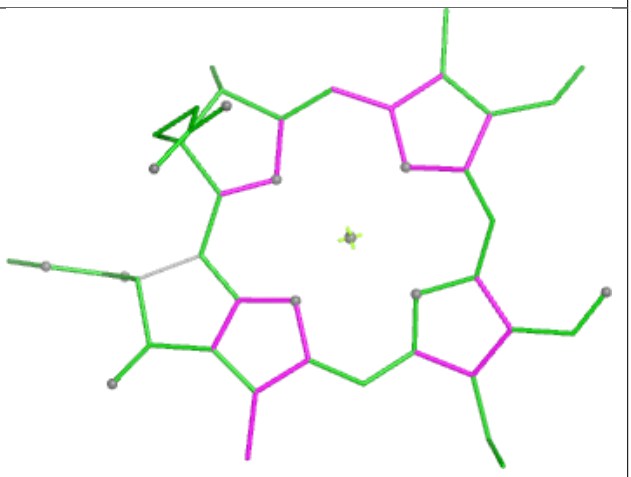
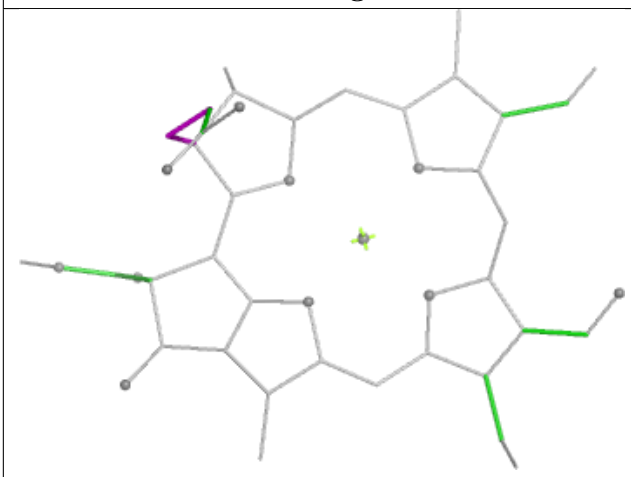


Bond angles



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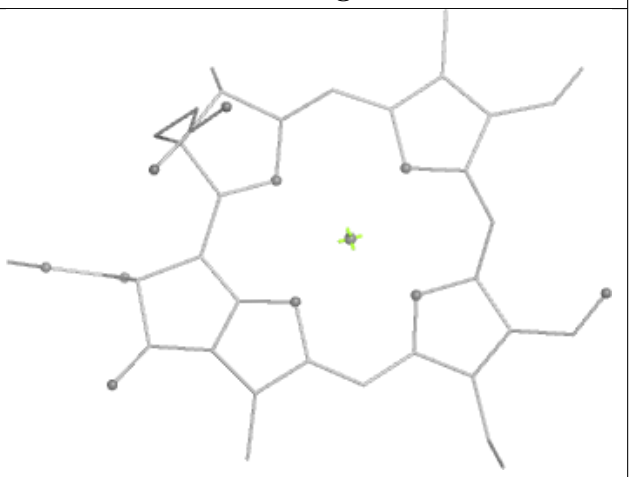
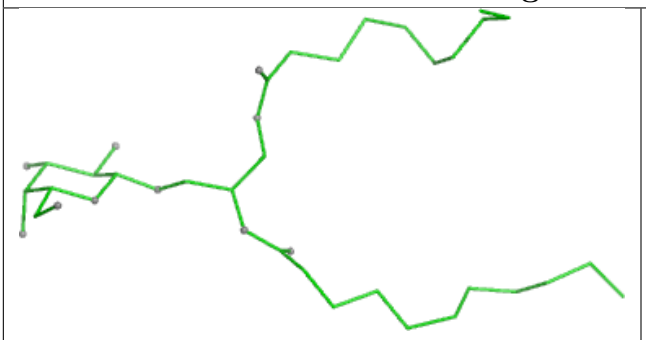


Rings

Ligand LMG L 201



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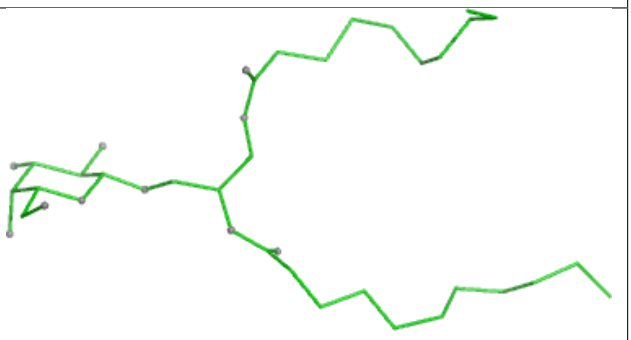
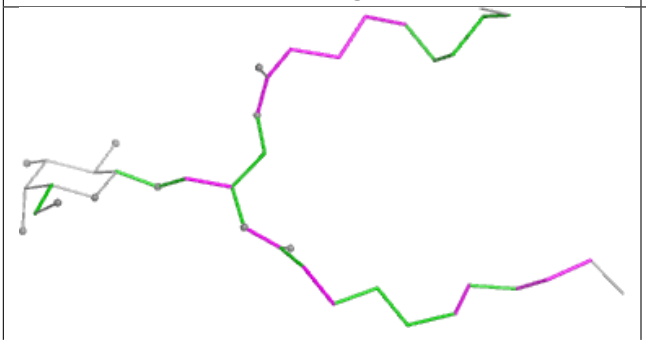


Bond angles



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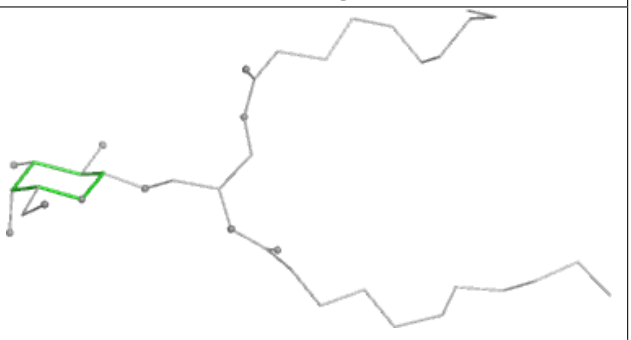
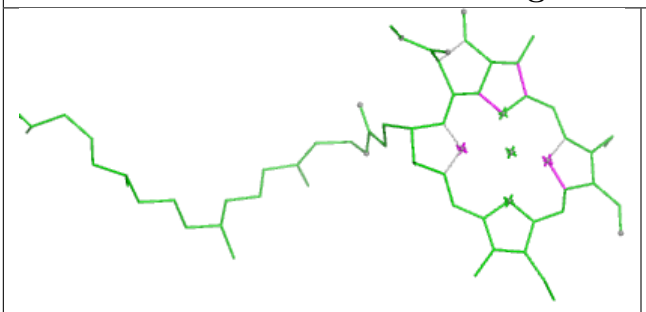
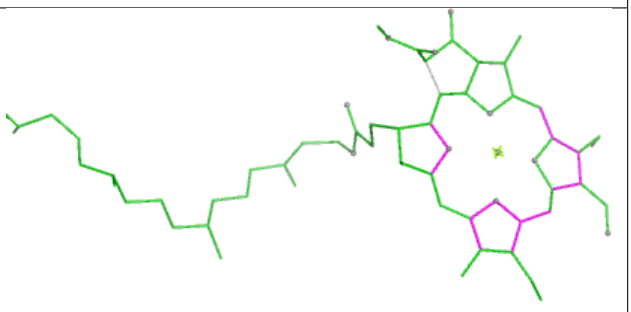


Rings

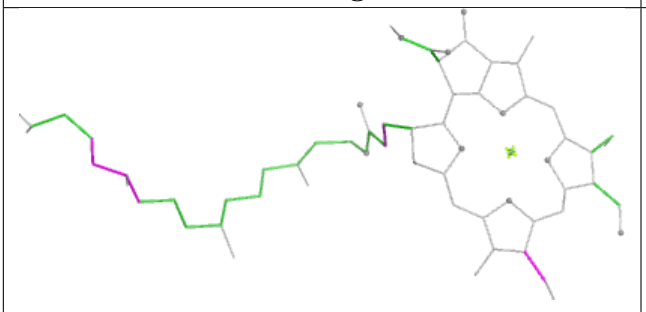
Ligand CHL 3 306



Bond lengths



Bond angles



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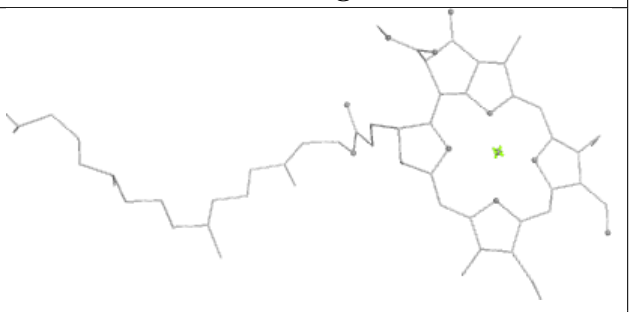
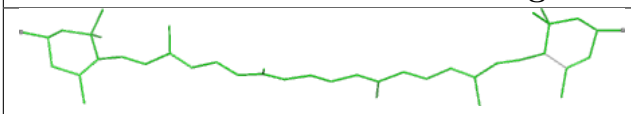
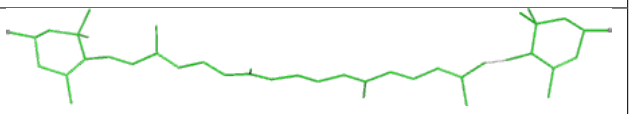
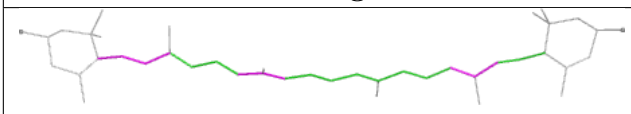
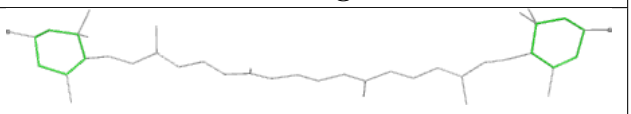


Rings

Ligand LUT 5 324	
 Bond lengths	 Bond angles
 Torsions	 Rings

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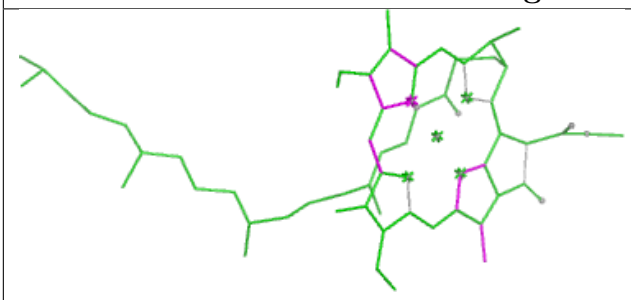
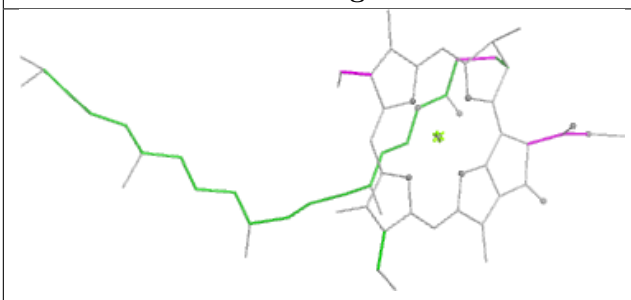
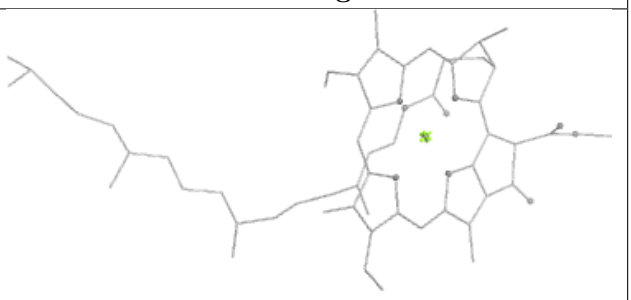
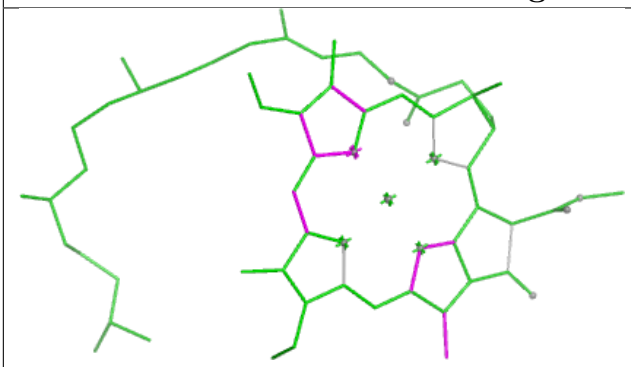
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA 7 609



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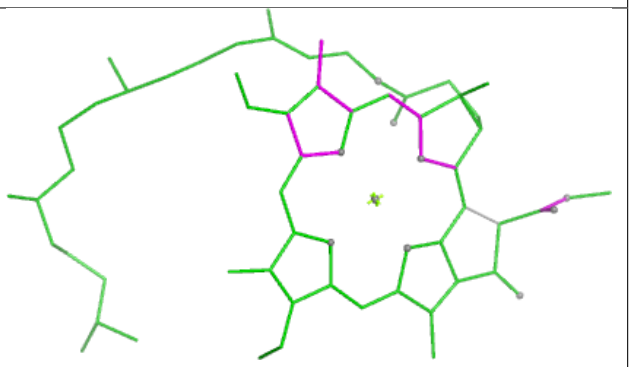
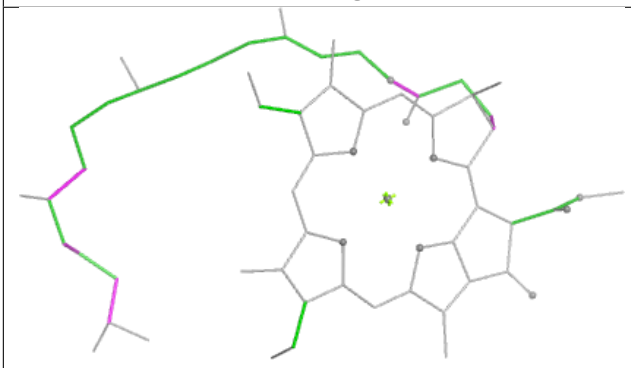


Bond angles



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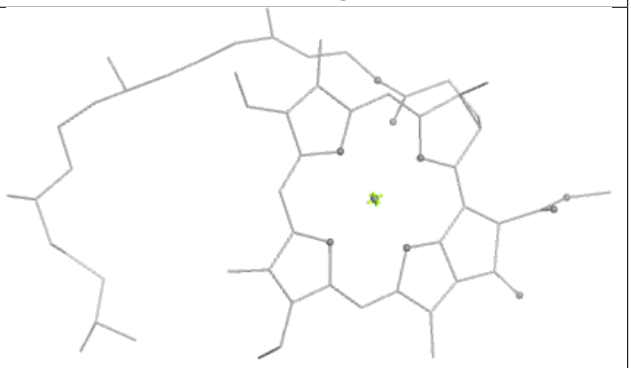
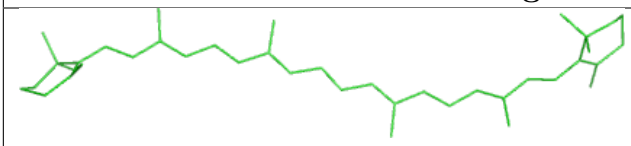


Rings

Ligand BCR B 847



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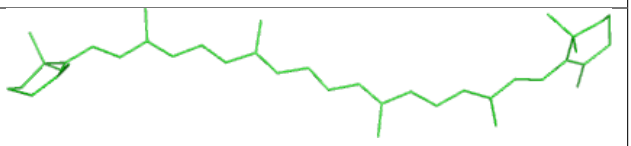

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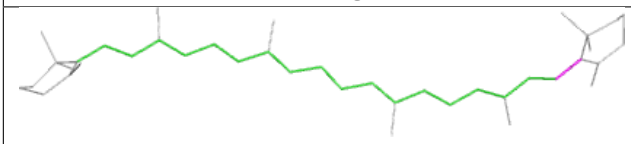

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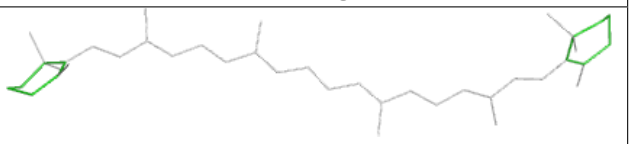
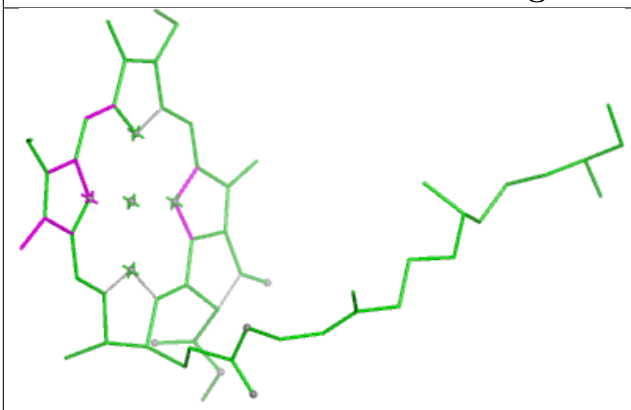


Rings

Ligand CLA 3 307



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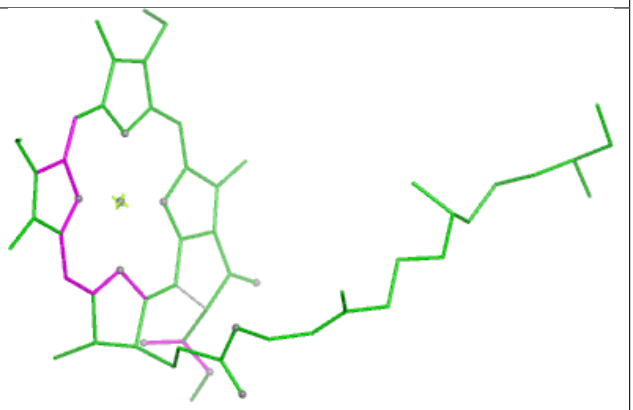

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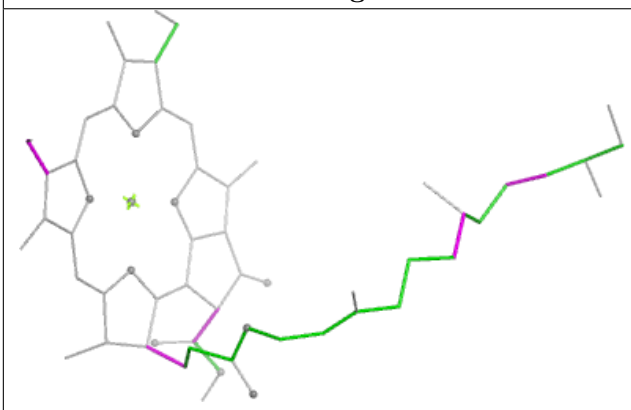

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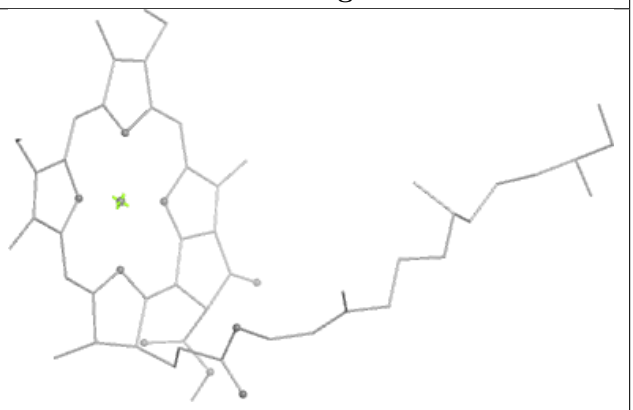
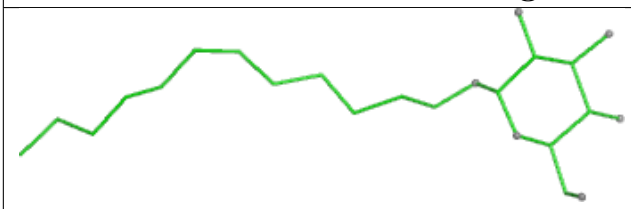


Rings

Ligand LMU A 857



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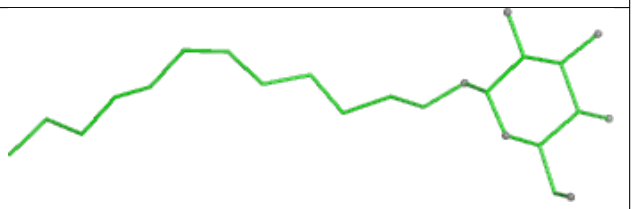
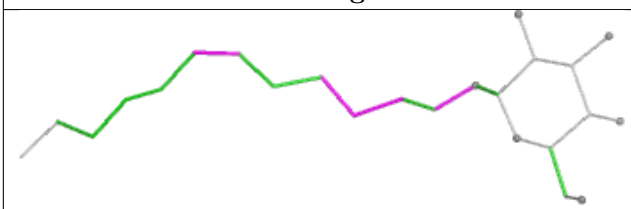


Bond angles



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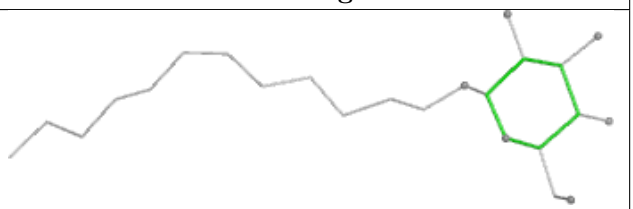

Rings

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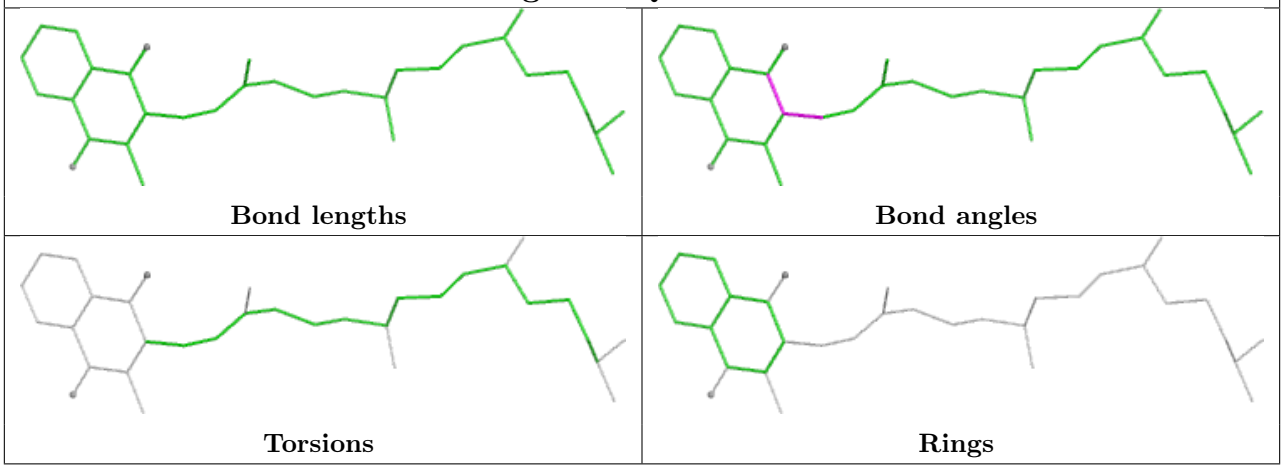
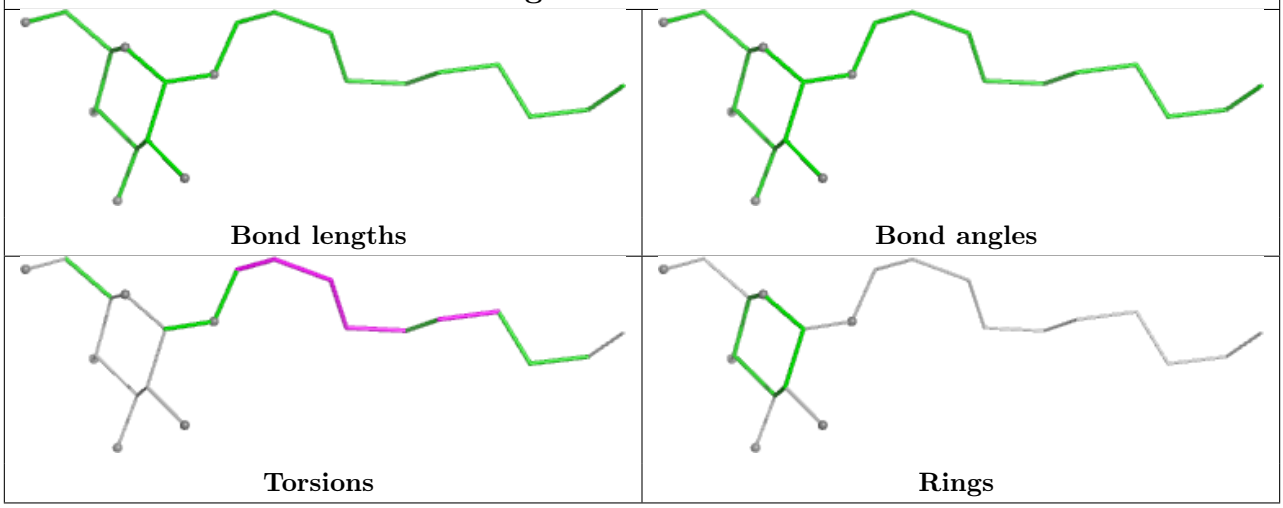


Ligand LMU 1 322



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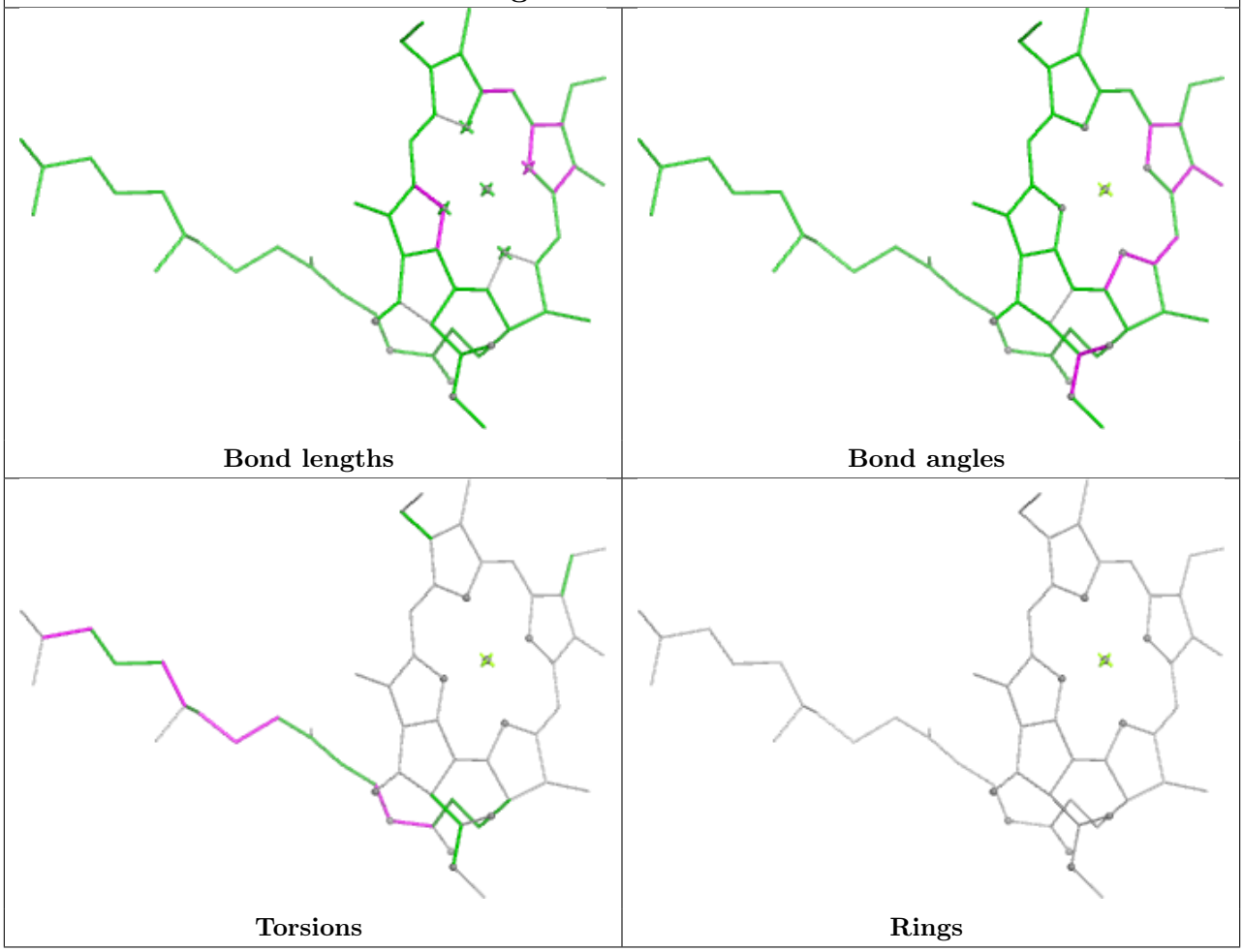

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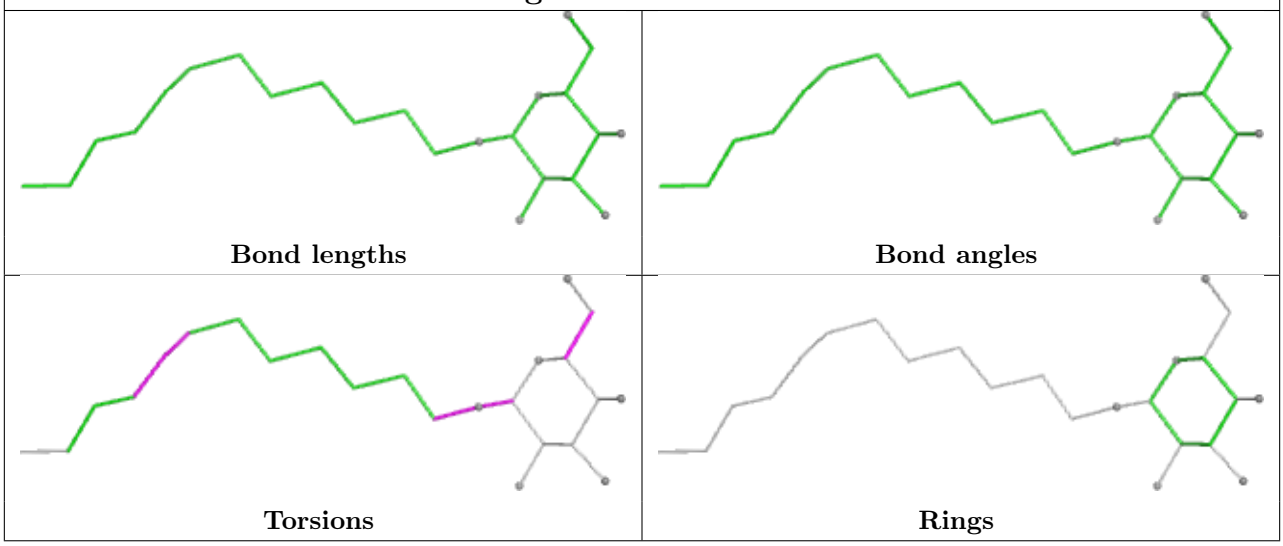

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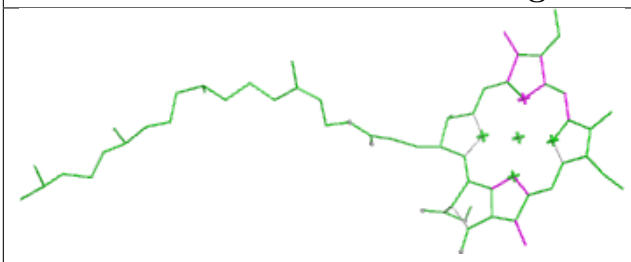
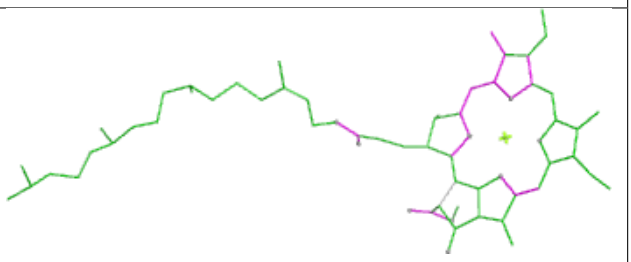


Bond lengths



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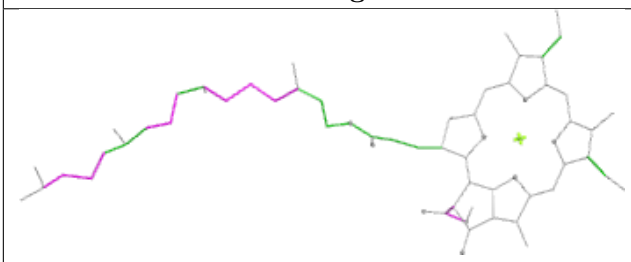

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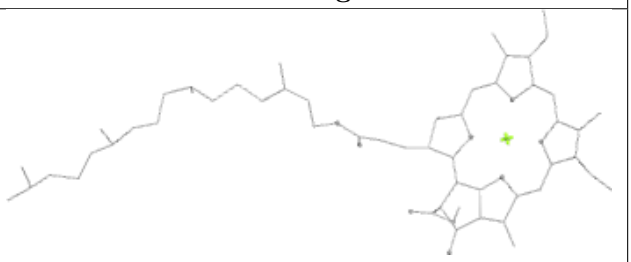
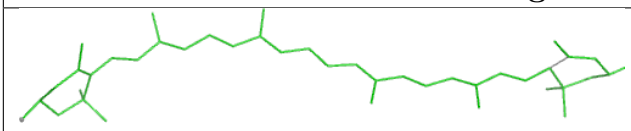


Rings

Ligand LUT 7 615



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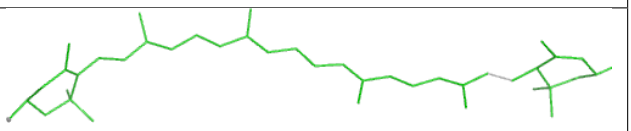

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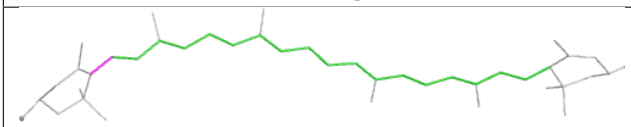

Torsions

Rings

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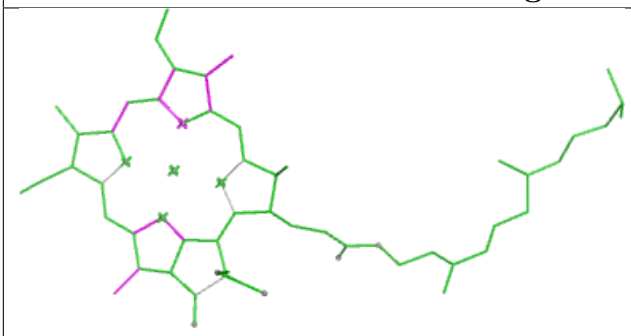

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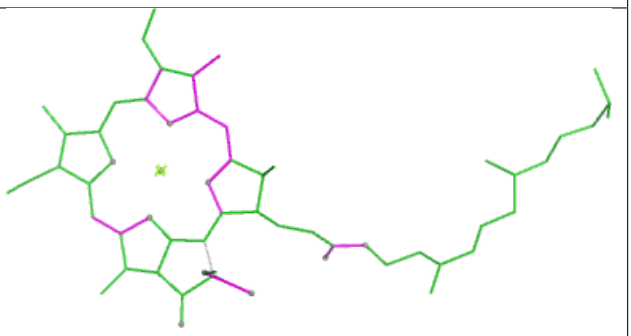

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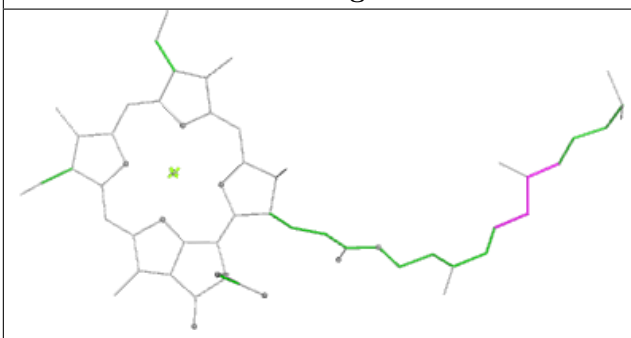

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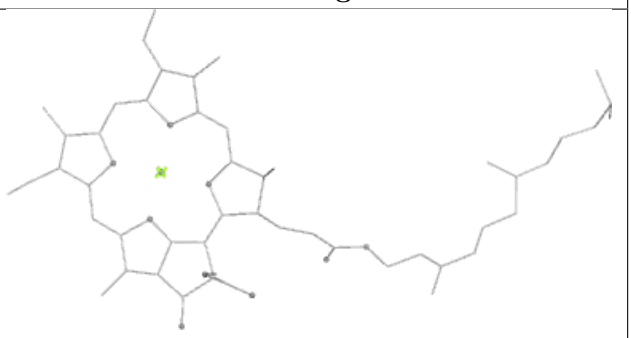
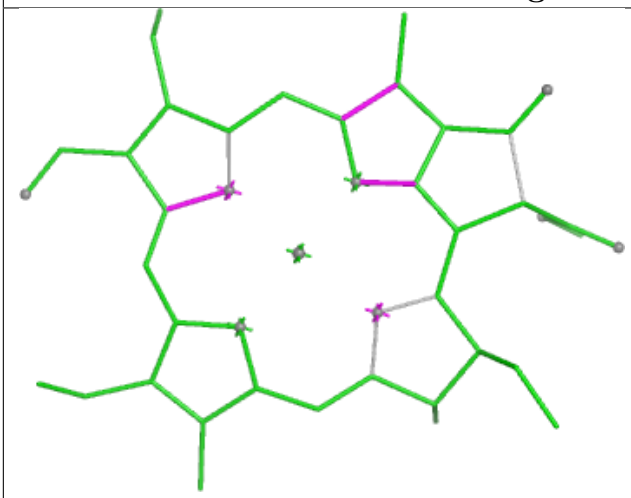


Rings

Ligand CHL 6 317



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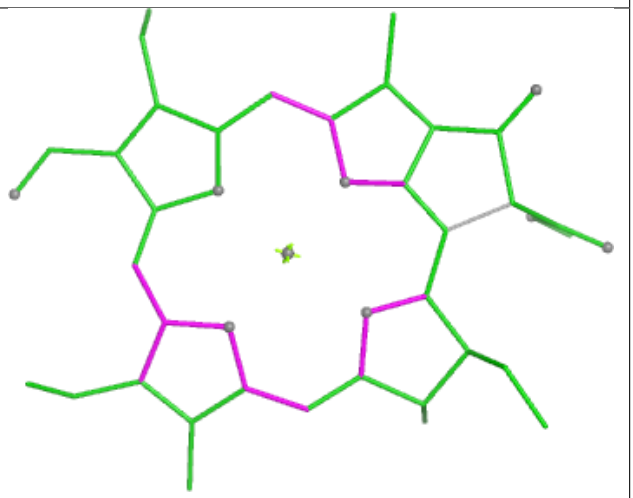

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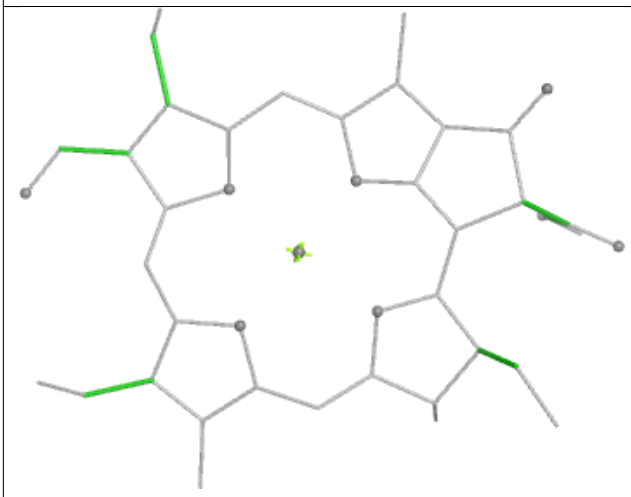

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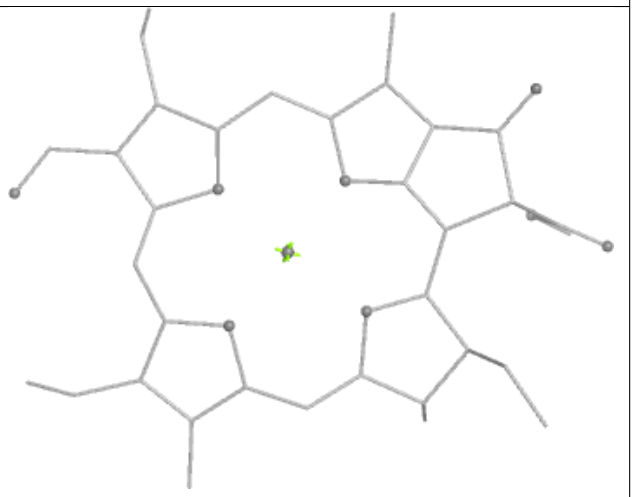
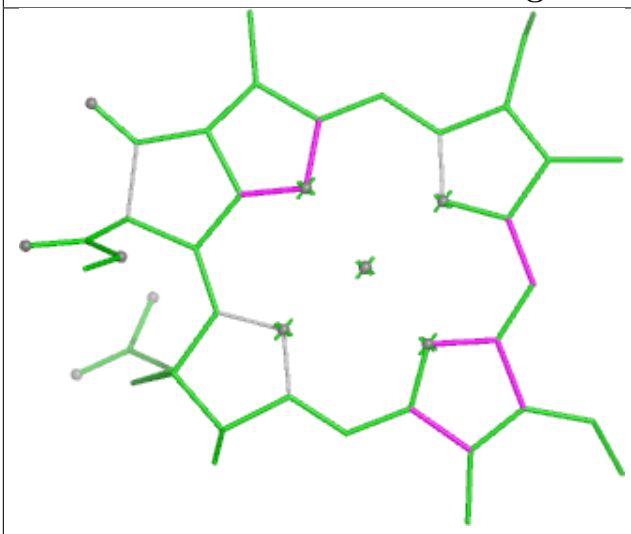


Rings

Ligand CLA L 204



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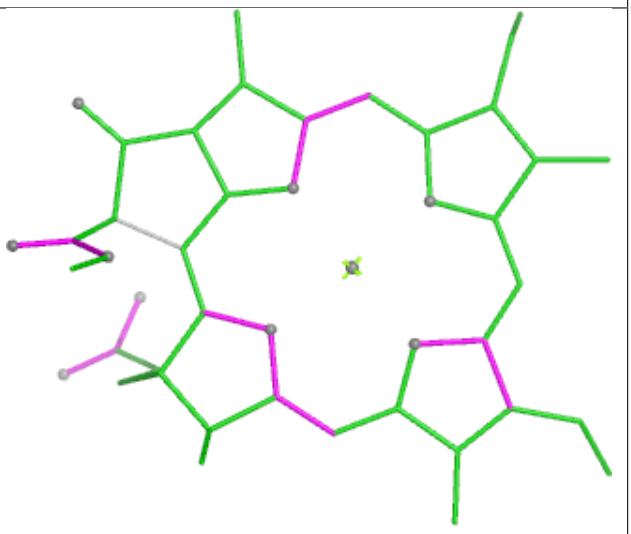

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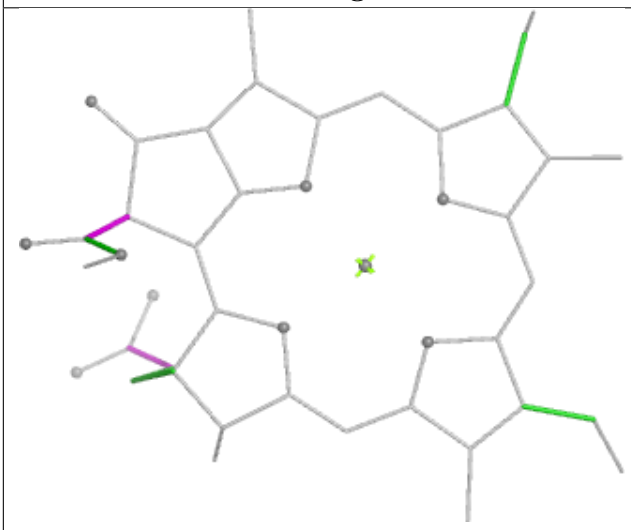

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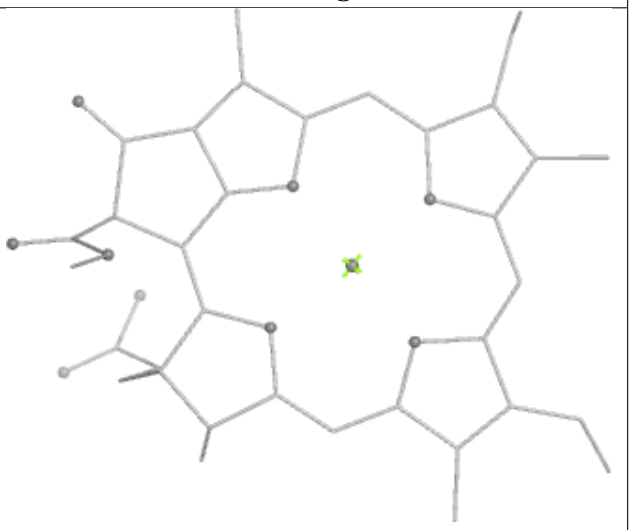
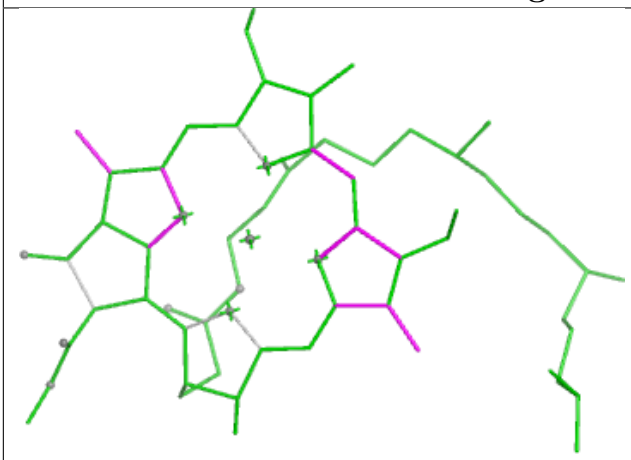


Rings

Ligand CLA 8 312



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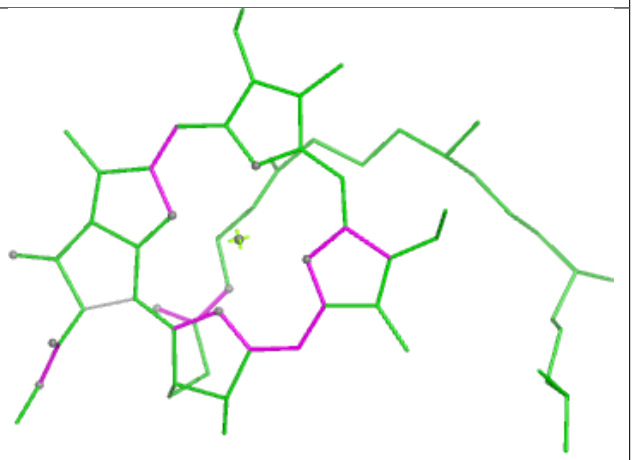

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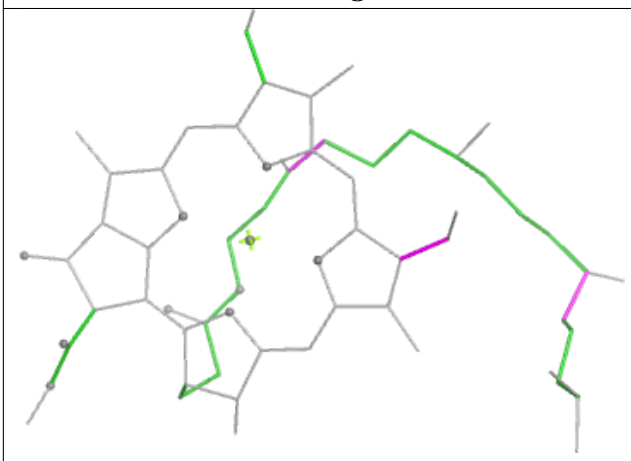

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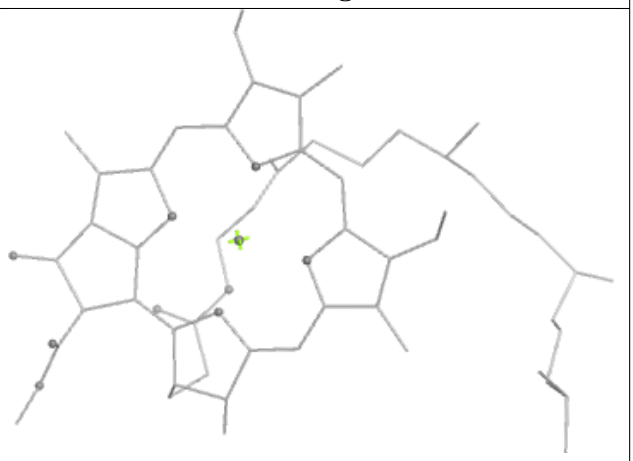
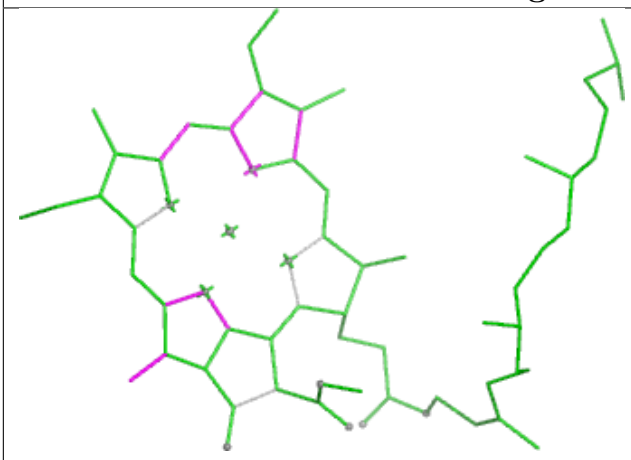


Rings

Ligand CLA 8 303



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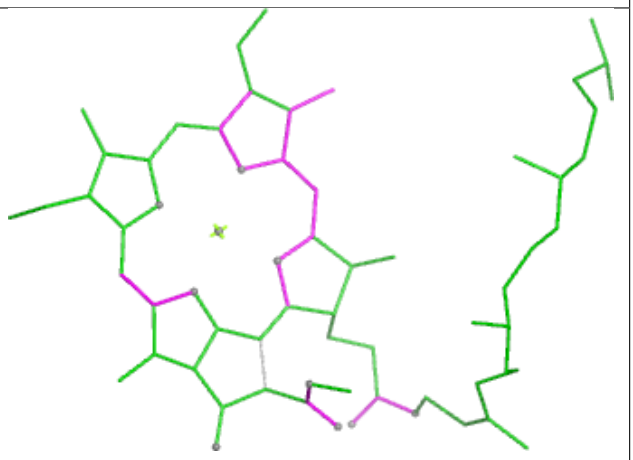
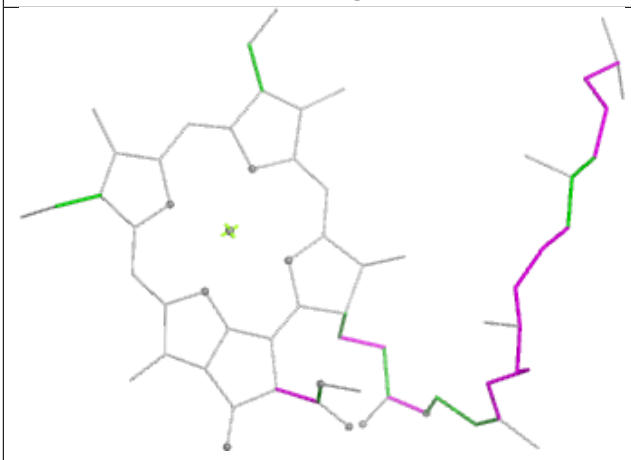


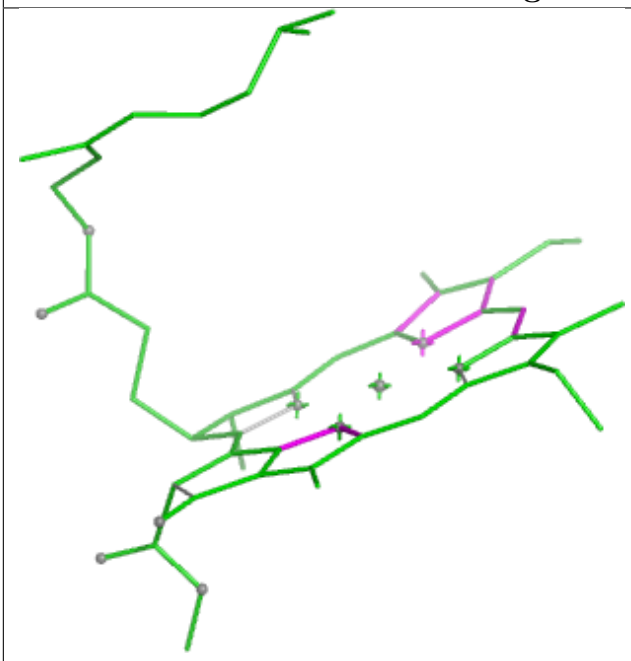
Bond angles



Torsions

Rings

Ligand CLA A 816



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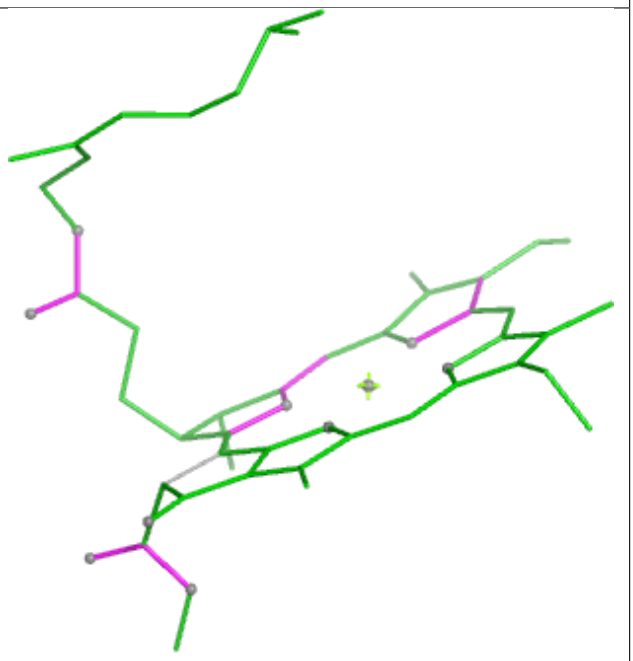
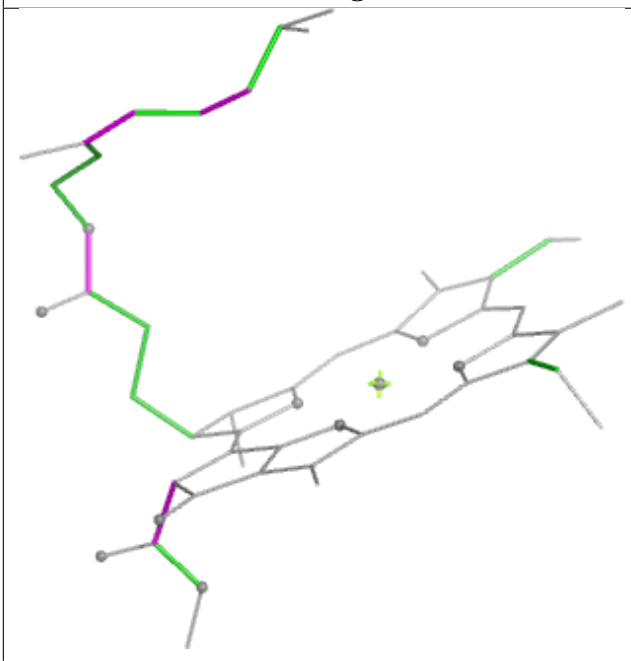


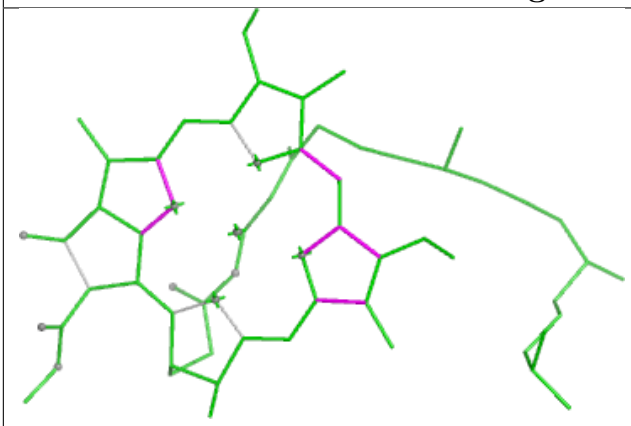
Bond angles



Torsions

Rings

Ligand CLA 1 312



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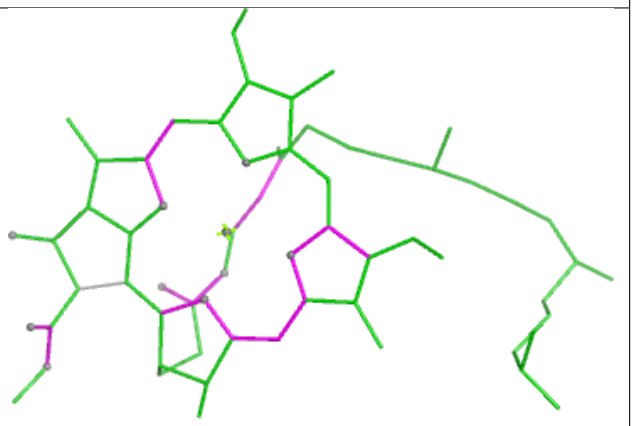

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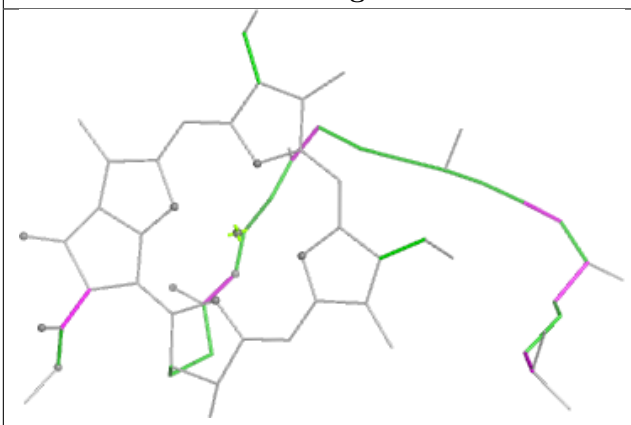

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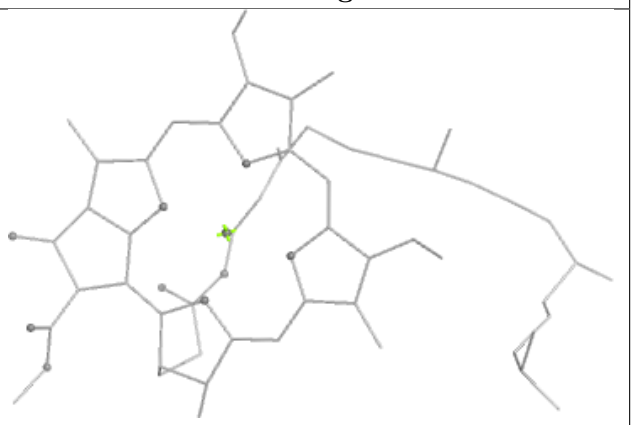
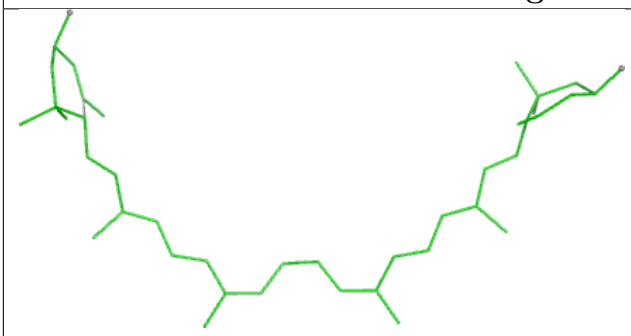


Rings

Ligand LUT F 305



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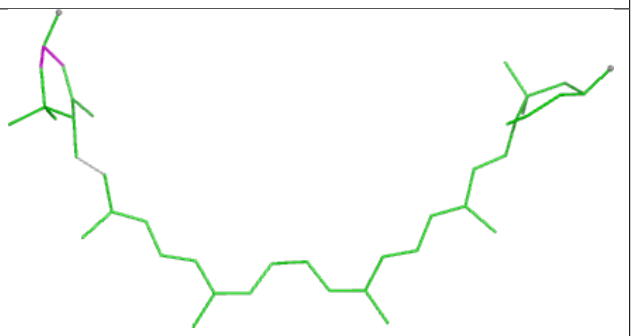

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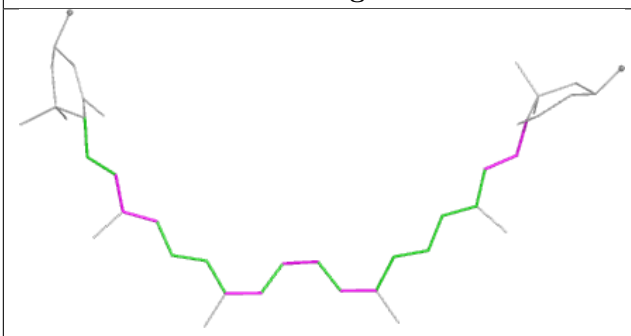
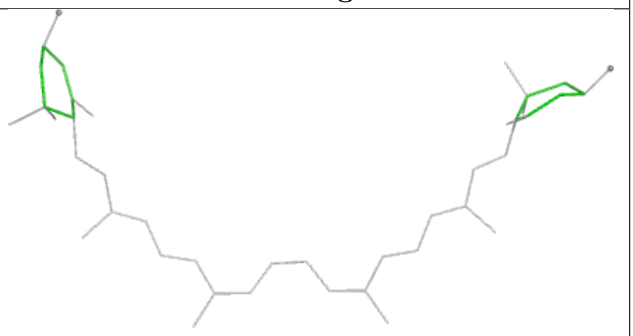
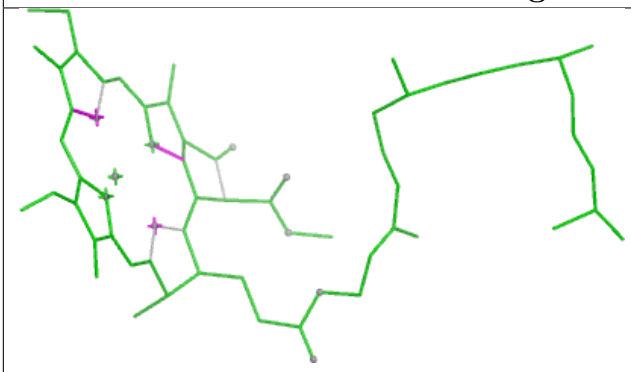


Torsions

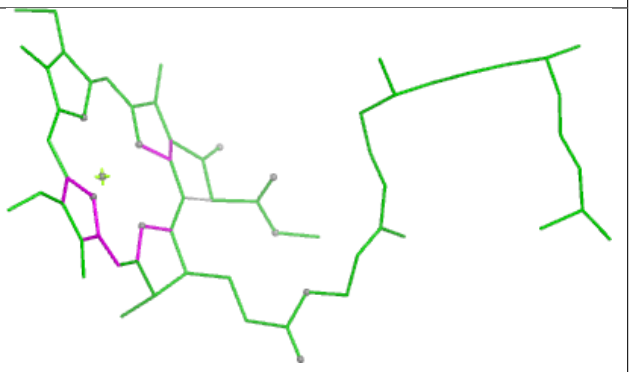


Rings

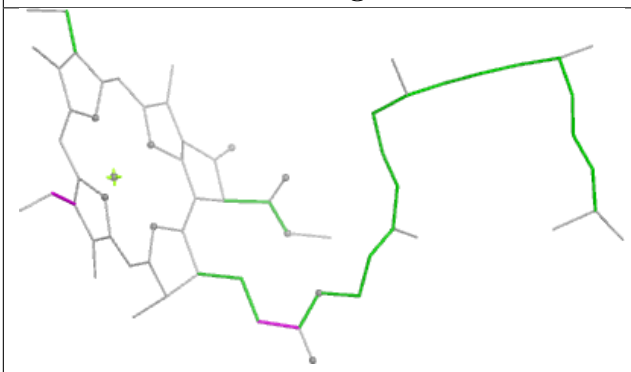
Ligand CL0 A 802



Bond lengths



Bond angles



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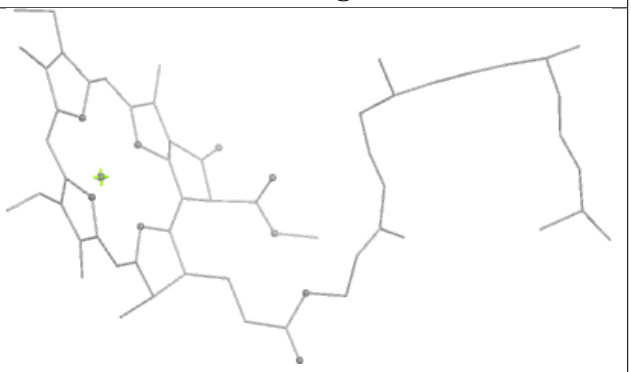
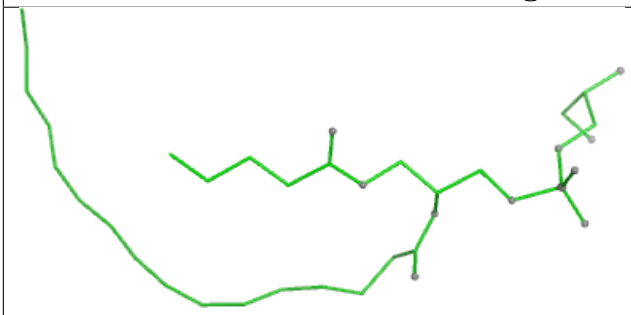


Rings

Ligand LHG A 848



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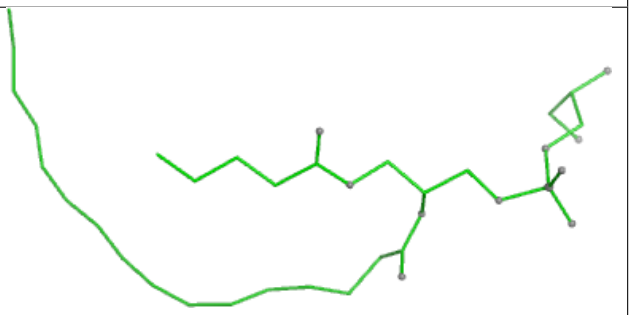

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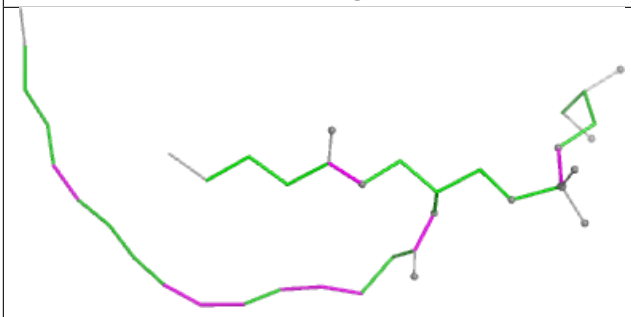

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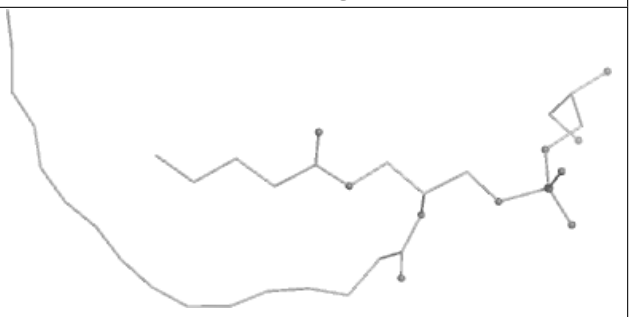
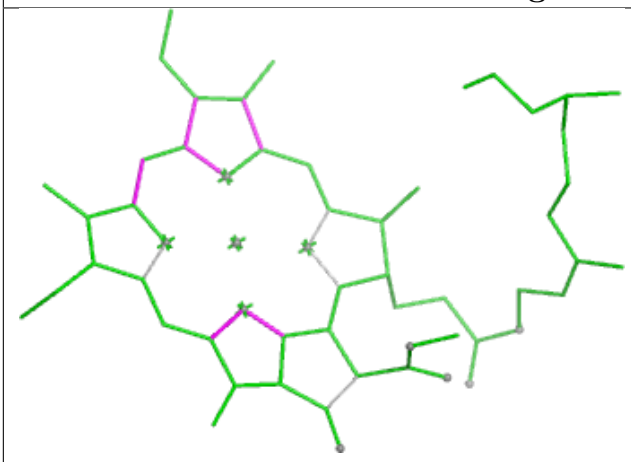


Rings

Ligand CLA 1 303



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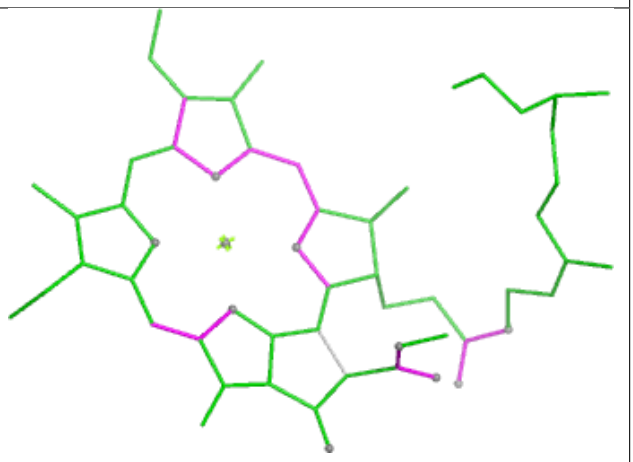

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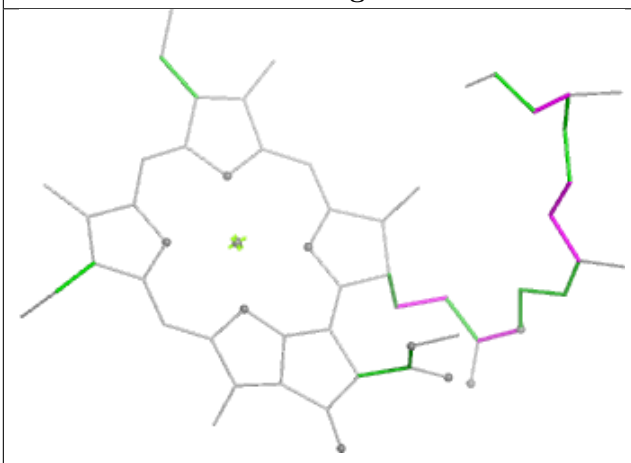

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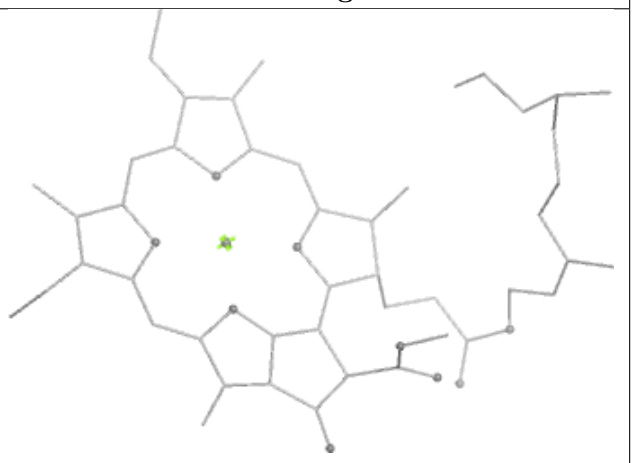
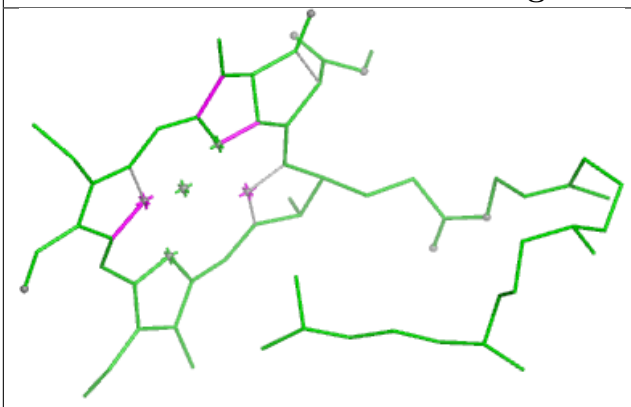


Rings

Ligand CHL 6 315



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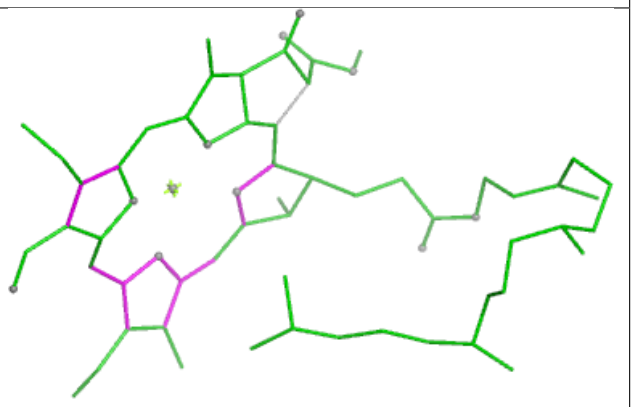

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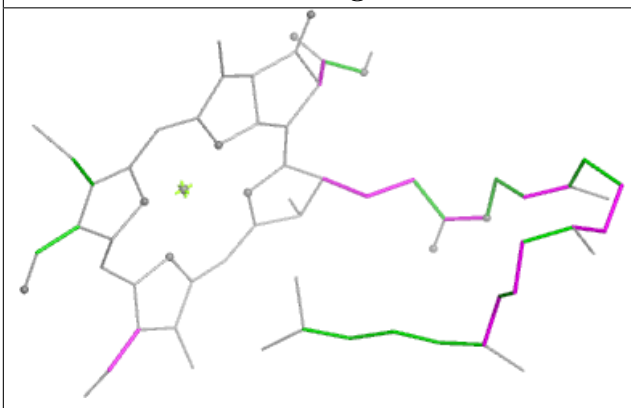

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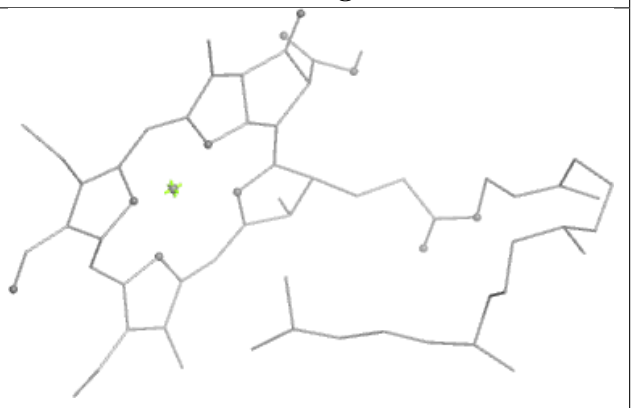
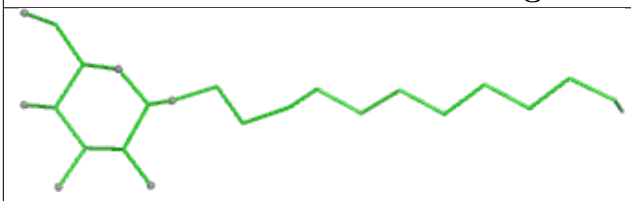


Rings

Ligand LMU 8 319



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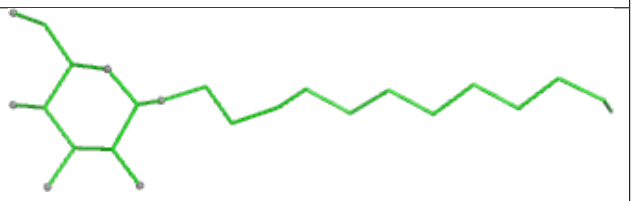

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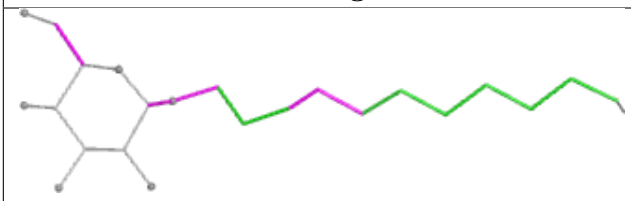

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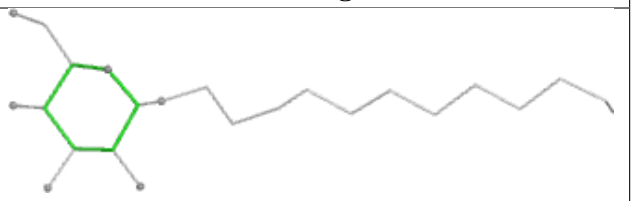
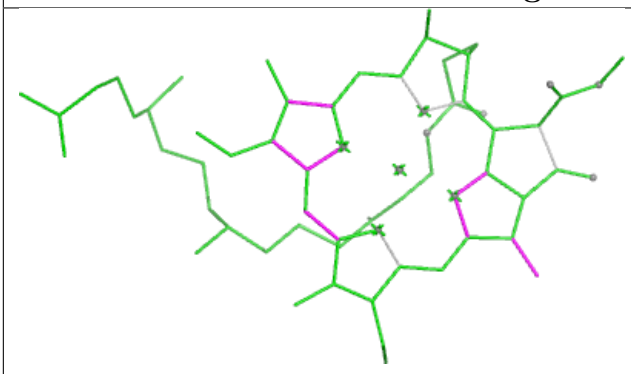


Rings

Ligand CLA A 814



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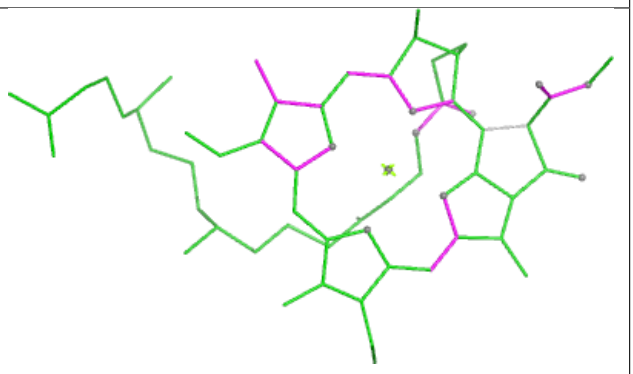

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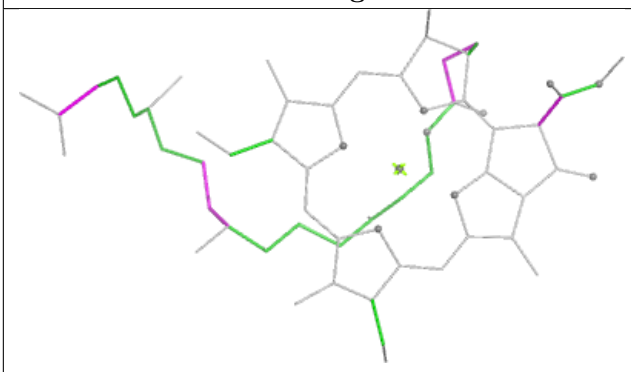

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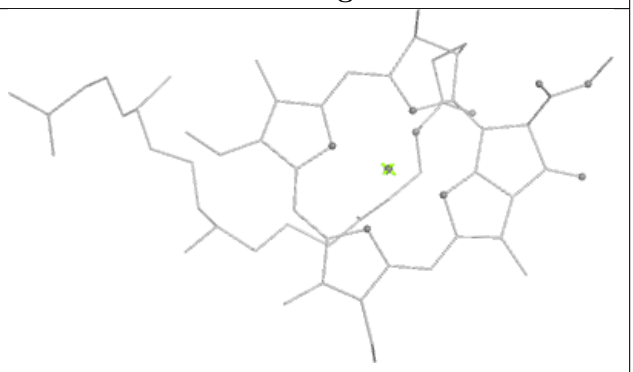
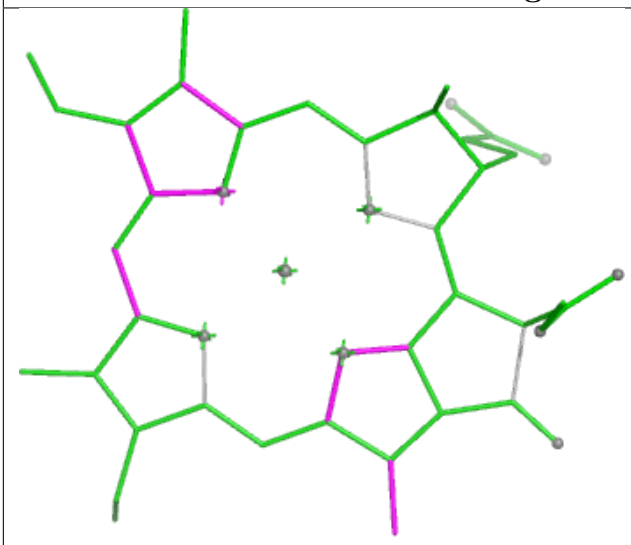


Rings

Ligand CLA B 831



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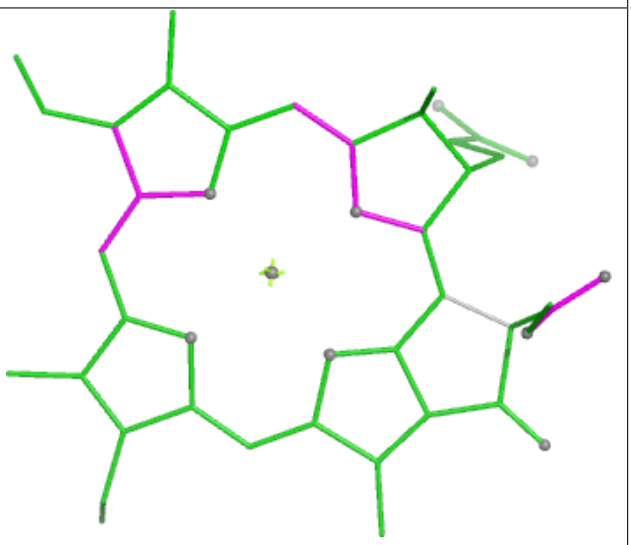

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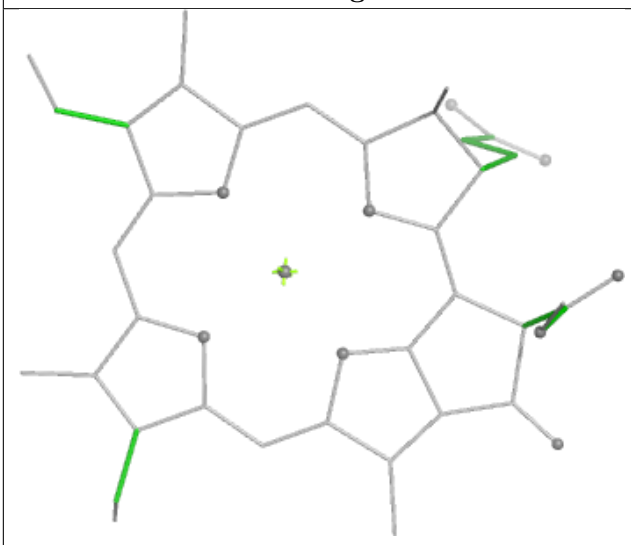

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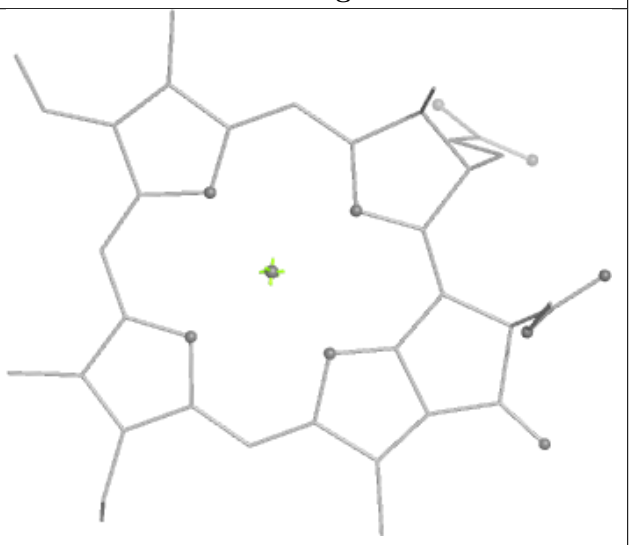
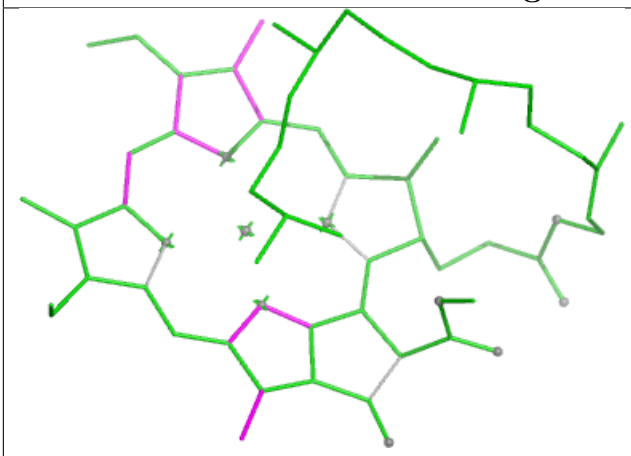


Rings

Ligand CLA A 808



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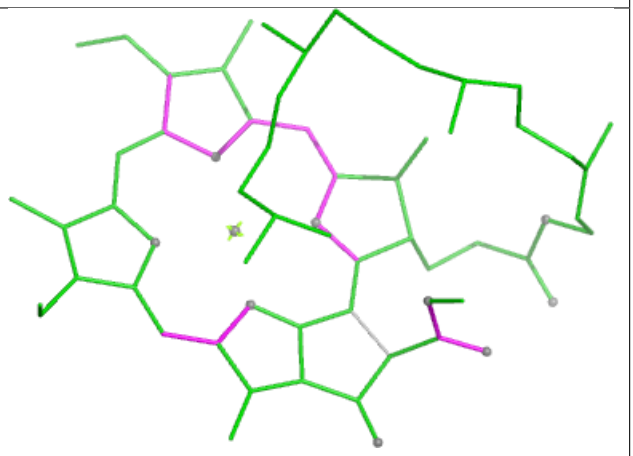
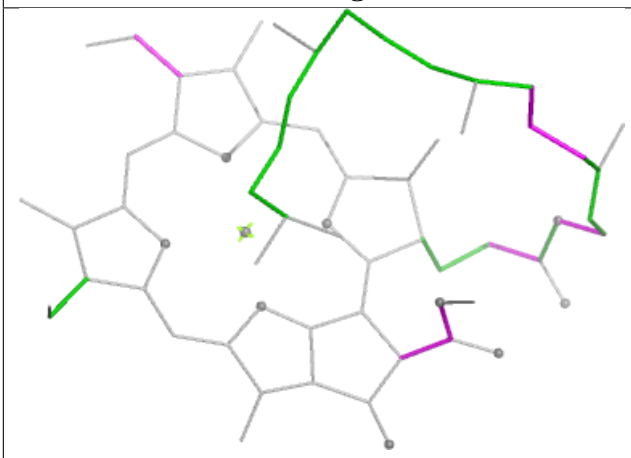


Bond angles



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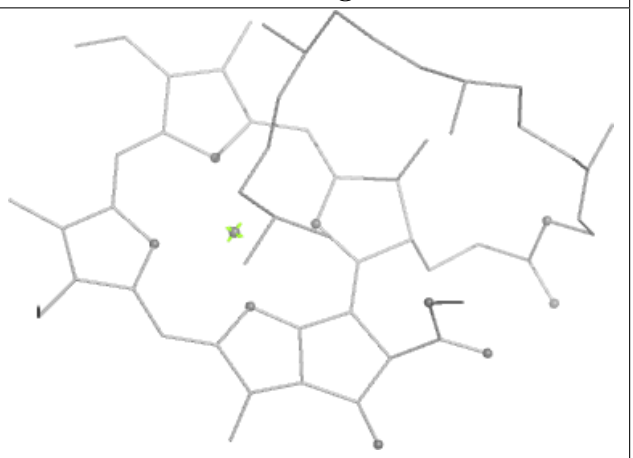
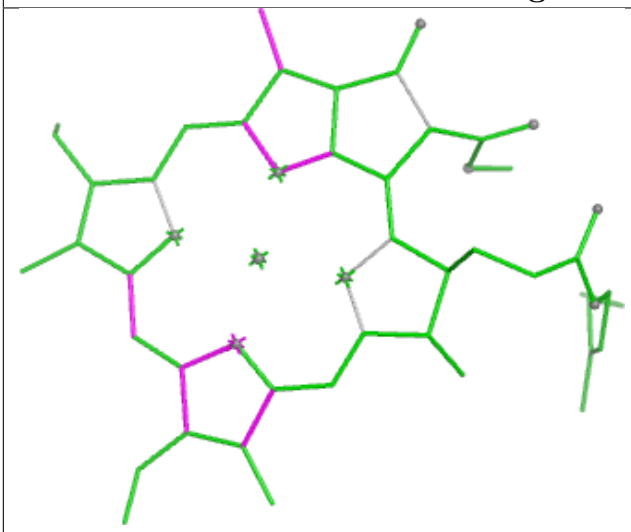


Rings

Ligand CLA 7 611



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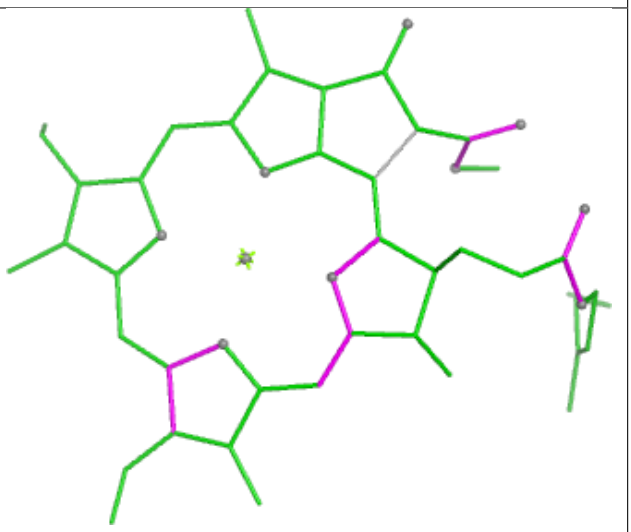

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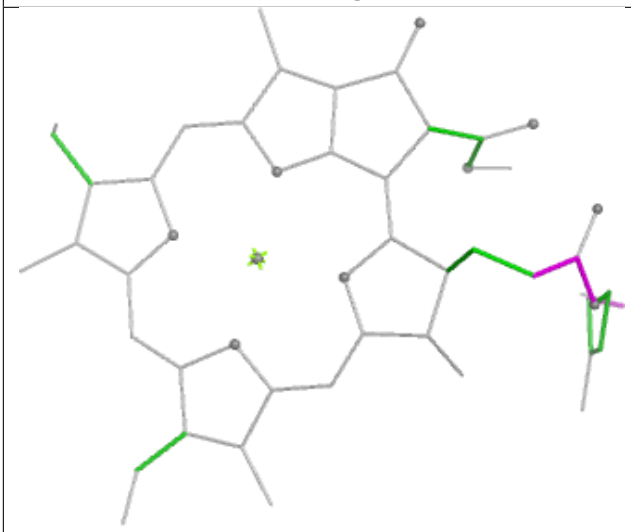

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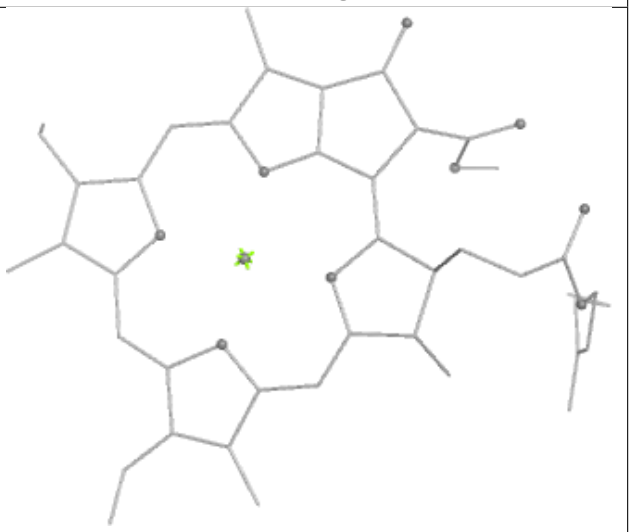
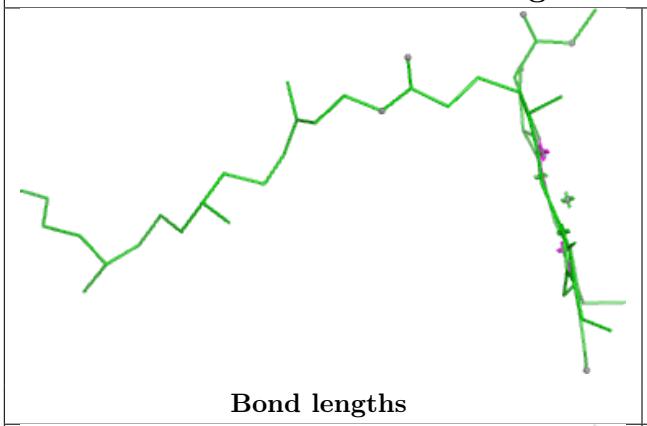


Rings

Ligand CHL 6 302



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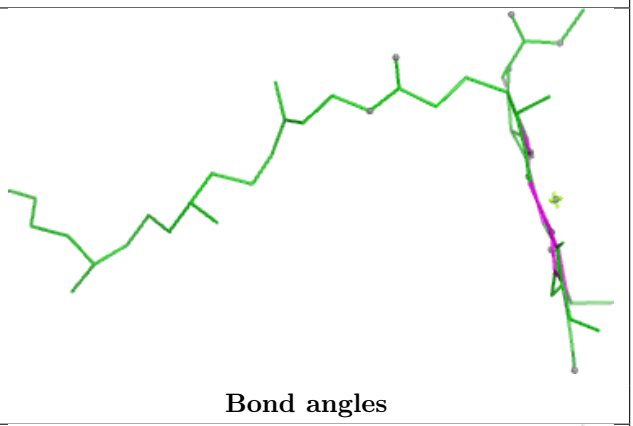

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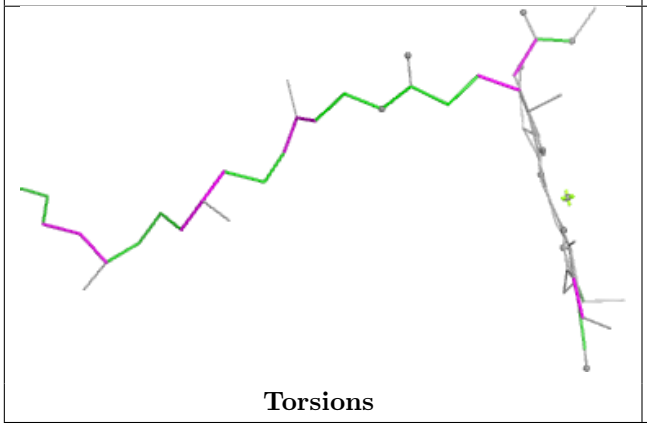

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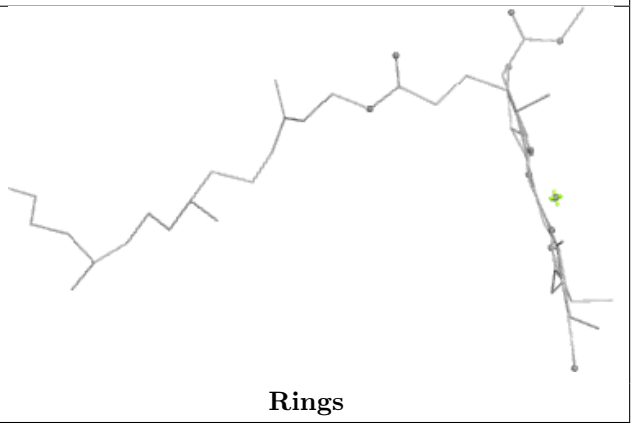
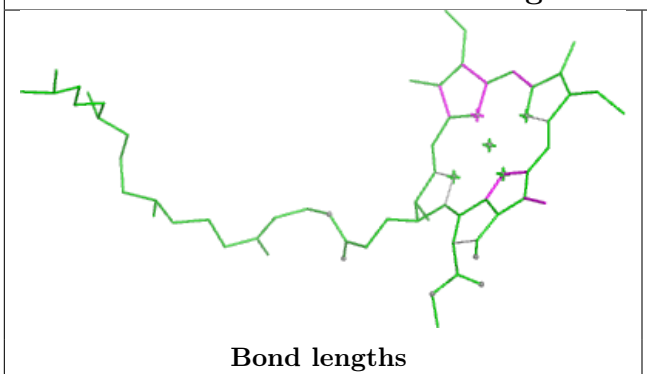


Rings

Ligand CLA B 801



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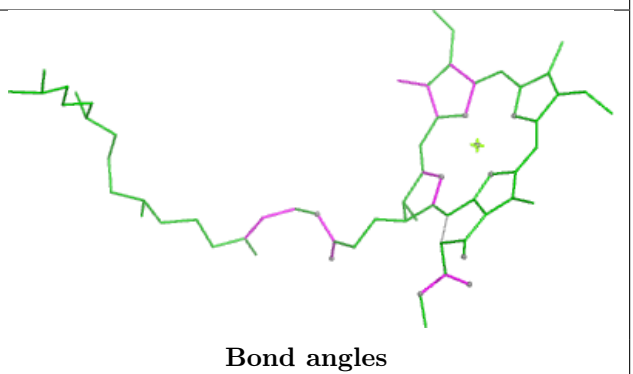
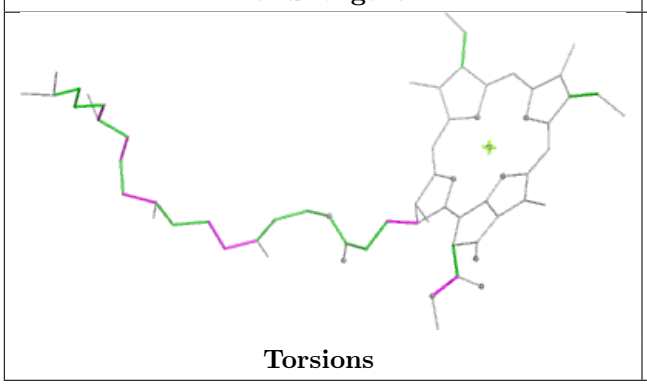


Bond angles



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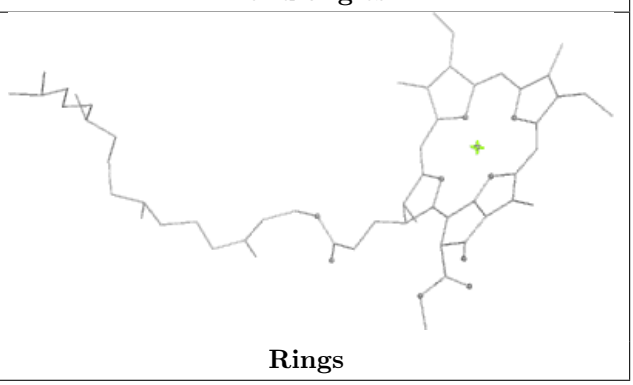
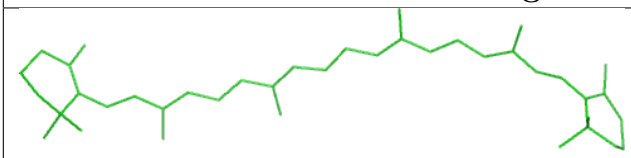


Rings

Ligand BCR B 848



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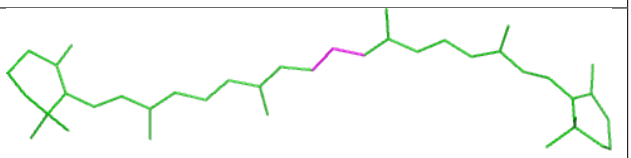
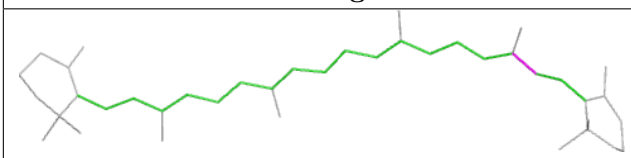


Bond angles



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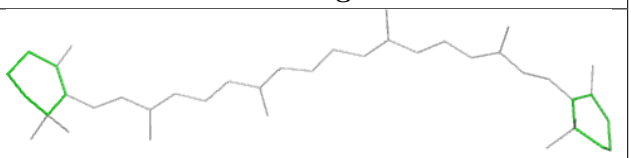
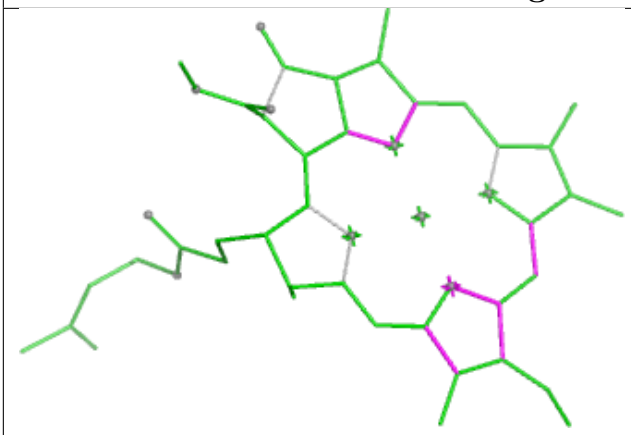


Rings

Ligand CLA 8 307



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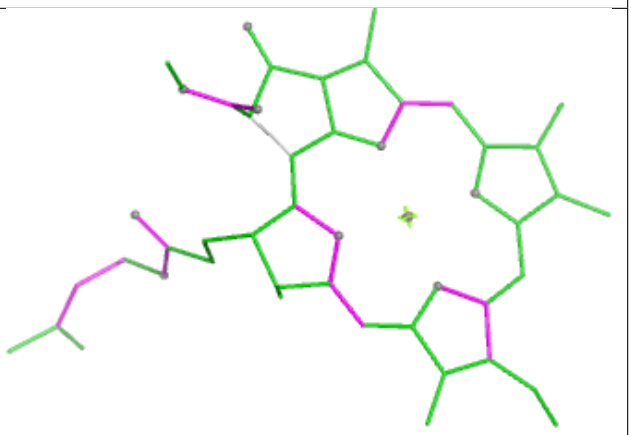
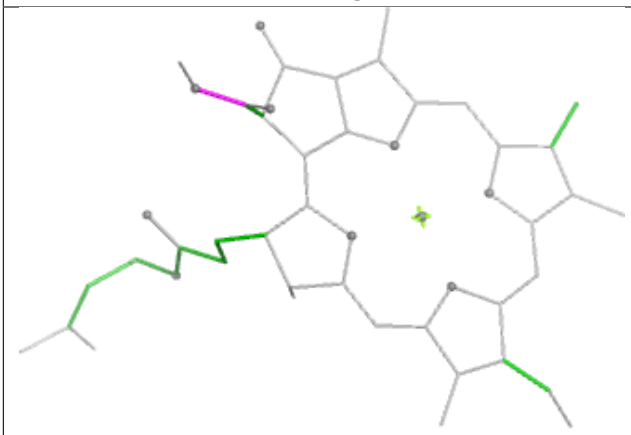


Bond angles



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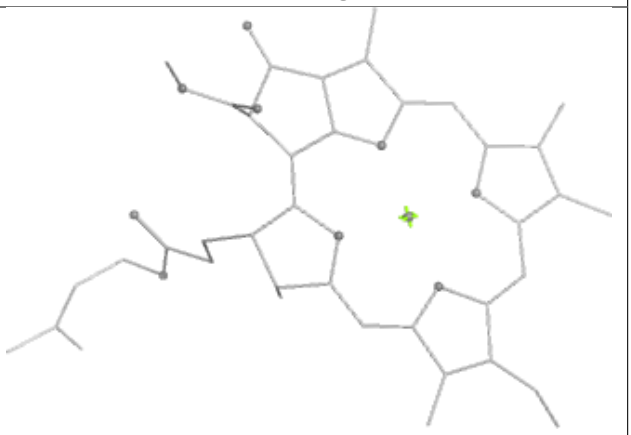
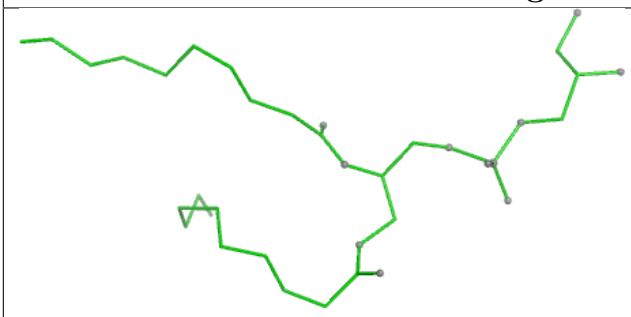


Rings

Ligand LHG 5 321



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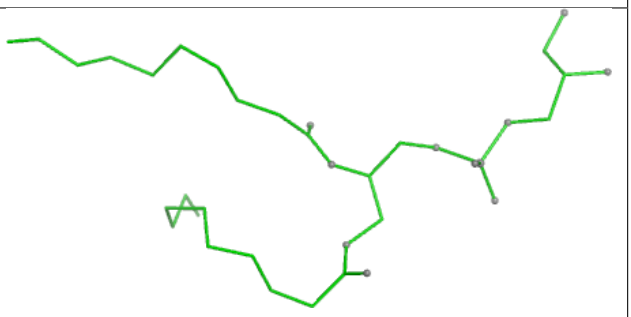
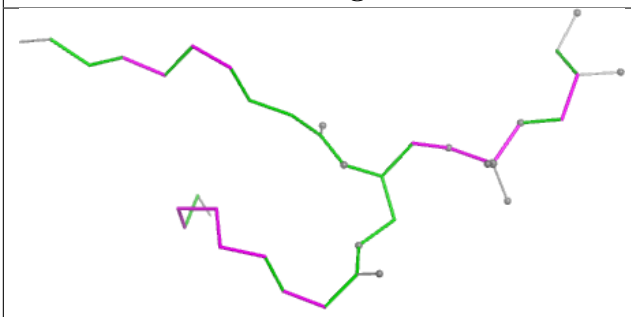


Bond angles



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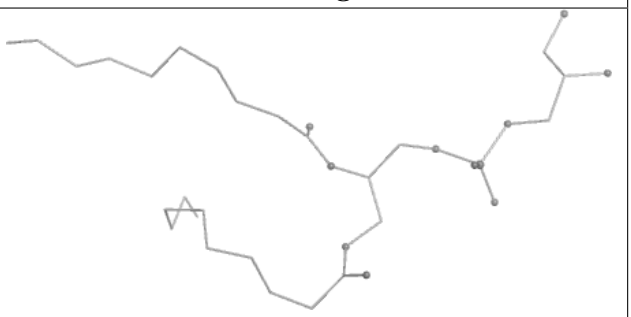
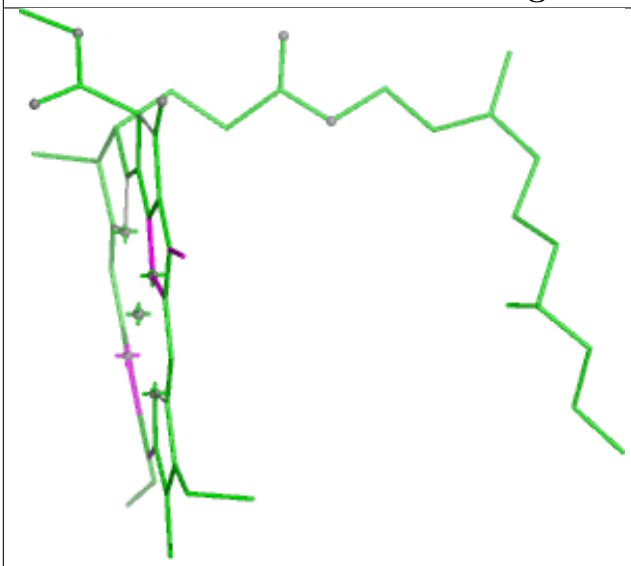
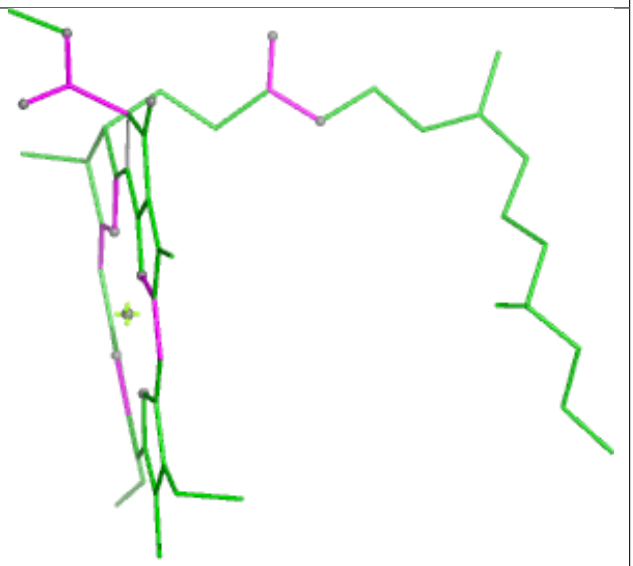


Rings

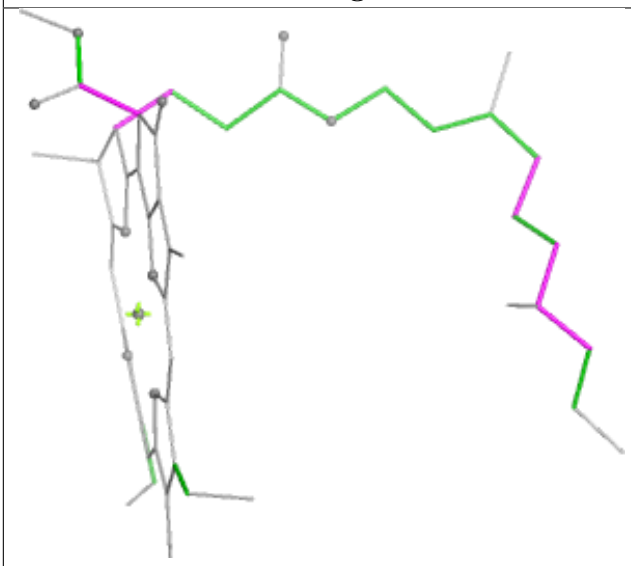
Ligand CLA 8 313



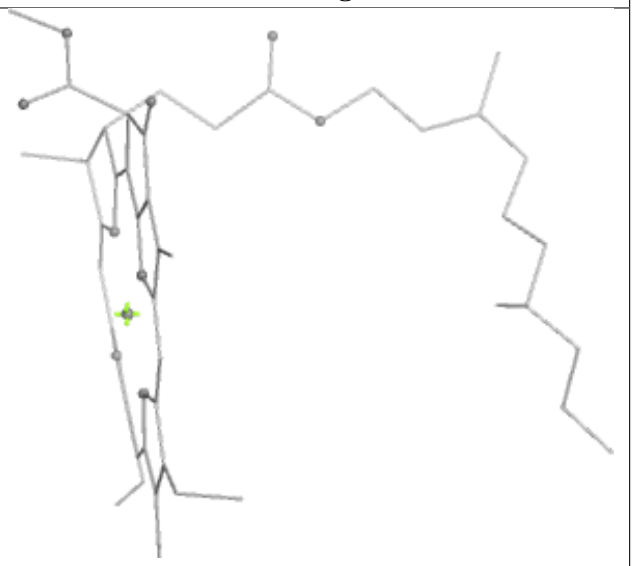
Bond lengths



Bond angles

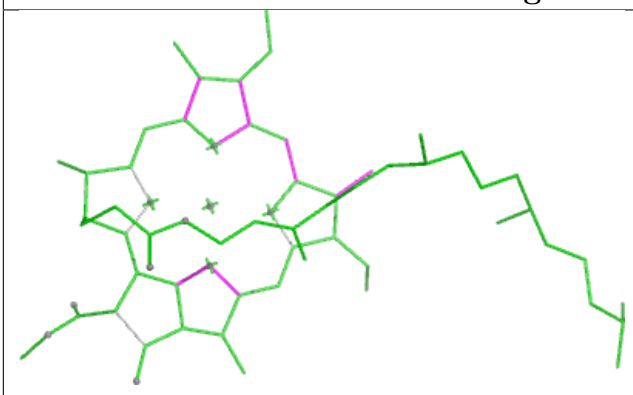


Torsions



Rings

Ligand CLA A 819



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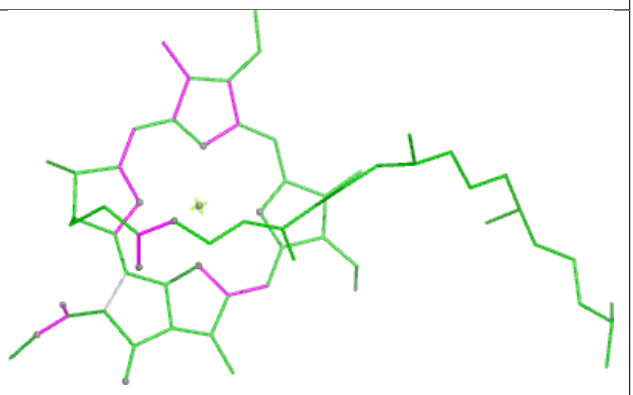
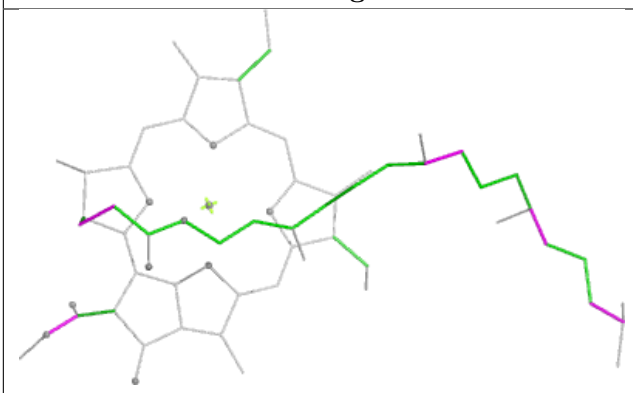


Bond angles



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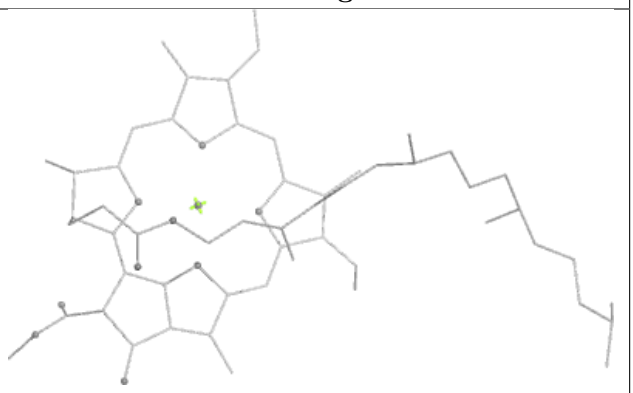
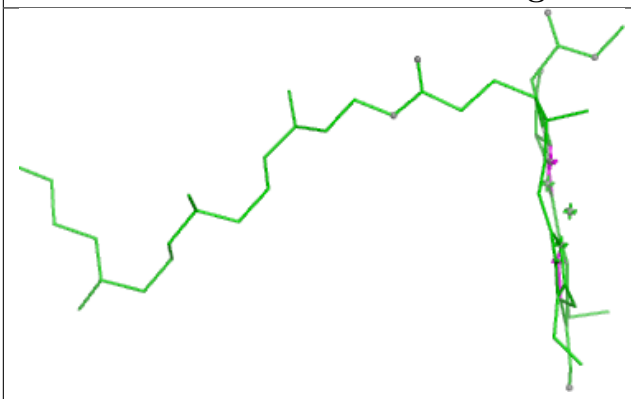


Rings

Ligand CHL 4 601



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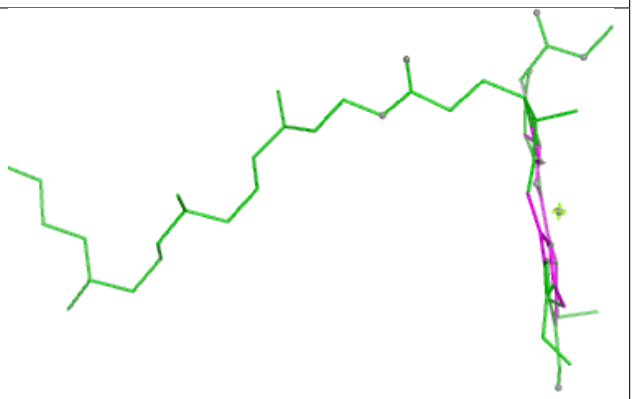

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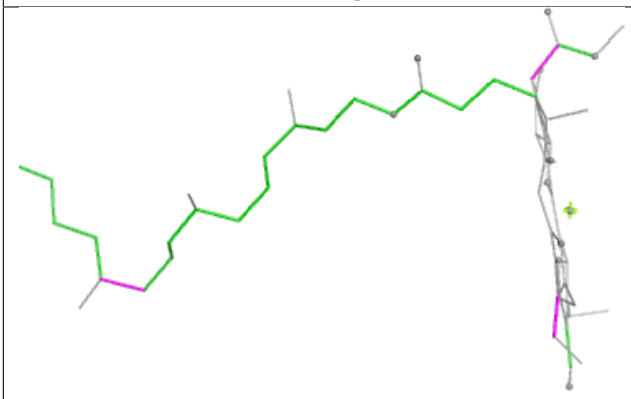

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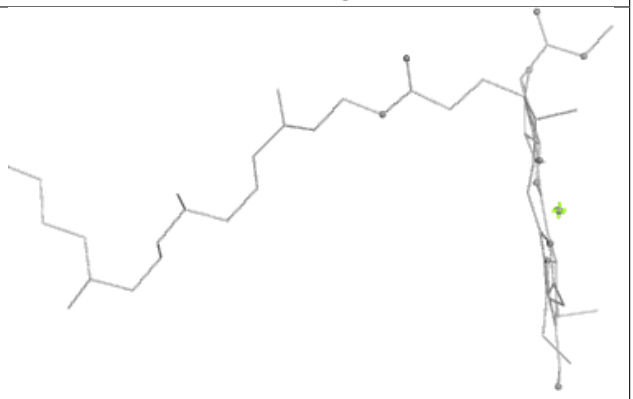
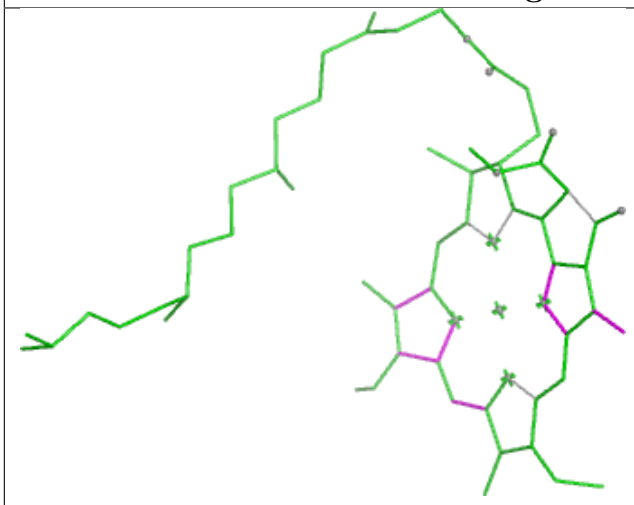


Rings

Ligand CLA B 825



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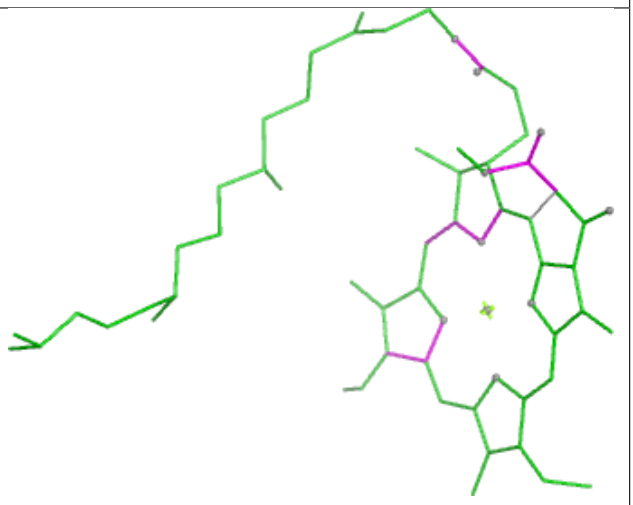

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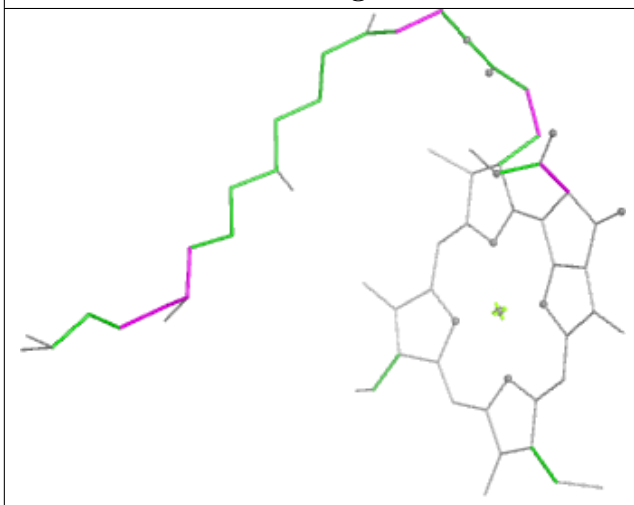

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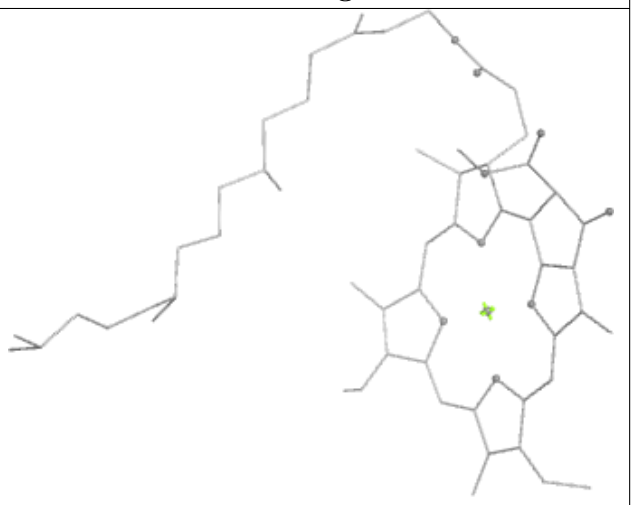
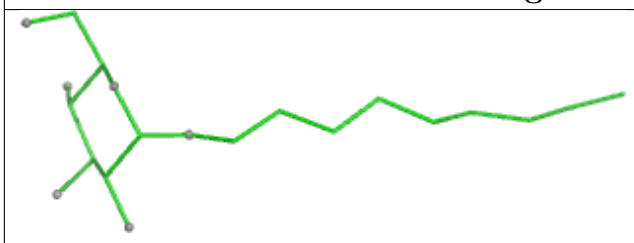


Rings

Ligand LMU 7 619



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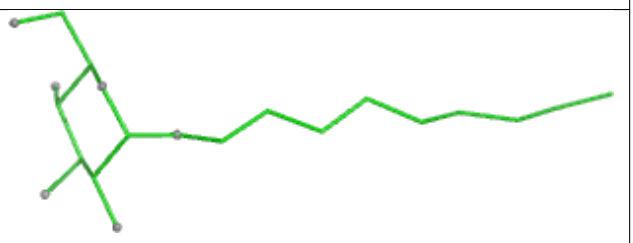
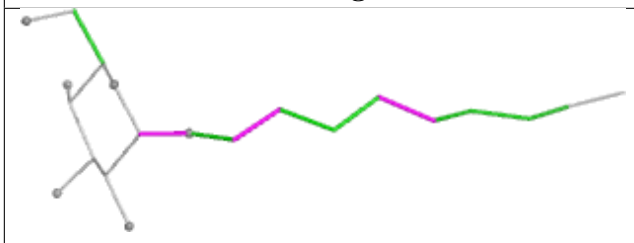


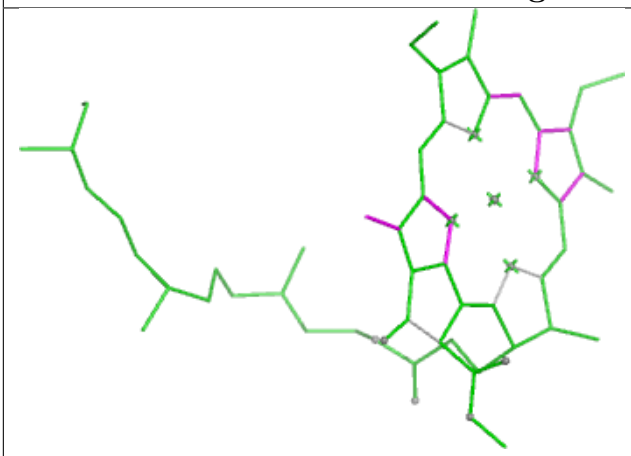
Bond angles



Torsions

Rings

Ligand CLA 1 310



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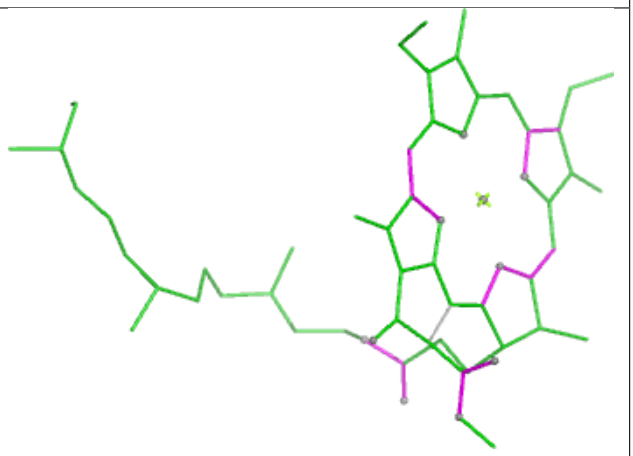
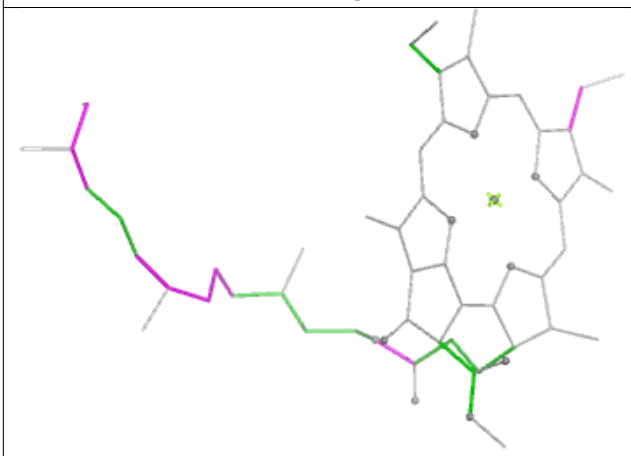


Bond angles



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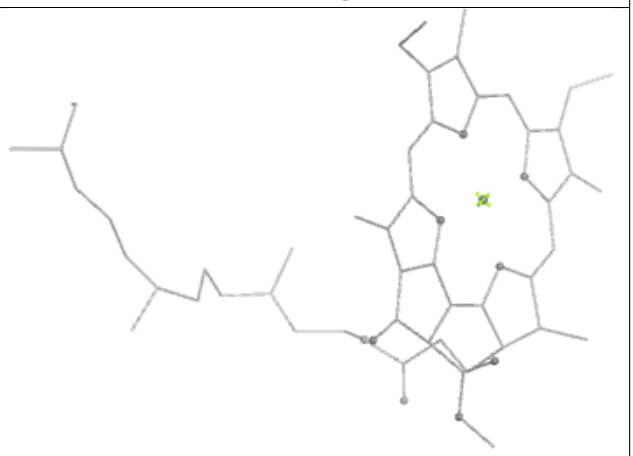
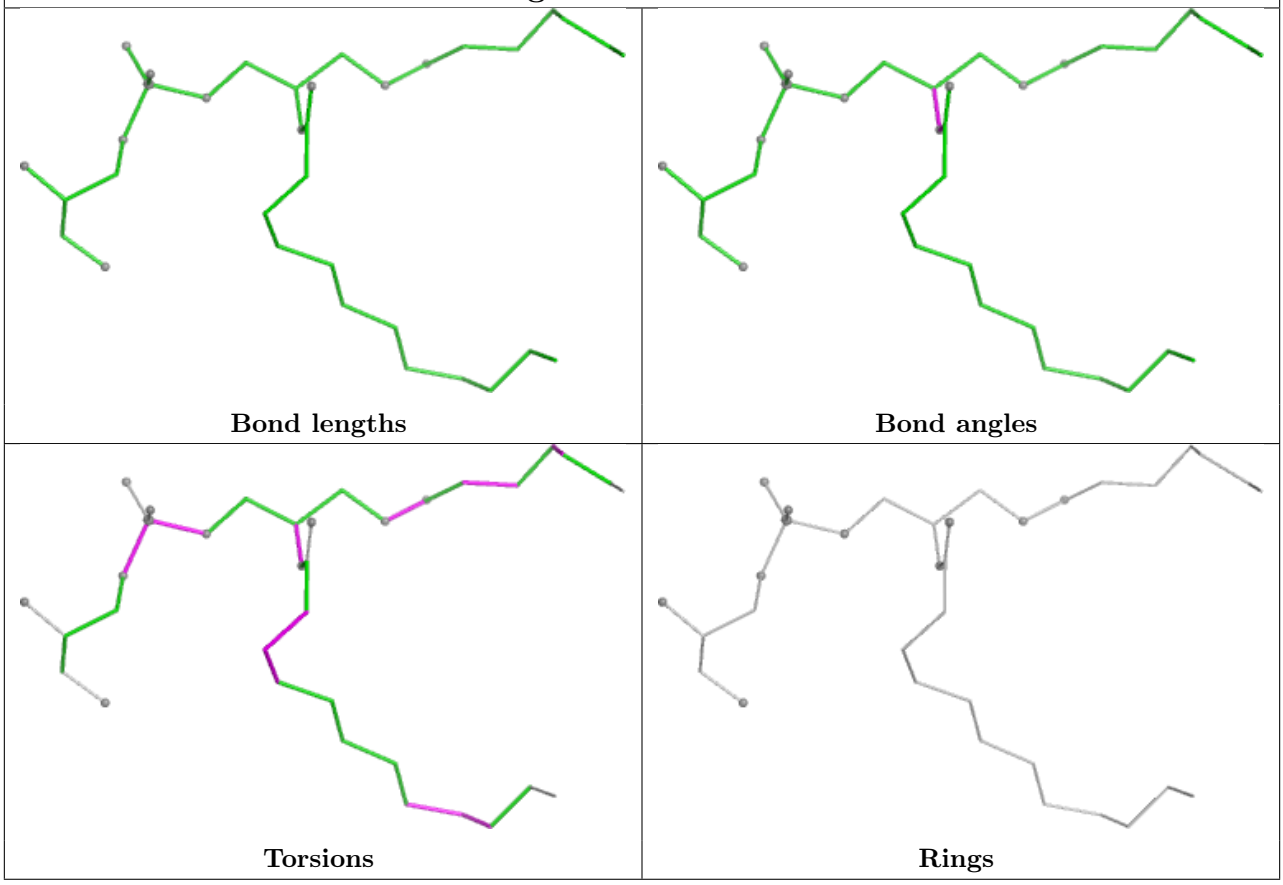
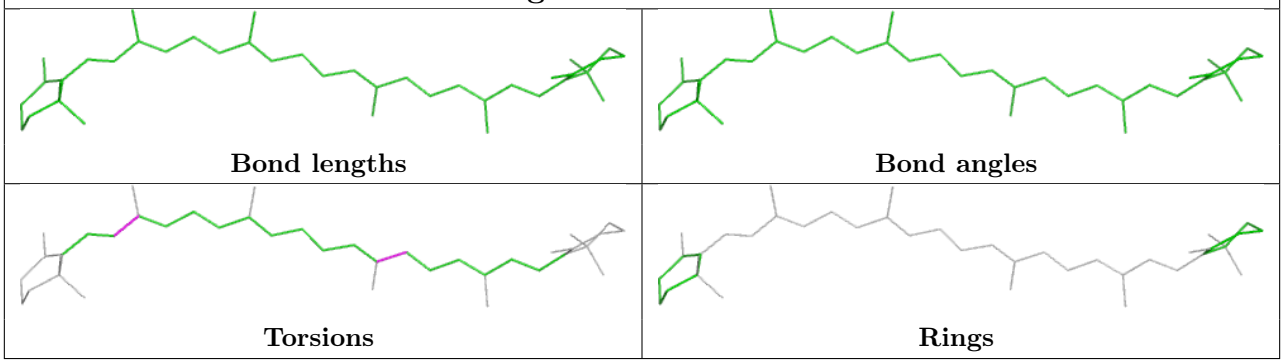


Rings

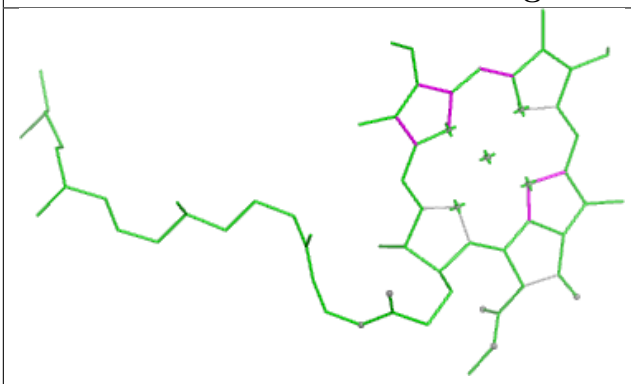
Ligand LHG 6 325



Ligand BCR 7 617



Ligand CLA A 803



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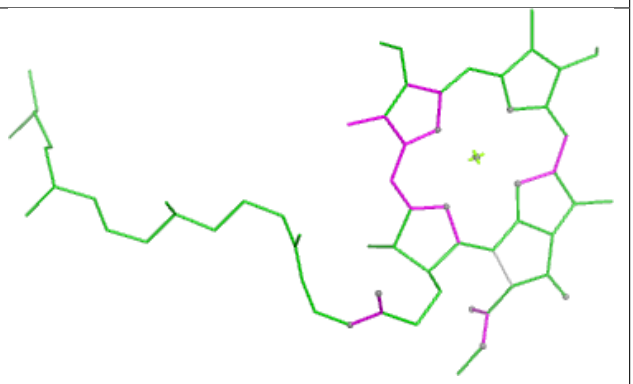
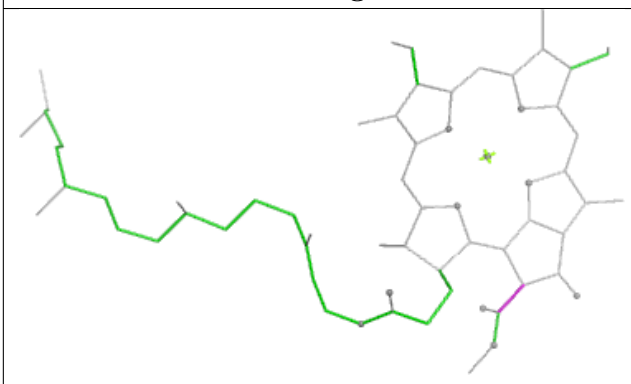


Bond angles



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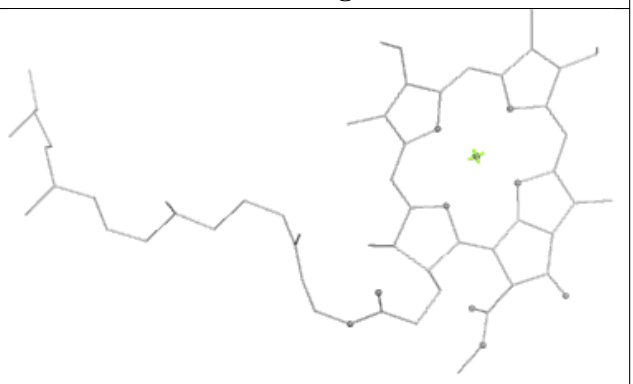
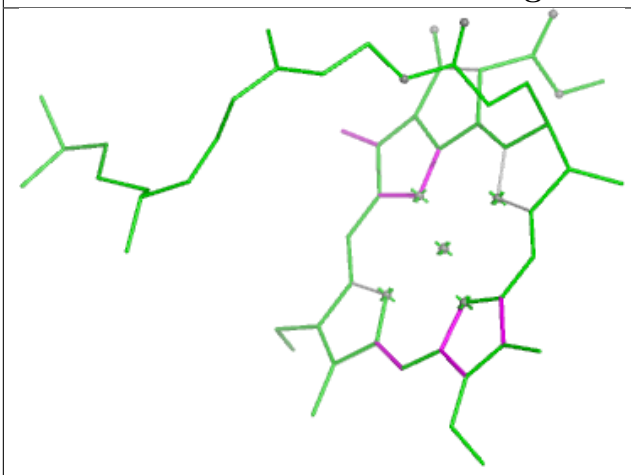


Rings

Ligand CLA B 815



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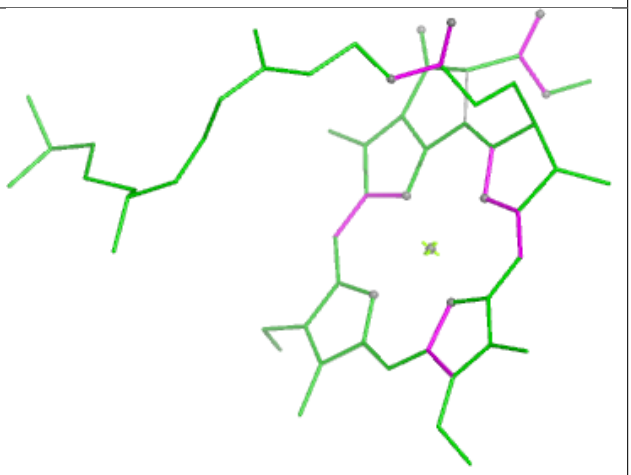
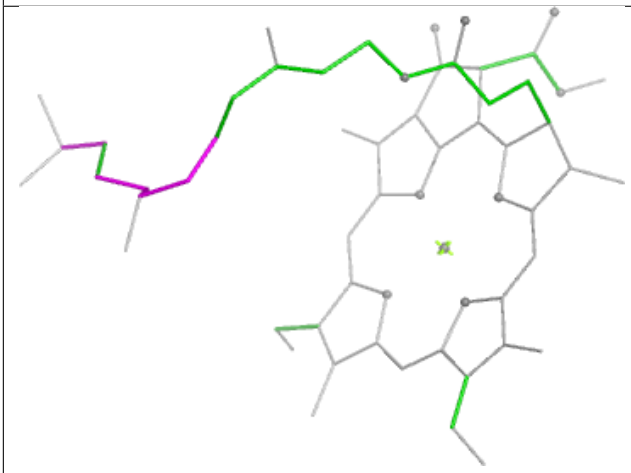


Bond angles



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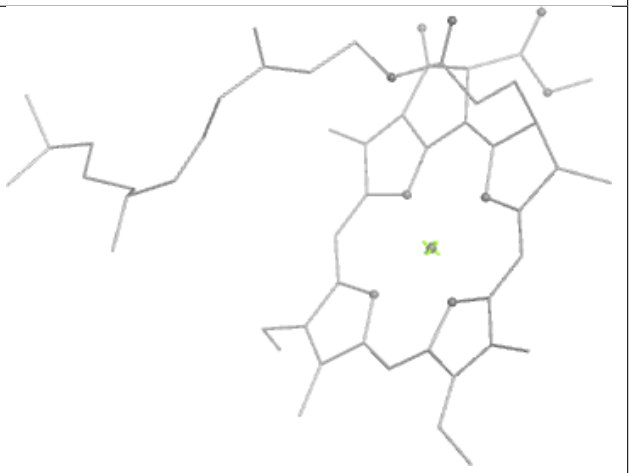
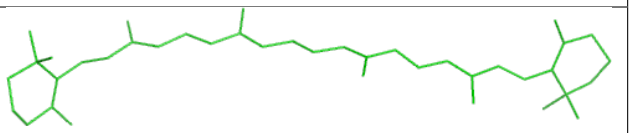


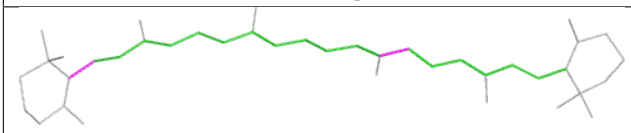
Rings

Ligand BCR 3 318

Bond lengths



Bond angles



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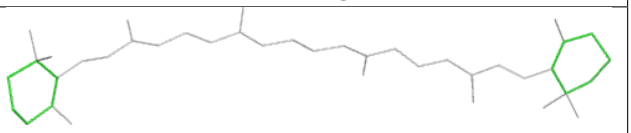
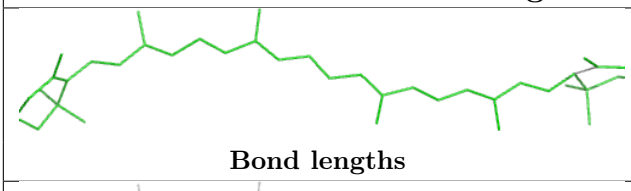


Rings

Ligand LUT Z 615



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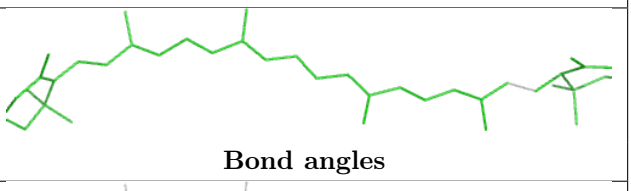
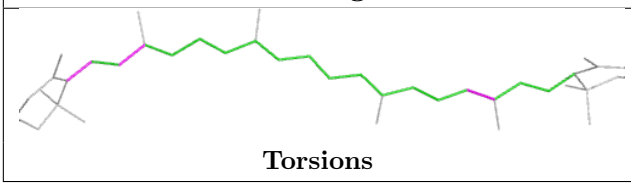


Bond angles



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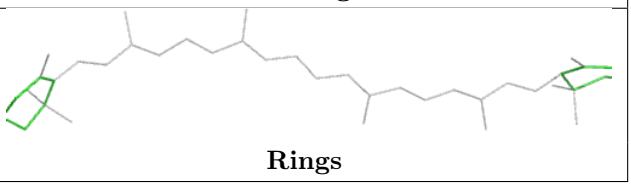
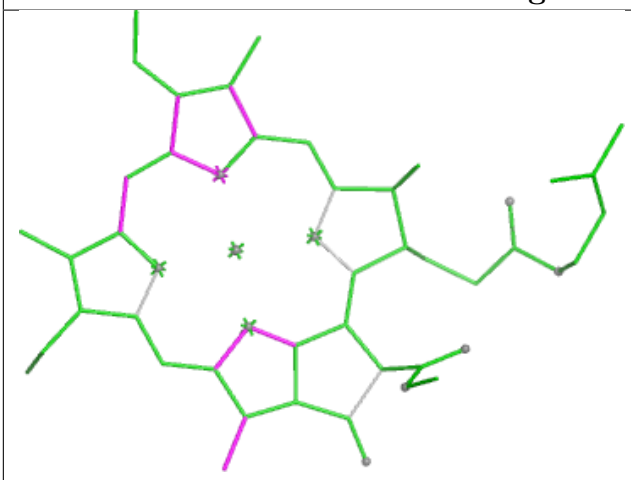


Rings

Ligand CLA 5 304



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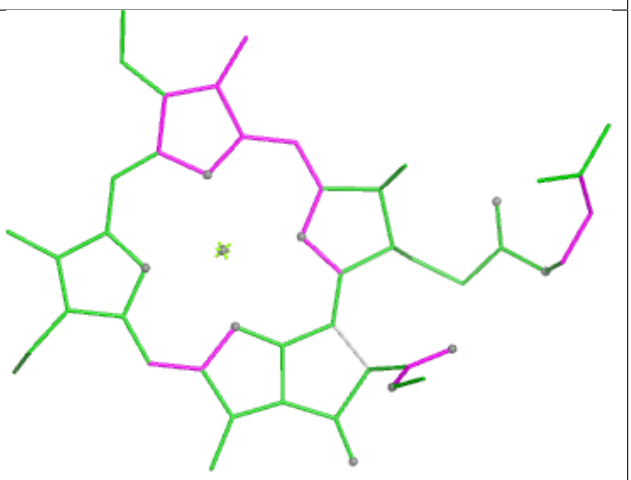
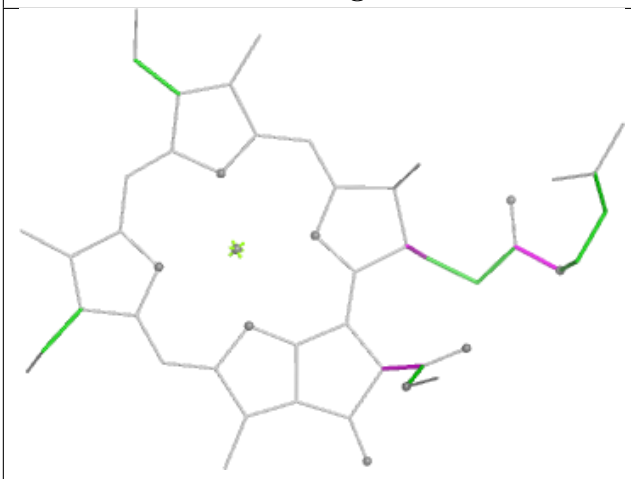


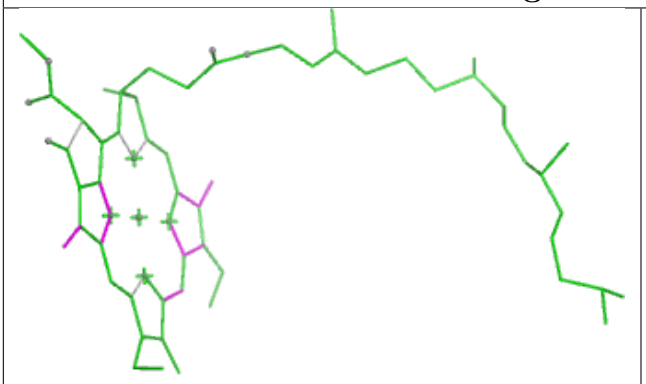
Bond angles



Torsions

Rings

Ligand CLA A 837



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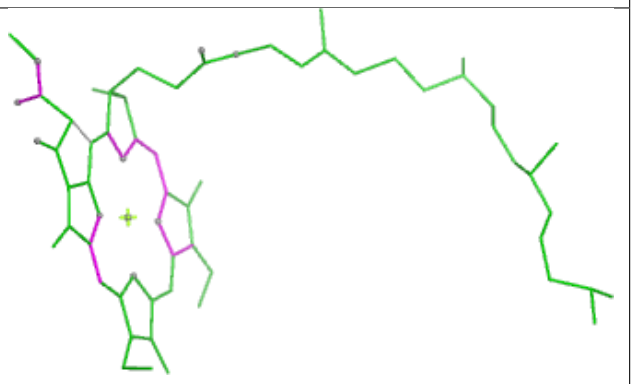
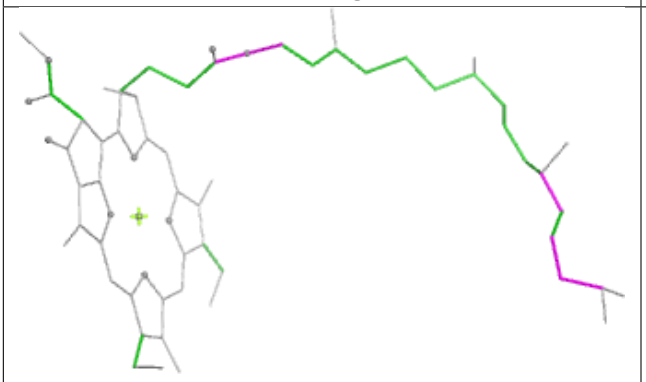


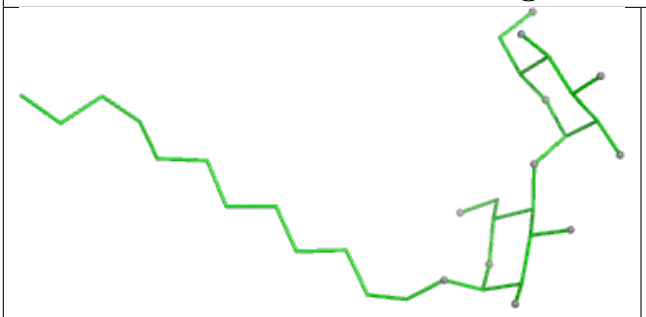
Bond angles



Torsions

Rings

Ligand LMU B 853



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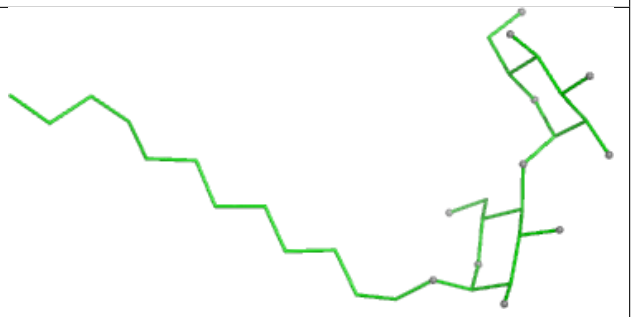
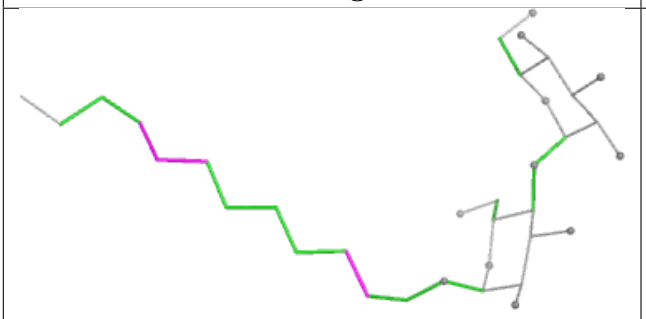


Bond angles



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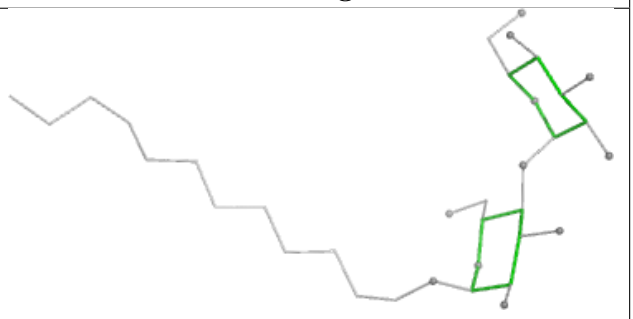
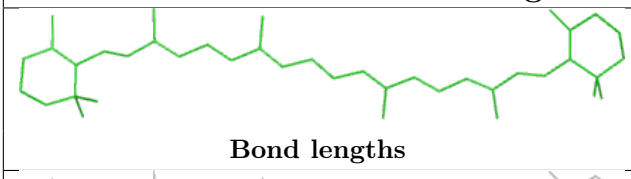


Rings

Ligand BCR L 205



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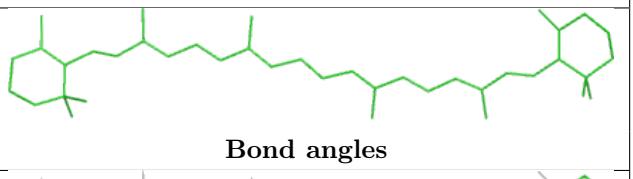


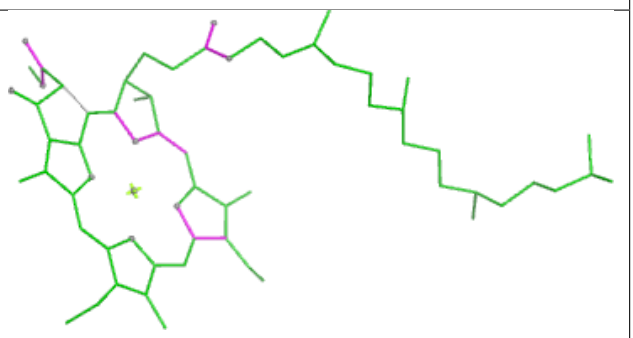
Bond angles

Torsions

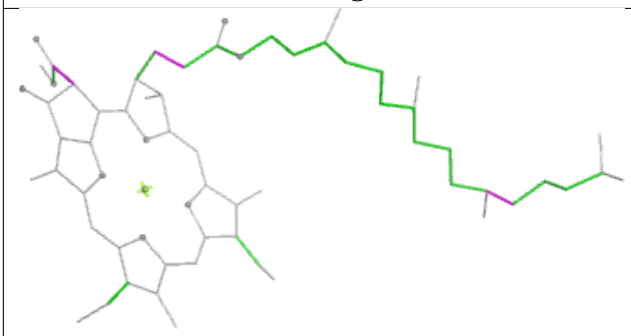
Rings

Ligand CLA A 810

Bond lengths



Bond angles



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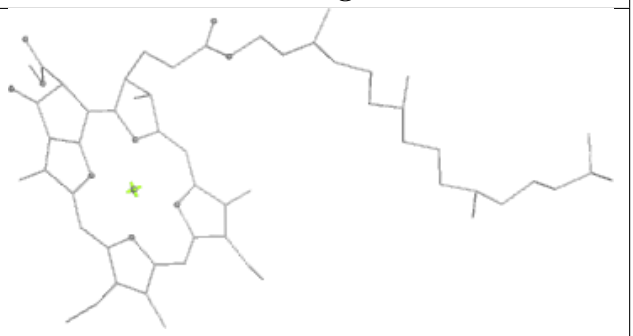
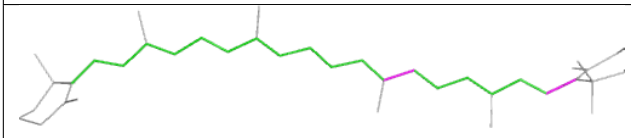


Rings

Ligand BCR 3 319

Bond lengths

Bond angles



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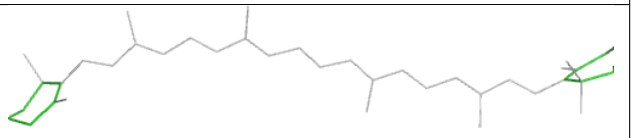
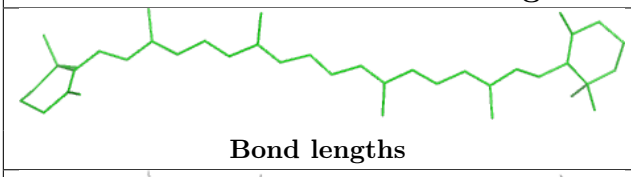
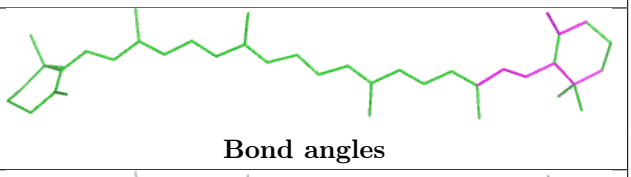


Rings

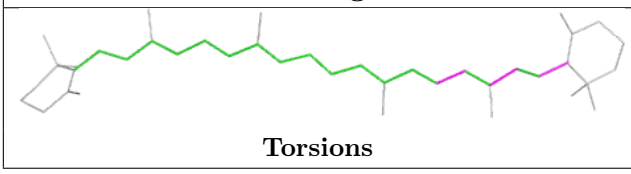
Ligand BCR B 844



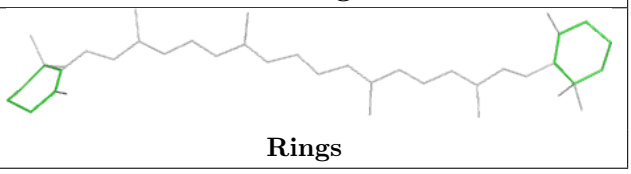
Bond lengths



Bond angles

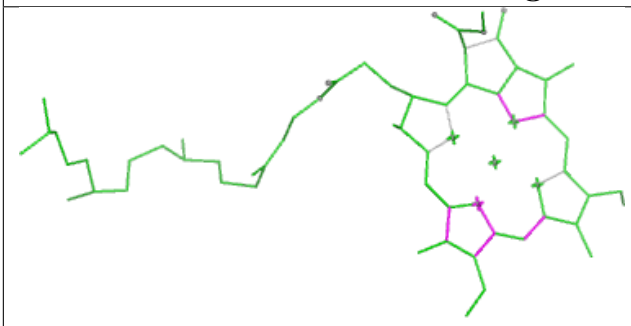


Torsions



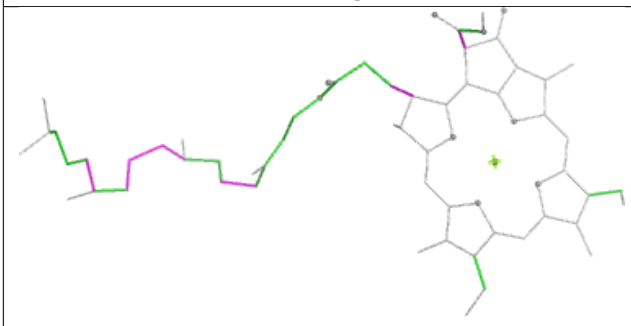
Rings

Ligand CLA B 814



Bond lengths

Bond angles

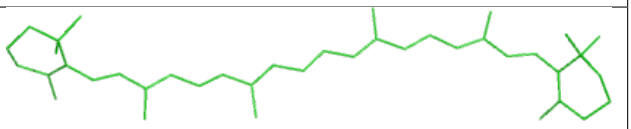


Torsions

Rings

Ligand BCR J 103

Bond lengths

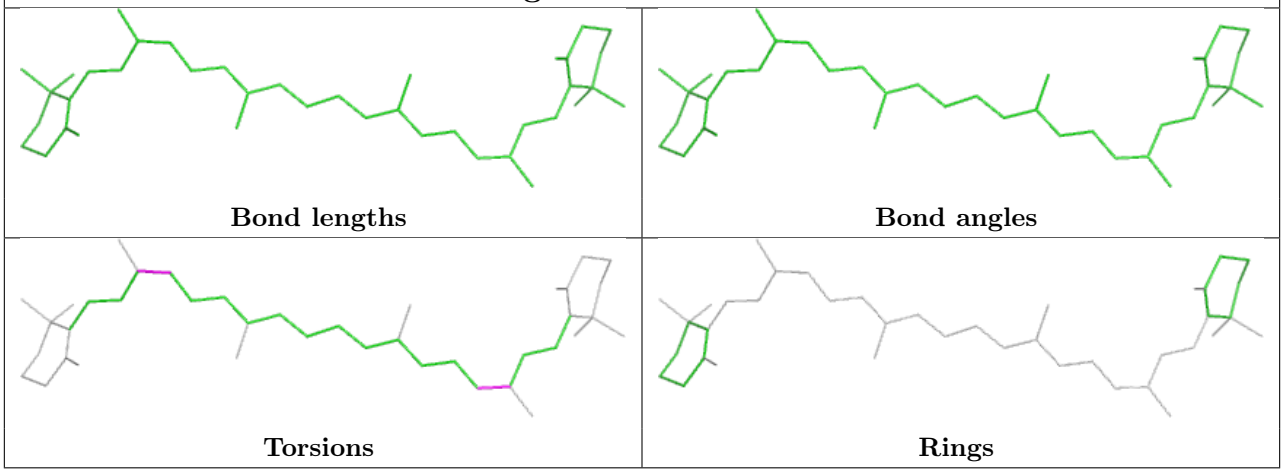


Bond angles

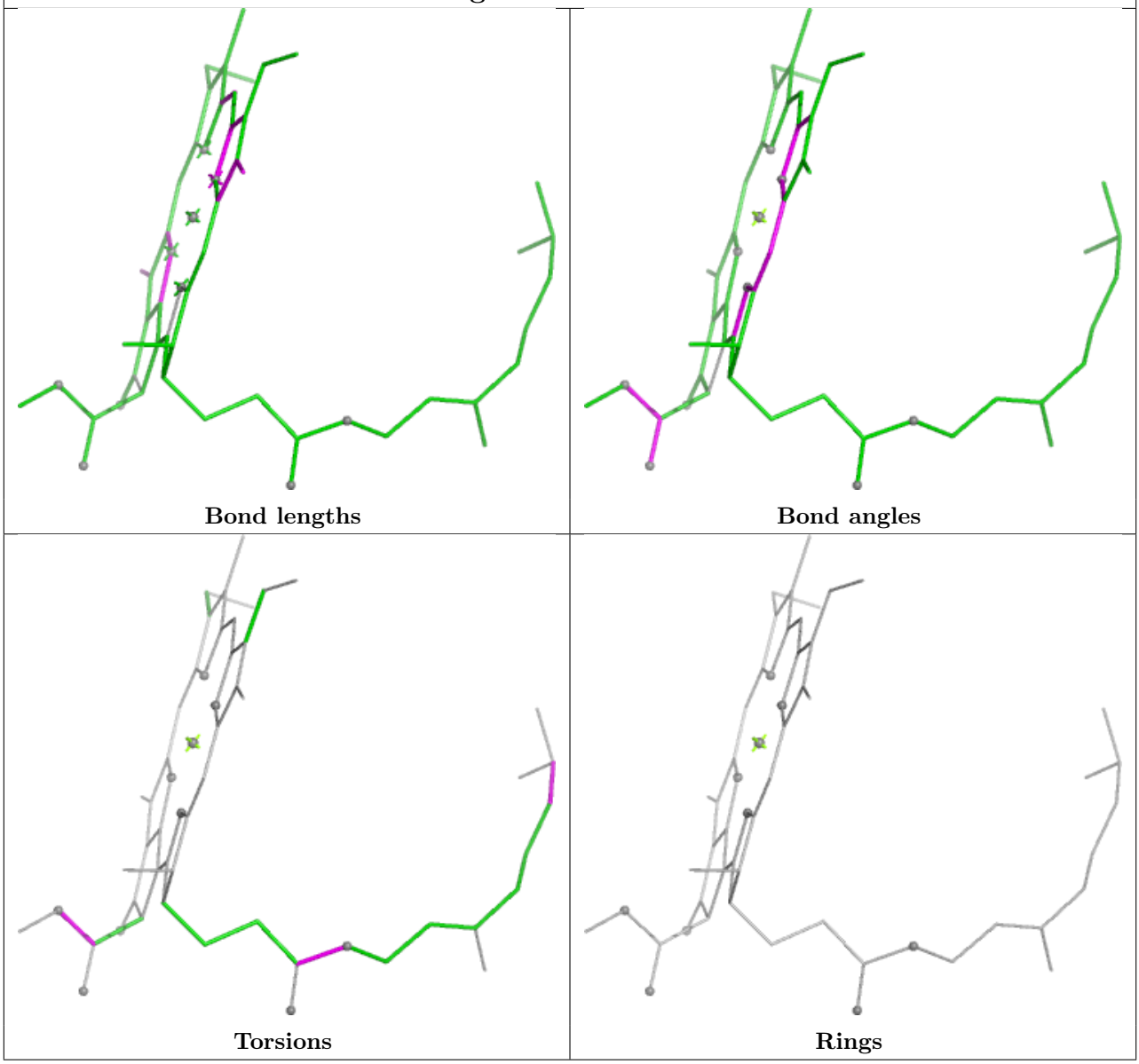
Torsions

Rings

Ligand BCR B 846

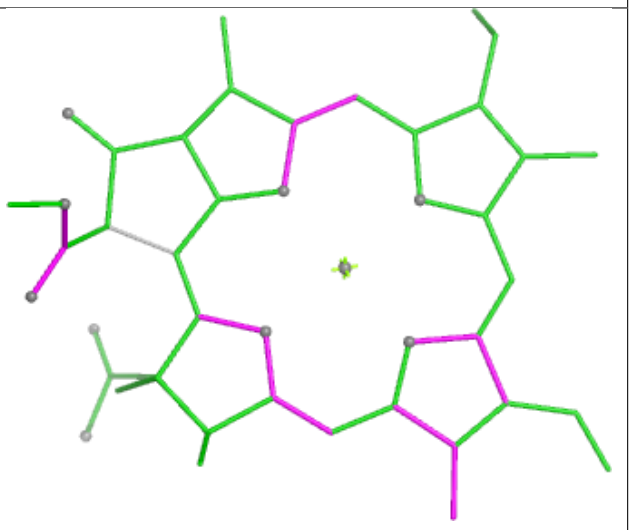


Ligand CLA 5 305



Ligand CLA A 846

Bond lengths



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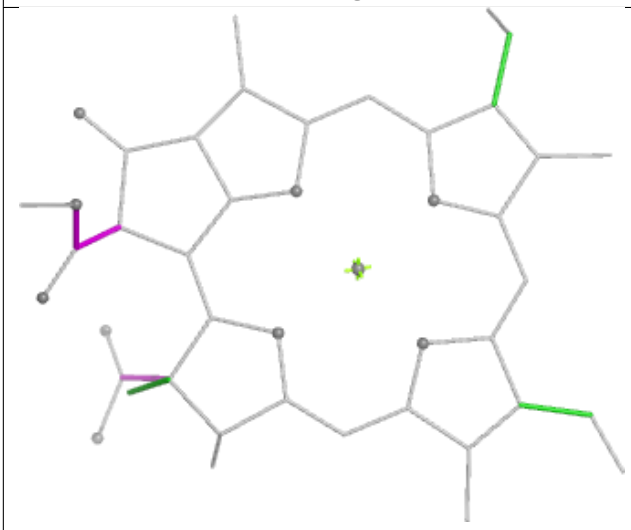

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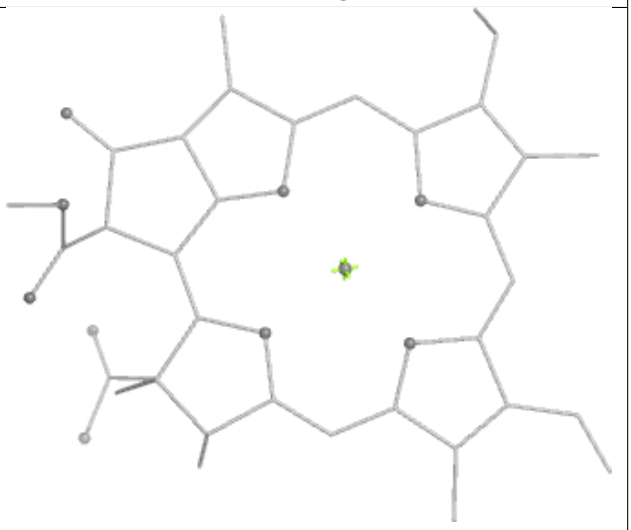
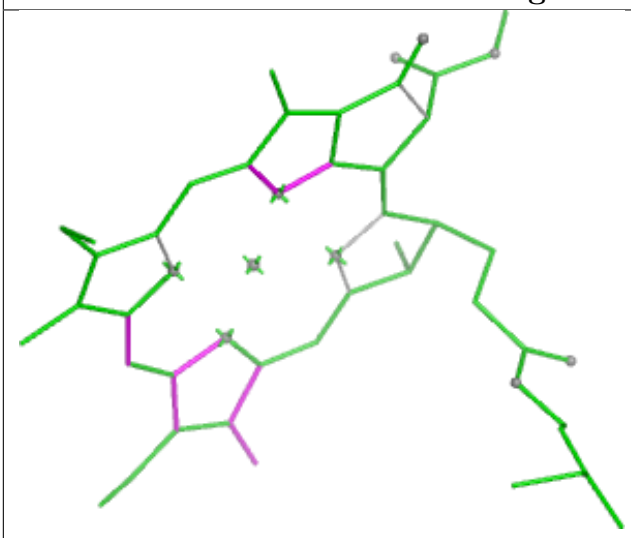


Rings

Ligand CLA 3 305



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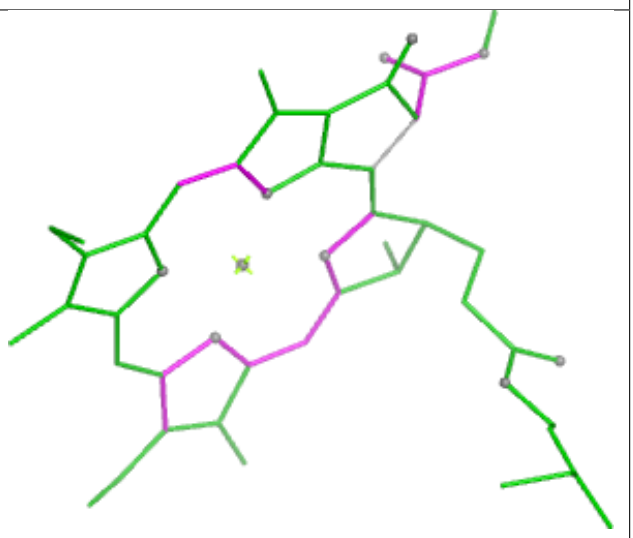
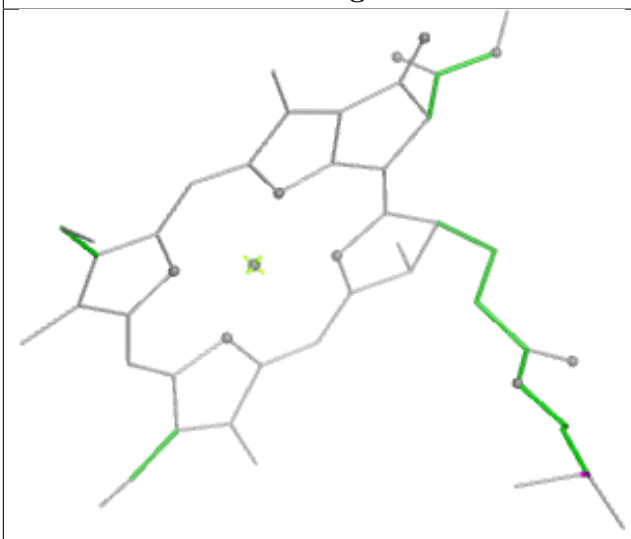


Bond angles



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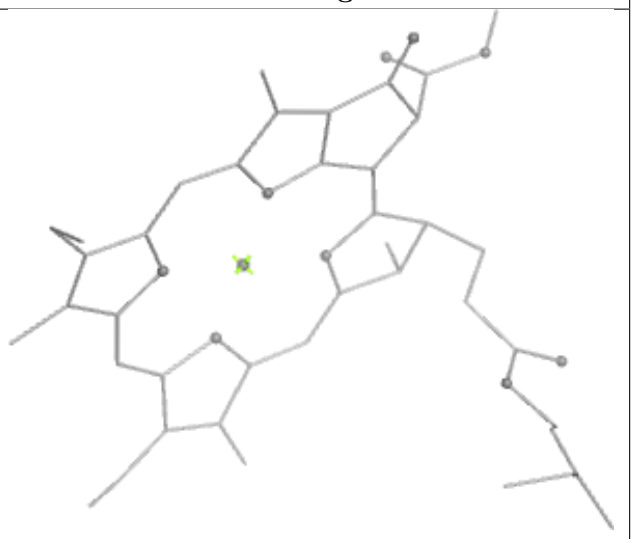
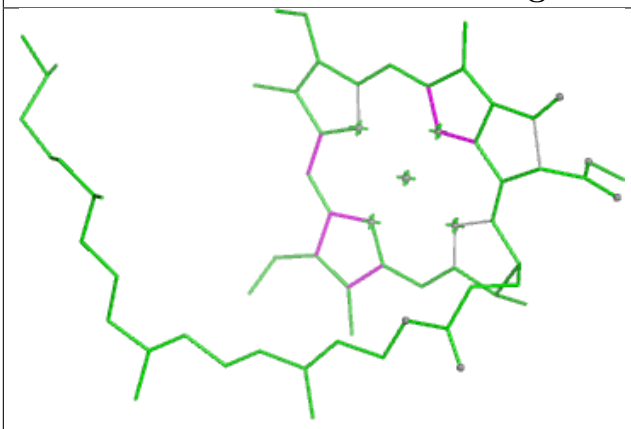


Rings

Ligand CLA 6 303



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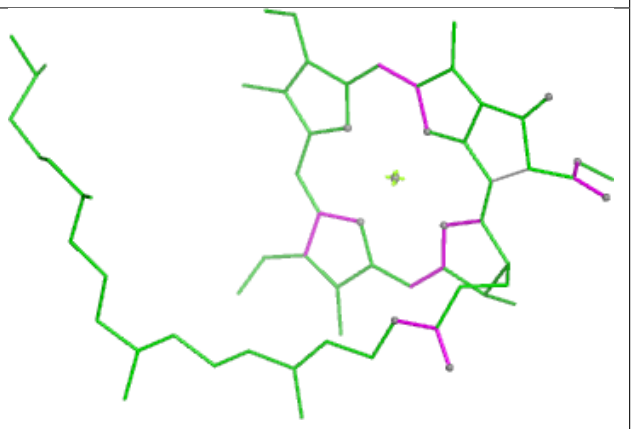
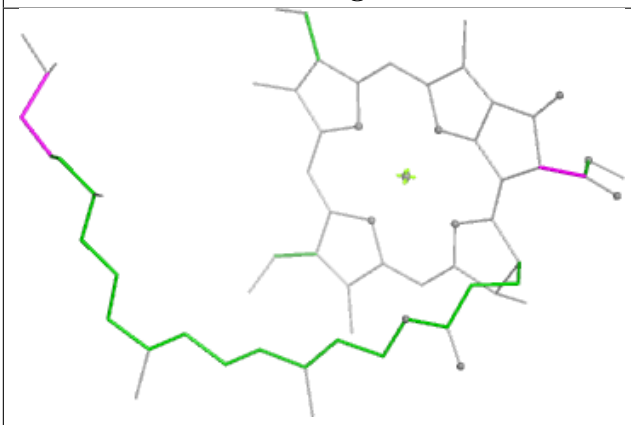


Bond angles



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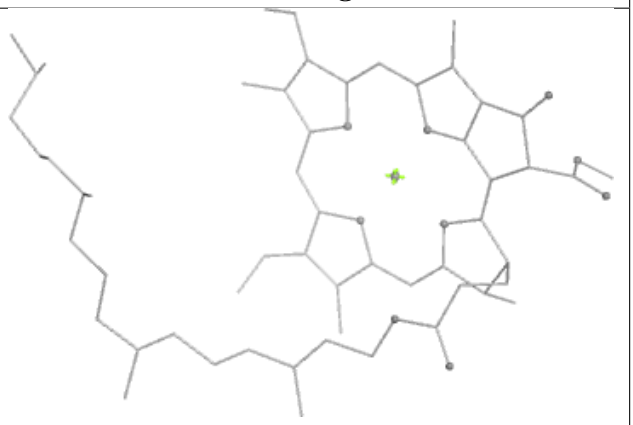
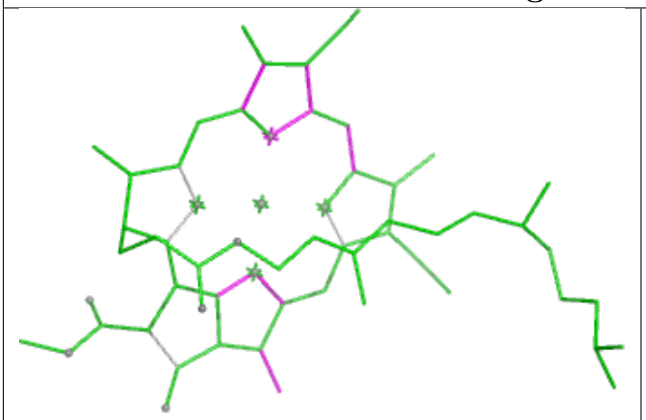


Rings

Ligand CLA Z 614



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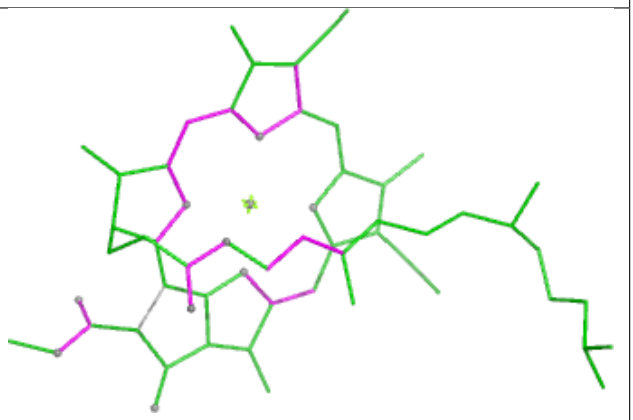
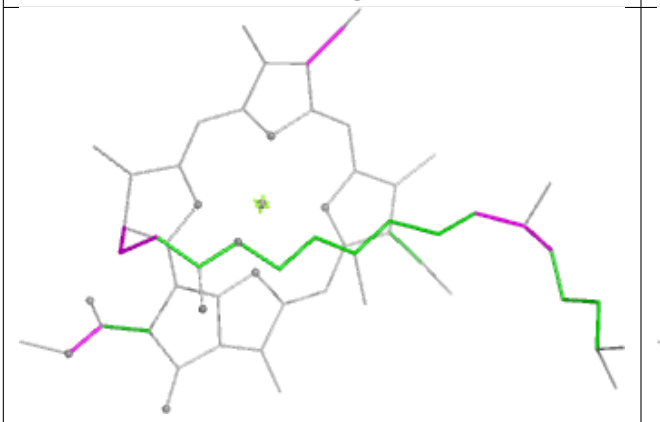


Bond angles



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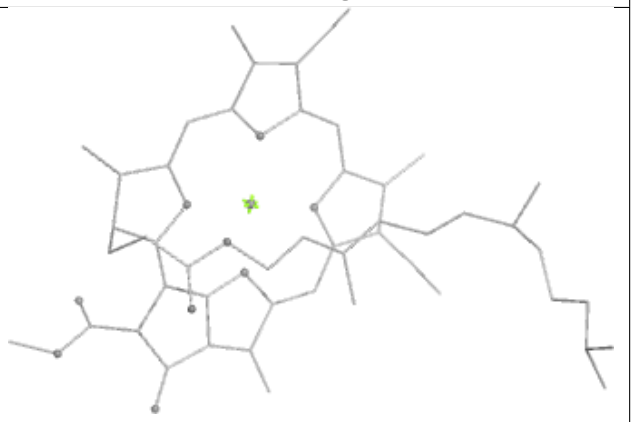

Rings

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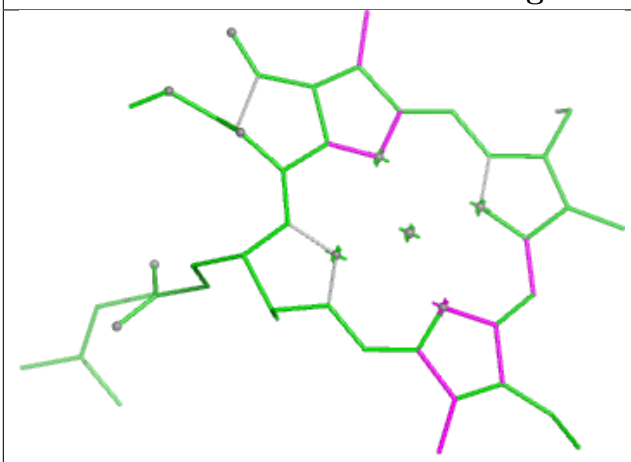

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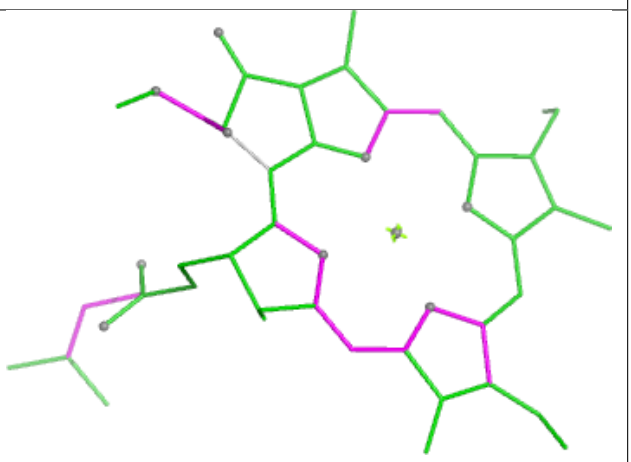
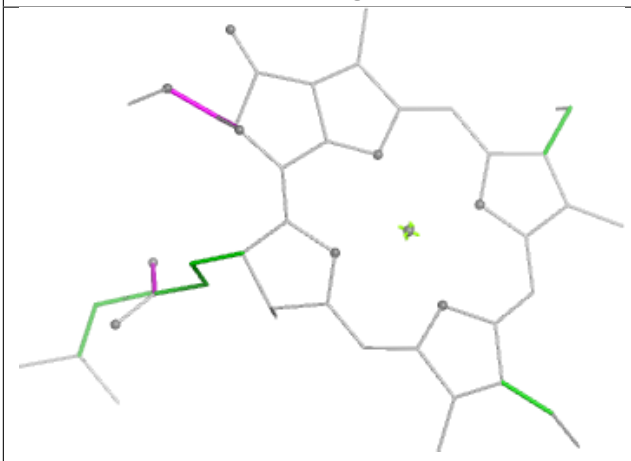


Bond angles



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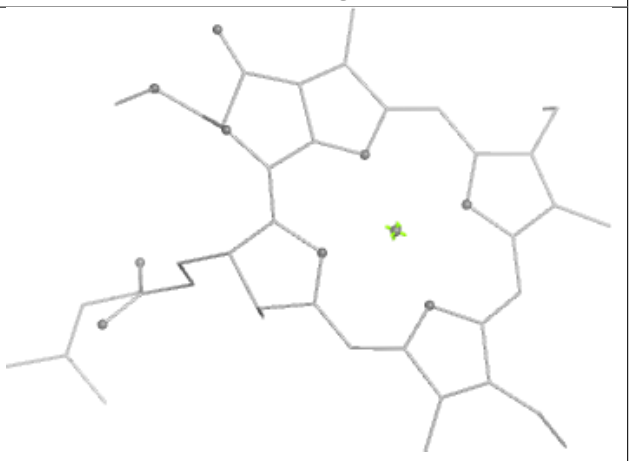
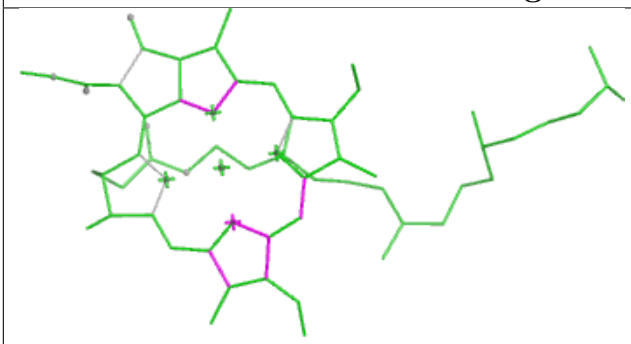


Rings

Ligand CLA B 817



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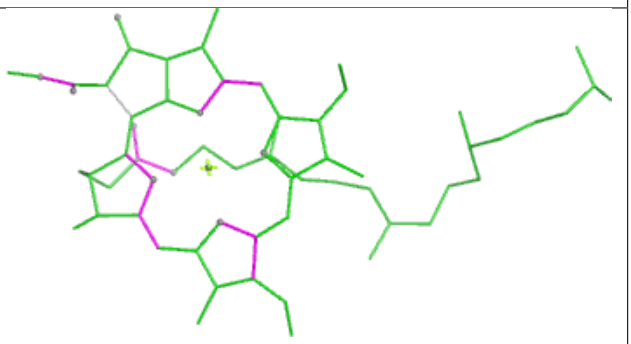

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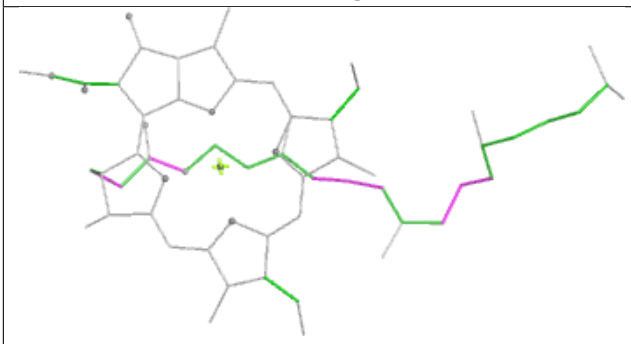

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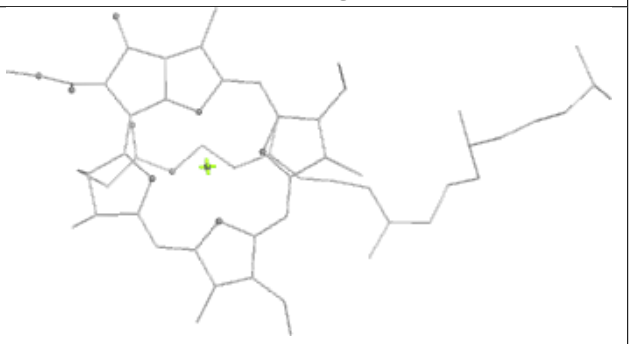
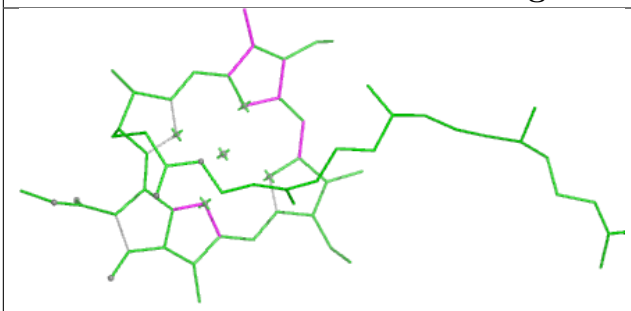


Rings

Ligand CLA 7 612



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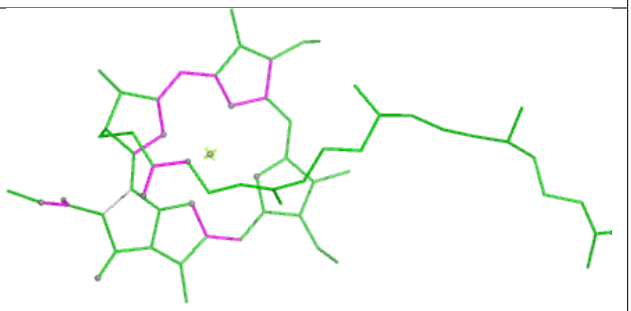
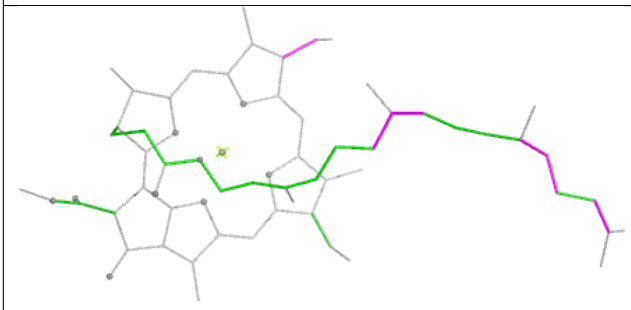


Bond angles



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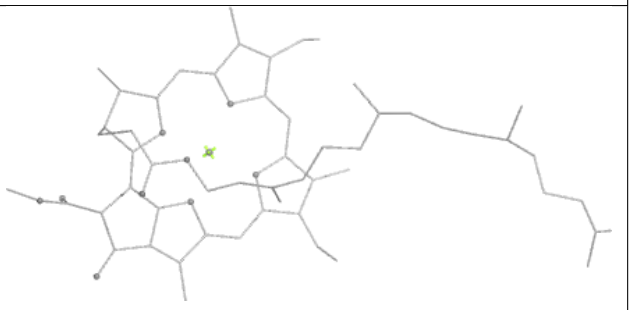
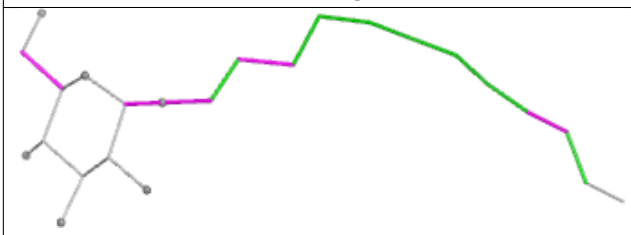


Rings

Ligand LMU 3 325

Bond lengths

Bond angles



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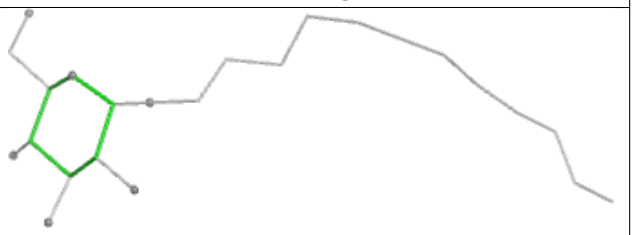
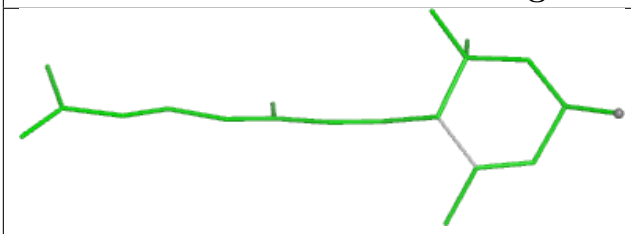


Rings

Ligand LUT 3 320



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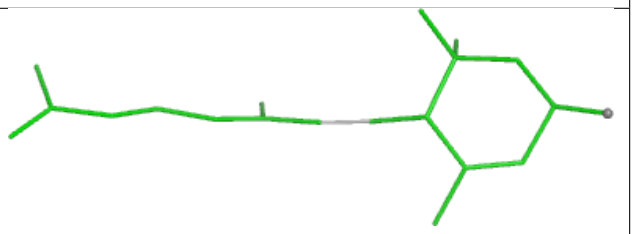
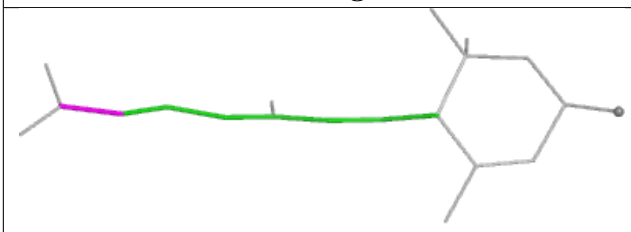


Bond angles



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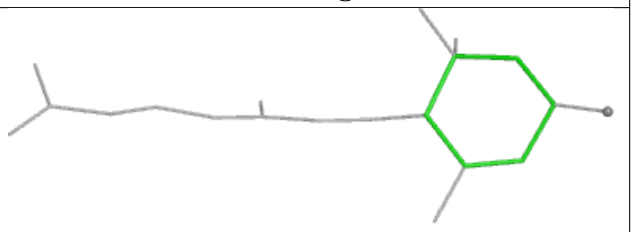
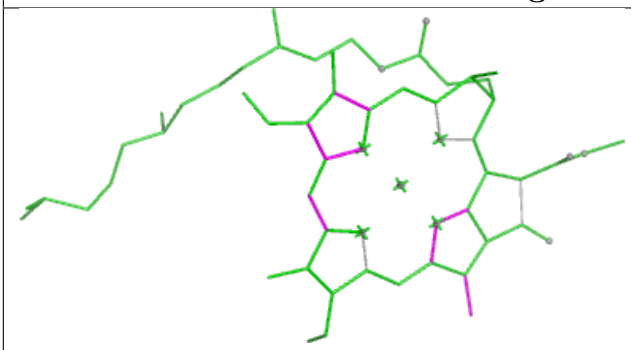


Rings

Ligand CLA 4 609



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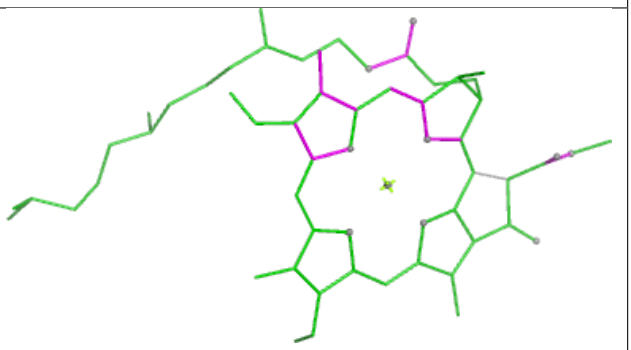
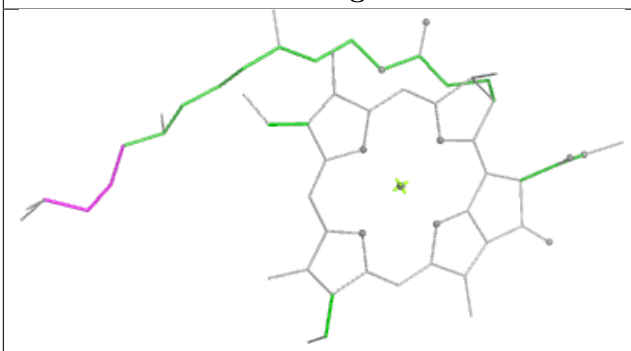


Bond angles



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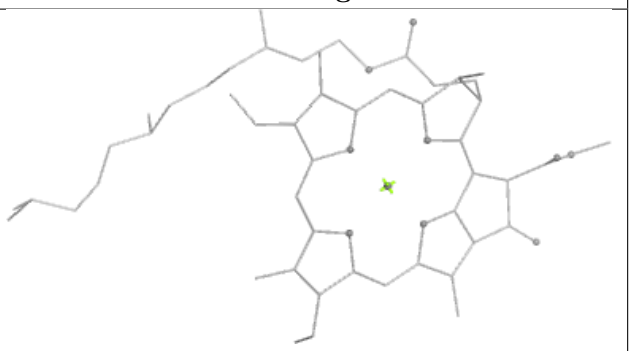
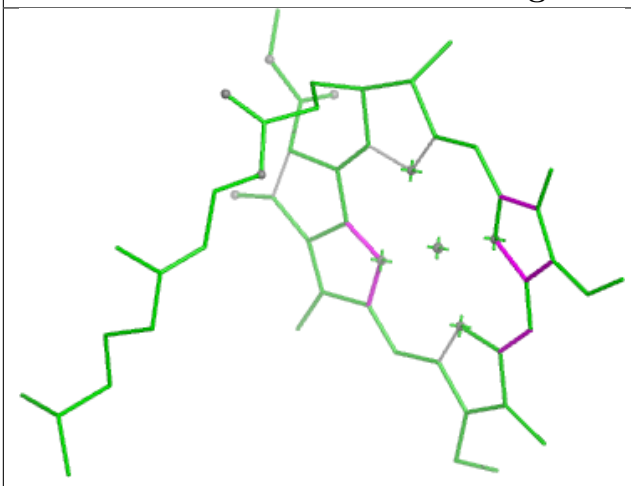


Rings

Ligand CLA 5 311



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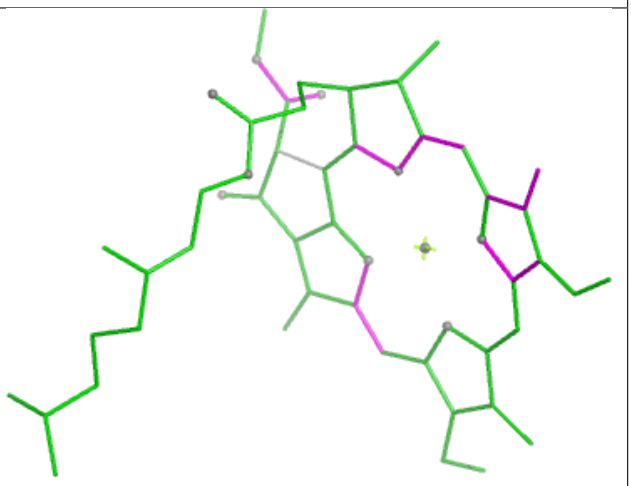
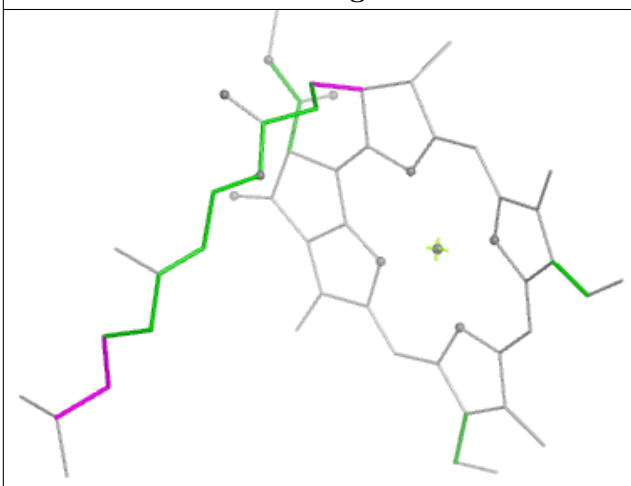


Bond angles



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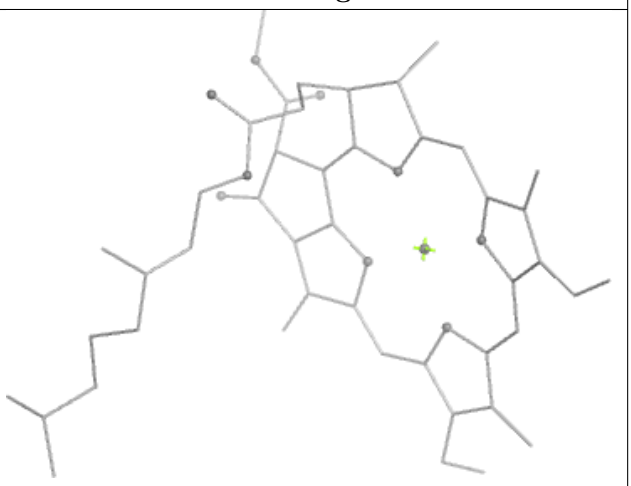
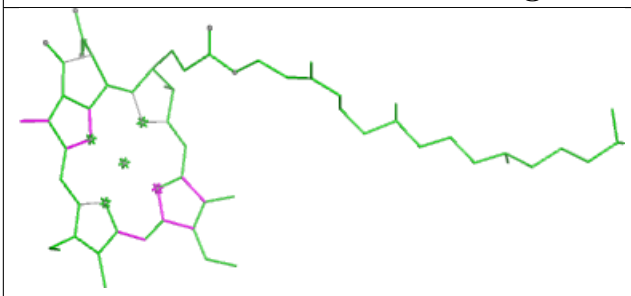


Rings

Ligand CLA A 836



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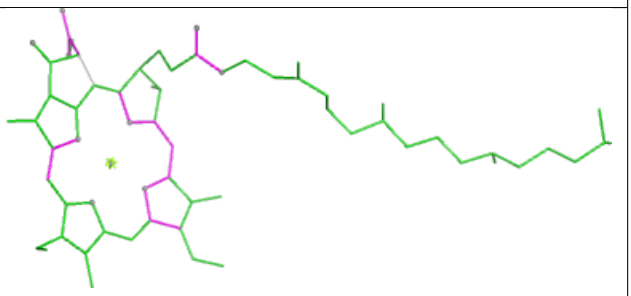
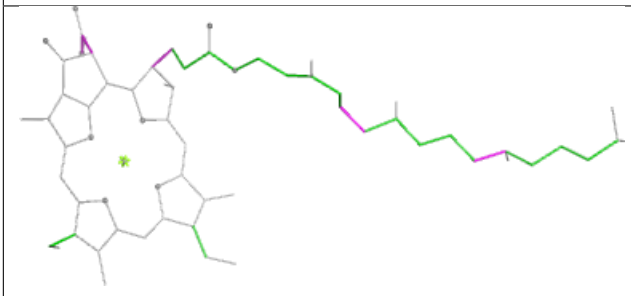


Bond angles



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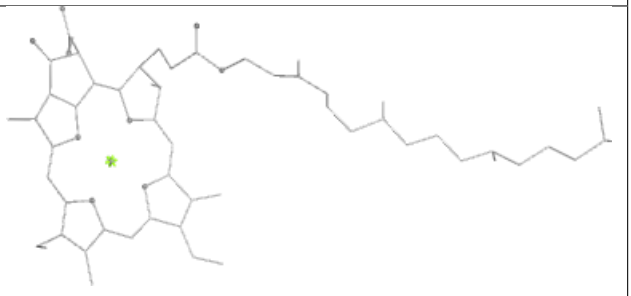
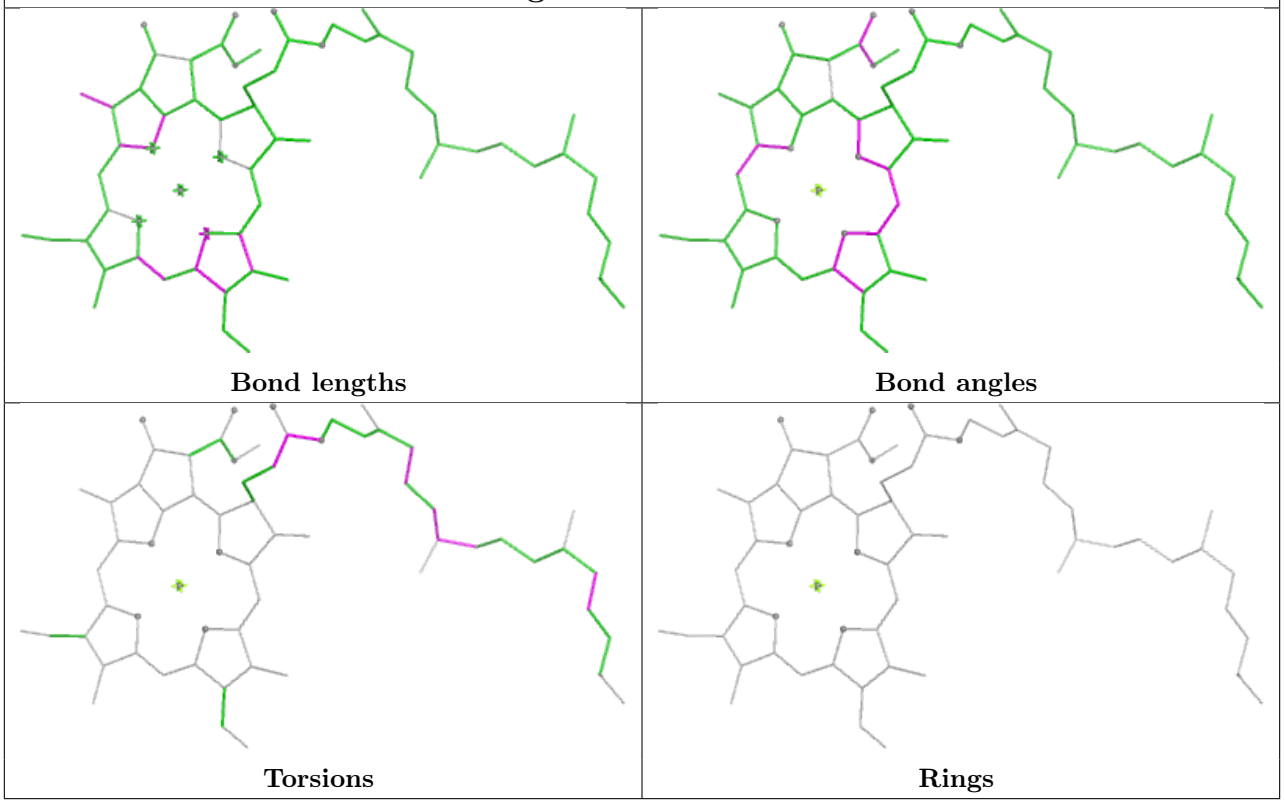
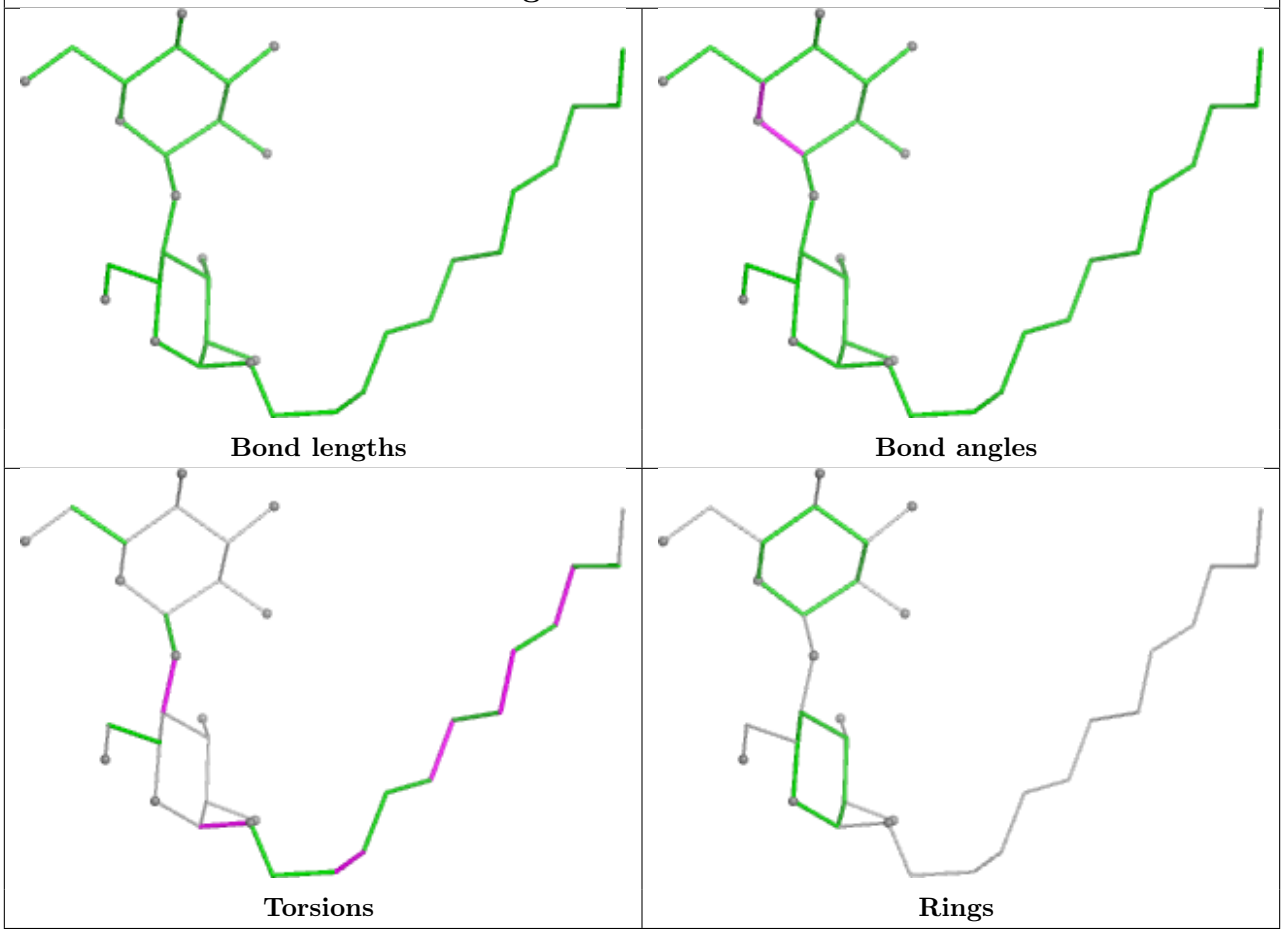


Rings

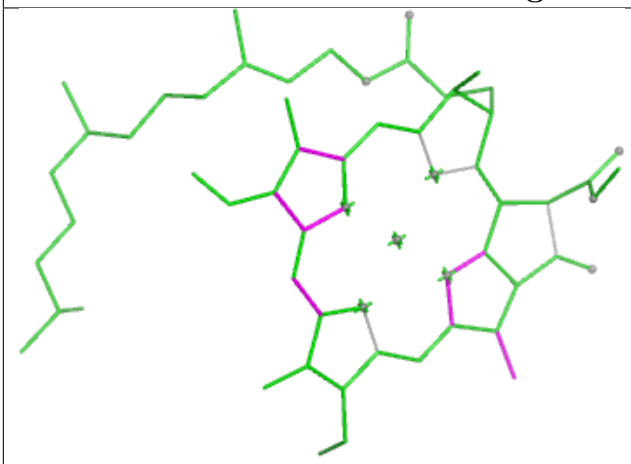
Ligand CLA Z 603



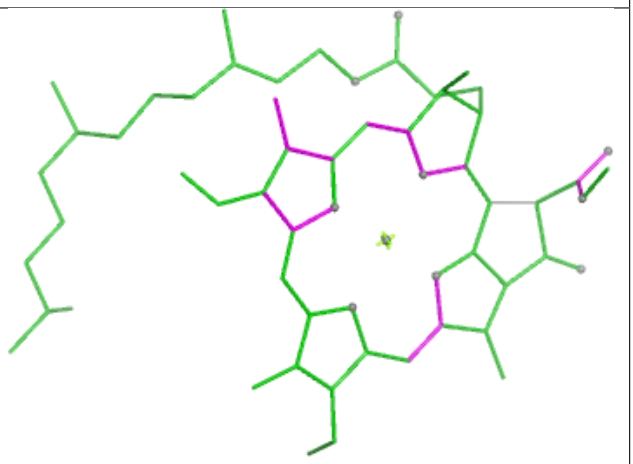
Ligand LMU F 306



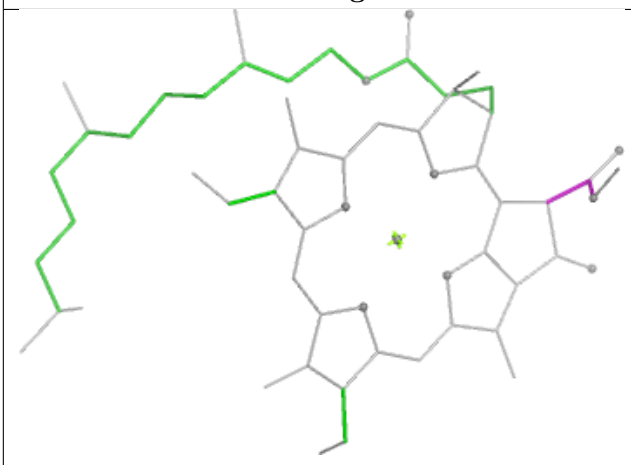
Ligand CLA Z 602



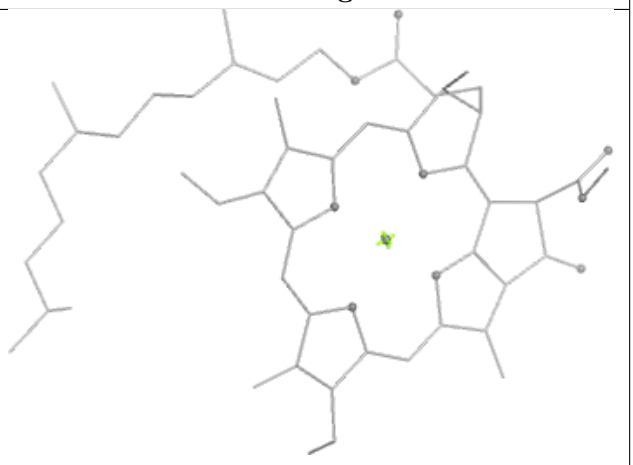
Bond lengths



Bond angles

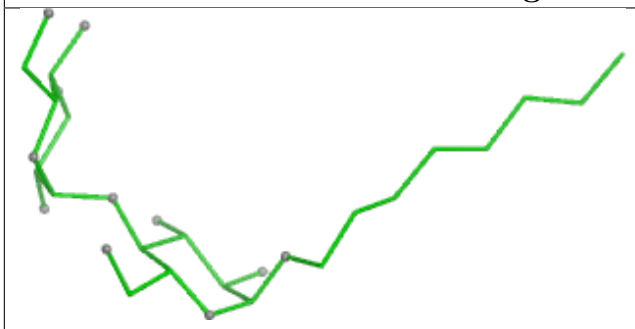


Torsions



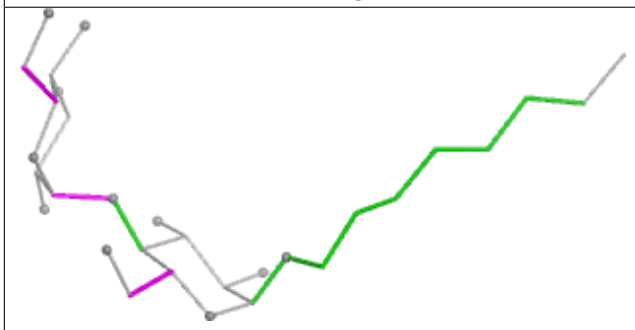
Rings

Ligand LMU Z 619

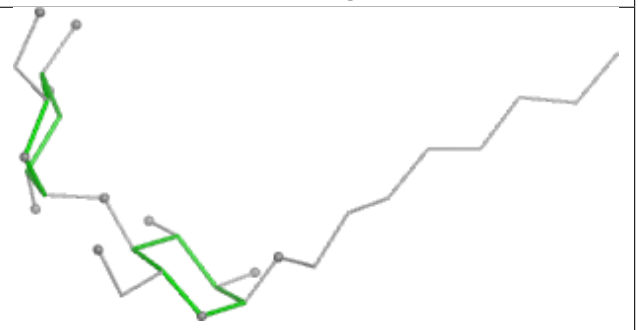


Bond lengths

Bond angles

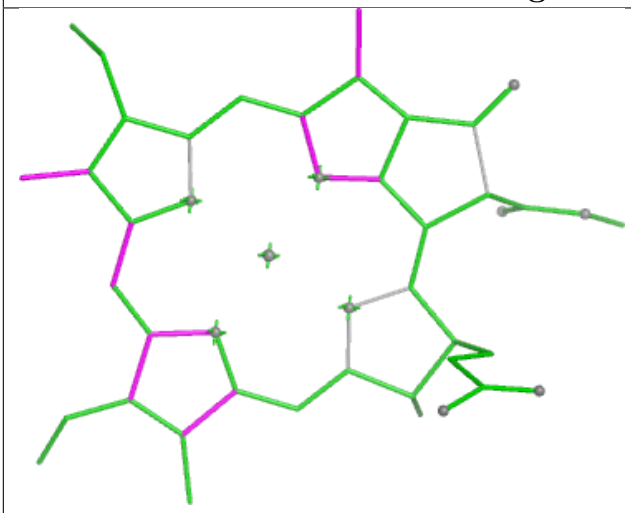


Torsions



Rings

Ligand CLA 3 314



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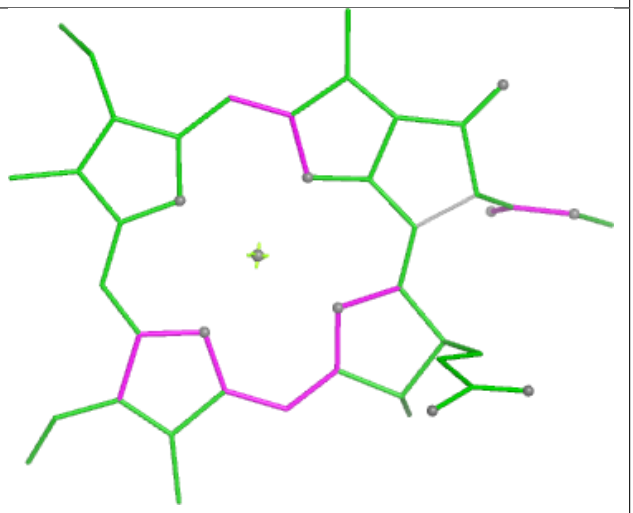
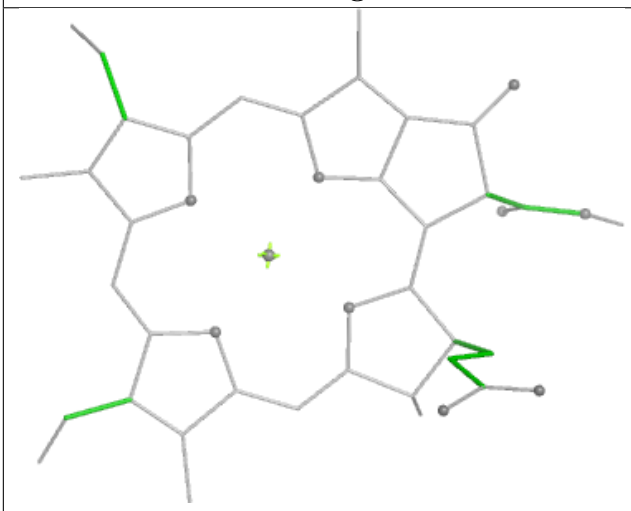


Bond angles



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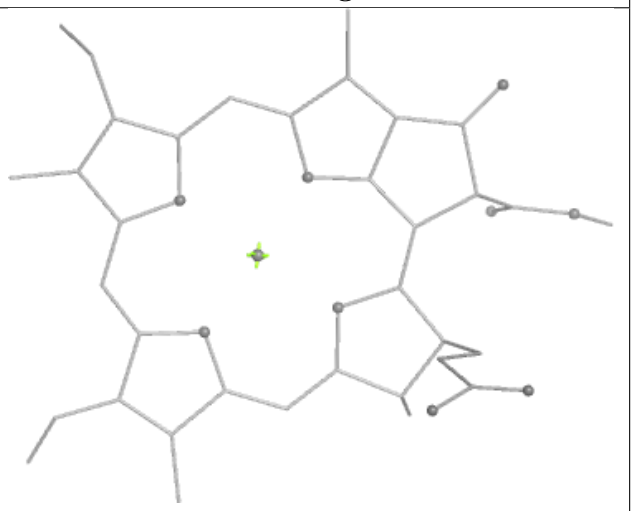
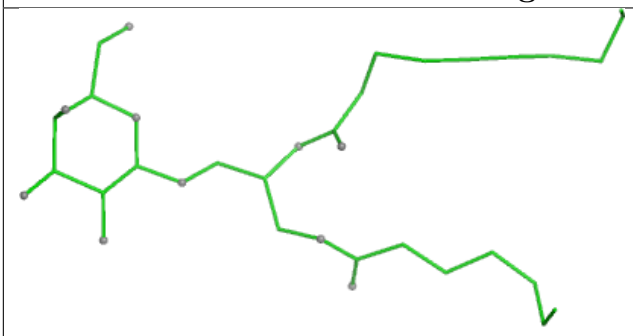


Rings

Ligand LMG G 201



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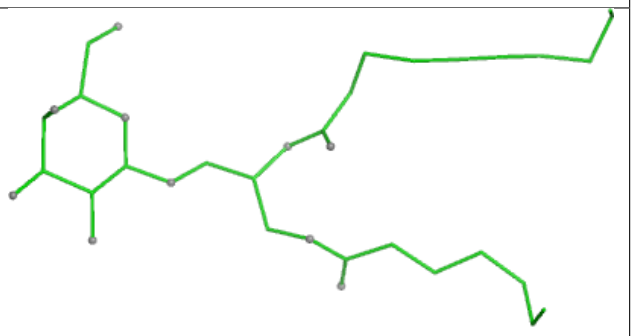
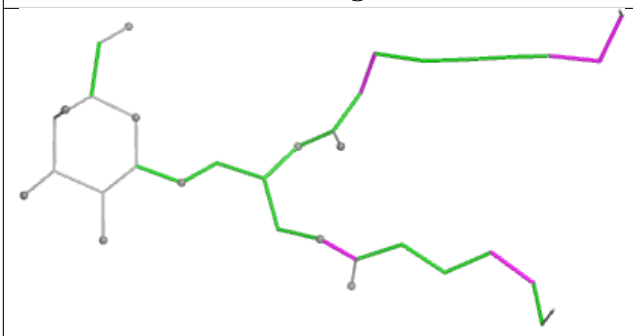


Bond angles



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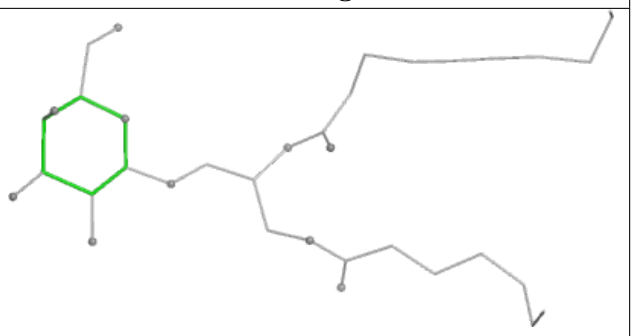
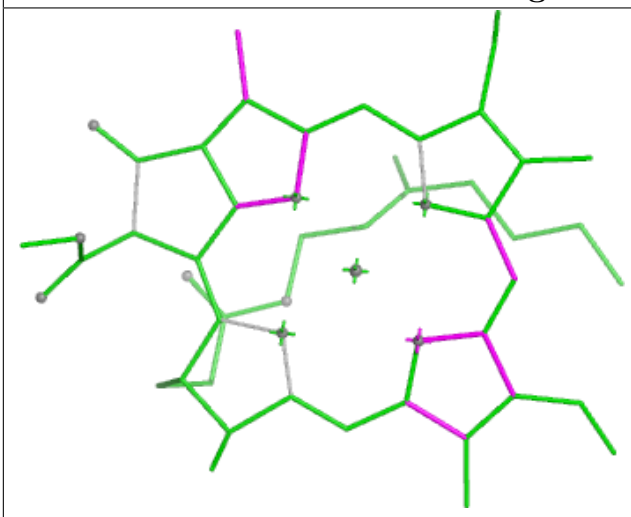


Rings

Ligand CLA 6 327



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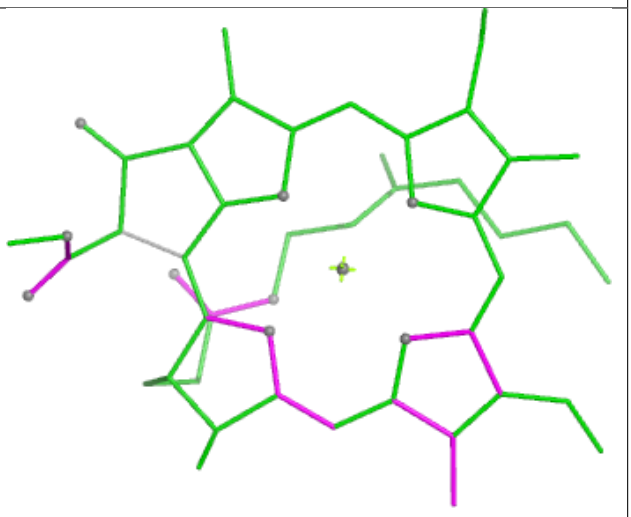

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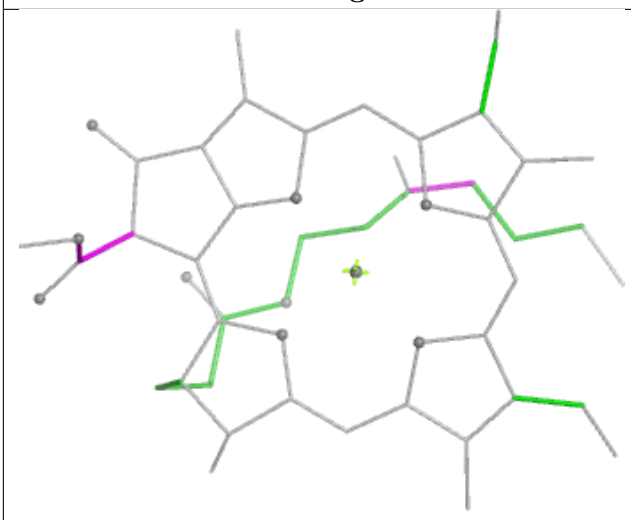

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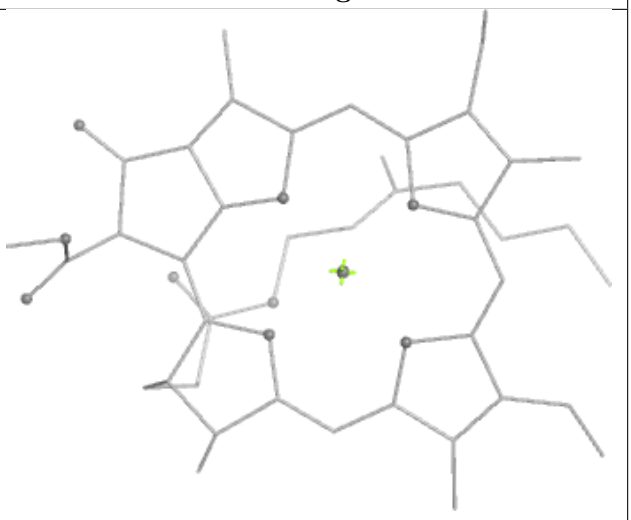
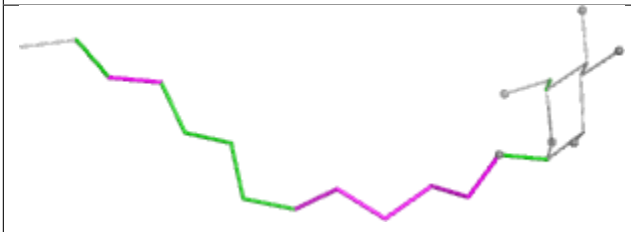


Rings

Ligand LMU 4 624

Bond lengths

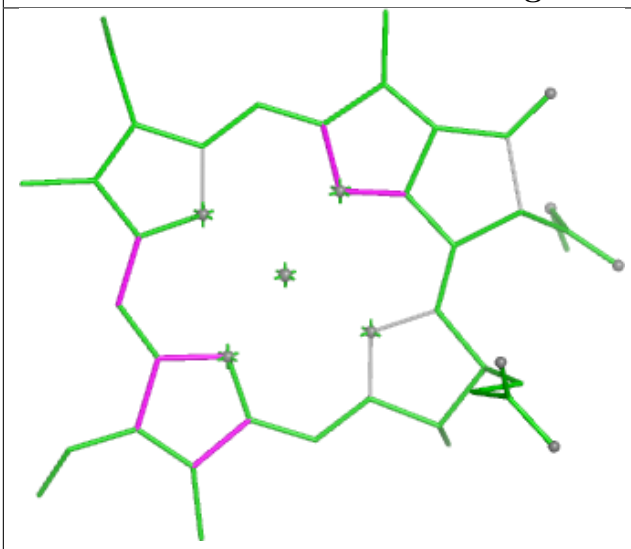
Bond angles



Torsions

Rings

Ligand CLA B 805



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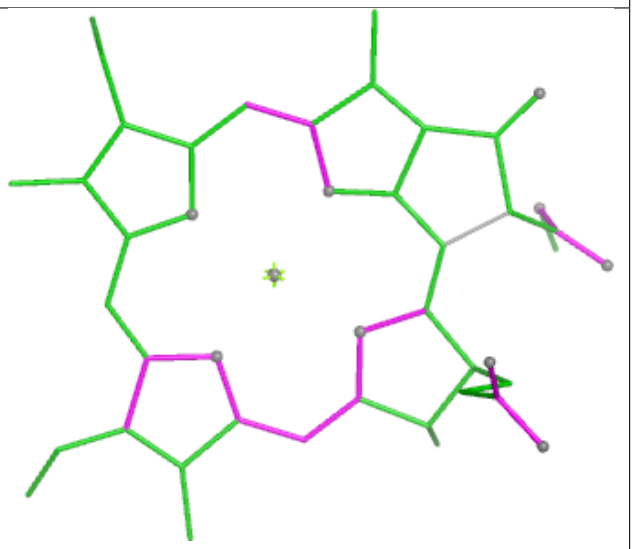
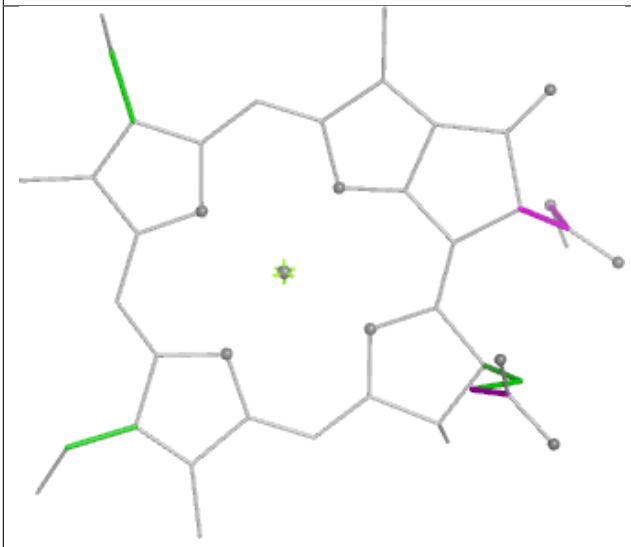


Bond angles



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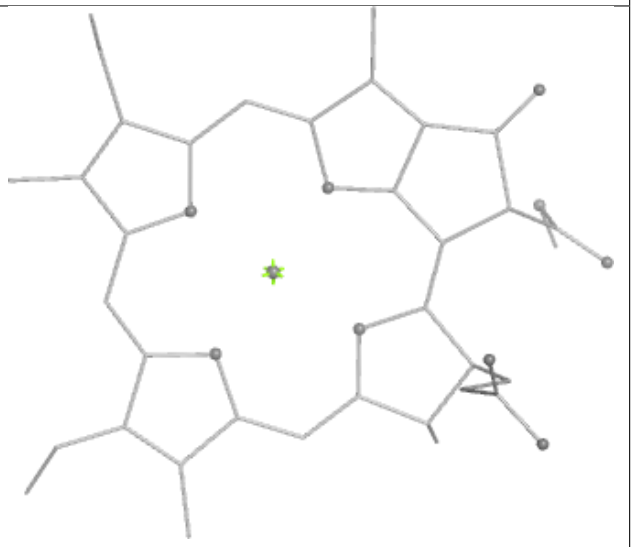
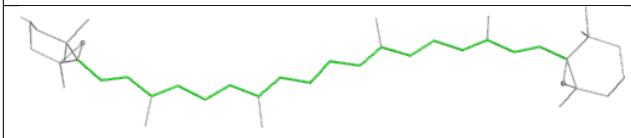


Rings

Ligand XAT 8 316

Bond lengths

Bond angles



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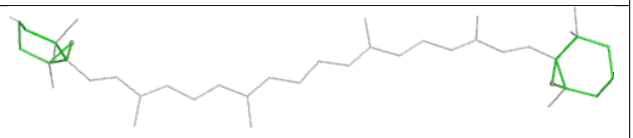
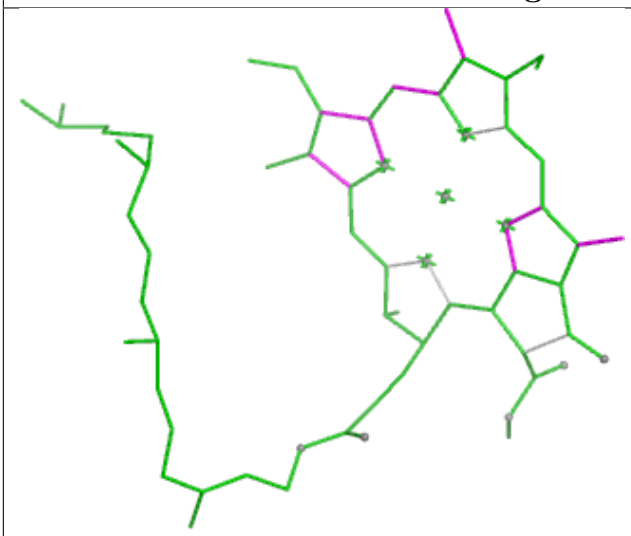


Rings

Ligand CLA B 824



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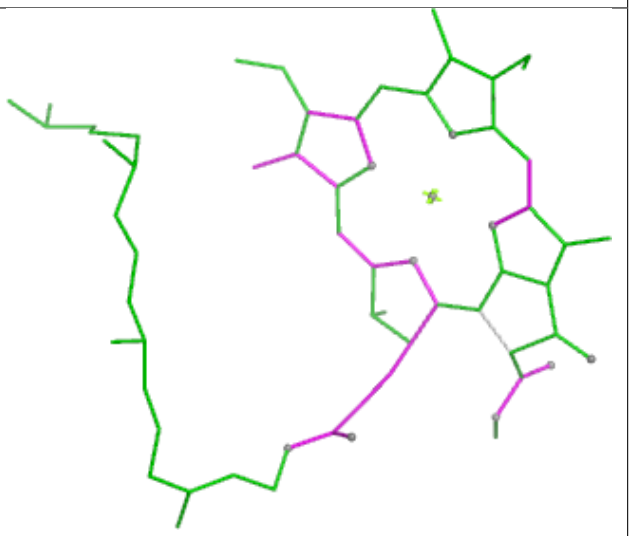
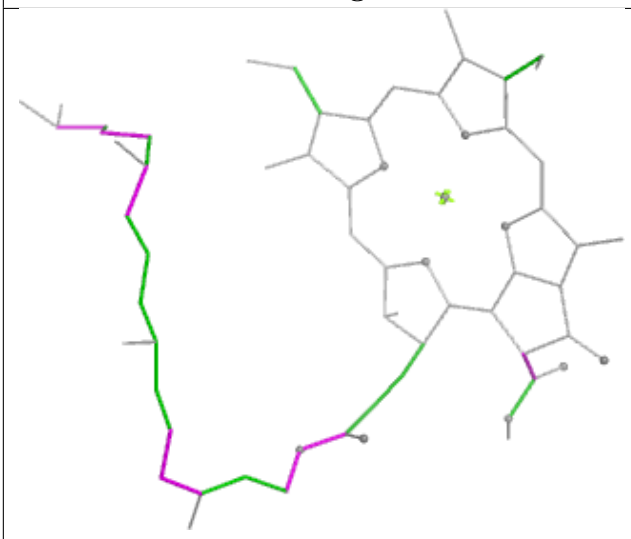


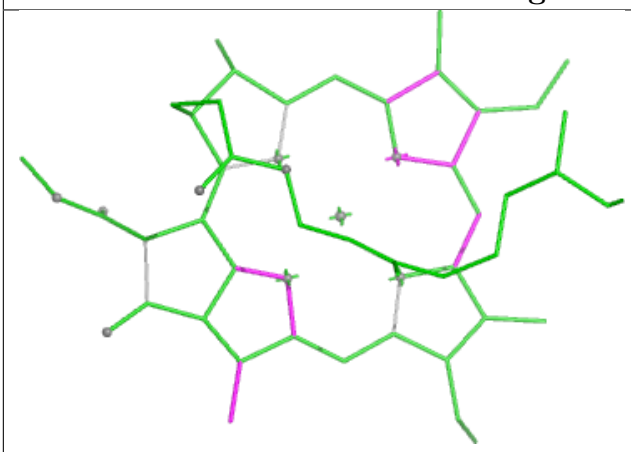
Bond angles



Torsions

Rings

Ligand CLA 5 313



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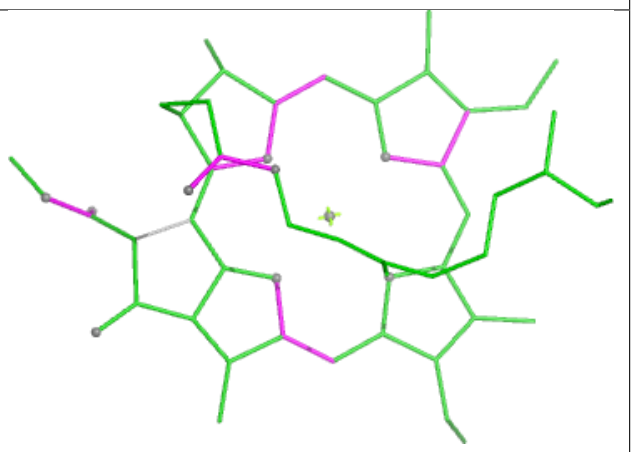
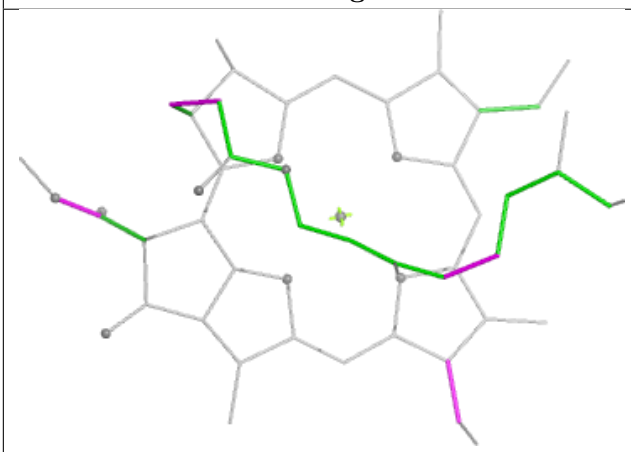


Bond angles



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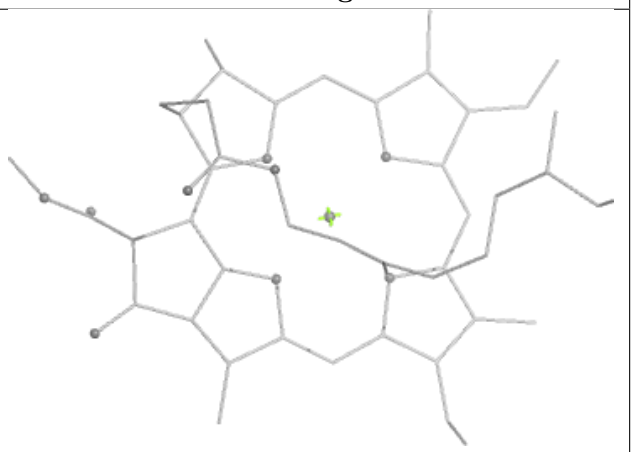
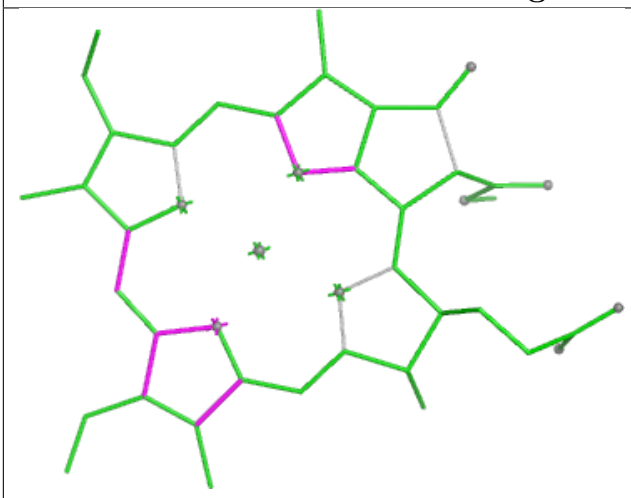


Rings

Ligand CLA 5 312



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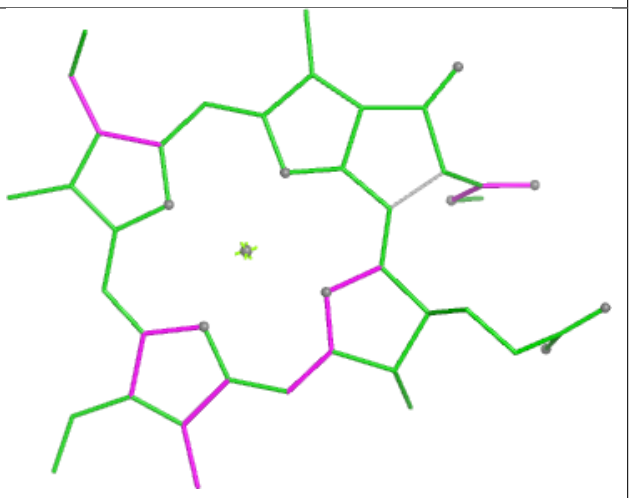
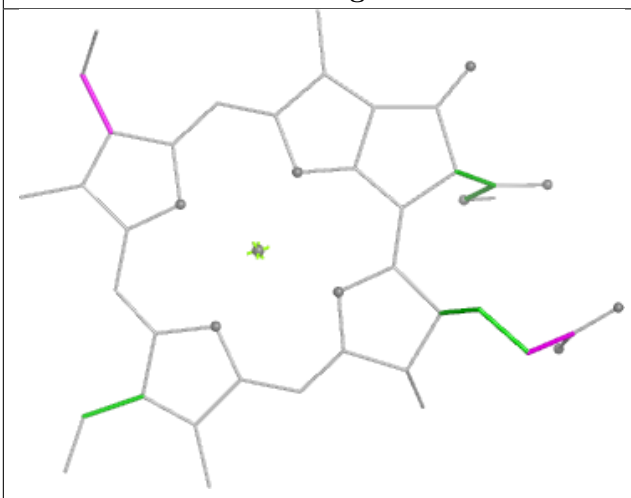
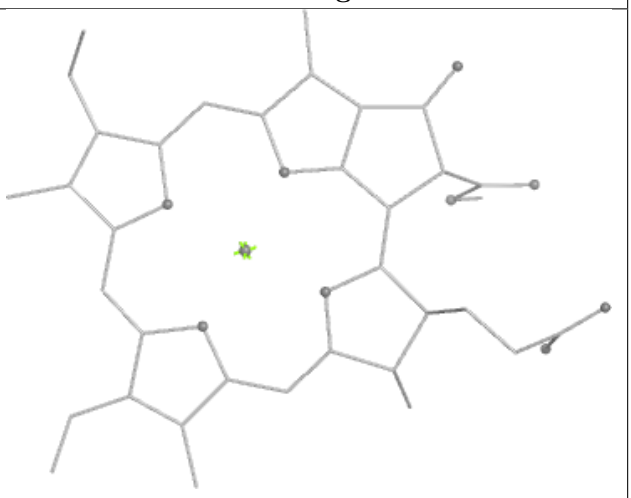


Bond angles

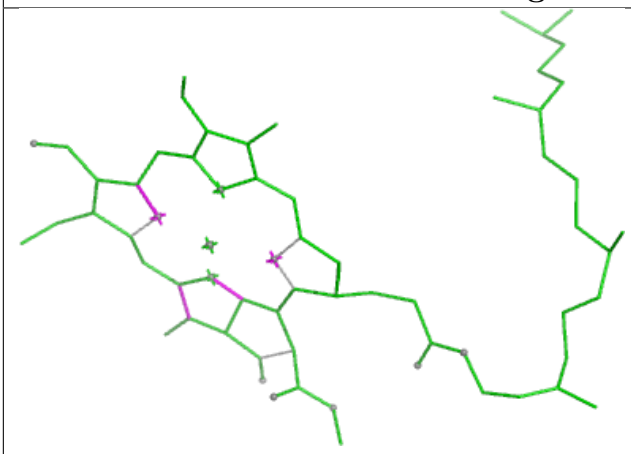


Torsions



Rings

Ligand CHL 4 605



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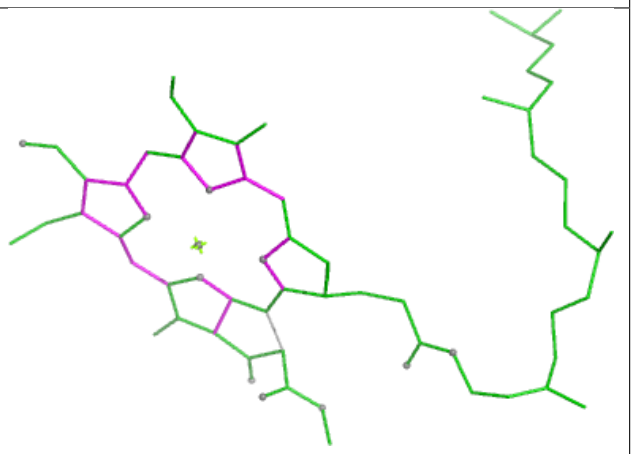
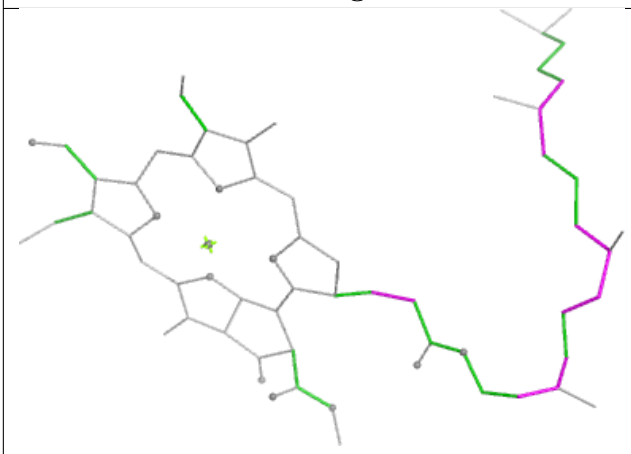


Bond angles



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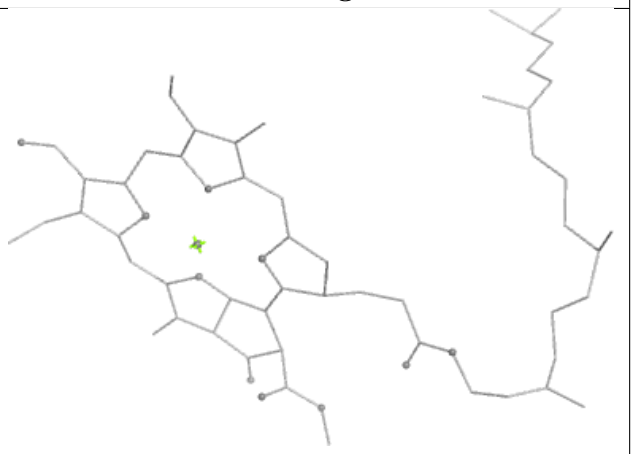
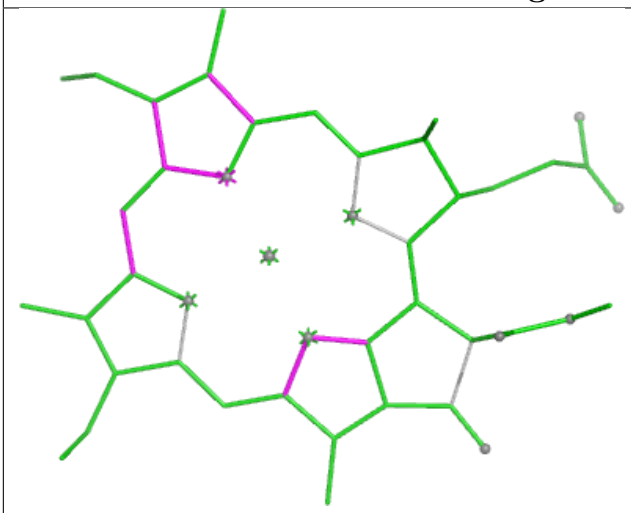


Rings

Ligand CLA 8 310



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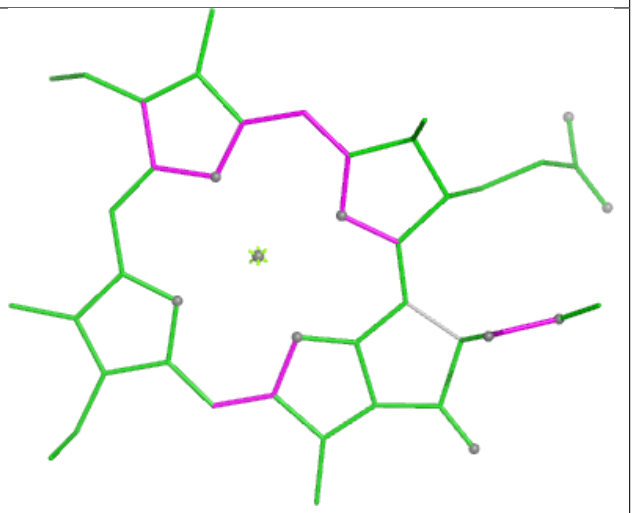
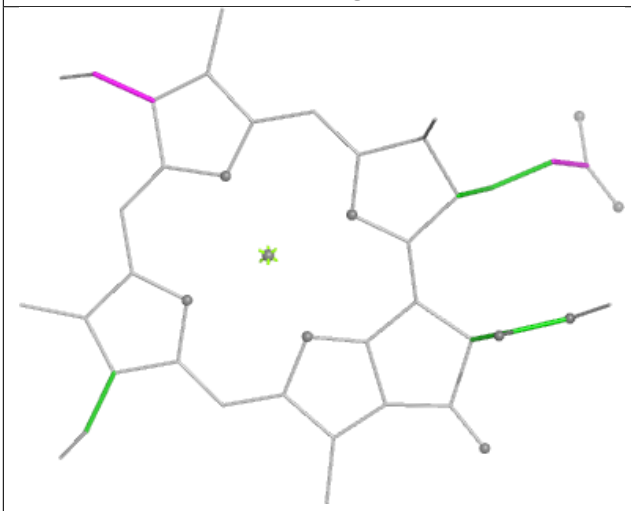


Bond angles



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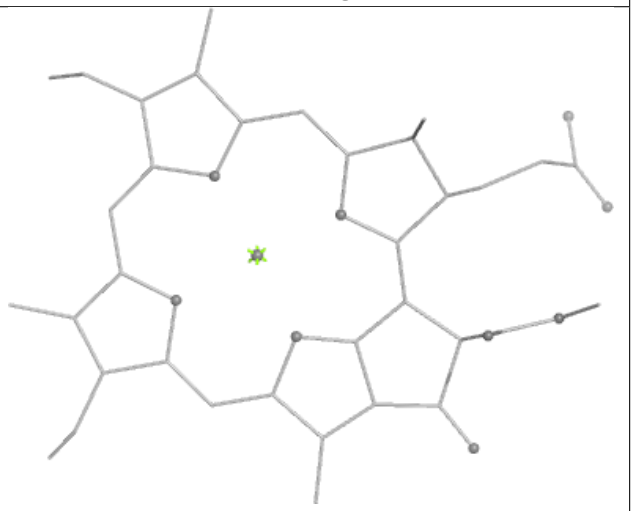
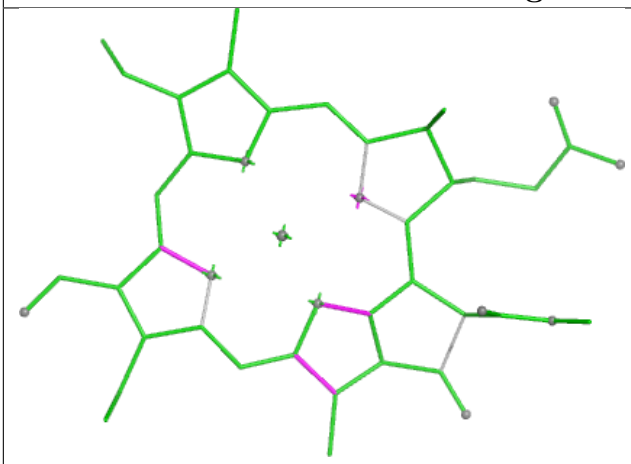


Rings

Ligand CHL Z 605



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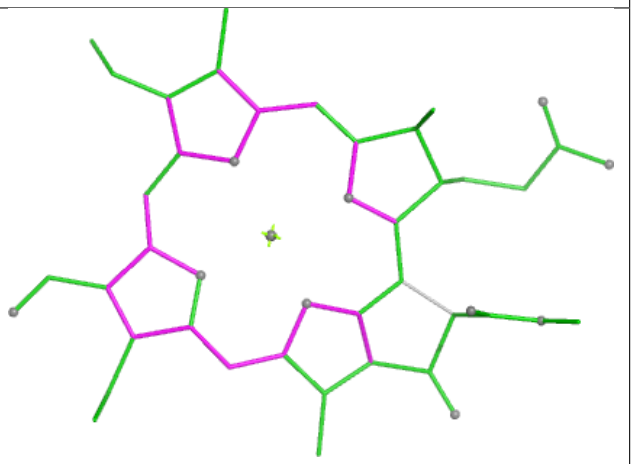
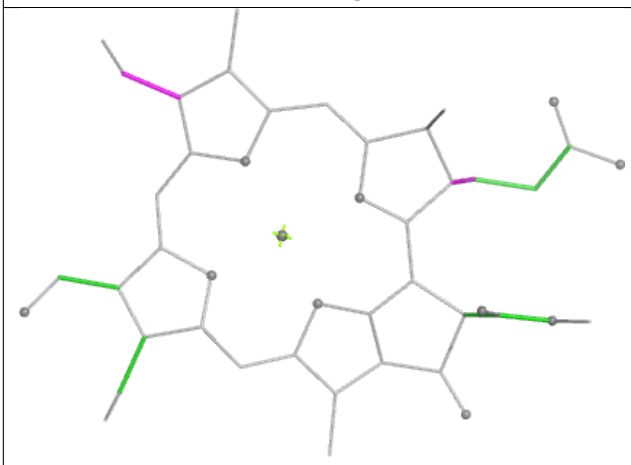


Bond angles



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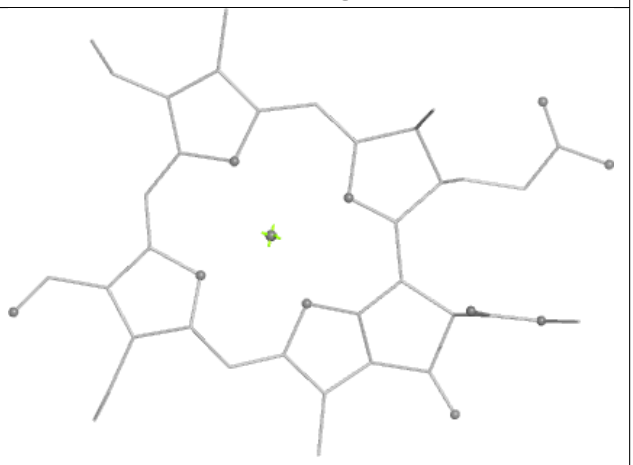
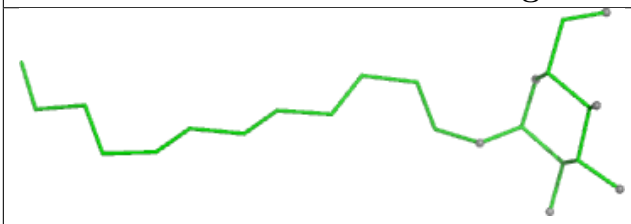


Rings

Ligand LMU Z 620



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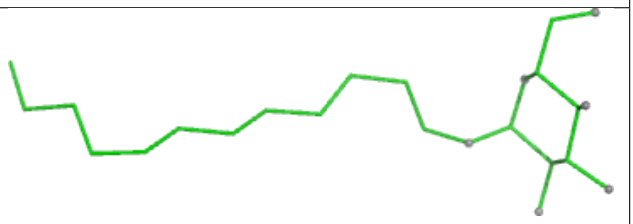
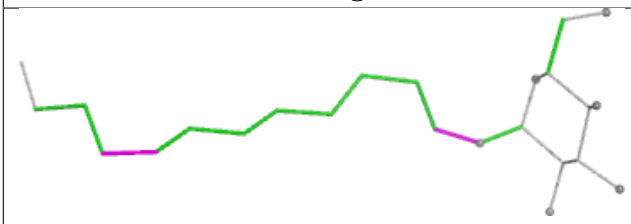


Bond angles



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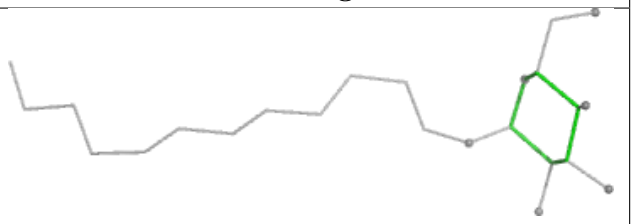
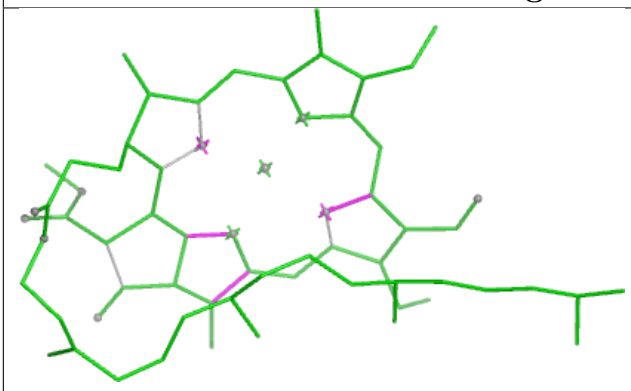


Rings

Ligand CHL Z 606



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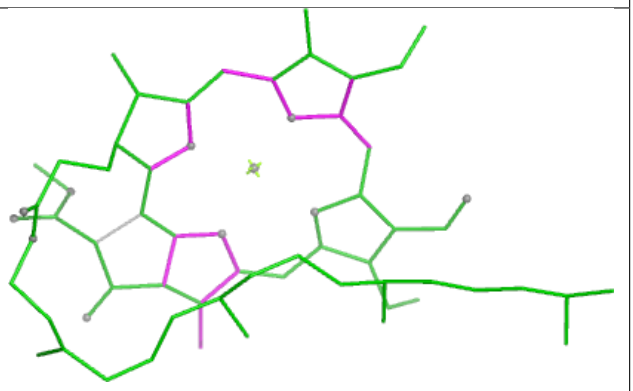
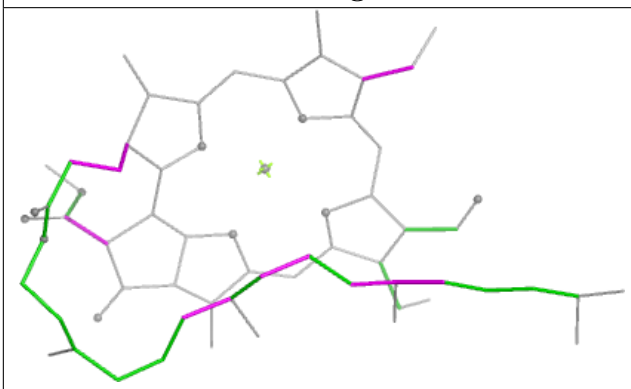


Bond angles



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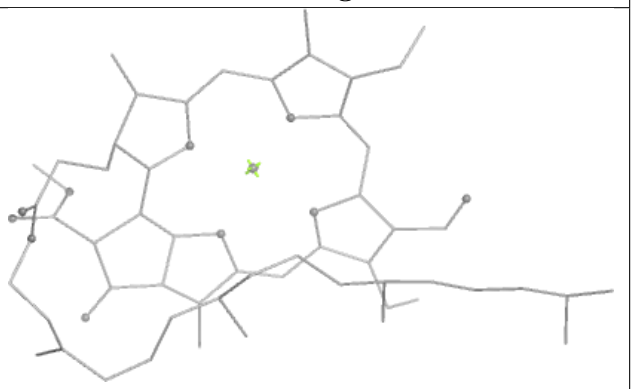
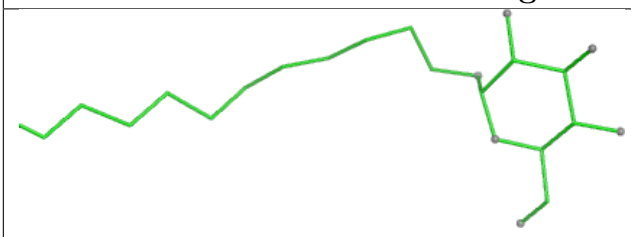


Rings

Ligand LMU K 201



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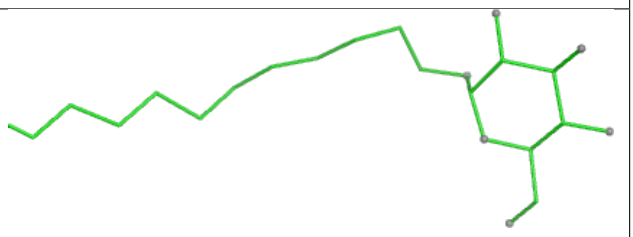
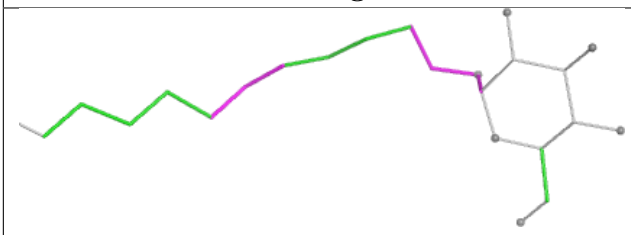
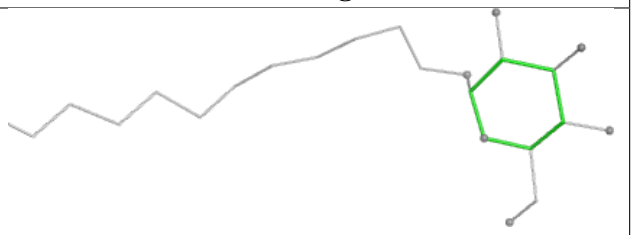


Bond angles

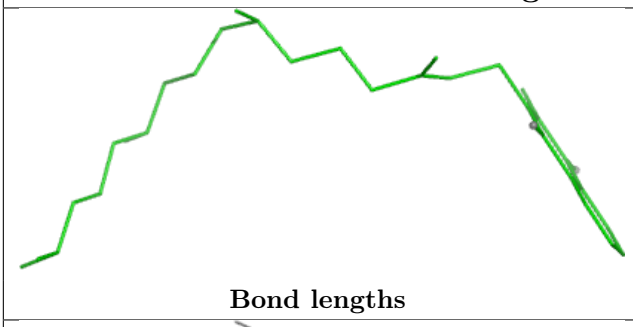


Torsions

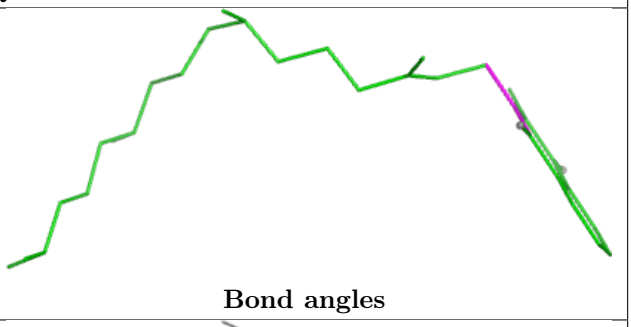


Rings

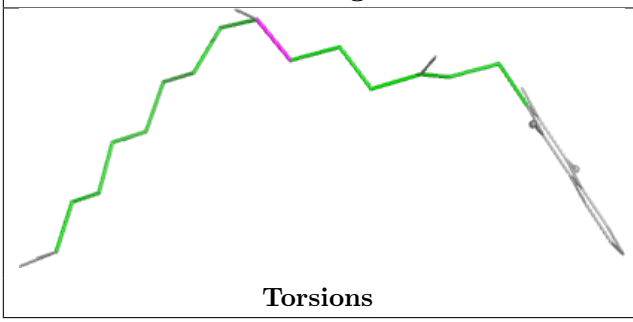
Ligand PQN B 843



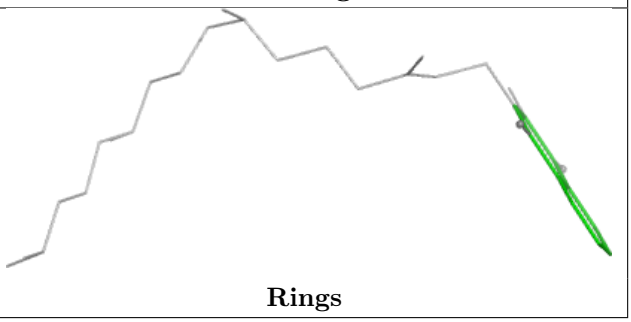
Bond lengths



Bond angles

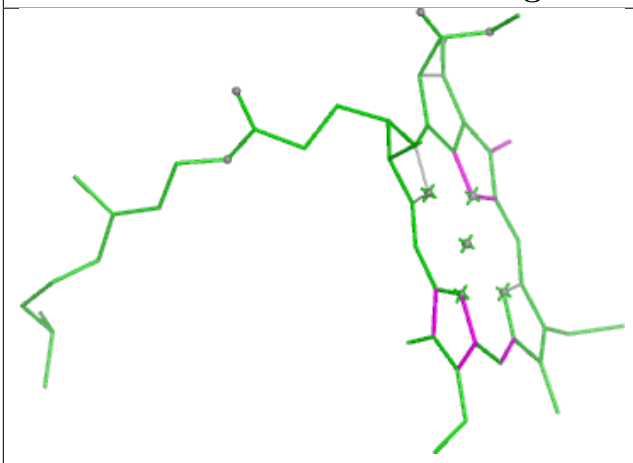


Torsions



Rings

Ligand CLA A 833



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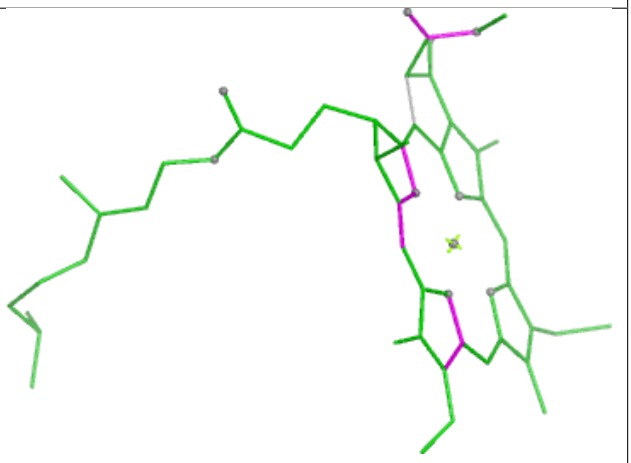
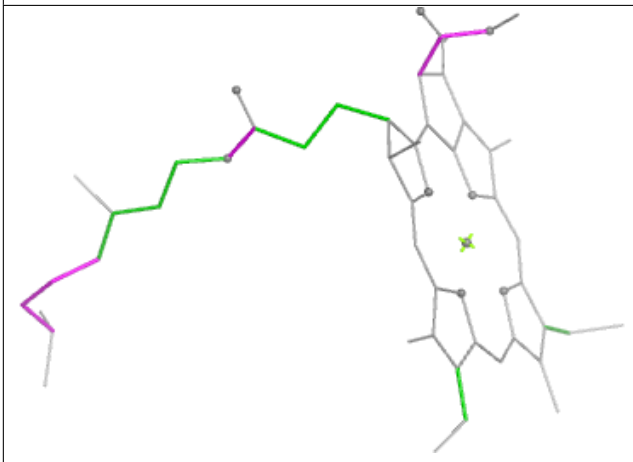


Bond angles



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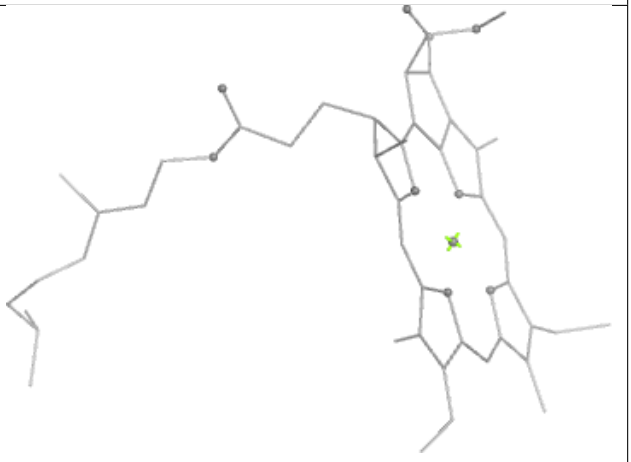
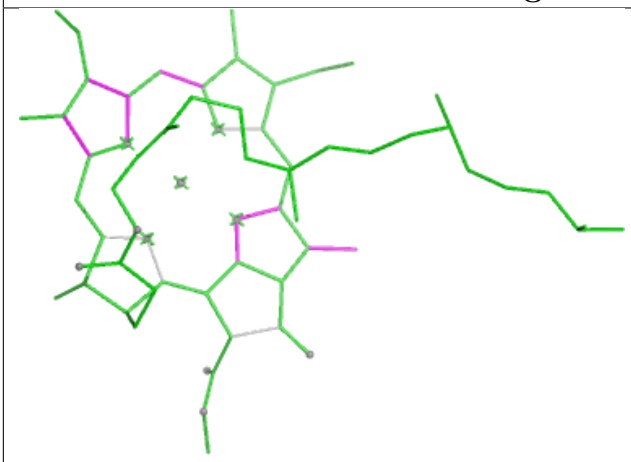


Rings

Ligand CLA B 828



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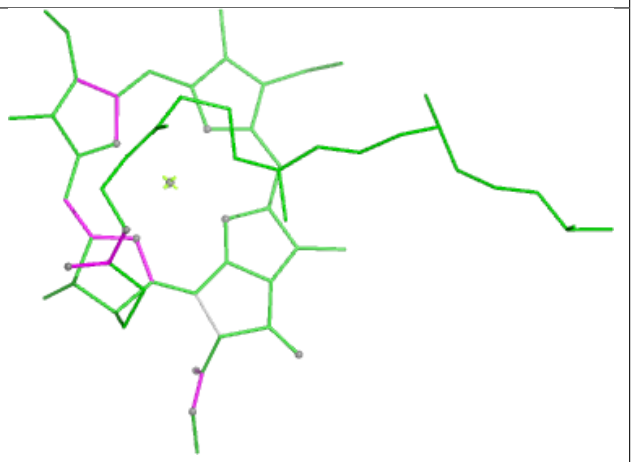

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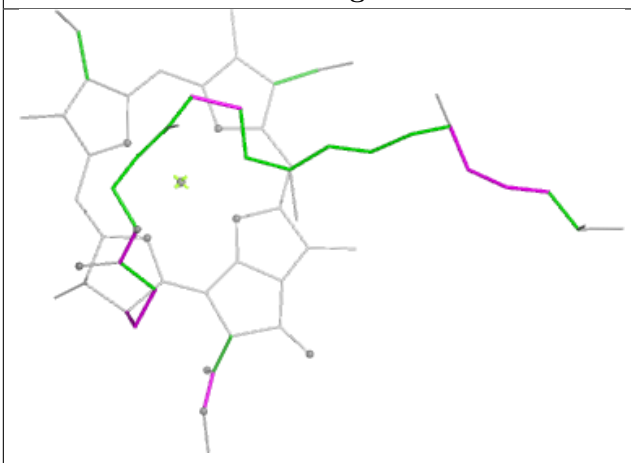

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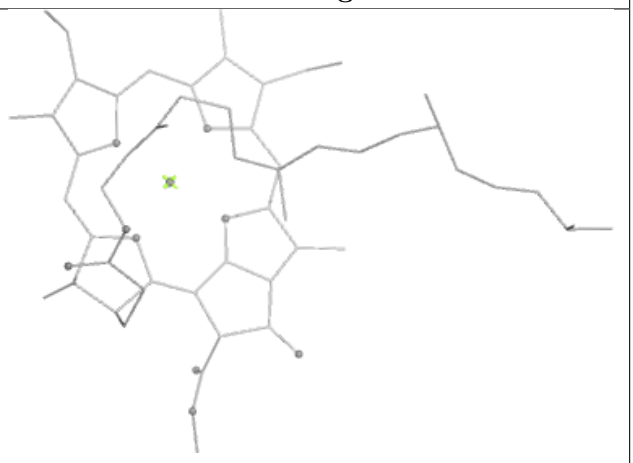
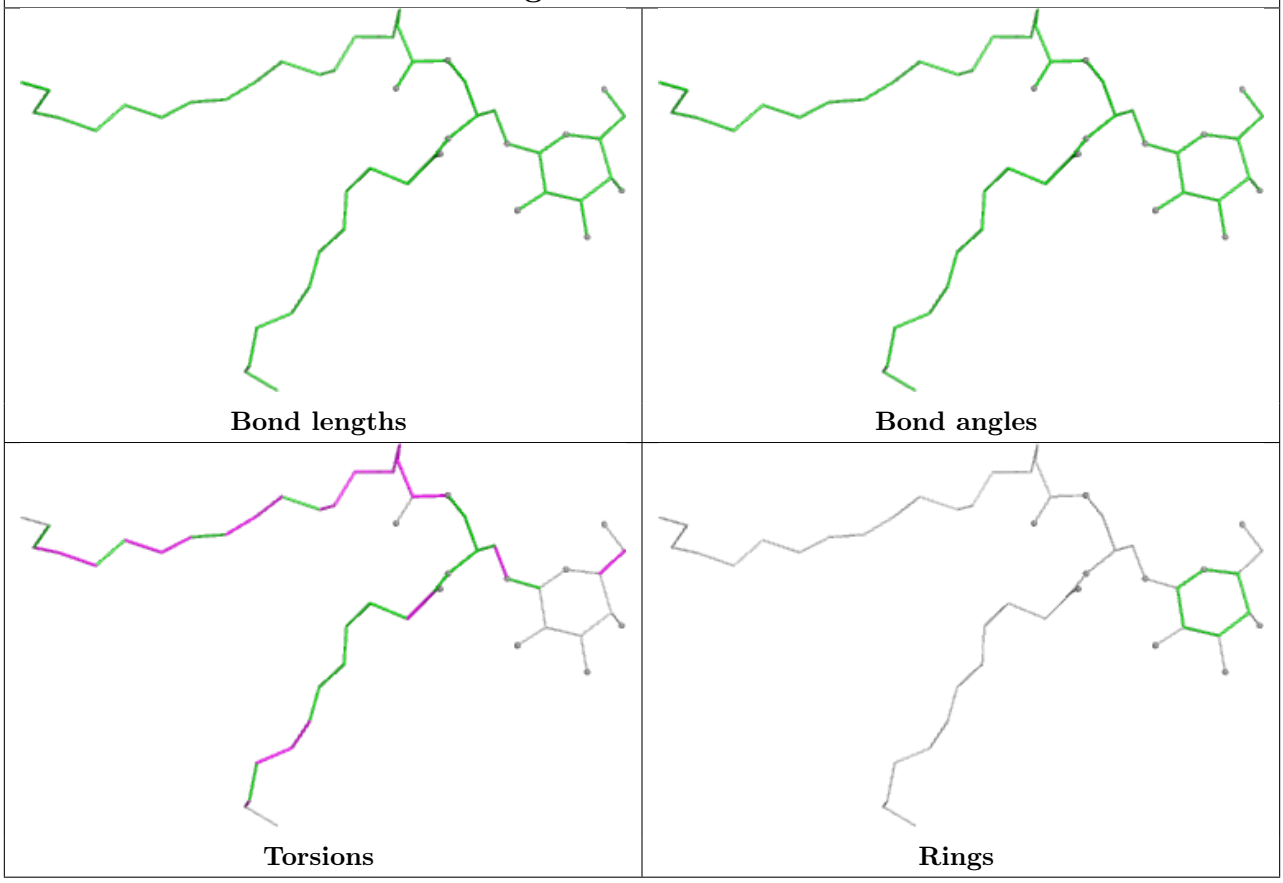
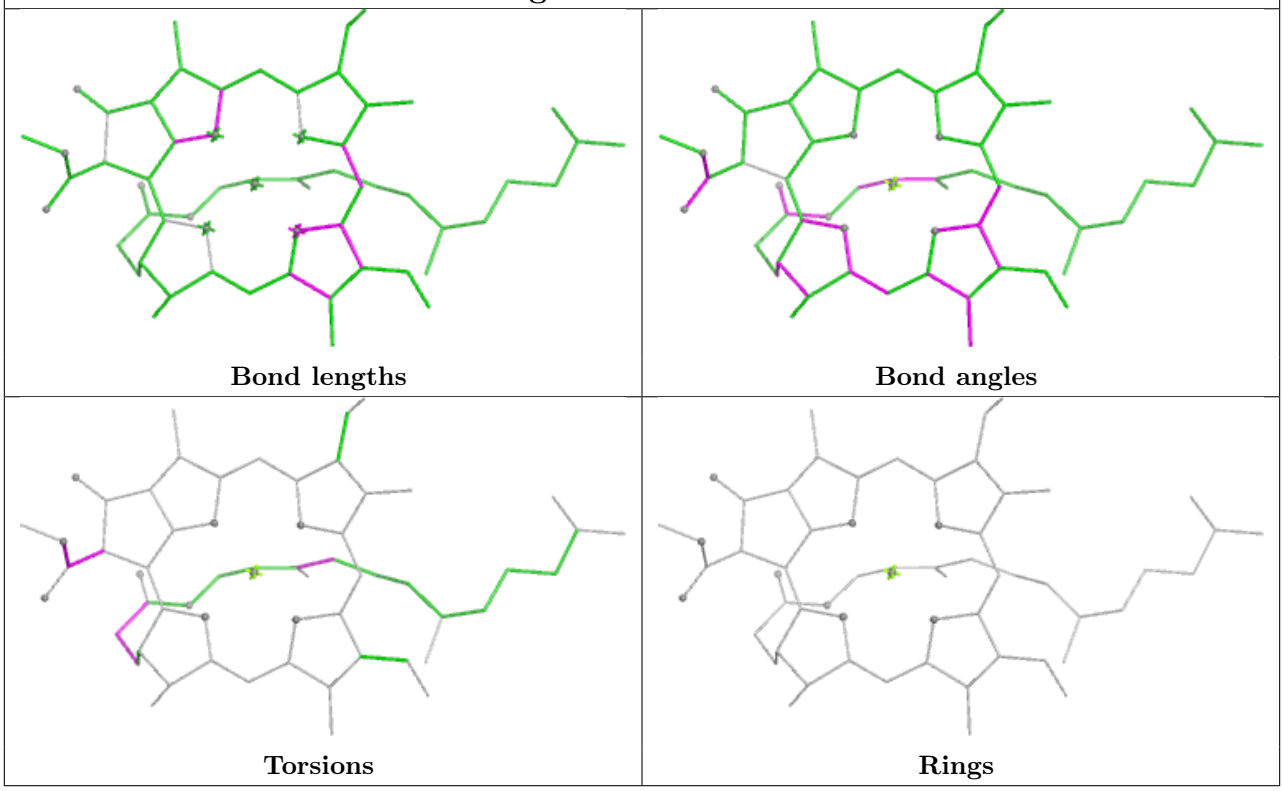


Rings

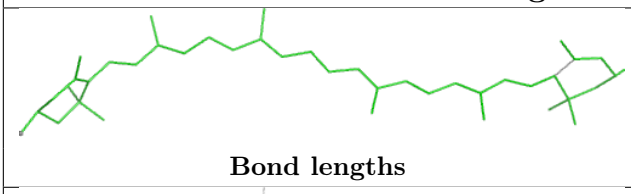
Ligand LMG 8 321



Ligand CLA 3 313



Ligand LUT 4 616



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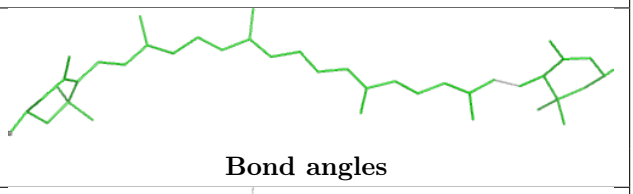
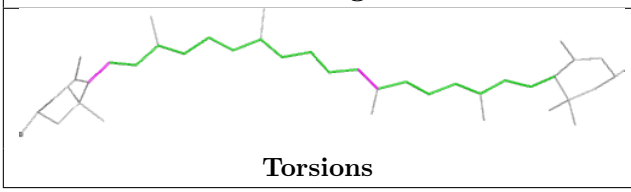


Bond angles



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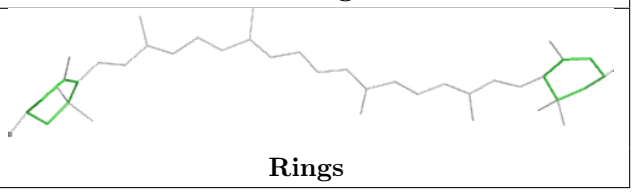
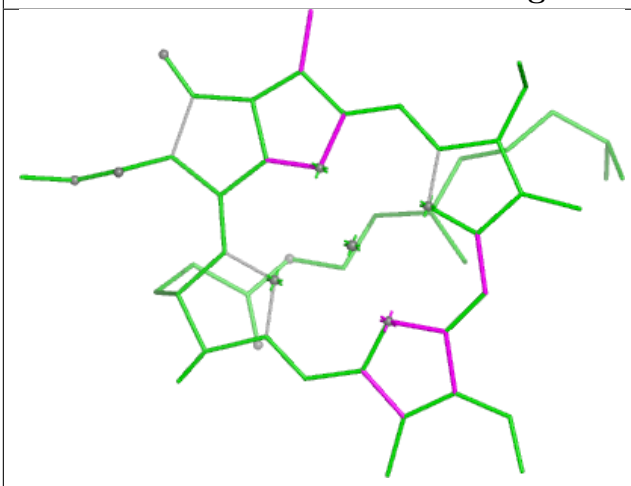


Rings

Ligand CLA J 102



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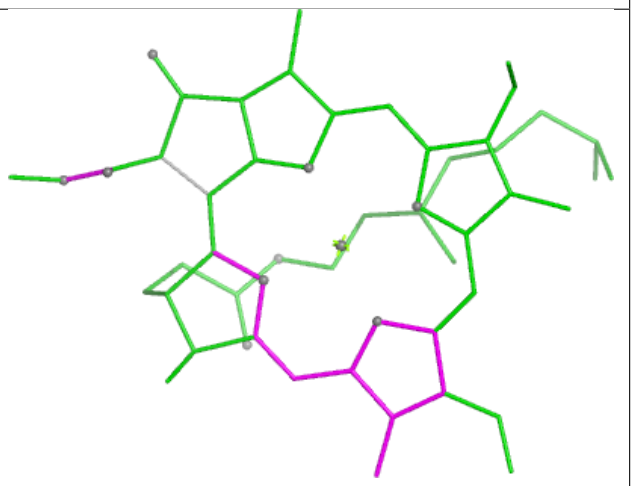
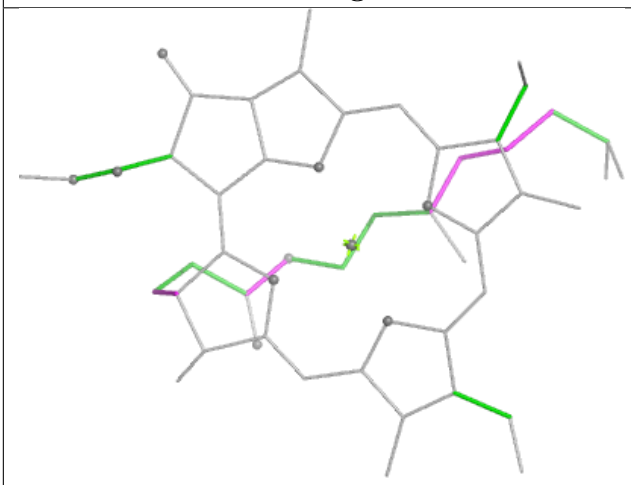


Bond angles



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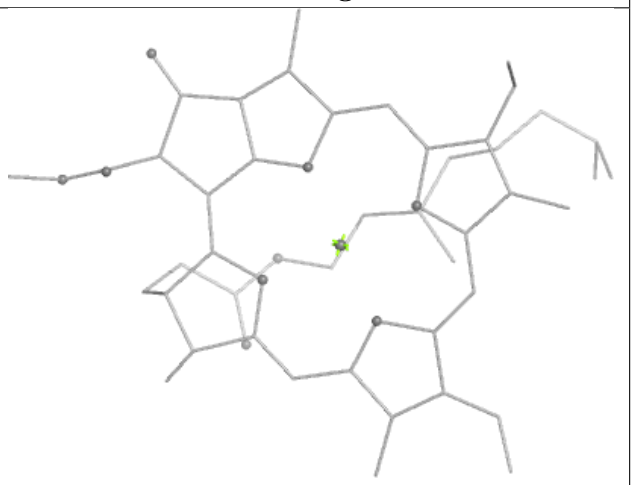
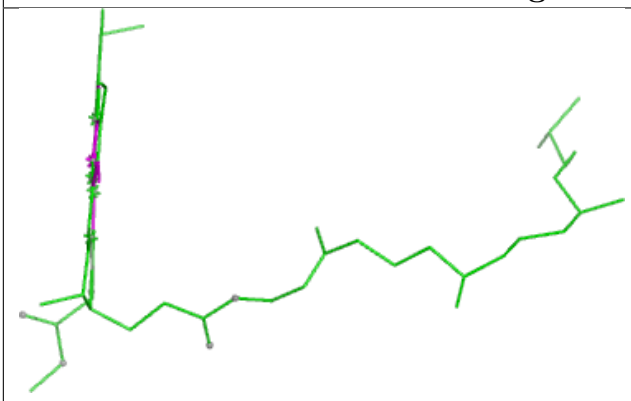


Rings

Ligand CLA 3 303



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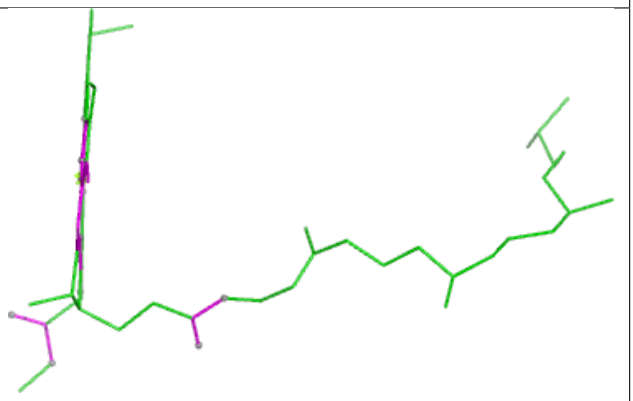
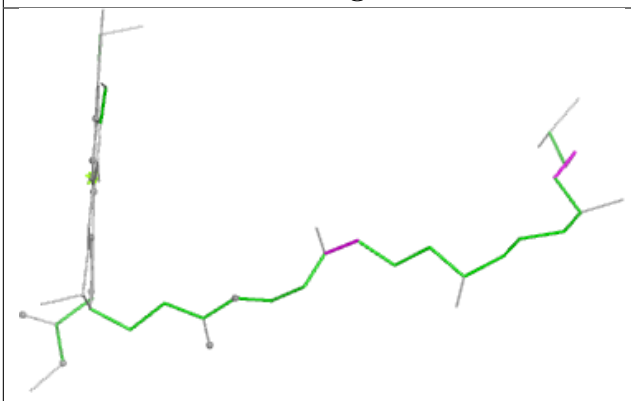


Bond angles



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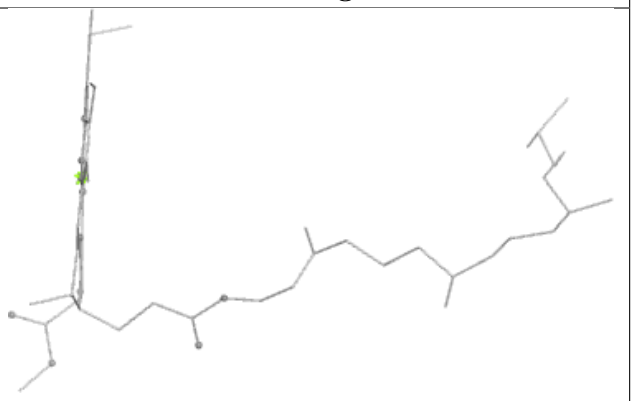
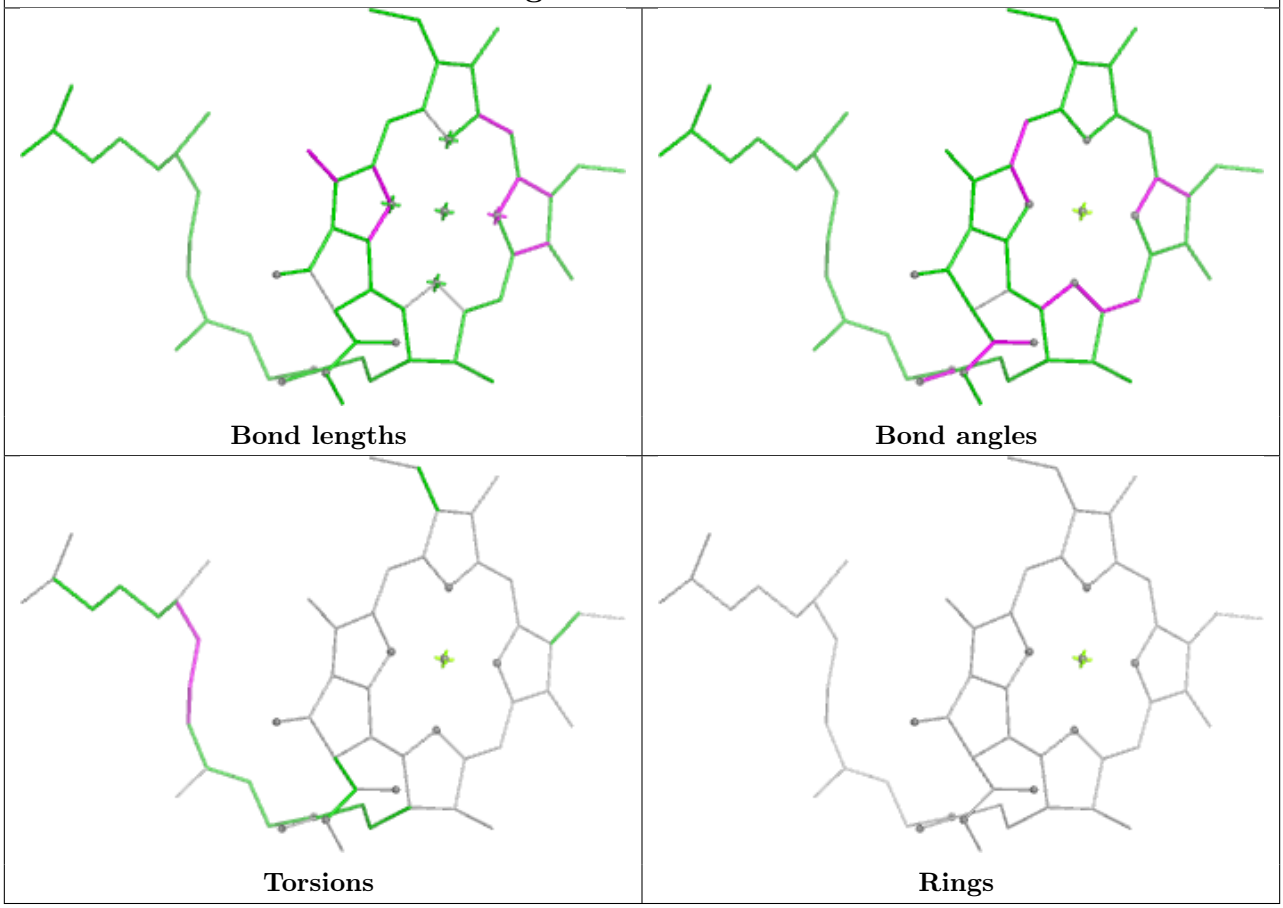
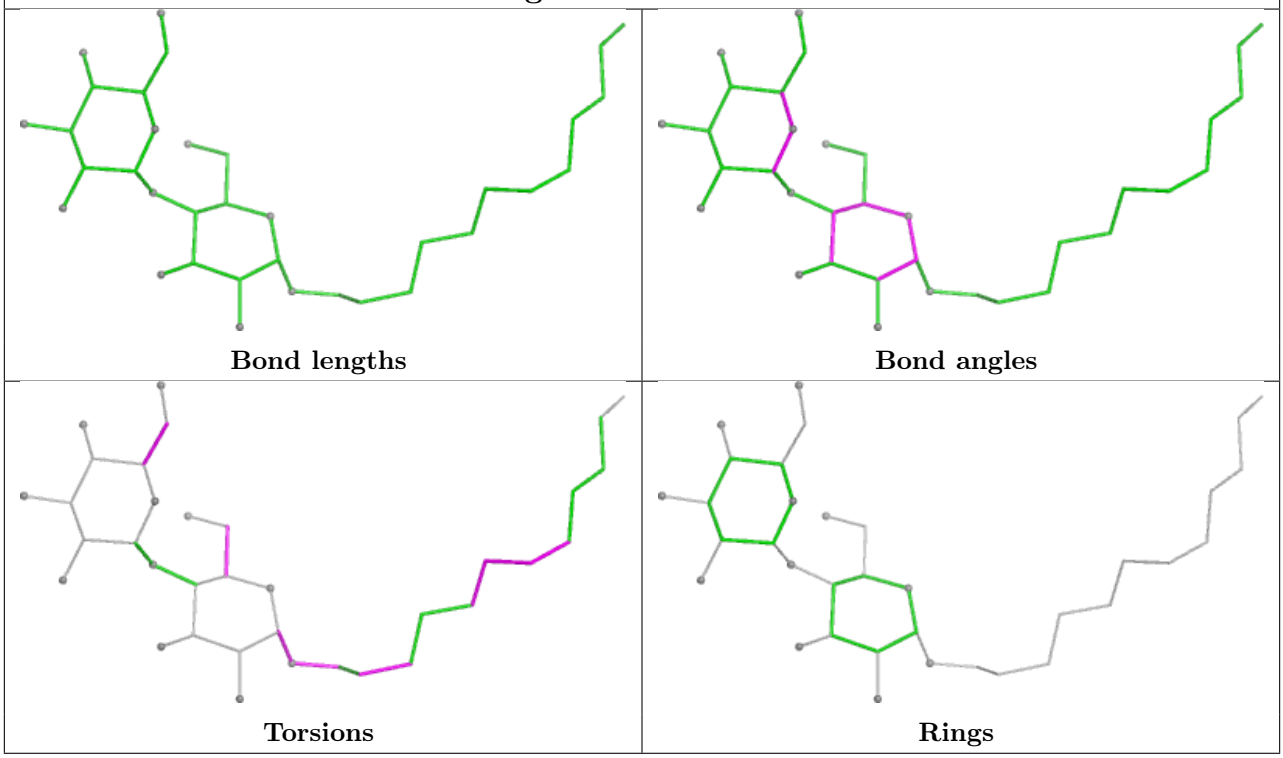


Rings

Ligand CLA B 835



Ligand LMU 3 324



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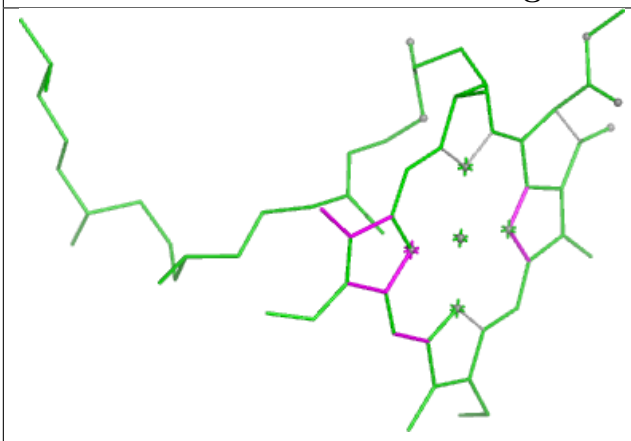

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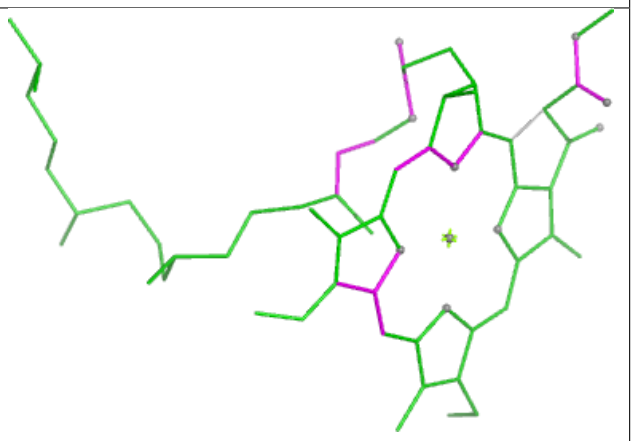
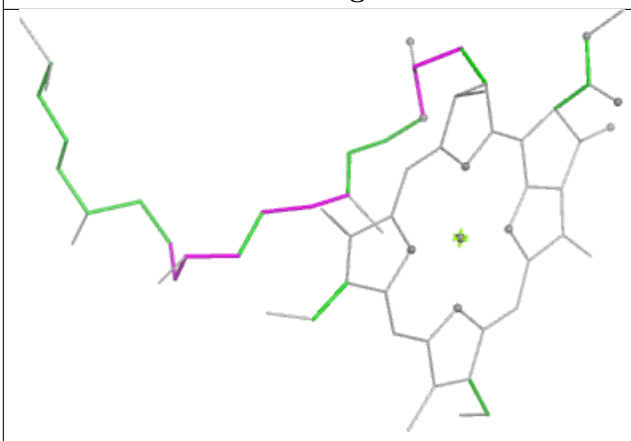


Bond angles



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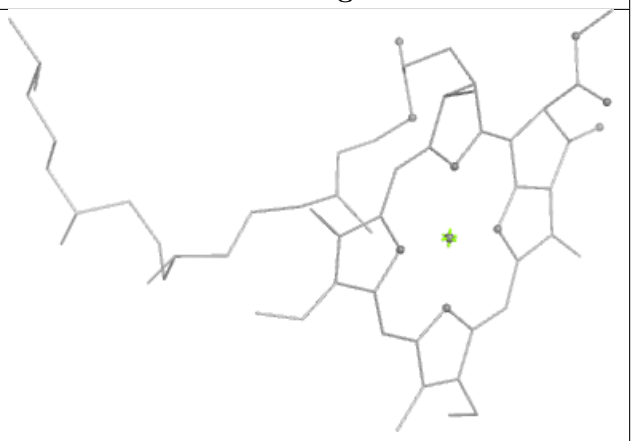
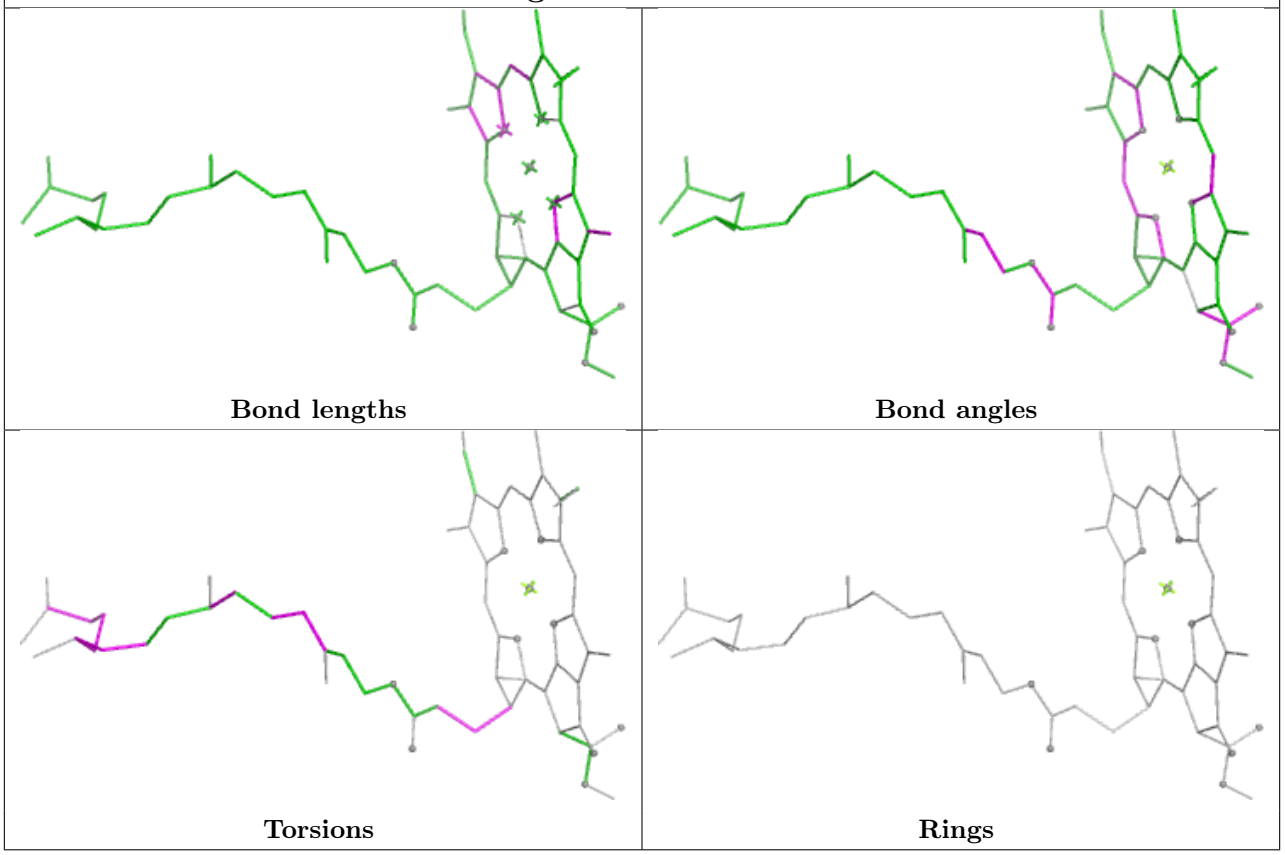
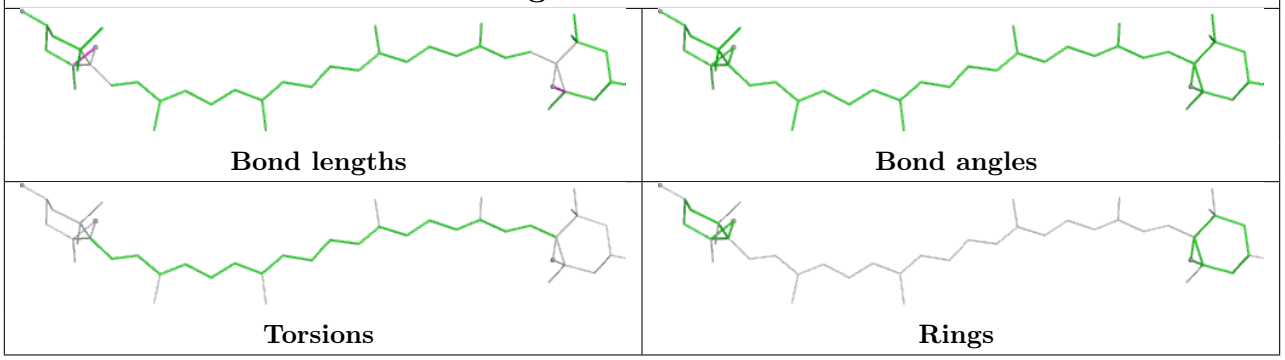


Rings

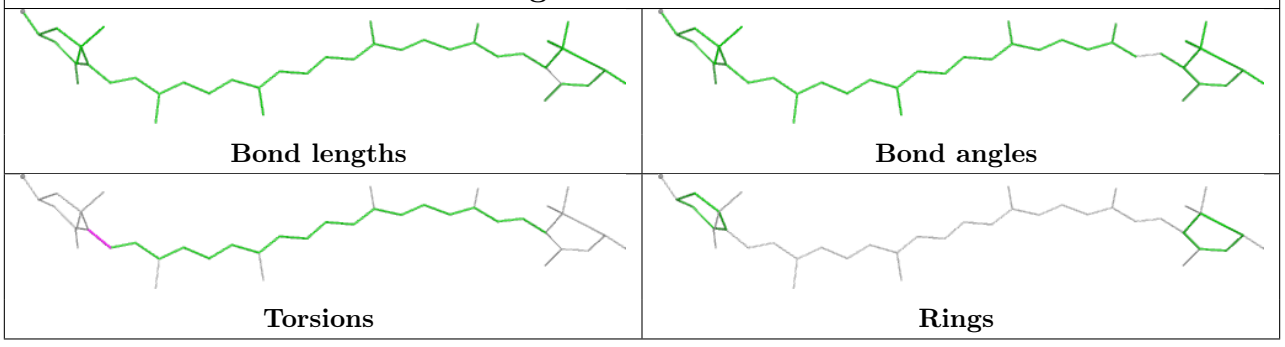
Ligand CLA L 203



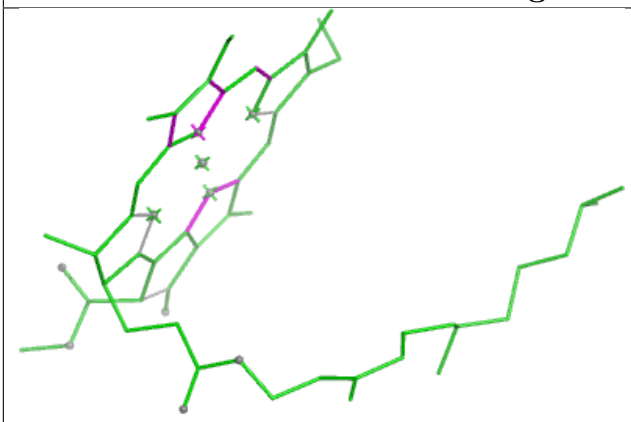
Ligand XAT 1 316



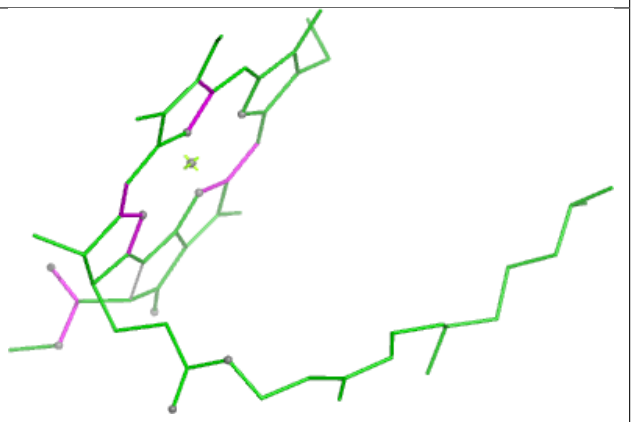
Ligand LUT 3 317



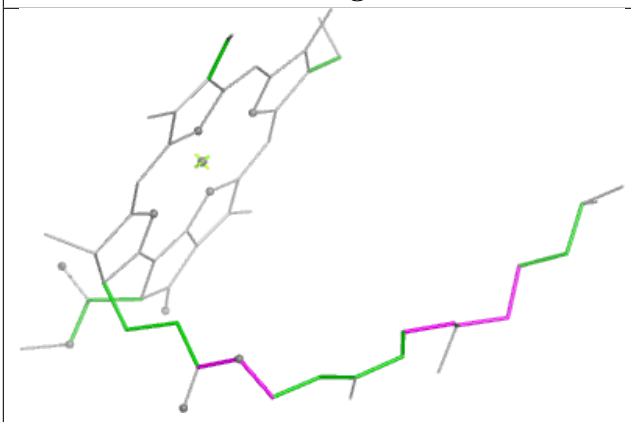
Ligand CLA 8 304



Bond lengths



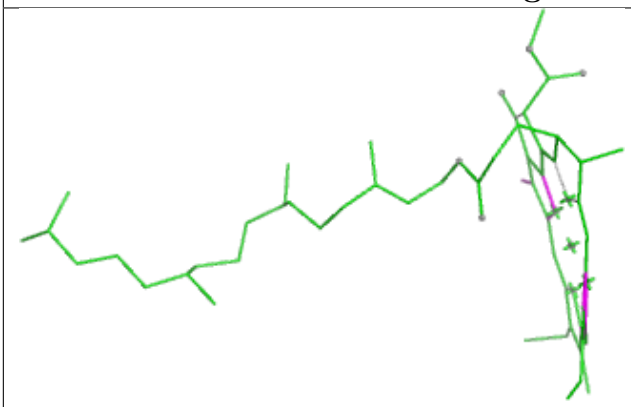
Bond angles



Torsions

Rings

Ligand CLA A 830



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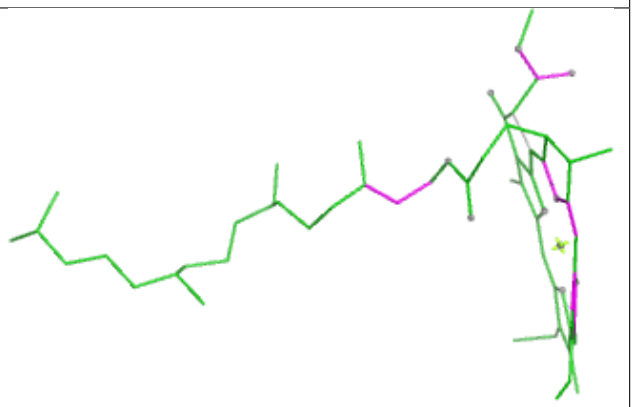
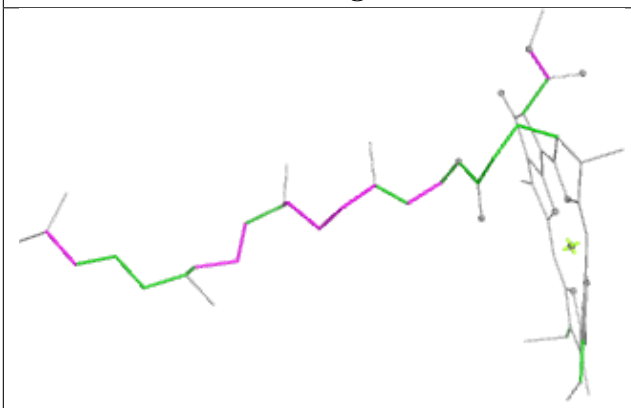
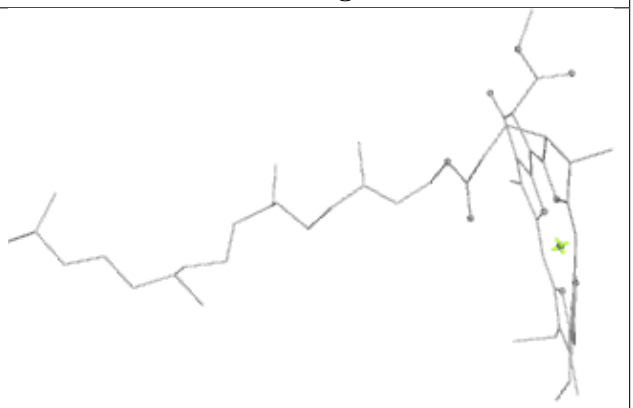


Bond angles

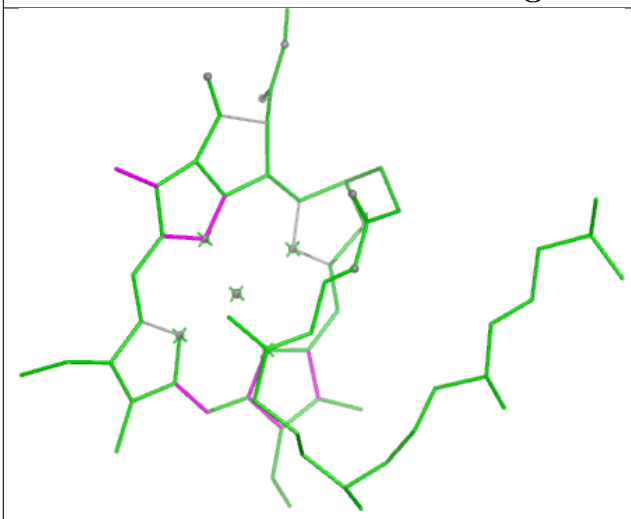


Torsions



Rings

Ligand CLA B 813



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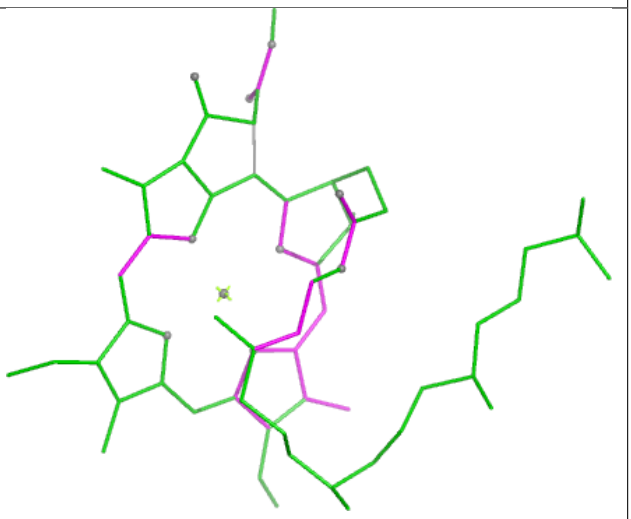
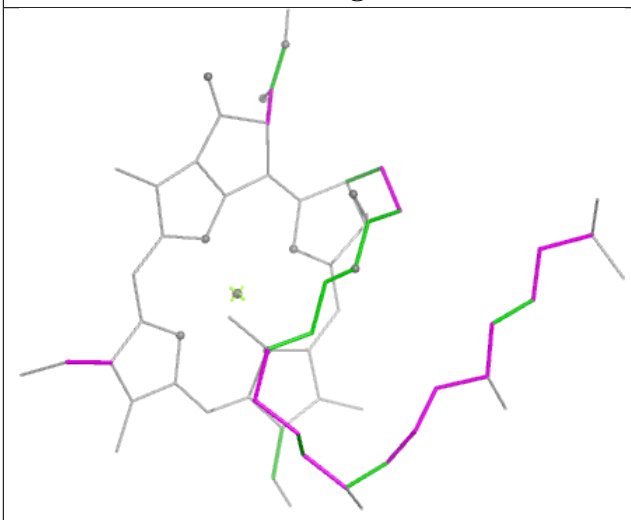


Bond angles



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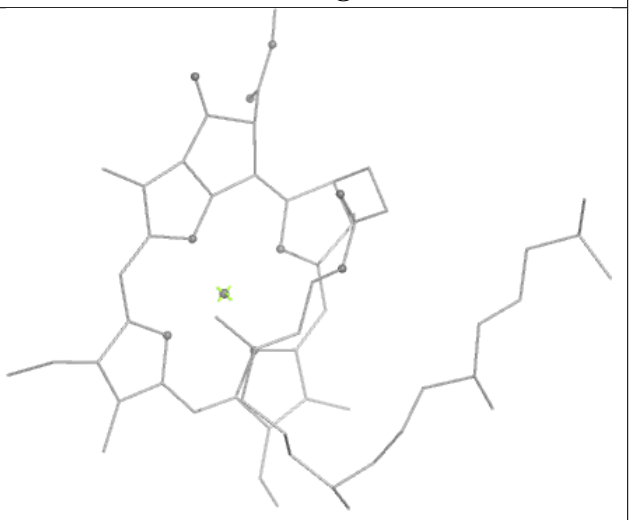
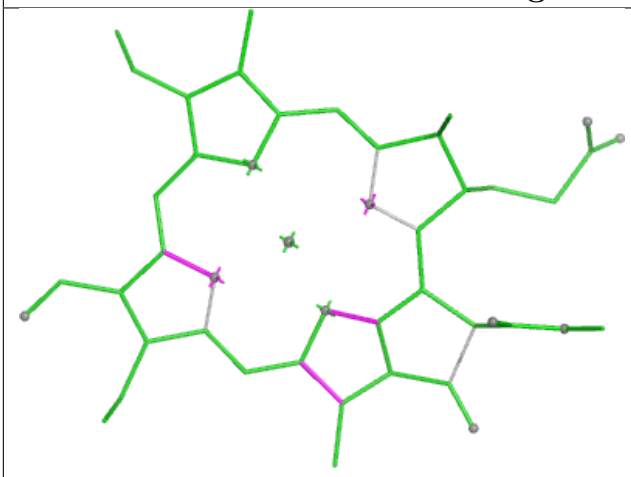
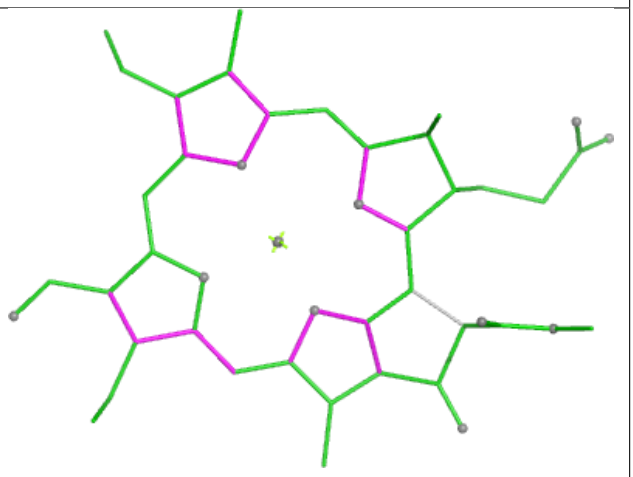


Rings

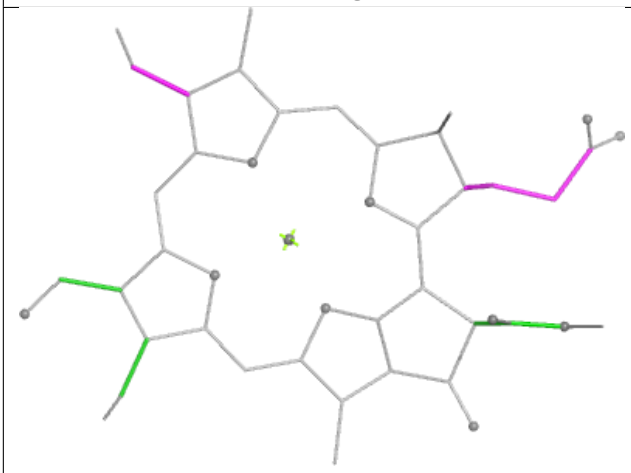
Ligand CHL 5 306



Bond lengths



Bond angles



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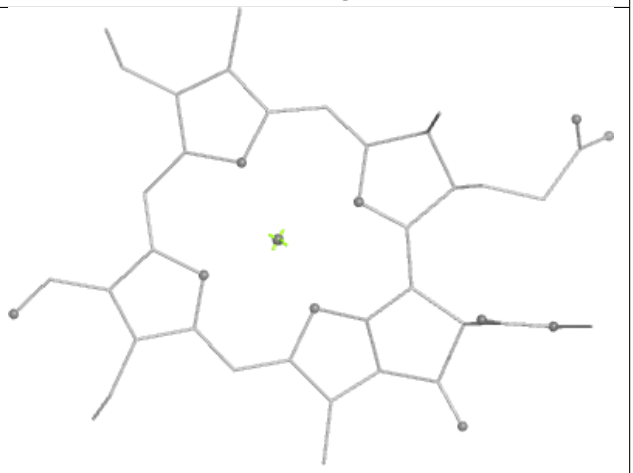
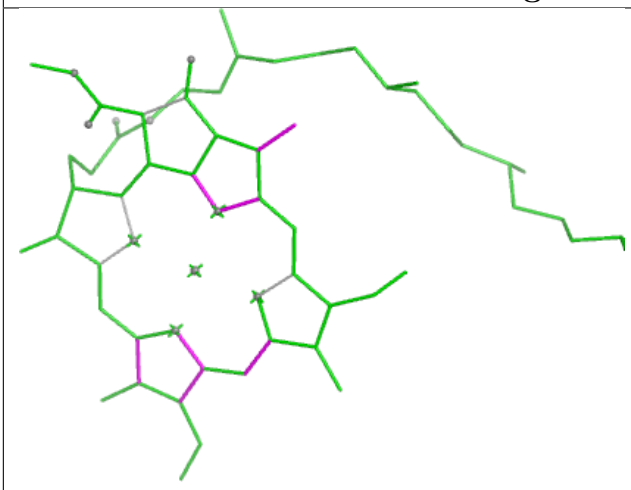


Rings

Ligand CLA A 831



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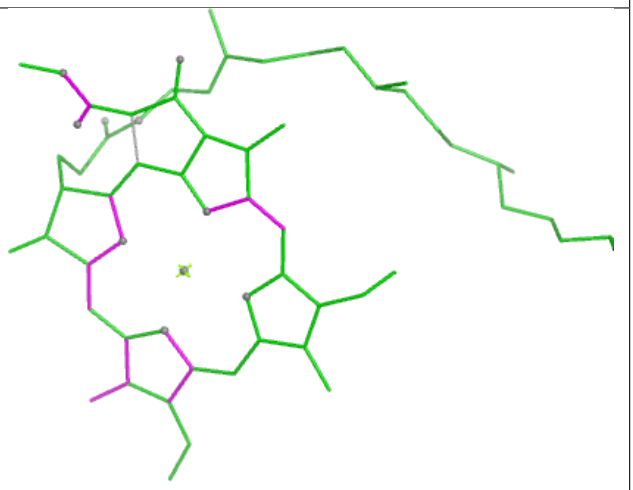
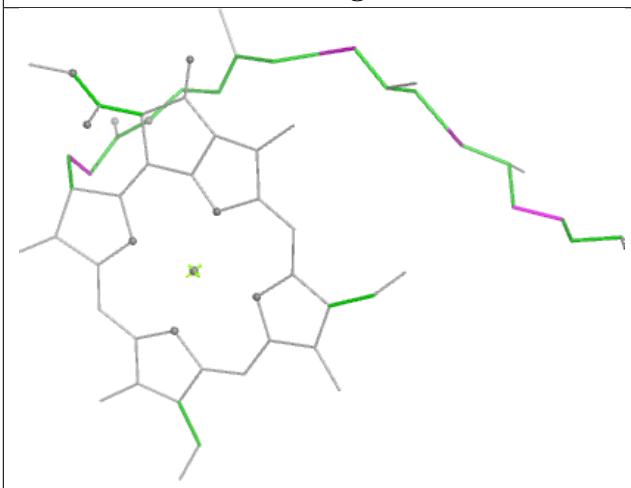


Bond angles



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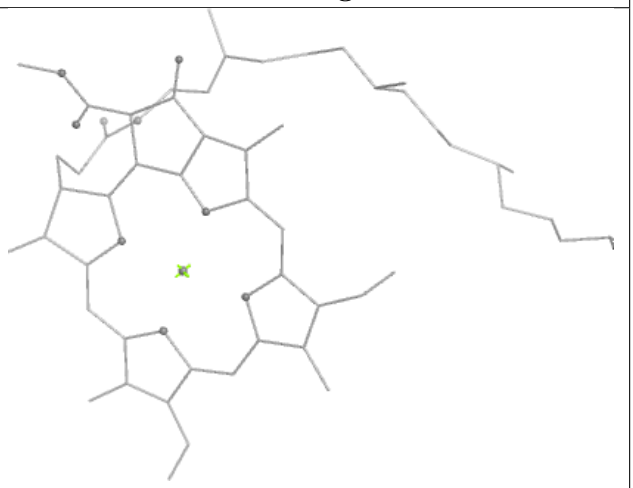
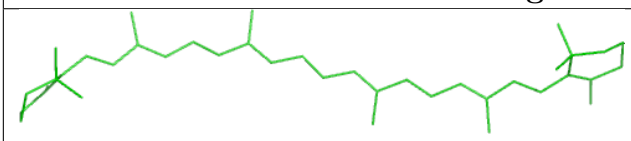


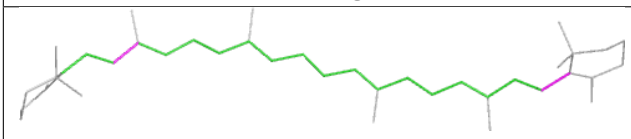
Rings

Ligand BCR 8 317



Bond lengths

Bond angles



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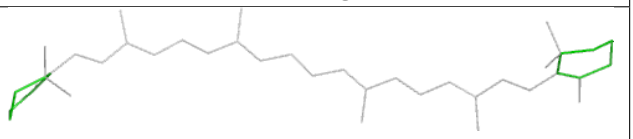
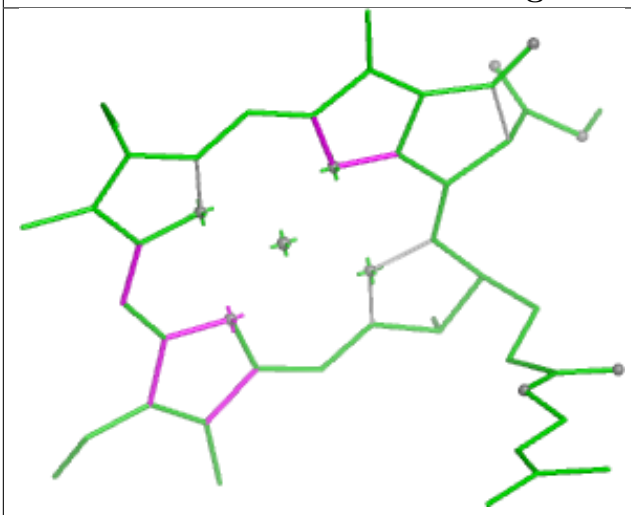
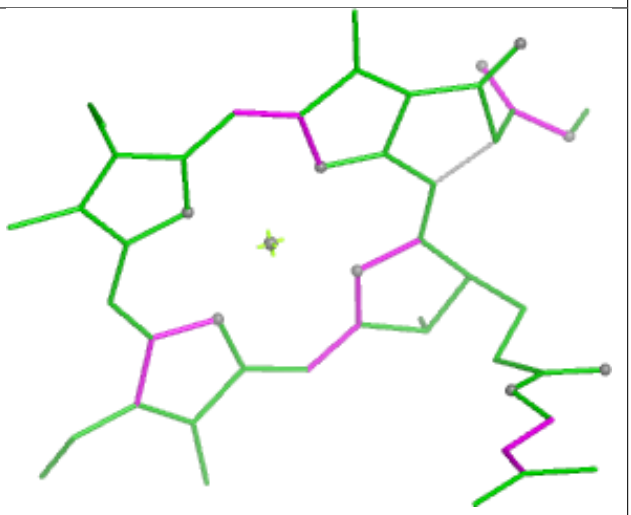


Rings

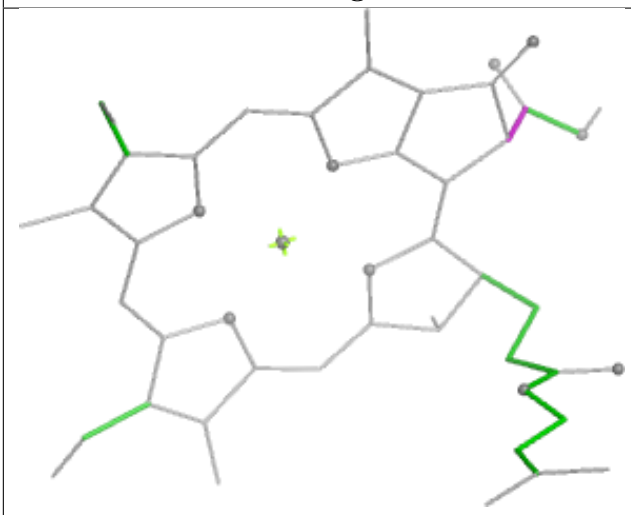
Ligand CLA Z 613



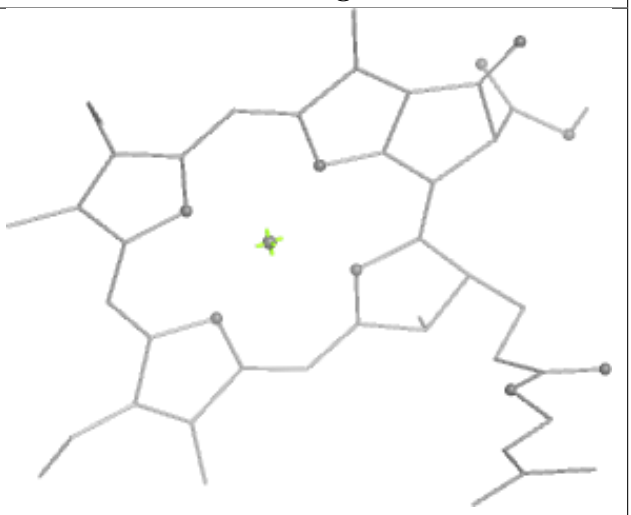
Bond lengths



Bond angles

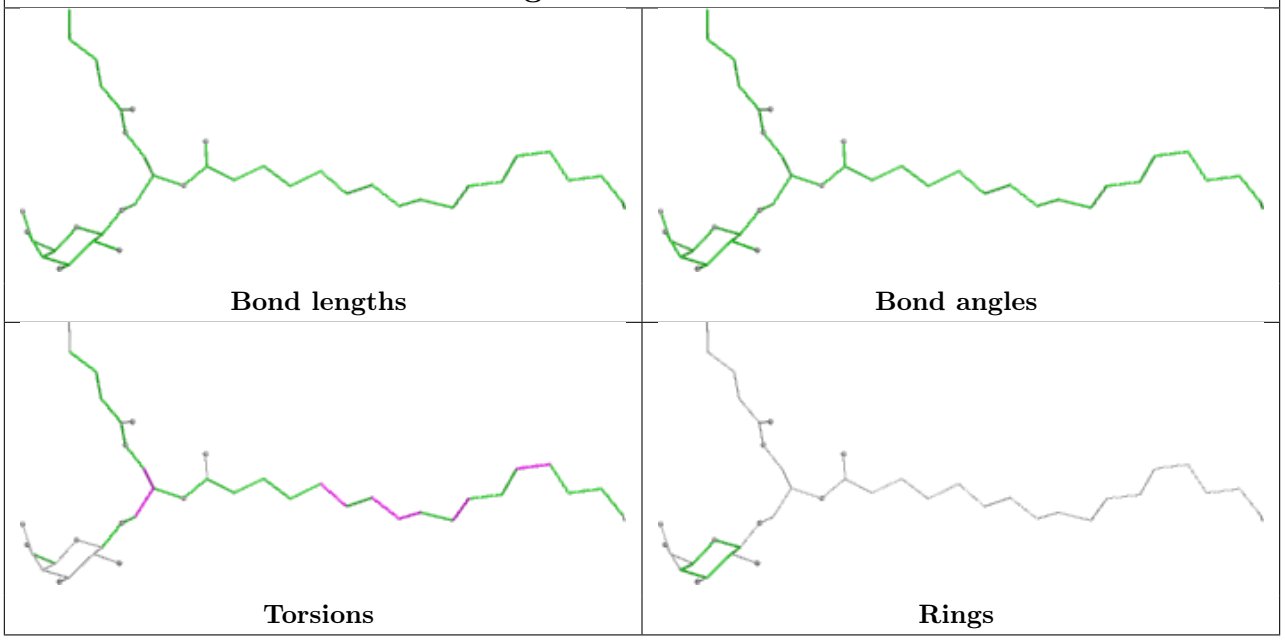


Torsions

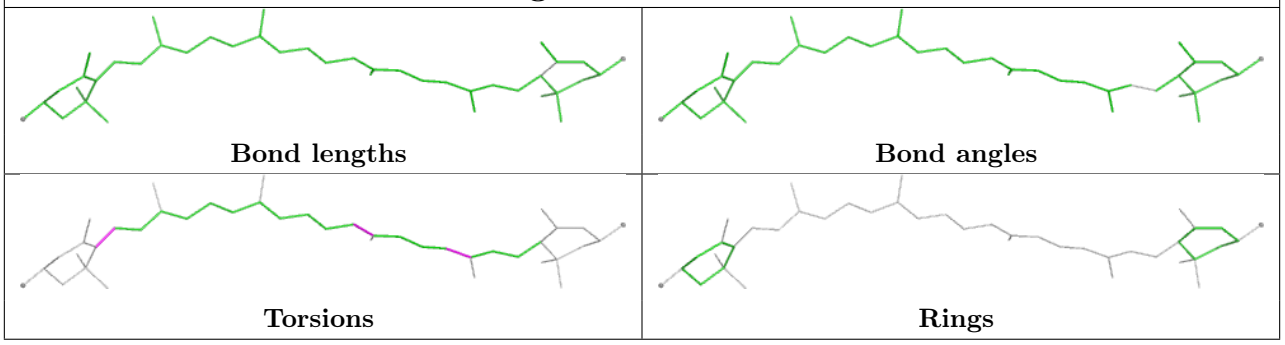


Rings

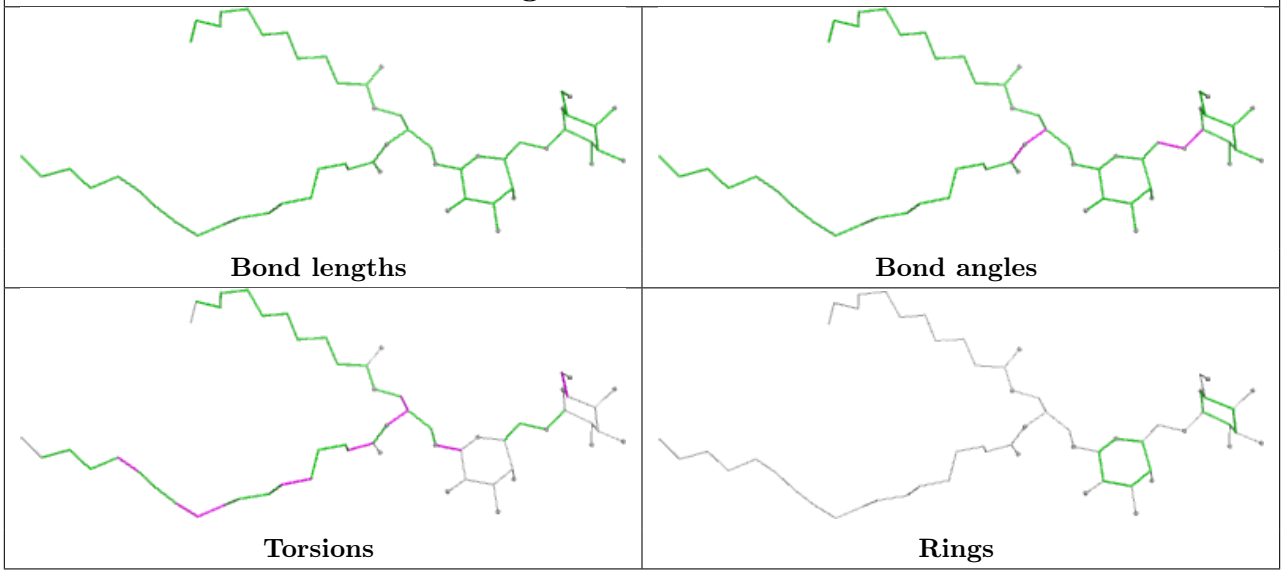
Ligand LMG J 104



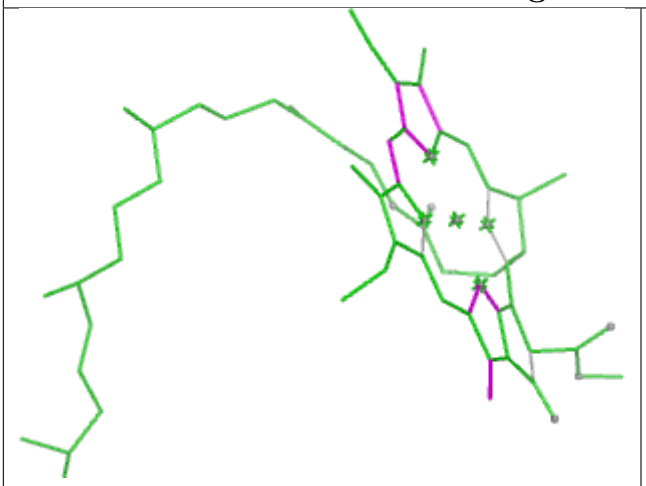
Ligand LUT 1 317



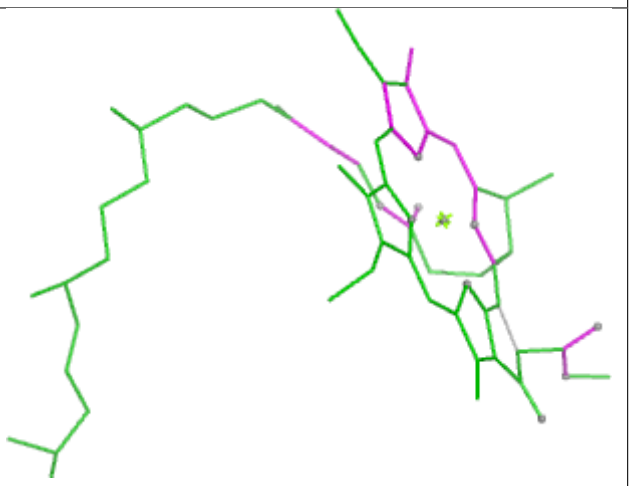
Ligand DGD B 850



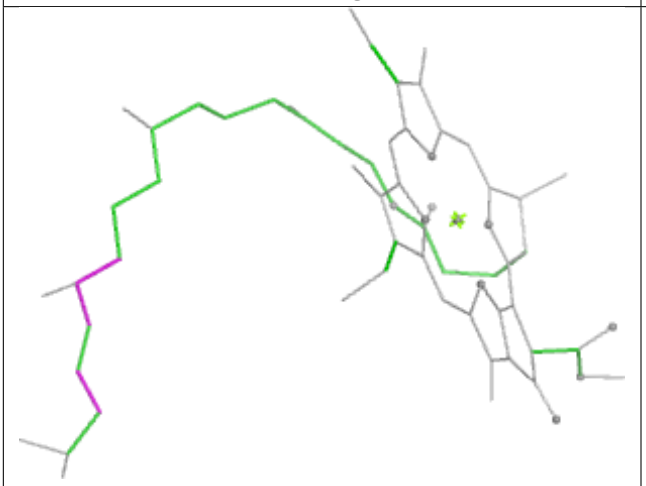
Ligand CLA 3 308



Bond lengths



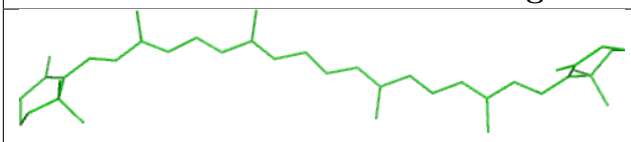
Bond angles



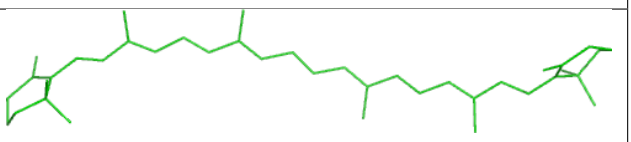
Torsions

Rings

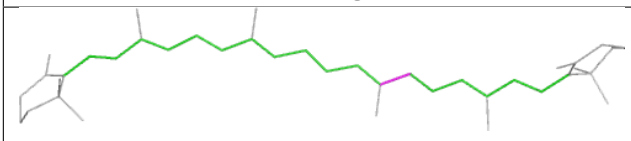
Ligand BCR 6 321



Bond lengths



Bond angles



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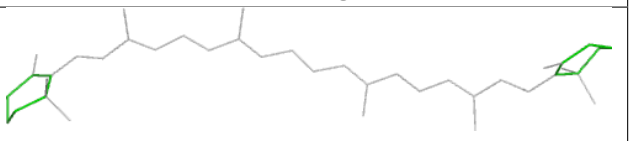
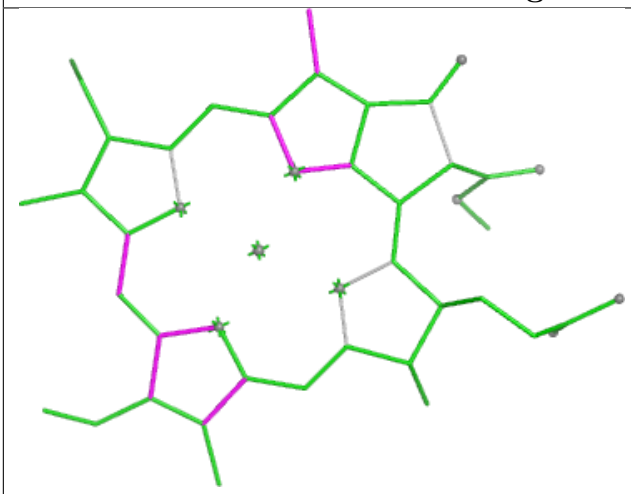


Rings

Ligand CLA Z 611



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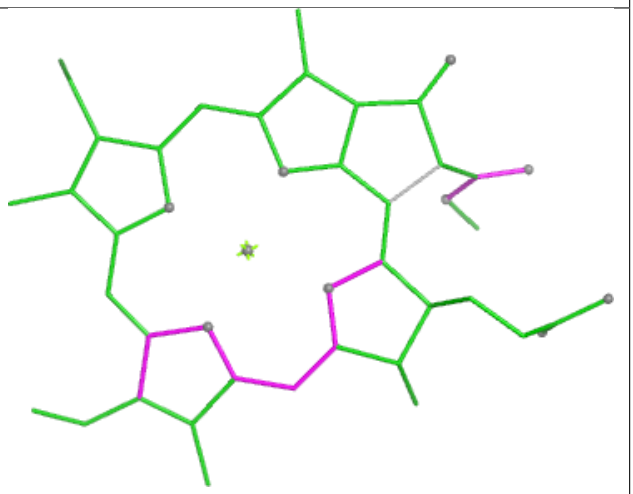
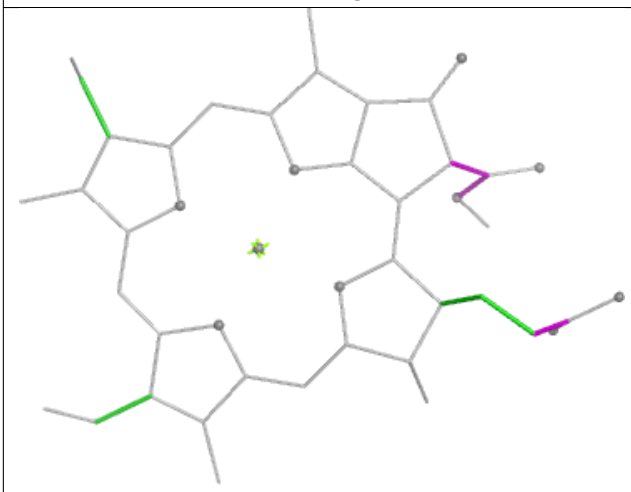


Bond angles



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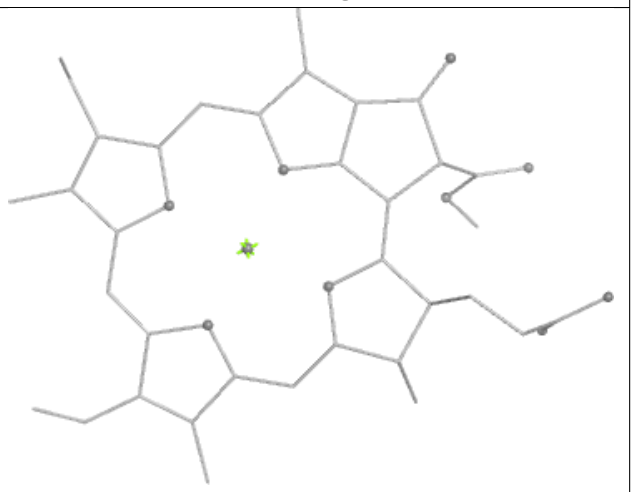
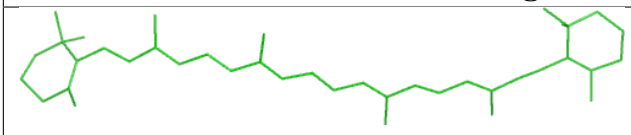
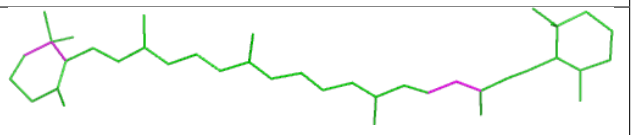


Rings

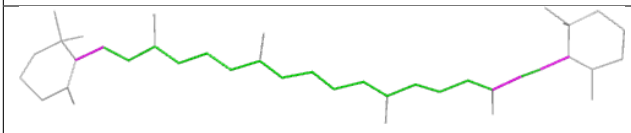
Ligand BCR A 858



Bond lengths



Bond angles



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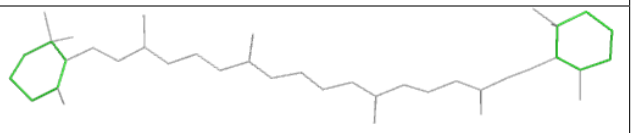
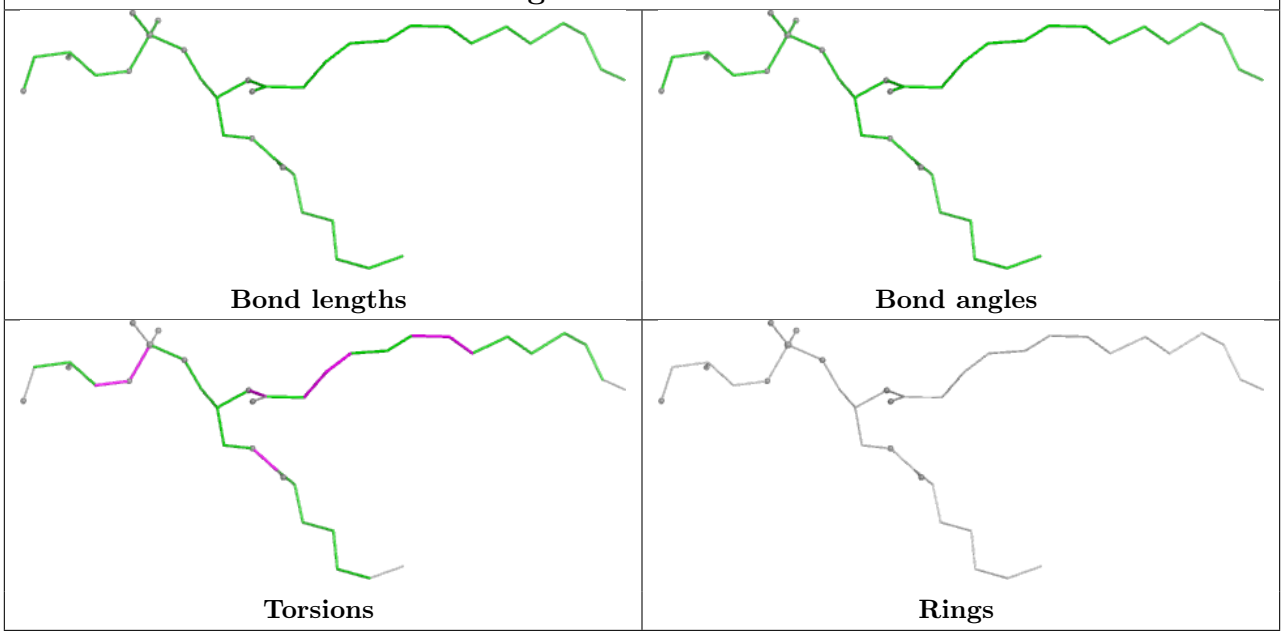
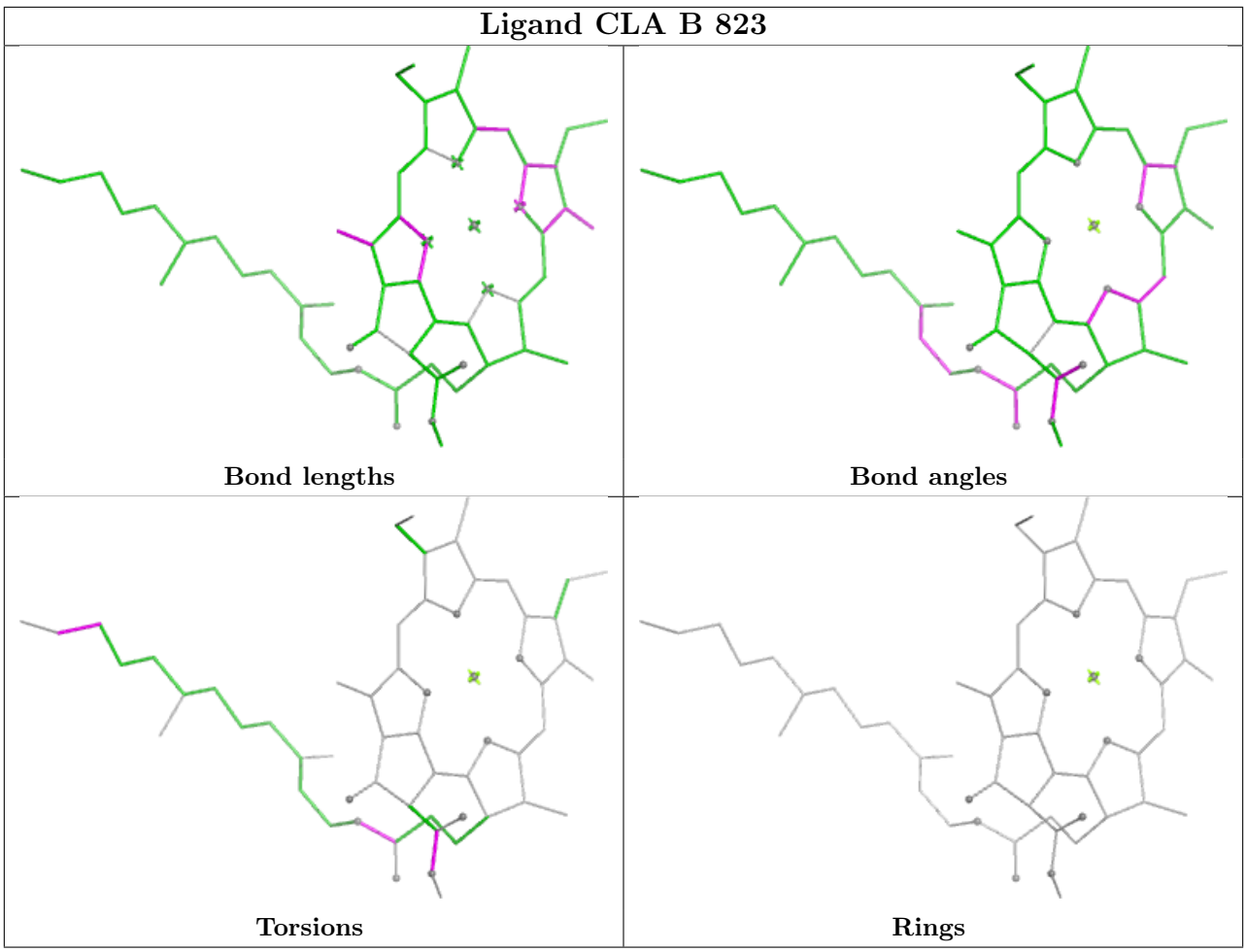


Rings

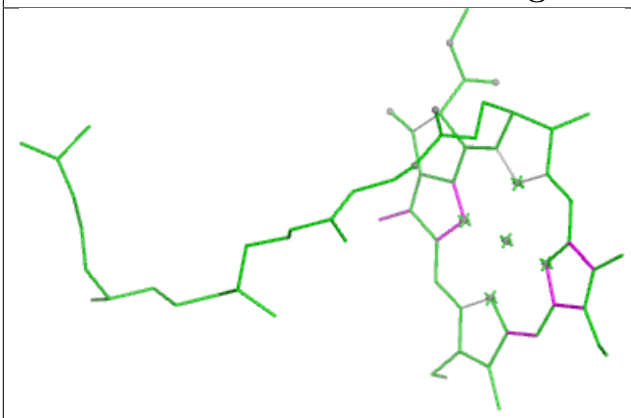
Ligand LHG 5 301



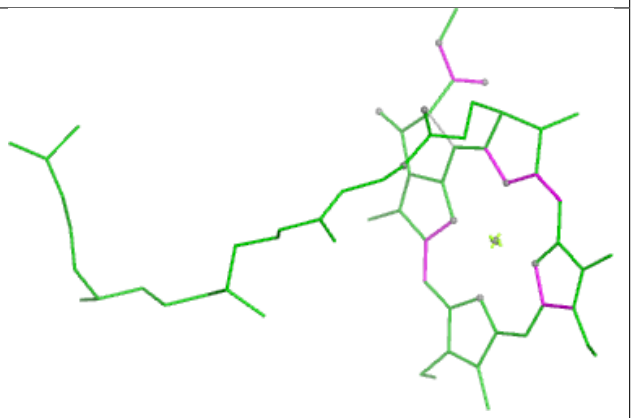
Ligand CLA B 823



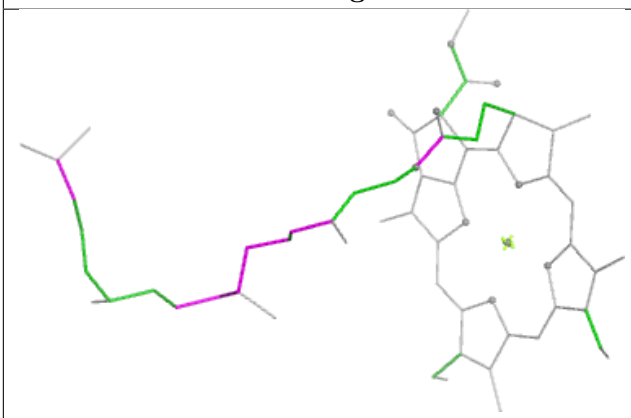
Ligand CLA 5 309



Bond lengths



Bond angles



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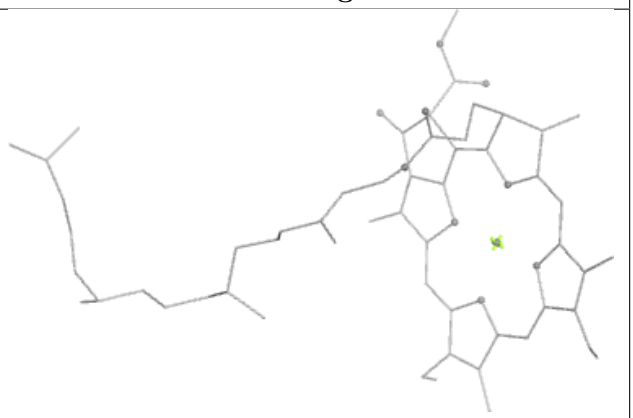
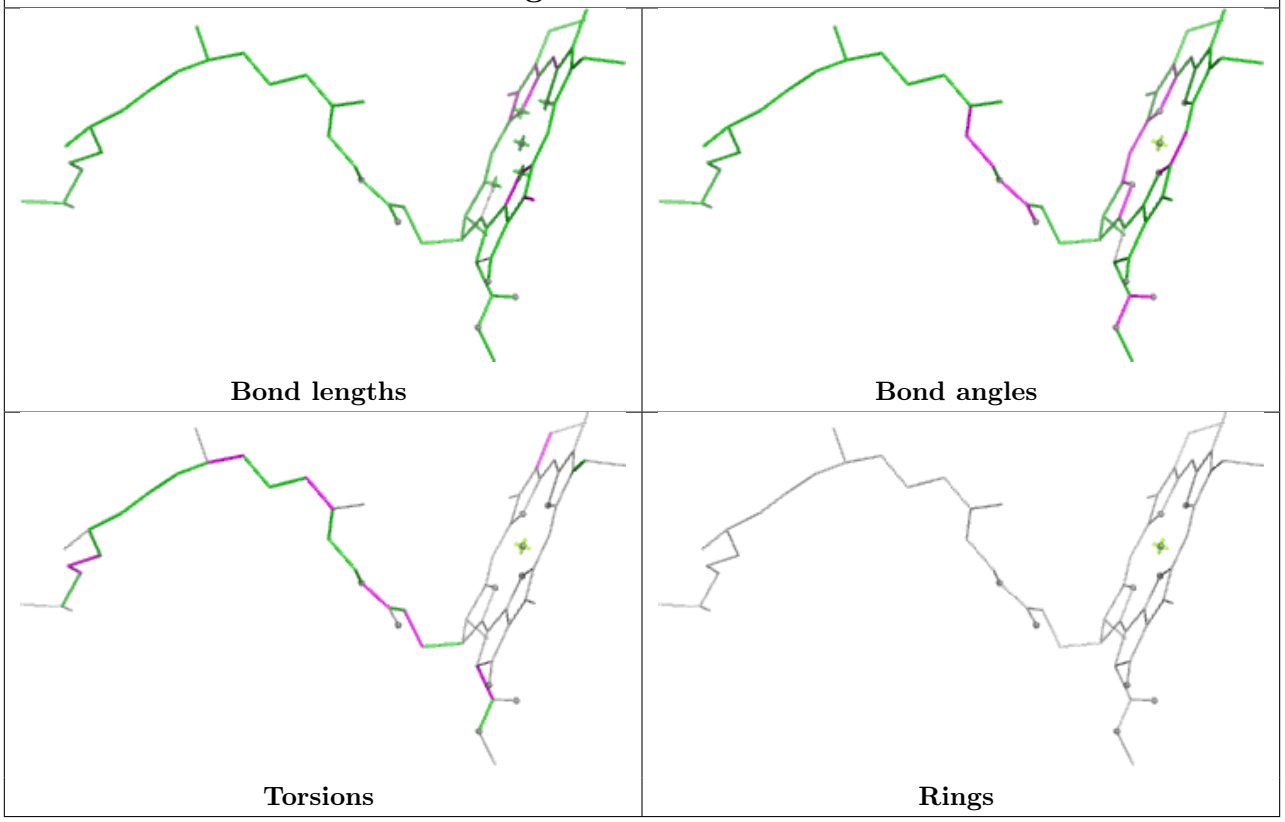
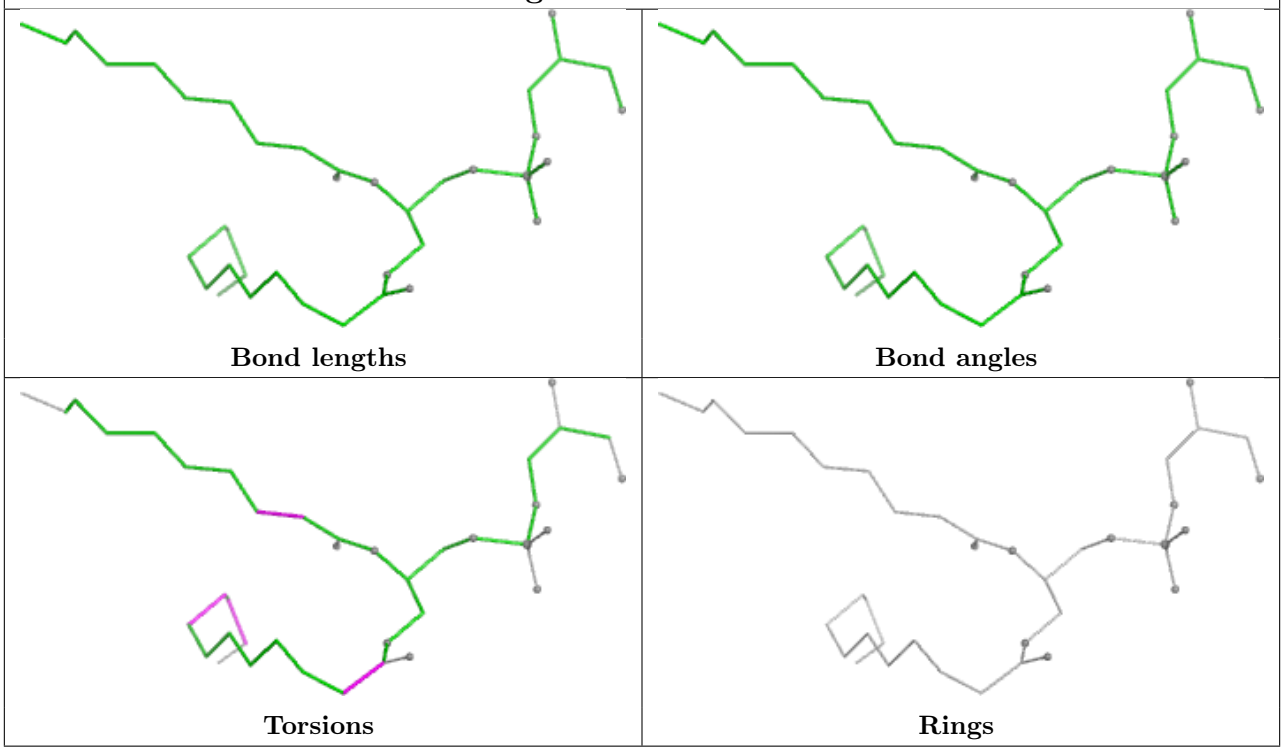


Rings

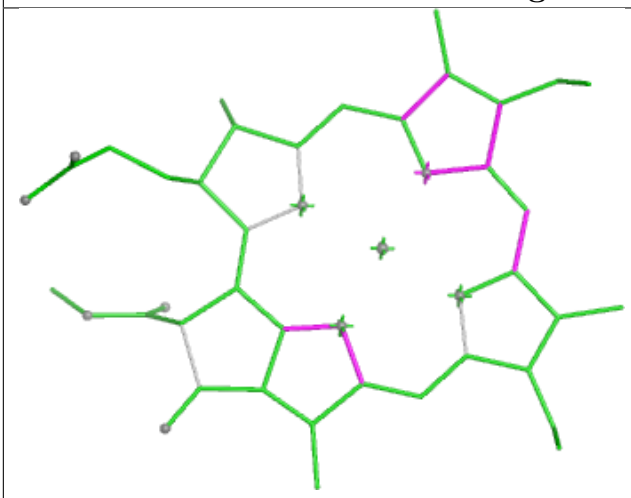
Ligand CLA B 840



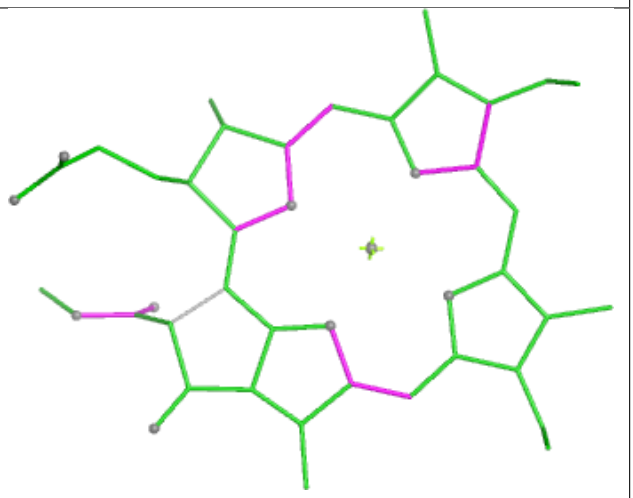
Ligand LHG Z 618



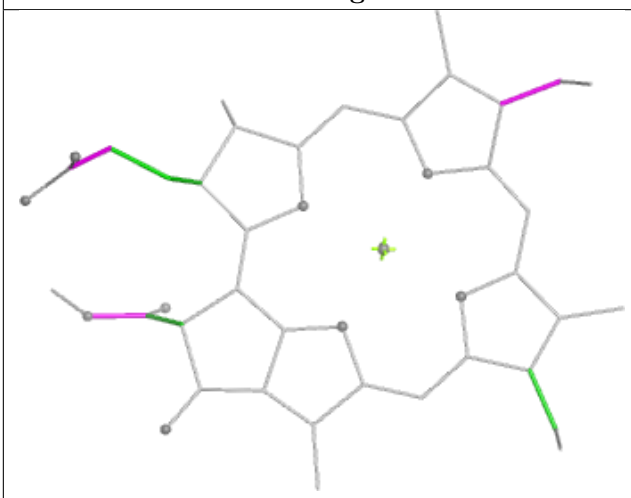
Ligand CLA 3 312



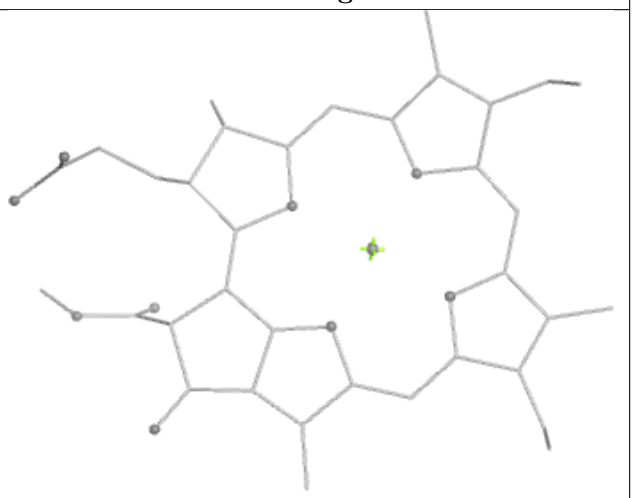
Bond lengths



Bond angles

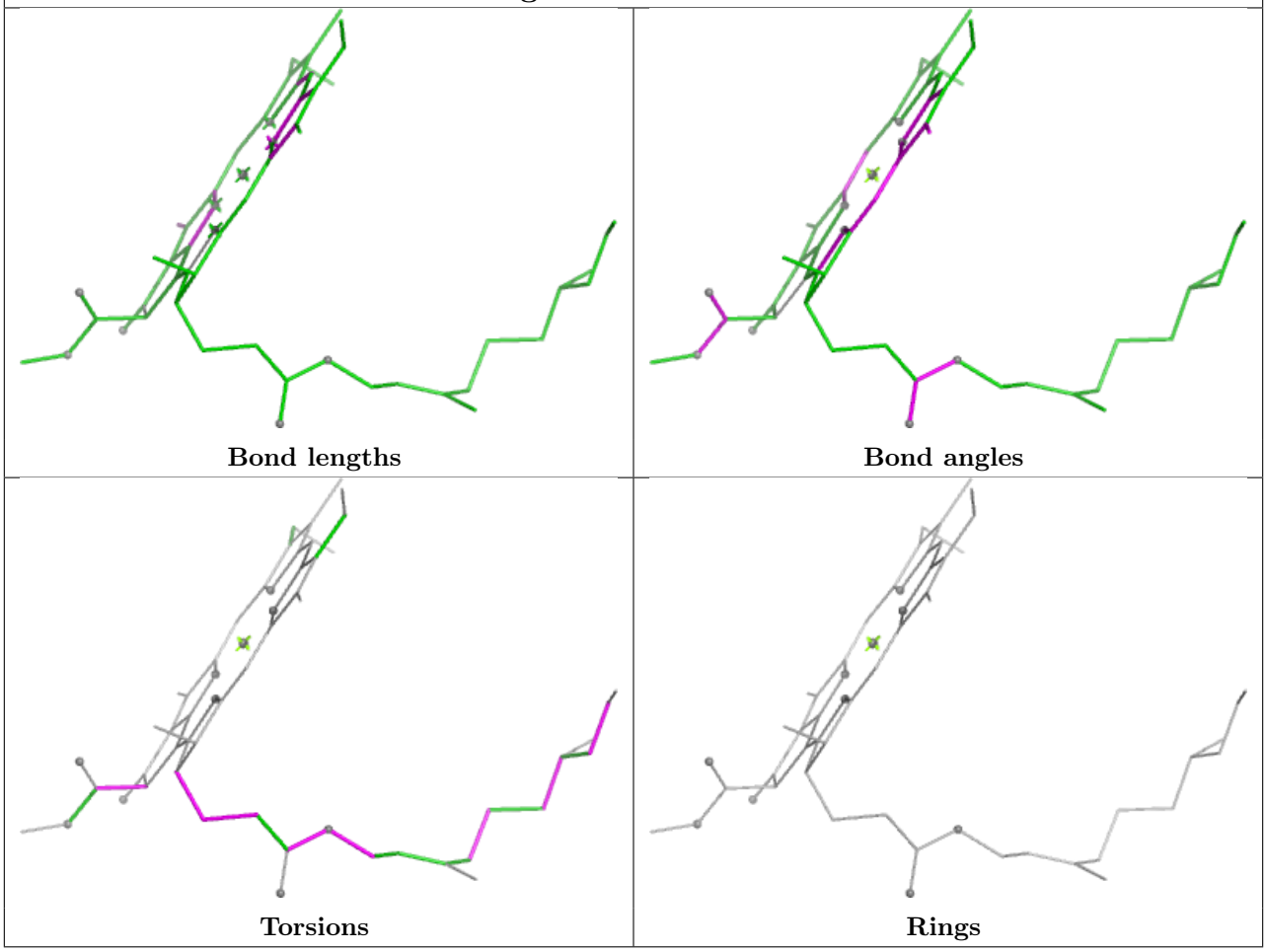


Torsions

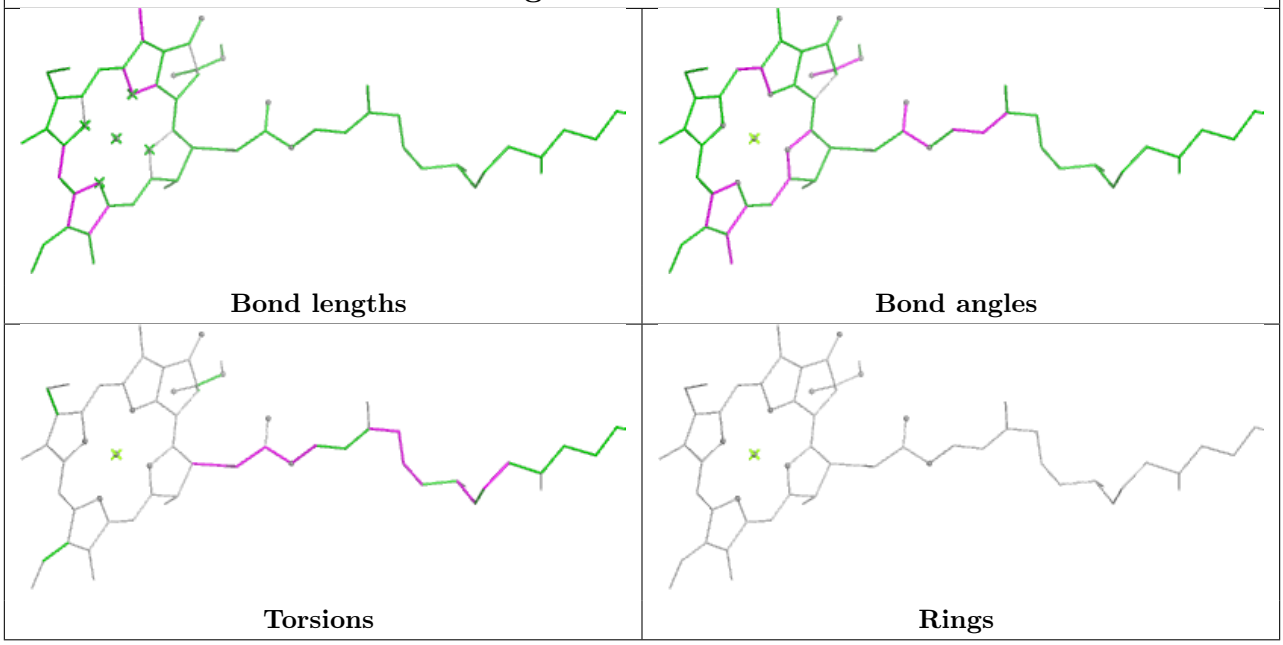


Rings

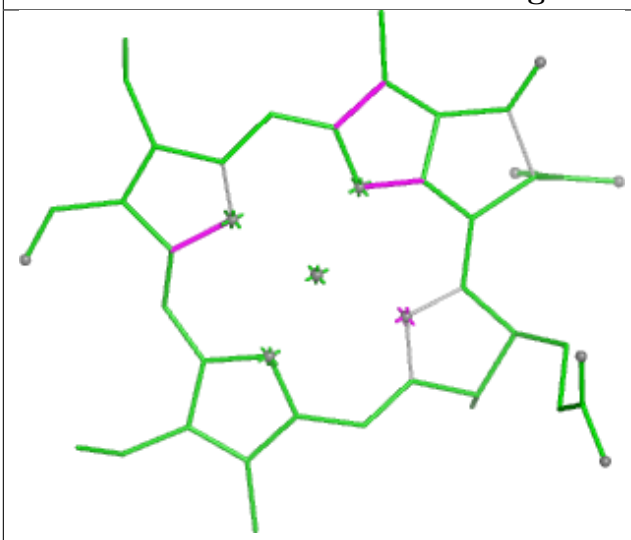
Ligand CLA Z 604



Ligand CLA A 811



Ligand CHL 4 615



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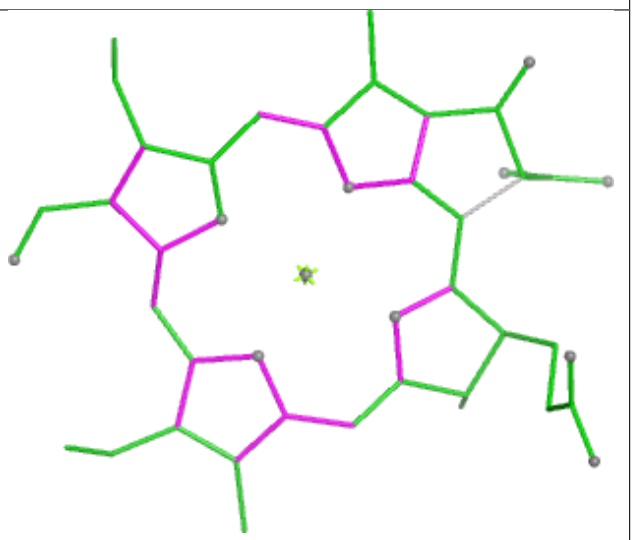
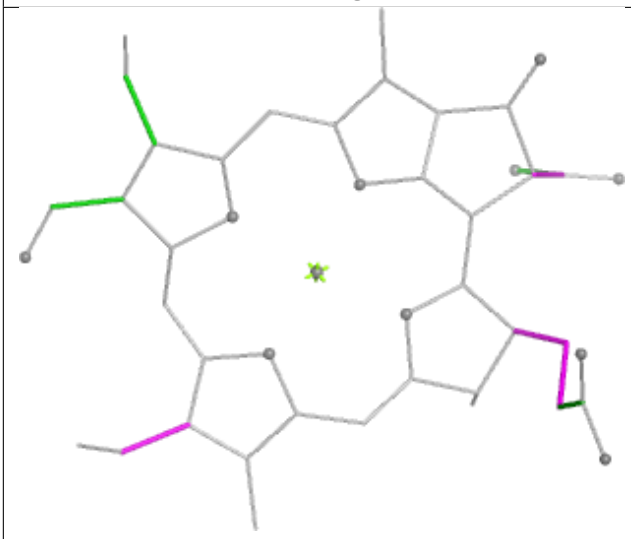
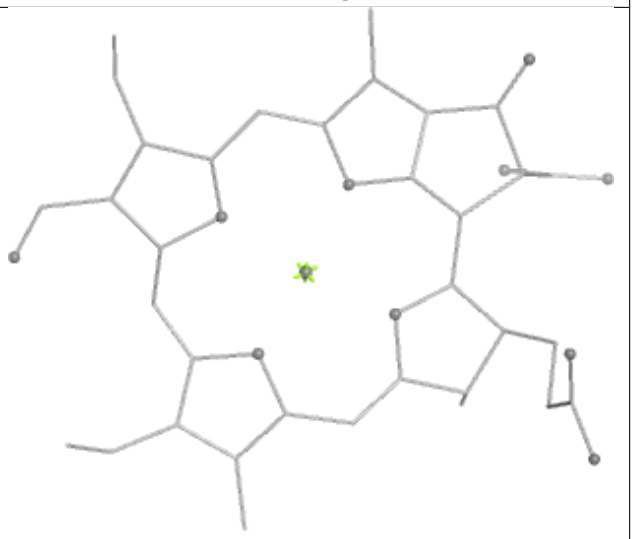


Bond angles

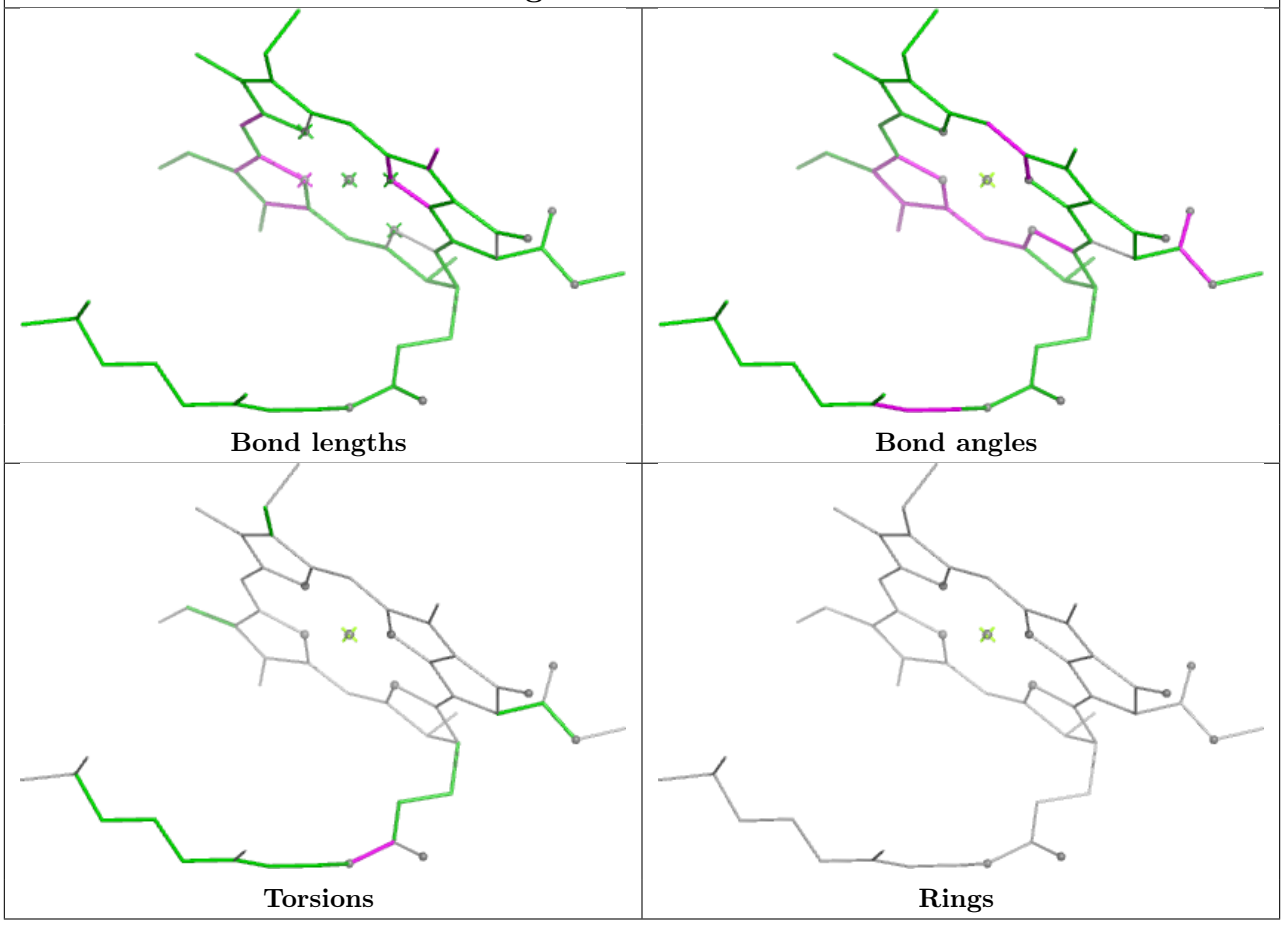


Torsions



Rings

Ligand CLA B 832



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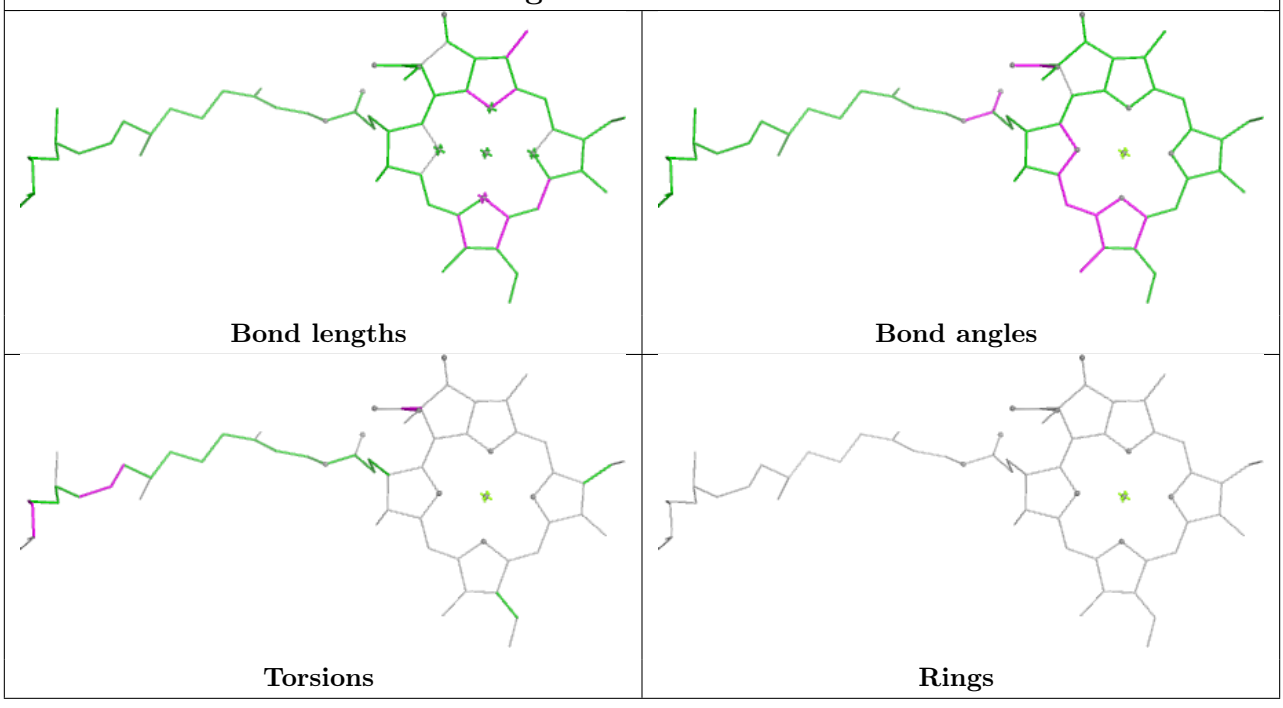

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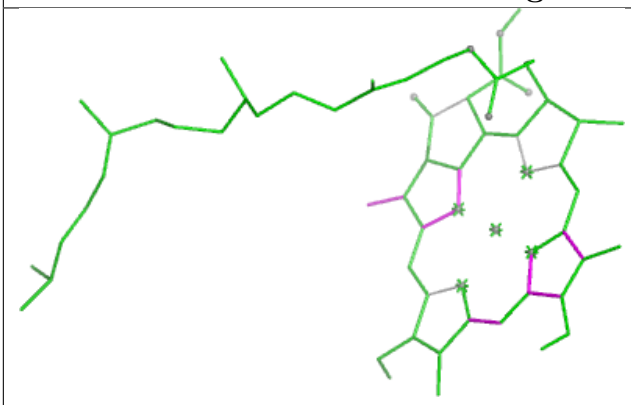

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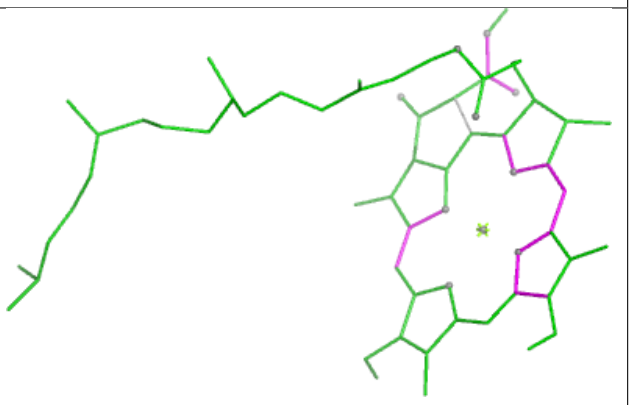
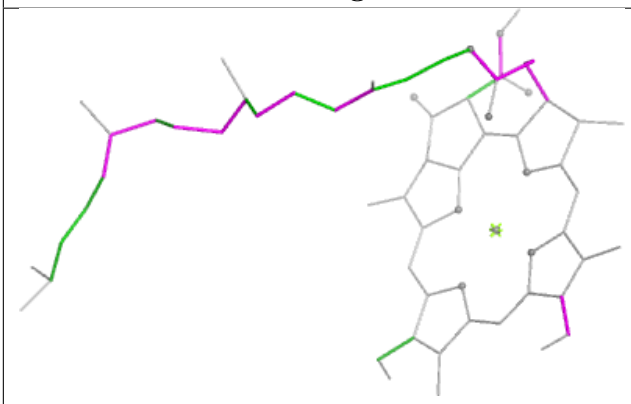


Bond angles



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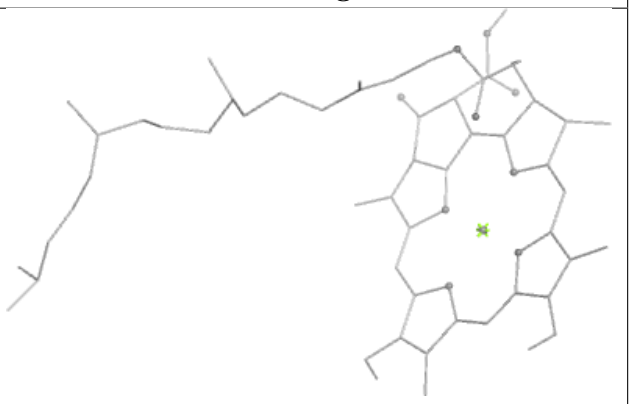
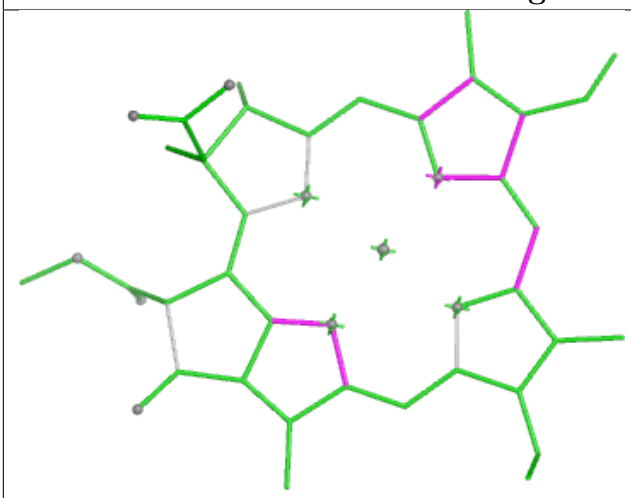


Rings

Ligand CLA 5 314



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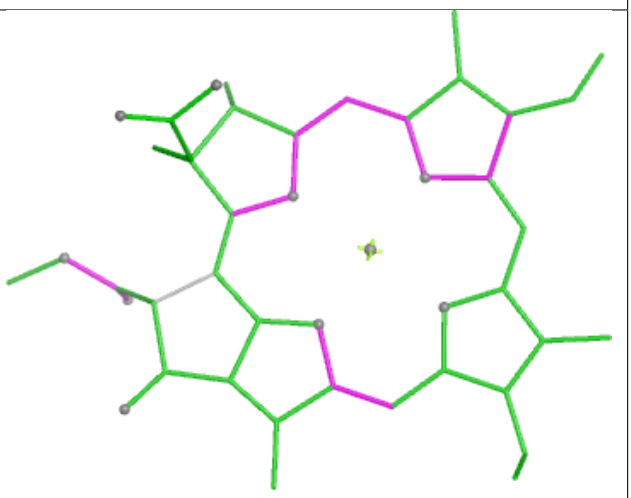
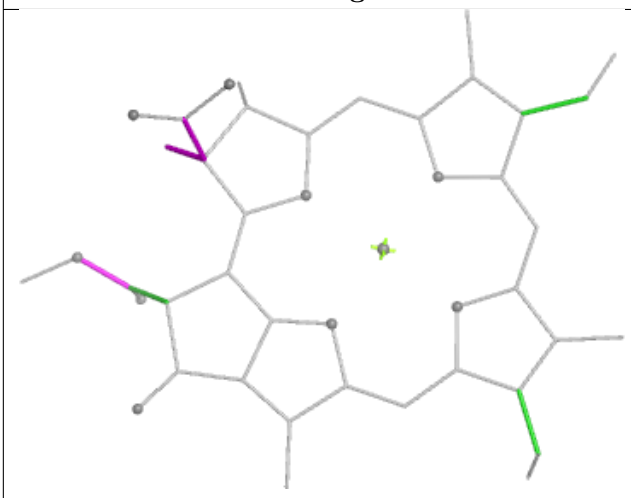


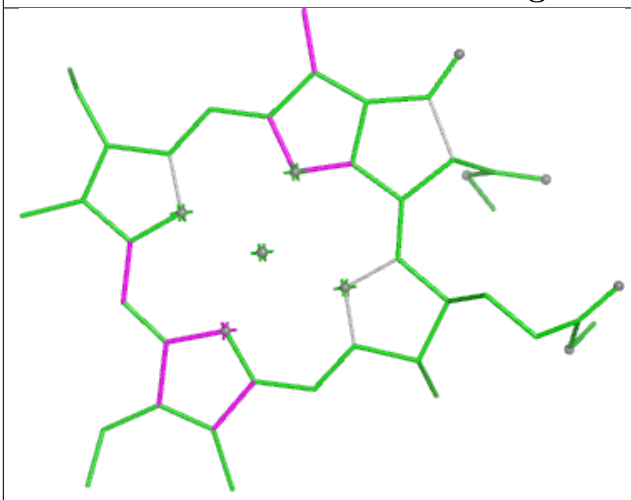
Bond angles



Torsions

Rings

Ligand CLA 3 310



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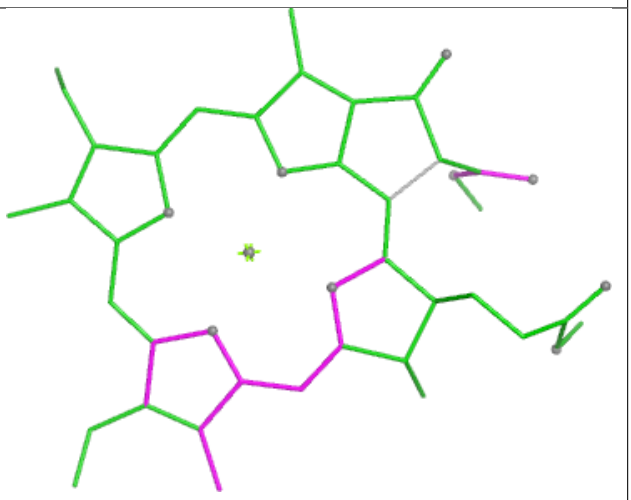
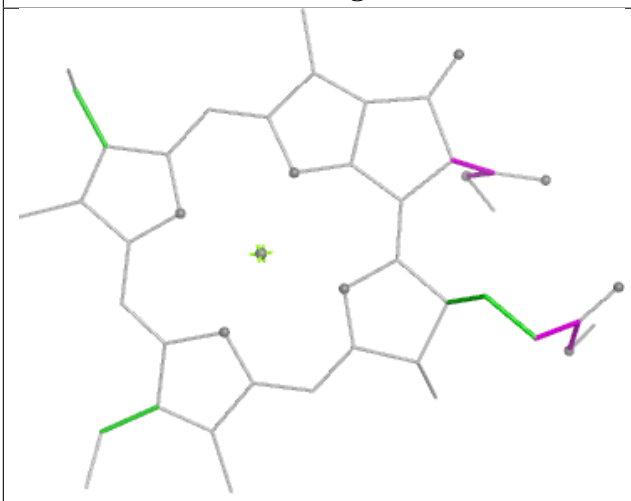


Bond angles



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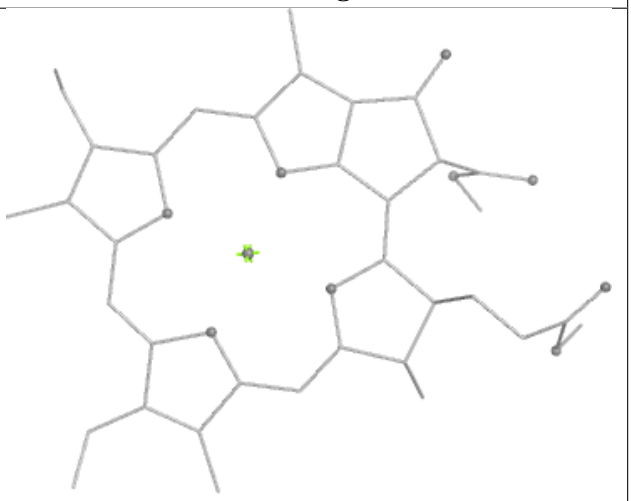
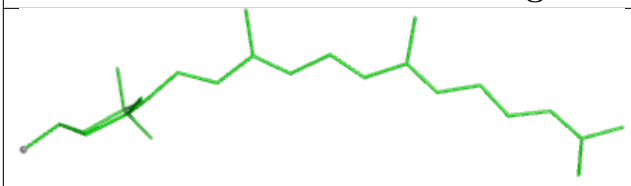


Rings

Ligand LUT Z 617



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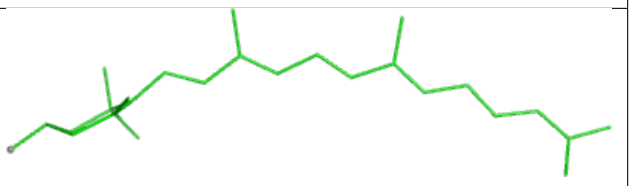
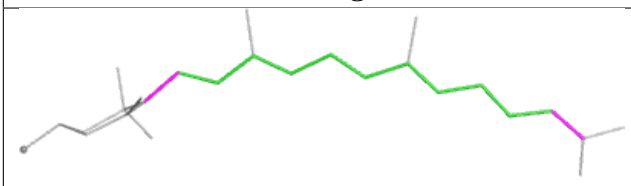


Bond angles



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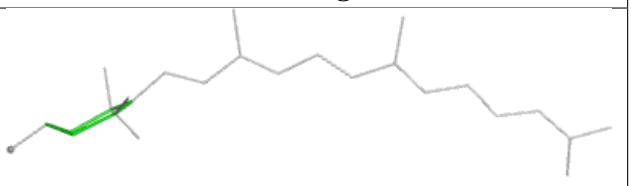
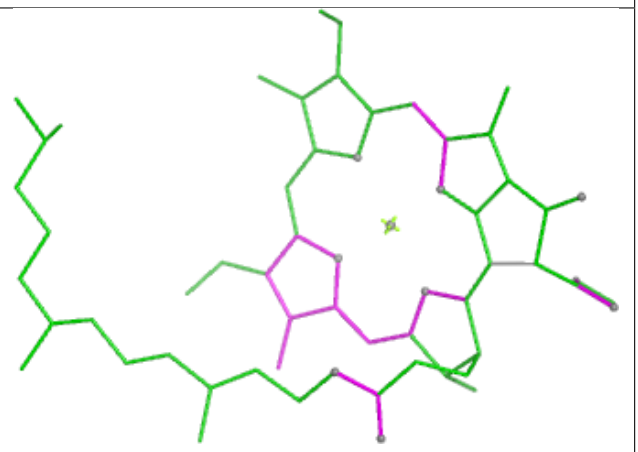


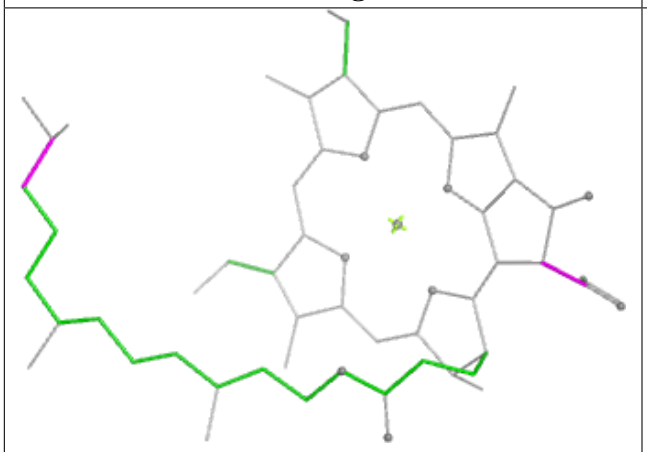
Rings

Ligand CLA 3 301

Bond lengths



Bond angles

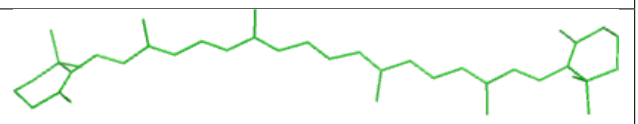


Torsions

Rings

Ligand BCR A 849

Bond lengths

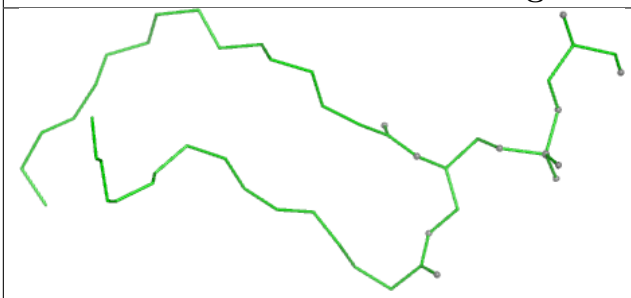


Bond angles

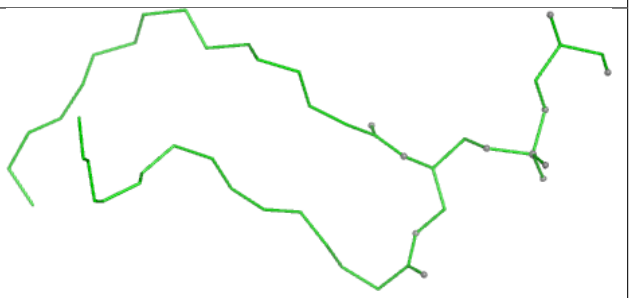
Torsions

Rings

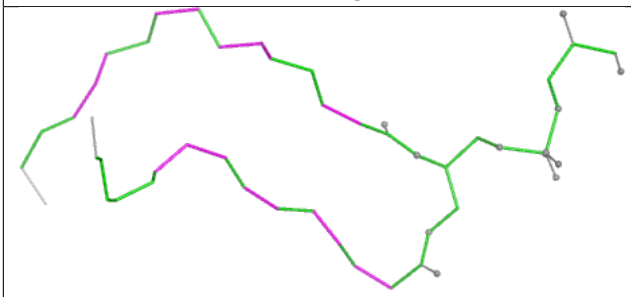
Ligand LHG 4 619



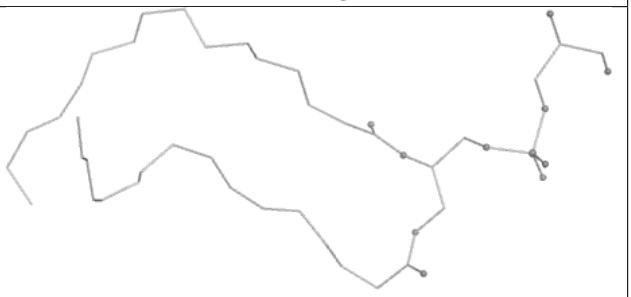
Bond lengths



Bond angles

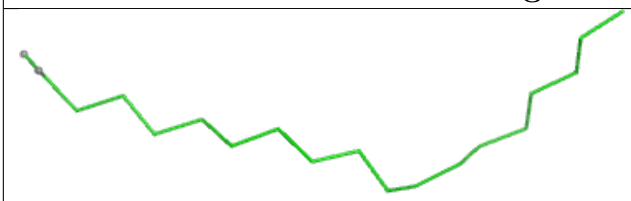


Torsions



Rings

Ligand LMG 6 326



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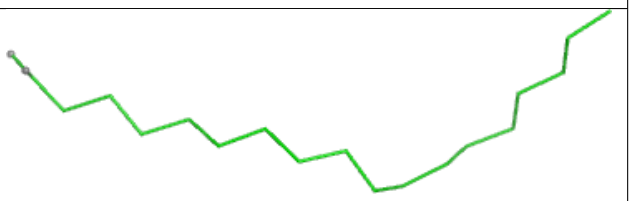

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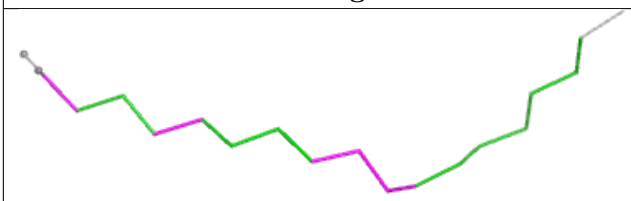

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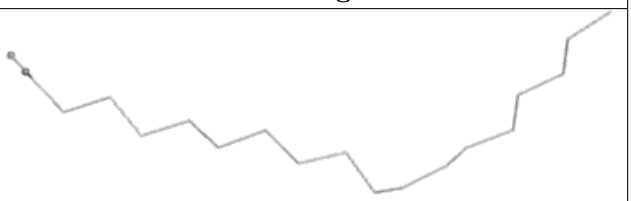
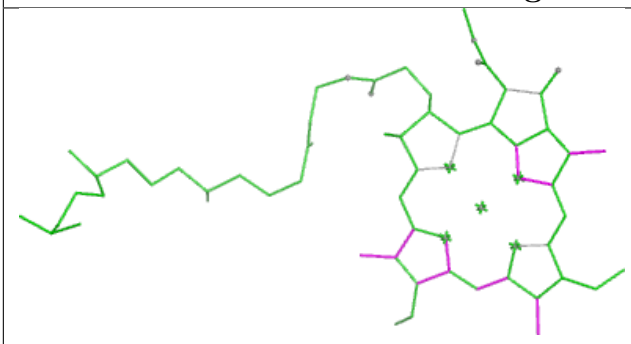


Rings

Ligand CLA B 804



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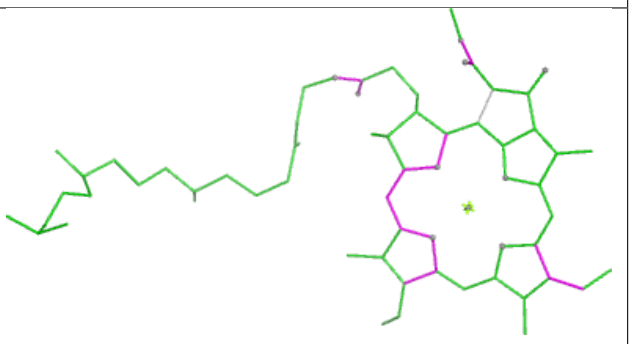

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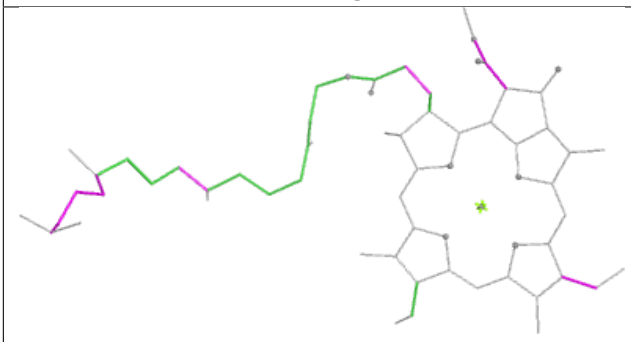

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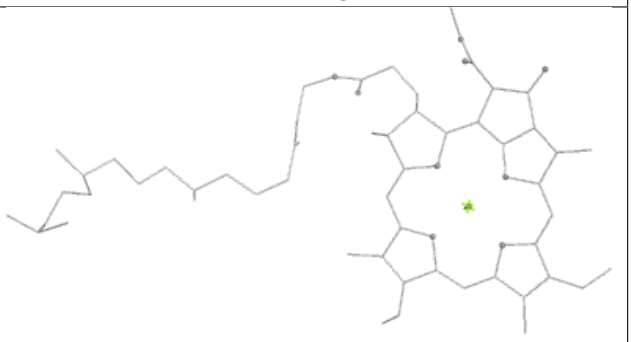
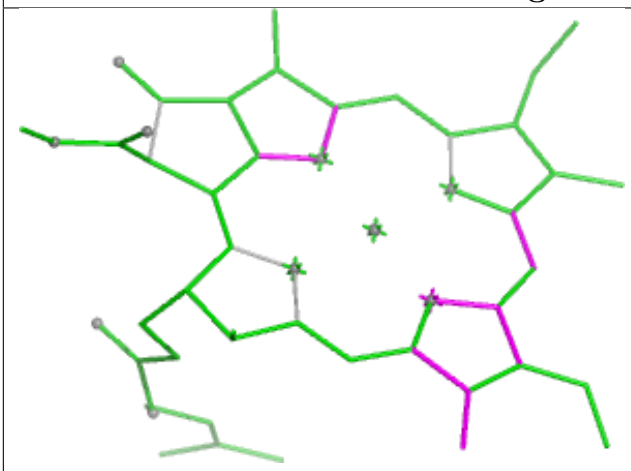


Rings

Ligand CLA 4 604



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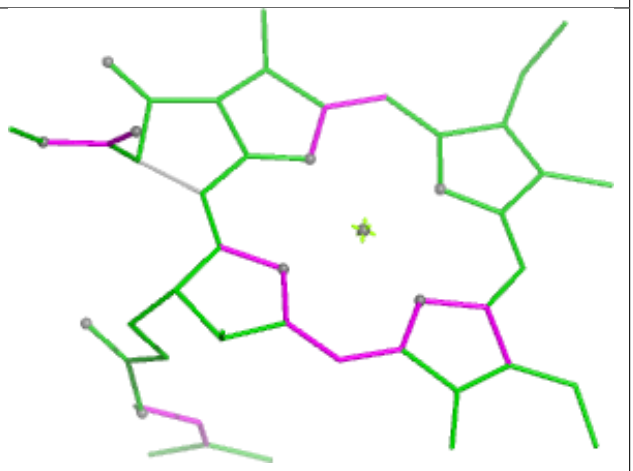
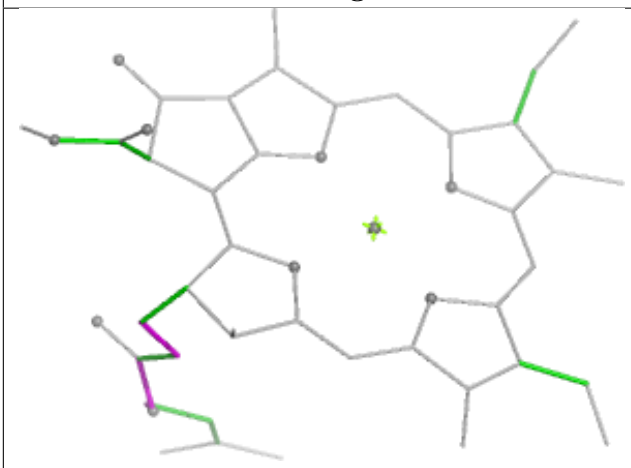


Bond angles



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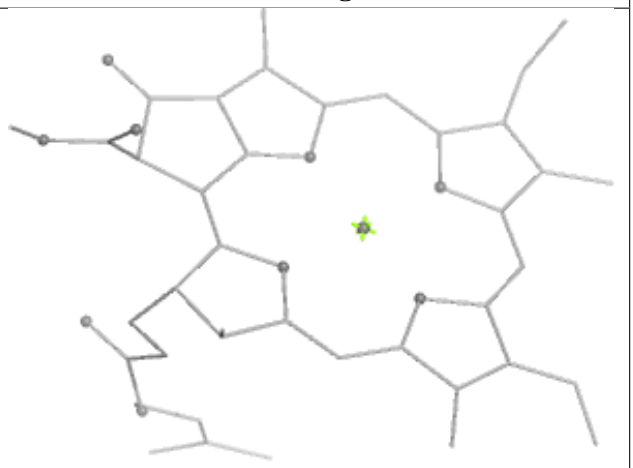
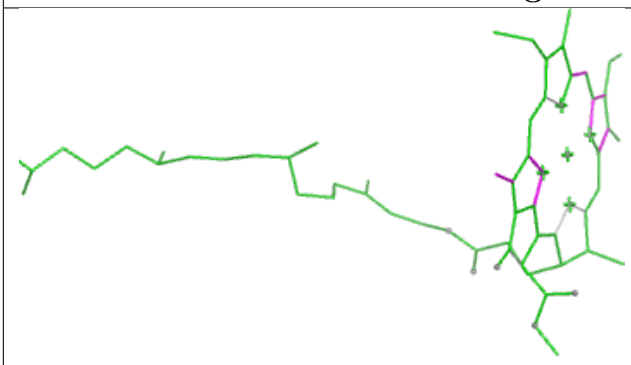


Rings

Ligand CLA B 829



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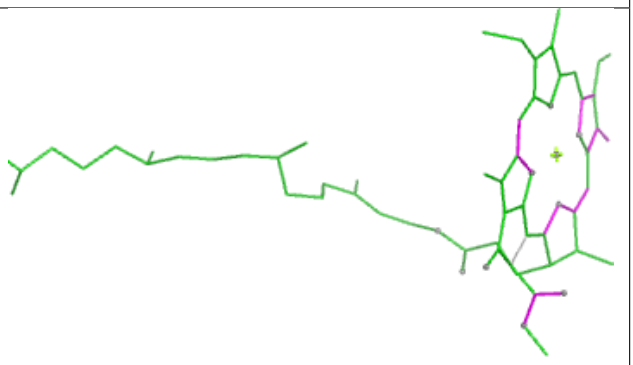

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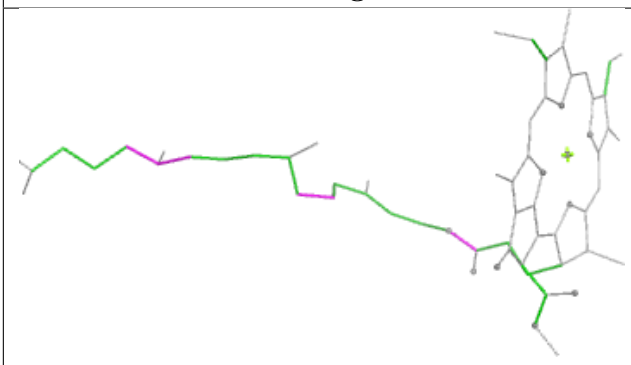

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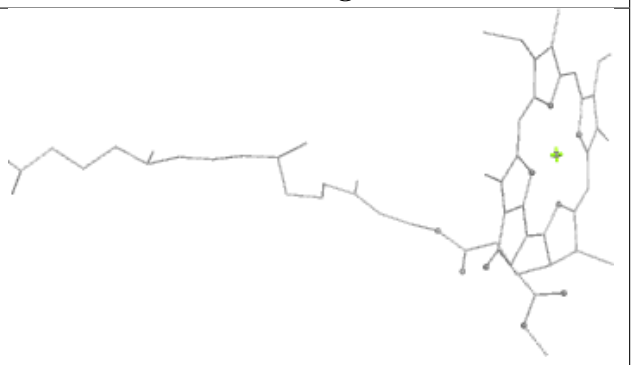
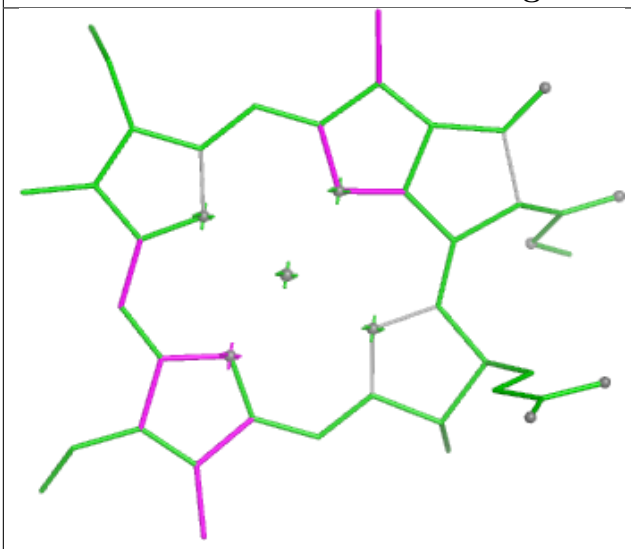


Rings

Ligand CLA K 205



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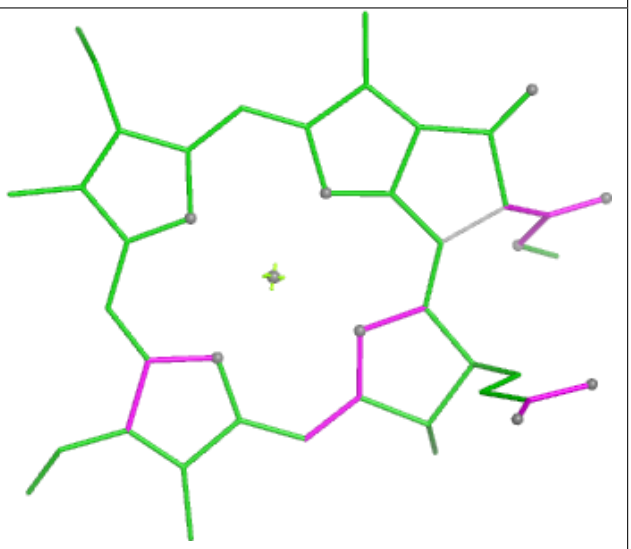

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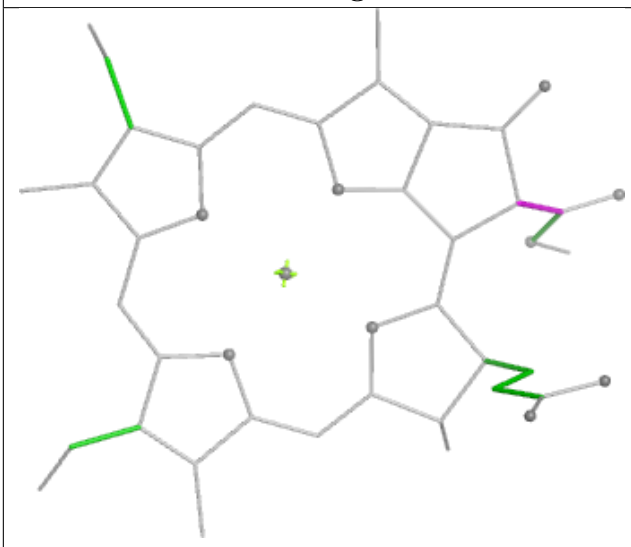

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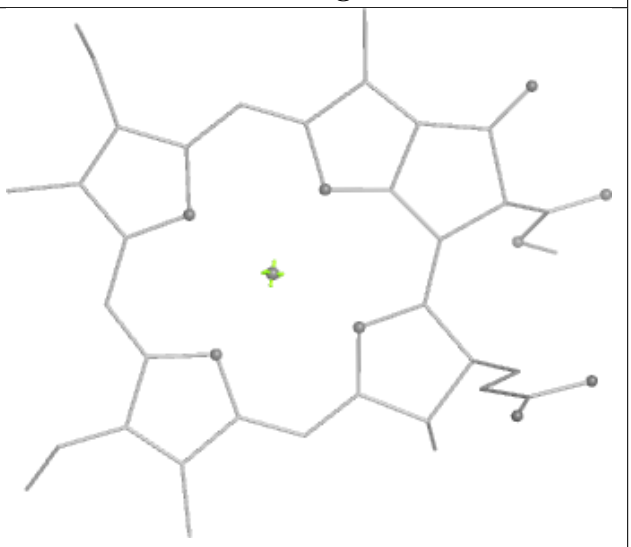
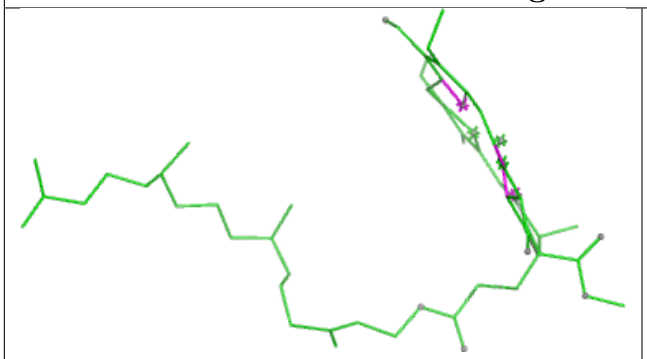


Rings

Ligand CHL 5 307



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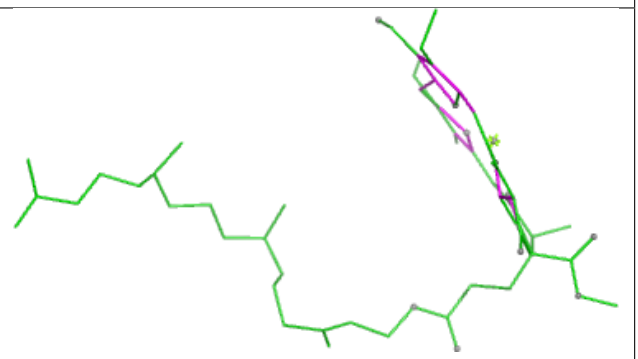

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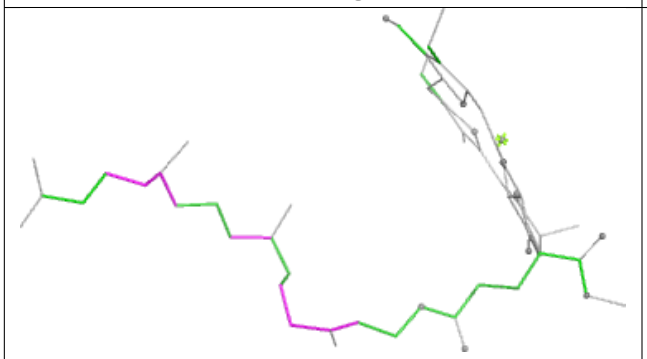
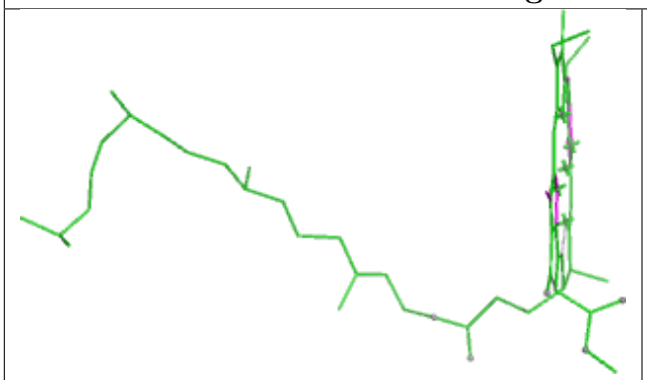


Torsions

Rings

Ligand CLA B 841



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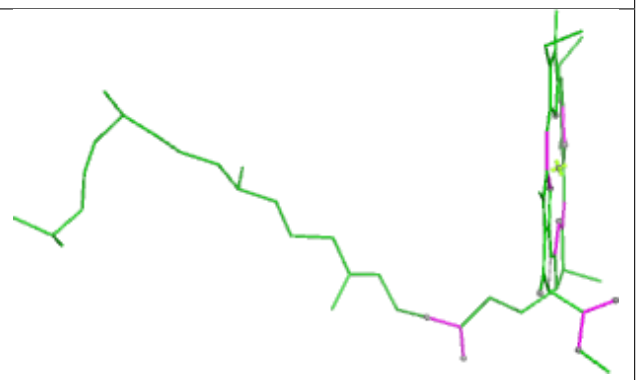
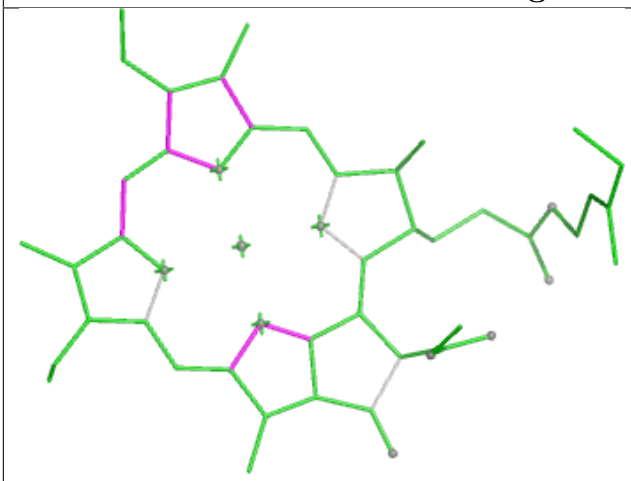


Bond angles

Torsions

Rings

Ligand CLA 6 304



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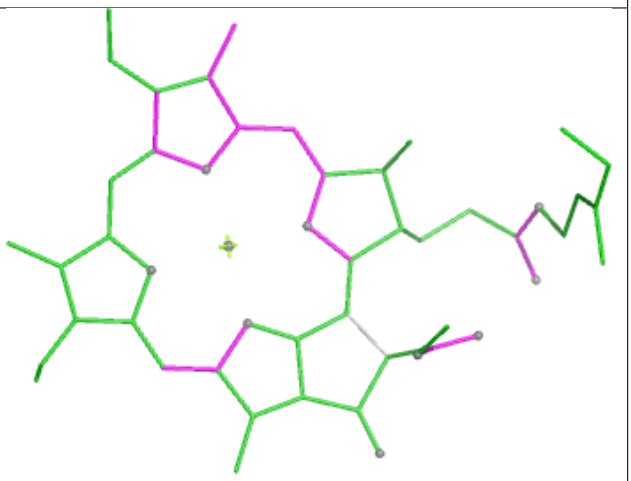

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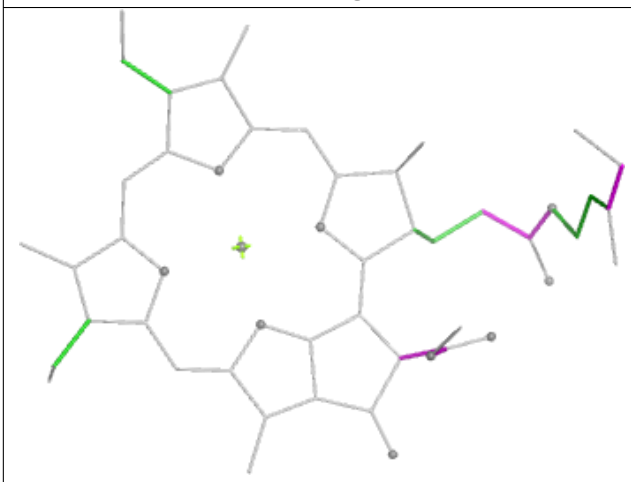

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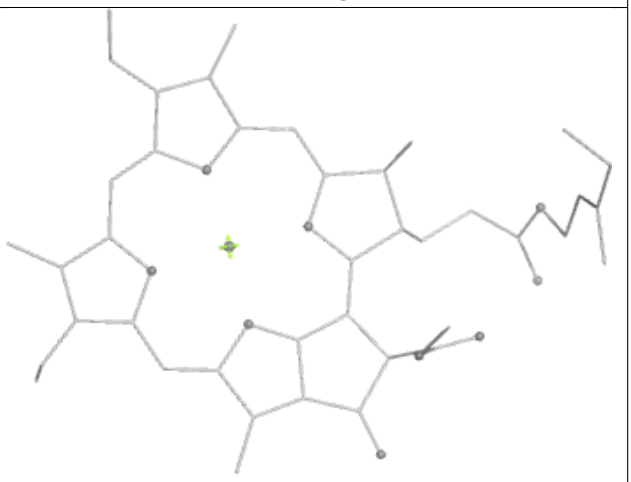
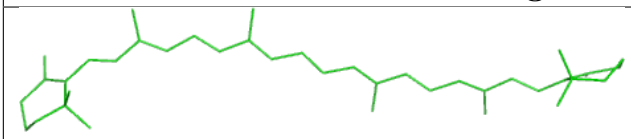


Rings

Ligand BCR 3 315



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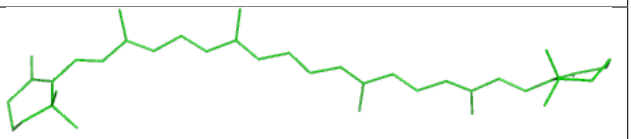
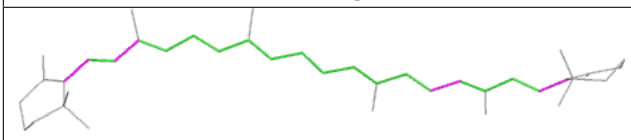


Bond angles



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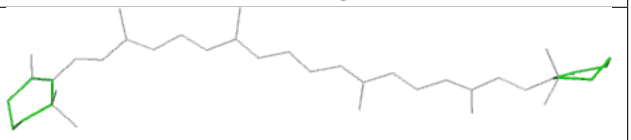
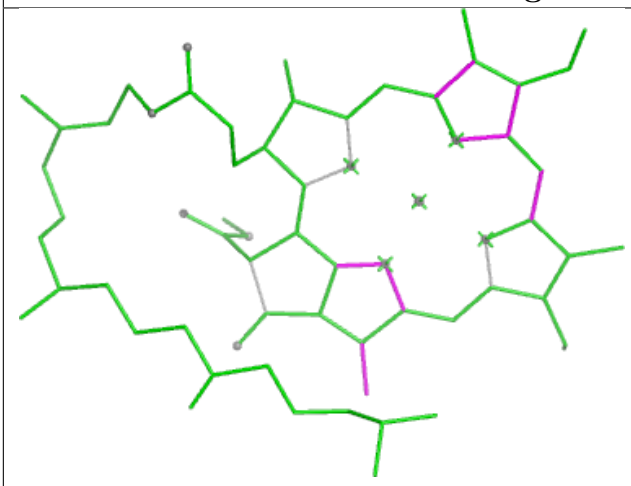


Rings

Ligand CLA B 806



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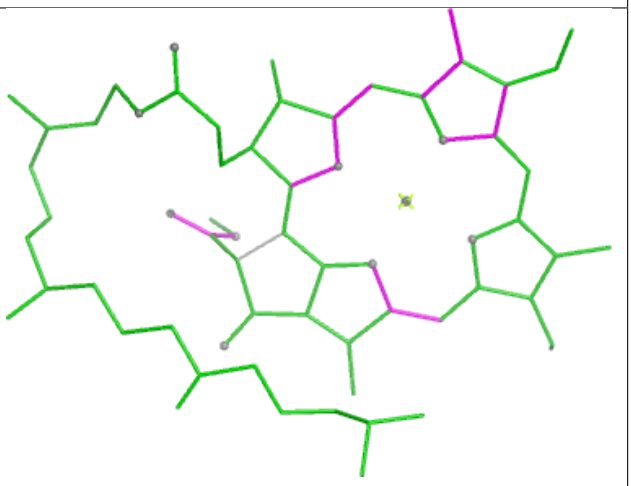
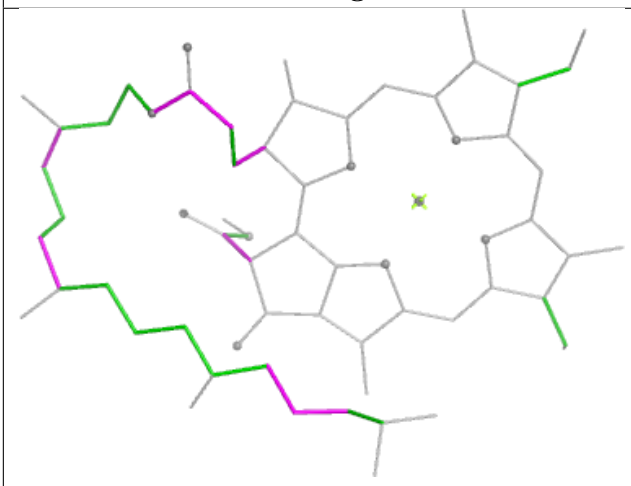


Bond angles



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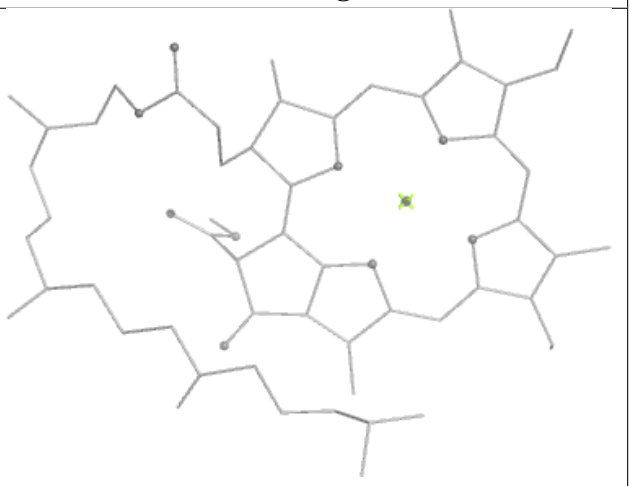
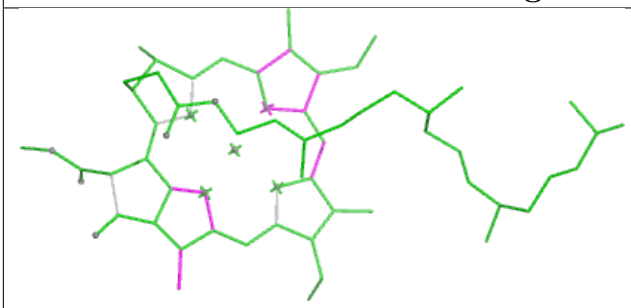
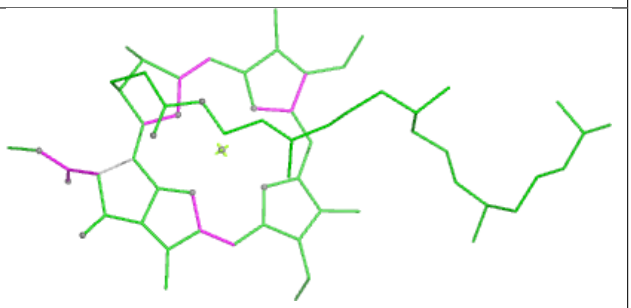
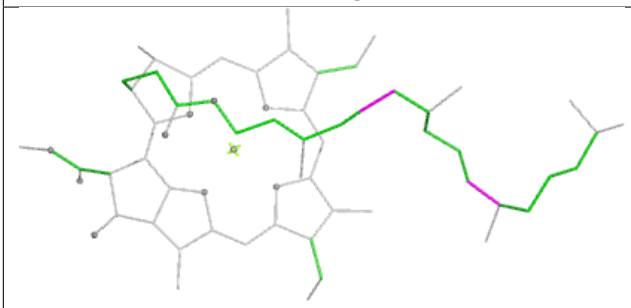
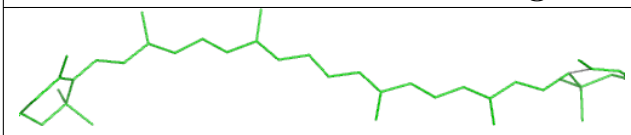
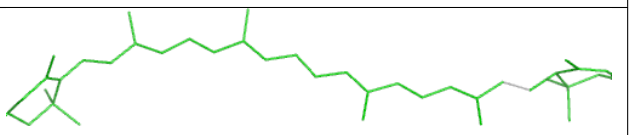
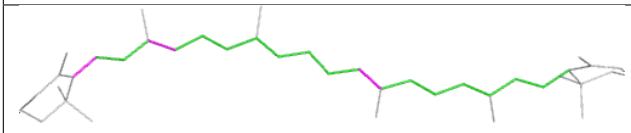
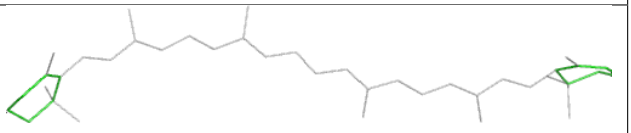
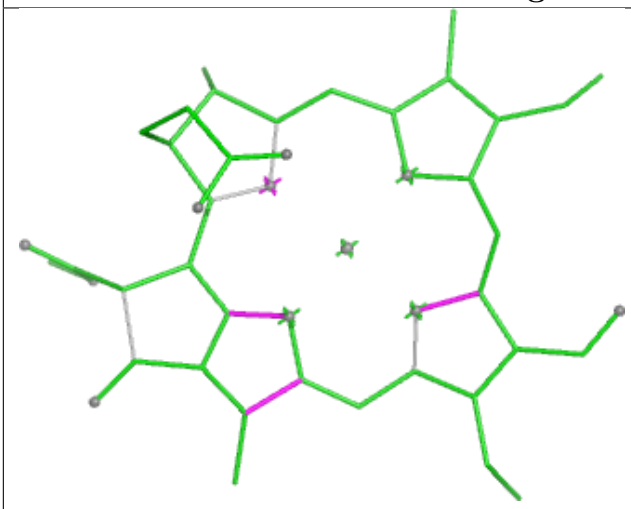


Rings

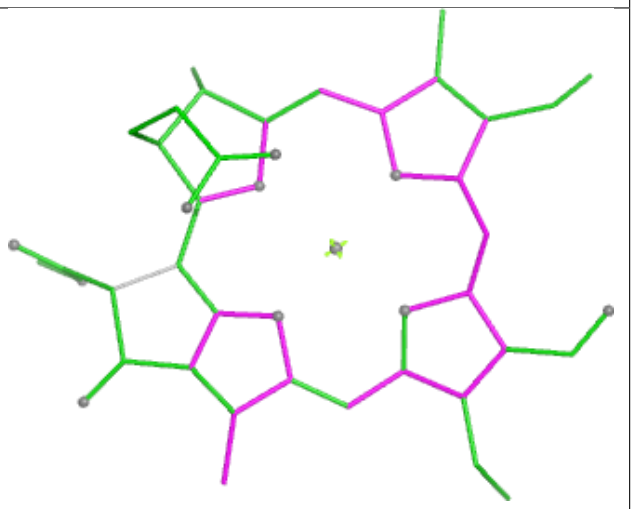
Ligand CLA B 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 1 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

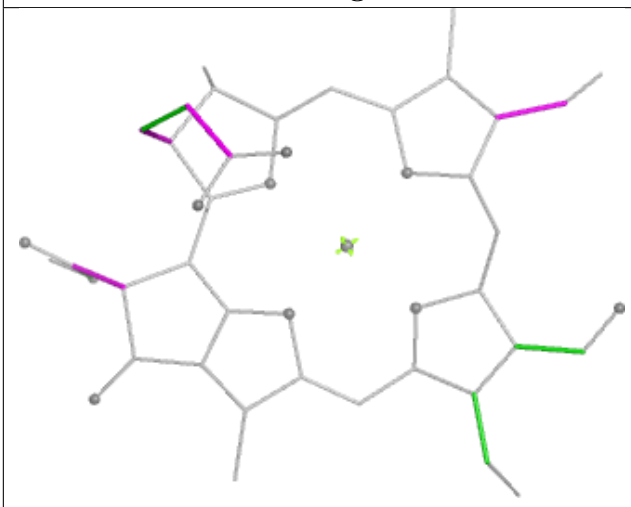
Ligand CHL 1 306



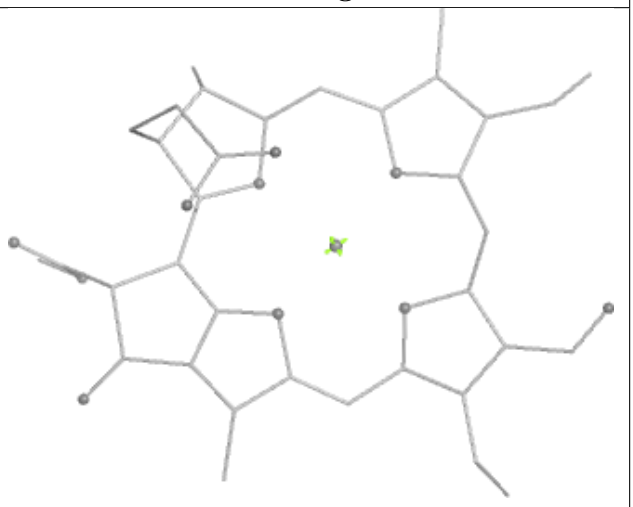
Bond lengths



Bond angles

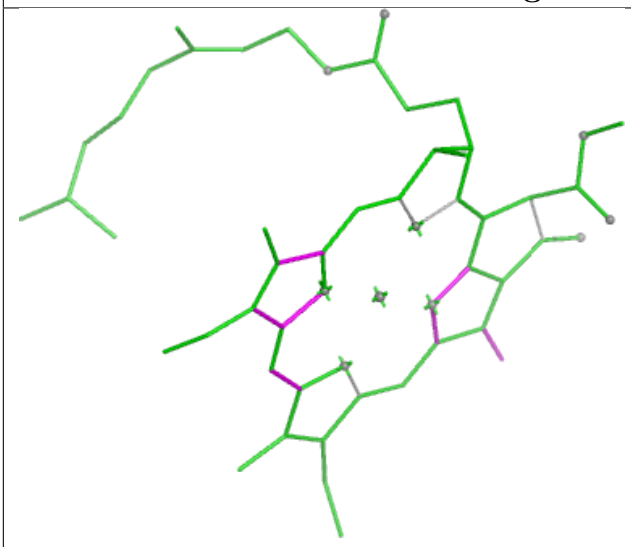


Torsions

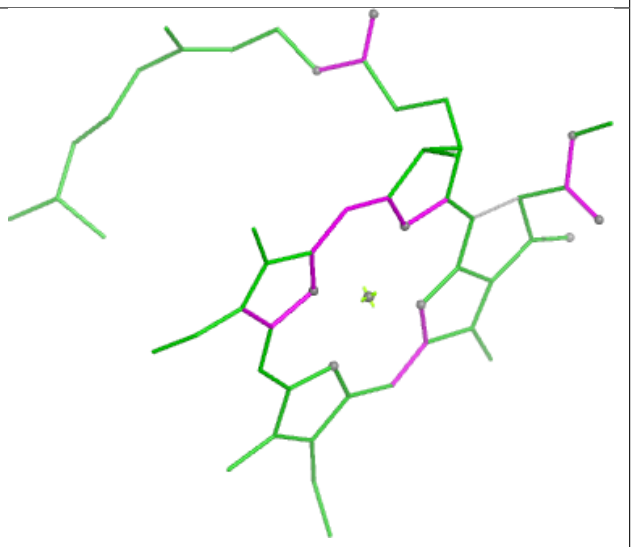


Rings

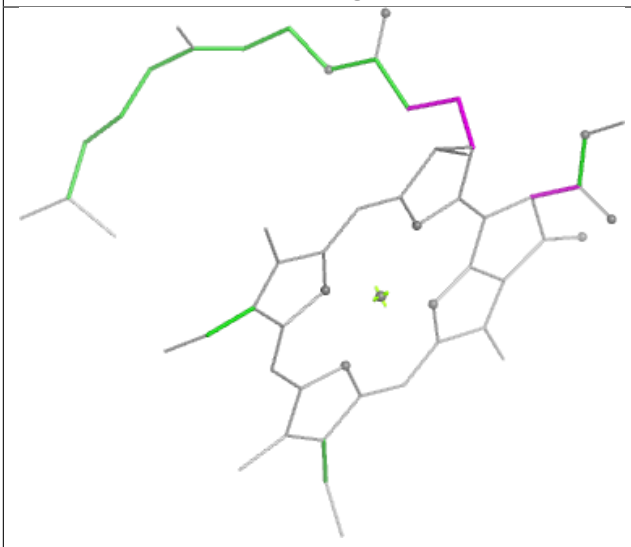
Ligand CLA A 826



Bond lengths



Bond angles



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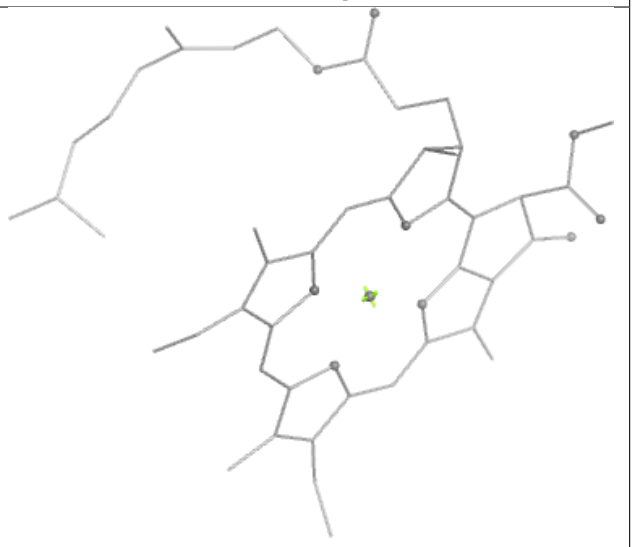
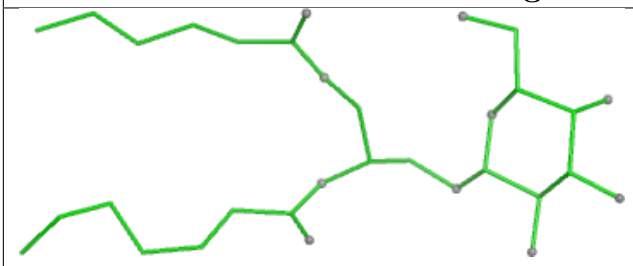
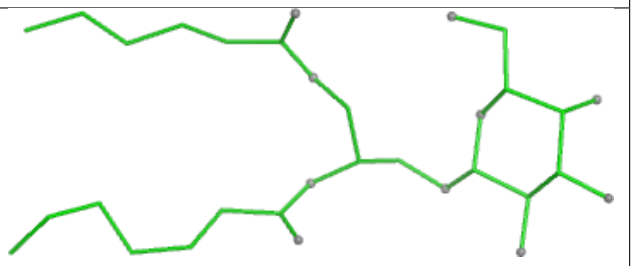


Rings

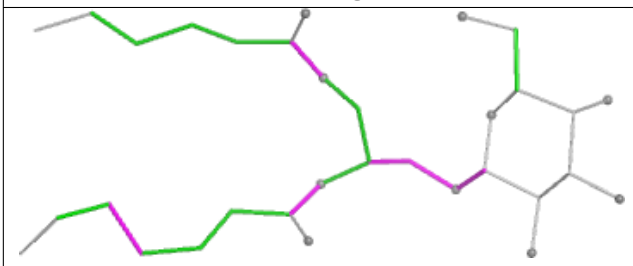
Ligand LMG 7 622



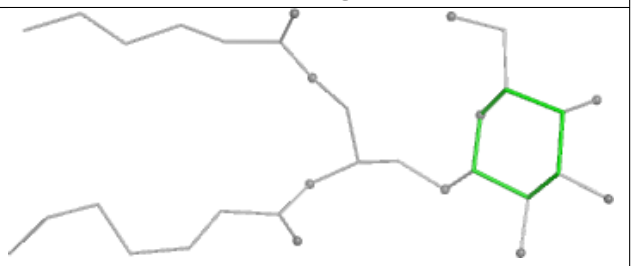
Bond lengths



Bond angles

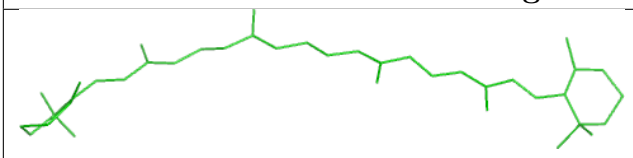


Torsions



Rings

Ligand BCR B 802



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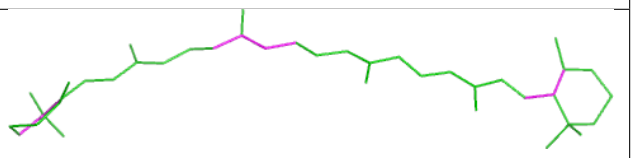

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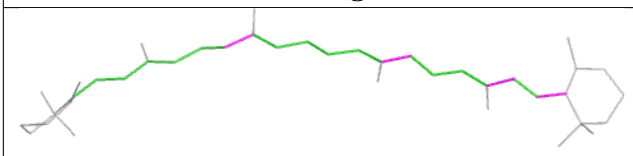

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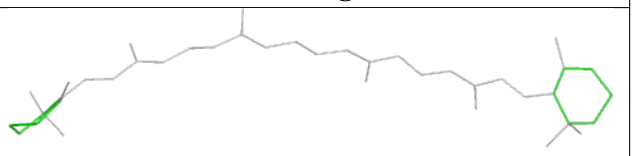
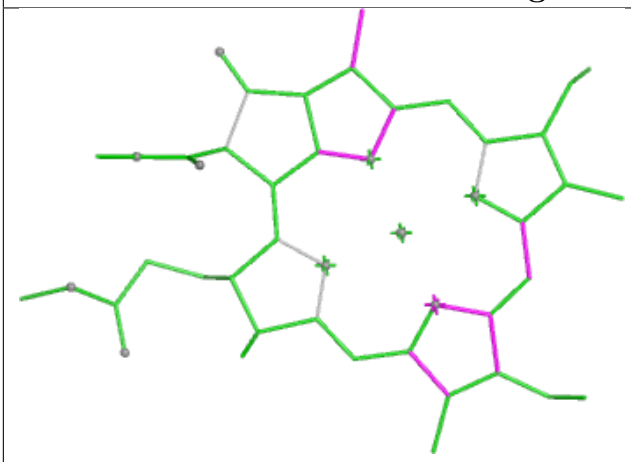


Rings

Ligand CLA 7 614



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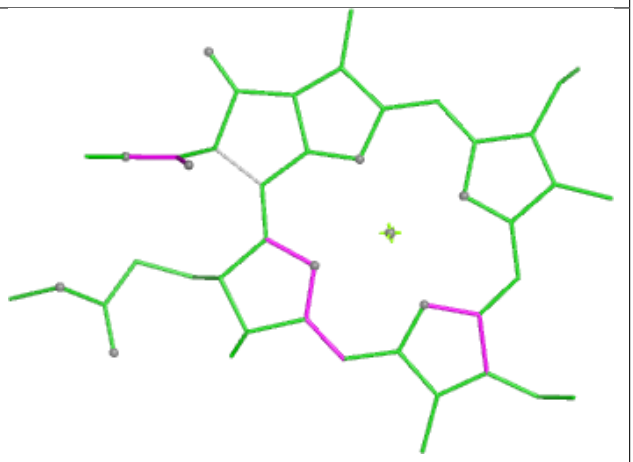
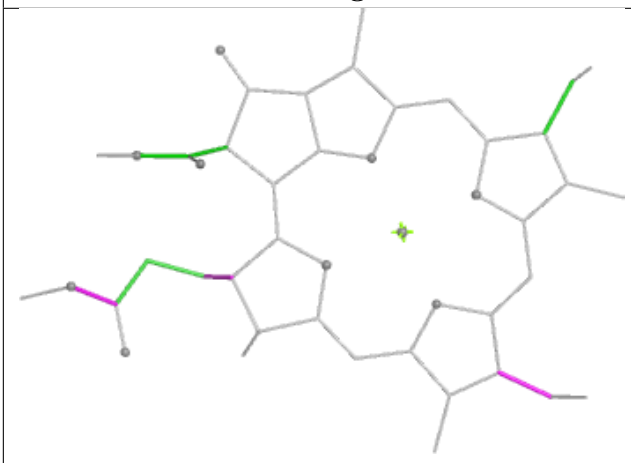


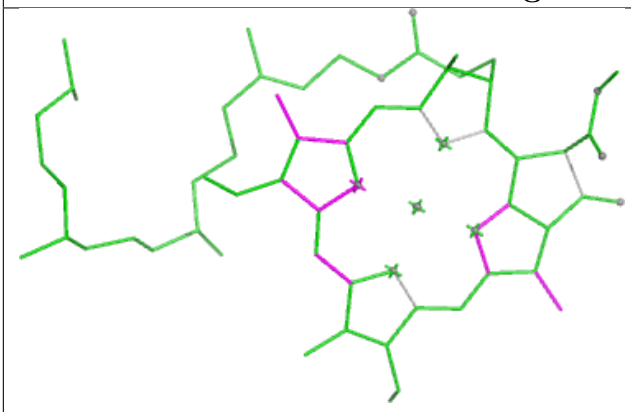
Bond angles



Torsions

Rings

Ligand CLA A 821



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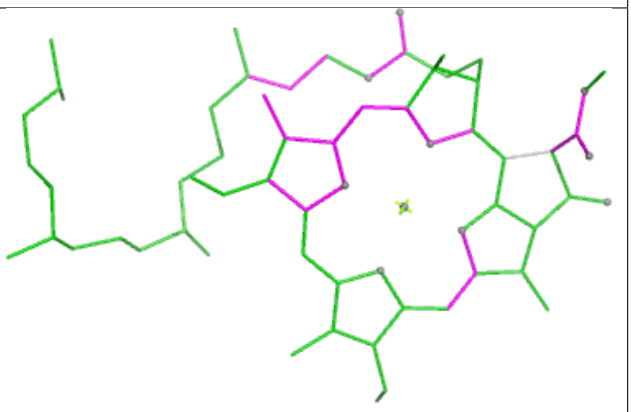
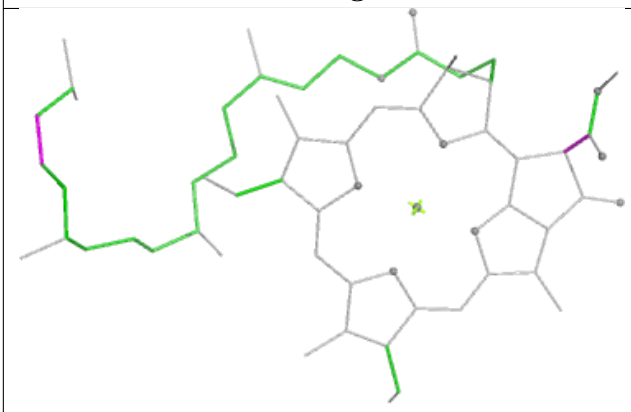


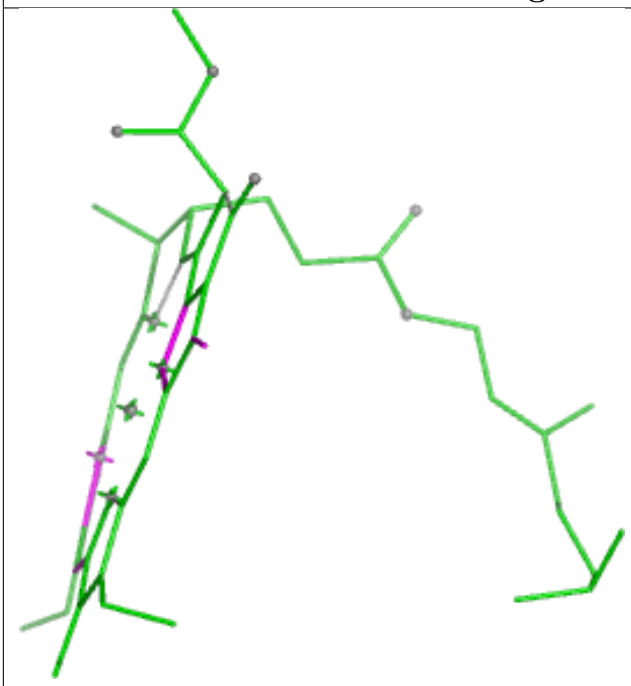
Bond angles



Torsions

Rings

Ligand CLA 4 613



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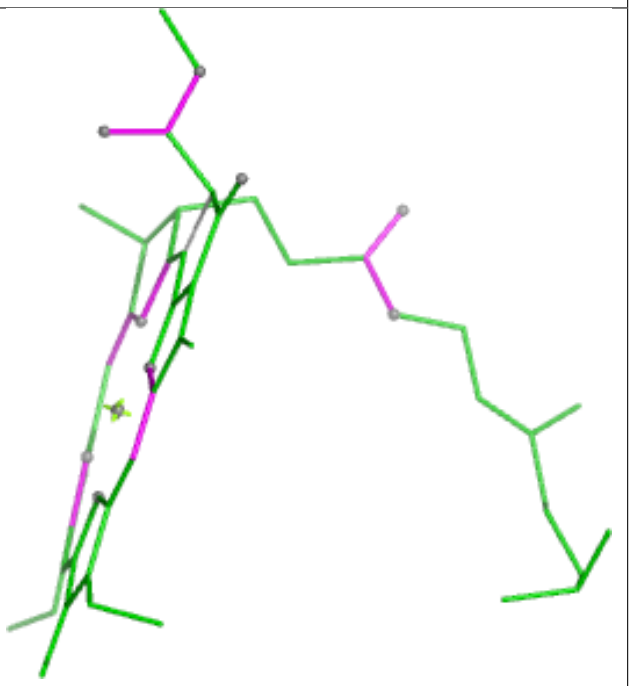
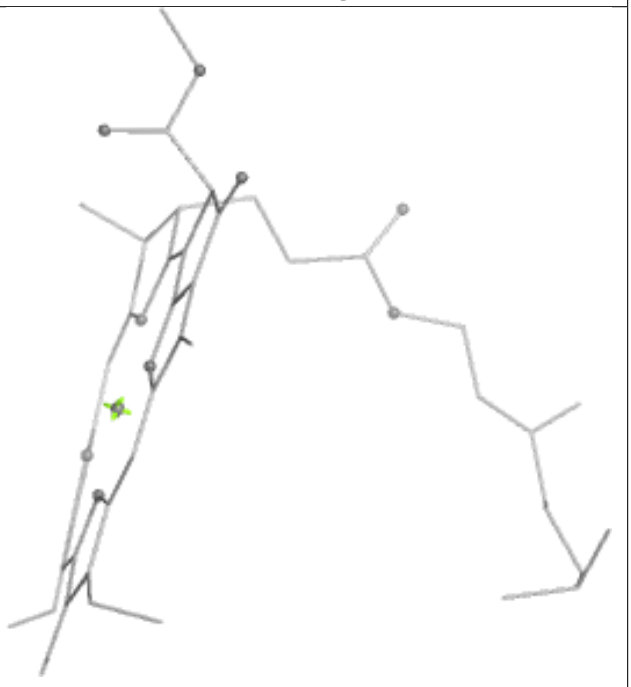


Bond angles

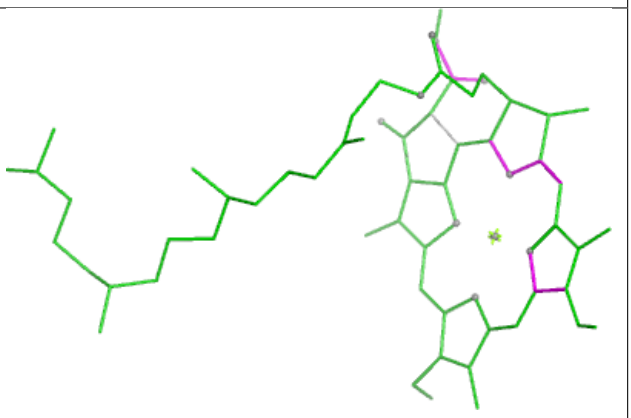
Torsions



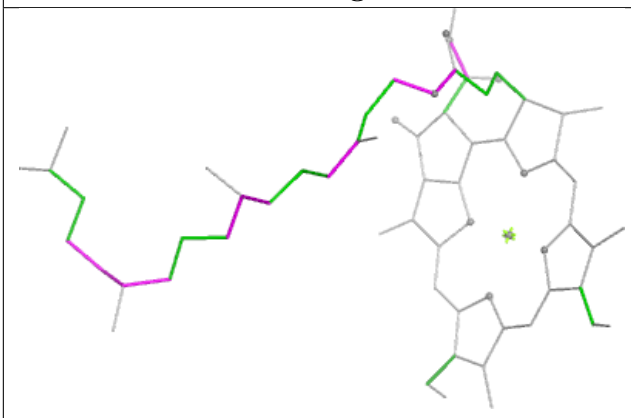
Rings

Ligand CLA 1 308

Bond lengths



Bond angles

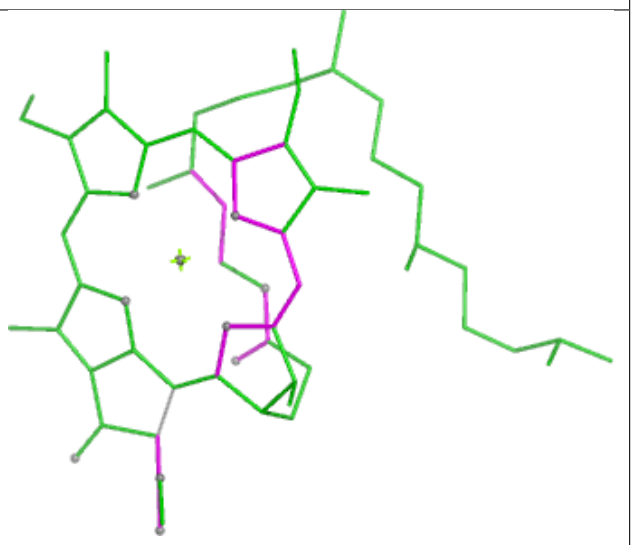


Torsions

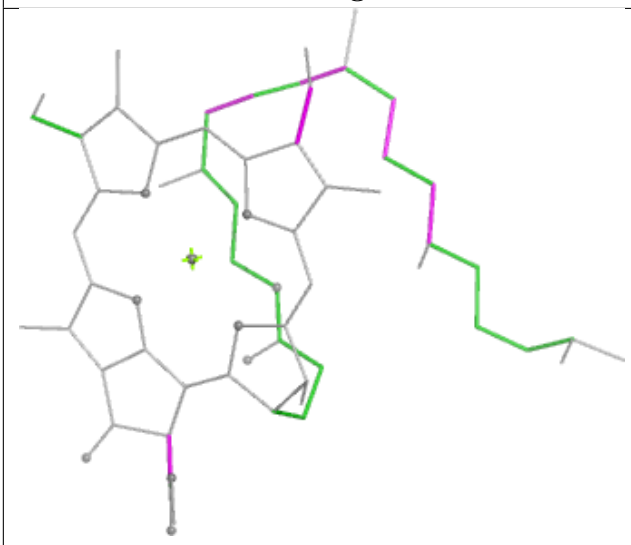
Rings

Ligand CLA B 809

Bond lengths



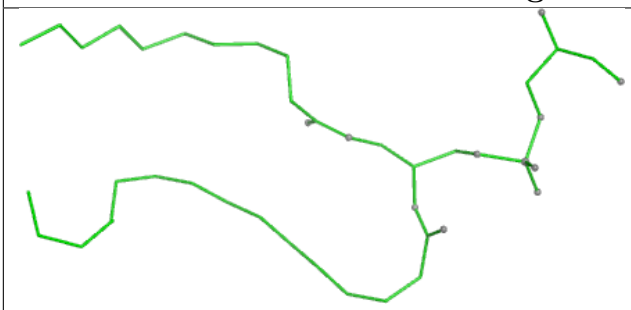
Bond angles



Torsions

Rings

Ligand LHG 8 318



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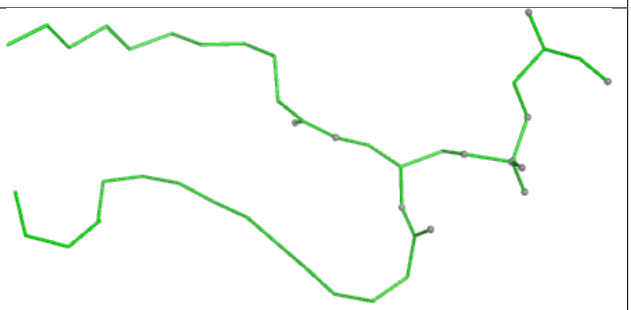
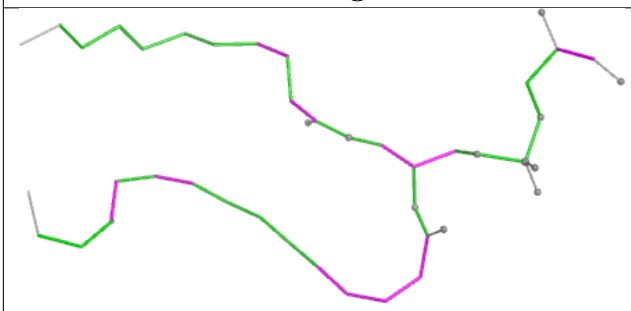


Bond angles



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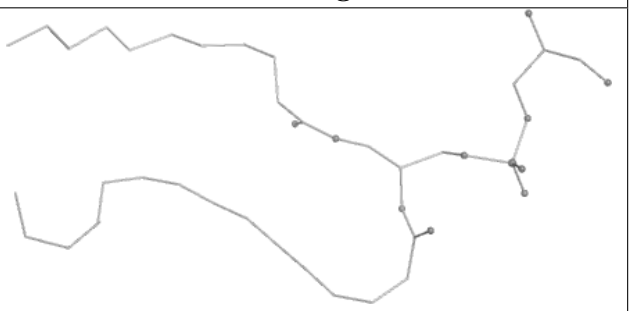
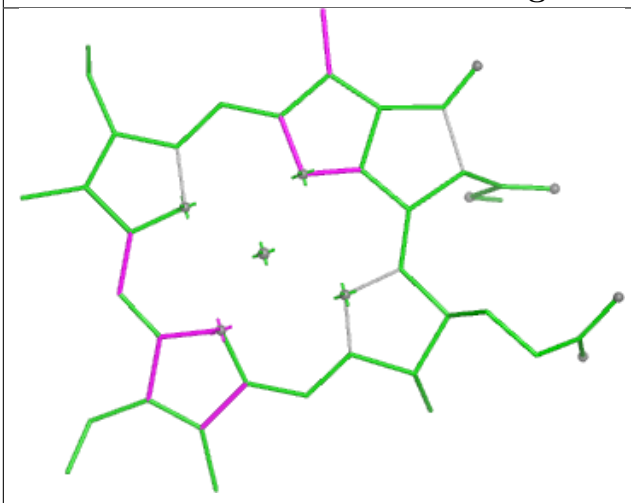


Rings

Ligand CLA 6 312



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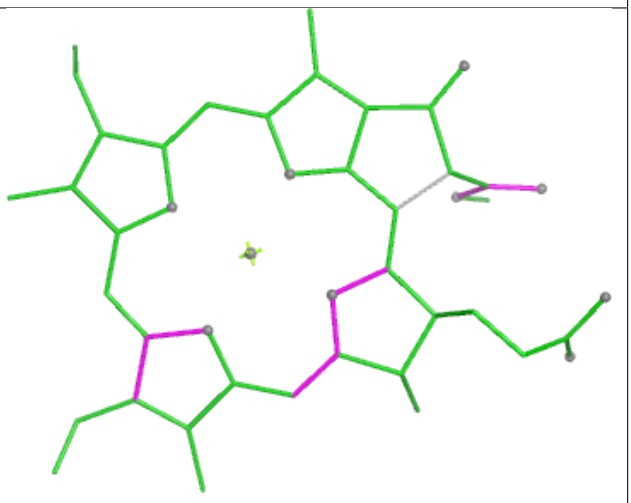

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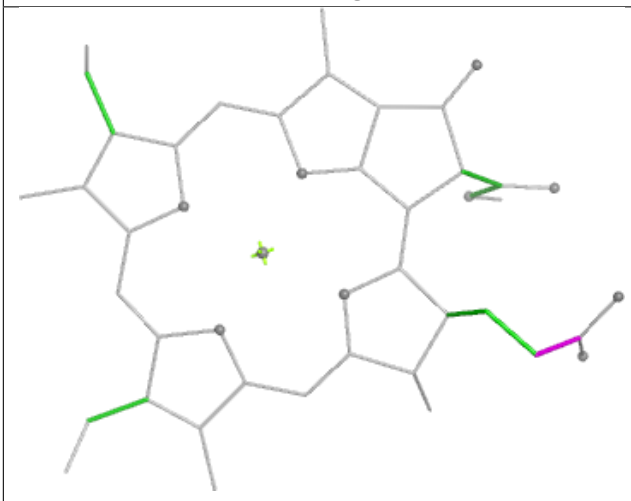

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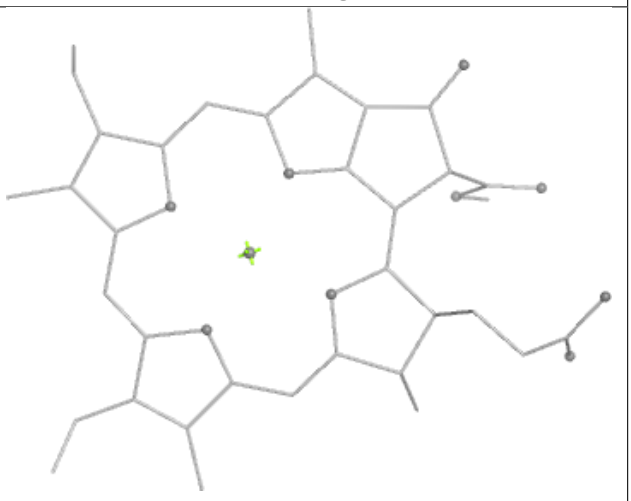
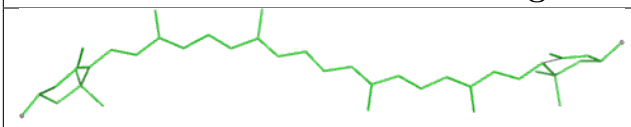


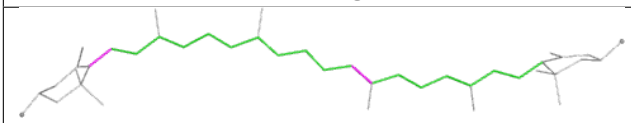
Rings

Ligand LUT 3 316



Bond lengths

Bond angles



Torsions

Rings

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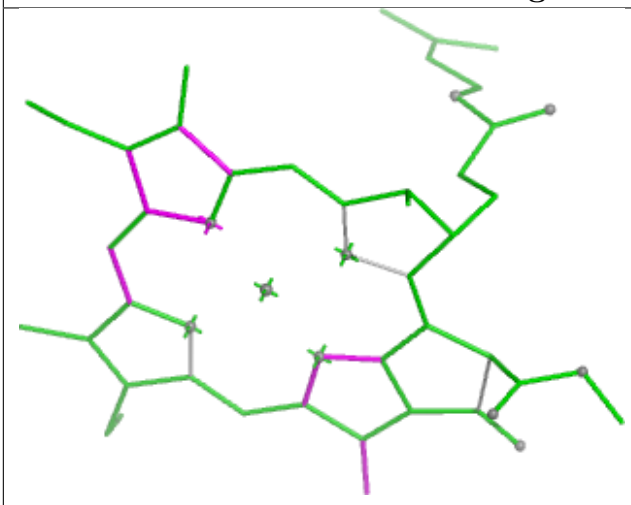

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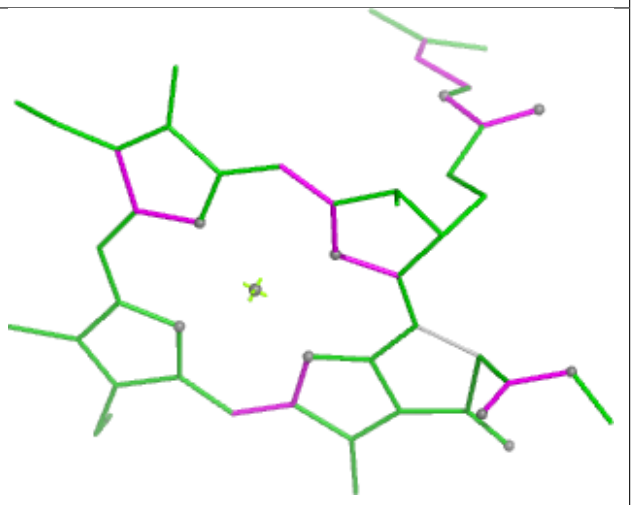
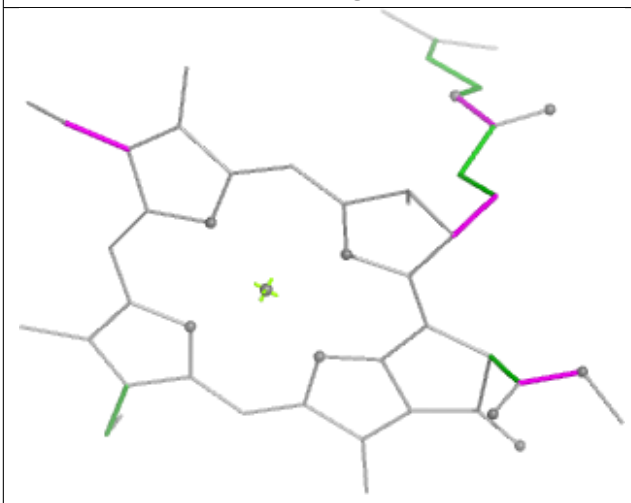


Bond angles



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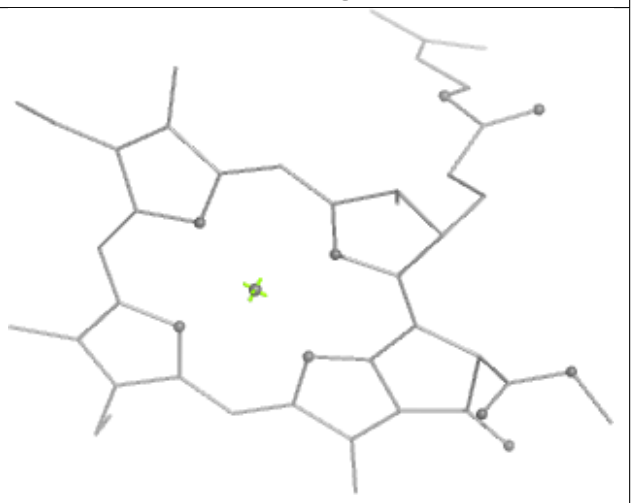
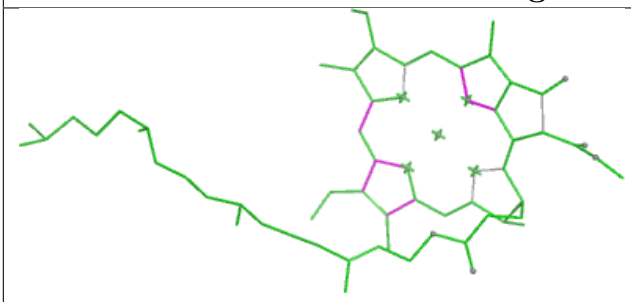
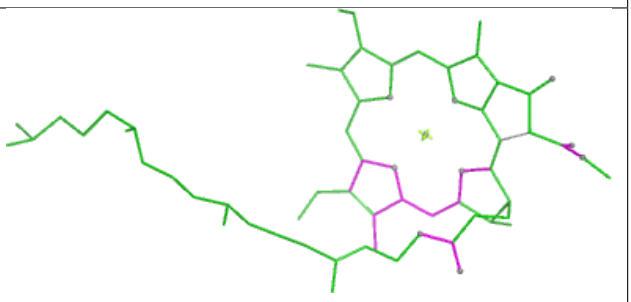


Rings

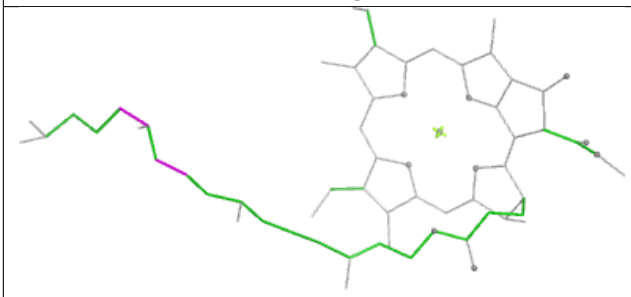
Ligand CLA 1 309



Bond lengths



Bond angles



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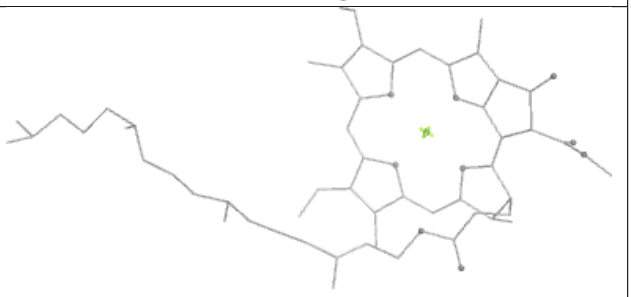
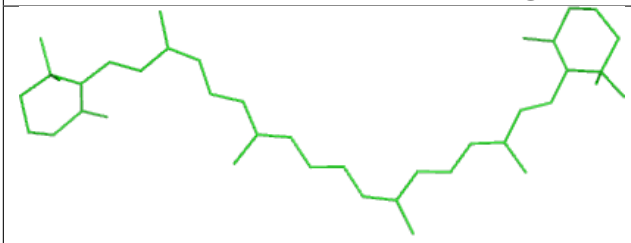


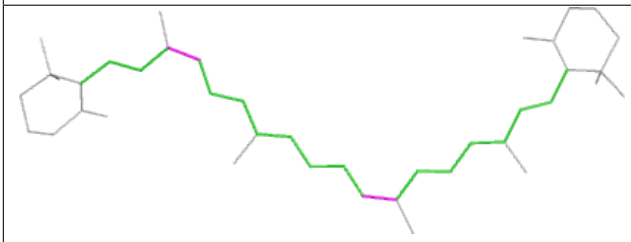
Rings

Ligand BCR A 853



Bond lengths

Bond angles



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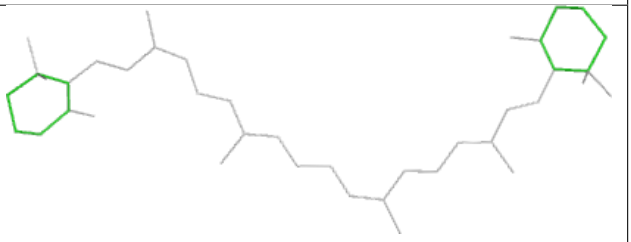
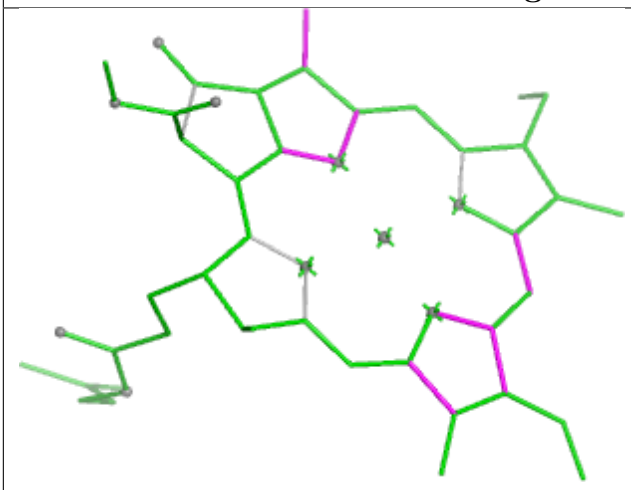


Rings

Ligand CLA B 839



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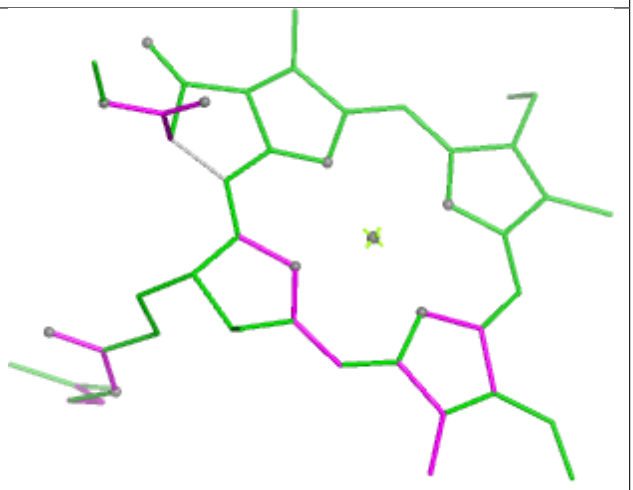
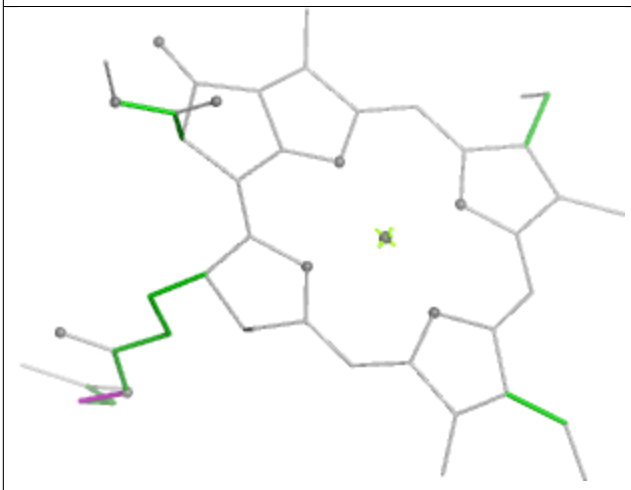


Bond angles



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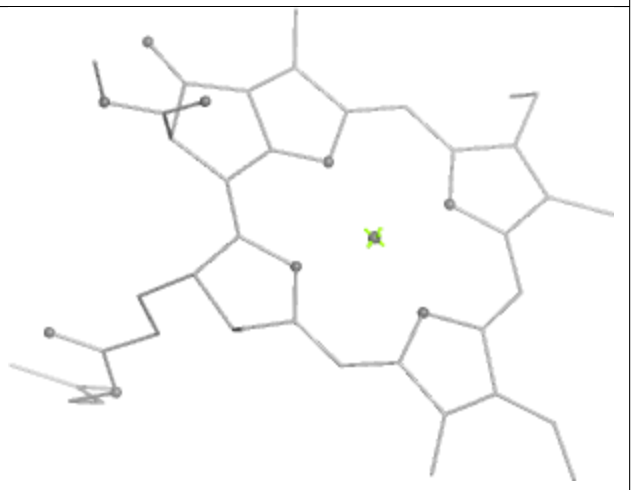
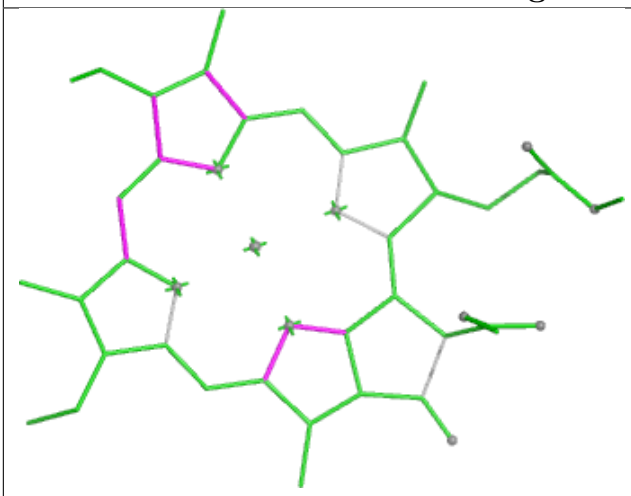


Rings

Ligand CLA 5 319



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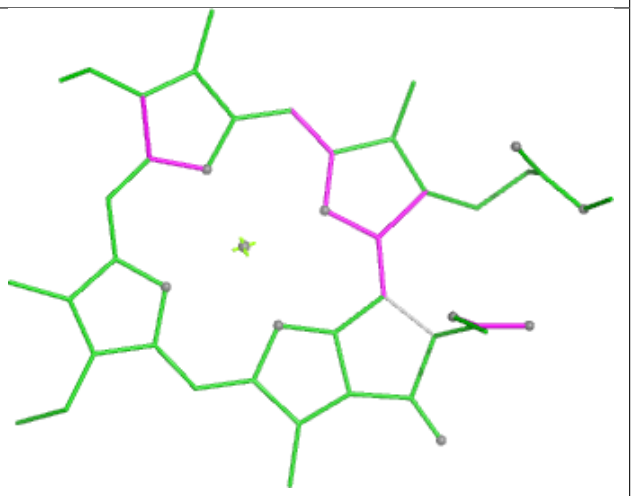
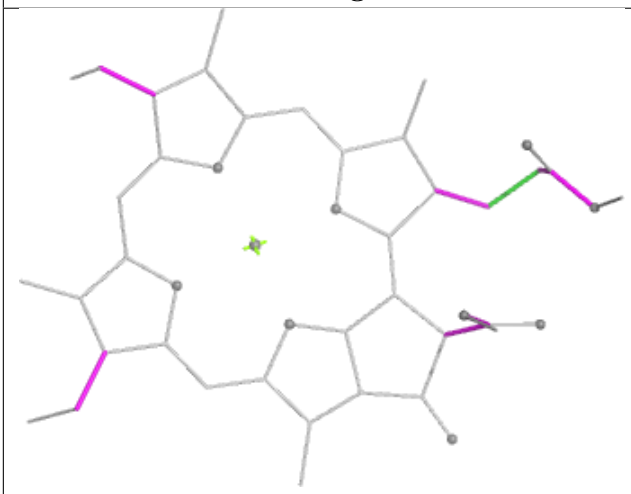


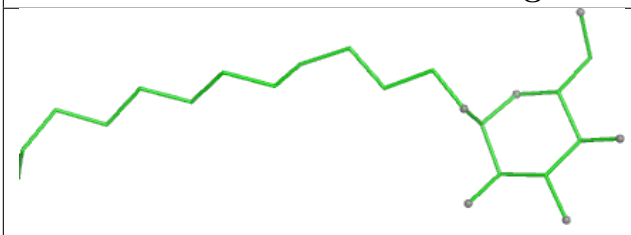
Bond angles



Torsions

Rings

Ligand LMU 6 324



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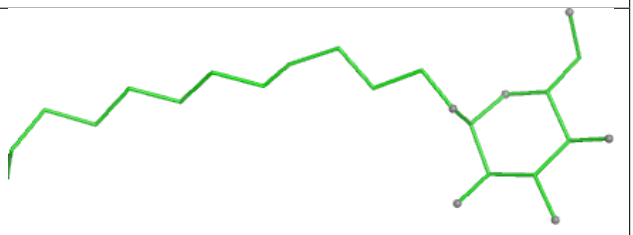
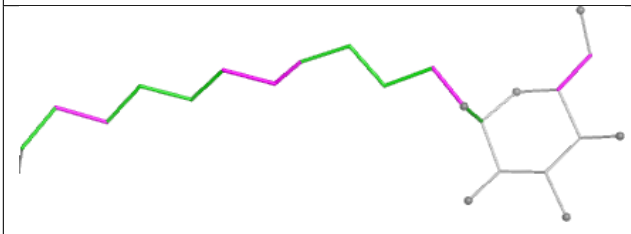


Bond angles



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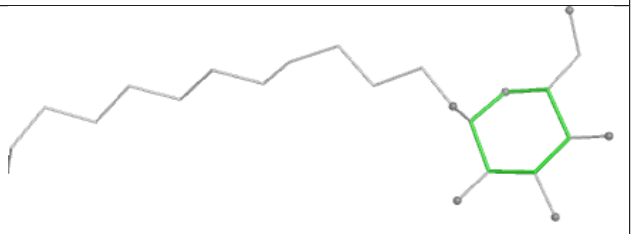
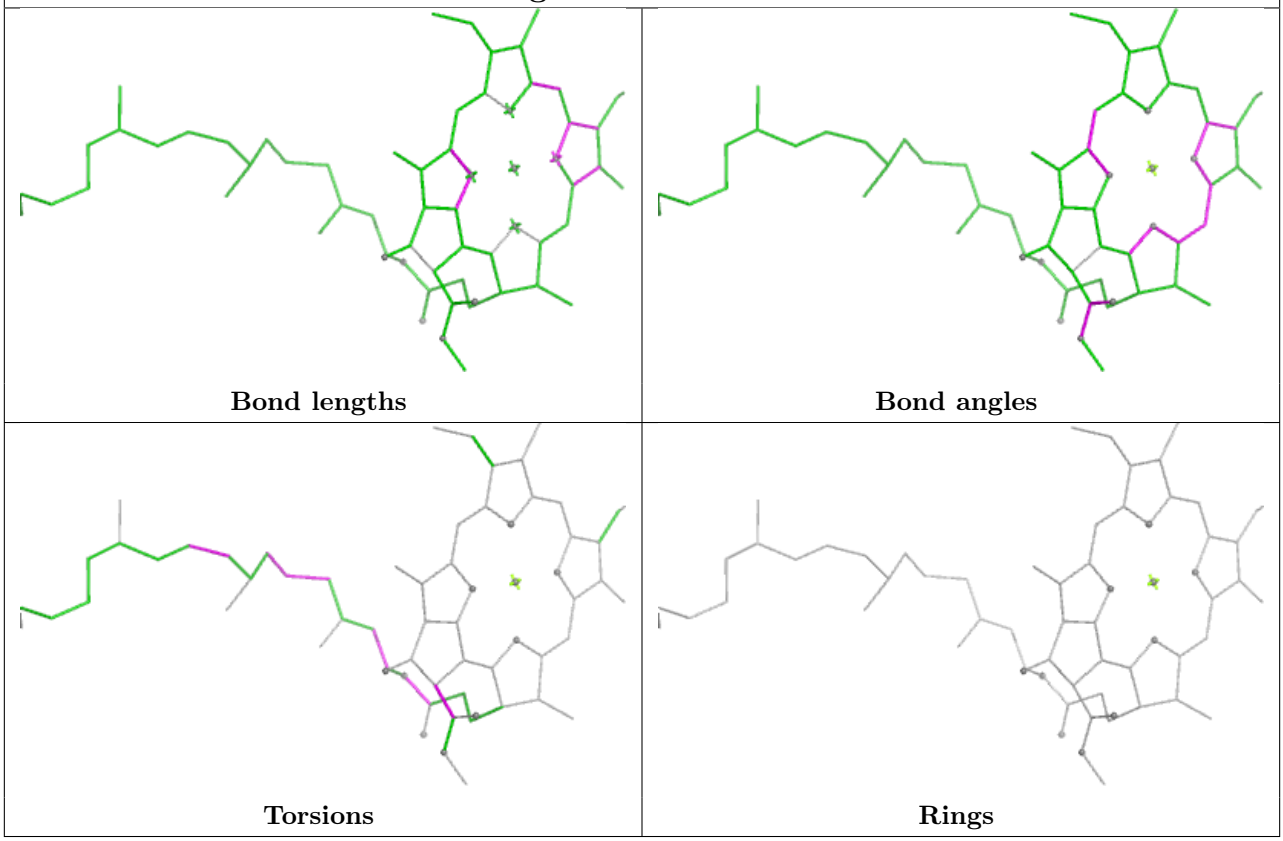
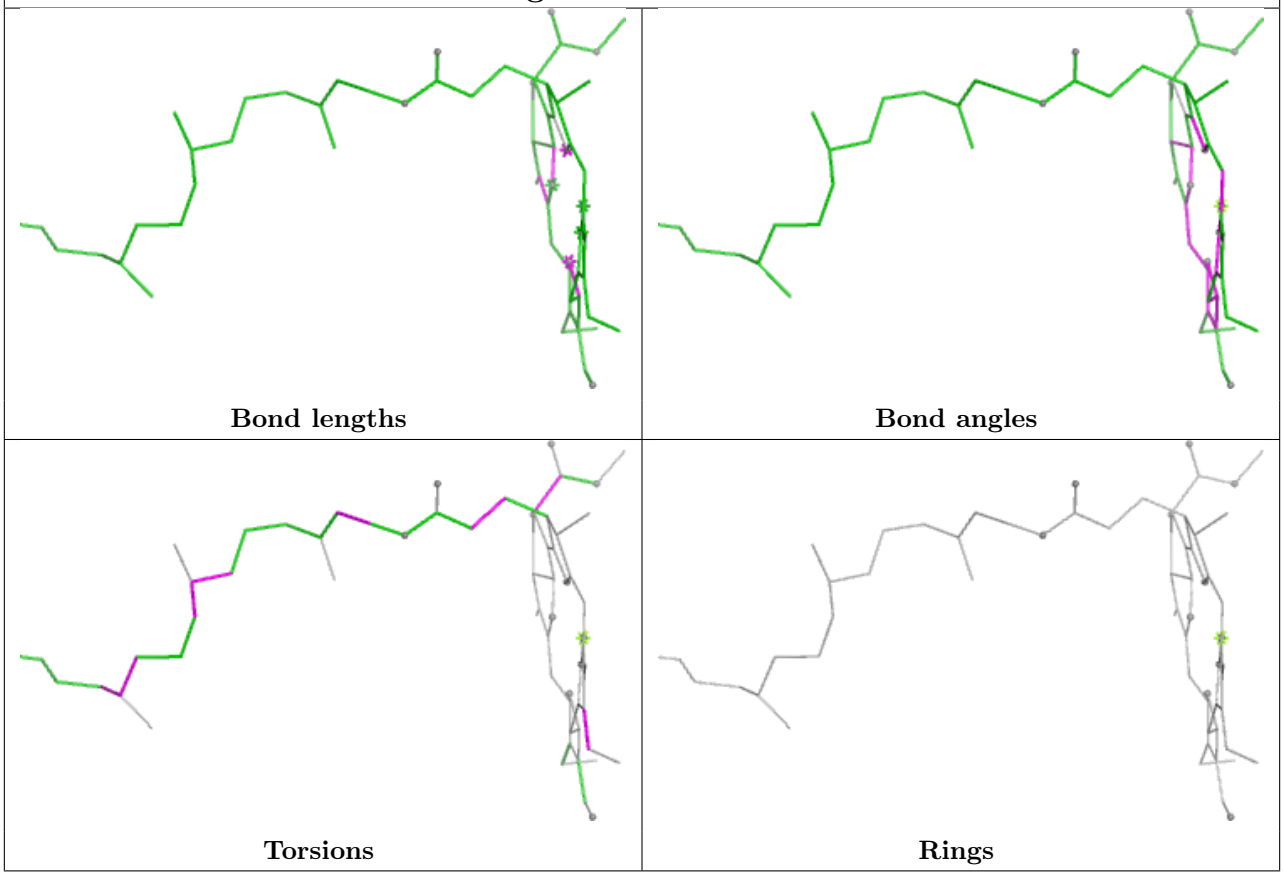


Rings

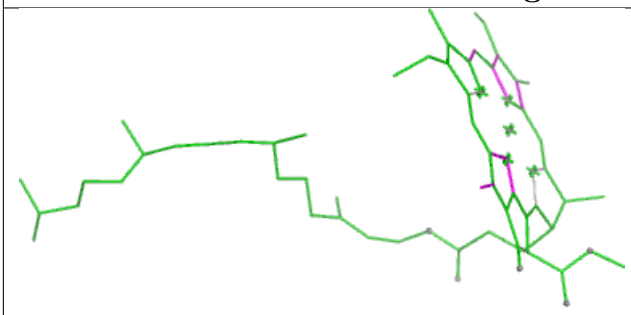
Ligand CLA 7 610



Ligand CHL Z 601

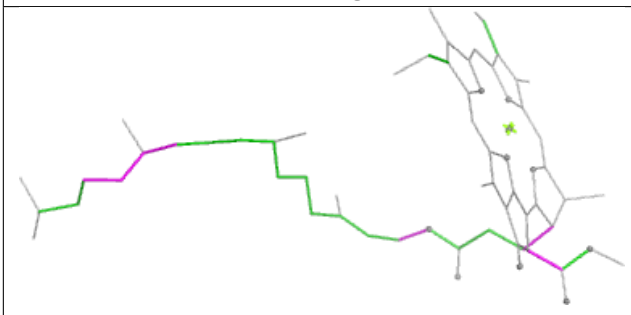


Ligand CLA A 813



Bond lengths

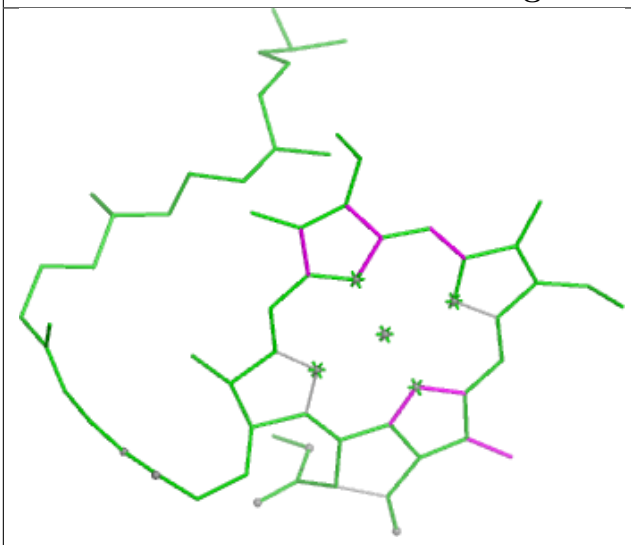
Bond angles



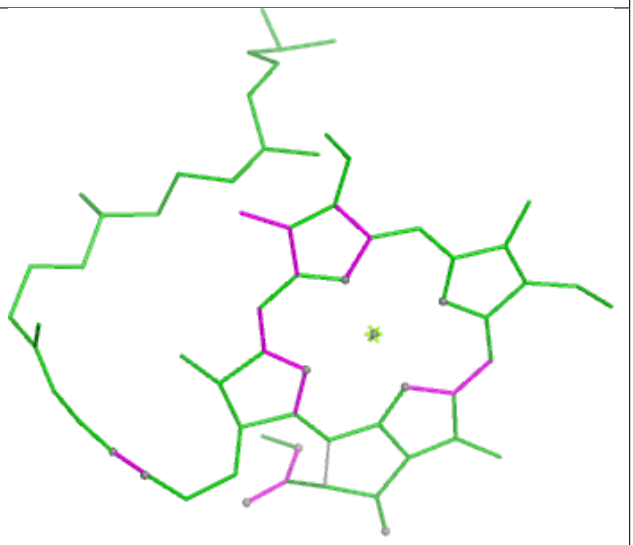
Torsions

Rings

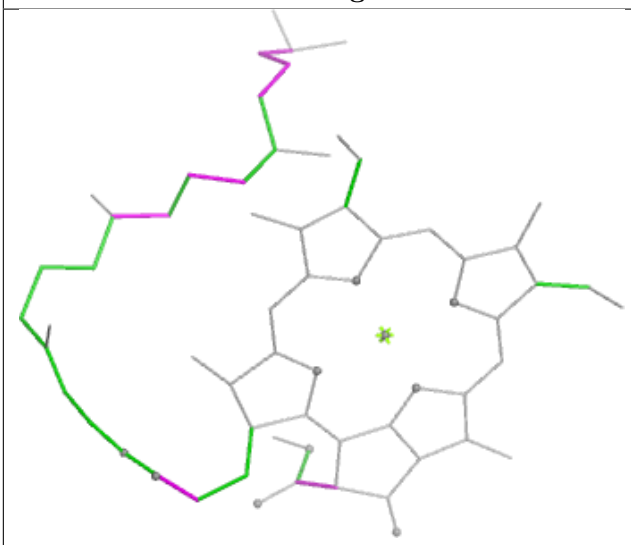
Ligand CLA A 815



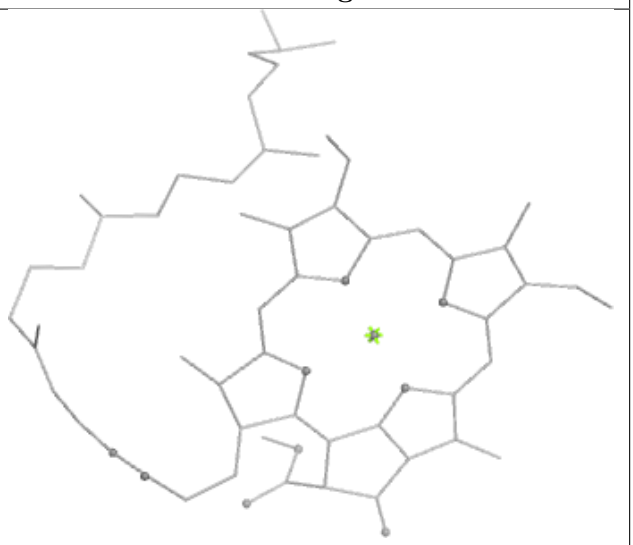
Bond lengths



Bond angles



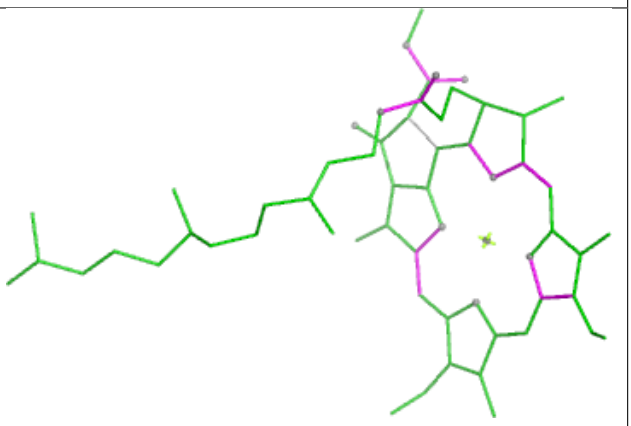
Torsions



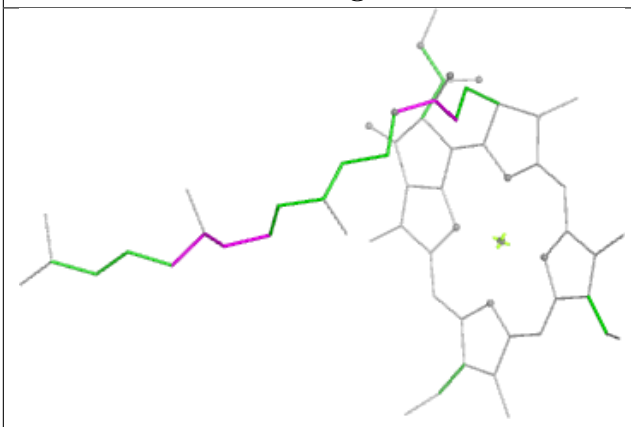
Rings

Ligand CLA 4 608

Bond lengths



Bond angles



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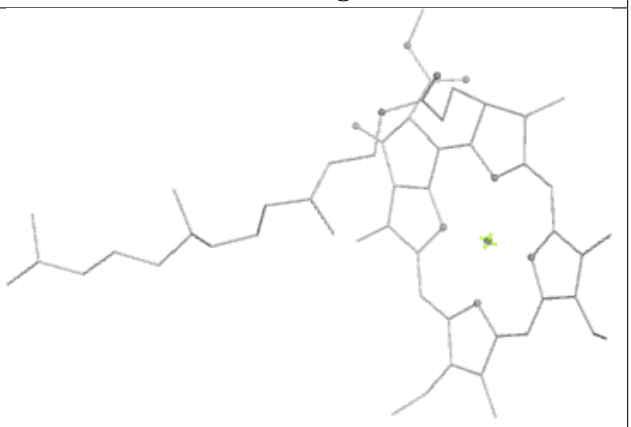
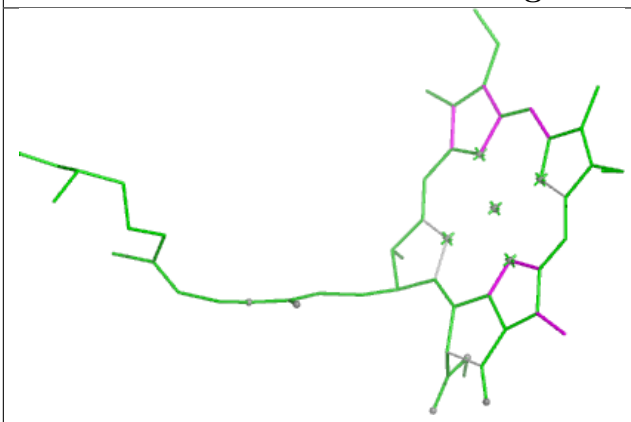


Rings

Ligand CLA B 834



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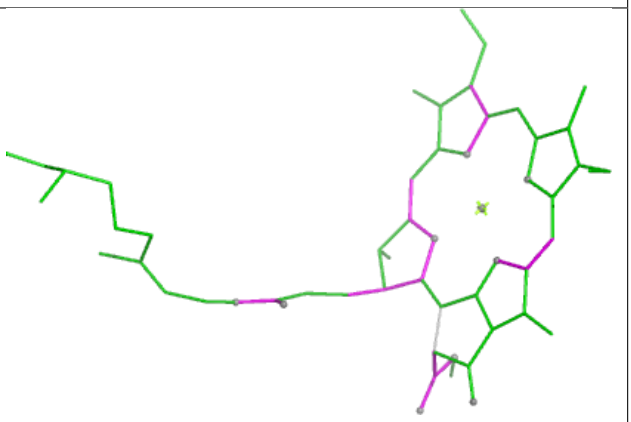
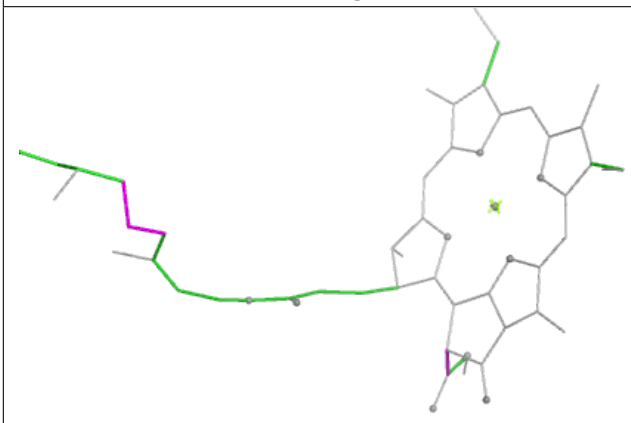


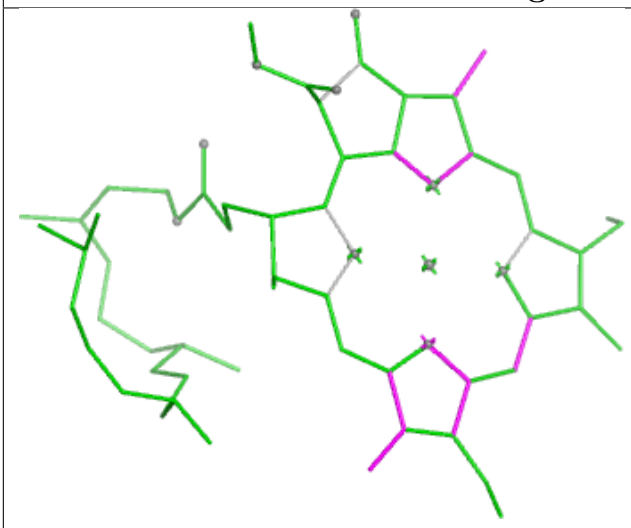
Bond angles



Torsions

Rings

Ligand CLA 1 307



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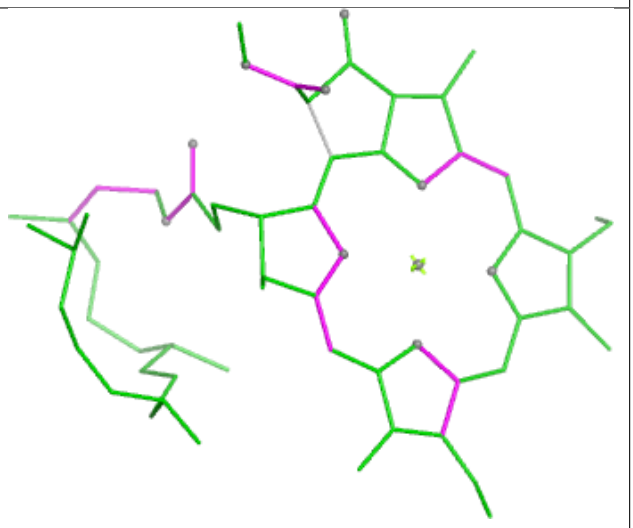
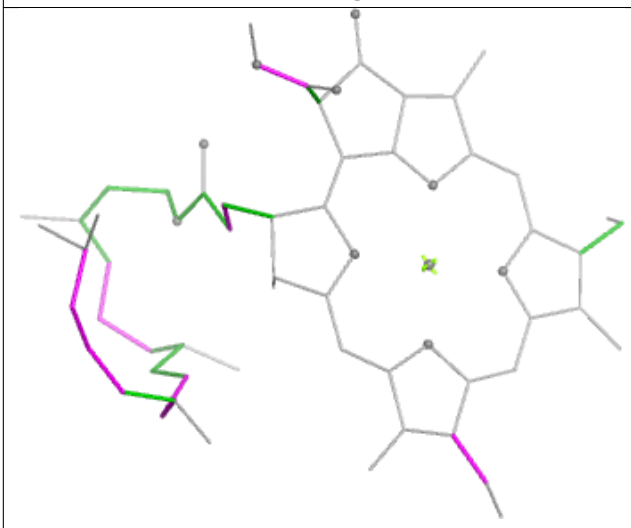


Bond angles



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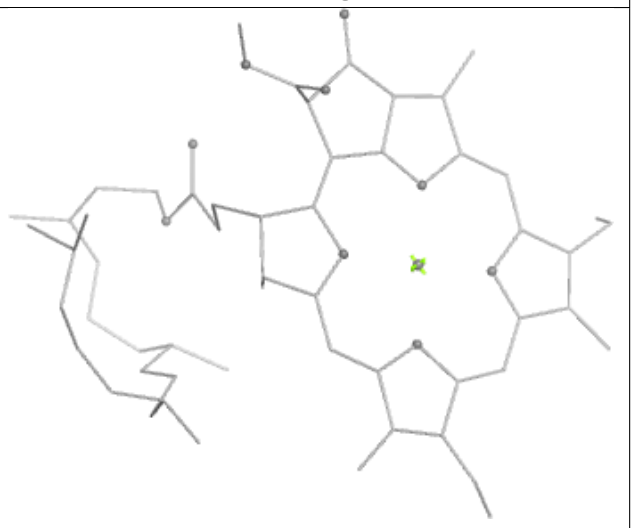
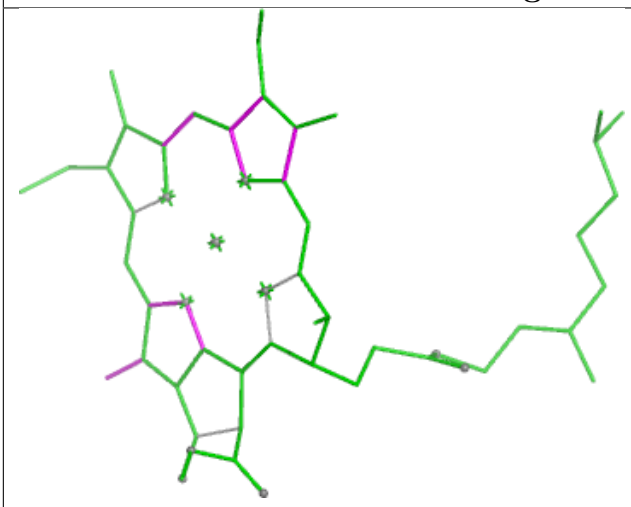


Rings

Ligand CLA A 822



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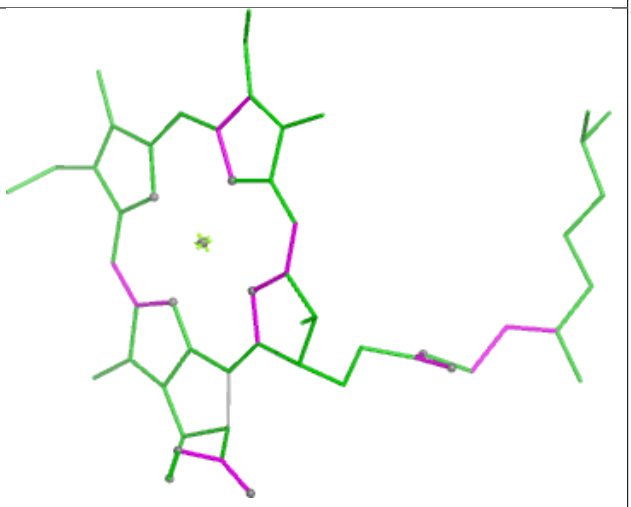
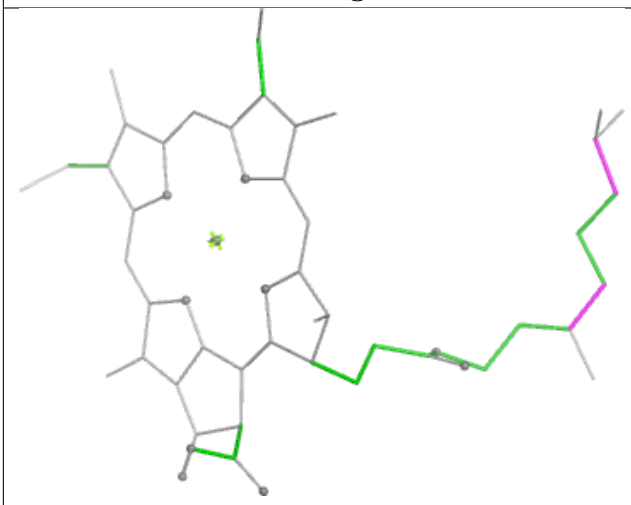


Bond angles



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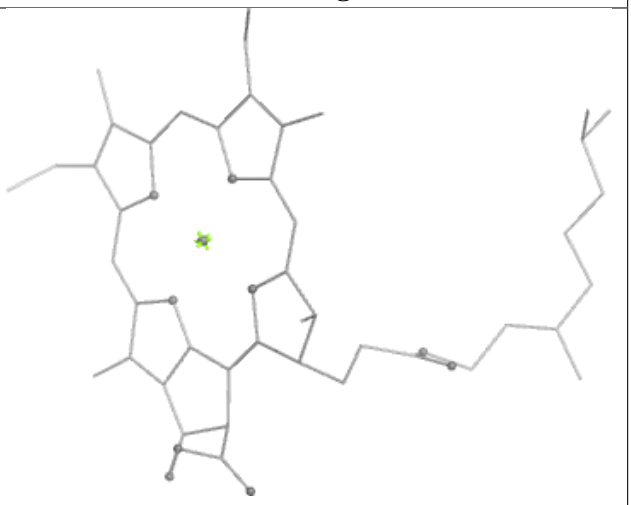
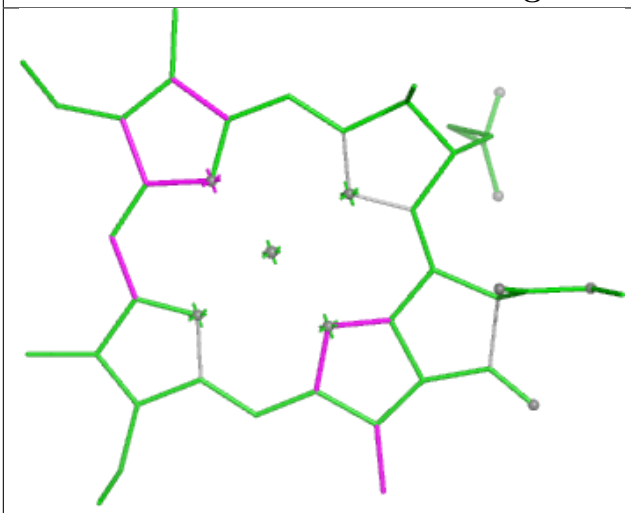


Rings

Ligand CLA A 825



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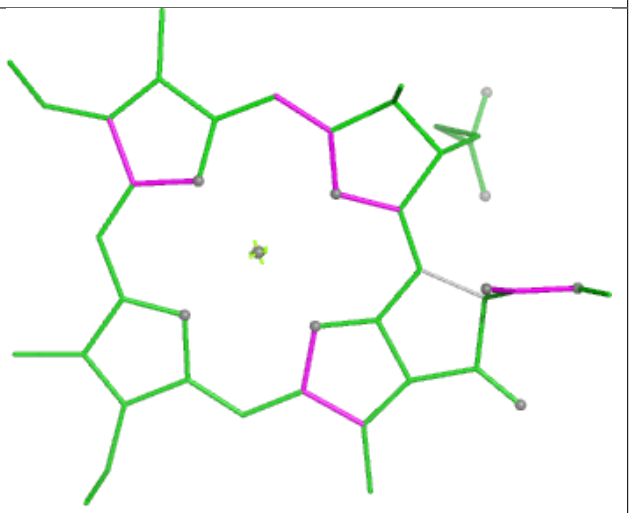
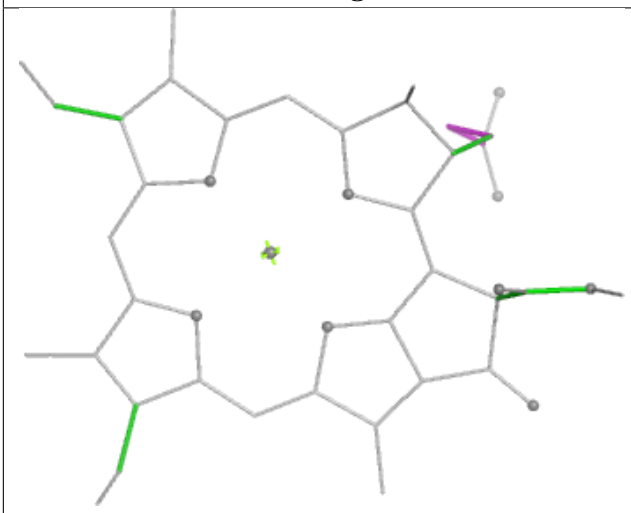


Bond angles



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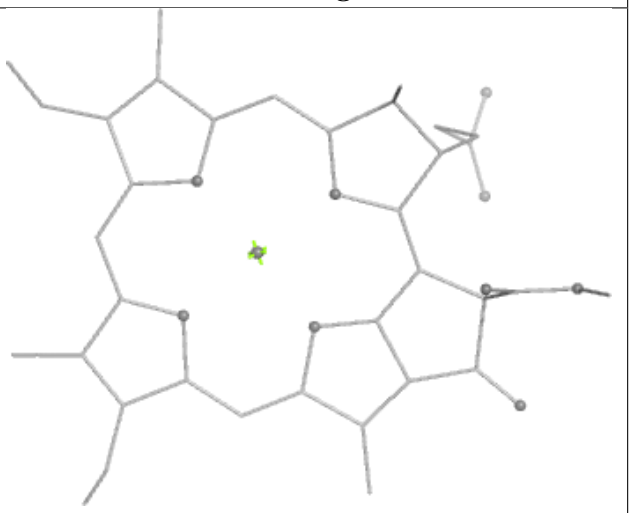
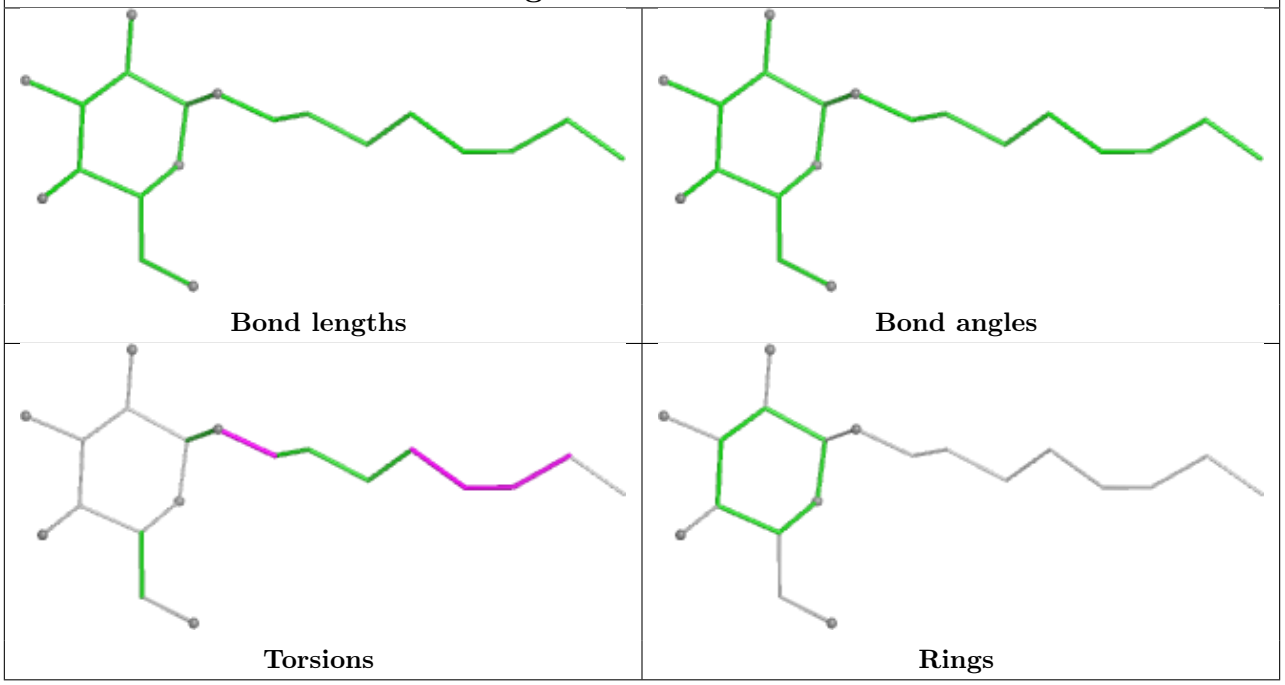
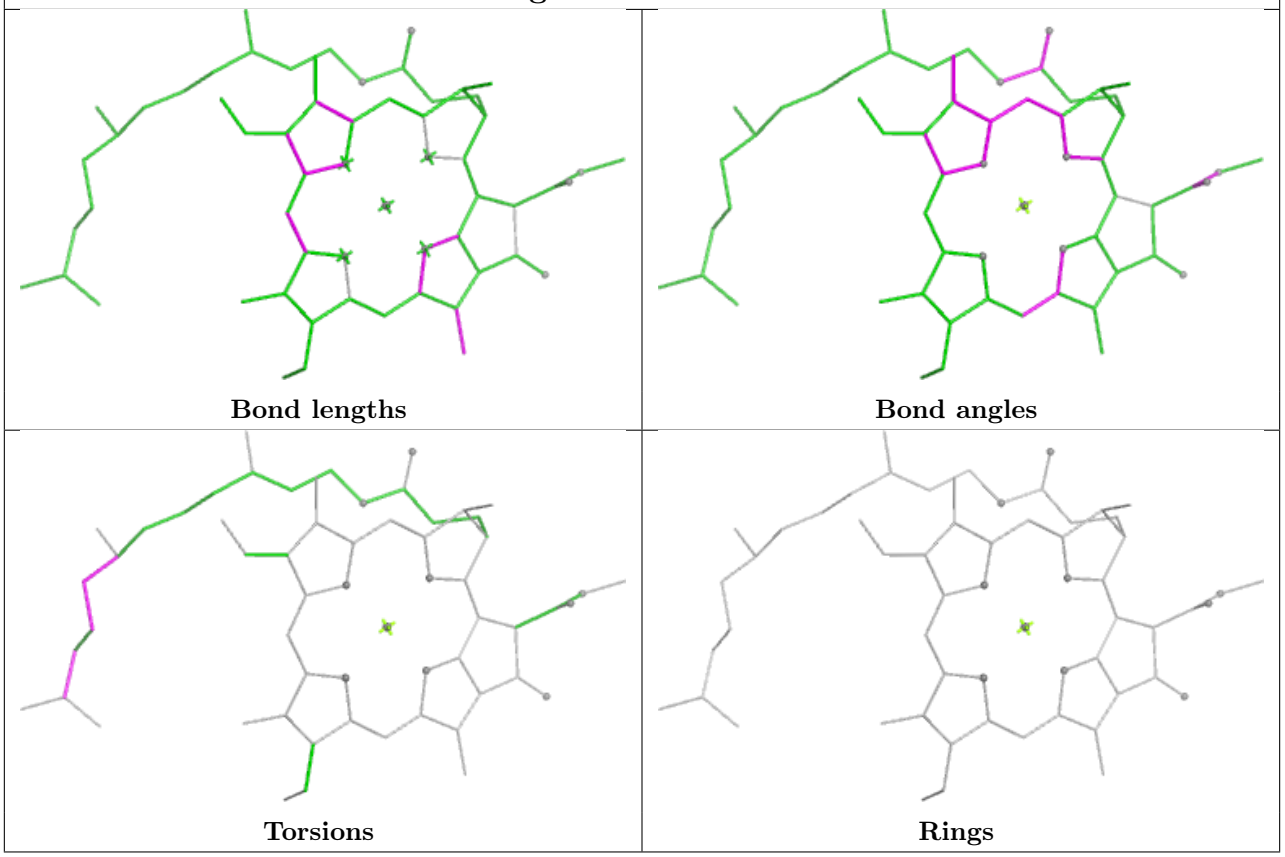


Rings

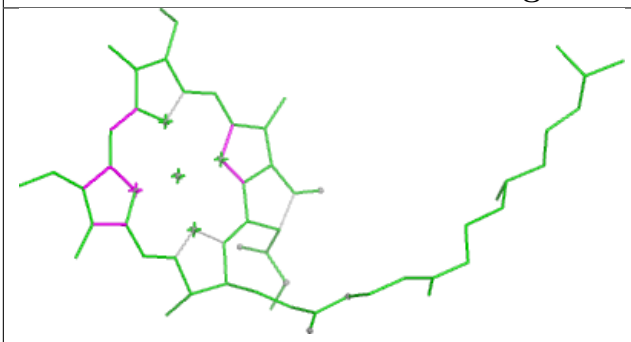
Ligand LMU 4 623



Ligand CLA 5 310



Ligand CLA K 203



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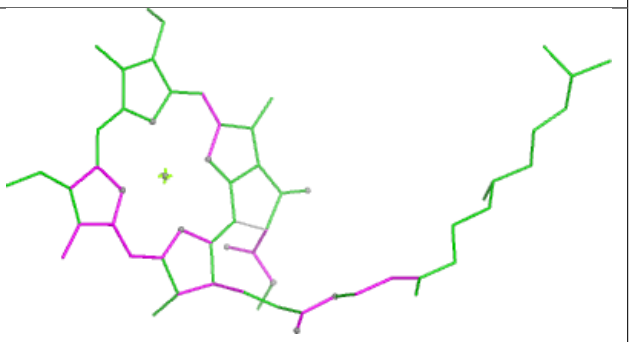
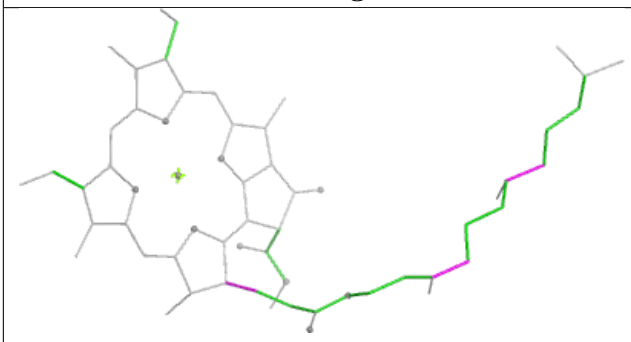


Bond angles



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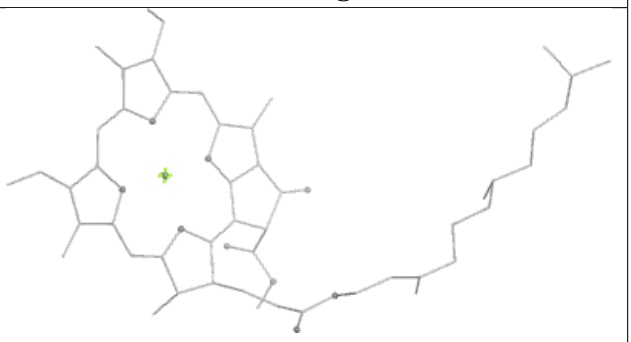
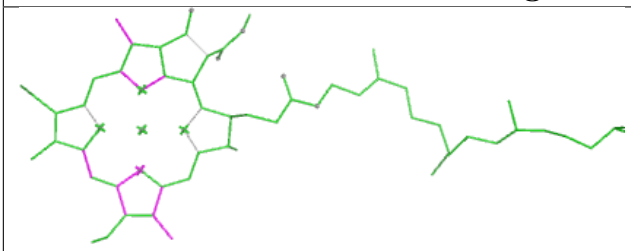


Rings

Ligand CLA A 835



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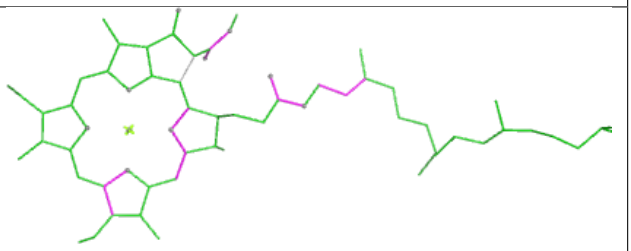

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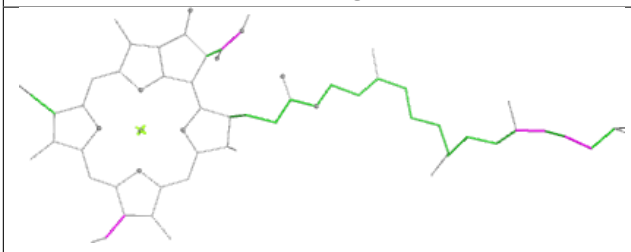

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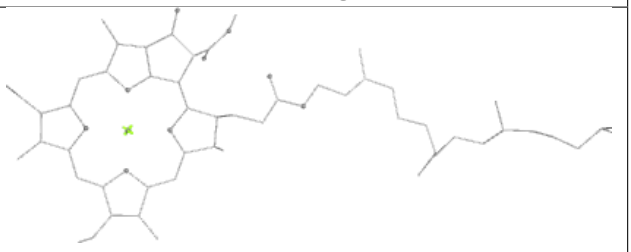
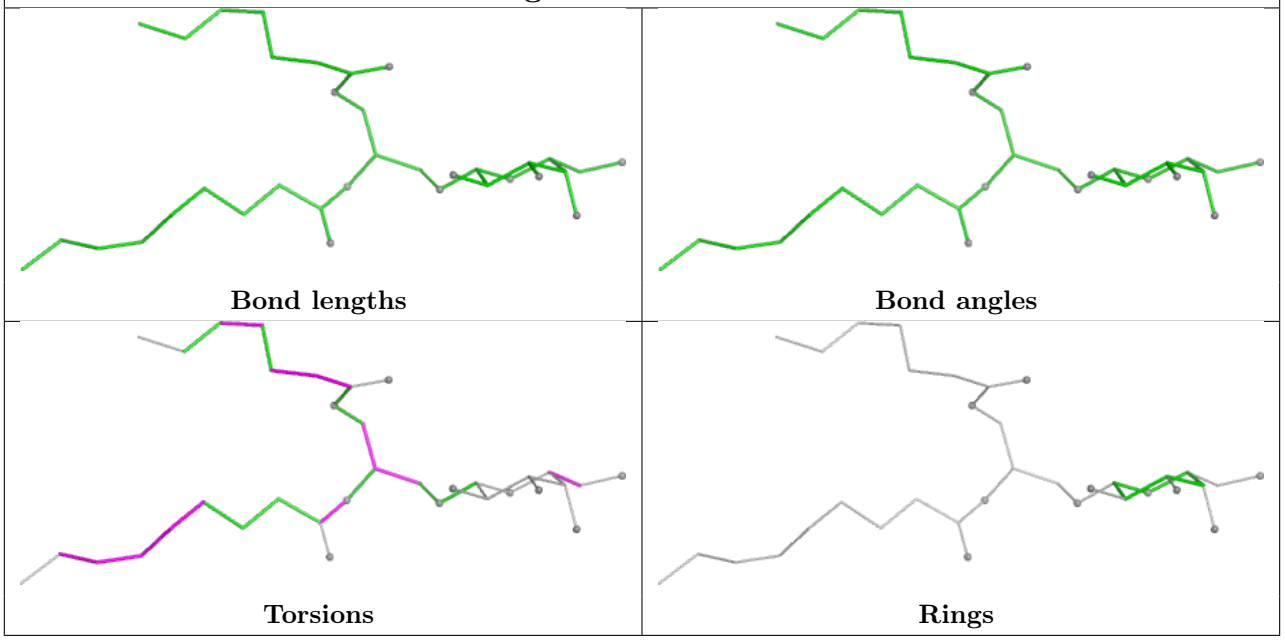
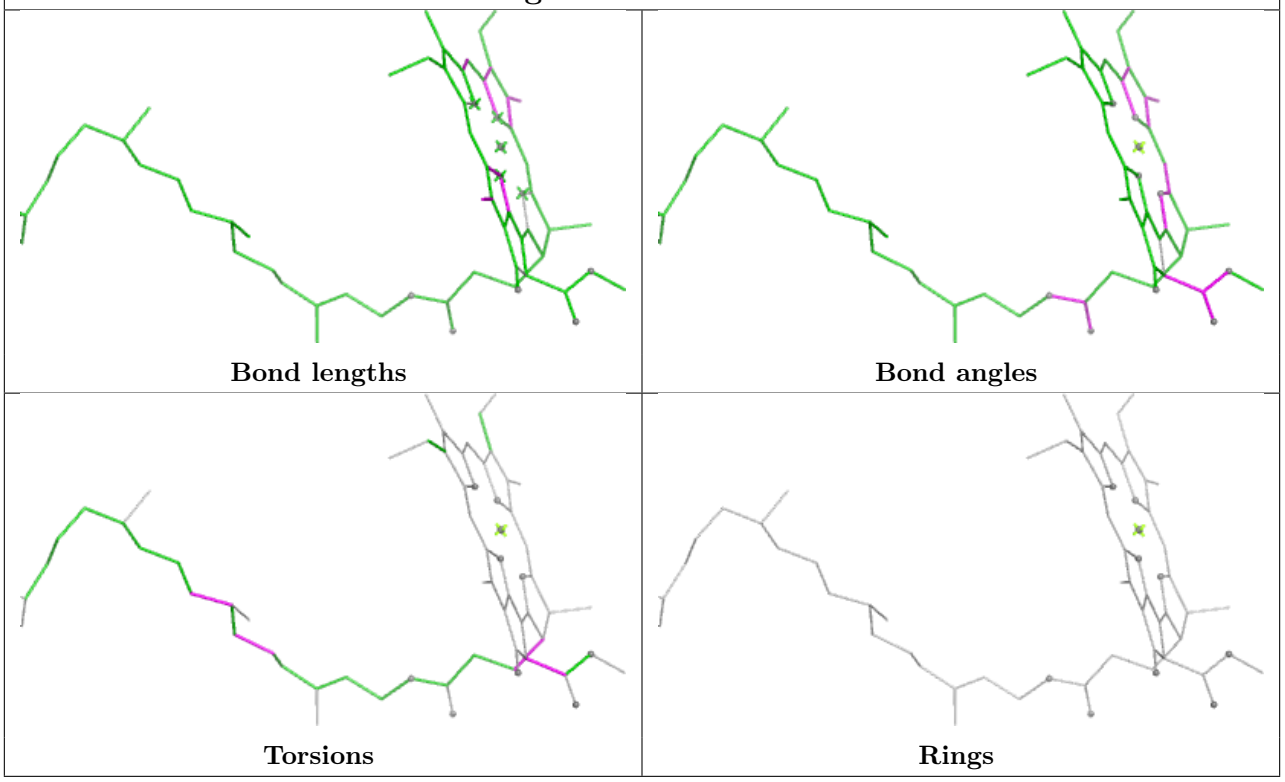


Rings

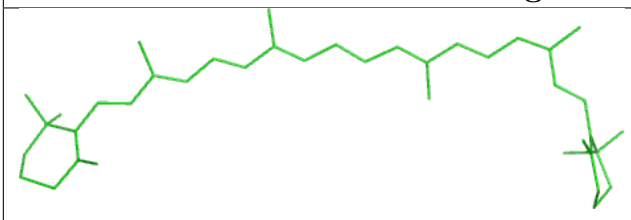
Ligand LMG J 105



Ligand CLA A 832



Ligand BCR L 202



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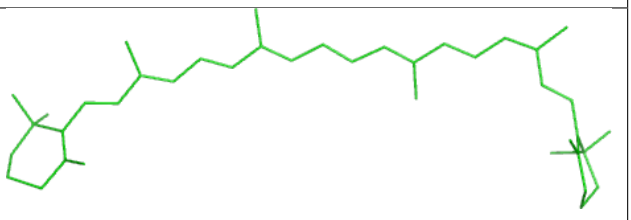
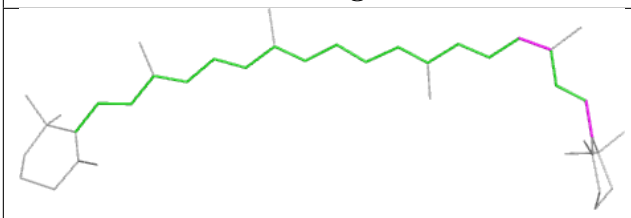


Bond angles



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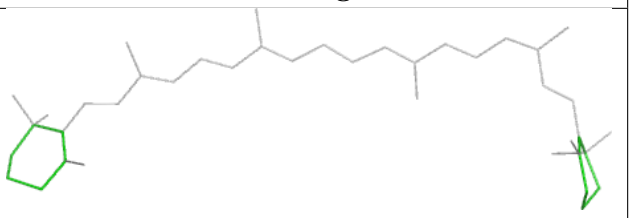
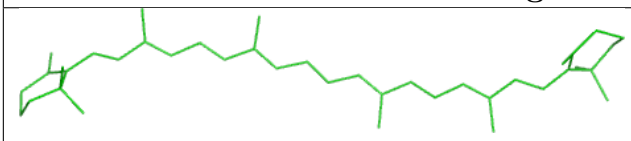


Rings

Ligand BCR 5 320



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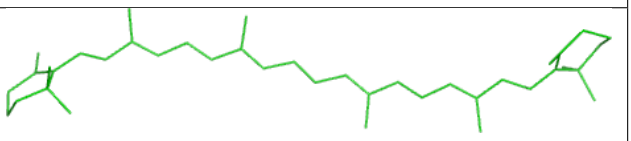
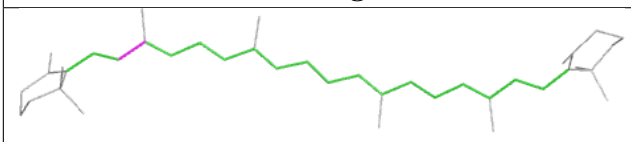


Bond angles



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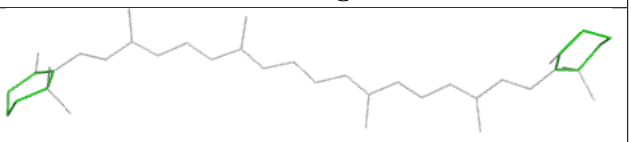
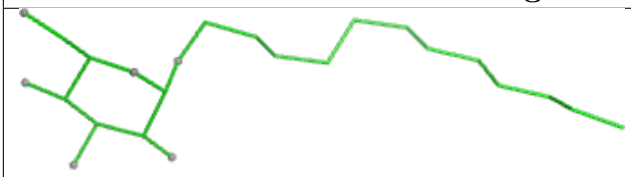


Rings

Ligand LMU 1 321



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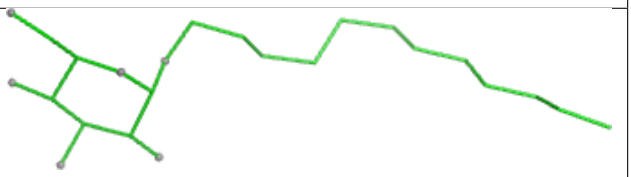
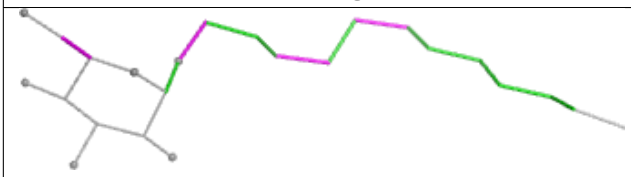


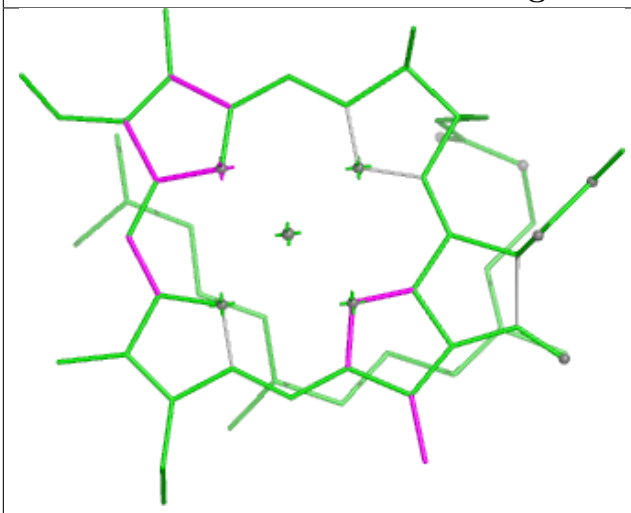
Bond angles



Torsions

Rings

Ligand CLA 1 313



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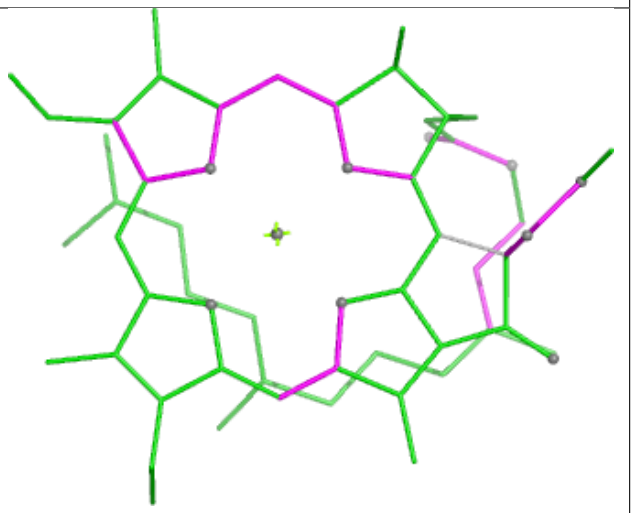
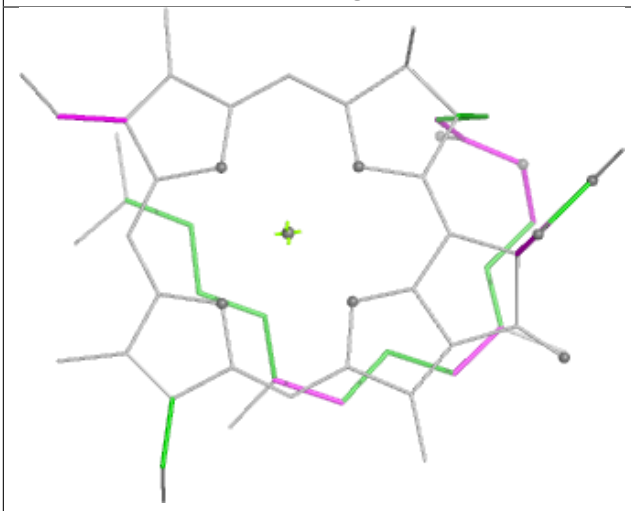


Bond angles



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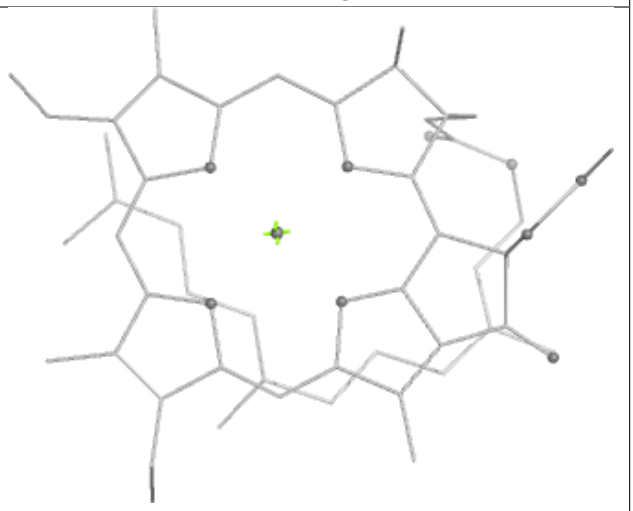
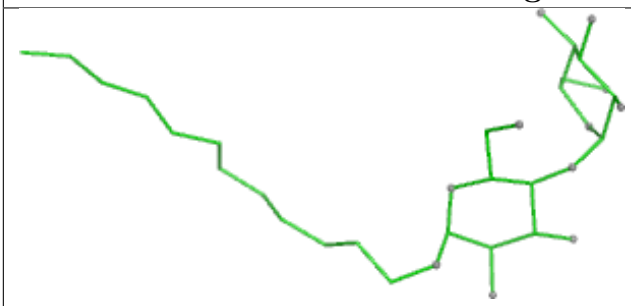


Rings

Ligand LMU 1 301



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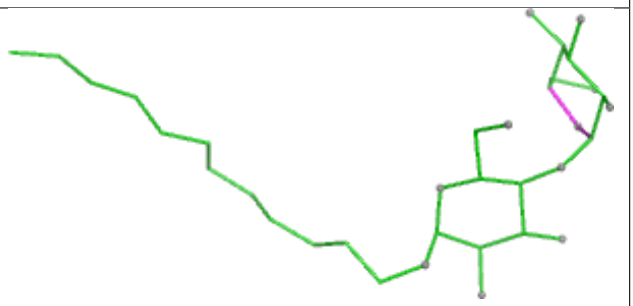
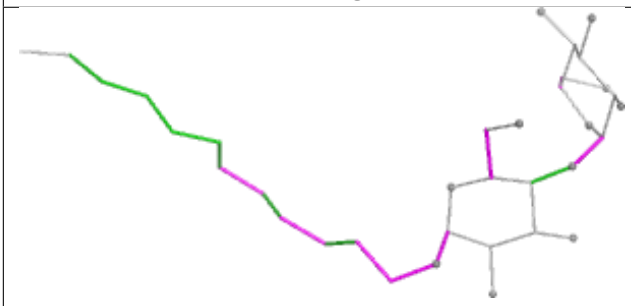


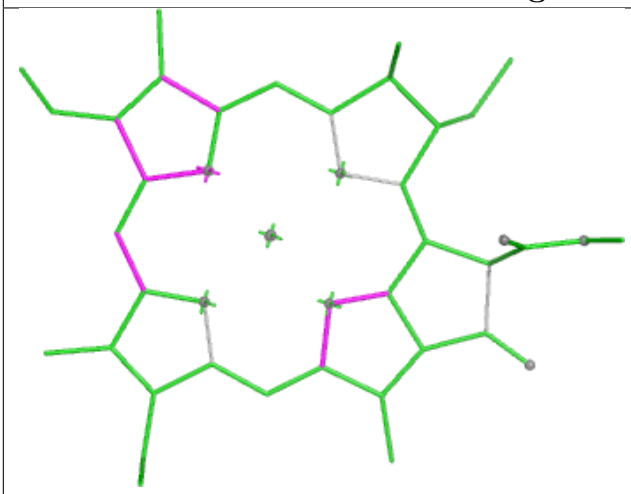
Bond angles



Torsions

Rings

Ligand CLA 3 304



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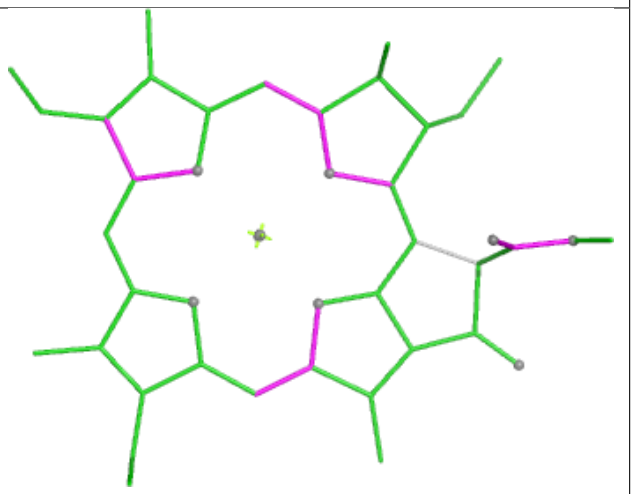
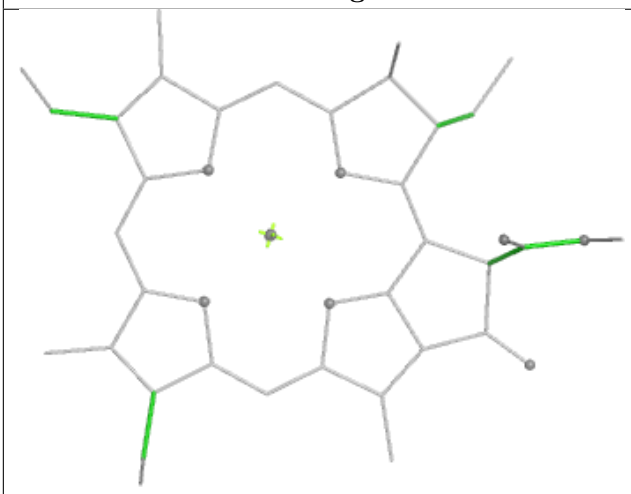


Bond angles



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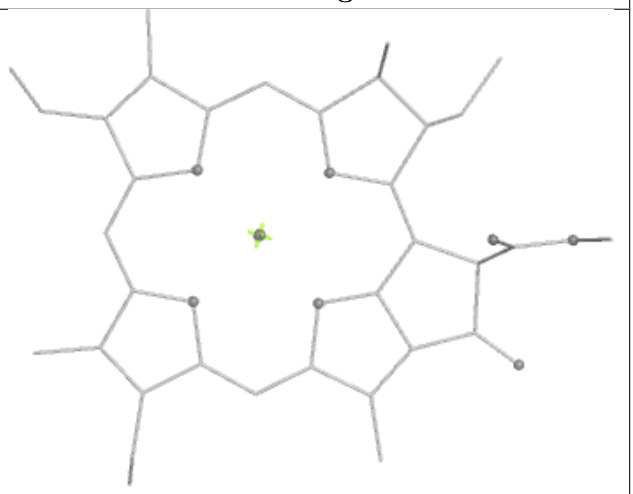
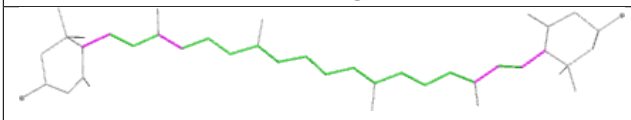


Rings

Ligand LUT 8 301

Bond lengths

Bond angles



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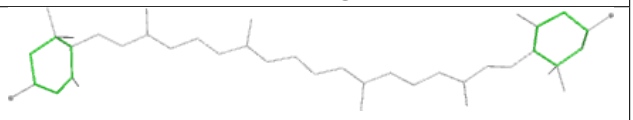
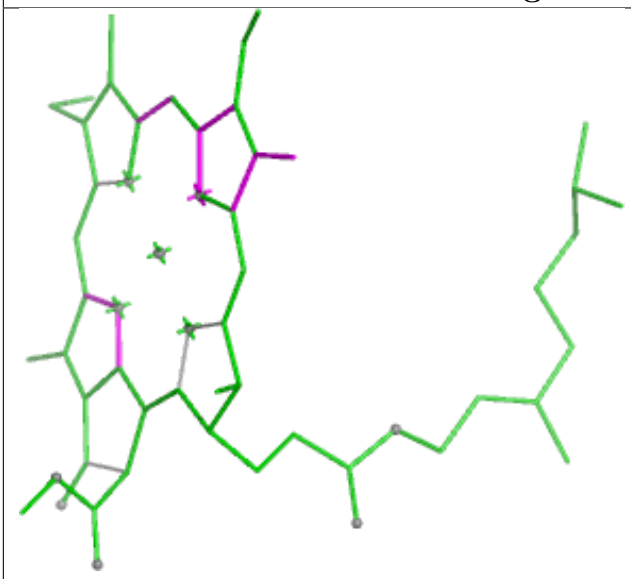
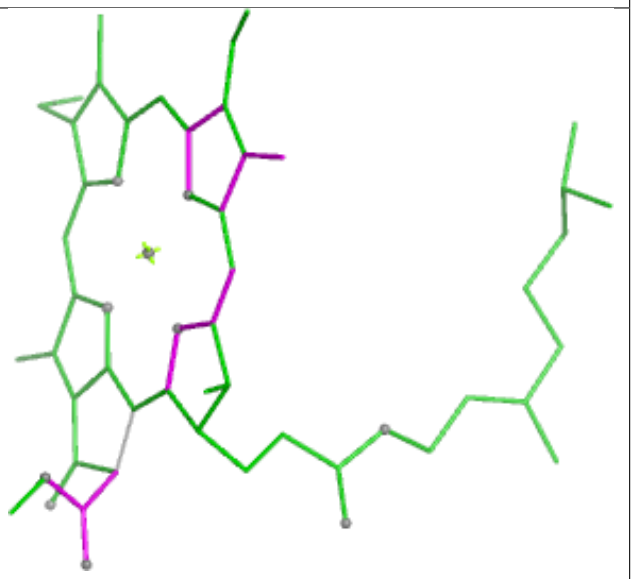


Rings

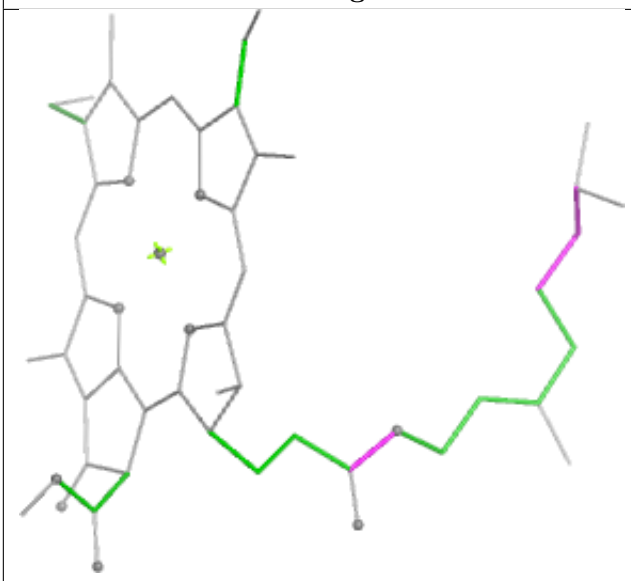
Ligand CLA A 818



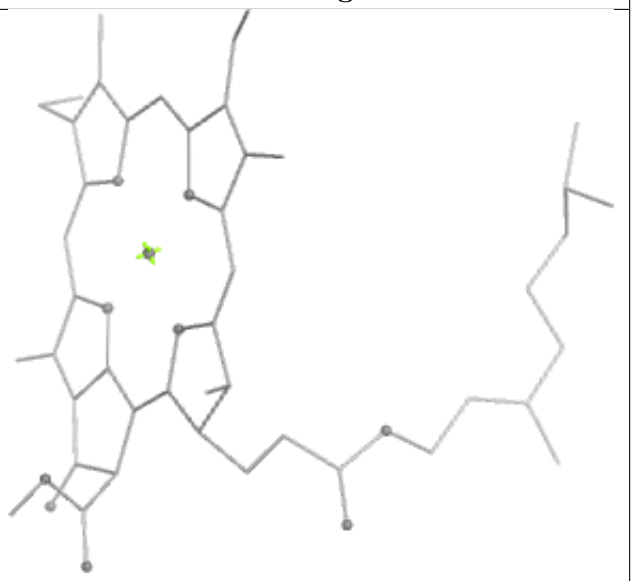
Bond lengths



Bond angles

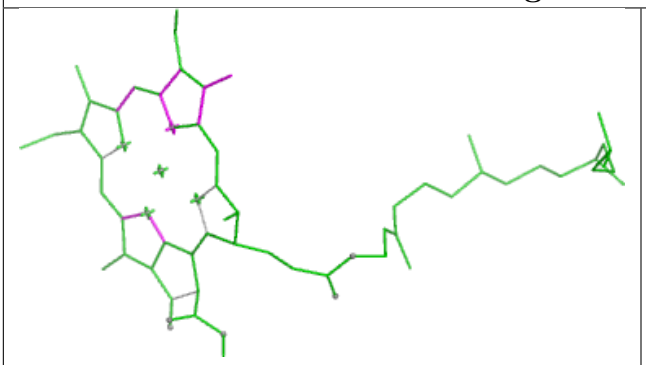


Torsions



Rings

Ligand CLA B 810



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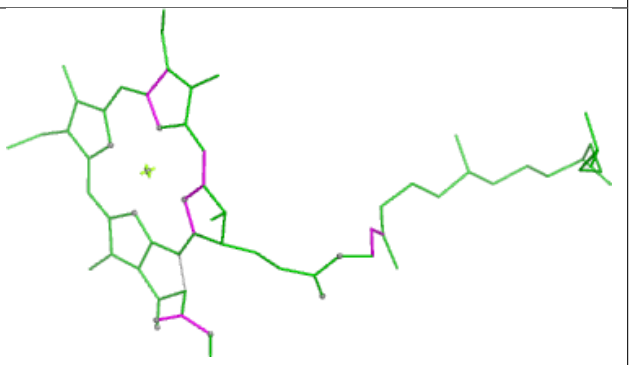

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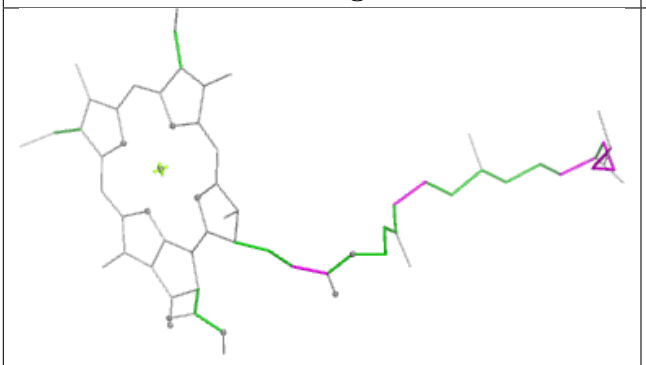

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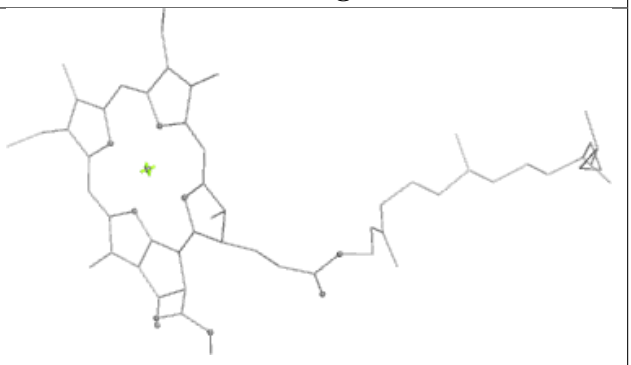
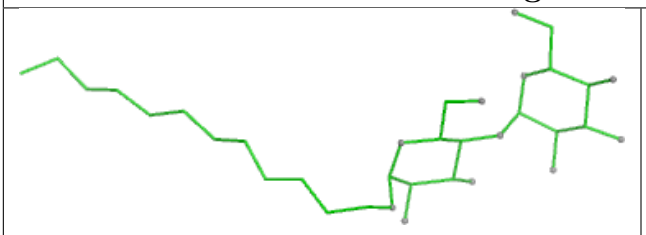


Rings

Ligand LMU 1 319



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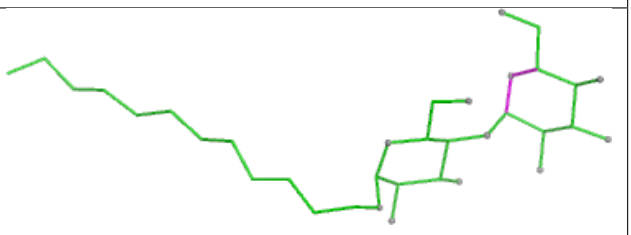

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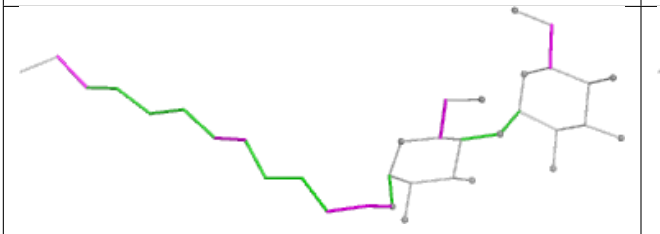

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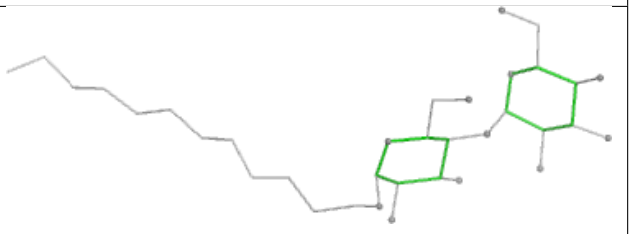
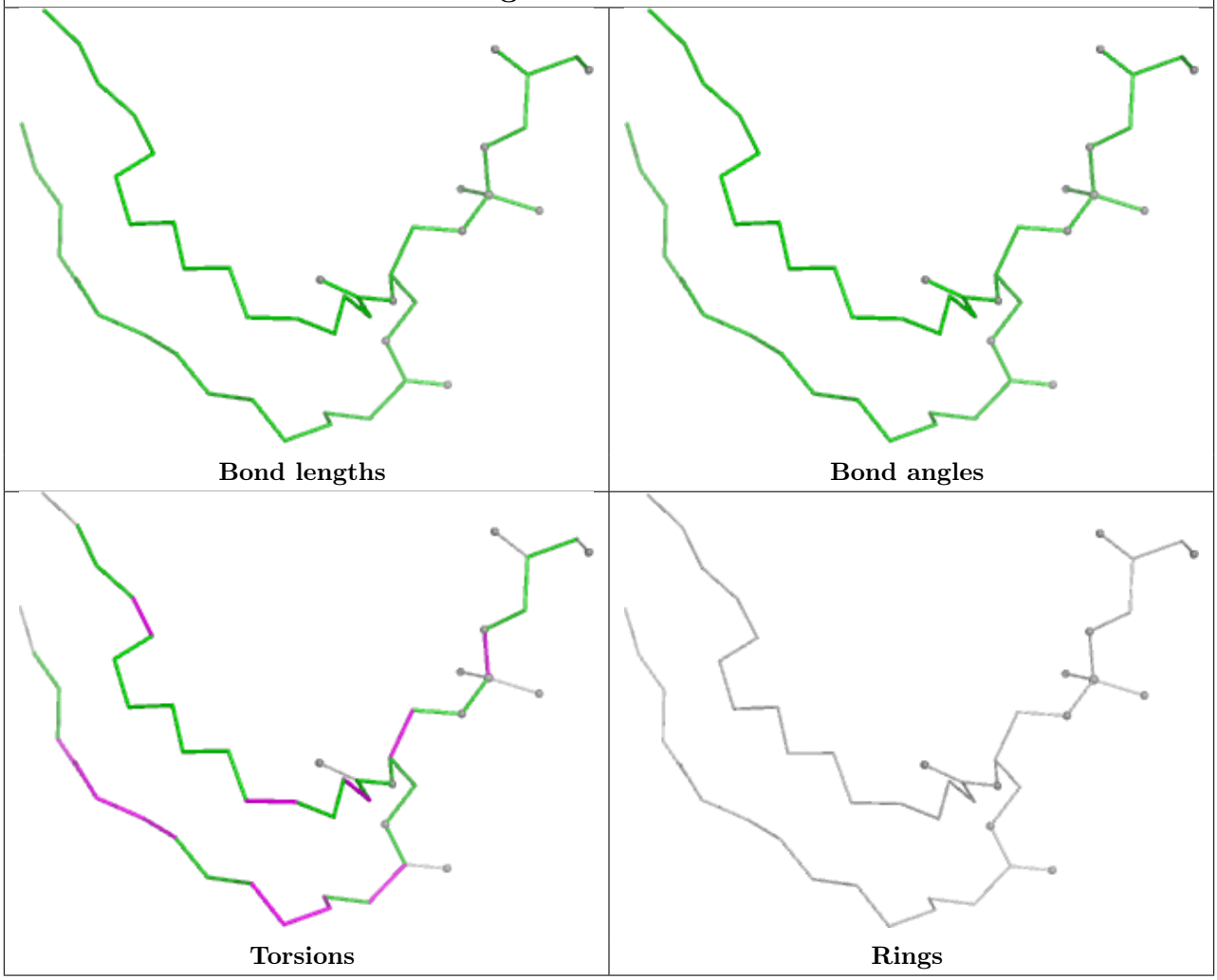
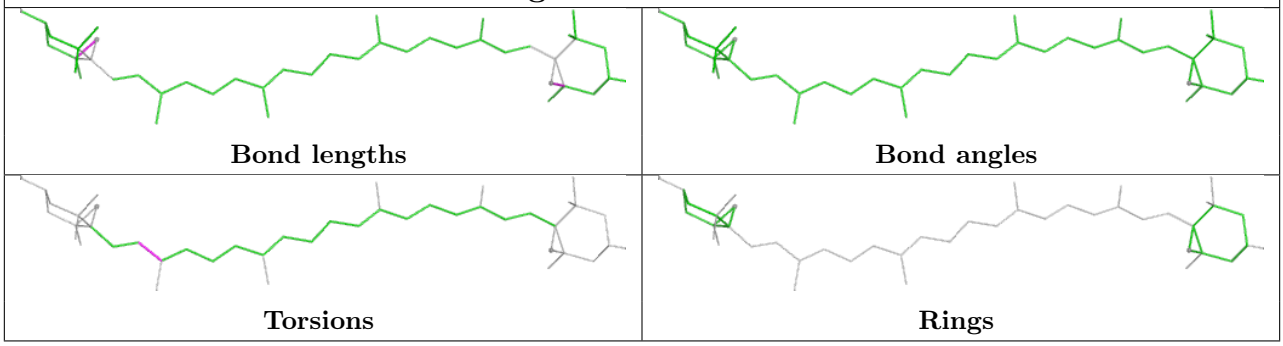


Rings

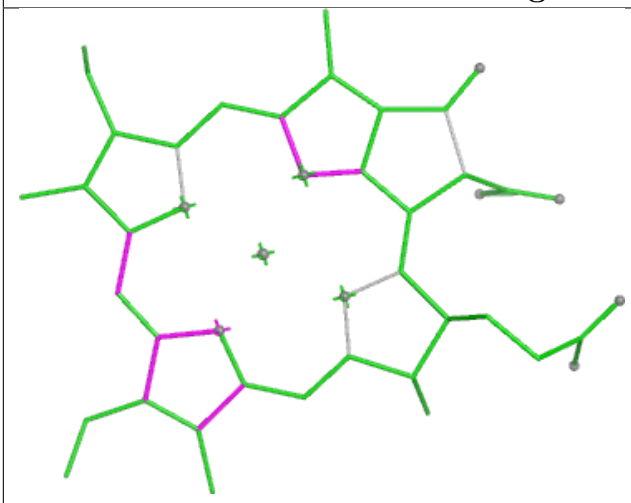
Ligand LHG 7 618



Ligand XAT 5 322



Ligand CLA 4 611



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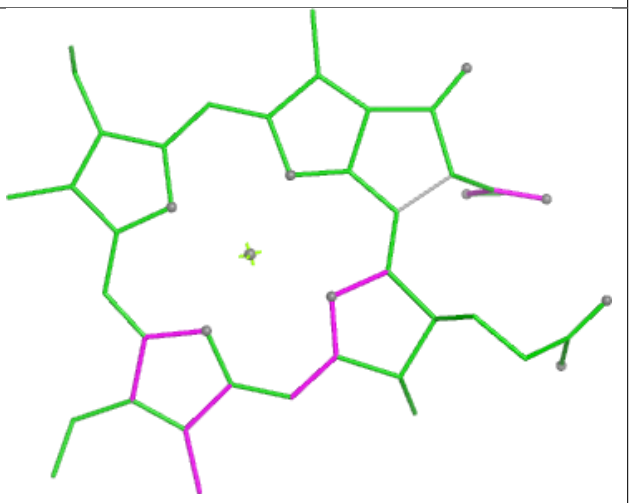

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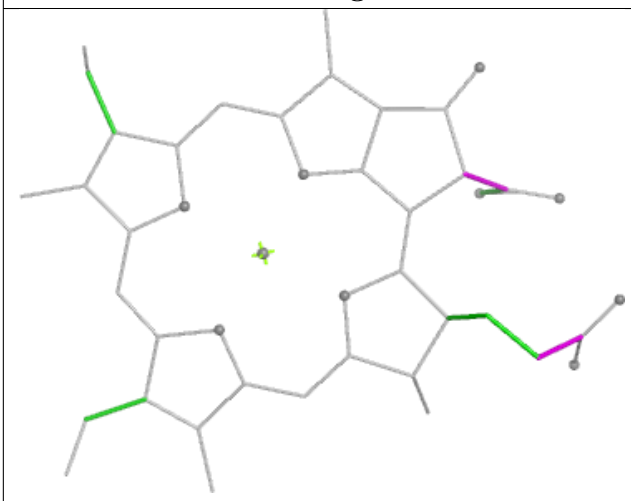

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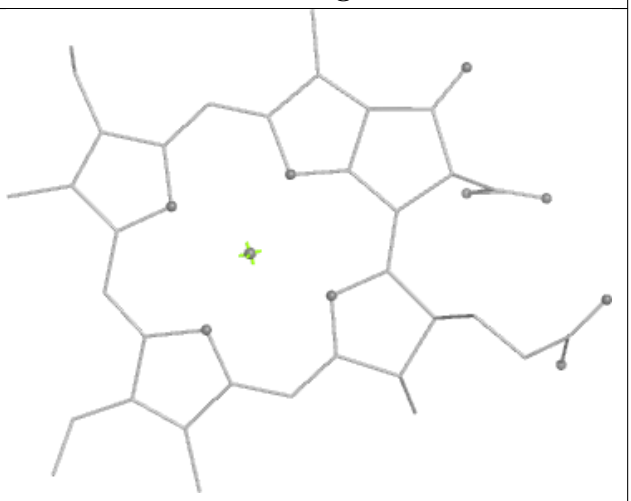
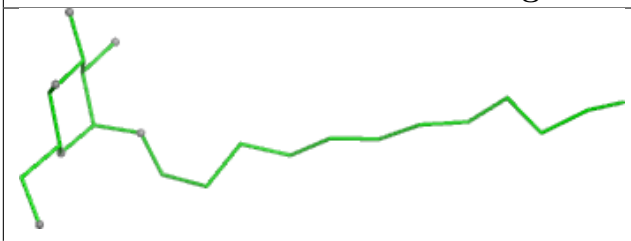


Rings

Ligand LMU Z 621



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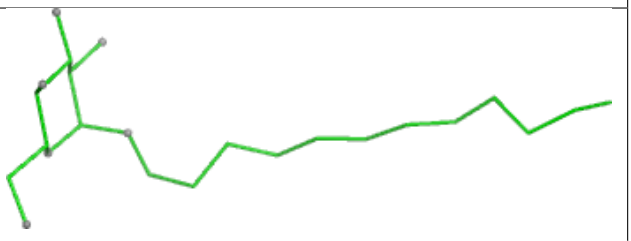

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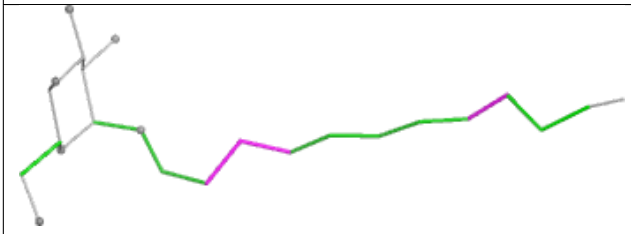

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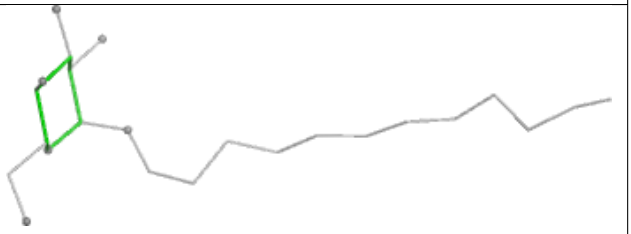
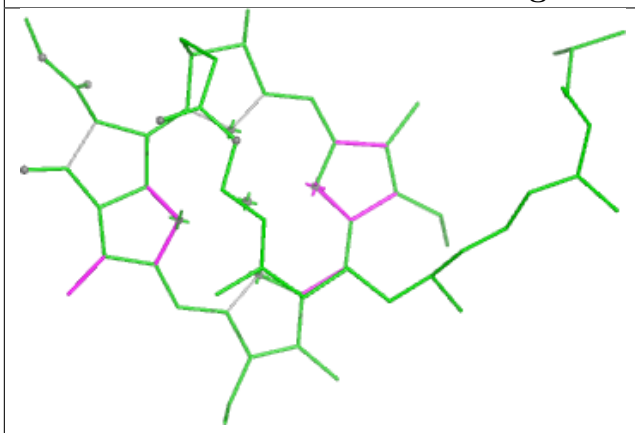


Rings

Ligand CLA 6 313



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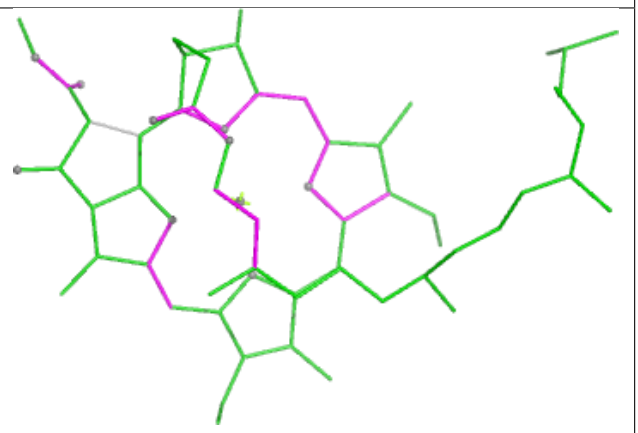

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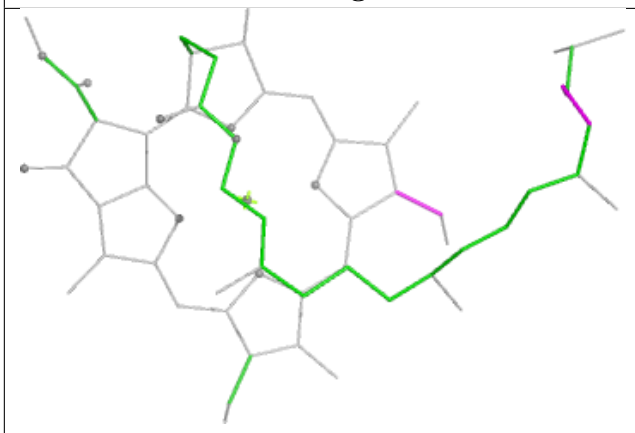

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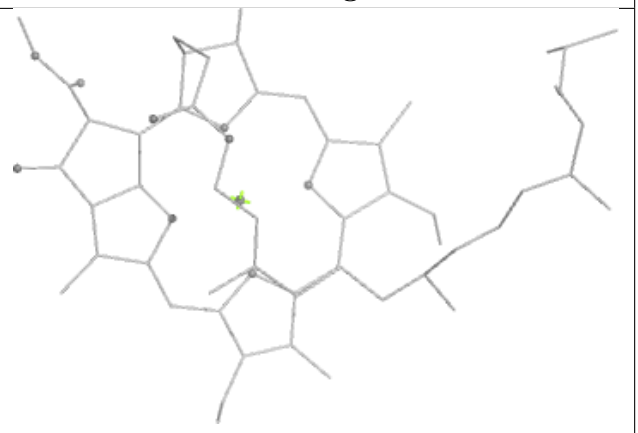
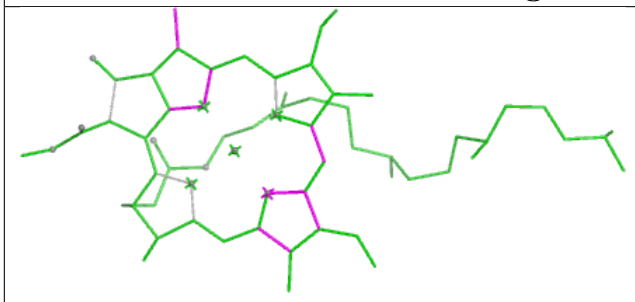


Rings

Ligand CLA A 840



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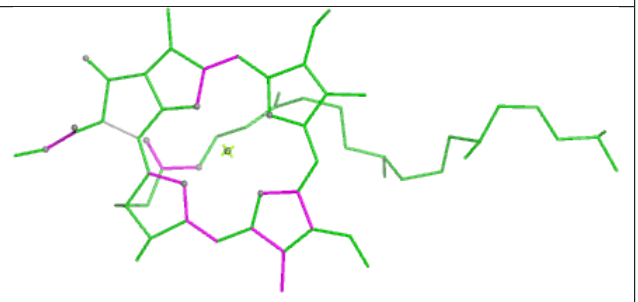

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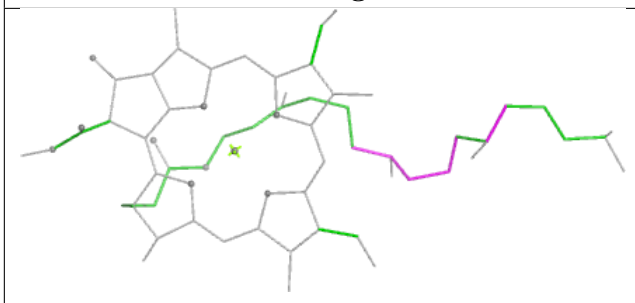

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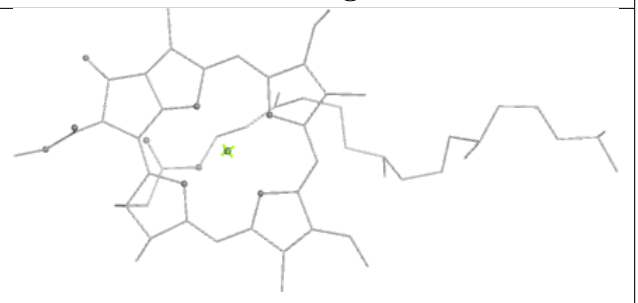
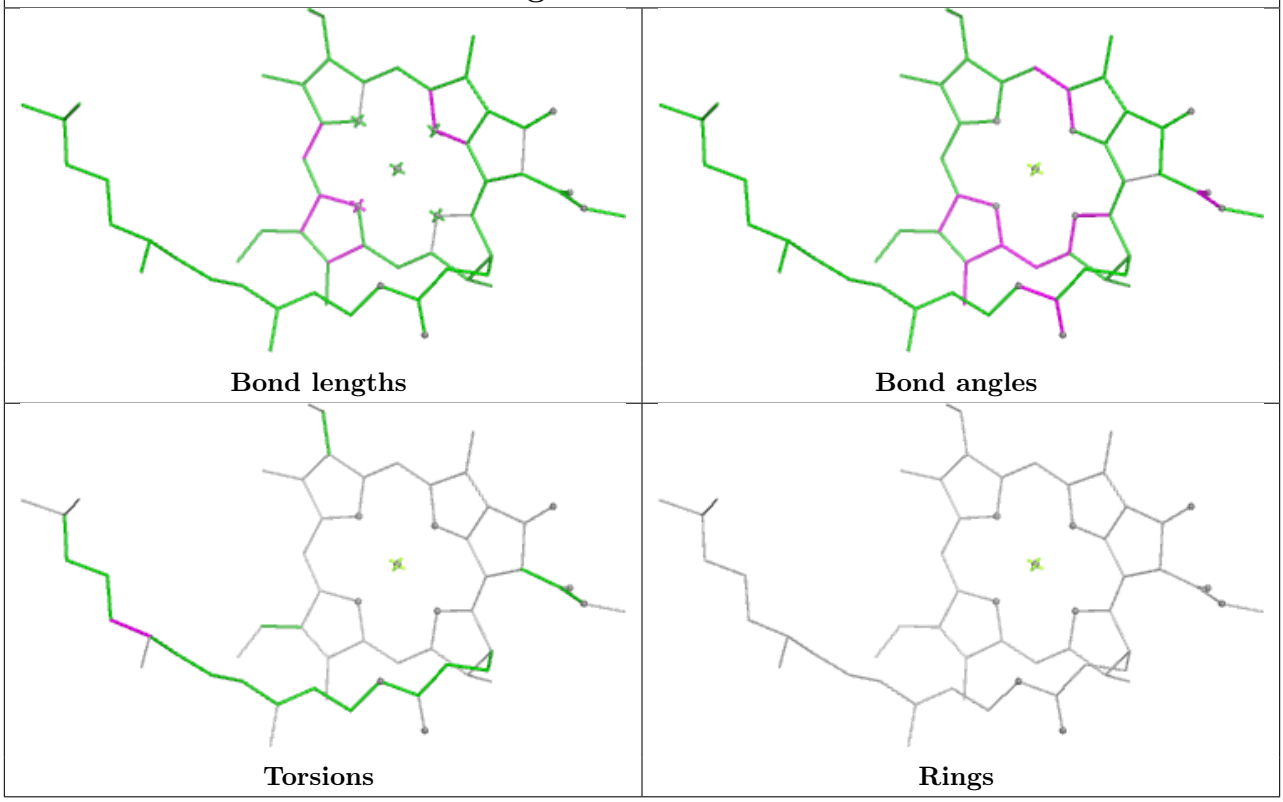
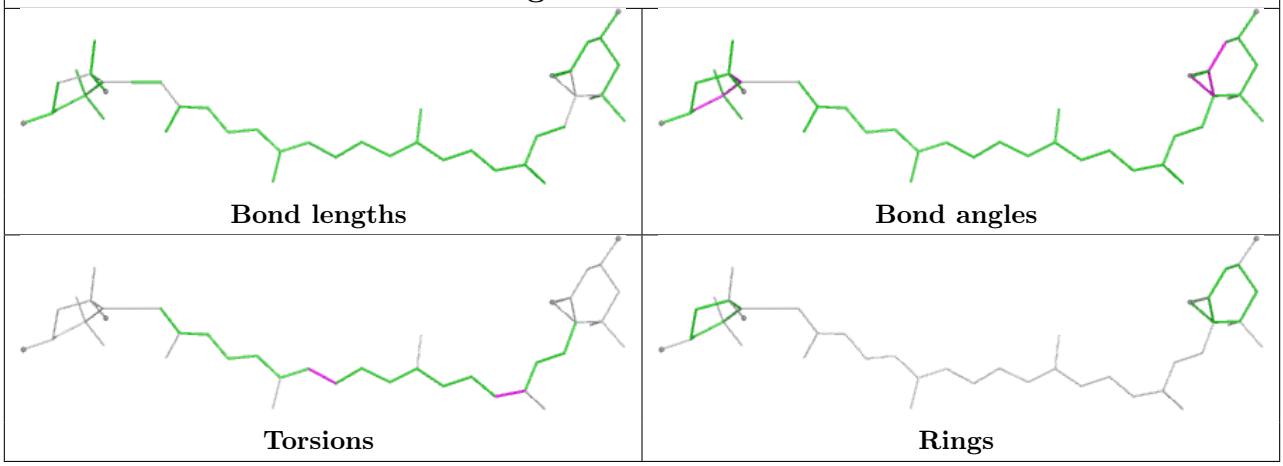


Rings

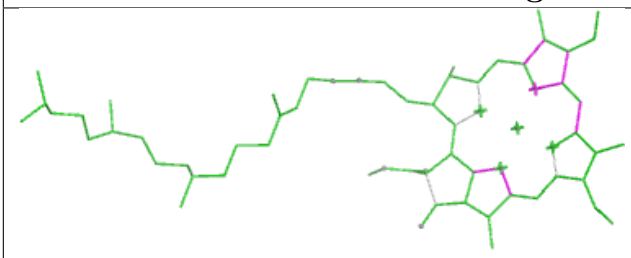
Ligand CLA Z 609



Ligand NEX 6 323



Ligand CLA F 302



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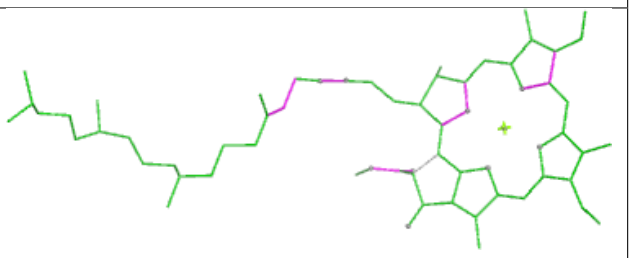
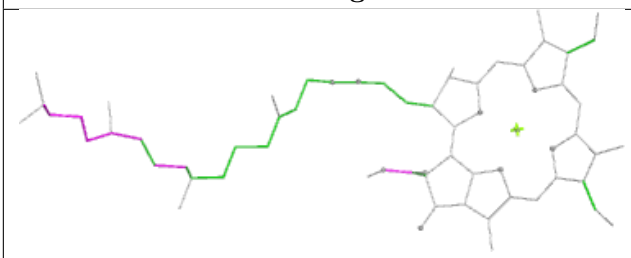


Bond angles



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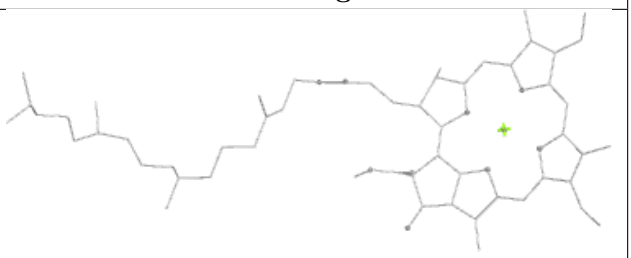
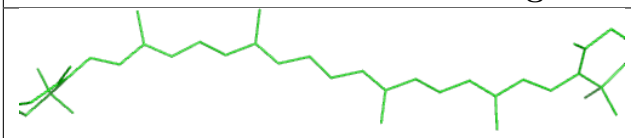


Rings

Ligand BCR 4 618



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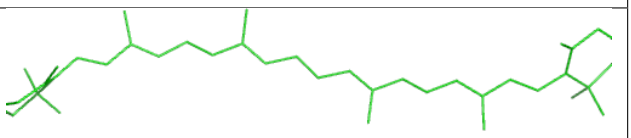

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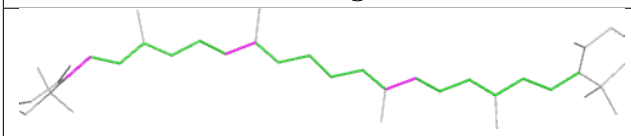

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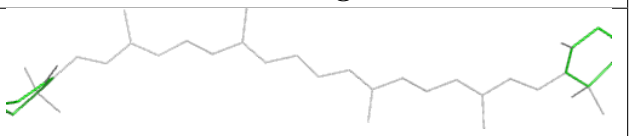
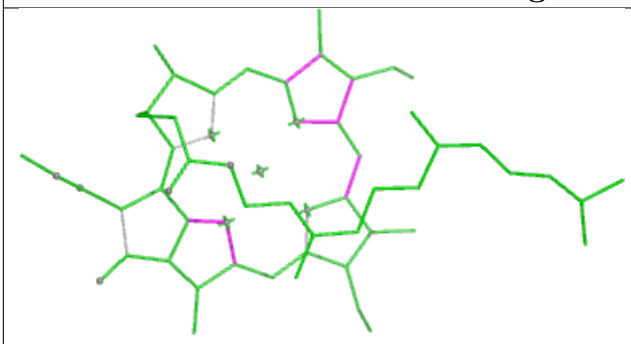


Rings

Ligand CLA 3 311



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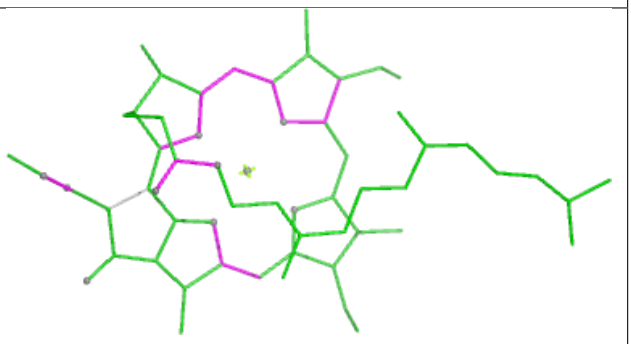
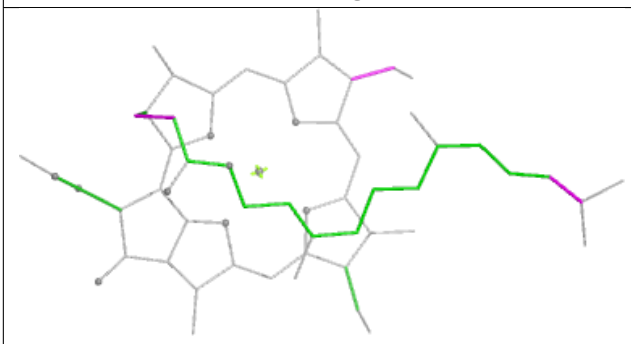


Bond angles



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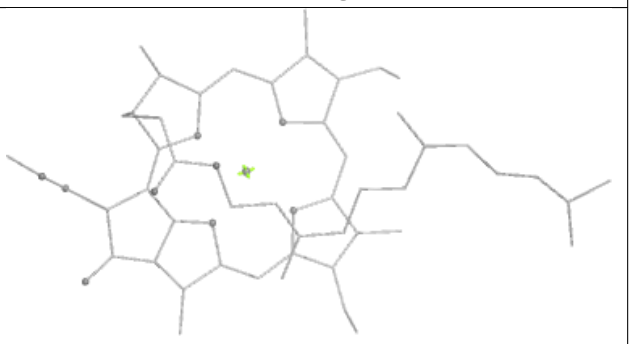
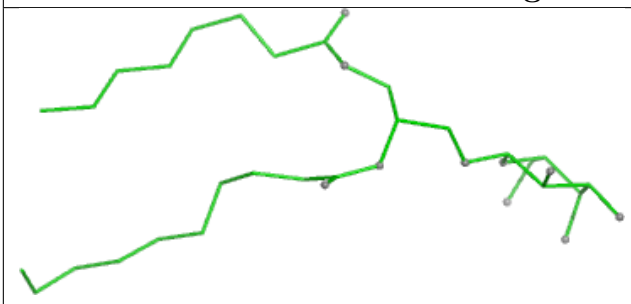


Rings

Ligand LMG 3 321



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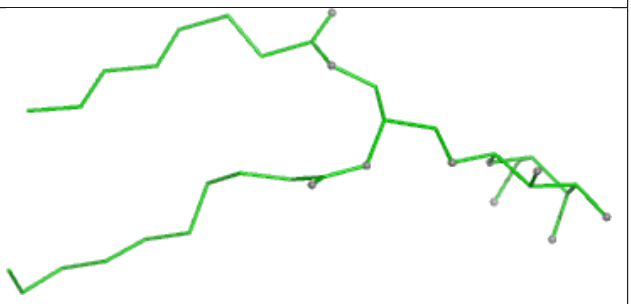

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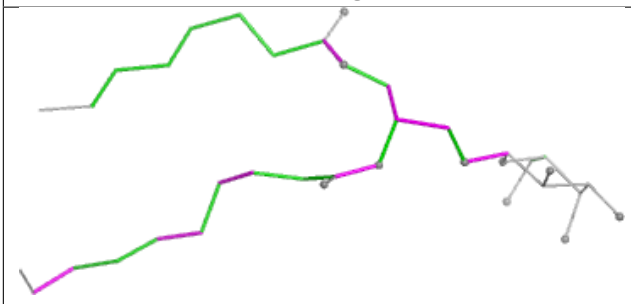

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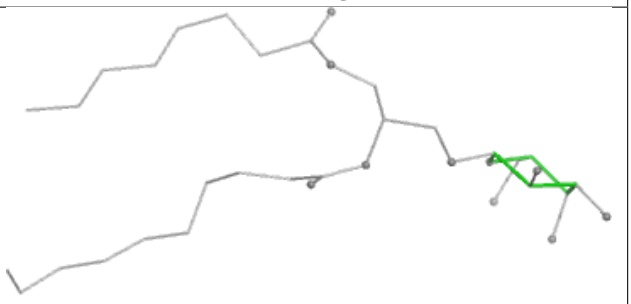
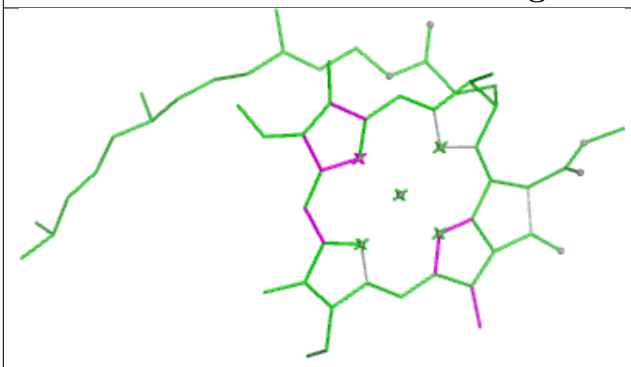


Rings

Ligand CLA 6 310



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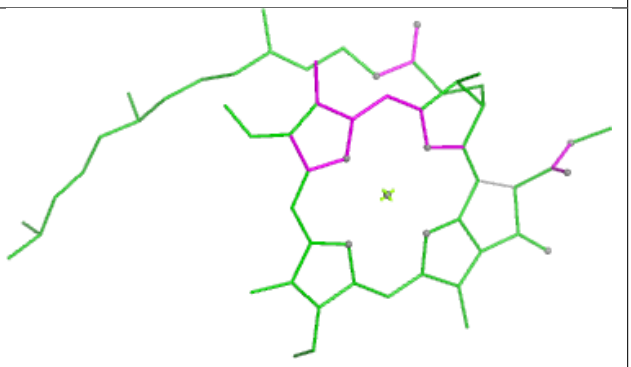

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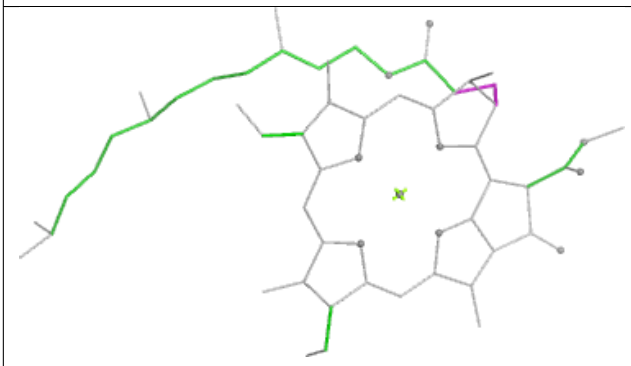

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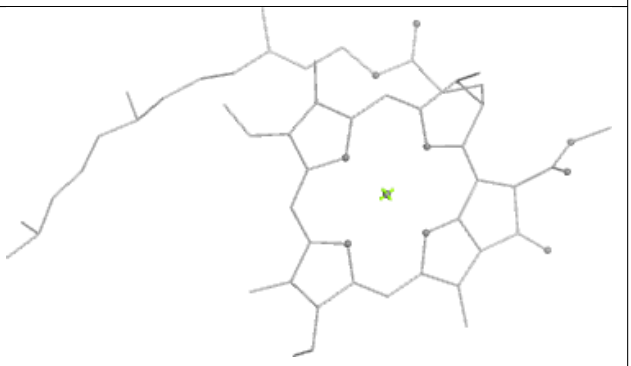
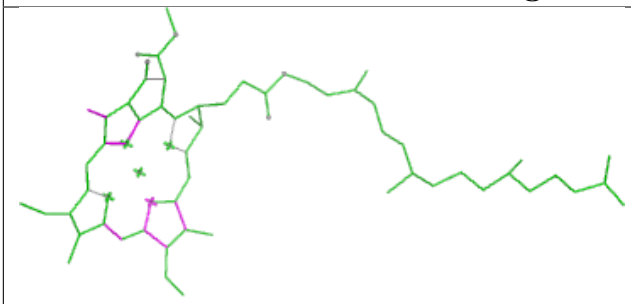


Rings

Ligand CLA A 804



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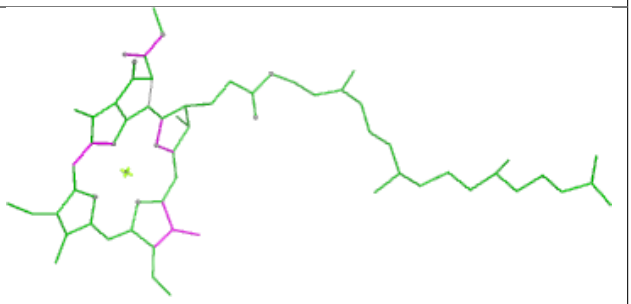
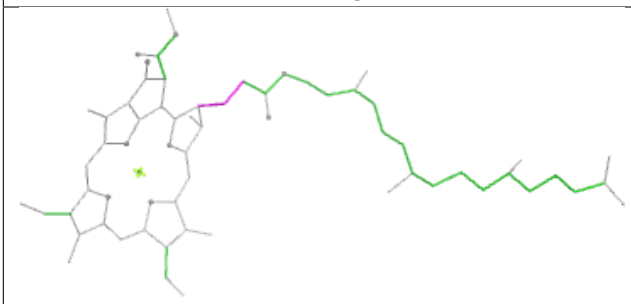


Bond angles



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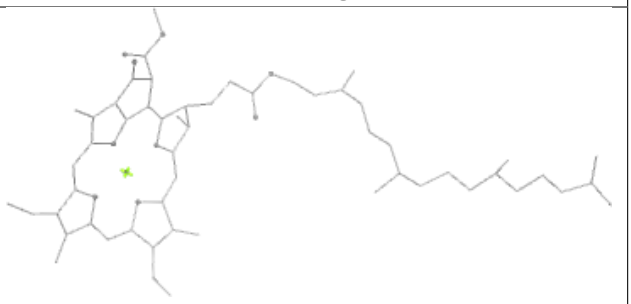
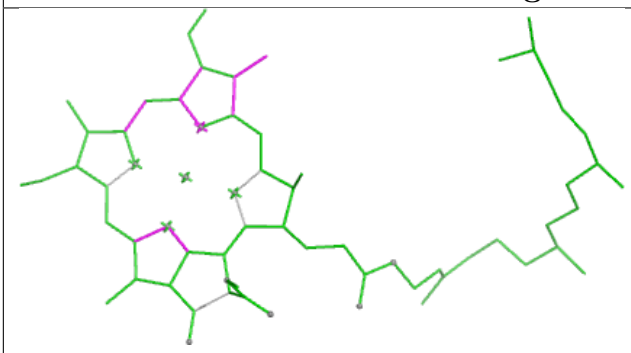


Rings

Ligand CLA A 829



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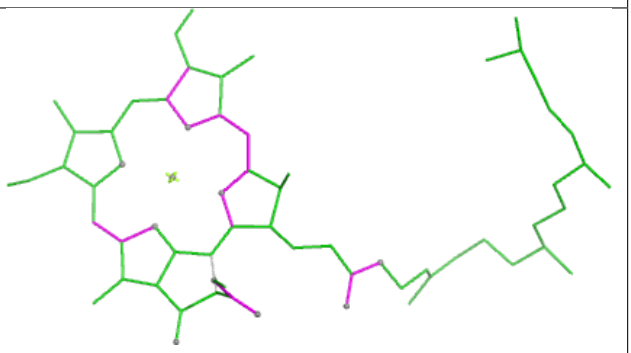
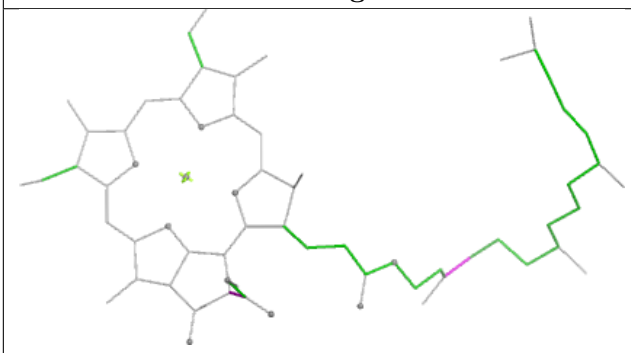
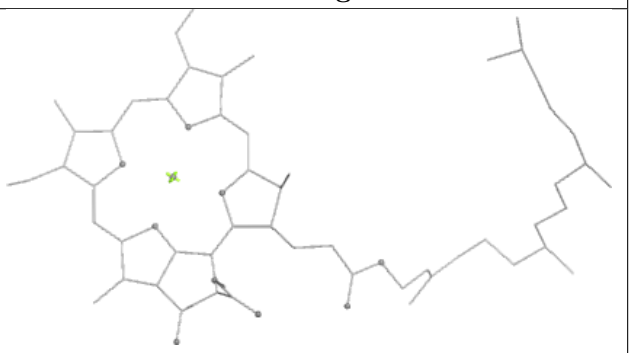


Bond angles

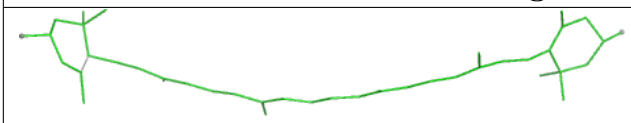


Torsions



Rings

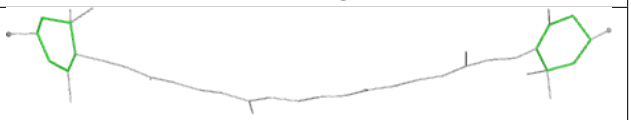
Ligand LUT J 101



Bond lengths

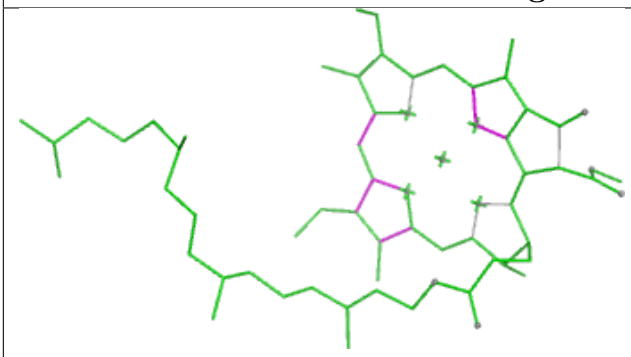
Bond angles

Torsions



Rings

Ligand CLA 8 302



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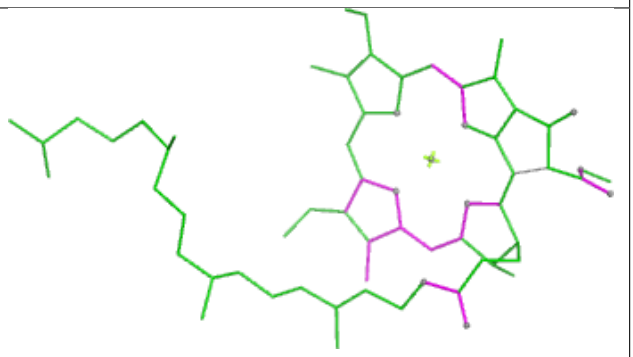

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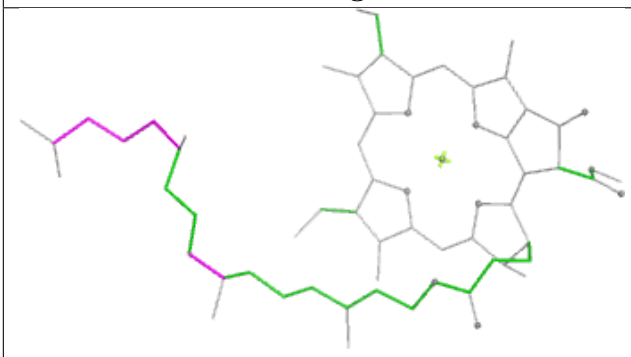

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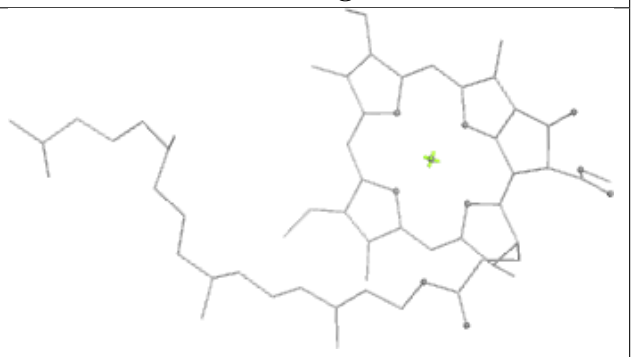
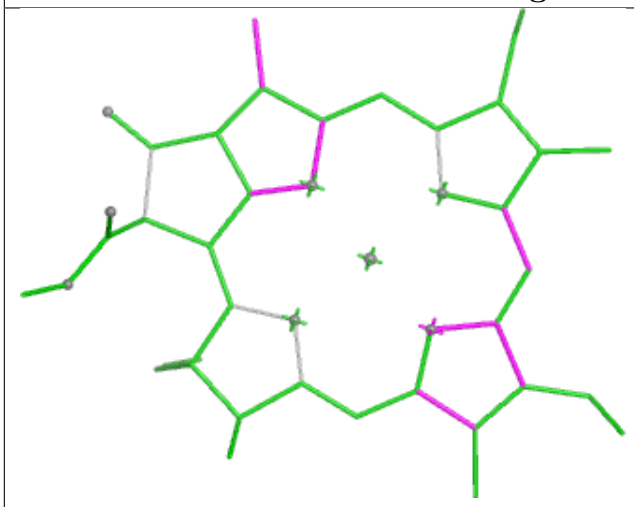


Rings

Ligand CLA 7 613



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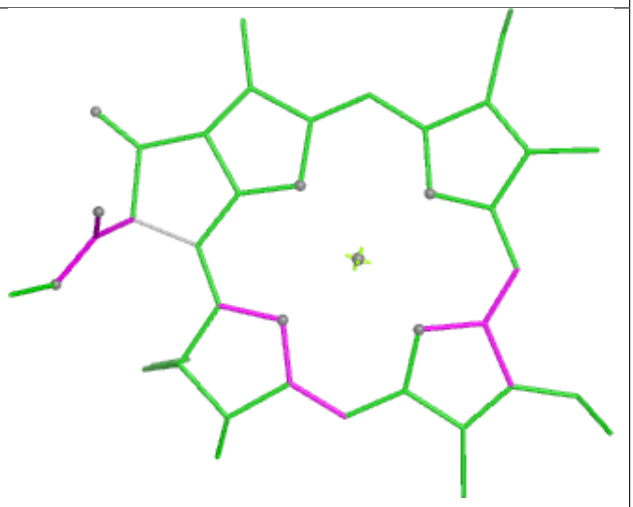

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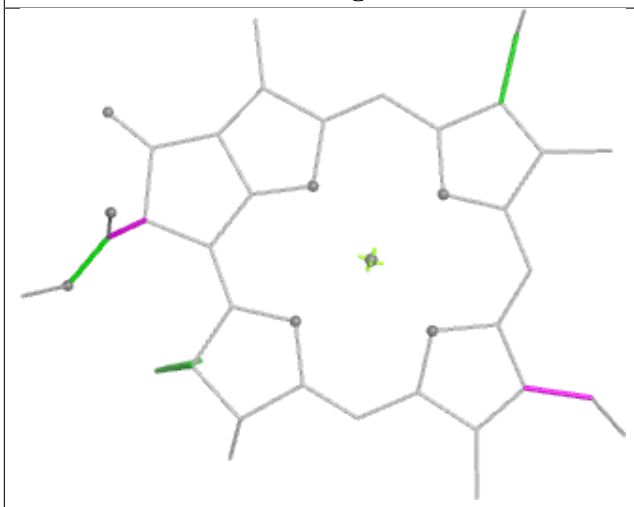

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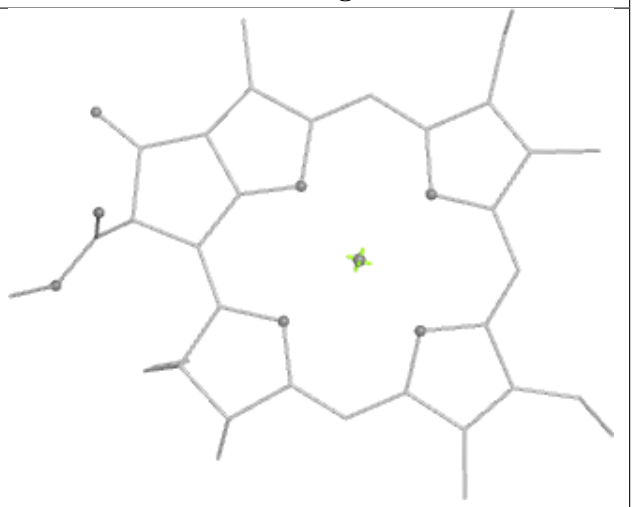
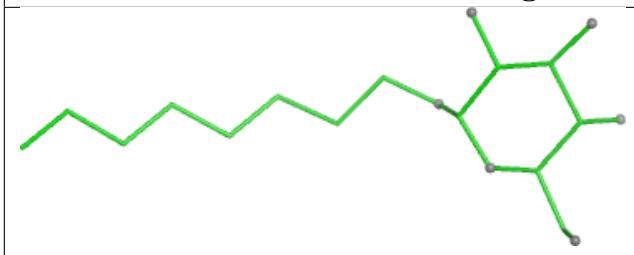


Rings

Ligand LMU A 856



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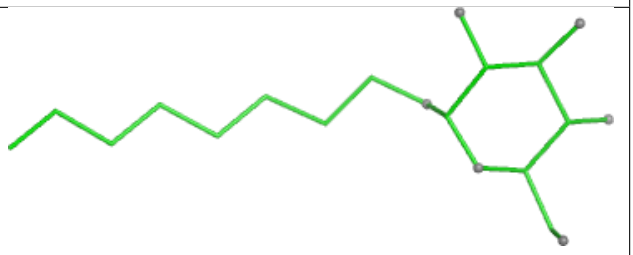

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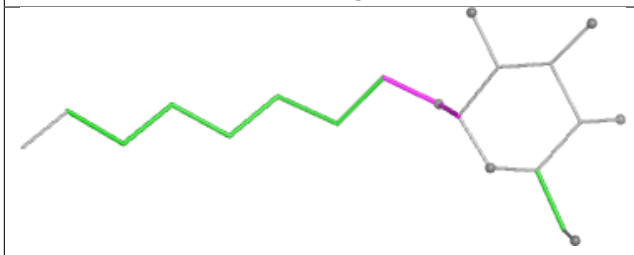

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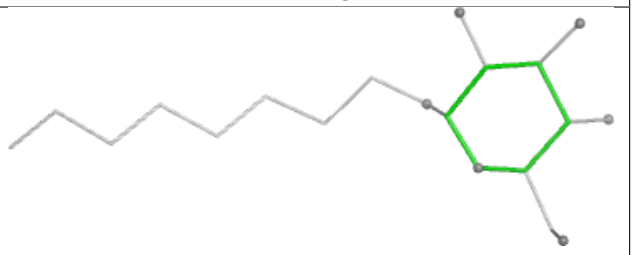
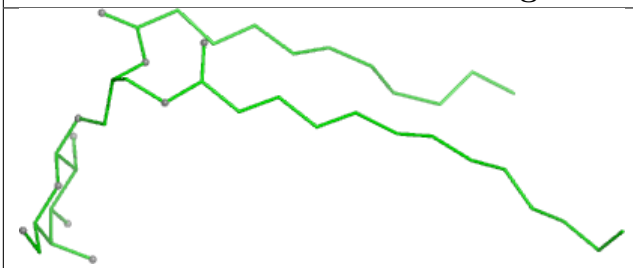


Rings

Ligand LMG B 852



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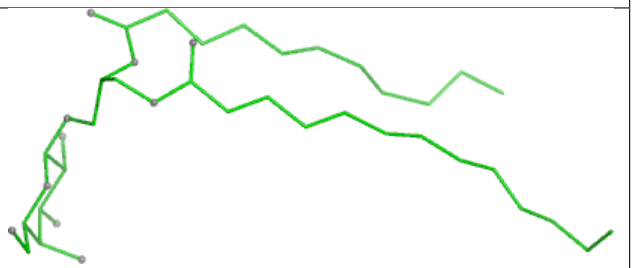
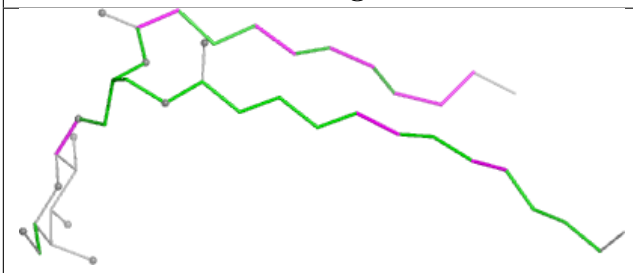


Bond angles



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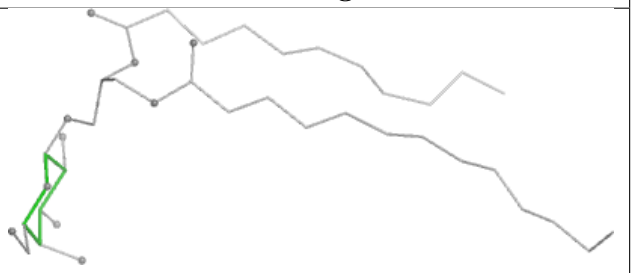
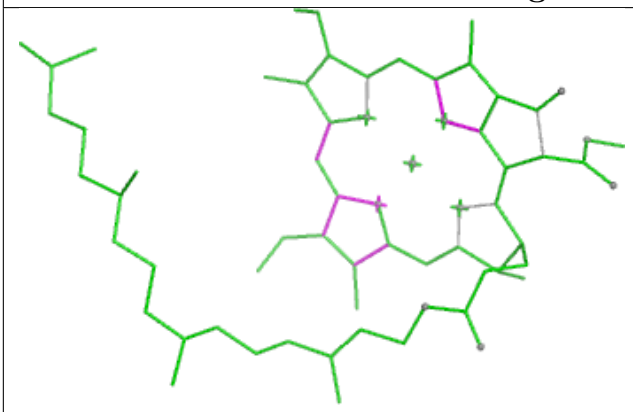
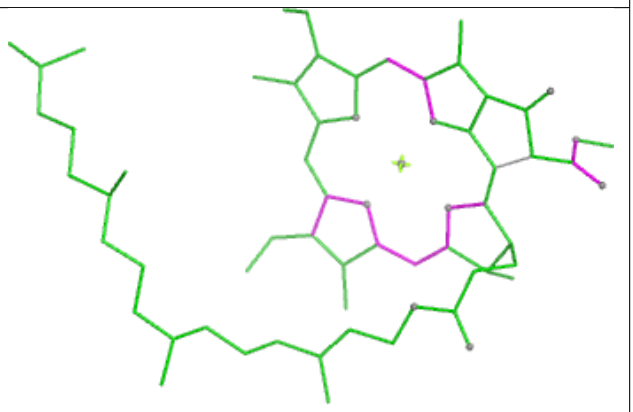


Rings

Ligand CLA 5 303



Bond lengths



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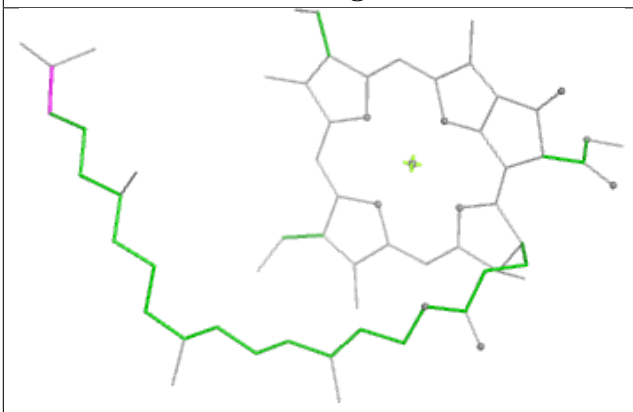

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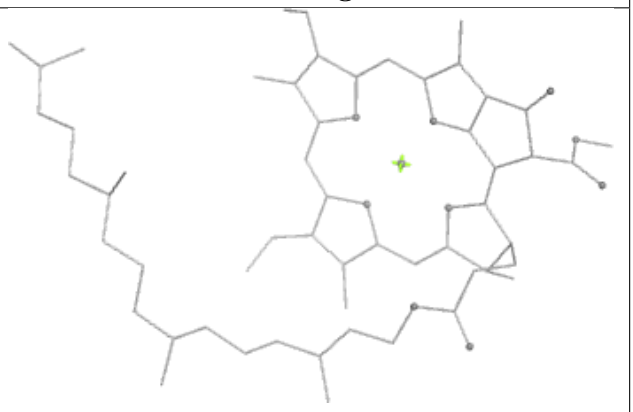
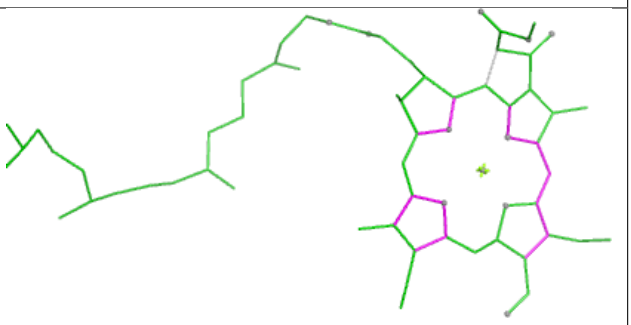


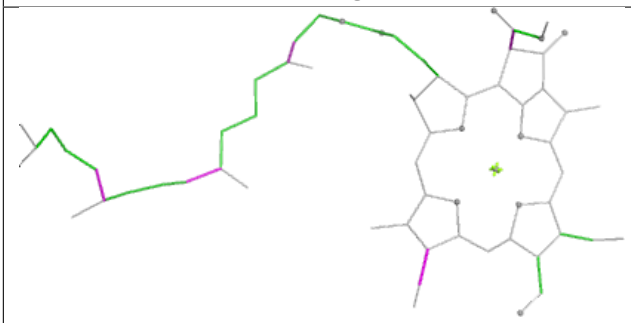
Rings

Ligand CHL 8 320

Bond lengths



Bond angles



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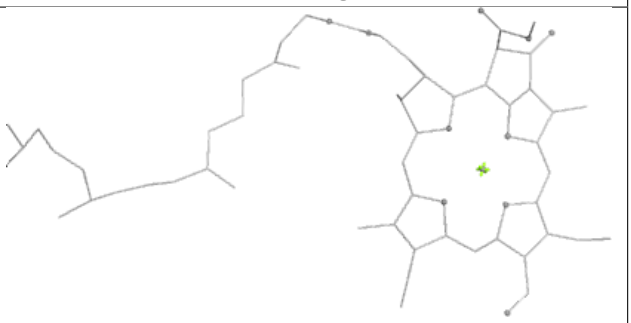
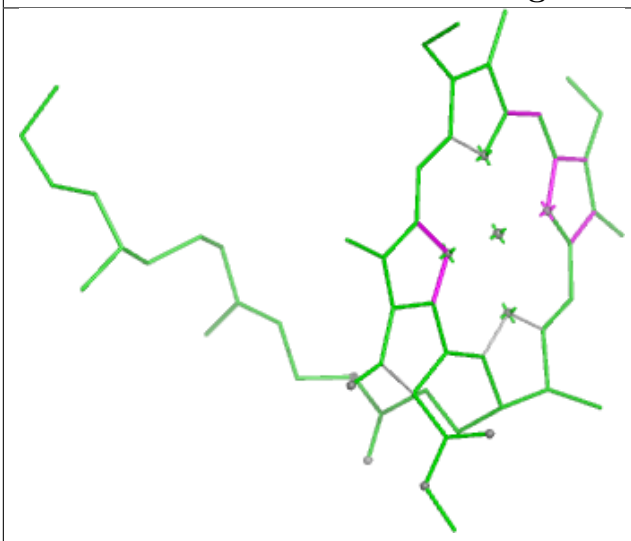


Rings

Ligand CLA 6 311



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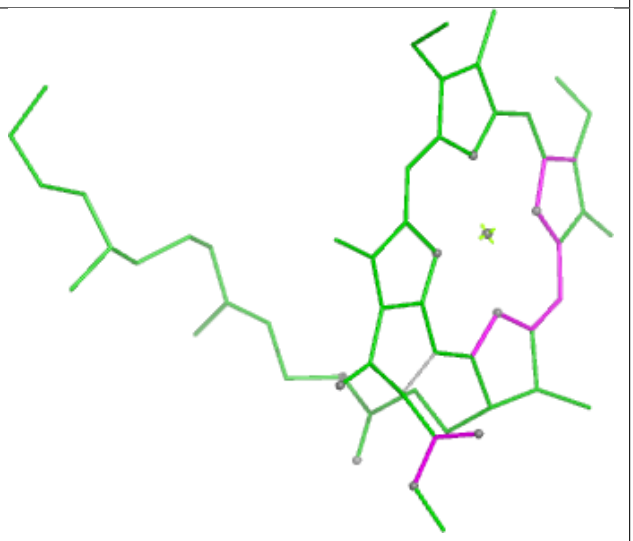

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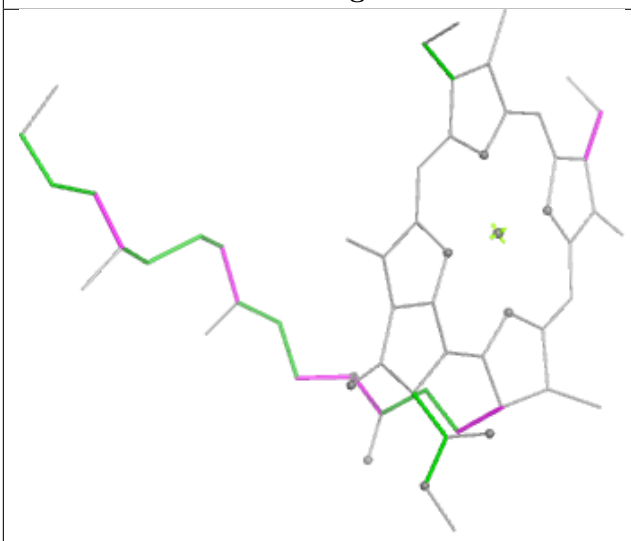
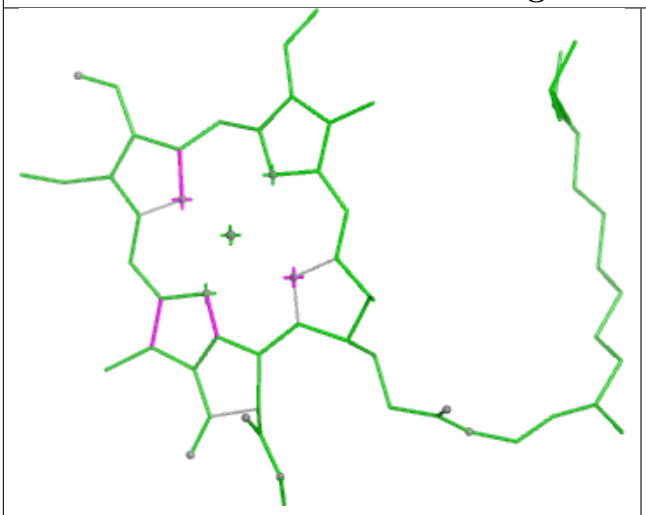


Torsions

Rings

Ligand CHL 8 305



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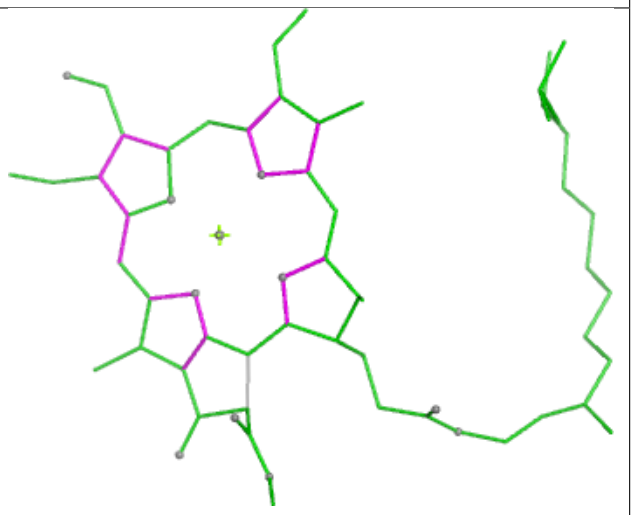
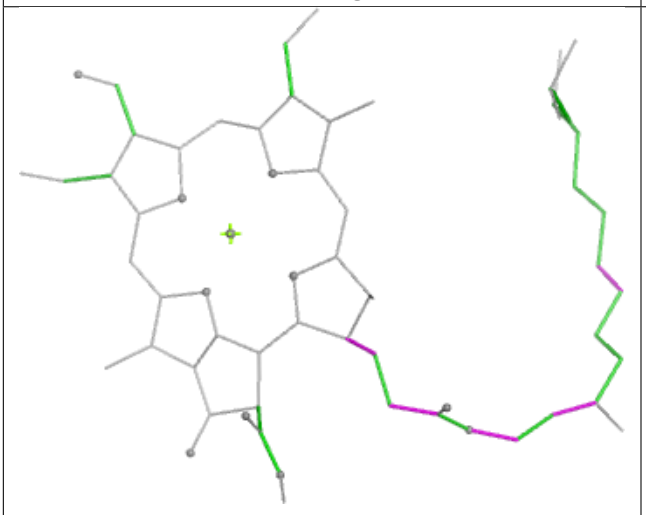


Bond angles



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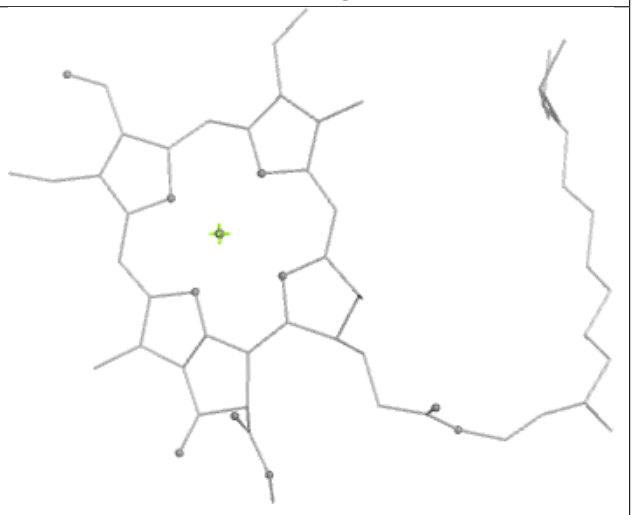
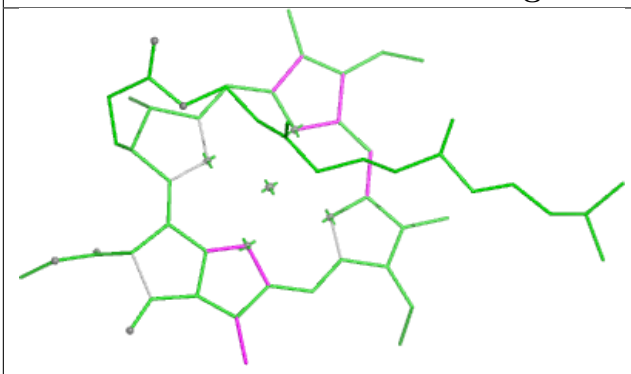


Rings

Ligand CLA A 820



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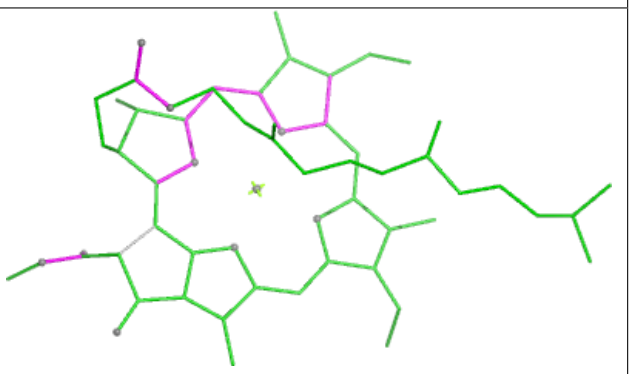
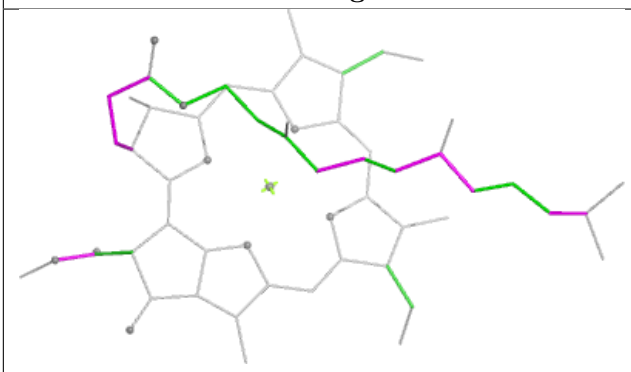


Bond angles



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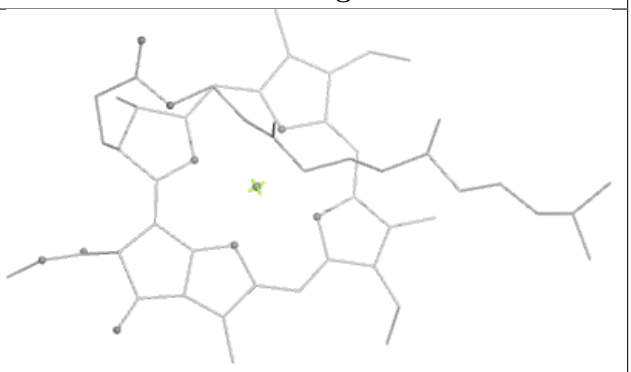
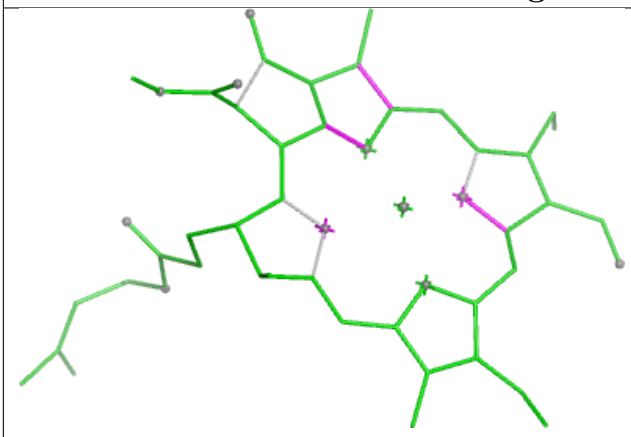


Rings

Ligand CHL 5 308



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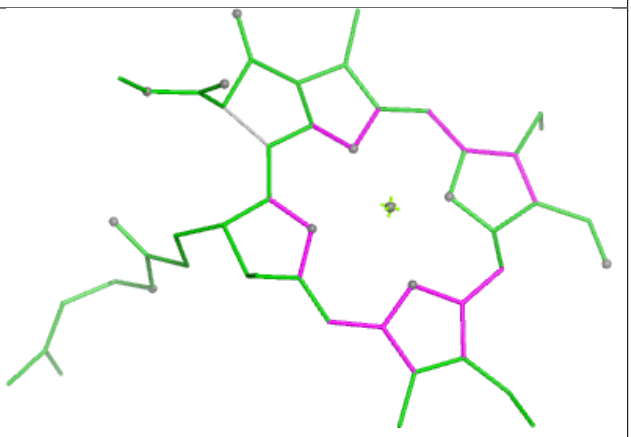

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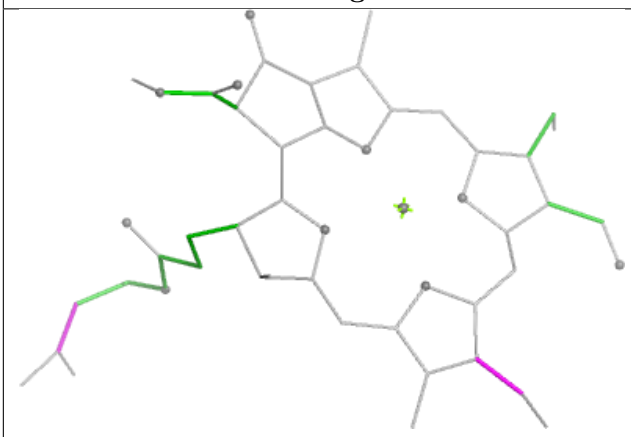

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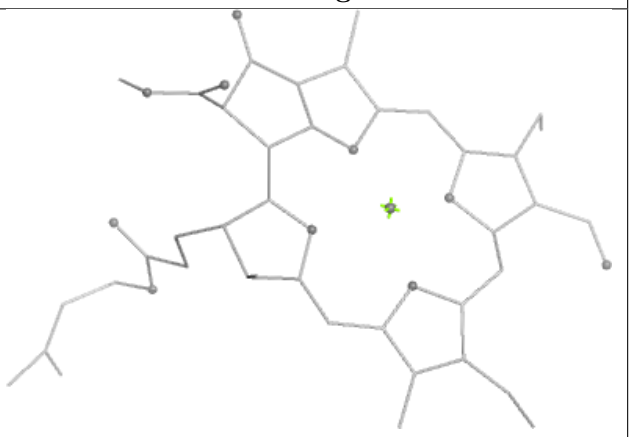
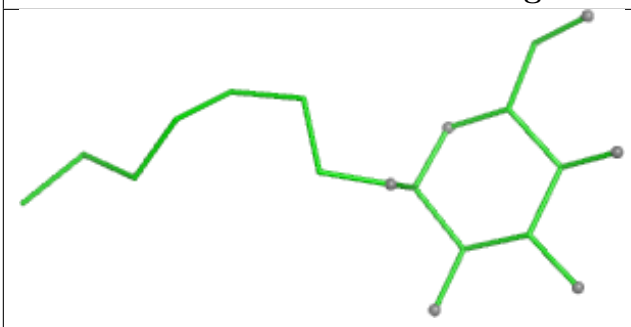


Rings

Ligand LMU 1 320



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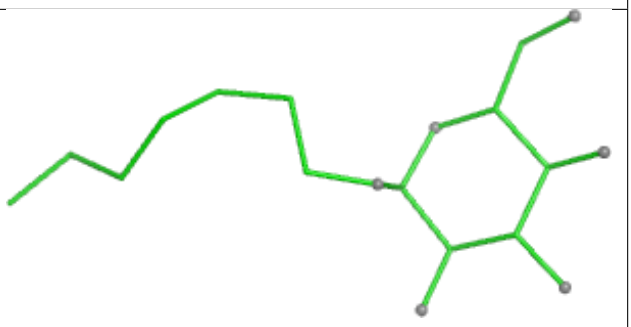

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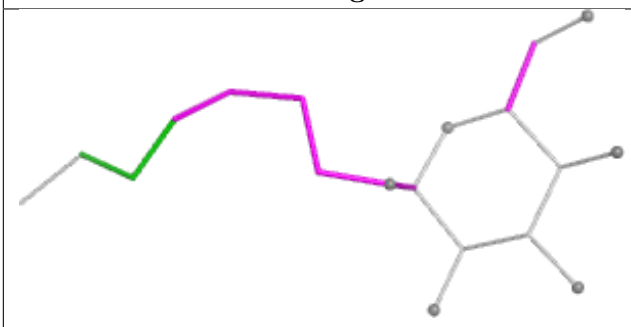

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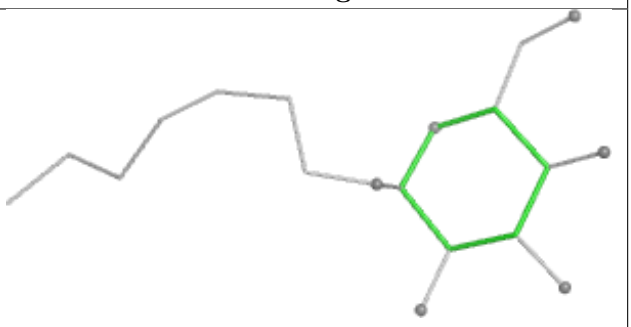
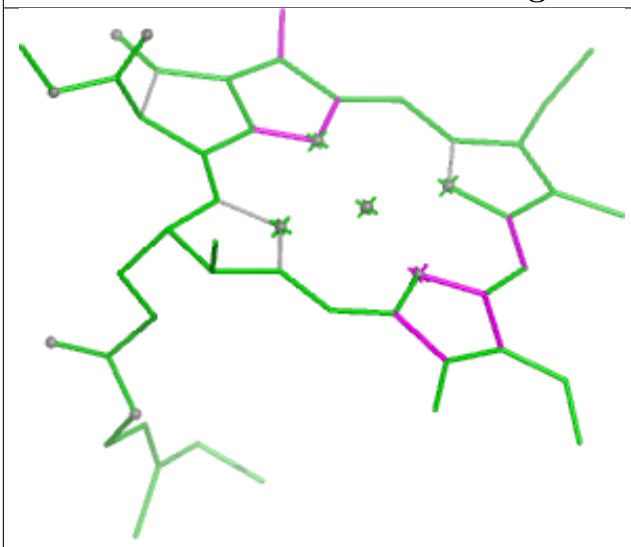


Rings

Ligand CLA 7 604



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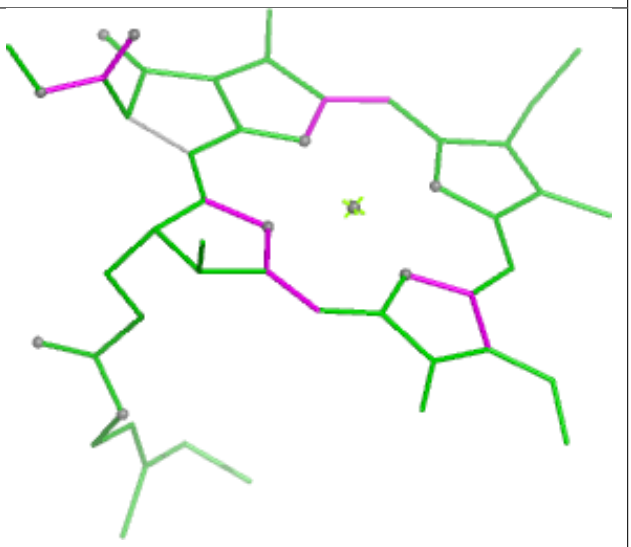
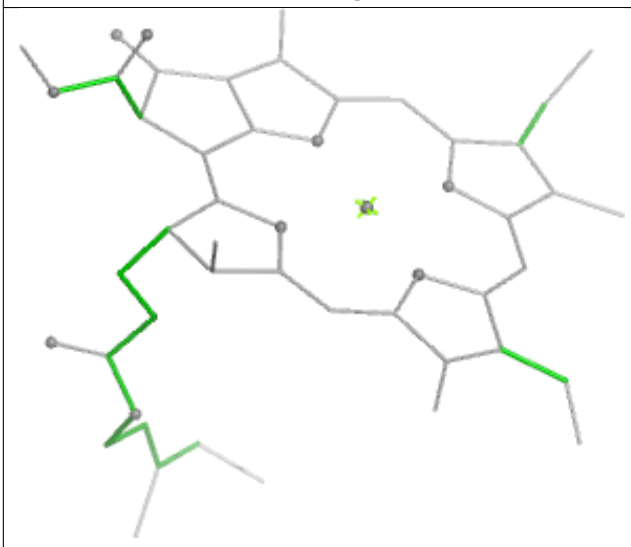


Bond angles



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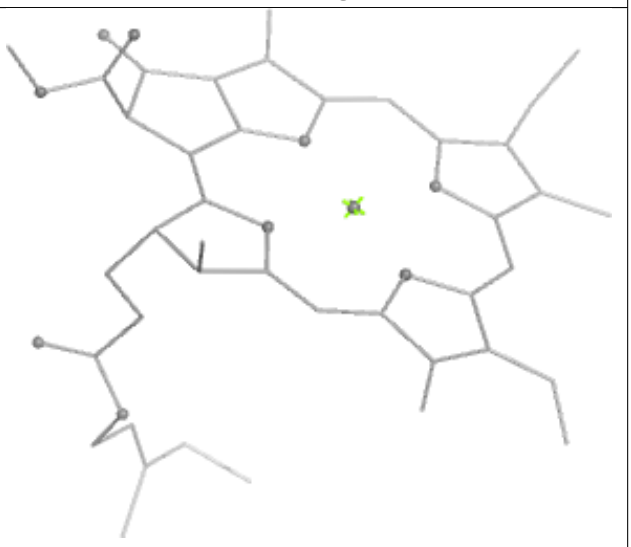
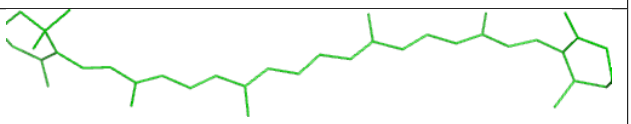


Rings

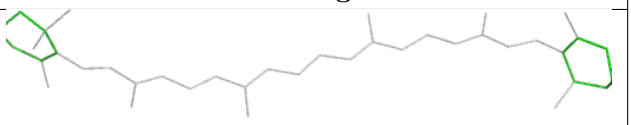
Ligand BCR K 206

Bond lengths



Bond angles

Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	142:SER	C	157:ALA	N	10.13

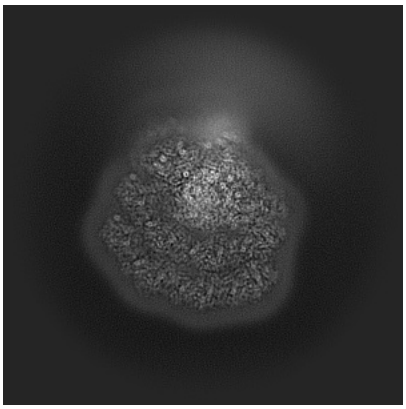
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54803. These allow visual inspection of the internal detail of the map and identification of artifacts.

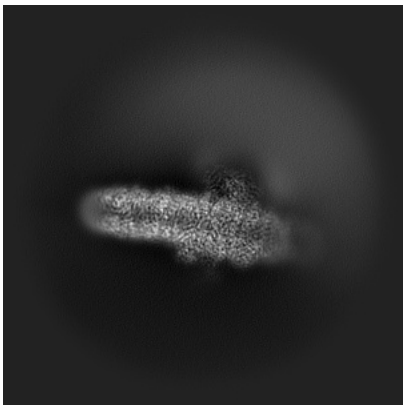
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

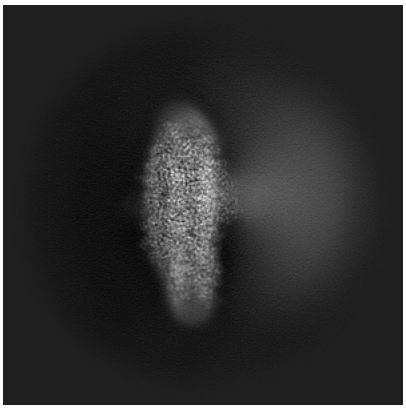
6.1.1 Primary map



X

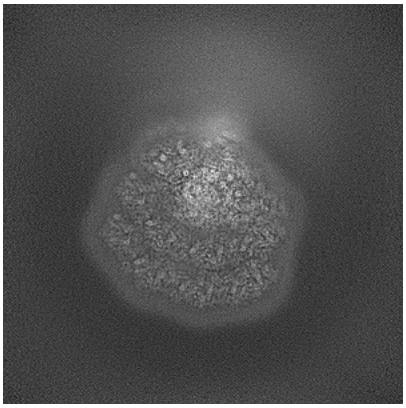


Y

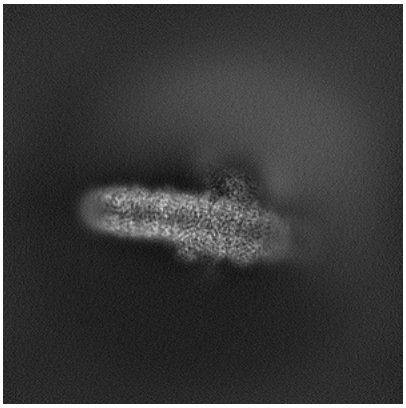


Z

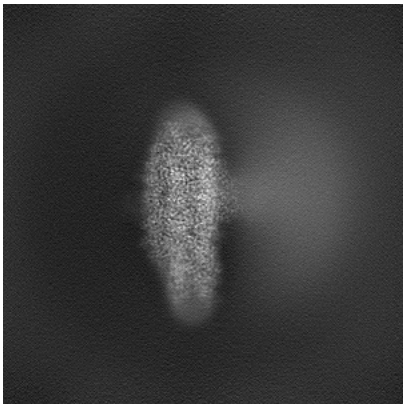
6.1.2 Raw map



X



Y

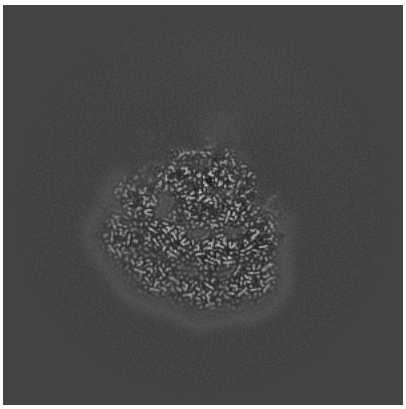


Z

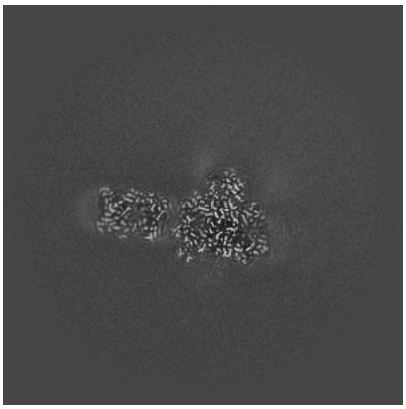
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

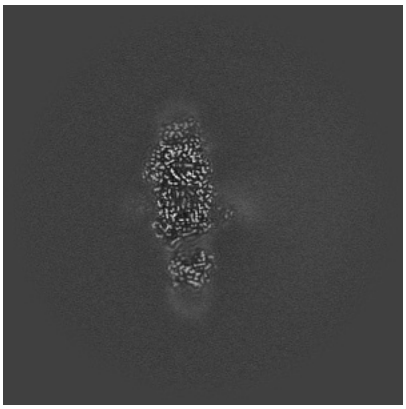
6.2.1 Primary map



X Index: 256

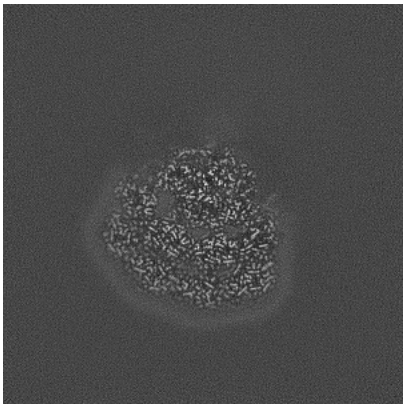


Y Index: 256

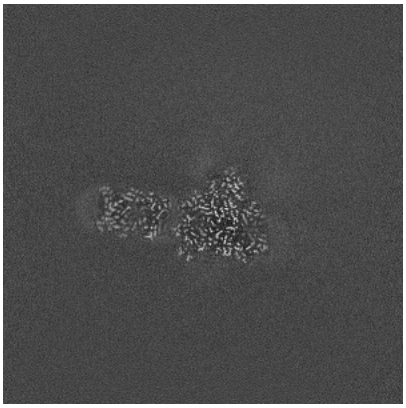


Z Index: 256

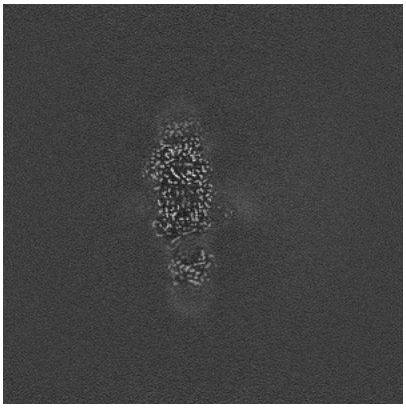
6.2.2 Raw map



X Index: 256



Y Index: 256

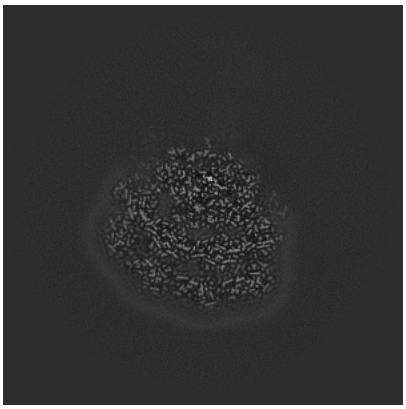


Z Index: 256

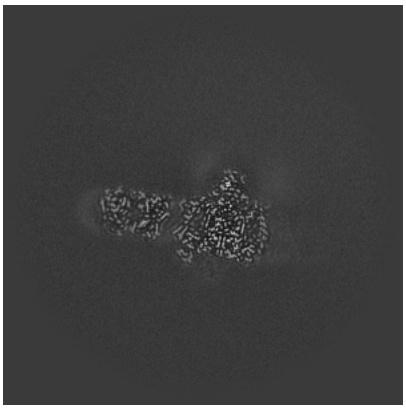
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

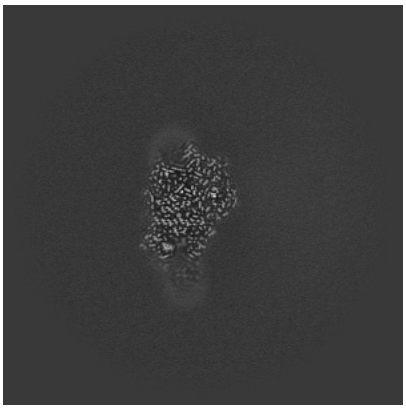
6.3.1 Primary map



X Index: 253

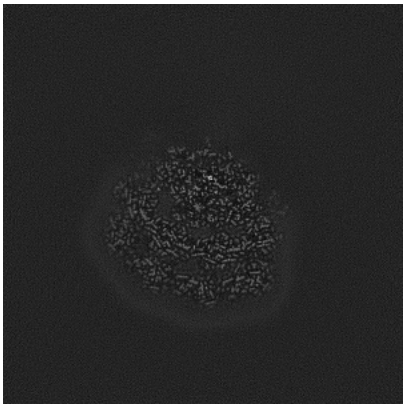


Y Index: 261

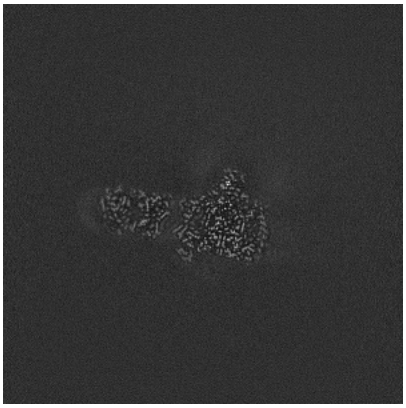


Z Index: 296

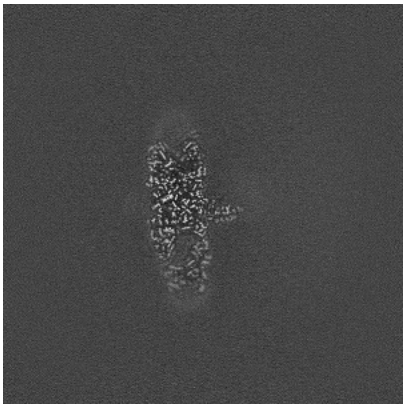
6.3.2 Raw map



X Index: 253



Y Index: 261

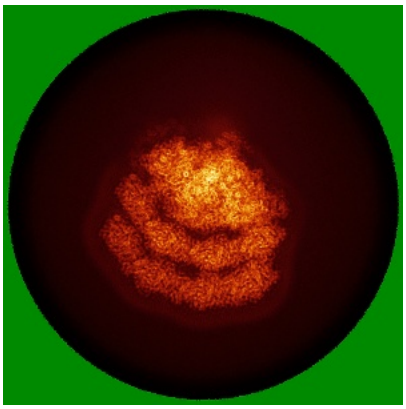


Z Index: 276

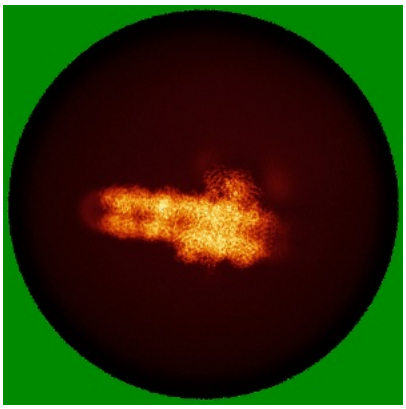
The images above show the largest variance slices of the map in three orthogonal directions.

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

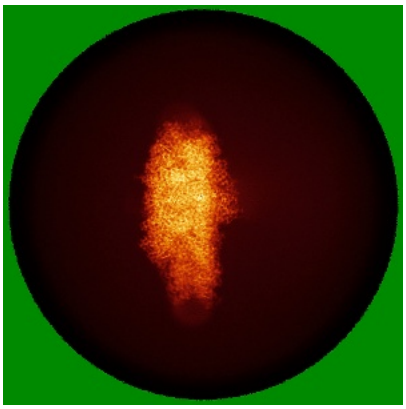
6.4.1 Primary map



X

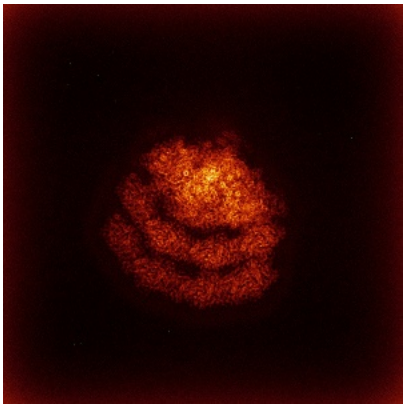


Y

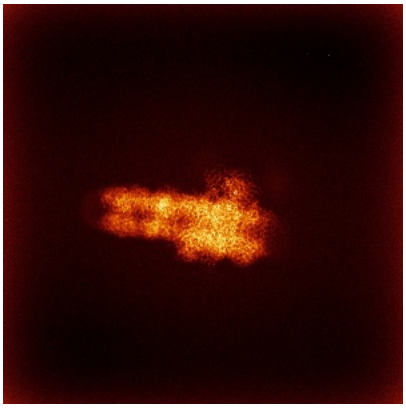


Z

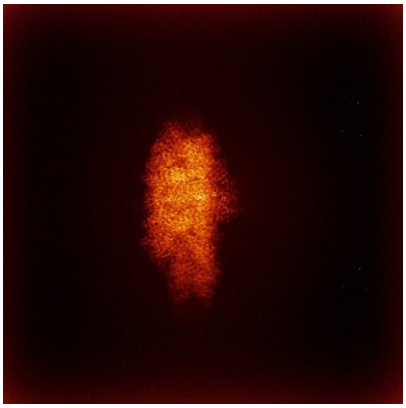
6.4.2 Raw map



X



Y

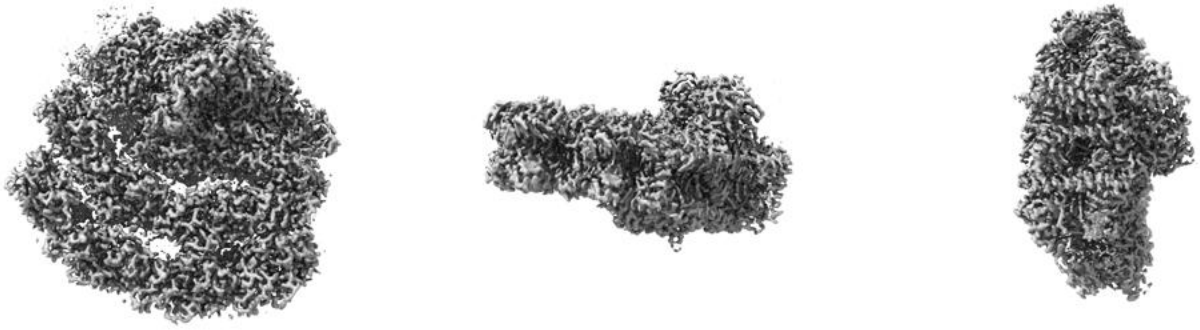


Z

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)

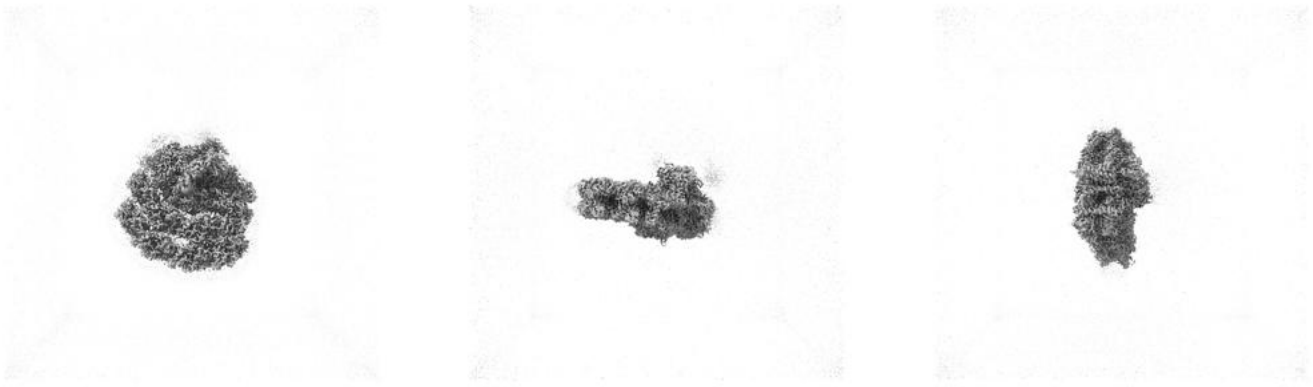
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

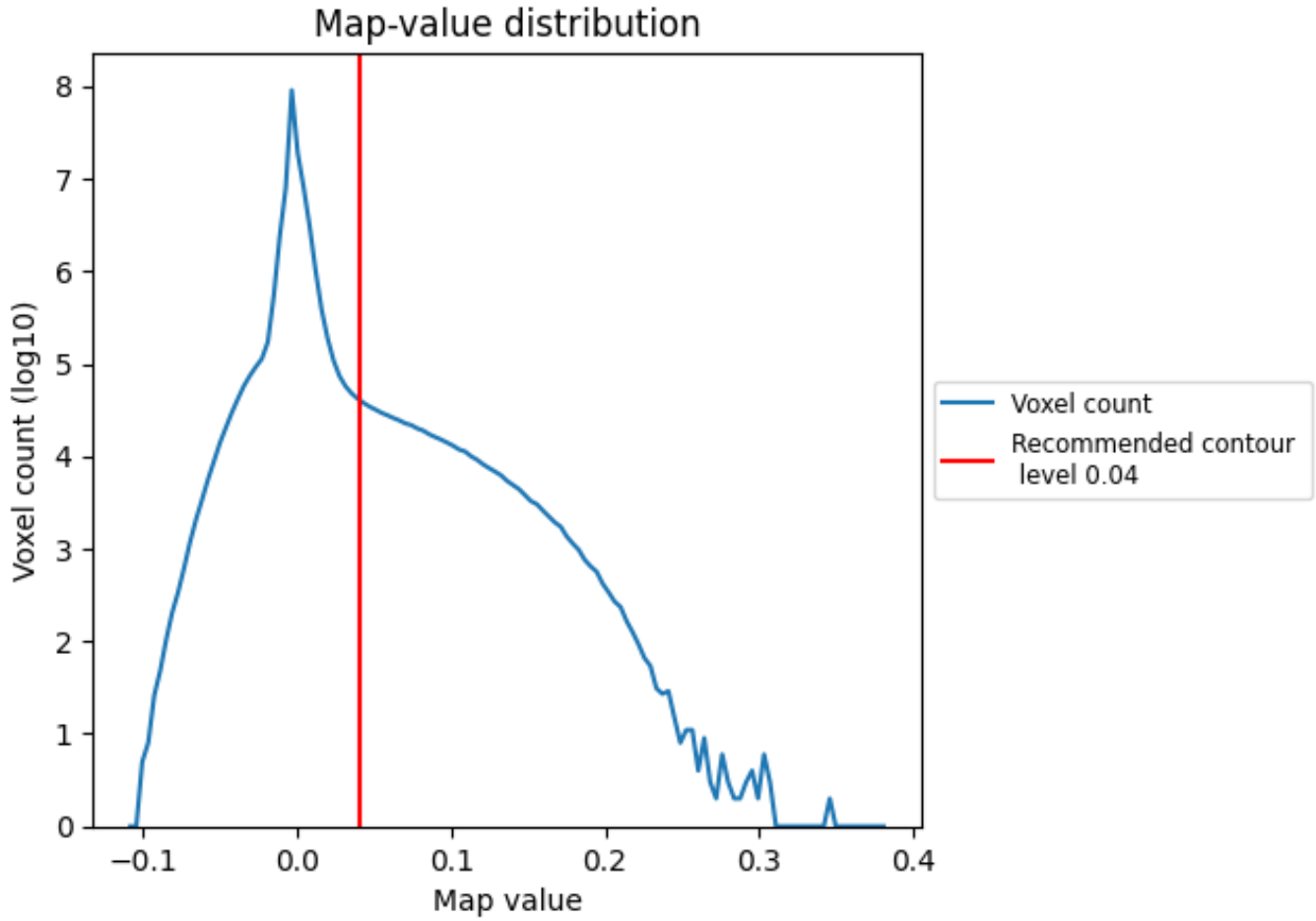
6.6 Mask visualisation (i)

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

7 Map analysis

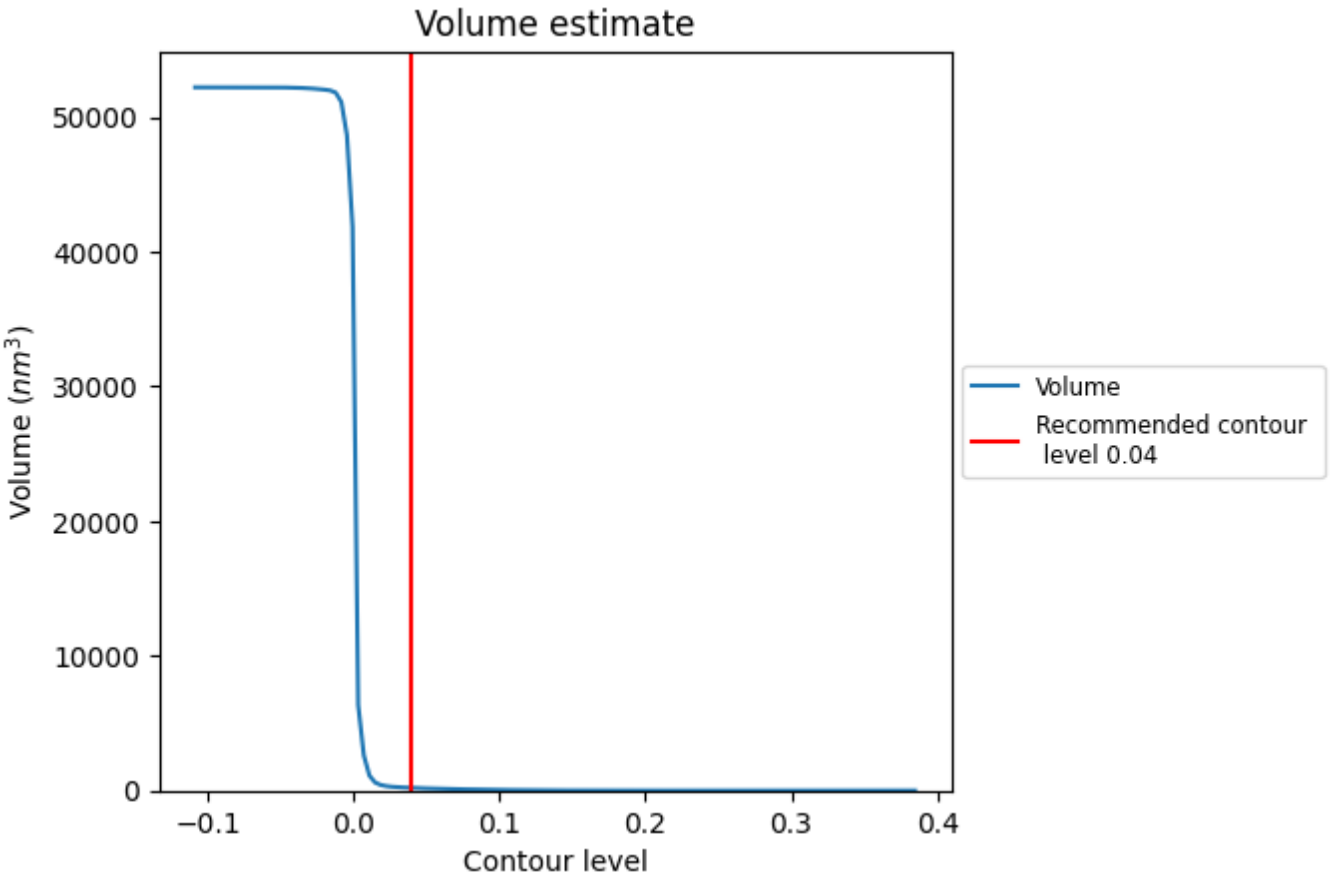
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

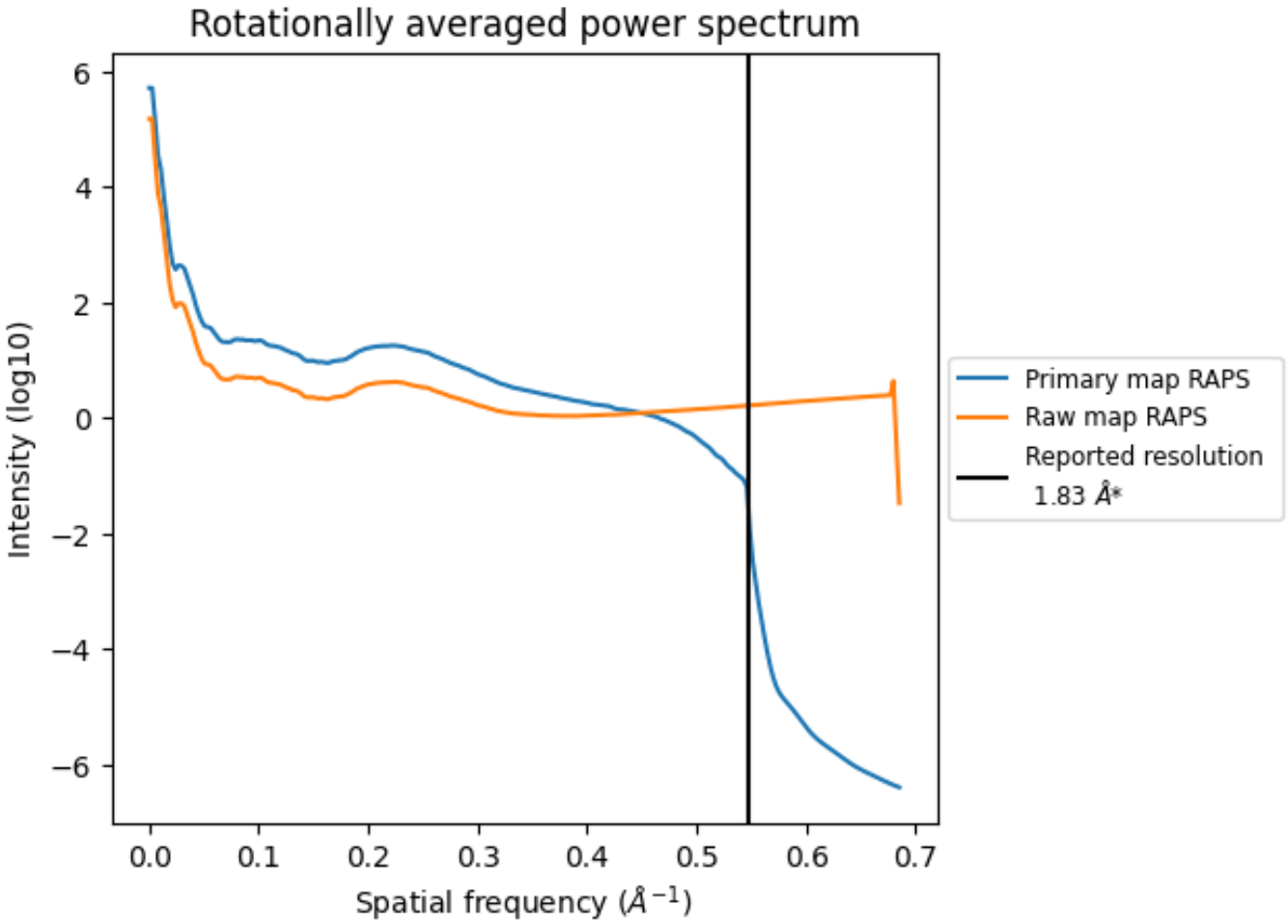
7.2 Volume estimate (i)



The volume at the recommended contour level is 200 nm^3; this corresponds to an approximate mass of 181 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)

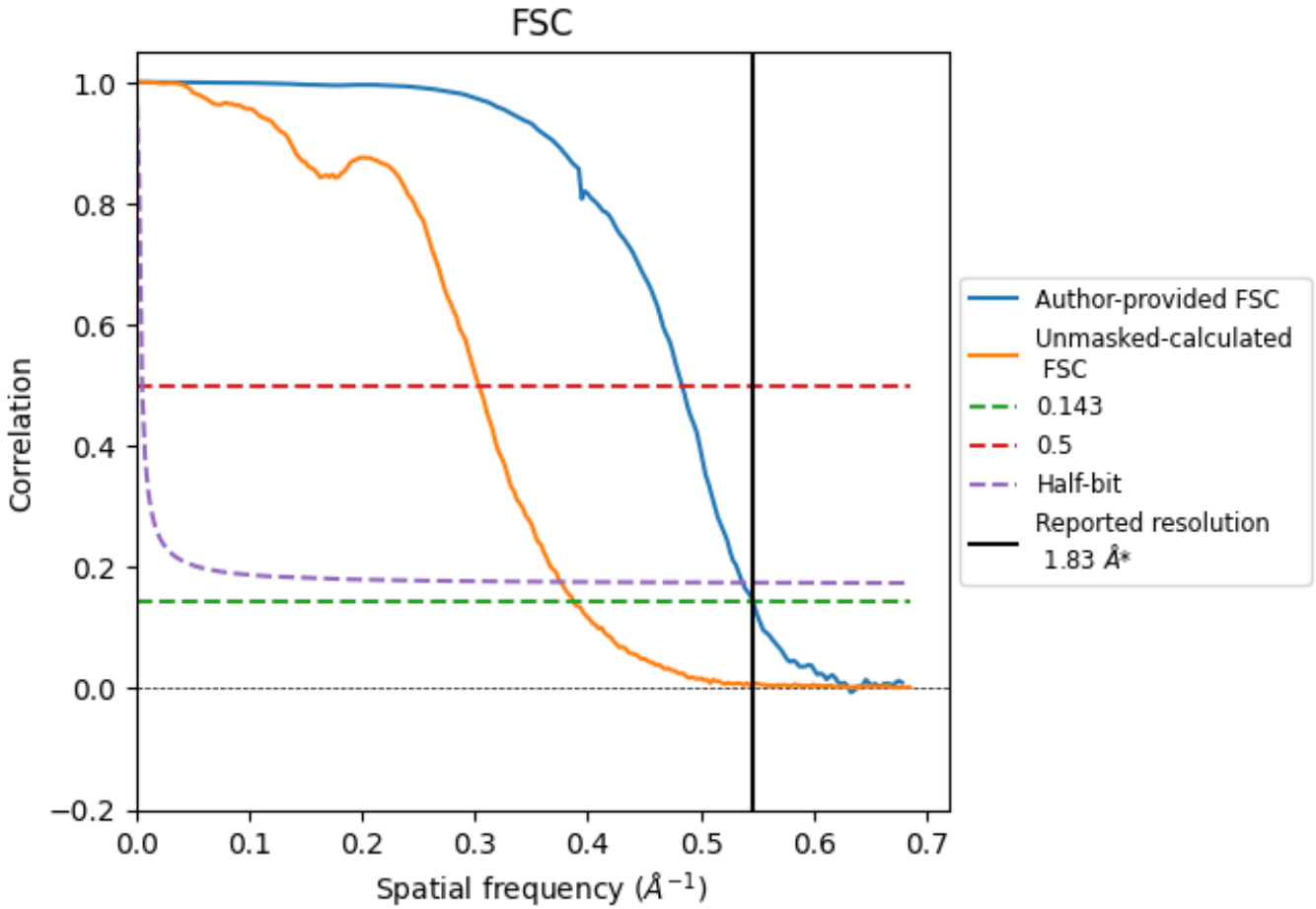


*Reported resolution corresponds to spatial frequency of 0.546 Å^{-1}

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 0.546 Å^{-1}

8.2 Resolution estimates (i)

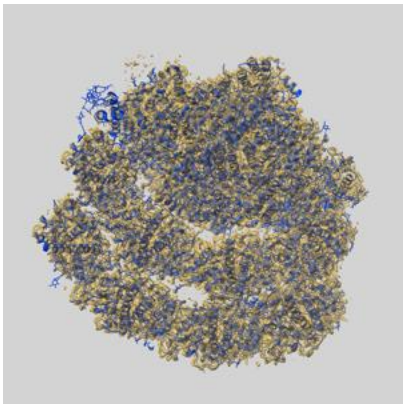
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.83	-	-
Author-provided FSC curve	1.83	2.07	1.86
Unmasked-calculated*	2.58	3.30	2.66

*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 2.58 differs from the reported value 1.83 by more than 10 %

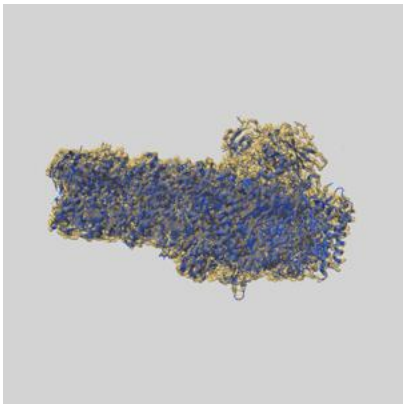
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54803 and PDB model 9SE6. Per-residue inclusion information can be found in section 3 on page 30.

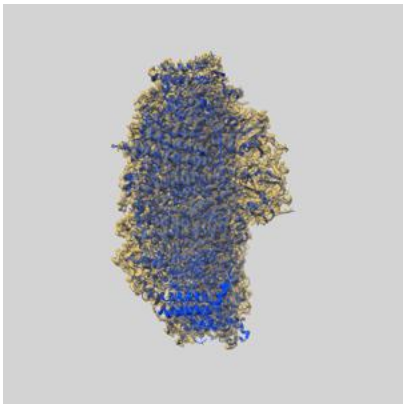
9.1 Map-model overlay



X



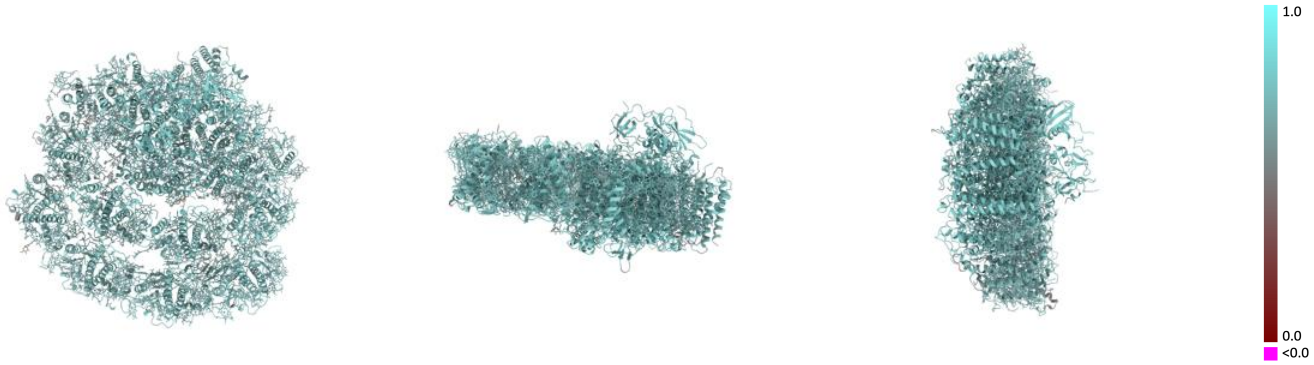
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

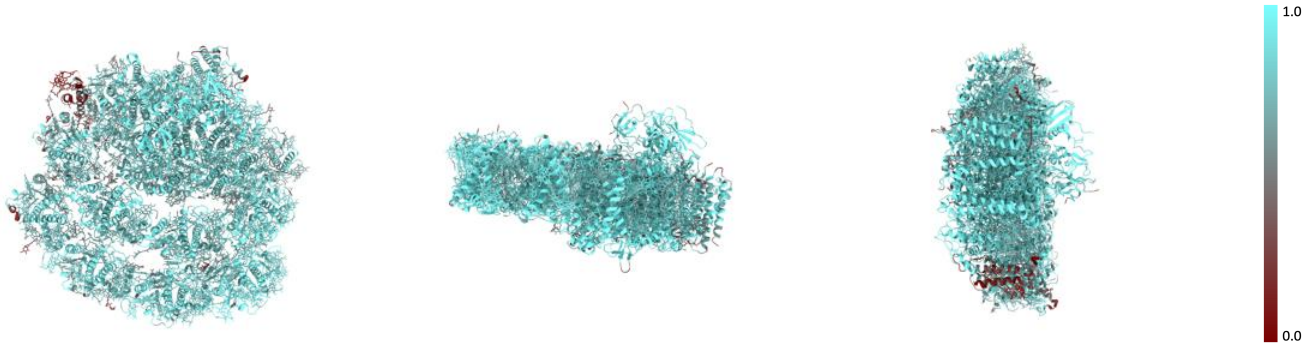
9.2 Q-score mapped to coordinate model



X Y Z

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

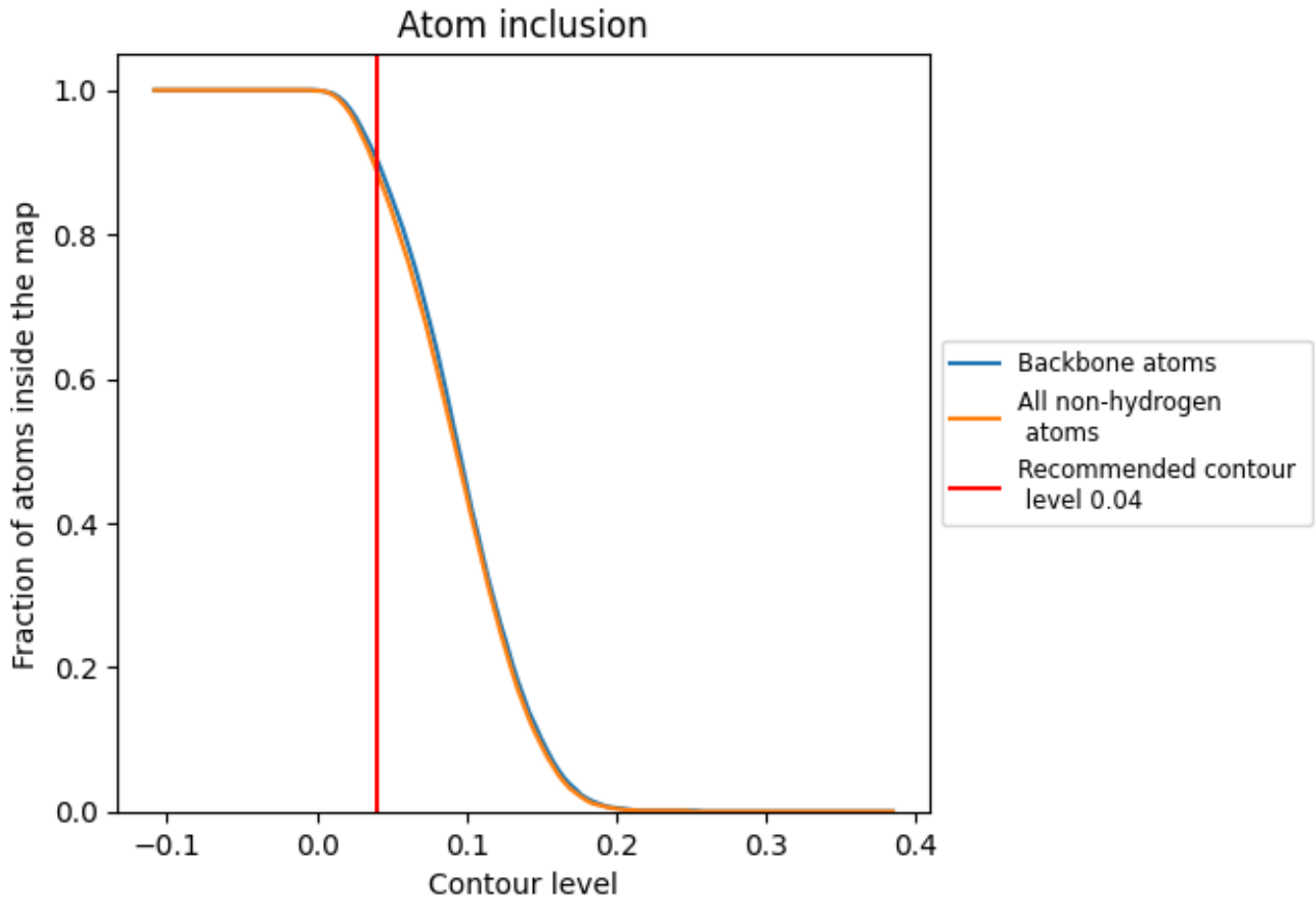
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.7200
1	0.8090	0.6830
3	0.9120	0.7230
4	0.8430	0.6810
5	0.9080	0.7020
6	0.8810	0.6960
7	0.9240	0.7300
8	0.9120	0.7250
A	0.9490	0.7540
B	0.9300	0.7430
C	0.9820	0.7630
D	0.9240	0.7400
E	0.8900	0.7250
F	0.8920	0.7270
G	0.1770	0.6260
I	0.8650	0.7140
J	0.9100	0.7350
K	0.7540	0.6890
L	0.7230	0.6770
Z	0.7830	0.6680