wwPDB EM Validation Summary Report

Sep 9, 2026 – 04:29 pm BST

PDB ID	:	9S1M / pdb_00009s1m
EMDB ID	:	EMD-54456
Title	:	Cryo-EM structure of Posidonia oceanica L-PSI-LHCI-LHCII supercomplex
Authors	:	Capaldi, S.; Amelii, A.; Sanita, G.; Esposito, M.; Bassi, R.
Deposited on	:	2025-07-18
Resolution	:	3.31 Å(reported)
Based on initial model	:	5ZJI

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:

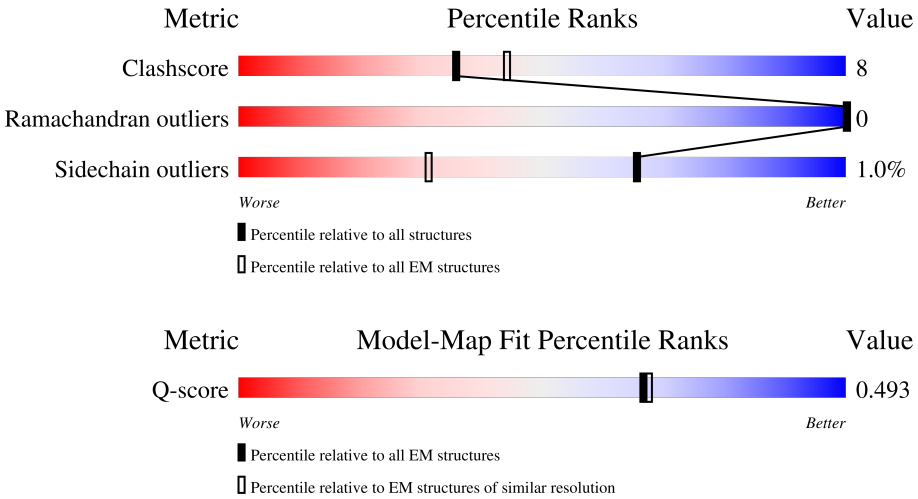
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.31 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.



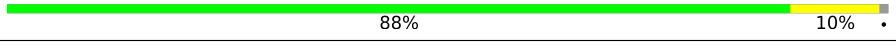
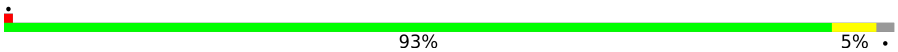
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14550 (2.81 - 3.81)

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

Mol	Chain	Length	Quality of chain
1	1	200	88% 11%
1	5	200	24% 80% 16%
2	2	211	79% 17%
3	3	232	11% 78% 13% 8%

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Mol	Chain	Length	Quality of chain
4	4	200	
4	6	200	
5	A	750	
6	B	734	
7	C	81	
8	D	155	
9	E	93	
10	F	159	
11	G	100	
12	H	95	
13	I	36	
14	J	42	
15	K	84	
16	L	170	
17	O	89	
18	X	228	
18	Z	228	
19	Y	228	

2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 49325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 6 (Lhca1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	198	Total	C	N	O	S	0	0
			1536	1004	256	271	5		
1	5	194	Total	C	N	O	S	0	0
			1504	981	252	266	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2 (Lhca2).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	203	Total	C	N	O	S	0	0
			1579	1031	257	285	6		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	213	Total	C	N	O	S	0	0
			1638	1074	263	295	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4 (Lhca4).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1557	1017	254	283	3		
4	6	198	Total	C	N	O	S	0	0
			1557	1017	254	283	3		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1 (PsaA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	724	Total	C	N	O	S	0	0
			5684	3726	968	972	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 (PsaB).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5858	3847	996	1002	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center (PsaC).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			614	380	106	117	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-1, chloroplastic (PsaD1).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	140	Total	C	N	O	S	0	0
			1103	708	190	201	4		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV B (PsaE2).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			519	333	92	94		

- Molecule 10 is a protein called Photosystem I reaction center subunit III (PsaF).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	155	Total	C	N	O	S	0	0
			1224	794	209	217	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit V (PsaG).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	98	Total	C	N	O	S	0	0
			768	500	128	139	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-1 (PsaH).

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	94	Total	C	N	O	0	0
			736	483	114	139		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII (PsaI).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	32	Total	C	N	O	S	0	0
			246	167	39	39	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	40	Total	C	N	O	0	0
			319	216	49	54		

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK (PsaK).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	80	Total	C	N	O	S	0	0
			566	360	97	105	4		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI (PsaL).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	162	Total	C	N	O	S	0	0
			1222	808	191	220	3		

- Molecule 17 is a protein called Photosystem I subunit O (PsaO).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	89	Total	C	N	O	S	0	0
			716	481	116	117	2		

- Molecule 18 is a protein called Chlorophyll a-b binding protein 1 (Lhcb1).

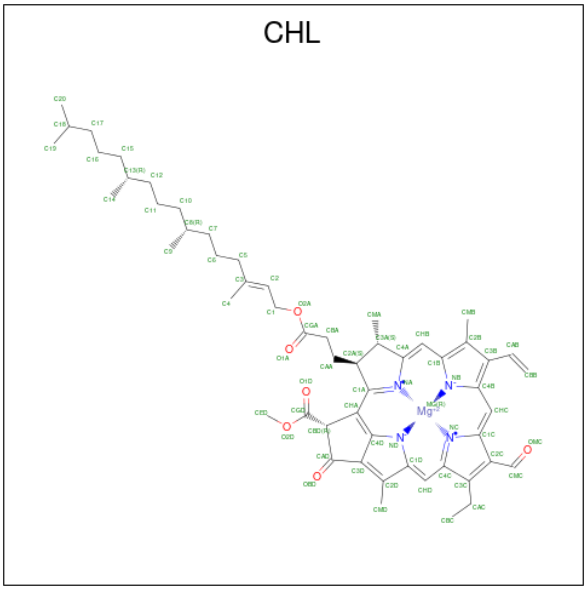
Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	218	Total	C	N	O	S	0	0
			1659	1076	269	307	7		
18	Z	218	Total	C	N	O	S	0	0
			1659	1076	269	307	7		

- Molecule 19 is a protein called Chlorophyll a-b binding protein 2 (Lhcb2).

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Y	227	Total	C	N	O	P	S	0	0
			1744	1130	286	321	1	6		

- 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	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
20	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	5	1	Total	C	Mg	N	O	0
			55	44	1	4	6	

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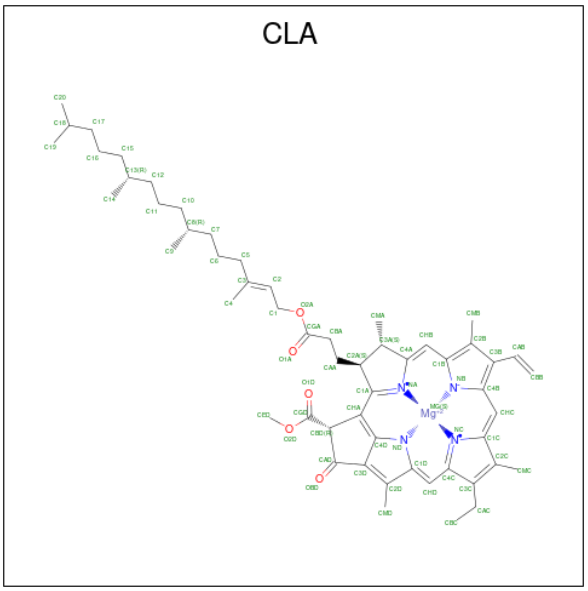
Mol	Chain	Residues	Atoms					AltConf
20	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	X	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	Y	1	Total	C	Mg	N	O	0
			47	36	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
			46	35	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
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
20	Z	1	Total 42	C 33	Mg 1	N 4	O 4	0
20	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0

- Molecule 21 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
21	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	6	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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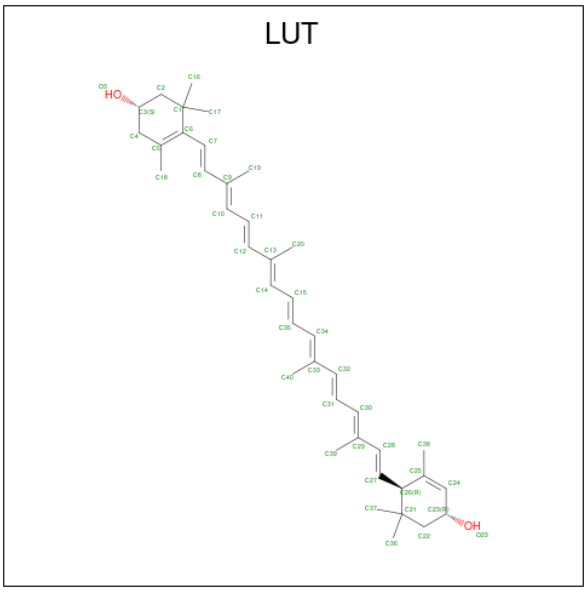
Mol	Chain	Residues	Atoms					AltConf
21	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
21	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
21	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	O	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	O	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	X	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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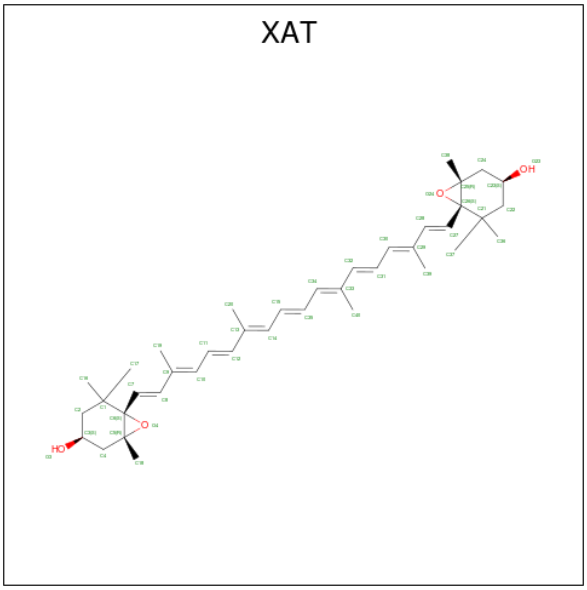
Mol	Chain	Residues	Atoms					AltConf
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- 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).



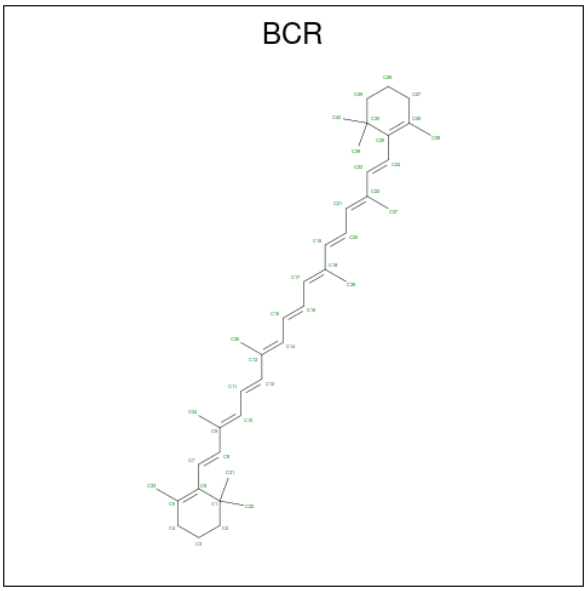
Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			42	40	2	
22	2	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			42	40	2	
22	4	1	Total	C	O	0
			42	40	2	
22	5	1	Total	C	O	0
			42	40	2	
22	5	1	Total	C	O	0
			42	40	2	
22	6	1	Total	C	O	0
			42	40	2	
22	F	1	Total	C	O	0
			42	40	2	
22	X	1	Total	C	O	0
			42	40	2	
22	X	1	Total	C	O	0
			42	40	2	
22	Y	1	Total	C	O	0
			42	40	2	
22	Y	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
			42	40	2	

- Molecule 23 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
23	1	1	Total	C	O	0
			44	40	4	
23	2	1	Total	C	O	0
			44	40	4	
23	3	1	Total	C	O	0
			44	40	4	
23	4	1	Total	C	O	0
			44	40	4	
23	5	1	Total	C	O	0
			44	40	4	
23	6	1	Total	C	O	0
			44	40	4	
23	O	1	Total	C	O	0
			44	40	4	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



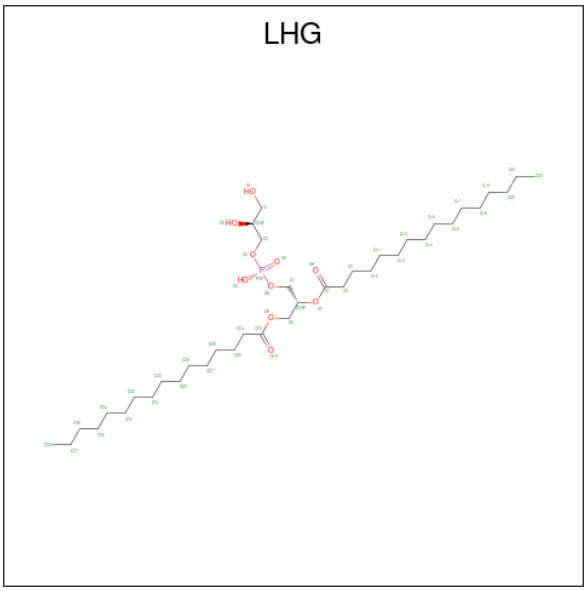
Mol	Chain	Residues	Atoms	AltConf
24	1	1	Total C 40 40	0
24	2	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	4	1	Total C 40 40	0
24	5	1	Total C 40 40	0
24	6	1	Total C 40 40	0
24	6	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0

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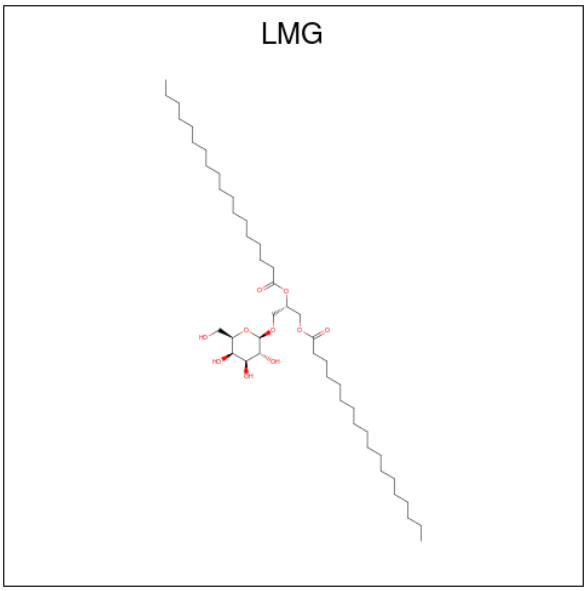
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	O	1	Total C 40 40	0
24	O	1	Total C 40 40	0
24	O	1	Total C 40 40	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



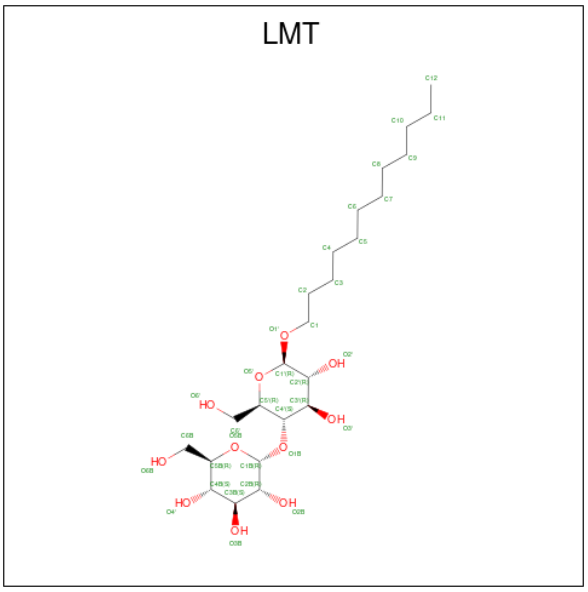
Mol	Chain	Residues	Atoms				AltConf
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			38	27	10	1	
25	2	1	Total	C	O	P	0
			37	26	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			30	19	10	1	
25	X	1	Total	C	O	P	0
			37	26	10	1	
25	Y	1	Total	C	O	P	0
			35	24	10	1	
25	Z	1	Total	C	O	P	0
			32	21	10	1	

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



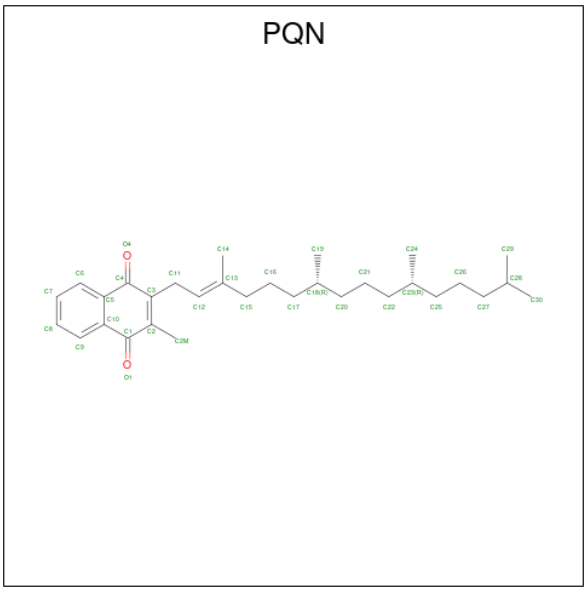
Mol	Chain	Residues	Atoms	AltConf
26	1	1	Total C O 53 43 10	0
26	1	1	Total C O 49 39 10	0
26	4	1	Total C O 36 26 10	0
26	5	1	Total C O 53 43 10	0
26	5	1	Total C O 49 39 10	0
26	6	1	Total C O 36 26 10	0
26	B	1	Total C O 52 42 10	0
26	F	1	Total C O 47 37 10	0
26	F	1	Total C O 30 20 10	0
26	G	1	Total C O 50 40 10	0

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



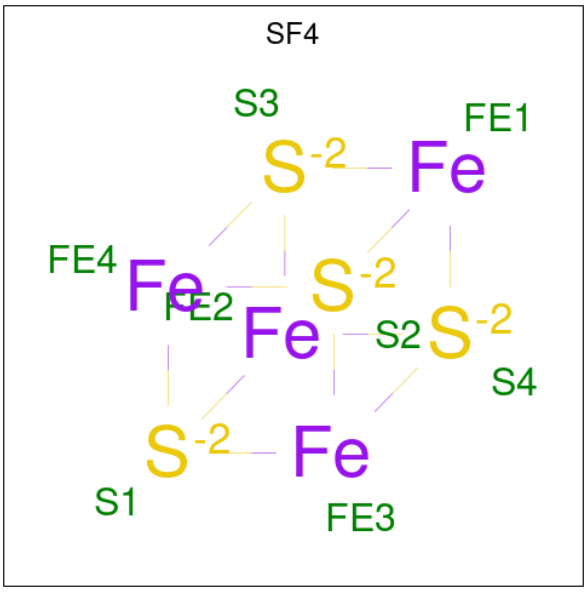
Mol	Chain	Residues	Atoms	AltConf
27	4	1	Total C O 35 24 11	0
27	6	1	Total C O 35 24 11	0
27	A	1	Total C O 35 24 11	0
27	F	1	Total C O 35 24 11	0
27	G	1	Total C O 35 24 11	0

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



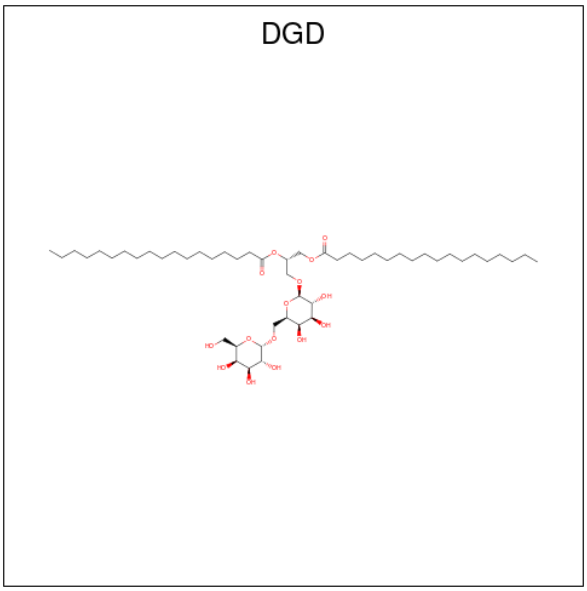
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	

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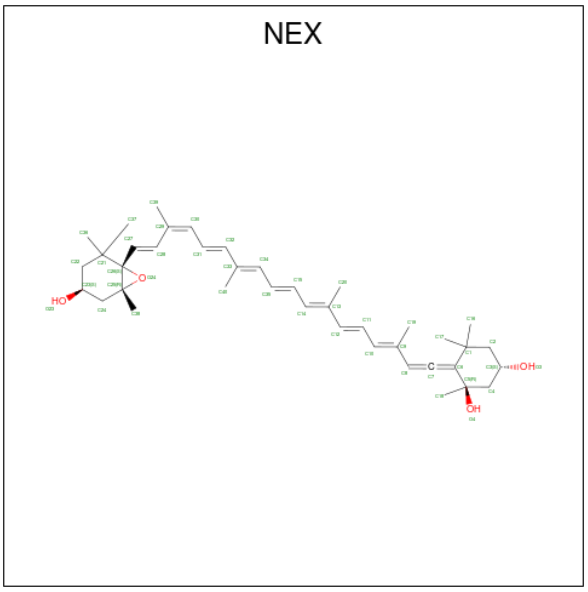
Mol	Chain	Residues	Atoms			AltConf
29	C	1	Total 8	Fe 4	S 4	0
29	C	1	Total 8	Fe 4	S 4	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total 61	C 46	O 15	0

- Molecule 31 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).

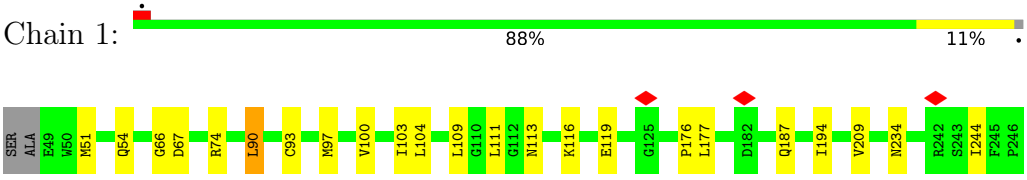


Mol	Chain	Residues	Atoms	AltConf
31	X	1	Total C O 44 40 4	0
31	Y	1	Total C O 44 40 4	0
31	Z	1	Total C O 44 40 4	0

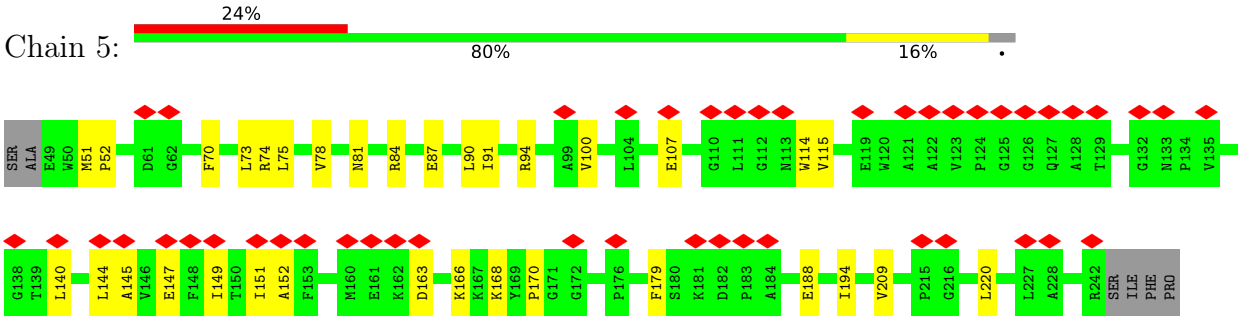
3 Residue-property plots (i)

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

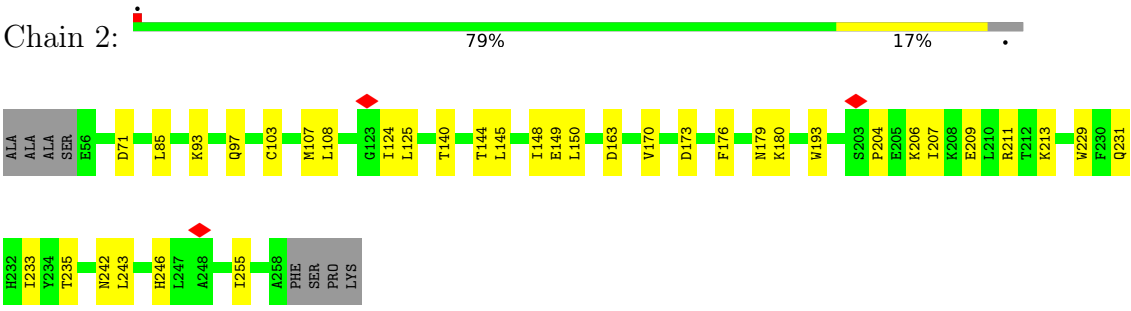
• Molecule 1: Chlorophyll a-b binding protein 6 (Lhca1)



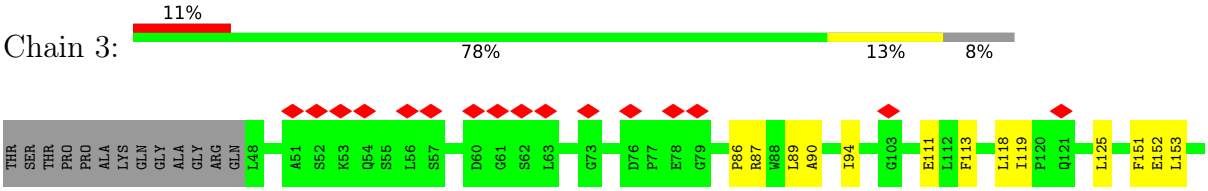
• Molecule 1: Chlorophyll a-b binding protein 6 (Lhca1)



• Molecule 2: Photosystem I chlorophyll a/b-binding protein 2 (Lhca2)

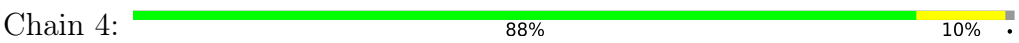


• Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3)



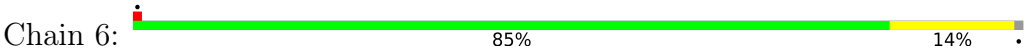


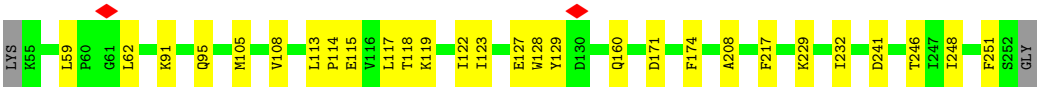
• Molecule 4: Chlorophyll a-b binding protein 4 (Lhca4)



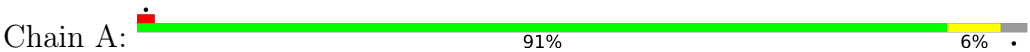


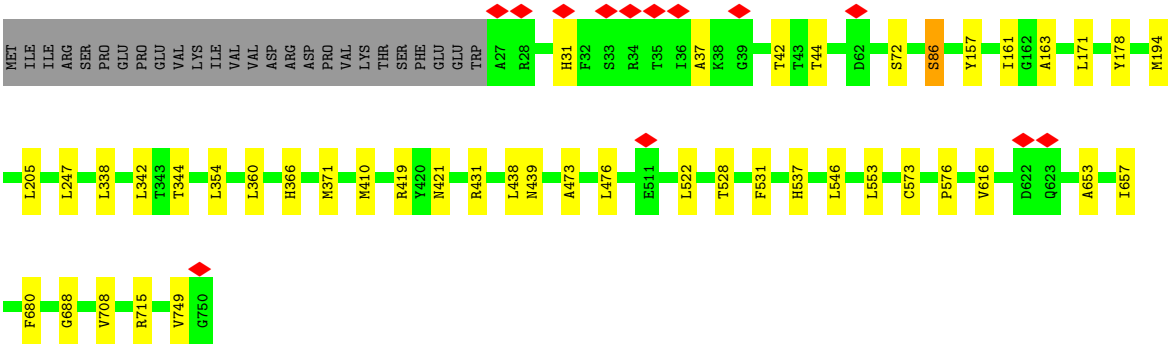
• Molecule 4: Chlorophyll a-b binding protein 4 (Lhca4)



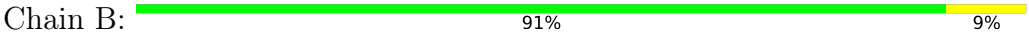


• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1 (PsaA)



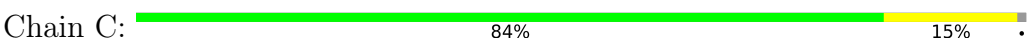


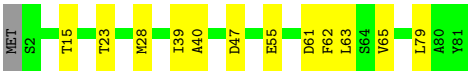
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2 (PsaB)





• Molecule 7: Photosystem I iron-sulfur center (PsaC)





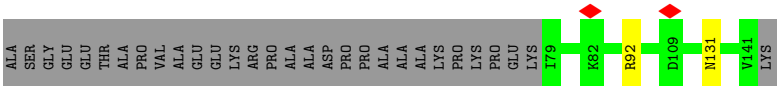
• Molecule 8: Photosystem I reaction center subunit II-1, chloroplastic (PsaD1)



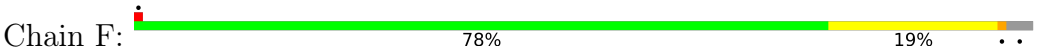


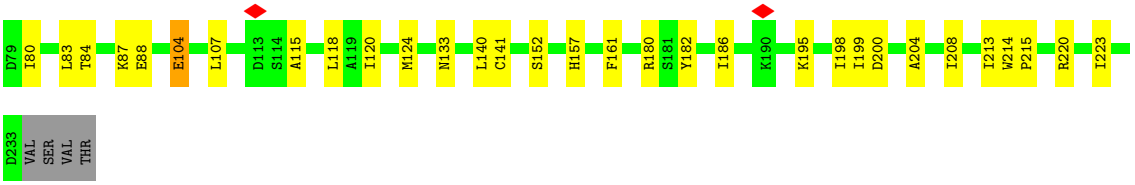
• Molecule 9: Photosystem I reaction center subunit IV B (PsaE2)



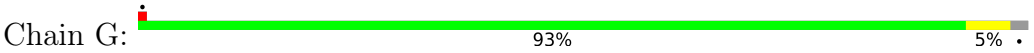


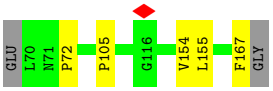
• Molecule 10: Photosystem I reaction center subunit III (PsaF)



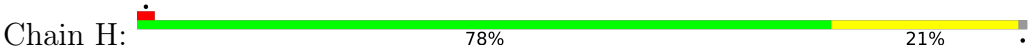


• Molecule 11: Photosystem I reaction center subunit V (PsaG)



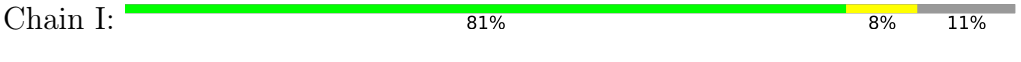


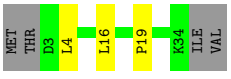
• Molecule 12: Photosystem I reaction center subunit VI-1 (PsaH)





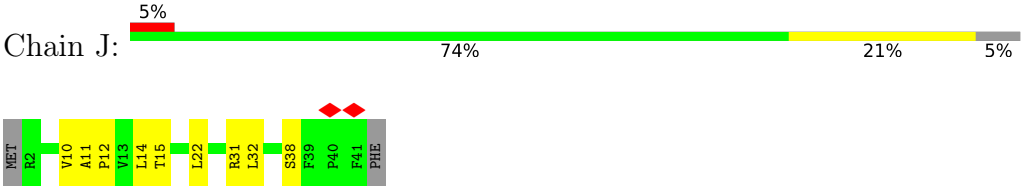
• Molecule 13: Photosystem I reaction center subunit VIII (PsaI)





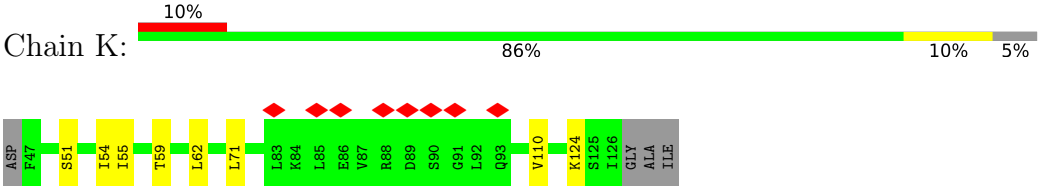
• Molecule 14: Photosystem I reaction center subunit IX

Chain J:



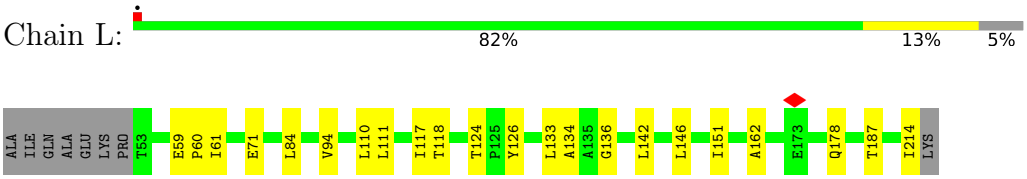
• Molecule 15: Photosystem I reaction center subunit psaK (PsaK)

Chain K:



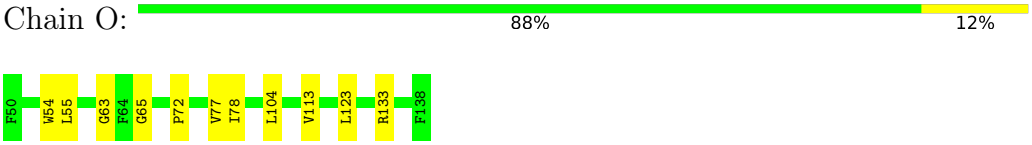
• Molecule 16: Photosystem I reaction center subunit XI (PsaL)

Chain L:



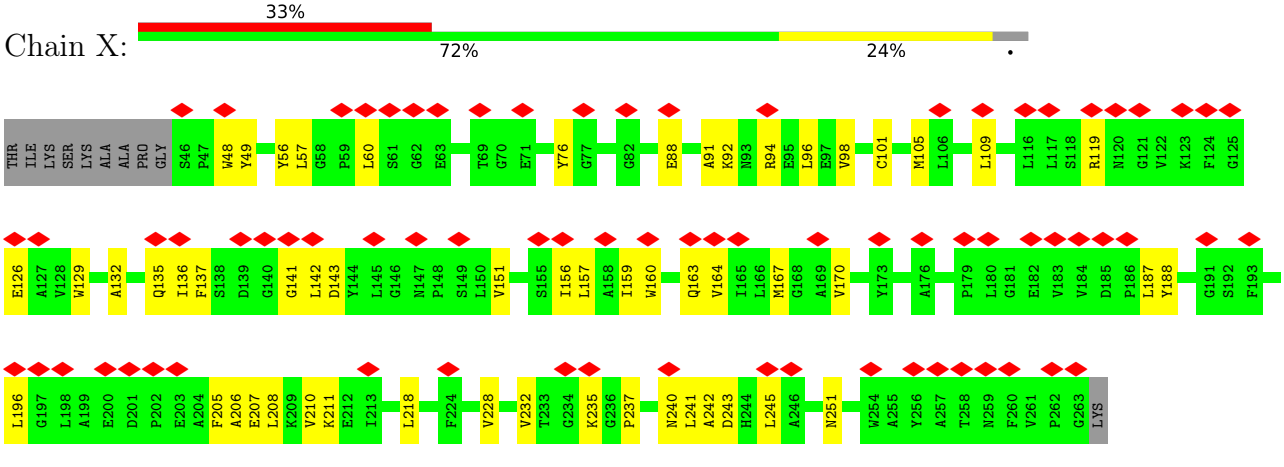
• Molecule 17: Photosystem I subunit O (PsaO)

Chain O:



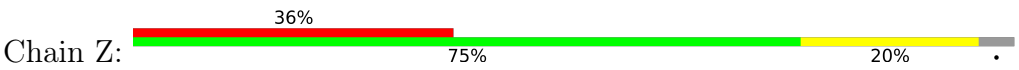
• Molecule 18: Chlorophyll a-b binding protein 1 (Lhcb1)

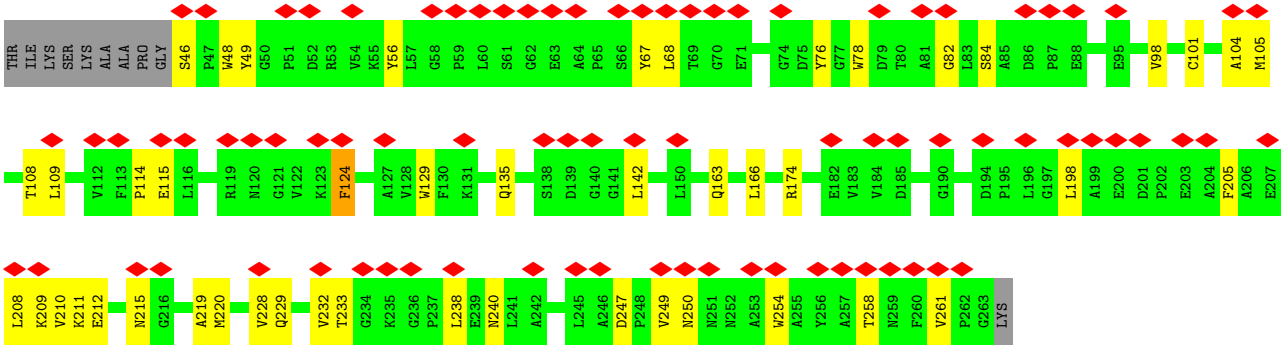
Chain X:



• Molecule 18: Chlorophyll a-b binding protein 1 (Lhcb1)

Chain Z:

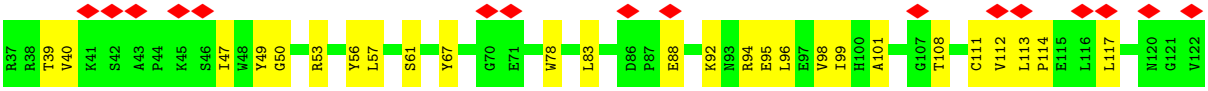


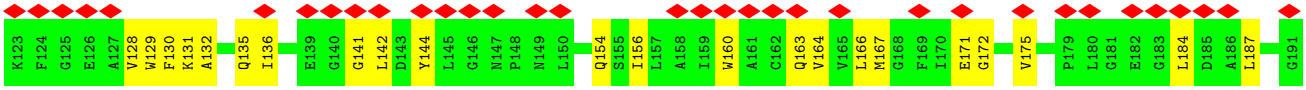


• Molecule 19: Chlorophyll a-b binding protein 2 (Lhcb2)

Chain Y:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	45.582	Depositor
Minimum map value	-16.918	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.985	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1	0.16	0/1587	0.33	0/2166
1	5	0.13	0/1553	0.34	0/2119
2	2	0.15	0/1634	0.29	0/2236
3	3	0.15	0/1690	0.34	0/2292
4	4	0.17	0/1606	0.32	0/2191
4	6	0.15	0/1606	0.34	0/2191
5	A	0.20	0/5878	0.32	0/8020
6	B	0.21	0/6070	0.33	0/8291
7	C	0.20	0/626	0.40	0/849
8	D	0.16	0/1131	0.37	0/1530
9	E	0.16	0/531	0.27	0/721
10	F	0.17	0/1253	0.33	0/1691
11	G	0.15	0/788	0.33	0/1069
12	H	0.17	0/759	0.40	0/1030
13	I	0.16	0/252	0.31	0/343
14	J	0.15	0/328	0.36	0/448
15	K	0.15	0/572	0.35	0/772
16	L	0.15	0/1259	0.29	0/1723
17	O	0.15	0/746	0.30	0/1015
18	X	0.11	0/1710	0.31	0/2331
18	Z	0.12	0/1710	0.33	0/2331
19	Y	0.14	0/1784	0.34	0/2425
All	All	0.17	0/35073	0.33	0/47784

There are no bond length outliers.

There are no bond angle outliers.

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	1	1536	0	1523	18	0
1	5	1504	0	1491	29	0
2	2	1579	0	1524	26	0
3	3	1638	0	1602	23	0
4	4	1557	0	1519	15	0
4	6	1557	0	1519	22	0
5	A	5684	0	5539	35	0
6	B	5858	0	5635	48	0
7	C	614	0	593	11	0
8	D	1103	0	1114	14	0
9	E	519	0	512	4	0
10	F	1224	0	1257	23	0
11	G	768	0	748	4	0
12	H	736	0	723	18	0
13	I	246	0	265	2	0
14	J	319	0	330	8	0
15	K	566	0	596	5	0
16	L	1222	0	1224	15	0
17	O	716	0	683	9	0
18	X	1659	0	1595	49	0
18	Z	1659	0	1595	44	0
19	Y	1744	0	1688	47	0
20	1	96	0	68	3	0
20	2	226	0	150	8	0
20	3	47	0	31	1	0
20	4	194	0	138	5	0
20	5	96	0	68	3	0
20	6	194	0	138	7	0
20	X	226	0	151	9	0
20	Y	319	0	213	13	0
20	Z	272	0	182	13	0
21	1	628	0	553	12	0
21	2	504	0	433	12	0
21	3	601	0	463	10	0
21	4	502	0	418	6	0
21	5	574	0	461	12	0
21	6	533	0	425	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	2452	0	2391	61	0
21	B	2282	0	2215	50	0
21	F	41	0	29	0	0
21	G	132	0	97	2	0
21	H	60	0	59	2	0
21	J	84	0	62	4	0
21	K	167	0	116	3	0
21	L	215	0	197	10	0
21	O	199	0	161	9	0
21	X	413	0	309	20	0
21	Y	390	0	319	11	0
21	Z	336	0	263	19	0
22	1	42	0	56	4	0
22	2	42	0	56	4	0
22	3	42	0	56	6	0
22	4	42	0	56	4	0
22	5	84	0	112	9	0
22	6	42	0	56	3	0
22	F	42	0	56	3	0
22	X	84	0	112	16	0
22	Y	84	0	112	16	0
22	Z	84	0	112	13	0
23	1	44	0	56	1	0
23	2	44	0	56	0	0
23	3	44	0	56	2	0
23	4	44	0	56	1	0
23	5	44	0	56	1	0
23	6	44	0	56	2	0
23	O	44	0	56	4	0
24	1	40	0	56	0	0
24	2	40	0	56	2	0
24	3	40	0	56	2	0
24	4	40	0	56	2	0
24	5	40	0	56	1	0
24	6	80	0	112	5	0
24	A	240	0	336	16	0
24	B	280	0	392	17	0
24	F	80	0	112	2	0
24	G	40	0	56	2	0
24	I	40	0	56	1	0
24	J	40	0	56	4	0
24	K	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	L	160	0	224	15	0
24	O	120	0	168	6	0
25	1	136	0	194	8	0
25	2	37	0	44	2	0
25	5	49	0	74	2	0
25	A	79	0	104	3	0
25	X	37	0	44	3	0
25	Y	35	0	40	3	0
25	Z	32	0	34	2	0
26	1	102	0	150	1	0
26	4	36	0	42	0	0
26	5	102	0	150	2	0
26	6	36	0	42	1	0
26	B	52	0	77	3	0
26	F	77	0	97	1	0
26	G	50	0	70	1	0
27	4	35	0	46	1	0
27	6	35	0	46	0	0
27	A	35	0	46	0	0
27	F	35	0	46	0	0
27	G	35	0	46	0	0
28	A	33	0	46	0	0
28	B	33	0	46	4	0
29	A	8	0	0	1	0
29	C	16	0	0	0	0
30	B	61	0	83	2	0
31	X	44	0	56	1	0
31	Y	44	0	56	2	0
31	Z	44	0	56	3	0
All	All	49325	0	48144	762	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 762 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)
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.58	0.83
5:A:680:PHE:HA	21:A:802:CLA:HAB	1.60	0.82
21:B:821:CLA:HBA1	21:B:821:CLA:HBD	1.63	0.81
7:C:61:ASP:HB3	9:E:131:ASN:HD21	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:610:CLA:HED3	21:X:610:CLA:H2A	1.65	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	196/200 (98%)	192 (98%)	4 (2%)	0	100	100
1	5	192/200 (96%)	187 (97%)	5 (3%)	0	100	100
2	2	201/211 (95%)	197 (98%)	4 (2%)	0	100	100
3	3	211/232 (91%)	204 (97%)	7 (3%)	0	100	100
4	4	196/200 (98%)	190 (97%)	6 (3%)	0	100	100
4	6	196/200 (98%)	188 (96%)	8 (4%)	0	100	100
5	A	722/750 (96%)	698 (97%)	24 (3%)	0	100	100
6	B	731/734 (100%)	704 (96%)	27 (4%)	0	100	100
7	C	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
8	D	138/155 (89%)	129 (94%)	9 (6%)	0	100	100
9	E	61/93 (66%)	58 (95%)	3 (5%)	0	100	100
10	F	153/159 (96%)	147 (96%)	6 (4%)	0	100	100
11	G	96/100 (96%)	90 (94%)	6 (6%)	0	100	100
12	H	92/95 (97%)	86 (94%)	6 (6%)	0	100	100
13	I	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
14	J	38/42 (90%)	37 (97%)	1 (3%)	0	100	100
15	K	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
16	L	160/170 (94%)	154 (96%)	6 (4%)	0	100	100
17	O	87/89 (98%)	85 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	X	216/228 (95%)	211 (98%)	5 (2%)	0	100	100
18	Z	216/228 (95%)	212 (98%)	4 (2%)	0	100	100
19	Y	224/228 (98%)	214 (96%)	10 (4%)	0	100	100
All	All	4312/4515 (96%)	4157 (96%)	155 (4%)	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	1	159/160 (99%)	158 (99%)	1 (1%)	78	80
1	5	155/160 (97%)	155 (100%)	0	100	100
2	2	164/169 (97%)	161 (98%)	3 (2%)	51	69
3	3	166/181 (92%)	164 (99%)	2 (1%)	63	74
4	4	166/167 (99%)	164 (99%)	2 (1%)	63	74
4	6	166/167 (99%)	165 (99%)	1 (1%)	78	80
5	A	582/608 (96%)	577 (99%)	5 (1%)	70	77
6	B	597/598 (100%)	589 (99%)	8 (1%)	61	73
7	C	70/71 (99%)	69 (99%)	1 (1%)	59	72
8	D	119/130 (92%)	117 (98%)	2 (2%)	53	70
9	E	58/79 (73%)	58 (100%)	0	100	100
10	F	128/132 (97%)	125 (98%)	3 (2%)	44	66
11	G	82/83 (99%)	82 (100%)	0	100	100
12	H	79/80 (99%)	79 (100%)	0	100	100
13	I	28/32 (88%)	28 (100%)	0	100	100
14	J	35/37 (95%)	35 (100%)	0	100	100
15	K	60/62 (97%)	59 (98%)	1 (2%)	53	70
16	L	128/134 (96%)	127 (99%)	1 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	O	73/73 (100%)	73 (100%)	0	100 100
18	X	168/175 (96%)	168 (100%)	0	100 100
18	Z	168/175 (96%)	167 (99%)	1 (1%)	78 80
19	Y	174/175 (99%)	170 (98%)	4 (2%)	44 66
All	All	3525/3648 (97%)	3490 (99%)	35 (1%)	65 75

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	K	62	LEU
16	L	133	LEU
19	Y	67	TYR
5	A	371	MET
5	A	366	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
11	G	148	HIS
18	Z	215	ASN
15	K	53	ASN
18	X	240	ASN
5	A	177	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\|>2$
19	TPO	Y	39	19	8,10,11	2.43	1 (12%)	10,14,16	1.26	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TPO	Y	39	19	-	6/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	39	TPO	P-OG1	6.72	1.72	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	39	TPO	OG1-P-O1P	-2.35	100.33	109.39

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	Y	39	TPO	N-CA-CB-CG2
19	Y	39	TPO	N-CA-CB-OG1
19	Y	39	TPO	C-CA-CB-CG2
19	Y	39	TPO	O-C-CA-CB
19	Y	39	TPO	CB-OG1-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

318 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	$\#\|Z\| > 2$
21	CLA	B	828	6	60,64,73	1.31	7 (11%)	72,102,113	1.73	9 (12%)
21	CLA	B	805	6	69,73,73	1.21	8 (11%)	83,113,113	1.74	12 (14%)
21	CLA	Z	304	-	49,53,73	1.42	8 (16%)	59,89,113	1.70	8 (13%)
24	BCR	O	205	-	41,41,41	0.11	0	56,56,56	0.22	0
26	LMG	4	318	-	36,36,55	0.20	0	44,44,63	0.19	0
21	CLA	B	825	6	66,70,73	1.27	7 (10%)	79,109,113	1.78	13 (16%)
21	CLA	L	301	-	69,73,73	1.22	8 (11%)	83,113,113	1.68	9 (10%)
21	CLA	6	602	4	64,68,73	1.27	8 (12%)	77,107,113	1.72	10 (12%)
20	CHL	X	601	18	50,54,74	1.52	8 (16%)	56,90,114	1.98	10 (17%)
21	CLA	X	611	18	49,53,73	1.41	7 (14%)	59,89,113	1.83	9 (15%)
21	CLA	2	608	2	49,53,73	1.40	7 (14%)	59,89,113	1.81	8 (13%)
20	CHL	2	601	2	51,55,74	1.46	6 (11%)	57,91,114	2.09	12 (21%)
20	CHL	6	615	4	44,49,74	1.54	7 (15%)	51,84,114	2.29	11 (21%)
21	CLA	2	611	2	49,53,73	1.42	8 (16%)	59,89,113	1.87	8 (13%)
24	BCR	O	201	-	41,41,41	0.13	0	56,56,56	0.63	2 (3%)
21	CLA	B	827	6	69,73,73	1.24	8 (11%)	83,113,113	1.69	11 (13%)
21	CLA	A	830	5	69,73,73	1.24	7 (10%)	83,113,113	1.68	11 (13%)
21	CLA	6	603	4	49,53,73	1.41	8 (16%)	59,89,113	1.79	9 (15%)
21	CLA	1	608	1	69,73,73	1.23	8 (11%)	83,113,113	1.61	11 (13%)
26	LMG	1	621	-	49,49,55	0.19	0	57,57,63	0.16	0
21	CLA	B	816	-	63,67,73	1.27	6 (9%)	75,105,113	1.74	11 (14%)
21	CLA	X	618	-	49,53,73	1.42	7 (14%)	59,89,113	1.73	10 (16%)
20	CHL	4	314	-	44,49,74	1.53	7 (15%)	51,84,114	2.32	13 (25%)
20	CHL	3	608	-	51,55,74	1.45	6 (11%)	57,91,114	2.11	16 (28%)
24	BCR	5	617	-	41,41,41	0.10	0	56,56,56	0.23	0
21	CLA	Y	603	-	49,53,73	1.42	8 (16%)	59,89,113	1.77	8 (13%)
21	CLA	6	609	4	58,62,73	1.34	8 (13%)	69,99,113	1.79	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	X	609	18	49,53,73	1.41	7 (14%)	59,89,113	2.03	9 (15%)
20	CHL	Y	608	-	50,54,74	1.52	8 (16%)	56,90,114	2.05	13 (23%)
21	CLA	3	611	-	47,51,73	1.42	8 (17%)	56,86,113	1.89	9 (16%)
21	CLA	B	802	-	69,73,73	1.25	6 (8%)	83,113,113	1.55	14 (16%)
21	CLA	A	809	5	59,63,73	1.33	8 (13%)	71,101,113	1.74	11 (15%)
21	CLA	5	609	1	49,53,73	1.41	8 (16%)	59,89,113	1.83	10 (16%)
29	SF4	A	850	5,6	0,12,12	-	-	-		
21	CLA	Z	310	-	49,53,73	1.42	7 (14%)	59,89,113	1.79	9 (15%)
26	LMG	G	206	-	50,50,55	0.20	0	58,58,63	0.18	0
21	CLA	A	820	5	49,53,73	1.41	8 (16%)	59,89,113	1.85	9 (15%)
21	CLA	B	830	6	47,51,73	1.40	8 (17%)	56,86,113	1.89	7 (12%)
21	CLA	L	303	16	49,53,73	1.41	8 (16%)	59,89,113	1.83	7 (11%)
21	CLA	L	305	-	49,53,73	1.42	8 (16%)	59,89,113	1.87	8 (13%)
21	CLA	B	823	-	69,73,73	1.23	8 (11%)	83,113,113	1.66	12 (14%)
24	BCR	3	601	-	41,41,41	0.12	0	56,56,56	0.26	0
21	CLA	X	612	18	49,53,73	1.41	7 (14%)	59,89,113	1.74	10 (16%)
24	BCR	B	847	-	41,41,41	0.13	0	56,56,56	0.29	0
21	CLA	2	618	4	50,54,73	1.38	8 (16%)	60,90,113	1.80	9 (15%)
20	CHL	1	606	1	44,49,74	1.46	5 (11%)	48,84,114	2.24	11 (22%)
26	LMG	5	621	-	49,49,55	0.19	0	57,57,63	0.14	0
25	LHG	1	620	-	48,48,48	0.30	0	51,54,54	0.30	0
21	CLA	4	308	4	58,62,73	1.33	7 (12%)	69,99,113	1.80	11 (15%)
26	LMG	5	620	-	53,53,55	0.18	0	61,61,63	0.14	0
28	PQN	B	841	-	34,34,34	0.24	0	42,45,45	0.50	1 (2%)
21	CLA	4	313	4	54,58,73	1.38	8 (14%)	65,95,113	1.84	10 (15%)
21	CLA	5	607	-	47,52,73	1.44	7 (14%)	56,88,113	1.85	6 (10%)
21	CLA	A	814	-	49,53,73	1.42	8 (16%)	59,89,113	1.86	8 (13%)
23	XAT	2	616	-	39,47,47	0.10	0	54,74,74	0.75	3 (5%)
23	XAT	4	316	-	39,47,47	0.12	0	54,74,74	0.88	3 (5%)
21	CLA	B	811	6	47,51,73	1.40	6 (12%)	56,86,113	1.86	8 (14%)
21	CLA	3	605	-	51,55,73	1.39	8 (15%)	61,91,113	1.88	11 (18%)
21	CLA	K	202	-	49,53,73	1.41	8 (16%)	59,89,113	1.86	9 (15%)
21	CLA	5	610	25	49,53,73	1.41	8 (16%)	59,89,113	1.90	8 (13%)
20	CHL	2	614	2	47,51,74	1.43	5 (10%)	52,86,114	2.16	9 (17%)
20	CHL	Z	301	-	50,54,74	1.53	8 (16%)	56,90,114	1.85	11 (19%)
20	CHL	Z	306	-	50,54,74	1.51	8 (16%)	56,90,114	2.10	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	A	854	-	41,41,41	0.24	0	56,56,56	0.47	0
21	CLA	3	609	3	49,53,73	1.42	8 (16%)	59,89,113	1.89	9 (15%)
25	LHG	Y	618	21	34,34,48	0.35	0	37,40,54	0.32	0
20	CHL	6	607	-	55,59,74	1.47	7 (12%)	62,96,114	2.08	12 (19%)
20	CHL	Y	609	19	50,54,74	1.53	8 (16%)	56,90,114	2.06	10 (17%)
21	CLA	A	815	5	46,50,73	1.41	8 (17%)	55,85,113	1.88	9 (16%)
20	CHL	5	606	1	44,49,74	1.49	5 (11%)	48,84,114	2.03	10 (20%)
24	BCR	1	617	-	41,41,41	0.12	0	56,56,56	0.24	0
21	CLA	A	831	5	54,58,73	1.39	8 (14%)	65,95,113	1.87	9 (13%)
21	CLA	B	806	6	56,60,73	1.36	8 (14%)	67,97,113	1.85	11 (16%)
24	BCR	2	619	-	41,41,41	0.26	0	56,56,56	0.57	1 (1%)
22	LUT	5	619	-	42,43,43	1.64	8 (19%)	51,60,60	1.62	11 (21%)
30	DGD	B	849	-	62,62,67	0.16	0	76,76,81	0.17	0
21	CLA	B	812	6	69,73,73	1.22	9 (13%)	83,113,113	1.71	10 (12%)
21	CLA	6	604	-	49,53,73	1.41	8 (16%)	59,89,113	1.85	8 (13%)
22	LUT	3	615	-	42,43,43	1.61	8 (19%)	51,60,60	1.70	11 (21%)
21	CLA	A	829	5	69,73,73	1.23	8 (11%)	83,113,113	1.66	10 (12%)
25	LHG	X	617	21	36,36,48	0.34	0	39,42,54	0.31	0
28	PQN	A	844	-	34,34,34	0.24	0	42,45,45	0.51	1 (2%)
21	CLA	A	843	-	61,65,73	1.30	8 (13%)	73,103,113	1.79	14 (19%)
21	CLA	Z	305	-	54,58,73	1.39	7 (12%)	65,95,113	1.78	7 (10%)
21	CLA	X	603	-	57,61,73	1.35	8 (14%)	68,98,113	1.74	11 (16%)
21	CLA	B	804	6	69,73,73	1.24	9 (13%)	83,113,113	1.75	9 (10%)
21	CLA	2	609	2	59,63,73	1.33	8 (13%)	71,101,113	1.75	10 (14%)
20	CHL	Y	605	-	46,50,74	1.48	6 (13%)	51,85,114	1.99	10 (19%)
21	CLA	4	309	-	64,68,73	1.28	8 (12%)	77,107,113	1.74	11 (14%)
21	CLA	1	605	-	43,48,73	1.42	8 (18%)	52,82,113	1.90	6 (11%)
24	BCR	B	845	-	41,41,41	0.13	0	56,56,56	0.34	0
22	LUT	6	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.58	11 (21%)
21	CLA	B	833	6	64,68,73	1.30	8 (12%)	77,107,113	1.72	12 (15%)
21	CLA	Z	313	-	50,54,73	1.41	8 (16%)	60,90,113	1.78	8 (13%)
21	CLA	G	202	-	49,53,73	1.42	8 (16%)	59,89,113	1.86	8 (13%)
22	LUT	1	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.54	11 (21%)
21	CLA	X	602	18	49,53,73	1.42	8 (16%)	59,89,113	1.86	8 (13%)
24	BCR	L	302	-	41,41,41	0.14	0	56,56,56	0.27	0
24	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	1	607	-	47,52,73	1.42	8 (17%)	56,88,113	1.74	6 (10%)
21	CLA	2	602	2	69,73,73	1.23	8 (11%)	83,113,113	1.65	11 (13%)
21	CLA	2	604	-	69,73,73	1.24	8 (11%)	83,113,113	1.65	13 (15%)
21	CLA	A	839	5	54,58,73	1.38	8 (14%)	65,95,113	1.82	11 (16%)
21	CLA	1	609	1	63,67,73	1.29	8 (12%)	76,106,113	1.68	11 (14%)
20	CHL	Y	619	-	51,55,74	1.47	6 (11%)	57,91,114	2.03	13 (22%)
25	LHG	A	851	-	48,48,48	0.29	0	51,54,54	0.29	0
24	BCR	B	846	-	41,41,41	0.12	0	56,56,56	0.32	0
20	CHL	Y	606	19	50,54,74	1.54	8 (16%)	56,90,114	1.94	11 (19%)
21	CLA	O	202	25	54,58,73	1.39	8 (14%)	65,95,113	1.88	10 (15%)
21	CLA	5	613	1	49,53,73	1.42	7 (14%)	59,89,113	1.80	8 (13%)
21	CLA	A	836	5	49,53,73	1.41	8 (16%)	59,89,113	1.90	8 (13%)
21	CLA	A	821	-	69,73,73	1.23	8 (11%)	83,113,113	1.72	11 (13%)
21	CLA	G	203	11	46,50,73	1.40	8 (17%)	55,85,113	1.88	8 (14%)
21	CLA	K	204	15	41,47,73	1.46	8 (19%)	49,81,113	1.92	7 (14%)
21	CLA	A	816	-	49,53,73	1.42	8 (16%)	59,89,113	1.91	9 (15%)
25	LHG	1	622	21	37,37,48	0.34	0	40,43,54	0.30	0
21	CLA	3	613	-	43,48,73	1.47	8 (18%)	51,83,113	1.80	6 (11%)
21	CLA	B	807	-	69,73,73	1.21	8 (11%)	83,113,113	1.71	12 (14%)
21	CLA	4	312	4	49,53,73	1.41	8 (16%)	59,89,113	1.83	8 (13%)
21	CLA	B	822	6	64,68,73	1.29	8 (12%)	77,107,113	1.67	11 (14%)
24	BCR	L	308	-	41,41,41	0.13	0	56,56,56	0.24	0
21	CLA	X	613	18	49,53,73	1.42	8 (16%)	59,89,113	1.79	9 (15%)
21	CLA	3	607	3	49,53,73	1.41	8 (16%)	59,89,113	1.85	8 (13%)
29	SF4	C	102	7	0,12,12	-	-	-		
24	BCR	G	205	-	41,41,41	0.12	0	56,56,56	0.31	0
21	CLA	B	818	-	59,63,73	1.34	8 (13%)	71,101,113	1.72	10 (14%)
22	LUT	F	301	-	42,43,43	1.65	8 (19%)	51,60,60	1.60	11 (21%)
21	CLA	A	834	-	69,73,73	1.23	8 (11%)	83,113,113	1.68	10 (12%)
21	CLA	K	203	15	50,54,73	1.39	7 (14%)	60,90,113	1.90	7 (11%)
21	CLA	A	819	5	69,73,73	1.23	8 (11%)	83,113,113	1.64	11 (13%)
25	LHG	A	853	21	29,29,48	0.38	0	32,35,54	0.33	0
21	CLA	6	601	4	50,54,73	1.39	8 (16%)	60,90,113	1.73	7 (11%)
20	CHL	4	306	-	55,59,74	1.47	7 (12%)	62,96,114	2.03	15 (24%)
21	CLA	A	810	5	54,58,73	1.39	7 (12%)	65,95,113	1.75	11 (16%)
21	CLA	3	602	3	64,68,73	1.29	8 (12%)	77,107,113	1.68	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	836	6	69,73,73	1.23	8 (11%)	83,113,113	1.63	10 (12%)
21	CLA	Y	610	19	49,53,73	1.42	8 (16%)	59,89,113	1.79	8 (13%)
21	CLA	B	819	6	54,58,73	1.39	8 (14%)	65,95,113	1.80	10 (15%)
24	BCR	L	307	-	41,41,41	0.14	0	56,56,56	0.29	0
22	LUT	Z	314	-	42,43,43	1.63	8 (19%)	51,60,60	1.55	10 (19%)
21	CLA	A	811	5	69,73,73	1.23	8 (11%)	83,113,113	1.66	10 (12%)
22	LUT	X	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.73	9 (17%)
21	CLA	A	841	5	69,73,73	1.22	8 (11%)	83,113,113	1.70	11 (13%)
21	CLA	B	824	-	54,58,73	1.39	6 (11%)	65,95,113	1.73	10 (15%)
21	CLA	1	604	-	53,57,73	1.36	8 (15%)	62,93,113	1.82	7 (11%)
20	CHL	Z	308	-	46,50,74	1.46	6 (13%)	51,85,114	2.20	12 (23%)
21	CLA	A	801	5	69,73,73	1.22	8 (11%)	83,113,113	1.67	13 (15%)
21	CLA	A	826	-	69,73,73	1.24	7 (10%)	83,113,113	1.65	12 (14%)
21	CLA	B	814	6	59,63,73	1.34	8 (13%)	71,101,113	1.82	9 (12%)
21	CLA	L	304	16	64,68,73	1.28	8 (12%)	77,107,113	1.72	11 (14%)
21	CLA	Z	303	18	64,68,73	1.28	7 (10%)	77,107,113	1.84	10 (12%)
21	CLA	6	613	4	49,53,73	1.41	7 (14%)	59,89,113	1.72	9 (15%)
21	CLA	A	832	5	60,64,73	1.32	8 (13%)	72,102,113	1.76	11 (15%)
21	CLA	A	804	5	59,63,73	1.32	8 (13%)	71,101,113	1.85	13 (18%)
21	CLA	4	301	4	64,68,73	1.27	8 (12%)	77,107,113	1.75	10 (12%)
25	LHG	1	618	21	48,48,48	0.29	0	51,54,54	0.28	0
22	LUT	4	315	-	42,43,43	1.66	8 (19%)	51,60,60	1.59	13 (25%)
21	CLA	F	304	10	45,49,73	1.45	8 (17%)	54,84,113	2.00	8 (14%)
21	CLA	Y	613	19	59,63,73	1.32	8 (13%)	71,101,113	1.69	12 (16%)
21	CLA	B	834	-	46,50,73	1.42	8 (17%)	55,85,113	1.88	7 (12%)
24	BCR	O	204	-	41,41,41	0.14	0	56,56,56	0.20	0
21	CLA	3	603	3	59,63,73	1.33	8 (13%)	71,101,113	1.75	10 (14%)
23	XAT	6	617	-	39,47,47	0.13	0	54,74,74	0.89	3 (5%)
24	BCR	K	205	-	41,41,41	0.12	0	56,56,56	0.21	0
31	NEX	X	616	-	38,46,46	0.41	1 (2%)	50,70,70	0.42	0
21	CLA	B	810	6	58,62,73	1.34	9 (15%)	73,100,113	2.06	13 (17%)
21	CLA	5	605	-	43,48,73	1.42	7 (16%)	52,82,113	1.85	10 (19%)
21	CLA	K	201	15	42,45,73	1.52	8 (19%)	50,78,113	1.88	9 (18%)
21	CLA	A	806	5	69,73,73	1.22	8 (11%)	83,113,113	1.76	11 (13%)
24	BCR	F	302	-	41,41,41	0.15	0	56,56,56	0.34	0
21	CLA	3	617	5	59,63,73	1.32	7 (11%)	71,101,113	1.77	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	835	-	54,58,73	1.40	8 (14%)	65,95,113	1.92	11 (16%)
27	LMT	G	201	-	36,36,36	0.10	0	47,47,47	0.16	0
23	XAT	3	616	-	39,47,47	0.10	0	54,74,74	0.88	4 (7%)
21	CLA	1	610	25	59,63,73	1.34	8 (13%)	71,101,113	1.78	9 (12%)
24	BCR	B	843	-	41,41,41	0.18	0	56,56,56	0.55	0
21	CLA	3	606	-	44,49,73	1.44	8 (18%)	52,84,113	1.83	7 (13%)
21	CLA	B	801	-	69,73,73	1.22	8 (11%)	83,113,113	1.70	12 (14%)
24	BCR	A	849	-	41,41,41	0.19	0	56,56,56	0.53	1 (1%)
20	CHL	Z	309	18	50,54,74	1.51	7 (14%)	56,90,114	1.90	13 (23%)
21	CLA	O	206	-	53,57,73	1.36	8 (15%)	62,93,113	1.74	9 (14%)
24	BCR	F	305	-	41,41,41	0.13	0	56,56,56	0.34	0
21	CLA	5	603	1	49,53,73	1.41	8 (16%)	59,89,113	1.91	7 (11%)
20	CHL	X	606	18	50,54,74	1.53	8 (16%)	56,90,114	1.87	11 (19%)
21	CLA	6	614	4	54,58,73	1.38	8 (14%)	65,95,113	1.81	10 (15%)
21	CLA	3	614	3	43,48,73	1.48	8 (18%)	51,83,113	1.75	7 (13%)
21	CLA	B	826	6	64,68,73	1.26	8 (12%)	77,107,113	1.76	11 (14%)
20	CHL	1	601	1	58,63,74	1.44	7 (12%)	65,101,114	1.88	13 (20%)
21	CLA	4	302	4	49,53,73	1.42	8 (16%)	59,89,113	1.82	10 (16%)
21	CLA	4	307	4	49,53,73	1.42	8 (16%)	59,89,113	1.84	7 (11%)
27	LMT	A	852	-	36,36,36	0.12	0	47,47,47	0.24	0
24	BCR	B	842	-	41,41,41	0.16	0	56,56,56	0.31	0
21	CLA	4	303	-	49,53,73	1.40	7 (14%)	59,89,113	1.82	10 (16%)
21	CLA	2	603	2	47,52,73	1.43	8 (17%)	56,88,113	1.77	7 (12%)
20	CHL	6	605	-	60,64,74	1.43	7 (11%)	68,102,114	1.86	16 (23%)
21	CLA	5	604	-	53,57,73	1.37	7 (13%)	62,93,113	1.79	9 (14%)
21	CLA	5	612	1	69,73,73	1.23	8 (11%)	83,113,113	1.60	13 (15%)
20	CHL	X	607	-	50,54,74	1.54	8 (16%)	56,90,114	2.02	12 (21%)
21	CLA	A	838	5	59,63,73	1.33	8 (13%)	71,101,113	1.75	10 (14%)
21	CLA	B	809	-	69,73,73	1.23	7 (10%)	83,113,113	1.57	11 (13%)
25	LHG	Z	317	21	31,31,48	0.36	0	34,37,54	0.33	0
21	CLA	B	829	6	47,51,73	1.41	7 (14%)	56,86,113	1.90	7 (12%)
20	CHL	4	305	-	50,54,74	1.51	7 (14%)	56,90,114	2.05	9 (16%)
29	SF4	C	101	7	0,12,12	-	-	-		
21	CLA	2	613	-	47,51,73	1.40	8 (17%)	56,86,113	1.82	7 (12%)
21	CLA	G	204	11	49,53,73	1.42	8 (16%)	59,89,113	1.90	9 (15%)
21	CLA	Y	612	19	49,53,73	1.42	8 (16%)	59,89,113	1.81	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	838	-	69,73,73	1.23	8 (11%)	83,113,113	1.66	10 (12%)
21	CLA	A	805	5	49,53,73	1.41	7 (14%)	59,89,113	1.85	9 (15%)
21	CLA	A	808	5	54,58,73	1.39	8 (14%)	65,95,113	1.86	10 (15%)
21	CLA	5	608	1	49,53,73	1.42	6 (12%)	59,89,113	2.12	8 (13%)
21	CLA	1	603	1	59,63,73	1.31	8 (13%)	71,101,113	1.80	12 (16%)
20	CHL	5	601	1	58,63,74	1.44	7 (12%)	65,101,114	1.87	11 (16%)
21	CLA	5	611	1	49,53,73	1.42	8 (16%)	59,89,113	1.88	8 (13%)
21	CLA	A	833	5	69,73,73	1.22	8 (11%)	83,113,113	1.73	12 (14%)
21	CLA	O	207	17	40,46,73	1.47	8 (20%)	48,80,113	1.76	6 (12%)
21	CLA	A	802	-	69,73,73	1.24	8 (11%)	83,113,113	1.72	12 (14%)
24	BCR	6	618	-	41,41,41	0.13	0	56,56,56	0.37	0
21	CLA	Y	611	25	49,53,73	1.42	8 (16%)	59,89,113	1.81	9 (15%)
20	CHL	X	605	18	46,50,74	1.47	6 (13%)	51,85,114	2.05	11 (21%)
21	CLA	B	820	6	59,63,73	1.33	7 (11%)	71,101,113	1.71	11 (15%)
21	CLA	B	808	6	59,63,73	1.33	8 (13%)	71,101,113	1.90	11 (15%)
21	CLA	1	612	1	69,73,73	1.22	8 (11%)	83,113,113	1.66	12 (14%)
21	CLA	A	823	-	45,49,73	1.44	8 (17%)	54,84,113	1.81	9 (16%)
22	LUT	5	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.58	8 (15%)
24	BCR	J	103	-	41,41,41	0.14	0	56,56,56	0.29	0
20	CHL	4	304	-	60,64,74	1.43	7 (11%)	68,102,114	1.82	15 (22%)
27	LMT	6	621	-	36,36,36	0.11	0	47,47,47	0.19	0
20	CHL	X	608	18	50,54,74	1.52	8 (16%)	56,90,114	2.08	11 (19%)
21	CLA	4	311	4	61,65,73	1.30	8 (13%)	73,103,113	1.73	10 (13%)
31	NEX	Z	316	-	38,46,46	0.37	1 (2%)	50,70,70	0.52	1 (2%)
21	CLA	3	604	-	49,53,73	1.41	8 (16%)	59,89,113	1.83	9 (15%)
21	CLA	1	614	1	49,53,73	1.41	8 (16%)	59,89,113	1.88	9 (15%)
27	LMT	F	303	-	36,36,36	0.12	0	47,47,47	0.46	0
22	LUT	Z	315	-	42,43,43	1.71	8 (19%)	51,60,60	1.93	10 (19%)
21	CLA	A	818	5	63,67,73	1.27	8 (12%)	75,105,113	1.75	12 (16%)
21	CLA	J	102	-	46,50,73	1.41	8 (17%)	55,85,113	1.85	8 (14%)
21	CLA	5	602	1	65,69,73	1.27	8 (12%)	78,108,113	1.69	9 (11%)
23	XAT	1	616	-	39,47,47	0.11	0	54,74,74	0.86	3 (5%)
20	CHL	Y	607	-	50,54,74	1.54	8 (16%)	56,90,114	1.90	11 (19%)
20	CHL	2	605	2	46,50,74	1.48	5 (10%)	52,85,114	2.00	10 (19%)
24	BCR	A	847	-	41,41,41	0.14	0	56,56,56	0.38	0
21	CLA	B	839	6	69,73,73	1.23	8 (11%)	83,113,113	1.74	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	1	602	1	65,69,73	1.26	8 (12%)	78,108,113	1.70	10 (12%)
27	LMT	4	319	-	36,36,36	0.11	0	47,47,47	0.16	0
24	BCR	A	846	-	41,41,41	0.16	0	56,56,56	0.56	1 (1%)
24	BCR	B	848	-	41,41,41	0.24	0	56,56,56	0.64	1 (1%)
21	CLA	6	610	-	49,53,73	1.43	7 (14%)	59,89,113	1.65	8 (13%)
21	CLA	A	824	5	59,63,73	1.33	8 (13%)	71,101,113	1.68	10 (14%)
26	LMG	1	619	-	53,53,55	0.18	0	61,61,63	0.17	0
21	CLA	3	612	3	47,52,73	1.44	8 (17%)	56,88,113	1.77	7 (12%)
24	BCR	I	101	-	41,41,41	0.15	0	56,56,56	0.23	0
21	CLA	2	612	-	59,63,73	1.33	8 (13%)	71,101,113	1.84	12 (16%)
21	CLA	1	611	1	49,53,73	1.42	8 (16%)	59,89,113	1.87	9 (15%)
23	XAT	5	616	-	39,47,47	0.09	0	54,74,74	0.67	2 (3%)
24	BCR	L	306	-	41,41,41	0.15	0	56,56,56	0.34	0
21	CLA	Z	311	25	49,53,73	1.42	7 (14%)	59,89,113	1.73	8 (13%)
21	CLA	A	817	5	64,68,73	1.28	8 (12%)	77,107,113	1.69	13 (16%)
21	CLA	B	831	6	69,73,73	1.23	8 (11%)	83,113,113	1.77	11 (13%)
21	CLA	Z	312	-	49,53,73	1.42	8 (16%)	59,89,113	1.77	8 (13%)
24	BCR	A	848	-	41,41,41	0.15	0	56,56,56	0.37	0
21	CLA	A	827	5	69,73,73	1.23	8 (11%)	83,113,113	1.76	11 (13%)
21	CLA	A	822	5	46,50,73	1.40	7 (15%)	55,85,113	1.73	6 (10%)
21	CLA	B	817	6	64,68,73	1.27	8 (12%)	77,107,113	1.76	13 (16%)
21	CLA	Y	604	-	49,53,73	1.42	8 (16%)	59,89,113	1.78	7 (11%)
20	CHL	6	606	-	50,54,74	1.52	7 (14%)	56,90,114	2.05	9 (16%)
21	CLA	A	835	5	49,53,73	1.42	6 (12%)	59,89,113	1.79	7 (11%)
21	CLA	O	203	-	66,70,73	1.25	7 (10%)	79,109,113	1.75	11 (13%)
21	CLA	X	610	25	49,53,73	1.41	7 (14%)	59,89,113	1.94	9 (15%)
25	LHG	2	617	21	36,36,48	0.34	0	39,42,54	0.32	0
21	CLA	A	813	5	69,73,73	1.21	7 (10%)	83,113,113	1.77	12 (14%)
22	LUT	Y	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.54	9 (17%)
21	CLA	H	201	12	64,68,73	1.27	7 (10%)	77,107,113	1.59	12 (15%)
24	BCR	A	845	-	41,41,41	0.15	0	56,56,56	0.25	0
21	CLA	B	821	6	59,63,73	1.32	8 (13%)	71,101,113	1.72	11 (15%)
21	CLA	A	803	-	69,73,73	1.21	7 (10%)	83,113,113	1.58	13 (15%)
20	CHL	Z	307	-	50,54,74	1.52	7 (14%)	56,90,114	1.89	12 (21%)
21	CLA	B	813	6	69,73,73	1.24	7 (10%)	83,113,113	1.68	10 (12%)
26	LMG	6	619	-	36,36,55	0.20	0	44,44,63	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	3	610	3	45,49,73	1.45	7 (15%)	54,84,113	1.90	9 (16%)
21	CLA	B	840	25	69,73,73	1.23	8 (11%)	83,113,113	1.74	12 (14%)
21	CLA	4	310	4	44,49,73	1.44	8 (18%)	52,84,113	1.85	4 (7%)
21	CLA	2	610	25	45,49,73	1.46	8 (17%)	54,84,113	1.86	7 (12%)
21	CLA	B	815	6	59,63,73	1.33	8 (13%)	71,101,113	1.80	9 (12%)
20	CHL	2	606	-	47,51,74	1.44	5 (10%)	52,86,114	2.00	10 (19%)
22	LUT	X	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.68	11 (21%)
21	CLA	X	604	-	49,53,73	1.42	7 (14%)	59,89,113	1.80	9 (15%)
21	CLA	A	825	-	69,73,73	1.22	8 (11%)	83,113,113	1.62	9 (10%)
26	LMG	F	307	-	30,30,55	0.21	0	38,38,63	0.16	0
26	LMG	F	306	-	47,47,55	0.21	0	55,55,63	0.18	0
21	CLA	Y	614	19	49,53,73	1.41	8 (16%)	59,89,113	1.82	9 (15%)
21	CLA	A	837	5	55,59,73	1.36	9 (16%)	66,96,113	1.99	11 (16%)
25	LHG	5	618	21	48,48,48	0.29	0	51,54,54	0.28	0
31	NEX	Y	617	-	38,46,46	0.39	1 (2%)	50,70,70	0.46	0
21	CLA	B	832	-	49,53,73	1.41	8 (16%)	59,89,113	1.76	6 (10%)
24	BCR	6	620	-	41,41,41	0.18	0	56,56,56	0.47	0
24	BCR	4	317	-	41,41,41	0.13	0	56,56,56	0.30	0
20	CHL	2	607	-	55,59,74	1.47	7 (12%)	62,96,114	2.04	12 (19%)
21	CLA	A	840	5	69,73,73	1.21	7 (10%)	83,113,113	1.66	10 (12%)
21	CLA	J	101	-	46,50,73	1.41	8 (17%)	55,85,113	1.88	7 (12%)
20	CHL	Z	302	18	50,54,74	1.53	8 (16%)	56,90,114	2.04	14 (25%)
21	CLA	5	614	1	49,53,73	1.39	7 (14%)	59,89,113	1.85	8 (13%)
21	CLA	B	803	6	45,49,73	1.44	7 (15%)	54,84,113	1.91	10 (18%)
21	CLA	6	608	4	49,53,73	1.42	8 (16%)	59,89,113	1.82	8 (13%)
21	CLA	A	812	5	58,62,73	1.33	8 (13%)	69,99,113	1.83	12 (17%)
21	CLA	A	828	-	69,73,73	1.22	7 (10%)	83,113,113	1.68	12 (14%)
21	CLA	B	837	6	51,55,73	1.37	8 (15%)	61,91,113	1.86	10 (16%)
21	CLA	Y	602	19	69,73,73	1.24	8 (11%)	83,113,113	1.69	9 (10%)
21	CLA	6	611	-	44,49,73	1.44	8 (18%)	52,84,113	1.93	5 (9%)
21	CLA	A	842	-	69,73,73	1.22	8 (11%)	83,113,113	1.60	10 (12%)
23	XAT	O	208	-	39,47,47	0.10	0	54,74,74	0.86	2 (3%)
22	LUT	Y	616	-	42,43,43	1.64	8 (19%)	51,60,60	1.60	11 (21%)
26	LMG	B	850	-	52,52,55	0.20	0	60,60,63	0.14	0
21	CLA	A	807	5	69,73,73	1.22	9 (13%)	83,113,113	1.73	11 (13%)
22	LUT	2	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.52	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	1	613	1	49,53,73	1.40	6 (12%)	59,89,113	1.81	10 (16%)
20	CHL	Y	601	19	50,54,74	1.51	7 (14%)	56,90,114	2.09	13 (23%)
21	CLA	6	612	4	61,65,73	1.31	8 (13%)	73,103,113	1.72	12 (16%)

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
21	CLA	B	828	6	-	13/29/105/115	-
21	CLA	B	805	6	-	18/39/115/115	-
21	CLA	Z	304	-	-	11/15/91/115	-
24	BCR	O	205	-	-	2/29/63/63	0/2/2/2
26	LMG	4	318	-	-	9/31/51/70	0/1/1/1
21	CLA	B	825	6	-	13/36/112/115	-
21	CLA	L	301	-	-	16/39/115/115	-
21	CLA	6	602	4	-	9/33/109/115	-
20	CHL	X	601	18	-	9/17/93/117	-
21	CLA	X	611	18	-	7/15/91/115	-
21	CLA	2	608	2	-	6/15/91/115	-
20	CHL	2	601	2	-	4/19/95/117	-
20	CHL	6	615	4	-	0/10/86/117	-
21	CLA	2	611	2	-	5/15/91/115	-
24	BCR	O	201	-	-	3/29/63/63	0/2/2/2
21	CLA	B	827	6	-	18/39/115/115	-
21	CLA	A	830	5	-	9/39/115/115	-
21	CLA	6	603	4	-	5/15/91/115	-
21	CLA	1	608	1	-	17/39/115/115	-
26	LMG	1	621	-	-	8/44/64/70	0/1/1/1
21	CLA	B	816	-	-	17/32/108/115	-
21	CLA	X	618	-	-	7/15/91/115	-
20	CHL	4	314	-	-	2/10/86/117	-
20	CHL	3	608	-	-	9/19/95/117	-
24	BCR	5	617	-	-	2/29/63/63	0/2/2/2
21	CLA	Y	603	-	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	609	4	-	4/26/102/115	-
21	CLA	X	609	18	-	7/15/91/115	-
20	CHL	Y	608	-	-	8/17/93/117	-
21	CLA	3	611	-	-	4/13/89/115	-
21	CLA	B	802	-	-	15/39/115/115	-
21	CLA	A	809	5	-	5/27/103/115	-
21	CLA	5	609	1	-	8/15/91/115	-
29	SF4	A	850	5,6	-	-	0/6/5/5
21	CLA	Z	310	-	-	10/15/91/115	-
26	LMG	G	206	-	-	12/45/65/70	0/1/1/1
21	CLA	A	820	5	-	7/15/91/115	-
21	CLA	B	830	6	-	2/13/89/115	-
21	CLA	L	303	16	-	6/15/91/115	-
21	CLA	L	305	-	-	6/15/91/115	-
21	CLA	B	823	-	-	21/39/115/115	-
24	BCR	3	601	-	-	0/29/63/63	0/2/2/2
21	CLA	X	612	18	-	6/15/91/115	-
24	BCR	B	847	-	-	0/29/63/63	0/2/2/2
21	CLA	2	618	4	-	7/17/93/115	-
20	CHL	1	606	1	-	2/10/86/117	-
26	LMG	5	621	-	-	7/44/64/70	0/1/1/1
25	LHG	1	620	-	-	11/53/53/53	-
21	CLA	4	308	4	-	4/26/102/115	-
26	LMG	5	620	-	-	10/48/68/70	0/1/1/1
28	PQN	B	841	-	-	8/23/43/43	0/2/2/2
21	CLA	4	313	4	-	7/21/97/115	-
21	CLA	5	607	-	-	3/13/89/115	-
21	CLA	A	814	-	-	5/15/91/115	-
23	XAT	2	616	-	-	0/31/93/93	0/4/4/4
23	XAT	4	316	-	-	0/31/93/93	0/4/4/4
21	CLA	B	811	6	-	5/13/89/115	-
21	CLA	3	605	-	-	6/18/94/115	-
21	CLA	K	202	-	-	3/15/91/115	-
21	CLA	5	610	25	-	3/15/91/115	-
20	CHL	2	614	2	-	2/14/90/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	Z	301	-	-	10/17/93/117	-
20	CHL	Z	306	-	-	6/17/93/117	-
24	BCR	A	854	-	-	3/29/63/63	0/2/2/2
21	CLA	3	609	3	-	5/15/91/115	-
25	LHG	Y	618	21	-	9/39/39/53	-
20	CHL	6	607	-	-	10/23/99/117	-
20	CHL	Y	609	19	-	3/17/93/117	-
21	CLA	A	815	5	-	5/12/88/115	-
20	CHL	5	606	1	-	1/10/86/117	-
24	BCR	1	617	-	-	0/29/63/63	0/2/2/2
21	CLA	A	831	5	-	5/21/97/115	-
21	CLA	B	806	6	-	5/24/100/115	-
24	BCR	2	619	-	-	14/29/63/63	0/2/2/2
22	LUT	5	619	-	-	2/29/67/67	0/2/2/2
30	DGD	B	849	-	-	7/50/90/95	0/2/2/2
21	CLA	B	812	6	-	19/39/115/115	-
21	CLA	6	604	-	-	4/15/91/115	-
22	LUT	3	615	-	-	2/29/67/67	0/2/2/2
21	CLA	A	829	5	-	16/39/115/115	-
25	LHG	X	617	21	-	11/41/41/53	-
28	PQN	A	844	-	-	6/23/43/43	0/2/2/2
21	CLA	A	843	-	-	12/30/106/115	-
21	CLA	Z	305	-	-	11/21/97/115	-
21	CLA	X	603	-	-	12/25/101/115	-
21	CLA	B	804	6	-	16/39/115/115	-
21	CLA	2	609	2	-	8/27/103/115	-
20	CHL	Y	605	-	-	5/12/88/117	-
21	CLA	4	309	-	-	11/33/109/115	-
21	CLA	1	605	-	-	3/10/82/115	-
24	BCR	B	845	-	-	0/29/63/63	0/2/2/2
22	LUT	6	616	-	-	1/29/67/67	0/2/2/2
21	CLA	B	833	6	-	6/33/109/115	-
21	CLA	Z	313	-	-	9/17/93/115	-
21	CLA	G	202	-	-	7/15/91/115	-
22	LUT	1	615	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	X	602	18	-	8/15/91/115	-
24	BCR	L	302	-	-	4/29/63/63	0/2/2/2
24	BCR	B	844	-	-	4/29/63/63	0/2/2/2
21	CLA	1	607	-	-	1/13/89/115	-
21	CLA	2	602	2	-	14/39/115/115	-
21	CLA	2	604	-	-	17/39/115/115	-
21	CLA	A	839	5	-	4/21/97/115	-
21	CLA	1	609	1	-	7/31/107/115	-
20	CHL	Y	619	-	-	7/19/95/117	-
25	LHG	A	851	-	-	8/53/53/53	-
24	BCR	B	846	-	-	3/29/63/63	0/2/2/2
20	CHL	Y	606	19	-	0/17/93/117	-
21	CLA	O	202	25	-	10/21/97/115	-
21	CLA	5	613	1	-	2/15/91/115	-
21	CLA	A	836	5	-	4/15/91/115	-
21	CLA	A	821	-	-	13/39/115/115	-
21	CLA	G	203	11	-	4/12/88/115	-
21	CLA	K	204	15	-	2/8/80/115	-
21	CLA	A	816	-	-	4/15/91/115	-
25	LHG	1	622	21	-	4/42/42/53	-
21	CLA	3	613	-	-	2/8/84/115	-
21	CLA	B	807	-	-	14/39/115/115	-
21	CLA	4	312	4	-	5/15/91/115	-
21	CLA	B	822	6	-	18/33/109/115	-
24	BCR	L	308	-	-	6/29/63/63	0/2/2/2
21	CLA	X	613	18	-	7/15/91/115	-
21	CLA	3	607	3	-	7/15/91/115	-
29	SF4	C	102	7	-	-	0/6/5/5
24	BCR	G	205	-	-	0/29/63/63	0/2/2/2
21	CLA	B	818	-	-	12/27/103/115	-
22	LUT	F	301	-	-	2/29/67/67	0/2/2/2
21	CLA	A	834	-	-	12/39/115/115	-
21	CLA	K	203	15	-	4/17/93/115	-
21	CLA	A	819	5	-	18/39/115/115	-
25	LHG	A	853	21	-	6/34/34/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	601	4	-	6/17/93/115	-
20	CHL	4	306	-	-	9/23/99/117	-
21	CLA	A	810	5	-	6/21/97/115	-
21	CLA	3	602	3	-	10/33/109/115	-
21	CLA	B	836	6	-	11/39/115/115	-
21	CLA	Y	610	19	-	10/15/91/115	-
21	CLA	B	819	6	-	7/21/97/115	-
24	BCR	L	307	-	-	2/29/63/63	0/2/2/2
22	LUT	Z	314	-	-	2/29/67/67	0/2/2/2
21	CLA	A	811	5	-	12/39/115/115	-
22	LUT	X	614	-	-	0/29/67/67	0/2/2/2
21	CLA	A	841	5	-	16/39/115/115	-
21	CLA	B	824	-	-	4/21/97/115	-
21	CLA	1	604	-	-	5/20/96/115	-
20	CHL	Z	308	-	-	5/12/88/117	-
21	CLA	A	801	5	-	19/39/115/115	-
21	CLA	A	826	-	-	16/39/115/115	-
21	CLA	B	814	6	-	9/27/103/115	-
21	CLA	L	304	16	-	11/33/109/115	-
21	CLA	Z	303	18	-	19/33/109/115	-
21	CLA	6	613	4	-	5/15/91/115	-
21	CLA	A	832	5	-	7/29/105/115	-
21	CLA	A	804	5	-	12/27/103/115	-
21	CLA	4	301	4	-	6/33/109/115	-
25	LHG	1	618	21	-	5/53/53/53	-
22	LUT	4	315	-	-	1/29/67/67	0/2/2/2
21	CLA	F	304	10	-	2/10/86/115	-
21	CLA	Y	613	19	-	8/27/103/115	-
21	CLA	B	834	-	-	4/12/88/115	-
24	BCR	O	204	-	-	4/29/63/63	0/2/2/2
21	CLA	3	603	3	-	12/27/103/115	-
23	XAT	6	617	-	-	0/31/93/93	0/4/4/4
24	BCR	K	205	-	-	4/29/63/63	0/2/2/2
31	NEX	X	616	-	-	2/27/83/83	0/3/3/3
21	CLA	B	810	6	-	9/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	605	-	-	2/10/82/115	-
21	CLA	K	201	15	-	0/4/76/115	-
21	CLA	A	806	5	-	22/39/115/115	-
24	BCR	F	302	-	-	0/29/63/63	0/2/2/2
21	CLA	3	617	5	-	14/27/103/115	-
21	CLA	B	835	-	-	4/21/97/115	-
27	LMT	G	201	-	-	2/21/61/61	0/2/2/2
23	XAT	3	616	-	-	0/31/93/93	0/4/4/4
21	CLA	1	610	25	-	6/27/103/115	-
24	BCR	B	843	-	-	3/29/63/63	0/2/2/2
21	CLA	3	606	-	-	4/10/86/115	-
21	CLA	B	801	-	-	13/39/115/115	-
24	BCR	A	849	-	-	7/29/63/63	0/2/2/2
20	CHL	Z	309	18	-	5/17/93/117	-
21	CLA	O	206	-	-	7/20/96/115	-
24	BCR	F	305	-	-	2/29/63/63	0/2/2/2
21	CLA	5	603	1	-	5/15/91/115	-
20	CHL	X	606	18	-	6/17/93/117	-
21	CLA	6	614	4	-	9/21/97/115	-
21	CLA	3	614	3	-	0/8/84/115	-
21	CLA	B	826	6	-	13/33/109/115	-
20	CHL	1	601	1	-	9/27/103/117	-
21	CLA	4	302	4	-	5/15/91/115	-
21	CLA	4	307	4	-	4/15/91/115	-
27	LMT	A	852	-	-	4/21/61/61	0/2/2/2
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
21	CLA	4	303	-	-	5/15/91/115	-
21	CLA	2	603	2	-	3/13/89/115	-
20	CHL	6	605	-	-	12/29/105/117	-
21	CLA	5	604	-	-	6/20/96/115	-
21	CLA	5	612	1	-	19/39/115/115	-
20	CHL	X	607	-	-	4/17/93/117	-
21	CLA	A	838	5	-	6/27/103/115	-
21	CLA	B	809	-	-	17/39/115/115	-
25	LHG	Z	317	21	-	3/36/36/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	829	6	-	5/13/89/115	-
20	CHL	4	305	-	-	6/17/93/117	-
29	SF4	C	101	7	-	-	0/6/5/5
21	CLA	2	613	-	-	2/13/89/115	-
21	CLA	G	204	11	-	7/15/91/115	-
21	CLA	Y	612	19	-	5/15/91/115	-
21	CLA	B	838	-	-	15/39/115/115	-
21	CLA	A	805	5	-	4/15/91/115	-
21	CLA	A	808	5	-	8/21/97/115	-
21	CLA	5	608	1	-	5/15/91/115	-
21	CLA	1	603	1	-	6/27/103/115	-
20	CHL	5	601	1	-	7/27/103/117	-
21	CLA	5	611	1	-	7/15/91/115	-
21	CLA	A	833	5	-	19/39/115/115	-
21	CLA	O	207	17	-	1/6/78/115	-
21	CLA	A	802	-	-	9/39/115/115	-
24	BCR	6	618	-	-	2/29/63/63	0/2/2/2
21	CLA	Y	611	25	-	2/15/91/115	-
20	CHL	X	605	18	-	2/12/88/117	-
21	CLA	B	820	6	-	11/27/103/115	-
21	CLA	B	808	6	-	7/27/103/115	-
21	CLA	1	612	1	-	19/39/115/115	-
21	CLA	A	823	-	-	1/10/86/115	-
22	LUT	5	615	-	-	2/29/67/67	0/2/2/2
24	BCR	J	103	-	-	2/29/63/63	0/2/2/2
20	CHL	4	304	-	-	16/29/105/117	-
27	LMT	6	621	-	-	4/21/61/61	0/2/2/2
20	CHL	X	608	18	-	5/17/93/117	-
21	CLA	4	311	4	-	12/30/106/115	-
31	NEX	Z	316	-	-	5/27/83/83	0/3/3/3
21	CLA	3	604	-	-	5/15/91/115	-
21	CLA	1	614	1	-	8/15/91/115	-
27	LMT	F	303	-	-	6/21/61/61	0/2/2/2
22	LUT	Z	315	-	-	4/29/67/67	0/2/2/2
21	CLA	A	818	5	-	15/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	J	102	-	-	6/12/88/115	-
21	CLA	5	602	1	-	14/35/111/115	-
23	XAT	1	616	-	-	0/31/93/93	0/4/4/4
20	CHL	Y	607	-	-	9/17/93/117	-
20	CHL	2	605	2	-	5/12/88/117	-
24	BCR	A	847	-	-	2/29/63/63	0/2/2/2
21	CLA	B	839	6	-	12/39/115/115	-
21	CLA	1	602	1	-	10/35/111/115	-
27	LMT	4	319	-	-	4/21/61/61	0/2/2/2
24	BCR	A	846	-	-	3/29/63/63	0/2/2/2
24	BCR	B	848	-	-	6/29/63/63	0/2/2/2
21	CLA	6	610	-	-	5/15/91/115	-
21	CLA	A	824	5	-	13/27/103/115	-
26	LMG	1	619	-	-	11/48/68/70	0/1/1/1
21	CLA	3	612	3	-	2/13/89/115	-
24	BCR	I	101	-	-	0/29/63/63	0/2/2/2
21	CLA	2	612	-	-	10/27/103/115	-
21	CLA	1	611	1	-	4/15/91/115	-
23	XAT	5	616	-	-	0/31/93/93	0/4/4/4
24	BCR	L	306	-	-	4/29/63/63	0/2/2/2
21	CLA	Z	311	25	-	6/15/91/115	-
21	CLA	A	817	5	-	16/33/109/115	-
21	CLA	B	831	6	-	12/39/115/115	-
21	CLA	Z	312	-	-	8/15/91/115	-
24	BCR	A	848	-	-	4/29/63/63	0/2/2/2
21	CLA	A	827	5	-	14/39/115/115	-
21	CLA	A	822	5	-	4/12/88/115	-
21	CLA	B	817	6	-	20/33/109/115	-
21	CLA	Y	604	-	-	9/15/91/115	-
20	CHL	6	606	-	-	6/17/93/117	-
21	CLA	A	835	5	-	3/15/91/115	-
21	CLA	O	203	-	-	15/36/112/115	-
21	CLA	X	610	25	-	9/15/91/115	-
25	LHG	2	617	21	-	10/41/41/53	-
21	CLA	A	813	5	-	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LUT	Y	615	-	-	2/29/67/67	0/2/2/2
21	CLA	H	201	12	-	15/33/109/115	-
24	BCR	A	845	-	-	4/29/63/63	0/2/2/2
21	CLA	B	821	6	-	12/27/103/115	-
21	CLA	A	803	-	-	15/39/115/115	-
20	CHL	Z	307	-	-	8/17/93/117	-
21	CLA	B	813	6	-	18/39/115/115	-
26	LMG	6	619	-	-	10/31/51/70	0/1/1/1
21	CLA	3	610	3	-	3/10/86/115	-
21	CLA	B	840	25	-	25/39/115/115	-
21	CLA	4	310	4	-	2/10/86/115	-
21	CLA	2	610	25	-	2/10/86/115	-
21	CLA	B	815	6	-	5/27/103/115	-
20	CHL	2	606	-	-	7/14/90/117	-
22	LUT	X	615	-	-	3/29/67/67	0/2/2/2
21	CLA	X	604	-	-	7/15/91/115	-
21	CLA	A	825	-	-	20/39/115/115	-
26	LMG	F	307	-	-	3/25/45/70	0/1/1/1
26	LMG	F	306	-	-	9/42/62/70	0/1/1/1
21	CLA	Y	614	19	-	6/15/91/115	-
21	CLA	A	837	5	-	8/23/99/115	-
25	LHG	5	618	21	-	7/53/53/53	-
31	NEX	Y	617	-	-	3/27/83/83	0/3/3/3
21	CLA	B	832	-	-	3/15/91/115	-
24	BCR	6	620	-	-	11/29/63/63	0/2/2/2
24	BCR	4	317	-	-	0/29/63/63	0/2/2/2
20	CHL	2	607	-	-	9/23/99/117	-
21	CLA	A	840	5	-	19/39/115/115	-
21	CLA	J	101	-	-	0/12/88/115	-
20	CHL	Z	302	18	-	7/17/93/117	-
21	CLA	5	614	1	-	9/15/91/115	-
21	CLA	B	803	6	-	4/10/86/115	-
21	CLA	6	608	4	-	5/15/91/115	-
21	CLA	A	812	5	-	10/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	828	-	-	13/39/115/115	-
21	CLA	B	837	6	-	5/18/94/115	-
21	CLA	Y	602	19	-	28/39/115/115	-
21	CLA	6	611	-	-	0/10/86/115	-
21	CLA	A	842	-	-	10/39/115/115	-
23	XAT	O	208	-	-	1/31/93/93	0/4/4/4
22	LUT	Y	616	-	-	0/29/67/67	0/2/2/2
26	LMG	B	850	-	-	12/47/67/70	0/1/1/1
21	CLA	A	807	5	-	21/39/115/115	-
22	LUT	2	615	-	-	1/29/67/67	0/2/2/2
21	CLA	1	613	1	-	4/15/91/115	-
20	CHL	Y	601	19	-	10/17/93/117	-
21	CLA	6	612	4	-	12/30/106/115	-

The worst 5 of 1864 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	X	605	CHL	CMC-C2C	5.48	1.56	1.45
20	X	607	CHL	CMC-C2C	5.47	1.56	1.45
20	5	606	CHL	CMC-C2C	5.46	1.56	1.45
20	X	606	CHL	CMC-C2C	5.45	1.56	1.45
20	Y	607	CHL	CMC-C2C	5.45	1.56	1.45

The worst 5 of 2453 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	608	CLA	C4A-NA-C1A	12.06	112.13	106.71
21	X	609	CLA	C4A-NA-C1A	11.26	111.77	106.71
21	Z	303	CLA	C4A-NA-C1A	11.10	111.70	106.71
20	6	607	CHL	C4A-NA-C1A	11.06	111.68	106.71
21	A	806	CLA	C4A-NA-C1A	10.99	111.65	106.71

There are no chirality outliers.

5 of 2288 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	601	CHL	C2B-C3B-CAB-CBB
20	1	601	CHL	C4B-C3B-CAB-CBB
20	2	605	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	2	605	CHL	C3A-C2A-CAA-CBA
20	2	606	CHL	C1A-C2A-CAA-CBA

There are no ring outliers.

239 monomers are involved in 453 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	828	CLA	2	0
21	B	805	CLA	1	0
24	O	205	BCR	3	0
21	B	825	CLA	2	0
21	L	301	CLA	4	0
21	6	602	CLA	3	0
20	X	601	CHL	3	0
21	X	611	CLA	4	0
21	2	608	CLA	1	0
20	2	601	CHL	3	0
21	2	611	CLA	3	0
24	O	201	BCR	2	0
21	B	827	CLA	1	0
21	A	830	CLA	2	0
21	B	816	CLA	2	0
21	X	618	CLA	2	0
20	4	314	CHL	1	0
20	3	608	CHL	1	0
24	5	617	BCR	1	0
21	Y	603	CLA	1	0
21	6	609	CLA	1	0
21	X	609	CLA	4	0
20	Y	608	CHL	3	0
21	B	802	CLA	5	0
21	A	809	CLA	2	0
21	5	609	CLA	1	0
29	A	850	SF4	1	0
21	Z	310	CLA	4	0
26	G	206	LMG	1	0
21	A	820	CLA	1	0
21	L	305	CLA	2	0
21	B	823	CLA	1	0
24	3	601	BCR	2	0
24	B	847	BCR	3	0
20	1	606	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	5	621	LMG	1	0
25	1	620	LHG	2	0
21	4	308	CLA	1	0
26	5	620	LMG	1	0
28	B	841	PQN	4	0
21	4	313	CLA	2	0
23	4	316	XAT	1	0
21	B	811	CLA	1	0
21	3	605	CLA	1	0
21	K	202	CLA	1	0
20	2	614	CHL	1	0
20	Z	301	CHL	2	0
24	A	854	BCR	4	0
21	3	609	CLA	1	0
25	Y	618	LHG	3	0
20	6	607	CHL	1	0
20	Y	609	CHL	1	0
24	2	619	BCR	2	0
22	5	619	LUT	3	0
30	B	849	DGD	2	0
21	B	812	CLA	3	0
22	3	615	LUT	6	0
21	A	829	CLA	3	0
25	X	617	LHG	3	0
21	Z	305	CLA	3	0
21	X	603	CLA	3	0
21	B	804	CLA	2	0
21	2	609	CLA	2	0
20	Y	605	CHL	1	0
21	1	605	CLA	1	0
24	B	845	BCR	1	0
22	6	616	LUT	3	0
21	Z	313	CLA	3	0
22	1	615	LUT	4	0
21	X	602	CLA	2	0
24	L	302	BCR	5	0
21	2	602	CLA	1	0
21	2	604	CLA	1	0
21	A	839	CLA	1	0
21	1	609	CLA	3	0
20	Y	619	CHL	2	0
25	A	851	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	846	BCR	2	0
20	Y	606	CHL	2	0
21	O	202	CLA	2	0
21	5	613	CLA	1	0
21	A	821	CLA	1	0
21	G	203	CLA	2	0
21	K	204	CLA	1	0
21	A	816	CLA	1	0
25	1	622	LHG	1	0
21	B	807	CLA	1	0
21	B	822	CLA	2	0
24	L	308	BCR	5	0
21	X	613	CLA	1	0
21	3	607	CLA	1	0
24	G	205	BCR	2	0
22	F	301	LUT	3	0
21	A	834	CLA	2	0
21	K	203	CLA	1	0
21	A	819	CLA	2	0
25	A	853	LHG	2	0
21	6	601	CLA	1	0
20	4	306	CHL	2	0
21	A	810	CLA	3	0
21	Y	610	CLA	1	0
24	L	307	BCR	2	0
22	Z	314	LUT	7	0
21	A	811	CLA	2	0
22	X	614	LUT	8	0
21	A	841	CLA	2	0
21	B	824	CLA	1	0
21	1	604	CLA	1	0
20	Z	308	CHL	1	0
21	A	801	CLA	1	0
21	A	826	CLA	2	0
21	L	304	CLA	4	0
21	Z	303	CLA	5	0
21	A	832	CLA	2	0
21	A	804	CLA	3	0
21	4	301	CLA	1	0
25	1	618	LHG	5	0
22	4	315	LUT	4	0
21	Y	613	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	O	204	BCR	1	0
21	3	603	CLA	1	0
23	6	617	XAT	2	0
31	X	616	NEX	1	0
21	B	810	CLA	1	0
21	5	605	CLA	2	0
21	A	806	CLA	1	0
24	F	302	BCR	1	0
21	3	617	CLA	1	0
23	3	616	XAT	2	0
24	B	843	BCR	1	0
21	B	801	CLA	1	0
24	A	849	BCR	4	0
20	Z	309	CHL	3	0
21	O	206	CLA	4	0
24	F	305	BCR	1	0
20	X	606	CHL	1	0
21	B	826	CLA	4	0
20	1	601	CHL	2	0
24	B	842	BCR	2	0
21	4	303	CLA	1	0
20	6	605	CHL	4	0
21	5	604	CLA	3	0
21	5	612	CLA	4	0
20	X	607	CHL	2	0
21	A	838	CLA	1	0
21	B	809	CLA	6	0
25	Z	317	LHG	2	0
20	4	305	CHL	1	0
21	2	613	CLA	1	0
21	B	838	CLA	6	0
21	A	805	CLA	1	0
21	A	808	CLA	1	0
21	5	608	CLA	1	0
21	1	603	CLA	2	0
20	5	601	CHL	3	0
21	5	611	CLA	1	0
21	A	802	CLA	7	0
24	6	618	BCR	1	0
20	X	605	CHL	1	0
21	B	820	CLA	1	0
21	B	808	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	612	CLA	3	0
22	5	615	LUT	6	0
24	J	103	BCR	4	0
20	4	304	CHL	2	0
20	X	608	CHL	2	0
21	4	311	CLA	1	0
31	Z	316	NEX	3	0
21	1	614	CLA	1	0
22	Z	315	LUT	6	0
21	A	818	CLA	3	0
21	J	102	CLA	2	0
21	5	602	CLA	1	0
23	1	616	XAT	1	0
20	Y	607	CHL	2	0
20	2	605	CHL	2	0
24	A	847	BCR	1	0
21	B	839	CLA	3	0
27	4	319	LMT	1	0
24	A	846	BCR	4	0
24	B	848	BCR	8	0
21	6	610	CLA	3	0
21	A	824	CLA	3	0
26	1	619	LMG	1	0
21	3	612	CLA	3	0
24	I	101	BCR	1	0
21	2	612	CLA	2	0
23	5	616	XAT	1	0
24	L	306	BCR	3	0
21	A	817	CLA	2	0
21	B	831	CLA	1	0
21	Z	312	CLA	4	0
24	A	848	BCR	2	0
21	A	827	CLA	2	0
21	B	817	CLA	1	0
21	Y	604	CLA	2	0
20	6	606	CHL	2	0
21	O	203	CLA	3	0
21	X	610	CLA	3	0
25	2	617	LHG	2	0
21	A	813	CLA	5	0
22	Y	615	LUT	8	0
21	H	201	CLA	2	0

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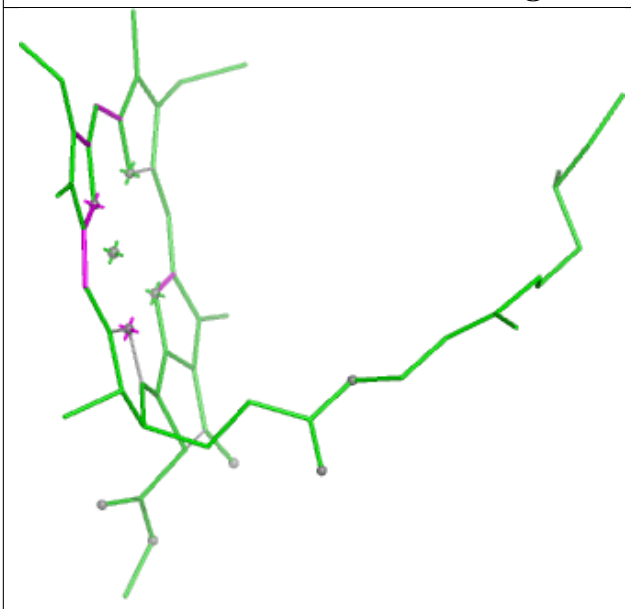
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	845	BCR	2	0
21	B	821	CLA	1	0
21	A	803	CLA	3	0
20	Z	307	CHL	3	0
21	B	813	CLA	2	0
26	6	619	LMG	1	0
21	3	610	CLA	2	0
21	B	840	CLA	2	0
21	2	610	CLA	1	0
20	2	606	CHL	1	0
22	X	615	LUT	8	0
21	X	604	CLA	1	0
21	A	825	CLA	1	0
26	F	306	LMG	1	0
21	A	837	CLA	2	0
25	5	618	LHG	2	0
31	Y	617	NEX	2	0
24	6	620	BCR	4	0
24	4	317	BCR	2	0
20	2	607	CHL	2	0
21	A	840	CLA	1	0
21	J	101	CLA	2	0
20	Z	302	CHL	4	0
21	A	812	CLA	1	0
21	A	828	CLA	3	0
21	B	837	CLA	1	0
21	Y	602	CLA	6	0
21	A	842	CLA	3	0
23	O	208	XAT	4	0
22	Y	616	LUT	8	0
26	B	850	LMG	3	0
21	A	807	CLA	1	0
22	2	615	LUT	4	0
21	1	613	CLA	1	0
20	Y	601	CHL	2	0
21	6	612	CLA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLA B 828



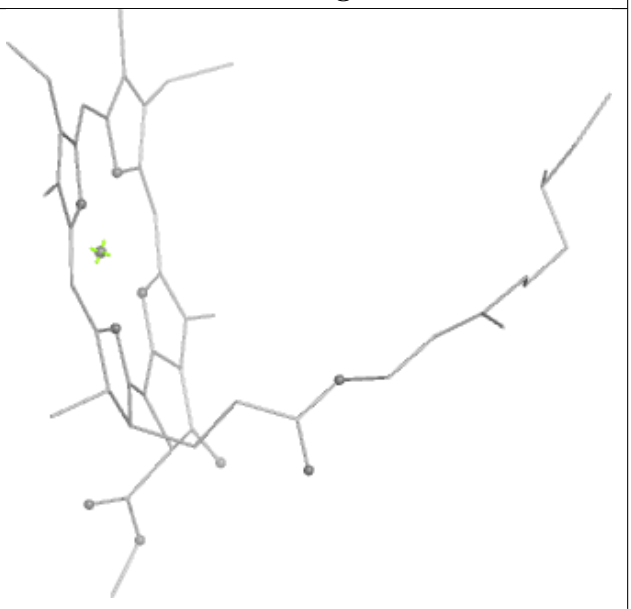
Bond lengths



Bond angles

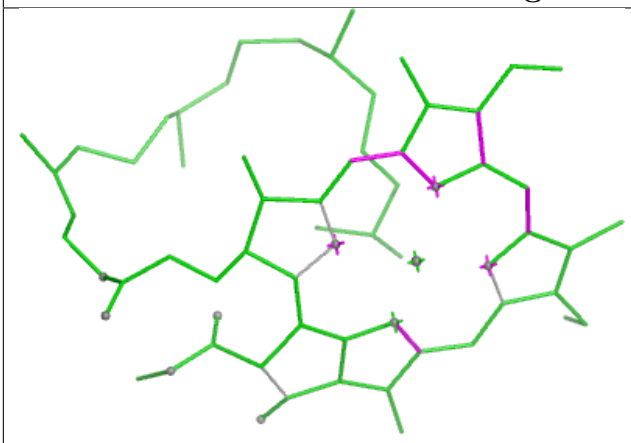


Torsions

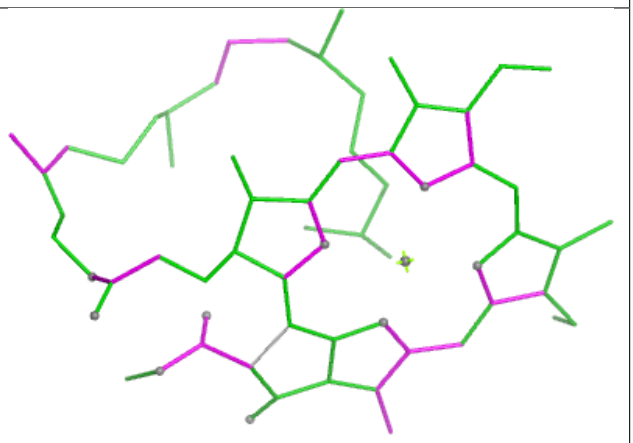


Rings

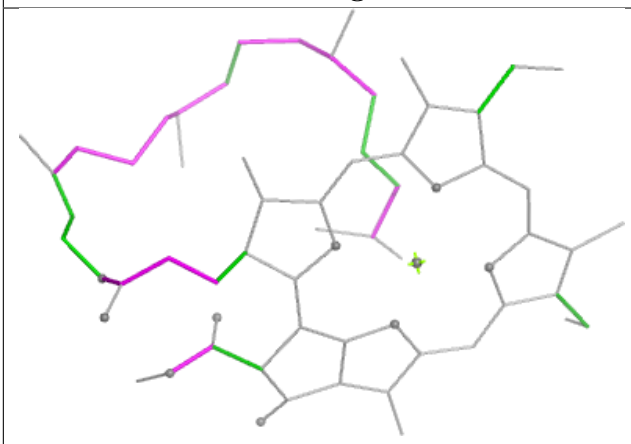
Ligand CLA B 805



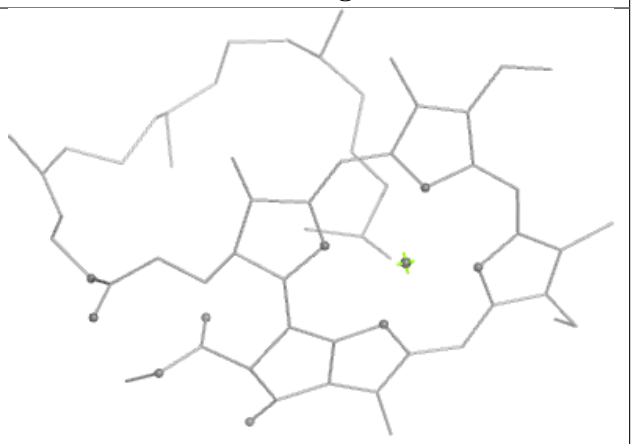
Bond lengths



Bond angles

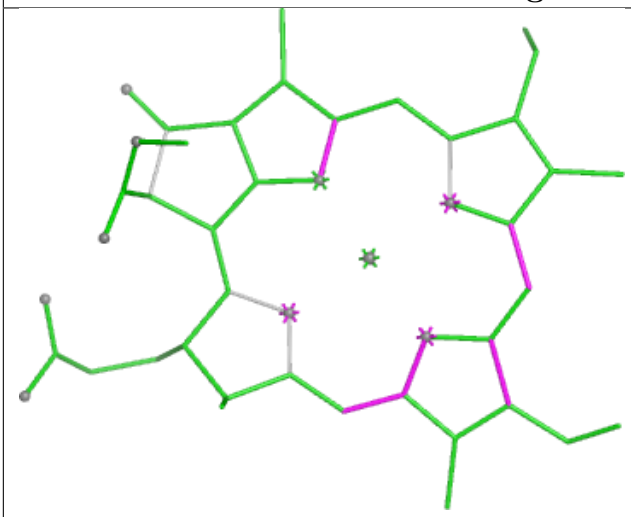


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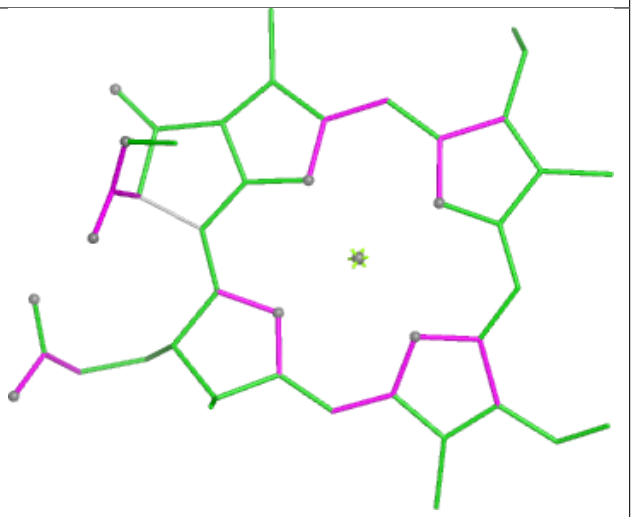


Rings

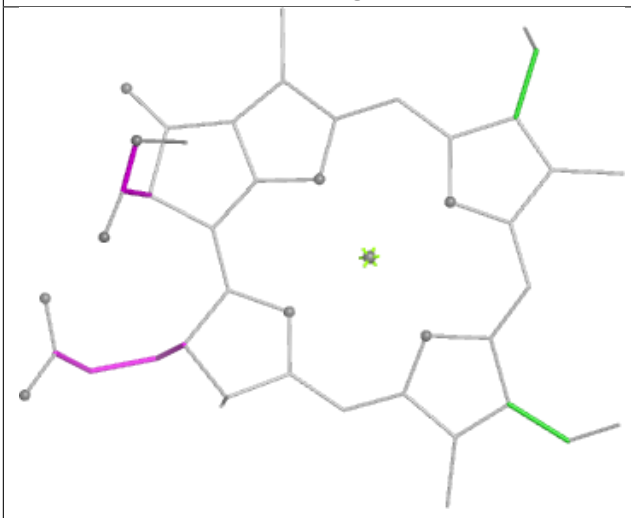
Ligand CLA Z 304



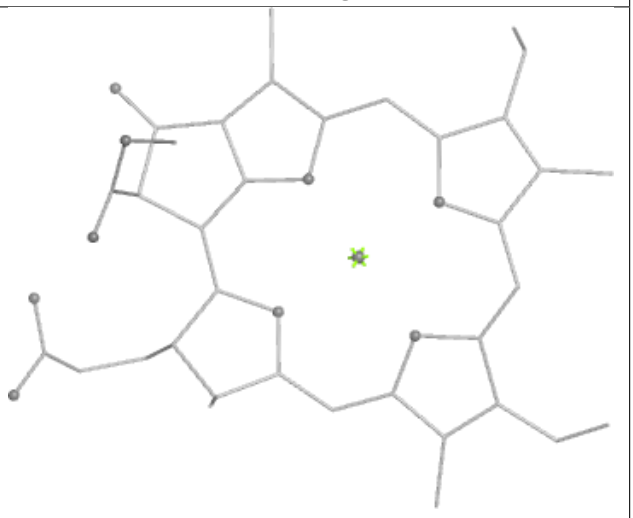
Bond lengths



Bond angles



Torsions



Rings

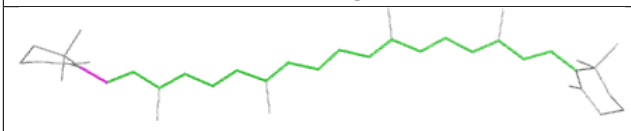
Ligand BCR O 205



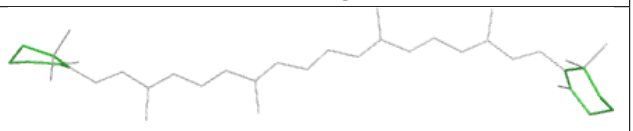
Bond lengths



Bond angles

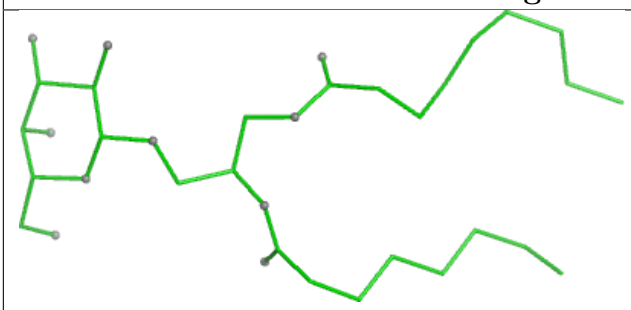


Torsions

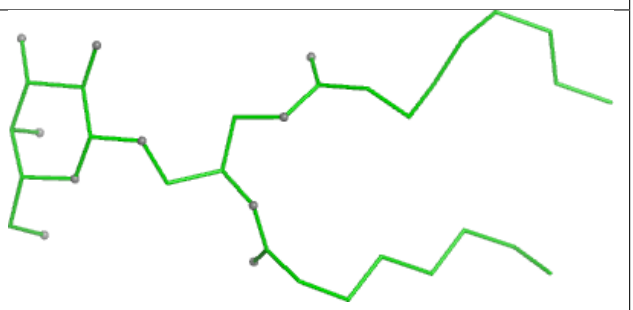


Rings

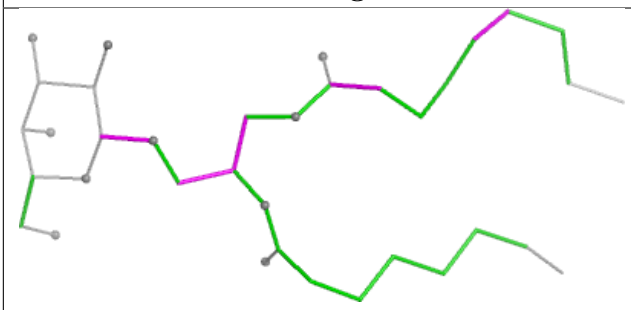
Ligand LMG 4 318



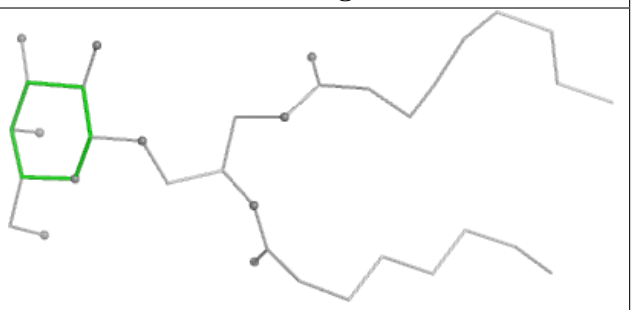
Bond lengths



Bond angles

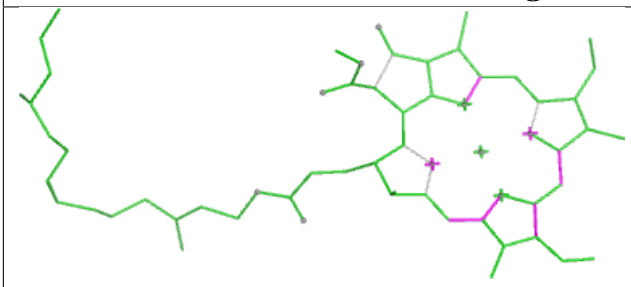


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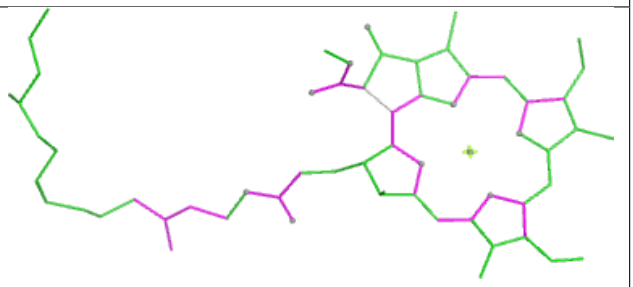


Rings

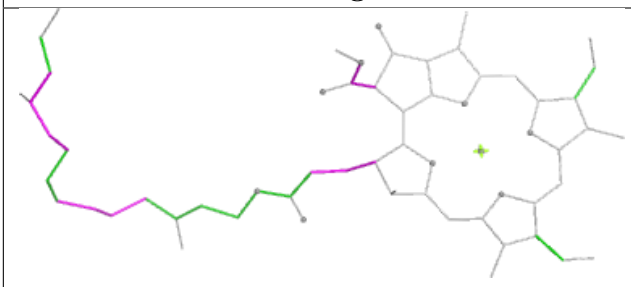
Ligand CLA B 825



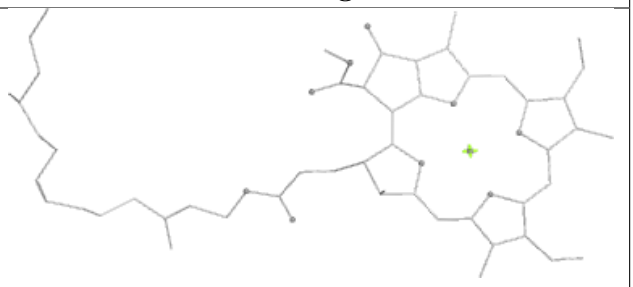
Bond lengths



Bond angles



Torsions

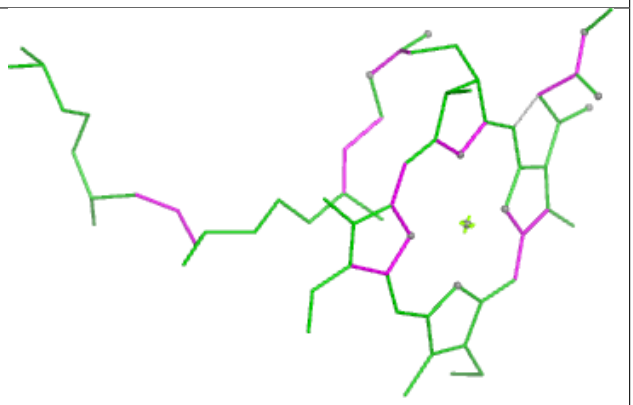


Rings

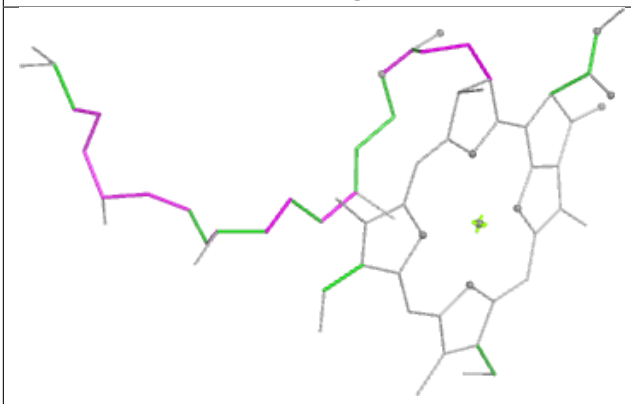
Ligand CLA L 301



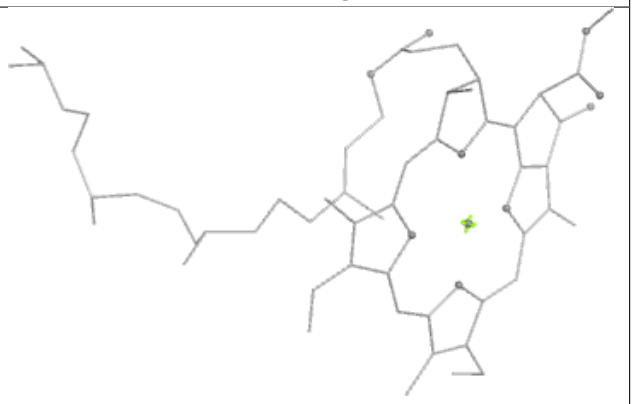
Bond lengths



Bond angles

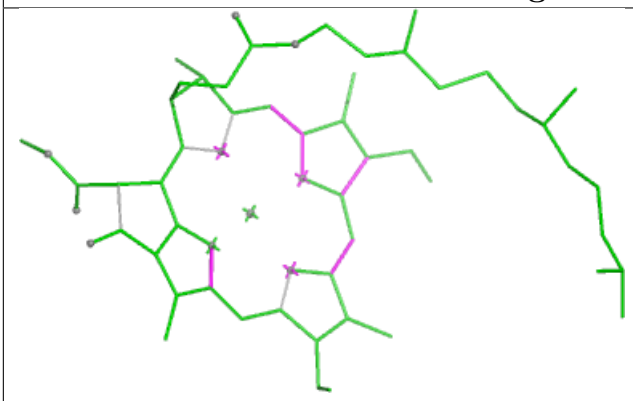


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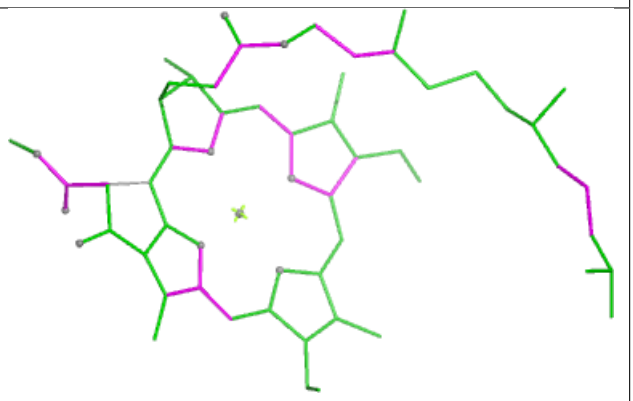


Rings

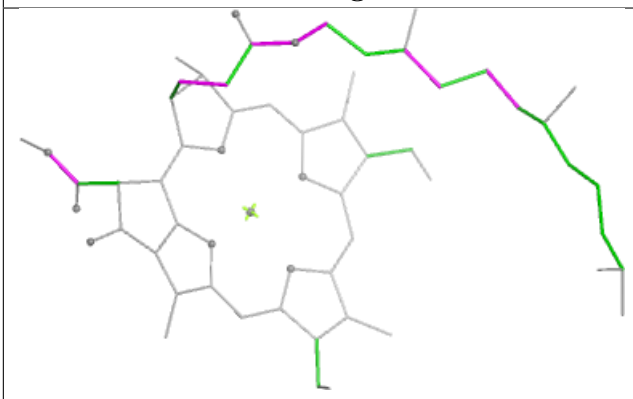
Ligand CLA 6 602



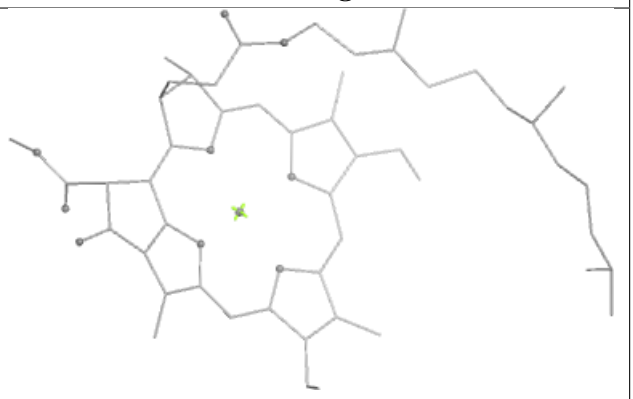
Bond lengths



Bond angles

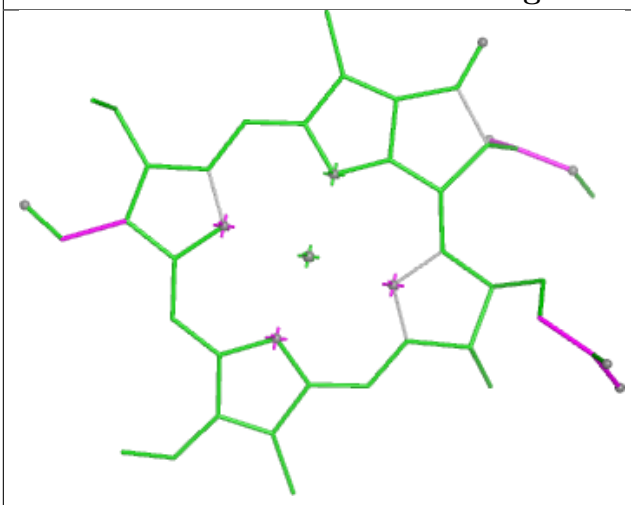


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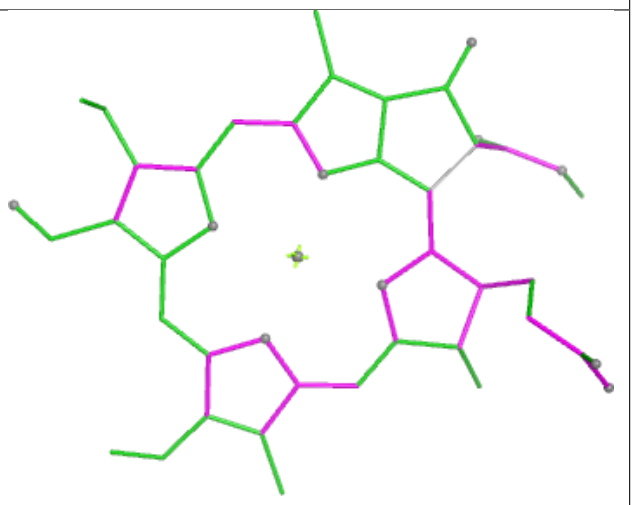


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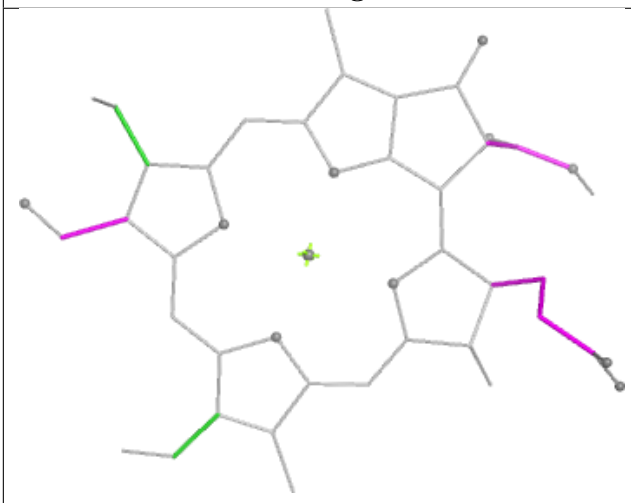
Ligand CHL X 601



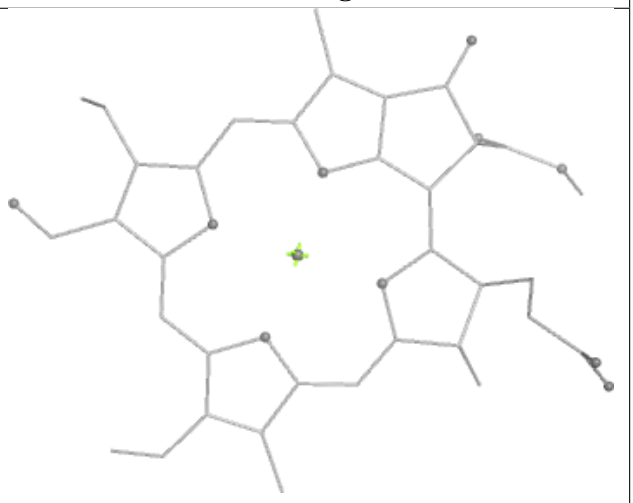
Bond lengths



Bond angles

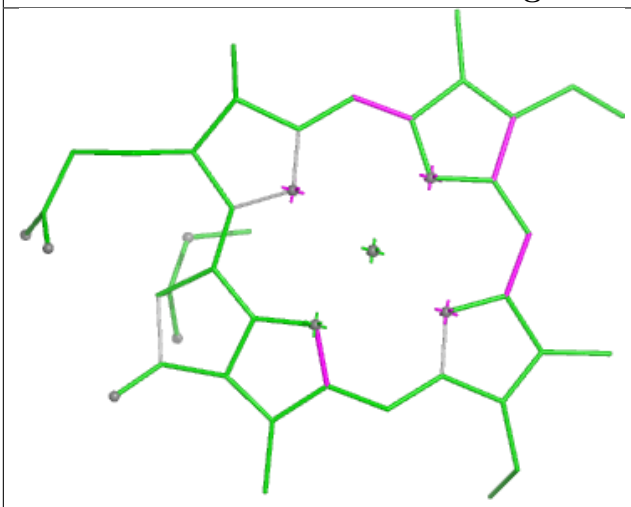


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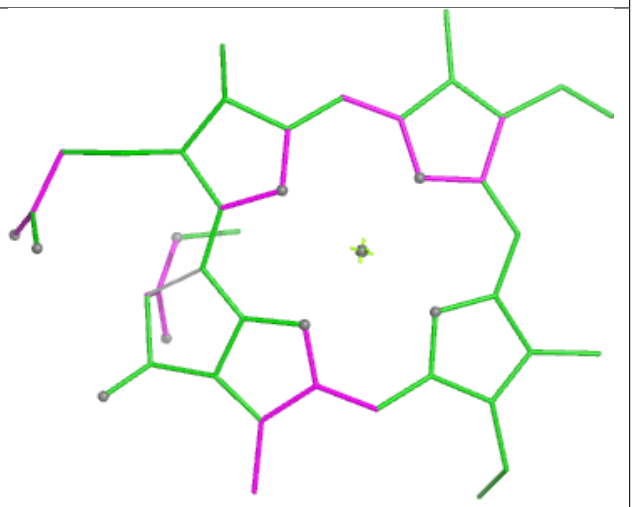


Rings

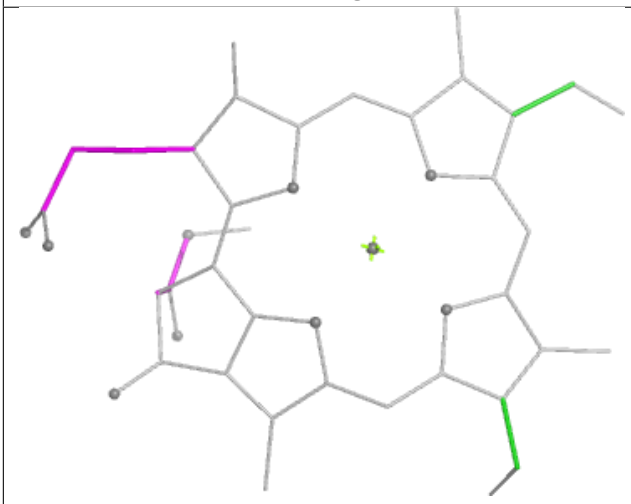
Ligand CLA X 611



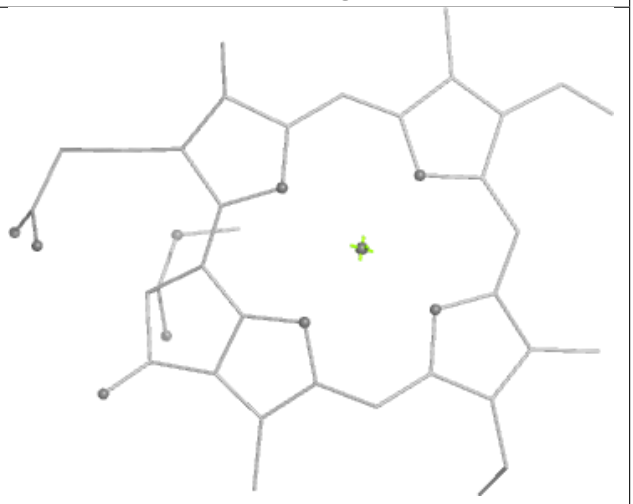
Bond lengths



Bond angles

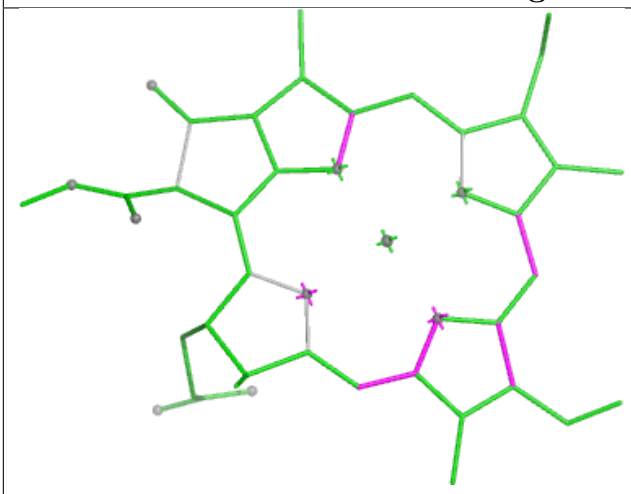


Torsions

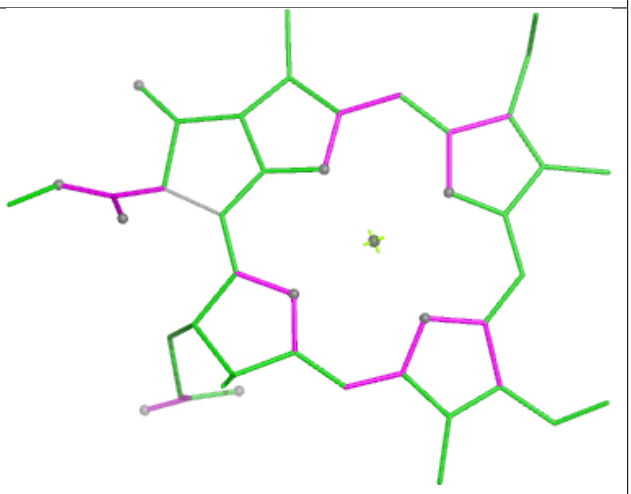


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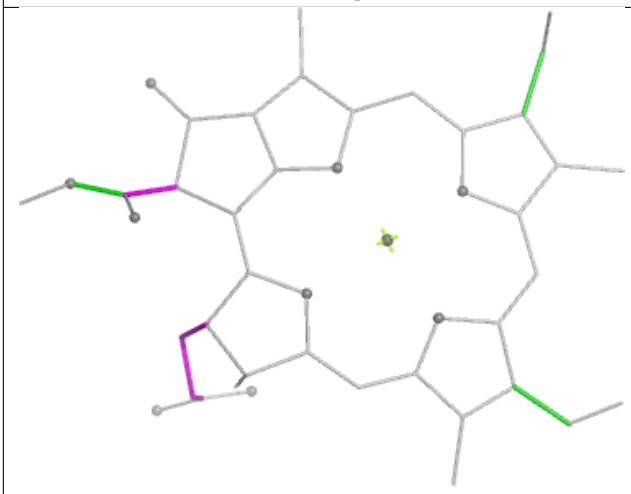
Ligand CLA 2 608



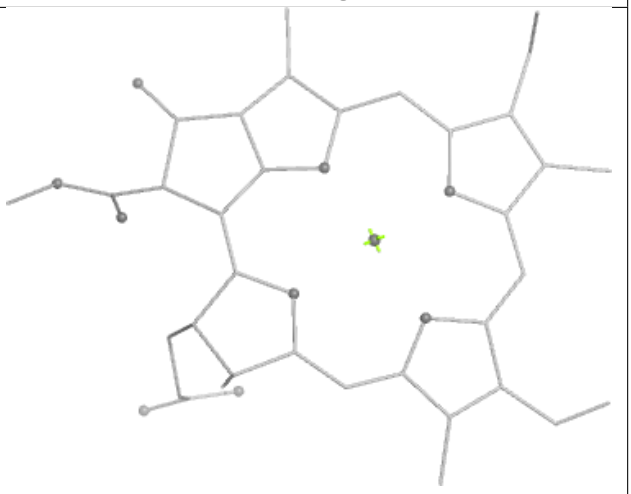
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Bond angles

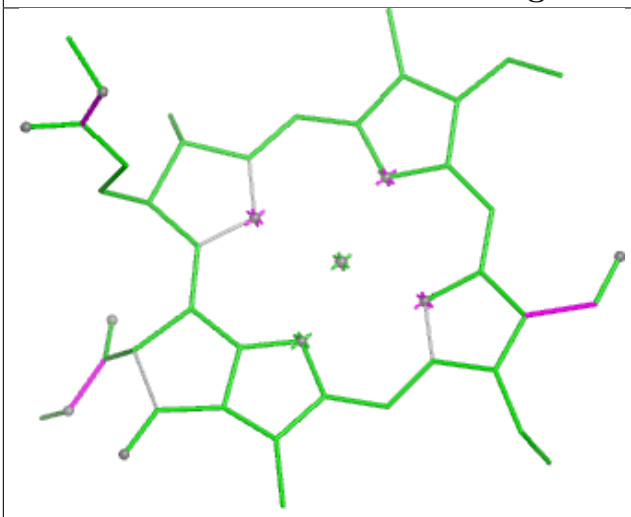


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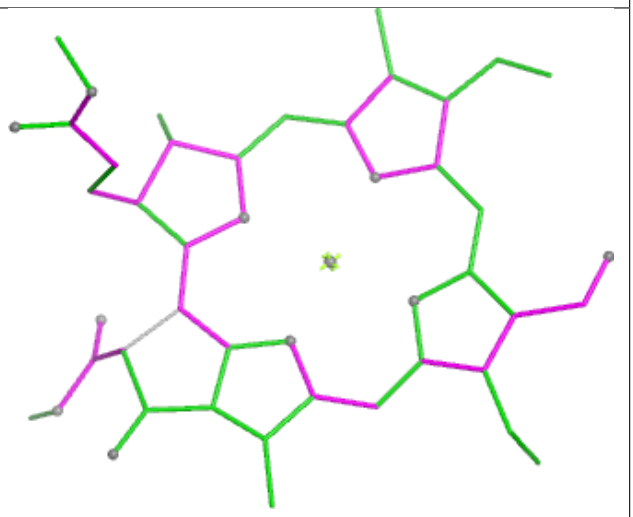


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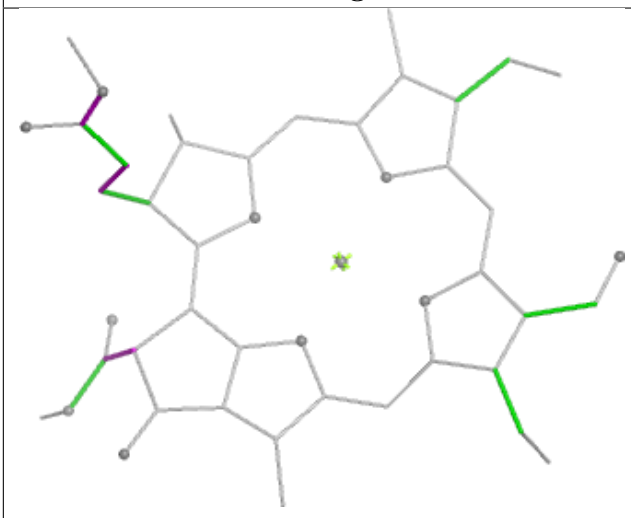
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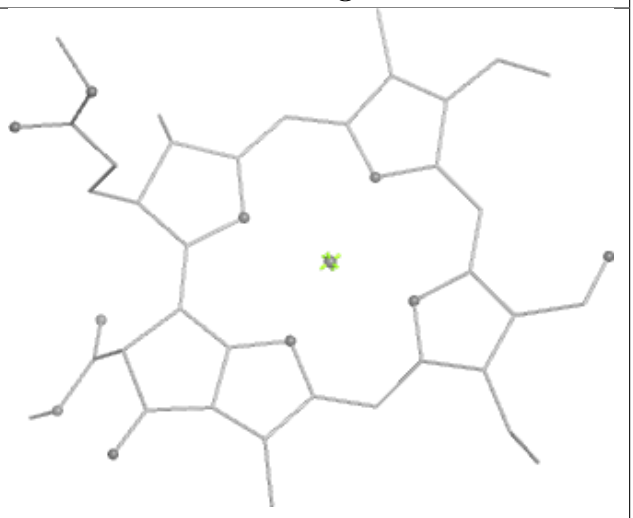
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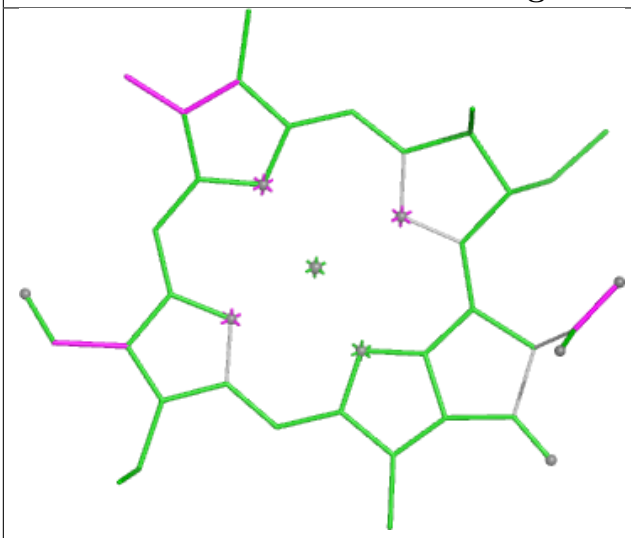


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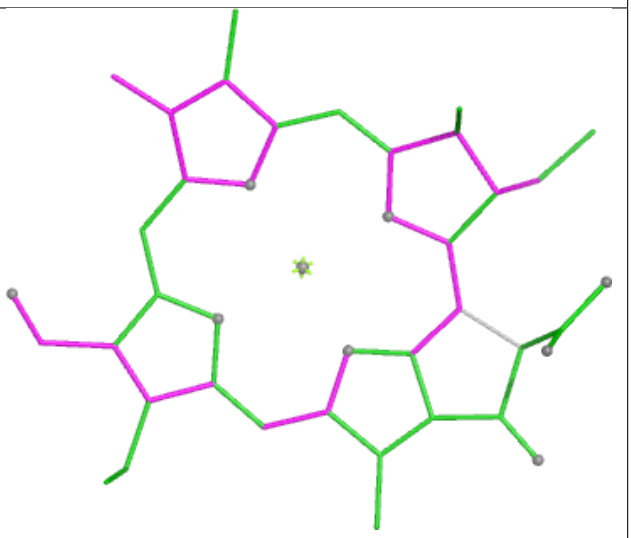


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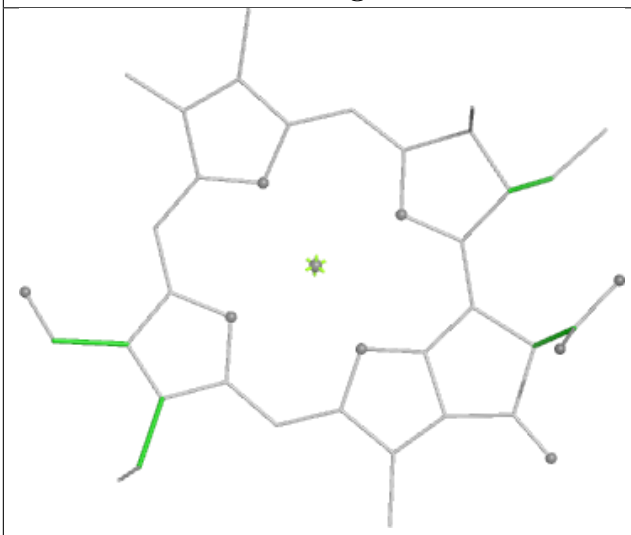
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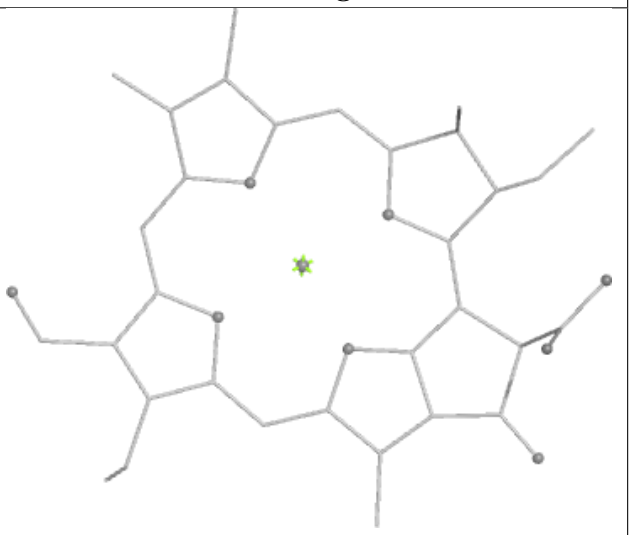
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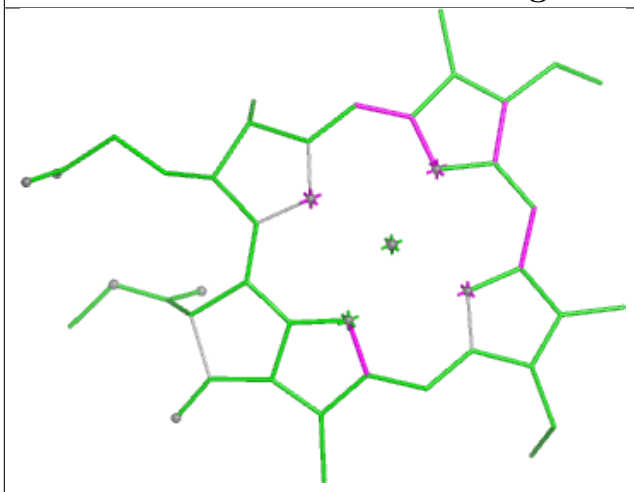


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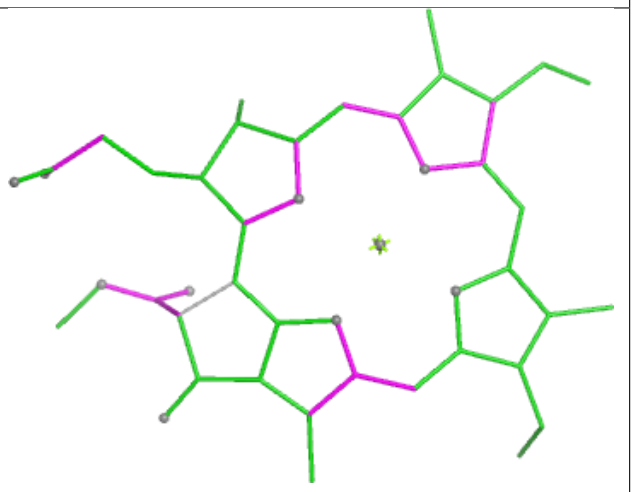


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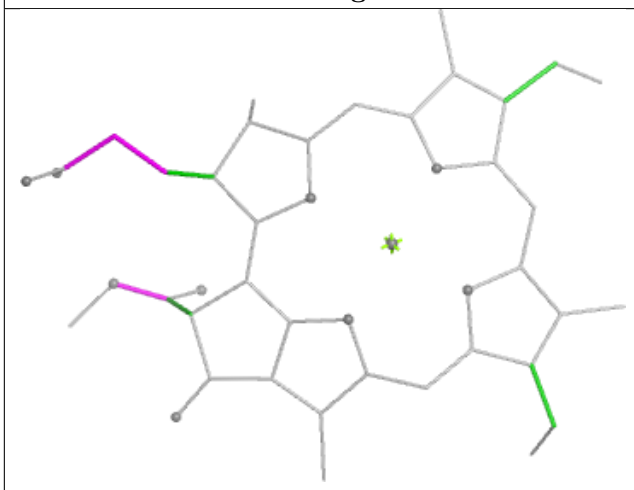
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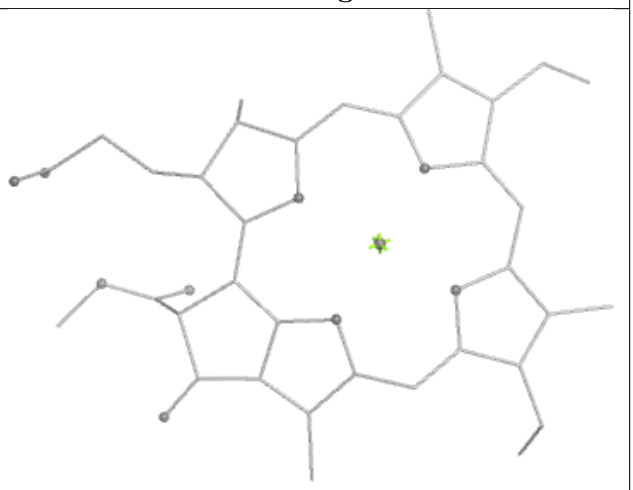
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Bond angles



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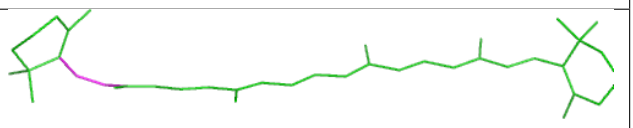


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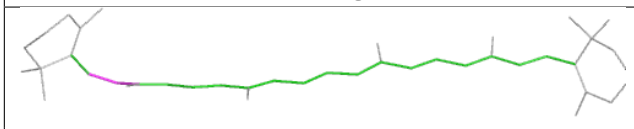
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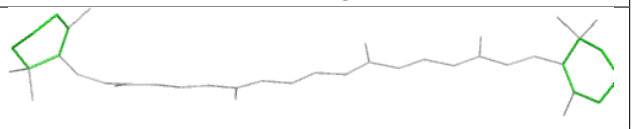
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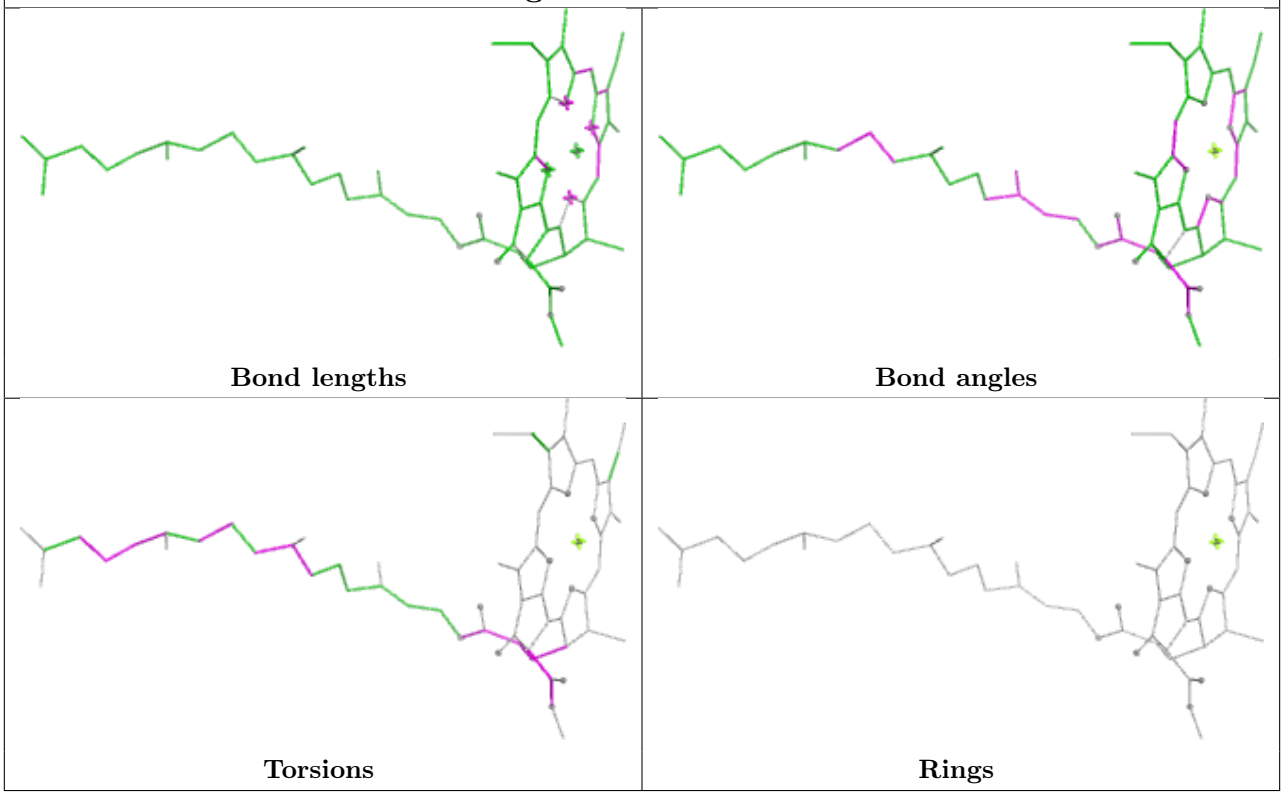


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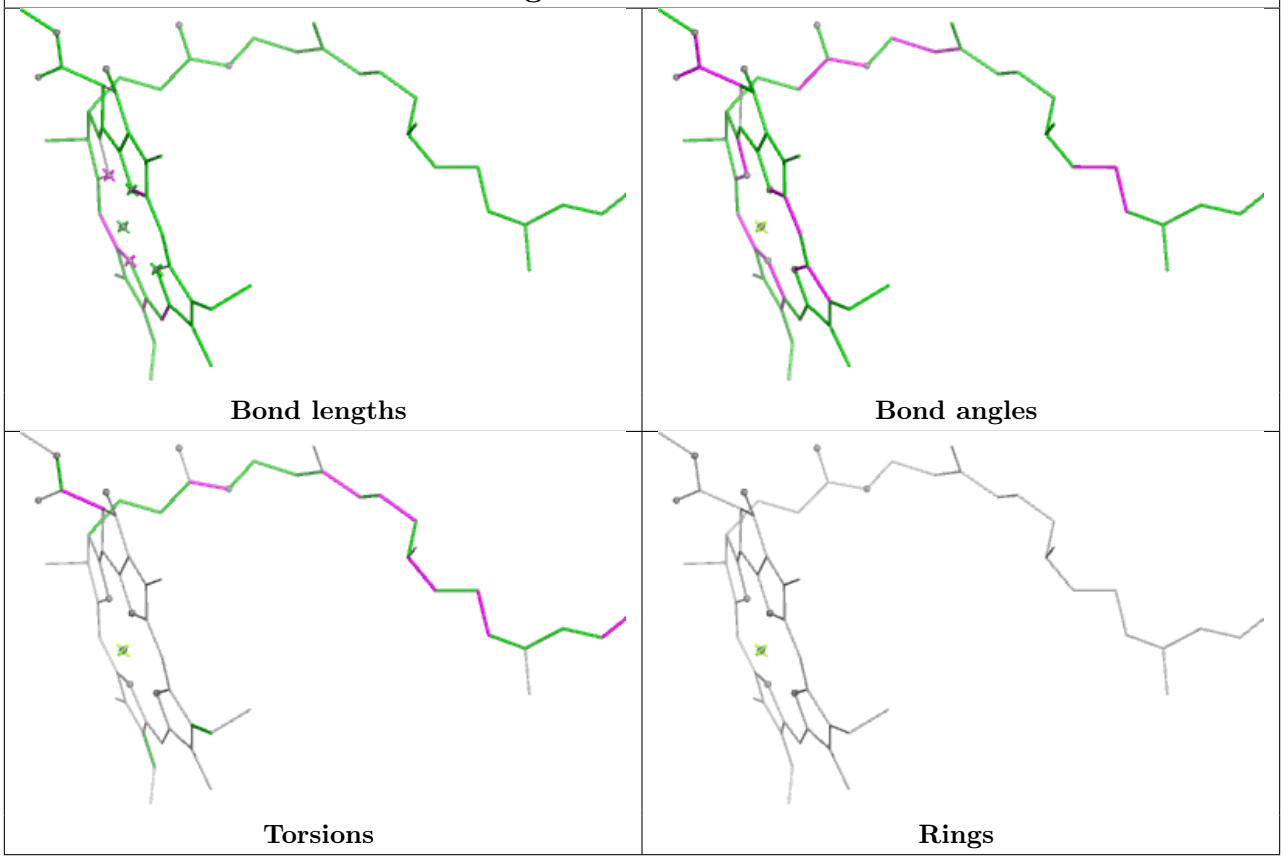


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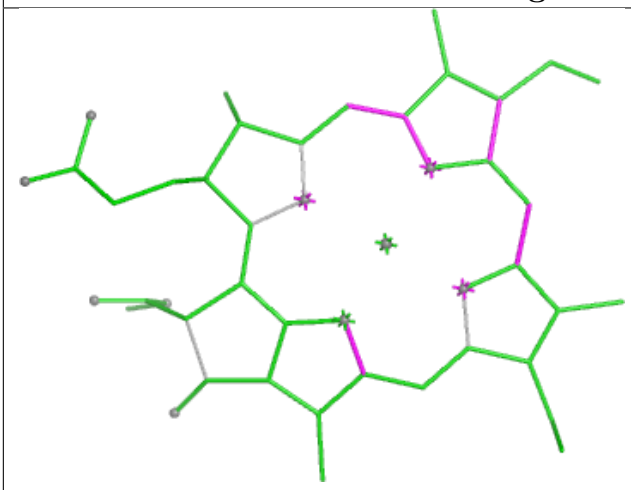
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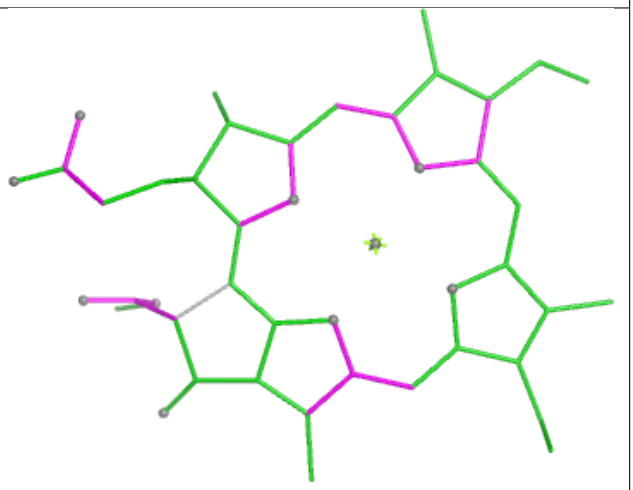
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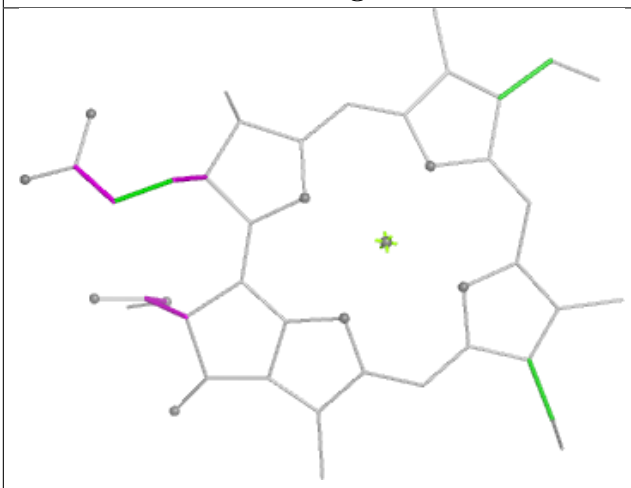
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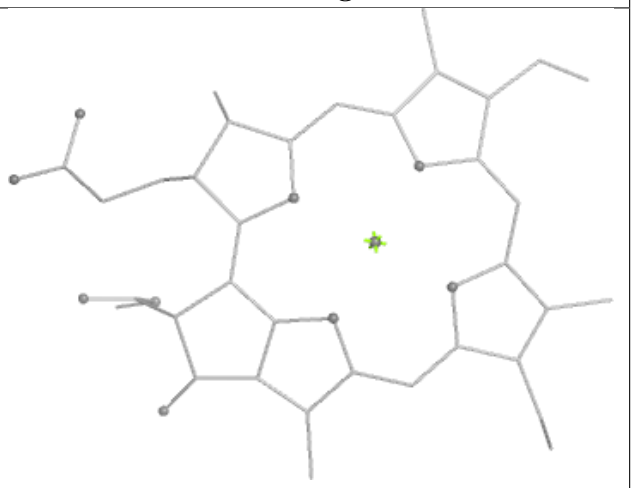
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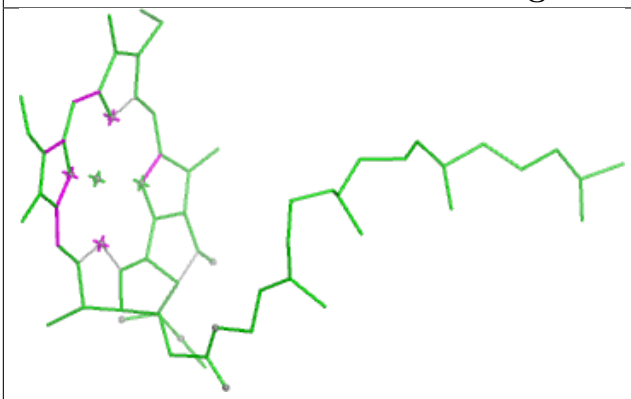


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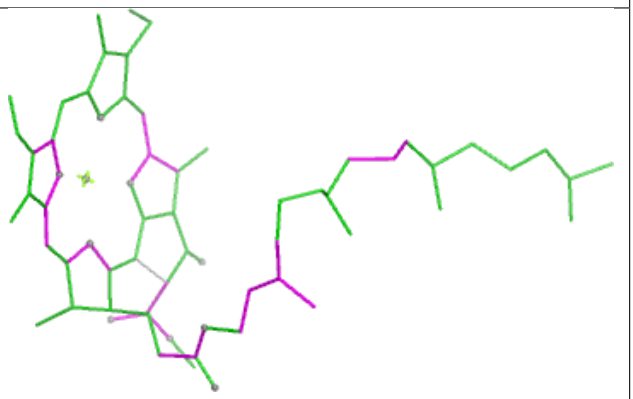


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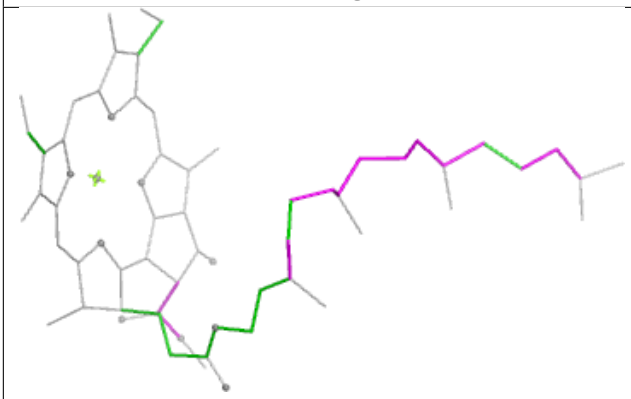
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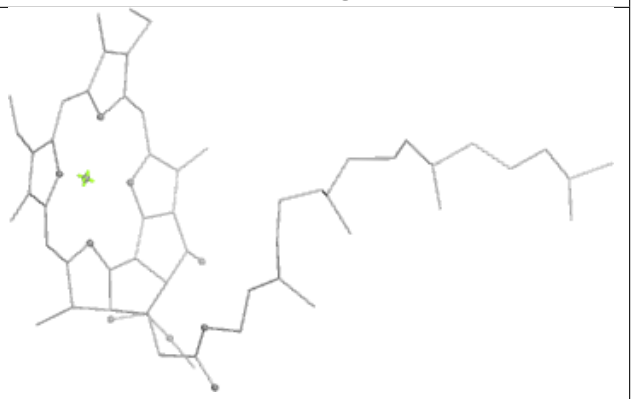
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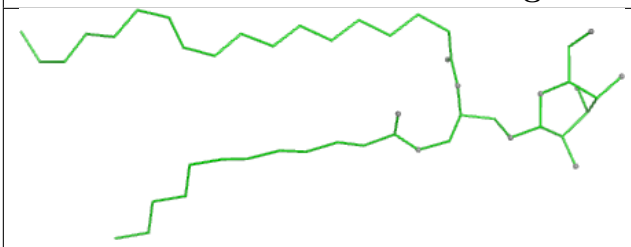


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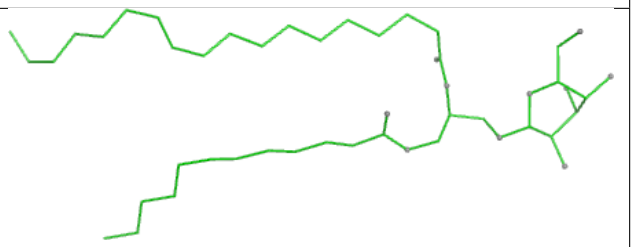


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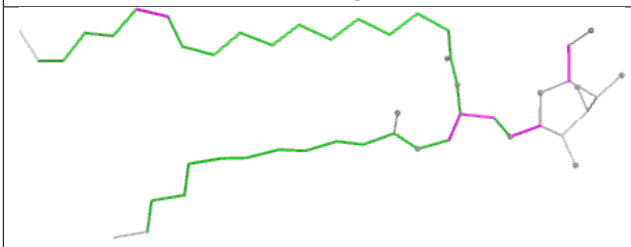
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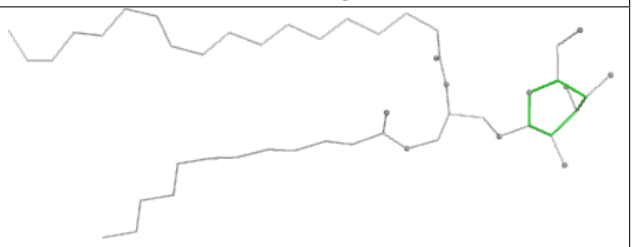
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Bond angles

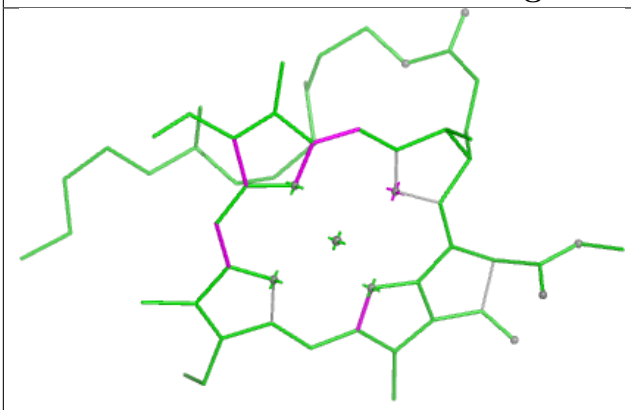


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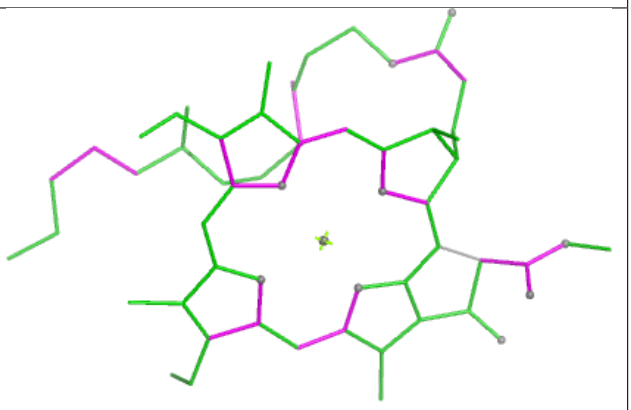


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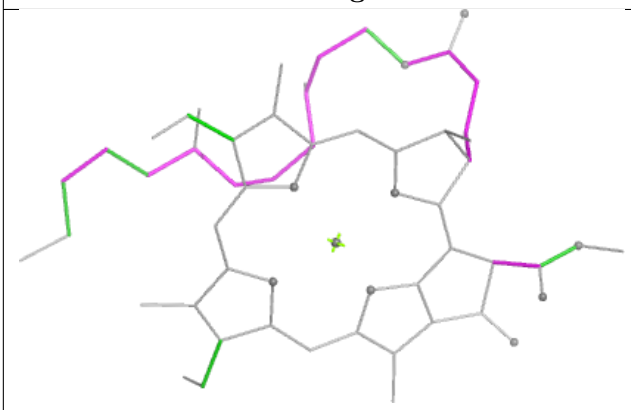
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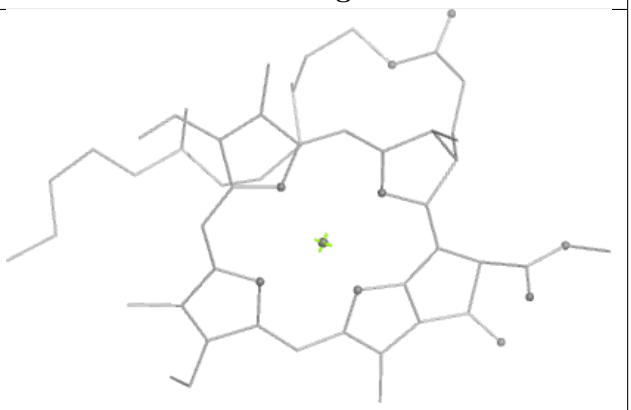
Bond lengths



Bond angles

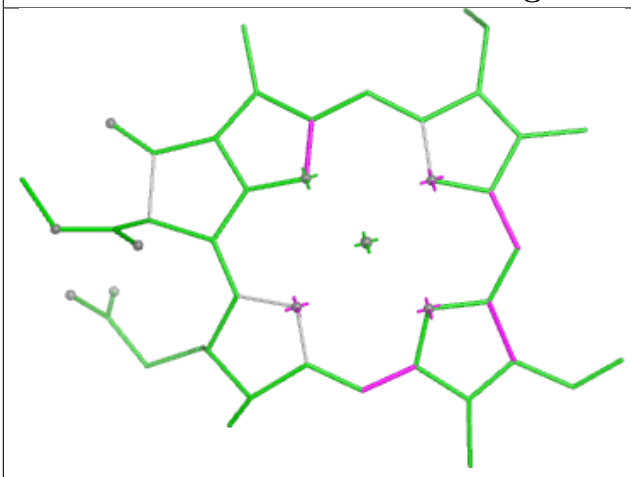


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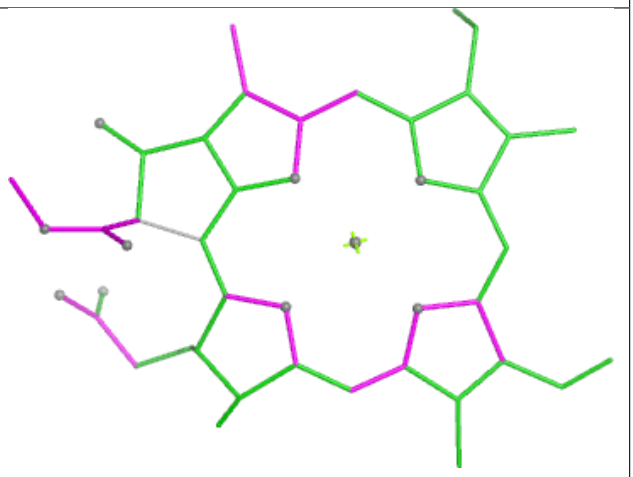


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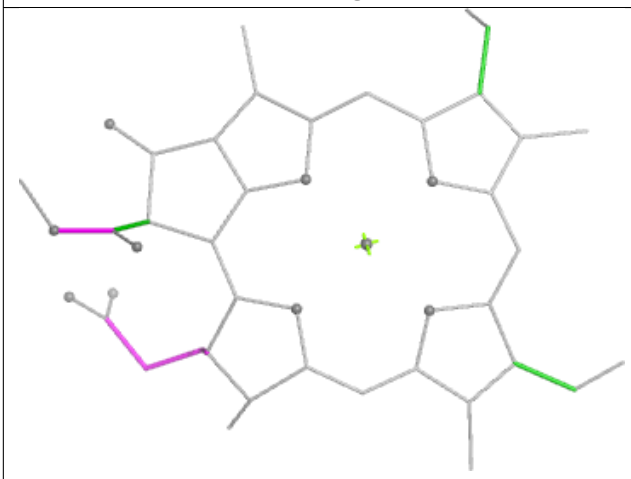
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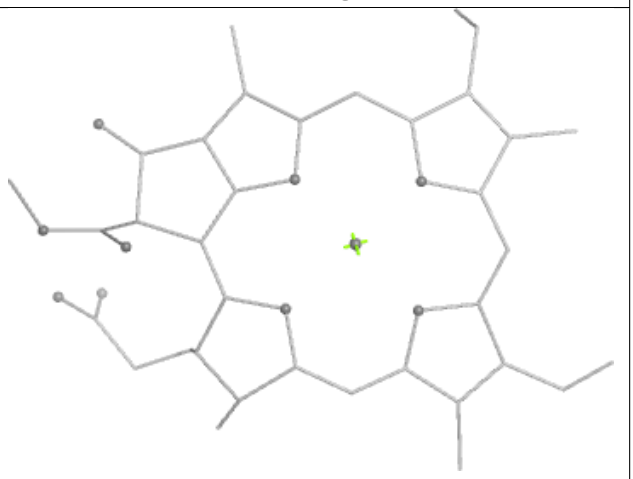
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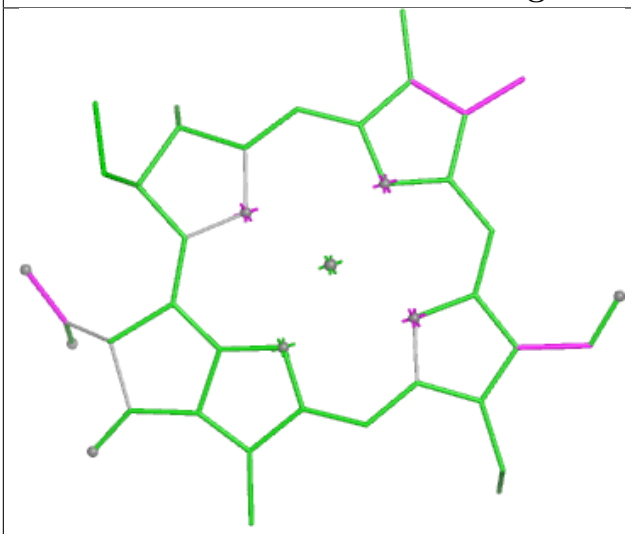


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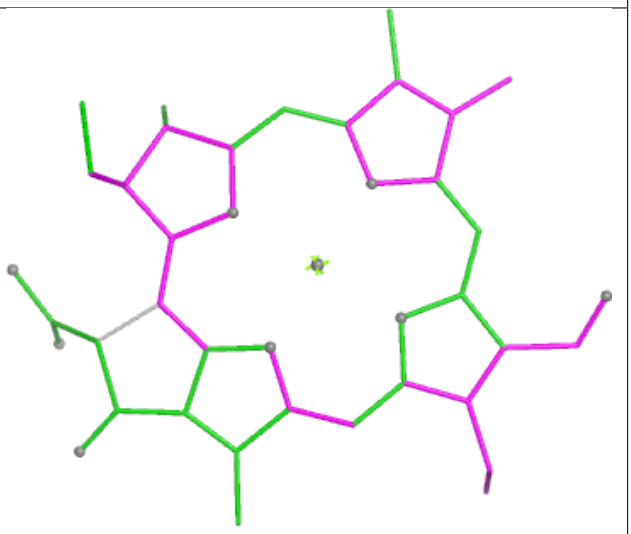


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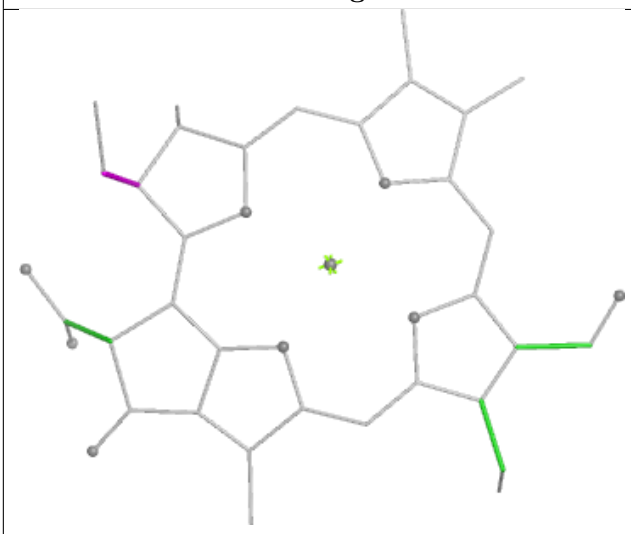
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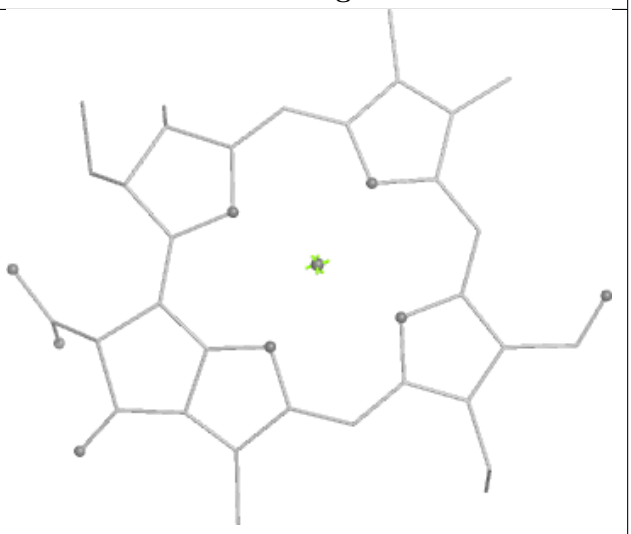
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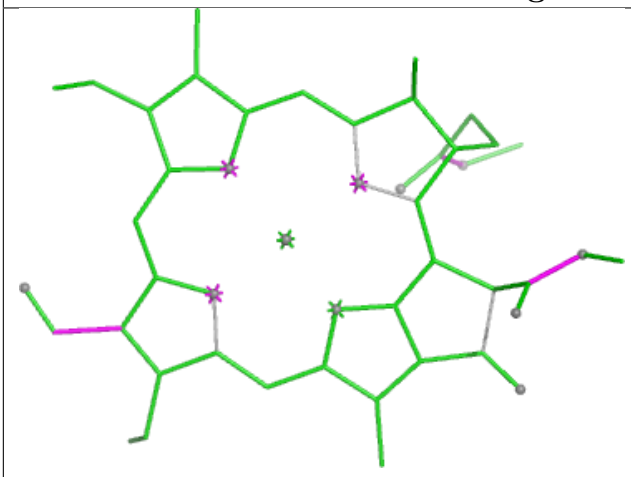


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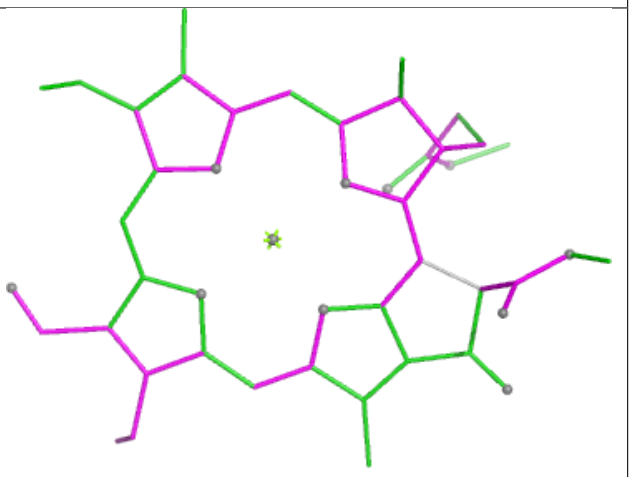


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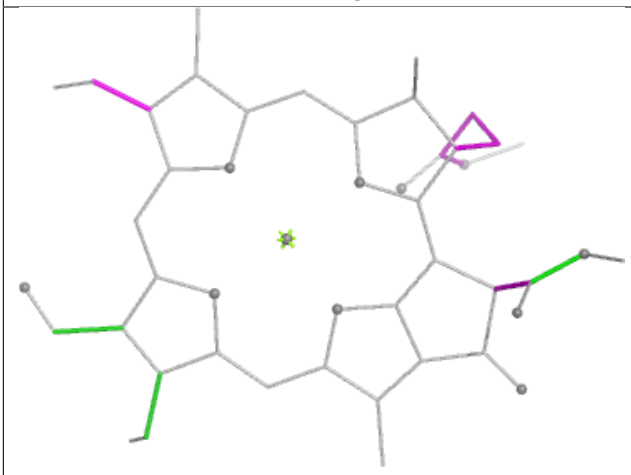
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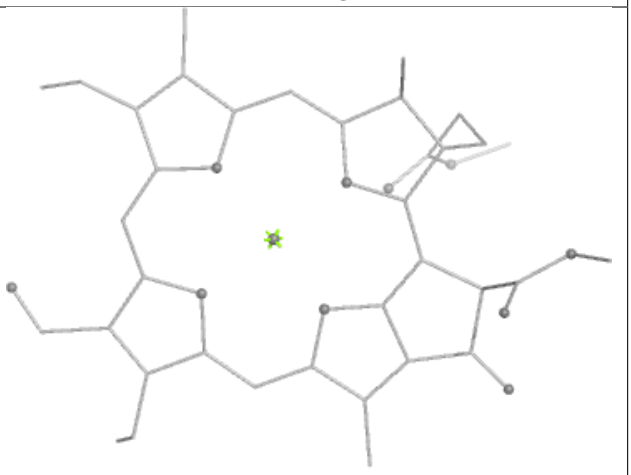
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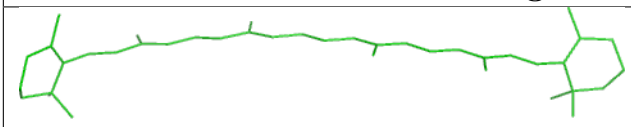


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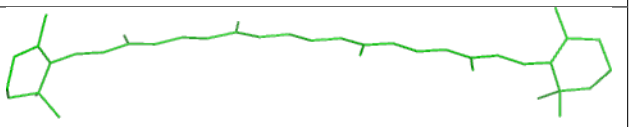


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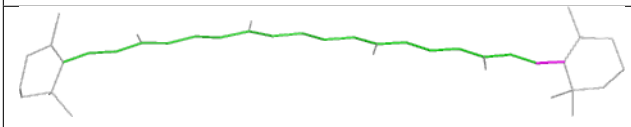
Ligand BCR 5 617



Bond lengths



Bond angles

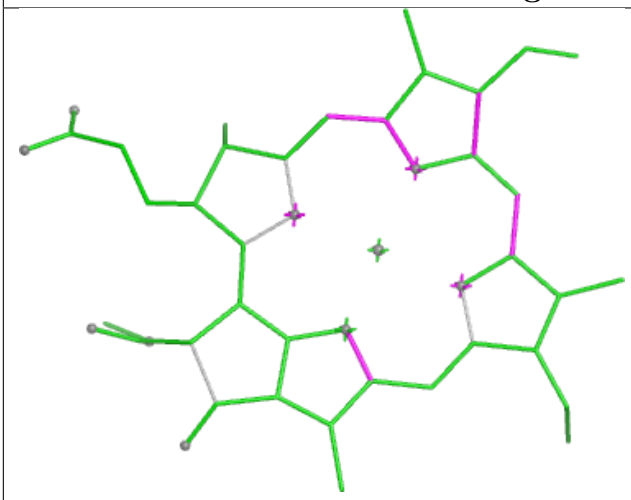


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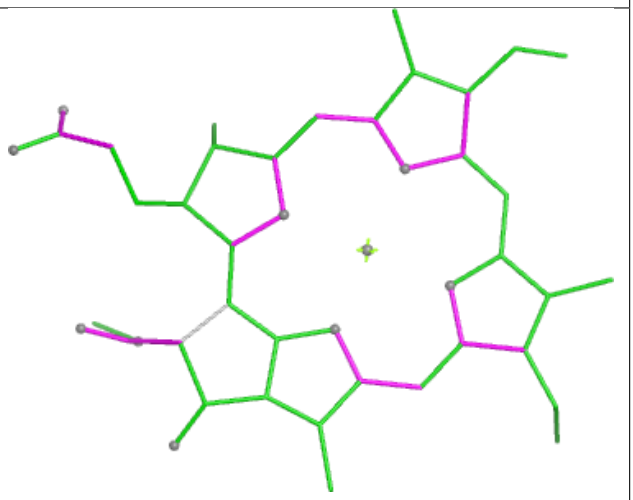


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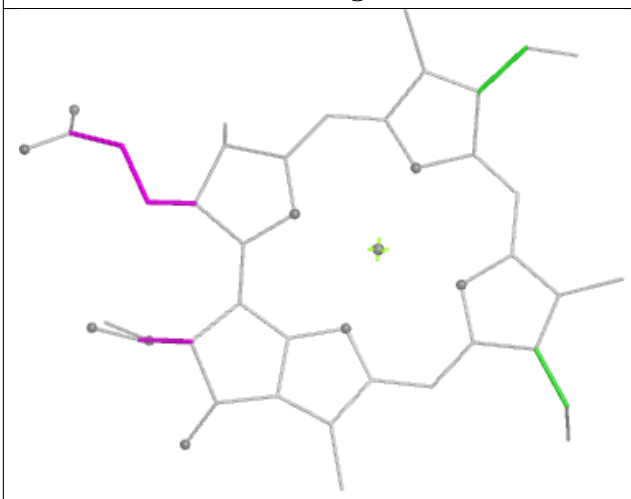
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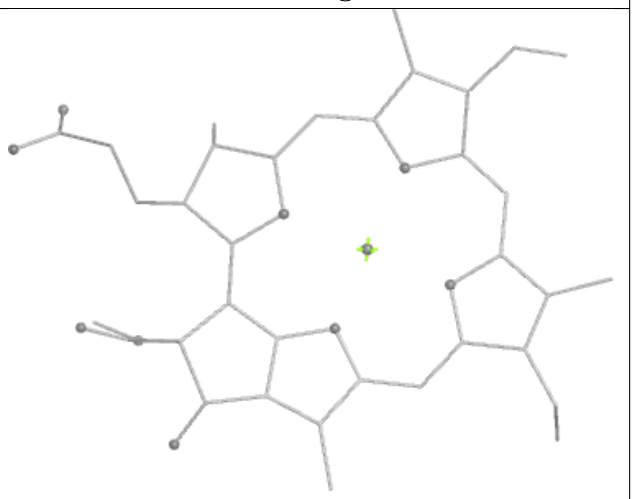
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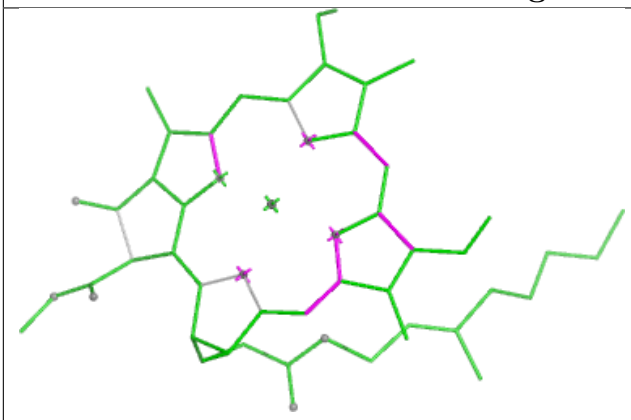


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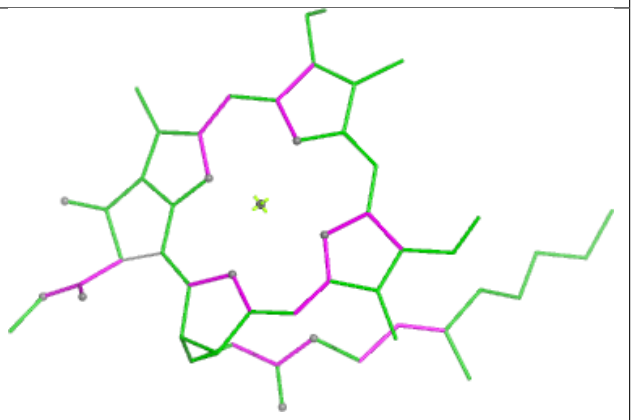


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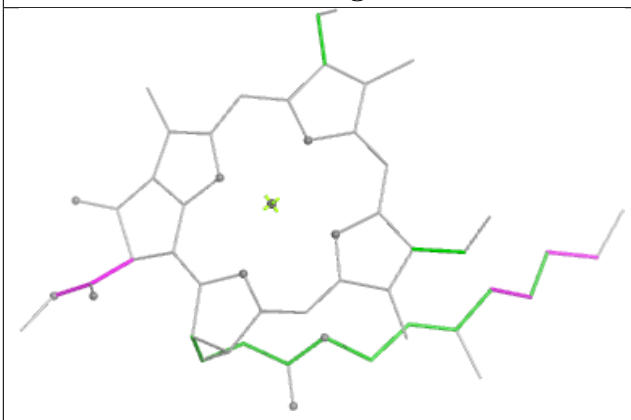
Ligand CLA 6 609



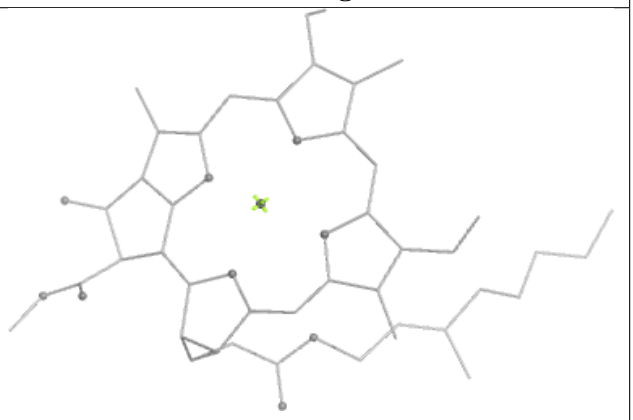
Bond lengths



Bond angles

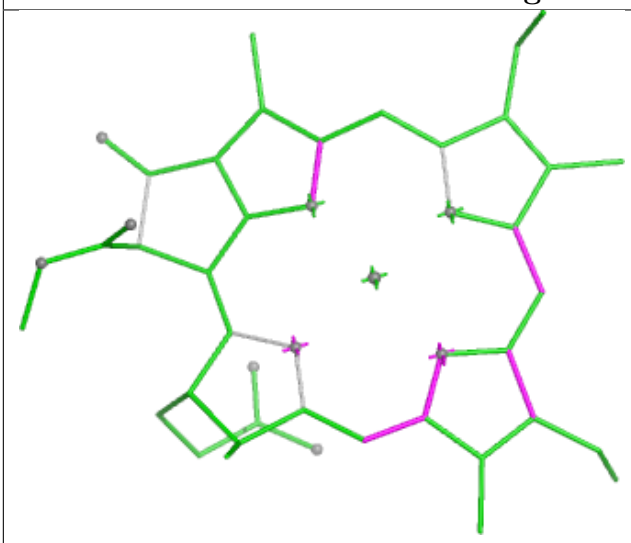


Torsions

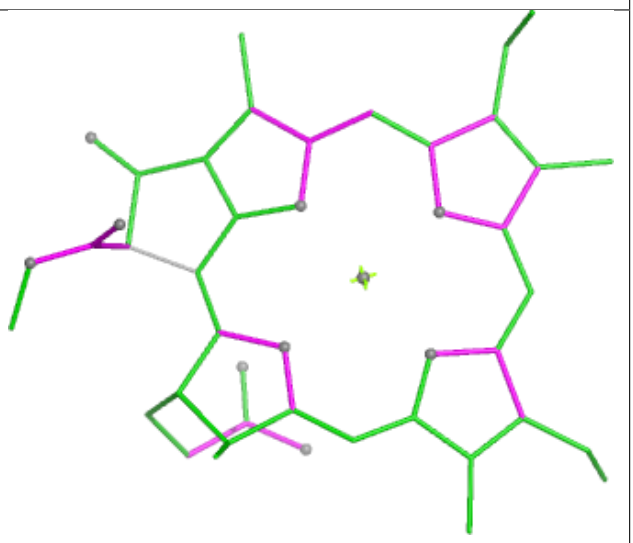


Rings

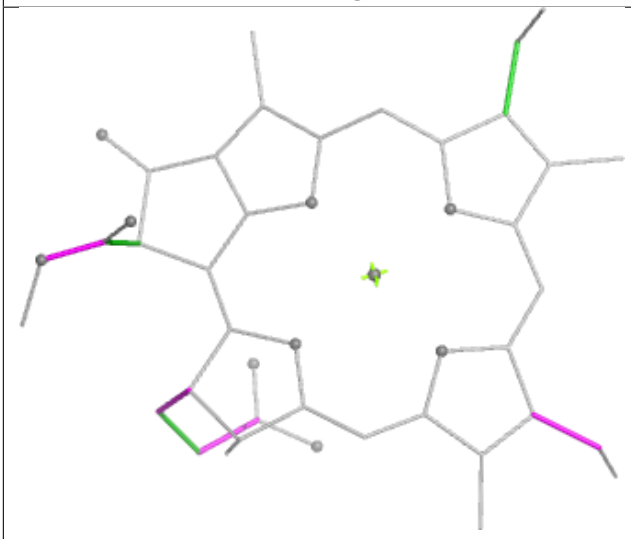
Ligand CLA X 609



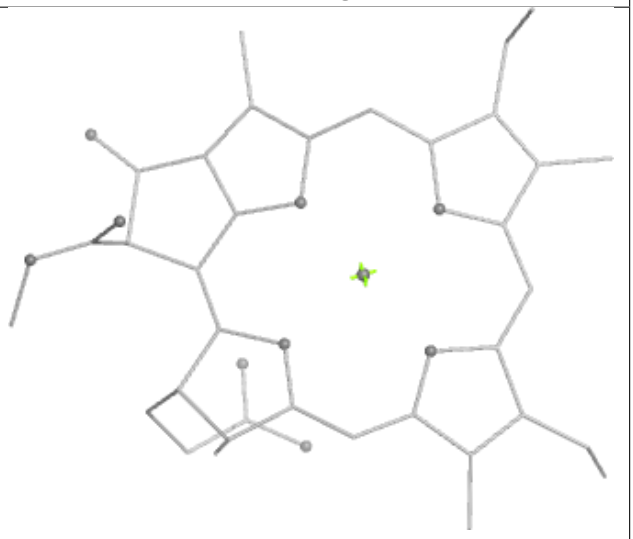
Bond lengths



Bond angles

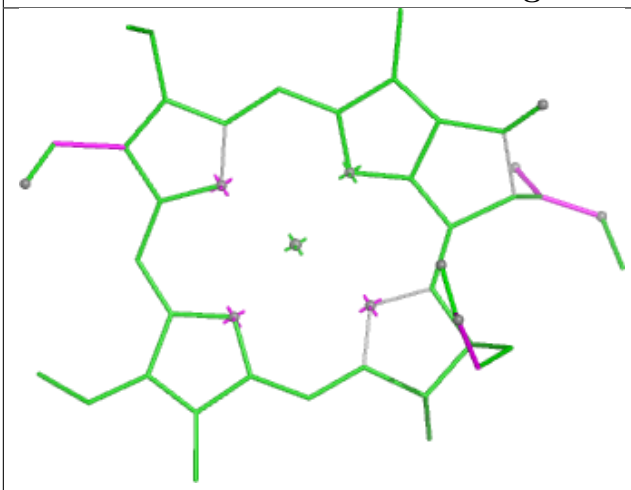


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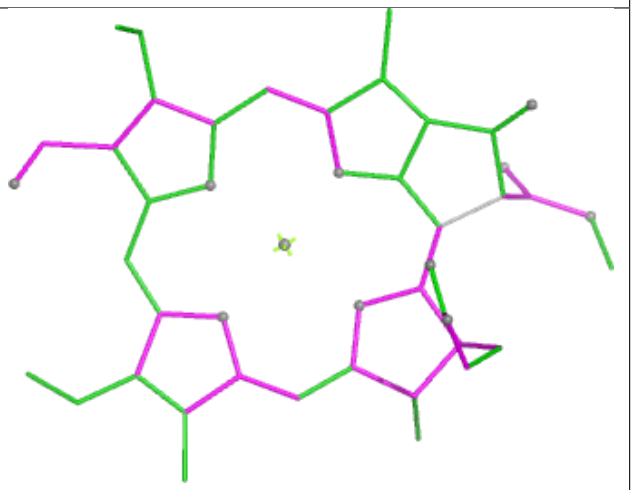


Rings

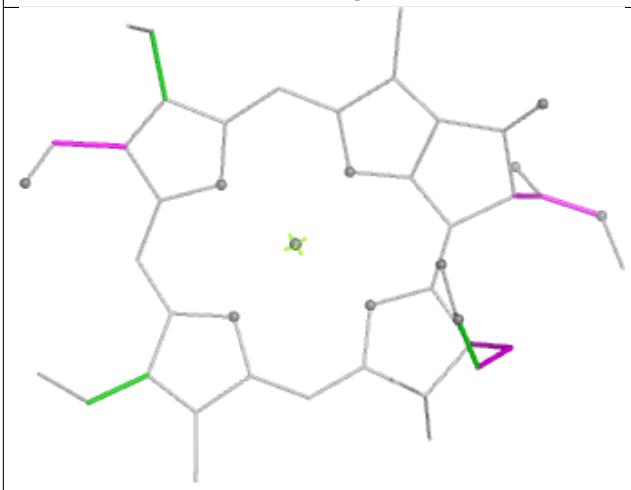
Ligand CHL Y 608



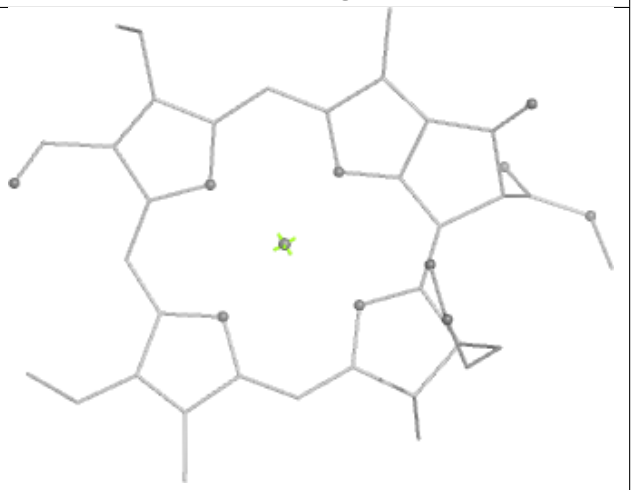
Bond lengths



Bond angles

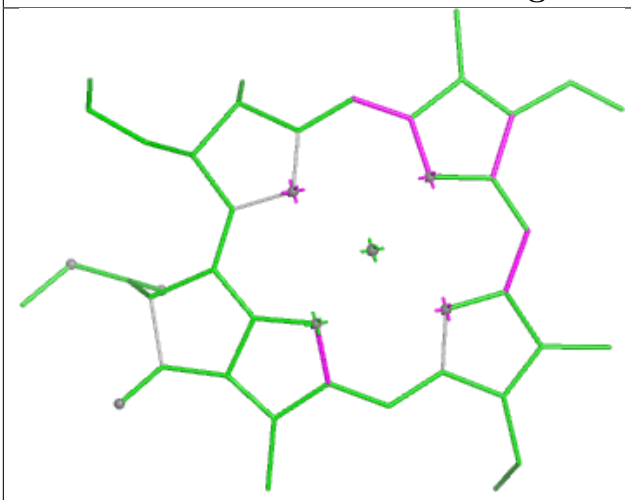


Torsions

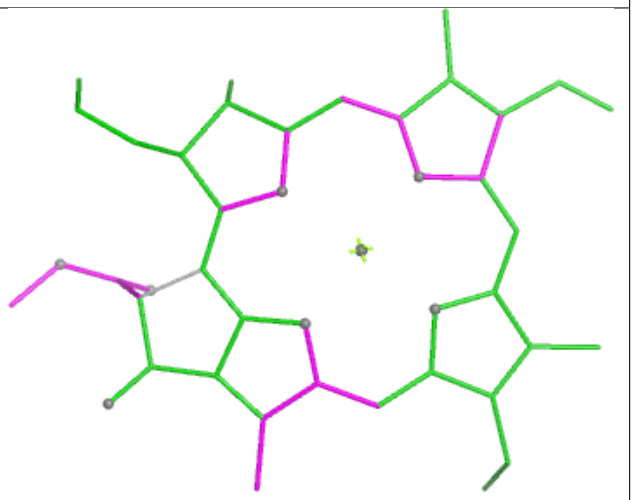


Rings

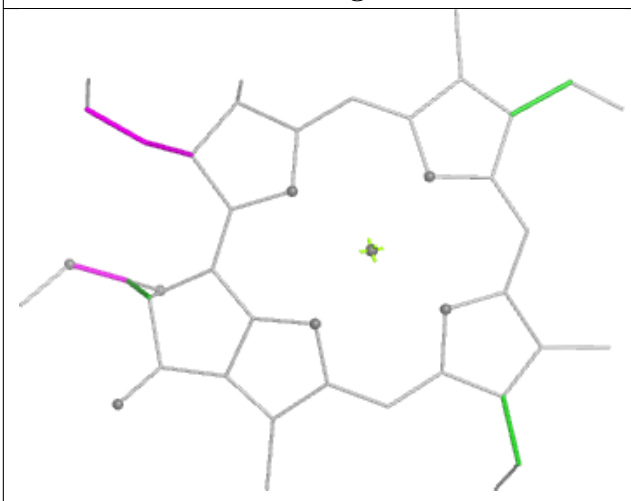
Ligand CLA 3 611



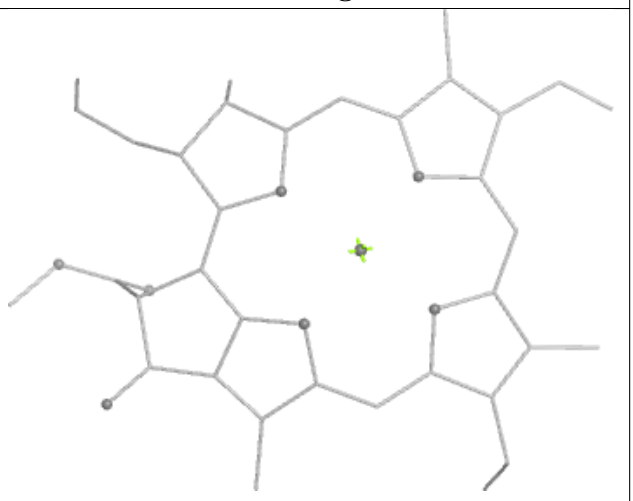
Bond lengths



Bond angles

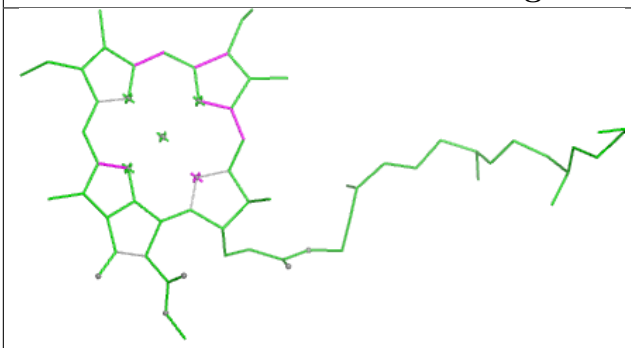


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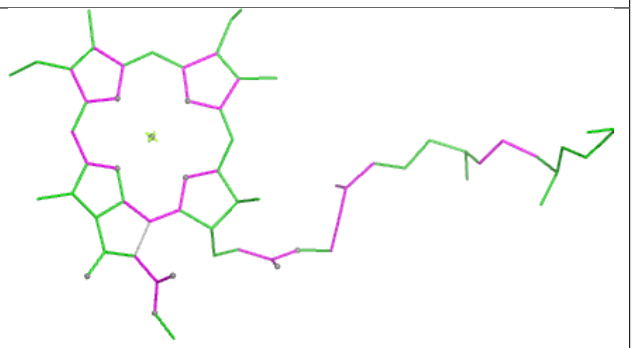


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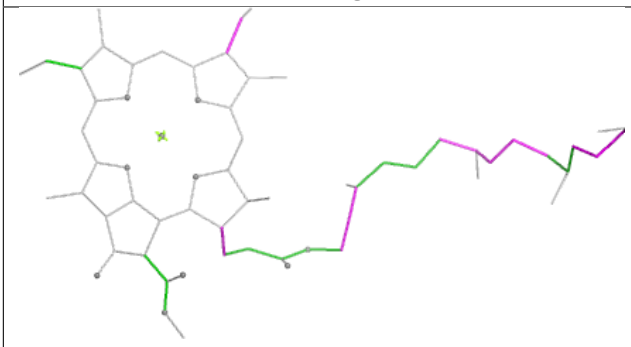
Ligand CLA B 802



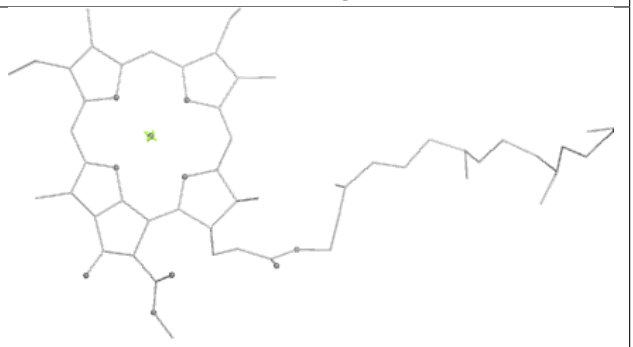
Bond lengths



Bond angles

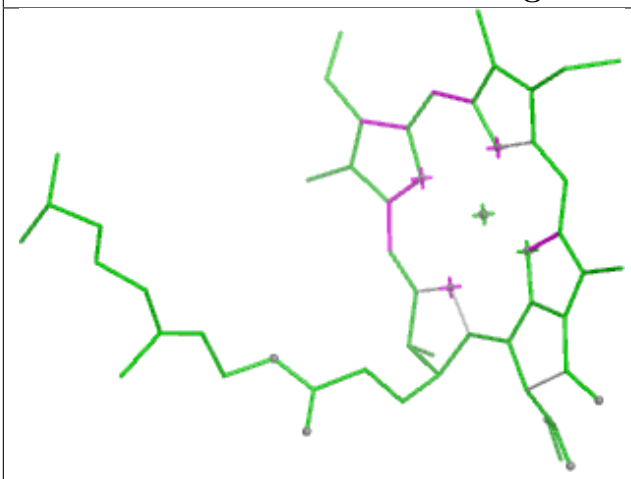


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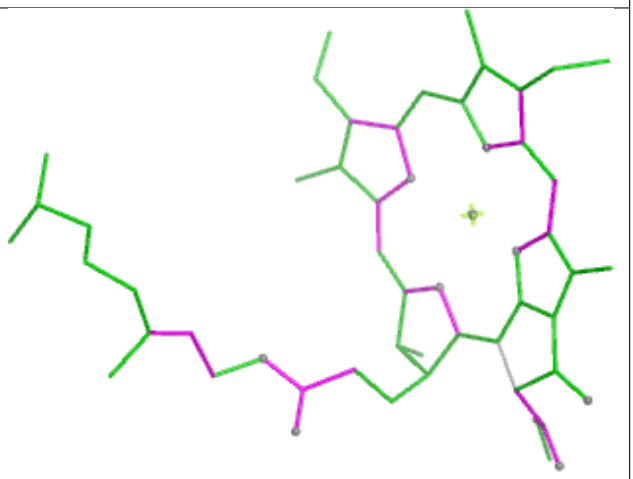


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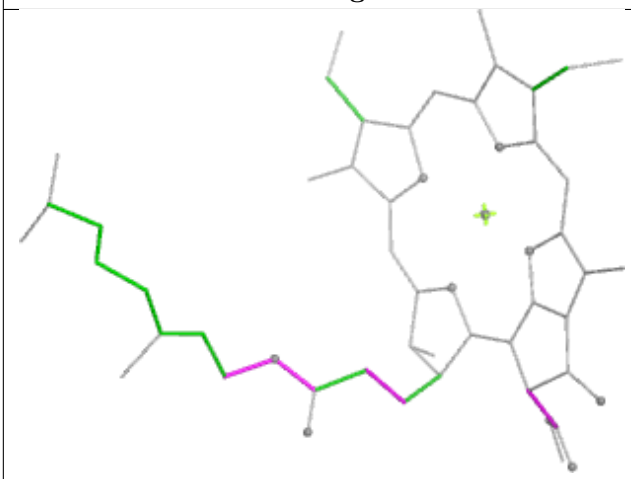
Ligand CLA A 809



Bond lengths



Bond angles

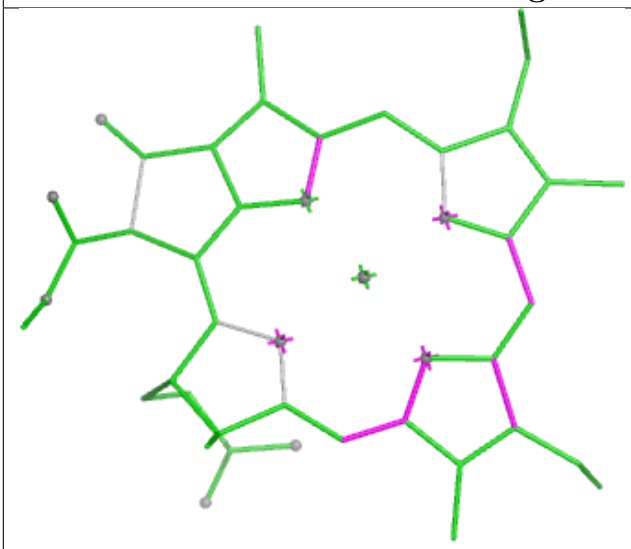


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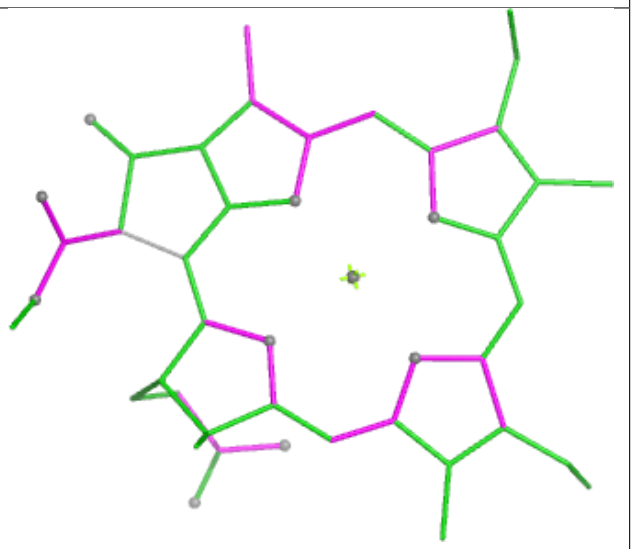


Rings

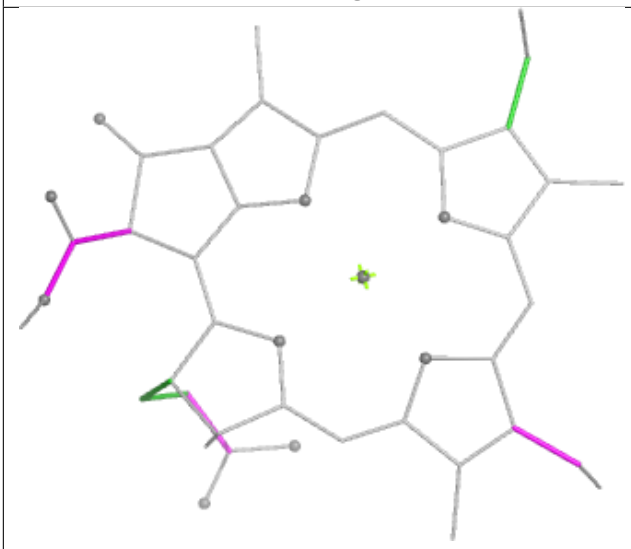
Ligand CLA 5 609



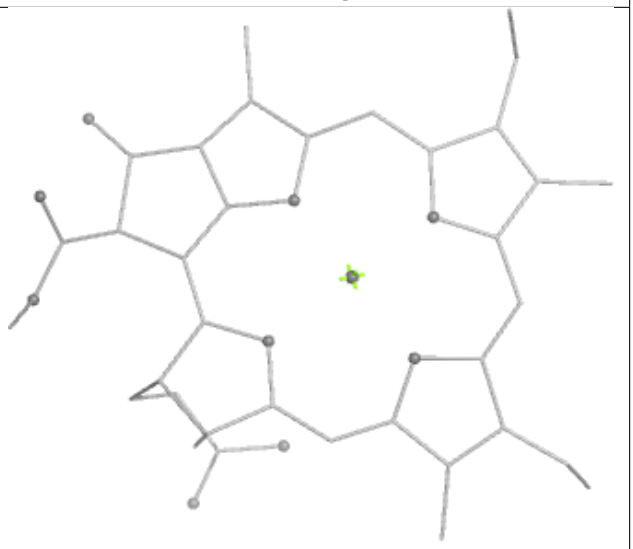
Bond lengths



Bond angles

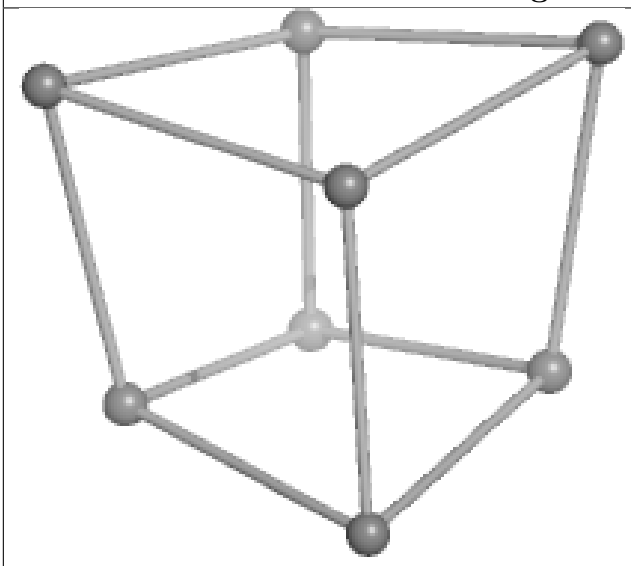


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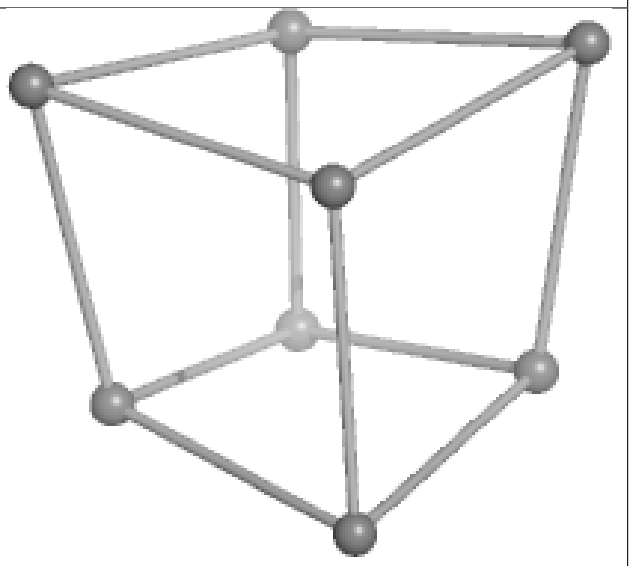


Rings

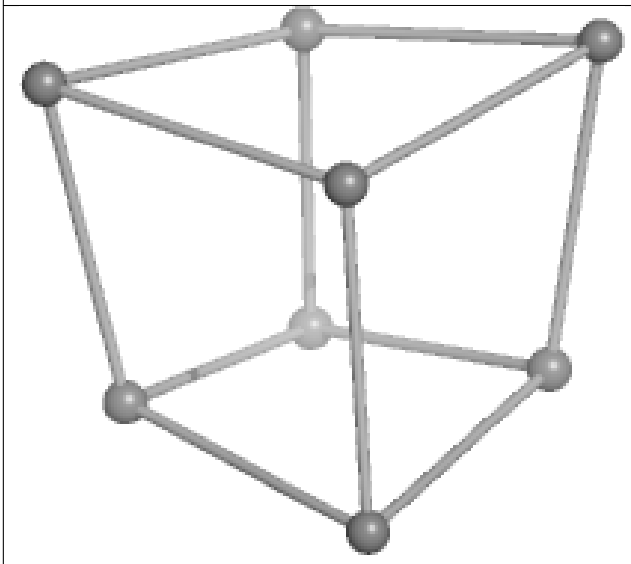
Ligand SF4 A 850



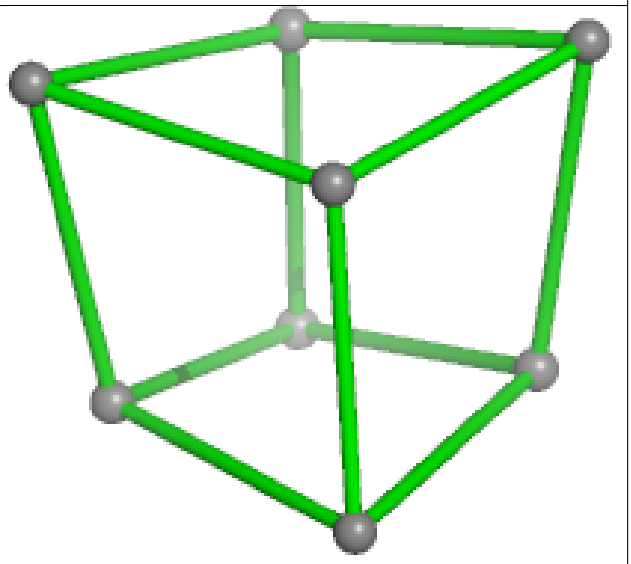
Bond lengths



Bond angles

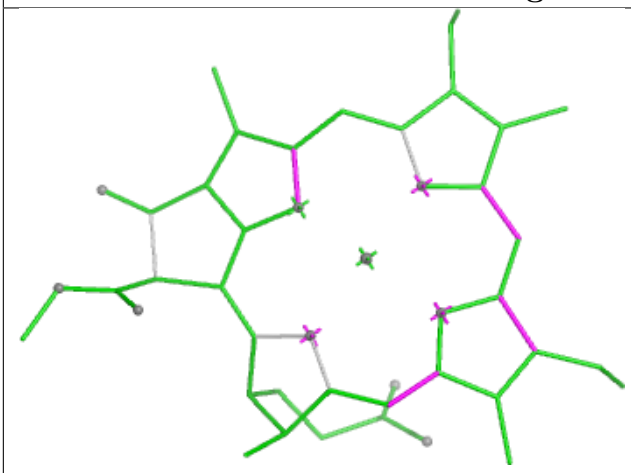


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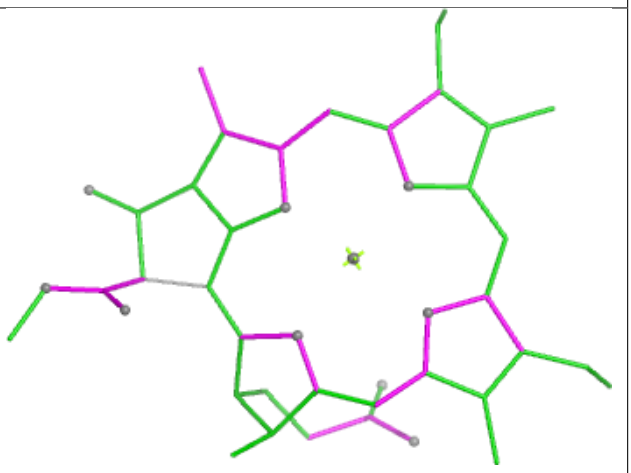


Rings

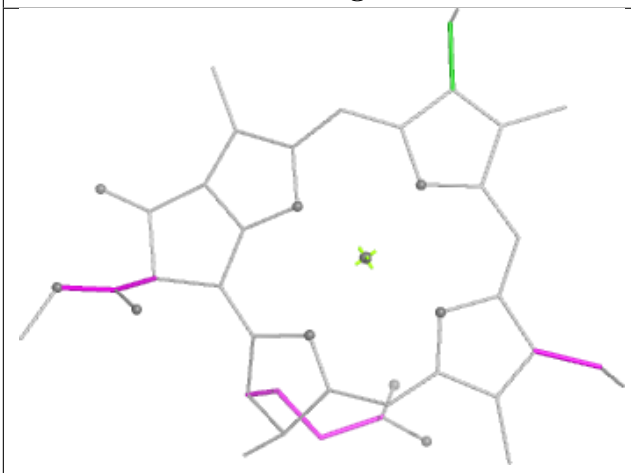
Ligand CLA Z 310



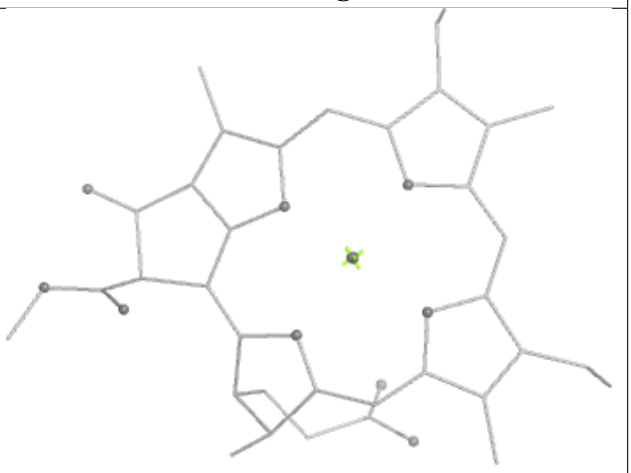
Bond lengths



Bond angles

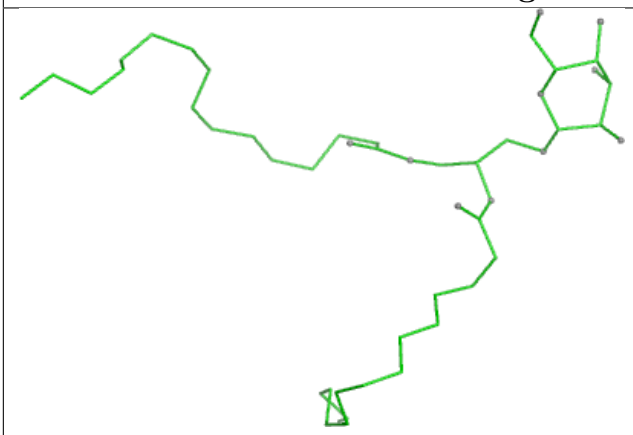


Torsions

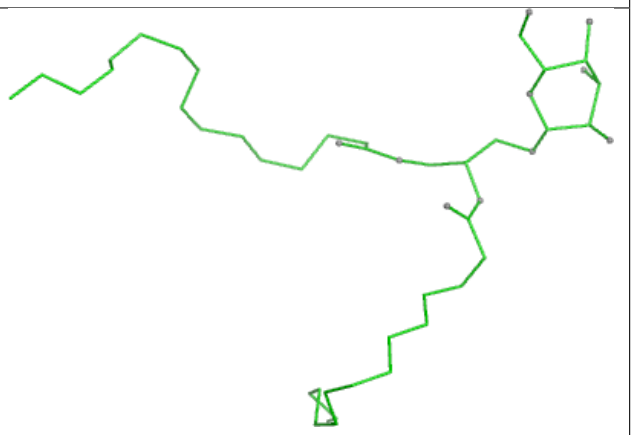


Rings

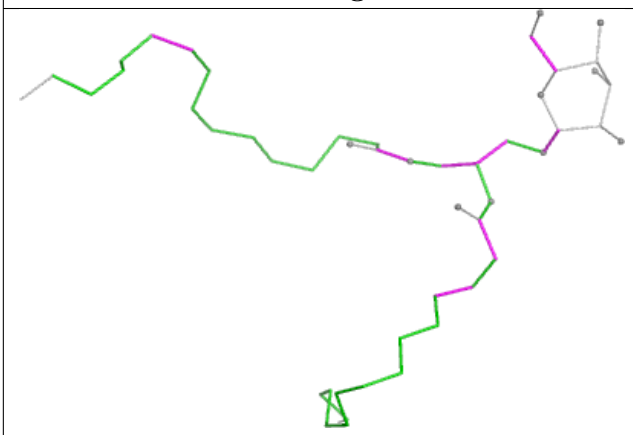
Ligand LMG G 206



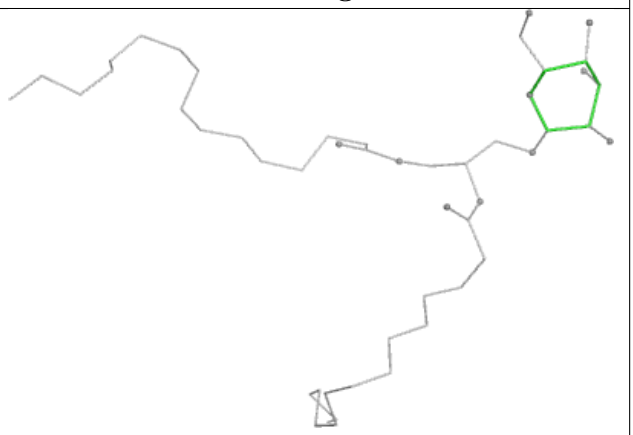
Bond lengths



Bond angles

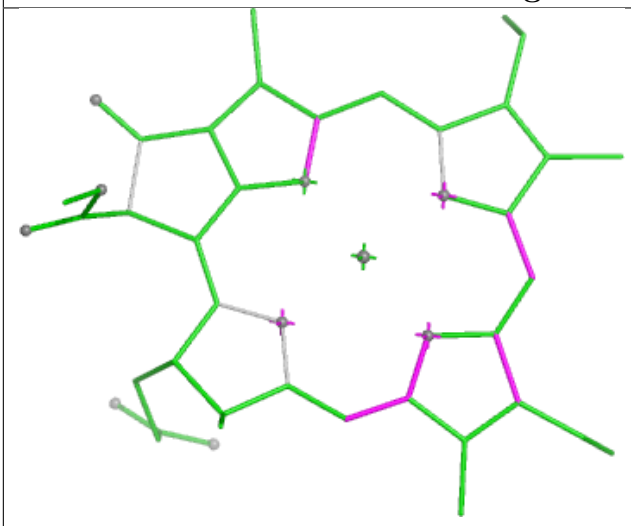


Torsions

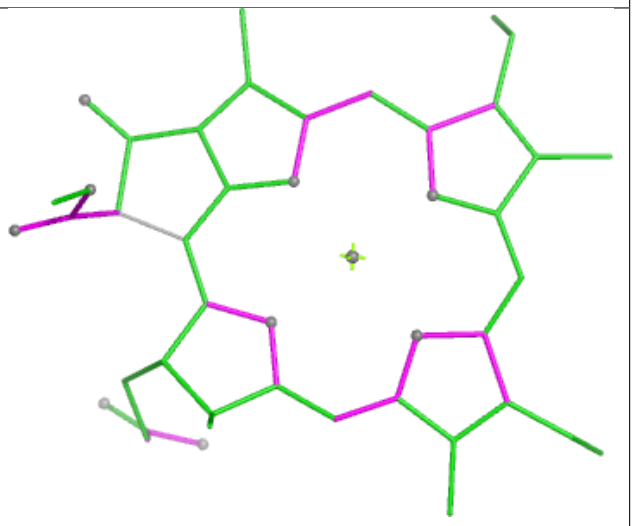


Rings

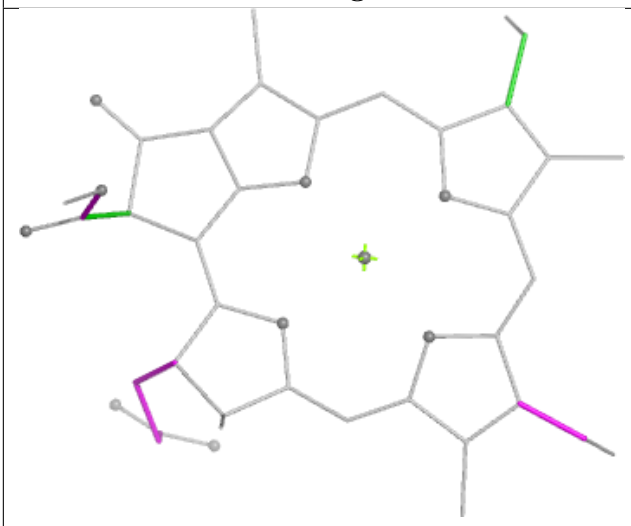
Ligand CLA A 820



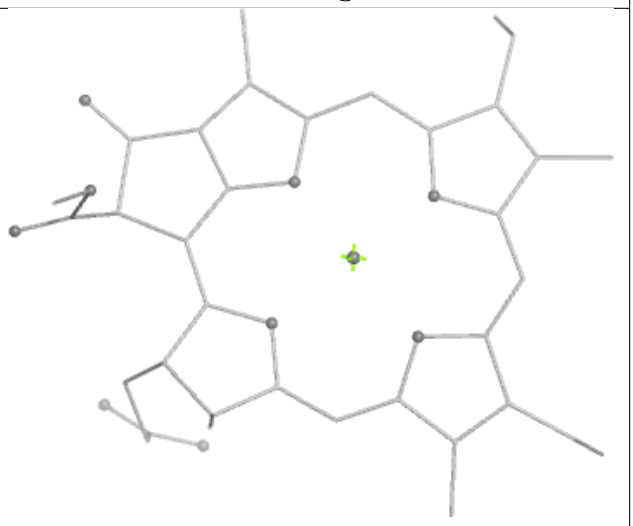
Bond lengths



Bond angles

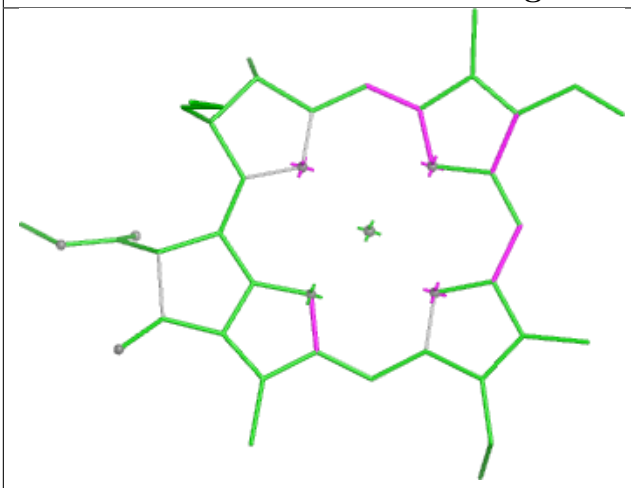


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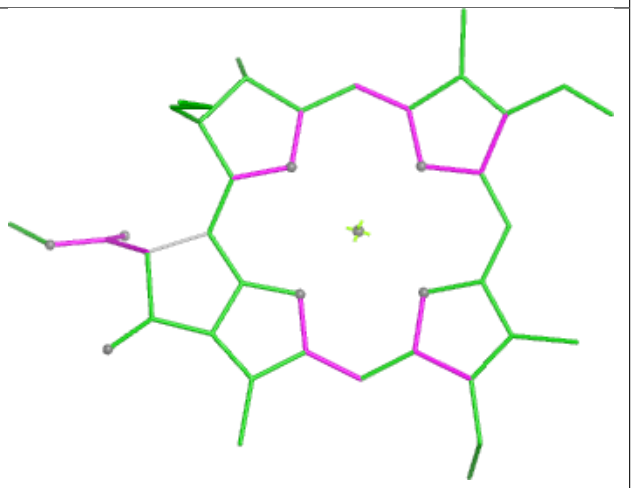


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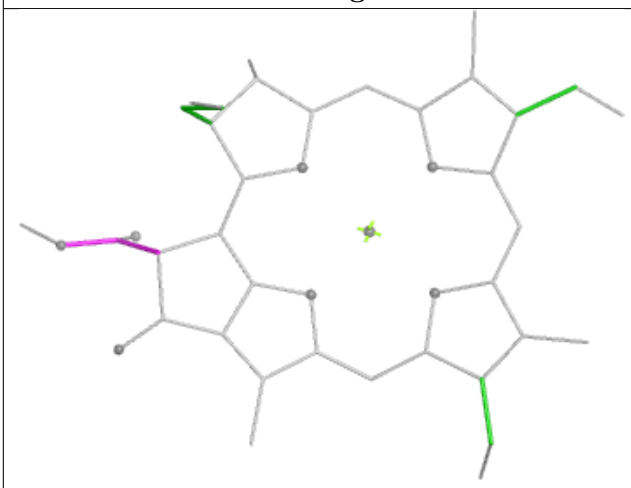
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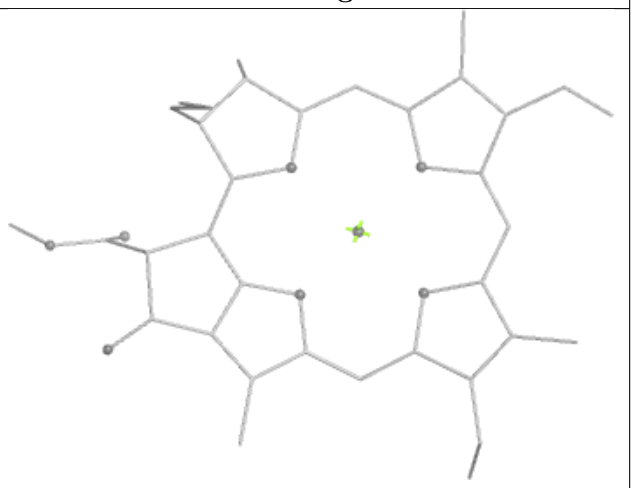
Bond lengths



Bond angles

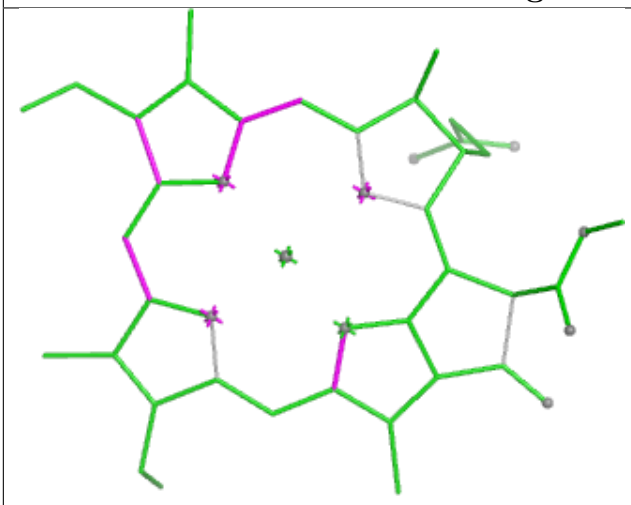


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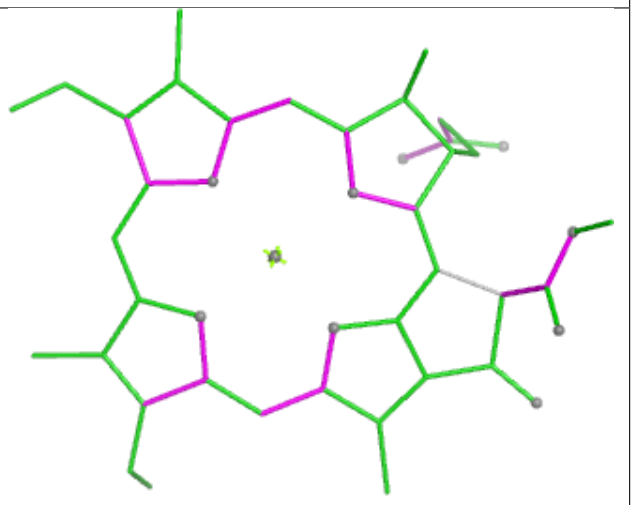


Rings

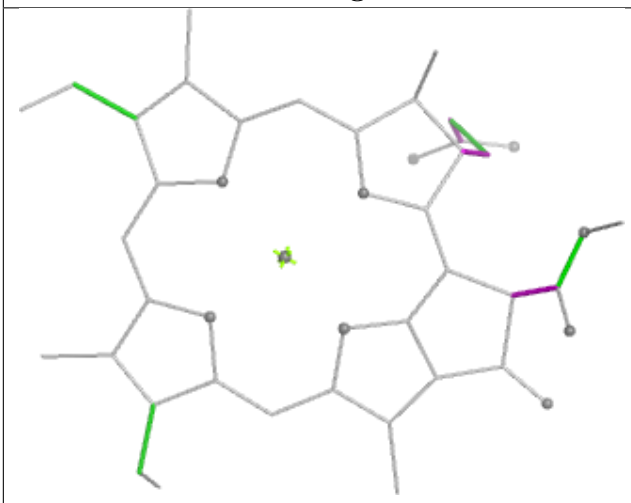
Ligand CLA L 303



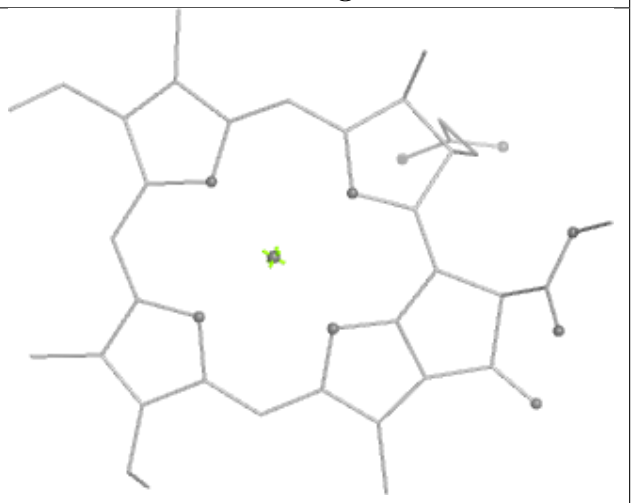
Bond lengths



Bond angles

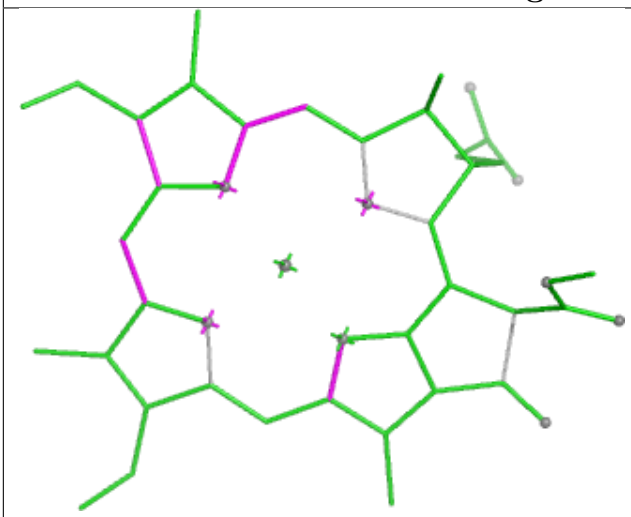


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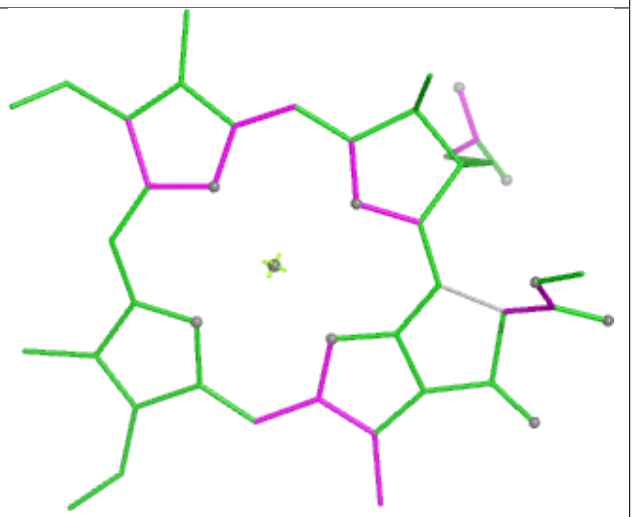


Rings

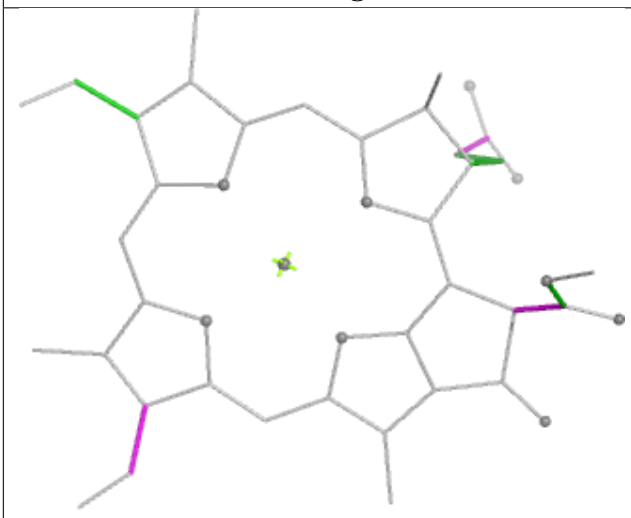
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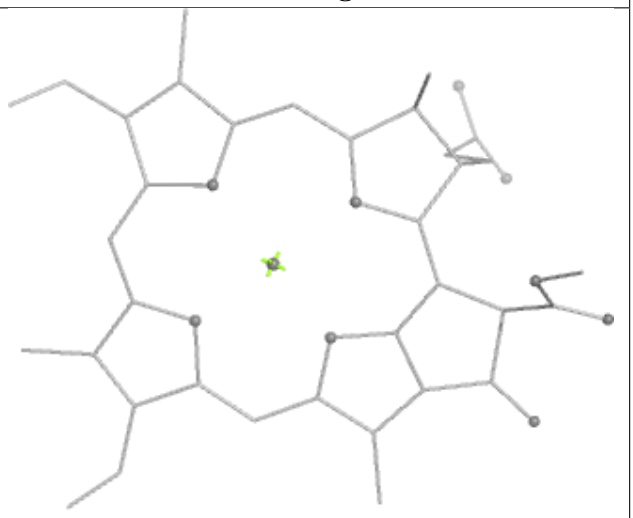
Bond lengths



Bond angles

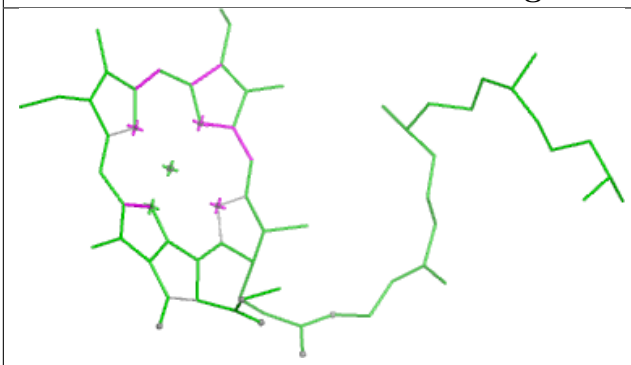


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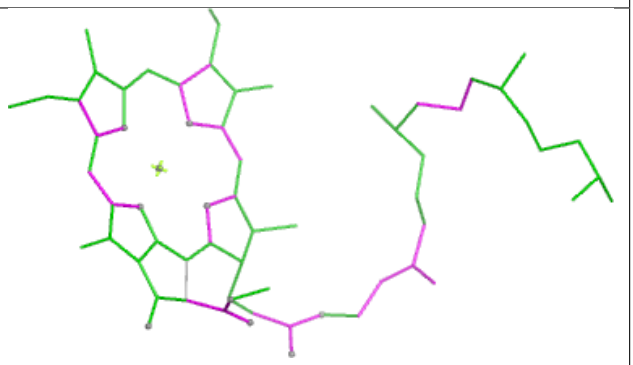


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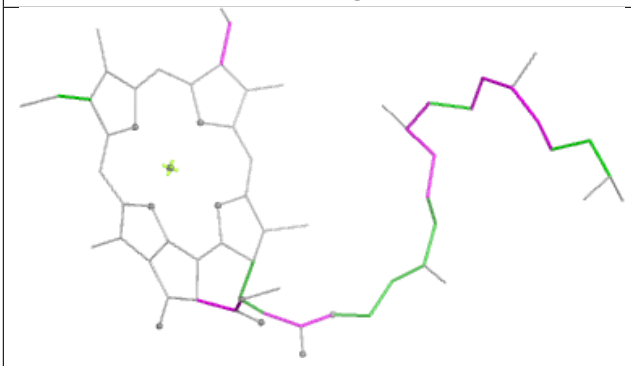
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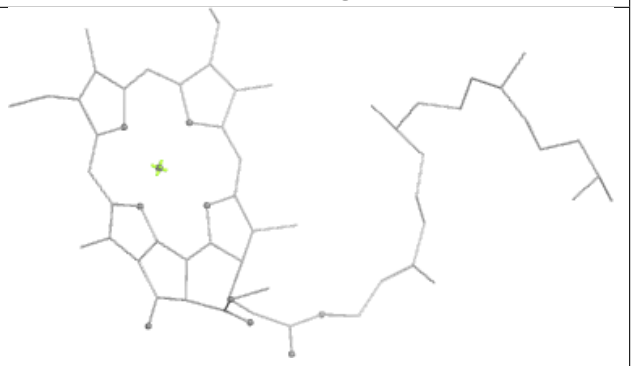
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR 3 601



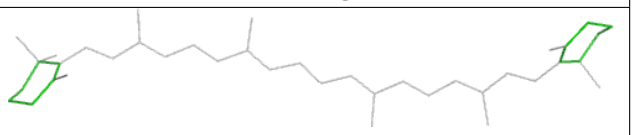
Bond lengths



Bond angles

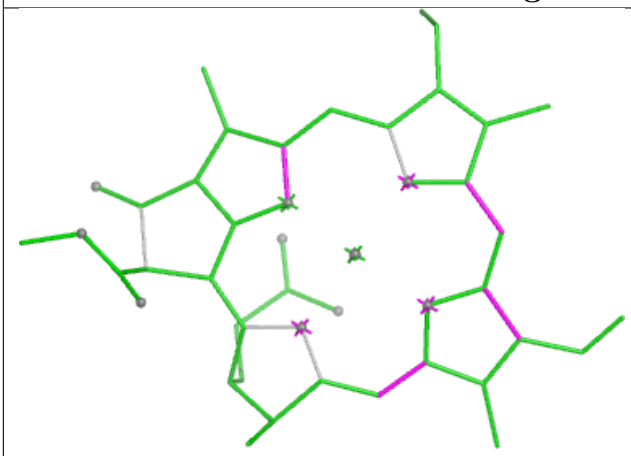


Torsions

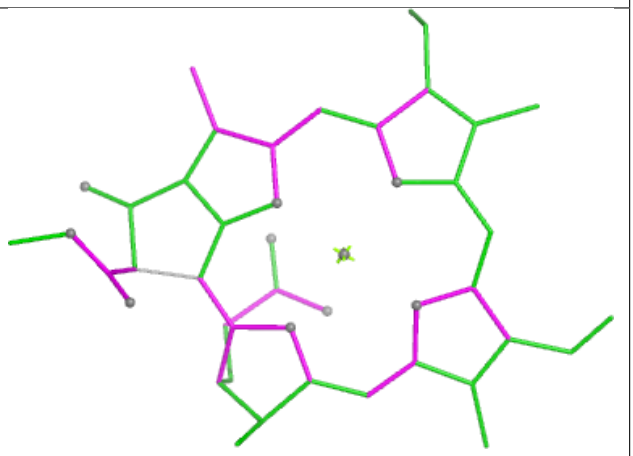


Rings

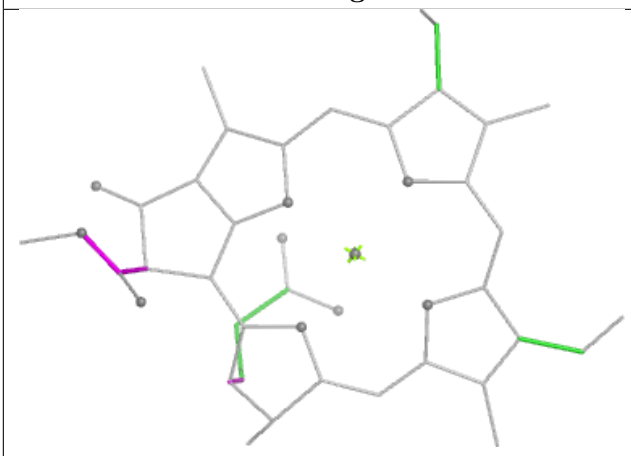
Ligand CLA X 612



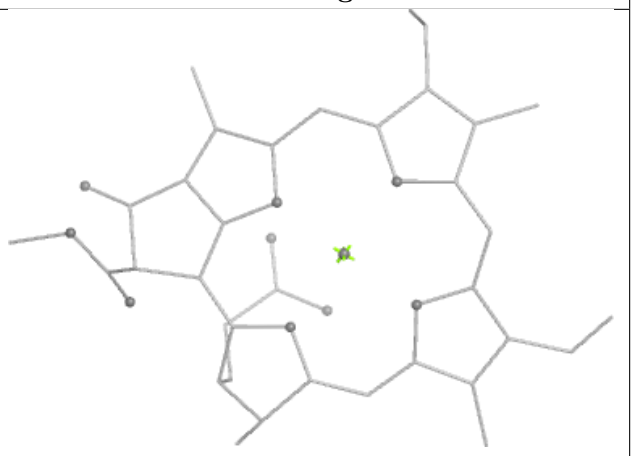
Bond lengths



Bond angles



Torsions



Rings

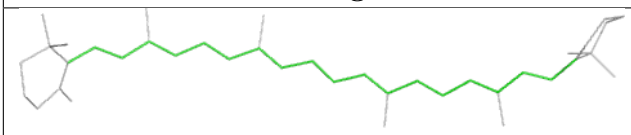
Ligand BCR B 847



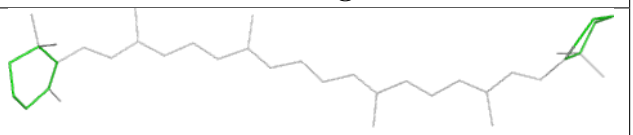
Bond lengths



Bond angles

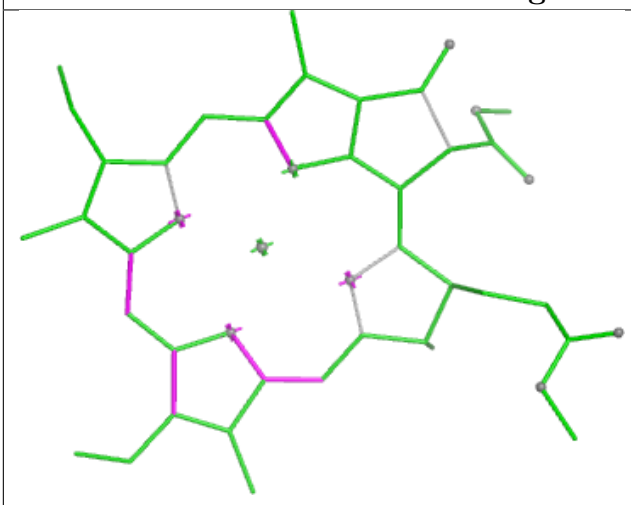


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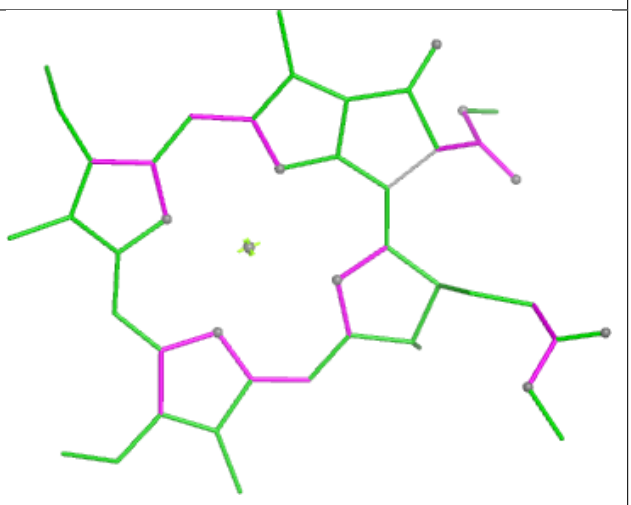


Rings

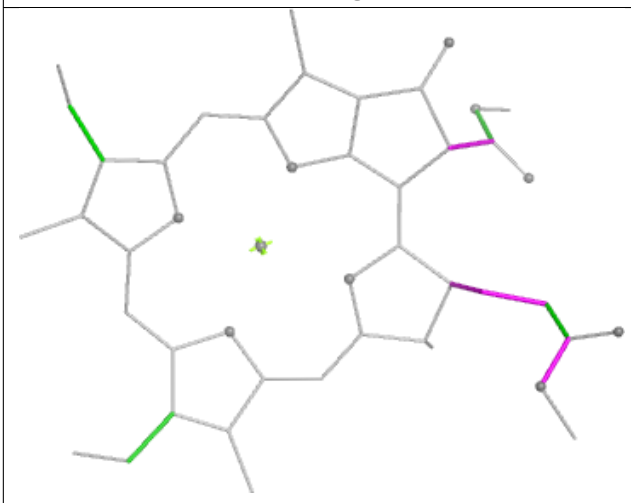
Ligand CLA 2 618



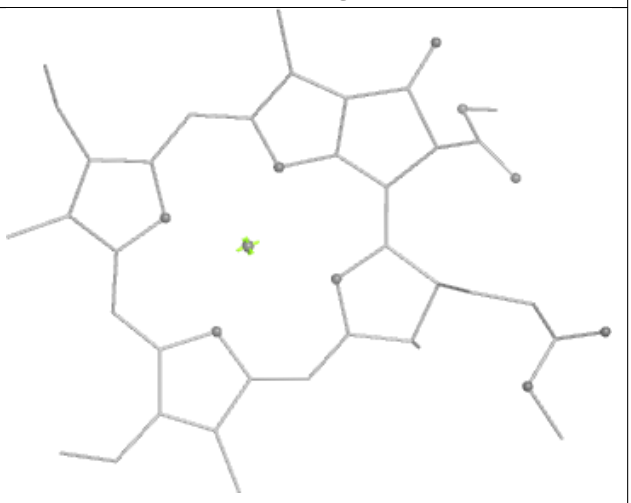
Bond lengths



Bond angles

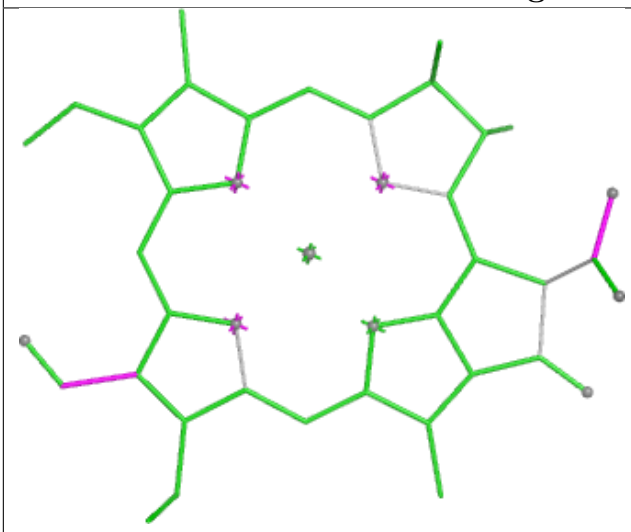


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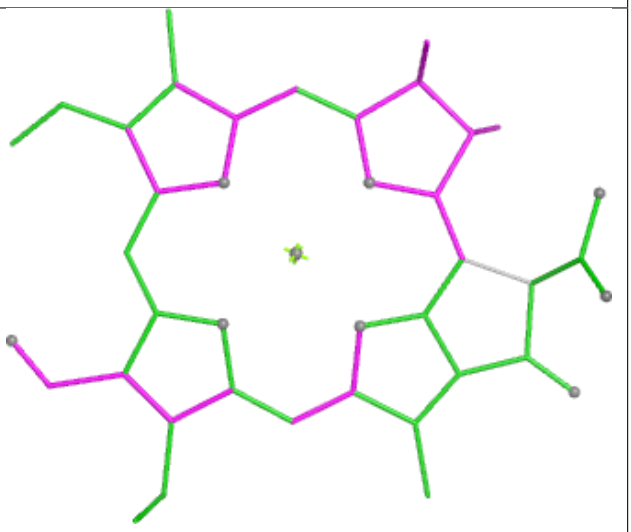


Rings

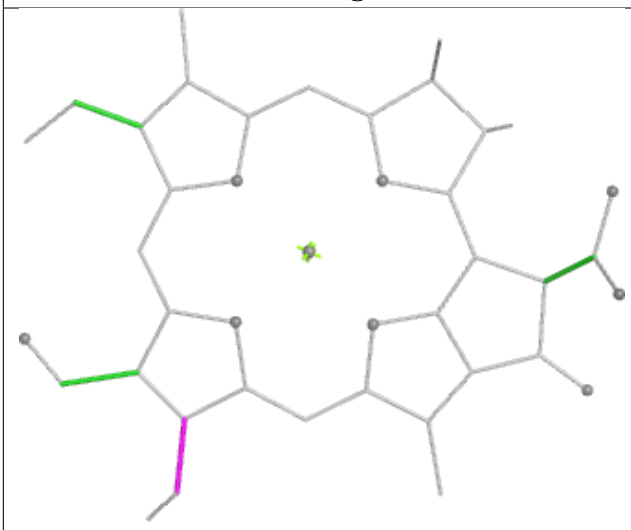
Ligand CHL 1 606



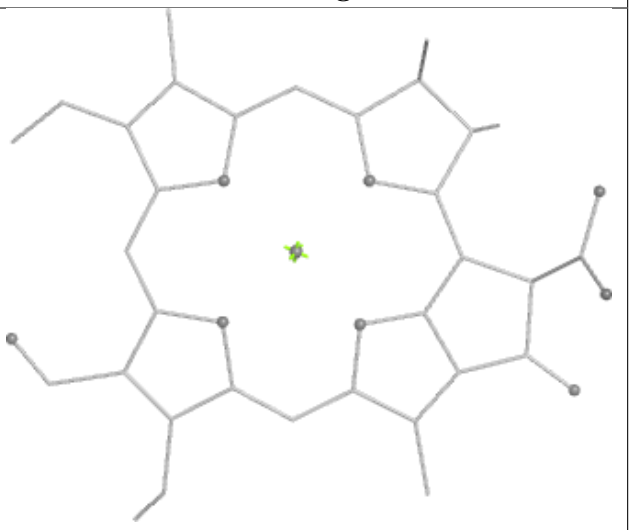
Bond lengths



Bond angles

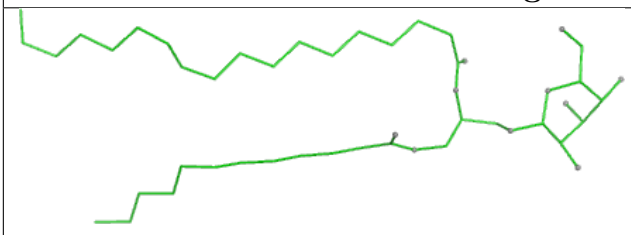


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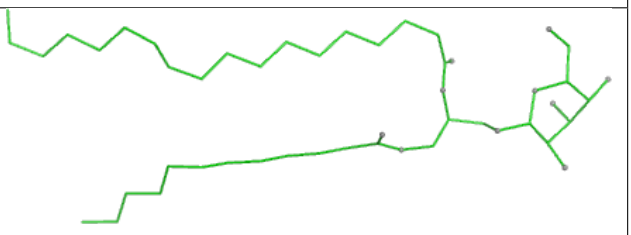


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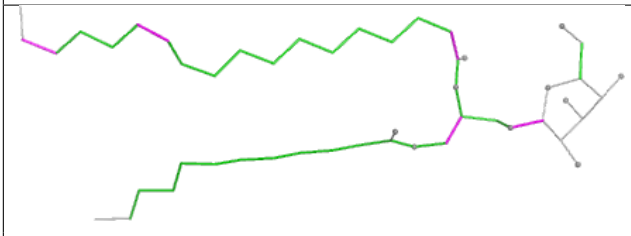
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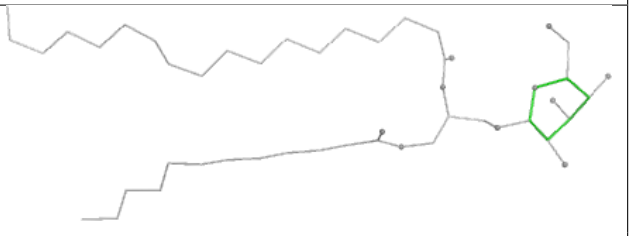
Bond lengths



Bond angles

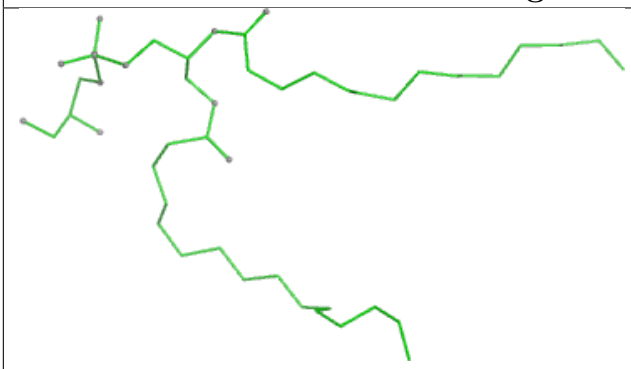


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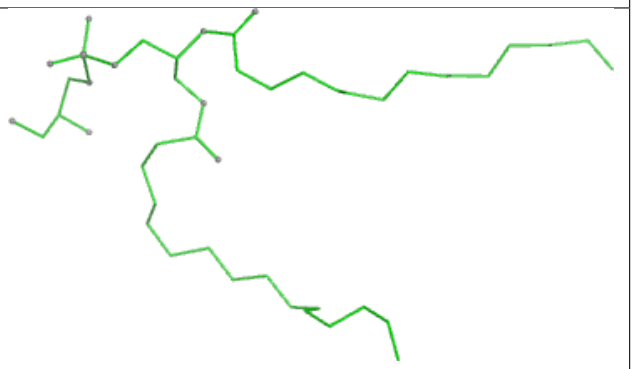


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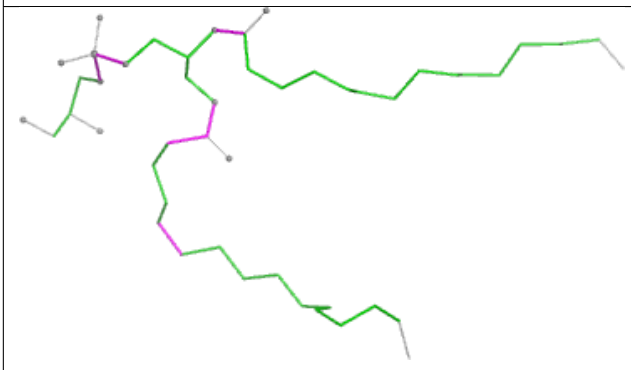
Ligand LHG 1 620



Bond lengths



Bond angles

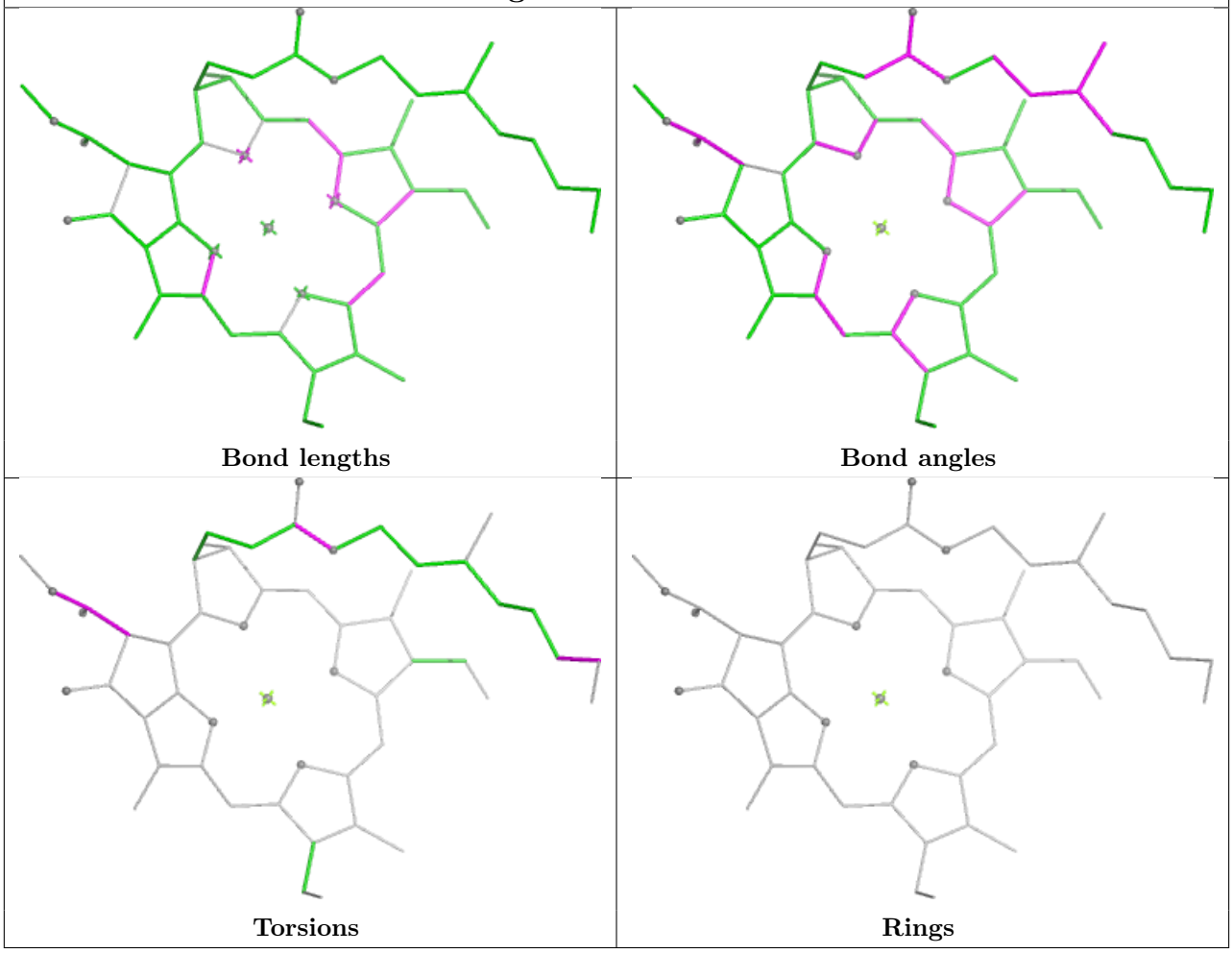


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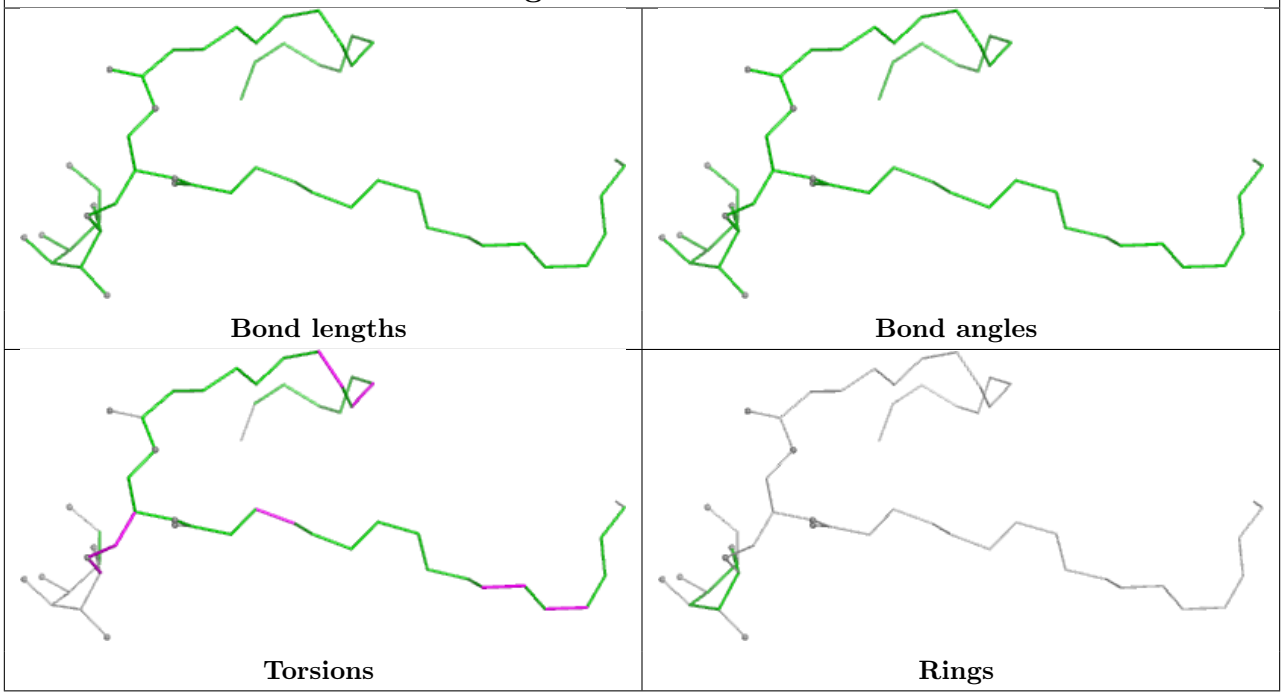


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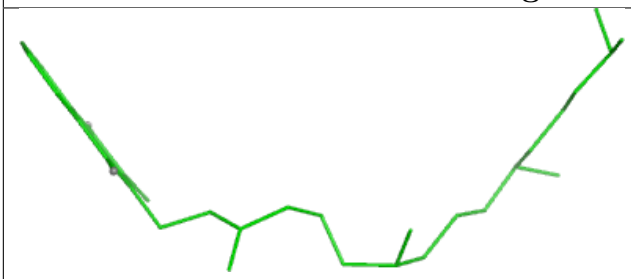
Ligand CLA 4 308



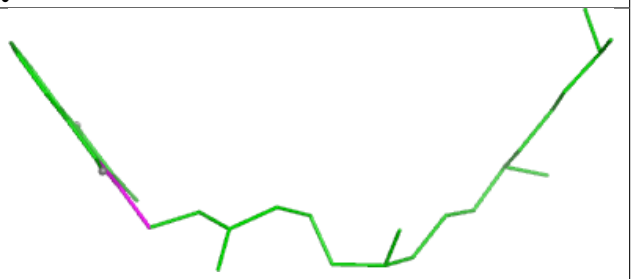
Ligand LMG 5 620



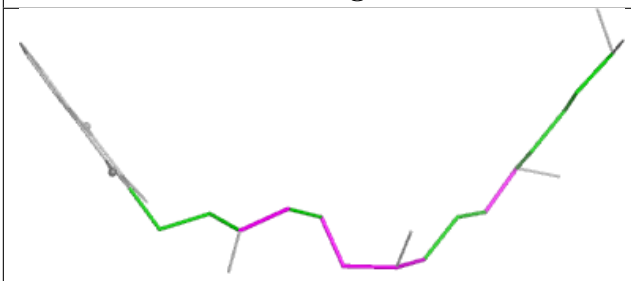
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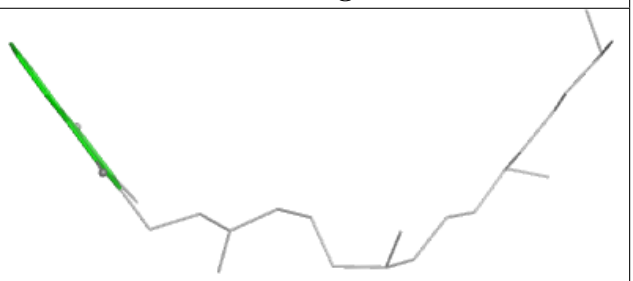
Bond lengths



Bond angles

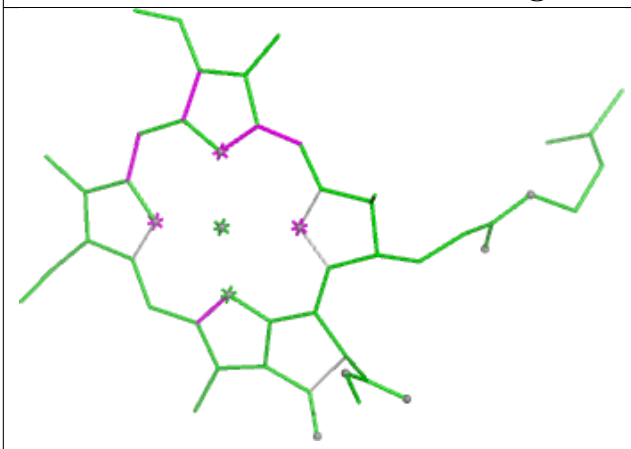


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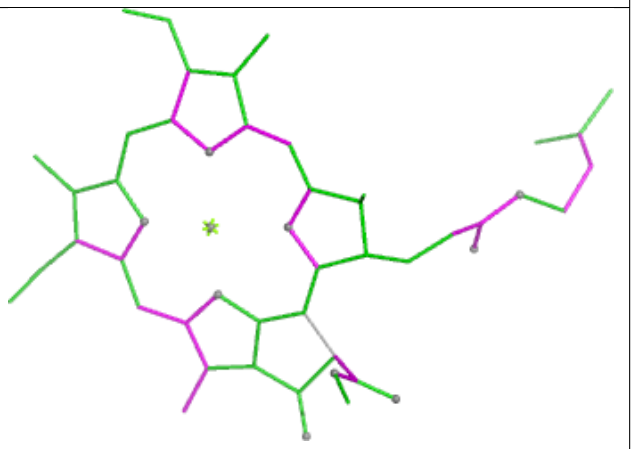


Rings

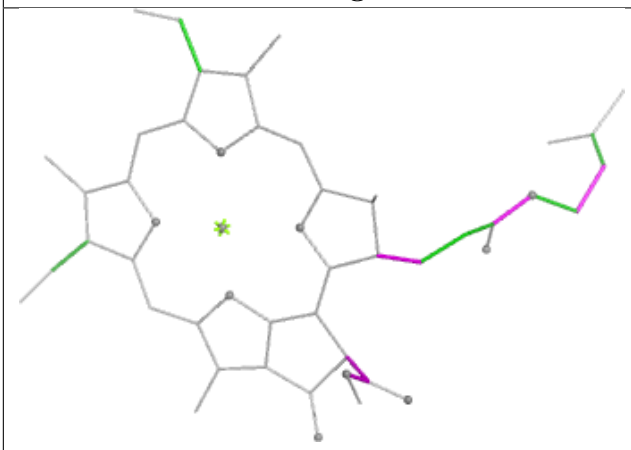
Ligand CLA 4 313



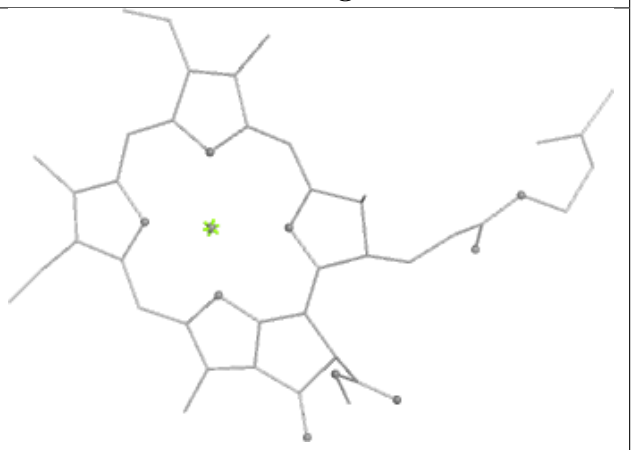
Bond lengths



Bond angles

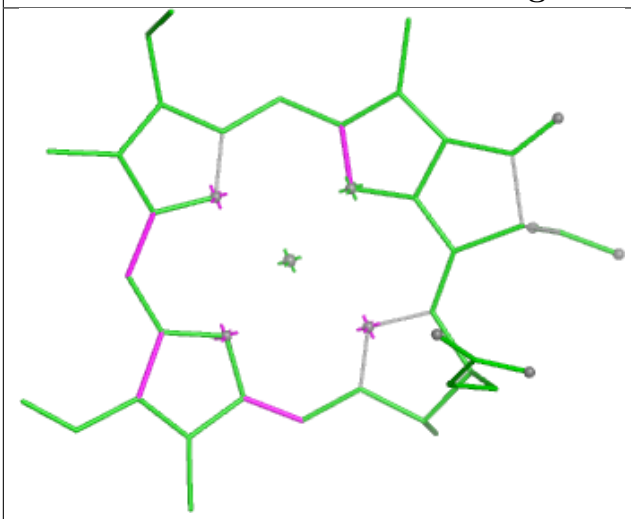


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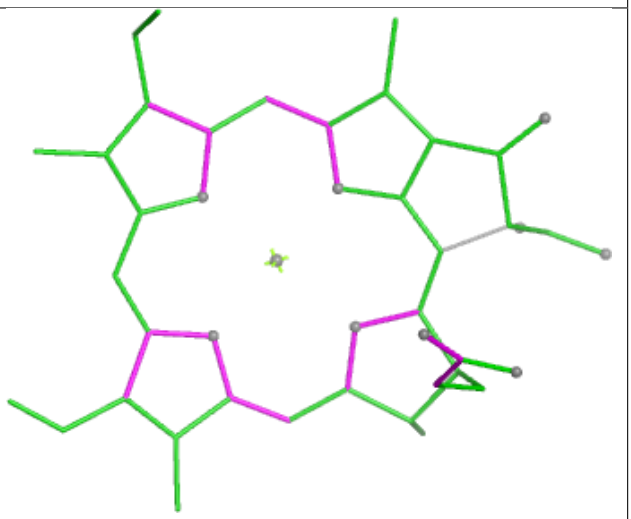


Rings

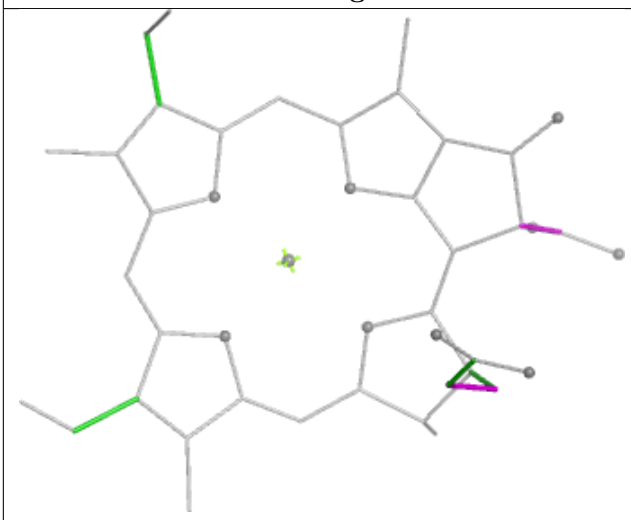
Ligand CLA 5 607



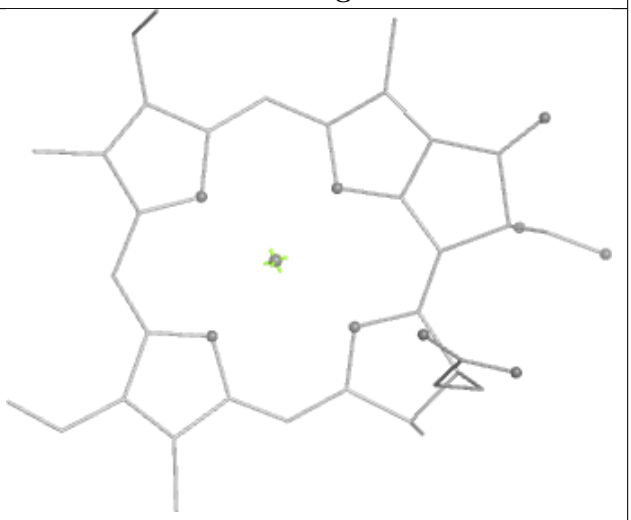
Bond lengths



Bond angles

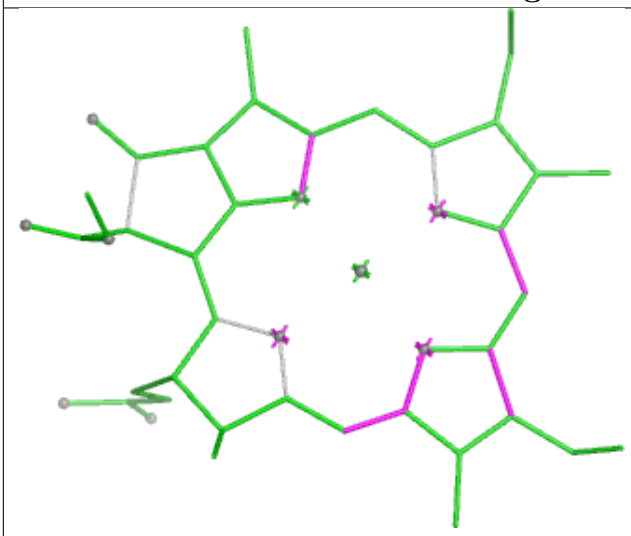


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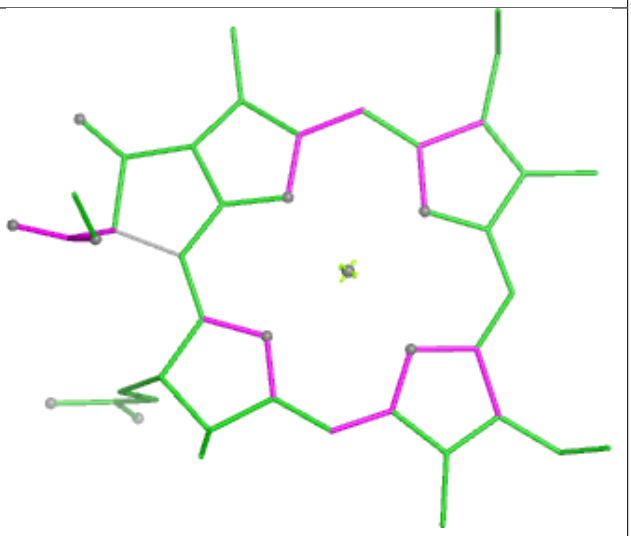


Rings

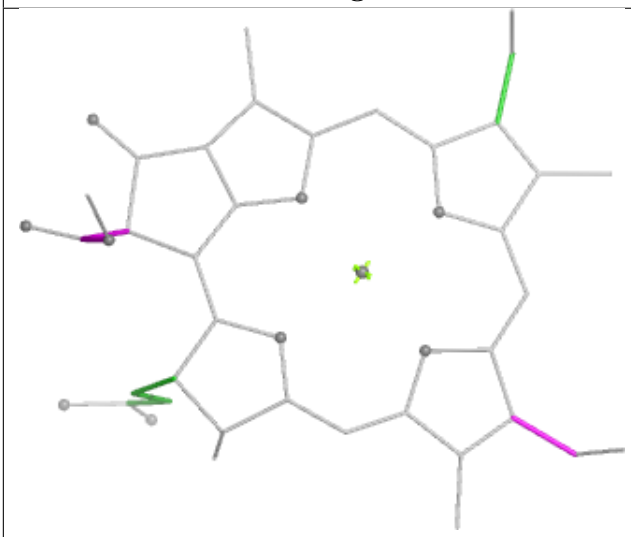
Ligand CLA A 814



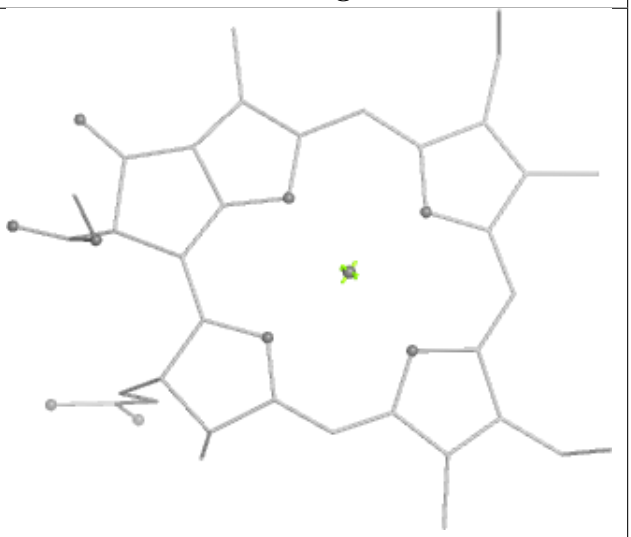
Bond lengths



Bond angles



Torsions

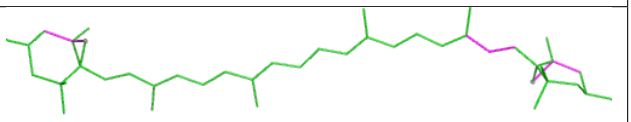


Rings

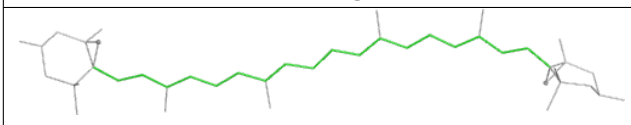
Ligand XAT 2 616



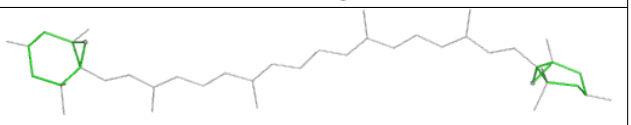
Bond lengths



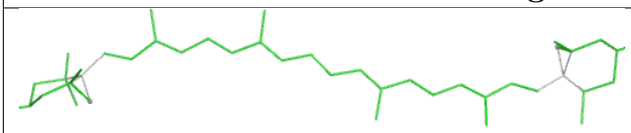
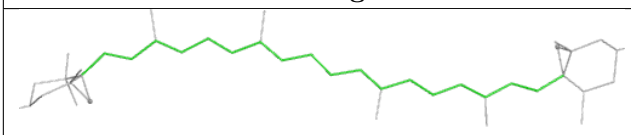
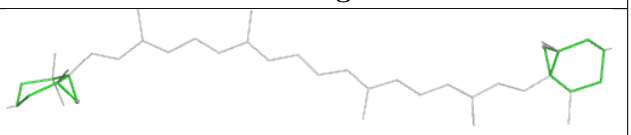
Bond angles

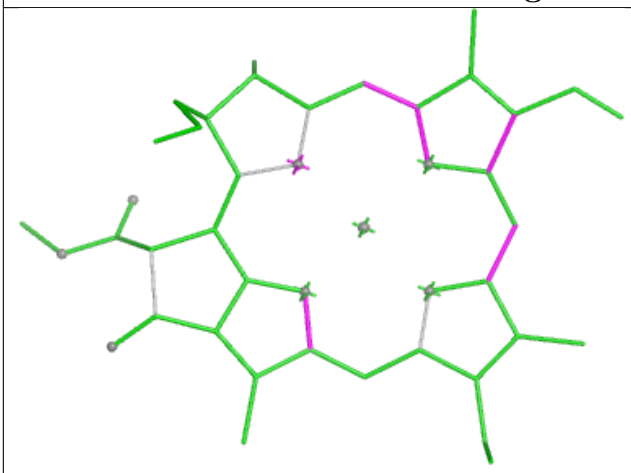
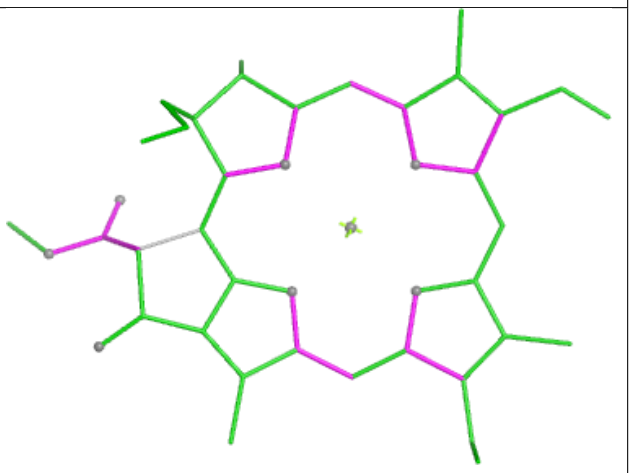
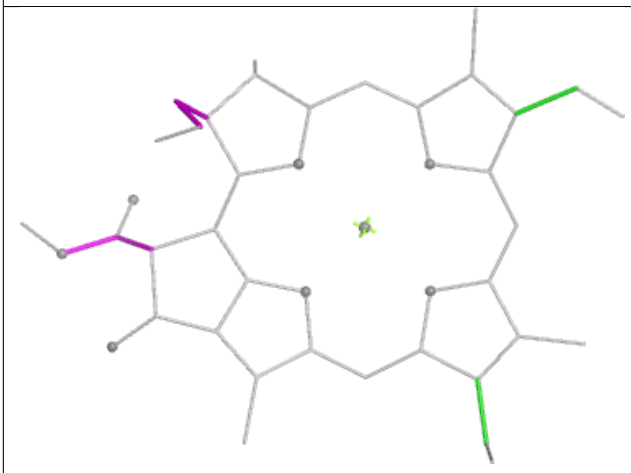
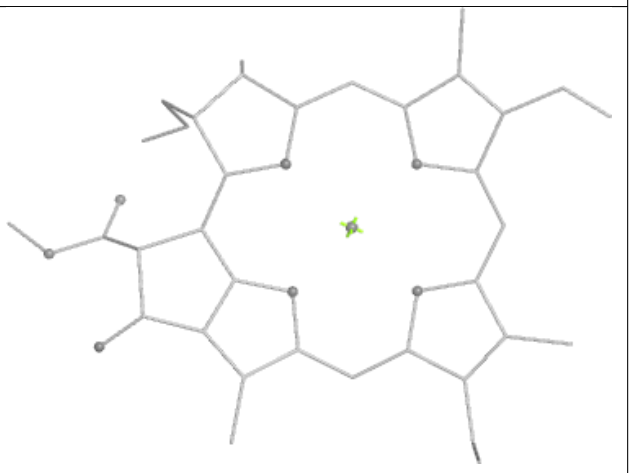


Torsions

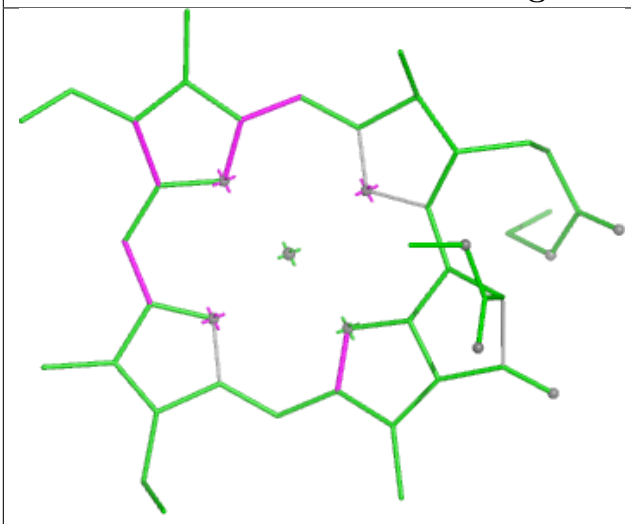


Rings

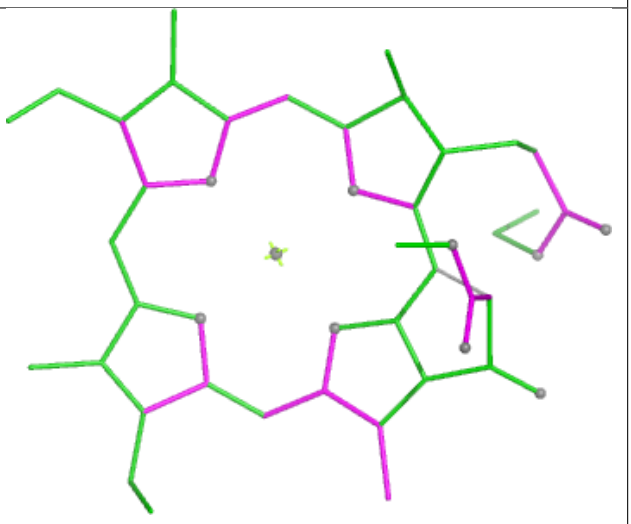
Ligand XAT 4 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

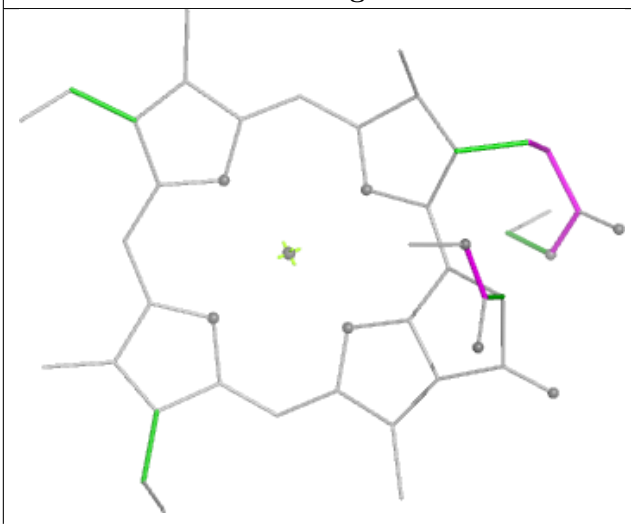
Ligand CLA 3 605



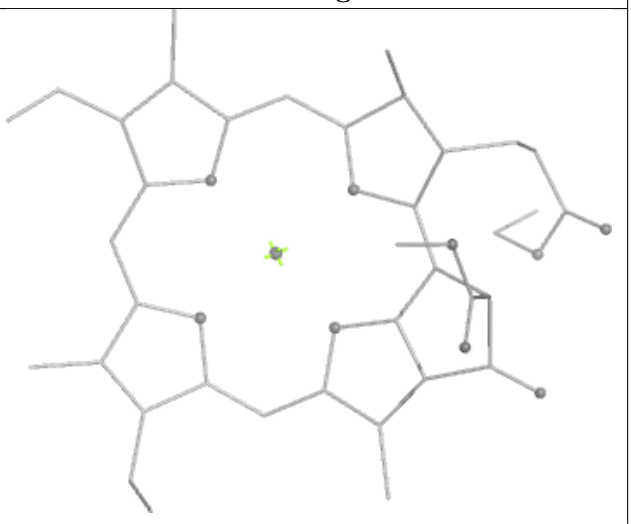
Bond lengths



Bond angles

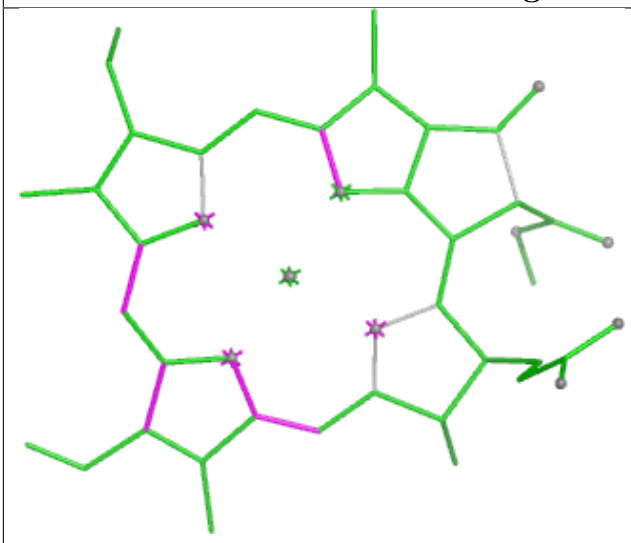


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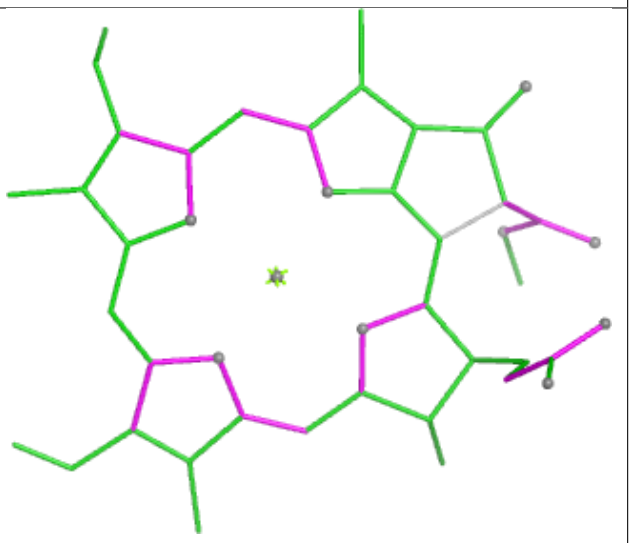


Rings

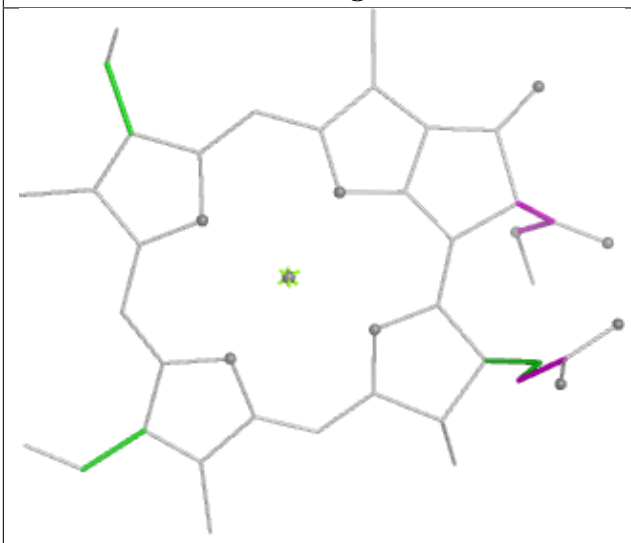
Ligand CLA K 202



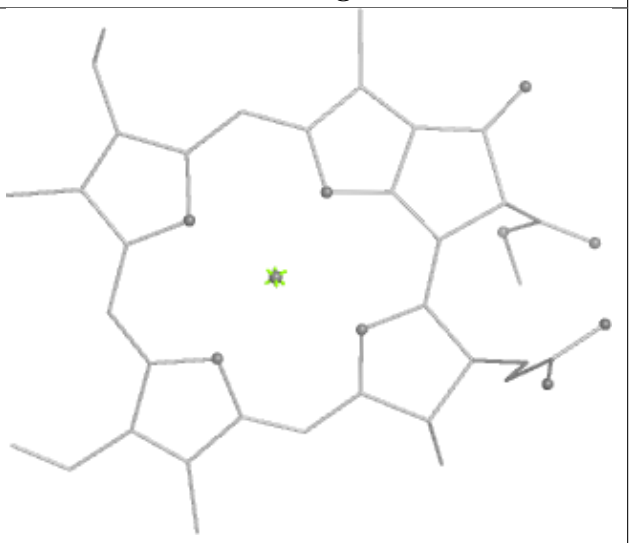
Bond lengths



Bond angles

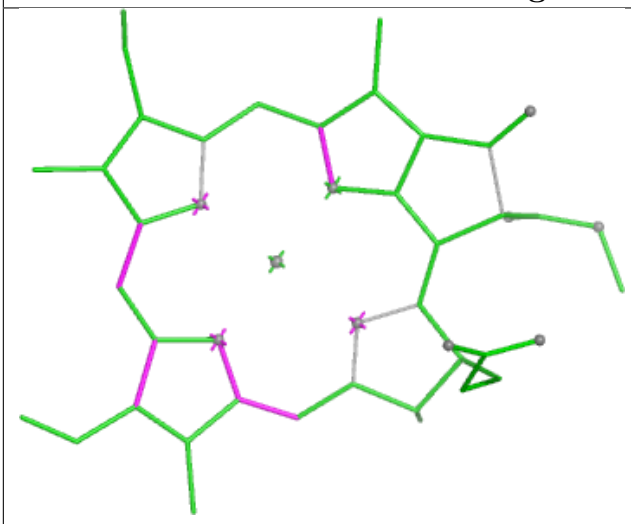


Torsions

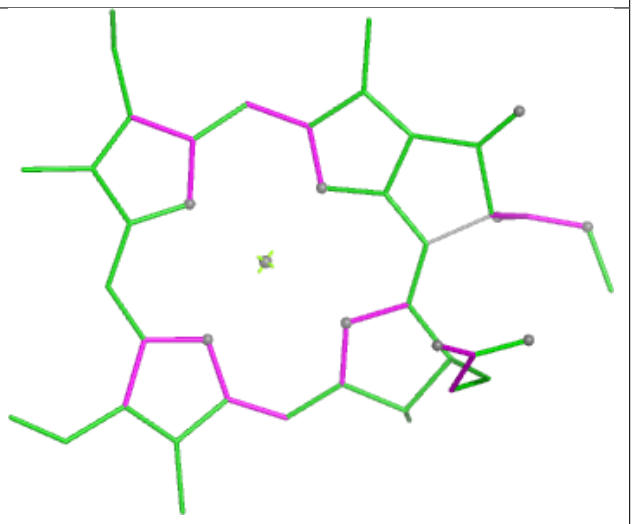


Rings

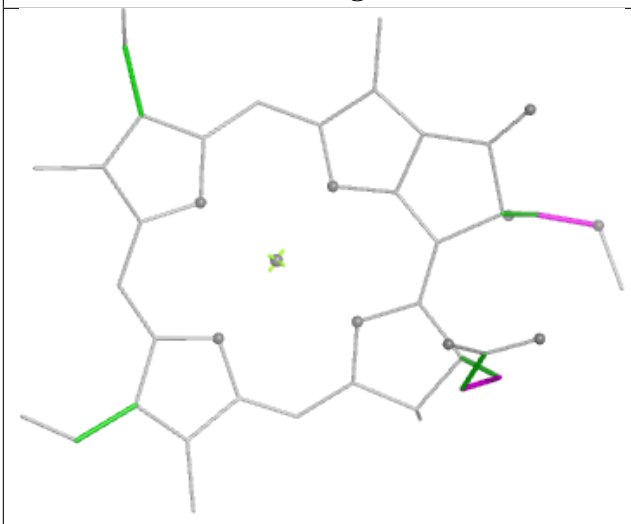
Ligand CLA 5 610



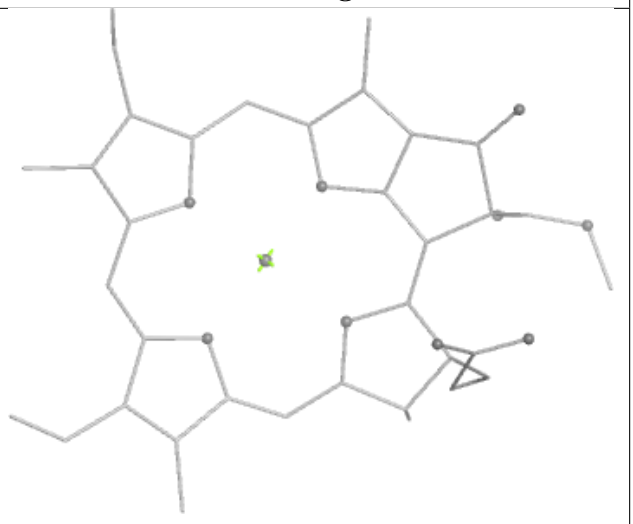
Bond lengths



Bond angles

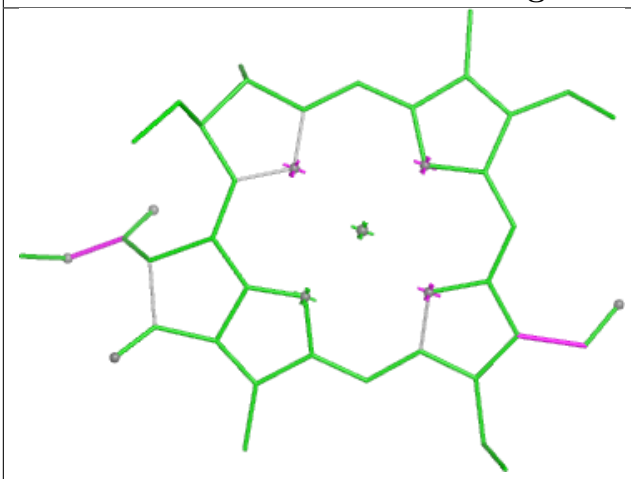


Torsions

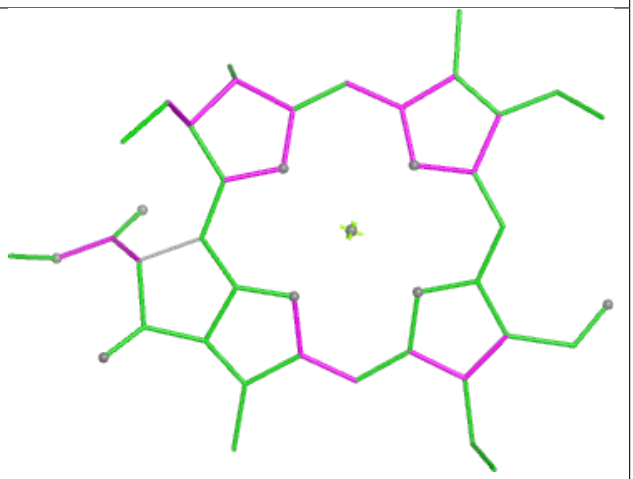


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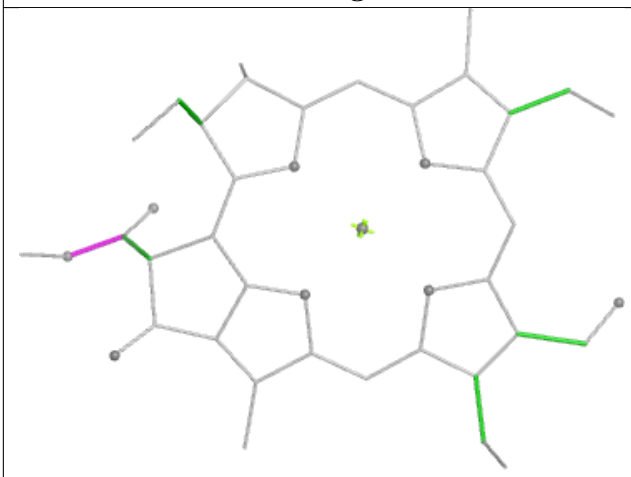
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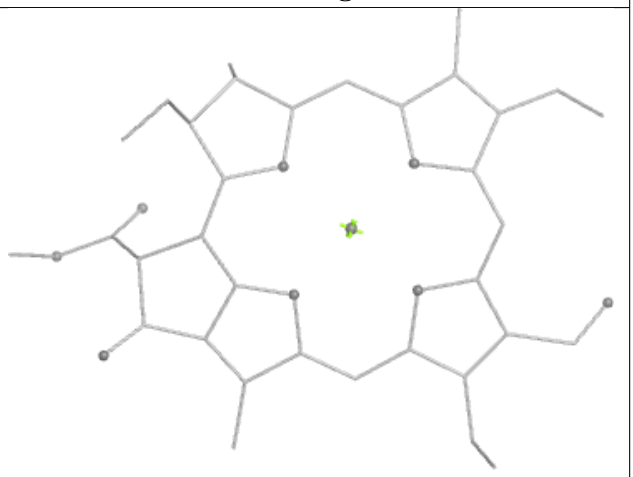
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Bond angles

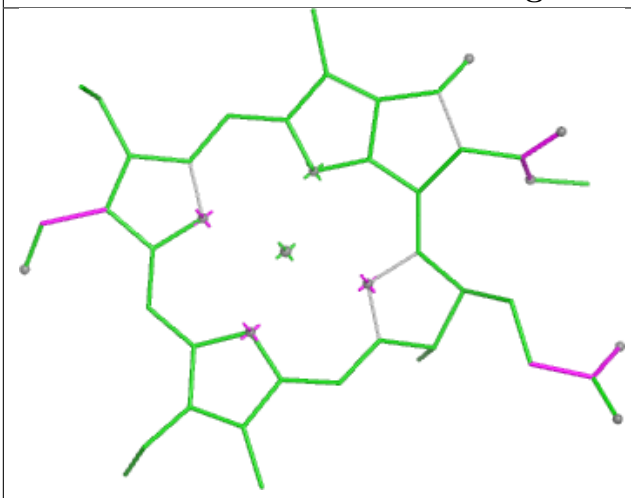


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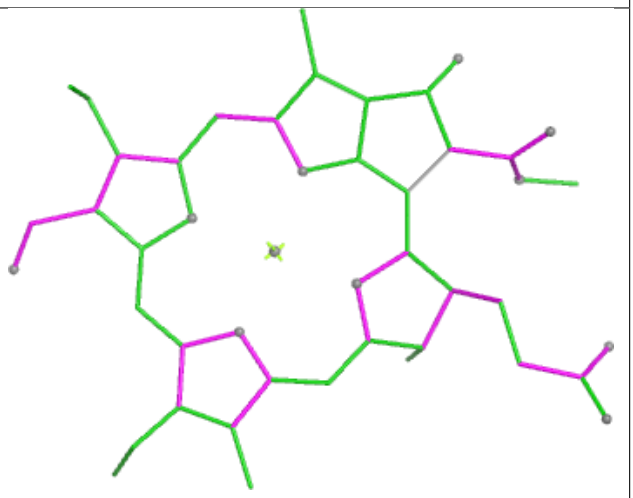


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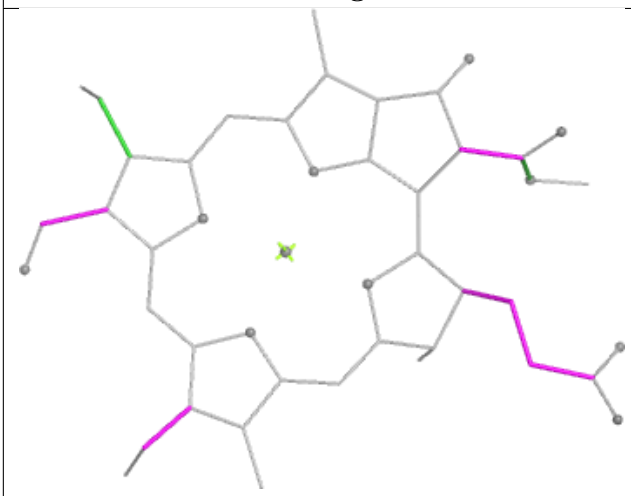
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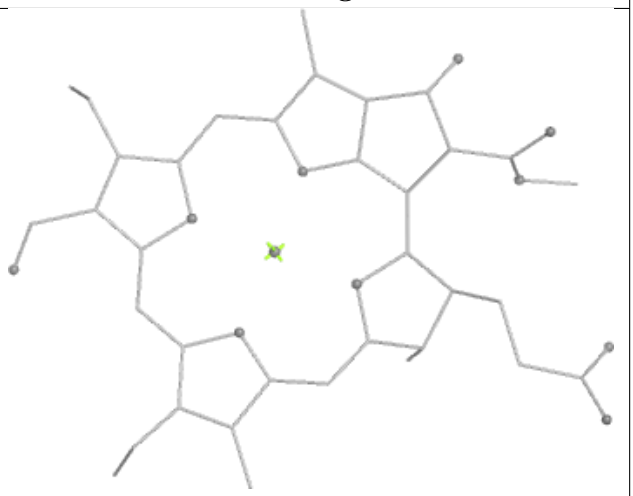
Bond lengths



Bond angles

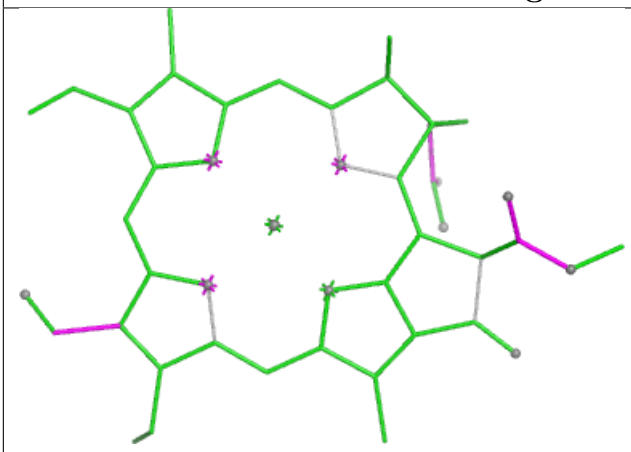


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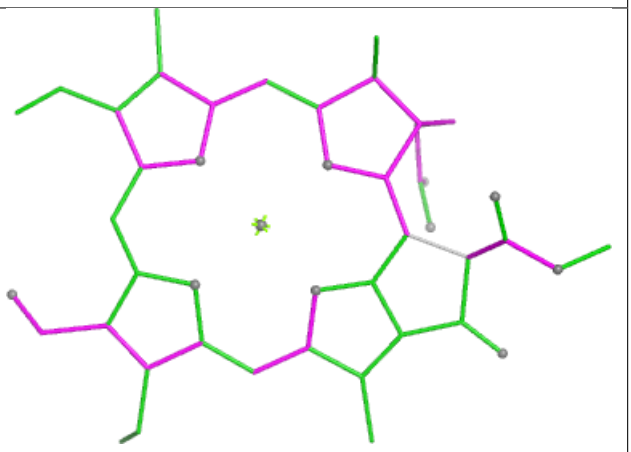


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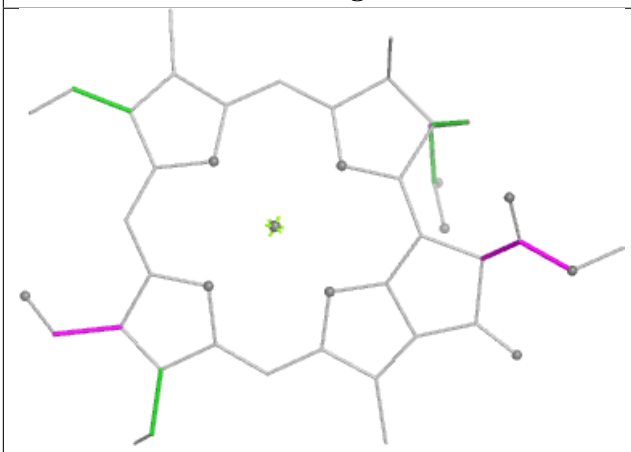
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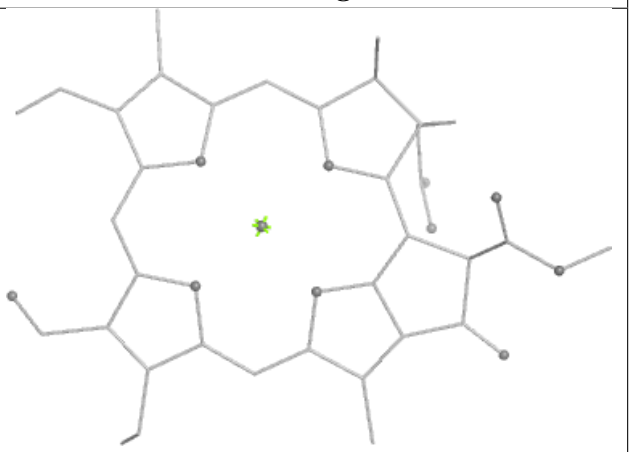
Bond lengths



Bond angles

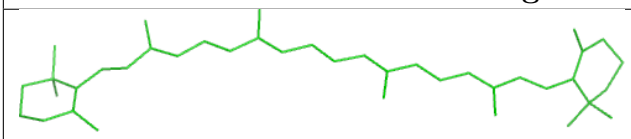


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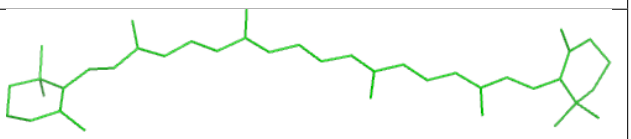


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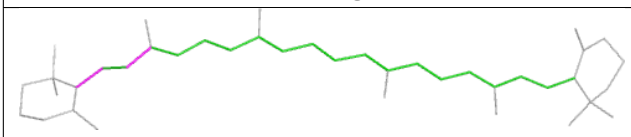
Ligand BCR A 854



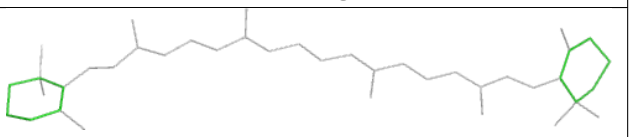
Bond lengths



Bond angles

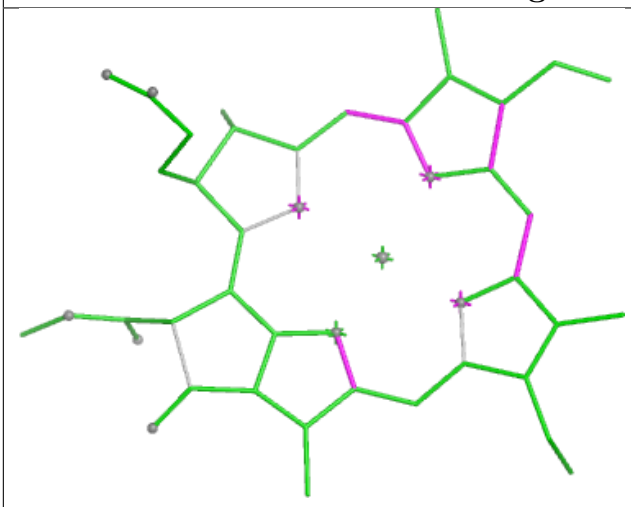


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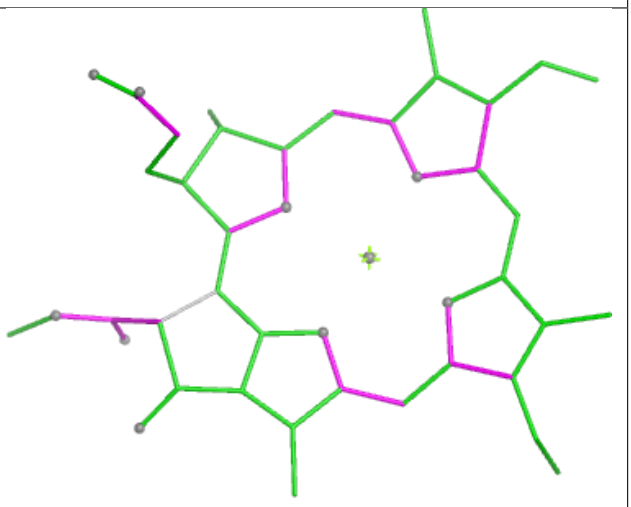


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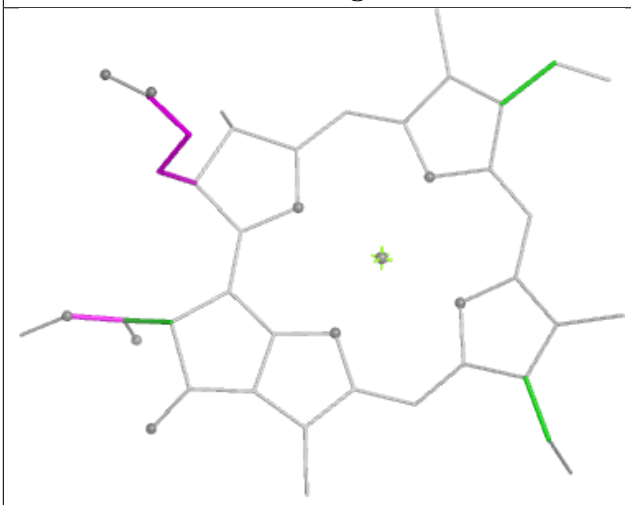
Ligand CLA 3 609



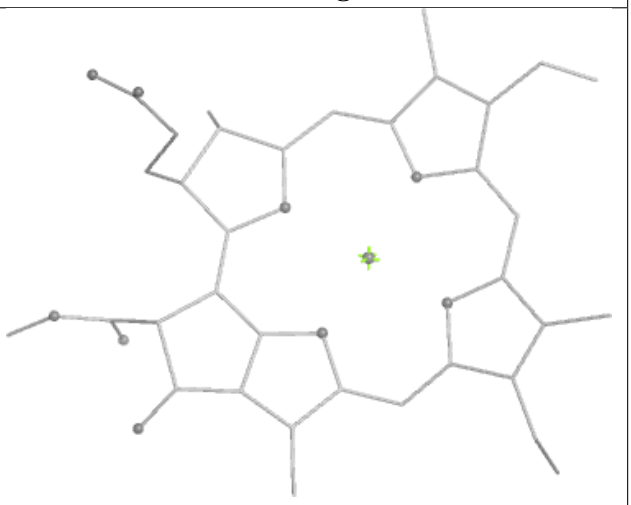
Bond lengths



Bond angles

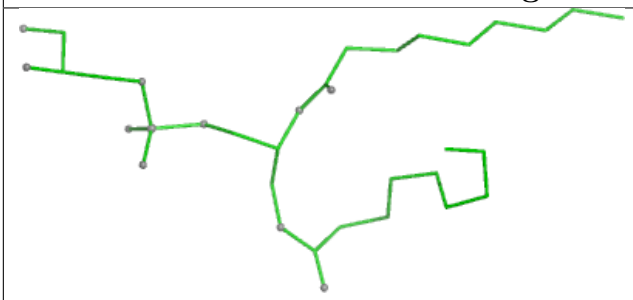


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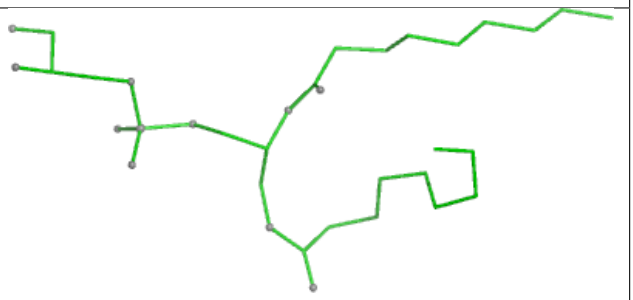


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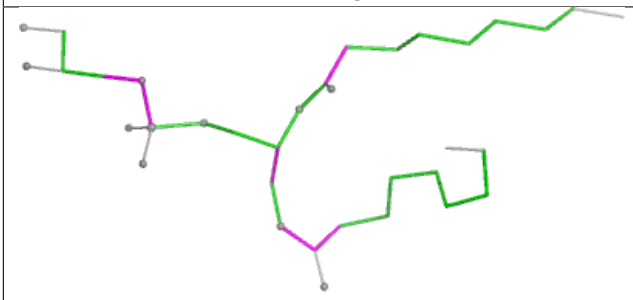
Ligand LHG Y 618



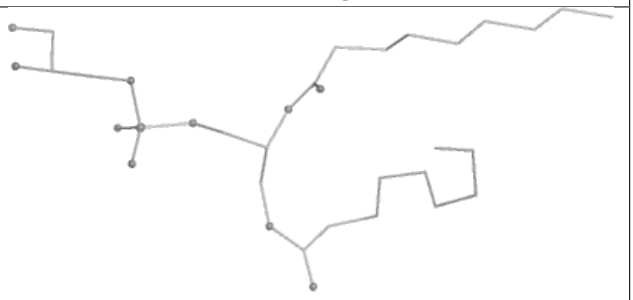
Bond lengths



Bond angles

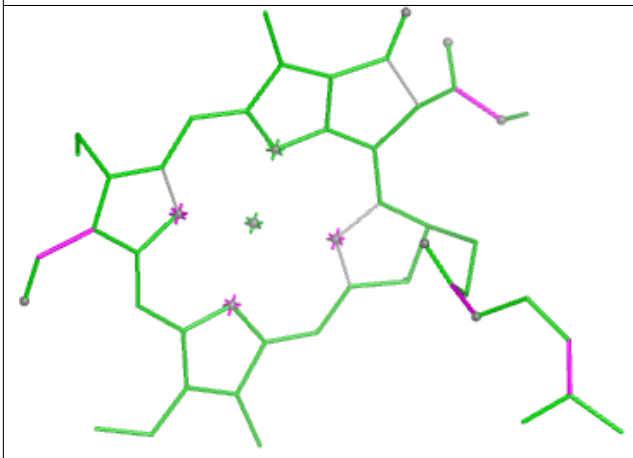


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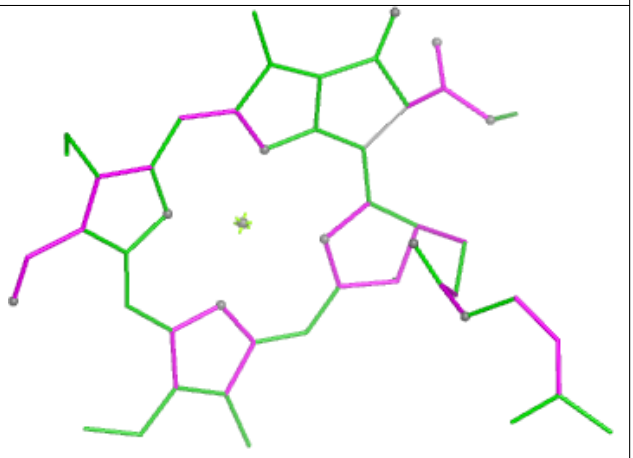


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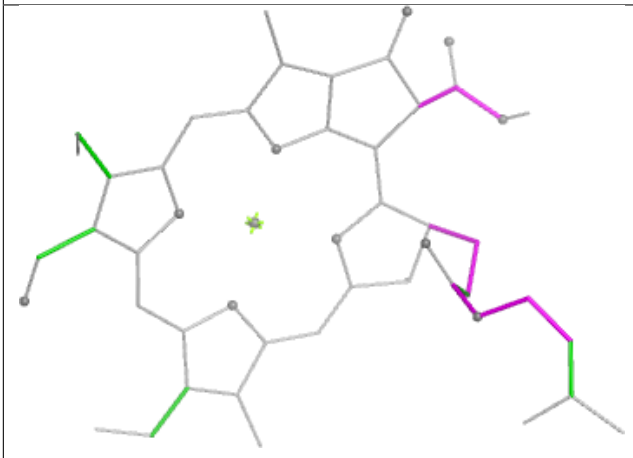
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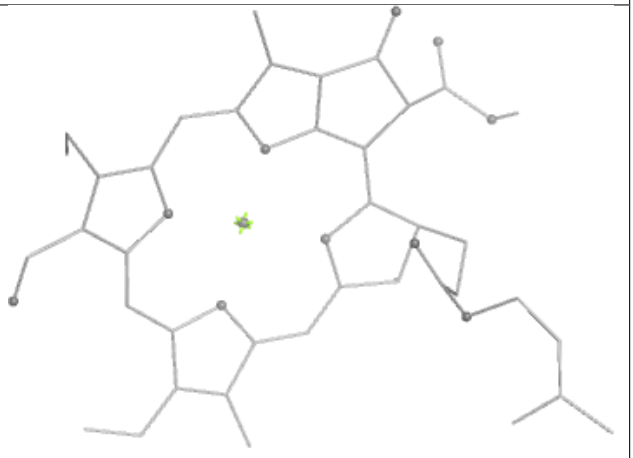
Bond lengths



Bond angles

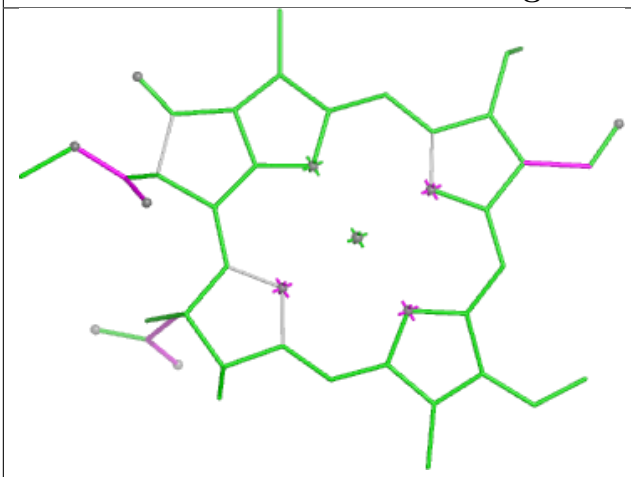


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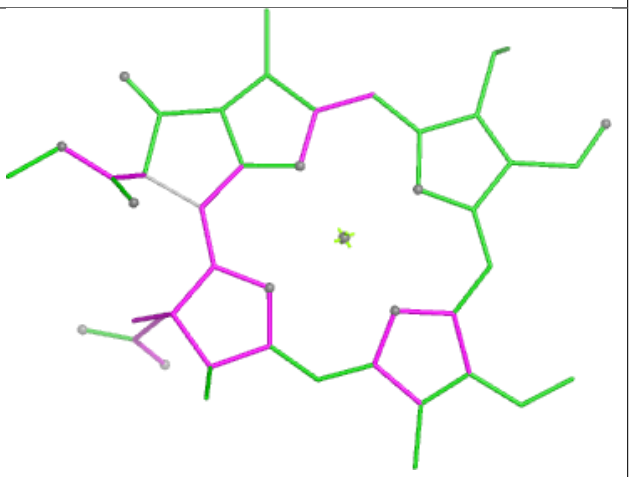


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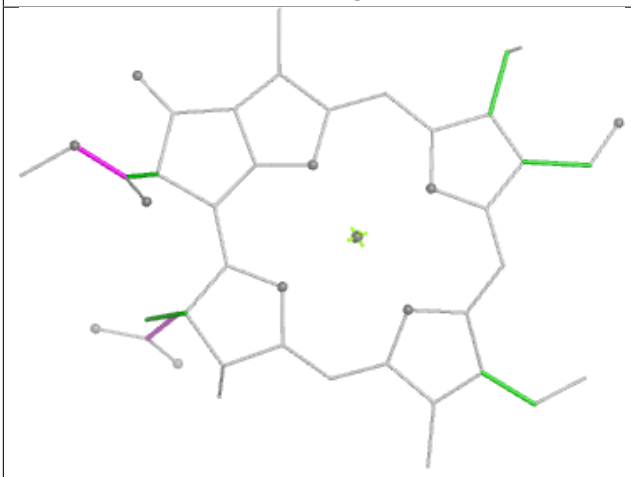
Ligand CHL Y 609



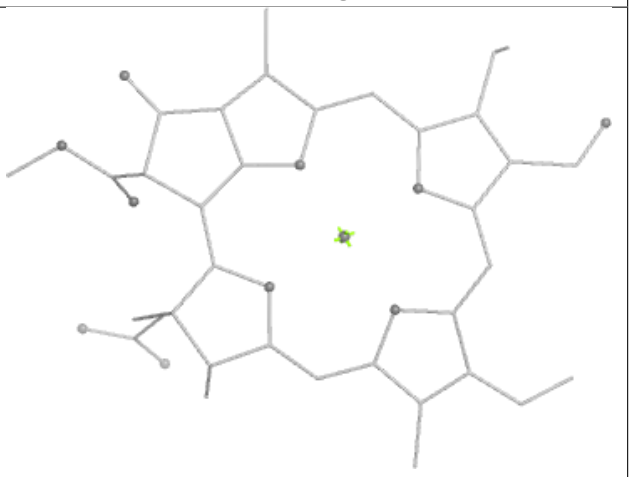
Bond lengths



Bond angles

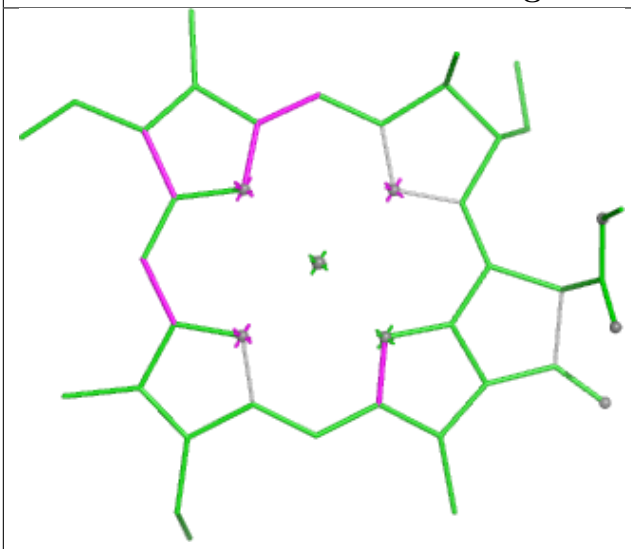


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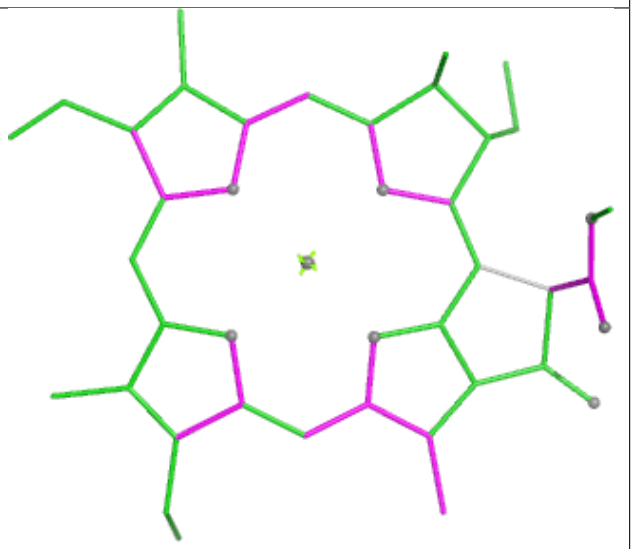


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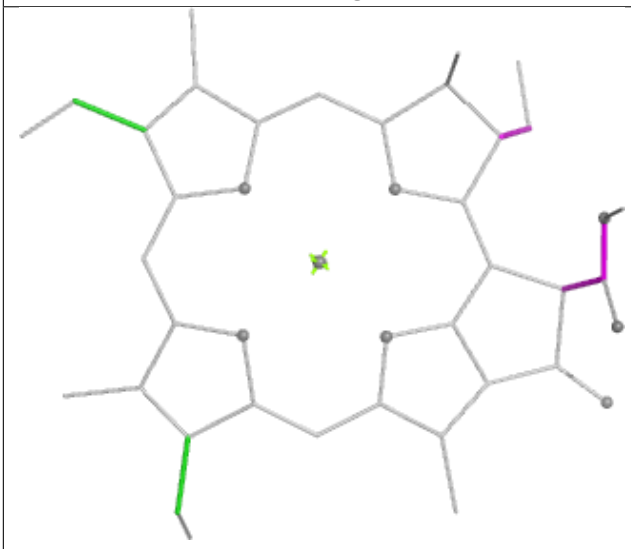
Ligand CLA A 815



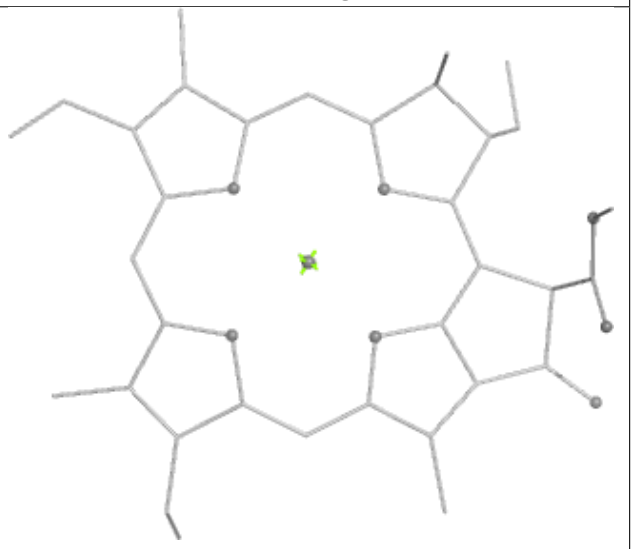
Bond lengths



Bond angles

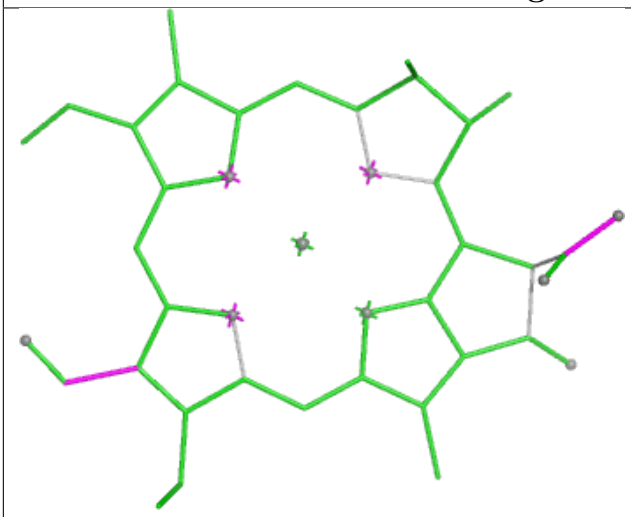


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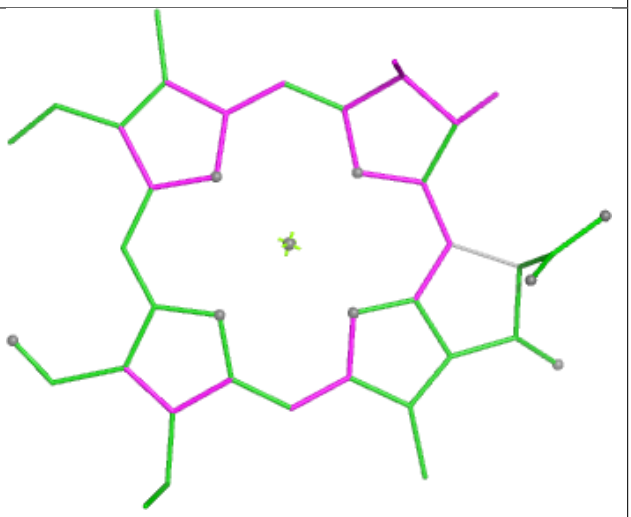


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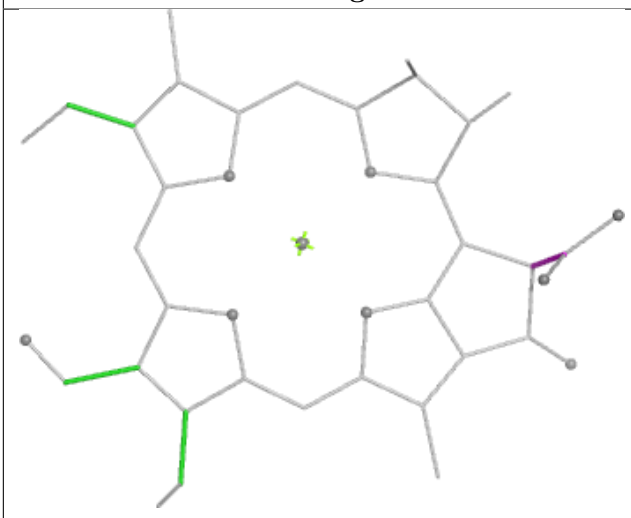
Ligand CHL 5 606



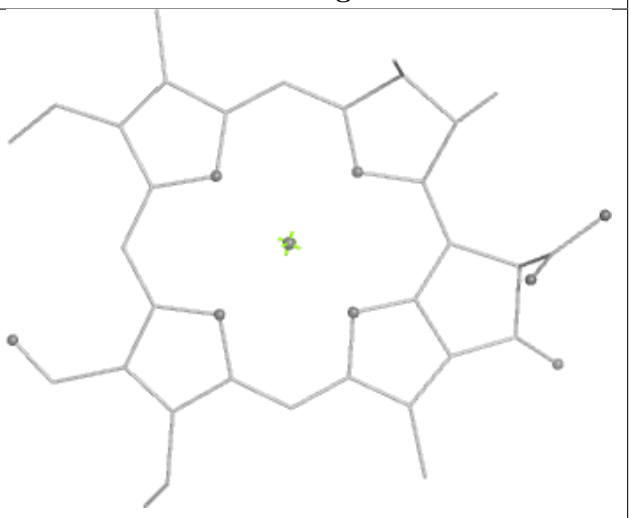
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Bond angles



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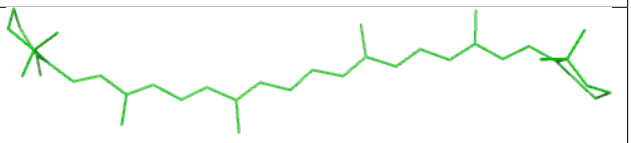


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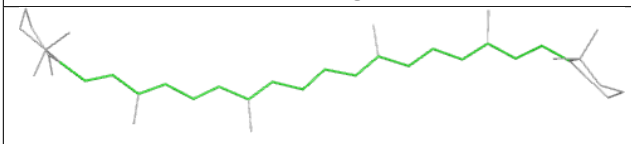
Ligand BCR 1 617



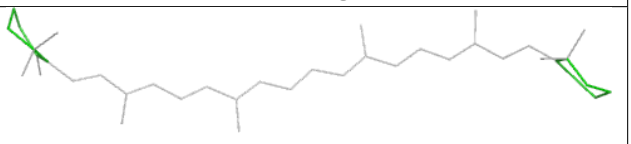
Bond lengths



Bond angles

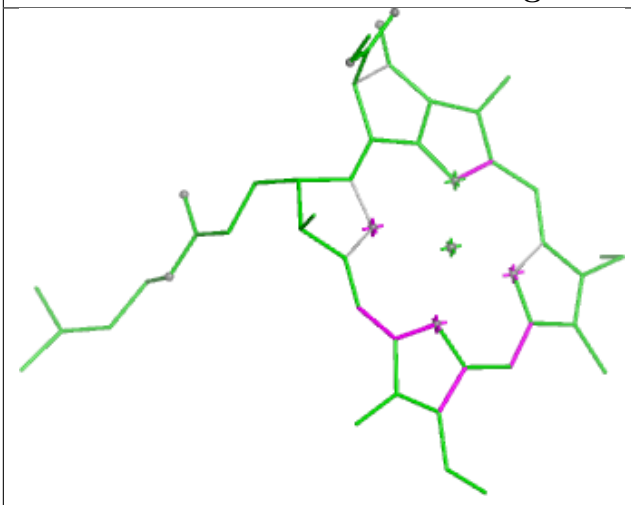


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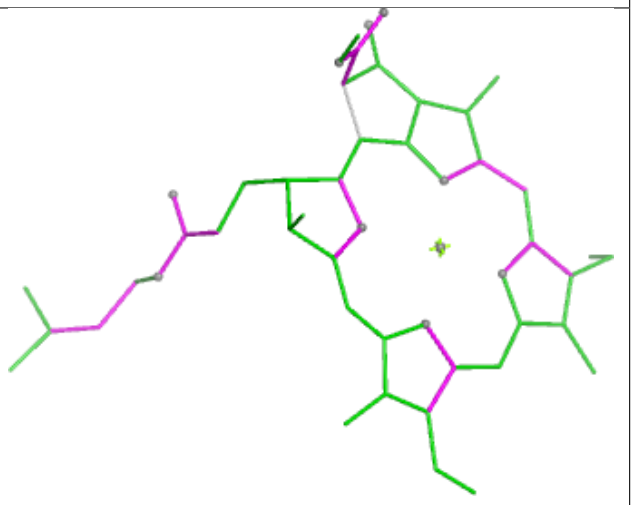


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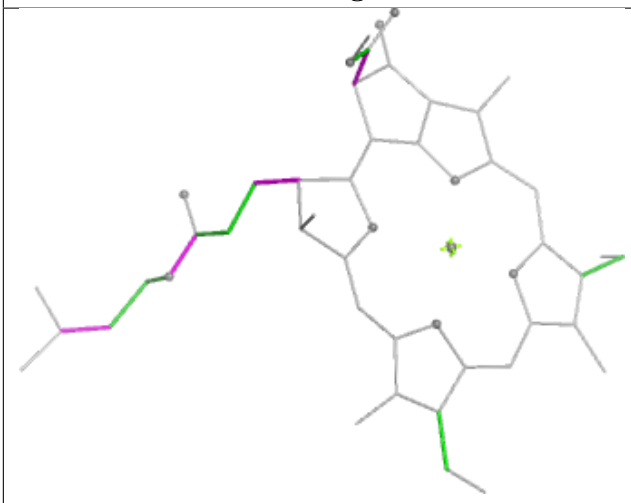
Ligand CLA A 831



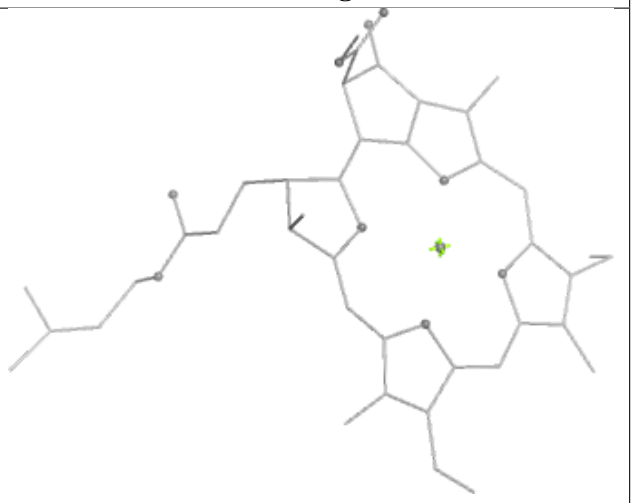
Bond lengths



Bond angles

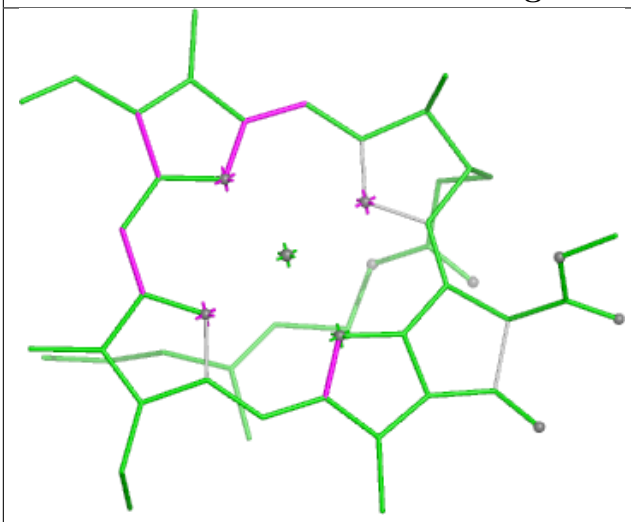


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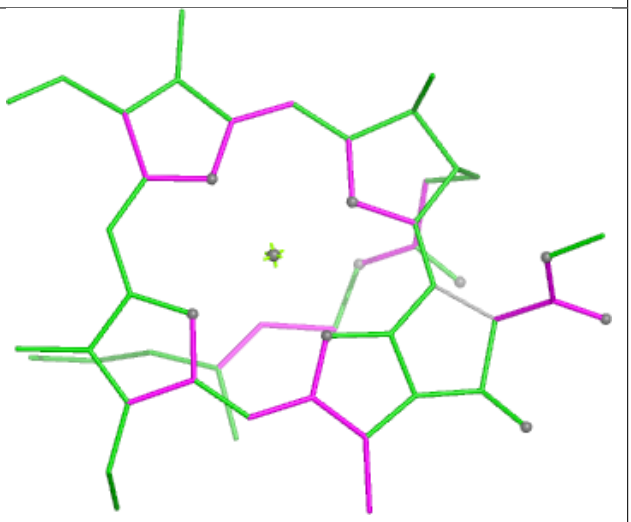


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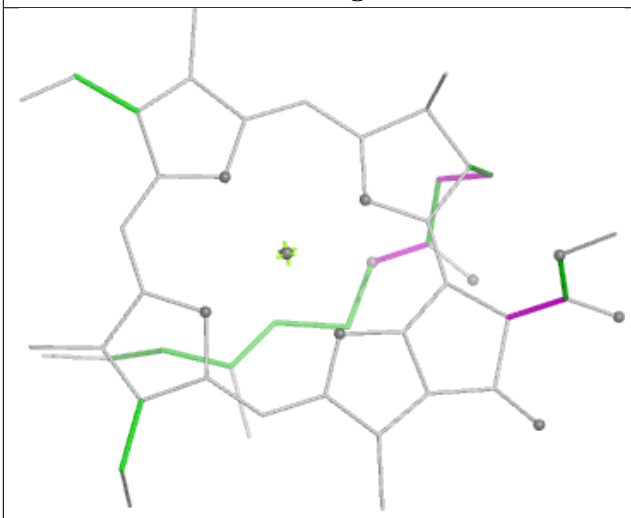
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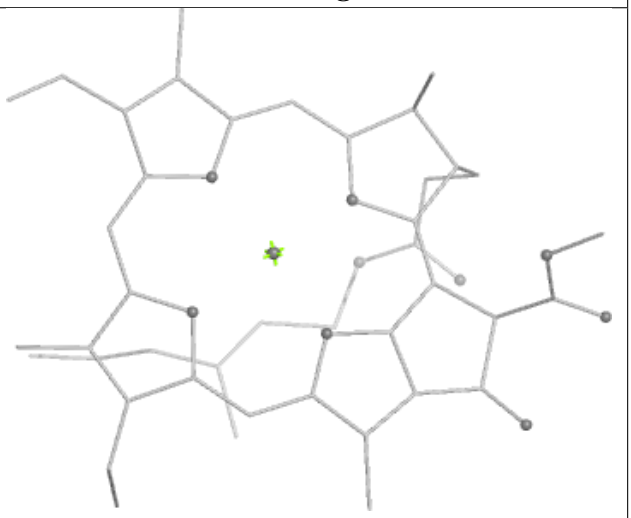
Bond lengths



Bond angles

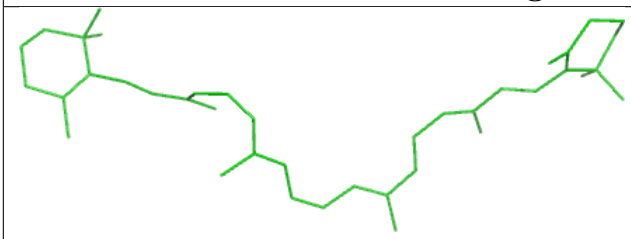


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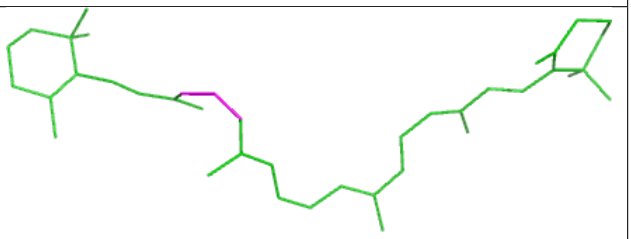


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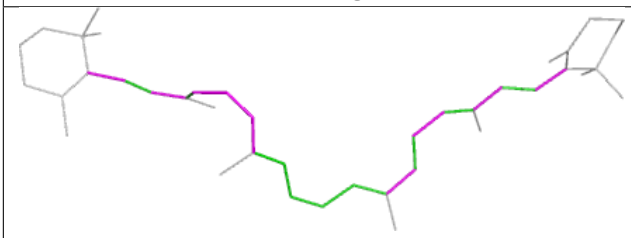
Ligand BCR 2 619



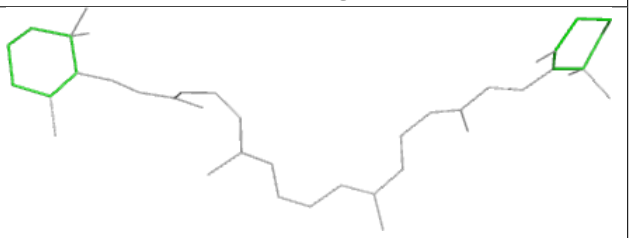
Bond lengths



Bond angles

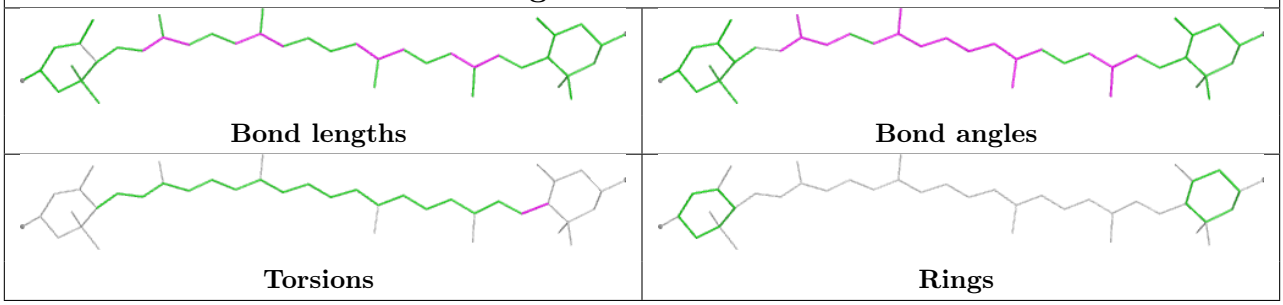


Torsions

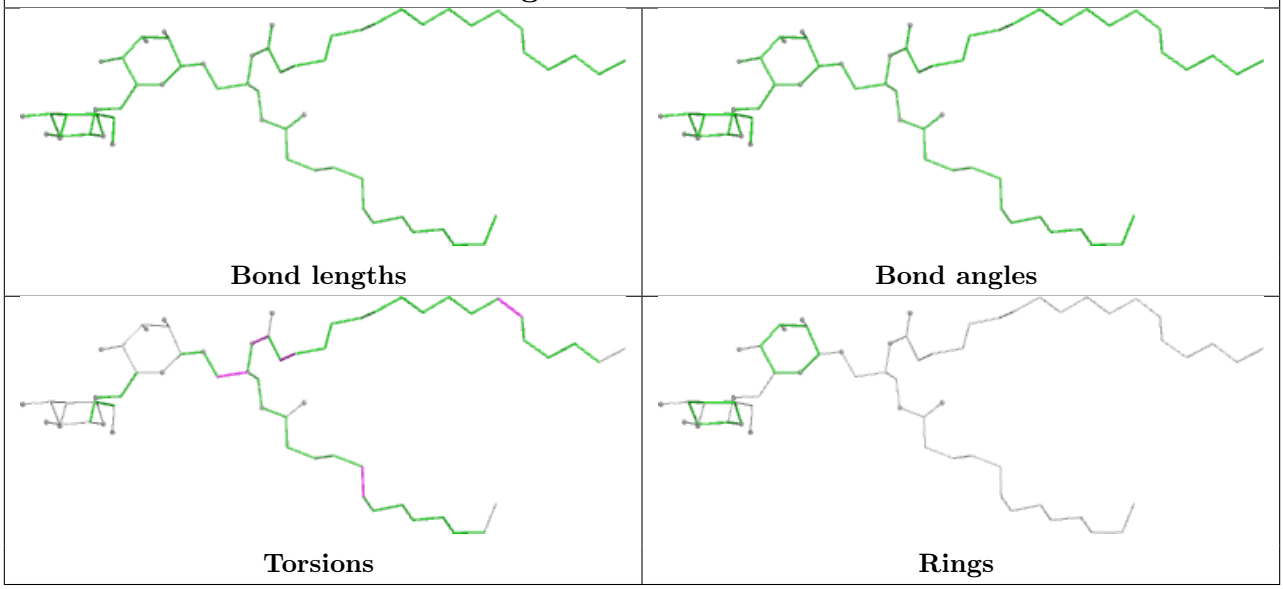


Rings

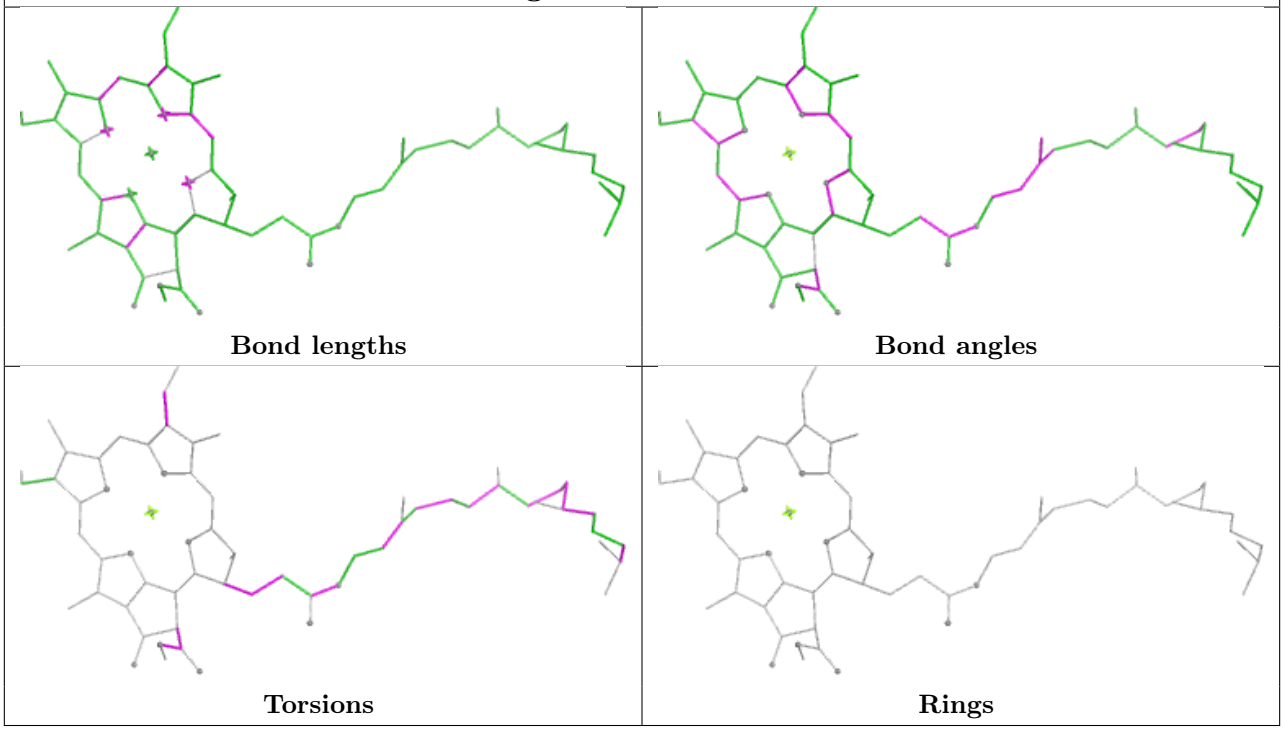
Ligand LUT 5 619



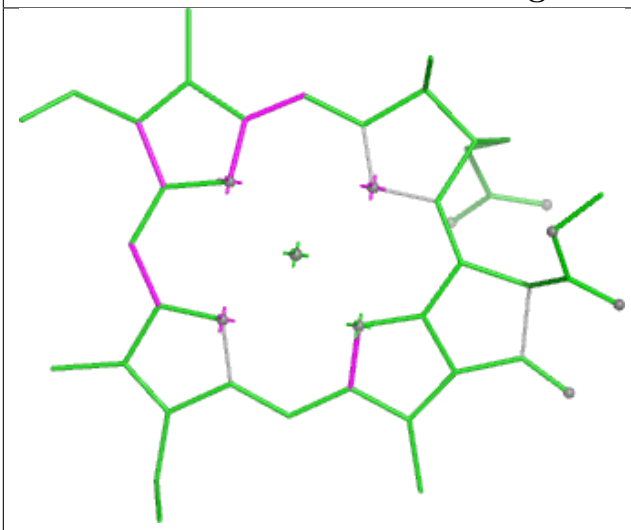
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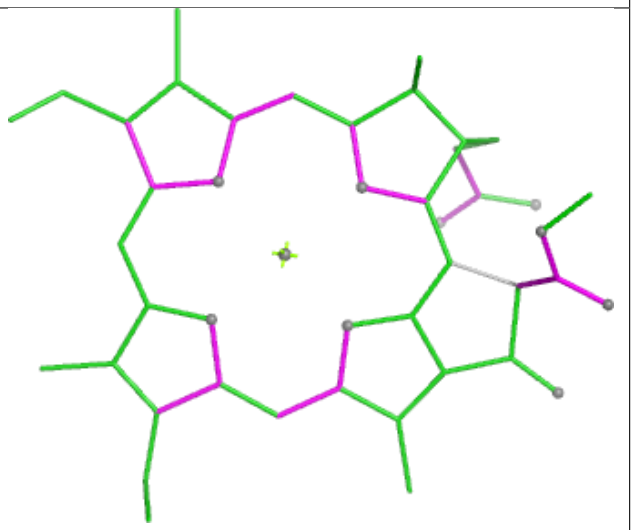
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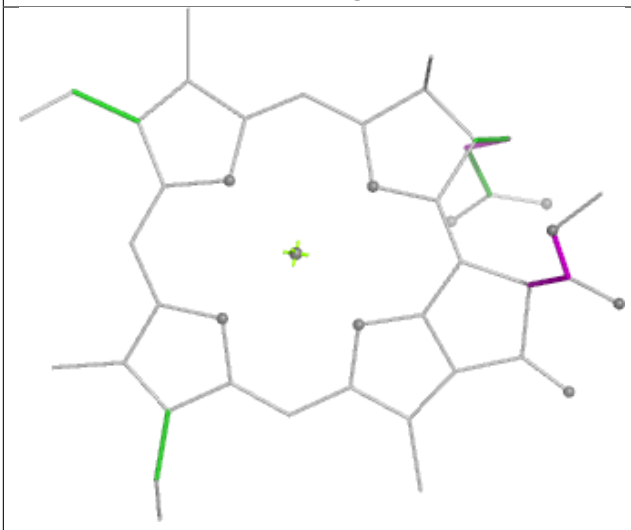
Ligand CLA 6 604



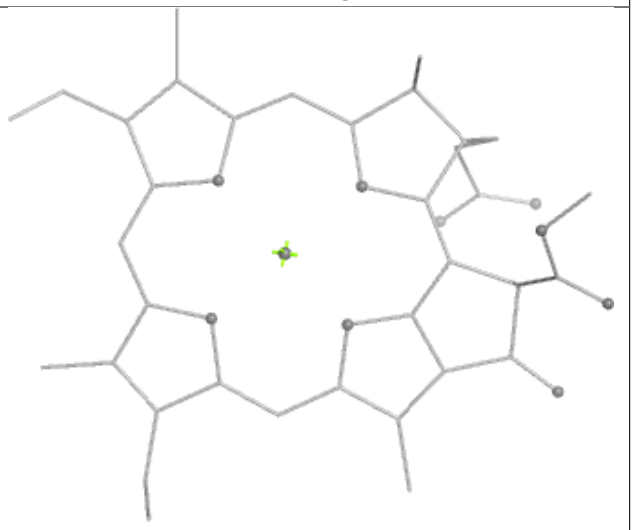
Bond lengths



Bond angles

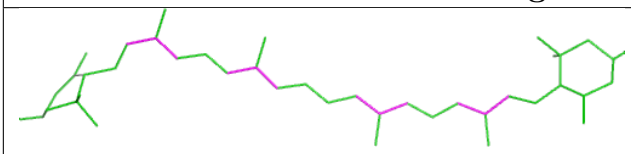


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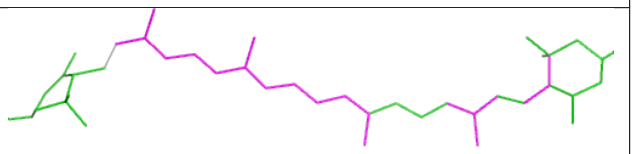


Rings

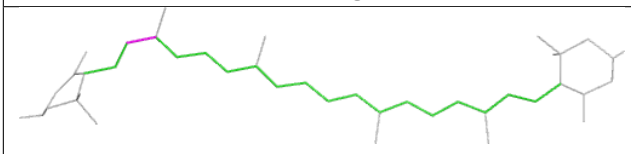
Ligand LUT 3 615



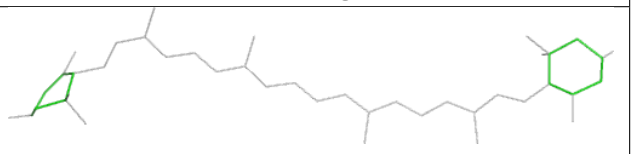
Bond lengths



Bond angles

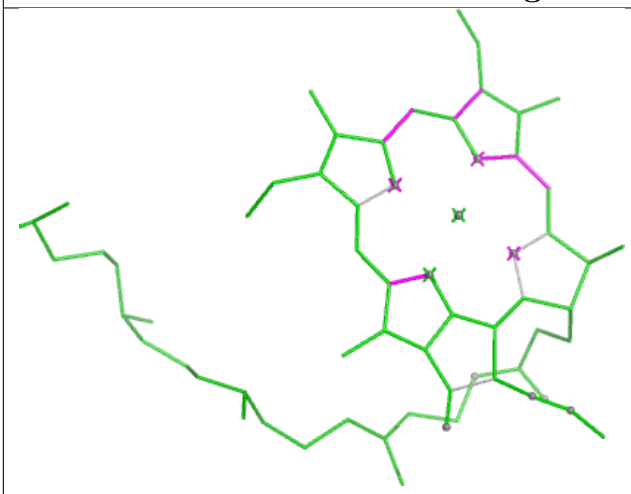


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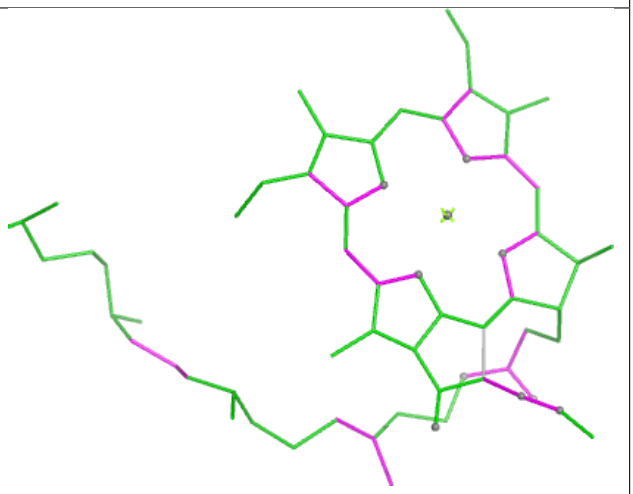


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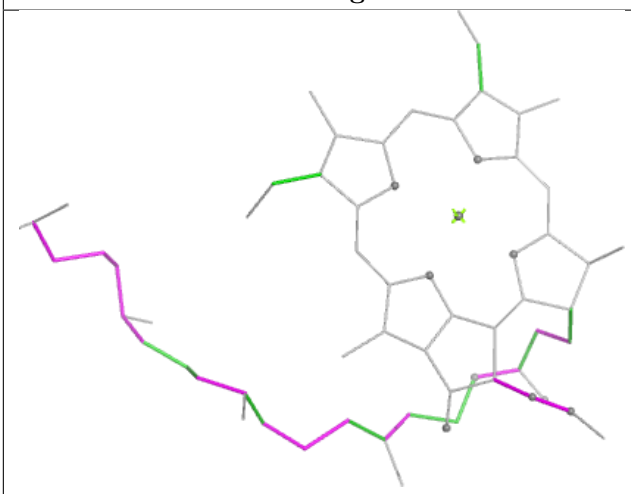
Ligand CLA A 829



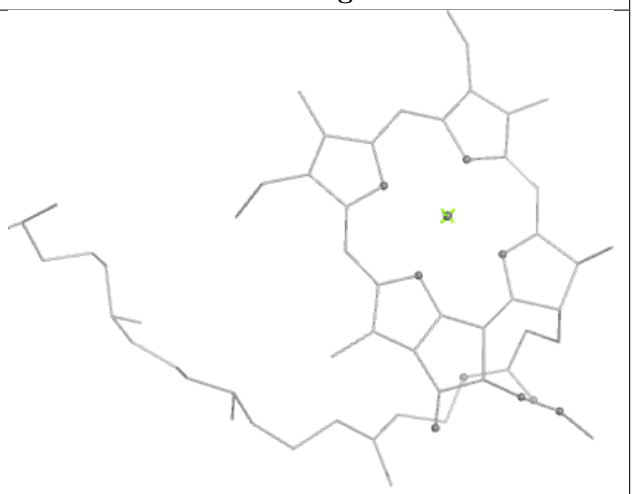
Bond lengths



Bond angles

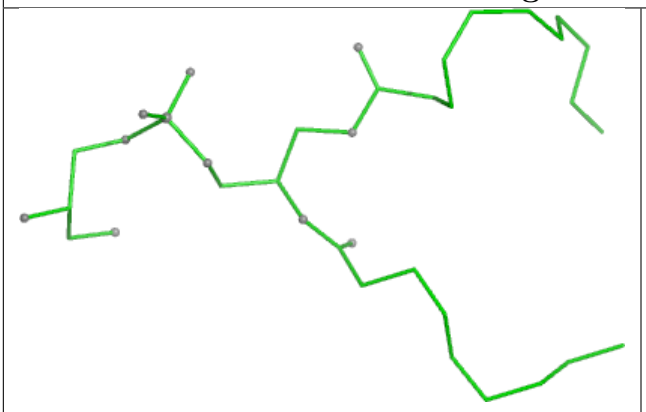


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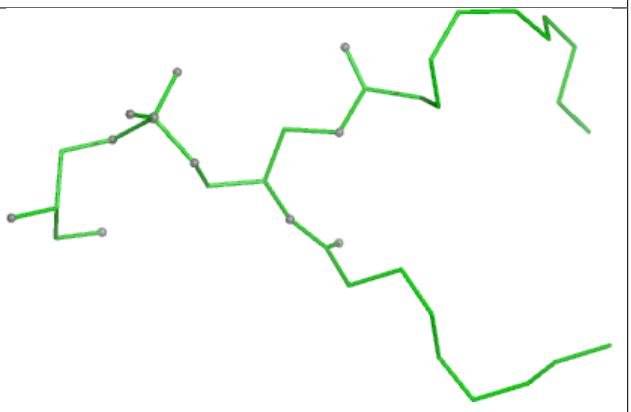


Rings

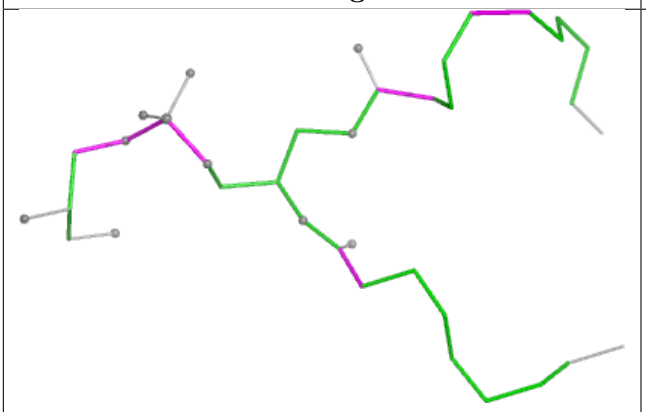
Ligand LHG X 617



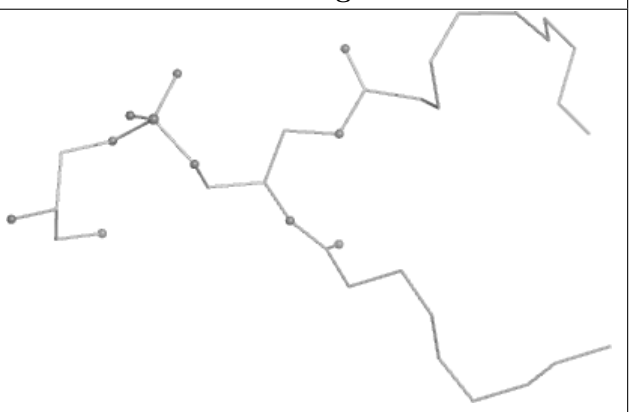
Bond lengths



Bond angles

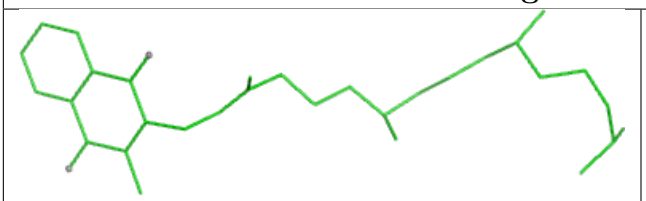


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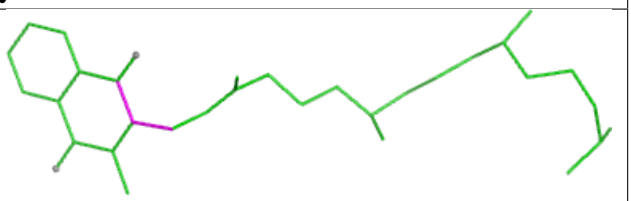


Rings

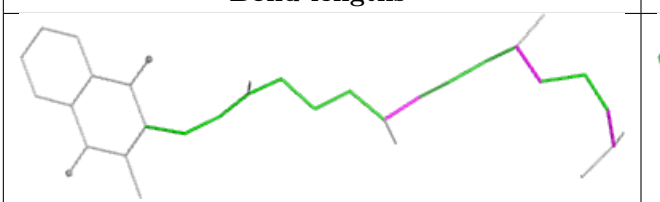
Ligand PQN A 844



Bond lengths



Bond angles

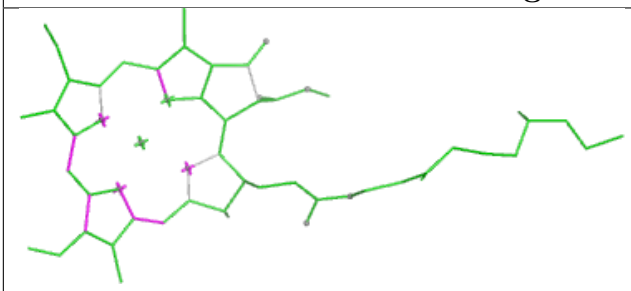


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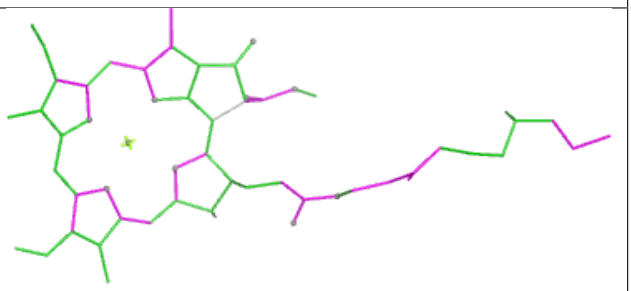


Rings

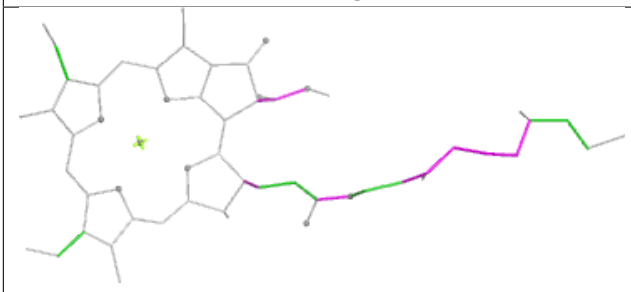
Ligand CLA A 843



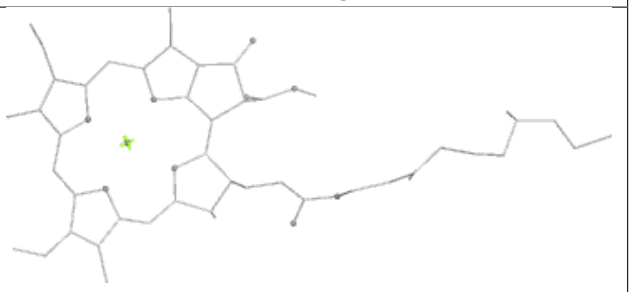
Bond lengths



Bond angles

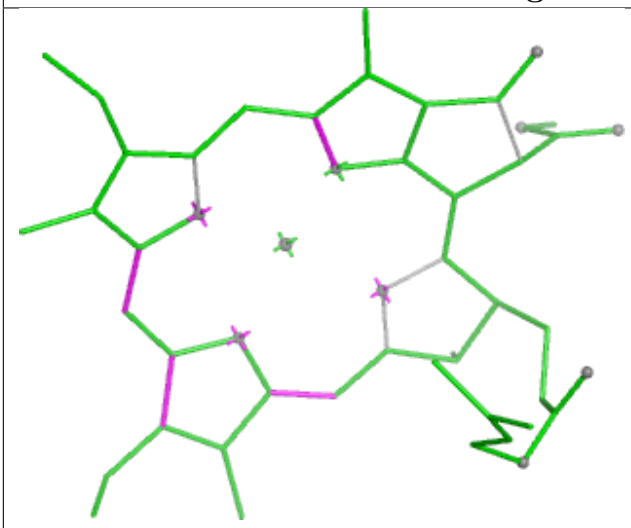


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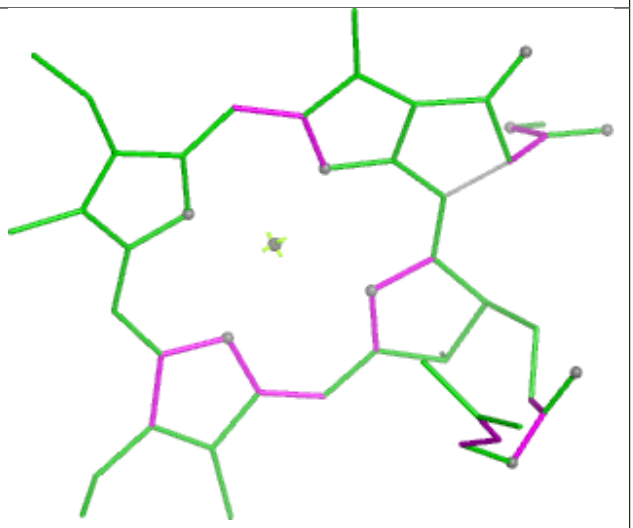


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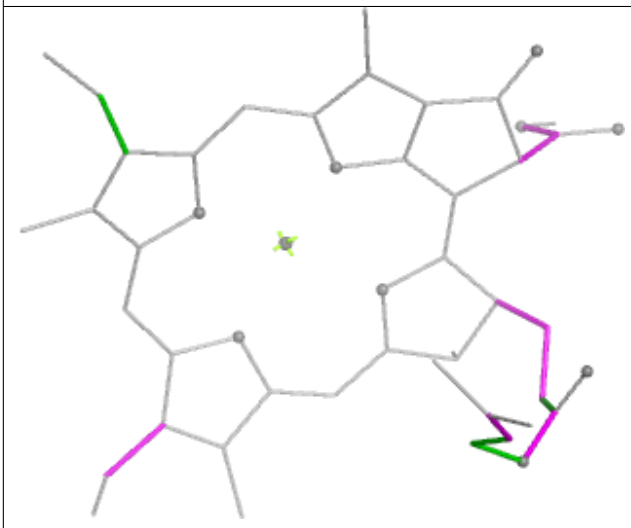
Ligand CLA Z 305



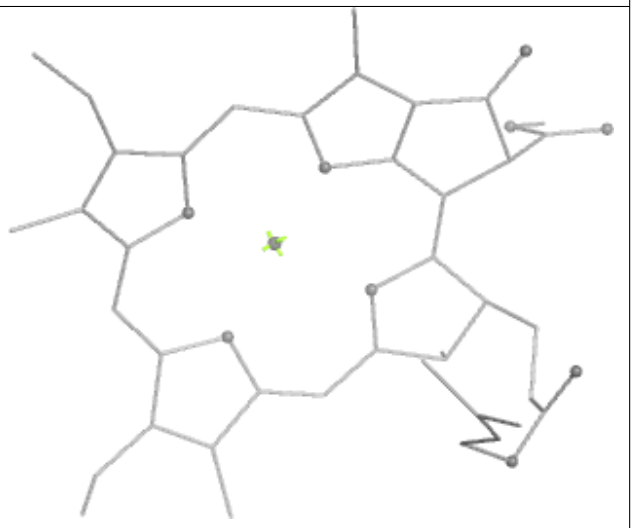
Bond lengths



Bond angles

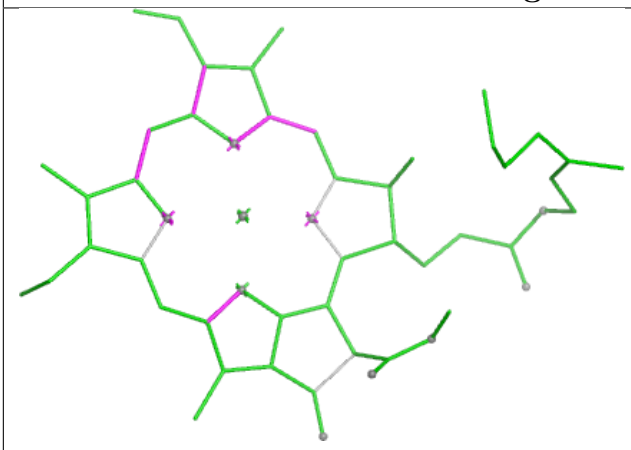


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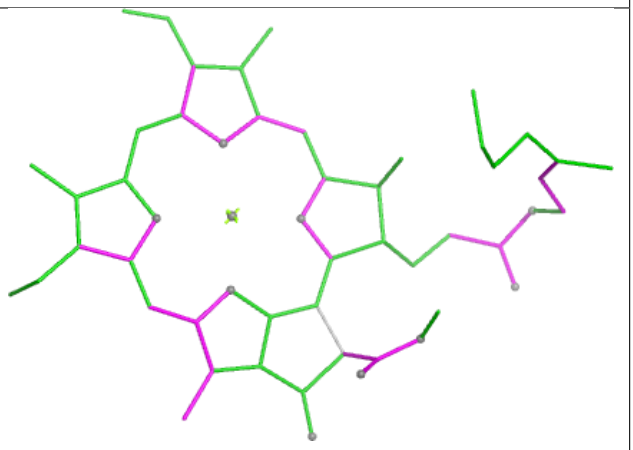


Rings

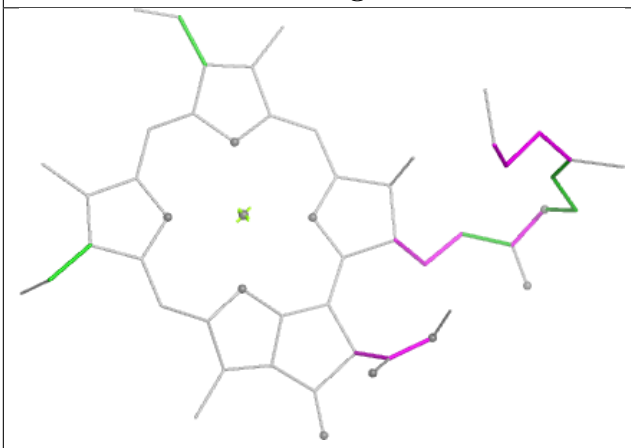
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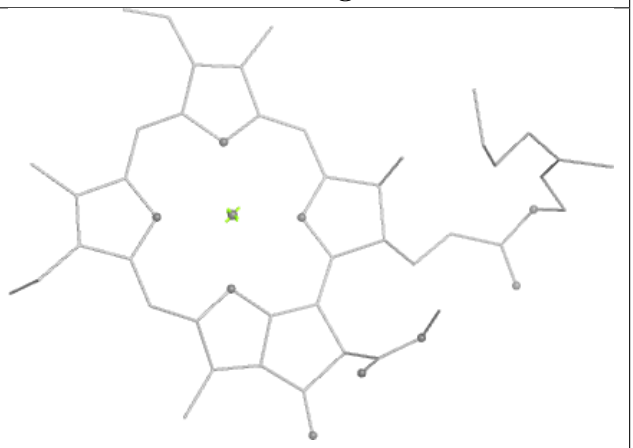
Bond lengths



Bond angles

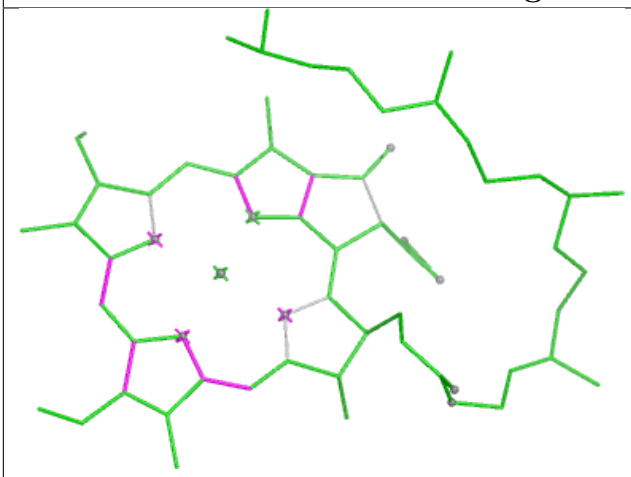


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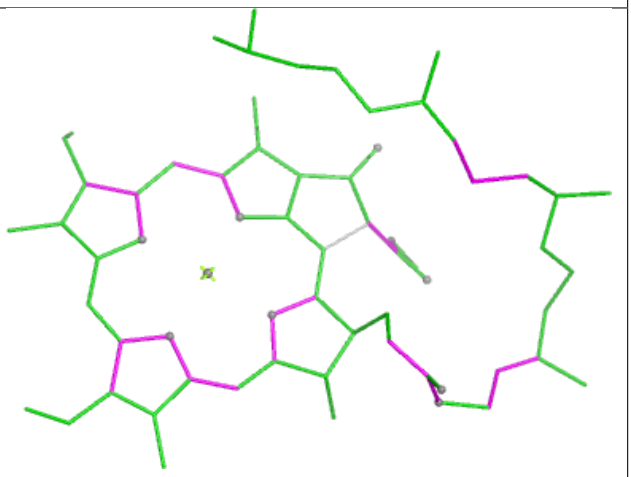


Rings

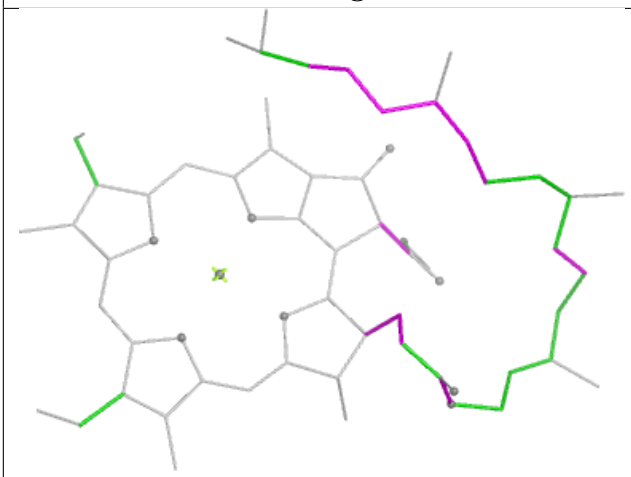
Ligand CLA B 804



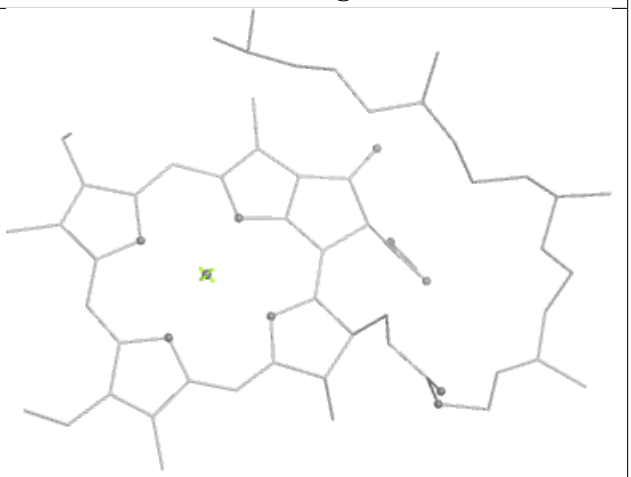
Bond lengths



Bond angles

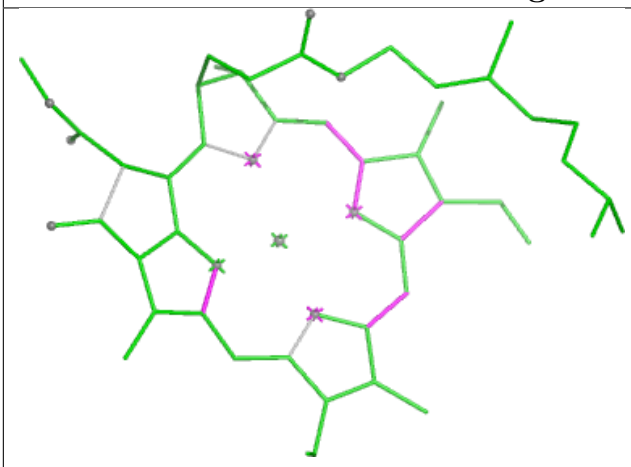


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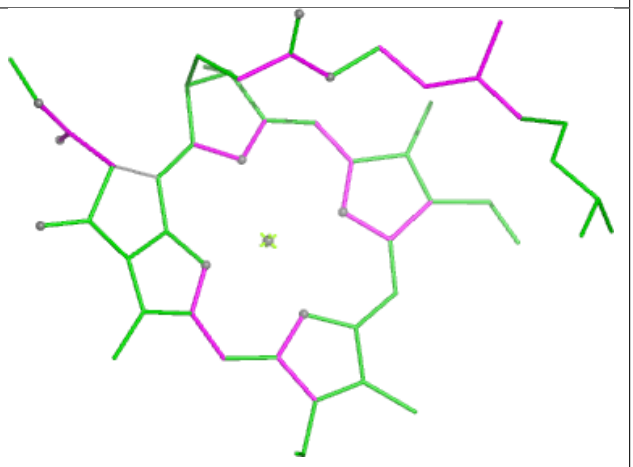


Rings

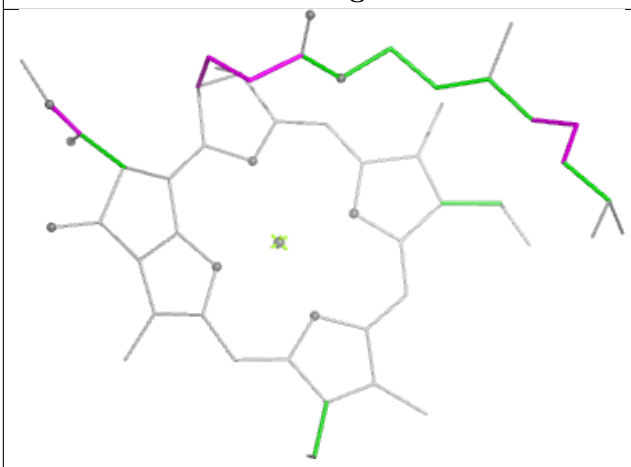
Ligand CLA 2 609



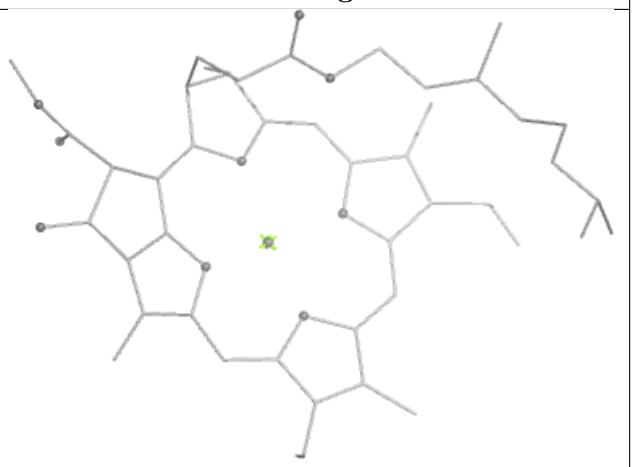
Bond lengths



Bond angles

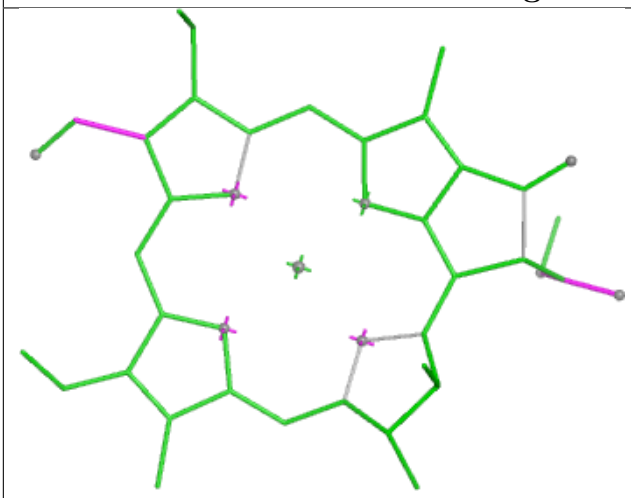


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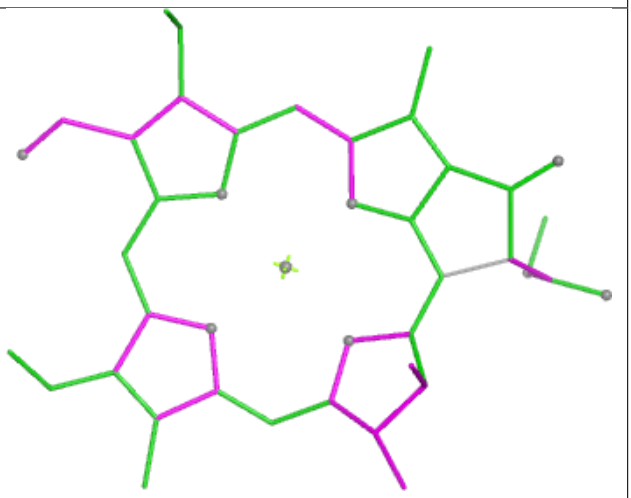


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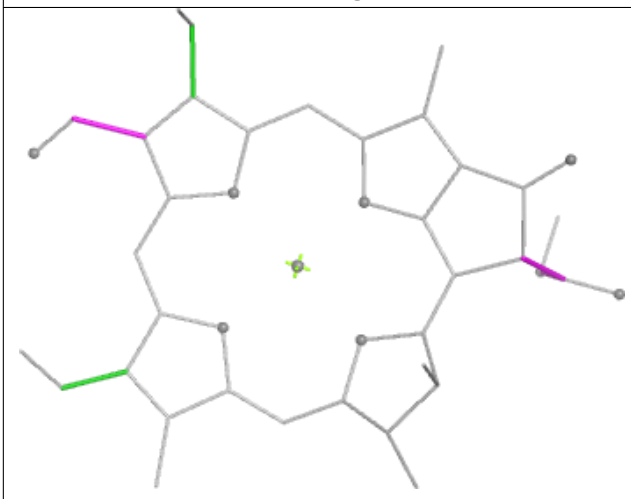
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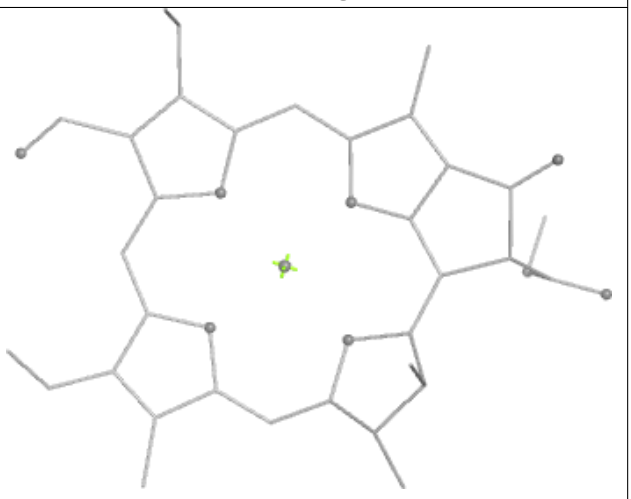
Bond lengths



Bond angles

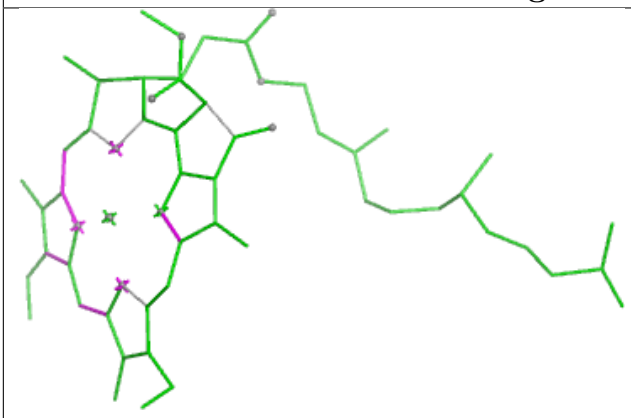


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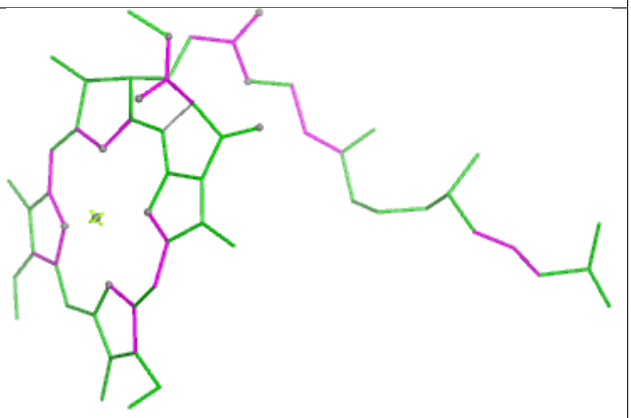


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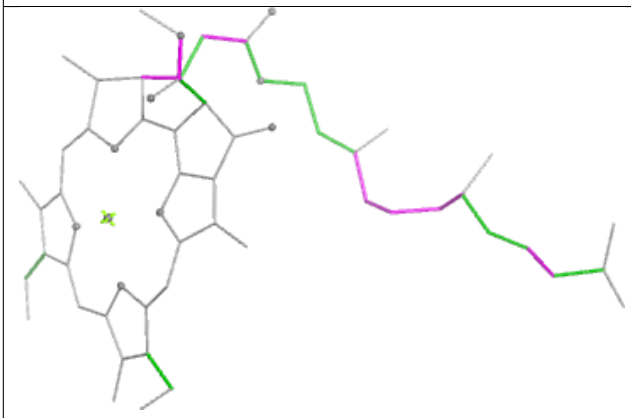
Ligand CLA 4 309



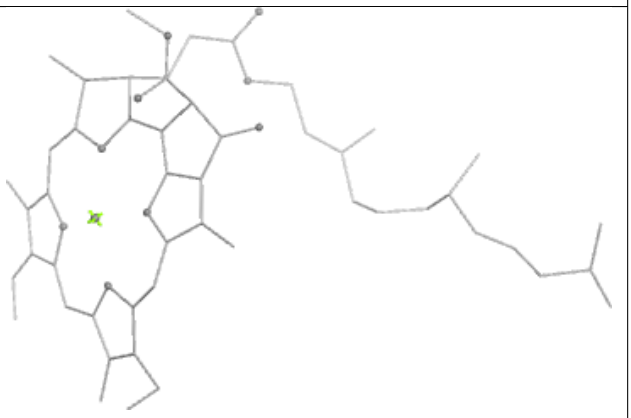
Bond lengths



Bond angles

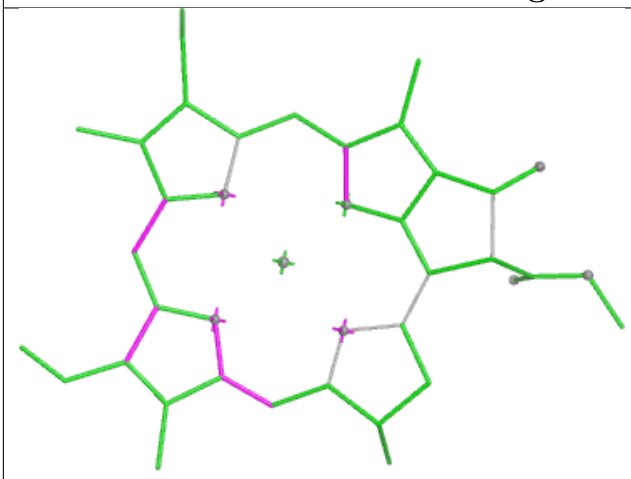


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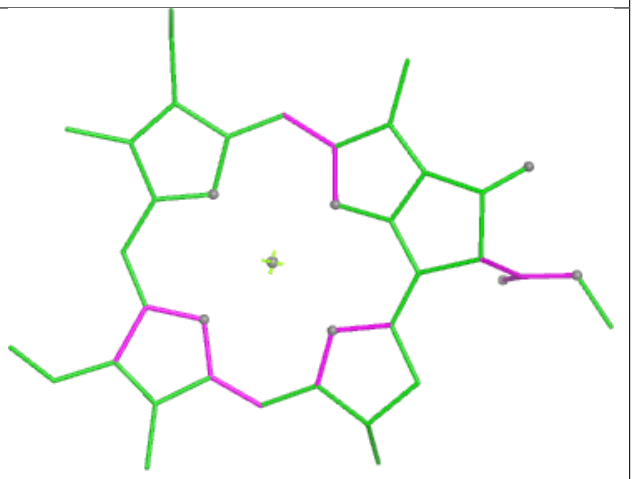


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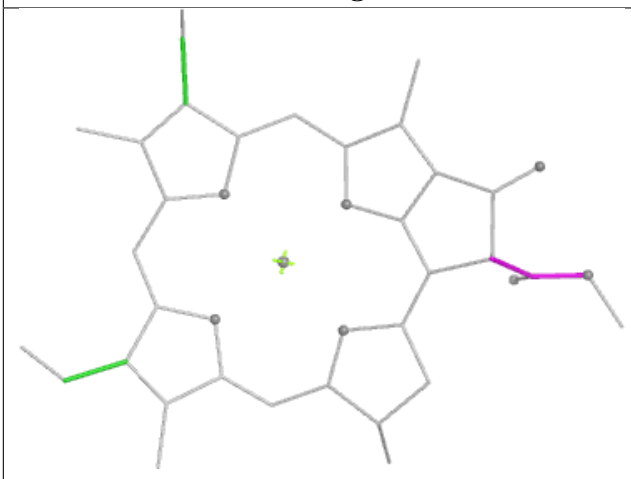
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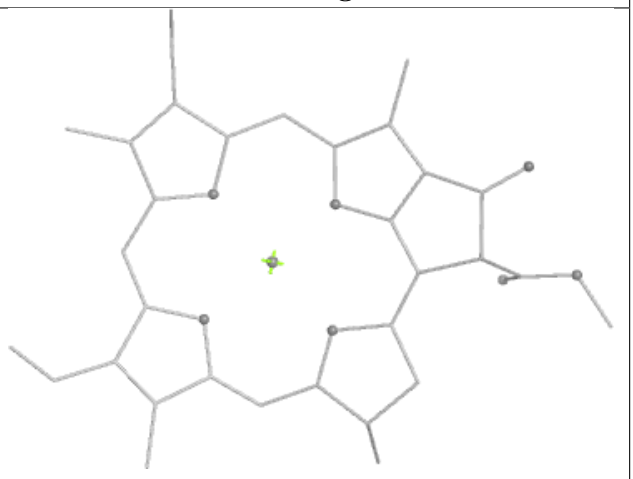
Bond lengths



Bond angles

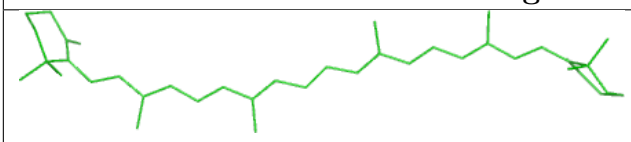


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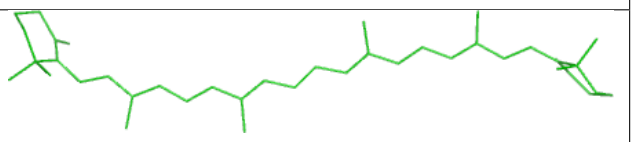


Rings

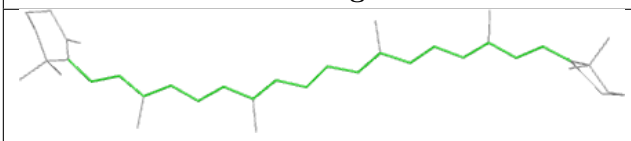
Ligand BCR B 845



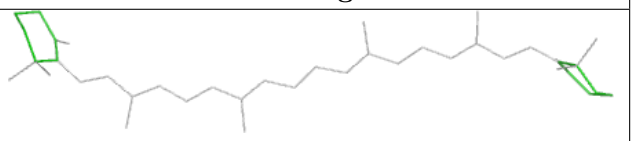
Bond lengths



Bond angles

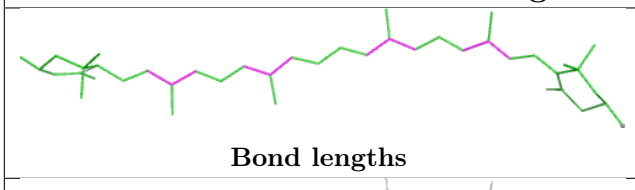


Torsions

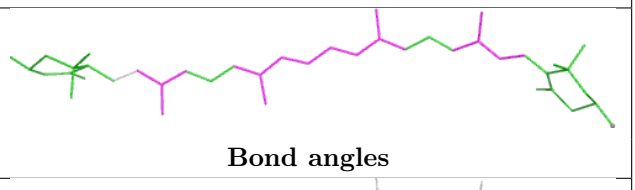


Rings

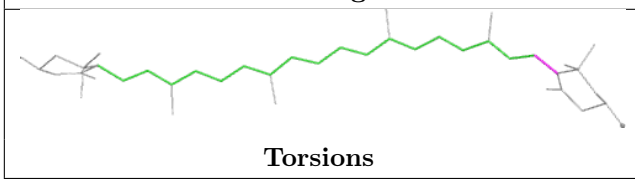
Ligand LUT 6 616



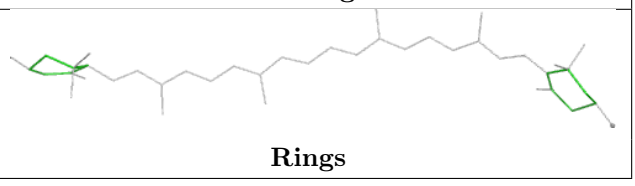
Bond lengths



Bond angles

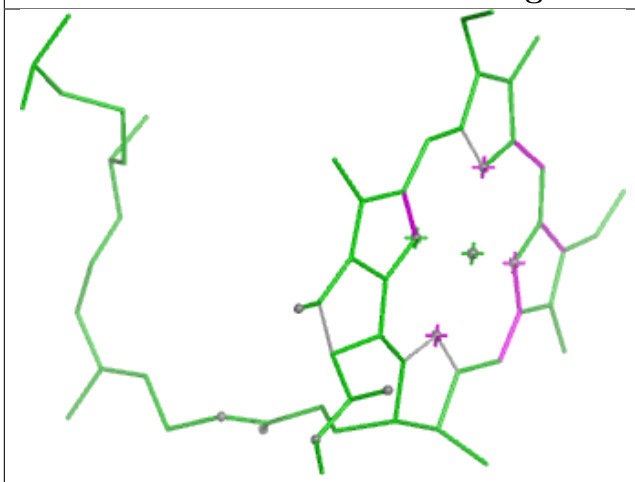


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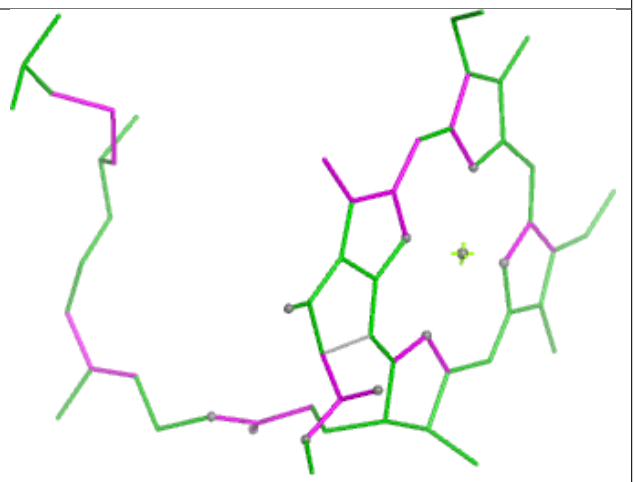


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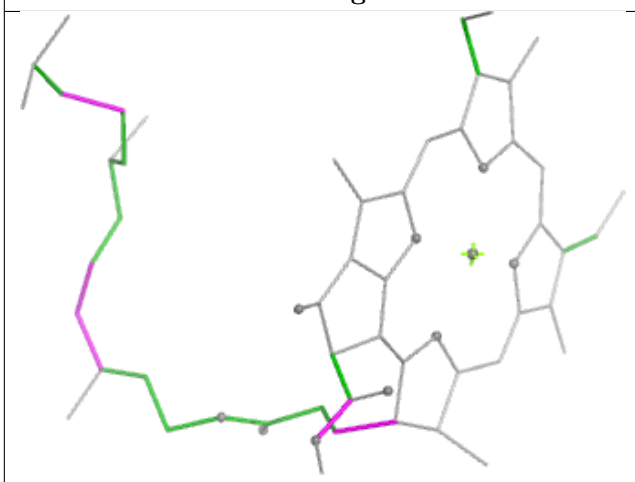
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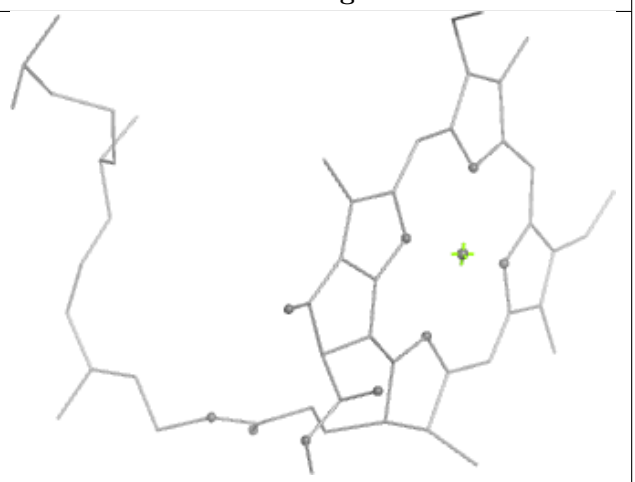
Bond lengths



Bond angles

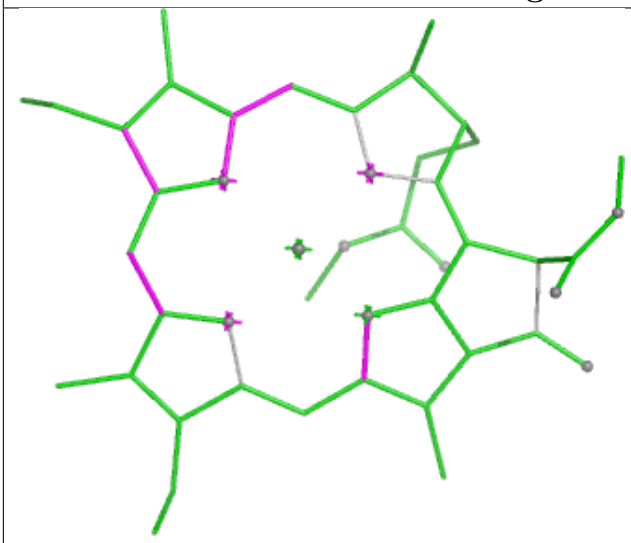


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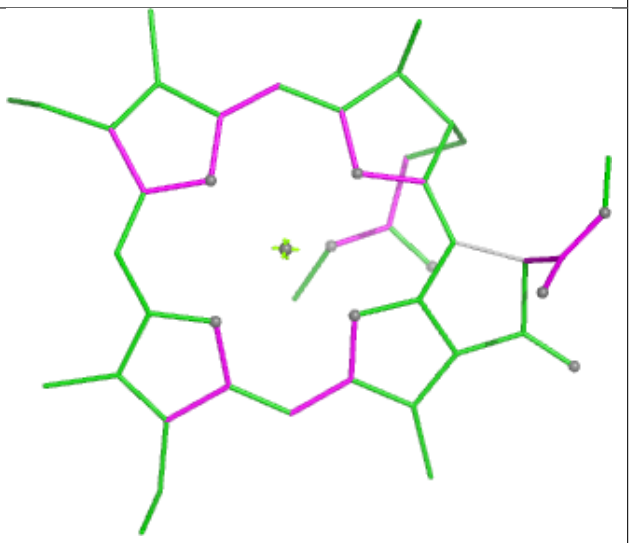


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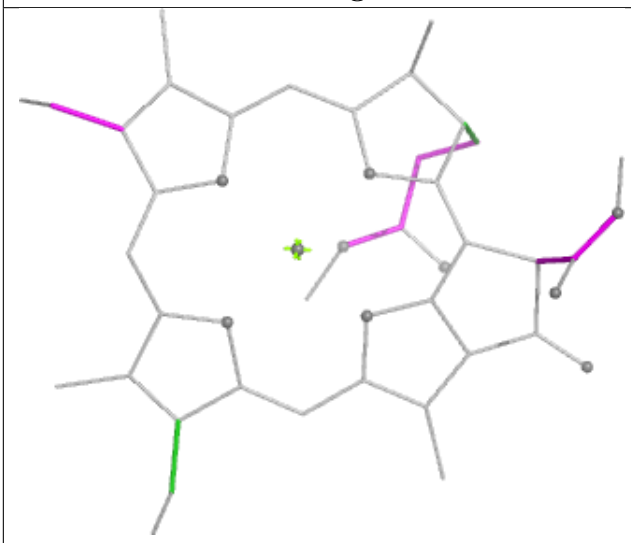
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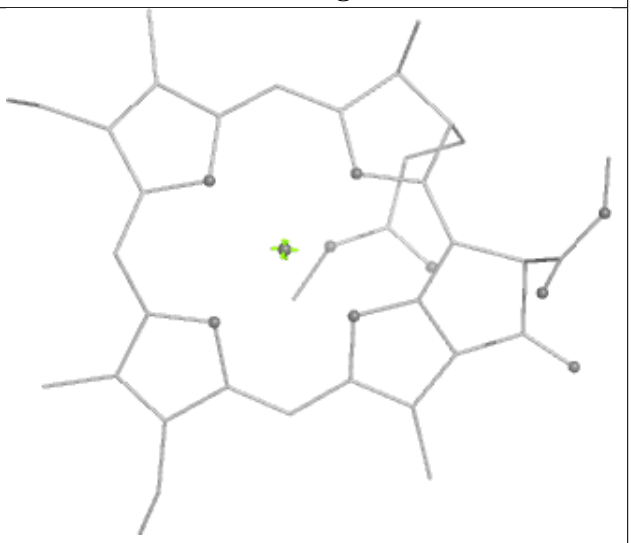
Bond lengths



Bond angles

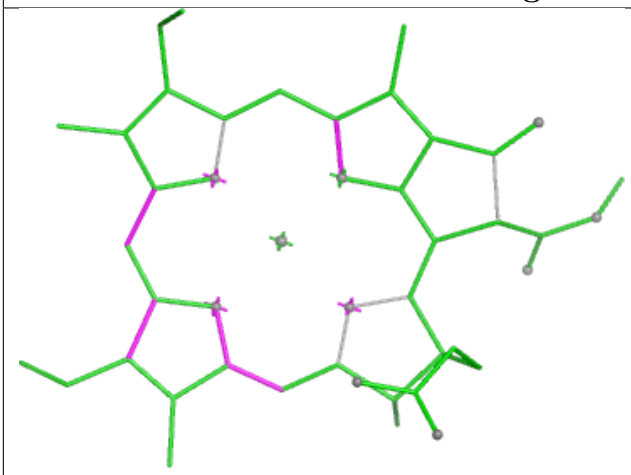


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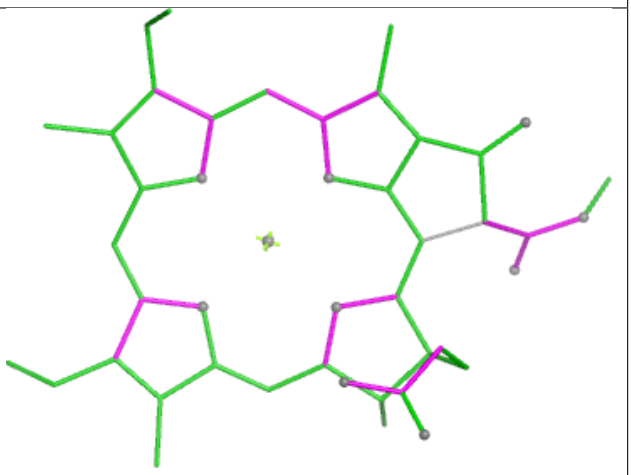


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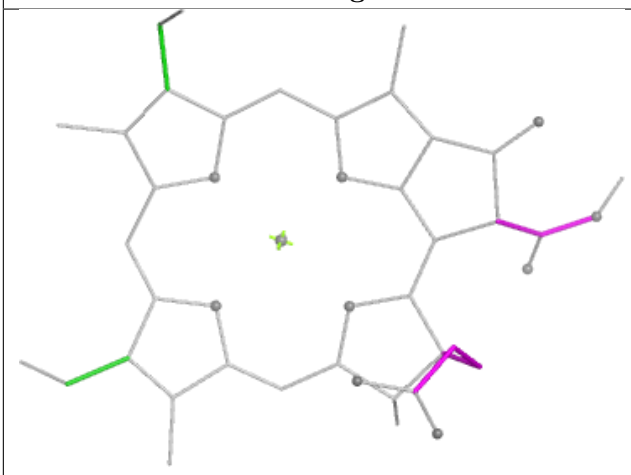
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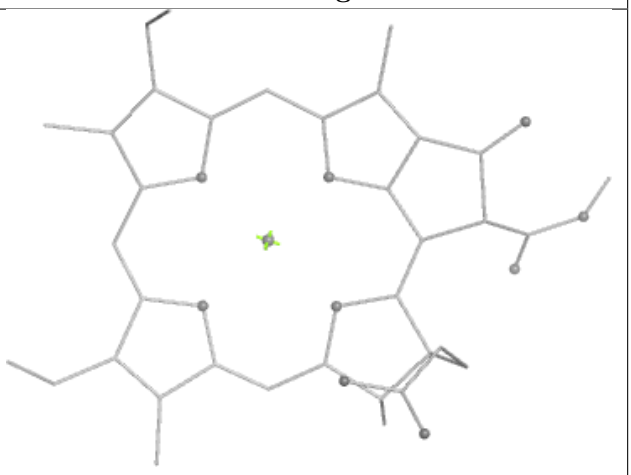
Bond lengths



Bond angles



Torsions

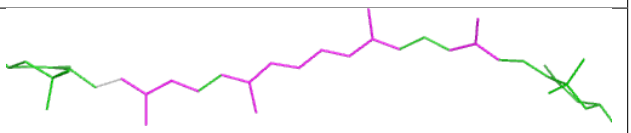


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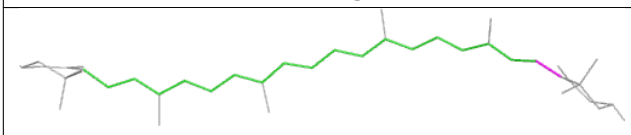
Ligand LUT 1 615



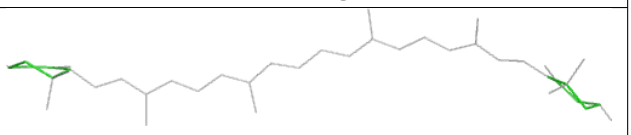
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Bond angles

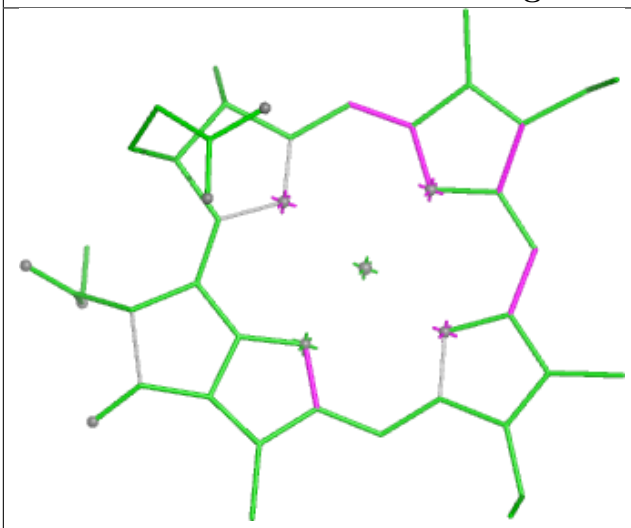


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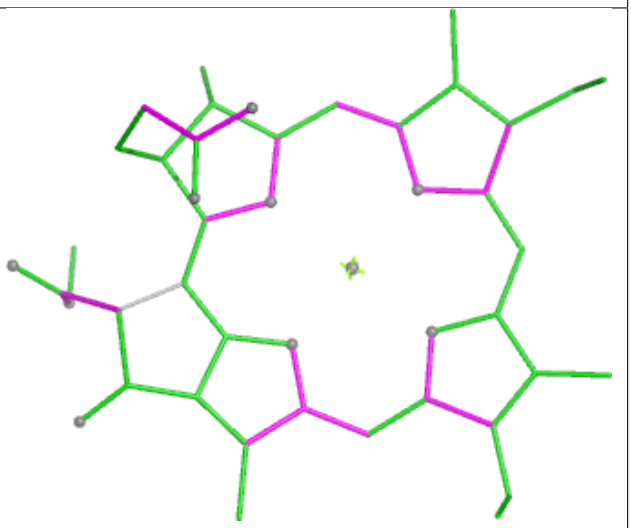


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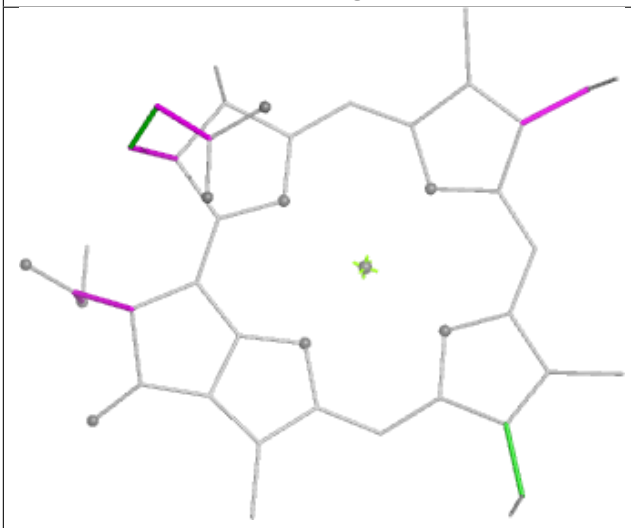
Ligand CLA X 602



Bond lengths



Bond angles



Torsions

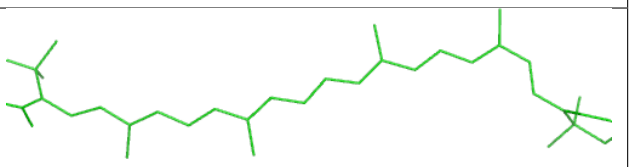


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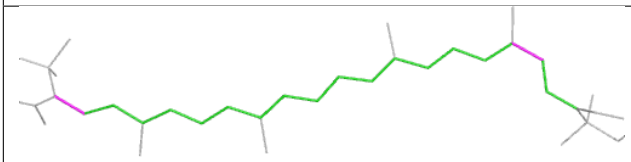
Ligand BCR L 302



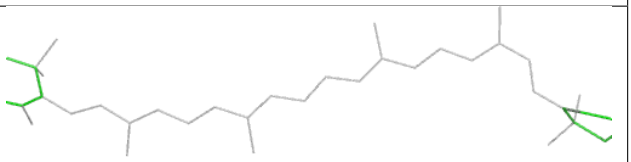
Bond lengths



Bond angles

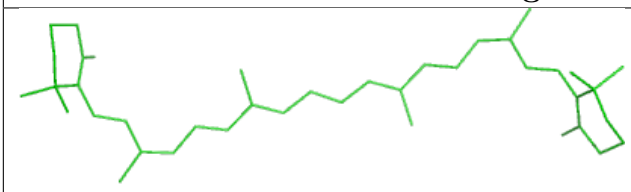


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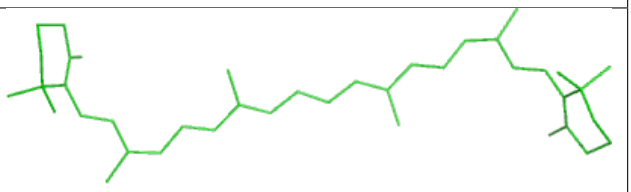


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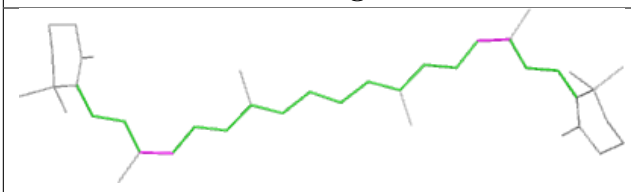
Ligand BCR B 844



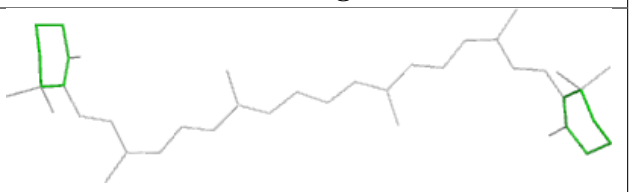
Bond lengths



Bond angles

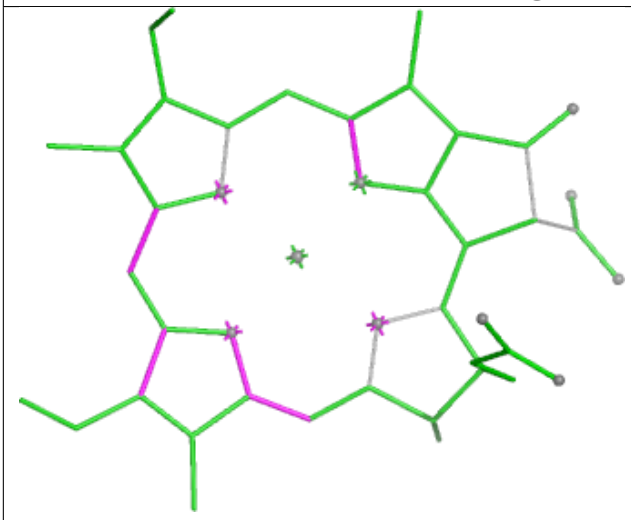


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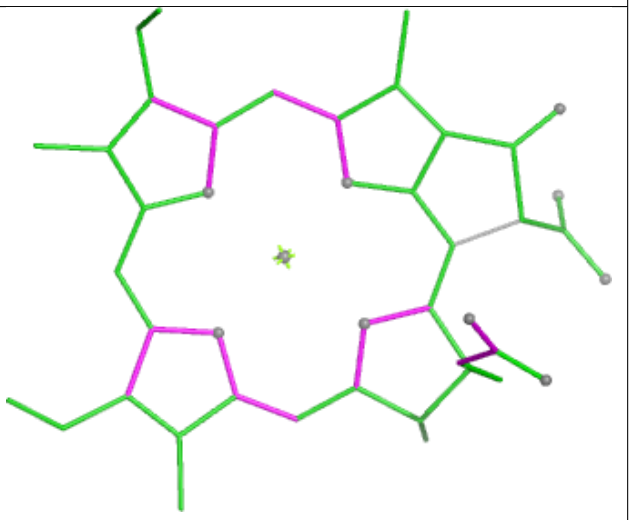


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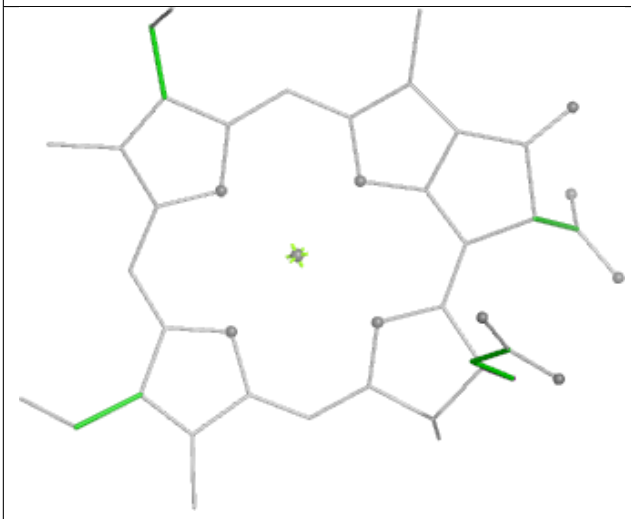
Ligand CLA 1 607



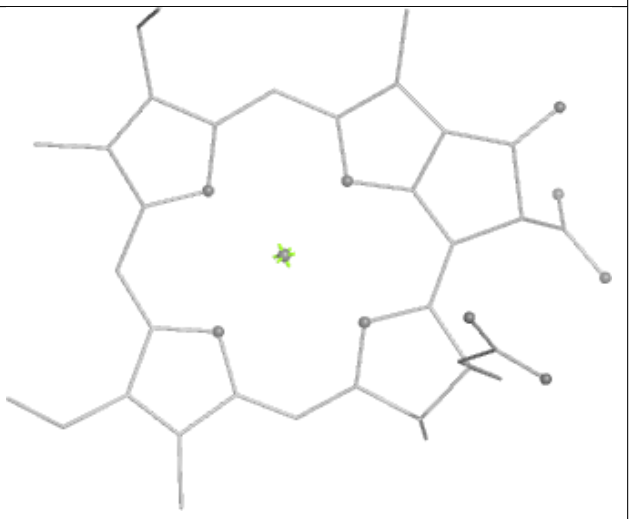
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Bond angles

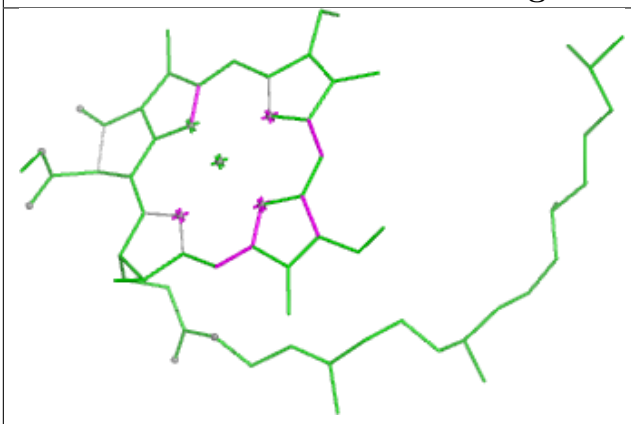


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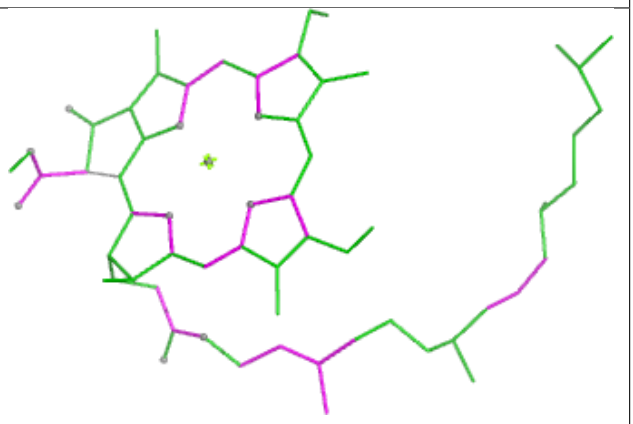


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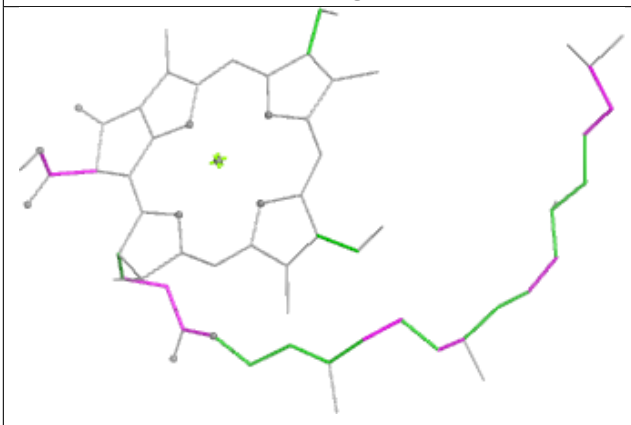
Ligand CLA 2 602



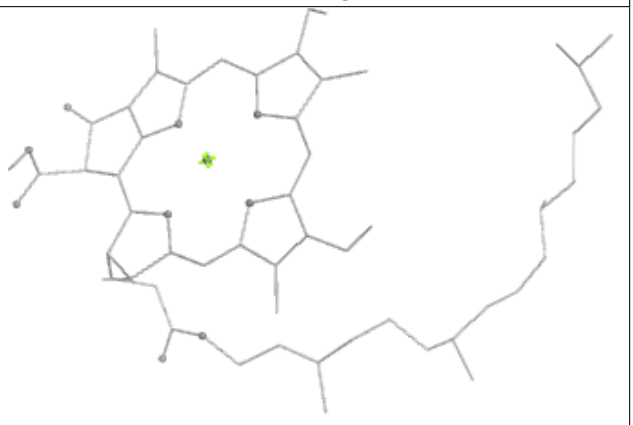
Bond lengths



Bond angles

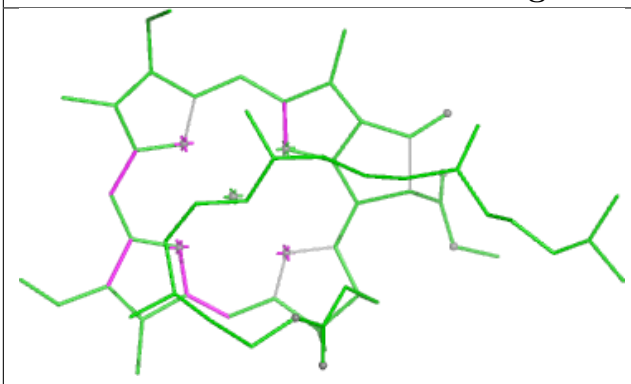


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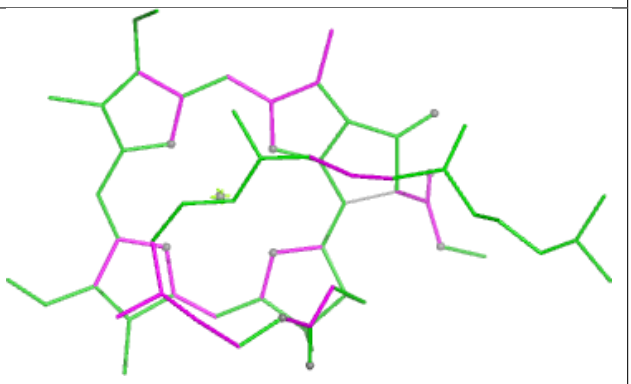


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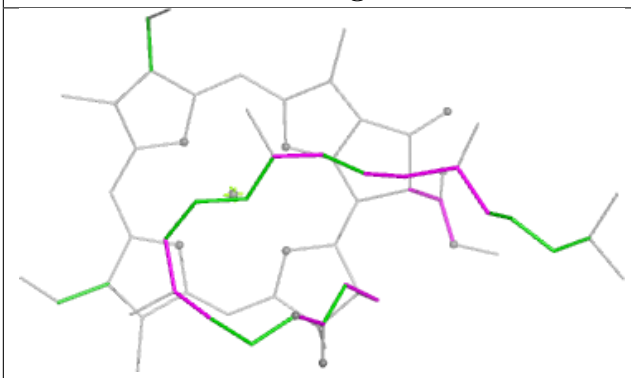
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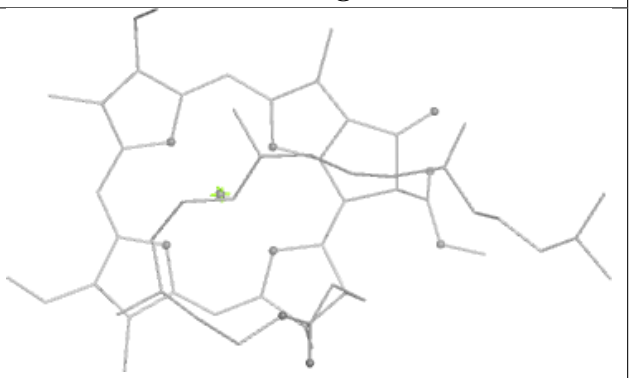
Bond lengths



Bond angles

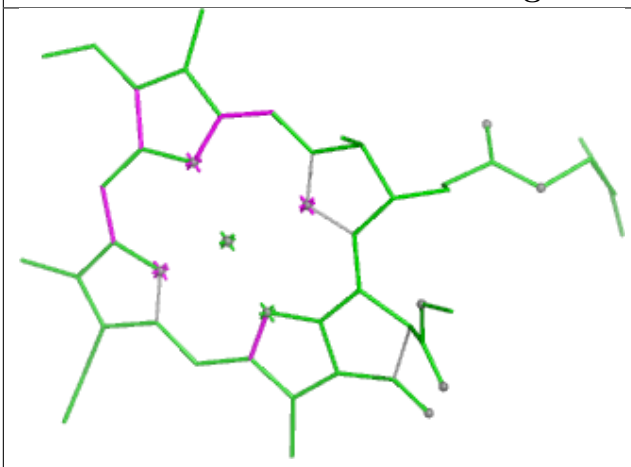


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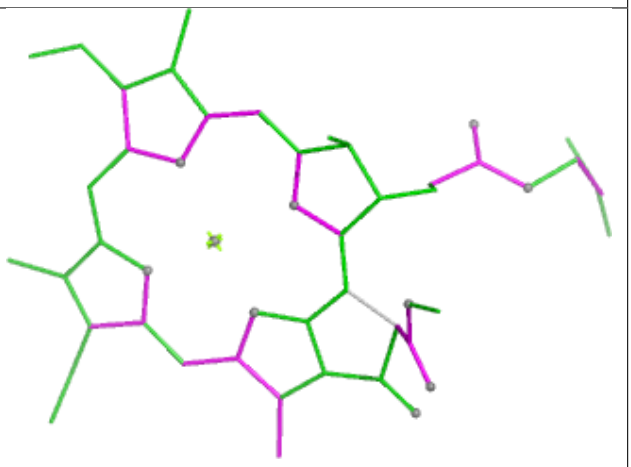


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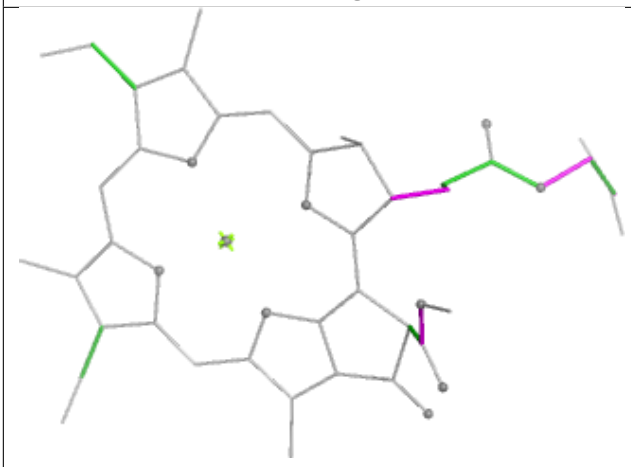
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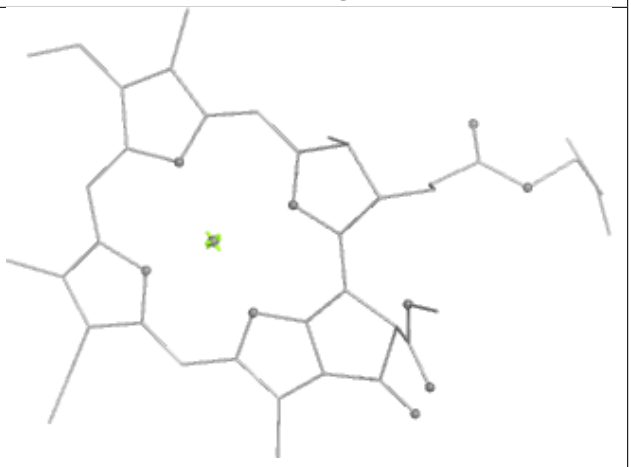
Bond lengths



Bond angles

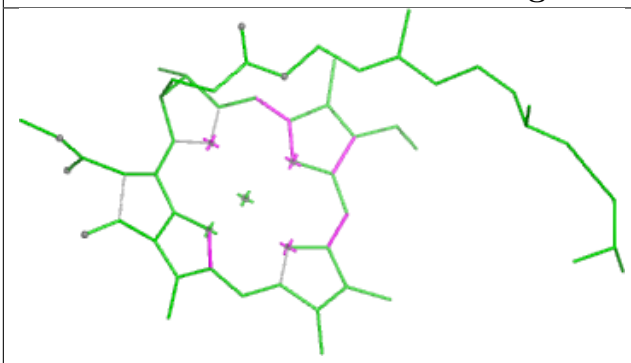


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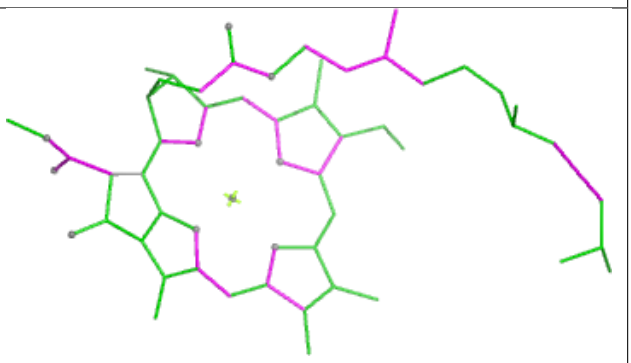


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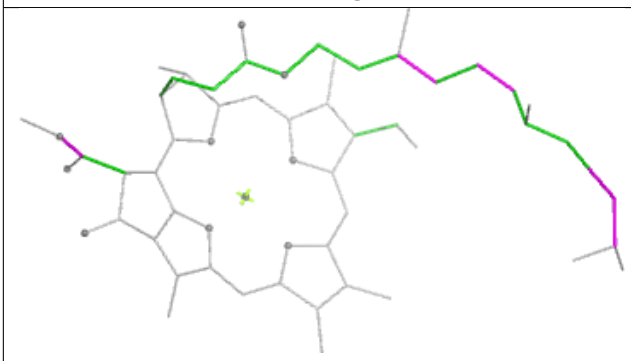
Ligand CLA 1 609



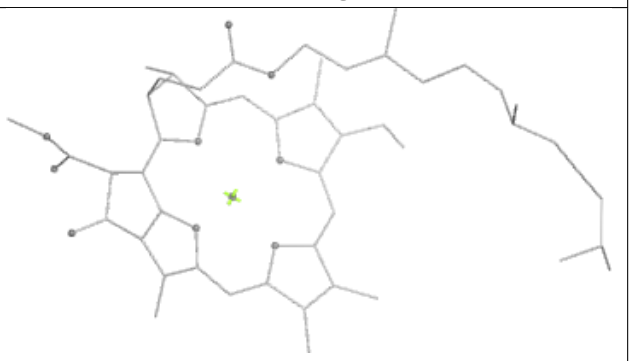
Bond lengths



Bond angles

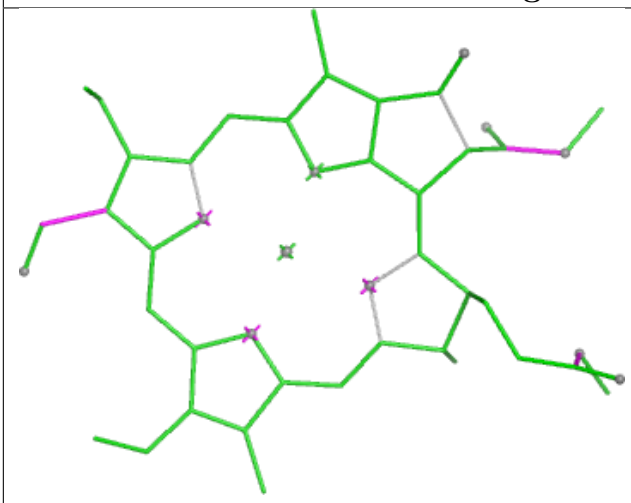


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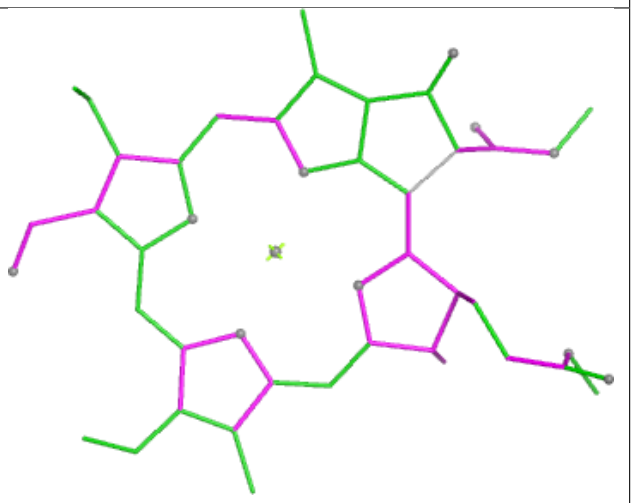


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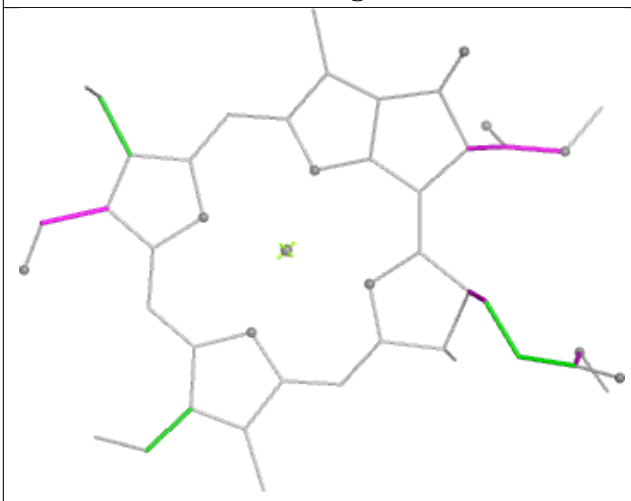
Ligand CHL Y 619



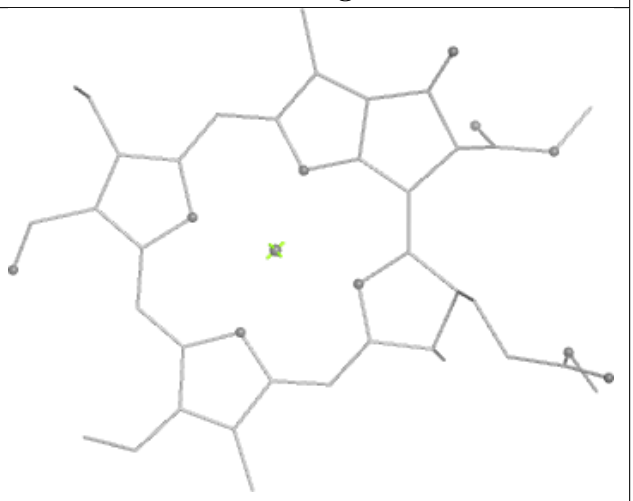
Bond lengths



Bond angles

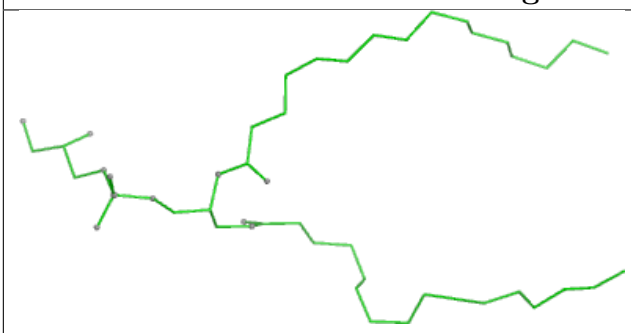


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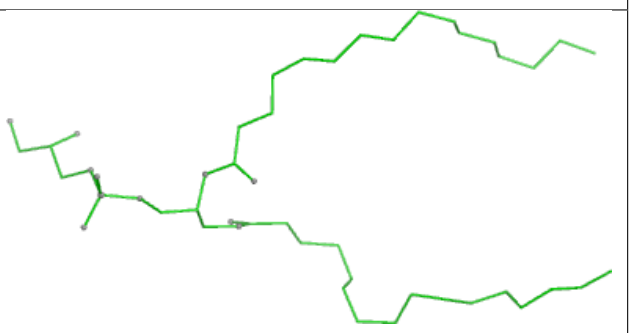


Rings

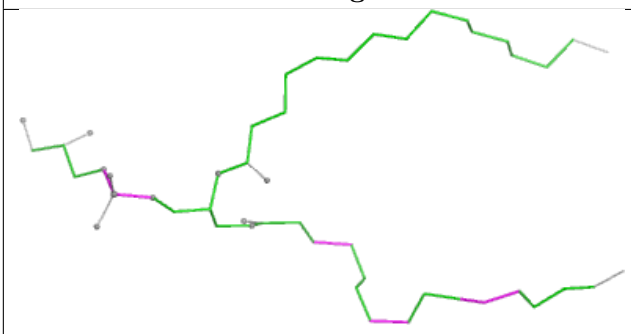
Ligand LHG A 851



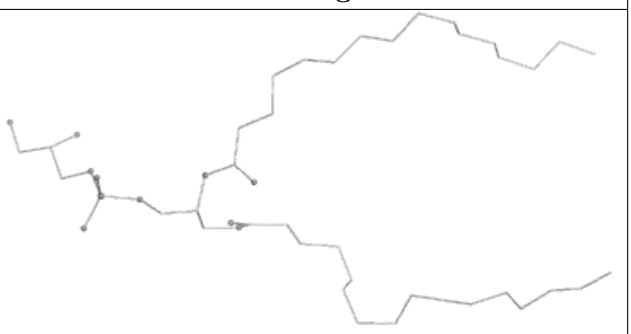
Bond lengths



Bond angles

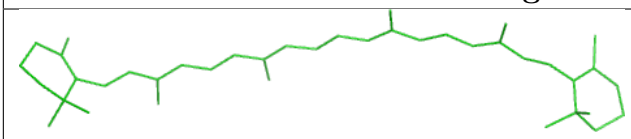


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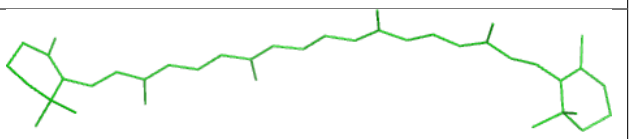


Rings

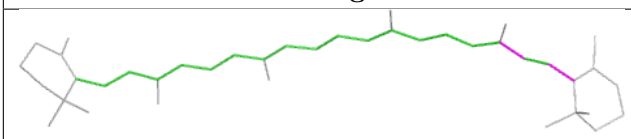
Ligand BCR B 846



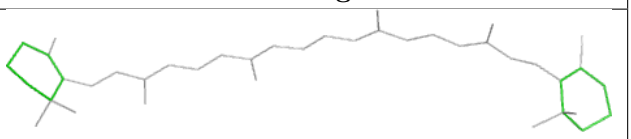
Bond lengths



Bond angles

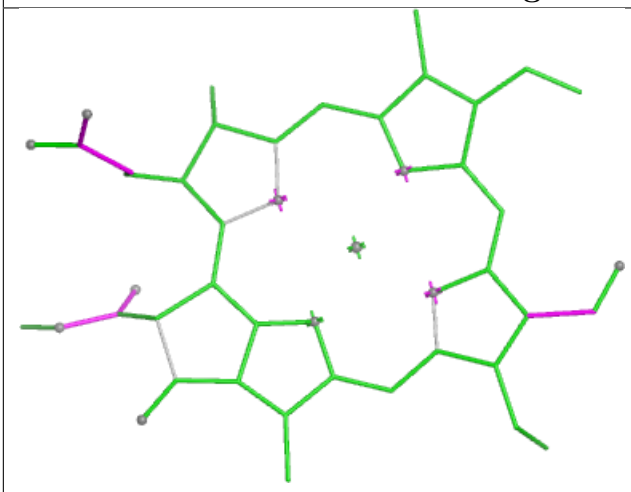


Torsions

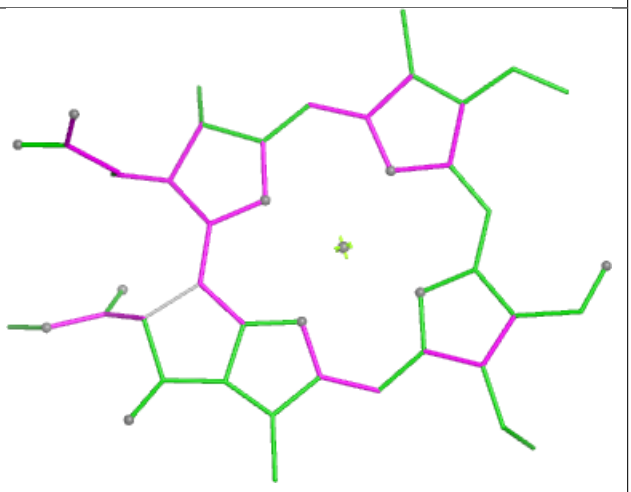


Rings

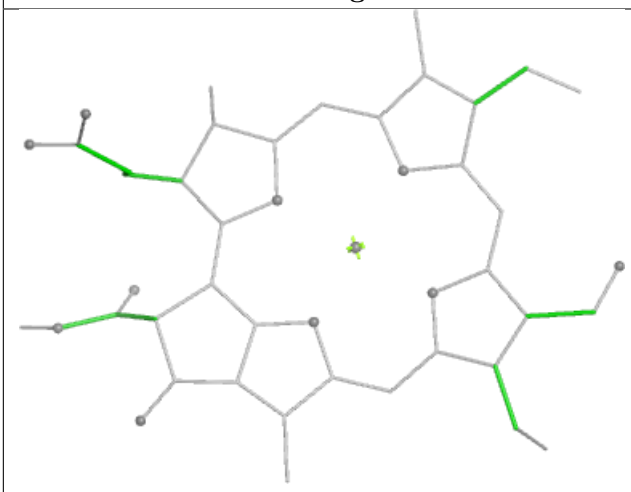
Ligand CHL Y 606



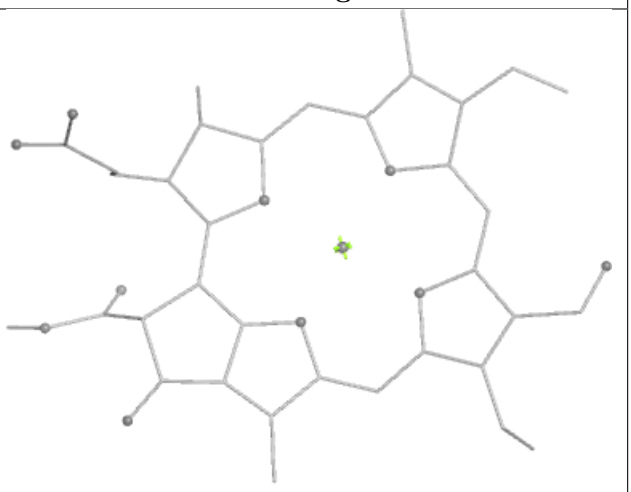
Bond lengths



Bond angles

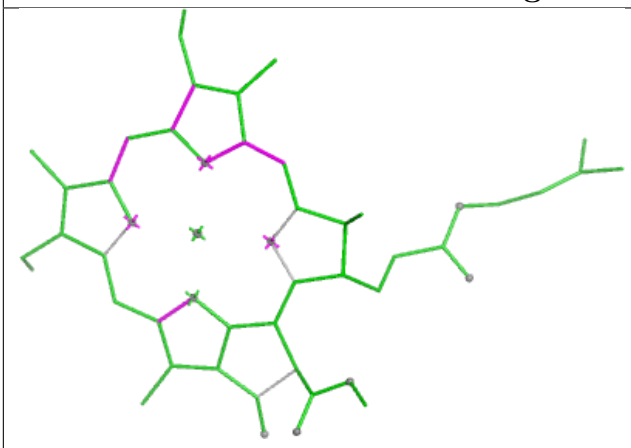


Torsions

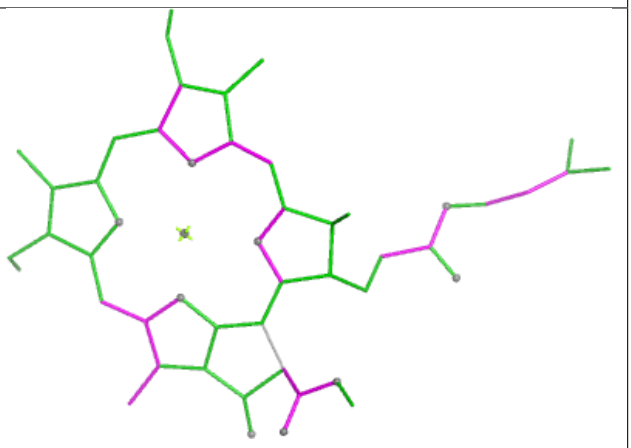


Rings

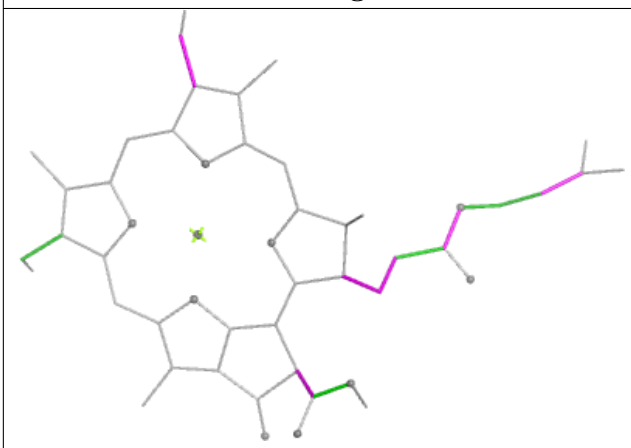
Ligand CLA O 202



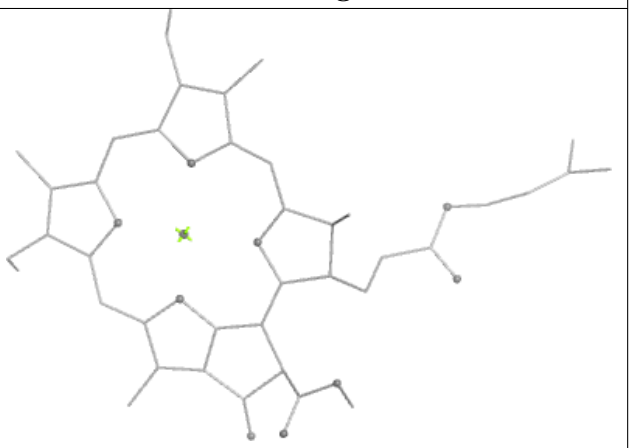
Bond lengths



Bond angles

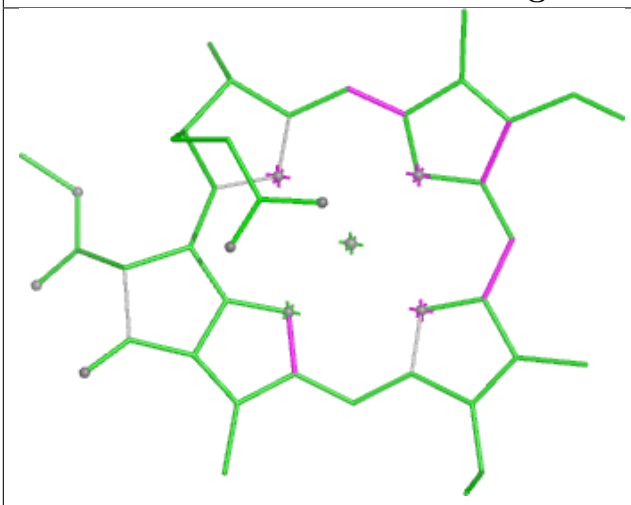


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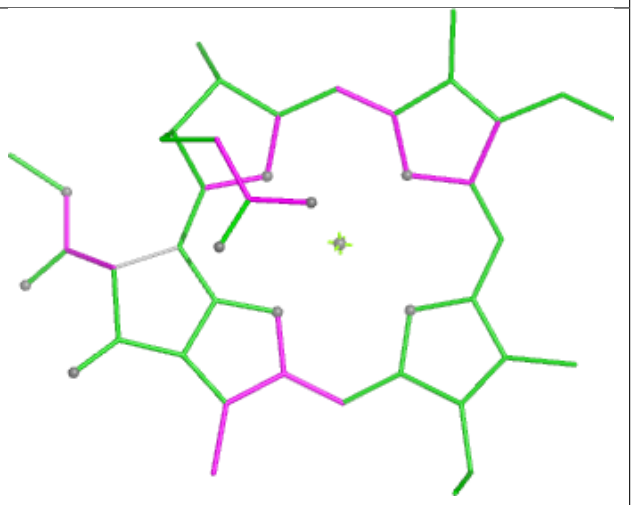


Rings

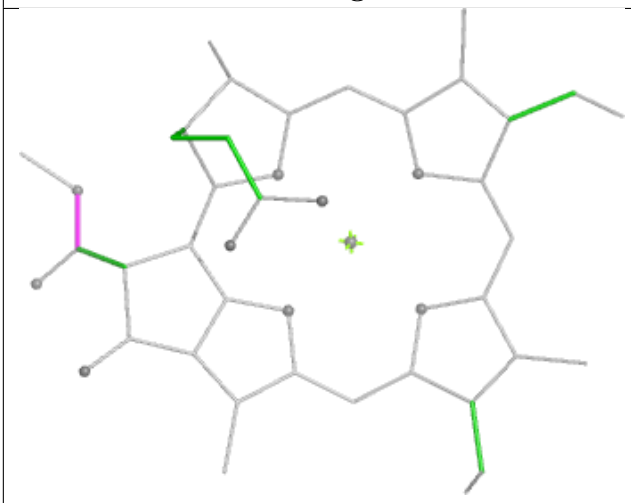
Ligand CLA 5 613



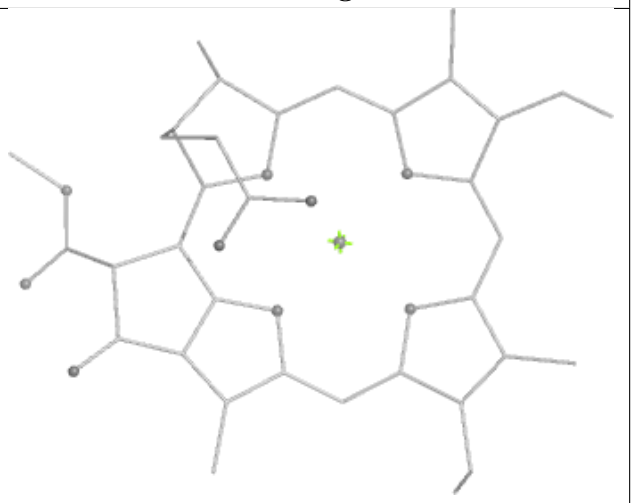
Bond lengths



Bond angles

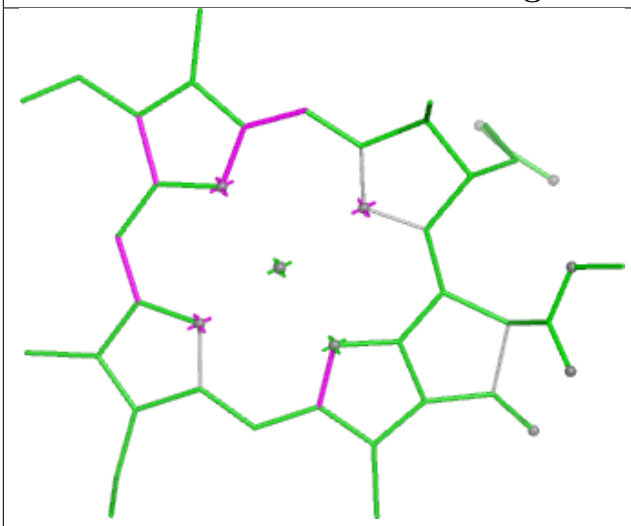


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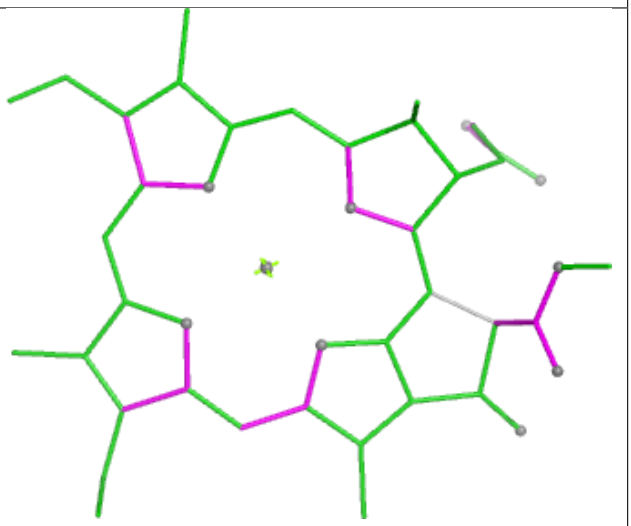


Rings

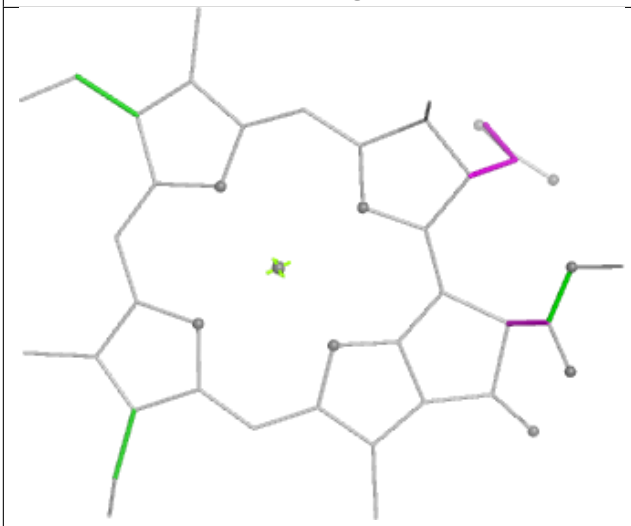
Ligand CLA A 836



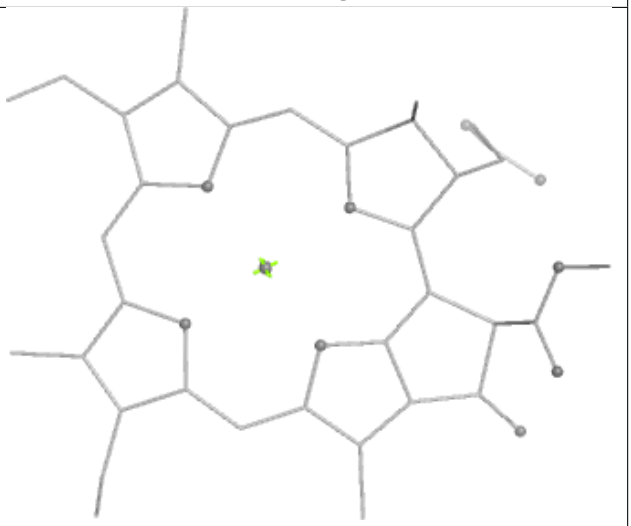
Bond lengths



Bond angles

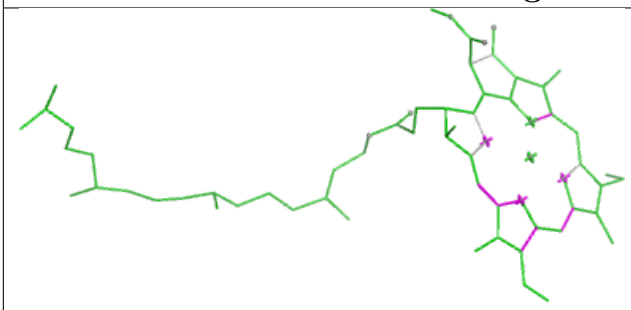


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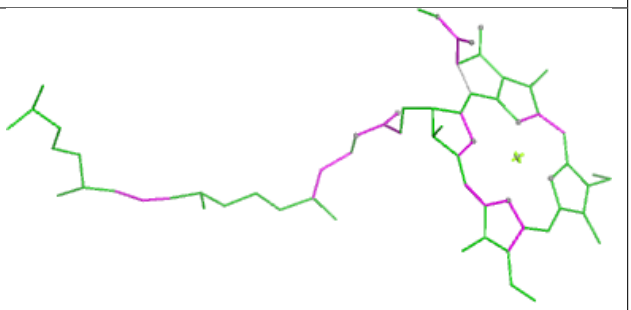


Rings

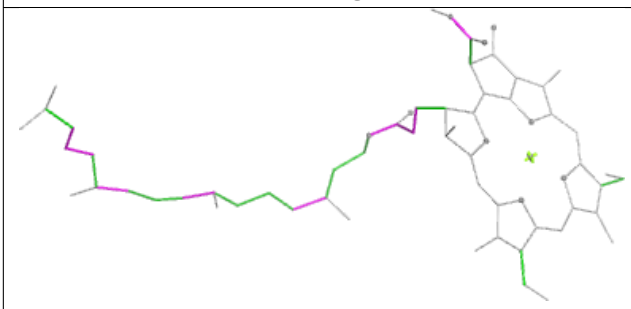
Ligand CLA A 821



Bond lengths



Bond angles

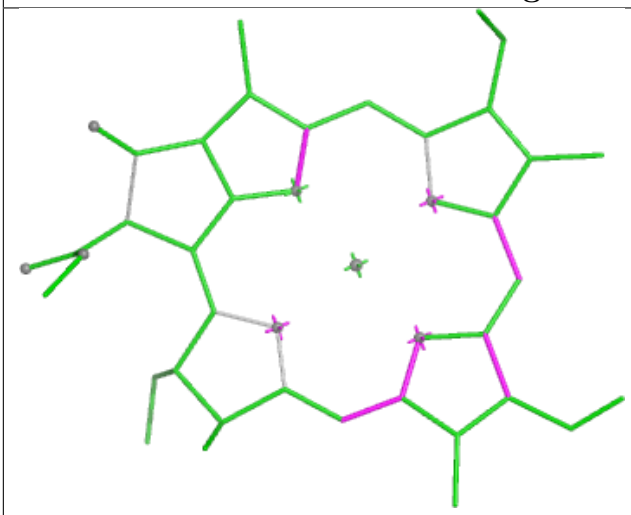


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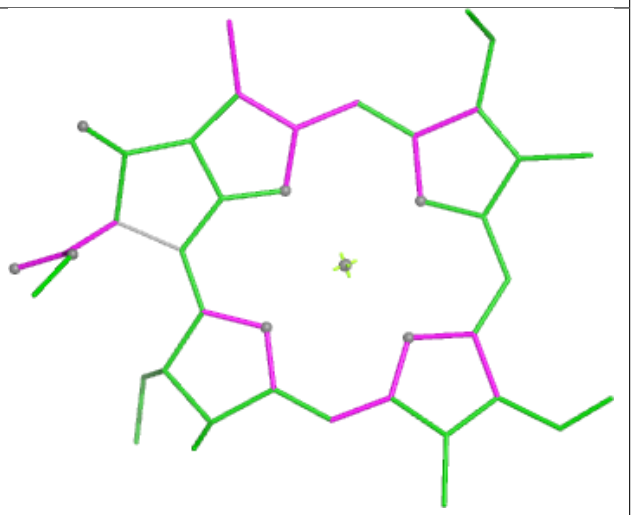


Rings

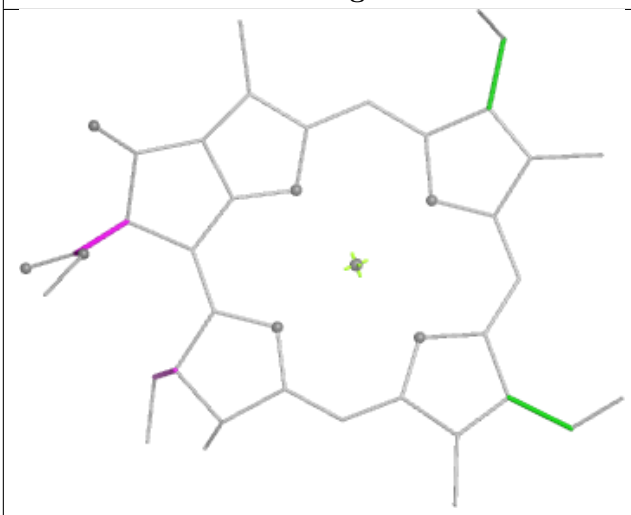
Ligand CLA G 203



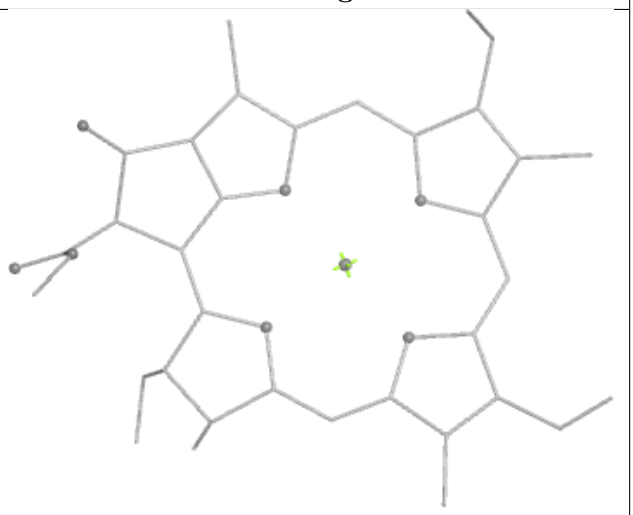
Bond lengths



Bond angles

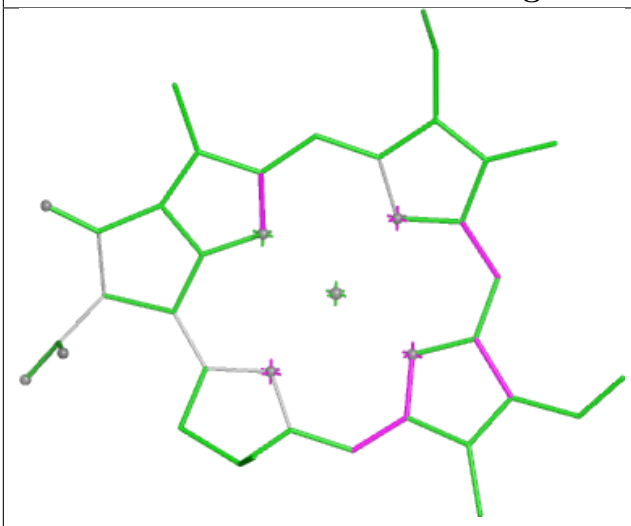


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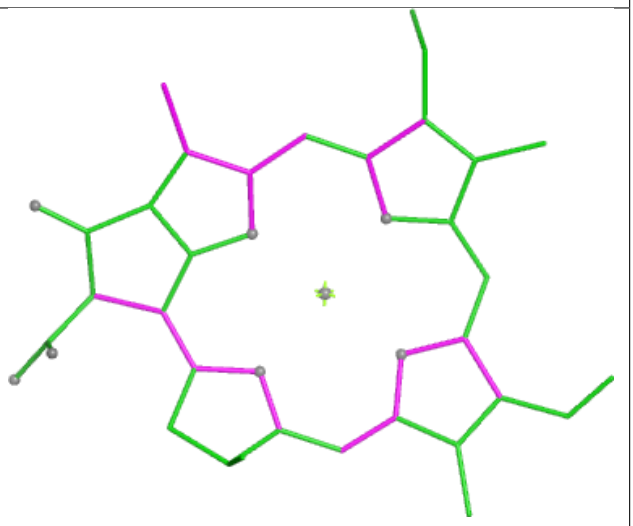


Rings

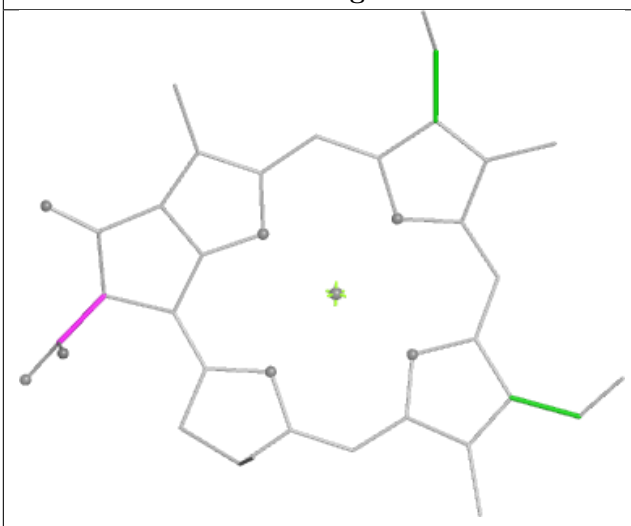
Ligand CLA K 204



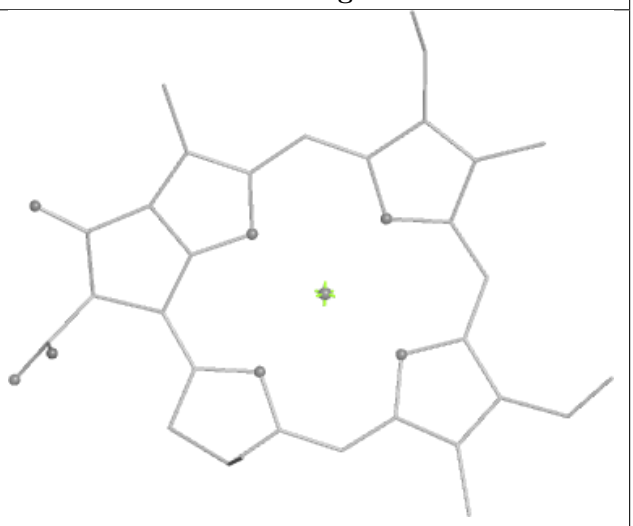
Bond lengths



Bond angles

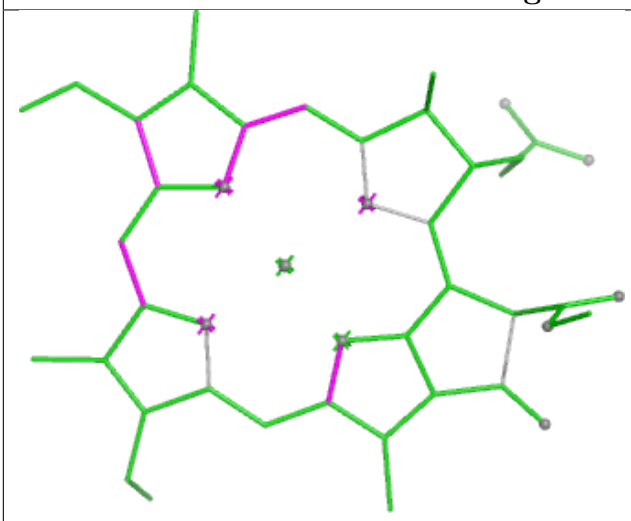


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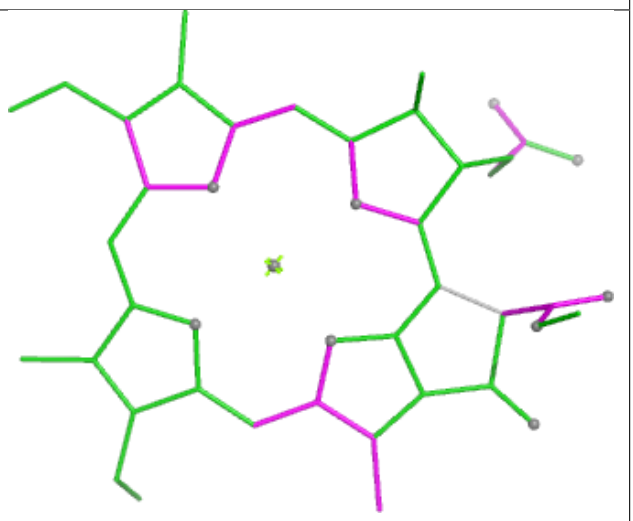


Rings

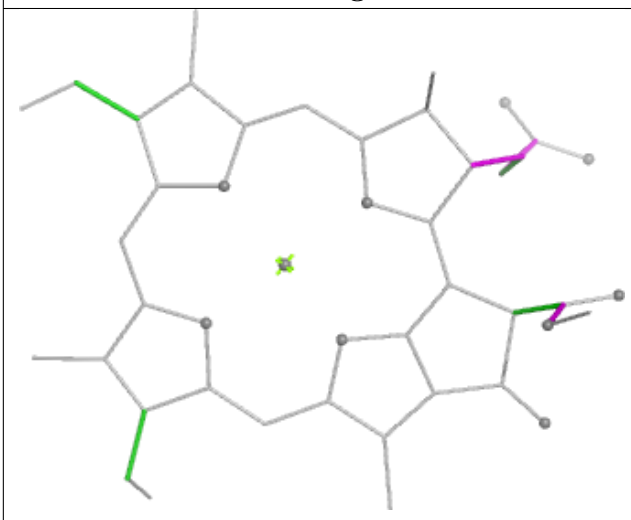
Ligand CLA A 816



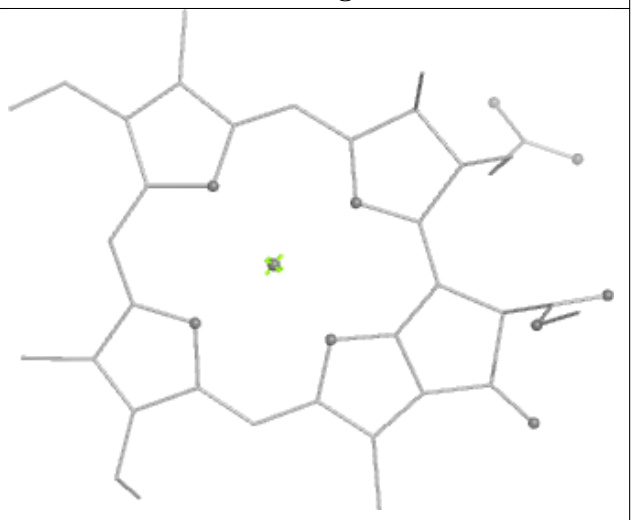
Bond lengths



Bond angles

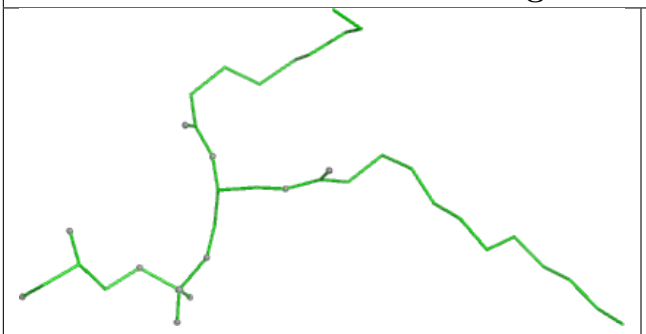


Torsions

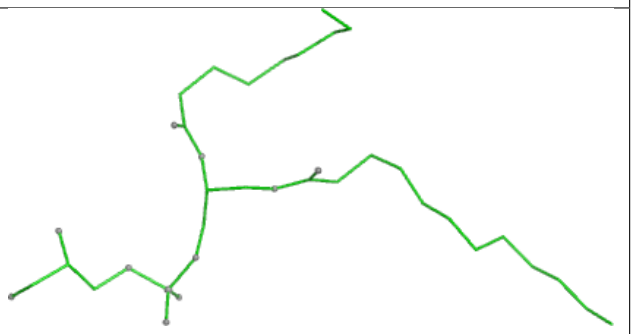


Rings

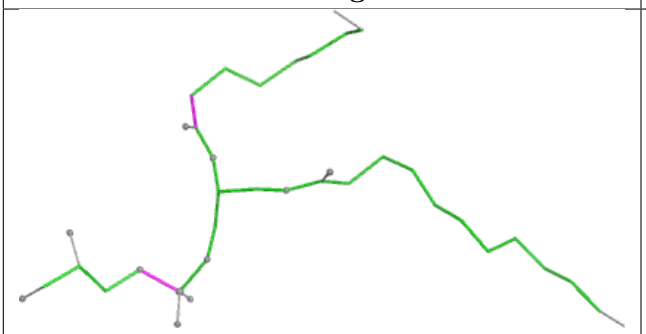
Ligand LHG 1 622



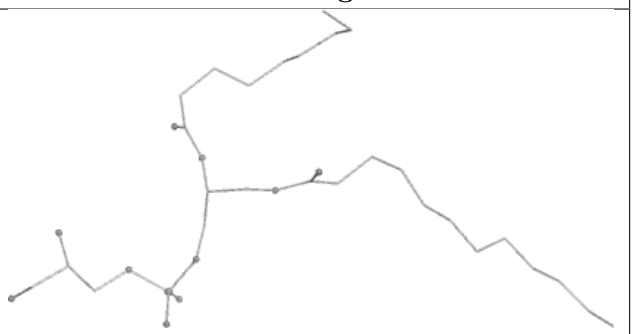
Bond lengths



Bond angles

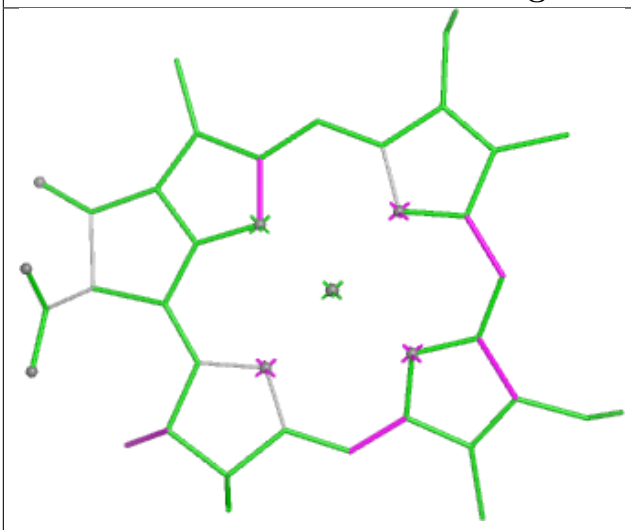


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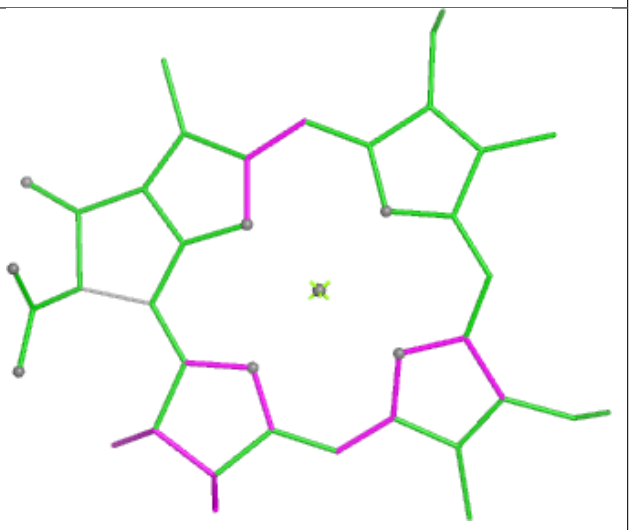


Rings

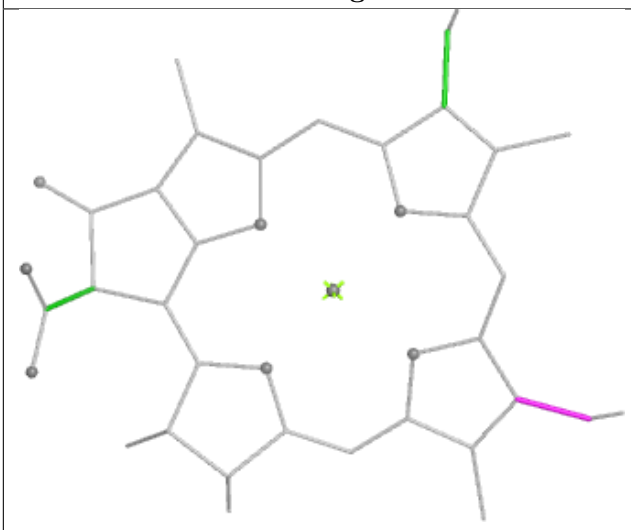
Ligand CLA 3 613



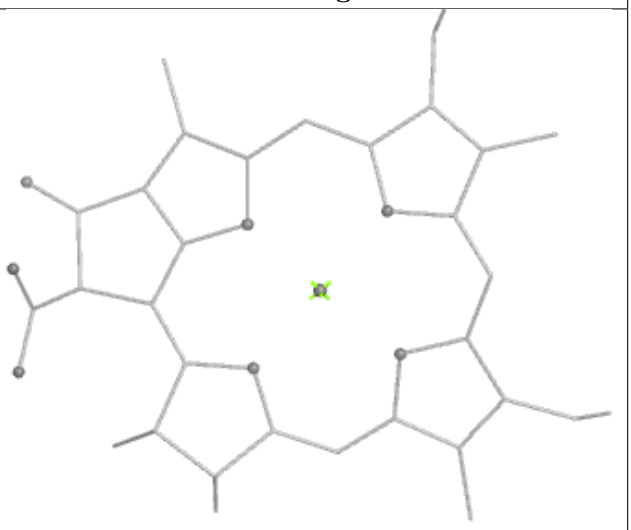
Bond lengths



Bond angles

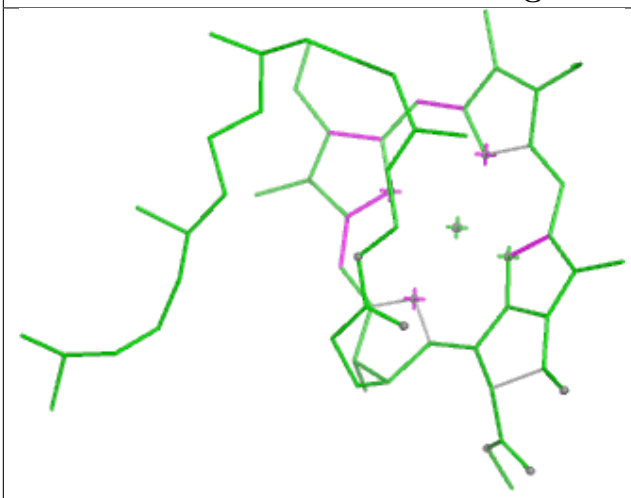


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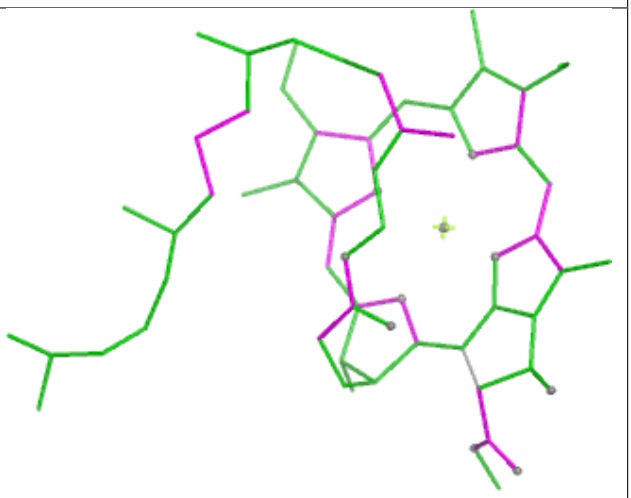


Rings

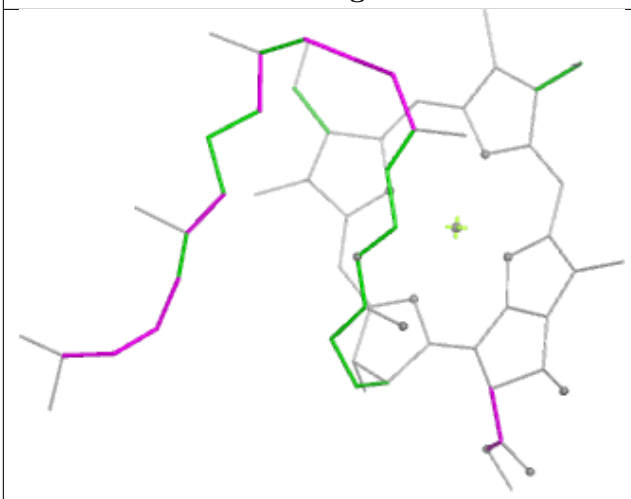
Ligand CLA B 807



Bond lengths



Bond angles

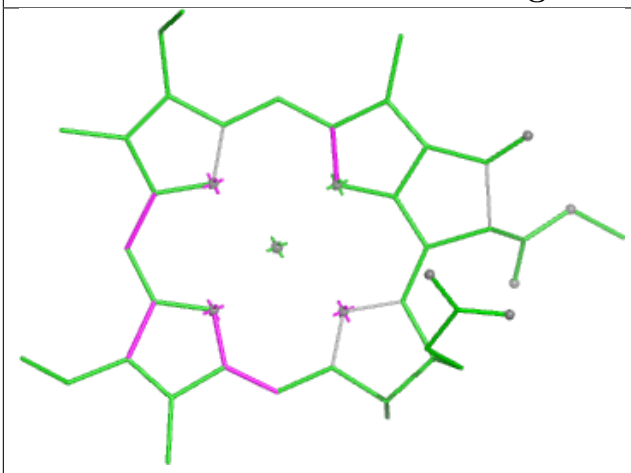


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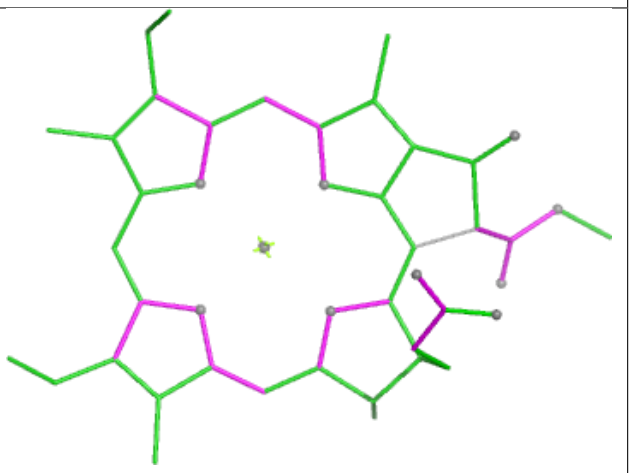


Rings

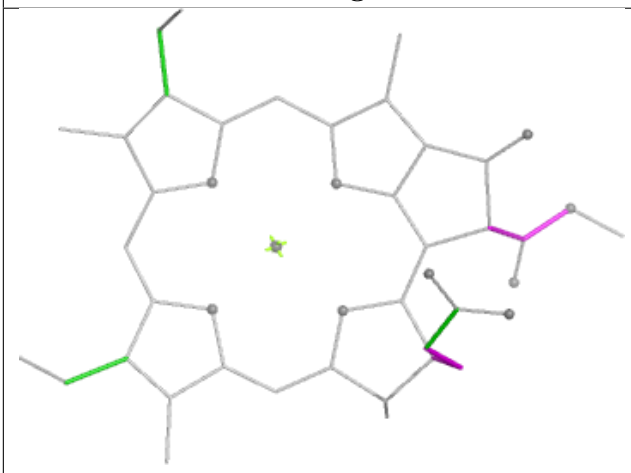
Ligand CLA 4 312



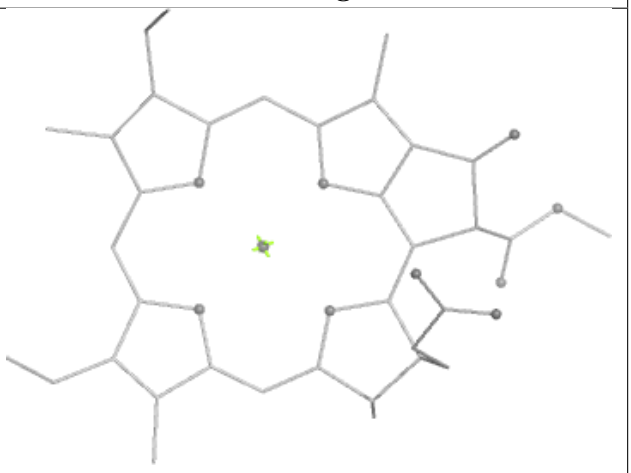
Bond lengths



Bond angles

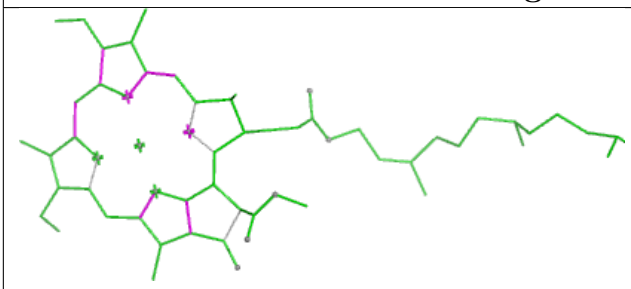


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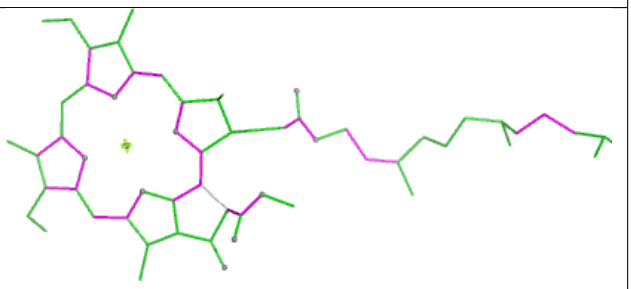


Rings

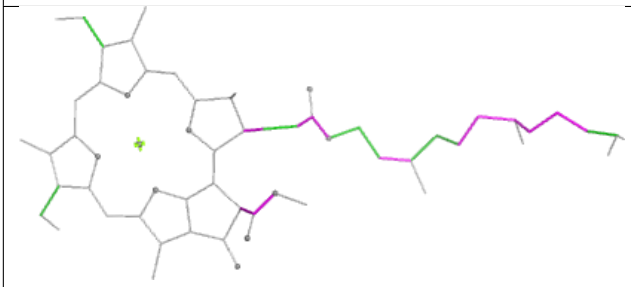
Ligand CLA B 822



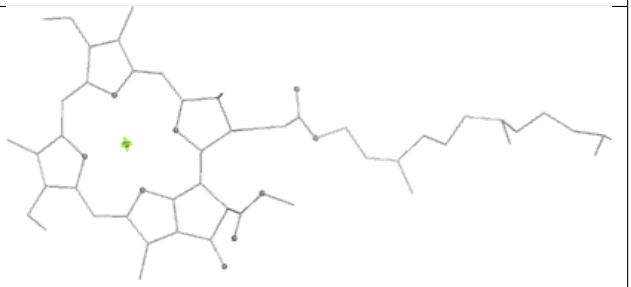
Bond lengths



Bond angles

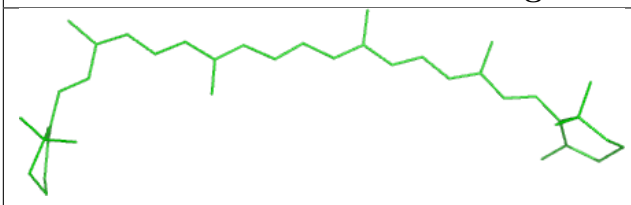


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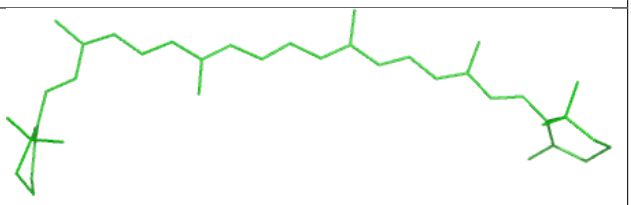


Rings

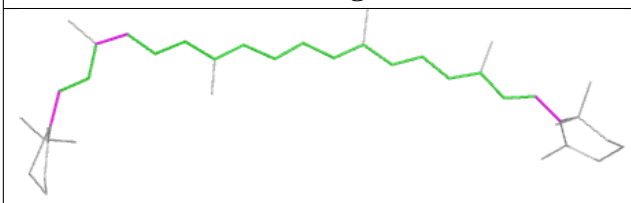
Ligand BCR L 308



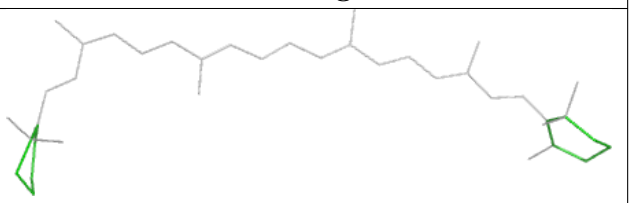
Bond lengths



Bond angles

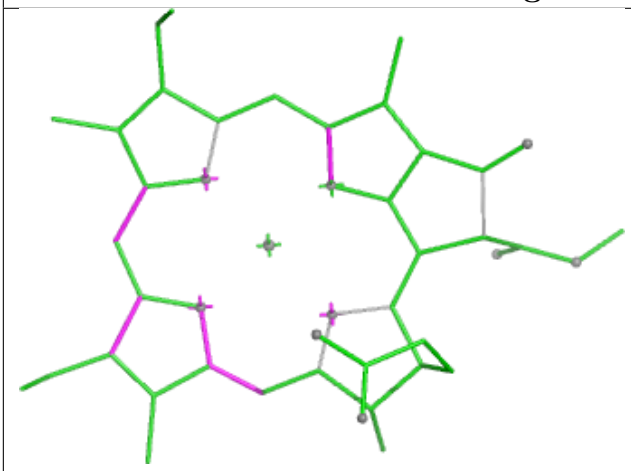


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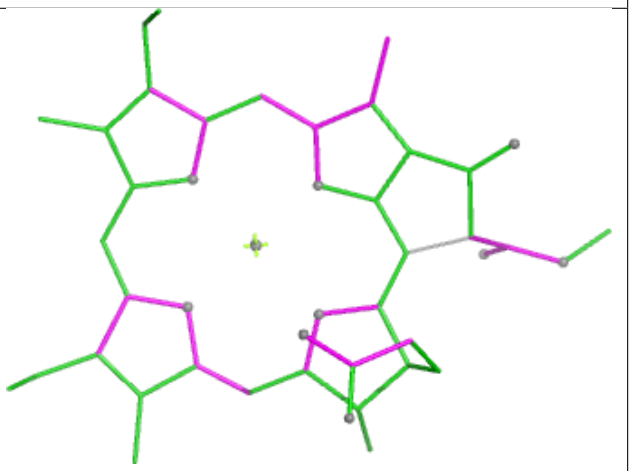


Rings

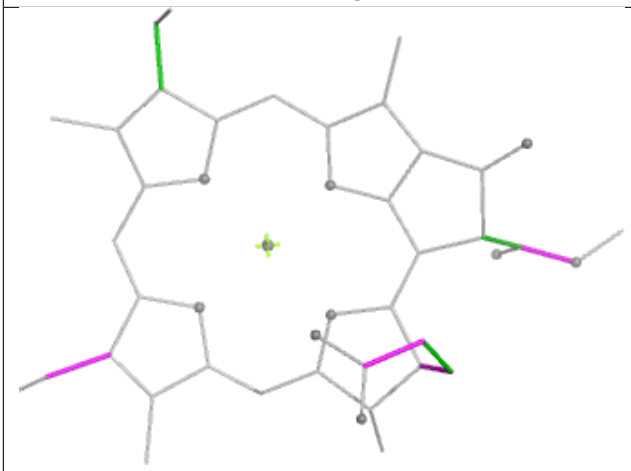
Ligand CLA X 613



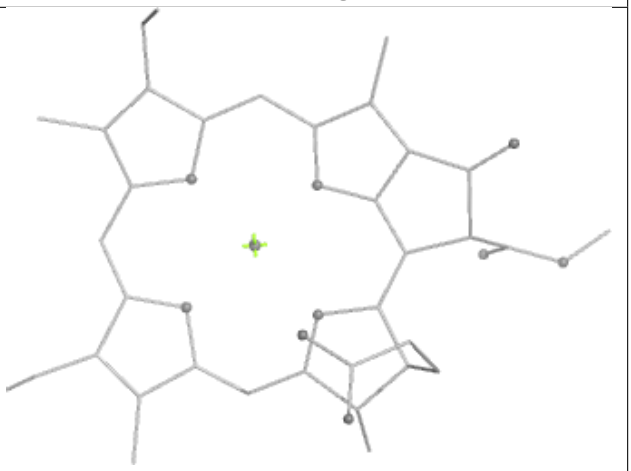
Bond lengths



Bond angles

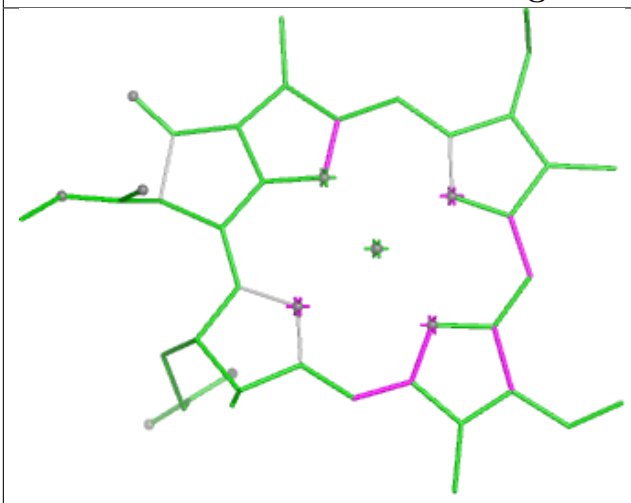


Torsions

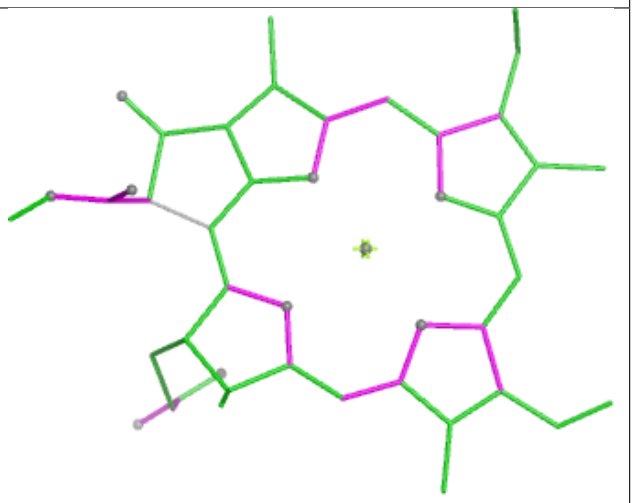


Rings

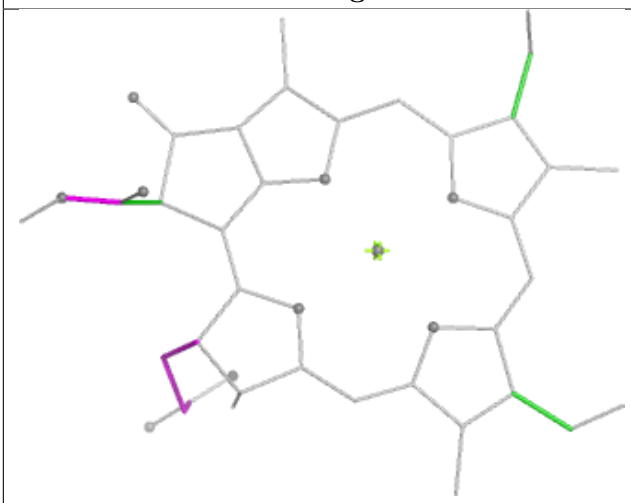
Ligand CLA 3 607



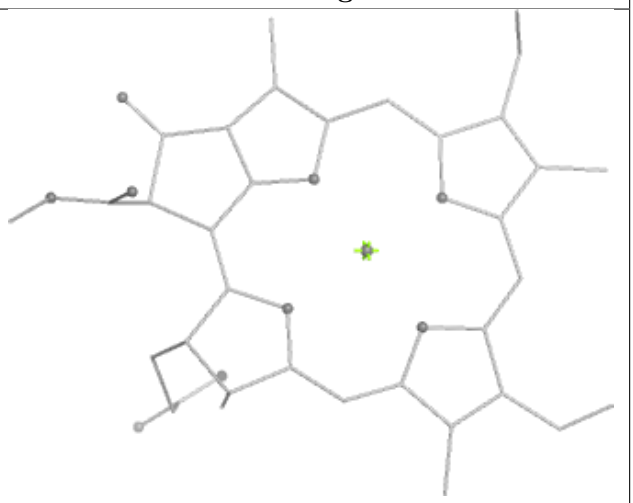
Bond lengths



Bond angles

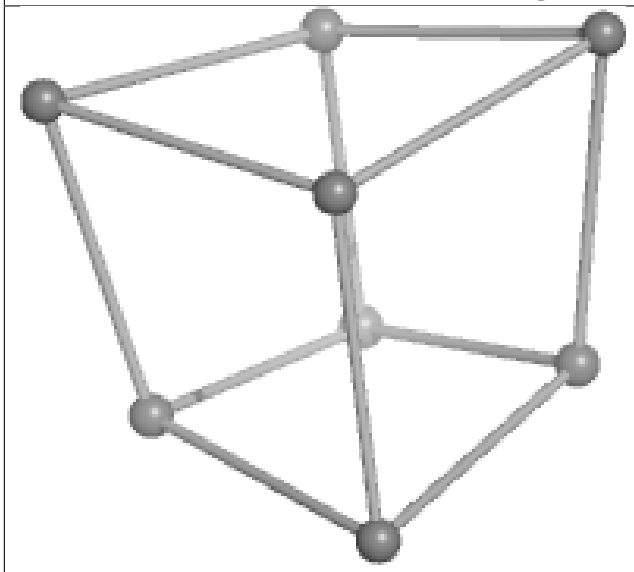


Torsions

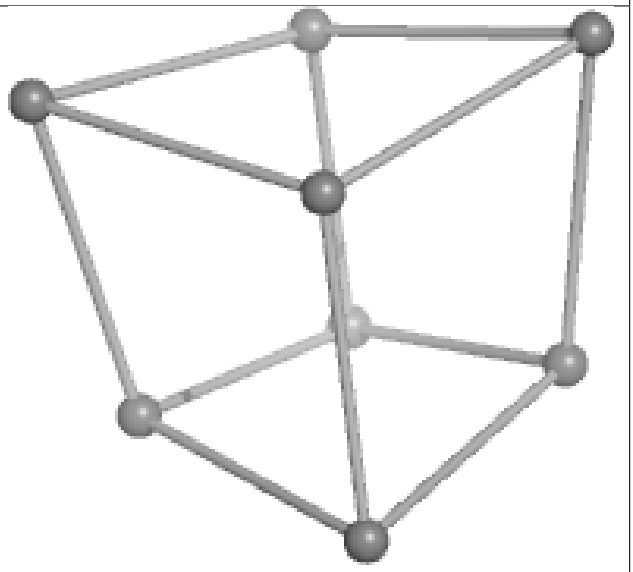


Rings

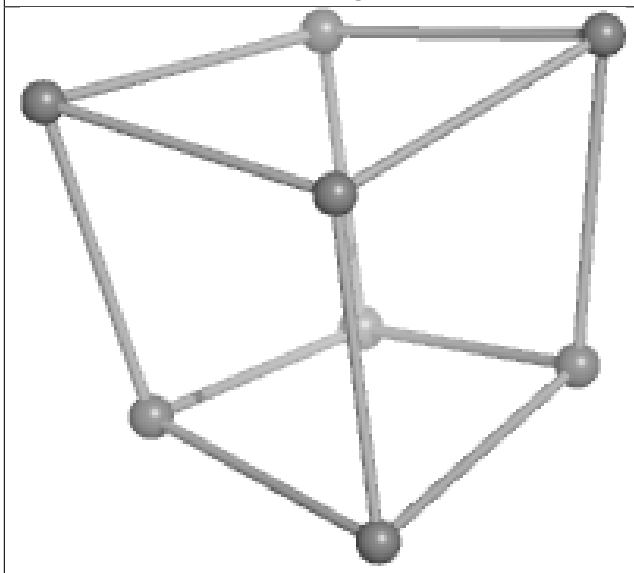
Ligand SF4 C 102



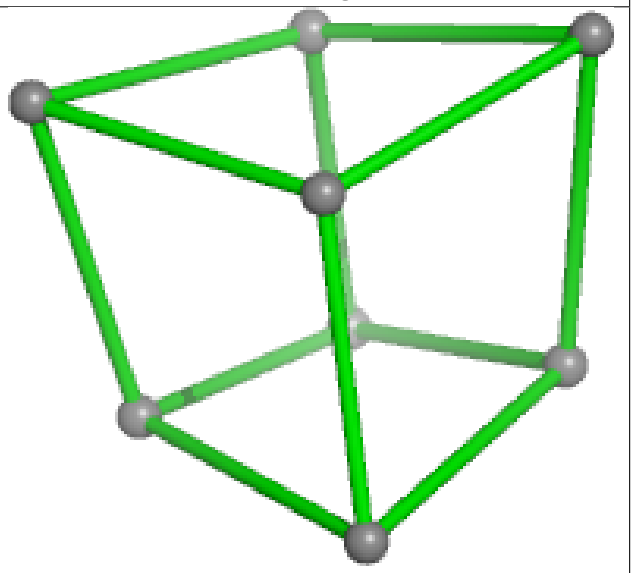
Bond lengths



Bond angles

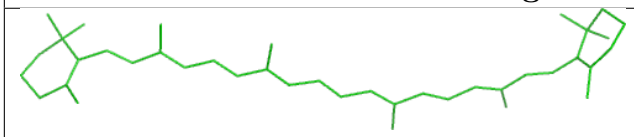


Torsions

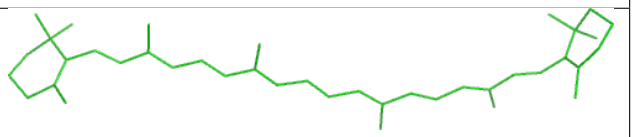


Rings

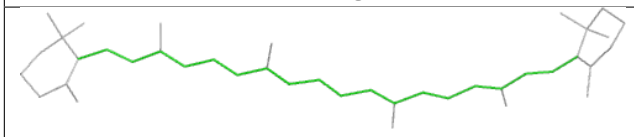
Ligand BCR G 205



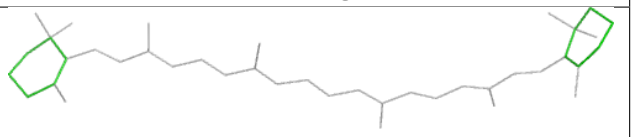
Bond lengths



Bond angles



Torsions

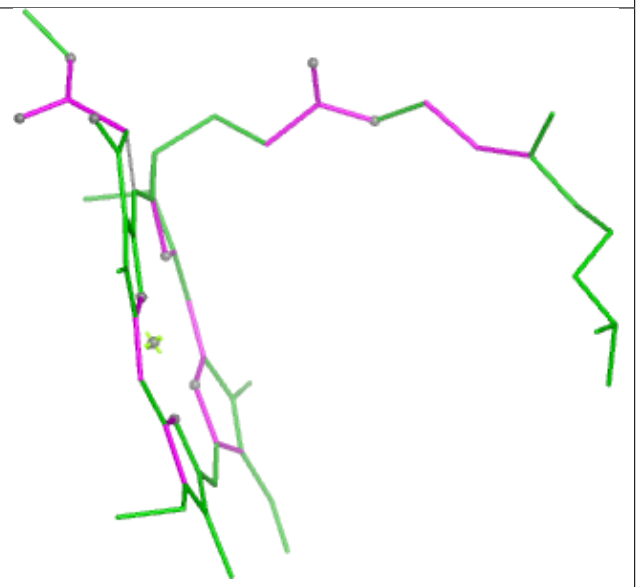


Rings

Ligand CLA B 818



Bond lengths



Bond angles



Torsions



Rings

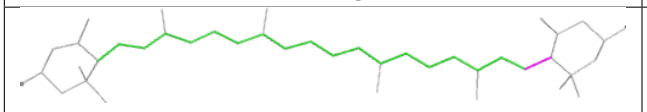
Ligand LUT F 301



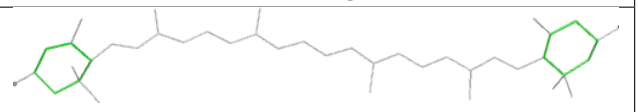
Bond lengths



Bond angles

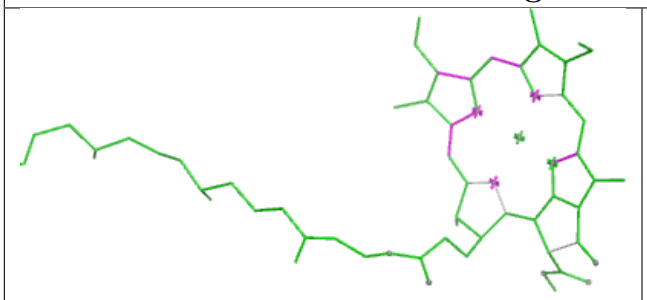


Torsions

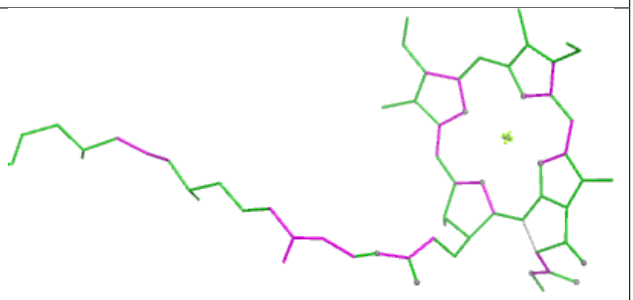


Rings

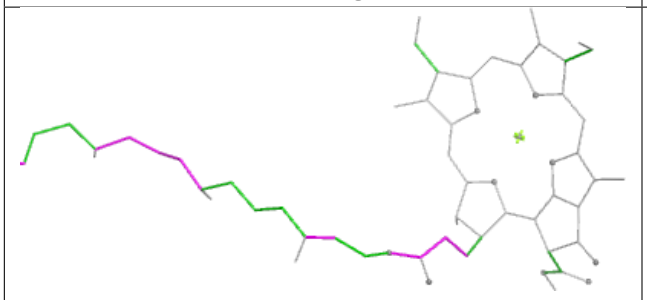
Ligand CLA A 834



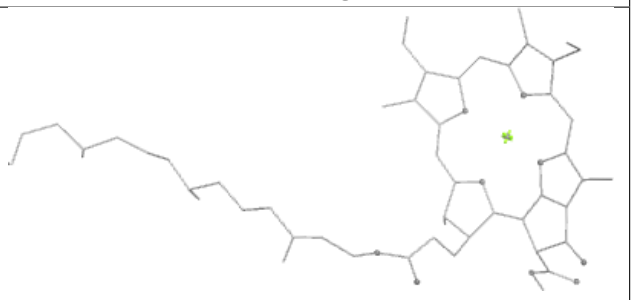
Bond lengths



Bond angles

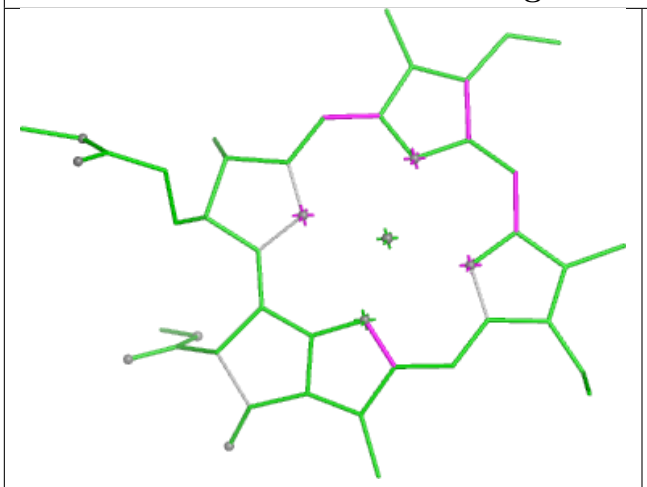


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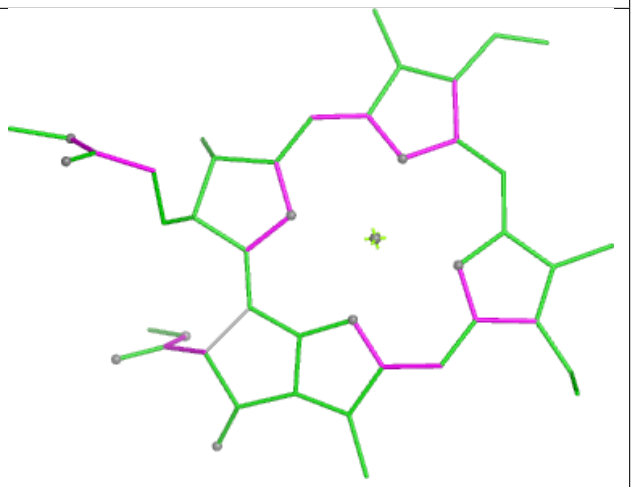


Rings

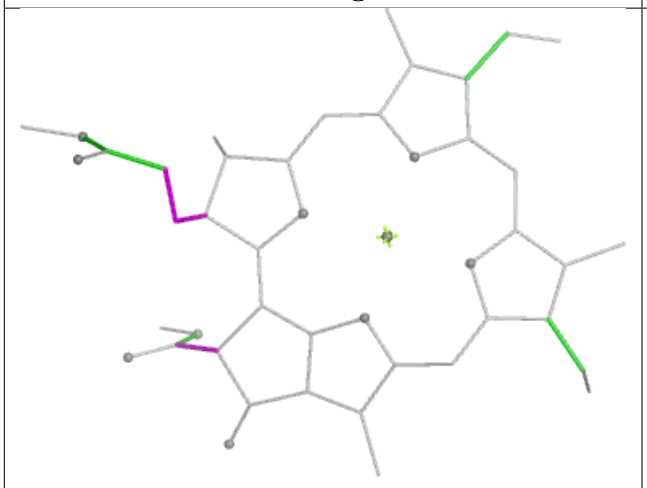
Ligand CLA K 203



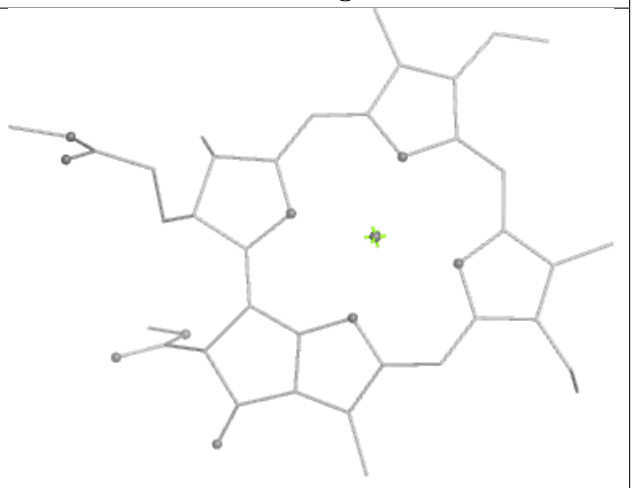
Bond lengths



Bond angles

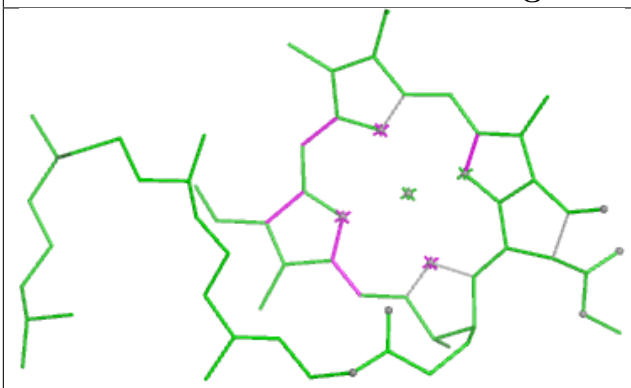


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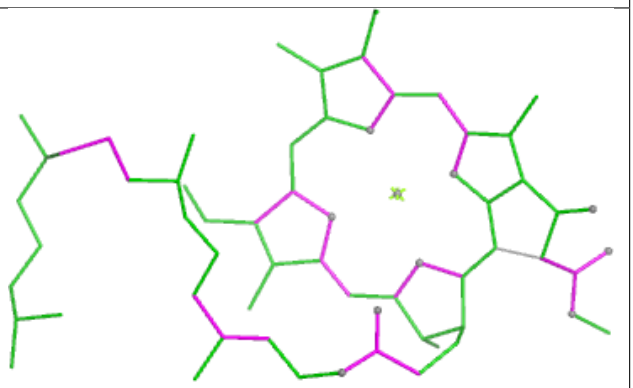


Rings

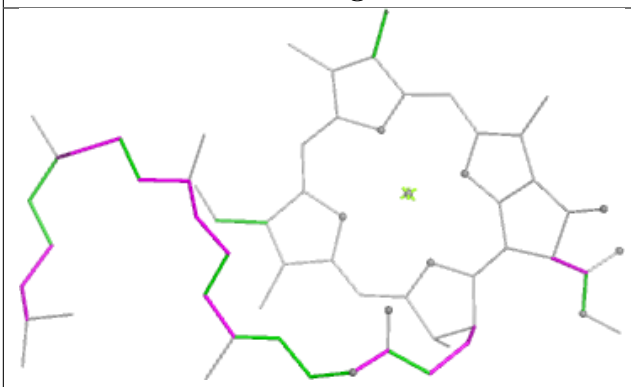
Ligand CLA A 819



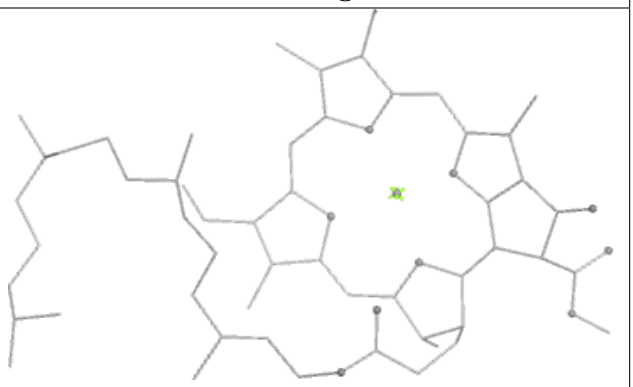
Bond lengths



Bond angles

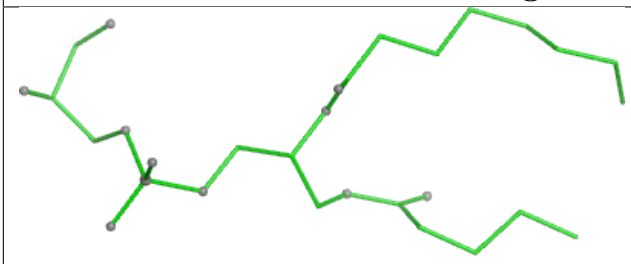


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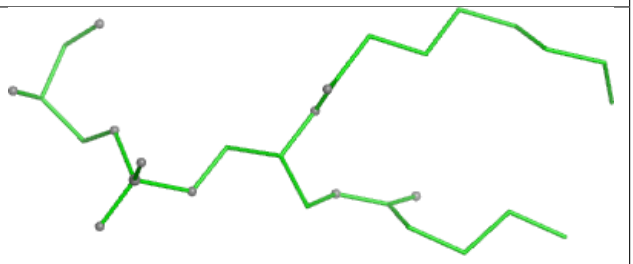


Rings

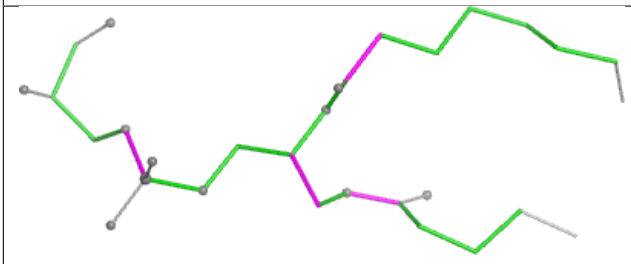
Ligand LHG A 853



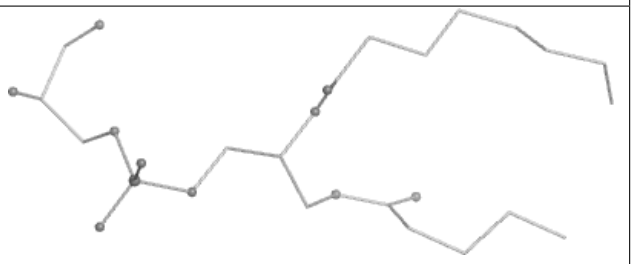
Bond lengths



Bond angles

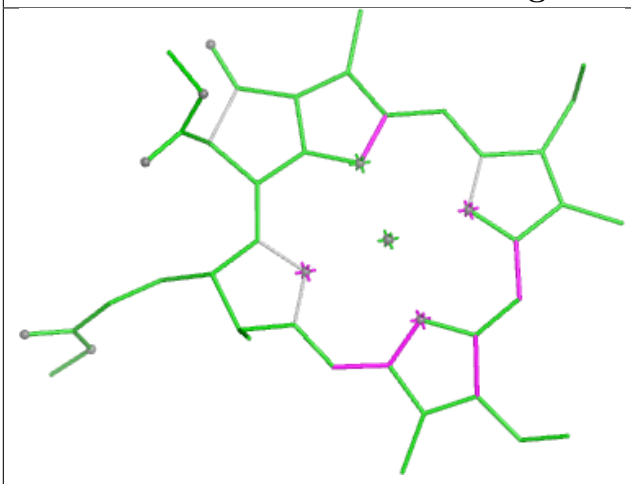


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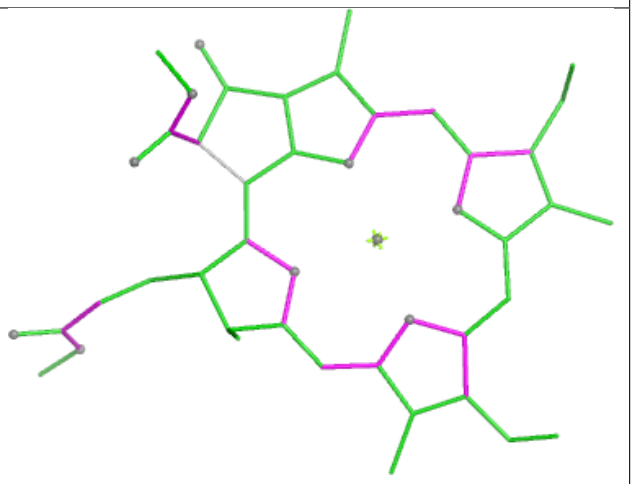


Rings

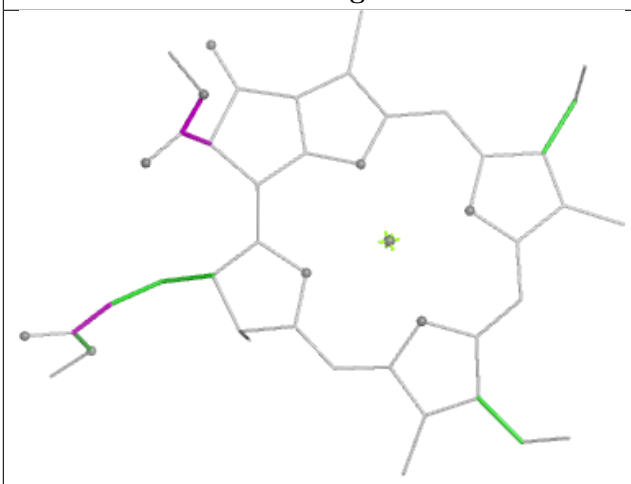
Ligand CLA 6 601



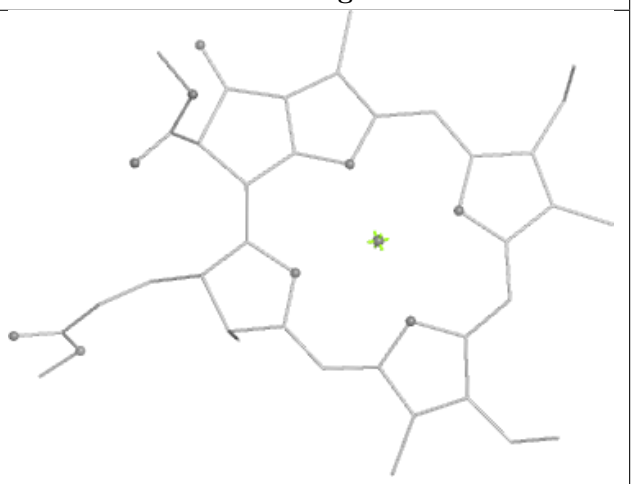
Bond lengths



Bond angles

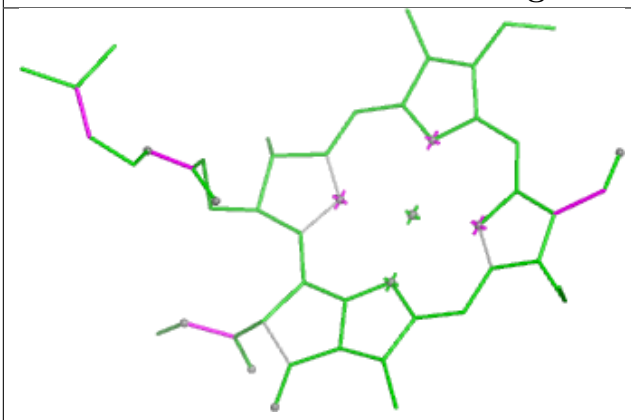


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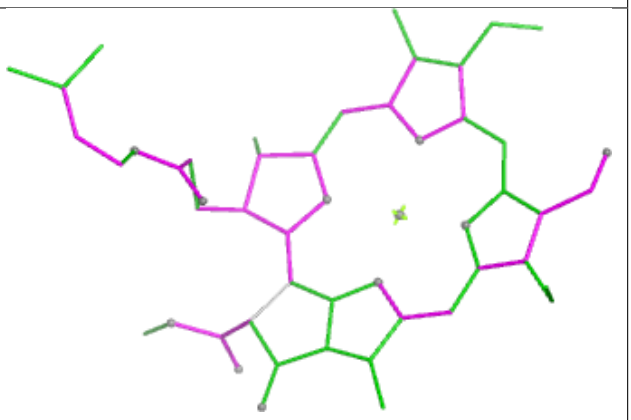


Rings

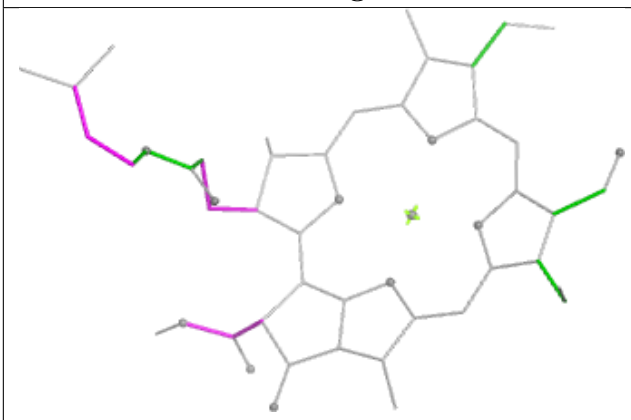
Ligand CHL 4 306



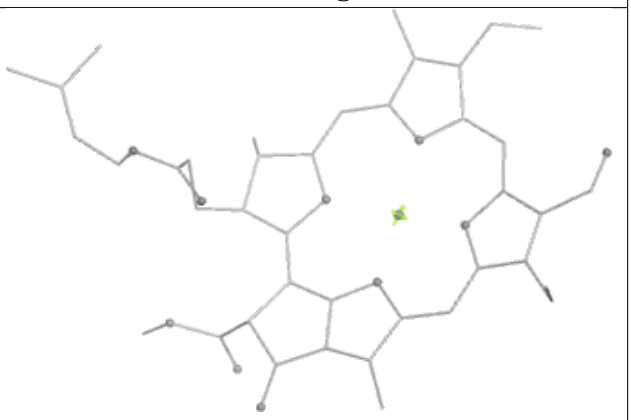
Bond lengths



Bond angles

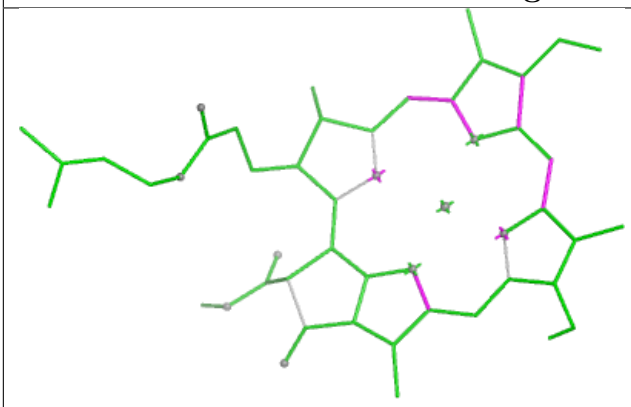


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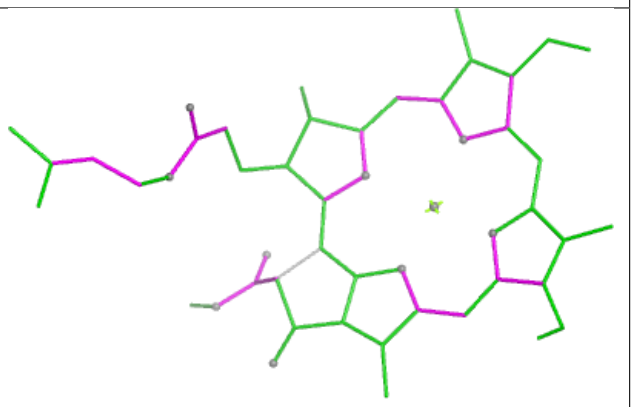


Rings

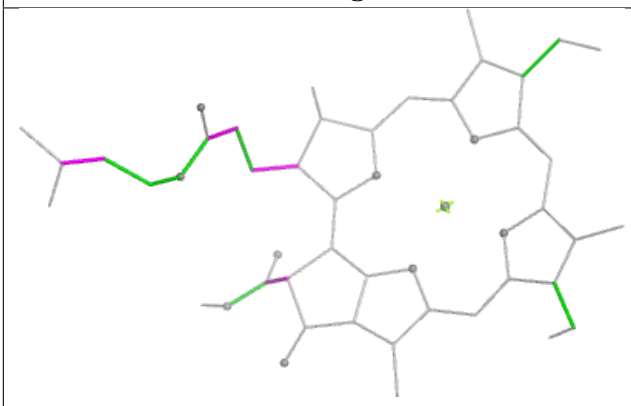
Ligand CLA A 810



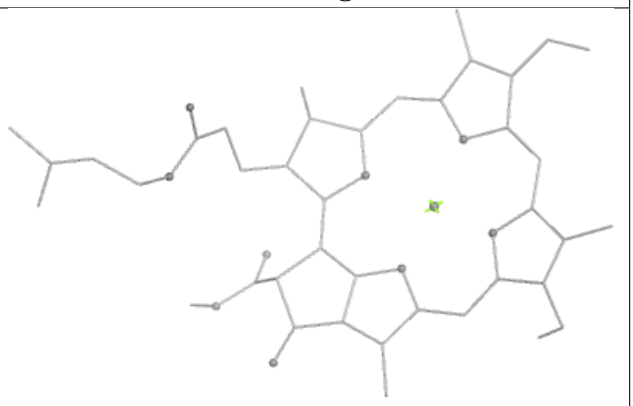
Bond lengths



Bond angles

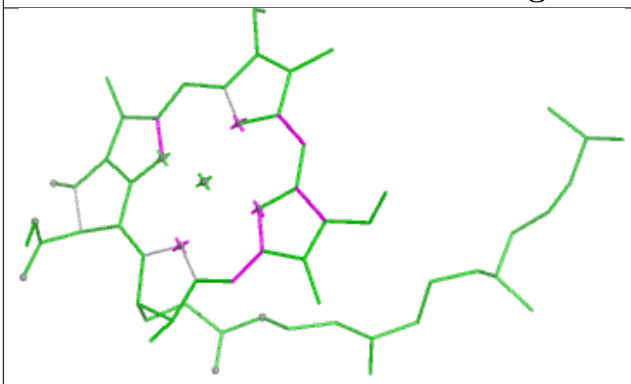


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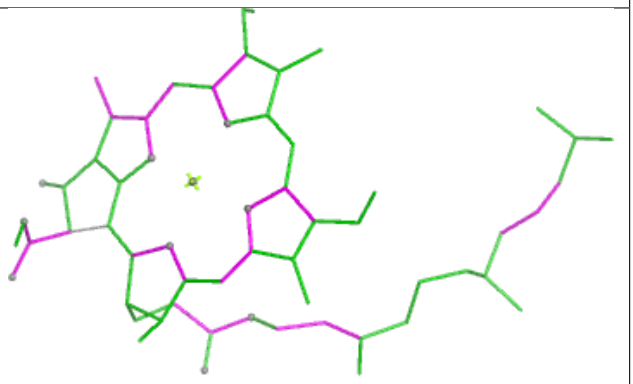


Rings

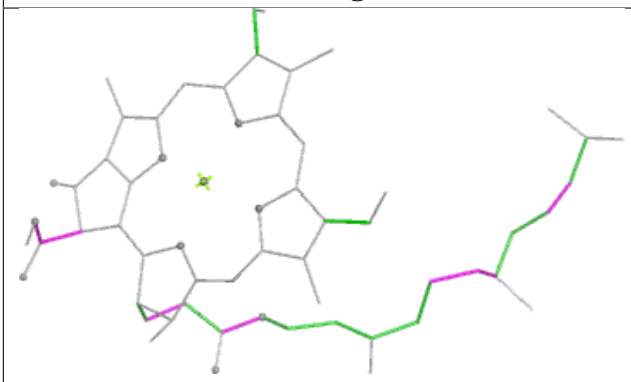
Ligand CLA 3 602



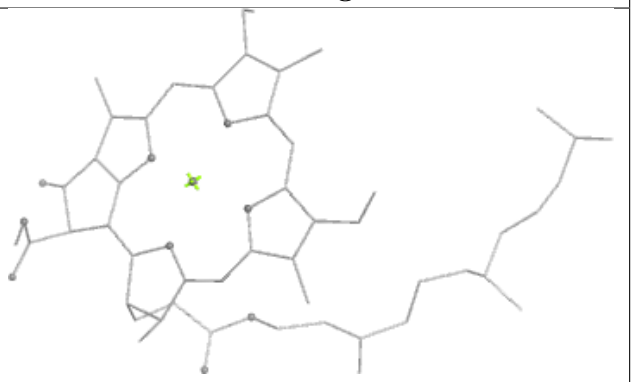
Bond lengths



Bond angles

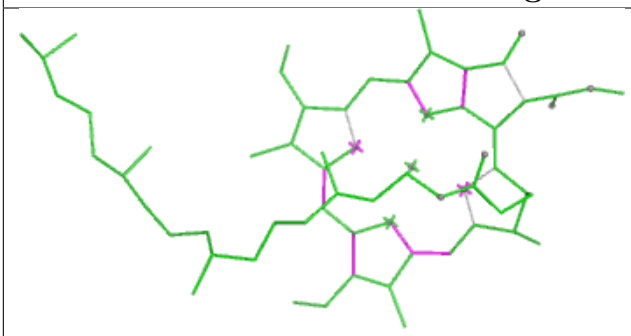


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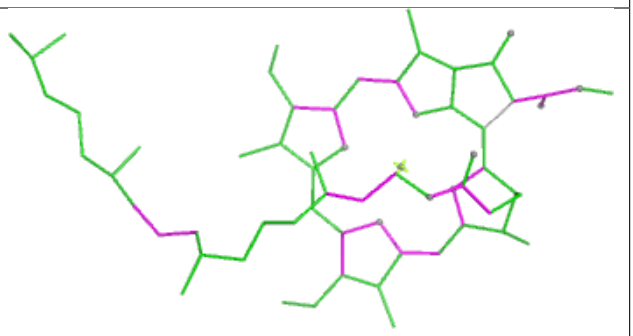


Rings

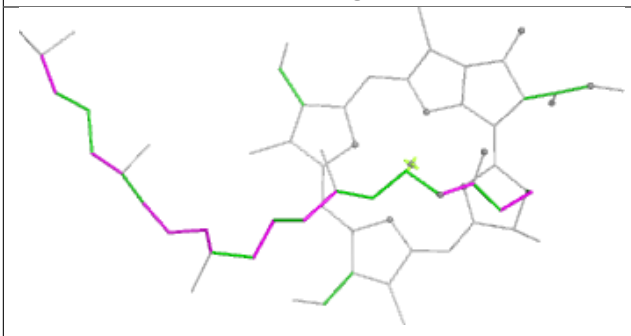
Ligand CLA B 836



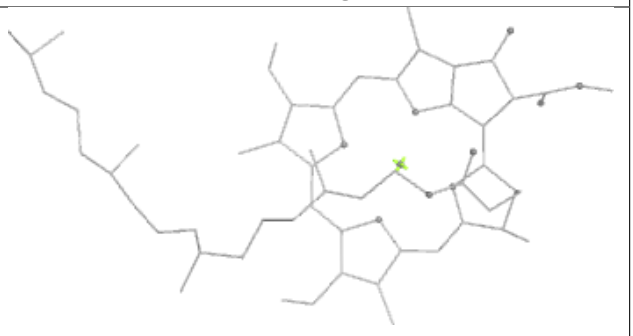
Bond lengths



Bond angles

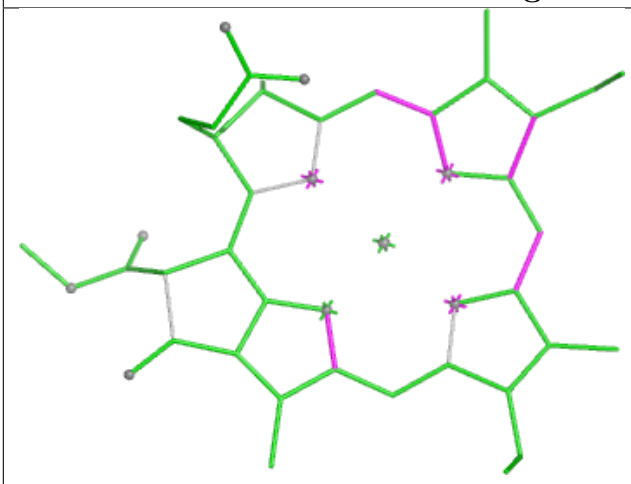


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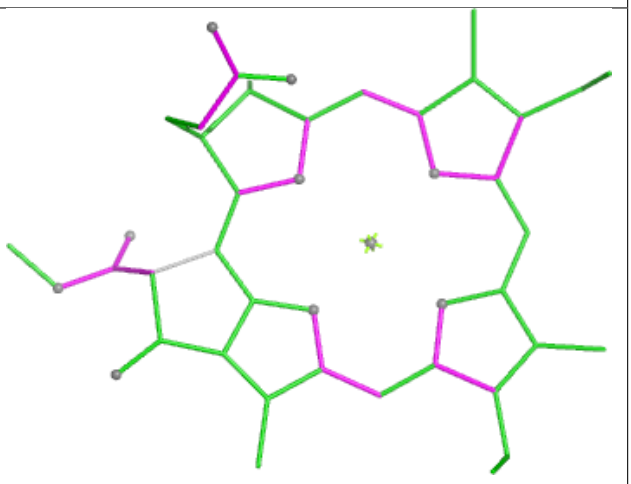


Rings

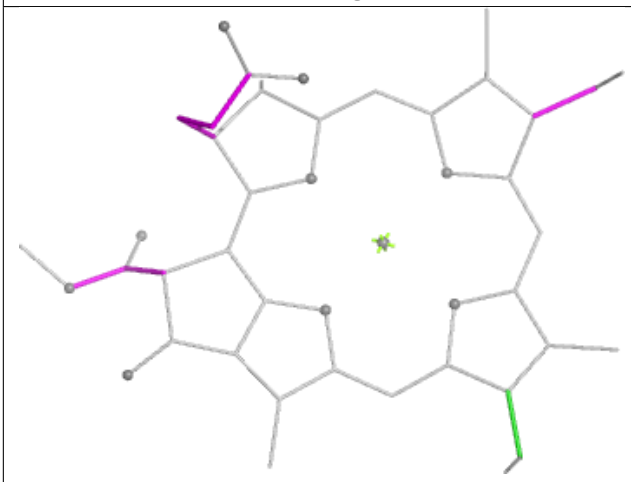
Ligand CLA Y 610



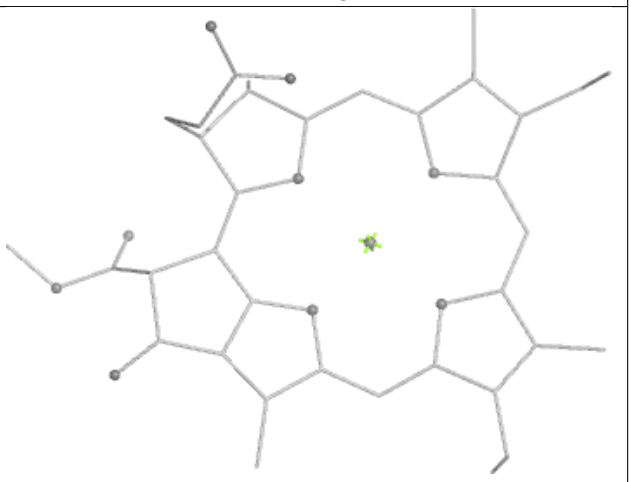
Bond lengths



Bond angles

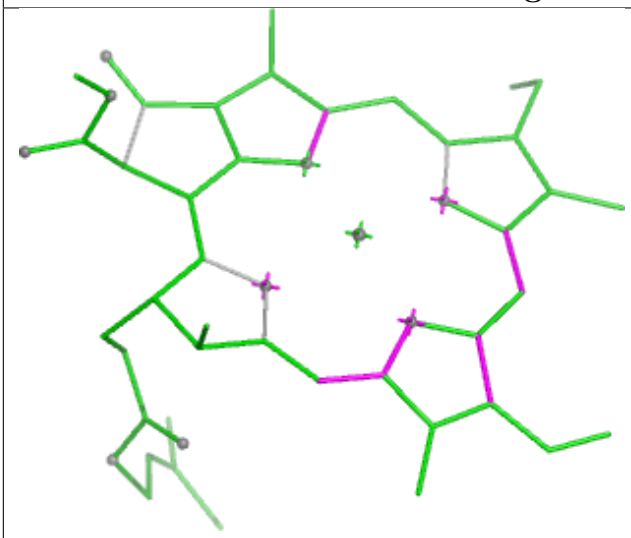


Torsions

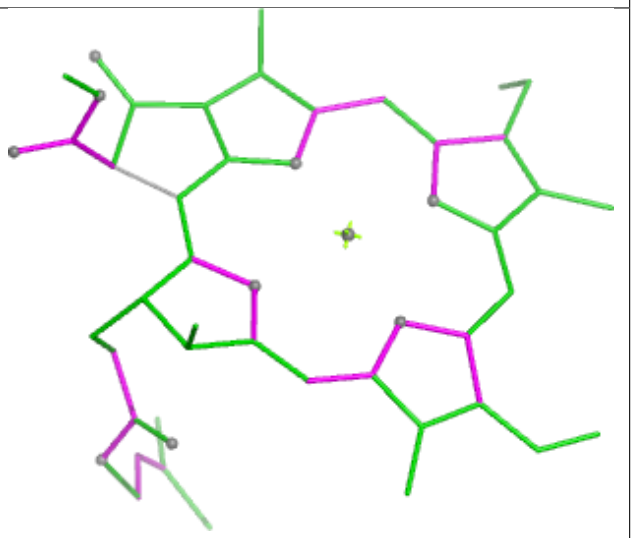


Rings

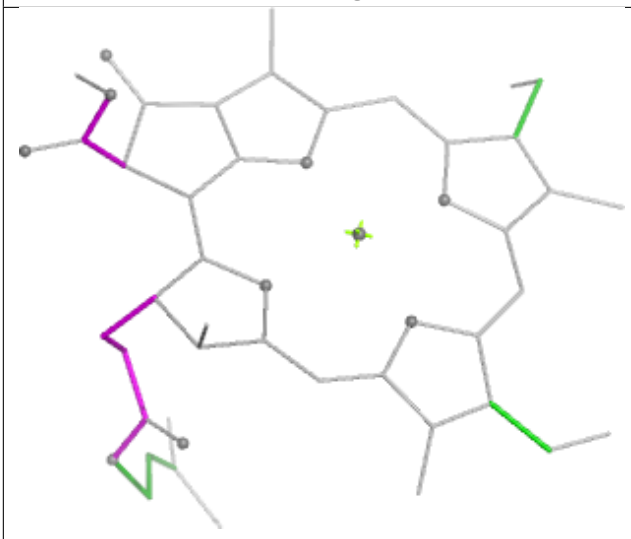
Ligand CLA B 819



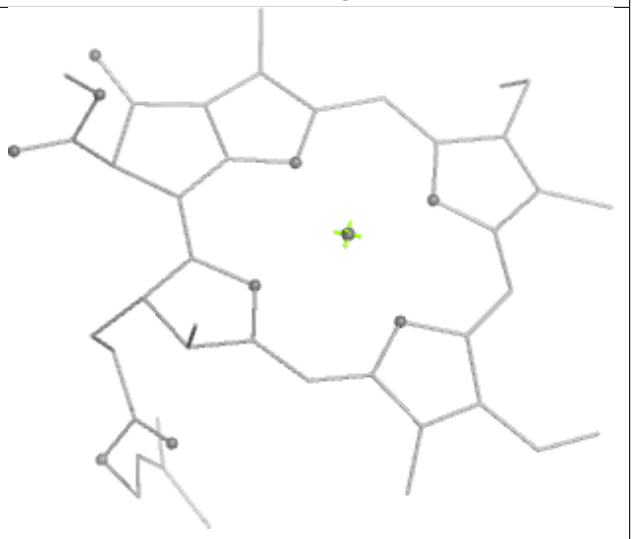
Bond lengths



Bond angles



Torsions



Rings

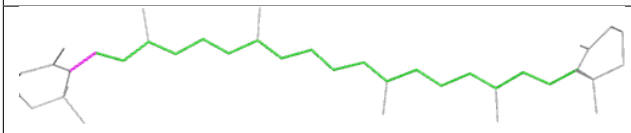
Ligand BCR L 307



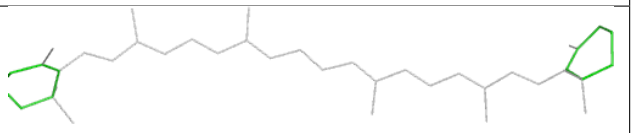
Bond lengths



Bond angles

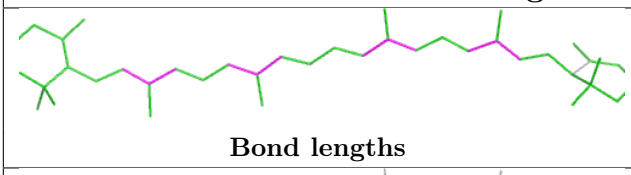


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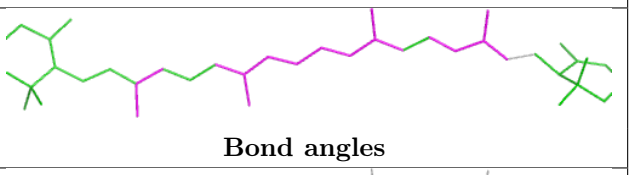


Rings

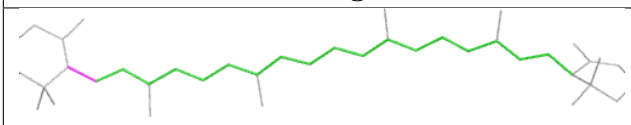
Ligand LUT Z 314



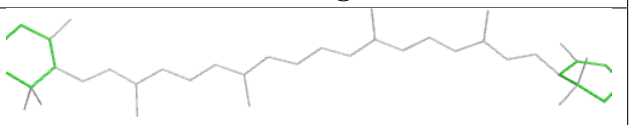
Bond lengths



Bond angles

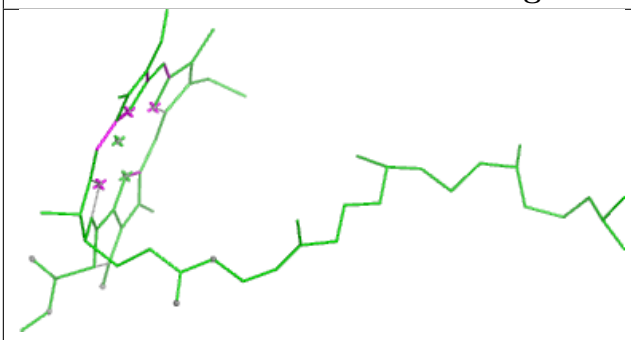


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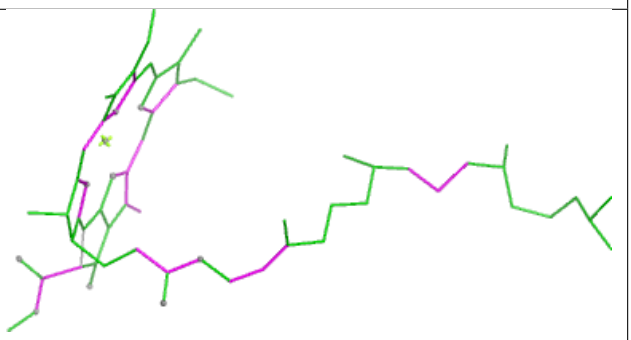


Rings

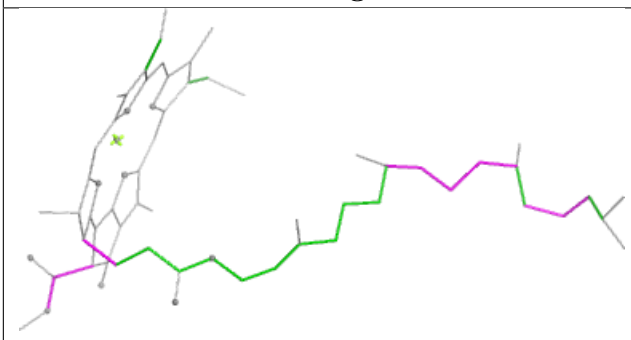
Ligand CLA A 811



Bond lengths



Bond angles

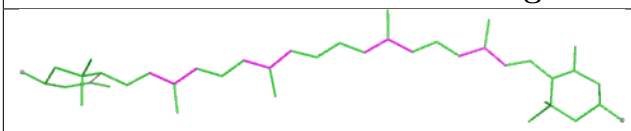


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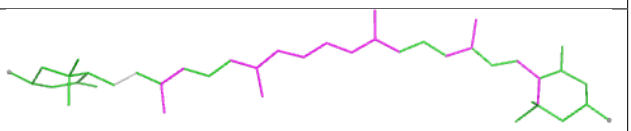


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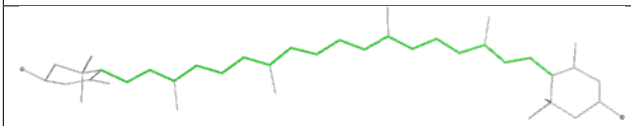
Ligand LUT X 614



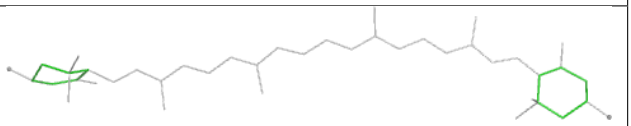
Bond lengths



Bond angles

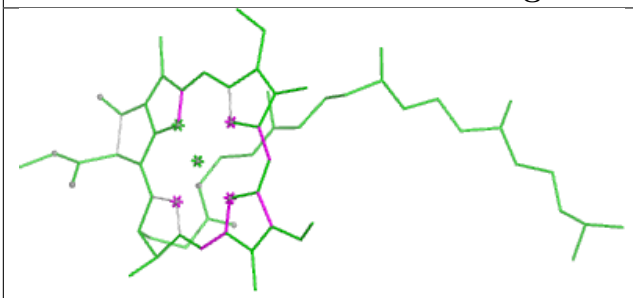


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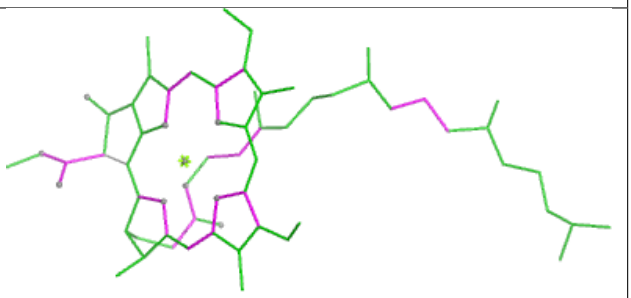


Rings

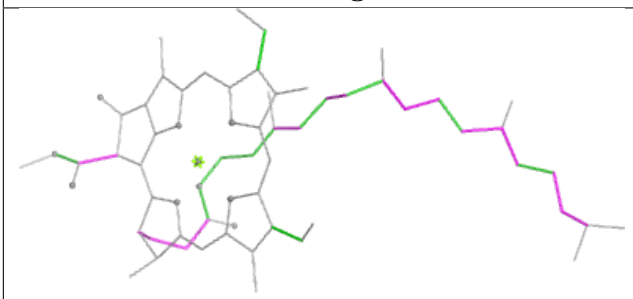
Ligand CLA A 841



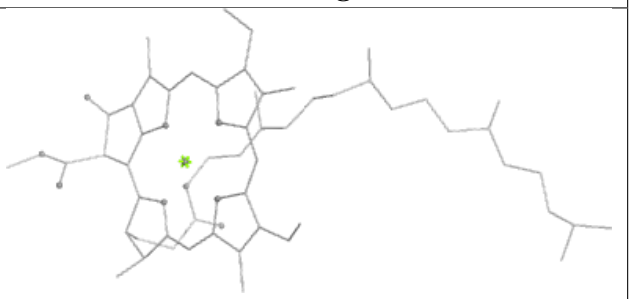
Bond lengths



Bond angles

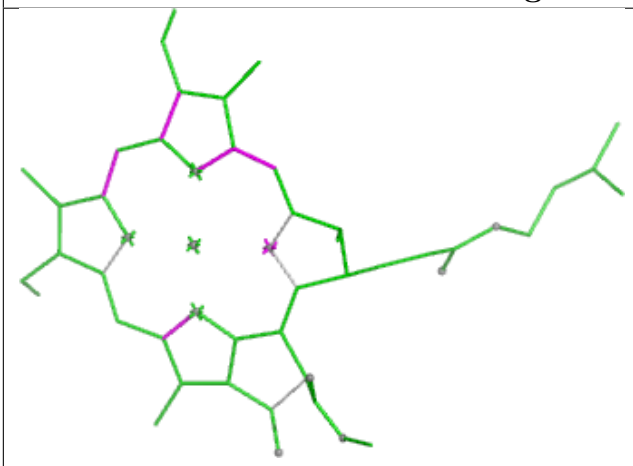


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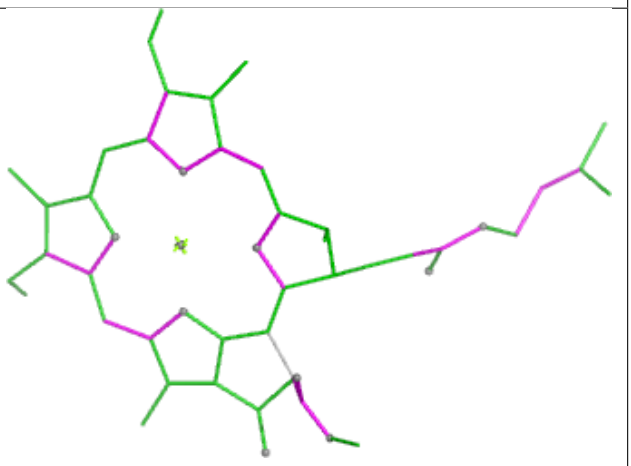


Rings

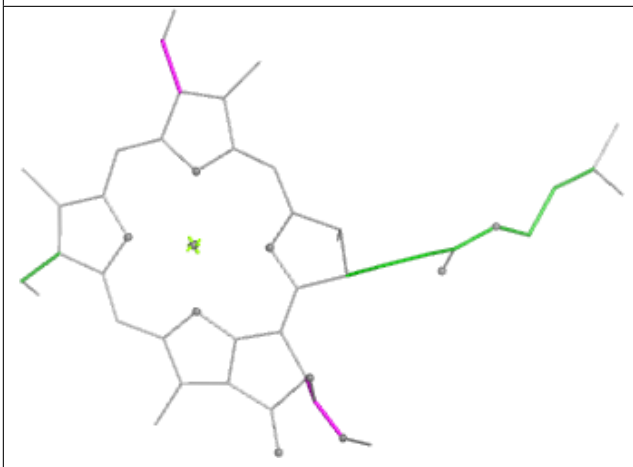
Ligand CLA B 824



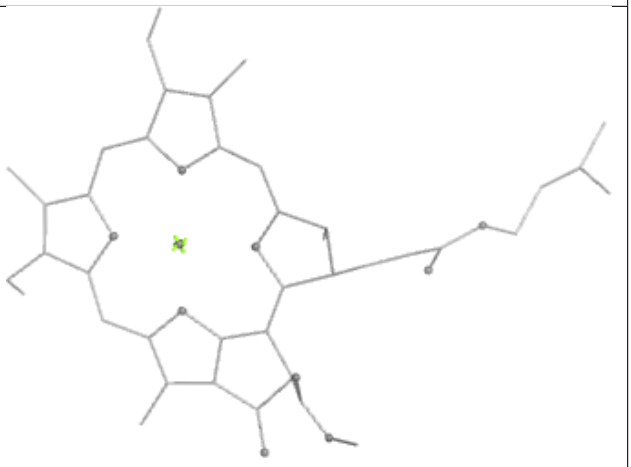
Bond lengths



Bond angles

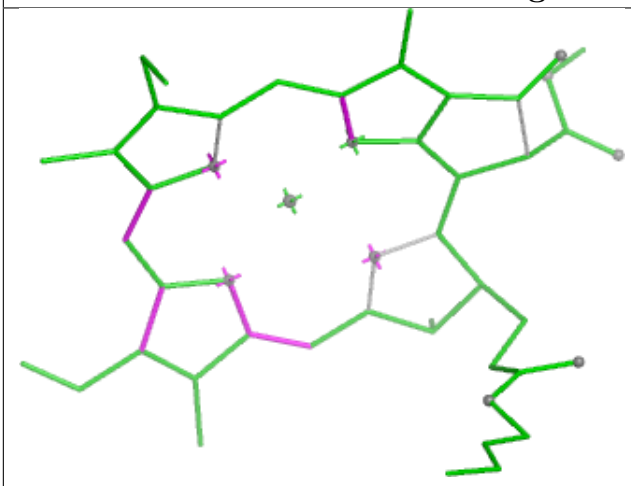


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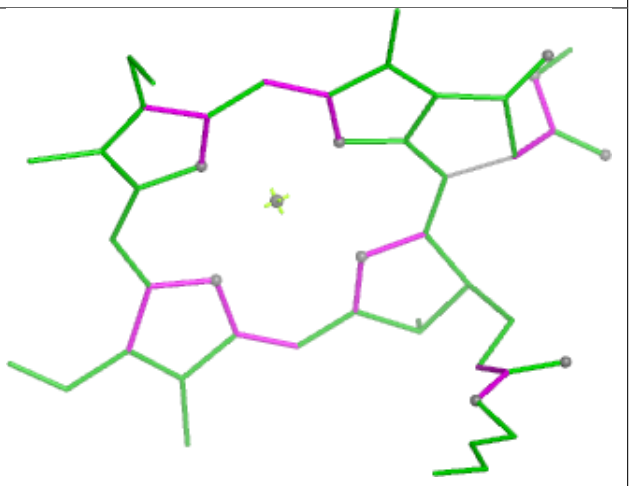


Rings

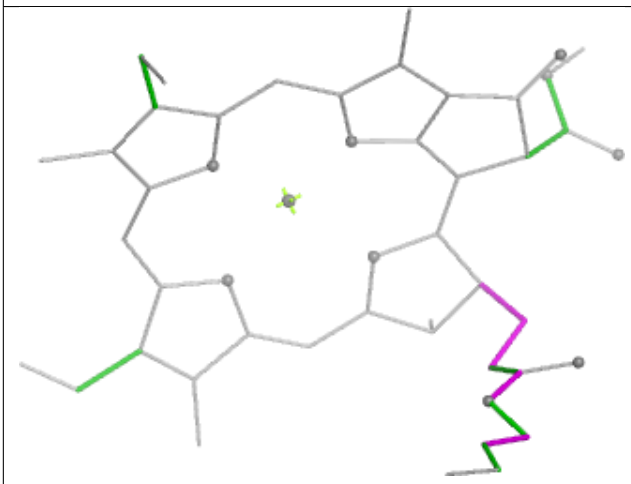
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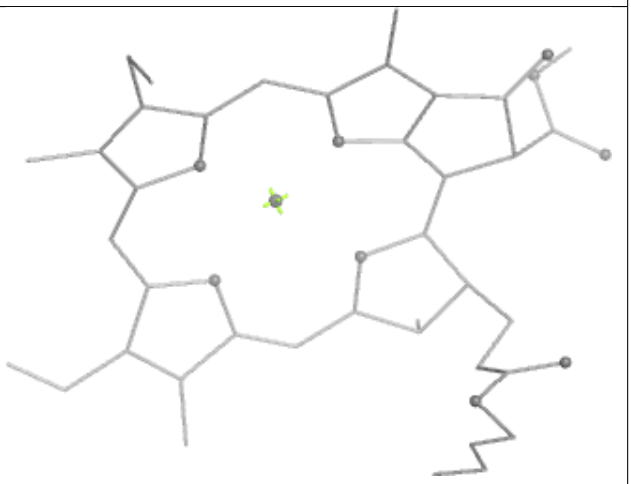
Bond lengths



Bond angles

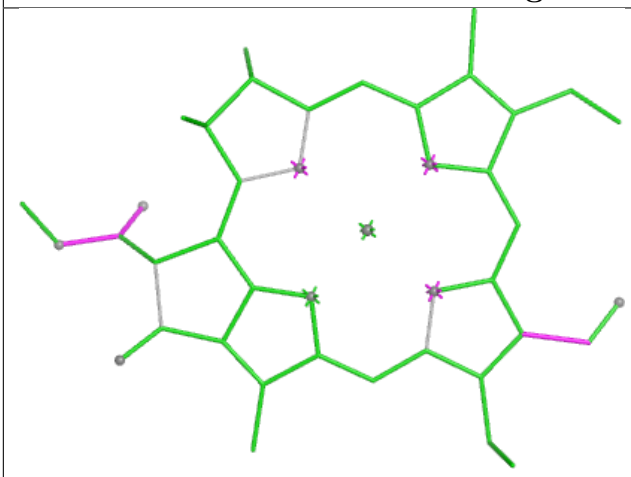


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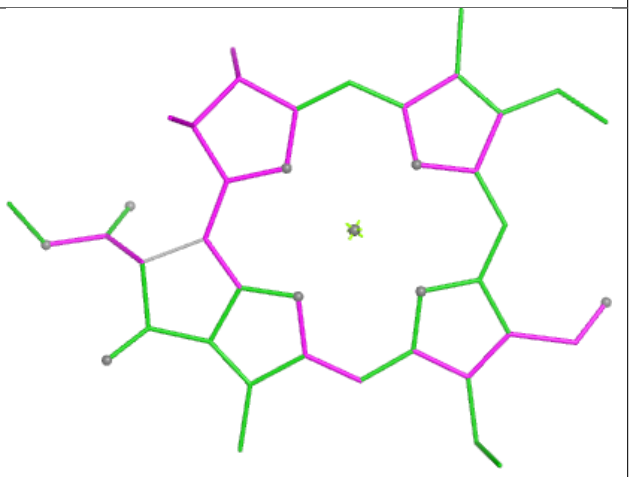


Rings

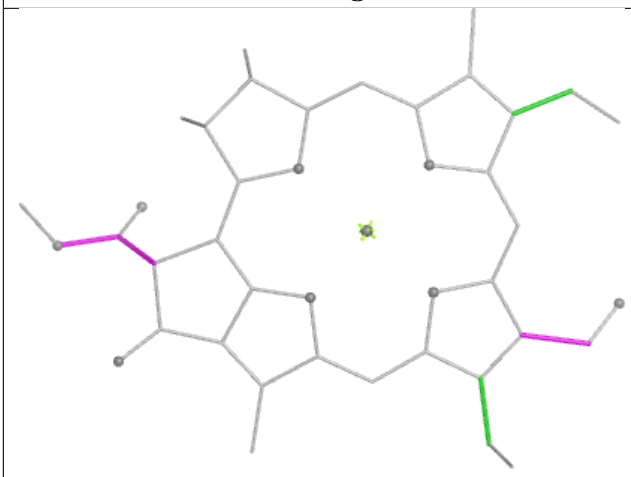
Ligand CHL Z 308



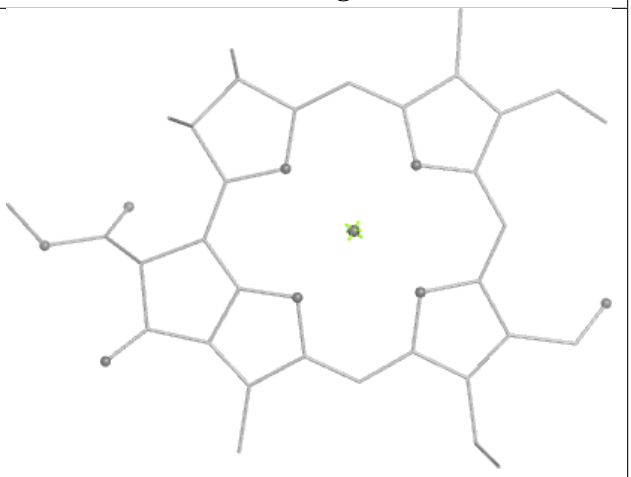
Bond lengths



Bond angles

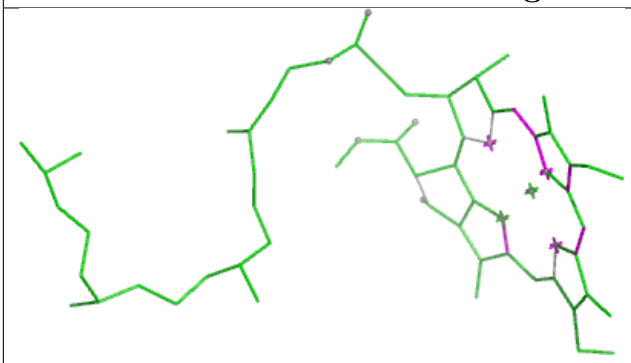


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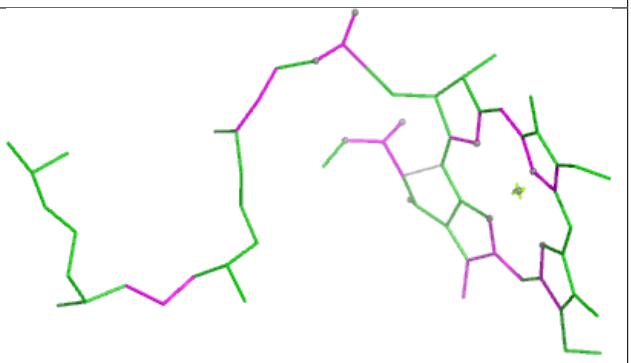


Rings

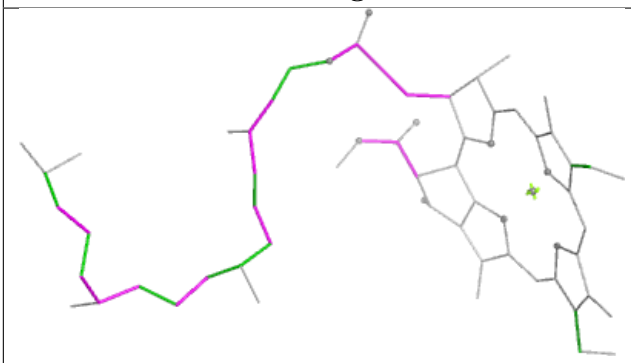
Ligand CLA A 801



Bond lengths



Bond angles

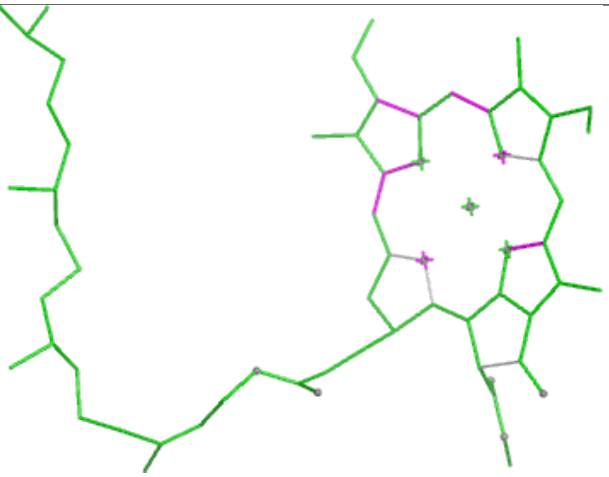


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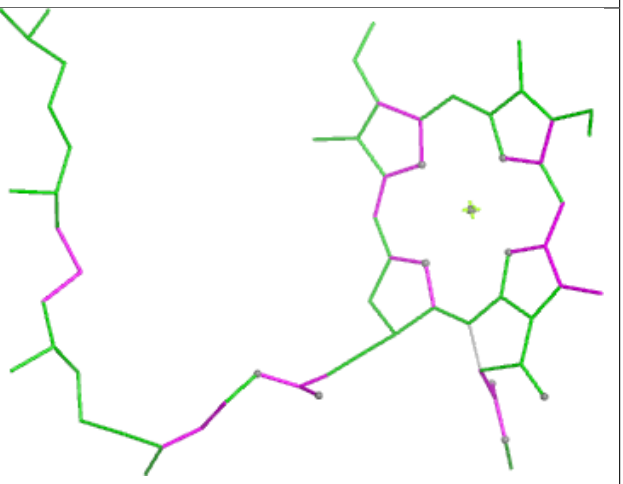


Rings

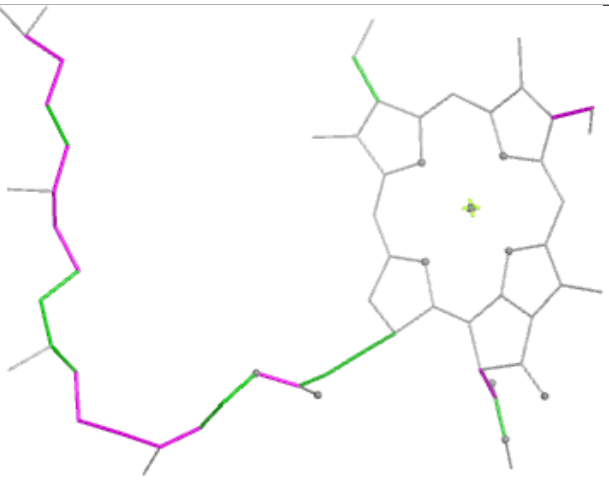
Ligand CLA A 826



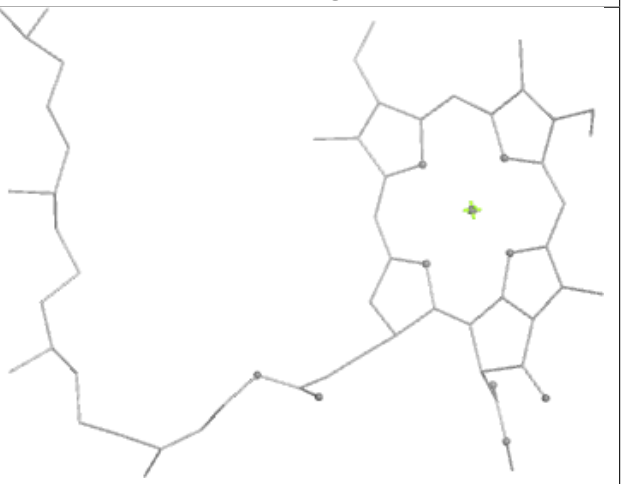
Bond lengths



Bond angles

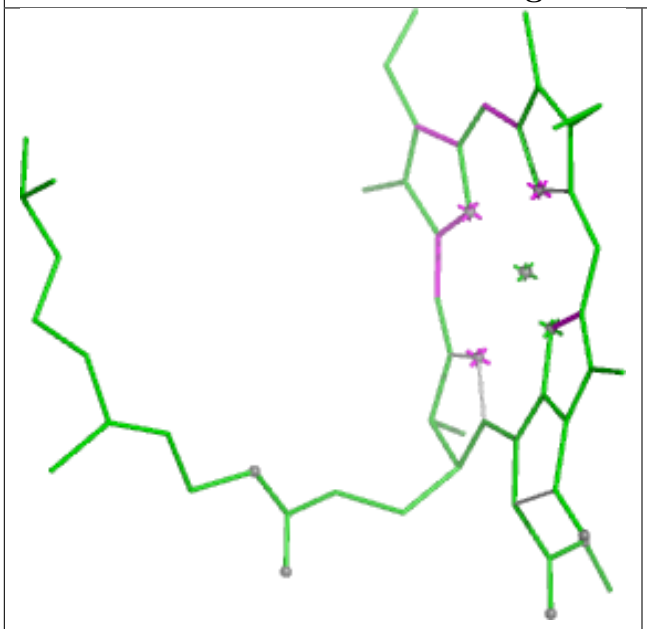


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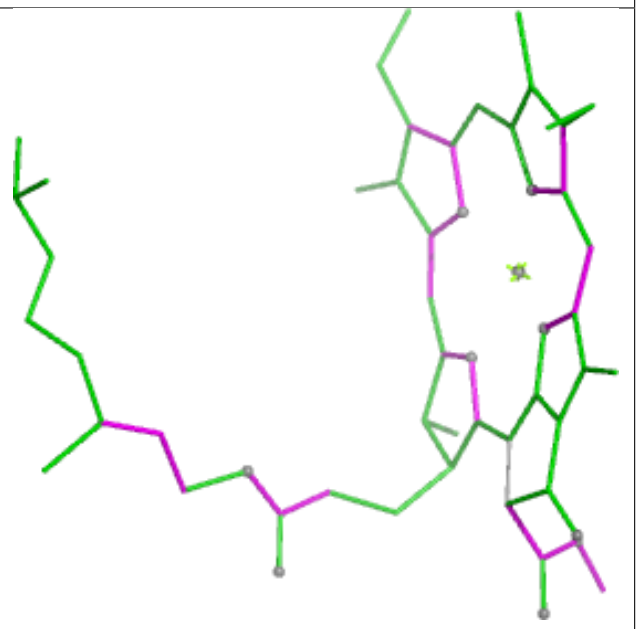


Rings

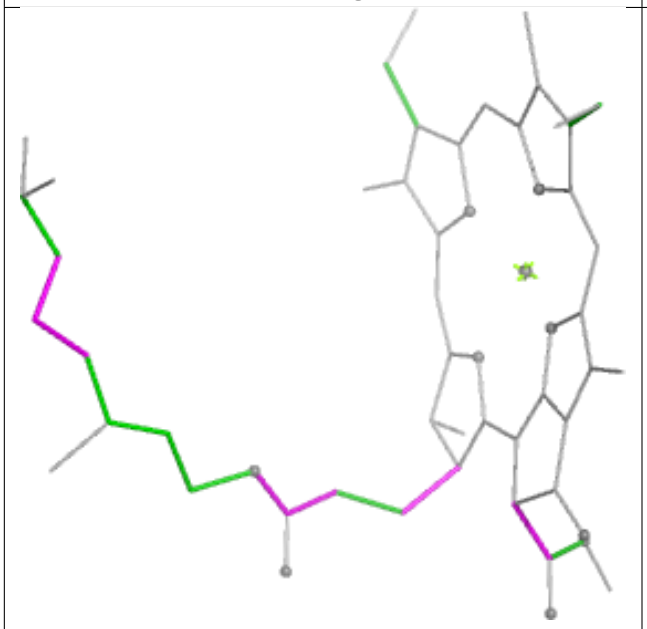
Ligand CLA B 814



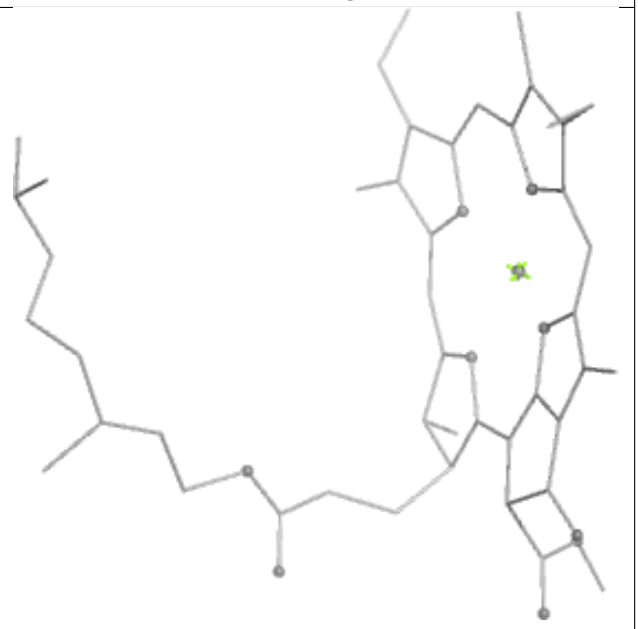
Bond lengths



Bond angles

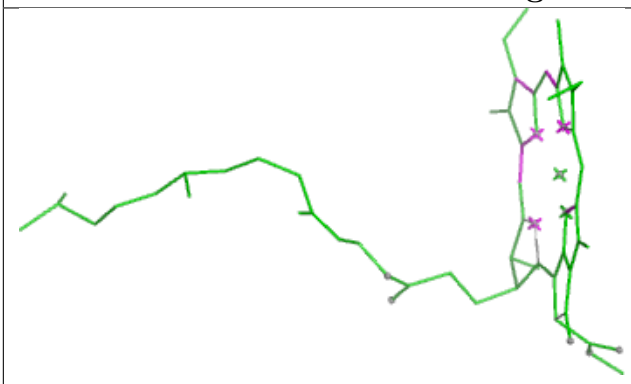


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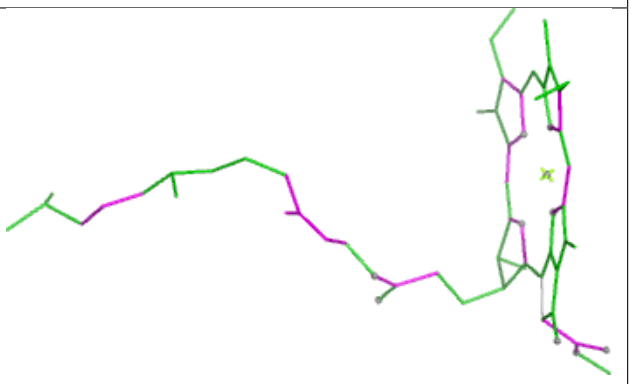


Rings

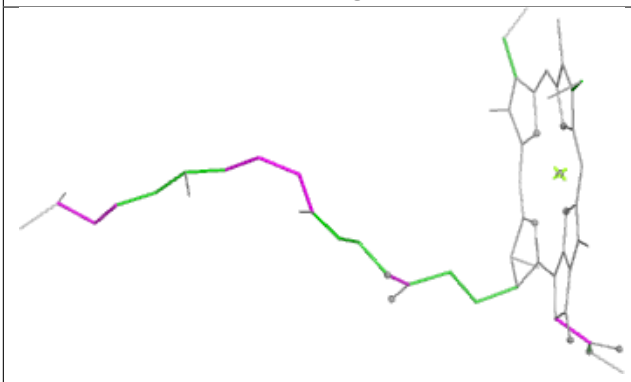
Ligand CLA L 304



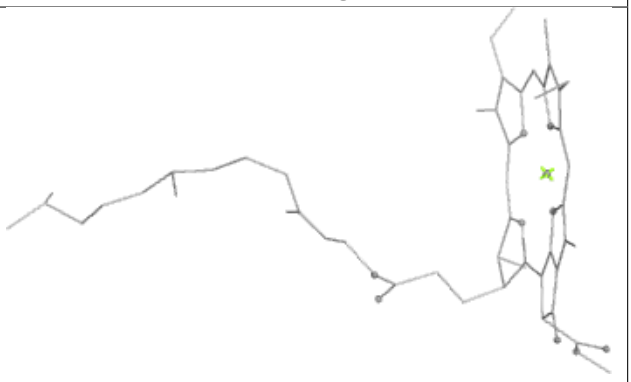
Bond lengths



Bond angles

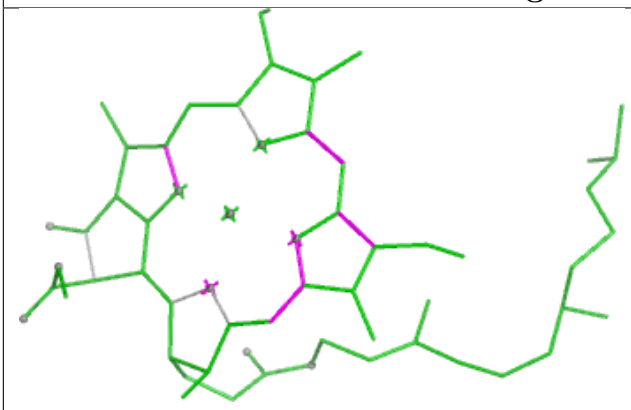


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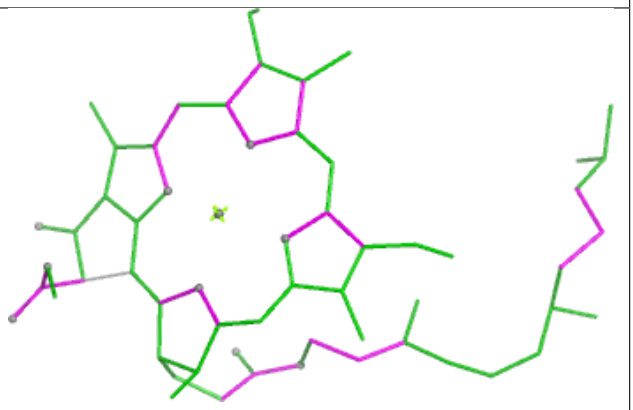


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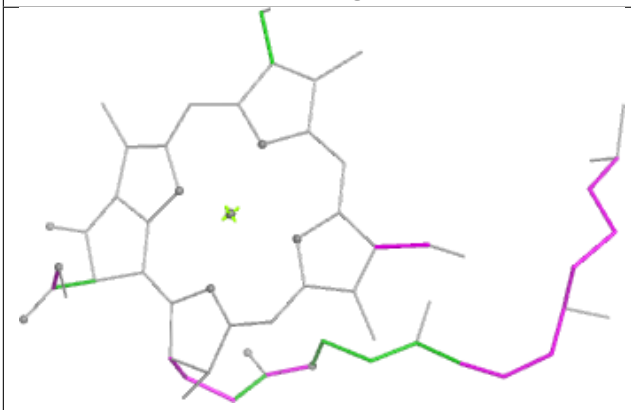
Ligand CLA Z 303



Bond lengths



Bond angles

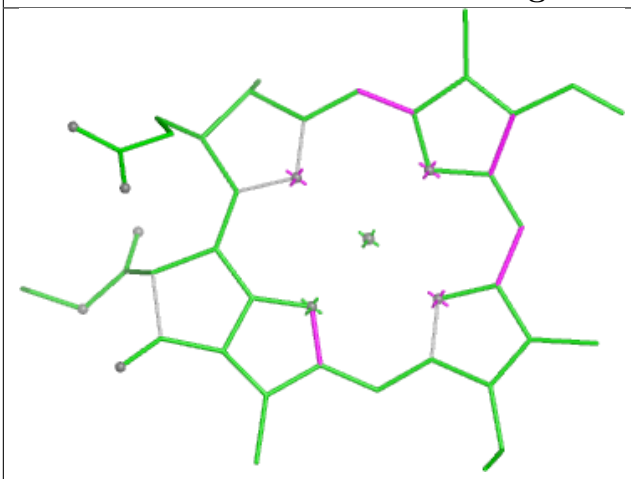


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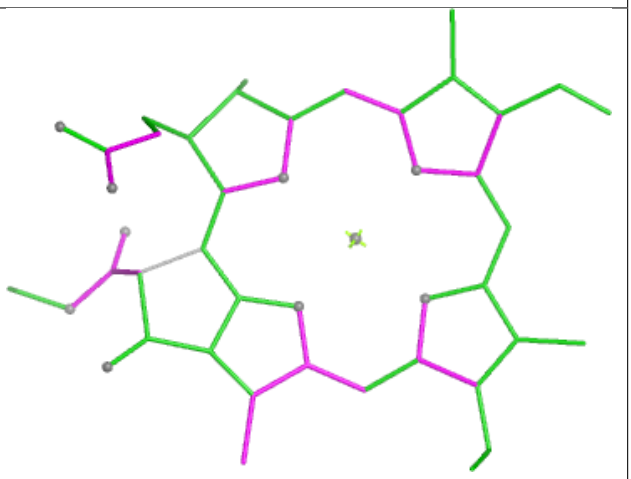


Rings

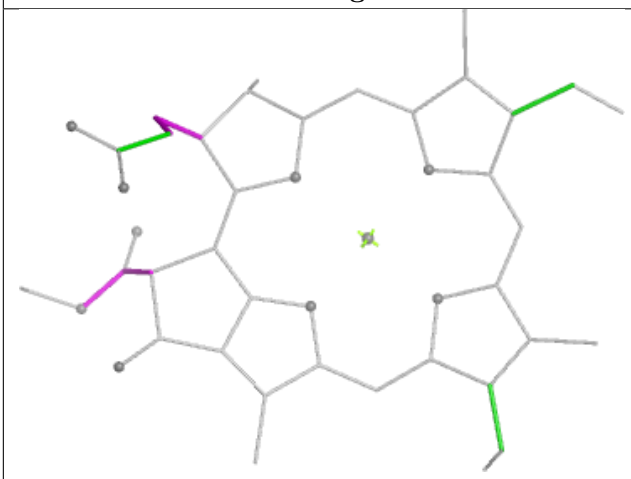
Ligand CLA 6 613



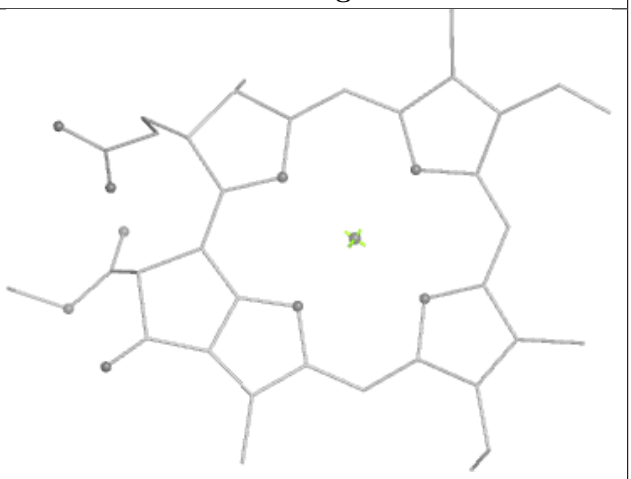
Bond lengths



Bond angles

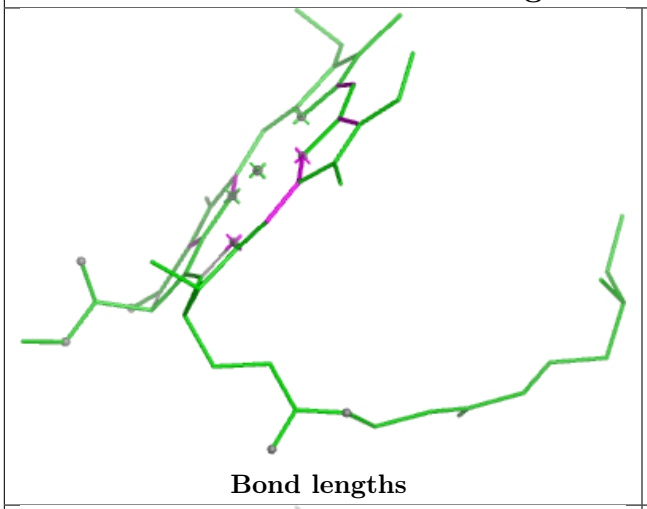


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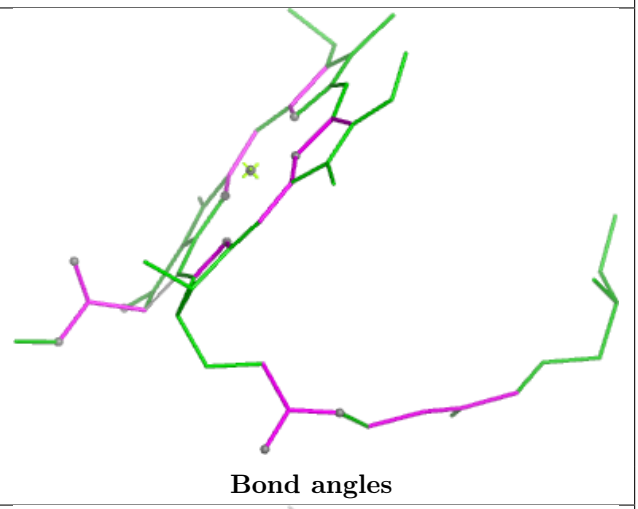


Rings

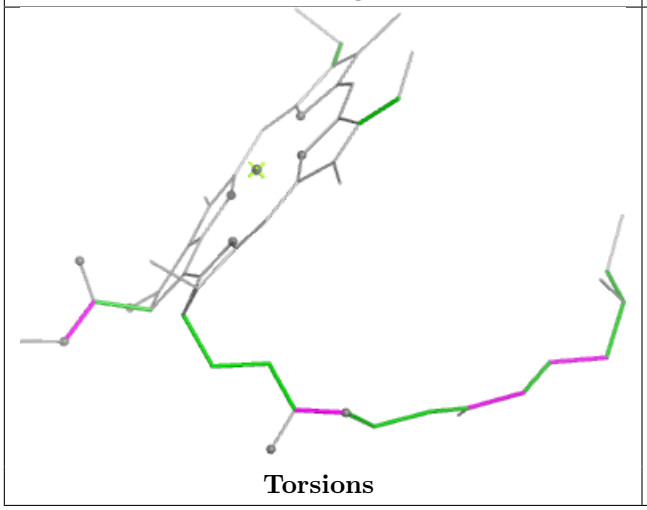
Ligand CLA A 832



Bond lengths



Bond angles

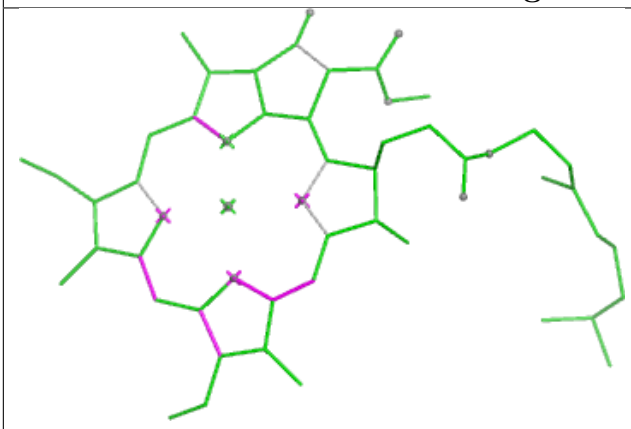


Torsions

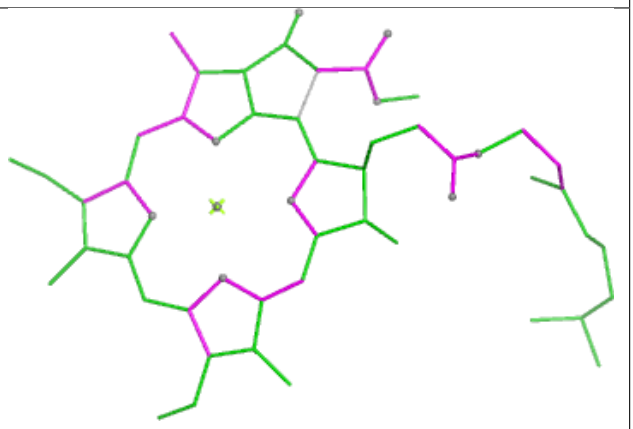


Rings

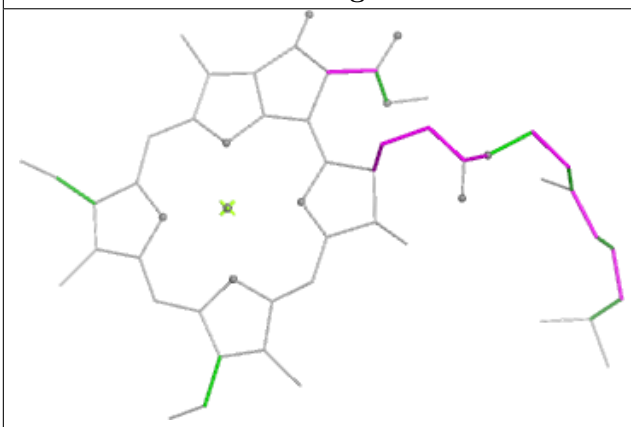
Ligand CLA A 804



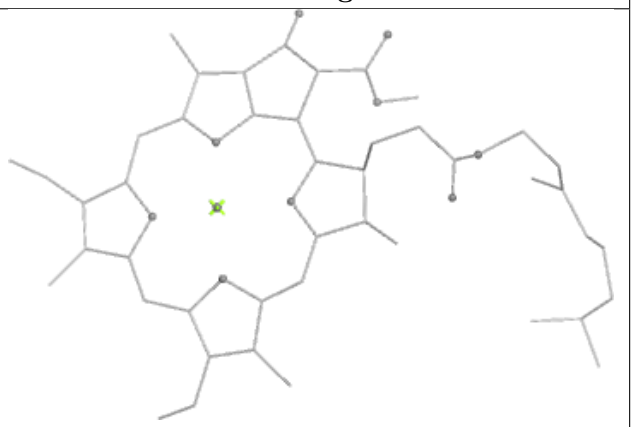
Bond lengths



Bond angles

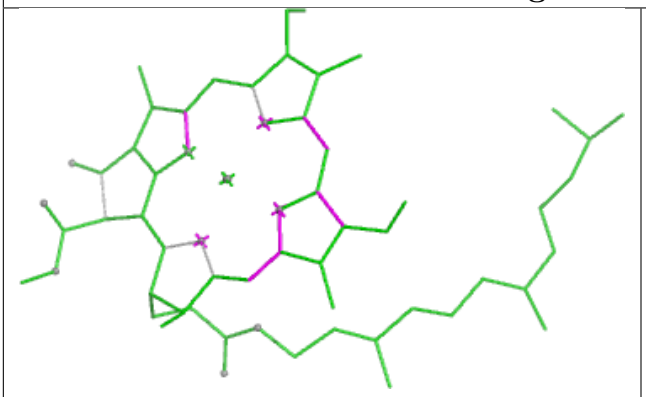


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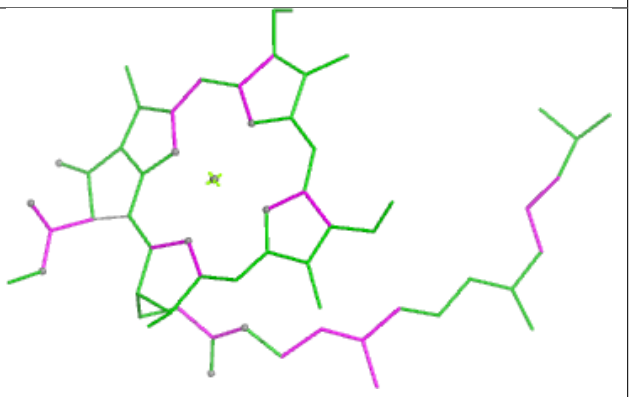


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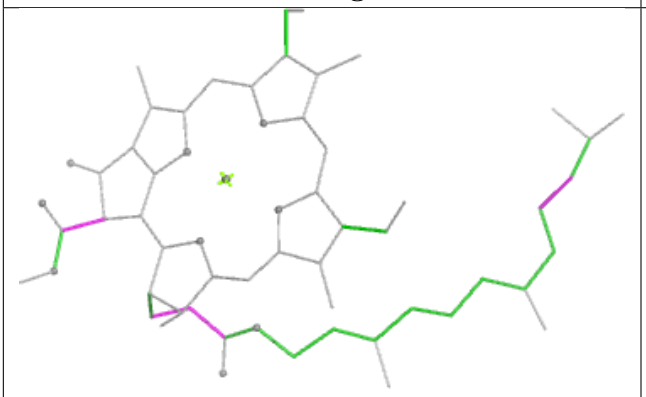
Ligand CLA 4 301



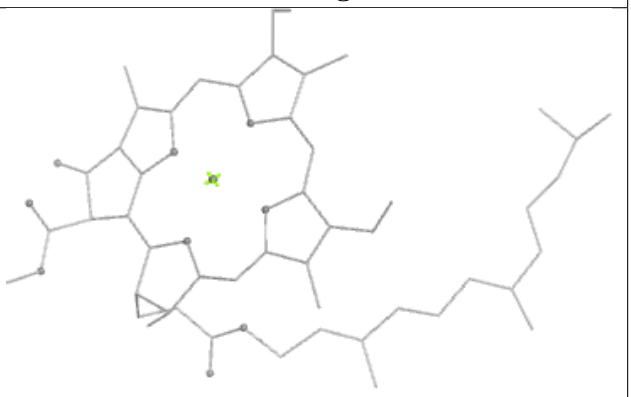
Bond lengths



Bond angles

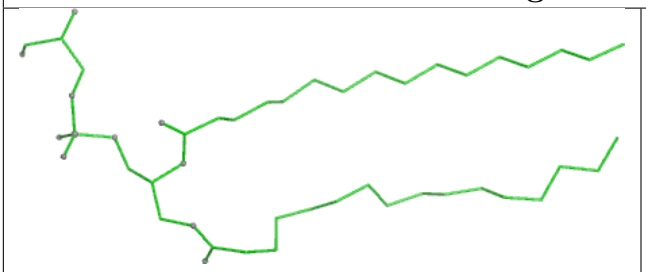


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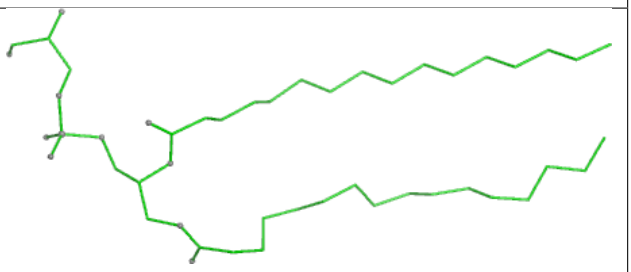


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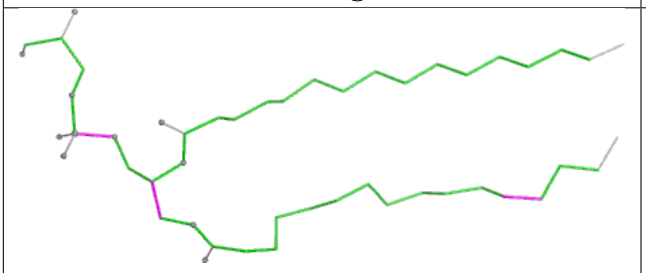
Ligand LHG 1 618



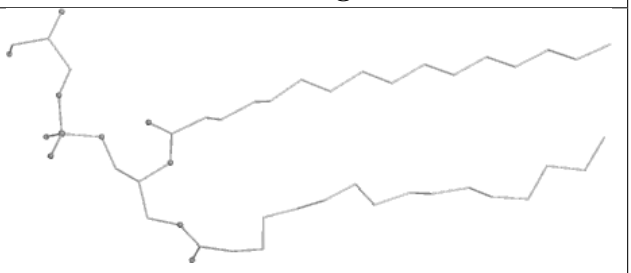
Bond lengths



Bond angles



Torsions

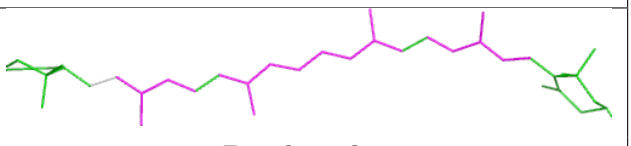


Rings

Ligand LUT 4 315



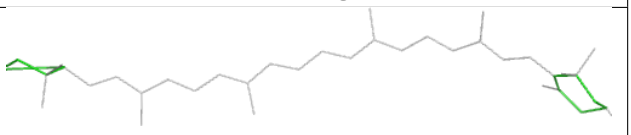
Bond lengths



Bond angles

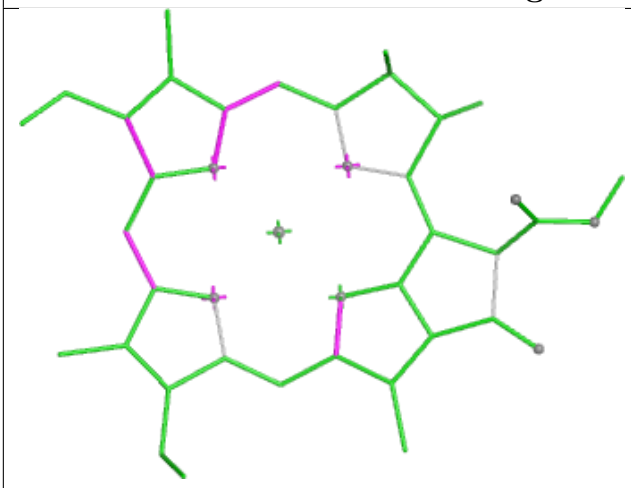


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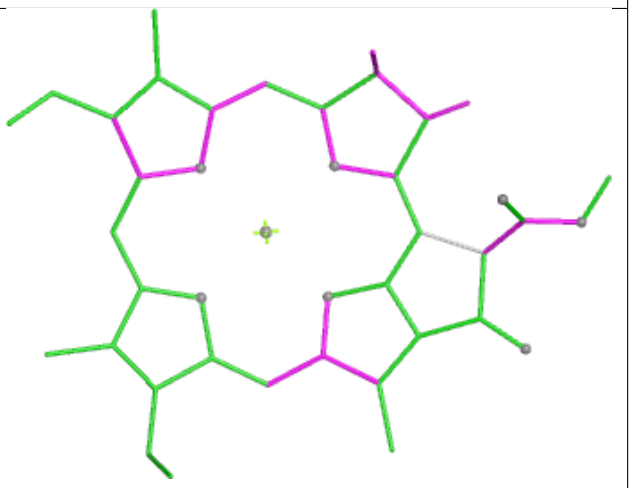


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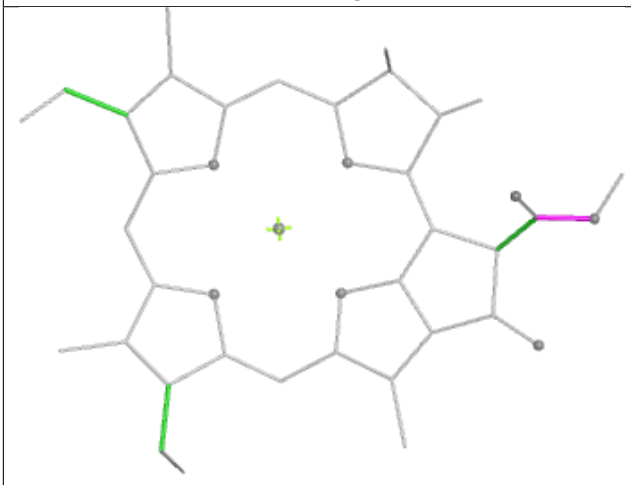
Ligand CLA F 304



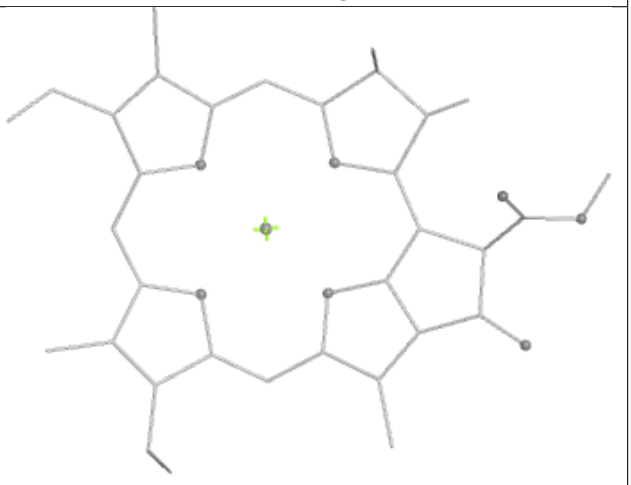
Bond lengths



Bond angles

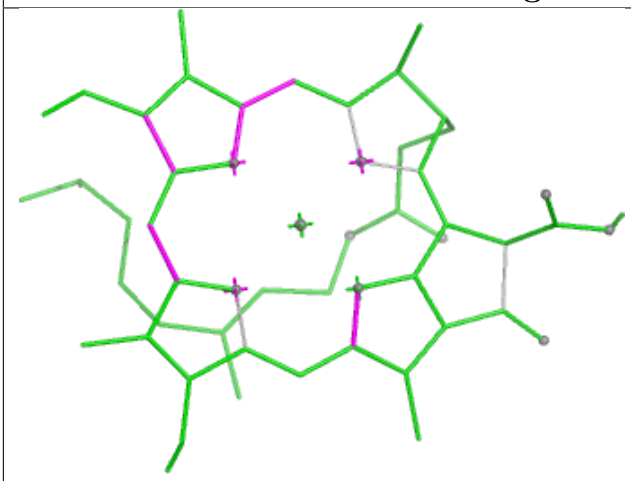


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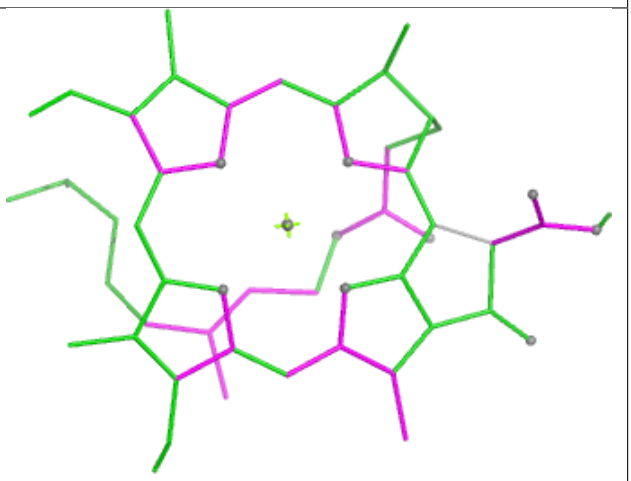


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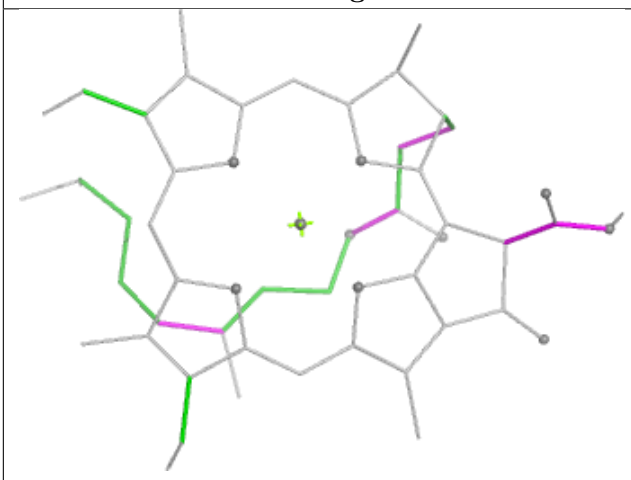
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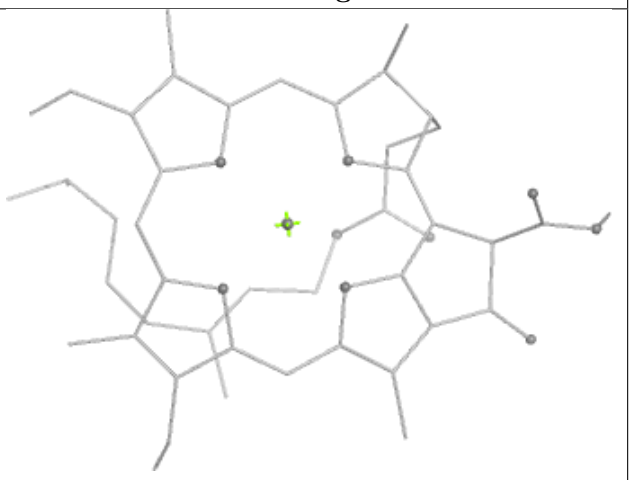
Bond lengths



Bond angles

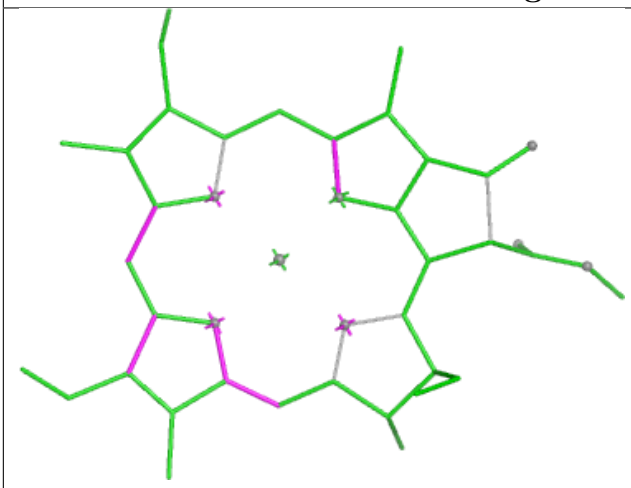


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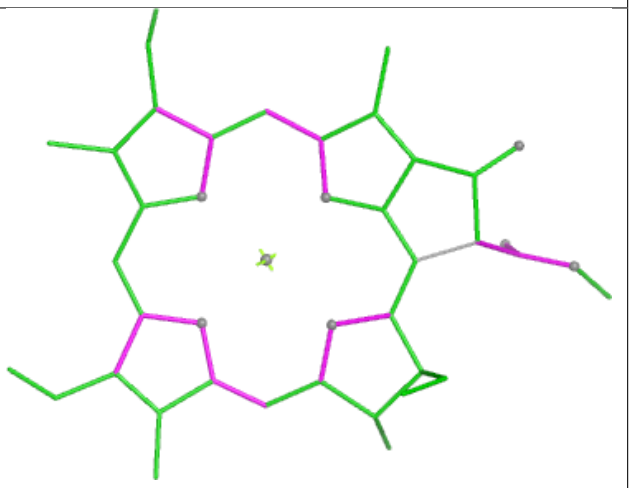


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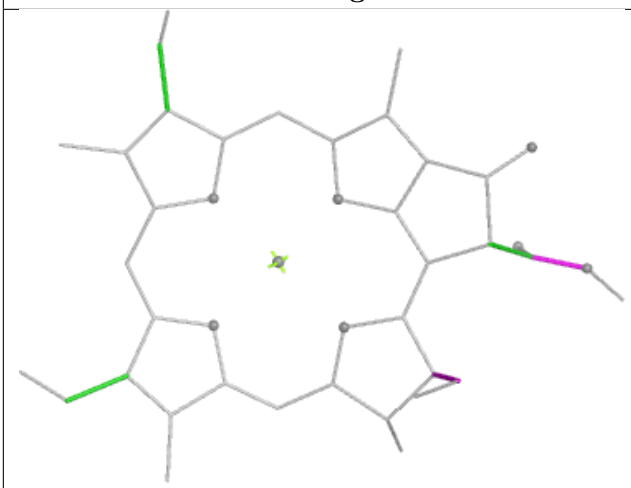
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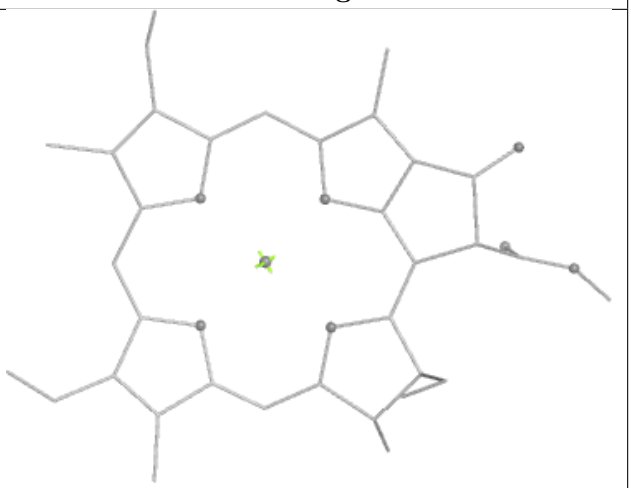
Bond lengths



Bond angles

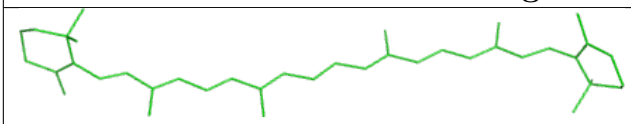


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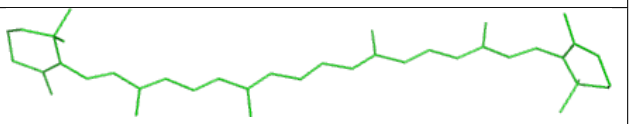


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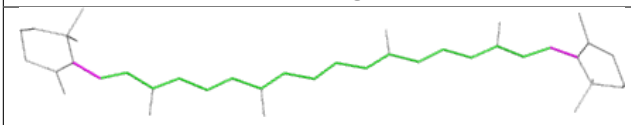
Ligand BCR O 204



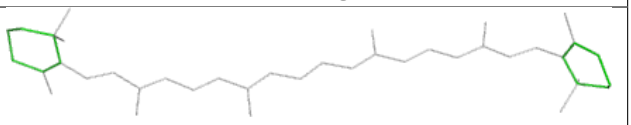
Bond lengths



Bond angles

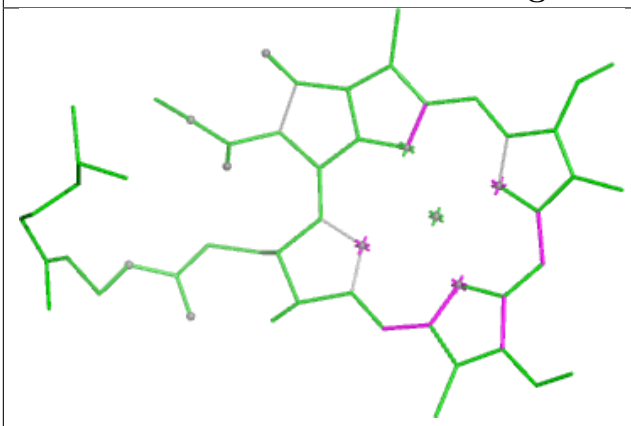


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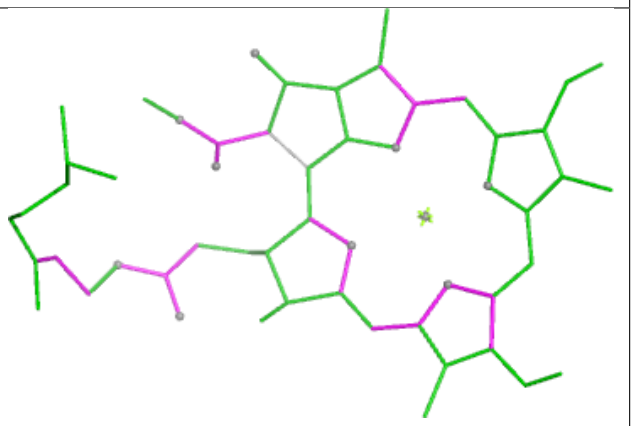


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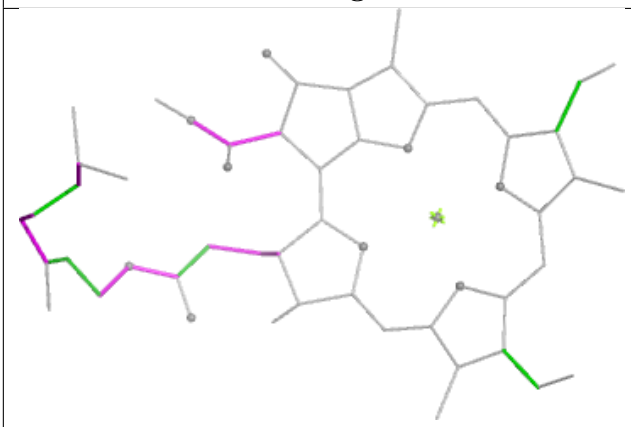
Ligand CLA 3 603



Bond lengths



Bond angles

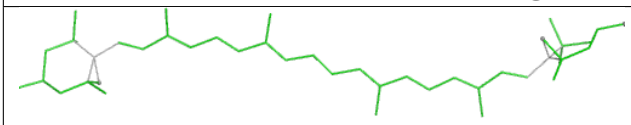


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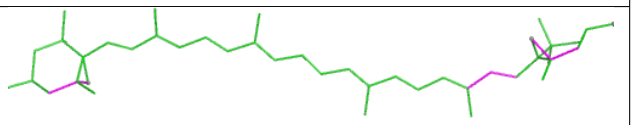


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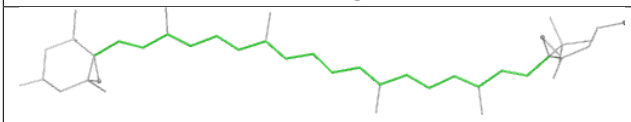
Ligand XAT 6 617



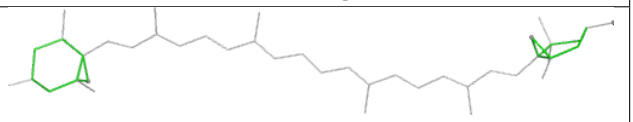
Bond lengths



Bond angles



Torsions



Rings

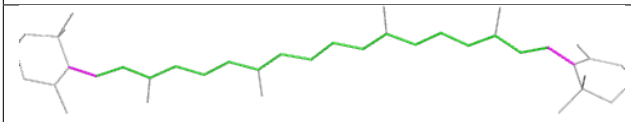
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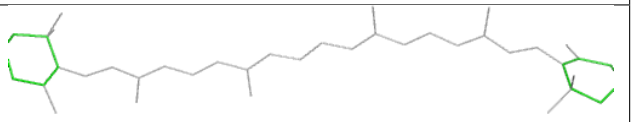
Bond lengths



Bond angles

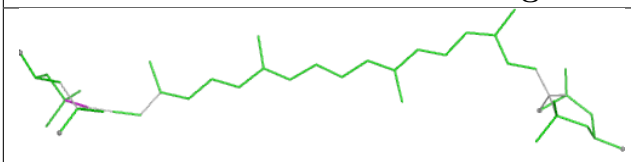


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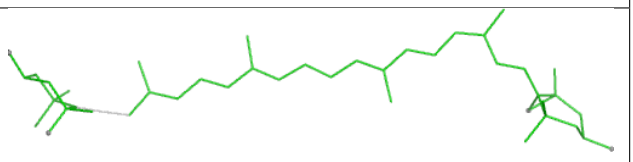


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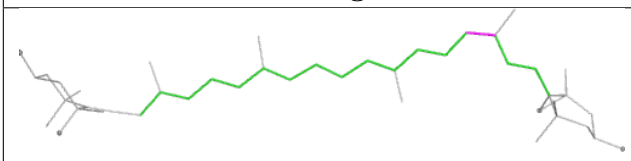
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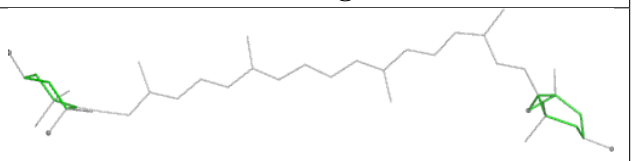
Bond lengths



Bond angles

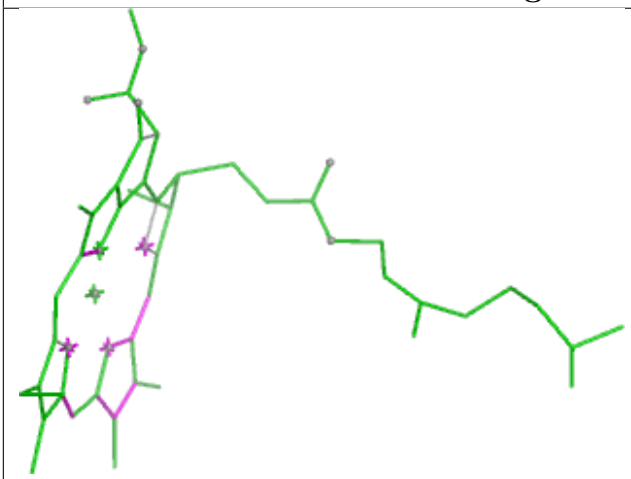


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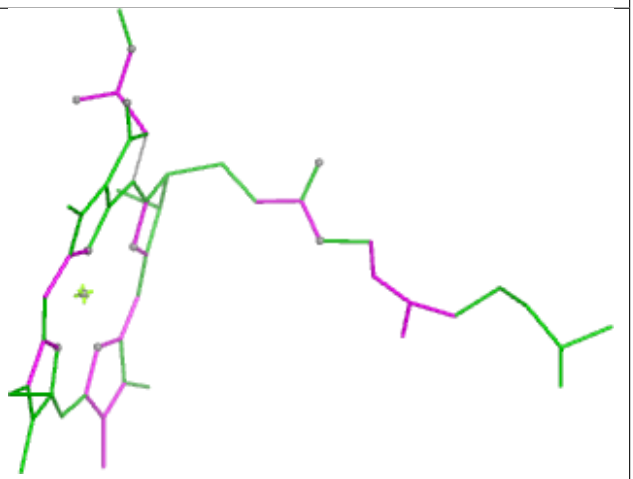


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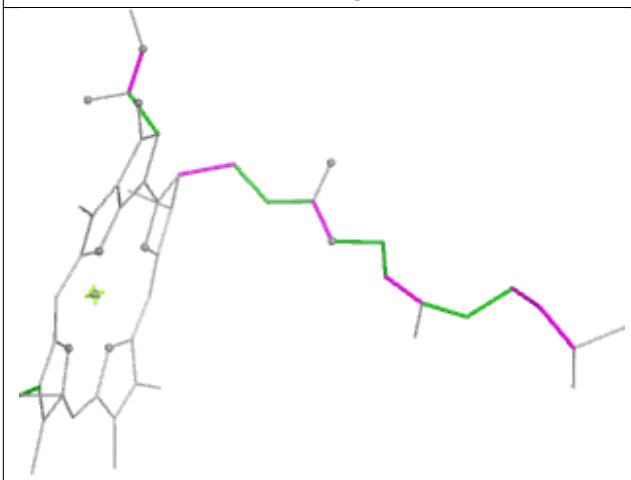
Ligand CLA B 810



Bond lengths



Bond angles

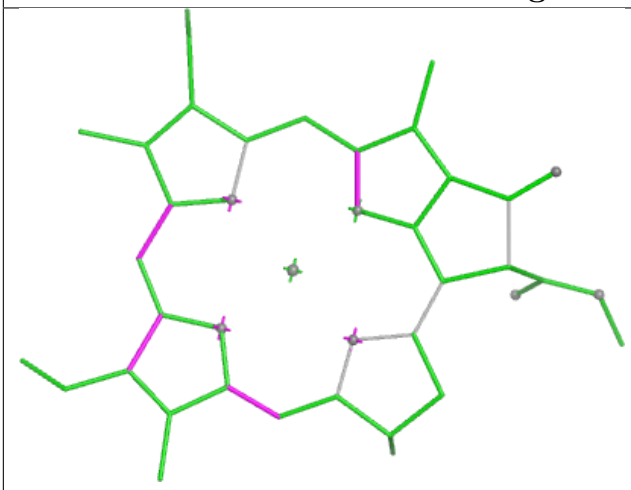


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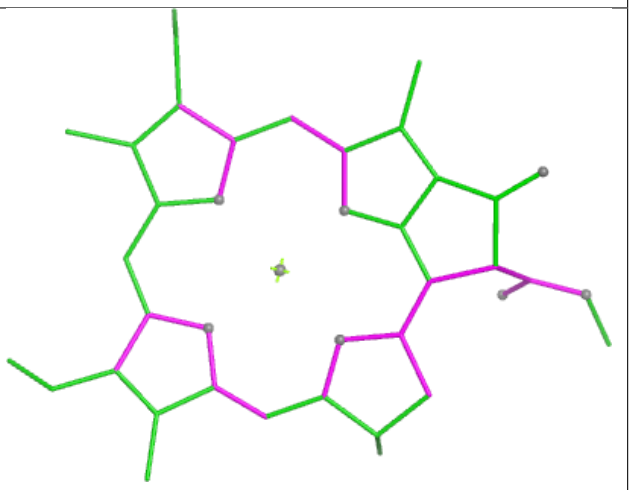


Rings

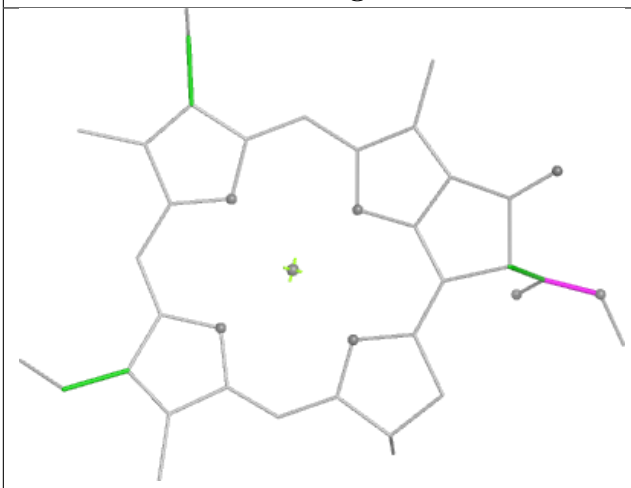
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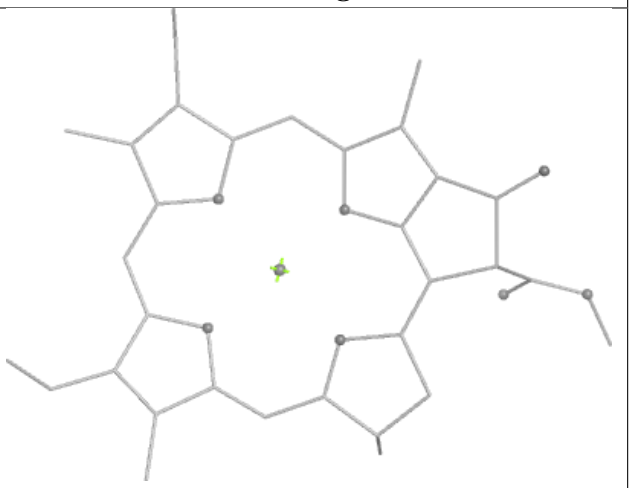
Bond lengths



Bond angles

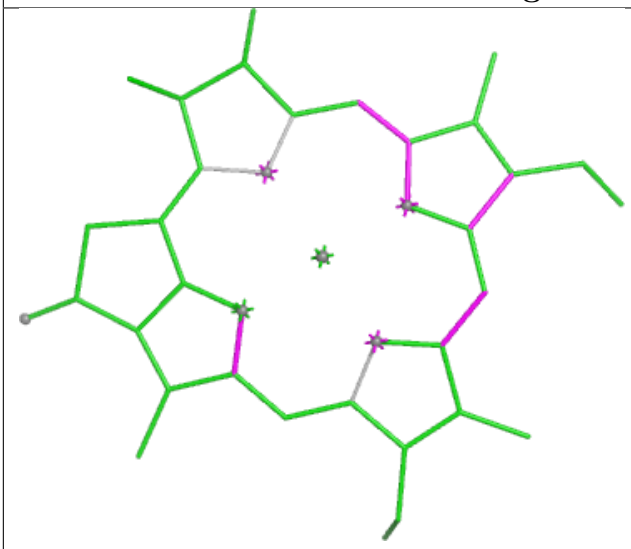


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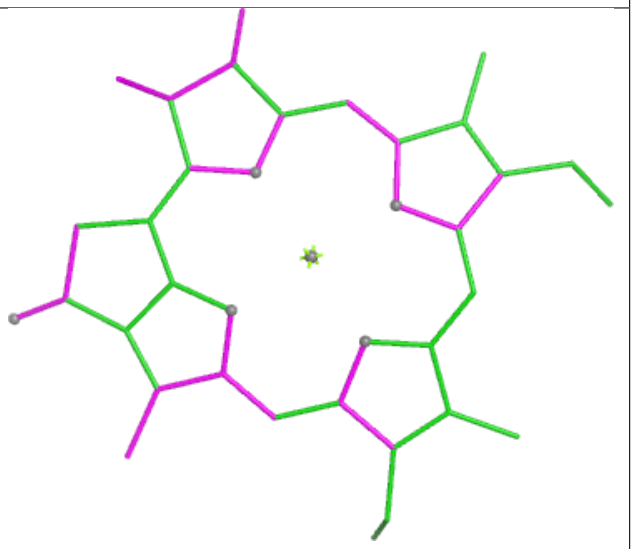


Rings

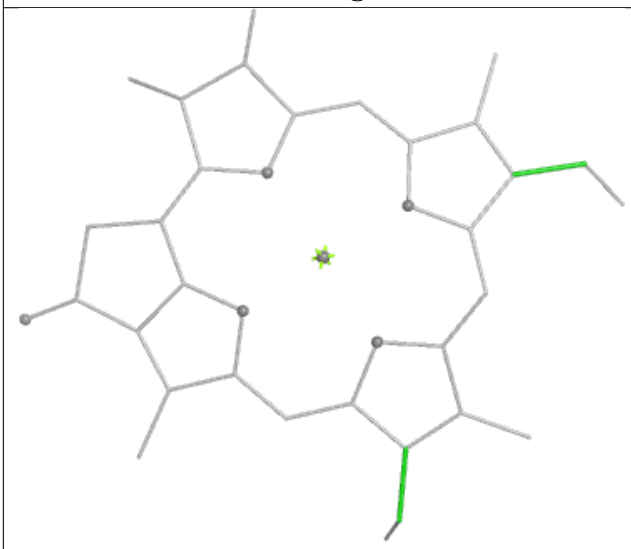
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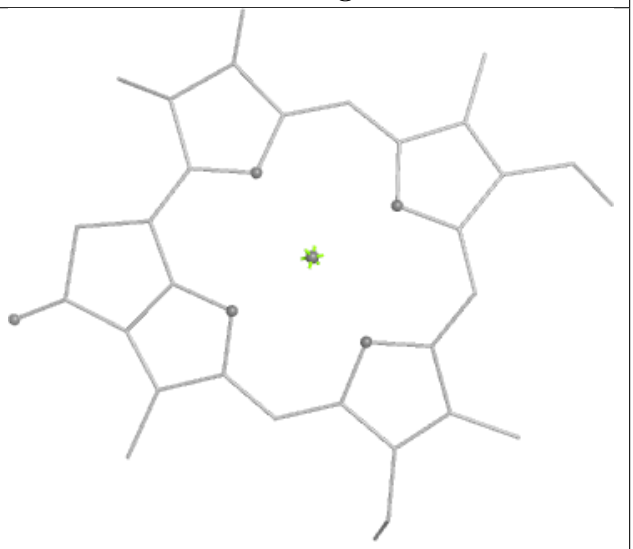
Bond lengths



Bond angles

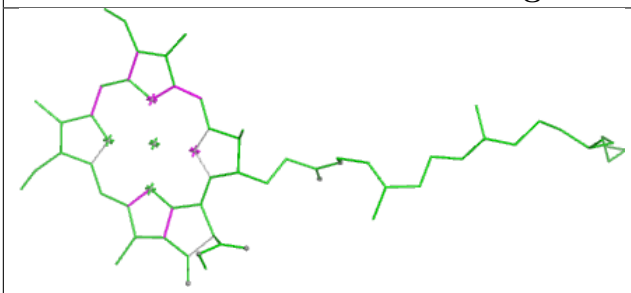


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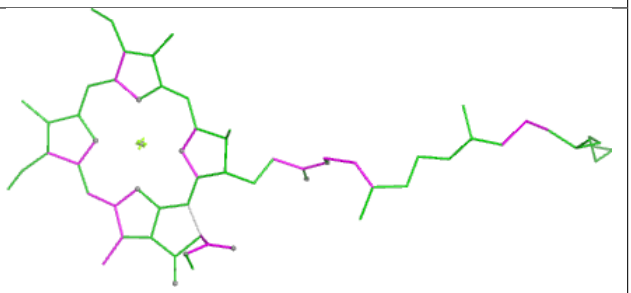


Rings

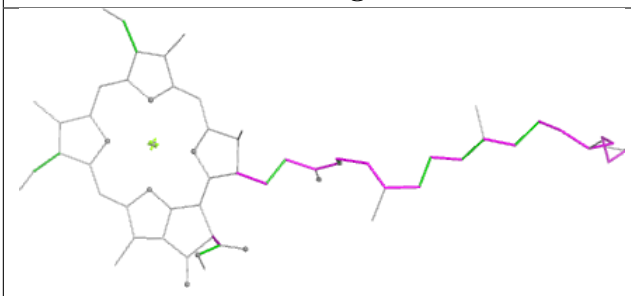
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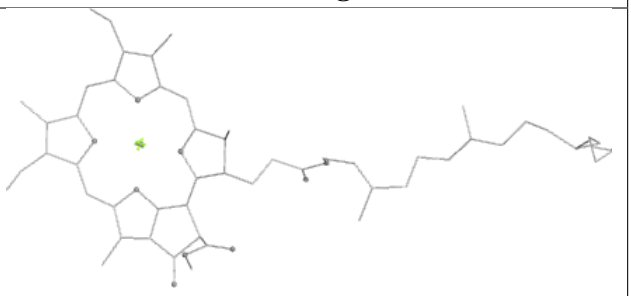
Bond lengths



Bond angles

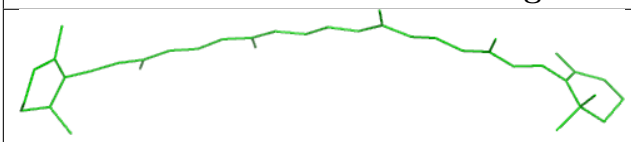


Torsions

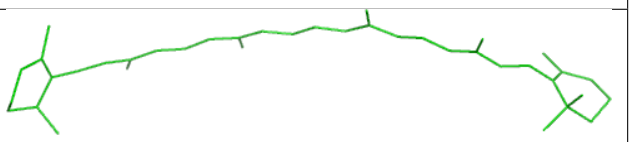


Rings

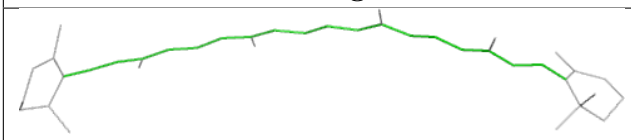
Ligand BCR F 302



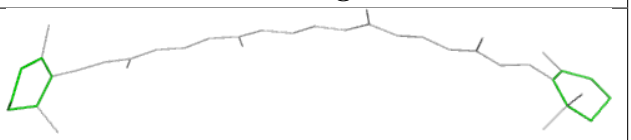
Bond lengths



Bond angles

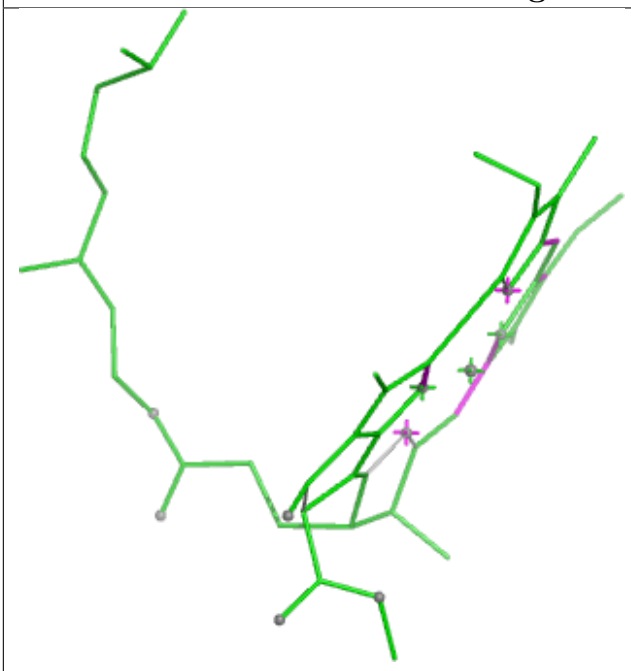


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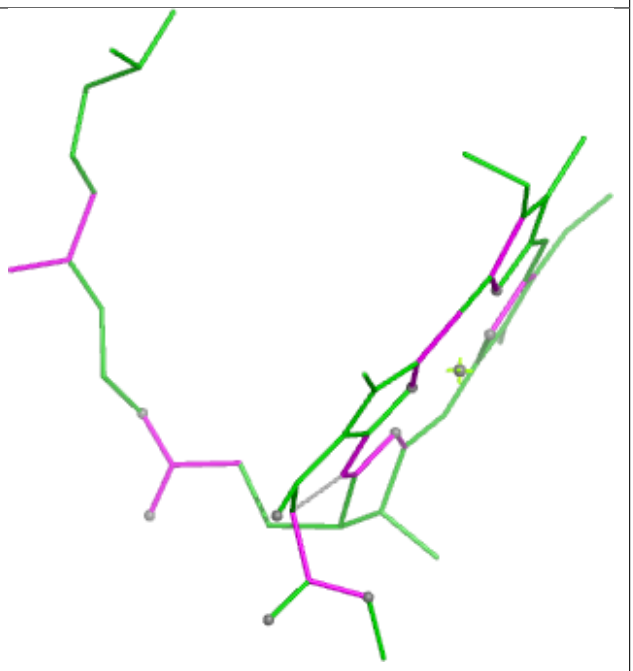


Rings

Ligand CLA 3 617



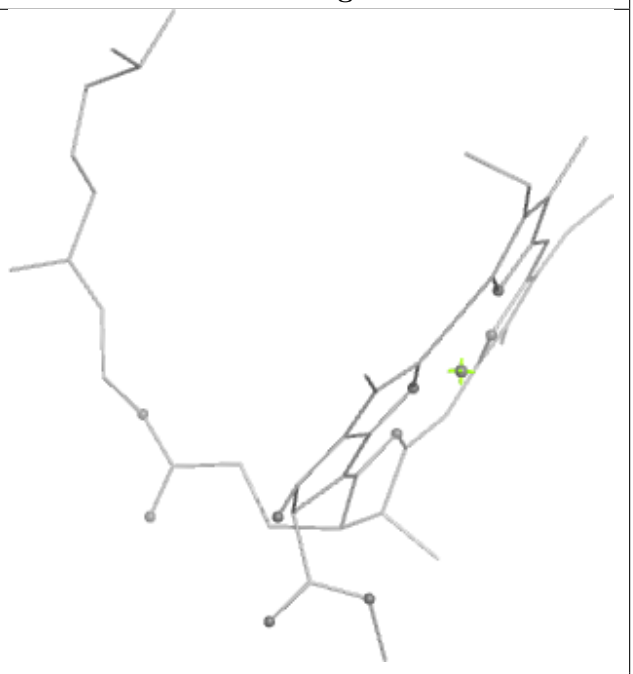
Bond lengths



Bond angles

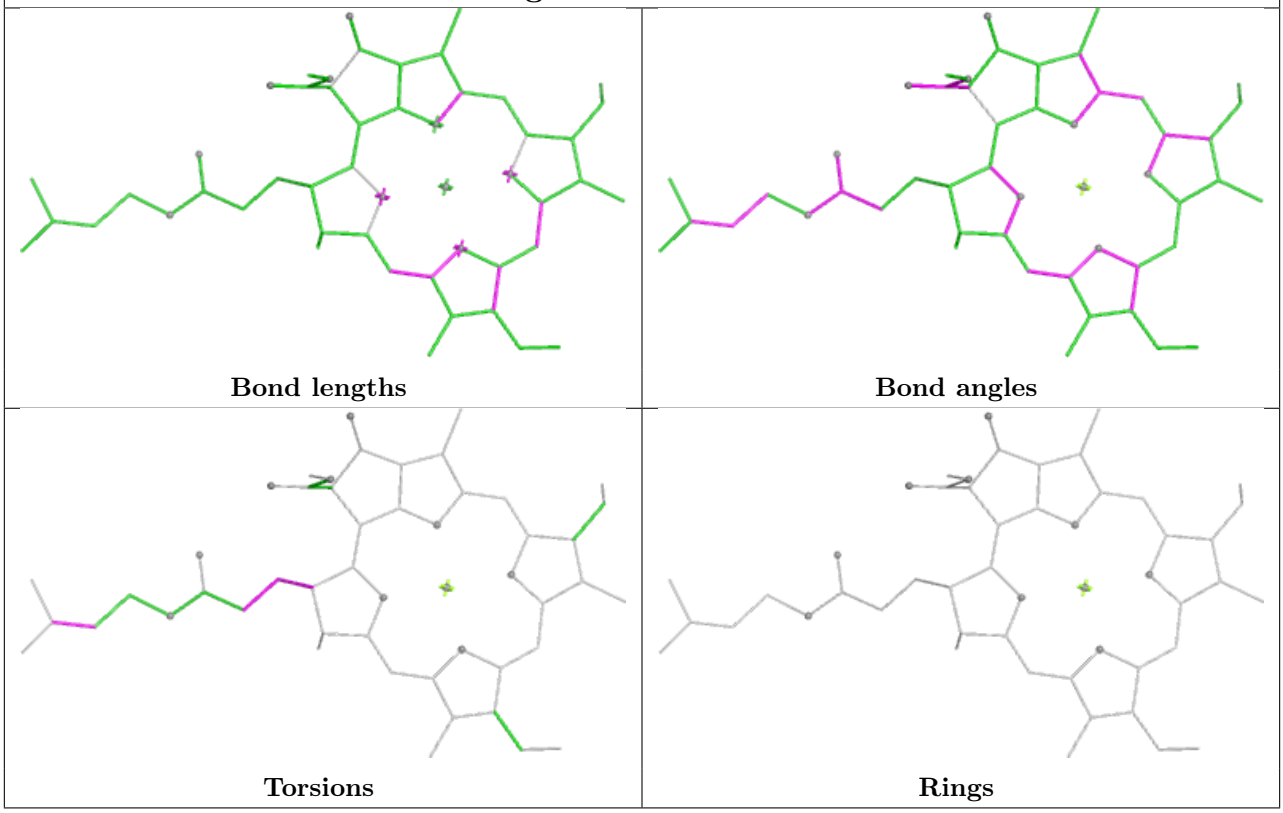


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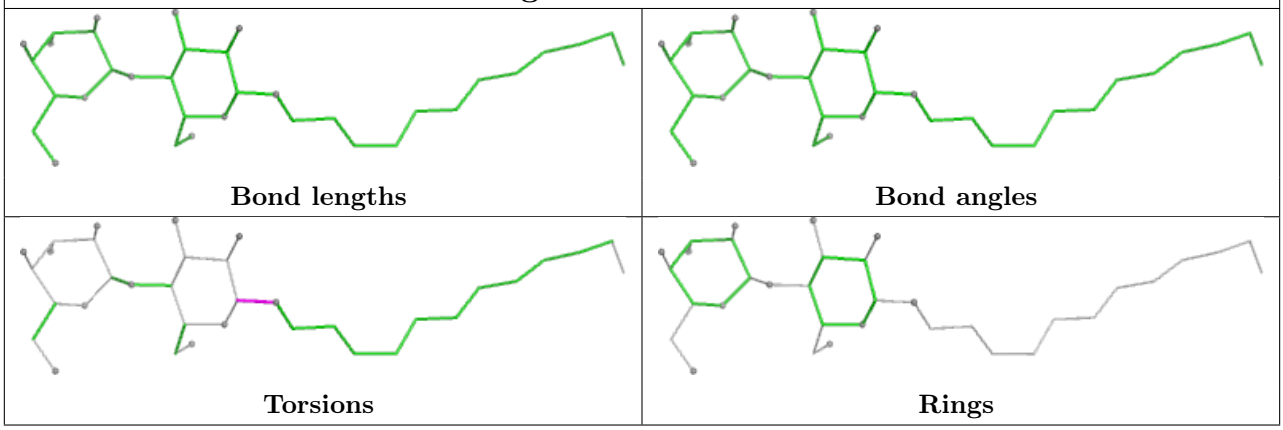


Rings

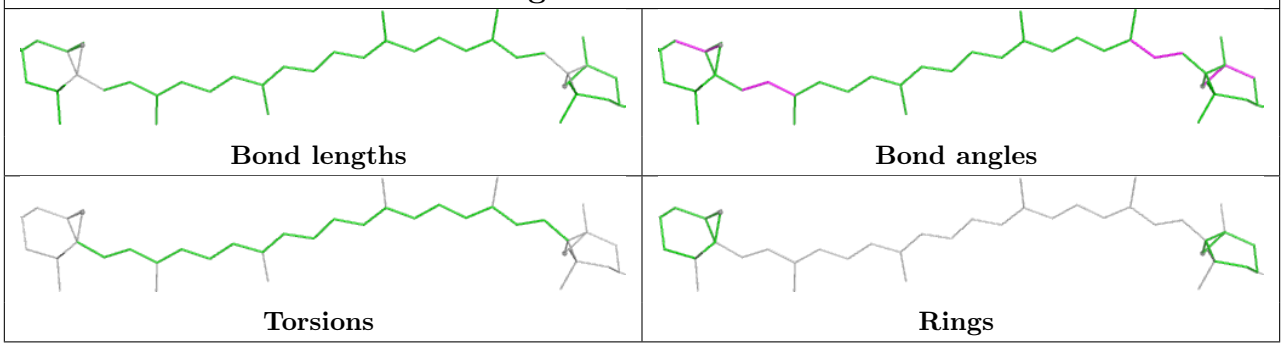
Ligand CLA B 835



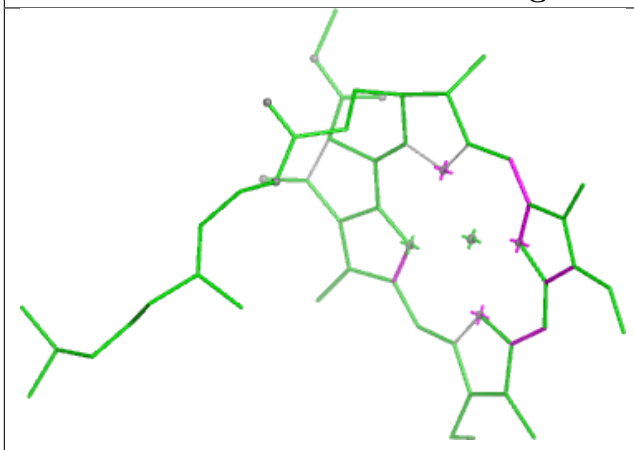
Ligand LMT G 201



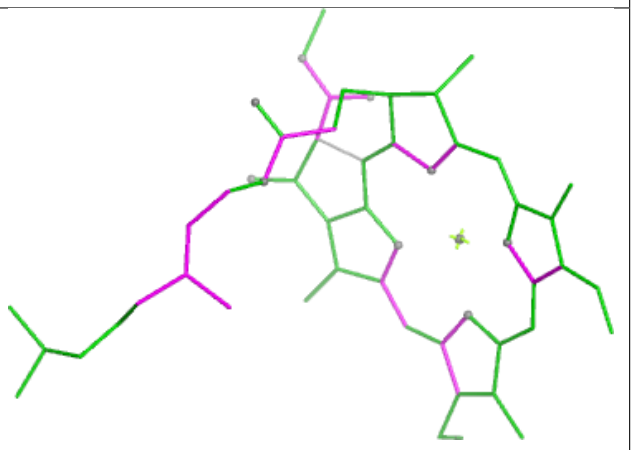
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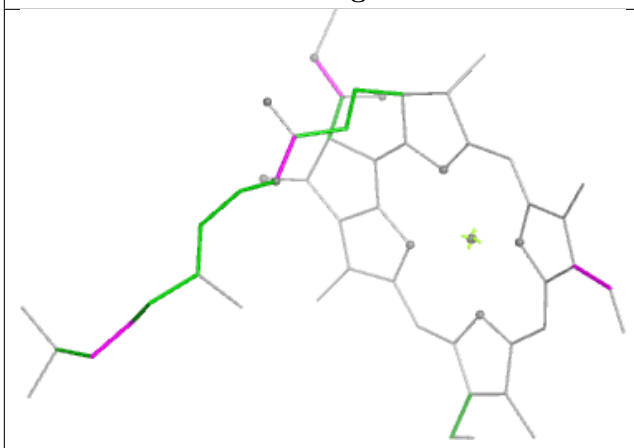
Ligand CLA 1 610



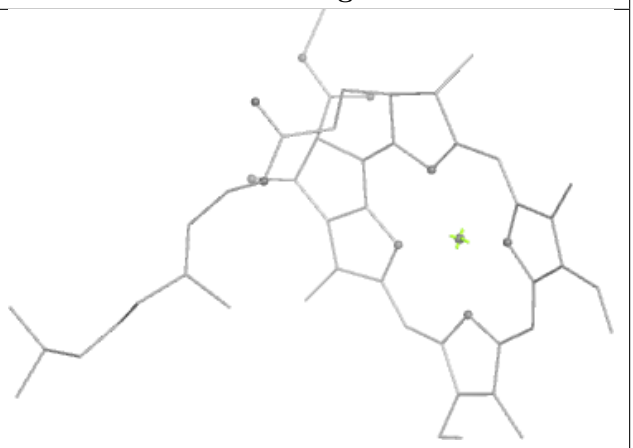
Bond lengths



Bond angles

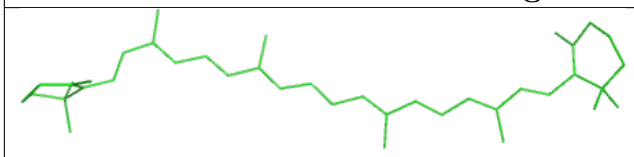


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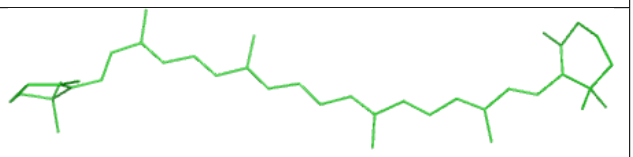


Rings

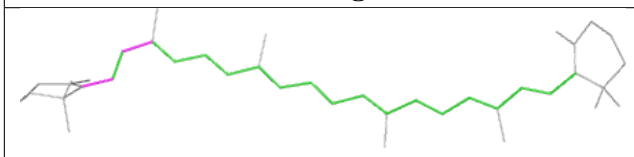
Ligand BCR B 843



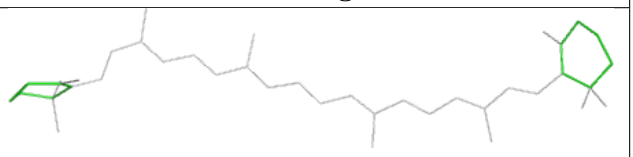
Bond lengths



Bond angles

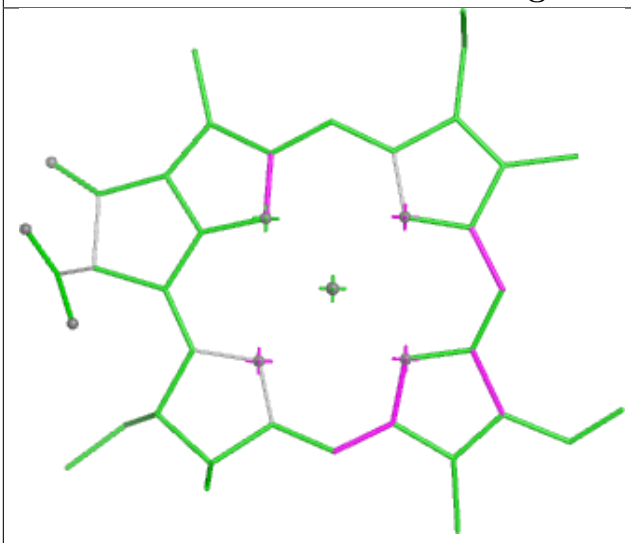


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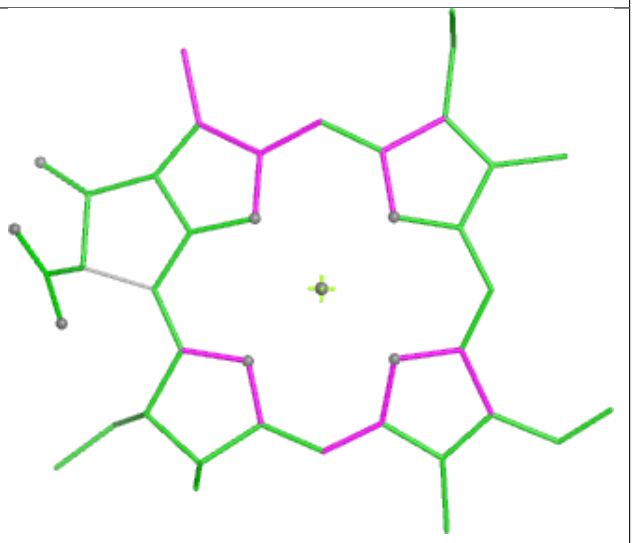


Rings

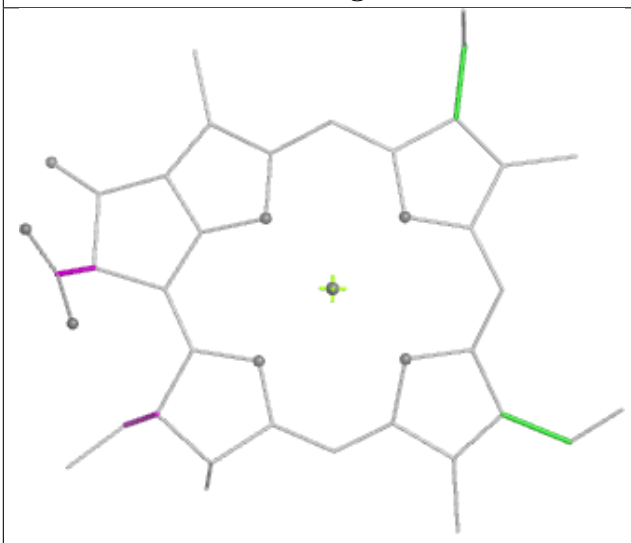
Ligand CLA 3 606



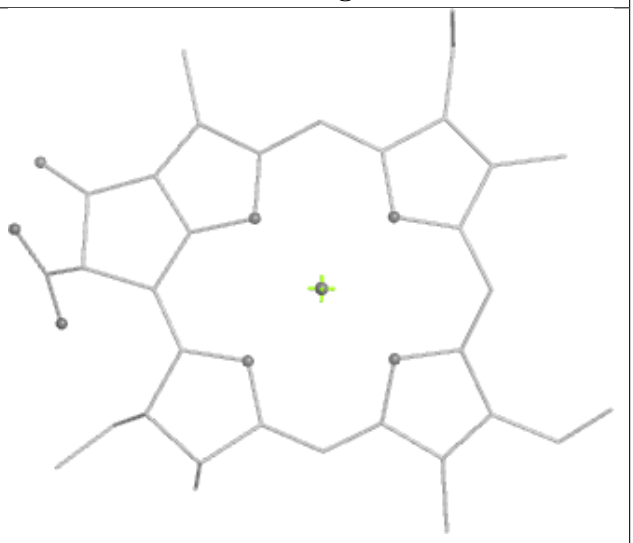
Bond lengths



Bond angles

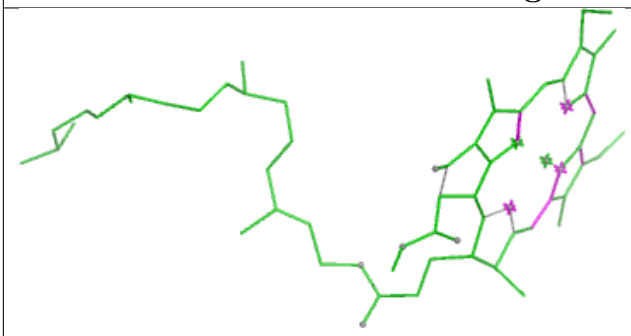


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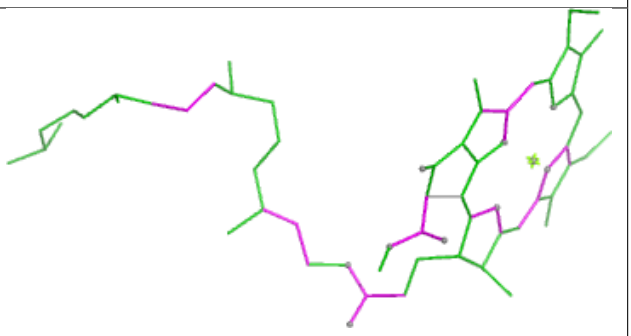


Rings

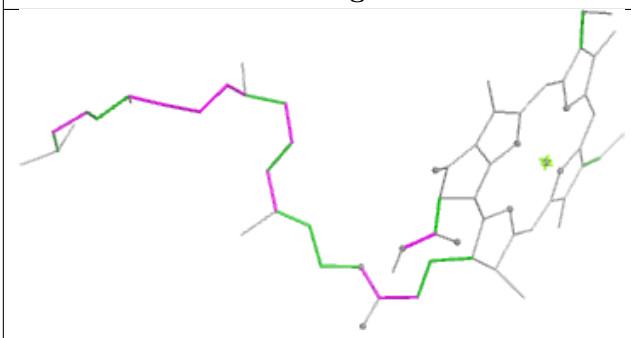
Ligand CLA B 801



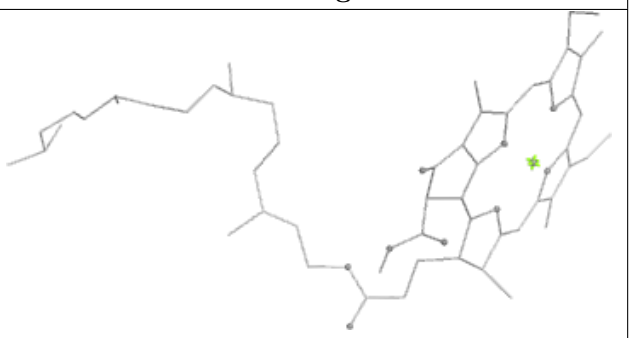
Bond lengths



Bond angles

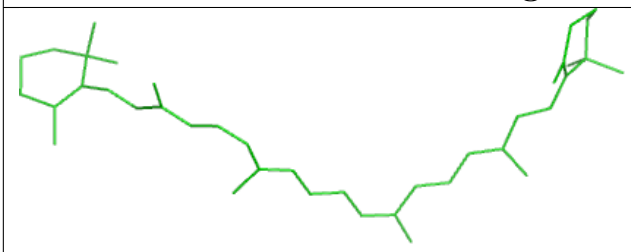


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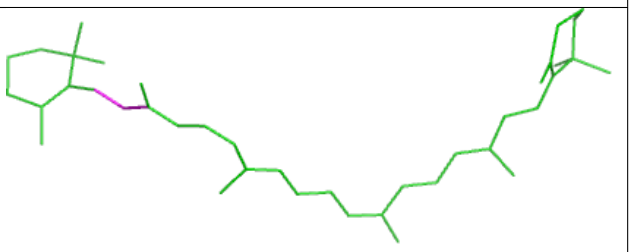


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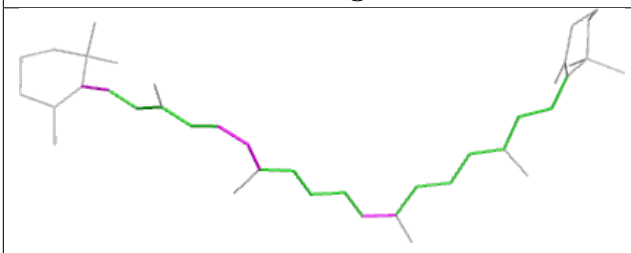
Ligand BCR A 849



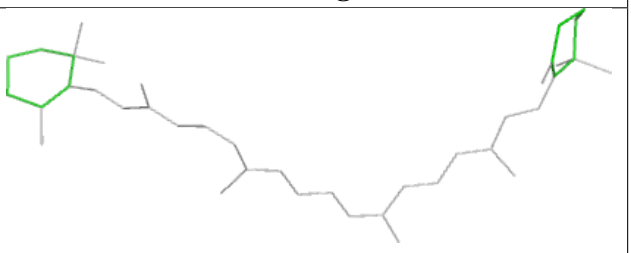
Bond lengths



Bond angles

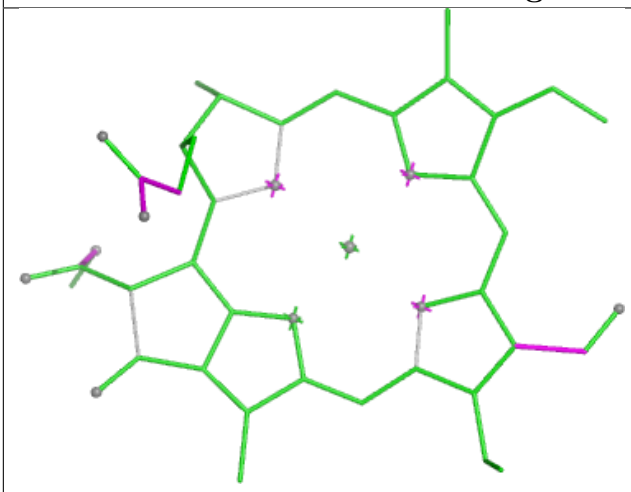


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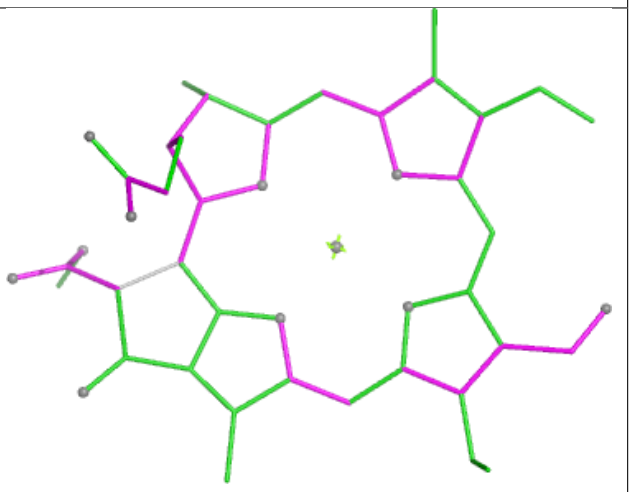


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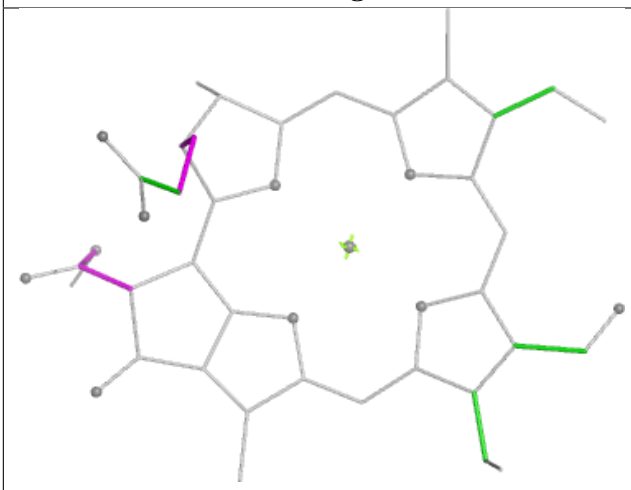
Ligand CHL Z 309



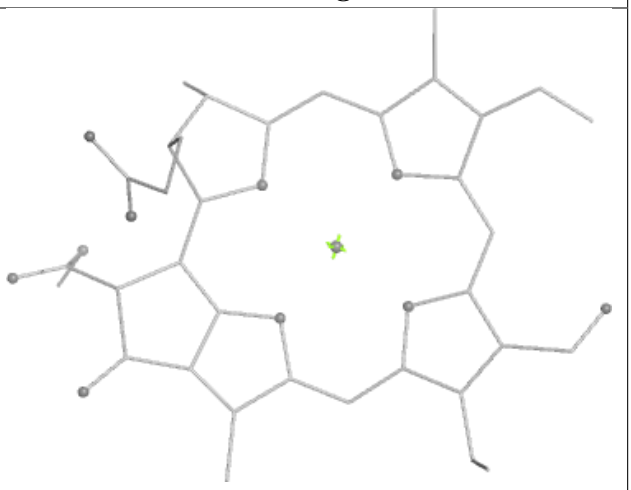
Bond lengths



Bond angles

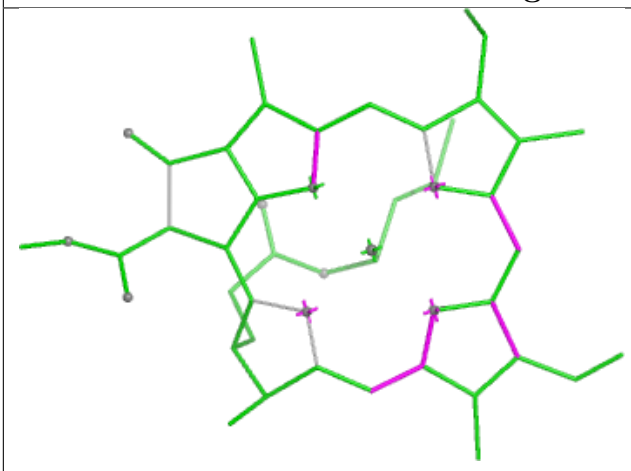


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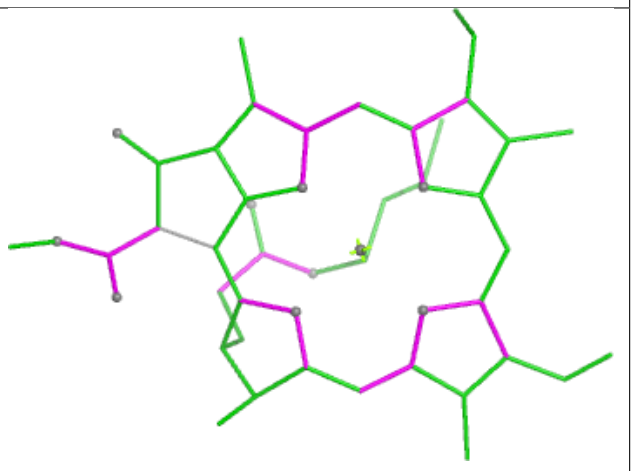


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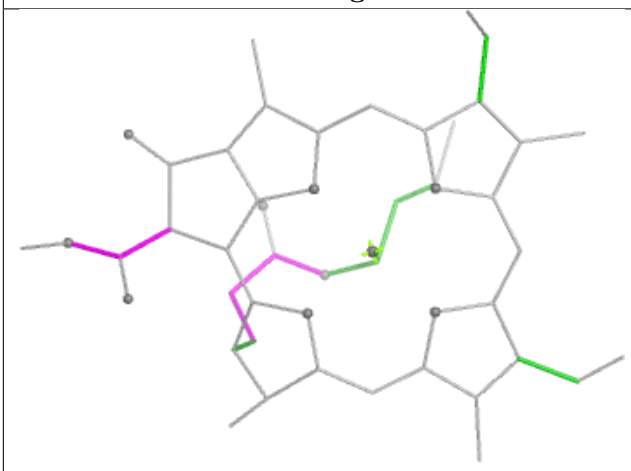
Ligand CLA O 206



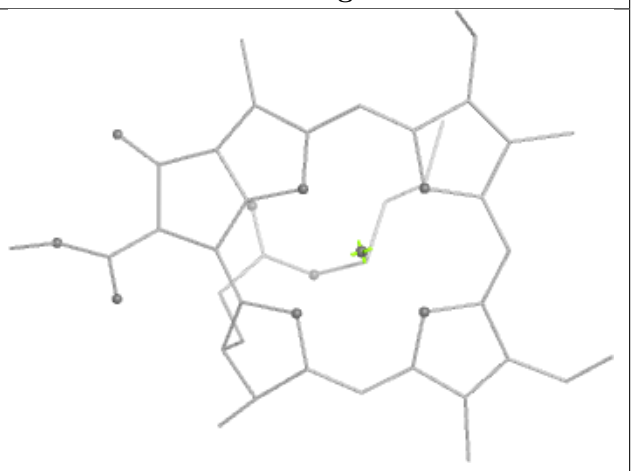
Bond lengths



Bond angles

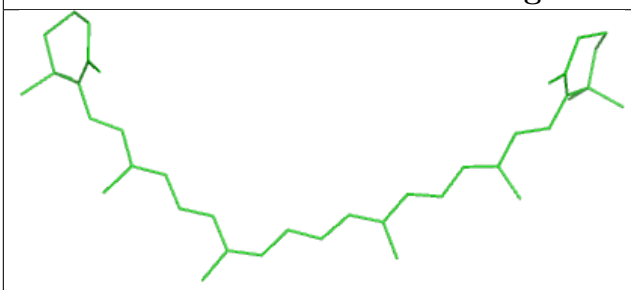


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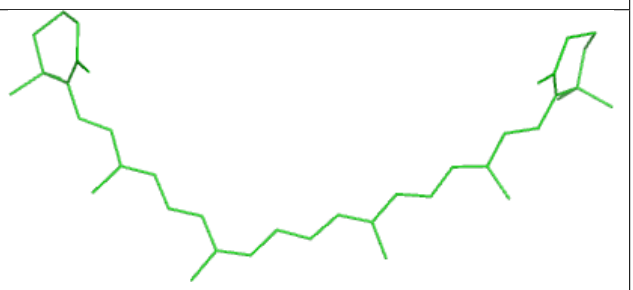


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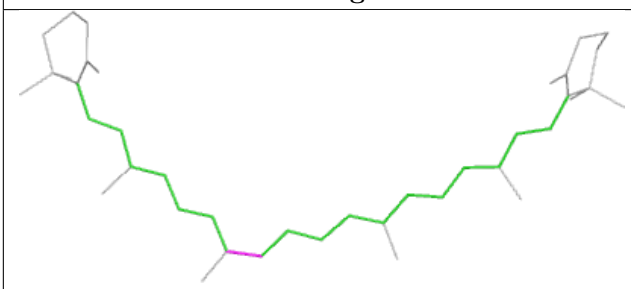
Ligand BCR F 305



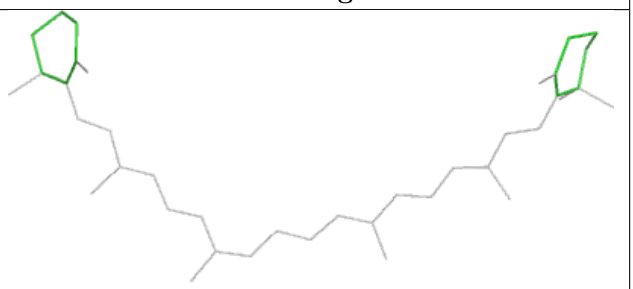
Bond lengths



Bond angles

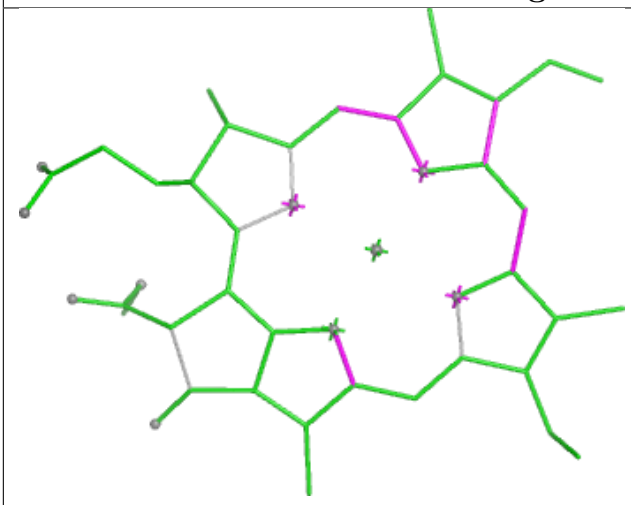


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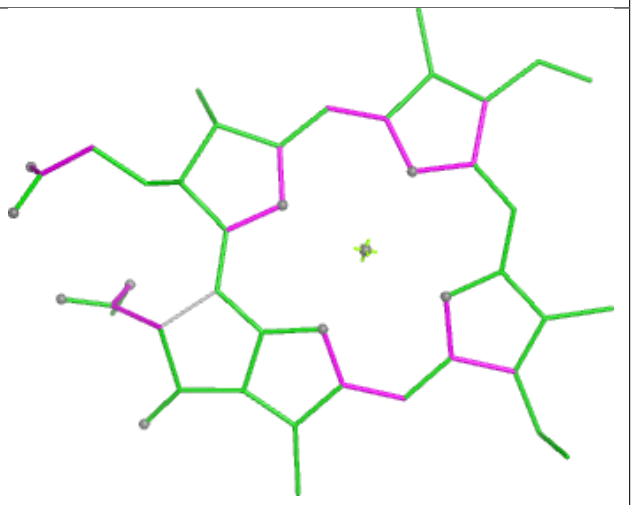


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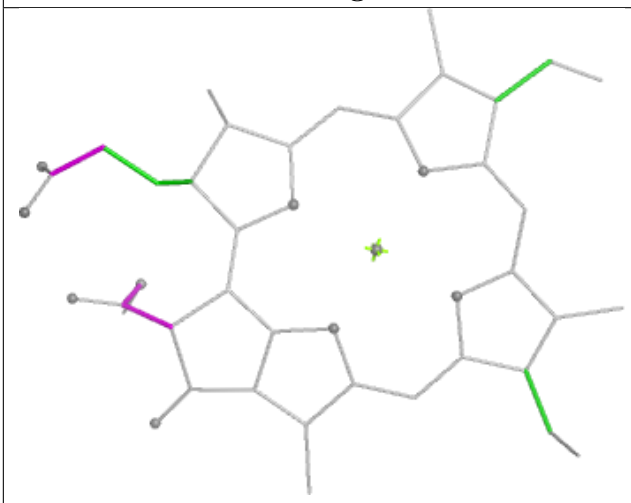
Ligand CLA 5 603



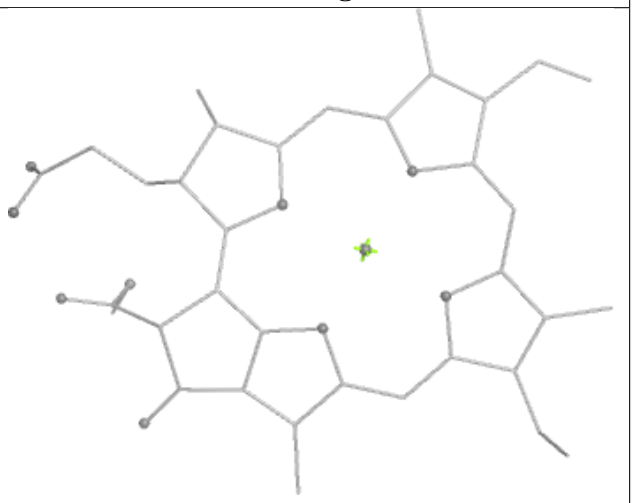
Bond lengths



Bond angles

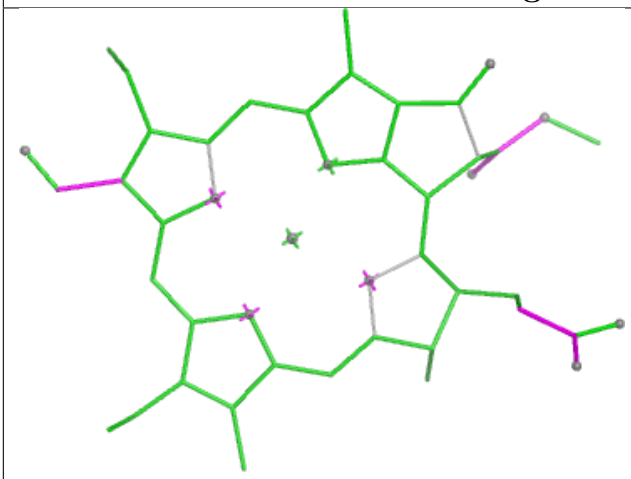


Torsions

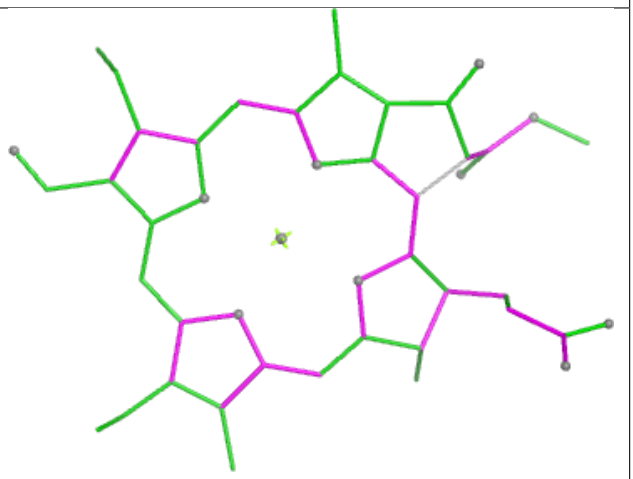


Rings

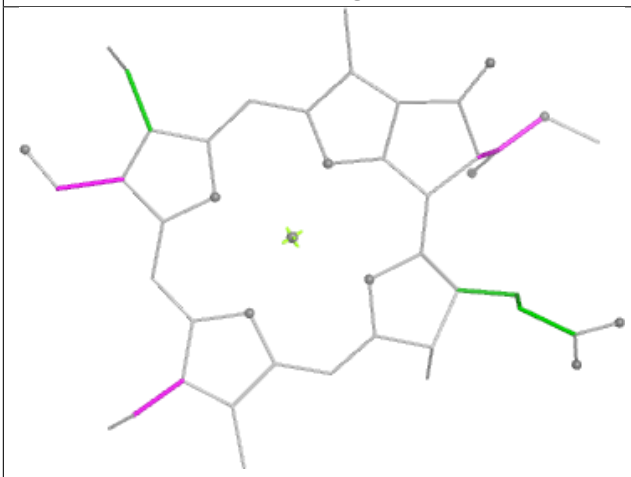
Ligand CHL X 606



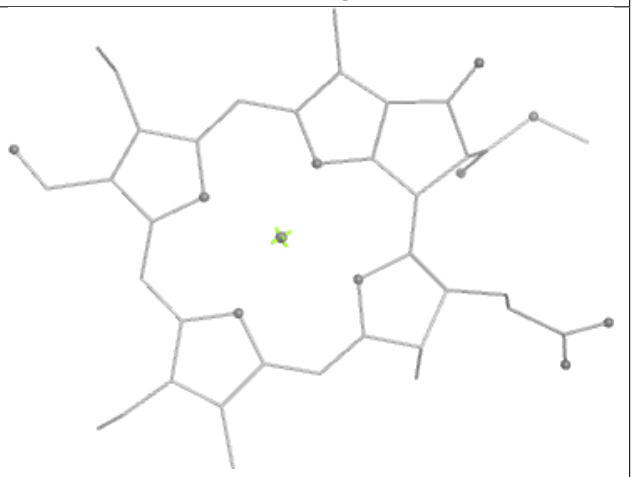
Bond lengths



Bond angles

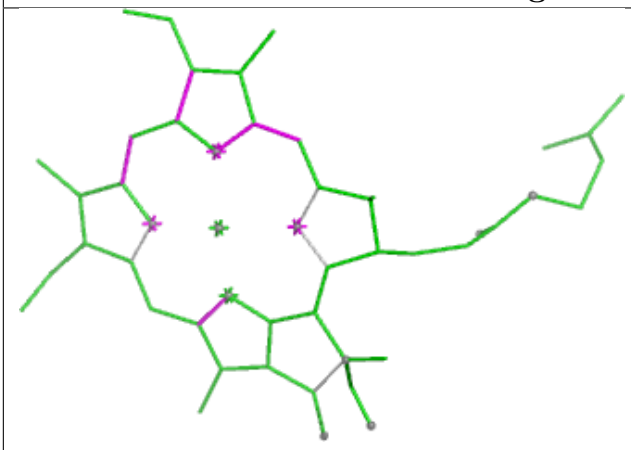


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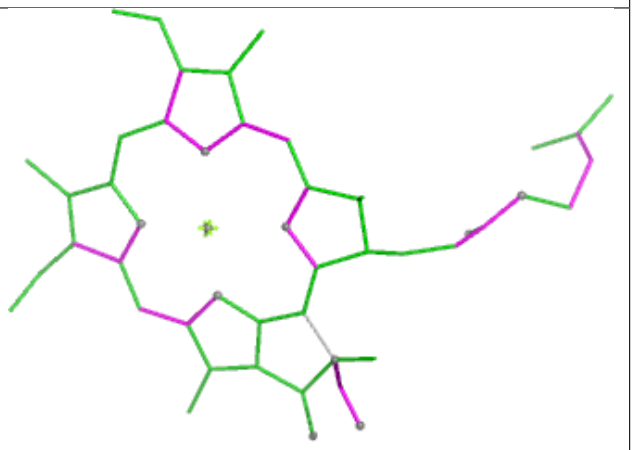


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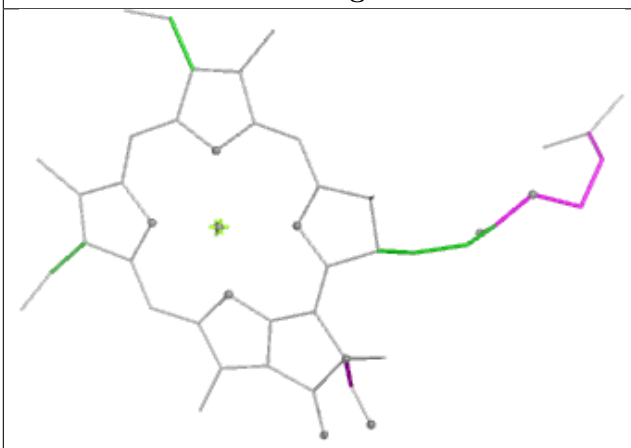
Ligand CLA 6 614



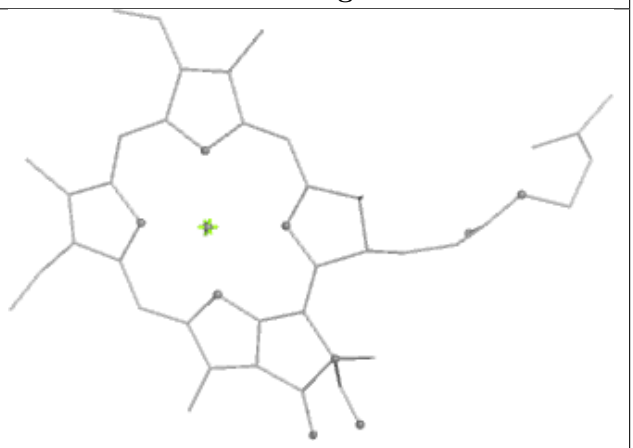
Bond lengths



Bond angles

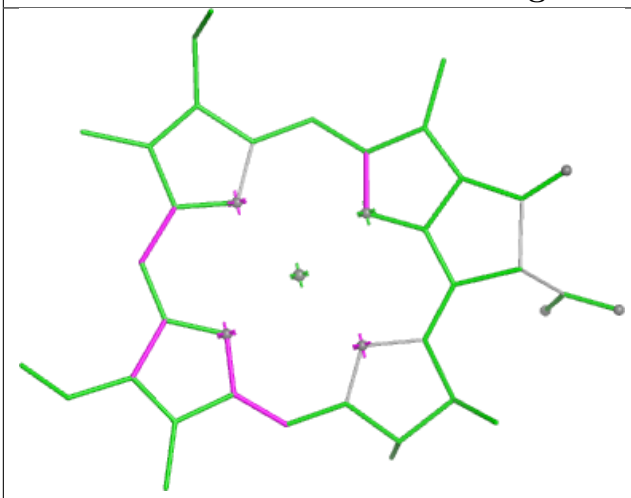


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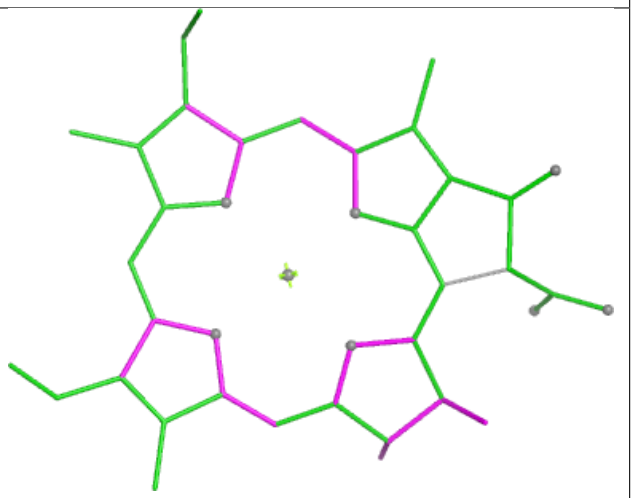


Rings

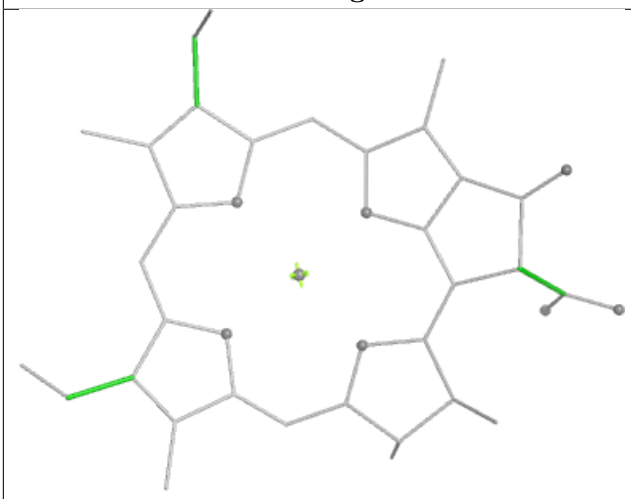
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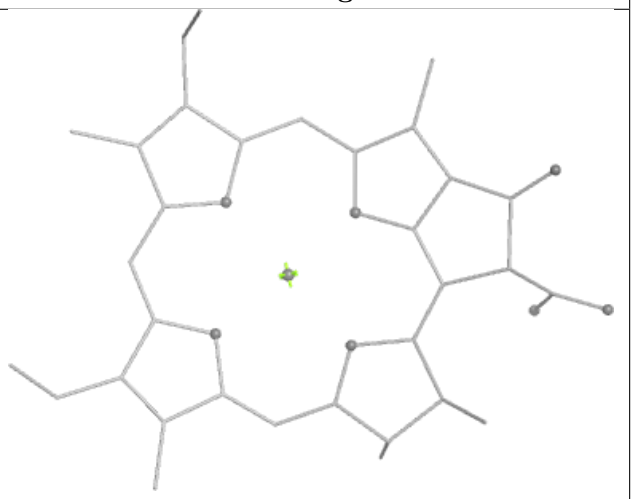
Bond lengths



Bond angles

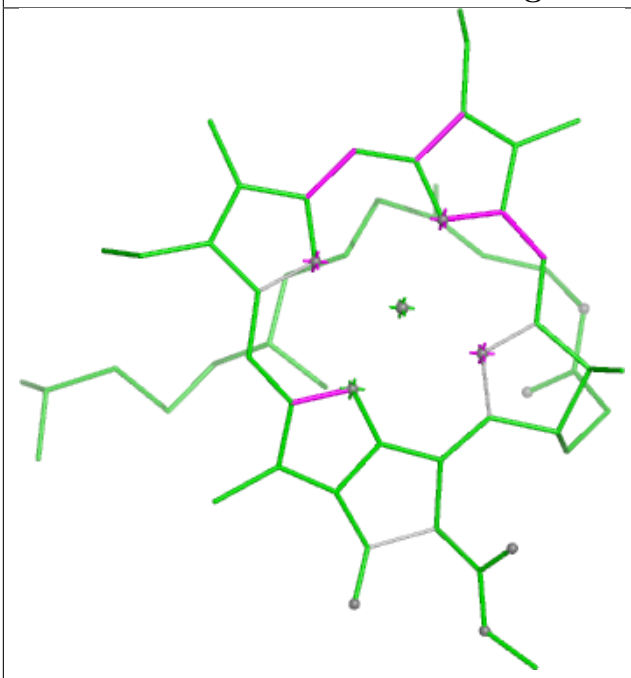


Torsions

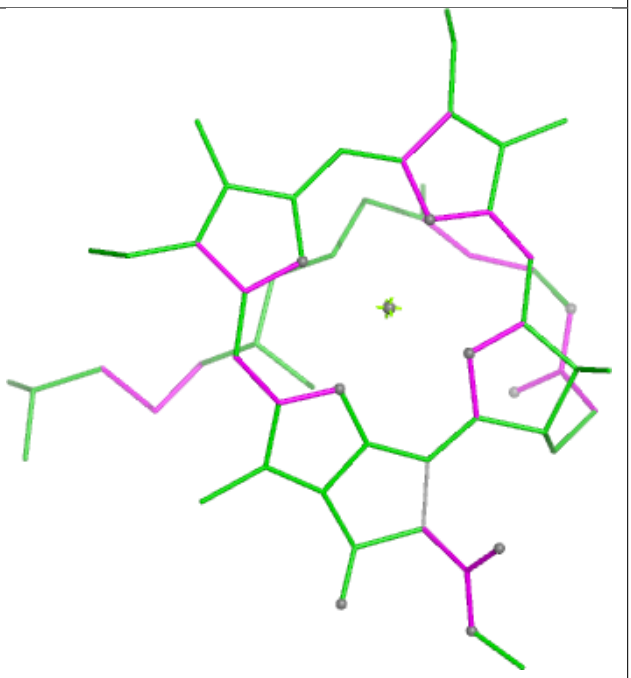


Rings

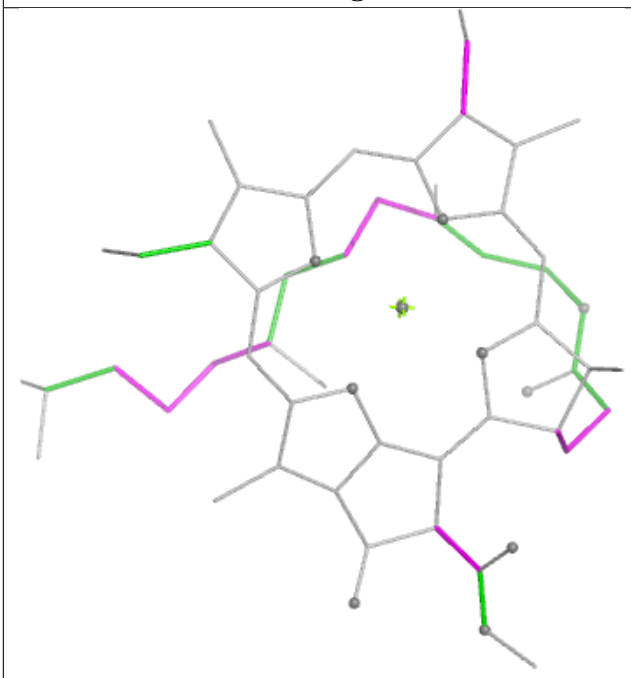
Ligand CLA B 826



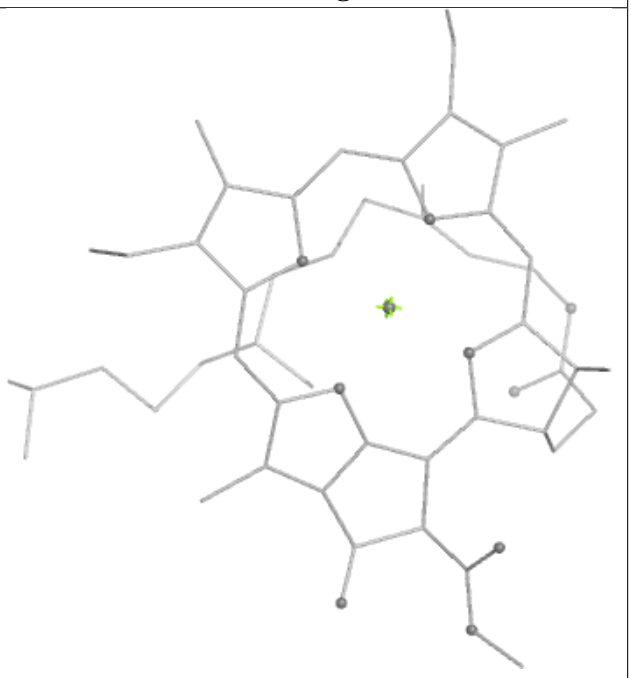
Bond lengths



Bond angles

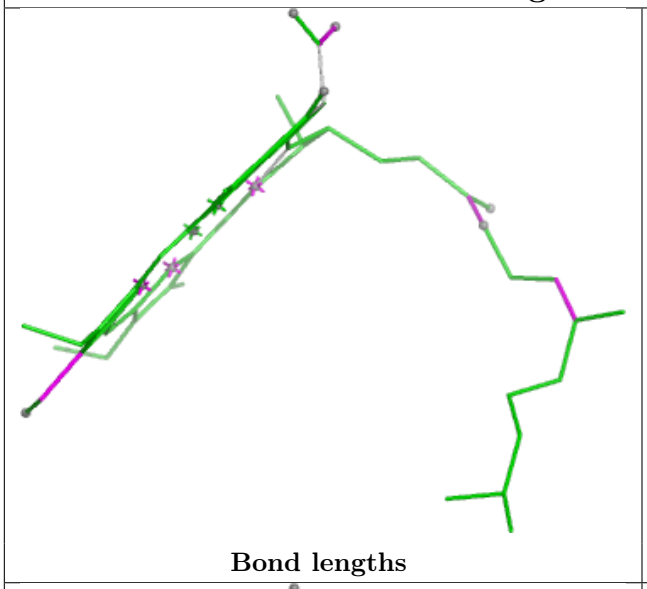


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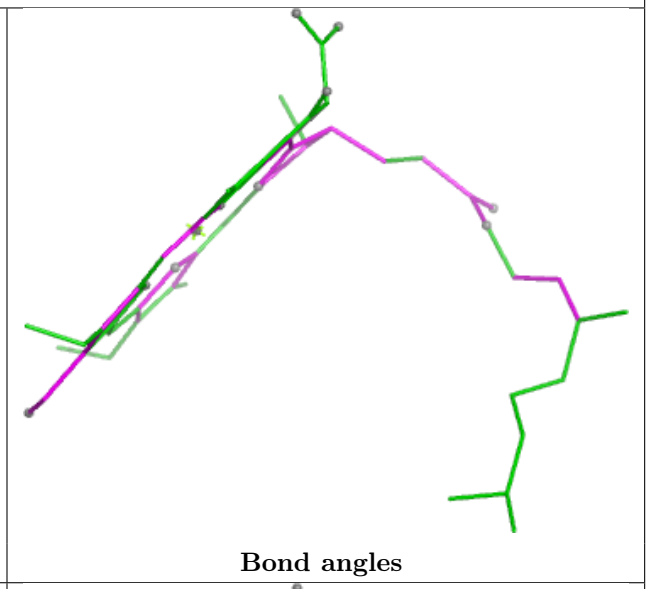


Rings

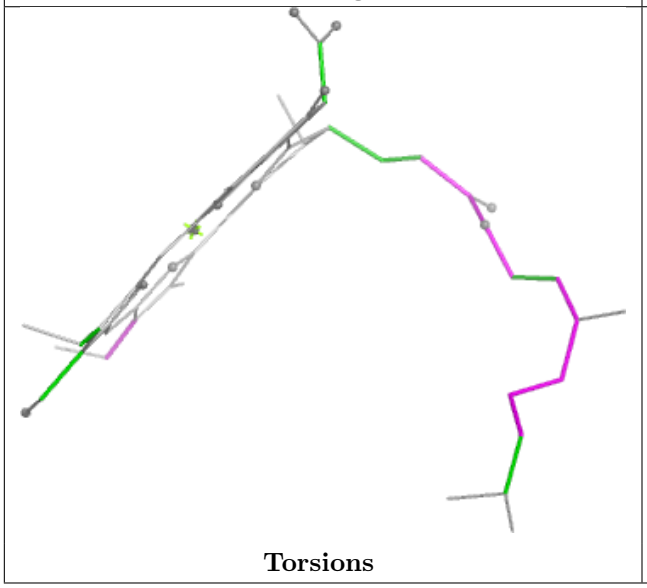
Ligand CHL 1 601



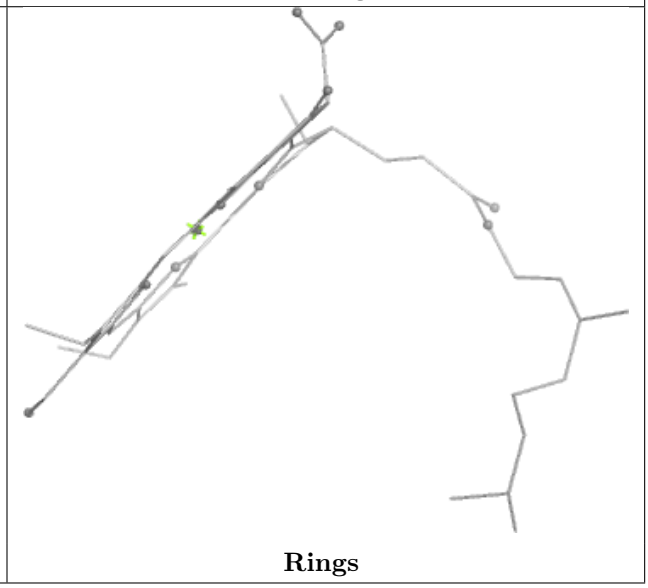
Bond lengths



Bond angles

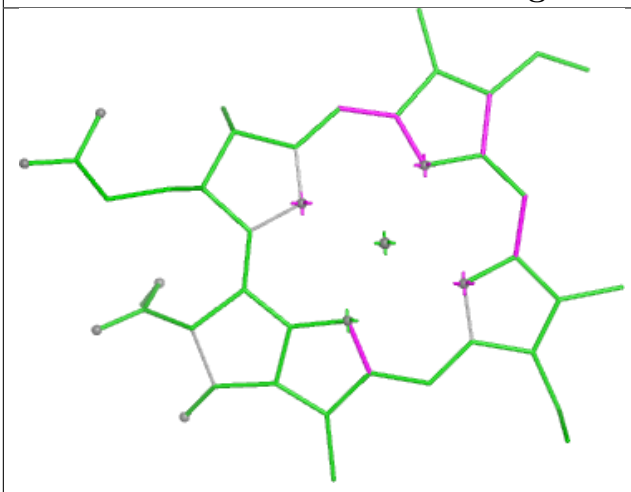


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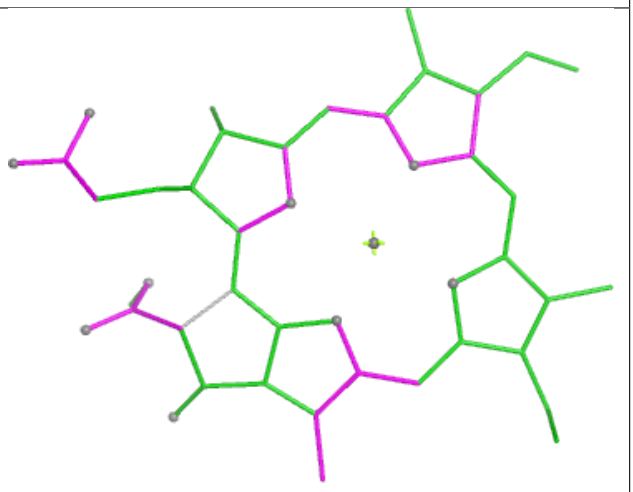


Rings

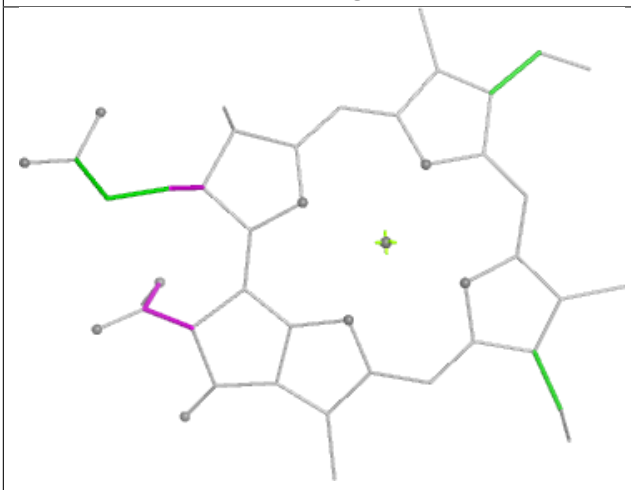
Ligand CLA 4 302



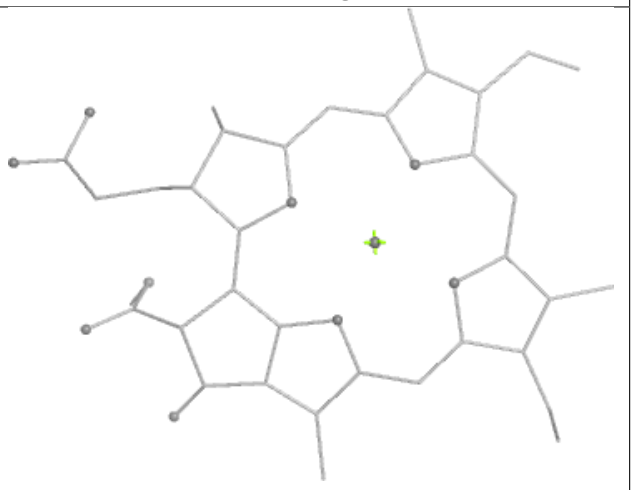
Bond lengths



Bond angles

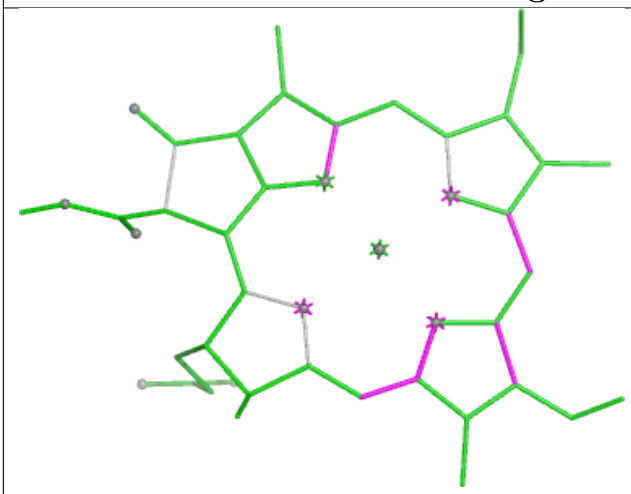


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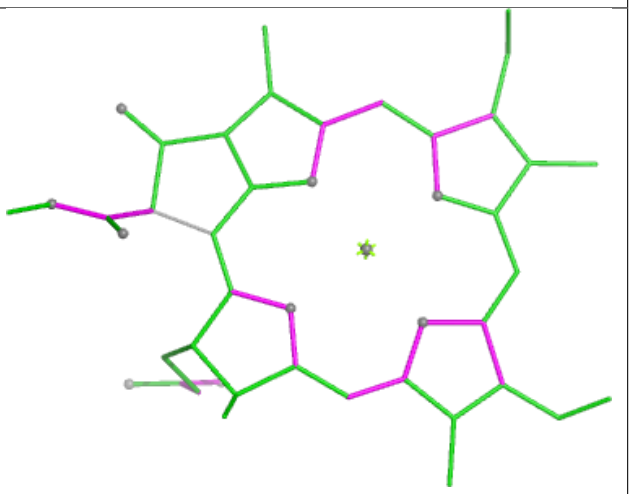


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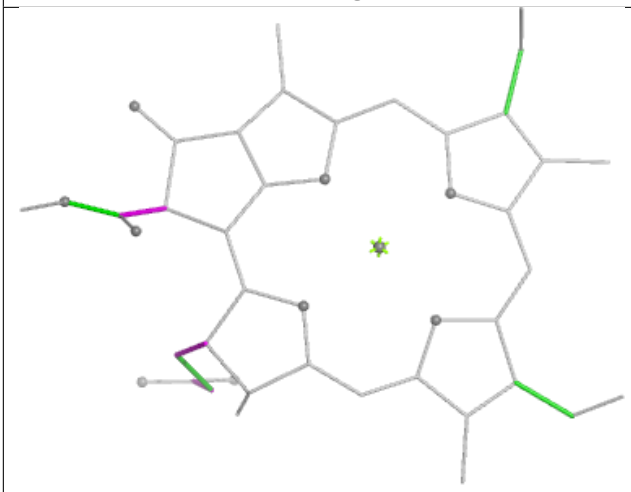
Ligand CLA 4 307



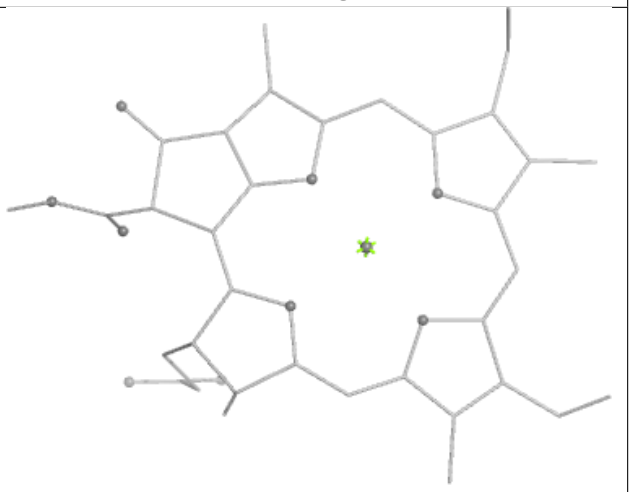
Bond lengths



Bond angles

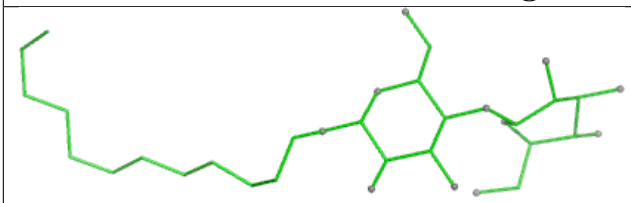


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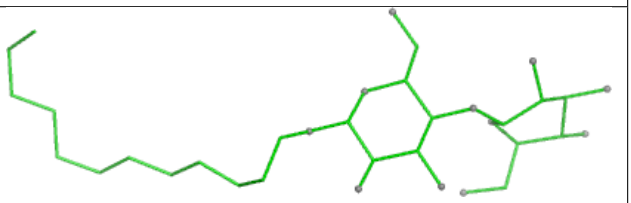


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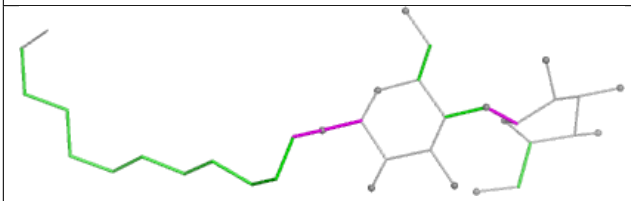
Ligand LMT A 852



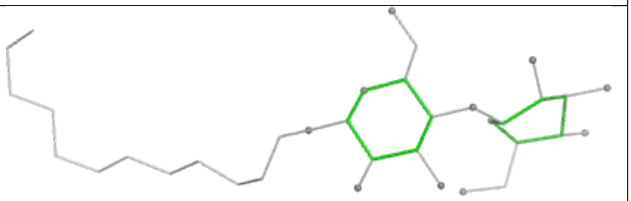
Bond lengths



Bond angles



Torsions



Rings

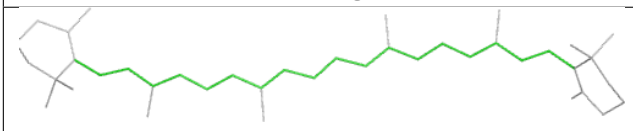
Ligand BCR B 842



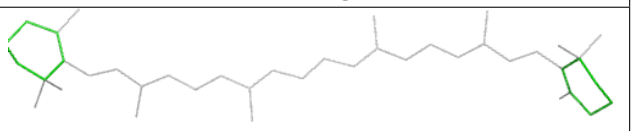
Bond lengths



Bond angles

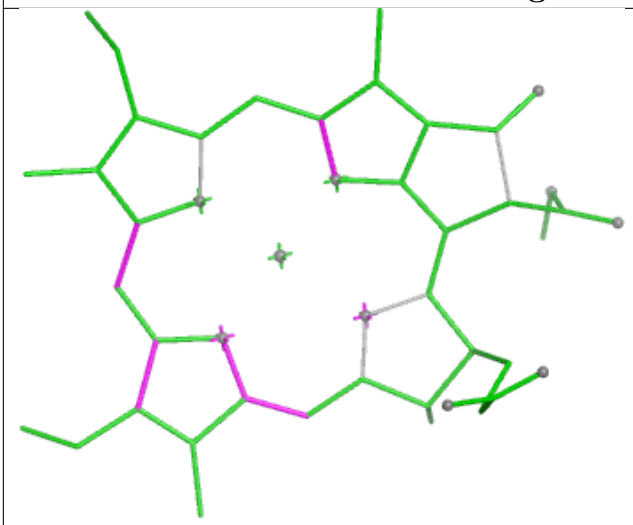


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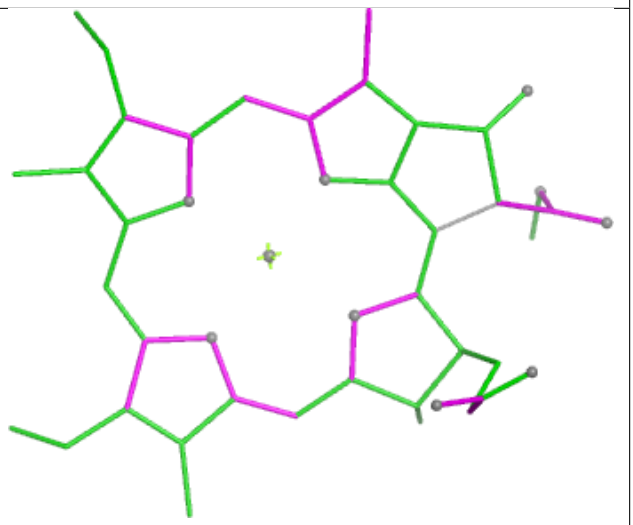


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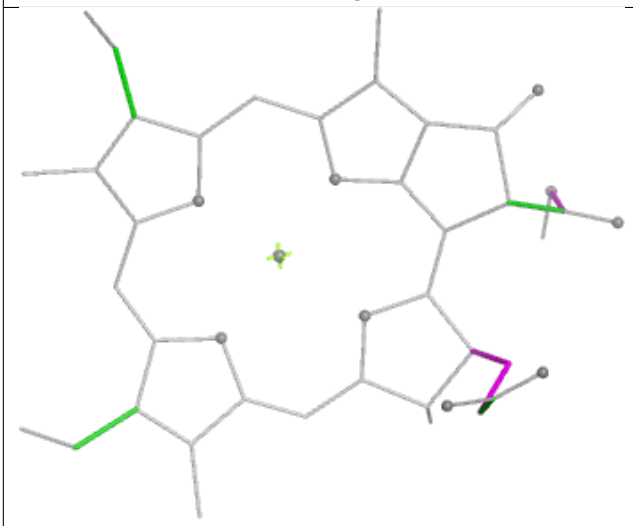
Ligand CLA 4 303



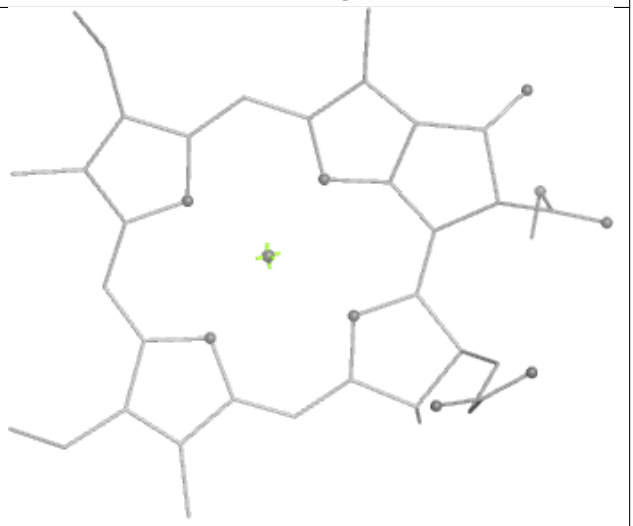
Bond lengths



Bond angles

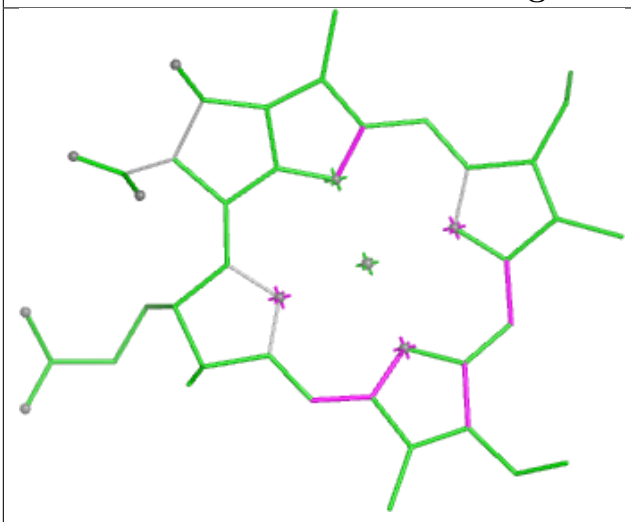


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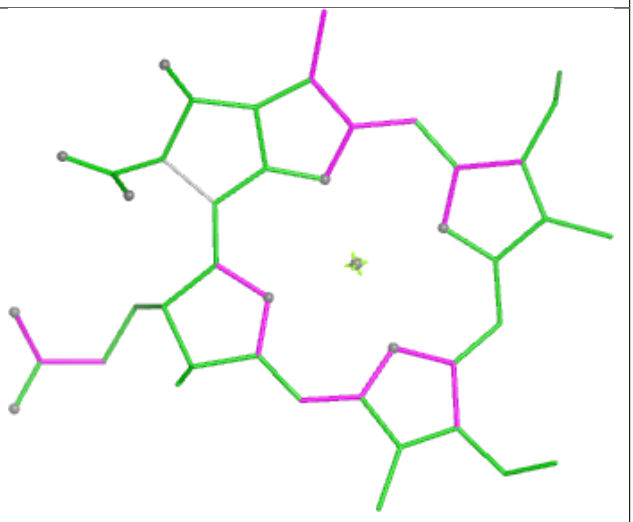


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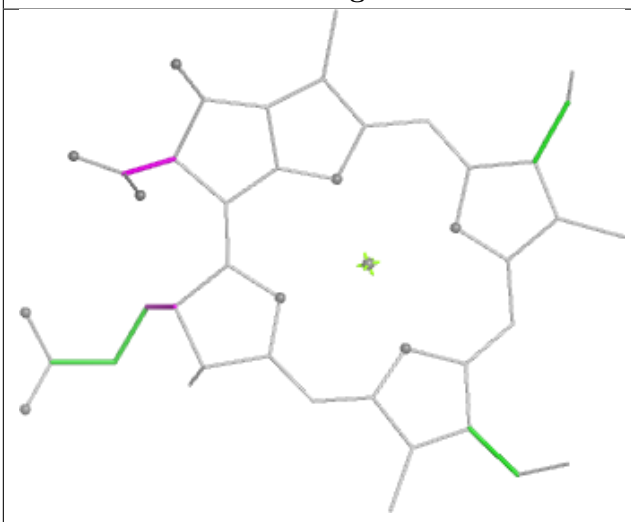
Ligand CLA 2 603



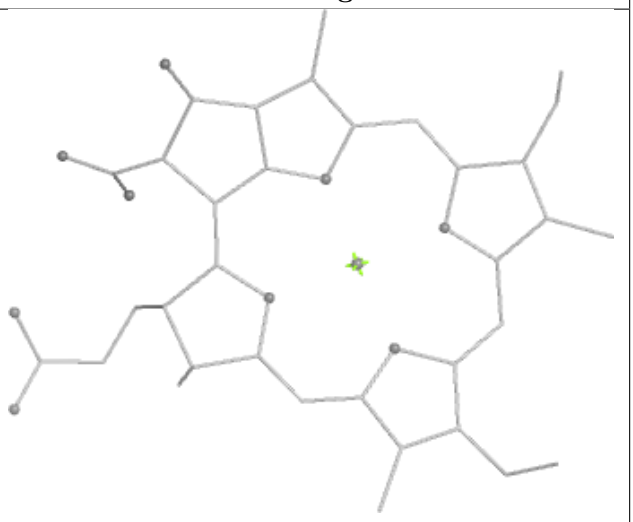
Bond lengths



Bond angles

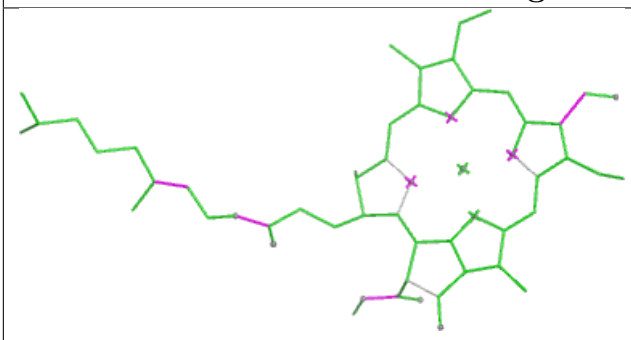


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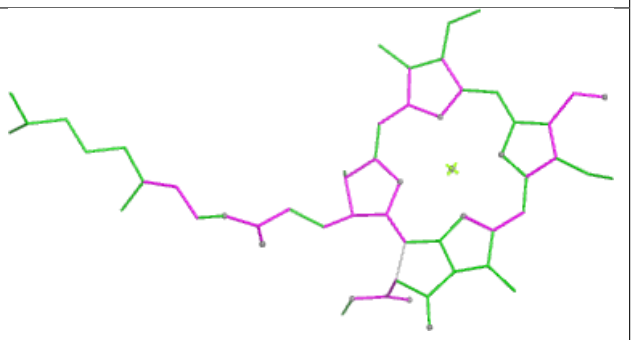


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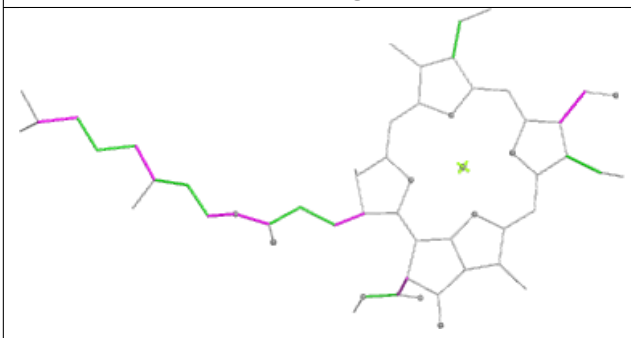
Ligand CHL 6 605



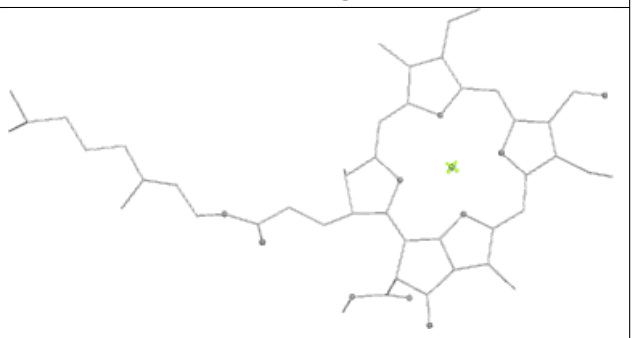
Bond lengths



Bond angles

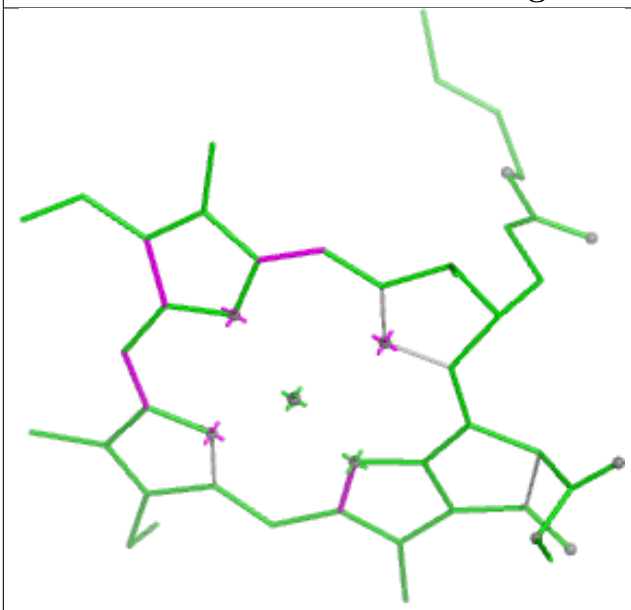


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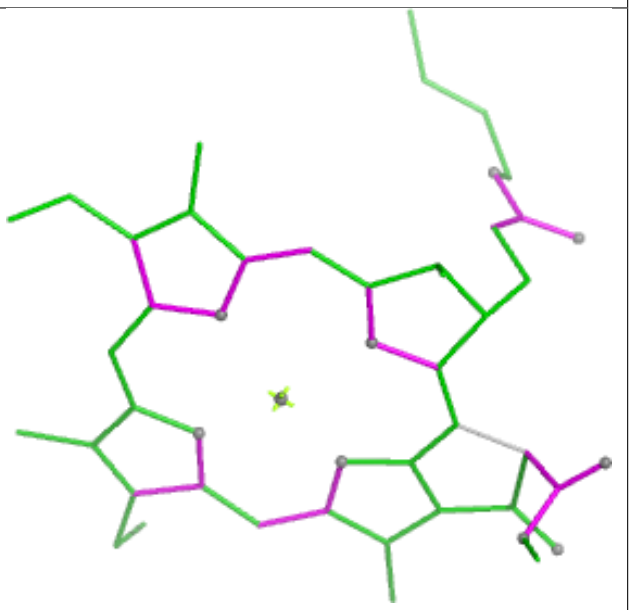


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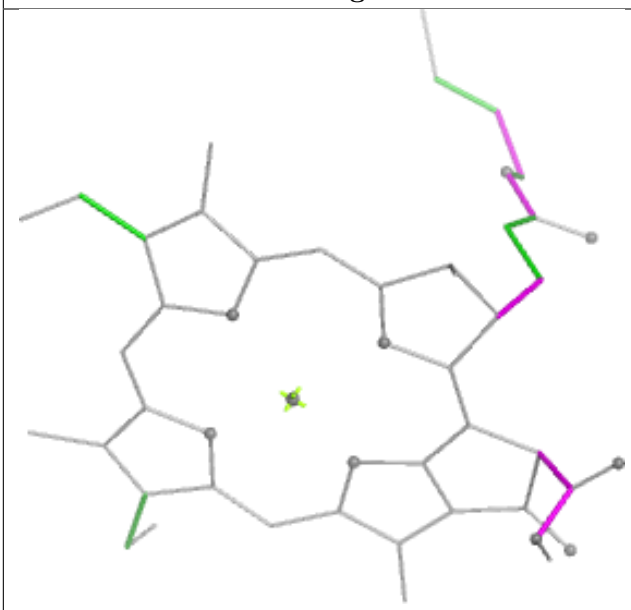
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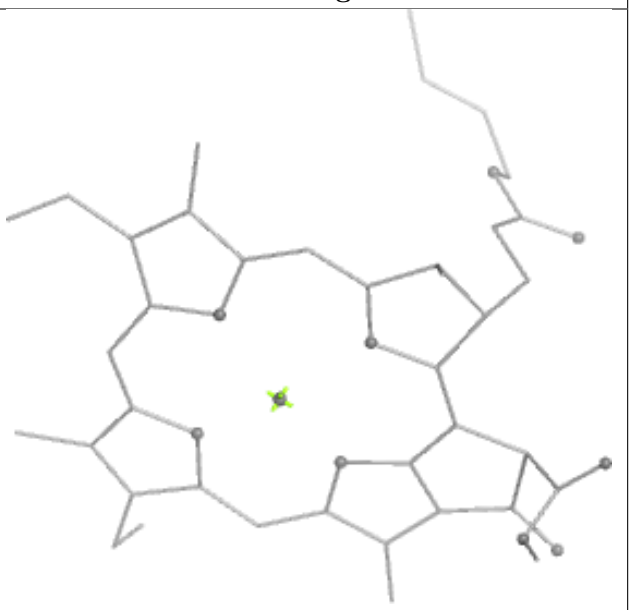
Bond lengths



Bond angles

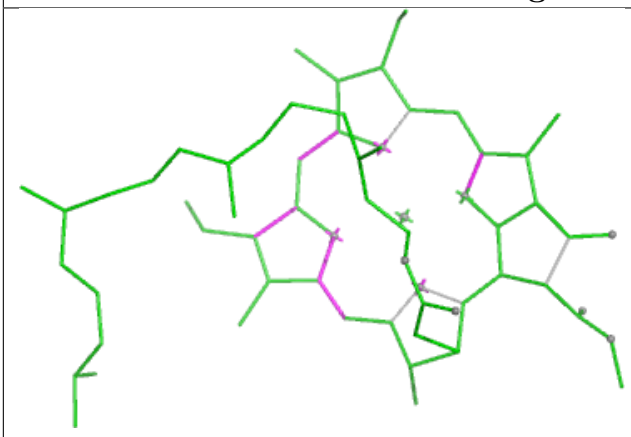


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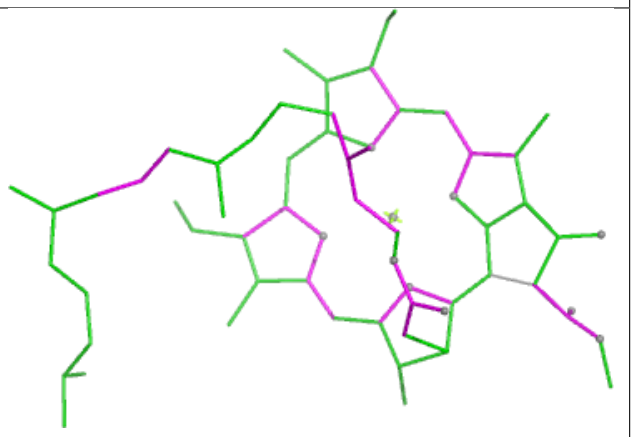


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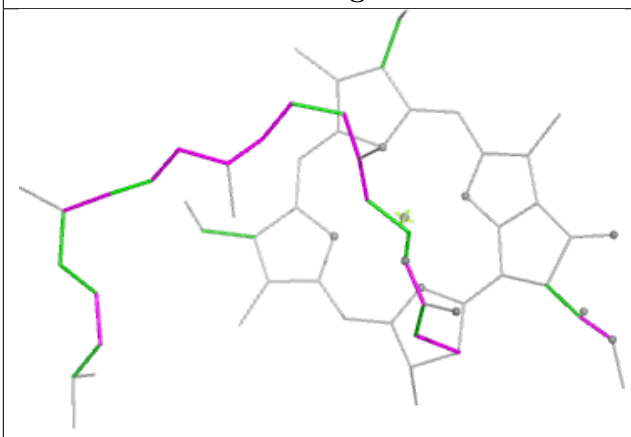
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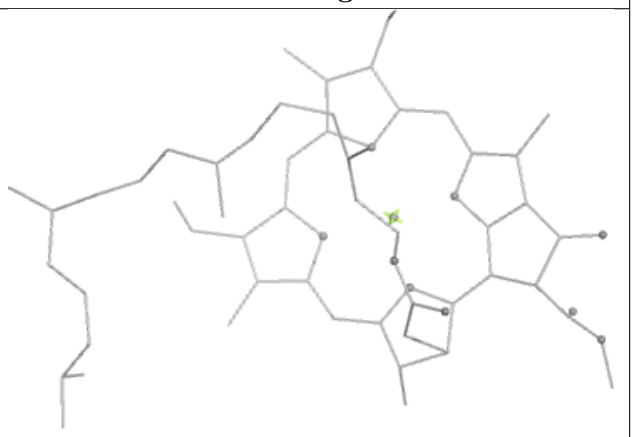
Bond lengths



Bond angles

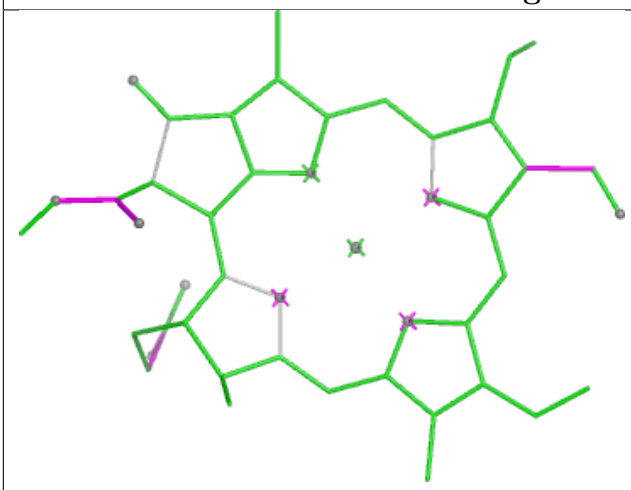


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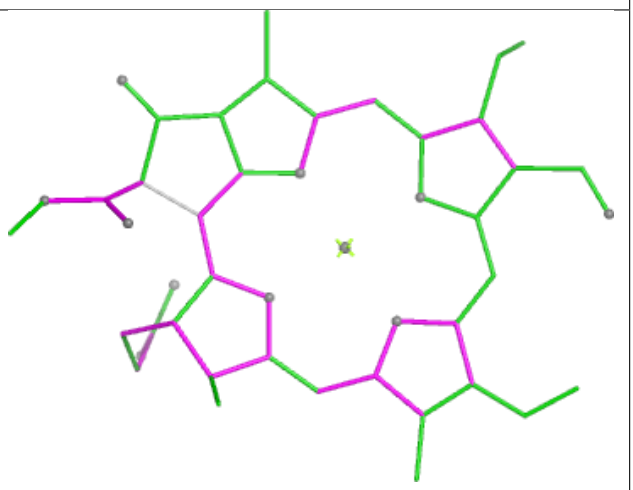


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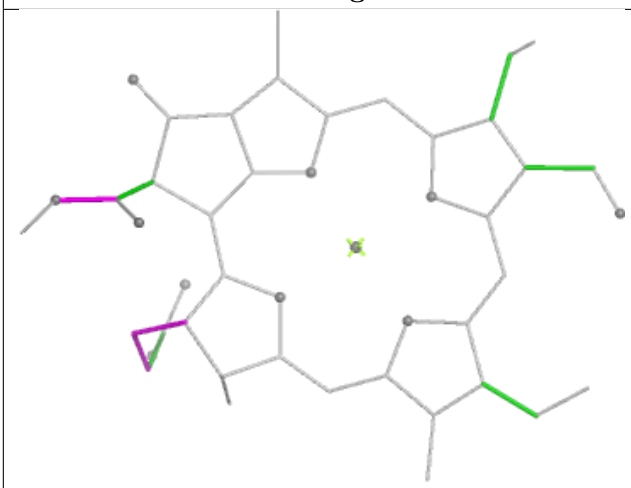
Ligand CHL X 607



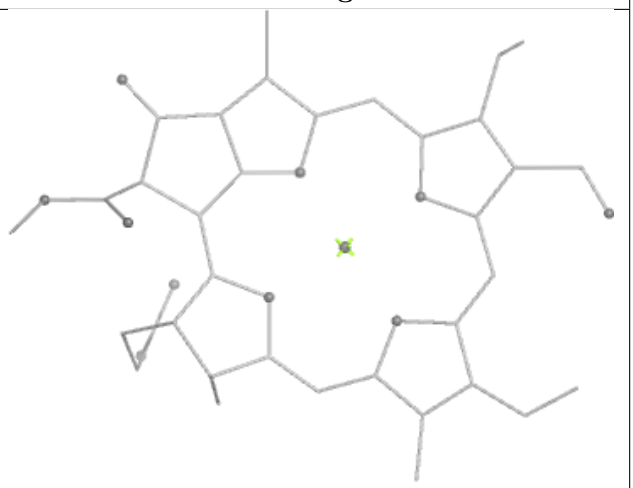
Bond lengths



Bond angles

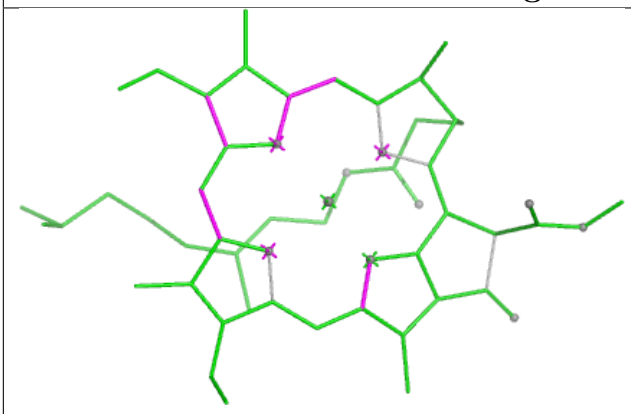


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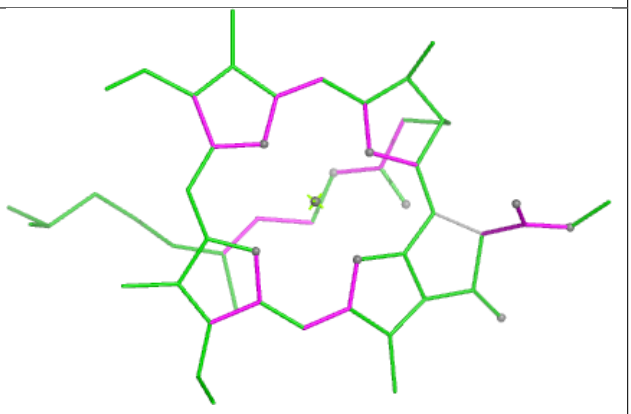


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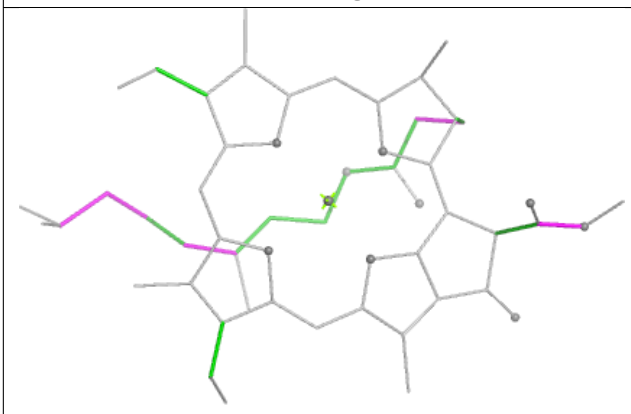
Ligand CLA A 838



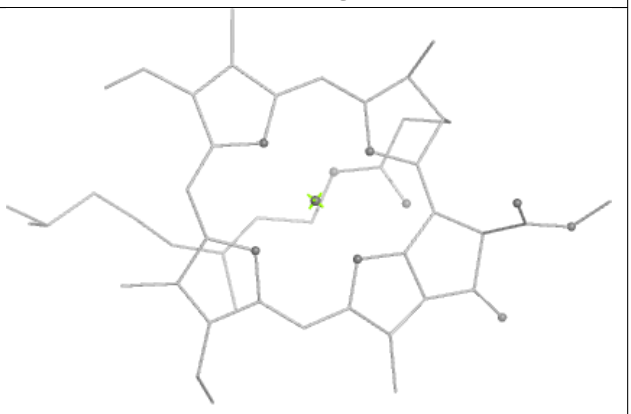
Bond lengths



Bond angles

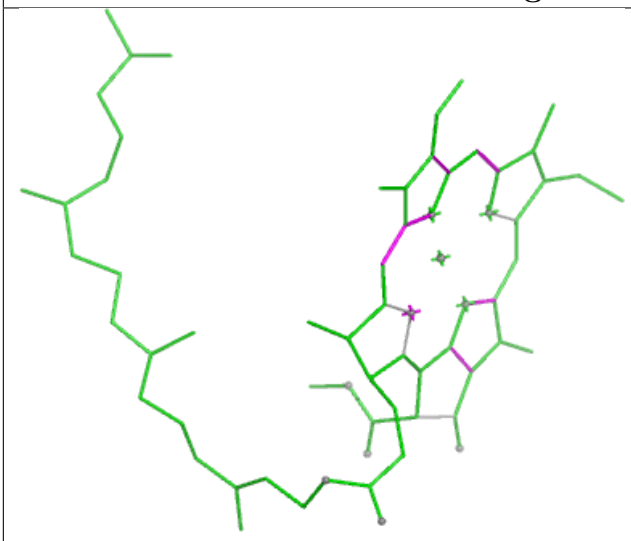


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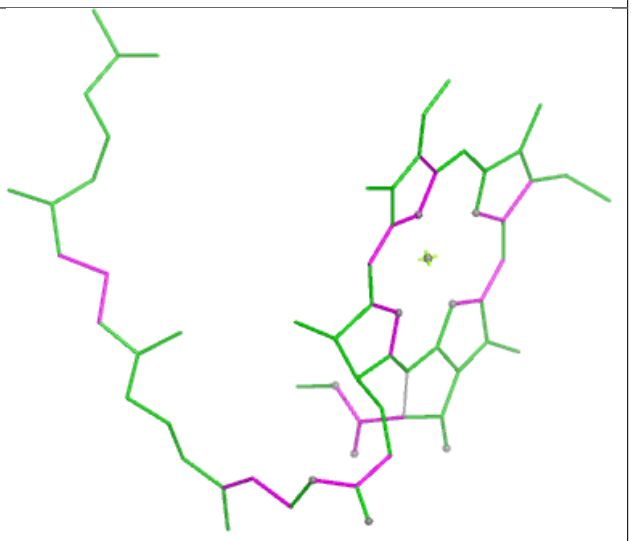


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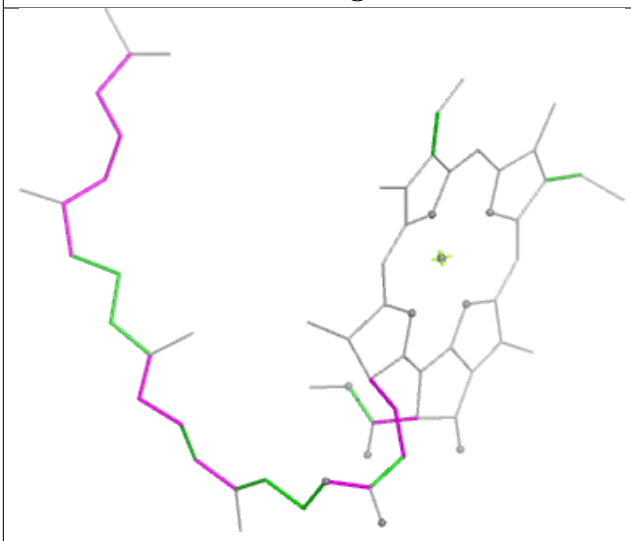
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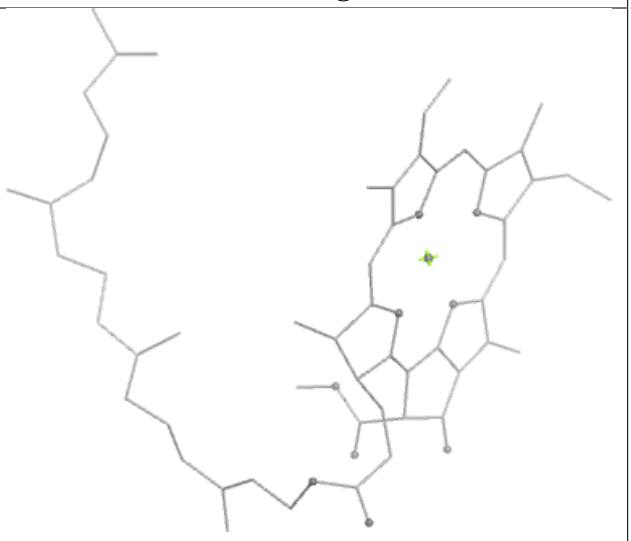
Bond lengths



Bond angles

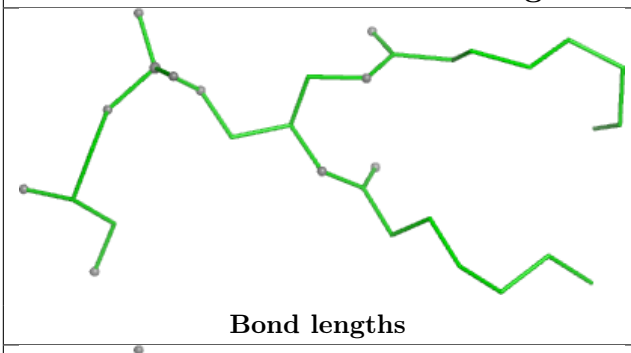


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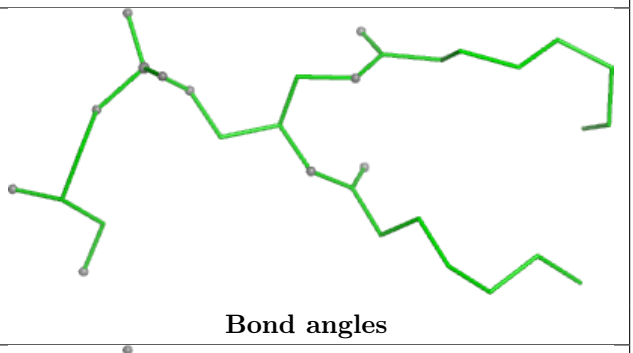


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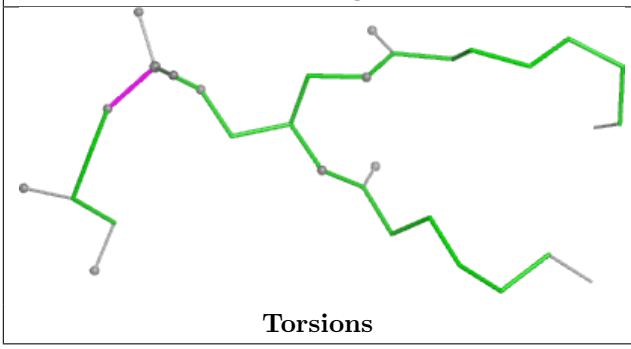
Ligand LHG Z 317



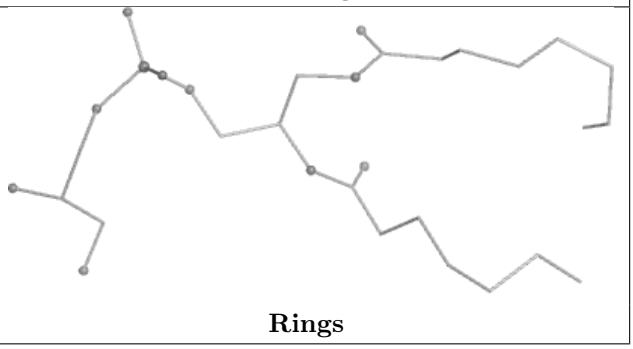
Bond lengths



Bond angles

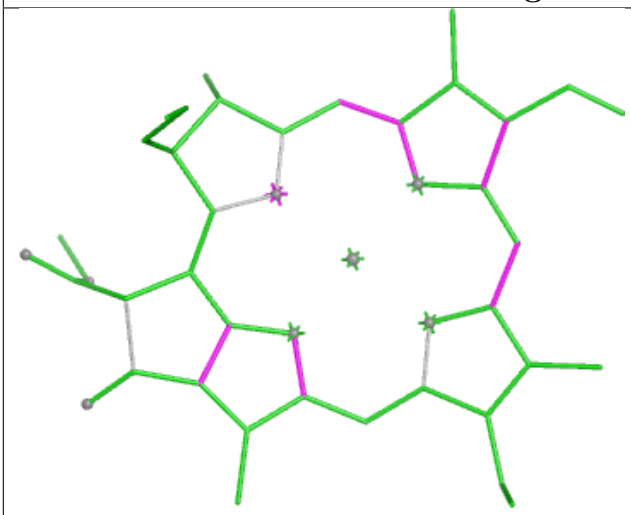


Torsions

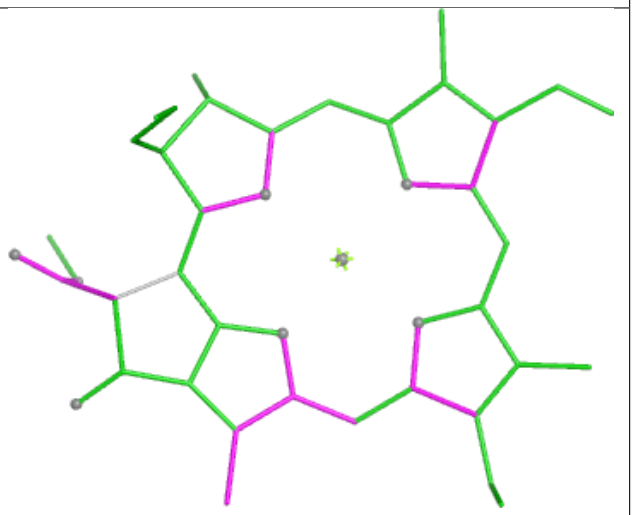


Rings

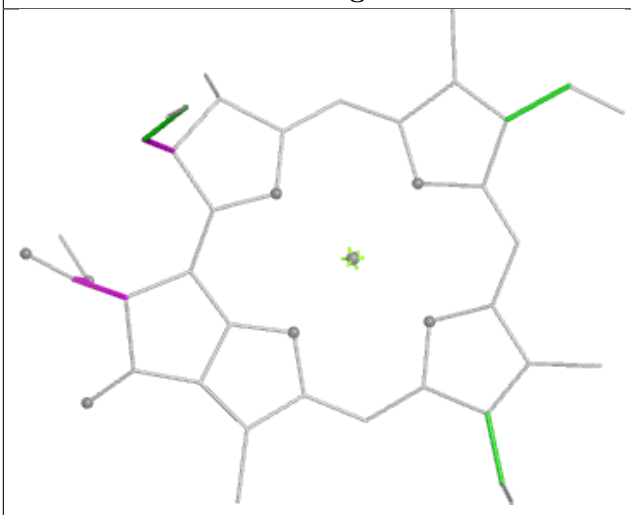
Ligand CLA B 829



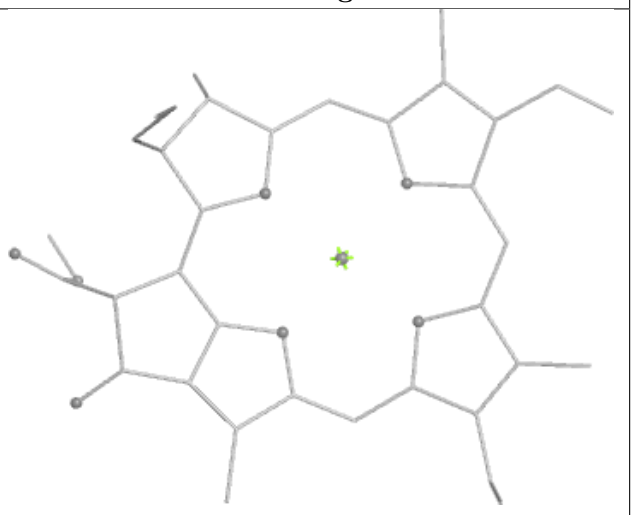
Bond lengths



Bond angles

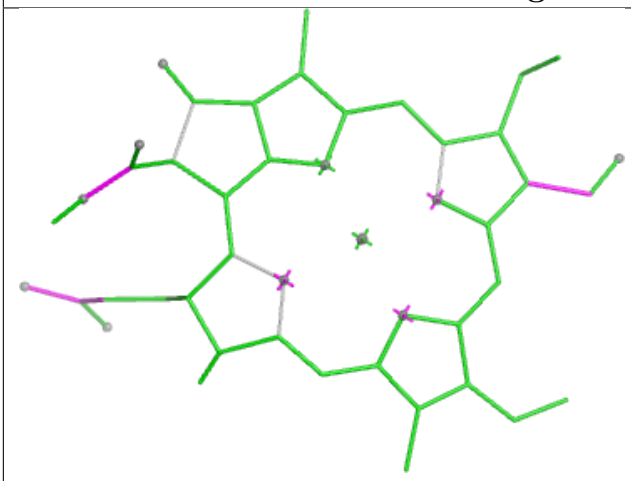


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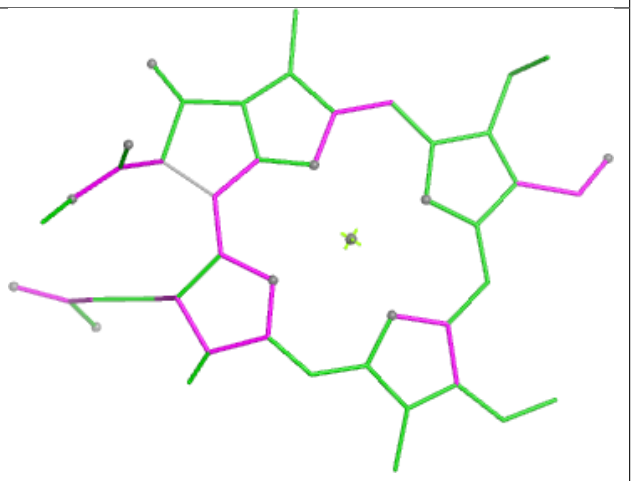


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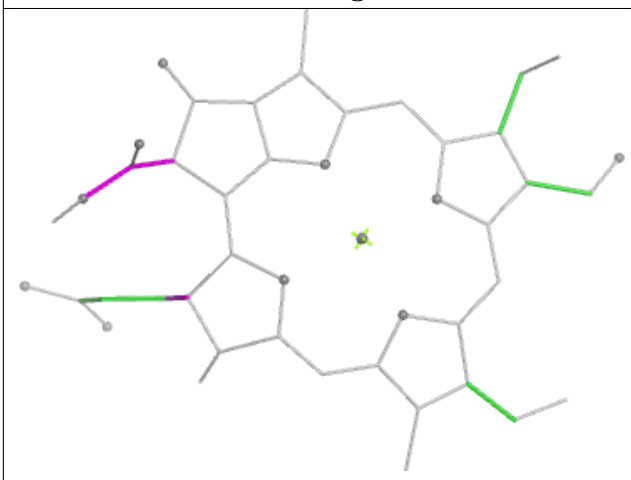
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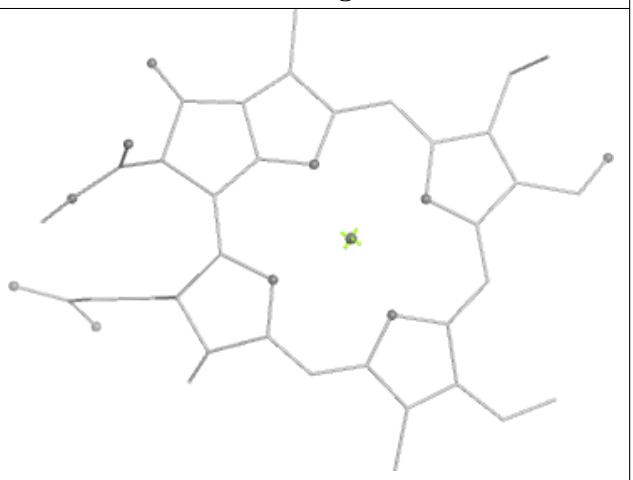
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Bond angles

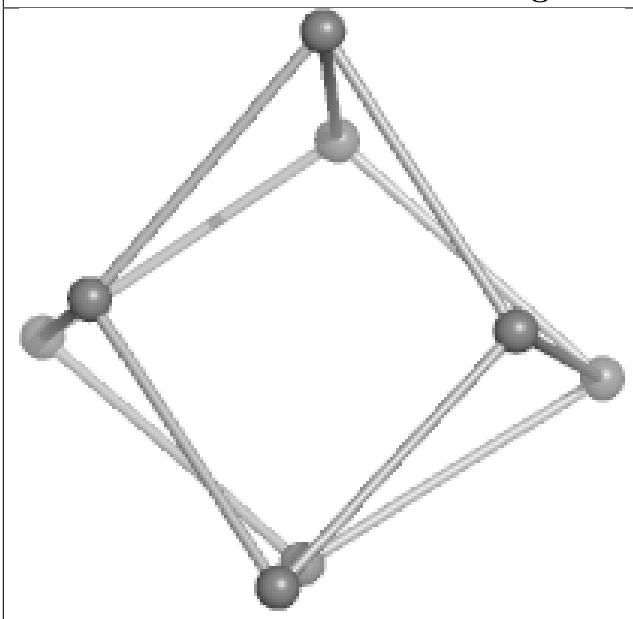


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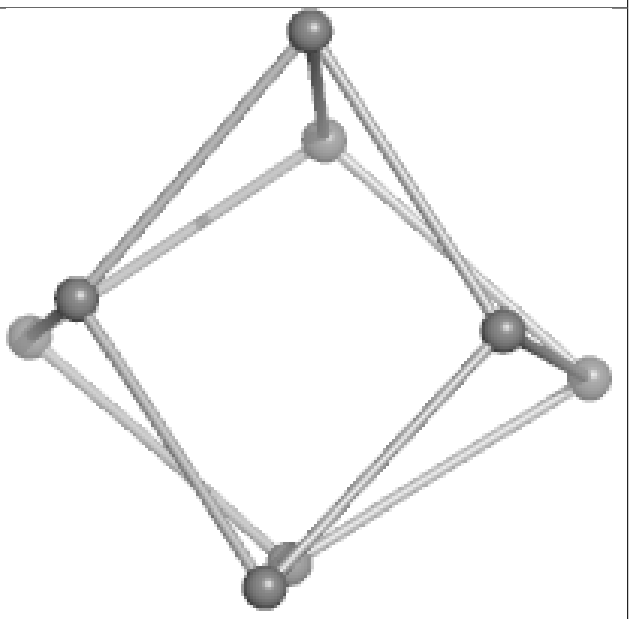


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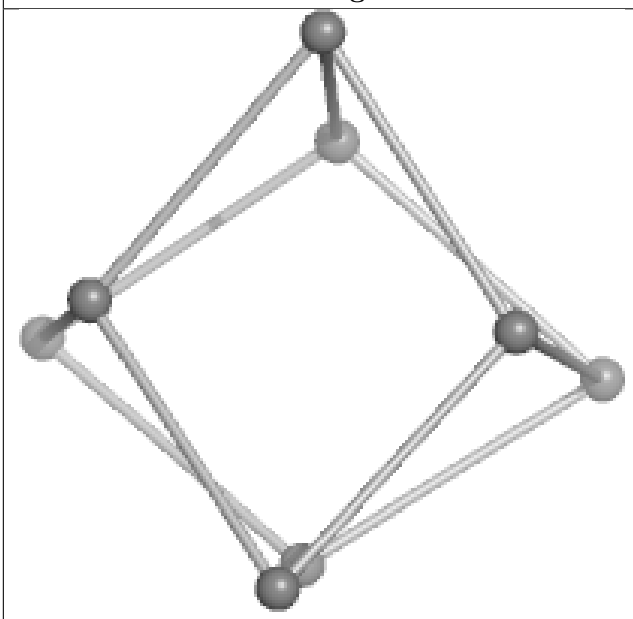
Ligand SF4 C 101



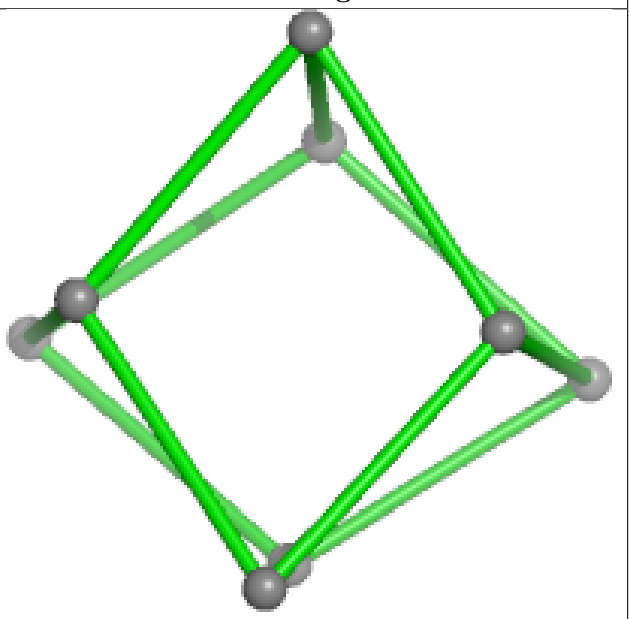
Bond lengths



Bond angles

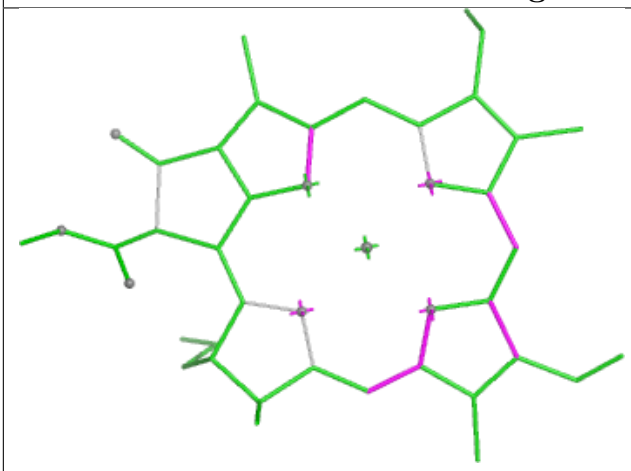


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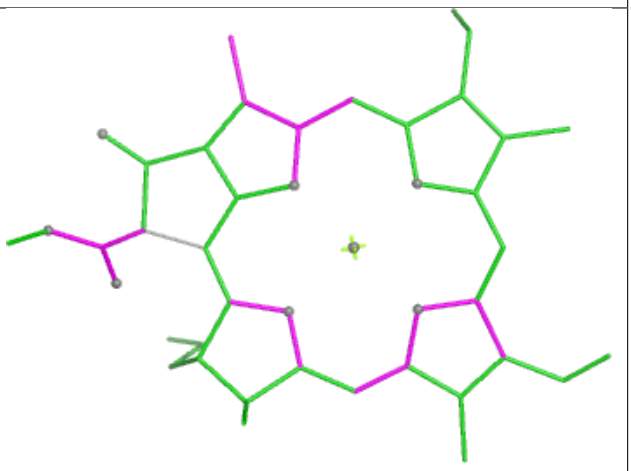


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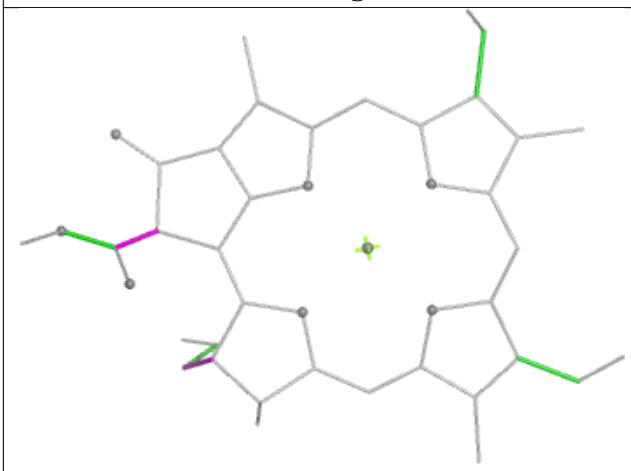
Ligand CLA 2 613



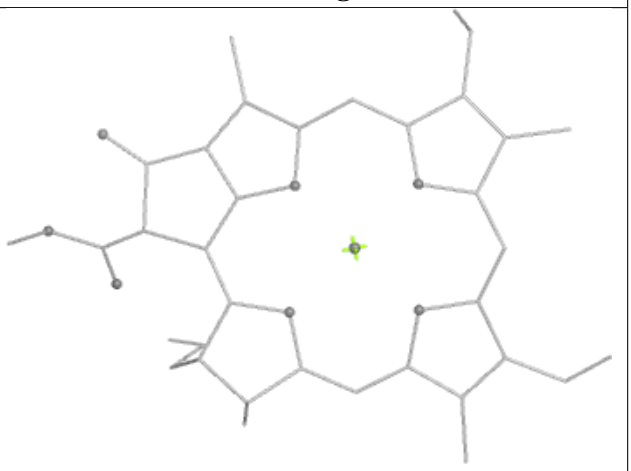
Bond lengths



Bond angles

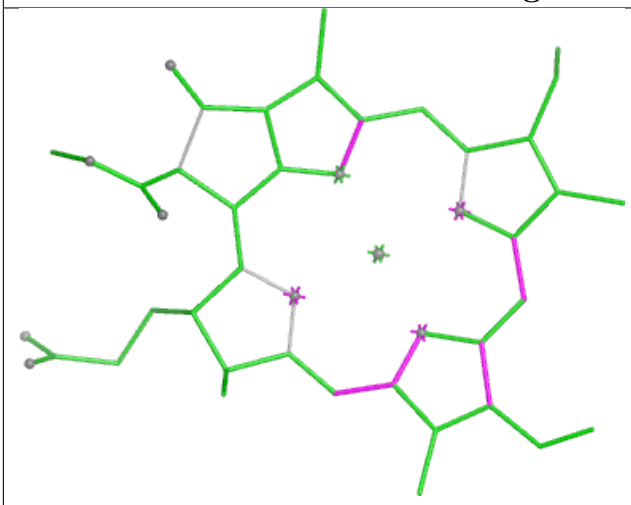


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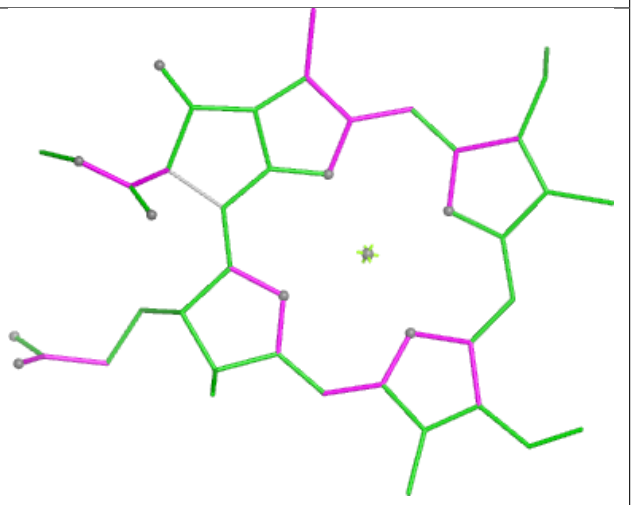


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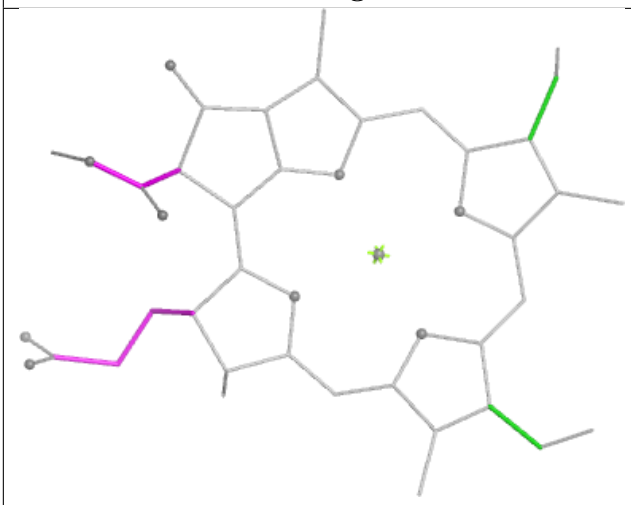
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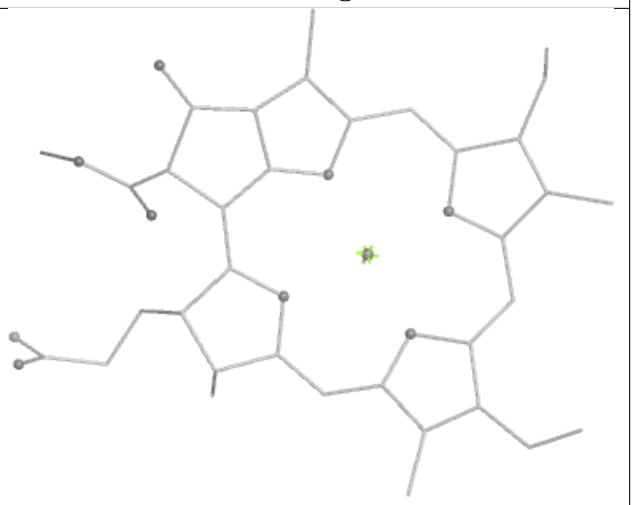
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Bond angles

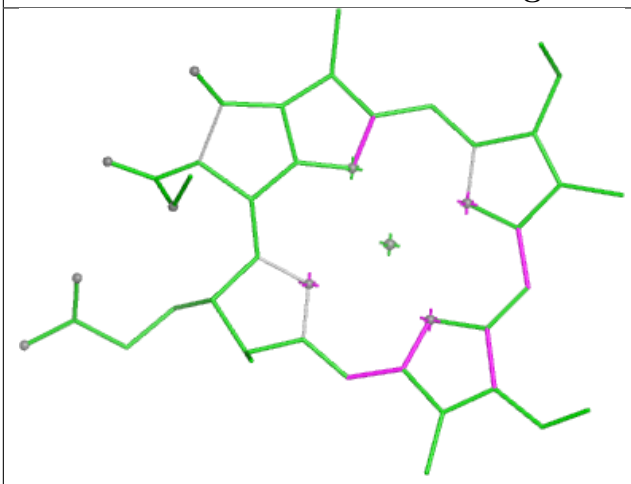


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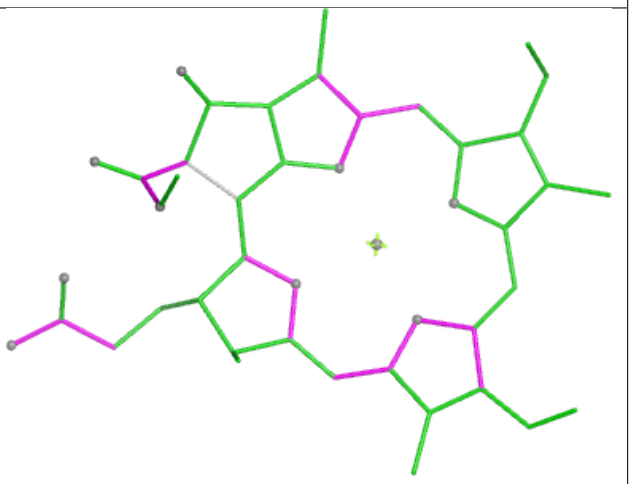


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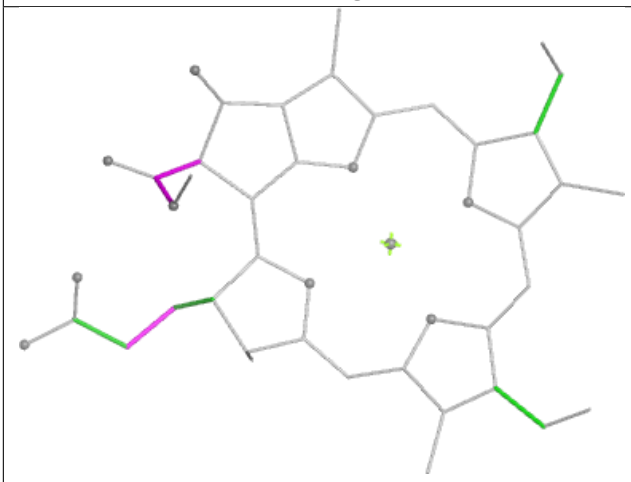
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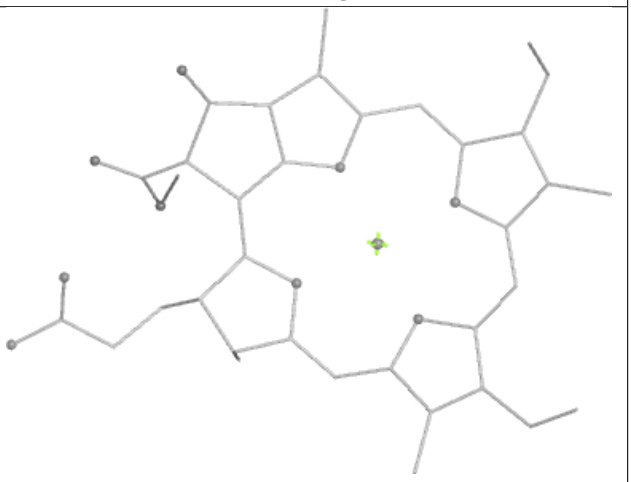
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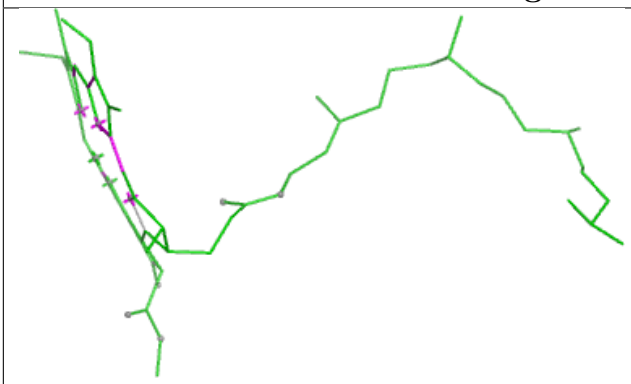


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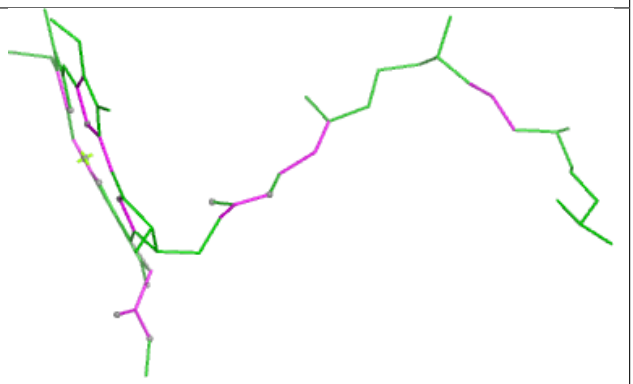


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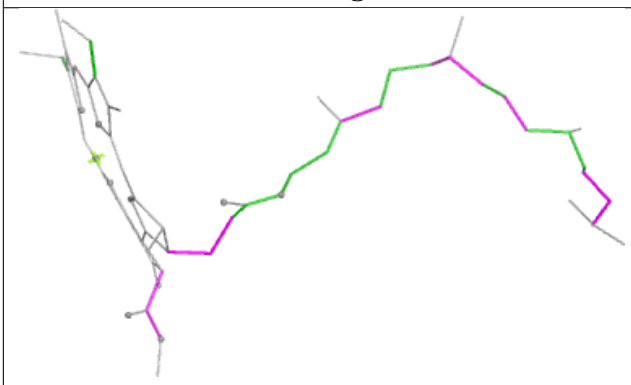
Ligand CLA B 838



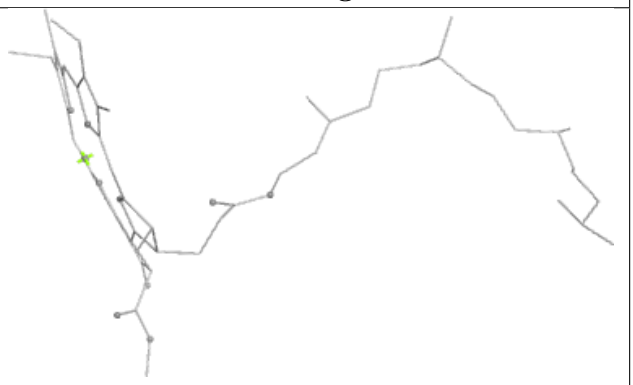
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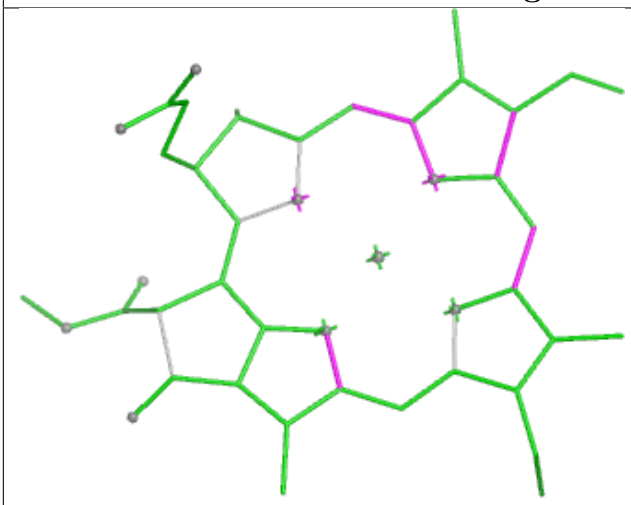


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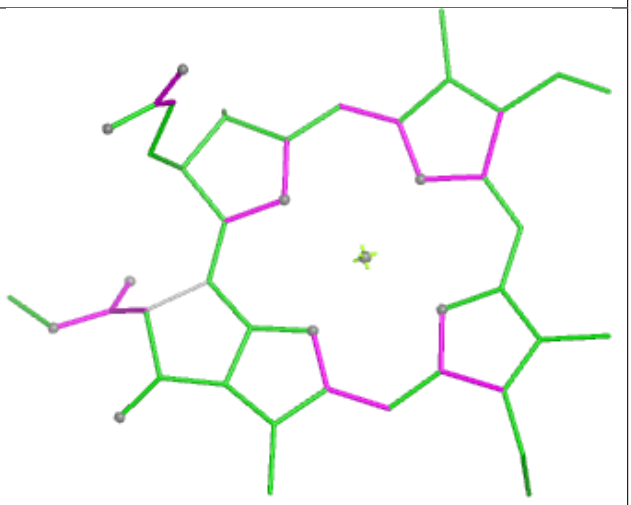


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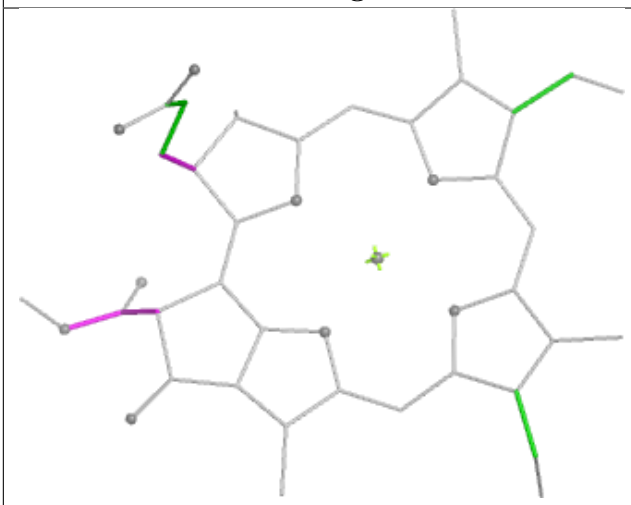
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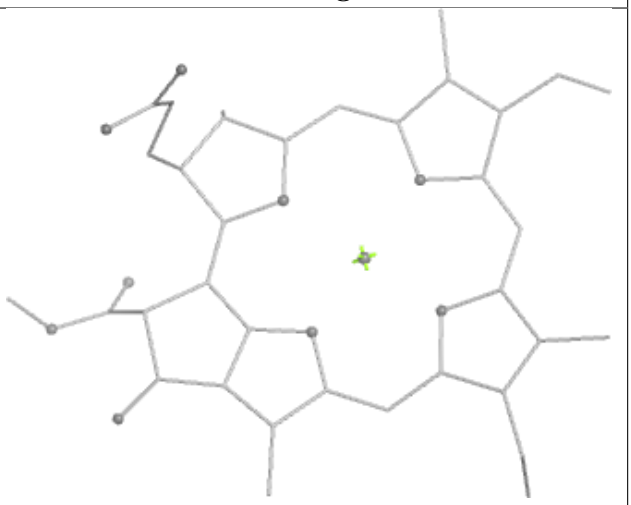
Bond lengths



Bond angles

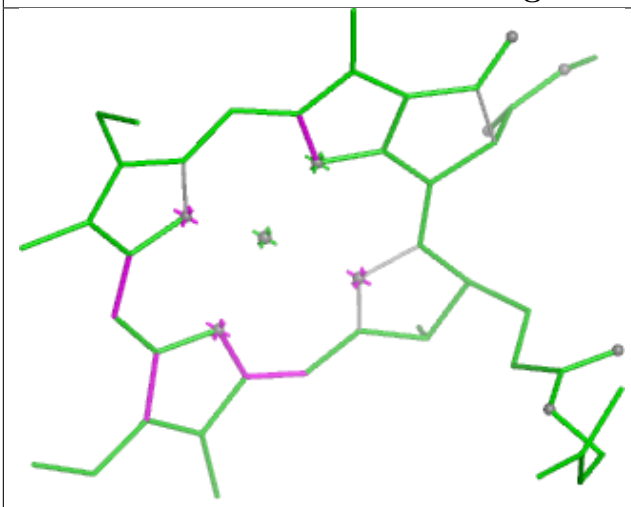


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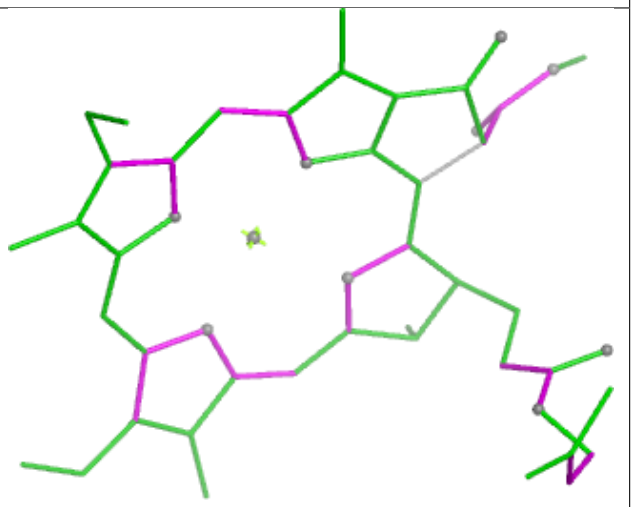


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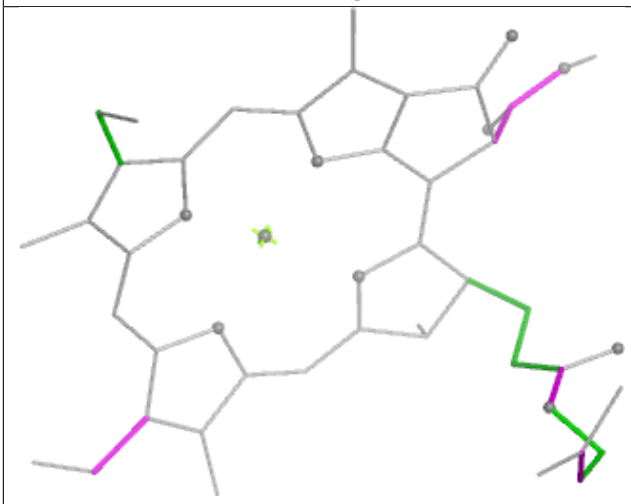
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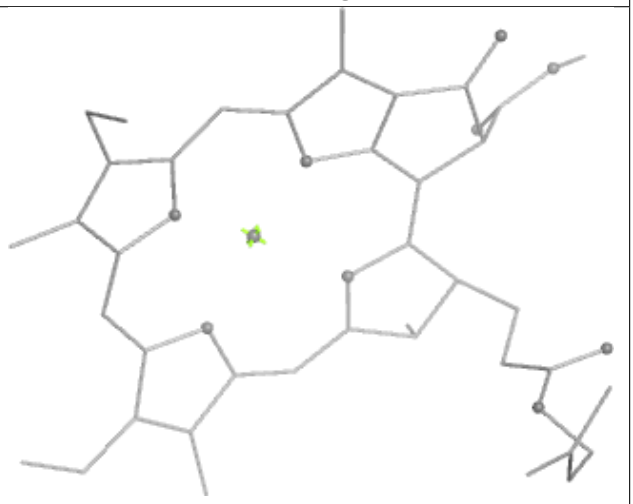
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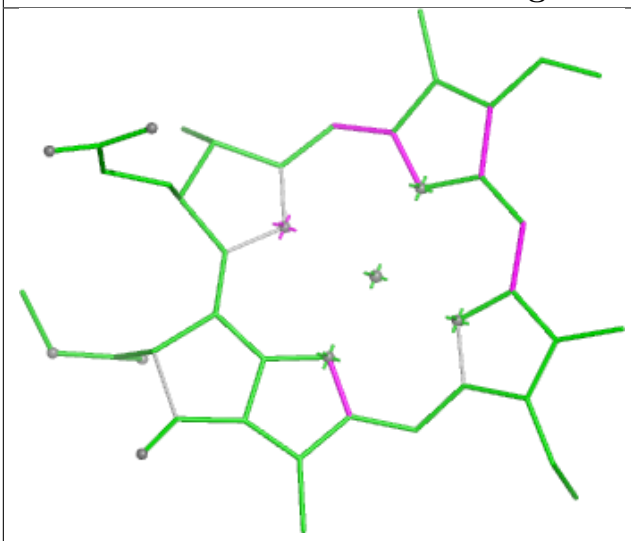


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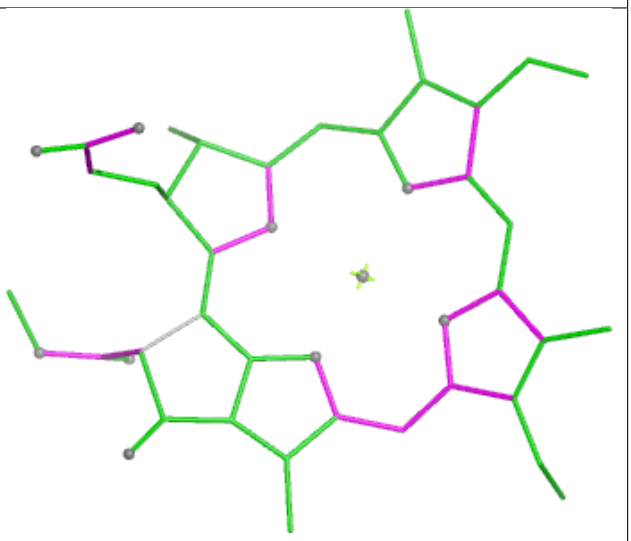


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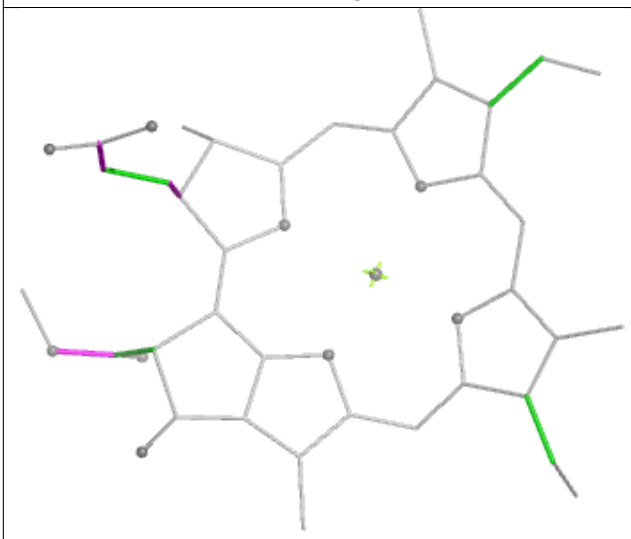
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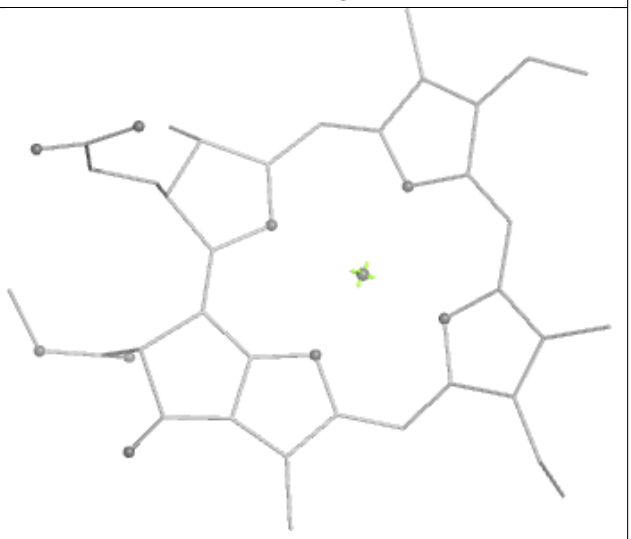
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Bond angles

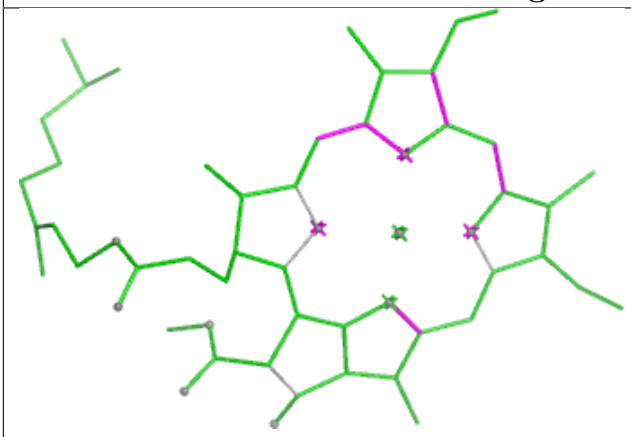


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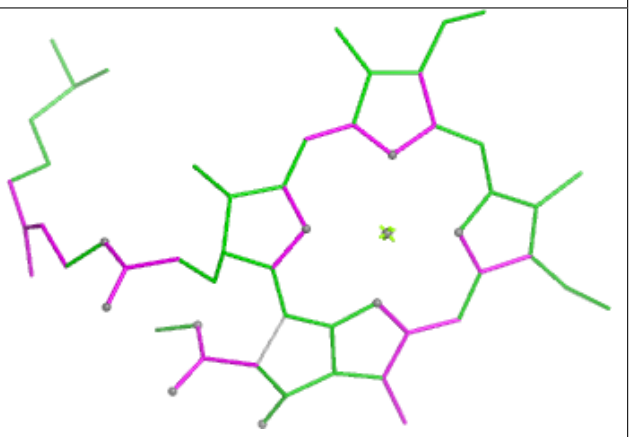


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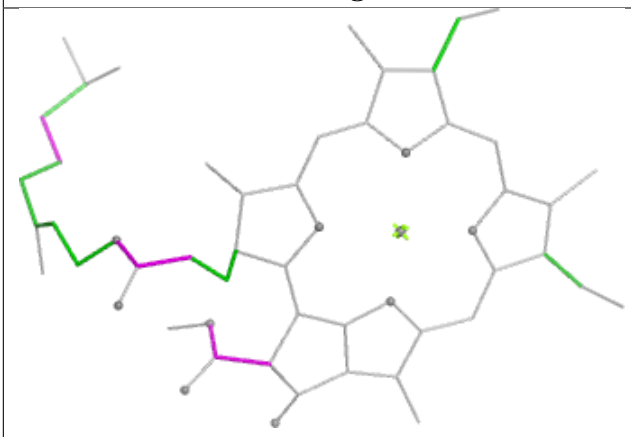
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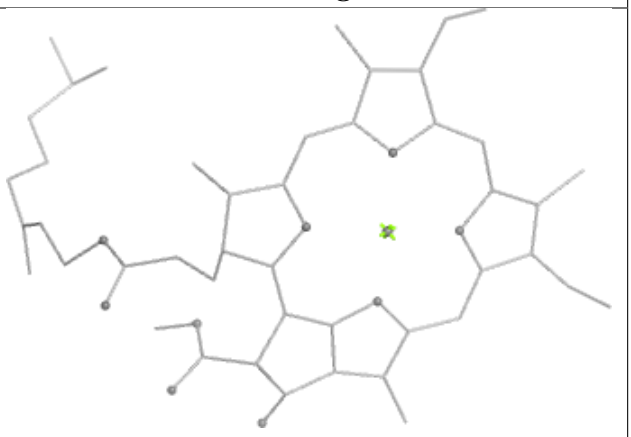
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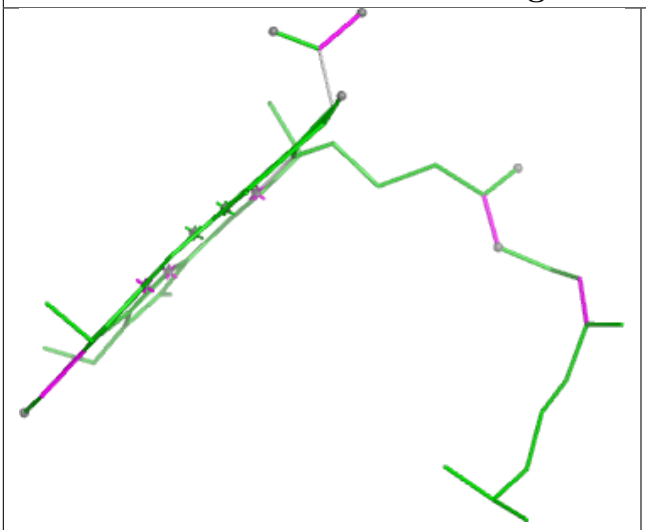


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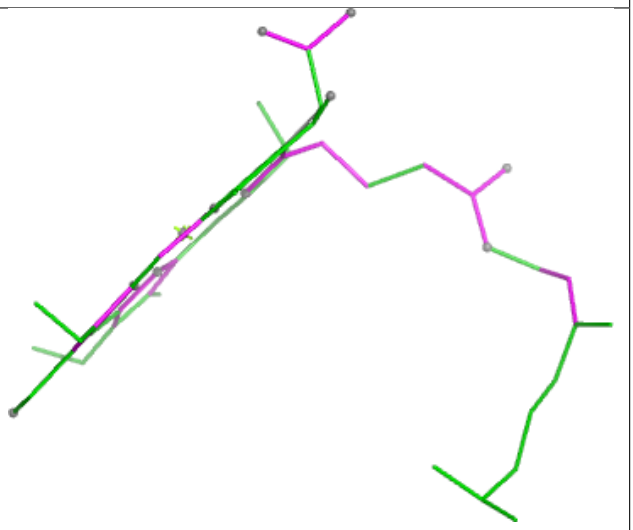


Rings

Ligand CHL 5 601



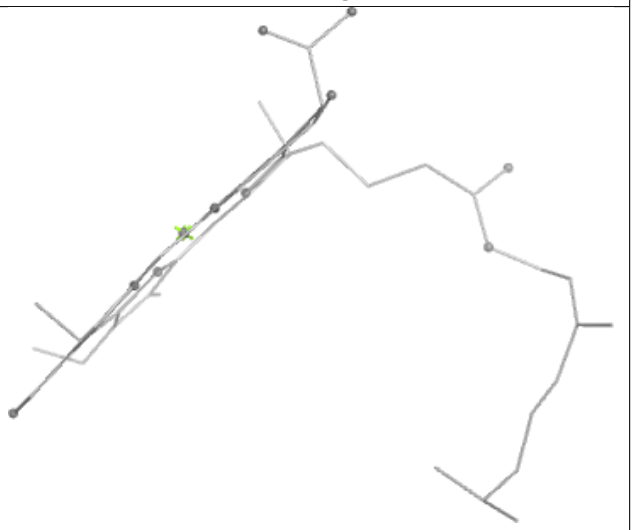
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Bond angles

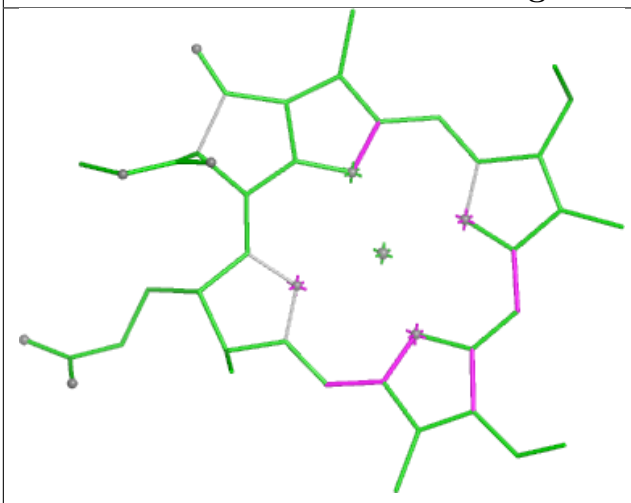


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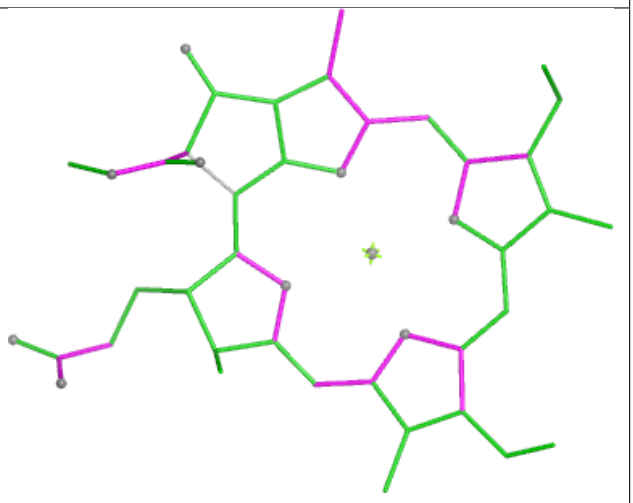


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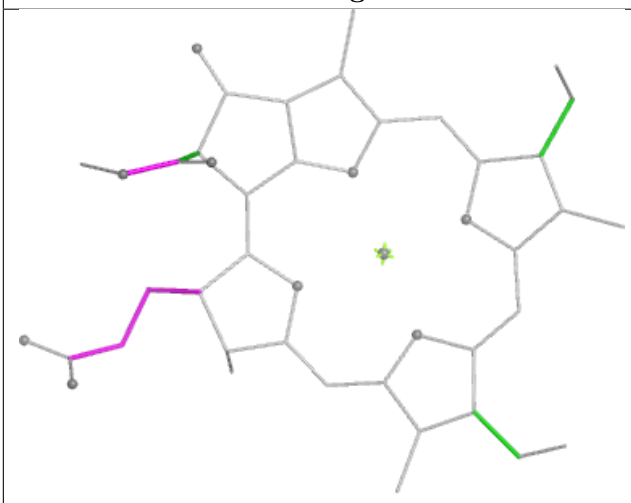
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Bond lengths



Bond angles

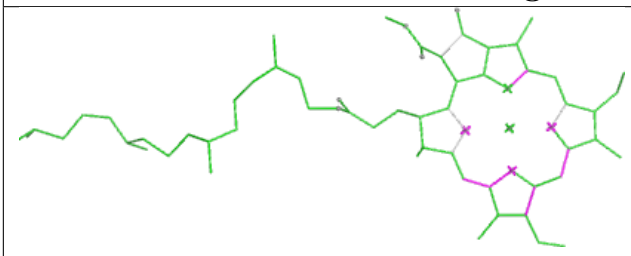


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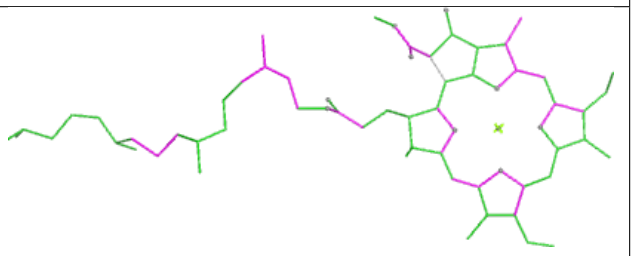


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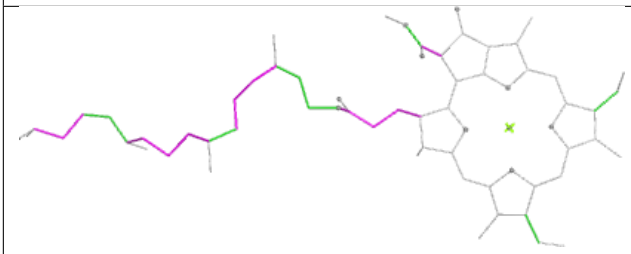
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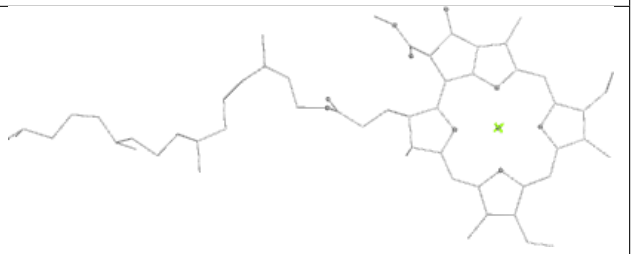
Bond lengths



Bond angles

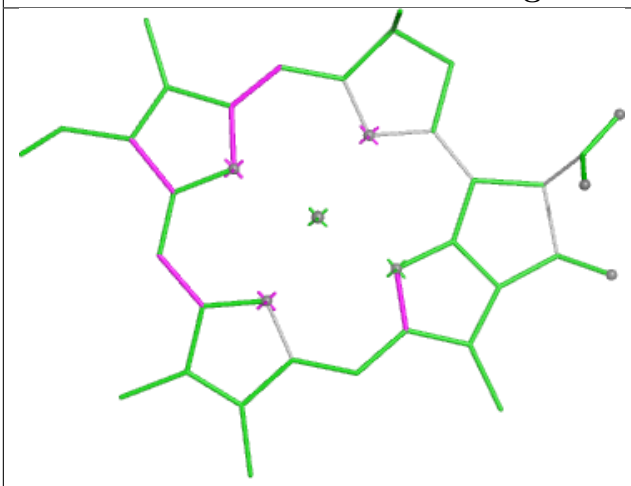


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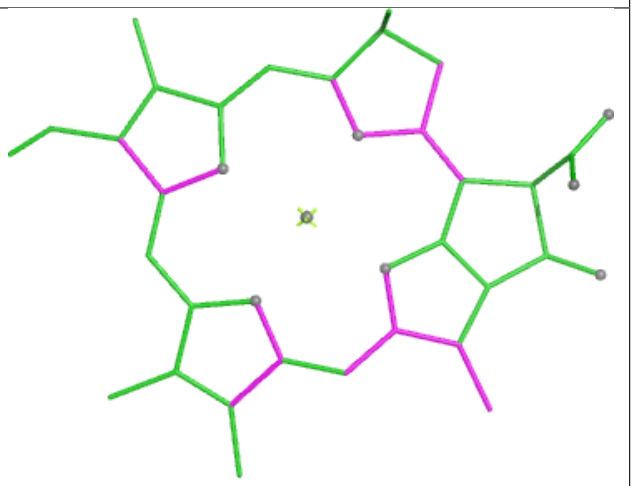


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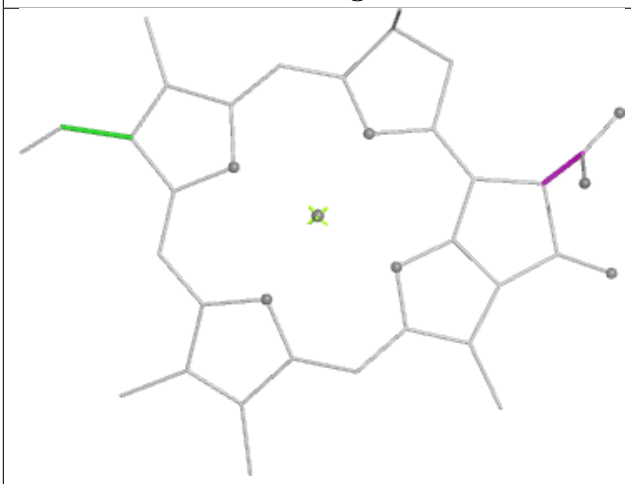
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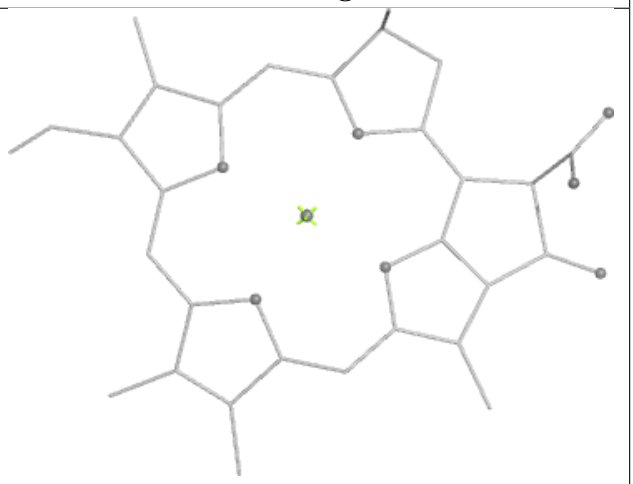
Bond lengths



Bond angles

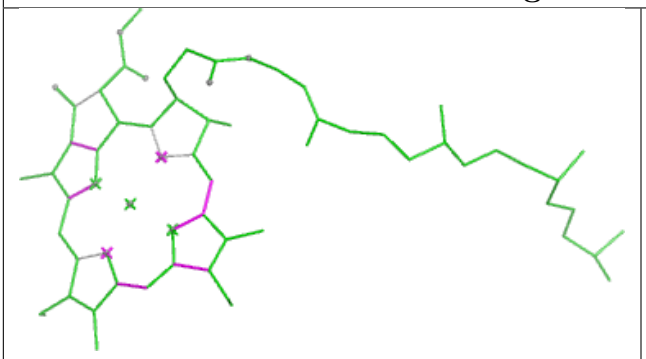


Torsions

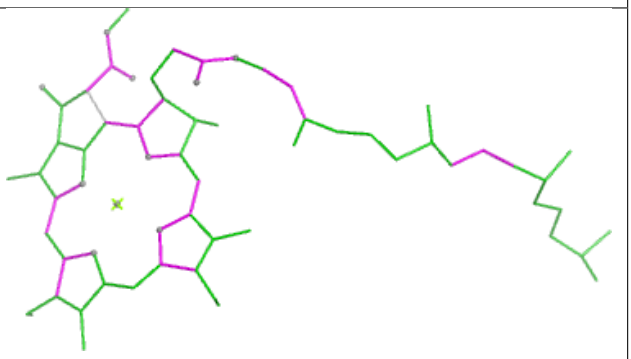


Rings

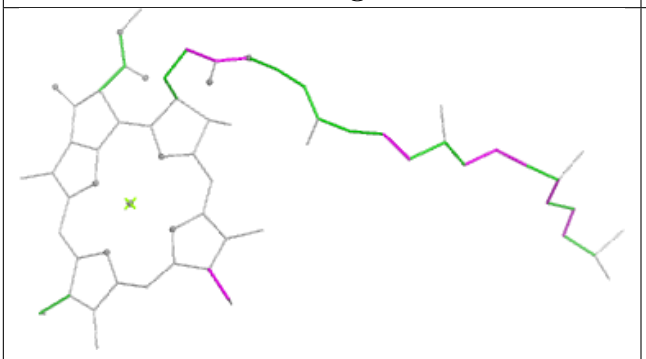
Ligand CLA A 802



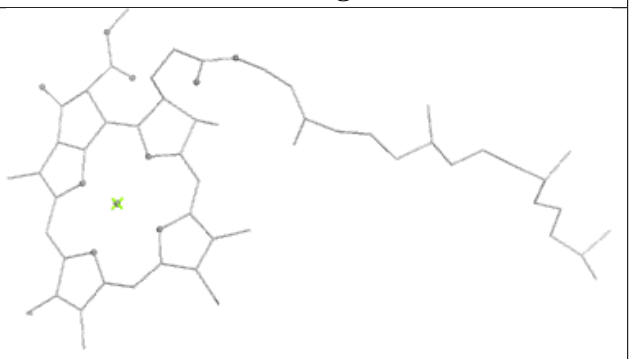
Bond lengths



Bond angles



Torsions

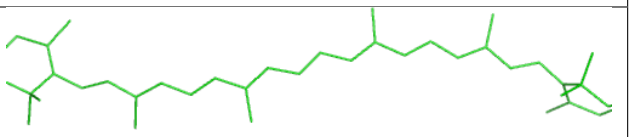


Rings

Ligand BCR 6 618



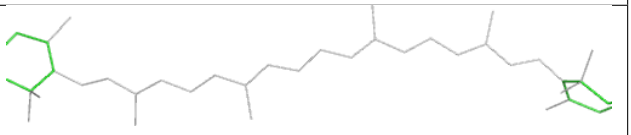
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Bond angles

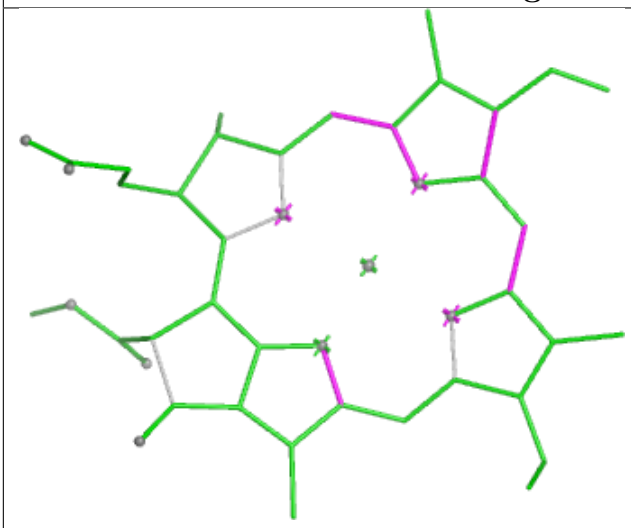


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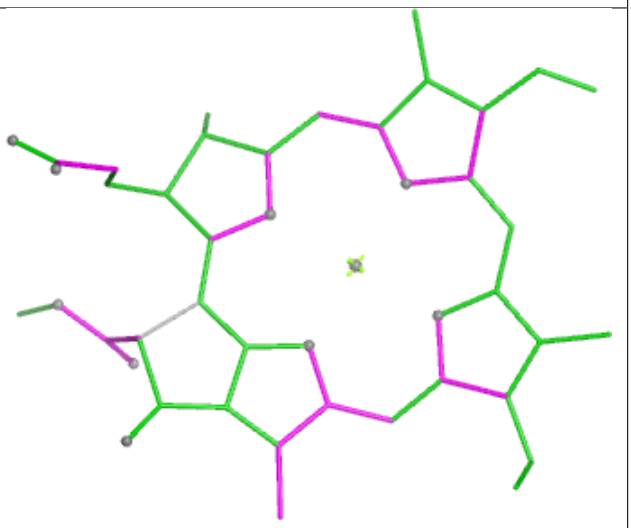


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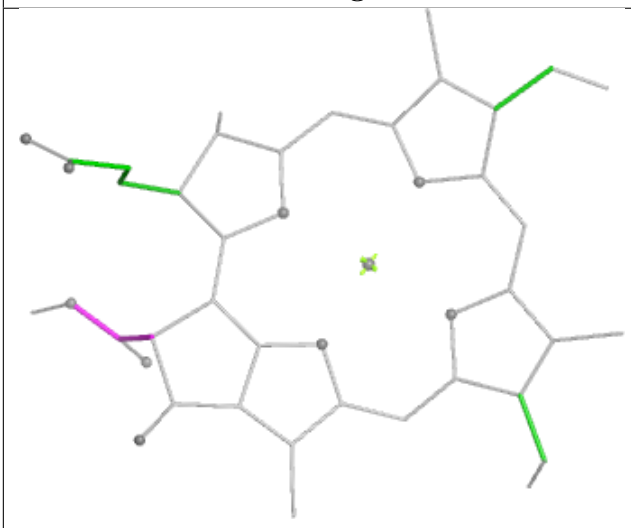
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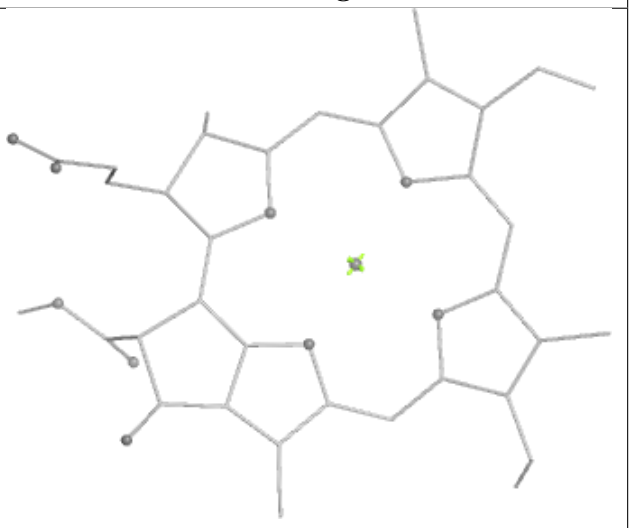
Bond lengths



Bond angles

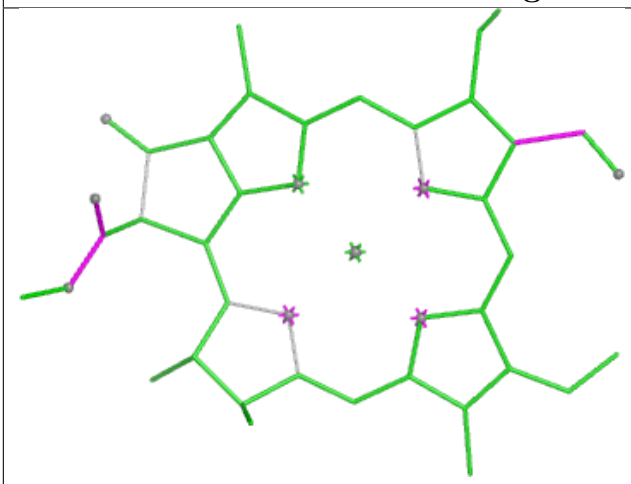


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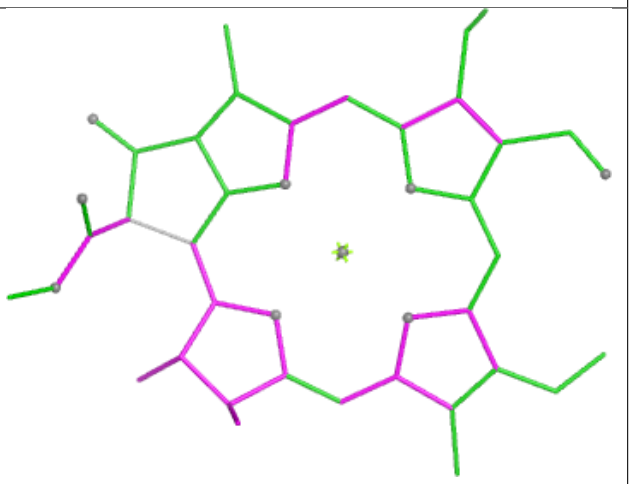


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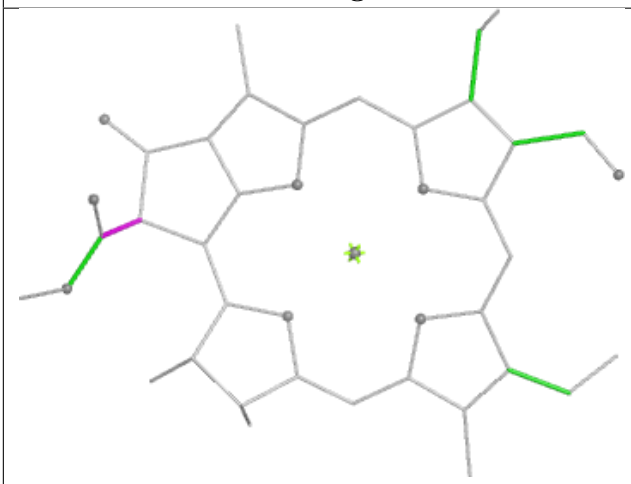
Ligand CHL X 605



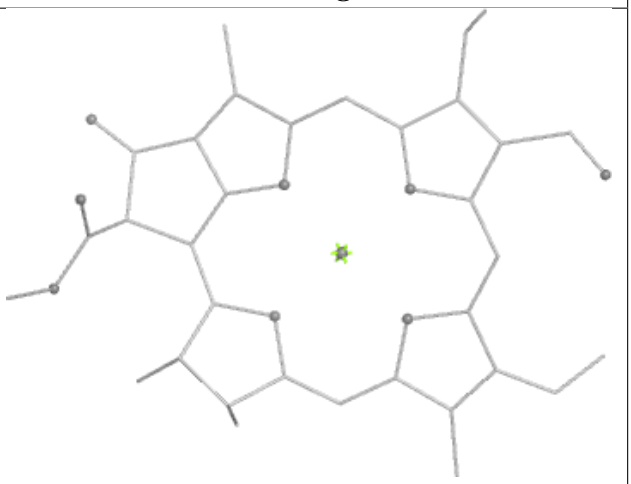
Bond lengths



Bond angles

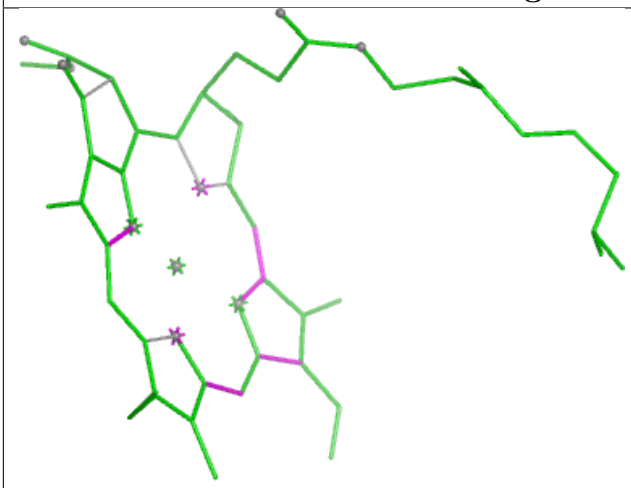


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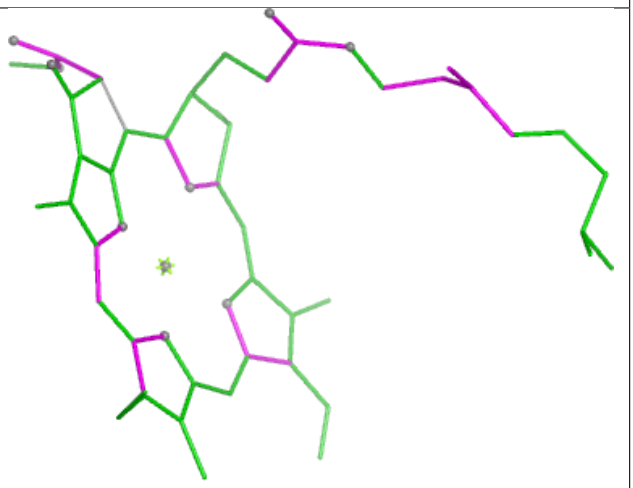


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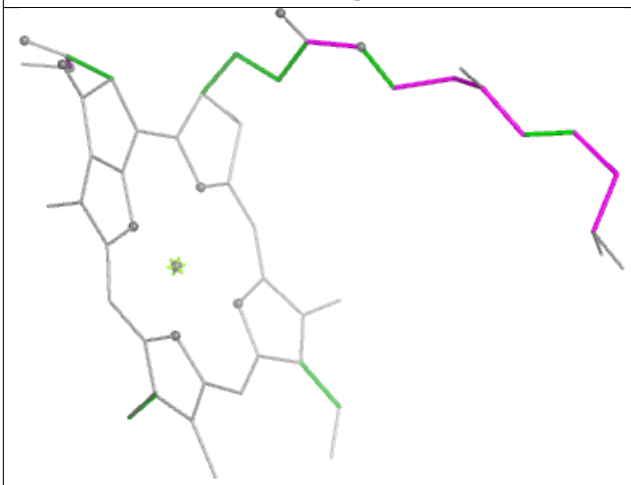
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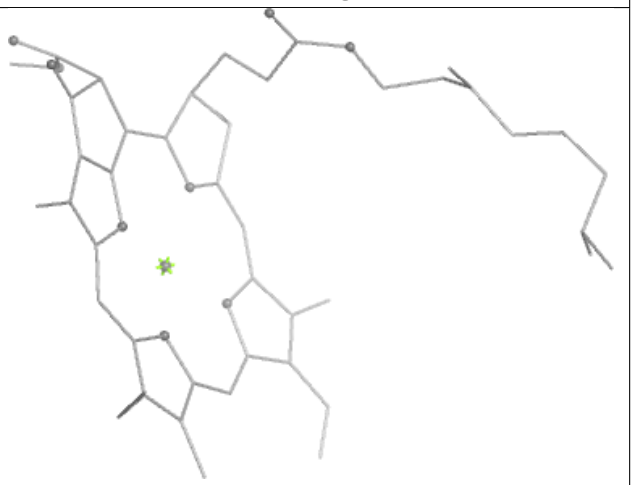
Bond lengths



Bond angles

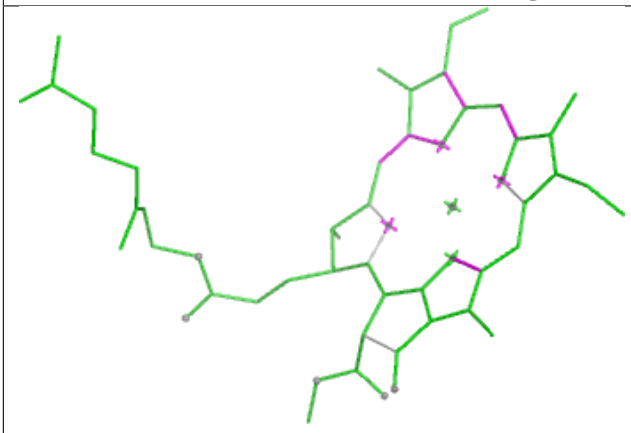


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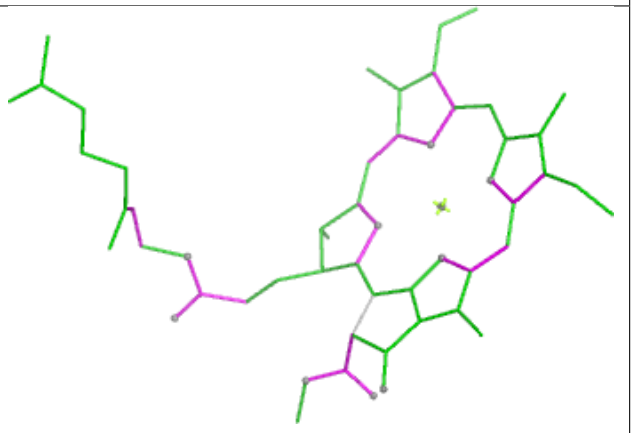


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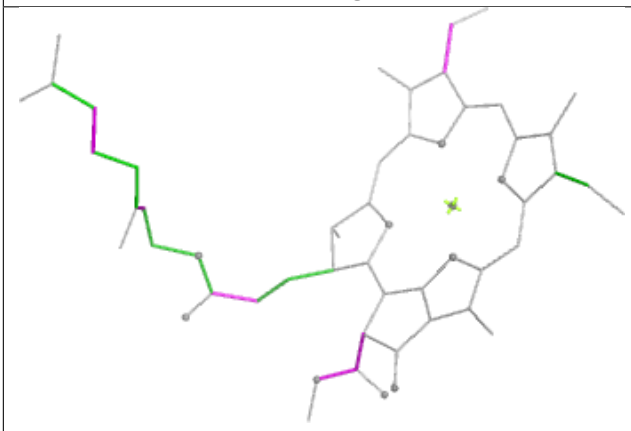
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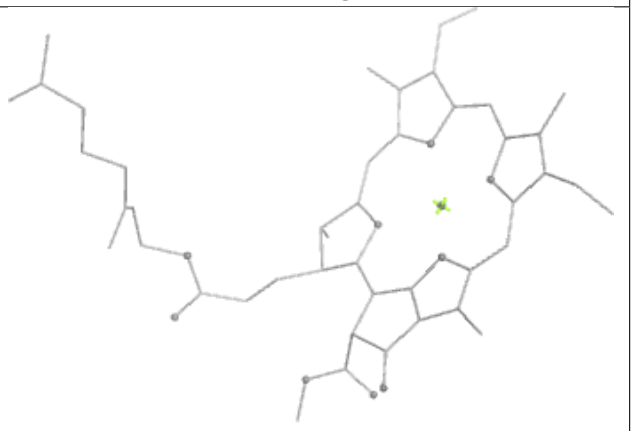
Bond lengths



Bond angles

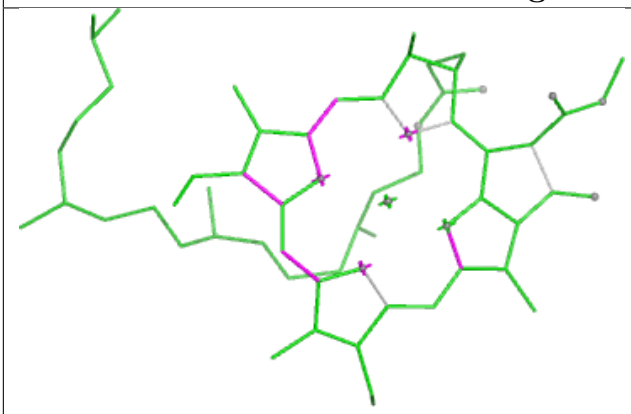


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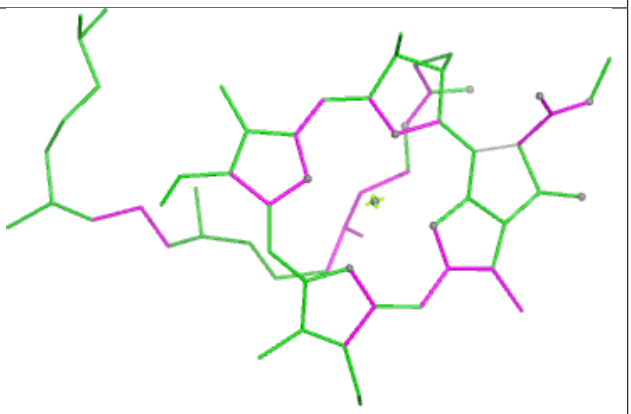


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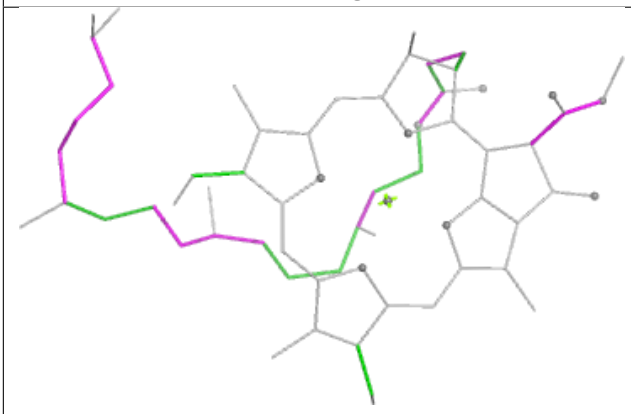
Ligand CLA 1 612



Bond lengths



Bond angles

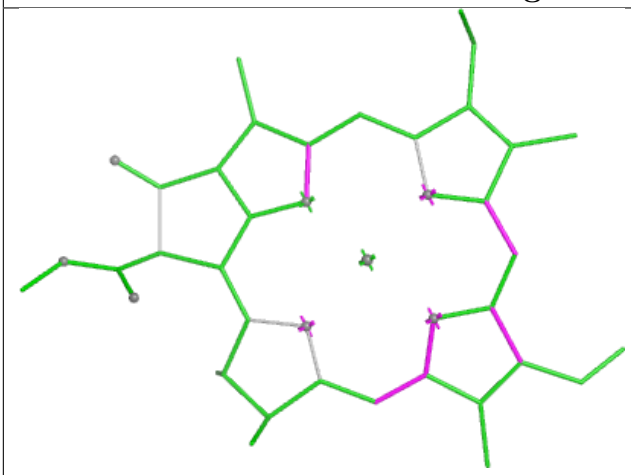


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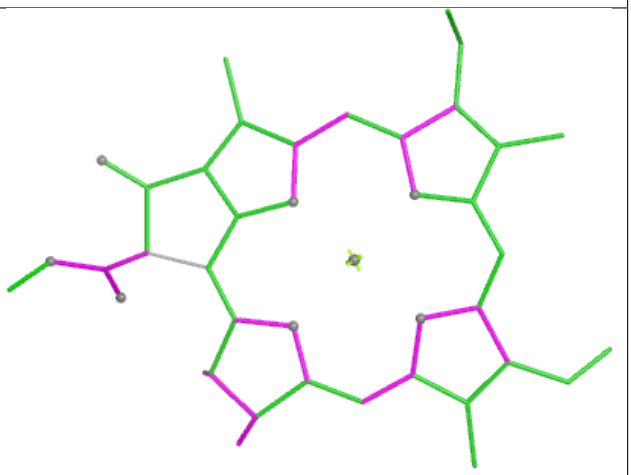


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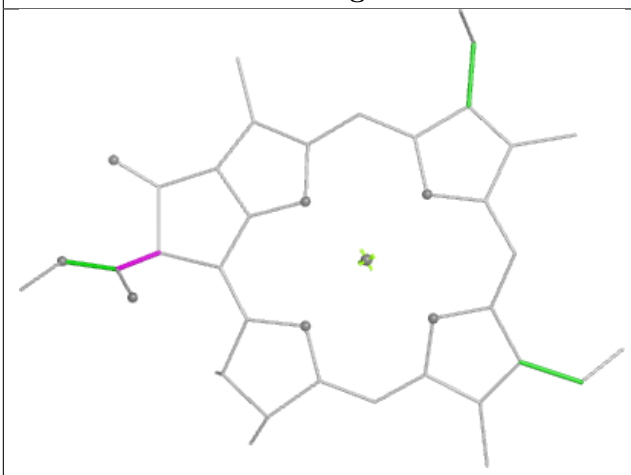
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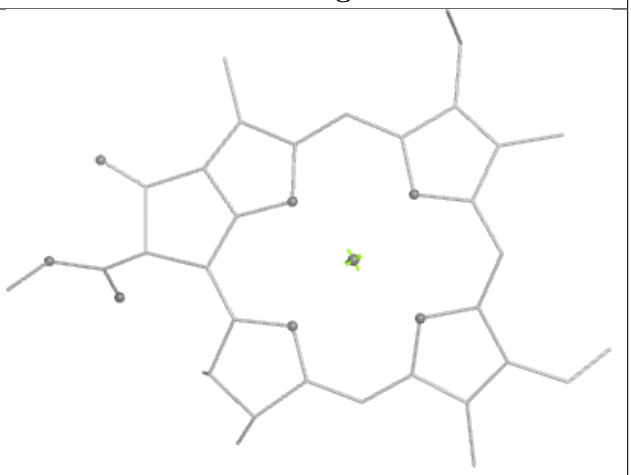
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Bond angles

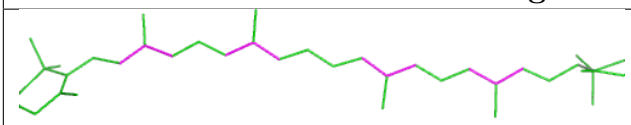


Torsions



Rings

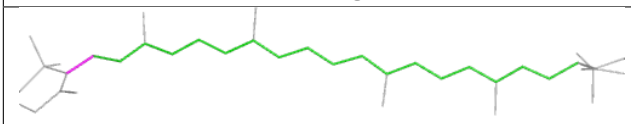
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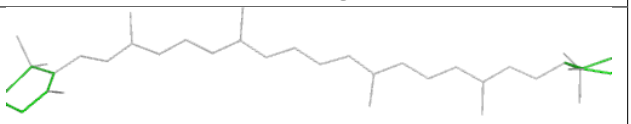
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Bond angles

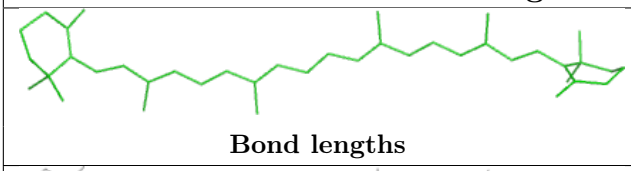


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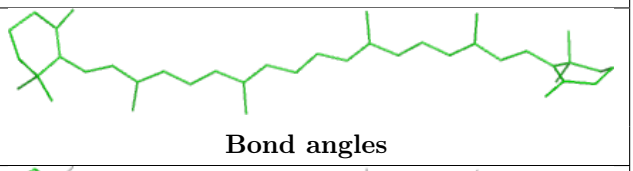


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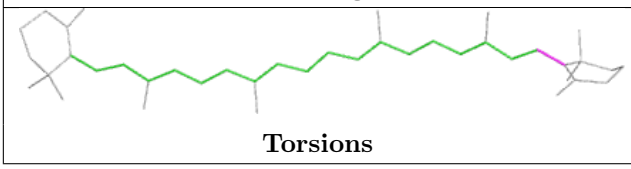
Ligand BCR J 103



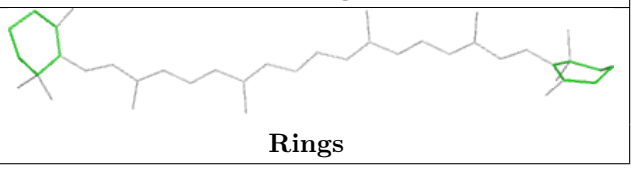
Bond lengths



Bond angles

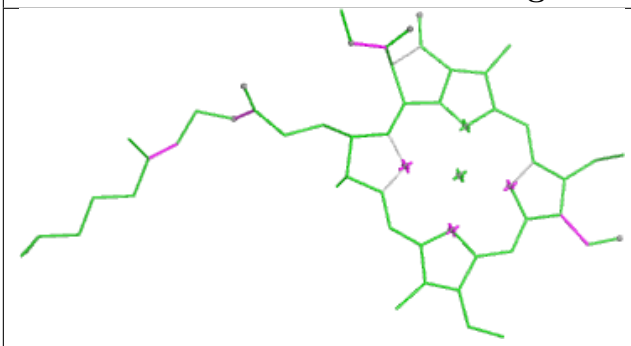


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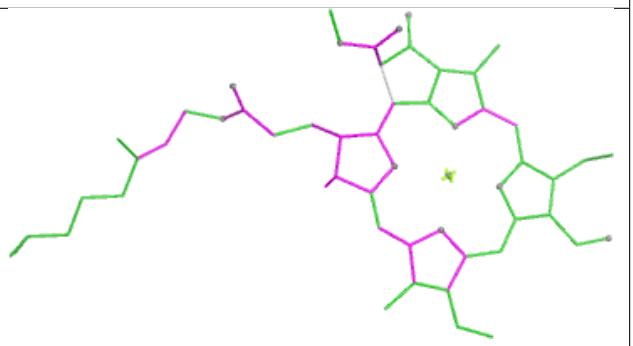


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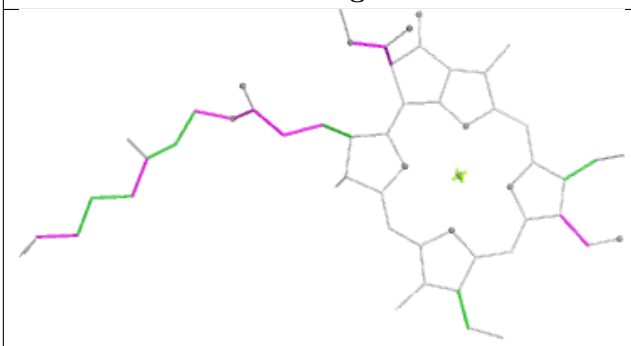
Ligand CHL 4 304



Bond lengths



Bond angles

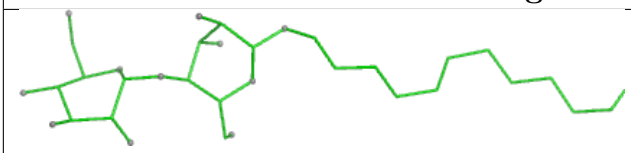


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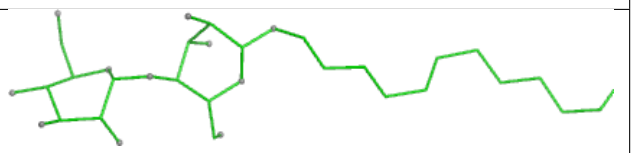


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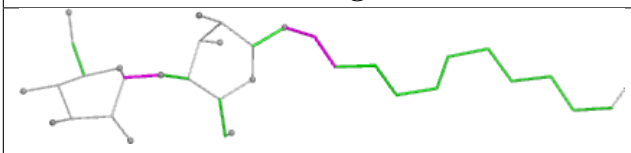
Ligand LMT 6 621



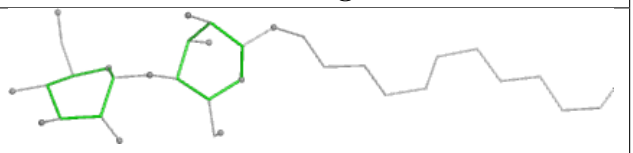
Bond lengths



Bond angles

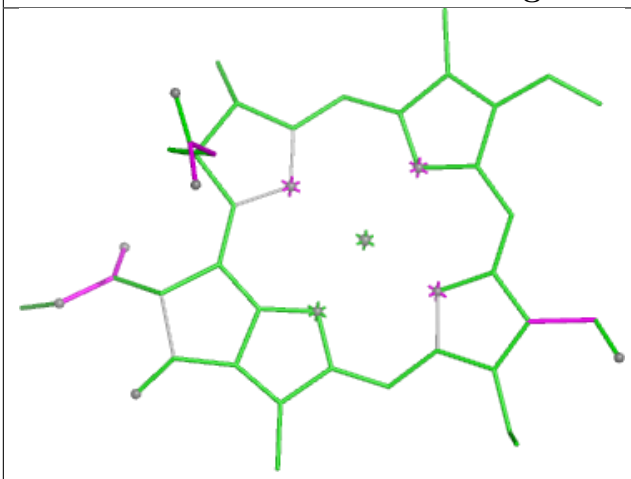


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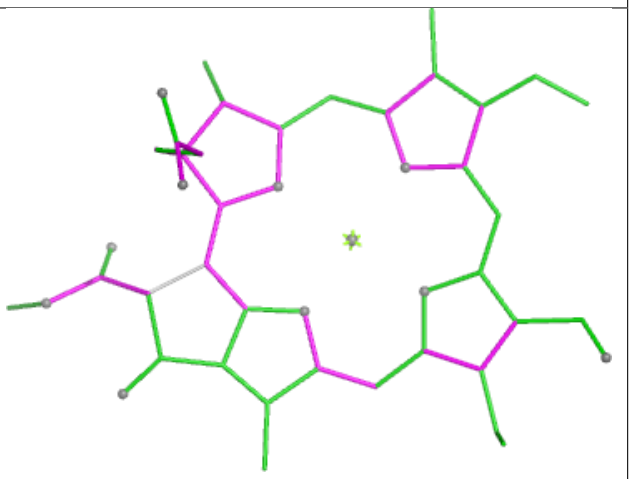


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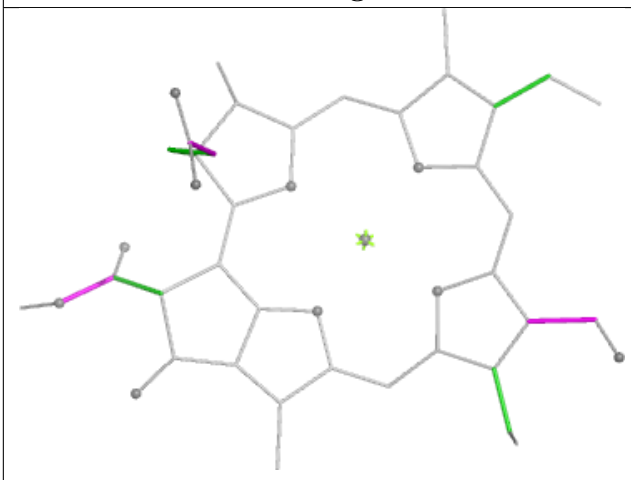
Ligand CHL X 608



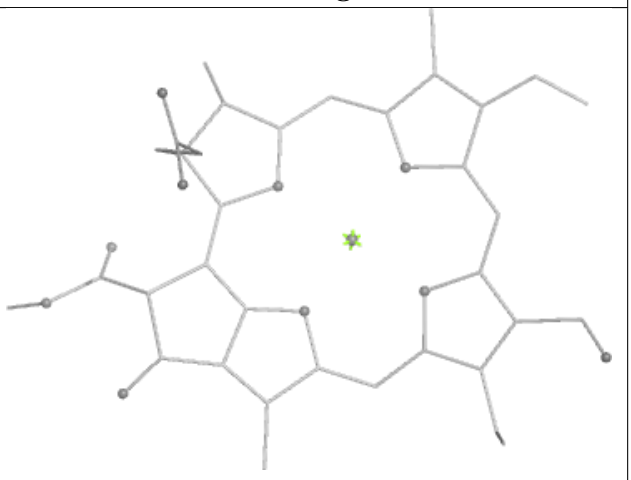
Bond lengths



Bond angles



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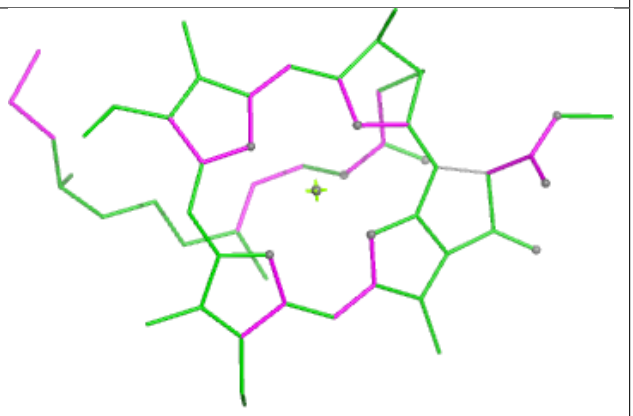


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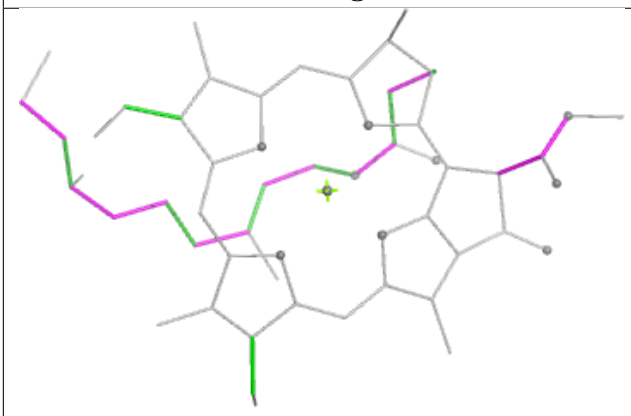
Ligand CLA 4 311



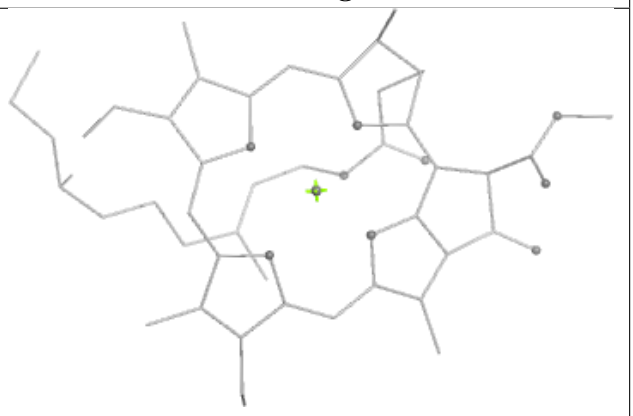
Bond lengths



Bond angles



Torsions



Rings

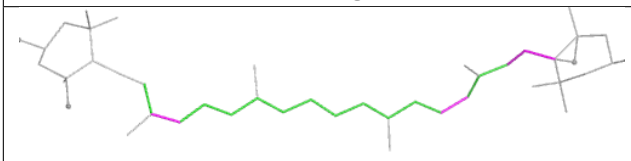
Ligand NEX Z 316



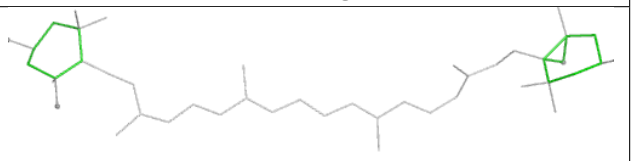
Bond lengths



Bond angles

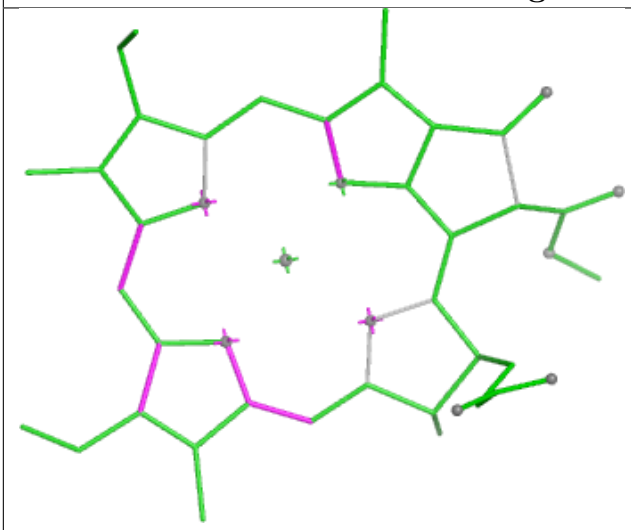


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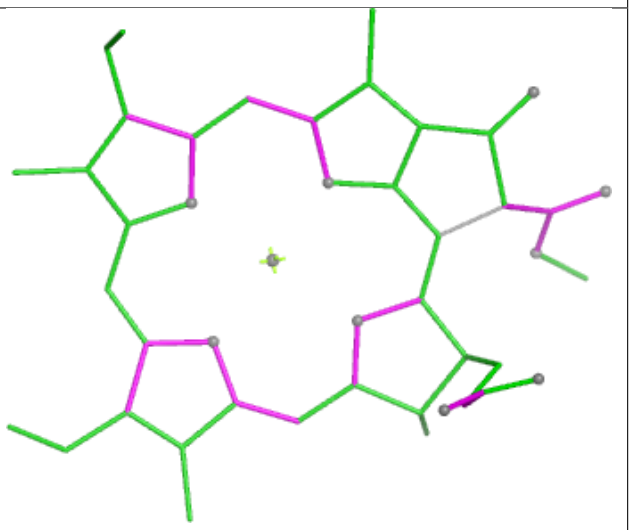


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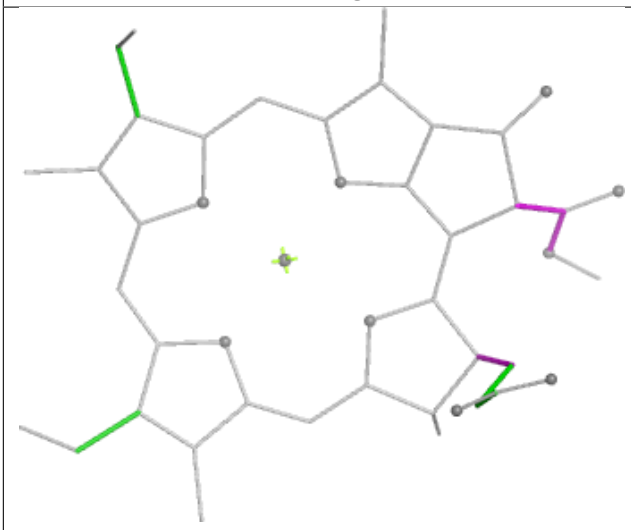
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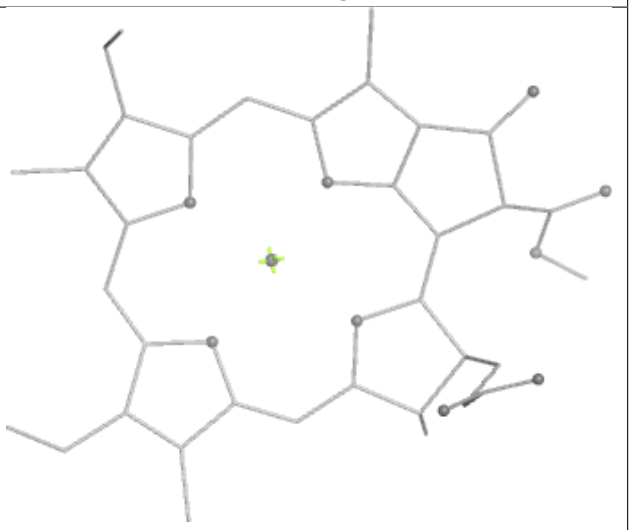
Bond lengths



Bond angles

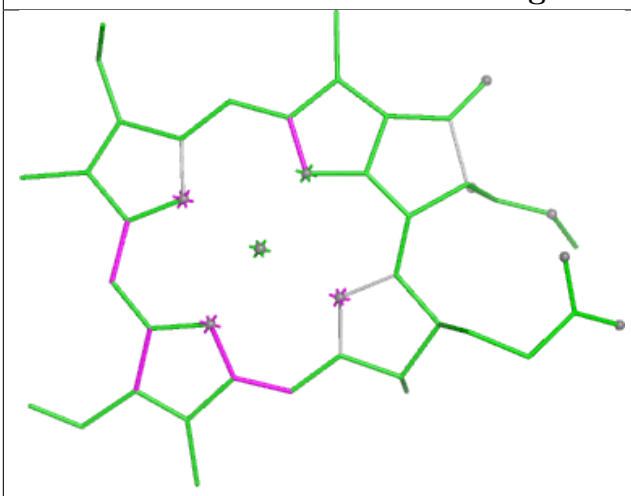


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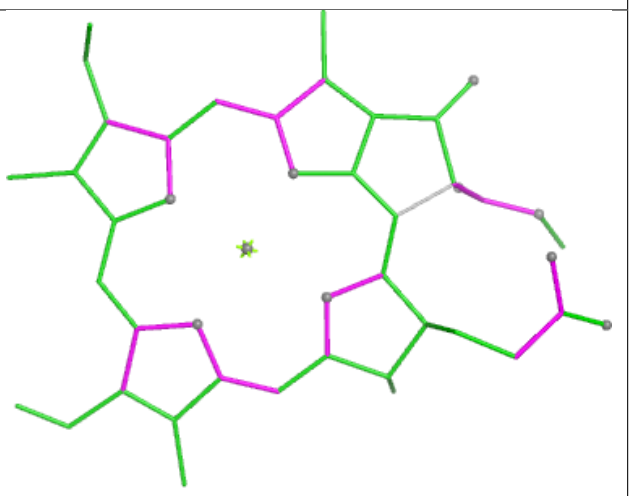


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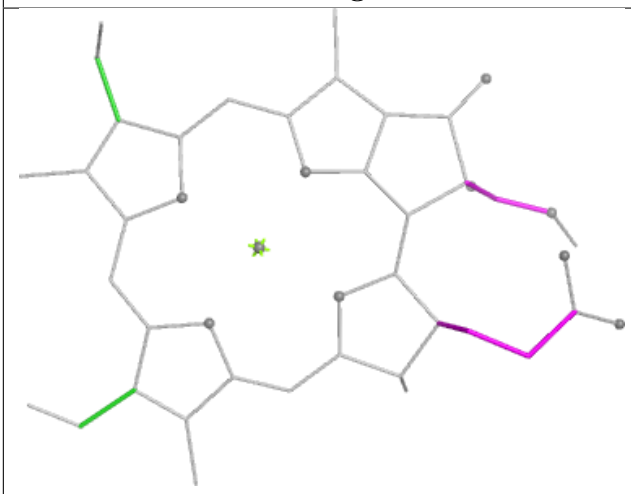
Ligand CLA 1 614



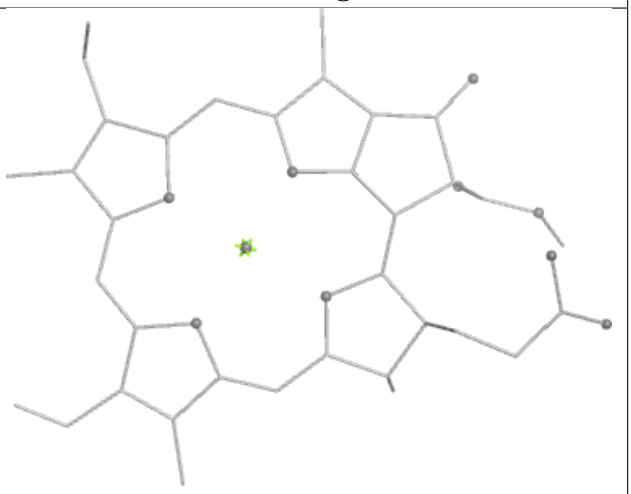
Bond lengths



Bond angles

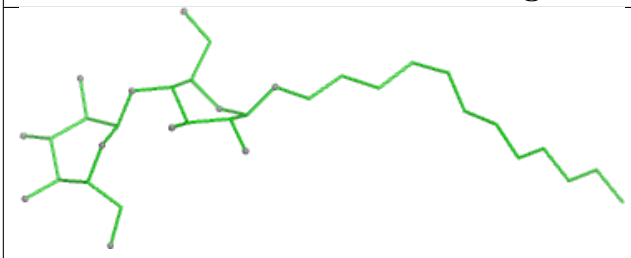


Torsions

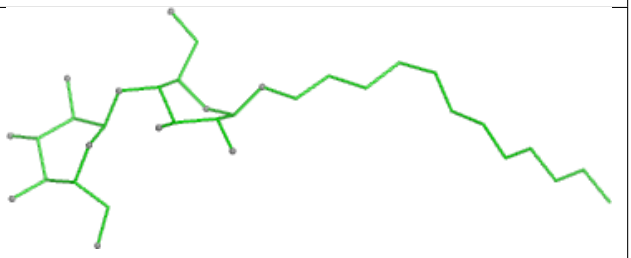


Rings

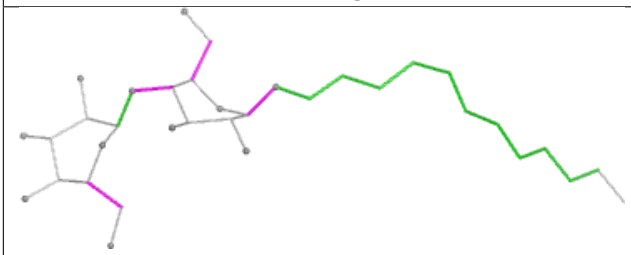
Ligand LMT F 303



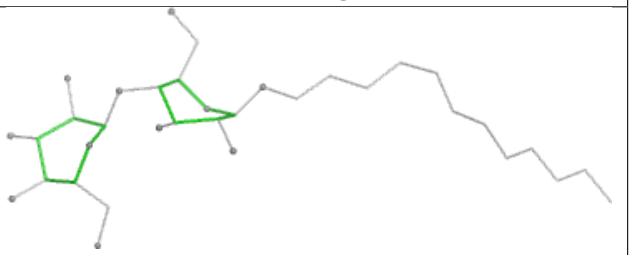
Bond lengths



Bond angles

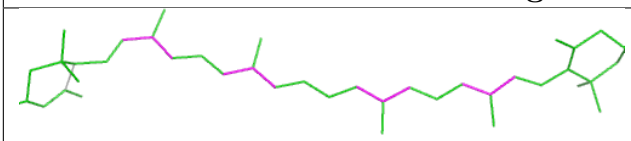


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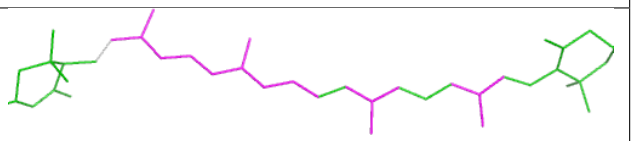


Rings

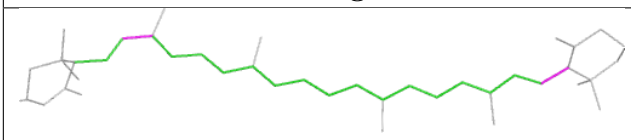
Ligand LUT Z 315



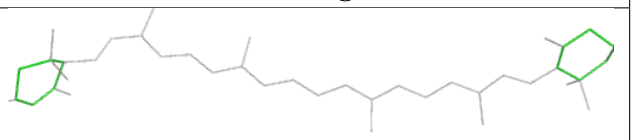
Bond lengths



Bond angles

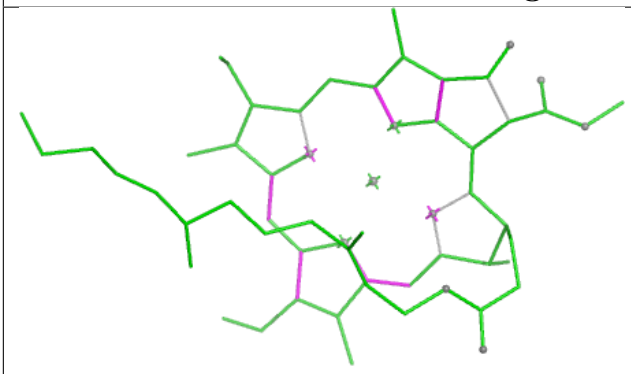


Torsions

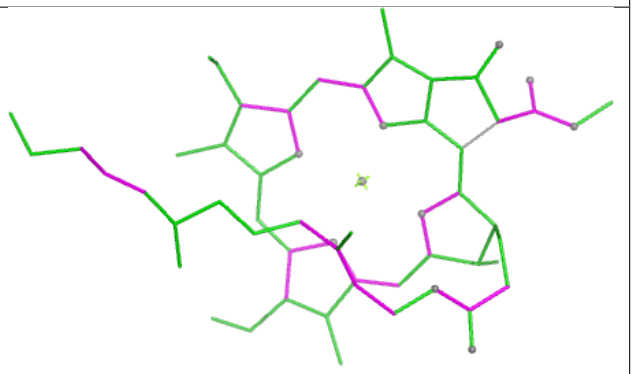


Rings

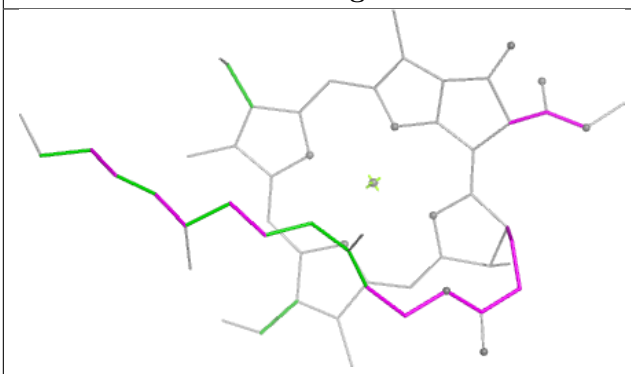
Ligand CLA A 818



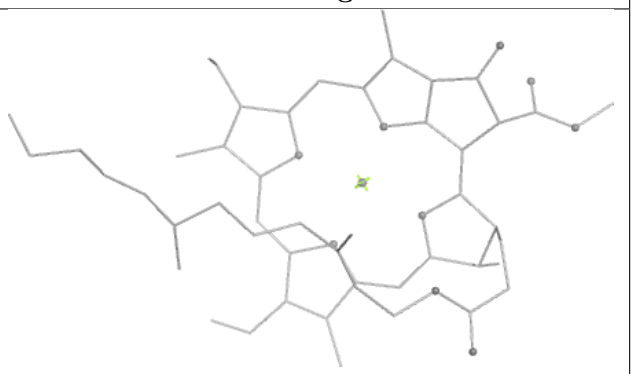
Bond lengths



Bond angles

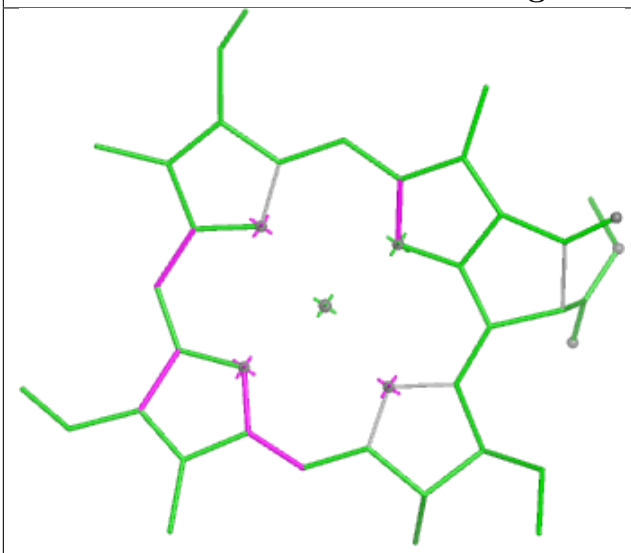


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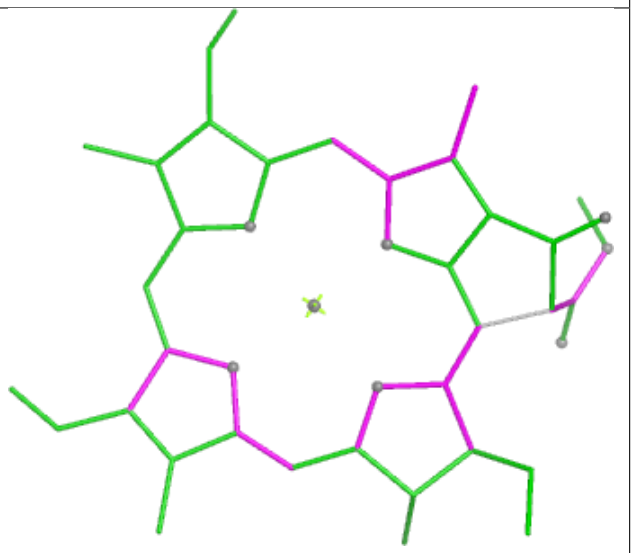


Rings

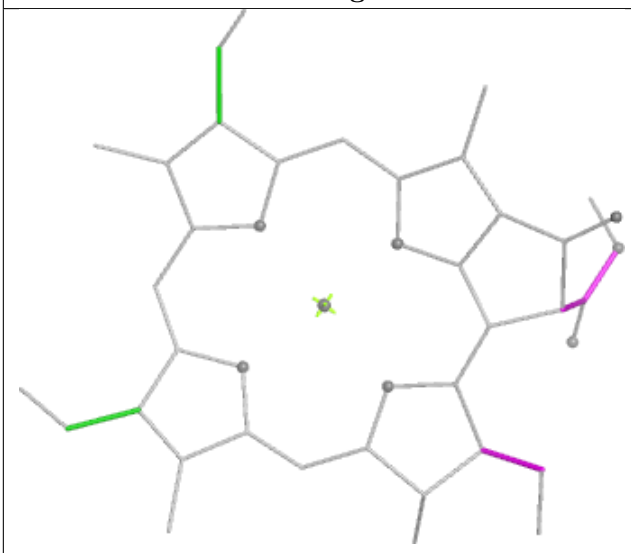
Ligand CLA J 102



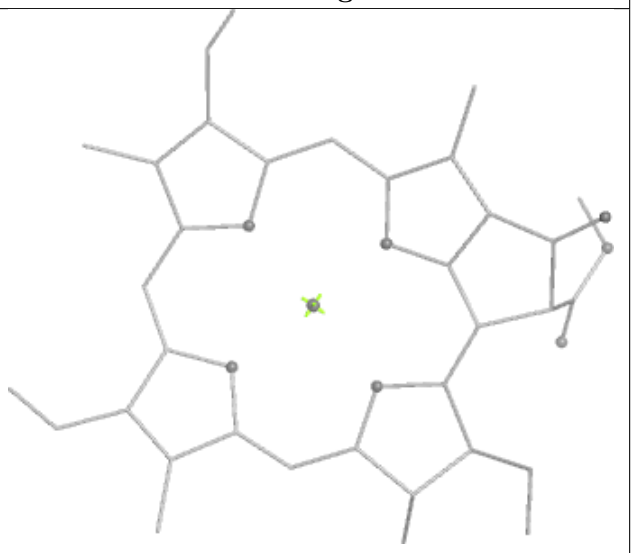
Bond lengths



Bond angles

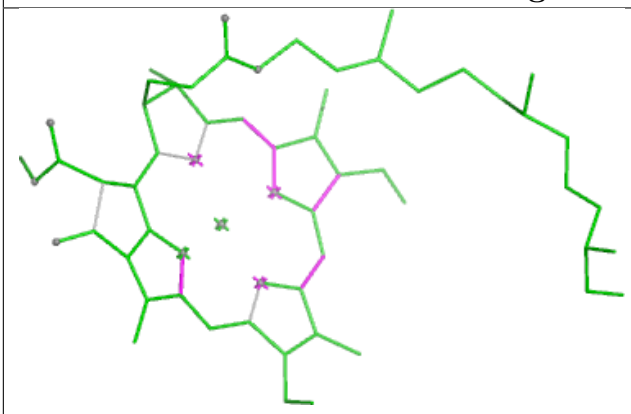


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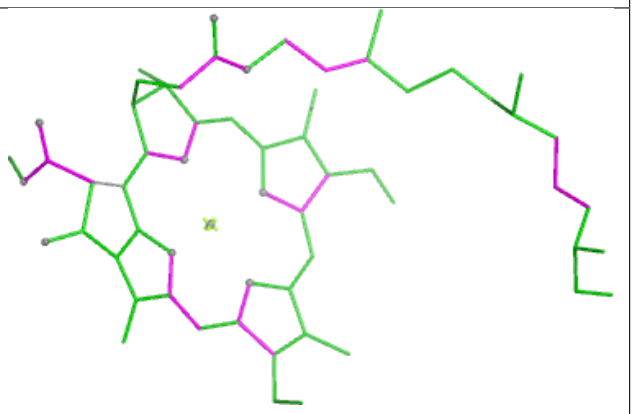


Rings

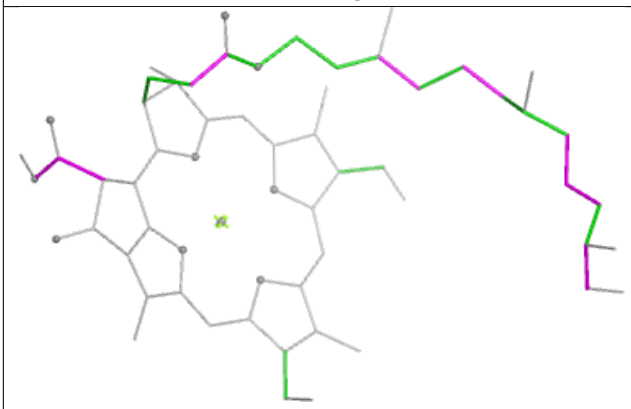
Ligand CLA 5 602



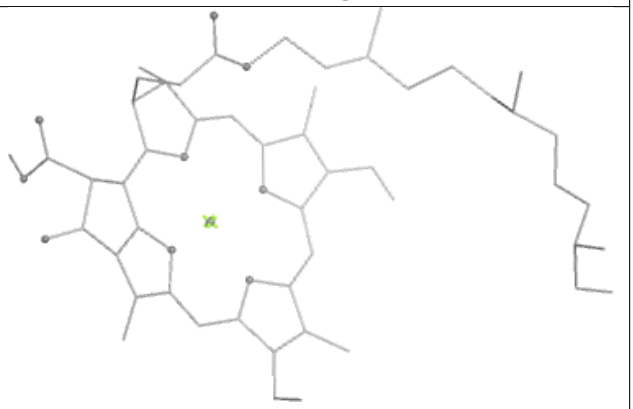
Bond lengths



Bond angles

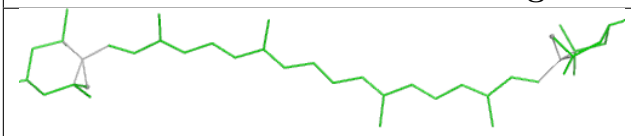


Torsions



Rings

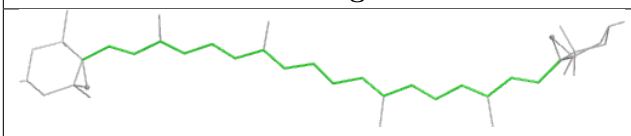
Ligand XAT 1 616



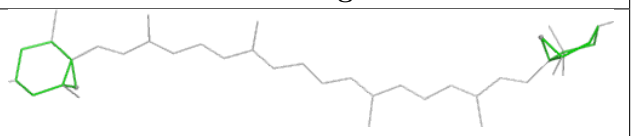
Bond lengths



Bond angles

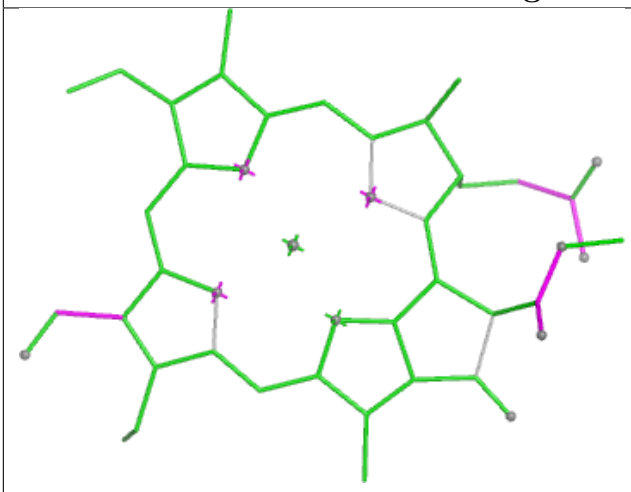


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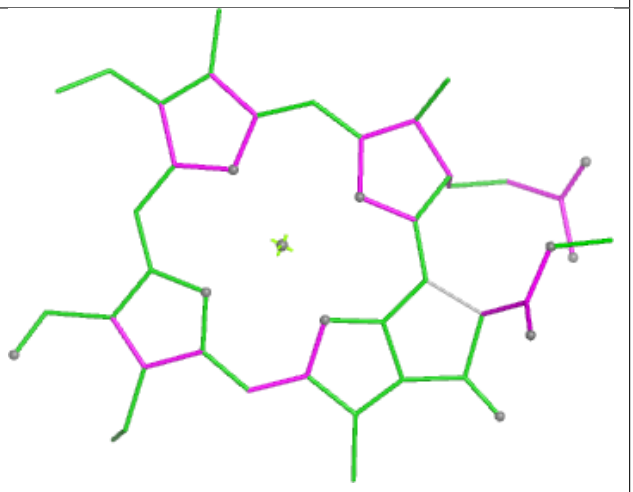


Rings

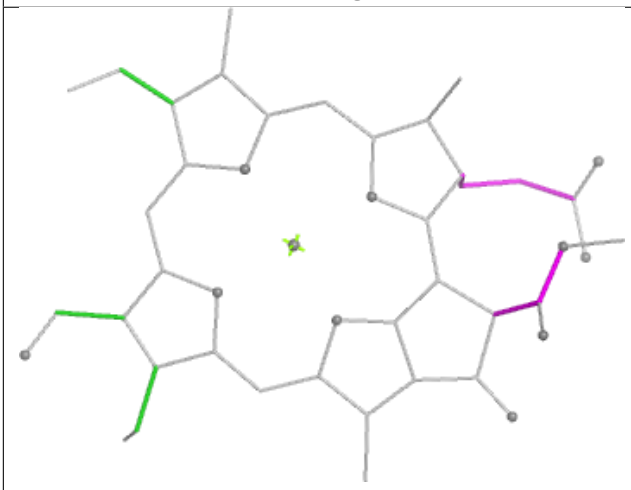
Ligand CHL Y 607



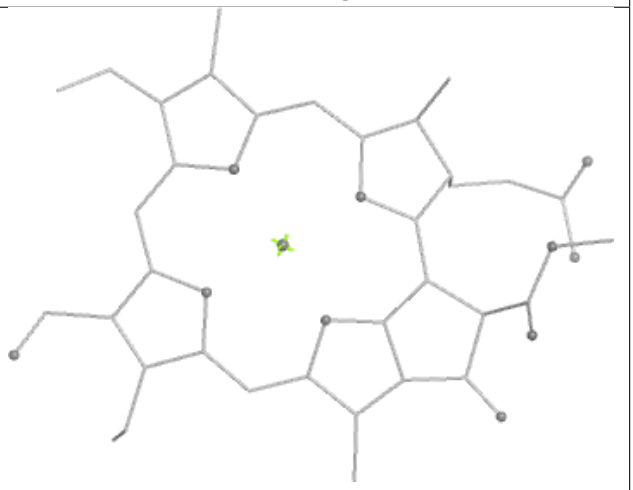
Bond lengths



Bond angles

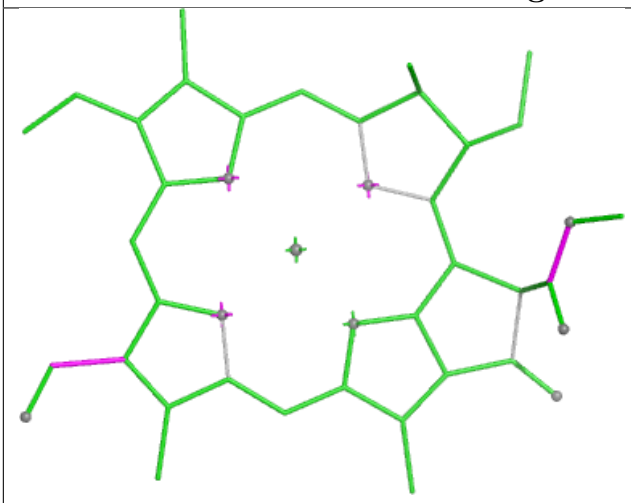


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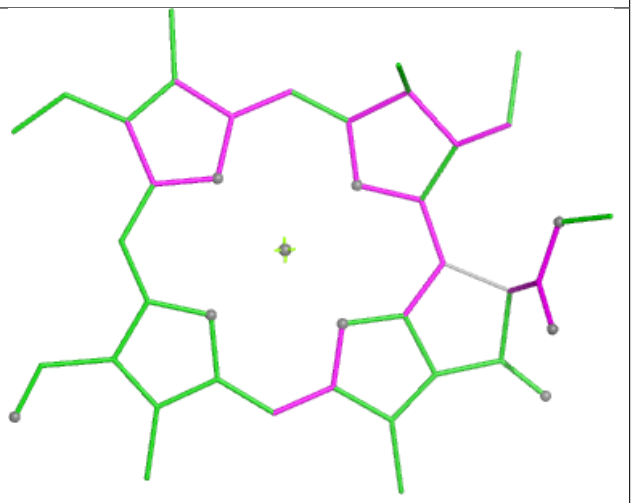


Rings

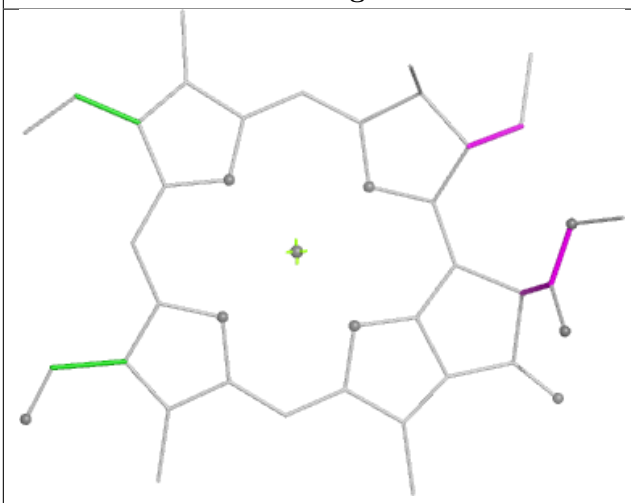
Ligand CHL 2 605



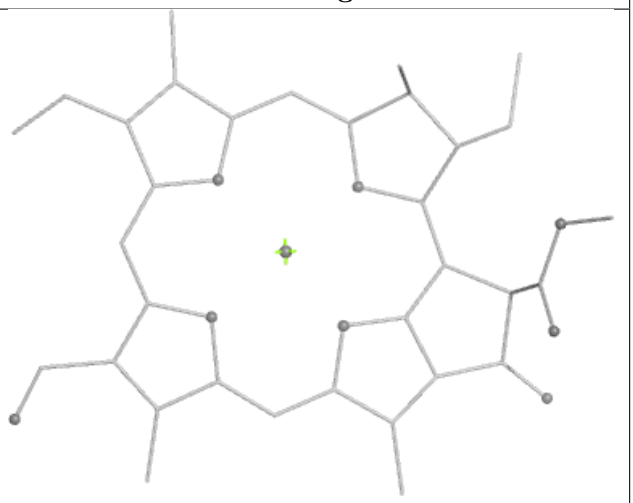
Bond lengths



Bond angles

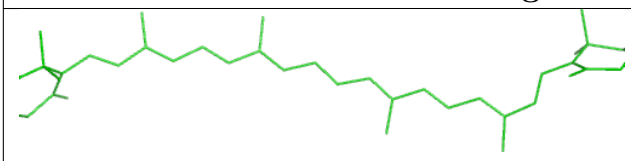


Torsions

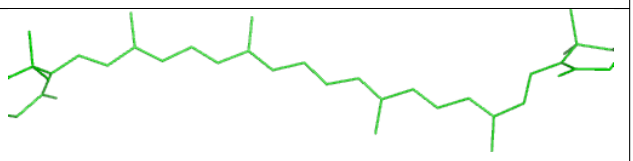


Rings

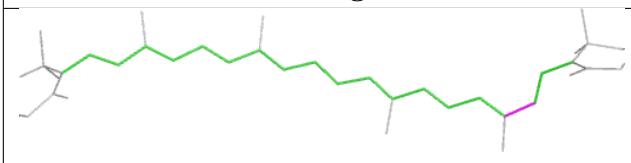
Ligand BCR A 847



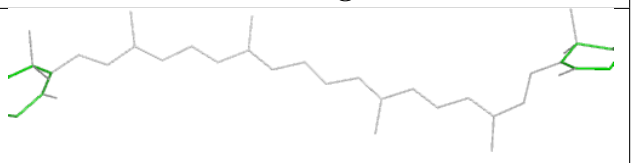
Bond lengths



Bond angles

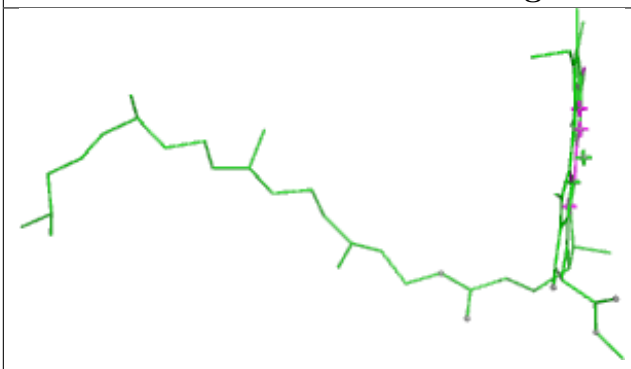


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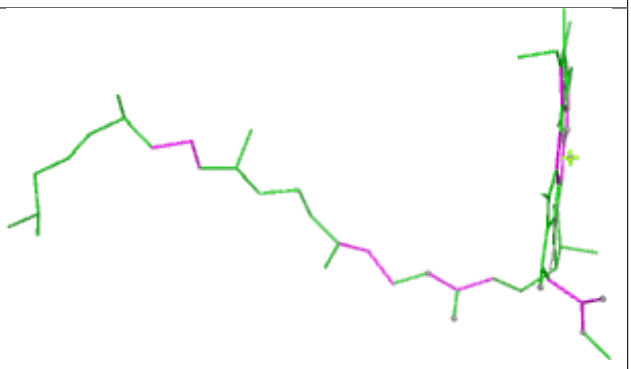


Rings

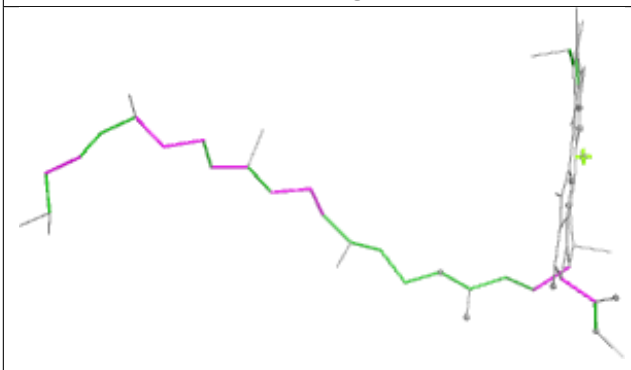
Ligand CLA B 839



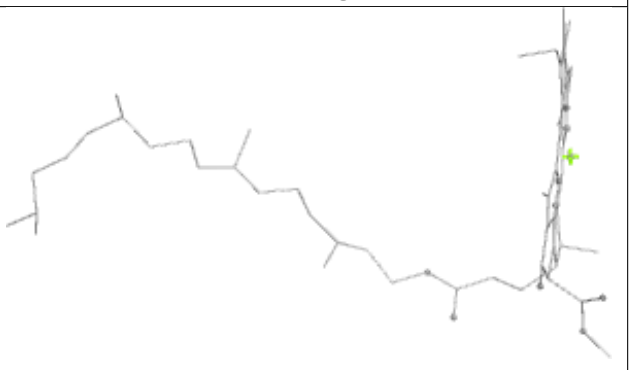
Bond lengths



Bond angles

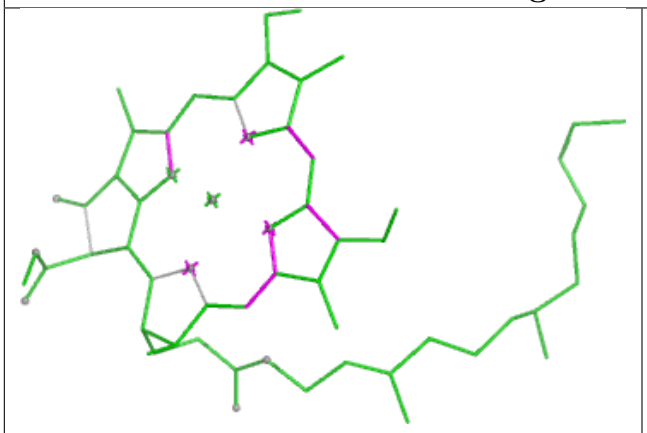


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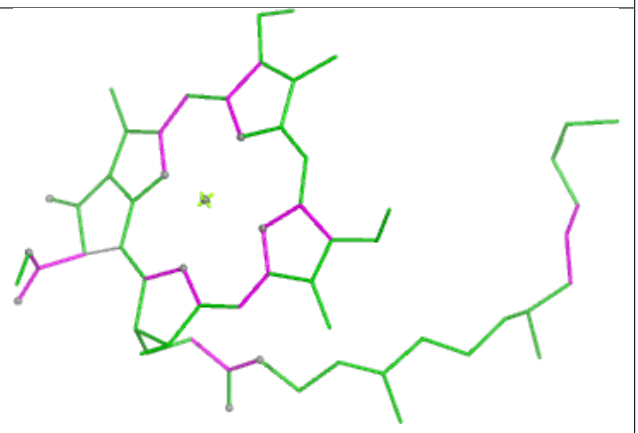


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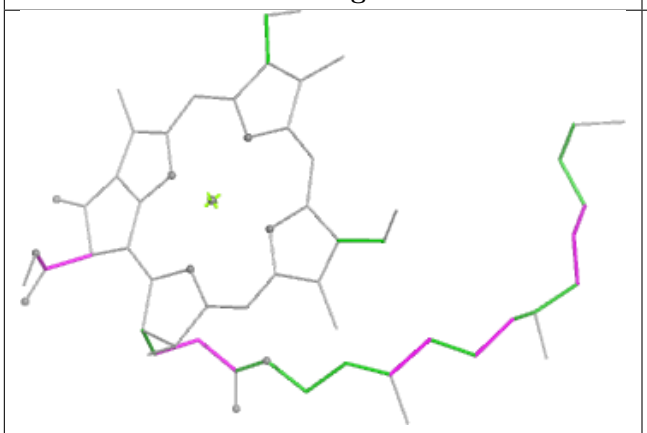
Ligand CLA 1 602



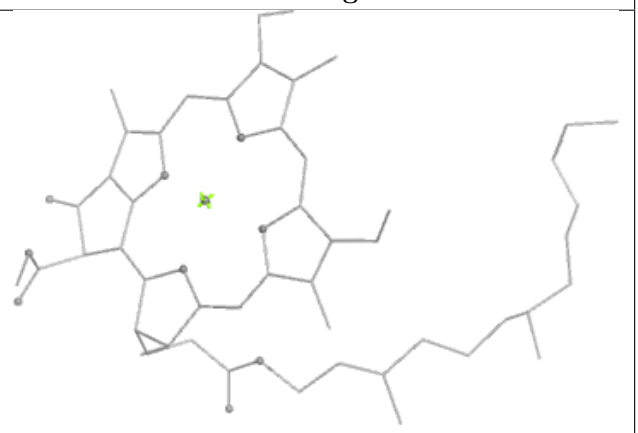
Bond lengths



Bond angles

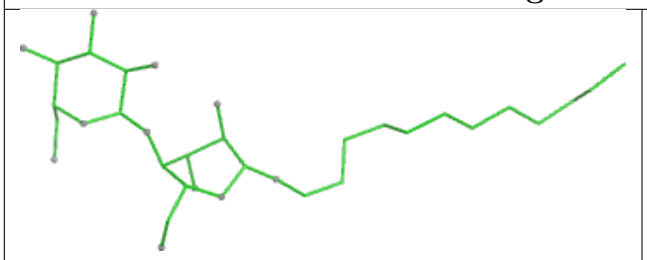


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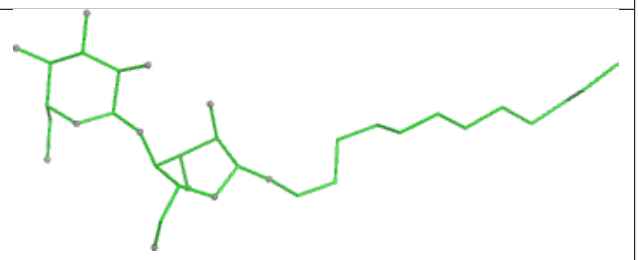


Rings

Ligand LMT 4 319



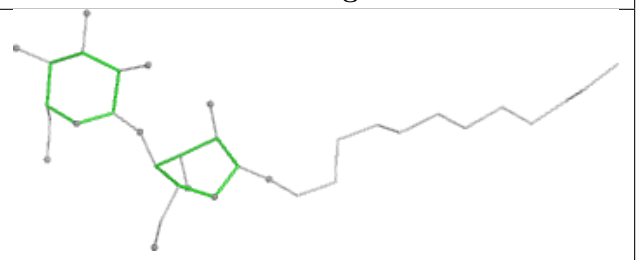
Bond lengths



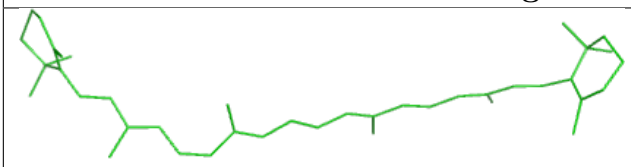
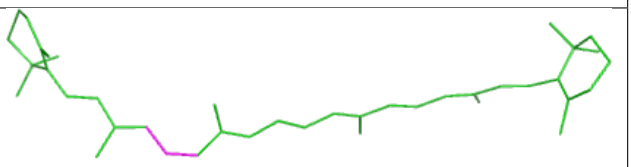
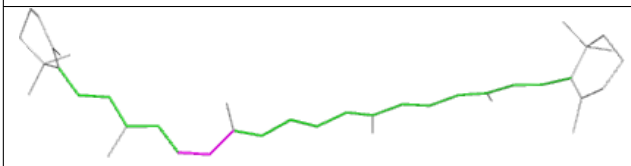
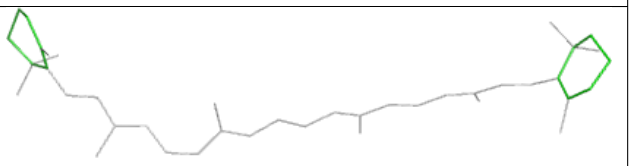
Bond angles

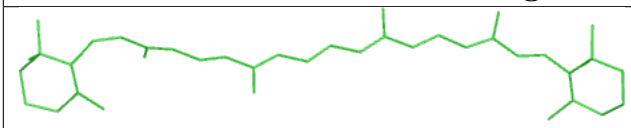
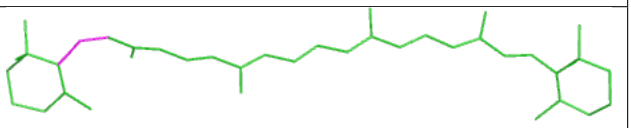
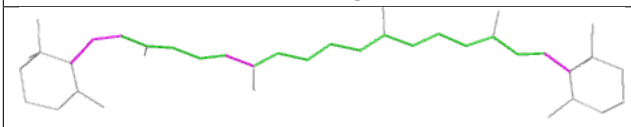
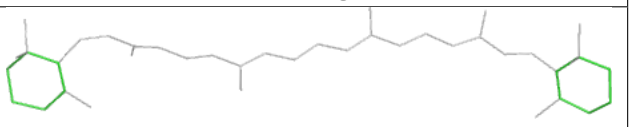


Torsions

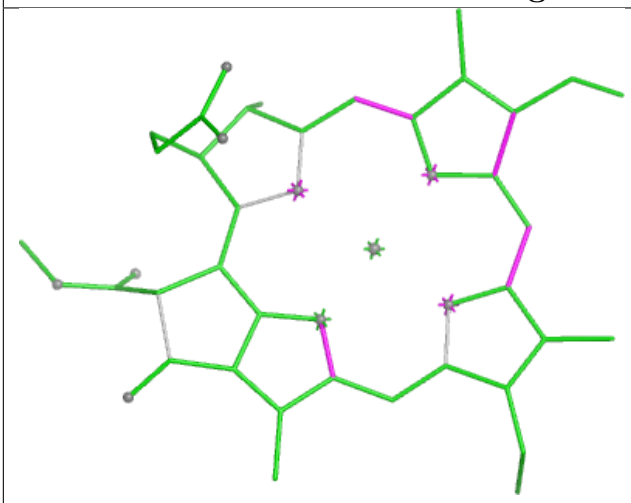


Rings

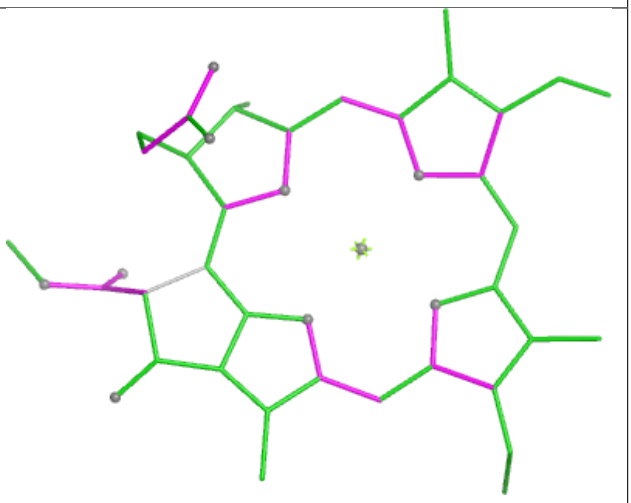
Ligand BCR A 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

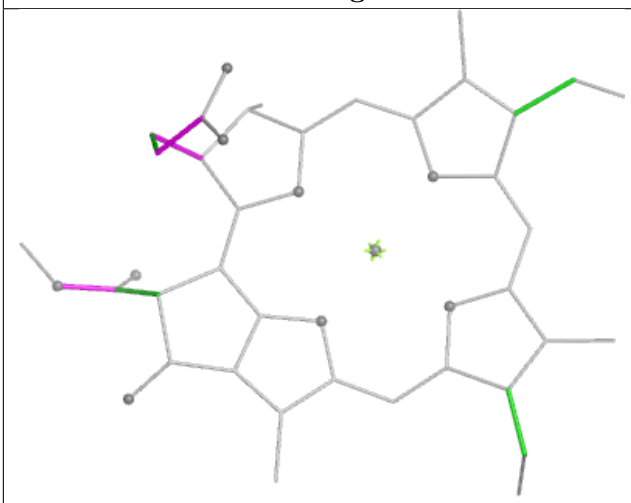
Ligand CLA 6 610



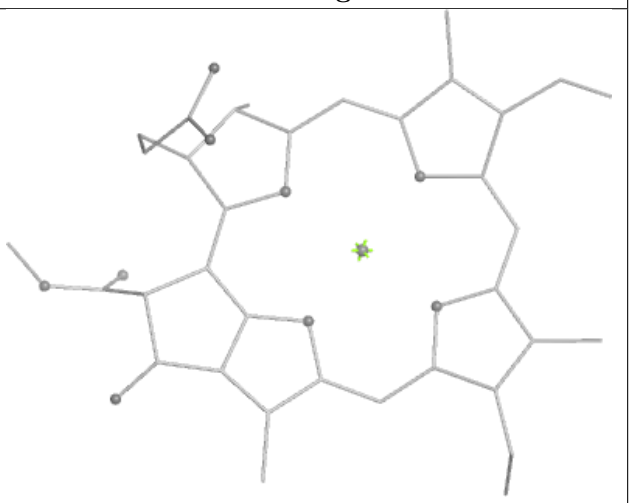
Bond lengths



Bond angles

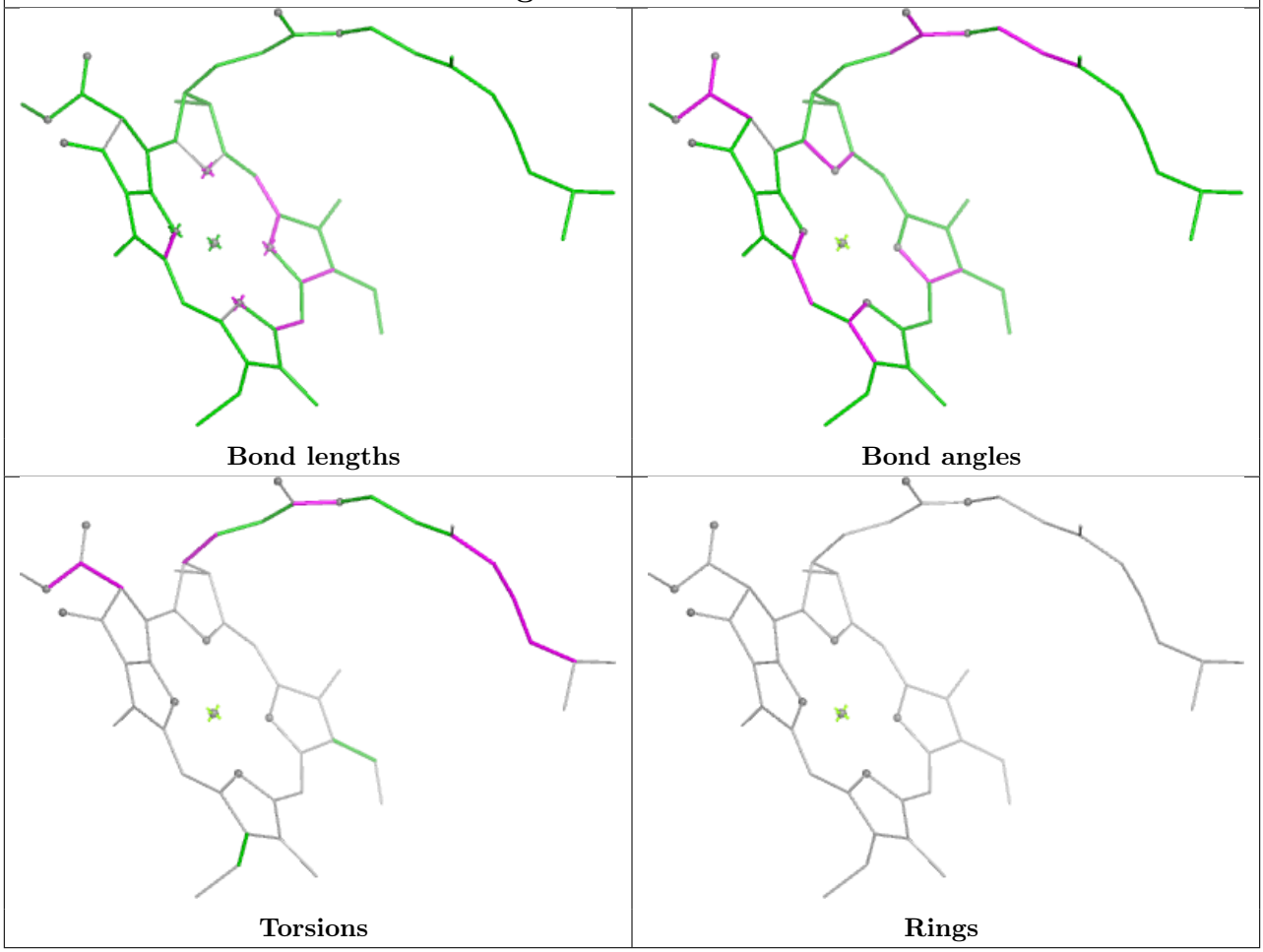


Torsions

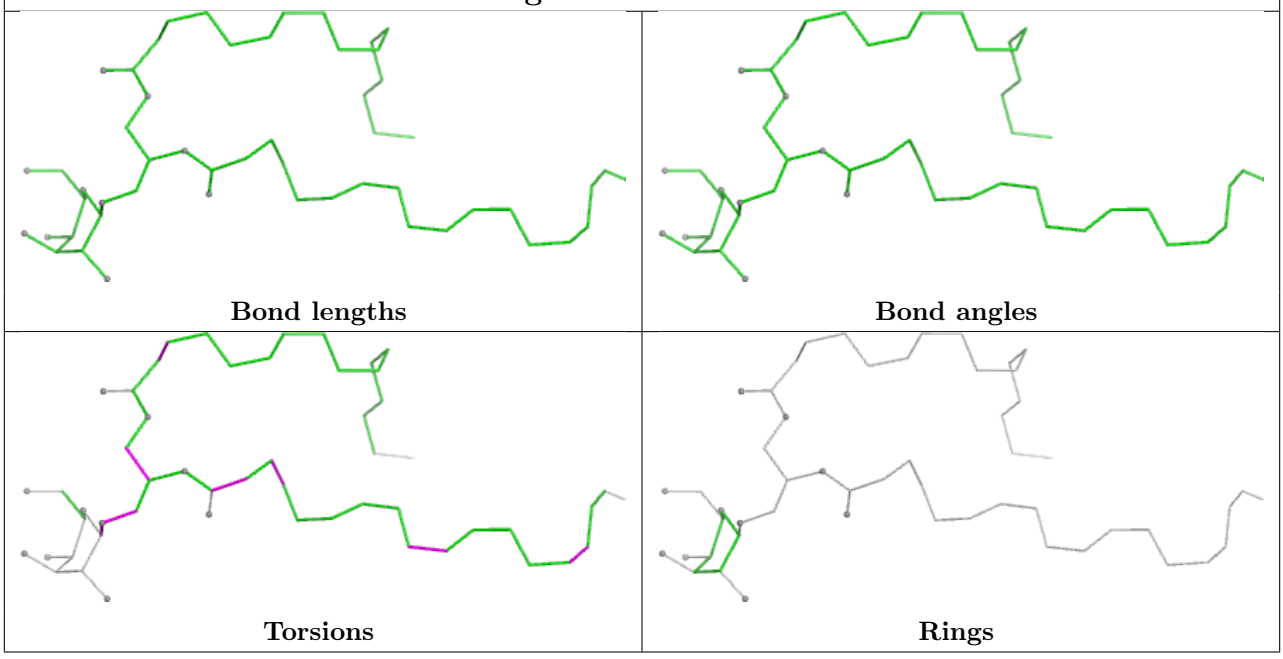


Rings

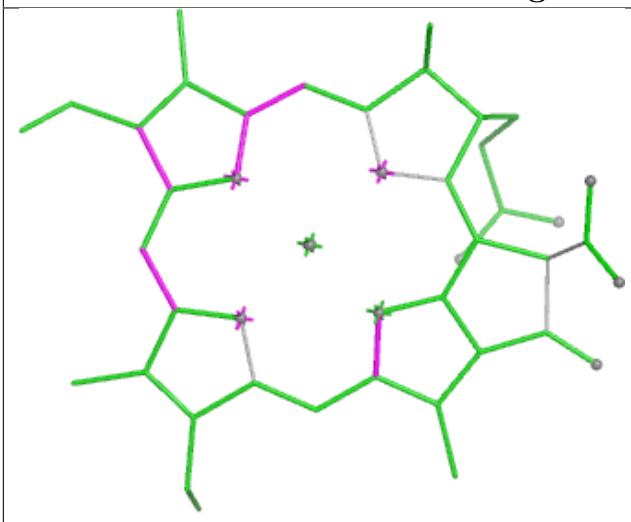
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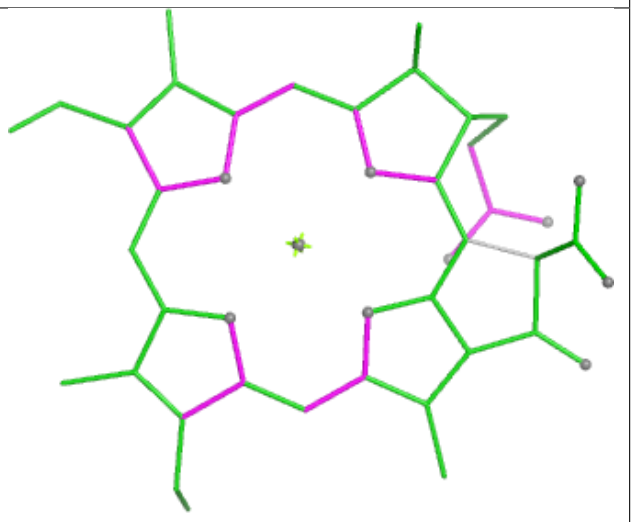
Ligand LMG 1 619



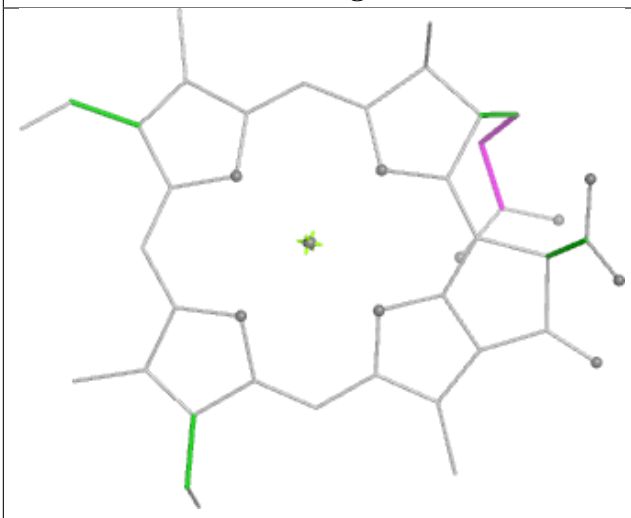
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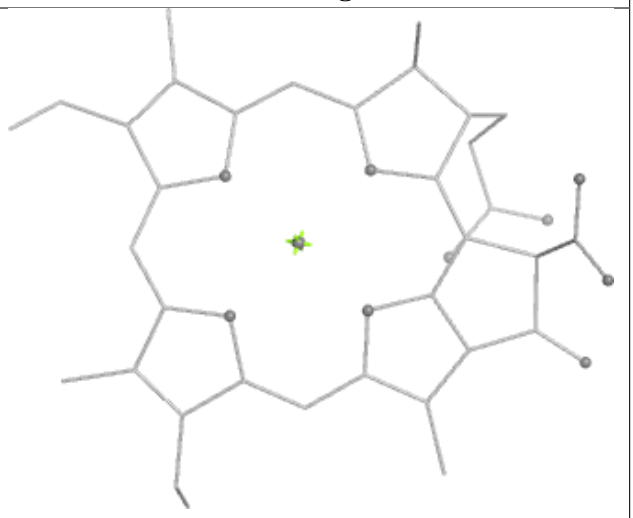
Bond lengths



Bond angles

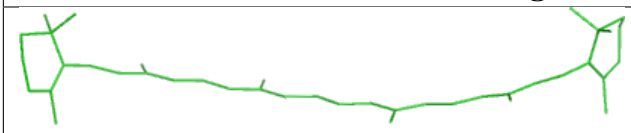


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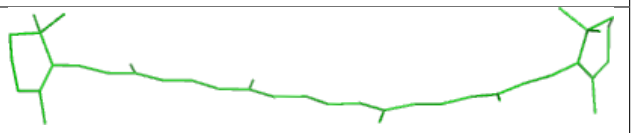


Rings

Ligand BCR I 101



Bond lengths



Bond angles

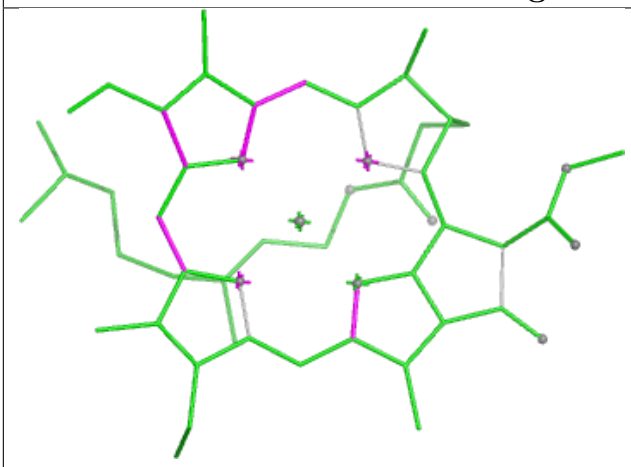


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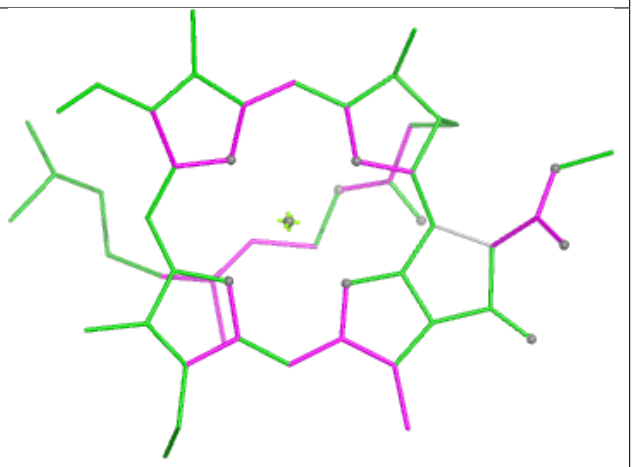


Rings

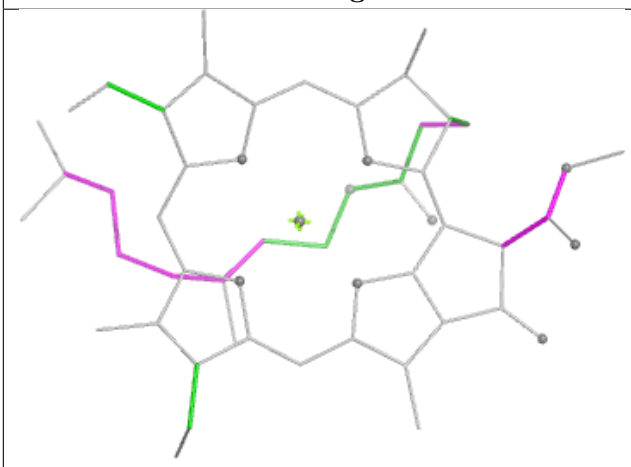
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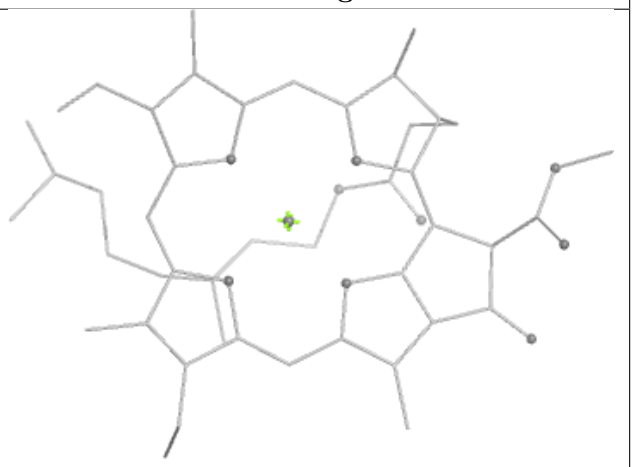
Bond lengths



Bond angles

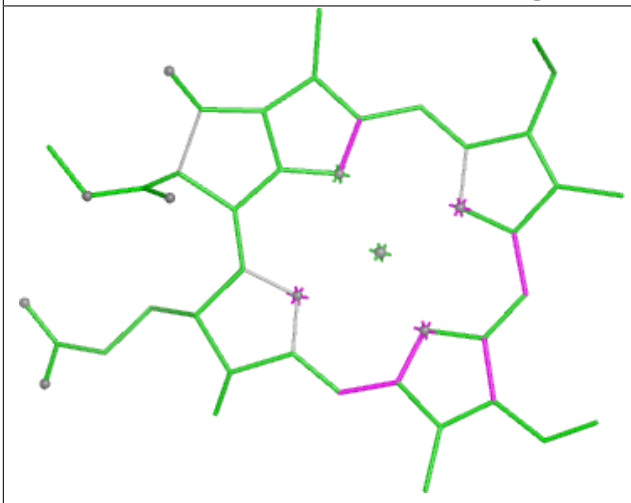


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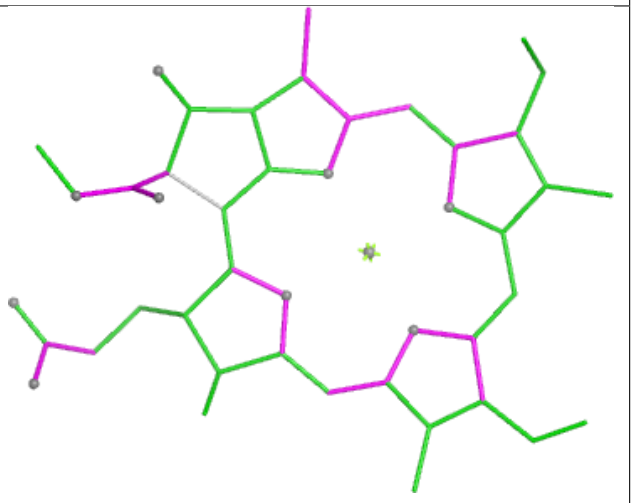


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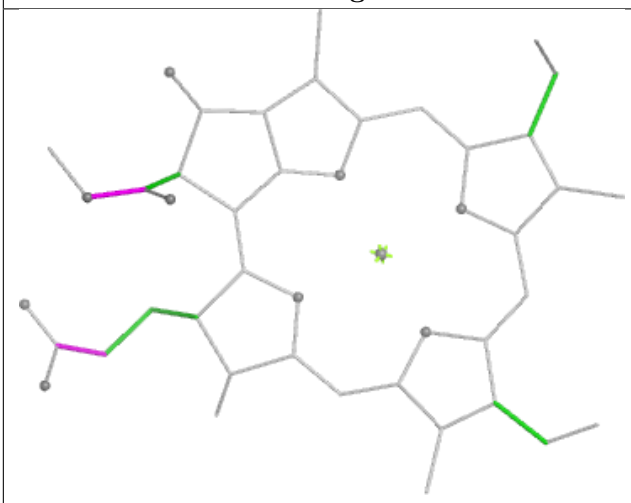
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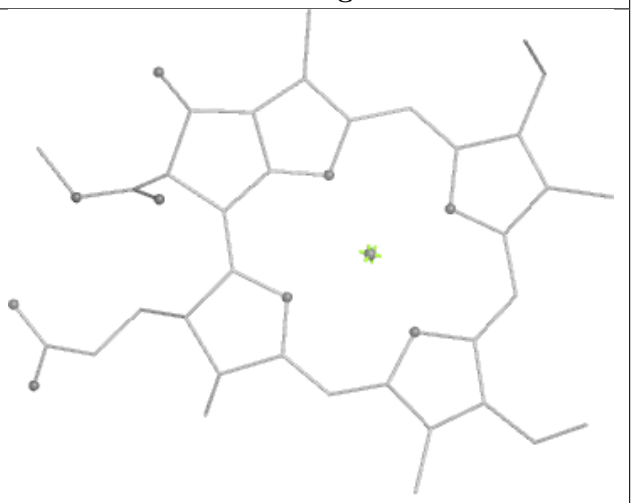
Bond lengths



Bond angles

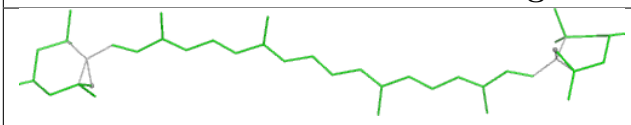


Torsions



Rings

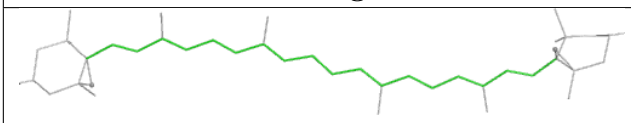
Ligand XAT 5 616



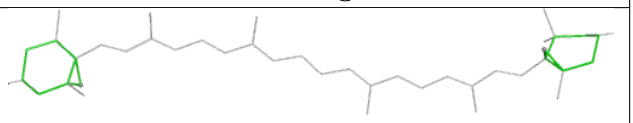
Bond lengths



Bond angles

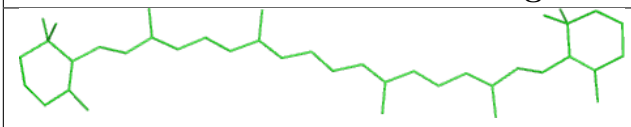


Torsions



Rings

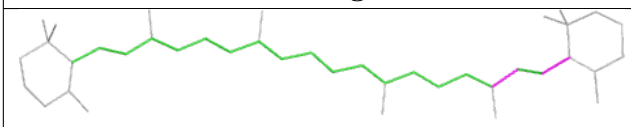
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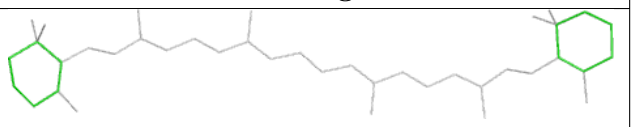
Bond lengths



Bond angles

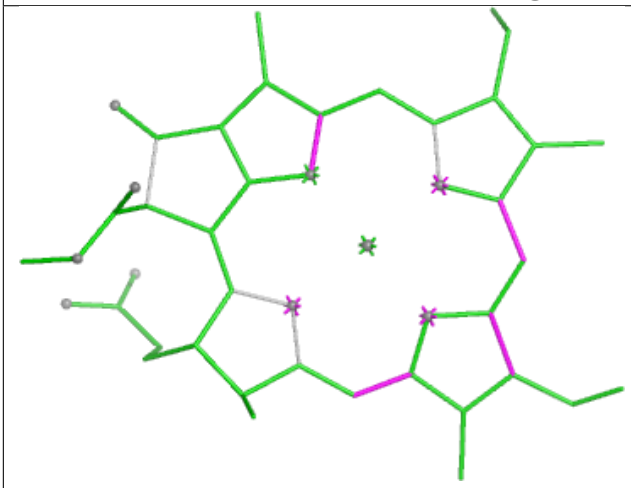


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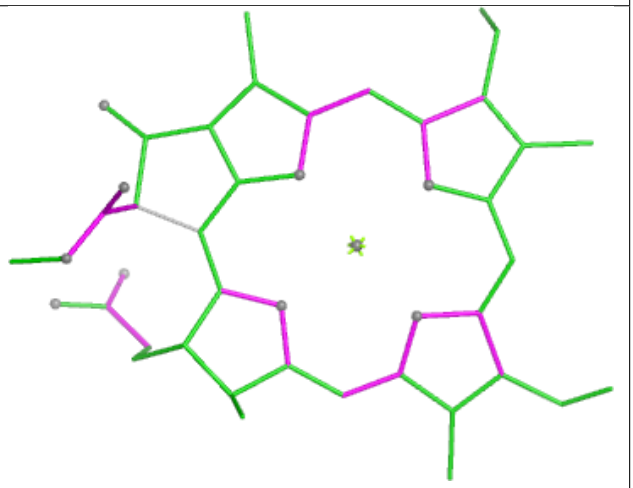


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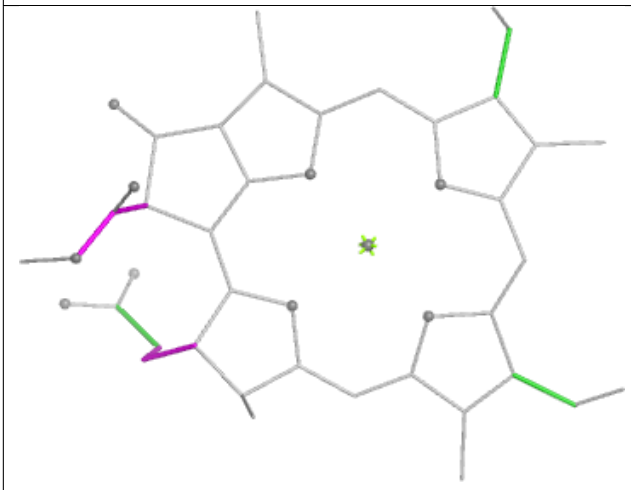
Ligand CLA Z 311



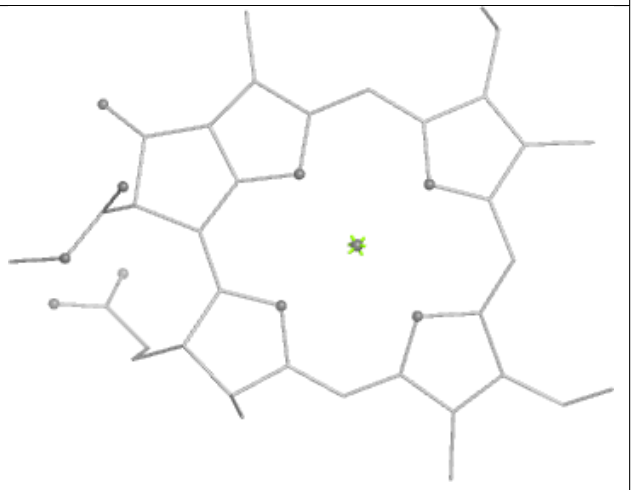
Bond lengths



Bond angles

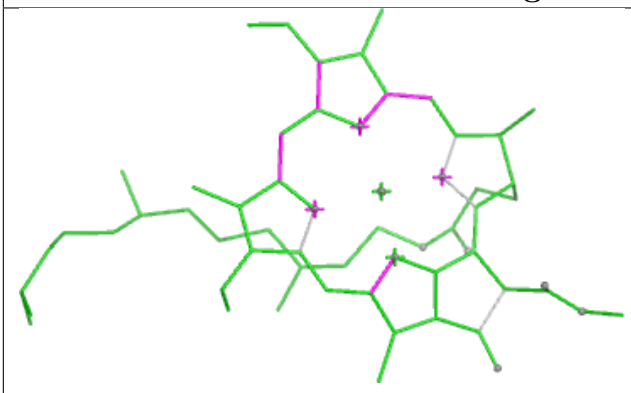


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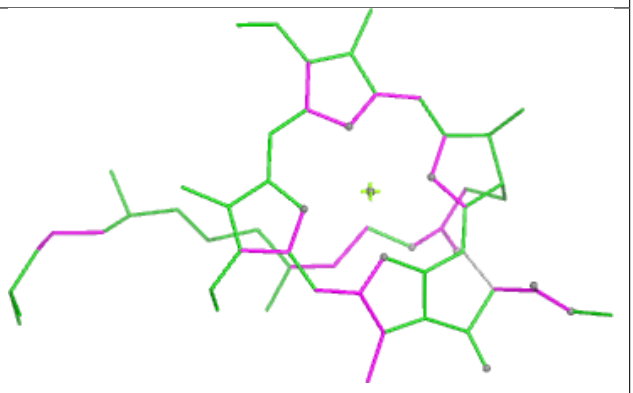


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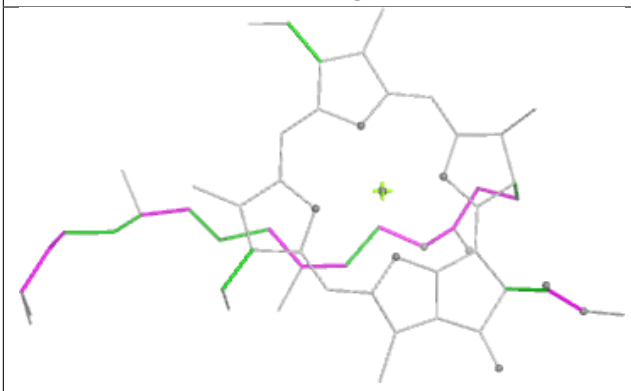
Ligand CLA A 817



Bond lengths



Bond angles

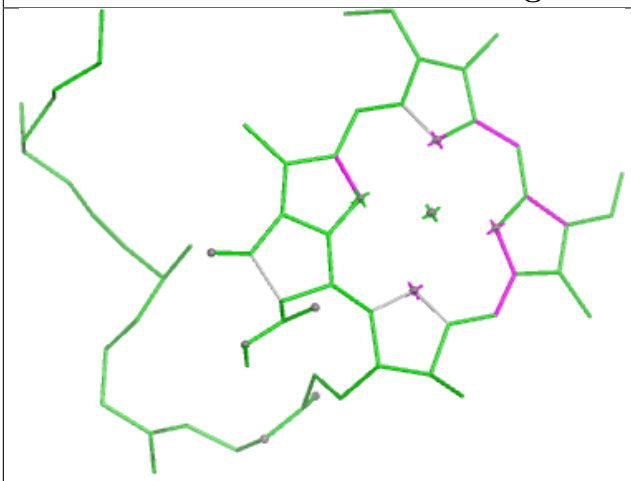


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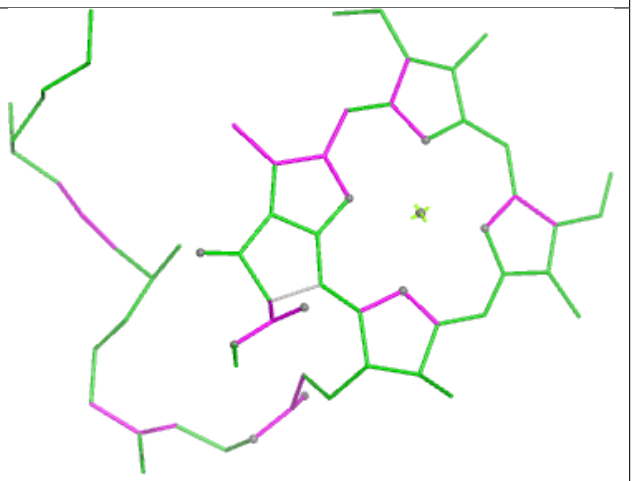


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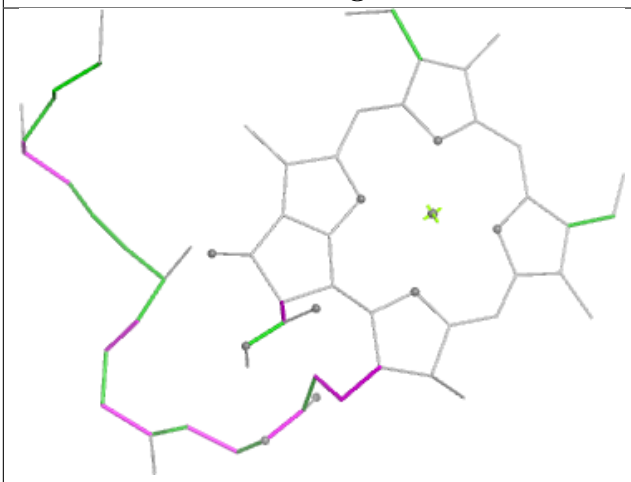
Ligand CLA B 831



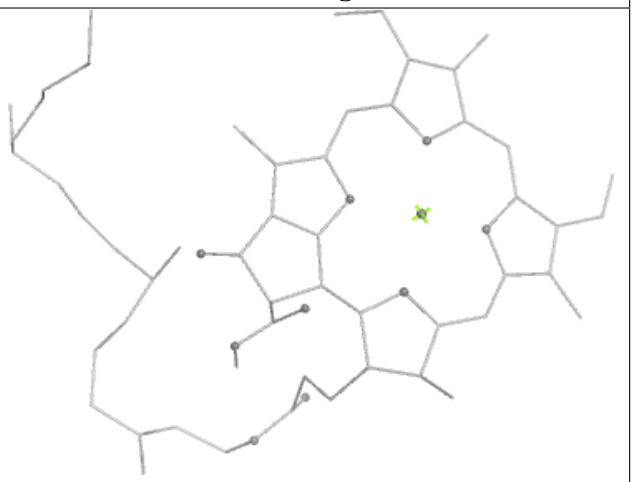
Bond lengths



Bond angles

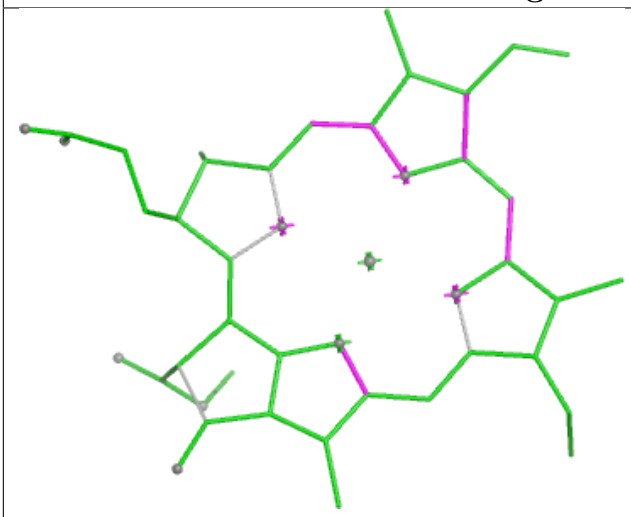


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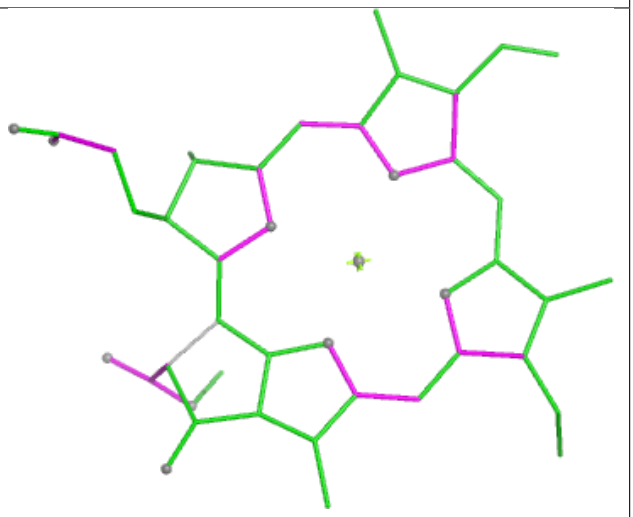


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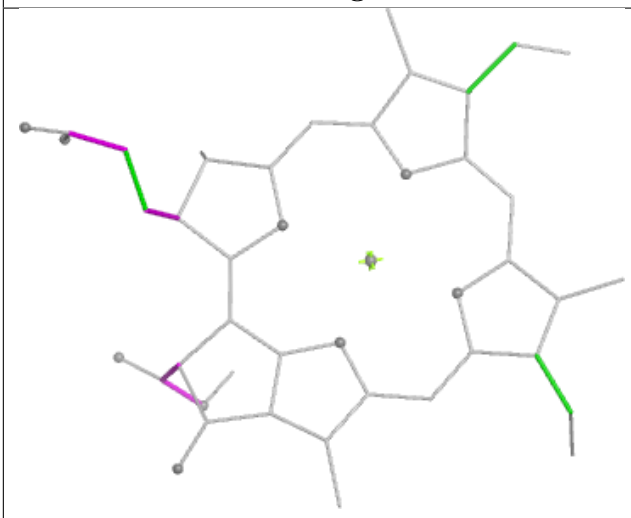
Ligand CLA Z 312



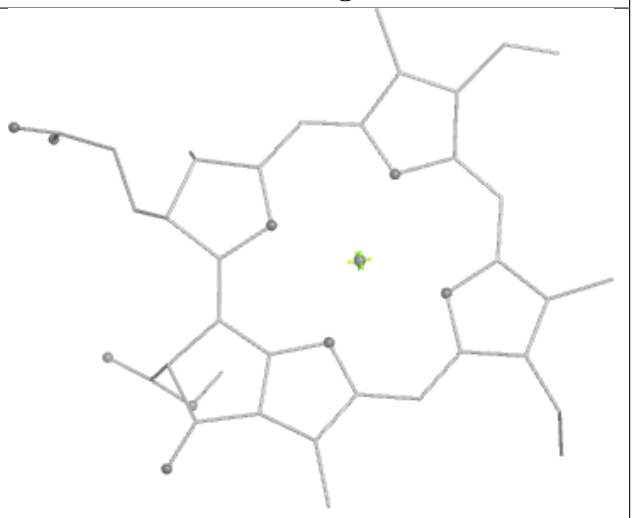
Bond lengths



Bond angles

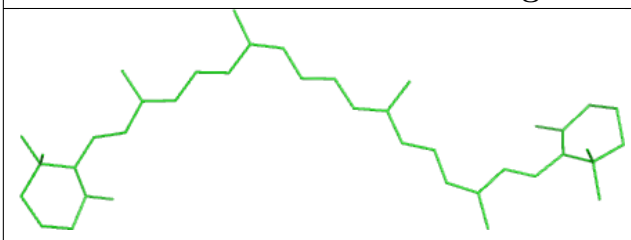


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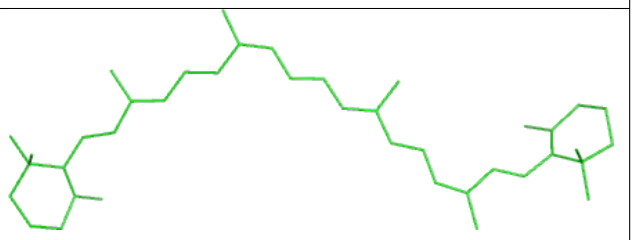


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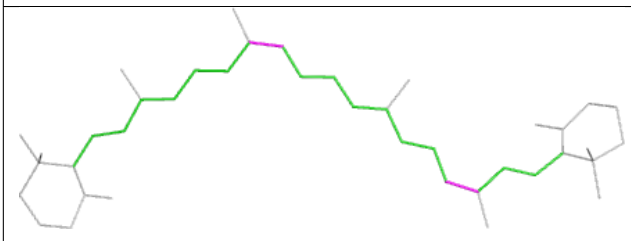
Ligand BCR A 848



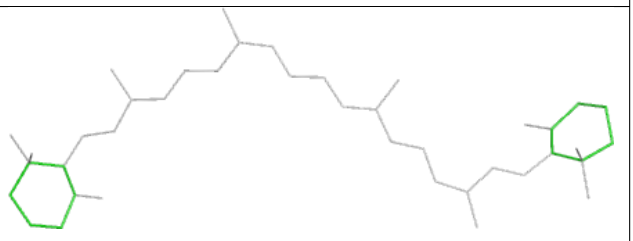
Bond lengths



Bond angles

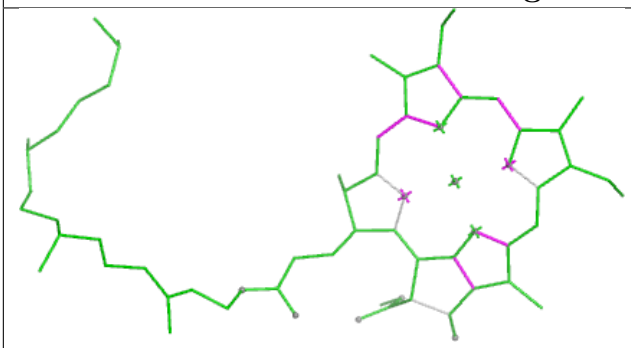


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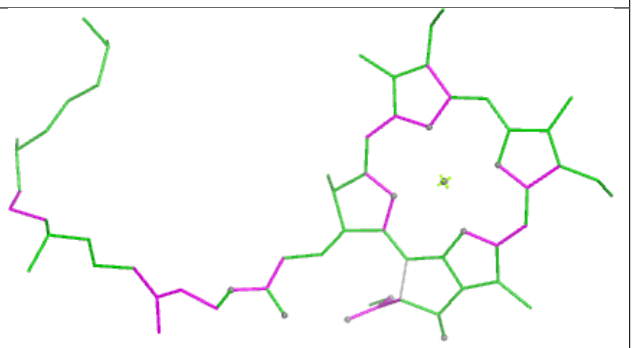


Rings

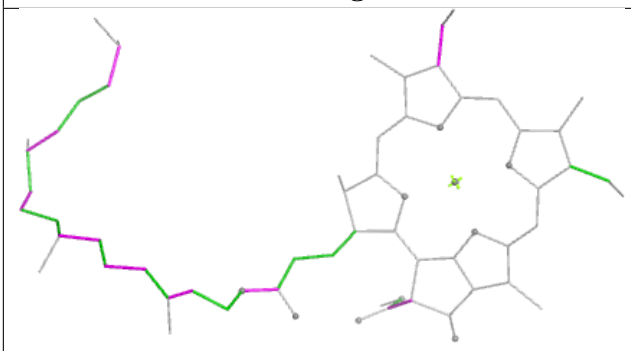
Ligand CLA A 827



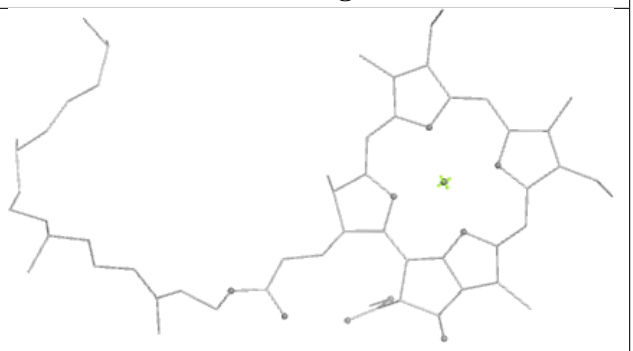
Bond lengths



Bond angles

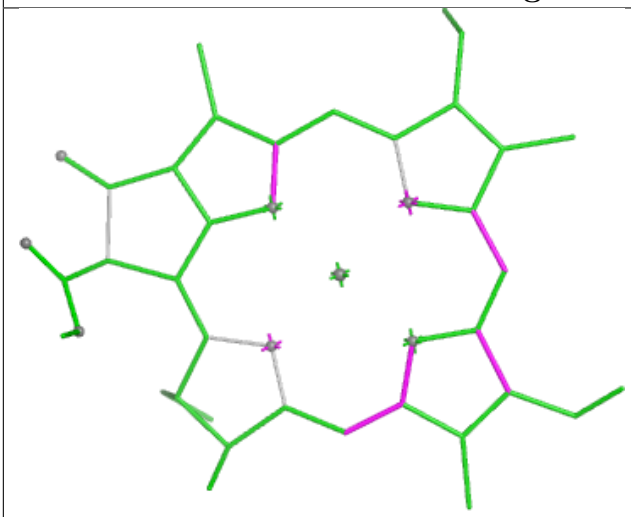


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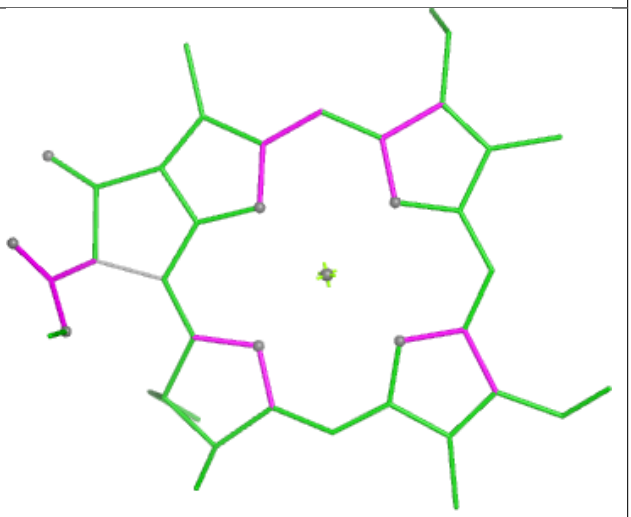


Rings

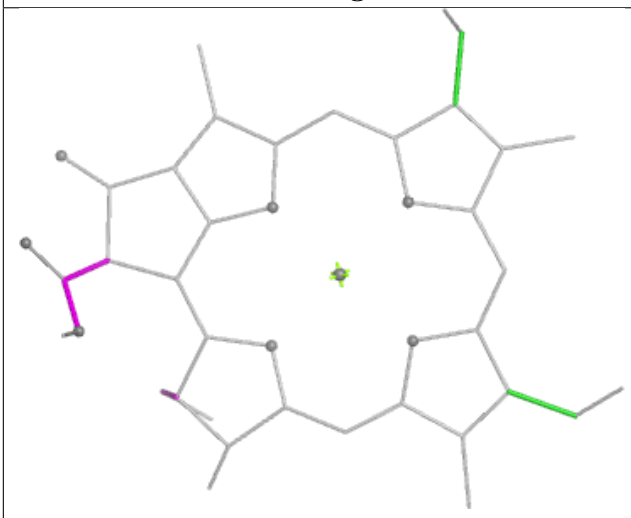
Ligand CLA A 822



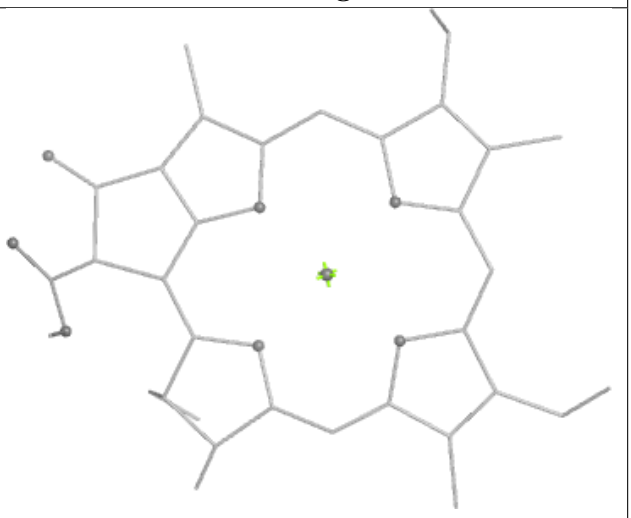
Bond lengths



Bond angles

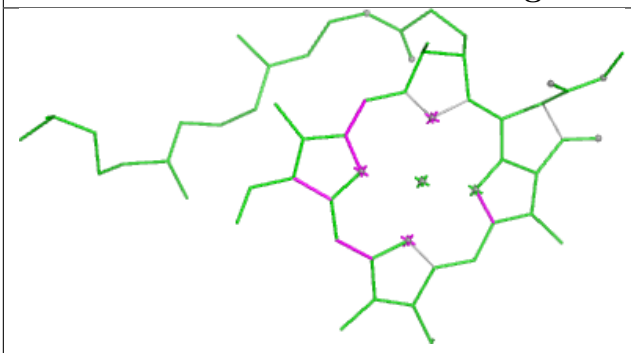


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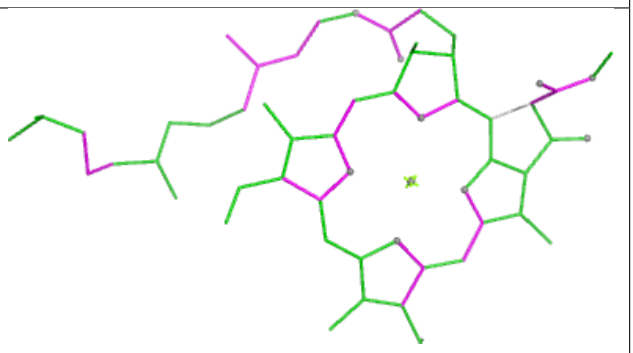


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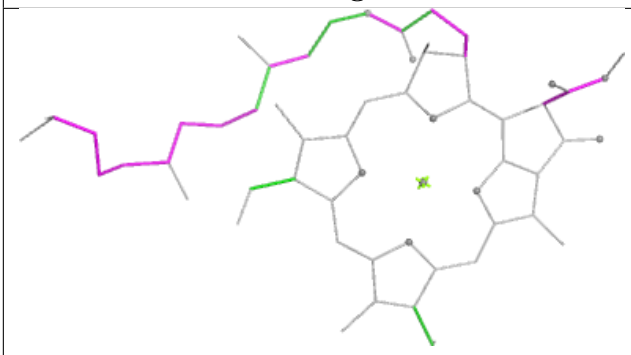
Ligand CLA B 817



Bond lengths



Bond angles

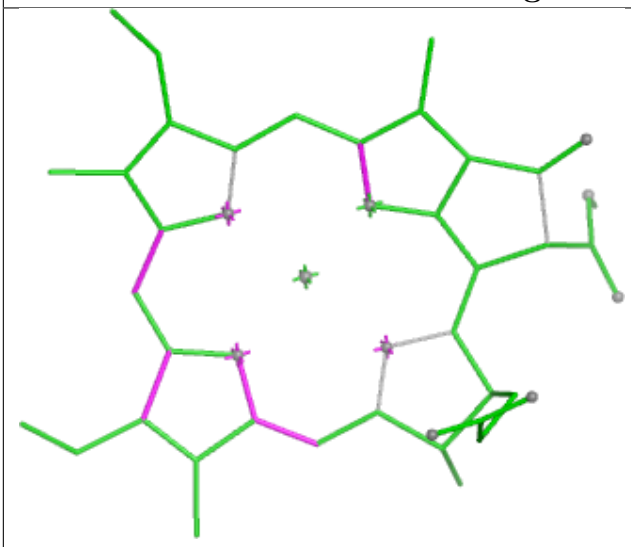


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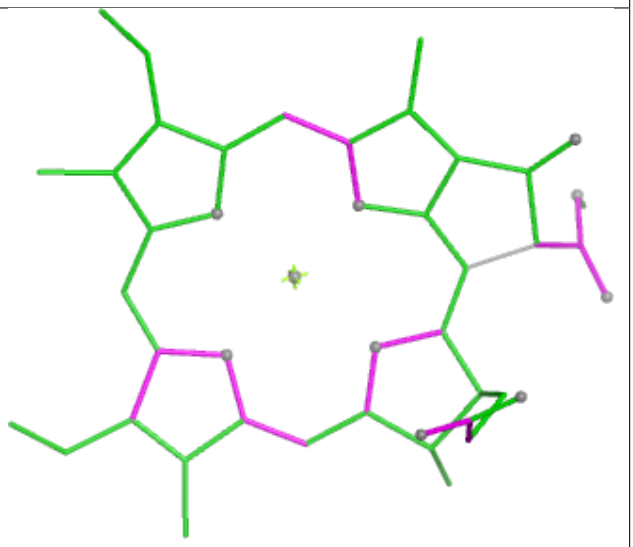


Rings

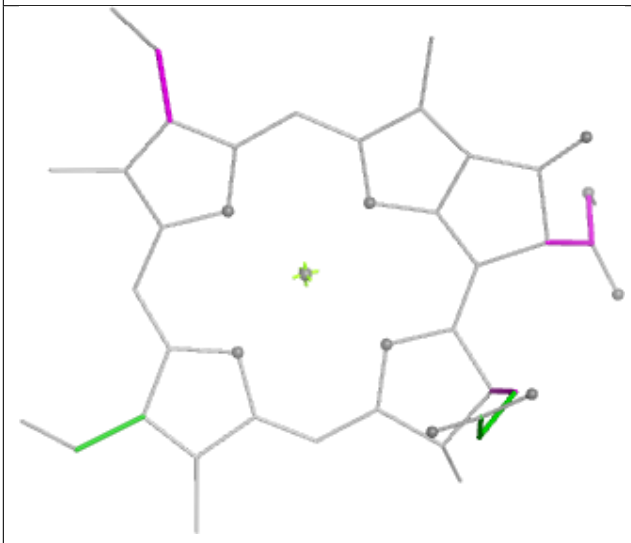
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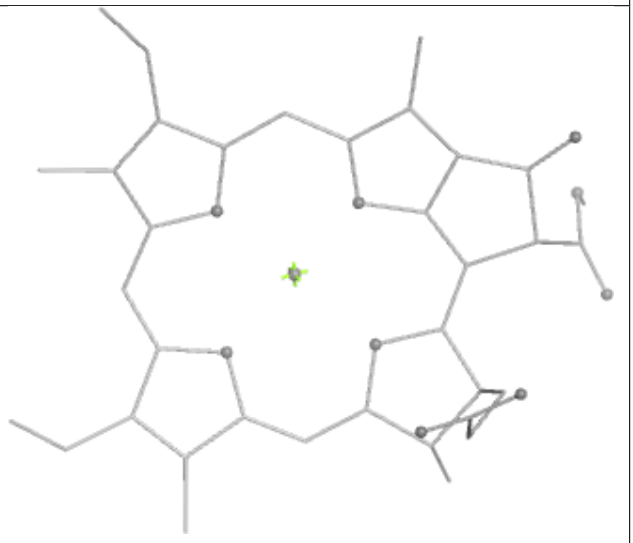
Bond lengths



Bond angles

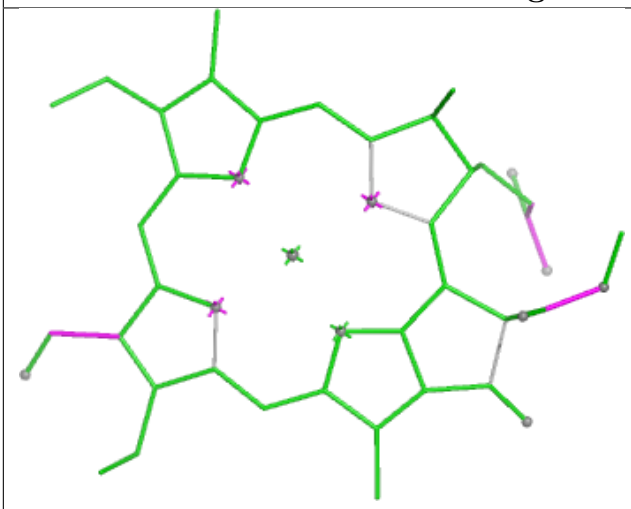


Torsions

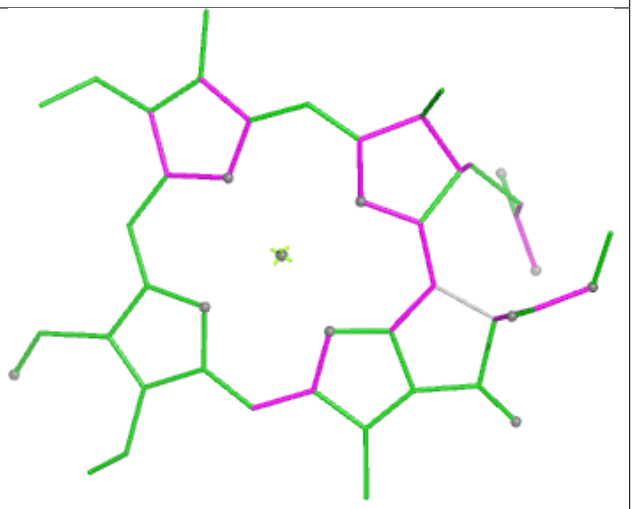


Rings

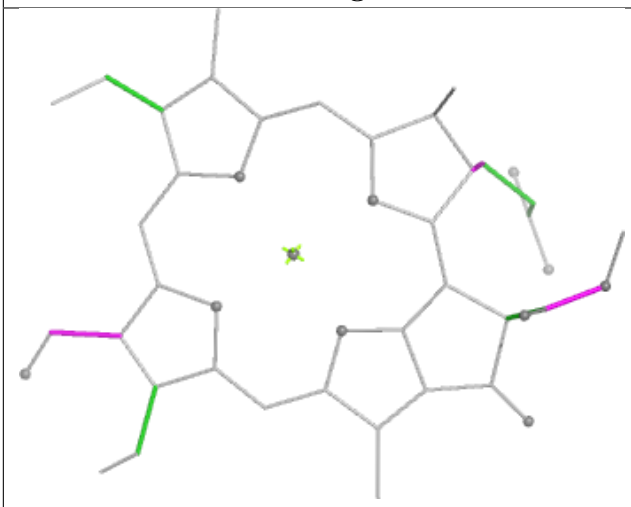
Ligand CHL 6 606



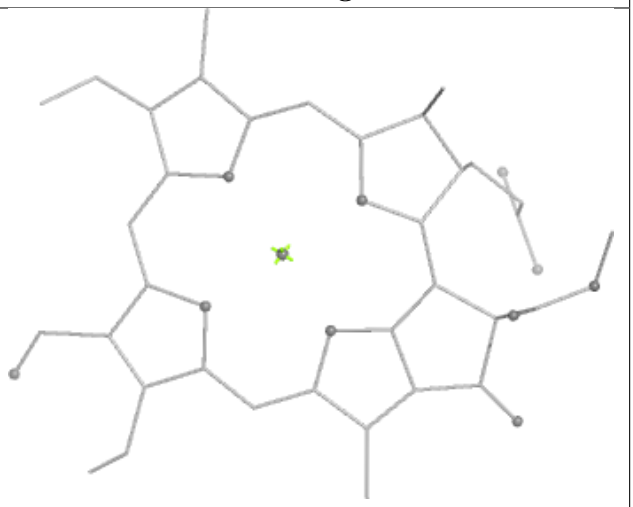
Bond lengths



Bond angles

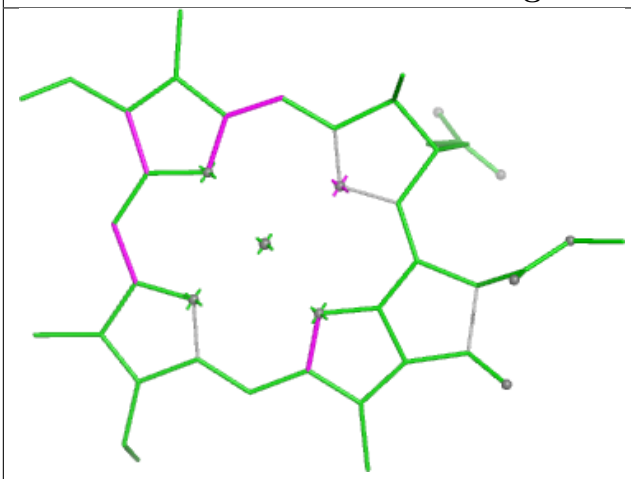


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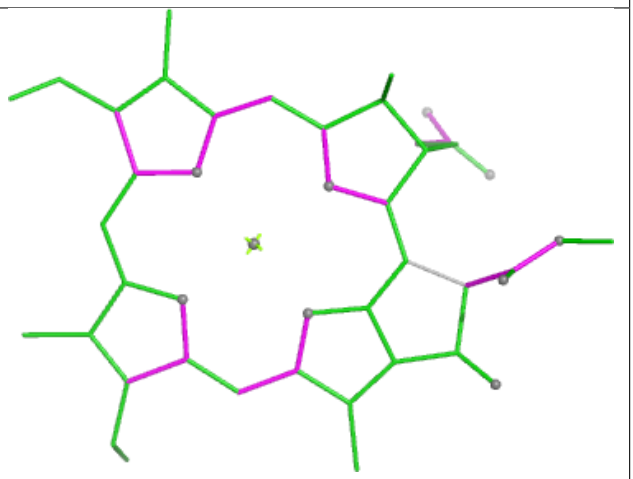


Rings

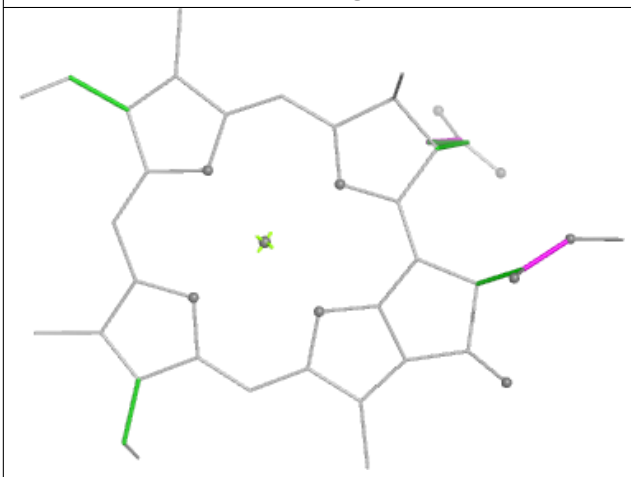
Ligand CLA A 835



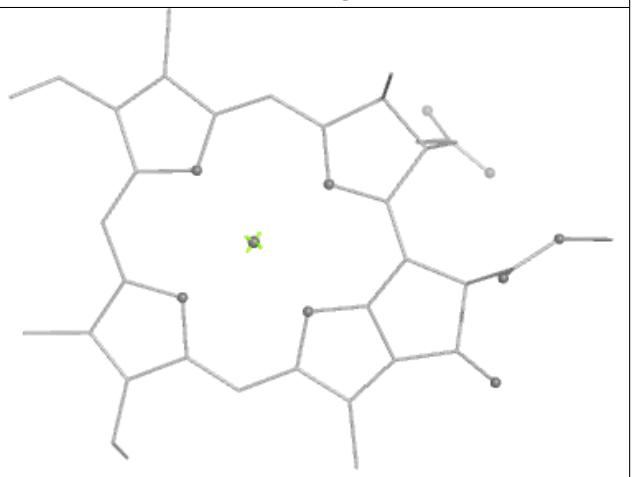
Bond lengths



Bond angles

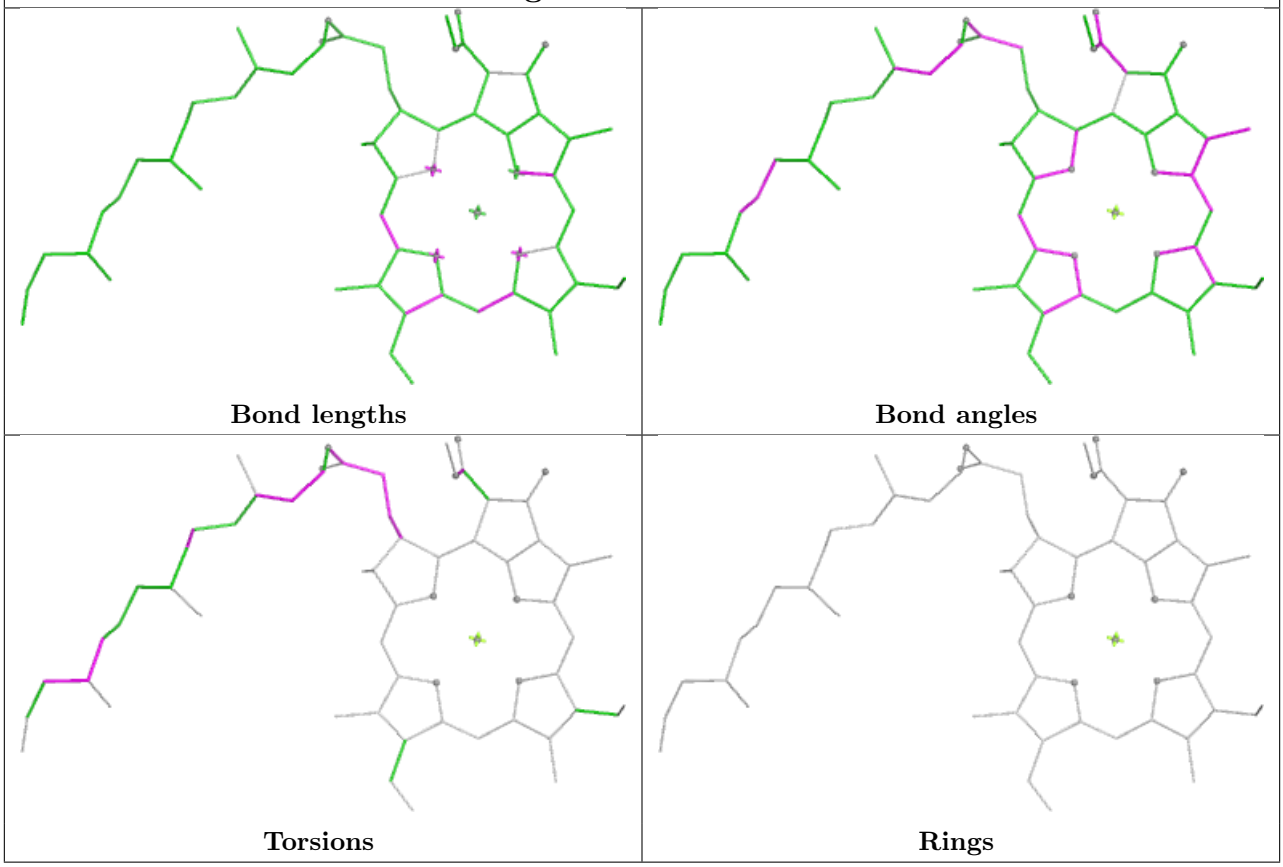


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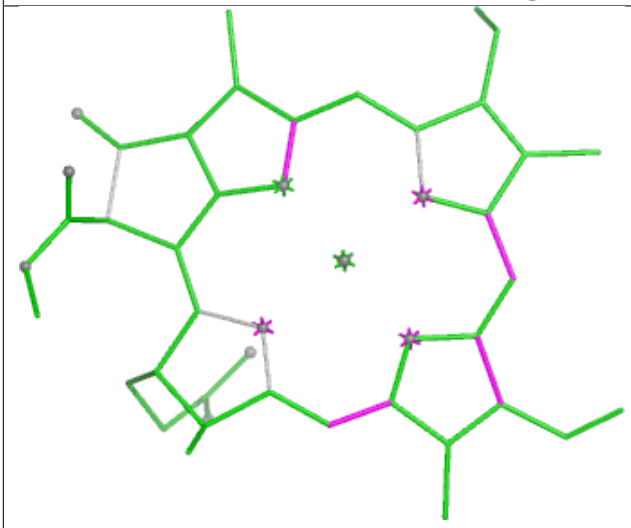


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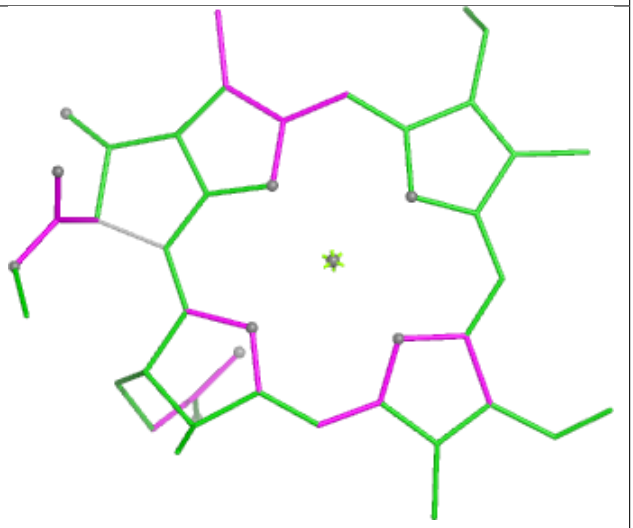
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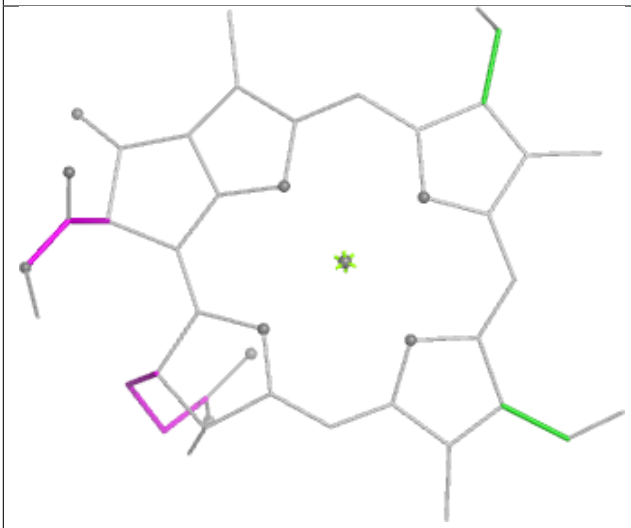
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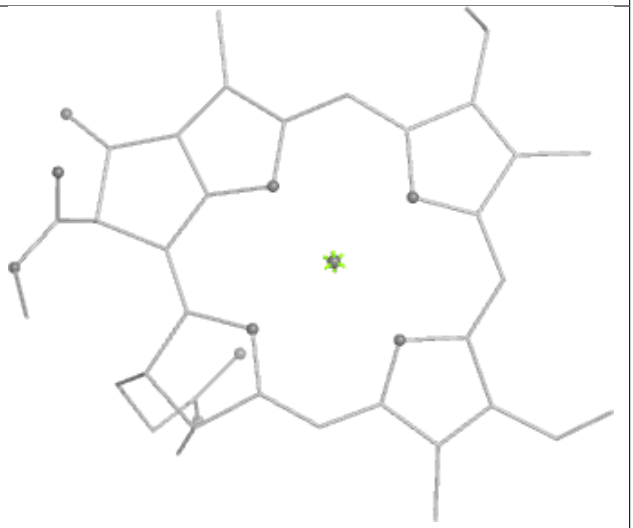
Bond lengths



Bond angles

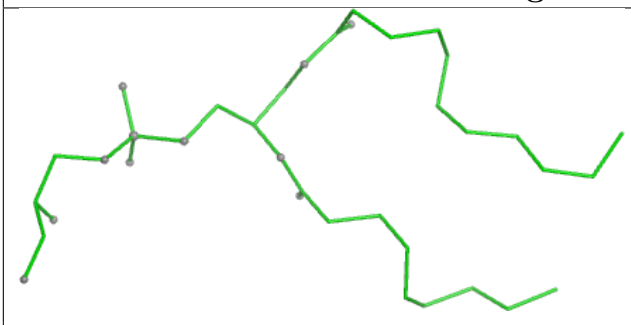


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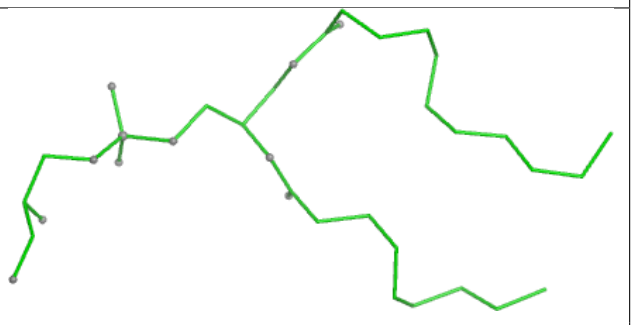


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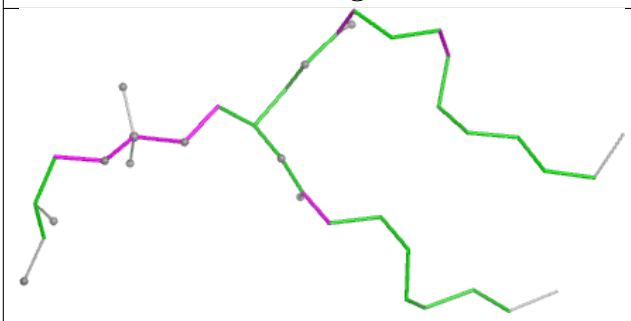
Ligand LHG 2 617



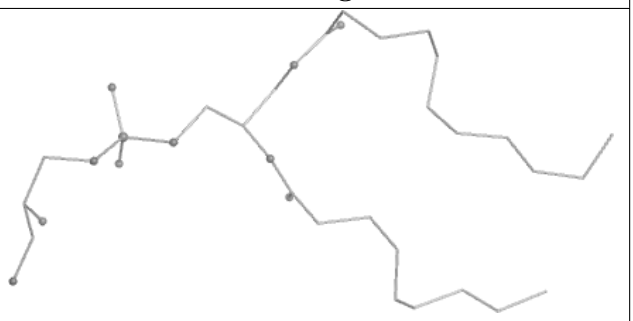
Bond lengths



Bond angles

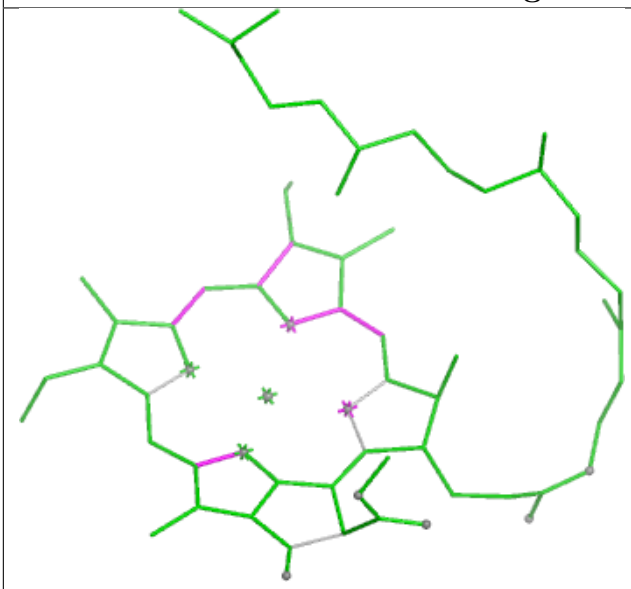


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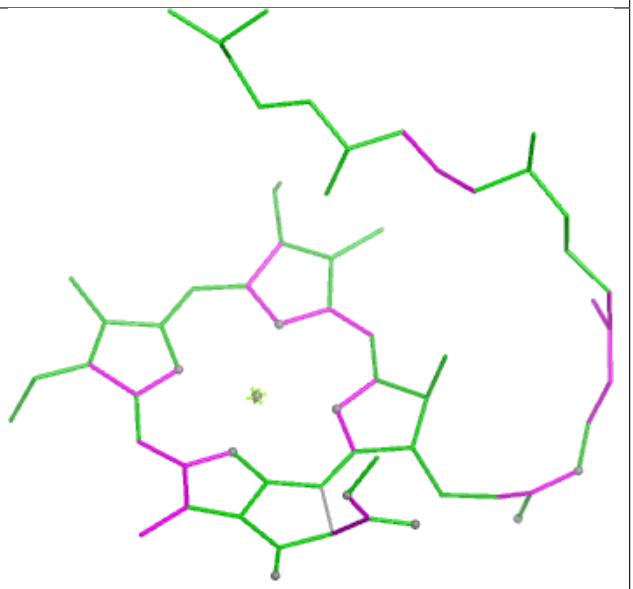


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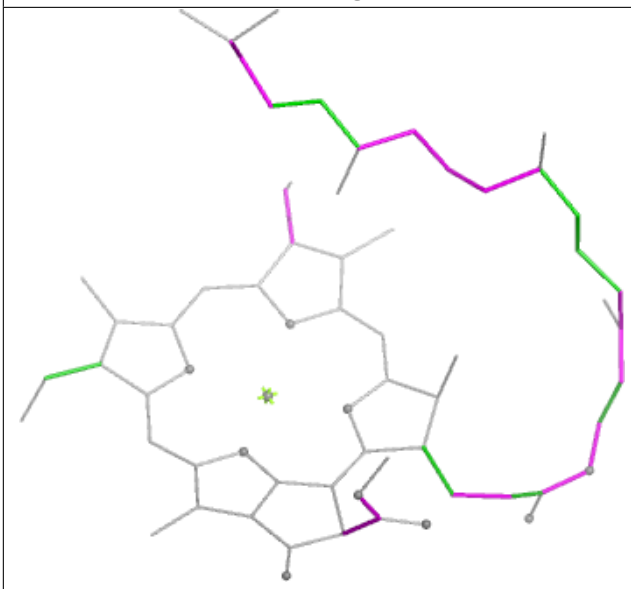
Ligand CLA A 813



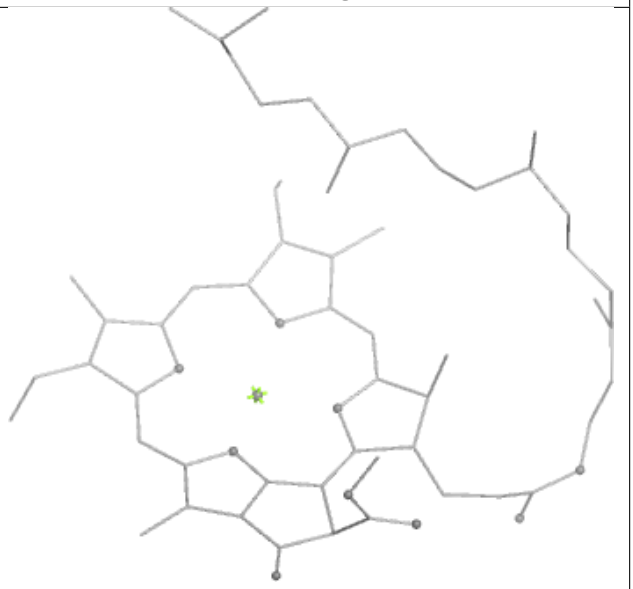
Bond lengths



Bond angles

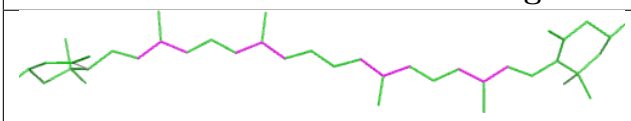


Torsions



Rings

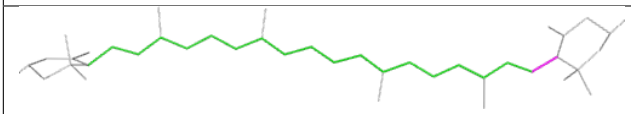
Ligand LUT Y 615



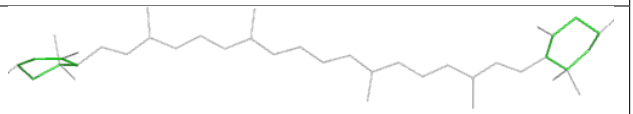
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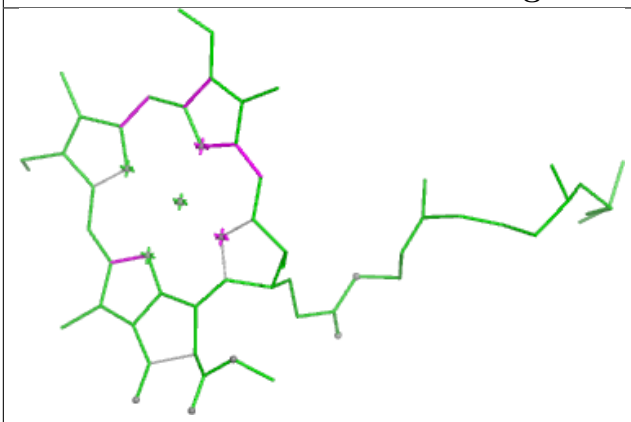


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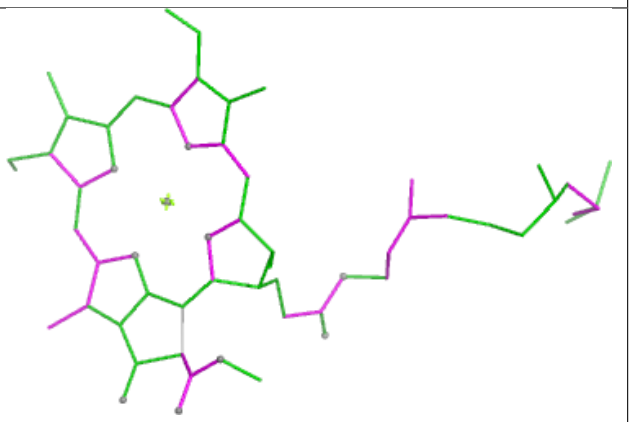


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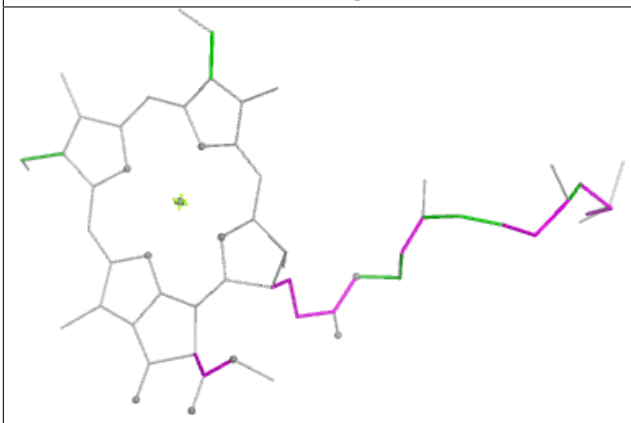
Ligand CLA H 201



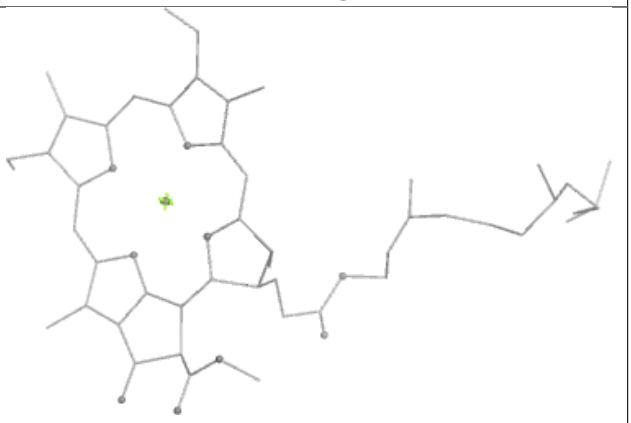
Bond lengths



Bond angles

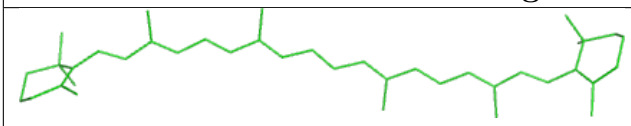


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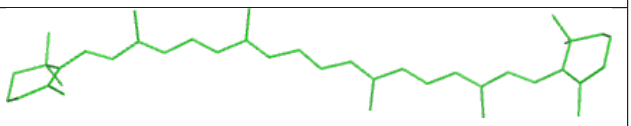


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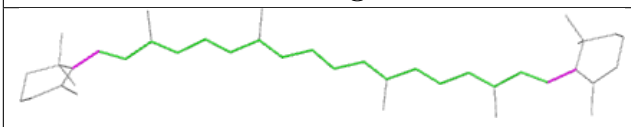
Ligand BCR A 845



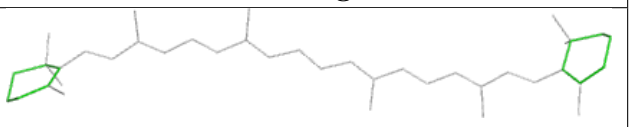
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Bond angles

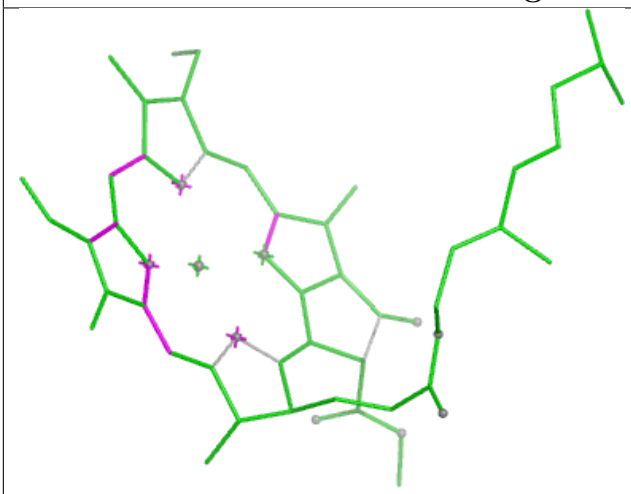


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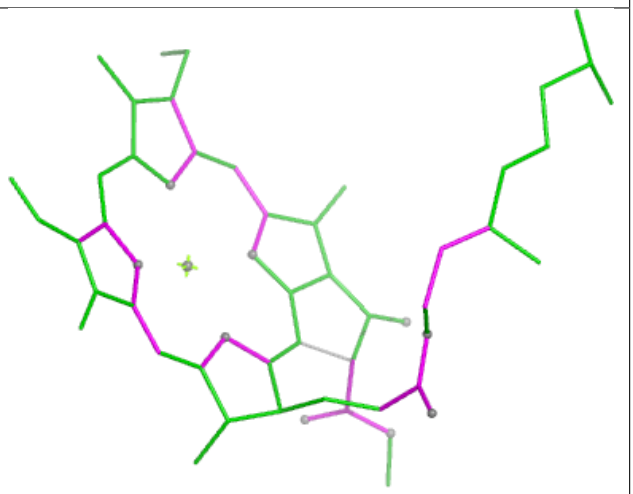


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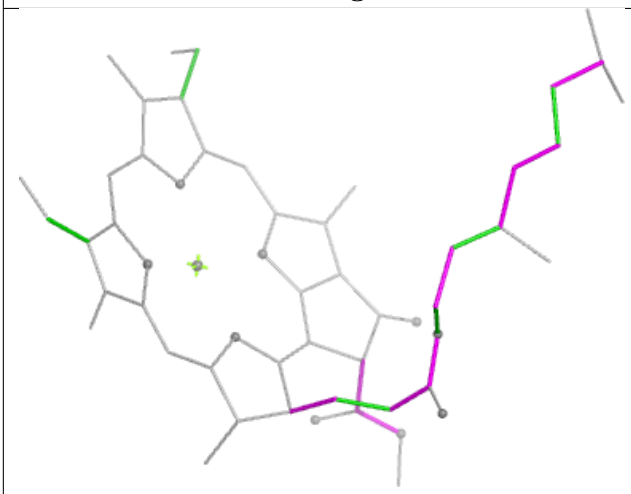
Ligand CLA B 821



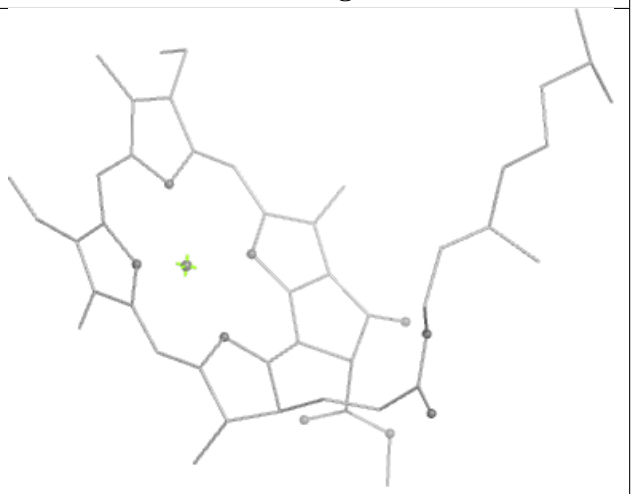
Bond lengths



Bond angles

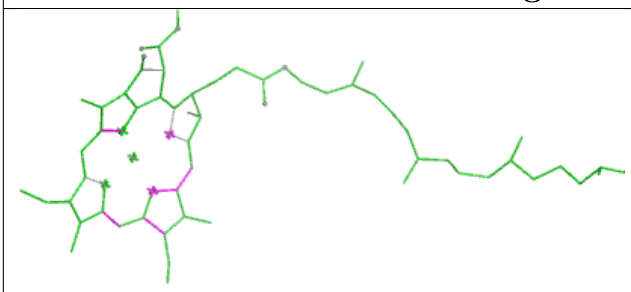


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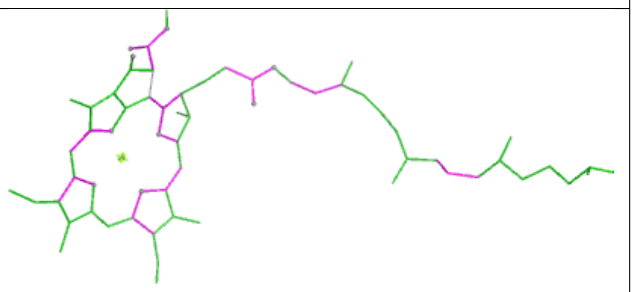


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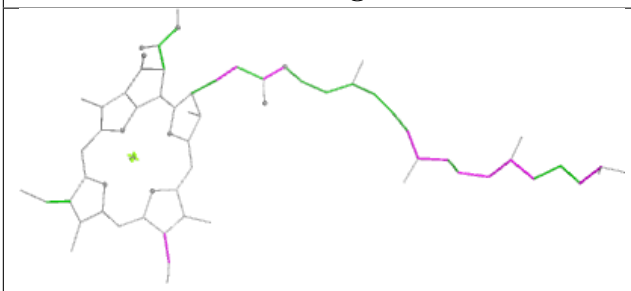
Ligand CLA A 803



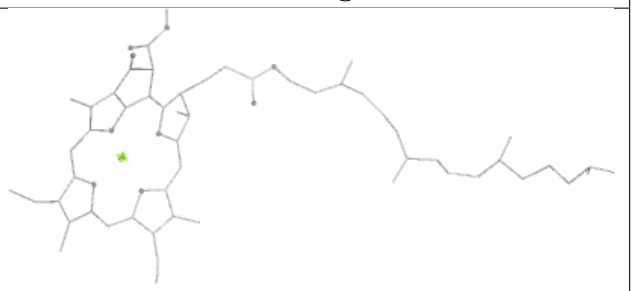
Bond lengths



Bond angles

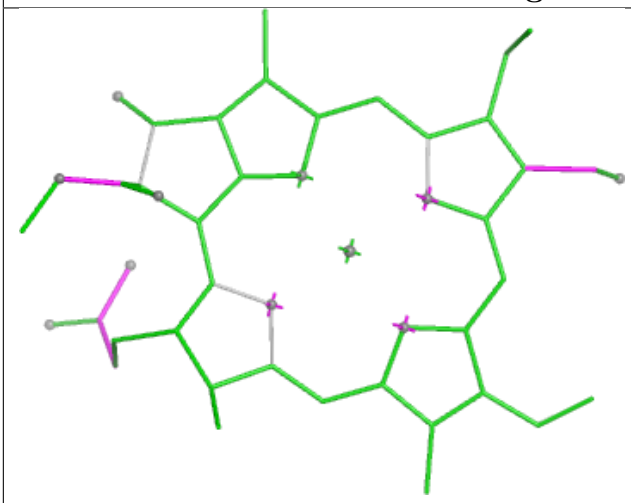


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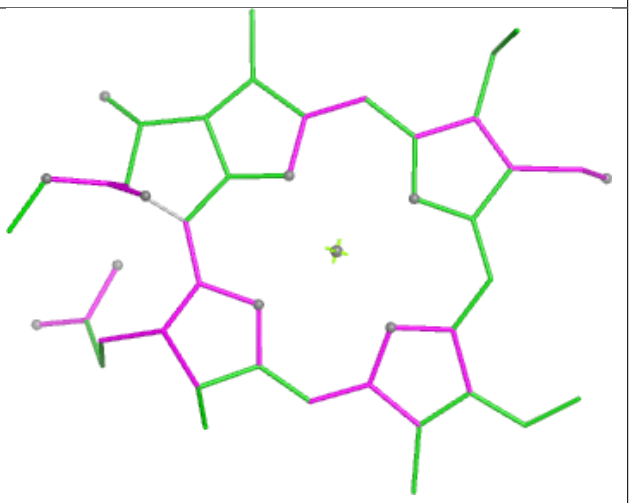


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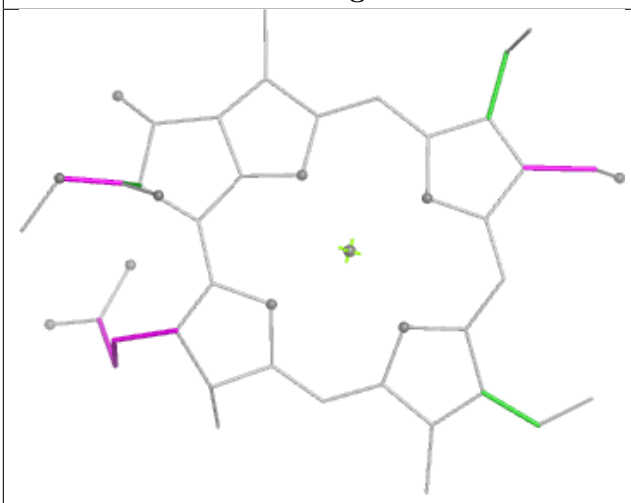
Ligand CHL Z 307



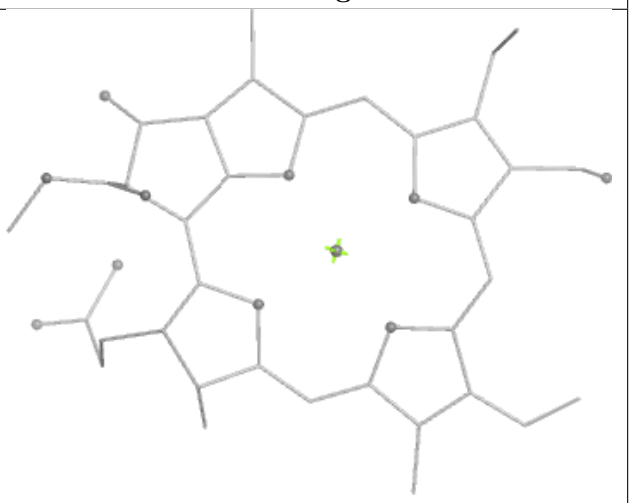
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Bond angles

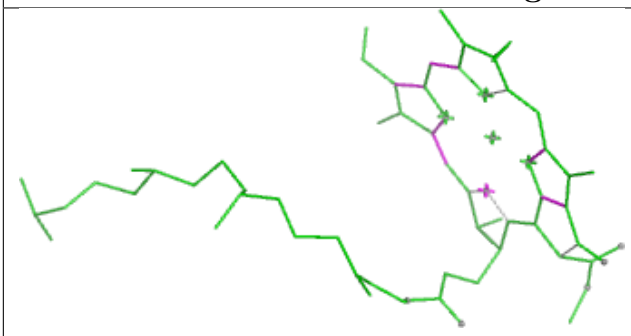


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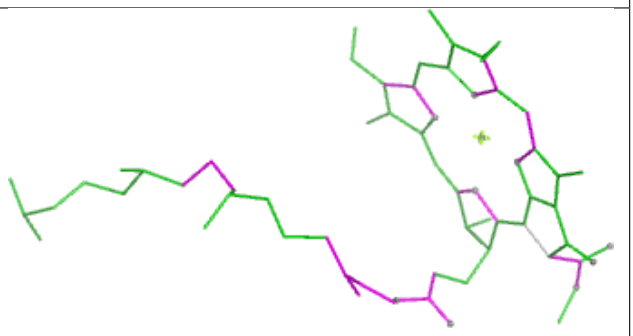


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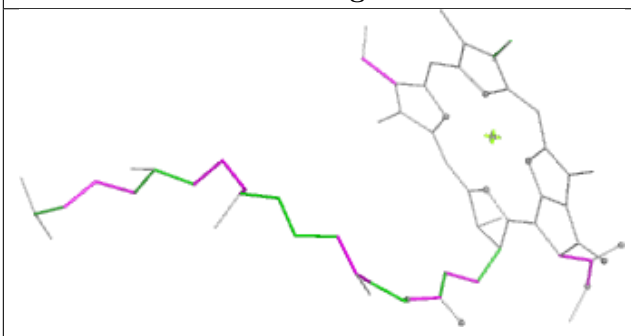
Ligand CLA B 813



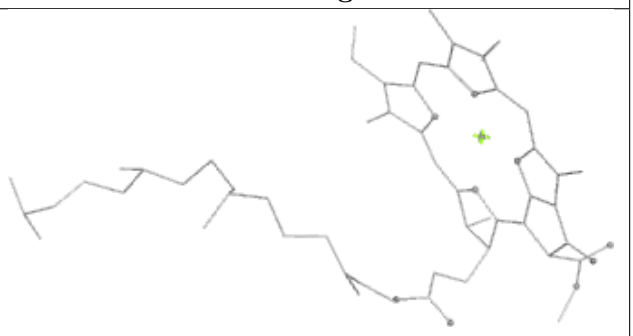
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Bond angles

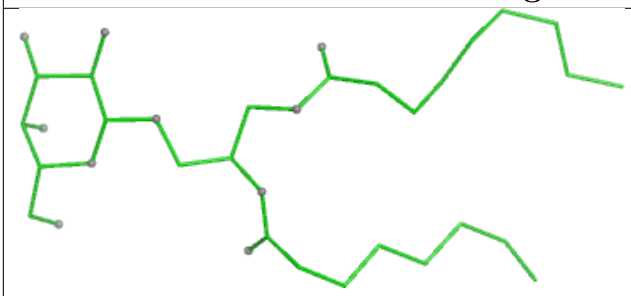


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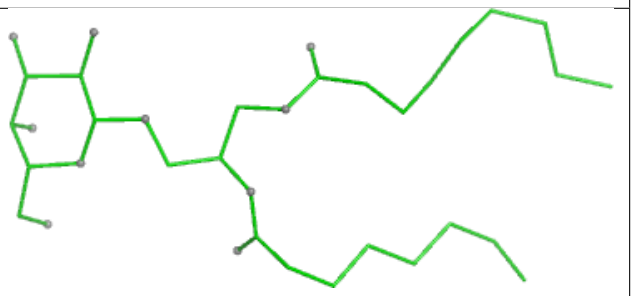


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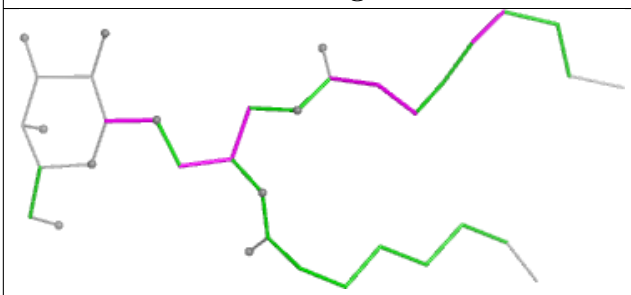
Ligand LMG 6 619



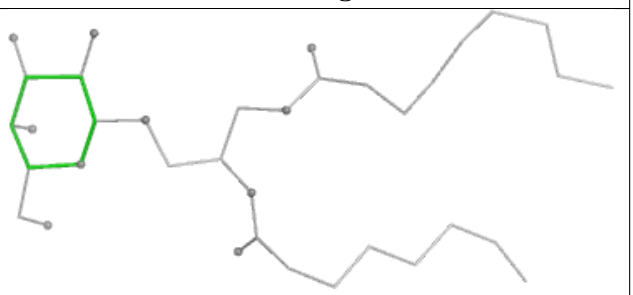
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Bond angles

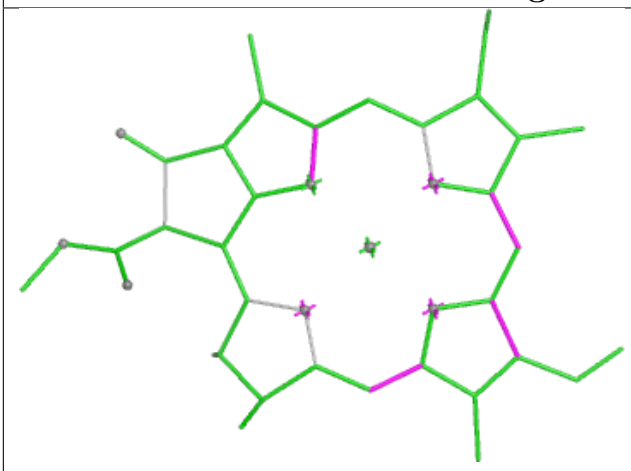


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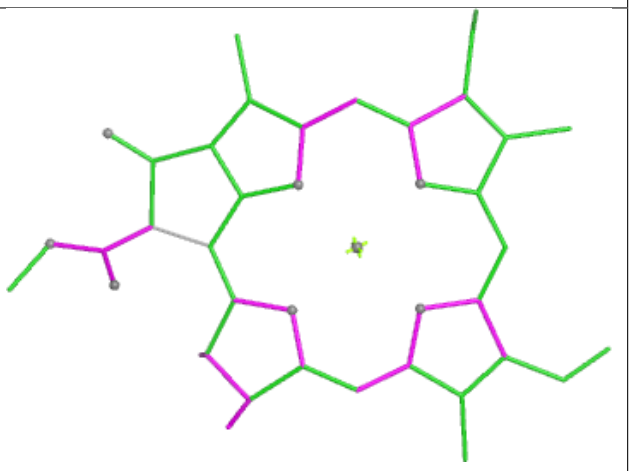


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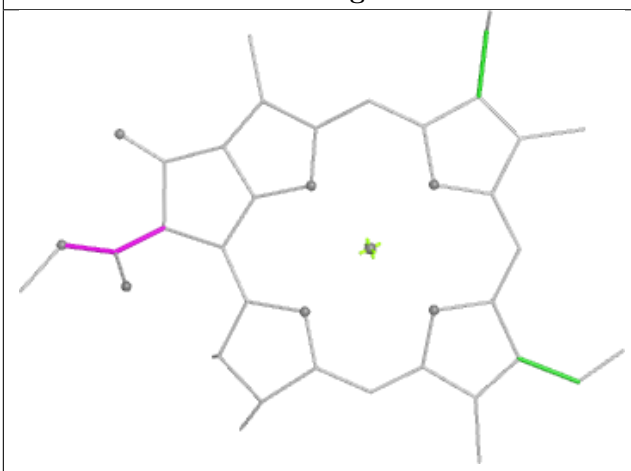
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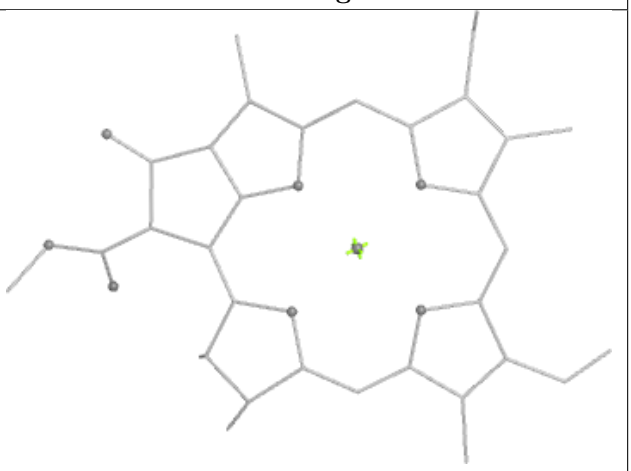
Bond lengths



Bond angles

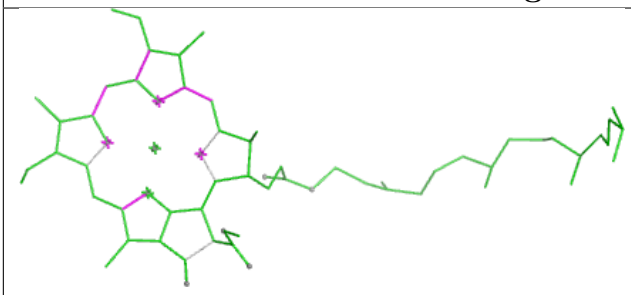


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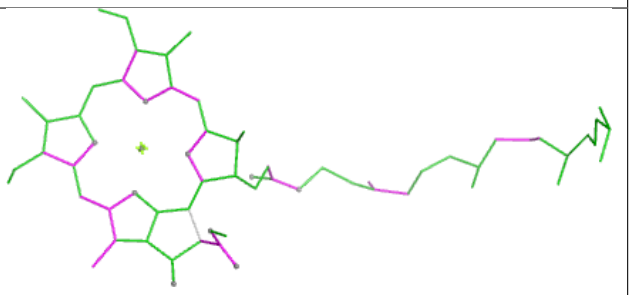


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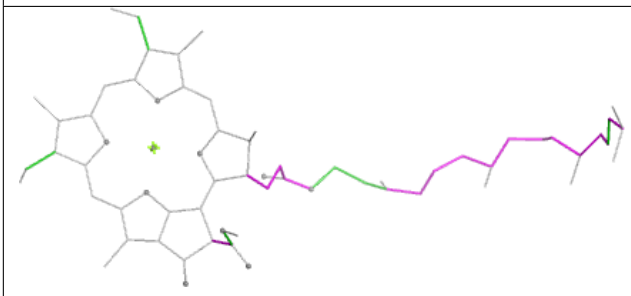
Ligand CLA B 840



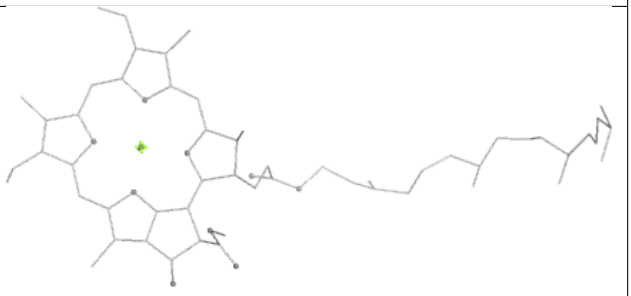
Bond lengths



Bond angles

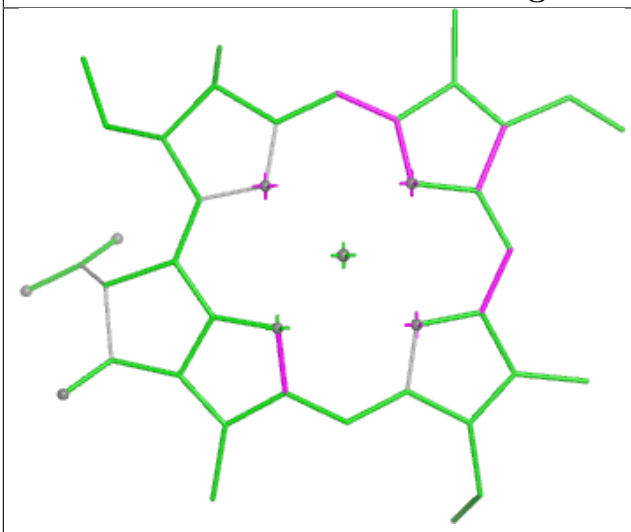


Torsions

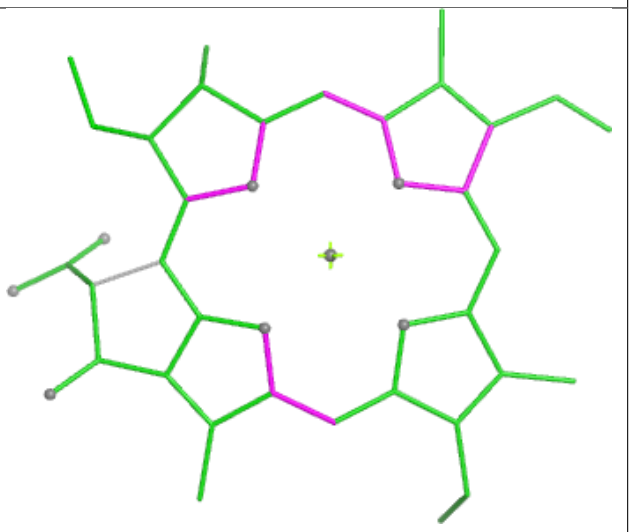


Rings

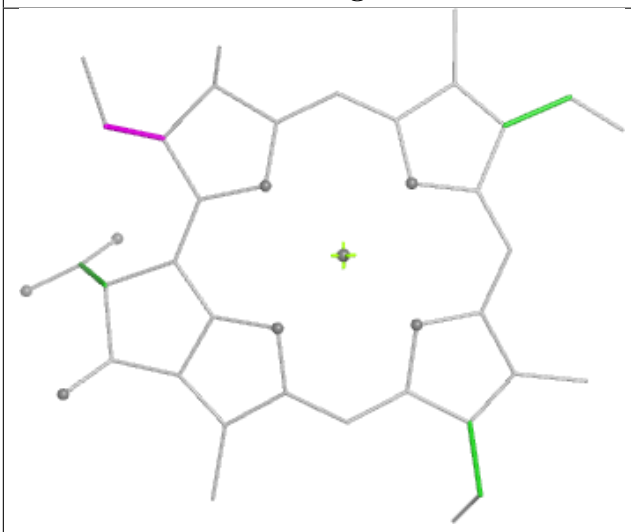
Ligand CLA 4 310



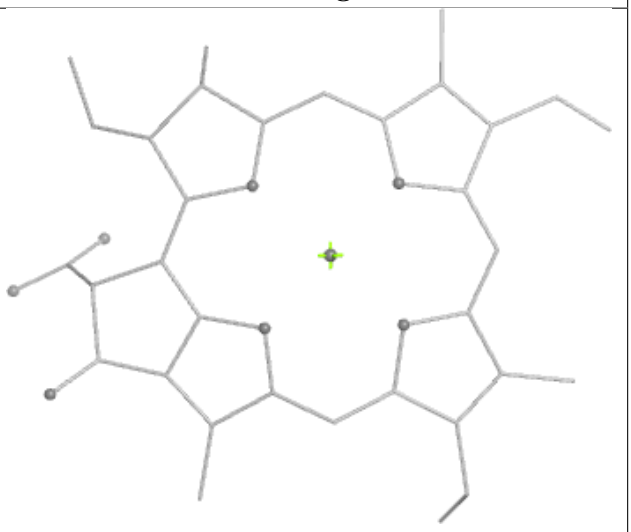
Bond lengths



Bond angles

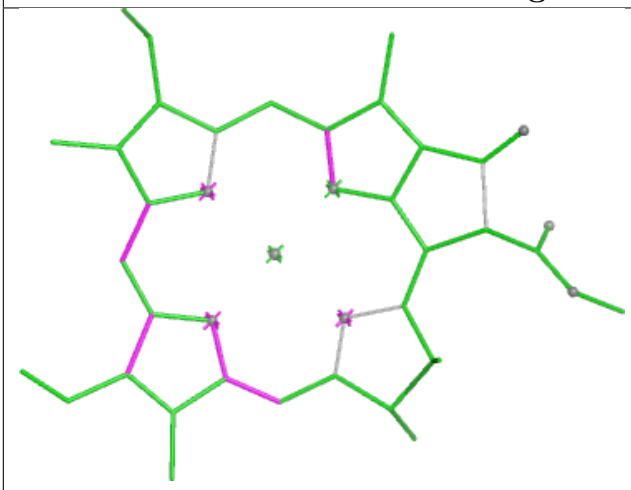


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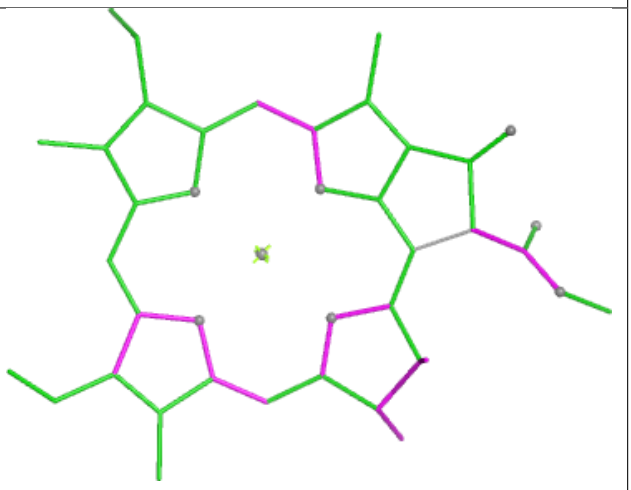


Rings

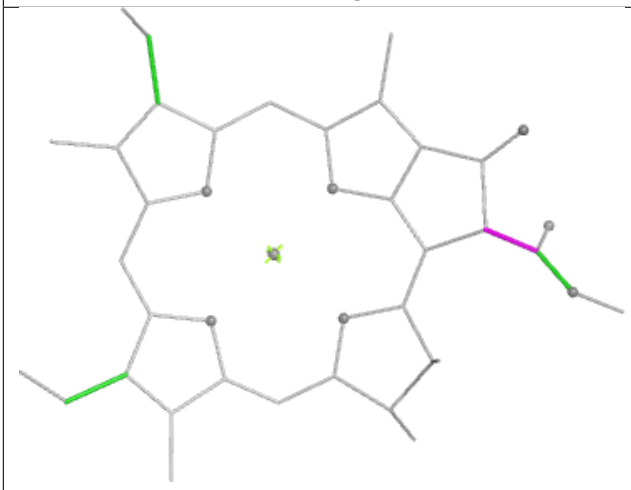
Ligand CLA 2 610



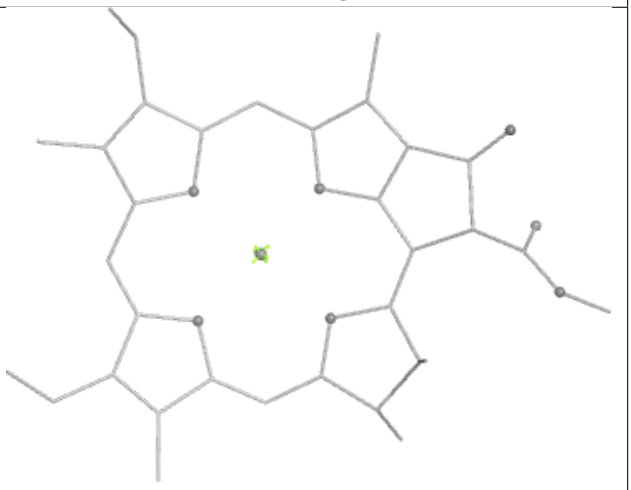
Bond lengths



Bond angles

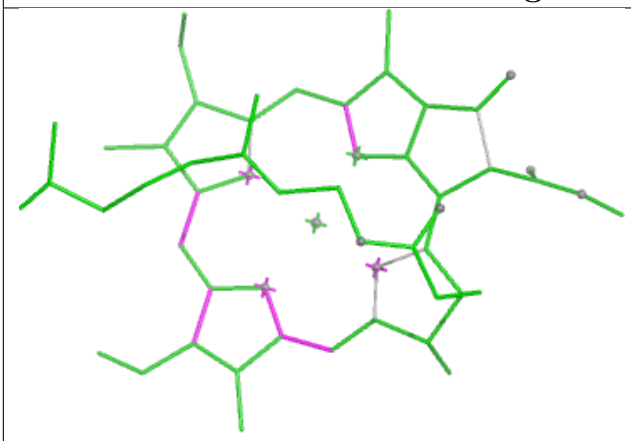


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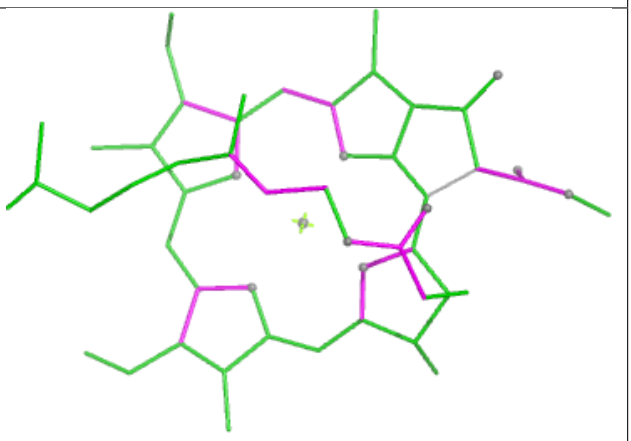


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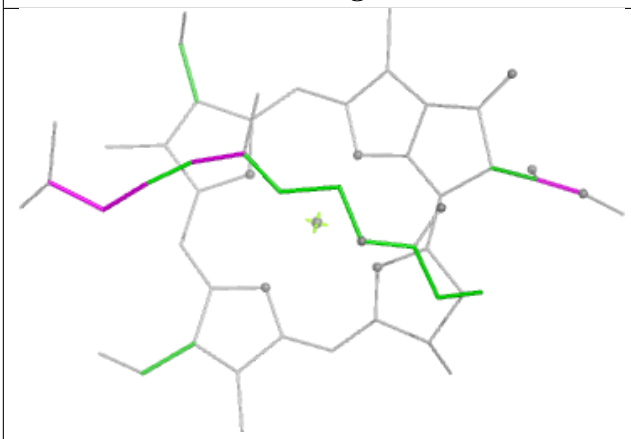
Ligand CLA B 815



Bond lengths



Bond angles

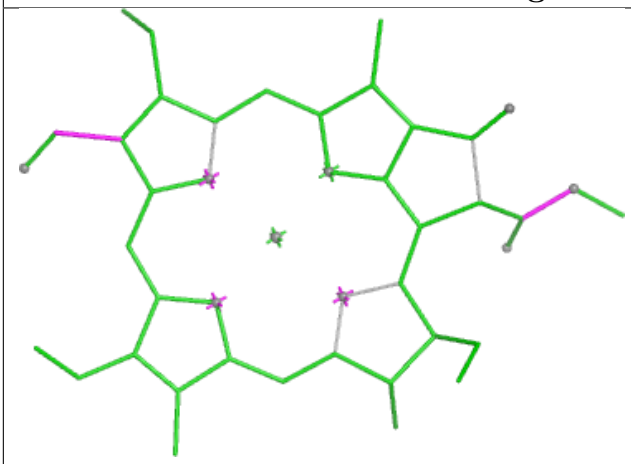


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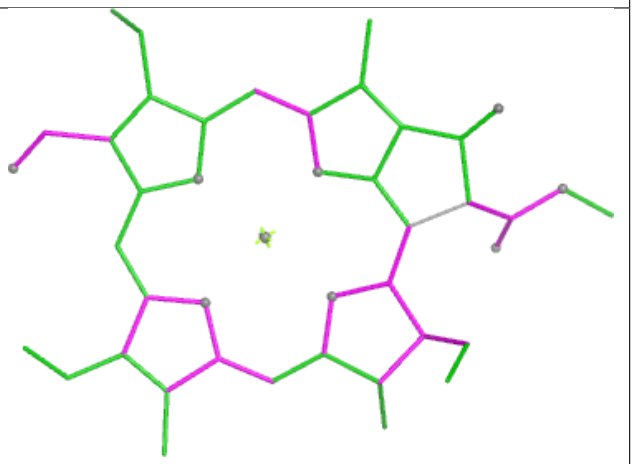


Rings

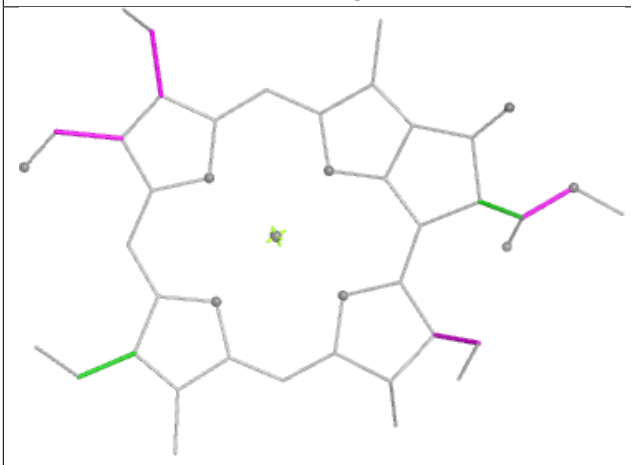
Ligand CHL 2 606



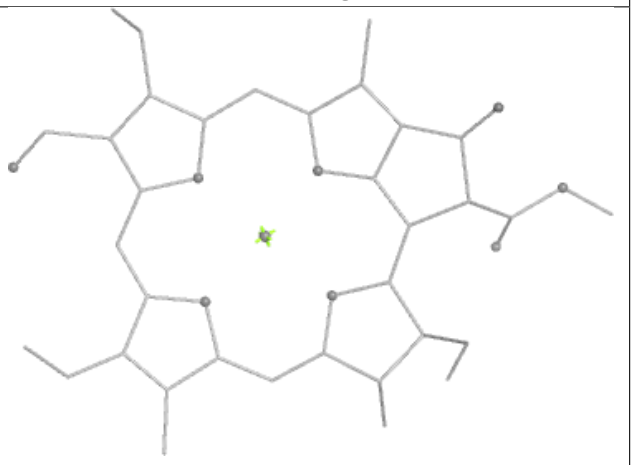
Bond lengths



Bond angles

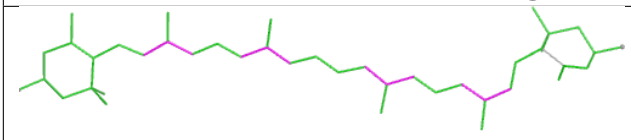


Torsions



Rings

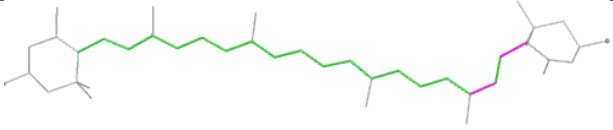
Ligand LUT X 615



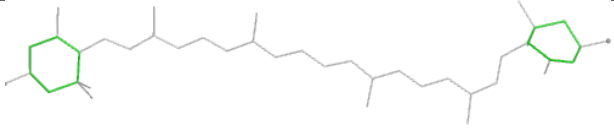
Bond lengths



Bond angles

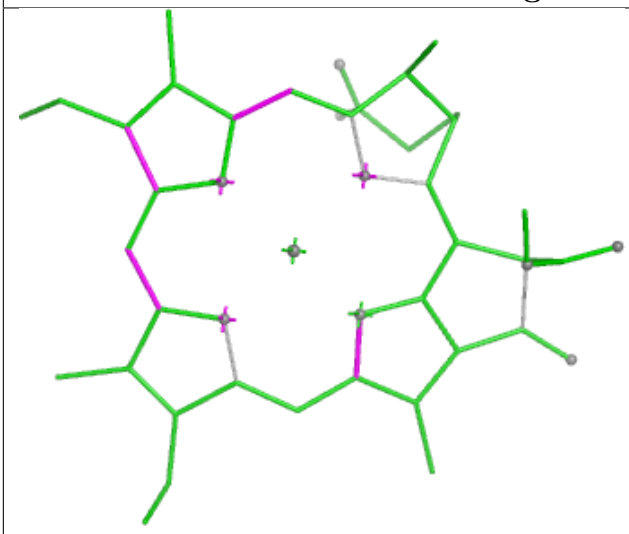


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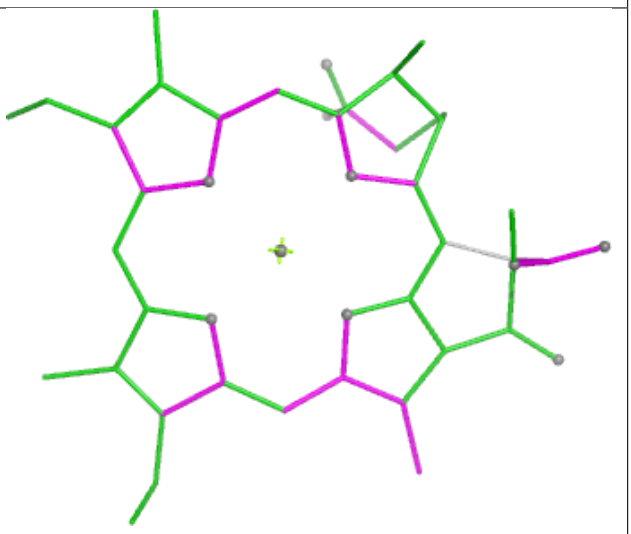


Rings

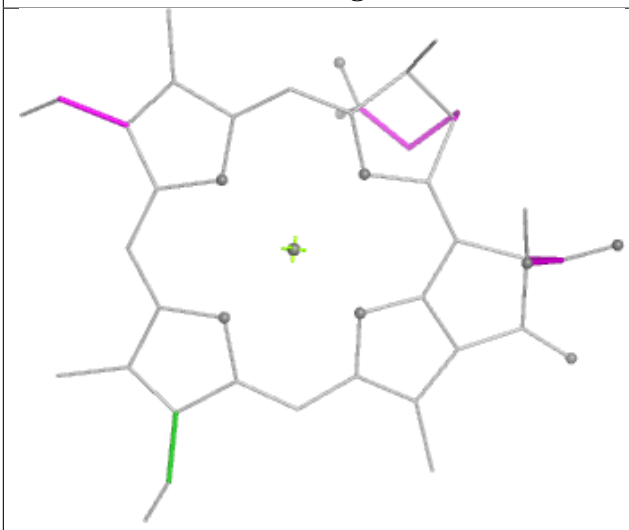
Ligand CLA X 604



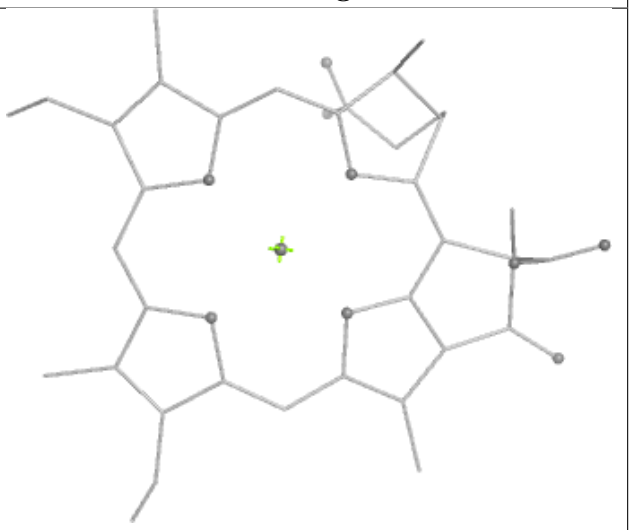
Bond lengths



Bond angles

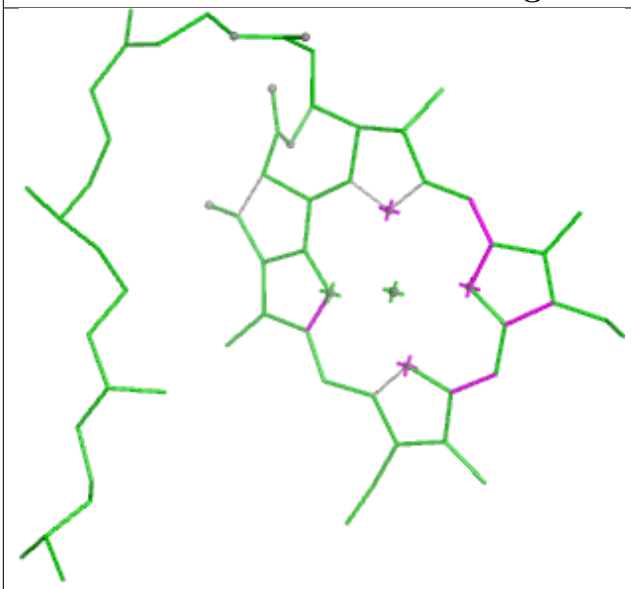


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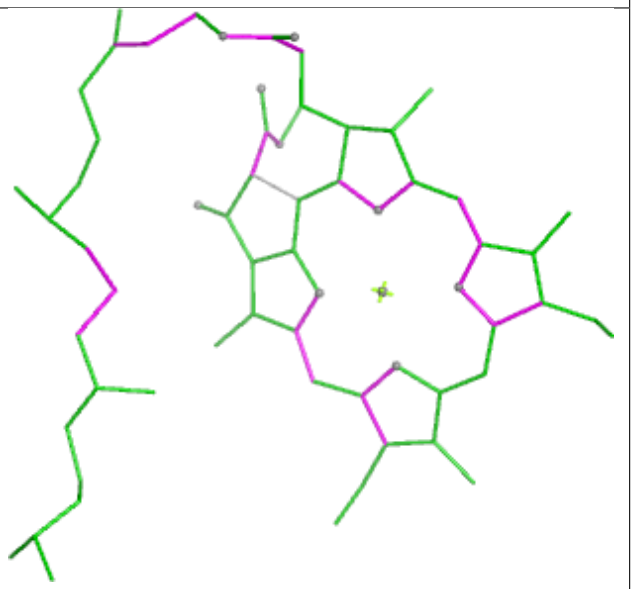


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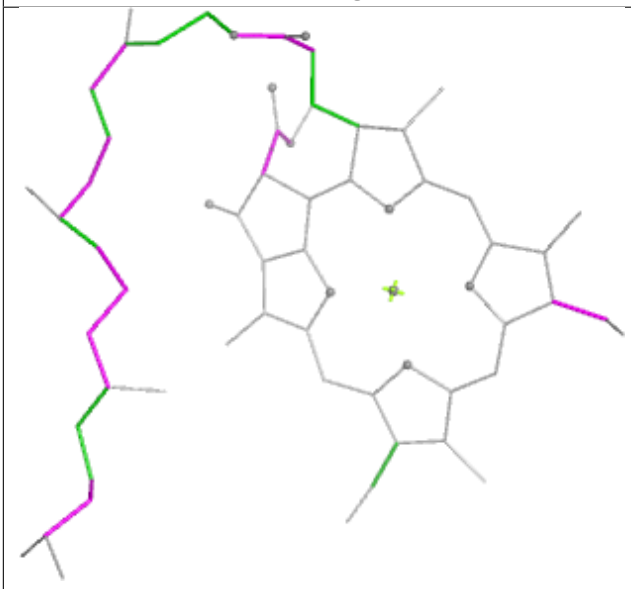
Ligand CLA A 825



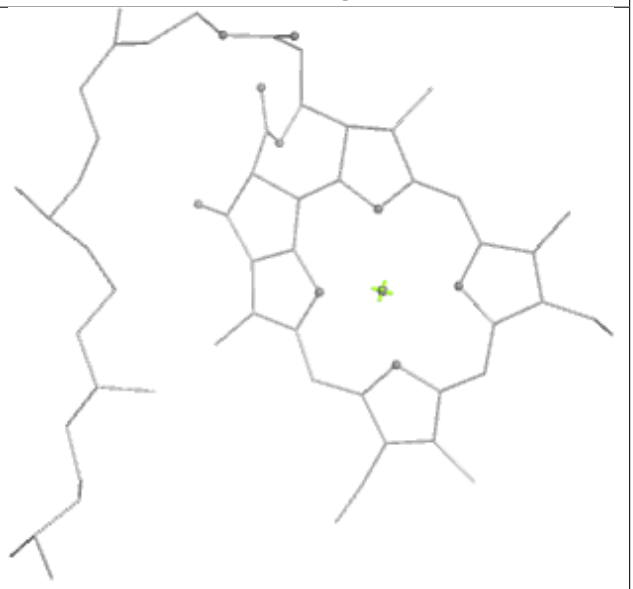
Bond lengths



Bond angles

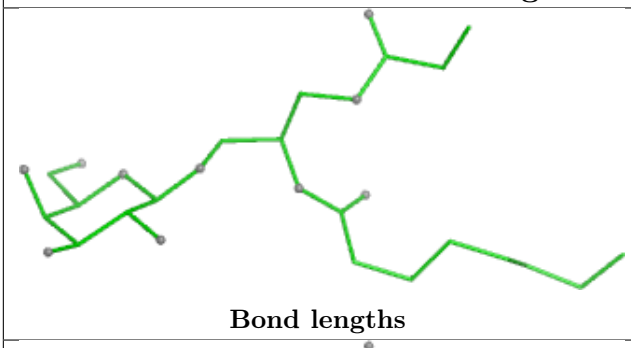


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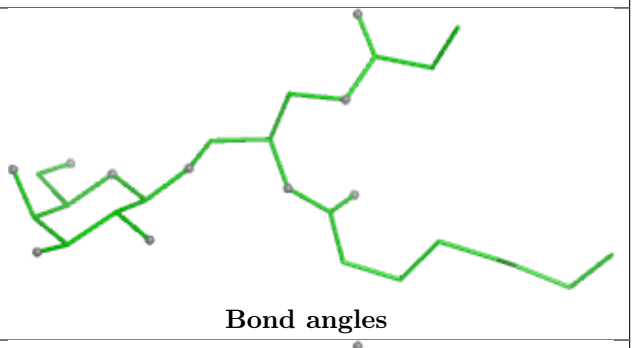


Rings

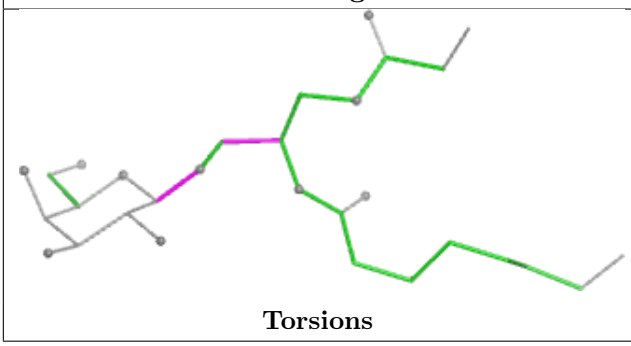
Ligand LMG F 307



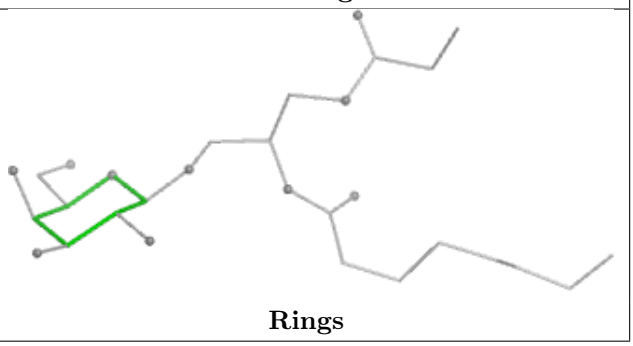
Bond lengths



Bond angles

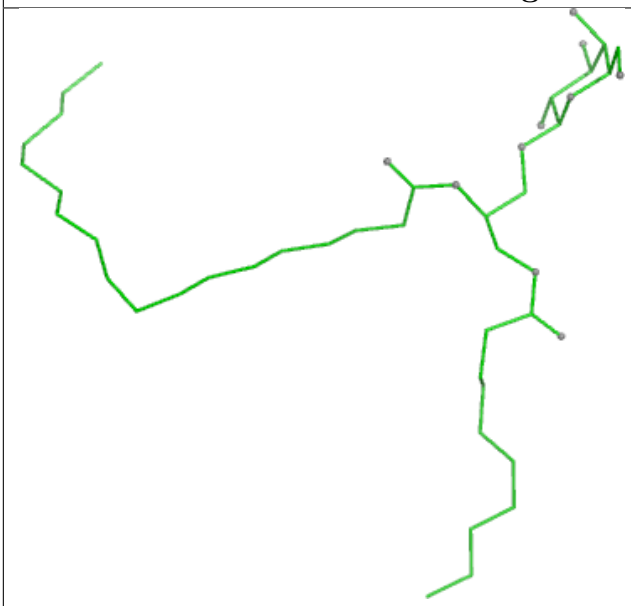


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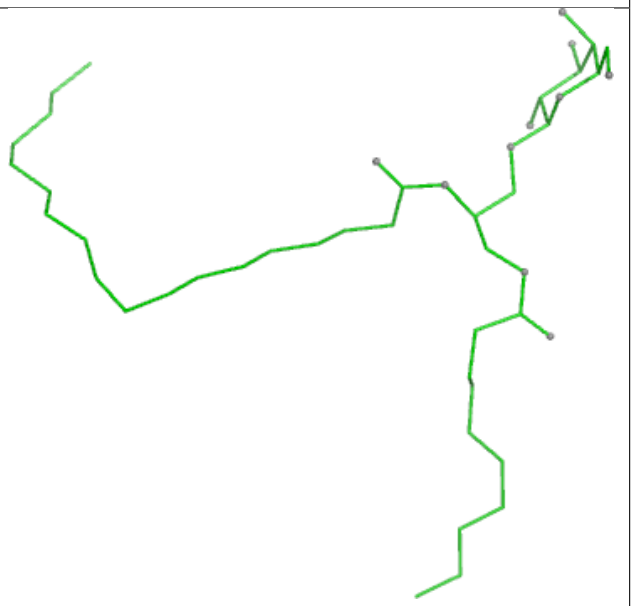


Rings

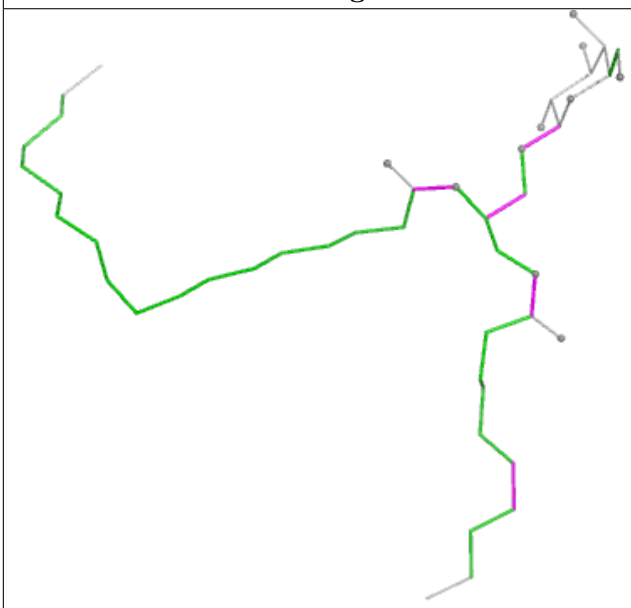
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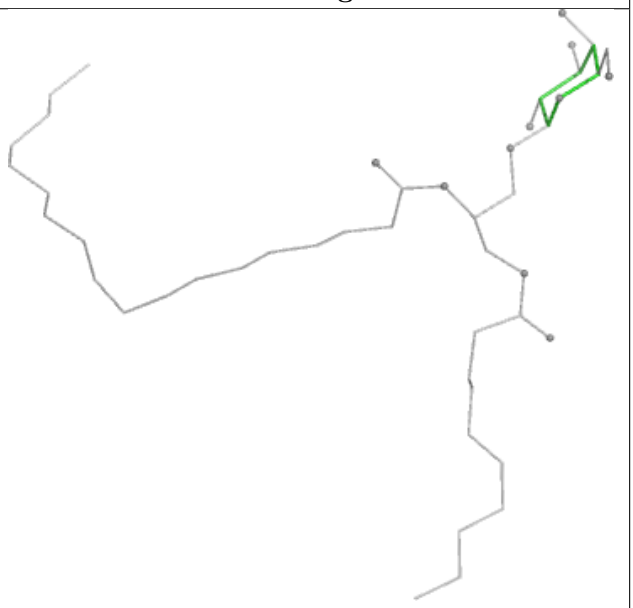
Bond lengths



Bond angles

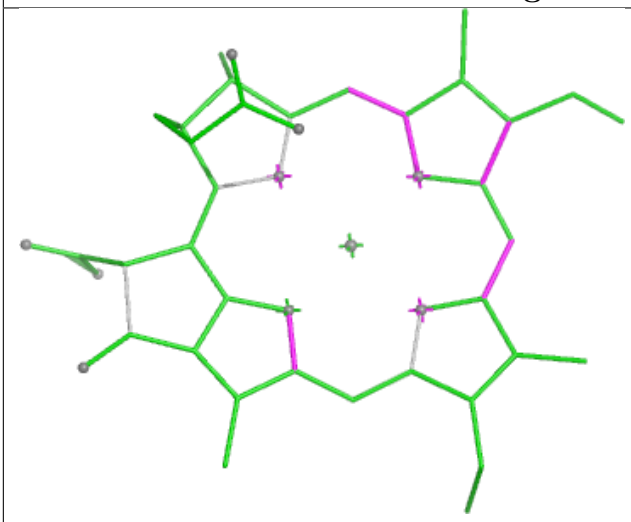


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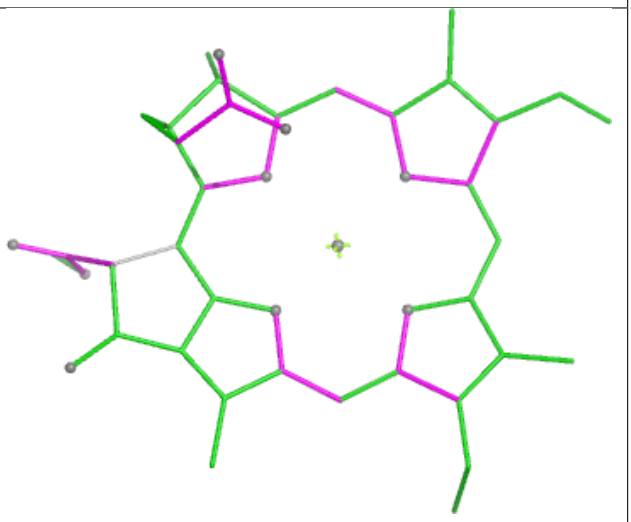


Rings

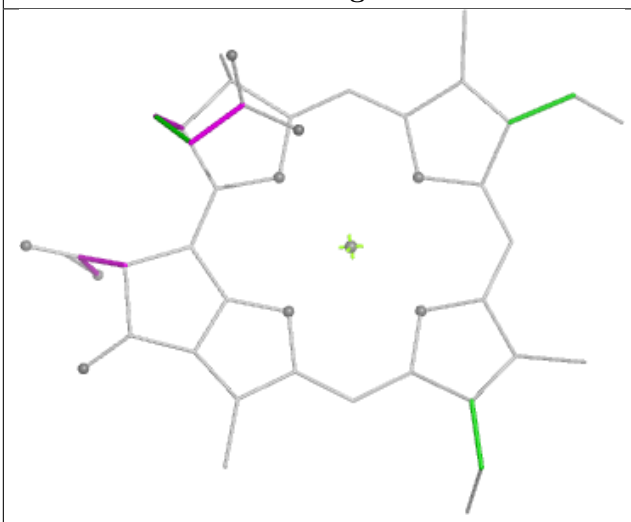
Ligand CLA Y 614



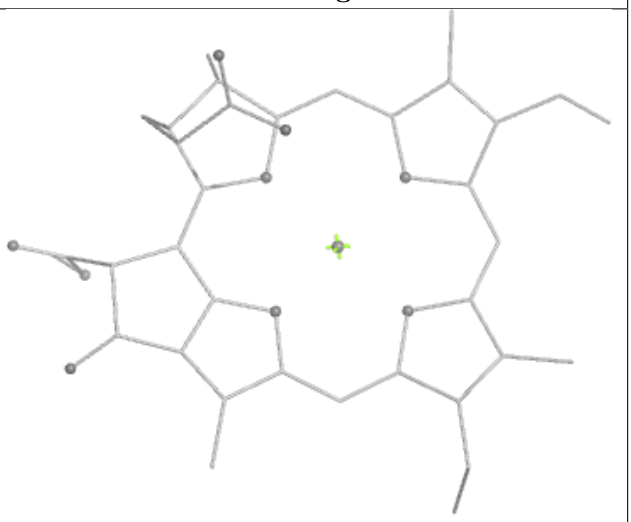
Bond lengths



Bond angles

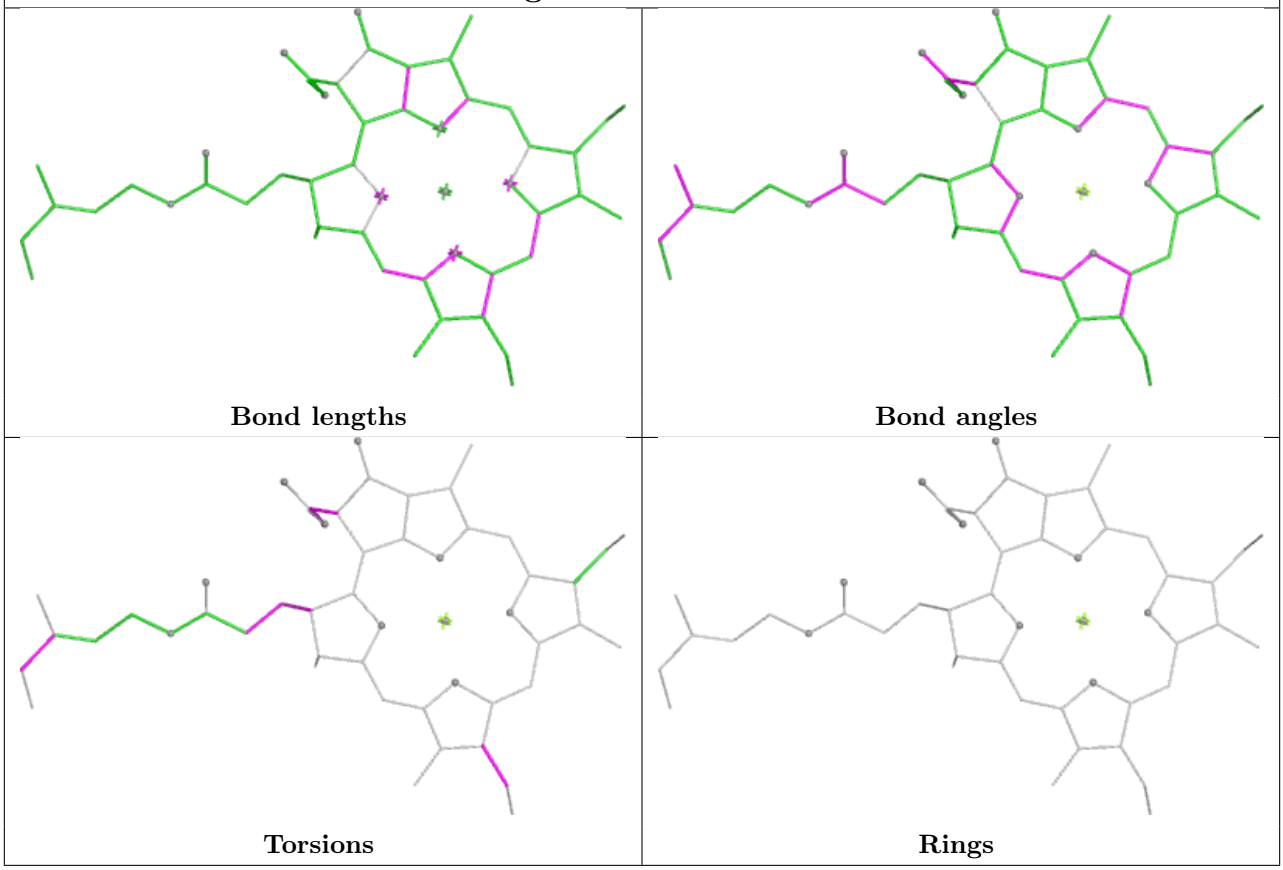


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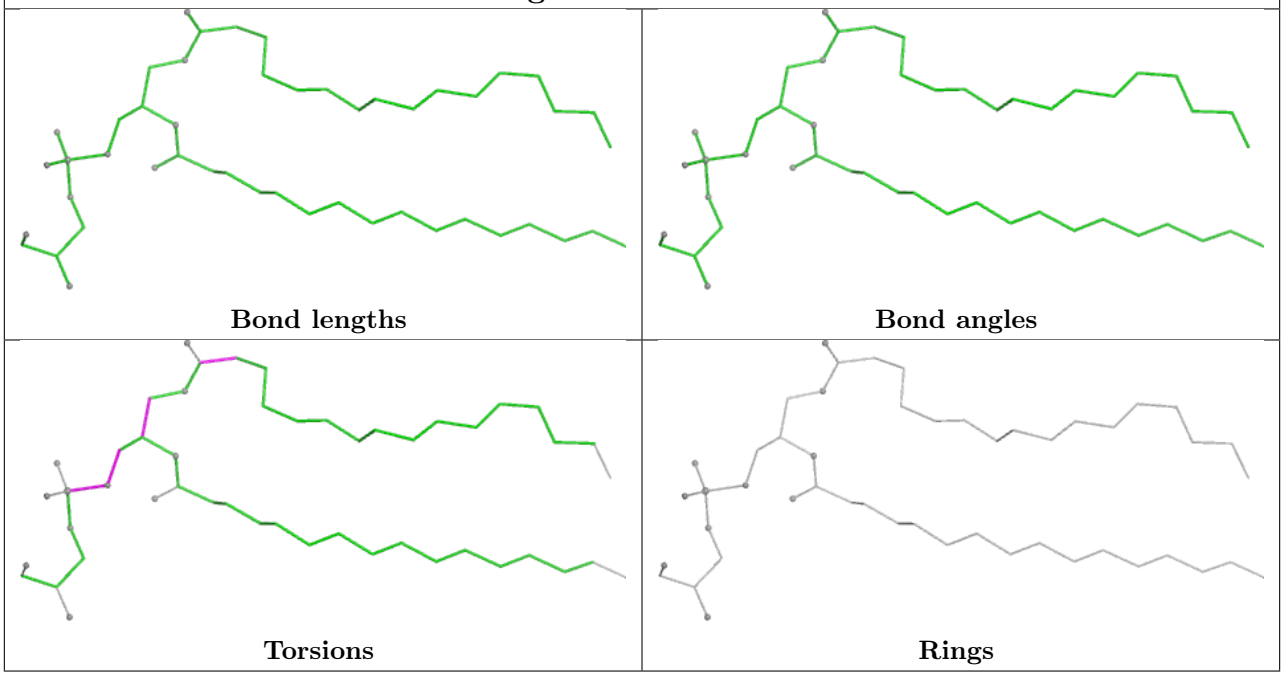


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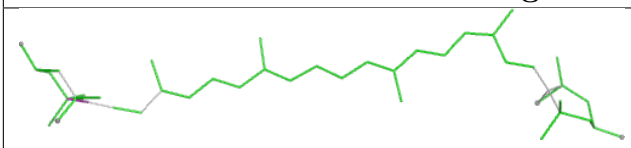
Ligand CLA A 837



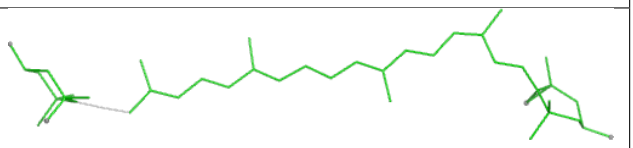
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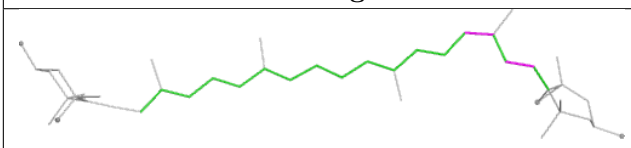
Ligand NEX Y 617



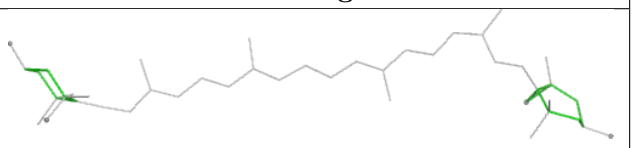
Bond lengths



Bond angles

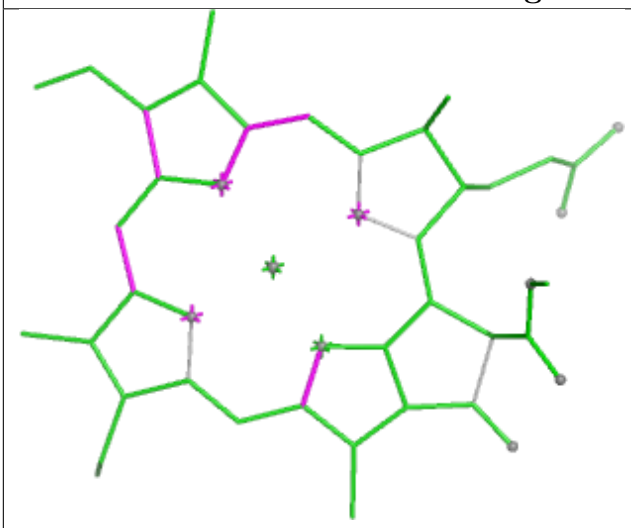


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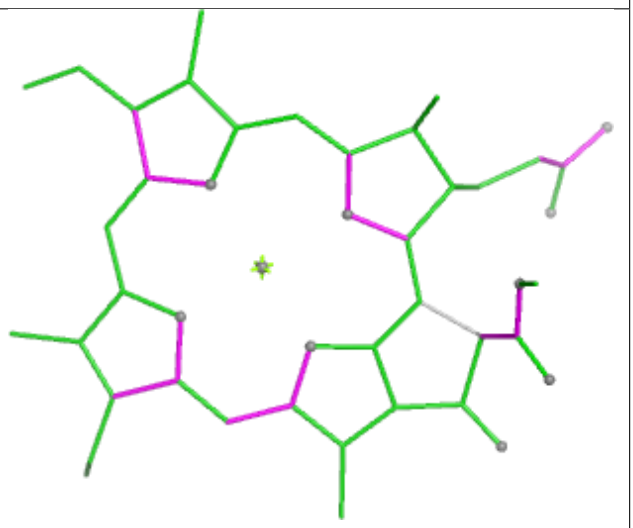


Rings

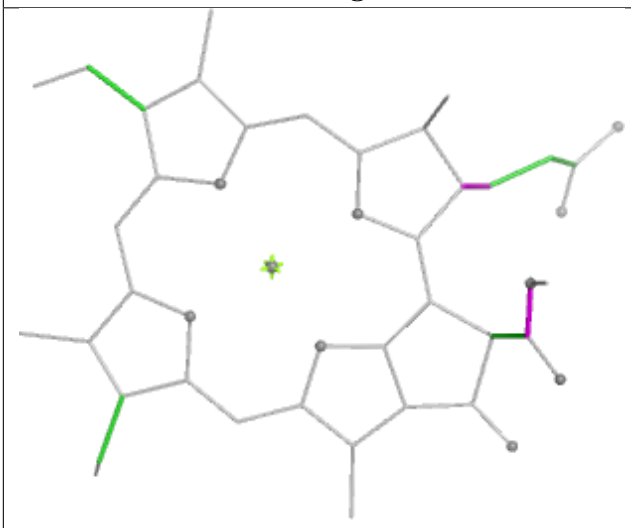
Ligand CLA B 832



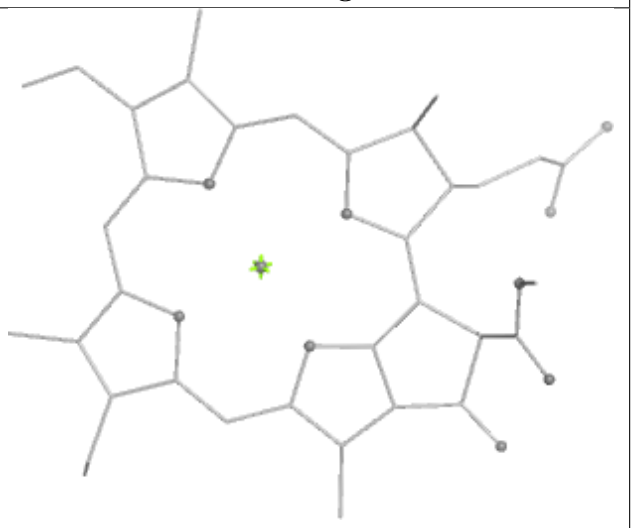
Bond lengths



Bond angles

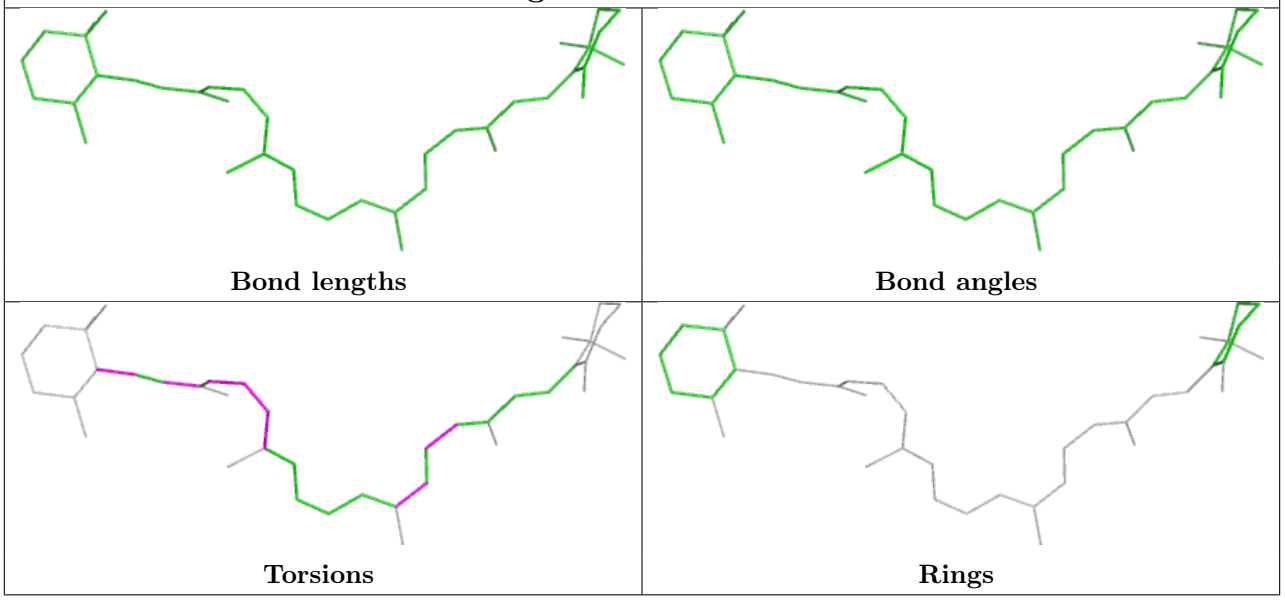


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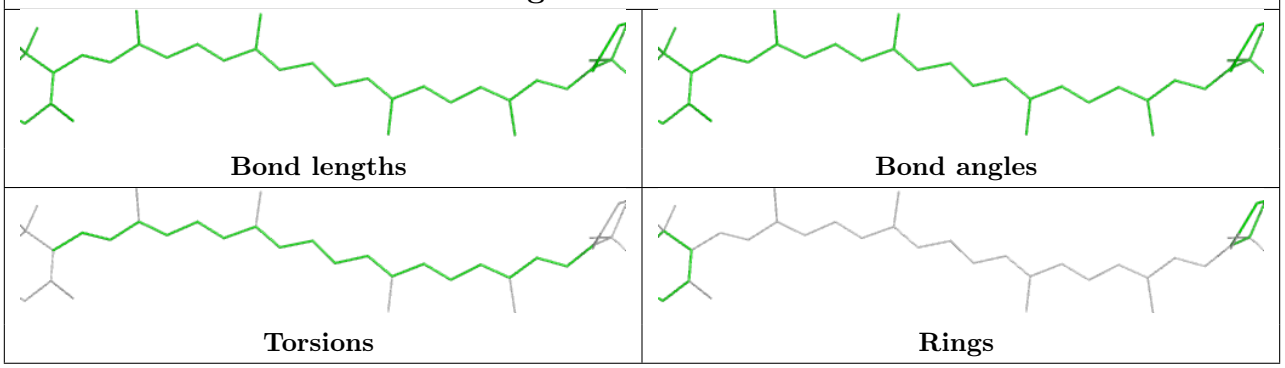


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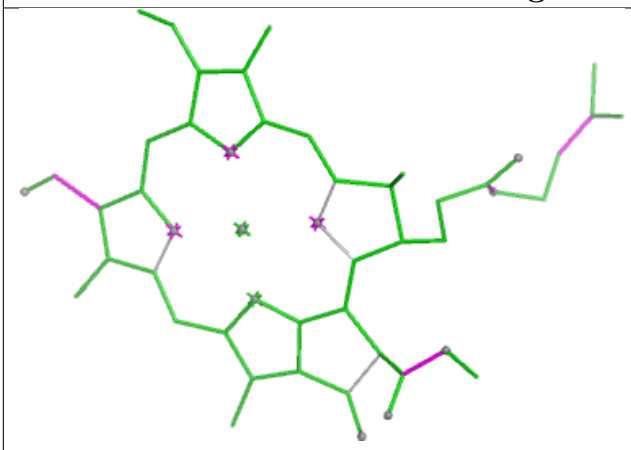
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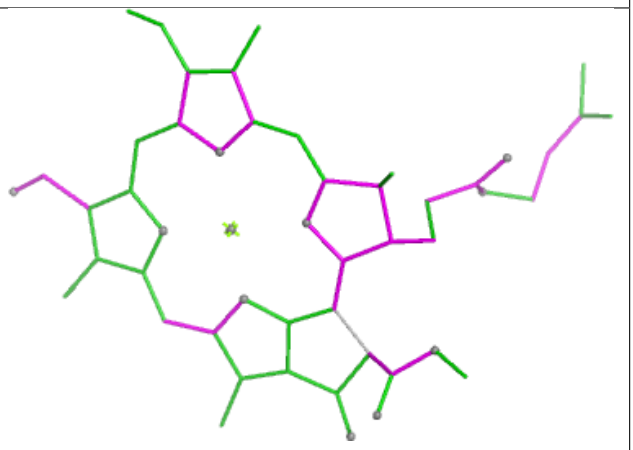
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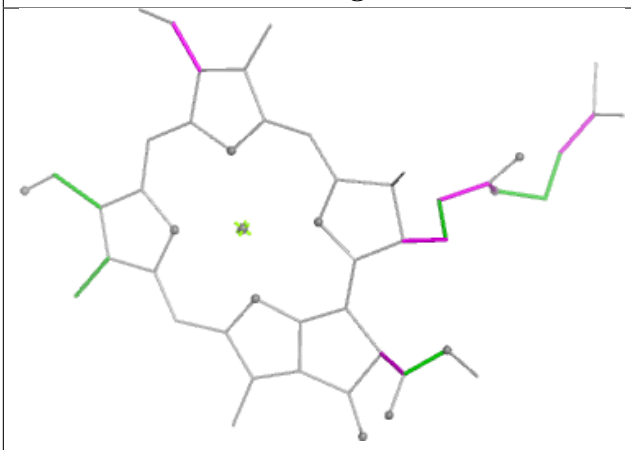
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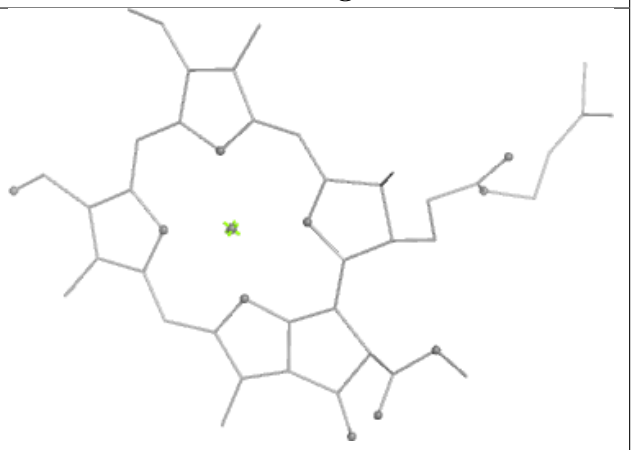
Bond lengths



Bond angles

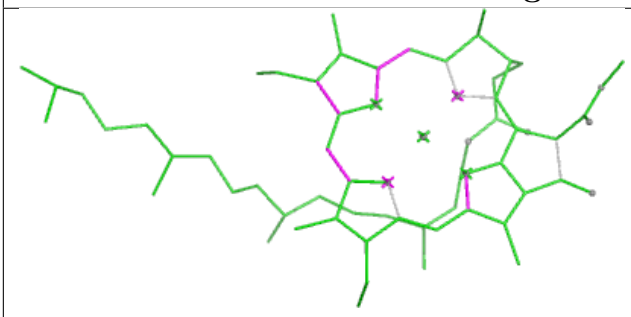


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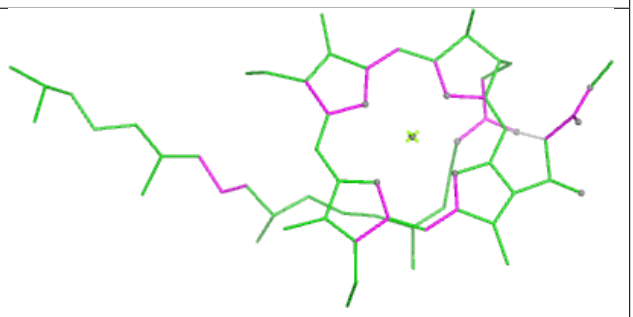


Rings

Ligand CLA A 840



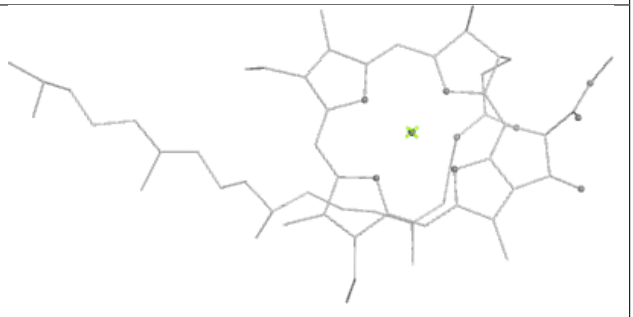
Bond lengths



Bond angles

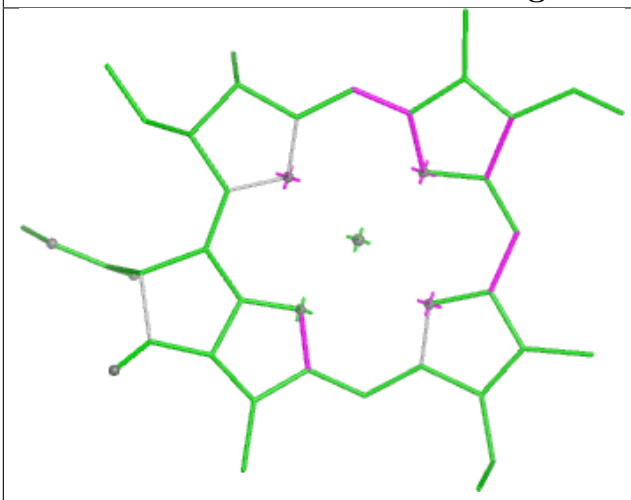


Torsions

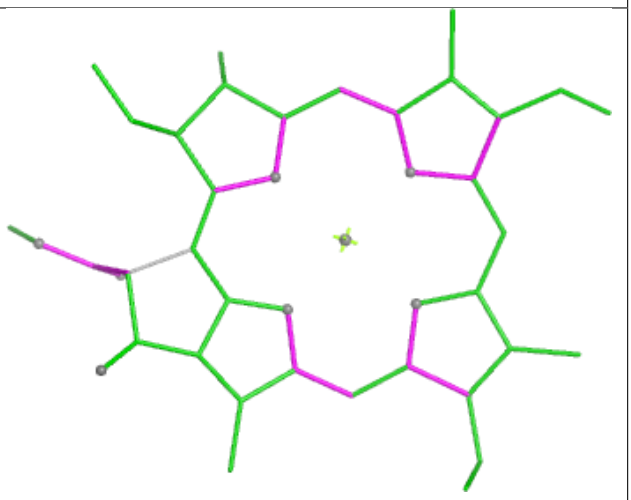


Rings

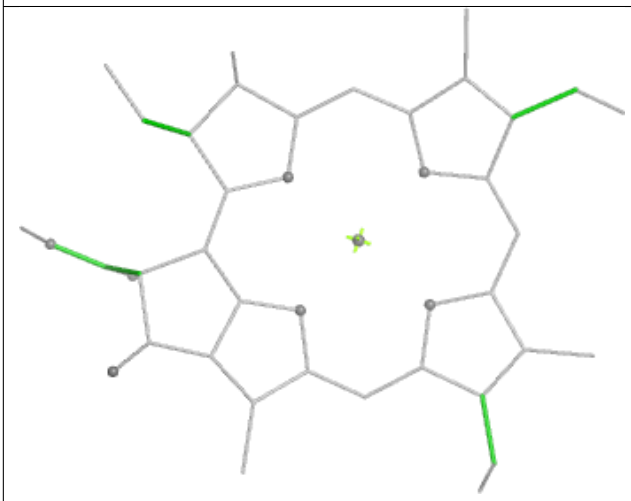
Ligand CLA J 101



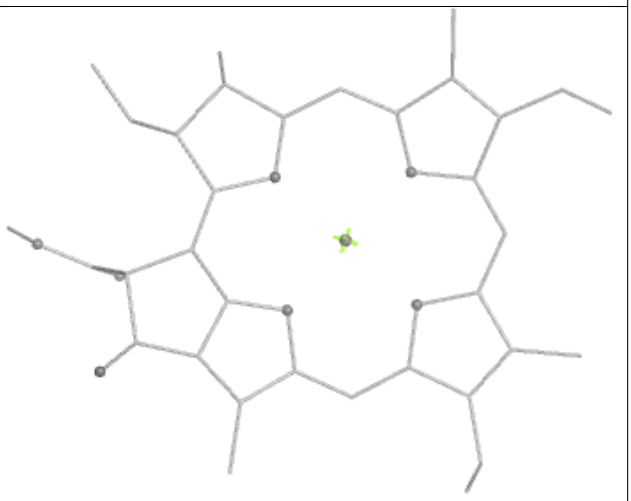
Bond lengths



Bond angles

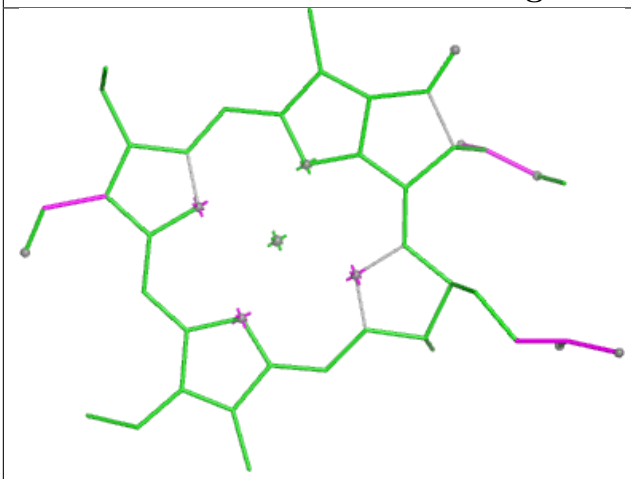


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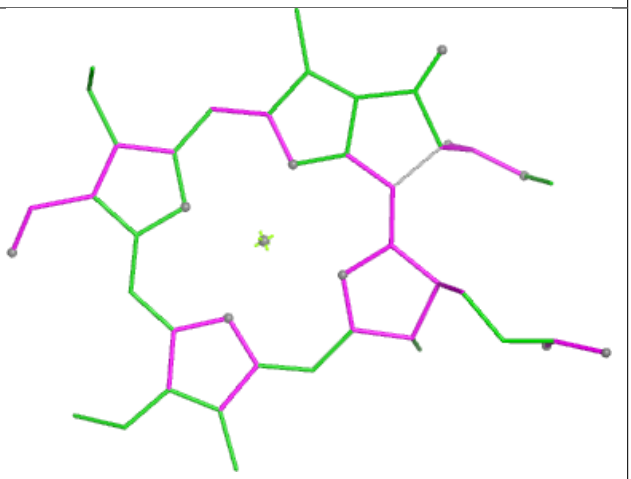


Rings

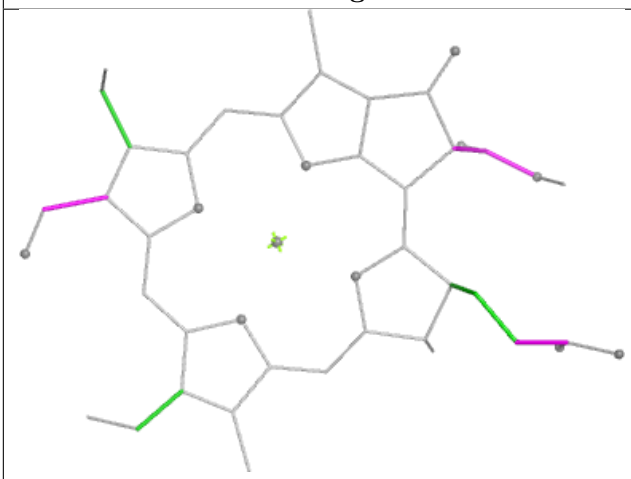
Ligand CHL Z 302



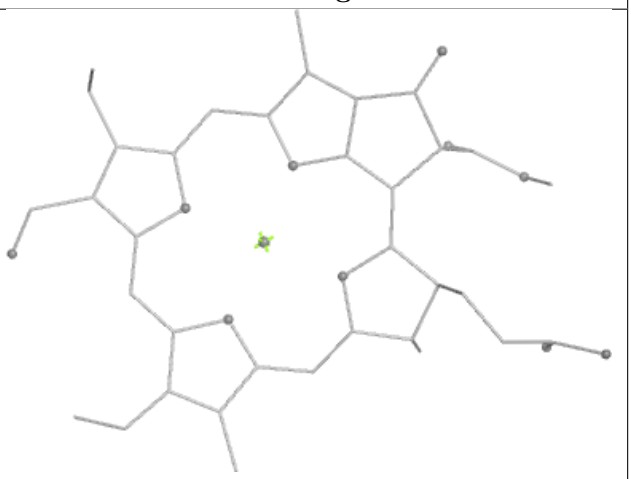
Bond lengths



Bond angles

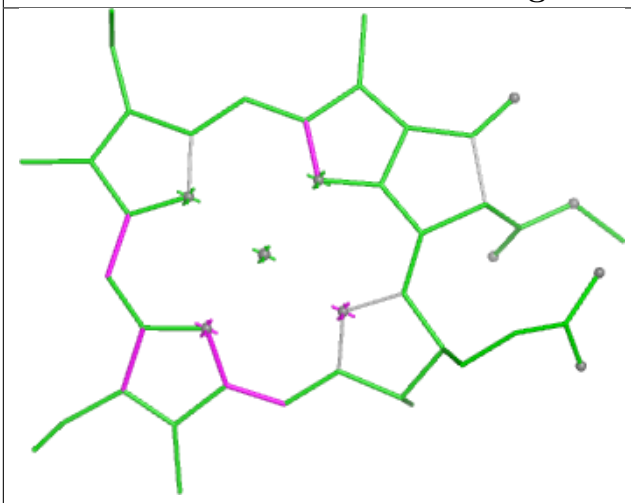


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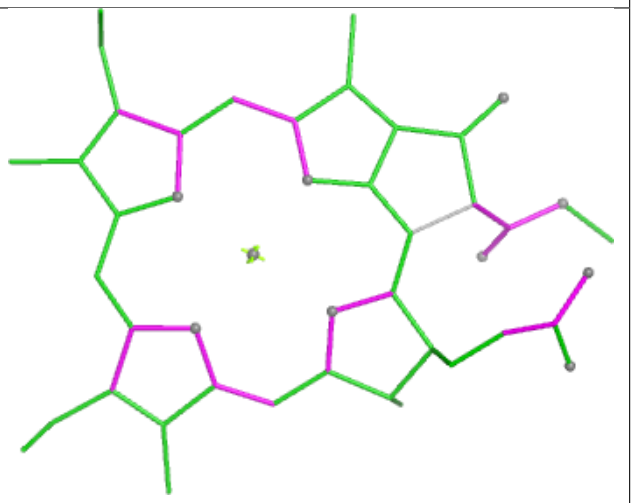


Rings

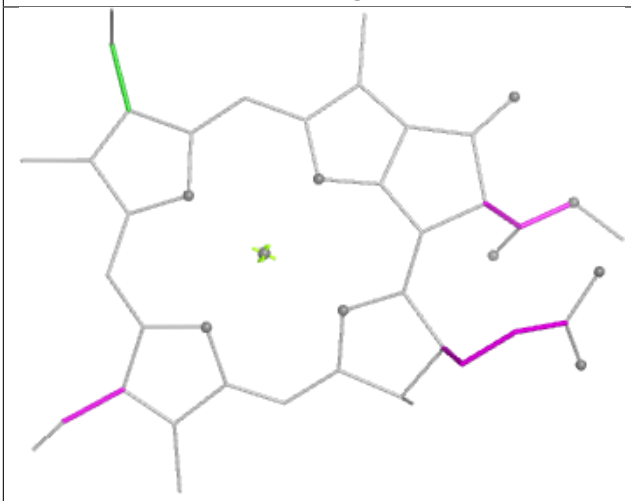
Ligand CLA 5 614



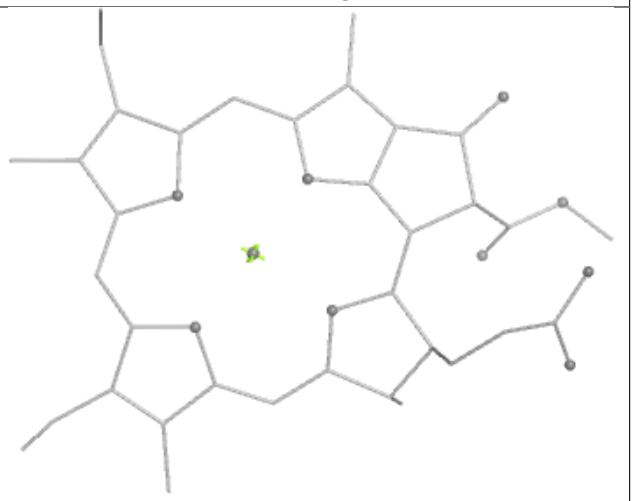
Bond lengths



Bond angles

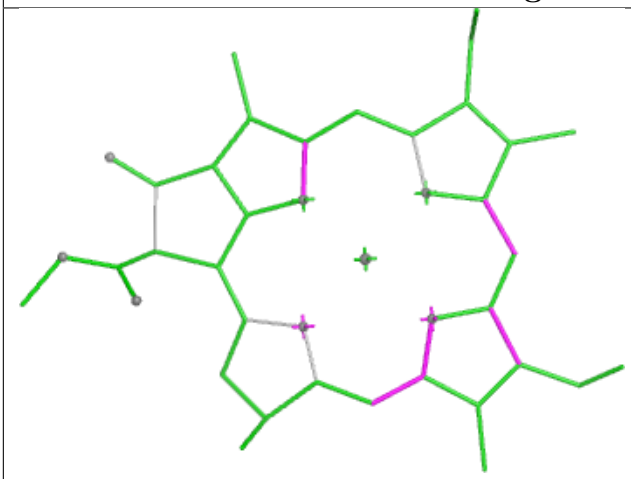


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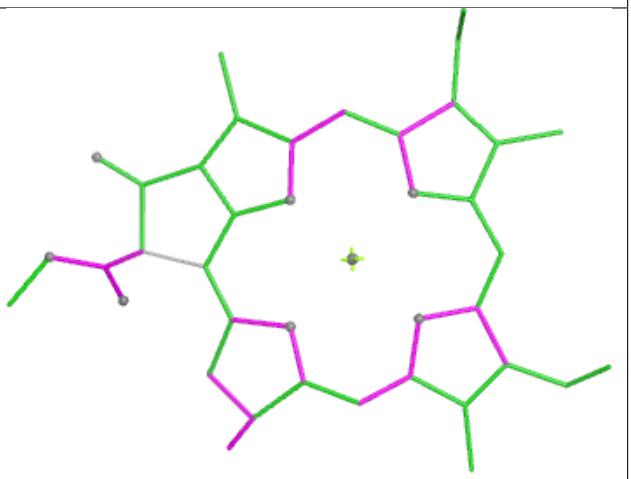


Rings

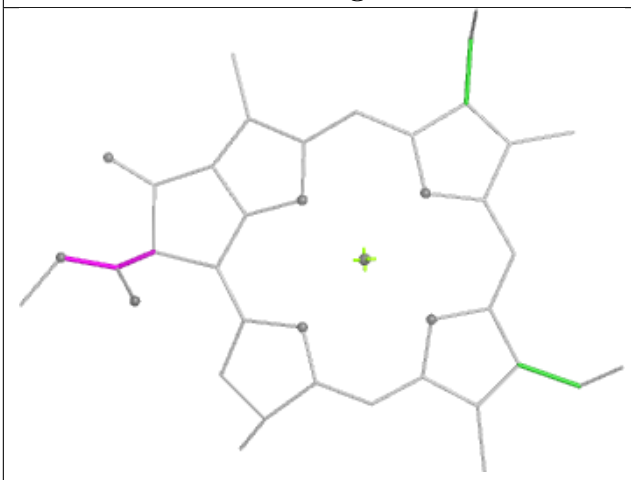
Ligand CLA B 803



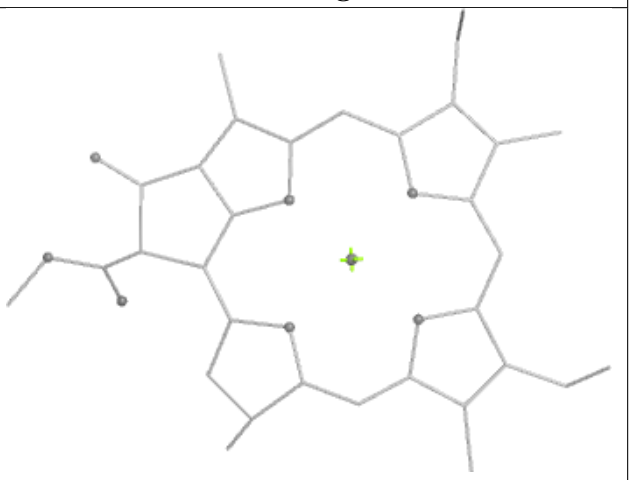
Bond lengths



Bond angles

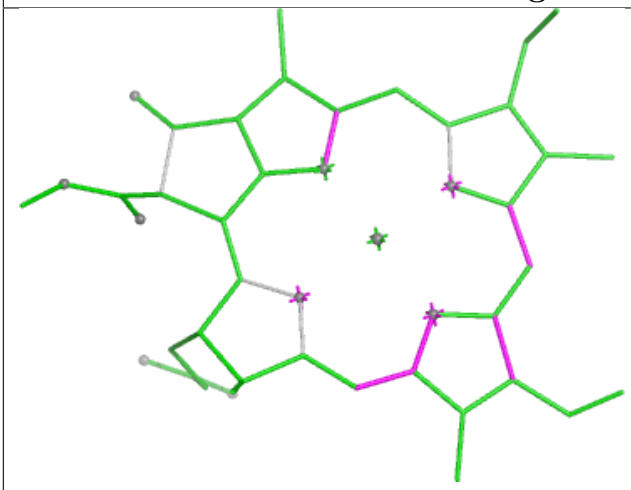


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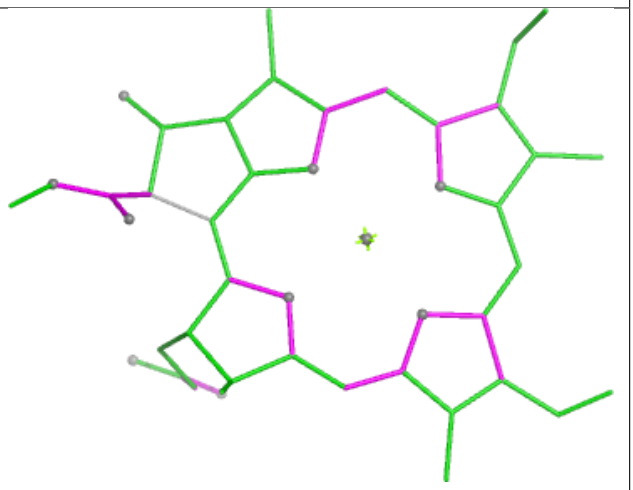


Rings

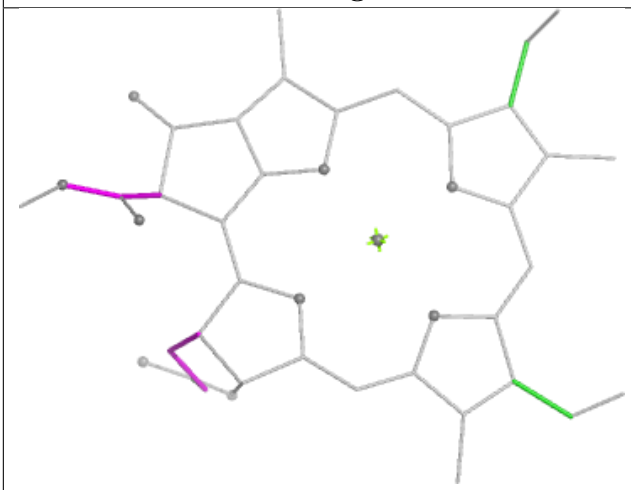
Ligand CLA 6 608



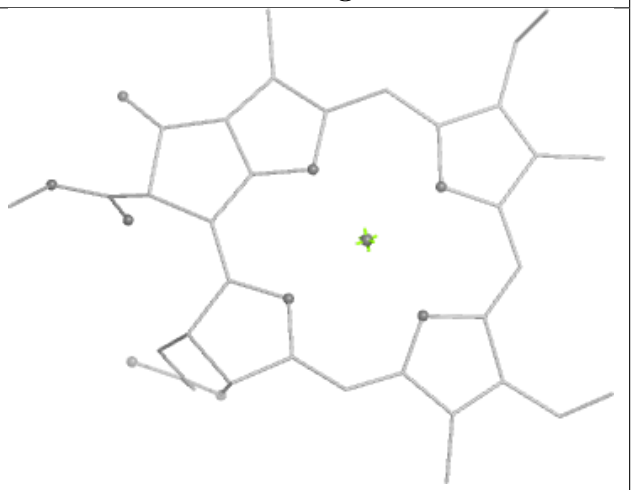
Bond lengths



Bond angles

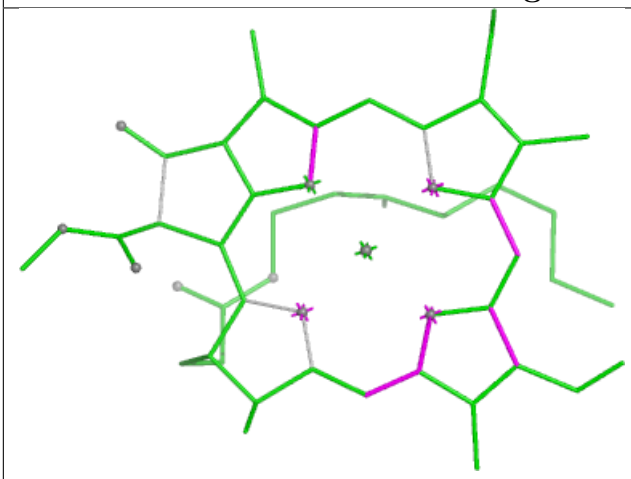


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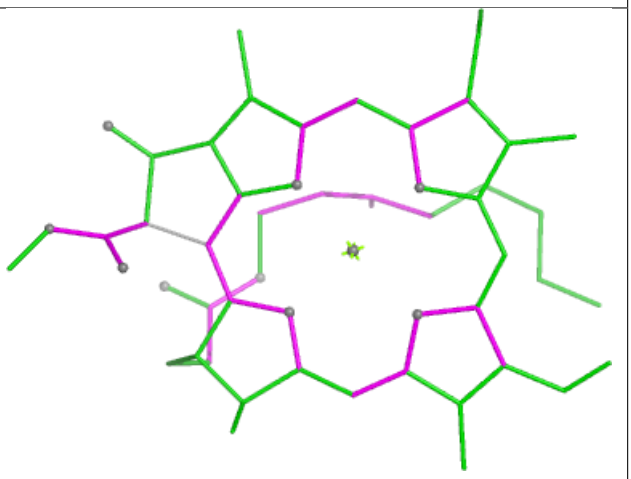


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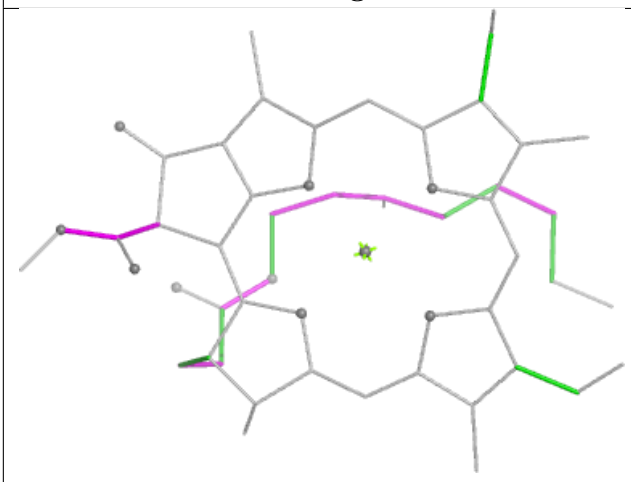
Ligand CLA A 812



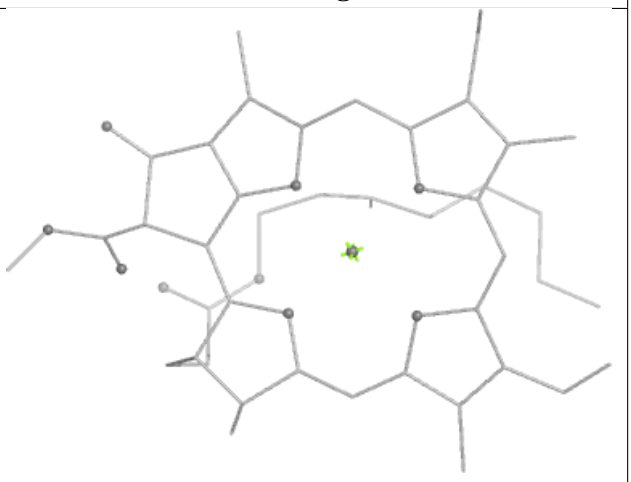
Bond lengths



Bond angles

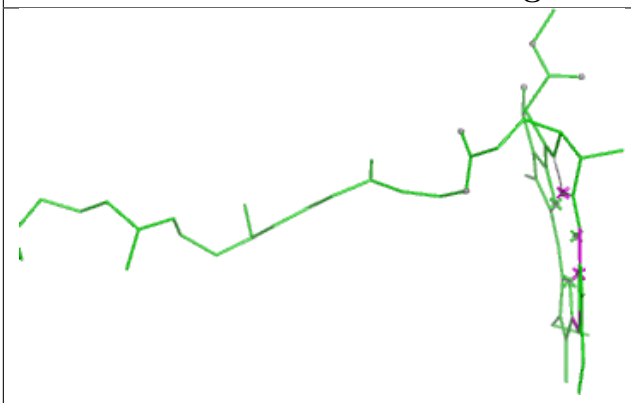


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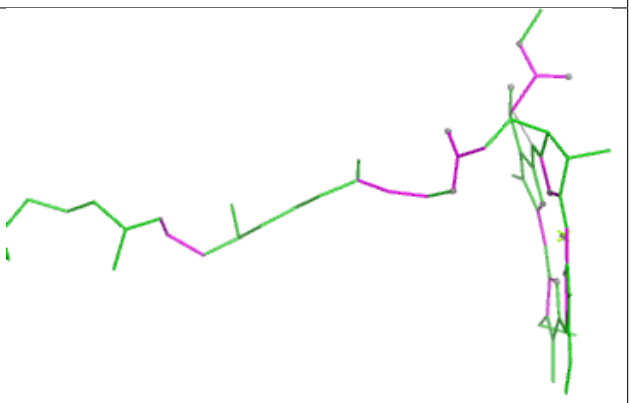


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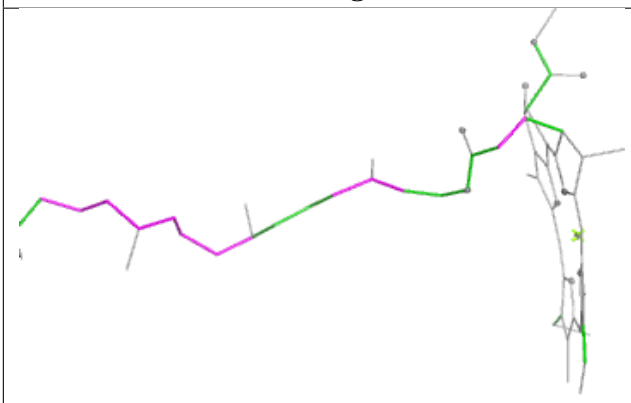
Ligand CLA A 828



Bond lengths



Bond angles

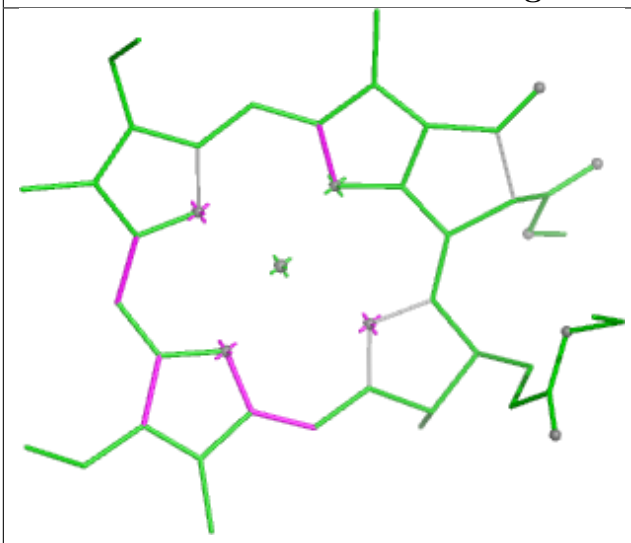


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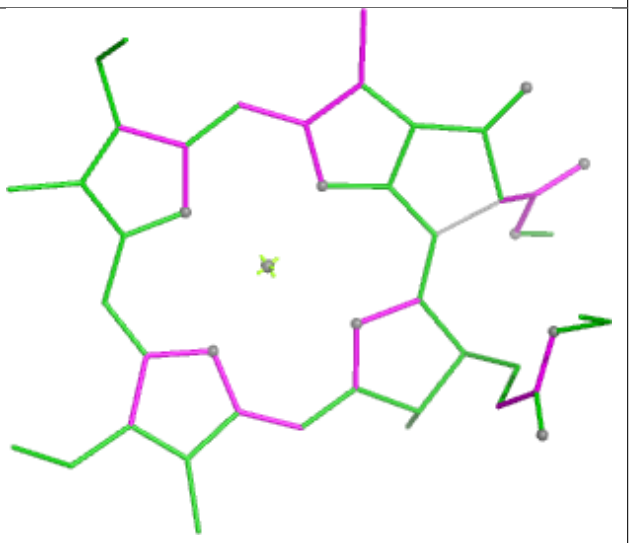


Rings

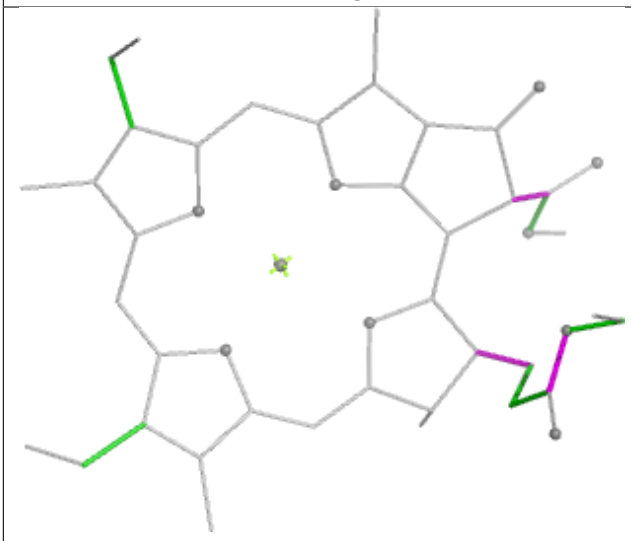
Ligand CLA B 837



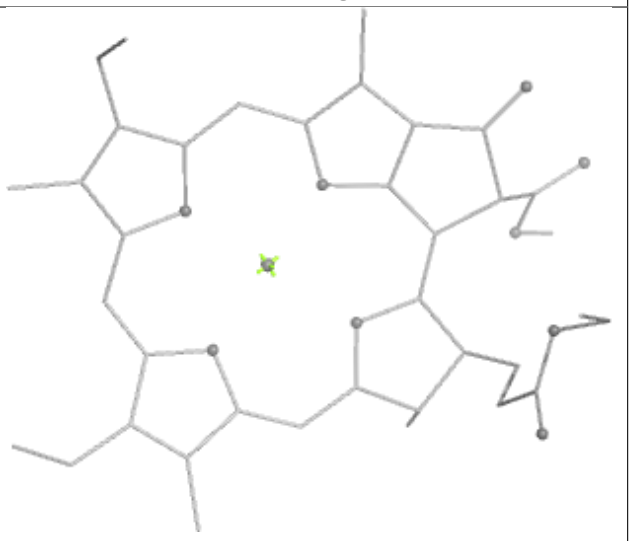
Bond lengths



Bond angles

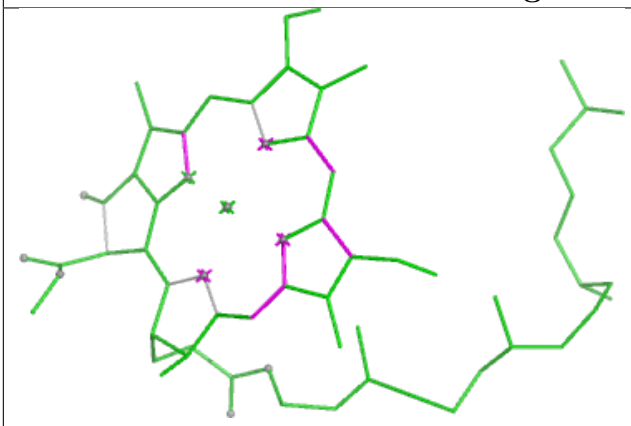


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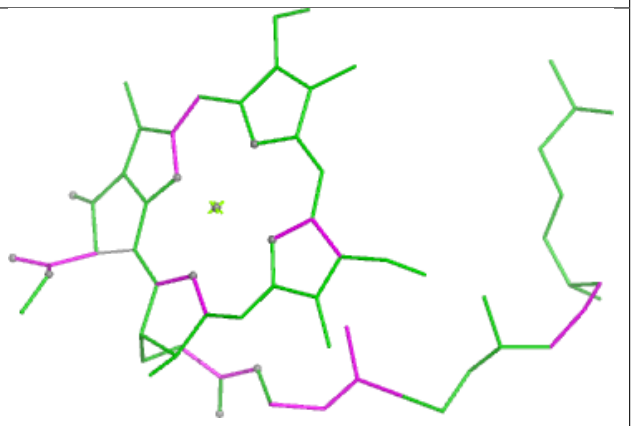


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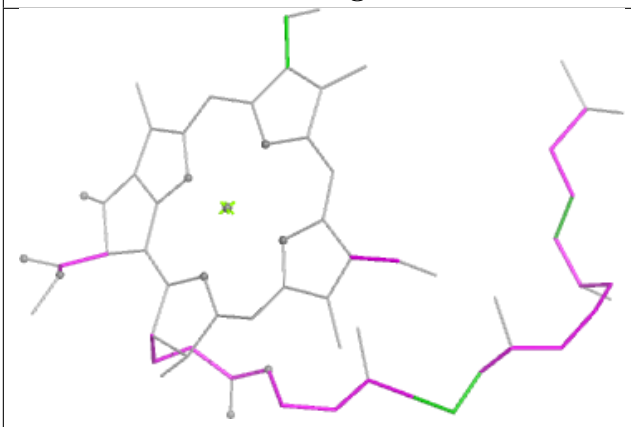
Ligand CLA Y 602



Bond lengths



Bond angles

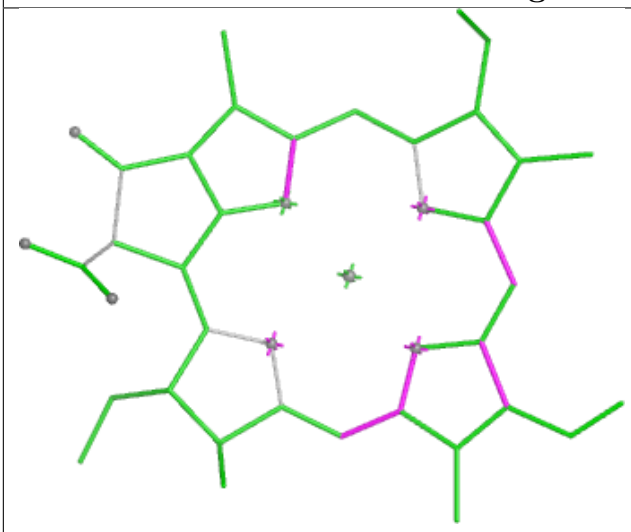


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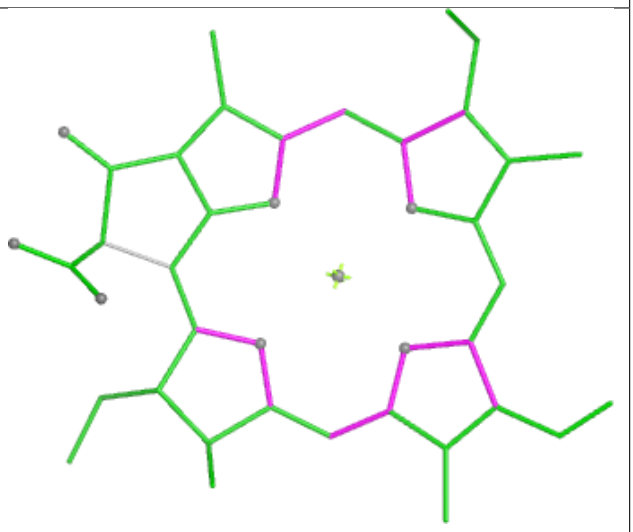


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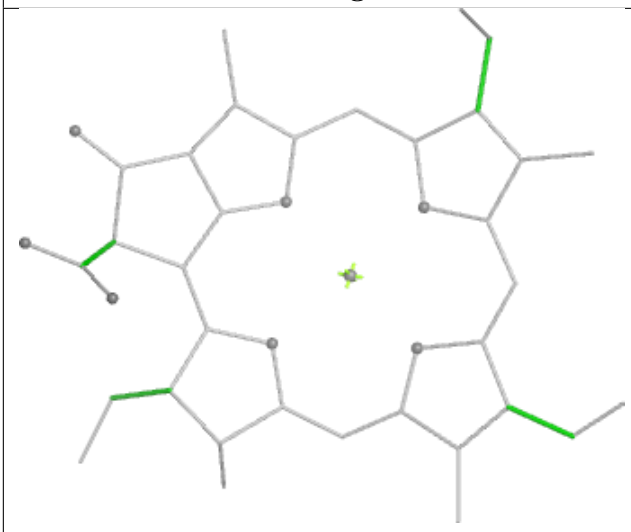
Ligand CLA 6 611



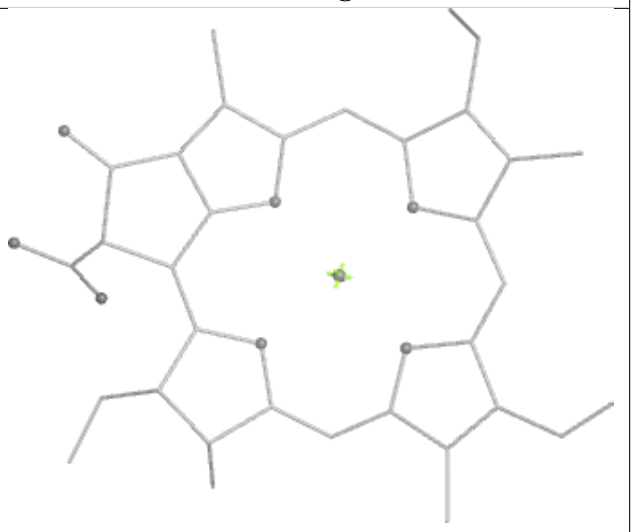
Bond lengths



Bond angles



Torsions

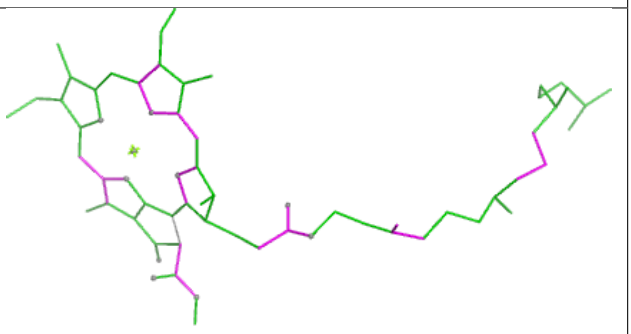


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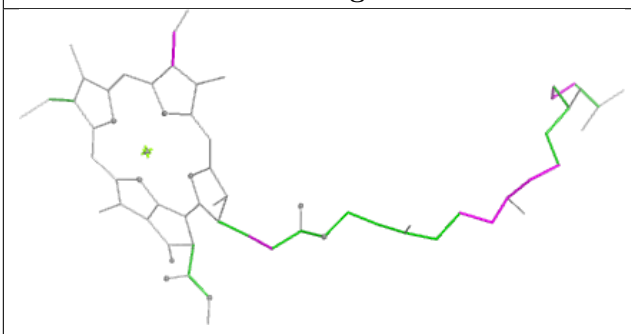
Ligand CLA A 842



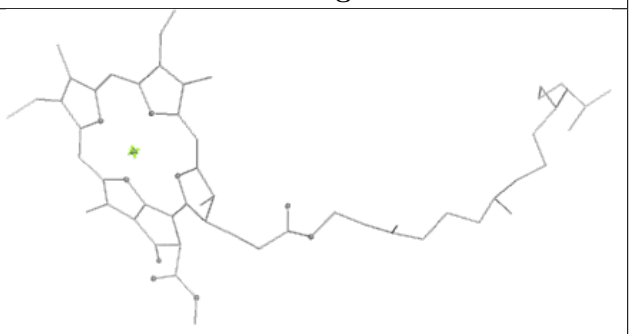
Bond lengths



Bond angles

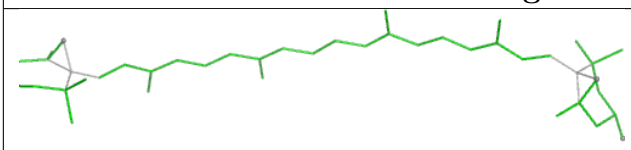


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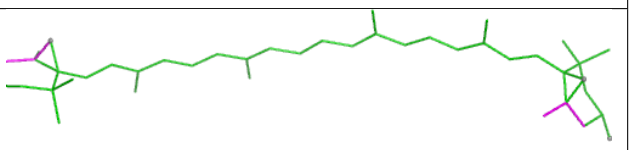


Rings

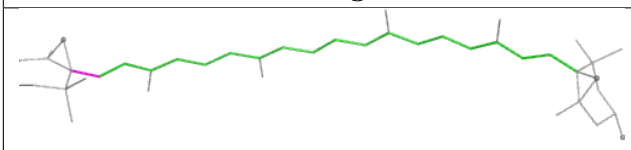
Ligand XAT O 208



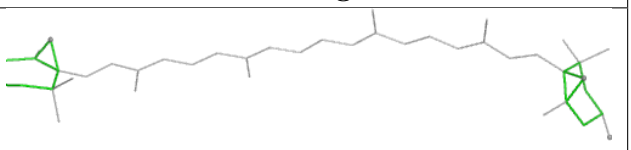
Bond lengths



Bond angles

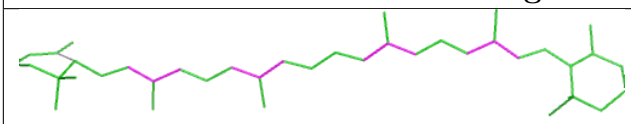


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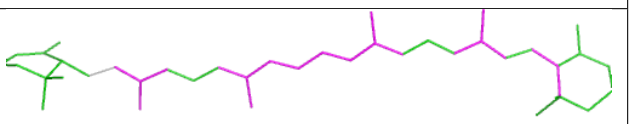


Rings

Ligand LUT Y 616



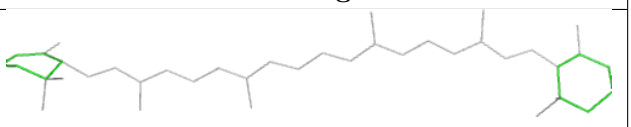
Bond lengths



Bond angles

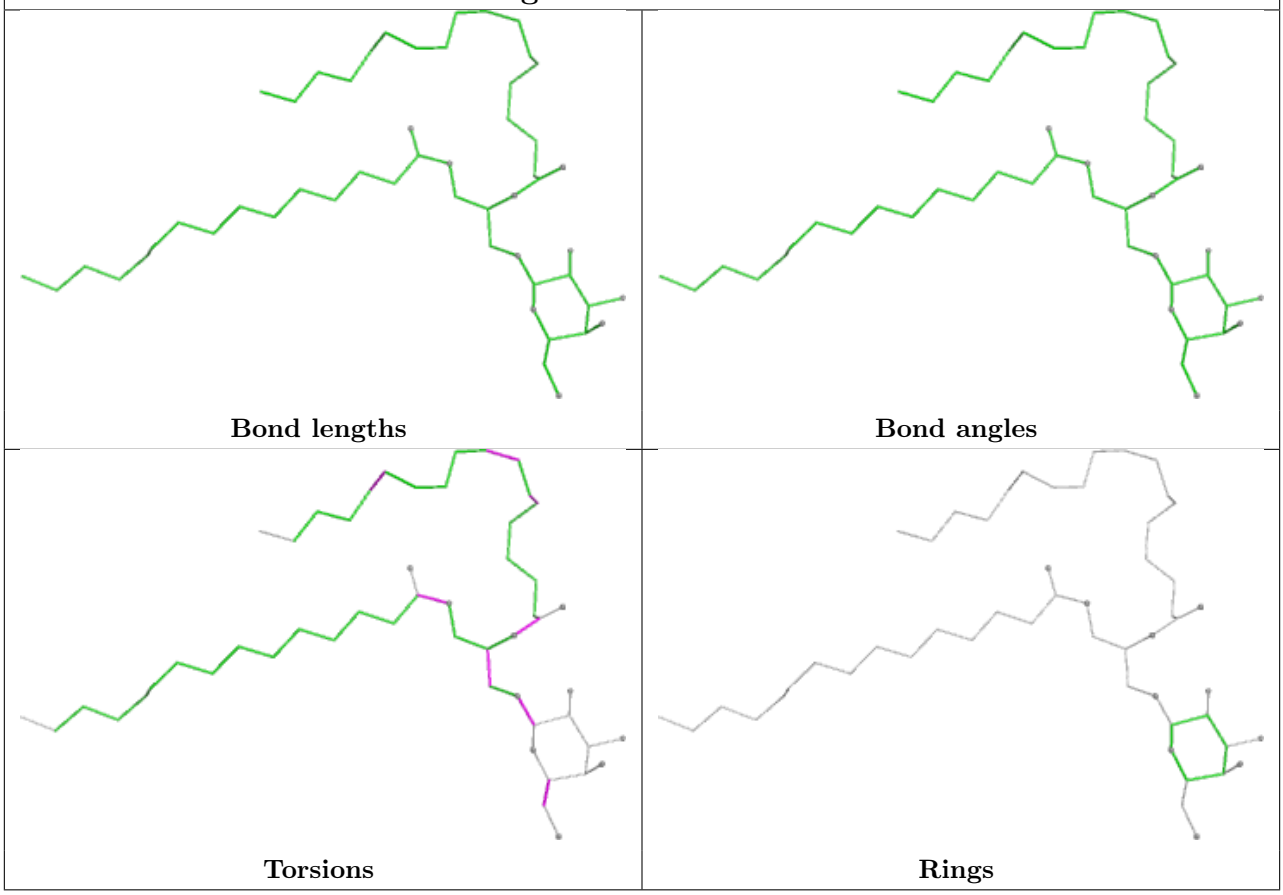


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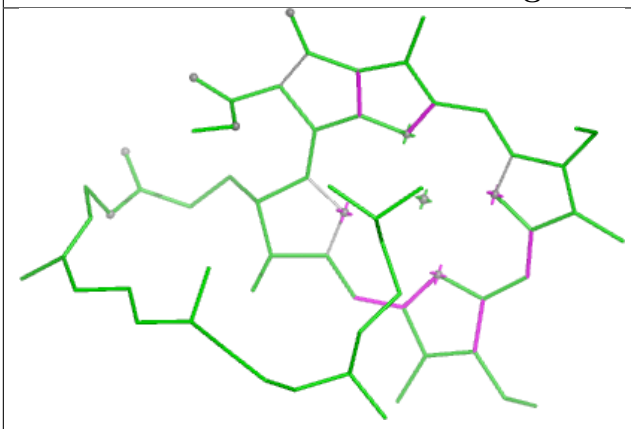


Rings

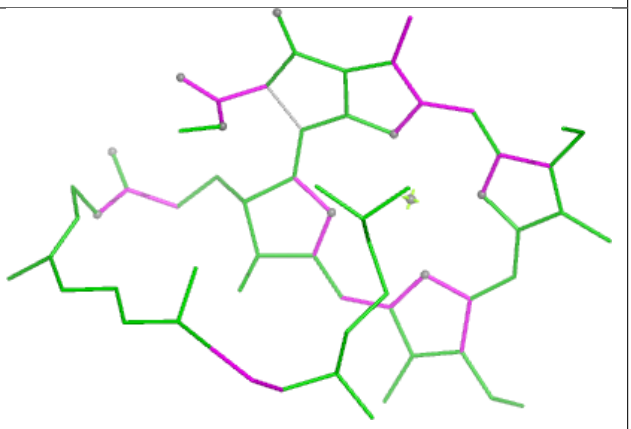
Ligand LMG B 850



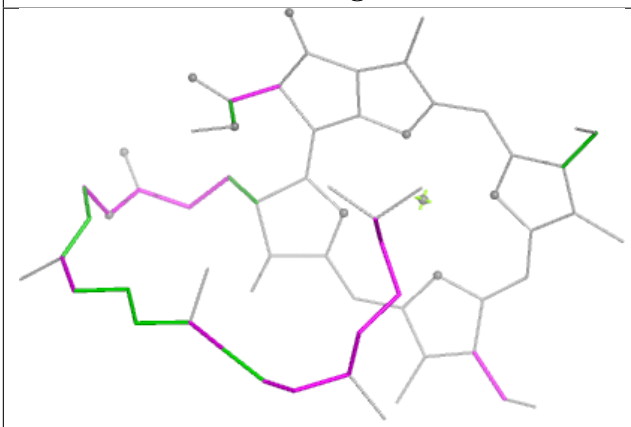
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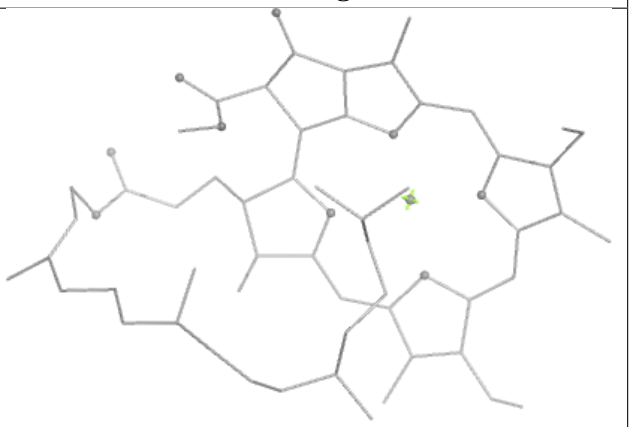
Bond lengths



Bond angles

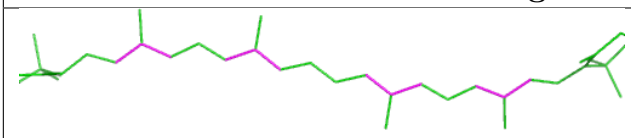


Torsions



Rings

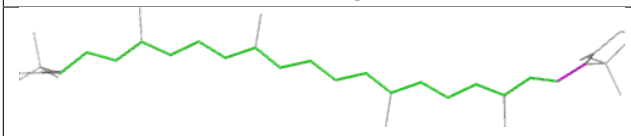
Ligand LUT 2 615



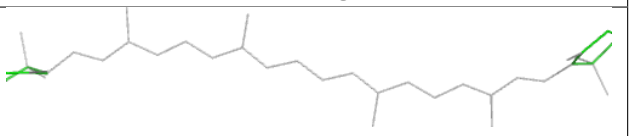
Bond lengths



Bond angles

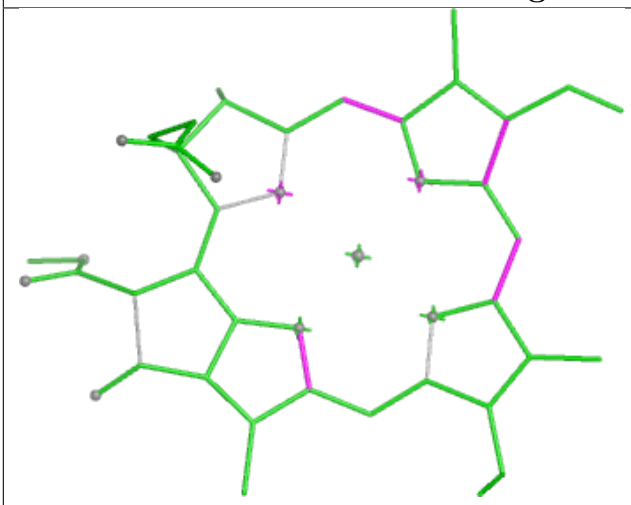


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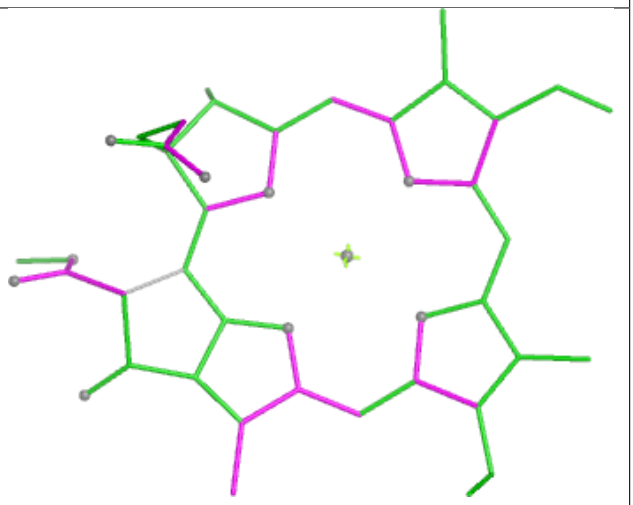


Rings

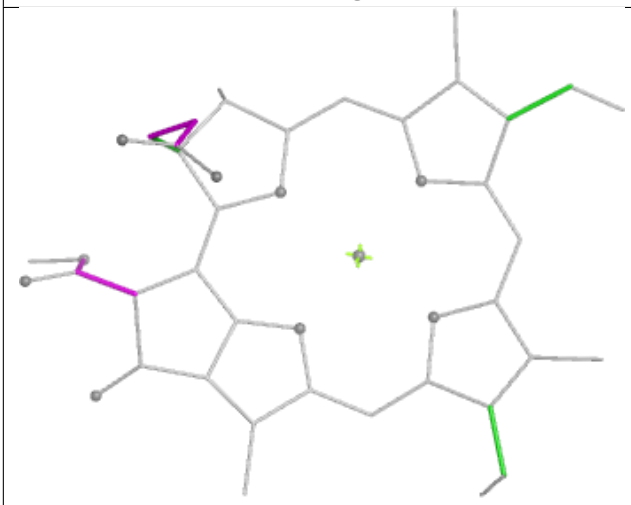
Ligand CLA 1 613



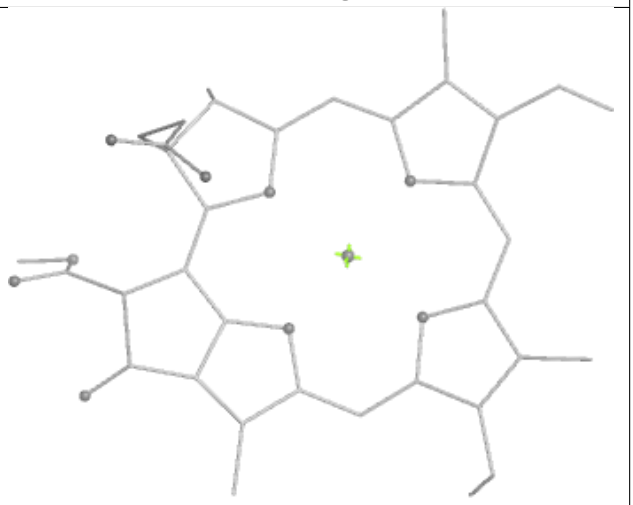
Bond lengths



Bond angles

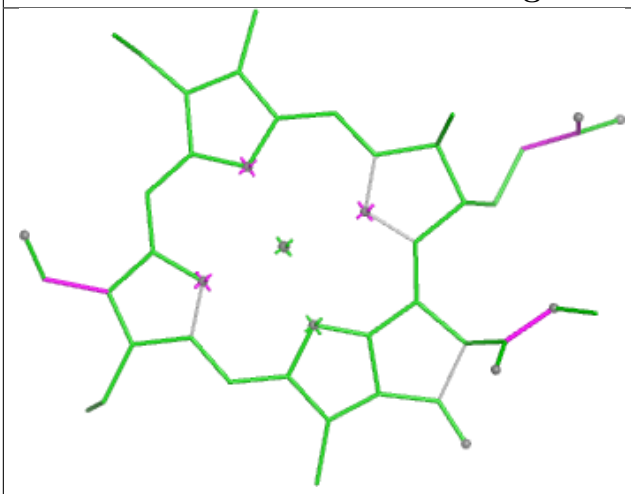


Torsions

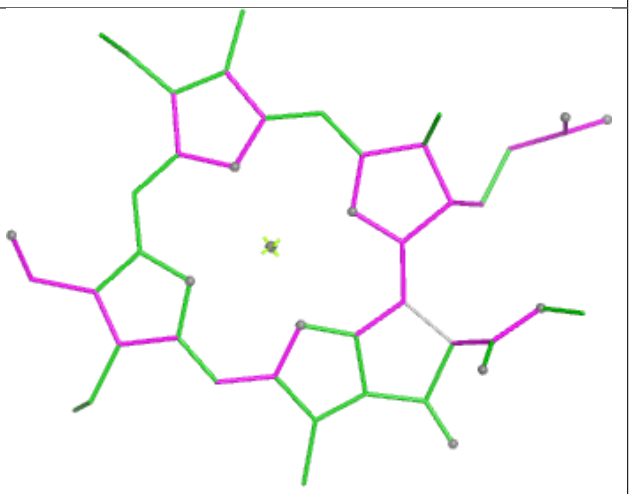


Rings

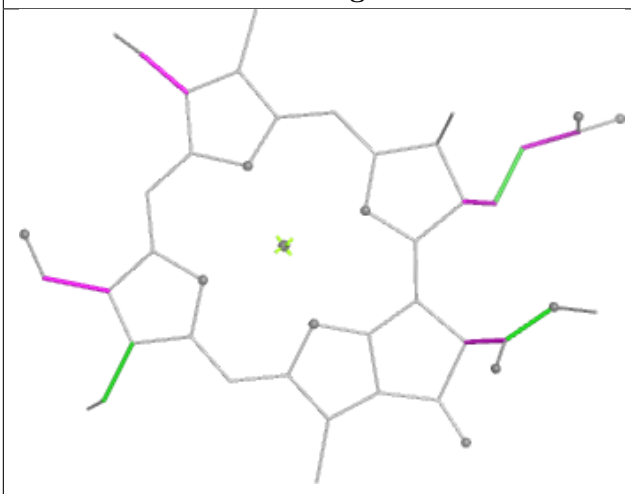
Ligand CHL Y 601



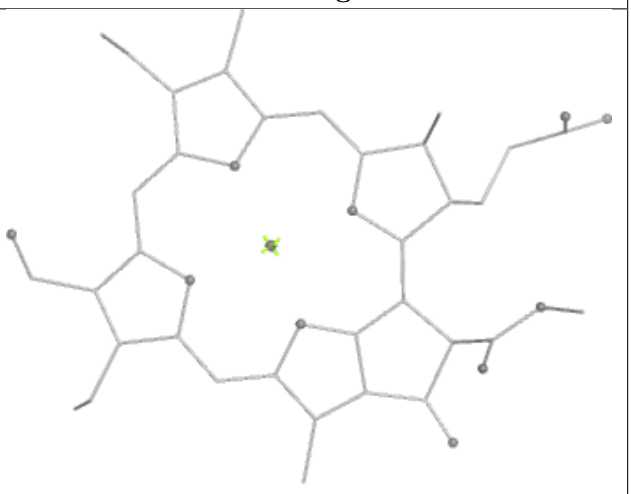
Bond lengths



Bond angles

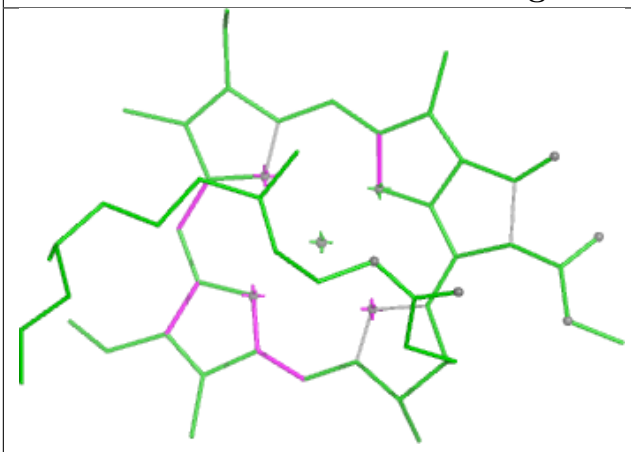


Torsions

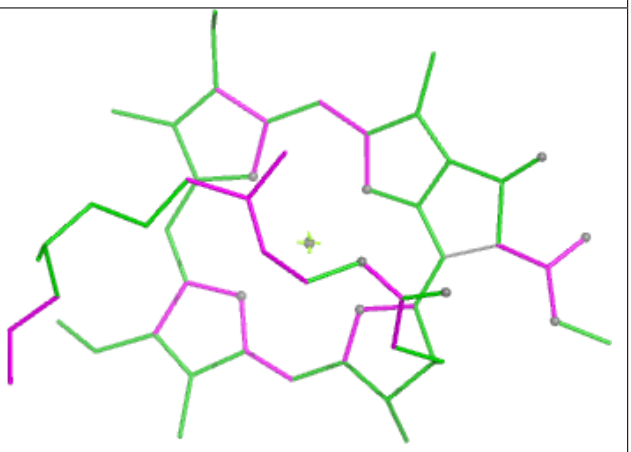


Rings

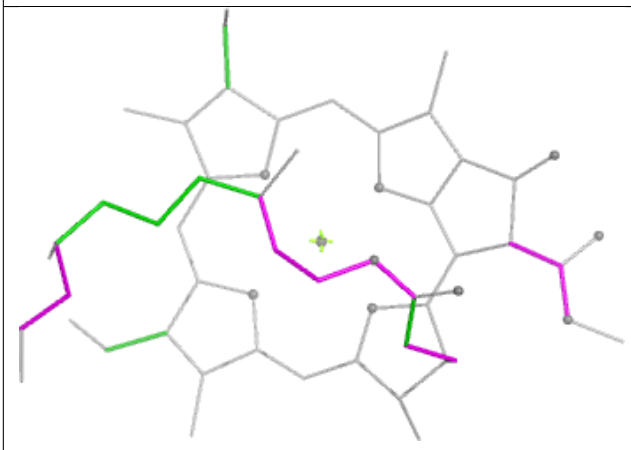
Ligand CLA 6 612



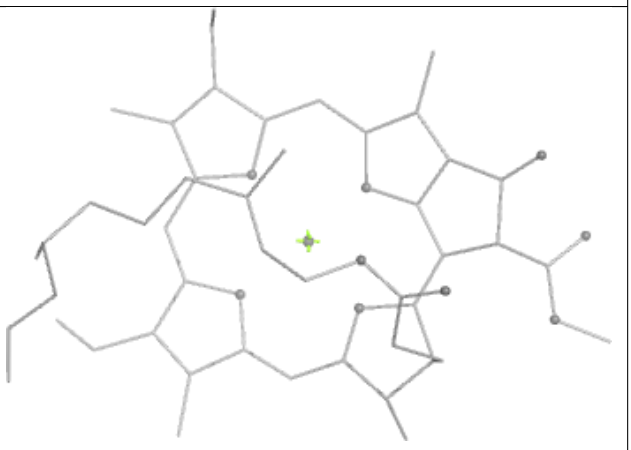
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

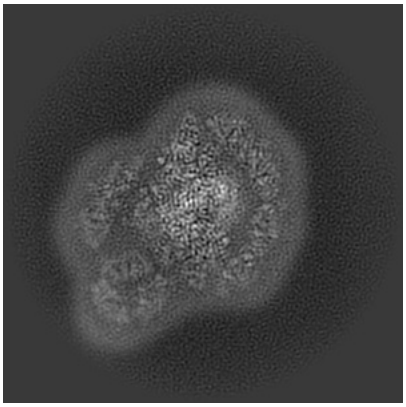
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54456. These allow visual inspection of the internal detail of the map and identification of artifacts.

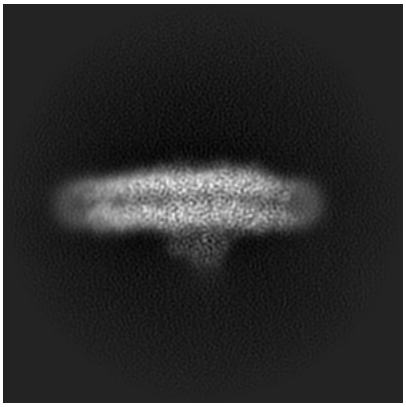
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

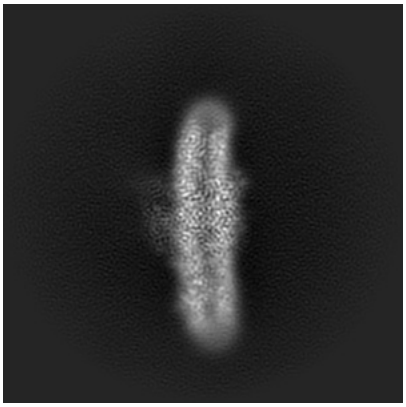
6.1.1 Primary map



X



Y

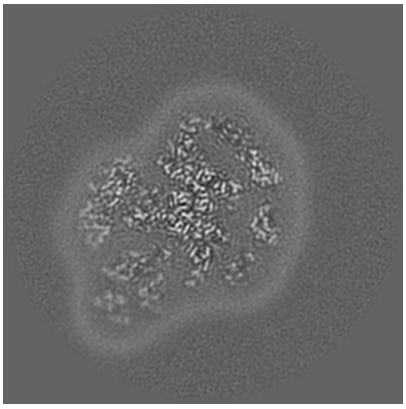


Z

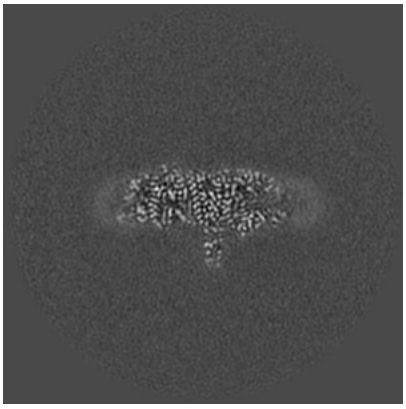
The images above show the map projected in three orthogonal directions.

6.2 Central slices

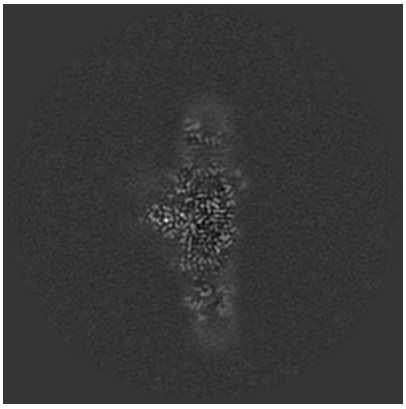
6.2.1 Primary map



X Index: 200



Y Index: 200

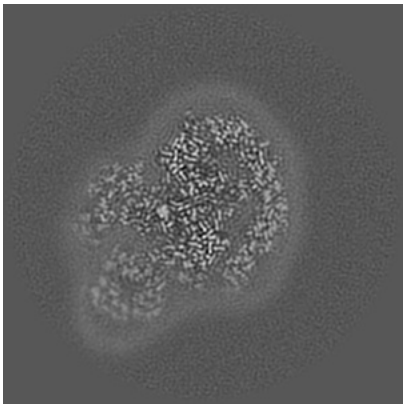


Z Index: 200

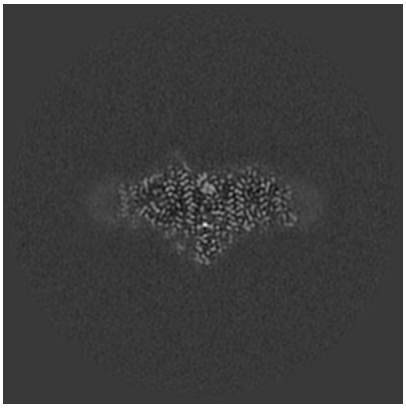
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

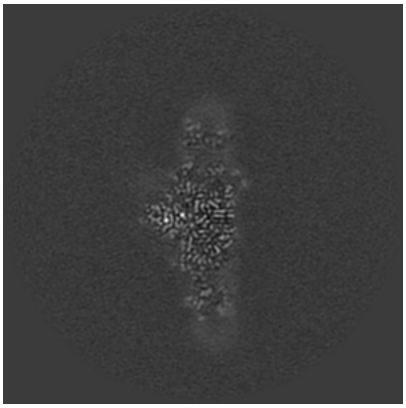
6.3.1 Primary map



X Index: 191



Y Index: 188

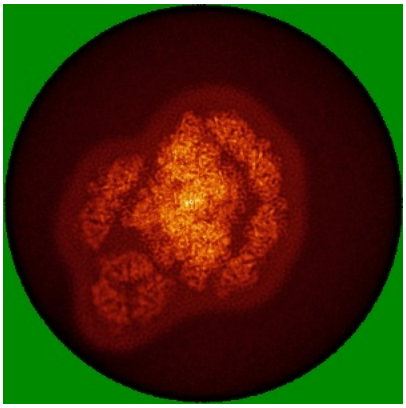


Z Index: 201

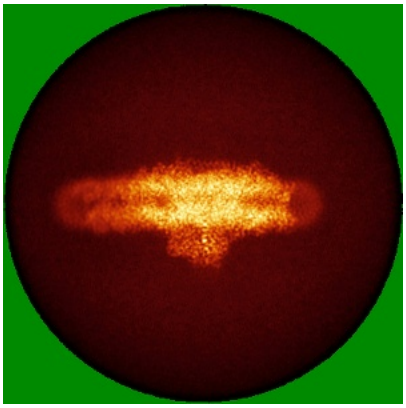
The images above show the largest variance slices of the map in three orthogonal directions.

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

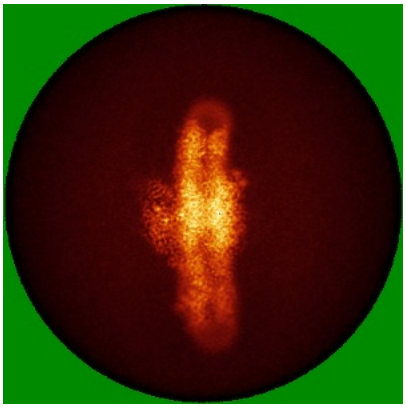
6.4.1 Primary map



X



Y

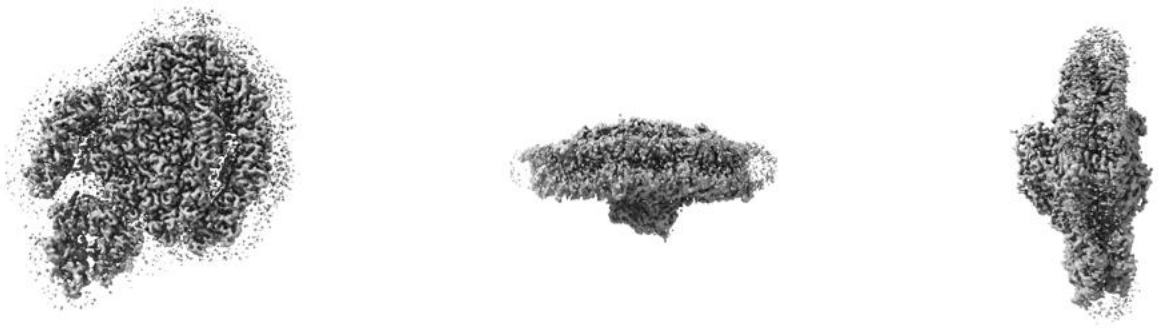


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

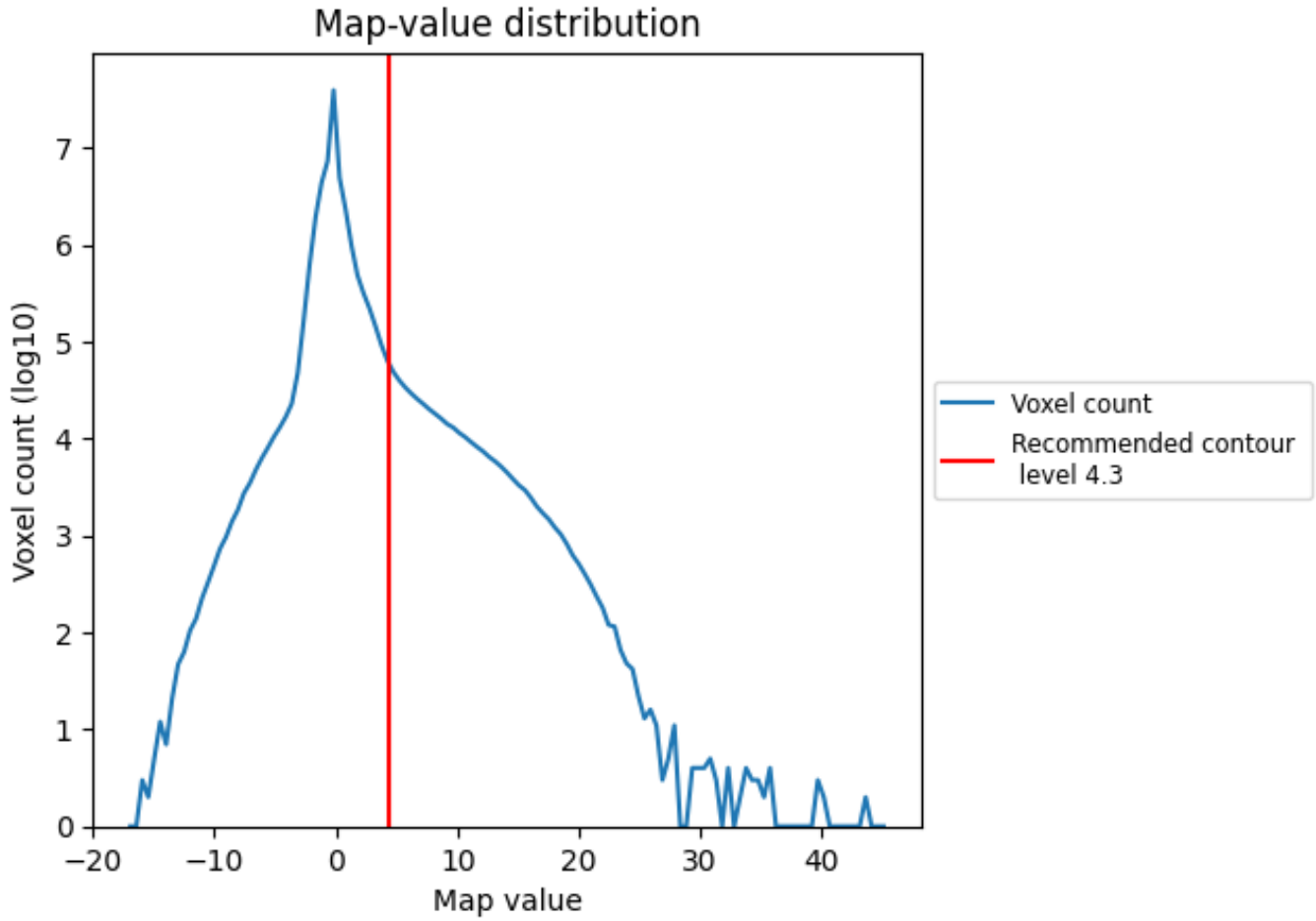
6.6 Mask visualisation (i)

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

7 Map analysis

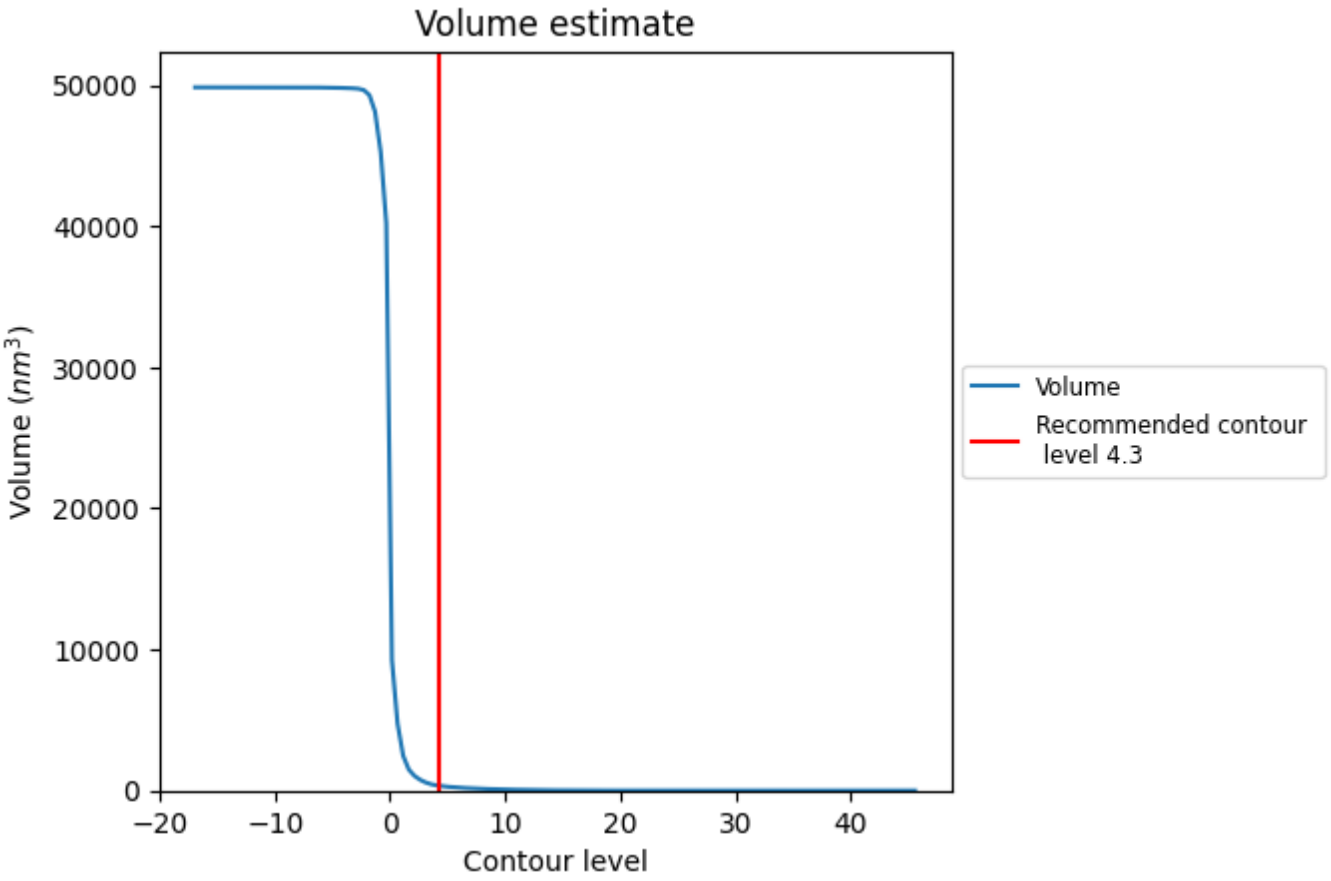
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

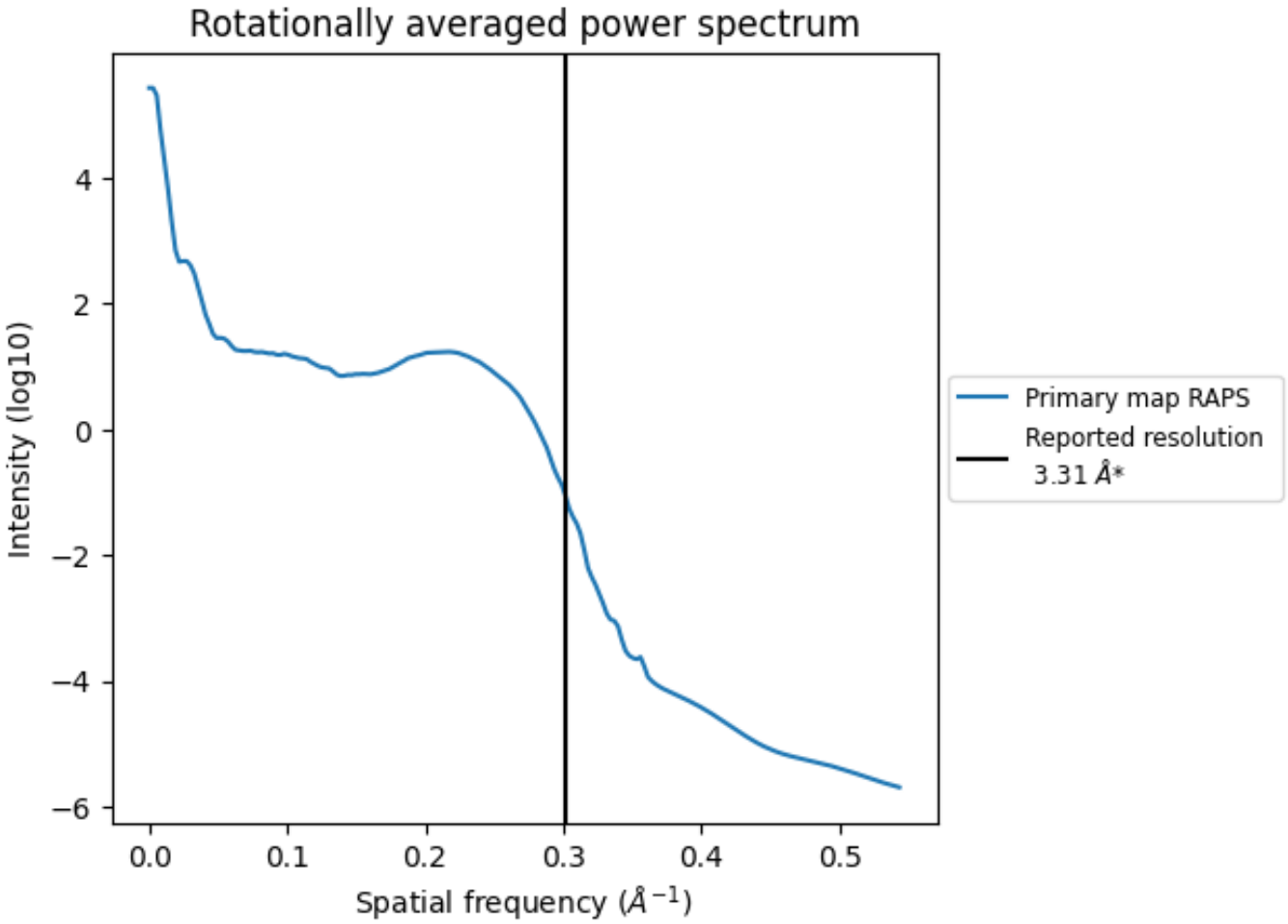
7.2 Volume estimate (i)



The volume at the recommended contour level is 337 nm^3; this corresponds to an approximate mass of 304 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 0.302 Å^{-1}

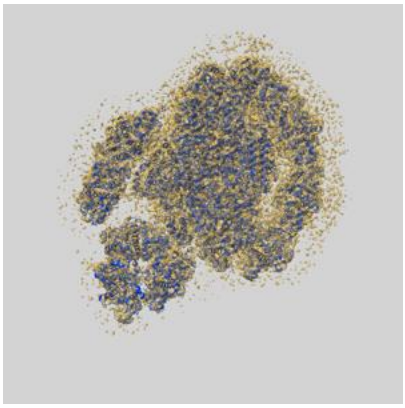
8 Fourier-Shell correlation

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

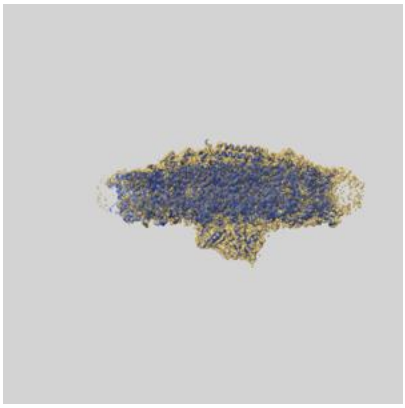
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54456 and PDB model 9S1M. Per-residue inclusion information can be found in section 3 on page 29.

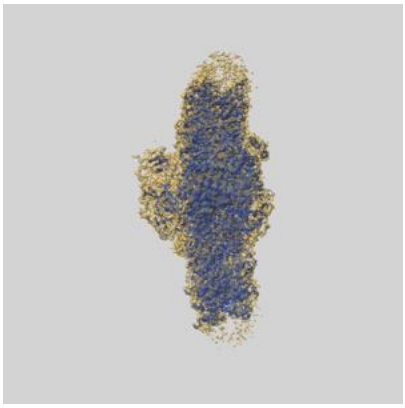
9.1 Map-model overlay



X



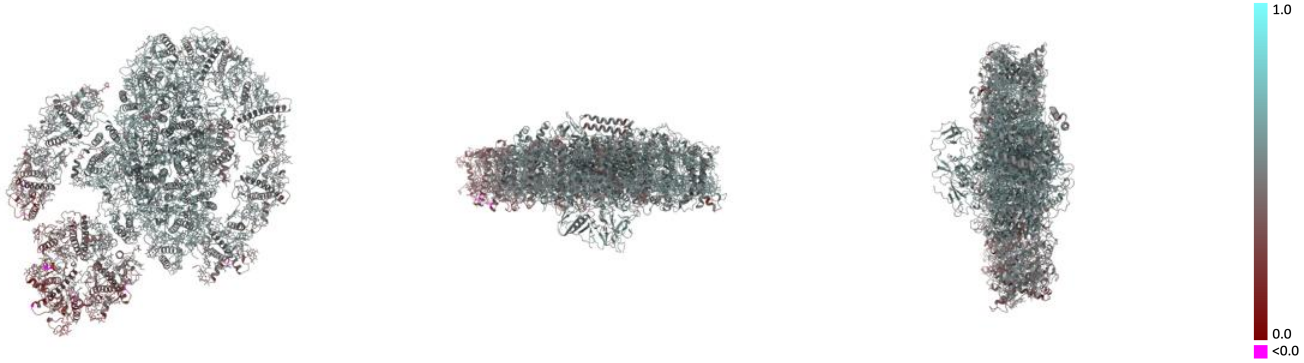
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

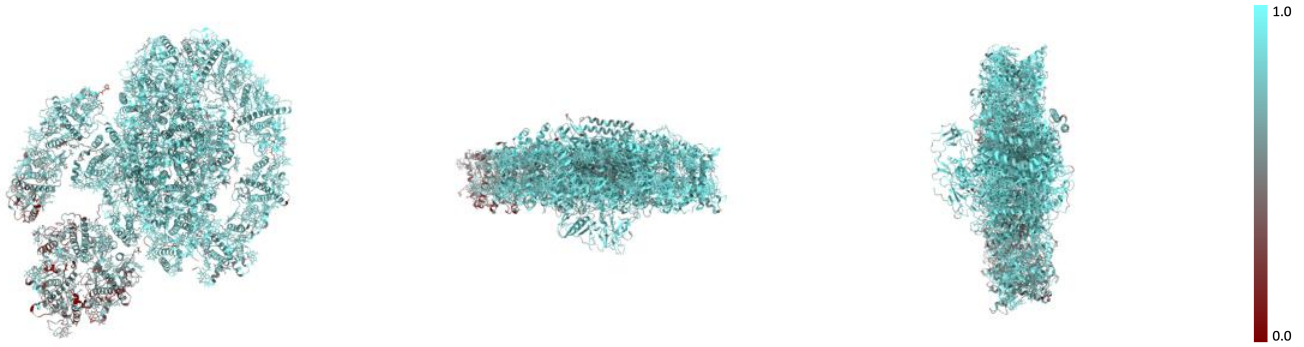
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

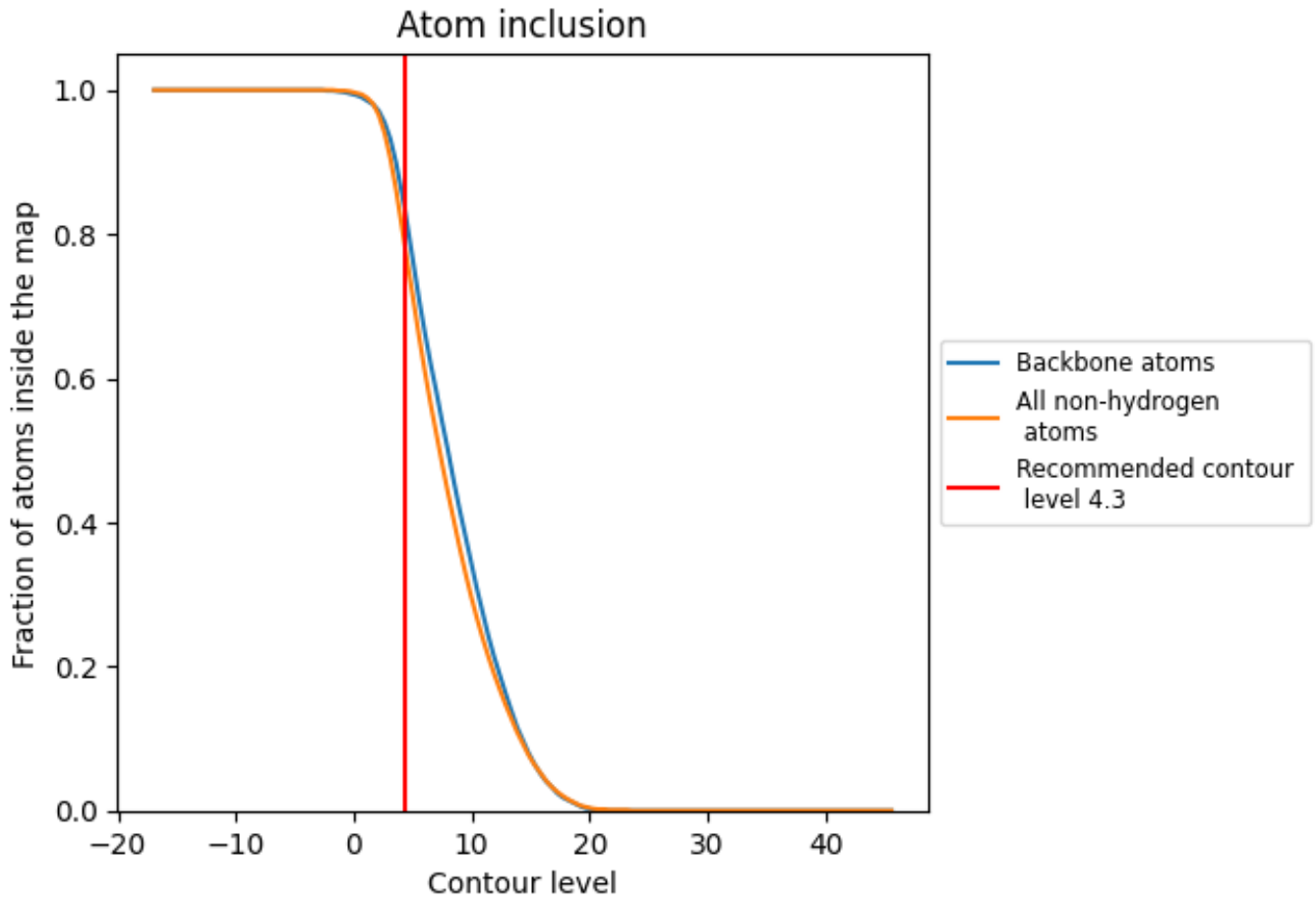
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.3).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7880	0.4930
1	0.8350	0.5180
2	0.8140	0.4840
3	0.7400	0.4600
4	0.8620	0.5100
5	0.6240	0.4050
6	0.7770	0.4890
A	0.8810	0.5520
B	0.8990	0.5550
C	0.9140	0.5450
D	0.8550	0.5360
E	0.8210	0.5350
F	0.7850	0.5050
G	0.8270	0.5140
H	0.7990	0.5020
I	0.8710	0.5380
J	0.7060	0.4890
K	0.7150	0.4700
L	0.8570	0.5360
O	0.8010	0.5230
X	0.5110	0.2930
Y	0.6080	0.4050
Z	0.5120	0.3490

