wwPDB EM Validation Summary Report

Sep 9, 2026 – 10:51 pm BST

PDB ID	:	7BGI / pdb_00007bgi
EMDB ID	:	EMD-12180
Title	:	Photosystem I of a temperature sensitive mutant Chlamydomonas reinhardtii
Authors	:	Caspy, I.; Nelson, N.
Deposited on	:	2021-01-07
Resolution	:	2.54 Å(reported)
Based on initial model	:	6JO5

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

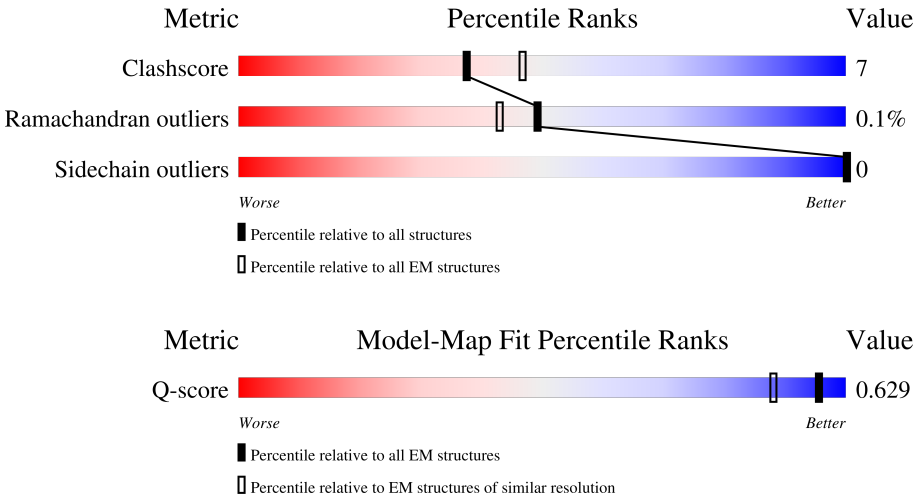
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.54 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	7403 (2.04 - 3.04)

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

Mol	Chain	Length	Quality of chain
1	A	741	87% 13%
2	B	733	86% 14%
3	C	80	95% 5%
4	D	144	90% 10%

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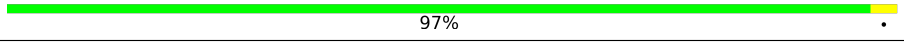
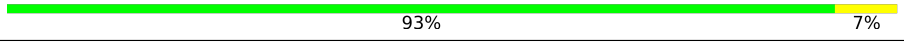
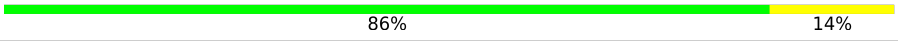
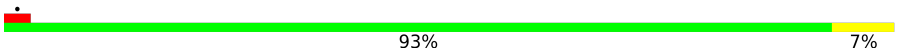
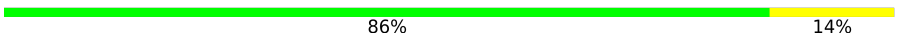
Mol	Chain	Length	Quality of chain
5	E	63	
6	F	165	
7	G	91	
8	I	37	
9	J	39	
10	K	84	
11	L	138	
12	1	194	
12	Z	194	
13	3	219	
14	7	213	
15	8	217	
16	4	210	
17	5	227	
18	6	229	
19	2	198	
20	9	183	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	RRX	F	4001	X	-	-	-
37	C7Z	1	503	X	-	-	-
37	C7Z	5	505	X	-	-	-
37	C7Z	J	4002	X	-	-	-
39	LUT	2	501	X	-	-	-
39	LUT	2	503	X	-	-	-
40	CHL	1	609	X	-	-	-
40	CHL	2	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CHL	3	611	X	-	-	-
40	CHL	4	610	X	-	-	-
40	CHL	4	613	X	-	-	-
40	CHL	5	610	X	-	-	-
40	CHL	6	610	X	-	-	-
40	CHL	6	613	X	-	-	-
40	CHL	8	610	X	-	-	-
40	CHL	8	613	X	-	-	-
40	CHL	9	610	X	-	-	-
40	CHL	Z	609	X	-	-	-
40	CHL	Z	610	X	-	-	-
42	QTB	Z	504	X	-	-	-

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 52213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5820	3805	993	1000	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5825	3825	977	1005	18	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	144	1135	725	201	202	7	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	63	497	316	87	94	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	74	Total	C	N	O	0	0
			550	354	94	102		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			282	195	39	47	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			321	219	45	56	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			571	362	98	109	2		

- Molecule 11 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	126	Total	C	N	O	S	0	0
			914	595	148	168	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
12	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	219	Total	C	N	O	S	0	0
			1674	1092	270	304	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	213	Total	C	N	O	S	0	0
			1650	1072	274	298	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1650	1073	280	293	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	210	Total	C	N	O	S	0	0
			1628	1068	262	293	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	227	Total	C	N	O	S	0	0
			1775	1154	297	316	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1766	1164	292	304	6		

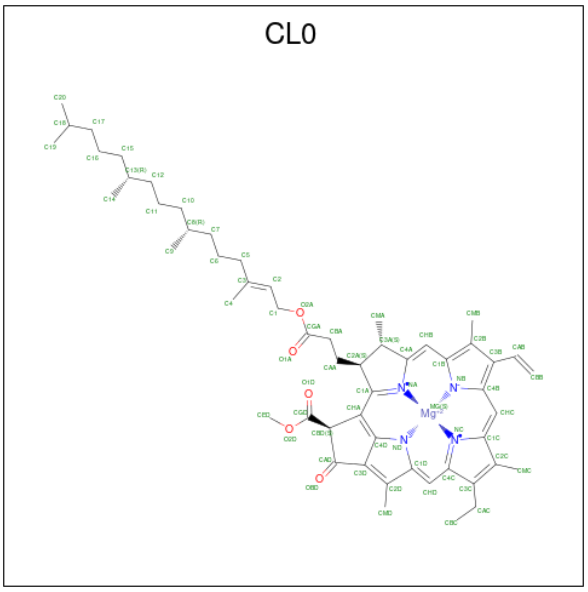
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	2	198	Total	C	N	O	S	0	0
			1518	983	249	276	10		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

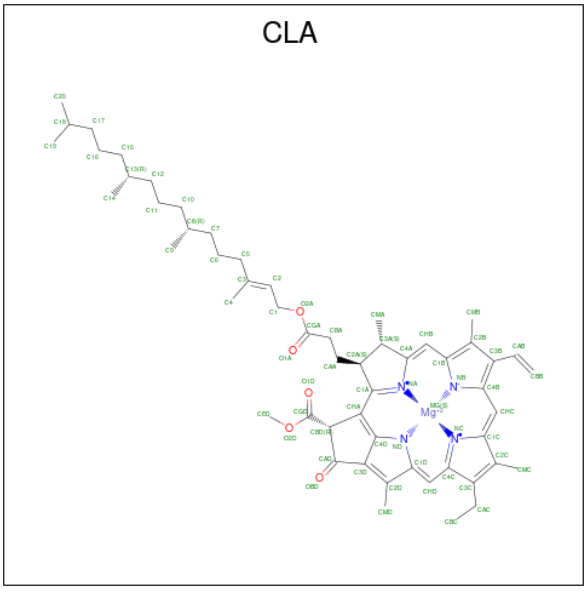
Mol	Chain	Residues	Atoms					AltConf	Trace
20	9	183	Total	C	N	O	S	0	0
			1406	910	235	254	7		

- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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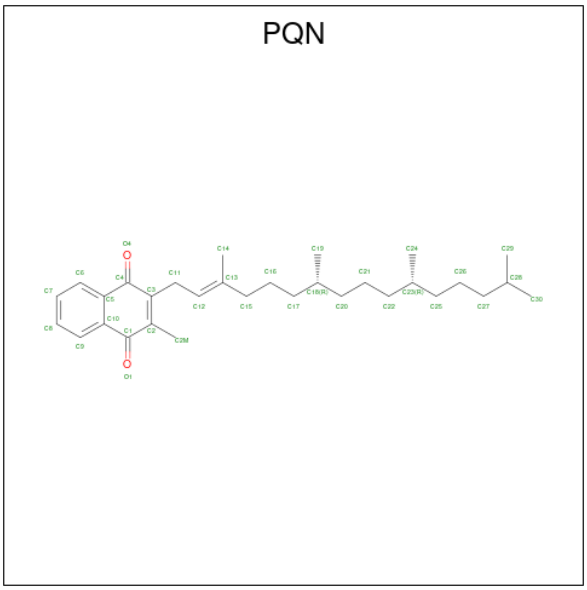
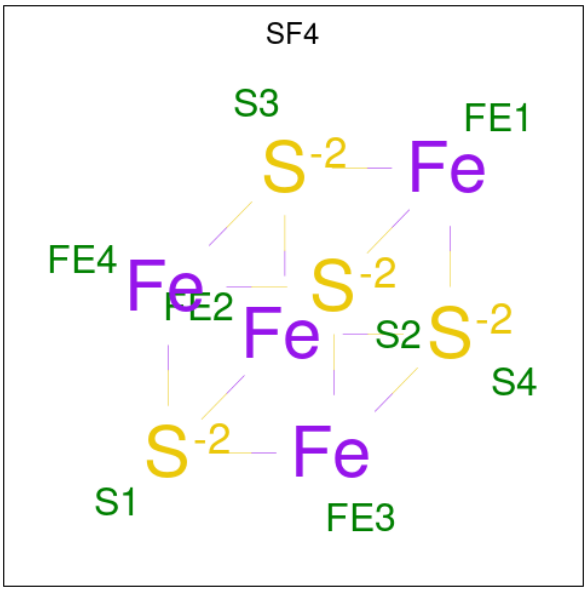
Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



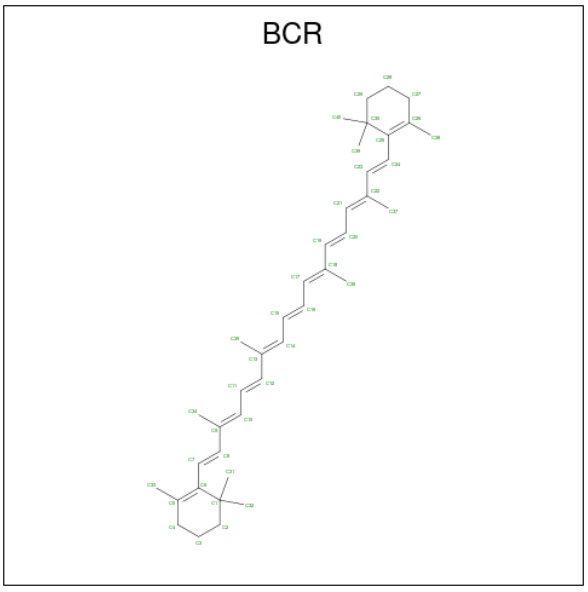
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	31	2	
23	B	1	Total	C	O	0
			33	31	2	

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0

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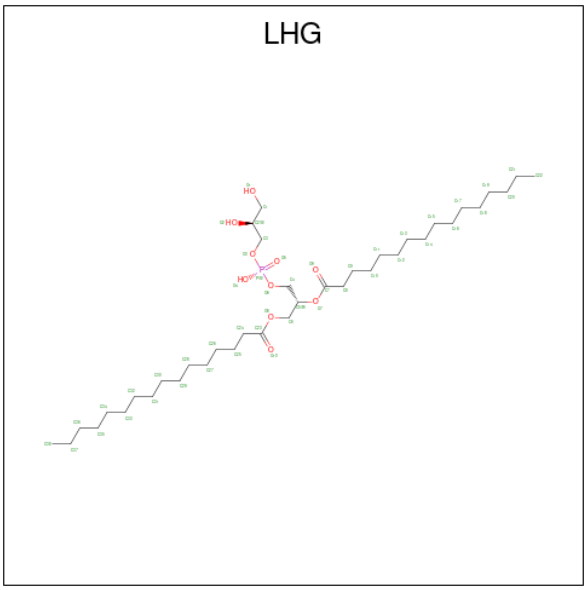
Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	6	1	Total C 40 40	0

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



Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C O P 35 24 10 1	0
26	A	1	Total C O P 49 38 10 1	0

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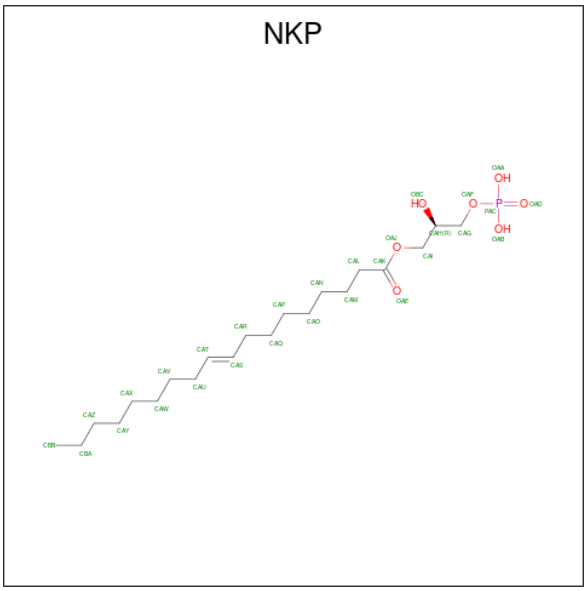
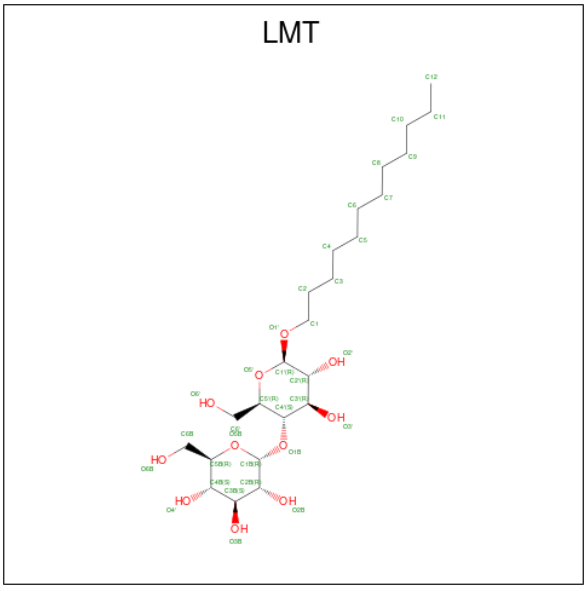
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	P	0
			23	12	10	1	
26	B	1	Total	C	O	P	0
			20	9	10	1	
26	B	1	Total	C	O	P	0
			33	22	10	1	
26	1	1	Total	C	O	P	0
			43	32	10	1	
26	Z	1	Total	C	O	P	0
			43	32	10	1	
26	3	1	Total	C	O	P	0
			20	9	10	1	
26	7	1	Total	C	O	P	0
			37	26	10	1	
26	8	1	Total	C	O	P	0
			38	27	10	1	
26	4	1	Total	C	O	P	0
			49	38	10	1	
26	4	1	Total	C	O	P	0
			32	21	10	1	
26	5	1	Total	C	O	P	0
			37	26	10	1	
26	6	1	Total	C	O	P	0
			49	38	10	1	
26	2	1	Total	C	O	P	0
			34	23	10	1	
26	9	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 27 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: $C_{21}H_{41}O_7P$).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			29	21	7	1	
27	3	1	Total	C	O	P	0
			16	8	7	1	
27	8	1	Total	C	O	P	0
			29	21	7	1	

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	

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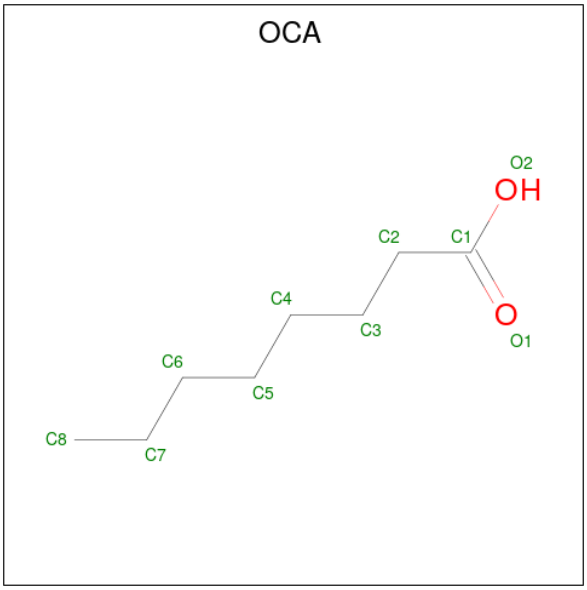
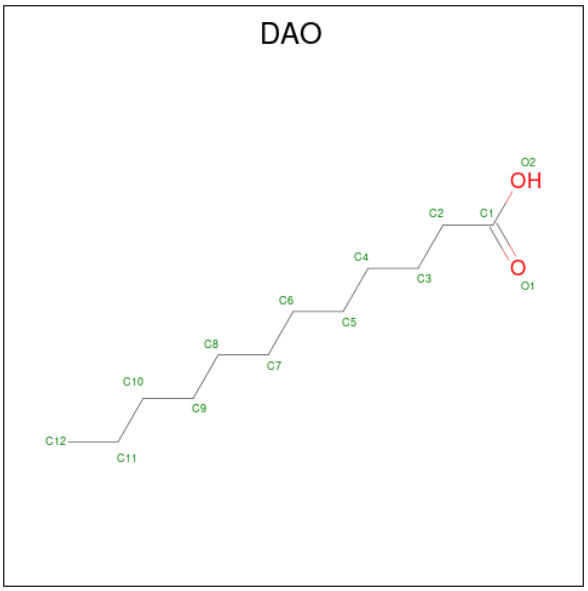
Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C O 35 24 11	0
28	B	1	Total C O 35 24 11	0
28	F	1	Total C O 35 24 11	0
28	1	1	Total C O 35 24 11	0
28	8	1	Total C O 35 24 11	0
28	4	1	Total C O 35 24 11	0
28	9	1	Total C O 35 24 11	0

- Molecule 29 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $C_8H_{16}O_2$).



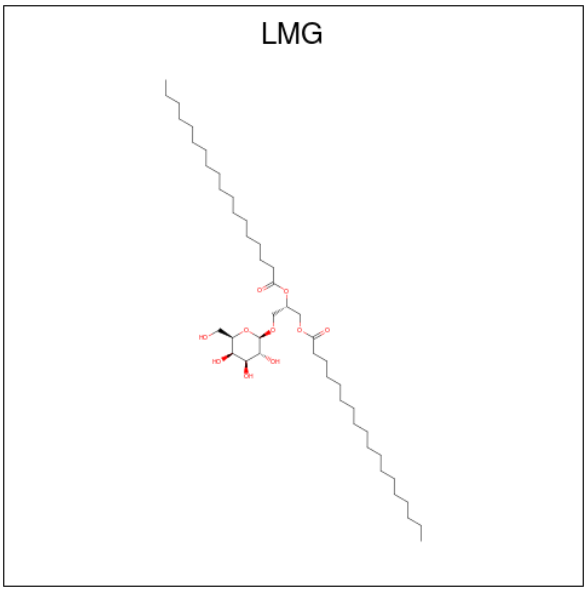
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C O 10 8 2	0

- Molecule 30 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



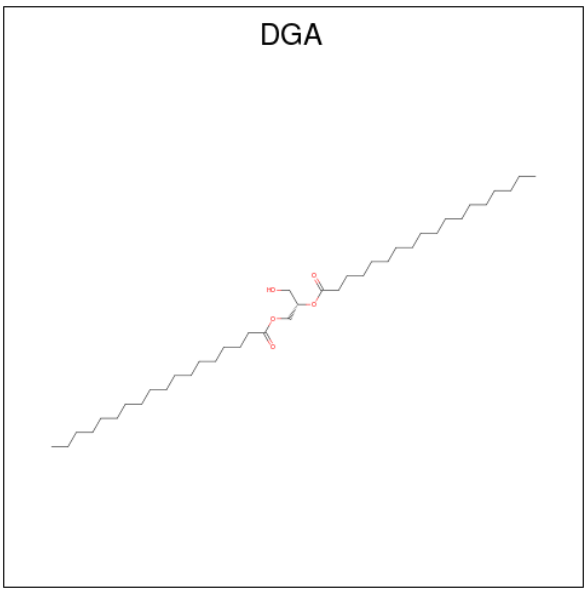
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			14	12	2	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



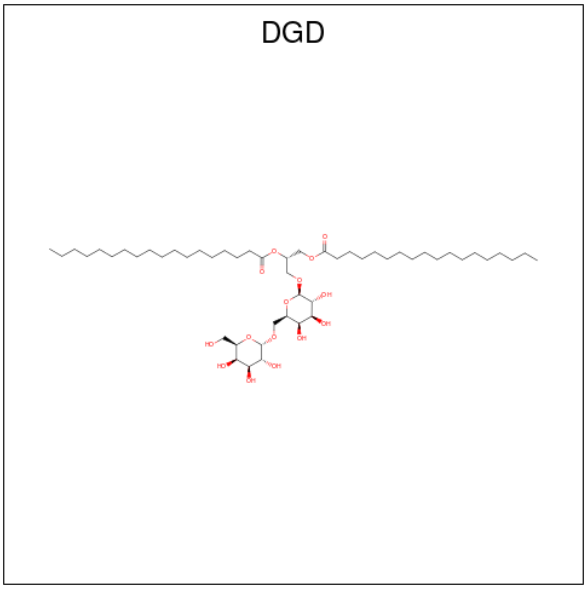
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			29	19	10	
31	J	1	Total	C	O	0
			35	25	10	

- Molecule 32 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C O 44 39 5	0
32	9	1	Total C O 39 34 5	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

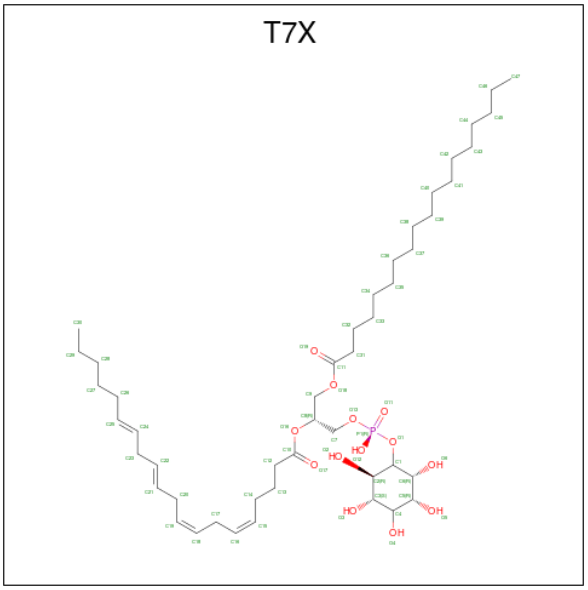


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	B	1	66	51	15	0

- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

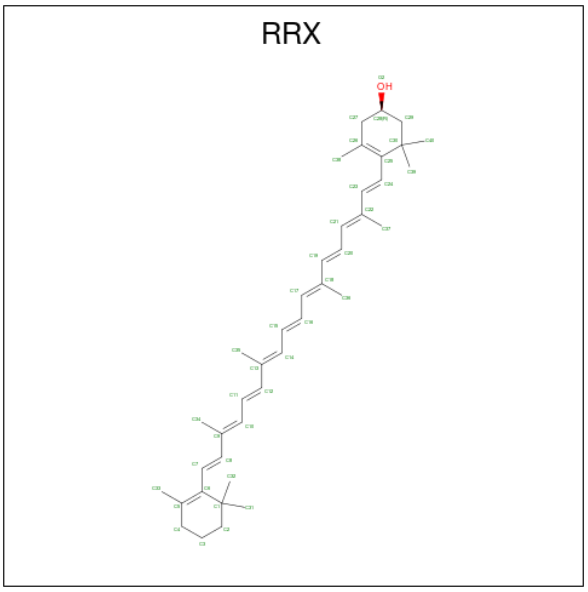
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
34	B	1	1	1	0

- Molecule 35 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



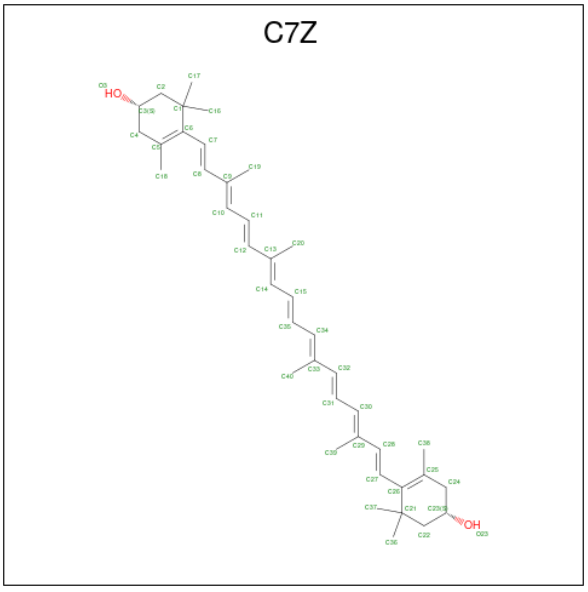
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
35	B	1	49	35	13	1	0

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	F	1	41	40	1	0

- Molecule 37 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E}, 15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



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

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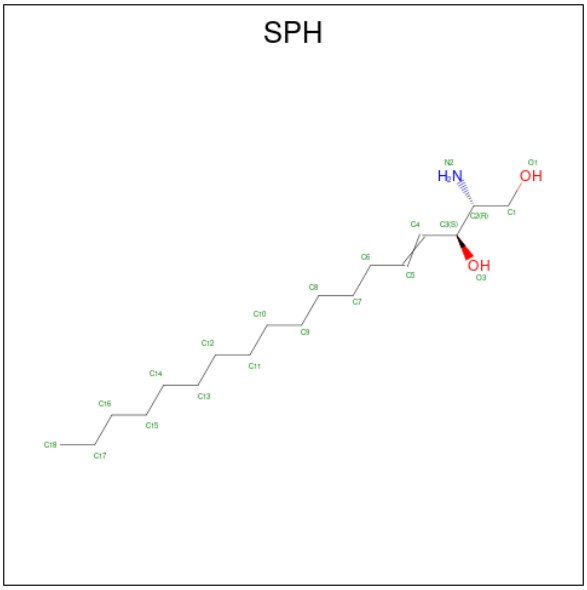
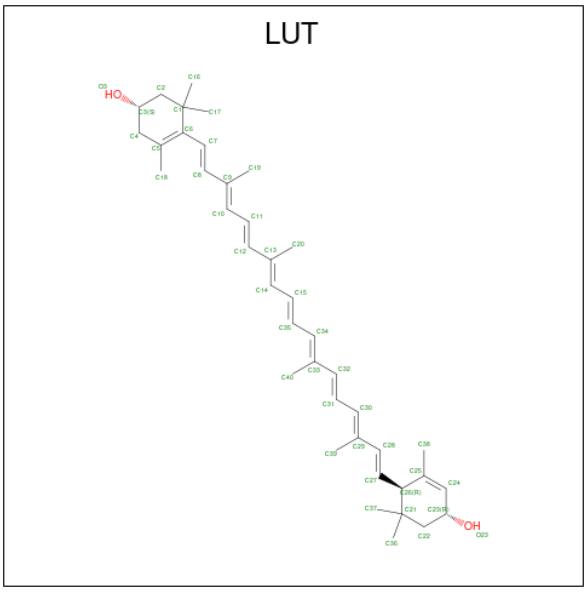
Mol	Chain	Residues	Atoms	AltConf
37	1	1	Total C O 42 40 2	0
37	5	1	Total C O 42 40 2	0

- Molecule 38 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms	AltConf
38	K	1	Total C N O 21 18 1 2	0
38	7	1	Total C N O 21 18 1 2	0
38	7	1	Total C N O 21 18 1 2	0

- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
39	1	1	Total C O 42 40 2	0
39	1	1	Total C O 42 40 2	0
39	Z	1	Total C O 42 40 2	0
39	Z	1	Total C O 42 40 2	0
39	Z	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	3	1	Total C O 42 40 2	0
39	7	1	Total C O 42 40 2	0
39	7	1	Total C O 42 40 2	0
39	8	1	Total C O 42 40 2	0
39	8	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	4	1	Total C O 42 40 2	0
39	5	1	Total C O 42 40 2	0

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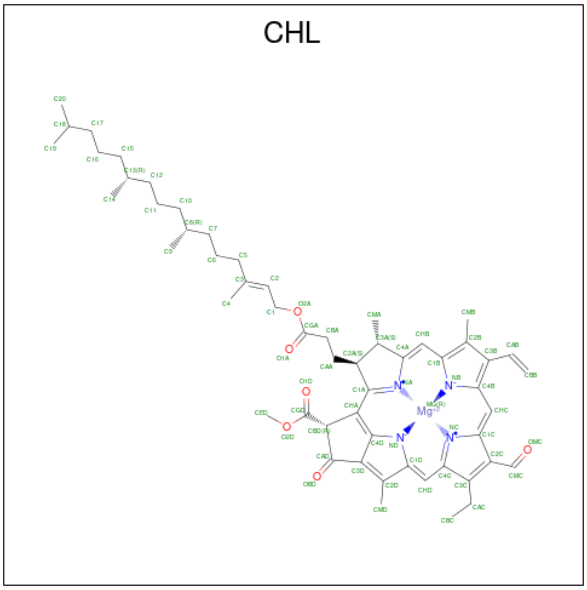
Mol	Chain	Residues	Atoms	AltConf
39	5	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0
39	6	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	2	1	Total C O 42 40 2	0
39	9	1	Total C O 42 40 2	0
39	9	1	Total C O 42 40 2	0

- Molecule 40 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms	AltConf
40	1	1	Total C Mg N O 48 37 1 4 6	0
40	1	1	Total C Mg N O 58 47 1 4 6	0
40	Z	1	Total C Mg N O 66 55 1 4 6	0

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Mol	Chain	Residues	Atoms					AltConf
40	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
40	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
40	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
40	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
40	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
40	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
40	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
40	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
40	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
40	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
40	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
40	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
40	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
40	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
40	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
40	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
40	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
40	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
40	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
40	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
40	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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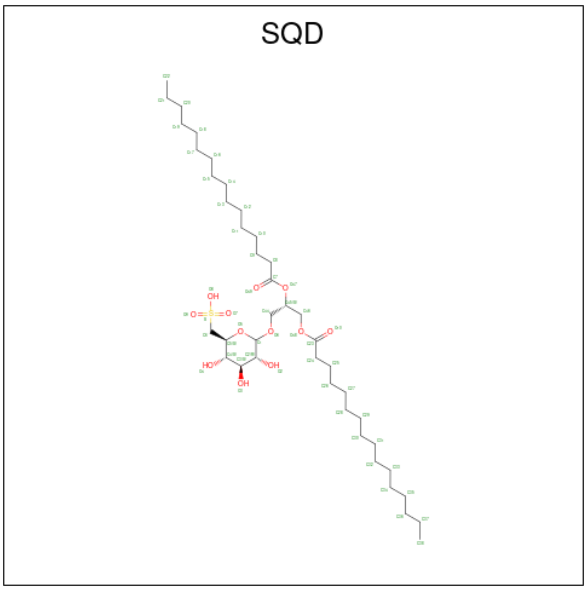
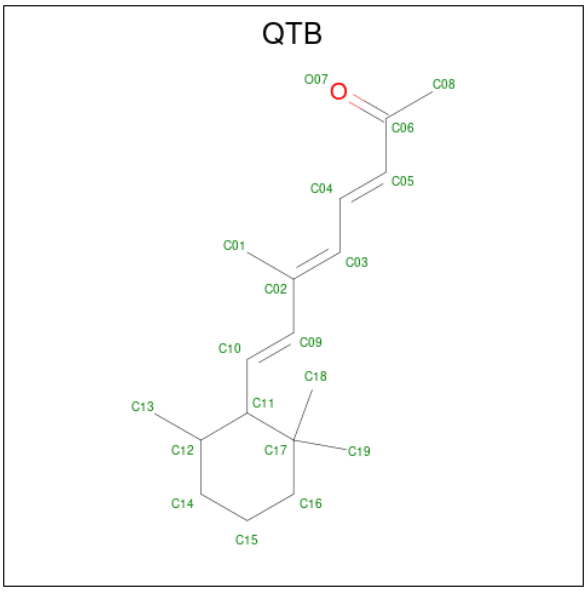
Mol	Chain	Residues	Atoms					AltConf
40	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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



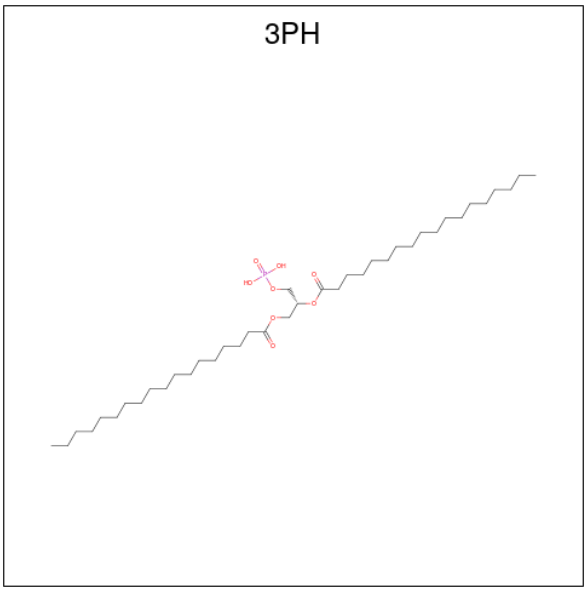
Mol	Chain	Residues	Atoms				AltConf
41	1	1	Total	C	O	S	0
			48	35	12	1	
41	2	1	Total	C	O	S	0
			43	30	12	1	

- Molecule 42 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: $C_{18}H_{28}O$).



Mol	Chain	Residues	Atoms	AltConf
42	Z	1	Total C O 19 18 1	0

- Molecule 43 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms	AltConf
43	7	1	Total C O P 39 30 8 1	0
43	8	1	Total C O P 30 21 8 1	0

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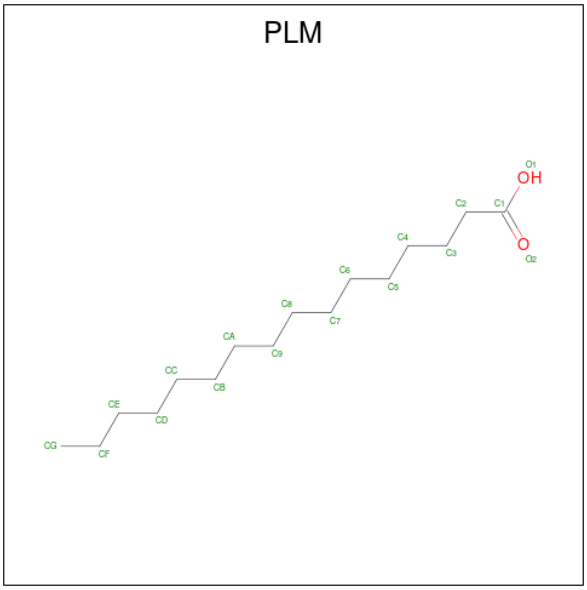
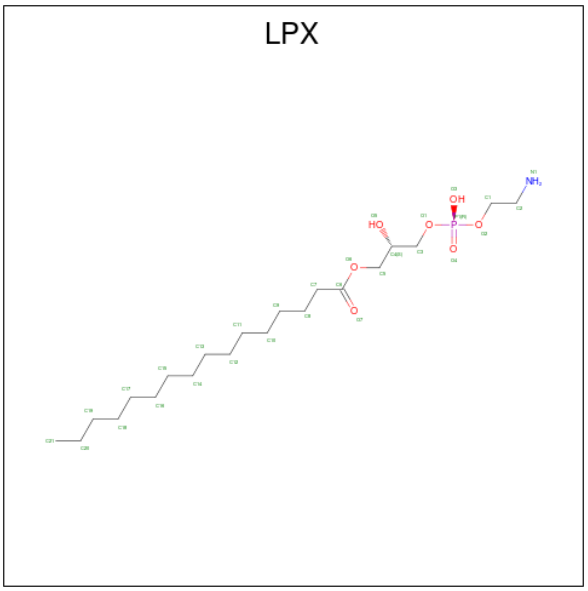
Mol	Chain	Residues	Atoms				AltConf
43	5	1	Total	C	O	P	0
			23	14	8	1	
43	6	1	Total	C	O	P	0
			29	20	8	1	
43	2	1	Total	C	O	P	0
			27	18	8	1	

- Molecule 44 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
44	7	1	Total	C	O	0
			18	16	2	

- Molecule 45 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms	AltConf
45	8	1	Total C N O P 30 21 1 7 1	0

- Molecule 46 is water.

Mol	Chain	Residues	Atoms	AltConf
46	A	2	Total O 2 2	0
46	A	15	Total O 15 15	0
46	A	2	Total O 2 2	0
46	A	6	Total O 6 6	0
46	A	9	Total O 9 9	0
46	A	2	Total O 2 2	0
46	A	7	Total O 7 7	0
46	A	18	Total O 18 18	0
46	A	8	Total O 8 8	0
46	A	14	Total O 14 14	0
46	A	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	2	Total O 2 2	0
46	B	12	Total O 12 12	0
46	B	10	Total O 10 10	0
46	B	16	Total O 16 16	0
46	B	2	Total O 2 2	0
46	B	2	Total O 2 2	0
46	B	1	Total O 1 1	0
46	B	28	Total O 28 28	0
46	B	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
46	C	1	Total O 1 1	0
46	C	1	Total O 1 1	0
46	C	1	Total O 1 1	0
46	C	1	Total O 1 1	0
46	C	1	Total O 1 1	0
46	C	12	Total O 12 12	0
46	C	1	Total O 1 1	0
46	C	1	Total O 1 1	0
46	D	1	Total O 1 1	0
46	D	1	Total O 1 1	0
46	D	1	Total O 1 1	0
46	D	2	Total O 2 2	0
46	D	1	Total O 1 1	0
46	D	2	Total O 2 2	0
46	D	1	Total O 1 1	0
46	D	2	Total O 2 2	0
46	D	1	Total O 1 1	0
46	E	1	Total O 1 1	0
46	E	4	Total O 4 4	0
46	E	1	Total O 1 1	0
46	E	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
46	F	1	Total O 1 1	0
46	F	1	Total O 1 1	0
46	F	2	Total O 2 2	0
46	F	8	Total O 8 8	0
46	F	1	Total O 1 1	0
46	F	1	Total O 1 1	0
46	J	2	Total O 2 2	0
46	J	1	Total O 1 1	0
46	K	2	Total O 2 2	0
46	L	1	Total O 1 1	0
46	L	1	Total O 1 1	0
46	L	1	Total O 1 1	0
46	L	2	Total O 2 2	0
46	1	16	Total O 16 16	0
46	Z	1	Total O 1 1	0
46	Z	7	Total O 7 7	0
46	3	17	Total O 17 17	0
46	7	18	Total O 18 18	0
46	8	1	Total O 1 1	0
46	8	15	Total O 15 15	0
46	4	7	Total O 7 7	0

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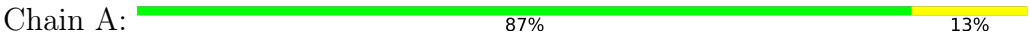
Mol	Chain	Residues	Atoms	AltConf
46	5	9	Total O 9 9	0
46	6	8	Total O 8 8	0
46	2	4	Total O 4 4	0
46	9	2	Total O 2 2	0

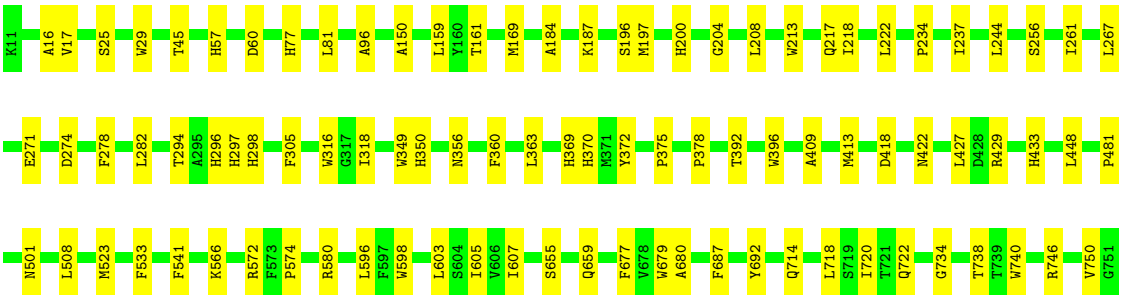
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

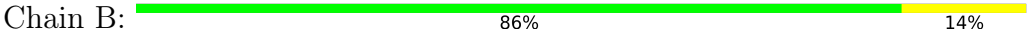
Chain A:





• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:





• Molecule 3: Photosystem I iron-sulfur center

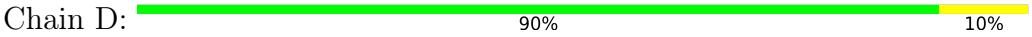
Chain C:

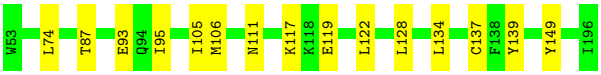




• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

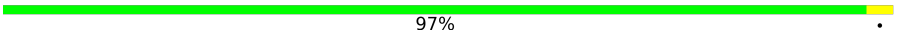
Chain D:





• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

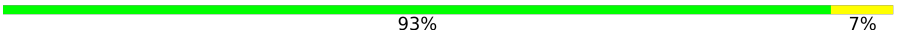
Chain E:





• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:

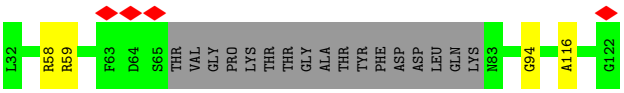




• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:

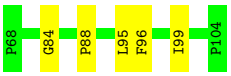




• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:





• Molecule 9: Photosystem I reaction center subunit IX

Chain J:

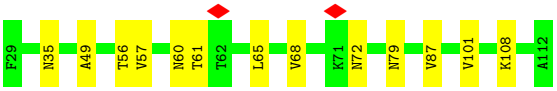




• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:

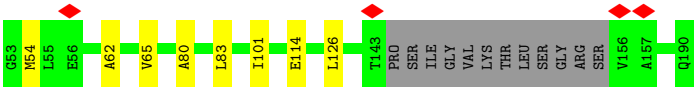




• Molecule 11: PSI subunit V

Chain L:

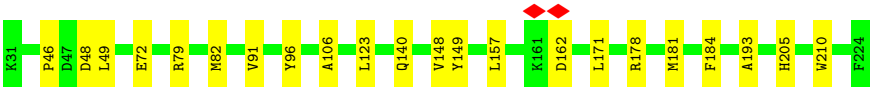




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

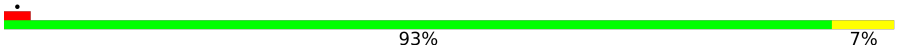
Chain 1:





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

Chain Z:





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

Chain 3:





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

Chain 7:





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

Chain 8:



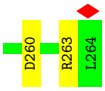


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:







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

Chain 5:





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

Chain 6:

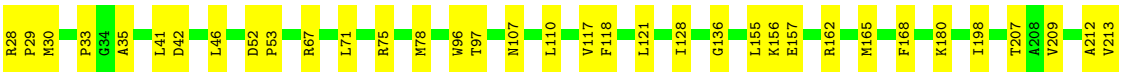




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



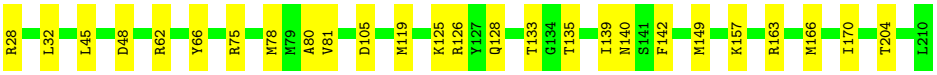




• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103082	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	264.64, 264.64, 264.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PLM, LHG, LUT, DAO, CHL, NKP, T7X, BCR, QTB, PQN, LMT, CL0, CA, 3PH, SF4, C7Z, DGA, SPH, SQD, SNC, OCA, LPX, DGD, RRX, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.22	0/6016	0.48	0/8201
2	B	0.24	0/6037	0.50	1/8242 (0.0%)
3	C	0.16	0/611	0.47	0/826
4	D	0.17	0/1154	0.48	0/1556
5	E	0.14	0/507	0.36	0/689
6	F	0.20	0/1292	0.45	0/1747
7	G	0.17	0/561	0.42	0/760
8	I	0.28	0/294	0.58	0/406
9	J	0.23	0/332	0.42	0/454
10	K	0.15	0/576	0.40	0/779
11	L	0.19	0/935	0.42	0/1277
12	1	0.17	0/1491	0.40	0/2028
12	Z	0.15	0/1491	0.38	0/2028
13	3	0.22	0/1722	0.48	0/2336
14	7	0.19	0/1702	0.46	0/2310
15	8	0.19	0/1701	0.42	0/2315
16	4	0.19	0/1683	0.43	0/2296
17	5	0.17	0/1830	0.38	0/2492
18	6	0.18	0/1828	0.39	0/2497
19	2	0.20	0/1556	0.50	0/2109
20	9	0.23	0/1447	0.52	0/1967
All	All	0.20	0/34766	0.46	1/47315 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	669	ARG	N-CA-C	5.37	117.57	111.02

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	A	5820	0	5670	74	0
2	B	5825	0	5579	79	0
3	C	601	0	581	3	0
4	D	1135	0	1148	8	0
5	E	497	0	491	1	0
6	F	1266	0	1301	9	0
7	G	550	0	532	3	0
8	I	282	0	292	4	0
9	J	321	0	322	4	0
10	K	571	0	606	11	0
11	L	914	0	921	5	0
12	1	1445	0	1396	17	0
12	Z	1445	0	1396	12	0
13	3	1674	0	1633	21	0
14	7	1650	0	1589	19	0
15	8	1650	0	1629	17	0
16	4	1628	0	1576	25	0
17	5	1775	0	1746	23	0
18	6	1766	0	1765	21	0
19	2	1518	0	1512	34	0
20	9	1406	0	1386	21	0
21	A	65	0	72	5	0
22	1	712	0	712	24	0
22	2	500	0	398	10	0
22	3	748	0	720	28	0
22	4	613	0	567	19	0
22	5	799	0	758	28	0
22	6	759	0	741	28	0
22	7	790	0	752	24	0
22	8	694	0	671	27	0
22	9	531	0	464	16	0
22	A	2699	0	2865	115	0
22	B	2680	0	2837	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	110	0	105	5	0
22	G	96	0	72	0	0
22	J	42	0	31	3	0
22	K	205	0	168	7	0
22	L	115	0	110	1	0
22	Z	622	0	584	17	0
23	A	33	0	46	1	0
23	B	33	0	46	0	0
24	A	8	0	0	0	0
24	C	16	0	0	1	0
25	3	160	0	211	9	0
25	4	40	0	53	2	0
25	5	80	0	105	6	0
25	6	80	0	106	4	0
25	7	80	0	106	4	0
25	8	40	0	53	1	0
25	A	200	0	264	14	0
25	B	280	0	370	18	0
25	G	40	0	53	1	0
25	I	40	0	52	3	0
25	J	40	0	53	4	0
25	K	80	0	106	5	0
25	L	80	0	106	3	0
26	1	43	0	56	1	0
26	2	34	0	38	2	0
26	3	20	0	12	0	0
26	4	81	0	108	1	0
26	5	37	0	44	0	0
26	6	49	0	74	4	0
26	7	37	0	44	2	0
26	8	38	0	46	0	0
26	9	33	0	36	0	0
26	A	84	0	114	7	0
26	B	76	0	64	2	0
26	Z	43	0	56	1	0
27	3	16	0	12	0	0
27	8	29	0	39	0	0
27	A	29	0	39	0	0
28	1	35	0	45	2	0
28	4	35	0	44	1	0
28	8	35	0	46	1	0
28	9	35	0	45	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	35	0	46	1	0
28	B	70	0	90	5	0
28	F	35	0	45	0	0
29	A	10	0	15	0	0
30	A	14	0	23	0	0
31	A	29	0	28	1	0
31	J	35	0	40	1	0
32	9	39	0	63	4	0
32	A	44	0	76	5	0
33	B	66	0	96	4	0
34	B	1	0	0	0	0
35	B	49	0	0	0	0
36	F	41	0	56	1	0
37	1	42	0	0	0	0
37	5	42	0	0	0	0
37	J	42	0	0	0	0
38	7	42	0	74	2	0
38	K	21	0	37	1	0
39	1	84	0	110	6	0
39	2	126	0	165	6	0
39	3	84	0	110	7	0
39	4	84	0	110	11	0
39	5	84	0	110	8	0
39	6	84	0	110	4	0
39	7	84	0	110	3	0
39	8	84	0	110	6	0
39	9	84	0	110	6	0
39	Z	126	0	165	8	0
40	1	106	0	82	2	0
40	2	150	0	105	6	0
40	3	66	0	69	3	0
40	4	201	0	146	5	0
40	5	160	0	134	7	0
40	6	206	0	156	3	0
40	7	54	0	42	3	0
40	8	122	0	115	4	0
40	9	108	0	97	2	0
40	Z	178	0	168	9	0
41	1	48	0	62	1	0
41	2	43	0	49	1	0
42	Z	19	0	0	0	0
43	2	27	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	5	23	0	19	0	0
43	6	29	0	31	0	0
43	7	39	0	51	1	0
43	8	30	0	33	0	0
44	7	18	0	31	0	0
45	8	30	0	43	1	0
46	1	16	0	0	0	0
46	2	4	0	0	0	0
46	3	17	0	0	0	0
46	4	7	0	0	0	0
46	5	9	0	0	0	0
46	6	8	0	0	0	0
46	7	18	0	0	0	0
46	8	16	0	0	0	0
46	9	2	0	0	0	0
46	A	91	0	0	1	0
46	B	79	0	0	1	0
46	C	19	0	0	0	0
46	D	12	0	0	0	0
46	E	7	0	0	0	0
46	F	14	0	0	0	0
46	J	3	0	0	0	0
46	K	2	0	0	0	0
46	L	5	0	0	0	0
46	Z	8	0	0	0	0
All	All	52213	0	51749	775	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 7.

The worst 5 of 775 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:117:VAL:O	19:2:121:LEU:HD13	1.73	0.88
1:A:396:TRP:CD1	22:A:1126:CLA:HAB	2.15	0.82
22:A:1138:CLA:H121	22:A:1138:CLA:HAB	1.64	0.79
22:B:1240:CLA:HBB1	22:1:605:CLA:H12	1.68	0.74
22:F:1301:CLA:HBB1	36:F:4001:RRX:H11	1.67	0.74

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	720 (97%)	19 (3%)	0	100	100
2	B	731/733 (100%)	707 (97%)	24 (3%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	141/144 (98%)	135 (96%)	6 (4%)	0	100	100
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	21	29
7	G	70/91 (77%)	70 (100%)	0	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
9	J	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
11	L	122/138 (88%)	119 (98%)	3 (2%)	0	100	100
12	1	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
12	Z	192/194 (99%)	188 (98%)	4 (2%)	0	100	100
13	3	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
14	7	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
15	8	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
16	4	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
17	5	225/227 (99%)	221 (98%)	3 (1%)	1 (0%)	30	39
18	6	227/229 (99%)	223 (98%)	4 (2%)	0	100	100
19	2	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	24	34
20	9	181/183 (99%)	170 (94%)	10 (6%)	1 (1%)	21	29
All	All	4323/4399 (98%)	4187 (97%)	132 (3%)	4 (0%)	49	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	150	PHE
17	5	243	GLN
19	2	180	LYS
20	9	139	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/601 (100%)	601 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	120/120 (100%)	120 (100%)	0	100	100
5	E	54/54 (100%)	54 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	G	54/68 (79%)	54 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	58/58 (100%)	58 (100%)	0	100	100
11	L	92/102 (90%)	92 (100%)	0	100	100
12	1	137/137 (100%)	137 (100%)	0	100	100
12	Z	137/137 (100%)	137 (100%)	0	100	100
13	3	167/167 (100%)	167 (100%)	0	100	100
14	7	164/164 (100%)	164 (100%)	0	100	100
15	8	163/163 (100%)	163 (100%)	0	100	100
16	4	164/165 (99%)	164 (100%)	0	100	100
17	5	184/184 (100%)	184 (100%)	0	100	100
18	6	183/183 (100%)	183 (100%)	0	100	100
19	2	154/156 (99%)	154 (100%)	0	100	100
20	9	141/141 (100%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3431/3458 (99%)	3431 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
15	8	230	HIS
16	4	175	ASN
2	B	628	ASN
2	B	505	ASN
18	6	206	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
4	SNC	D	137	4	4,7,8	1.06	0	1,7,9	3.60	1 (100%)

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
4	SNC	D	137	4	-	0/0/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	137	SNC	CA-CB-SG	-3.60	105.28	112.76

There are no chirality outliers.

There are no torsion outliers.

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)

Of 354 ligands modelled in this entry, 1 is monoatomic - leaving 353 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	8	603	-	69,73,73	1.35	7 (10%)	83,113,113	2.14	21 (25%)
22	CLA	A	1132	-	69,73,73	1.37	6 (8%)	83,113,113	2.00	19 (22%)
40	CHL	7	610	-	58,62,74	0.87	2 (3%)	65,99,114	1.41	13 (20%)
22	CLA	A	1122	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	19 (22%)
39	LUT	2	502	-	42,43,43	2.32	1 (2%)	51,60,60	1.94	13 (25%)
22	CLA	5	612	-	69,73,73	1.34	6 (8%)	83,113,113	1.91	17 (20%)
22	CLA	B	1232	-	49,53,73	1.61	7 (14%)	59,89,113	2.00	16 (27%)
39	LUT	9	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	15 (29%)
40	CHL	1	610	-	52,56,74	0.91	2 (3%)	58,92,114	1.31	9 (15%)
40	CHL	5	611	-	55,59,74	0.91	2 (3%)	62,96,114	1.38	10 (16%)
40	CHL	9	613	-	46,50,74	1.40	3 (6%)	51,85,114	1.39	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	8	601	-	64,68,73	1.42	8 (12%)	77,107,113	2.02	19 (24%)
40	CHL	4	613	-	60,64,74	0.89	2 (3%)	68,102,114	1.33	12 (17%)
31	LMG	J	5001	-	35,35,55	0.48	0	43,43,63	1.12	2 (4%)
40	CHL	Z	613	-	50,54,74	0.93	2 (4%)	56,90,114	1.32	8 (14%)
22	CLA	3	608	-	49,53,73	1.61	7 (14%)	59,89,113	2.10	14 (23%)
22	CLA	A	1104	1	69,73,73	1.36	8 (11%)	83,113,113	1.92	20 (24%)
40	CHL	6	617	-	47,51,74	0.98	2 (4%)	52,86,114	1.38	10 (19%)
22	CLA	A	1126	-	69,73,73	1.37	8 (11%)	83,113,113	1.94	19 (22%)
37	C7Z	1	503	-	43,43,43	5.39	27 (62%)	58,60,60	2.30	20 (34%)
25	BCR	B	4005	-	41,41,41	1.86	4 (9%)	56,56,56	4.49	16 (28%)
25	BCR	A	4002	-	41,41,41	1.83	5 (12%)	56,56,56	4.18	14 (25%)
22	CLA	3	604	-	64,68,73	1.39	8 (12%)	77,107,113	2.07	19 (24%)
22	CLA	L	1502	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
22	CLA	B	1226	-	69,73,73	1.43	8 (11%)	83,113,113	2.02	21 (25%)
26	LHG	5	801	-	36,36,48	0.43	0	39,42,54	1.17	4 (10%)
22	CLA	B	1207	2	69,73,73	1.36	6 (8%)	83,113,113	1.91	19 (22%)
22	CLA	8	608	-	59,63,73	1.46	6 (10%)	71,101,113	1.99	18 (25%)
22	CLA	6	604	-	69,73,73	1.37	7 (10%)	83,113,113	1.97	21 (25%)
22	CLA	1	602	-	49,53,73	1.63	8 (16%)	59,89,113	2.00	16 (27%)
26	LHG	4	801	-	48,48,48	0.39	0	51,54,54	1.11	4 (7%)
39	LUT	6	502	-	42,43,43	2.32	1 (2%)	51,60,60	1.85	13 (25%)
40	CHL	2	613	-	55,59,74	0.95	2 (3%)	62,96,114	1.33	8 (12%)
22	CLA	9	603	-	64,68,73	1.43	6 (9%)	77,107,113	2.14	19 (24%)
22	CLA	K	1403	10	53,57,73	1.56	6 (11%)	62,93,113	2.12	16 (25%)
22	CLA	3	616	-	60,64,73	1.45	7 (11%)	72,102,113	2.12	20 (27%)
22	CLA	5	609	17	69,73,73	1.37	7 (10%)	83,113,113	1.89	19 (22%)
22	CLA	6	612	-	54,58,73	1.53	7 (12%)	65,95,113	2.17	18 (27%)
22	CLA	3	610	13	64,68,73	1.43	7 (10%)	77,107,113	1.98	20 (25%)
40	CHL	6	611	-	55,59,74	0.90	2 (3%)	62,96,114	1.34	10 (16%)
22	CLA	5	607	-	65,69,73	1.40	7 (10%)	78,108,113	1.94	18 (23%)
26	LHG	A	5001	22	34,34,48	0.46	0	37,40,54	1.18	4 (10%)
25	BCR	5	504	-	41,41,41	1.84	5 (12%)	56,56,56	4.50	22 (39%)
22	CLA	F	1301	-	69,73,73	1.35	7 (10%)	83,113,113	1.94	22 (26%)
31	LMG	A	5003	-	29,29,55	0.56	0	37,37,63	1.20	3 (8%)
27	NKP	A	5004	-	28,28,28	1.52	3 (10%)	31,32,32	1.25	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	1224	-	69,73,73	1.39	8 (11%)	83,113,113	1.96	18 (21%)
22	CLA	B	1237	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	15 (18%)
22	CLA	2	602	-	50,54,73	1.59	6 (12%)	60,90,113	2.10	17 (28%)
22	CLA	6	619	18	69,73,73	1.37	7 (10%)	83,113,113	1.97	18 (21%)
22	CLA	5	618	-	69,73,73	1.35	6 (8%)	83,113,113	1.96	18 (21%)
43	3PH	5	802	-	22,22,47	1.23	3 (13%)	26,27,52	1.27	2 (7%)
22	CLA	9	605	-	59,63,73	1.48	7 (11%)	71,101,113	2.05	19 (26%)
28	LMT	A	5006	-	36,36,36	1.20	6 (16%)	47,47,47	1.04	1 (2%)
22	CLA	2	606	-	50,54,73	1.60	7 (14%)	60,90,113	2.10	13 (21%)
22	CLA	B	1239	2	69,73,73	1.36	6 (8%)	83,113,113	1.98	18 (21%)
22	CLA	3	612	-	64,68,73	1.40	8 (12%)	77,107,113	1.97	17 (22%)
22	CLA	B	1203	-	69,73,73	1.36	7 (10%)	83,113,113	1.85	18 (21%)
22	CLA	B	1236	-	69,73,73	1.38	8 (11%)	83,113,113	1.93	18 (21%)
22	CLA	B	1230	-	62,66,73	1.41	6 (9%)	74,104,113	2.08	20 (27%)
22	CLA	A	1140	-	69,73,73	1.38	8 (11%)	83,113,113	1.90	19 (22%)
22	CLA	5	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.00	18 (23%)
22	CLA	3	601	-	69,73,73	1.37	7 (10%)	83,113,113	1.99	21 (25%)
26	LHG	4	802	-	31,31,48	0.47	0	34,37,54	1.12	2 (5%)
39	LUT	7	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	13 (25%)
26	LHG	B	5001	-	22,22,48	0.55	0	25,28,54	1.30	1 (4%)
39	LUT	4	501	-	42,43,43	2.37	1 (2%)	51,60,60	1.84	12 (23%)
22	CLA	A	1116	-	64,68,73	1.43	9 (14%)	77,107,113	1.99	19 (24%)
43	3PH	8	806	-	29,29,47	1.08	4 (13%)	33,34,52	1.18	2 (6%)
30	DAO	A	5007	-	13,13,13	0.79	1 (7%)	13,13,13	0.97	0
43	3PH	6	802	-	28,28,47	1.11	4 (14%)	32,33,52	1.25	2 (6%)
22	CLA	2	615	-	50,54,73	1.58	6 (12%)	60,90,113	2.07	16 (26%)
25	BCR	A	4004	-	41,41,41	1.82	5 (12%)	56,56,56	4.32	19 (33%)
22	CLA	Z	605	-	69,73,73	1.35	8 (11%)	83,113,113	1.95	20 (24%)
22	CLA	4	609	16	64,68,73	1.41	7 (10%)	77,107,113	1.97	18 (23%)
22	CLA	B	1221	-	69,73,73	1.38	9 (13%)	83,113,113	2.07	20 (24%)
22	CLA	4	604	-	64,68,73	1.42	7 (10%)	77,107,113	1.98	19 (24%)
25	BCR	3	505	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	12 (21%)
28	LMT	1	803	-	36,36,36	1.19	5 (13%)	47,47,47	0.98	2 (4%)
25	BCR	3	506	-	41,41,41	1.86	4 (9%)	56,56,56	4.40	15 (26%)
22	CLA	6	609	18	69,73,73	1.35	7 (10%)	83,113,113	1.98	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	9	612	-	54,58,73	1.56	8 (14%)	65,95,113	2.12	18 (27%)
25	BCR	L	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	14 (25%)
21	CL0	A	1011	-	69,73,73	2.35	20 (28%)	83,113,113	2.54	24 (28%)
25	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.23	15 (26%)
22	CLA	A	1107	1	69,73,73	1.39	6 (8%)	83,113,113	1.88	15 (18%)
22	CLA	6	607	-	59,63,73	1.48	7 (11%)	71,101,113	2.03	17 (23%)
22	CLA	2	601	-	64,68,73	1.41	8 (12%)	77,107,113	2.04	19 (24%)
22	CLA	B	1021	-	69,73,73	1.37	8 (11%)	83,113,113	1.89	17 (20%)
22	CLA	B	1227	-	54,58,73	1.55	8 (14%)	65,95,113	2.01	19 (29%)
40	CHL	4	617	-	47,51,74	0.97	2 (4%)	52,86,114	1.36	10 (19%)
22	CLA	3	602	-	50,54,73	1.58	7 (14%)	60,90,113	1.99	14 (23%)
22	CLA	B	1208	-	60,64,73	1.46	8 (13%)	72,102,113	2.06	18 (25%)
25	BCR	A	4003	-	41,41,41	1.82	4 (9%)	56,56,56	4.33	19 (33%)
22	CLA	6	601	-	64,68,73	1.43	7 (10%)	77,107,113	2.02	19 (24%)
22	CLA	6	602	-	56,60,73	1.52	7 (12%)	67,97,113	2.12	18 (26%)
22	CLA	A	1131	-	69,73,73	1.36	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	A	1129	-	54,58,73	1.55	8 (14%)	65,95,113	2.07	17 (26%)
25	BCR	6	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.28	14 (25%)
22	CLA	2	612	-	54,58,73	1.55	7 (12%)	65,95,113	2.13	19 (29%)
22	CLA	5	608	-	49,53,73	1.60	7 (14%)	59,89,113	2.10	16 (27%)
26	LHG	2	801	-	33,33,48	0.45	0	36,39,54	1.22	3 (8%)
28	LMT	8	805	-	36,36,36	1.21	6 (16%)	47,47,47	1.15	3 (6%)
22	CLA	A	1118	1	64,68,73	1.40	7 (10%)	77,107,113	2.06	20 (25%)
22	CLA	B	1212	-	61,65,73	1.46	6 (9%)	73,103,113	2.09	20 (27%)
25	BCR	3	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.17	16 (28%)
22	CLA	A	1102	-	59,63,73	1.48	7 (11%)	71,101,113	2.09	21 (29%)
22	CLA	K	1402	-	59,63,73	1.47	7 (11%)	71,101,113	2.11	19 (26%)
22	CLA	B	1214	-	63,67,73	1.41	7 (11%)	75,105,113	2.15	22 (29%)
25	BCR	B	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.19	10 (17%)
27	NKP	3	802	-	15,15,28	2.07	3 (20%)	18,19,32	1.53	2 (11%)
42	QTB	Z	504	-	19,19,19	2.46	5 (26%)	20,26,26	2.76	7 (35%)
40	CHL	Z	610	-	70,74,74	0.77	2 (2%)	80,114,114	1.18	10 (12%)
22	CLA	3	607	-	64,68,73	1.42	8 (12%)	77,107,113	2.10	19 (24%)
40	CHL	6	610	-	60,64,74	0.85	2 (3%)	68,102,114	1.33	12 (17%)
22	CLA	6	615	-	65,69,73	1.40	7 (10%)	78,108,113	2.05	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	1222	-	69,73,73	1.36	7 (10%)	83,113,113	1.90	21 (25%)
22	CLA	K	1401	-	50,54,73	1.60	6 (12%)	60,90,113	2.01	15 (25%)
22	CLA	7	604	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	22 (26%)
22	CLA	L	1503	-	54,58,73	1.54	6 (11%)	65,95,113	2.14	18 (27%)
22	CLA	A	1109	-	69,73,73	1.36	7 (10%)	83,113,113	1.98	18 (21%)
26	LHG	Z	801	-	42,42,48	0.41	0	45,48,54	1.16	4 (8%)
22	CLA	Z	603	-	54,58,73	1.53	7 (12%)	65,95,113	2.19	20 (30%)
22	CLA	B	1206	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	16 (19%)
40	CHL	2	610	-	52,56,74	0.91	2 (3%)	58,92,114	1.33	9 (15%)
32	DGA	A	5005	-	43,43,43	1.15	3 (6%)	45,45,45	1.49	3 (6%)
22	CLA	A	1013	-	69,73,73	1.39	8 (11%)	83,113,113	1.82	19 (22%)
22	CLA	G	1601	7	54,58,73	1.54	6 (11%)	65,95,113	2.11	19 (29%)
22	CLA	6	606	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	17 (20%)
22	CLA	9	601	-	64,68,73	1.42	6 (9%)	77,107,113	2.06	18 (23%)
22	CLA	A	1141	26	56,60,73	1.51	7 (12%)	67,97,113	2.19	19 (28%)
25	BCR	A	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.13	15 (26%)
22	CLA	B	1022	46	69,73,73	1.38	6 (8%)	83,113,113	1.88	21 (25%)
38	SPH	7	804	-	19,20,20	0.64	0	18,21,21	1.11	1 (5%)
32	DGA	9	802	-	38,38,43	1.15	3 (7%)	40,40,45	1.61	3 (7%)
22	CLA	6	608	-	59,63,73	1.48	8 (13%)	71,101,113	2.08	17 (23%)
22	CLA	B	1211	-	64,68,73	1.40	6 (9%)	77,107,113	2.12	19 (24%)
24	SF4	A	3001	2,1	0,12,12	-	-	-		
23	PQN	A	2001	-	34,34,34	0.39	0	42,45,45	1.07	2 (4%)
22	CLA	A	1108	1	69,73,73	1.37	6 (8%)	83,113,113	1.95	20 (24%)
22	CLA	1	613	-	50,54,73	1.61	8 (16%)	60,90,113	2.02	16 (26%)
39	LUT	8	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.86	15 (29%)
41	SQD	1	802	-	47,48,54	0.83	0	56,59,65	0.94	2 (3%)
28	LMT	B	5005	-	36,36,36	1.21	6 (16%)	47,47,47	1.11	3 (6%)
22	CLA	B	1225	-	69,73,73	1.38	8 (11%)	83,113,113	1.79	14 (16%)
25	BCR	B	4001	-	41,41,41	1.83	5 (12%)	56,56,56	4.12	15 (26%)
22	CLA	1	604	-	64,68,73	1.41	7 (10%)	77,107,113	1.99	18 (23%)
22	CLA	B	1204	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	17 (20%)
22	CLA	A	1119	-	69,73,73	1.37	7 (10%)	83,113,113	1.76	16 (19%)
22	CLA	A	1117	-	69,73,73	1.38	7 (10%)	83,113,113	1.93	17 (20%)
25	BCR	8	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.26	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LUT	2	503	-	42,43,43	2.40	1 (2%)	51,60,60	2.63	23 (45%)
38	SPH	7	803	-	19,20,20	0.67	0	18,21,21	0.96	1 (5%)
22	CLA	A	1112	-	64,68,73	1.42	7 (10%)	77,107,113	2.00	18 (23%)
26	LHG	1	801	-	42,42,48	0.44	0	45,48,54	1.18	4 (8%)
39	LUT	Z	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.87	13 (25%)
22	CLA	7	612	-	54,58,73	1.55	6 (11%)	65,95,113	2.12	17 (26%)
26	LHG	7	801	-	36,36,48	0.45	0	39,42,54	1.17	3 (7%)
22	CLA	1	603	-	69,73,73	1.35	7 (10%)	83,113,113	1.99	20 (24%)
22	CLA	A	1110	1	69,73,73	1.38	8 (11%)	83,113,113	1.97	19 (22%)
22	CLA	7	603	14	69,73,73	1.36	7 (10%)	83,113,113	2.10	21 (25%)
25	BCR	4	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	16 (28%)
22	CLA	6	605	18	59,63,73	1.48	7 (11%)	71,101,113	2.06	20 (28%)
22	CLA	7	609	14	69,73,73	1.34	7 (10%)	83,113,113	1.97	18 (21%)
25	BCR	6	504	-	41,41,41	1.89	4 (9%)	56,56,56	4.30	15 (26%)
24	SF4	C	3003	3	0,12,12	-	-	-		
22	CLA	1	605	-	59,63,73	1.47	8 (13%)	71,101,113	2.10	19 (26%)
27	NKP	8	802	-	28,28,28	1.50	2 (7%)	31,32,32	1.25	3 (9%)
22	CLA	B	1215	-	64,68,73	1.41	7 (10%)	77,107,113	1.98	16 (20%)
22	CLA	Z	606	-	61,65,73	1.44	7 (11%)	73,103,113	2.09	18 (24%)
25	BCR	5	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	15 (26%)
25	BCR	J	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.22	16 (28%)
22	CLA	2	608	-	49,53,73	1.61	7 (14%)	59,89,113	2.13	16 (27%)
22	CLA	5	602	-	65,69,73	1.41	8 (12%)	78,108,113	1.90	18 (23%)
22	CLA	9	608	-	49,53,73	1.61	8 (16%)	59,89,113	2.05	15 (25%)
33	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.02	4 (4%)
40	CHL	6	613	-	60,64,74	0.88	2 (3%)	68,102,114	1.17	9 (13%)
22	CLA	4	603	-	69,73,73	1.37	7 (10%)	83,113,113	2.04	21 (25%)
22	CLA	1	615	12	69,73,73	1.38	7 (10%)	83,113,113	1.84	16 (19%)
22	CLA	B	1216	-	69,73,73	1.35	7 (10%)	83,113,113	1.89	18 (21%)
22	CLA	B	1223	-	69,73,73	1.38	8 (11%)	83,113,113	1.91	20 (24%)
22	CLA	B	1231	2	69,73,73	1.36	7 (10%)	83,113,113	1.89	17 (20%)
22	CLA	7	611	-	54,58,73	1.51	7 (12%)	65,95,113	2.20	18 (27%)
26	LHG	3	801	-	19,19,48	0.92	1 (5%)	20,24,54	1.34	1 (5%)
22	CLA	4	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.05	21 (27%)
22	CLA	Z	615	12	50,54,73	1.59	7 (14%)	60,90,113	2.08	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LUT	Z	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.91	12 (23%)
22	CLA	A	1128	-	69,73,73	1.40	6 (8%)	83,113,113	1.89	15 (18%)
22	CLA	7	607	-	69,73,73	1.36	7 (10%)	83,113,113	1.89	18 (21%)
23	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.04	2 (4%)
22	CLA	5	613	-	59,63,73	1.47	8 (13%)	71,101,113	1.98	17 (23%)
22	CLA	5	615	17	54,58,73	1.54	7 (12%)	65,95,113	2.19	20 (30%)
22	CLA	1	607	-	64,68,73	1.43	7 (10%)	77,107,113	2.00	18 (23%)
22	CLA	6	618	-	50,54,73	1.59	7 (14%)	60,90,113	2.09	16 (26%)
40	CHL	8	610	-	60,64,74	0.89	2 (3%)	68,102,114	1.35	11 (16%)
22	CLA	Z	611	-	59,63,73	1.46	7 (11%)	71,101,113	2.09	21 (29%)
40	CHL	2	609	19	55,59,74	0.99	3 (5%)	62,96,114	1.38	9 (14%)
22	CLA	K	1404	-	59,63,73	1.49	7 (11%)	71,101,113	2.10	17 (23%)
41	SQD	2	803	-	42,43,54	0.88	0	51,54,65	0.97	2 (3%)
22	CLA	Z	601	-	64,68,73	1.40	7 (10%)	77,107,113	2.01	19 (24%)
22	CLA	3	605	13	69,73,73	1.38	8 (11%)	83,113,113	1.85	19 (22%)
40	CHL	1	609	12	62,66,74	0.86	2 (3%)	70,104,114	1.29	10 (14%)
39	LUT	7	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.91	12 (23%)
22	CLA	1	606	-	65,69,73	1.40	8 (12%)	78,108,113	1.97	17 (21%)
22	CLA	4	608	-	59,63,73	1.47	7 (11%)	71,101,113	2.06	18 (25%)
24	SF4	C	3002	3	0,12,12	-	-	-		
22	CLA	5	606	-	54,58,73	1.54	6 (11%)	65,95,113	2.16	16 (24%)
22	CLA	A	1105	-	69,73,73	1.36	8 (11%)	83,113,113	1.93	19 (22%)
25	BCR	3	504	-	41,41,41	1.87	5 (12%)	56,56,56	4.31	16 (28%)
22	CLA	3	618	-	50,54,73	1.60	8 (16%)	60,90,113	2.03	15 (25%)
22	CLA	F	1302	-	49,53,73	1.59	7 (14%)	59,89,113	2.01	15 (25%)
36	RRX	F	4001	-	42,42,42	4.83	24 (57%)	57,58,58	2.50	24 (42%)
22	CLA	A	1113	1	69,73,73	1.37	6 (8%)	83,113,113	1.92	17 (20%)
22	CLA	7	601	-	64,68,73	1.44	8 (12%)	77,107,113	2.06	20 (25%)
28	LMT	4	803	-	36,36,36	1.17	5 (13%)	47,47,47	1.01	1 (2%)
39	LUT	9	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.83	14 (27%)
22	CLA	A	1115	-	64,68,73	1.42	7 (10%)	77,107,113	1.84	16 (20%)
22	CLA	A	1135	-	55,59,73	1.55	9 (16%)	66,96,113	2.17	20 (30%)
40	CHL	5	617	-	47,51,74	0.97	2 (4%)	52,86,114	1.35	9 (17%)
28	LMT	B	6101	-	36,36,36	1.19	5 (13%)	47,47,47	1.08	3 (6%)
25	BCR	B	4003	-	41,41,41	1.86	5 (12%)	56,56,56	4.26	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	4	612	-	54,58,73	1.52	7 (12%)	65,95,113	2.22	18 (27%)
22	CLA	Z	612	-	69,73,73	1.36	6 (8%)	83,113,113	1.91	18 (21%)
40	CHL	4	611	-	55,59,74	0.89	2 (3%)	62,96,114	1.32	10 (16%)
40	CHL	5	610	-	70,74,74	0.82	2 (2%)	80,114,114	1.22	9 (11%)
22	CLA	B	1241	-	69,73,73	1.35	8 (11%)	83,113,113	2.05	21 (25%)
25	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.34	15 (26%)
22	CLA	8	602	-	69,73,73	1.36	6 (8%)	83,113,113	1.89	17 (20%)
43	3PH	7	802	-	38,38,47	0.94	3 (7%)	42,43,52	1.12	2 (4%)
22	CLA	A	1139	1	69,73,73	1.36	7 (10%)	83,113,113	1.95	19 (22%)
22	CLA	7	608	-	47,51,73	1.64	7 (14%)	56,86,113	2.11	15 (26%)
22	CLA	B	1238	-	69,73,73	1.35	7 (10%)	83,113,113	1.97	17 (20%)
39	LUT	8	501	-	42,43,43	2.30	1 (2%)	51,60,60	1.92	13 (25%)
22	CLA	B	1218	-	69,73,73	1.37	8 (11%)	83,113,113	2.03	18 (21%)
22	CLA	4	605	-	69,73,73	1.36	9 (13%)	83,113,113	1.91	18 (21%)
22	CLA	1	611	-	69,73,73	1.35	7 (10%)	83,113,113	1.97	20 (24%)
22	CLA	A	1101	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	21 (25%)
22	CLA	3	606	-	69,73,73	1.36	7 (10%)	83,113,113	2.02	16 (19%)
40	CHL	3	611	-	70,74,74	0.81	3 (4%)	80,114,114	1.37	12 (15%)
22	CLA	A	1106	-	69,73,73	1.37	9 (13%)	83,113,113	1.98	18 (21%)
22	CLA	3	613	46	59,63,73	1.46	6 (10%)	71,101,113	2.02	16 (22%)
37	C7Z	5	505	-	43,43,43	5.41	25 (58%)	58,60,60	2.25	19 (32%)
22	CLA	B	1229	2	69,73,73	1.35	8 (11%)	83,113,113	1.97	21 (25%)
28	LMT	9	803	-	36,36,36	1.18	5 (13%)	47,47,47	1.04	3 (6%)
22	CLA	2	604	-	60,64,73	1.46	8 (13%)	72,102,113	2.17	17 (23%)
26	LHG	B	5006	-	32,32,48	0.45	0	35,38,54	1.20	3 (8%)
22	CLA	A	1114	-	65,69,73	1.41	7 (10%)	78,108,113	1.97	17 (21%)
22	CLA	A	1120	-	59,63,73	1.46	7 (11%)	71,101,113	2.15	21 (29%)
22	CLA	A	1111	-	69,73,73	1.37	7 (10%)	83,113,113	1.97	18 (21%)
39	LUT	3	502	-	42,43,43	2.38	1 (2%)	51,60,60	1.97	14 (27%)
26	LHG	8	801	-	37,37,48	0.43	0	40,43,54	1.07	2 (5%)
22	CLA	A	1133	1	69,73,73	1.35	6 (8%)	83,113,113	1.87	15 (18%)
22	CLA	2	607	-	50,54,73	1.62	7 (14%)	60,90,113	2.08	15 (25%)
22	CLA	4	607	-	59,63,73	1.48	8 (13%)	71,101,113	2.06	17 (23%)
22	CLA	9	607	-	59,63,73	1.48	6 (10%)	71,101,113	2.05	18 (25%)
22	CLA	A	1121	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	7	605	14	65,69,73	1.39	7 (10%)	78,108,113	1.98	21 (26%)
22	CLA	A	1103	1	69,73,73	1.32	6 (8%)	83,113,113	1.95	17 (20%)
22	CLA	5	603	-	60,64,73	1.44	6 (10%)	72,102,113	2.21	20 (27%)
22	CLA	B	1209	2	69,73,73	1.38	7 (10%)	83,113,113	1.98	18 (21%)
22	CLA	8	615	15	50,54,73	1.60	7 (14%)	60,90,113	2.12	16 (26%)
40	CHL	9	610	-	70,74,74	0.86	3 (4%)	80,114,114	1.21	11 (13%)
22	CLA	8	609	15	69,73,73	1.37	8 (11%)	83,113,113	1.97	19 (22%)
22	CLA	9	606	-	54,58,73	1.53	8 (14%)	65,95,113	2.13	18 (27%)
22	CLA	G	1602	-	50,54,73	1.60	7 (14%)	60,90,113	2.06	14 (23%)
22	CLA	A	1134	1	59,63,73	1.47	7 (11%)	71,101,113	2.13	20 (28%)
39	LUT	1	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.84	13 (25%)
22	CLA	5	605	-	59,63,73	1.48	8 (13%)	71,101,113	2.13	23 (32%)
39	LUT	2	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.36	13 (25%)
25	BCR	B	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.16	13 (23%)
39	LUT	Z	503	-	42,43,43	2.35	1 (2%)	51,60,60	2.08	13 (25%)
22	CLA	1	601	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	21 (25%)
22	CLA	4	602	-	56,60,73	1.51	7 (12%)	67,97,113	2.12	19 (28%)
22	CLA	8	605	-	69,73,73	1.38	8 (11%)	83,113,113	1.88	19 (22%)
22	CLA	Z	602	-	50,54,73	1.60	7 (14%)	60,90,113	2.02	13 (21%)
22	CLA	Z	604	-	69,73,73	1.37	8 (11%)	83,113,113	1.95	20 (24%)
44	PLM	7	805	-	17,17,17	0.56	0	17,17,17	1.11	1 (5%)
37	C7Z	J	4002	-	43,43,43	5.37	27 (62%)	58,60,60	2.23	20 (34%)
22	CLA	B	1228	2	69,73,73	1.36	6 (8%)	83,113,113	1.91	19 (22%)
22	CLA	B	1023	-	69,73,73	1.36	6 (8%)	83,113,113	2.01	17 (20%)
25	BCR	G	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.20	14 (25%)
22	CLA	8	612	-	50,54,73	1.59	7 (14%)	60,90,113	2.02	13 (21%)
22	CLA	B	1234	-	64,68,73	1.44	8 (12%)	77,107,113	1.97	19 (24%)
22	CLA	A	1137	-	69,73,73	1.37	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	A	1123	-	69,73,73	1.39	7 (10%)	83,113,113	1.95	18 (21%)
25	BCR	7	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.47	18 (32%)
38	SPH	K	5001	-	19,20,20	0.61	0	18,21,21	1.12	2 (11%)
22	CLA	A	1136	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	16 (19%)
22	CLA	B	1235	2	69,73,73	1.37	8 (11%)	83,113,113	1.96	17 (20%)
22	CLA	A	1138	1	69,73,73	1.36	6 (8%)	83,113,113	1.97	16 (19%)
22	CLA	A	1125	-	69,73,73	1.38	7 (10%)	83,113,113	1.99	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	3PH	2	802	-	26,26,47	1.14	4 (15%)	30,31,52	1.30	2 (6%)
26	LHG	6	801	-	48,48,48	0.40	0	51,54,54	1.08	4 (7%)
22	CLA	2	603	-	59,63,73	1.48	7 (11%)	71,101,113	2.21	21 (29%)
22	CLA	A	1012	-	69,73,73	1.39	7 (10%)	83,113,113	1.95	20 (24%)
22	CLA	B	1217	2	60,64,73	1.46	8 (13%)	72,102,113	2.04	20 (27%)
22	CLA	9	604	-	69,73,73	1.38	9 (13%)	83,113,113	2.00	23 (27%)
22	CLA	6	603	-	69,73,73	1.37	7 (10%)	83,113,113	2.07	19 (22%)
40	CHL	4	610	-	55,59,74	0.87	2 (3%)	62,96,114	1.43	12 (19%)
22	CLA	Z	608	-	60,64,73	1.45	8 (13%)	72,102,113	2.01	18 (25%)
22	CLA	8	607	-	59,63,73	1.48	6 (10%)	71,101,113	1.99	17 (23%)
22	CLA	9	602	-	49,53,73	1.63	7 (14%)	59,89,113	1.99	13 (22%)
25	BCR	B	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.14	14 (25%)
22	CLA	A	1124	46	69,73,73	1.38	7 (10%)	83,113,113	1.90	18 (21%)
22	CLA	J	1901	-	46,50,73	1.65	7 (15%)	55,85,113	2.14	18 (32%)
29	OCA	A	5008	-	9,9,9	0.70	0	9,9,9	1.36	1 (11%)
22	CLA	5	622	-	50,54,73	1.61	7 (14%)	60,90,113	2.10	15 (25%)
25	BCR	7	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	15 (26%)
39	LUT	5	501	-	42,43,43	2.44	2 (4%)	51,60,60	1.91	12 (23%)
22	CLA	7	602	-	54,58,73	1.53	6 (11%)	65,95,113	2.08	18 (27%)
25	BCR	A	4005	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	12 (21%)
26	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	0.98	2 (3%)
22	CLA	8	606	-	64,68,73	1.42	7 (10%)	77,107,113	1.94	18 (23%)
22	CLA	B	1240	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	22 (26%)
22	CLA	A	1127	-	69,73,73	1.39	6 (8%)	83,113,113	1.82	16 (19%)
22	CLA	7	616	-	64,68,73	1.41	7 (10%)	77,107,113	2.05	19 (24%)
25	BCR	I	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	16 (28%)
22	CLA	3	603	-	69,73,73	1.37	8 (11%)	83,113,113	2.04	18 (21%)
40	CHL	8	613	-	70,74,74	0.85	2 (2%)	80,114,114	1.21	12 (15%)
22	CLA	B	1220	-	69,73,73	1.35	6 (8%)	83,113,113	1.88	17 (20%)
22	CLA	4	606	-	54,58,73	1.53	7 (12%)	65,95,113	2.10	20 (30%)
45	LPX	8	803	-	29,29,29	1.00	2 (6%)	31,33,33	1.00	1 (3%)
25	BCR	L	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.21	15 (26%)
22	CLA	B	1213	2	69,73,73	1.38	7 (10%)	83,113,113	2.01	19 (22%)
22	CLA	1	608	-	64,68,73	1.38	7 (10%)	77,107,113	2.01	17 (22%)
22	CLA	1	612	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	1130	1	69,73,73	1.36	6 (8%)	83,113,113	1.88	17 (20%)
39	LUT	4	502	-	42,43,43	2.29	1 (2%)	51,60,60	1.81	12 (23%)
39	LUT	1	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.89	14 (27%)
22	CLA	B	1210	-	69,73,73	1.38	7 (10%)	83,113,113	2.06	20 (24%)
40	CHL	Z	609	12	70,74,74	0.84	3 (4%)	80,114,114	1.25	11 (13%)
28	LMT	F	5001	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
22	CLA	4	615	-	45,49,73	1.68	8 (17%)	54,84,113	2.16	16 (29%)
26	LHG	B	5002	-	19,19,48	0.84	1 (5%)	20,24,54	1.36	1 (5%)
26	LHG	9	801	-	32,32,48	0.45	0	35,38,54	1.11	2 (5%)
22	CLA	B	1201	-	49,53,73	1.60	8 (16%)	59,89,113	2.04	17 (28%)
22	CLA	B	1202	-	69,73,73	1.35	7 (10%)	83,113,113	2.01	20 (24%)
22	CLA	Z	607	-	61,65,73	1.45	7 (11%)	73,103,113	2.00	19 (26%)
22	CLA	B	1205	-	69,73,73	1.36	6 (8%)	83,113,113	2.02	19 (22%)
39	LUT	3	501	-	42,43,43	2.32	1 (2%)	51,60,60	1.95	12 (23%)
22	CLA	8	604	-	66,70,73	1.40	7 (10%)	79,109,113	2.02	23 (29%)
22	CLA	7	606	-	60,64,73	1.46	7 (11%)	72,102,113	2.05	16 (22%)
22	CLA	8	611	-	54,58,73	1.52	7 (12%)	65,95,113	2.19	18 (27%)
22	CLA	B	1219	-	63,67,73	1.44	7 (11%)	75,105,113	2.06	18 (24%)
22	CLA	9	609	20	50,54,73	1.62	7 (14%)	60,90,113	2.07	16 (26%)
39	LUT	6	501	-	42,43,43	2.38	1 (2%)	51,60,60	1.87	14 (27%)
22	CLA	7	613	-	46,50,73	1.67	7 (15%)	55,85,113	2.10	17 (30%)
22	CLA	5	604	-	69,73,73	1.36	8 (11%)	83,113,113	1.96	22 (26%)
22	CLA	2	605	-	54,58,73	1.56	8 (14%)	65,95,113	2.14	19 (29%)
35	T7X	B	5004	-	49,49,61	0.93	4 (8%)	59,61,73	1.03	3 (5%)
39	LUT	5	502	-	42,43,43	2.26	1 (2%)	51,60,60	1.77	11 (21%)
22	CLA	7	615	14	62,66,73	1.44	7 (11%)	74,104,113	2.05	20 (27%)
25	BCR	K	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.24	19 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	8	603	-	-	10/39/115/115	-
22	CLA	A	1132	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CHL	7	610	-	-	4/27/103/117	-
22	CLA	A	1122	-	-	23/39/115/115	-
39	LUT	2	502	-	-	5/29/67/67	0/2/2/2
22	CLA	5	612	-	-	13/39/115/115	-
22	CLA	B	1232	-	-	5/15/91/115	-
39	LUT	9	501	-	-	4/29/67/67	0/2/2/2
40	CHL	1	610	-	-	8/20/96/117	-
40	CHL	5	611	-	-	3/23/99/117	-
40	CHL	9	613	-	-	0/12/88/117	-
40	CHL	4	613	-	1/1/13/21	2/29/105/117	-
22	CLA	8	601	-	-	12/33/109/115	-
31	LMG	J	5001	-	-	14/30/50/70	0/1/1/1
40	CHL	Z	613	-	-	5/17/93/117	-
22	CLA	3	608	-	-	7/15/91/115	-
22	CLA	A	1104	1	-	23/39/115/115	-
40	CHL	6	617	-	-	2/14/90/117	-
22	CLA	A	1126	-	-	22/39/115/115	-
37	C7Z	1	503	-	1/1/12/26	8/29/67/67	0/2/2/2
25	BCR	B	4005	-	-	15/29/63/63	0/2/2/2
25	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
22	CLA	3	604	-	-	6/33/109/115	-
22	CLA	L	1502	-	-	24/39/115/115	-
22	CLA	B	1226	-	-	13/39/115/115	-
26	LHG	5	801	-	-	27/41/41/53	-
22	CLA	B	1207	2	-	18/39/115/115	-
22	CLA	8	608	-	-	10/27/103/115	-
22	CLA	6	604	-	-	13/39/115/115	-
22	CLA	1	602	-	-	7/15/91/115	-
26	LHG	4	801	-	-	30/53/53/53	-
39	LUT	6	502	-	-	4/29/67/67	0/2/2/2
40	CHL	2	613	-	-	6/23/99/117	-
22	CLA	9	603	-	-	14/33/109/115	-
22	CLA	K	1403	10	-	10/20/96/115	-
22	CLA	3	616	-	-	13/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	609	17	-	21/39/115/115	-
22	CLA	6	612	-	-	9/21/97/115	-
22	CLA	3	610	13	-	13/33/109/115	-
40	CHL	6	611	-	-	5/23/99/117	-
22	CLA	5	607	-	-	14/35/111/115	-
26	LHG	A	5001	22	-	16/39/39/53	-
25	BCR	5	504	-	-	11/29/63/63	0/2/2/2
22	CLA	F	1301	-	-	13/39/115/115	-
31	LMG	A	5003	-	-	8/24/44/70	0/1/1/1
27	NKP	A	5004	-	-	12/28/28/28	-
22	CLA	B	1224	-	-	17/39/115/115	-
22	CLA	B	1237	-	-	20/39/115/115	-
22	CLA	2	602	-	-	12/17/93/115	-
22	CLA	6	619	18	-	17/39/115/115	-
22	CLA	5	618	-	-	19/39/115/115	-
43	3PH	5	802	-	-	7/24/24/49	-
22	CLA	9	605	-	-	8/27/103/115	-
28	LMT	A	5006	-	-	9/21/61/61	0/2/2/2
22	CLA	2	606	-	-	10/17/93/115	-
22	CLA	B	1239	2	-	15/39/115/115	-
22	CLA	3	612	-	-	11/33/109/115	-
22	CLA	B	1203	-	-	19/39/115/115	-
22	CLA	B	1236	-	-	25/39/115/115	-
22	CLA	B	1230	-	-	16/31/107/115	-
22	CLA	A	1140	-	-	10/39/115/115	-
22	CLA	5	601	-	-	14/33/109/115	-
22	CLA	3	601	-	-	16/39/115/115	-
26	LHG	4	802	-	-	25/36/36/53	-
39	LUT	7	502	-	-	3/29/67/67	0/2/2/2
26	LHG	B	5001	-	-	13/26/26/53	-
39	LUT	4	501	-	-	3/29/67/67	0/2/2/2
22	CLA	A	1116	-	-	12/33/109/115	-
43	3PH	8	806	-	-	19/31/31/49	-
30	DAO	A	5007	-	-	3/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	3PH	6	802	-	-	12/30/30/49	-
22	CLA	2	615	-	-	8/17/93/115	-
25	BCR	A	4004	-	-	14/29/63/63	0/2/2/2
22	CLA	Z	605	-	-	15/39/115/115	-
22	CLA	4	609	16	-	12/33/109/115	-
22	CLA	B	1221	-	-	12/39/115/115	-
22	CLA	4	604	-	-	11/33/109/115	-
25	BCR	3	505	-	-	11/29/63/63	0/2/2/2
28	LMT	1	803	-	-	4/21/61/61	0/2/2/2
25	BCR	3	506	-	-	15/29/63/63	0/2/2/2
22	CLA	6	609	18	-	11/39/115/115	-
22	CLA	9	612	-	-	3/21/97/115	-
25	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
21	CL0	A	1011	-	-	13/39/115/115	-
25	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
22	CLA	A	1107	1	-	13/39/115/115	-
22	CLA	6	607	-	-	12/27/103/115	-
22	CLA	2	601	-	-	16/33/109/115	-
22	CLA	B	1021	-	-	9/39/115/115	-
22	CLA	B	1227	-	-	11/21/97/115	-
40	CHL	4	617	-	-	2/14/90/117	-
22	CLA	3	602	-	-	6/17/93/115	-
22	CLA	B	1208	-	-	10/29/105/115	-
25	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
22	CLA	6	601	-	-	13/33/109/115	-
22	CLA	6	602	-	-	8/24/100/115	-
22	CLA	A	1131	-	-	16/39/115/115	-
22	CLA	A	1129	-	-	11/21/97/115	-
25	BCR	6	503	-	-	13/29/63/63	0/2/2/2
22	CLA	2	612	-	-	6/21/97/115	-
22	CLA	5	608	-	-	6/15/91/115	-
26	LHG	2	801	-	-	16/38/38/53	-
28	LMT	8	805	-	-	6/21/61/61	0/2/2/2
22	CLA	A	1118	1	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1212	-	-	15/30/106/115	-
25	BCR	3	503	-	-	10/29/63/63	0/2/2/2
22	CLA	A	1102	-	-	9/27/103/115	-
22	CLA	K	1402	-	-	16/27/103/115	-
22	CLA	B	1214	-	-	13/32/108/115	-
25	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
27	NKP	3	802	-	-	5/15/15/28	-
42	QTB	Z	504	-	1/1/5/10	7/11/28/28	0/1/1/1
40	CHL	Z	610	-	1/1/15/21	10/41/117/117	-
22	CLA	3	607	-	-	19/33/109/115	-
40	CHL	6	610	-	1/1/13/21	4/29/105/117	-
22	CLA	6	615	-	-	16/35/111/115	-
22	CLA	B	1222	-	-	10/39/115/115	-
22	CLA	K	1401	-	-	8/17/93/115	-
22	CLA	7	604	-	-	15/39/115/115	-
22	CLA	L	1503	-	-	11/21/97/115	-
22	CLA	A	1109	-	-	15/39/115/115	-
26	LHG	Z	801	-	-	29/47/47/53	-
22	CLA	Z	603	-	-	11/21/97/115	-
22	CLA	B	1206	-	-	21/39/115/115	-
40	CHL	2	610	-	1/1/11/21	1/20/96/117	-
32	DGA	A	5005	-	-	24/45/45/45	-
22	CLA	A	1013	-	-	14/39/115/115	-
22	CLA	G	1601	7	-	11/21/97/115	-
22	CLA	6	606	-	-	19/39/115/115	-
22	CLA	9	601	-	-	16/33/109/115	-
22	CLA	A	1141	26	-	10/24/100/115	-
25	BCR	A	4001	-	-	15/29/63/63	0/2/2/2
22	CLA	B	1022	46	-	9/39/115/115	-
38	SPH	7	804	-	-	7/21/21/21	-
32	DGA	9	802	-	-	21/40/40/45	-
22	CLA	6	608	-	-	12/27/103/115	-
22	CLA	B	1211	-	-	12/33/109/115	-
24	SF4	A	3001	2,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PQN	A	2001	-	-	5/23/43/43	0/2/2/2
22	CLA	A	1108	1	-	18/39/115/115	-
22	CLA	1	613	-	-	9/17/93/115	-
39	LUT	8	502	-	-	4/29/67/67	0/2/2/2
41	SQD	1	802	-	-	17/43/63/69	0/1/1/1
28	LMT	B	5005	-	-	6/21/61/61	0/2/2/2
22	CLA	B	1225	-	-	4/39/115/115	-
25	BCR	B	4001	-	-	12/29/63/63	0/2/2/2
22	CLA	1	604	-	-	13/33/109/115	-
22	CLA	B	1204	-	-	14/39/115/115	-
22	CLA	A	1119	-	-	13/39/115/115	-
22	CLA	A	1117	-	-	20/39/115/115	-
25	BCR	8	503	-	-	11/29/63/63	0/2/2/2
39	LUT	2	503	-	1/1/12/27	9/29/67/67	0/2/2/2
38	SPH	7	803	-	-	11/21/21/21	-
22	CLA	A	1112	-	-	11/33/109/115	-
26	LHG	1	801	-	-	26/47/47/53	-
39	LUT	Z	501	-	-	4/29/67/67	0/2/2/2
22	CLA	7	612	-	-	9/21/97/115	-
26	LHG	7	801	-	-	22/41/41/53	-
22	CLA	1	603	-	-	17/39/115/115	-
22	CLA	A	1110	1	-	18/39/115/115	-
22	CLA	7	603	14	-	15/39/115/115	-
25	BCR	4	503	-	-	15/29/63/63	0/2/2/2
22	CLA	6	605	18	-	16/27/103/115	-
22	CLA	7	609	14	-	20/39/115/115	-
25	BCR	6	504	-	-	12/29/63/63	0/2/2/2
24	SF4	C	3003	3	-	-	0/6/5/5
22	CLA	1	605	-	-	9/27/103/115	-
27	NKP	8	802	-	-	12/28/28/28	-
22	CLA	B	1215	-	-	16/33/109/115	-
22	CLA	Z	606	-	-	13/30/106/115	-
25	BCR	5	503	-	-	12/29/63/63	0/2/2/2
25	BCR	J	4001	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	608	-	-	7/15/91/115	-
22	CLA	5	602	-	-	13/35/111/115	-
22	CLA	9	608	-	-	8/15/91/115	-
33	DGD	B	5003	-	-	16/55/95/95	0/2/2/2
40	CHL	6	613	-	1/1/13/21	5/29/105/117	-
22	CLA	4	603	-	-	16/39/115/115	-
22	CLA	1	615	12	-	11/39/115/115	-
22	CLA	B	1216	-	-	28/39/115/115	-
22	CLA	B	1223	-	-	21/39/115/115	-
22	CLA	B	1231	2	-	18/39/115/115	-
22	CLA	7	611	-	-	5/21/97/115	-
26	LHG	3	801	-	-	13/22/22/53	-
22	CLA	4	601	-	-	13/33/109/115	-
22	CLA	Z	615	12	-	9/17/93/115	-
39	LUT	Z	502	-	-	2/29/67/67	0/2/2/2
22	CLA	A	1128	-	-	19/39/115/115	-
22	CLA	7	607	-	-	22/39/115/115	-
23	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
22	CLA	5	613	-	-	12/27/103/115	-
22	CLA	5	615	17	-	10/21/97/115	-
22	CLA	1	607	-	-	17/33/109/115	-
22	CLA	6	618	-	-	10/17/93/115	-
40	CHL	8	610	-	1/1/13/21	5/29/105/117	-
22	CLA	Z	611	-	-	10/27/103/115	-
40	CHL	2	609	19	-	4/23/99/117	-
22	CLA	K	1404	-	-	14/27/103/115	-
41	SQD	2	803	-	-	18/38/58/69	0/1/1/1
22	CLA	Z	601	-	-	13/33/109/115	-
22	CLA	3	605	13	-	8/39/115/115	-
40	CHL	1	609	12	1/1/13/21	3/32/108/117	-
39	LUT	7	501	-	-	3/29/67/67	0/2/2/2
22	CLA	1	606	-	-	12/35/111/115	-
22	CLA	4	608	-	-	16/27/103/115	-
24	SF4	C	3002	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	606	-	-	10/21/97/115	-
22	CLA	A	1105	-	-	15/39/115/115	-
25	BCR	3	504	-	-	12/29/63/63	0/2/2/2
22	CLA	3	618	-	-	10/17/93/115	-
22	CLA	F	1302	-	-	5/15/91/115	-
36	RRX	F	4001	-	1/1/11/25	9/29/65/65	0/2/2/2
22	CLA	A	1113	1	-	9/39/115/115	-
22	CLA	7	601	-	-	9/33/109/115	-
28	LMT	4	803	-	-	9/21/61/61	0/2/2/2
39	LUT	9	502	-	-	3/29/67/67	0/2/2/2
22	CLA	A	1115	-	-	11/33/109/115	-
22	CLA	A	1135	-	-	9/23/99/115	-
40	CHL	5	617	-	-	0/14/90/117	-
28	LMT	B	6101	-	-	10/21/61/61	0/2/2/2
25	BCR	B	4003	-	-	5/29/63/63	0/2/2/2
22	CLA	4	612	-	-	7/21/97/115	-
22	CLA	Z	612	-	-	17/39/115/115	-
40	CHL	4	611	-	-	5/23/99/117	-
40	CHL	5	610	-	1/1/15/21	6/41/117/117	-
22	CLA	B	1241	-	-	20/39/115/115	-
25	BCR	K	4001	-	-	16/29/63/63	0/2/2/2
22	CLA	8	602	-	-	18/39/115/115	-
43	3PH	7	802	-	-	19/40/40/49	-
22	CLA	A	1139	1	-	12/39/115/115	-
22	CLA	7	608	-	-	7/13/89/115	-
22	CLA	B	1238	-	-	13/39/115/115	-
39	LUT	8	501	-	-	3/29/67/67	0/2/2/2
22	CLA	B	1218	-	-	10/39/115/115	-
22	CLA	4	605	-	-	11/39/115/115	-
22	CLA	1	611	-	-	20/39/115/115	-
22	CLA	A	1101	-	-	17/39/115/115	-
22	CLA	3	606	-	-	18/39/115/115	-
40	CHL	3	611	-	1/1/15/21	1/41/117/117	-
22	CLA	A	1106	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	613	46	-	9/27/103/115	-
37	C7Z	5	505	-	1/1/12/26	10/29/67/67	0/2/2/2
22	CLA	B	1229	2	-	13/39/115/115	-
28	LMT	9	803	-	-	9/21/61/61	0/2/2/2
22	CLA	2	604	-	-	13/29/105/115	-
26	LHG	B	5006	-	-	17/37/37/53	-
22	CLA	A	1114	-	-	9/35/111/115	-
22	CLA	A	1120	-	-	12/27/103/115	-
22	CLA	A	1111	-	-	13/39/115/115	-
39	LUT	3	502	-	-	3/29/67/67	0/2/2/2
26	LHG	8	801	-	-	23/42/42/53	-
22	CLA	A	1133	1	-	17/39/115/115	-
22	CLA	2	607	-	-	11/17/93/115	-
22	CLA	4	607	-	-	11/27/103/115	-
22	CLA	9	607	-	-	11/27/103/115	-
22	CLA	A	1121	-	-	23/39/115/115	-
22	CLA	7	605	14	-	14/35/111/115	-
22	CLA	A	1103	1	-	11/39/115/115	-
22	CLA	5	603	-	-	10/29/105/115	-
22	CLA	B	1209	2	-	16/39/115/115	-
22	CLA	8	615	15	-	9/17/93/115	-
40	CHL	9	610	-	1/1/15/21	5/41/117/117	-
22	CLA	8	609	15	-	15/39/115/115	-
22	CLA	9	606	-	-	13/21/97/115	-
22	CLA	G	1602	-	-	7/17/93/115	-
22	CLA	A	1134	1	-	15/27/103/115	-
39	LUT	1	501	-	-	2/29/67/67	0/2/2/2
22	CLA	5	605	-	-	12/27/103/115	-
39	LUT	2	501	-	1/1/12/27	6/29/67/67	0/2/2/2
25	BCR	B	4007	-	-	13/29/63/63	0/2/2/2
39	LUT	Z	503	-	-	10/29/67/67	0/2/2/2
22	CLA	1	601	-	-	15/39/115/115	-
22	CLA	4	602	-	-	9/24/100/115	-
22	CLA	8	605	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Z	602	-	-	6/17/93/115	-
22	CLA	Z	604	-	-	18/39/115/115	-
44	PLM	7	805	-	-	3/15/15/15	-
37	C7Z	J	4002	-	1/1/12/26	13/29/67/67	0/2/2/2
22	CLA	B	1228	2	-	20/39/115/115	-
22	CLA	B	1023	-	-	15/39/115/115	-
25	BCR	G	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	8	612	-	-	11/17/93/115	-
22	CLA	B	1234	-	-	14/33/109/115	-
22	CLA	A	1137	-	-	15/39/115/115	-
22	CLA	A	1123	-	-	12/39/115/115	-
25	BCR	7	504	-	-	12/29/63/63	0/2/2/2
38	SPH	K	5001	-	-	12/21/21/21	-
22	CLA	A	1136	-	-	19/39/115/115	-
22	CLA	B	1235	2	-	17/39/115/115	-
22	CLA	A	1138	1	-	17/39/115/115	-
22	CLA	A	1125	-	-	17/39/115/115	-
43	3PH	2	802	-	-	8/28/28/49	-
26	LHG	6	801	-	-	37/53/53/53	-
22	CLA	2	603	-	-	10/27/103/115	-
22	CLA	A	1012	-	-	17/39/115/115	-
22	CLA	B	1217	2	-	12/29/105/115	-
22	CLA	9	604	-	-	13/39/115/115	-
22	CLA	6	603	-	-	19/39/115/115	-
40	CHL	4	610	-	1/1/12/21	4/23/99/117	-
22	CLA	Z	608	-	-	15/29/105/115	-
22	CLA	8	607	-	-	15/27/103/115	-
22	CLA	9	602	-	-	4/15/91/115	-
25	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
22	CLA	A	1124	46	-	17/39/115/115	-
22	CLA	J	1901	-	-	8/12/88/115	-
29	OCA	A	5008	-	-	0/7/7/7	-
22	CLA	5	622	-	-	7/17/93/115	-
25	BCR	7	503	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LUT	5	501	-	-	3/29/67/67	0/2/2/2
22	CLA	7	602	-	-	7/21/97/115	-
25	BCR	A	4005	-	-	12/29/63/63	0/2/2/2
26	LHG	A	5002	-	-	31/53/53/53	-
22	CLA	8	606	-	-	16/33/109/115	-
22	CLA	B	1240	-	-	23/39/115/115	-
22	CLA	A	1127	-	-	12/39/115/115	-
22	CLA	7	616	-	-	12/33/109/115	-
25	BCR	I	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	3	603	-	-	19/39/115/115	-
40	CHL	8	613	-	2/2/15/21	12/41/117/117	-
22	CLA	B	1220	-	-	21/39/115/115	-
22	CLA	4	606	-	-	10/21/97/115	-
45	LPX	8	803	-	-	10/31/31/31	-
25	BCR	L	4002	-	-	13/29/63/63	0/2/2/2
22	CLA	B	1213	2	-	17/39/115/115	-
22	CLA	1	608	-	-	13/33/109/115	-
22	CLA	1	612	-	-	26/39/115/115	-
22	CLA	A	1130	1	-	18/39/115/115	-
39	LUT	4	502	-	-	2/29/67/67	0/2/2/2
39	LUT	1	502	-	-	2/29/67/67	0/2/2/2
22	CLA	B	1210	-	-	21/39/115/115	-
40	CHL	Z	609	12	1/1/15/21	12/41/117/117	-
28	LMT	F	5001	-	-	6/21/61/61	0/2/2/2
22	CLA	4	615	-	-	6/10/86/115	-
26	LHG	B	5002	-	-	13/22/22/53	-
26	LHG	9	801	-	-	20/37/37/53	-
22	CLA	B	1201	-	-	4/15/91/115	-
22	CLA	B	1202	-	-	10/39/115/115	-
22	CLA	Z	607	-	-	17/30/106/115	-
22	CLA	B	1205	-	-	14/39/115/115	-
39	LUT	3	501	-	-	1/29/67/67	0/2/2/2
22	CLA	8	604	-	-	8/36/112/115	-
22	CLA	7	606	-	-	17/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	8	611	-	-	8/21/97/115	-
22	CLA	B	1219	-	-	17/32/108/115	-
22	CLA	9	609	20	-	9/17/93/115	-
39	LUT	6	501	-	-	5/29/67/67	0/2/2/2
22	CLA	7	613	-	-	4/12/88/115	-
22	CLA	5	604	-	-	11/39/115/115	-
22	CLA	2	605	-	-	11/21/97/115	-
35	T7X	B	5004	-	-	14/44/68/80	0/1/1/1
39	LUT	5	502	-	-	2/29/67/67	0/2/2/2
22	CLA	7	615	14	-	14/31/107/115	-
25	BCR	K	4002	-	-	11/29/63/63	0/2/2/2

The worst 5 of 1968 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	503	C7Z	C25-C26	15.92	1.62	1.34
37	5	505	C7Z	C25-C26	15.89	1.62	1.34
37	J	4002	C7Z	C25-C26	15.74	1.61	1.34
37	5	505	C7Z	C5-C6	15.41	1.61	1.34
37	1	503	C7Z	C5-C6	15.37	1.61	1.34

The worst 5 of 5205 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	504	BCR	C10-C11-C12	18.05	179.54	123.22
25	5	504	BCR	C10-C11-C12	17.86	178.96	123.22
25	7	504	BCR	C10-C11-C12	17.63	178.24	123.22
25	3	504	BCR	C10-C11-C12	17.62	178.19	123.22
25	A	4002	BCR	C10-C11-C12	17.57	178.04	123.22

5 of 21 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	F	4001	RRX	C28
37	J	4002	C7Z	C3
37	1	503	C7Z	C3
37	5	505	C7Z	C3
39	2	501	LUT	C26

5 of 4209 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	1011	CL0	C2B-C3B-CAB-CBB
21	A	1011	CL0	C4B-C3B-CAB-CBB
22	A	1012	CLA	CBD-CGD-O2D-CED
22	A	1012	CLA	C2-C3-C5-C6
22	A	1012	CLA	C4-C3-C5-C6

There are no ring outliers.

290 monomers are involved in 585 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	603	CLA	1	0
22	A	1132	CLA	1	0
40	7	610	CHL	3	0
22	A	1122	CLA	3	0
39	2	502	LUT	4	0
22	5	612	CLA	1	0
22	B	1232	CLA	1	0
39	9	501	LUT	4	0
40	1	610	CHL	1	0
40	9	613	CHL	1	0
22	8	601	CLA	6	0
40	4	613	CHL	1	0
31	J	5001	LMG	1	0
40	Z	613	CHL	4	0
22	3	608	CLA	1	0
22	A	1104	CLA	4	0
40	6	617	CHL	1	0
22	A	1126	CLA	9	0
25	B	4005	BCR	2	0
25	A	4002	BCR	4	0
22	3	604	CLA	4	0
22	L	1502	CLA	1	0
22	B	1226	CLA	3	0
22	B	1207	CLA	2	0
22	8	608	CLA	4	0
22	6	604	CLA	2	0
22	1	602	CLA	1	0
26	4	801	LHG	1	0
39	6	502	LUT	1	0
40	2	613	CHL	1	0
22	9	603	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	616	CLA	1	0
22	5	609	CLA	3	0
22	6	612	CLA	3	0
22	3	610	CLA	1	0
22	5	607	CLA	3	0
26	A	5001	LHG	3	0
25	5	504	BCR	2	0
22	F	1301	CLA	3	0
31	A	5003	LMG	1	0
22	B	1224	CLA	3	0
22	B	1237	CLA	3	0
22	2	602	CLA	1	0
22	6	619	CLA	3	0
22	5	618	CLA	5	0
22	9	605	CLA	3	0
28	A	5006	LMT	1	0
22	B	1239	CLA	2	0
22	3	612	CLA	5	0
22	B	1203	CLA	3	0
22	B	1236	CLA	6	0
22	B	1230	CLA	5	0
22	A	1140	CLA	1	0
22	5	601	CLA	3	0
22	3	601	CLA	3	0
39	7	502	LUT	1	0
26	B	5001	LHG	1	0
39	4	501	LUT	5	0
22	A	1116	CLA	6	0
25	A	4004	BCR	2	0
22	Z	605	CLA	4	0
22	4	609	CLA	4	0
22	B	1221	CLA	3	0
22	4	604	CLA	4	0
25	3	505	BCR	3	0
28	1	803	LMT	2	0
25	3	506	BCR	2	0
22	6	609	CLA	7	0
22	9	612	CLA	2	0
25	L	4001	BCR	1	0
21	A	1011	CL0	5	0
25	B	4004	BCR	4	0
22	A	1107	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	607	CLA	1	0
22	2	601	CLA	1	0
22	B	1021	CLA	6	0
22	B	1227	CLA	2	0
40	4	617	CHL	1	0
22	B	1208	CLA	3	0
25	A	4003	BCR	3	0
22	6	601	CLA	4	0
22	A	1131	CLA	1	0
22	A	1129	CLA	2	0
25	6	503	BCR	3	0
26	2	801	LHG	2	0
28	8	805	LMT	1	0
22	A	1118	CLA	3	0
22	B	1212	CLA	2	0
25	3	503	BCR	1	0
22	K	1402	CLA	2	0
22	B	1214	CLA	6	0
25	B	4002	BCR	3	0
40	Z	610	CHL	5	0
22	3	607	CLA	1	0
40	6	610	CHL	2	0
22	6	615	CLA	2	0
22	B	1222	CLA	4	0
22	K	1401	CLA	4	0
22	7	604	CLA	1	0
22	A	1109	CLA	3	0
26	Z	801	LHG	1	0
22	B	1206	CLA	2	0
40	2	610	CHL	2	0
32	A	5005	DGA	5	0
22	A	1013	CLA	5	0
22	6	606	CLA	1	0
22	9	601	CLA	3	0
25	A	4001	BCR	1	0
22	B	1022	CLA	1	0
38	7	804	SPH	1	0
32	9	802	DGA	4	0
22	6	608	CLA	2	0
22	B	1211	CLA	1	0
23	A	2001	PQN	1	0
22	A	1108	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	613	CLA	2	0
39	8	502	LUT	2	0
41	1	802	SQD	1	0
28	B	5005	LMT	3	0
22	B	1225	CLA	3	0
25	B	4001	BCR	2	0
22	1	604	CLA	2	0
22	B	1204	CLA	1	0
22	A	1119	CLA	3	0
22	A	1117	CLA	4	0
25	8	503	BCR	1	0
39	2	503	LUT	1	0
38	7	803	SPH	1	0
22	A	1112	CLA	2	0
26	1	801	LHG	1	0
39	Z	501	LUT	1	0
22	7	612	CLA	1	0
26	7	801	LHG	2	0
22	1	603	CLA	3	0
22	A	1110	CLA	2	0
22	7	603	CLA	5	0
25	4	503	BCR	2	0
22	6	605	CLA	2	0
22	7	609	CLA	2	0
25	6	504	BCR	1	0
24	C	3003	SF4	1	0
22	1	605	CLA	1	0
22	B	1215	CLA	3	0
22	Z	606	CLA	2	0
25	5	503	BCR	4	0
25	J	4001	BCR	4	0
22	5	602	CLA	2	0
33	B	5003	DGD	4	0
22	1	615	CLA	3	0
22	B	1216	CLA	4	0
22	B	1231	CLA	2	0
22	7	611	CLA	1	0
22	4	601	CLA	4	0
39	Z	502	LUT	4	0
22	A	1128	CLA	5	0
22	7	607	CLA	3	0
22	5	613	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	615	CLA	2	0
22	1	607	CLA	2	0
22	Z	611	CLA	2	0
40	2	609	CHL	3	0
22	K	1404	CLA	1	0
41	2	803	SQD	1	0
22	Z	601	CLA	3	0
22	3	605	CLA	3	0
40	1	609	CHL	1	0
39	7	501	LUT	2	0
22	1	606	CLA	1	0
22	4	608	CLA	1	0
22	5	606	CLA	1	0
22	A	1105	CLA	2	0
25	3	504	BCR	3	0
22	3	618	CLA	3	0
22	F	1302	CLA	2	0
36	F	4001	RRX	1	0
22	A	1113	CLA	1	0
22	7	601	CLA	4	0
28	4	803	LMT	1	0
39	9	502	LUT	2	0
22	A	1115	CLA	4	0
40	5	617	CHL	1	0
28	B	6101	LMT	2	0
25	B	4003	BCR	3	0
22	4	612	CLA	3	0
40	5	610	CHL	6	0
22	B	1241	CLA	1	0
25	K	4001	BCR	2	0
22	8	602	CLA	3	0
43	7	802	3PH	1	0
22	A	1139	CLA	2	0
22	B	1238	CLA	4	0
39	8	501	LUT	4	0
22	B	1218	CLA	1	0
22	4	605	CLA	2	0
22	1	611	CLA	3	0
22	A	1101	CLA	2	0
22	3	606	CLA	4	0
40	3	611	CHL	3	0
22	A	1106	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	613	CLA	3	0
22	B	1229	CLA	2	0
28	9	803	LMT	3	0
22	2	604	CLA	2	0
26	B	5006	LHG	1	0
22	A	1114	CLA	4	0
22	A	1120	CLA	2	0
22	A	1111	CLA	6	0
39	3	502	LUT	5	0
22	A	1133	CLA	5	0
22	2	607	CLA	3	0
22	A	1121	CLA	2	0
22	A	1103	CLA	4	0
22	5	603	CLA	3	0
22	B	1209	CLA	5	0
40	9	610	CHL	1	0
22	8	609	CLA	2	0
22	9	606	CLA	1	0
22	A	1134	CLA	1	0
39	1	501	LUT	2	0
22	5	605	CLA	2	0
39	2	501	LUT	1	0
25	B	4007	BCR	3	0
39	Z	503	LUT	3	0
22	1	601	CLA	4	0
22	4	602	CLA	1	0
22	8	605	CLA	3	0
22	Z	604	CLA	4	0
22	B	1228	CLA	1	0
22	B	1023	CLA	6	0
25	G	4001	BCR	1	0
22	8	612	CLA	1	0
22	B	1234	CLA	4	0
22	A	1137	CLA	4	0
22	A	1123	CLA	1	0
25	7	504	BCR	1	0
38	K	5001	SPH	1	0
22	A	1136	CLA	2	0
22	B	1235	CLA	3	0
22	A	1138	CLA	5	0
22	A	1125	CLA	3	0
26	6	801	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2	603	CLA	3	0
22	A	1012	CLA	7	0
22	B	1217	CLA	2	0
22	9	604	CLA	4	0
22	6	603	CLA	3	0
40	4	610	CHL	3	0
22	8	607	CLA	4	0
22	9	602	CLA	1	0
25	B	4006	BCR	2	0
22	A	1124	CLA	5	0
22	J	1901	CLA	3	0
22	5	622	CLA	1	0
25	7	503	BCR	3	0
39	5	501	LUT	4	0
22	7	602	CLA	2	0
25	A	4005	BCR	5	0
26	A	5002	LHG	4	0
22	8	606	CLA	4	0
22	B	1240	CLA	8	0
22	A	1127	CLA	6	0
22	7	616	CLA	3	0
25	I	4001	BCR	3	0
22	3	603	CLA	3	0
40	8	613	CHL	4	0
22	B	1220	CLA	5	0
22	4	606	CLA	1	0
45	8	803	LPX	1	0
25	L	4002	BCR	2	0
22	B	1213	CLA	4	0
22	1	608	CLA	4	0
22	A	1130	CLA	3	0
39	4	502	LUT	6	0
39	1	502	LUT	4	0
22	B	1210	CLA	4	0
40	Z	609	CHL	3	0
22	B	1202	CLA	2	0
22	Z	607	CLA	2	0
22	B	1205	CLA	3	0
39	3	501	LUT	2	0
22	8	604	CLA	1	0
22	7	606	CLA	2	0
22	8	611	CLA	1	0

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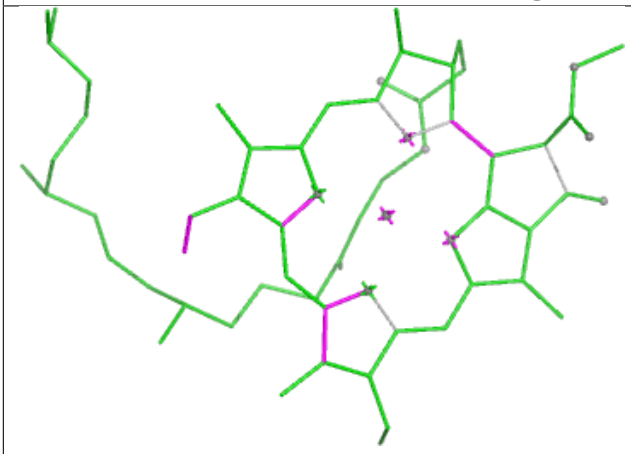
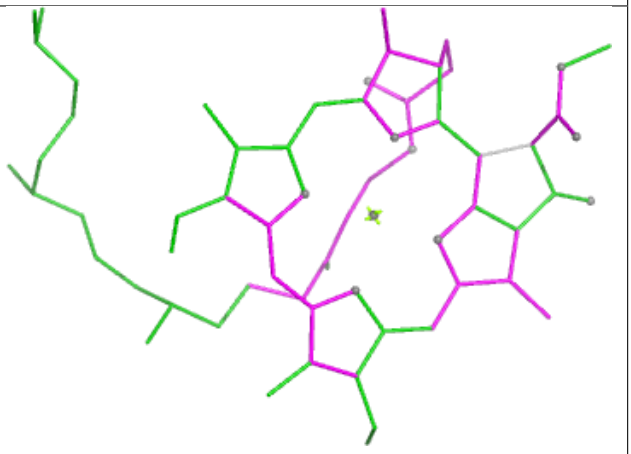
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	6	501	LUT	3	0
22	7	613	CLA	3	0
22	5	604	CLA	2	0
22	2	605	CLA	1	0
39	5	502	LUT	4	0
22	7	615	CLA	1	0
25	K	4002	BCR	3	0

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

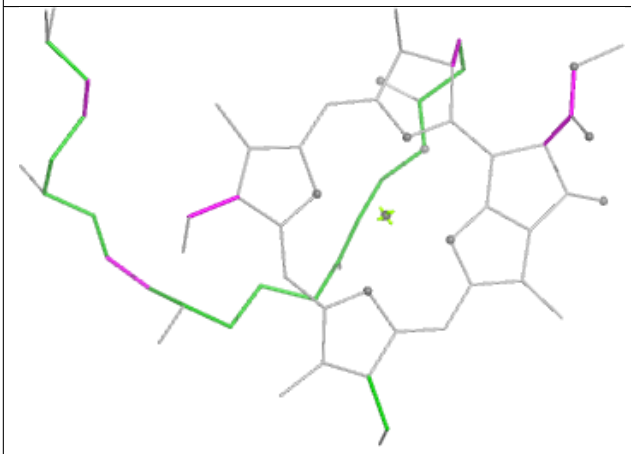
Ligand CLA 8 603



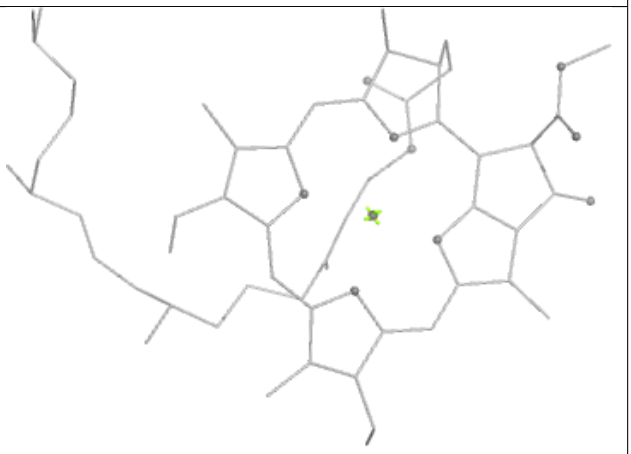
Bond lengths



Bond angles

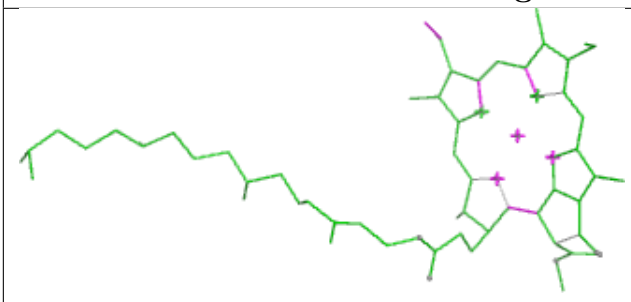


Torsions

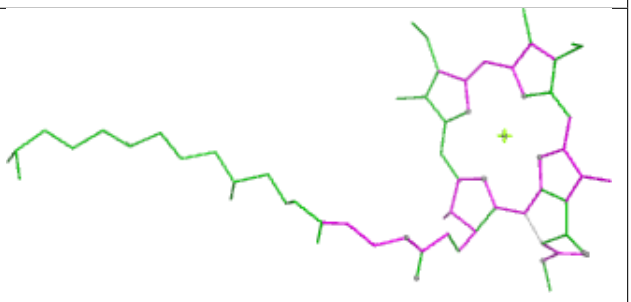


Rings

Ligand CLA A 1132



Bond lengths



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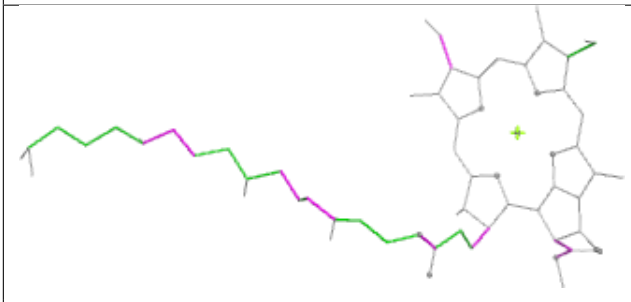
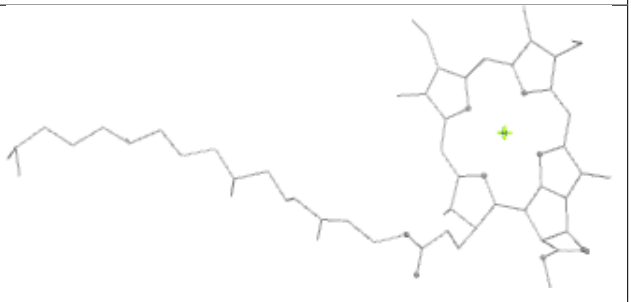
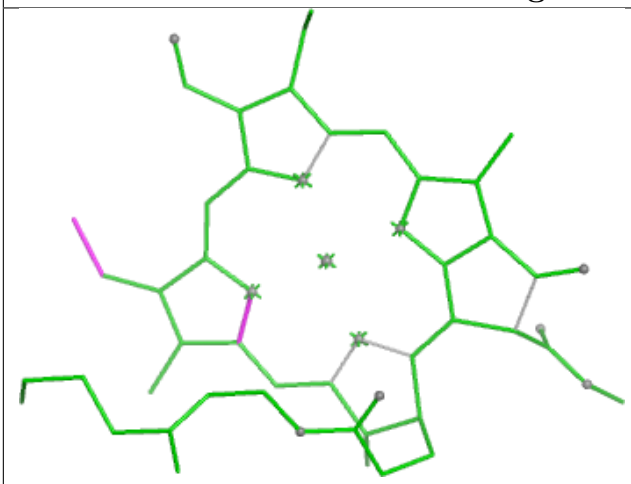


Torsions

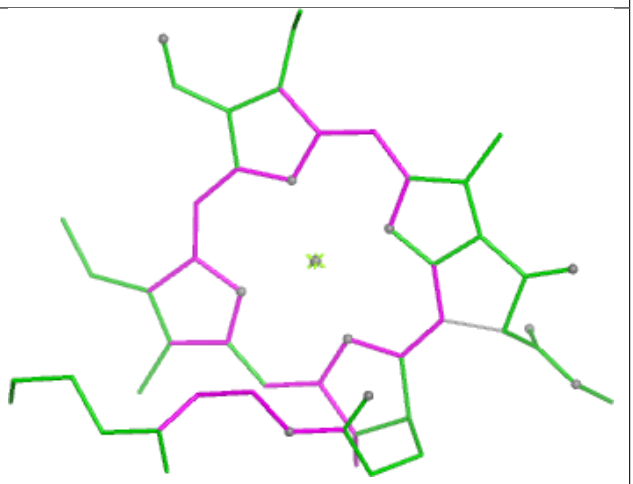


Rings

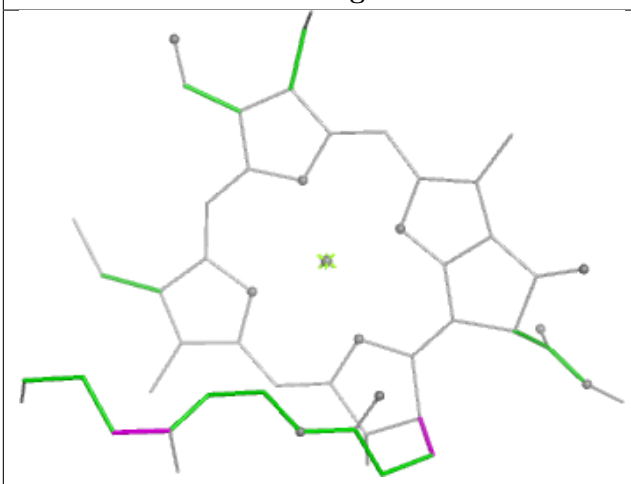
Ligand CHL 7 610



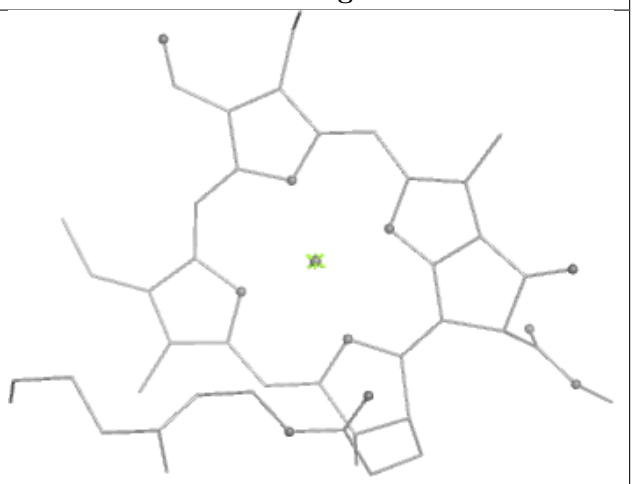
Bond lengths



Bond angles

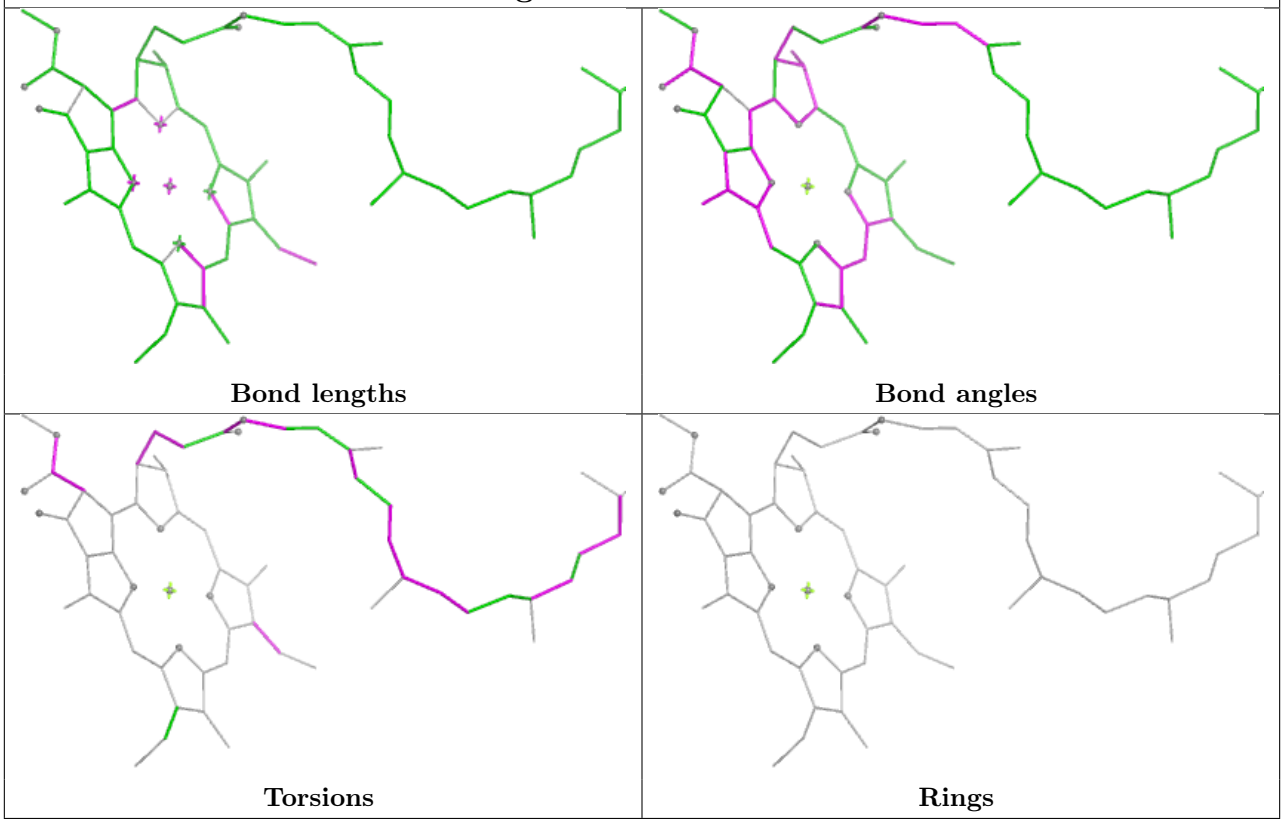


Torsions

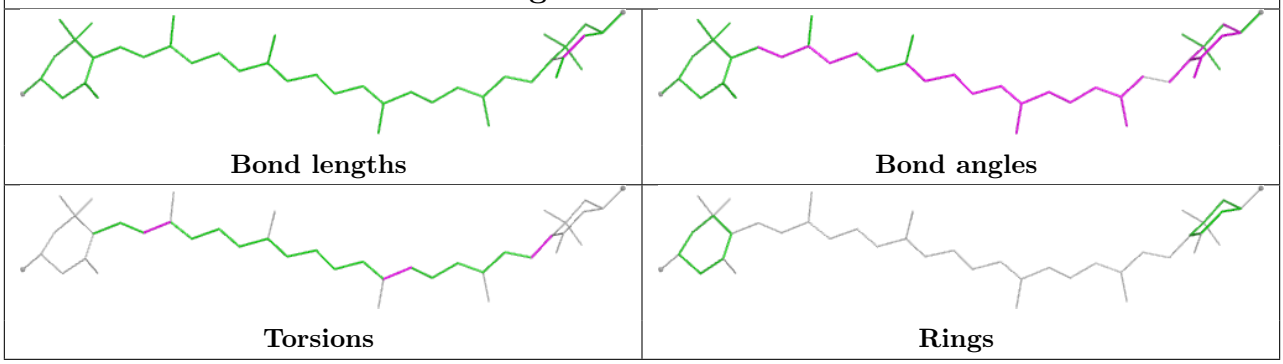


Rings

Ligand CLA A 1122



Ligand LUT 2 502



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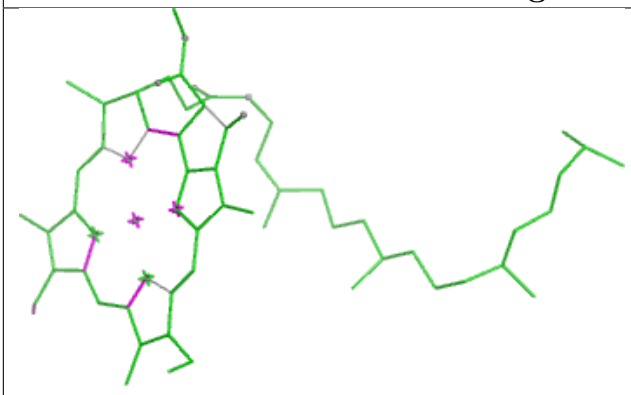
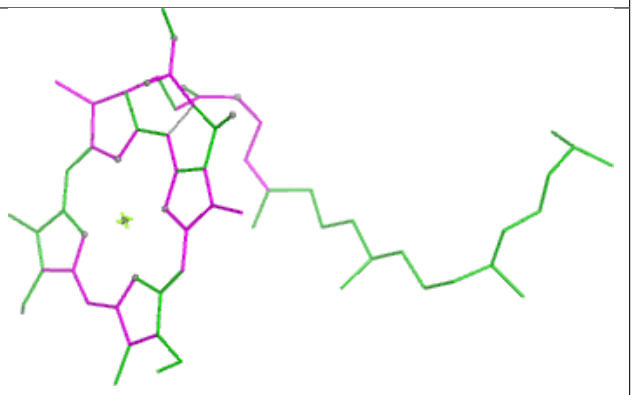
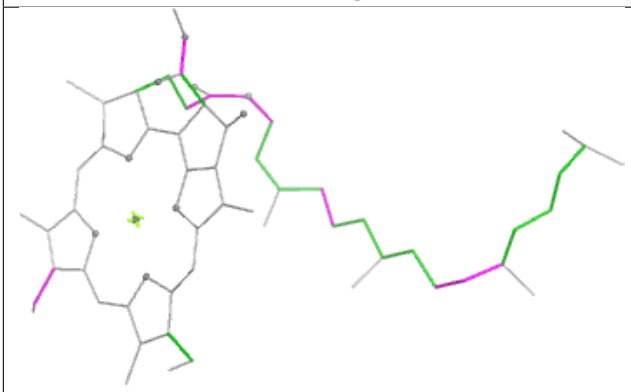


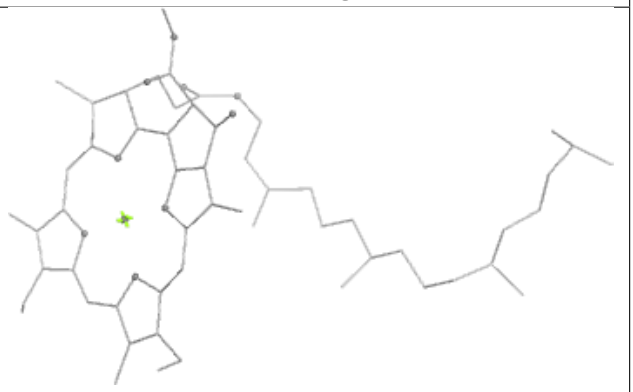
Bond lengths



Bond angles

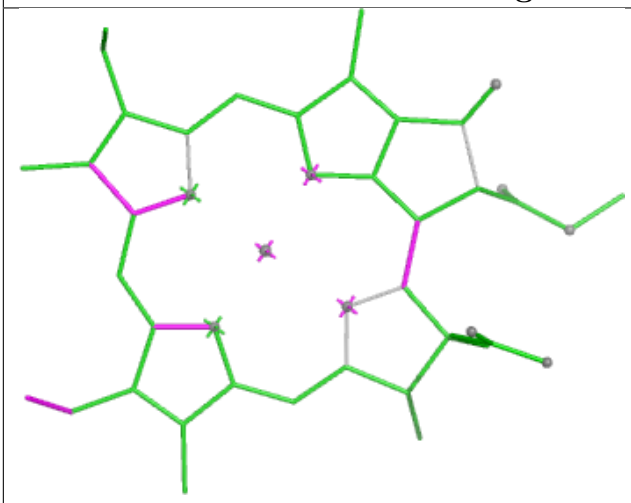


Torsions



Rings

Ligand CLA B 1232



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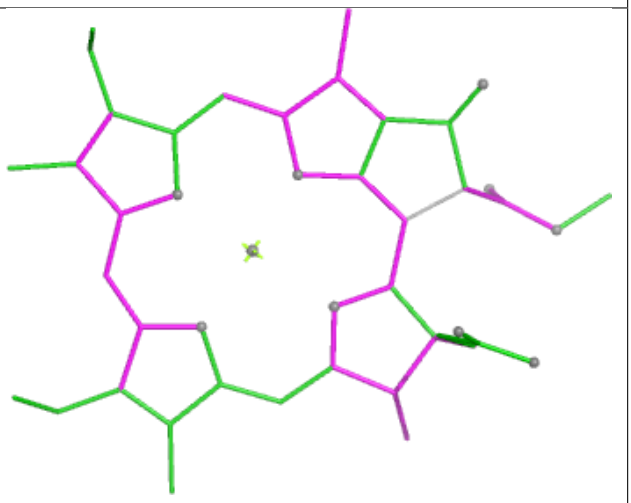
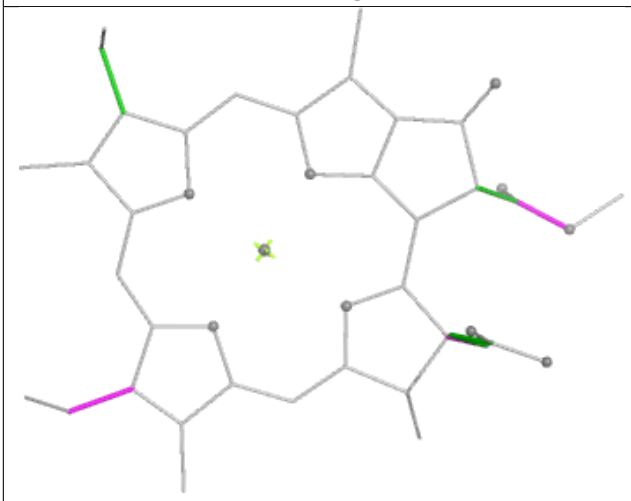


Bond angles



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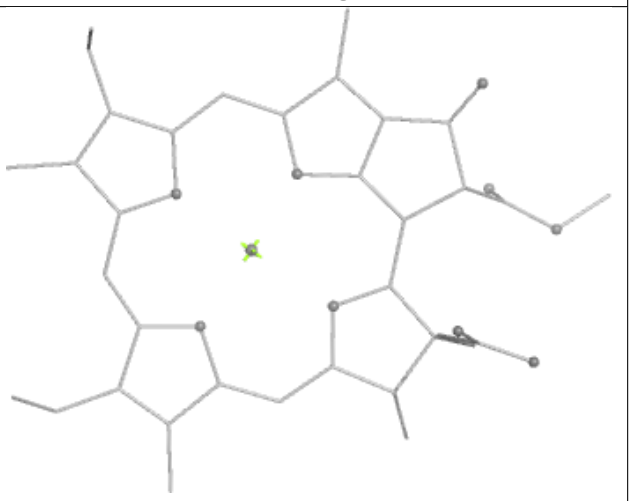

Rings

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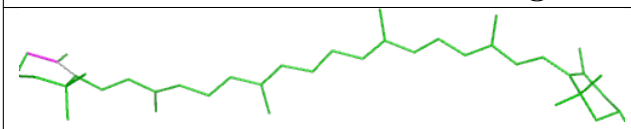

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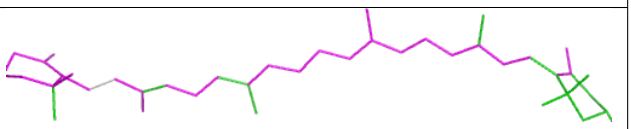
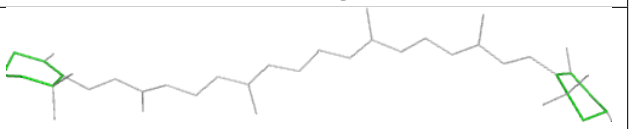


Bond angles

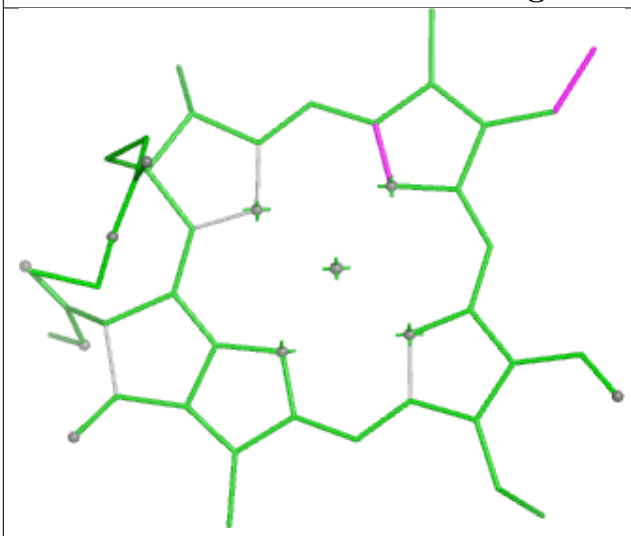


Torsions



Rings

Ligand CHL 1 610



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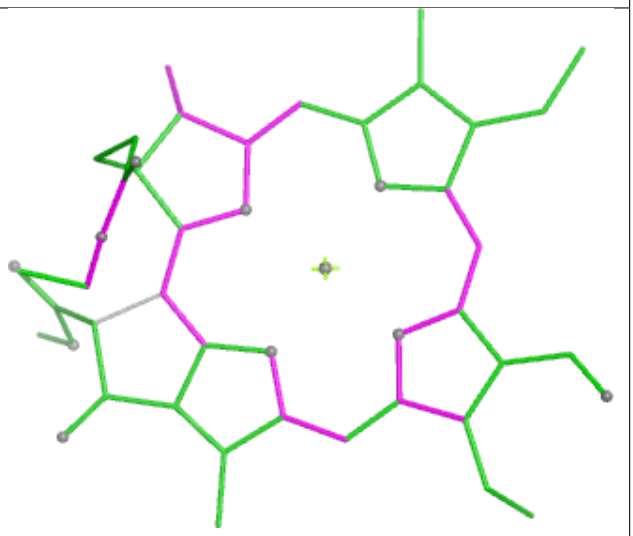

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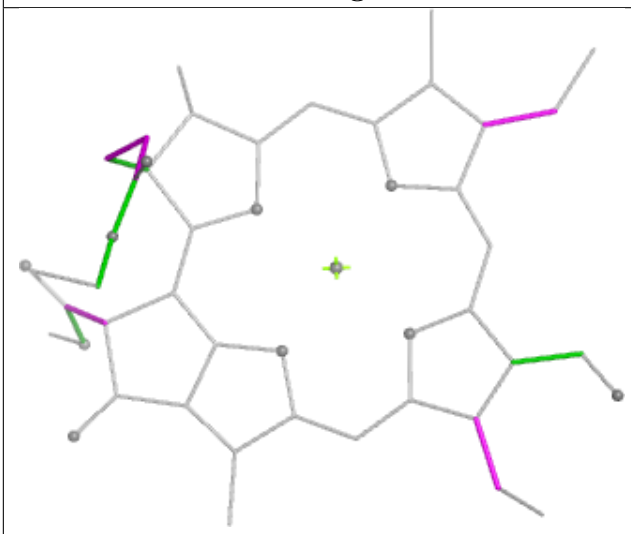

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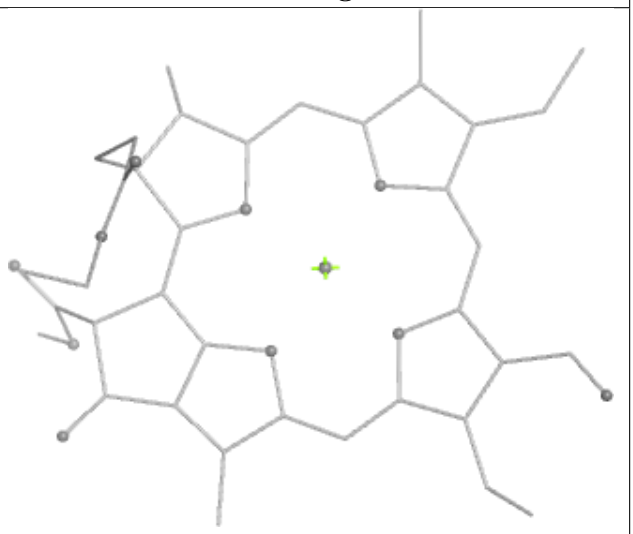

Rings

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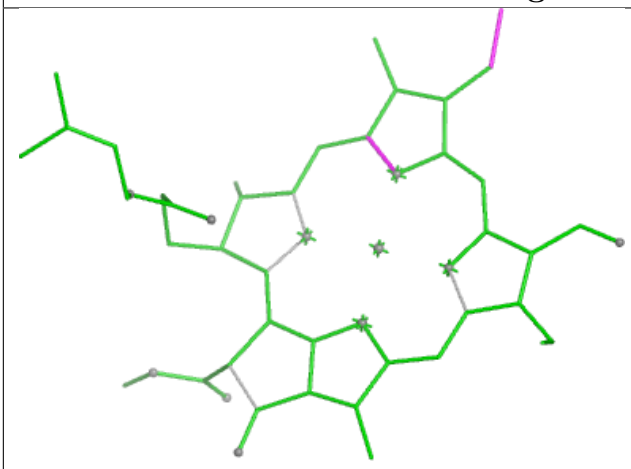

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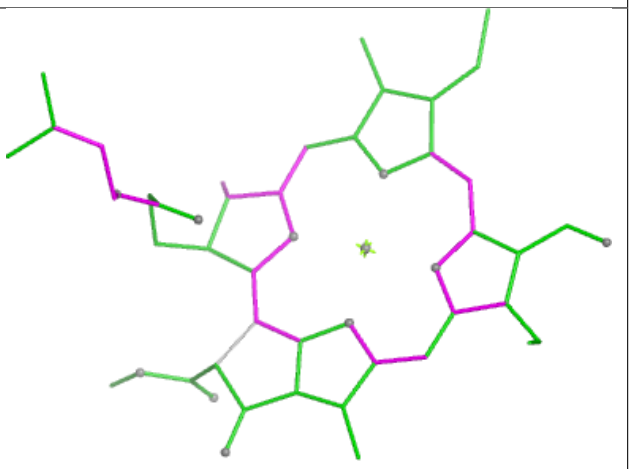

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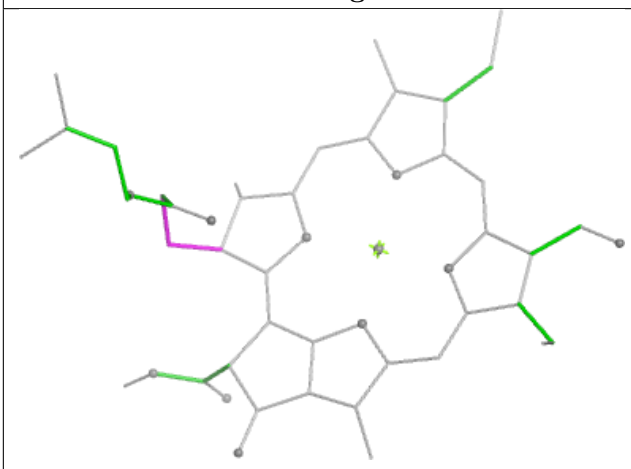

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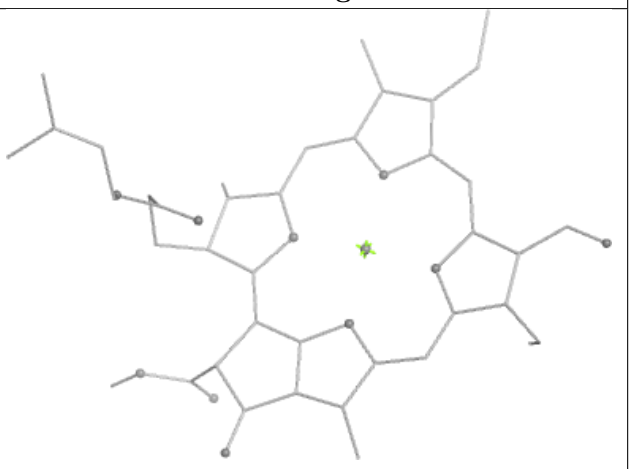
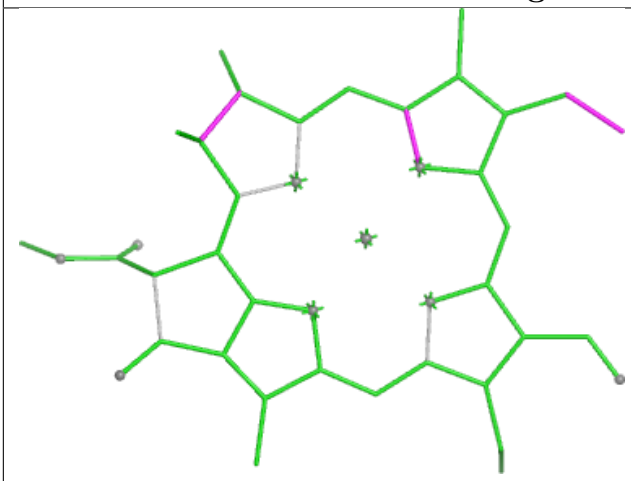


Rings

Ligand CHL 9 613



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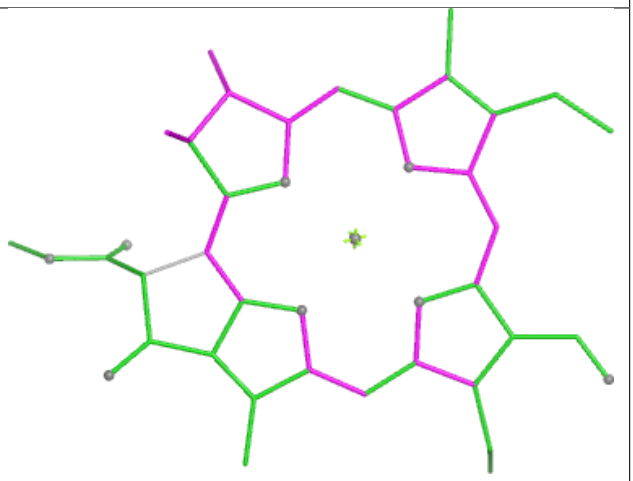
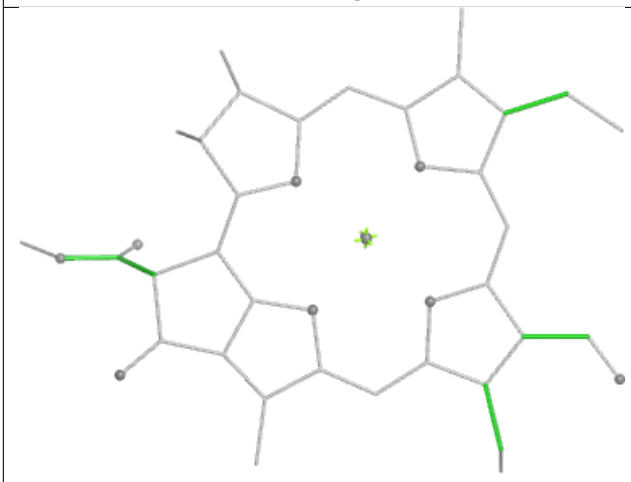


Bond angles



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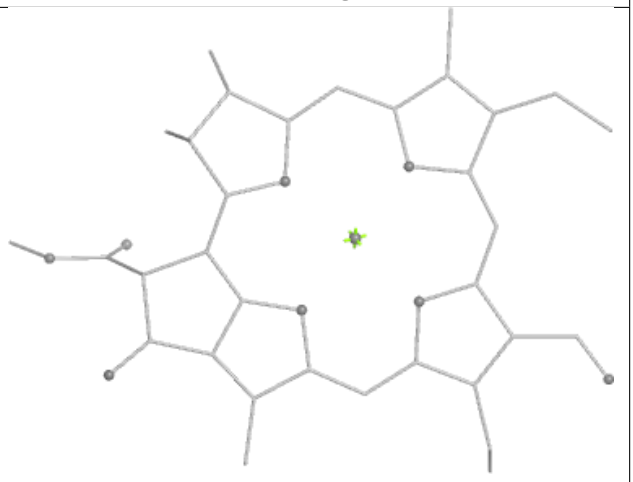
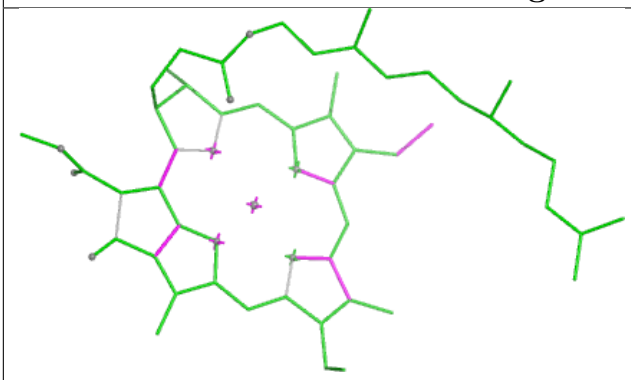


Rings

Ligand CLA 8 601



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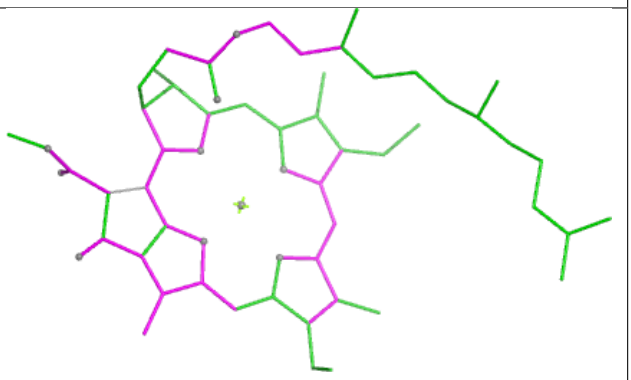
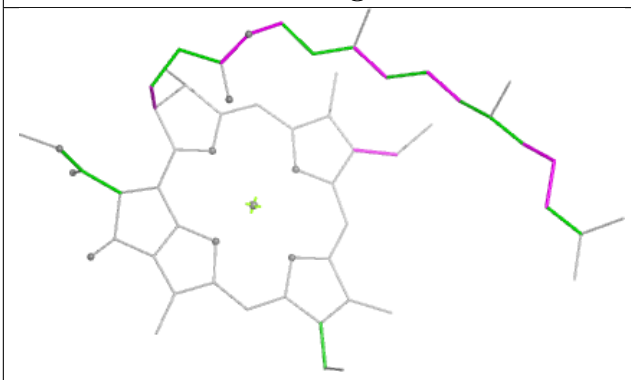
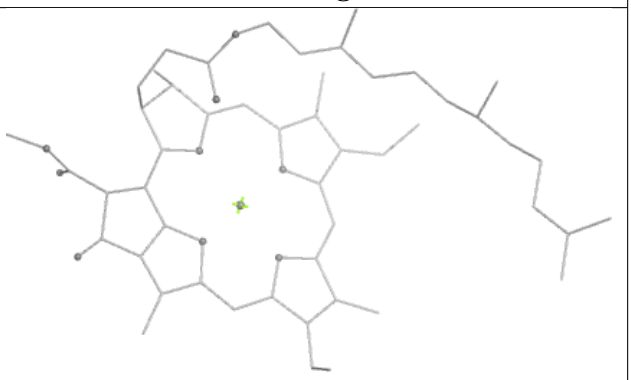


Bond angles

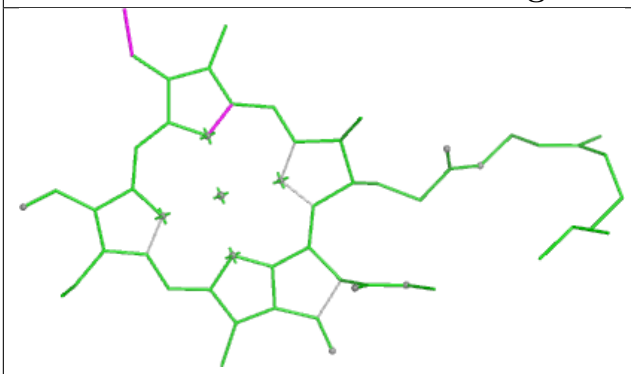


Torsions



Rings

Ligand CHL 4 613



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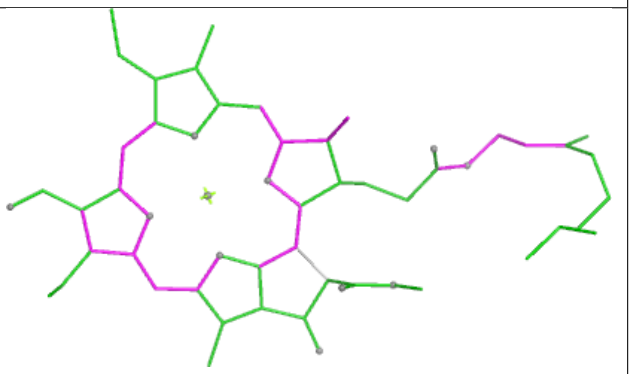
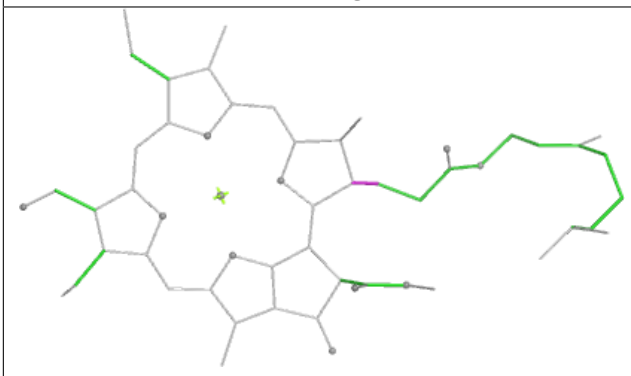


Bond angles



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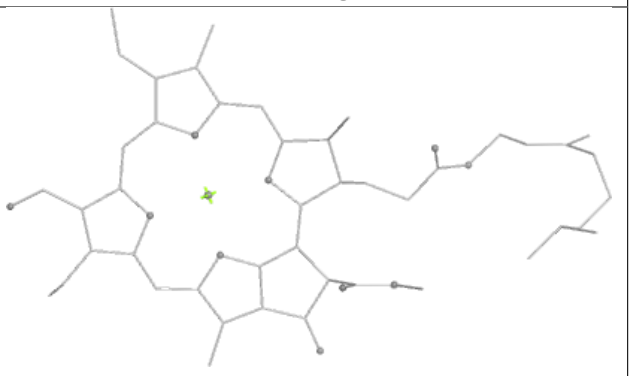
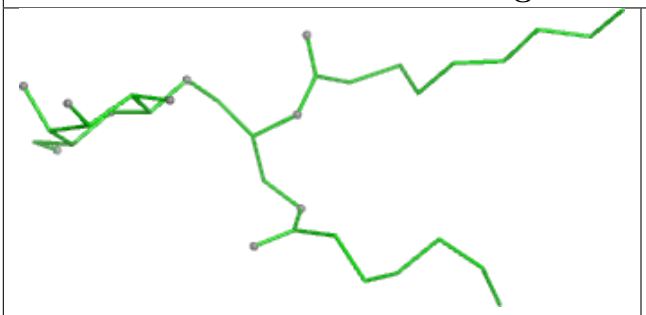


Rings

Ligand LMG J 5001



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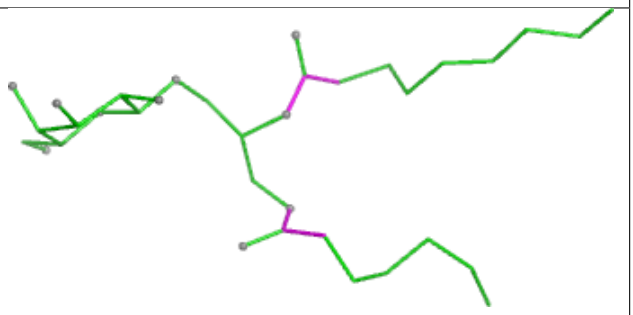

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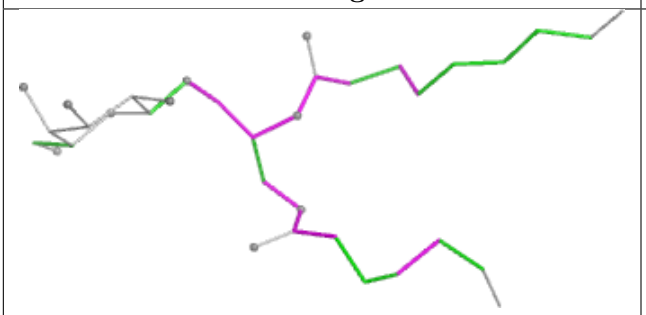

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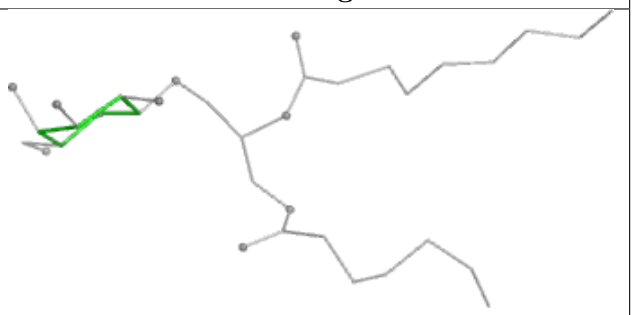
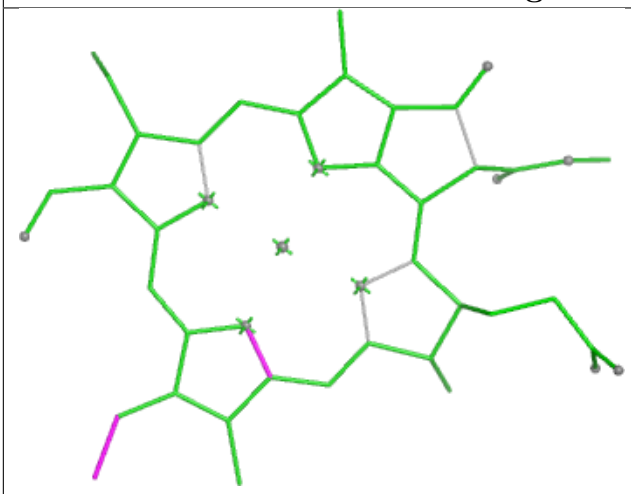


Rings

Ligand CHL Z 613



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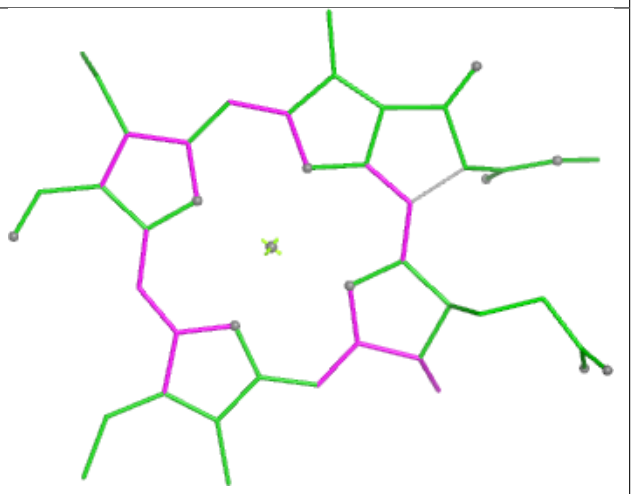

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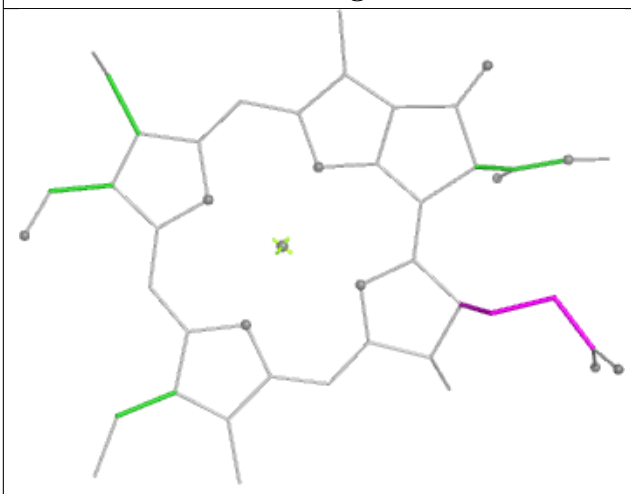

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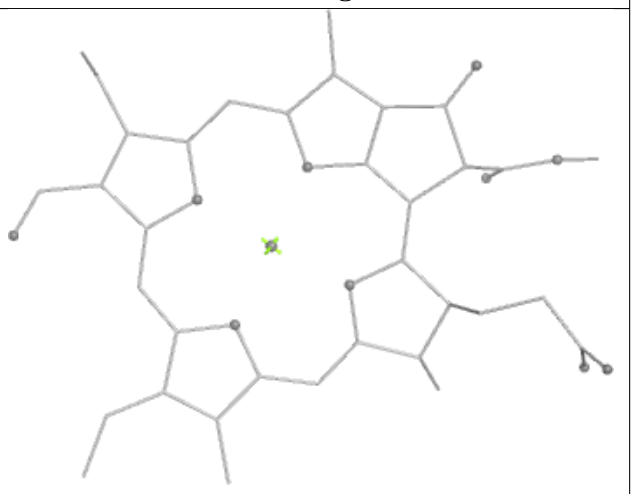
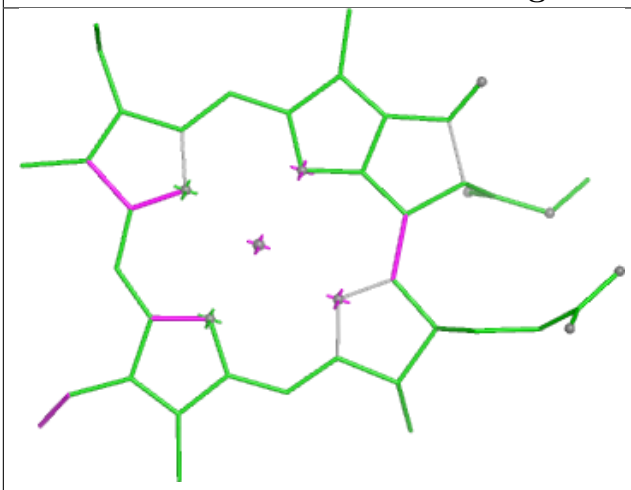


Rings

Ligand CLA 3 608



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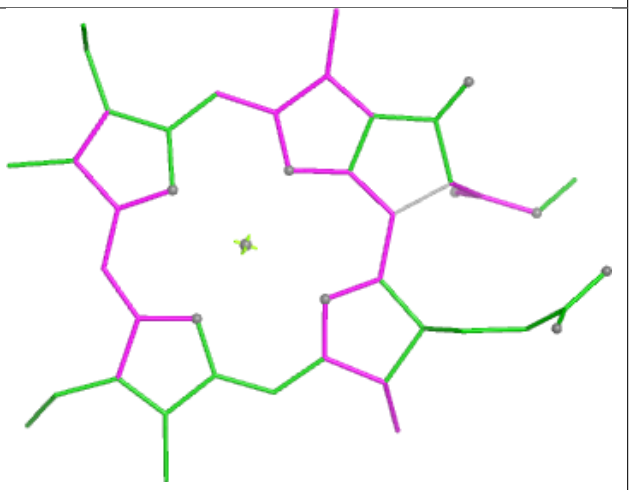

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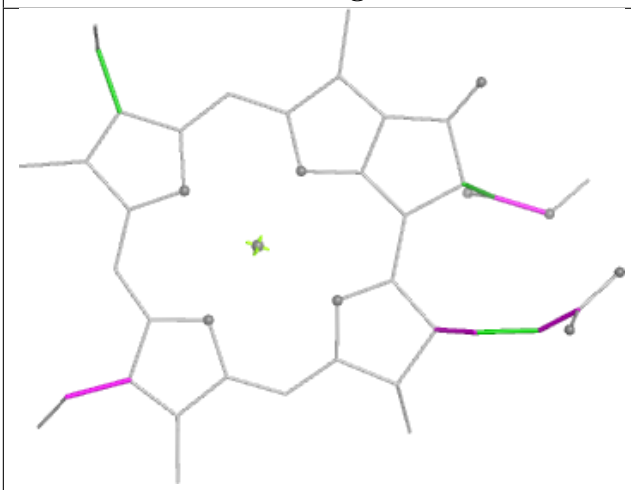

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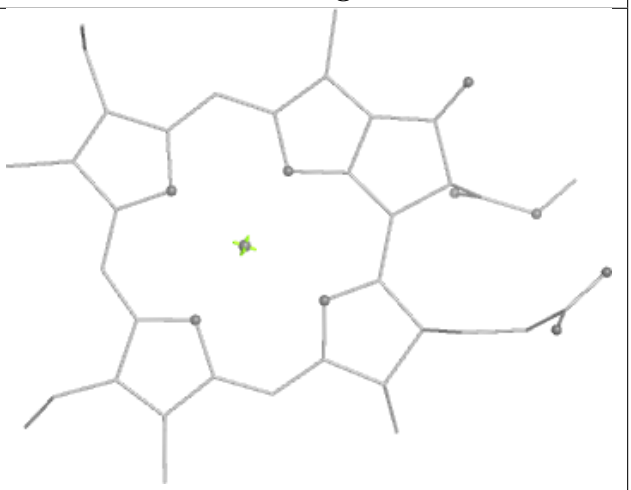
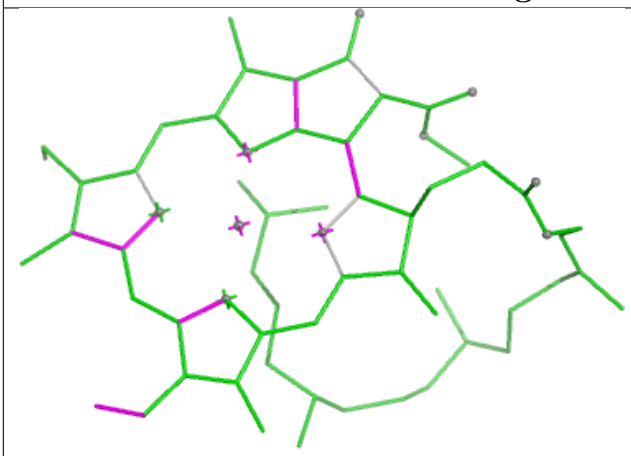


Rings

Ligand CLA A 1104



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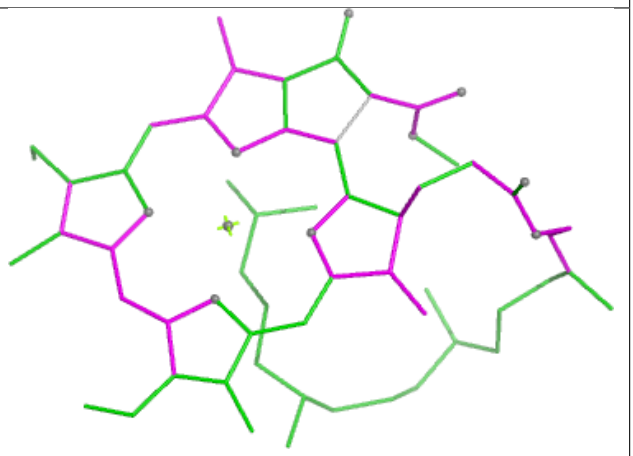

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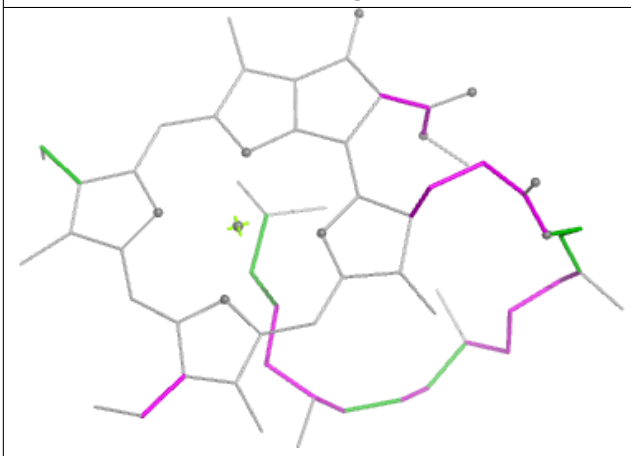

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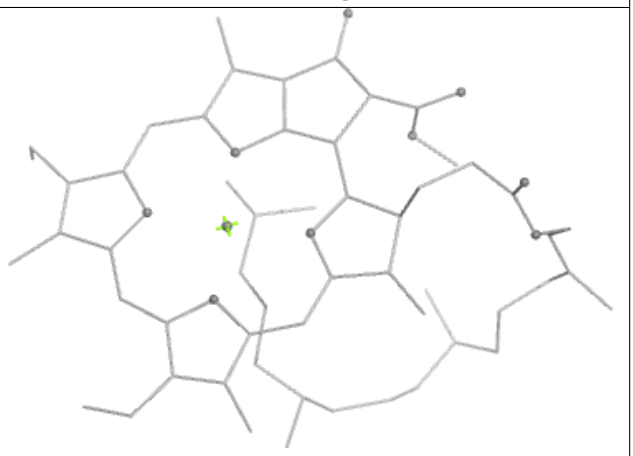
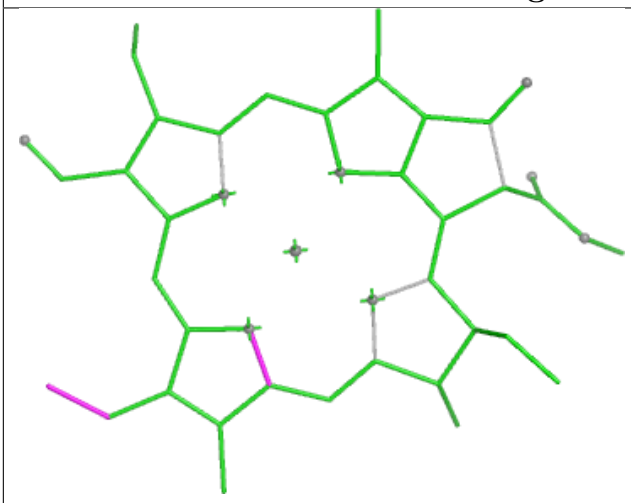


Rings

Ligand CHL 6 617



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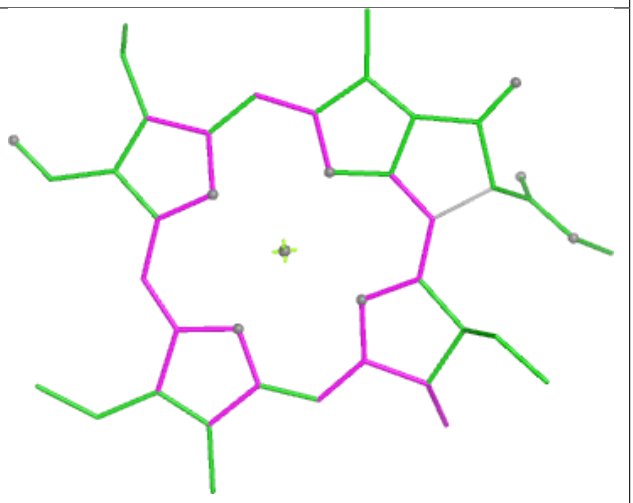
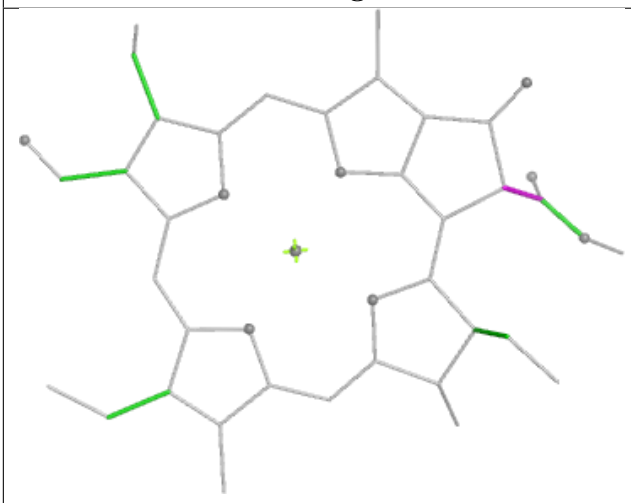


Bond angles



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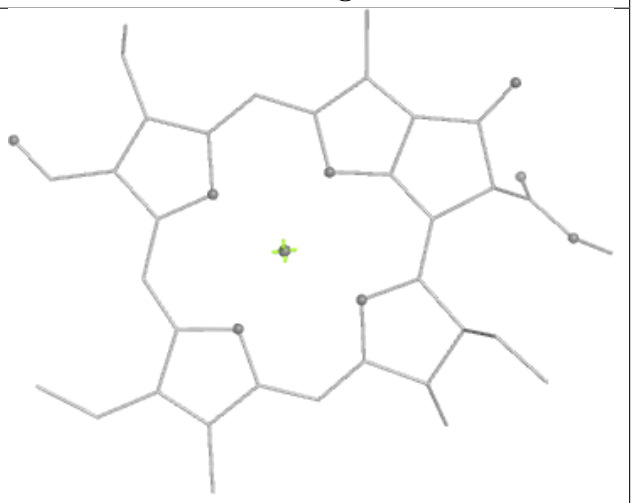
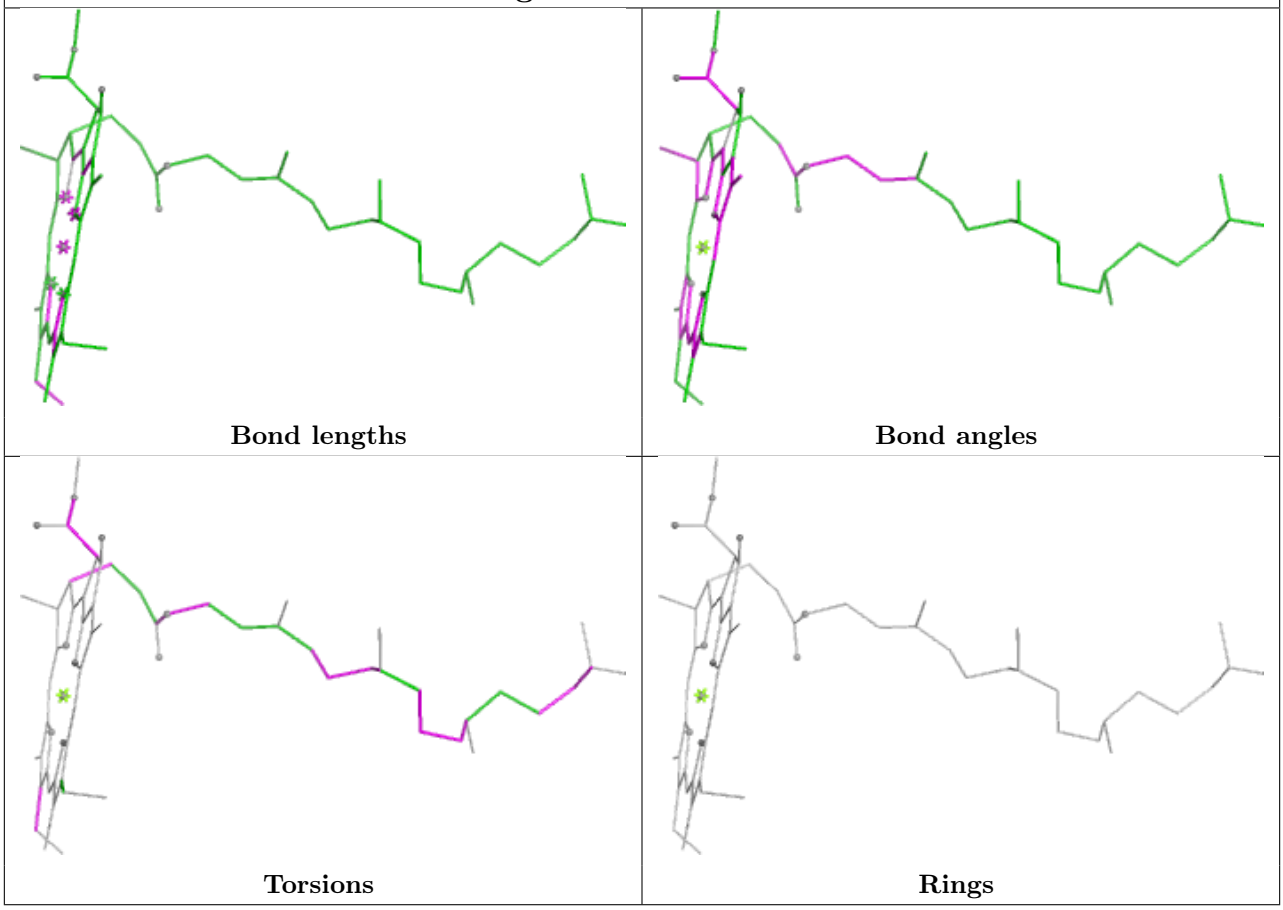
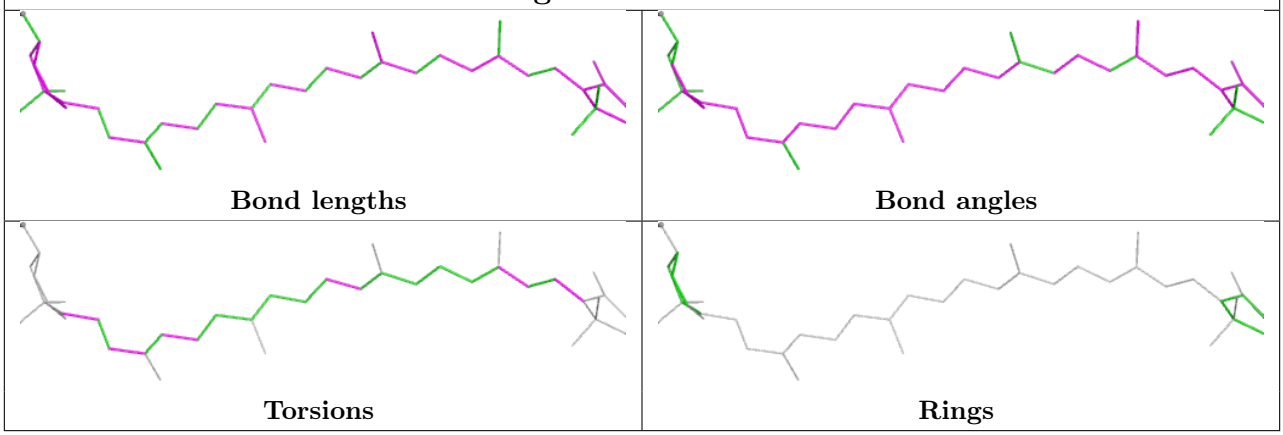


Rings

Ligand CLA A 1126



Ligand C7Z 1 503



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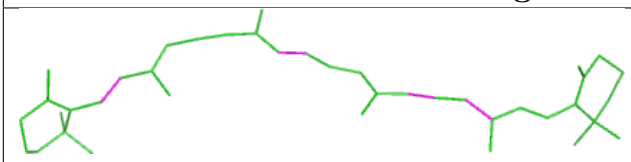
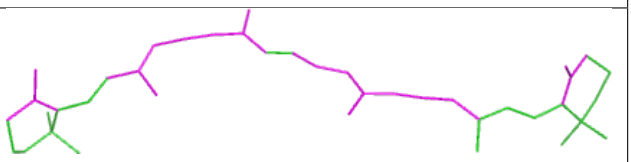
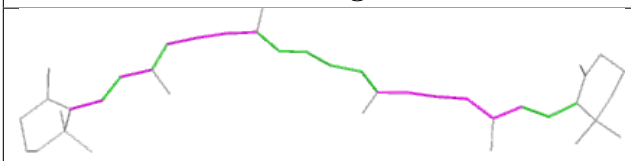
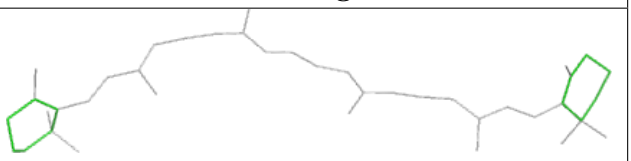
 Bond lengths	 Bond angles
 Torsions	 Rings

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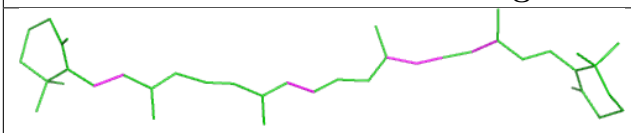
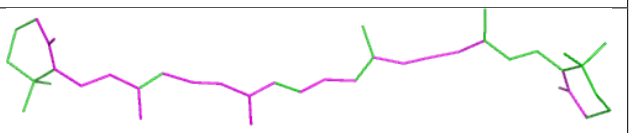
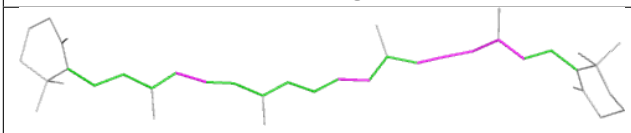
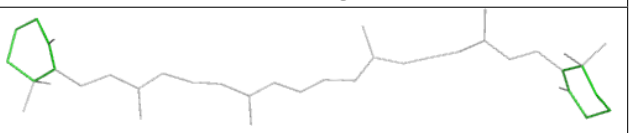
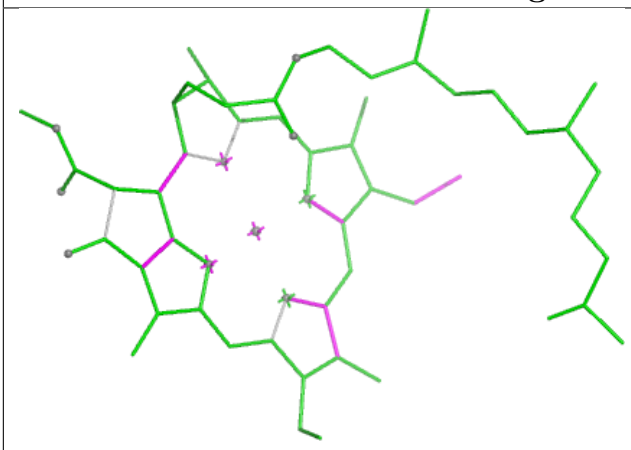
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 604



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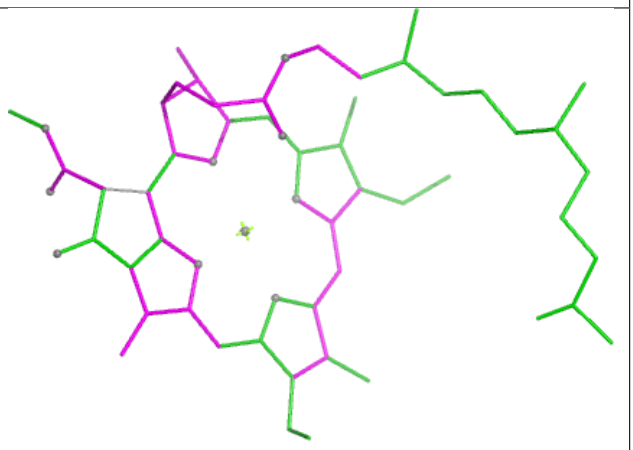
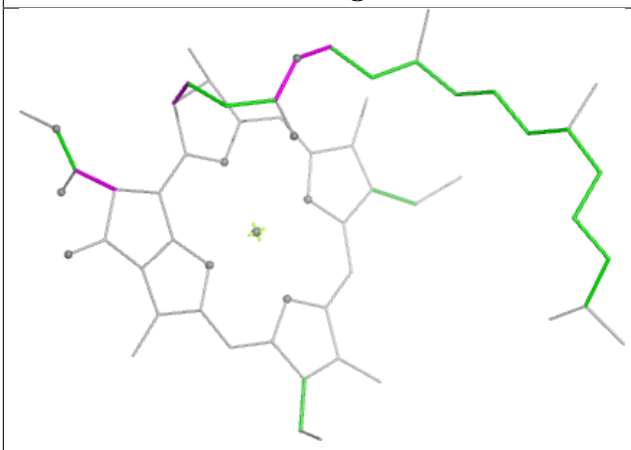


Bond angles

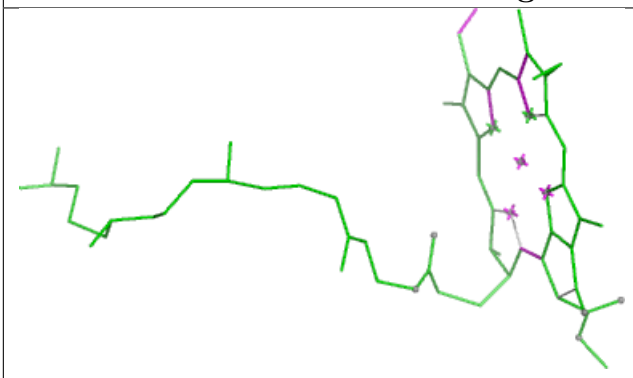


Torsions



Rings

Ligand CLA L 1502



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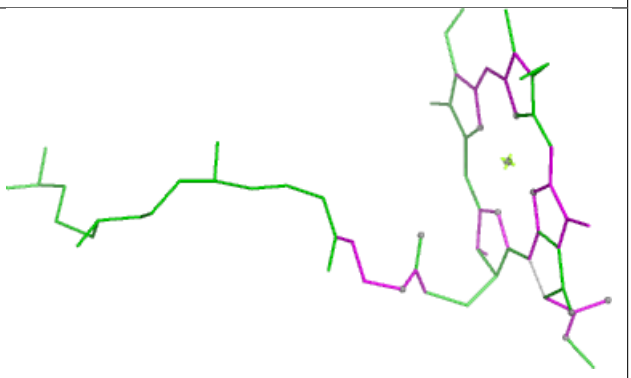
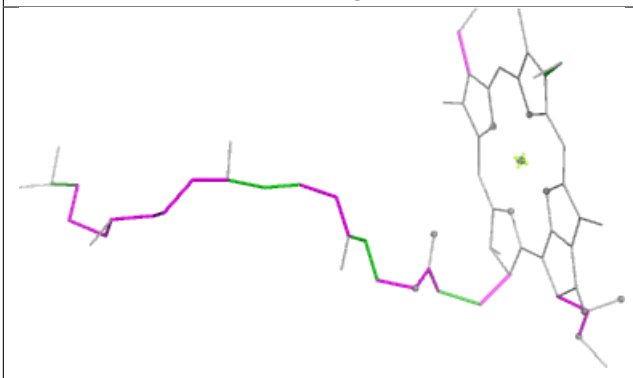


Bond angles

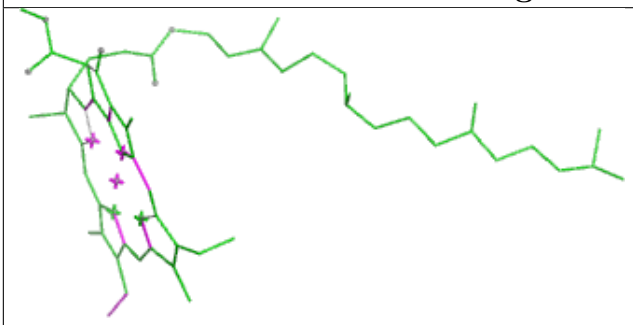


Torsions



Rings

Ligand CLA B 1226



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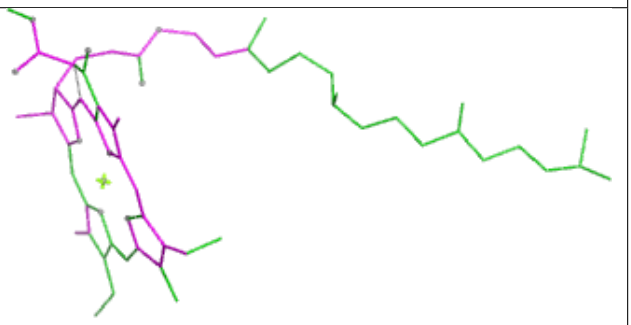

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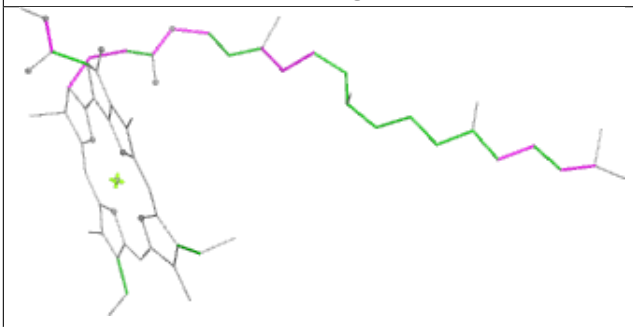

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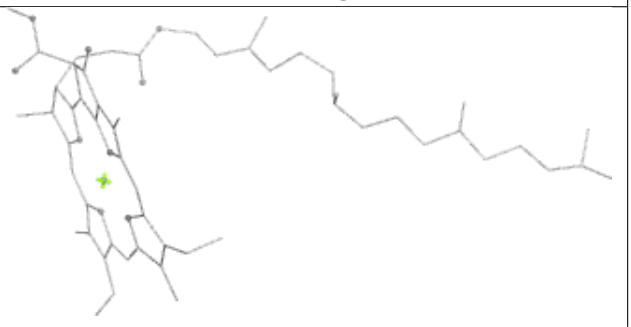
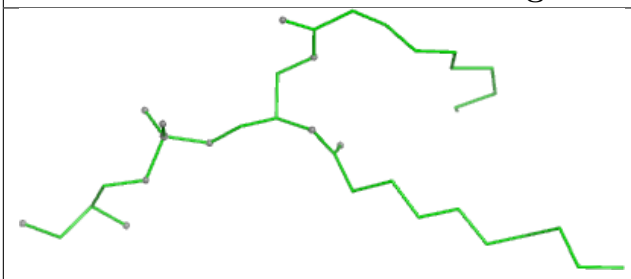


Rings

Ligand LHG 5 801



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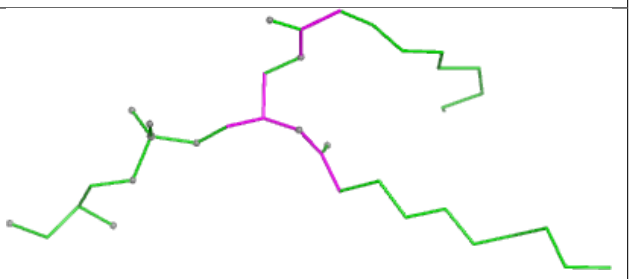

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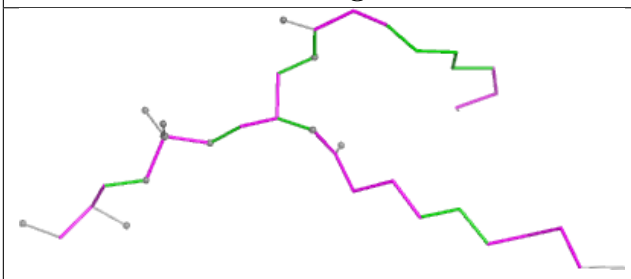

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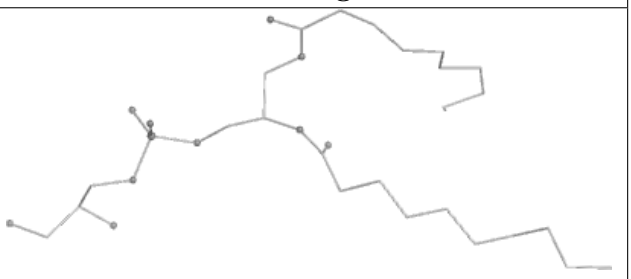
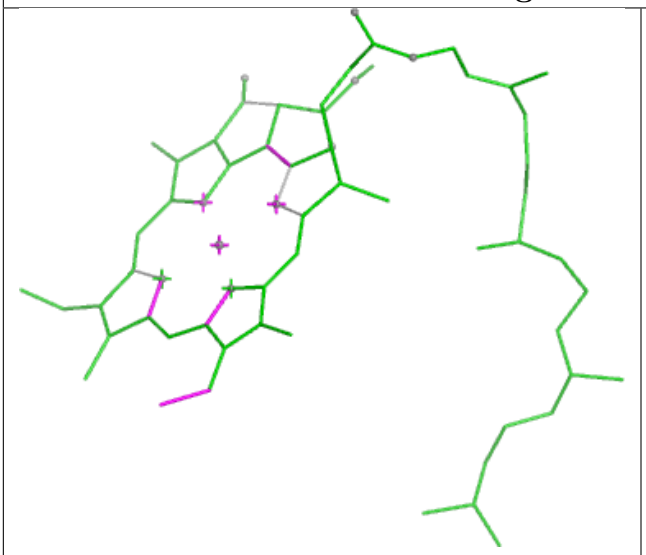
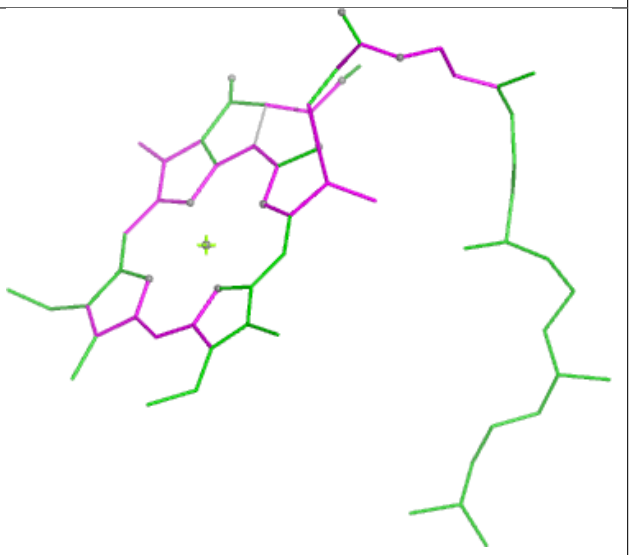


Rings

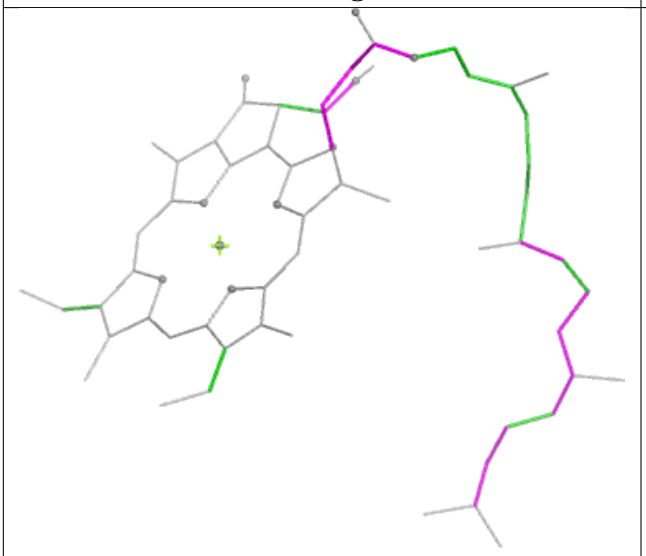
Ligand CLA B 1207



Bond lengths



Bond angles



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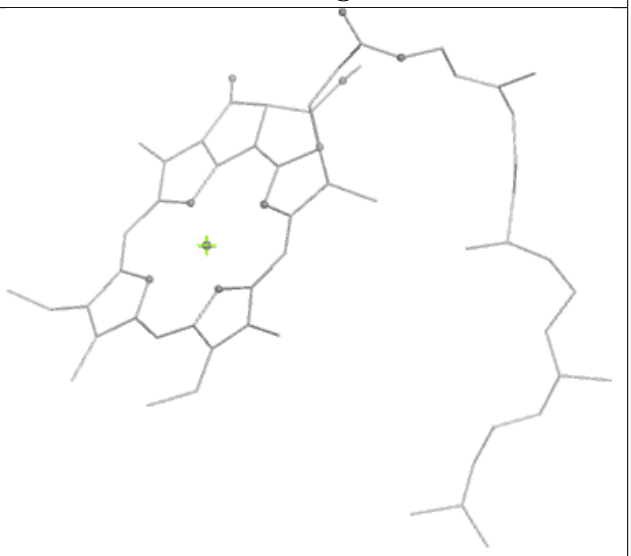
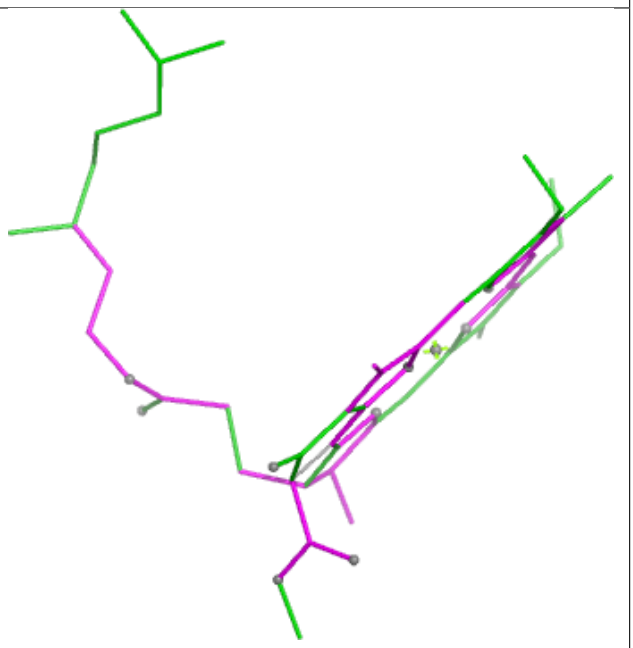


Rings

Ligand CLA 8 608



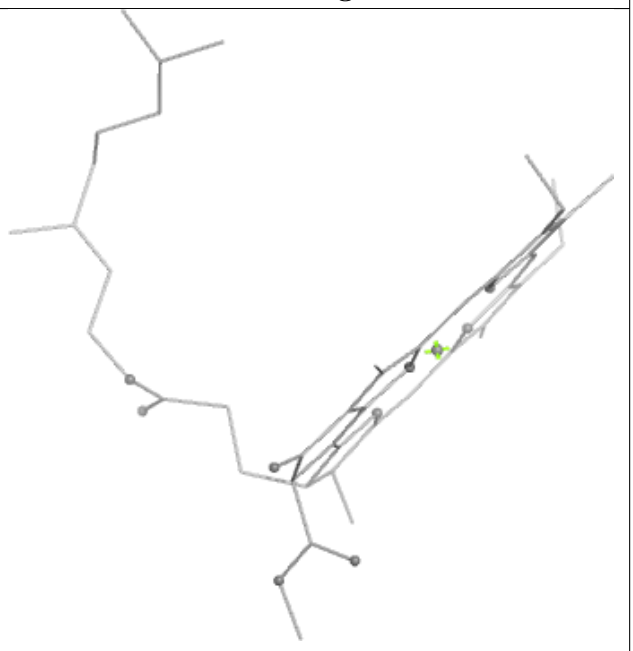
Bond lengths



Bond angles

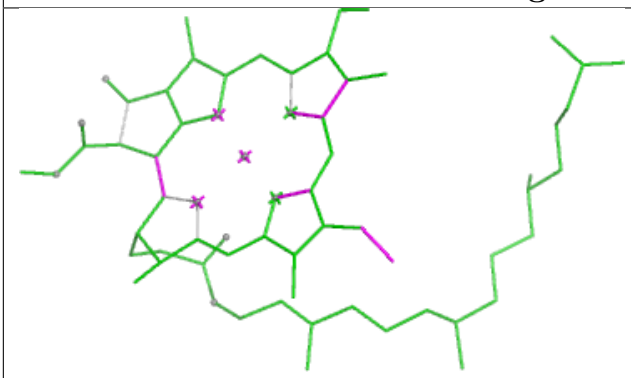


Torsions

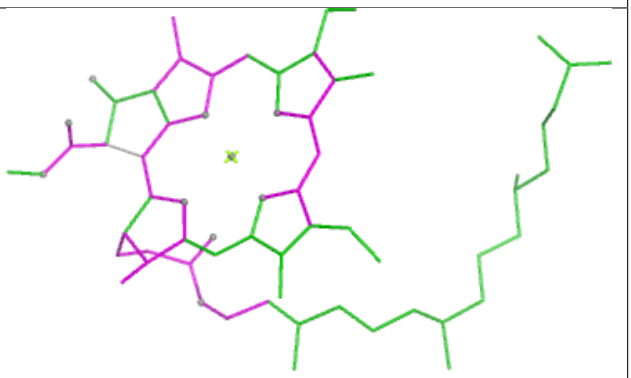


Rings

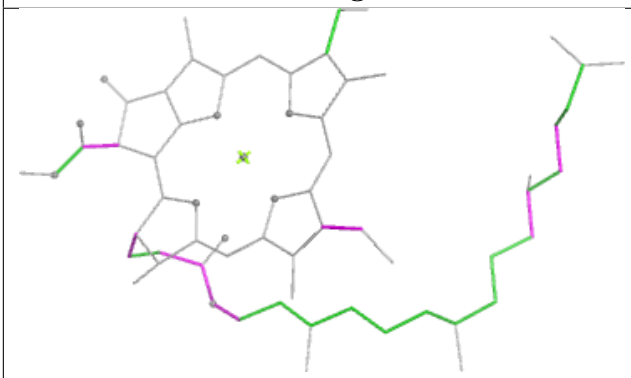
Ligand CLA 6 604



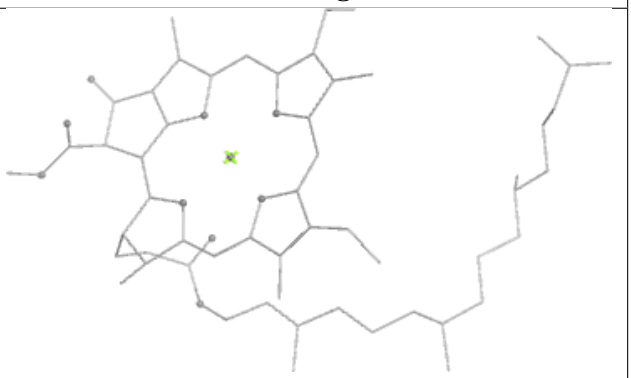
Bond lengths



Bond angles

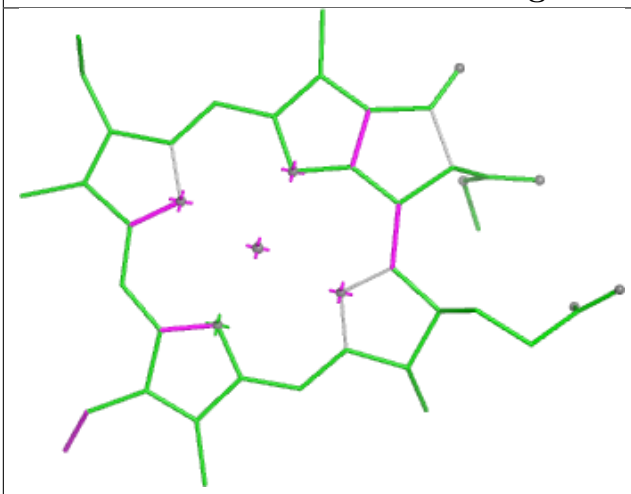


Torsions



Rings

Ligand CLA 1 602



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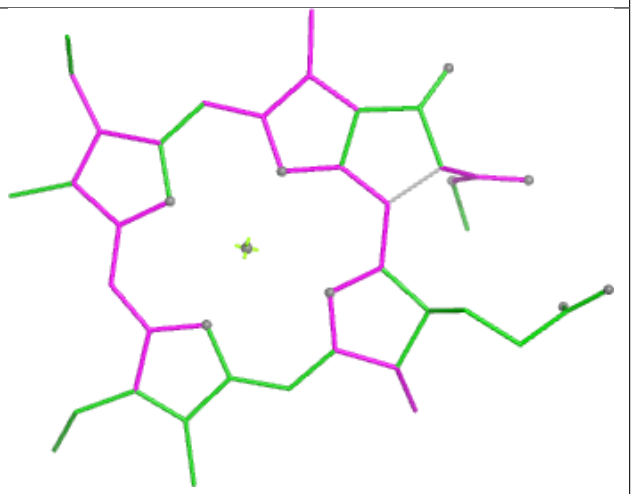

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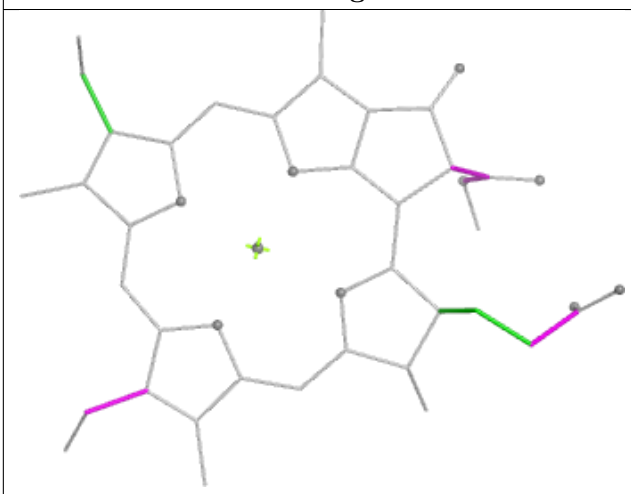

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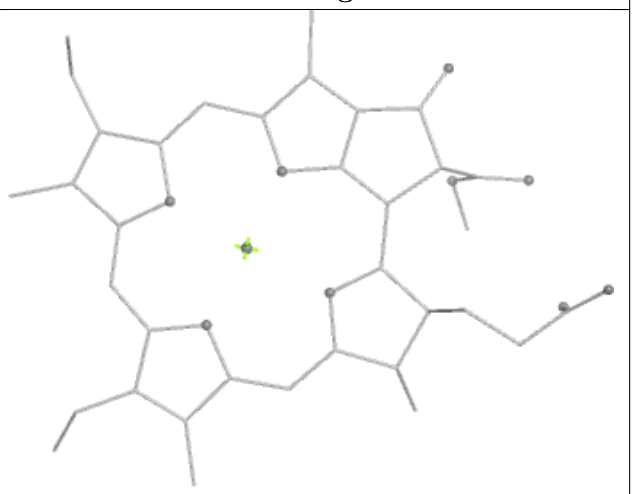
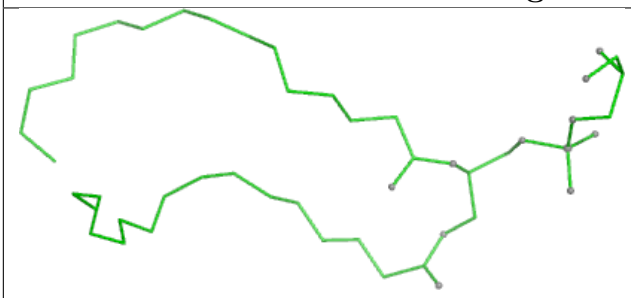


Rings

Ligand LHG 4 801



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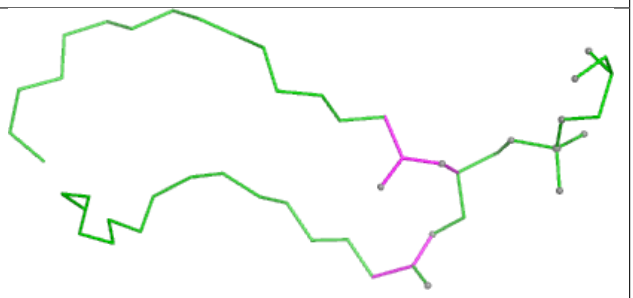

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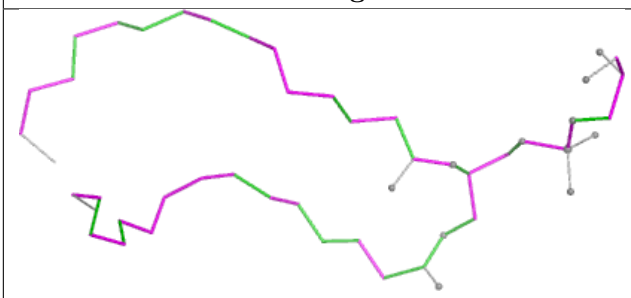

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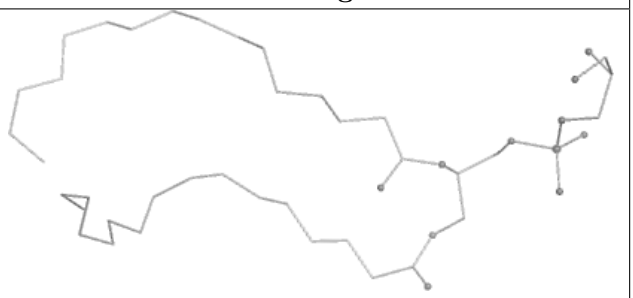


Rings

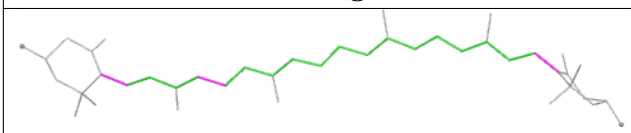
Ligand LUT 6 502



Bond lengths



Bond angles



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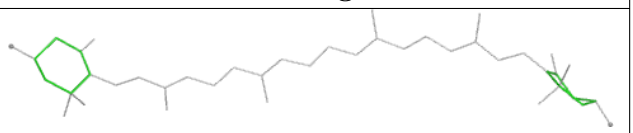
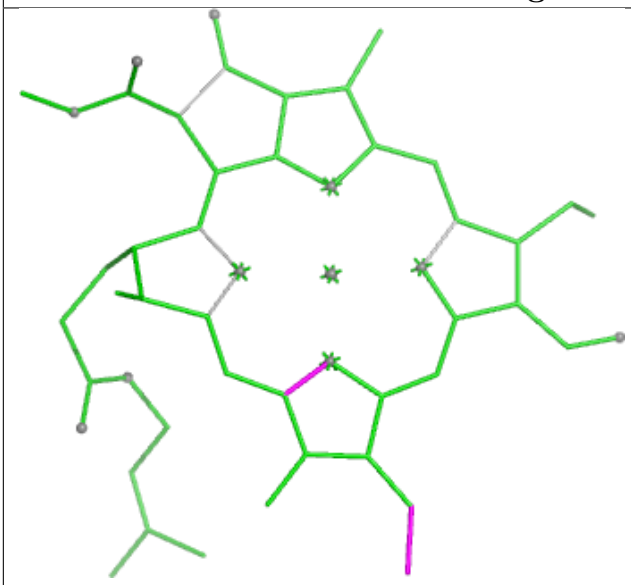


Rings

Ligand CHL 2 613



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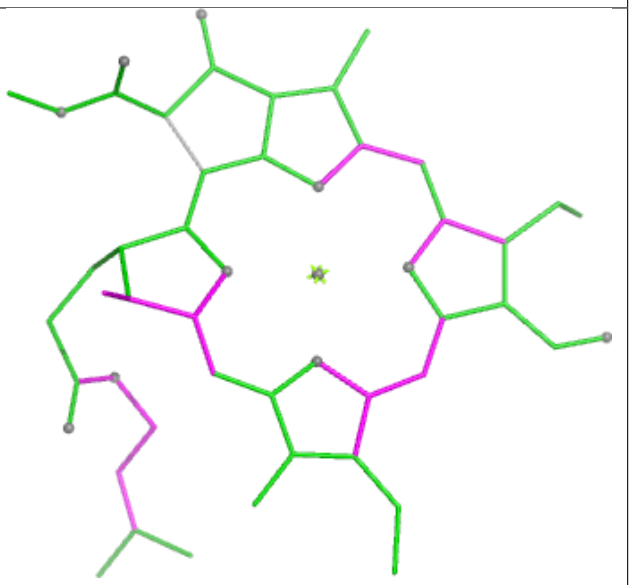

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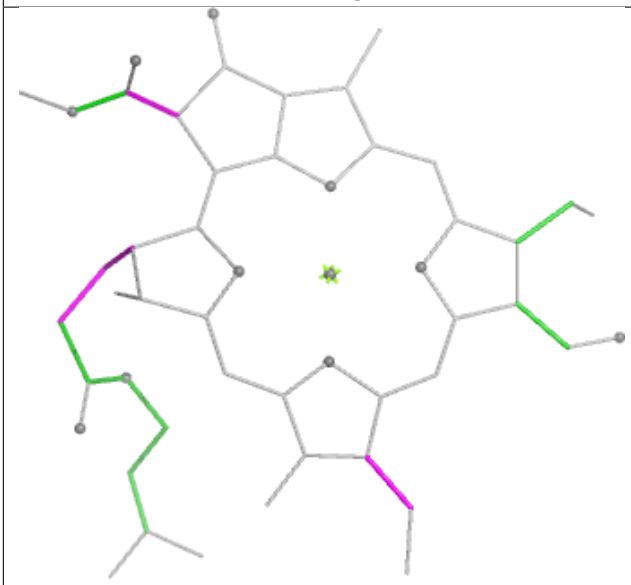

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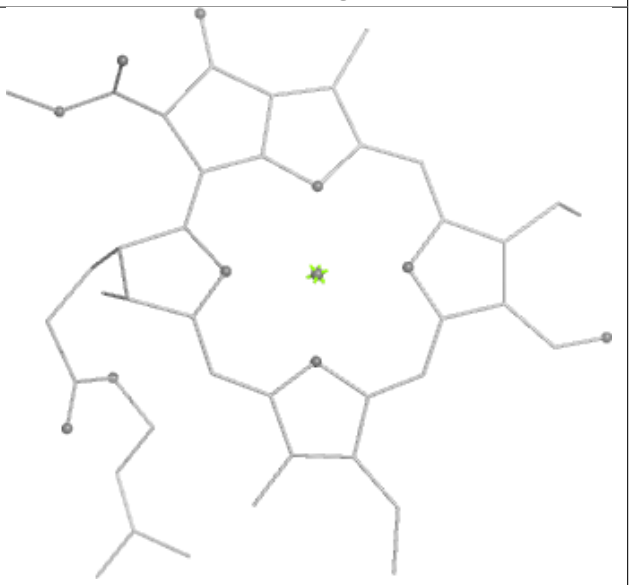
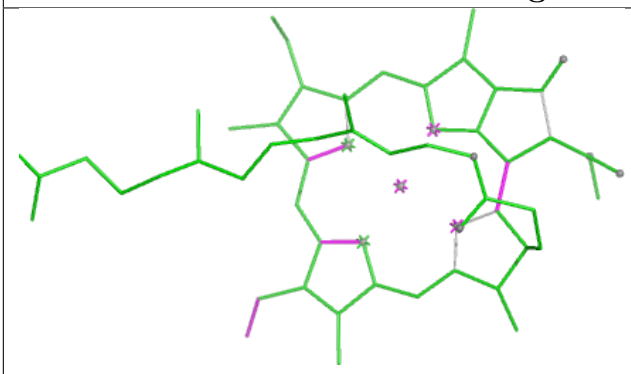


Rings

Ligand CLA 9 603



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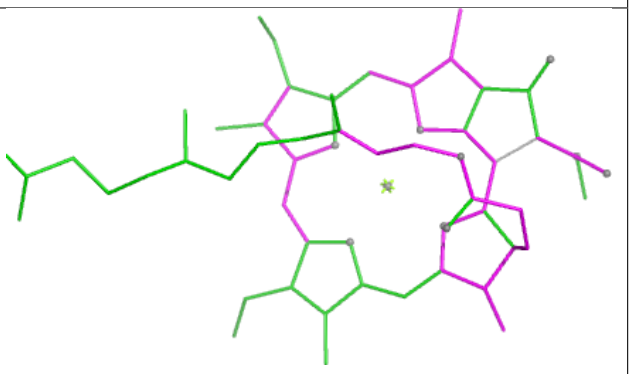

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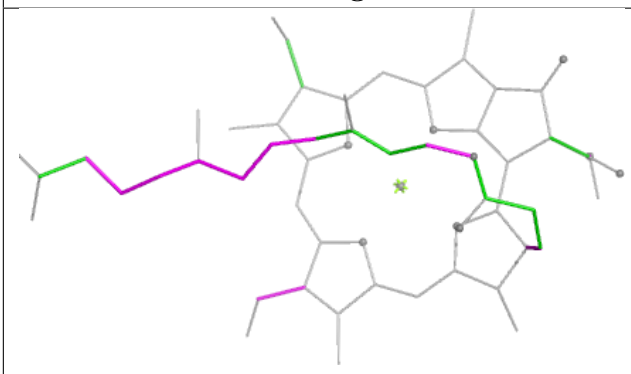

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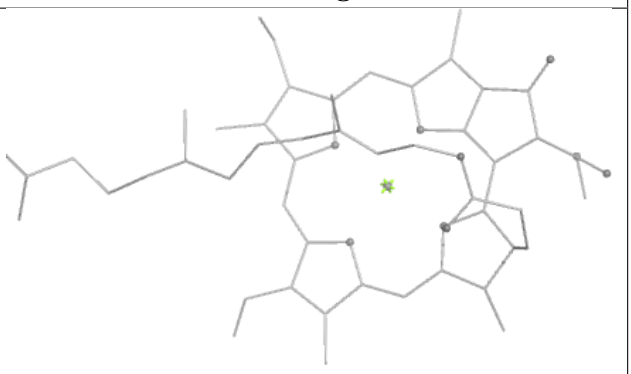

Rings

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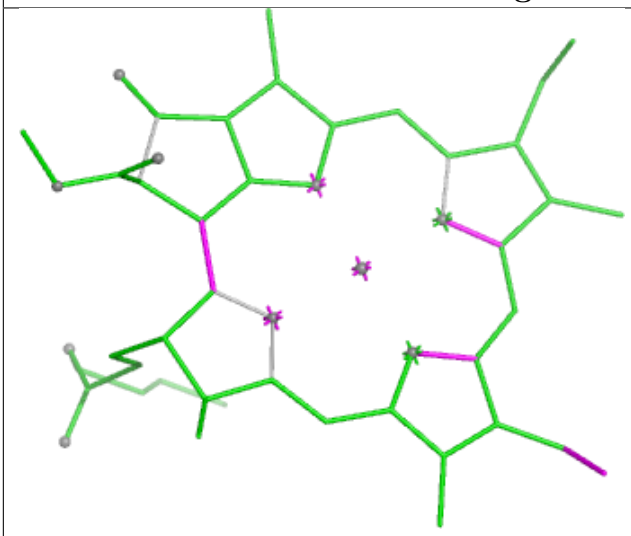

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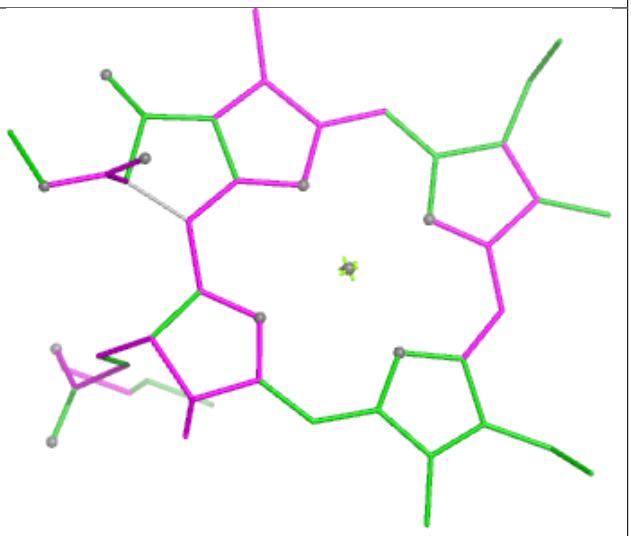

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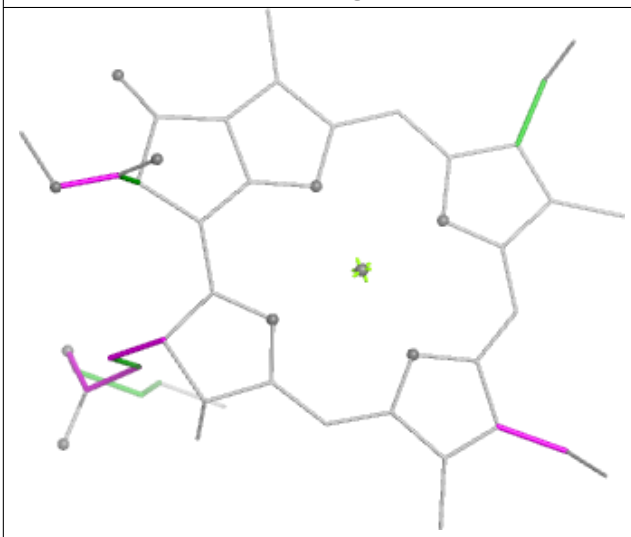

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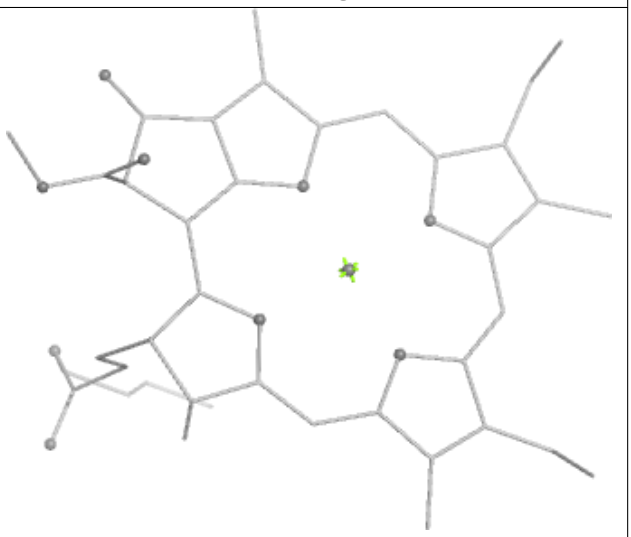
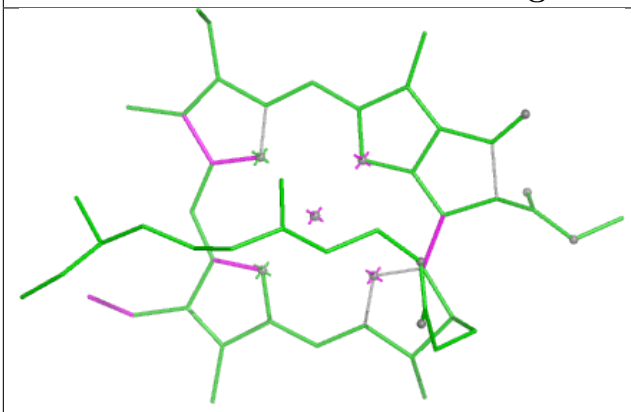


Rings

Ligand CLA 3 616



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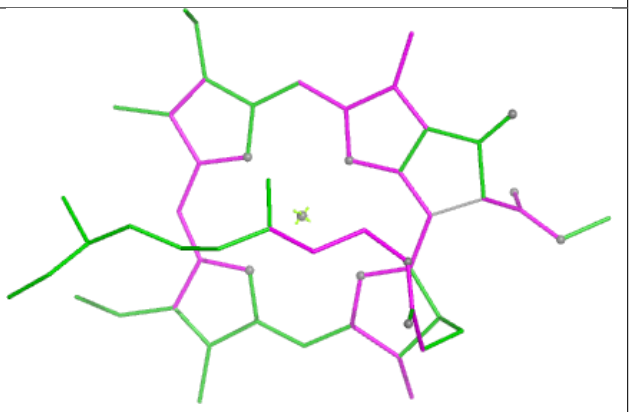

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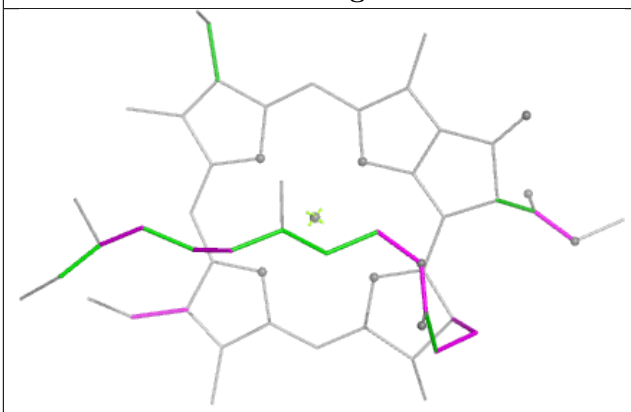

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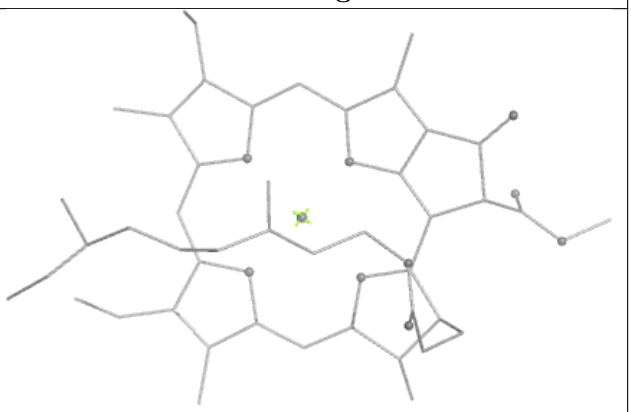

Rings

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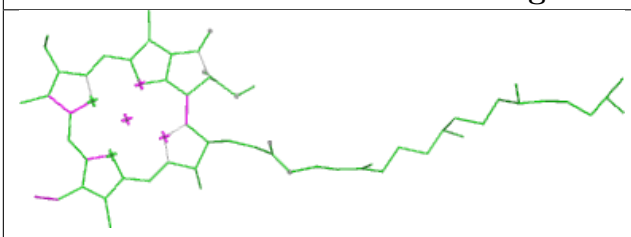

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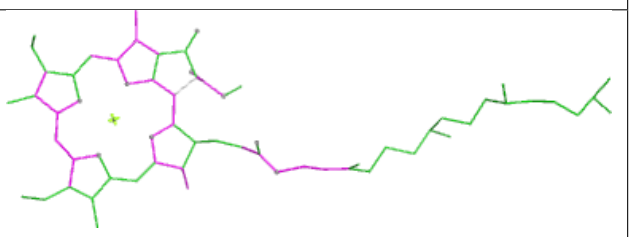

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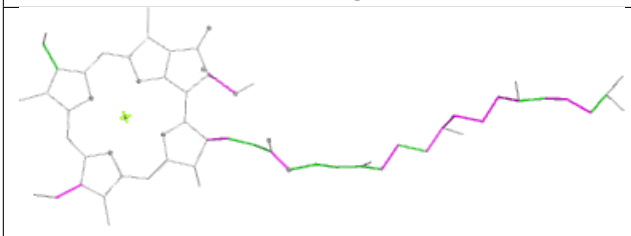

Torsions



Rings

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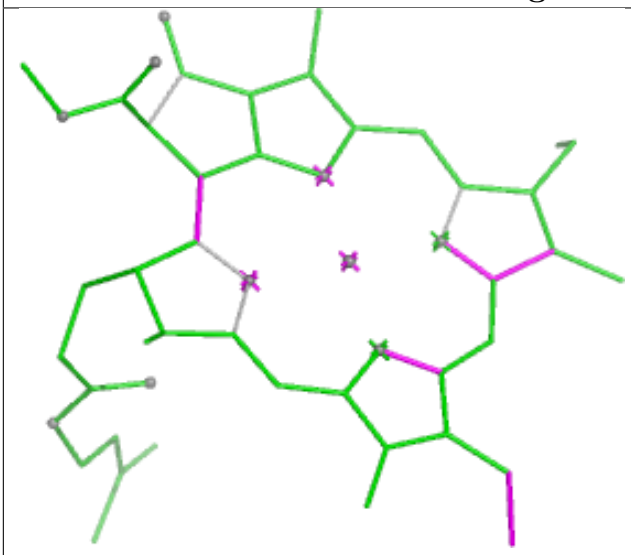

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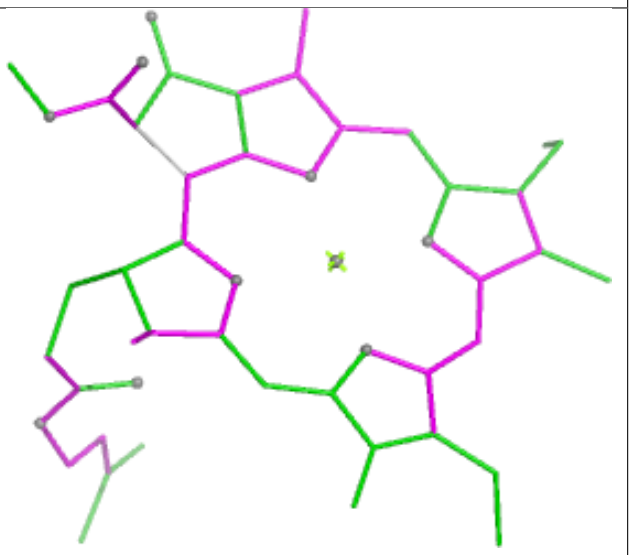

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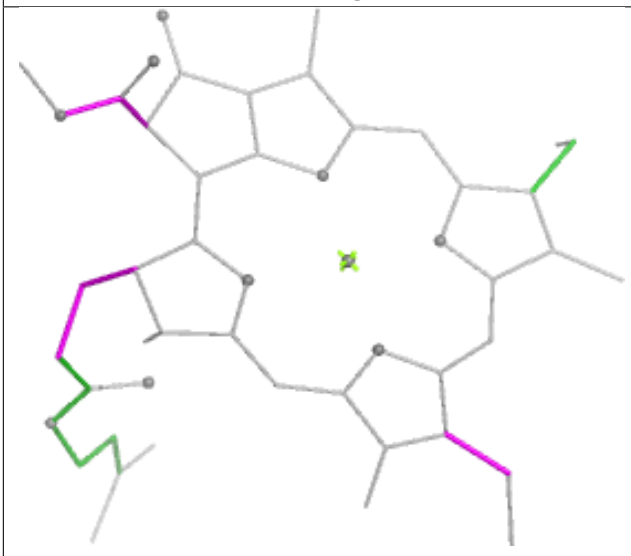

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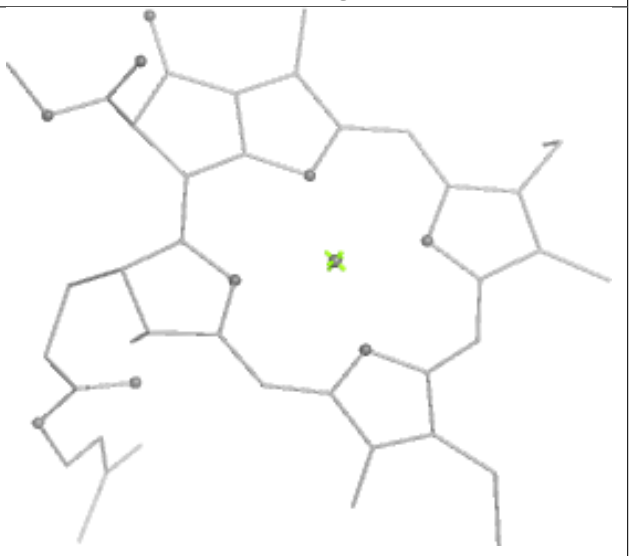

Rings

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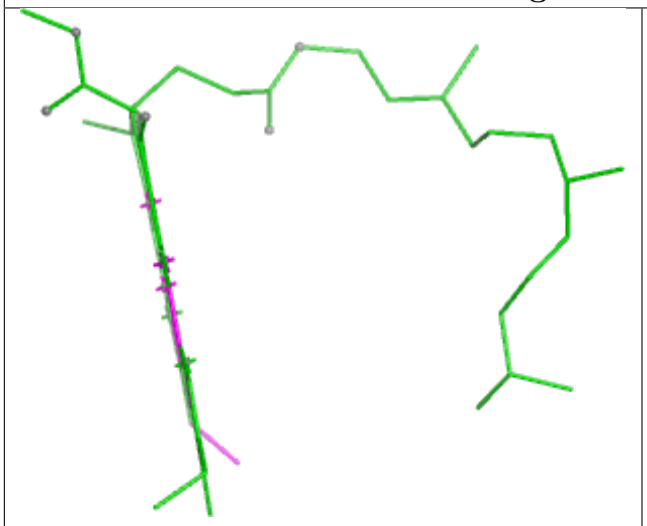

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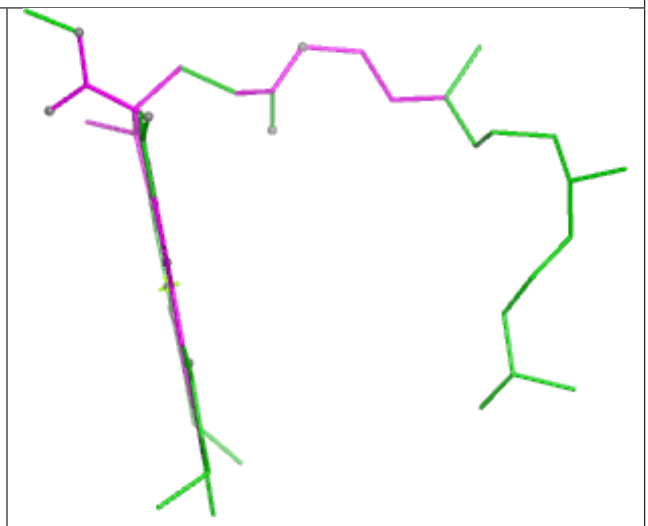

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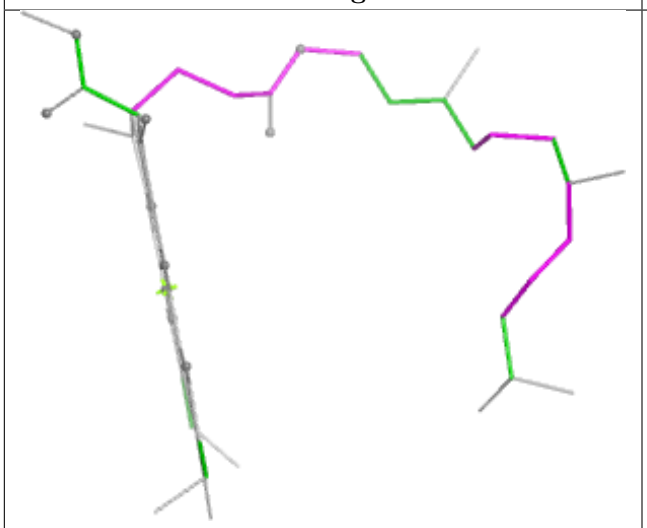

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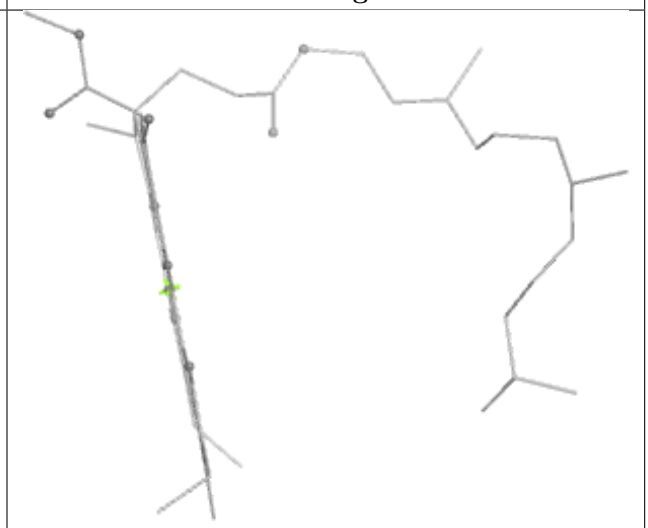

Rings

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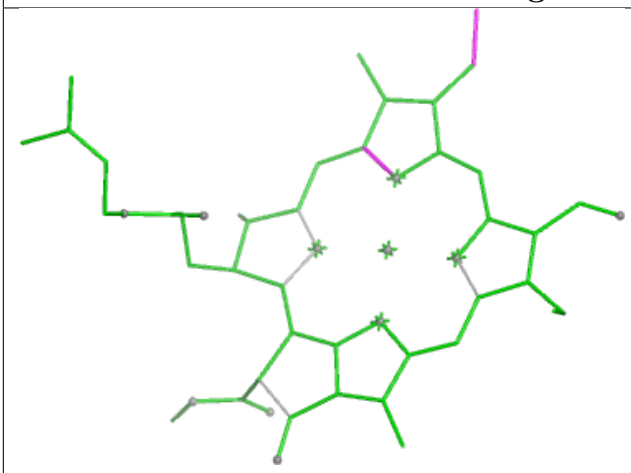

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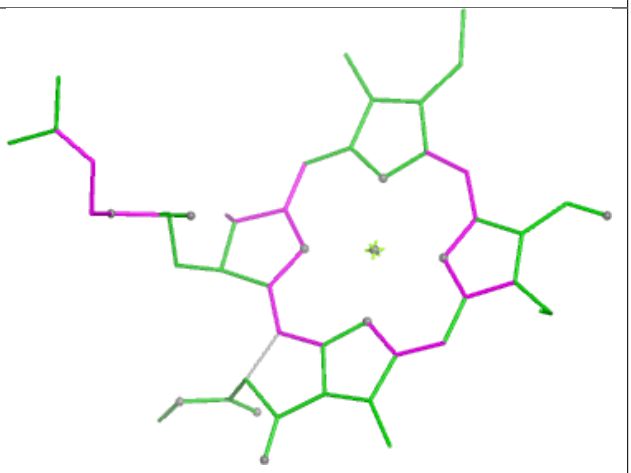

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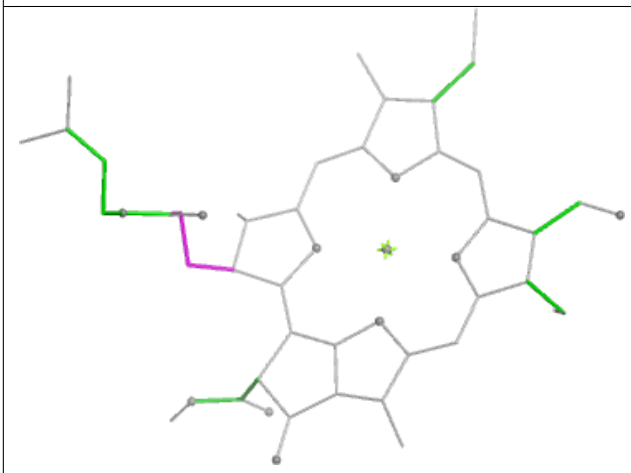

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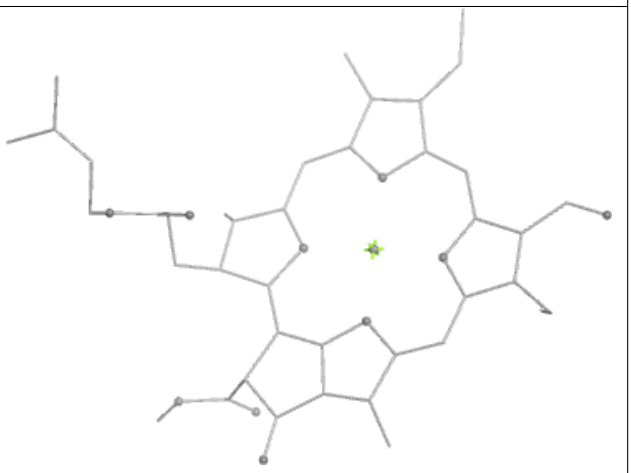

Rings

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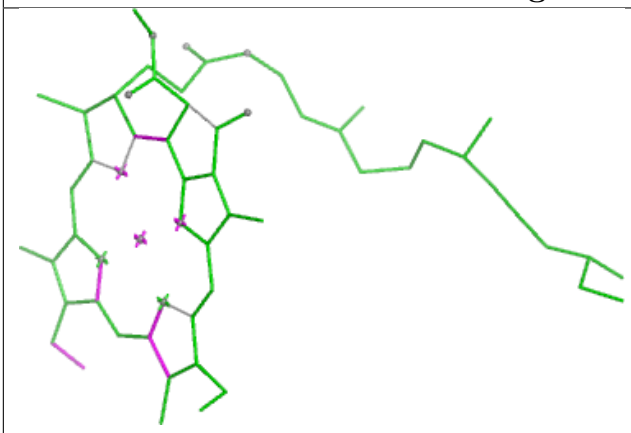

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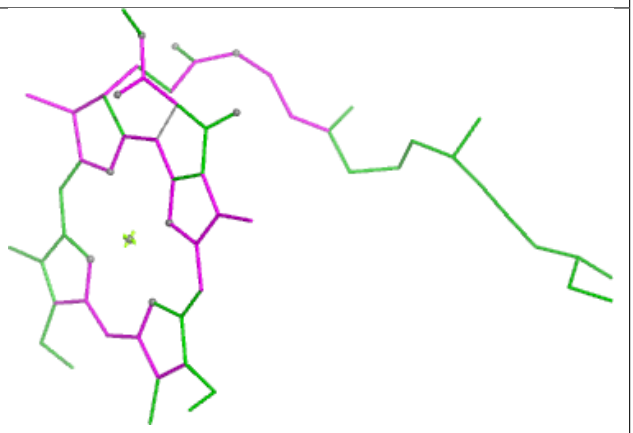

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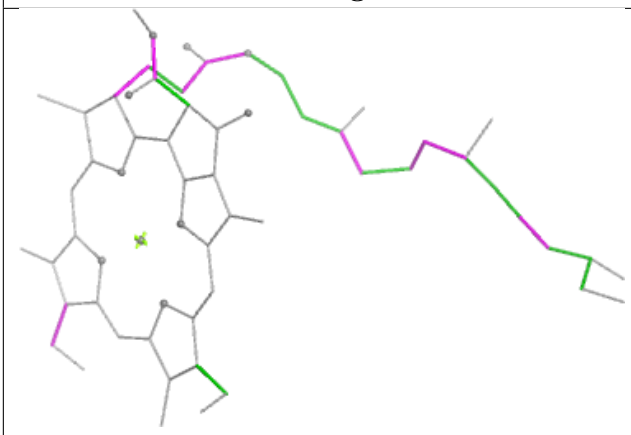

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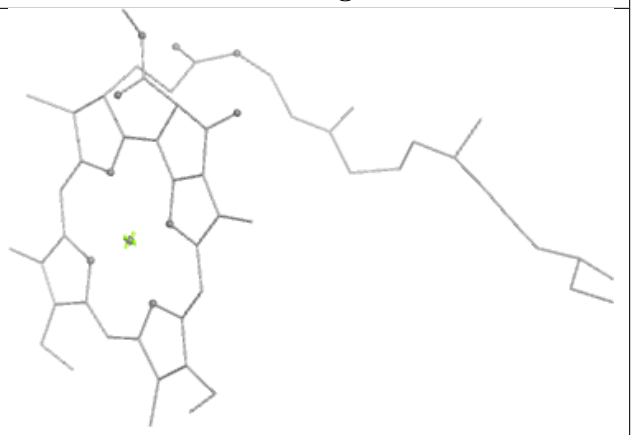
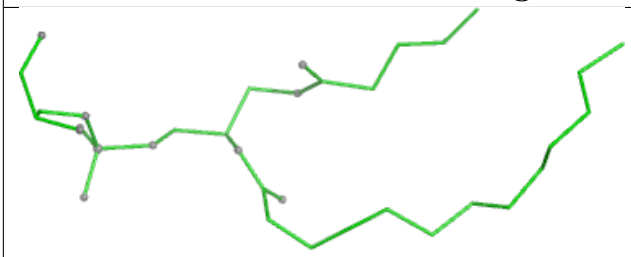


Rings

Ligand LHG A 5001



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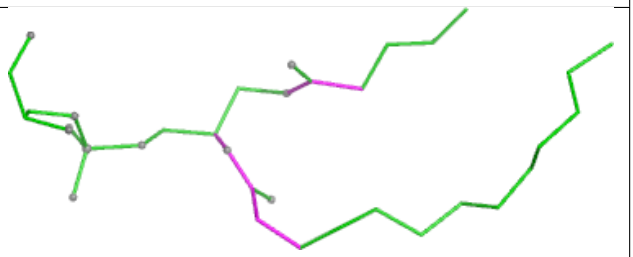

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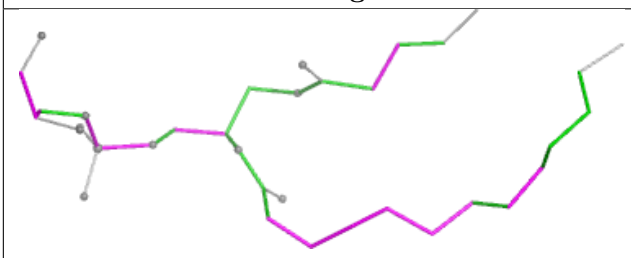

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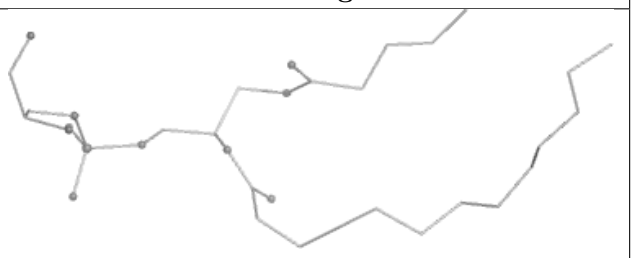
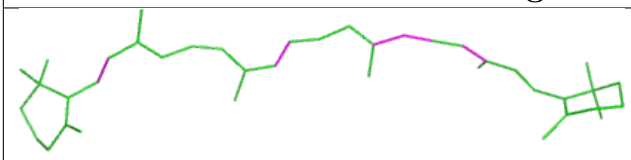


Rings

Ligand BCR 5 504



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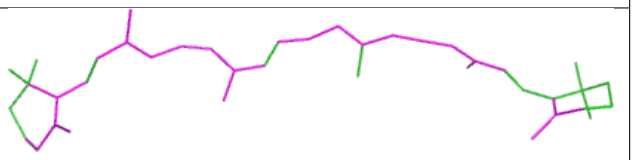
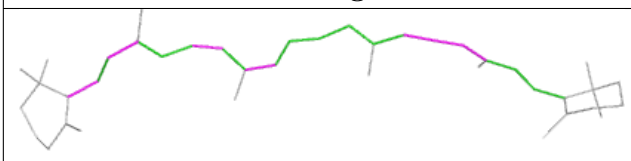


Bond angles



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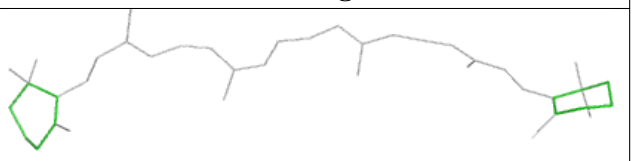
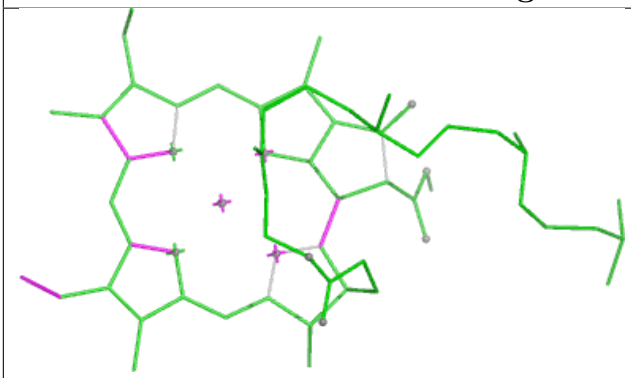


Rings

Ligand CLA F 1301



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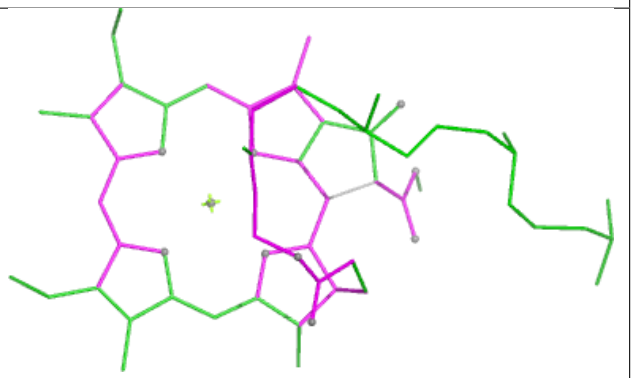
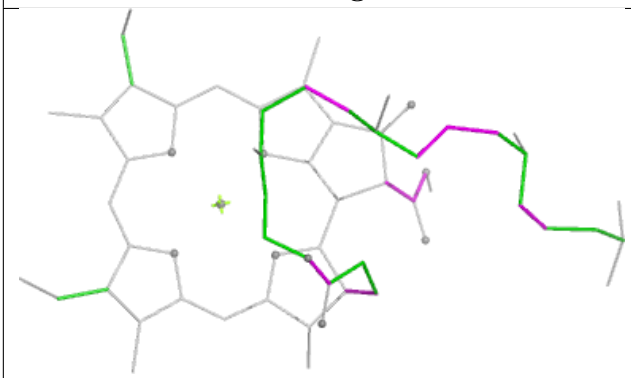


Bond angles



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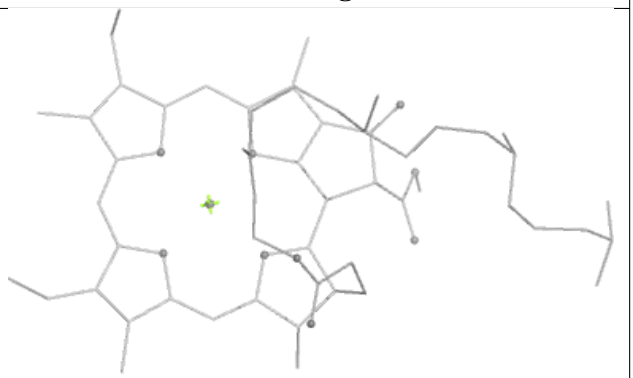
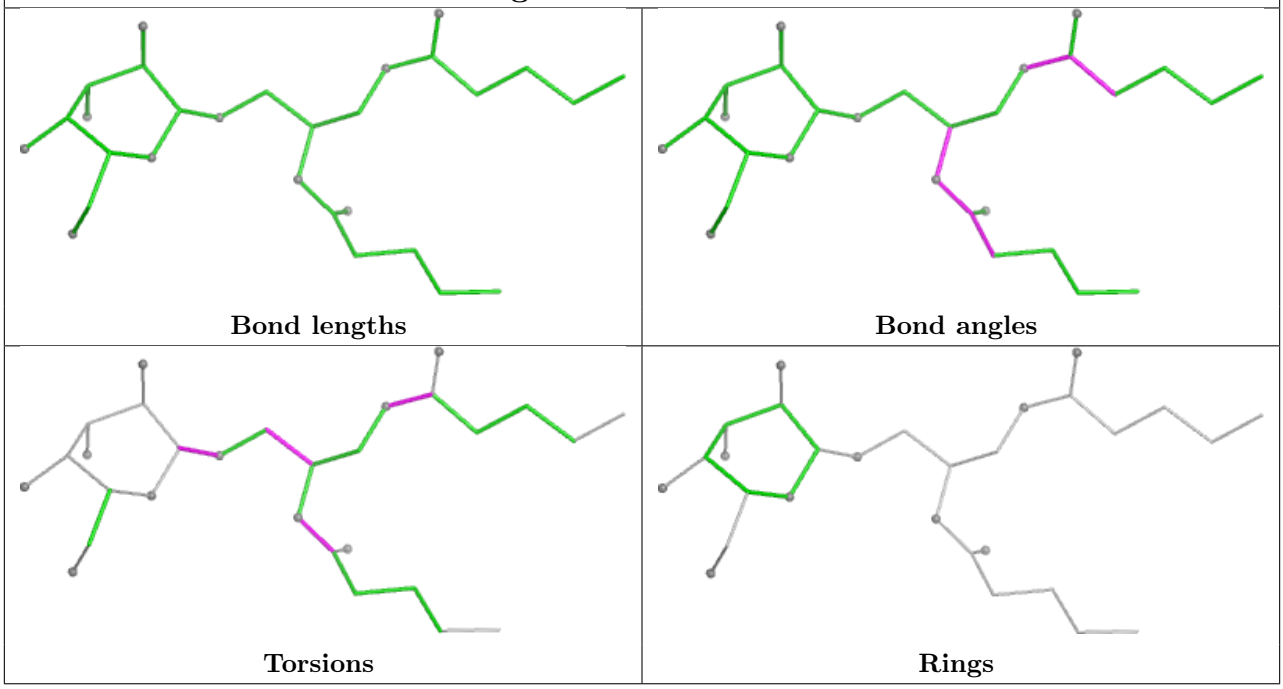
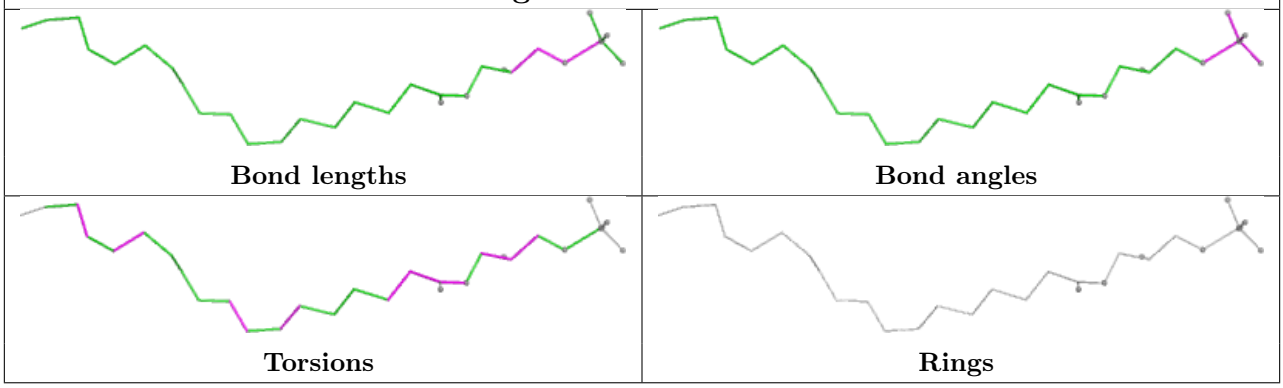


Rings

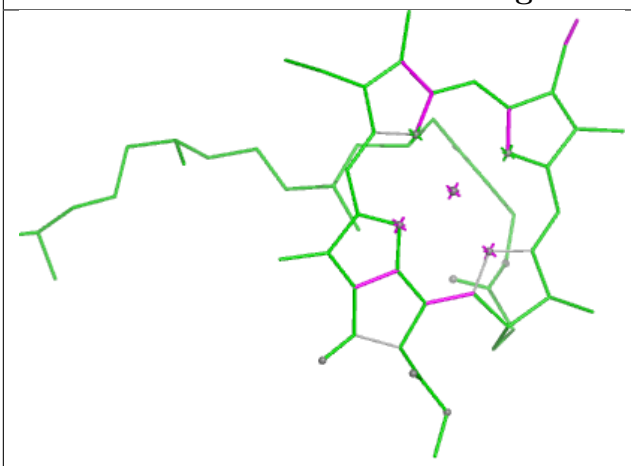
Ligand LMG A 5003



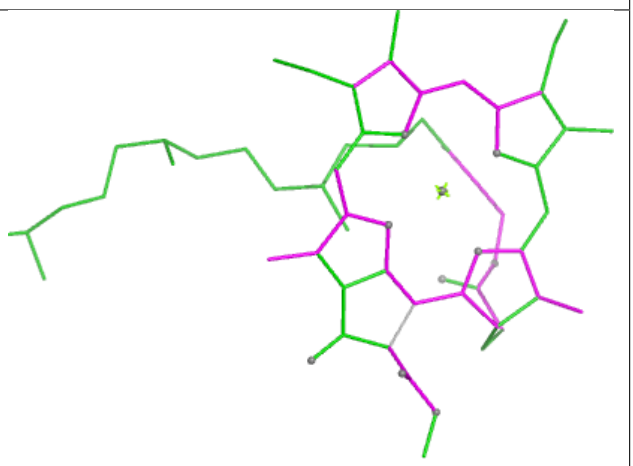
Ligand NKP A 5004



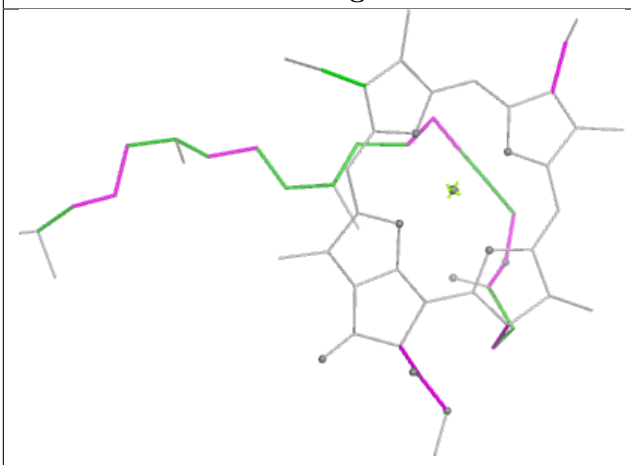
Ligand CLA B 1224



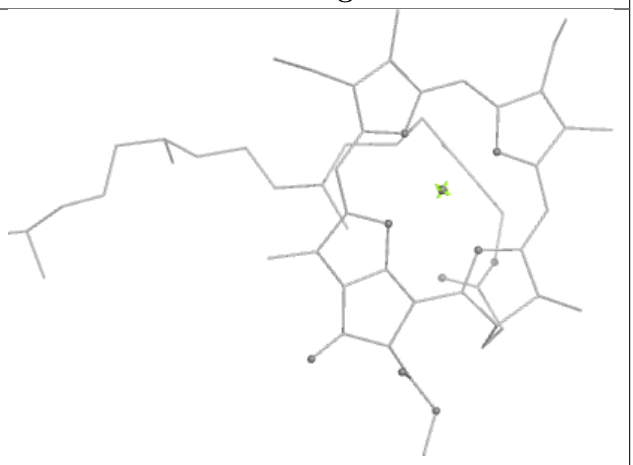
Bond lengths



Bond angles

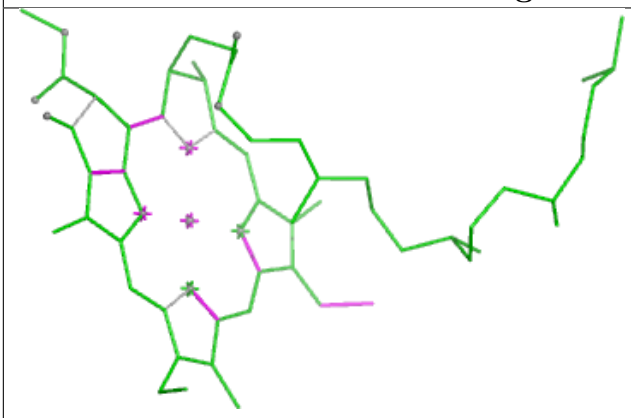


Torsions



Rings

Ligand CLA B 1237



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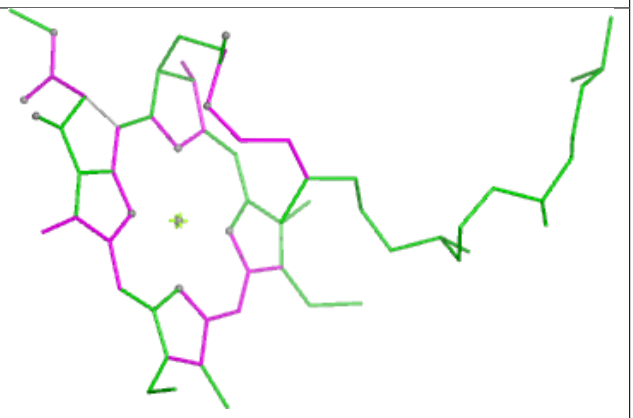

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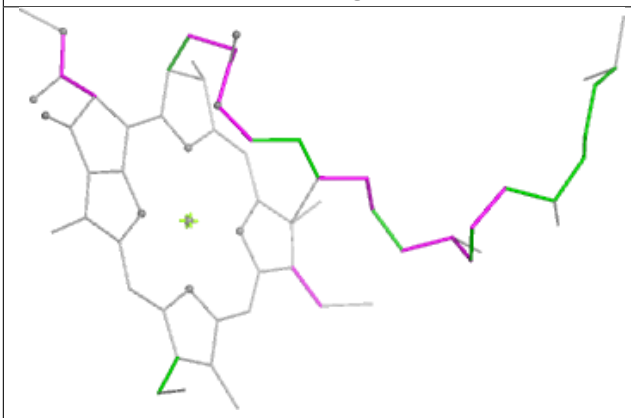

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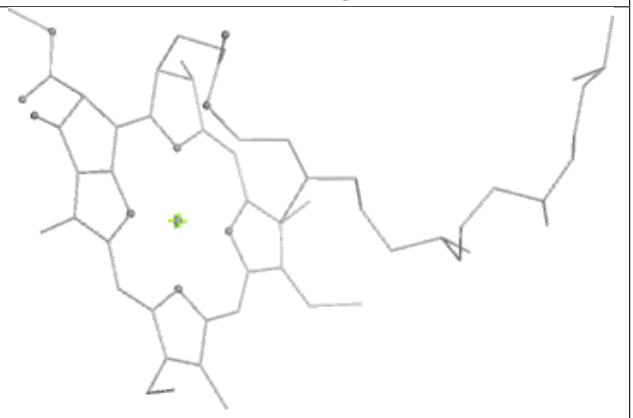
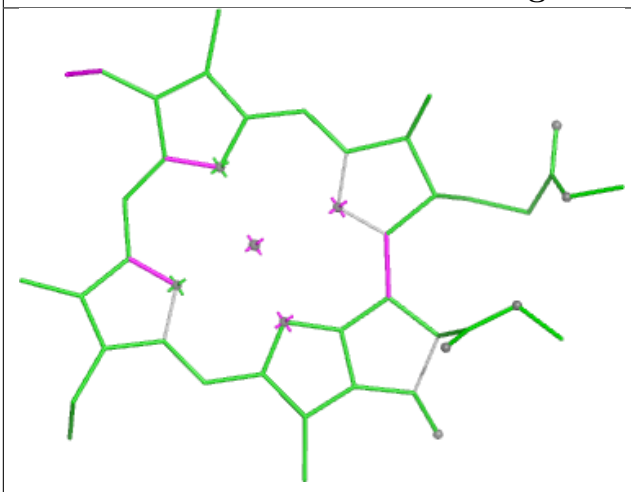


Rings

Ligand CLA 2 602



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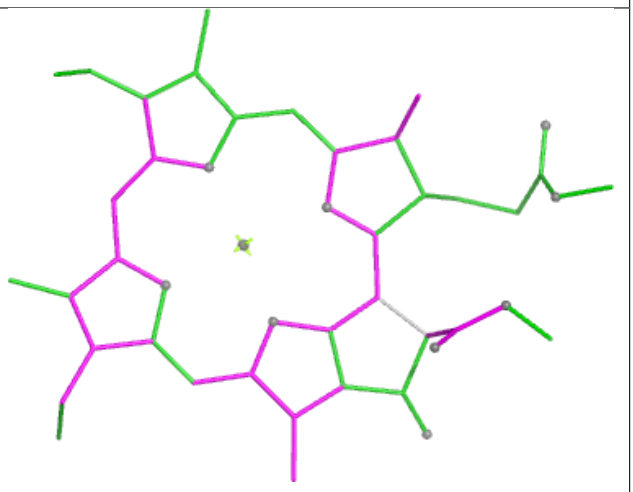
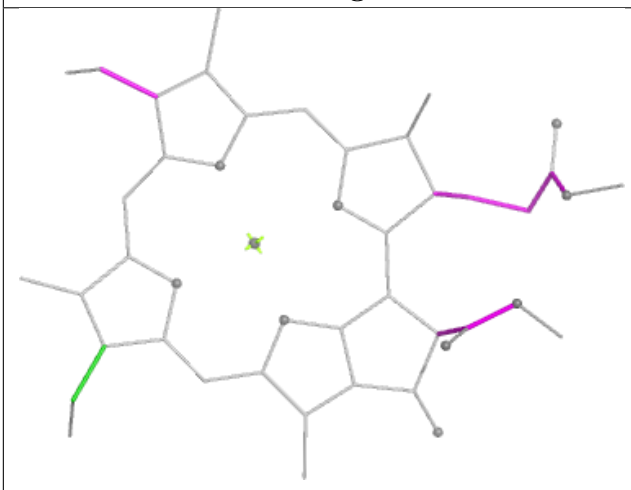


Bond angles



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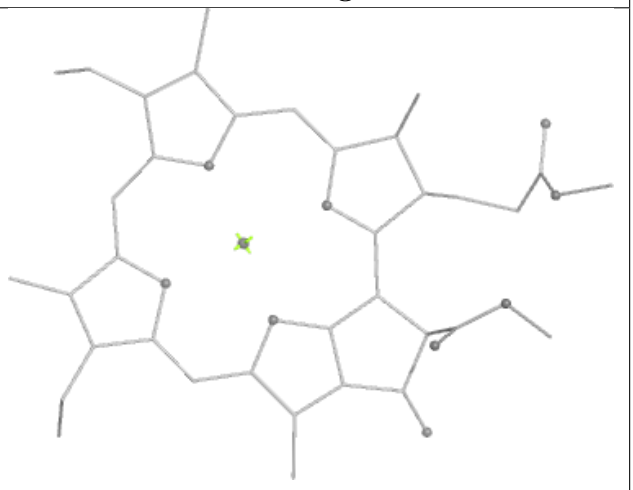
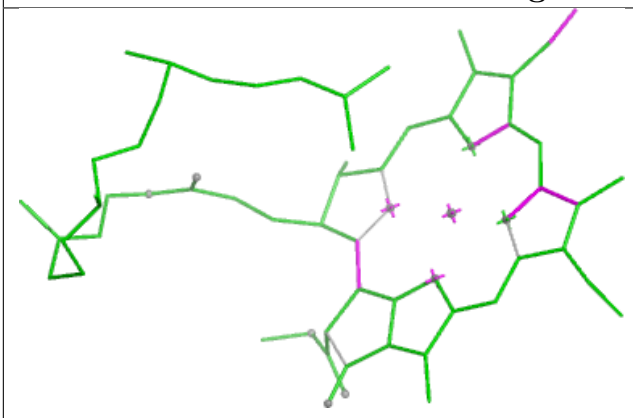


Rings

Ligand CLA 6 619



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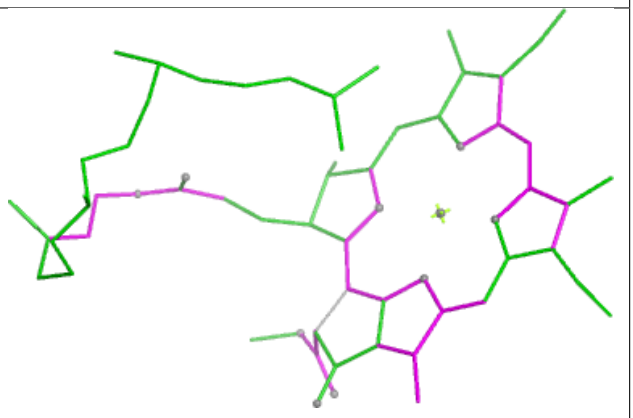
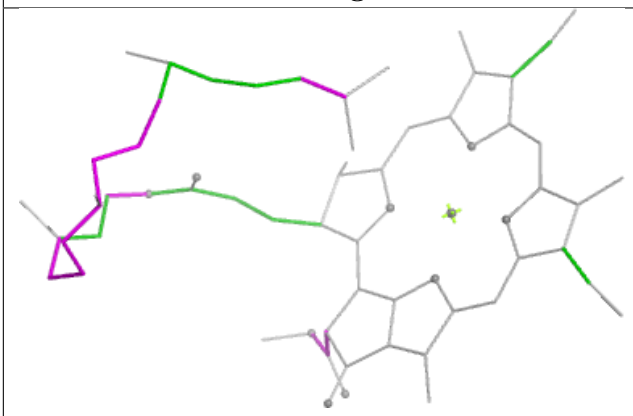


Bond angles



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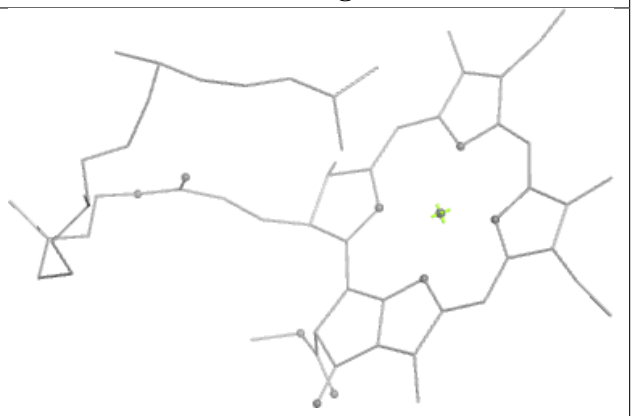
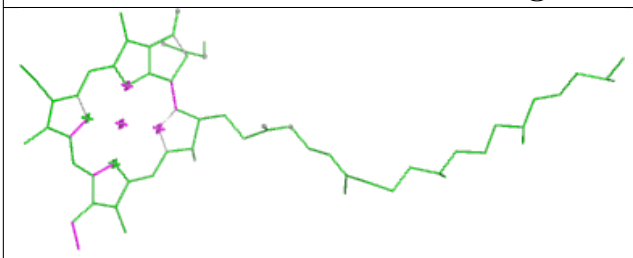


Rings

Ligand CLA 5 618



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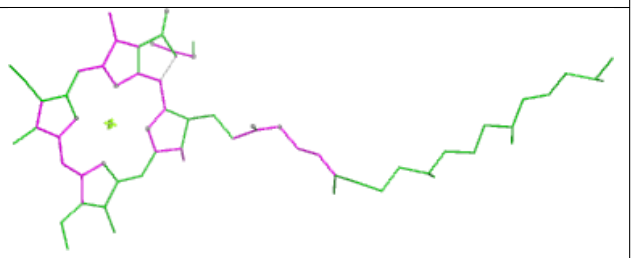
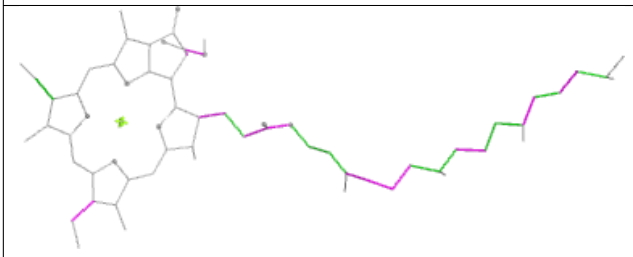


Bond angles



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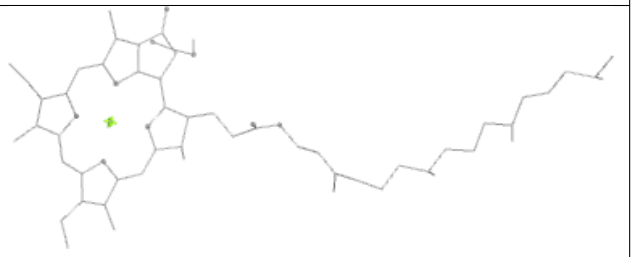
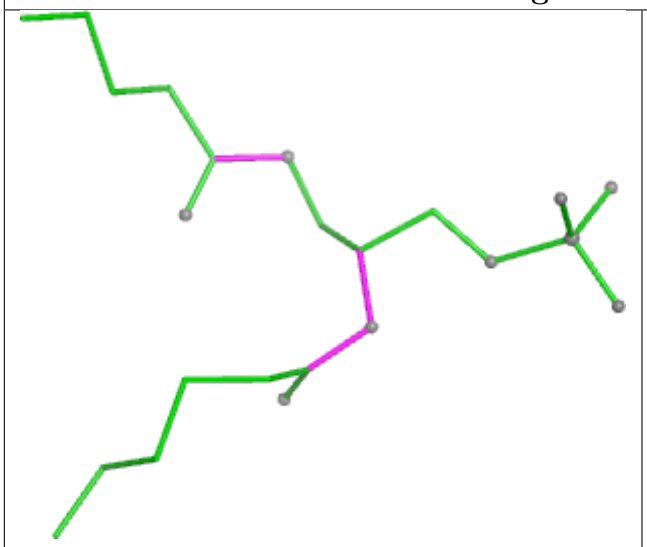


Rings

Ligand 3PH 5 802



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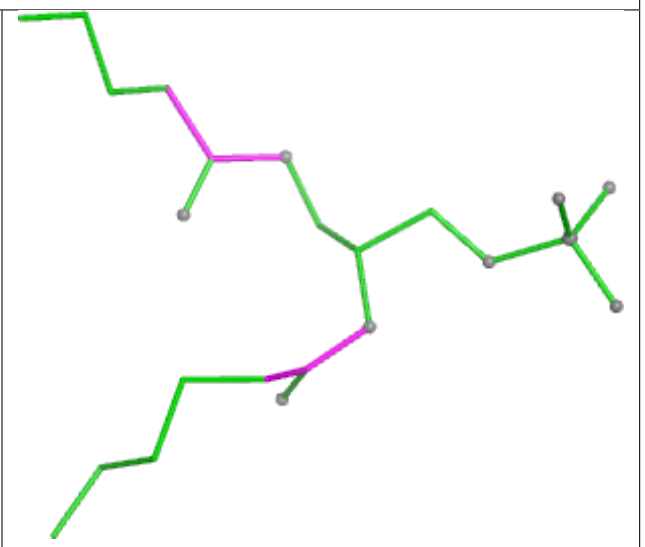

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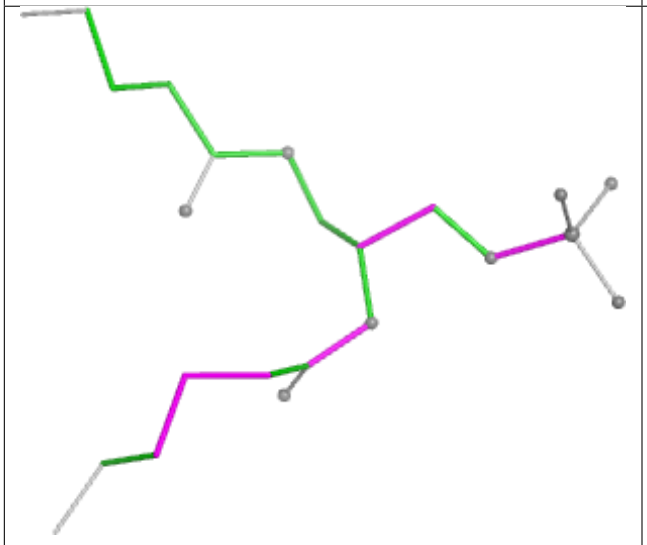

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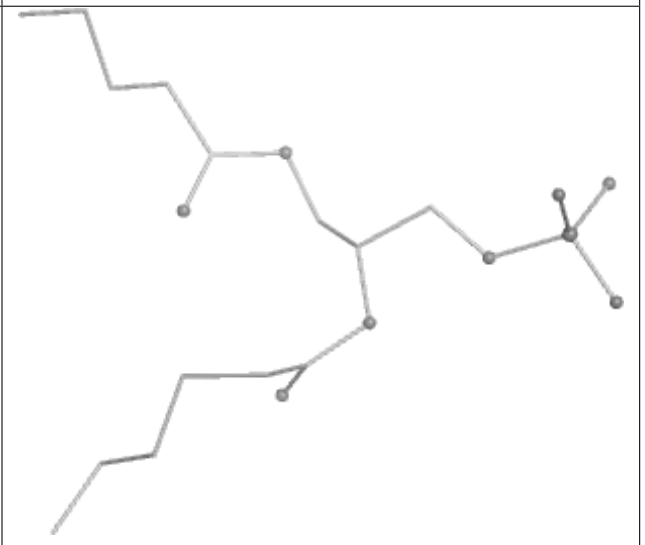
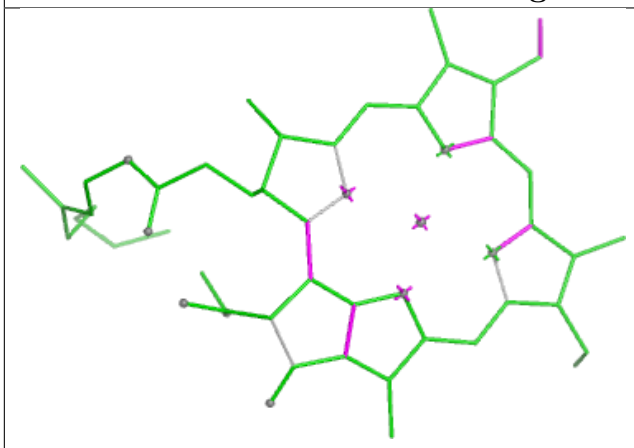


Rings

Ligand CLA 9 605



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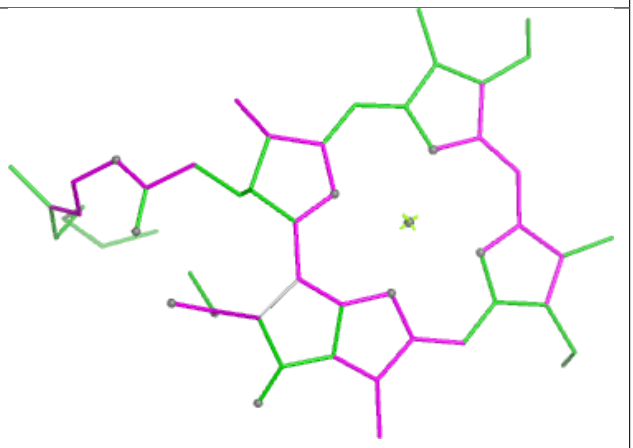
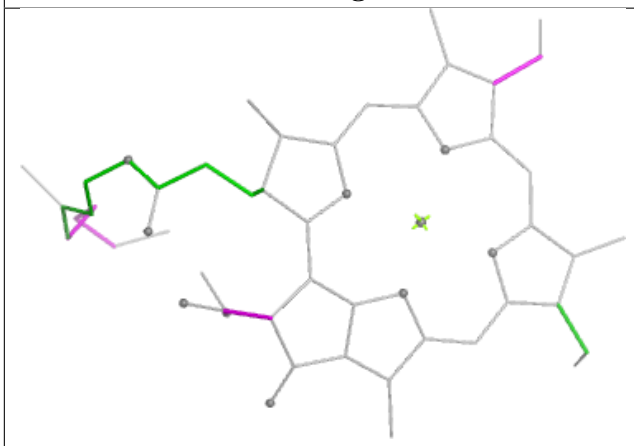


Bond angles



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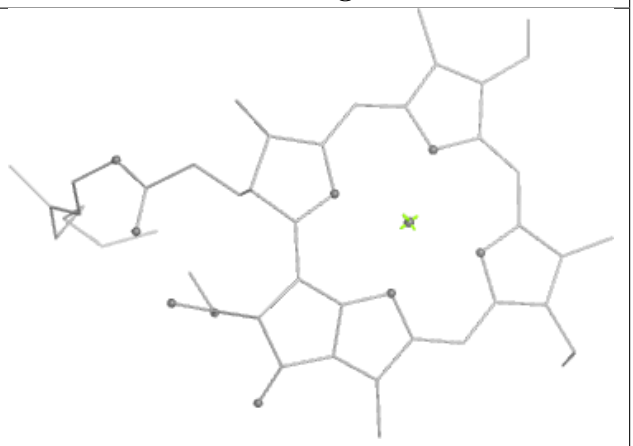
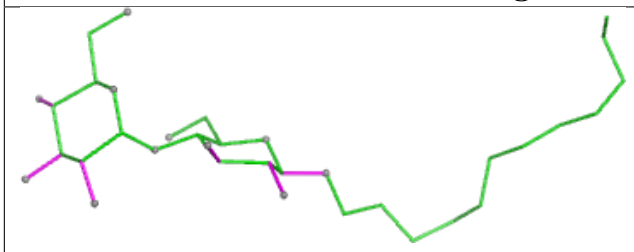


Rings

Ligand LMT A 5006



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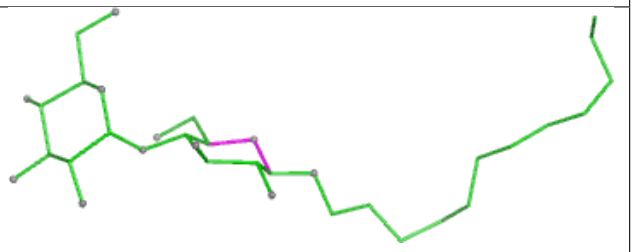
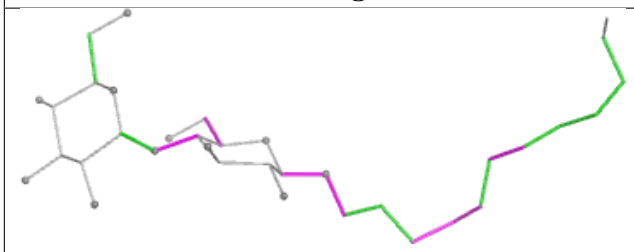


Bond angles



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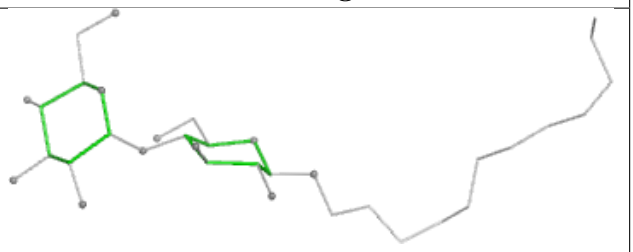
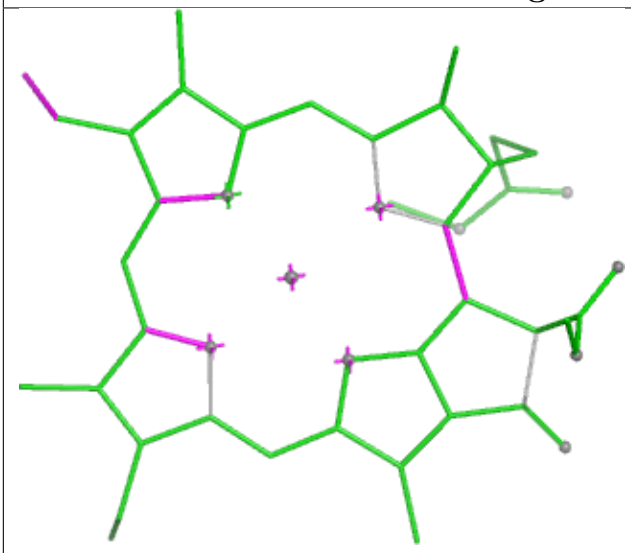


Rings

Ligand CLA 2 606



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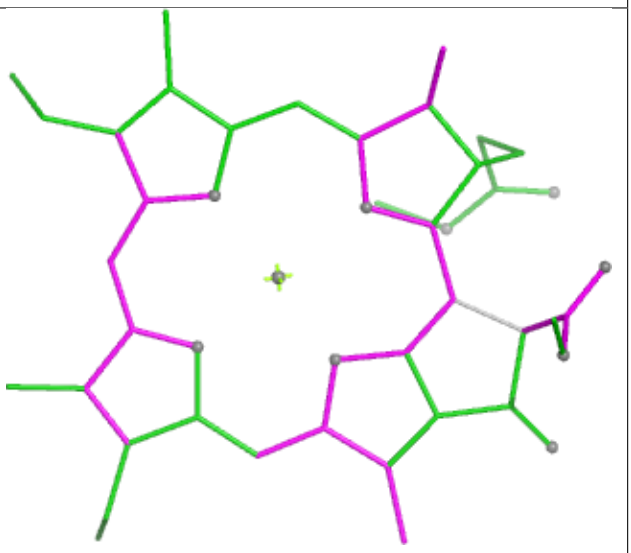
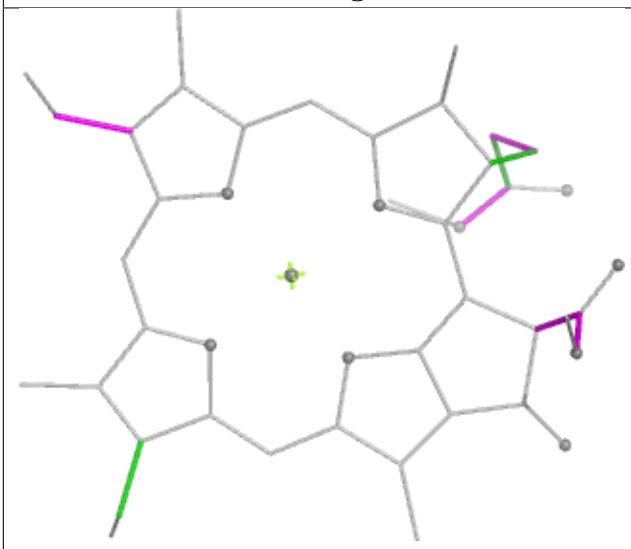


Bond angles



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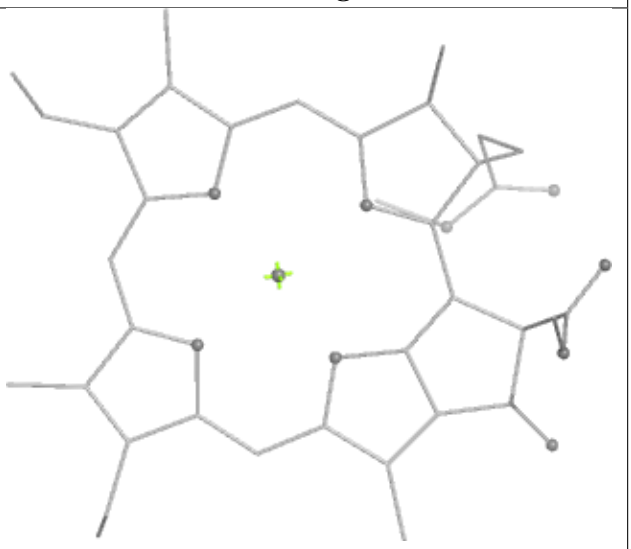
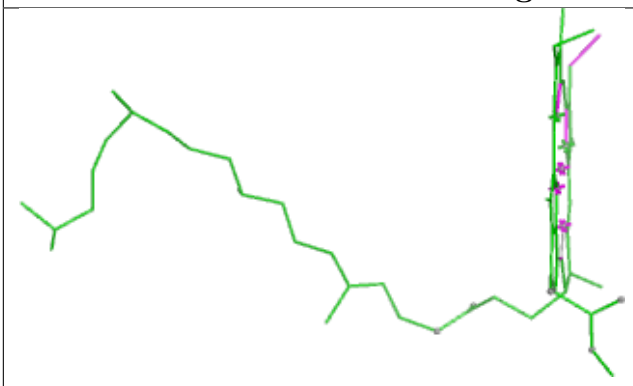


Rings

Ligand CLA B 1239



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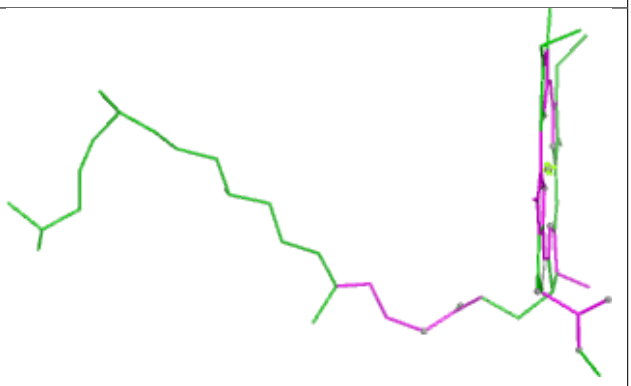
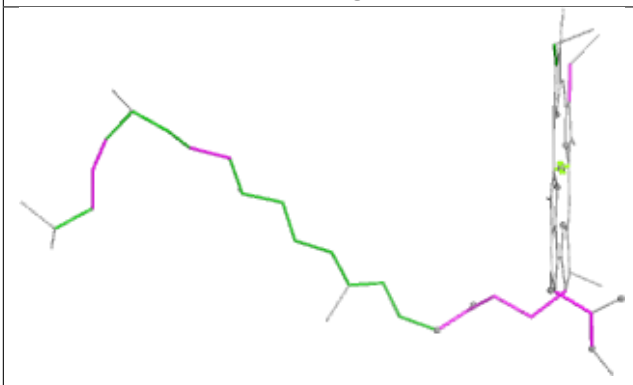
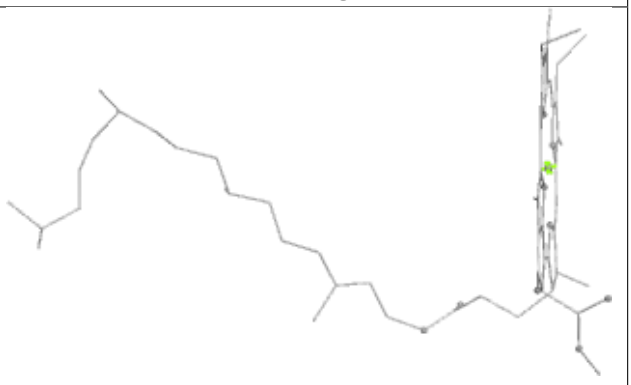


Bond angles

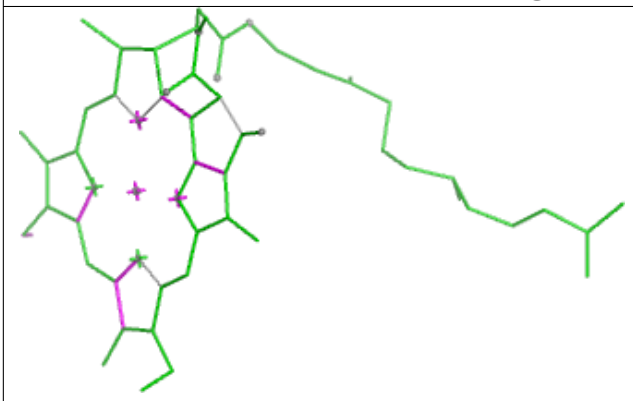


Torsions



Rings

Ligand CLA 3 612



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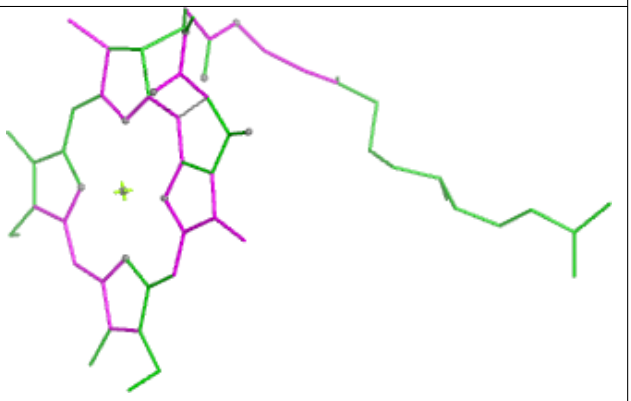

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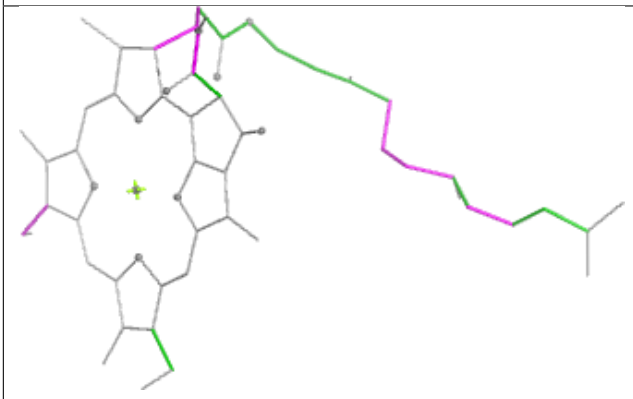
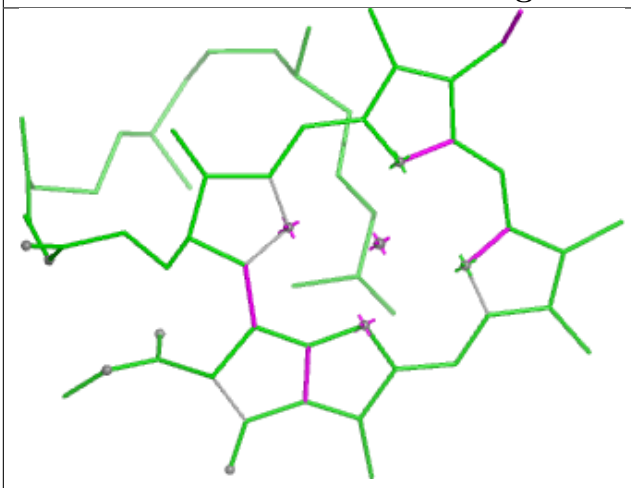


Torsions



Rings

Ligand CLA B 1203



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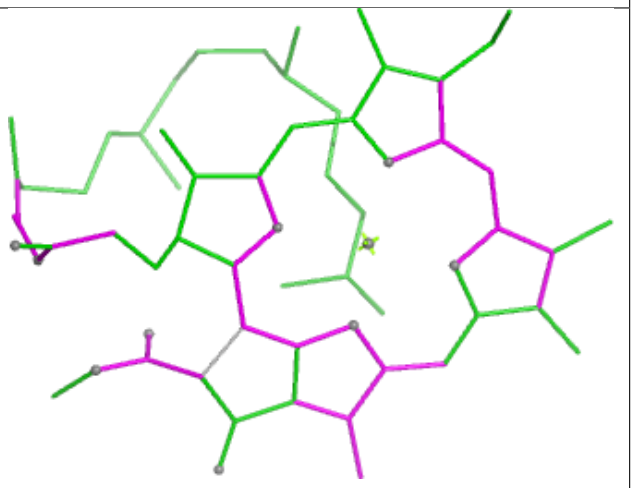
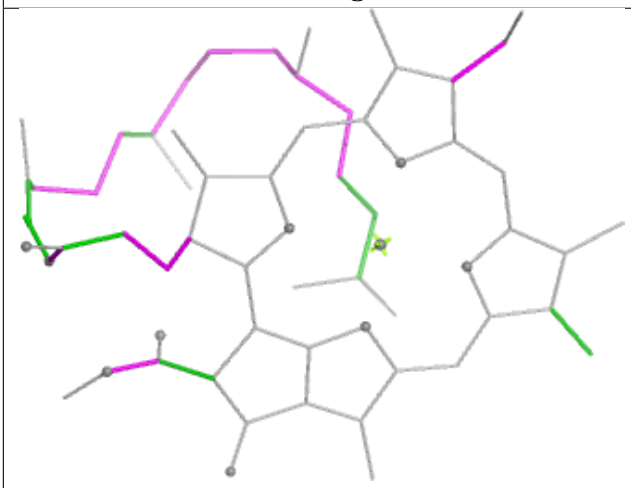


Bond angles



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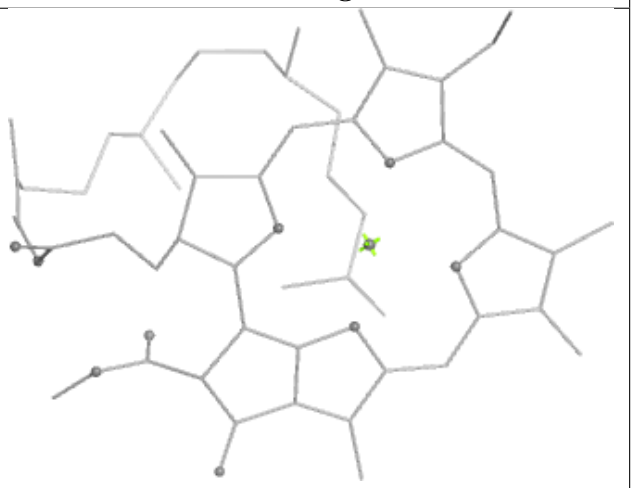
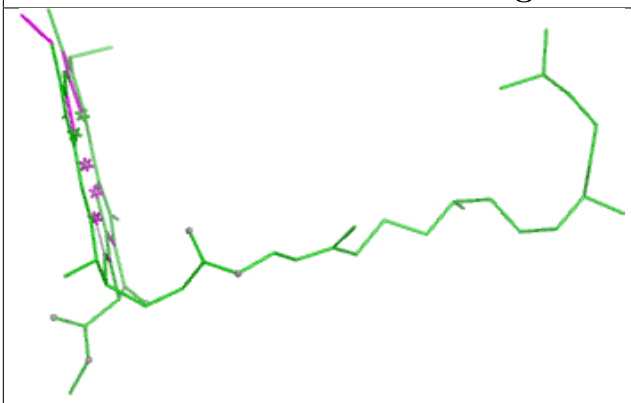


Rings

Ligand CLA B 1236



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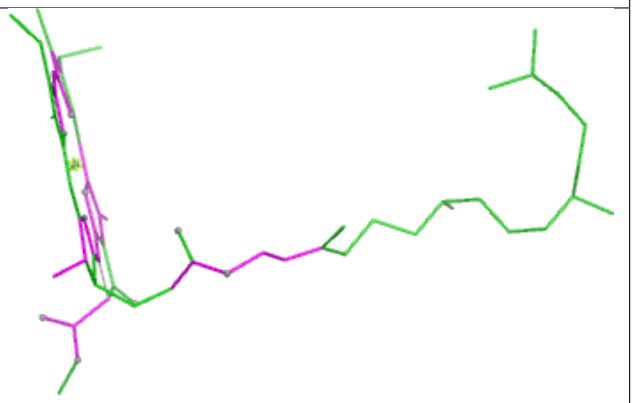
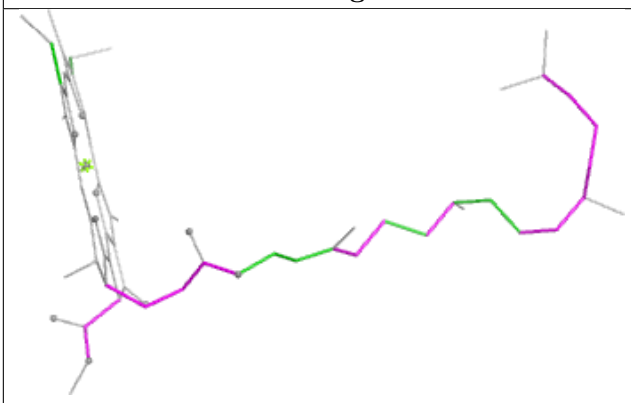


Bond angles



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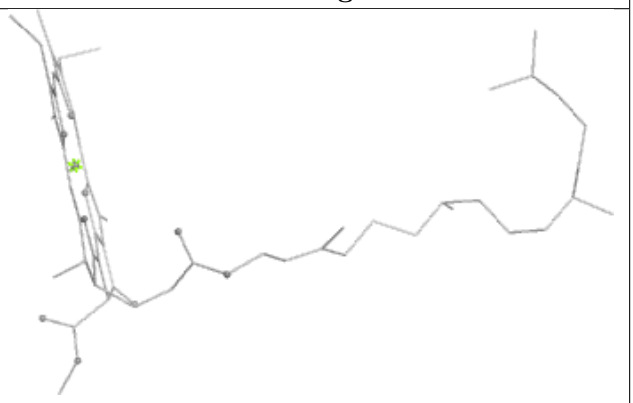
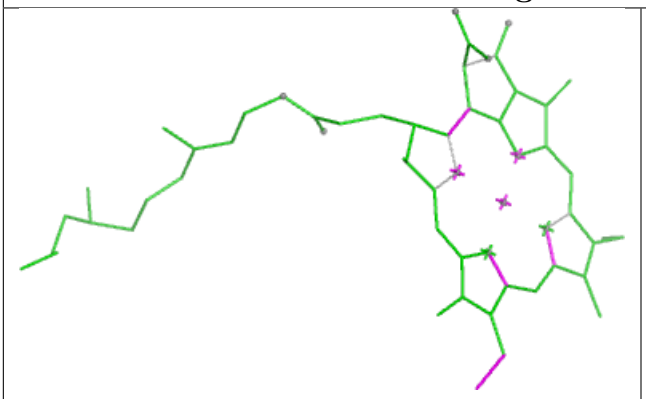
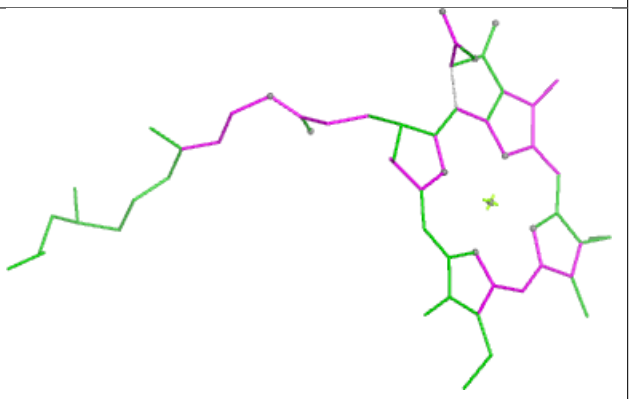


Rings

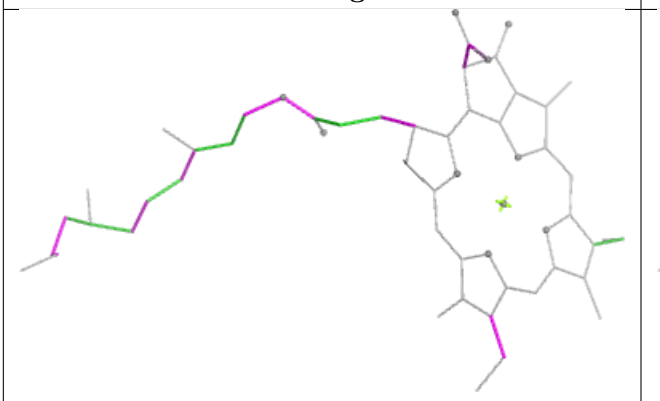
Ligand CLA B 1230



Bond lengths



Bond angles



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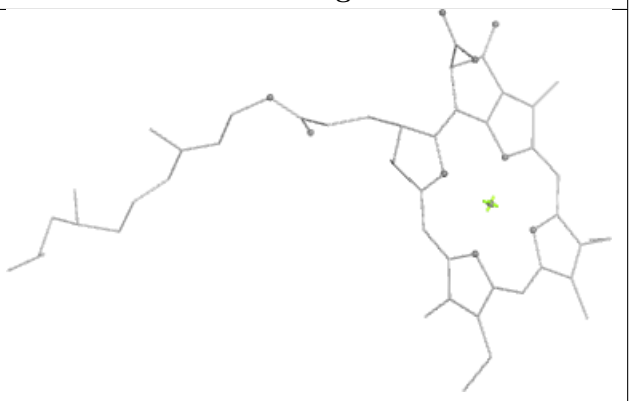
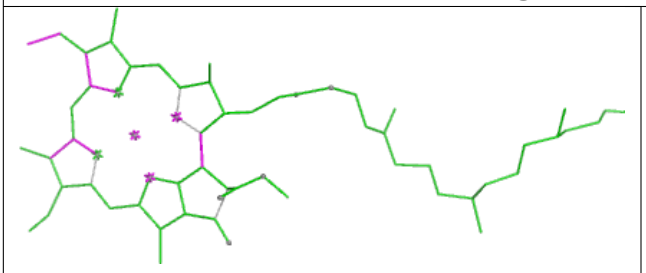
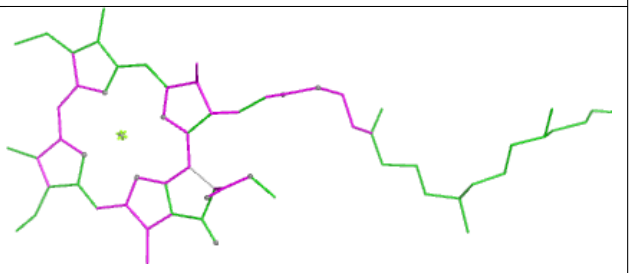


Rings

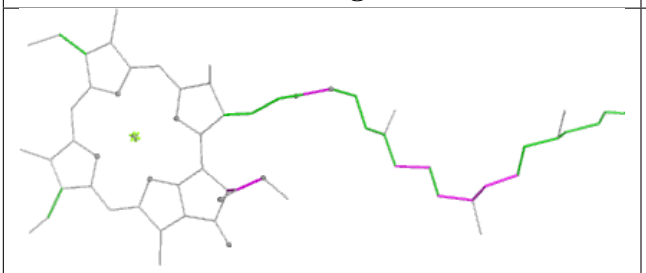
Ligand CLA A 1140



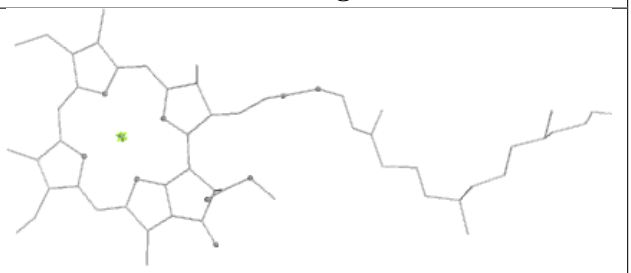
Bond lengths



Bond angles

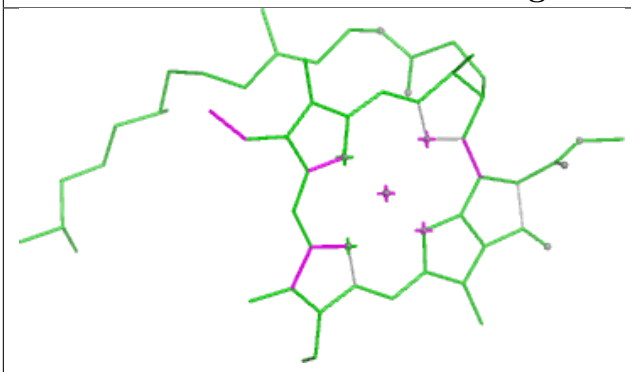


Torsions



Rings

Ligand CLA 5 601



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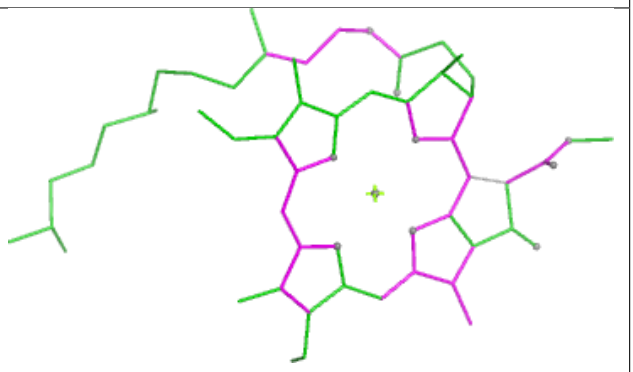

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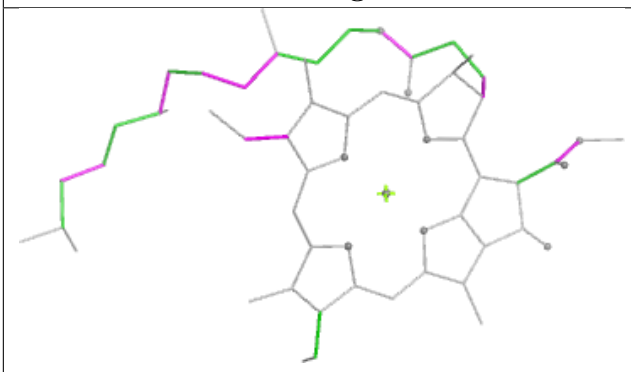

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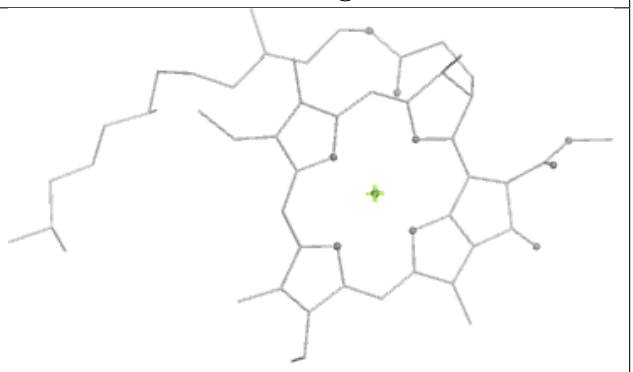
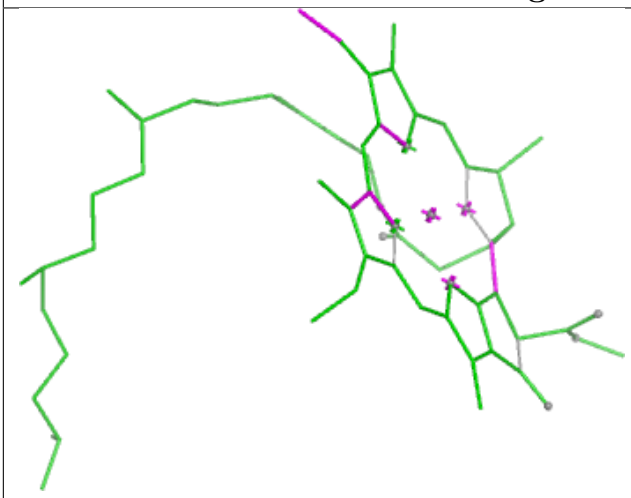


Rings

Ligand CLA 3 601



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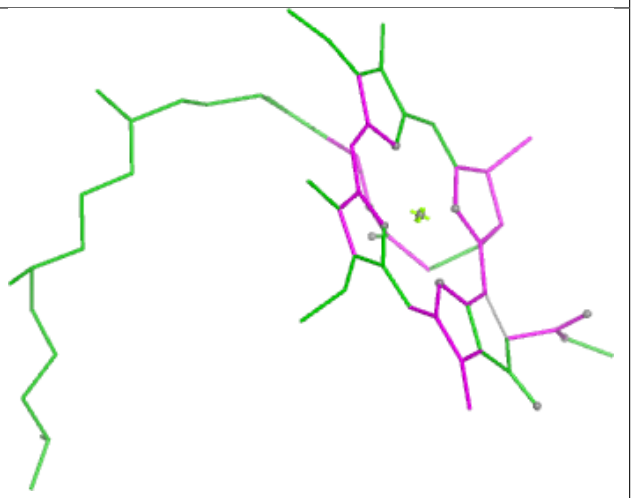


Bond angles

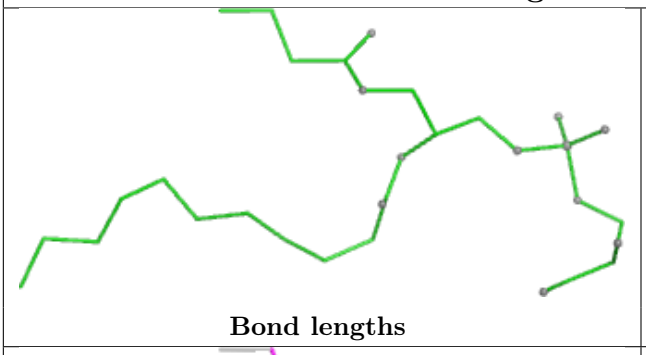


Torsions



Rings

Ligand LHG 4 802



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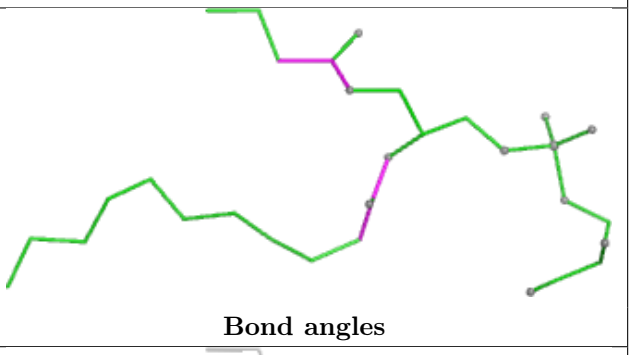
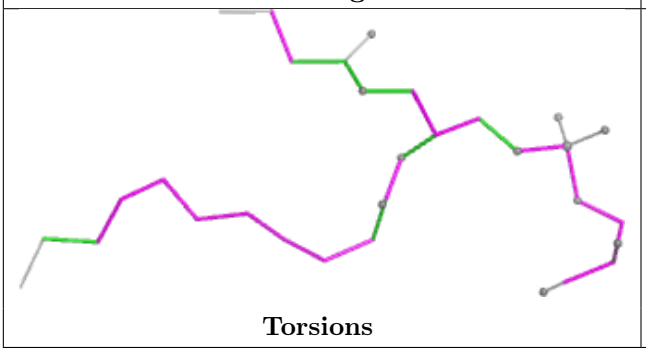


Bond angles



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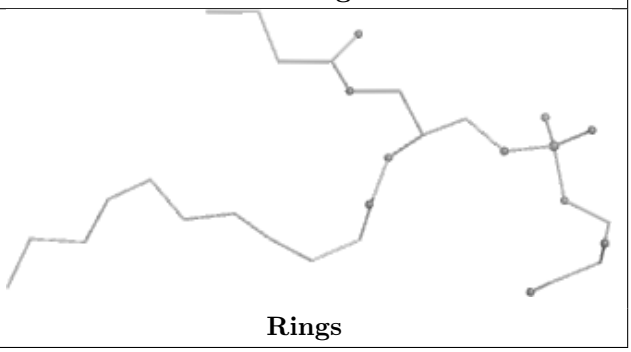
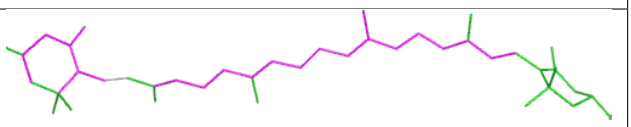


Rings

Ligand LUT 7 502



Bond lengths



Bond angles

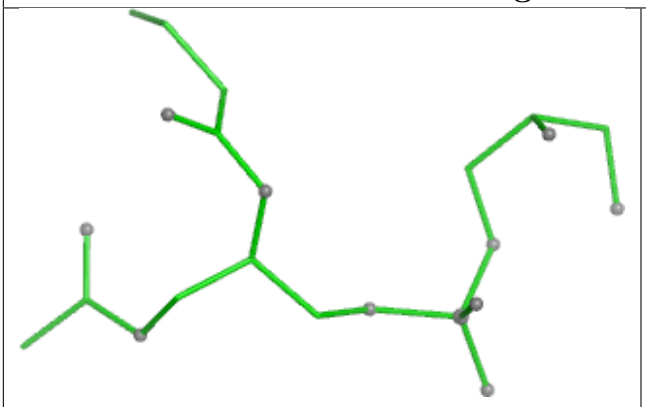


Torsions



Rings

Ligand LHG B 5001



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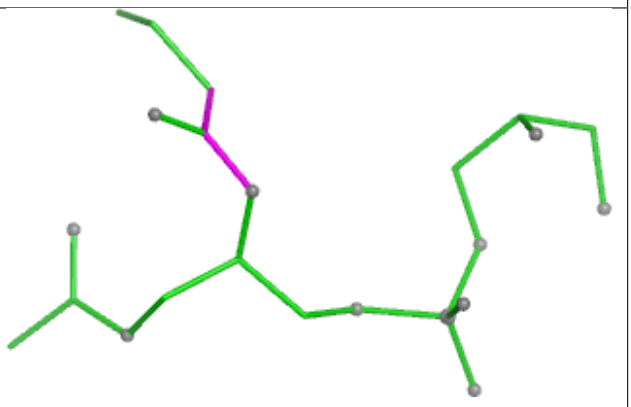
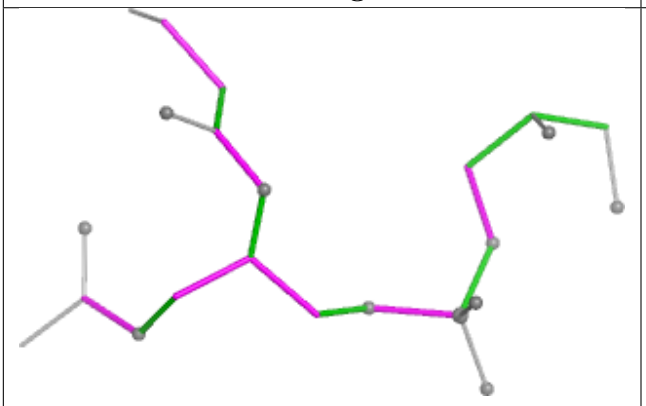


Bond angles



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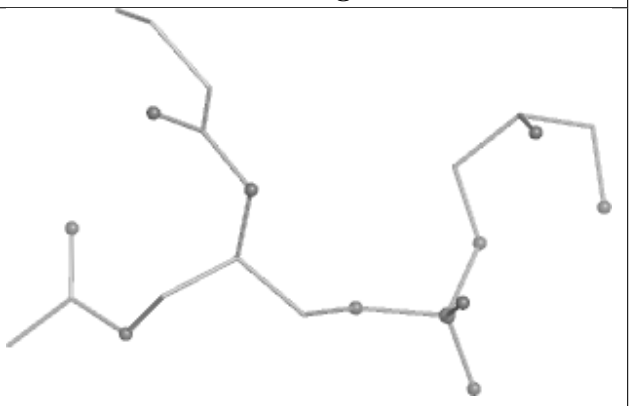


Rings

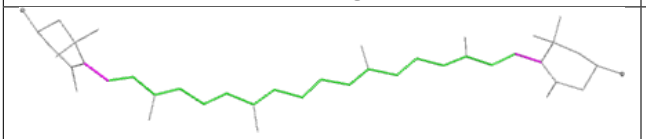
Ligand LUT 4 501



Bond lengths



Bond angles



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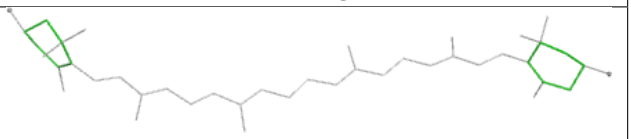
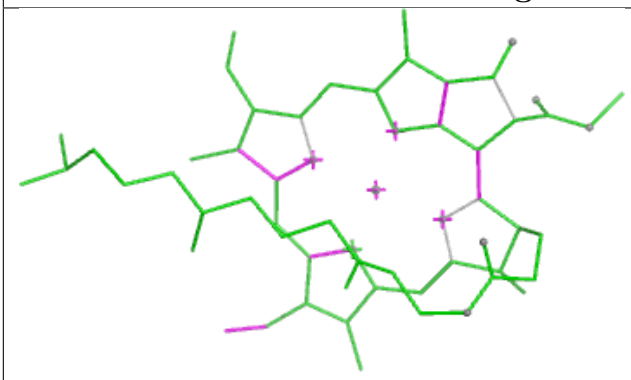
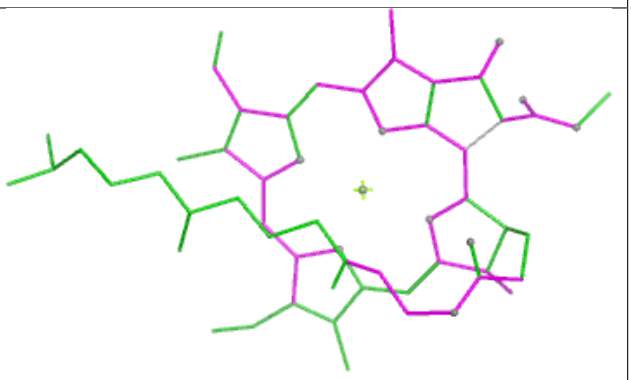


Rings

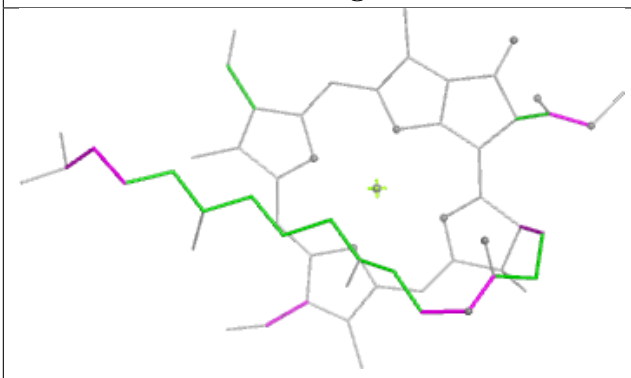
Ligand CLA A 1116



Bond lengths



Bond angles



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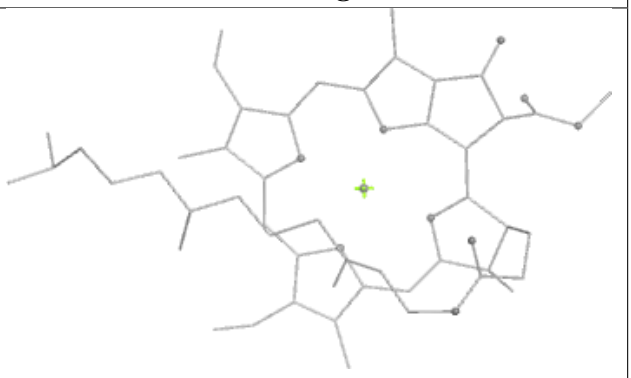


Rings

Ligand 3PH 8 806



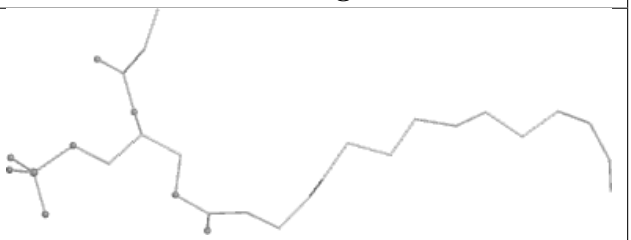
Bond lengths



Bond angles

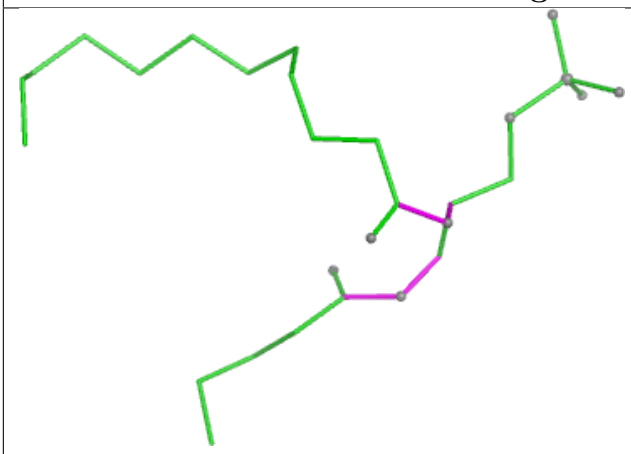


Torsions



Rings

Ligand 3PH 6 802



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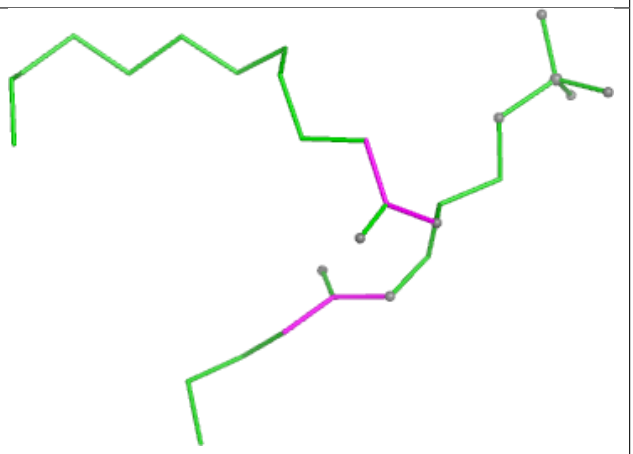
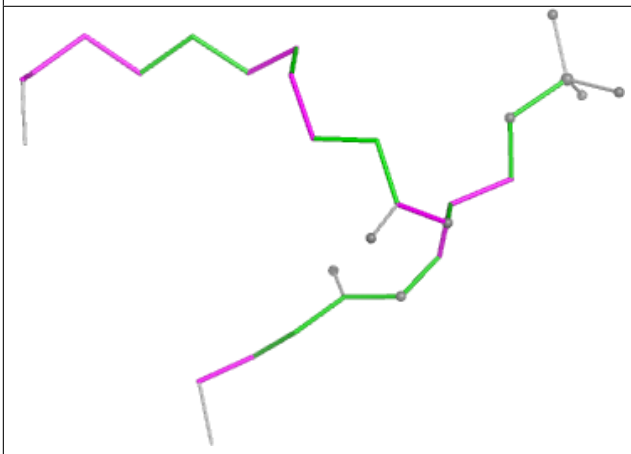


Bond angles



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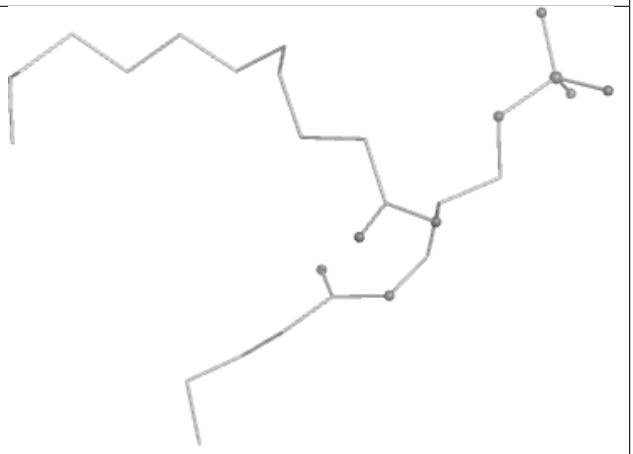
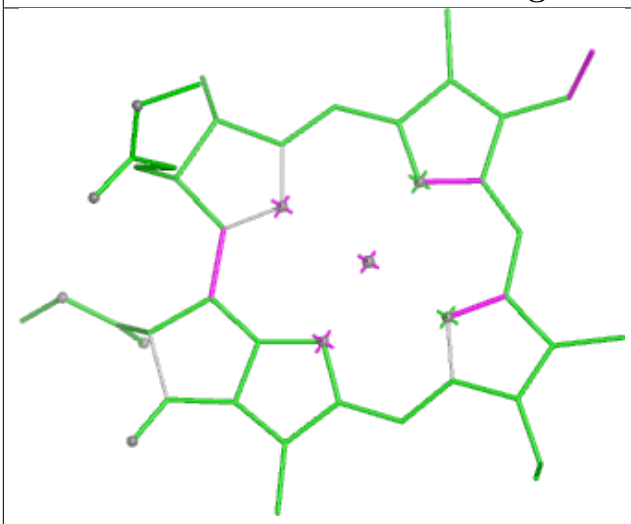


Rings

Ligand CLA 2 615



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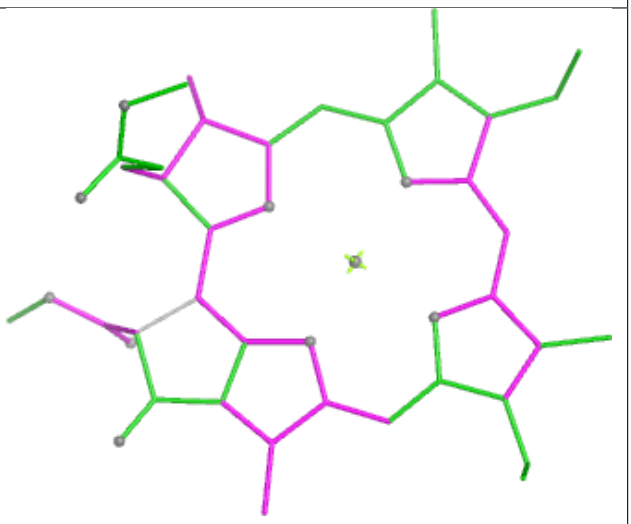

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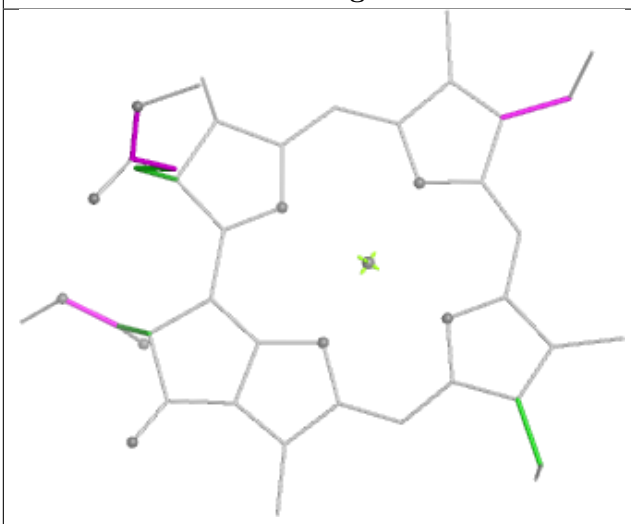

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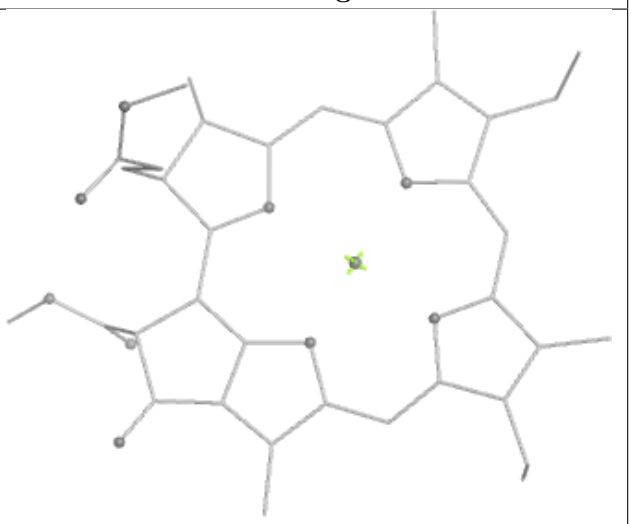
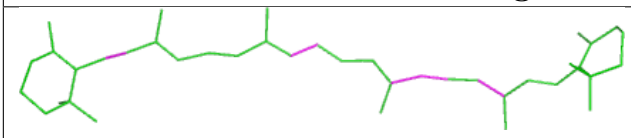


Rings

Ligand BCR A 4004



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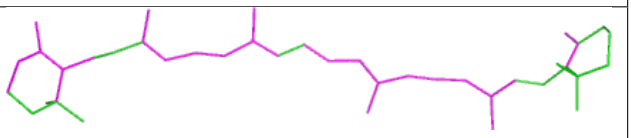
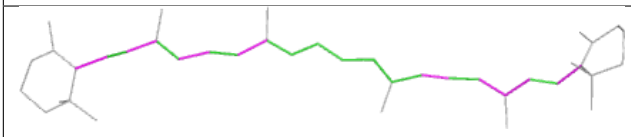


Bond angles



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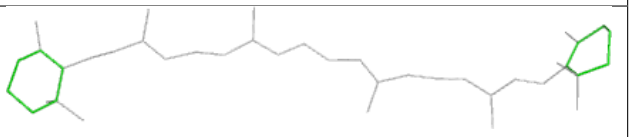
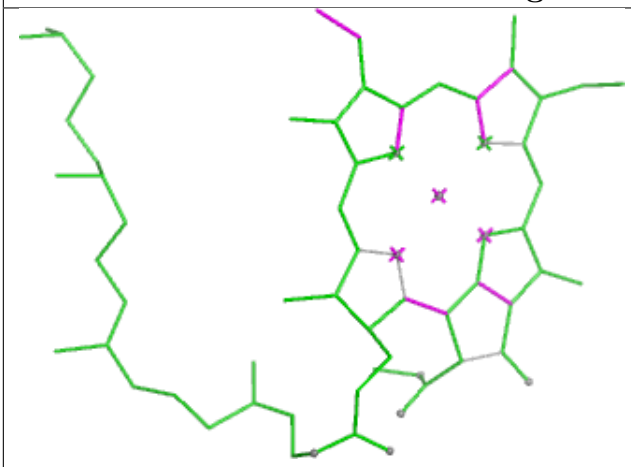


Rings

Ligand CLA Z 605



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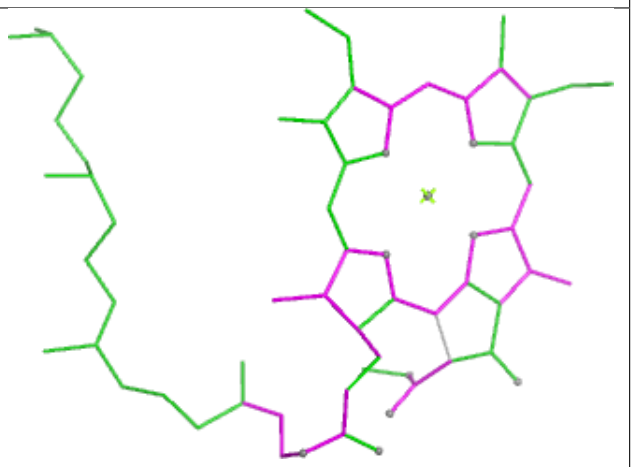
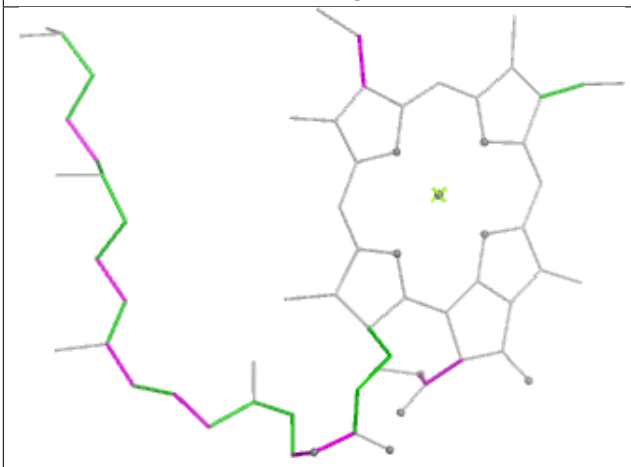


Bond angles

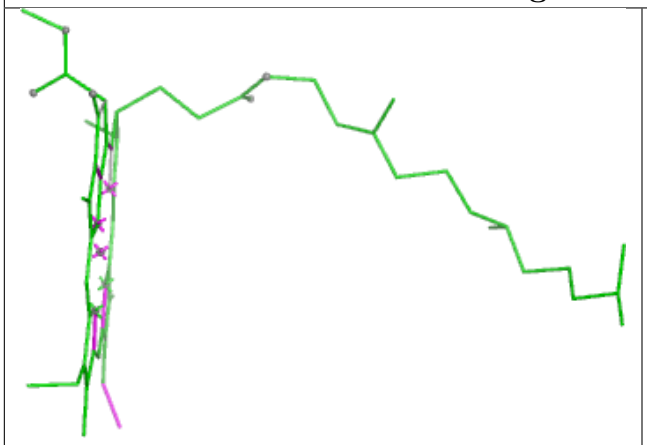


Torsions



Rings

Ligand CLA 4 609



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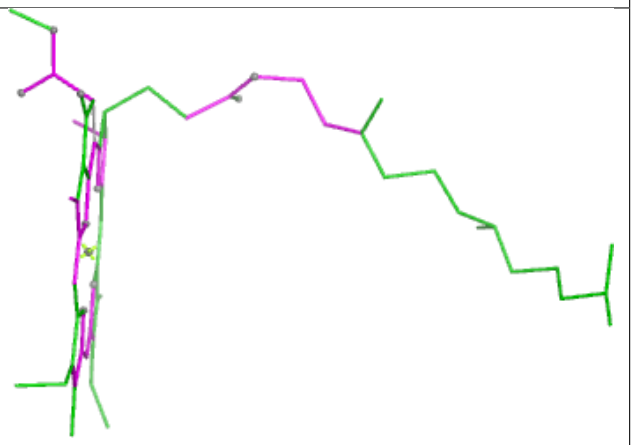
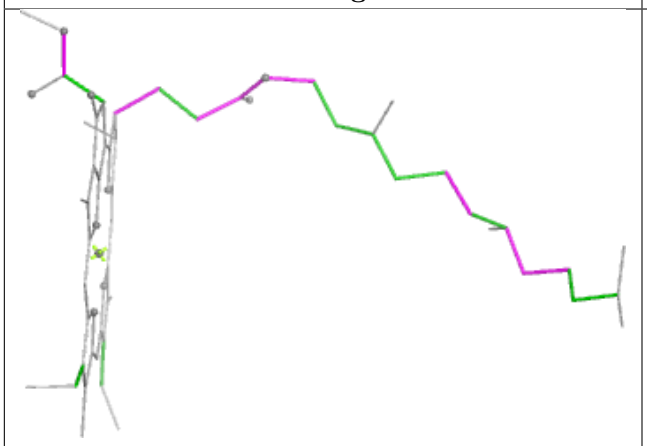


Bond angles



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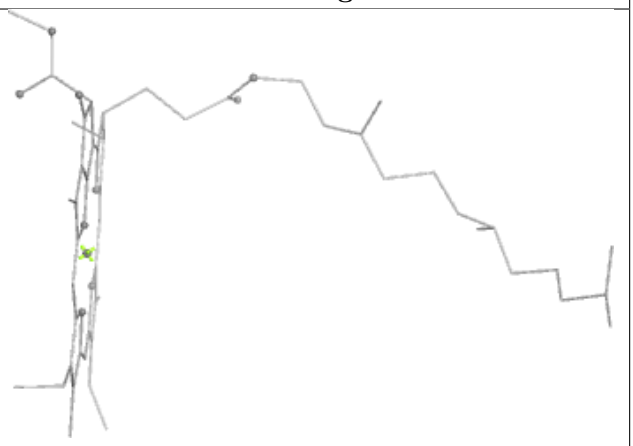
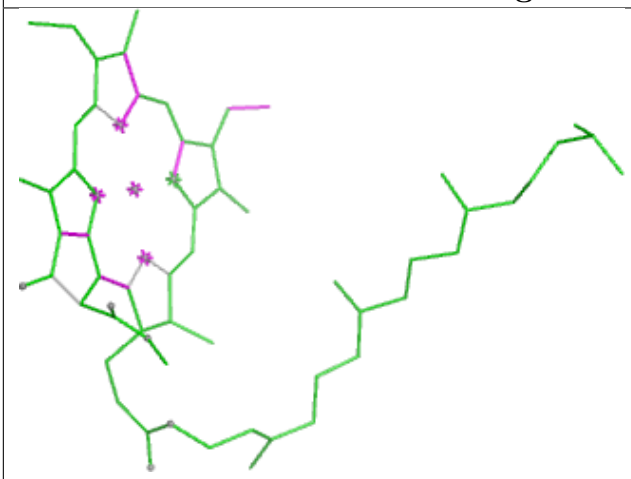


Rings

Ligand CLA B 1221



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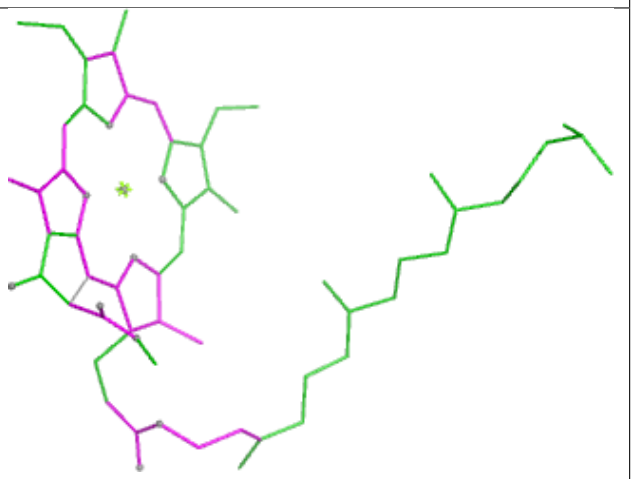
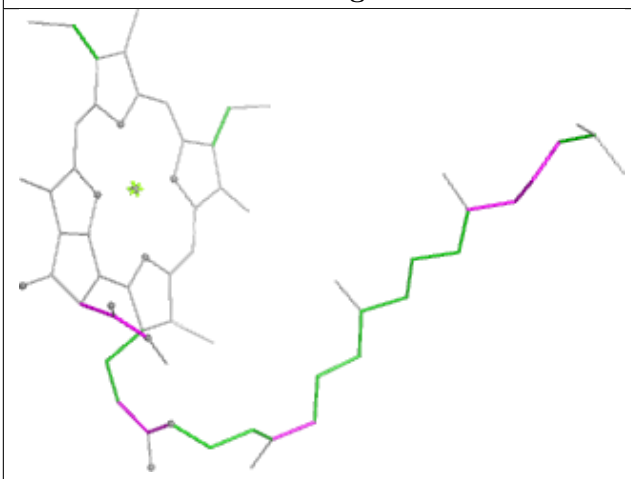


Bond angles



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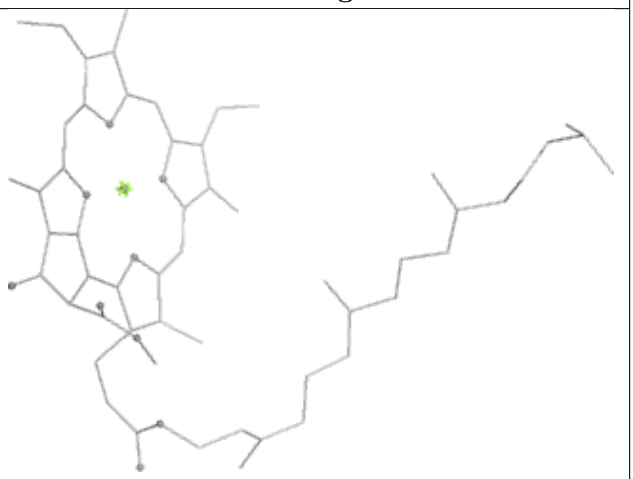
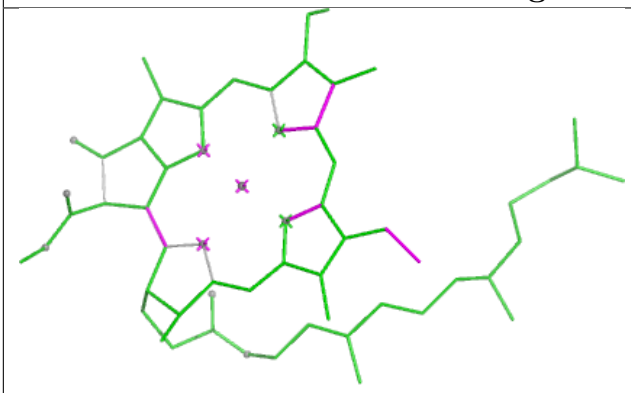


Rings

Ligand CLA 4 604



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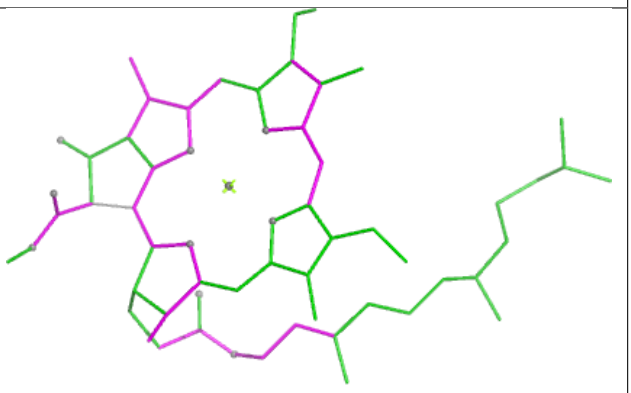
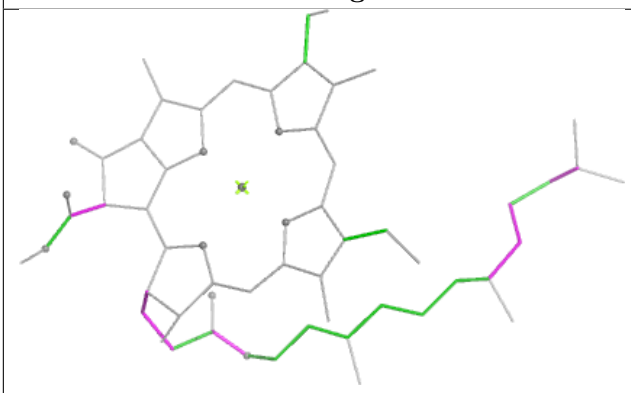


Bond angles



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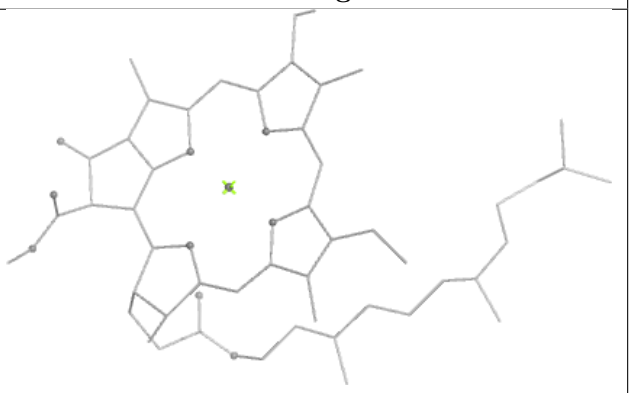
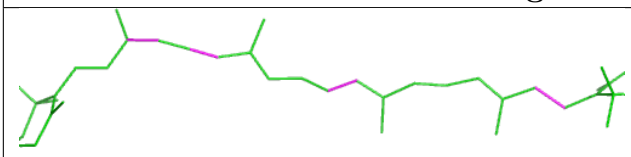


Rings

Ligand BCR 3 505



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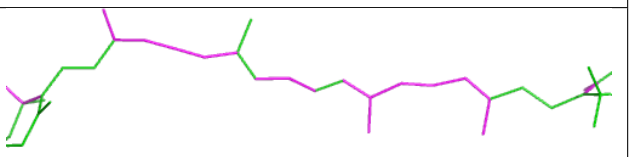
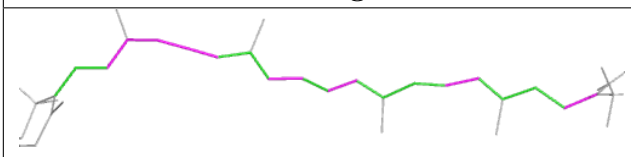


Bond angles



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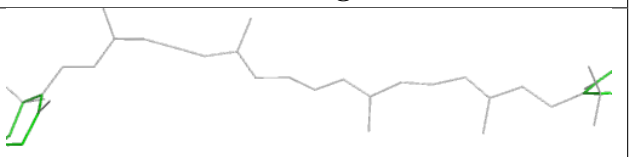
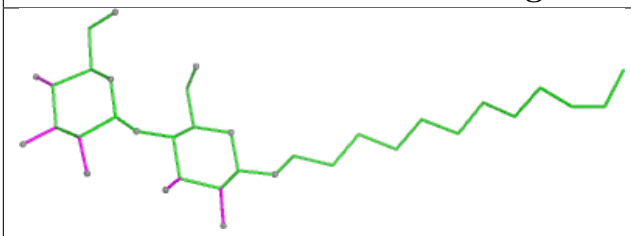


Rings

Ligand LMT 1 803



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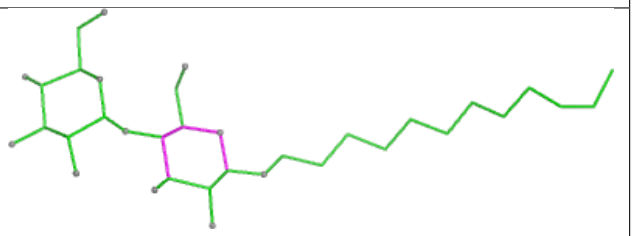
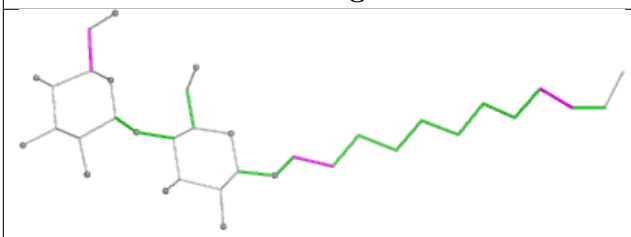
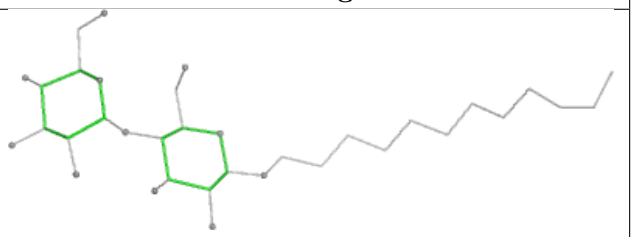


Bond angles

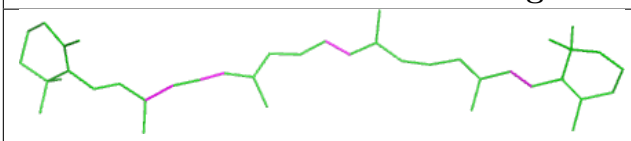


Torsions



Rings

Ligand BCR 3 506



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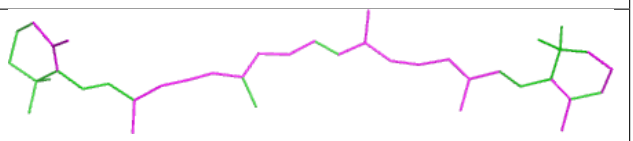
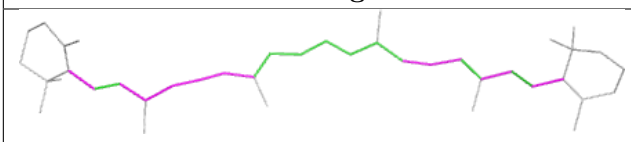


Bond angles



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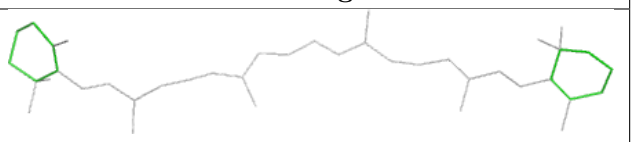
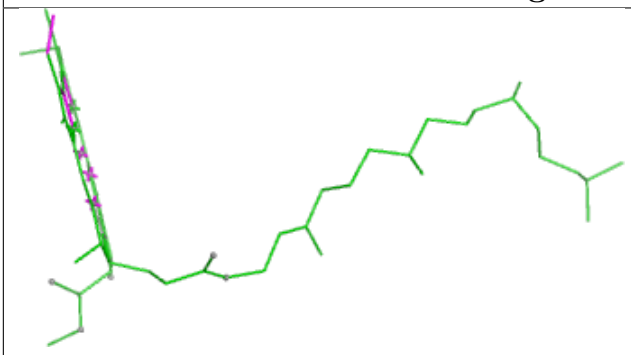


Rings

Ligand CLA 6 609



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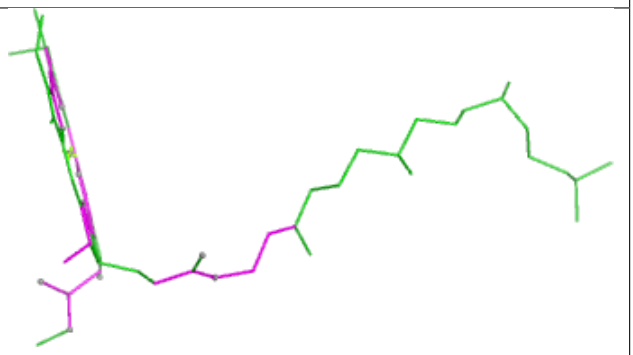

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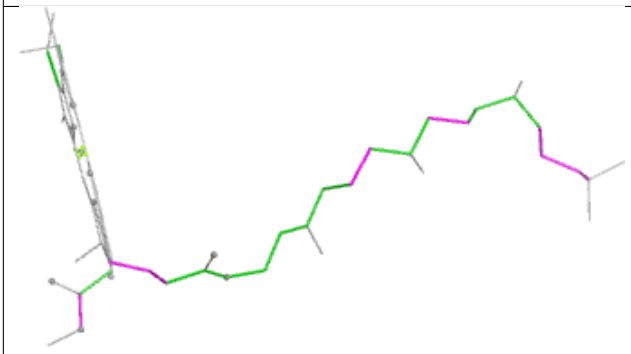
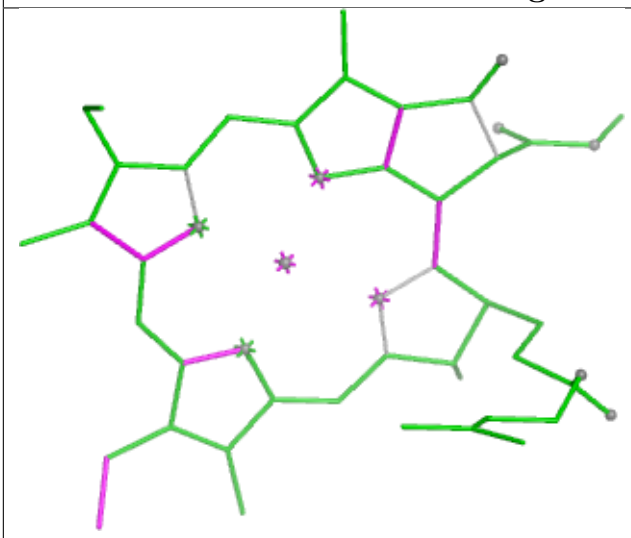


Torsions



Rings

Ligand CLA 9 612



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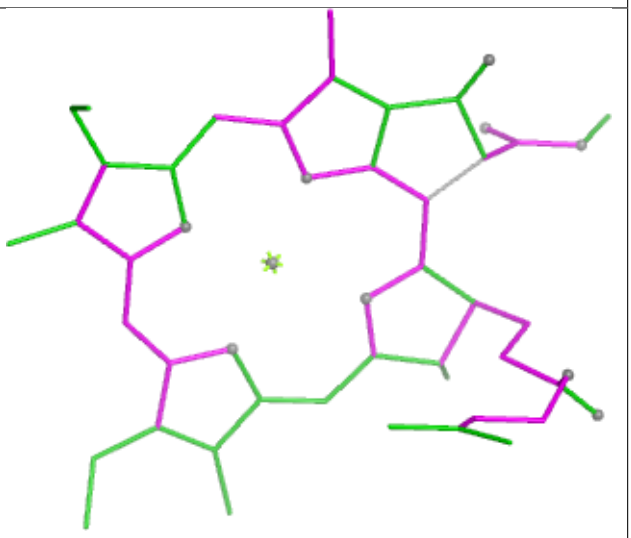

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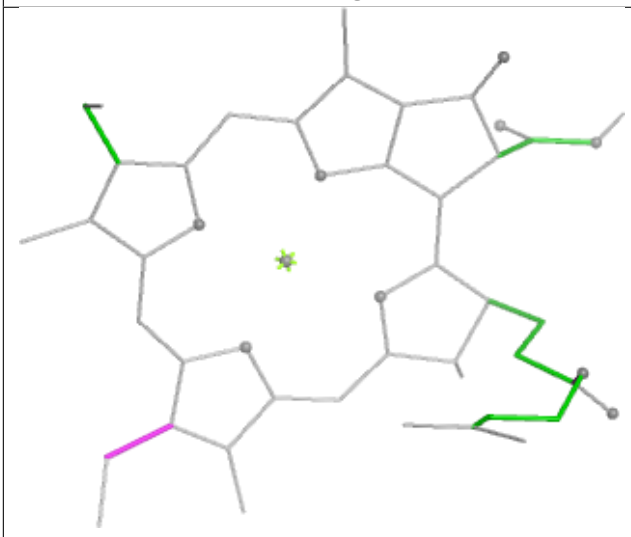

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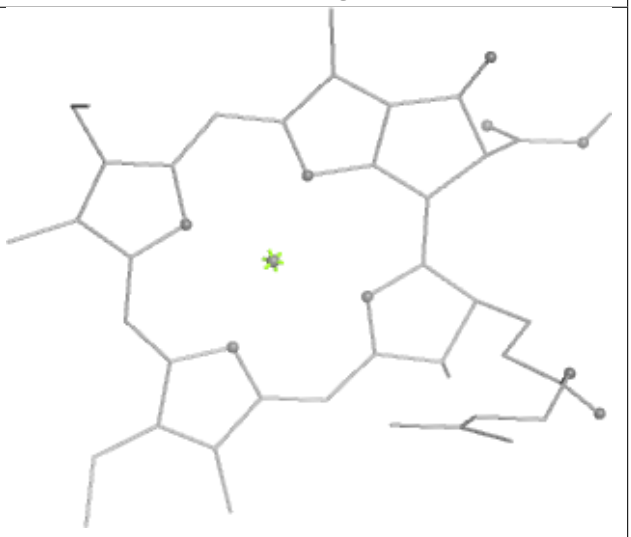
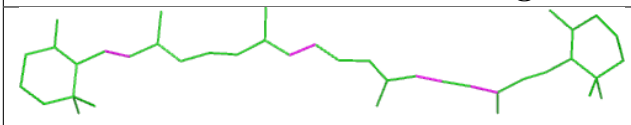


Rings

Ligand BCR L 4001



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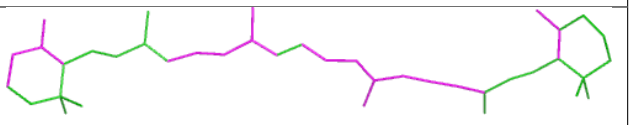

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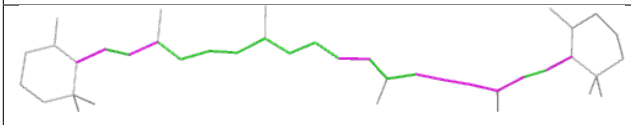
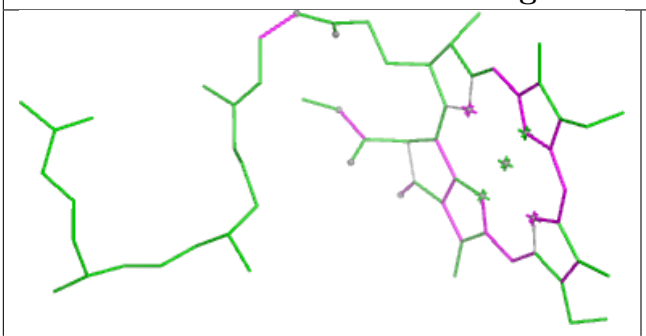


Torsions



Rings

Ligand CL0 A 1011



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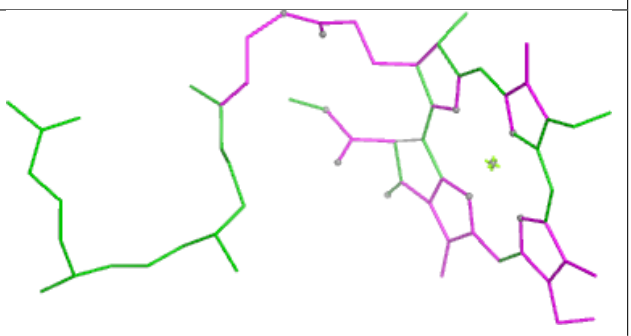

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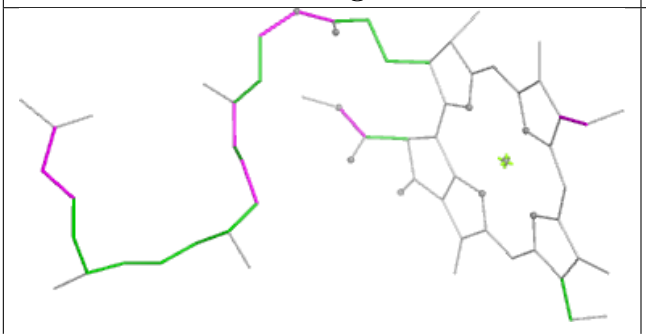

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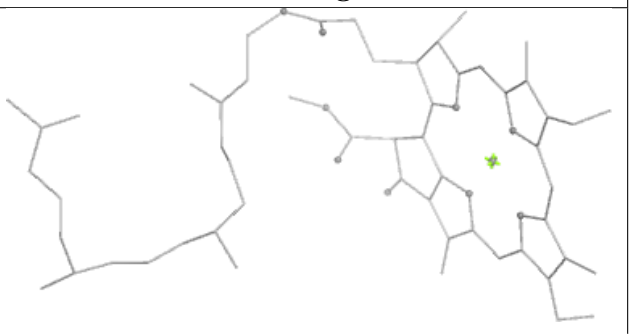
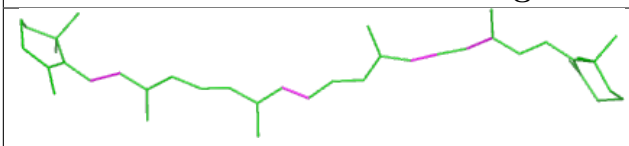


Rings

Ligand BCR B 4004



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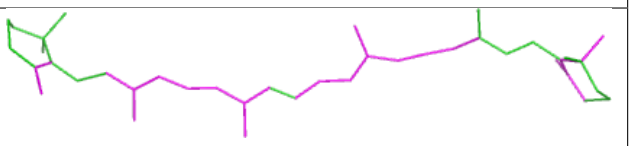

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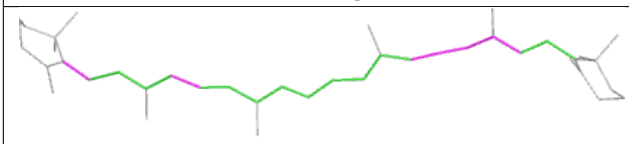

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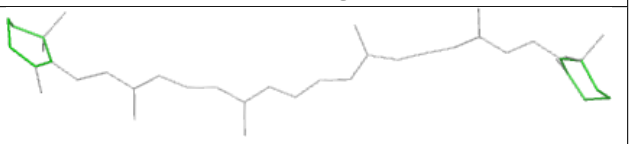
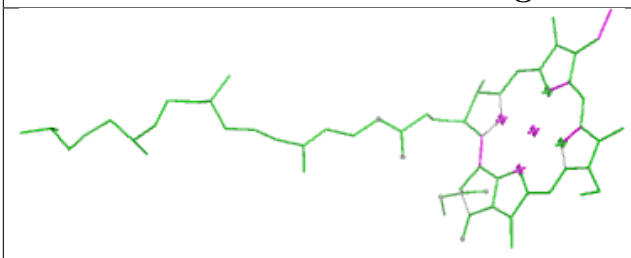


Rings

Ligand CLA A 1107



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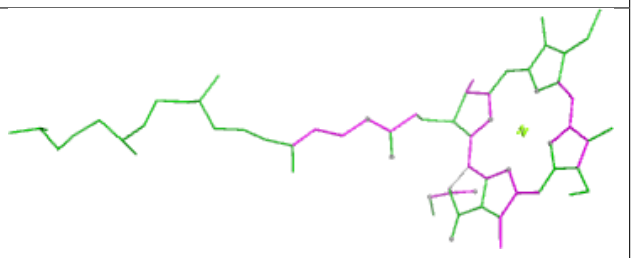

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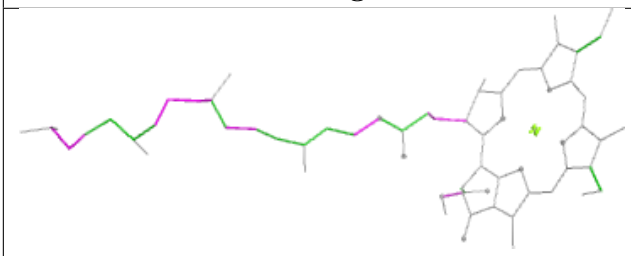

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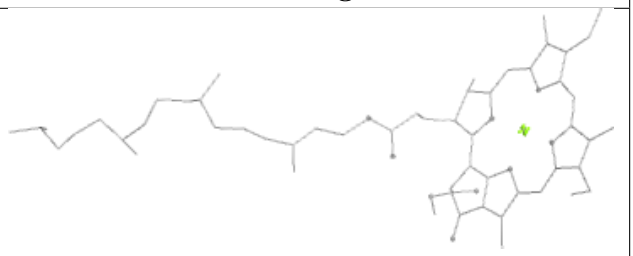
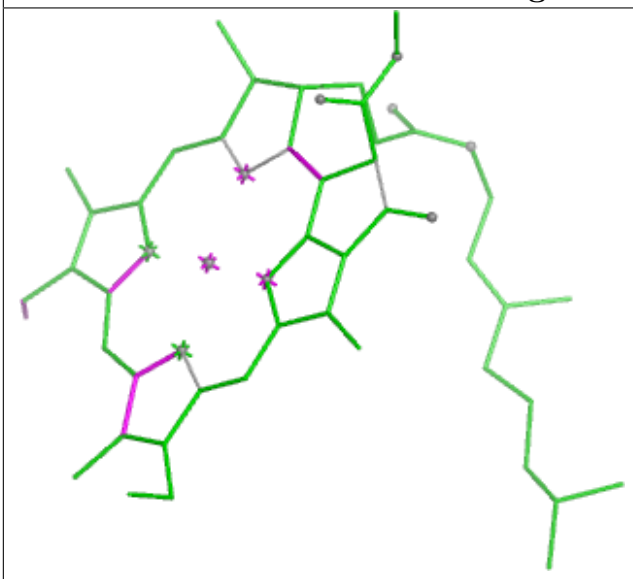


Rings

Ligand CLA 6 607



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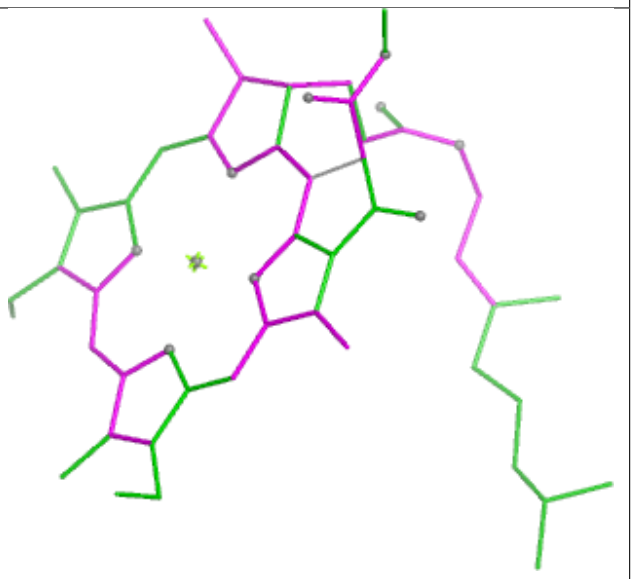

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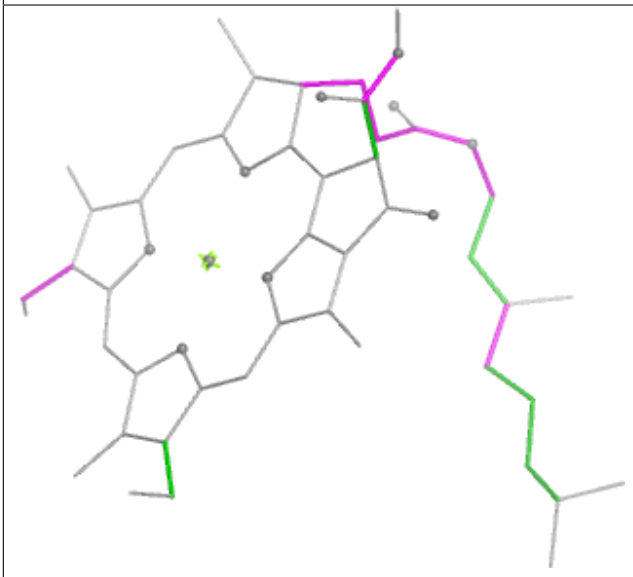
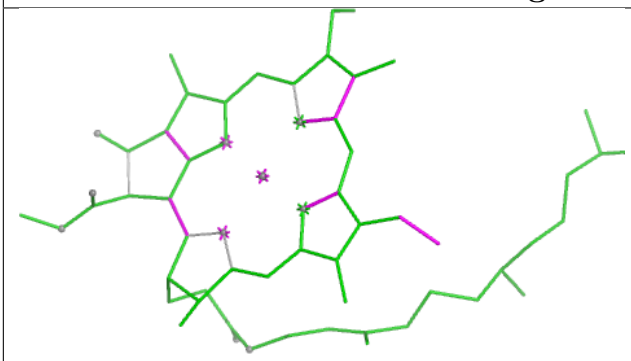


Torsions



Rings

Ligand CLA 2 601



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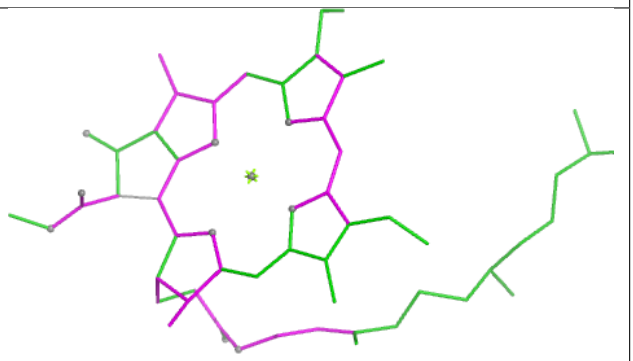

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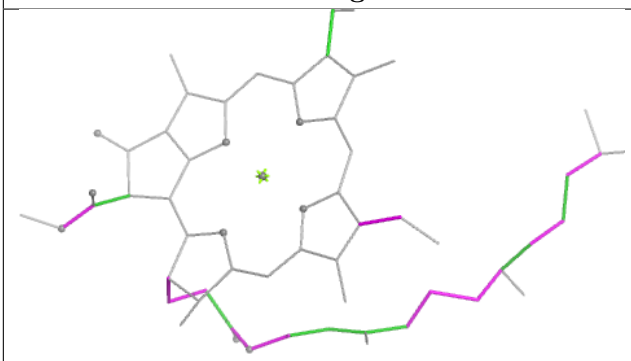

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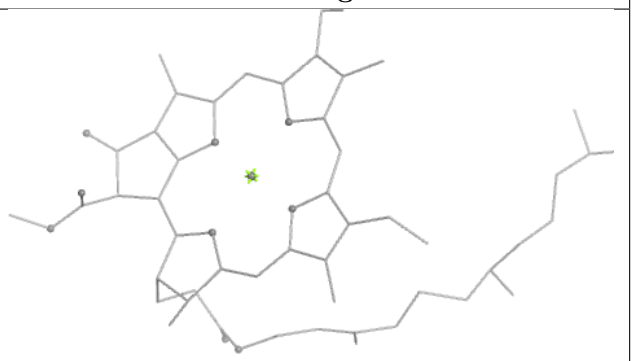
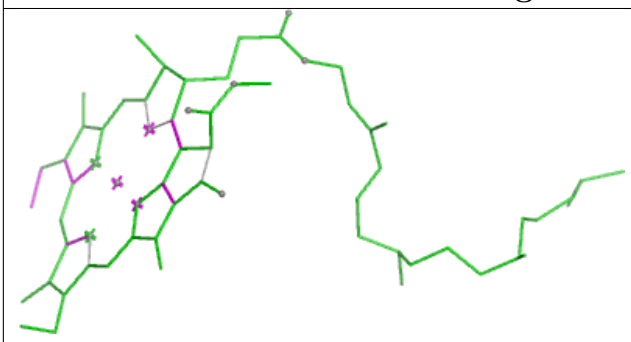


Rings

Ligand CLA B 1021



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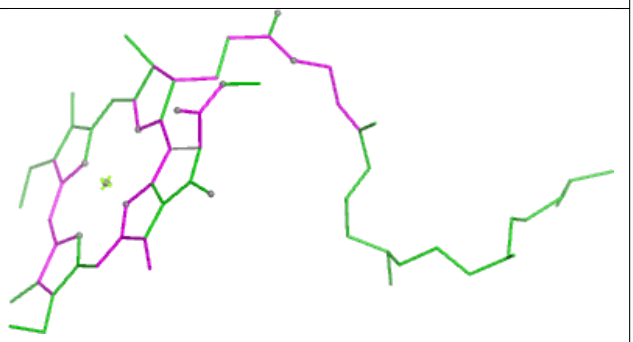

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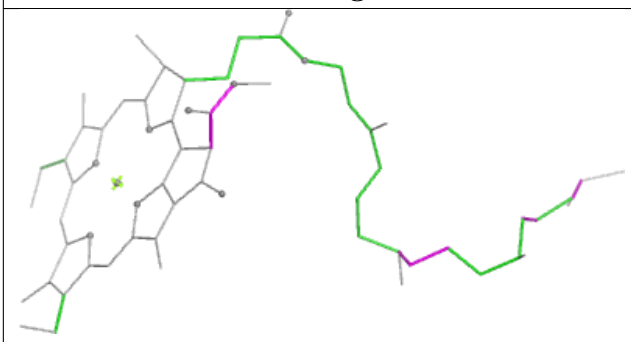

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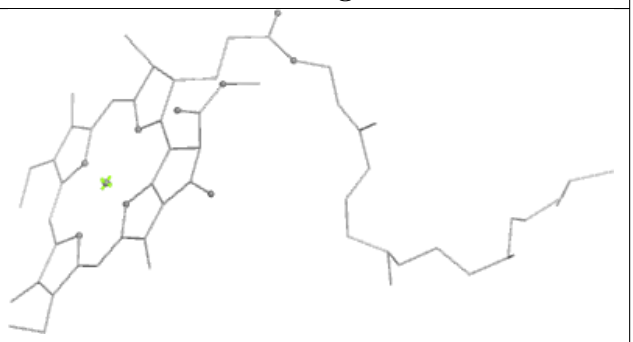
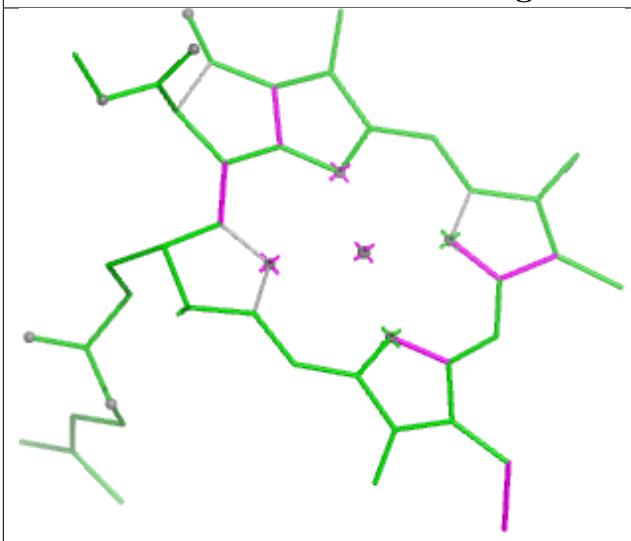


Rings

Ligand CLA B 1227



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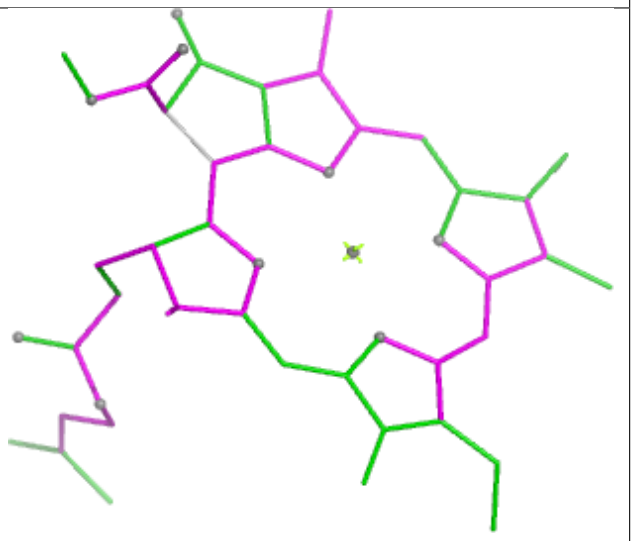
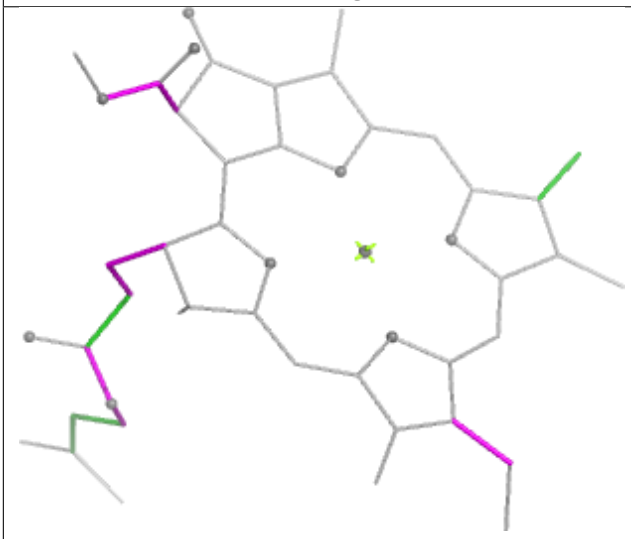


Bond angles



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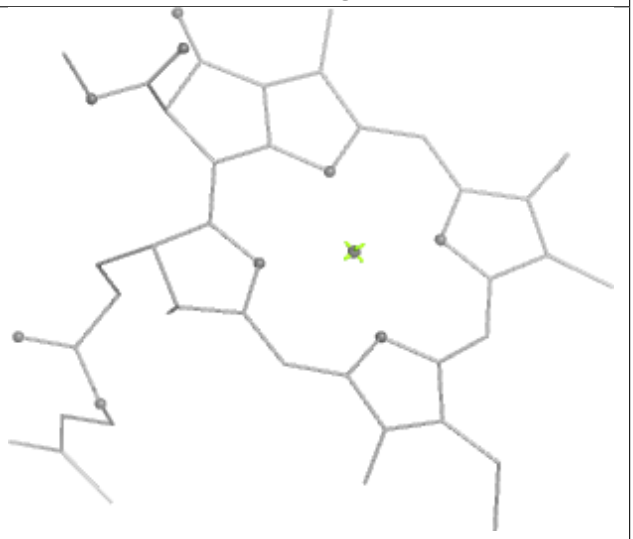
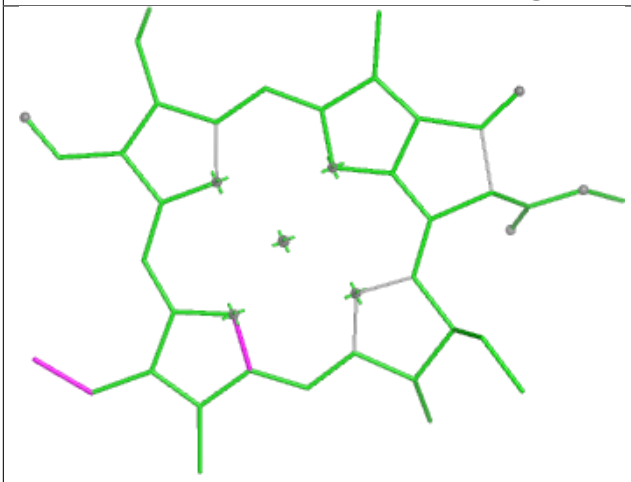


Rings

Ligand CHL 4 617



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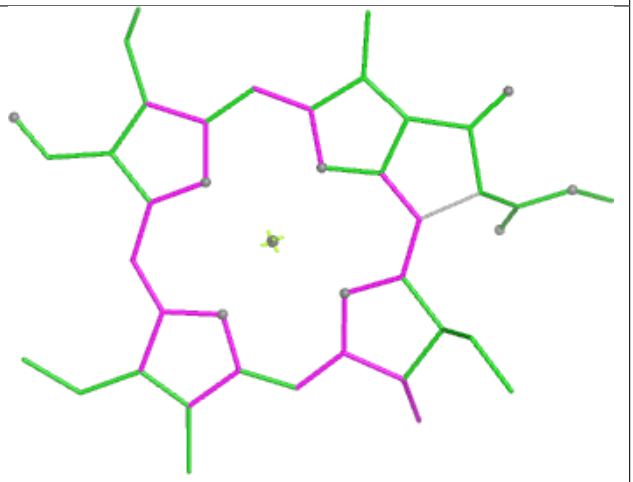

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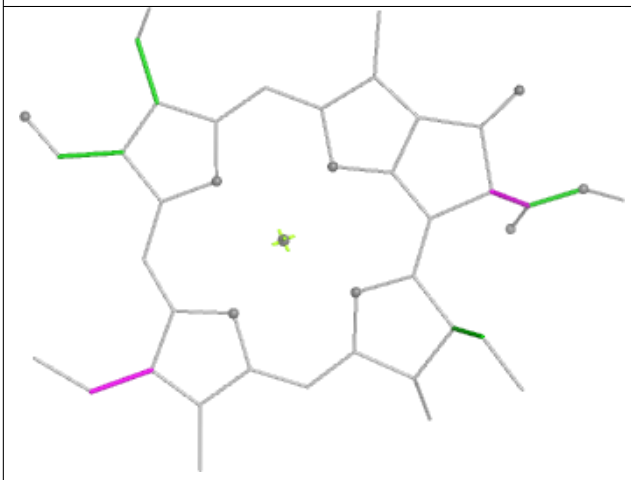

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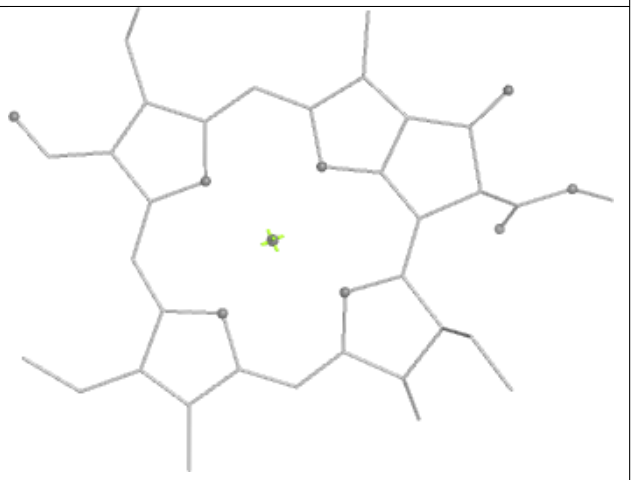
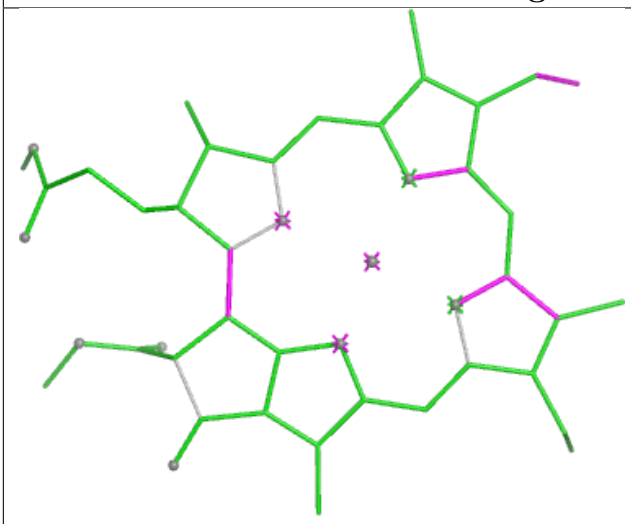


Rings

Ligand CLA 3 602



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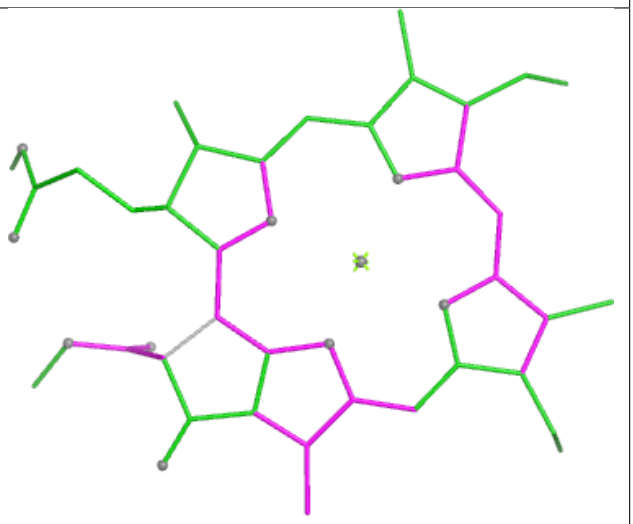
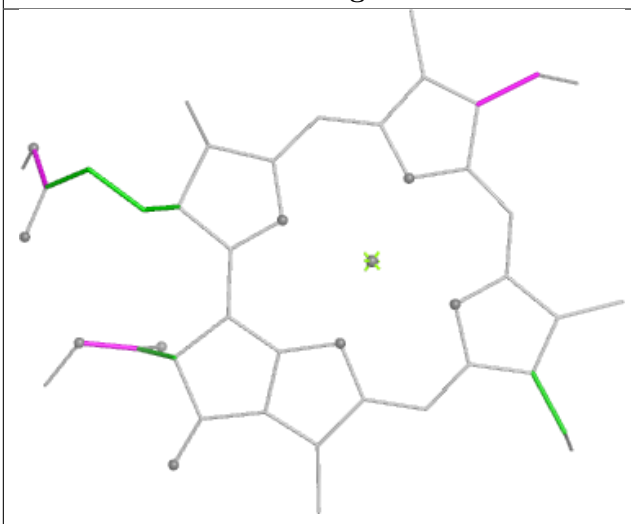


Bond angles



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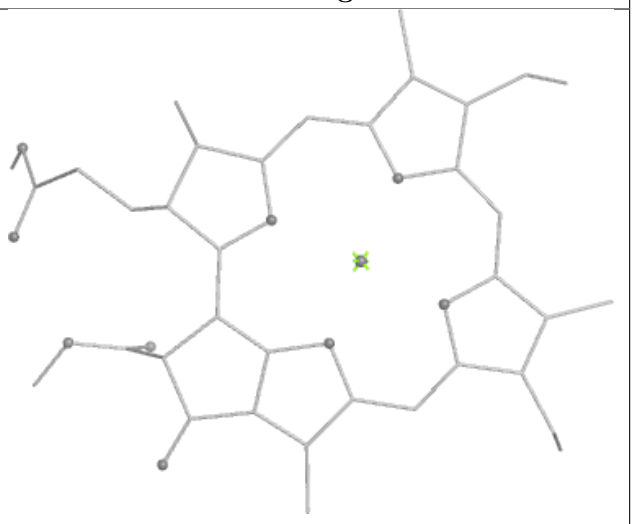
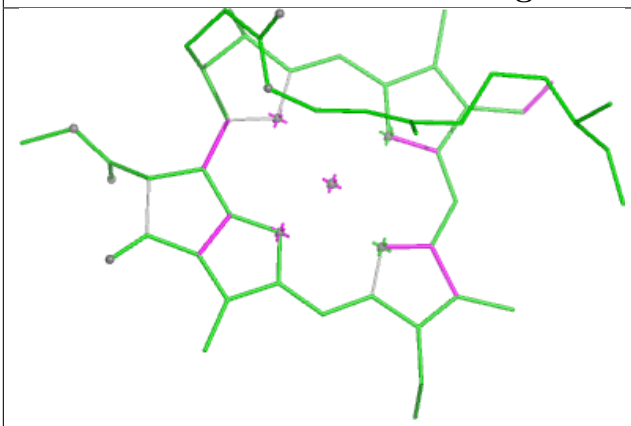


Rings

Ligand CLA B 1208



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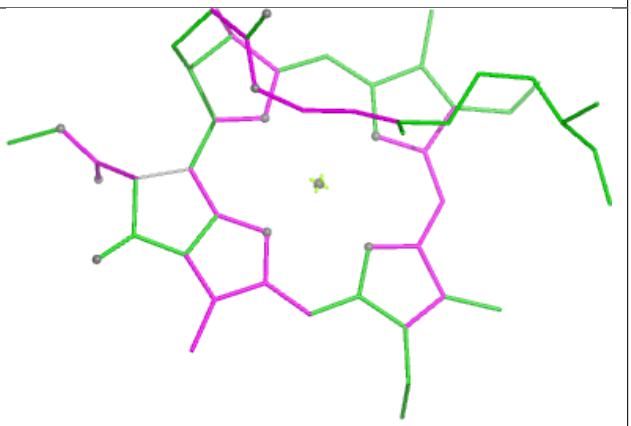
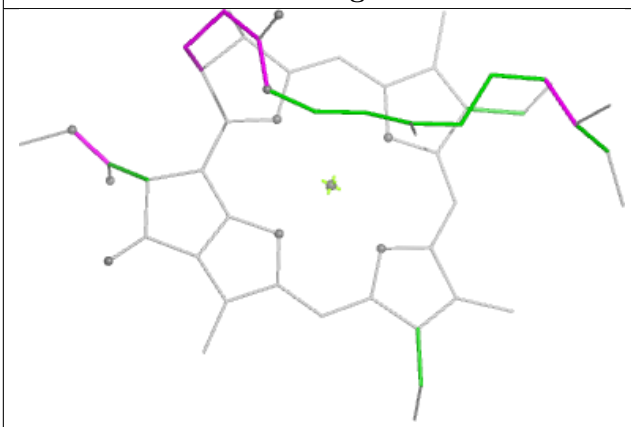


Bond angles



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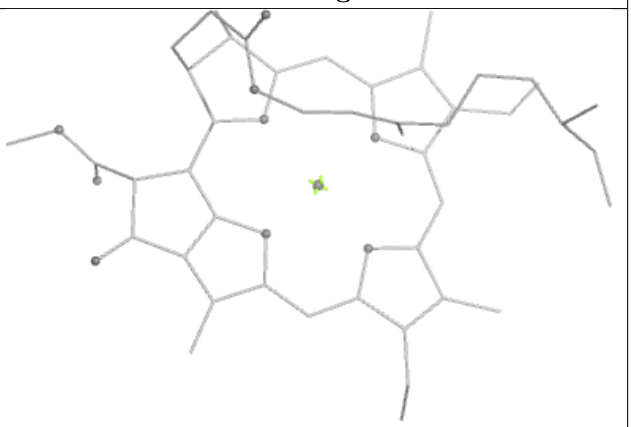
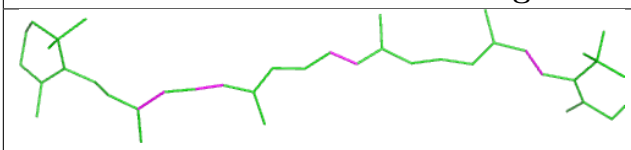


Rings

Ligand BCR A 4003



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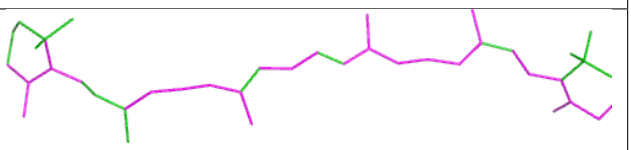
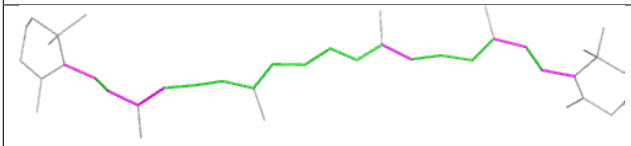


Bond angles



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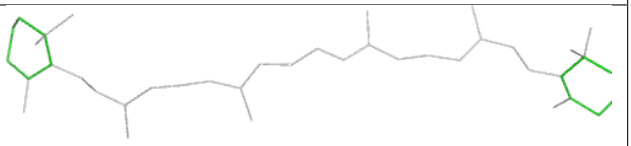
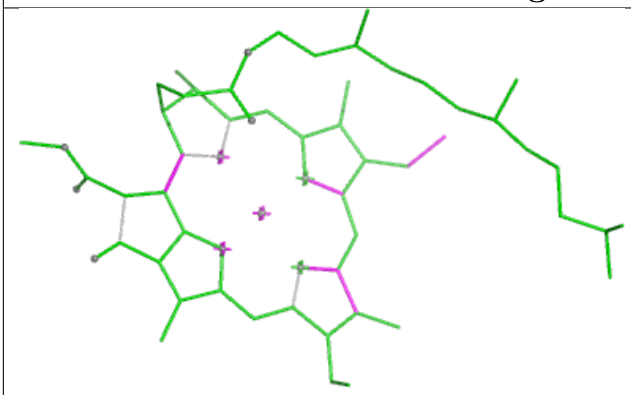


Rings

Ligand CLA 6 601



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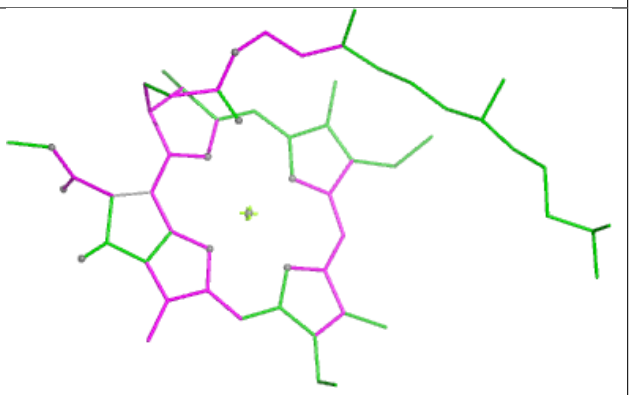
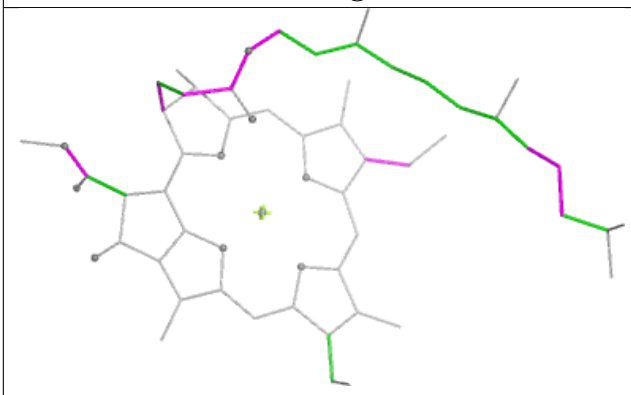
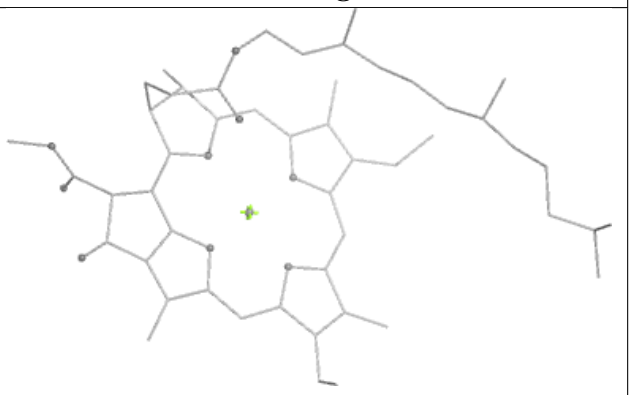


Bond angles

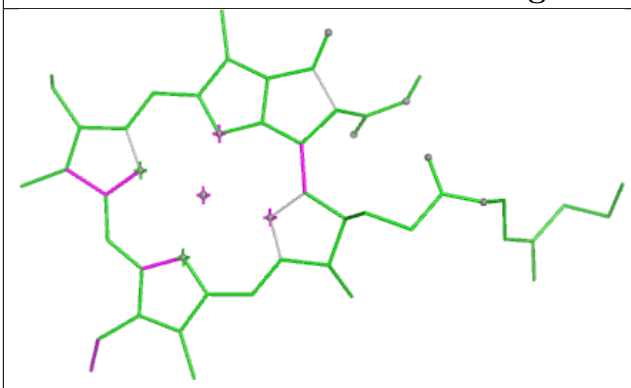


Torsions



Rings

Ligand CLA 6 602



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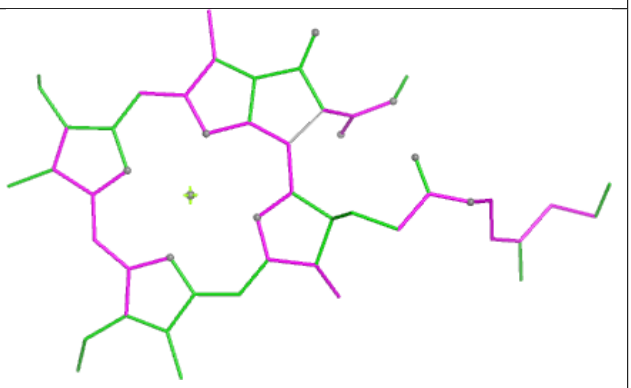

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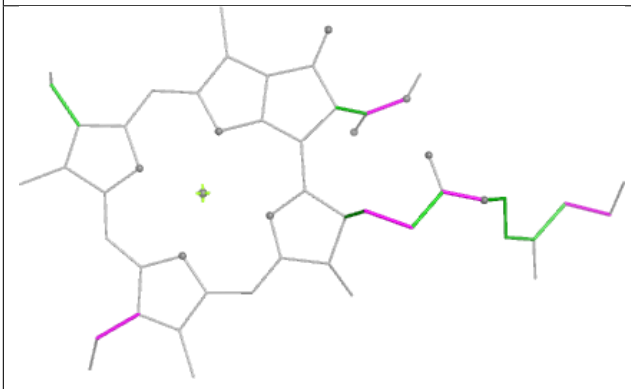

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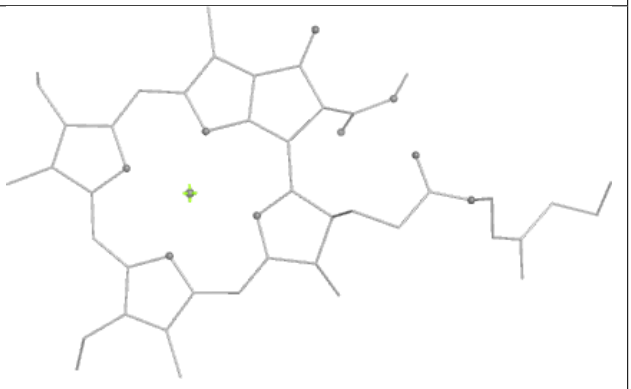
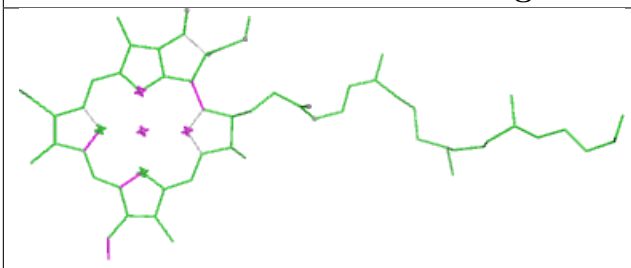


Rings

Ligand CLA A 1131



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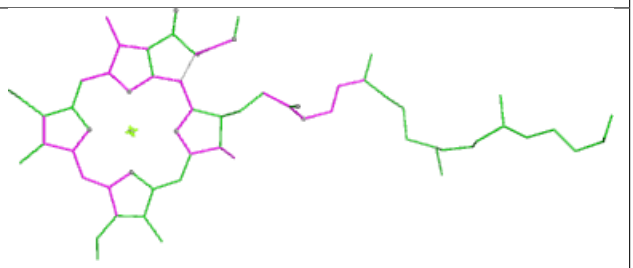
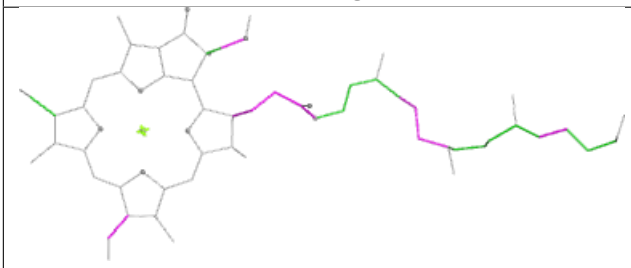


Bond angles



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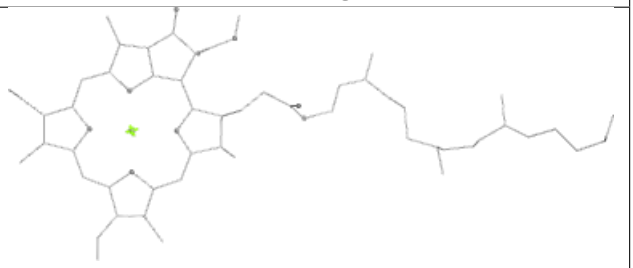
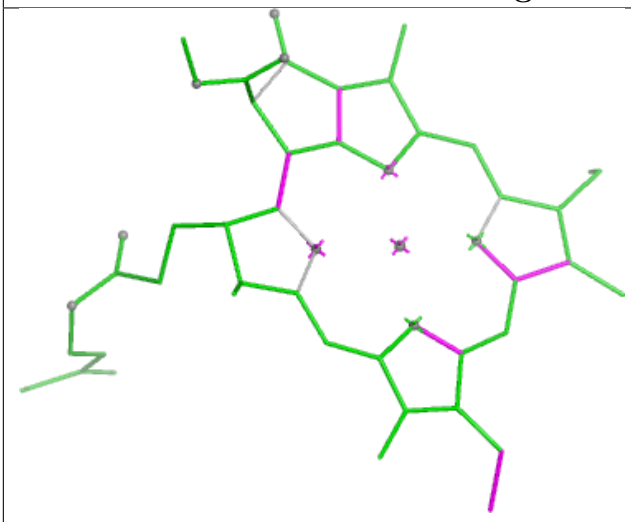


Rings

Ligand CLA A 1129



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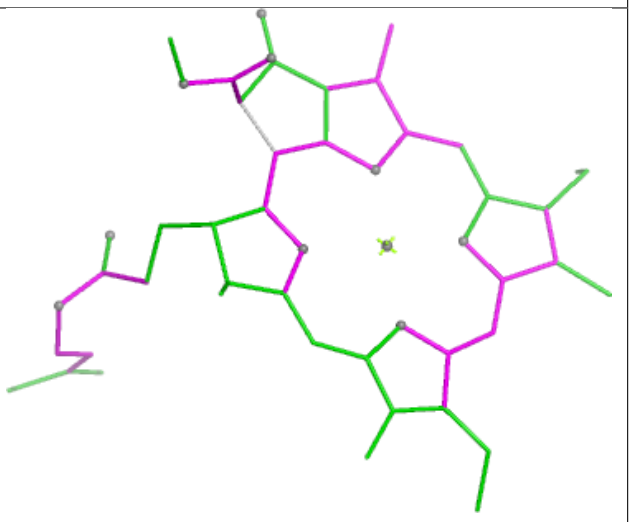

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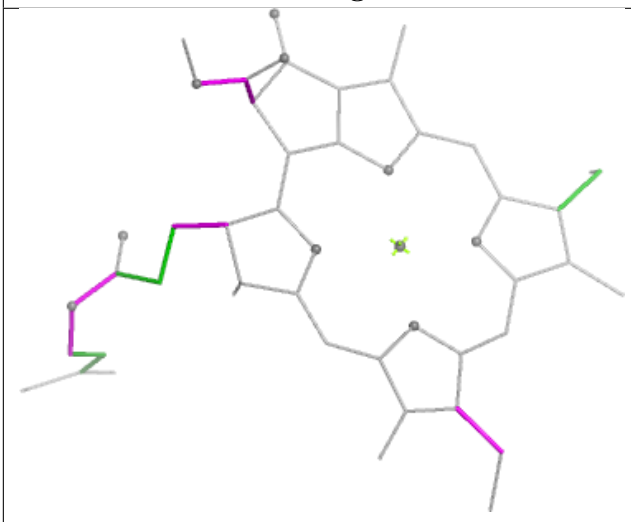

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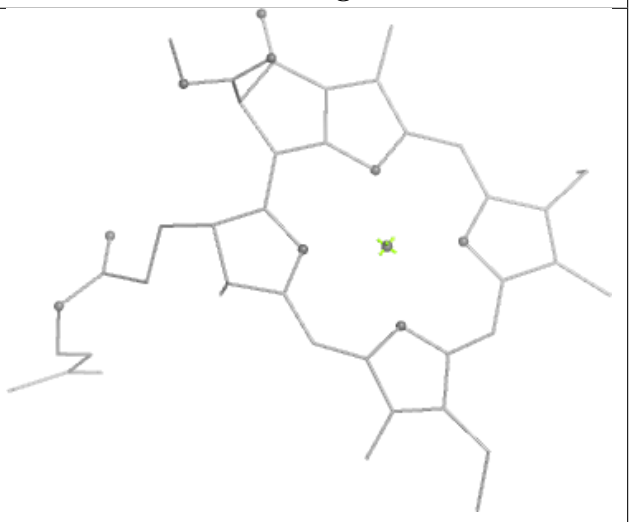
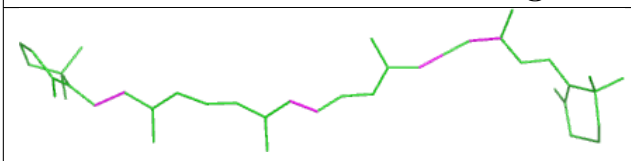


Rings

Ligand BCR 6 503



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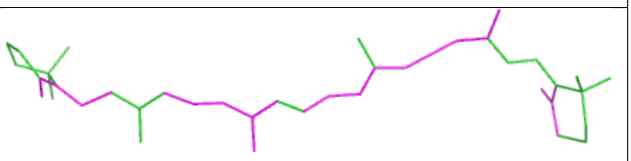

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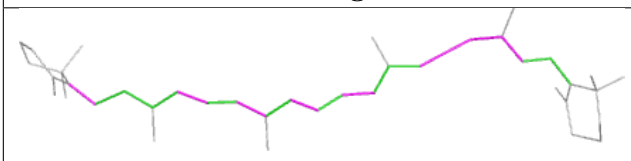

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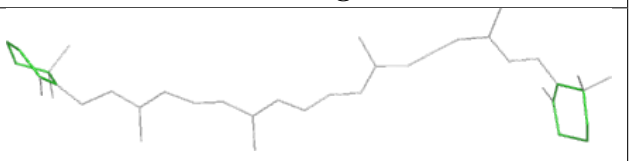
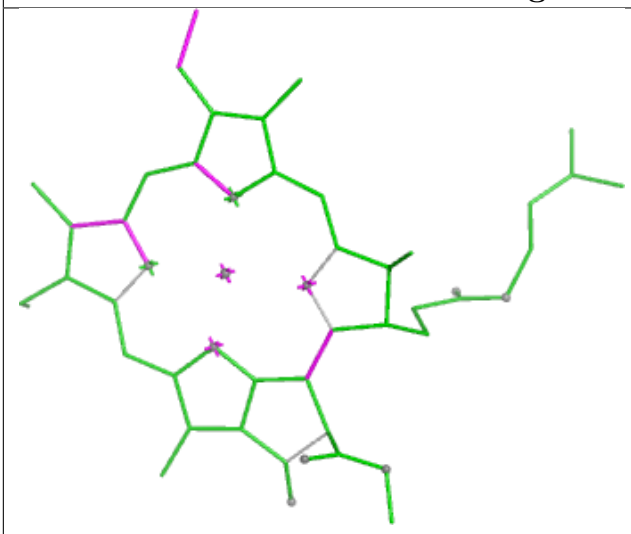


Rings

Ligand CLA 2 612



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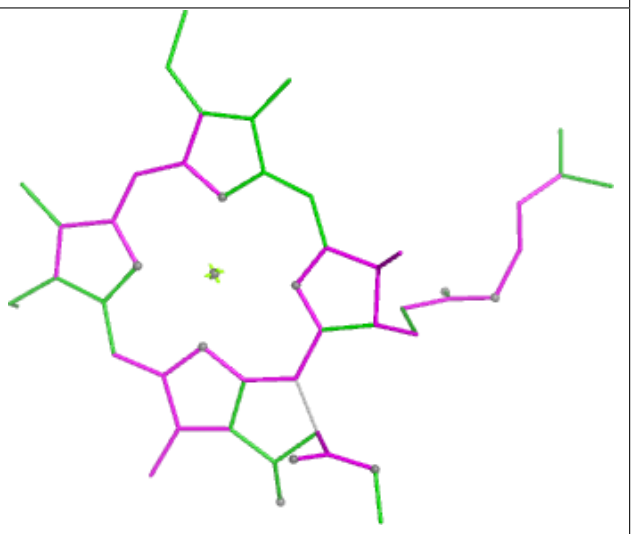

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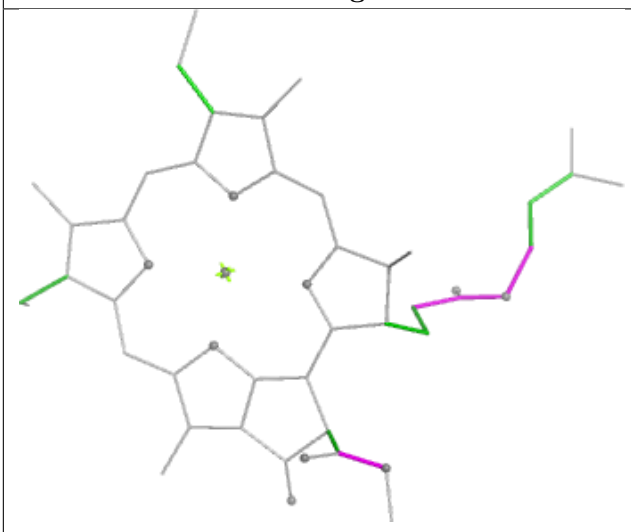

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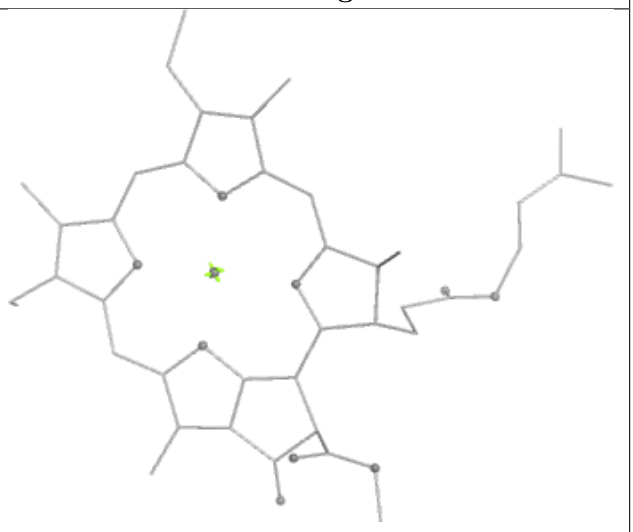
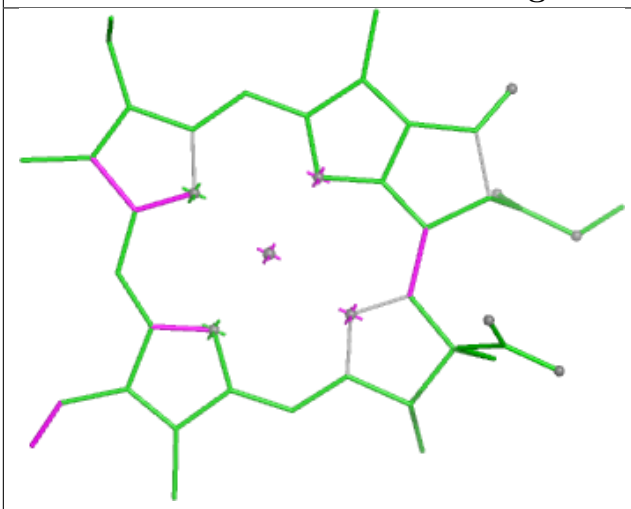


Rings

Ligand CLA 5 608



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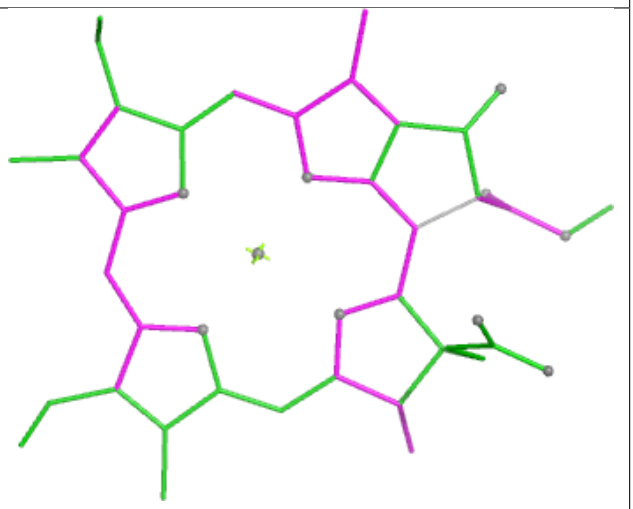

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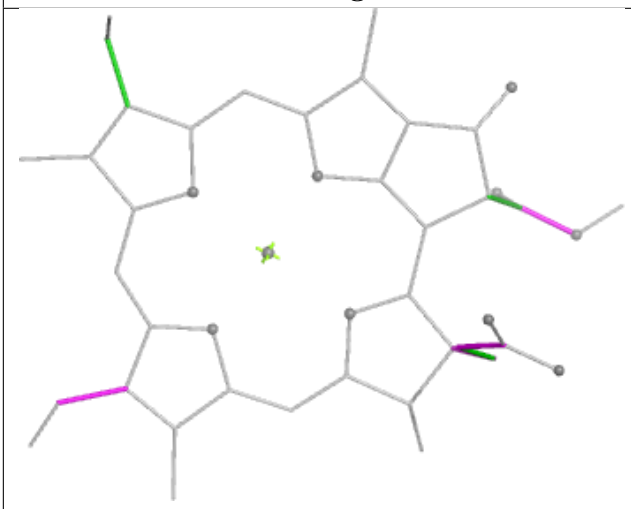

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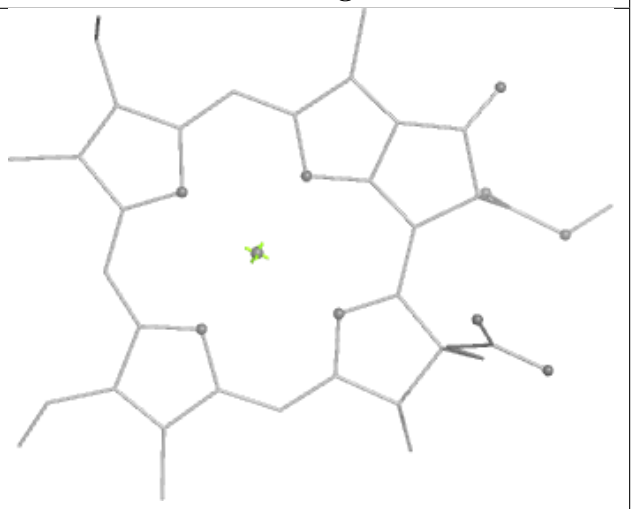
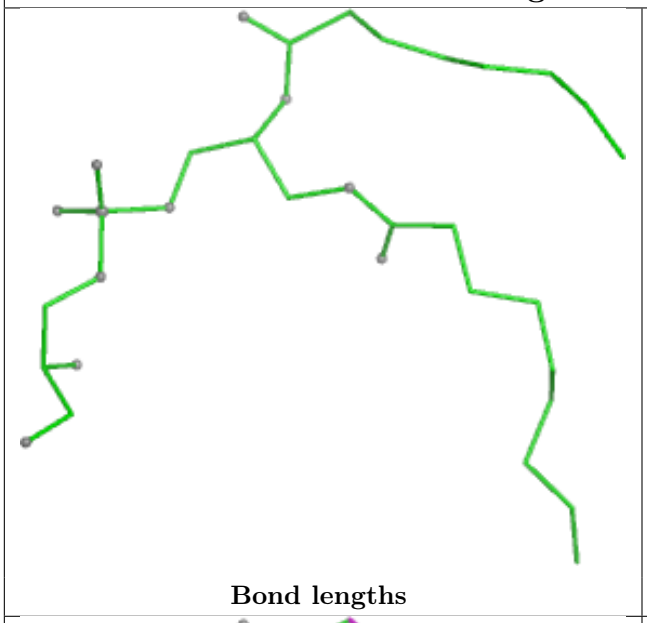


Rings

Ligand LHG 2 801



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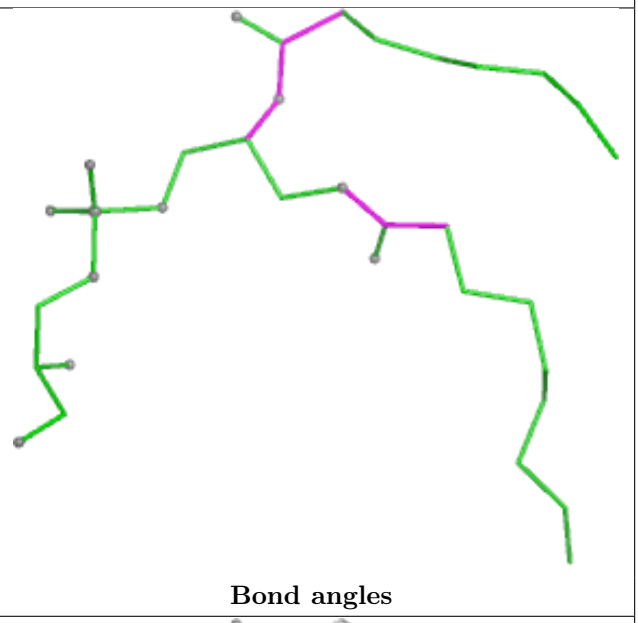
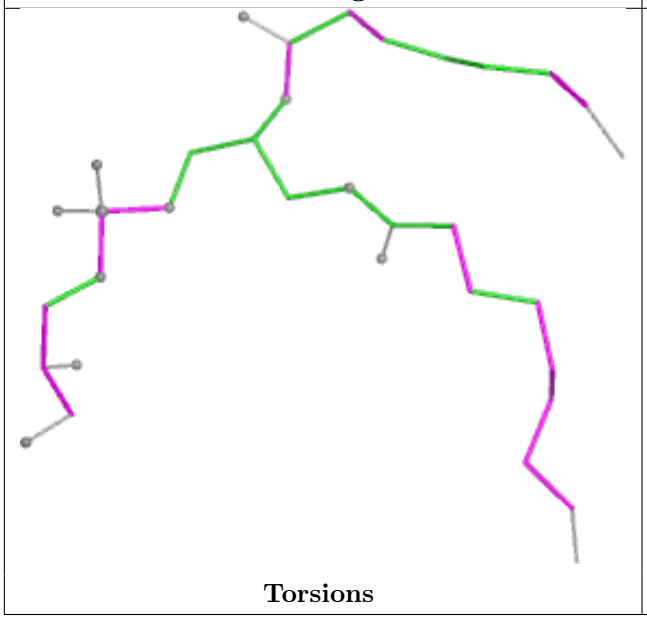


Bond angles



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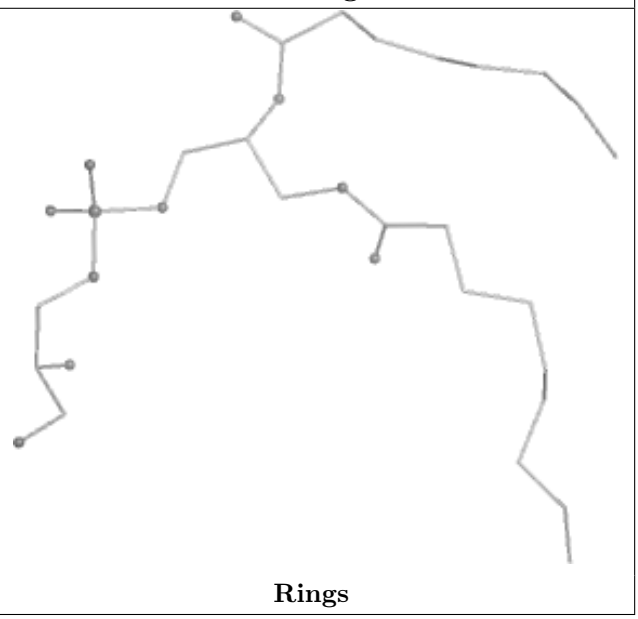
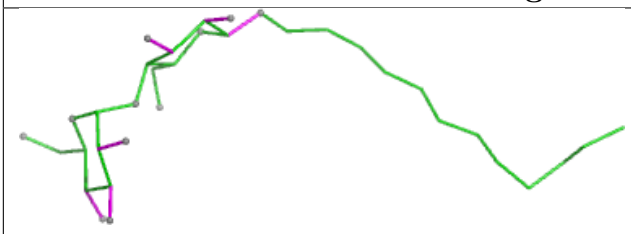


Rings

Ligand LMT 8 805



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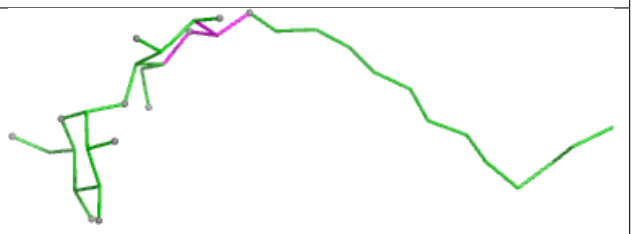
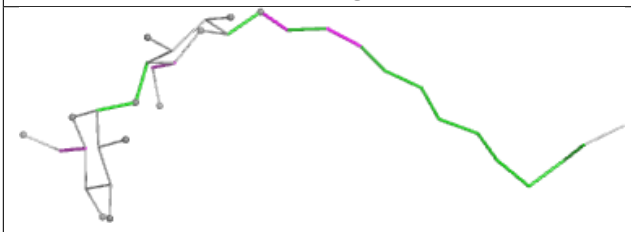


Bond angles



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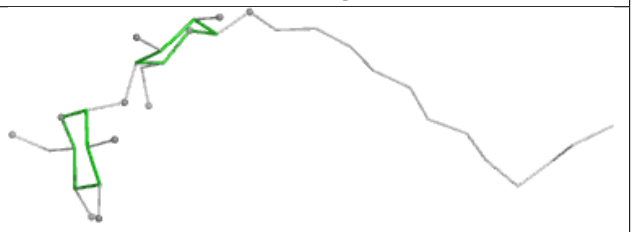
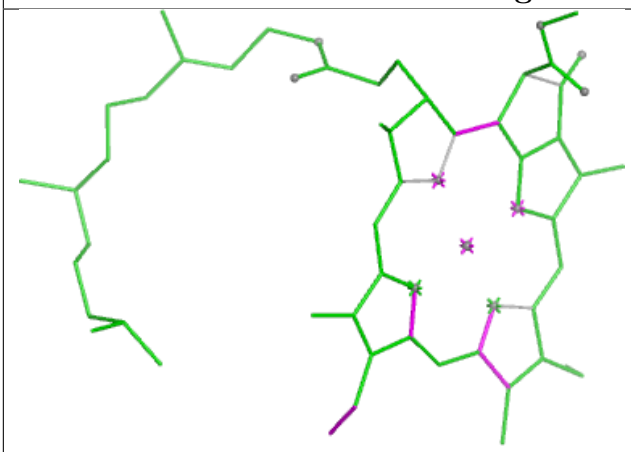


Rings

Ligand CLA A 1118



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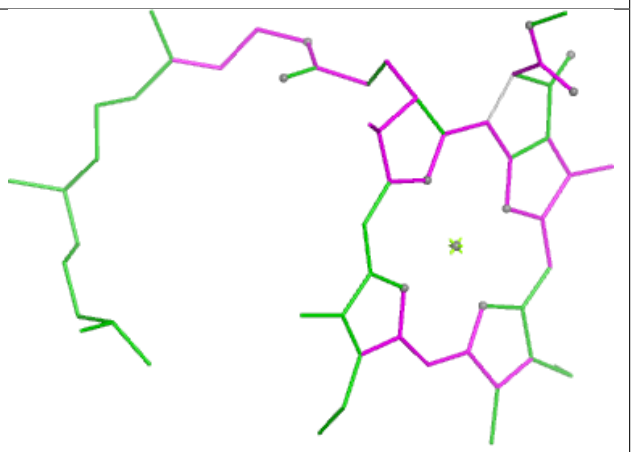

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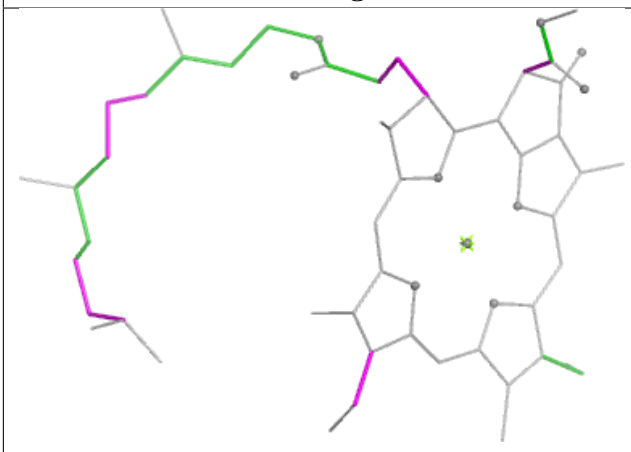

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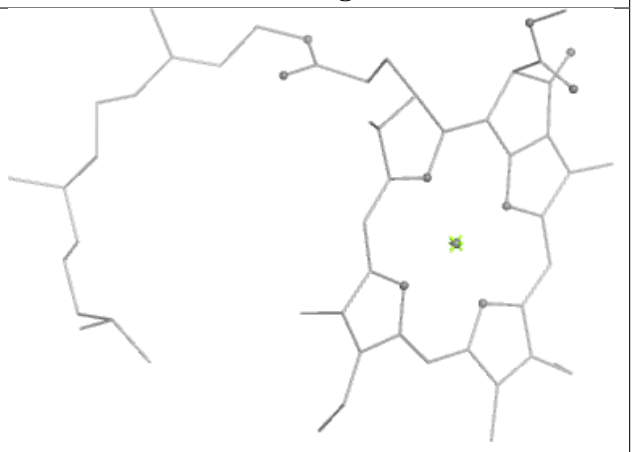
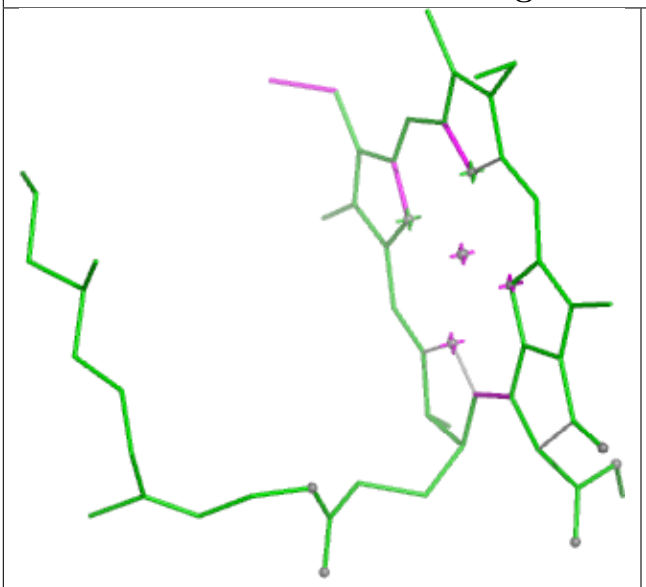


Rings

Ligand CLA B 1212



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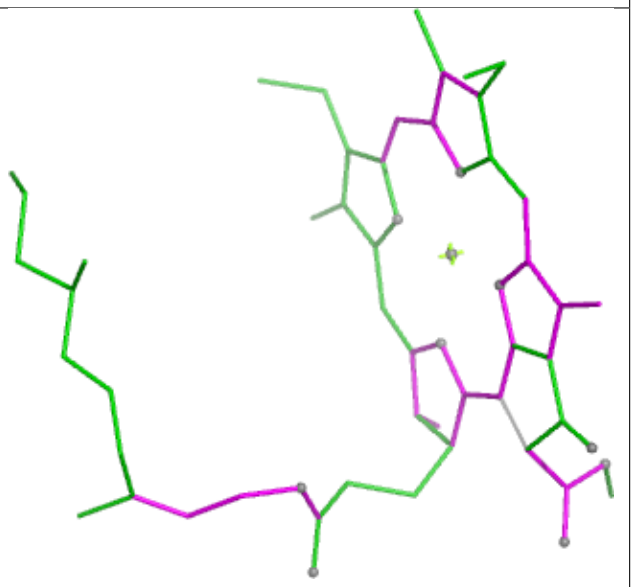
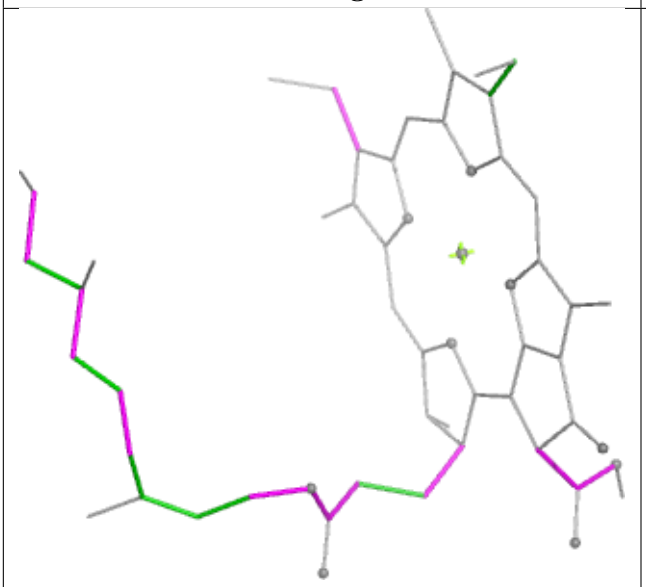


Bond angles



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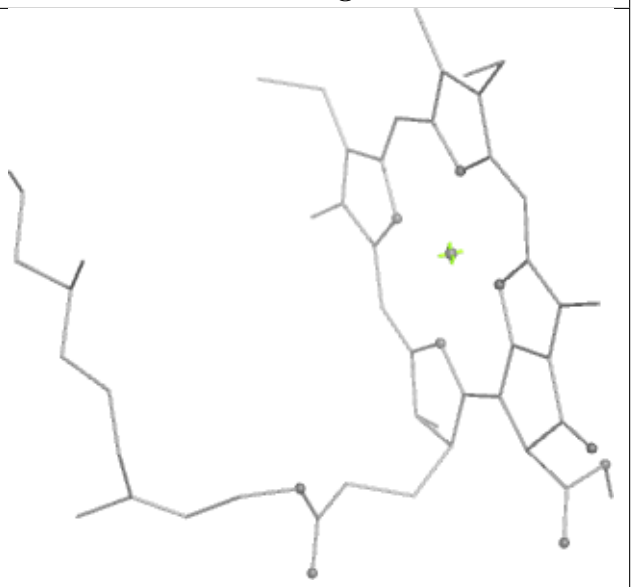


Rings

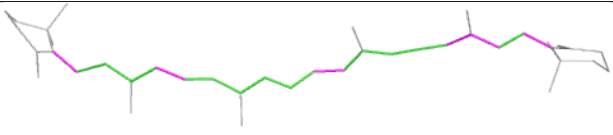
Ligand BCR 3 503



Bond lengths



Bond angles



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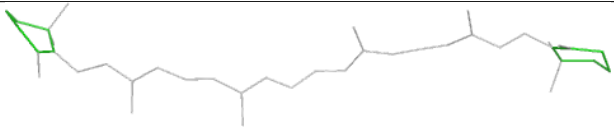
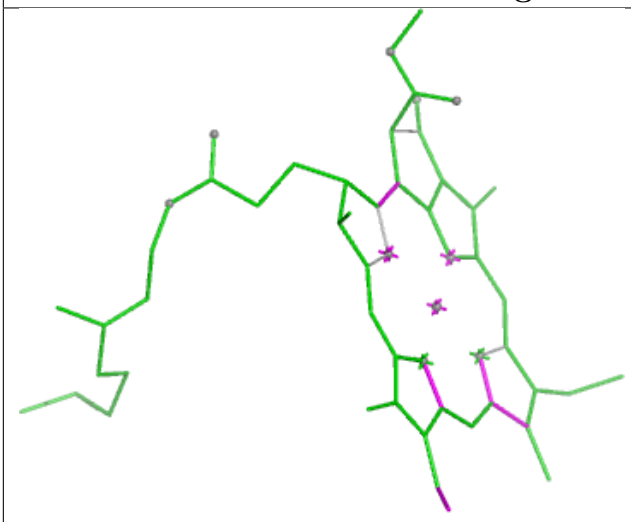
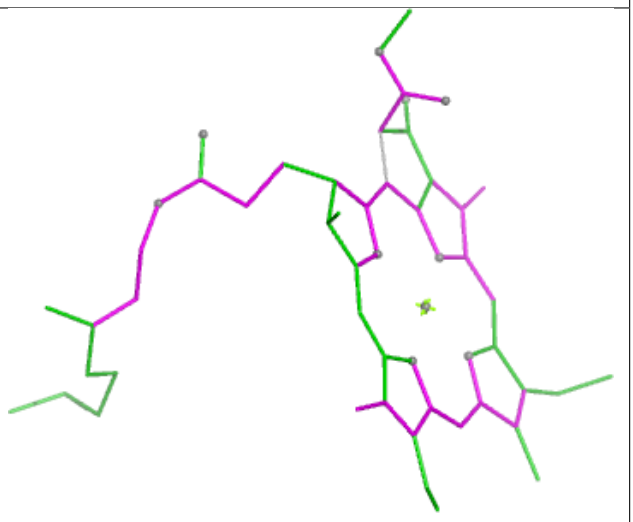


Rings

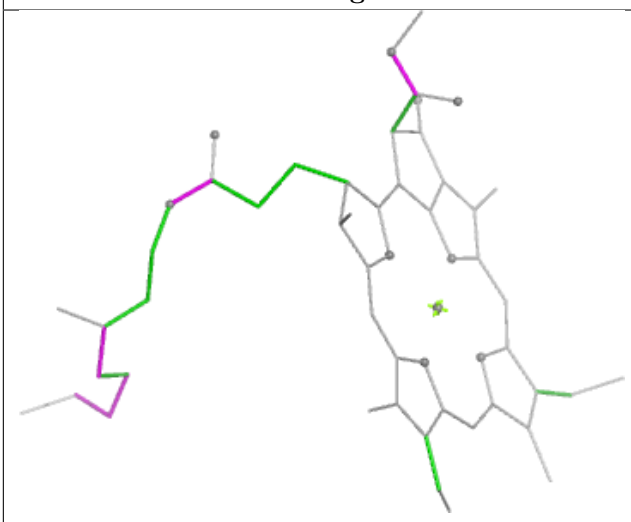
Ligand CLA A 1102



Bond lengths



Bond angles



Torsions

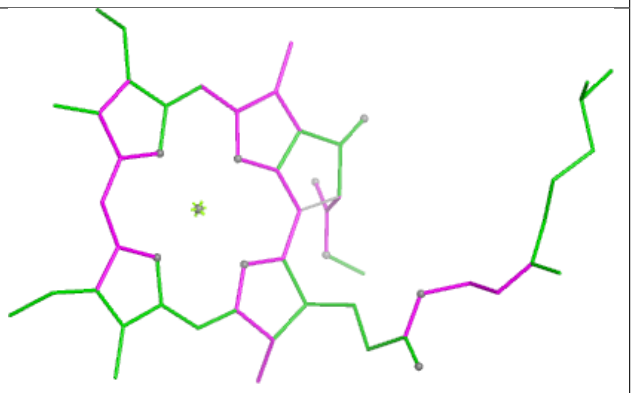


Rings

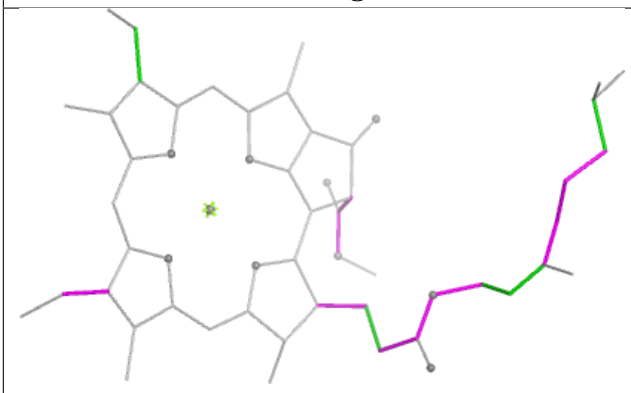
Ligand CLA K 1402



Bond lengths



Bond angles



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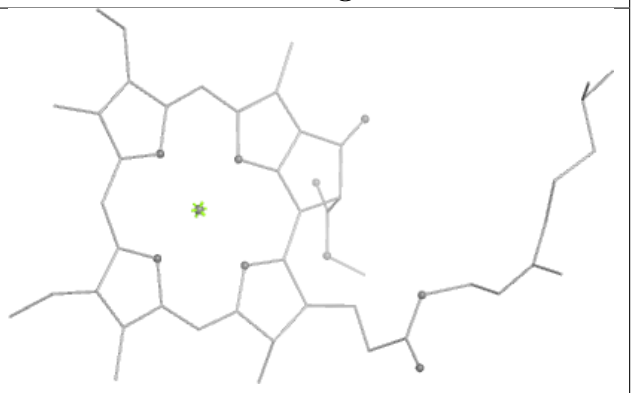
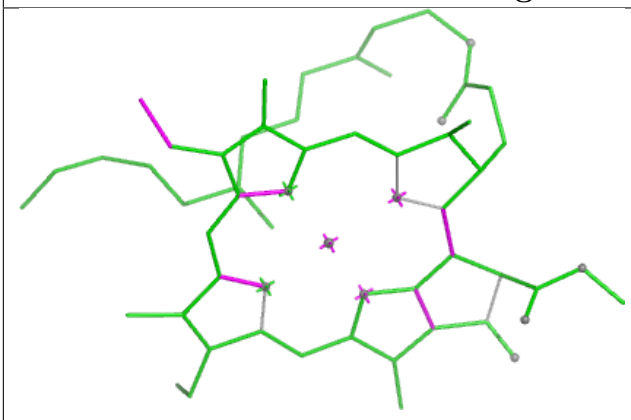
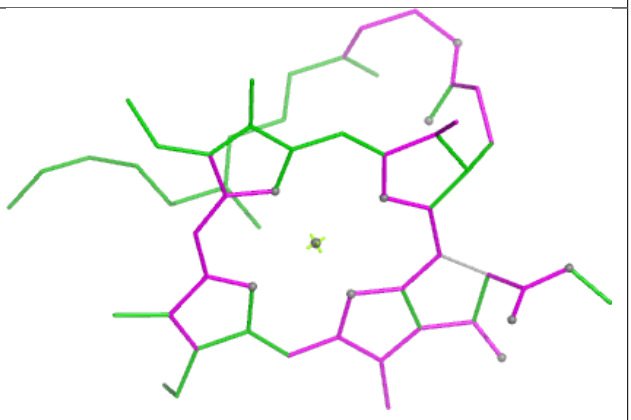


Rings

Ligand CLA B 1214



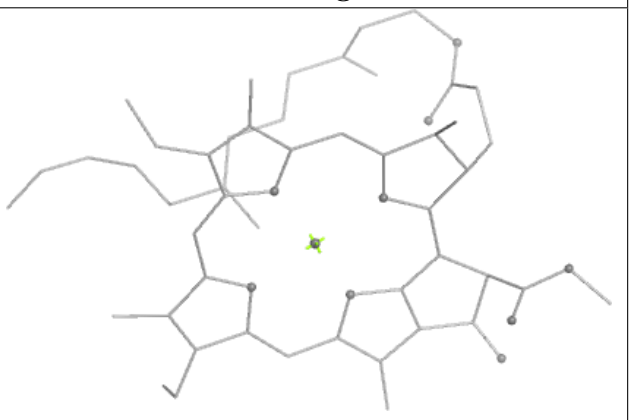
Bond lengths



Bond angles

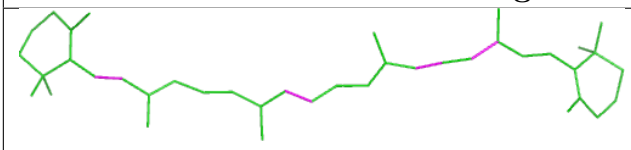


Torsions

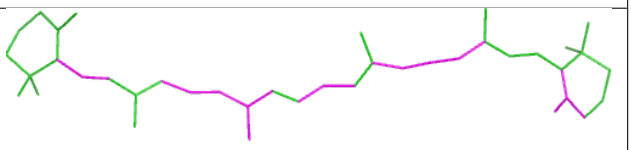


Rings

Ligand BCR B 4002



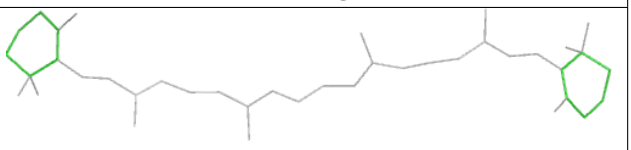
Bond lengths



Bond angles

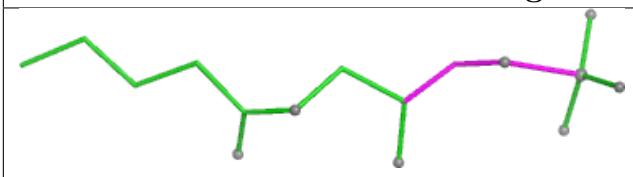


Torsions

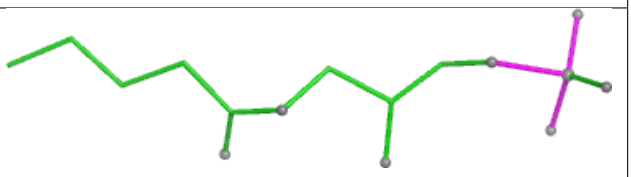


Rings

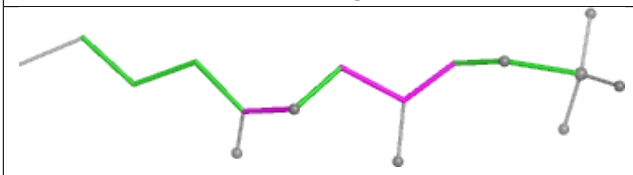
Ligand NKP 3 802



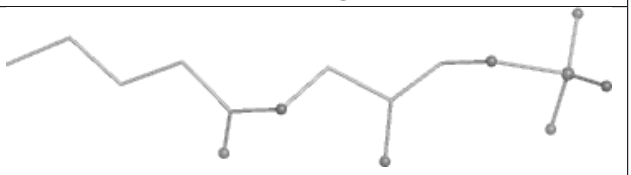
Bond lengths



Bond angles

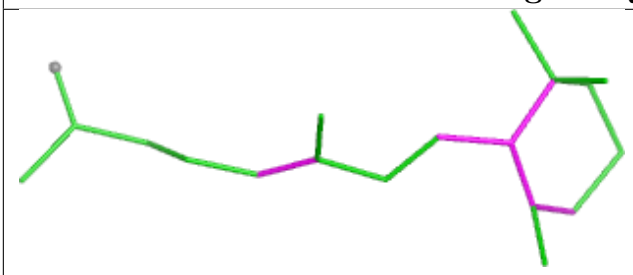


Torsions



Rings

Ligand QTB Z 504



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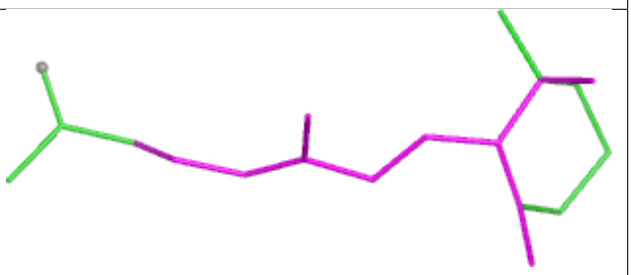

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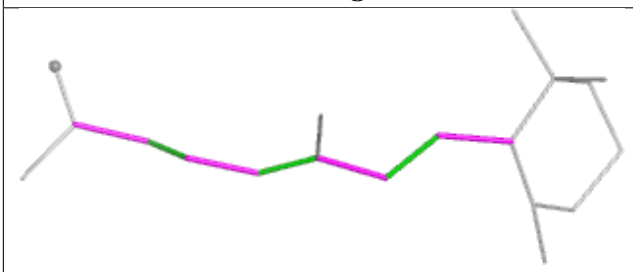

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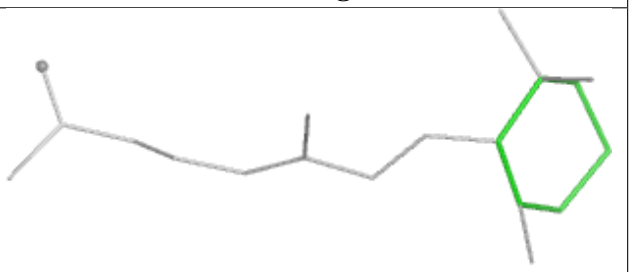
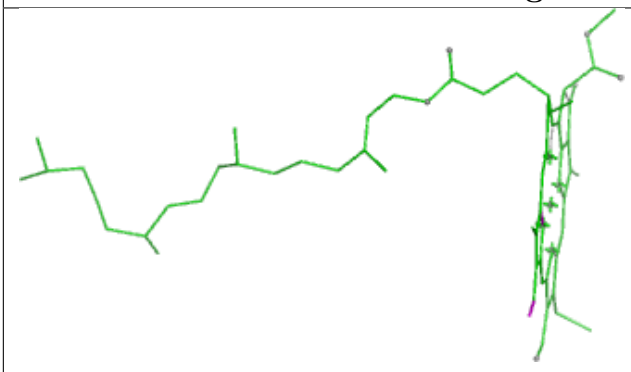


Rings

Ligand CHL Z 610



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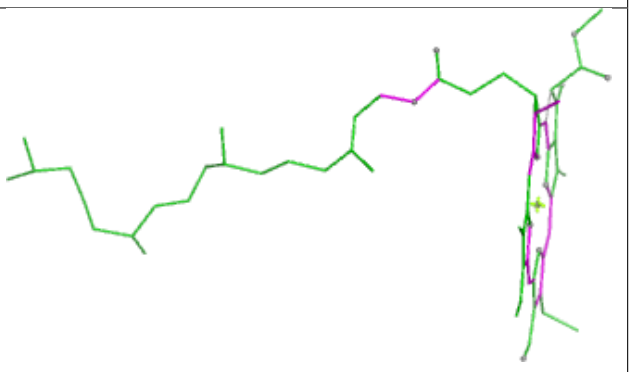

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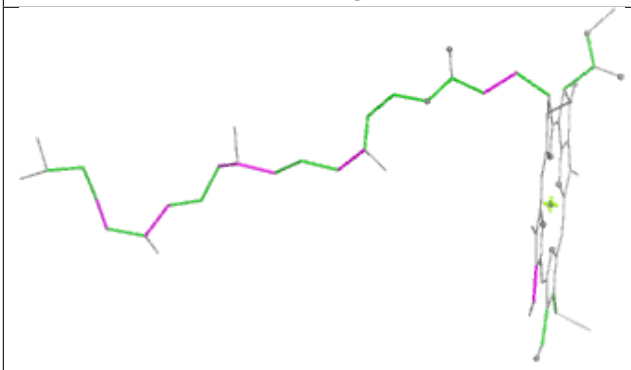

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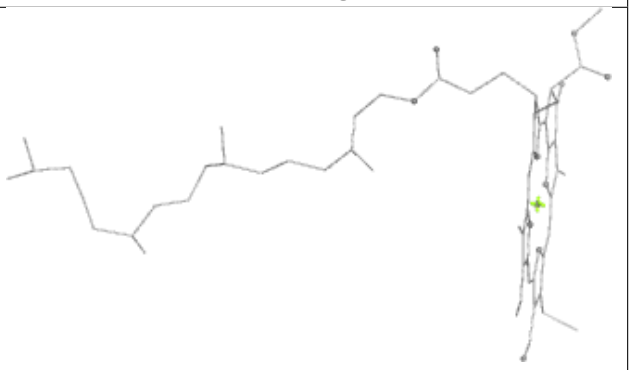
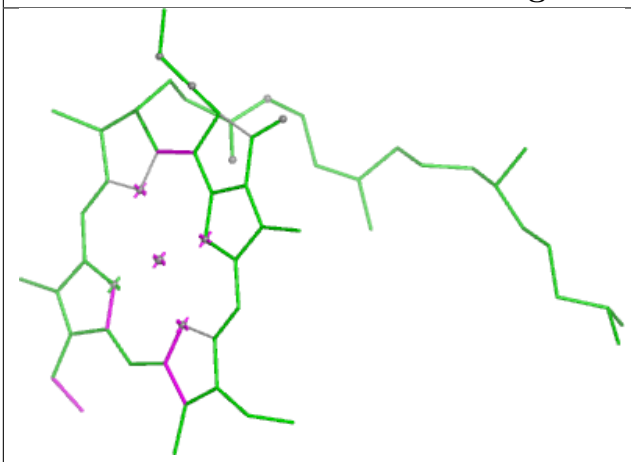


Rings

Ligand CLA 3 607



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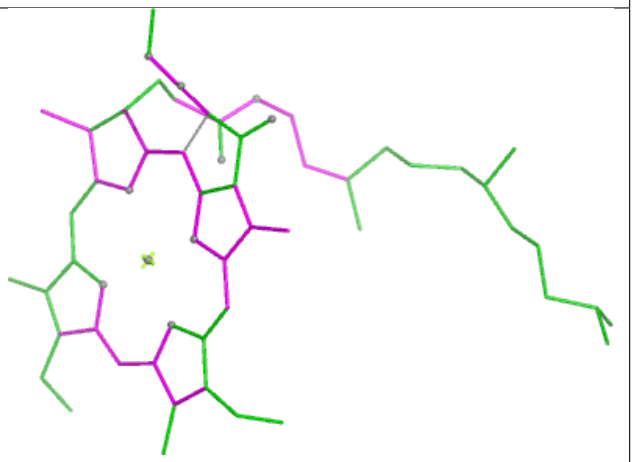
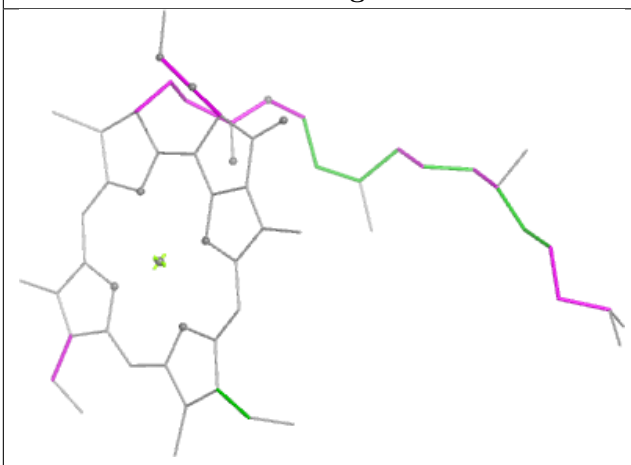


Bond angles



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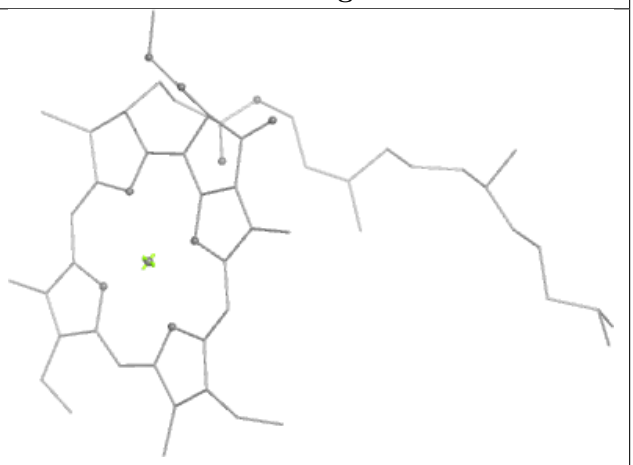
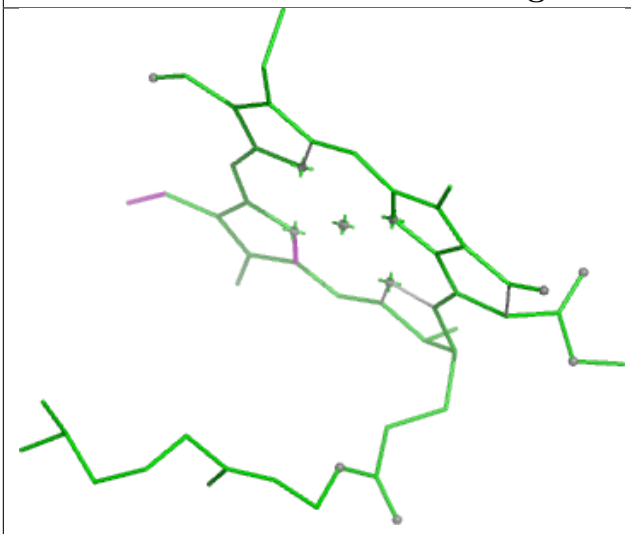


Rings

Ligand CHL 6 610



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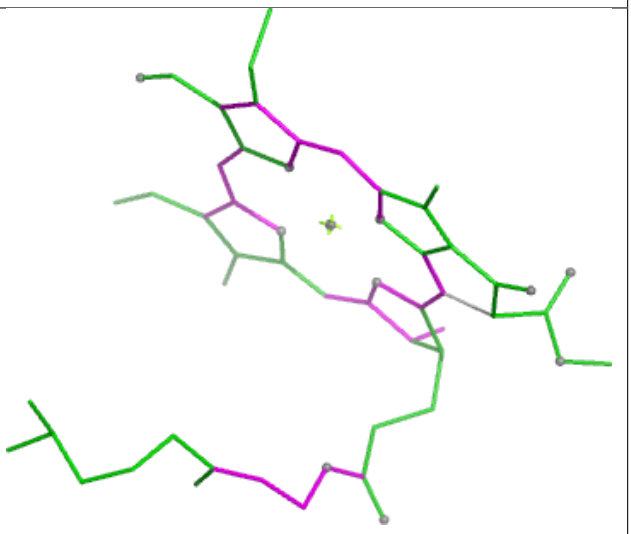
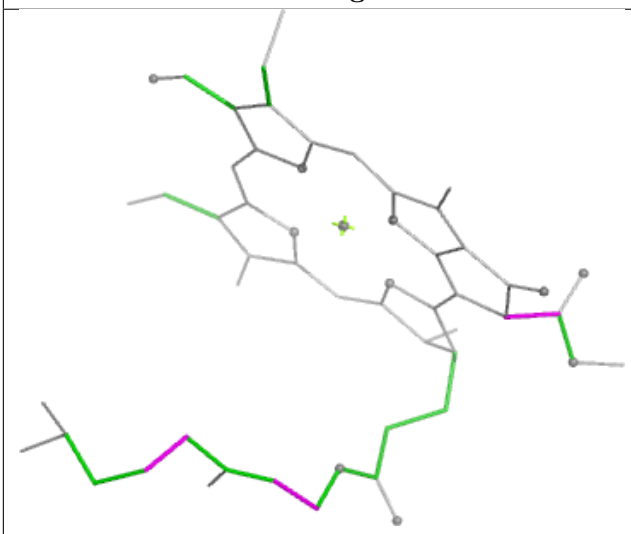


Bond angles



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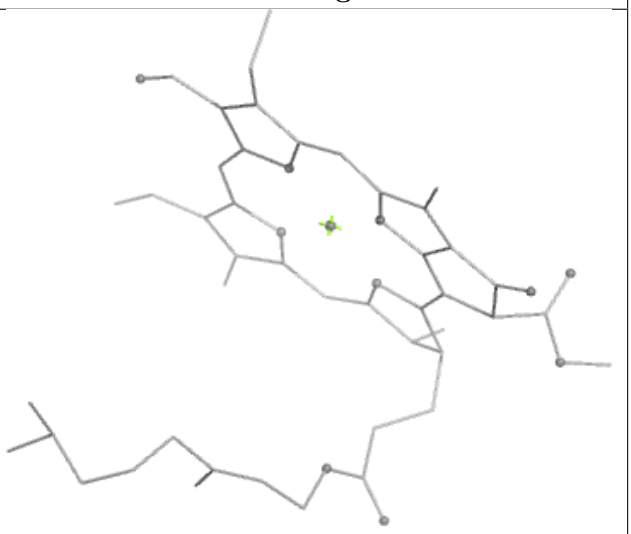
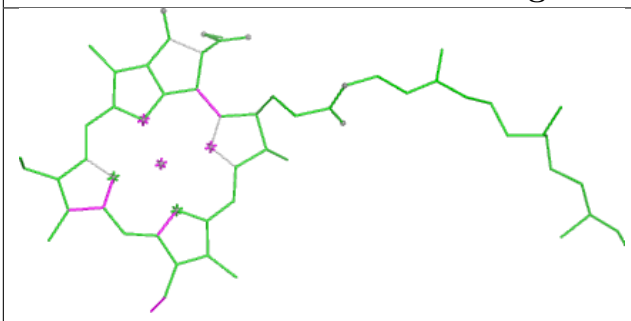


Rings

Ligand CLA 6 615



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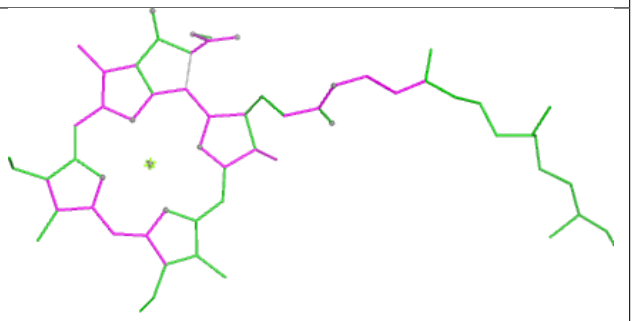

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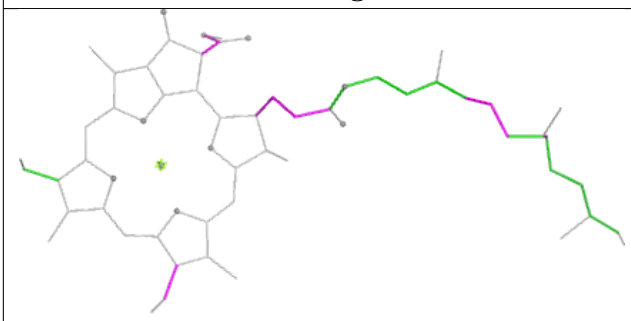

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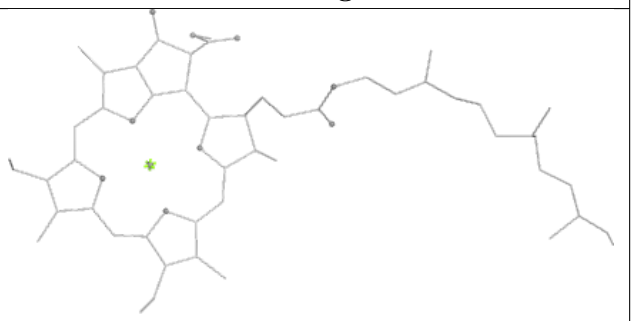
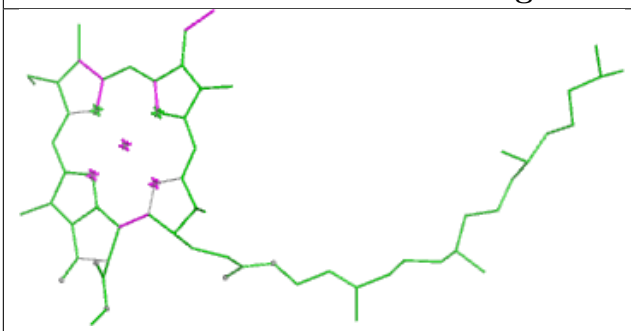


Rings

Ligand CLA B 1222



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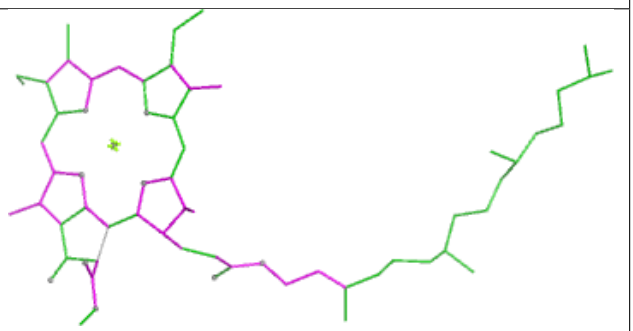
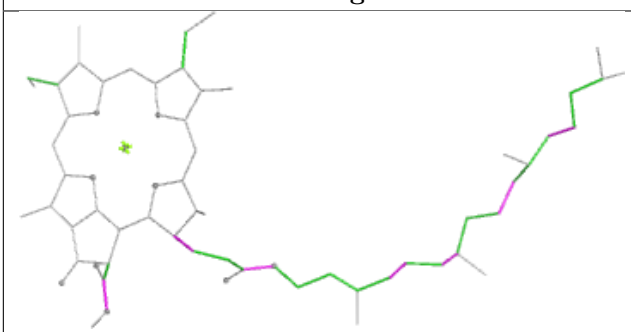


Bond angles

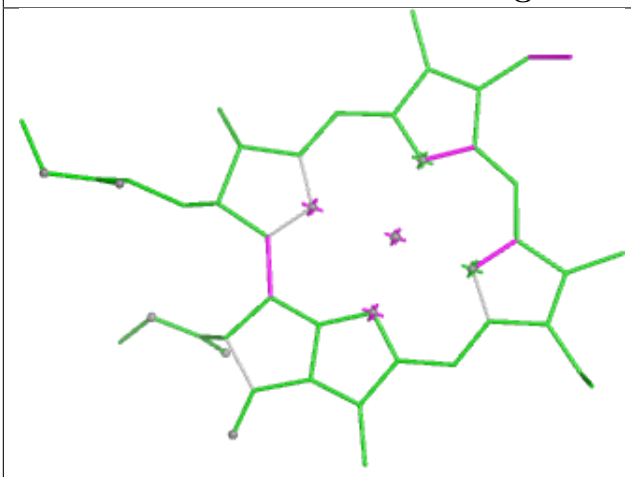


Torsions



Rings

Ligand CLA K 1401



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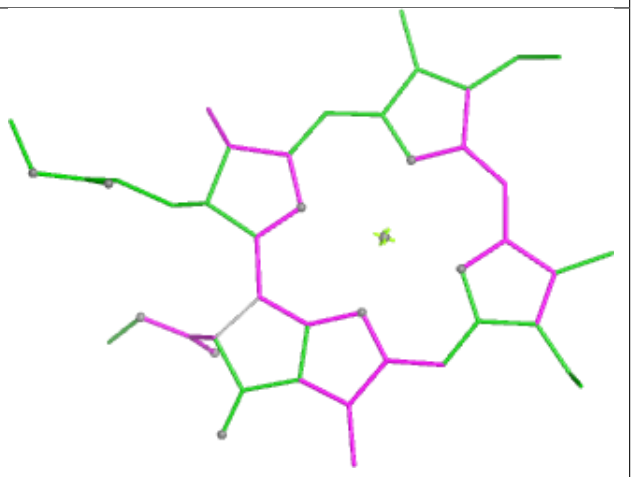
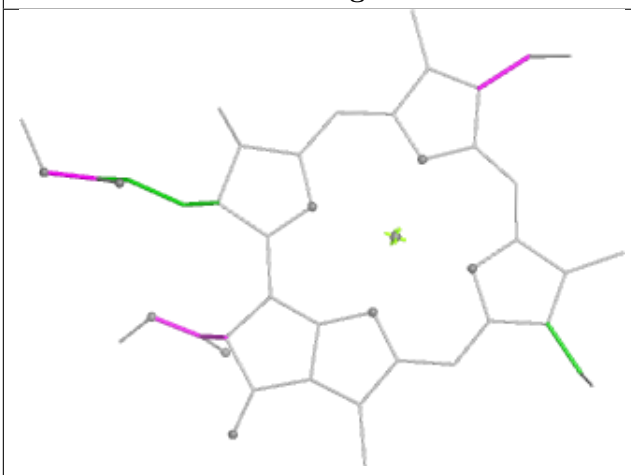


Bond angles



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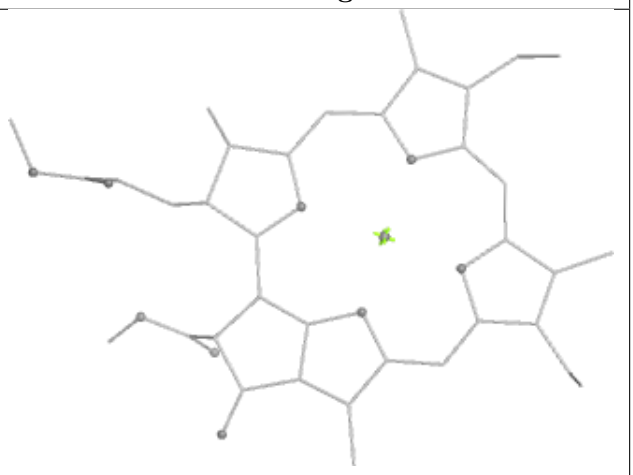
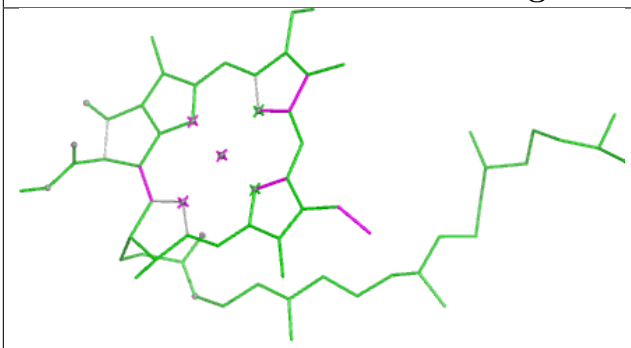


Rings

Ligand CLA 7 604



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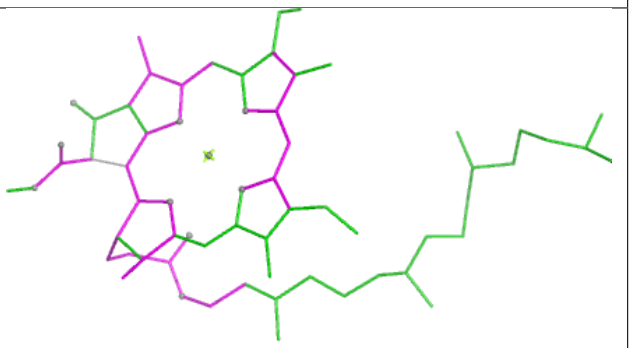

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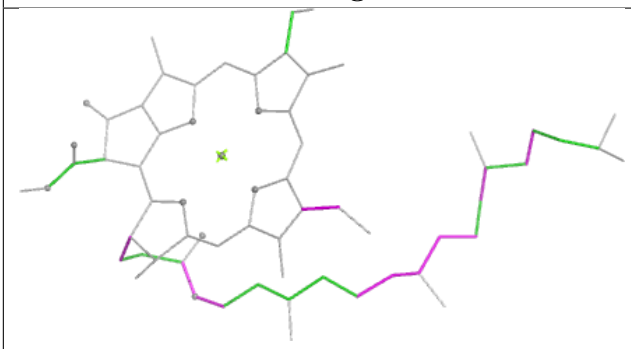

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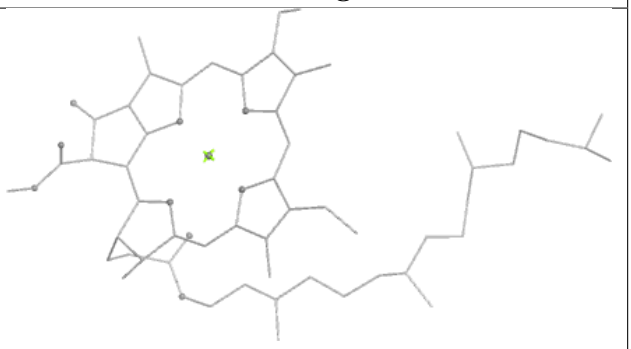
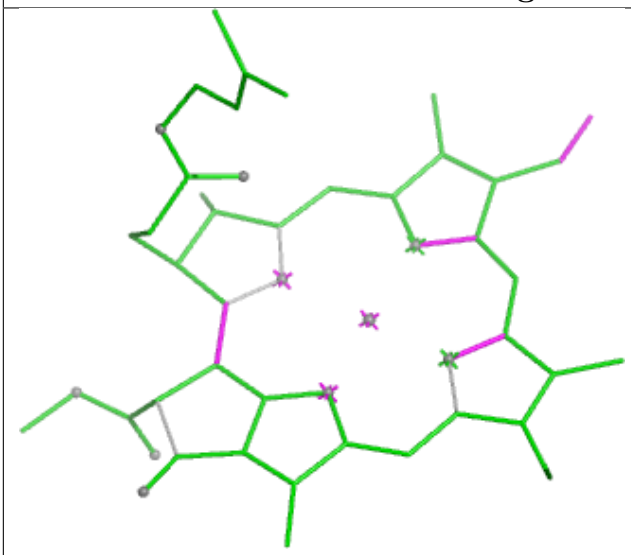


Rings

Ligand CLA L 1503



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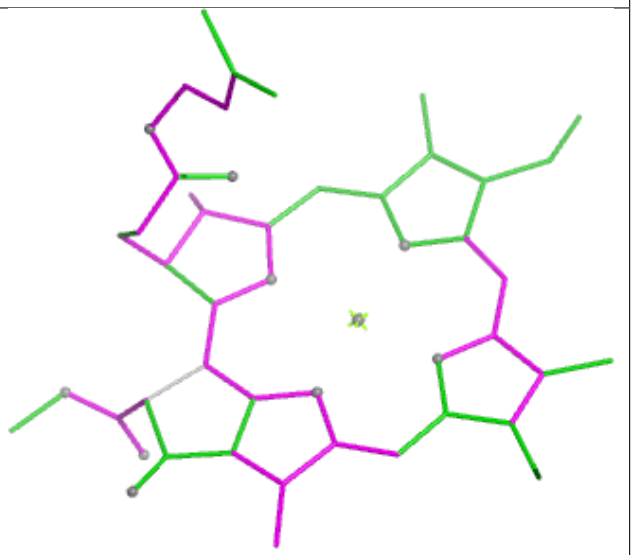
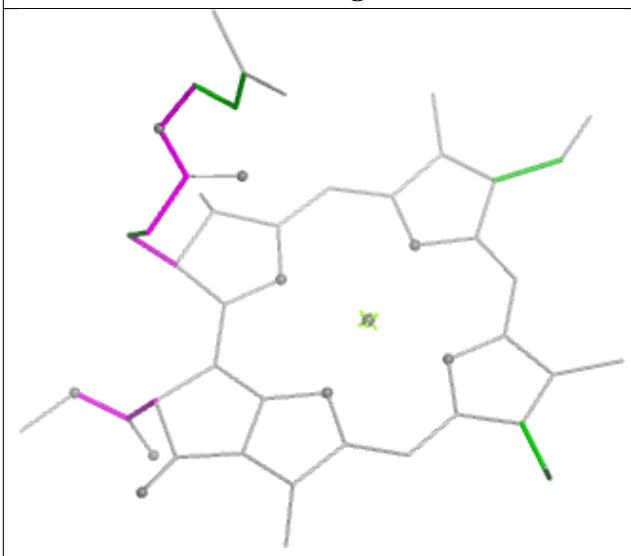


Bond angles



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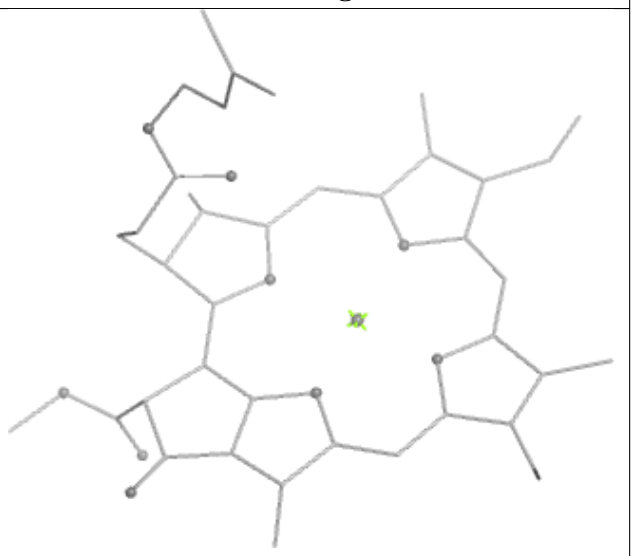
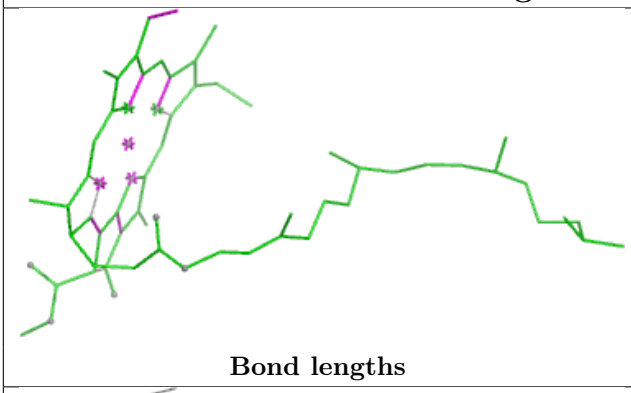


Rings

Ligand CLA A 1109



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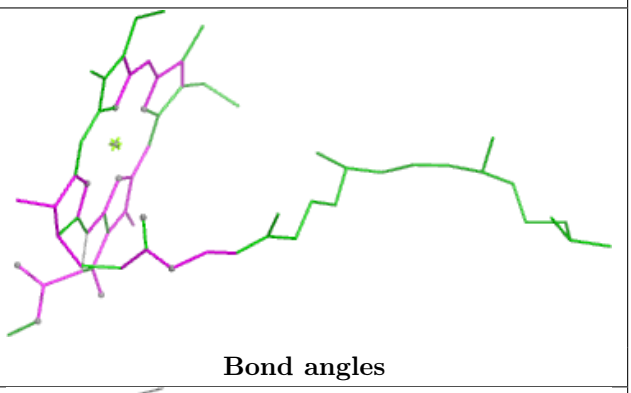
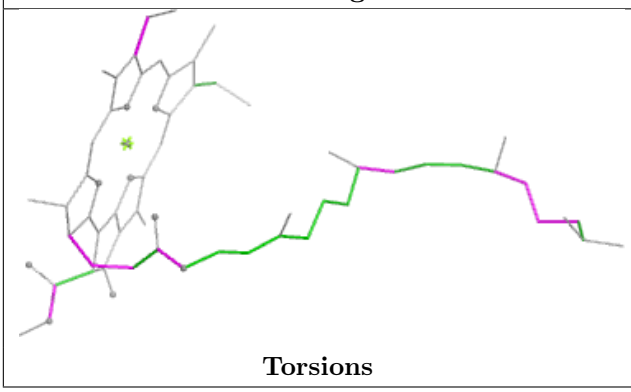


Bond angles



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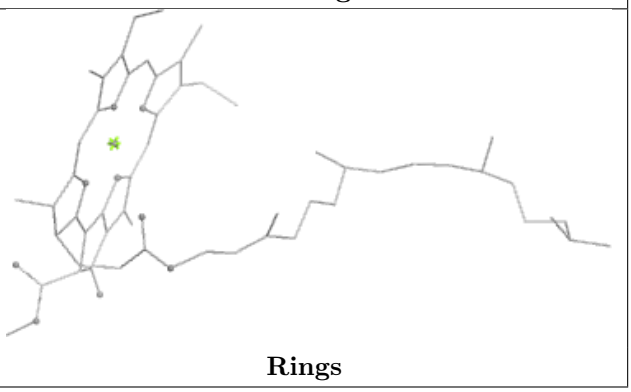
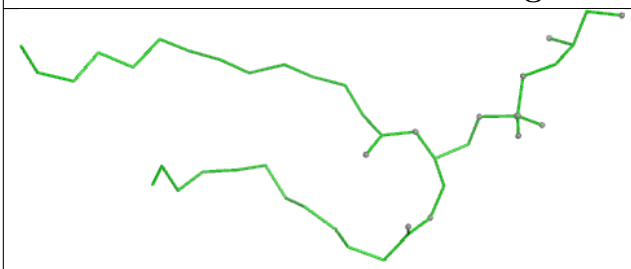


Rings

Ligand LHG Z 801



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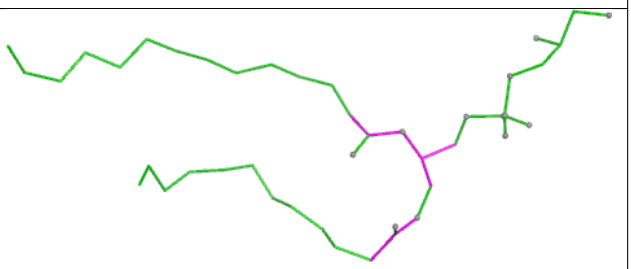
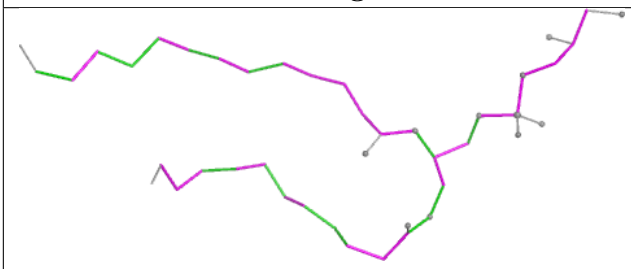


Bond angles



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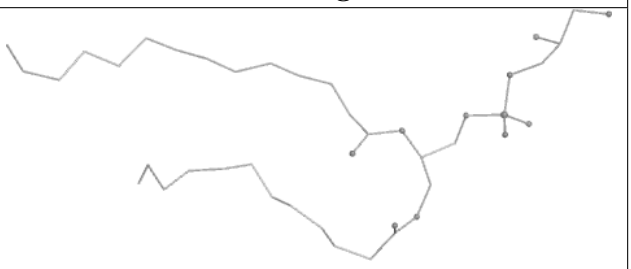
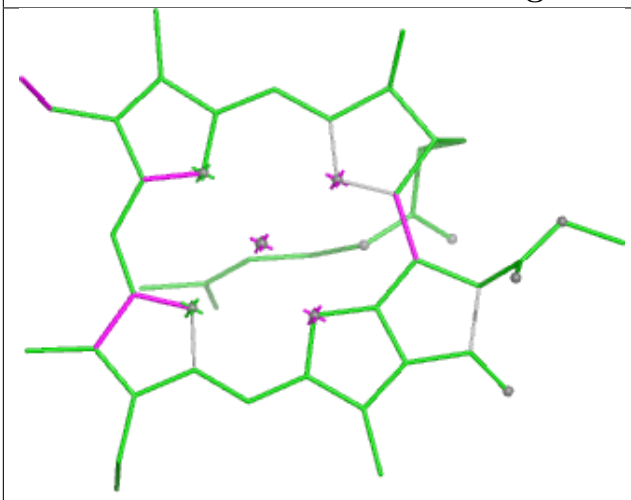


Rings

Ligand CLA Z 603



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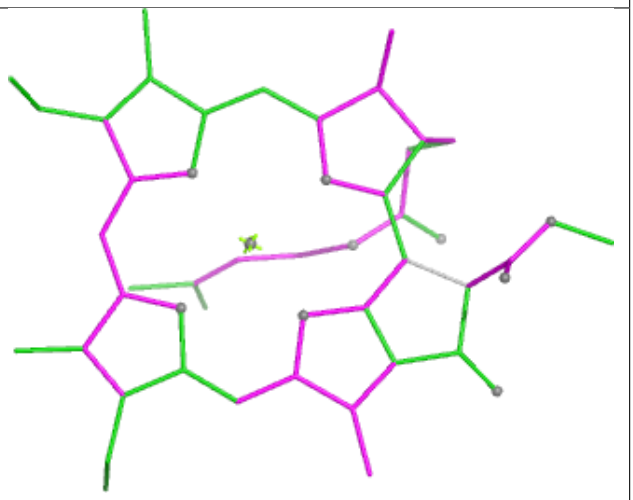
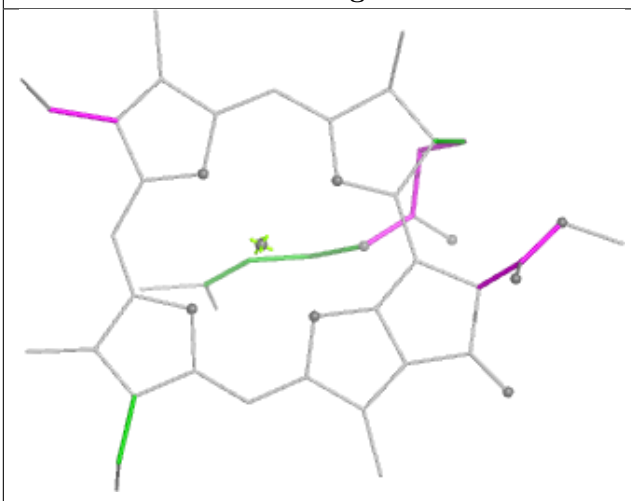


Bond angles



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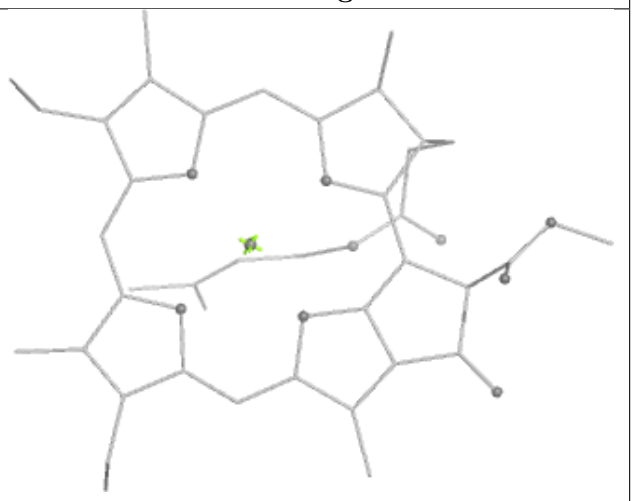
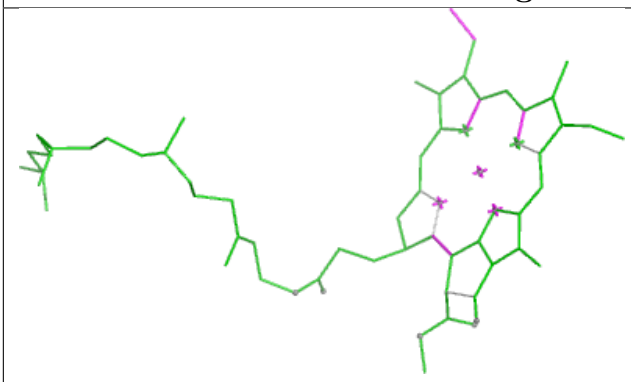


Rings

Ligand CLA B 1206



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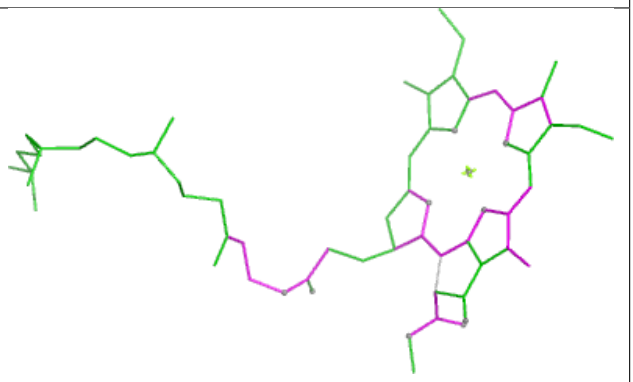
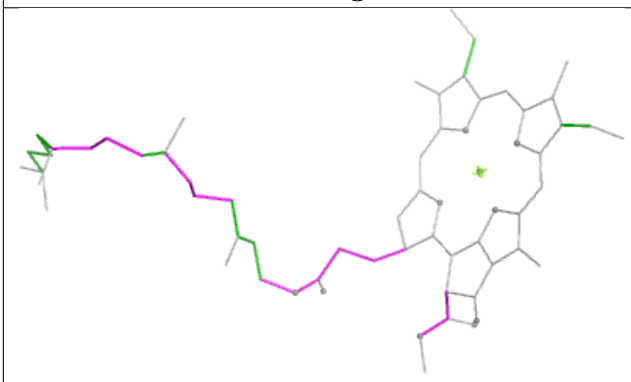


Bond angles



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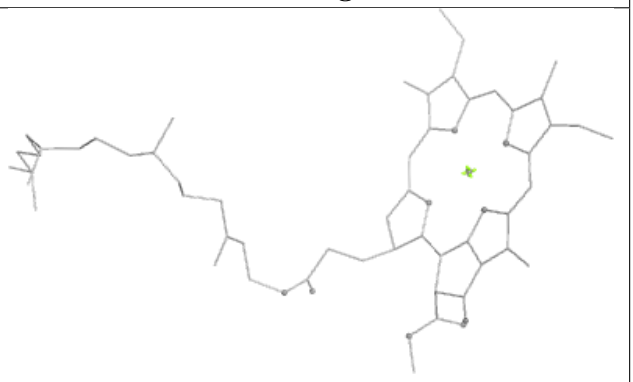
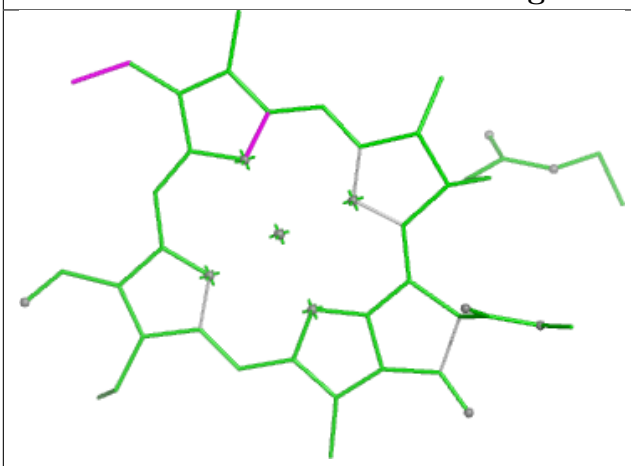


Rings

Ligand CHL 2 610



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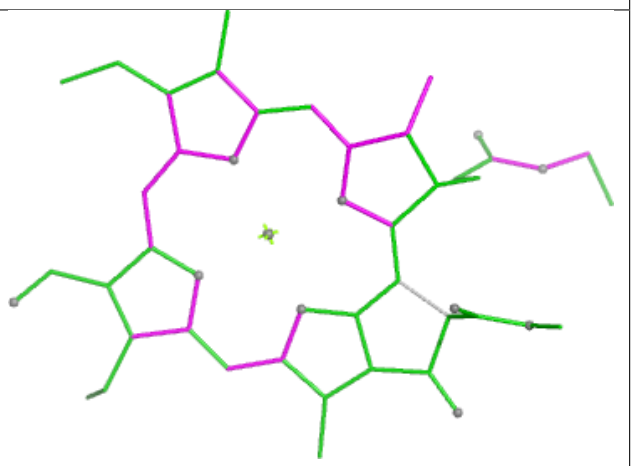
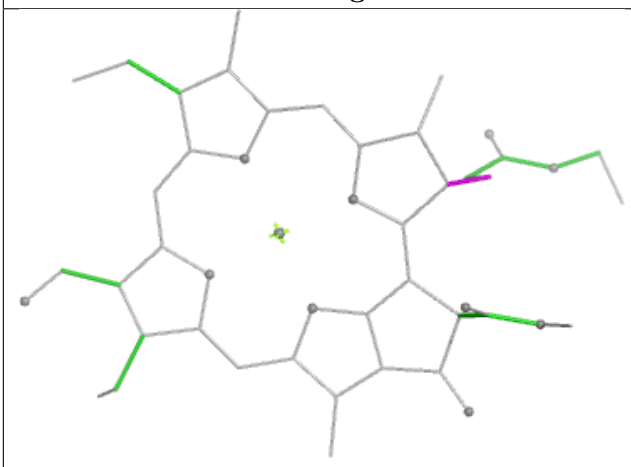


Bond angles



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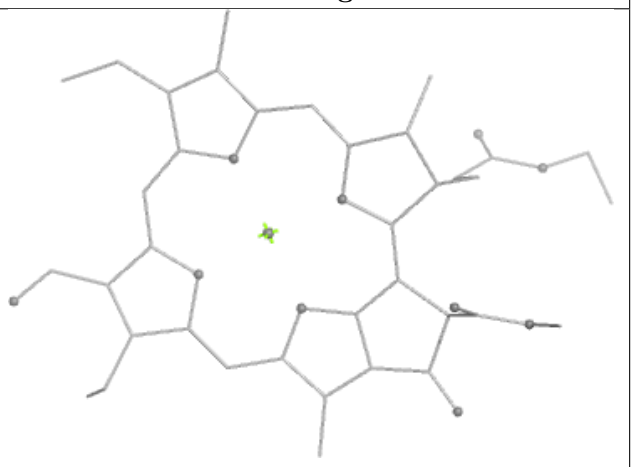
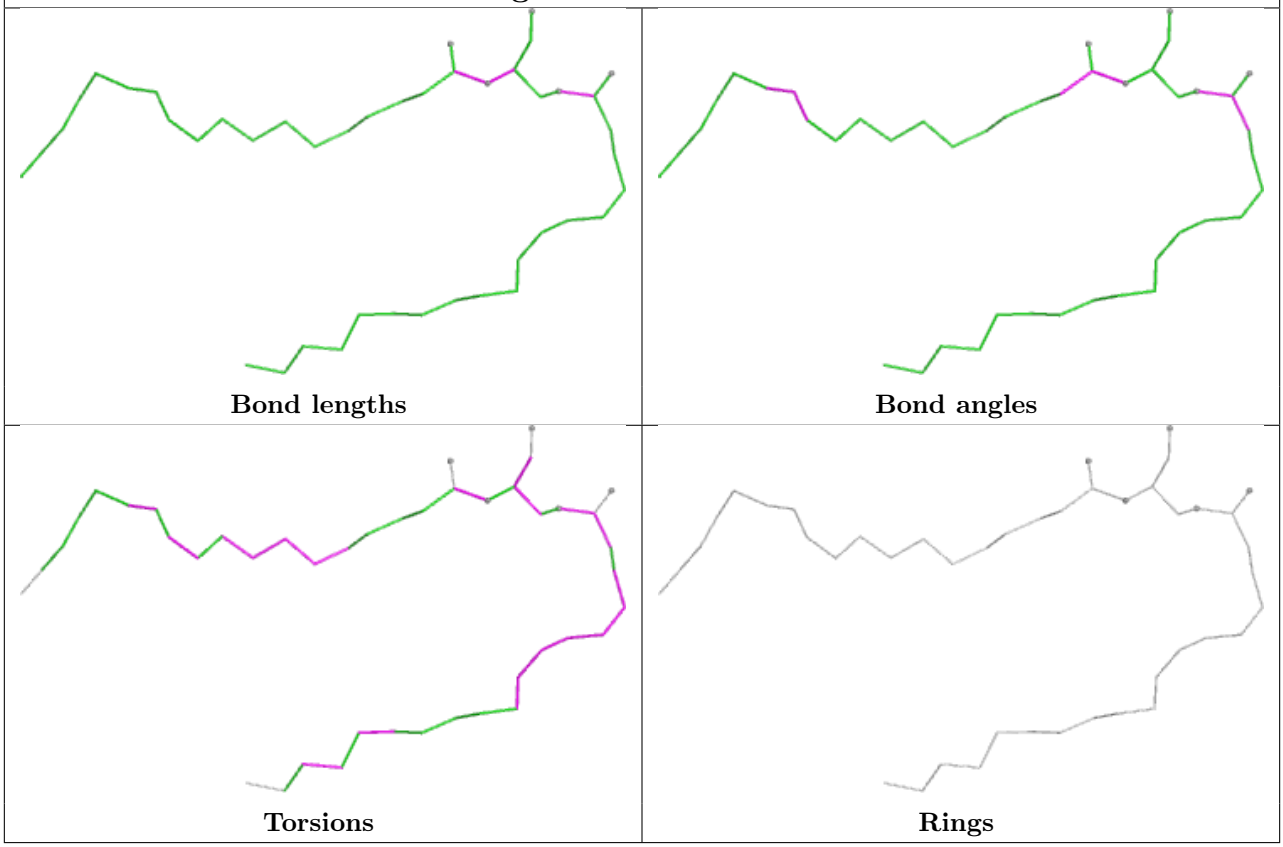
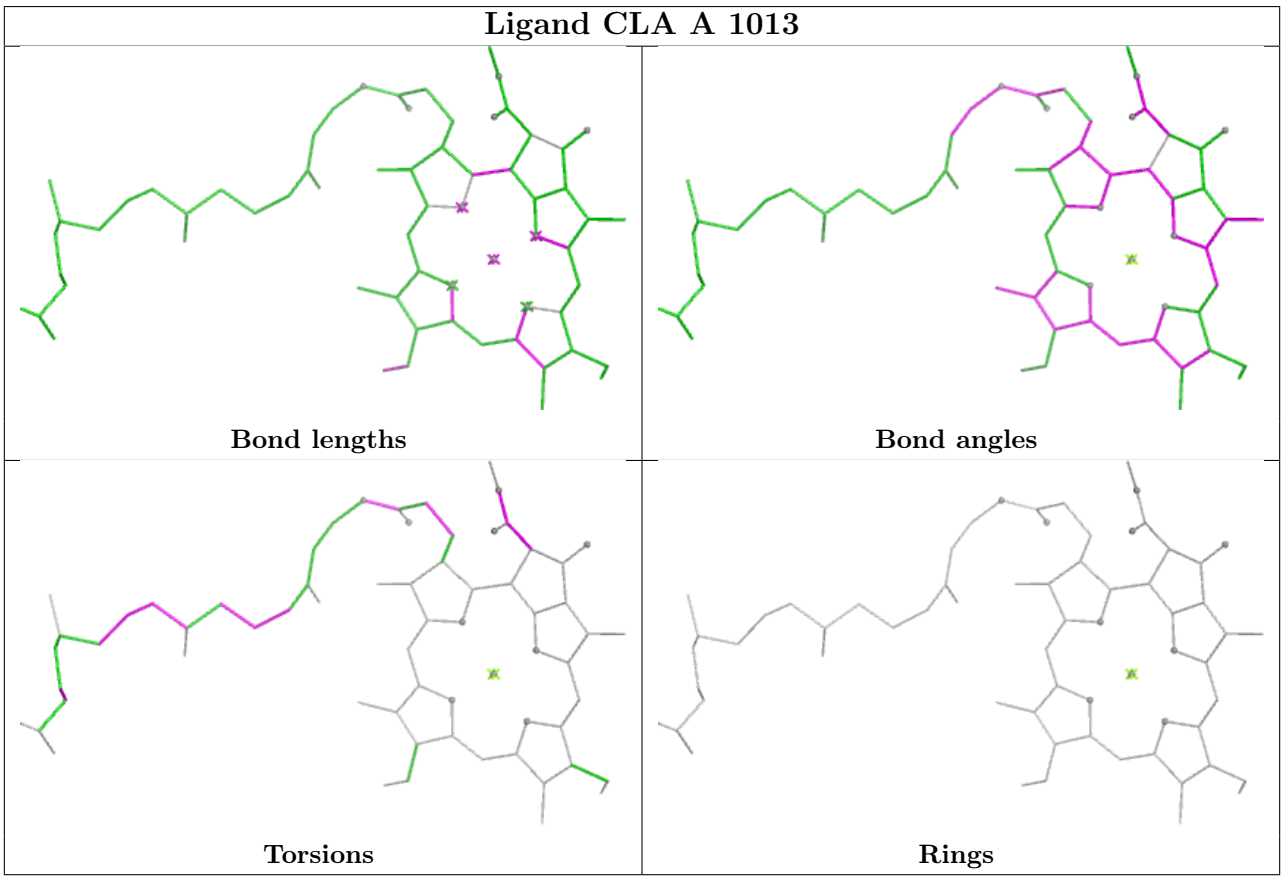


Rings

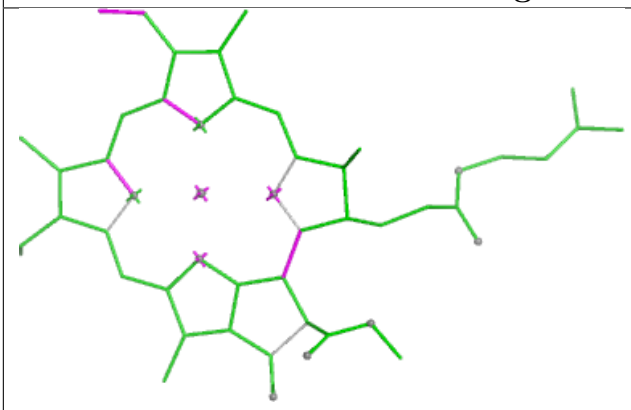
Ligand DGA A 5005



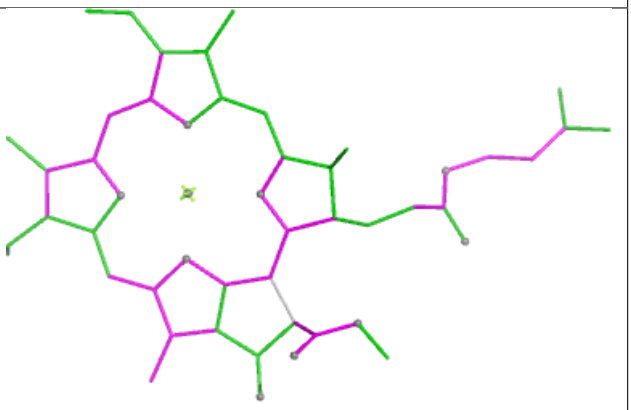
Ligand CLA A 1013



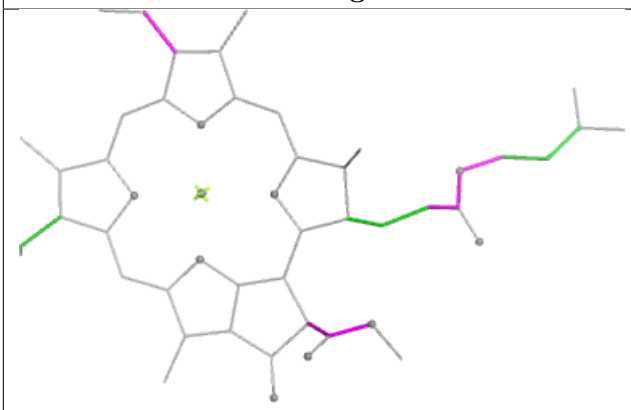
Ligand CLA G 1601



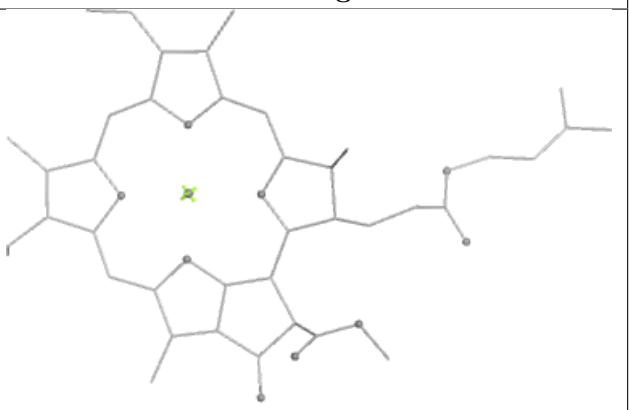
Bond lengths



Bond angles



Torsions

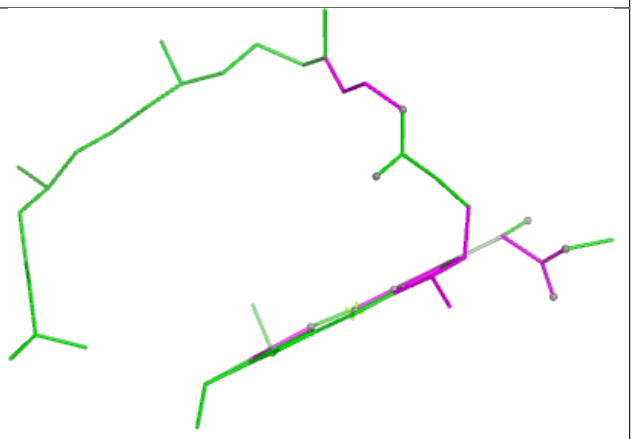


Rings

Ligand CLA 6 606



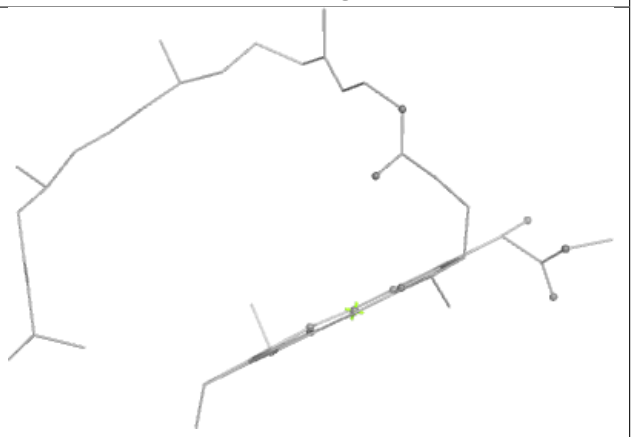
Bond lengths



Bond angles

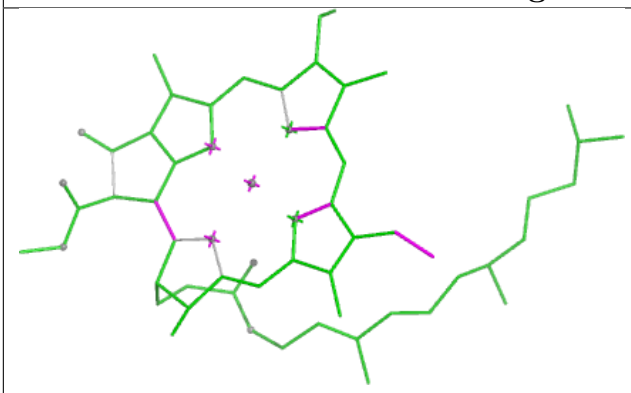


Torsions



Rings

Ligand CLA 9 601



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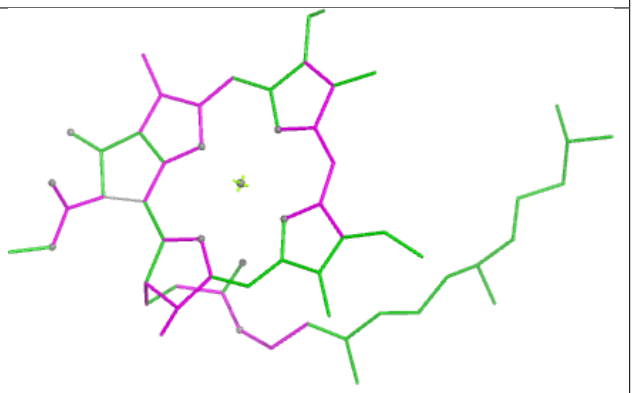
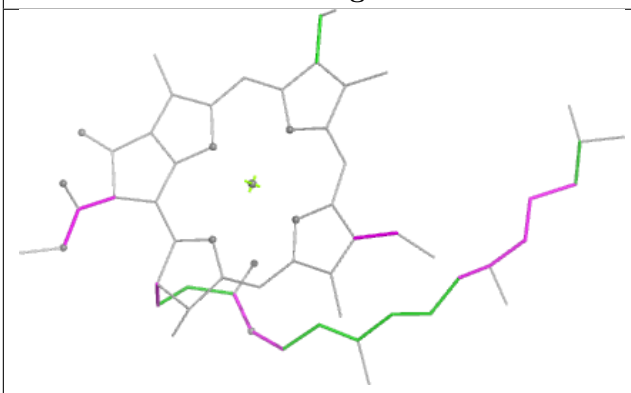


Bond angles



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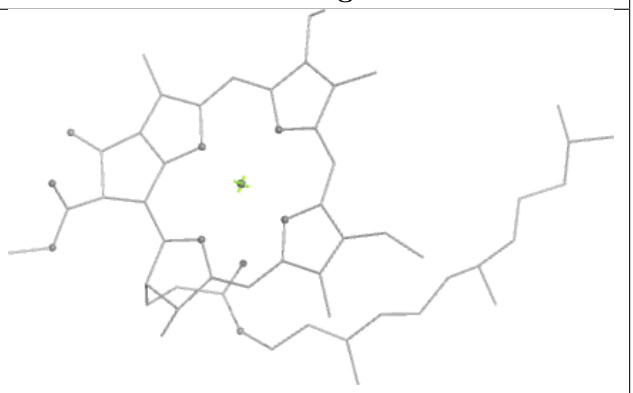
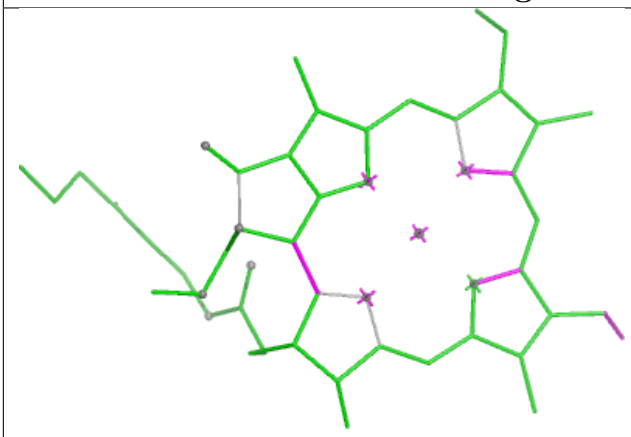


Rings

Ligand CLA A 1141



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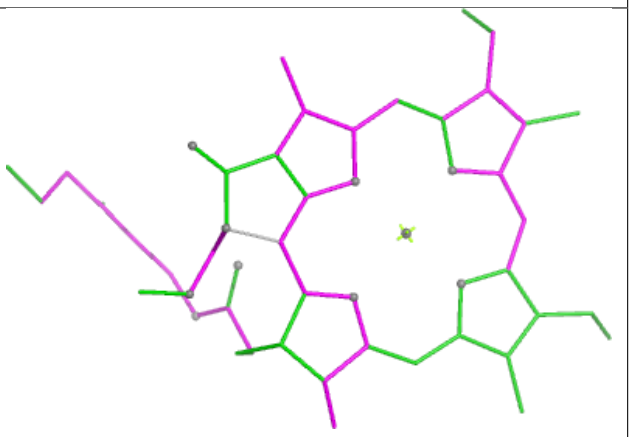
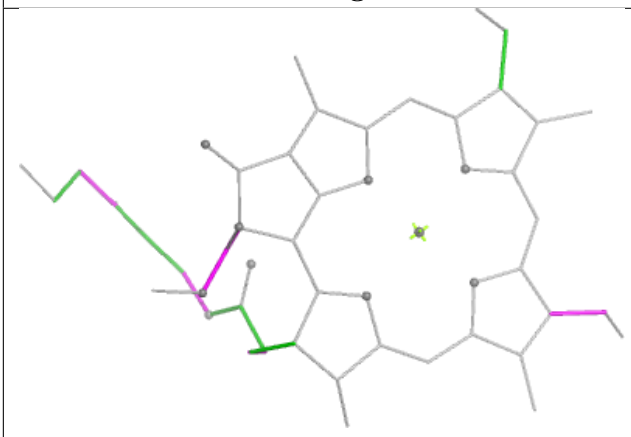


Bond angles



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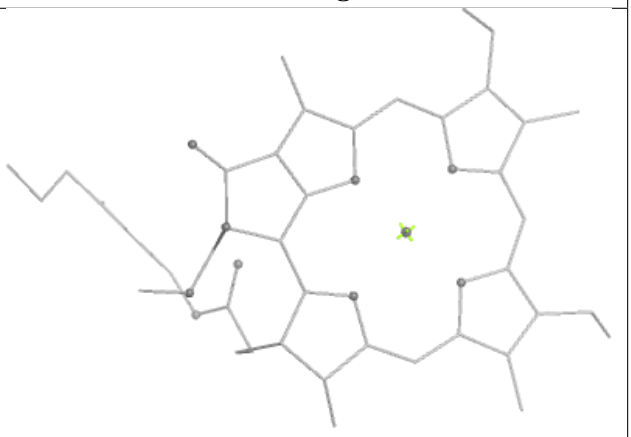
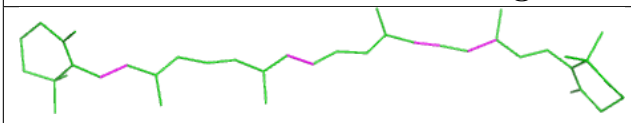


Rings

Ligand BCR A 4001



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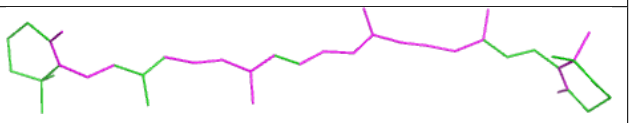

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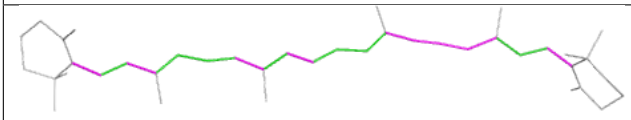

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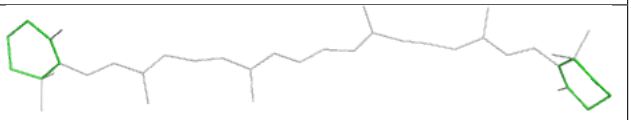
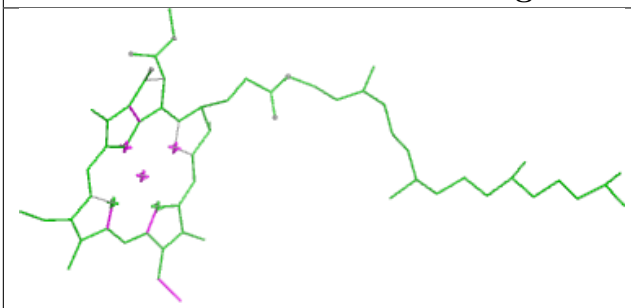


Rings

Ligand CLA B 1022



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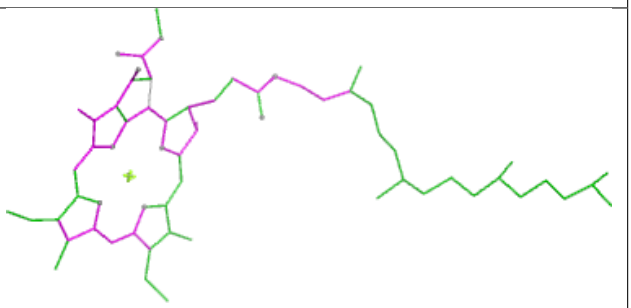

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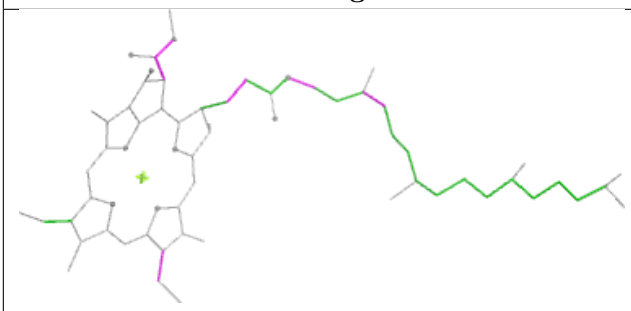

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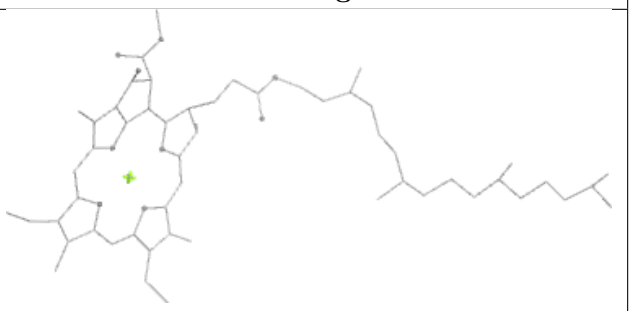
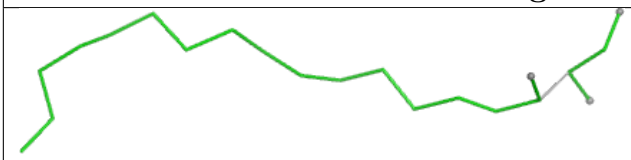


Rings

Ligand SPH 7 804



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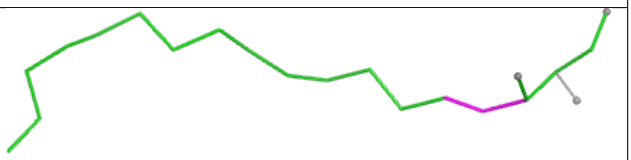
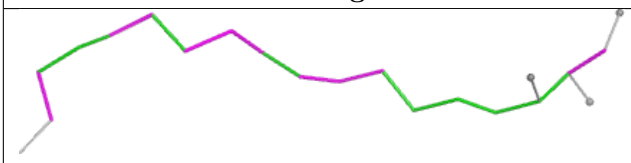


Bond angles



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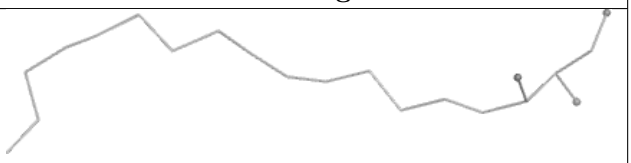
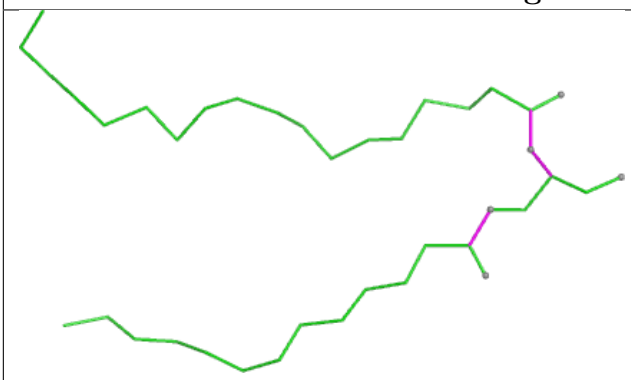


Rings

Ligand DGA 9 802



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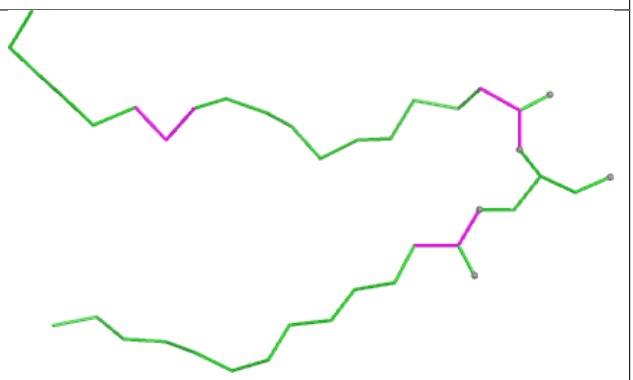
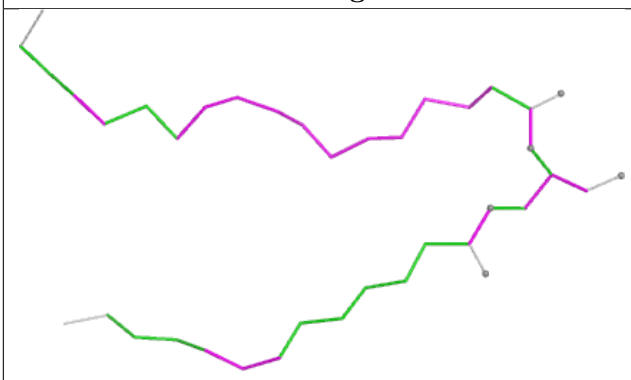


Bond angles



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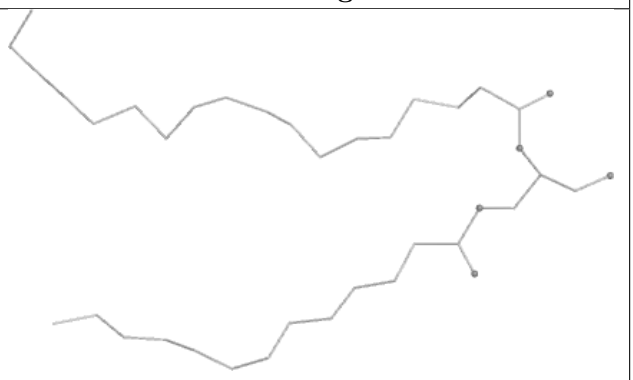


Rings

Ligand CLA 6 608



Bond lengths



Bond angles



Torsions



Rings

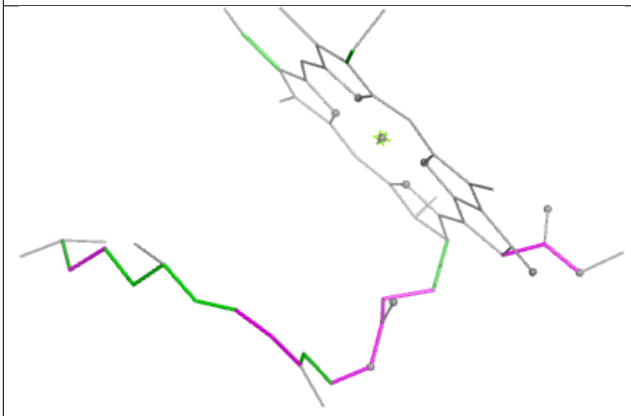
Ligand CLA B 1211



Bond lengths



Bond angles

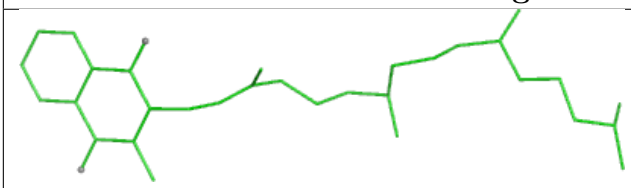


Torsions



Rings

Ligand PQN A 2001



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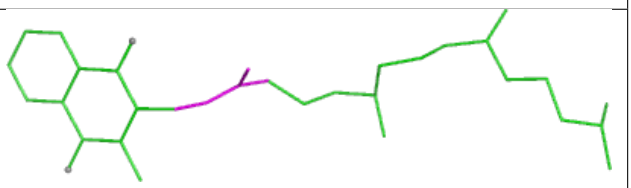
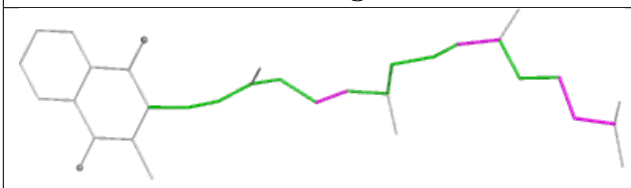


Bond angles



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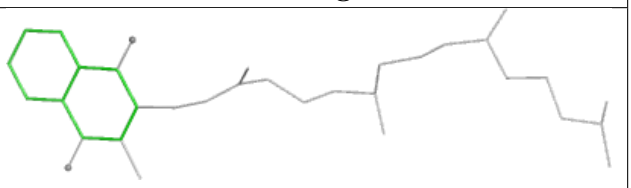
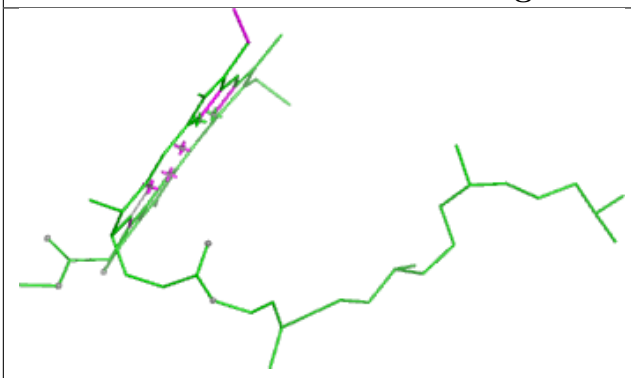


Rings

Ligand CLA A 1108



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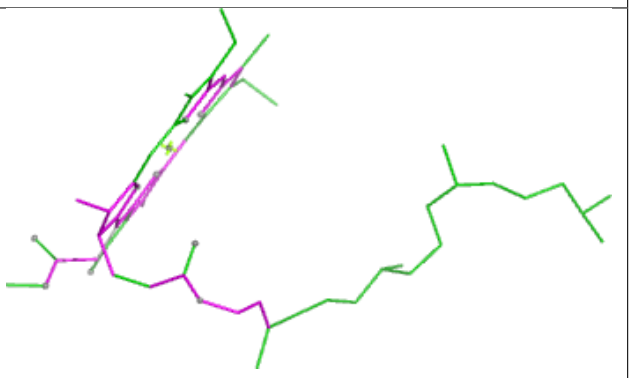
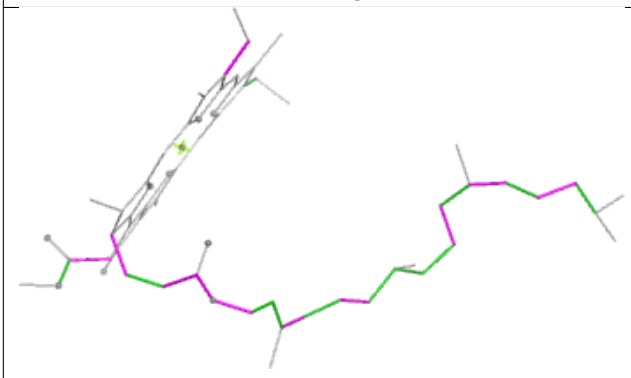


Bond angles

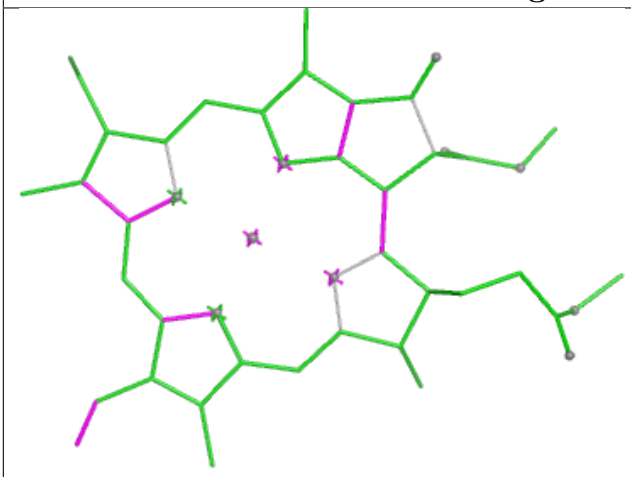


Torsions



Rings

Ligand CLA 1 613



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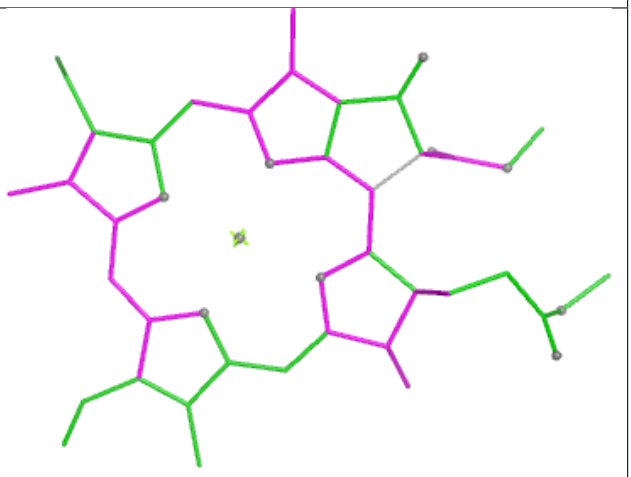
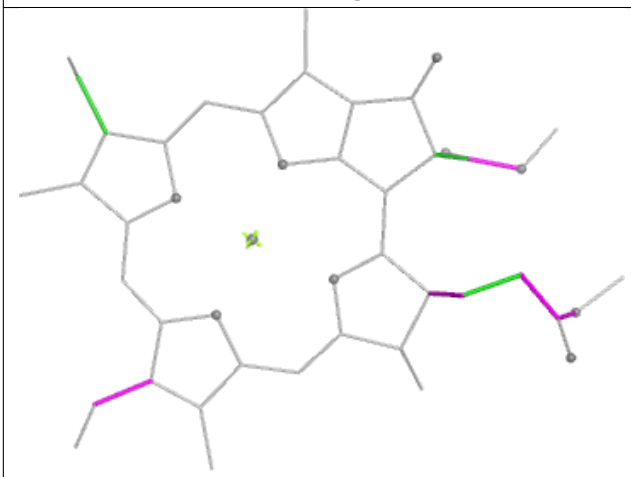


Bond angles



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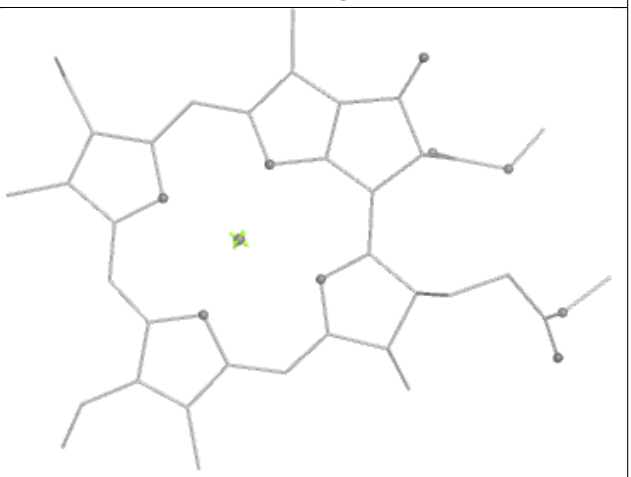
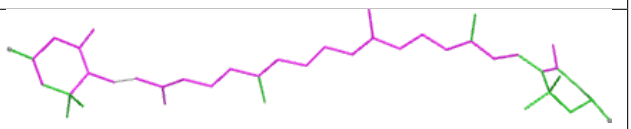


Rings

Ligand LUT 8 502



Bond lengths



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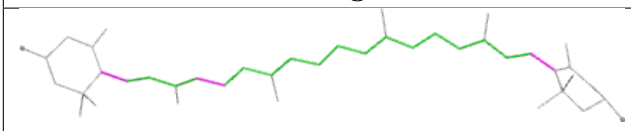

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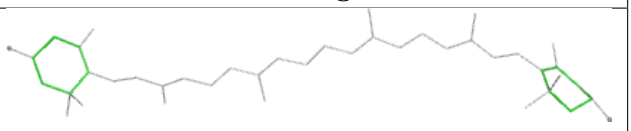
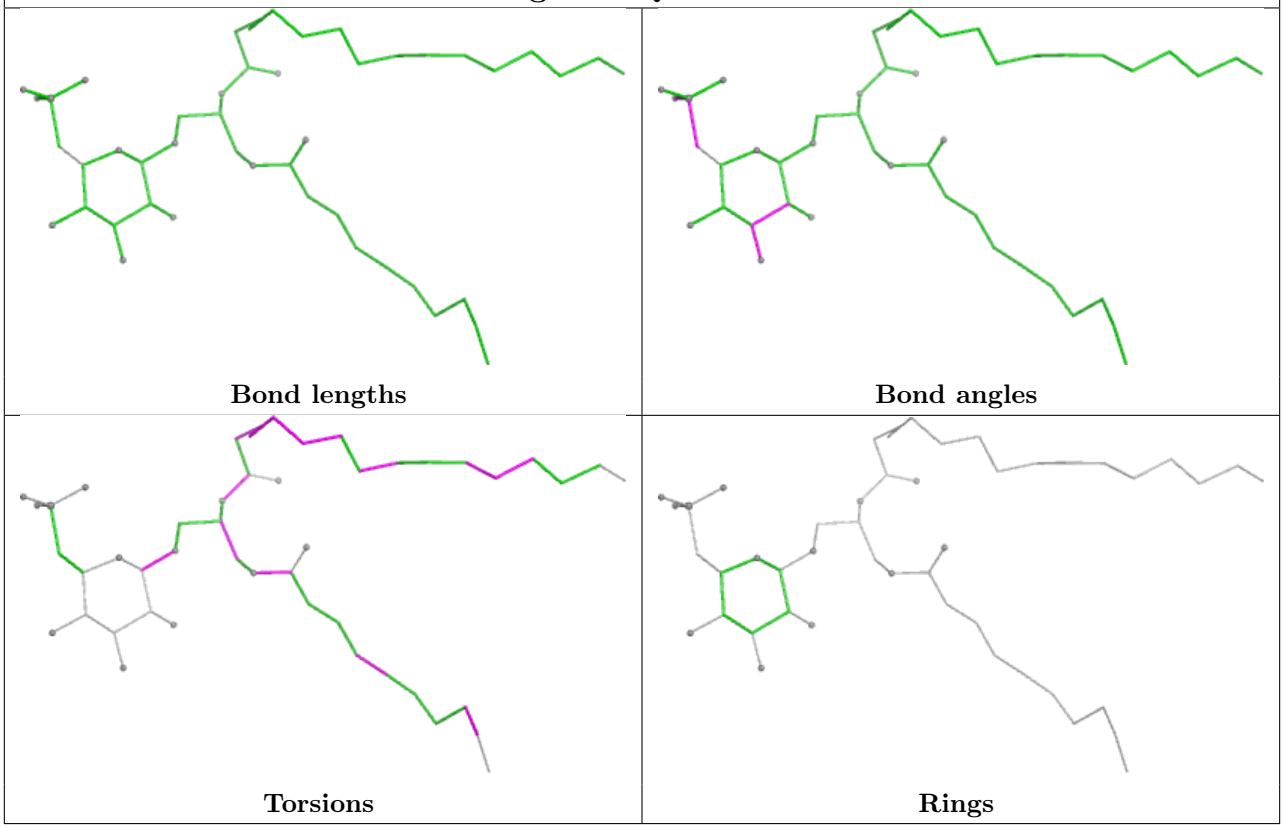
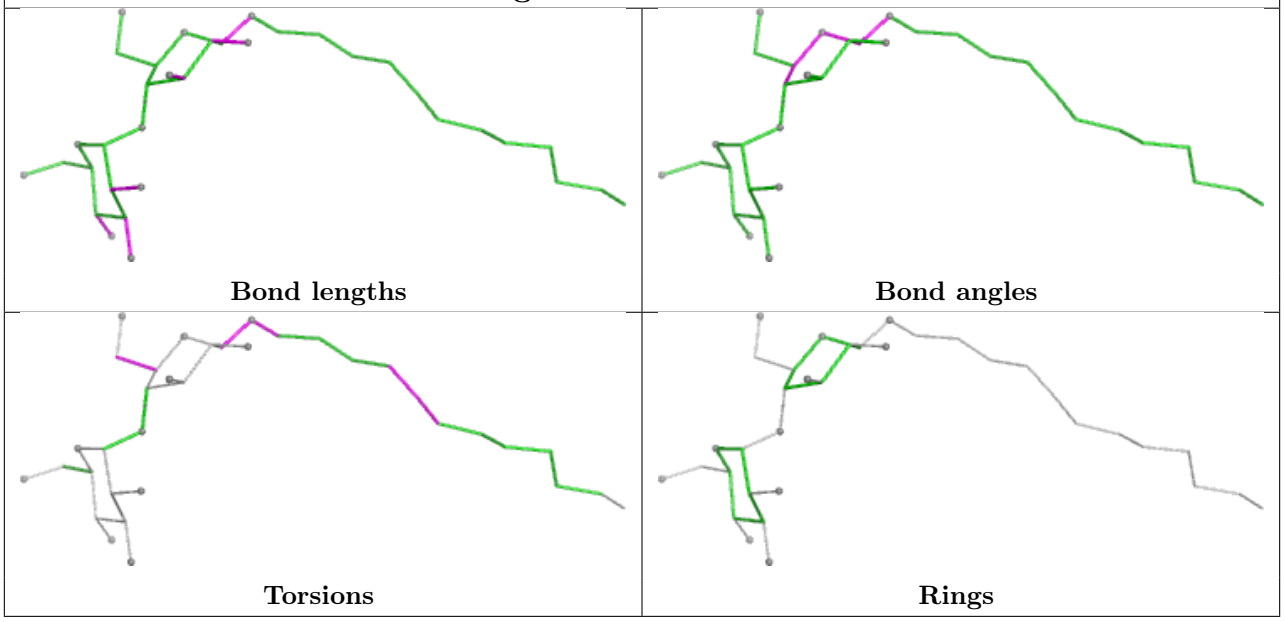


Rings

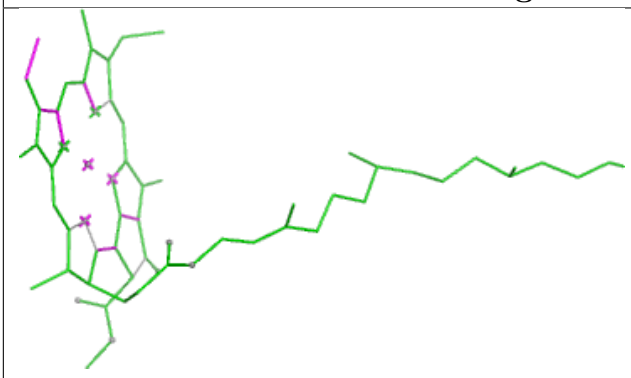
Ligand SQD 1 802



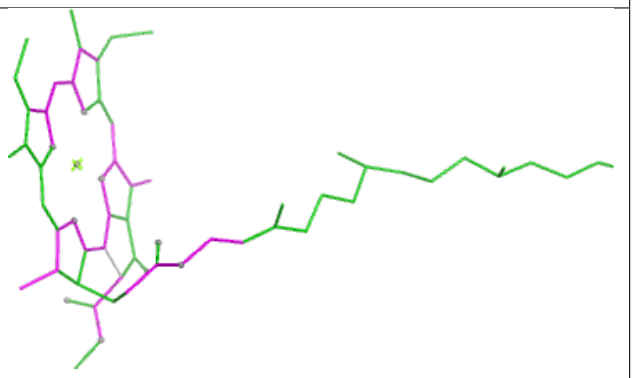
Ligand LMT B 5005



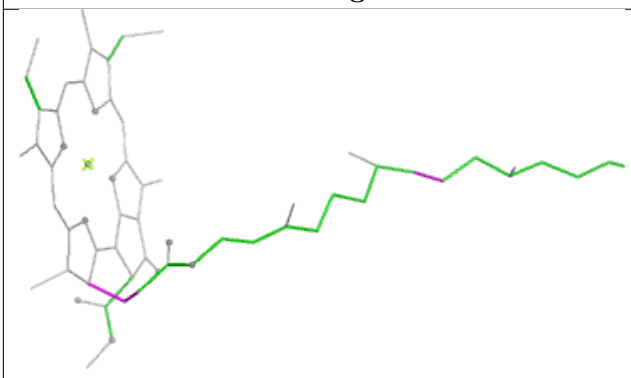
Ligand CLA B 1225



Bond lengths



Bond angles

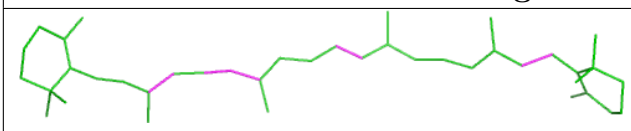


Torsions

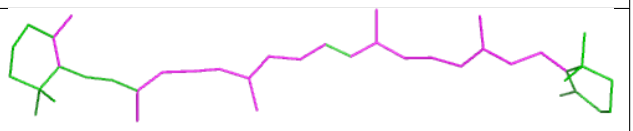


Rings

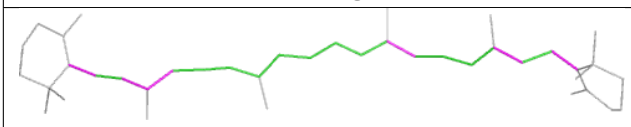
Ligand BCR B 4001



Bond lengths



Bond angles



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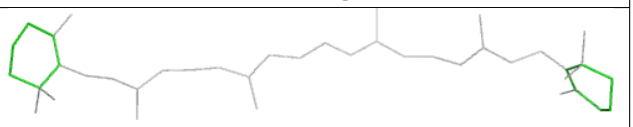
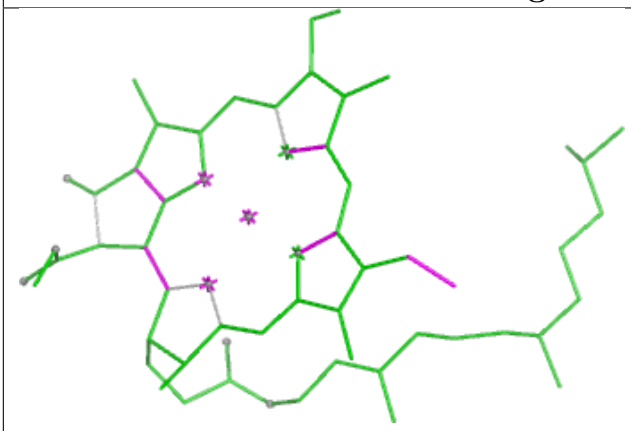


Rings

Ligand CLA 1 604



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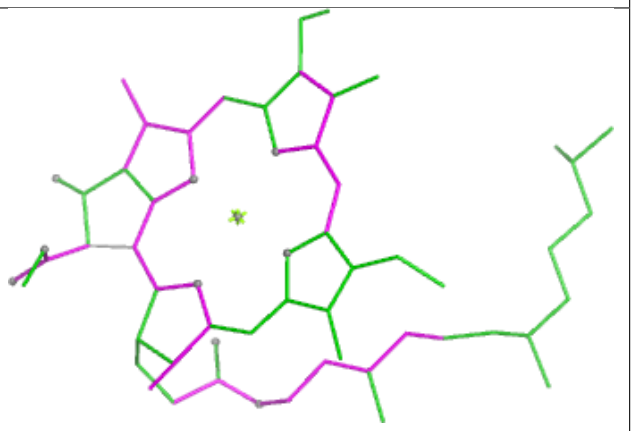
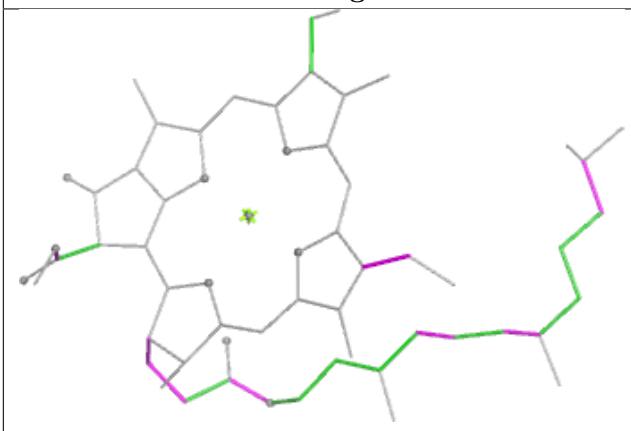
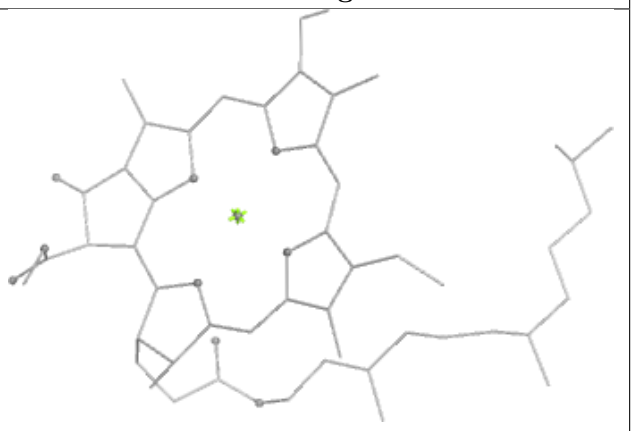


Bond angles



Torsions

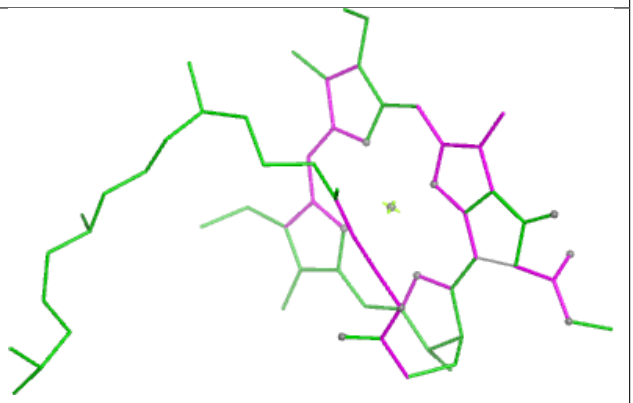


Rings

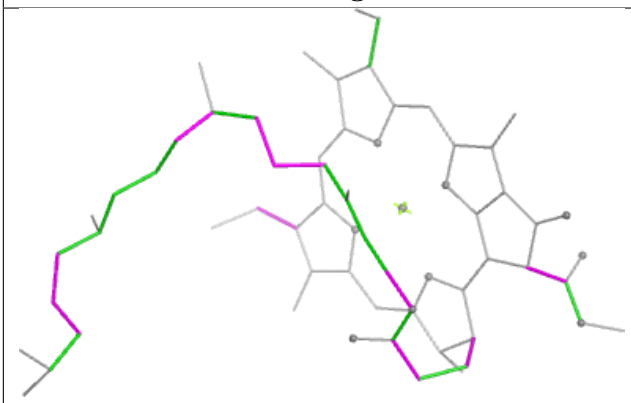
Ligand CLA B 1204



Bond lengths



Bond angles



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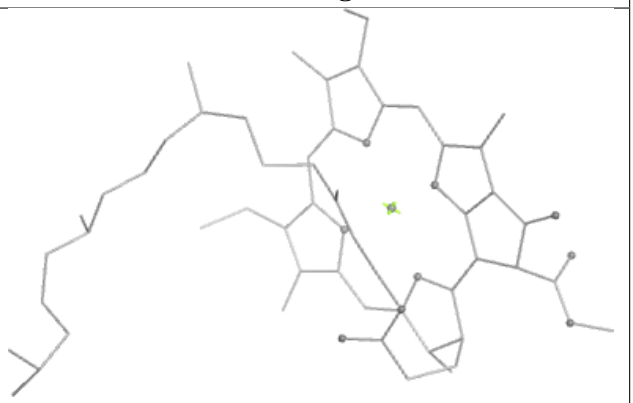
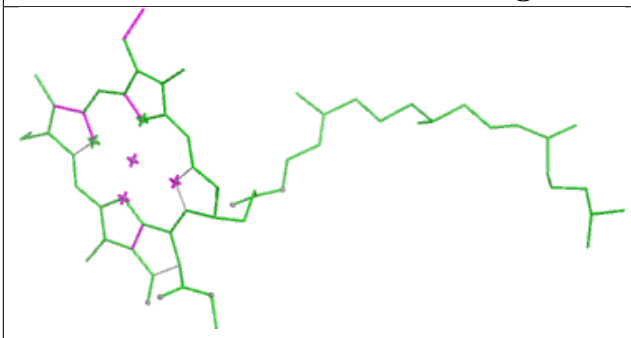


Rings

Ligand CLA A 1119



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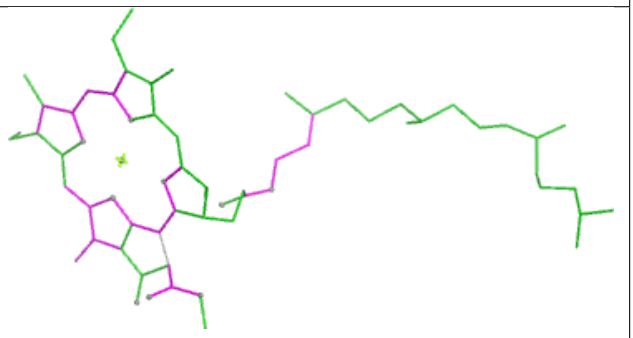
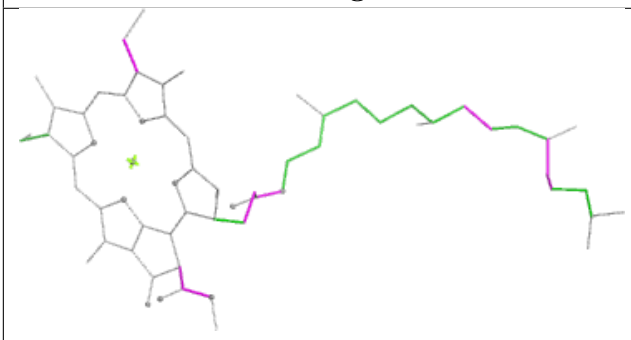


Bond angles



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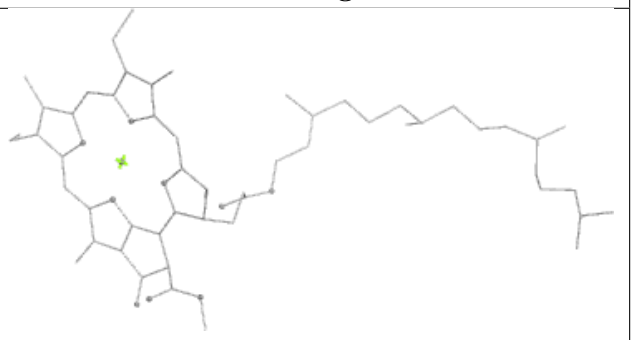
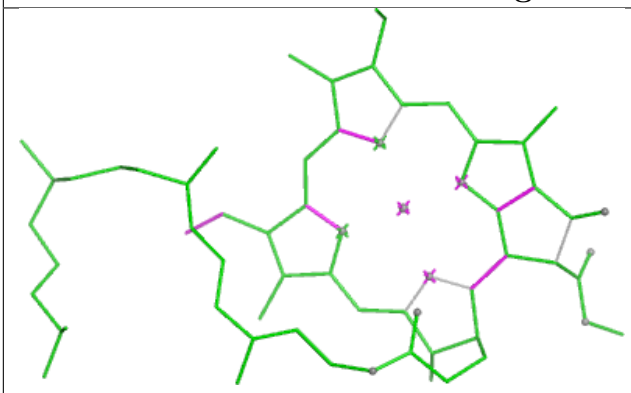


Rings

Ligand CLA A 1117



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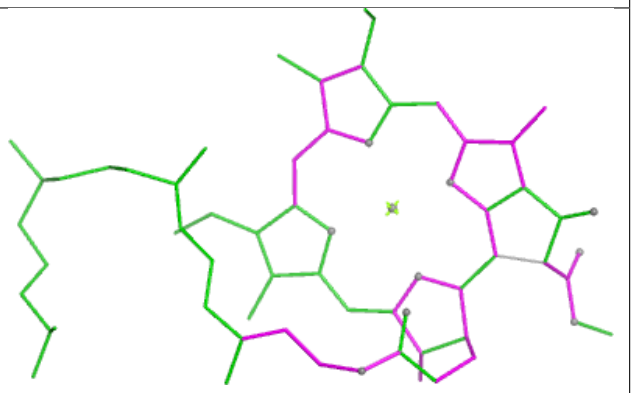
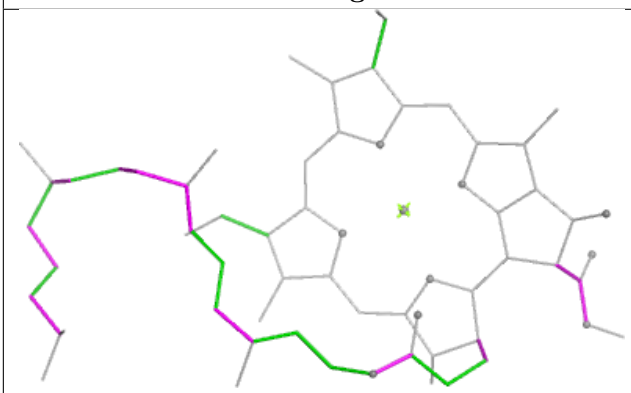


Bond angles

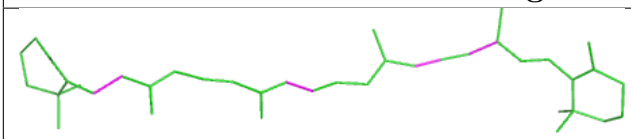


Torsions



Rings

Ligand BCR 8 503



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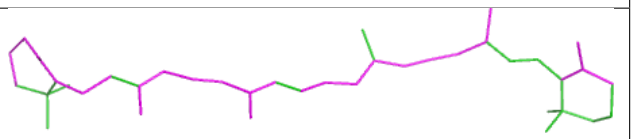

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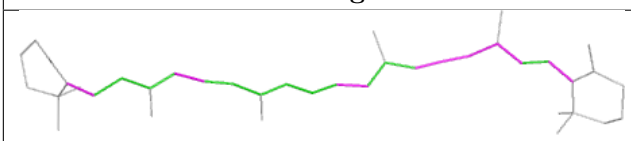

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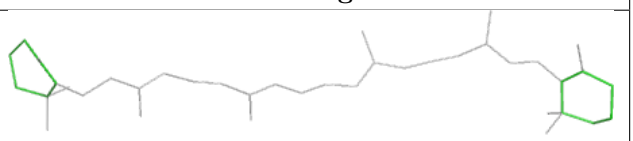
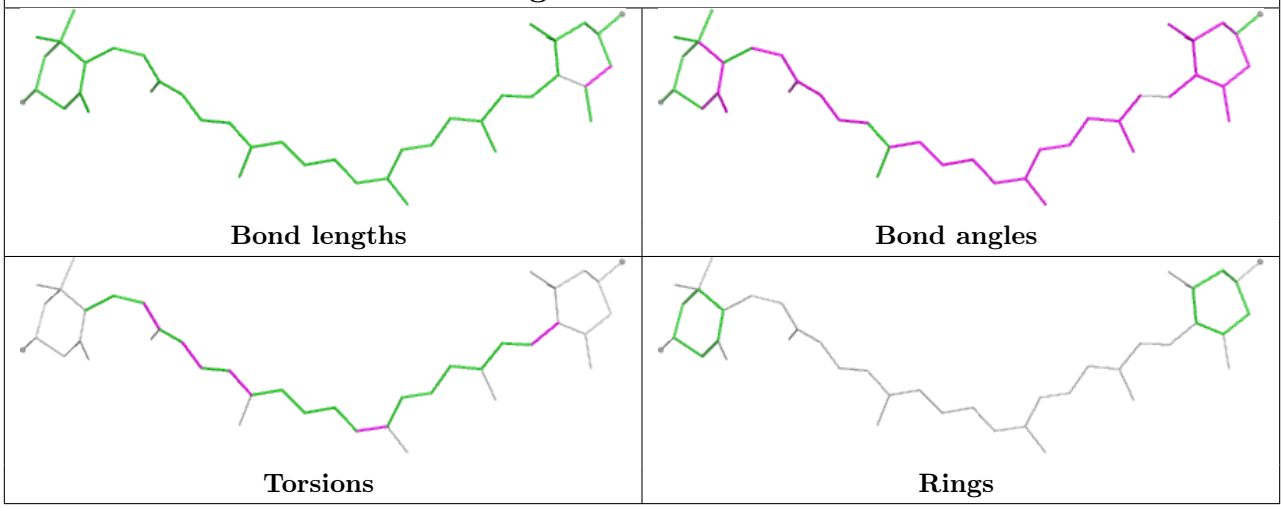
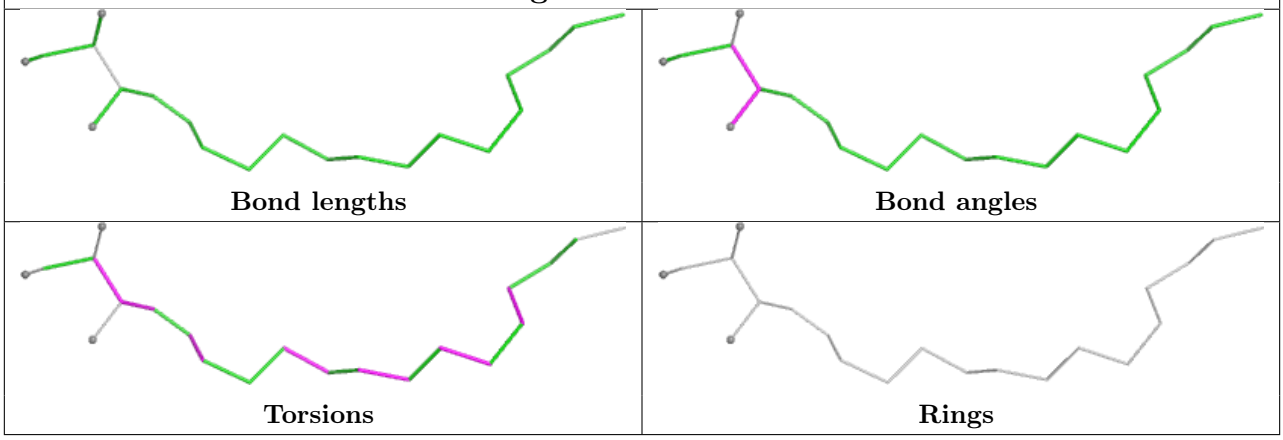


Rings

Ligand LUT 2 503



Ligand SPH 7 803



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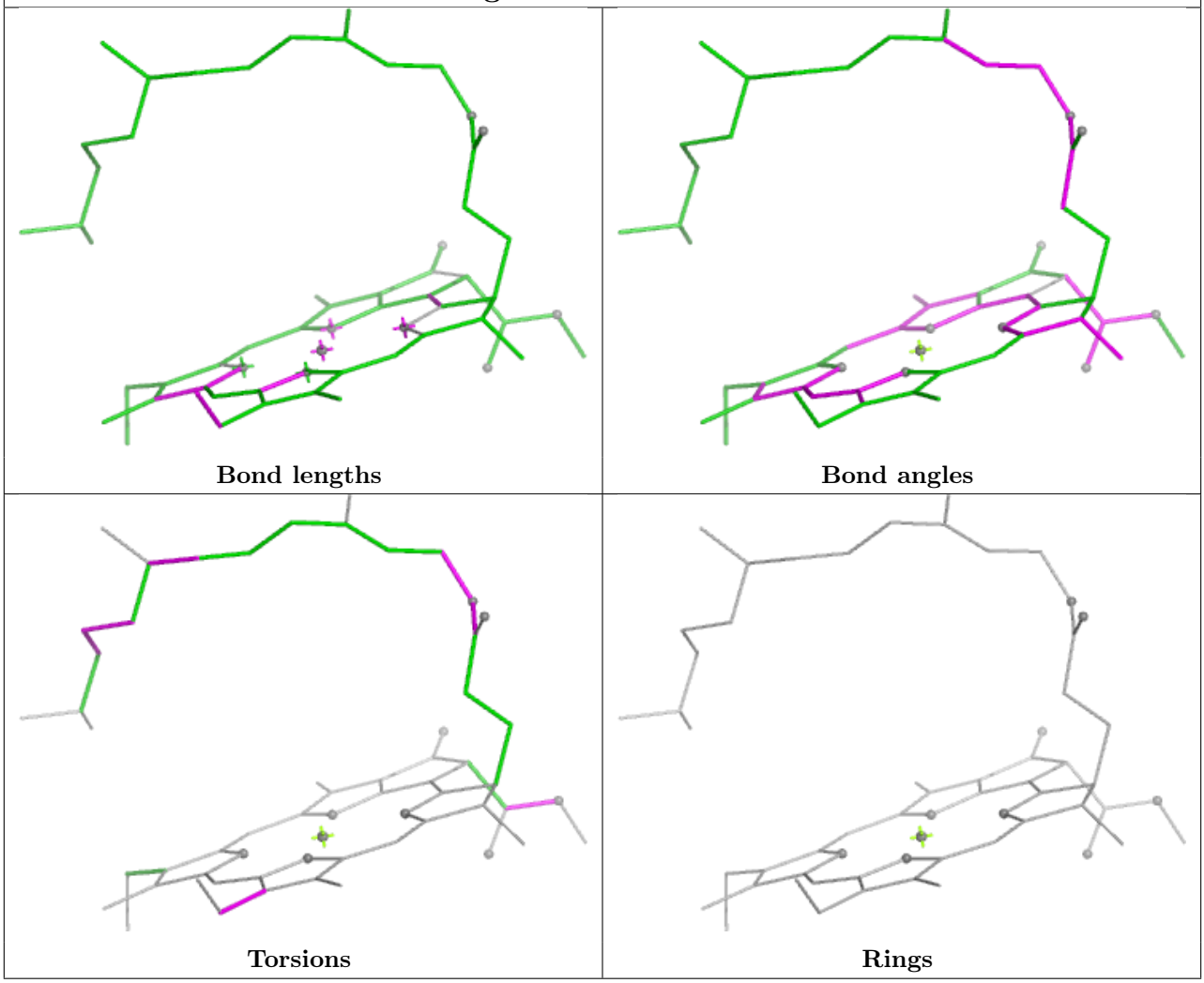

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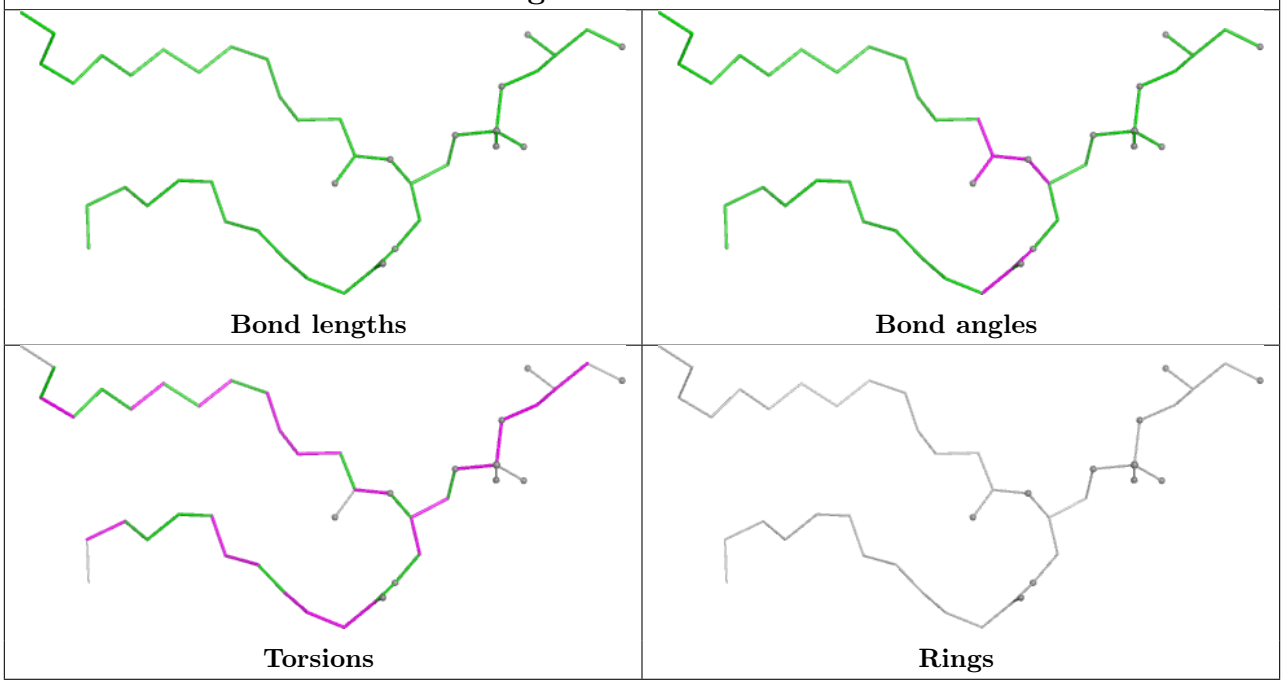

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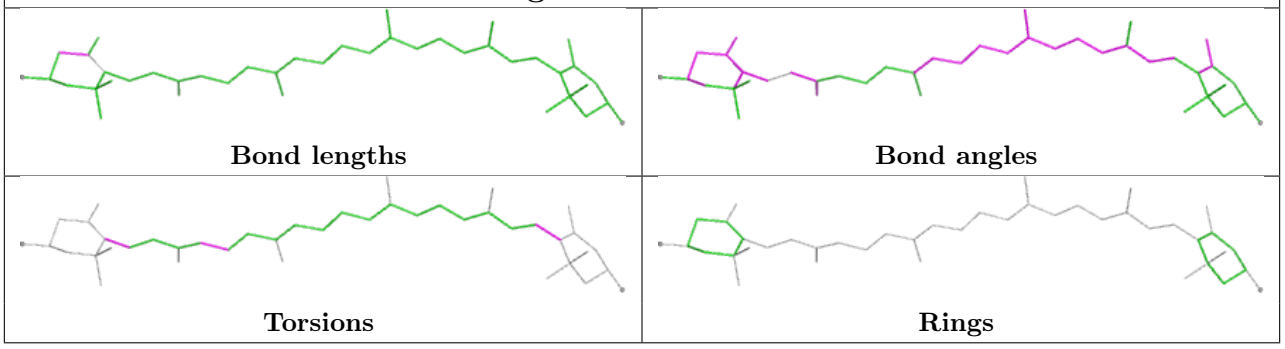

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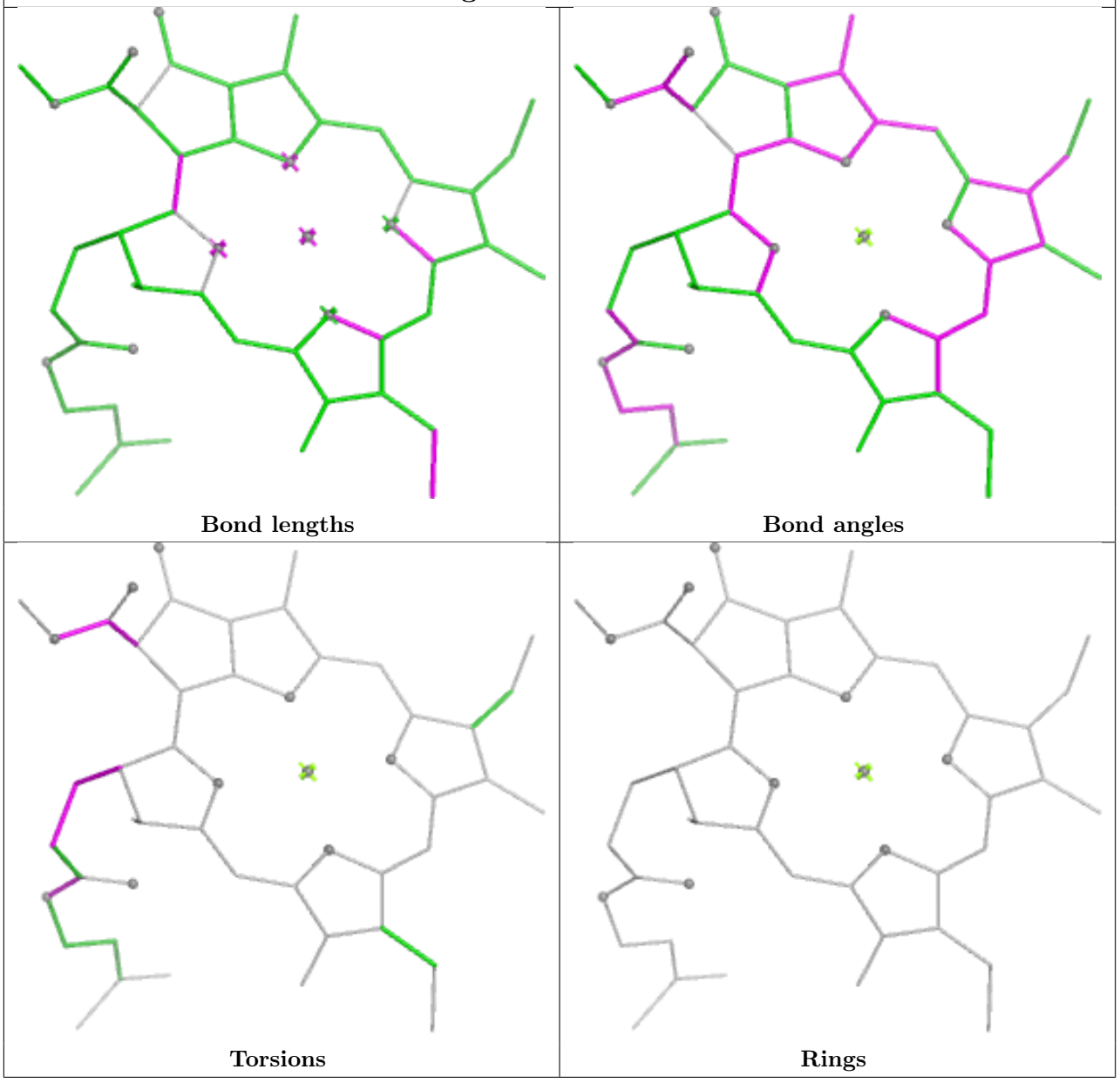

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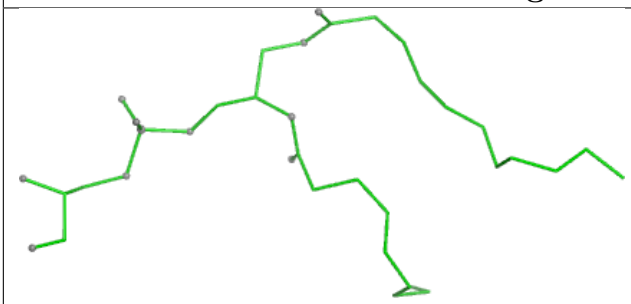
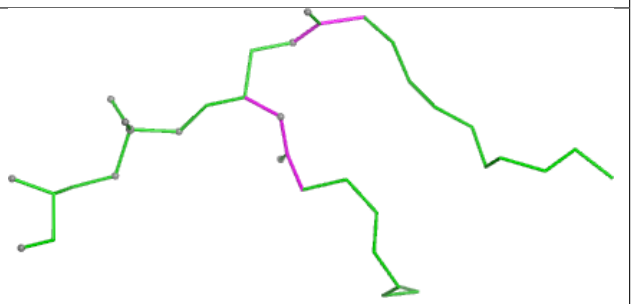
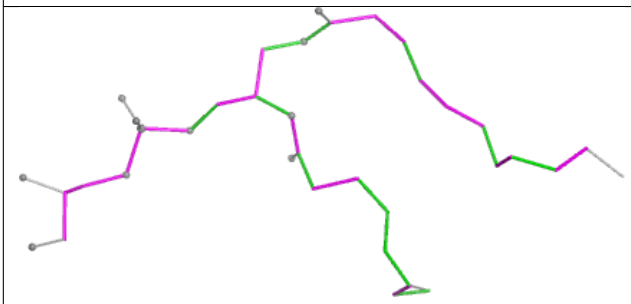


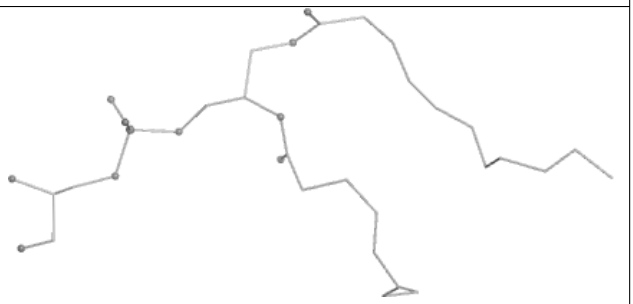
Bond lengths



Bond angles

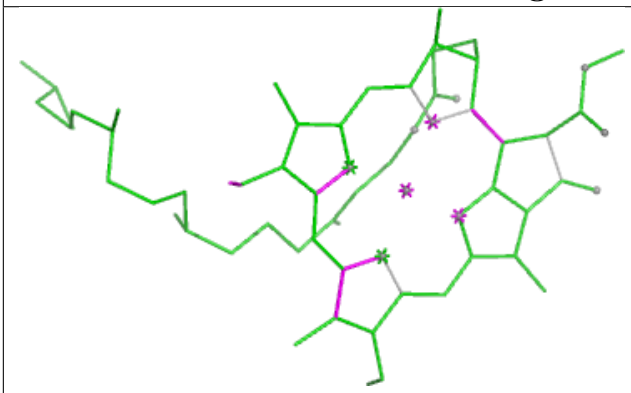


Torsions



Rings

Ligand CLA 1 603



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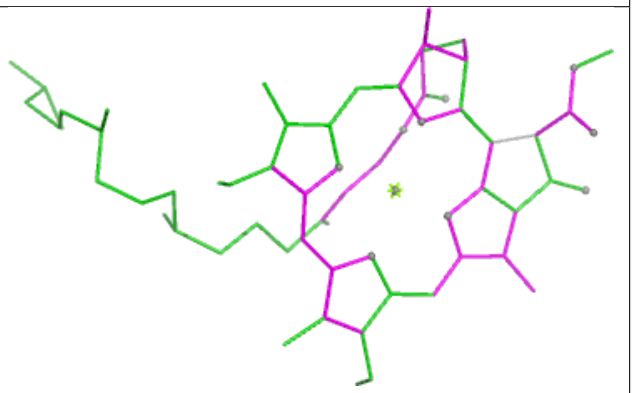

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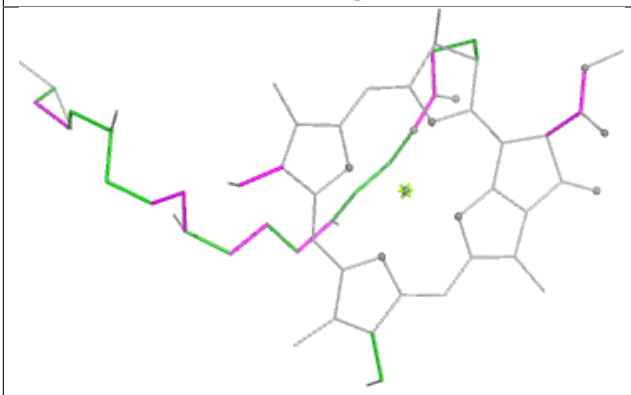
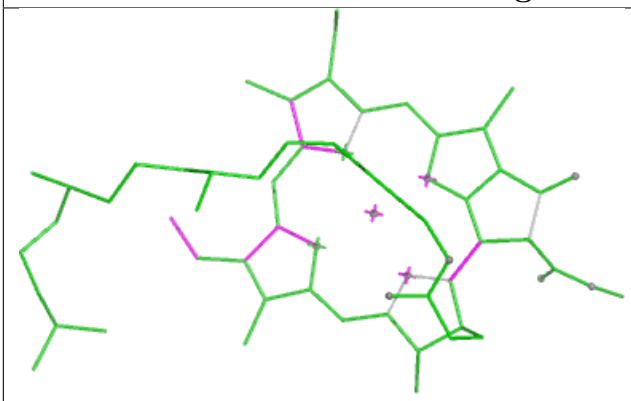


Torsions



Rings

Ligand CLA A 1110



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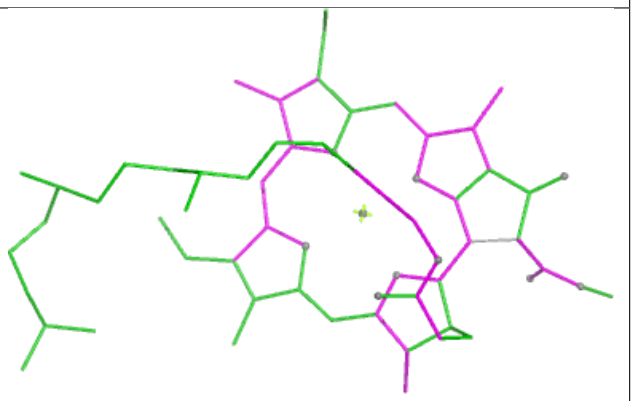
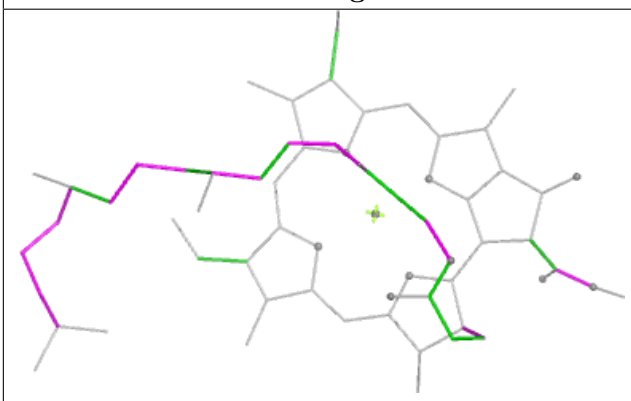


Bond angles



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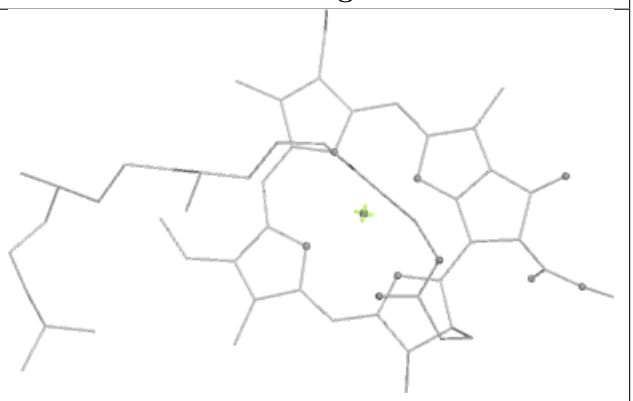
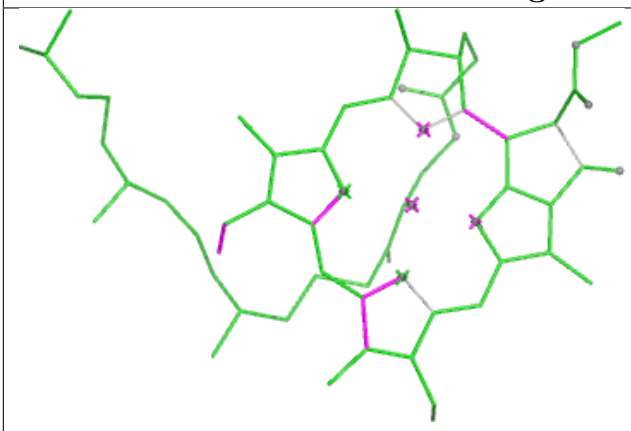


Rings

Ligand CLA 7 603



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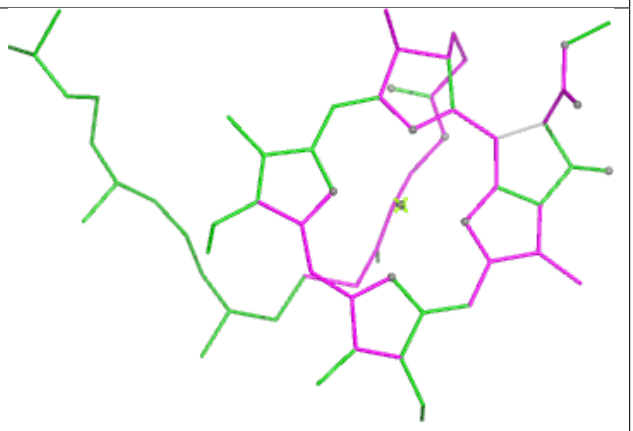

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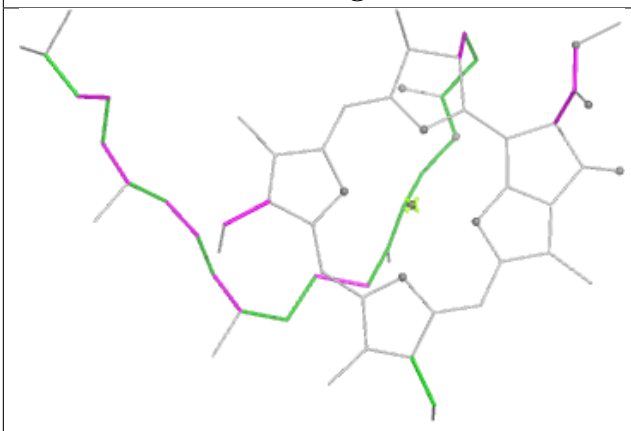

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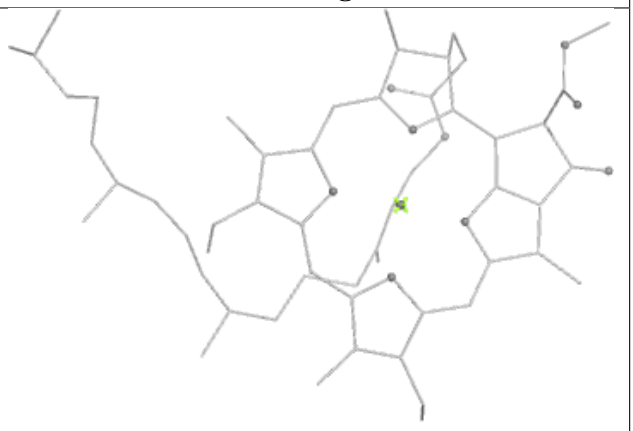
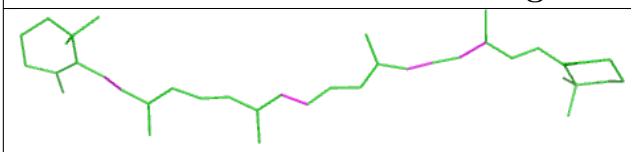


Rings

Ligand BCR 4 503



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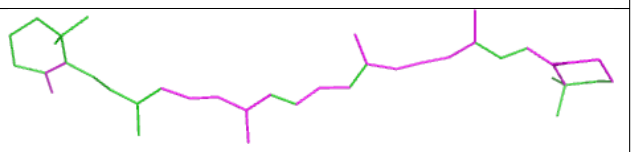
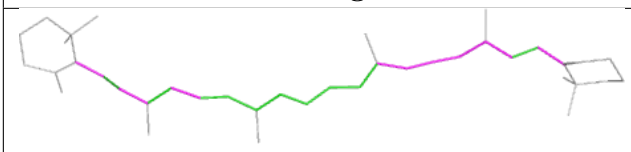


Bond angles



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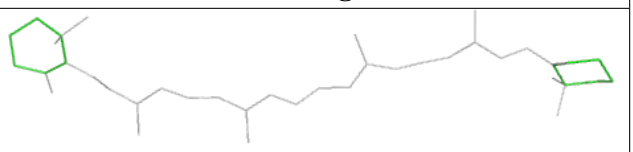
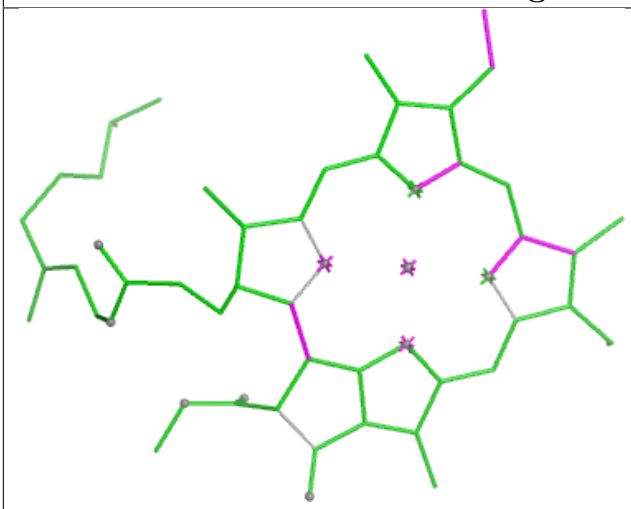


Rings

Ligand CLA 6 605



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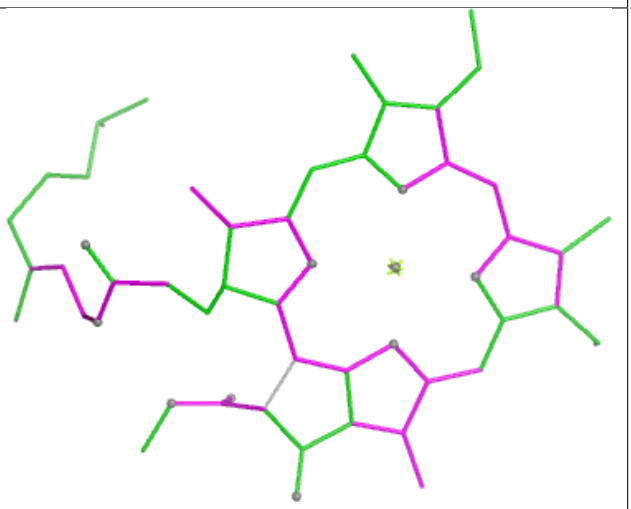
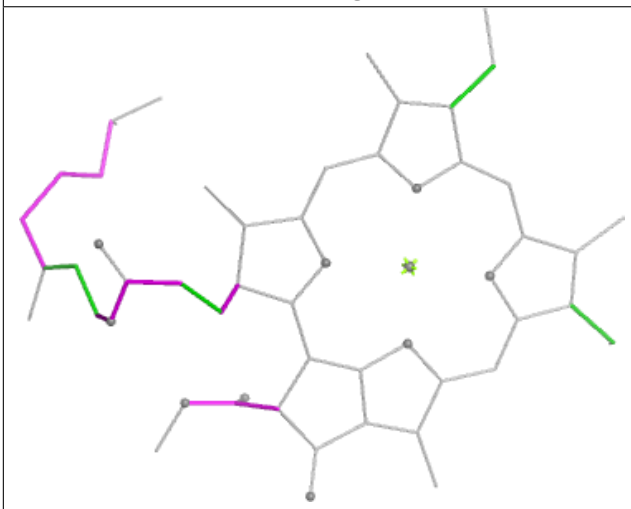


Bond angles



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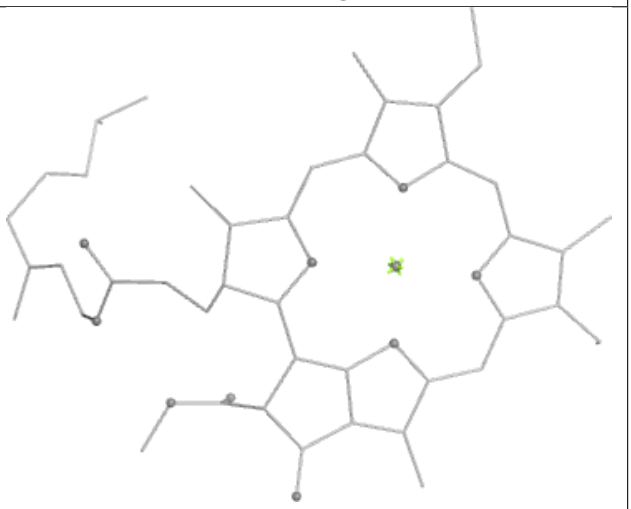
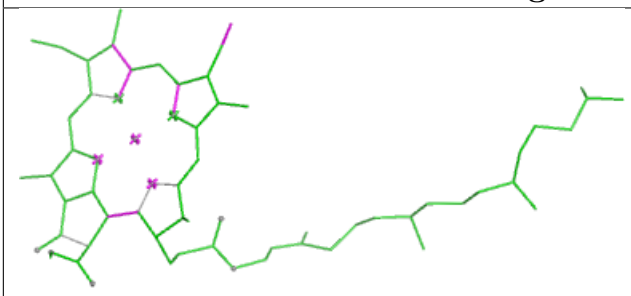


Rings

Ligand CLA 7 609



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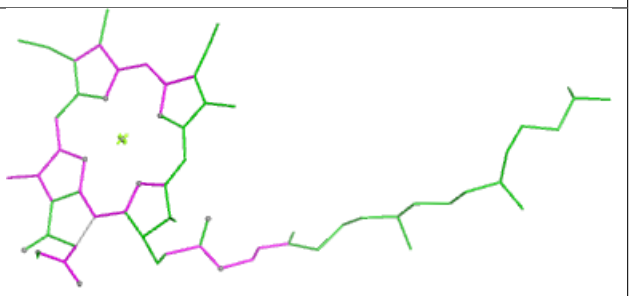
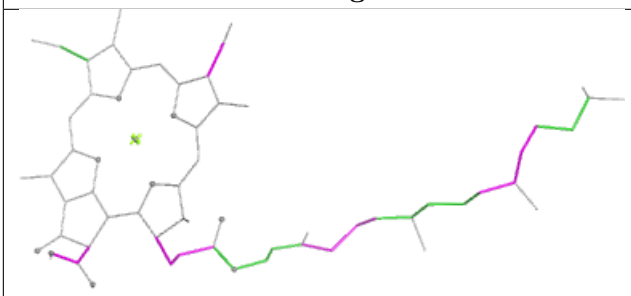


Bond angles



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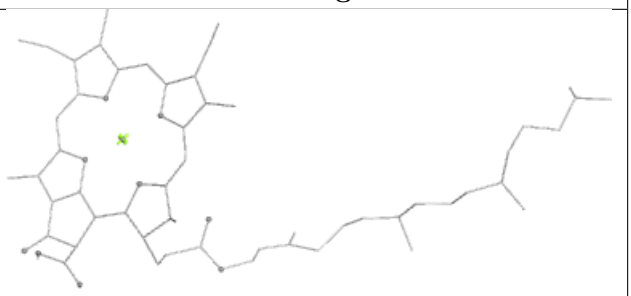
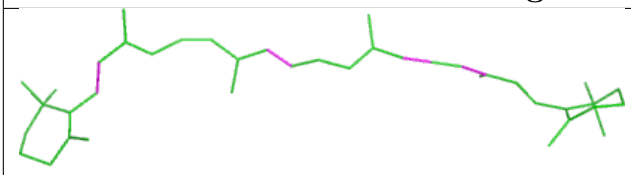


Rings

Ligand BCR 6 504



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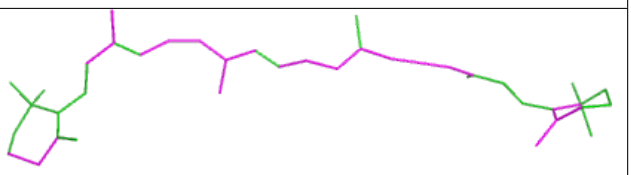
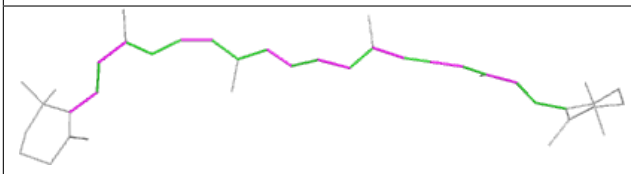


Bond angles



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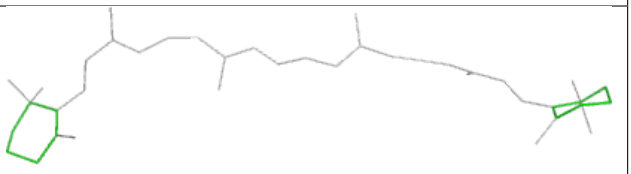
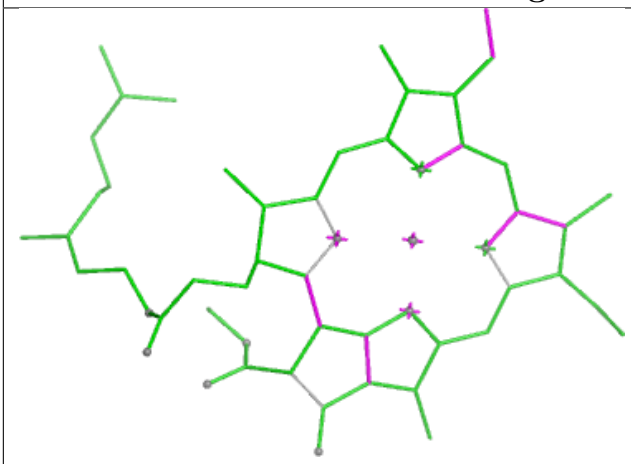


Rings

Ligand CLA 1 605



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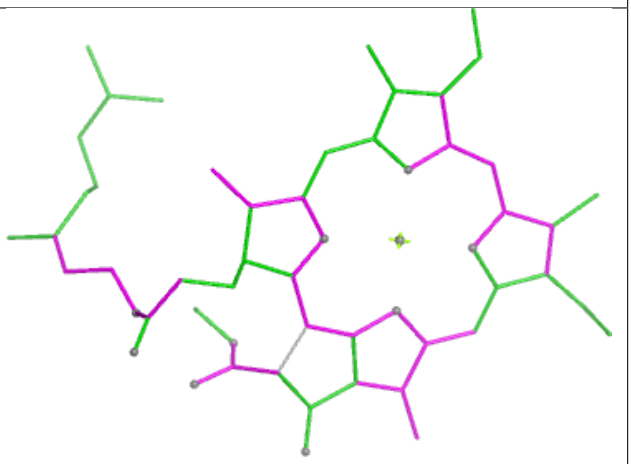
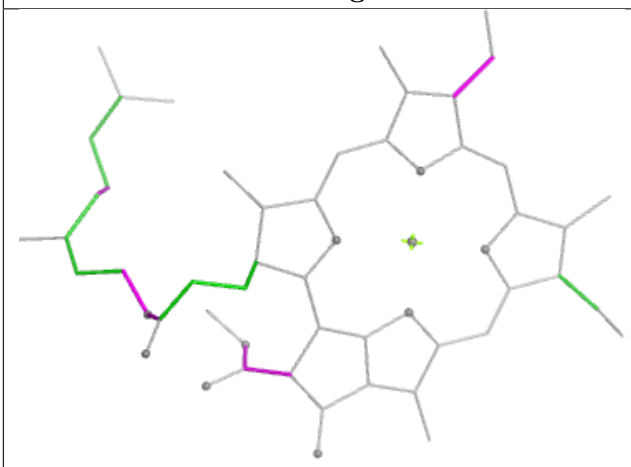


Bond angles



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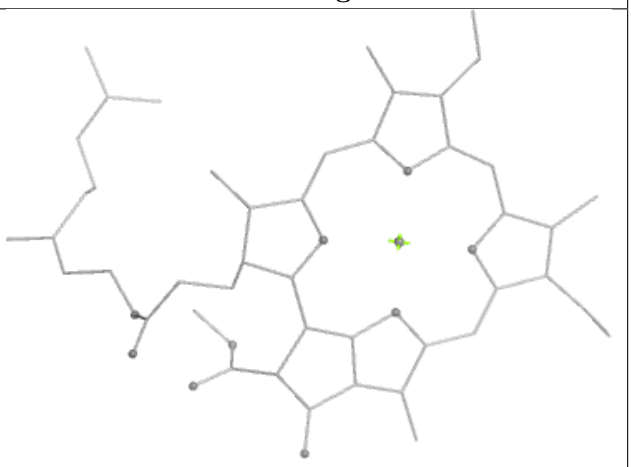
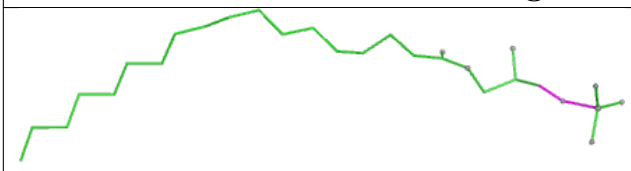
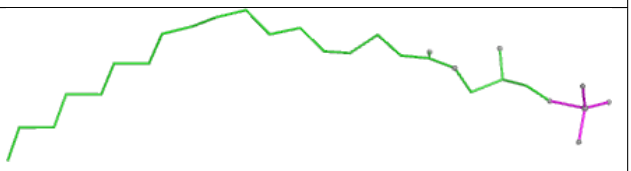


Rings

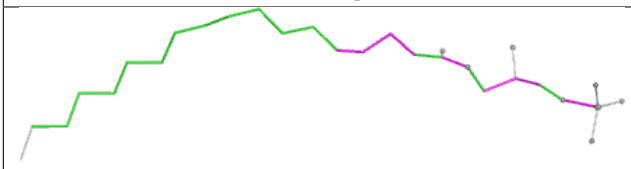
Ligand NKP 8 802



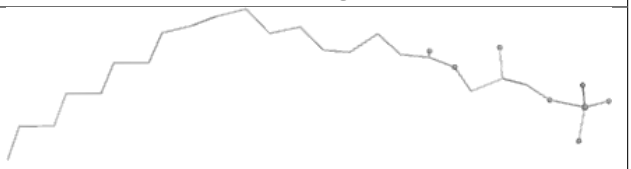
Bond lengths



Bond angles

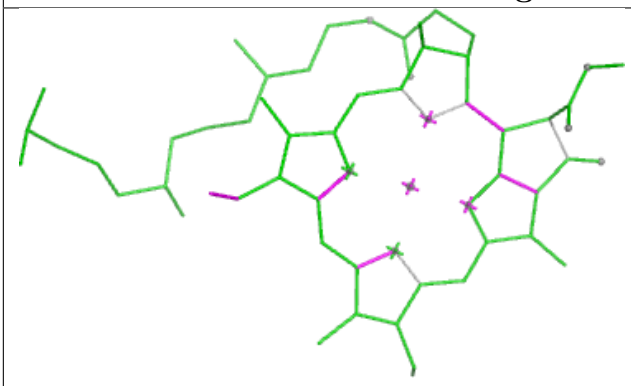


Torsions



Rings

Ligand CLA B 1215



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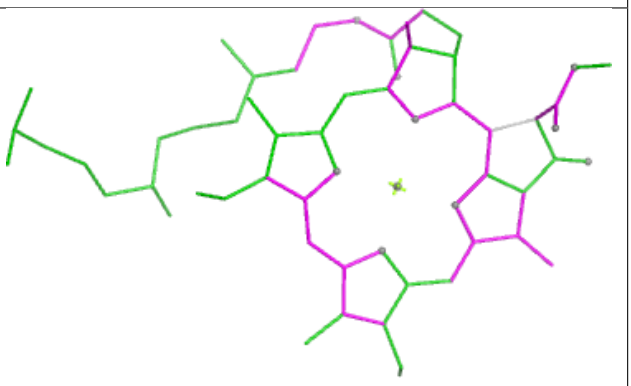

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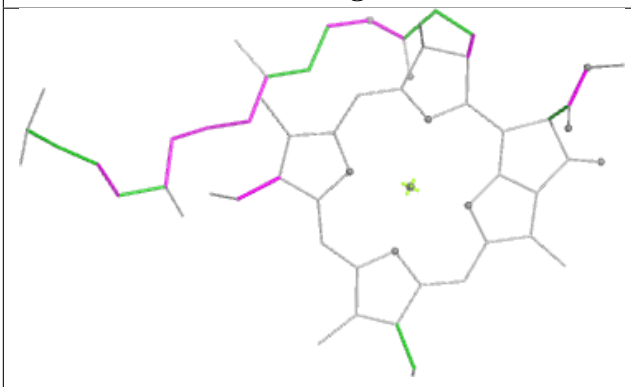

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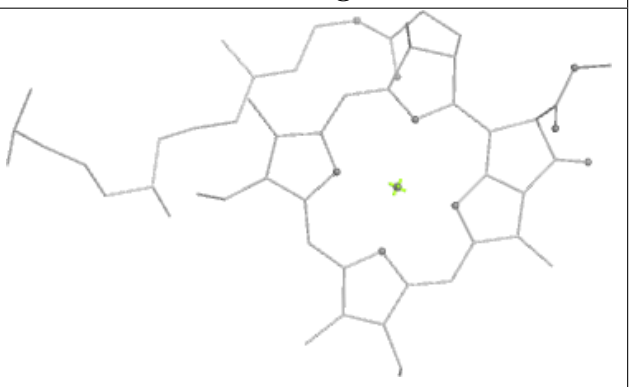
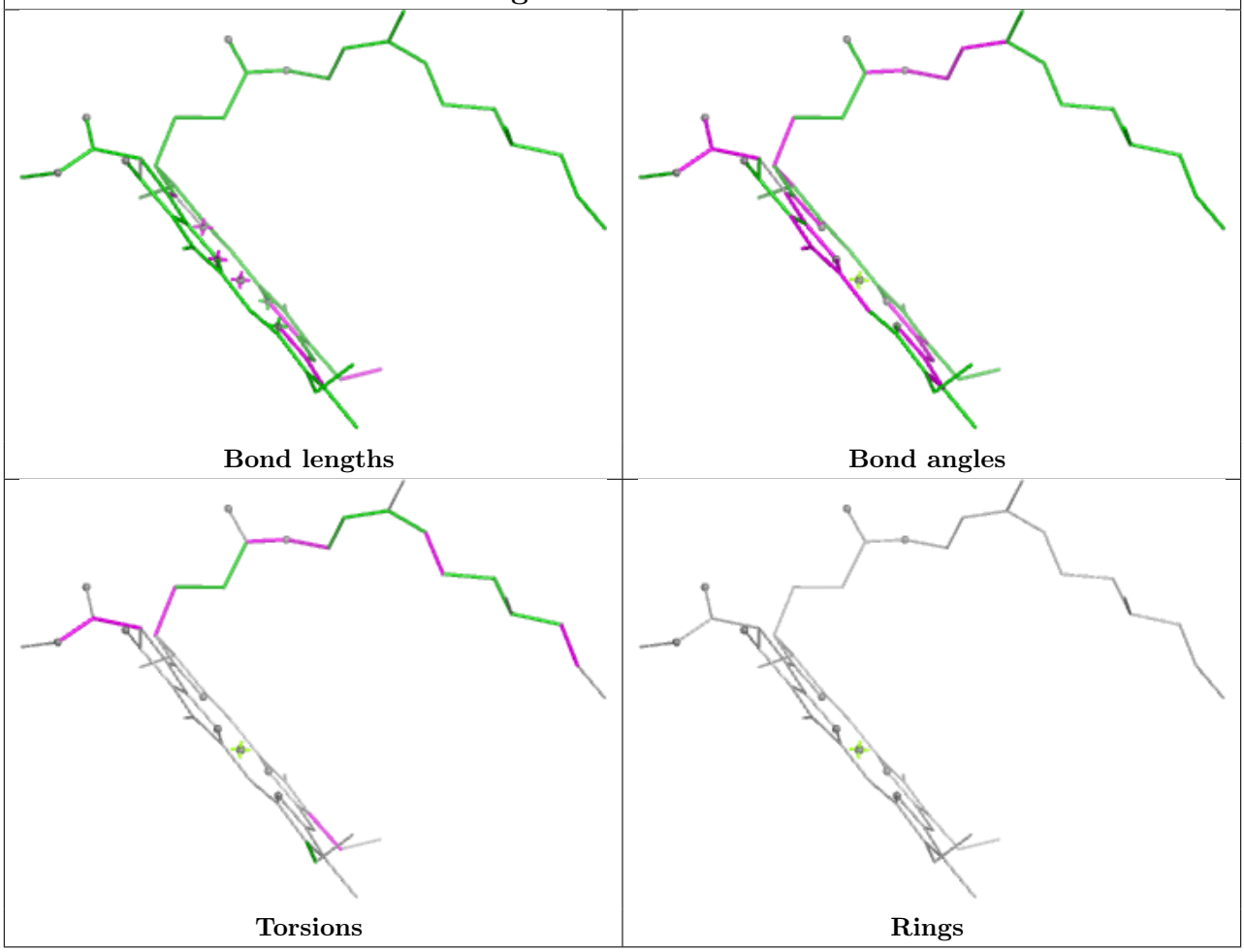
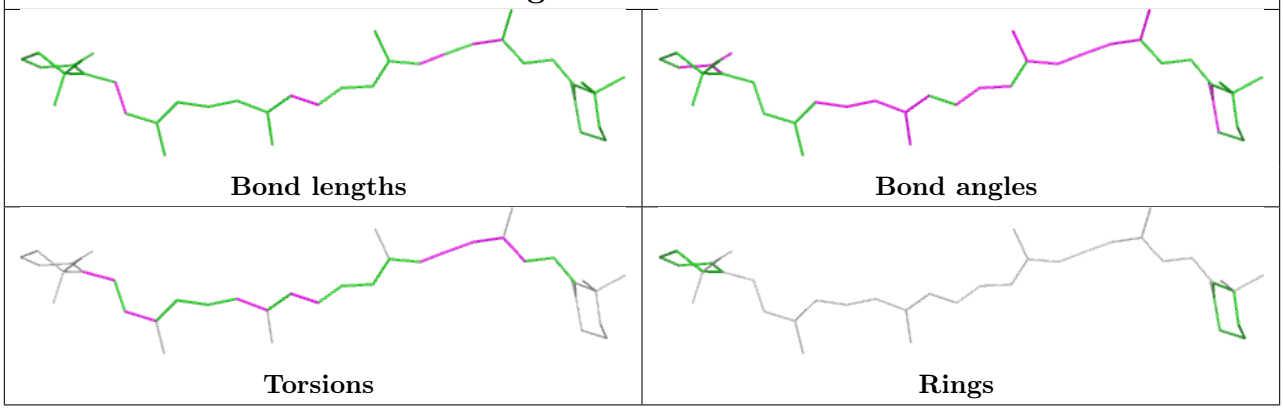


Rings

Ligand CLA Z 606



Ligand BCR 5 503



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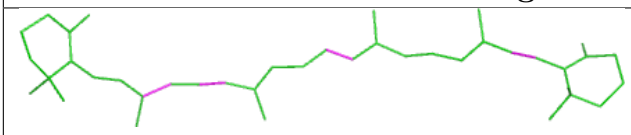

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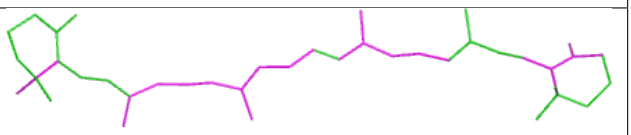

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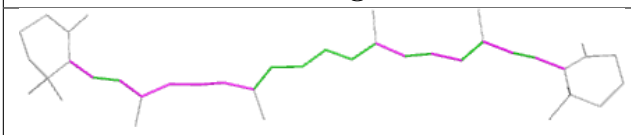

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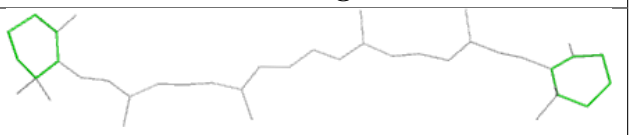
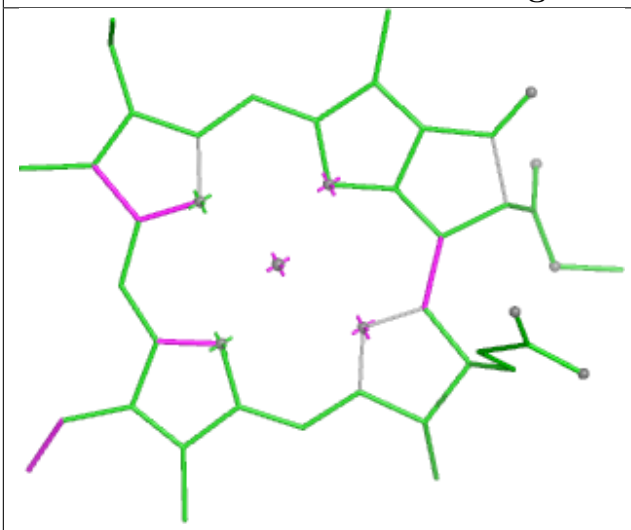


Rings

Ligand CLA 2 608



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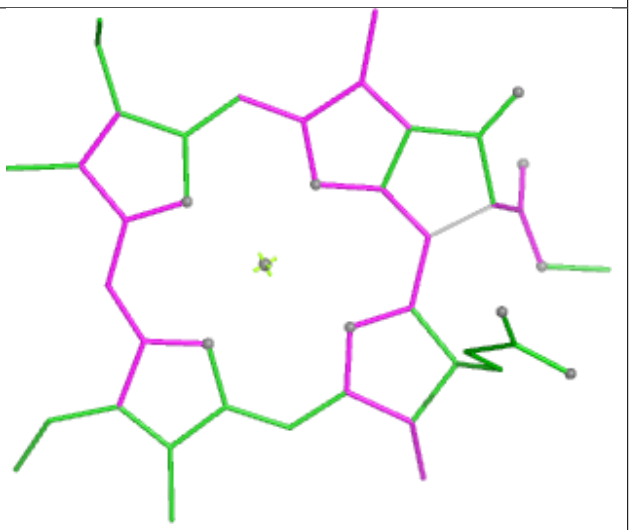

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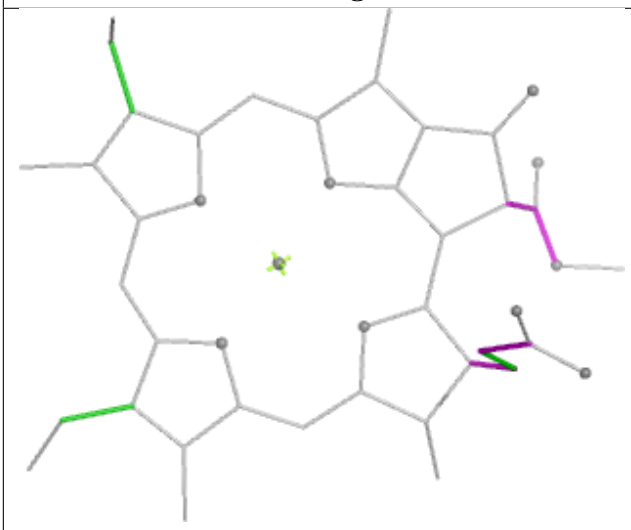

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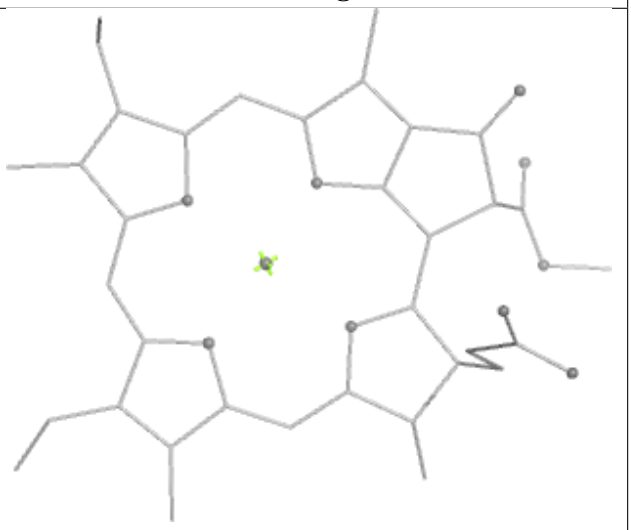
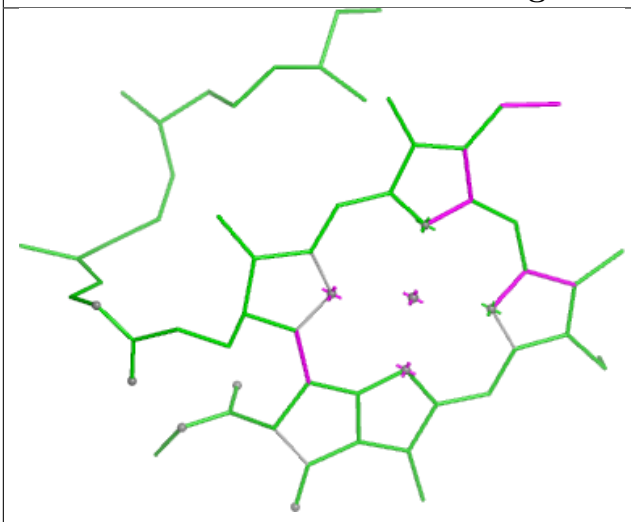


Rings

Ligand CLA 5 602



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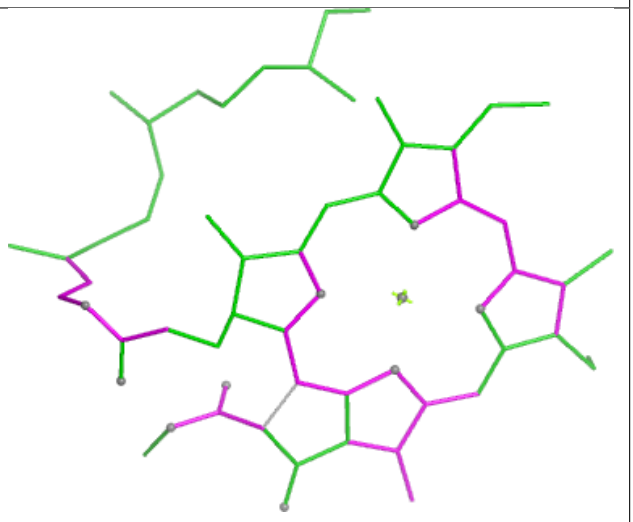

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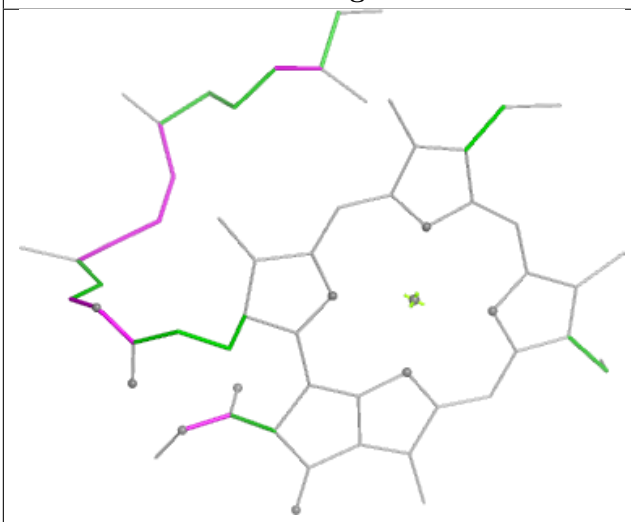
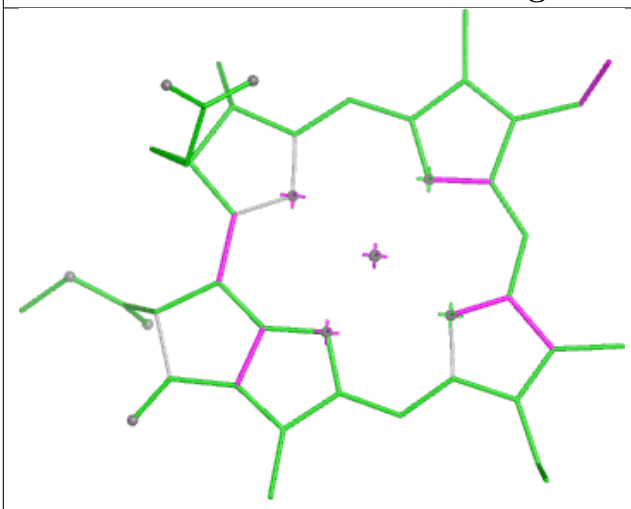


Torsions



Rings

Ligand CLA 9 608



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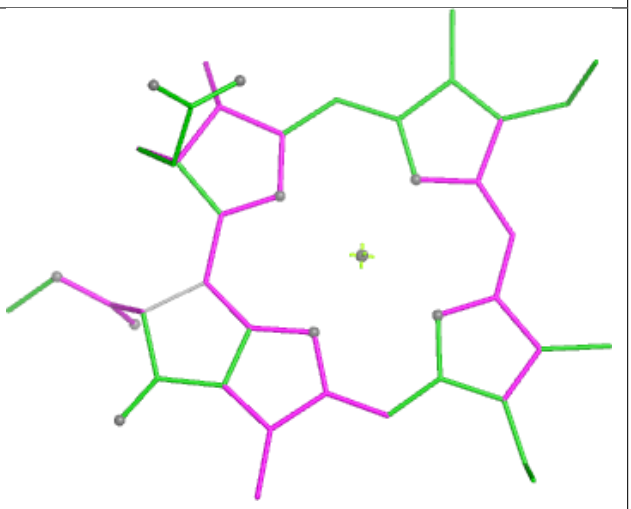

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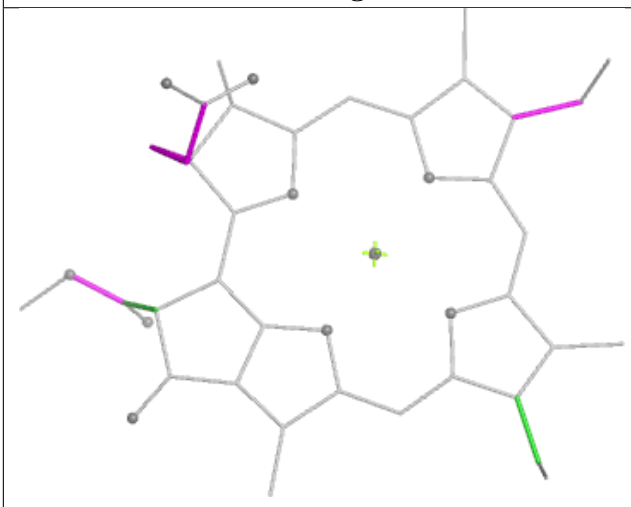

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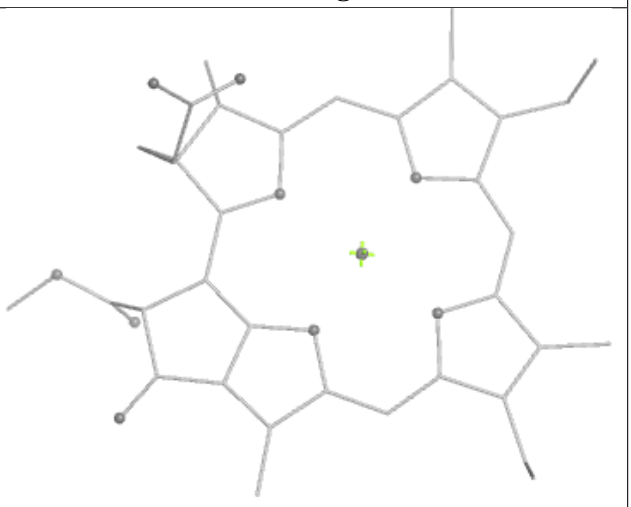
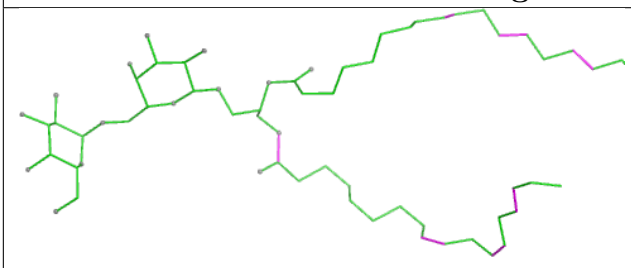


Rings

Ligand DGD B 5003



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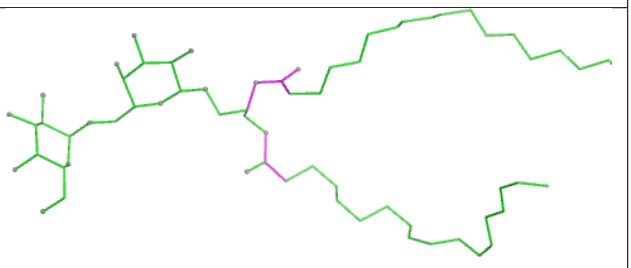

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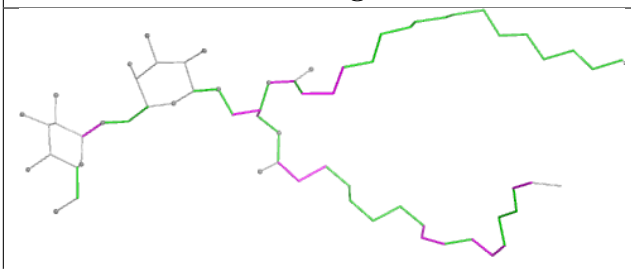

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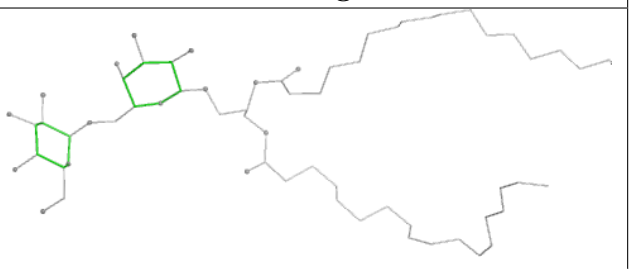
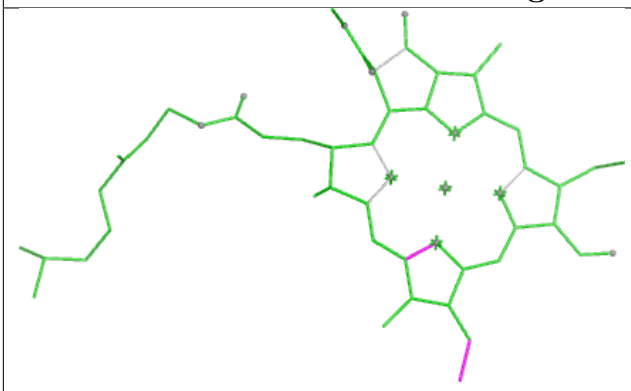


Rings

Ligand CHL 6 613



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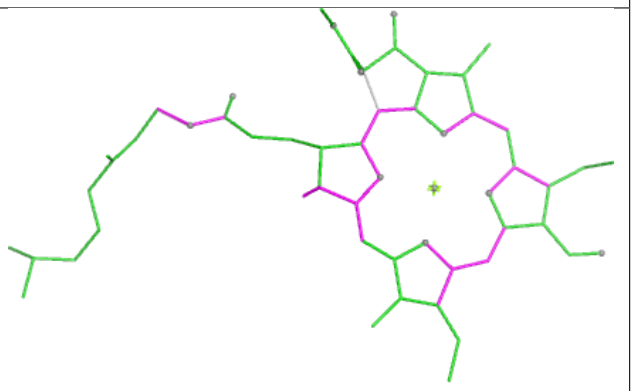

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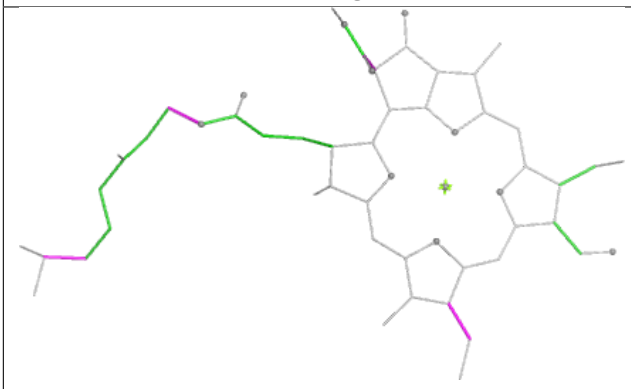

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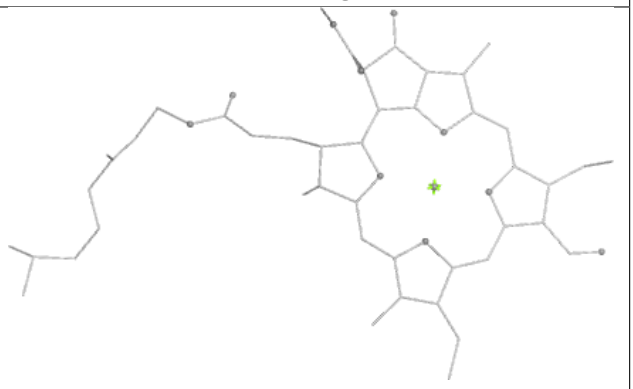
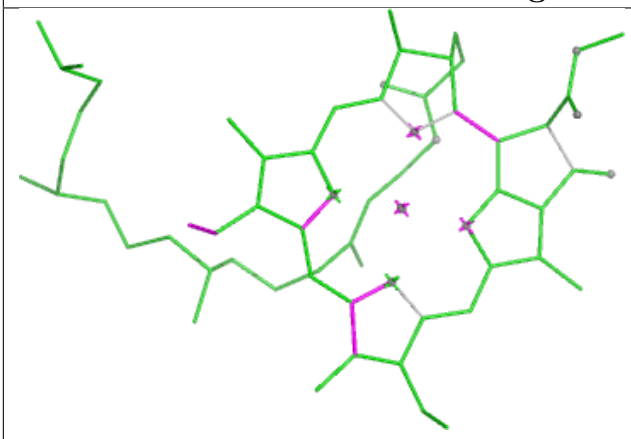


Rings

Ligand CLA 4 603



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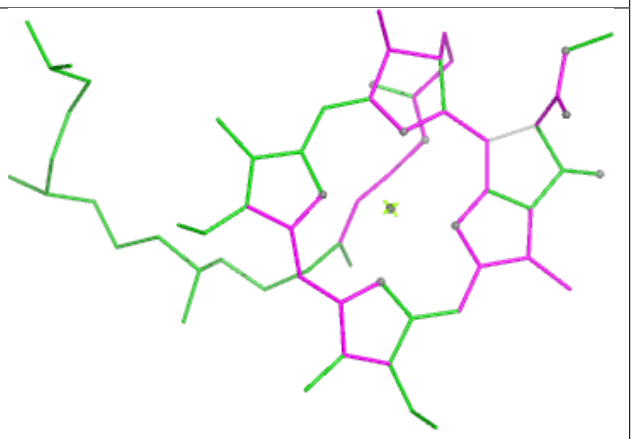
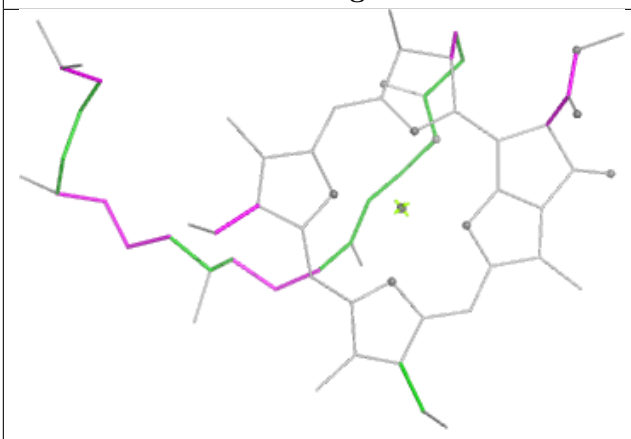


Bond angles

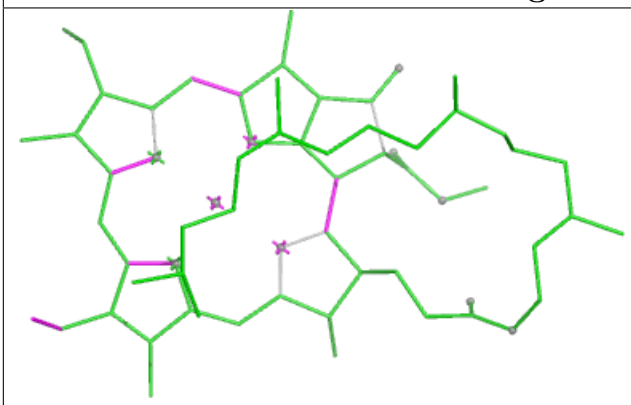


Torsions



Rings

Ligand CLA 1 615



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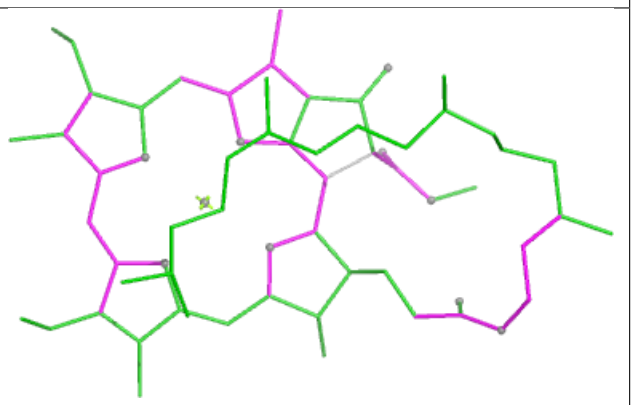
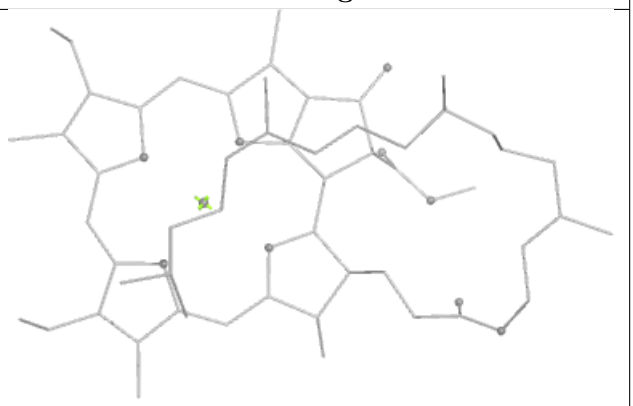


Bond angles

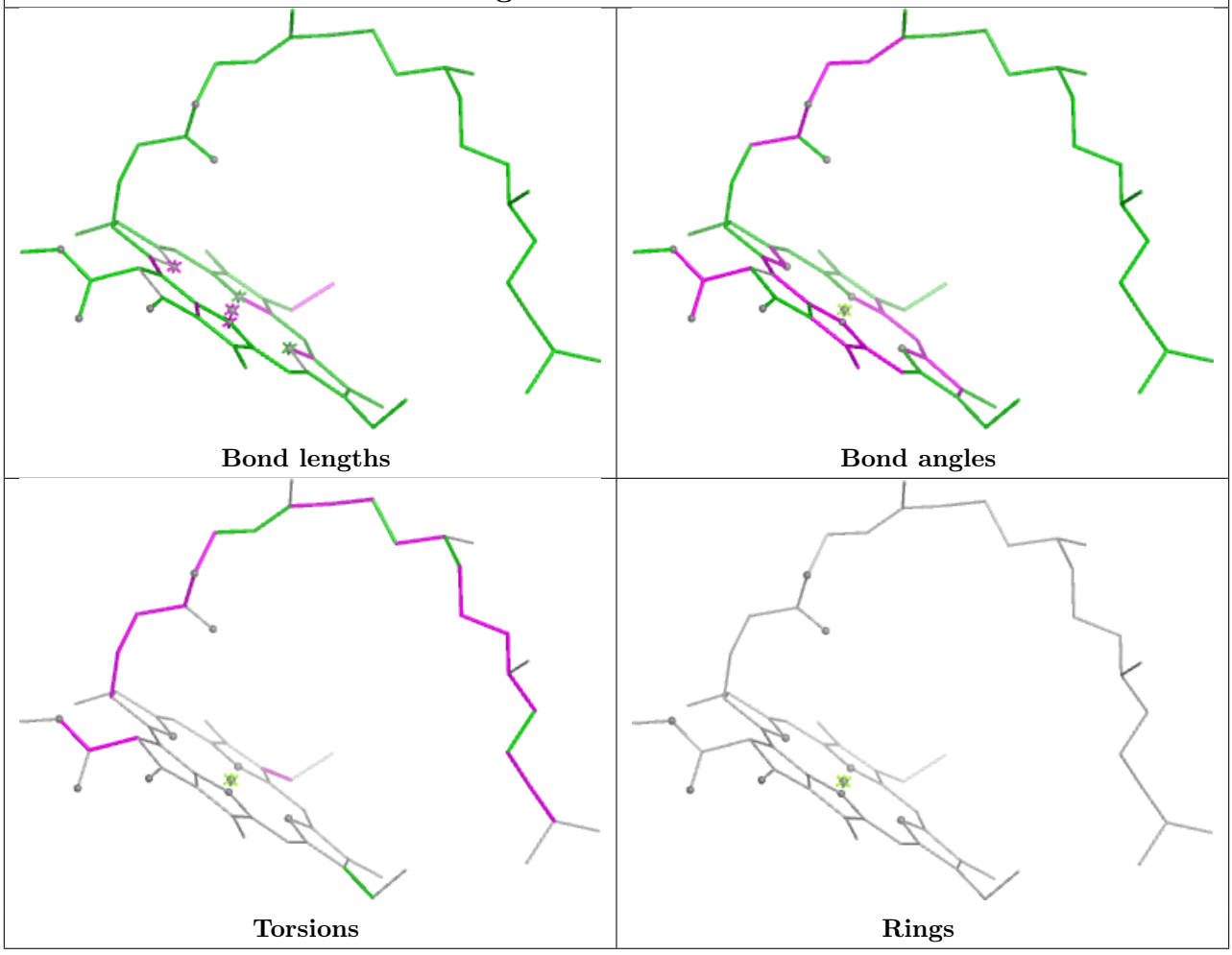


Torsions



Rings

Ligand CLA B 1216



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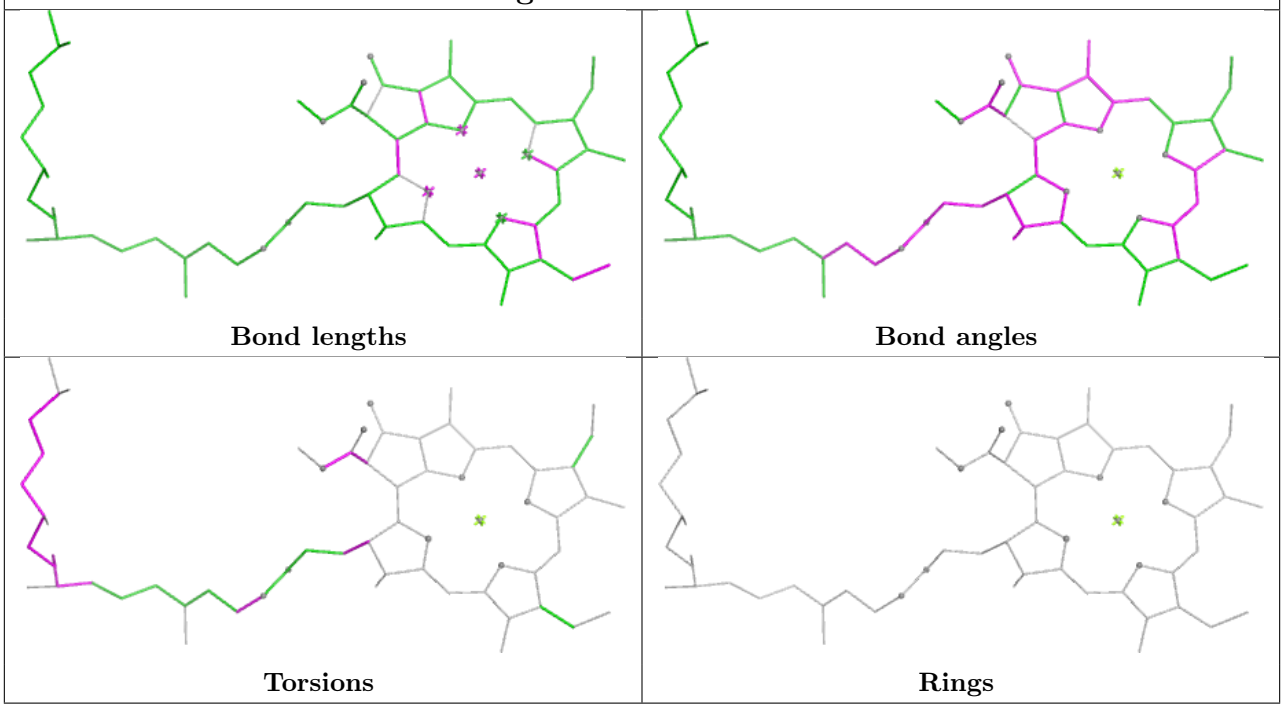

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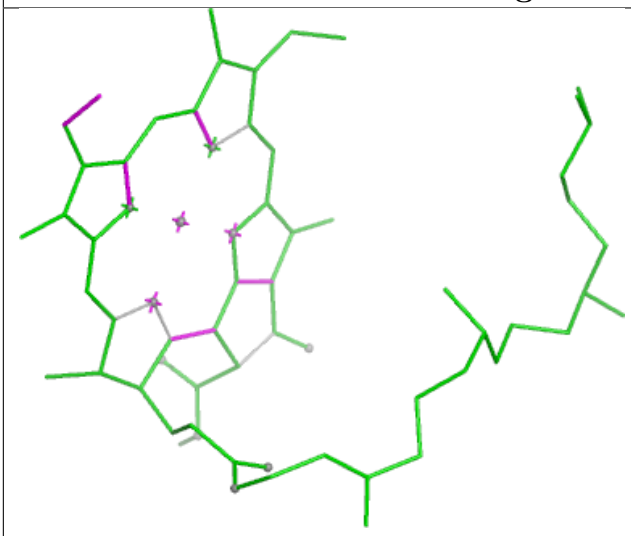

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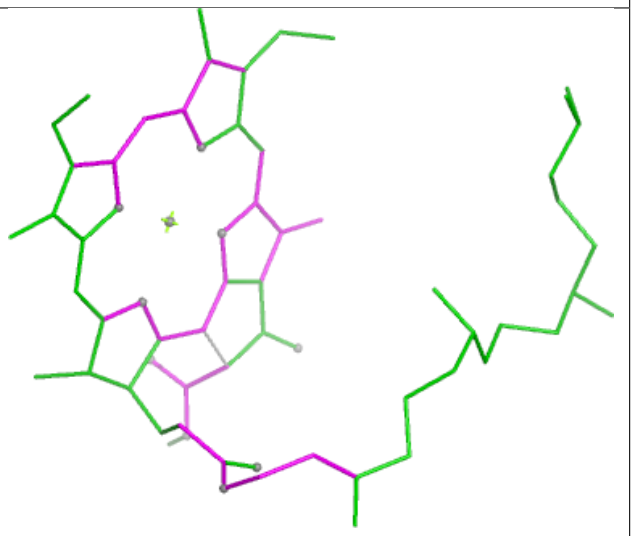
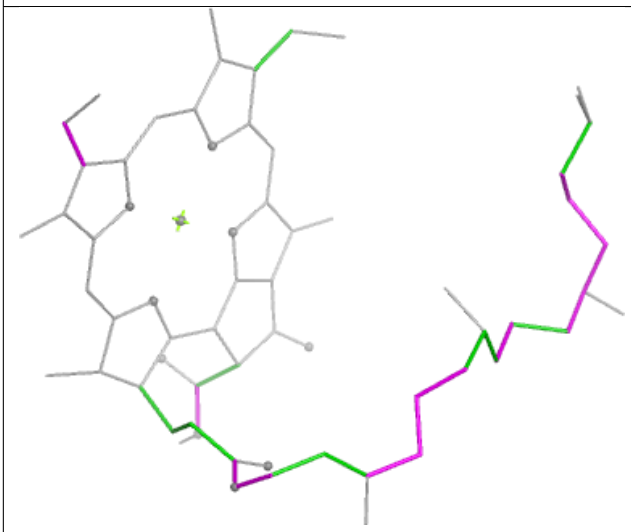


Bond angles



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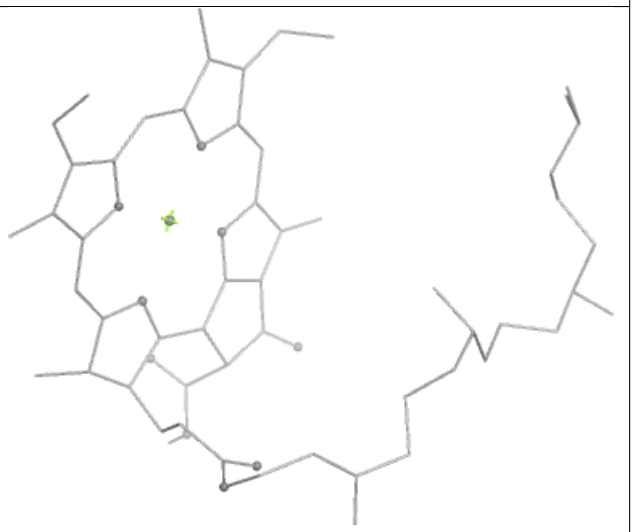
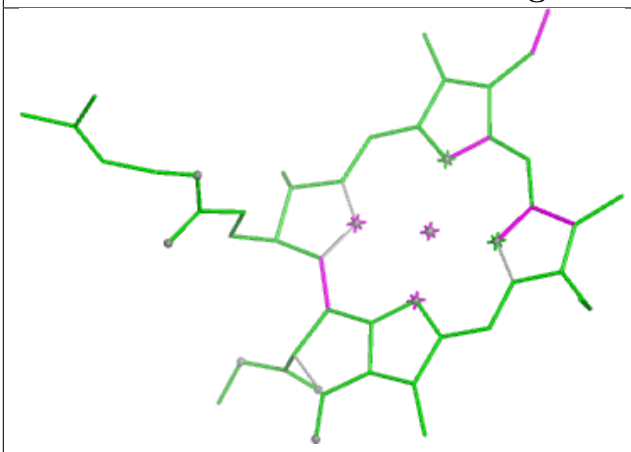


Rings

Ligand CLA 7 611



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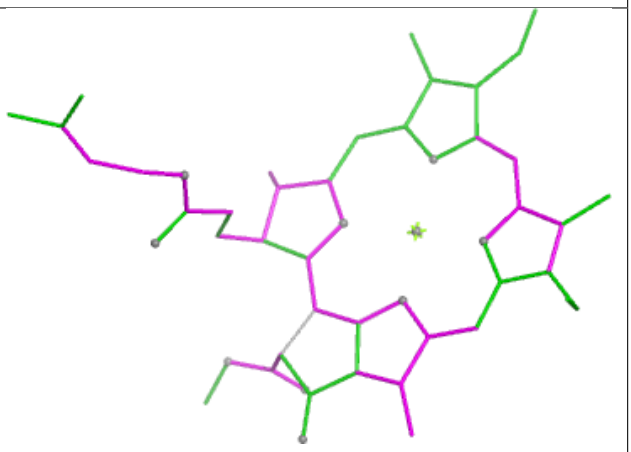

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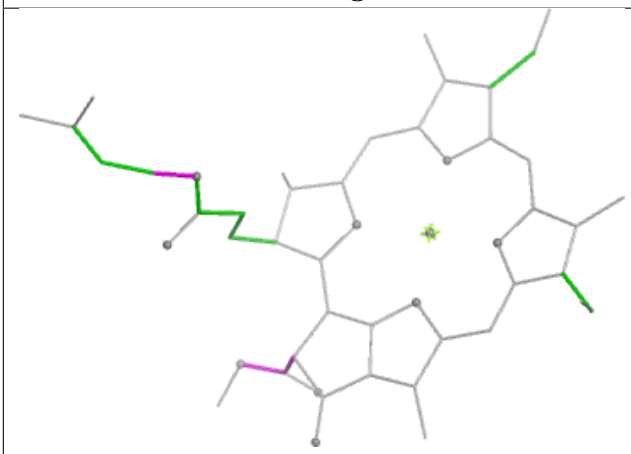

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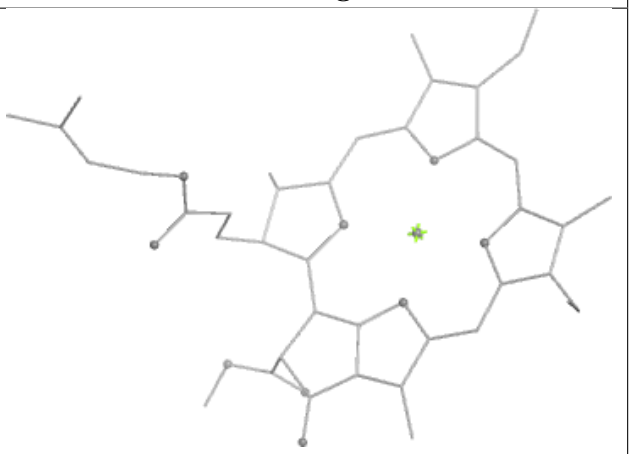
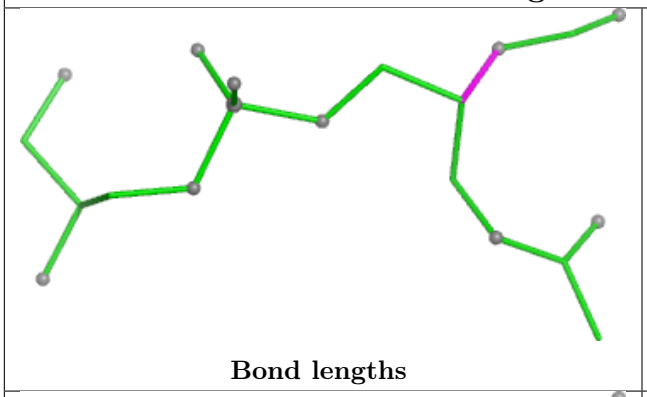


Rings

Ligand LHG 3 801



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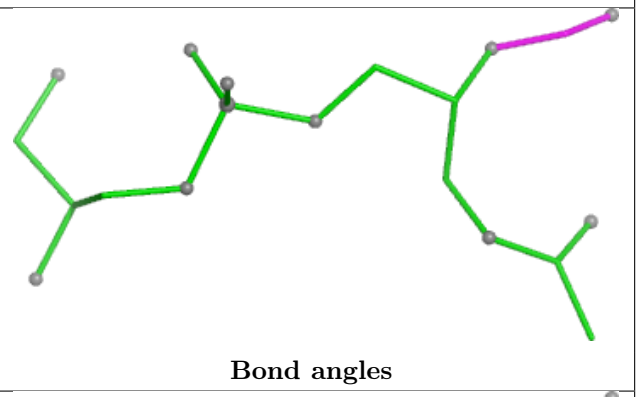
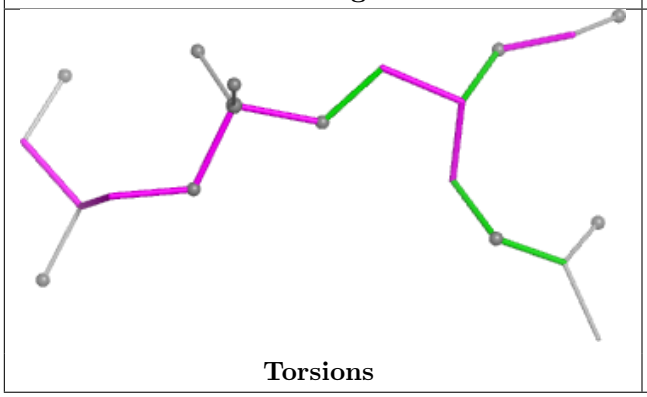


Bond angles



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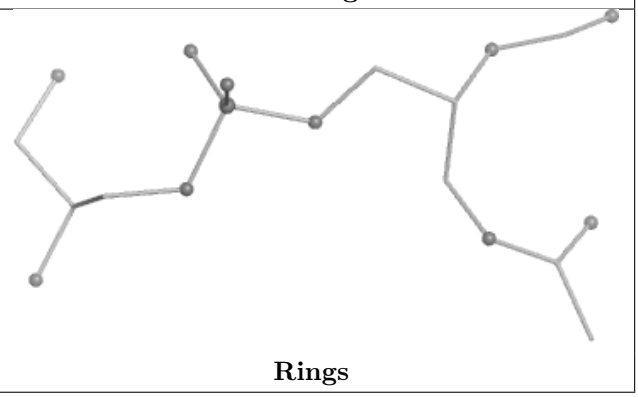
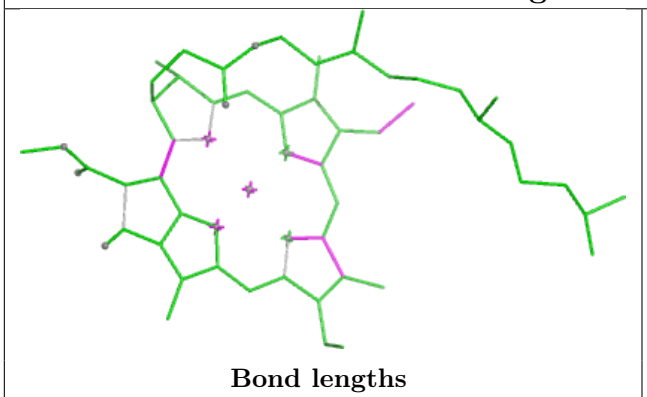


Rings

Ligand CLA 4 601



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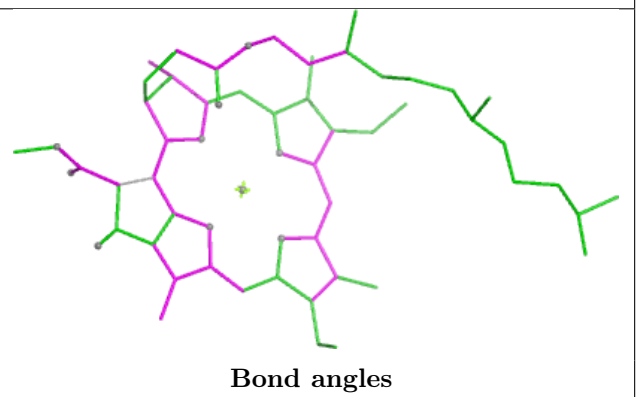

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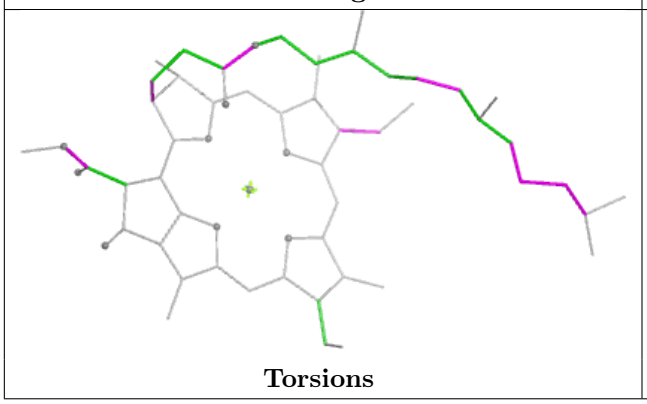

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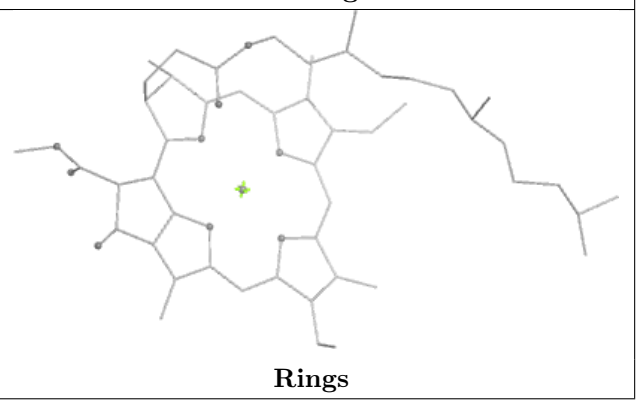
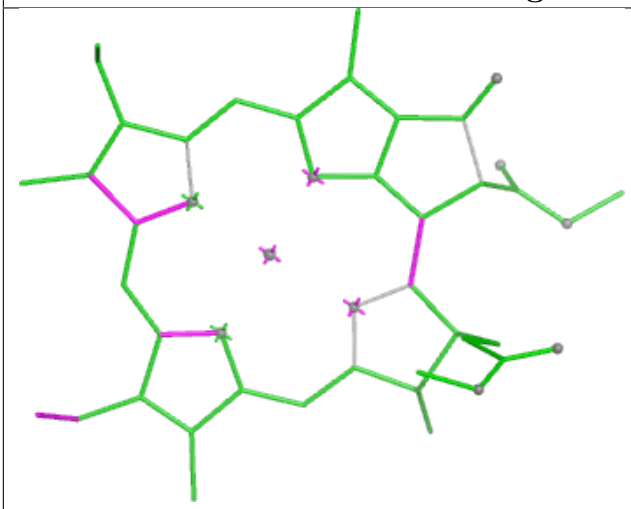


Rings

Ligand CLA Z 615



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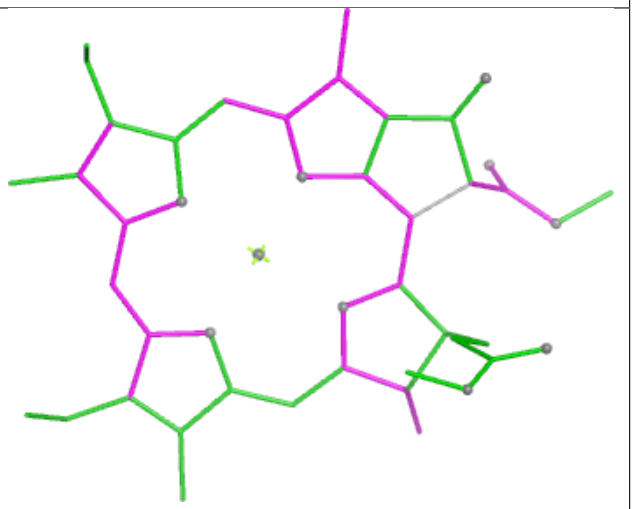
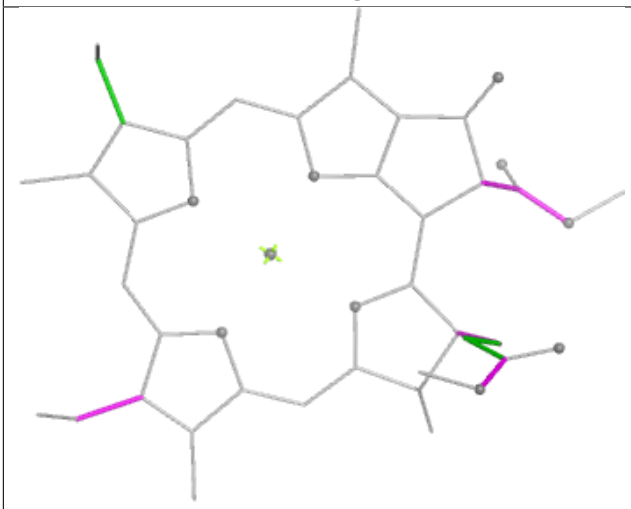
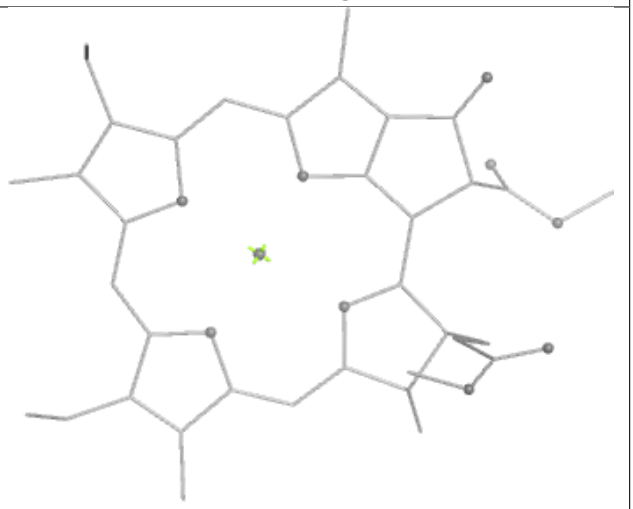


Bond angles

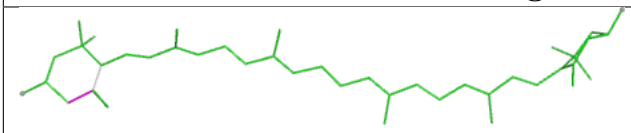


Torsions



Rings

Ligand LUT Z 502



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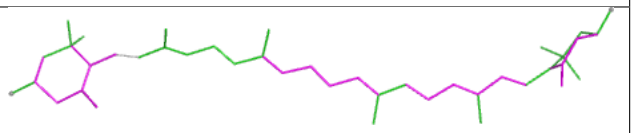
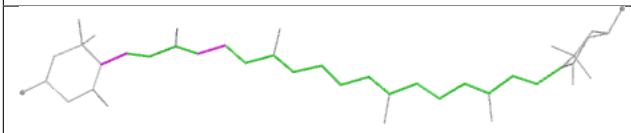


Bond angles



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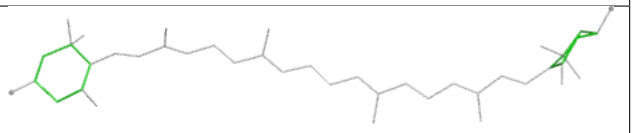
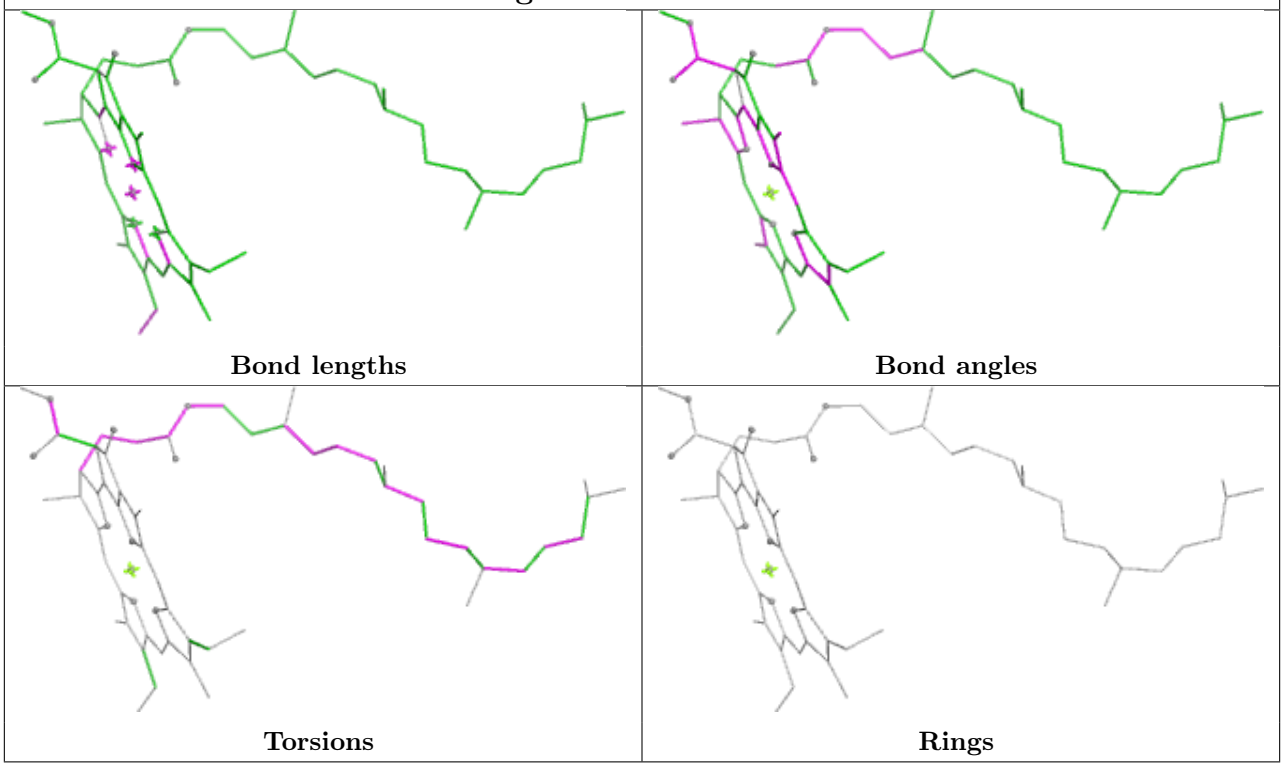


Rings

Ligand CLA A 1128



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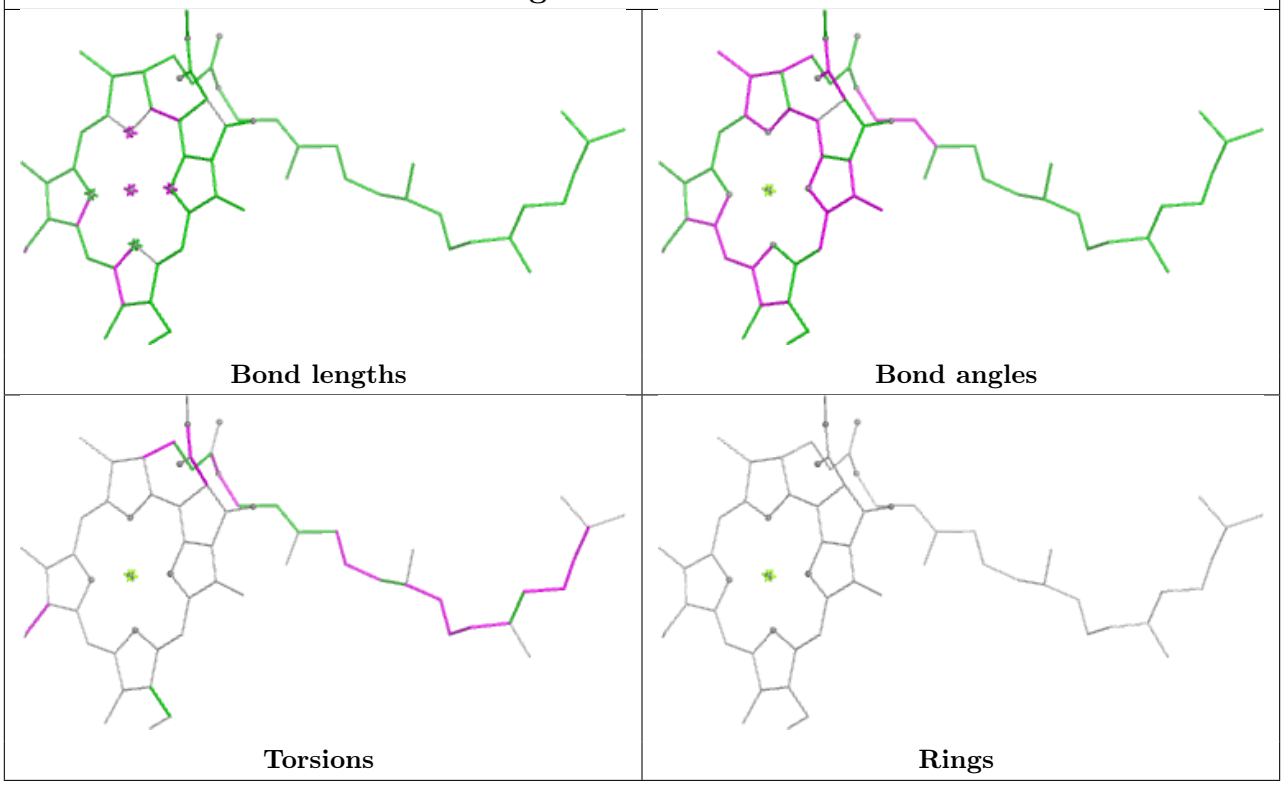

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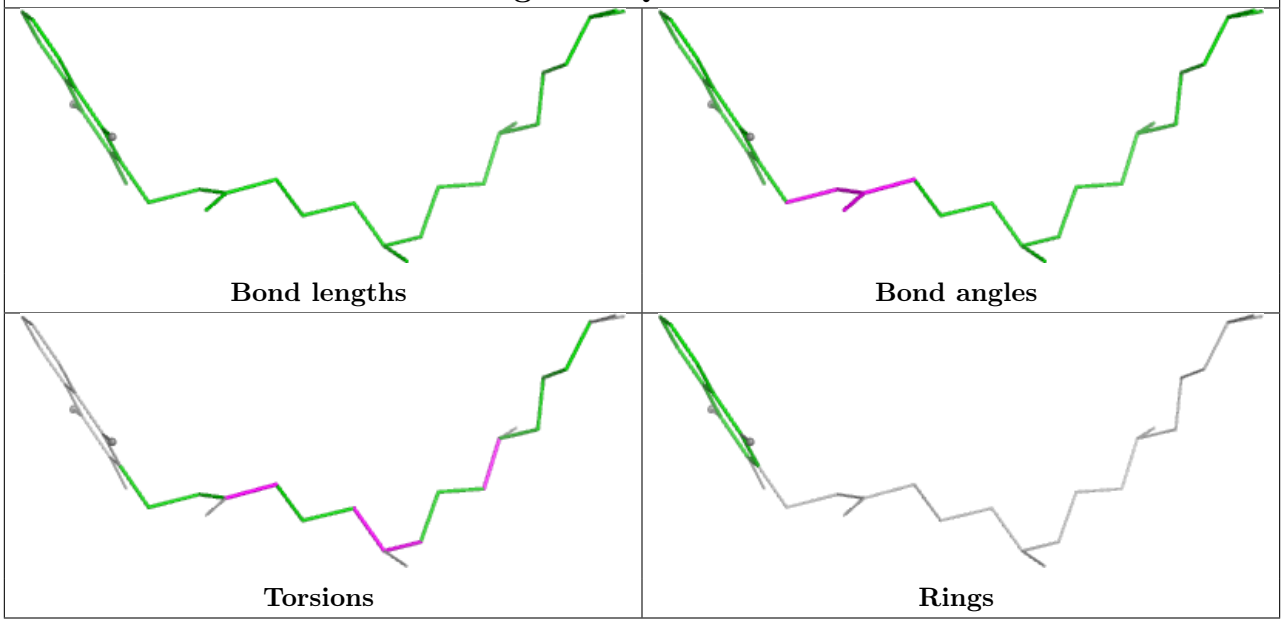

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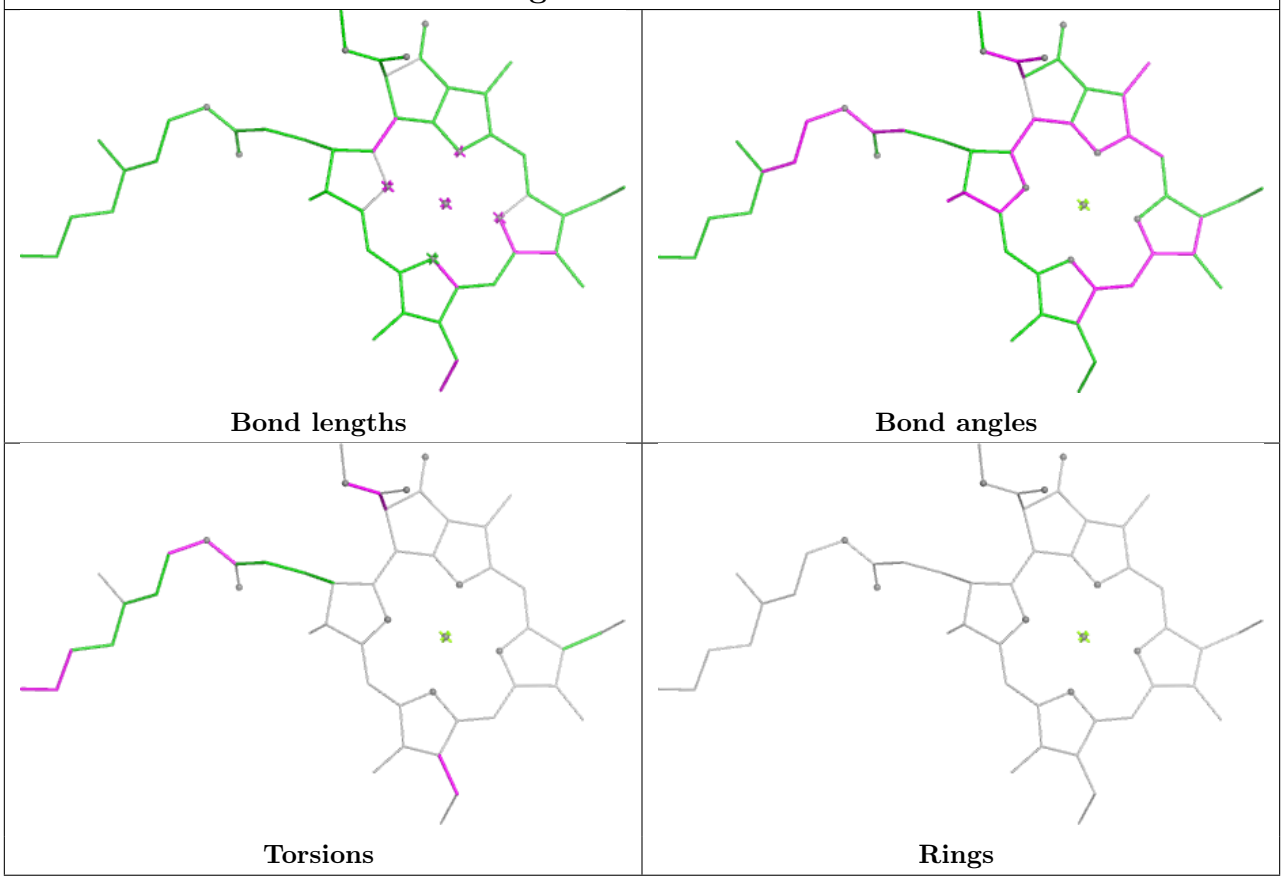

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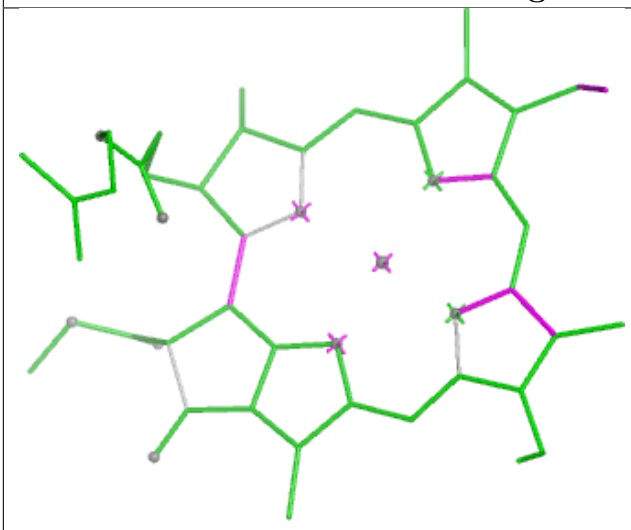

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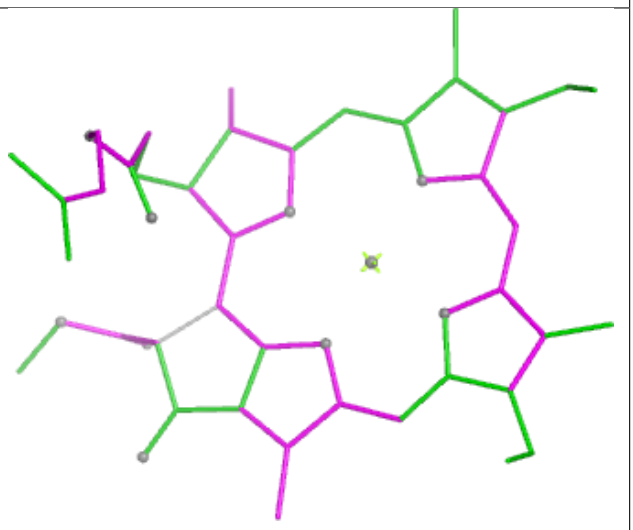
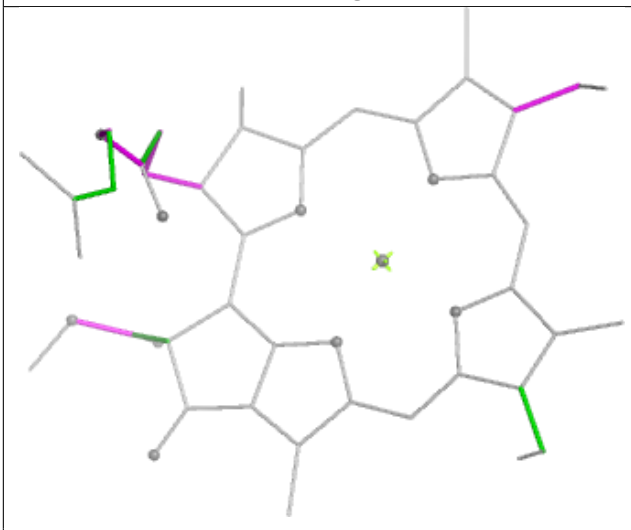


Bond angles



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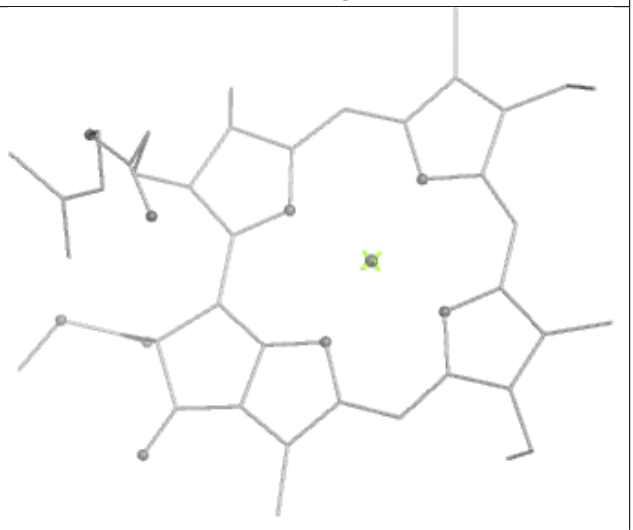

Rings

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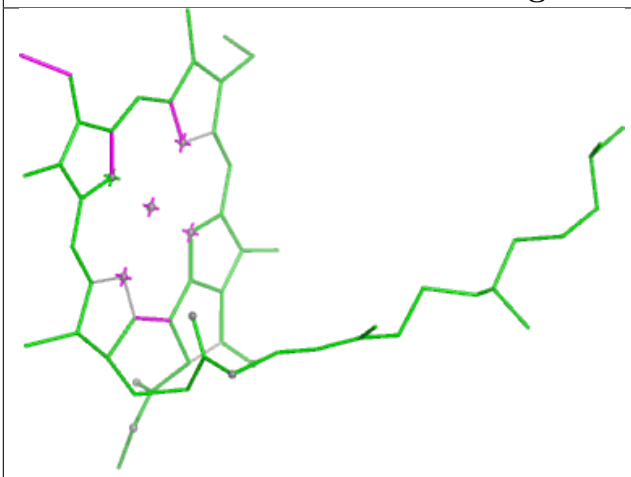

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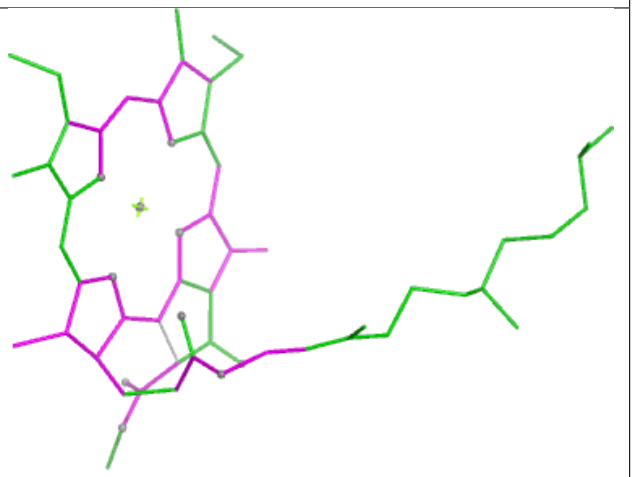

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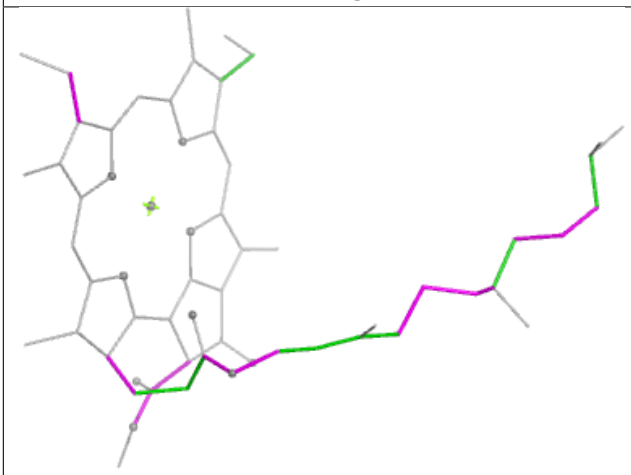

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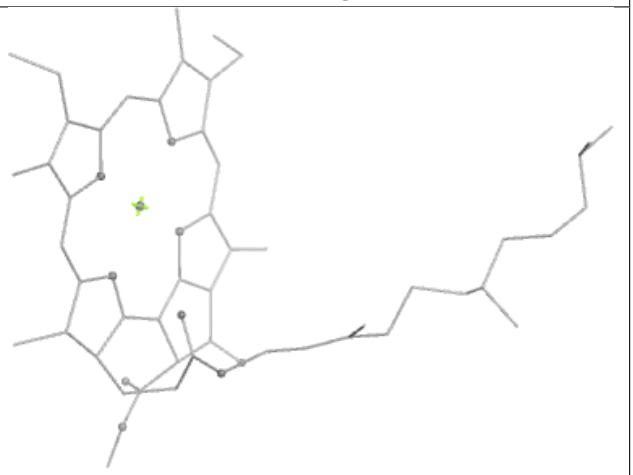

Rings

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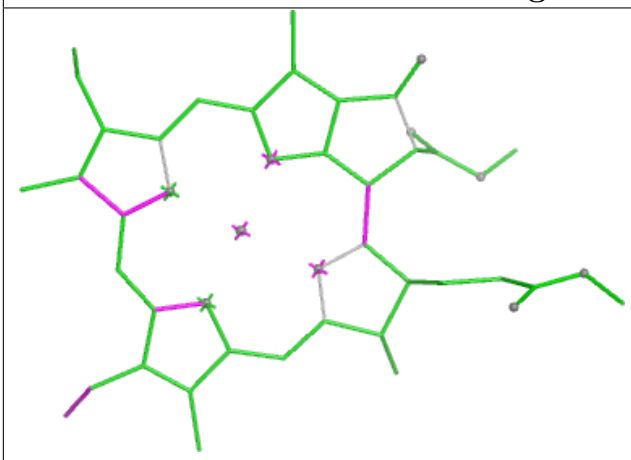

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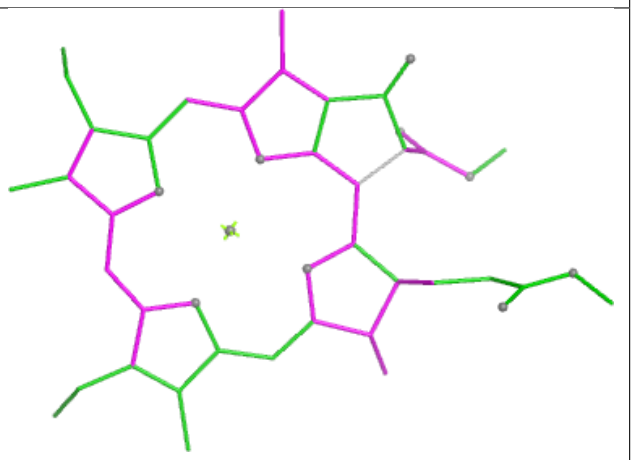

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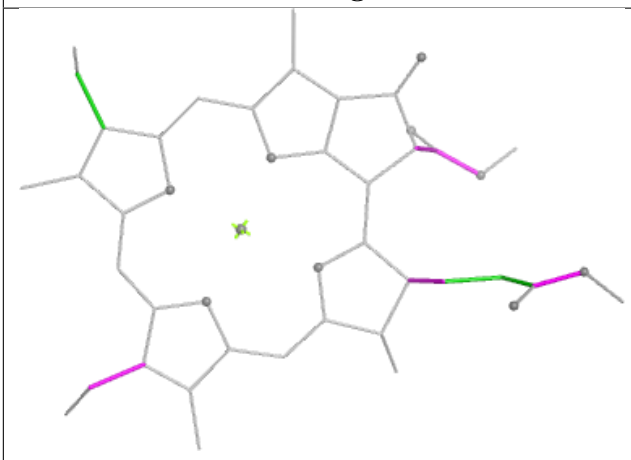

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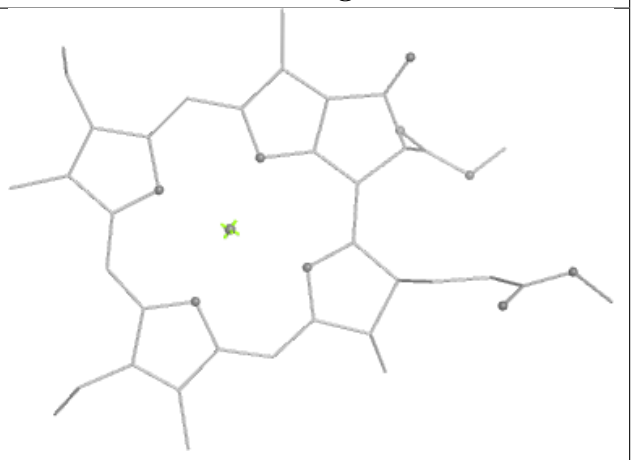

Rings

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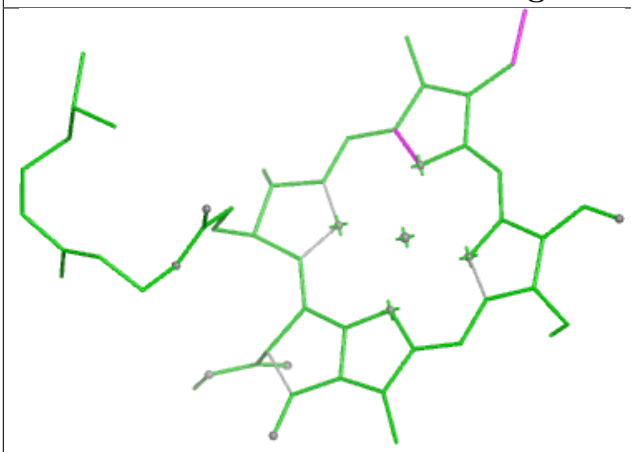

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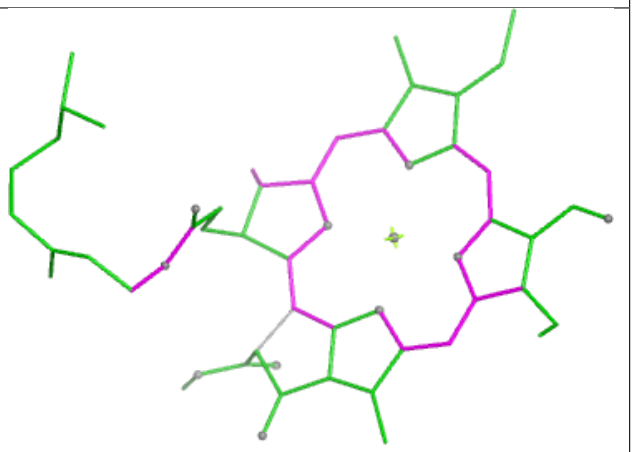

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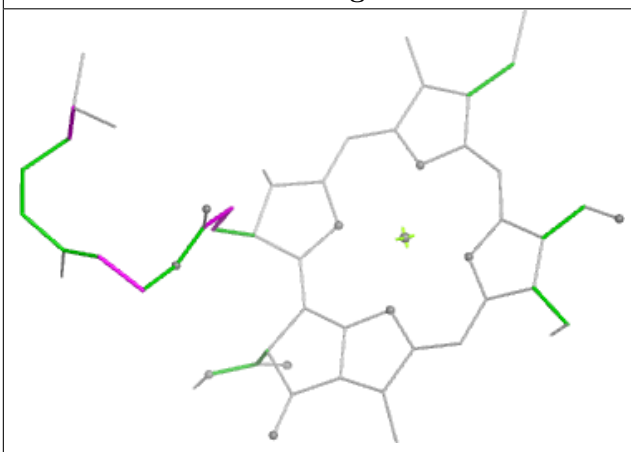

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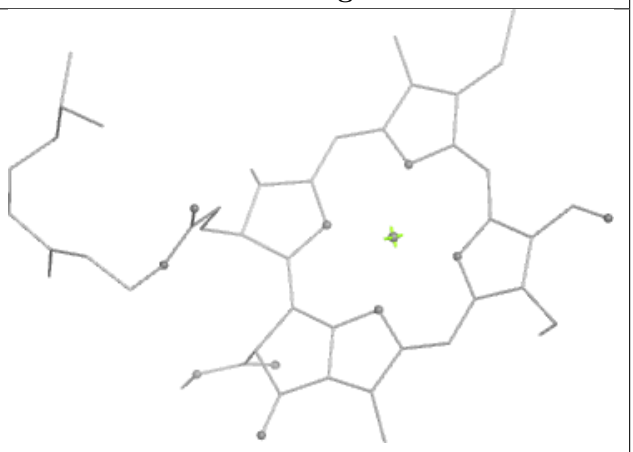

Rings

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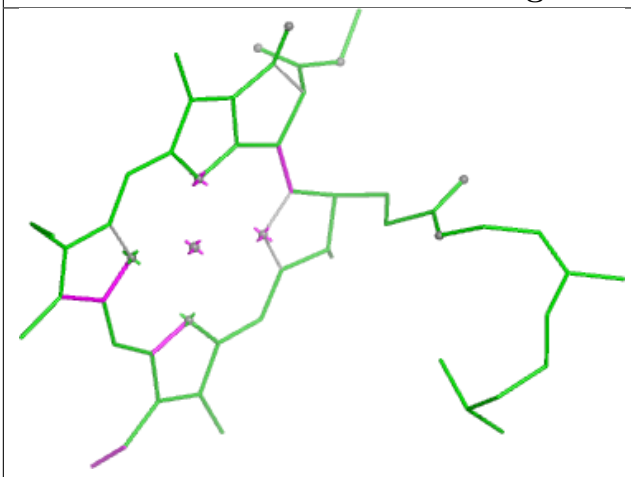

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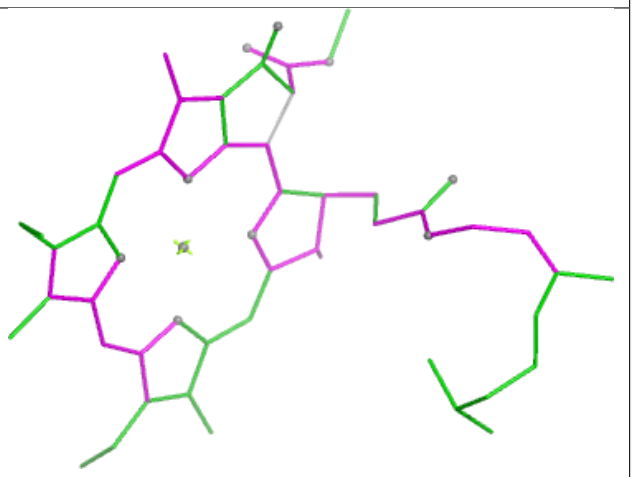

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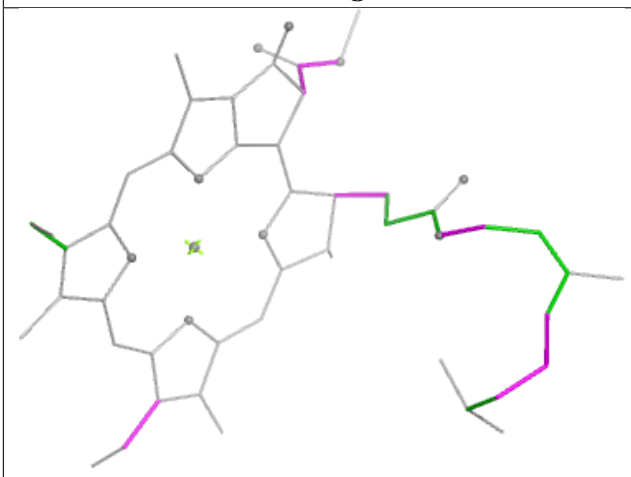

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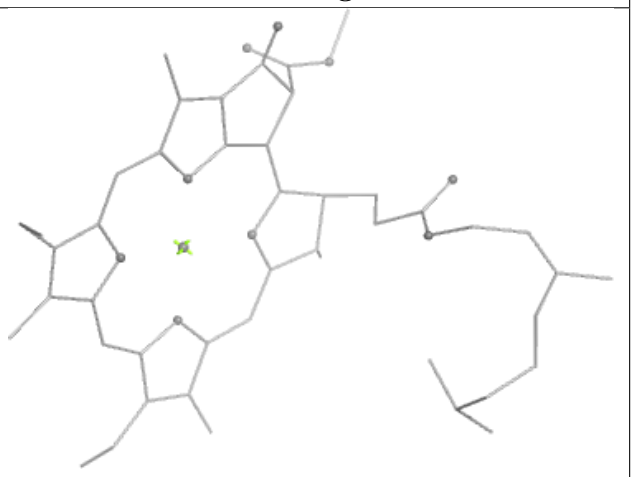

Rings

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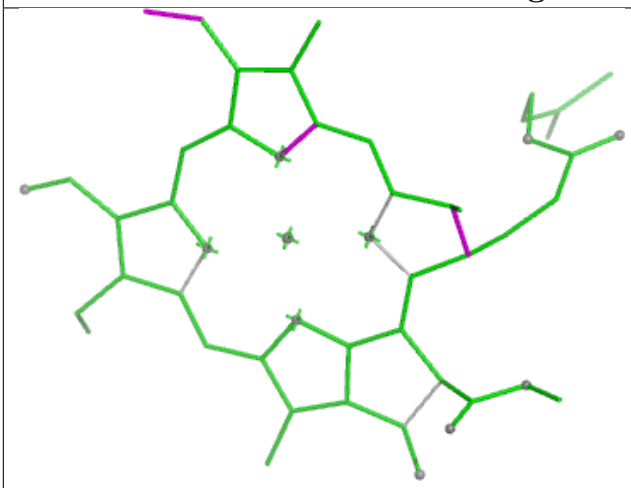

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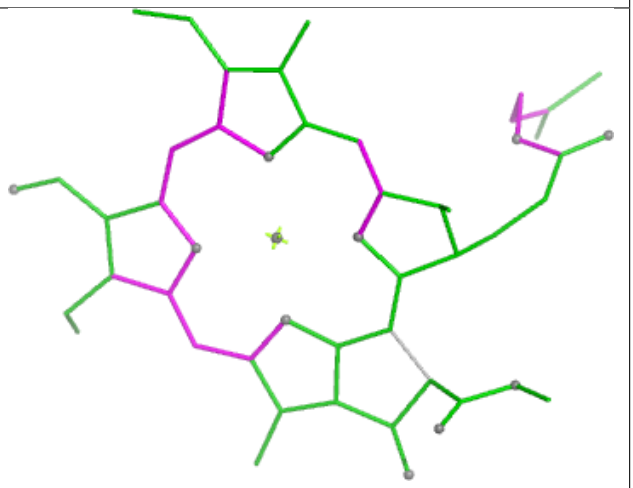

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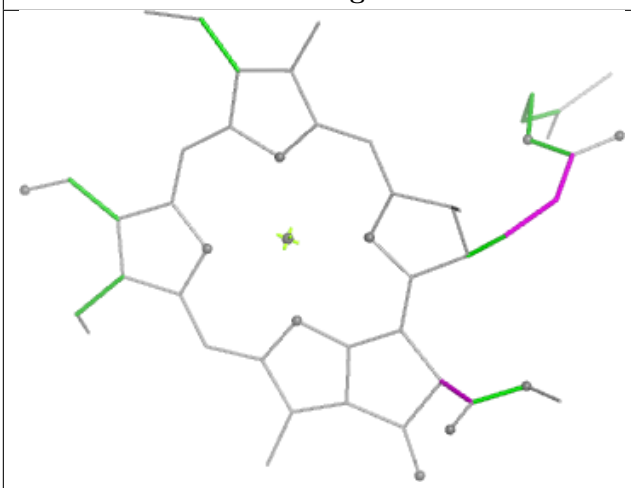

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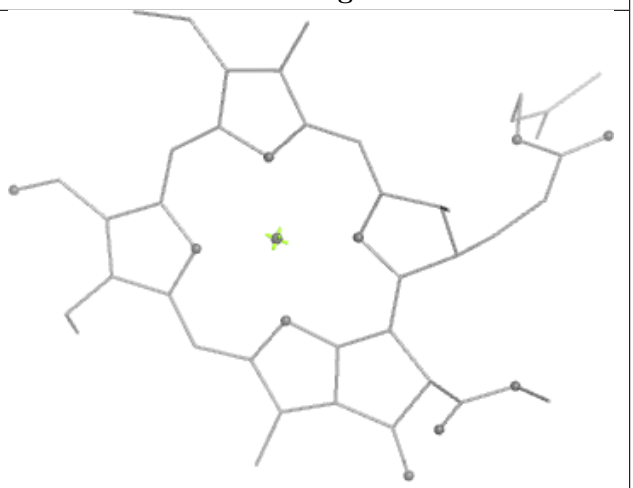

Rings

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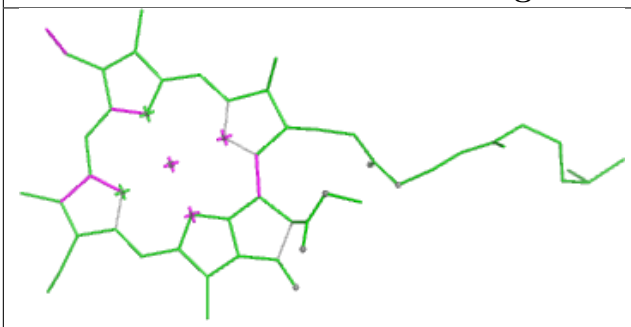

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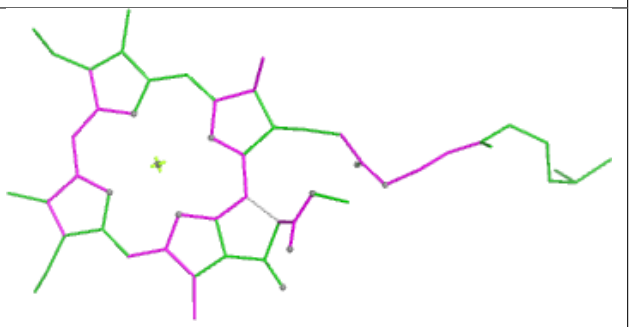

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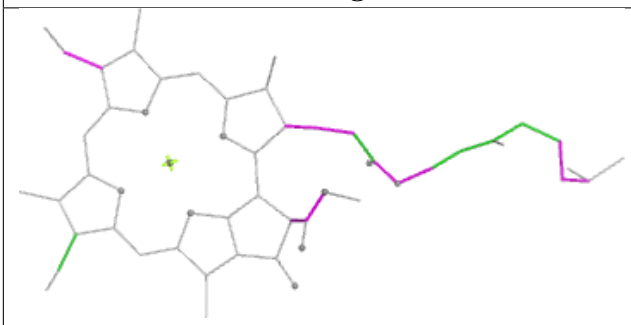

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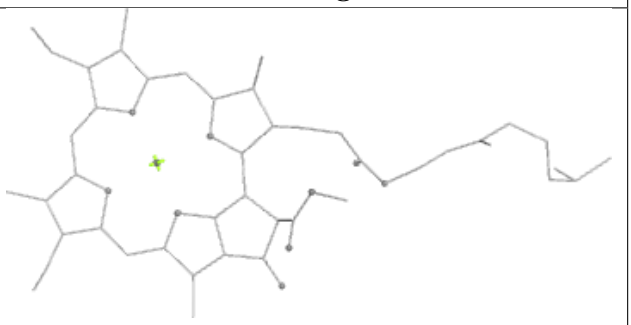
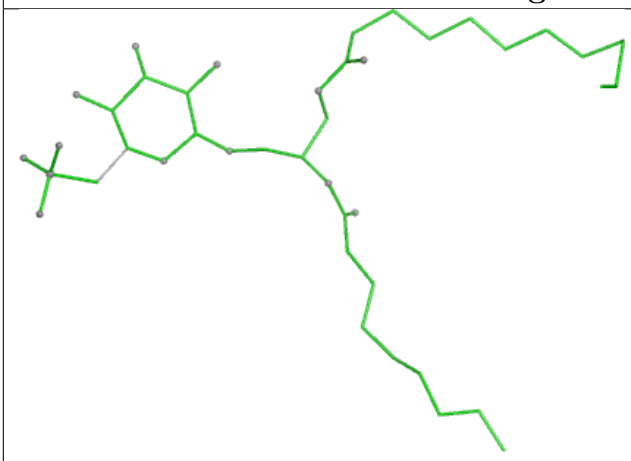


Rings

Ligand SQD 2 803



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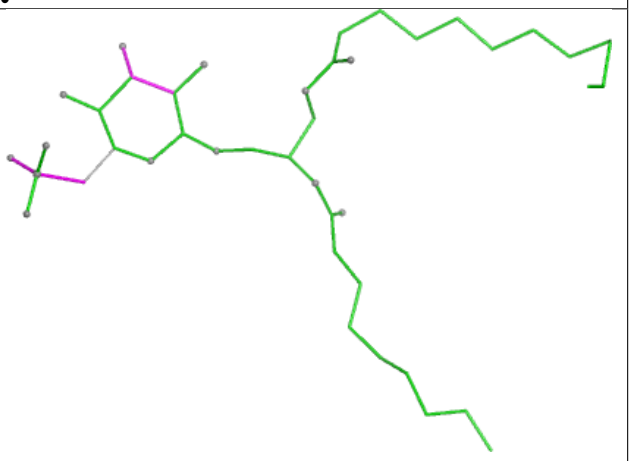

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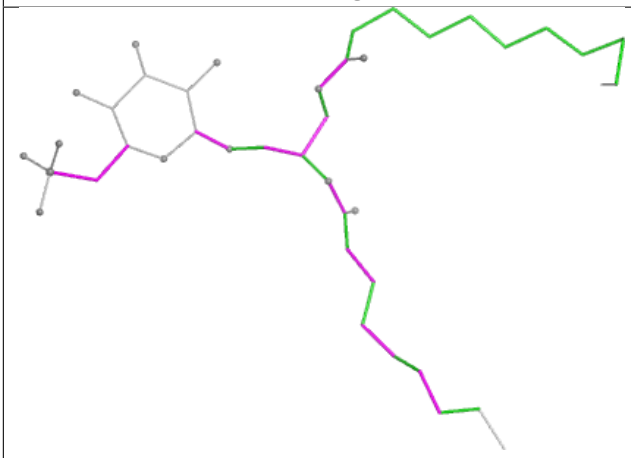

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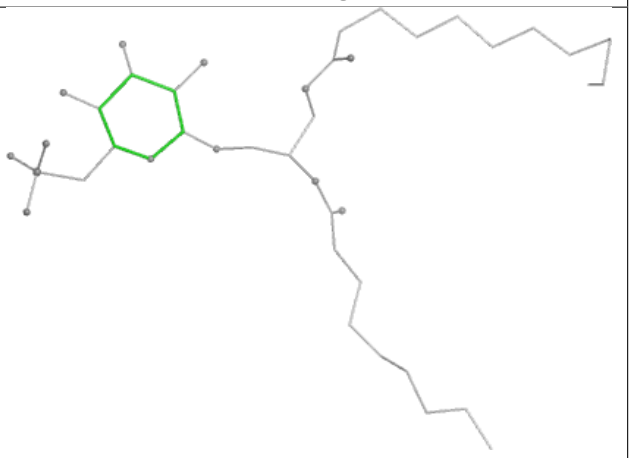
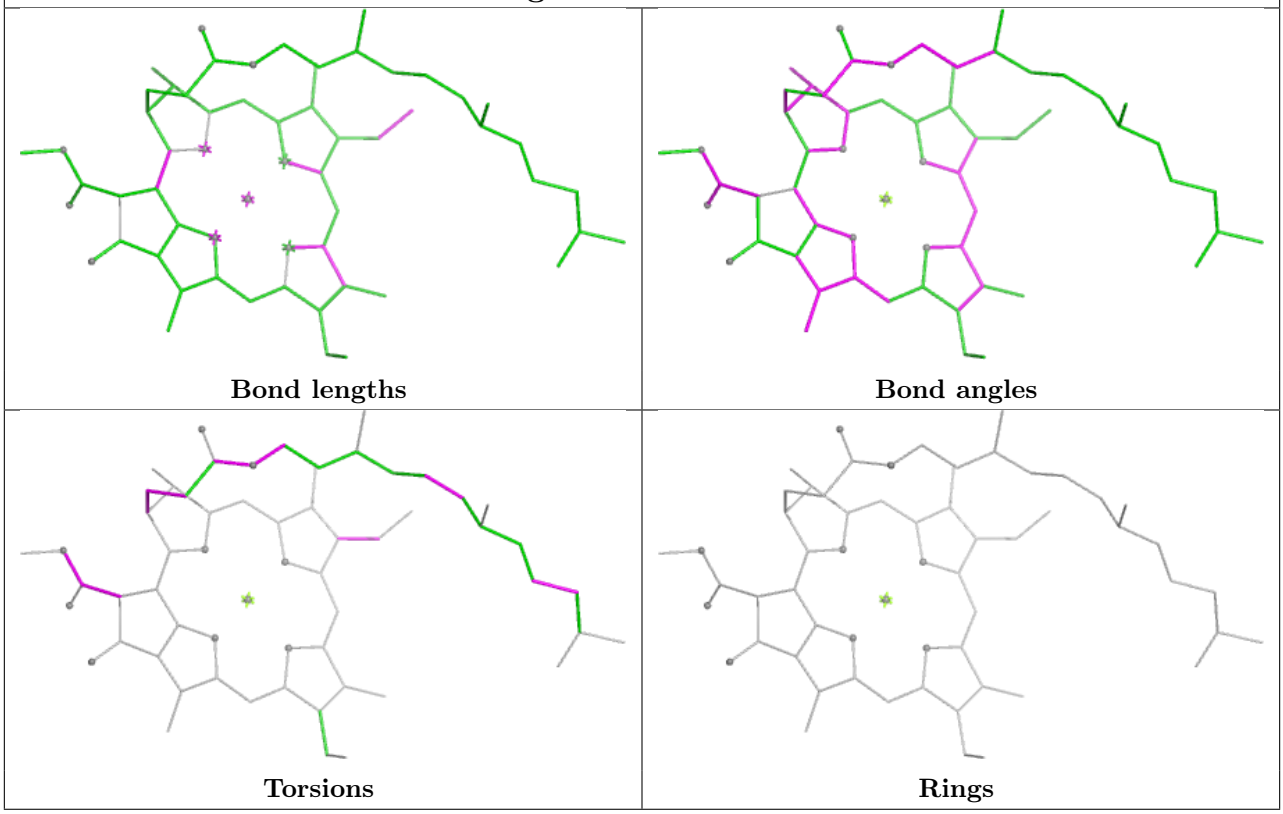


Rings

Ligand CLA Z 601



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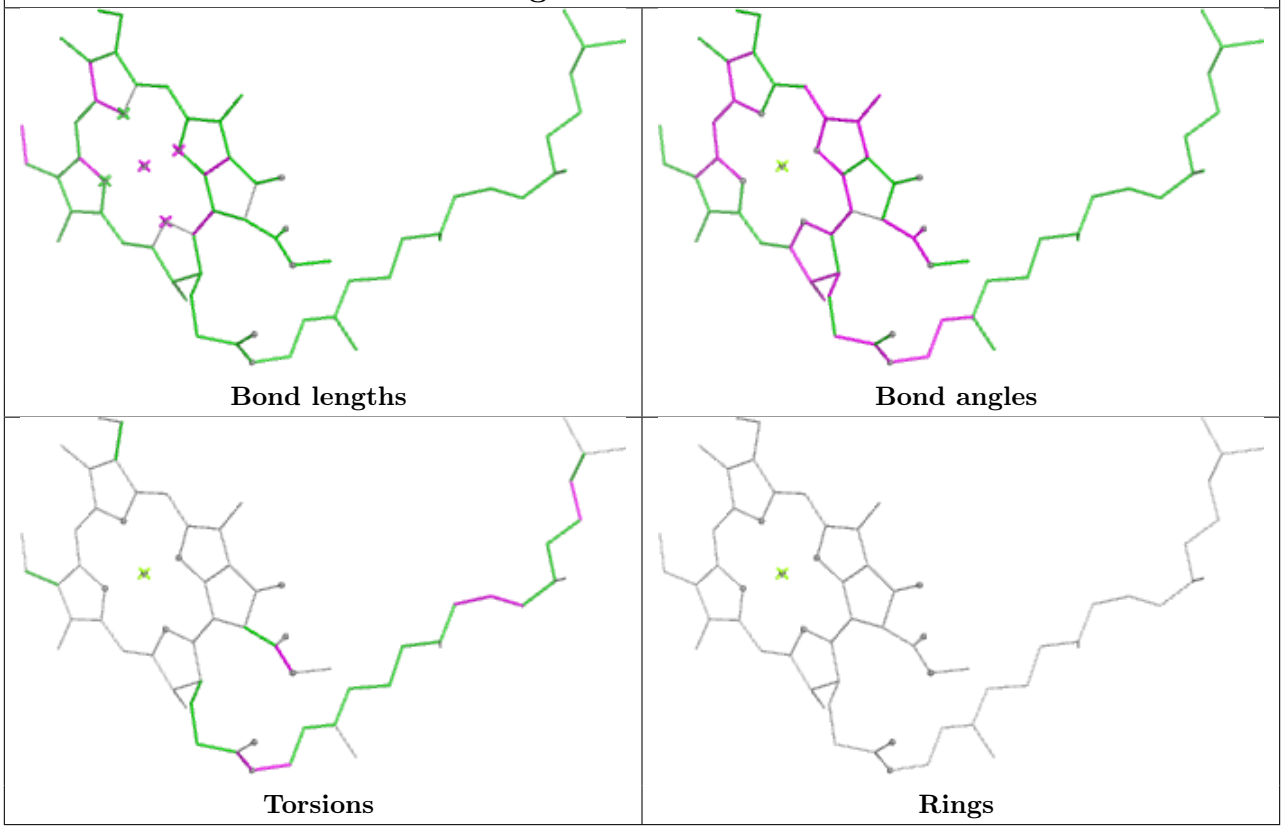

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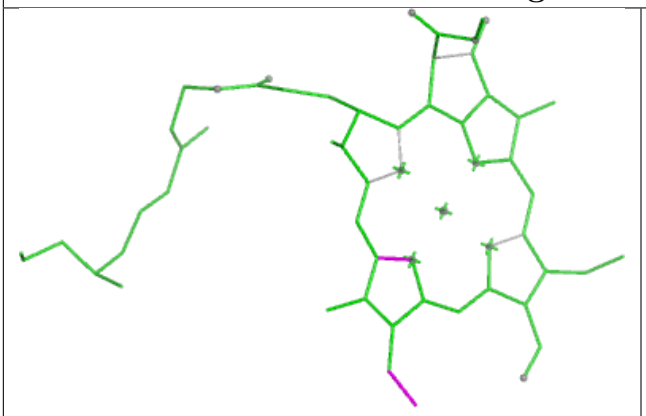

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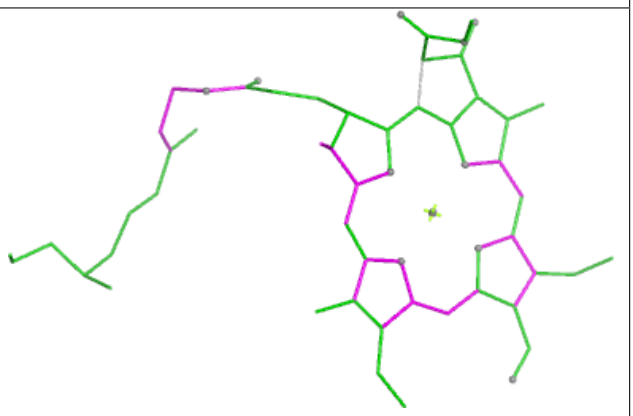

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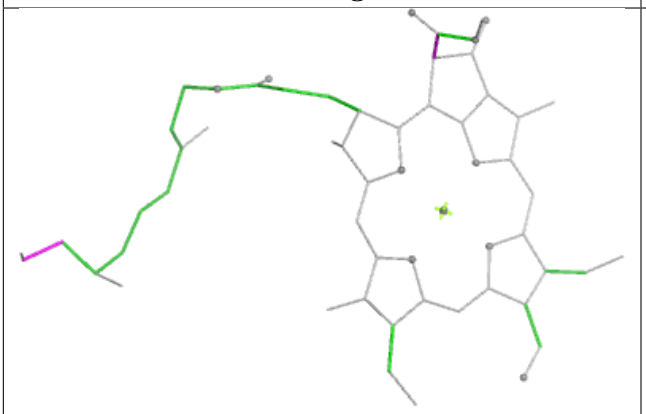

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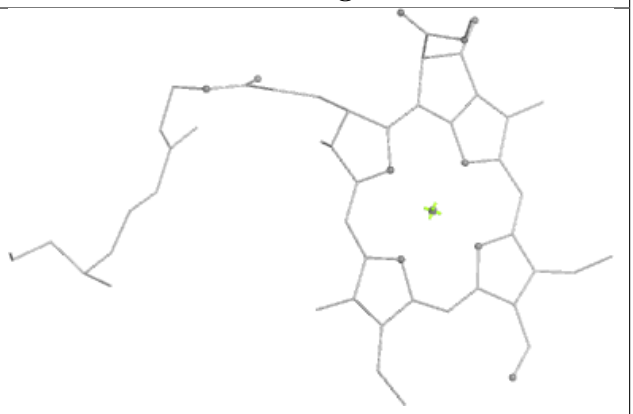

Rings

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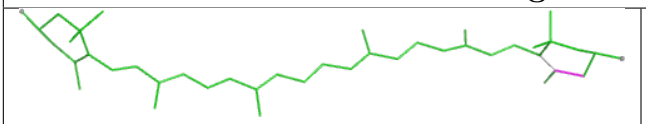

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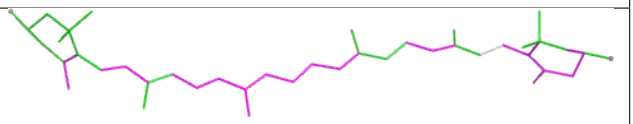

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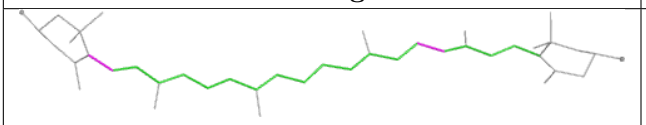

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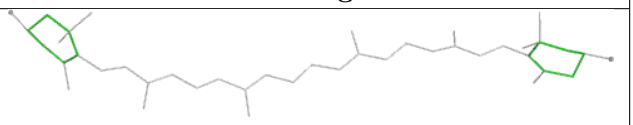
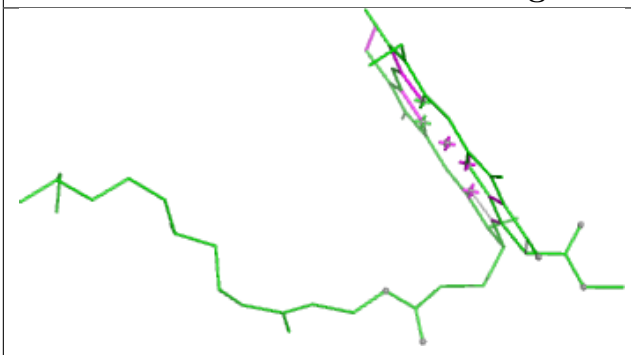


Rings

Ligand CLA 1 606



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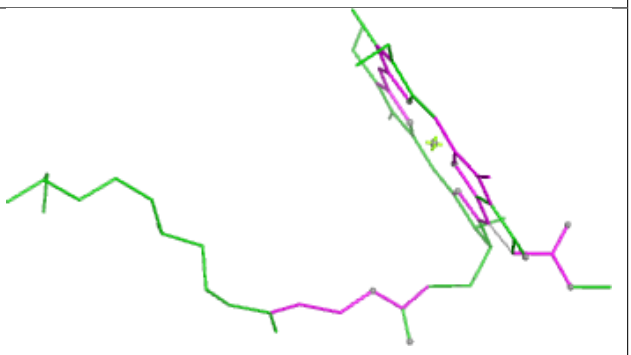

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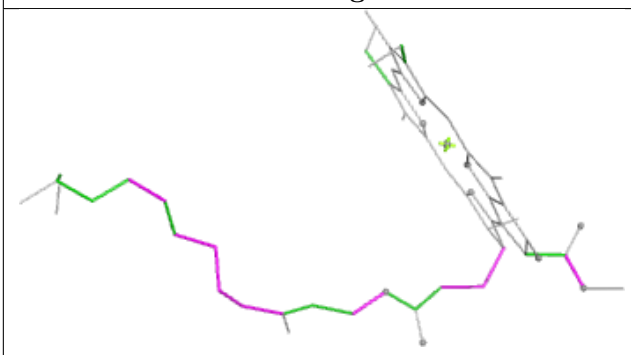

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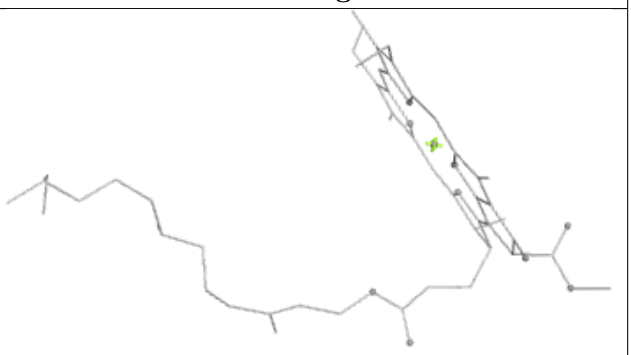
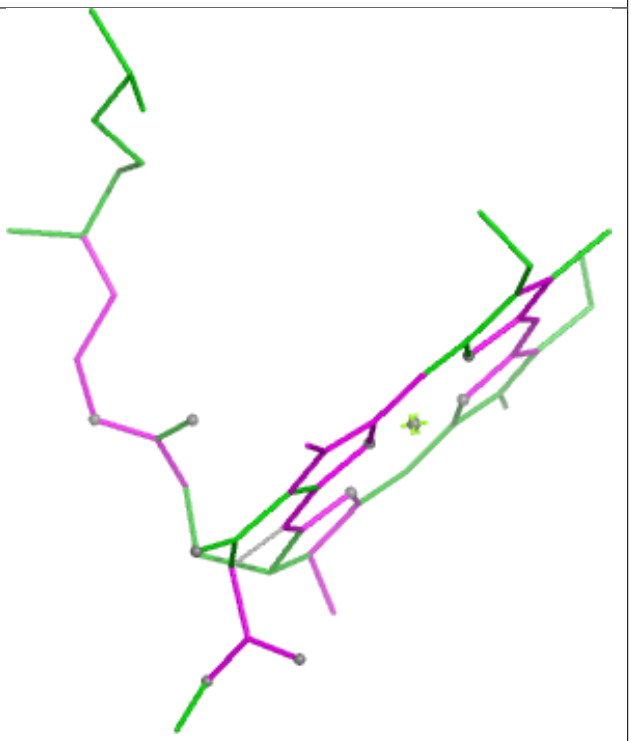


Rings

Ligand CLA 4 608



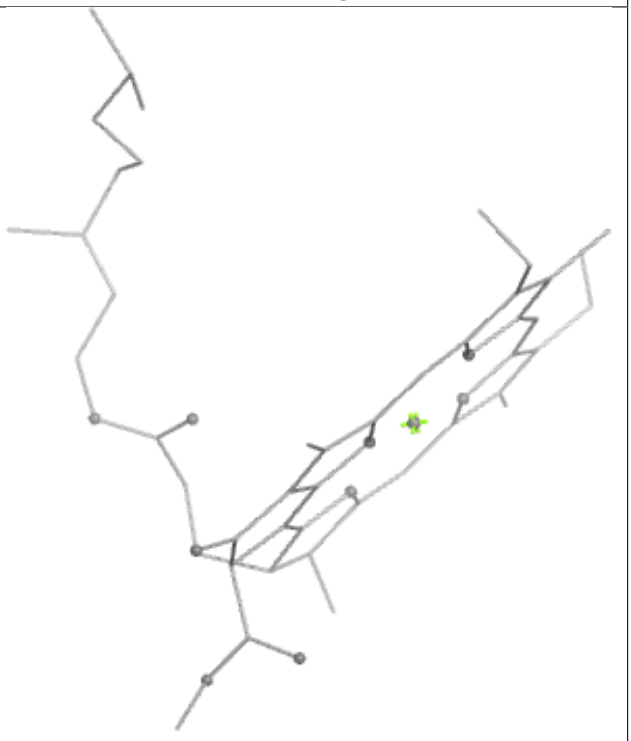
Bond lengths



Bond angles



Torsions



Rings

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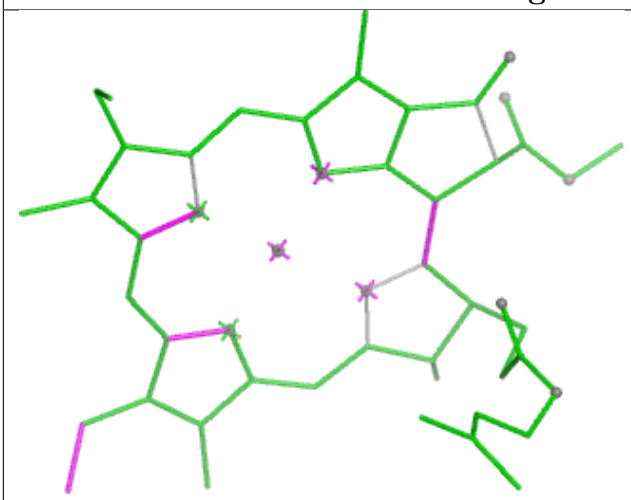
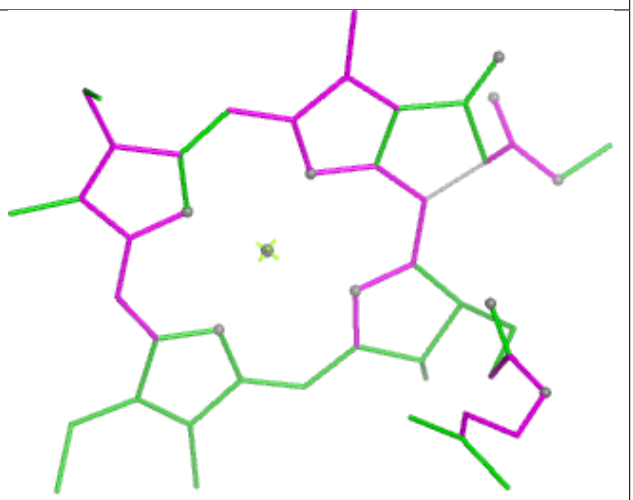
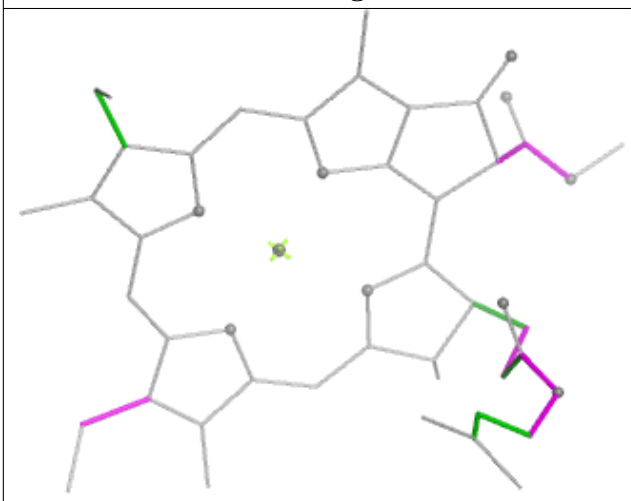


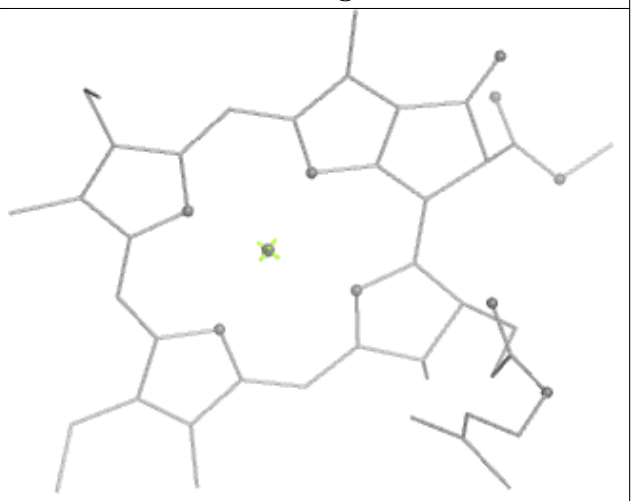
Bond lengths



Bond angles



Torsions

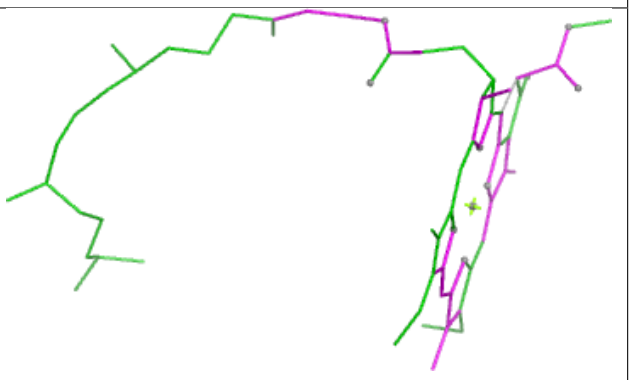


Rings

Ligand CLA A 1105



Bond lengths



Bond angles

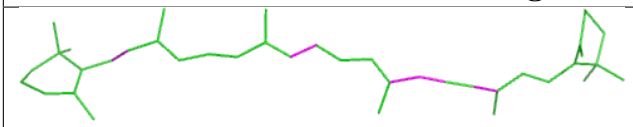


Torsions



Rings

Ligand BCR 3 504



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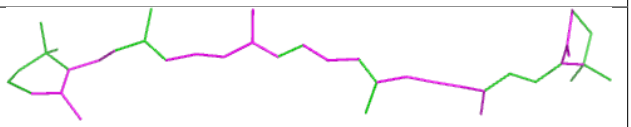
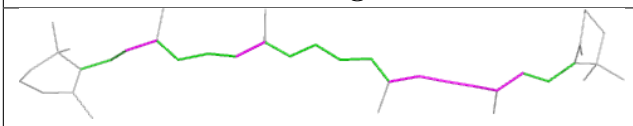


Bond angles



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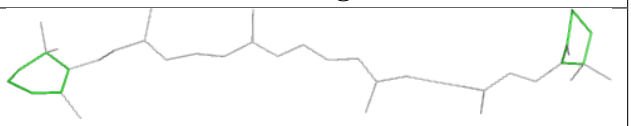
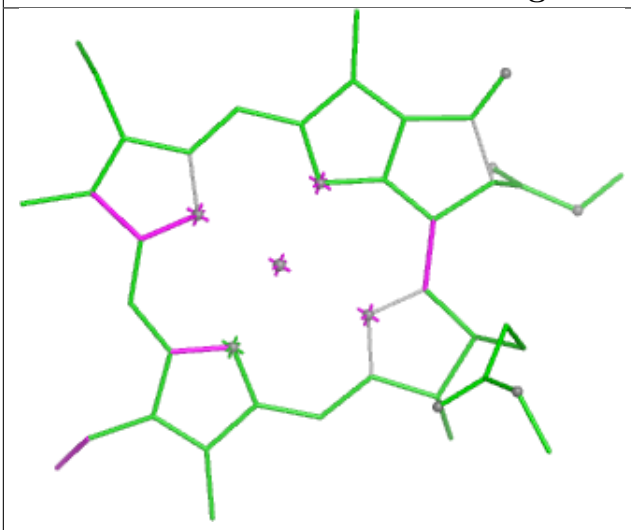


Rings

Ligand CLA 3 618



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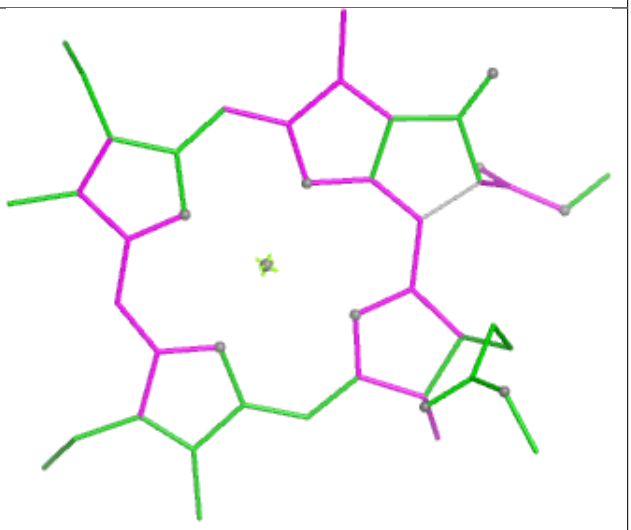
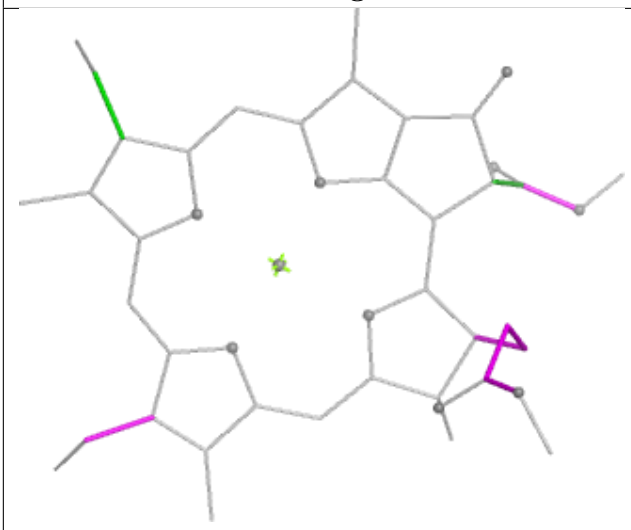


Bond angles



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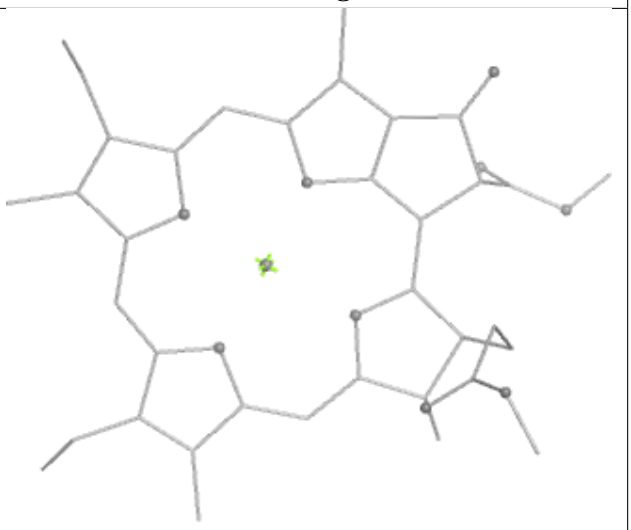
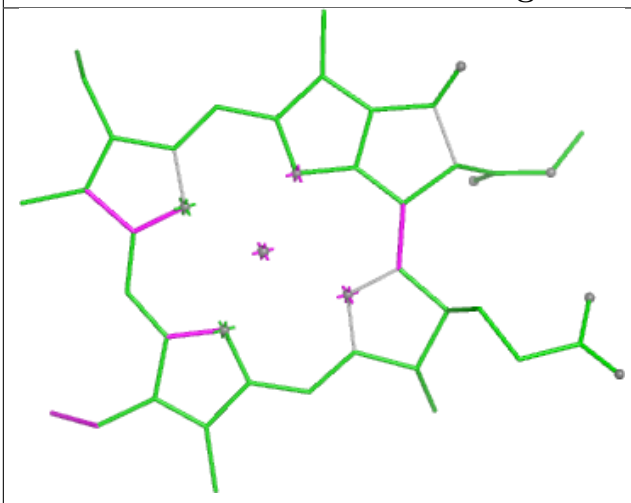


Rings

Ligand CLA F 1302



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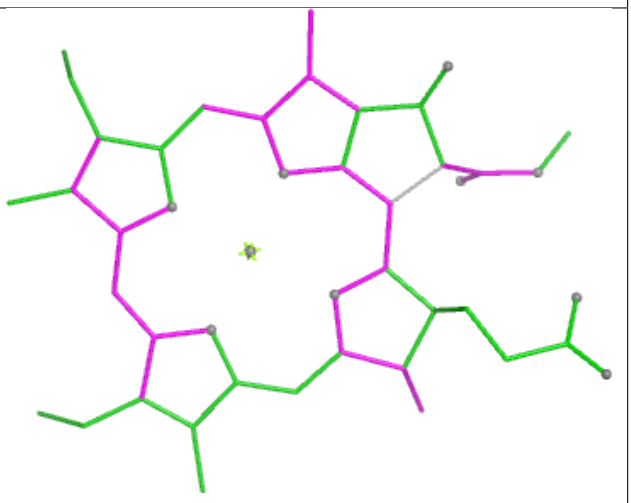
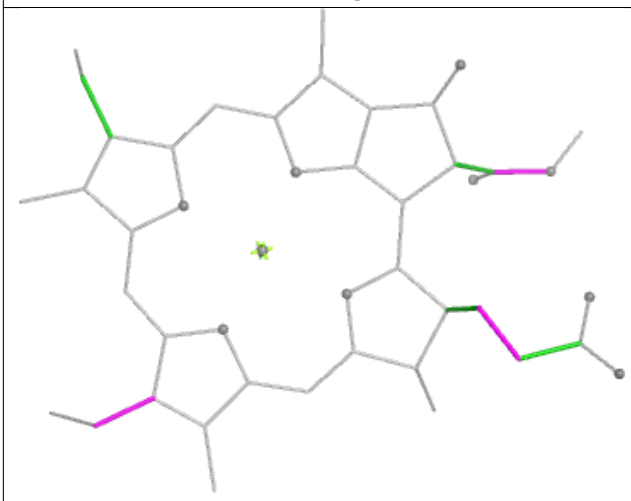


Bond angles



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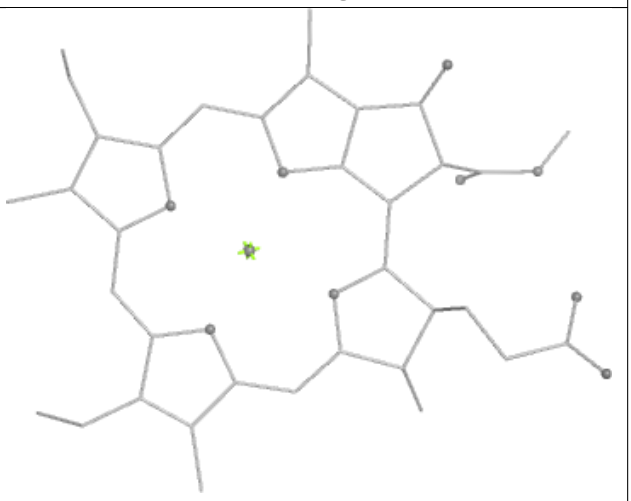
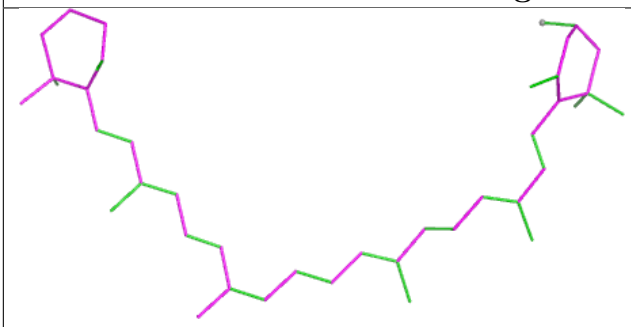


Rings

Ligand RRX F 4001



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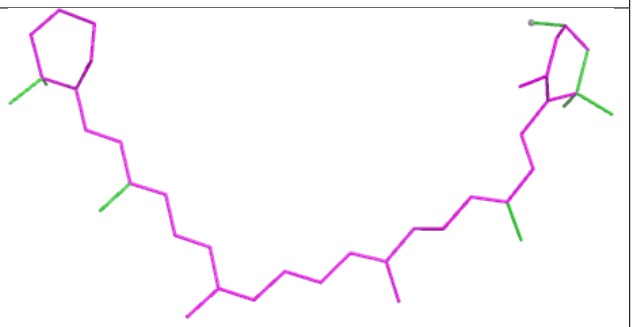
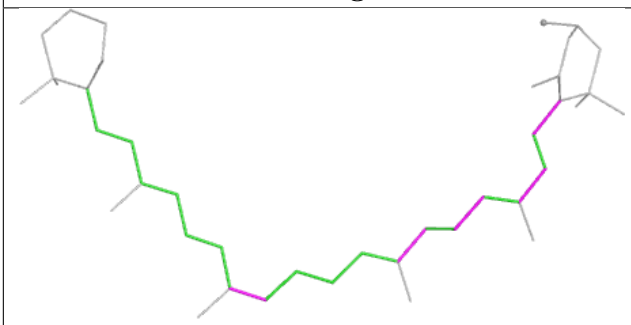


Bond angles



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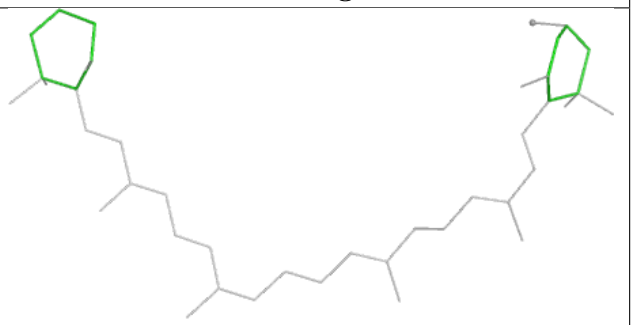
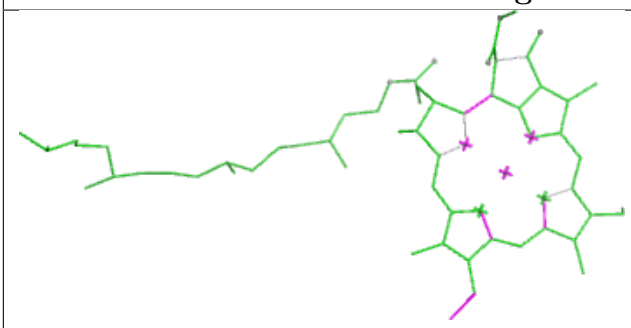


Rings

Ligand CLA A 1113



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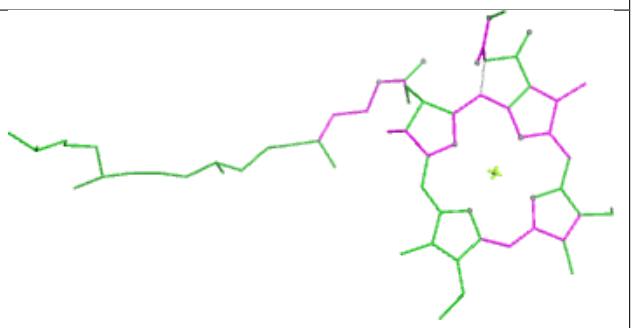

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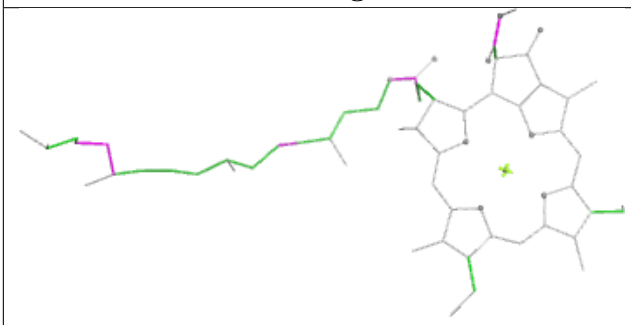

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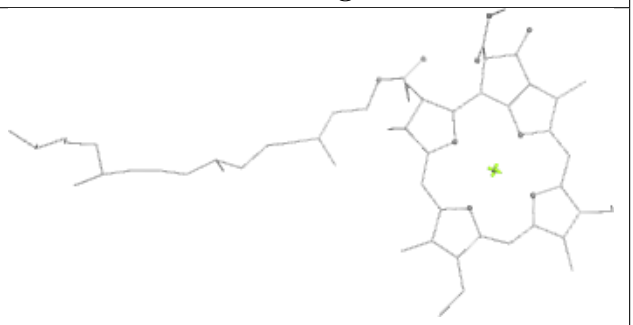
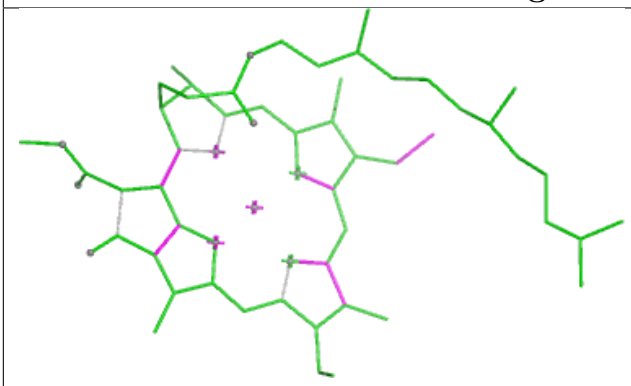


Rings

Ligand CLA 7 601



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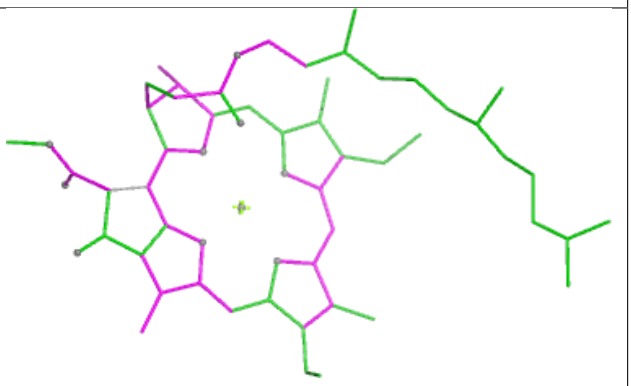

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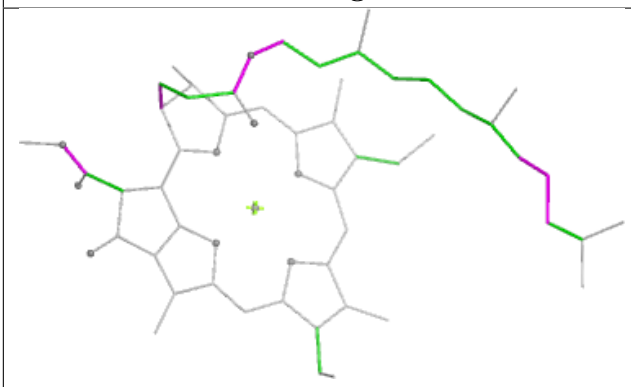

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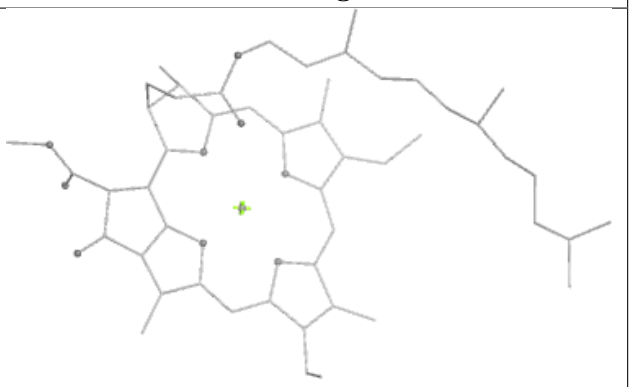
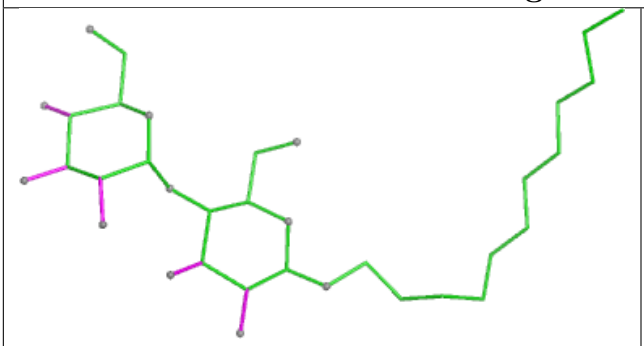


Rings

Ligand LMT 4 803



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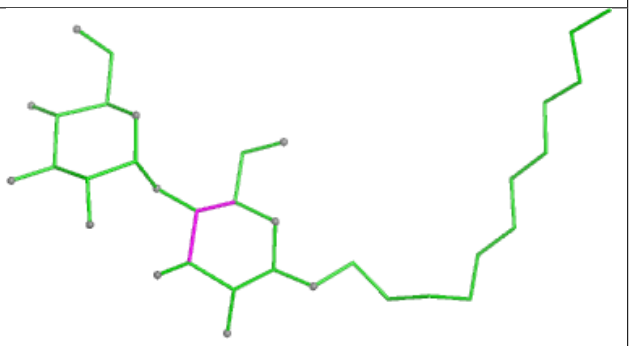

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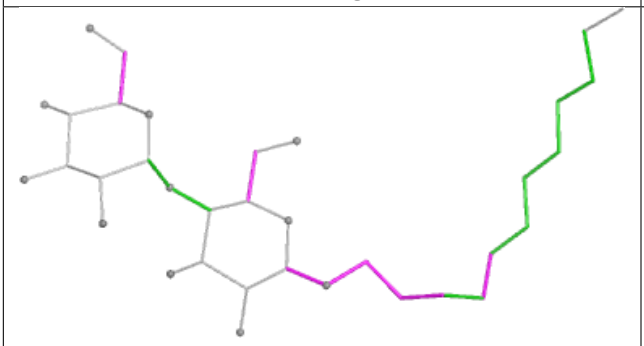

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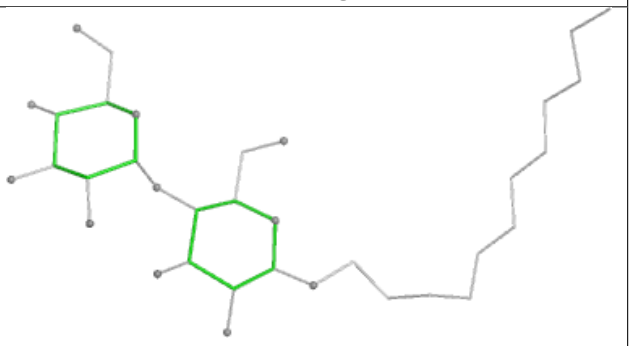
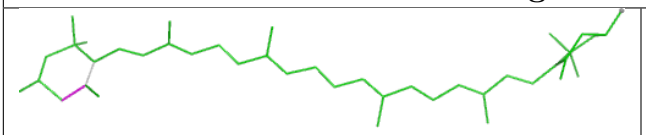


Rings

Ligand LUT 9 502



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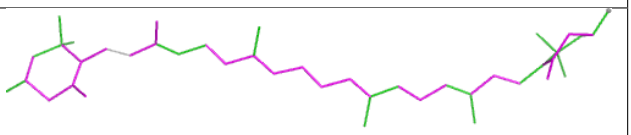
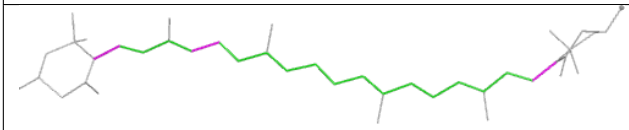


Bond angles



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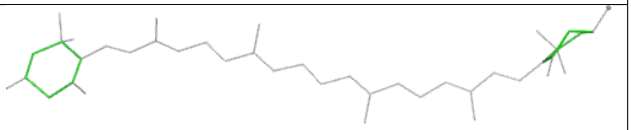
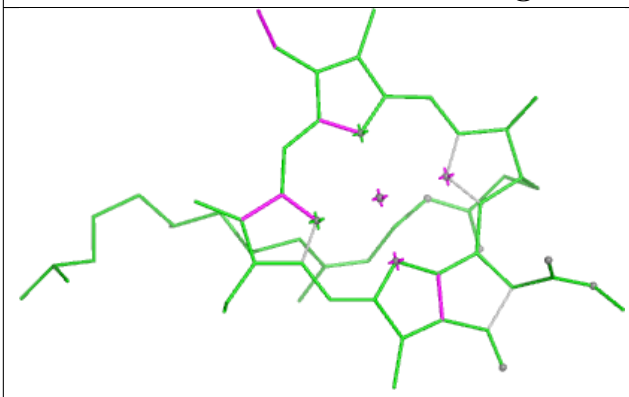


Rings

Ligand CLA A 1115



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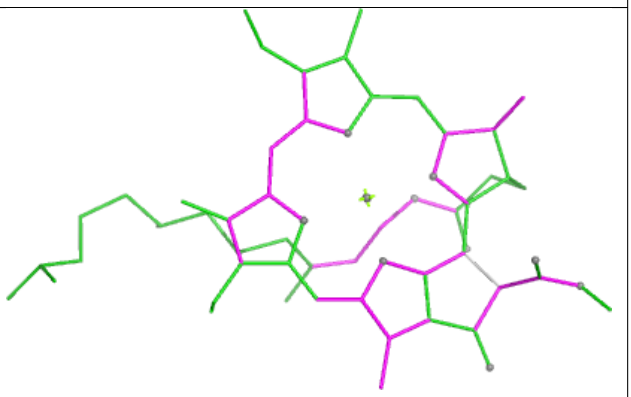

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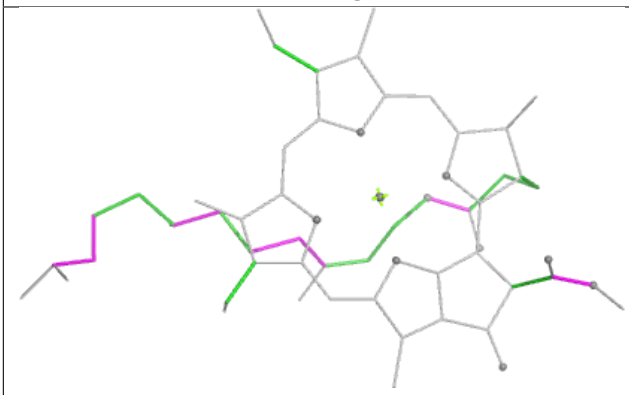

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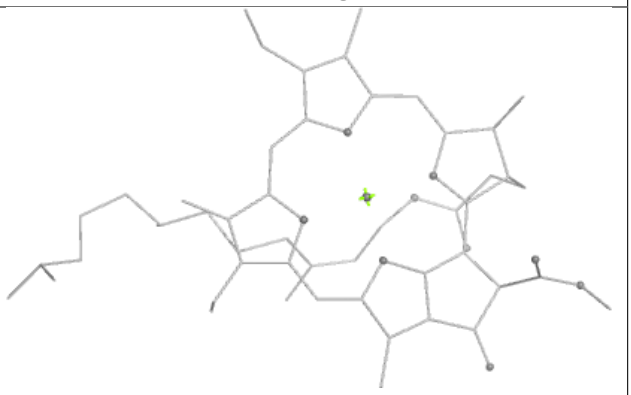
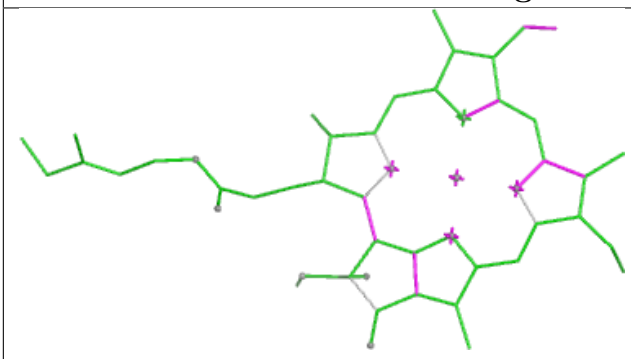


Rings

Ligand CLA A 1135



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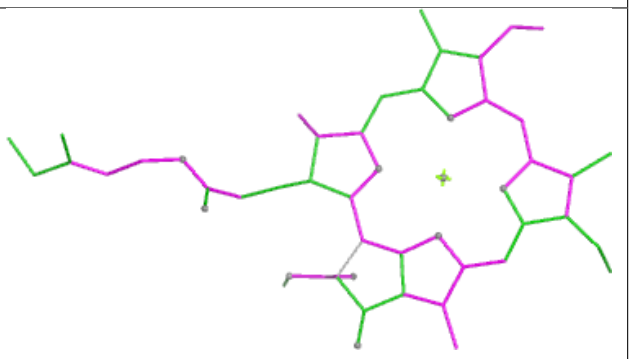
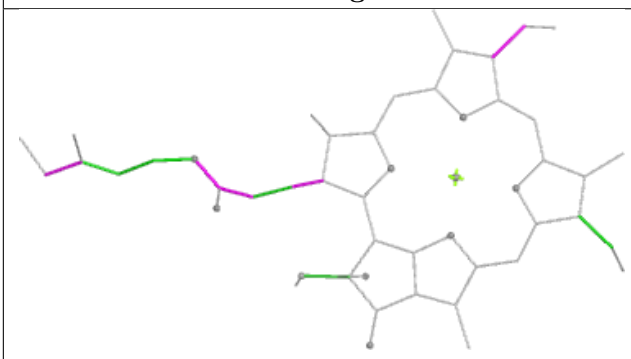


Bond angles



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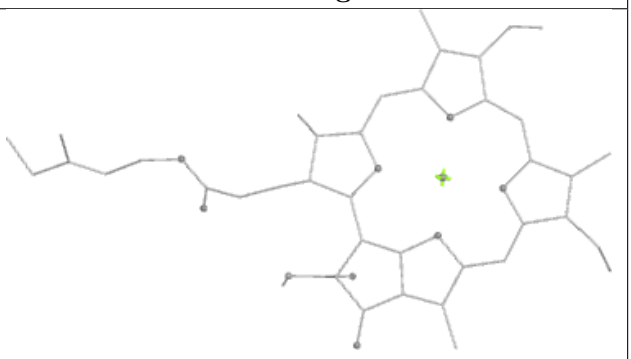
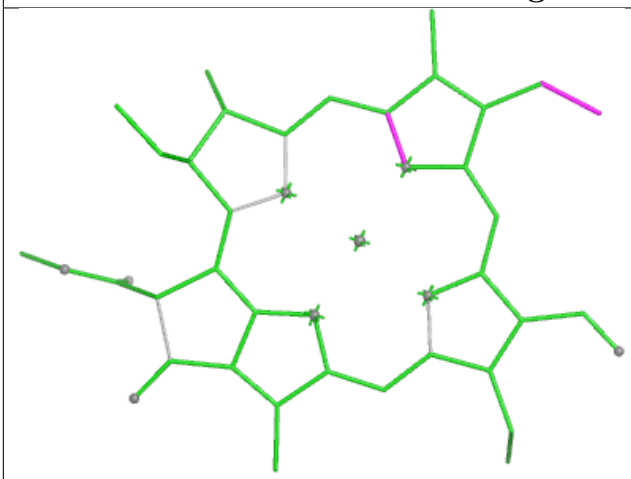


Rings

Ligand CHL 5 617



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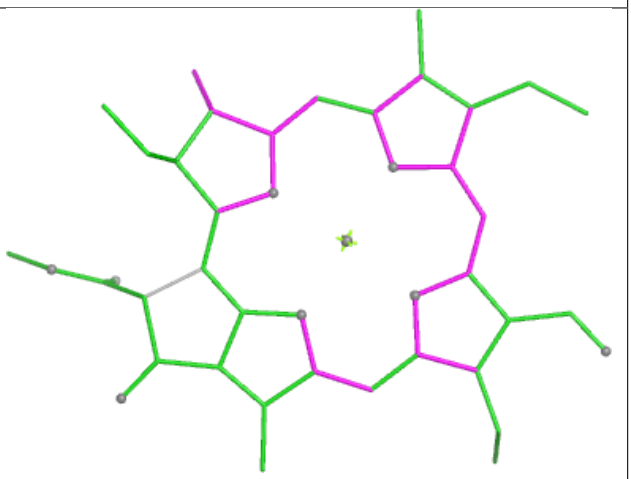
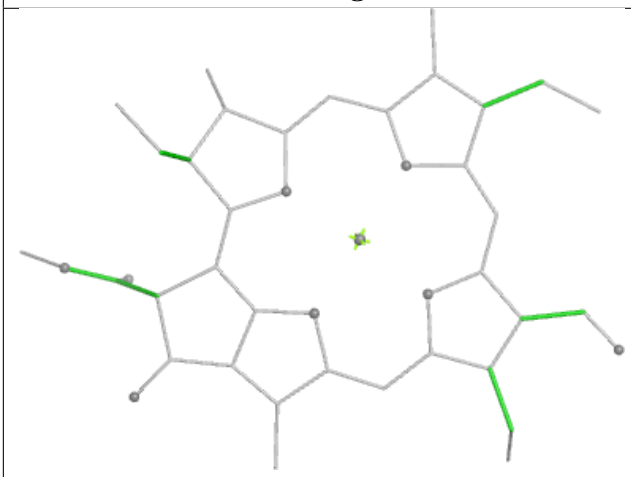


Bond angles



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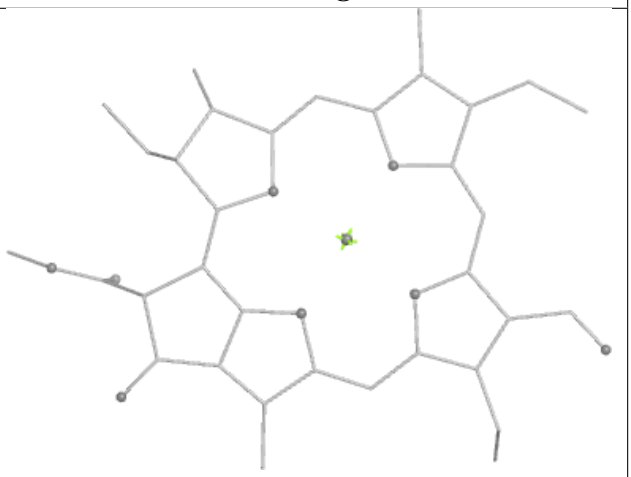
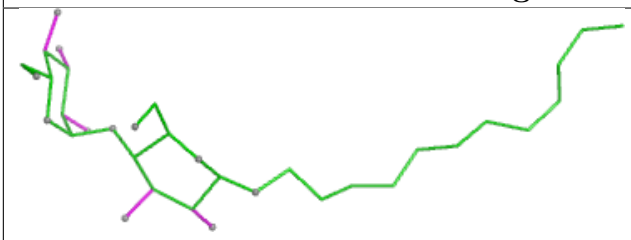
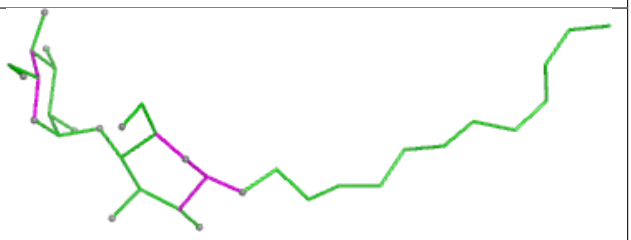


Rings

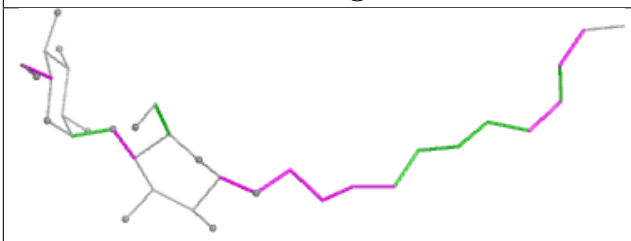
Ligand LMT B 6101



Bond lengths



Bond angles



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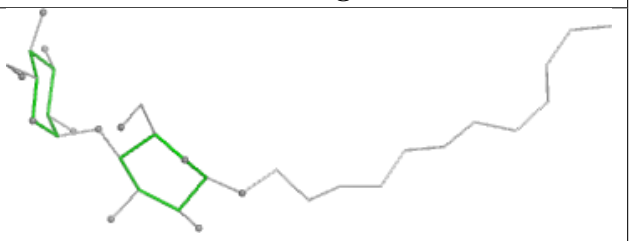
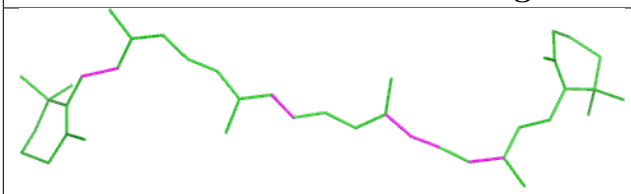
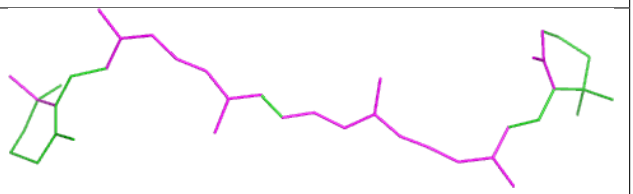


Rings

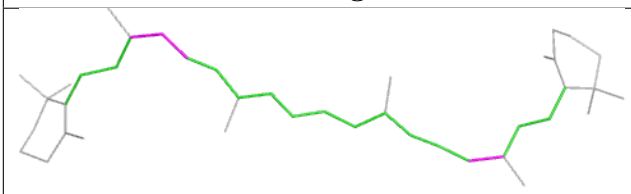
Ligand BCR B 4003



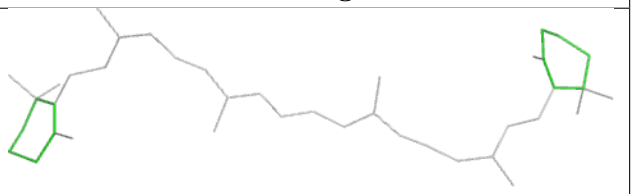
Bond lengths



Bond angles

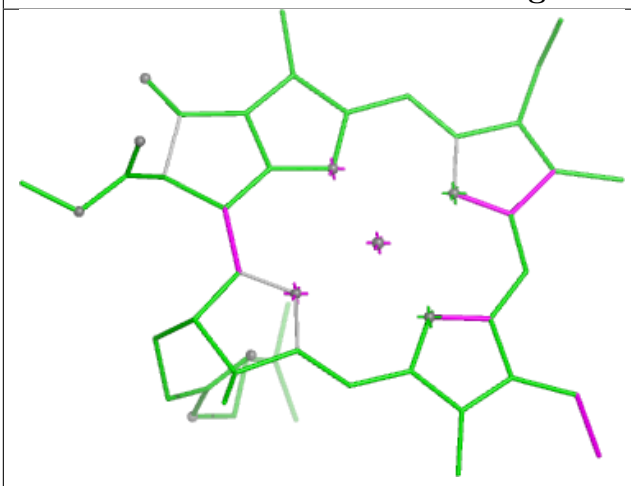


Torsions

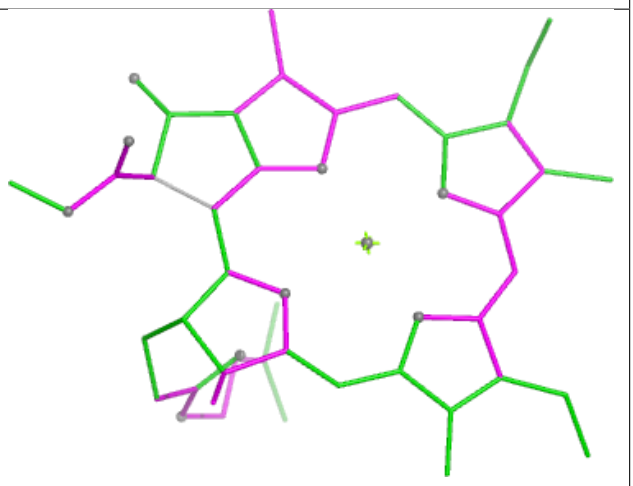


Rings

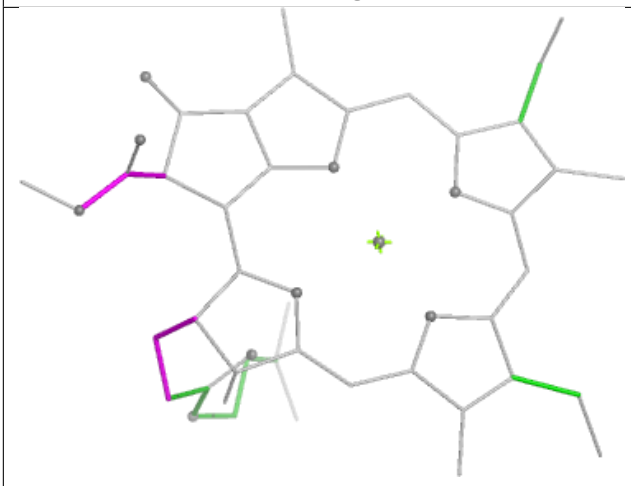
Ligand CLA 4 612



Bond lengths



Bond angles

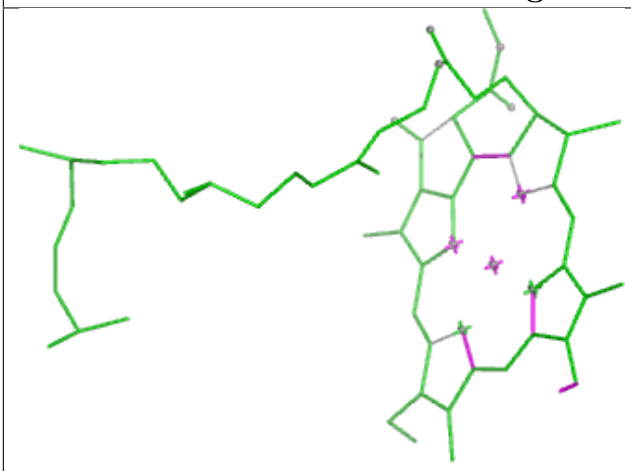


Torsions



Rings

Ligand CLA Z 612



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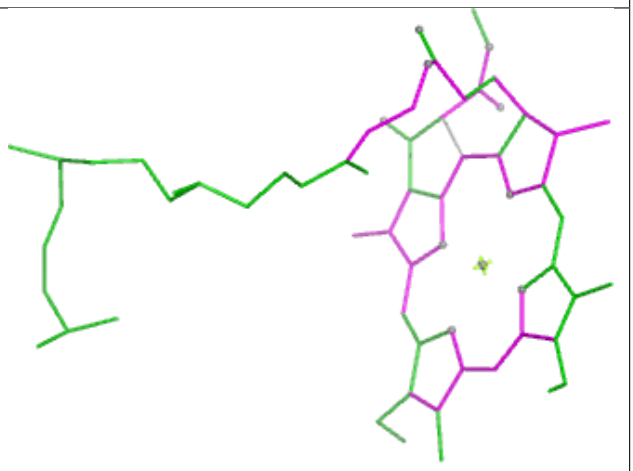
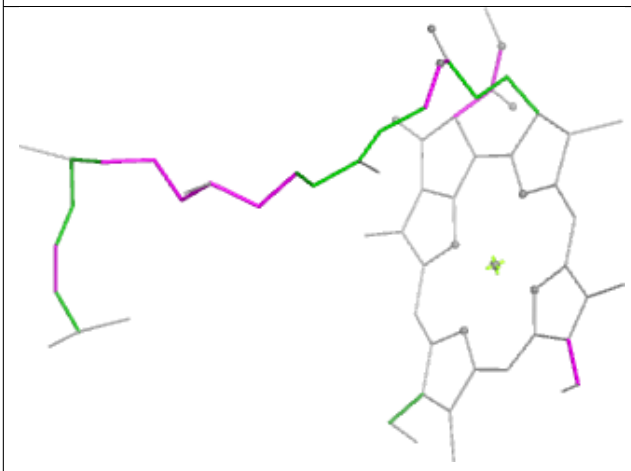


Bond angles

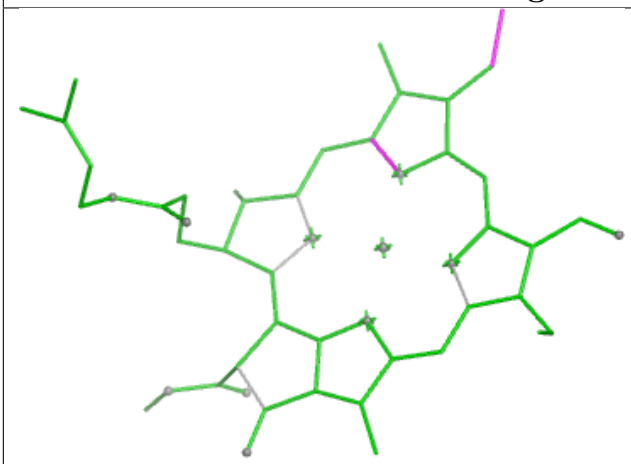


Torsions



Rings

Ligand CHL 4 611



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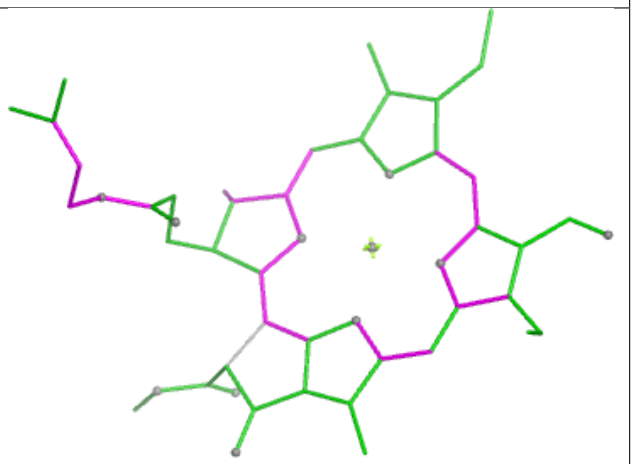

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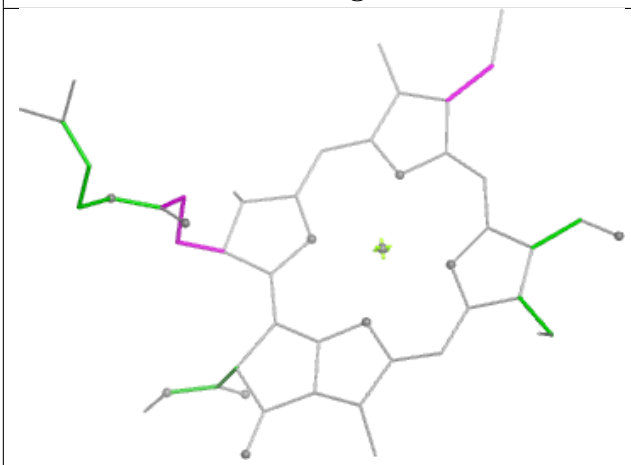

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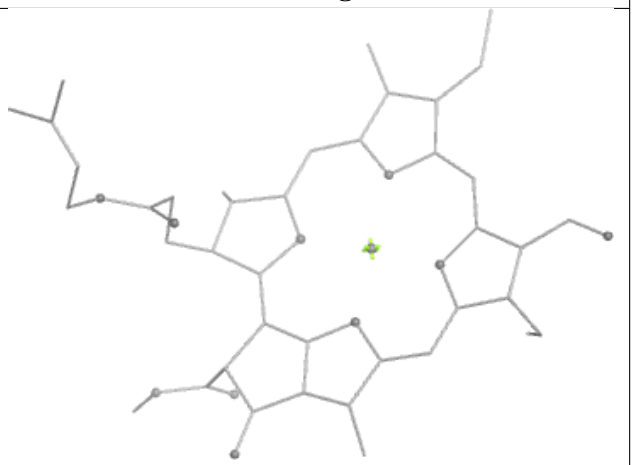

Rings

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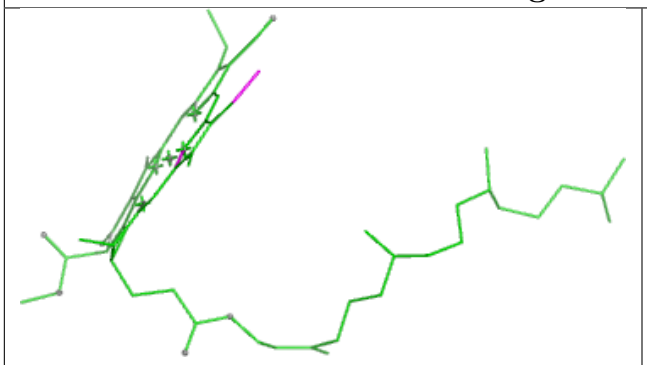

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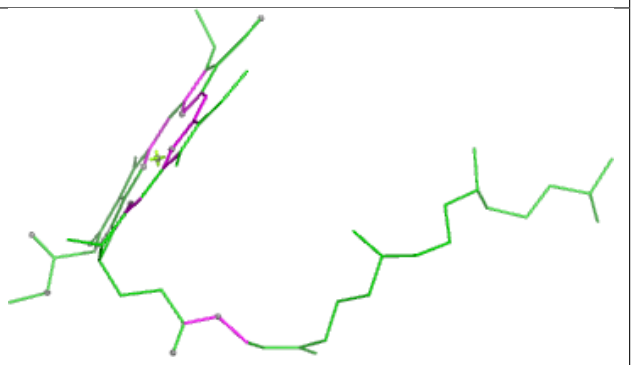

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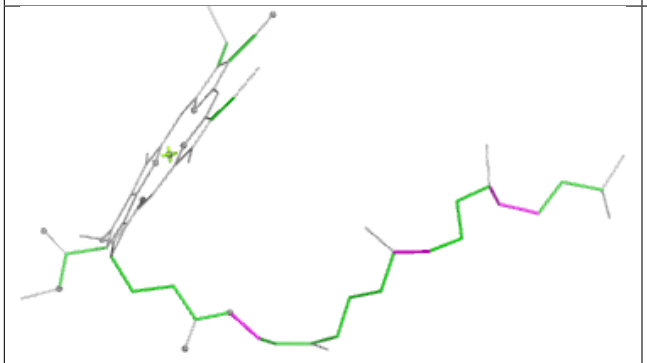
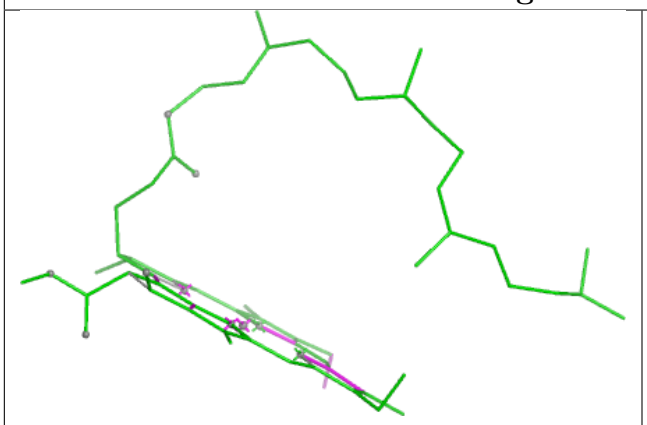


Torsions



Rings

Ligand CLA B 1241



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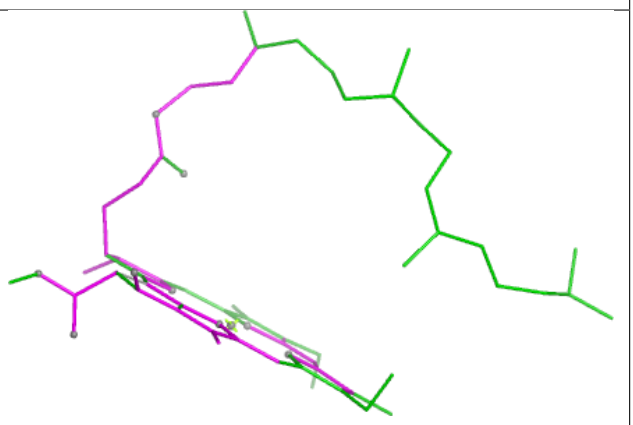

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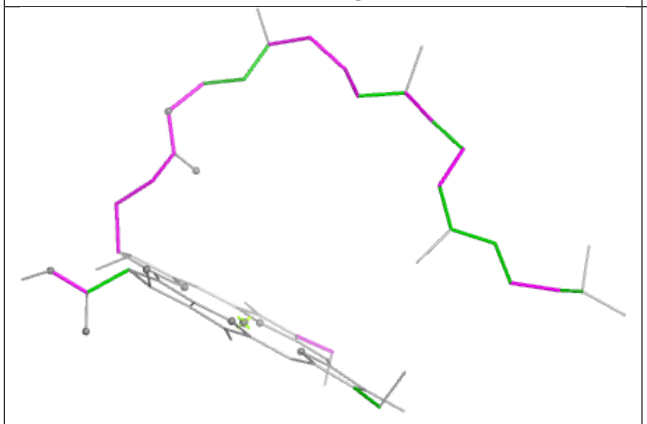

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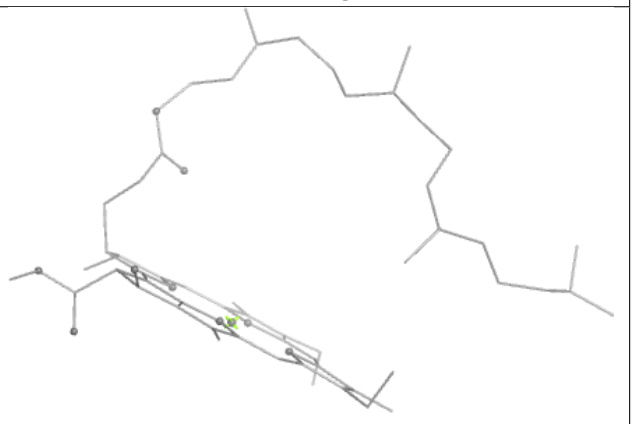
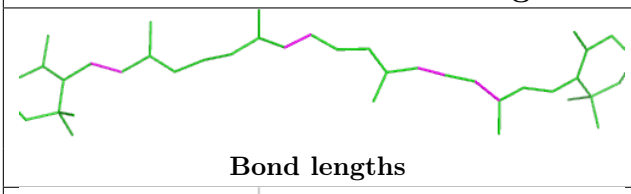


Rings

Ligand BCR K 4001



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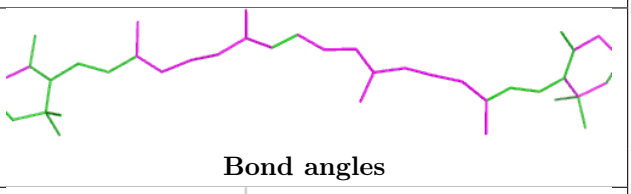

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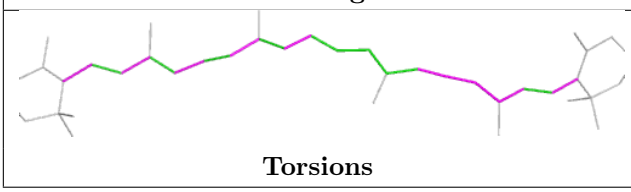

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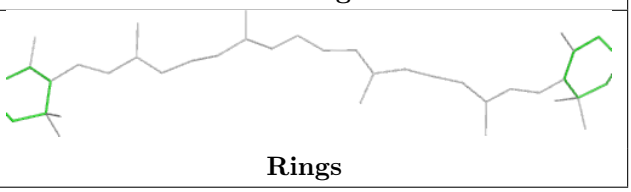
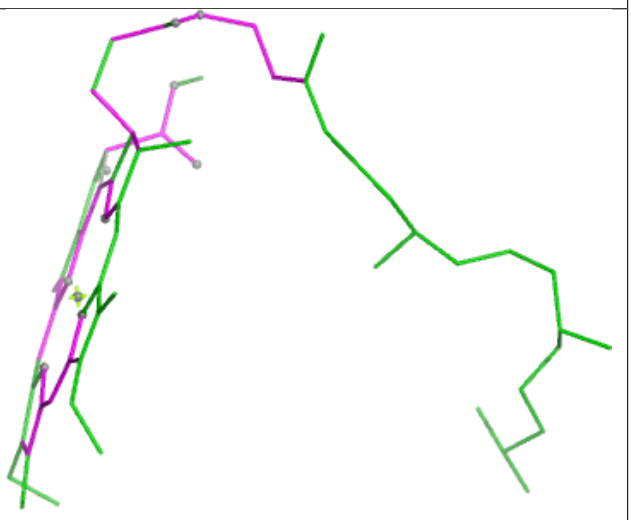


Rings

Ligand CLA 8 602



Bond lengths



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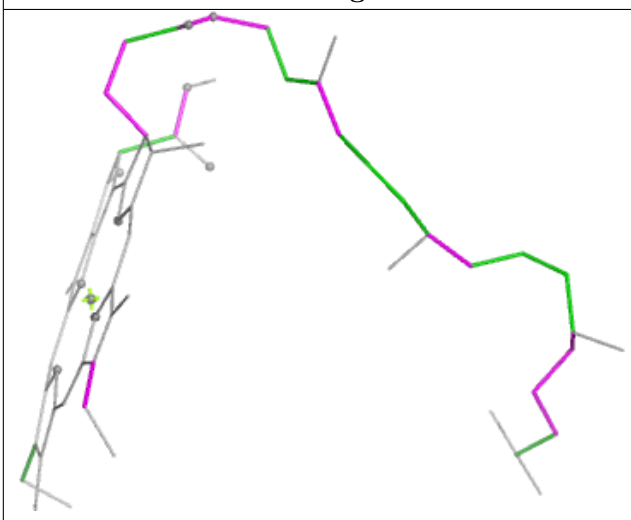
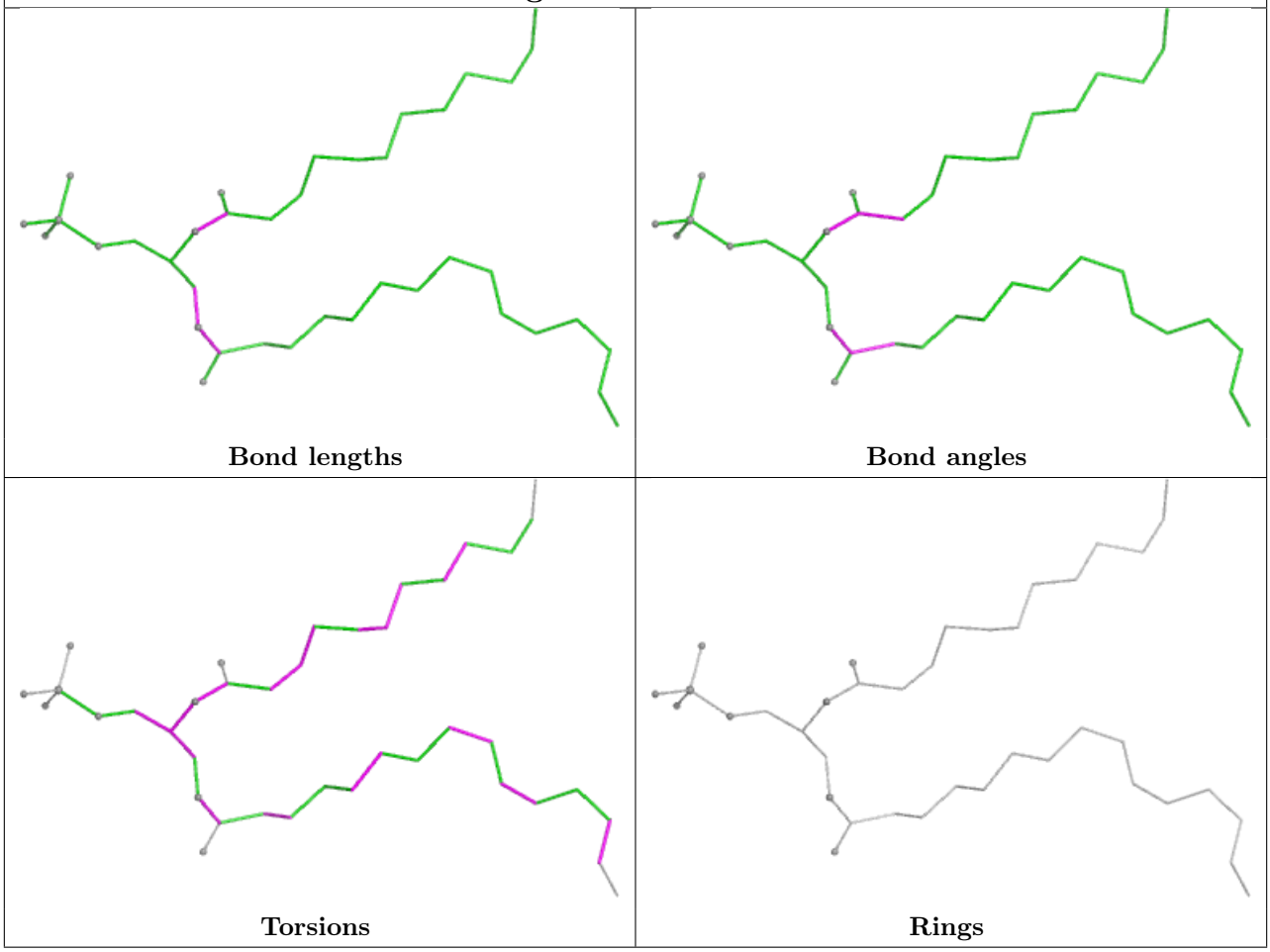


Torsions

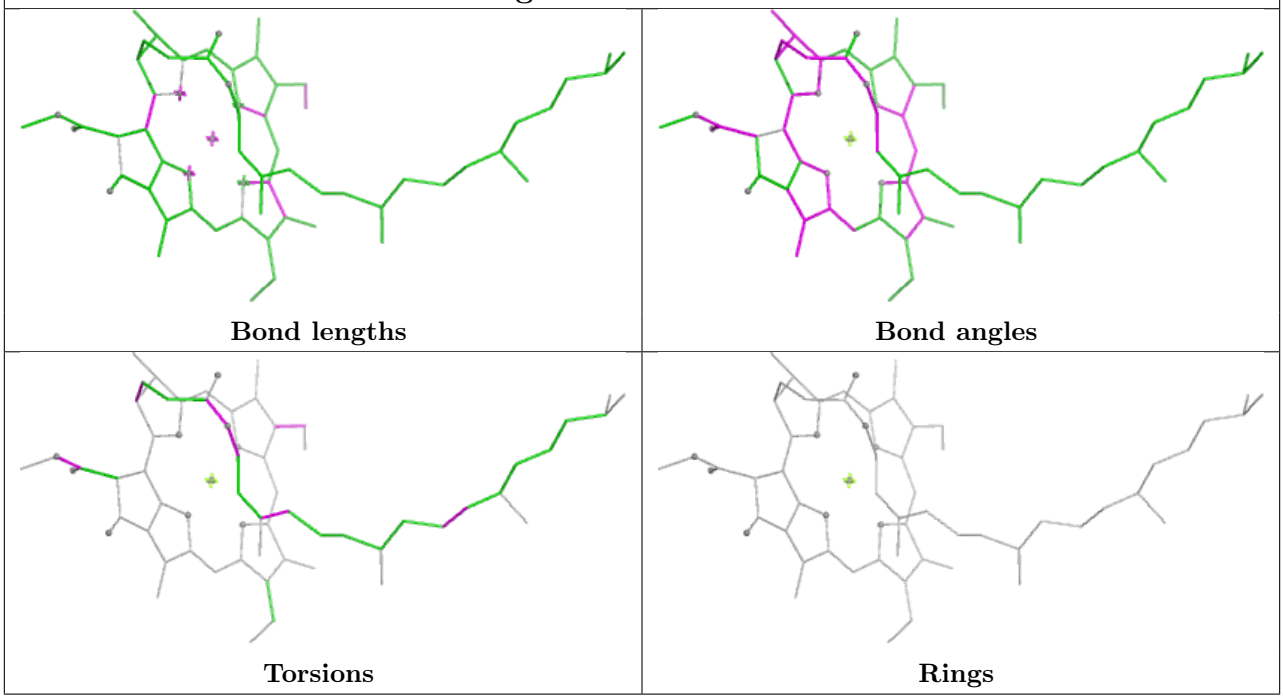


Rings

Ligand 3PH 7 802



Ligand CLA A 1139



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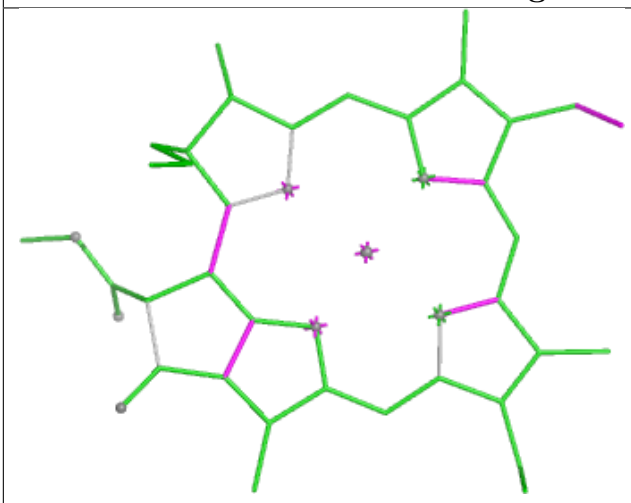

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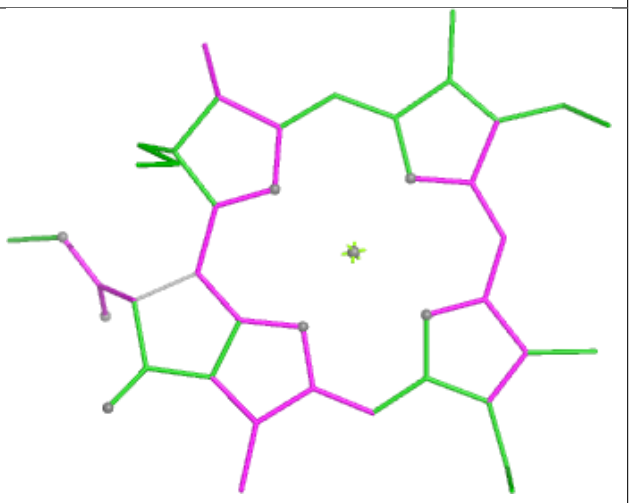

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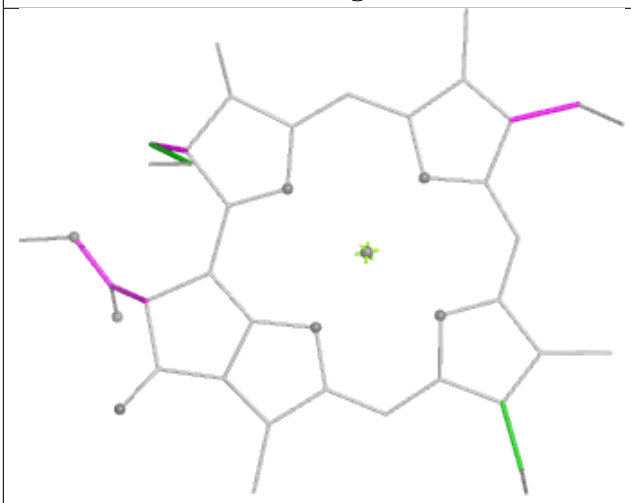

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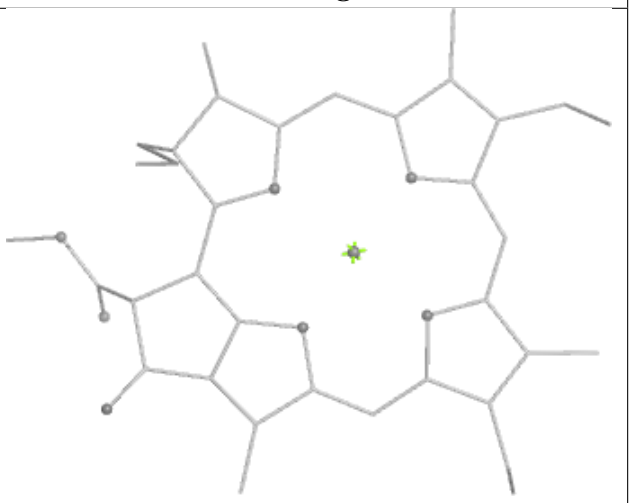
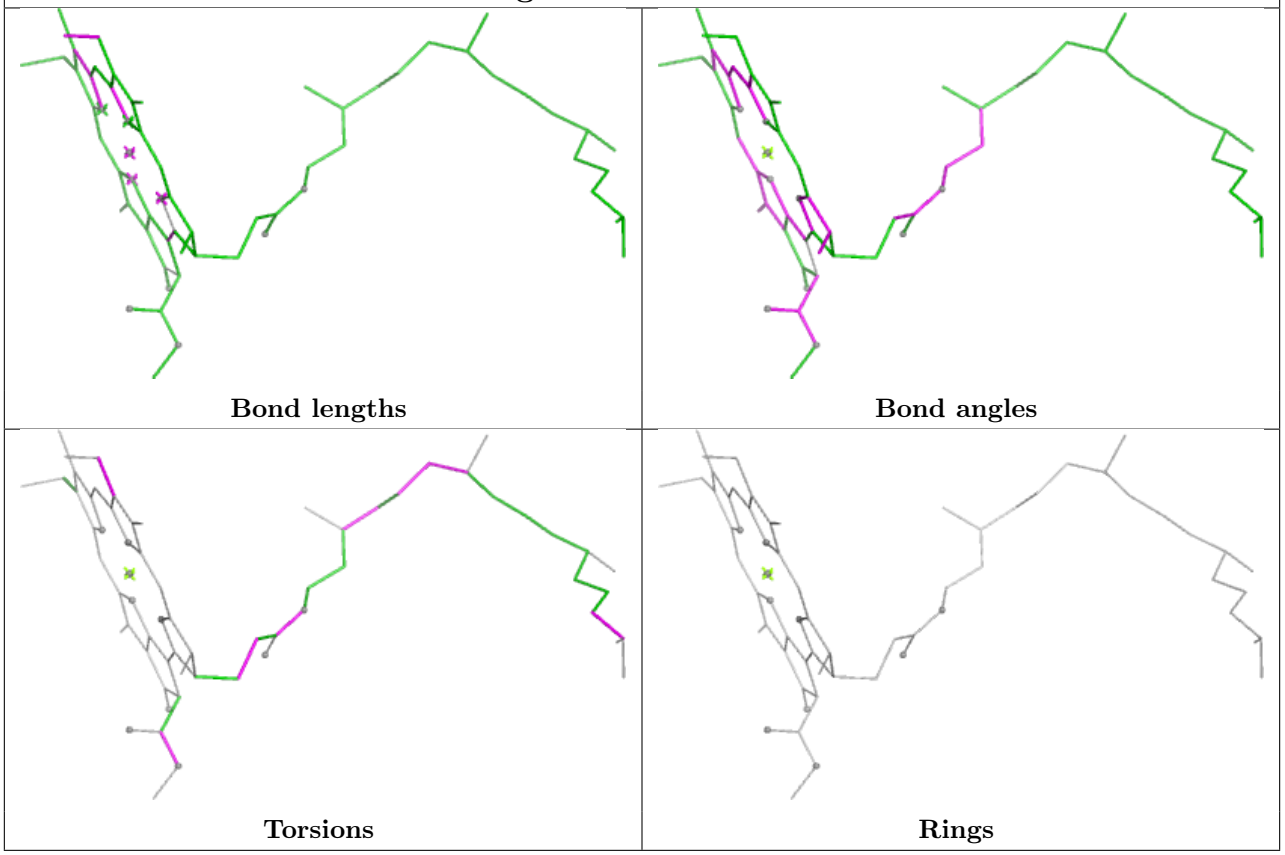


Rings

Ligand CLA B 1238



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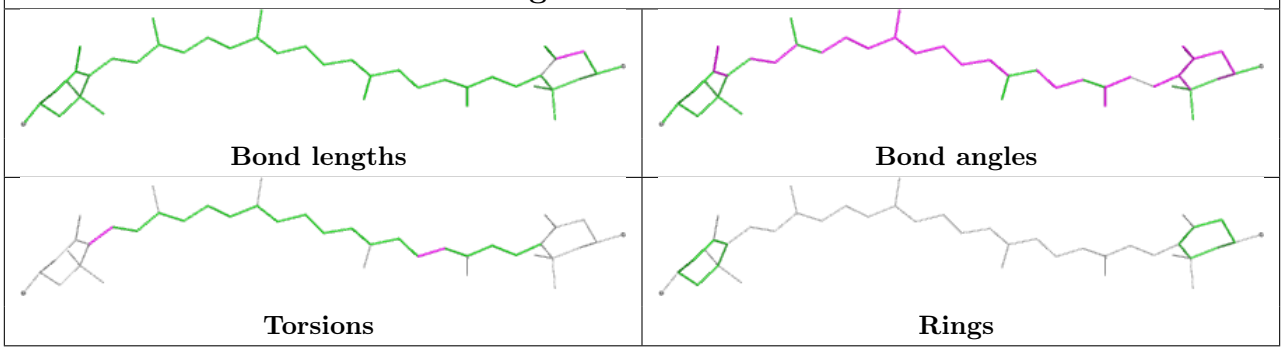

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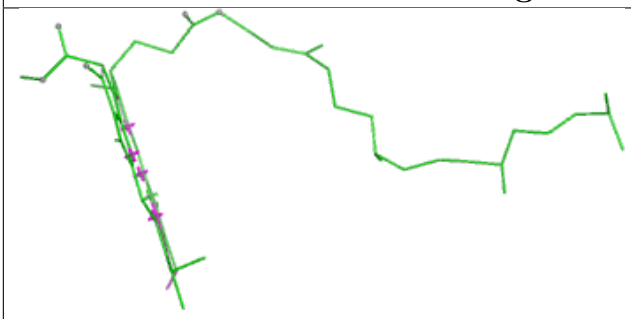

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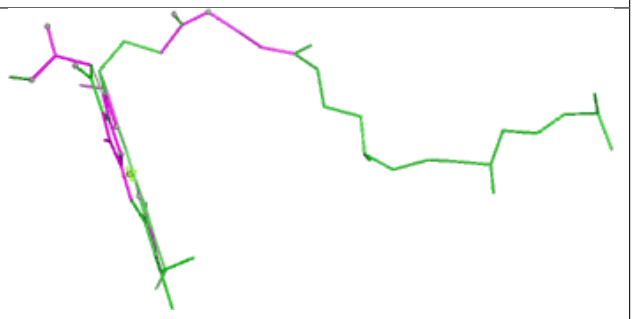

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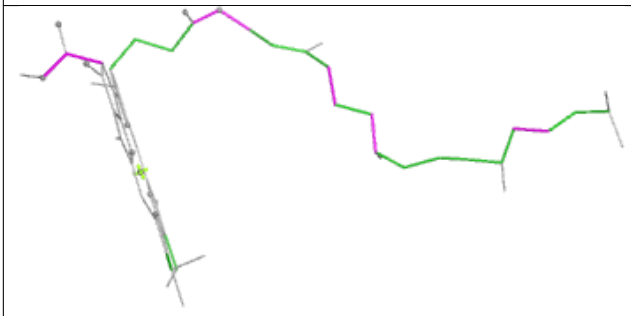
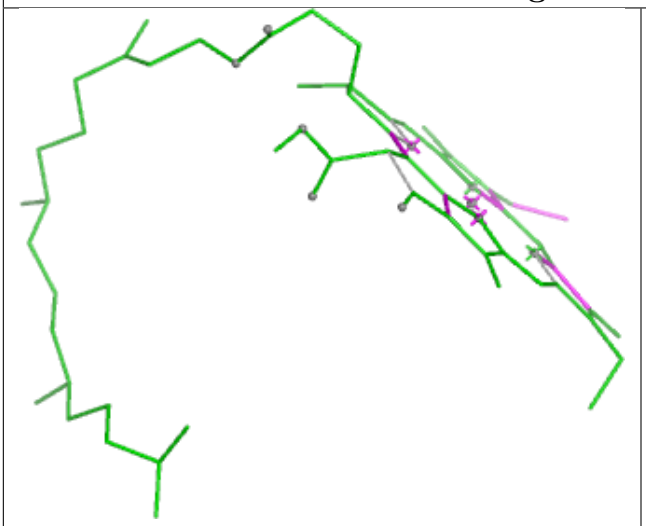


Torsions



Rings

Ligand CLA 4 605



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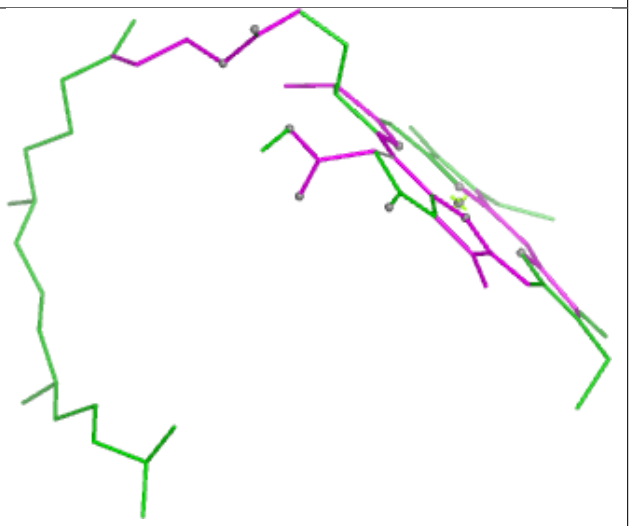

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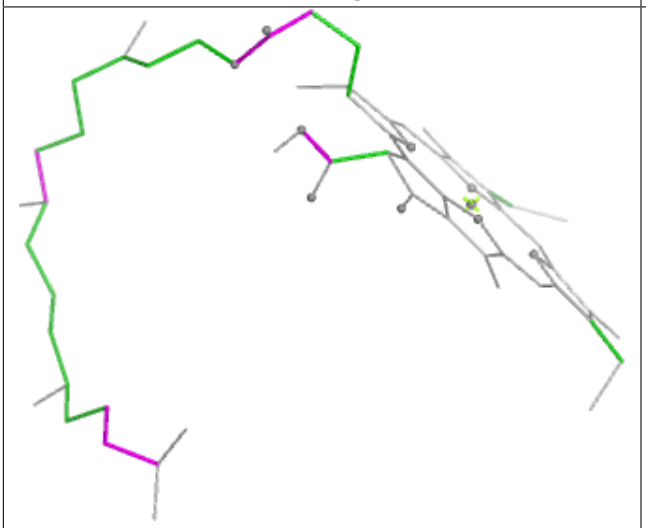

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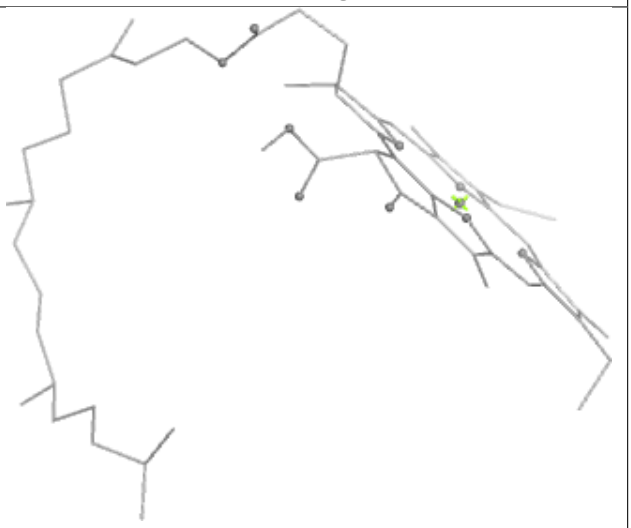
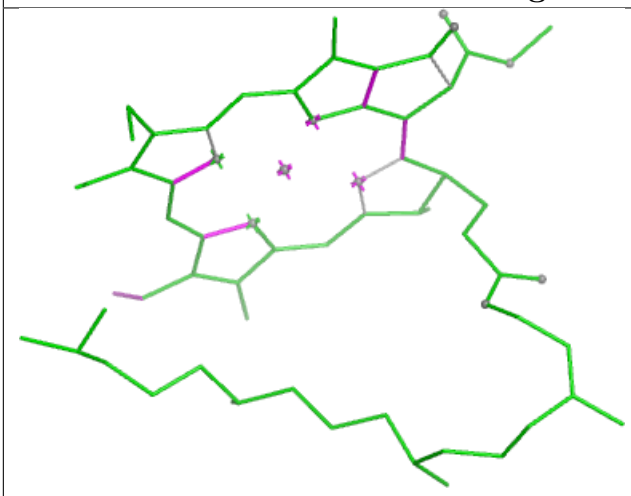


Rings

Ligand CLA 1 611



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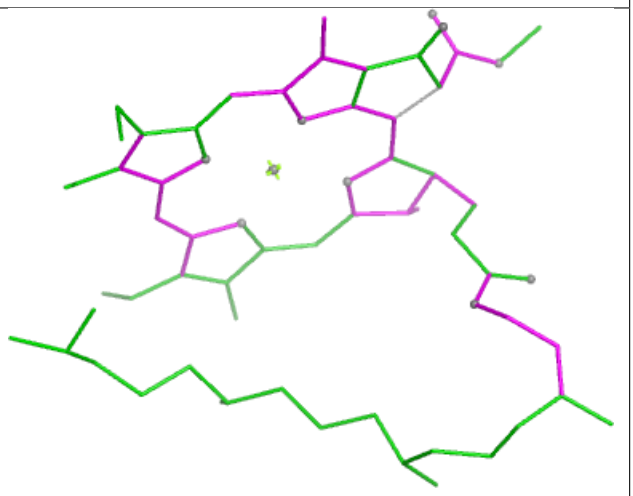

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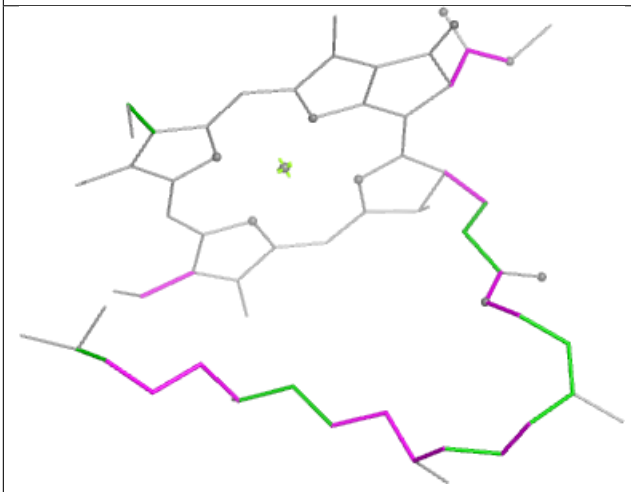

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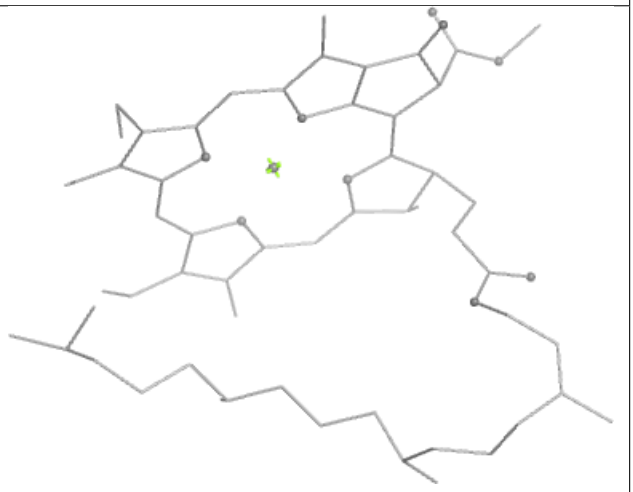
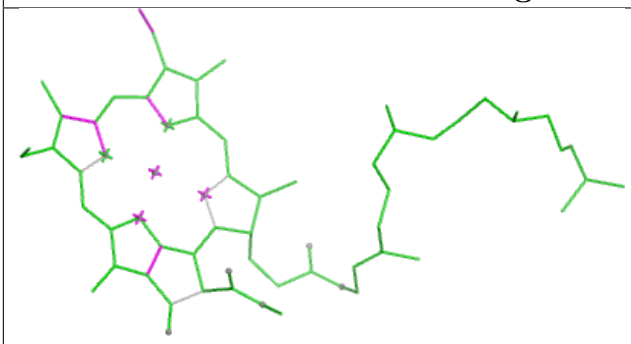


Rings

Ligand CLA A 1101



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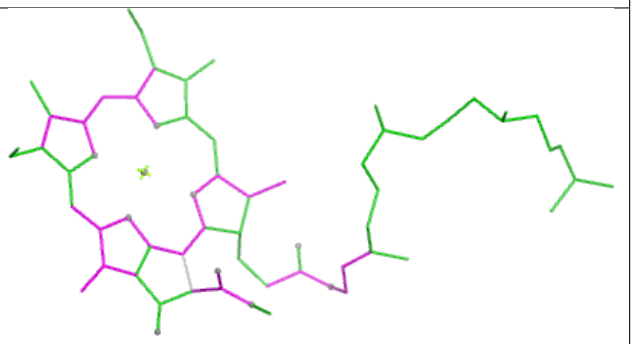

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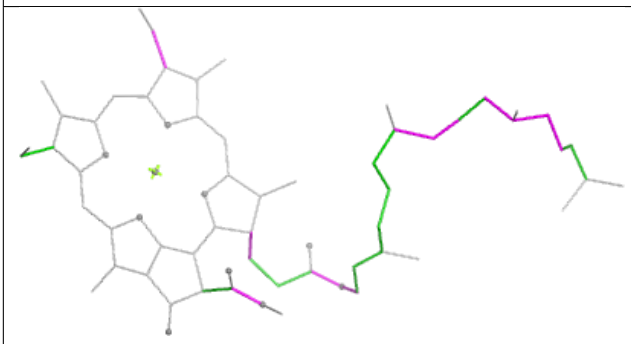

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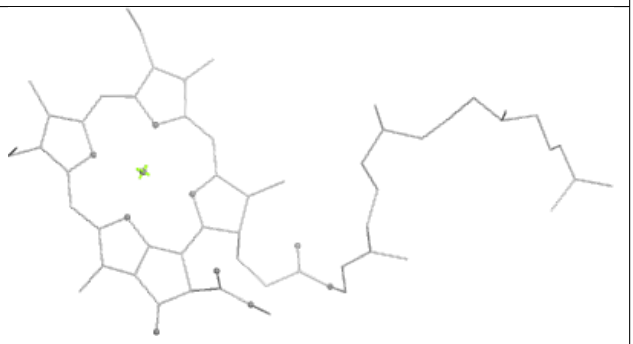
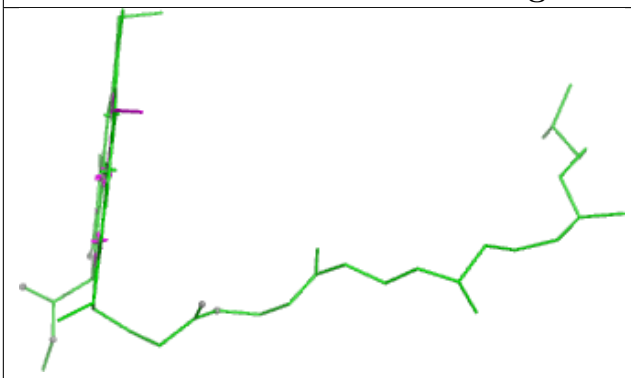


Rings

Ligand CLA 3 606



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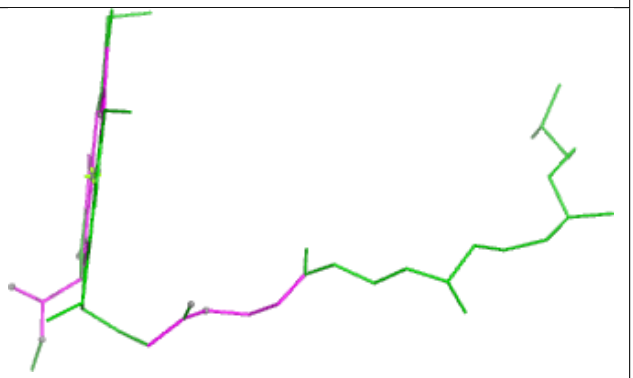
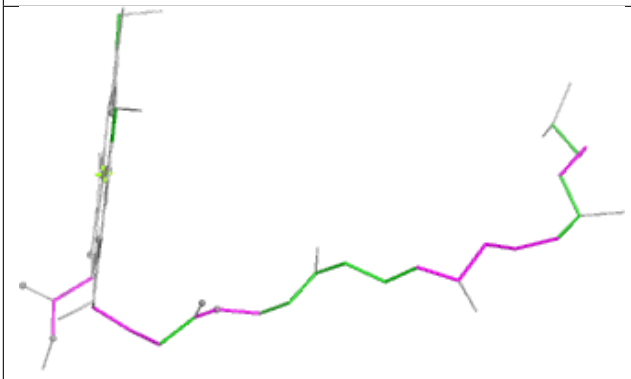


Bond angles

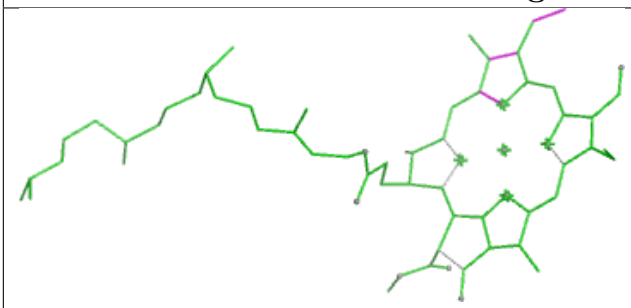


Torsions



Rings

Ligand CHL 3 611



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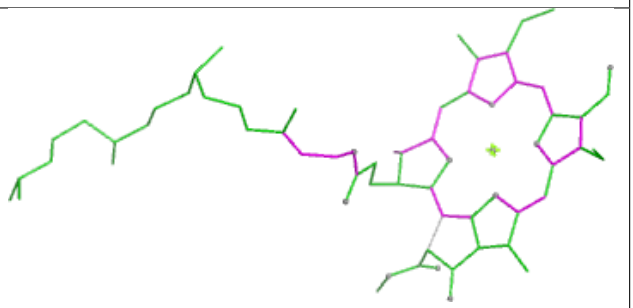
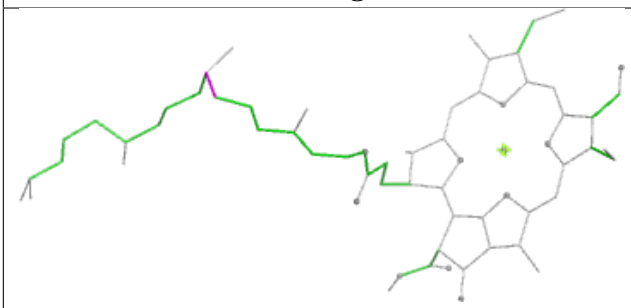


Bond angles



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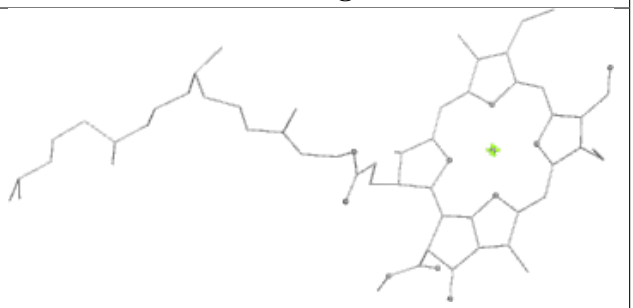
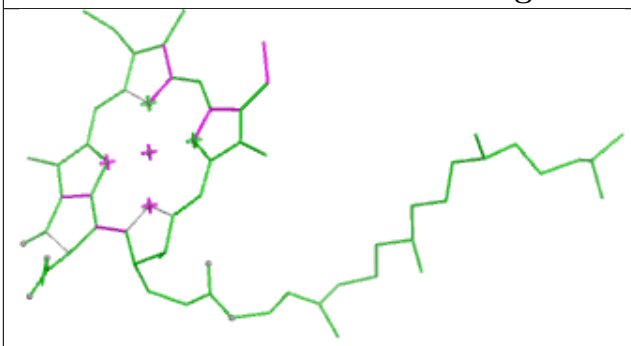


Rings

Ligand CLA A 1106



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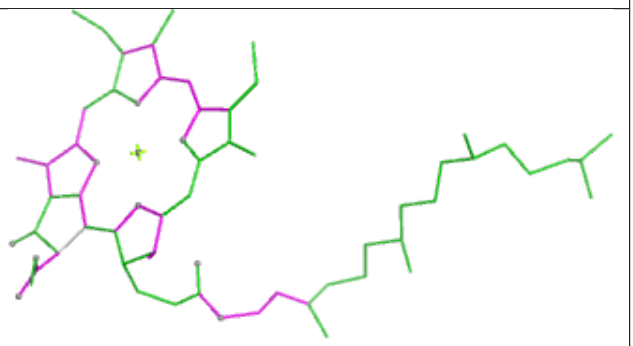
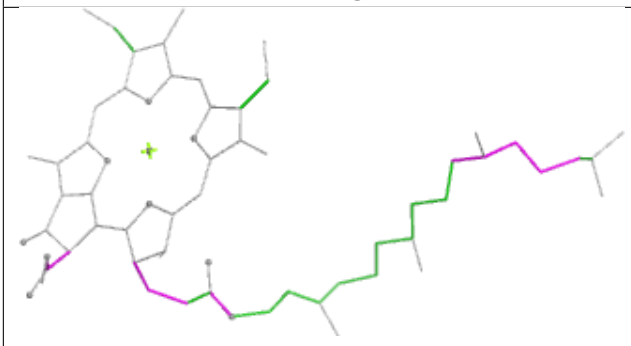


Bond angles



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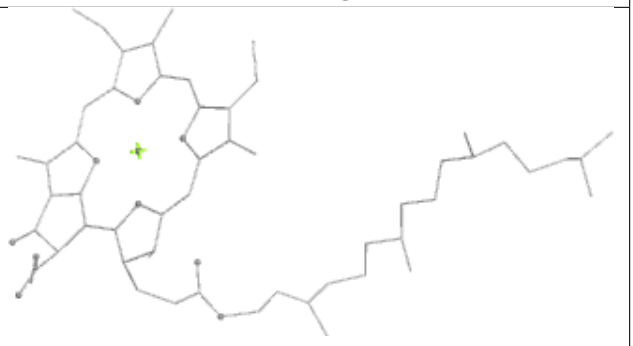
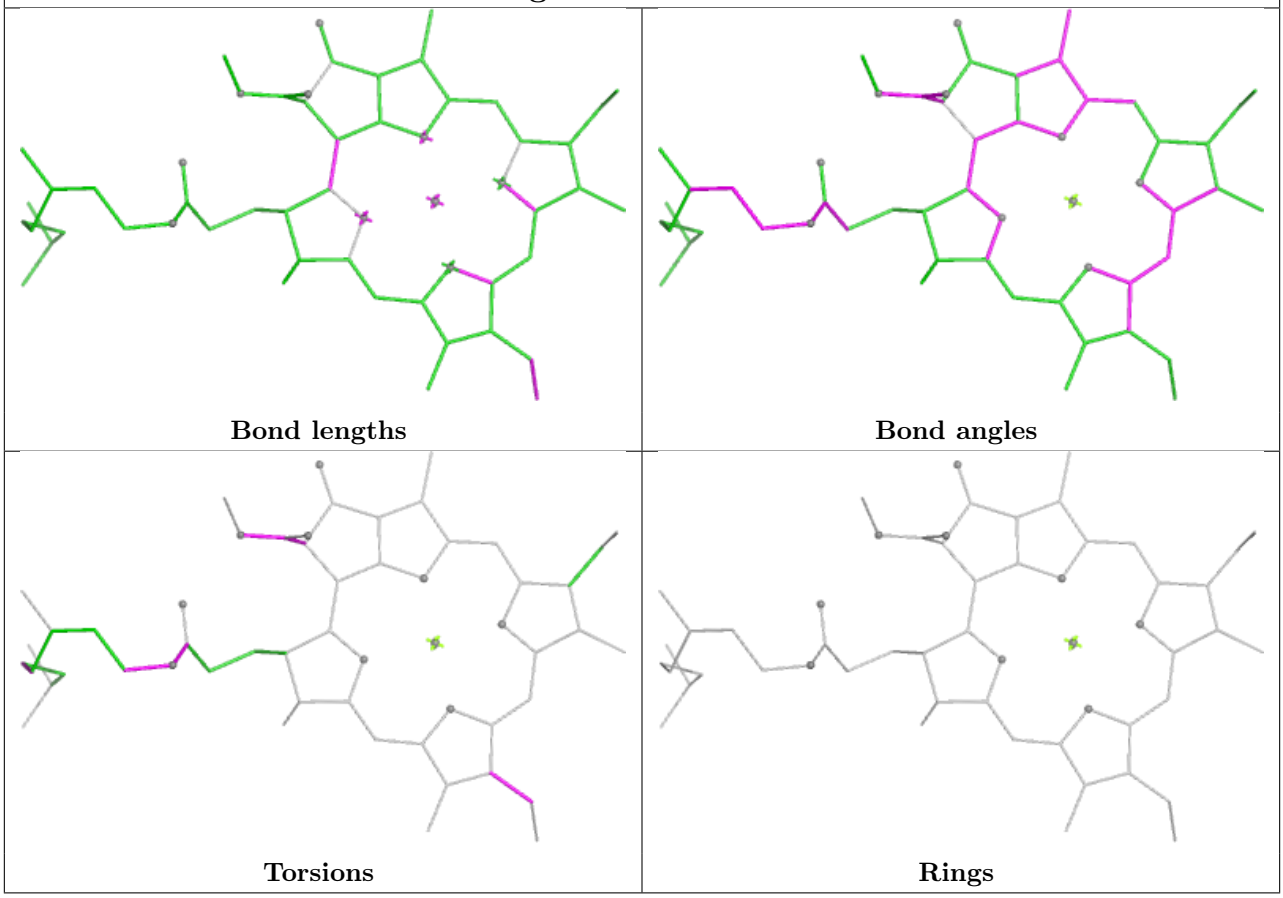
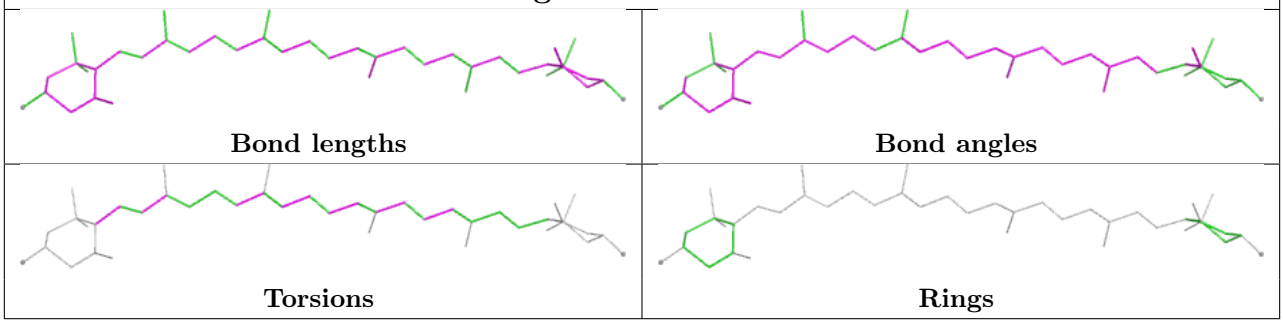


Rings

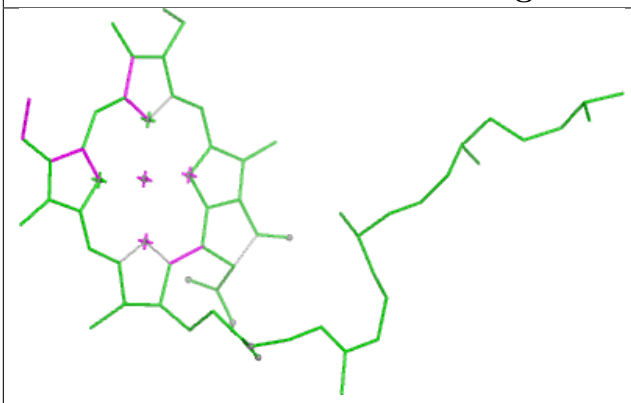
Ligand CLA 3 613



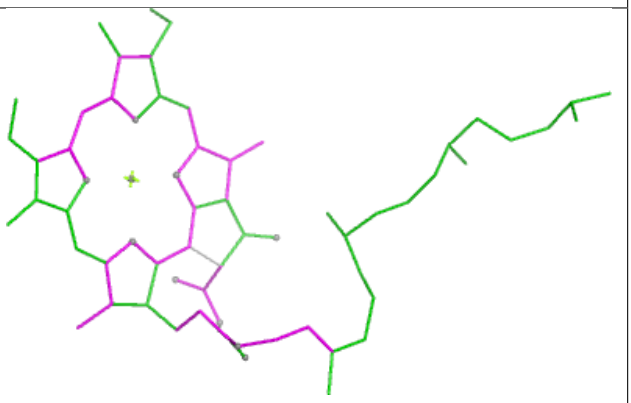
Ligand C7Z 5 505



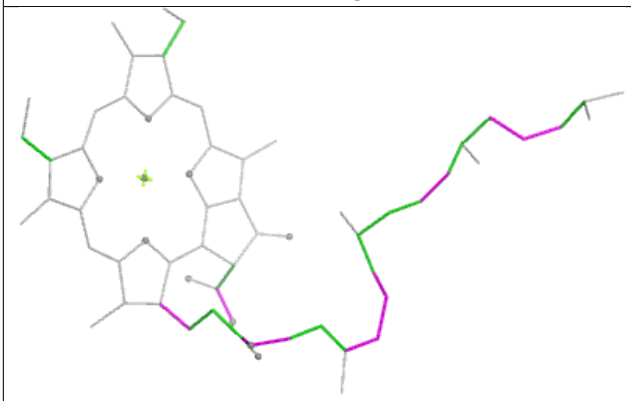
Ligand CLA B 1229



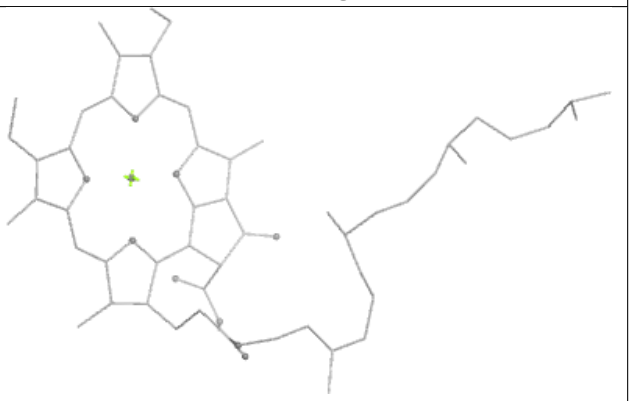
Bond lengths



Bond angles

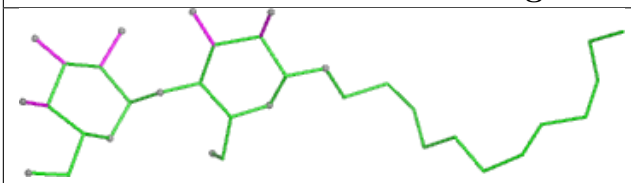


Torsions



Rings

Ligand LMT 9 803



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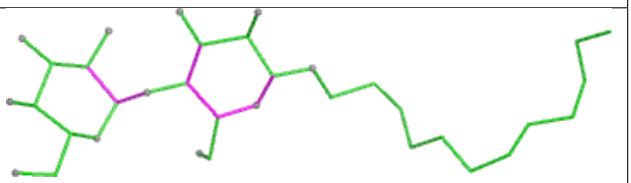
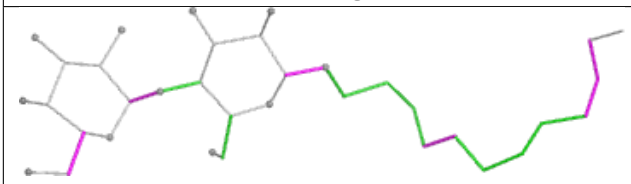


Bond angles



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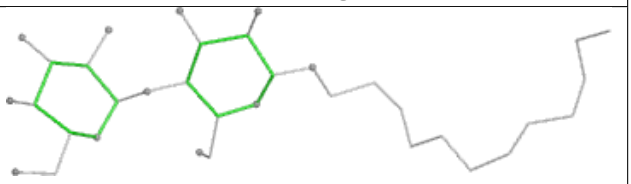
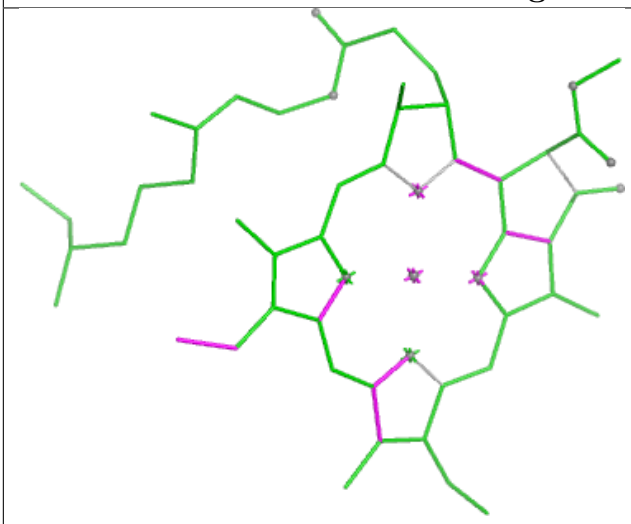


Rings

Ligand CLA 2 604



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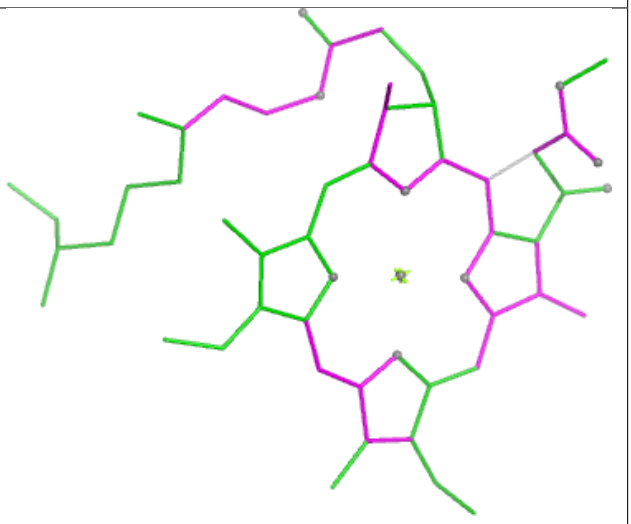

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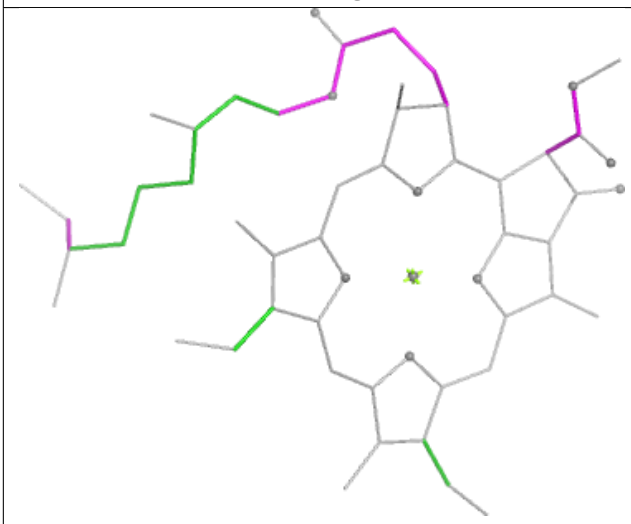

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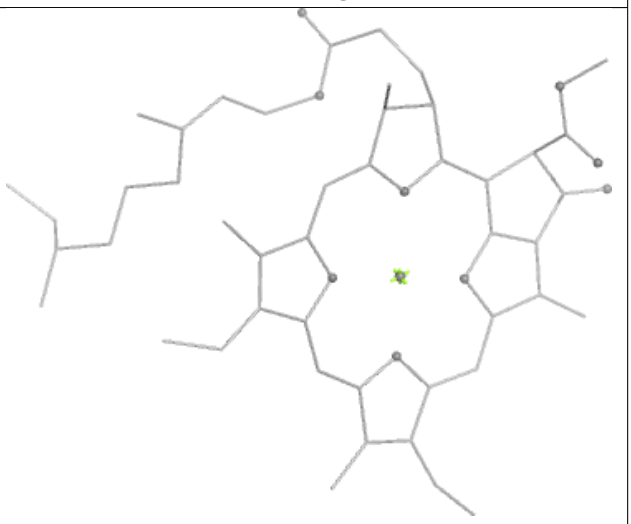
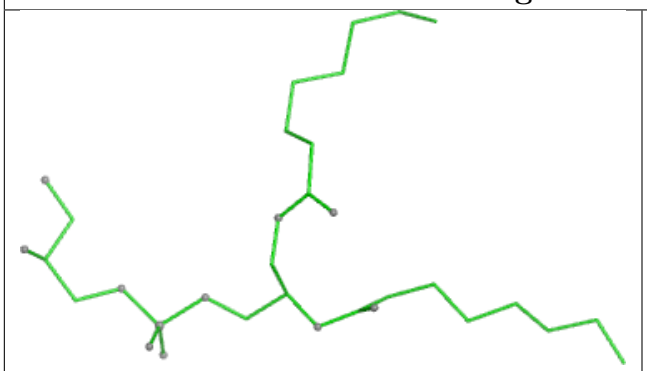


Rings

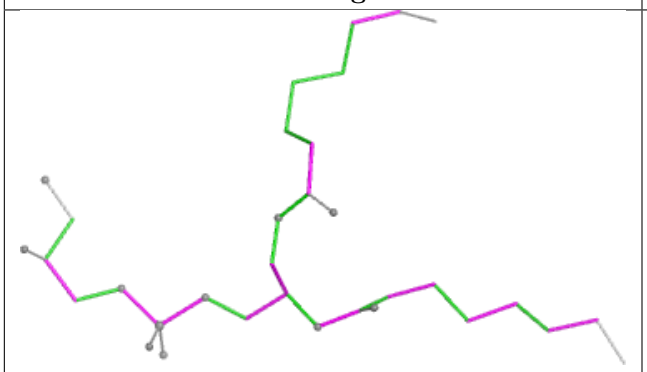
Ligand LHG B 5006



Bond lengths



Bond angles



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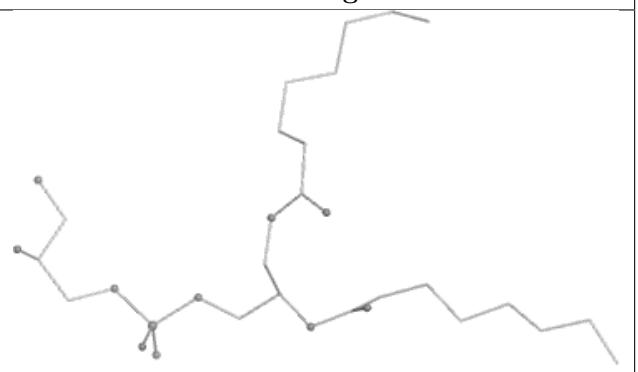
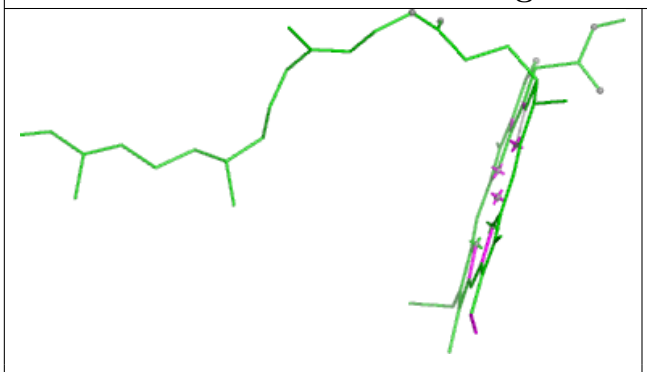


Rings

Ligand CLA A 1114



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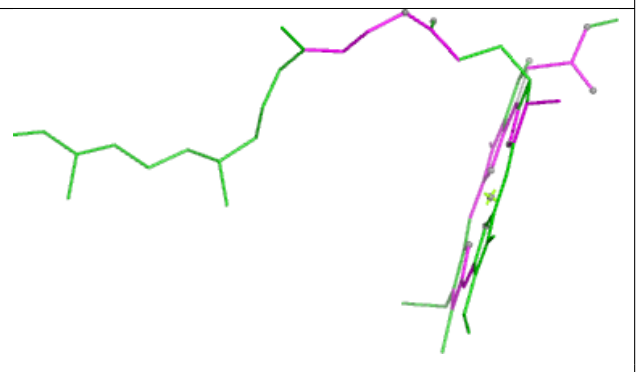
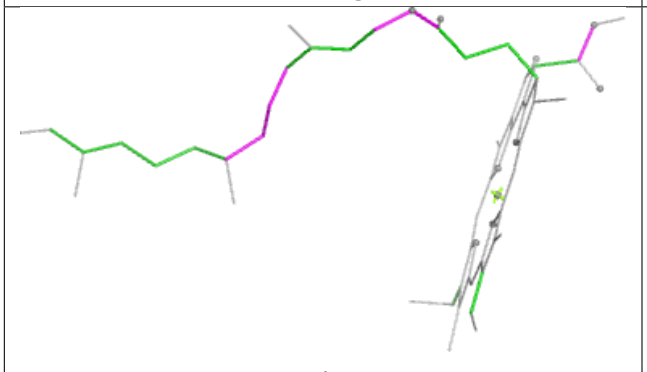


Bond angles

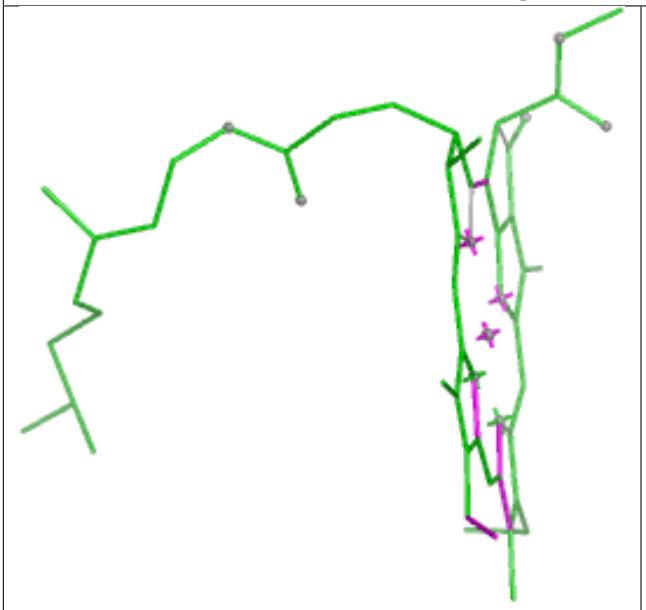


Torsions



Rings

Ligand CLA A 1120



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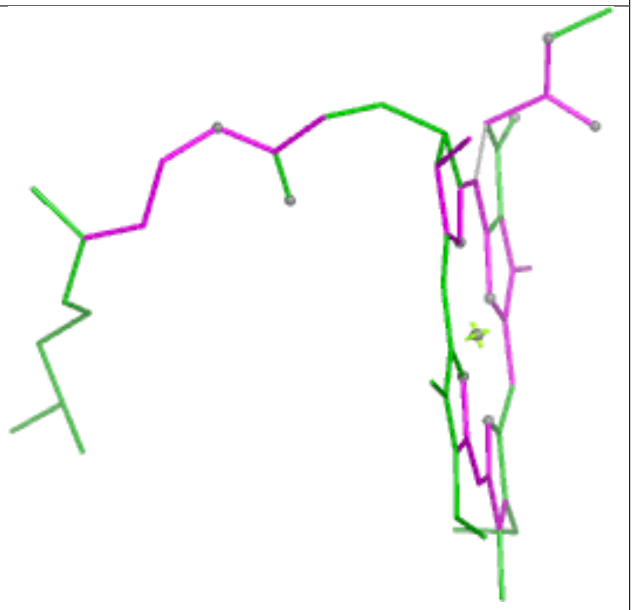
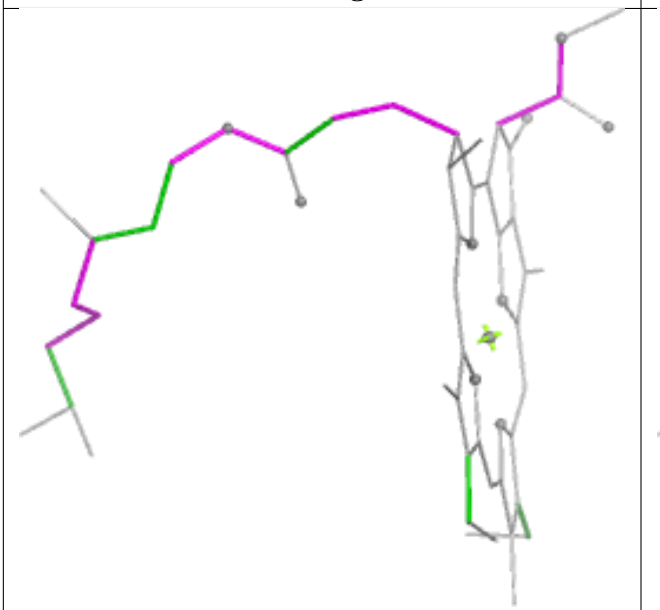


Bond angles



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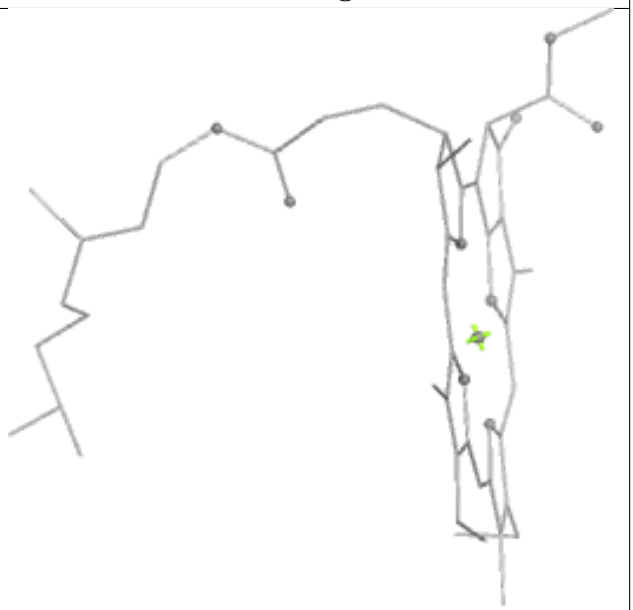
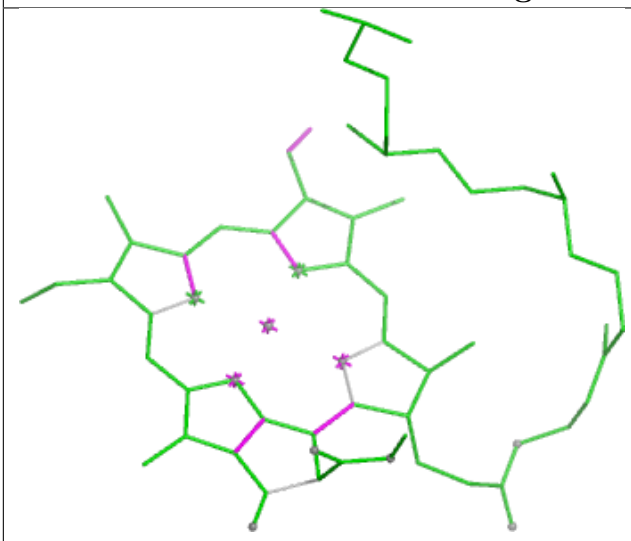


Rings

Ligand CLA A 1111



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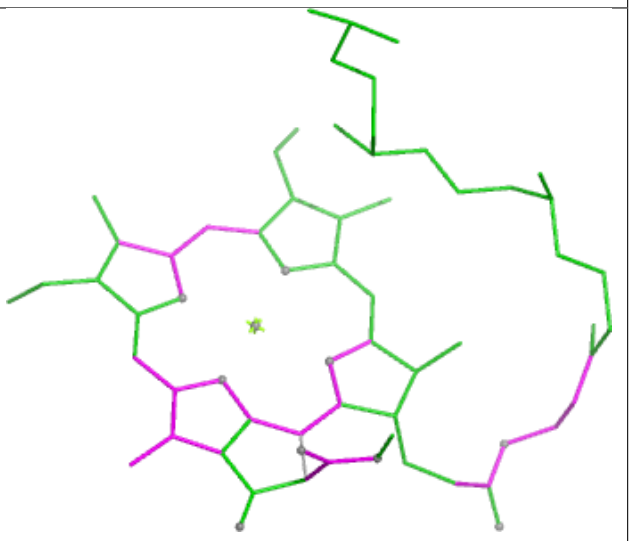

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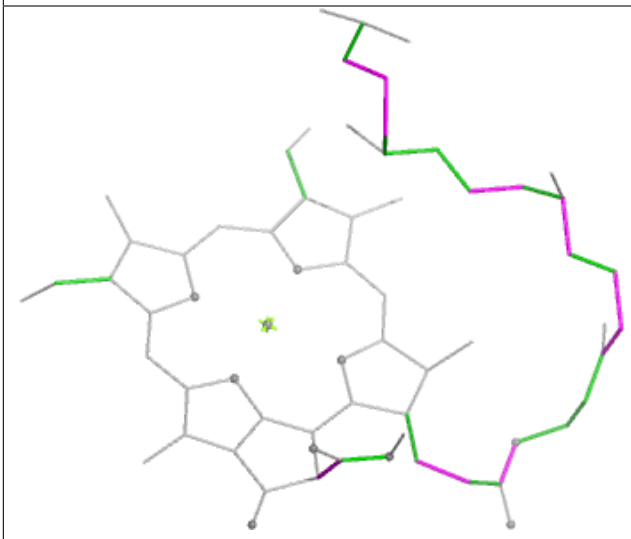

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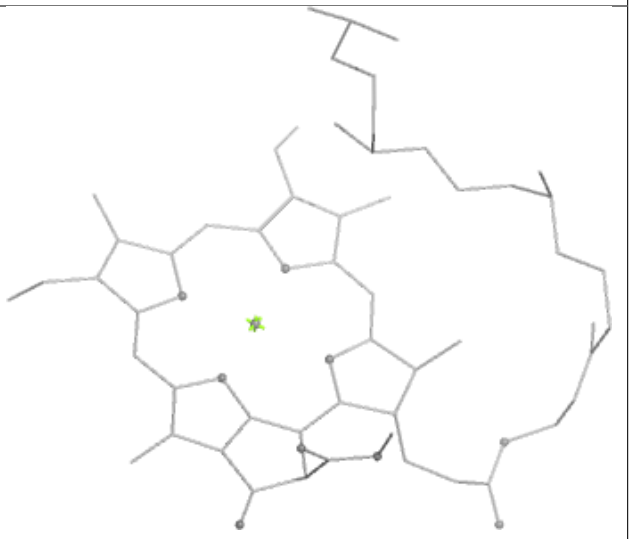
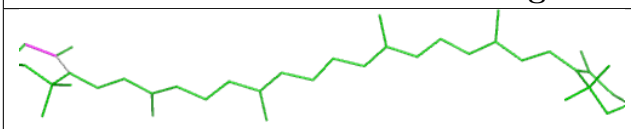


Rings

Ligand LUT 3 502



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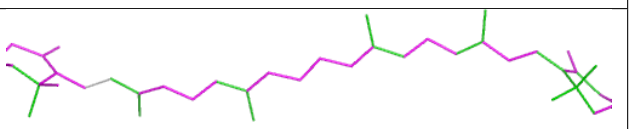
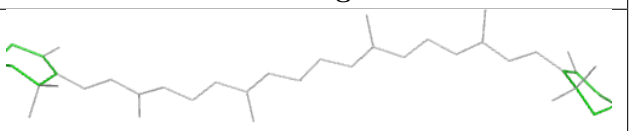


Bond angles

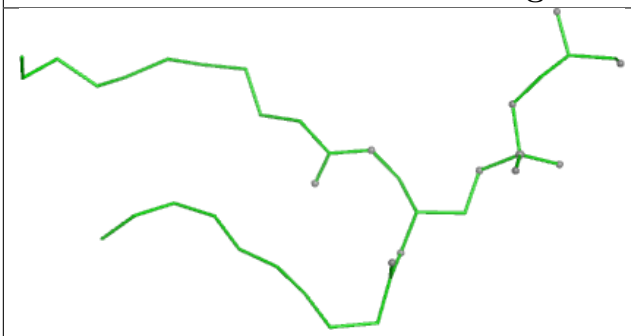


Torsions



Rings

Ligand LHG 8 801



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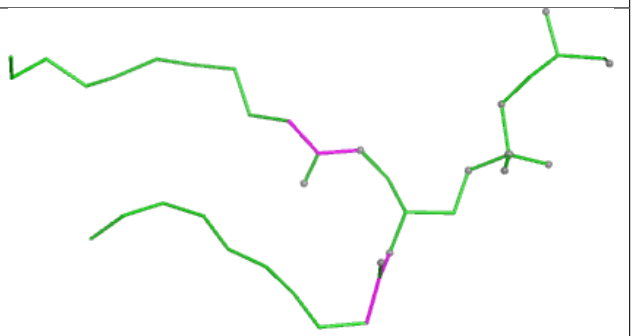
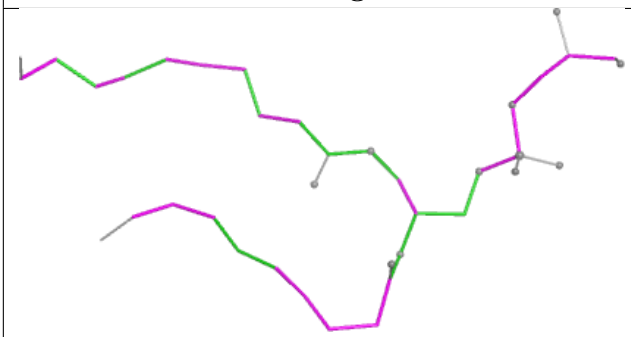


Bond angles

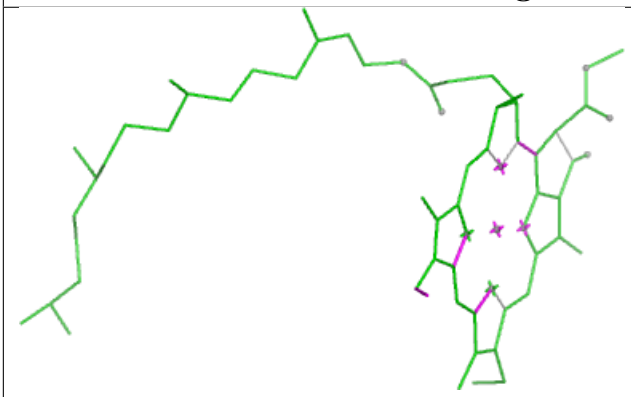


Torsions



Rings

Ligand CLA A 1133



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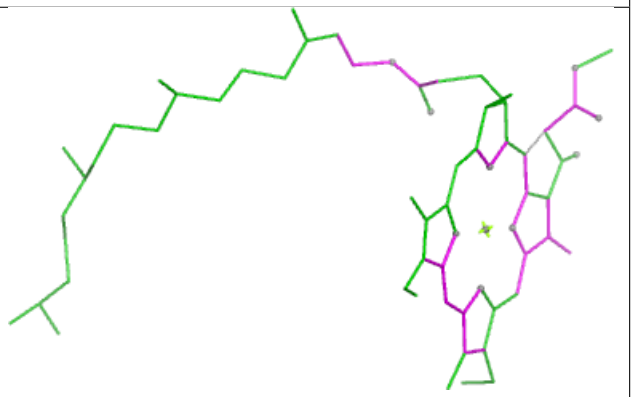
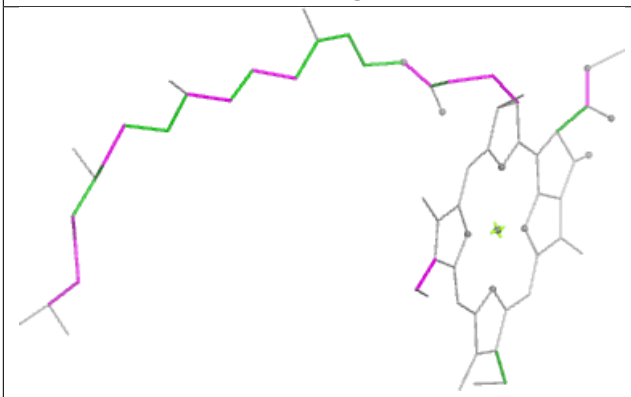


Bond angles



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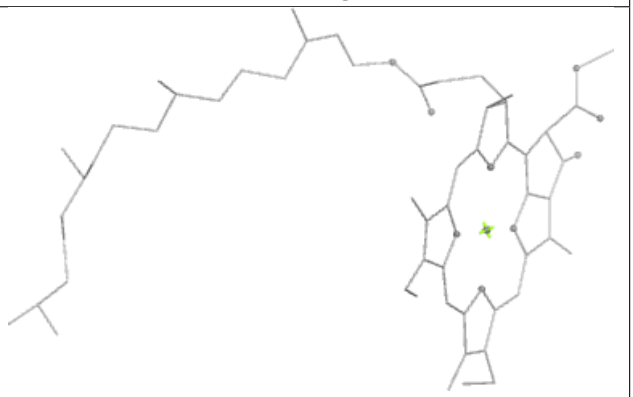
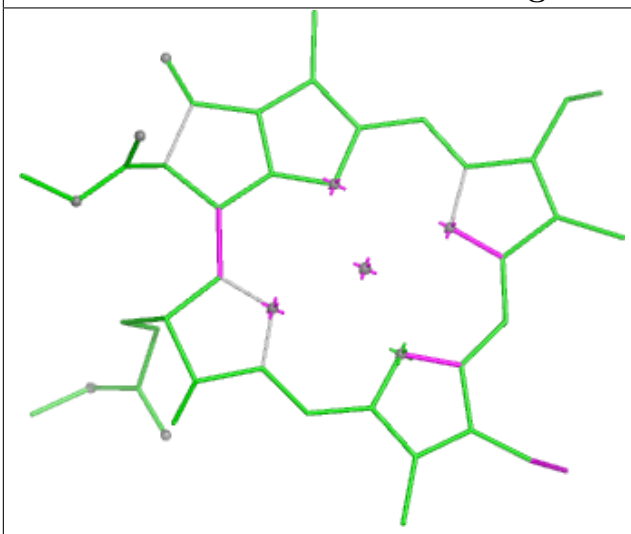


Rings

Ligand CLA 2 607



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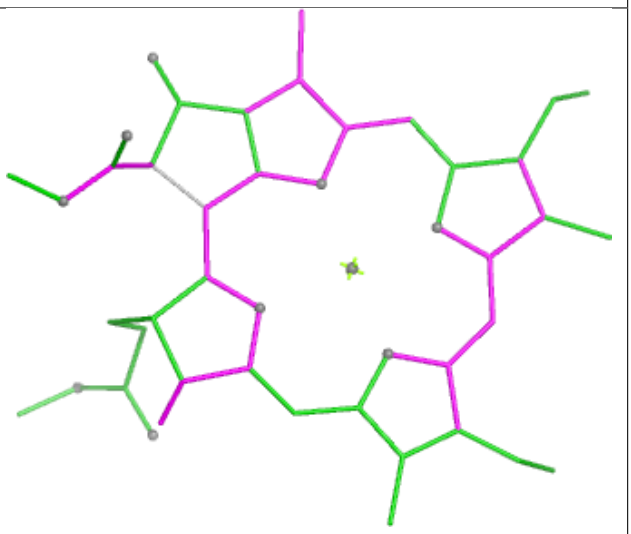
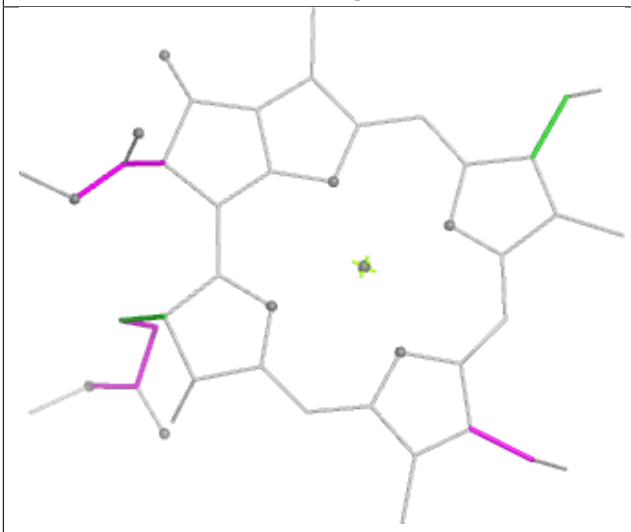


Bond angles



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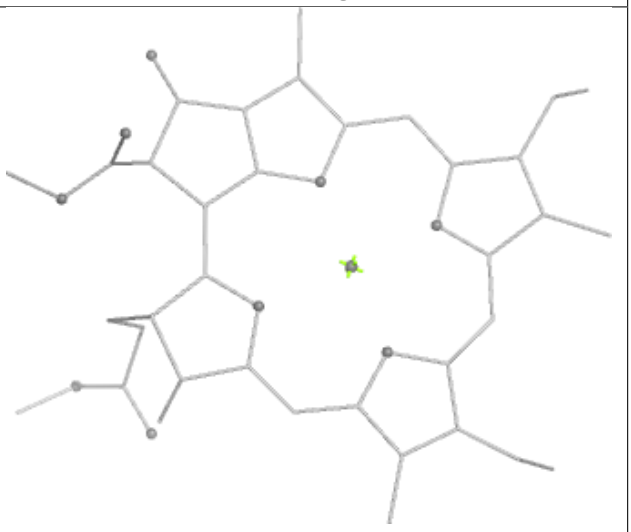
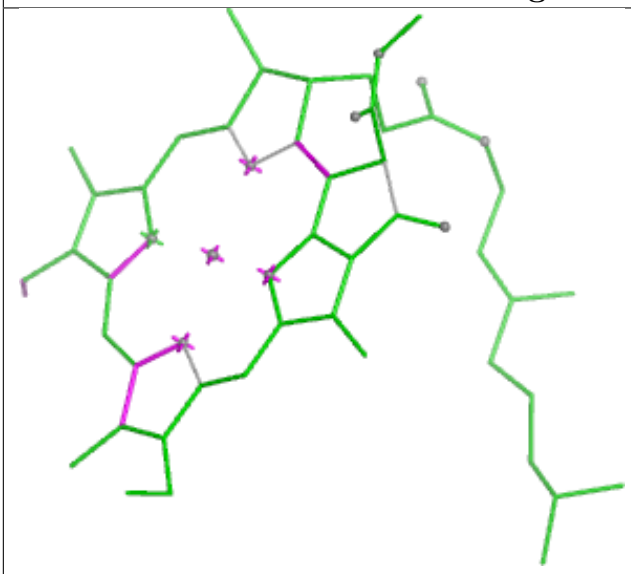


Rings

Ligand CLA 4 607



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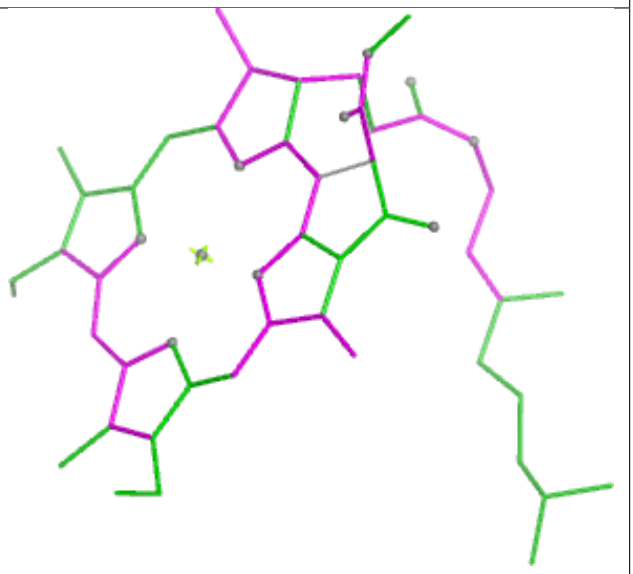
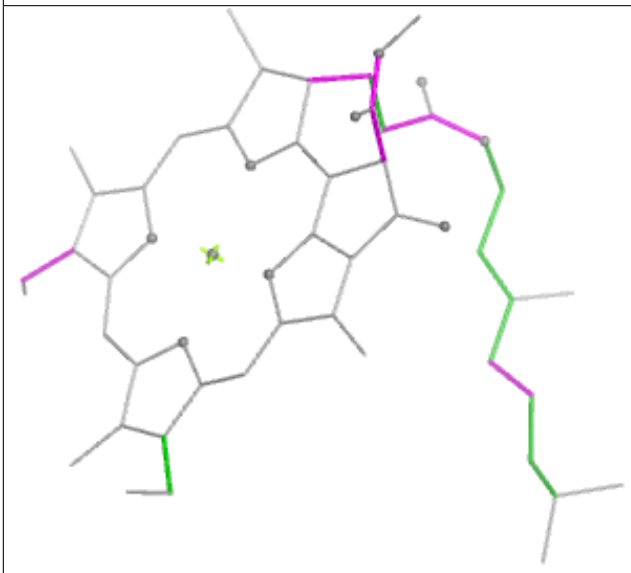


Bond angles

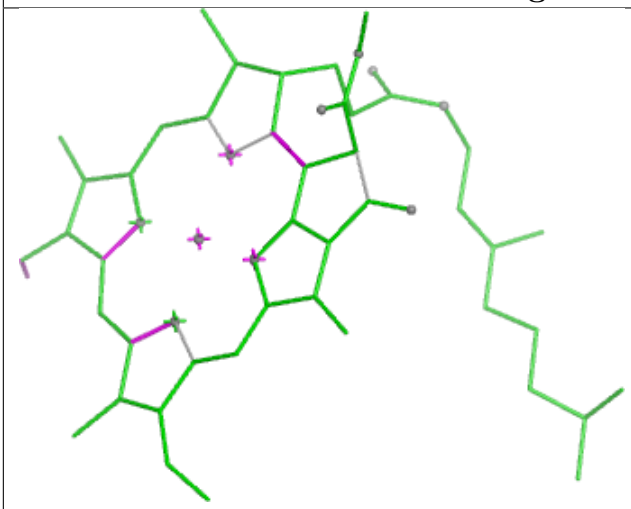


Torsions



Rings

Ligand CLA 9 607



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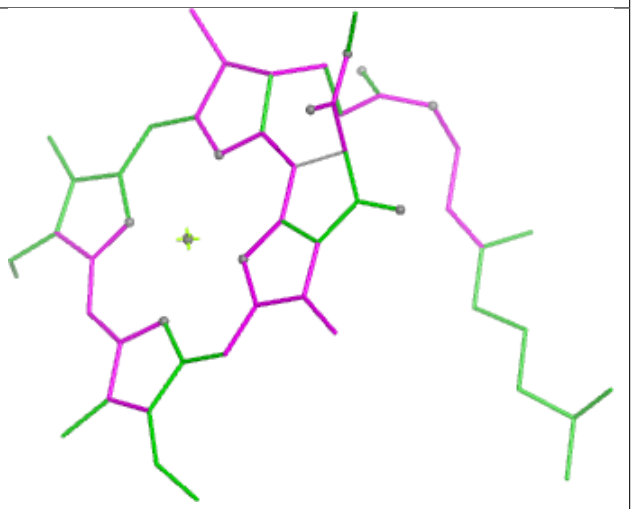

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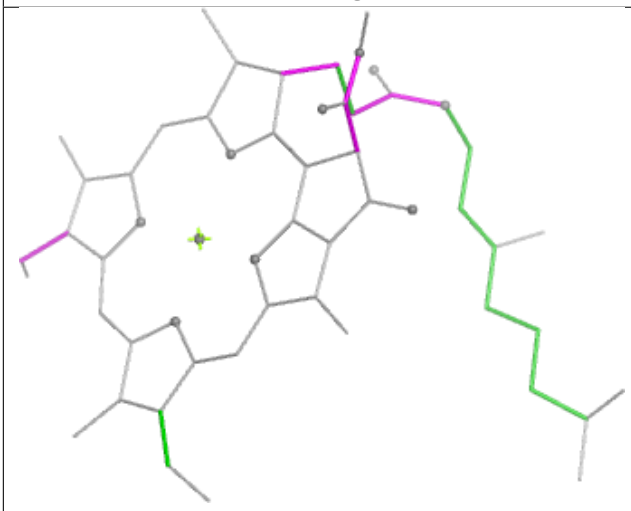

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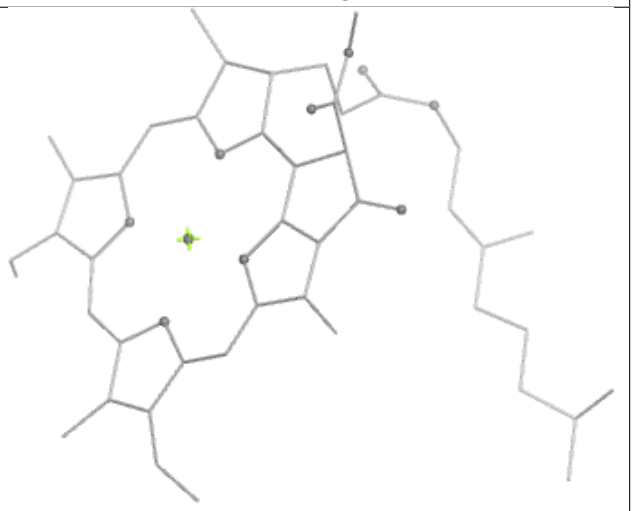
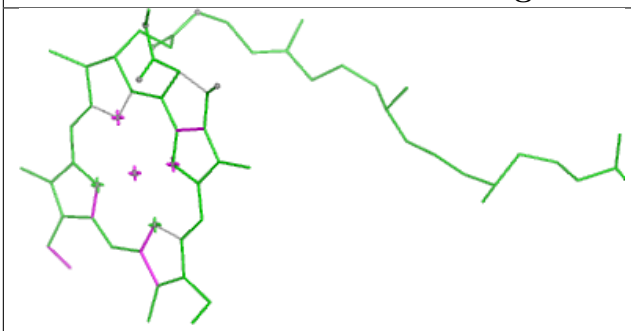


Rings

Ligand CLA A 1121



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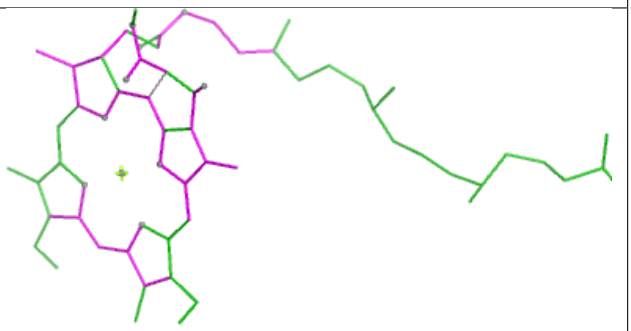
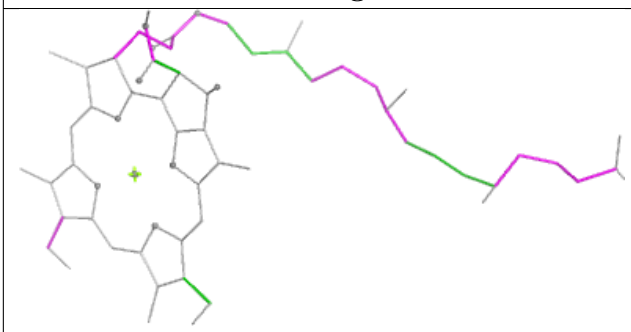


Bond angles

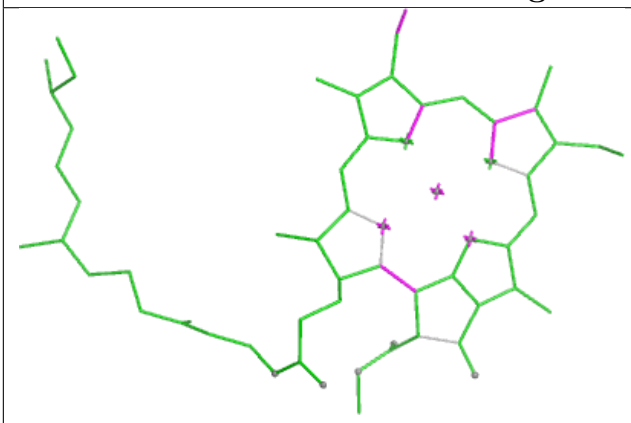


Torsions



Rings

Ligand CLA 7 605



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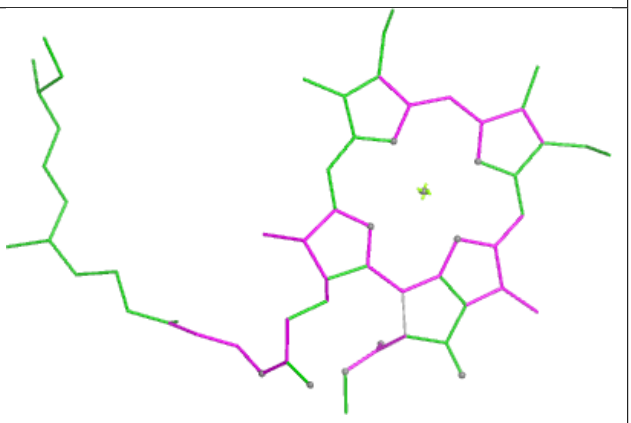
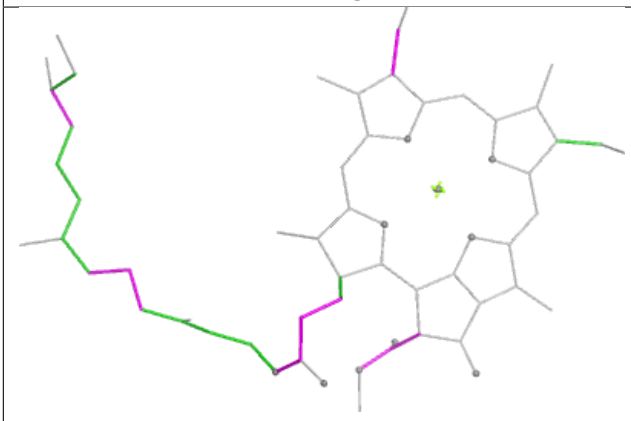
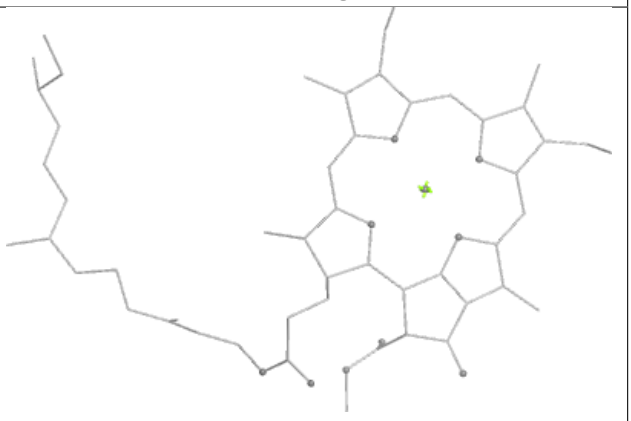


Bond angles

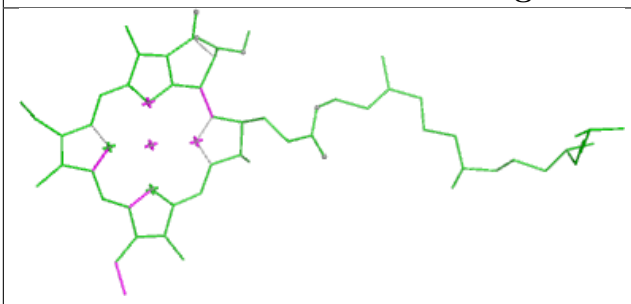


Torsions



Rings

Ligand CLA A 1103



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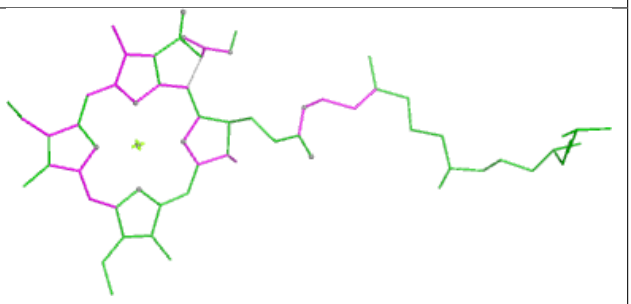
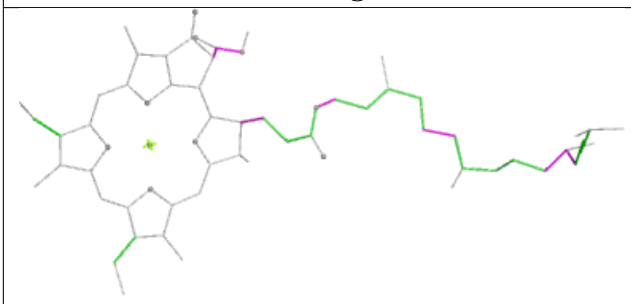


Bond angles



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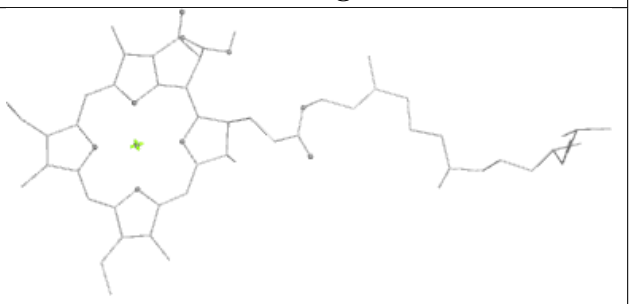
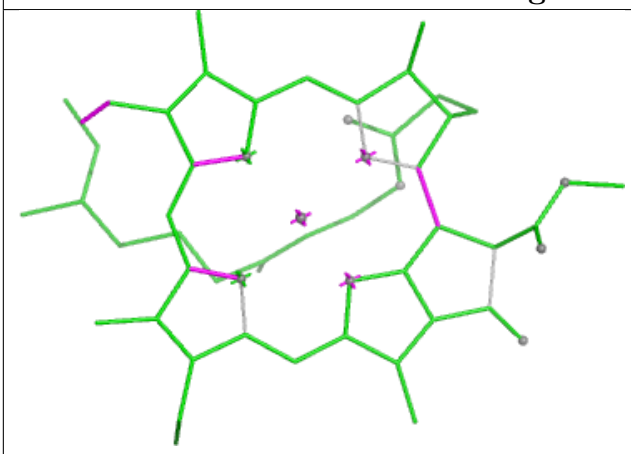
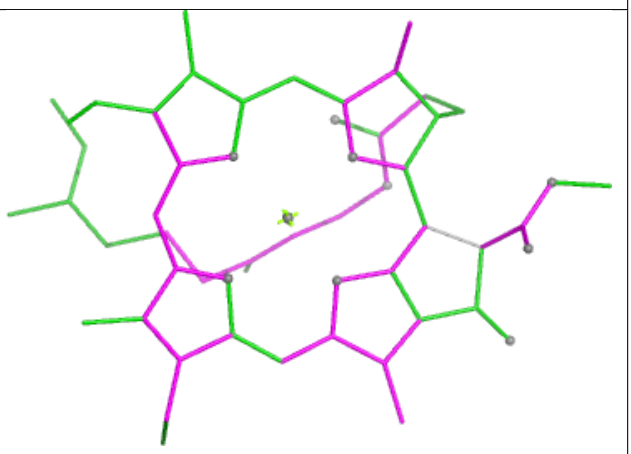


Rings

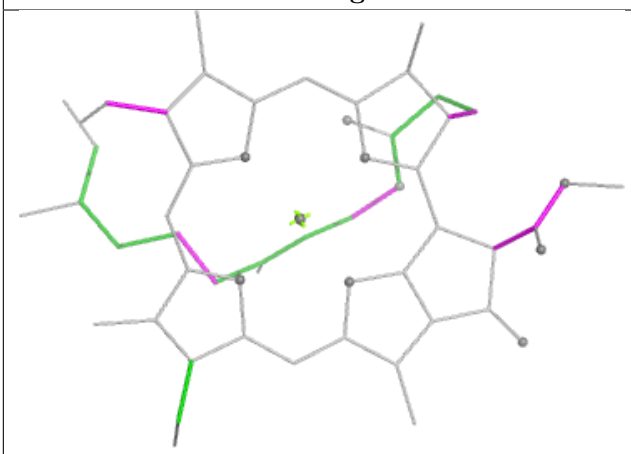
Ligand CLA 5 603



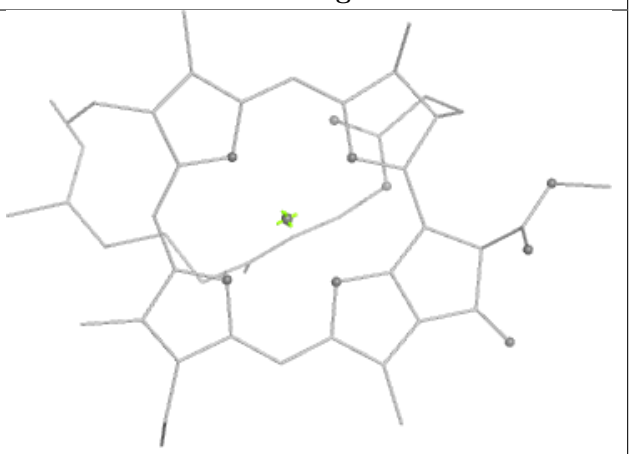
Bond lengths



Bond angles

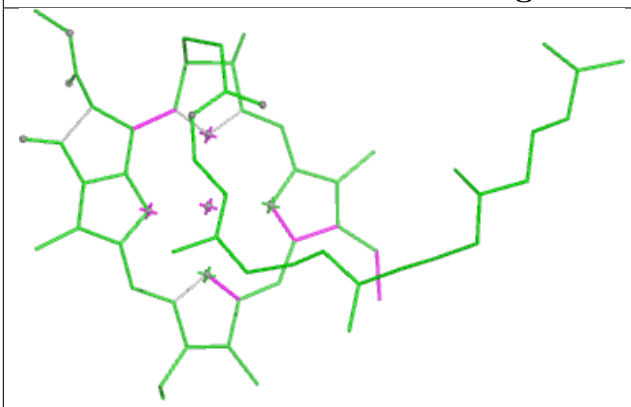


Torsions



Rings

Ligand CLA B 1209



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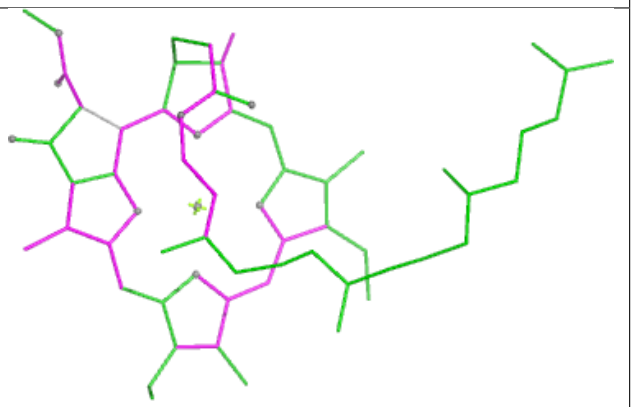

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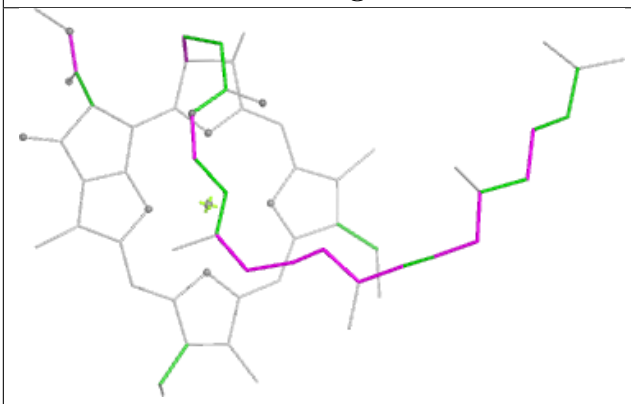

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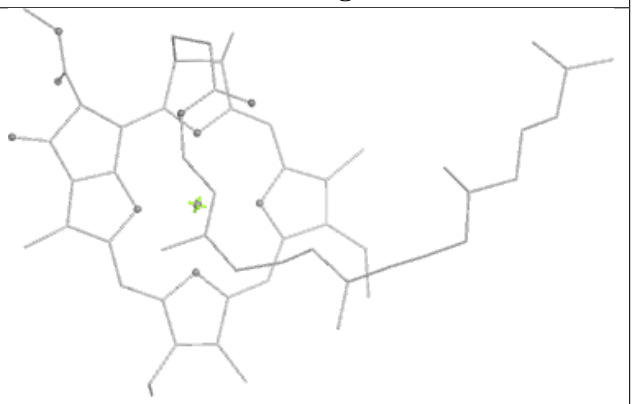
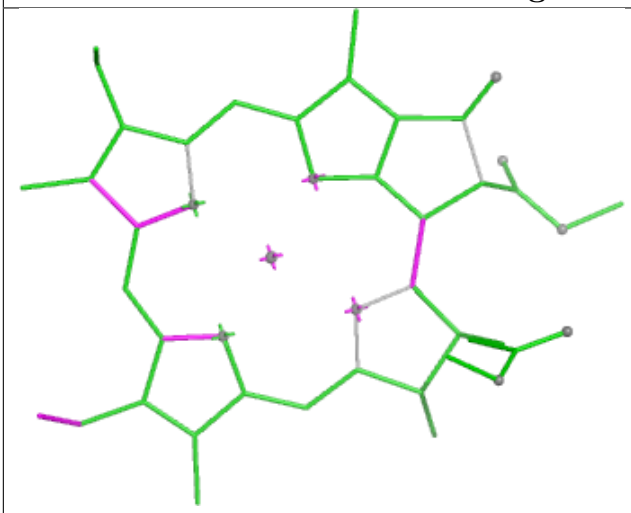


Rings

Ligand CLA 8 615



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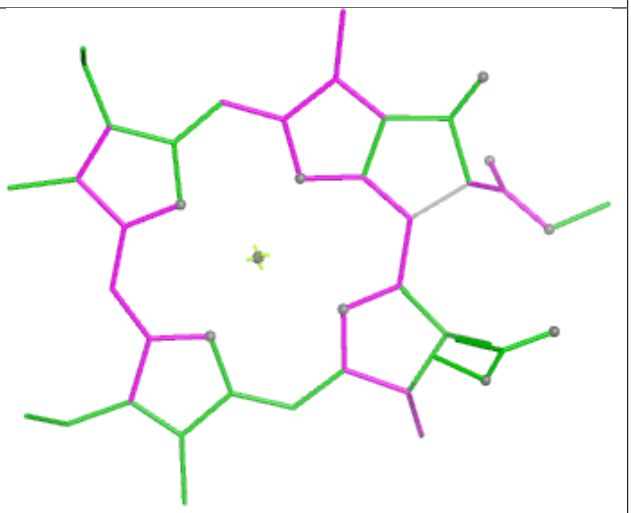
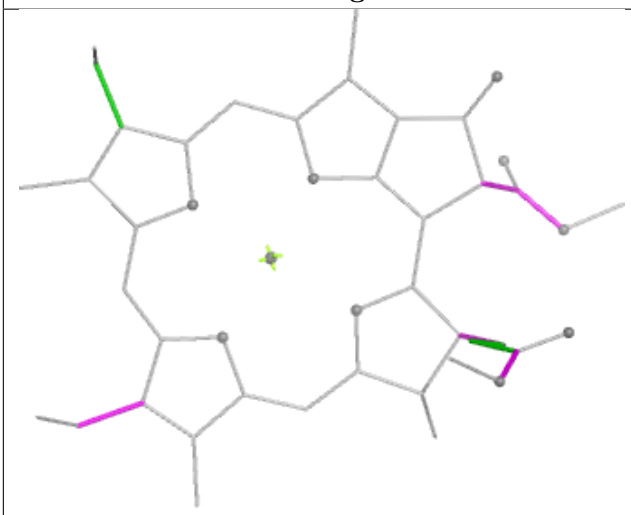


Bond angles



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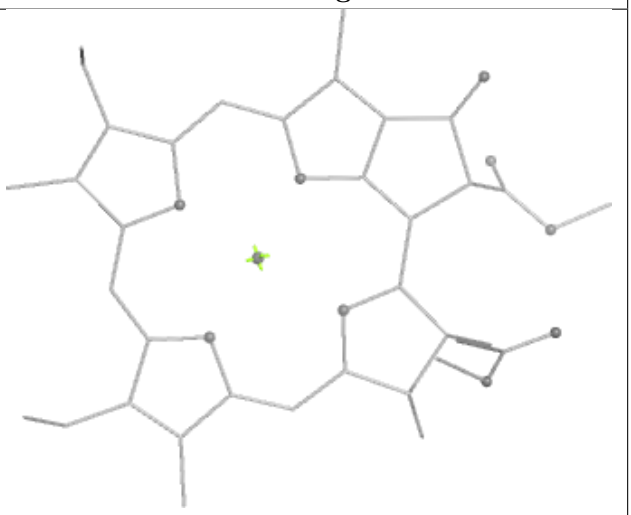
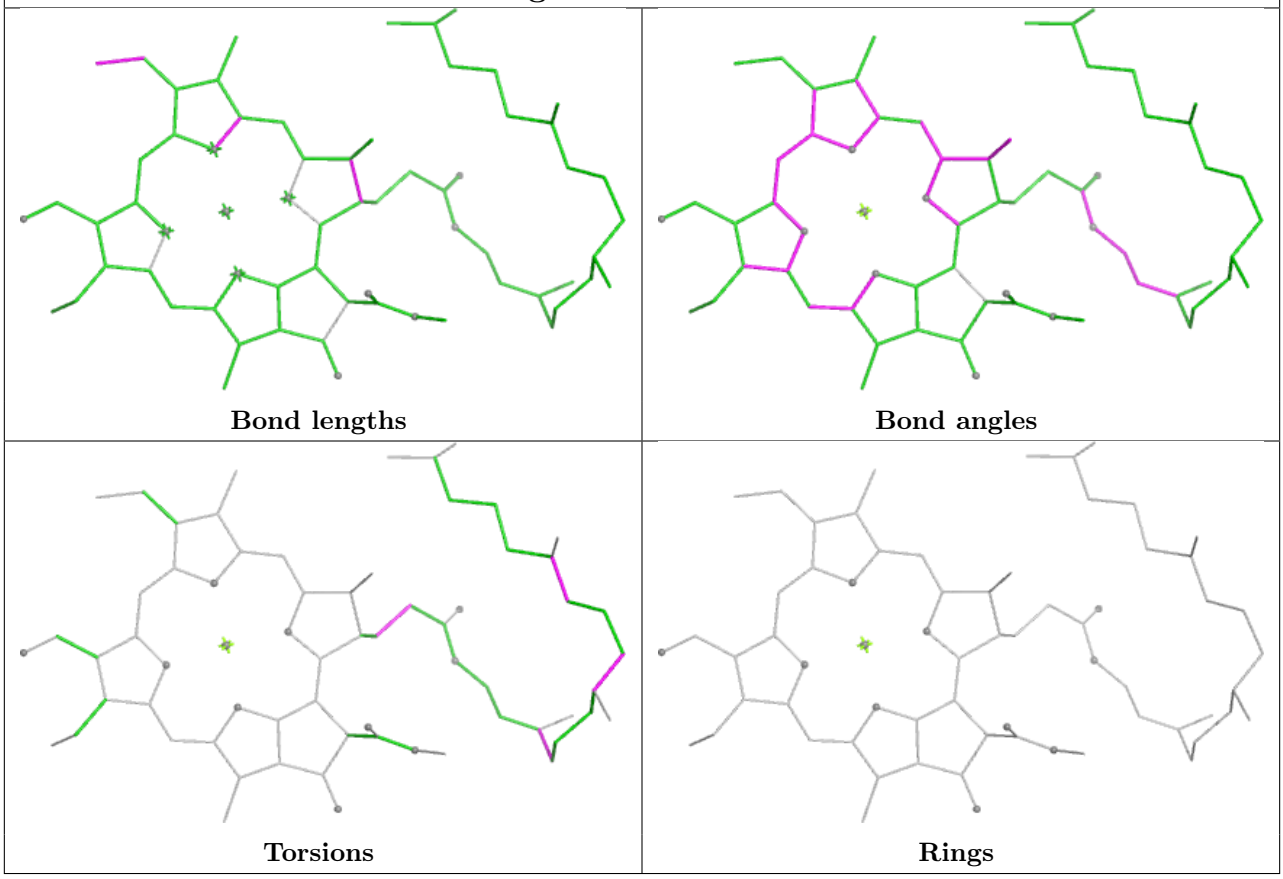


Rings

Ligand CHL 9 610



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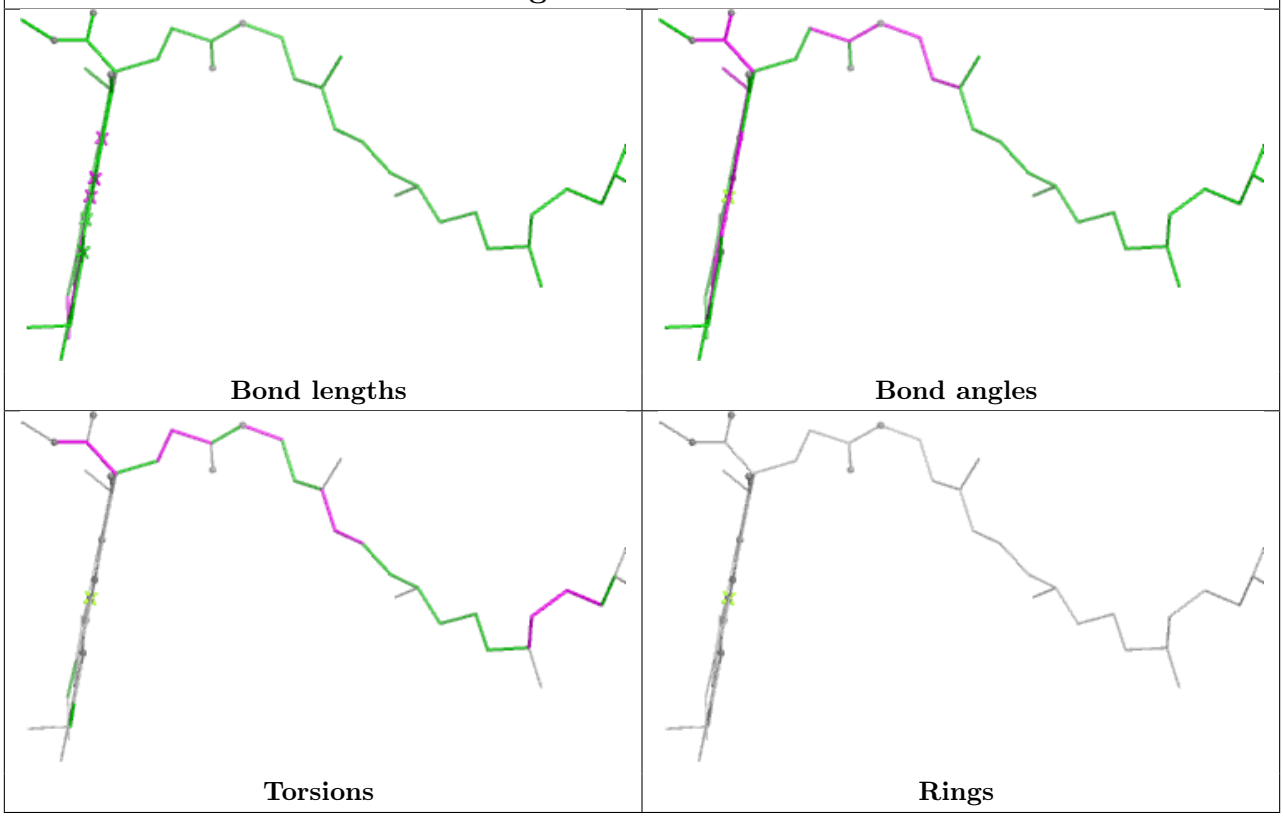

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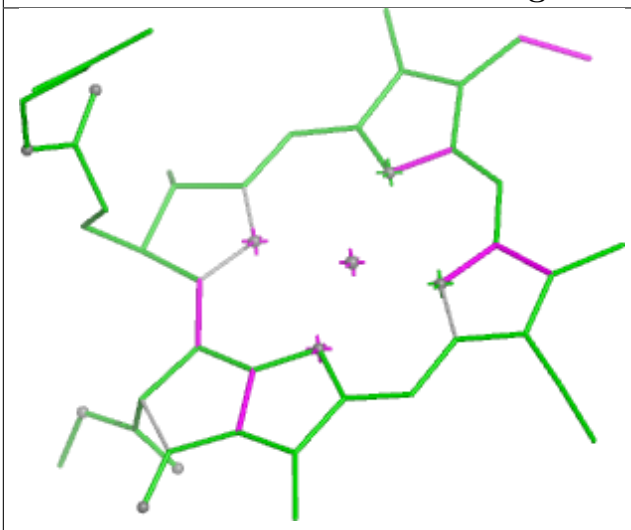

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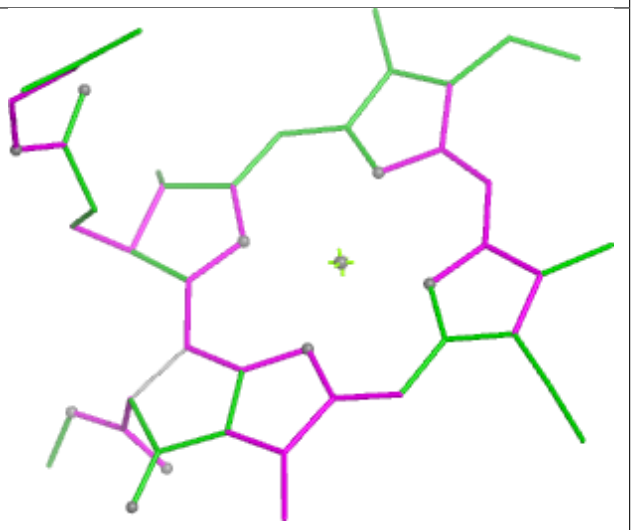
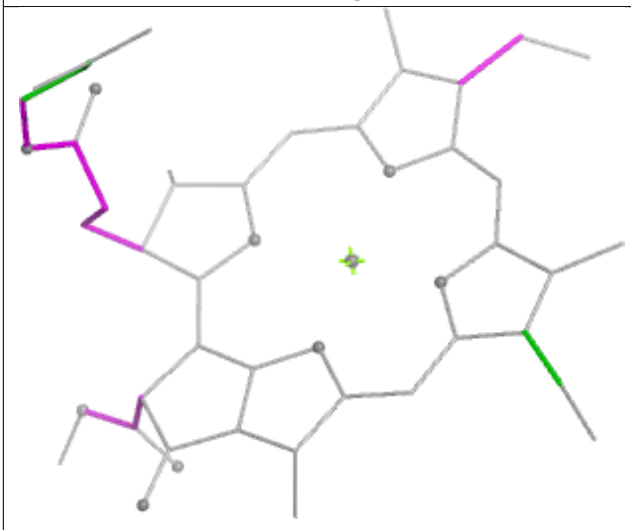


Bond angles



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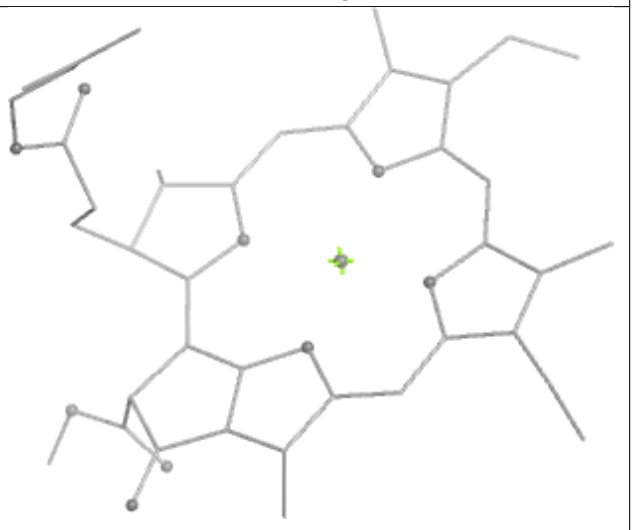
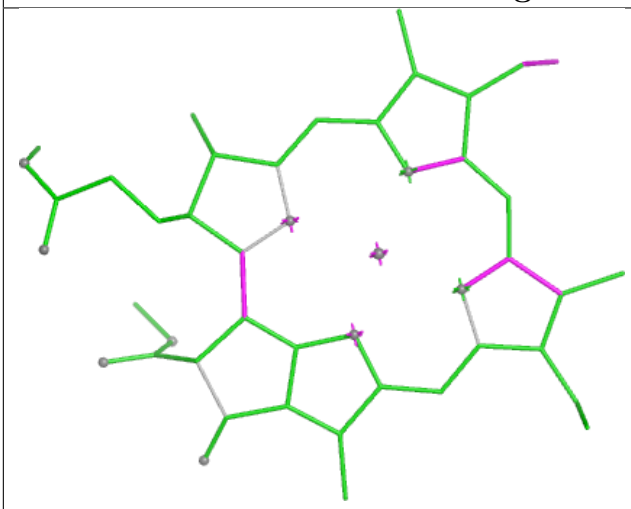


Rings

Ligand CLA G 1602



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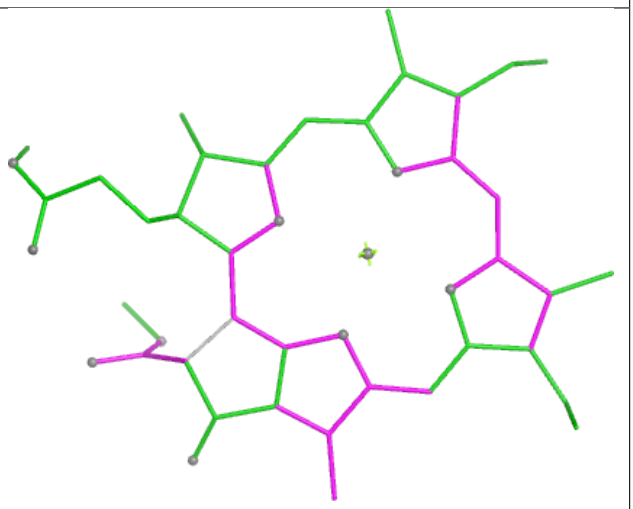
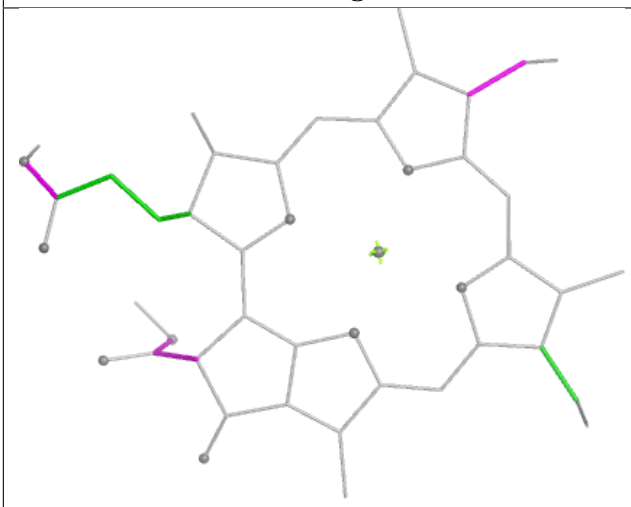


Bond angles



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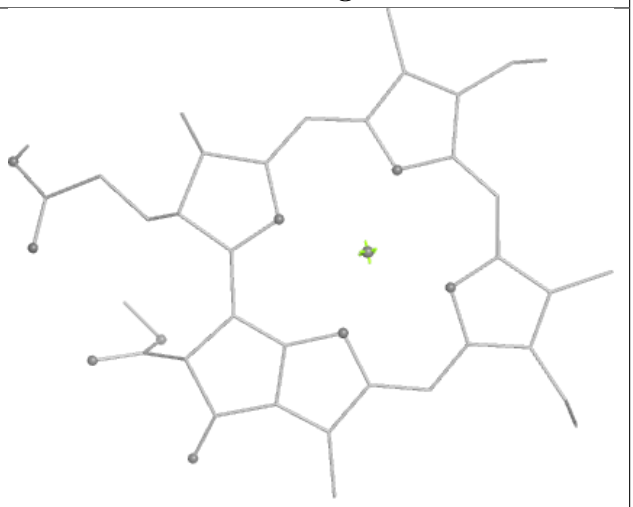
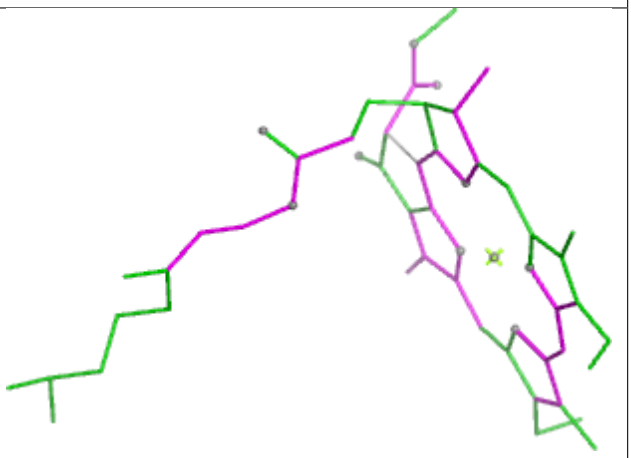


Rings

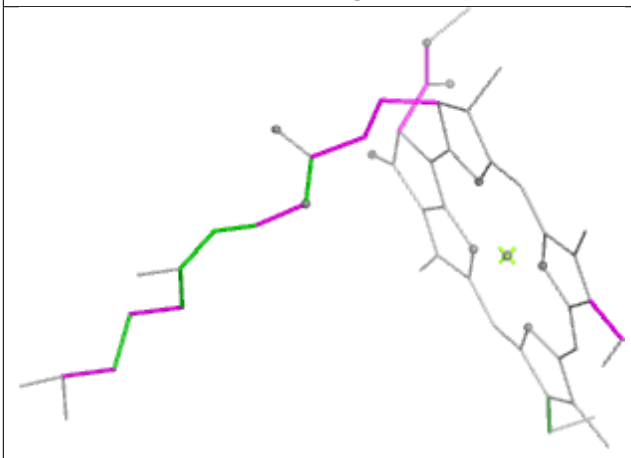
Ligand CLA A 1134



Bond lengths



Bond angles

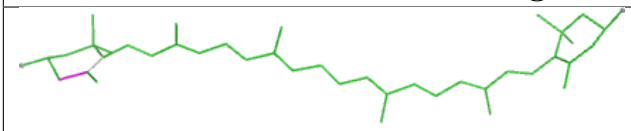


Torsions



Rings

Ligand LUT 1 501



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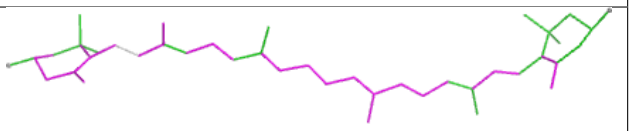
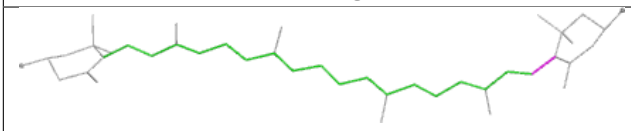


Bond angles



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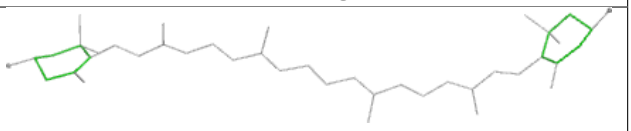
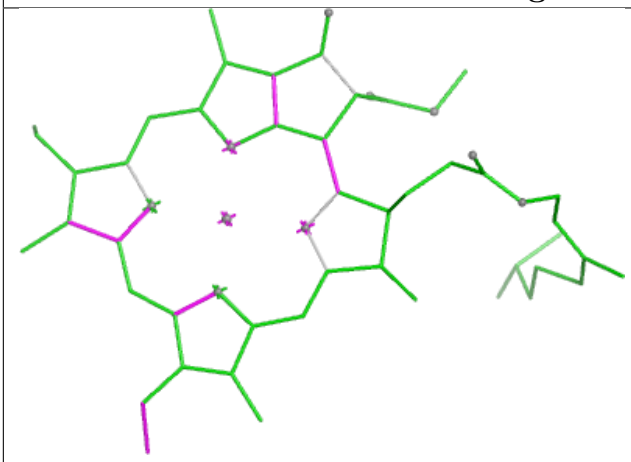


Rings

Ligand CLA 5 605



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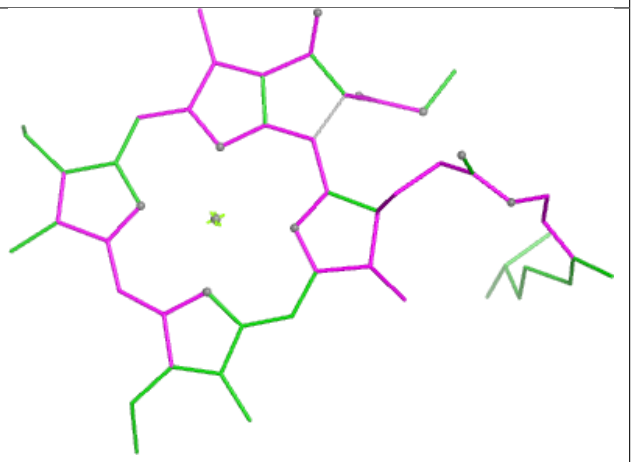
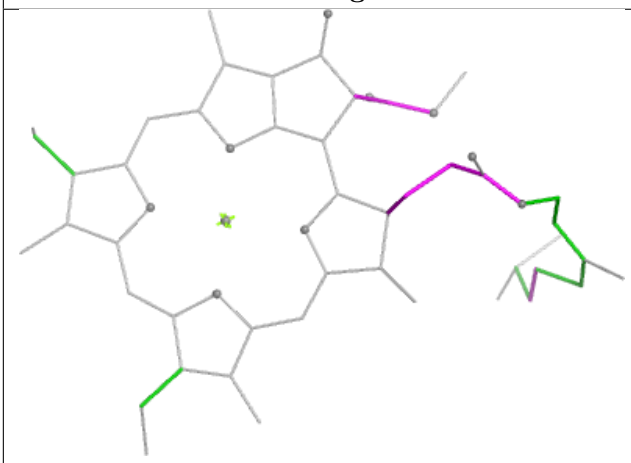


Bond angles



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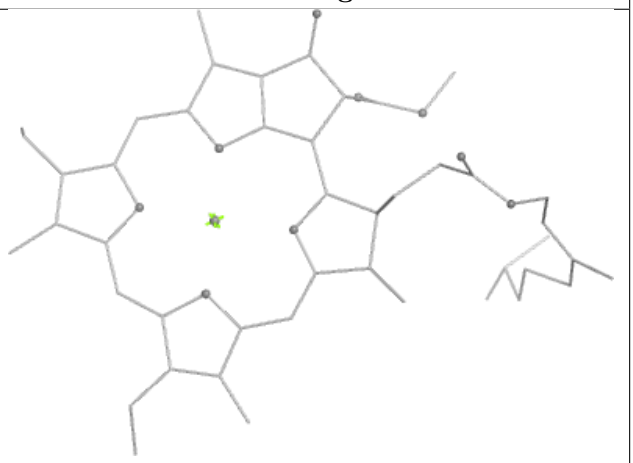
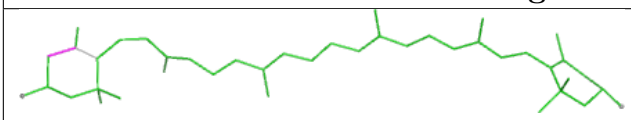


Rings

Ligand LUT 2 501



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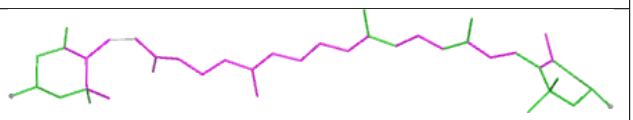
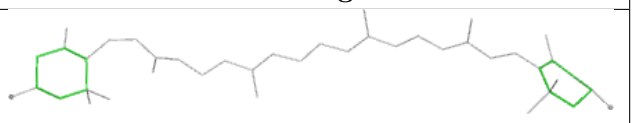


Bond angles

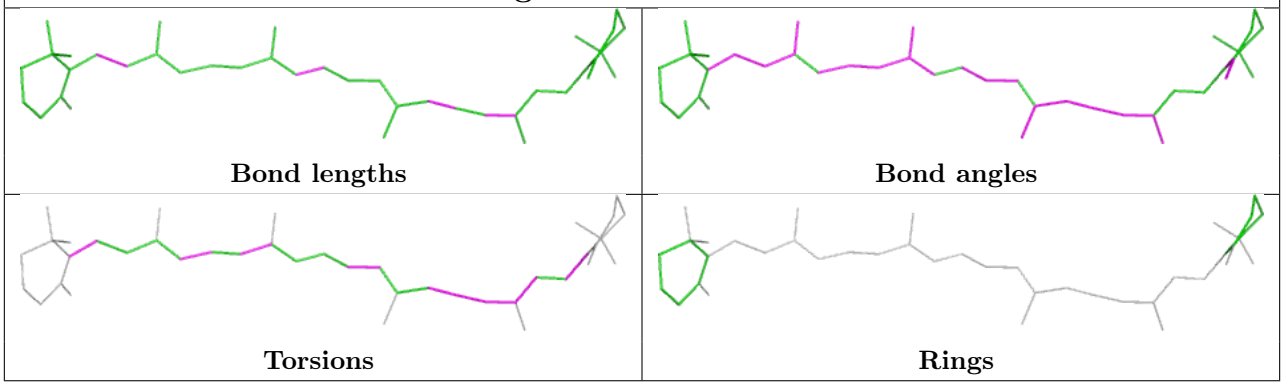


Torsions

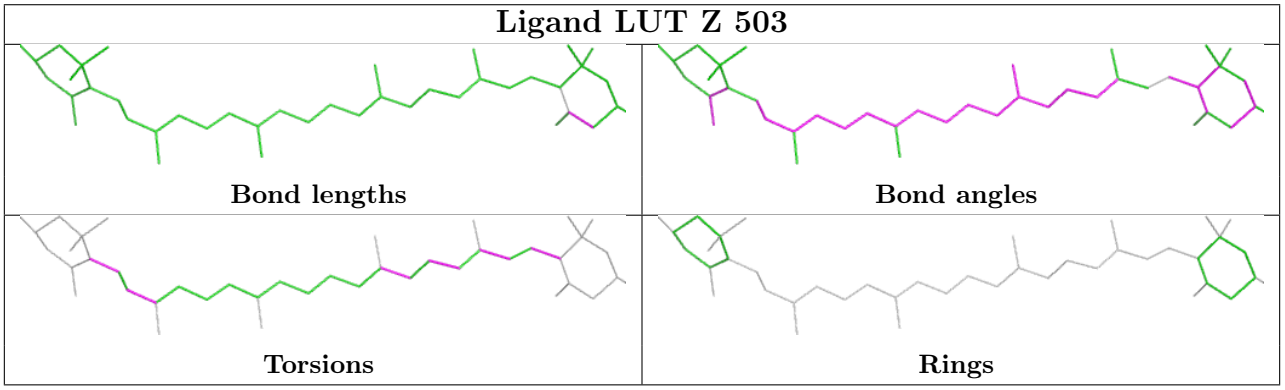


Rings

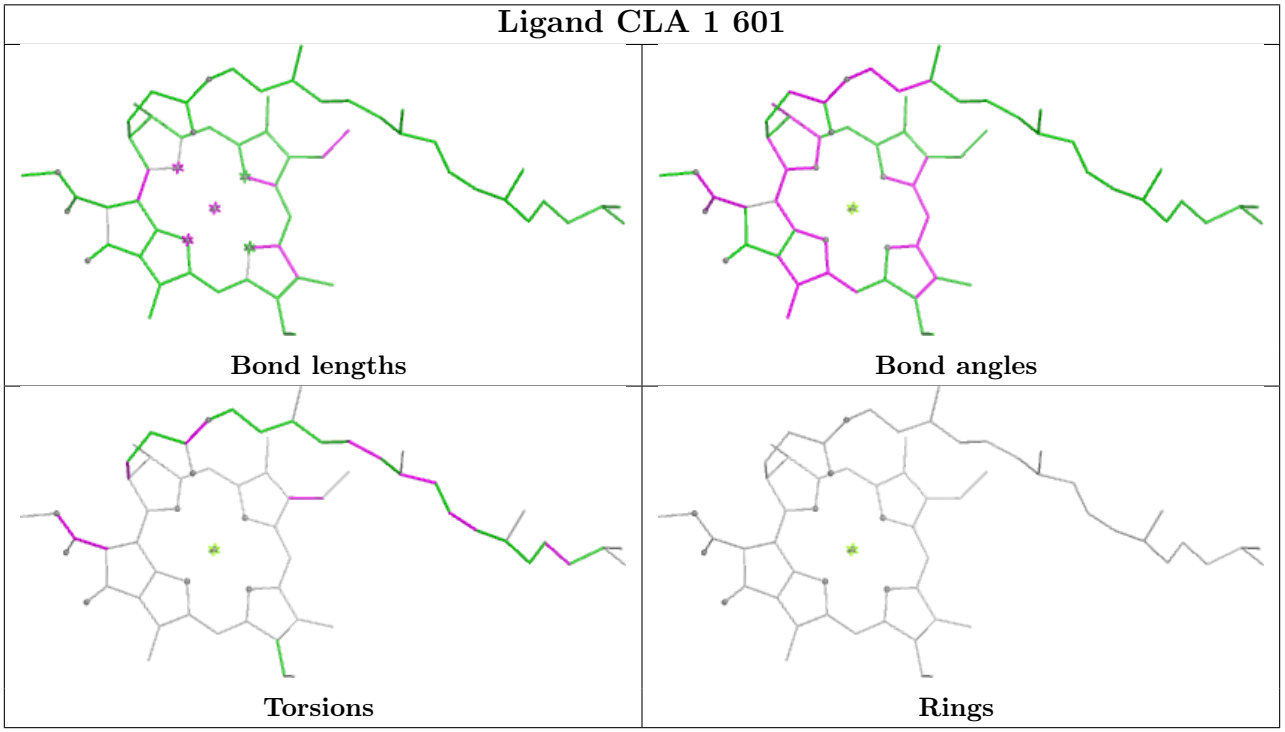
Ligand BCR B 4007



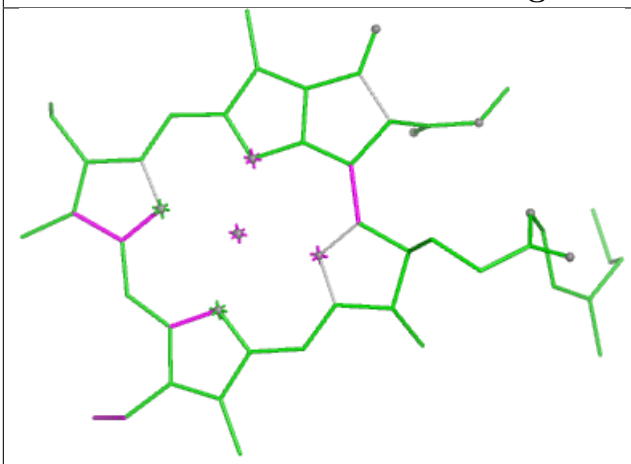
Ligand LUT Z 503



Ligand CLA 1 601



Ligand CLA 4 602



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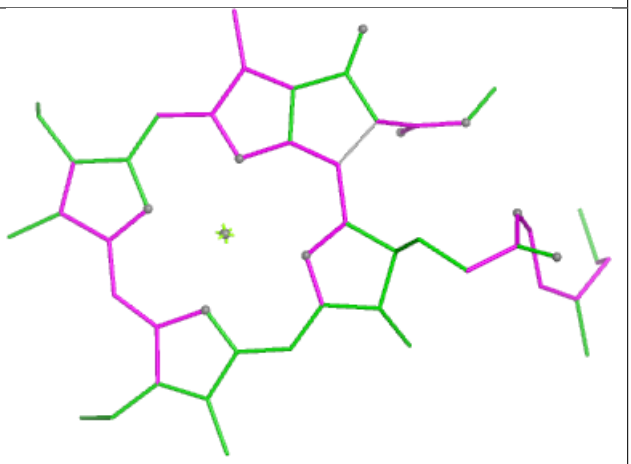
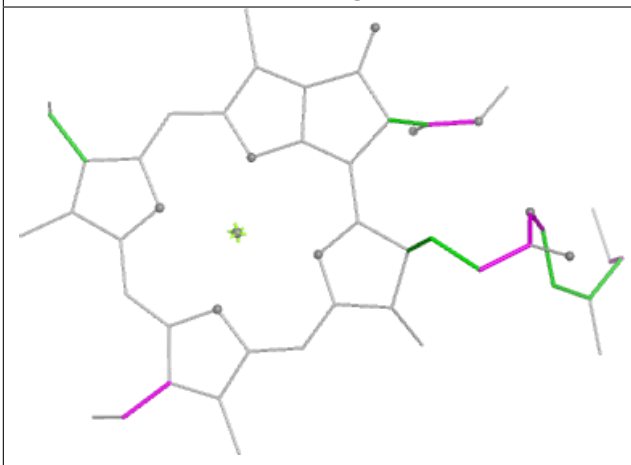


Bond angles



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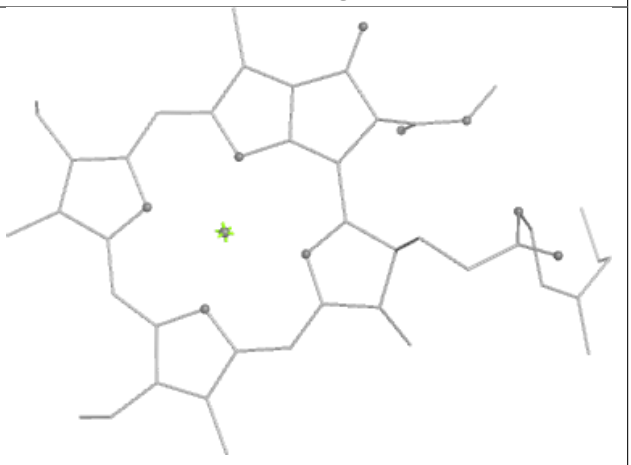
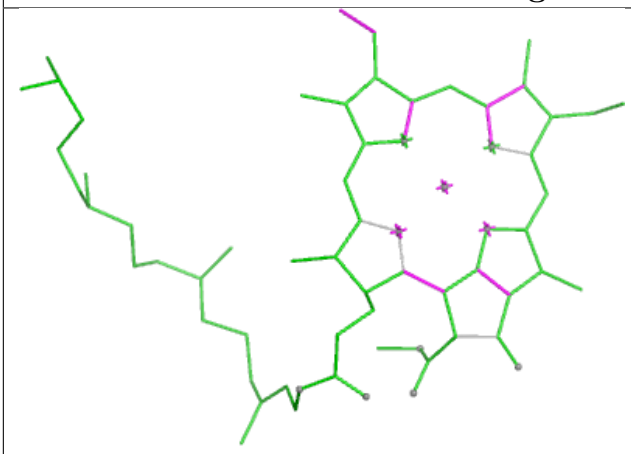


Rings

Ligand CLA 8 605



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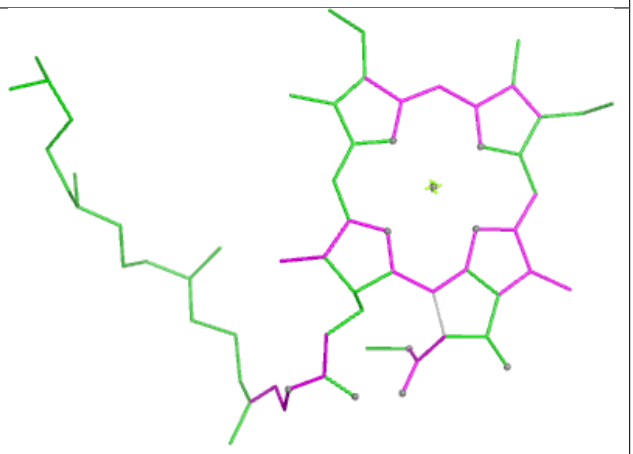
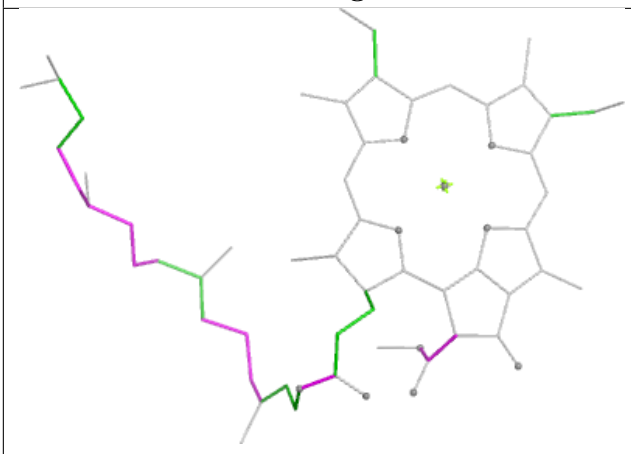


Bond angles



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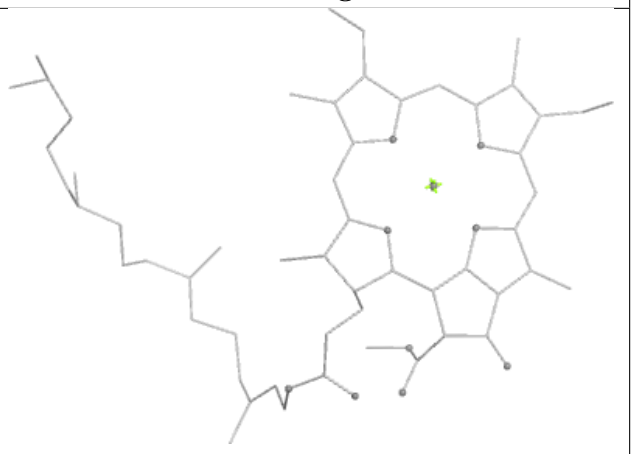
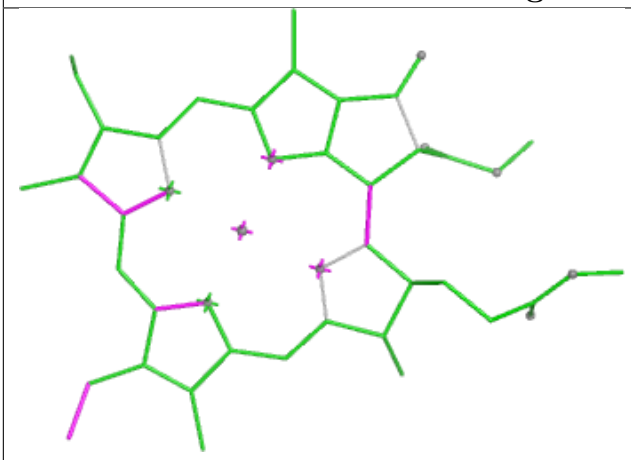


Rings

Ligand CLA Z 602



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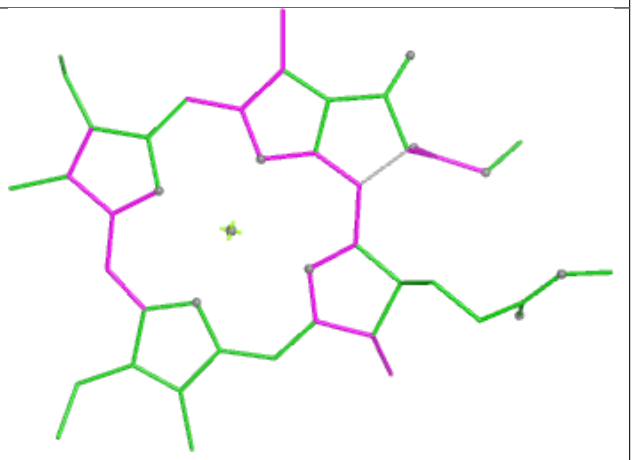
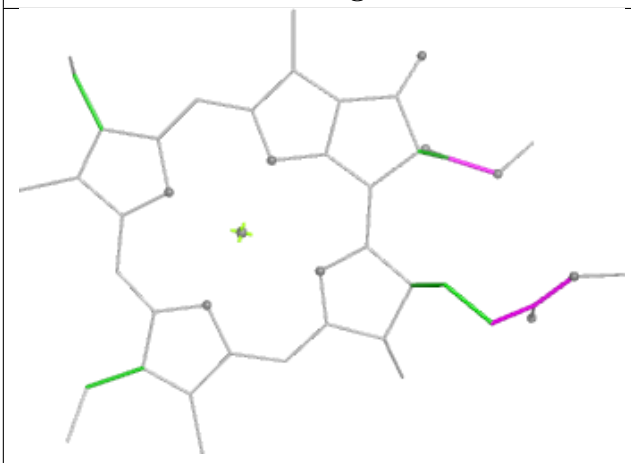


Bond angles



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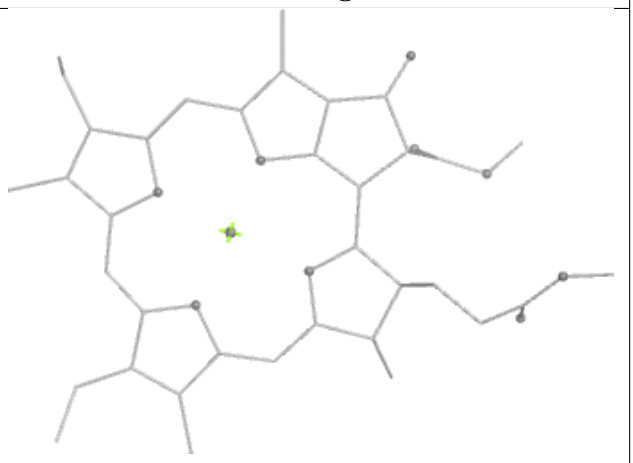
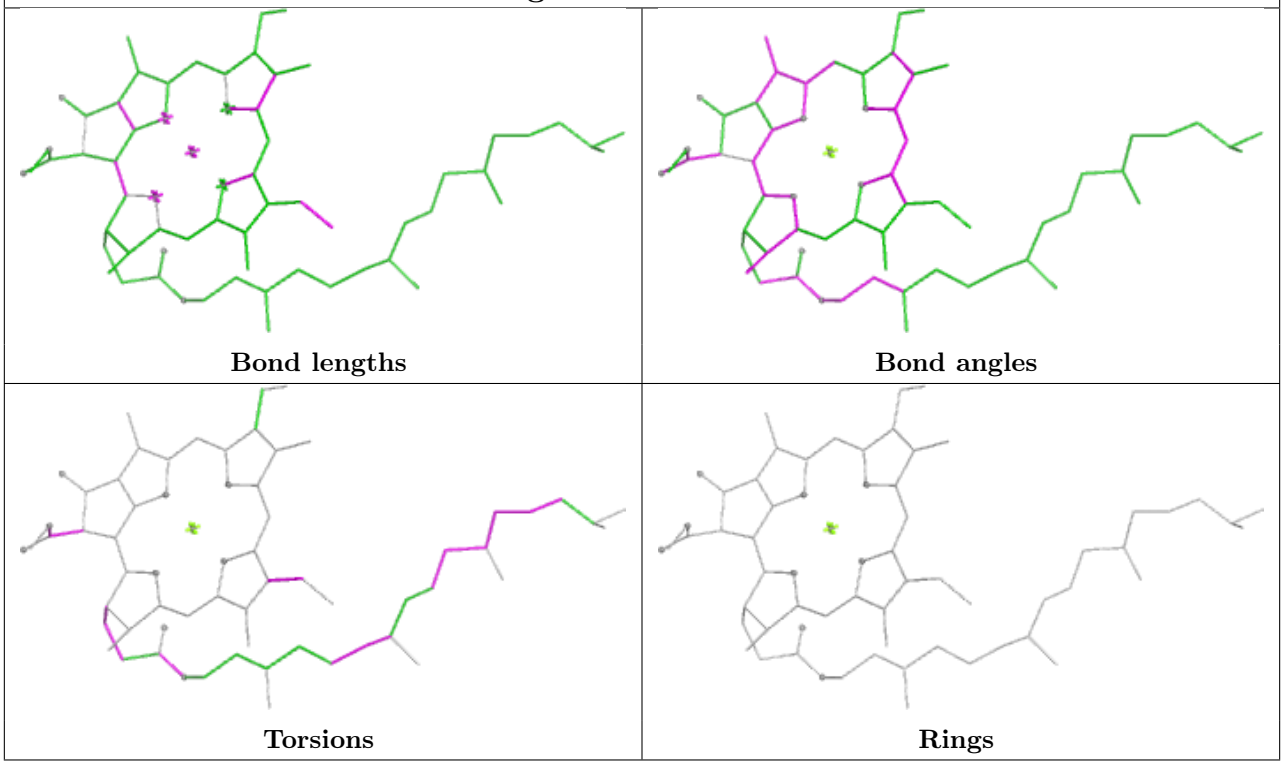
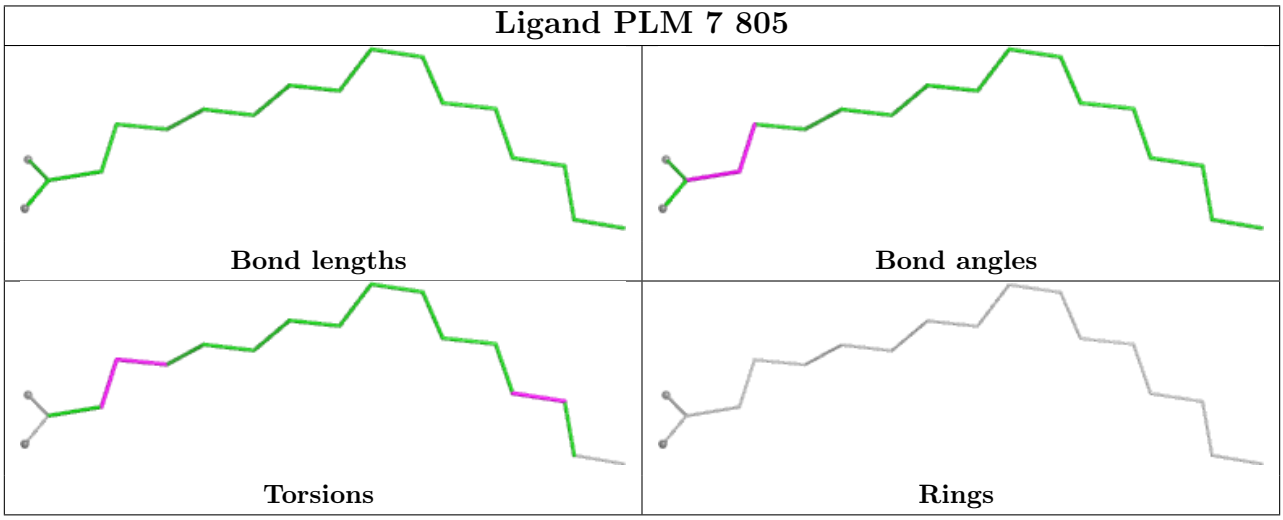


Rings

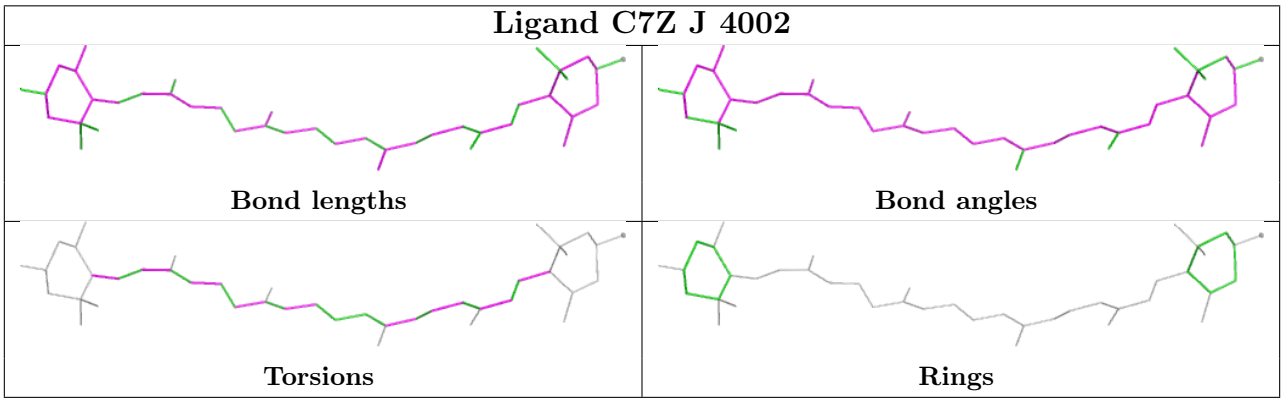
Ligand CLA Z 604



Ligand PLM 7 805



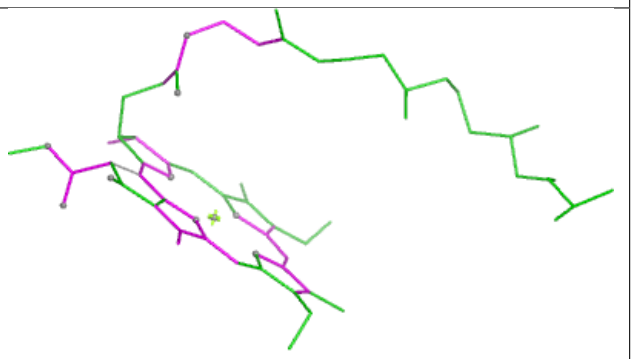
Ligand C7Z J 4002



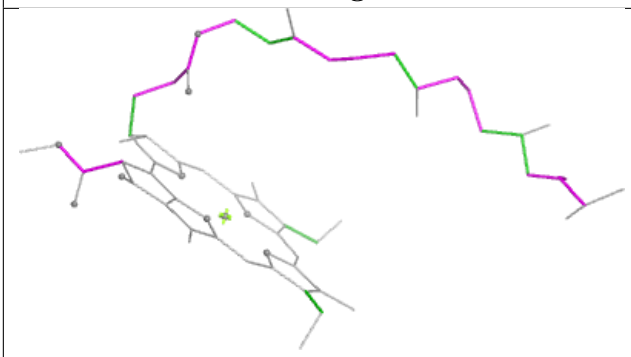
Ligand CLA B 1228



Bond lengths



Bond angles

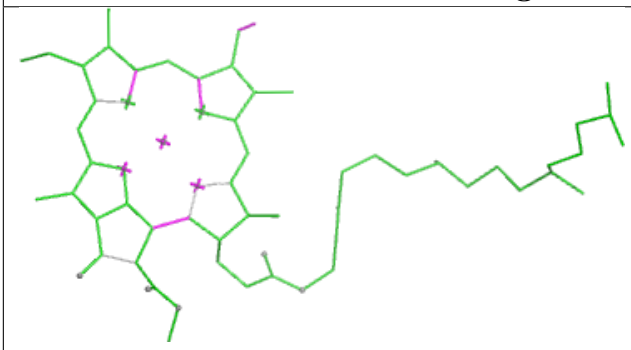


Torsions

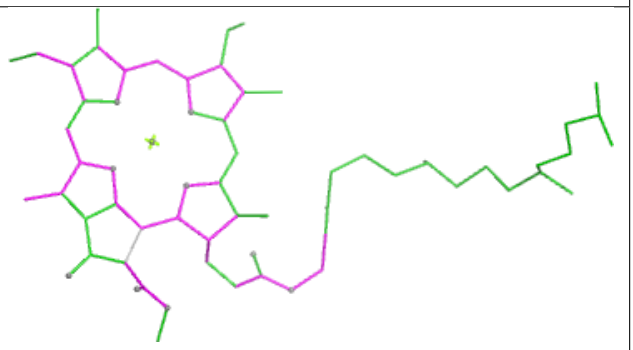


Rings

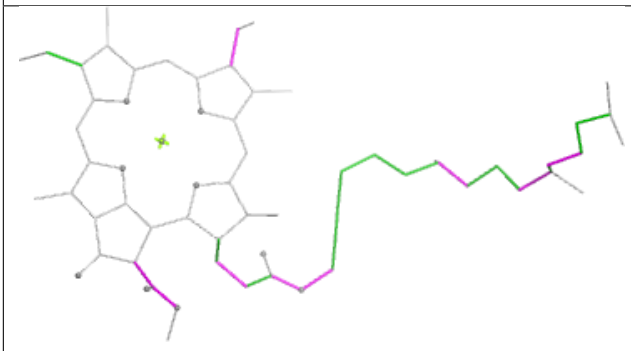
Ligand CLA B 1023



Bond lengths



Bond angles

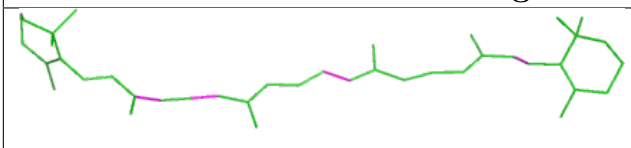


Torsions

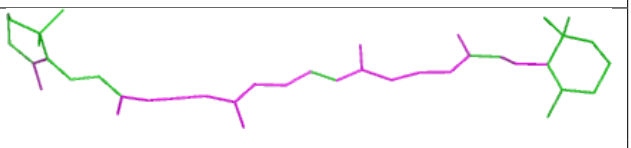


Rings

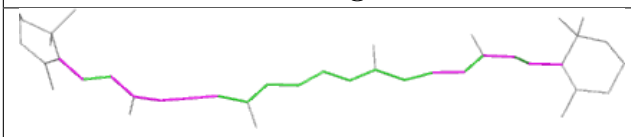
Ligand BCR G 4001



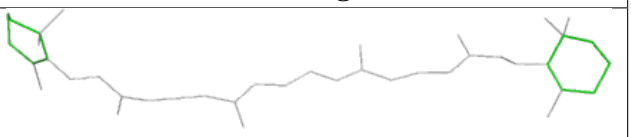
Bond lengths



Bond angles

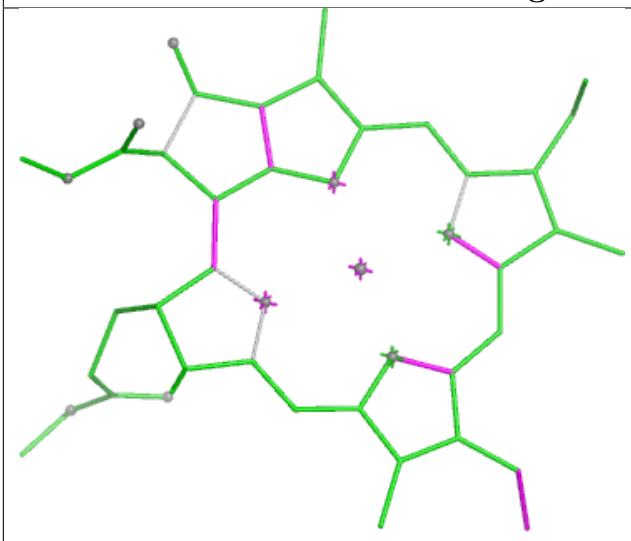


Torsions



Rings

Ligand CLA 8 612



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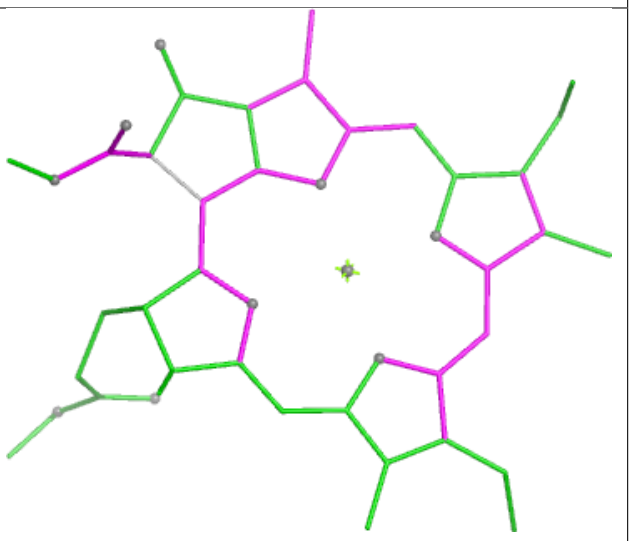

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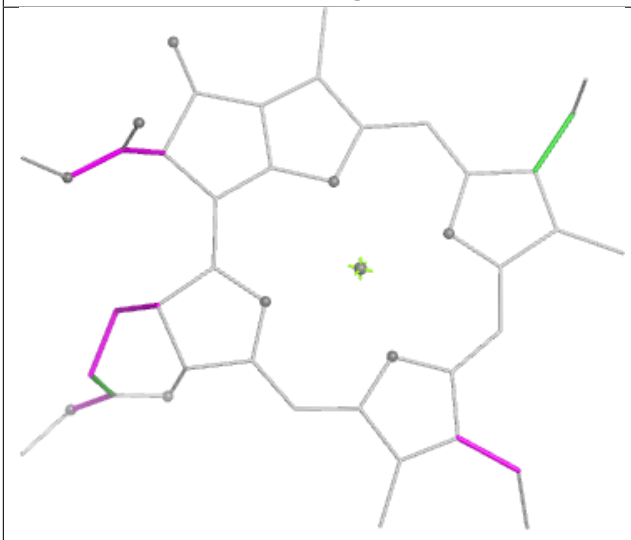

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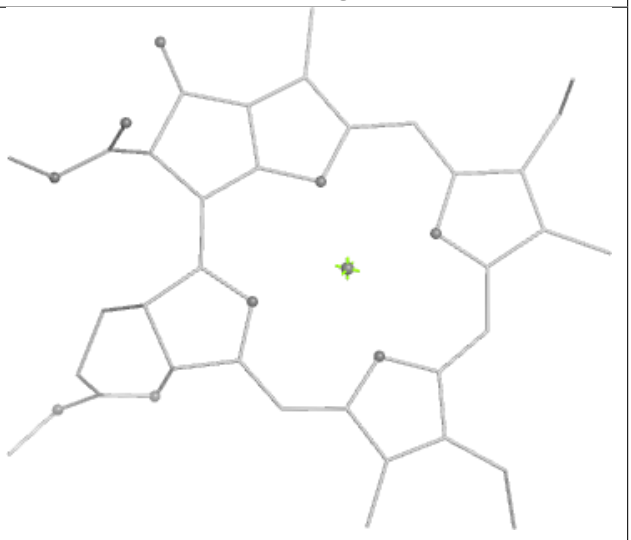
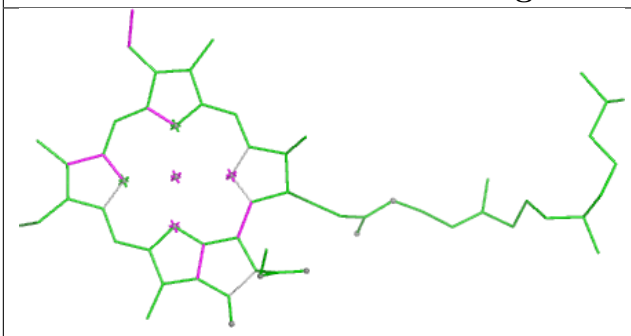


Rings

Ligand CLA B 1234



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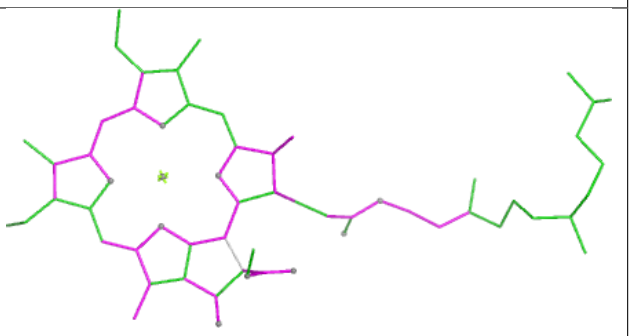
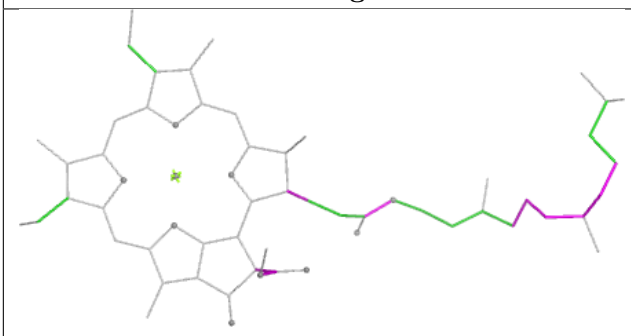


Bond angles



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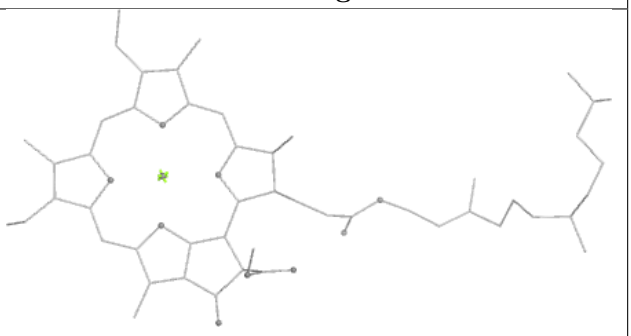
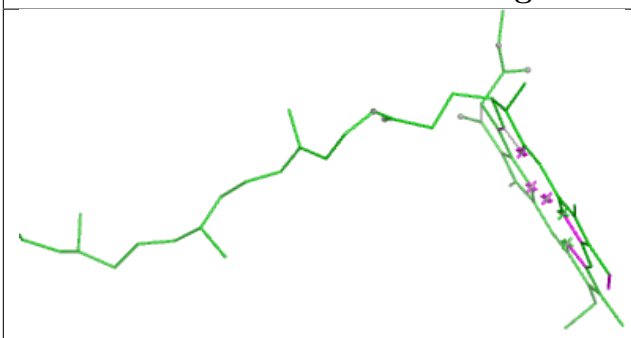


Rings

Ligand CLA A 1137



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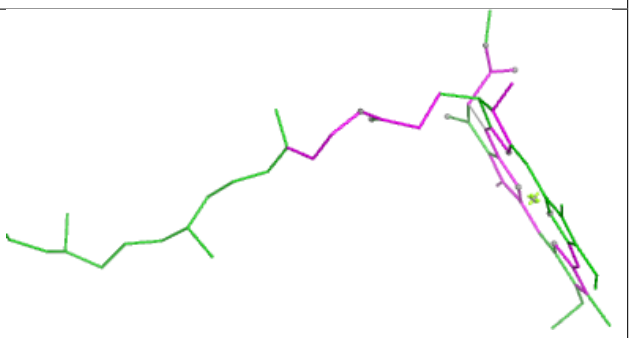
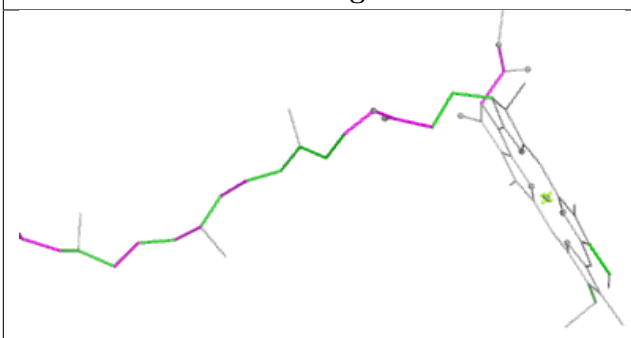


Bond angles



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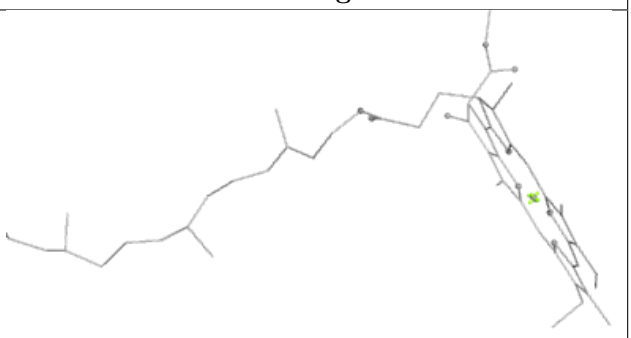
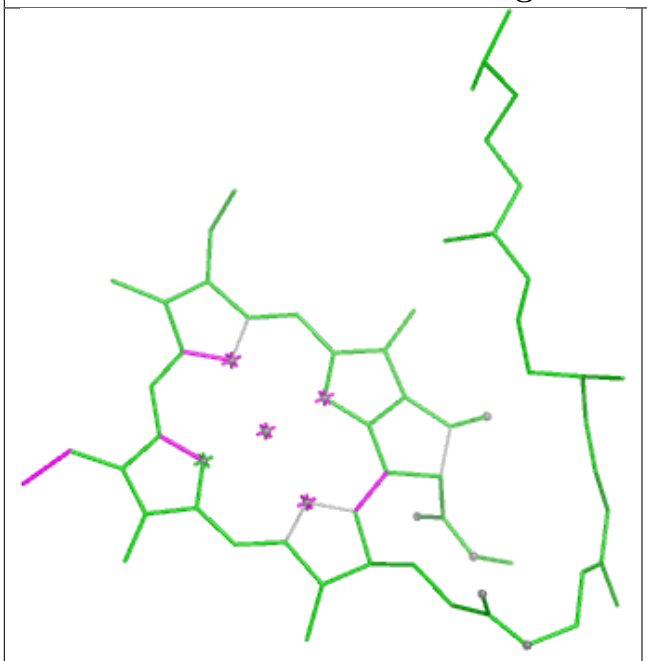


Rings

Ligand CLA A 1123



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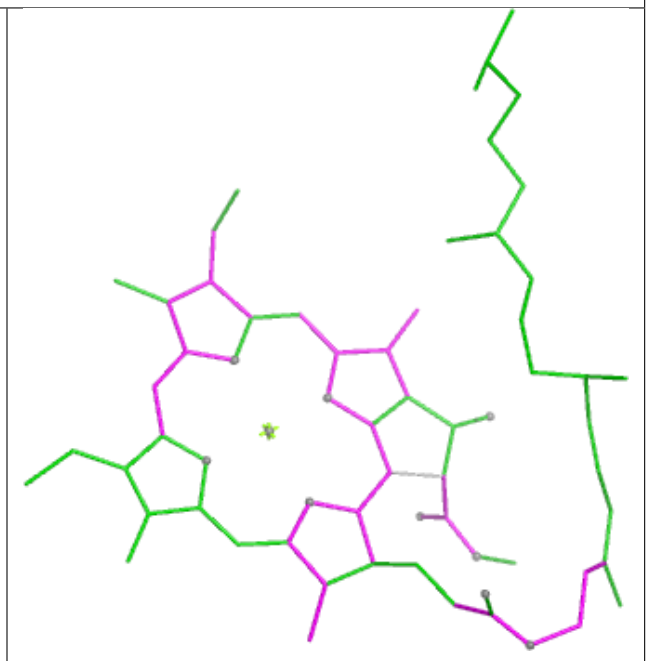
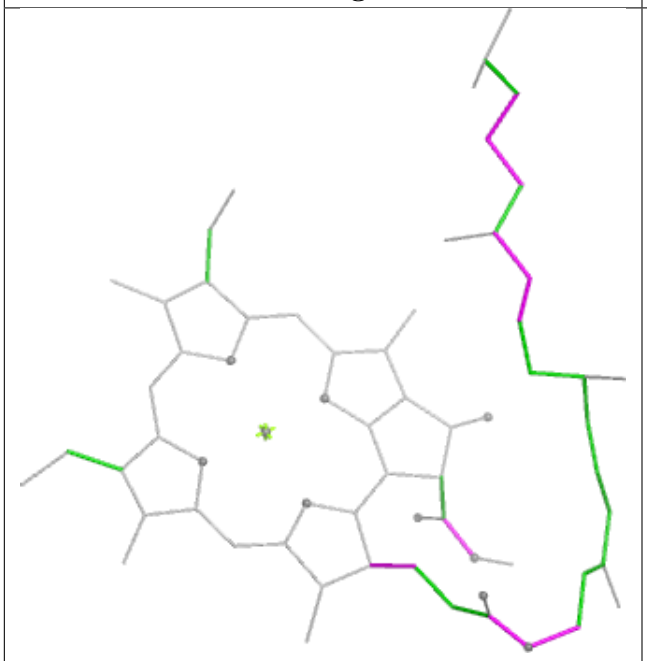


Bond angles



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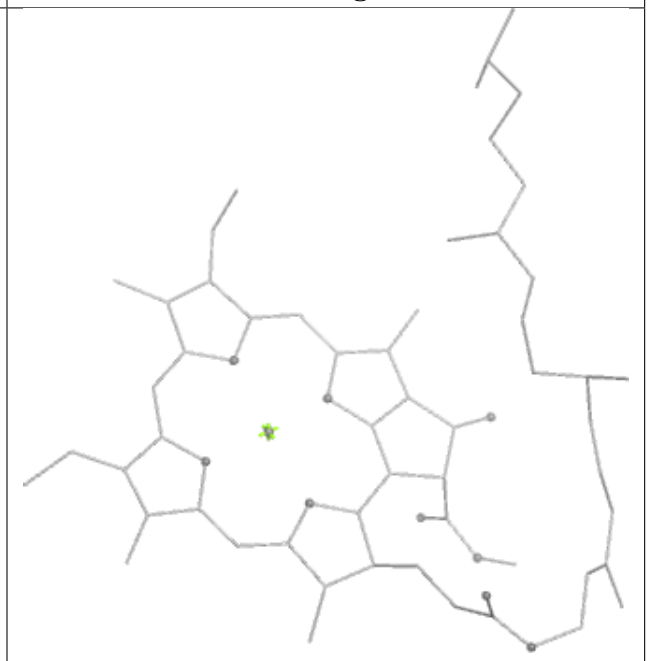
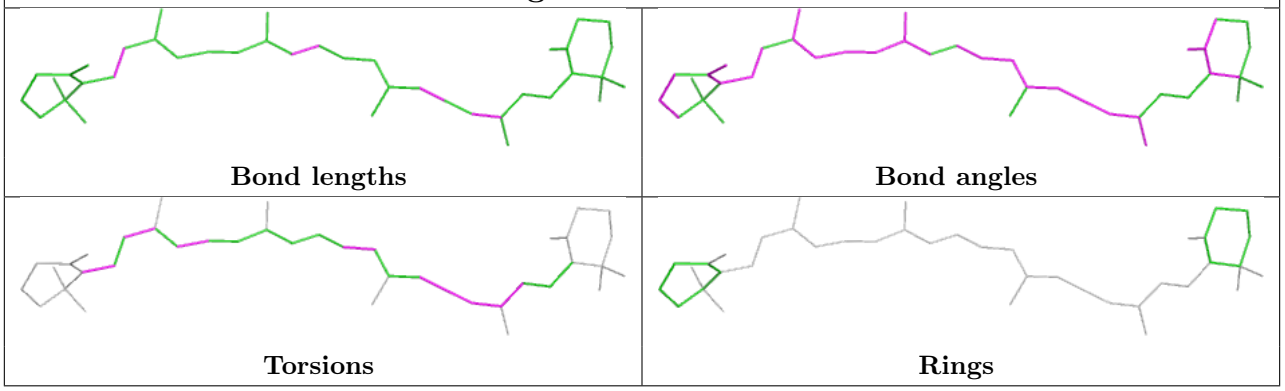
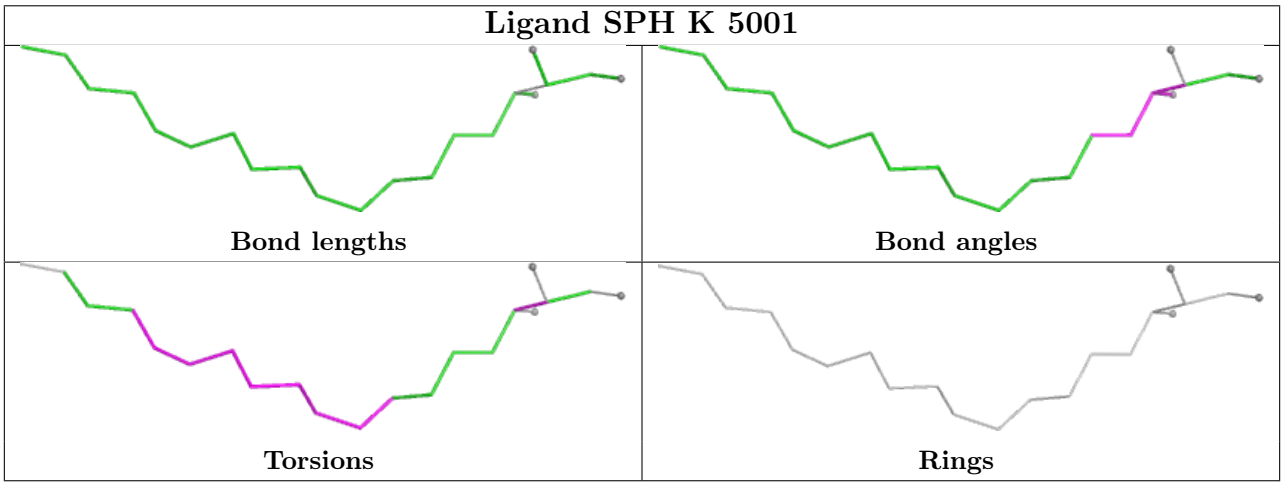


Rings

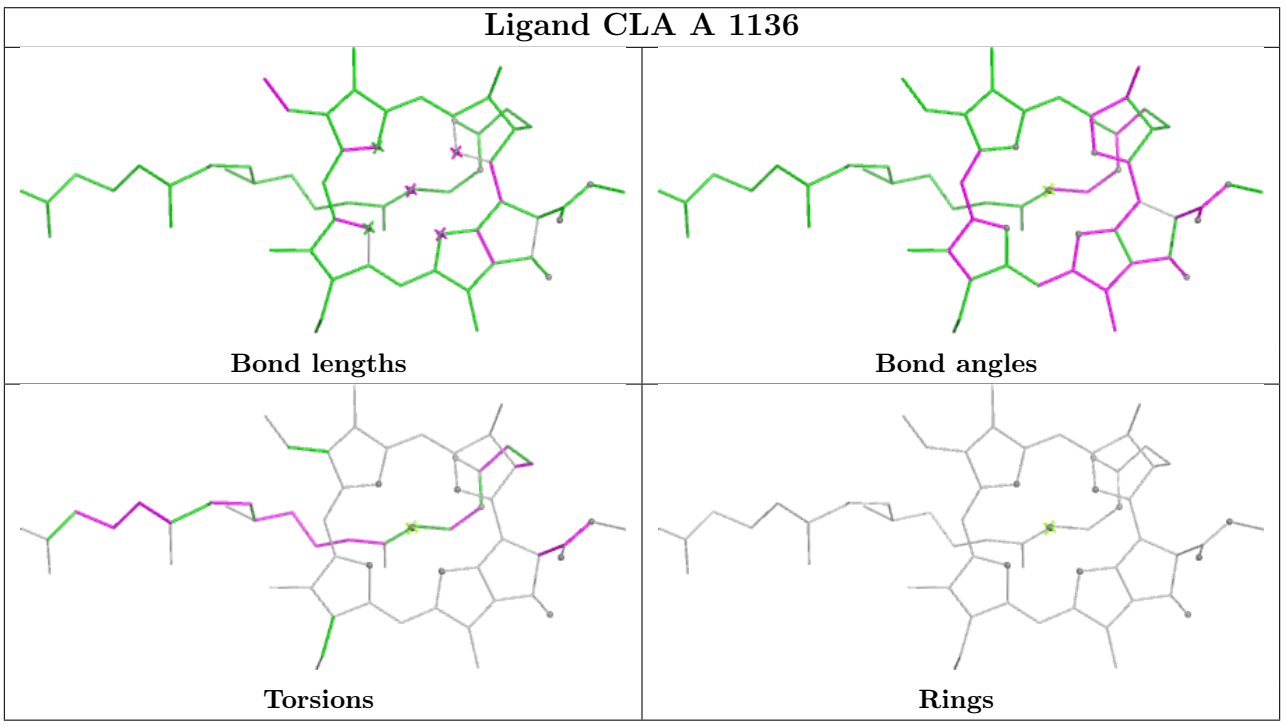
Ligand BCR 7 504



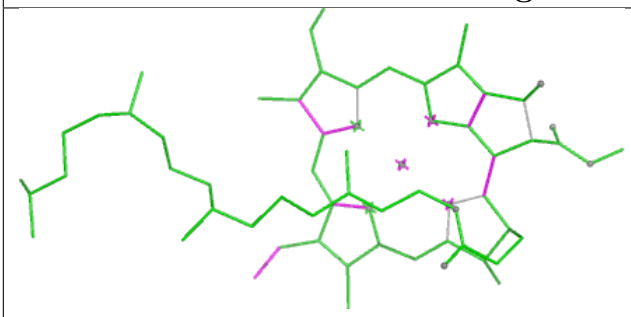
Ligand SPH K 5001



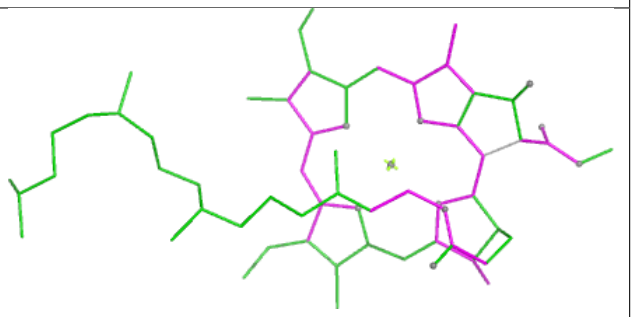
Ligand CLA A 1136



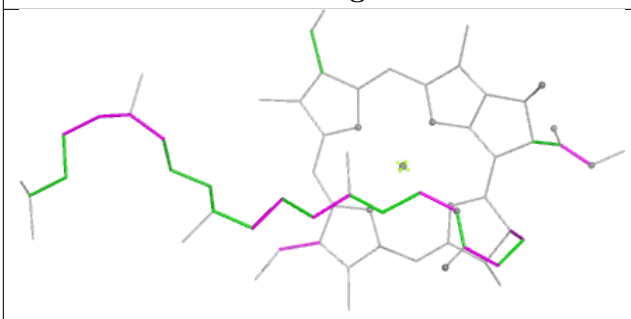
Ligand CLA B 1235



Bond lengths



Bond angles

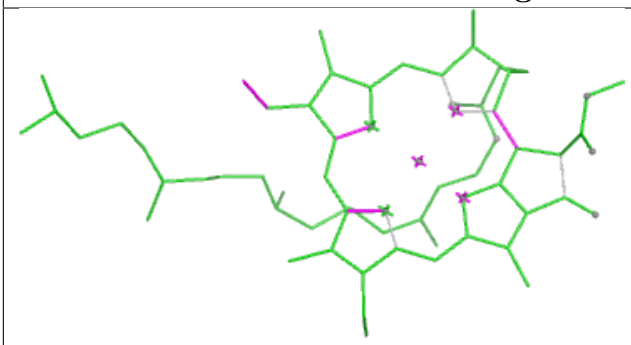


Torsions



Rings

Ligand CLA A 1138



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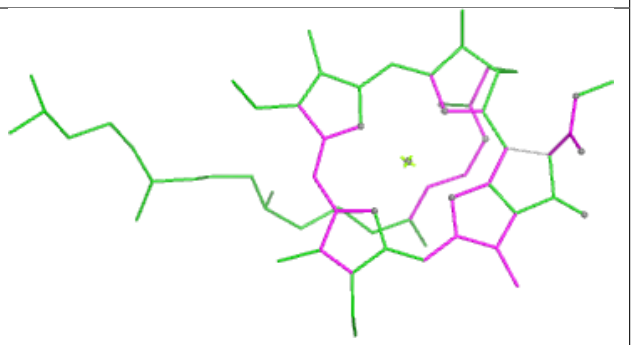
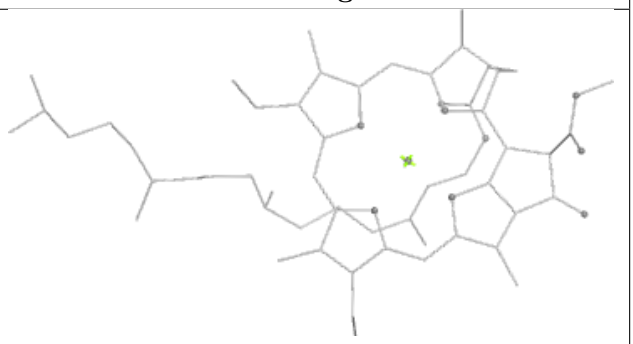


Bond angles

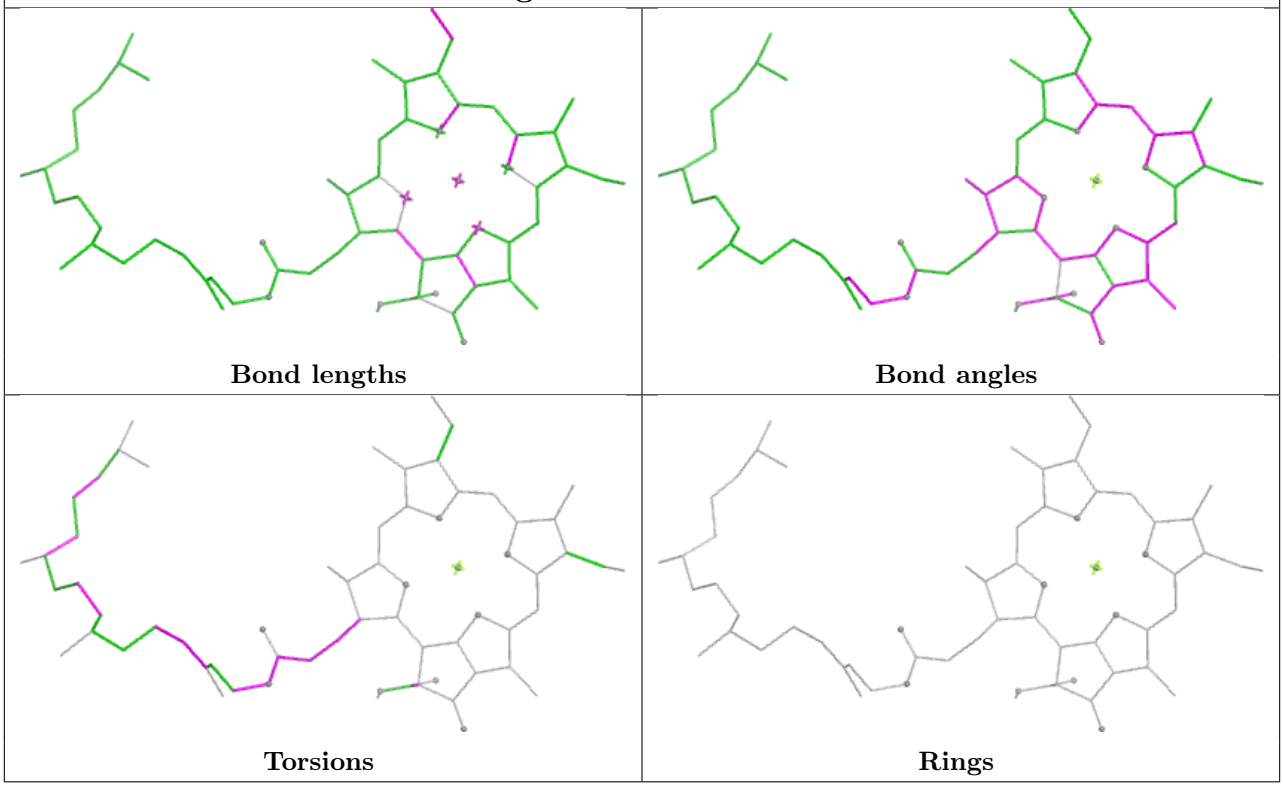


Torsions



Rings

Ligand CLA A 1125



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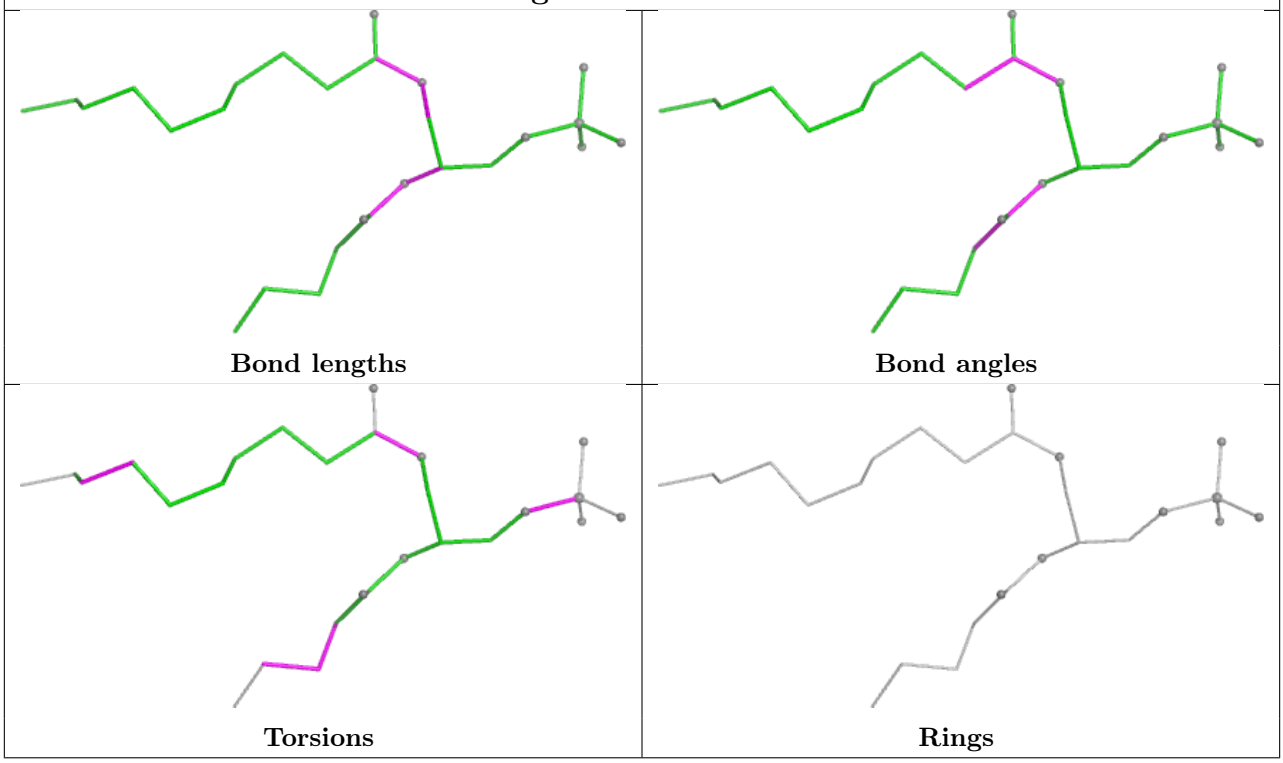
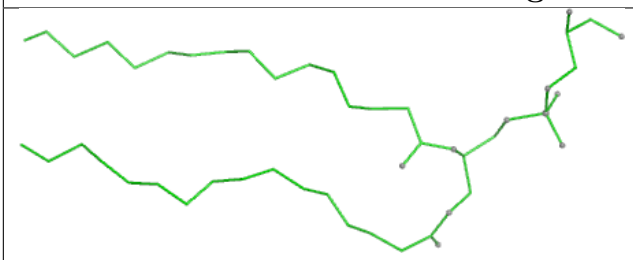


Ligand LHG 6 801



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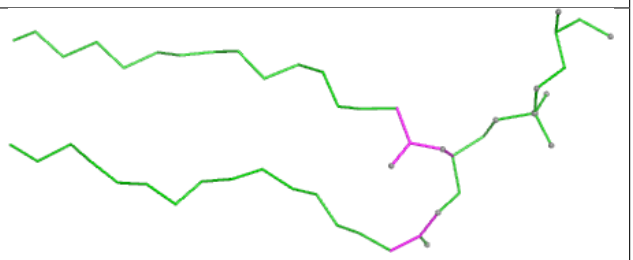
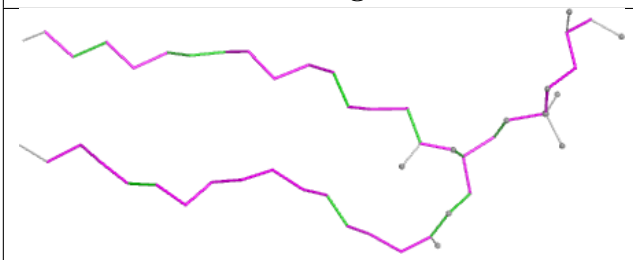


Bond angles



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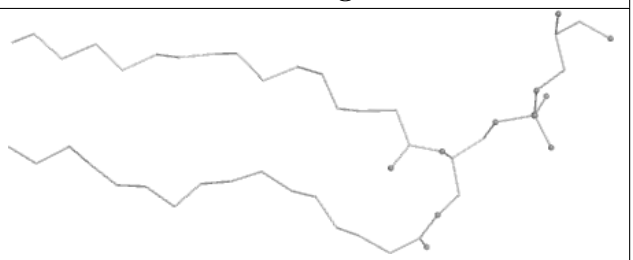
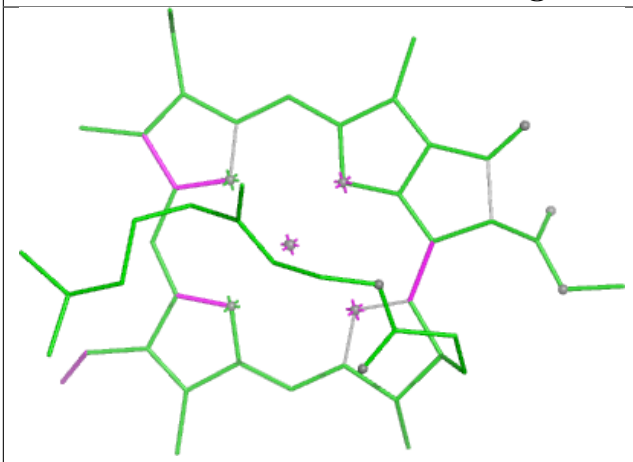


Rings

Ligand CLA 2 603



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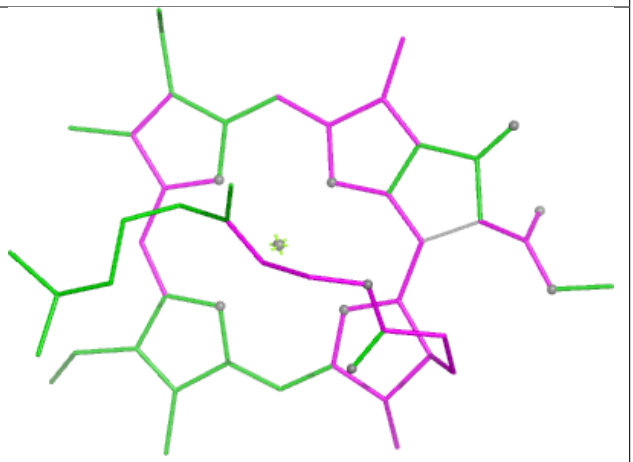
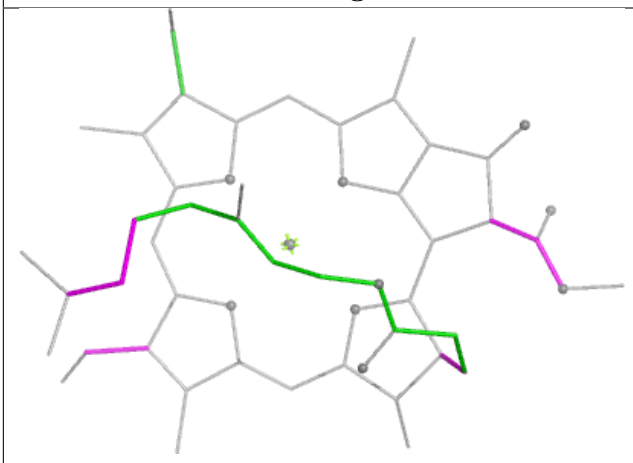
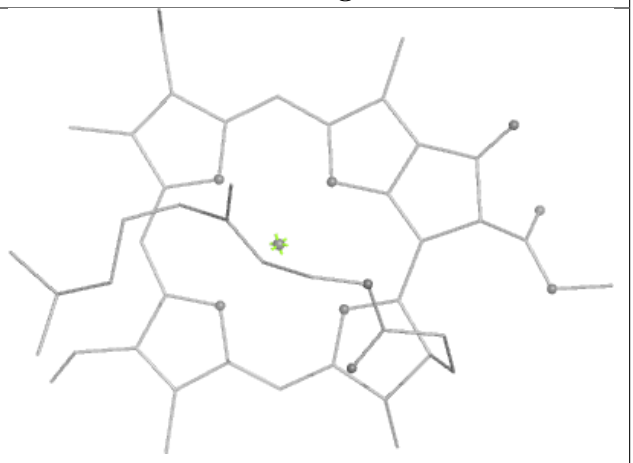


Bond angles

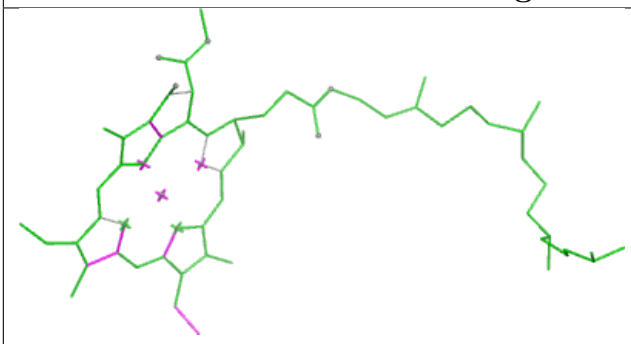


Torsions

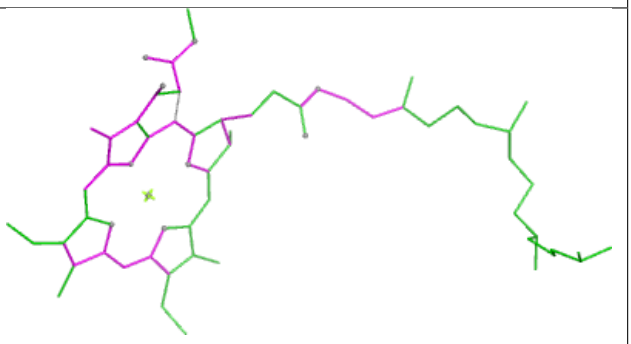


Rings

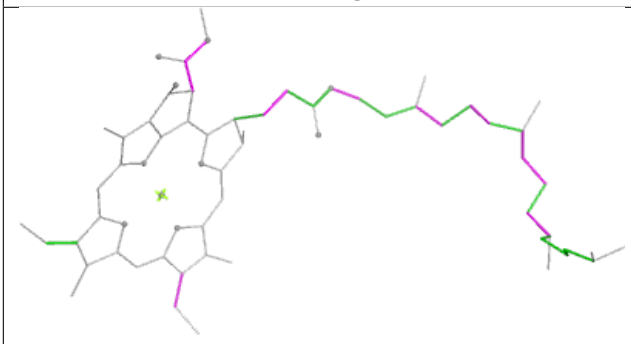
Ligand CLA A 1012



Bond lengths



Bond angles



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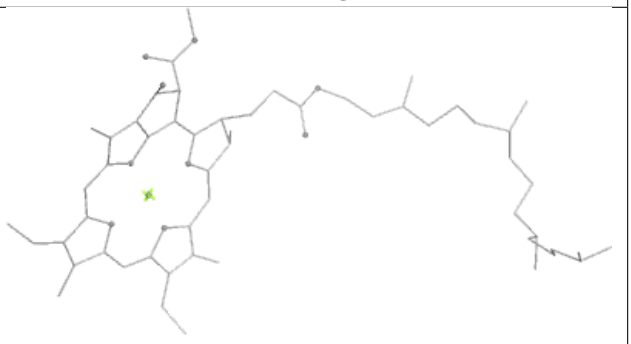
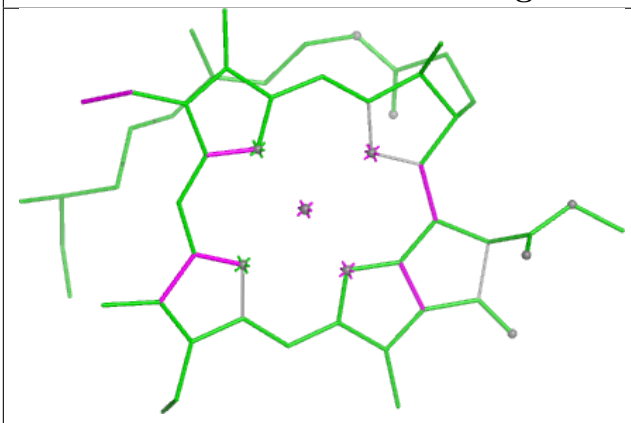


Rings

Ligand CLA B 1217



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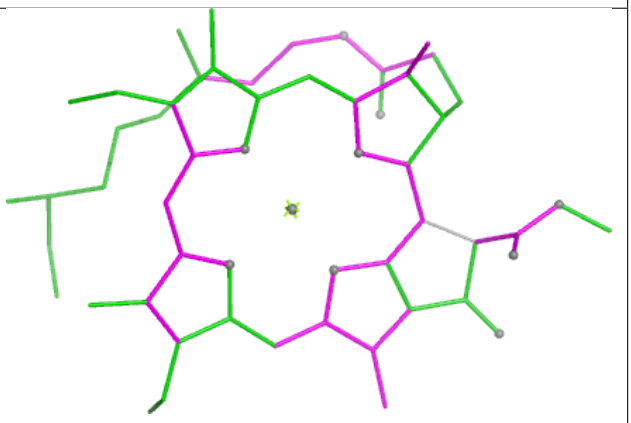
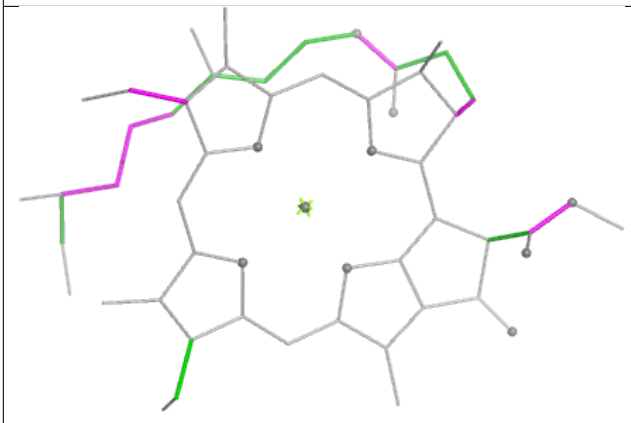


Bond angles



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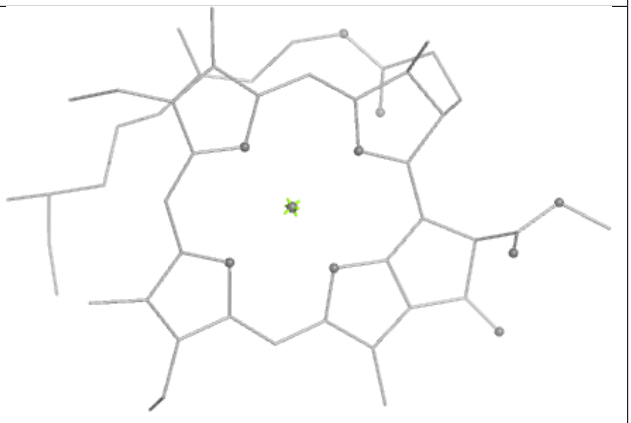
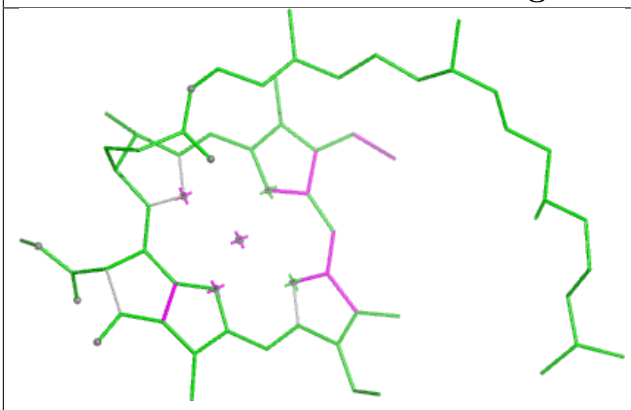


Rings

Ligand CLA 9 604



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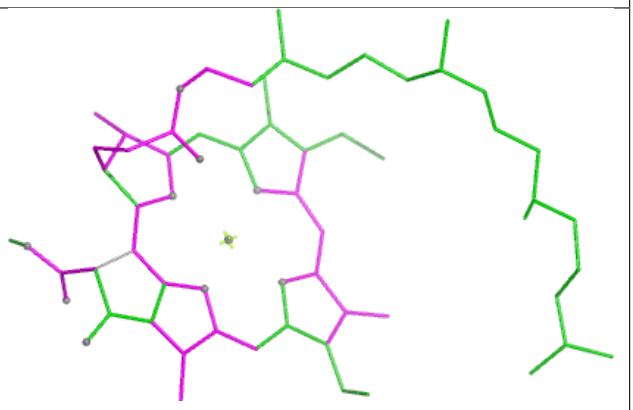
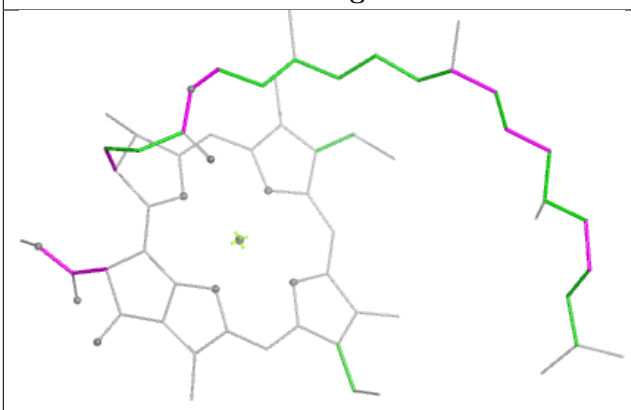


Bond angles



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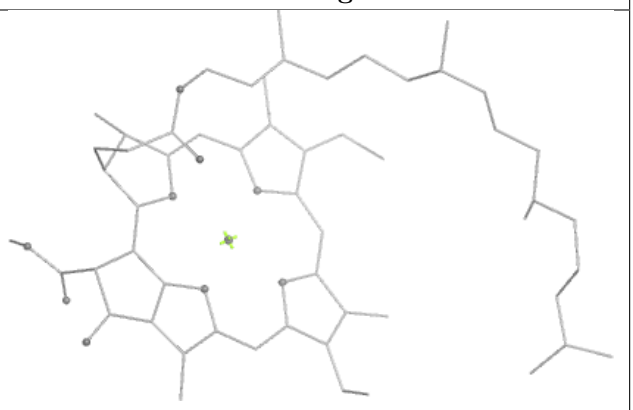
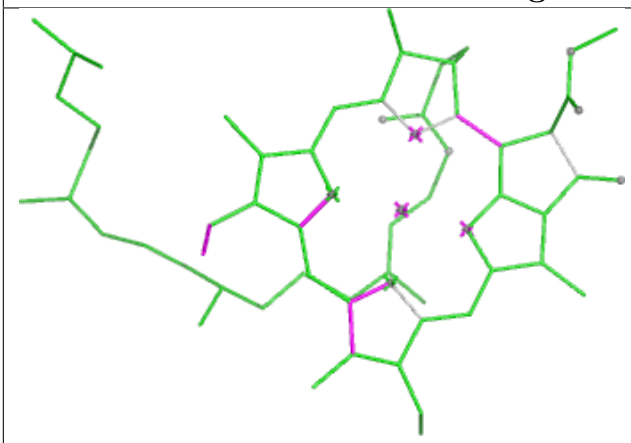


Rings

Ligand CLA 6 603



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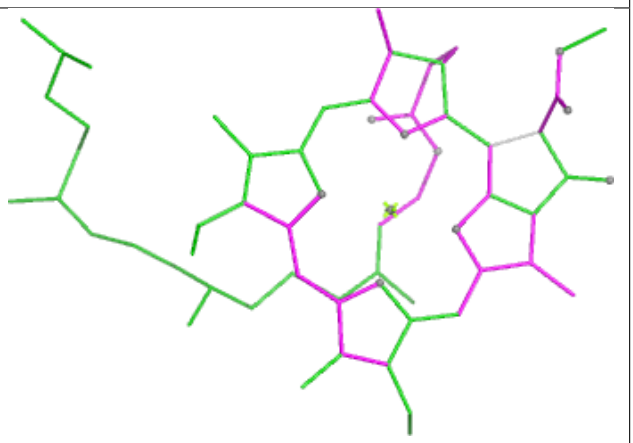
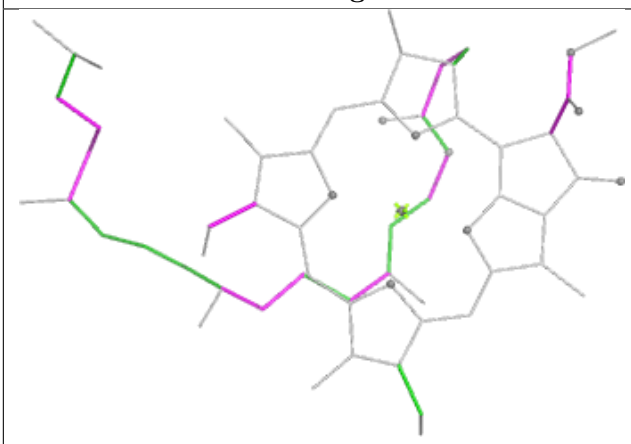


Bond angles



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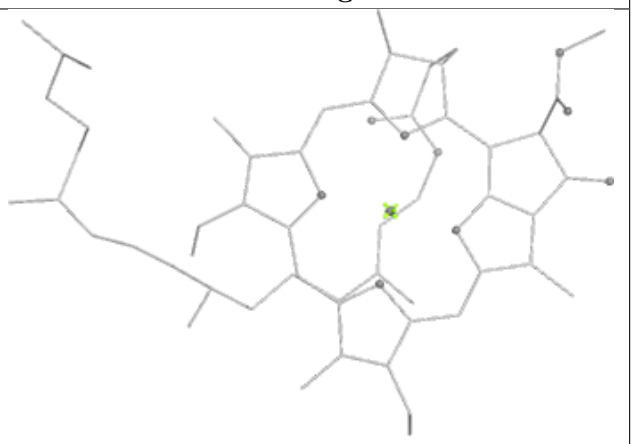
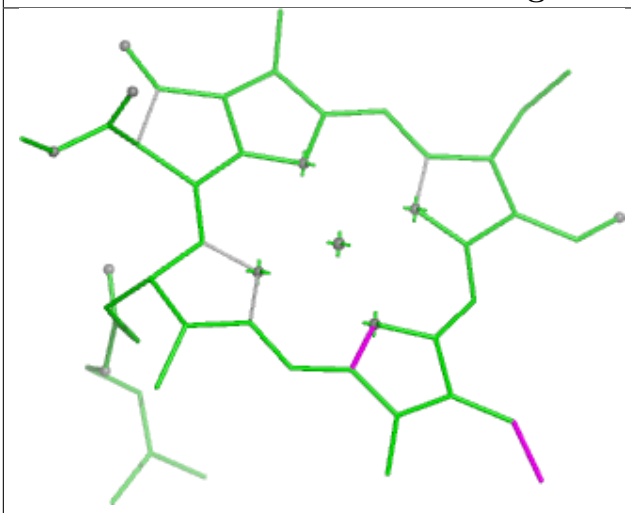


Rings

Ligand CHL 4 610



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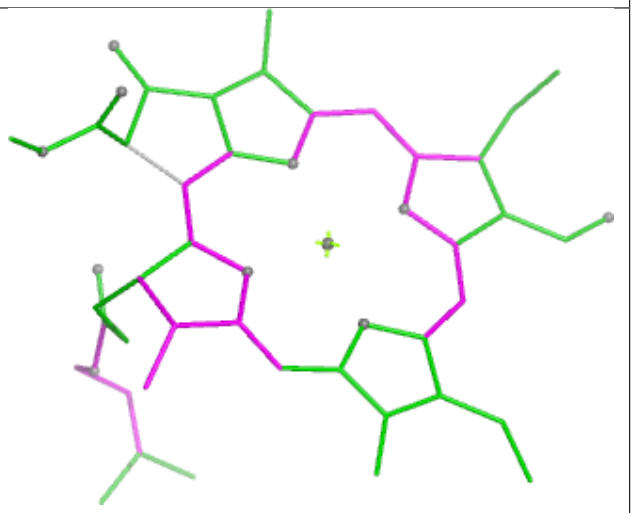
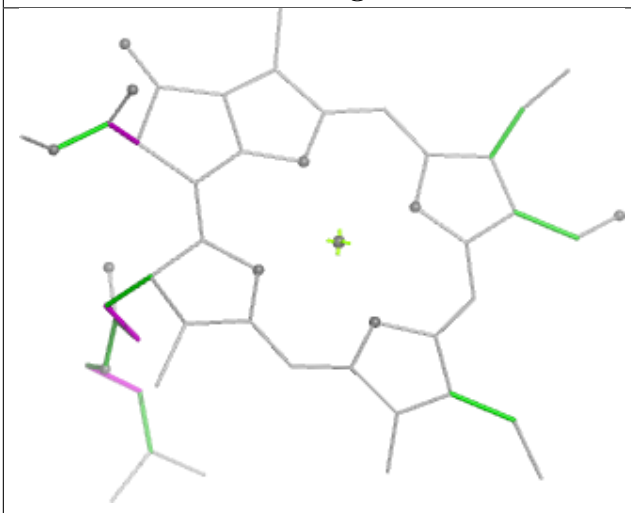


Bond angles



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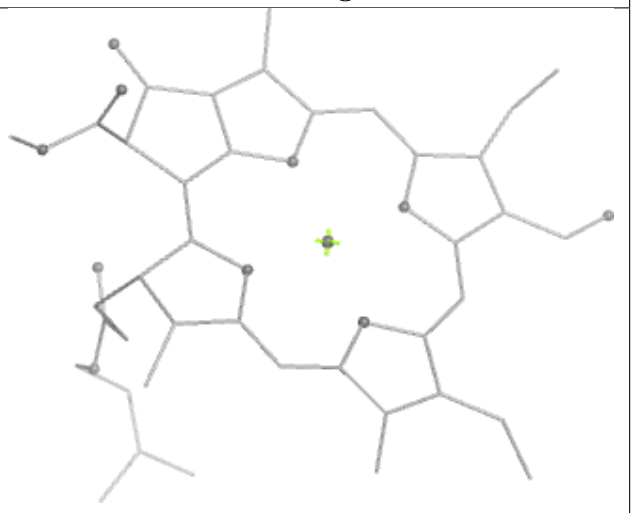
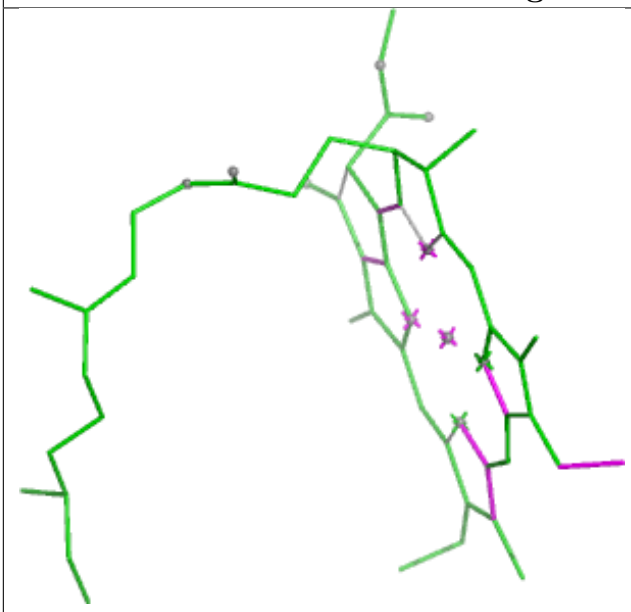
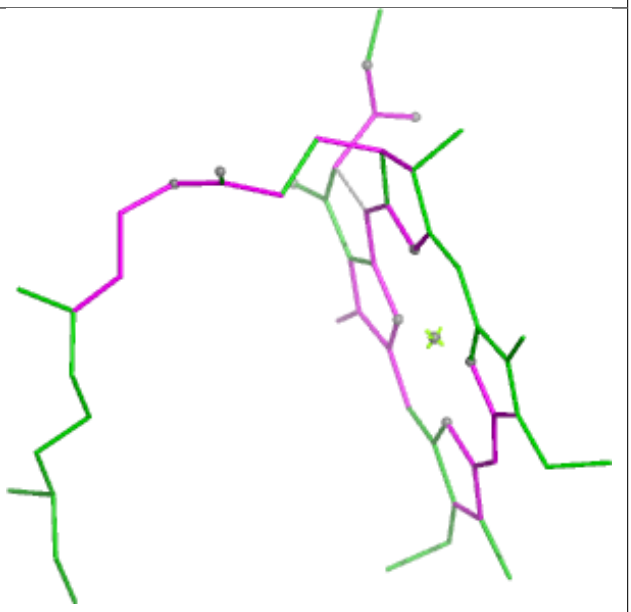


Rings

Ligand CLA Z 608



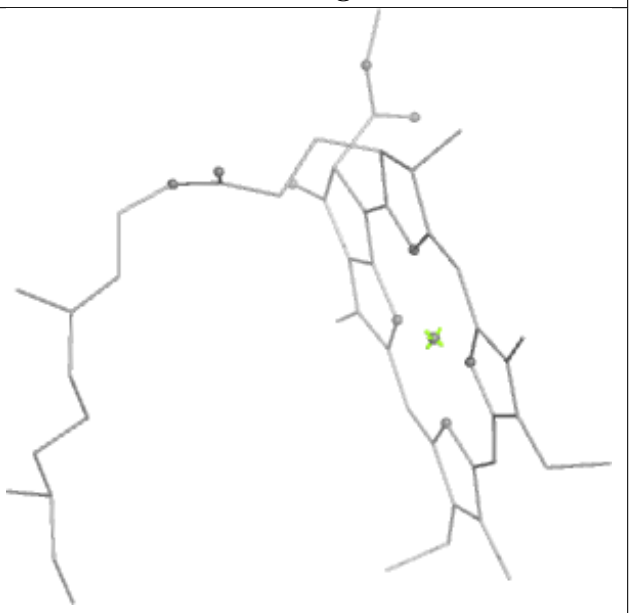
Bond lengths



Bond angles

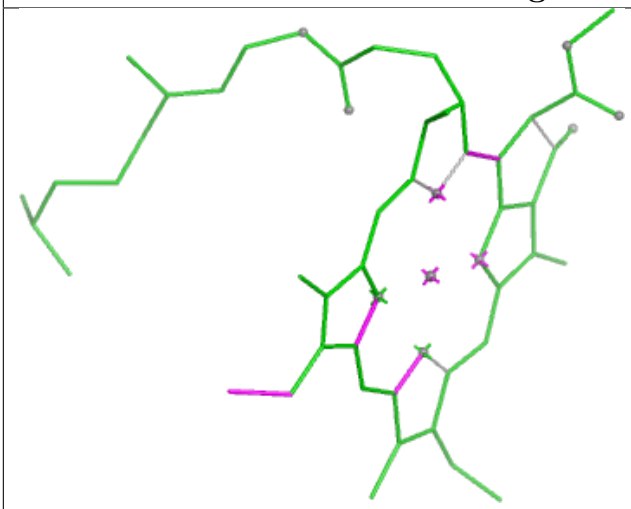


Torsions



Rings

Ligand CLA 8 607



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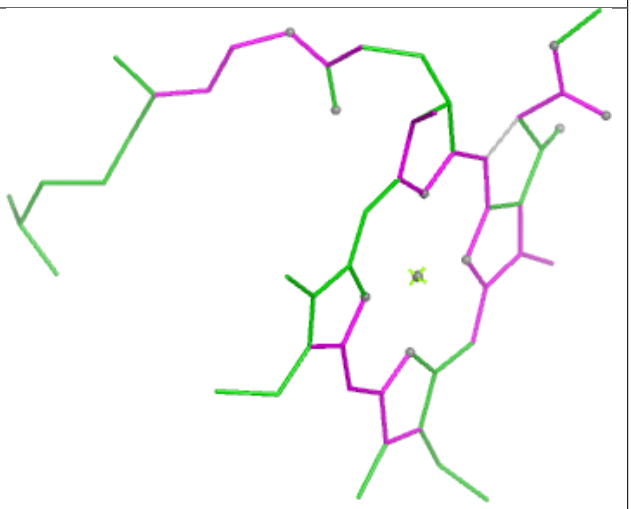

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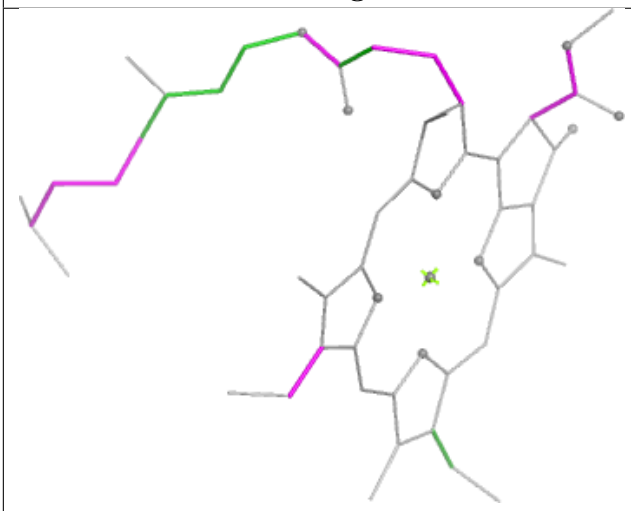

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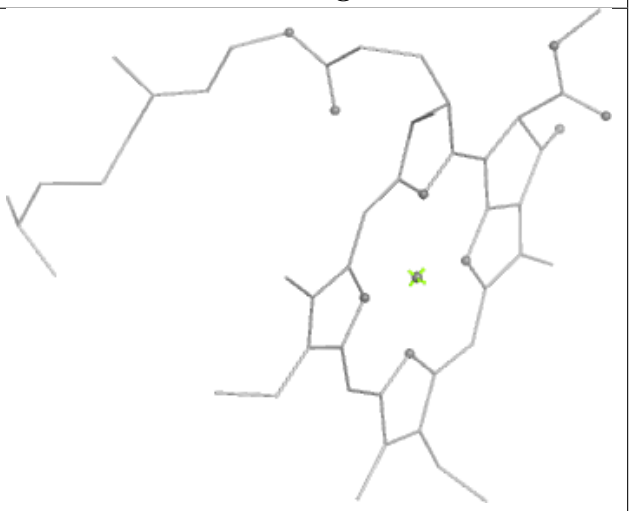
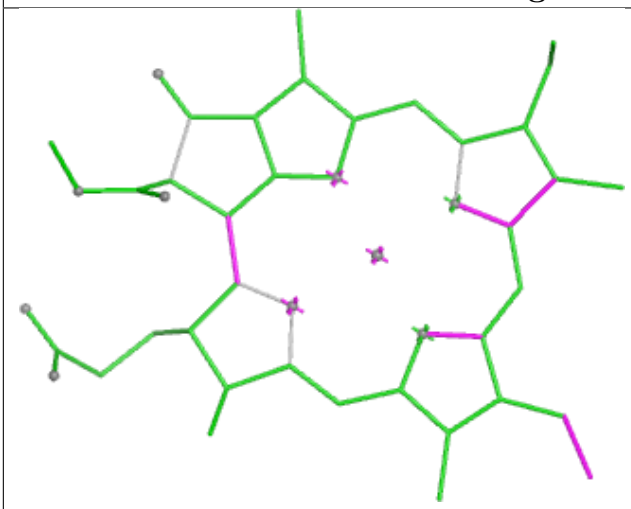


Rings

Ligand CLA 9 602



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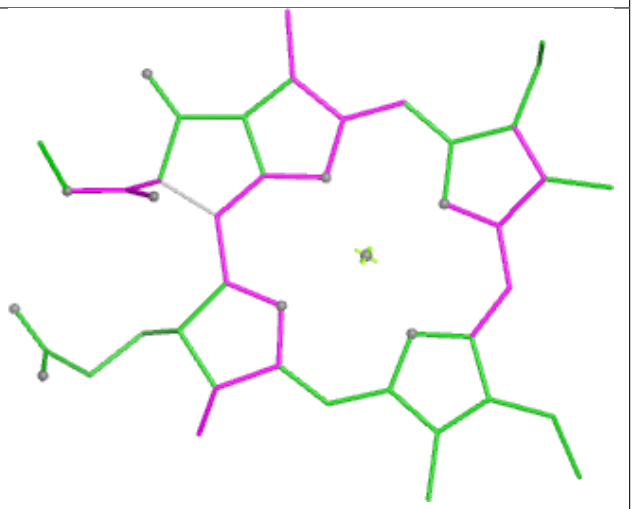

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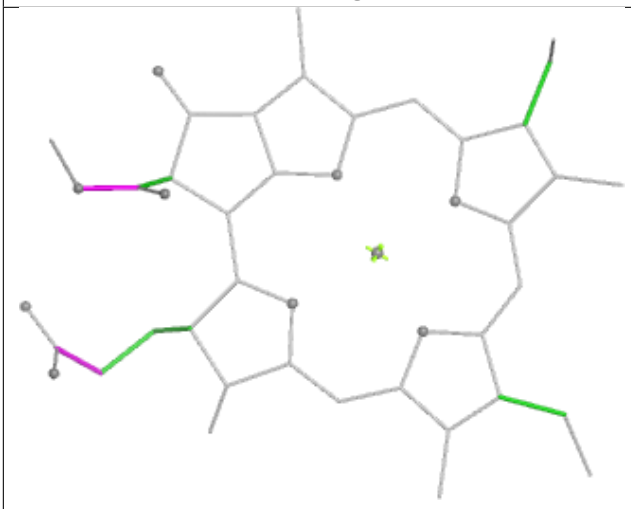
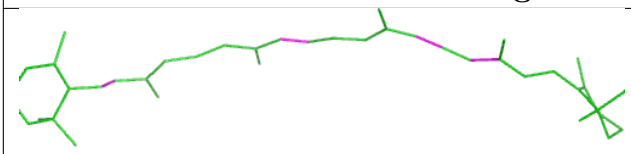


Torsions



Rings

Ligand BCR B 4006



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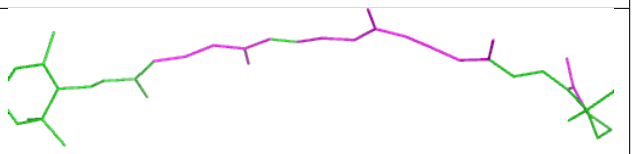

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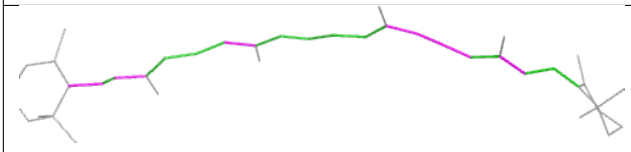

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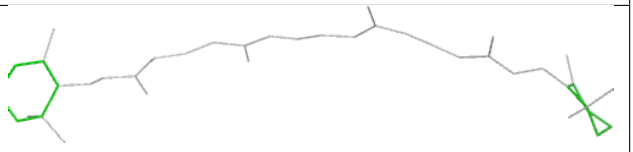
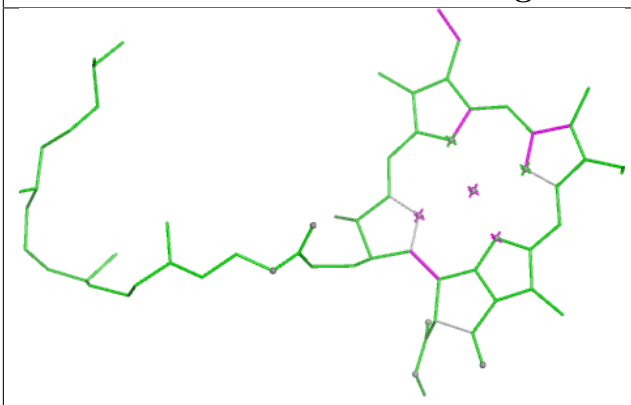


Rings

Ligand CLA A 1124



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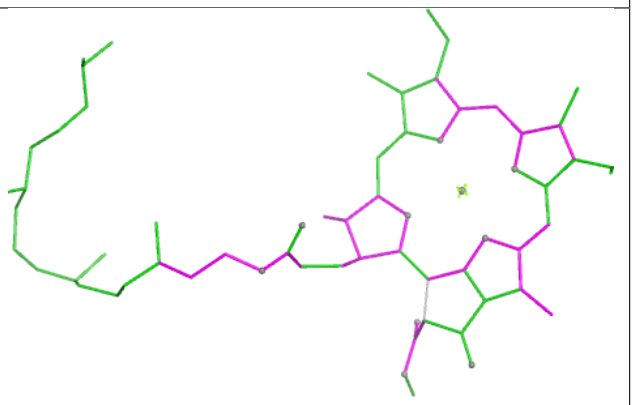

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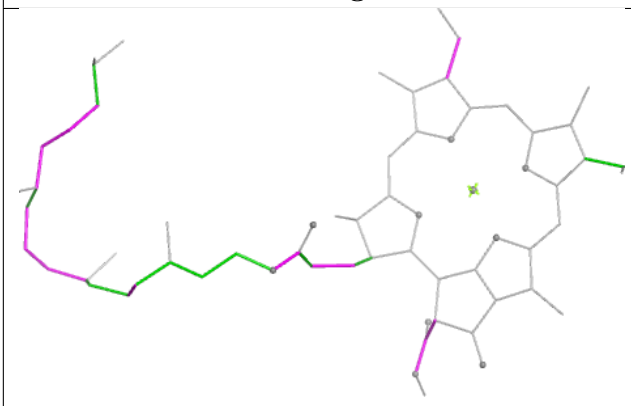

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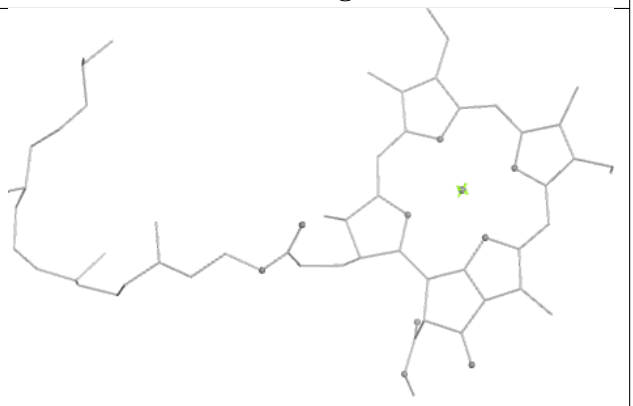
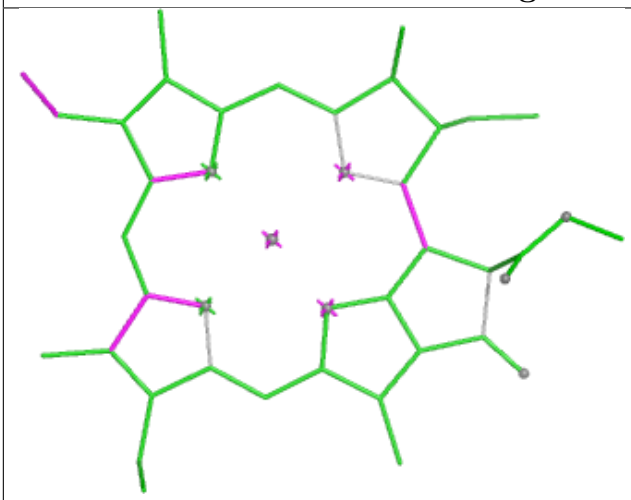


Rings

Ligand CLA J 1901



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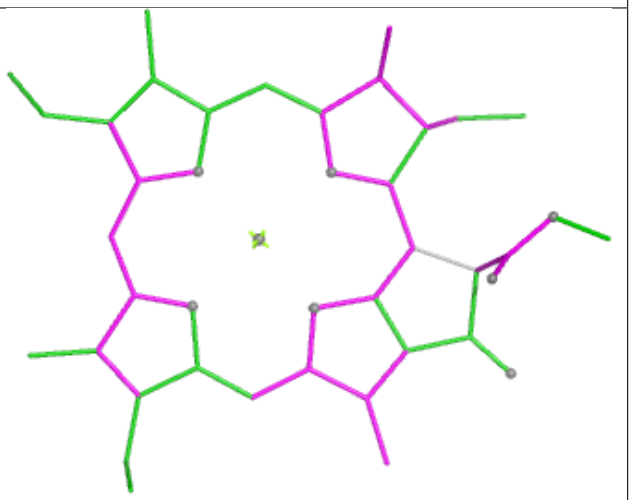
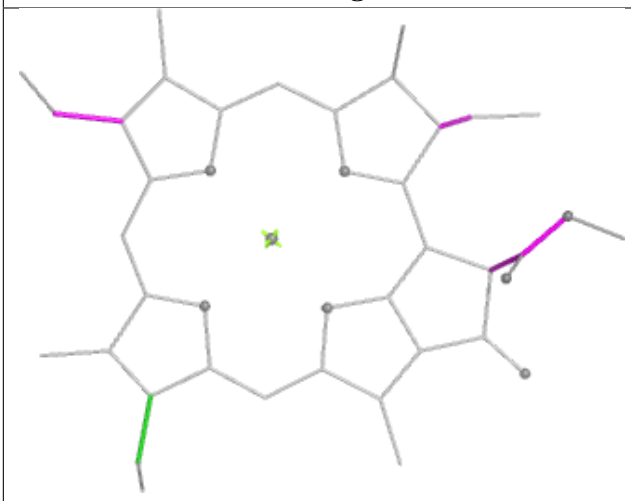


Bond angles



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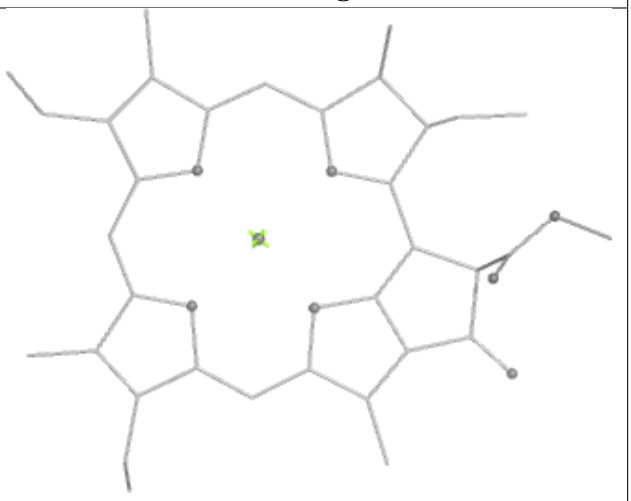
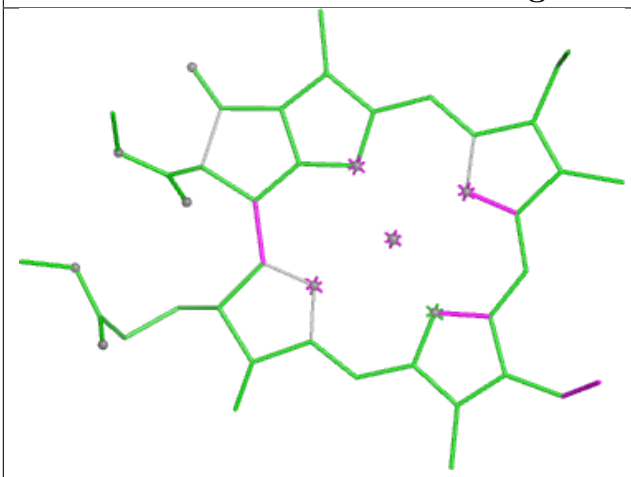


Rings

Ligand CLA 5 622



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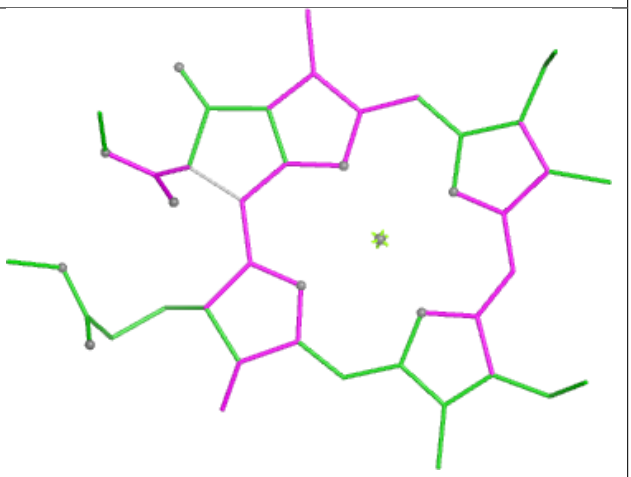

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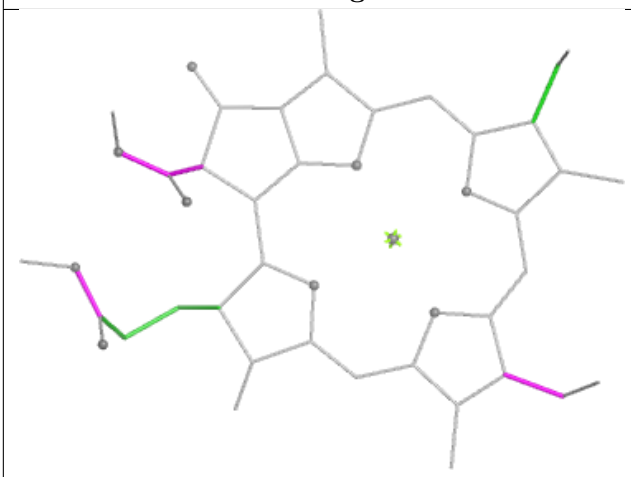

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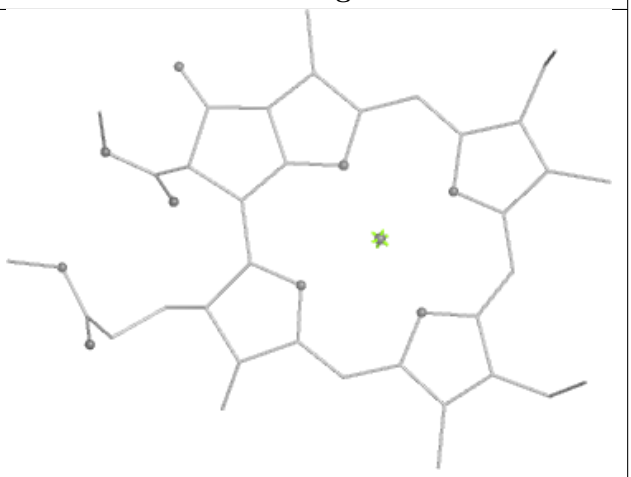
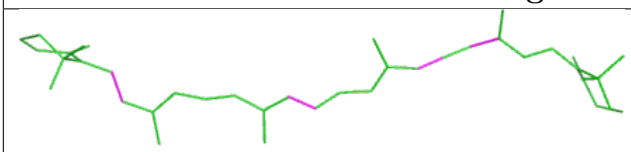


Rings

Ligand BCR 7 503



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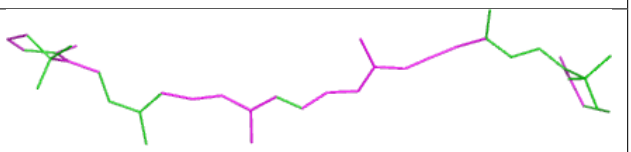

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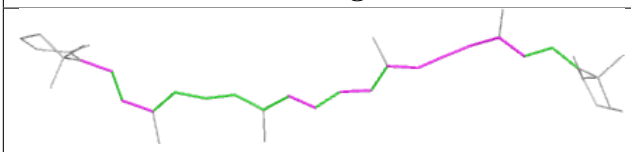

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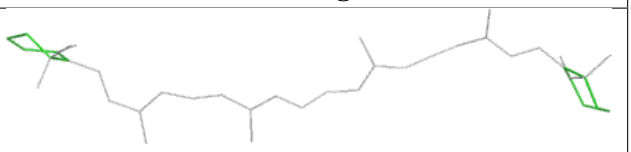
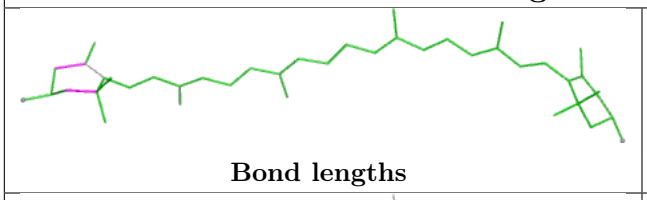


Rings

Ligand LUT 5 501



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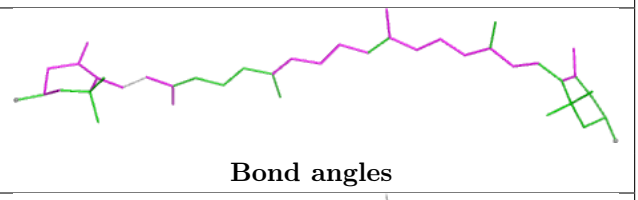

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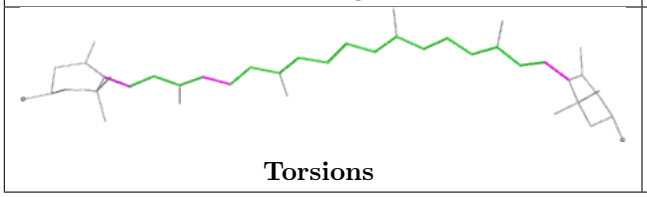

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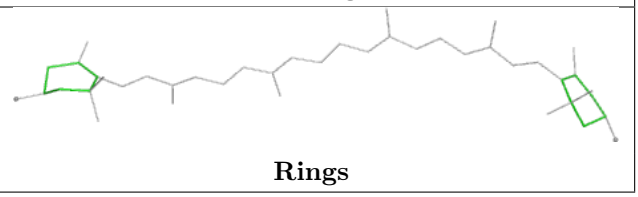
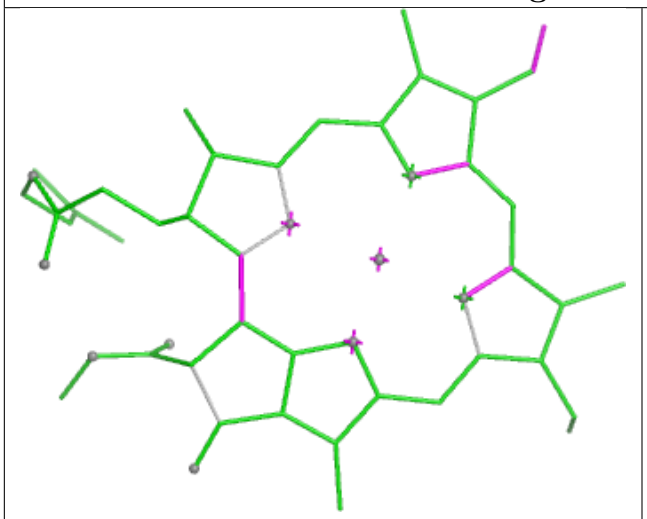


Rings

Ligand CLA 7 602



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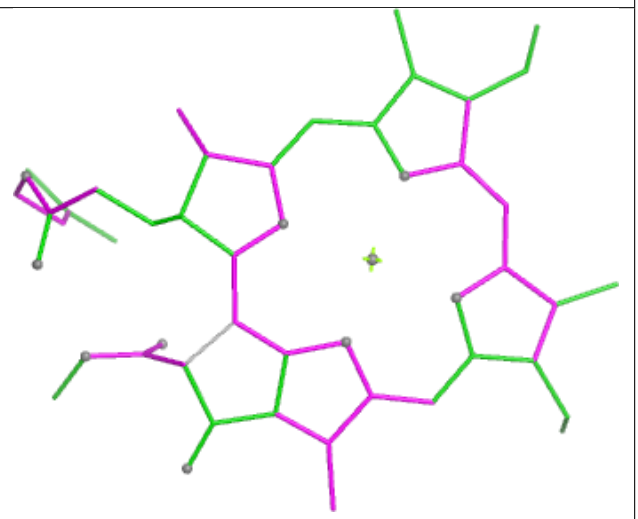

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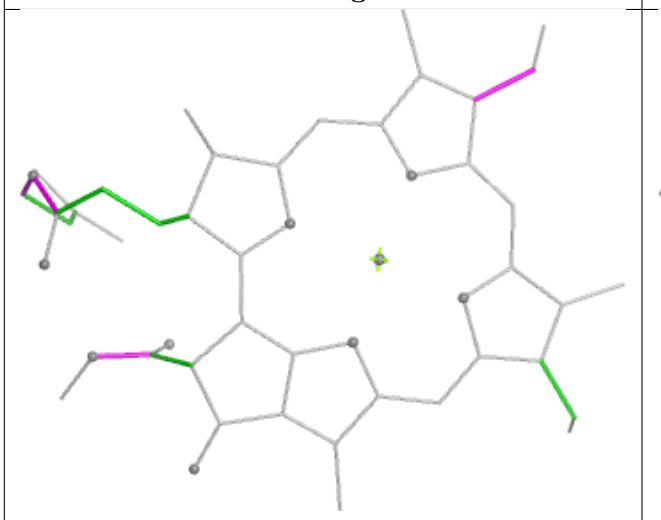

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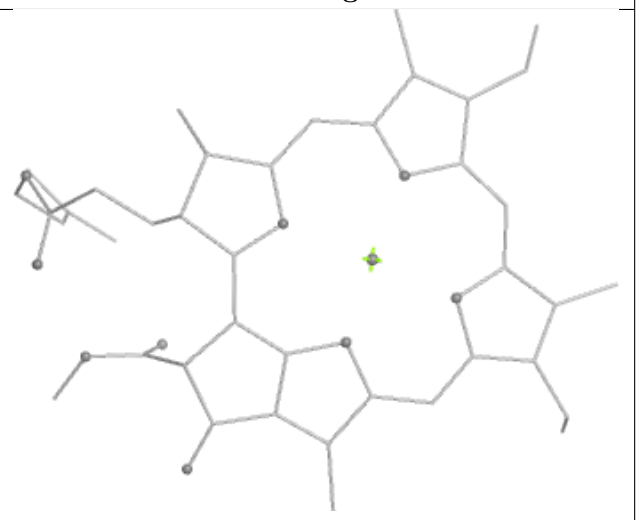
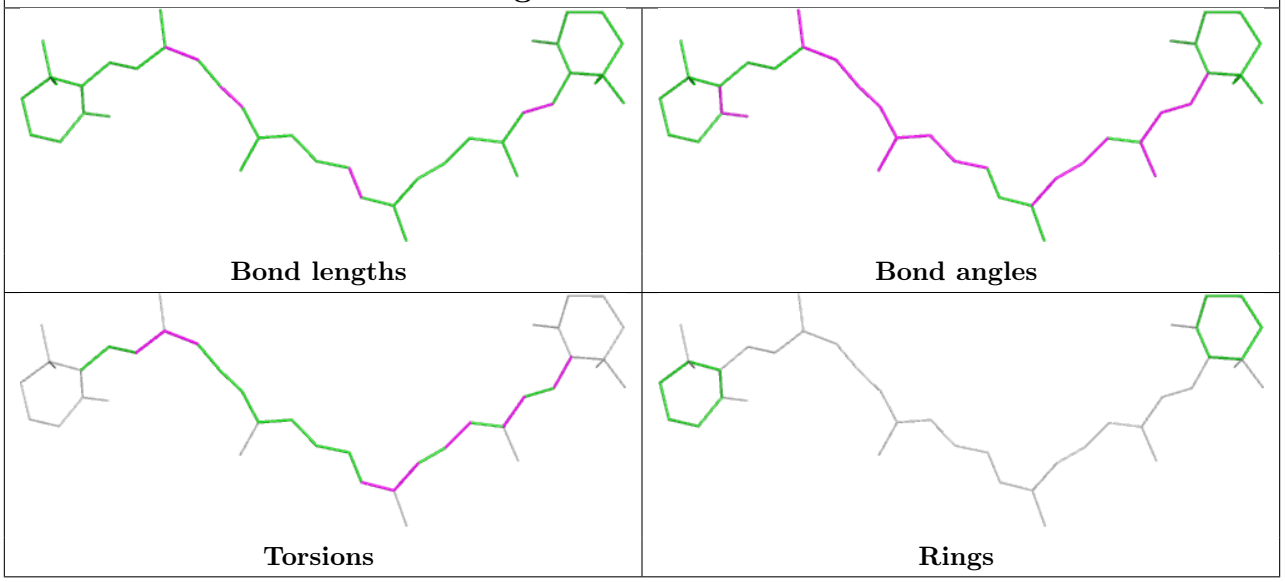
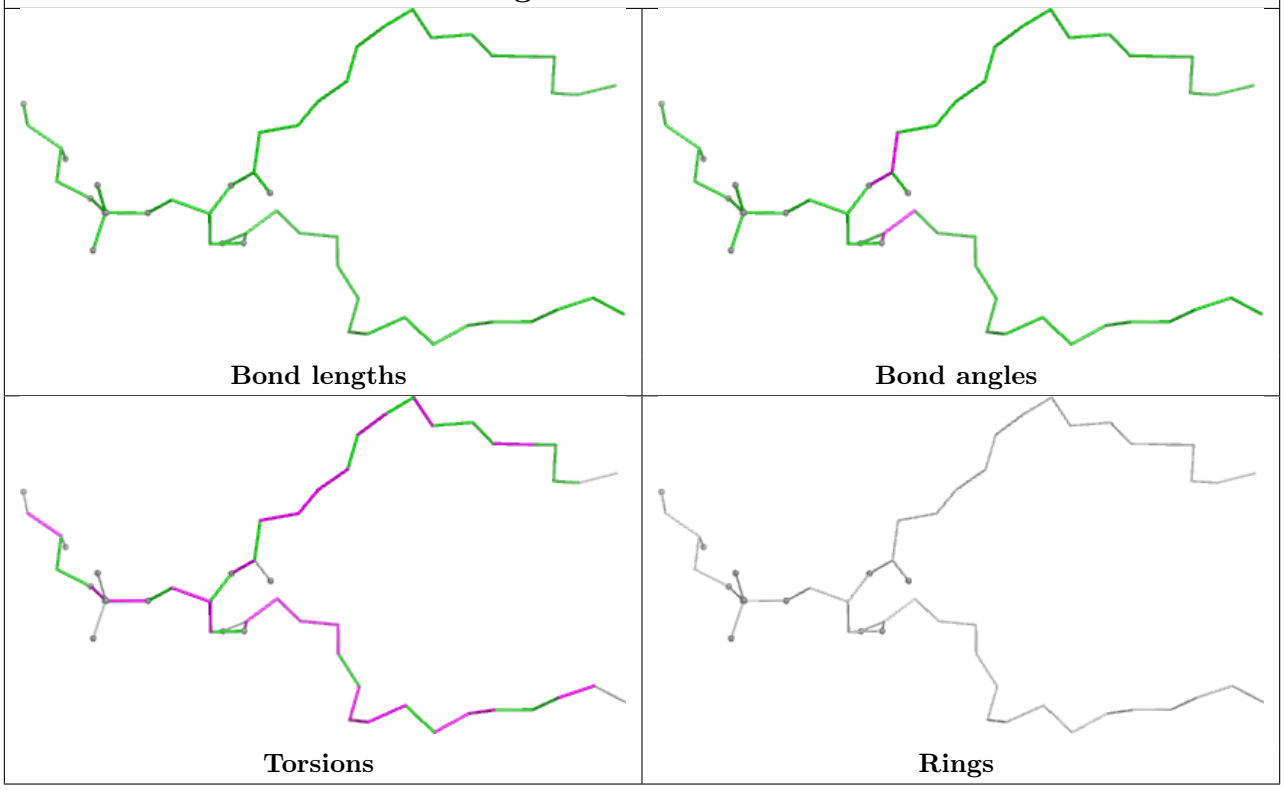


Rings

Ligand BCR A 4005



Ligand LHG A 5002



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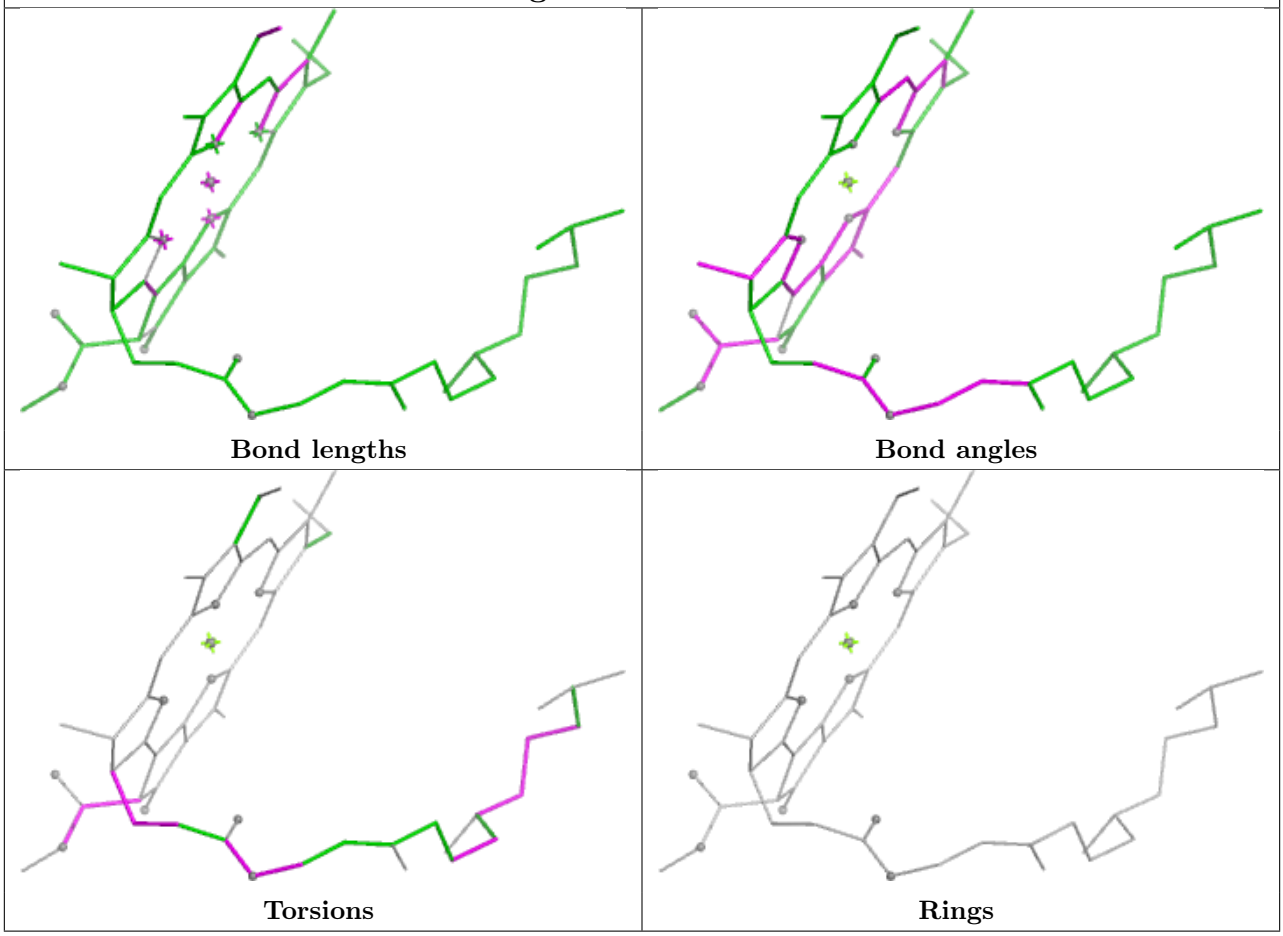
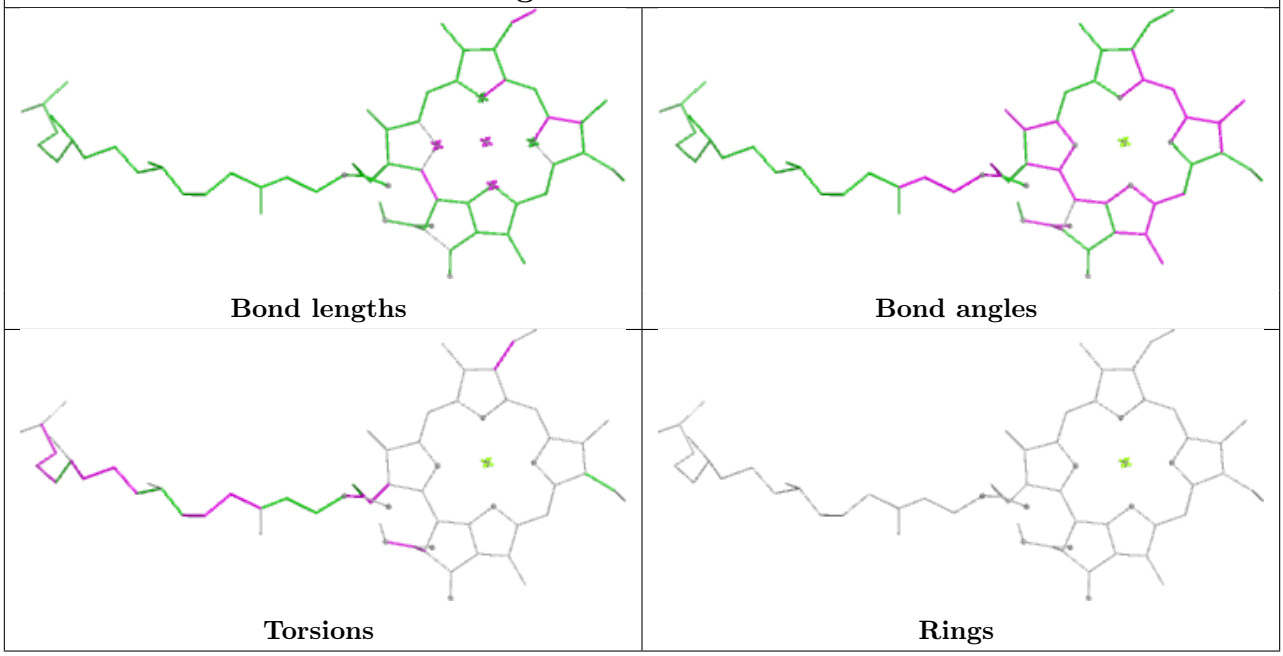
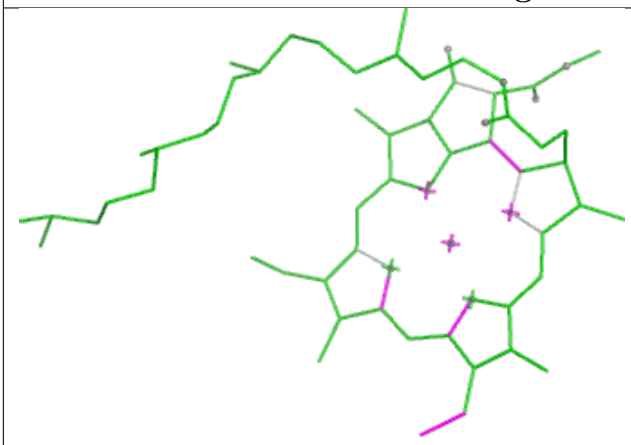


Ligand CLA B 1240



Ligand CLA A 1127



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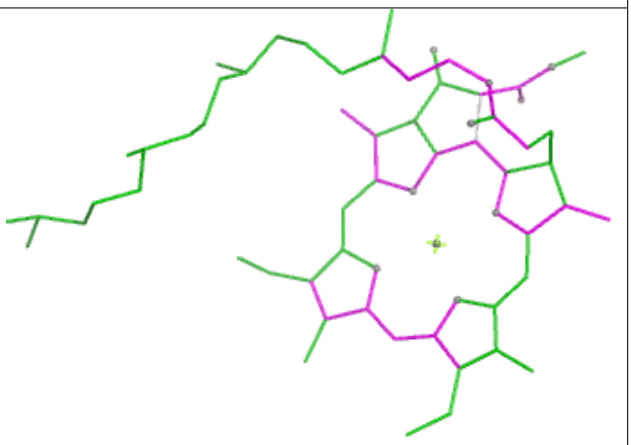
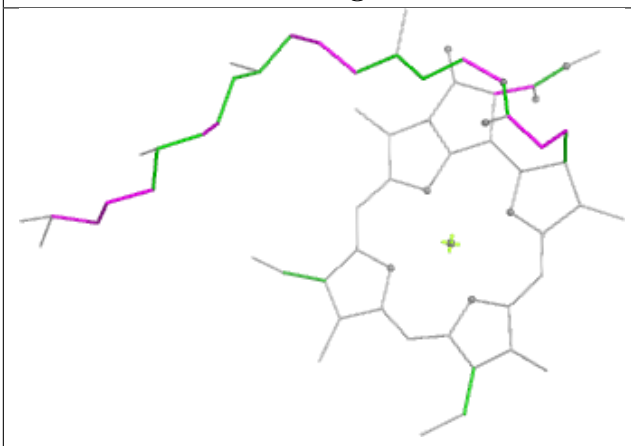


Bond angles

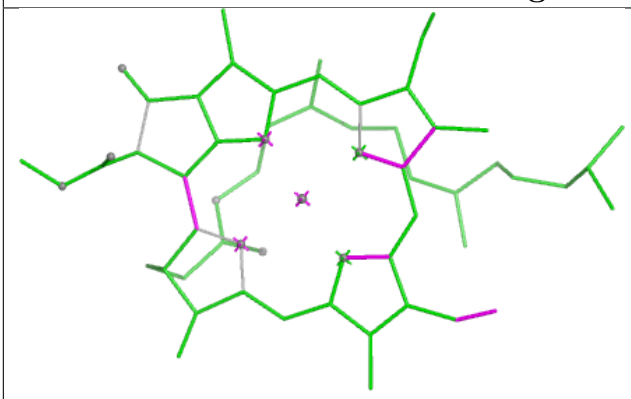


Torsions



Rings

Ligand CLA 7 616



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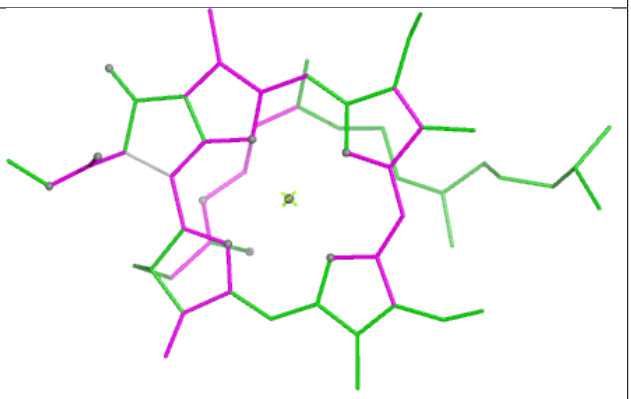
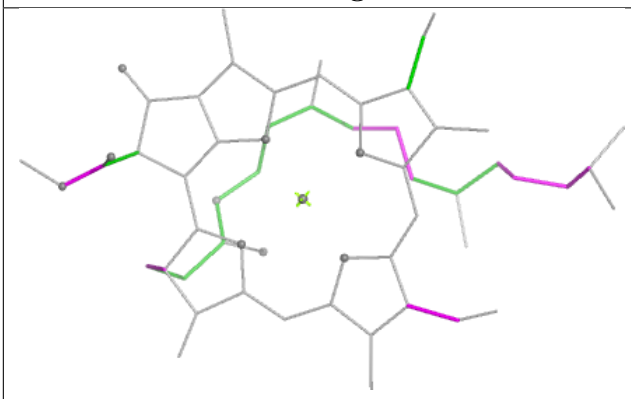
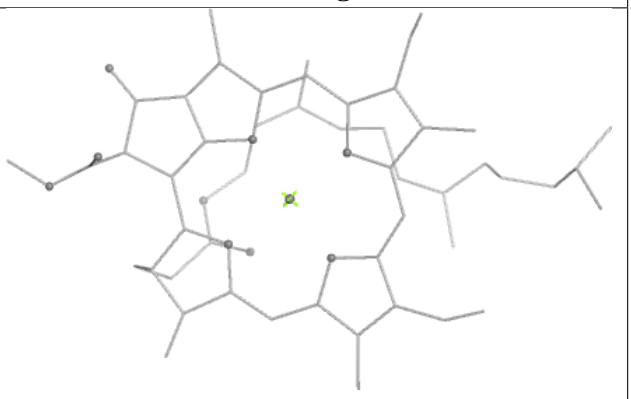


Bond angles

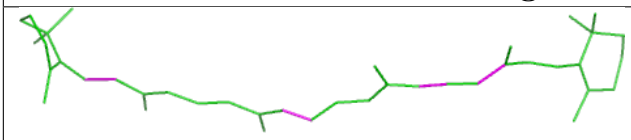


Torsions



Rings

Ligand BCR I 4001



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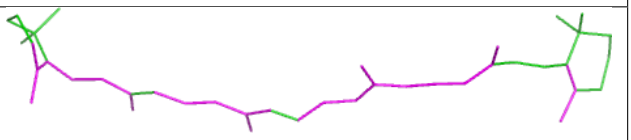
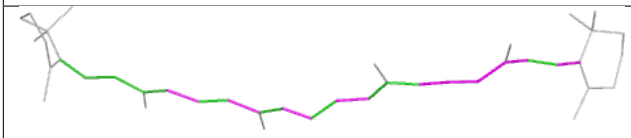


Bond angles



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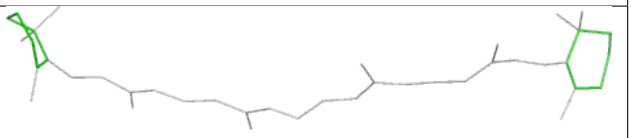
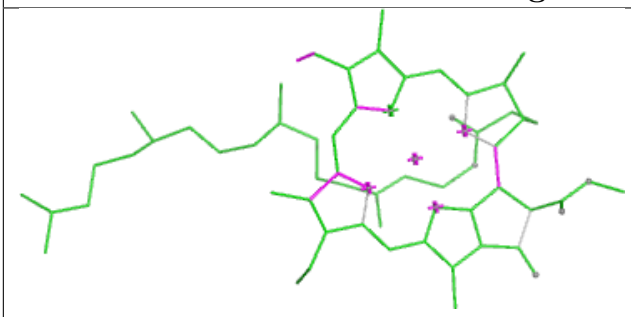


Rings

Ligand CLA 3 603



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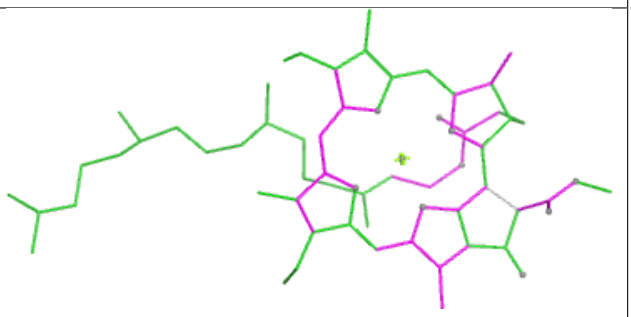
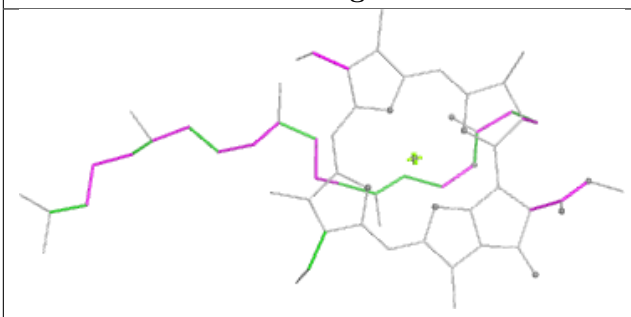


Bond angles

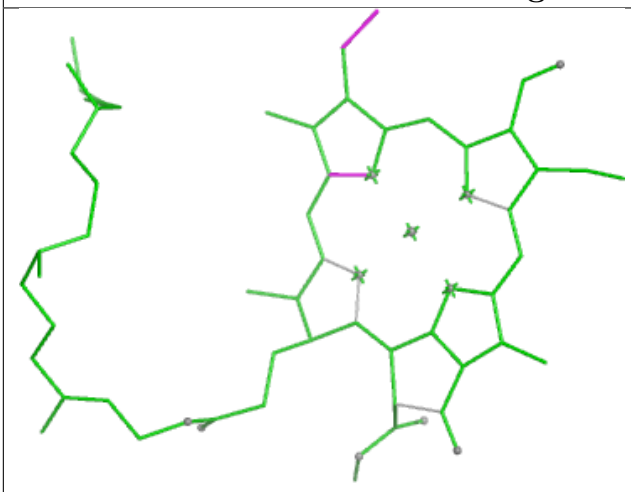


Torsions

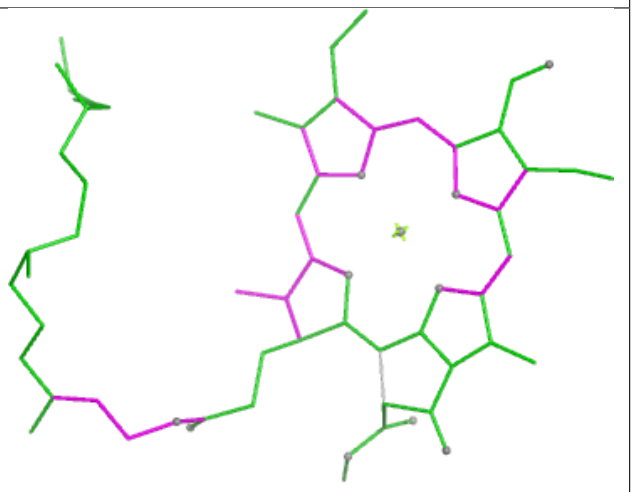


Rings

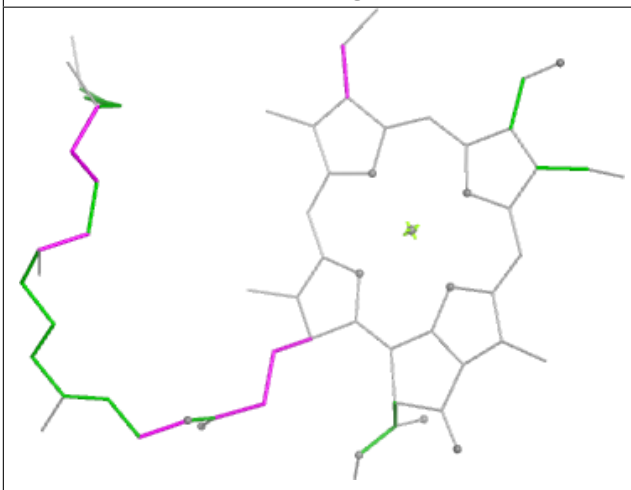
Ligand CHL 8 613



Bond lengths



Bond angles

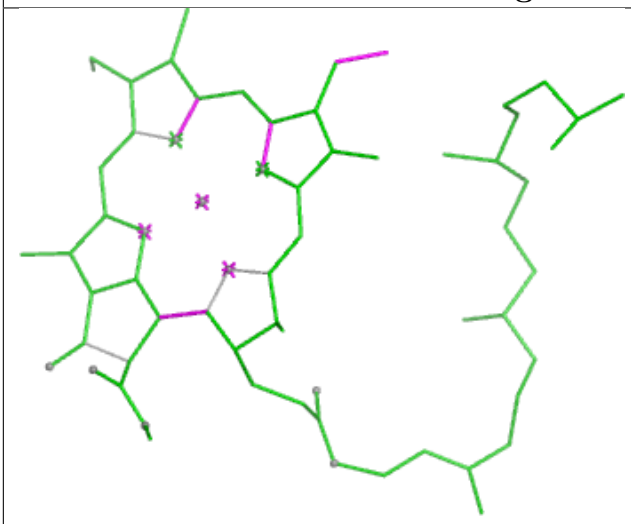


Torsions

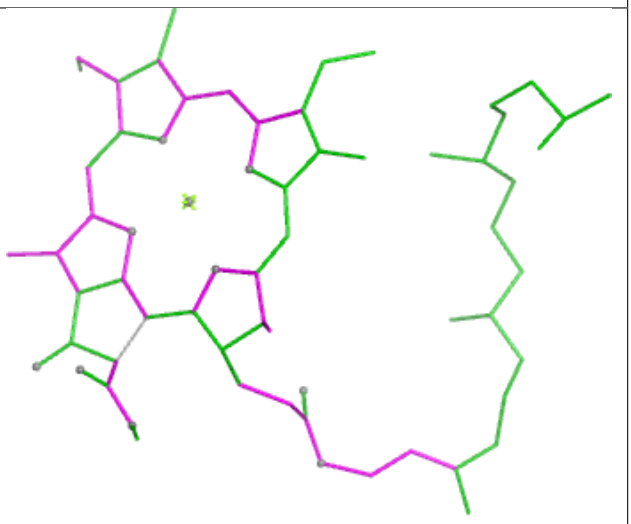


Rings

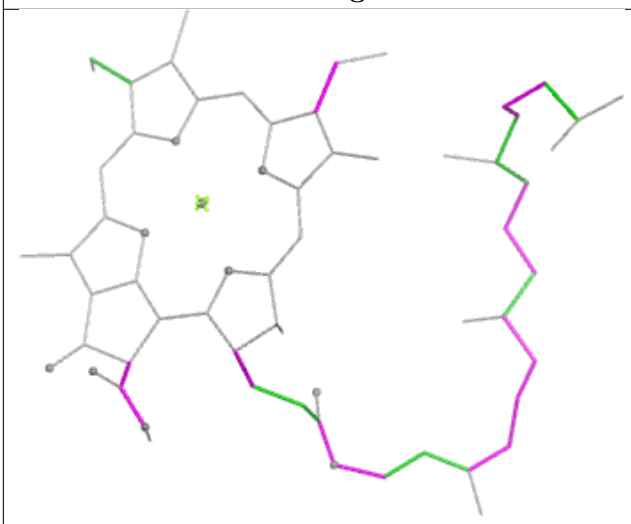
Ligand CLA B 1220



Bond lengths



Bond angles

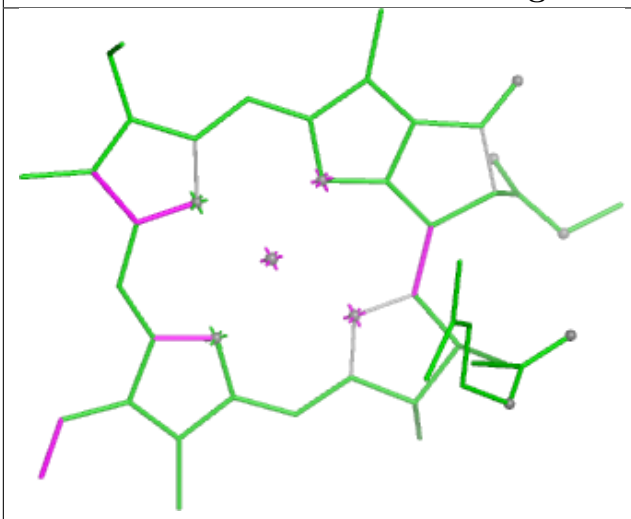


Torsions



Rings

Ligand CLA 4 606



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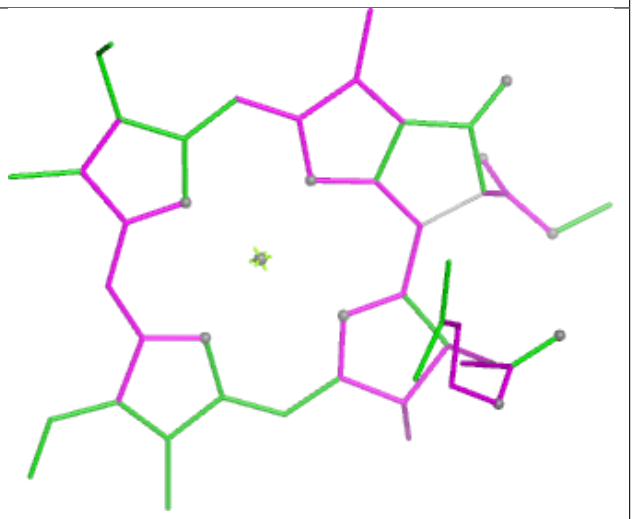

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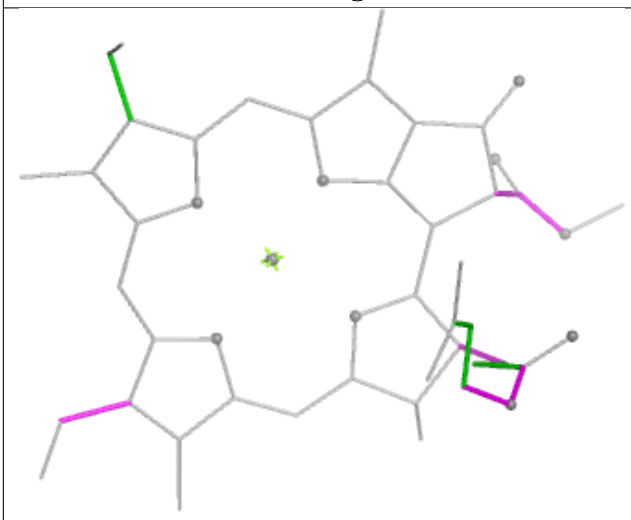

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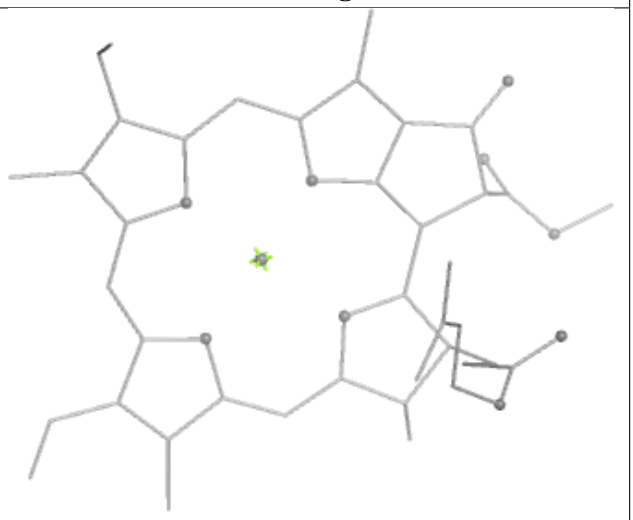
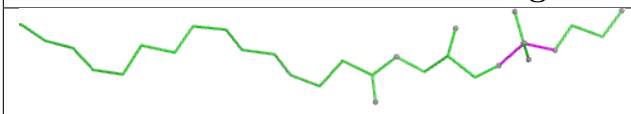


Rings

Ligand LPX 8 803



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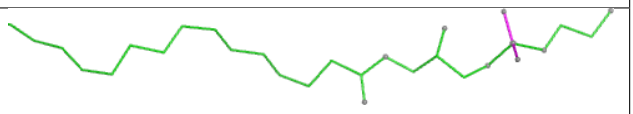

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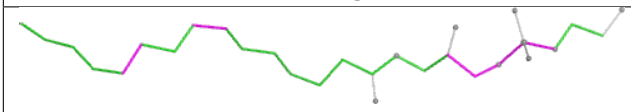

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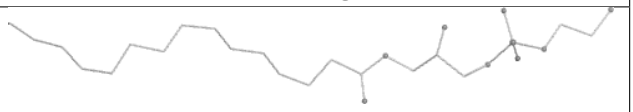
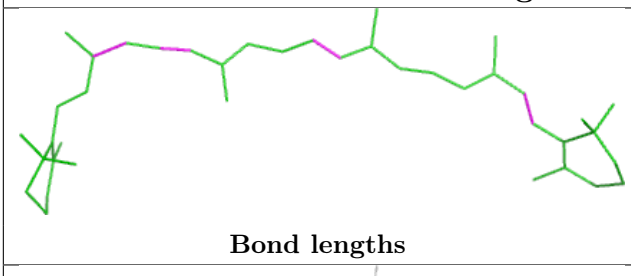


Rings

Ligand BCR L 4002



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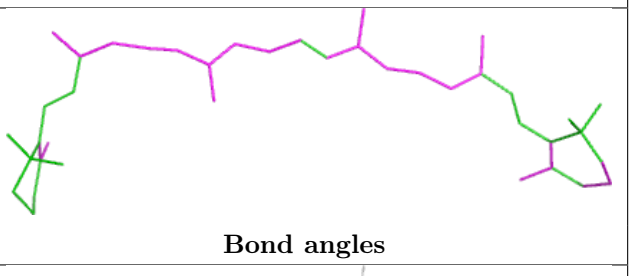

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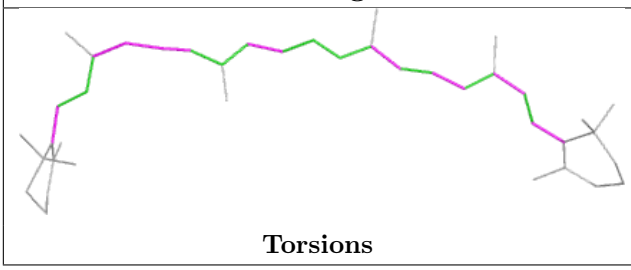

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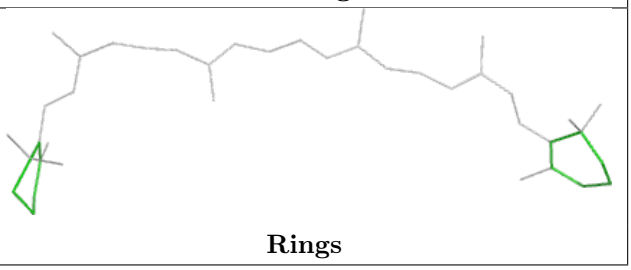
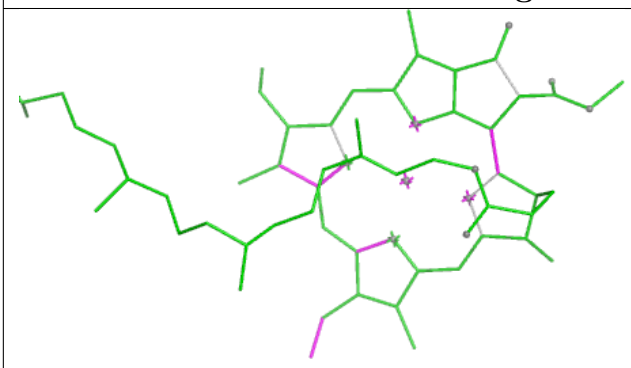


Rings

Ligand CLA B 1213



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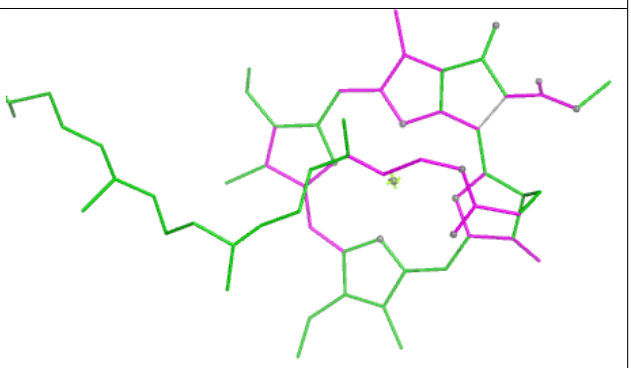
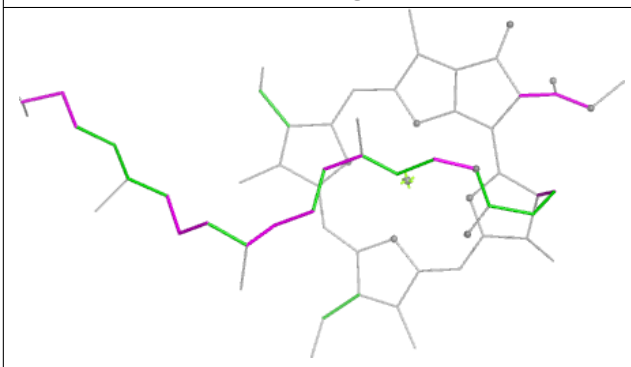


Bond angles



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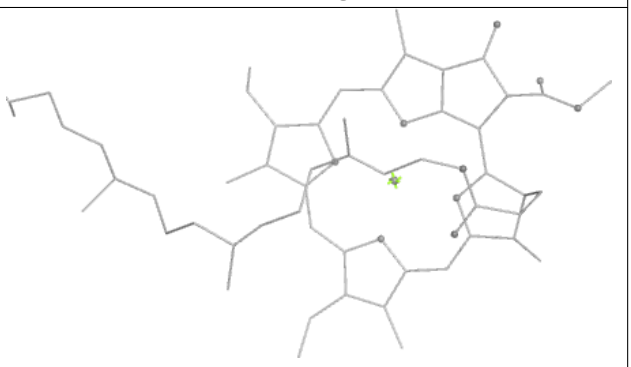
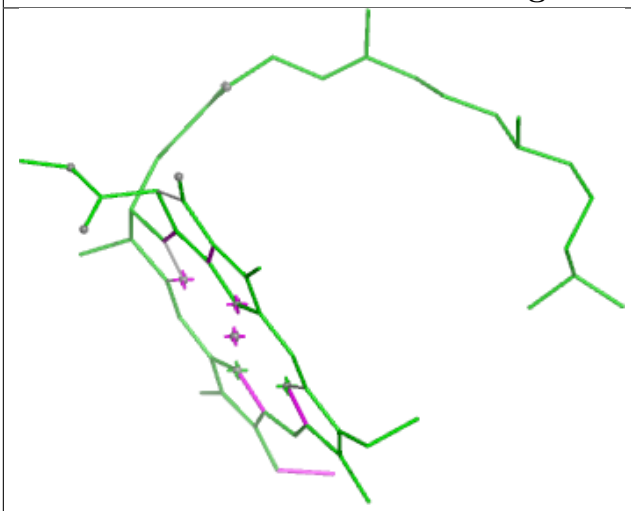


Rings

Ligand CLA 1 608



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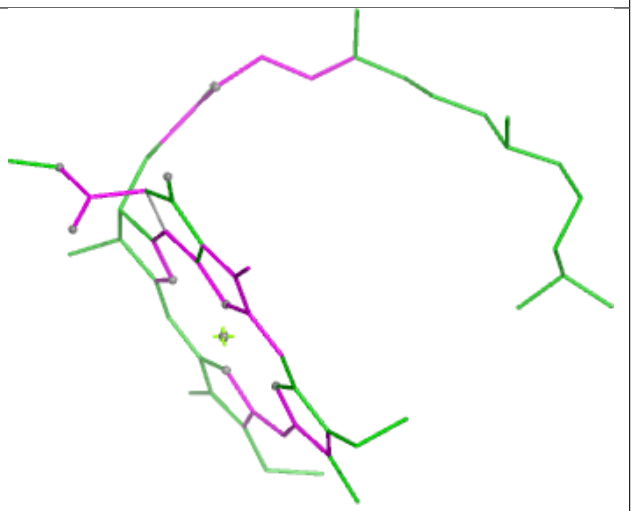

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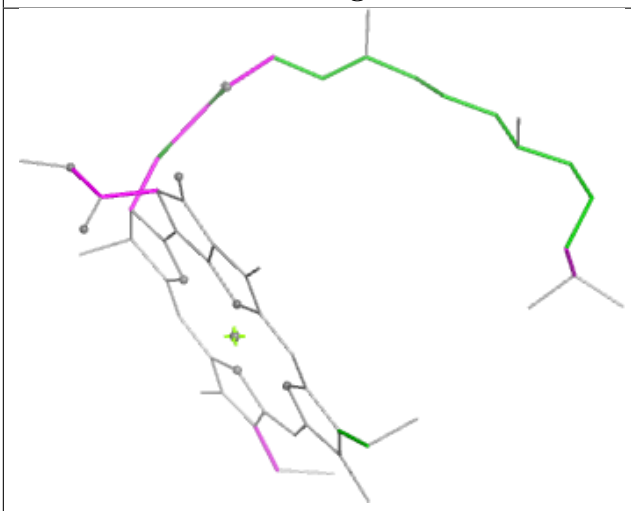

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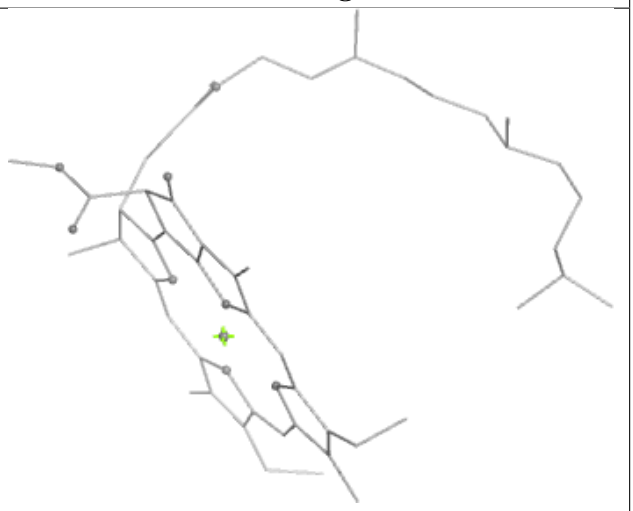

Rings

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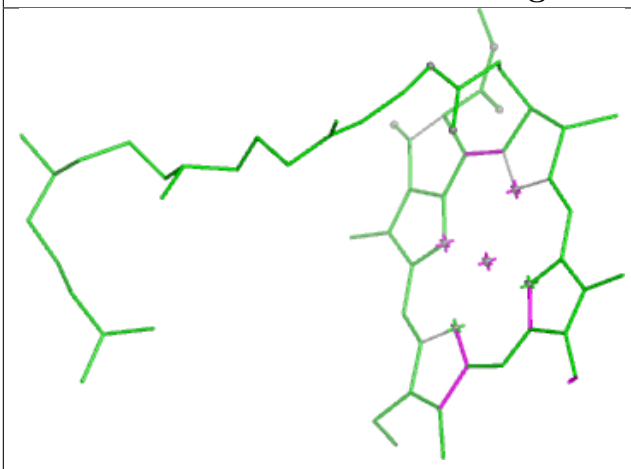

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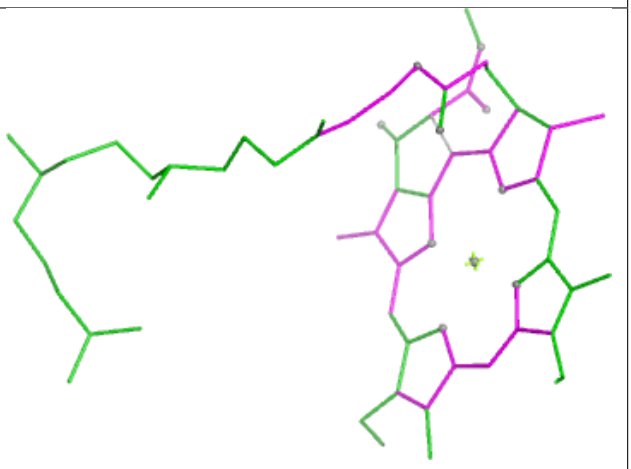

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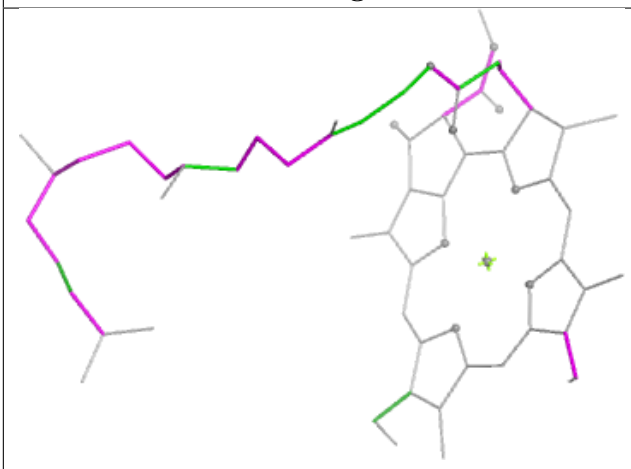

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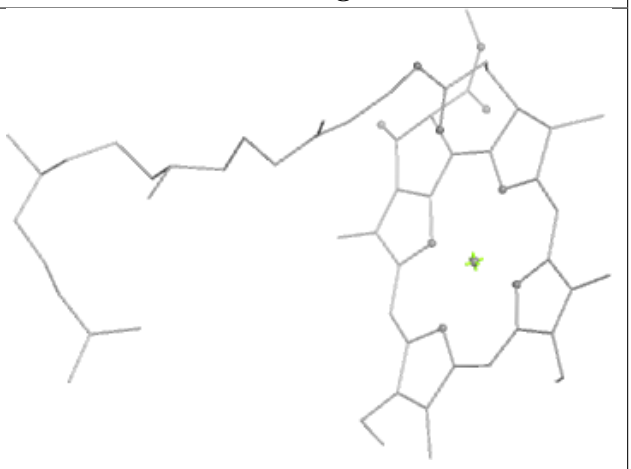

Rings

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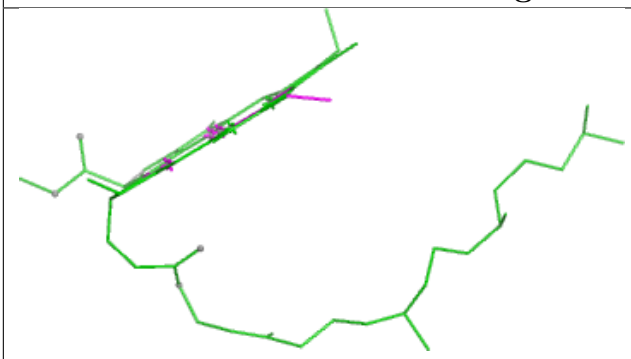

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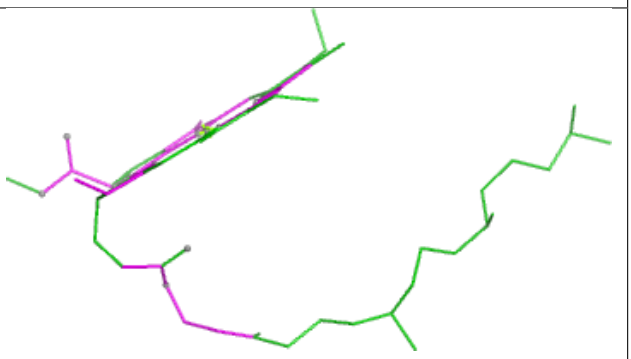

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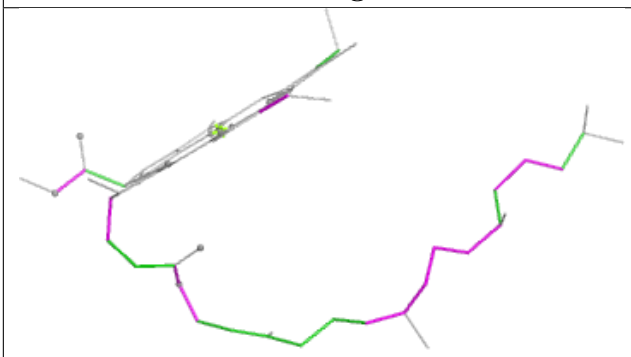
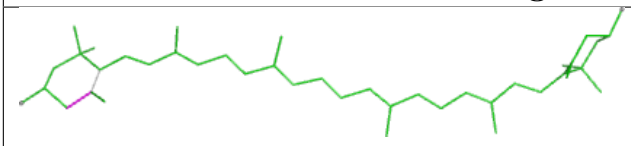


Torsions



Rings

Ligand LUT 4 502



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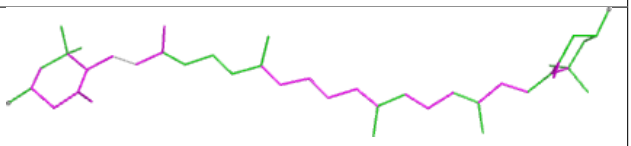

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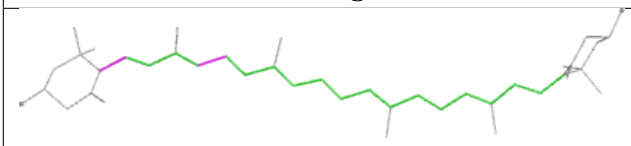

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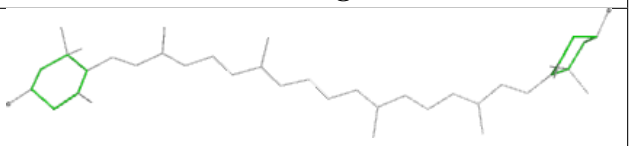

Rings

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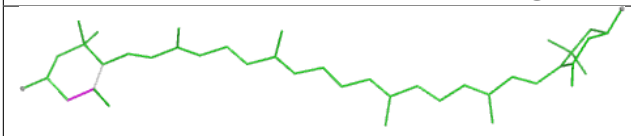

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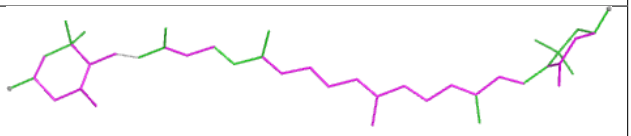
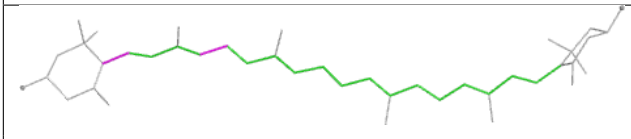


Bond angles



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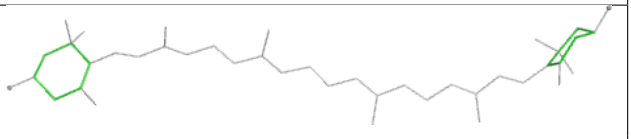
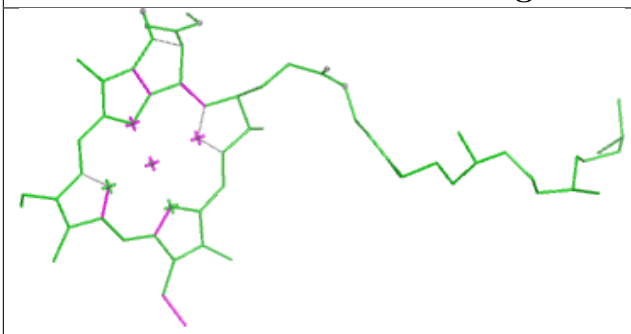


Rings

Ligand CLA B 1210



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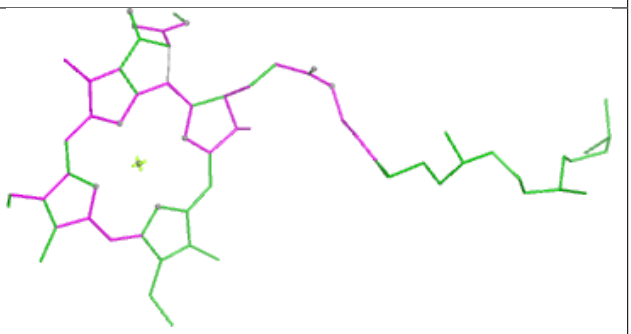

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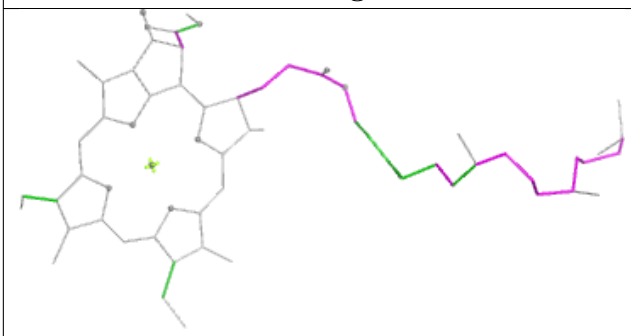

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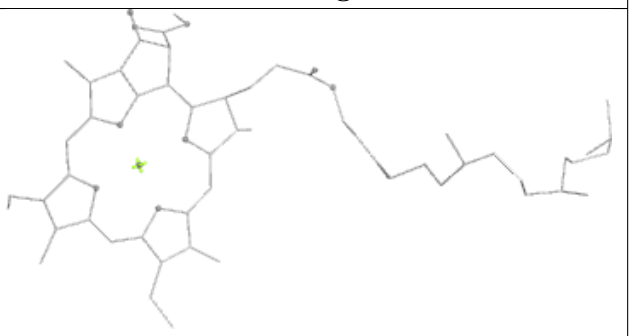
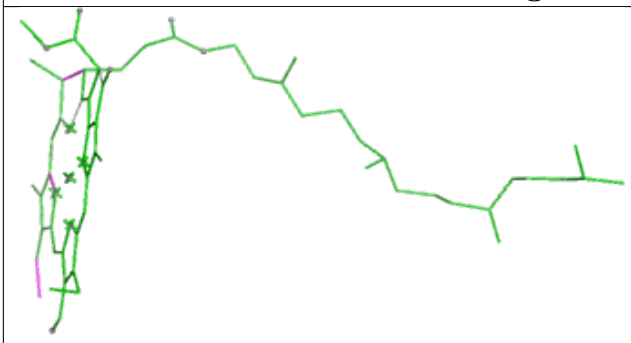


Rings

Ligand CHL Z 609



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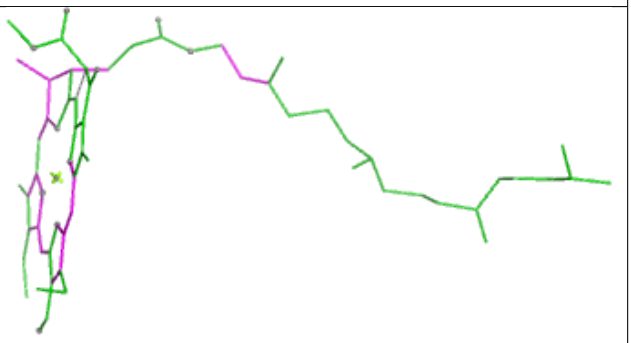
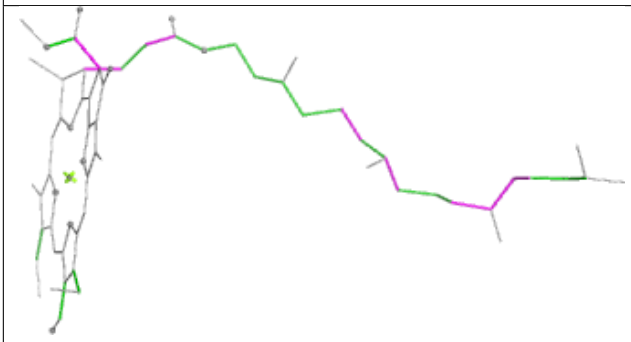


Bond angles



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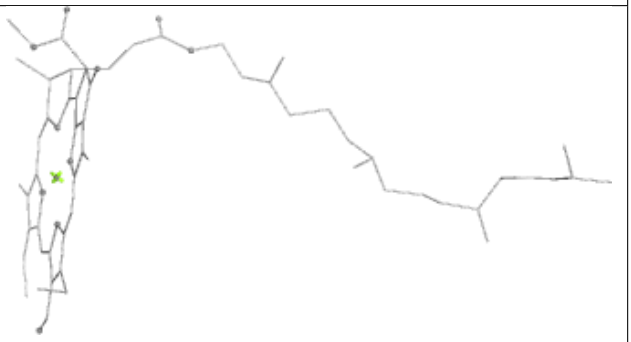
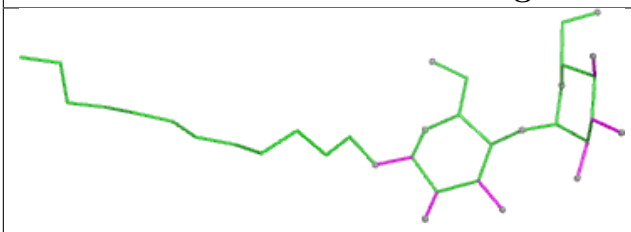


Rings

Ligand LMT F 5001



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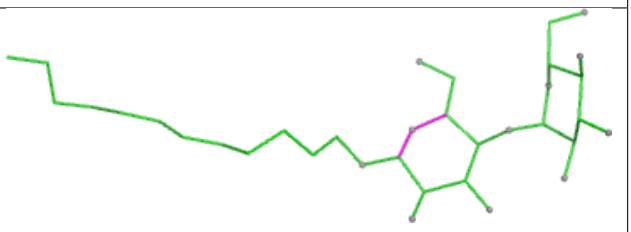
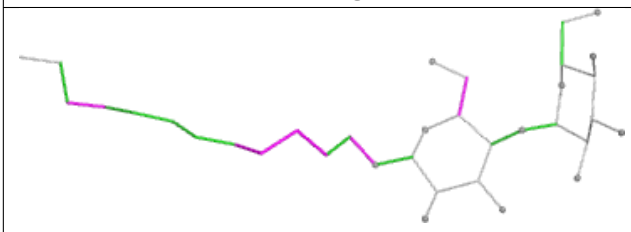


Bond angles



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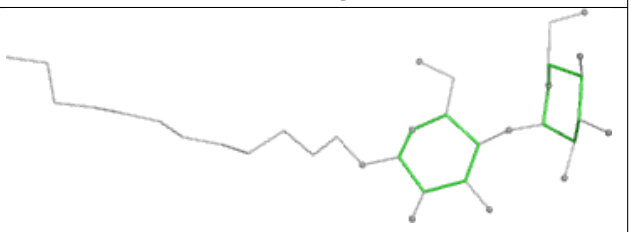
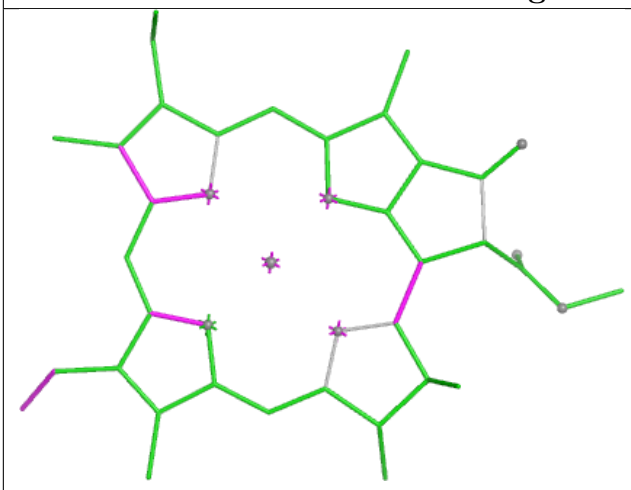


Rings

Ligand CLA 4 615



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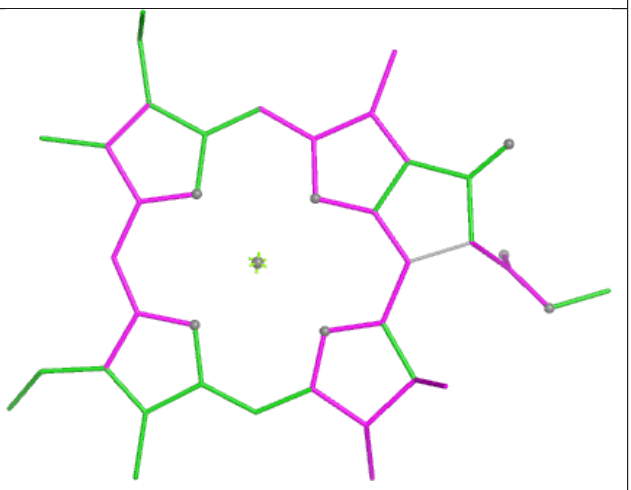
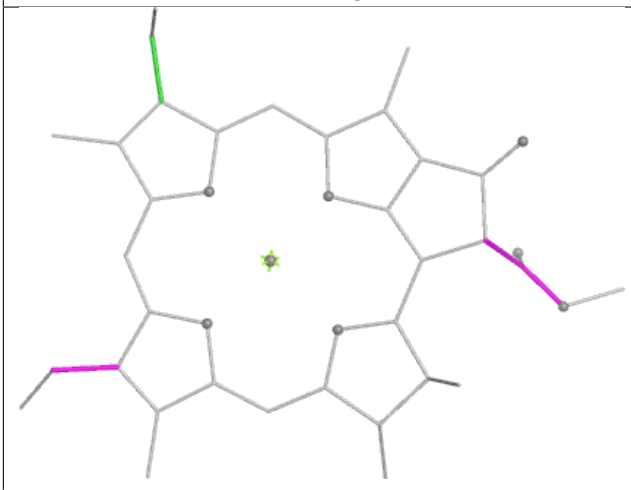


Bond angles



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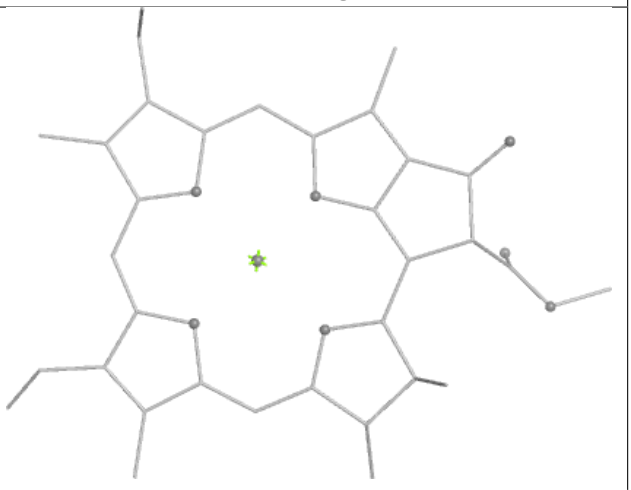
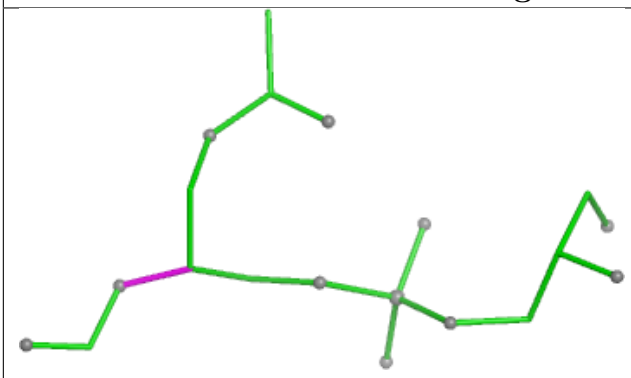
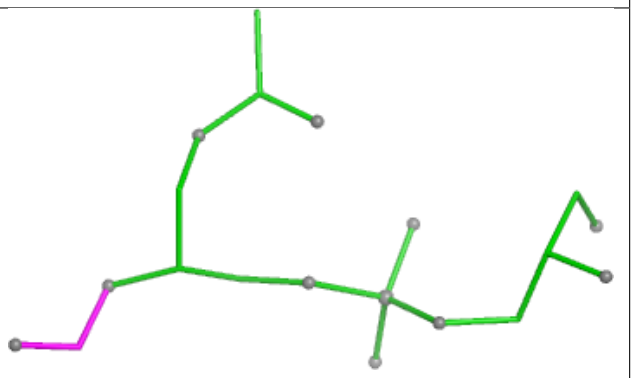


Rings

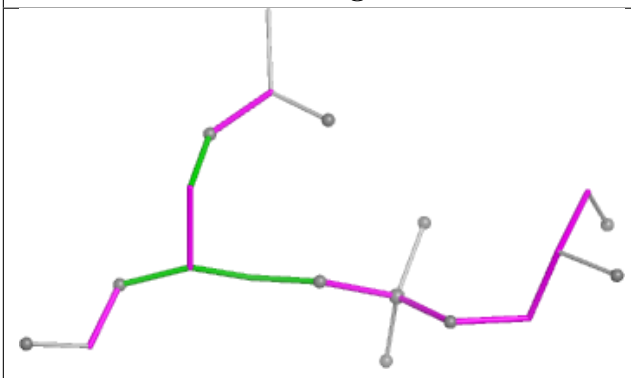
Ligand LHG B 5002



Bond lengths



Bond angles



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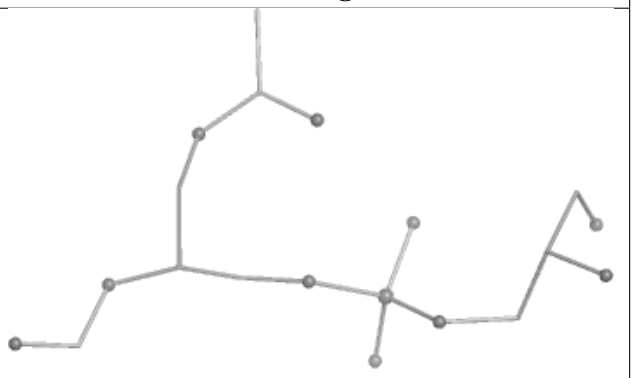
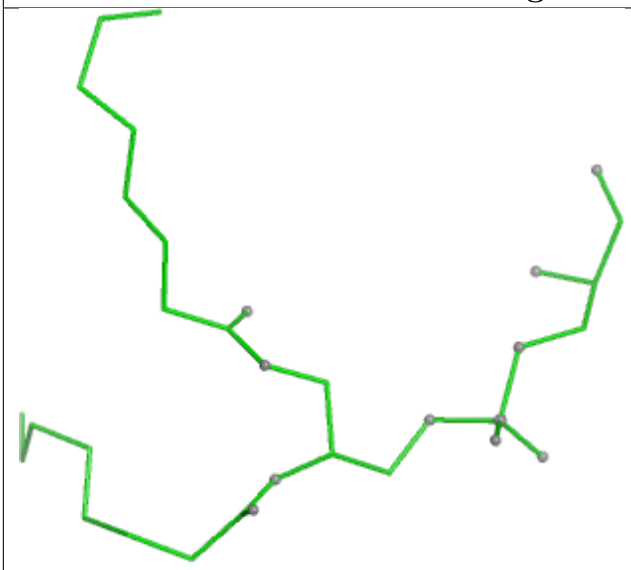
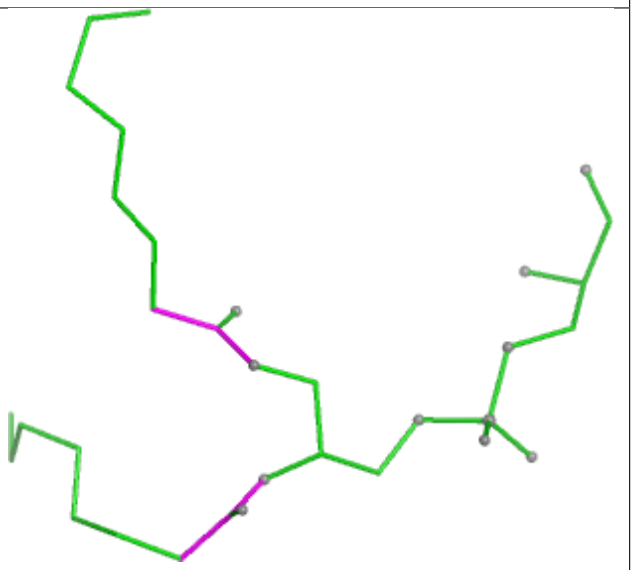


Rings

Ligand LHG 9 801



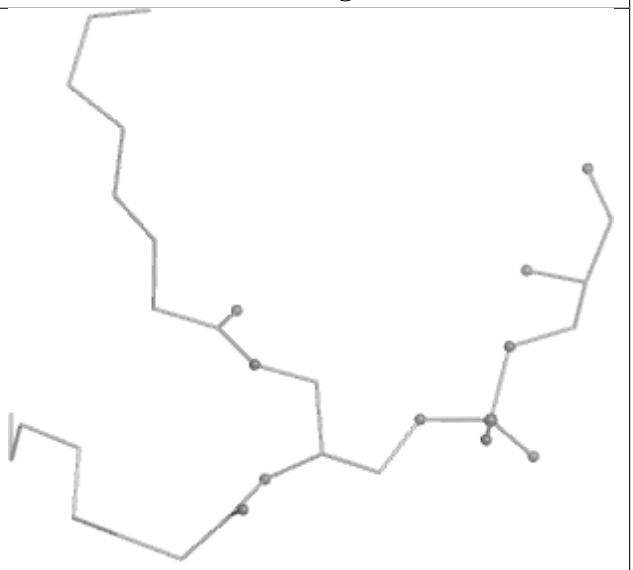
Bond lengths



Bond angles

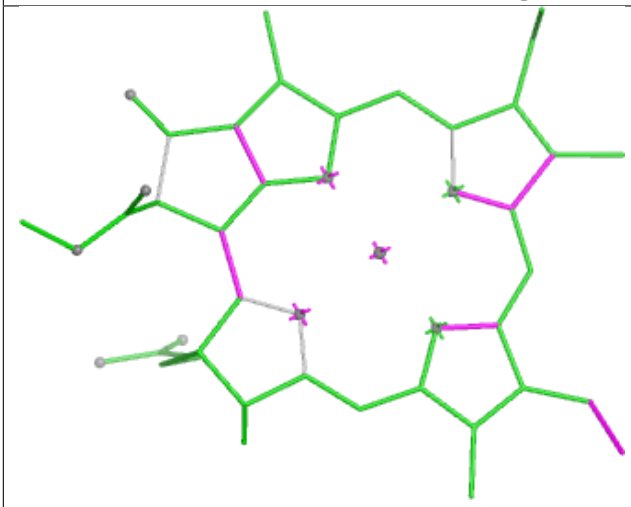


Torsions



Rings

Ligand CLA B 1201



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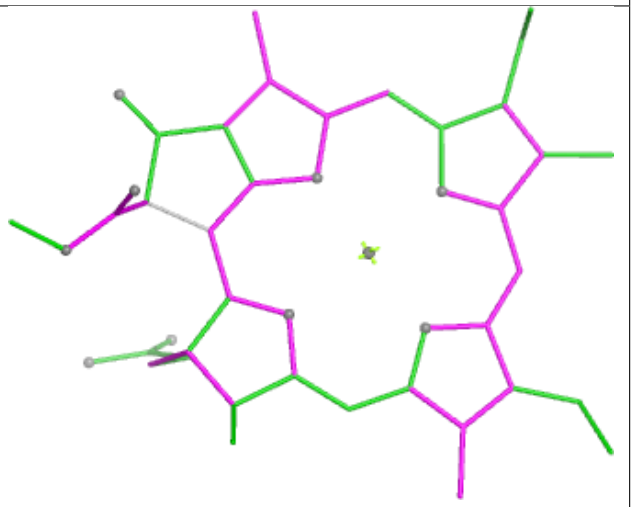
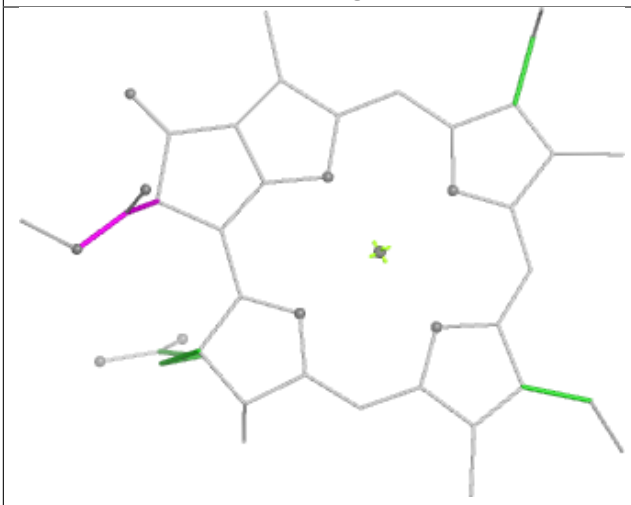


Bond angles



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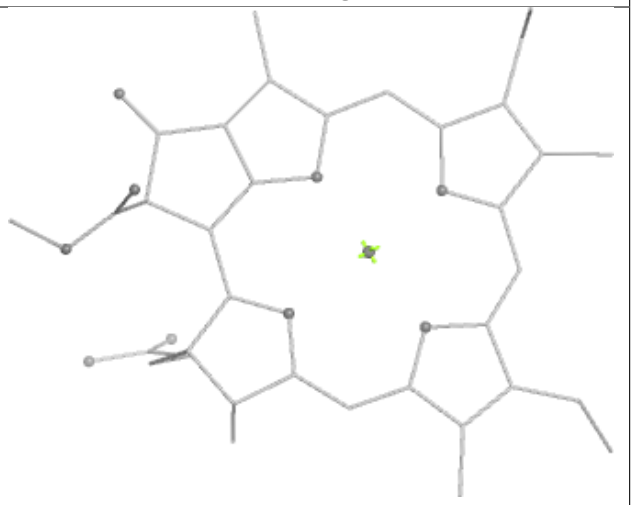
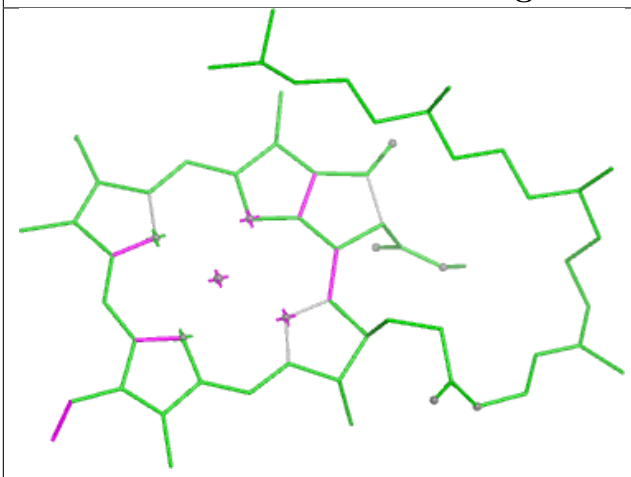


Rings

Ligand CLA B 1202



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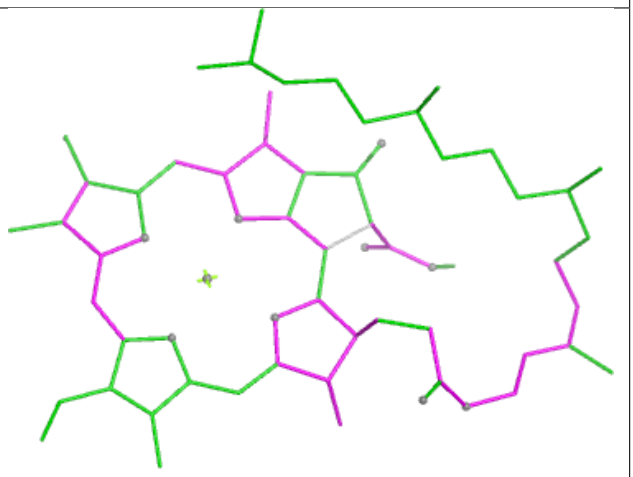
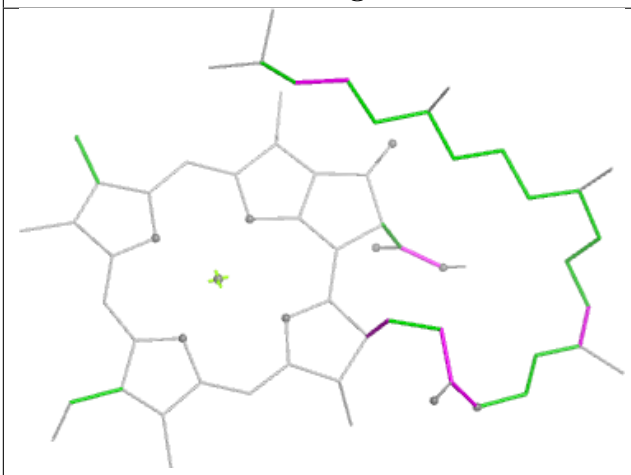


Bond angles



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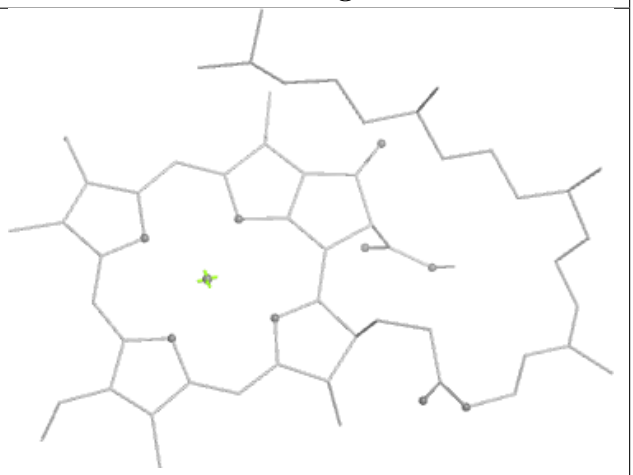
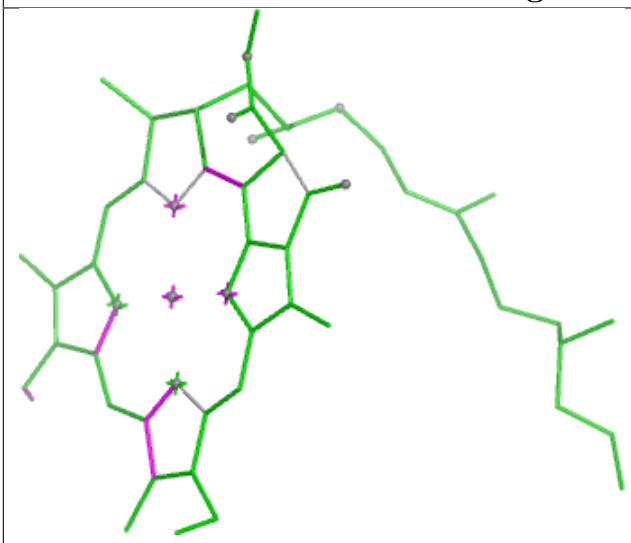


Rings

Ligand CLA Z 607



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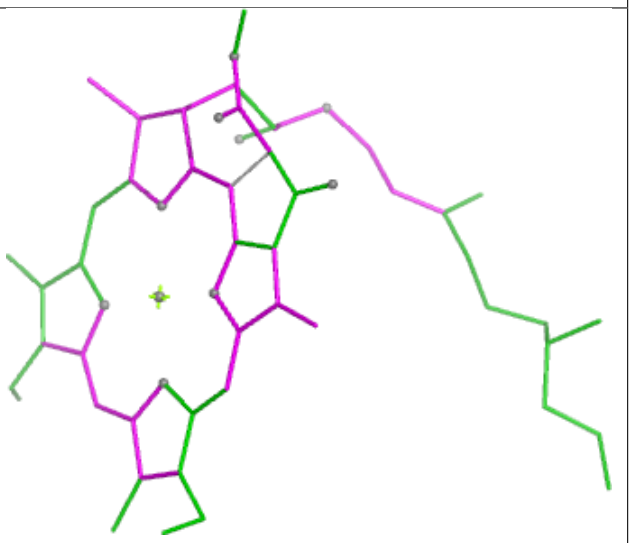
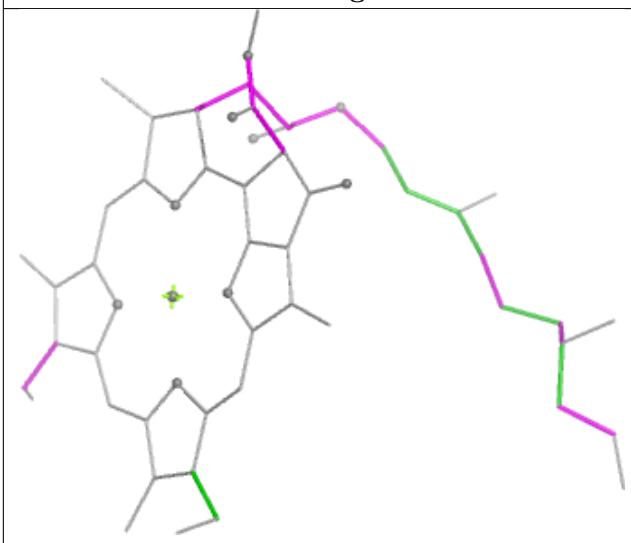


Bond angles



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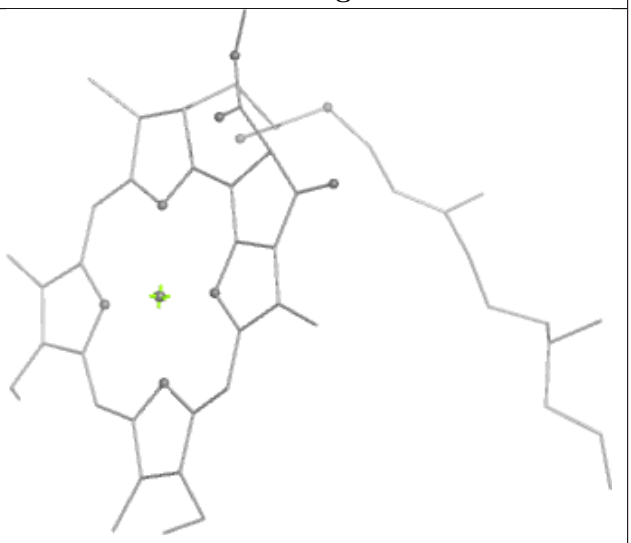
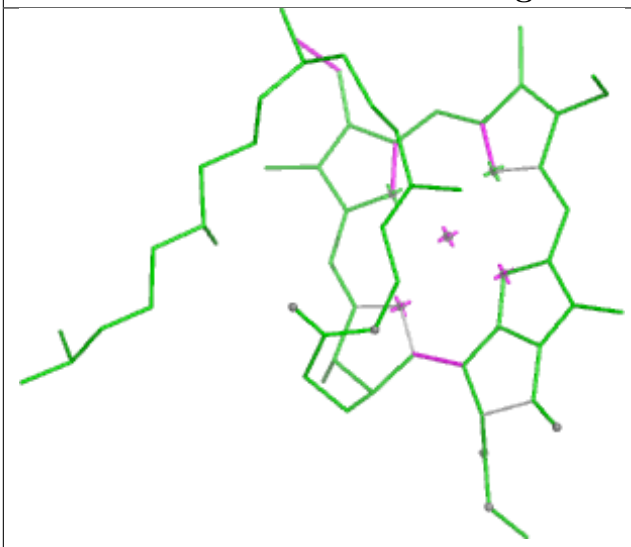


Rings

Ligand CLA B 1205



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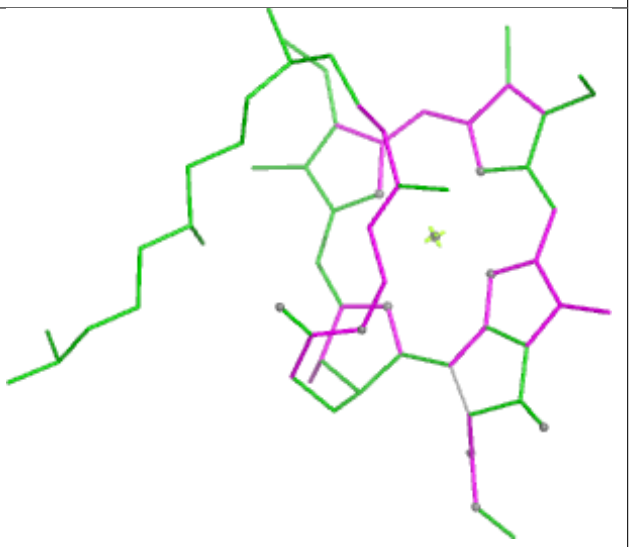
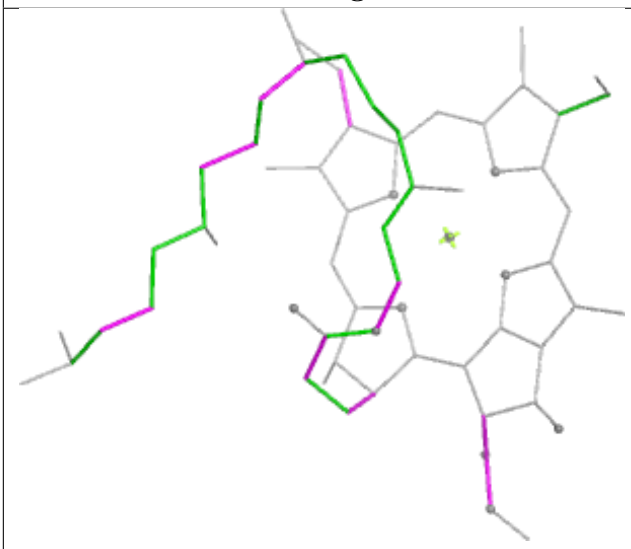


Bond angles

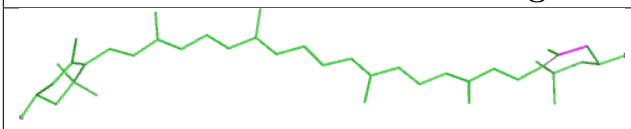


Torsions



Rings

Ligand LUT 3 501



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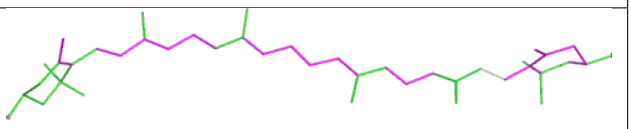
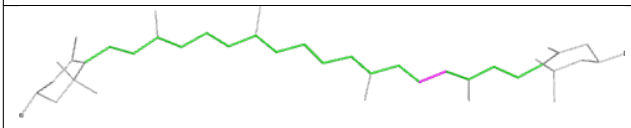


Bond angles



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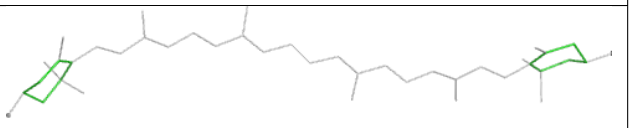
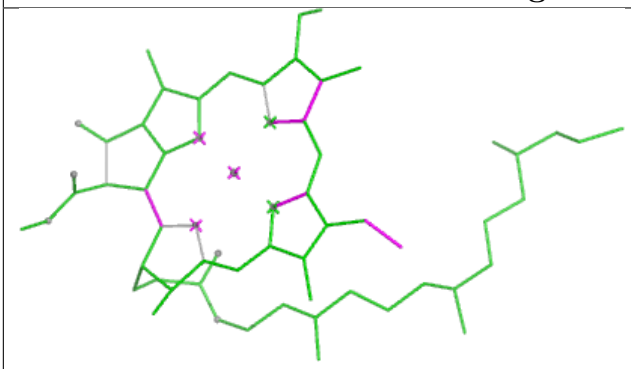


Rings

Ligand CLA 8 604



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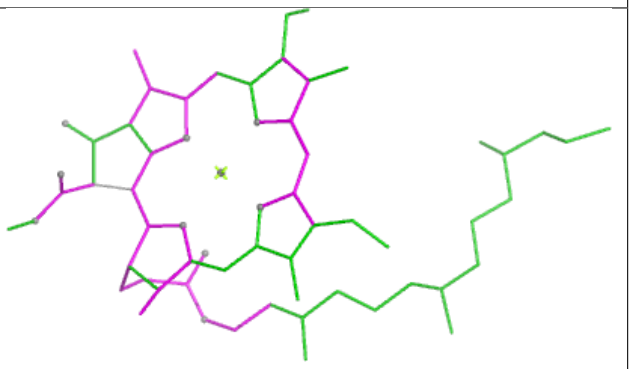

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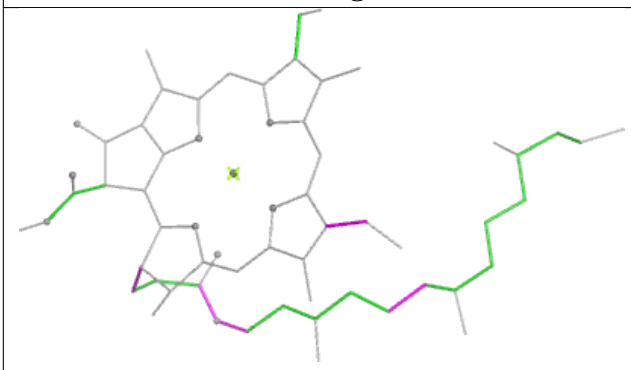

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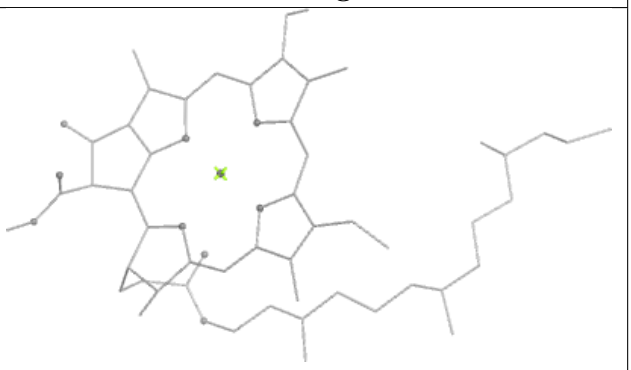
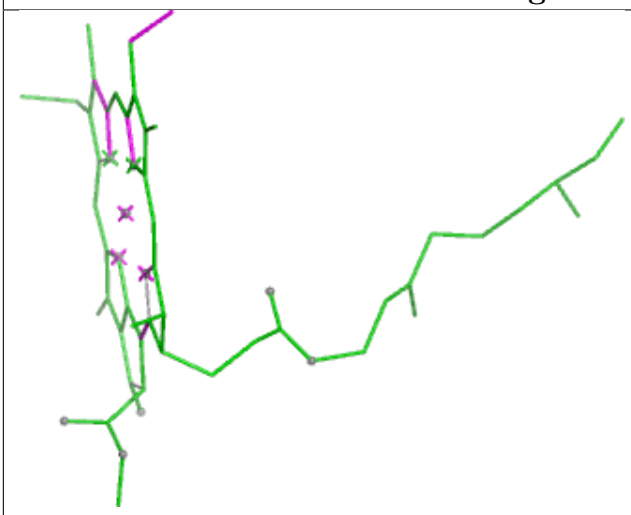


Rings

Ligand CLA 7 606



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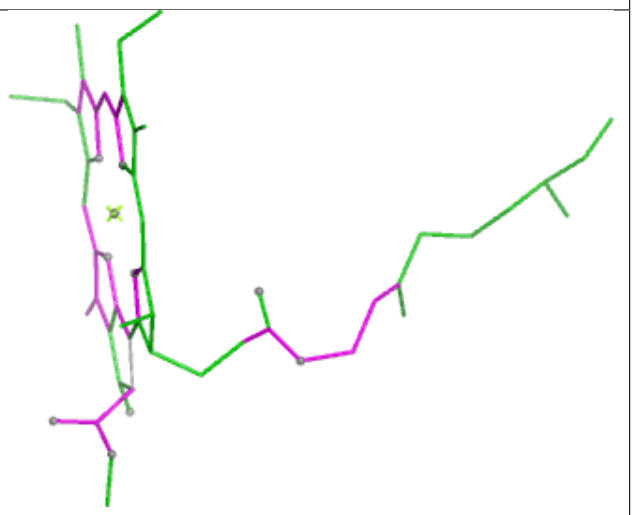
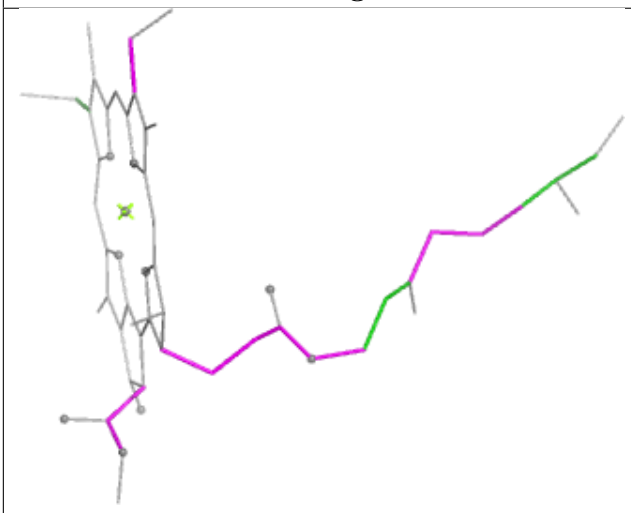


Bond angles

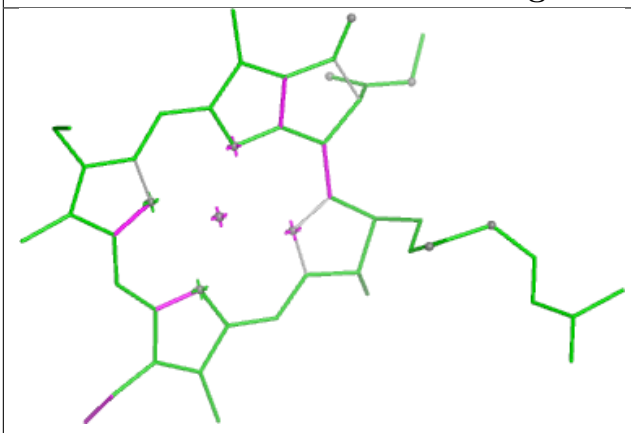


Torsions



Rings

Ligand CLA 8 611



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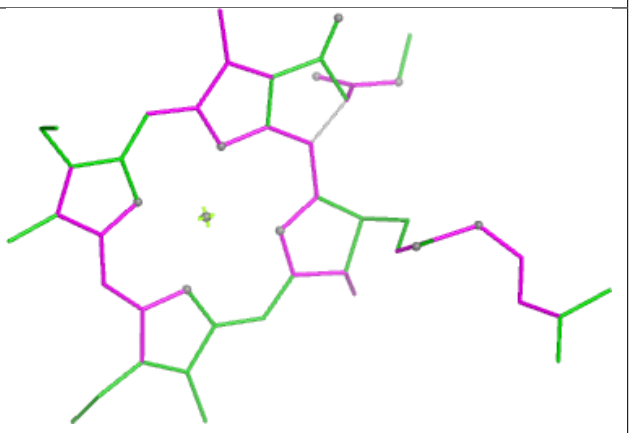
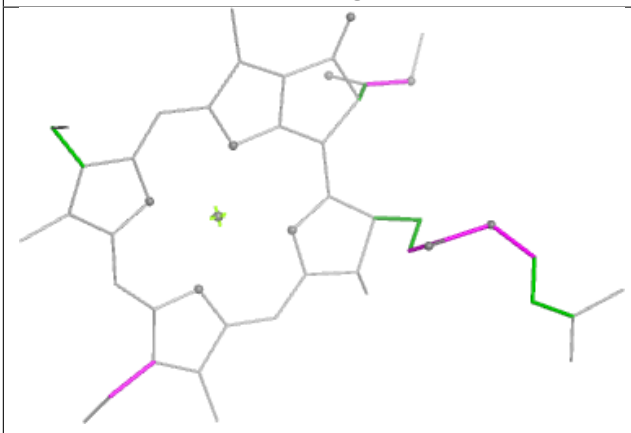


Bond angles



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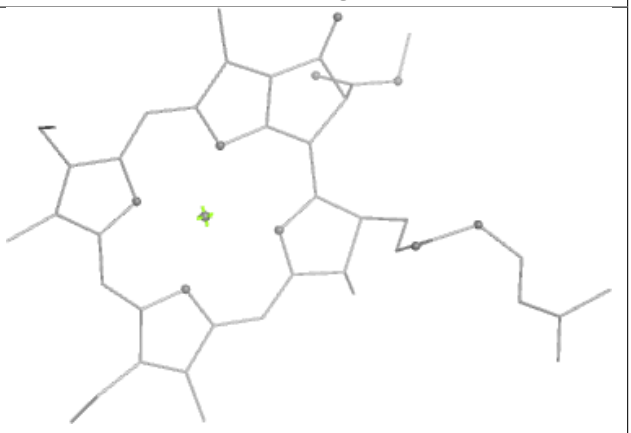
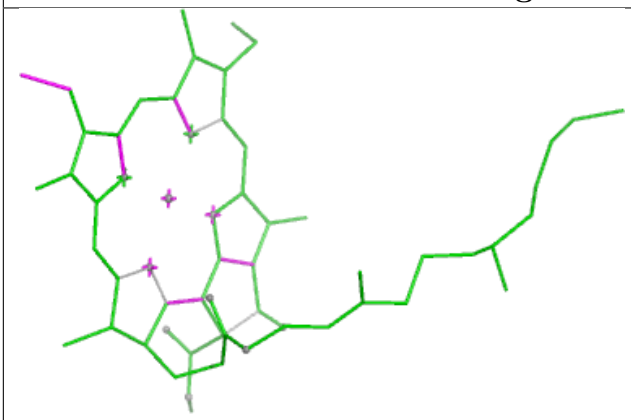


Rings

Ligand CLA B 1219



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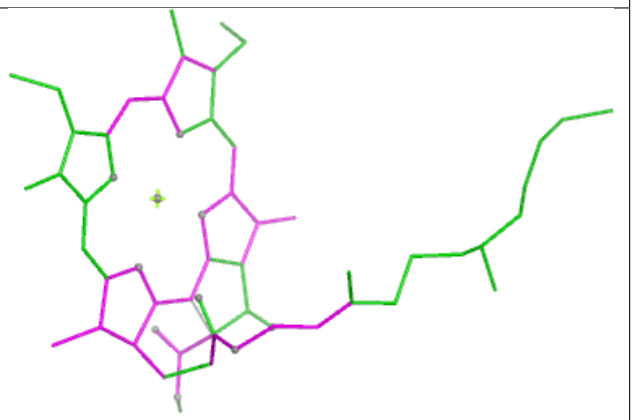
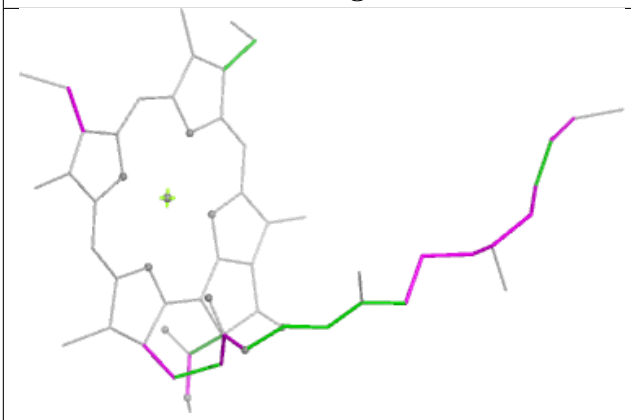


Bond angles

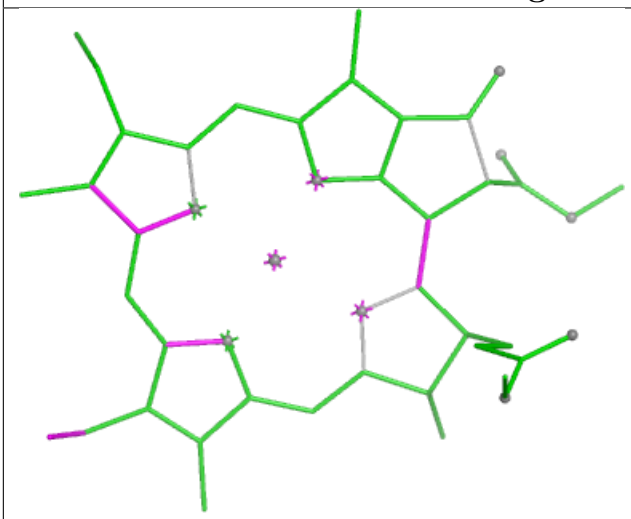


Torsions



Rings

Ligand CLA 9 609



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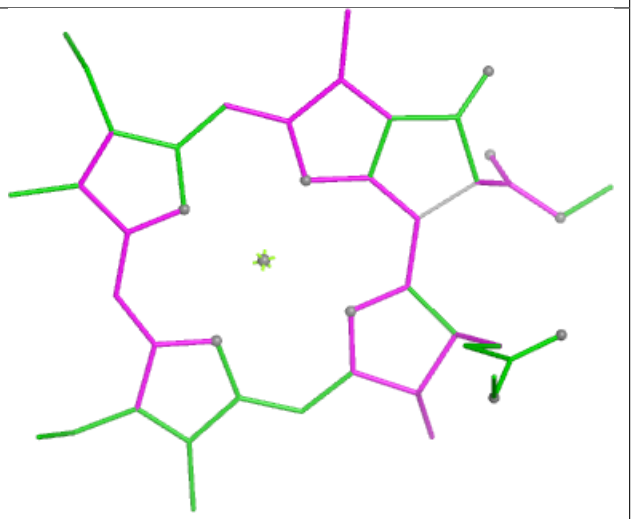

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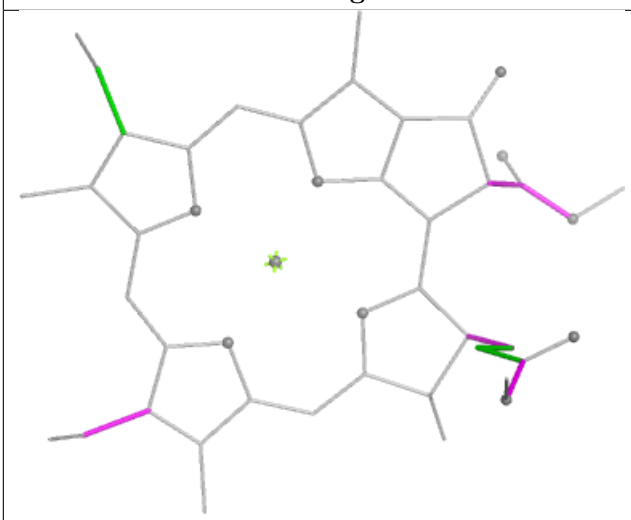

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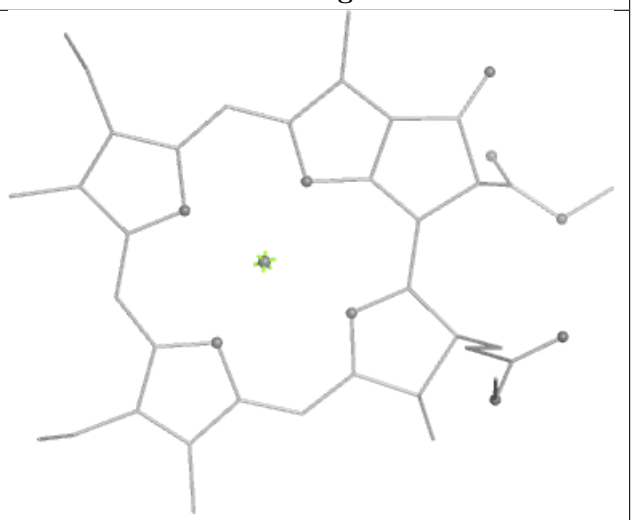


Rings

Ligand LUT 6 501



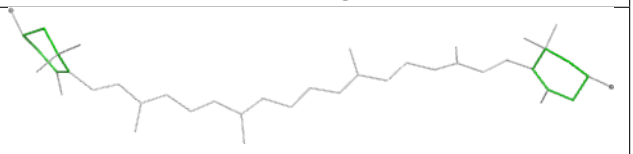
Bond lengths



Bond angles

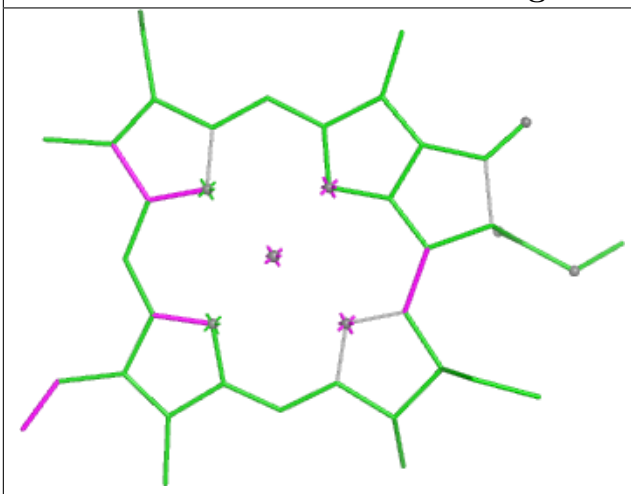


Torsions



Rings

Ligand CLA 7 613



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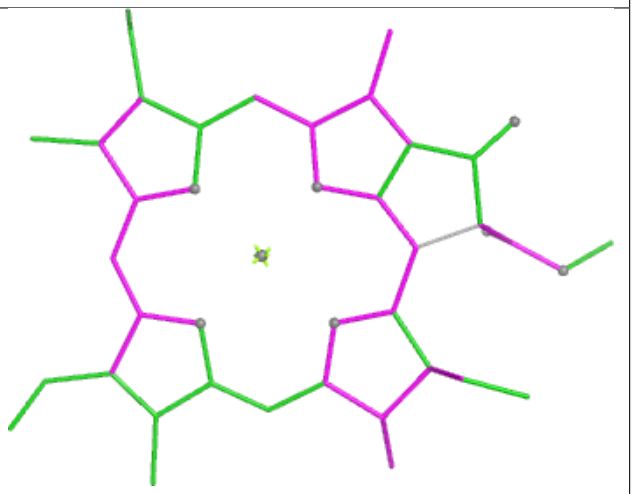
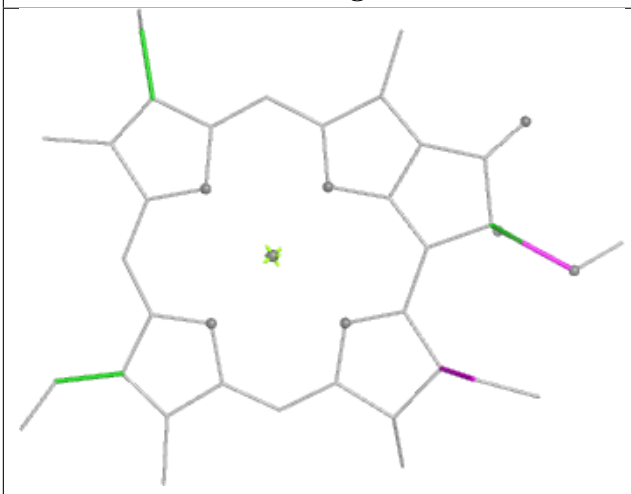


Bond angles



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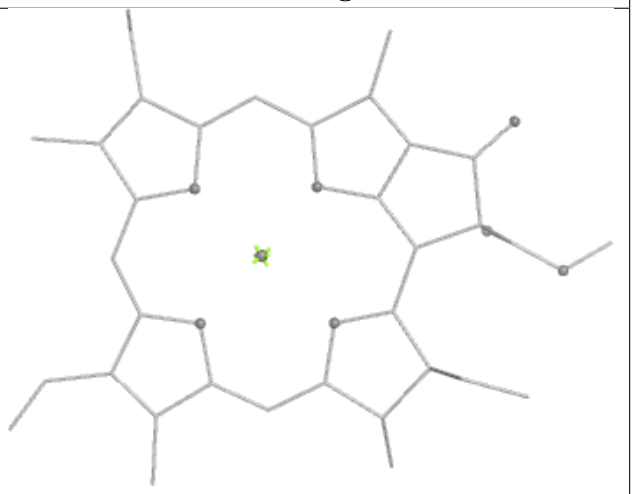
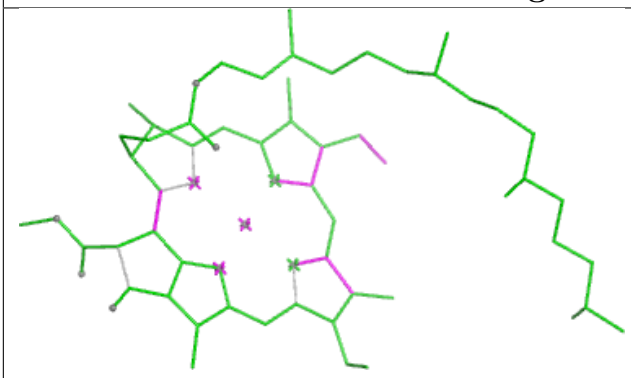


Rings

Ligand CLA 5 604



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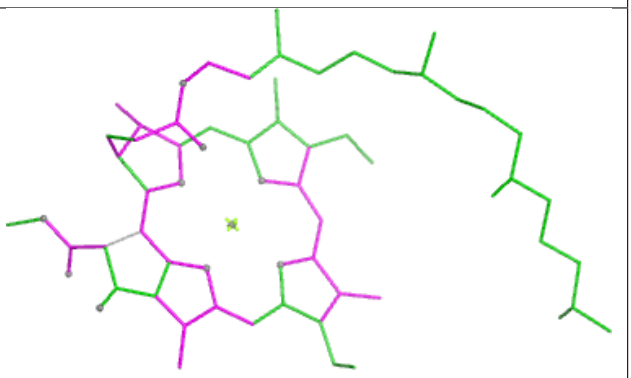
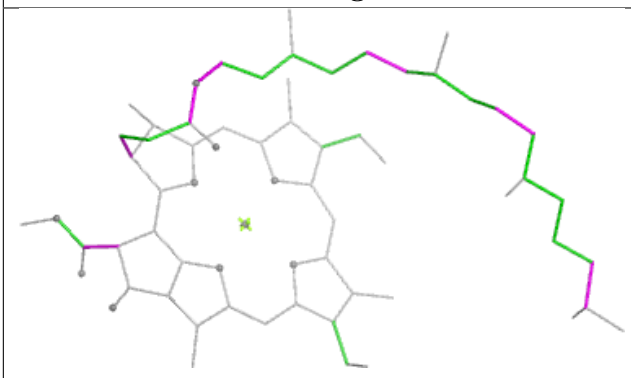


Bond angles



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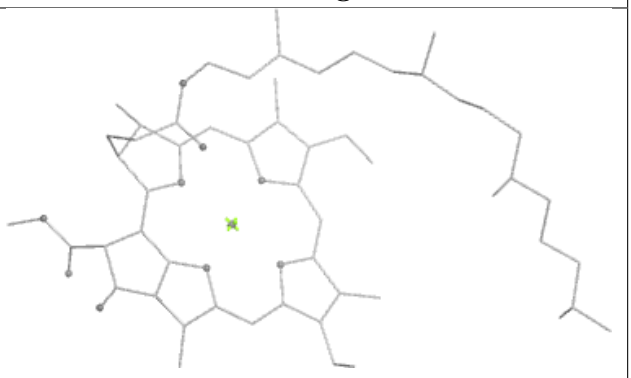
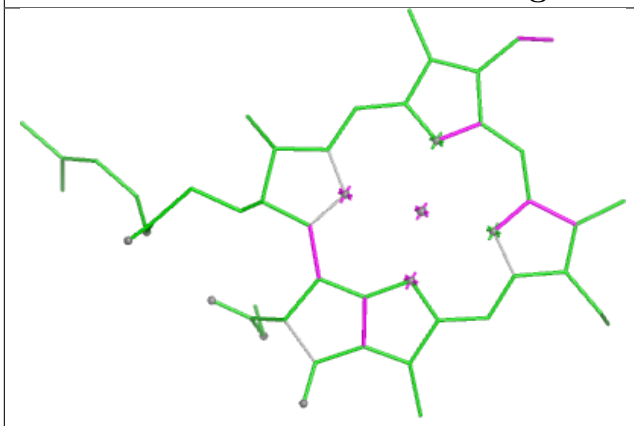


Rings

Ligand CLA 2 605



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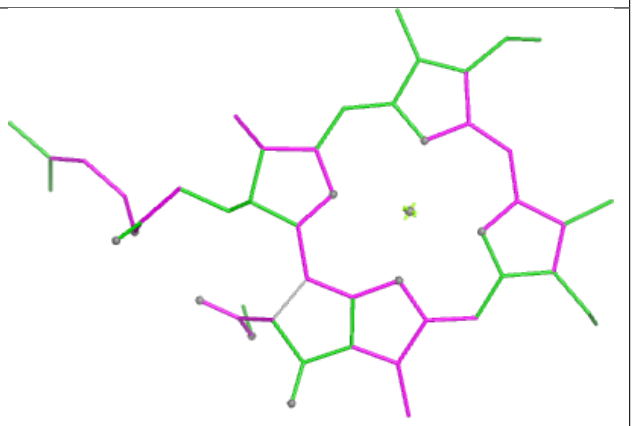
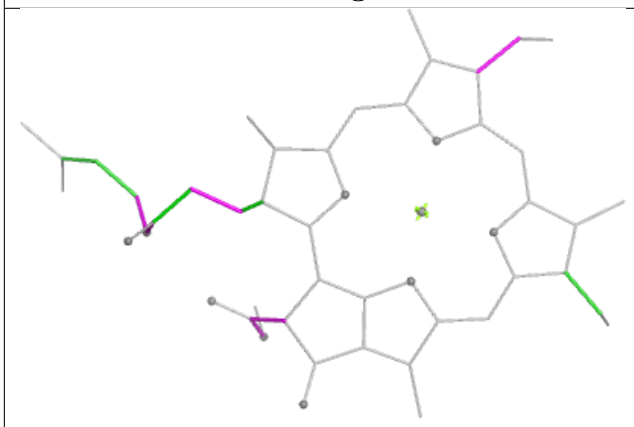
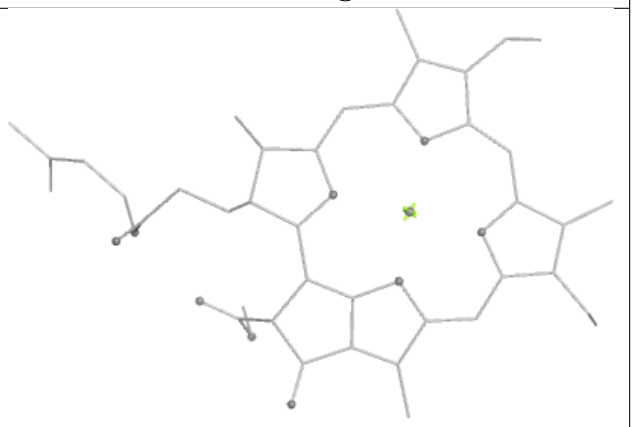


Bond angles

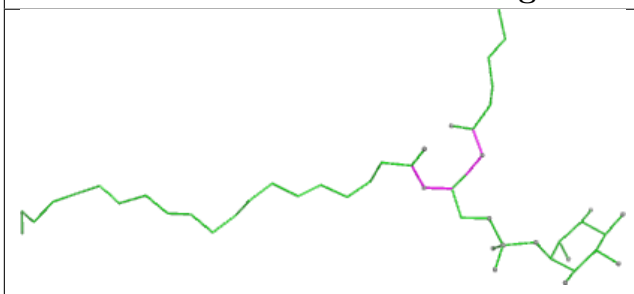


Torsions



Rings

Ligand T7X B 5004



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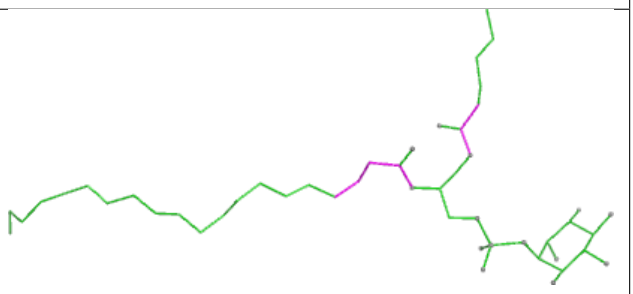
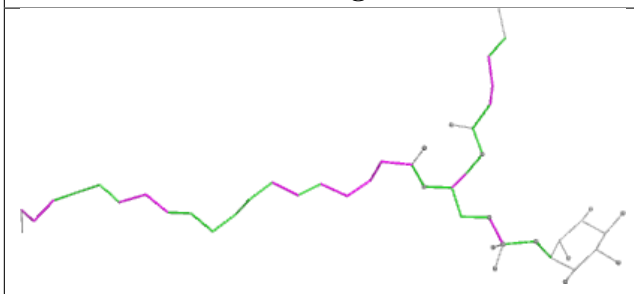


Bond angles



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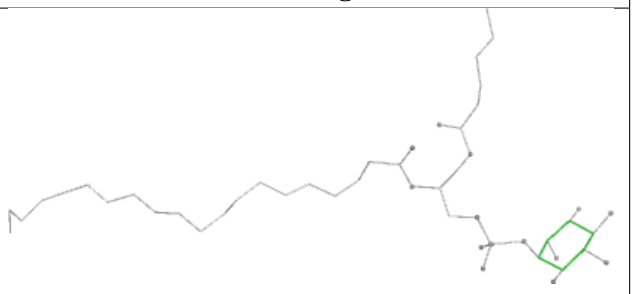
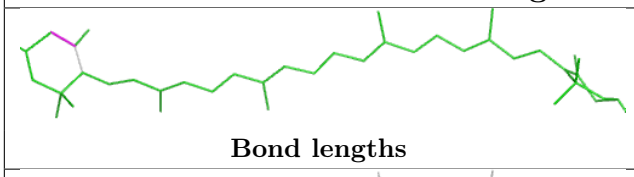


Rings

Ligand LUT 5 502



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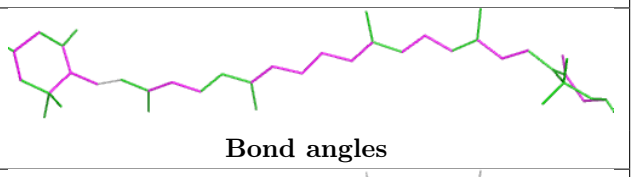
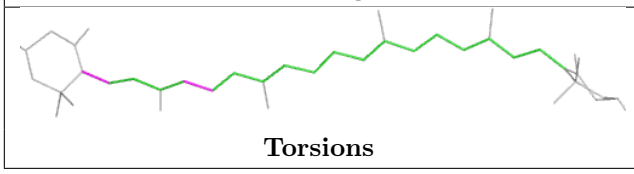
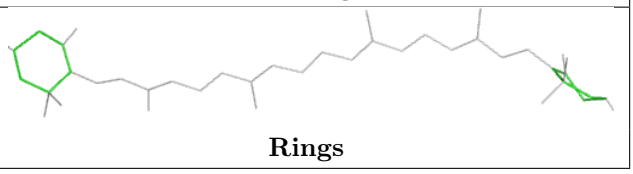


Bond angles

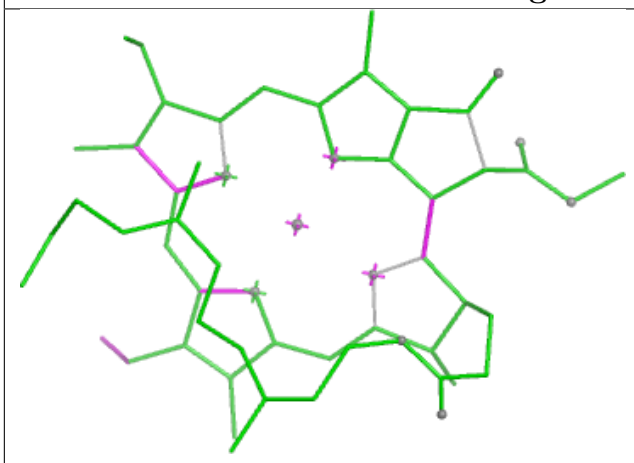


Torsions

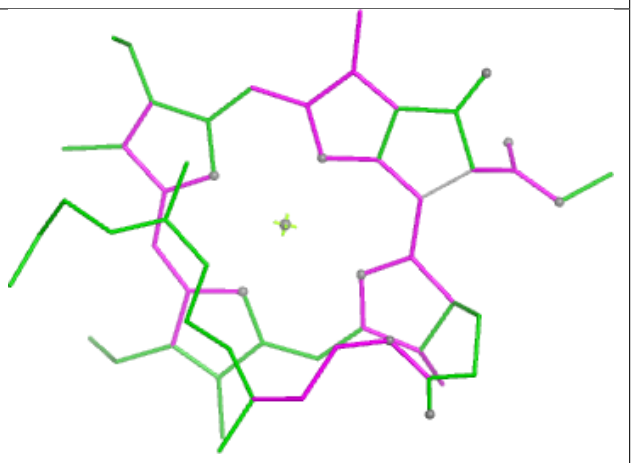


Rings

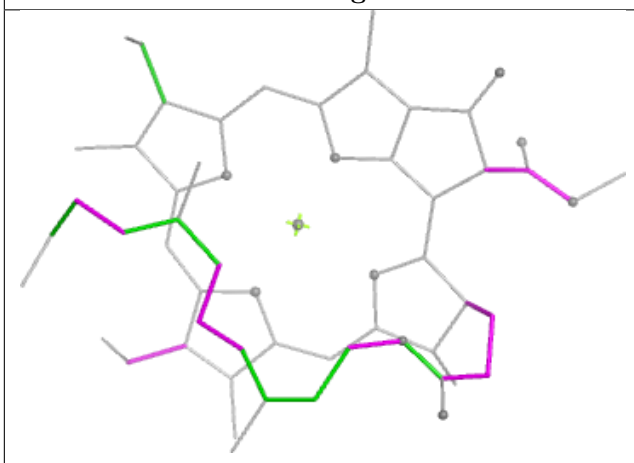
Ligand CLA 7 615



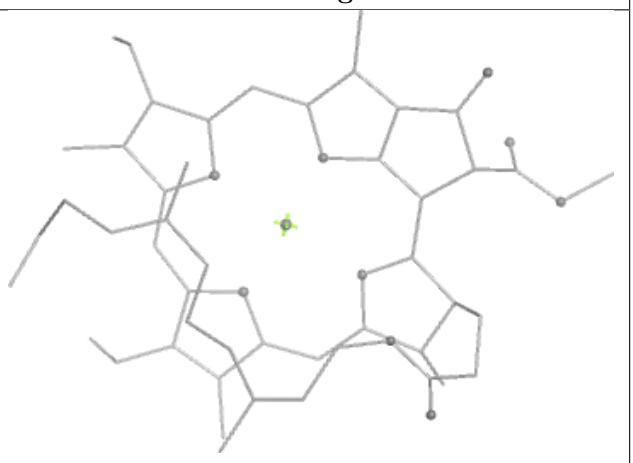
Bond lengths



Bond angles

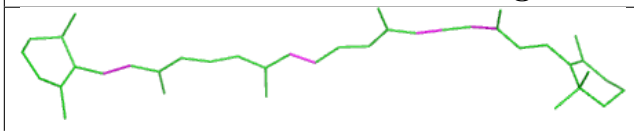


Torsions

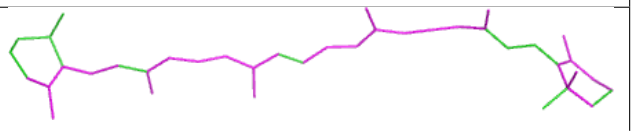


Rings

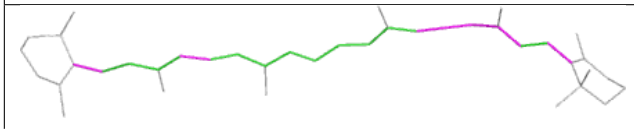
Ligand BCR K 4002



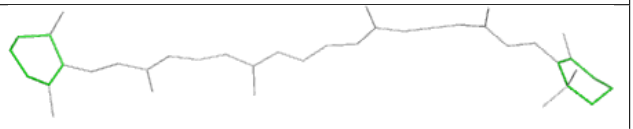
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

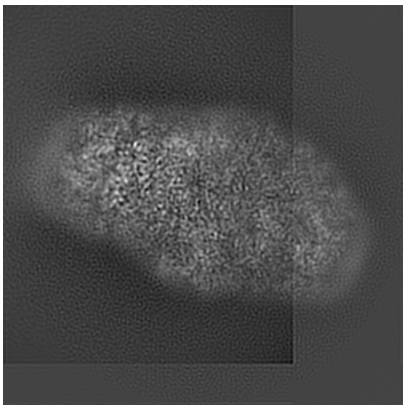
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12180. These allow visual inspection of the internal detail of the map and identification of artifacts.

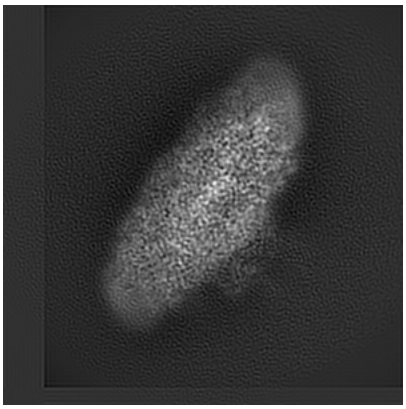
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

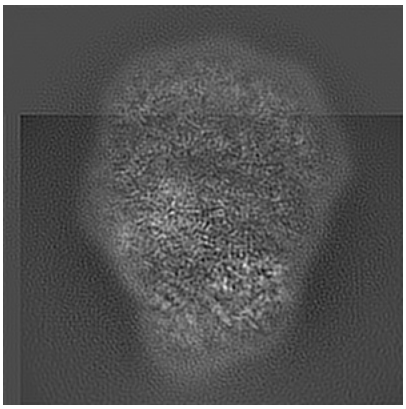
6.1.1 Primary map



X

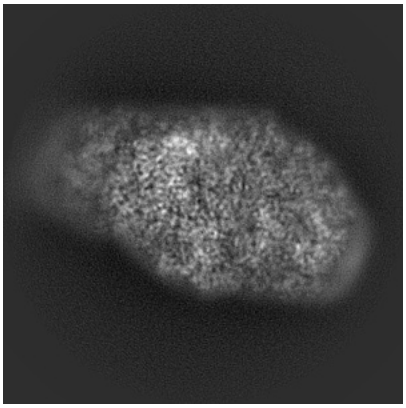


Y

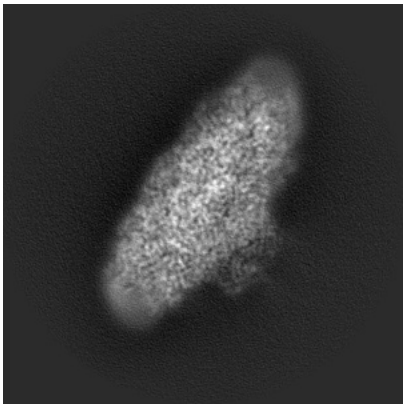


Z

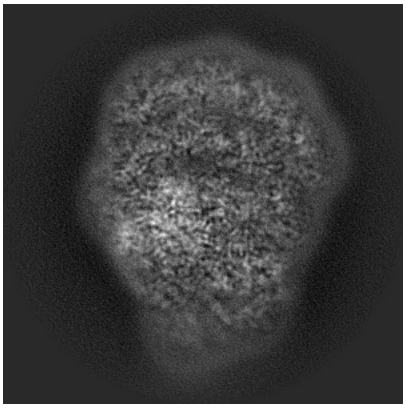
6.1.2 Raw map



X



Y

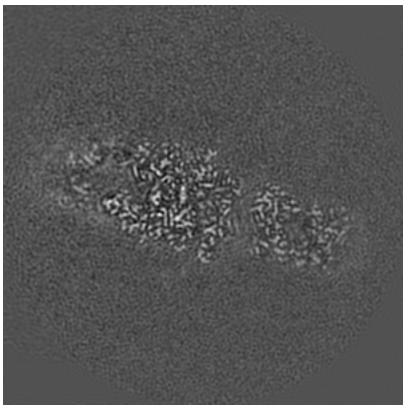


Z

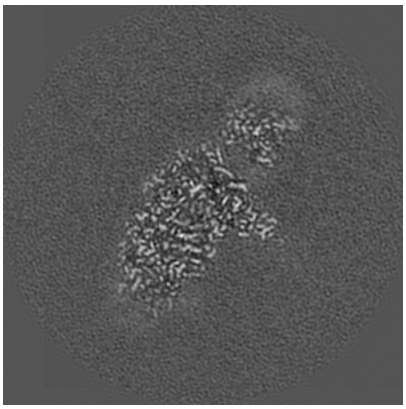
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

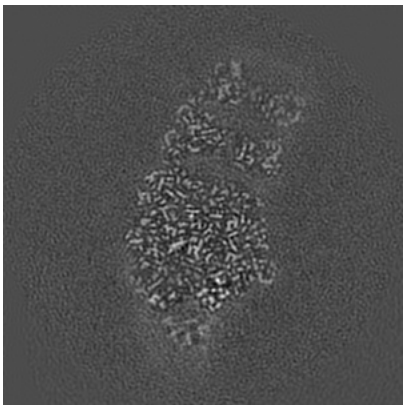
6.2.1 Primary map



X Index: 160

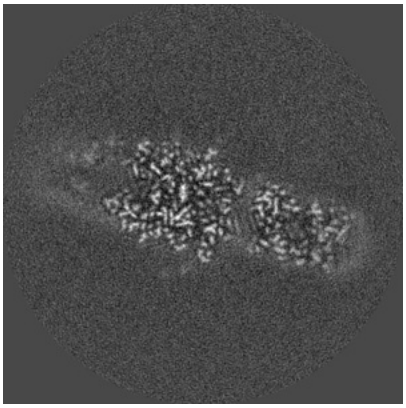


Y Index: 160

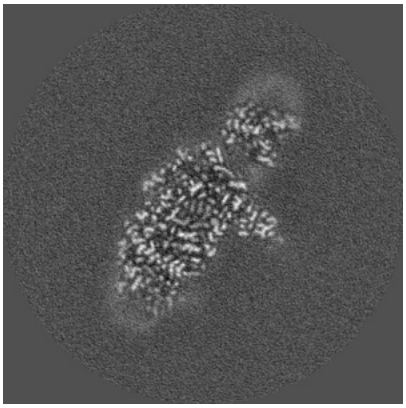


Z Index: 160

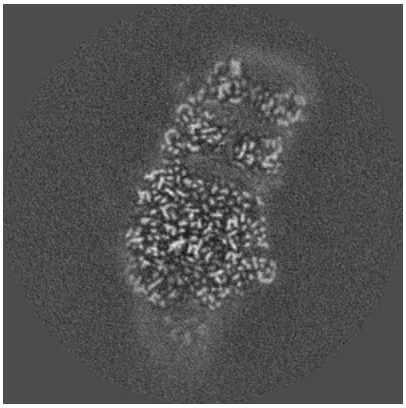
6.2.2 Raw map



X Index: 160



Y Index: 160

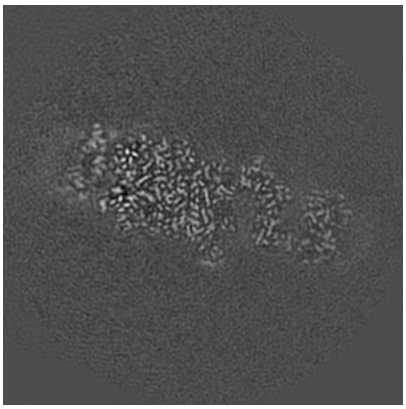


Z Index: 160

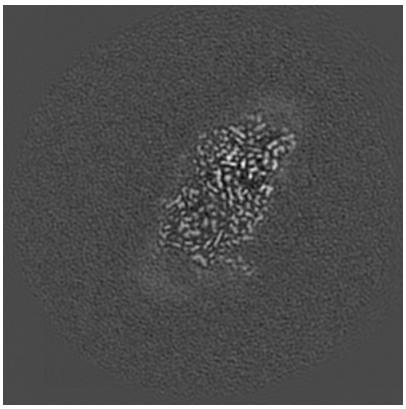
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

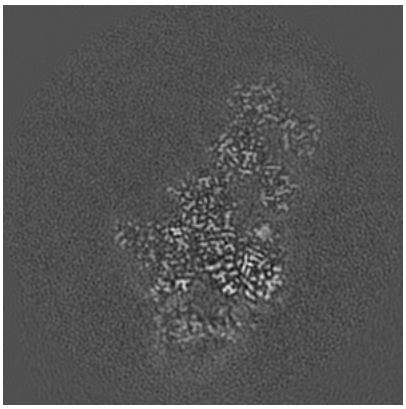
6.3.1 Primary map



X Index: 172

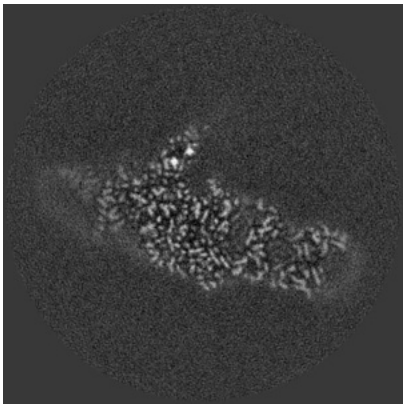


Y Index: 112

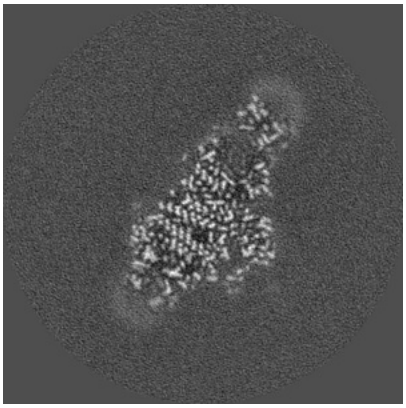


Z Index: 180

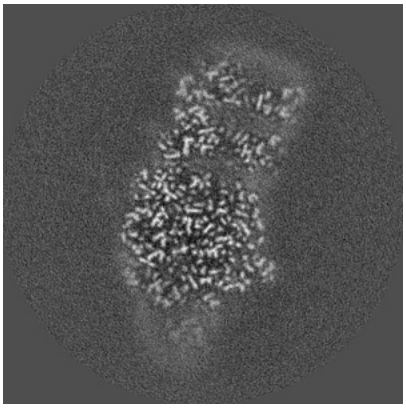
6.3.2 Raw map



X Index: 127



Y Index: 145

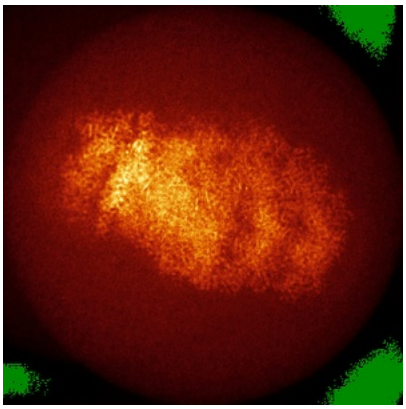


Z Index: 157

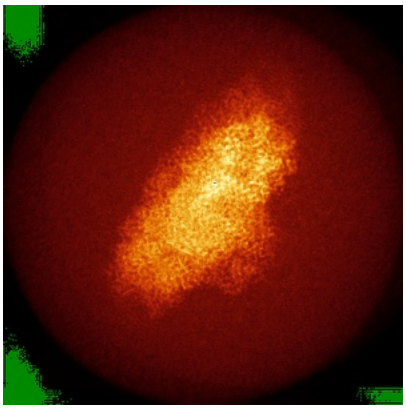
The images above show the largest variance slices of the map in three orthogonal directions.

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

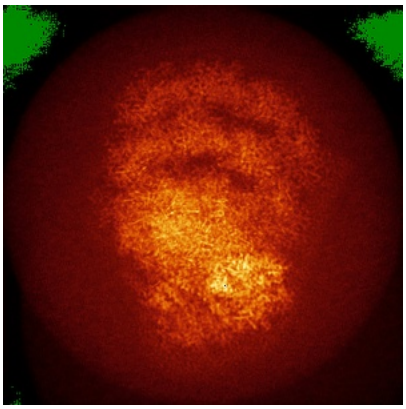
6.4.1 Primary map



X

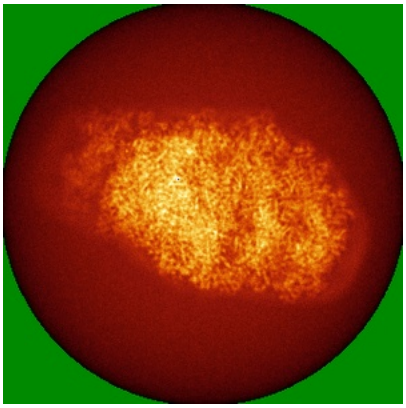


Y

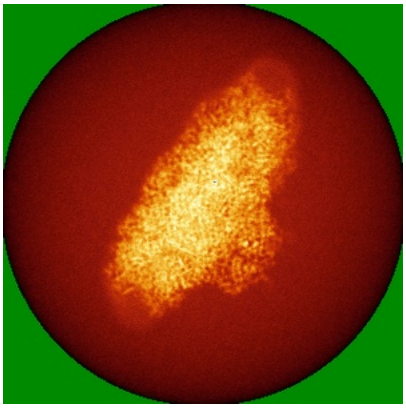


Z

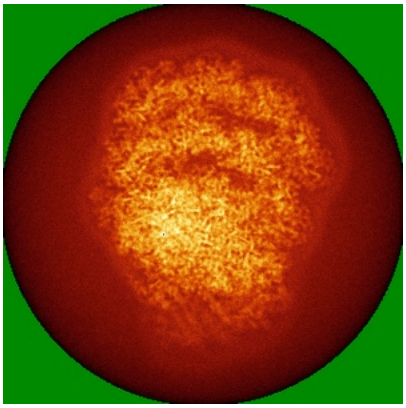
6.4.2 Raw map



X



Y

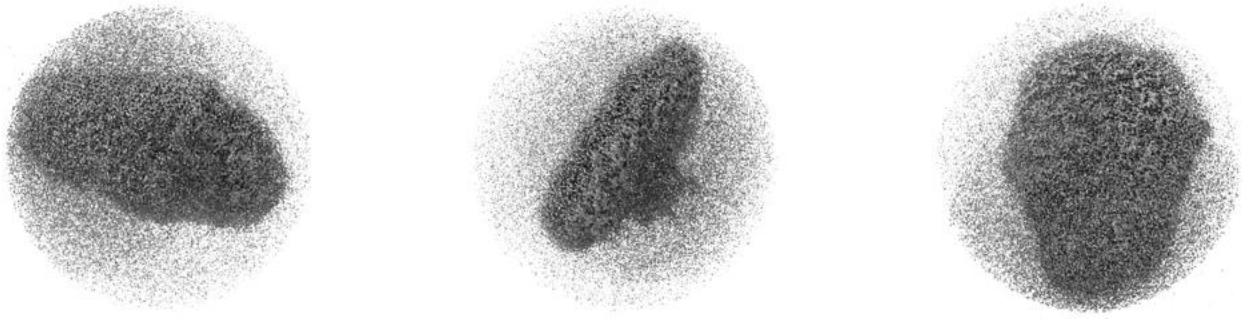


Z

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

6.5 Orthogonal surface views (i)

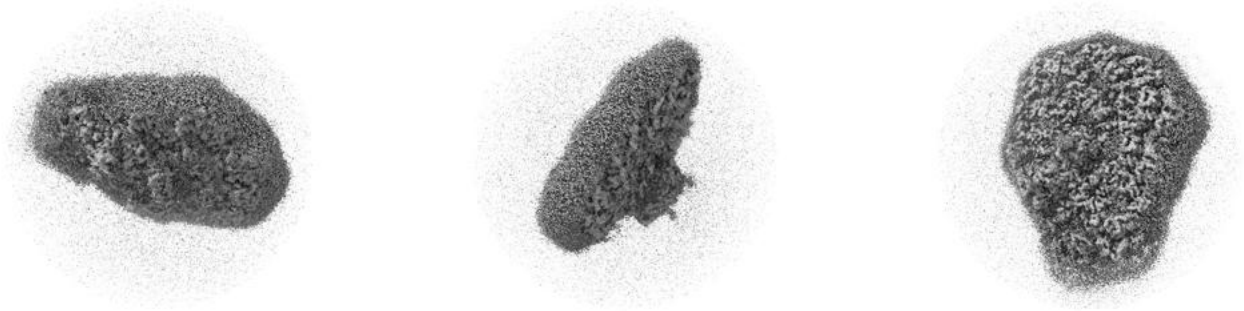
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

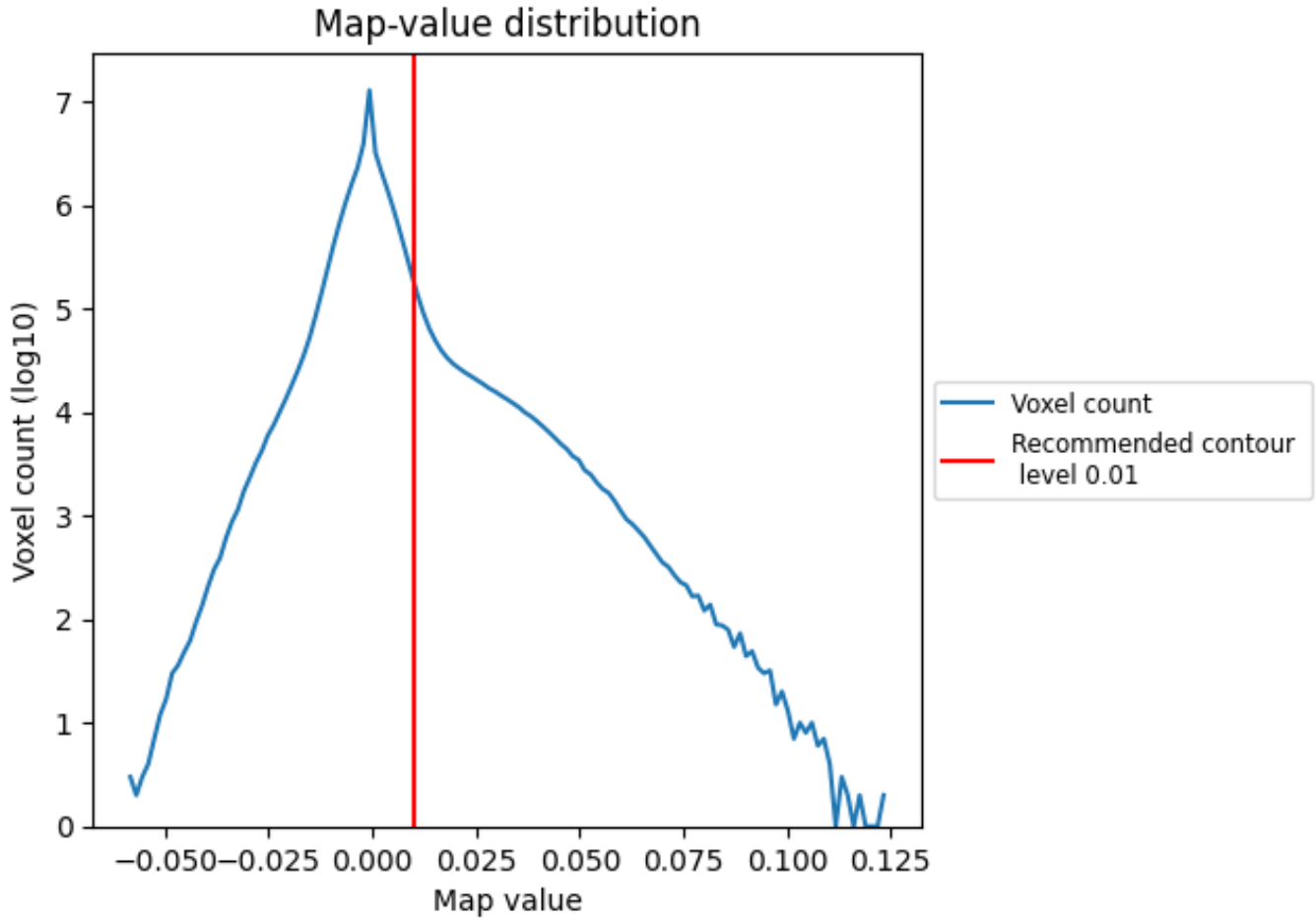
6.6 Mask visualisation (i)

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

7 Map analysis

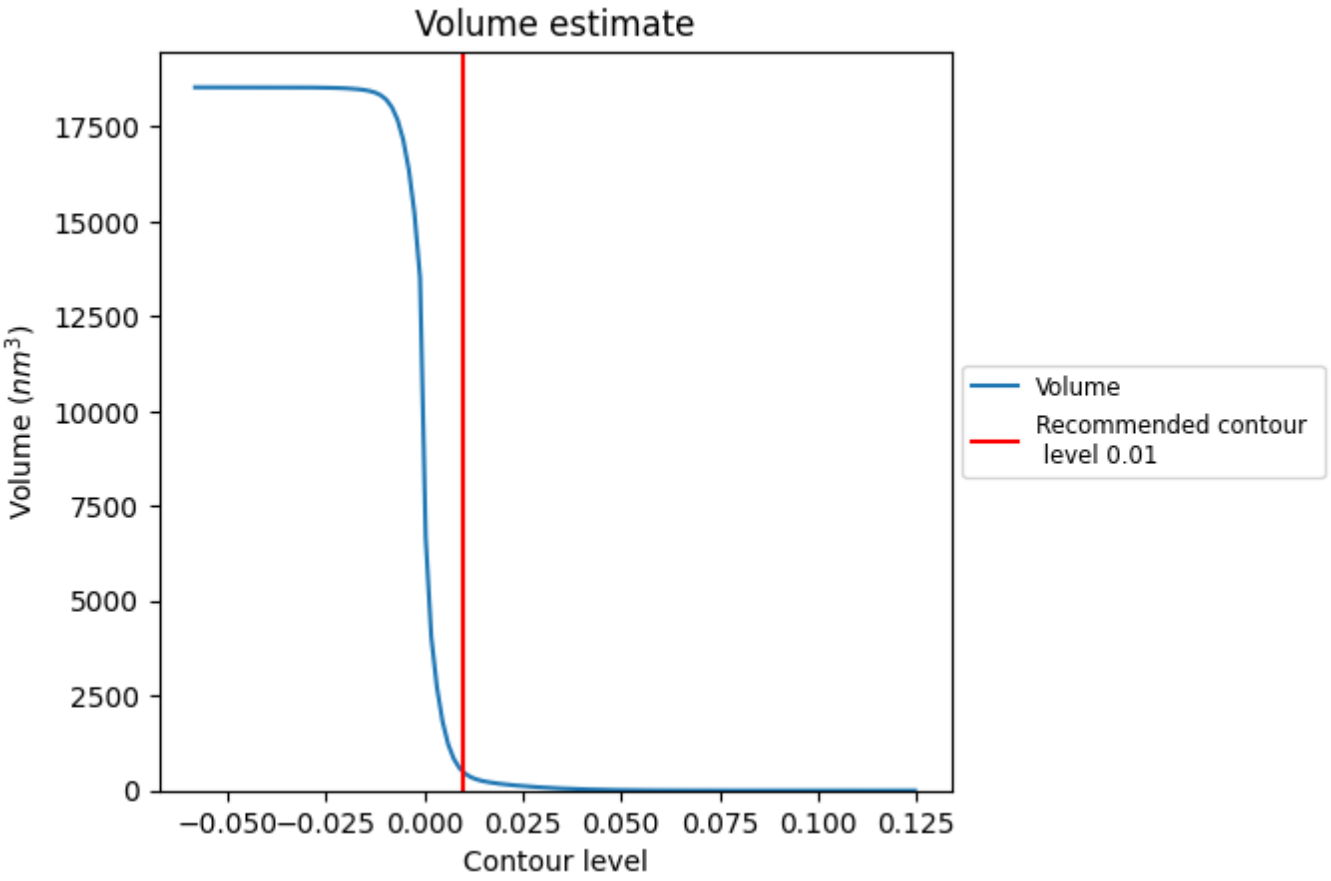
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

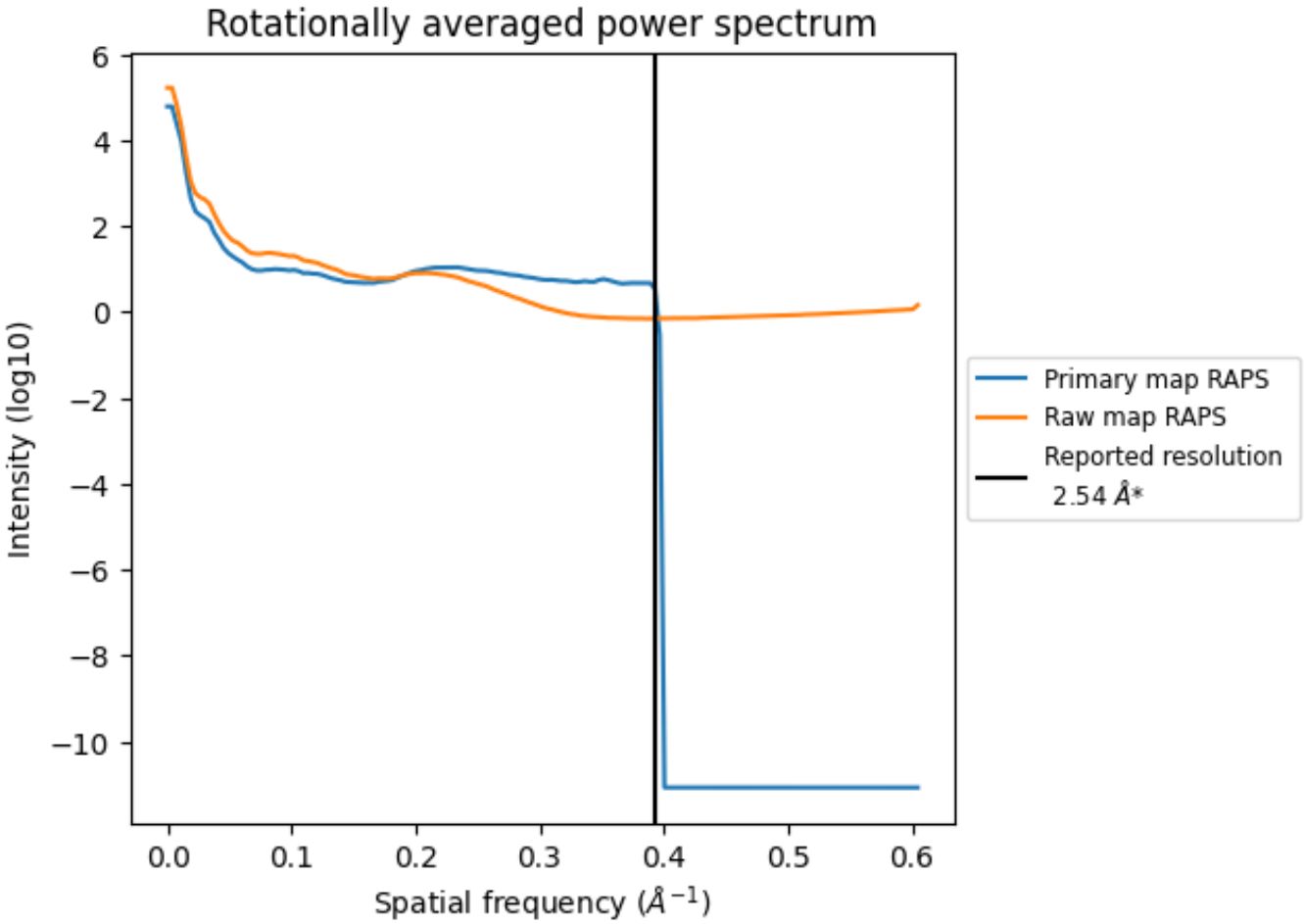
7.2 Volume estimate (i)



The volume at the recommended contour level is 483 nm^3; this corresponds to an approximate mass of 436 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)

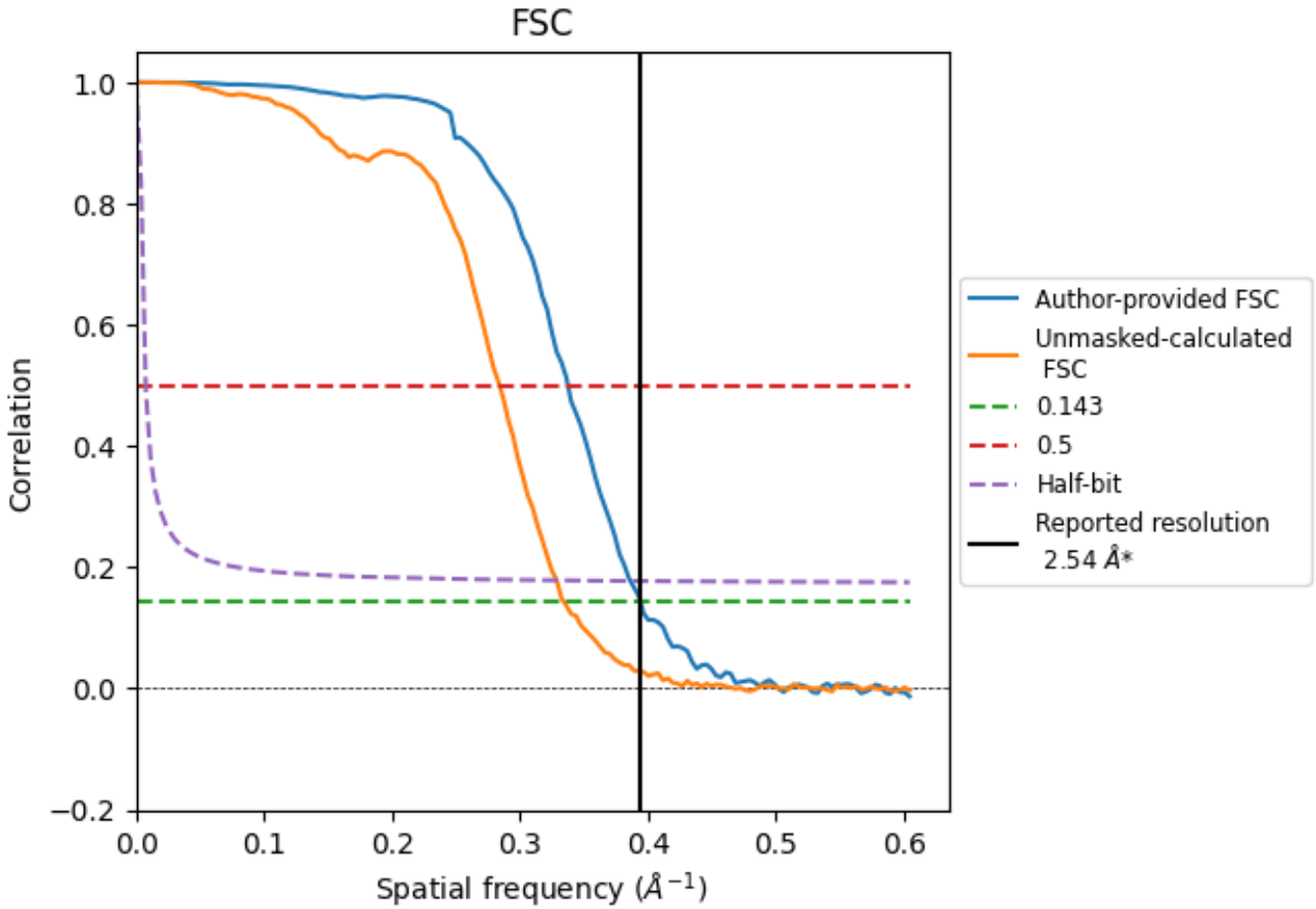


*Reported resolution corresponds to spatial frequency of 0.394 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.394 Å^{-1}

8.2 Resolution estimates (i)

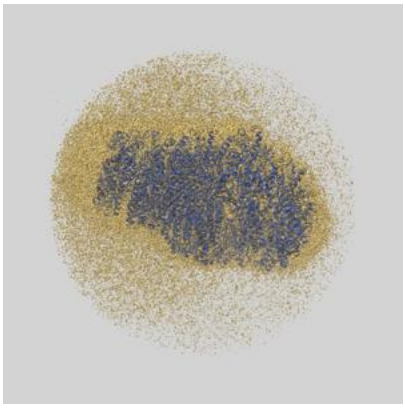
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.54	2.96	2.59
Unmasked-calculated*	2.99	3.52	3.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.54 by more than 10 %

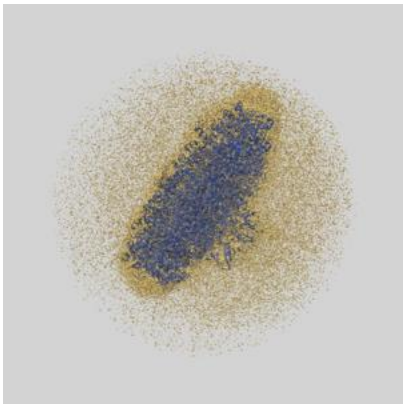
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12180 and PDB model 7BGI. Per-residue inclusion information can be found in section 3 on page 42.

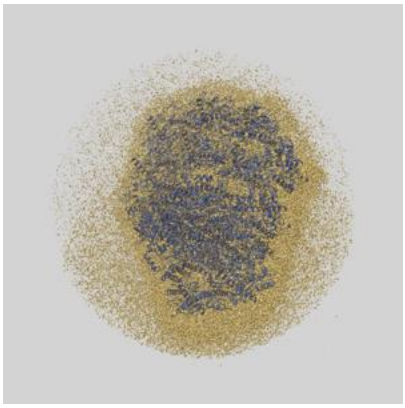
9.1 Map-model overlay



X



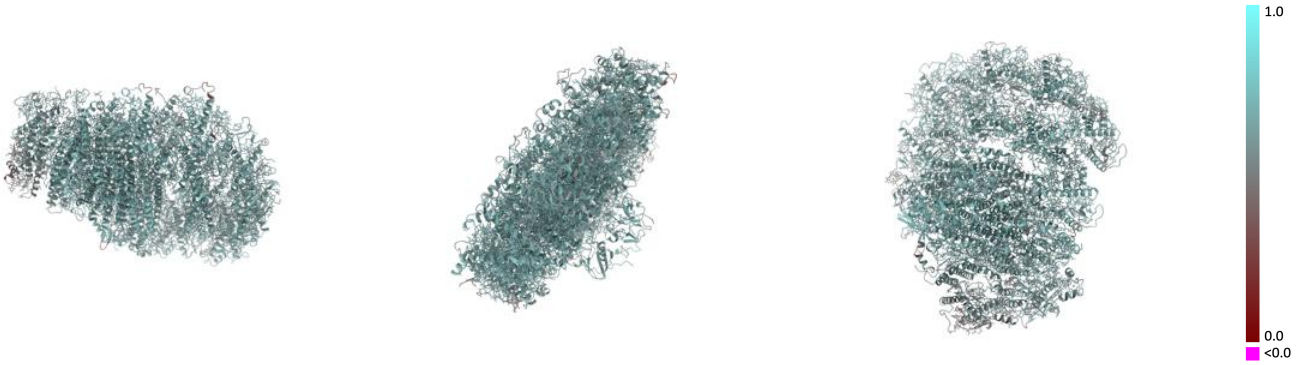
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

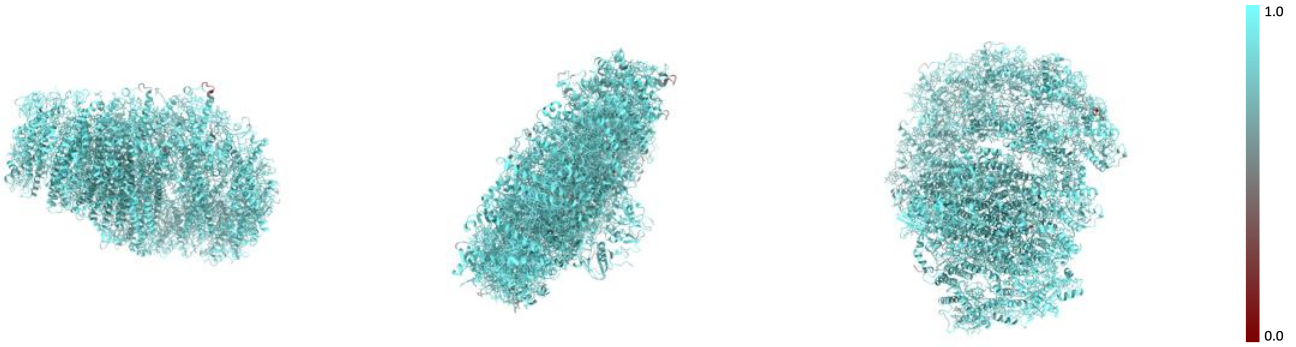
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

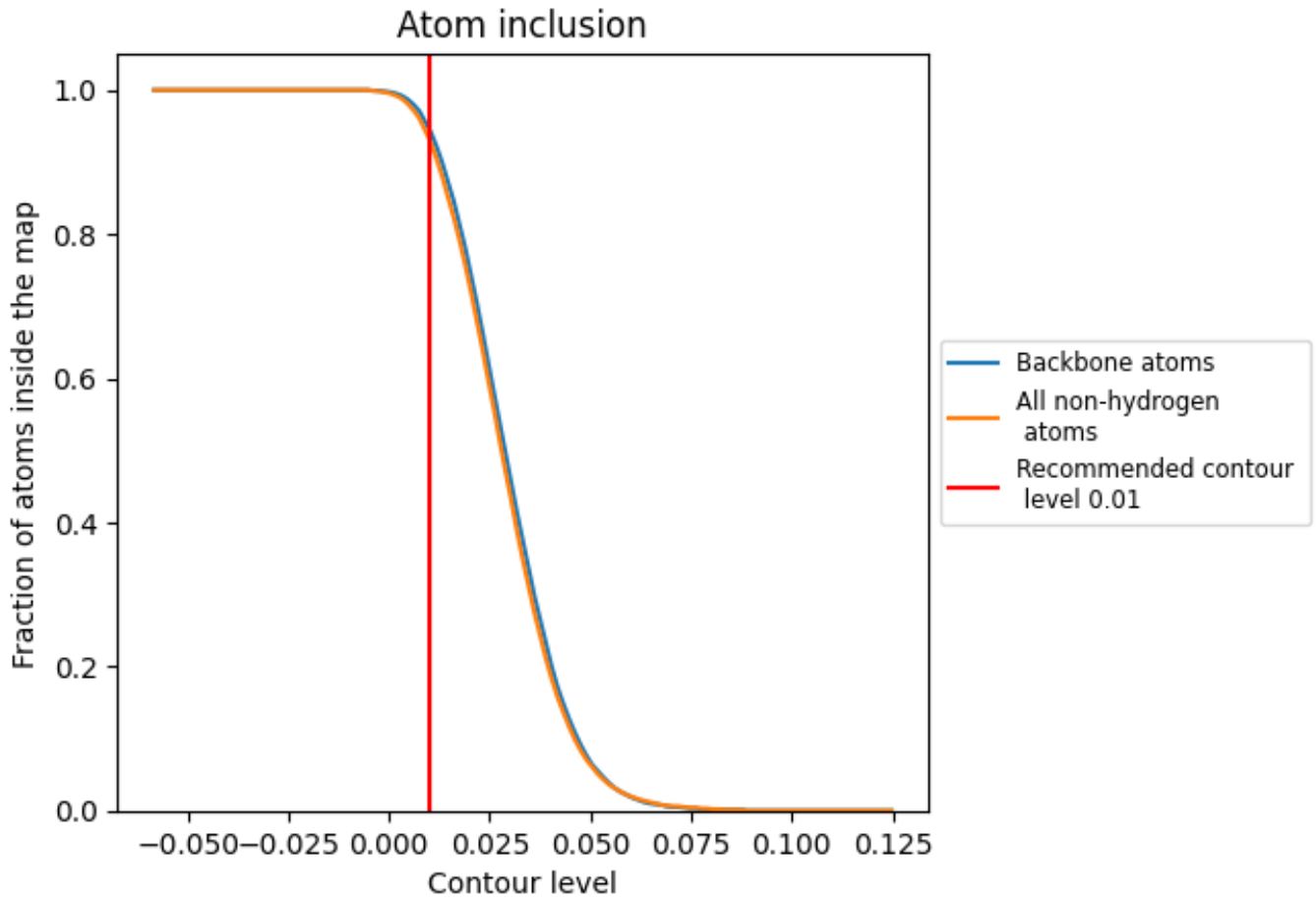
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9320	0.6290
1	0.9110	0.6250
2	0.8940	0.5190
3	0.9240	0.6360
4	0.8850	0.6060
5	0.8950	0.6180
6	0.9010	0.6180
7	0.9310	0.6430
8	0.9370	0.6450
9	0.9380	0.5690
A	0.9590	0.6640
B	0.9710	0.6600
C	0.9700	0.6640
D	0.9410	0.6380
E	0.9530	0.6430
F	0.9410	0.6430
G	0.9100	0.5900
I	0.9750	0.6150
J	0.9600	0.6600
K	0.8510	0.5850
L	0.9030	0.5770
Z	0.8490	0.5870

