wwPDB EM Validation Summary Report

Sep 10, 2026 – 04:11 pm BST

PDB ID	:	7BLX / pdb_00007blx
EMDB ID	:	EMD-12227
Title	:	Photosystem I of a temperature sensitive mutant Chlamydomonas reinhardtii
Authors	:	Caspy, I.; Nelson, N.
Deposited on	:	2021-01-19
Resolution	:	3.15 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:

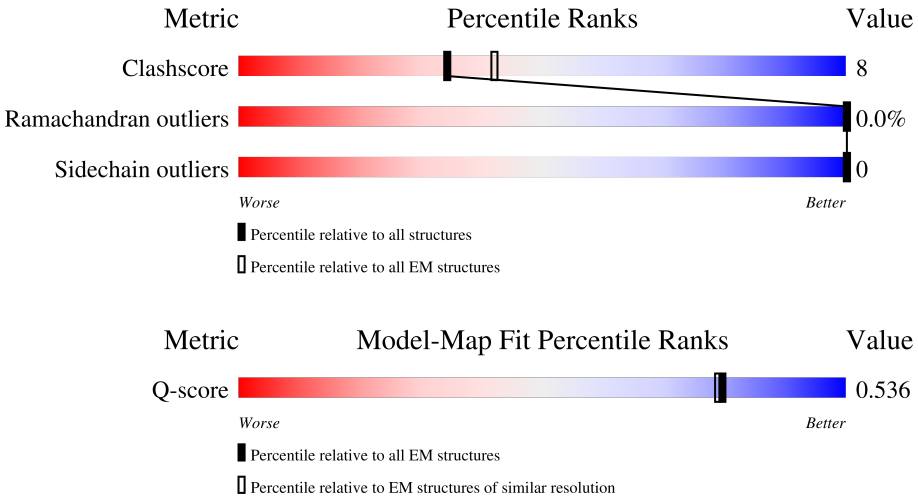
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.15 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	14486 (2.65 - 3.65)

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	17% 86% 14%
2	B	733	21% 86% 14%
3	C	80	21% 92% 8%
4	D	144	47% 95% 5%

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Mol	Chain	Length	Quality of chain
5	E	63	38% 97%
6	F	165	38% 91% 9%
7	G	91	77% 71% 10% 19%
8	I	37	70% 86% 14%
9	J	39	28% 82% 18%
10	K	84	88% 88% 12%
11	L	126	86% 88% 12%
12	1	194	59% 88% 12%
12	Z	194	86% 94% 6%
13	3	219	52% 82% 18%
14	7	213	37% 90% 10%
15	8	217	42% 87% 13%
16	4	210	85% 85% 15%
17	5	227	77% 87% 13%
18	6	229	79% 85% 15%

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
33	RRX	F	4001	X	-	-	-
34	C7Z	1	503	X	-	-	-
34	C7Z	5	505	X	-	-	-
34	C7Z	J	4002	X	-	-	-
37	CHL	1	609	X	-	-	-
37	CHL	3	611	X	-	-	-
37	CHL	4	610	X	-	-	-
37	CHL	4	613	X	-	-	-
37	CHL	5	610	X	-	-	-
37	CHL	6	610	X	-	-	-
37	CHL	6	613	X	-	-	-
37	CHL	8	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CHL	8	613	X	-	-	-
37	CHL	Z	609	X	-	-	-
37	CHL	Z	610	X	-	-	-
39	QTB	Z	504	X	-	-	-

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 47524 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		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	PRO	deletion	UNP A8IL32
L	?	-	SER	deletion	UNP A8IL32
L	?	-	ILE	deletion	UNP A8IL32
L	?	-	GLY	deletion	UNP A8IL32
L	?	-	VAL	deletion	UNP A8IL32
L	?	-	LYS	deletion	UNP A8IL32
L	?	-	THR	deletion	UNP A8IL32
L	?	-	LEU	deletion	UNP A8IL32
L	?	-	SER	deletion	UNP A8IL32
L	?	-	GLY	deletion	UNP A8IL32
L	?	-	ARG	deletion	UNP A8IL32

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	SER	deletion	UNP A8IL32

- 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		

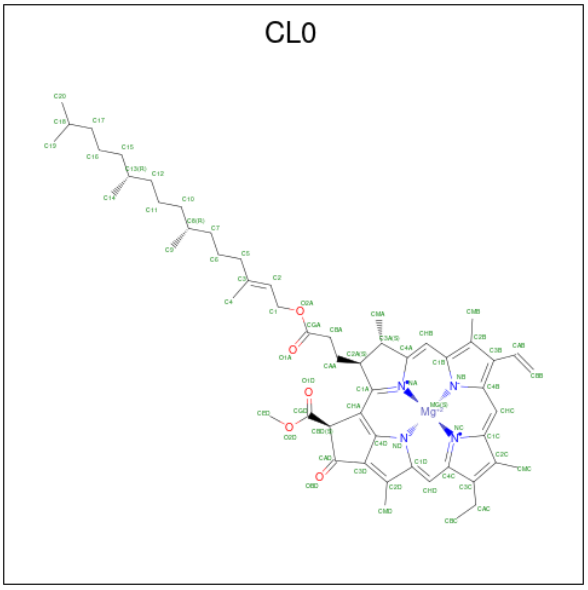
- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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.

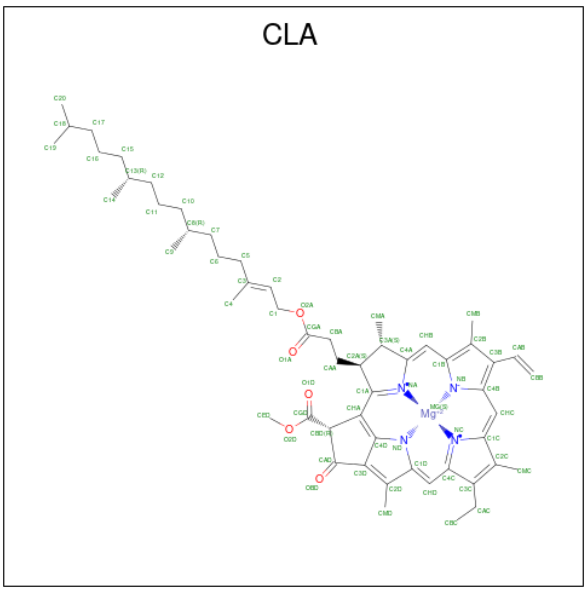
Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1766	1164	292	304	6		

- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	7	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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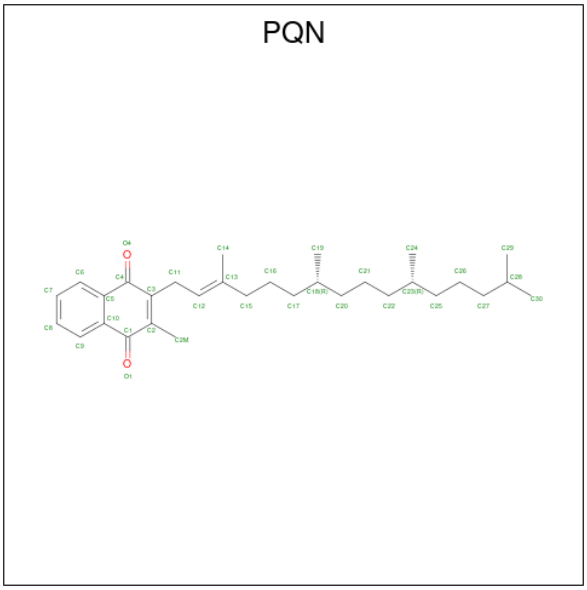
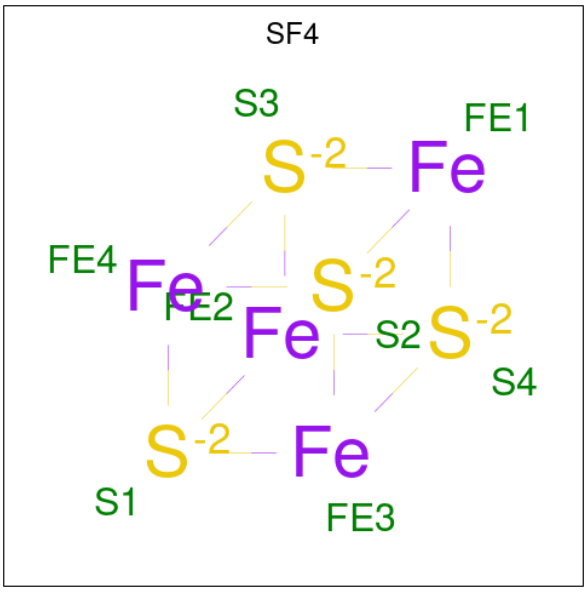
Mol	Chain	Residues	Atoms					AltConf
20	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



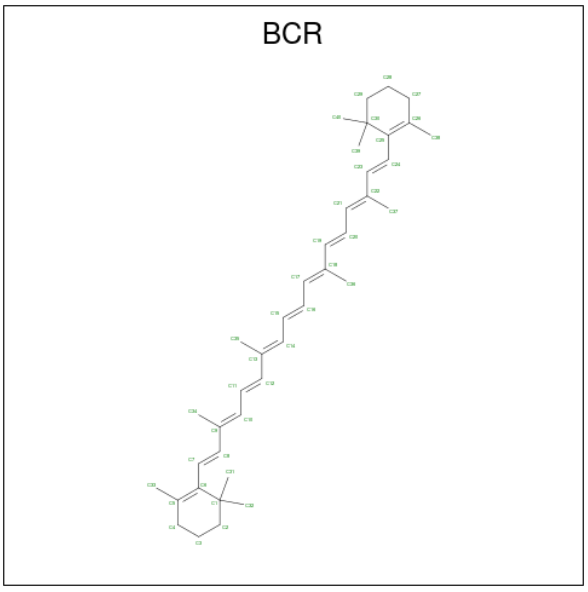
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			33	31	2	
21	B	1	Total	C	O	0
			33	31	2	

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0

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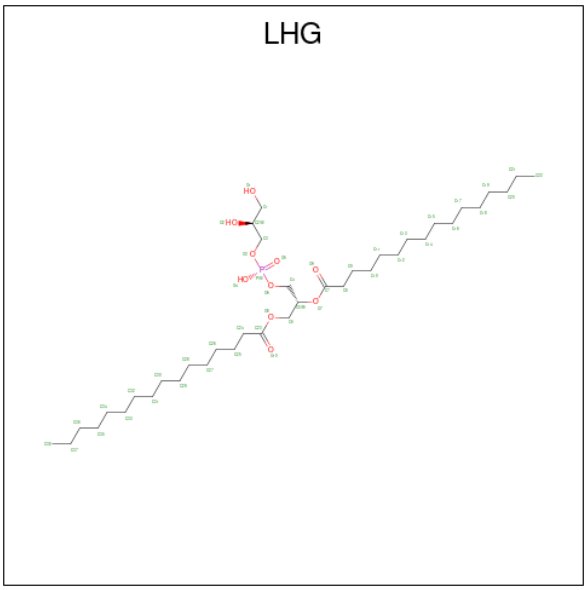
Mol	Chain	Residues	Atoms	AltConf
23	3	1	Total C 40 40	0
23	7	1	Total C 40 40	0
23	7	1	Total C 40 40	0
23	8	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	5	1	Total C 40 40	0
23	5	1	Total C 40 40	0
23	6	1	Total C 40 40	0
23	6	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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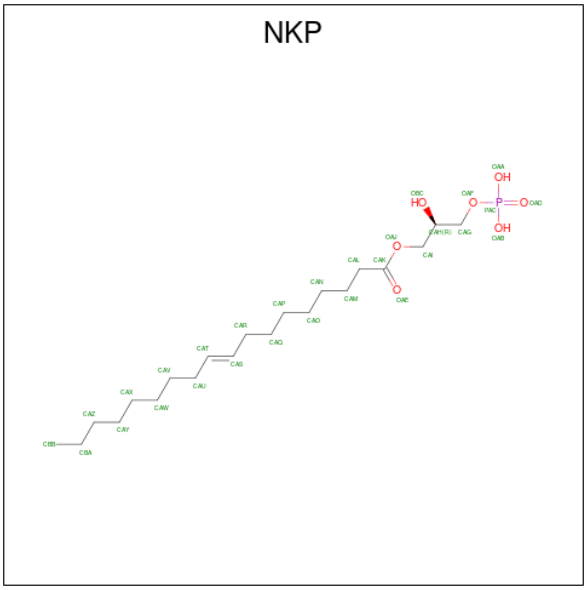
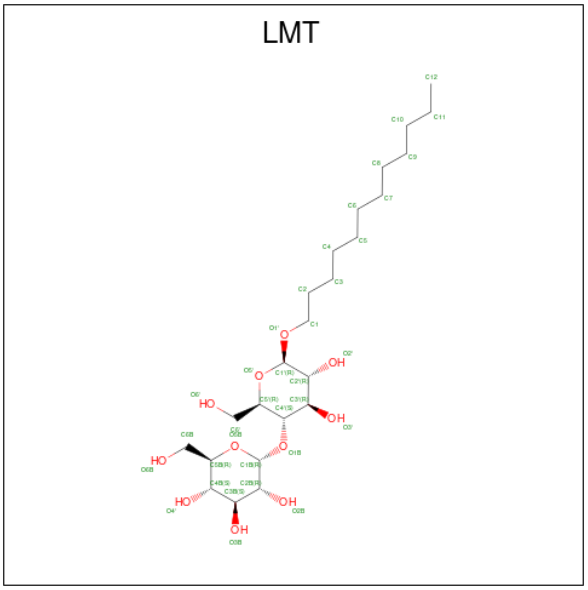
Mol	Chain	Residues	Atoms				AltConf
24	B	1	Total	C	O	P	0
			23	12	10	1	
24	B	1	Total	C	O	P	0
			20	9	10	1	
24	B	1	Total	C	O	P	0
			33	22	10	1	
24	1	1	Total	C	O	P	0
			43	32	10	1	
24	Z	1	Total	C	O	P	0
			43	32	10	1	
24	3	1	Total	C	O	P	0
			20	9	10	1	
24	7	1	Total	C	O	P	0
			37	26	10	1	
24	8	1	Total	C	O	P	0
			38	27	10	1	
24	4	1	Total	C	O	P	0
			49	38	10	1	
24	4	1	Total	C	O	P	0
			32	21	10	1	
24	5	1	Total	C	O	P	0
			37	26	10	1	
24	6	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: $C_{21}H_{41}O_7P$).



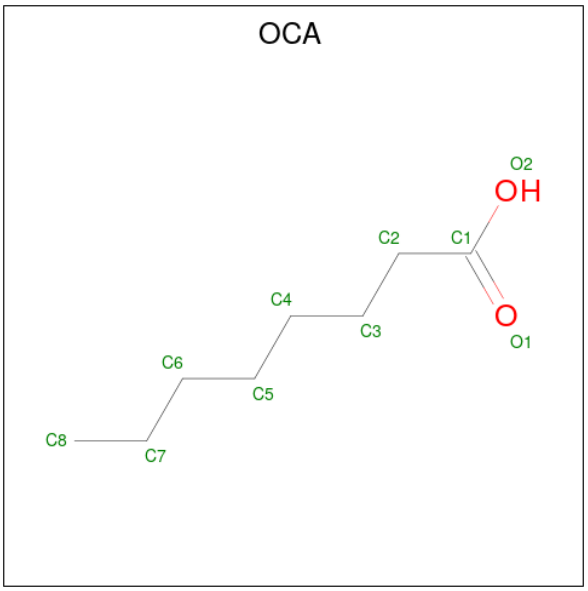
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C O P 29 21 7 1	0
25	3	1	Total C O P 16 8 7 1	0
25	8	1	Total C O P 29 21 7 1	0

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



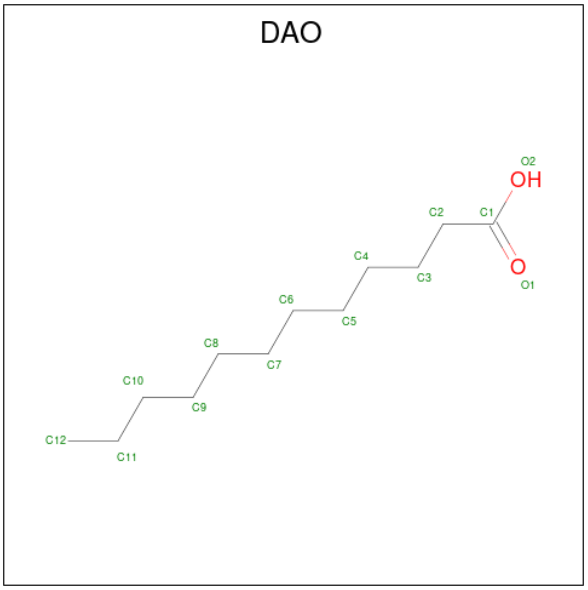
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C O 35 24 11	0
26	B	1	Total C O 35 24 11	0
26	B	1	Total C O 35 24 11	0
26	F	1	Total C O 35 24 11	0
26	1	1	Total C O 35 24 11	0
26	8	1	Total C O 35 24 11	0
26	4	1	Total C O 35 24 11	0

- Molecule 27 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $C_8H_{16}O_2$).



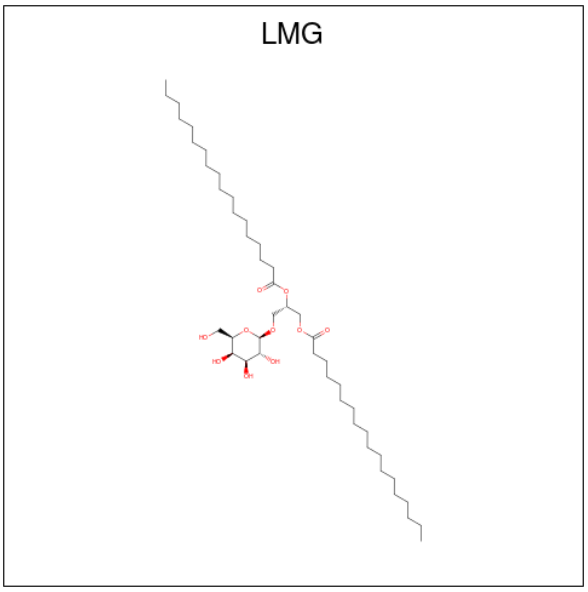
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			10	8	2	

- Molecule 28 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



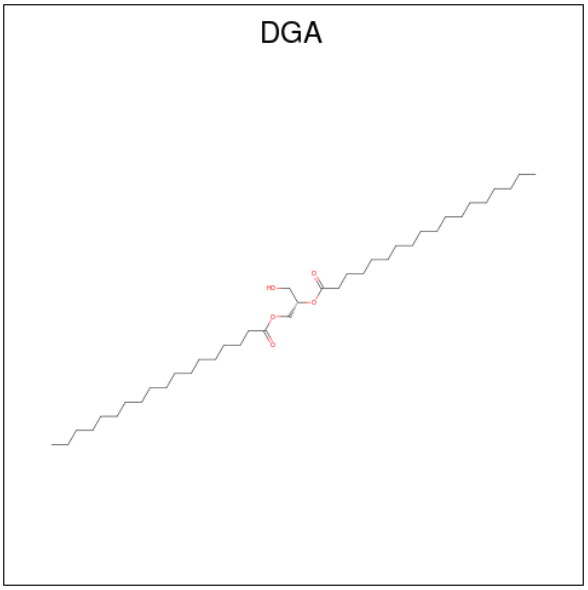
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			14	12	2	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

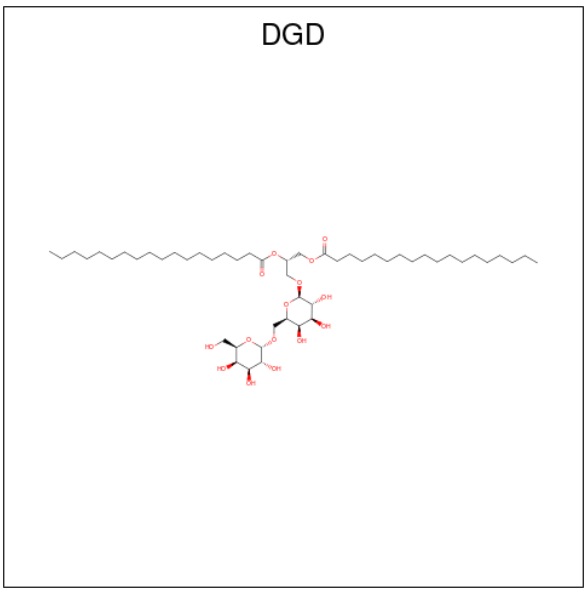
- Molecule 30 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total 44	C 39	O 5	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

$C_{51}H_{96}O_{15}$).

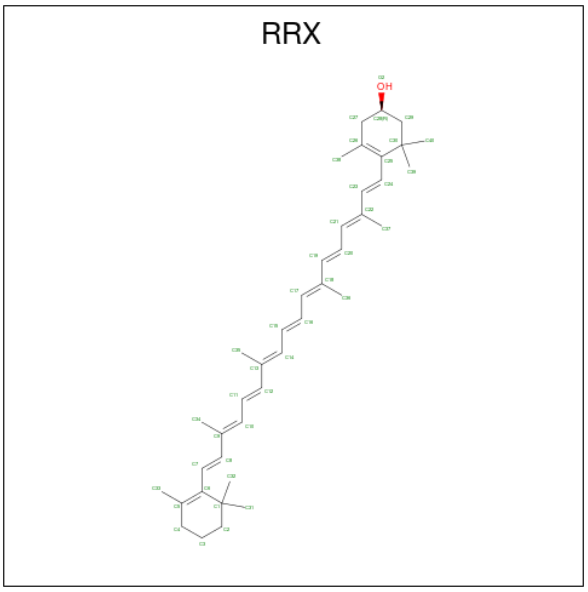


Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			66	51	15	

- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

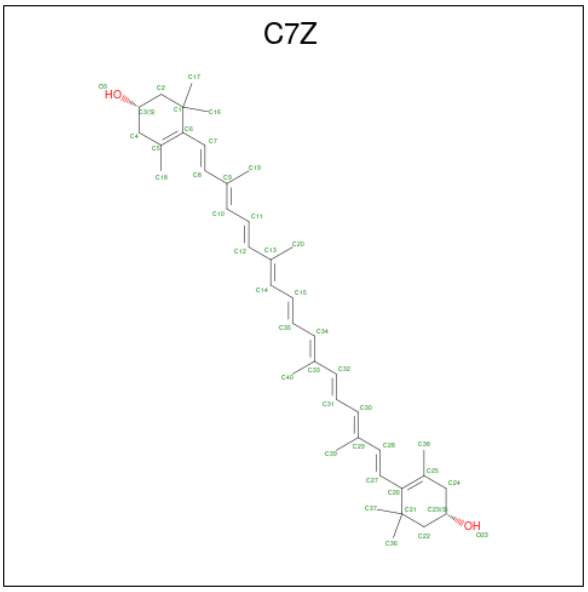
Mol	Chain	Residues	Atoms		AltConf
32	B	1	Total	Ca	0
			1	1	

- Molecule 33 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



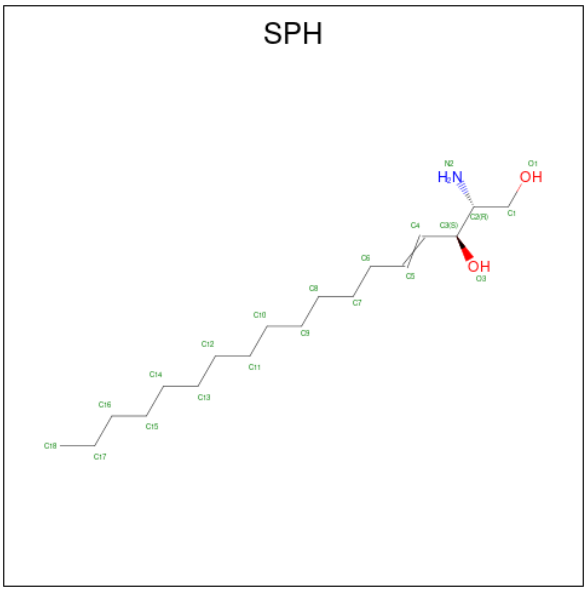
Mol	Chain	Residues	Atoms			AltConf
33	F	1	Total	C	O	0
			41	40	1	

- Molecule 34 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: $C_{40}H_{56}O_2$).



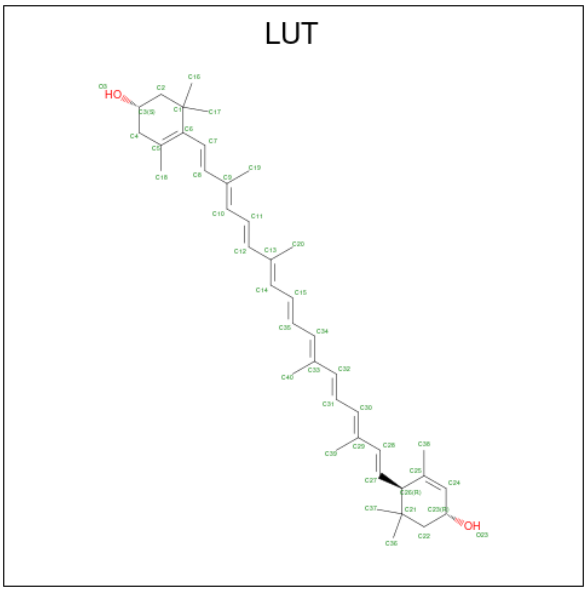
Mol	Chain	Residues	Atoms			AltConf
34	J	1	Total	C	O	0
			42	40	2	
34	1	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	

- Molecule 35 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



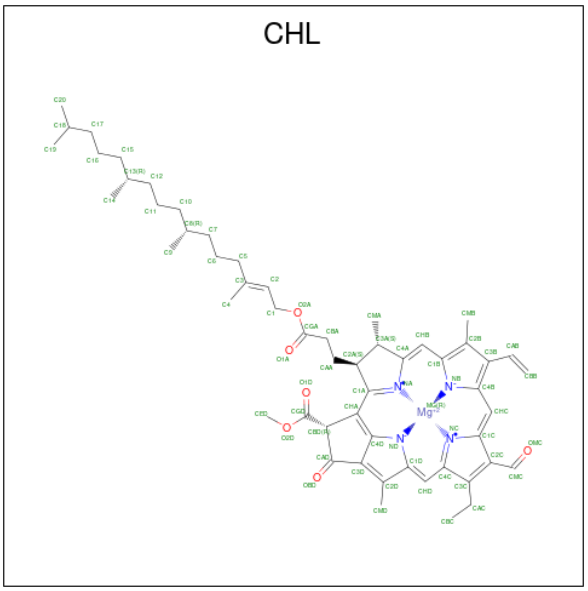
Mol	Chain	Residues	Atoms				AltConf
35	K	1	Total	C	N	O	0
			21	18	1	2	
35	7	1	Total	C	N	O	0
			21	18	1	2	
35	7	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 36 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
36	1	1	Total	C	O	0
			42	40	2	
36	1	1	Total	C	O	0
			42	40	2	
36	Z	1	Total	C	O	0
			42	40	2	
36	Z	1	Total	C	O	0
			42	40	2	
36	Z	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	7	1	Total	C	O	0
			42	40	2	
36	7	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	

- Molecule 37 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
37	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
37	1	1	Total 58	C 47	Mg 1	N 4	O 6	0
37	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
37	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	7	1	Total 54	C 43	Mg 1	N 4	O 6	0
37	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
37	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
37	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
37	4	1	Total 56	C 45	Mg 1	N 4	O 6	0
37	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
37	5	1	Total 66	C 55	Mg 1	N 4	O 6	0

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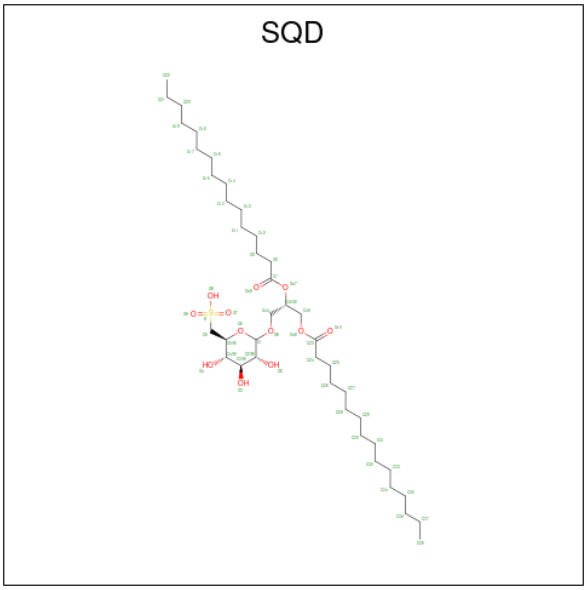
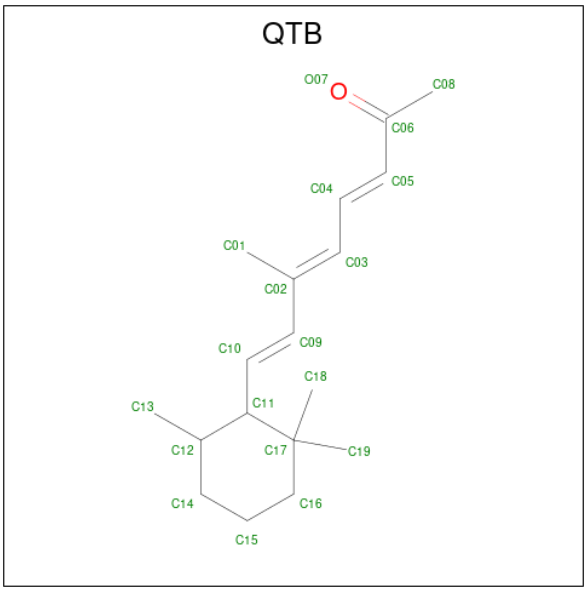
Mol	Chain	Residues	Atoms					AltConf
37	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
37	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
37	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
37	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
37	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
37	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



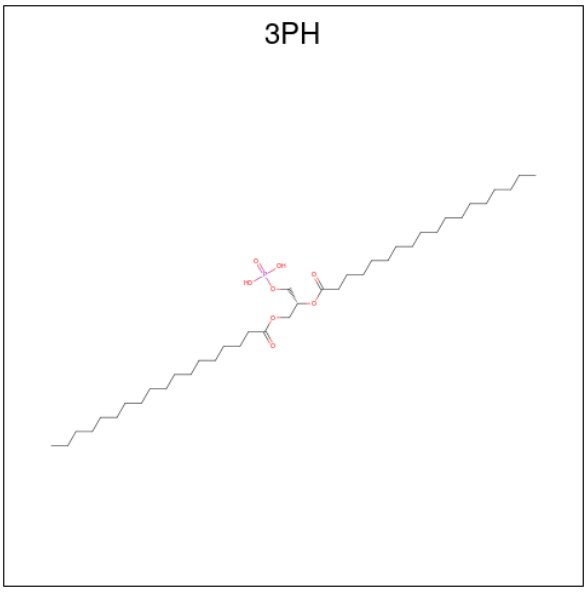
Mol	Chain	Residues	Atoms				AltConf
38	1	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 39 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
39	Z	1	Total C O 19 18 1	0

- Molecule 40 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms	AltConf
40	7	1	Total C O P 39 30 8 1	0
40	8	1	Total C O P 30 21 8 1	0

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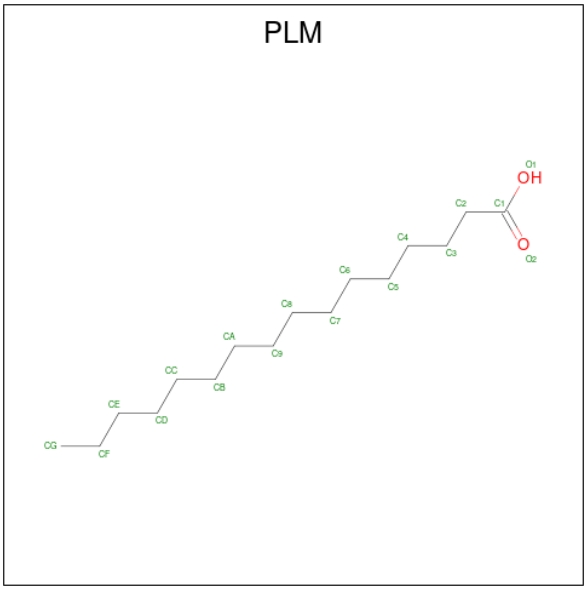
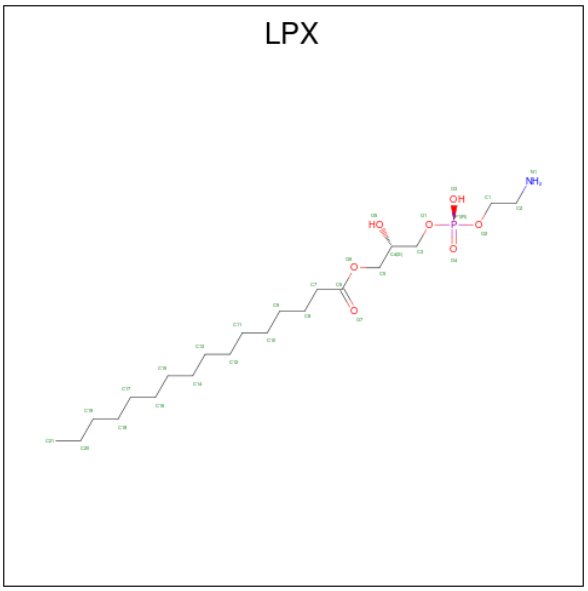
Mol	Chain	Residues	Atoms				AltConf
40	5	1	Total	C	O	P	0
			23	14	8	1	
40	6	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 41 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
41	7	1	Total	C	O	0
			18	16	2	

- Molecule 42 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
42	8	1	Total C N O P 30 21 1 7 1	0

- Molecule 43 is water.

Mol	Chain	Residues	Atoms	AltConf
43	A	3	Total O 3 3	0
43	A	10	Total O 10 10	0
43	A	17	Total O 17 17	0
43	A	7	Total O 7 7	0
43	A	6	Total O 6 6	0
43	A	3	Total O 3 3	0
43	A	5	Total O 5 5	0
43	A	14	Total O 14 14	0
43	A	3	Total O 3 3	0
43	A	16	Total O 16 16	0
43	A	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	B	2	Total O 2 2	0
43	B	1	Total O 1 1	0
43	B	1	Total O 1 1	0
43	B	1	Total O 1 1	0
43	B	5	Total O 5 5	0
43	B	15	Total O 15 15	0
43	B	4	Total O 4 4	0
43	B	12	Total O 12 12	0
43	B	18	Total O 18 18	0
43	B	2	Total O 2 2	0
43	B	15	Total O 15 15	0
43	B	3	Total O 3 3	0
43	C	1	Total O 1 1	0
43	C	1	Total O 1 1	0
43	C	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
43	C	1	Total O 1 1	0
43	C	2	Total O 2 2	0
43	C	8	Total O 8 8	0
43	C	1	Total O 1 1	0
43	C	1	Total O 1 1	0
43	C	1	Total O 1 1	0
43	C	1	Total O 1 1	0
43	C	1	Total O 1 1	0
43	D	1	Total O 1 1	0
43	D	1	Total O 1 1	0
43	D	1	Total O 1 1	0
43	D	1	Total O 1 1	0
43	D	1	Total O 1 1	0
43	D	1	Total O 1 1	0
43	D	1	Total O 1 1	0
43	D	2	Total O 2 2	0
43	D	2	Total O 2 2	0
43	D	1	Total O 1 1	0
43	E	1	Total O 1 1	0
43	E	1	Total O 1 1	0
43	E	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
43	E	4	Total O 4 4	0
43	F	1	Total O 1 1	0
43	F	1	Total O 1 1	0
43	F	1	Total O 1 1	0
43	F	3	Total O 3 3	0
43	F	6	Total O 6 6	0
43	F	1	Total O 1 1	0
43	F	1	Total O 1 1	0
43	J	1	Total O 1 1	0
43	J	2	Total O 2 2	0
43	K	1	Total O 1 1	0
43	K	1	Total O 1 1	0
43	L	1	Total O 1 1	0
43	L	4	Total O 4 4	0
43	1	15	Total O 15 15	0
43	1	1	Total O 1 1	0
43	Z	8	Total O 8 8	0
43	3	16	Total O 16 16	0
43	3	1	Total O 1 1	0
43	7	18	Total O 18 18	0
43	8	1	Total O 1 1	0

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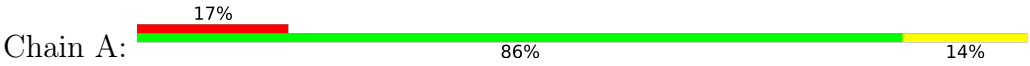
Mol	Chain	Residues	Atoms	AltConf
43	8	15	Total O 15 15	0
43	4	7	Total O 7 7	0
43	5	9	Total O 9 9	0
43	6	8	Total O 8 8	0

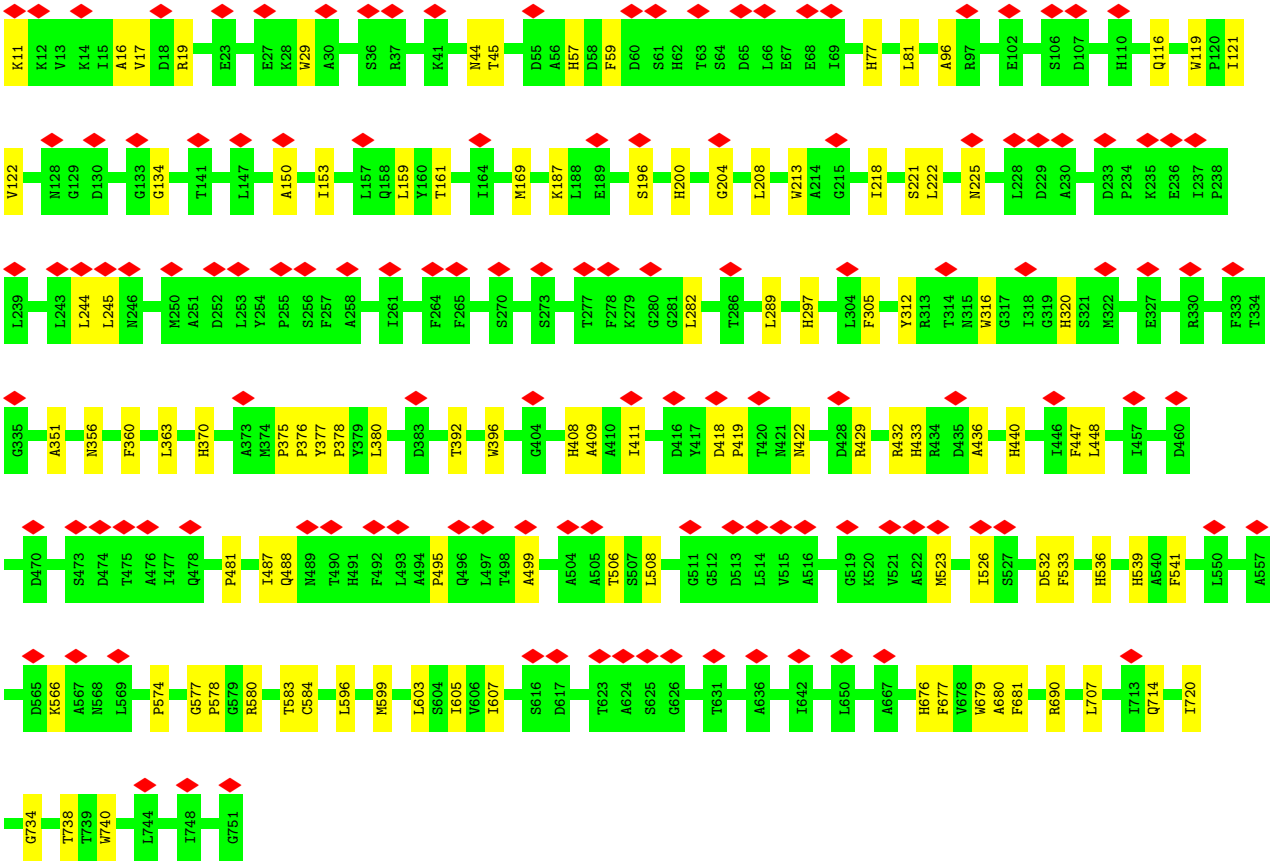
3 Residue-property plots (i)

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

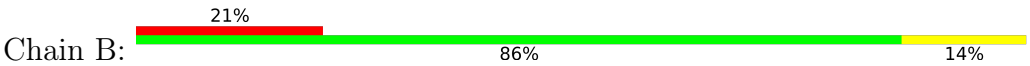
Chain A:

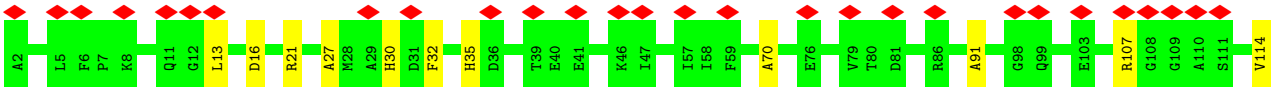


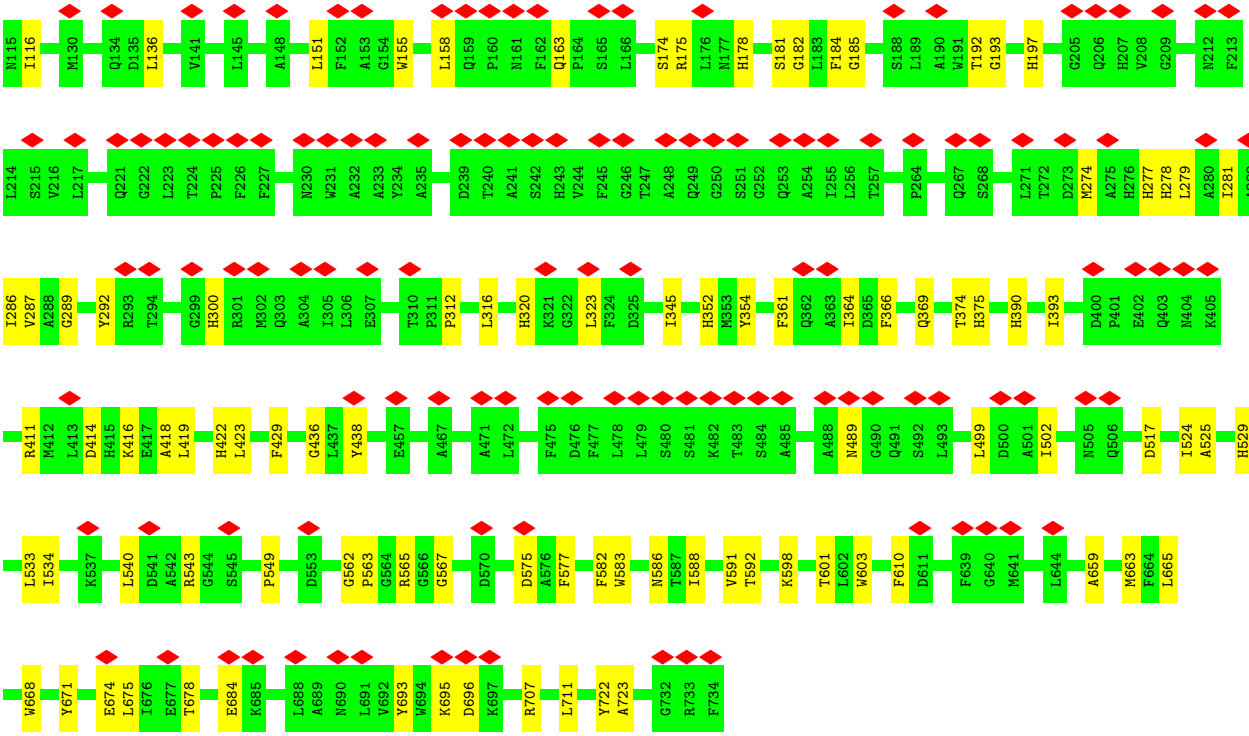


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

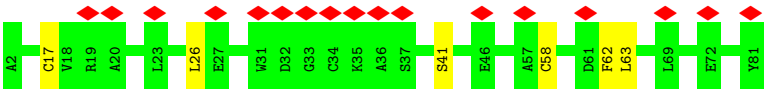




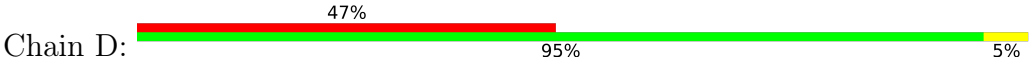


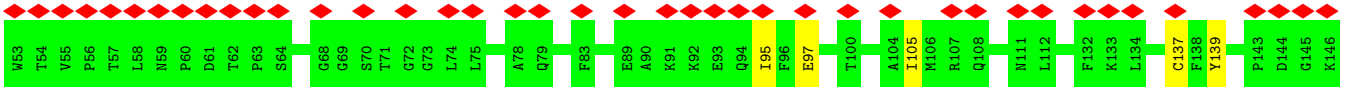
• Molecule 3: Photosystem I iron-sulfur center

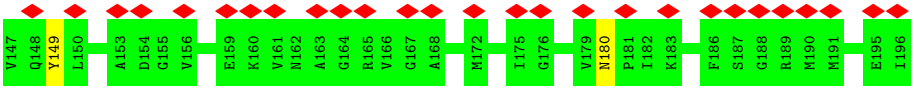




• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

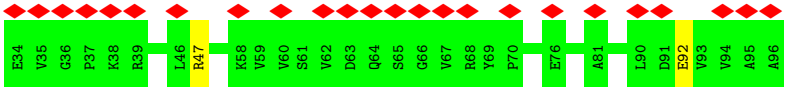






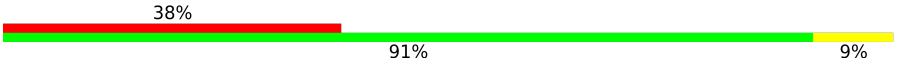
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

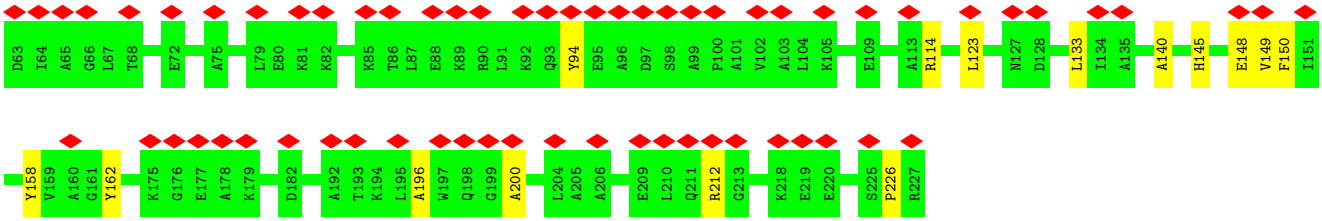




• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:

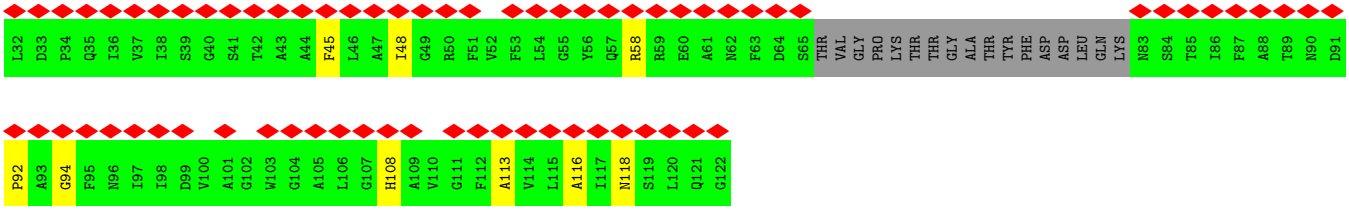




• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:

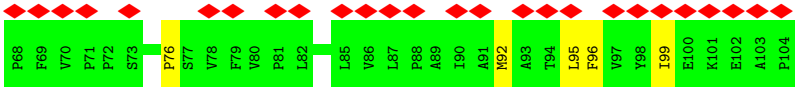




• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:

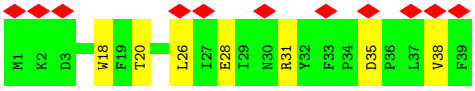




• Molecule 9: Photosystem I reaction center subunit IX

Chain J:

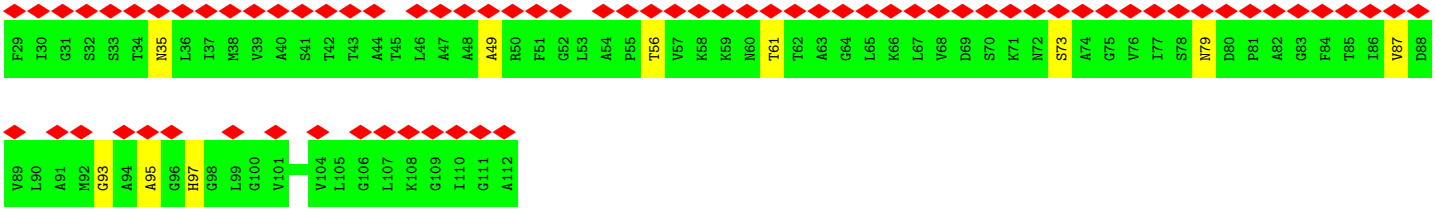




• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:

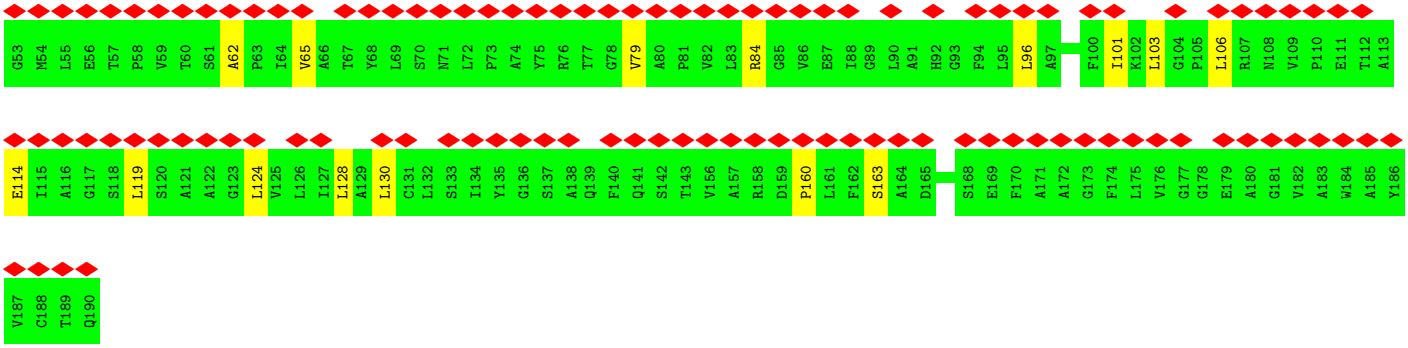




• Molecule 11: PSI subunit V

Chain L:

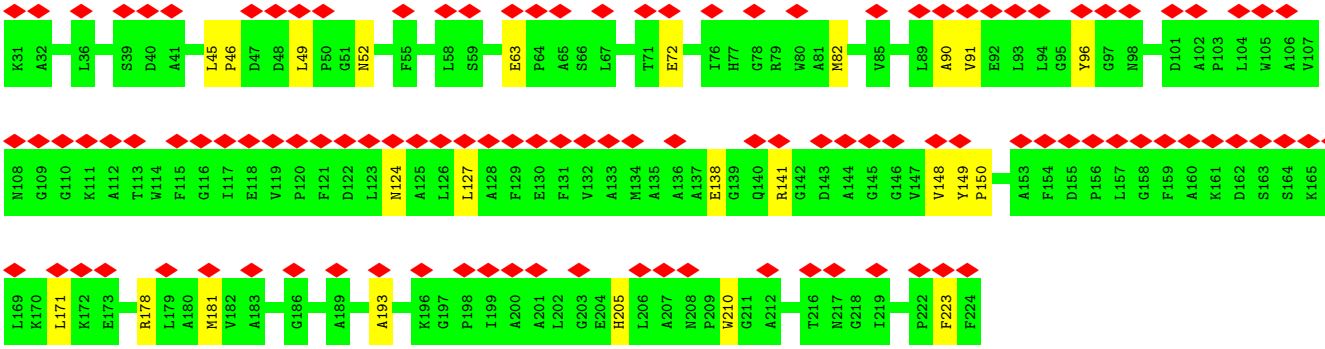




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

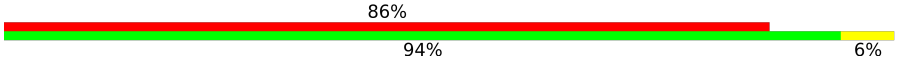
Chain 1:

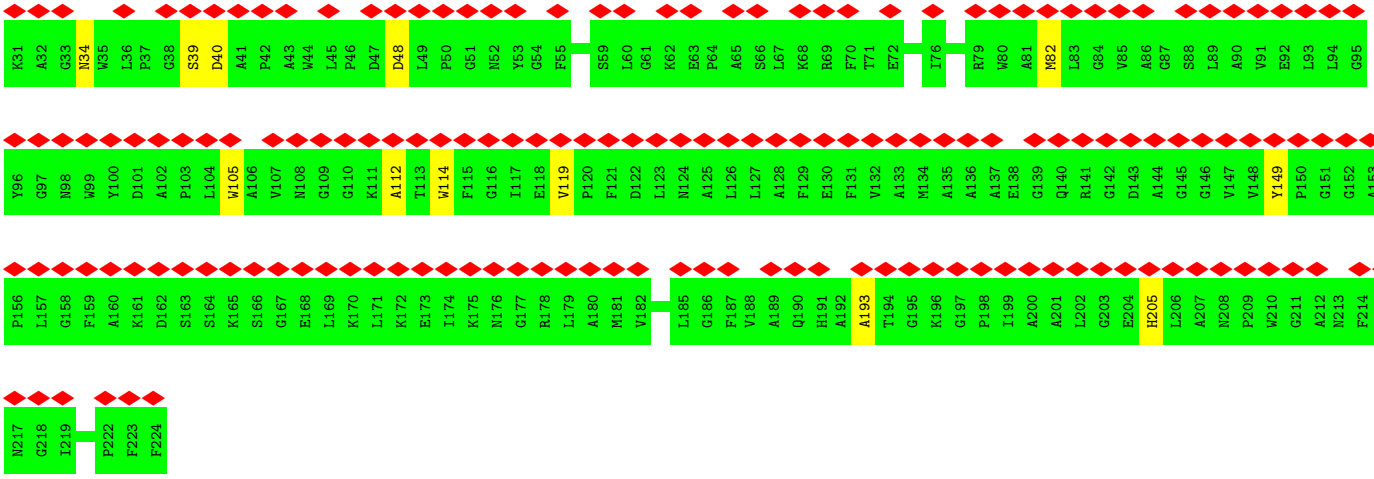




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

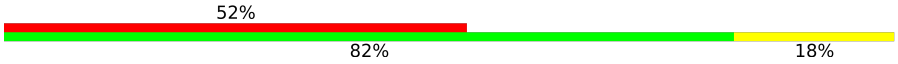
Chain Z:

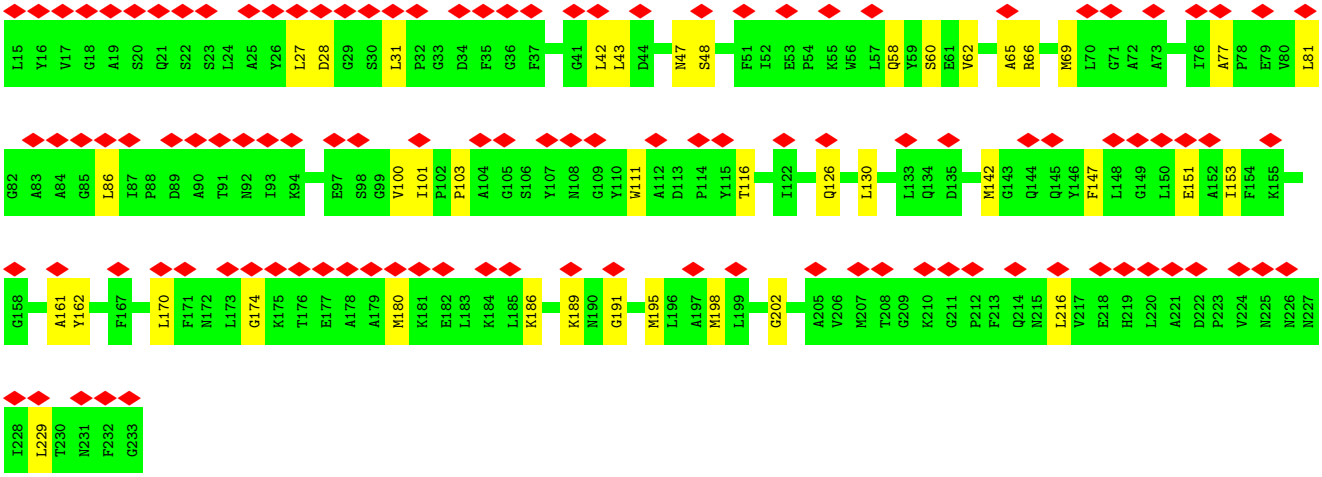




• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

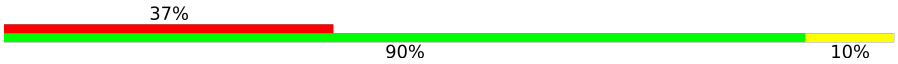
Chain 3:

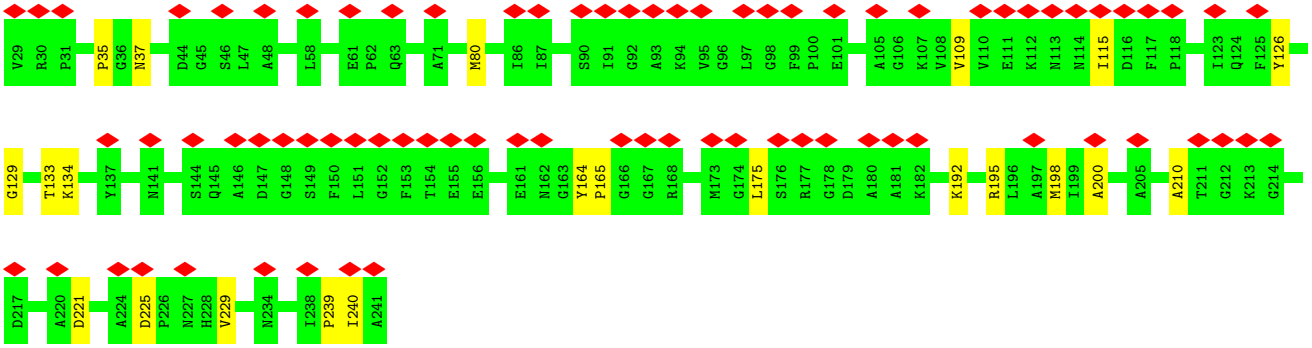




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7:

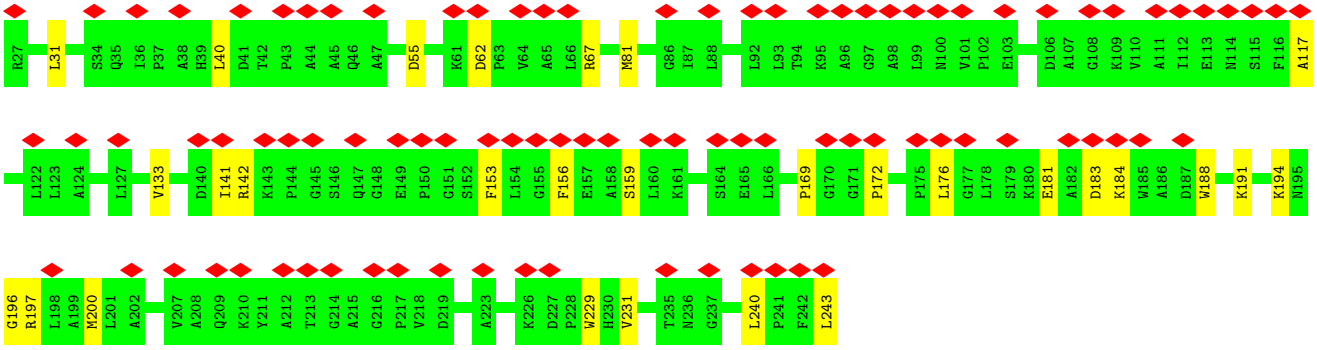




• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:

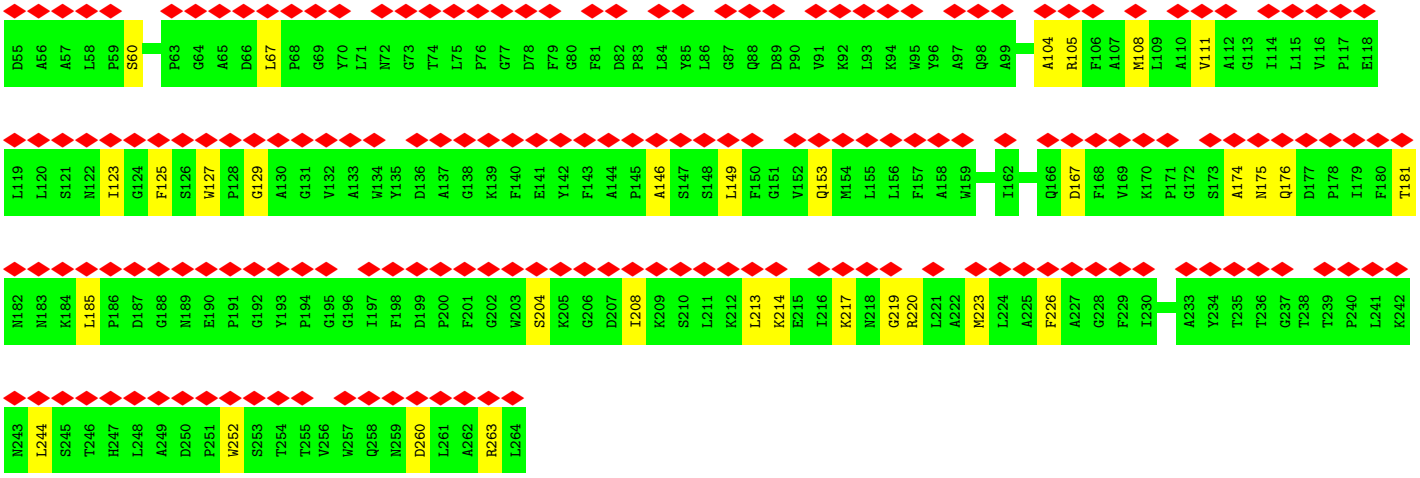




• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

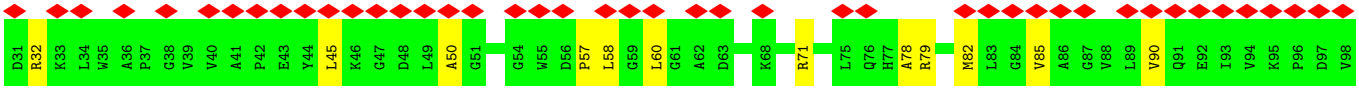


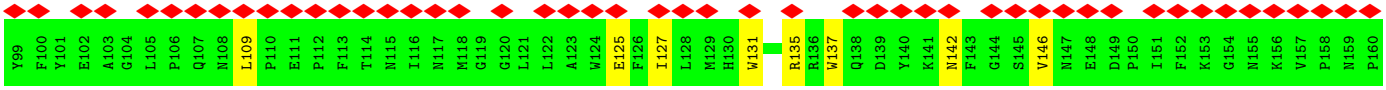


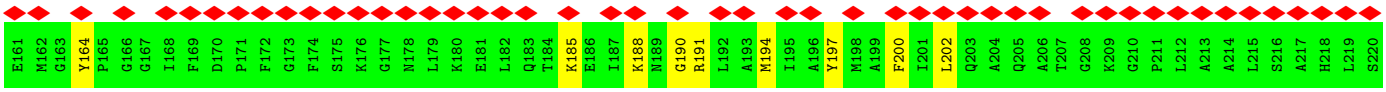
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

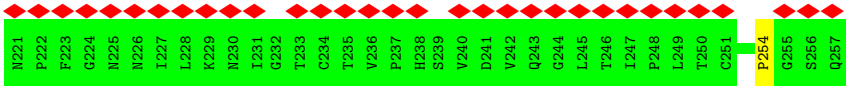
Chain 5:







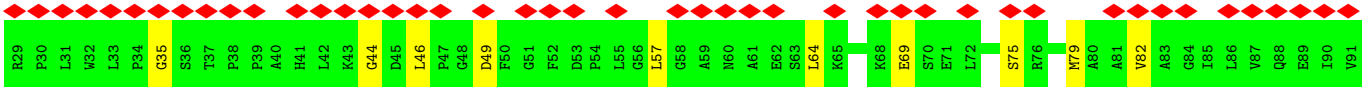


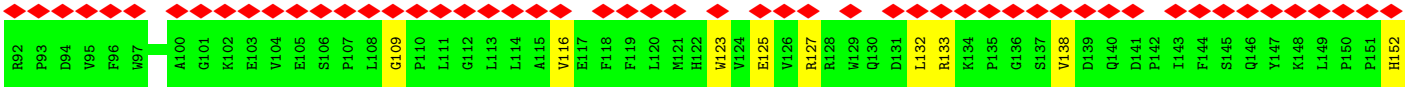


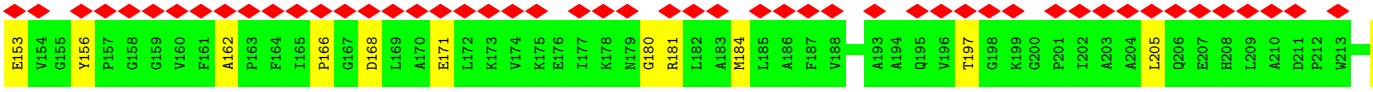
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

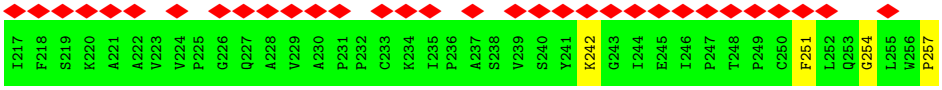
Chain 6:










I217
F218
S219
K220
A221
A222
V223
V224
P225
G226
Q227
A228
V229
A230
P231
P232
C233
K234
I235
P236
A237
S238
V239
S240
Y241
K242
G243
I244
E245
I246
P247
T248
P249
C250
F251
L252
Q253
G254
L255
W256
P257

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17311	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	0.060	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	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: OCA, DGD, LPX, QTB, 3PH, LMG, CL0, SNC, CHL, SPH, CA, SF4, LHG, C7Z, RRX, BCR, PQN, DAO, CLA, PLM, NKP, LMT, LUT, SQD, DGA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/6016	0.50	1/8201 (0.0%)
2	B	0.24	0/6037	0.50	0/8242
3	C	0.21	0/611	0.48	0/826
4	D	0.21	0/1154	0.51	0/1556
5	E	0.18	0/507	0.39	0/689
6	F	0.23	0/1292	0.50	0/1747
7	G	0.17	0/561	0.44	0/760
8	I	0.27	0/294	0.56	0/406
9	J	0.27	0/332	0.47	0/454
10	K	0.20	0/576	0.47	0/779
11	L	0.19	0/935	0.43	0/1277
12	1	0.20	0/1491	0.44	0/2028
12	Z	0.18	0/1491	0.42	0/2028
13	3	0.23	0/1722	0.48	0/2336
14	7	0.21	0/1702	0.44	0/2310
15	8	0.22	0/1701	0.46	0/2315
16	4	0.22	0/1683	0.46	0/2296
17	5	0.20	0/1830	0.45	0/2492
18	6	0.21	0/1828	0.44	0/2497
All	All	0.22	0/31763	0.47	1/43239 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	ASN	N-CA-C	-6.43	107.29	114.62

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	81	0
2	B	5825	0	5579	78	0
3	C	601	0	581	4	0
4	D	1135	0	1148	4	0
5	E	497	0	491	1	0
6	F	1266	0	1301	13	0
7	G	550	0	532	7	0
8	I	282	0	292	5	0
9	J	321	0	322	6	0
10	K	571	0	606	10	0
11	L	914	0	921	10	0
12	1	1445	0	1396	19	0
12	Z	1445	0	1396	10	0
13	3	1674	0	1633	36	0
14	7	1650	0	1589	20	0
15	8	1650	0	1629	22	0
16	4	1628	0	1576	24	0
17	5	1775	0	1746	29	0
18	6	1766	0	1765	29	0
19	A	65	0	72	3	0
20	1	712	0	712	26	0
20	3	748	0	720	24	0
20	4	613	0	566	20	0
20	5	799	0	757	24	0
20	6	759	0	741	34	0
20	7	790	0	751	29	0
20	8	694	0	672	24	0
20	A	2699	0	2866	129	0
20	B	2680	0	2834	111	0
20	F	110	0	105	9	0
20	G	96	0	72	2	0
20	J	42	0	30	0	0
20	K	205	0	168	8	0
20	L	115	0	110	3	0
20	Z	622	0	584	20	0
21	A	33	0	46	0	0
21	B	33	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	8	0	0	0	0
22	C	16	0	0	1	0
23	3	160	0	212	9	0
23	4	40	0	53	1	0
23	5	80	0	105	3	0
23	6	80	0	106	6	0
23	7	80	0	106	5	0
23	8	40	0	53	2	0
23	A	200	0	264	18	0
23	B	280	0	370	19	0
23	G	40	0	53	3	0
23	I	40	0	52	2	0
23	J	40	0	53	3	0
23	K	80	0	106	5	0
23	L	80	0	106	6	0
24	1	43	0	56	2	0
24	3	20	0	12	0	0
24	4	81	0	108	4	0
24	5	37	0	44	1	0
24	6	49	0	74	4	0
24	7	37	0	44	2	0
24	8	38	0	46	2	0
24	A	84	0	114	4	0
24	B	76	0	64	3	0
24	Z	43	0	56	0	0
25	3	16	0	12	1	0
25	8	29	0	39	0	0
25	A	29	0	39	0	0
26	1	35	0	45	1	0
26	4	35	0	43	2	0
26	8	35	0	45	2	0
26	A	35	0	42	2	0
26	B	70	0	89	2	0
26	F	35	0	45	0	0
27	A	10	0	15	0	0
28	A	14	0	23	0	0
29	A	29	0	28	0	0
29	J	35	0	40	0	0
30	A	44	0	76	5	0
31	B	66	0	96	5	0
32	B	1	0	0	0	0
33	F	41	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	1	42	0	0	0	0
34	5	42	0	0	0	0
34	J	42	0	0	0	0
35	7	42	0	74	3	0
35	K	21	0	37	2	0
36	1	84	0	110	4	0
36	3	84	0	110	11	0
36	4	84	0	110	9	0
36	5	84	0	110	11	0
36	6	84	0	110	5	0
36	7	84	0	110	1	0
36	8	84	0	110	5	0
36	Z	126	0	165	4	0
37	1	106	0	82	4	0
37	3	66	0	69	4	0
37	4	201	0	146	3	0
37	5	160	0	133	7	0
37	6	206	0	157	5	0
37	7	54	0	42	2	0
37	8	122	0	115	5	0
37	Z	178	0	168	8	0
38	1	48	0	62	1	0
39	Z	19	0	0	0	0
40	5	23	0	19	0	0
40	6	29	0	31	0	0
40	7	39	0	51	5	0
40	8	30	0	33	0	0
41	7	18	0	31	0	0
42	8	30	0	43	0	0
43	1	16	0	0	0	0
43	3	17	0	0	0	0
43	4	7	0	0	0	0
43	5	9	0	0	1	0
43	6	8	0	0	0	0
43	7	18	0	0	0	0
43	8	16	0	0	0	0
43	A	91	0	0	2	0
43	B	79	0	0	0	0
43	C	19	0	0	1	0
43	D	12	0	0	0	0
43	E	7	0	0	0	0
43	F	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	J	3	0	0	0	0
43	K	2	0	0	0	0
43	L	5	0	0	0	0
43	Z	8	0	0	0	0
All	All	47524	0	47243	762	0

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

The worst 5 of 762 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:4:502:LUT:H32	20:4:604:CLA:HAB	1.44	0.98
20:5:605:CLA:H52	20:5:622:CLA:HAB	1.66	0.77
20:B:1218:CLA:HMD2	23:B:4001:BCR:HC7	1.67	0.76
1:A:396:TRP:CD1	20:A:1126:CLA:HAB	2.23	0.74
20:F:1301:CLA:HBB1	33:F:4001:RRX:H11	1.70	0.73

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	716 (97%)	23 (3%)	0	100	100
2	B	731/733 (100%)	705 (96%)	26 (4%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	163/165 (99%)	157 (96%)	5 (3%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	80 (98%)	2 (2%)	0	100	100
11	L	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
12	1	192/194 (99%)	182 (95%)	10 (5%)	0	100	100
12	Z	192/194 (99%)	189 (98%)	3 (2%)	0	100	100
13	3	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
14	7	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
15	8	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
16	4	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
17	5	225/227 (99%)	221 (98%)	4 (2%)	0	100	100
18	6	227/229 (99%)	222 (98%)	5 (2%)	0	100	100
All	All	3946/4006 (98%)	3820 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	150	PHE

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	92/92 (100%)	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
All	All	3136/3151 (100%)	3136 (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 25 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	30	ASN
12	Z	52	ASN
18	6	140	GLN
12	1	52	ASN
13	3	190	ASN

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	1.00	0	1,7,9	3.26	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	-3.26	105.99	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 317 ligands modelled in this entry, 1 is monoatomic - leaving 316 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	$\#\|Z\| > 2$
20	CLA	7	609	14	69,73,73	1.35	7 (10%)	83,113,113	1.99	21 (25%)
23	BCR	6	504	-	41,41,41	1.84	4 (9%)	56,56,56	4.10	17 (30%)
24	LHG	7	801	-	36,36,48	0.46	0	39,42,54	1.17	3 (7%)
20	CLA	6	609	18	69,73,73	1.37	7 (10%)	83,113,113	1.91	17 (20%)
36	LUT	5	501	-	42,43,43	2.42	1 (2%)	51,60,60	1.94	11 (21%)
28	DAO	A	5007	-	13,13,13	0.81	1 (7%)	13,13,13	0.92	0
20	CLA	8	606	-	64,68,73	1.42	7 (10%)	77,107,113	1.93	16 (20%)
36	LUT	6	502	-	42,43,43	2.38	1 (2%)	51,60,60	1.88	16 (31%)
20	CLA	1	605	-	59,63,73	1.47	7 (11%)	71,101,113	2.05	19 (26%)
26	LMT	A	5006	-	36,36,36	1.22	6 (16%)	47,47,47	1.04	1 (2%)
23	BCR	B	4003	-	41,41,41	1.84	4 (9%)	56,56,56	4.30	18 (32%)
20	CLA	B	1229	-	69,73,73	1.35	9 (13%)	83,113,113	1.97	22 (26%)
30	DGA	A	5005	-	43,43,43	1.14	3 (6%)	45,45,45	1.48	3 (6%)
23	BCR	3	506	-	41,41,41	1.87	4 (9%)	56,56,56	4.48	15 (26%)
20	CLA	3	607	-	64,68,73	1.41	7 (10%)	77,107,113	2.06	19 (24%)
23	BCR	5	504	-	41,41,41	1.83	5 (12%)	56,56,56	4.57	21 (37%)
20	CLA	A	1106	-	69,73,73	1.37	8 (11%)	83,113,113	2.02	17 (20%)
20	CLA	A	1128	-	69,73,73	1.42	8 (11%)	83,113,113	1.90	15 (18%)
23	BCR	3	503	-	41,41,41	1.83	5 (12%)	56,56,56	4.19	16 (28%)
24	LHG	6	801	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
41	PLM	7	805	-	17,17,17	0.58	0	17,17,17	1.04	0
20	CLA	A	1116	-	64,68,73	1.43	7 (10%)	77,107,113	2.01	22 (28%)
20	CLA	5	613	-	59,63,73	1.49	7 (11%)	71,101,113	2.02	19 (26%)
20	CLA	A	1118	-	64,68,73	1.41	8 (12%)	77,107,113	2.02	19 (24%)
20	CLA	A	1122	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
20	CLA	A	1012	-	69,73,73	1.36	7 (10%)	83,113,113	2.02	19 (22%)
20	CLA	B	1222	-	69,73,73	1.39	7 (10%)	83,113,113	1.90	22 (26%)
20	CLA	A	1141	24	56,60,73	1.54	6 (10%)	67,97,113	2.13	18 (26%)
20	CLA	Z	612	-	69,73,73	1.37	6 (8%)	83,113,113	1.93	17 (20%)
37	CHL	7	610	-	58,62,74	0.93	2 (3%)	65,99,114	1.35	12 (18%)
20	CLA	1	601	-	69,73,73	1.37	6 (8%)	83,113,113	1.96	20 (24%)
20	CLA	A	1113	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	C7Z	J	4002	-	43,43,43	5.36	27 (62%)	58,60,60	2.29	20 (34%)
20	CLA	1	613	-	50,54,73	1.60	8 (16%)	60,90,113	2.08	15 (25%)
20	CLA	7	601	-	64,68,73	1.44	8 (12%)	77,107,113	2.06	21 (27%)
20	CLA	A	1136	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	16 (19%)
20	CLA	A	1107	1	69,73,73	1.38	8 (11%)	83,113,113	1.93	20 (24%)
23	BCR	B	4001	-	41,41,41	1.84	5 (12%)	56,56,56	4.19	13 (23%)
26	LMT	B	6101	-	36,36,36	1.18	5 (13%)	47,47,47	1.11	5 (10%)
20	CLA	B	1240	-	69,73,73	1.37	9 (13%)	83,113,113	1.89	20 (24%)
20	CLA	5	606	-	54,58,73	1.54	7 (12%)	65,95,113	2.16	18 (27%)
20	CLA	5	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.03	20 (25%)
20	CLA	7	613	-	46,50,73	1.68	7 (15%)	55,85,113	2.12	15 (27%)
20	CLA	A	1131	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	17 (20%)
20	CLA	6	605	-	59,63,73	1.50	8 (13%)	71,101,113	2.07	18 (25%)
20	CLA	B	1221	-	69,73,73	1.38	7 (10%)	83,113,113	1.99	18 (21%)
20	CLA	1	608	-	64,68,73	1.39	6 (9%)	77,107,113	1.99	17 (22%)
20	CLA	1	611	-	69,73,73	1.35	7 (10%)	83,113,113	1.94	21 (25%)
36	LUT	3	501	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	12 (23%)
20	CLA	4	608	-	59,63,73	1.49	8 (13%)	71,101,113	2.02	18 (25%)
36	LUT	Z	503	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	11 (21%)
20	CLA	B	1206	-	69,73,73	1.38	6 (8%)	83,113,113	1.91	17 (20%)
20	CLA	6	608	-	59,63,73	1.48	7 (11%)	71,101,113	2.11	18 (25%)
20	CLA	8	608	-	59,63,73	1.49	7 (11%)	71,101,113	1.99	17 (23%)
20	CLA	B	1212	-	61,65,73	1.45	6 (9%)	73,103,113	2.07	19 (26%)
20	CLA	1	615	12	69,73,73	1.39	7 (10%)	83,113,113	1.82	16 (19%)
20	CLA	Z	604	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	20 (24%)
20	CLA	7	611	-	54,58,73	1.53	7 (12%)	65,95,113	2.21	19 (29%)
24	LHG	B	5002	-	19,19,48	0.84	1 (5%)	20,24,54	1.34	1 (5%)
20	CLA	B	1223	-	69,73,73	1.38	6 (8%)	83,113,113	1.95	20 (24%)
20	CLA	6	607	-	59,63,73	1.47	7 (11%)	71,101,113	1.99	19 (26%)
20	CLA	A	1127	-	69,73,73	1.38	6 (8%)	83,113,113	1.82	18 (21%)
20	CLA	3	604	-	64,68,73	1.44	7 (10%)	77,107,113	2.09	21 (27%)
24	LHG	8	801	-	37,37,48	0.43	0	40,43,54	1.14	4 (10%)
20	CLA	A	1114	-	65,69,73	1.44	7 (10%)	78,108,113	1.97	15 (19%)
37	CHL	1	609	12	62,66,74	0.90	3 (4%)	70,104,114	1.31	12 (17%)
23	BCR	4	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	J	5001	-	35,35,55	0.46	0	43,43,63	1.13	2 (4%)
20	CLA	3	602	-	50,54,73	1.60	7 (14%)	60,90,113	1.98	13 (21%)
20	CLA	8	607	-	59,63,73	1.50	6 (10%)	71,101,113	2.03	16 (22%)
20	CLA	A	1111	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	18 (21%)
20	CLA	B	1023	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	18 (21%)
23	BCR	8	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.24	14 (25%)
20	CLA	A	1115	-	64,68,73	1.40	7 (10%)	77,107,113	2.01	19 (24%)
20	CLA	K	1404	-	59,63,73	1.48	7 (11%)	71,101,113	2.15	18 (25%)
19	CL0	A	1011	-	69,73,73	2.34	20 (28%)	83,113,113	2.58	26 (31%)
37	CHL	Z	609	12	70,74,74	0.88	3 (4%)	80,114,114	1.27	11 (13%)
35	SPH	7	803	-	19,20,20	0.66	0	18,21,21	0.90	0
20	CLA	7	602	-	54,58,73	1.53	7 (12%)	65,95,113	2.11	17 (26%)
23	BCR	G	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.30	15 (26%)
20	CLA	4	602	-	56,60,73	1.52	6 (10%)	67,97,113	2.13	17 (25%)
20	CLA	B	1218	-	69,73,73	1.38	7 (10%)	83,113,113	2.00	21 (25%)
20	CLA	3	601	-	69,73,73	1.38	8 (11%)	83,113,113	1.99	18 (21%)
23	BCR	7	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.28	14 (25%)
20	CLA	6	619	18	69,73,73	1.38	6 (8%)	83,113,113	1.91	17 (20%)
20	CLA	8	602	-	69,73,73	1.36	7 (10%)	83,113,113	2.00	21 (25%)
20	CLA	A	1125	-	69,73,73	1.37	6 (8%)	83,113,113	1.97	20 (24%)
20	CLA	B	1241	-	69,73,73	1.39	9 (13%)	83,113,113	1.94	18 (21%)
29	LMG	A	5003	-	29,29,55	0.55	0	37,37,63	1.26	4 (10%)
22	SF4	C	3002	3	0,12,12	-	-	-		
37	CHL	5	617	-	47,51,74	1.01	2 (4%)	52,86,114	1.40	9 (17%)
23	BCR	5	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.30	19 (33%)
20	CLA	B	1205	-	69,73,73	1.35	7 (10%)	83,113,113	2.00	17 (20%)
20	CLA	L	1503	-	54,58,73	1.53	6 (11%)	65,95,113	2.14	18 (27%)
20	CLA	8	611	-	54,58,73	1.53	7 (12%)	65,95,113	2.23	18 (27%)
20	CLA	4	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.03	18 (23%)
20	CLA	A	1102	-	59,63,73	1.46	8 (13%)	71,101,113	2.15	20 (28%)
23	BCR	B	4005	-	41,41,41	1.89	4 (9%)	56,56,56	4.48	17 (30%)
20	CLA	1	603	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	19 (22%)
24	LHG	A	5001	20	34,34,48	0.45	0	37,40,54	1.16	3 (8%)
20	CLA	6	604	-	69,73,73	1.36	6 (8%)	83,113,113	1.95	22 (26%)
20	CLA	6	603	-	69,73,73	1.36	6 (8%)	83,113,113	2.00	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	7	603	-	69,73,73	1.36	8 (11%)	83,113,113	2.12	22 (26%)
25	NKP	A	5004	-	28,28,28	1.56	3 (10%)	31,32,32	1.23	3 (9%)
20	CLA	8	603	-	69,73,73	1.36	7 (10%)	83,113,113	2.13	22 (26%)
20	CLA	B	1213	2	69,73,73	1.37	8 (11%)	83,113,113	2.07	23 (27%)
22	SF4	C	3003	3	0,12,12	-	-	-		
26	LMT	B	5005	-	36,36,36	1.24	5 (13%)	47,47,47	1.15	4 (8%)
20	CLA	B	1224	-	69,73,73	1.39	7 (10%)	83,113,113	1.96	18 (21%)
20	CLA	B	1232	-	49,53,73	1.63	7 (14%)	59,89,113	2.06	13 (22%)
20	CLA	7	604	-	69,73,73	1.37	6 (8%)	83,113,113	1.91	20 (24%)
20	CLA	Z	607	-	61,65,73	1.45	7 (11%)	73,103,113	2.01	17 (23%)
20	CLA	B	1217	2	60,64,73	1.47	7 (11%)	72,102,113	2.01	17 (23%)
36	LUT	6	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.85	11 (21%)
26	LMT	4	803	-	36,36,36	1.21	6 (16%)	47,47,47	1.05	3 (6%)
20	CLA	3	612	-	64,68,73	1.42	8 (12%)	77,107,113	1.97	17 (22%)
20	CLA	8	605	-	69,73,73	1.39	7 (10%)	83,113,113	1.92	18 (21%)
20	CLA	A	1138	-	69,73,73	1.35	7 (10%)	83,113,113	2.05	17 (20%)
20	CLA	Z	602	-	50,54,73	1.60	6 (12%)	60,90,113	2.00	13 (21%)
36	LUT	Z	501	-	42,43,43	2.29	1 (2%)	51,60,60	1.91	11 (21%)
20	CLA	A	1126	-	69,73,73	1.39	8 (11%)	83,113,113	1.93	17 (20%)
20	CLA	4	609	16	64,68,73	1.41	7 (10%)	77,107,113	1.99	19 (24%)
20	CLA	A	1101	-	69,73,73	1.36	6 (8%)	83,113,113	1.94	19 (22%)
20	CLA	5	604	-	69,73,73	1.37	8 (11%)	83,113,113	1.96	20 (24%)
20	CLA	B	1225	-	69,73,73	1.39	8 (11%)	83,113,113	1.80	16 (19%)
22	SF4	A	3001	2,1	0,12,12	-	-	-		
40	3PH	5	802	-	22,22,47	1.24	4 (18%)	26,27,52	1.35	2 (7%)
20	CLA	B	1226	-	69,73,73	1.41	7 (10%)	83,113,113	2.05	21 (25%)
20	CLA	B	1228	-	69,73,73	1.36	6 (8%)	83,113,113	1.92	19 (22%)
20	CLA	A	1120	-	59,63,73	1.46	7 (11%)	71,101,113	2.19	21 (29%)
20	CLA	4	604	-	64,68,73	1.42	7 (10%)	77,107,113	1.93	17 (22%)
20	CLA	5	609	-	69,73,73	1.37	9 (13%)	83,113,113	1.88	17 (20%)
20	CLA	J	1901	-	46,50,73	1.66	7 (15%)	55,85,113	2.17	16 (29%)
20	CLA	B	1022	43	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
25	NKP	3	802	-	15,15,28	2.07	3 (20%)	18,19,32	1.52	2 (11%)
24	LHG	Z	801	-	42,42,48	0.41	0	45,48,54	1.16	4 (8%)
31	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.07	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CHL	8	610	-	60,64,74	0.93	2 (3%)	68,102,114	1.35	12 (17%)
20	CLA	B	1215	-	64,68,73	1.42	7 (10%)	77,107,113	1.95	18 (23%)
25	NKP	8	802	-	28,28,28	1.51	2 (7%)	31,32,32	1.25	3 (9%)
23	BCR	A	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.11	14 (25%)
26	LMT	F	5001	-	36,36,36	1.21	6 (16%)	47,47,47	0.92	1 (2%)
33	RRX	F	4001	-	42,42,42	4.79	24 (57%)	57,58,58	2.53	23 (40%)
20	CLA	F	1302	-	49,53,73	1.62	8 (16%)	59,89,113	2.02	15 (25%)
26	LMT	1	803	-	36,36,36	1.17	5 (13%)	47,47,47	0.99	1 (2%)
36	LUT	1	502	-	42,43,43	2.31	1 (2%)	51,60,60	2.00	16 (31%)
20	CLA	6	601	-	64,68,73	1.43	7 (10%)	77,107,113	2.02	22 (28%)
36	LUT	4	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.83	14 (27%)
20	CLA	8	609	15	69,73,73	1.37	7 (10%)	83,113,113	1.96	20 (24%)
24	LHG	5	801	-	36,36,48	0.44	0	39,42,54	1.18	3 (7%)
38	SQD	1	802	-	47,48,54	0.83	0	56,59,65	0.94	2 (3%)
37	CHL	4	613	-	60,64,74	0.93	2 (3%)	68,102,114	1.32	10 (14%)
37	CHL	5	610	-	70,74,74	0.84	2 (2%)	80,114,114	1.19	10 (12%)
36	LUT	7	502	-	42,43,43	2.30	1 (2%)	51,60,60	1.96	12 (23%)
20	CLA	A	1135	-	55,59,73	1.54	8 (14%)	66,96,113	2.22	20 (30%)
37	CHL	4	610	-	55,59,74	0.93	2 (3%)	62,96,114	1.48	12 (19%)
20	CLA	A	1108	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	17 (20%)
20	CLA	1	607	-	64,68,73	1.43	6 (9%)	77,107,113	1.98	18 (23%)
23	BCR	B	4007	-	41,41,41	1.83	4 (9%)	56,56,56	4.18	16 (28%)
20	CLA	Z	606	-	61,65,73	1.48	9 (14%)	73,103,113	2.02	20 (27%)
26	LMT	8	805	-	36,36,36	1.20	5 (13%)	47,47,47	1.01	1 (2%)
20	CLA	8	615	15	50,54,73	1.59	7 (14%)	60,90,113	2.12	17 (28%)
23	BCR	B	4004	-	41,41,41	1.82	4 (9%)	56,56,56	4.25	14 (25%)
21	PQN	A	2001	-	34,34,34	0.39	0	42,45,45	1.15	2 (4%)
20	CLA	7	607	-	69,73,73	1.37	6 (8%)	83,113,113	1.98	18 (21%)
34	C7Z	1	503	-	43,43,43	5.38	26 (60%)	58,60,60	2.36	20 (34%)
20	CLA	A	1121	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	20 (24%)
20	CLA	3	616	-	60,64,73	1.45	6 (10%)	72,102,113	2.11	18 (25%)
23	BCR	K	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	14 (25%)
20	CLA	G	1601	-	54,58,73	1.52	6 (11%)	65,95,113	2.17	18 (27%)
20	CLA	Z	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.00	19 (24%)
24	LHG	B	5006	-	32,32,48	0.45	0	35,38,54	1.16	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	1130	-	69,73,73	1.37	7 (10%)	83,113,113	1.88	18 (21%)
21	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.09	2 (4%)
23	BCR	L	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.30	16 (28%)
23	BCR	6	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	15 (26%)
20	CLA	B	1207	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)
20	CLA	7	612	-	54,58,73	1.55	7 (12%)	65,95,113	2.08	17 (26%)
20	CLA	5	618	-	69,73,73	1.35	7 (10%)	83,113,113	2.06	19 (22%)
20	CLA	B	1227	-	54,58,73	1.57	7 (12%)	65,95,113	2.14	18 (27%)
20	CLA	5	615	17	54,58,73	1.54	6 (11%)	65,95,113	2.15	18 (27%)
20	CLA	7	615	14	62,66,73	1.44	8 (12%)	74,104,113	2.00	17 (22%)
20	CLA	B	1230	-	62,66,73	1.45	6 (9%)	74,104,113	2.07	19 (25%)
37	CHL	4	611	-	55,59,74	0.95	2 (3%)	62,96,114	1.37	10 (16%)
23	BCR	L	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.27	13 (23%)
20	CLA	Z	608	-	60,64,73	1.47	9 (15%)	72,102,113	2.04	19 (26%)
20	CLA	Z	611	-	59,63,73	1.47	8 (13%)	71,101,113	2.08	19 (26%)
20	CLA	6	602	-	56,60,73	1.53	6 (10%)	67,97,113	2.08	18 (26%)
20	CLA	B	1201	-	49,53,73	1.61	8 (16%)	59,89,113	2.10	20 (33%)
36	LUT	8	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.92	14 (27%)
24	LHG	A	5002	-	48,48,48	0.40	0	51,54,54	1.07	3 (5%)
36	LUT	8	501	-	42,43,43	2.30	1 (2%)	51,60,60	1.95	14 (27%)
20	CLA	3	608	-	49,53,73	1.62	7 (14%)	59,89,113	2.10	15 (25%)
20	CLA	A	1134	1	59,63,73	1.47	6 (10%)	71,101,113	2.12	17 (23%)
20	CLA	Z	615	-	50,54,73	1.58	6 (12%)	60,90,113	2.04	17 (28%)
20	CLA	K	1401	-	50,54,73	1.61	7 (14%)	60,90,113	2.00	15 (25%)
23	BCR	I	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.27	15 (26%)
20	CLA	B	1235	-	69,73,73	1.36	8 (11%)	83,113,113	1.97	17 (20%)
20	CLA	B	1239	-	69,73,73	1.34	7 (10%)	83,113,113	2.04	17 (20%)
36	LUT	3	502	-	42,43,43	2.43	1 (2%)	51,60,60	2.02	16 (31%)
20	CLA	4	603	-	69,73,73	1.35	6 (8%)	83,113,113	2.08	21 (25%)
20	CLA	5	602	-	65,69,73	1.40	8 (12%)	78,108,113	1.92	16 (20%)
20	CLA	G	1602	-	50,54,73	1.58	8 (16%)	60,90,113	2.18	17 (28%)
40	3PH	8	806	-	29,29,47	1.09	4 (13%)	33,34,52	1.11	2 (6%)
20	CLA	B	1208	-	60,64,73	1.46	7 (11%)	72,102,113	2.09	17 (23%)
23	BCR	B	4002	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	14 (25%)
24	LHG	B	5001	-	22,22,48	0.55	0	25,28,54	1.30	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	OCA	A	5008	-	9,9,9	0.65	0	9,9,9	0.97	0
24	LHG	4	802	-	31,31,48	0.46	0	34,37,54	1.13	2 (5%)
39	QTB	Z	504	-	19,19,19	2.50	5 (26%)	20,26,26	2.80	8 (40%)
20	CLA	K	1403	-	53,57,73	1.53	6 (11%)	62,93,113	2.13	18 (29%)
20	CLA	A	1119	-	69,73,73	1.38	6 (8%)	83,113,113	1.82	17 (20%)
20	CLA	1	606	-	65,69,73	1.42	7 (10%)	78,108,113	1.97	16 (20%)
20	CLA	3	618	-	50,54,73	1.62	7 (14%)	60,90,113	2.07	15 (25%)
20	CLA	A	1112	-	64,68,73	1.41	7 (10%)	77,107,113	1.99	20 (25%)
20	CLA	B	1238	-	69,73,73	1.36	8 (11%)	83,113,113	1.98	18 (21%)
20	CLA	7	606	-	60,64,73	1.47	6 (10%)	72,102,113	2.00	17 (23%)
20	CLA	4	605	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	18 (21%)
20	CLA	1	604	-	64,68,73	1.42	6 (9%)	77,107,113	1.98	19 (24%)
20	CLA	6	606	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	19 (22%)
20	CLA	4	607	-	59,63,73	1.48	7 (11%)	71,101,113	2.02	17 (23%)
20	CLA	6	615	-	65,69,73	1.40	6 (9%)	78,108,113	2.09	20 (25%)
20	CLA	7	605	14	65,69,73	1.38	7 (10%)	78,108,113	2.02	21 (26%)
20	CLA	3	605	-	69,73,73	1.37	8 (11%)	83,113,113	1.85	18 (21%)
20	CLA	5	603	-	60,64,73	1.44	6 (10%)	72,102,113	2.17	17 (23%)
37	CHL	1	610	-	52,56,74	0.93	2 (3%)	58,92,114	1.28	10 (17%)
35	SPH	7	804	-	19,20,20	0.69	0	18,21,21	1.06	1 (5%)
20	CLA	8	604	-	66,70,73	1.39	6 (9%)	79,109,113	2.03	22 (27%)
20	CLA	B	1209	-	69,73,73	1.36	7 (10%)	83,113,113	1.89	18 (21%)
36	LUT	5	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.77	12 (23%)
20	CLA	B	1231	-	69,73,73	1.36	6 (8%)	83,113,113	1.98	18 (21%)
23	BCR	A	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.14	12 (21%)
20	CLA	Z	603	-	54,58,73	1.55	7 (12%)	65,95,113	2.16	19 (29%)
20	CLA	7	608	-	47,51,73	1.67	9 (19%)	56,86,113	2.16	15 (26%)
20	CLA	4	612	-	54,58,73	1.56	6 (11%)	65,95,113	2.21	19 (29%)
23	BCR	A	4004	-	41,41,41	1.81	4 (9%)	56,56,56	4.37	16 (28%)
20	CLA	A	1123	-	69,73,73	1.38	8 (11%)	83,113,113	1.92	15 (18%)
20	CLA	A	1104	-	69,73,73	1.37	8 (11%)	83,113,113	1.97	21 (25%)
37	CHL	6	610	-	60,64,74	0.89	2 (3%)	68,102,114	1.31	11 (16%)
20	CLA	B	1216	-	69,73,73	1.36	8 (11%)	83,113,113	1.87	16 (19%)
20	CLA	A	1109	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	17 (20%)
37	CHL	6	611	-	55,59,74	0.96	2 (3%)	62,96,114	1.29	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	1140	-	69,73,73	1.37	7 (10%)	83,113,113	1.87	17 (20%)
20	CLA	8	612	-	50,54,73	1.61	8 (16%)	60,90,113	1.95	13 (21%)
20	CLA	8	601	15	64,68,73	1.43	7 (10%)	77,107,113	2.02	18 (23%)
37	CHL	3	611	-	70,74,74	0.87	2 (2%)	80,114,114	1.30	12 (15%)
20	CLA	B	1214	-	63,67,73	1.45	8 (12%)	75,105,113	2.12	23 (30%)
20	CLA	B	1219	-	63,67,73	1.44	7 (11%)	75,105,113	2.09	21 (28%)
20	CLA	B	1236	-	69,73,73	1.38	8 (11%)	83,113,113	1.97	17 (20%)
20	CLA	A	1139	1	69,73,73	1.37	7 (10%)	83,113,113	1.98	23 (27%)
20	CLA	5	605	-	59,63,73	1.49	7 (11%)	71,101,113	2.17	21 (29%)
20	CLA	A	1129	-	54,58,73	1.55	7 (12%)	65,95,113	2.10	16 (24%)
23	BCR	B	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.21	17 (30%)
20	CLA	Z	605	-	69,73,73	1.37	6 (8%)	83,113,113	1.92	20 (24%)
35	SPH	K	5001	-	19,20,20	0.66	0	18,21,21	1.00	0
42	LPX	8	803	-	29,29,29	1.02	2 (6%)	31,33,33	0.93	1 (3%)
40	3PH	7	802	-	38,38,47	0.98	3 (7%)	42,43,52	1.16	2 (4%)
23	BCR	3	505	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	11 (19%)
20	CLA	B	1203	-	69,73,73	1.35	8 (11%)	83,113,113	1.90	20 (24%)
20	CLA	A	1103	1	69,73,73	1.33	6 (8%)	83,113,113	1.98	17 (20%)
23	BCR	A	4003	-	41,41,41	1.80	4 (9%)	56,56,56	4.35	20 (35%)
20	CLA	L	1502	-	69,73,73	1.37	8 (11%)	83,113,113	1.97	19 (22%)
23	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.36	12 (21%)
37	CHL	4	617	-	47,51,74	1.01	2 (4%)	52,86,114	1.41	8 (15%)
20	CLA	A	1110	1	69,73,73	1.37	7 (10%)	83,113,113	2.05	17 (20%)
37	CHL	Z	610	-	70,74,74	0.80	2 (2%)	80,114,114	1.17	10 (12%)
20	CLA	A	1132	-	69,73,73	1.36	8 (11%)	83,113,113	1.94	18 (21%)
24	LHG	3	801	-	19,19,48	0.91	1 (5%)	20,24,54	1.44	1 (5%)
20	CLA	B	1234	-	64,68,73	1.44	7 (10%)	77,107,113	1.98	17 (22%)
20	CLA	B	1204	-	69,73,73	1.36	7 (10%)	83,113,113	1.98	17 (20%)
20	CLA	F	1301	-	69,73,73	1.35	6 (8%)	83,113,113	1.98	22 (26%)
24	LHG	4	801	-	48,48,48	0.40	0	51,54,54	1.13	4 (7%)
20	CLA	5	608	-	49,53,73	1.62	7 (14%)	59,89,113	2.16	15 (25%)
20	CLA	A	1117	-	69,73,73	1.37	7 (10%)	83,113,113	1.99	17 (20%)
37	CHL	5	611	-	55,59,74	0.89	2 (3%)	62,96,114	1.35	9 (14%)
20	CLA	3	603	-	69,73,73	1.36	7 (10%)	83,113,113	2.06	19 (22%)
20	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	$\#\|Z\|>2$
23	BCR	7	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.41	17 (30%)
20	CLA	B	1237	-	69,73,73	1.36	7 (10%)	83,113,113	1.86	17 (20%)
20	CLA	7	616	-	64,68,73	1.38	7 (10%)	77,107,113	2.14	18 (23%)
20	CLA	A	1105	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	19 (22%)
20	CLA	3	606	-	69,73,73	1.34	7 (10%)	83,113,113	2.01	19 (22%)
20	CLA	A	1013	-	69,73,73	1.39	8 (11%)	83,113,113	1.88	20 (24%)
37	CHL	6	617	-	47,51,74	0.96	2 (4%)	52,86,114	1.33	8 (15%)
20	CLA	B	1210	-	69,73,73	1.38	6 (8%)	83,113,113	1.95	18 (21%)
20	CLA	K	1402	-	59,63,73	1.48	9 (15%)	71,101,113	2.07	19 (26%)
20	CLA	B	1202	-	69,73,73	1.37	6 (8%)	83,113,113	1.99	20 (24%)
34	C7Z	5	505	-	43,43,43	5.43	26 (60%)	58,60,60	2.17	17 (29%)
20	CLA	B	1021	-	69,73,73	1.37	6 (8%)	83,113,113	1.95	19 (22%)
36	LUT	Z	502	-	42,43,43	2.29	1 (2%)	51,60,60	1.98	13 (25%)
37	CHL	Z	613	-	50,54,74	0.98	2 (4%)	56,90,114	1.30	8 (14%)
36	LUT	1	501	-	42,43,43	2.31	1 (2%)	51,60,60	1.80	10 (19%)
36	LUT	4	501	-	42,43,43	2.37	1 (2%)	51,60,60	1.94	13 (25%)
20	CLA	5	622	-	50,54,73	1.63	7 (14%)	60,90,113	2.11	14 (23%)
20	CLA	6	612	-	54,58,73	1.55	7 (12%)	65,95,113	2.16	18 (27%)
20	CLA	A	1124	-	69,73,73	1.37	6 (8%)	83,113,113	1.88	19 (22%)
20	CLA	6	618	-	50,54,73	1.58	6 (12%)	60,90,113	2.13	16 (26%)
20	CLA	3	613	-	59,63,73	1.48	7 (11%)	71,101,113	2.06	17 (23%)
20	CLA	4	606	-	54,58,73	1.53	8 (14%)	65,95,113	2.20	19 (29%)
20	CLA	4	615	-	45,49,73	1.68	6 (13%)	54,84,113	2.19	16 (29%)
20	CLA	A	1137	-	69,73,73	1.37	8 (11%)	83,113,113	2.01	21 (25%)
20	CLA	3	610	13	64,68,73	1.42	7 (10%)	77,107,113	1.98	20 (25%)
36	LUT	7	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.90	12 (23%)
37	CHL	6	613	-	60,64,74	0.90	2 (3%)	68,102,114	1.20	9 (13%)
37	CHL	8	613	-	70,74,74	0.91	3 (4%)	80,114,114	1.22	11 (13%)
24	LHG	1	801	-	42,42,48	0.45	0	45,48,54	1.11	2 (4%)
20	CLA	A	1133	1	69,73,73	1.38	7 (10%)	83,113,113	1.84	16 (19%)
20	CLA	B	1211	-	64,68,73	1.45	7 (10%)	77,107,113	1.86	14 (18%)
23	BCR	A	4005	-	41,41,41	1.83	5 (12%)	56,56,56	4.17	11 (19%)
23	BCR	J	4001	-	41,41,41	1.81	4 (9%)	56,56,56	4.27	17 (30%)
20	CLA	5	612	-	69,73,73	1.35	6 (8%)	83,113,113	1.86	17 (20%)
20	CLA	B	1220	-	69,73,73	1.37	6 (8%)	83,113,113	1.87	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	3	504	-	41,41,41	1.83	5 (12%)	56,56,56	4.28	15 (26%)
20	CLA	5	607	-	65,69,73	1.41	7 (10%)	78,108,113	1.97	19 (24%)
20	CLA	1	602	-	49,53,73	1.64	9 (18%)	59,89,113	2.04	14 (23%)
40	3PH	6	802	-	28,28,47	1.11	4 (14%)	32,33,52	1.29	2 (6%)

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
20	CLA	7	609	14	-	21/39/115/115	-
23	BCR	6	504	-	-	11/29/63/63	0/2/2/2
24	LHG	7	801	-	-	26/41/41/53	-
20	CLA	6	609	18	-	13/39/115/115	-
36	LUT	5	501	-	-	3/29/67/67	0/2/2/2
28	DAO	A	5007	-	-	1/11/11/11	-
20	CLA	8	606	-	-	13/33/109/115	-
36	LUT	6	502	-	-	2/29/67/67	0/2/2/2
20	CLA	1	605	-	-	11/27/103/115	-
26	LMT	A	5006	-	-	12/21/61/61	0/2/2/2
23	BCR	B	4003	-	-	9/29/63/63	0/2/2/2
20	CLA	B	1229	-	-	13/39/115/115	-
30	DGA	A	5005	-	-	21/45/45/45	-
23	BCR	3	506	-	-	15/29/63/63	0/2/2/2
20	CLA	3	607	-	-	23/33/109/115	-
23	BCR	5	504	-	-	11/29/63/63	0/2/2/2
20	CLA	A	1106	-	-	18/39/115/115	-
20	CLA	A	1128	-	-	19/39/115/115	-
23	BCR	3	503	-	-	10/29/63/63	0/2/2/2
24	LHG	6	801	-	-	33/53/53/53	-
41	PLM	7	805	-	-	7/15/15/15	-
20	CLA	A	1116	-	-	14/33/109/115	-
20	CLA	5	613	-	-	14/27/103/115	-
20	CLA	A	1118	-	-	16/33/109/115	-
20	CLA	A	1122	-	-	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1012	-	-	19/39/115/115	-
20	CLA	B	1222	-	-	15/39/115/115	-
20	CLA	A	1141	24	-	11/24/100/115	-
20	CLA	Z	612	-	-	18/39/115/115	-
37	CHL	7	610	-	-	5/27/103/117	-
20	CLA	1	601	-	-	17/39/115/115	-
20	CLA	A	1113	-	-	12/39/115/115	-
34	C7Z	J	4002	-	1/1/12/26	11/29/67/67	0/2/2/2
20	CLA	1	613	-	-	10/17/93/115	-
20	CLA	7	601	-	-	14/33/109/115	-
20	CLA	A	1136	-	-	16/39/115/115	-
20	CLA	A	1107	1	-	17/39/115/115	-
23	BCR	B	4001	-	-	13/29/63/63	0/2/2/2
26	LMT	B	6101	-	-	10/21/61/61	0/2/2/2
20	CLA	B	1240	-	-	21/39/115/115	-
20	CLA	5	606	-	-	14/21/97/115	-
20	CLA	5	601	-	-	17/33/109/115	-
20	CLA	7	613	-	-	6/12/88/115	-
20	CLA	A	1131	-	-	17/39/115/115	-
20	CLA	6	605	-	-	16/27/103/115	-
20	CLA	B	1221	-	-	16/39/115/115	-
20	CLA	1	608	-	-	14/33/109/115	-
20	CLA	1	611	-	-	16/39/115/115	-
36	LUT	3	501	-	-	1/29/67/67	0/2/2/2
20	CLA	4	608	-	-	10/27/103/115	-
36	LUT	Z	503	-	-	6/29/67/67	0/2/2/2
20	CLA	B	1206	-	-	18/39/115/115	-
20	CLA	6	608	-	-	14/27/103/115	-
20	CLA	8	608	-	-	13/27/103/115	-
20	CLA	B	1212	-	-	9/30/106/115	-
20	CLA	1	615	12	-	17/39/115/115	-
20	CLA	Z	604	-	-	19/39/115/115	-
20	CLA	7	611	-	-	4/21/97/115	-
24	LHG	B	5002	-	-	11/22/22/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1223	-	-	18/39/115/115	-
20	CLA	6	607	-	-	8/27/103/115	-
20	CLA	A	1127	-	-	14/39/115/115	-
20	CLA	3	604	-	-	9/33/109/115	-
24	LHG	8	801	-	-	20/42/42/53	-
37	CHL	1	609	12	1/1/13/21	5/32/108/117	-
20	CLA	A	1114	-	-	9/35/111/115	-
23	BCR	4	503	-	-	16/29/63/63	0/2/2/2
29	LMG	J	5001	-	-	10/30/50/70	0/1/1/1
20	CLA	3	602	-	-	6/17/93/115	-
20	CLA	8	607	-	-	16/27/103/115	-
20	CLA	A	1111	-	-	17/39/115/115	-
20	CLA	B	1023	-	-	17/39/115/115	-
23	BCR	8	503	-	-	11/29/63/63	0/2/2/2
20	CLA	A	1115	-	-	15/33/109/115	-
20	CLA	K	1404	-	-	13/27/103/115	-
19	CL0	A	1011	-	-	11/39/115/115	-
37	CHL	Z	609	12	1/1/15/21	12/41/117/117	-
35	SPH	7	803	-	-	7/21/21/21	-
20	CLA	7	602	-	-	7/21/97/115	-
23	BCR	G	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	4	602	-	-	8/24/100/115	-
20	CLA	B	1218	-	-	16/39/115/115	-
20	CLA	3	601	-	-	12/39/115/115	-
23	BCR	7	503	-	-	10/29/63/63	0/2/2/2
20	CLA	6	619	18	-	18/39/115/115	-
20	CLA	8	602	-	-	17/39/115/115	-
20	CLA	A	1125	-	-	22/39/115/115	-
20	CLA	B	1241	-	-	23/39/115/115	-
29	LMG	A	5003	-	-	8/24/44/70	0/1/1/1
22	SF4	C	3002	3	-	-	0/6/5/5
37	CHL	5	617	-	-	3/14/90/117	-
23	BCR	5	503	-	-	12/29/63/63	0/2/2/2
20	CLA	B	1205	-	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	L	1503	-	-	10/21/97/115	-
20	CLA	8	611	-	-	7/21/97/115	-
20	CLA	4	601	-	-	10/33/109/115	-
20	CLA	A	1102	-	-	15/27/103/115	-
23	BCR	B	4005	-	-	13/29/63/63	0/2/2/2
20	CLA	1	603	-	-	17/39/115/115	-
24	LHG	A	5001	20	-	22/39/39/53	-
20	CLA	6	604	-	-	12/39/115/115	-
20	CLA	6	603	-	-	21/39/115/115	-
20	CLA	7	603	-	-	15/39/115/115	-
25	NKP	A	5004	-	-	14/28/28/28	-
20	CLA	8	603	-	-	8/39/115/115	-
20	CLA	B	1213	2	-	21/39/115/115	-
26	LMT	B	5005	-	-	14/21/61/61	0/2/2/2
22	SF4	C	3003	3	-	-	0/6/5/5
20	CLA	B	1224	-	-	17/39/115/115	-
20	CLA	B	1232	-	-	4/15/91/115	-
20	CLA	7	604	-	-	15/39/115/115	-
20	CLA	Z	607	-	-	15/30/106/115	-
20	CLA	B	1217	2	-	17/29/105/115	-
36	LUT	6	501	-	-	4/29/67/67	0/2/2/2
26	LMT	4	803	-	-	11/21/61/61	0/2/2/2
20	CLA	3	612	-	-	11/33/109/115	-
20	CLA	8	605	-	-	19/39/115/115	-
20	CLA	A	1138	-	-	16/39/115/115	-
20	CLA	Z	602	-	-	4/17/93/115	-
36	LUT	Z	501	-	-	2/29/67/67	0/2/2/2
20	CLA	A	1126	-	-	22/39/115/115	-
20	CLA	4	609	16	-	15/33/109/115	-
20	CLA	A	1101	-	-	16/39/115/115	-
20	CLA	5	604	-	-	13/39/115/115	-
20	CLA	B	1225	-	-	11/39/115/115	-
22	SF4	A	3001	2,1	-	-	0/6/5/5
40	3PH	5	802	-	-	9/24/24/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1226	-	-	17/39/115/115	-
20	CLA	B	1228	-	-	18/39/115/115	-
20	CLA	A	1120	-	-	15/27/103/115	-
20	CLA	4	604	-	-	9/33/109/115	-
20	CLA	5	609	-	-	13/39/115/115	-
20	CLA	J	1901	-	-	4/12/88/115	-
20	CLA	B	1022	43	-	9/39/115/115	-
25	NKP	3	802	-	-	2/15/15/28	-
24	LHG	Z	801	-	-	29/47/47/53	-
31	DGD	B	5003	-	-	17/55/95/95	0/2/2/2
37	CHL	8	610	-	1/1/13/21	6/29/105/117	-
20	CLA	B	1215	-	-	17/33/109/115	-
25	NKP	8	802	-	-	15/28/28/28	-
23	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
26	LMT	F	5001	-	-	8/21/61/61	0/2/2/2
33	RRX	F	4001	-	1/1/11/25	9/29/65/65	0/2/2/2
20	CLA	F	1302	-	-	6/15/91/115	-
26	LMT	1	803	-	-	6/21/61/61	0/2/2/2
36	LUT	1	502	-	-	1/29/67/67	0/2/2/2
20	CLA	6	601	-	-	15/33/109/115	-
36	LUT	4	502	-	-	4/29/67/67	0/2/2/2
20	CLA	8	609	15	-	19/39/115/115	-
24	LHG	5	801	-	-	27/41/41/53	-
38	SQD	1	802	-	-	21/43/63/69	0/1/1/1
37	CHL	4	613	-	1/1/13/21	3/29/105/117	-
37	CHL	5	610	-	1/1/15/21	9/41/117/117	-
36	LUT	7	502	-	-	2/29/67/67	0/2/2/2
37	CHL	4	610	-	1/1/12/21	5/23/99/117	-
20	CLA	A	1135	-	-	11/23/99/115	-
20	CLA	A	1108	-	-	25/39/115/115	-
20	CLA	1	607	-	-	14/33/109/115	-
23	BCR	B	4007	-	-	12/29/63/63	0/2/2/2
20	CLA	Z	606	-	-	9/30/106/115	-
26	LMT	8	805	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	8	615	15	-	9/17/93/115	-
23	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
21	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
20	CLA	7	607	-	-	23/39/115/115	-
34	C7Z	1	503	-	1/1/12/26	6/29/67/67	0/2/2/2
20	CLA	A	1121	-	-	23/39/115/115	-
20	CLA	3	616	-	-	10/29/105/115	-
23	BCR	K	4002	-	-	8/29/63/63	0/2/2/2
20	CLA	G	1601	-	-	10/21/97/115	-
20	CLA	Z	601	-	-	12/33/109/115	-
24	LHG	B	5006	-	-	24/37/37/53	-
20	CLA	A	1130	-	-	17/39/115/115	-
21	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
23	BCR	L	4002	-	-	11/29/63/63	0/2/2/2
23	BCR	6	503	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1207	-	-	16/39/115/115	-
20	CLA	7	612	-	-	10/21/97/115	-
20	CLA	5	618	-	-	18/39/115/115	-
20	CLA	B	1227	-	-	11/21/97/115	-
20	CLA	5	615	17	-	7/21/97/115	-
20	CLA	7	615	14	-	17/31/107/115	-
20	CLA	B	1230	-	-	13/31/107/115	-
37	CHL	4	611	-	-	6/23/99/117	-
23	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	Z	608	-	-	13/29/105/115	-
20	CLA	Z	611	-	-	10/27/103/115	-
20	CLA	6	602	-	-	7/24/100/115	-
20	CLA	B	1201	-	-	4/15/91/115	-
36	LUT	8	502	-	-	2/29/67/67	0/2/2/2
24	LHG	A	5002	-	-	29/53/53/53	-
36	LUT	8	501	-	-	2/29/67/67	0/2/2/2
20	CLA	3	608	-	-	8/15/91/115	-
20	CLA	A	1134	1	-	12/27/103/115	-
20	CLA	Z	615	-	-	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	K	1401	-	-	7/17/93/115	-
23	BCR	I	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1235	-	-	17/39/115/115	-
20	CLA	B	1239	-	-	16/39/115/115	-
36	LUT	3	502	-	-	1/29/67/67	0/2/2/2
20	CLA	4	603	-	-	16/39/115/115	-
20	CLA	5	602	-	-	16/35/111/115	-
20	CLA	G	1602	-	-	8/17/93/115	-
40	3PH	8	806	-	-	13/31/31/49	-
20	CLA	B	1208	-	-	11/29/105/115	-
23	BCR	B	4002	-	-	12/29/63/63	0/2/2/2
24	LHG	B	5001	-	-	15/26/26/53	-
27	OCA	A	5008	-	-	2/7/7/7	-
24	LHG	4	802	-	-	20/36/36/53	-
39	QTB	Z	504	-	1/1/5/10	6/11/28/28	0/1/1/1
20	CLA	K	1403	-	-	12/20/96/115	-
20	CLA	A	1119	-	-	19/39/115/115	-
20	CLA	1	606	-	-	15/35/111/115	-
20	CLA	3	618	-	-	11/17/93/115	-
20	CLA	A	1112	-	-	15/33/109/115	-
20	CLA	B	1238	-	-	15/39/115/115	-
20	CLA	7	606	-	-	15/29/105/115	-
20	CLA	4	605	-	-	14/39/115/115	-
20	CLA	1	604	-	-	13/33/109/115	-
20	CLA	6	606	-	-	18/39/115/115	-
20	CLA	4	607	-	-	10/27/103/115	-
20	CLA	6	615	-	-	14/35/111/115	-
20	CLA	7	605	14	-	19/35/111/115	-
20	CLA	3	605	-	-	11/39/115/115	-
20	CLA	5	603	-	-	10/29/105/115	-
37	CHL	1	610	-	-	4/20/96/117	-
35	SPH	7	804	-	-	11/21/21/21	-
20	CLA	8	604	-	-	13/36/112/115	-
20	CLA	B	1209	-	-	25/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LUT	5	502	-	-	2/29/67/67	0/2/2/2
20	CLA	B	1231	-	-	12/39/115/115	-
23	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
20	CLA	Z	603	-	-	12/21/97/115	-
20	CLA	7	608	-	-	8/13/89/115	-
20	CLA	4	612	-	-	9/21/97/115	-
23	BCR	A	4004	-	-	15/29/63/63	0/2/2/2
20	CLA	A	1123	-	-	13/39/115/115	-
20	CLA	A	1104	-	-	21/39/115/115	-
37	CHL	6	610	-	1/1/13/21	9/29/105/117	-
20	CLA	B	1216	-	-	22/39/115/115	-
20	CLA	A	1109	-	-	13/39/115/115	-
37	CHL	6	611	-	-	7/23/99/117	-
20	CLA	A	1140	-	-	19/39/115/115	-
20	CLA	8	612	-	-	9/17/93/115	-
20	CLA	8	601	15	-	13/33/109/115	-
37	CHL	3	611	-	1/1/15/21	7/41/117/117	-
20	CLA	B	1214	-	-	15/32/108/115	-
20	CLA	B	1219	-	-	17/32/108/115	-
20	CLA	B	1236	-	-	24/39/115/115	-
20	CLA	A	1139	1	-	15/39/115/115	-
20	CLA	5	605	-	-	14/27/103/115	-
20	CLA	A	1129	-	-	9/21/97/115	-
23	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
20	CLA	Z	605	-	-	12/39/115/115	-
35	SPH	K	5001	-	-	14/21/21/21	-
42	LPX	8	803	-	-	11/31/31/31	-
40	3PH	7	802	-	-	21/40/40/49	-
23	BCR	3	505	-	-	10/29/63/63	0/2/2/2
20	CLA	B	1203	-	-	19/39/115/115	-
20	CLA	A	1103	1	-	17/39/115/115	-
23	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
20	CLA	L	1502	-	-	26/39/115/115	-
23	BCR	K	4001	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	4	617	-	-	1/14/90/117	-
20	CLA	A	1110	1	-	20/39/115/115	-
37	CHL	Z	610	-	1/1/15/21	5/41/117/117	-
20	CLA	A	1132	-	-	20/39/115/115	-
24	LHG	3	801	-	-	12/22/22/53	-
20	CLA	B	1234	-	-	21/33/109/115	-
20	CLA	B	1204	-	-	15/39/115/115	-
20	CLA	F	1301	-	-	15/39/115/115	-
24	LHG	4	801	-	-	33/53/53/53	-
20	CLA	5	608	-	-	7/15/91/115	-
20	CLA	A	1117	-	-	19/39/115/115	-
37	CHL	5	611	-	-	3/23/99/117	-
20	CLA	3	603	-	-	18/39/115/115	-
20	CLA	1	612	-	-	24/39/115/115	-
23	BCR	7	504	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1237	-	-	20/39/115/115	-
20	CLA	7	616	-	-	13/33/109/115	-
20	CLA	A	1105	-	-	14/39/115/115	-
20	CLA	3	606	-	-	20/39/115/115	-
20	CLA	A	1013	-	-	18/39/115/115	-
37	CHL	6	617	-	-	2/14/90/117	-
20	CLA	B	1210	-	-	20/39/115/115	-
20	CLA	K	1402	-	-	16/27/103/115	-
20	CLA	B	1202	-	-	17/39/115/115	-
34	C7Z	5	505	-	1/1/12/26	12/29/67/67	0/2/2/2
20	CLA	B	1021	-	-	15/39/115/115	-
36	LUT	Z	502	-	-	1/29/67/67	0/2/2/2
37	CHL	Z	613	-	-	3/17/93/117	-
36	LUT	1	501	-	-	5/29/67/67	0/2/2/2
36	LUT	4	501	-	-	5/29/67/67	0/2/2/2
20	CLA	5	622	-	-	7/17/93/115	-
20	CLA	6	612	-	-	9/21/97/115	-
20	CLA	A	1124	-	-	16/39/115/115	-
20	CLA	6	618	-	-	10/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	613	-	-	7/27/103/115	-
20	CLA	4	606	-	-	11/21/97/115	-
20	CLA	4	615	-	-	2/10/86/115	-
20	CLA	A	1137	-	-	13/39/115/115	-
20	CLA	3	610	13	-	14/33/109/115	-
36	LUT	7	501	-	-	3/29/67/67	0/2/2/2
37	CHL	6	613	-	1/1/13/21	3/29/105/117	-
37	CHL	8	613	-	2/2/15/21	10/41/117/117	-
24	LHG	1	801	-	-	24/47/47/53	-
20	CLA	A	1133	1	-	16/39/115/115	-
20	CLA	B	1211	-	-	16/33/109/115	-
23	BCR	A	4005	-	-	15/29/63/63	0/2/2/2
23	BCR	J	4001	-	-	17/29/63/63	0/2/2/2
20	CLA	5	612	-	-	10/39/115/115	-
20	CLA	B	1220	-	-	21/39/115/115	-
23	BCR	3	504	-	-	11/29/63/63	0/2/2/2
20	CLA	5	607	-	-	15/35/111/115	-
20	CLA	1	602	-	-	5/15/91/115	-
40	3PH	6	802	-	-	15/30/30/49	-

The worst 5 of 1775 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	J	4002	C7Z	C25-C26	15.76	1.61	1.34
34	5	505	C7Z	C5-C6	15.72	1.61	1.34
34	1	503	C7Z	C25-C26	15.70	1.61	1.34
34	5	505	C7Z	C25-C26	15.69	1.61	1.34
34	1	503	C7Z	C5-C6	15.12	1.60	1.34

The worst 5 of 4679 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	504	BCR	C10-C11-C12	18.18	179.94	123.22
23	5	504	BCR	C16-C15-C14	17.70	159.73	123.47
23	K	4001	BCR	C10-C11-C12	17.63	178.24	123.22
23	A	4003	BCR	C10-C11-C12	17.47	177.75	123.22
23	B	4007	BCR	C10-C11-C12	17.47	177.72	123.22

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	F	4001	RRX	C28
34	J	4002	C7Z	C3
34	1	503	C7Z	C3
34	5	505	C7Z	C3
37	1	609	CHL	C8

5 of 4013 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1012	CLA	CHA-CBD-CGD-O1D
20	A	1012	CLA	CBD-CGD-O2D-CED
20	A	1012	CLA	C2-C3-C5-C6
20	A	1102	CLA	CBD-CGD-O2D-CED
20	A	1104	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

264 monomers are involved in 581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	7	609	CLA	1	0
23	6	504	BCR	2	0
24	7	801	LHG	2	0
20	6	609	CLA	9	0
36	5	501	LUT	3	0
20	8	606	CLA	1	0
36	6	502	LUT	1	0
20	1	605	CLA	2	0
26	A	5006	LMT	2	0
23	B	4003	BCR	1	0
20	B	1229	CLA	2	0
30	A	5005	DGA	5	0
23	3	506	BCR	2	0
20	3	607	CLA	2	0
23	5	504	BCR	1	0
20	A	1106	CLA	7	0
20	A	1128	CLA	3	0
23	3	503	BCR	2	0
24	6	801	LHG	4	0
20	A	1116	CLA	5	0
20	5	613	CLA	1	0
20	A	1118	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1122	CLA	3	0
20	A	1012	CLA	7	0
20	B	1222	CLA	3	0
37	7	610	CHL	2	0
20	1	601	CLA	5	0
20	A	1113	CLA	4	0
20	1	613	CLA	3	0
20	7	601	CLA	4	0
20	A	1136	CLA	2	0
20	A	1107	CLA	4	0
23	B	4001	BCR	5	0
26	B	6101	LMT	1	0
20	B	1240	CLA	5	0
20	5	606	CLA	1	0
20	5	601	CLA	4	0
20	7	613	CLA	3	0
20	6	605	CLA	2	0
20	B	1221	CLA	4	0
20	1	608	CLA	2	0
20	1	611	CLA	3	0
36	3	501	LUT	6	0
20	4	608	CLA	1	0
36	Z	503	LUT	2	0
20	B	1206	CLA	2	0
20	6	608	CLA	6	0
20	8	608	CLA	1	0
20	B	1212	CLA	1	0
20	1	615	CLA	3	0
20	Z	604	CLA	4	0
20	7	611	CLA	1	0
20	B	1223	CLA	1	0
20	A	1127	CLA	5	0
20	3	604	CLA	3	0
24	8	801	LHG	2	0
20	A	1114	CLA	5	0
37	1	609	CHL	3	0
23	4	503	BCR	1	0
20	3	602	CLA	1	0
20	8	607	CLA	5	0
20	A	1111	CLA	6	0
20	B	1023	CLA	4	0
23	8	503	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1115	CLA	2	0
20	K	1404	CLA	1	0
19	A	1011	CL0	3	0
37	Z	609	CHL	4	0
35	7	803	SPH	1	0
20	7	602	CLA	1	0
23	G	4001	BCR	3	0
20	4	602	CLA	2	0
20	B	1218	CLA	5	0
20	3	601	CLA	5	0
23	7	503	BCR	2	0
20	6	619	CLA	4	0
20	8	602	CLA	3	0
20	A	1125	CLA	4	0
20	B	1241	CLA	2	0
37	5	617	CHL	1	0
23	5	503	BCR	2	0
20	B	1205	CLA	3	0
20	8	611	CLA	1	0
20	4	601	CLA	5	0
20	A	1102	CLA	1	0
23	B	4005	BCR	2	0
20	1	603	CLA	2	0
24	A	5001	LHG	1	0
20	6	604	CLA	3	0
20	6	603	CLA	3	0
20	7	603	CLA	2	0
20	8	603	CLA	3	0
20	B	1213	CLA	2	0
22	C	3003	SF4	1	0
26	B	5005	LMT	1	0
20	B	1224	CLA	6	0
20	B	1232	CLA	1	0
20	7	604	CLA	1	0
20	B	1217	CLA	1	0
36	6	501	LUT	4	0
26	4	803	LMT	2	0
20	3	612	CLA	3	0
20	8	605	CLA	2	0
20	A	1138	CLA	3	0
36	Z	501	LUT	1	0
20	A	1126	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	609	CLA	4	0
20	A	1101	CLA	3	0
20	5	604	CLA	5	0
20	B	1225	CLA	7	0
20	B	1226	CLA	7	0
20	A	1120	CLA	3	0
20	4	604	CLA	3	0
20	5	609	CLA	3	0
20	B	1022	CLA	1	0
25	3	802	NKP	1	0
31	B	5003	DGD	5	0
37	8	610	CHL	1	0
20	B	1215	CLA	3	0
23	A	4002	BCR	4	0
33	F	4001	RRX	4	0
20	F	1302	CLA	5	0
26	1	803	LMT	1	0
36	1	502	LUT	2	0
20	6	601	CLA	6	0
36	4	502	LUT	4	0
20	8	609	CLA	2	0
24	5	801	LHG	1	0
38	1	802	SQD	1	0
37	4	613	CHL	1	0
37	5	610	CHL	5	0
36	7	502	LUT	1	0
20	A	1135	CLA	1	0
37	4	610	CHL	1	0
20	1	607	CLA	1	0
23	B	4007	BCR	1	0
20	Z	606	CLA	2	0
26	8	805	LMT	2	0
23	B	4004	BCR	3	0
20	7	607	CLA	3	0
20	A	1121	CLA	2	0
23	K	4002	BCR	3	0
20	Z	601	CLA	3	0
24	B	5006	LHG	2	0
20	A	1130	CLA	2	0
21	B	2002	PQN	1	0
23	L	4002	BCR	2	0
23	6	503	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1207	CLA	5	0
20	7	612	CLA	1	0
20	5	618	CLA	4	0
20	B	1227	CLA	4	0
20	5	615	CLA	1	0
20	7	615	CLA	5	0
20	B	1230	CLA	3	0
23	L	4001	BCR	4	0
20	Z	608	CLA	2	0
20	Z	611	CLA	1	0
20	6	602	CLA	1	0
36	8	502	LUT	1	0
24	A	5002	LHG	3	0
36	8	501	LUT	4	0
20	Z	615	CLA	2	0
20	K	1401	CLA	5	0
23	I	4001	BCR	2	0
20	B	1235	CLA	6	0
20	B	1239	CLA	3	0
36	3	502	LUT	5	0
20	4	603	CLA	4	0
20	G	1602	CLA	2	0
20	B	1208	CLA	1	0
23	B	4002	BCR	5	0
24	B	5001	LHG	1	0
24	4	802	LHG	1	0
20	A	1119	CLA	4	0
20	1	606	CLA	2	0
20	A	1112	CLA	5	0
20	B	1238	CLA	5	0
20	7	606	CLA	3	0
20	1	604	CLA	3	0
20	6	606	CLA	2	0
20	4	607	CLA	1	0
20	6	615	CLA	4	0
20	7	605	CLA	1	0
20	3	605	CLA	1	0
20	5	603	CLA	1	0
37	1	610	CHL	1	0
35	7	804	SPH	2	0
20	8	604	CLA	2	0
20	B	1209	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	502	LUT	8	0
23	A	4001	BCR	2	0
20	Z	603	CLA	1	0
20	7	608	CLA	1	0
20	4	612	CLA	1	0
23	A	4004	BCR	3	0
20	A	1123	CLA	3	0
20	A	1104	CLA	3	0
37	6	610	CHL	1	0
20	B	1216	CLA	3	0
20	A	1109	CLA	3	0
20	A	1140	CLA	3	0
20	8	612	CLA	1	0
20	8	601	CLA	5	0
37	3	611	CHL	4	0
20	B	1214	CLA	4	0
20	B	1236	CLA	4	0
20	A	1139	CLA	4	0
20	5	605	CLA	1	0
20	A	1129	CLA	2	0
23	B	4006	BCR	4	0
20	Z	605	CLA	5	0
35	K	5001	SPH	2	0
40	7	802	3PH	5	0
23	3	505	BCR	2	0
20	B	1203	CLA	6	0
20	A	1103	CLA	5	0
23	A	4003	BCR	4	0
20	L	1502	CLA	3	0
23	K	4001	BCR	2	0
37	4	617	CHL	1	0
20	A	1110	CLA	3	0
37	Z	610	CHL	3	0
20	A	1132	CLA	2	0
20	B	1234	CLA	3	0
20	B	1204	CLA	1	0
20	F	1301	CLA	4	0
24	4	801	LHG	3	0
20	A	1117	CLA	4	0
37	5	611	CHL	1	0
20	3	603	CLA	2	0
20	1	612	CLA	3	0

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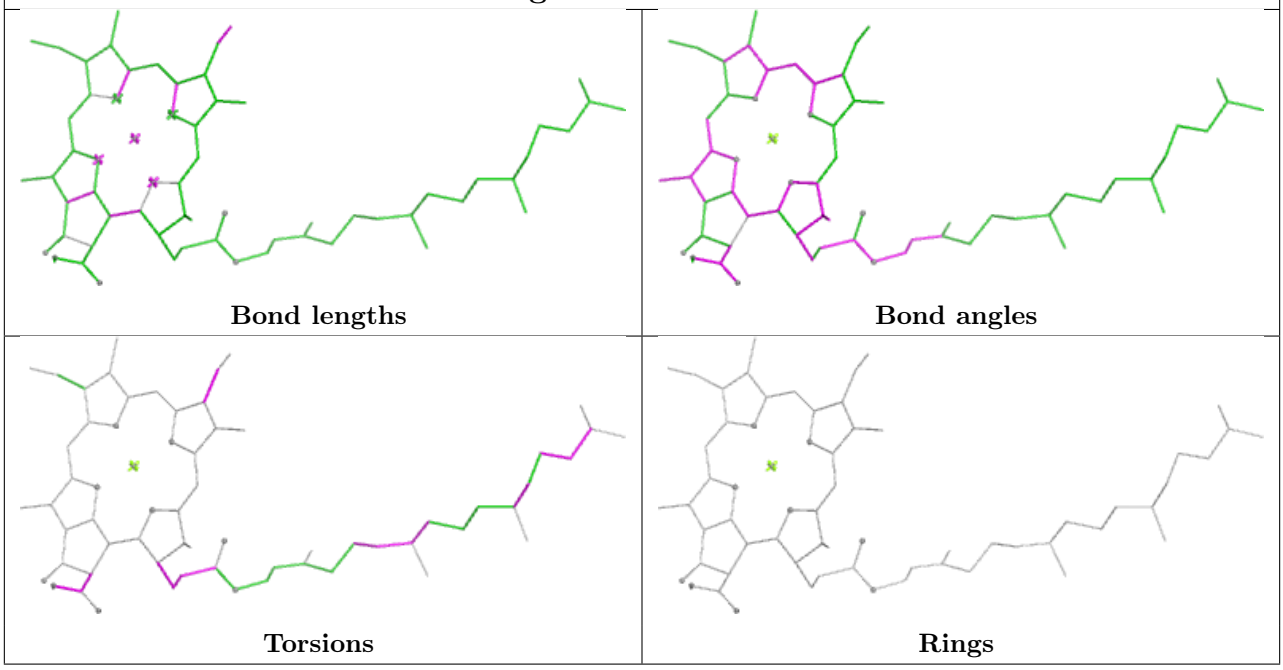
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	7	504	BCR	3	0
20	B	1237	CLA	1	0
20	7	616	CLA	5	0
20	A	1105	CLA	3	0
20	3	606	CLA	2	0
20	A	1013	CLA	7	0
37	6	617	CHL	1	0
20	B	1210	CLA	4	0
20	K	1402	CLA	2	0
20	B	1202	CLA	1	0
20	B	1021	CLA	5	0
36	Z	502	LUT	1	0
37	Z	613	CHL	3	0
36	1	501	LUT	2	0
36	4	501	LUT	5	0
20	5	622	CLA	1	0
20	6	612	CLA	2	0
20	A	1124	CLA	6	0
20	3	613	CLA	3	0
20	A	1137	CLA	2	0
20	3	610	CLA	3	0
37	6	613	CHL	3	0
37	8	613	CHL	4	0
24	1	801	LHG	2	0
20	A	1133	CLA	2	0
20	B	1211	CLA	1	0
23	A	4005	BCR	6	0
23	J	4001	BCR	3	0
20	5	612	CLA	2	0
20	B	1220	CLA	4	0
23	3	504	BCR	3	0
20	5	607	CLA	2	0

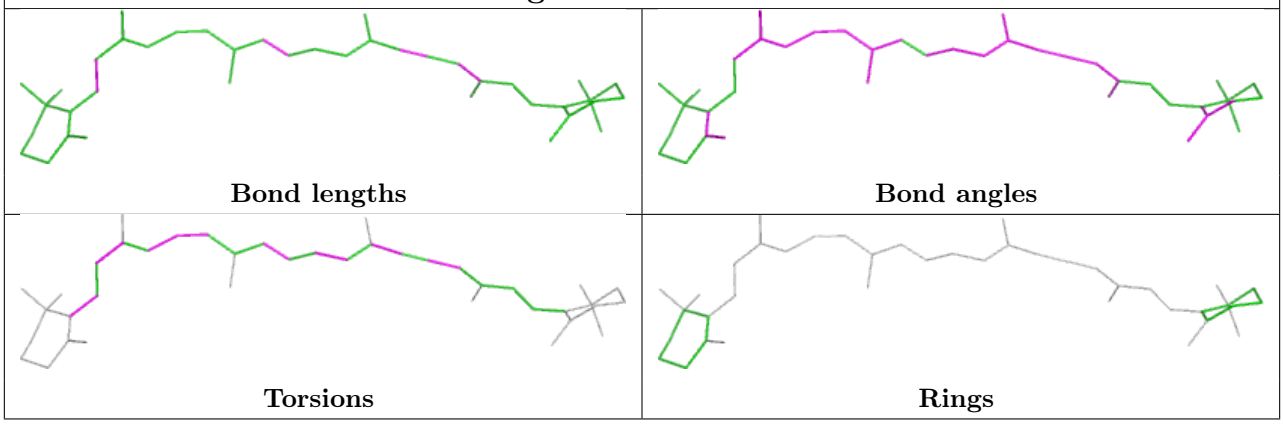
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

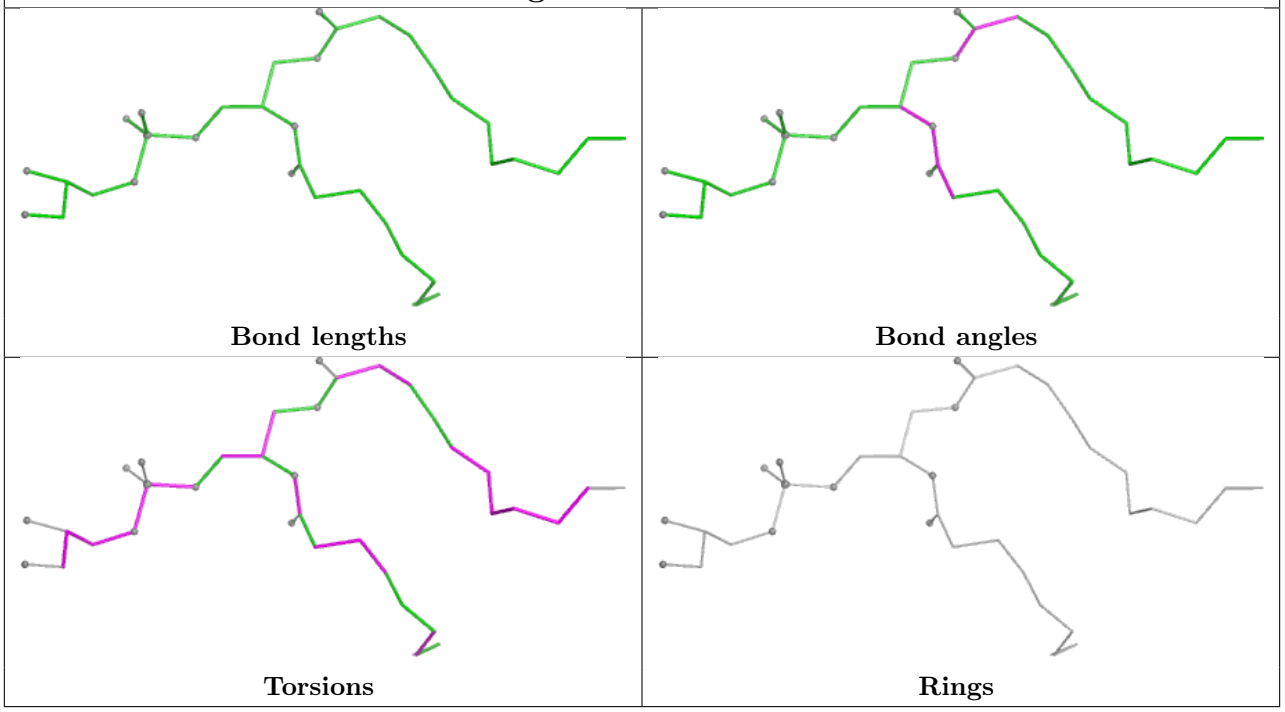
Ligand CLA 7 609



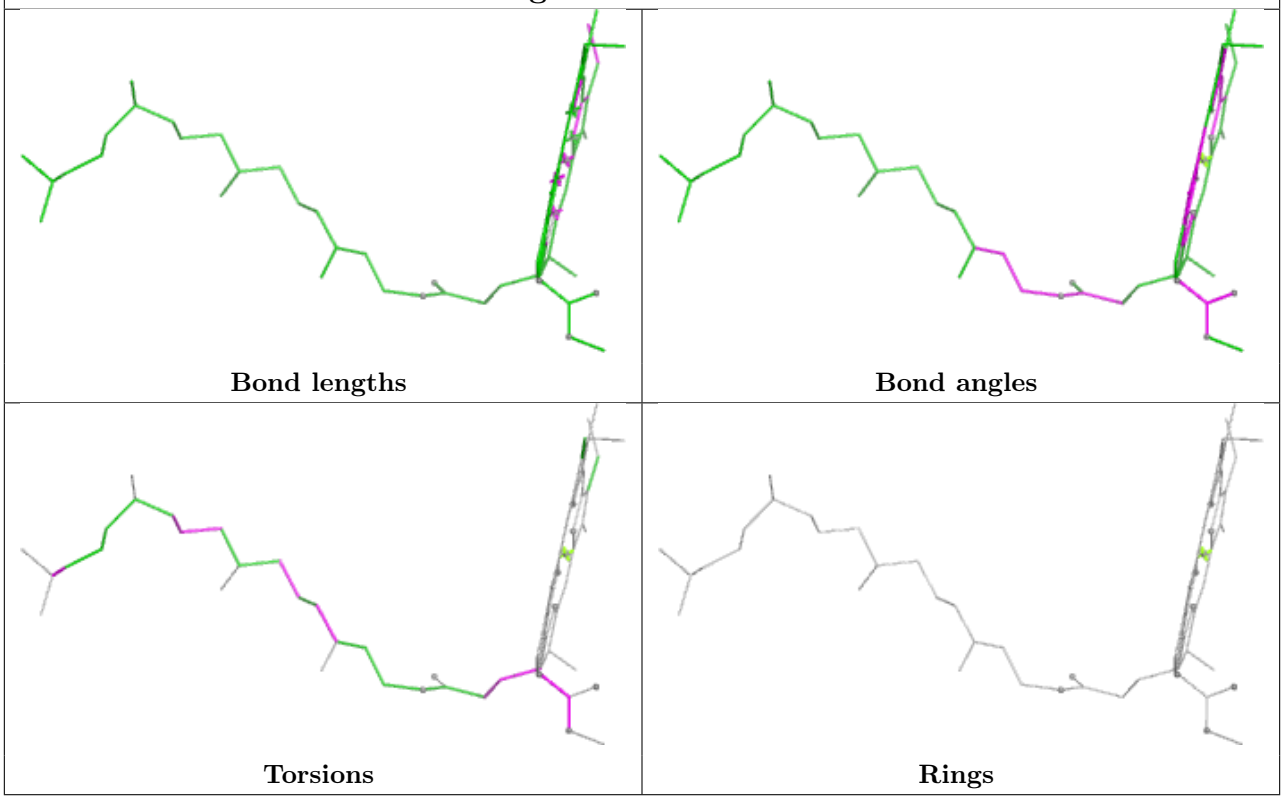
Ligand BCR 6 504



Ligand LHG 7 801



Ligand CLA 6 609



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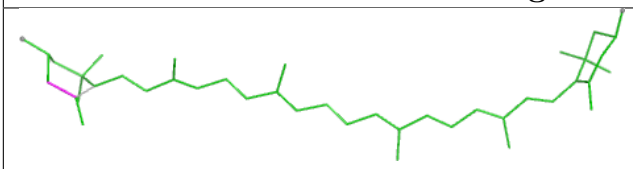
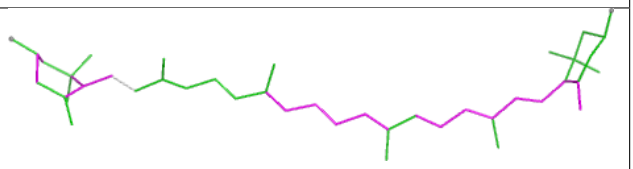
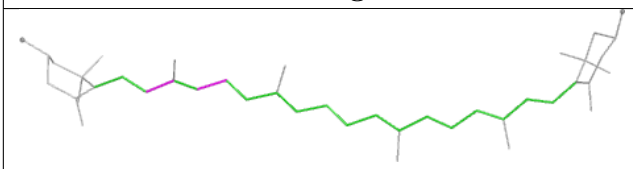


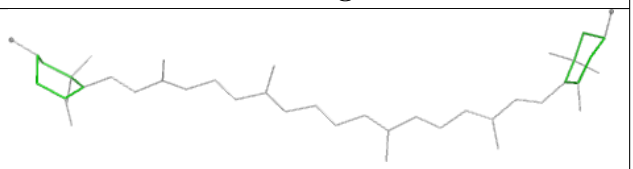
Bond lengths



Bond angles

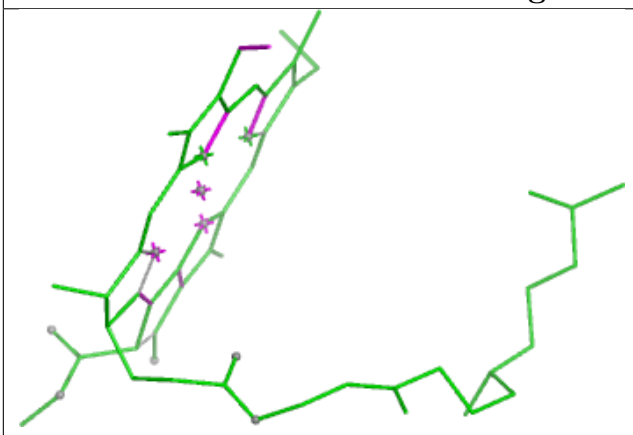


Torsions



Rings

Ligand CLA 8 606



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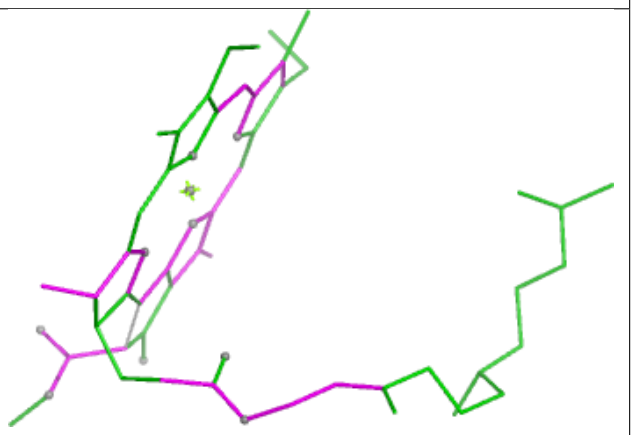


Bond angles

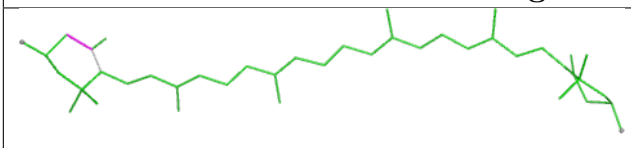


Torsions



Rings

Ligand LUT 6 502



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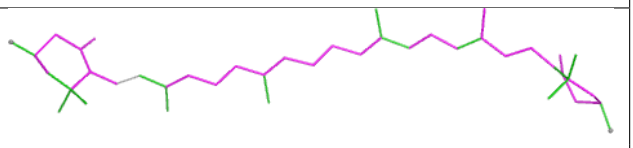
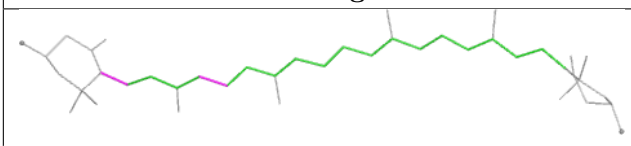


Bond angles



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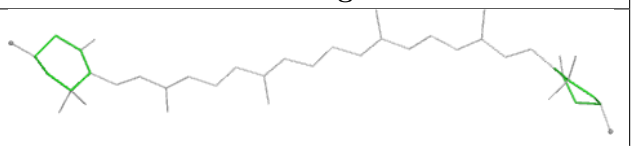
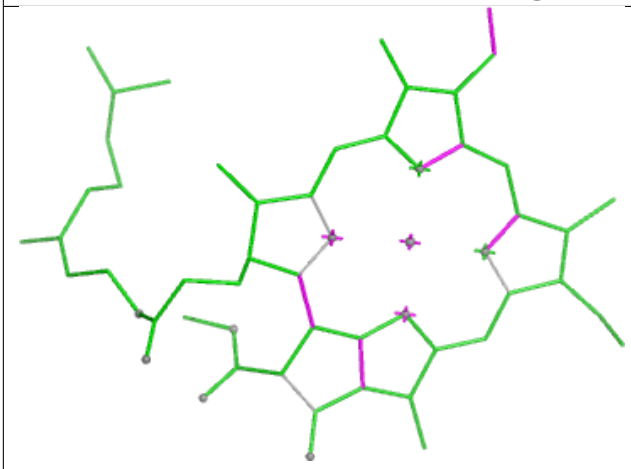


Rings

Ligand CLA 1 605



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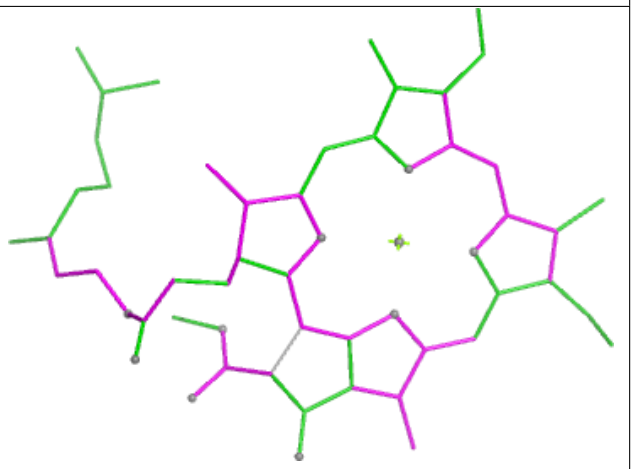
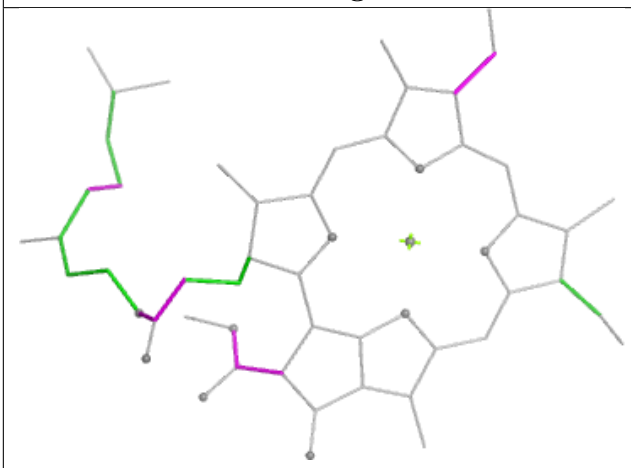
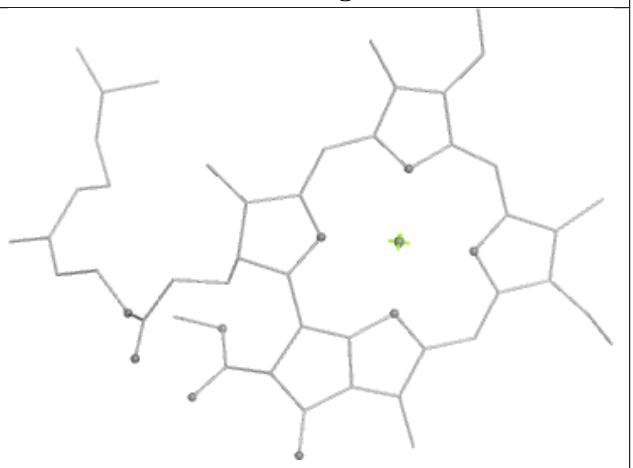


Bond angles

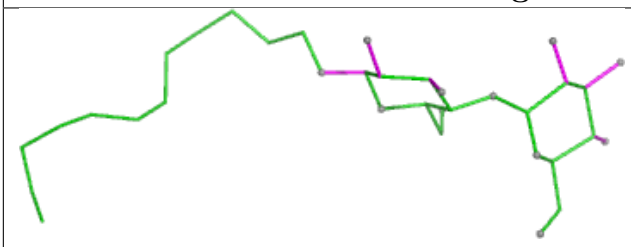


Torsions



Rings

Ligand LMT A 5006



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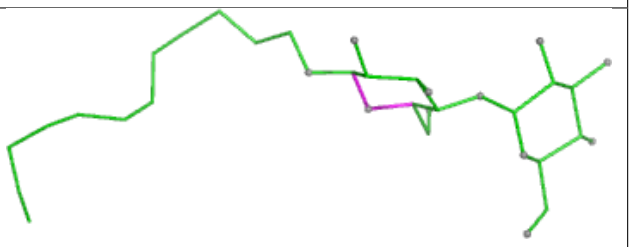
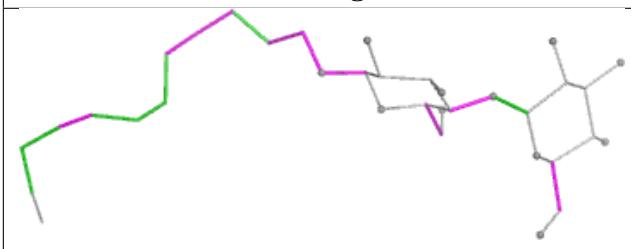


Bond angles



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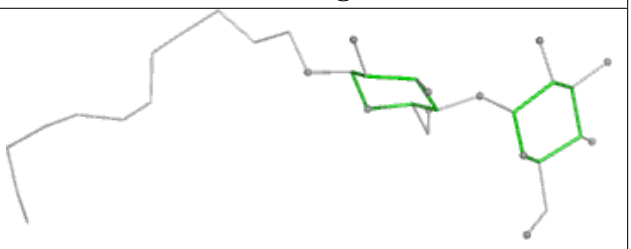
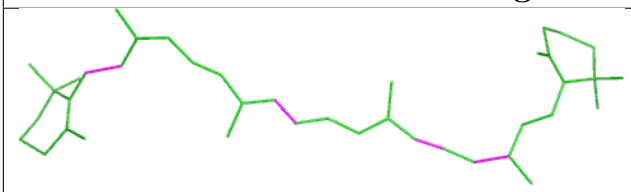


Rings

Ligand BCR B 4003



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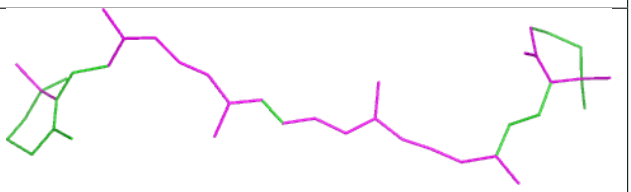
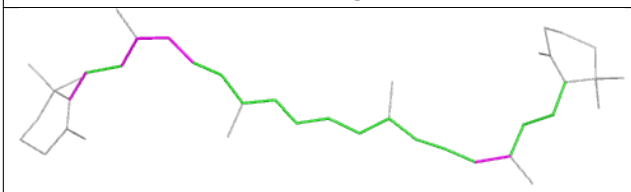


Bond angles



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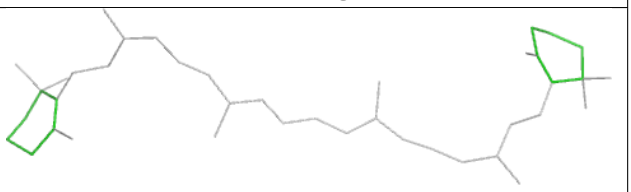
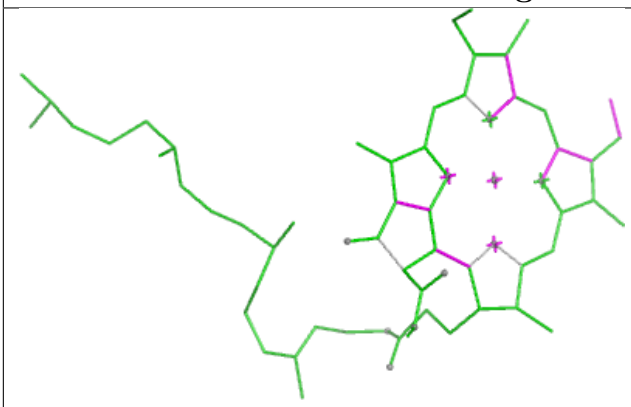


Rings

Ligand CLA B 1229



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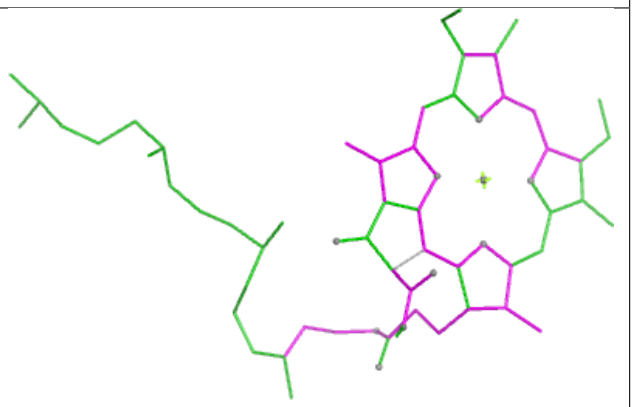
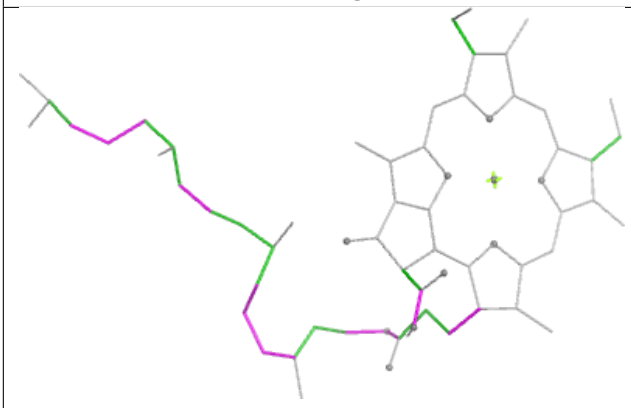


Bond angles



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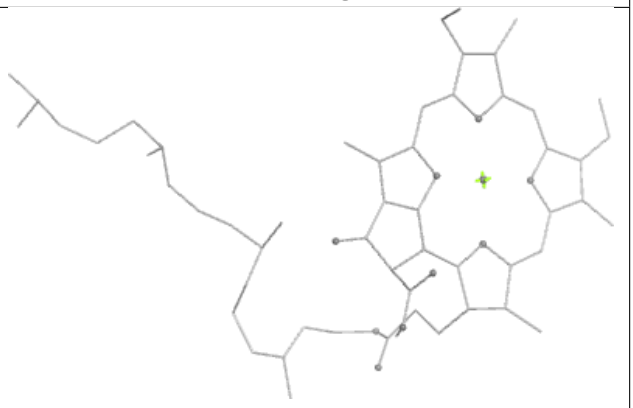
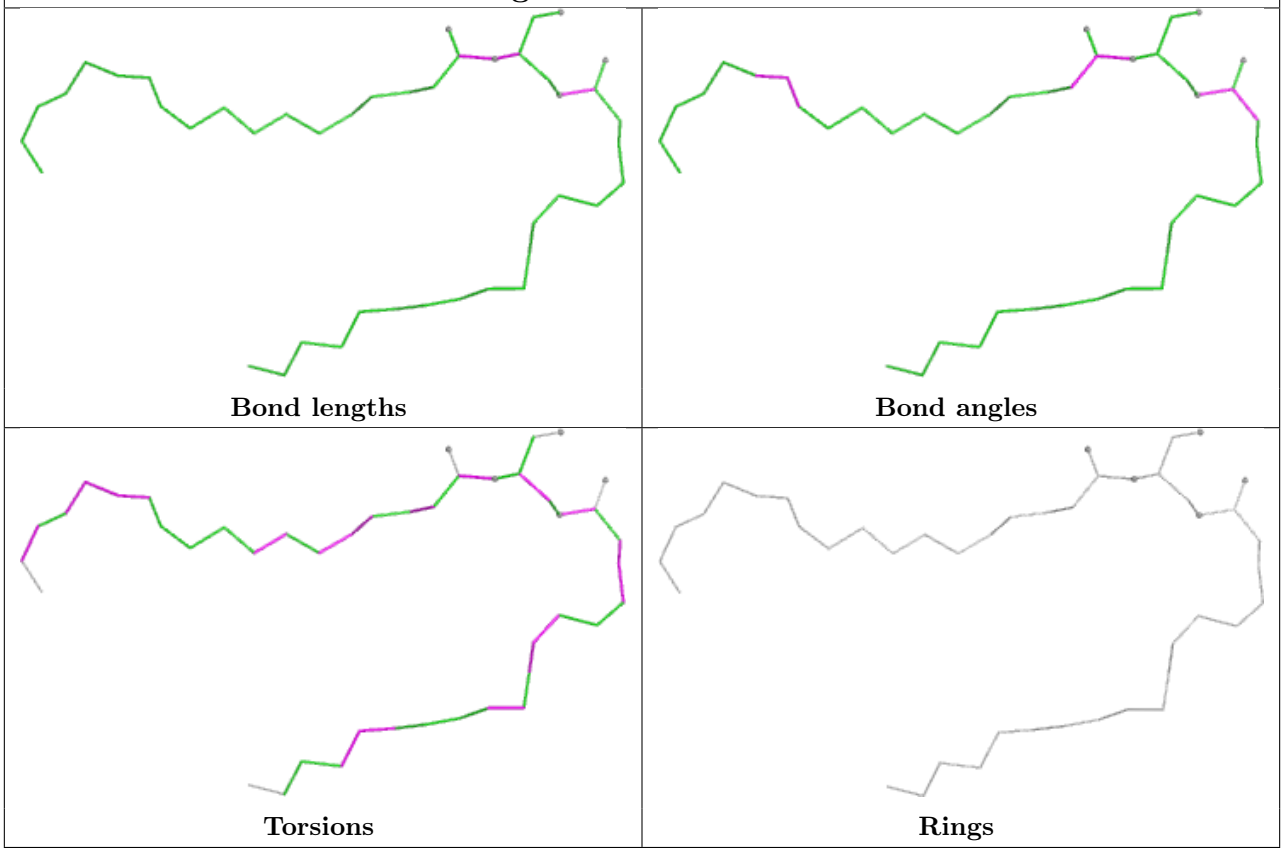
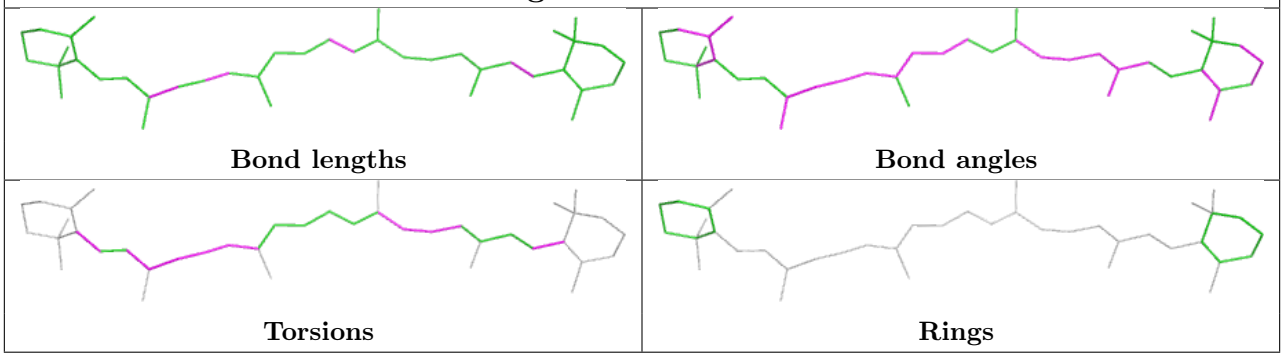


Rings

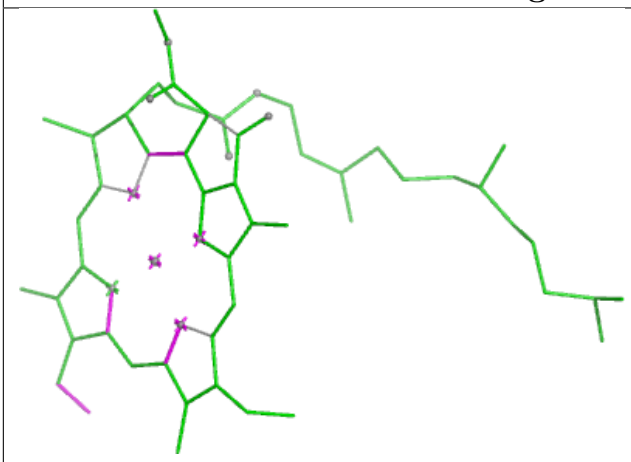
Ligand DGA A 5005



Ligand BCR 3 506



Ligand CLA 3 607



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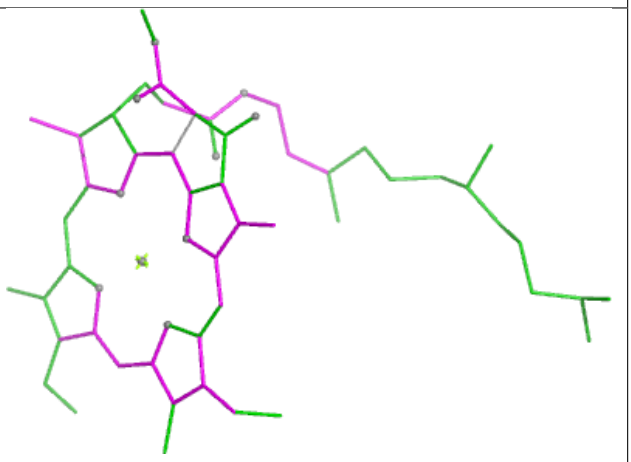
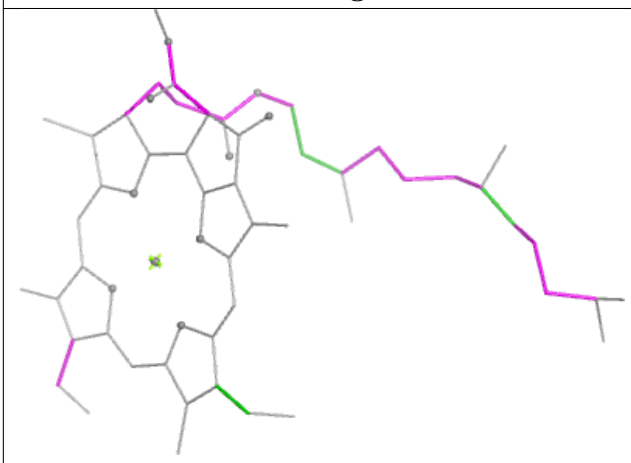


Bond angles

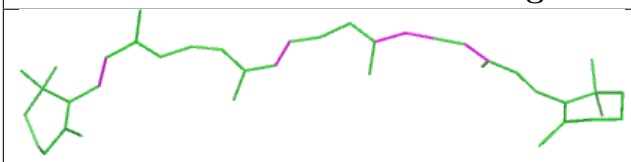


Torsions



Rings

Ligand BCR 5 504



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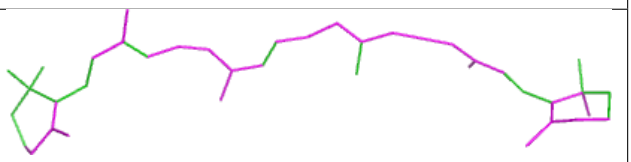
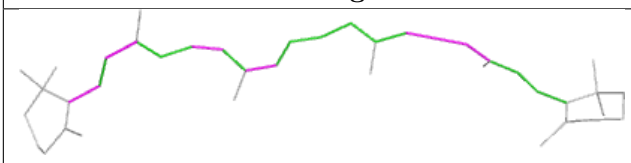


Bond angles



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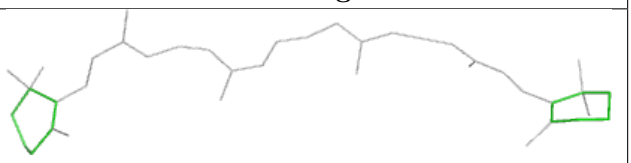
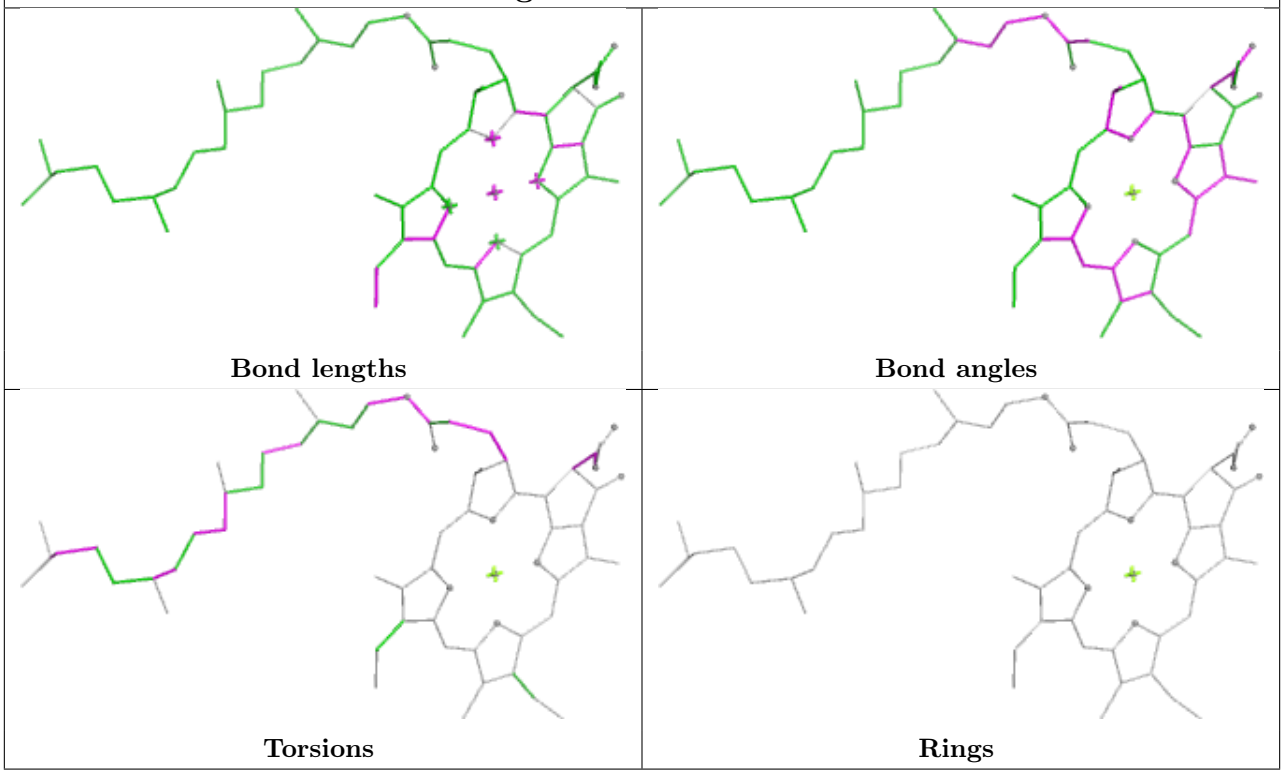


Rings

Ligand CLA A 1106



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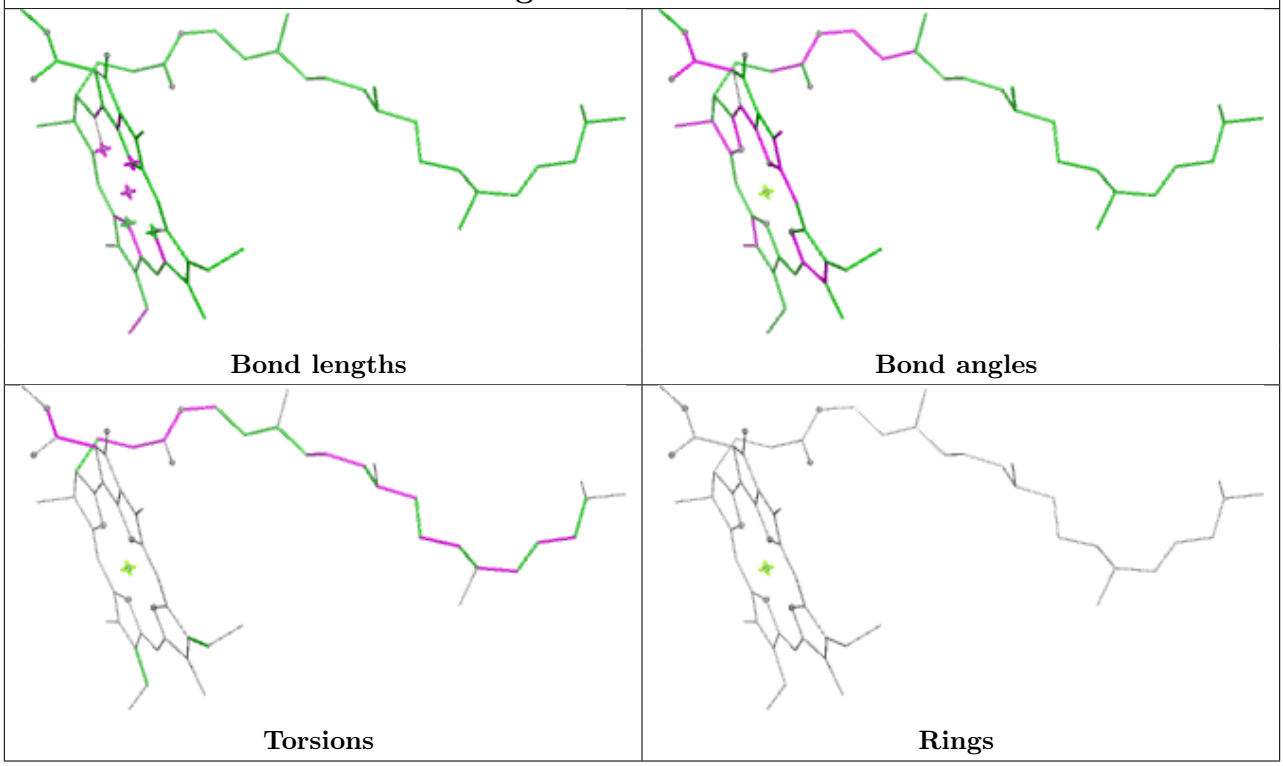

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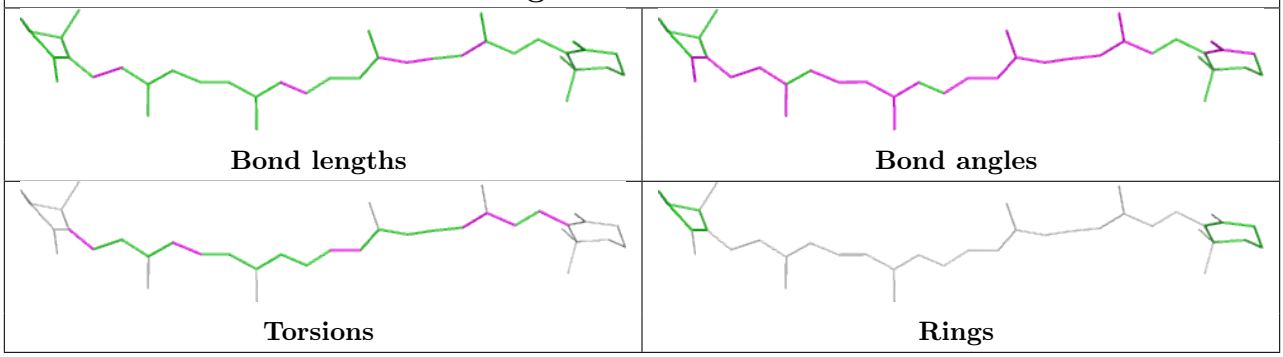
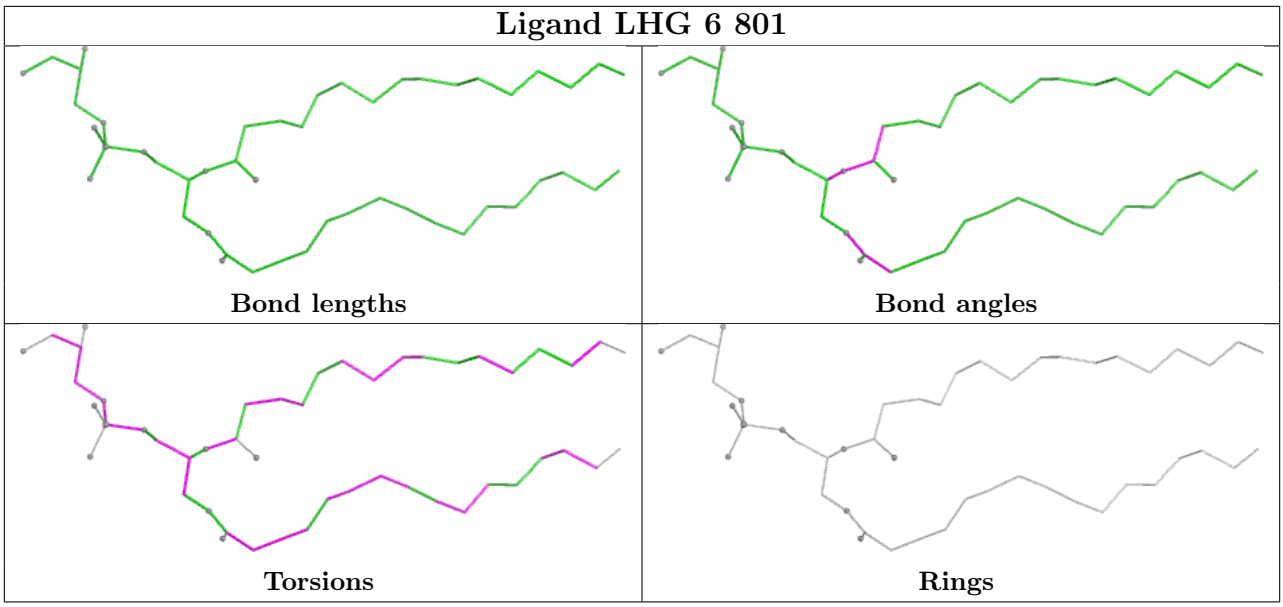


Ligand LHG 6 801



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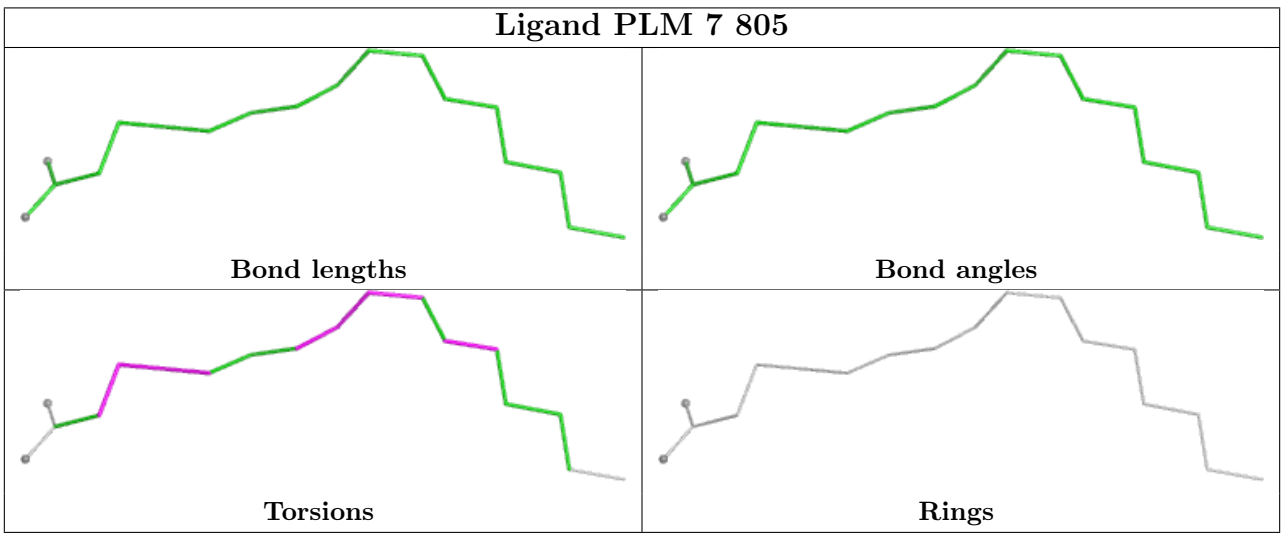
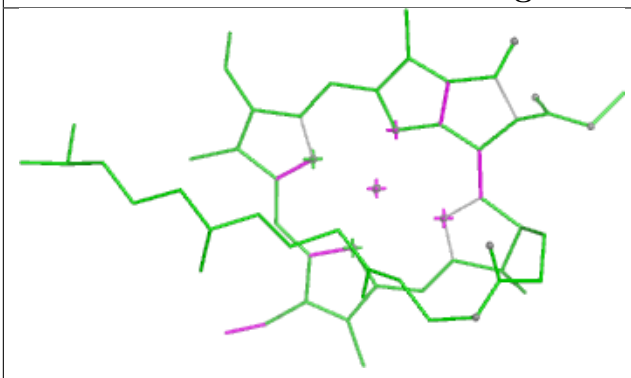
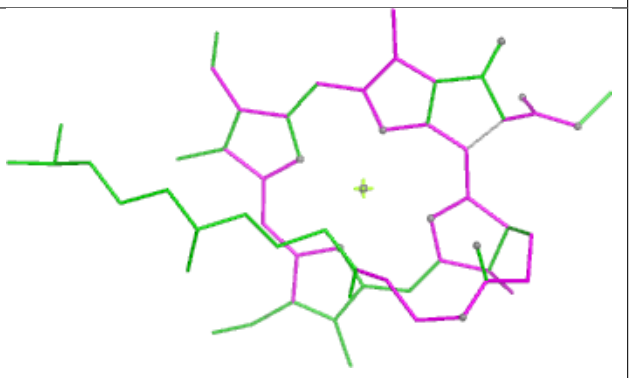


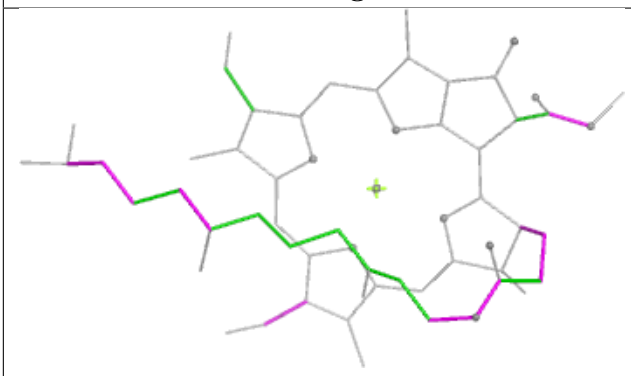
Ligand CLA A 1116



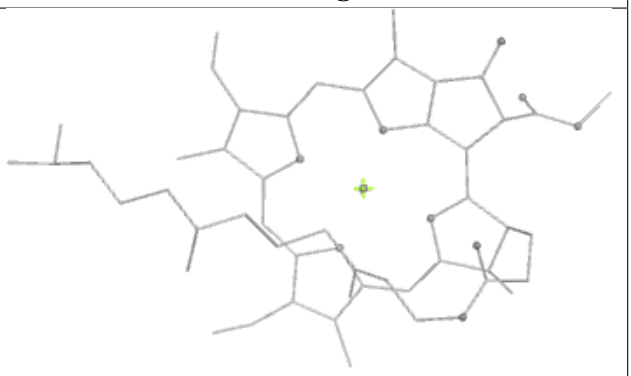
Bond lengths



Bond angles

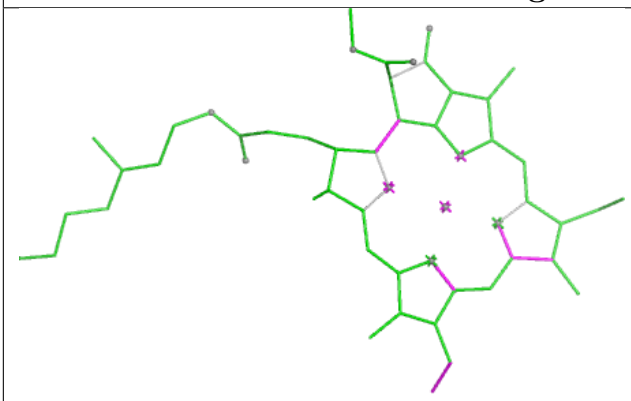


Torsions



Rings

Ligand CLA 5 613



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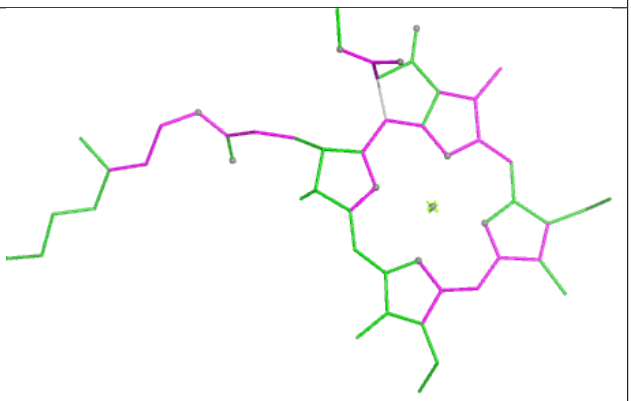
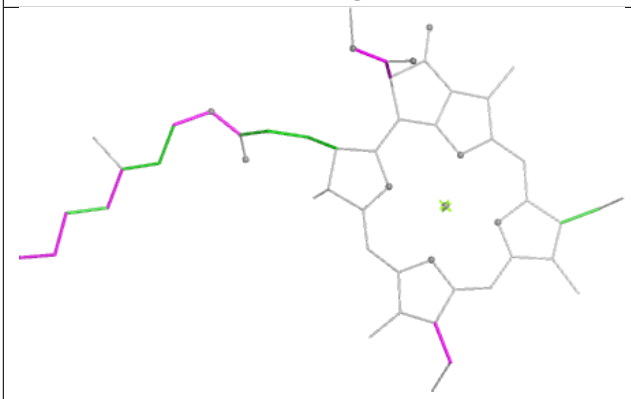


Bond angles



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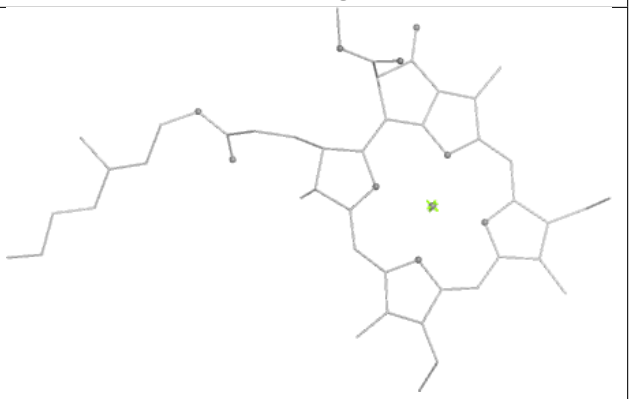
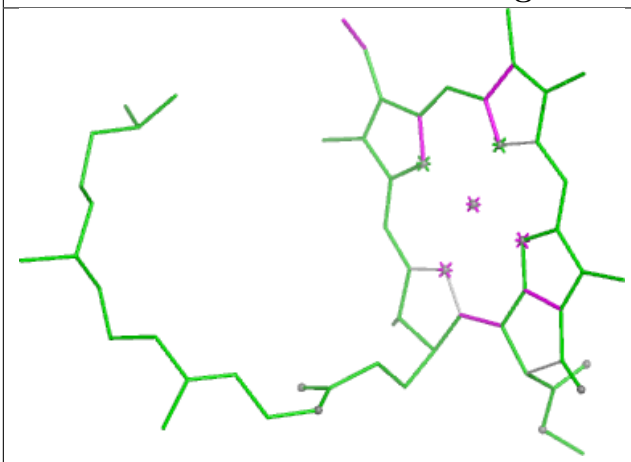
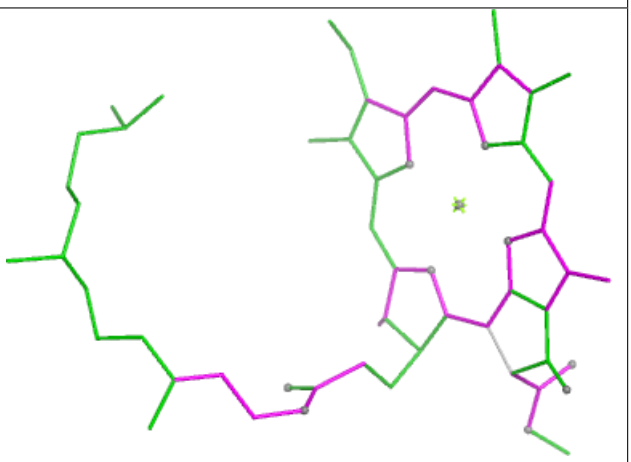


Rings

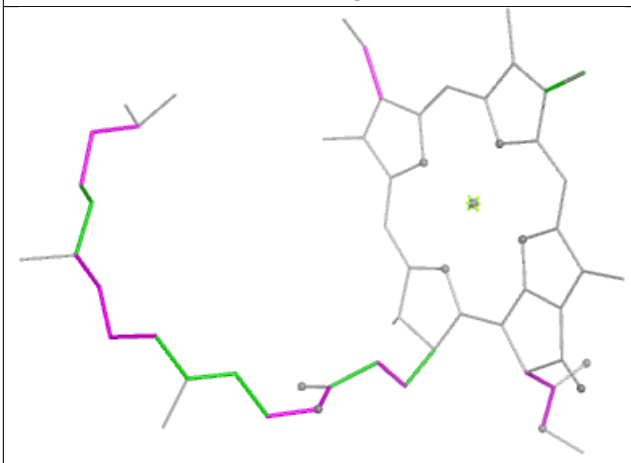
Ligand CLA A 1118



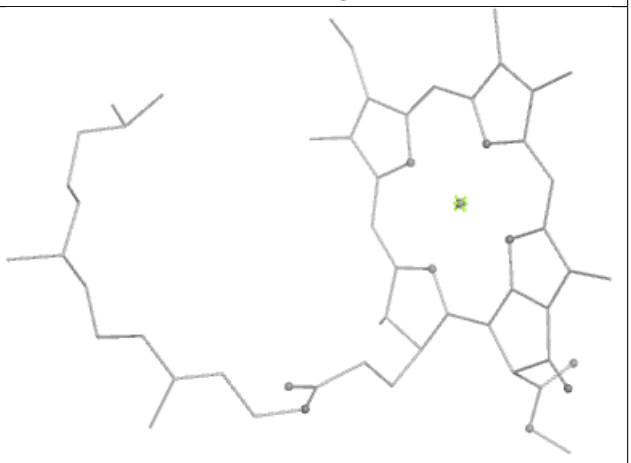
Bond lengths



Bond angles

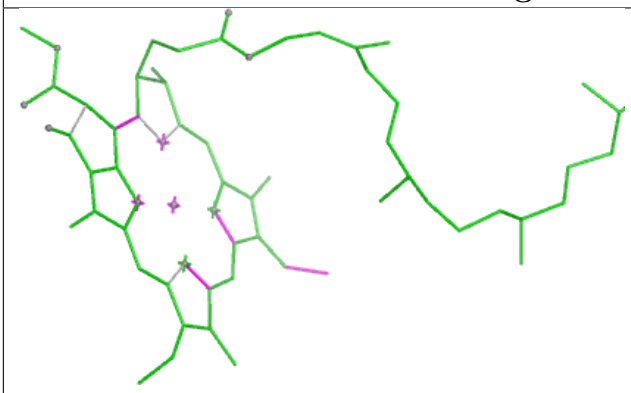


Torsions

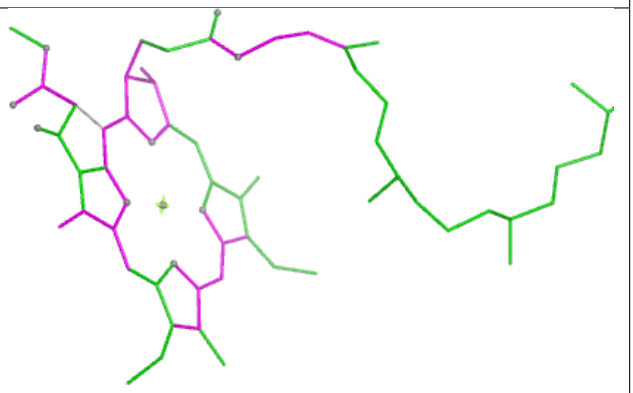


Rings

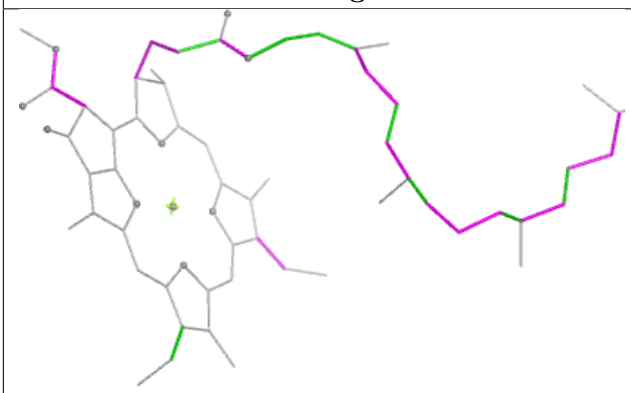
Ligand CLA A 1122



Bond lengths



Bond angles

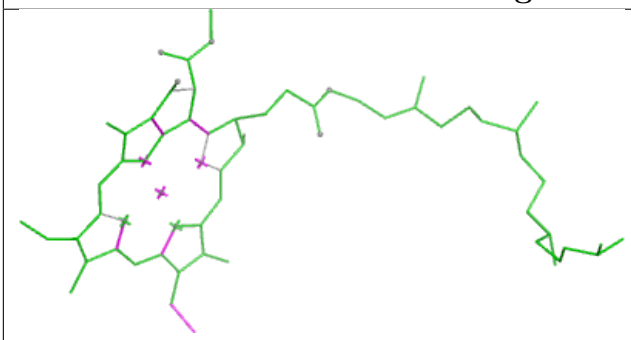


Torsions

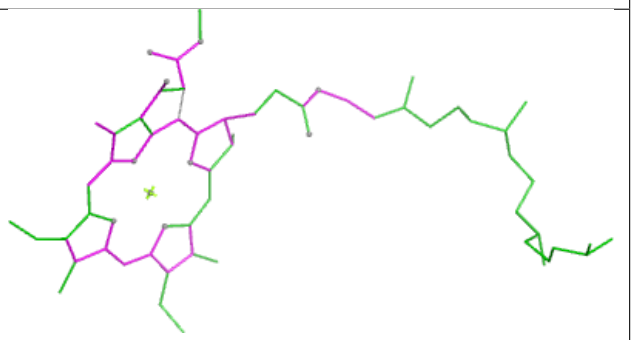


Rings

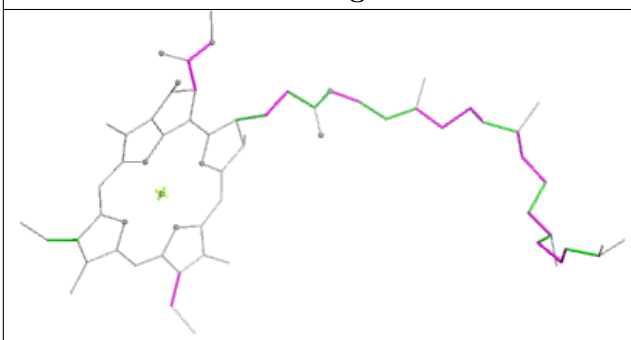
Ligand CLA A 1012



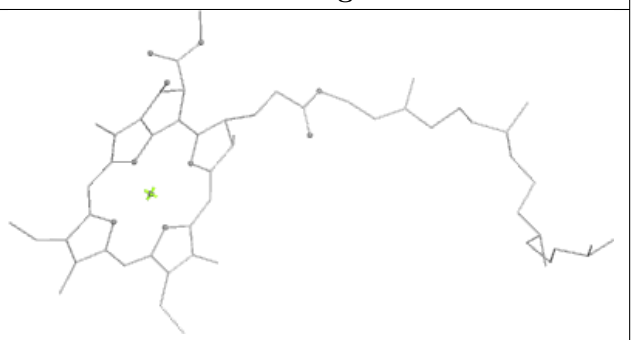
Bond lengths



Bond angles

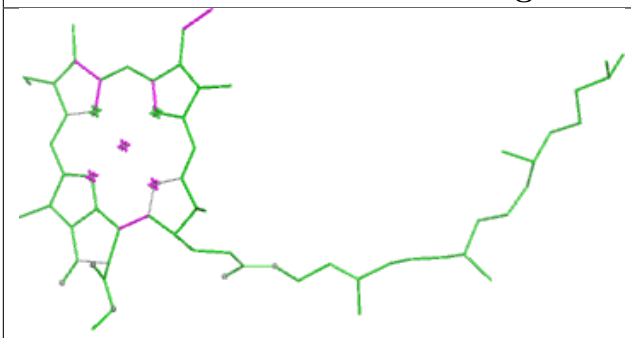


Torsions



Rings

Ligand CLA B 1222



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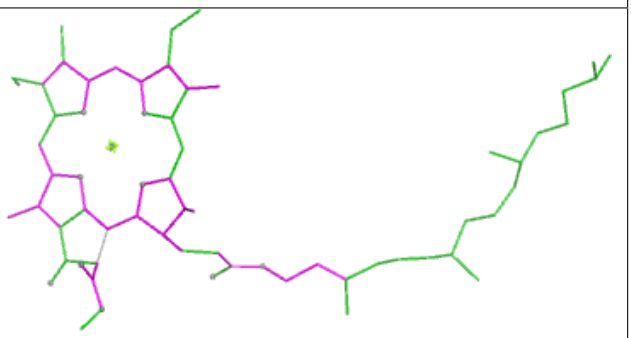

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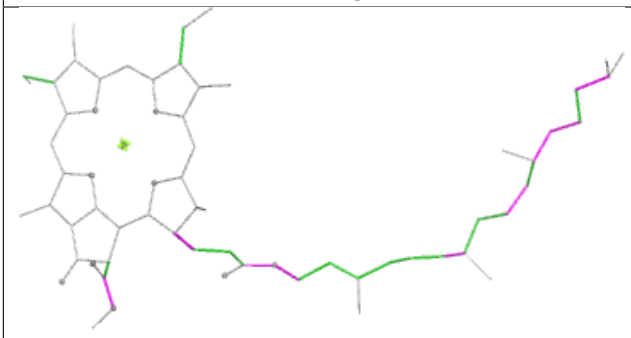

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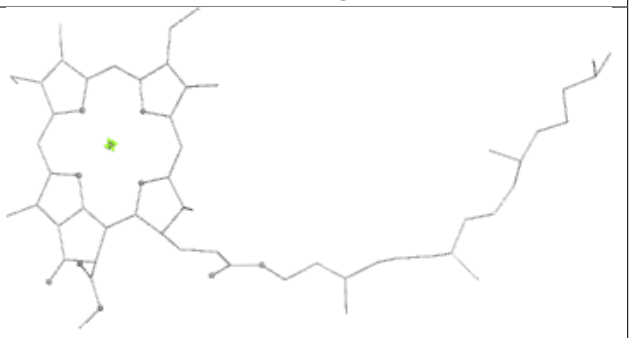
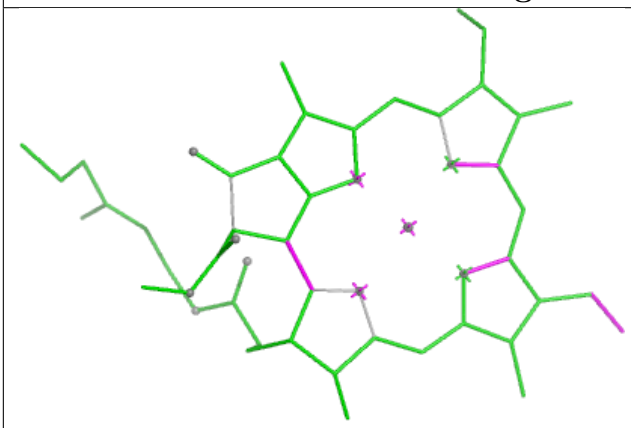


Rings

Ligand CLA A 1141



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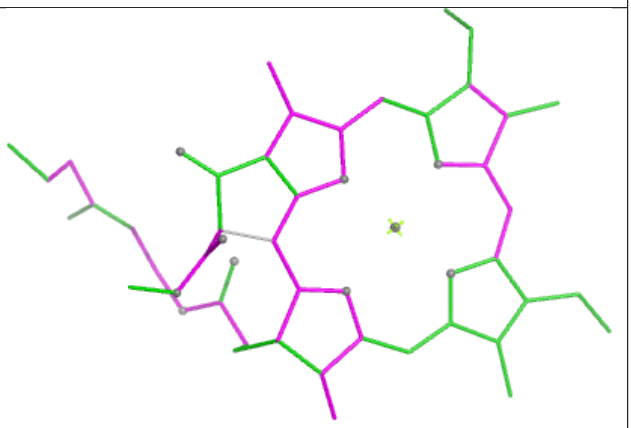

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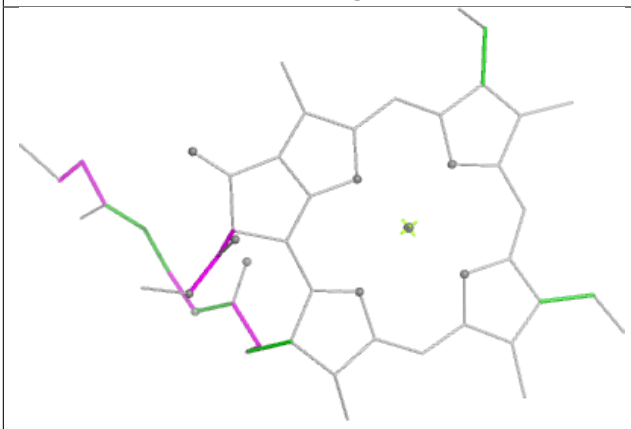

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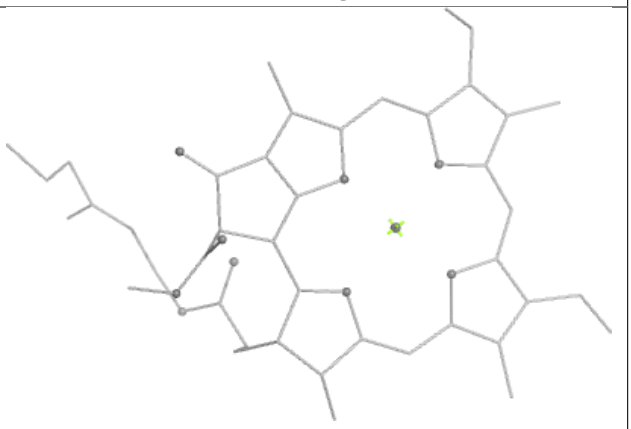
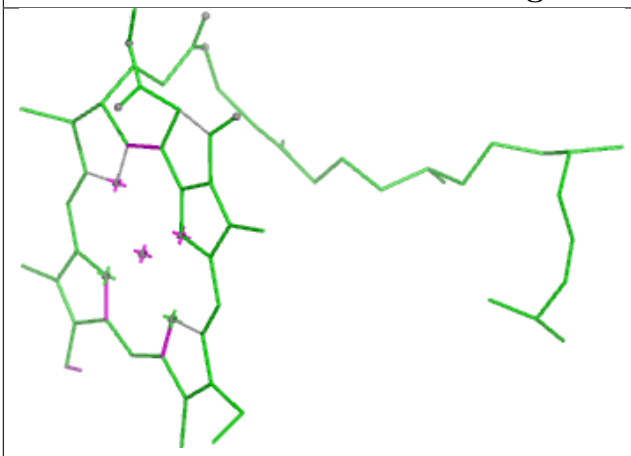


Rings

Ligand CLA Z 612



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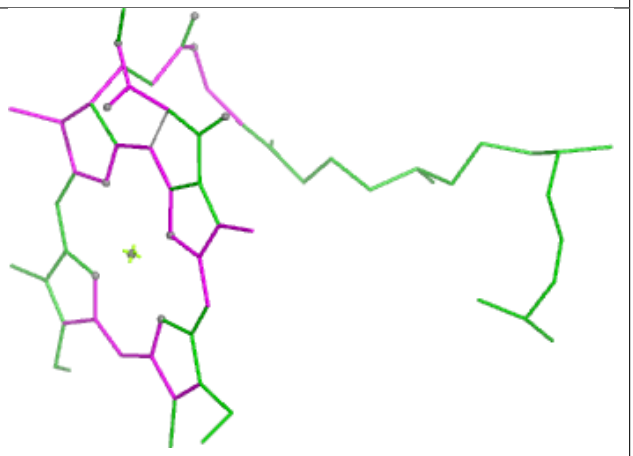
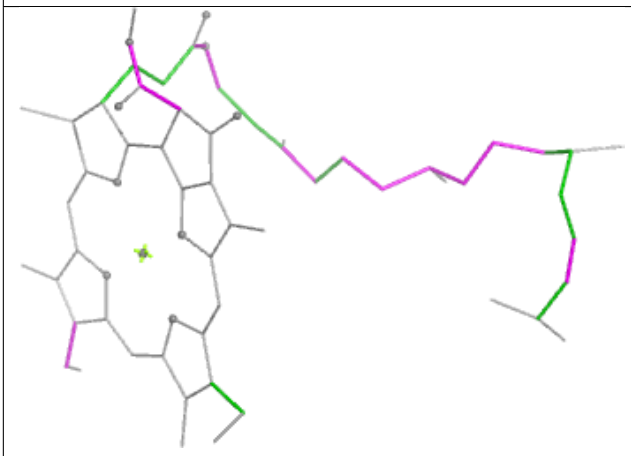


Bond angles

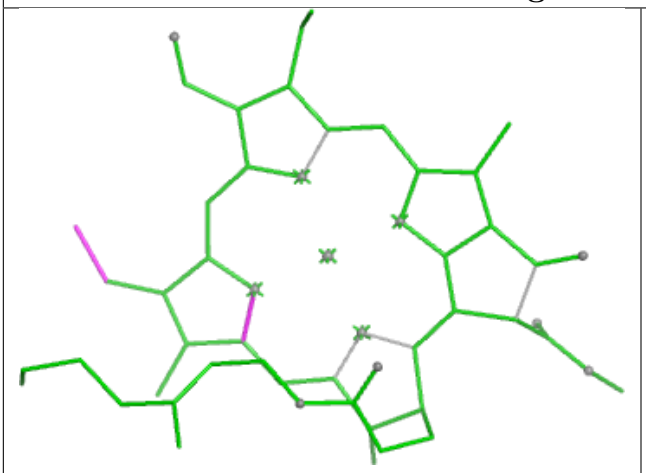


Torsions



Rings

Ligand CHL 7 610



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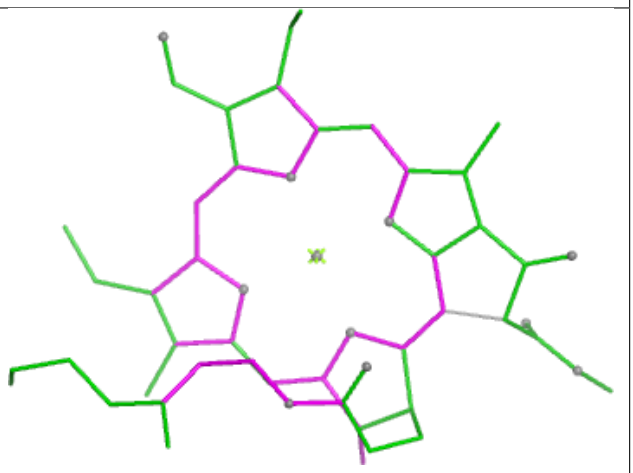
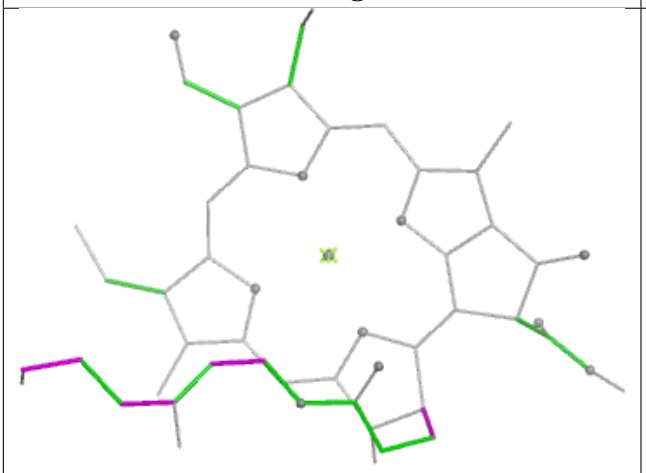


Bond angles



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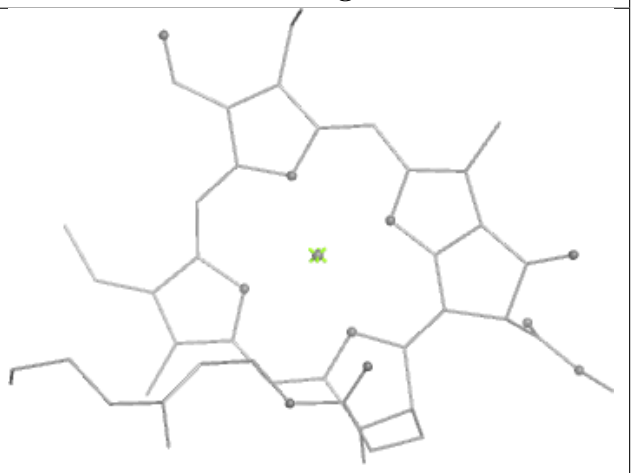
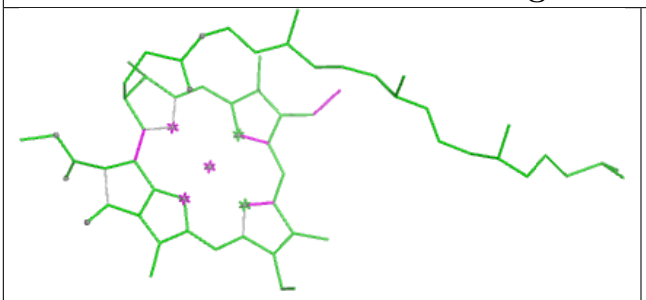


Rings

Ligand CLA 1 601



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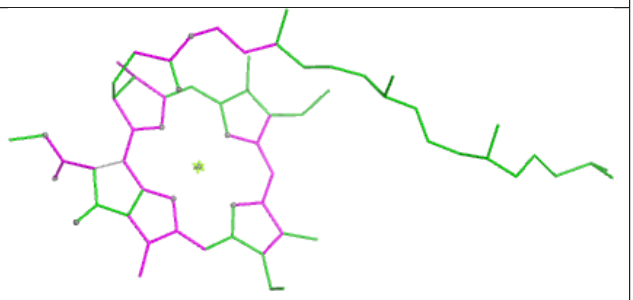

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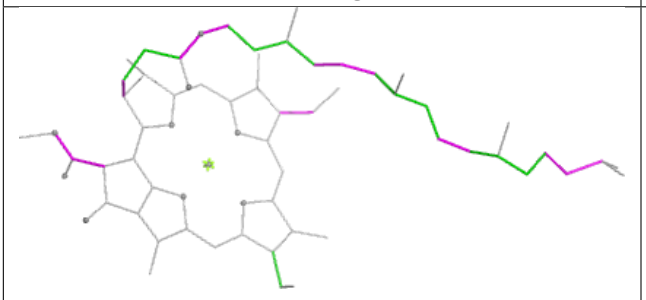

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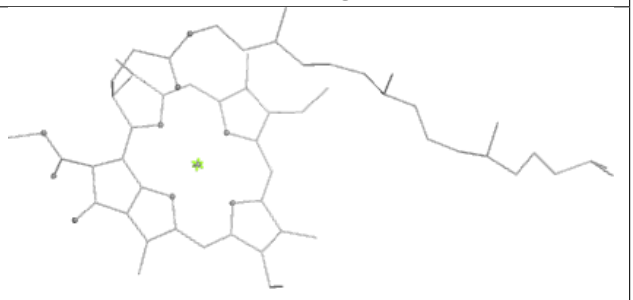
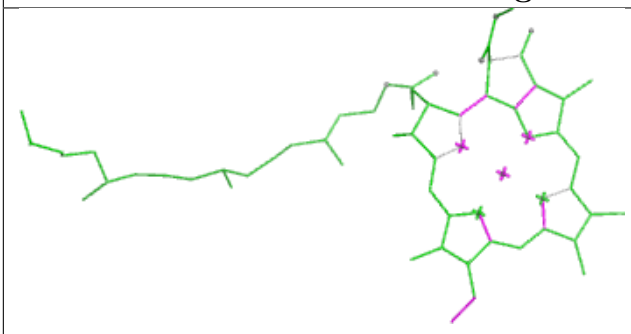


Rings

Ligand CLA A 1113



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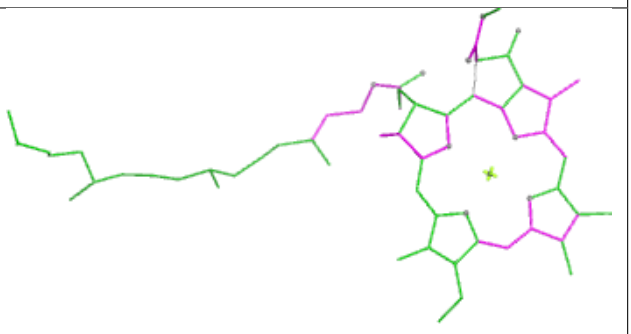
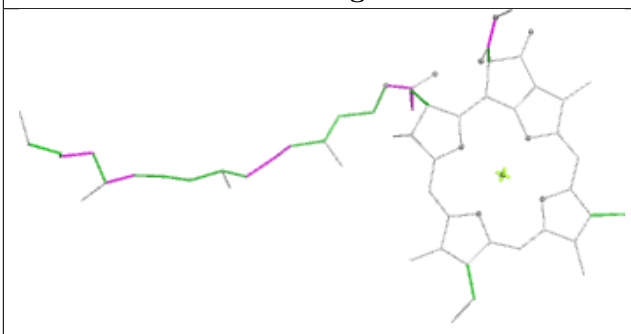


Bond angles



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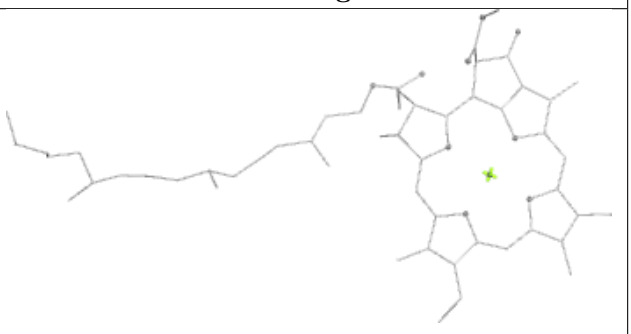
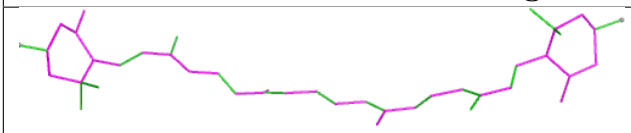


Rings

Ligand C7Z J 4002



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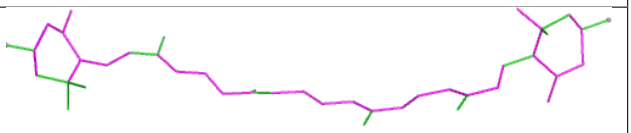
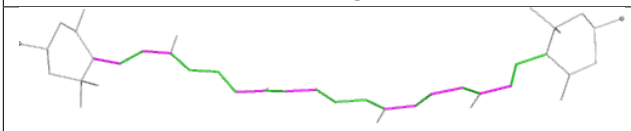


Bond angles



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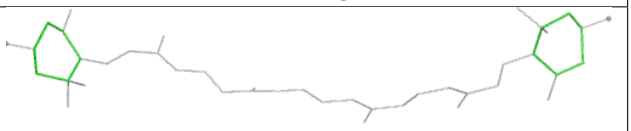
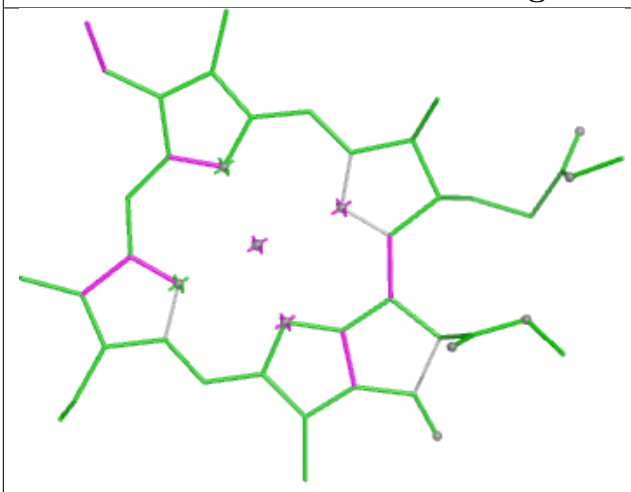


Rings

Ligand CLA 1 613



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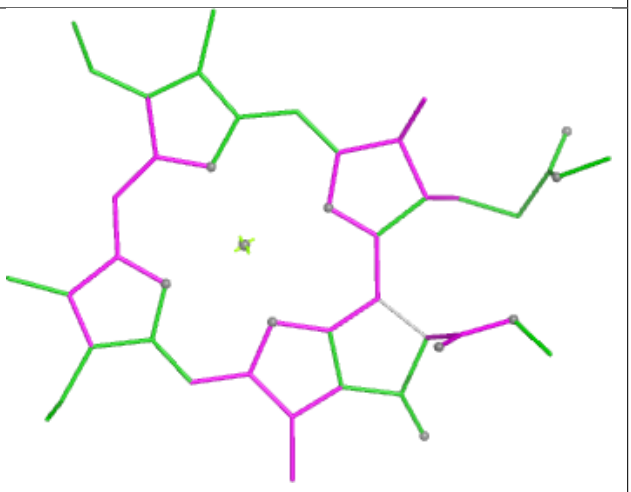
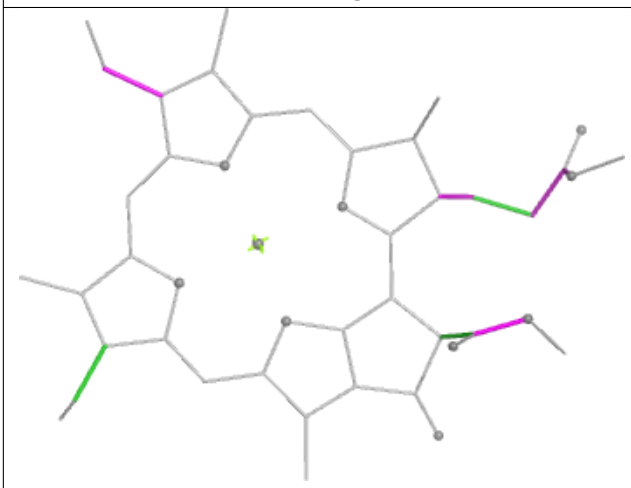


Bond angles



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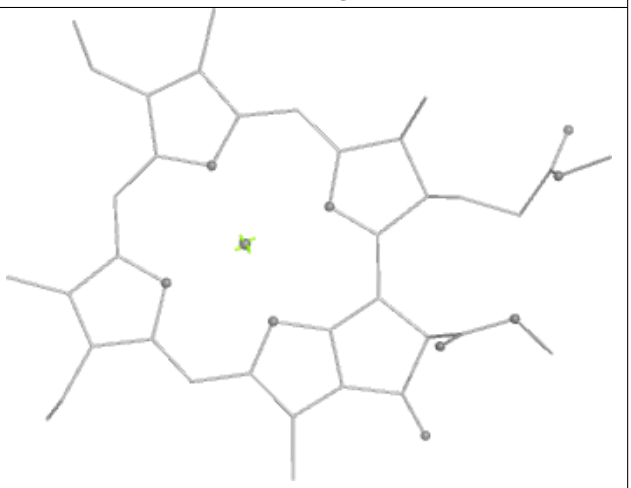
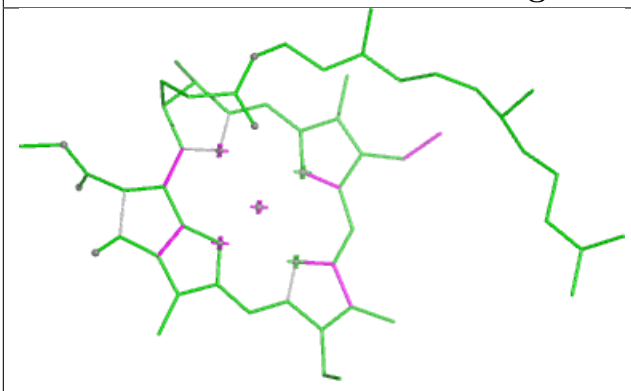


Rings

Ligand CLA 7 601



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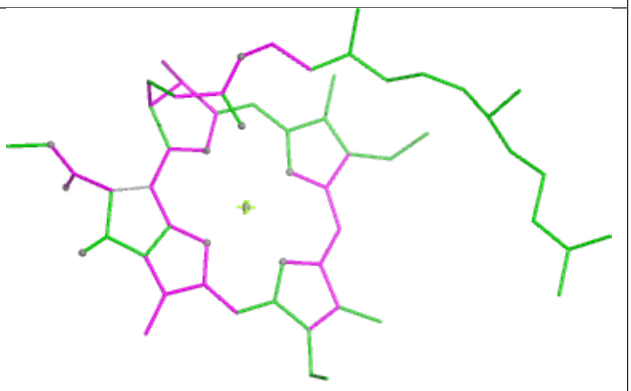
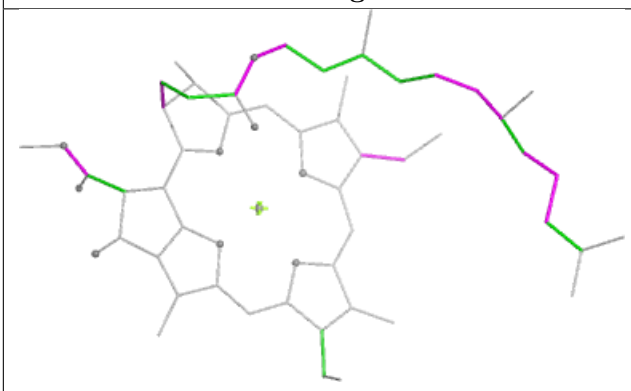


Bond angles

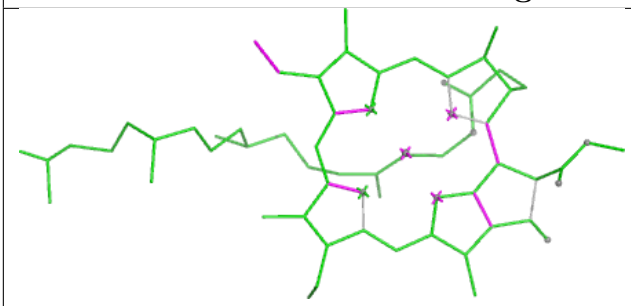


Torsions



Rings

Ligand CLA A 1136



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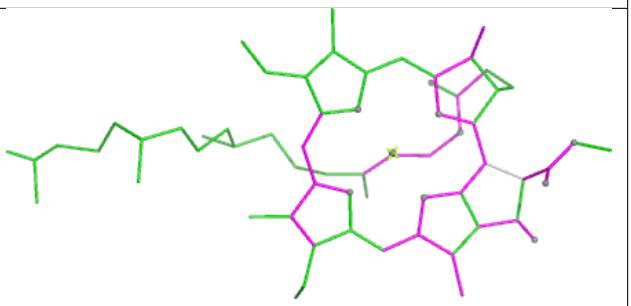
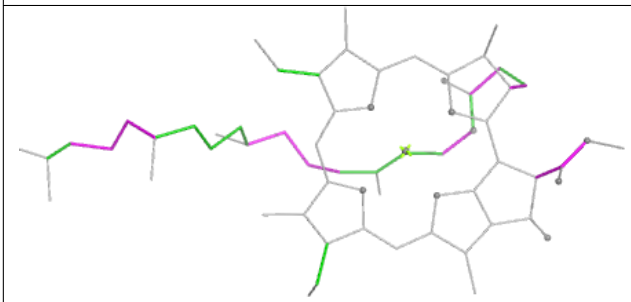


Bond angles



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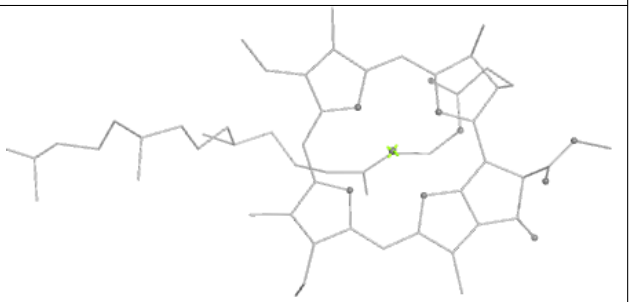
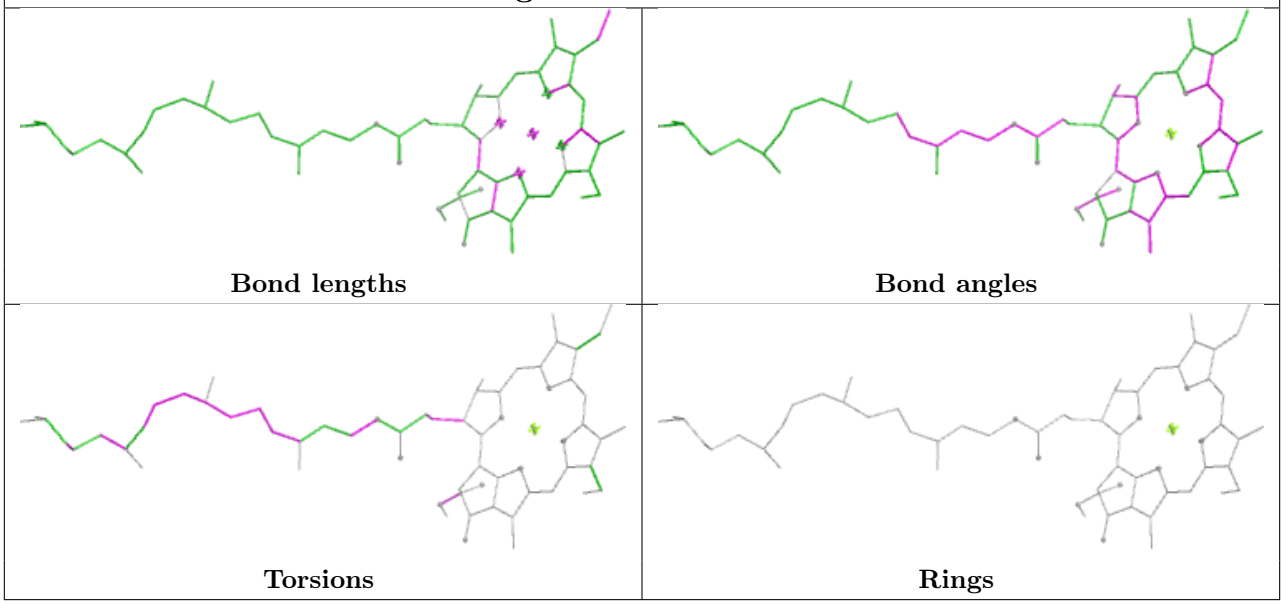
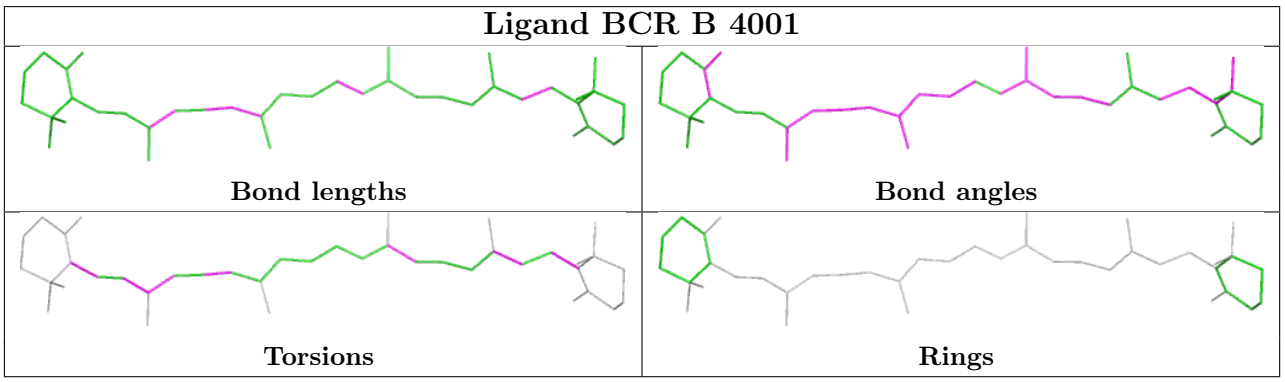


Rings

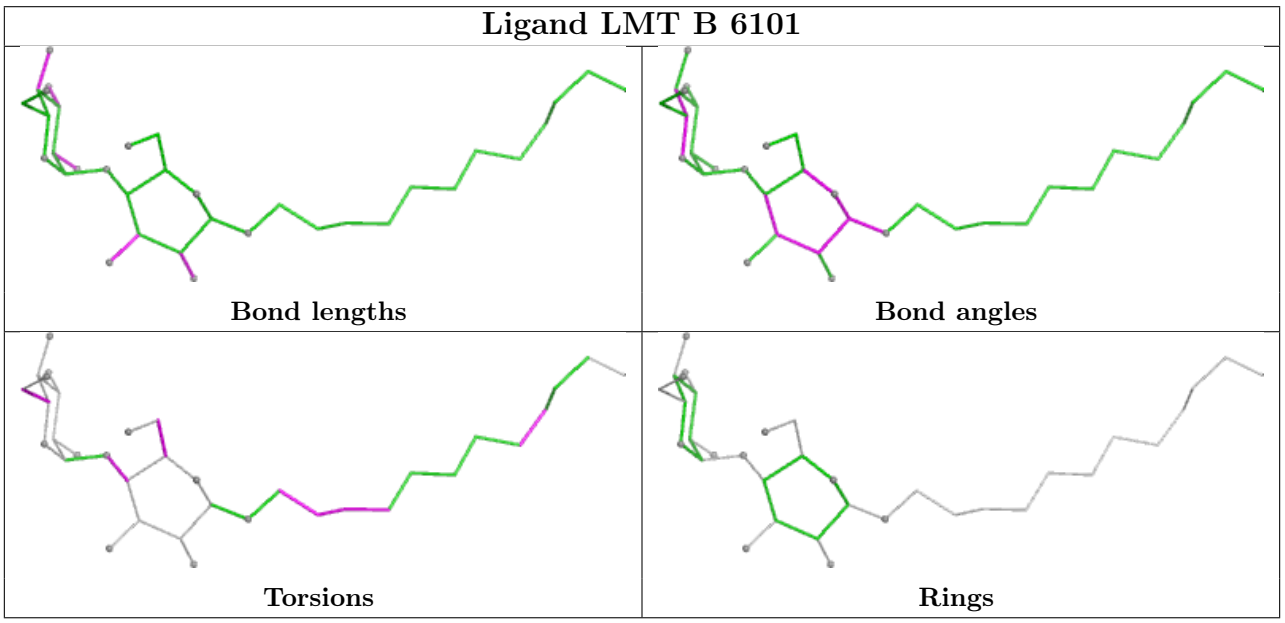
Ligand CLA A 1107



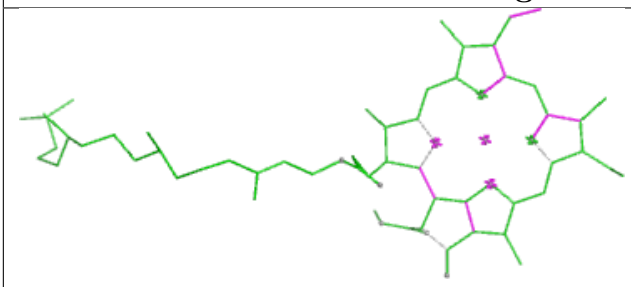
Ligand BCR B 4001



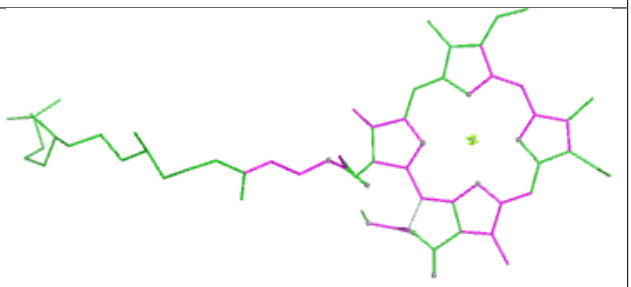
Ligand LMT B 6101



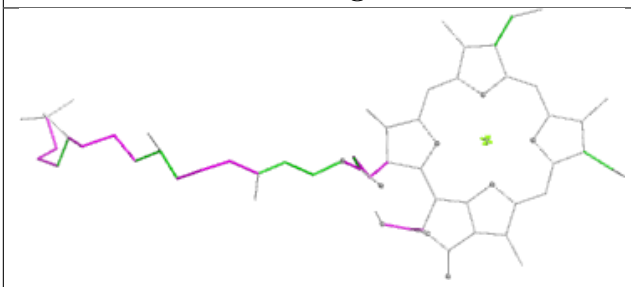
Ligand CLA B 1240



Bond lengths



Bond angles



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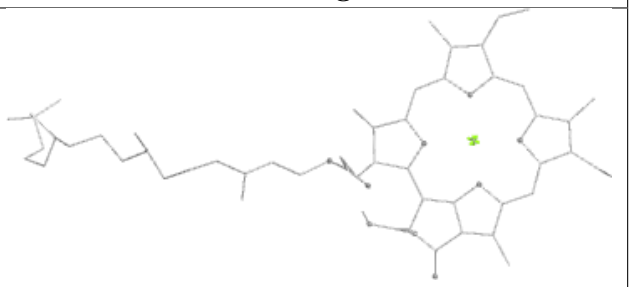
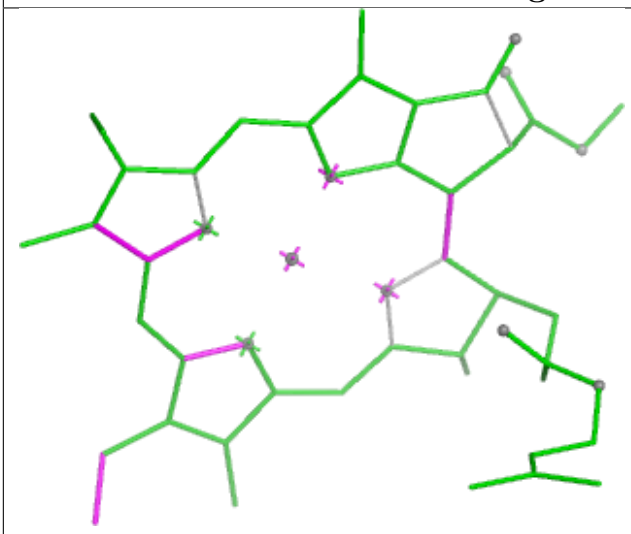


Rings

Ligand CLA 5 606



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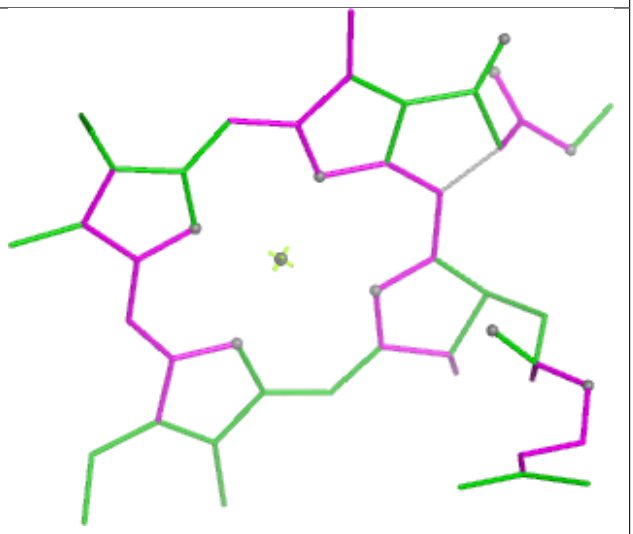
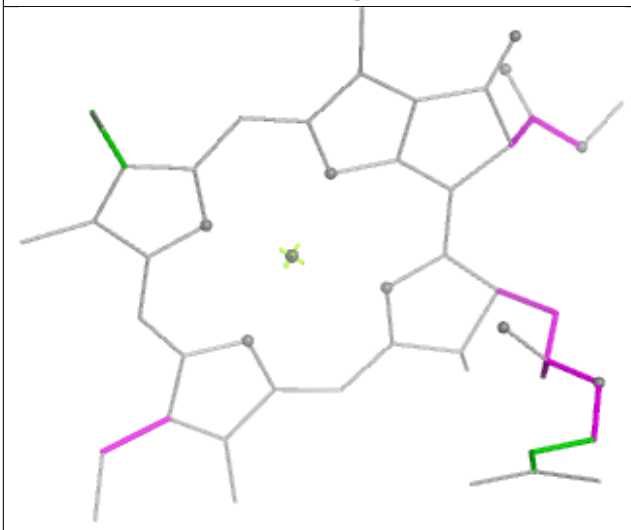


Bond angles



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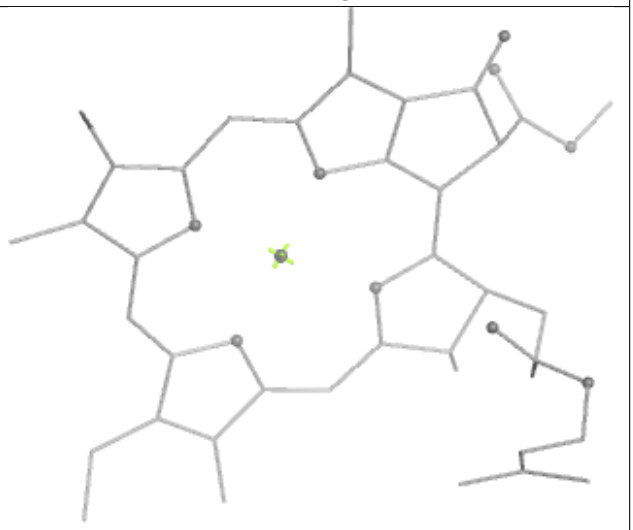
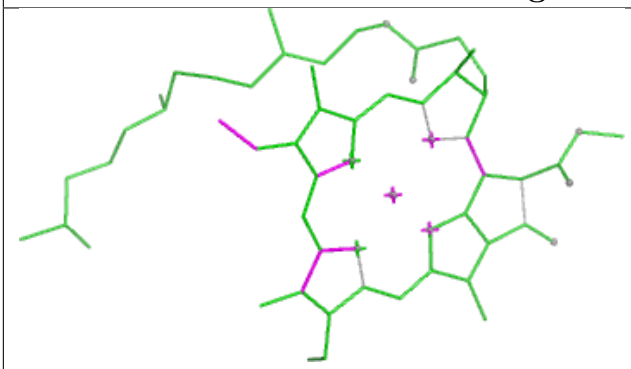


Rings

Ligand CLA 5 601



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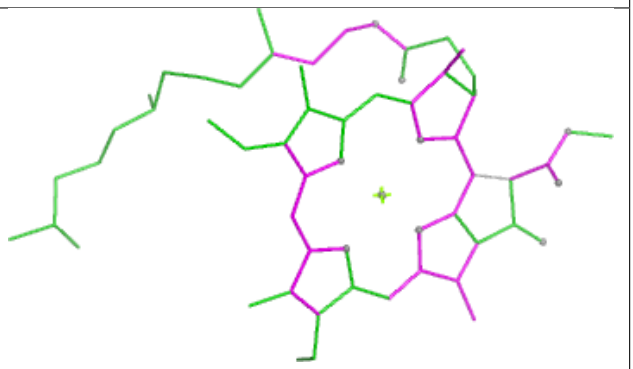
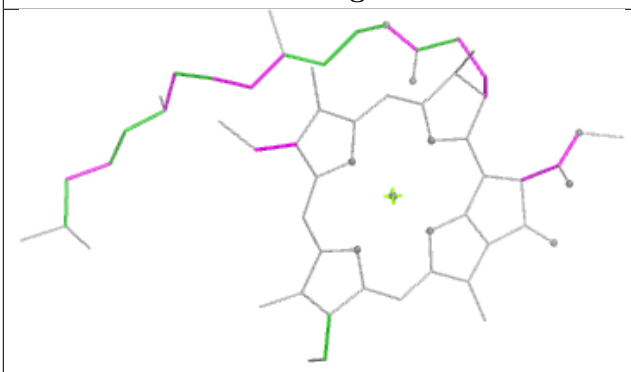


Bond angles



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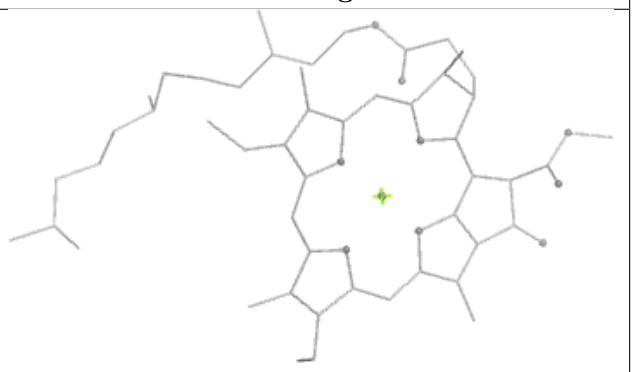
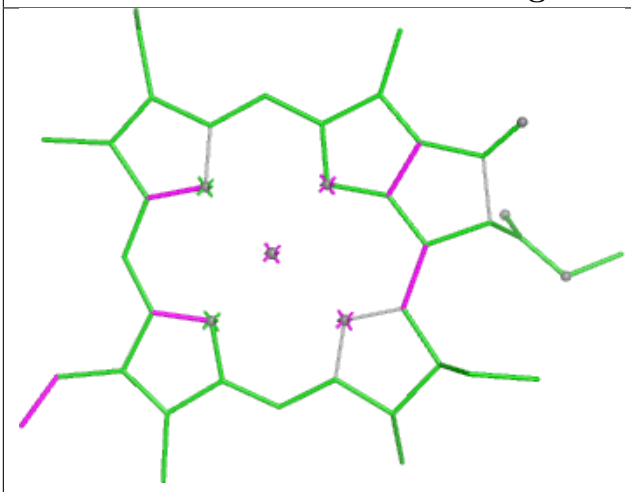
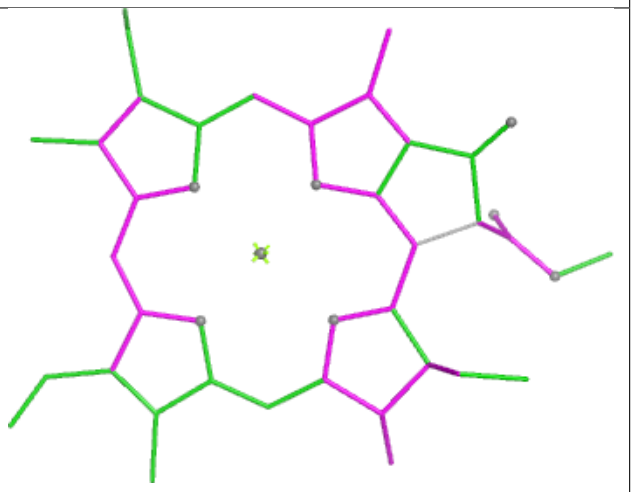


Rings

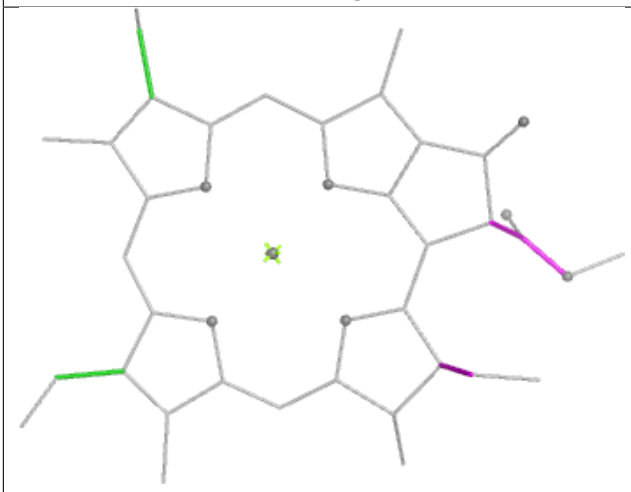
Ligand CLA 7 613



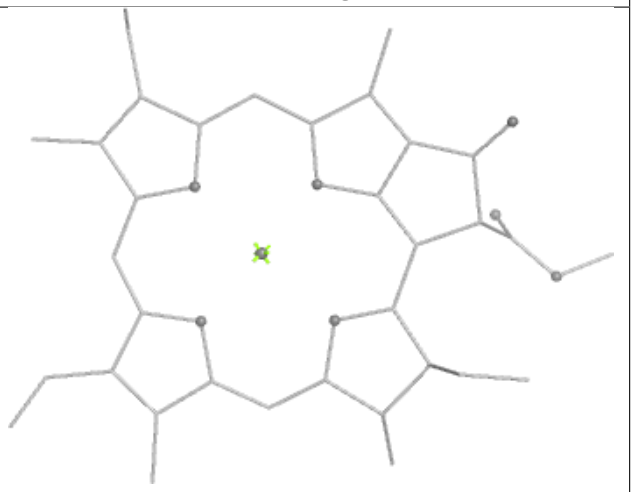
Bond lengths



Bond angles

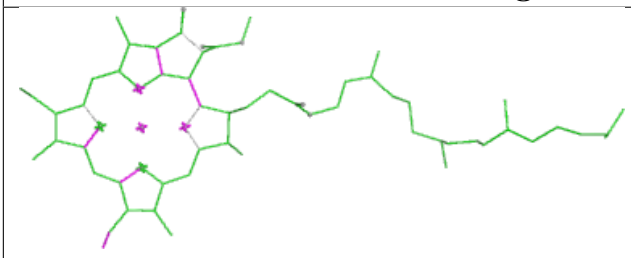


Torsions



Rings

Ligand CLA A 1131



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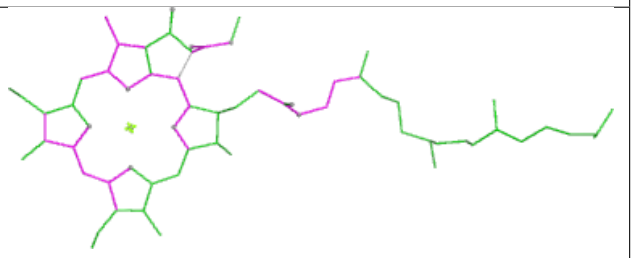
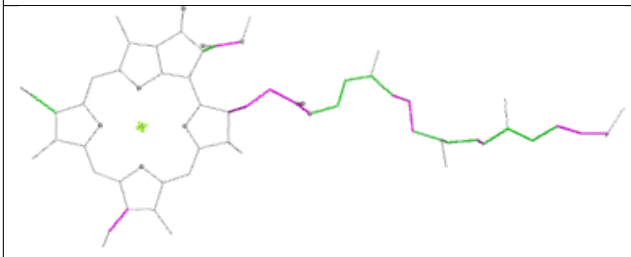


Bond angles



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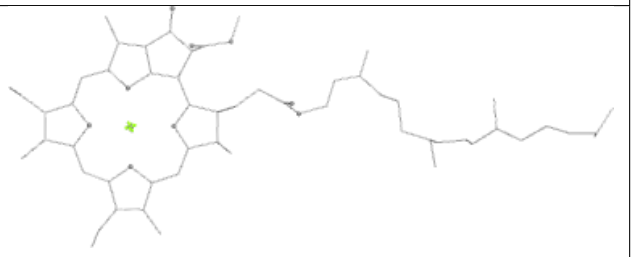
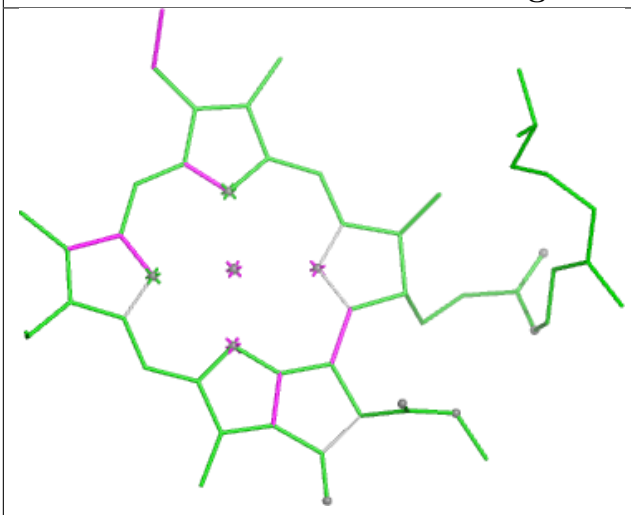


Rings

Ligand CLA 6 605



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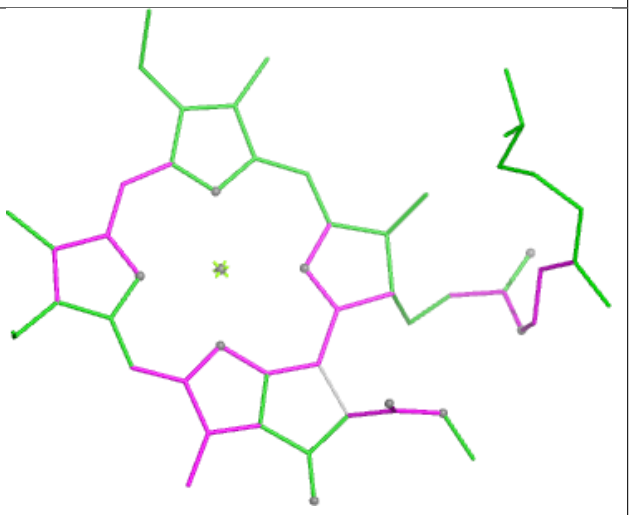
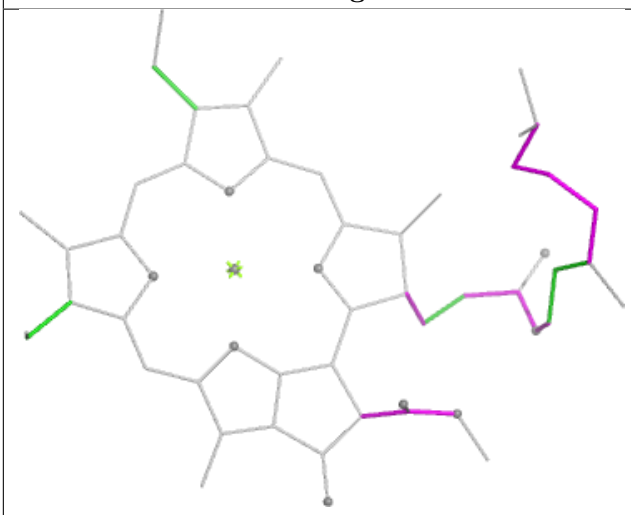


Bond angles



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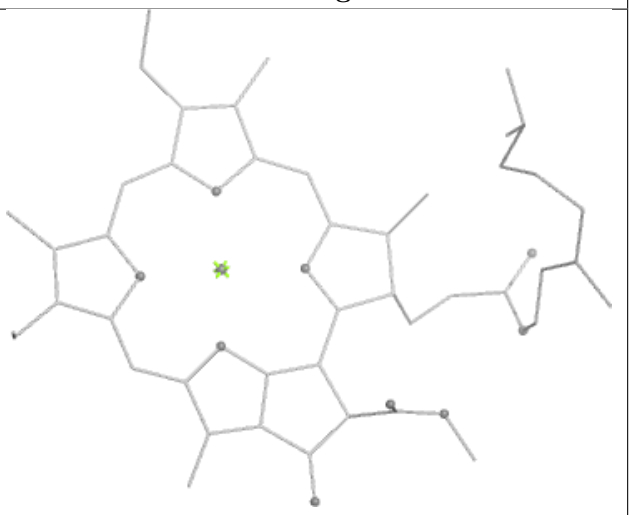
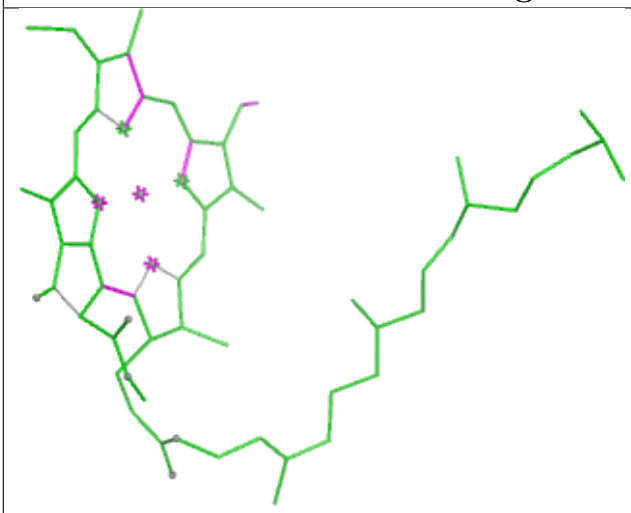


Rings

Ligand CLA B 1221



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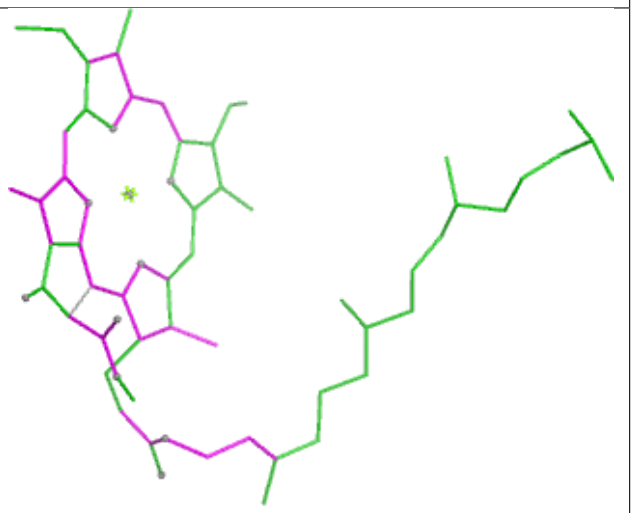
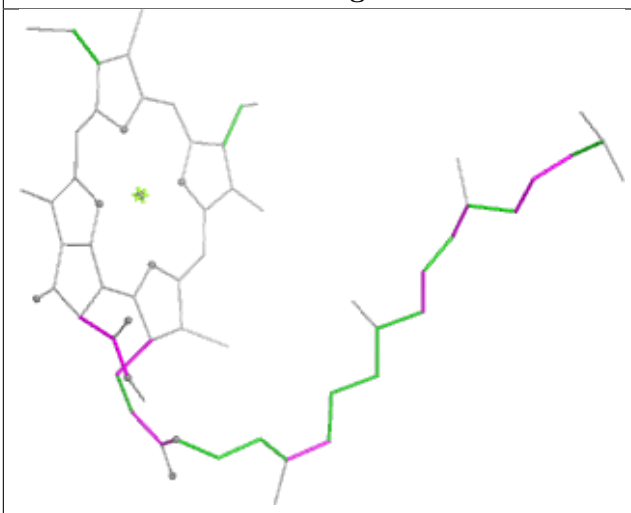


Bond angles



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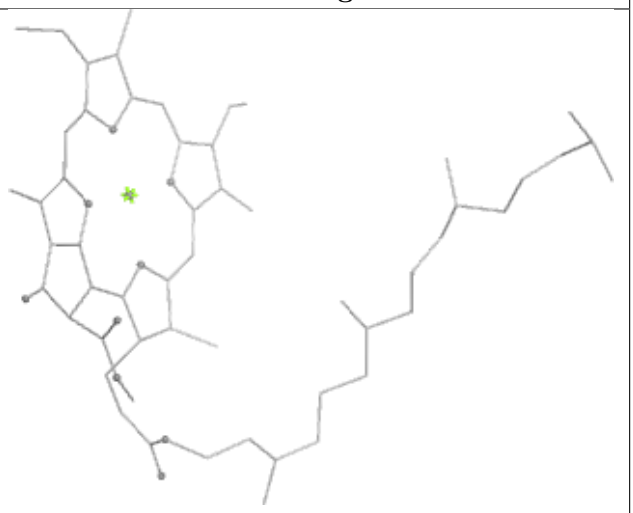
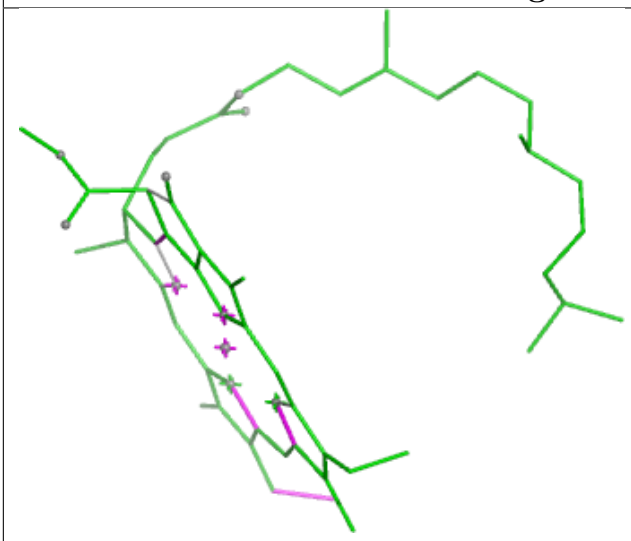


Rings

Ligand CLA 1 608



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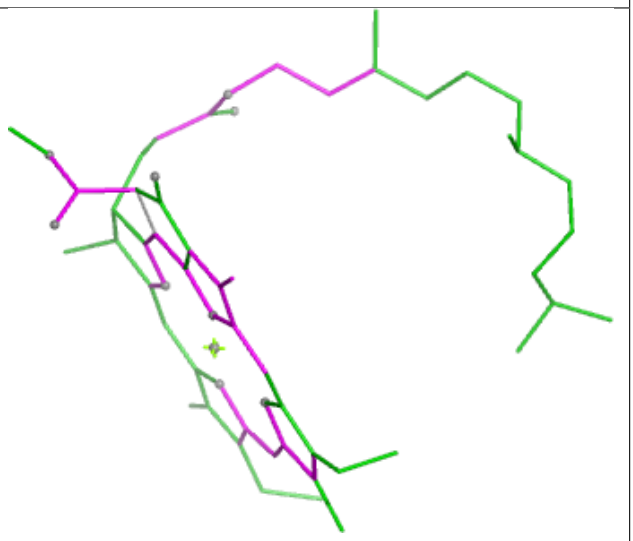
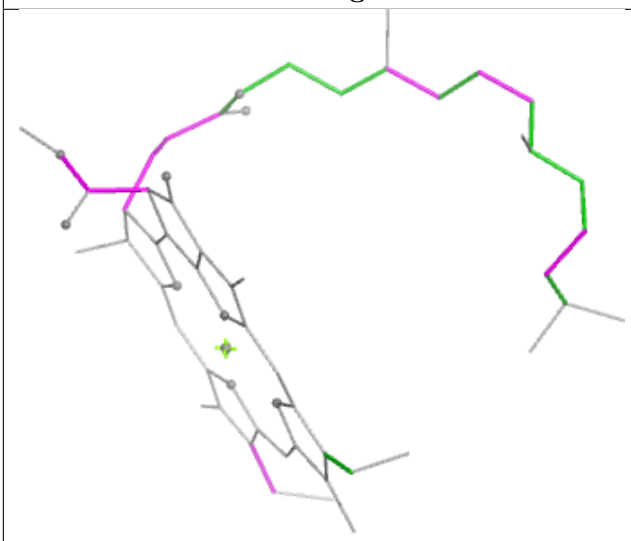


Bond angles

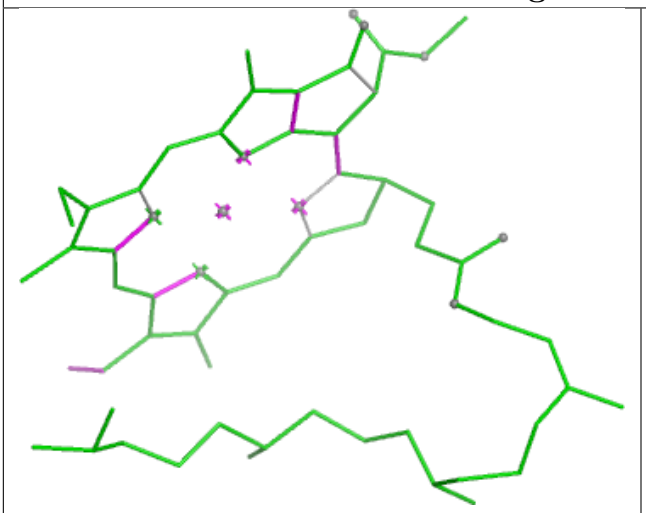


Torsions



Rings

Ligand CLA 1 611



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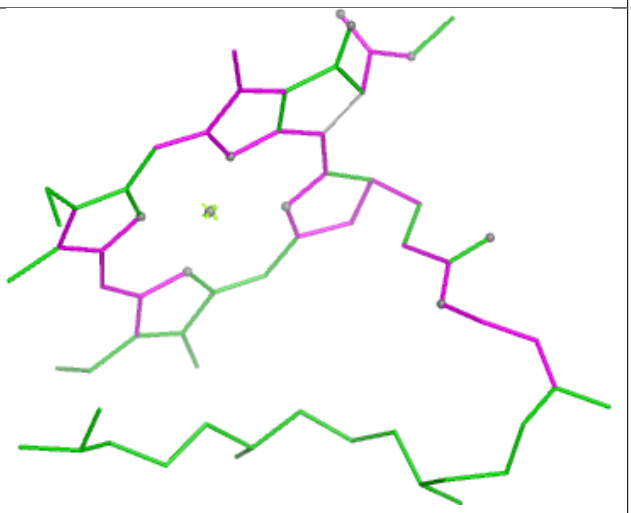
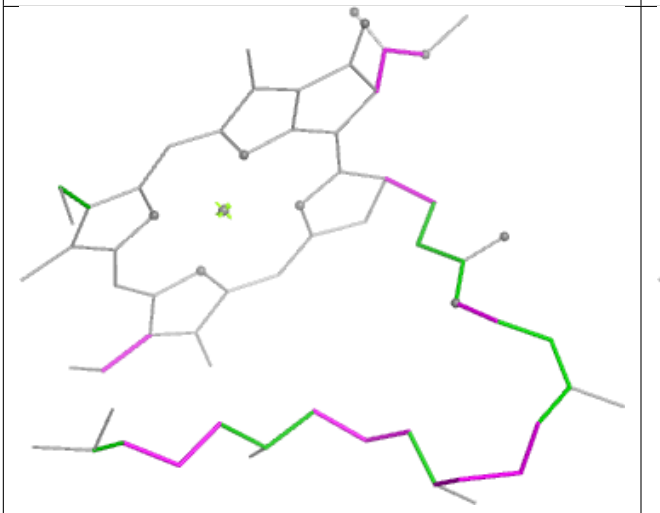


Bond angles



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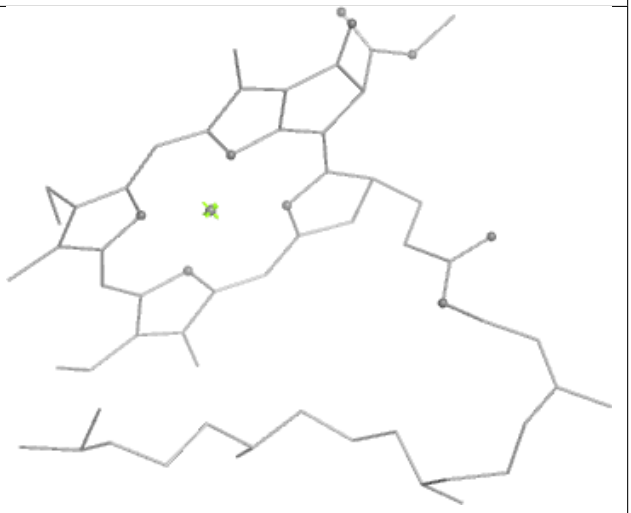
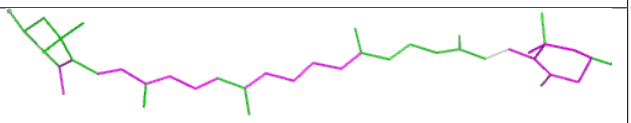


Rings

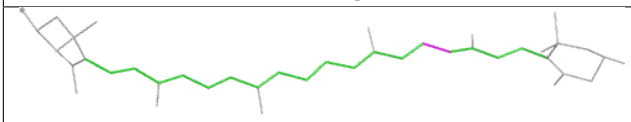
Ligand LUT 3 501



Bond lengths



Bond angles



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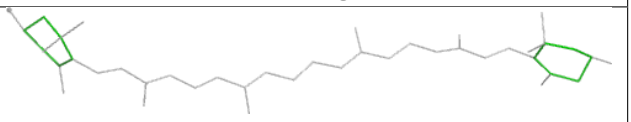
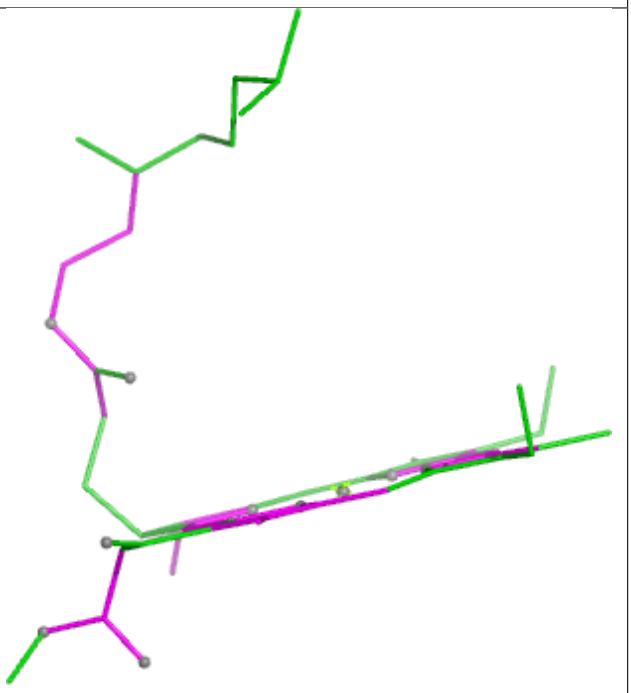


Rings

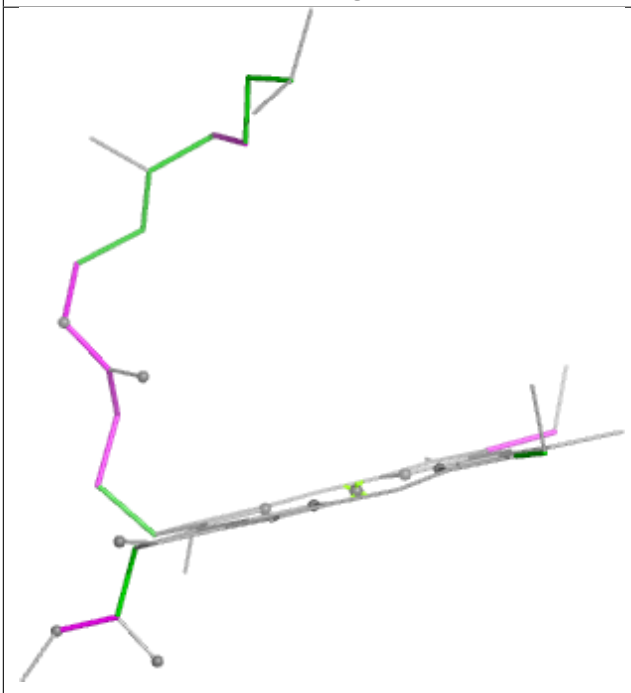
Ligand CLA 4 608



Bond lengths



Bond angles



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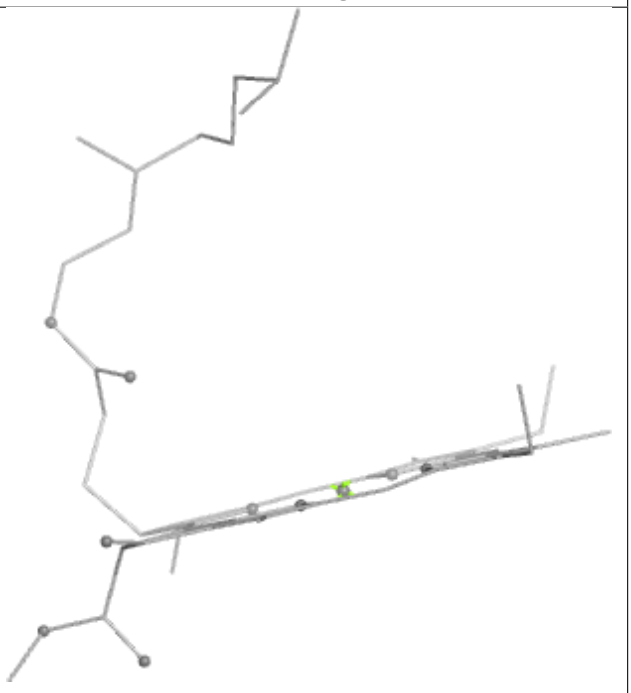
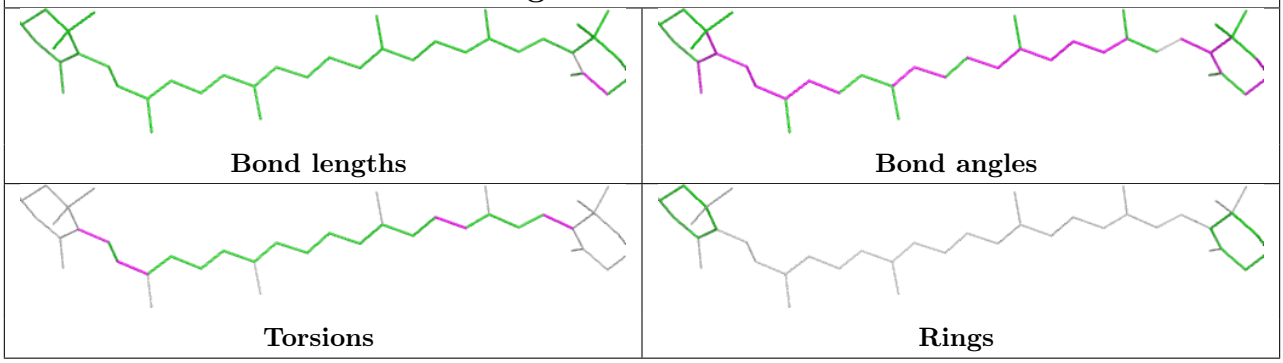


Rings

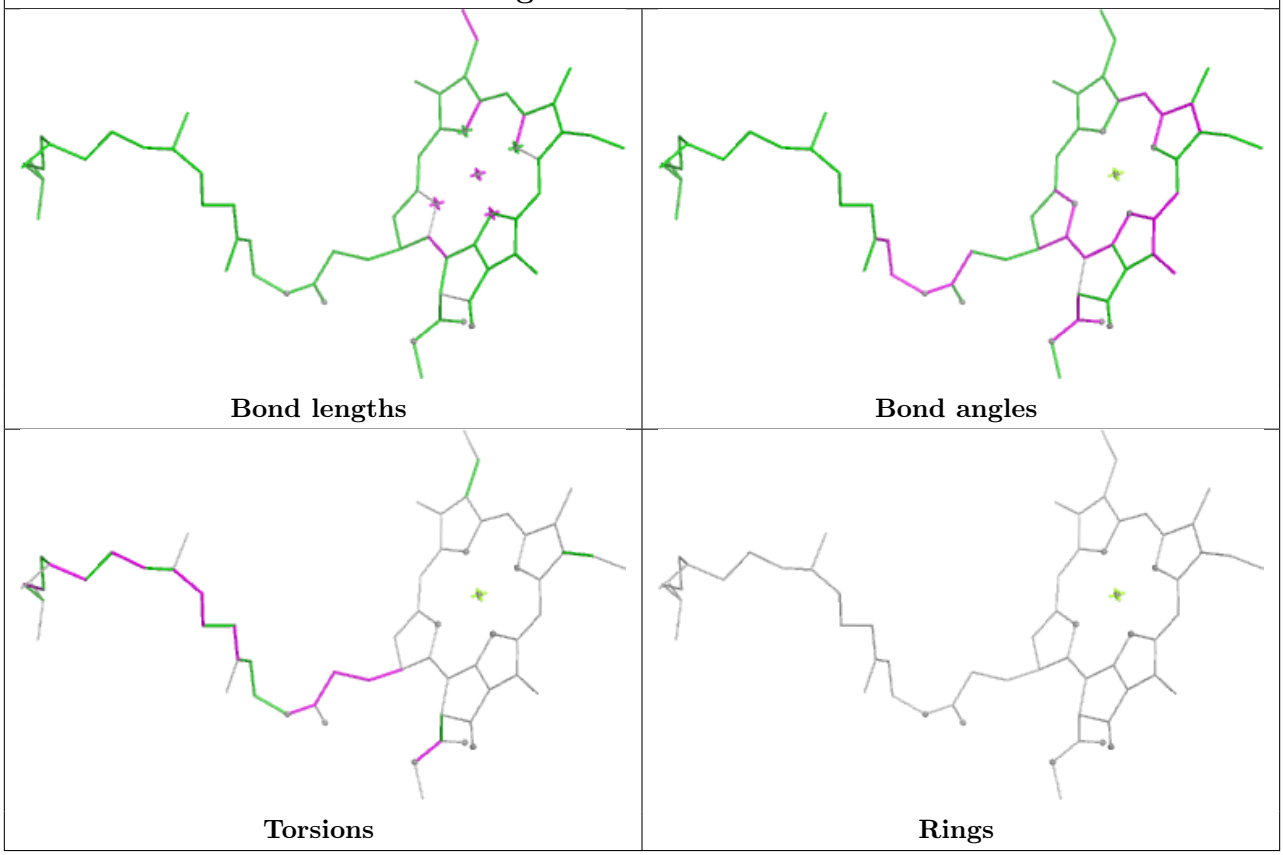
Ligand LUT Z 503



Bond lengths | Bond angles

Torsions | Rings

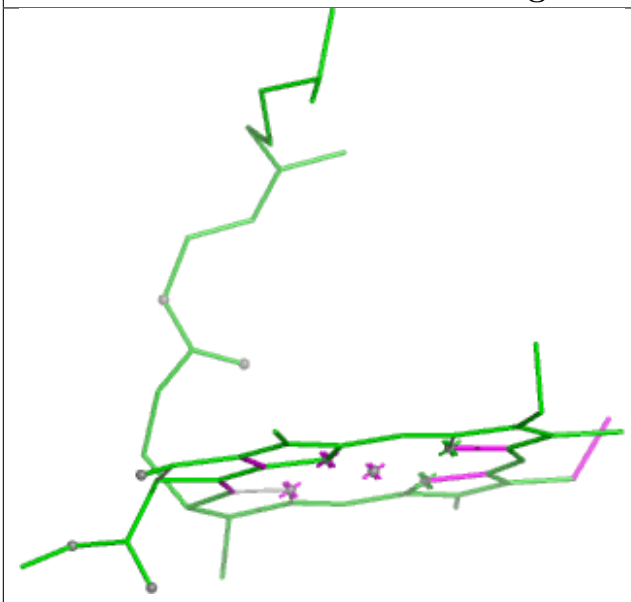
Ligand CLA B 1206



Bond lengths | Bond angles

Torsions | Rings

Ligand CLA 6 608



Bond lengths



Bond angles



Torsions

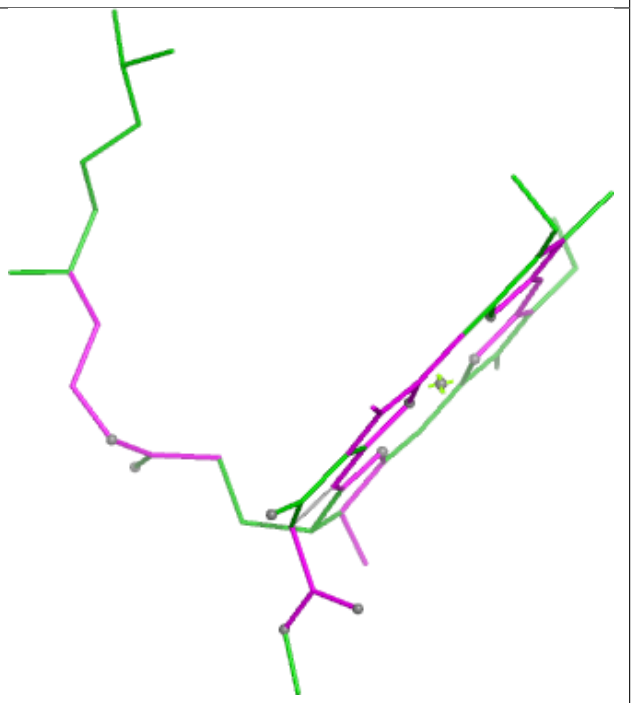


Rings

Ligand CLA 8 608



Bond lengths



Bond angles



Torsions

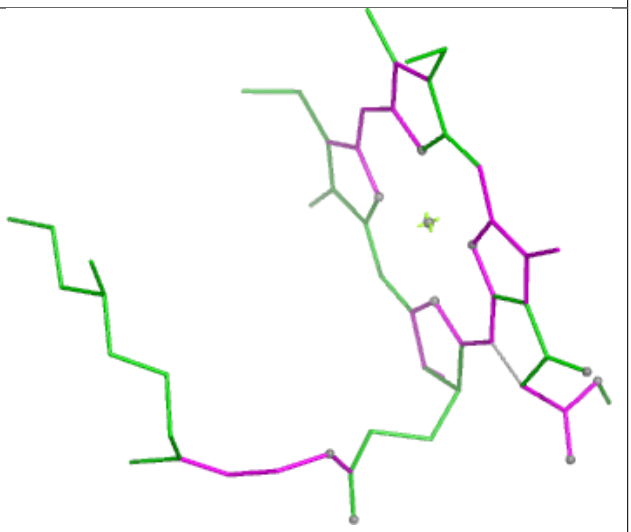


Rings

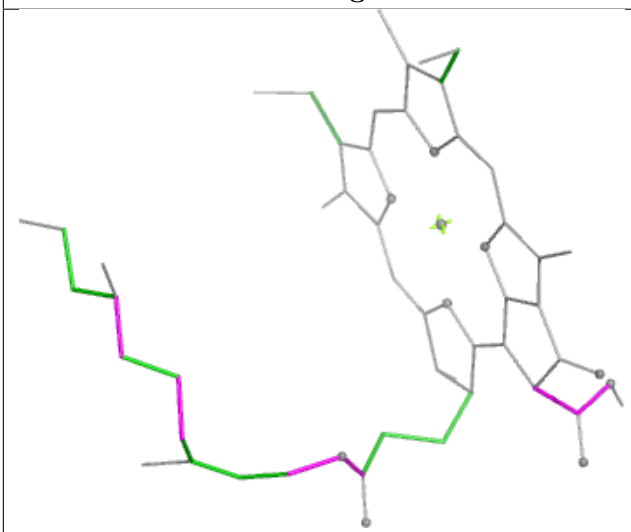
Ligand CLA B 1212



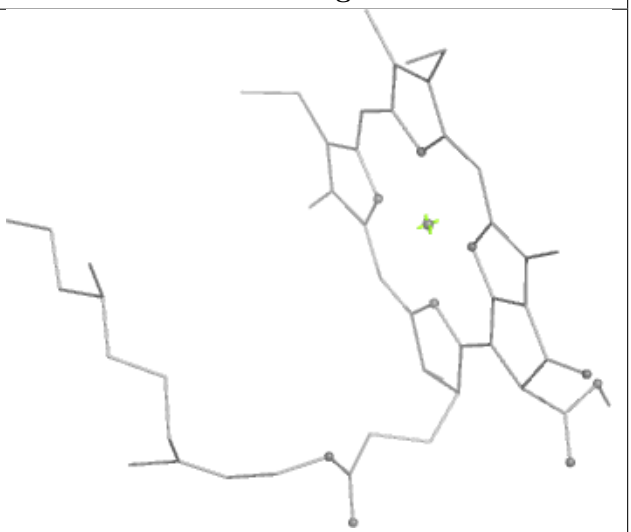
Bond lengths



Bond angles

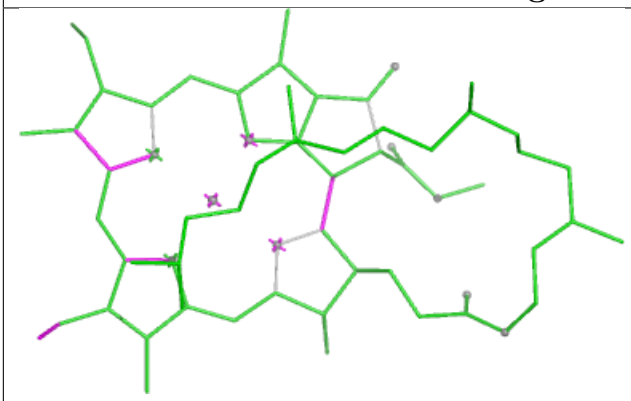


Torsions



Rings

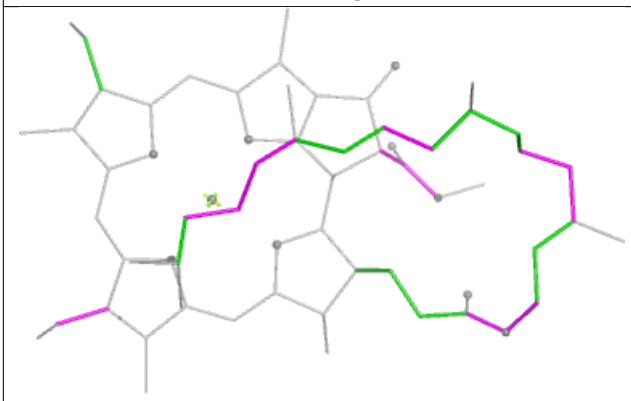
Ligand CLA 1 615



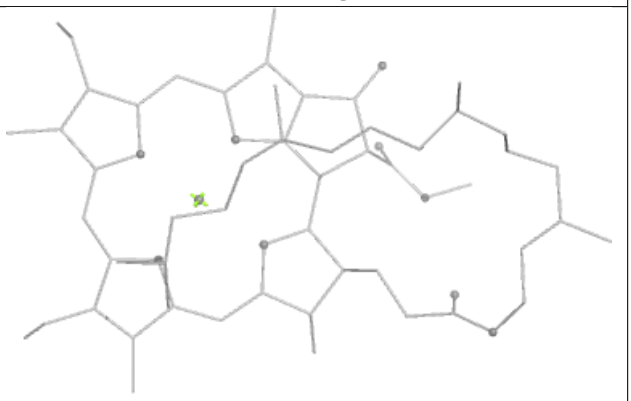
Bond lengths



Bond angles

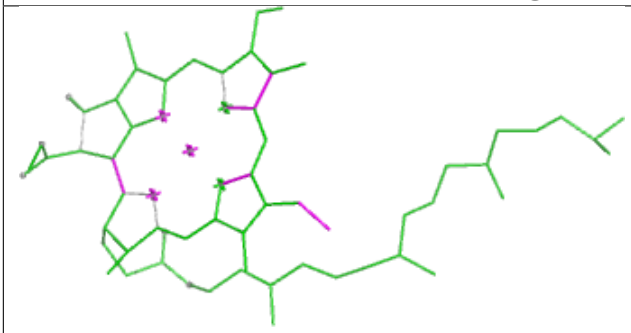


Torsions

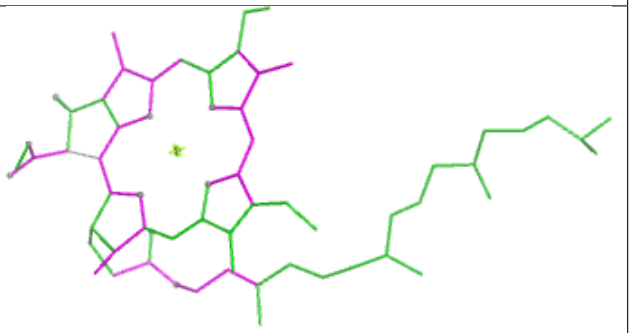


Rings

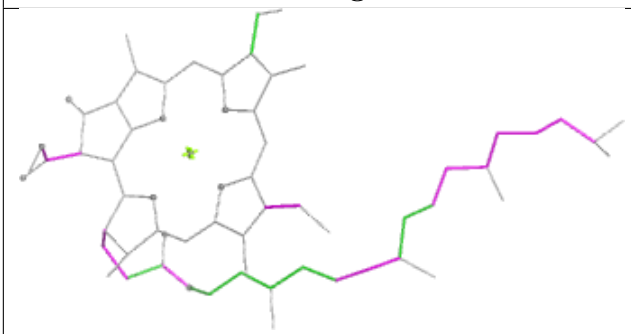
Ligand CLA Z 604



Bond lengths



Bond angles



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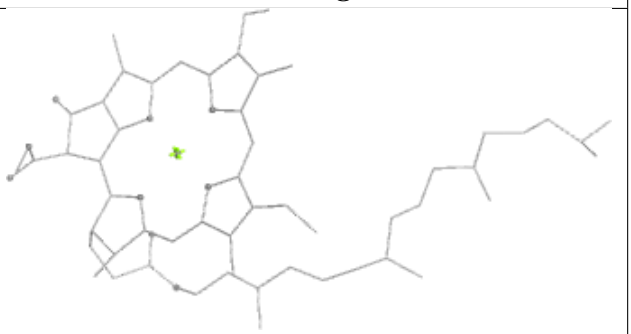
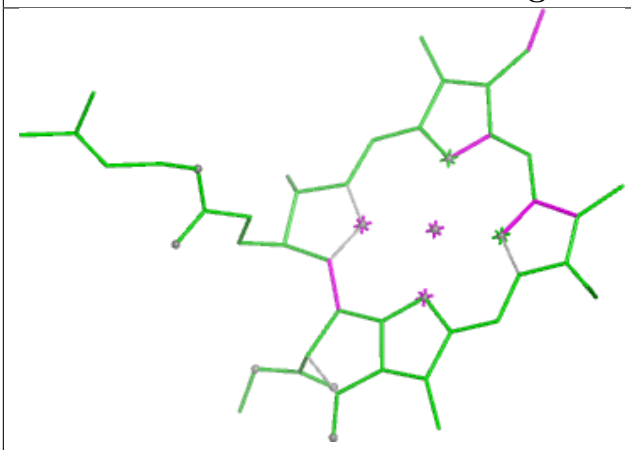


Rings

Ligand CLA 7 611



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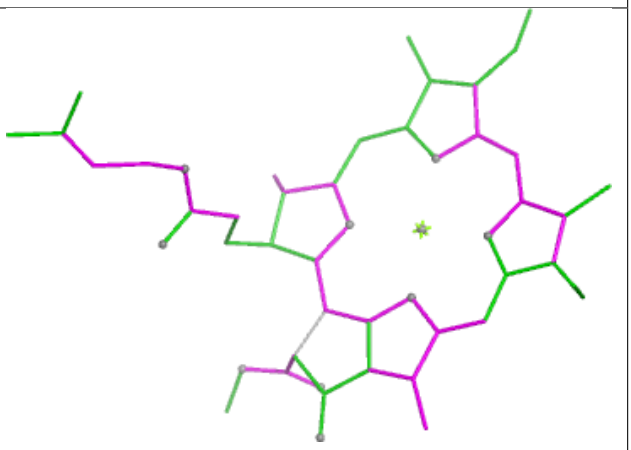
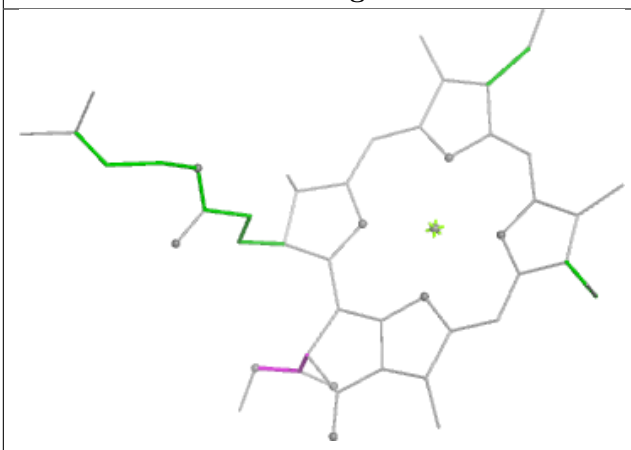


Bond angles



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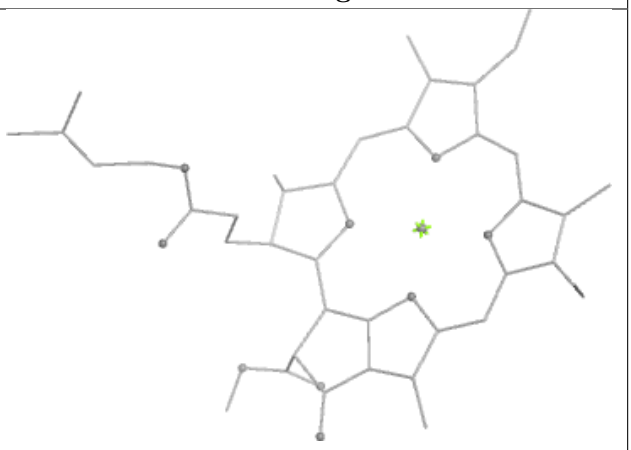
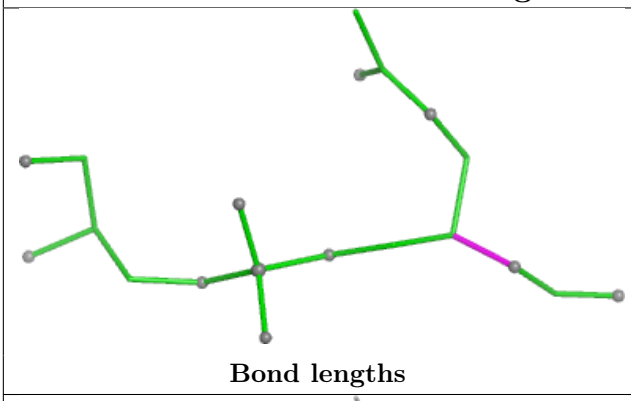
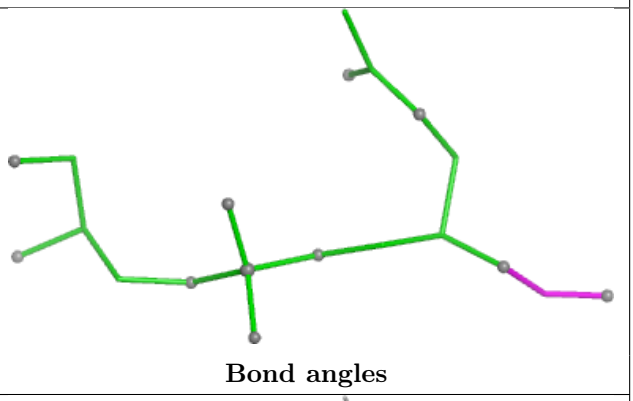


Rings

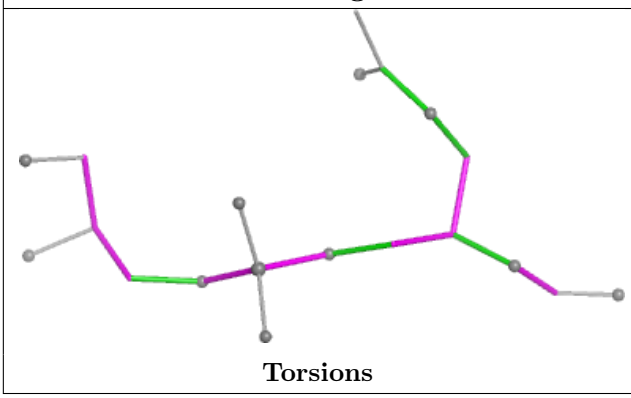
Ligand LHG B 5002



Bond lengths



Bond angles



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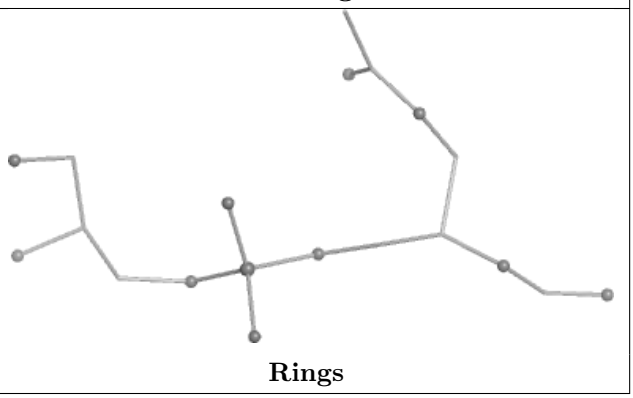
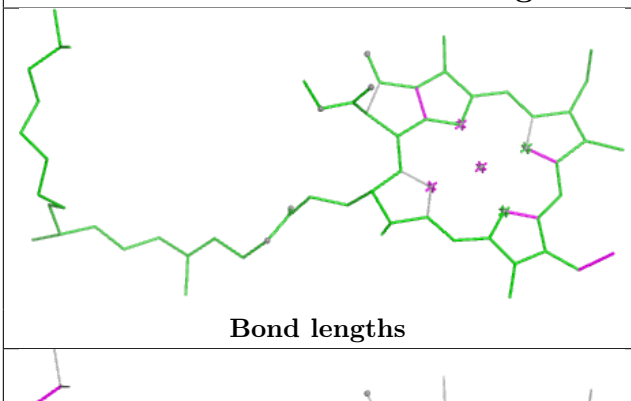
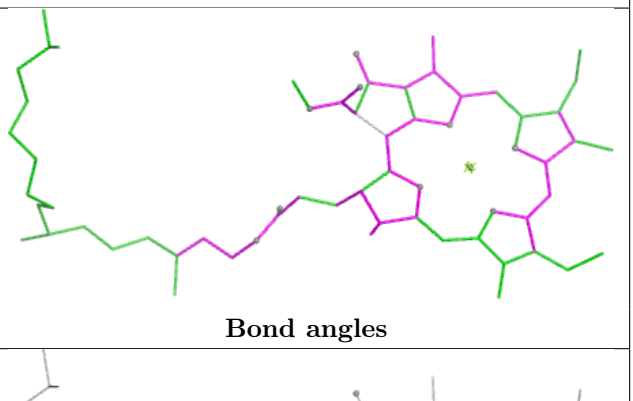


Rings

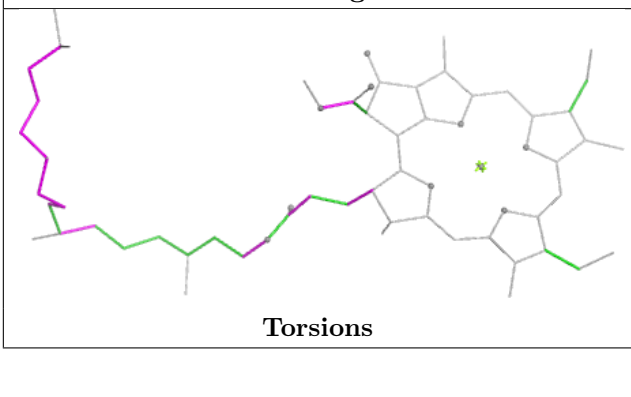
Ligand CLA B 1223



Bond lengths



Bond angles



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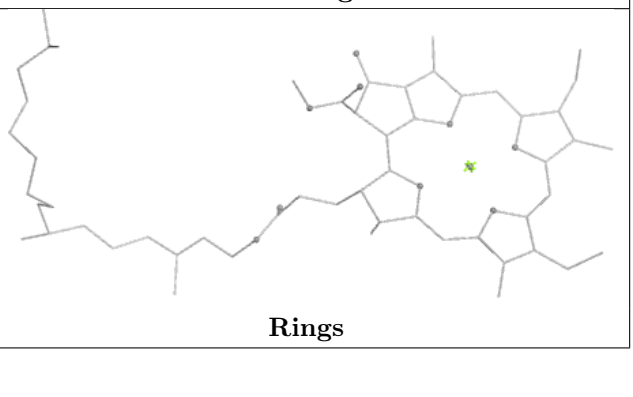
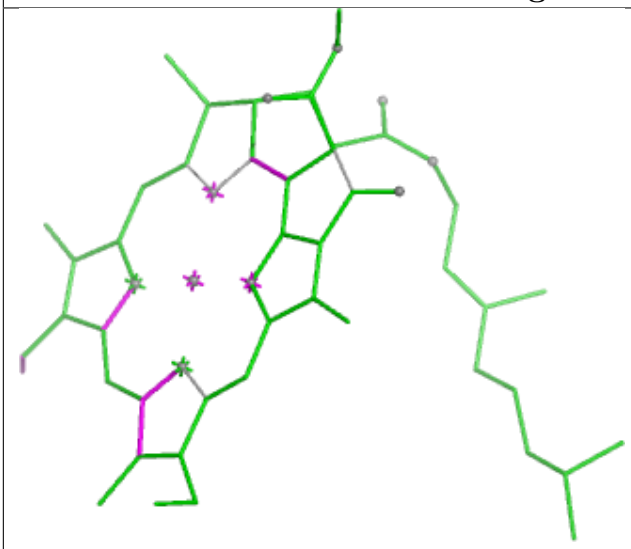


Rings

Ligand CLA 6 607



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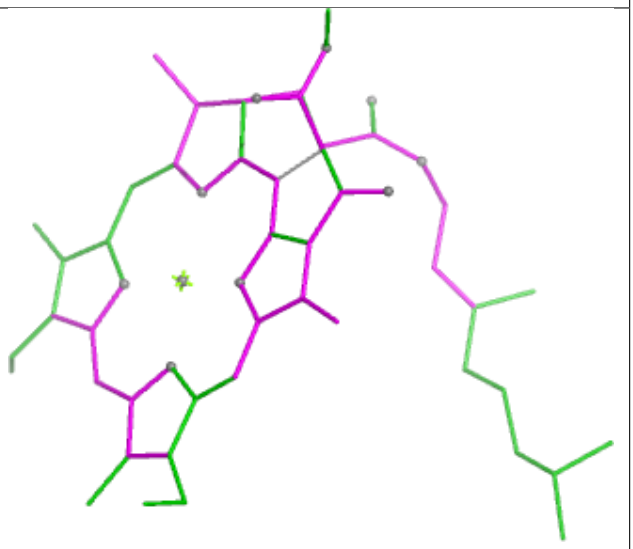
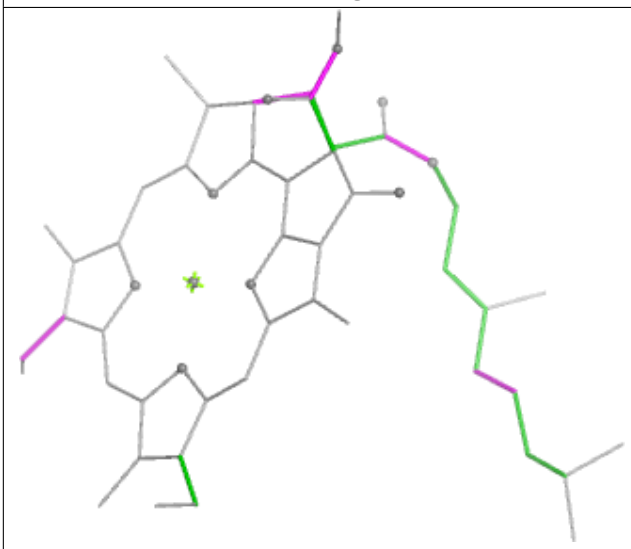


Bond angles



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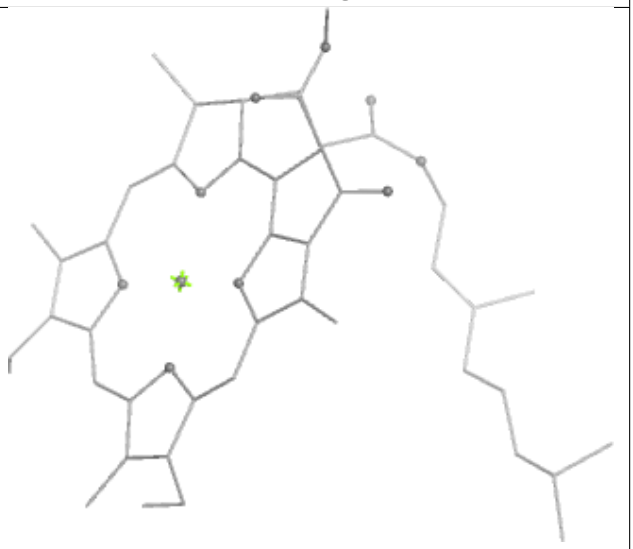
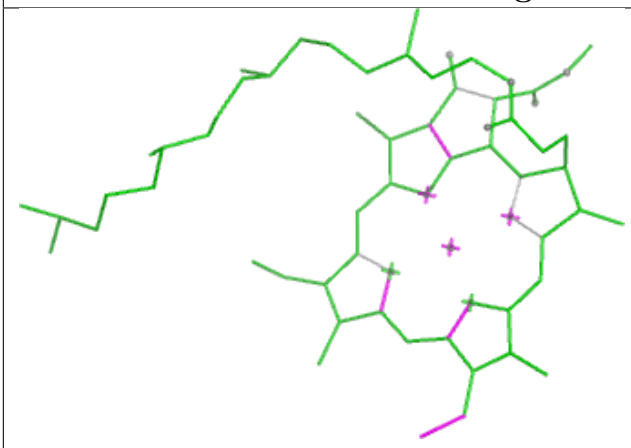
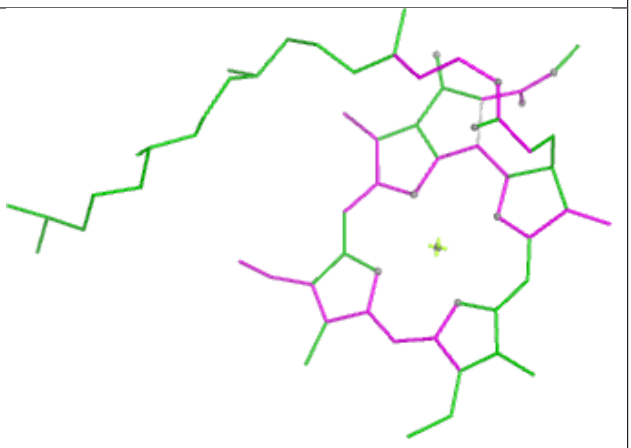


Rings

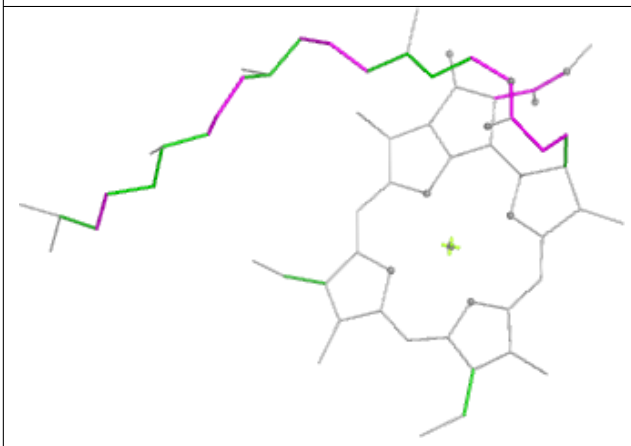
Ligand CLA A 1127



Bond lengths



Bond angles

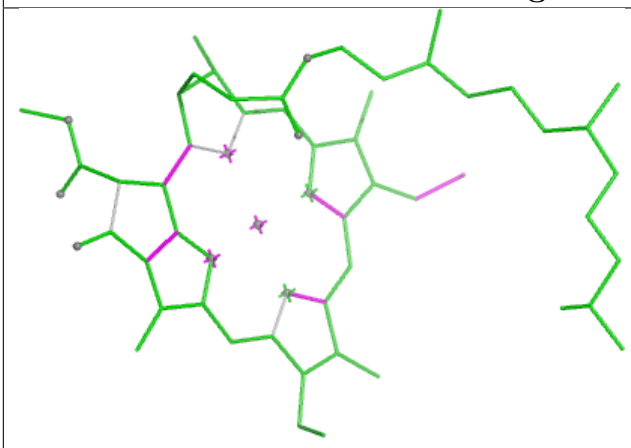


Torsions



Rings

Ligand CLA 3 604



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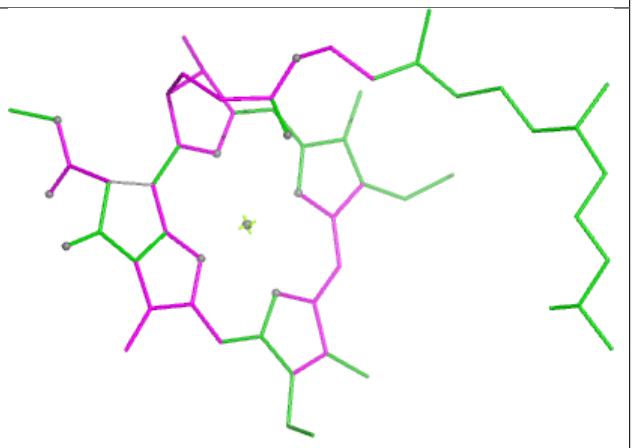

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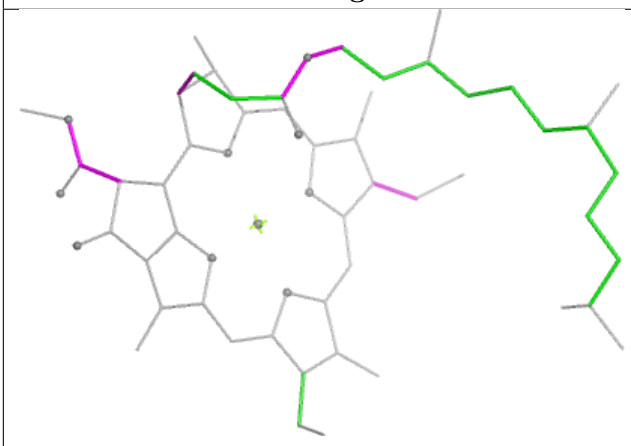

Torsions



Rings

Ligand LHG 8 801



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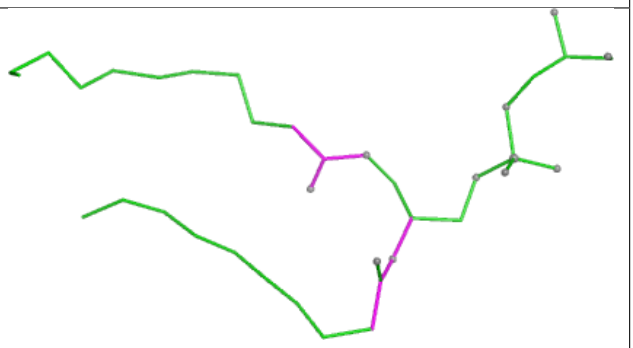

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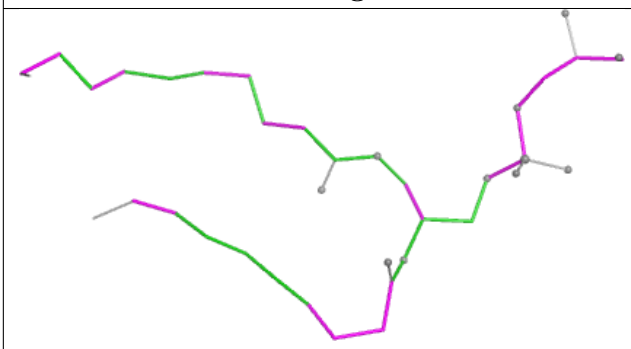
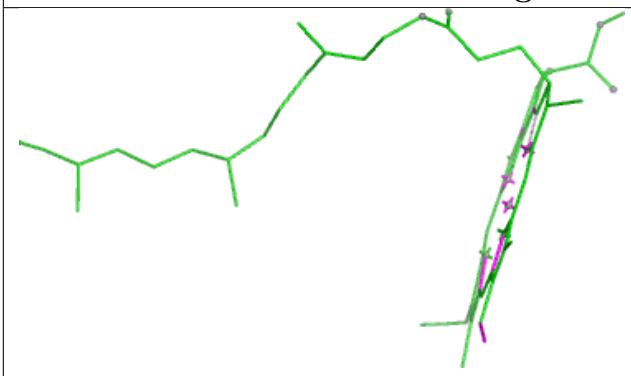


Torsions



Rings

Ligand CLA A 1114



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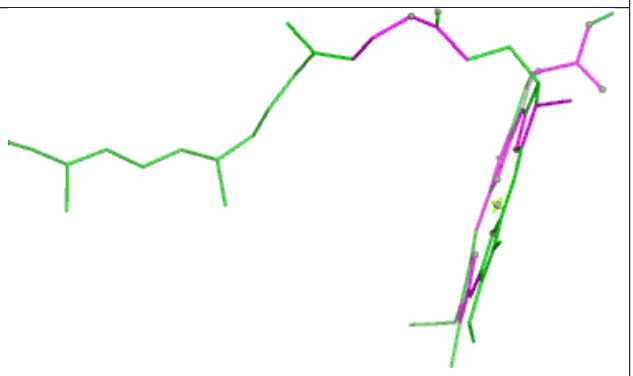

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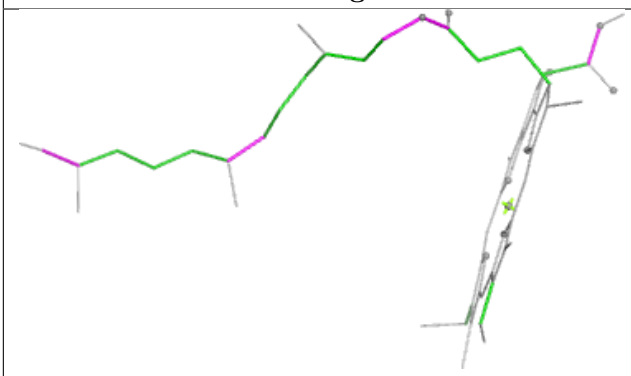
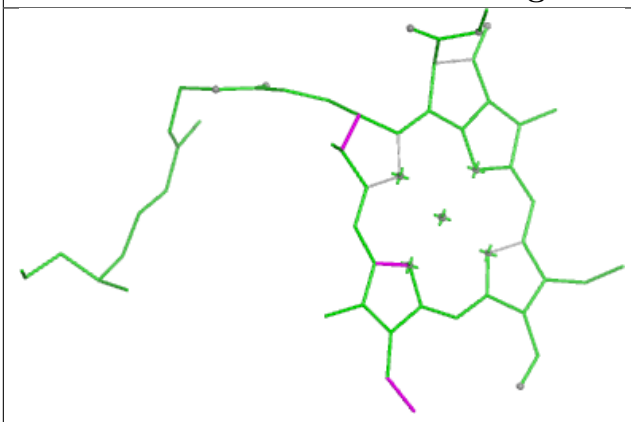


Torsions



Rings

Ligand CHL 1 609



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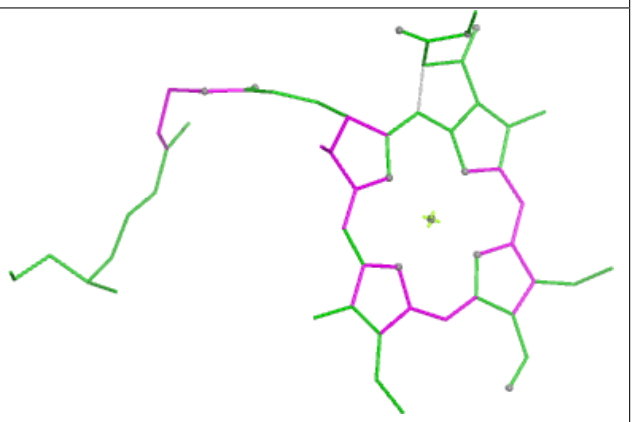

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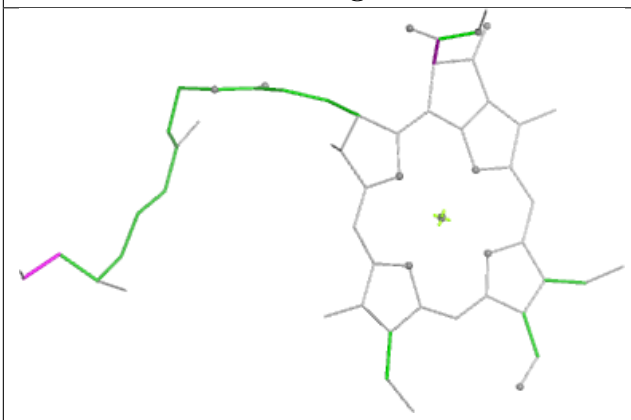

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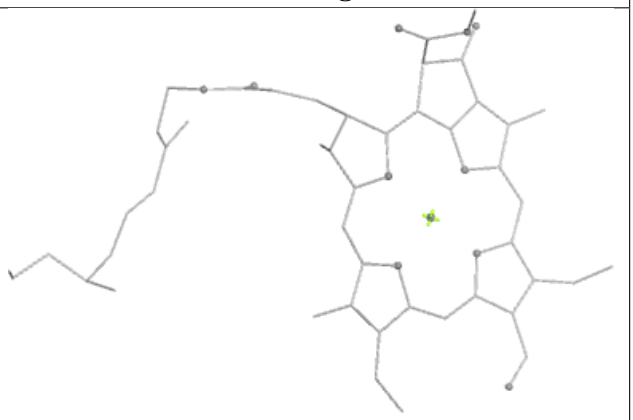
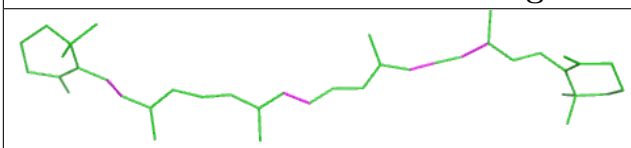


Rings

Ligand BCR 4 503



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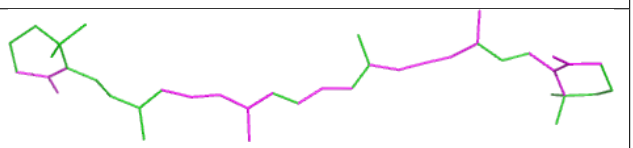

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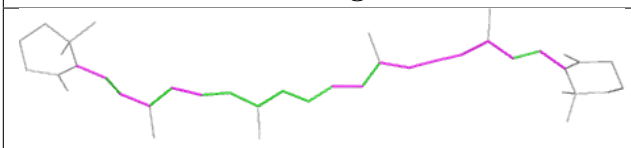

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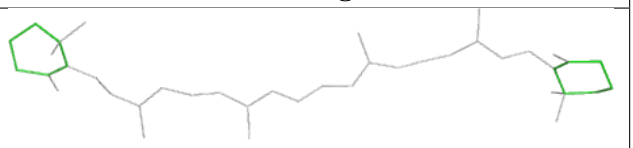
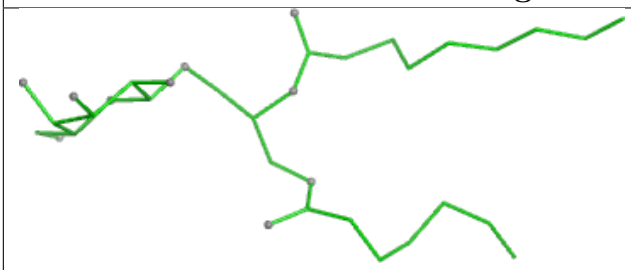


Rings

Ligand LMG J 5001



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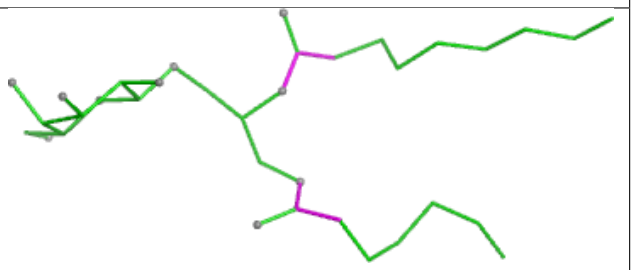

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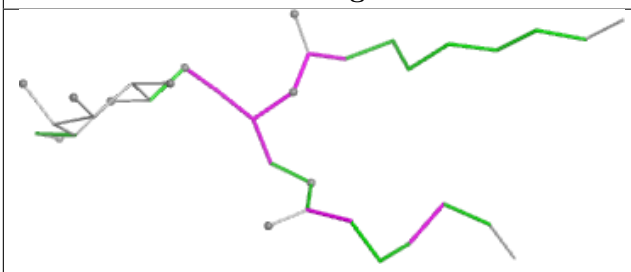

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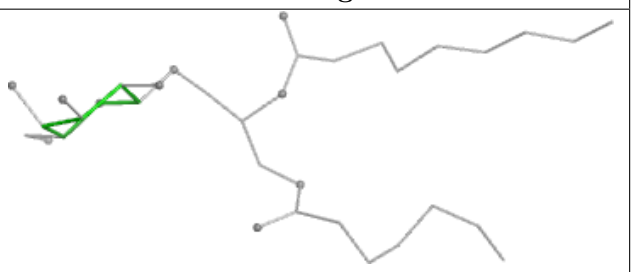
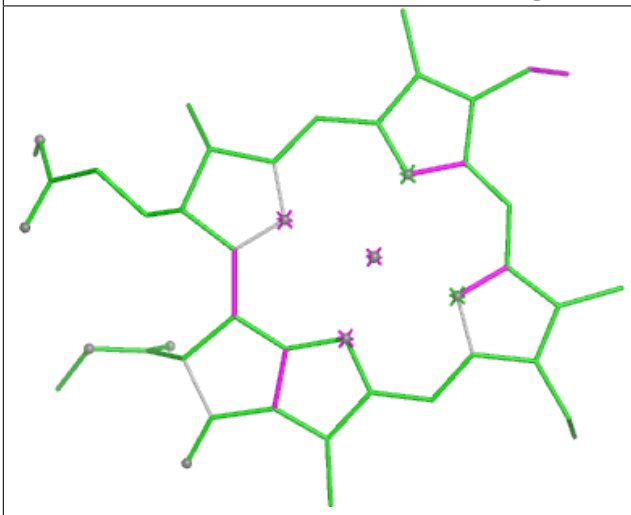


Rings

Ligand CLA 3 602



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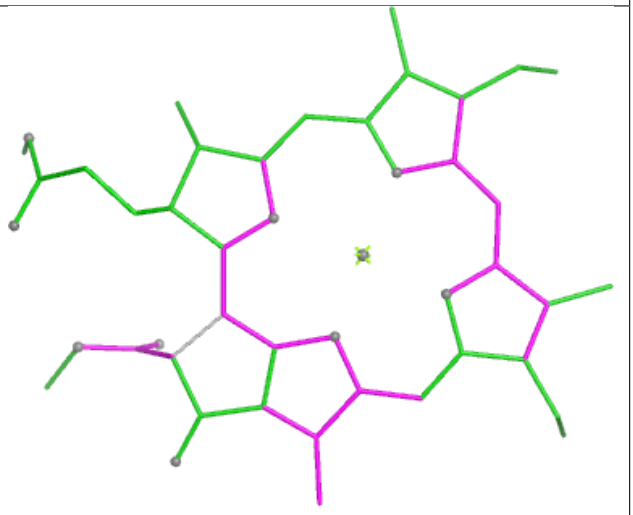
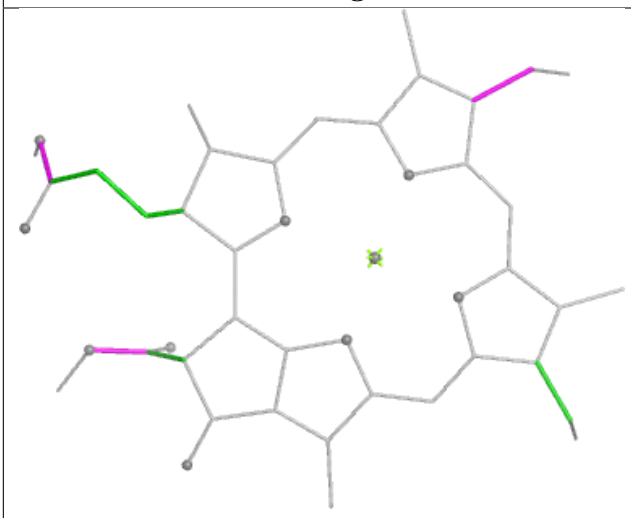


Bond angles



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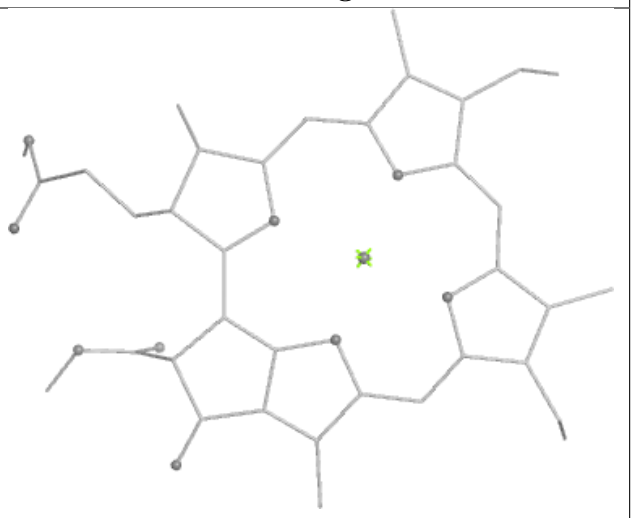
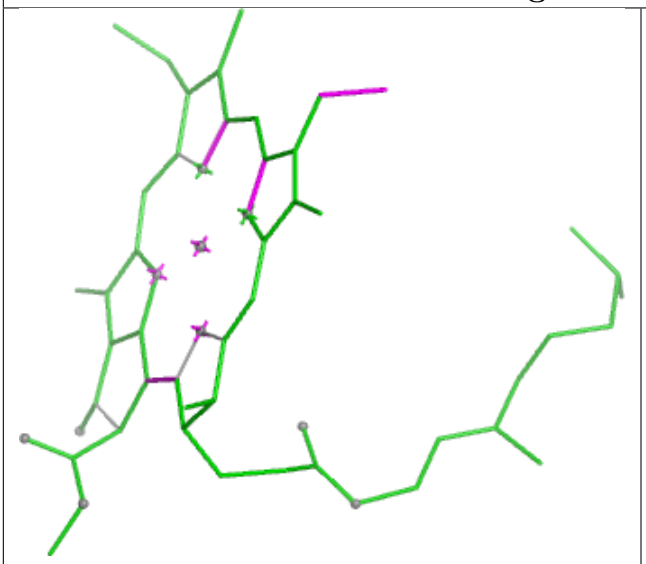


Rings

Ligand CLA 8 607



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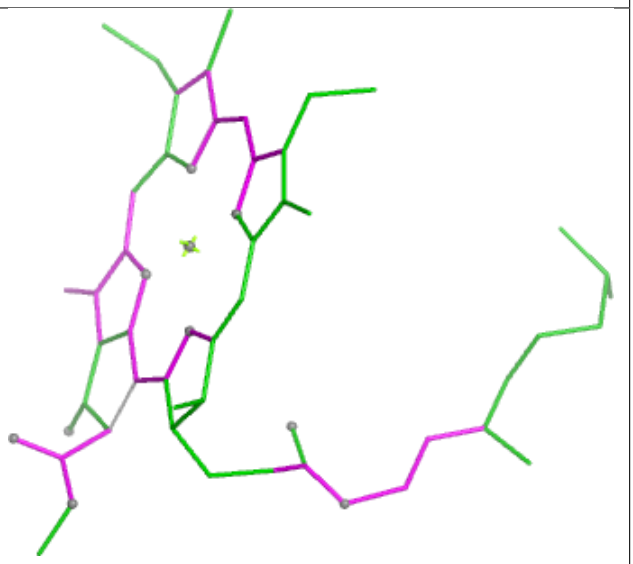

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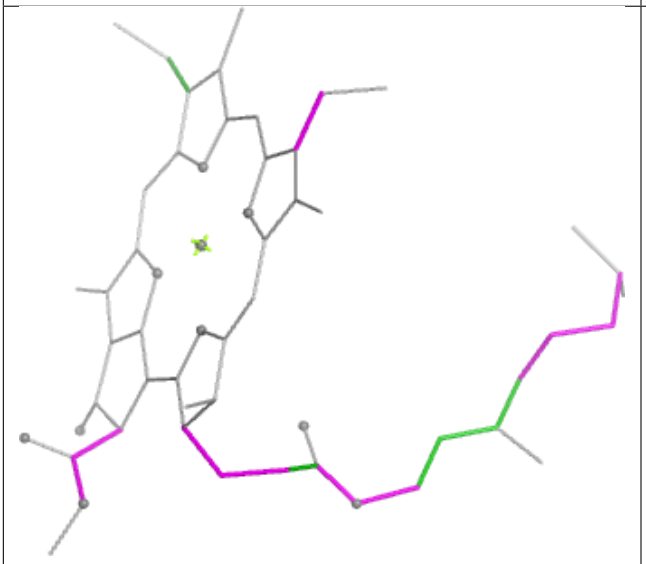

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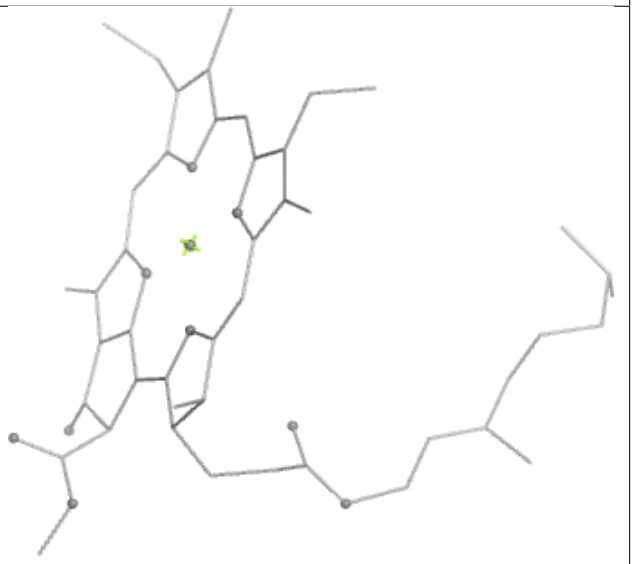
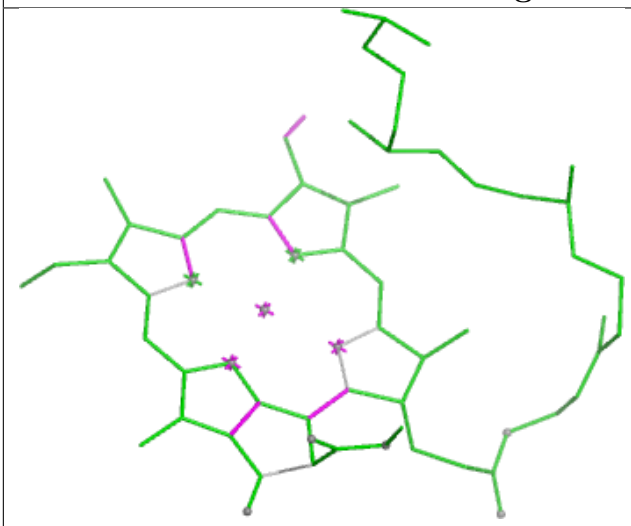


Rings

Ligand CLA A 1111



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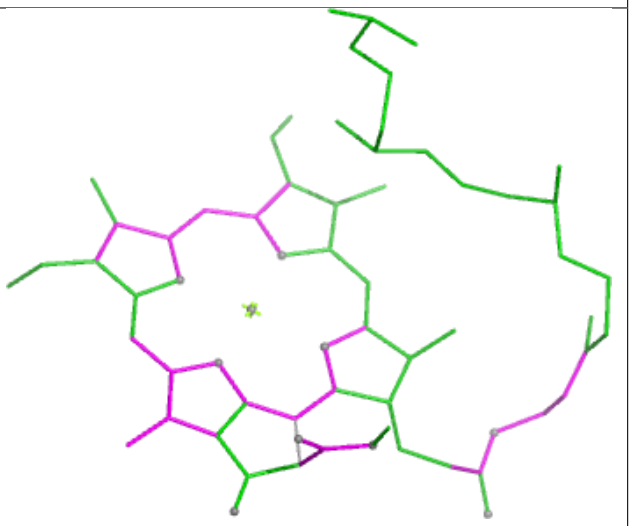

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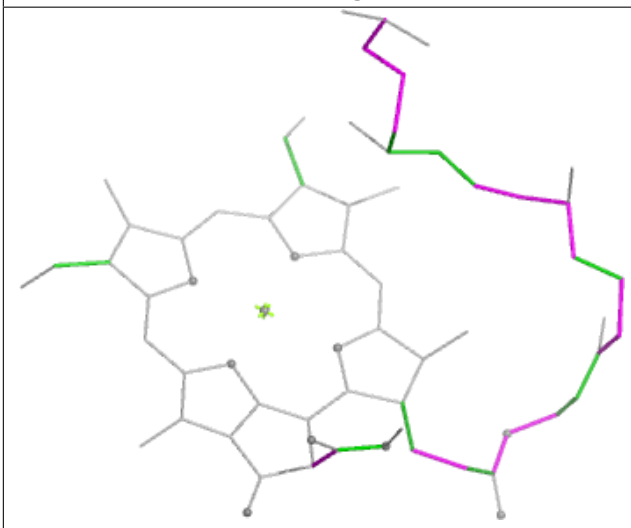

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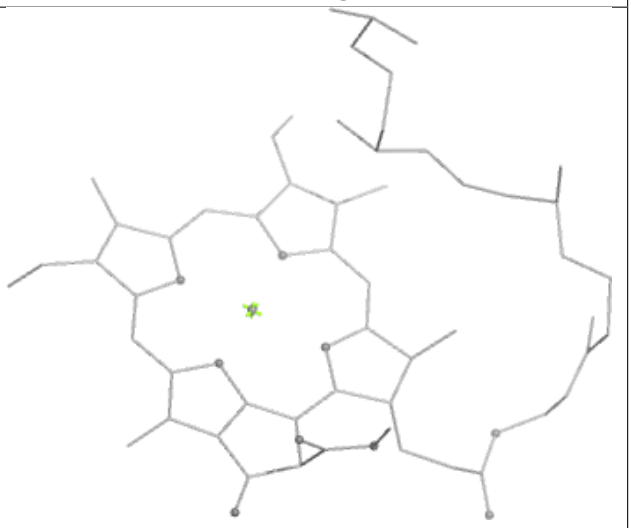
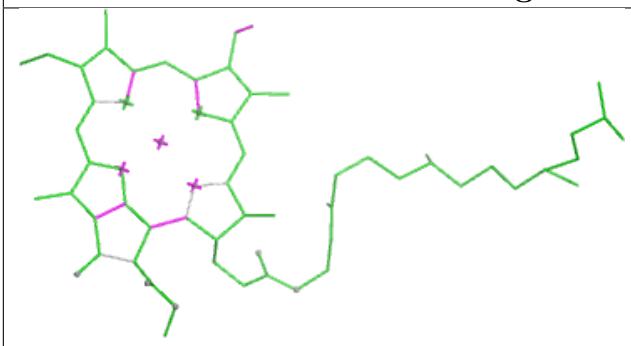


Rings

Ligand CLA B 1023



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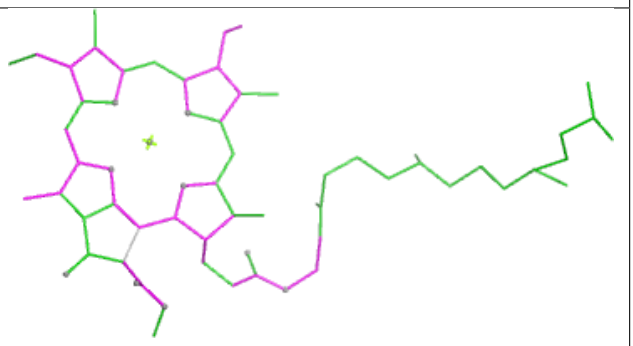
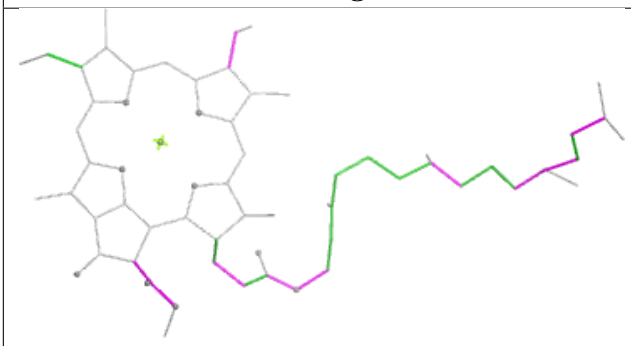


Bond angles



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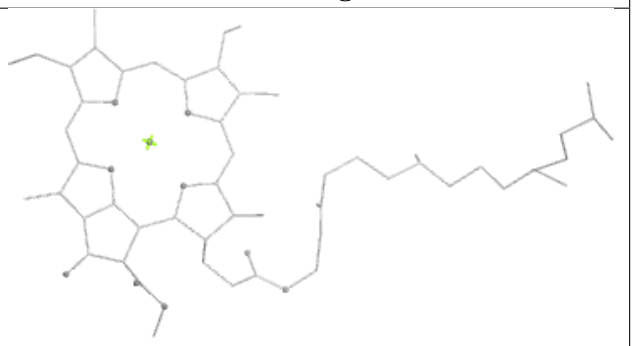
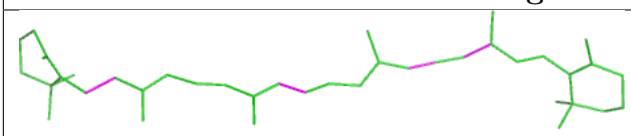


Rings

Ligand BCR 8 503



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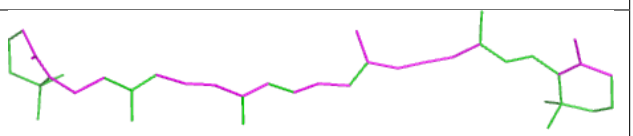

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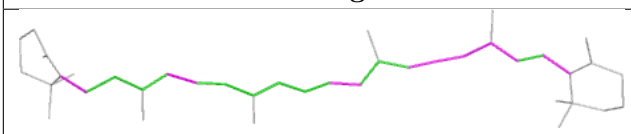

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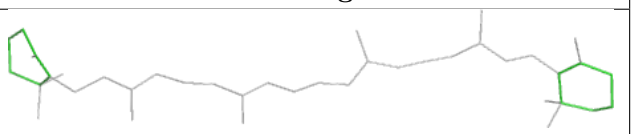
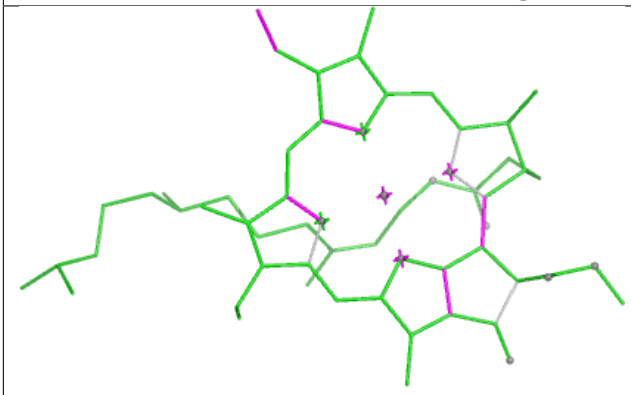


Rings

Ligand CLA A 1115



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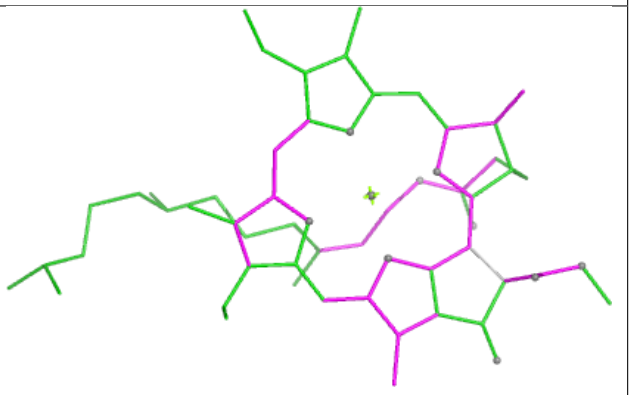
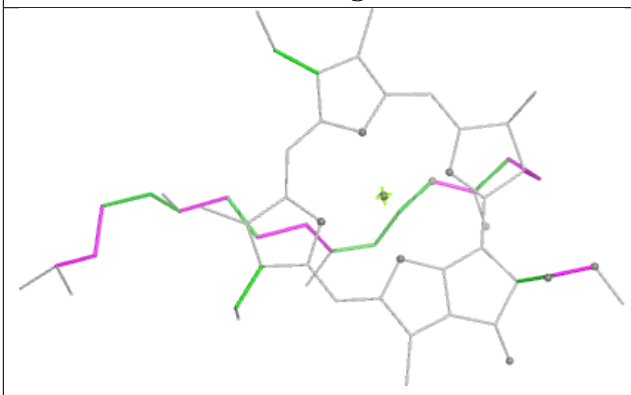


Bond angles



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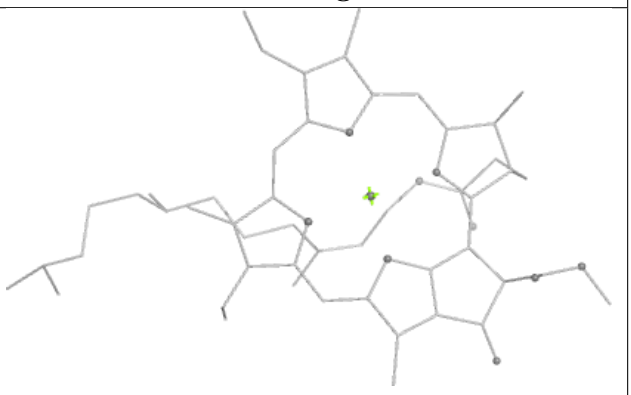
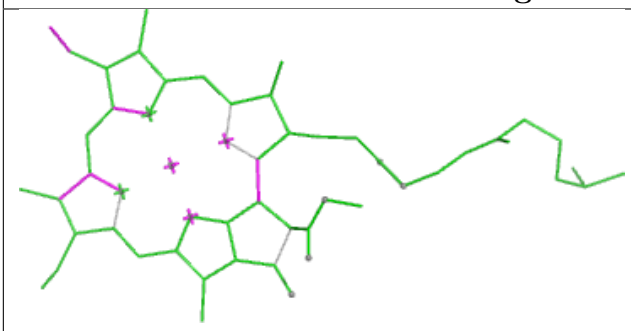


Rings

Ligand CLA K 1404



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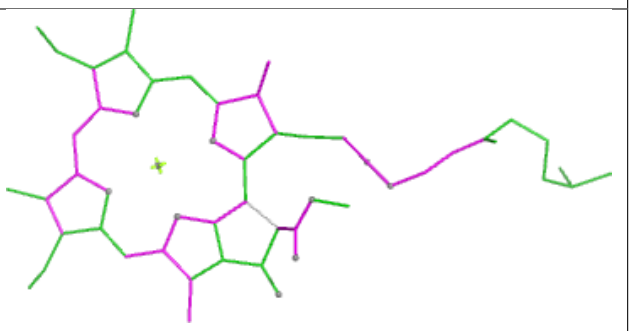
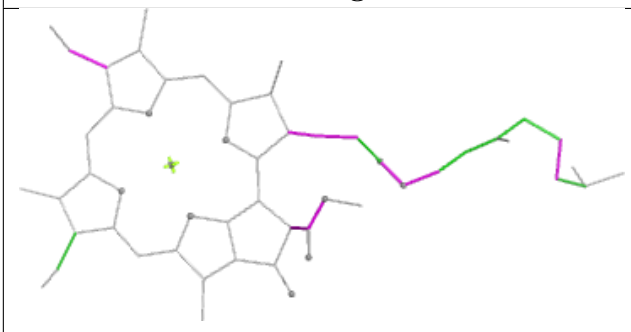


Bond angles



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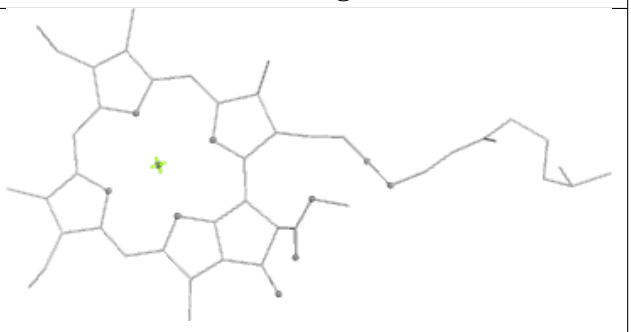
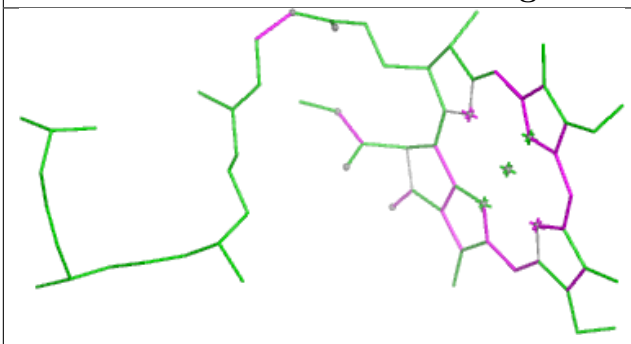


Rings

Ligand CL0 A 1011



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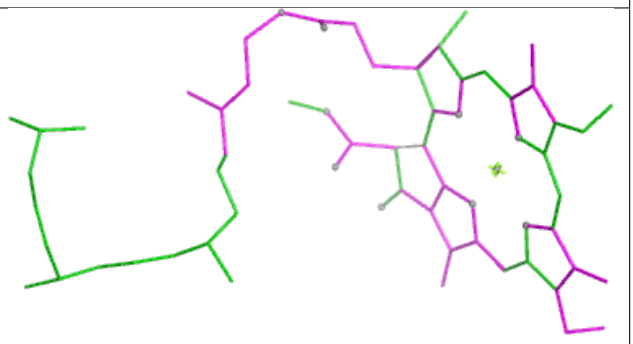
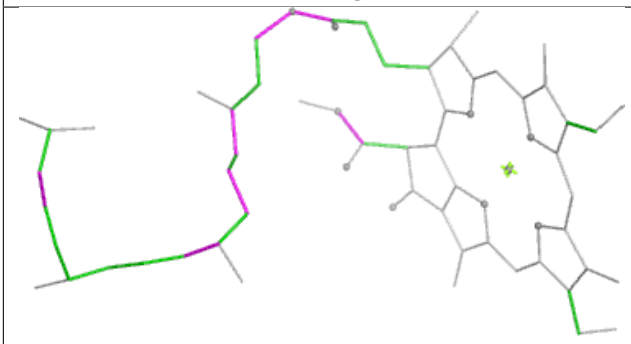
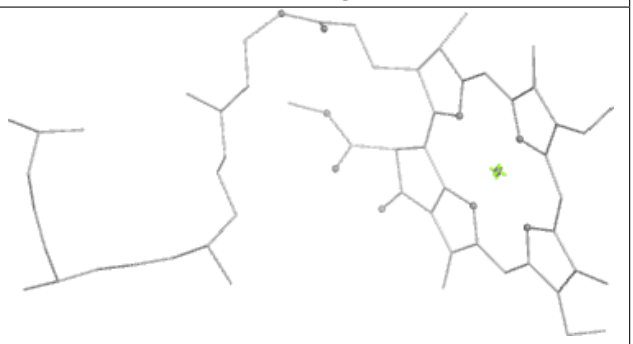


Bond angles

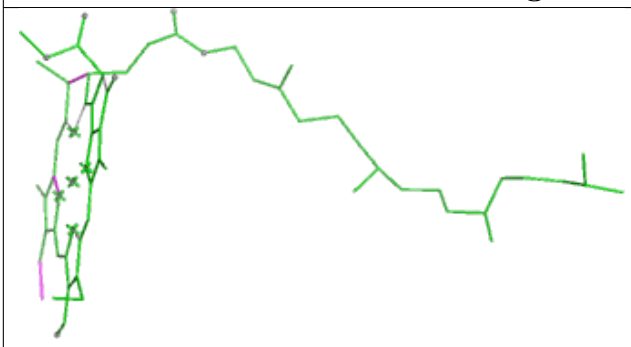


Torsions

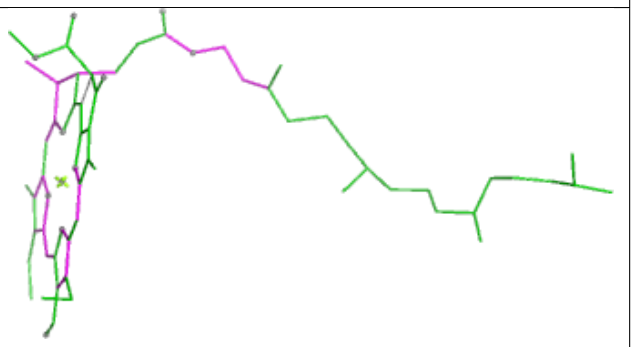


Rings

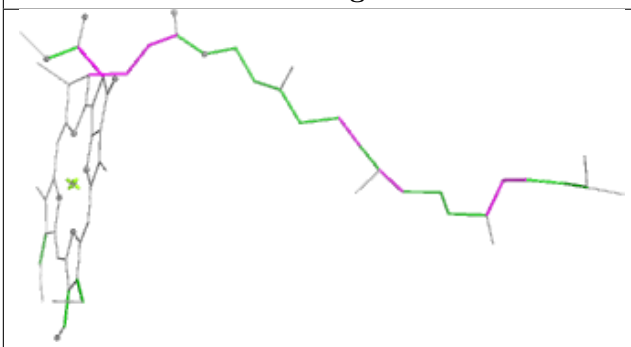
Ligand CHL Z 609



Bond lengths



Bond angles



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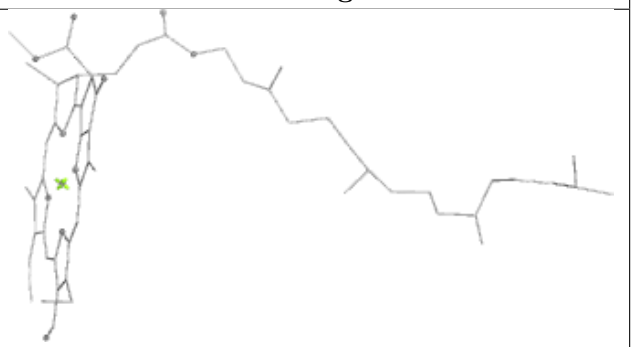
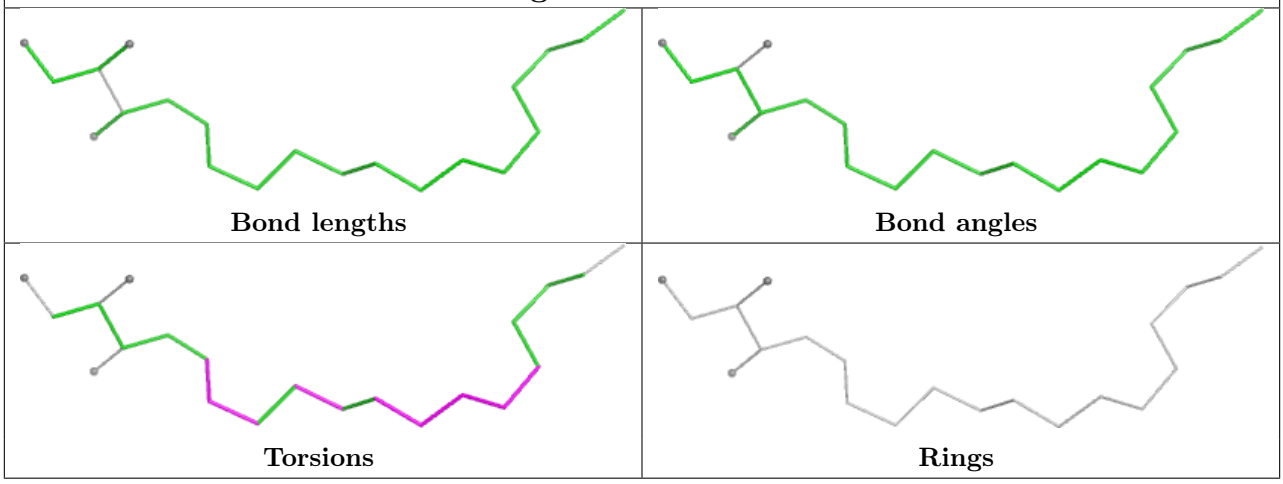
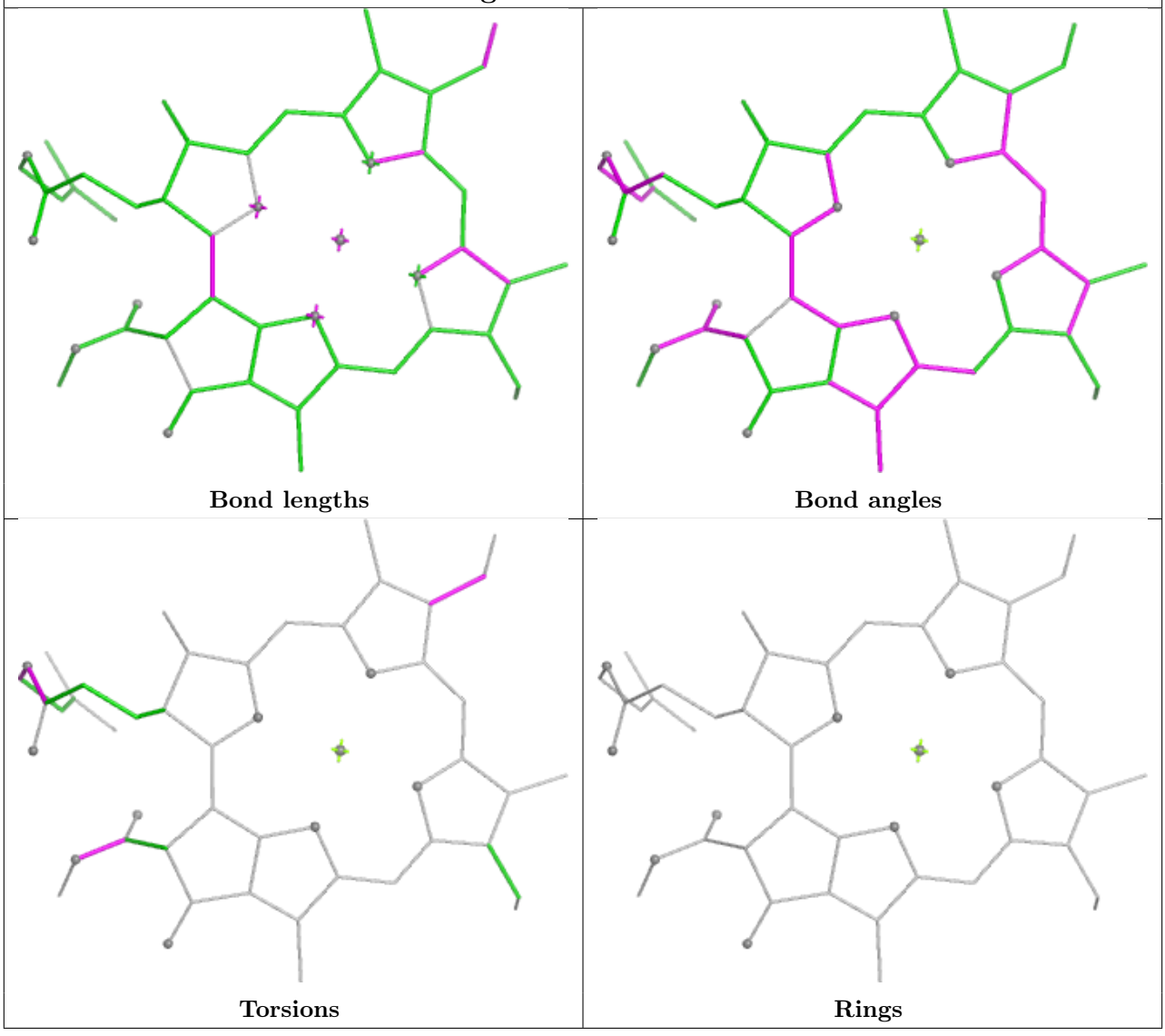


Rings

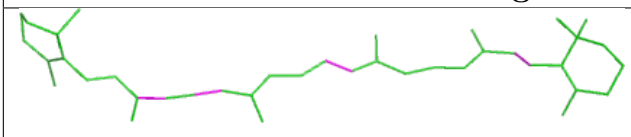
Ligand SPH 7 803



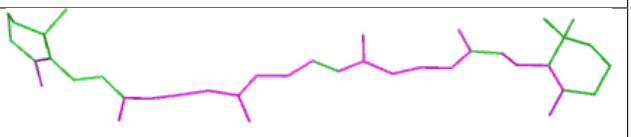
Ligand CLA 7 602



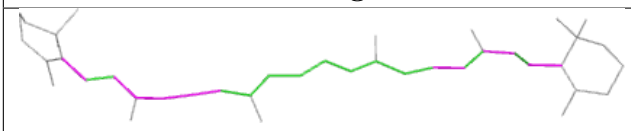
Ligand BCR G 4001



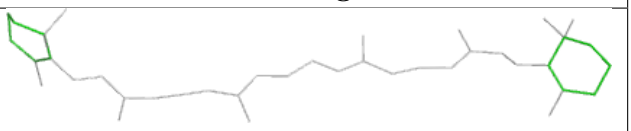
Bond lengths



Bond angles

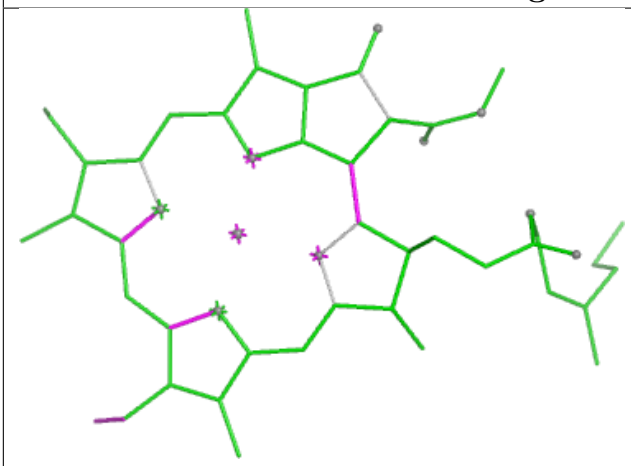


Torsions



Rings

Ligand CLA 4 602



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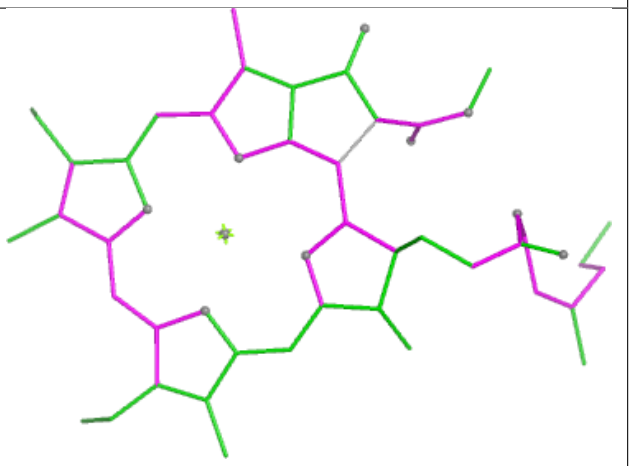

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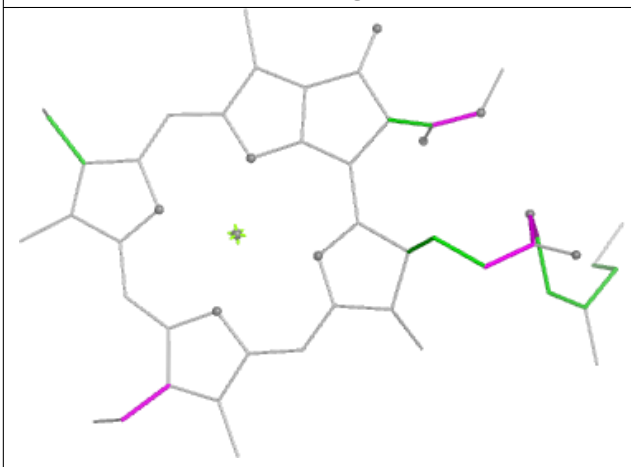

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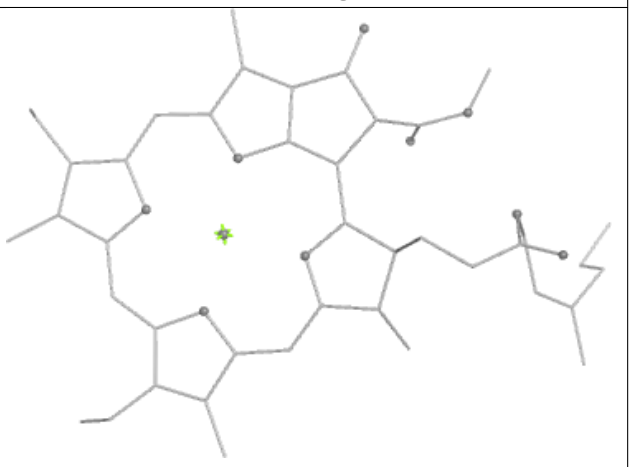
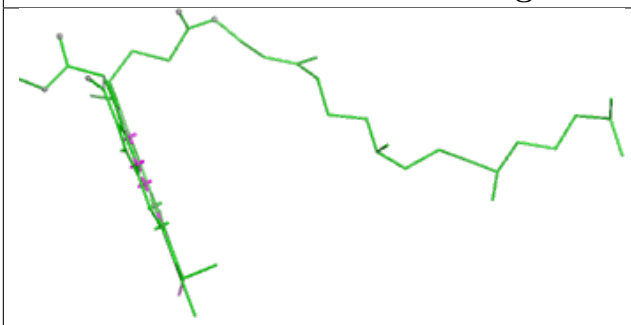


Rings

Ligand CLA B 1218



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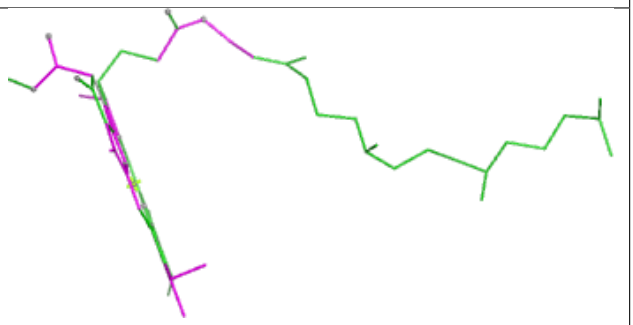
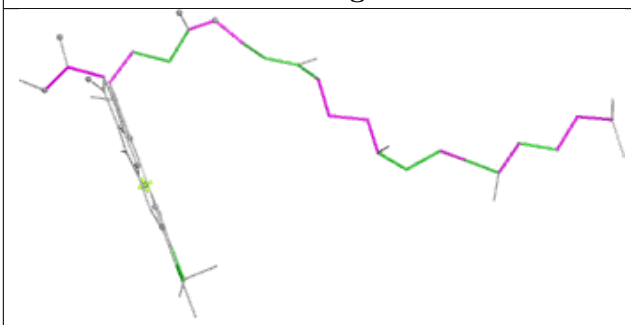


Bond angles

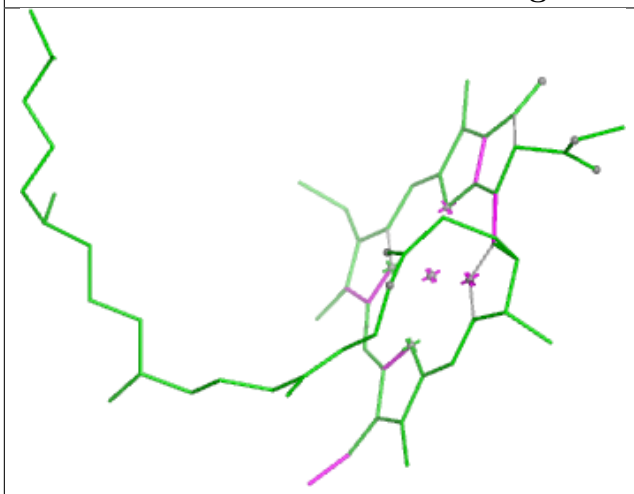


Torsions



Rings

Ligand CLA 3 601



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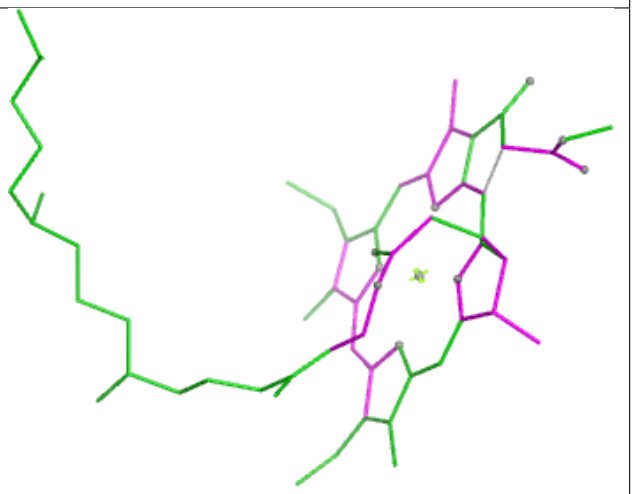

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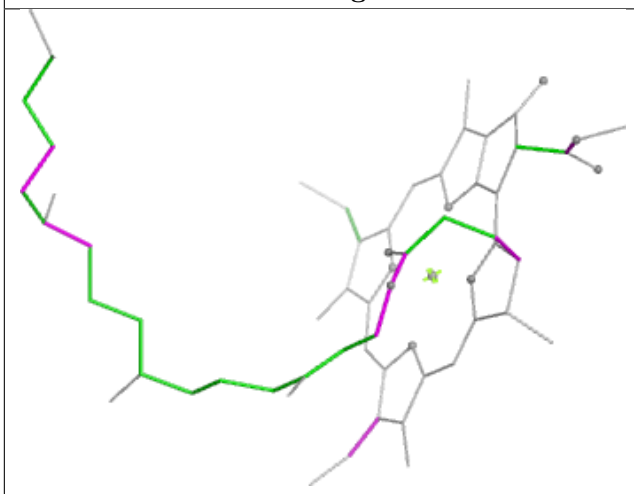

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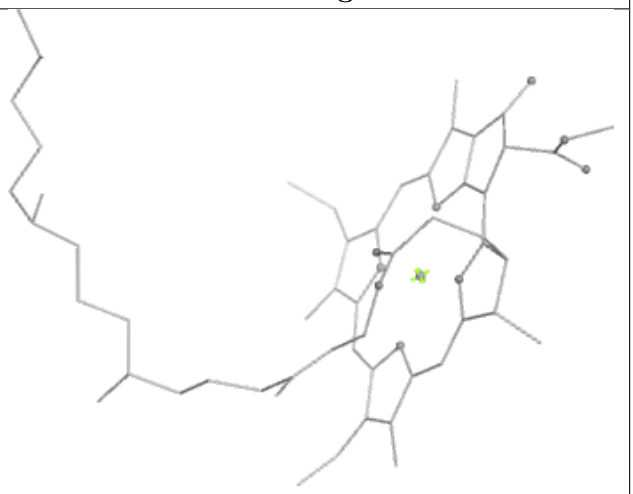
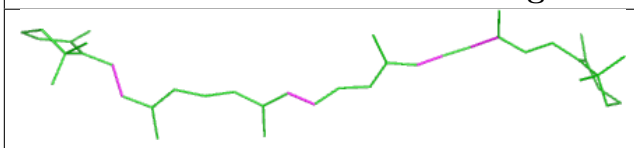


Rings

Ligand BCR 7 503



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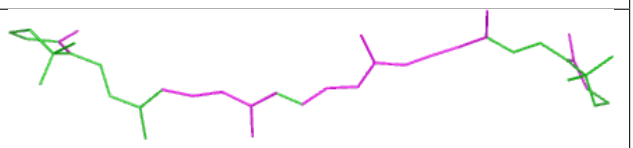
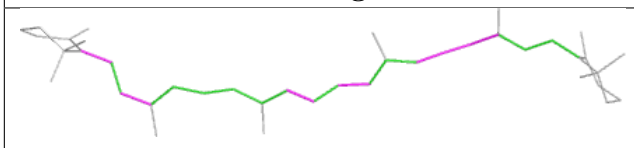


Bond angles



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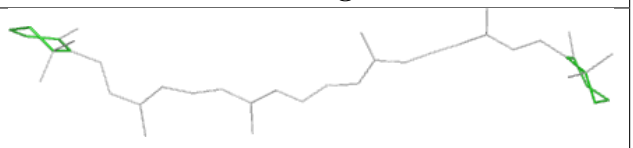
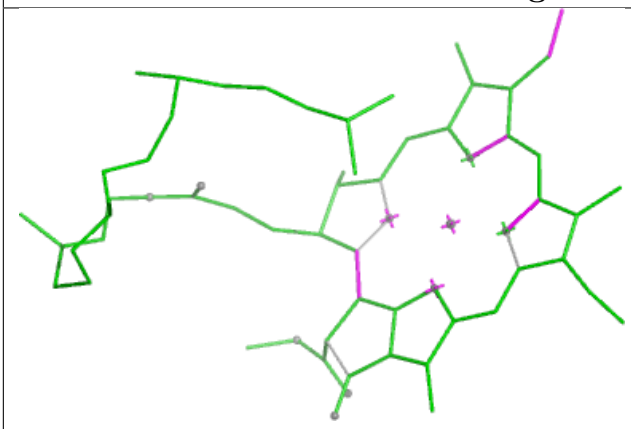


Rings

Ligand CLA 6 619



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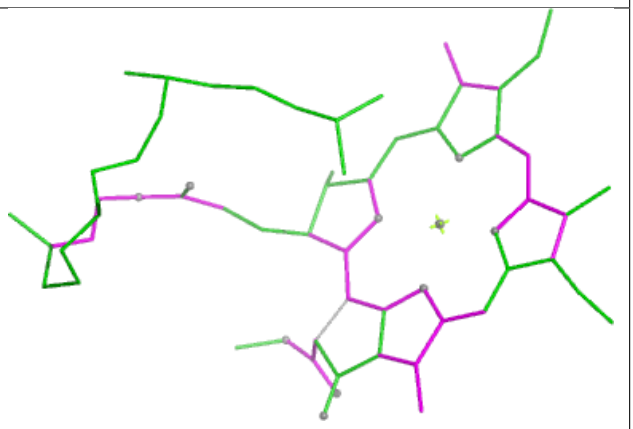

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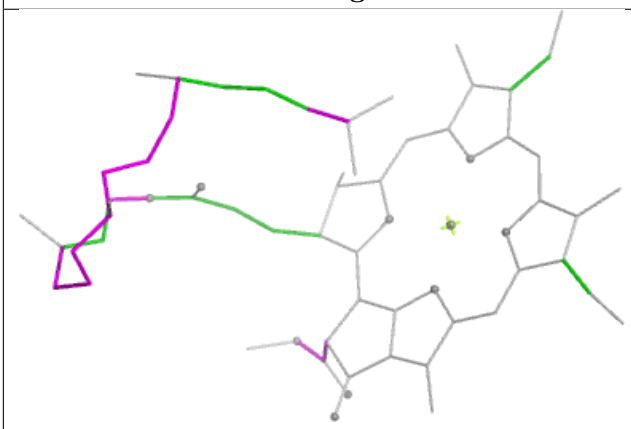

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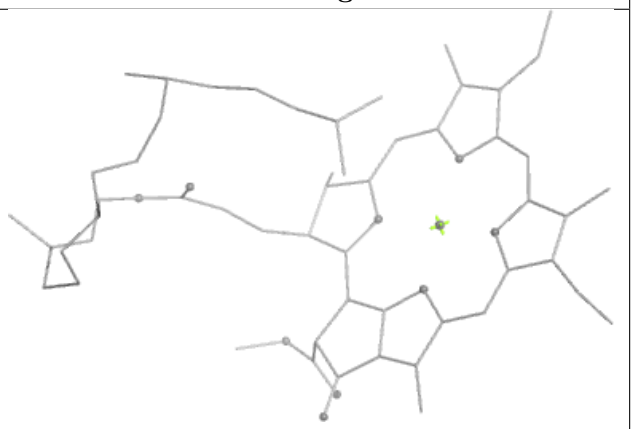
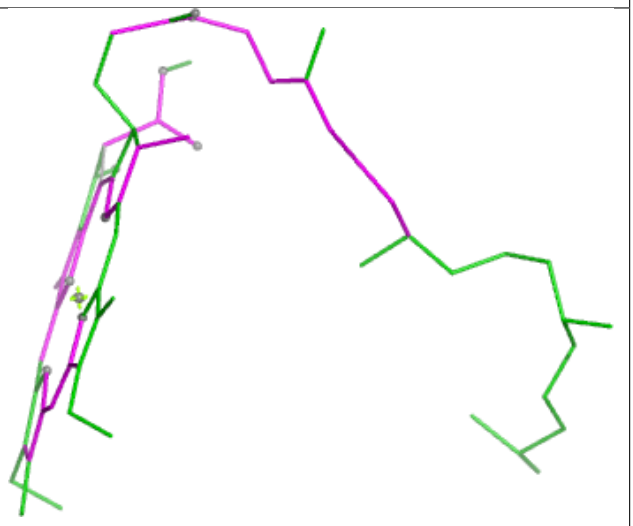


Rings

Ligand CLA 8 602



Bond lengths



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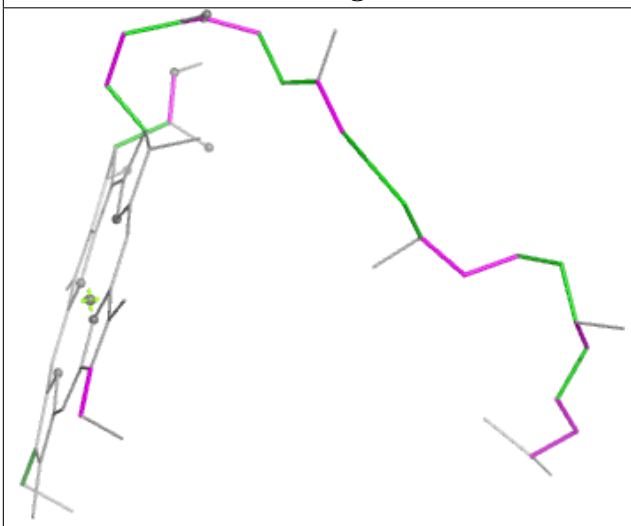
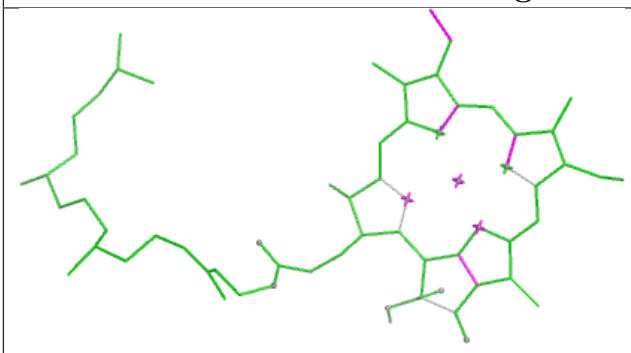


Torsions



Rings

Ligand CLA A 1125



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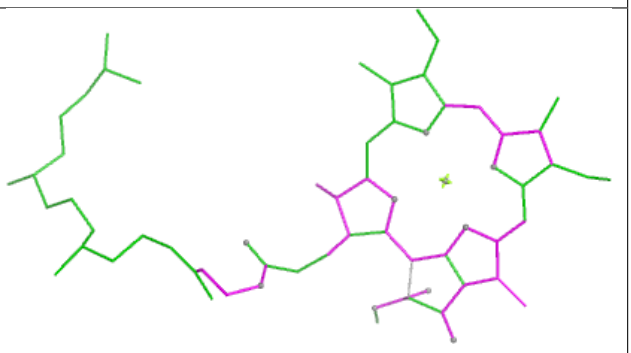

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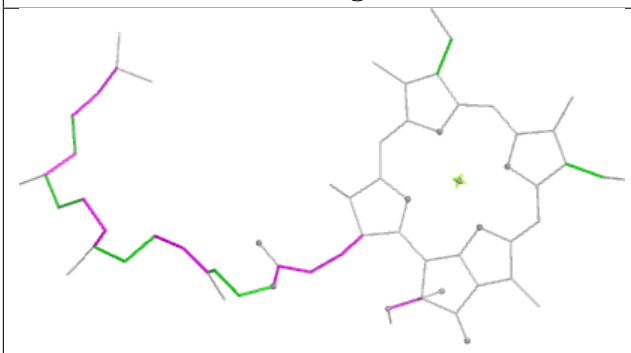

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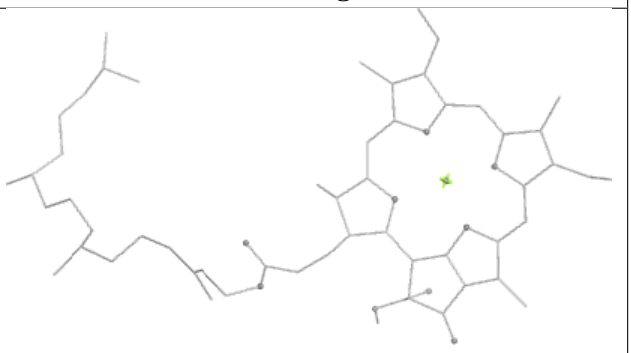
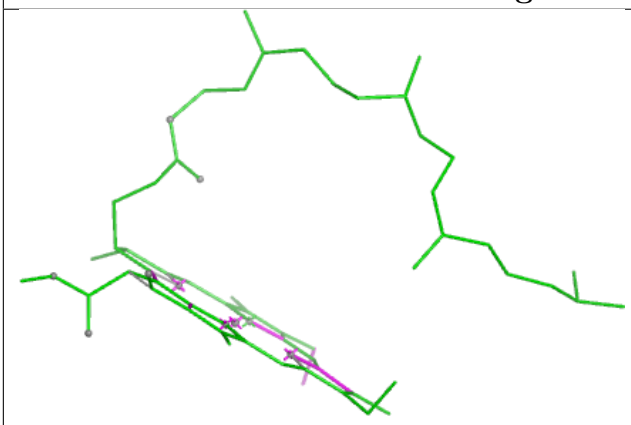


Rings

Ligand CLA B 1241



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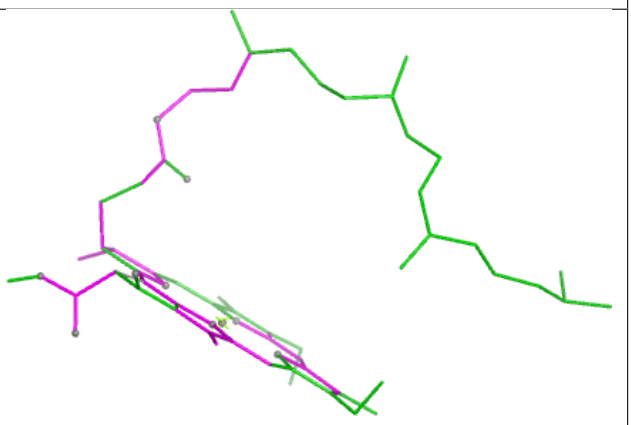
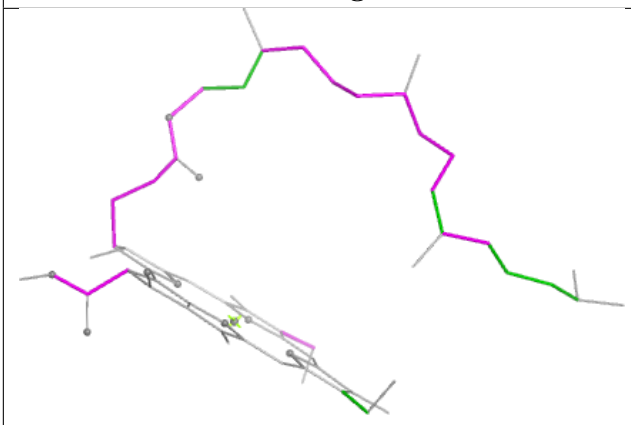


Bond angles



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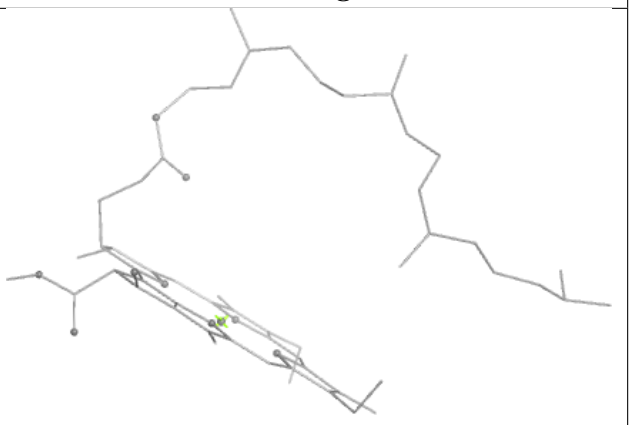
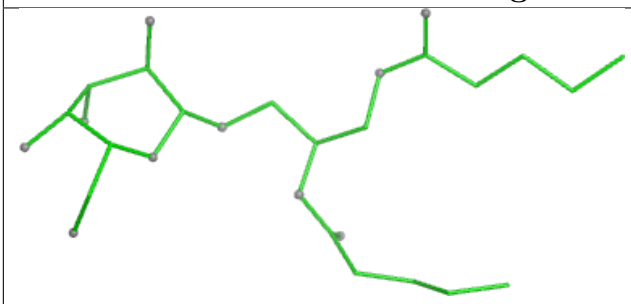


Rings

Ligand LMG A 5003



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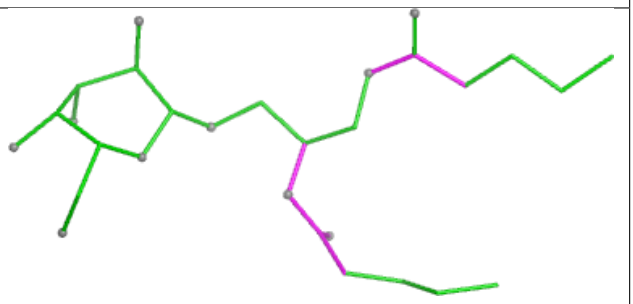
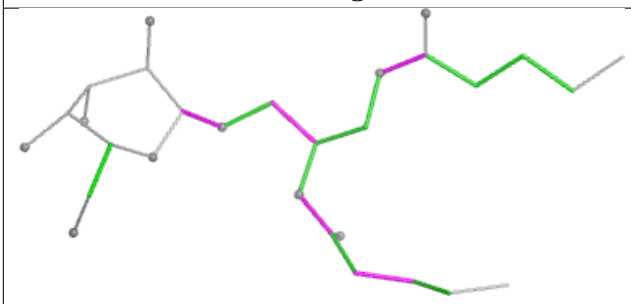


Bond angles



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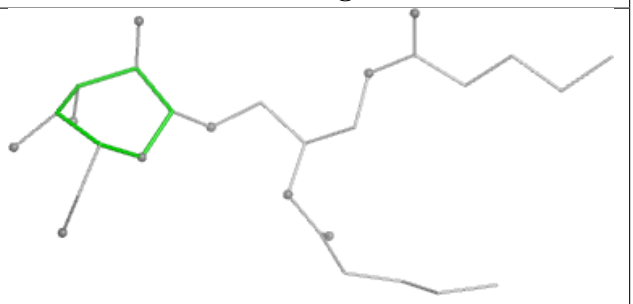
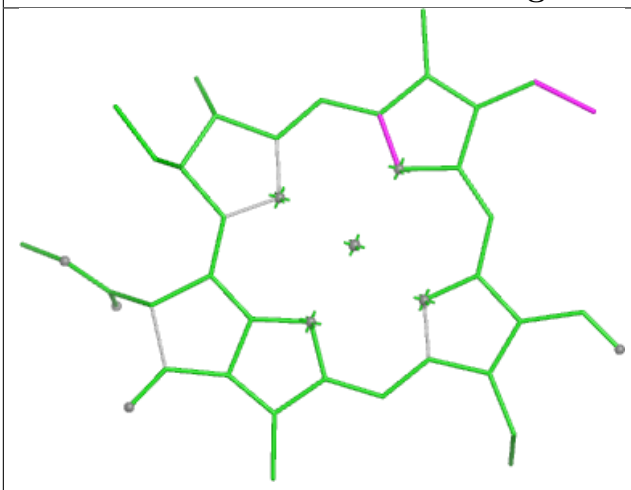


Rings

Ligand CHL 5 617



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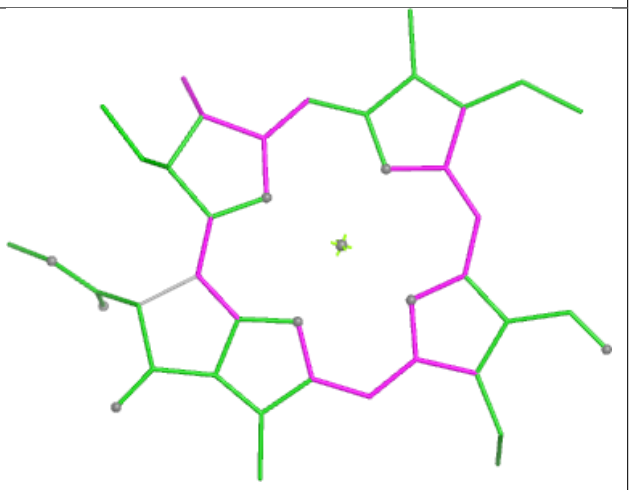
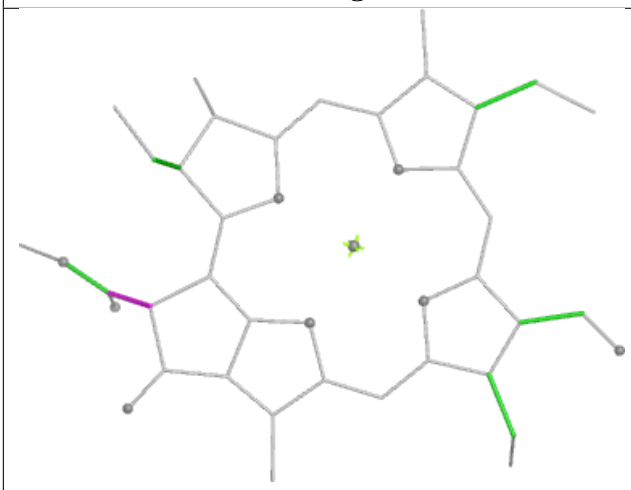


Bond angles



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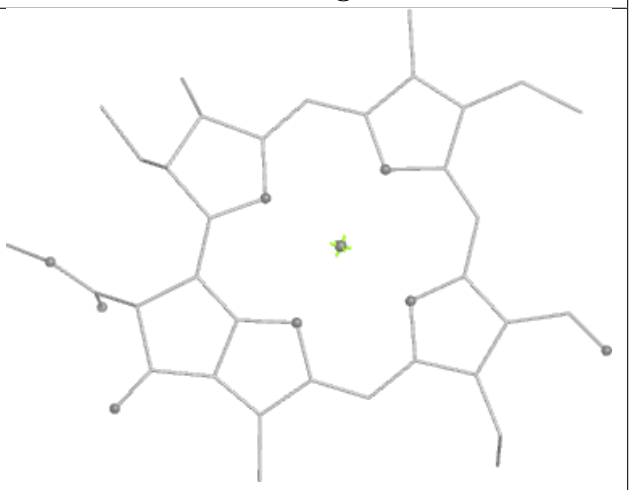
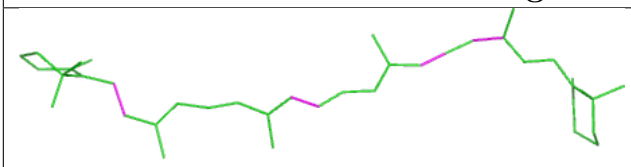


Rings

Ligand BCR 5 503



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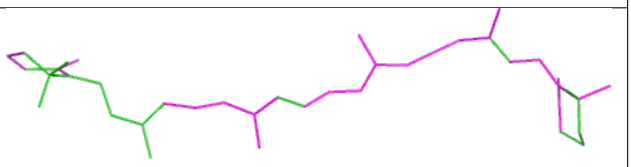
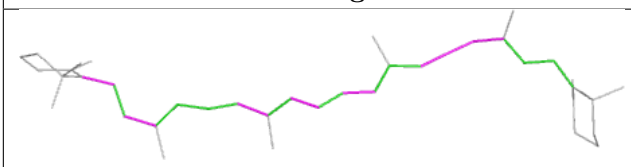


Bond angles



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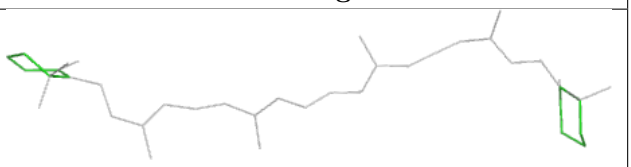
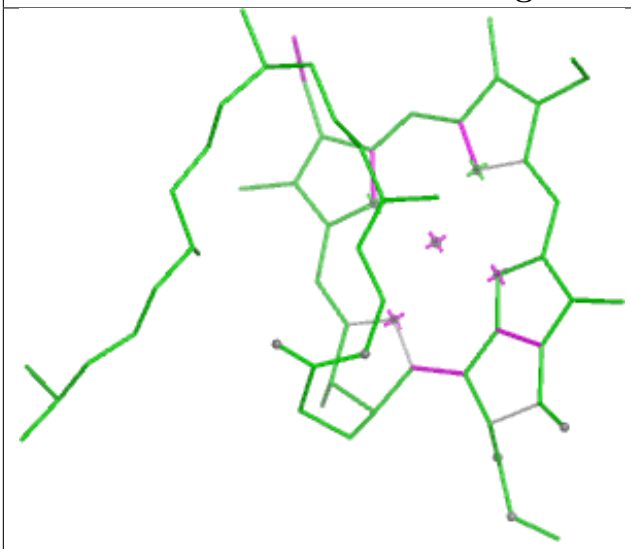


Rings

Ligand CLA B 1205



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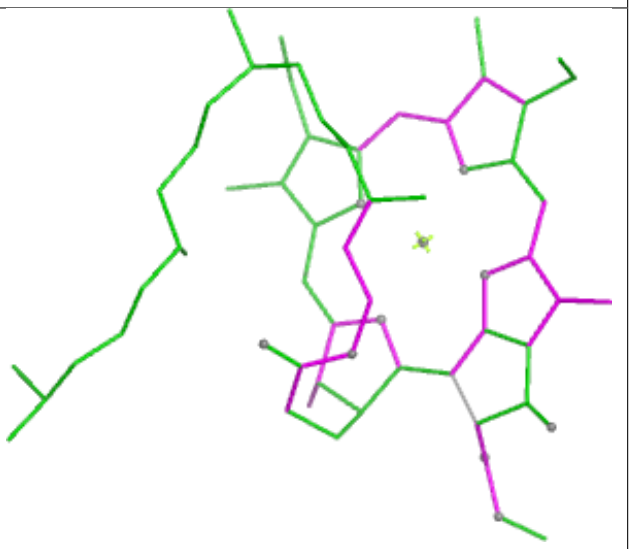
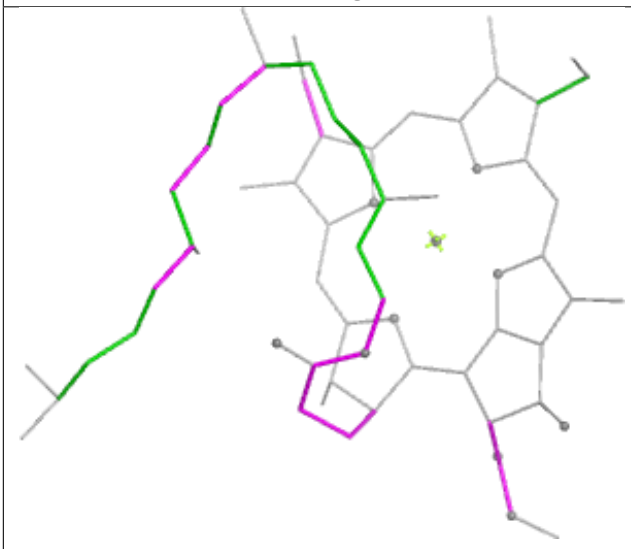


Bond angles

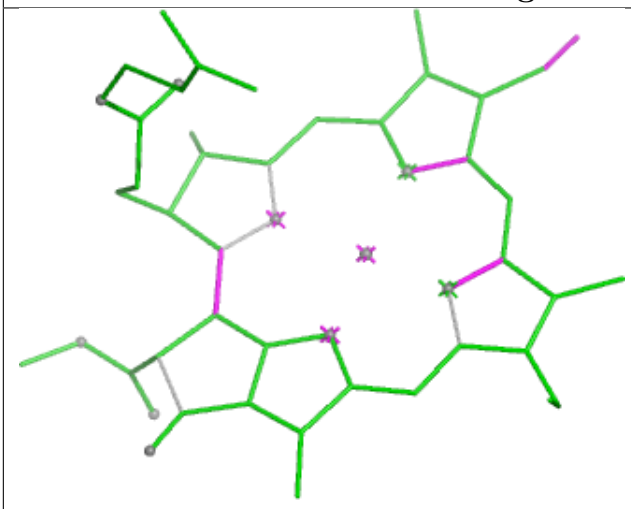


Torsions



Rings

Ligand CLA L 1503



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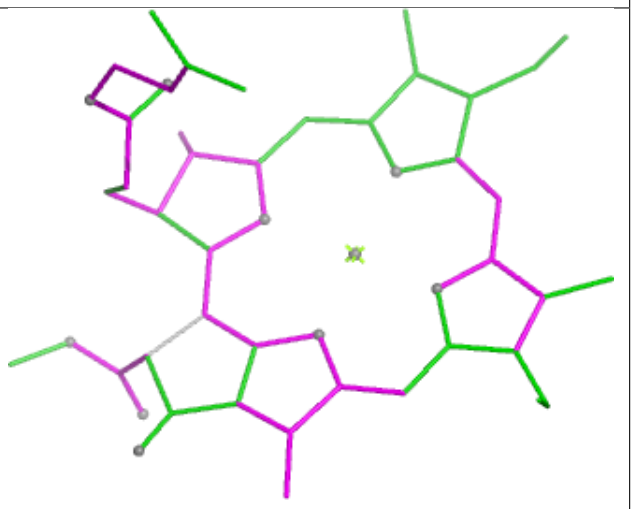
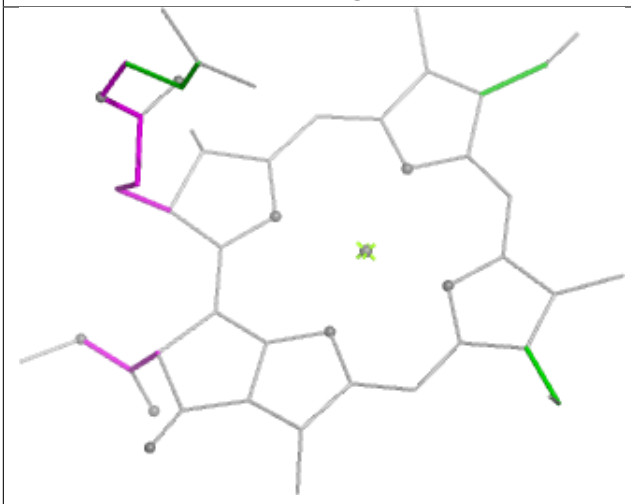


Bond angles



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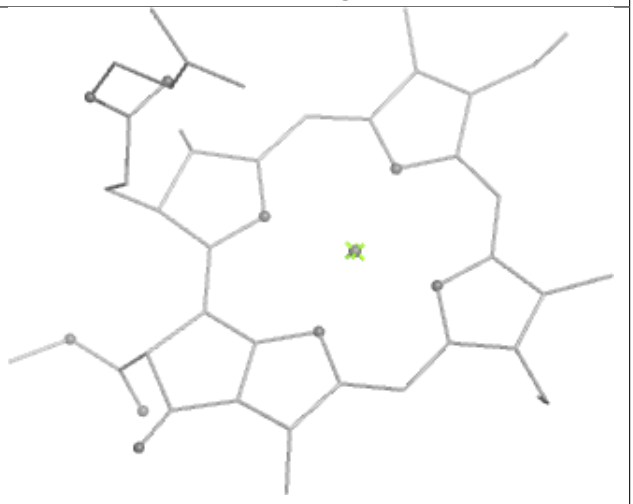
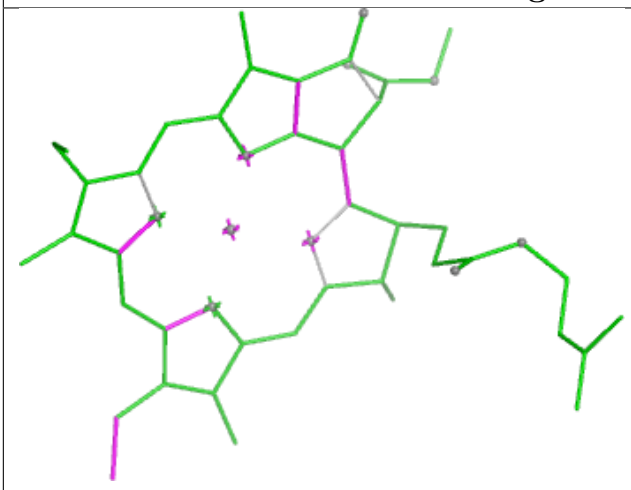


Rings

Ligand CLA 8 611



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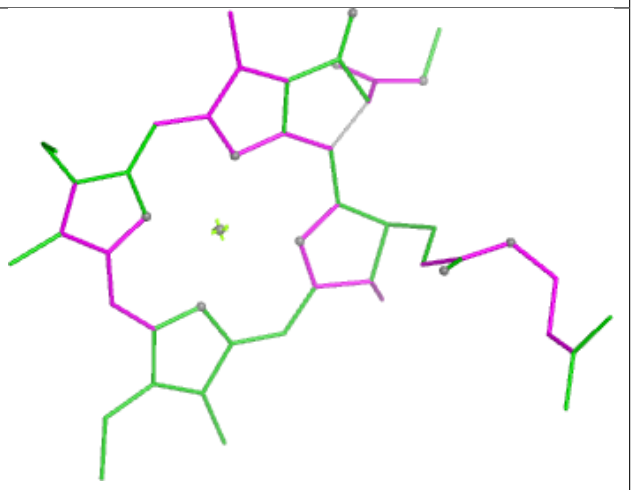
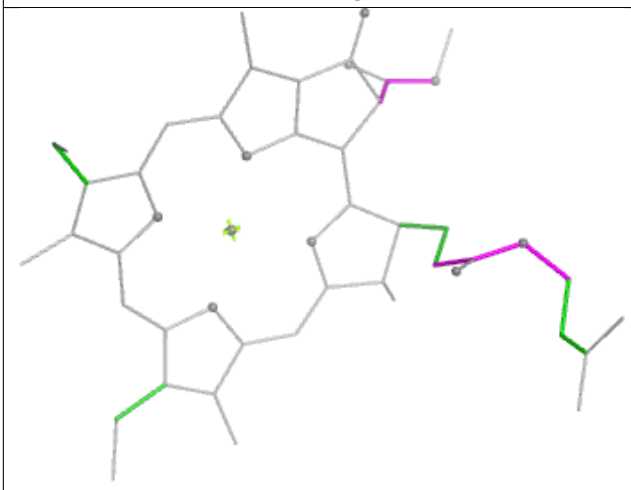


Bond angles



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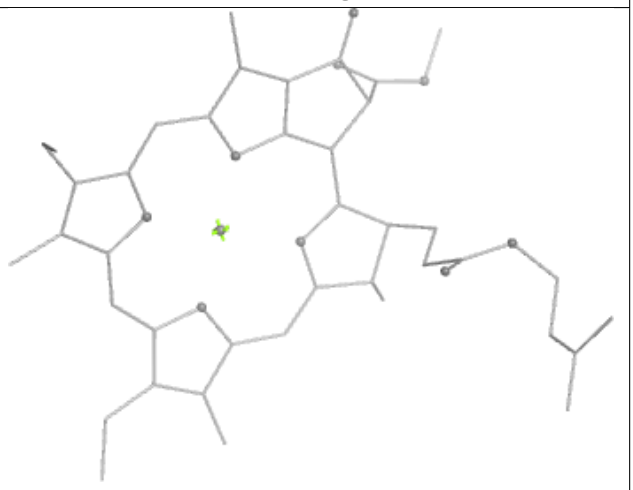
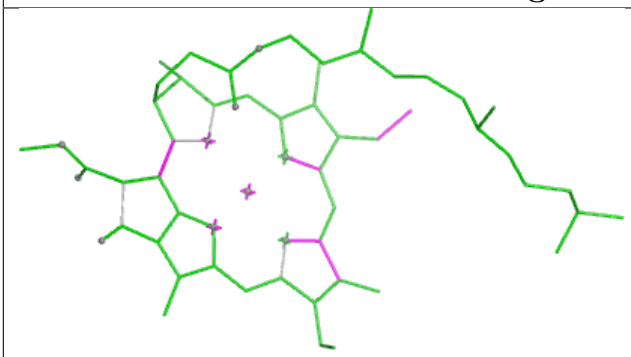
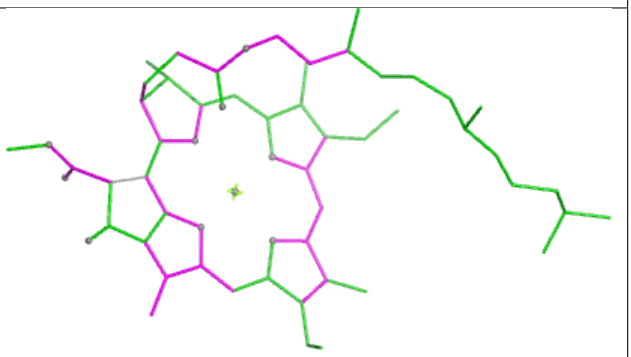


Rings

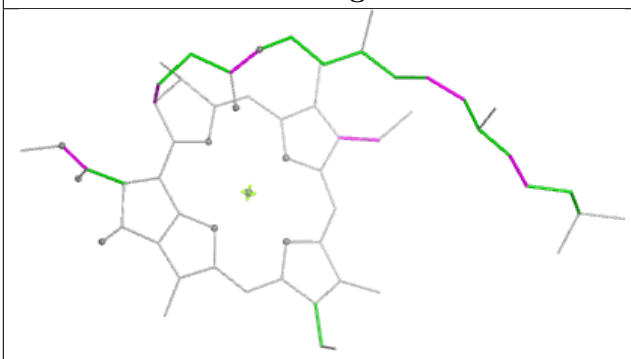
Ligand CLA 4 601



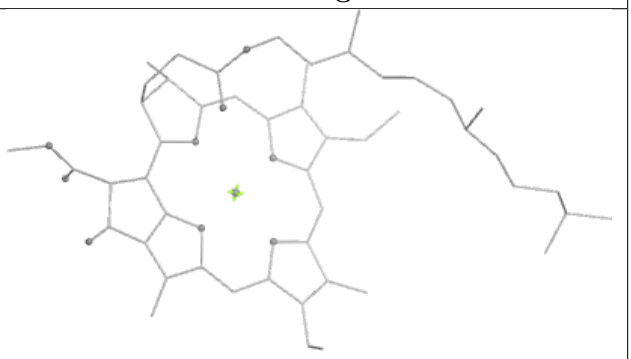
Bond lengths



Bond angles

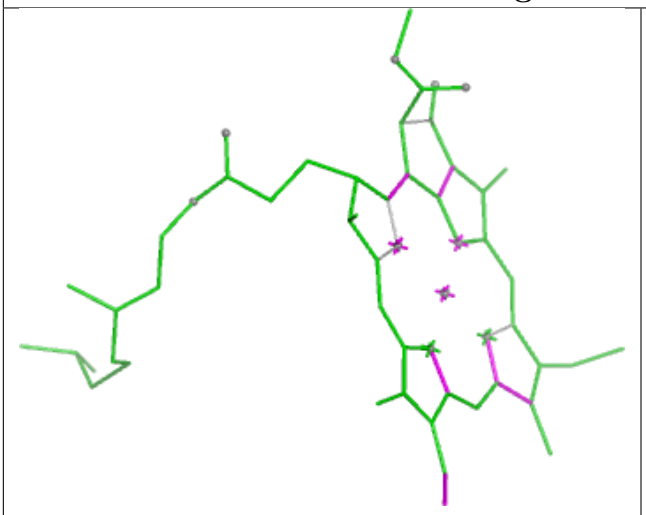


Torsions



Rings

Ligand CLA A 1102



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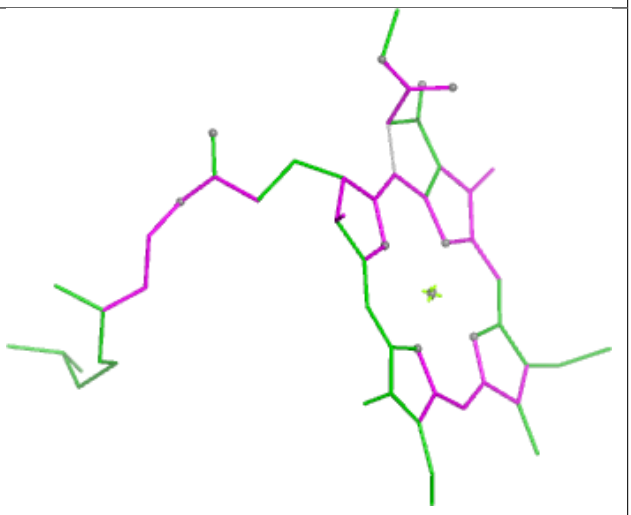

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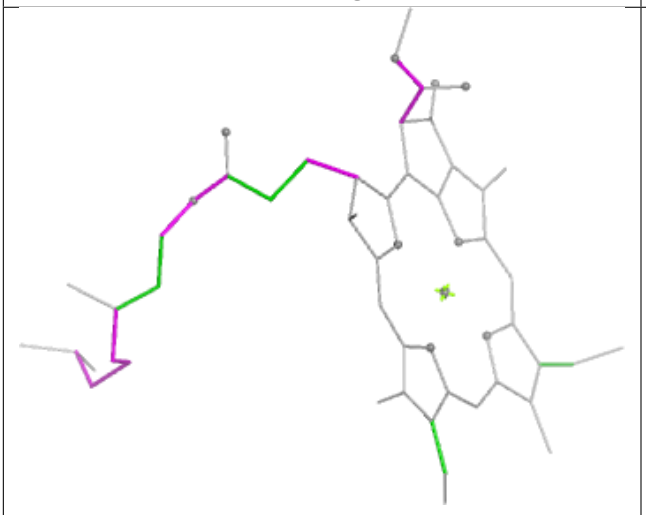

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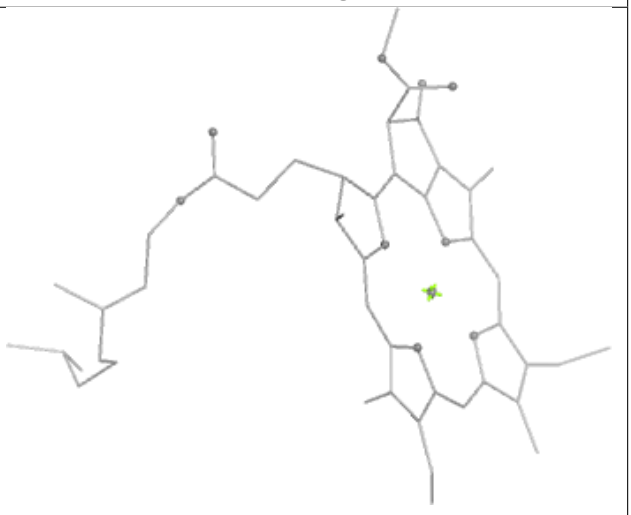
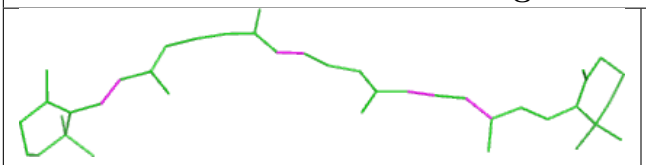


Rings

Ligand BCR B 4005



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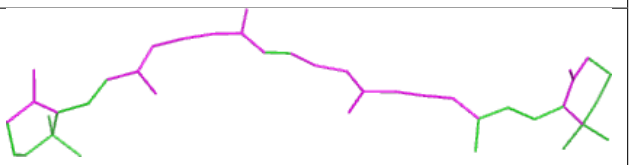

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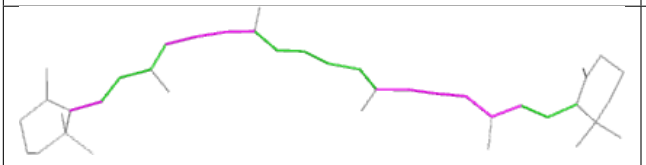

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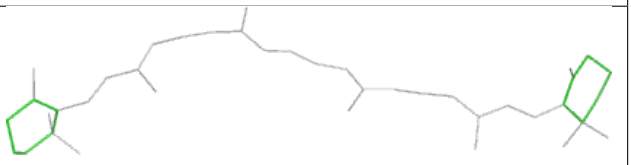
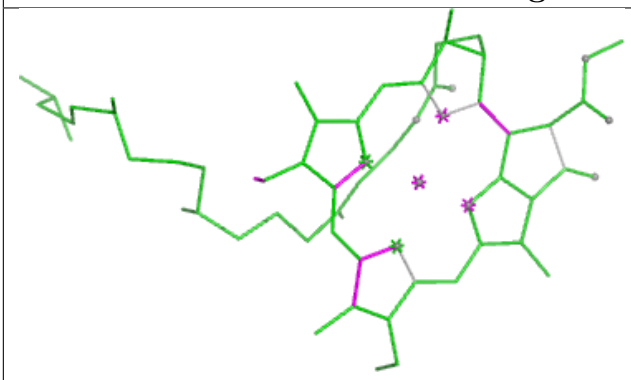


Rings

Ligand CLA 1 603



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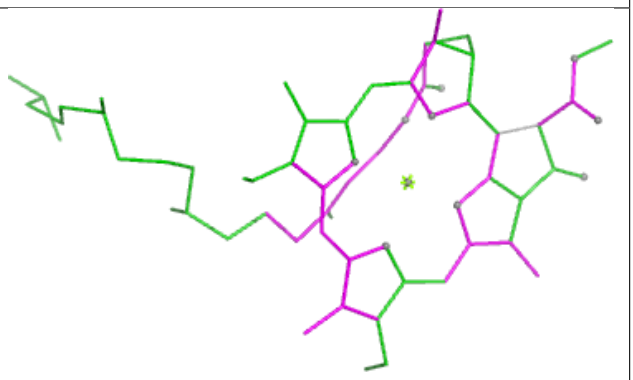

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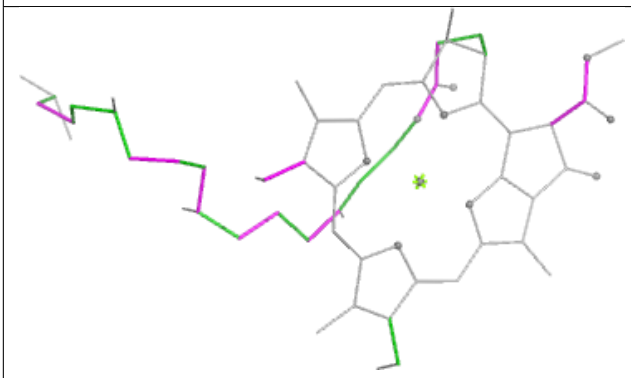

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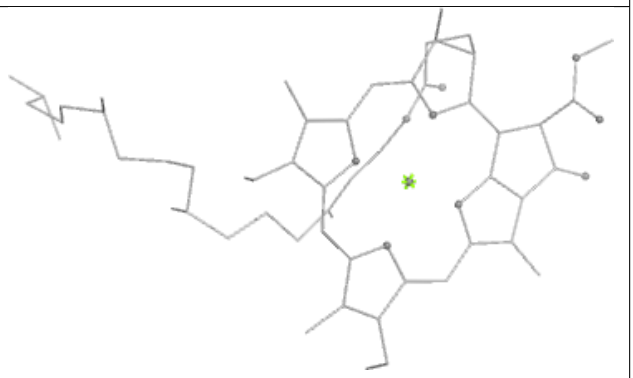
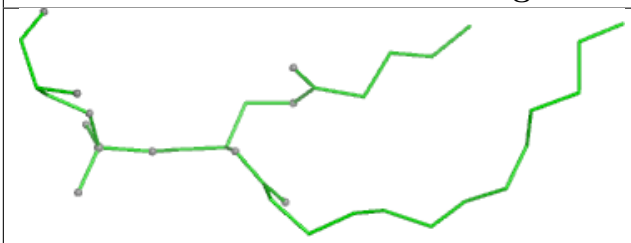


Rings

Ligand LHG A 5001



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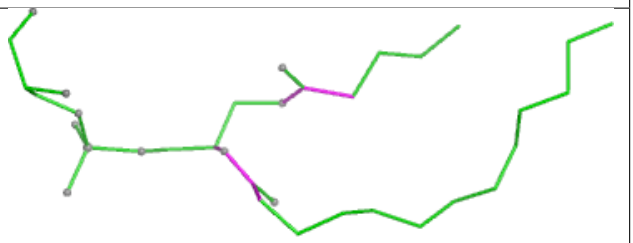

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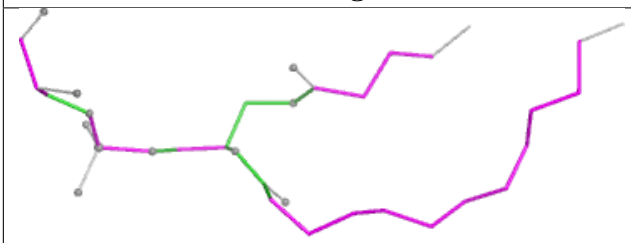

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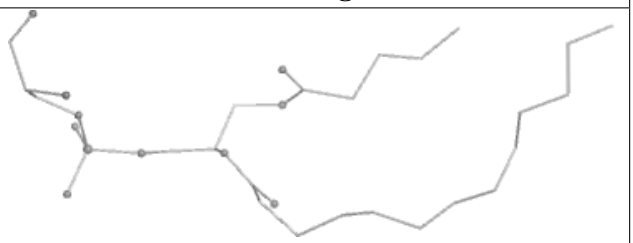
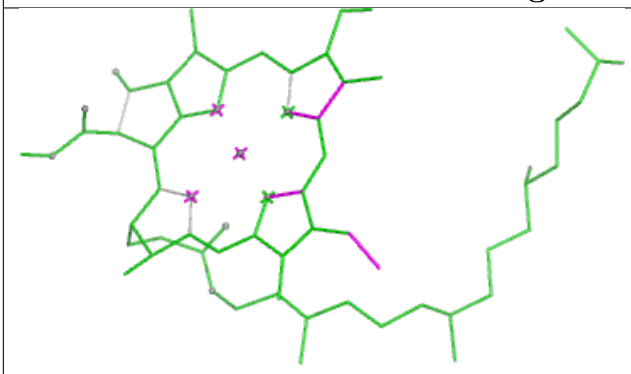


Rings

Ligand CLA 6 604



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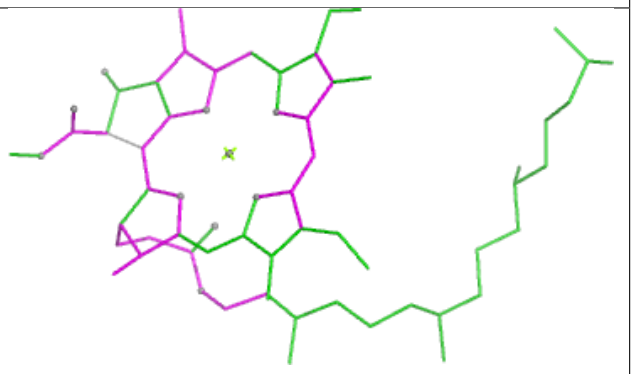

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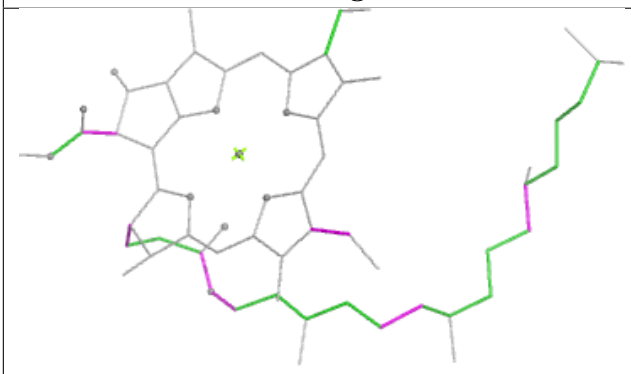

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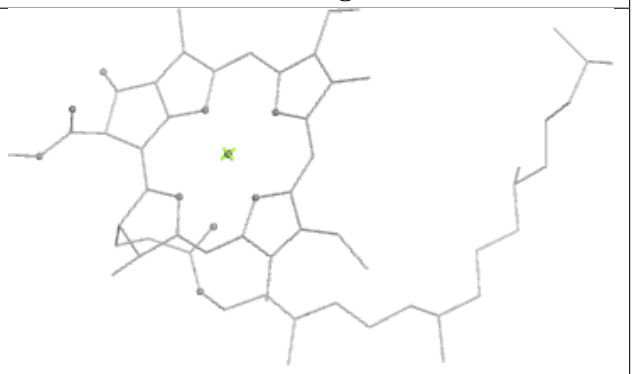
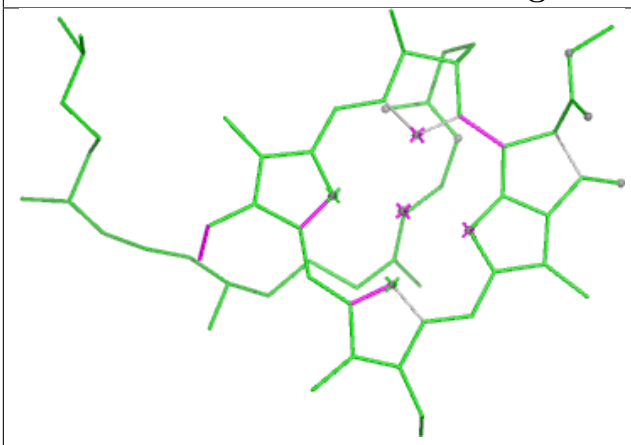


Rings

Ligand CLA 6 603



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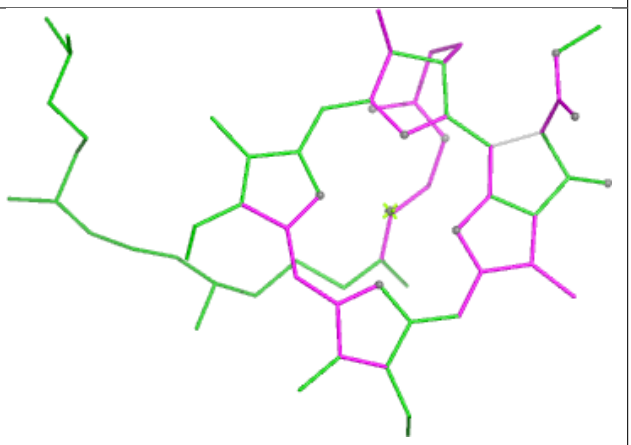
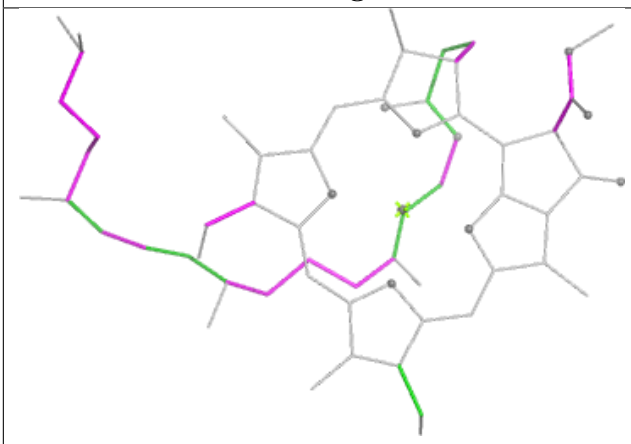


Bond angles



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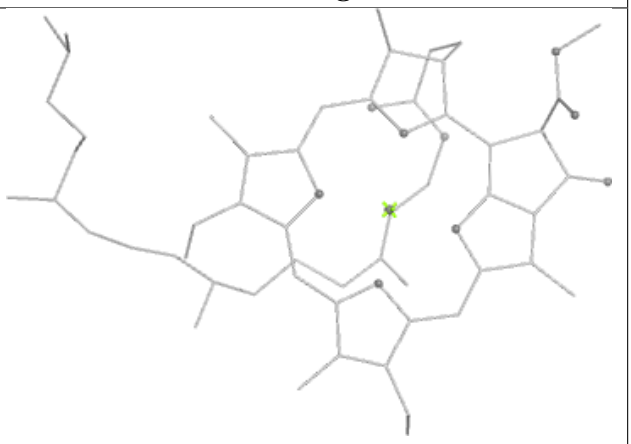
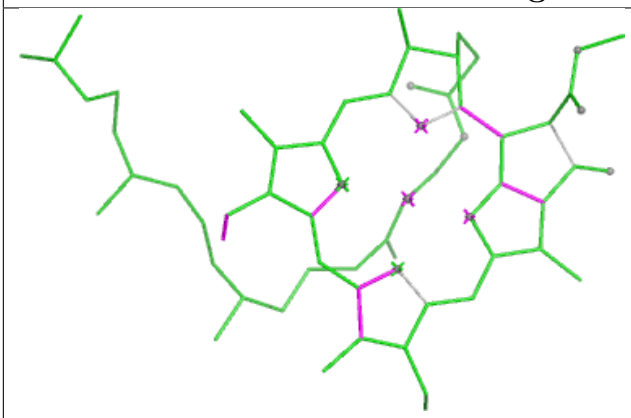


Rings

Ligand CLA 7 603



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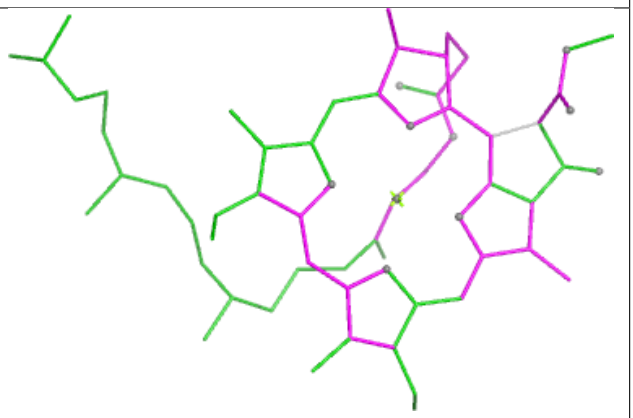

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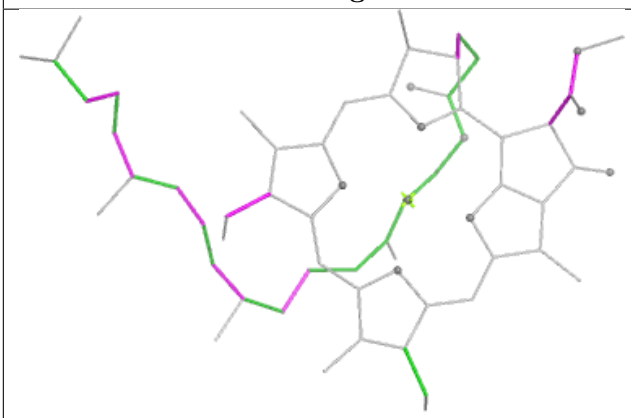

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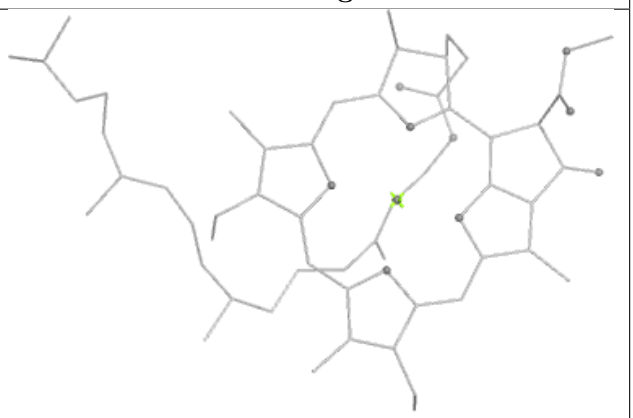
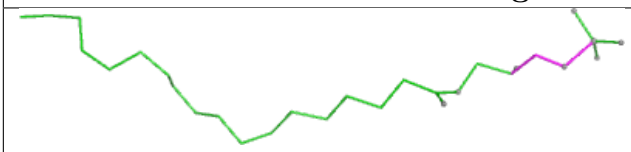


Rings

Ligand NKP A 5004



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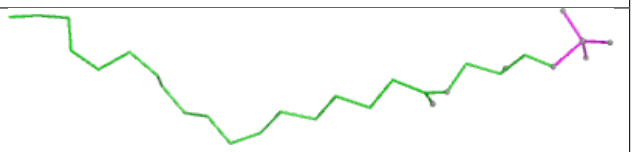
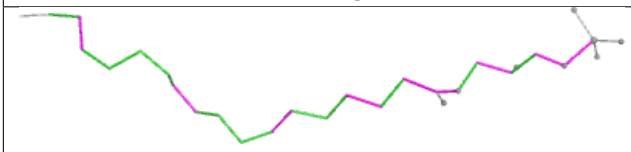


Bond angles



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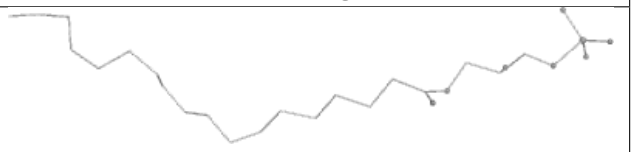
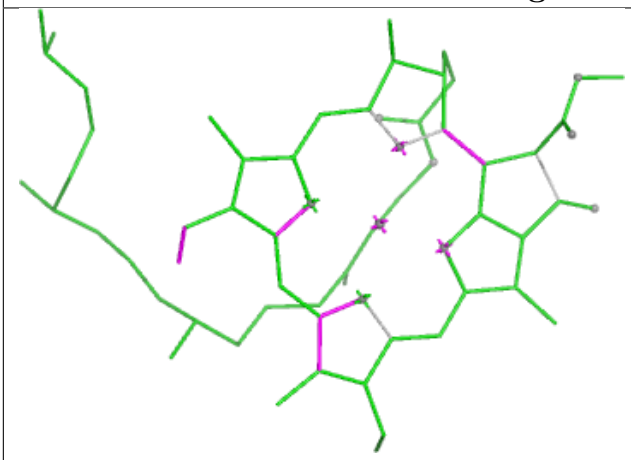


Rings

Ligand CLA 8 603



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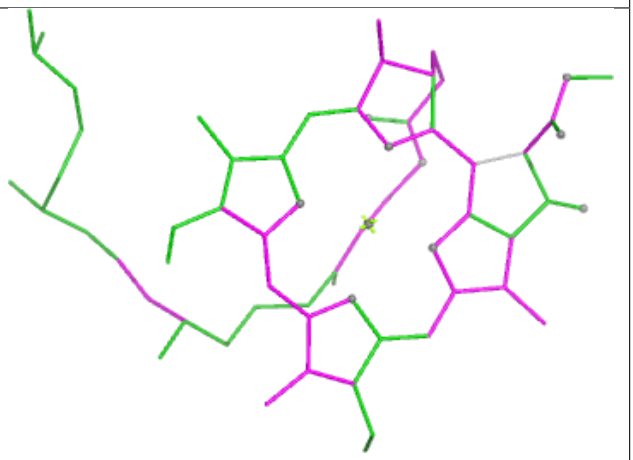

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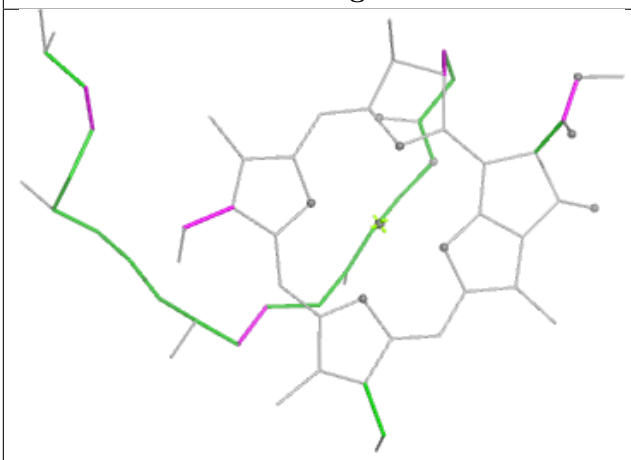

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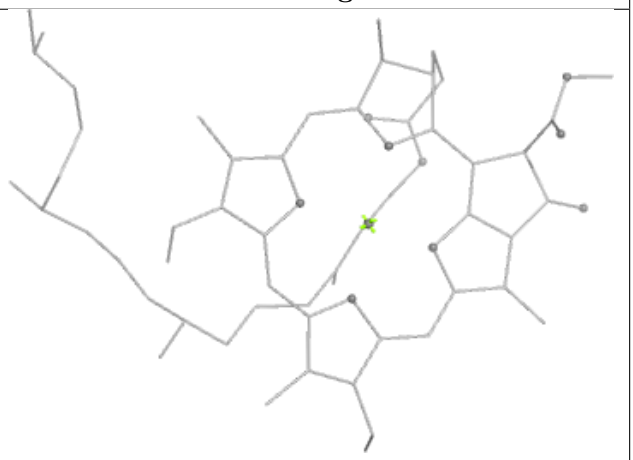
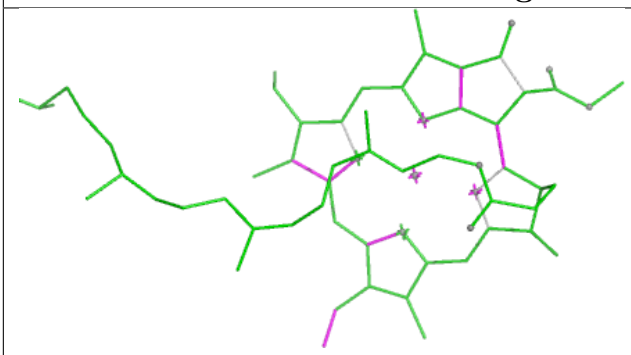


Rings

Ligand CLA B 1213



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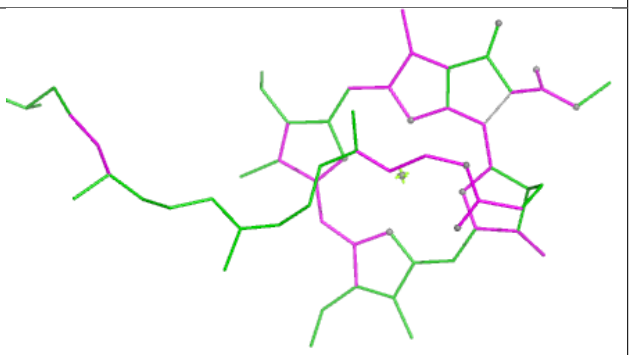
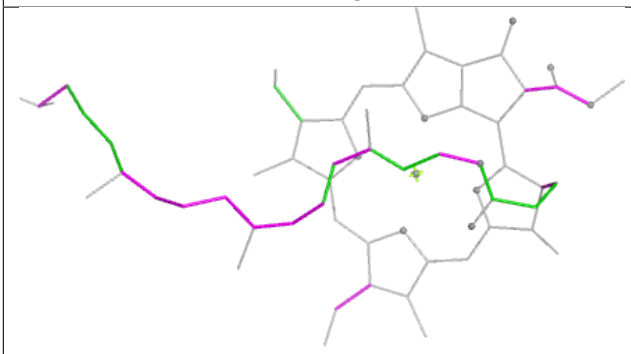


Bond angles

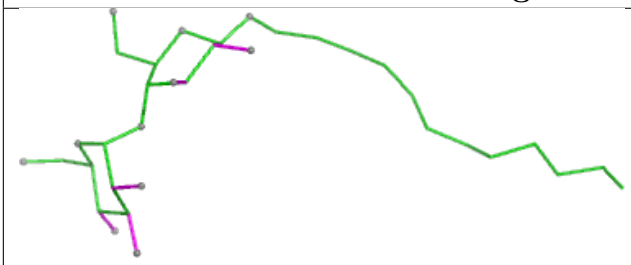


Torsions



Rings

Ligand LMT B 5005



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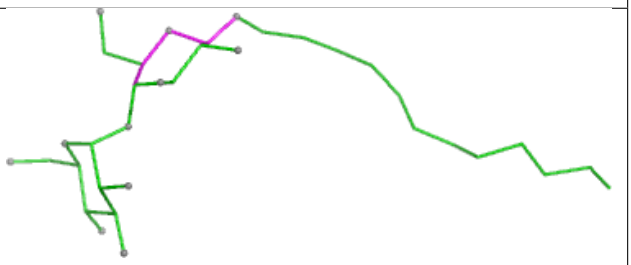
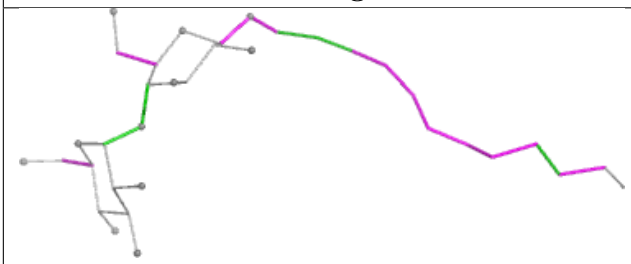


Bond angles



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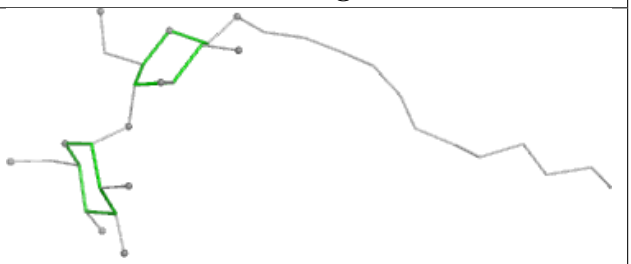
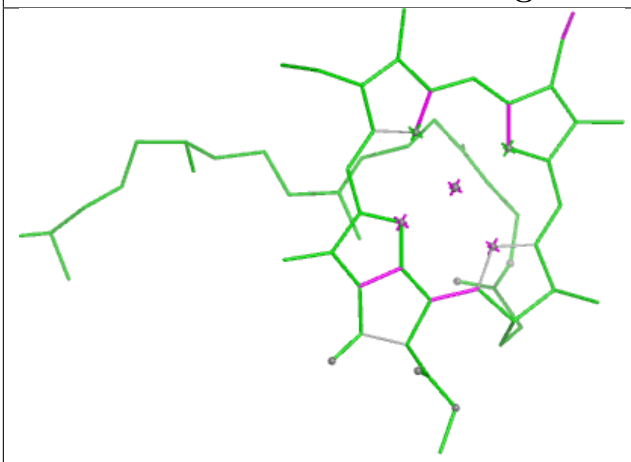


Rings

Ligand CLA B 1224



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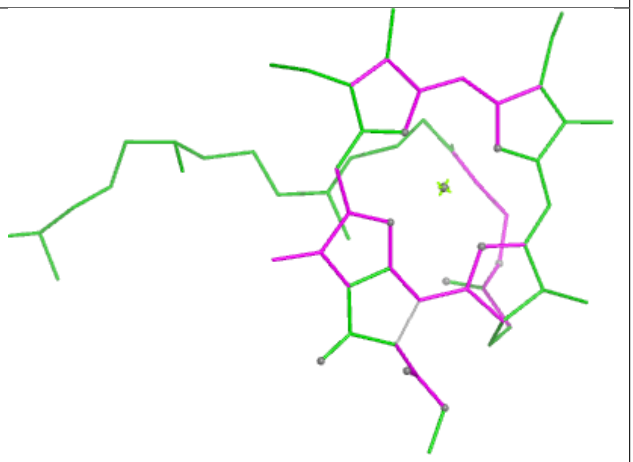
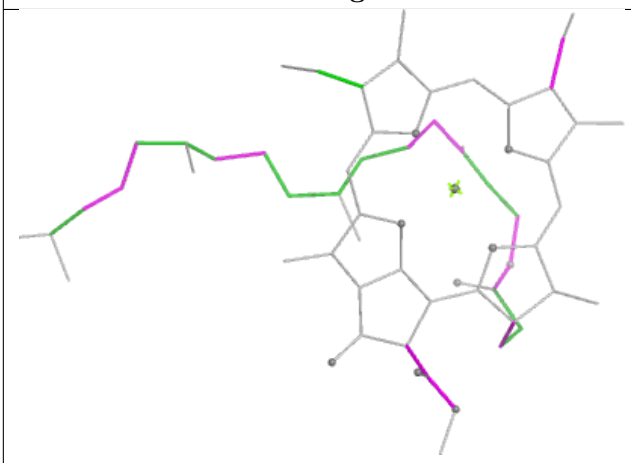


Bond angles

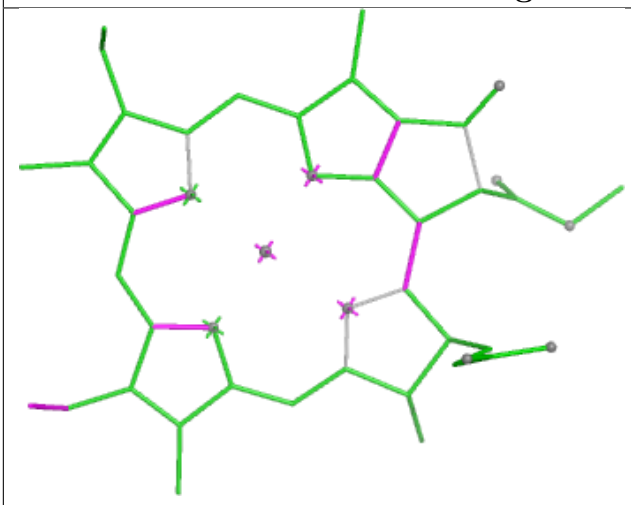


Torsions



Rings

Ligand CLA B 1232



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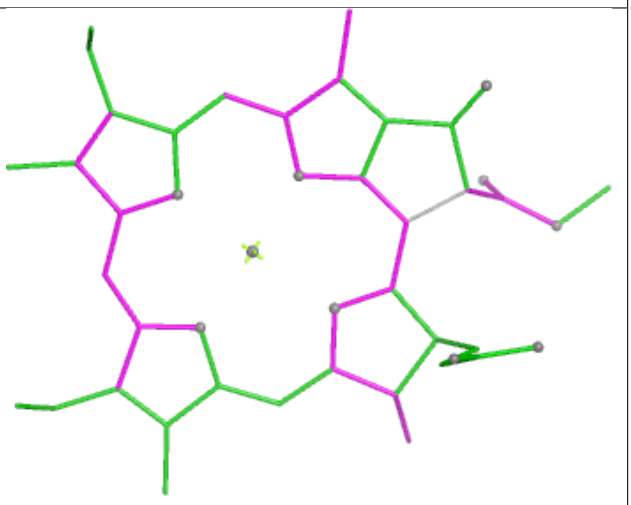
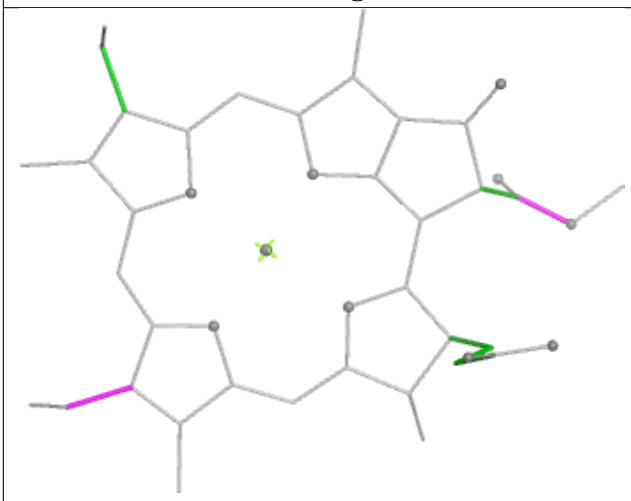


Bond angles



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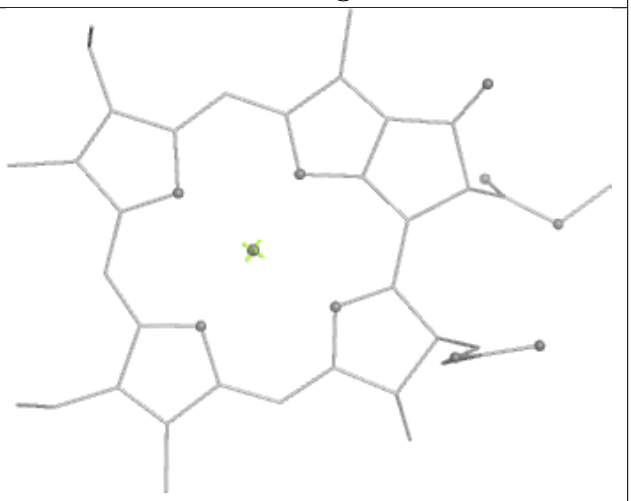
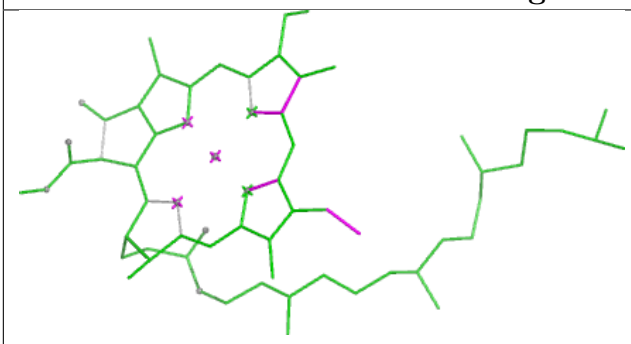


Rings

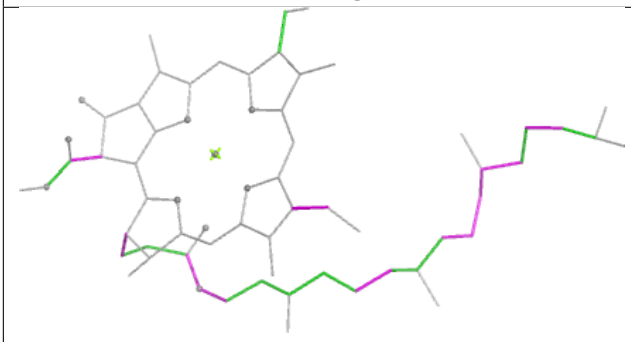
Ligand CLA 7 604



Bond lengths



Bond angles



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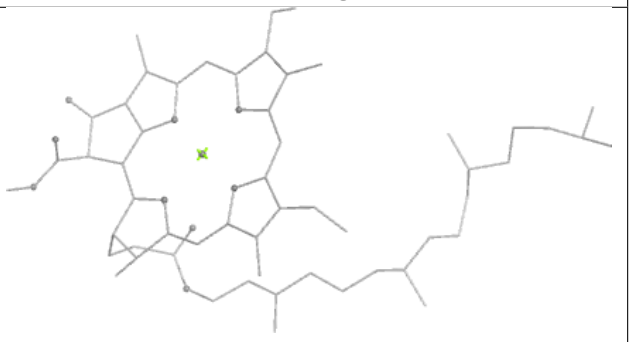
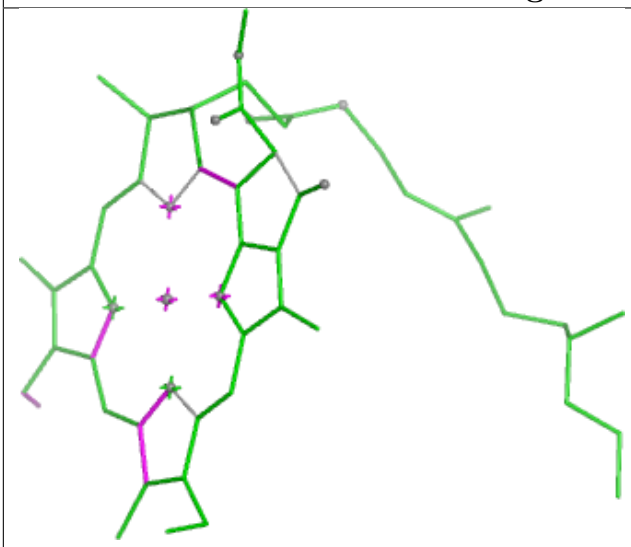
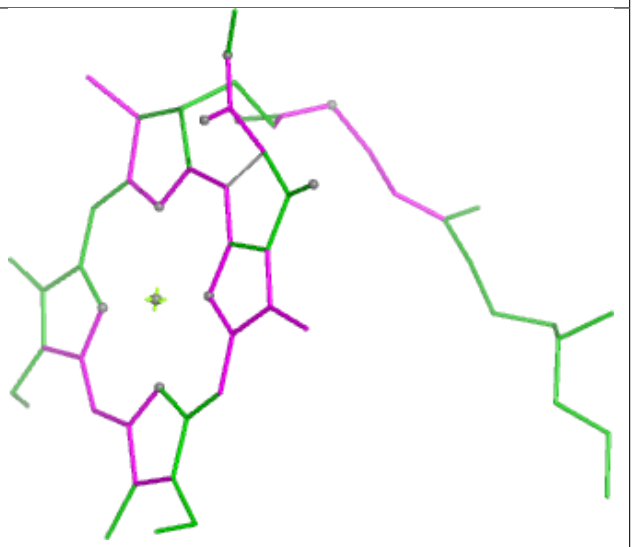


Rings

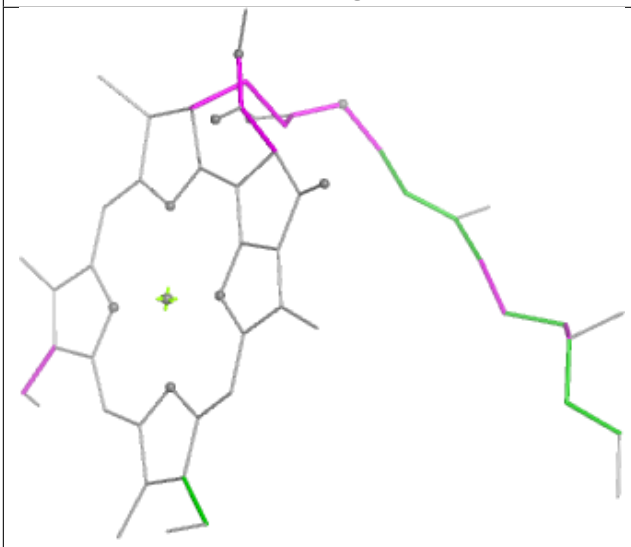
Ligand CLA Z 607



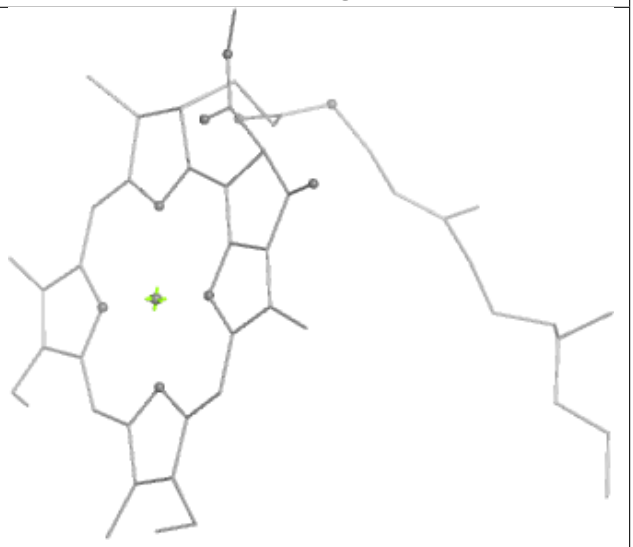
Bond lengths



Bond angles

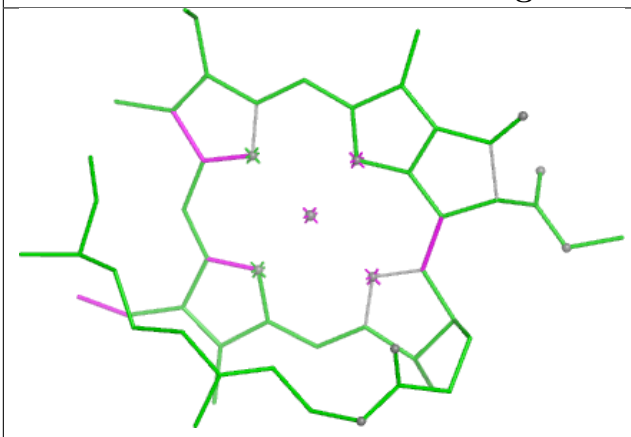


Torsions

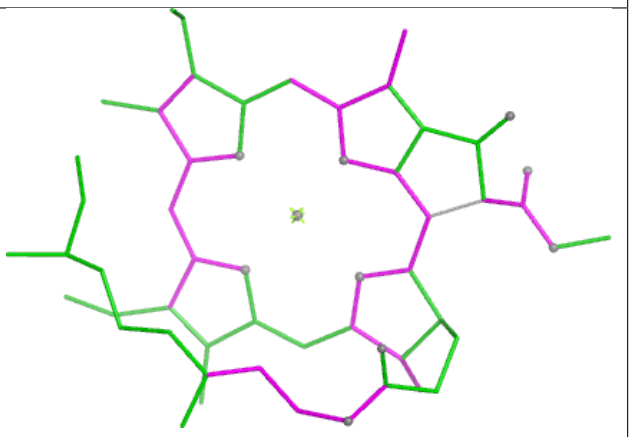


Rings

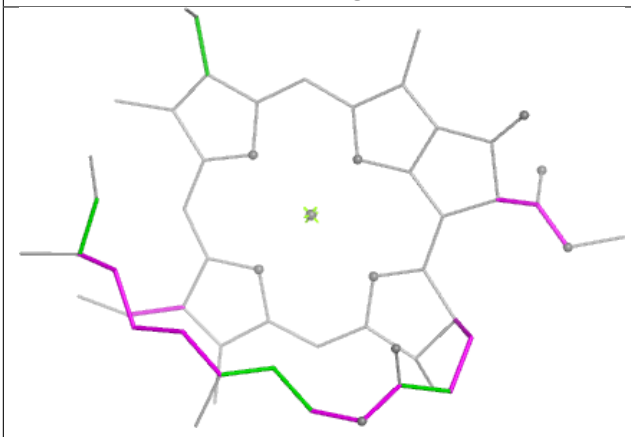
Ligand CLA B 1217



Bond lengths



Bond angles



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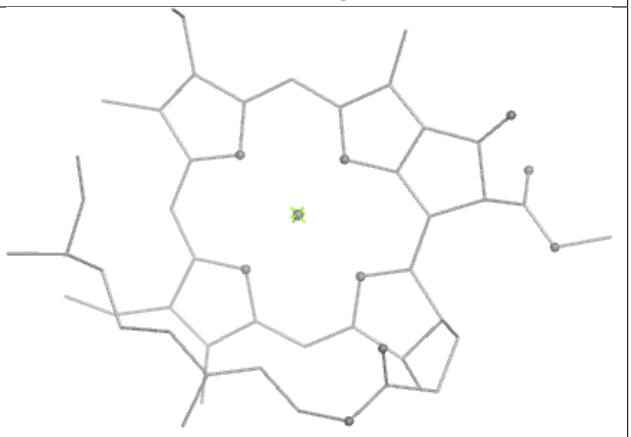
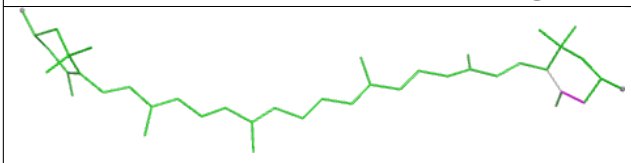


Rings

Ligand LUT 6 501



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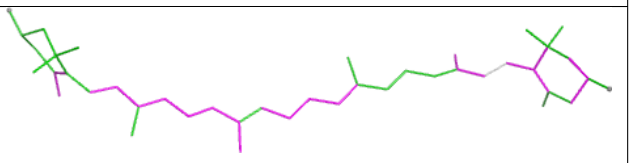

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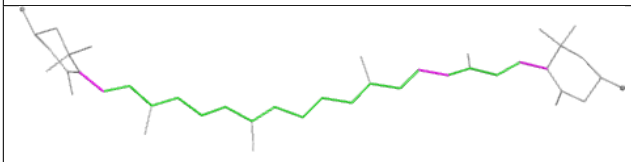

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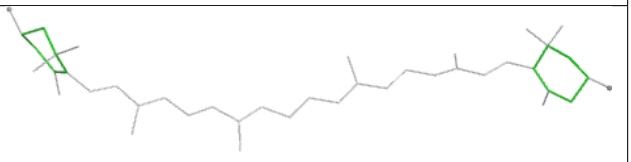
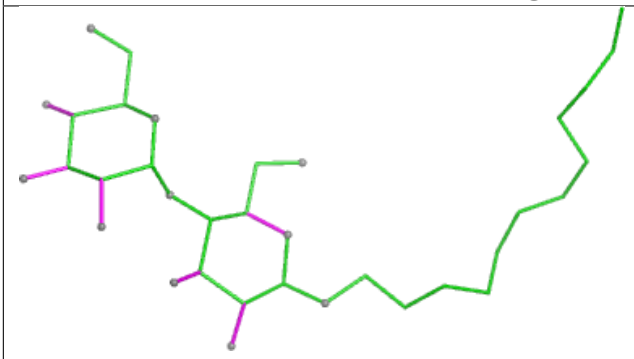


Rings

Ligand LMT 4 803



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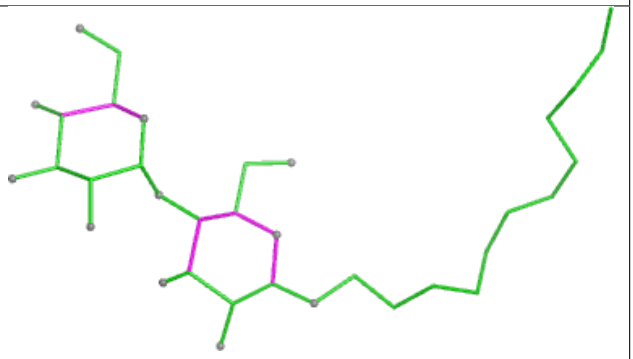
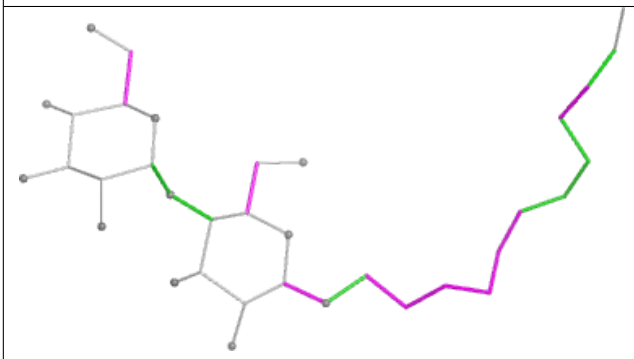


Bond angles



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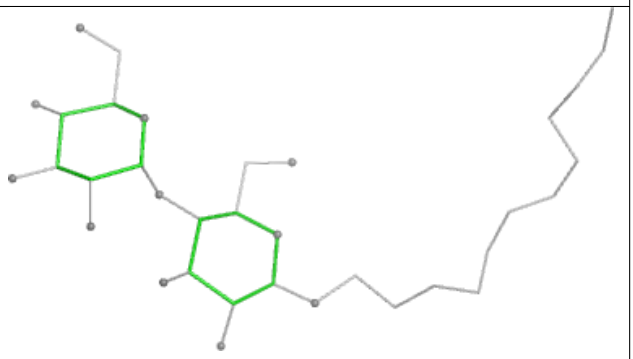
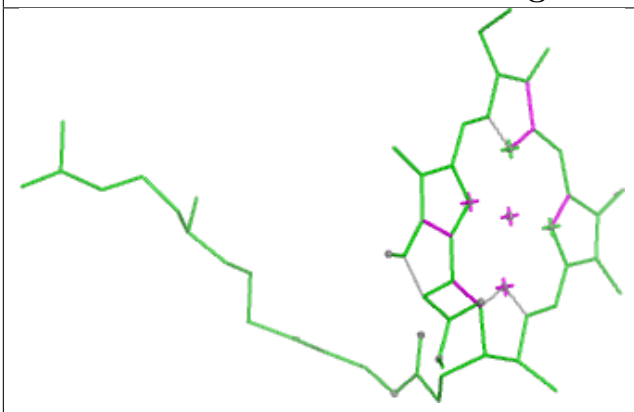


Rings

Ligand CLA 3 612



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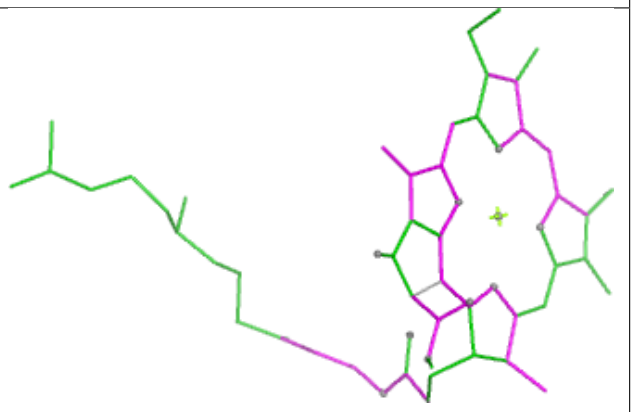
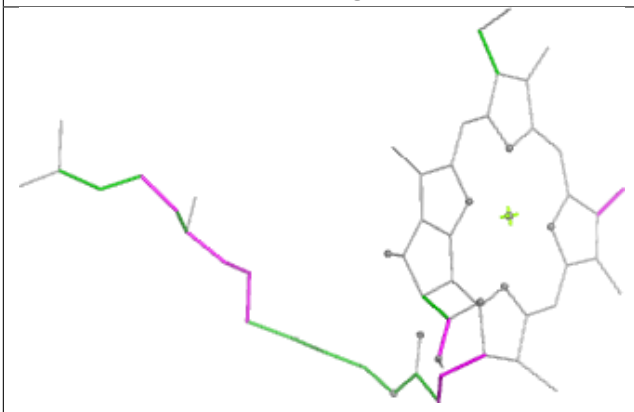


Bond angles

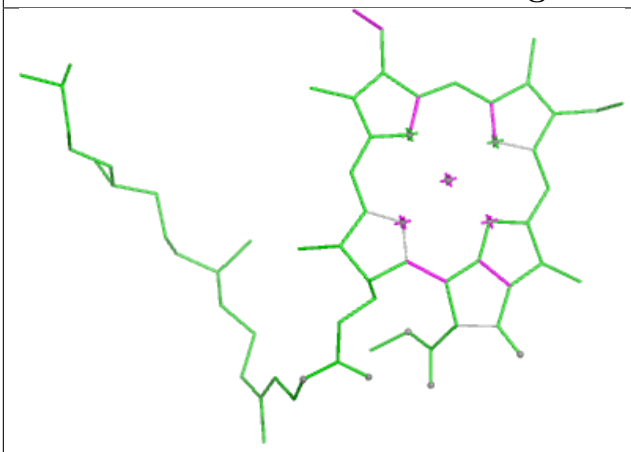


Torsions



Rings

Ligand CLA 8 605



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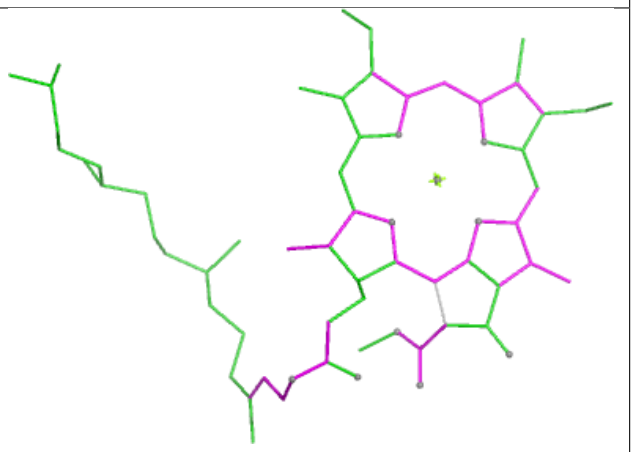
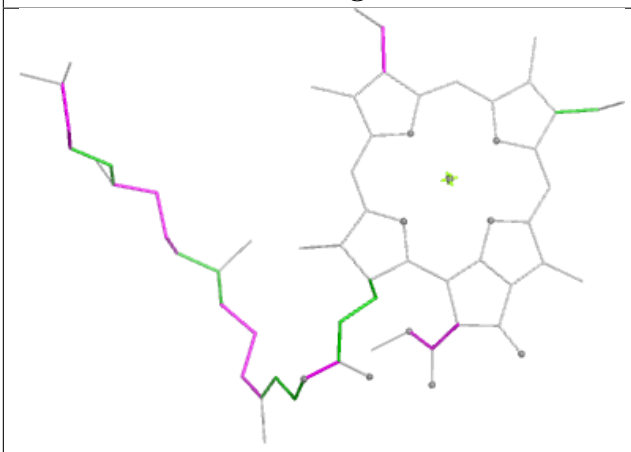


Bond angles



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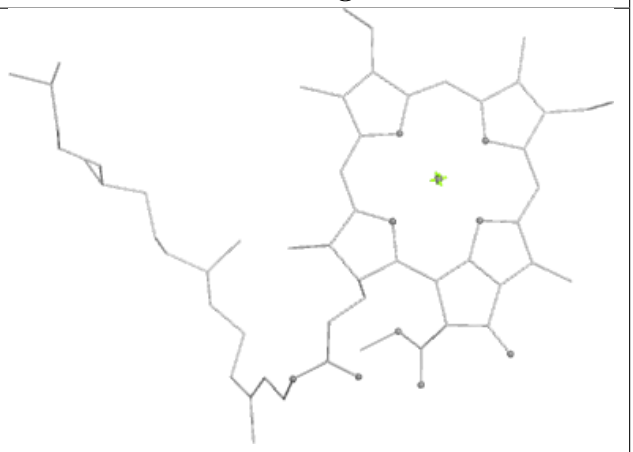
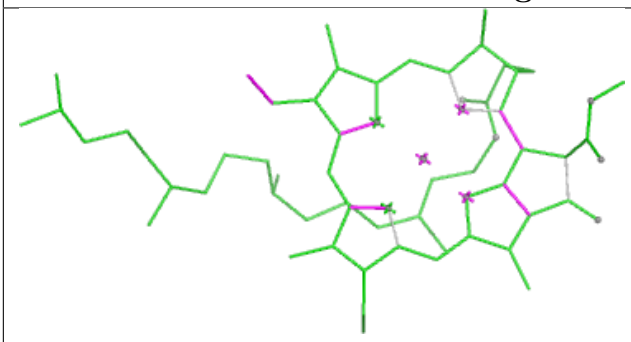
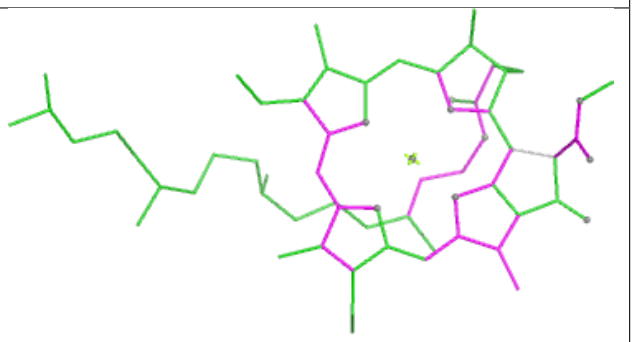
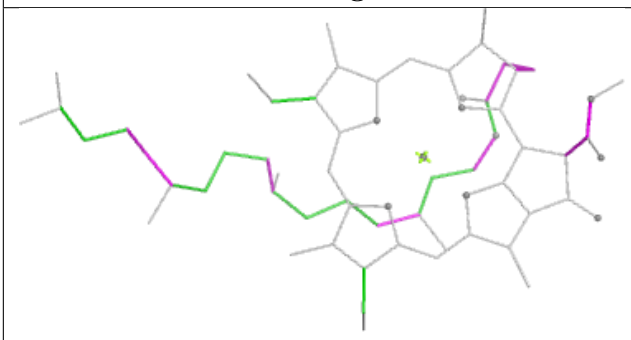
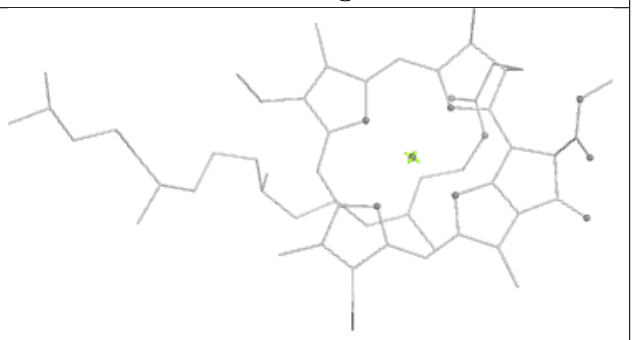
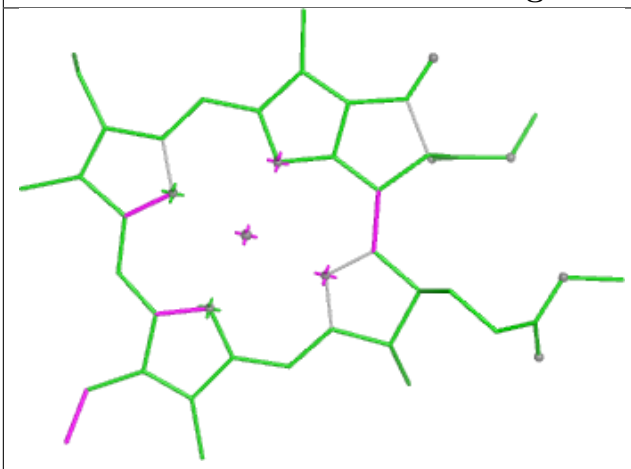


Rings

Ligand CLA A 1138	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA Z 602



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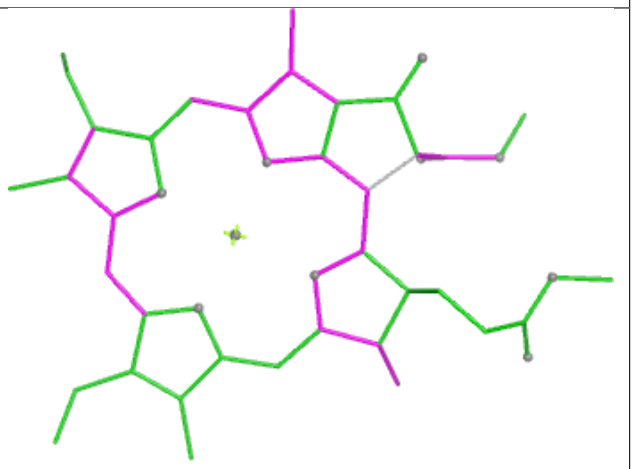
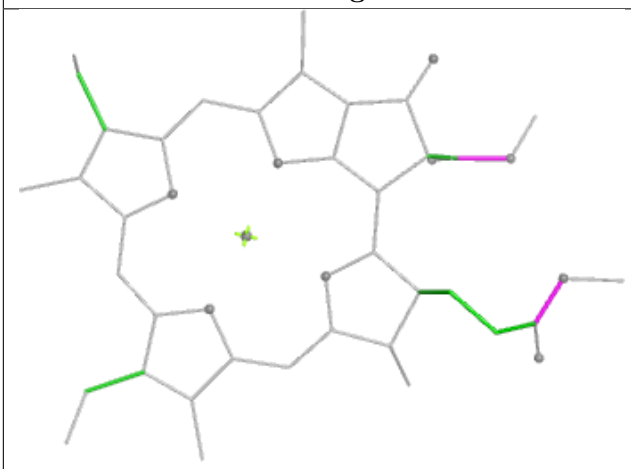


Bond angles



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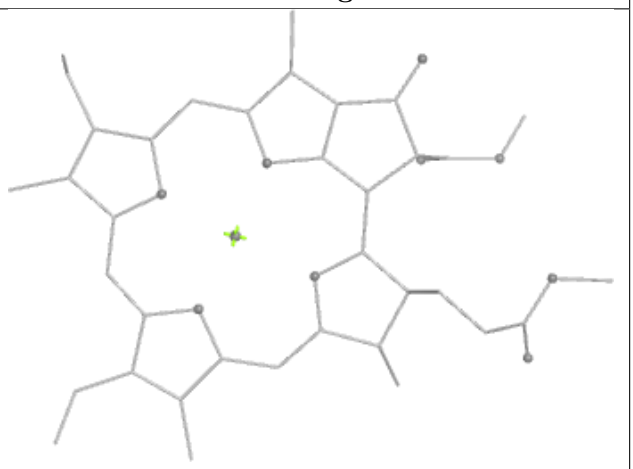


Rings

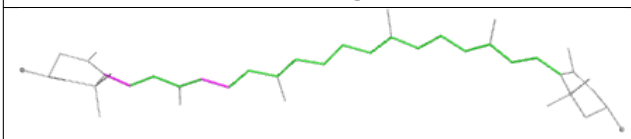
Ligand LUT Z 501



Bond lengths



Bond angles



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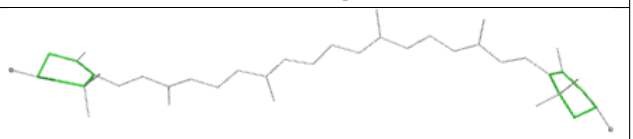
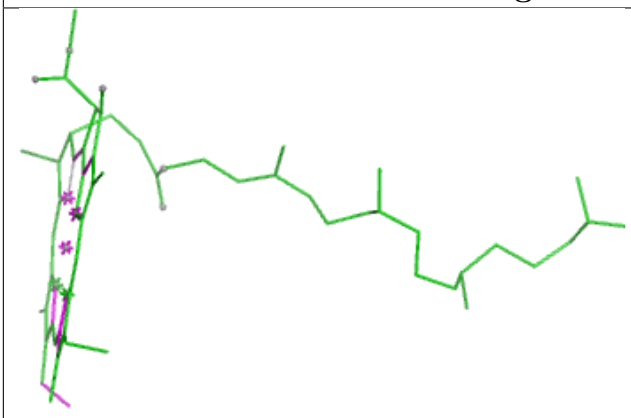
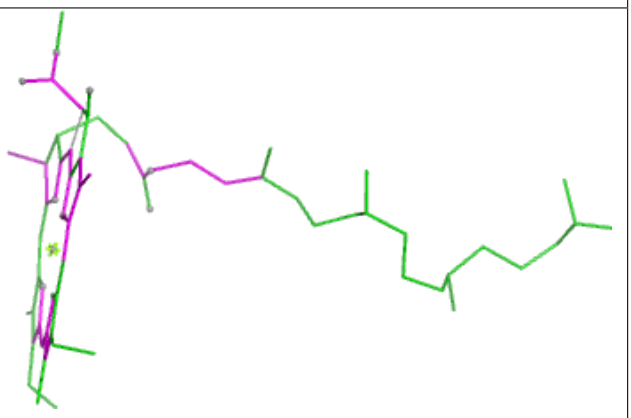


Rings

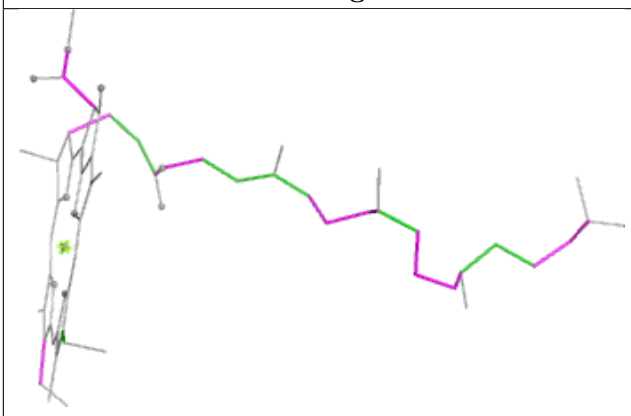
Ligand CLA A 1126



Bond lengths



Bond angles



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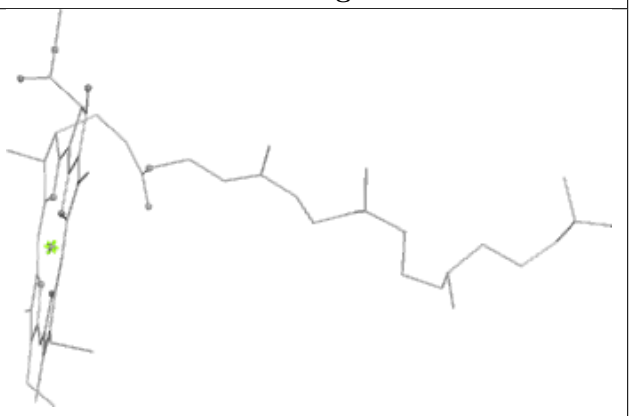
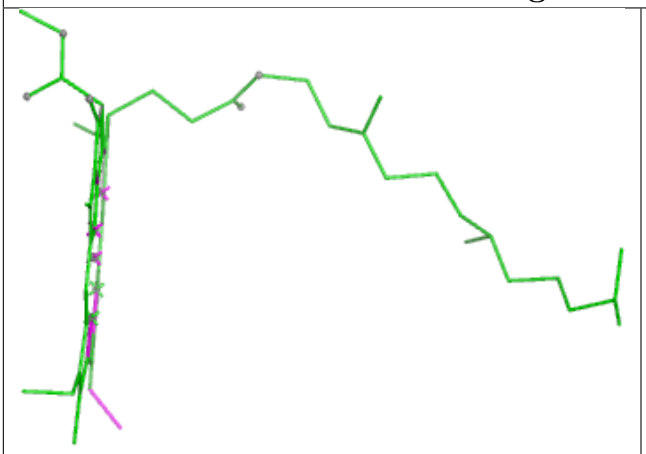


Rings

Ligand CLA 4 609



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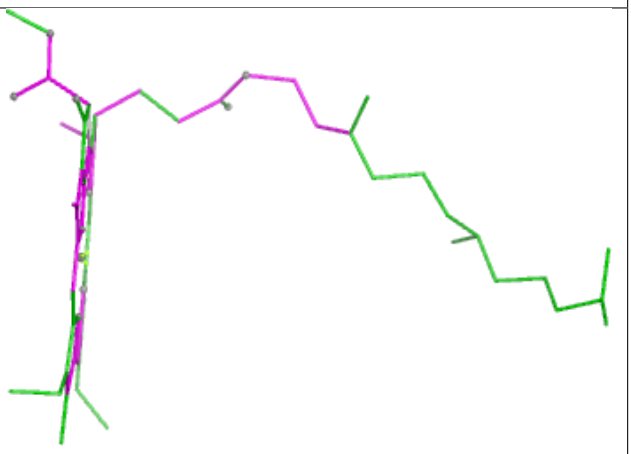
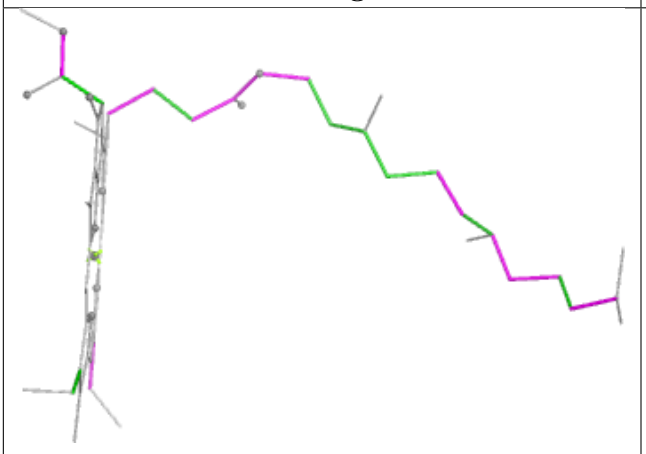


Bond angles



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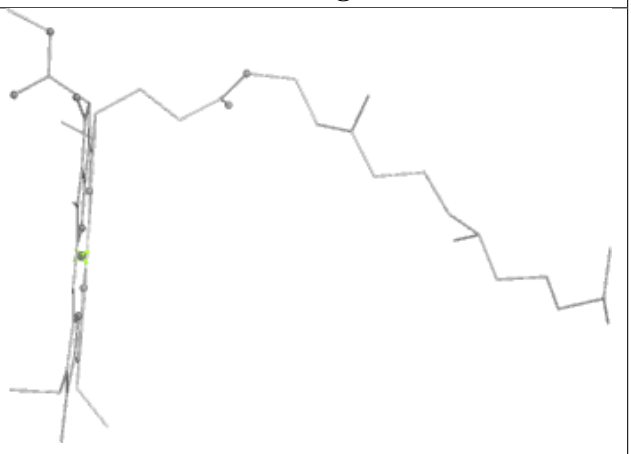
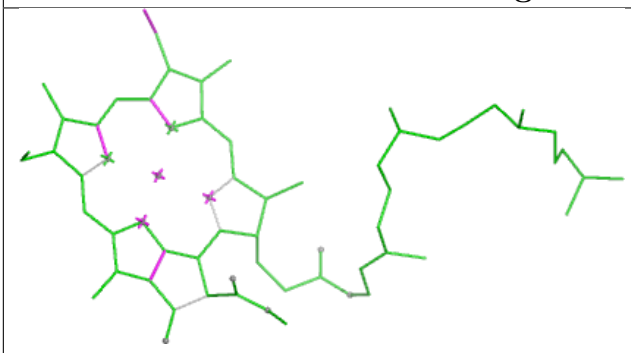


Rings

Ligand CLA A 1101



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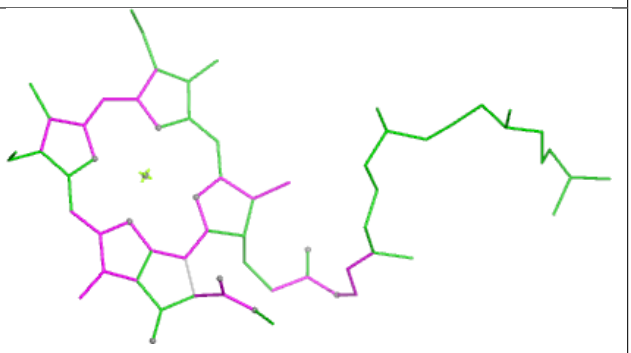
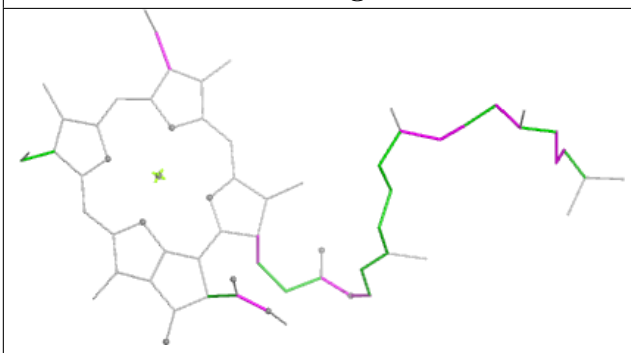


Bond angles



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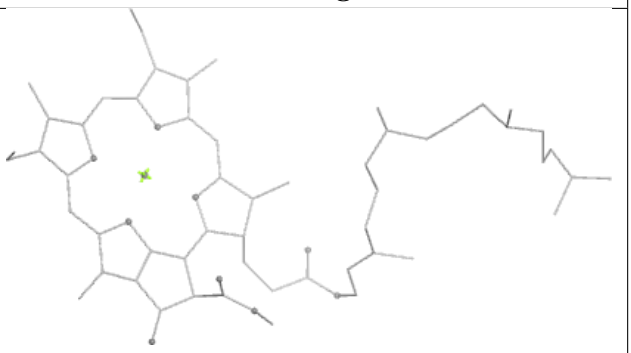
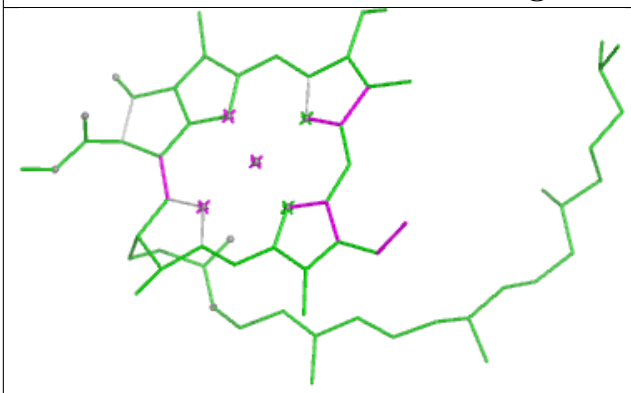


Rings

Ligand CLA 5 604



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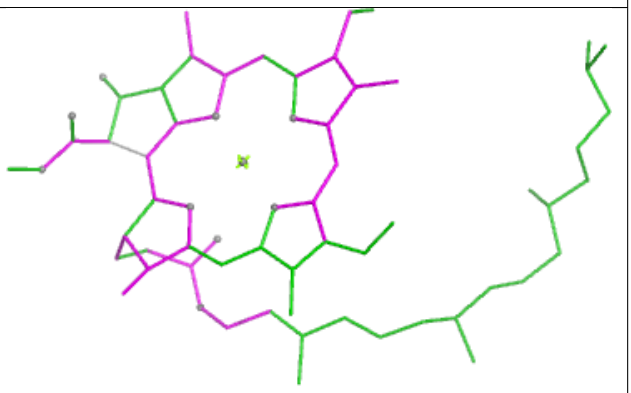
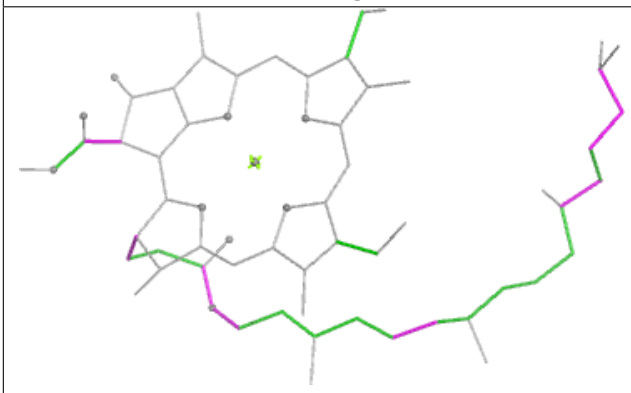


Bond angles



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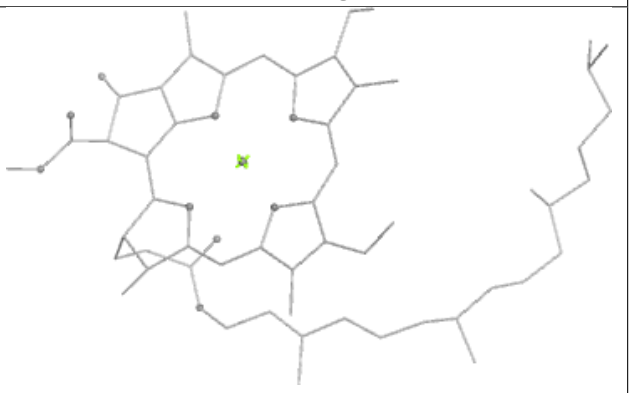
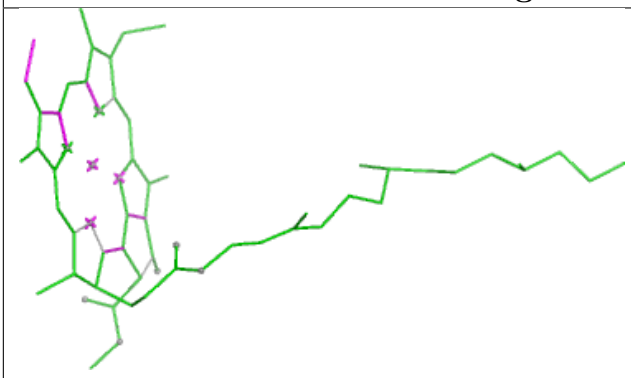


Rings

Ligand CLA B 1225



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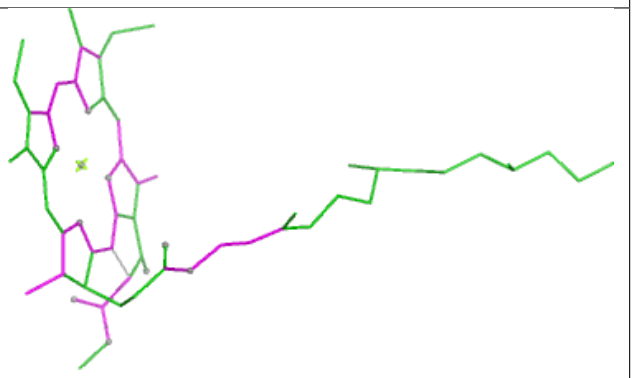
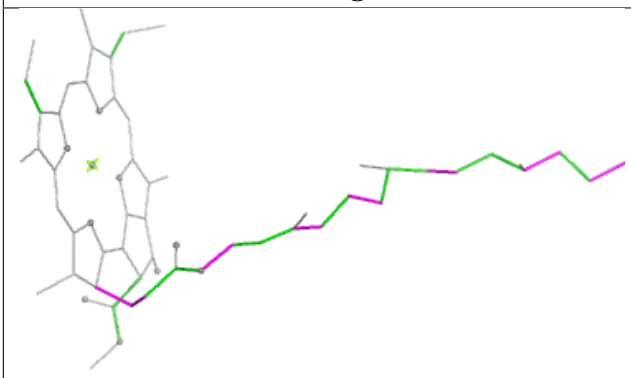


Bond angles

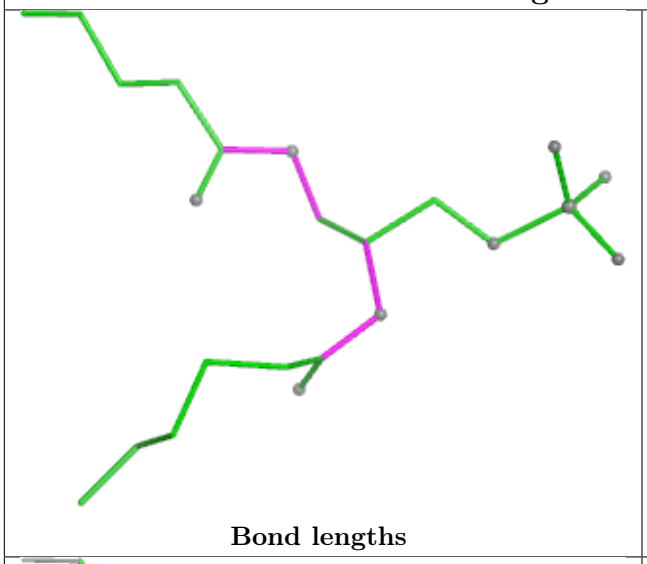


Torsions



Rings

Ligand 3PH 5 802



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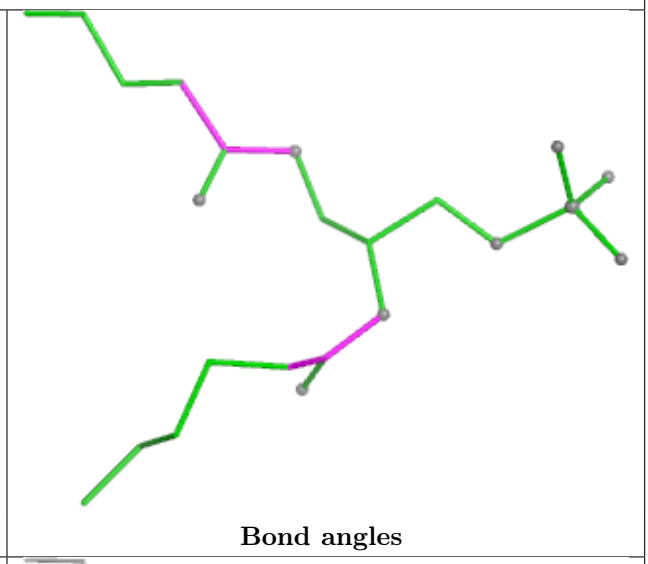
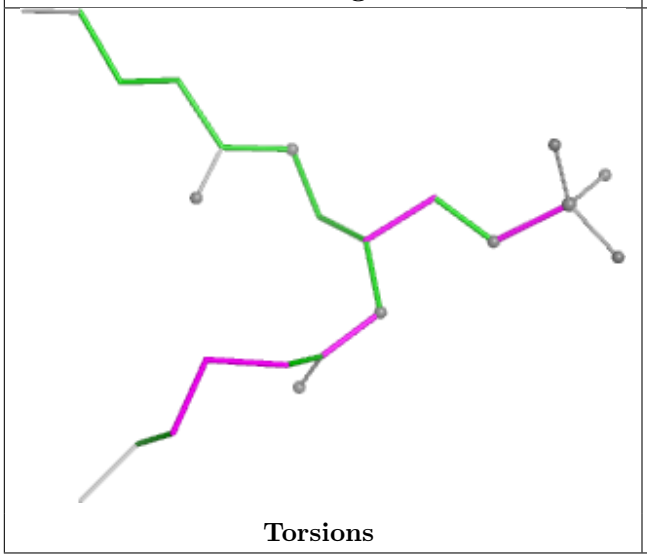


Bond angles



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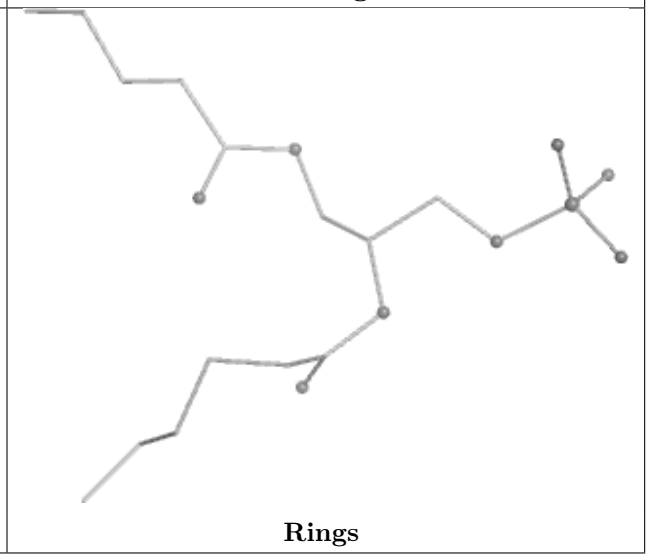
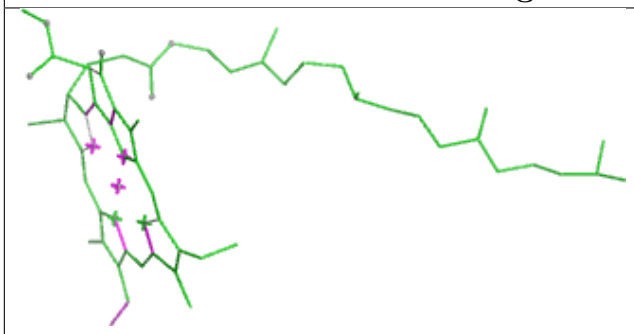
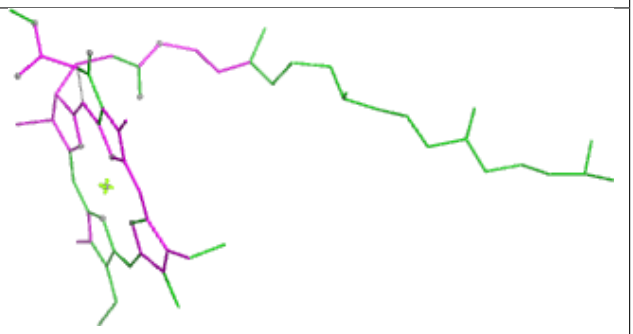


Rings

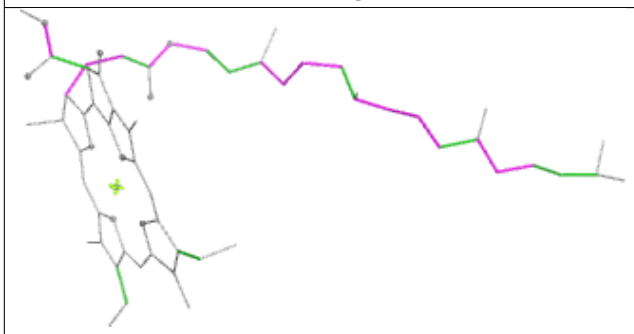
Ligand CLA B 1226



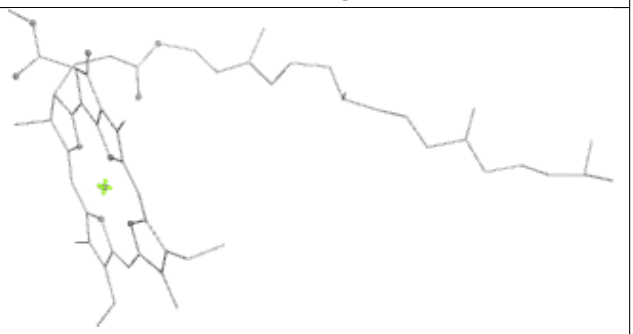
Bond lengths



Bond angles



Torsions

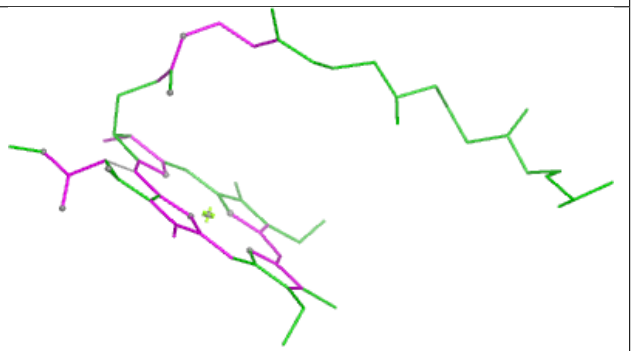


Rings

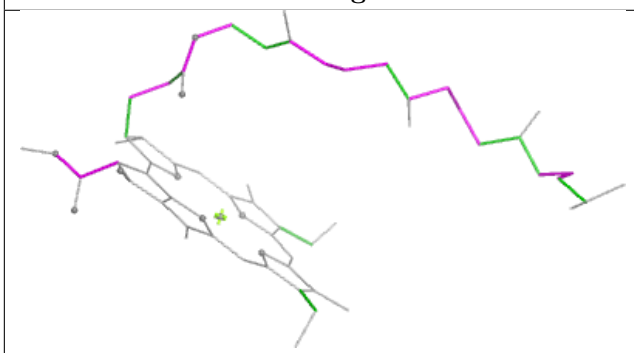
Ligand CLA B 1228



Bond lengths



Bond angles



Torsions



Rings

Ligand CLA A 1120



Bond lengths



Bond angles

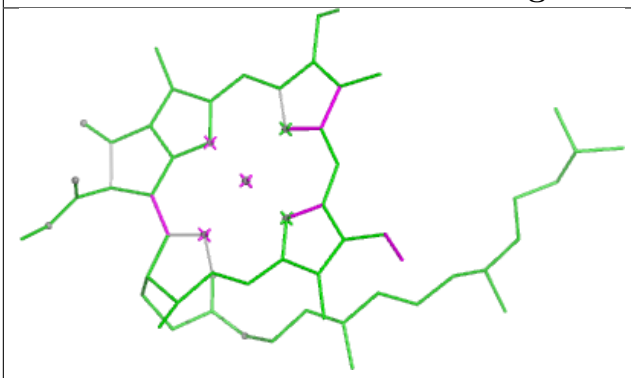


Torsions

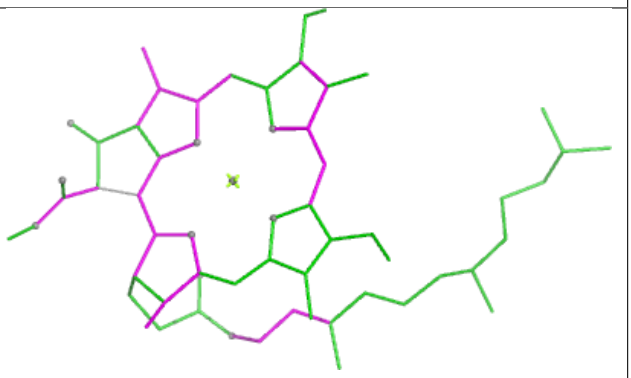


Rings

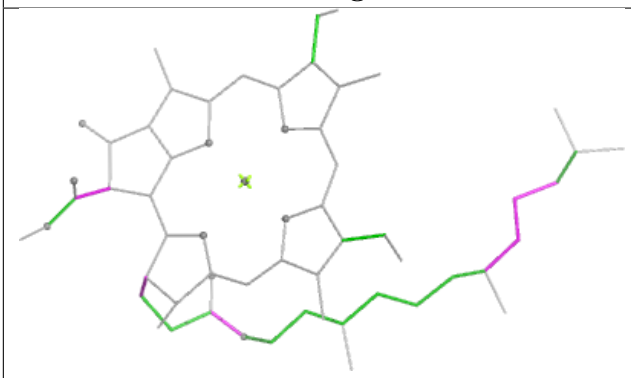
Ligand CLA 4 604



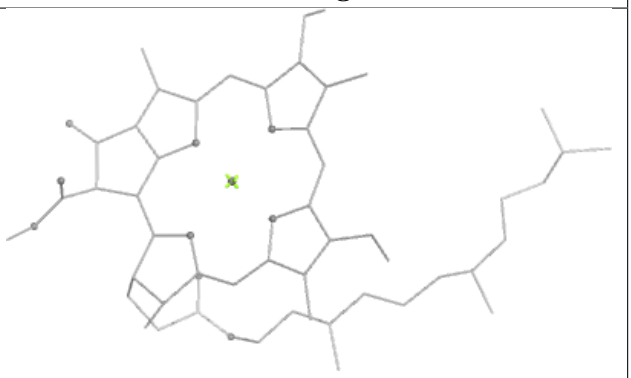
Bond lengths



Bond angles

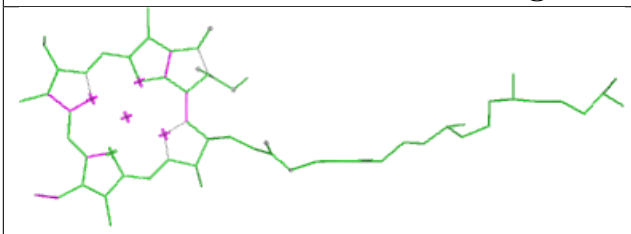


Torsions



Rings

Ligand CLA 5 609



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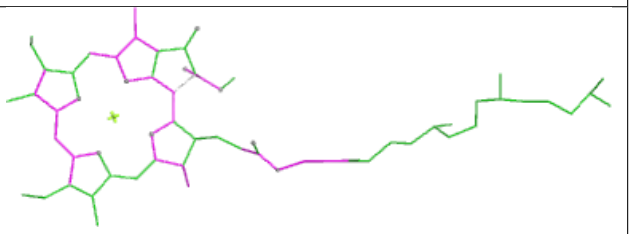
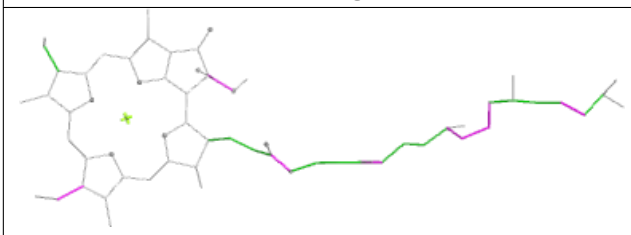


Bond angles



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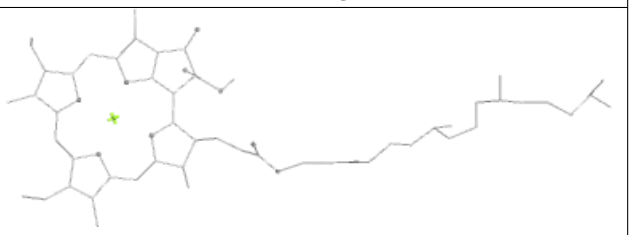
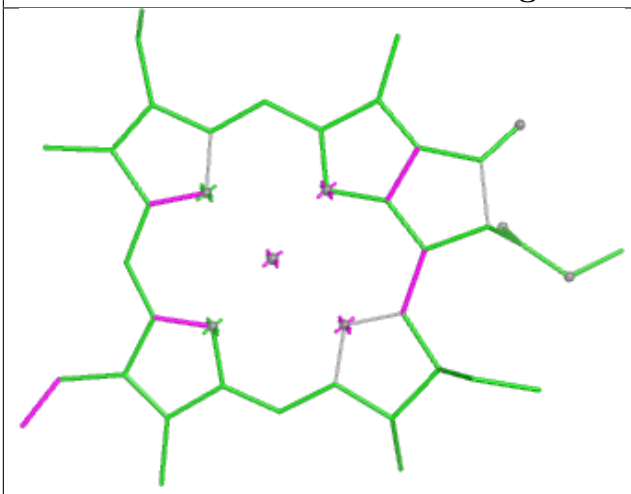
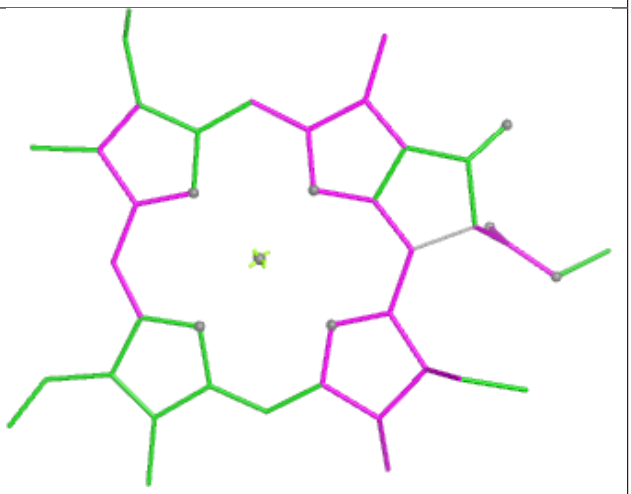


Rings

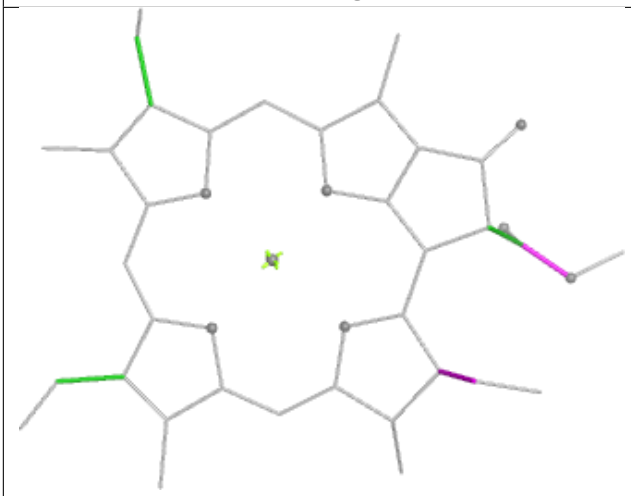
Ligand CLA J 1901



Bond lengths



Bond angles



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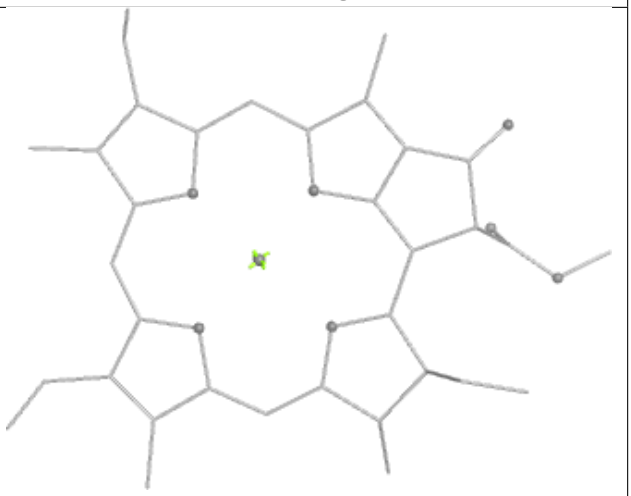
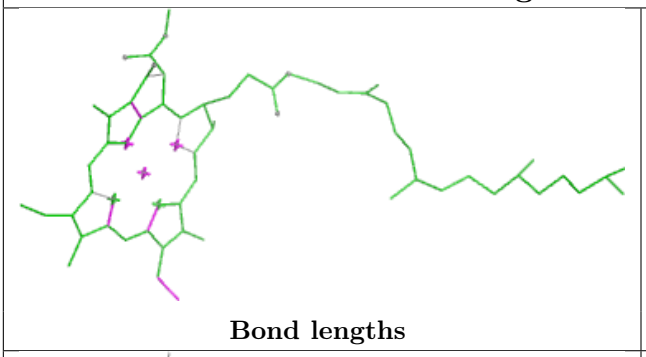


Rings

Ligand CLA B 1022



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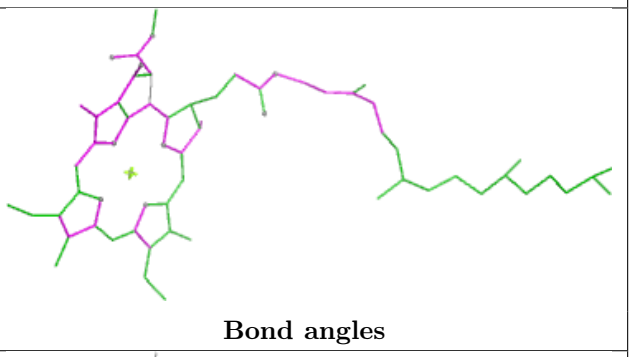
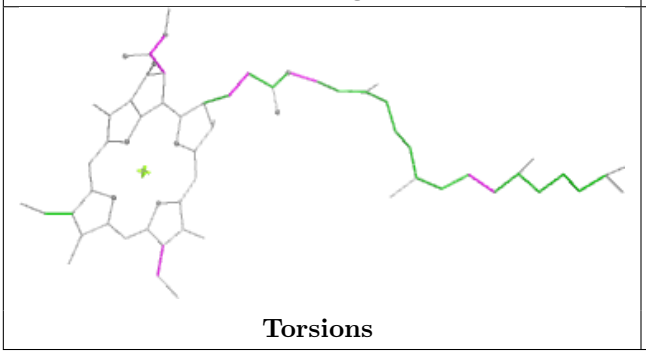


Bond angles



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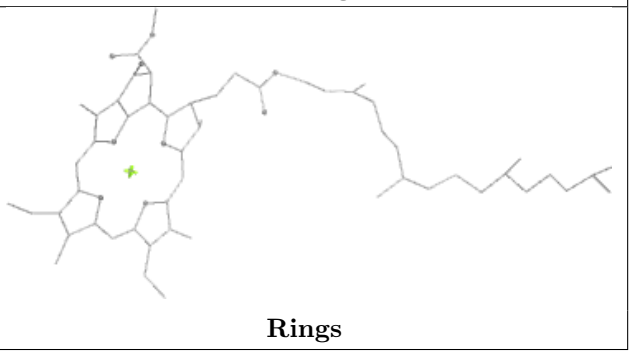
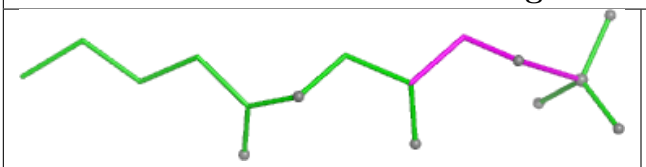


Rings

Ligand NKP 3 802



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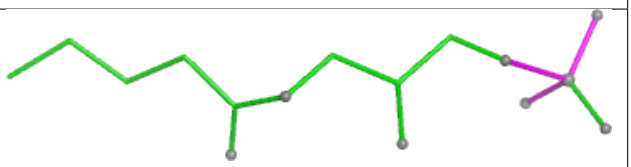
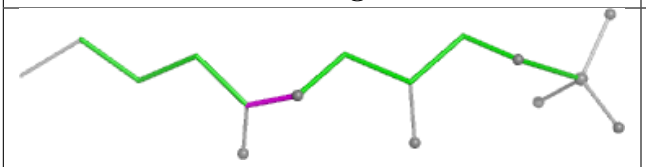


Bond angles



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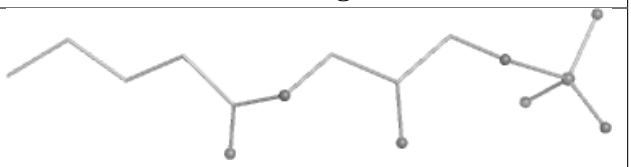

Rings

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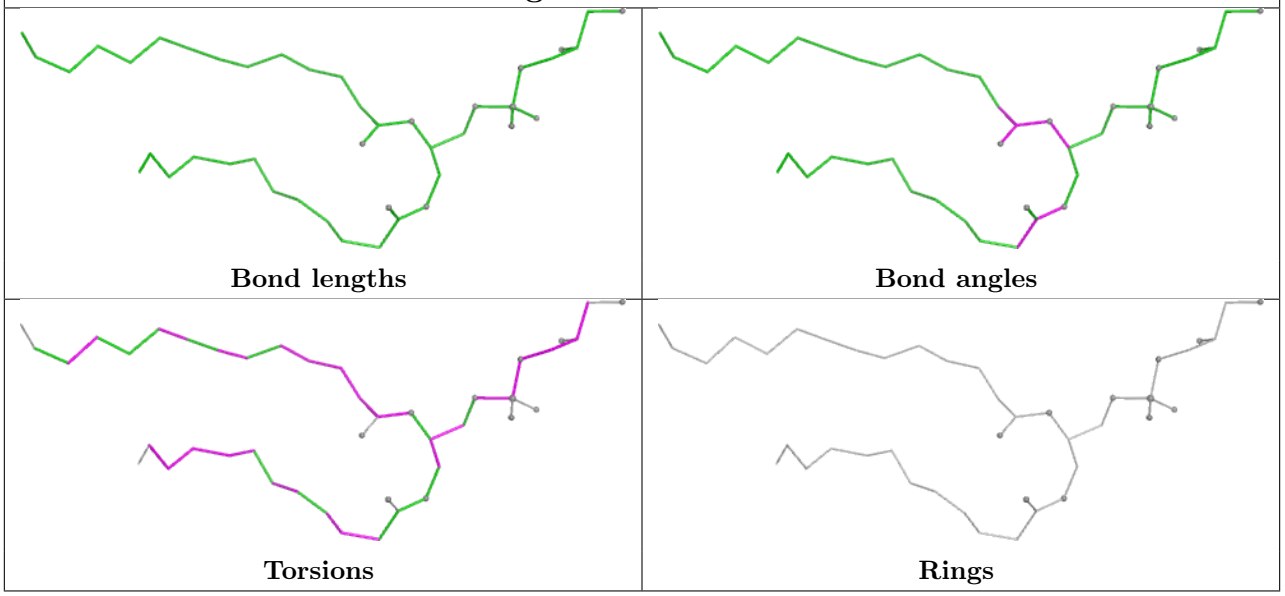

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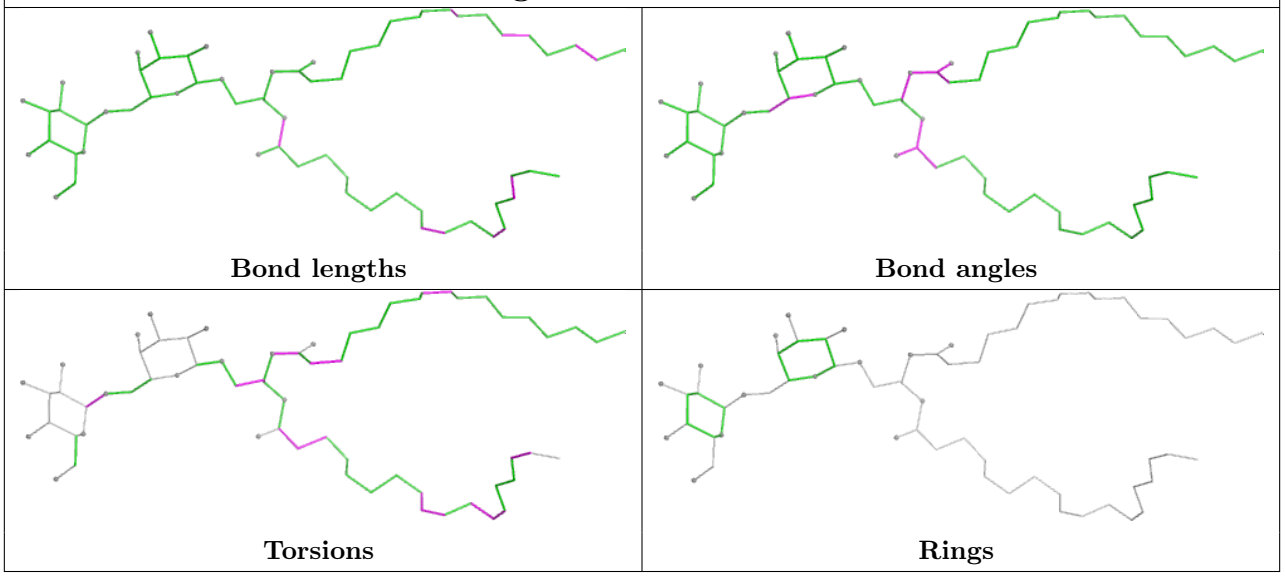
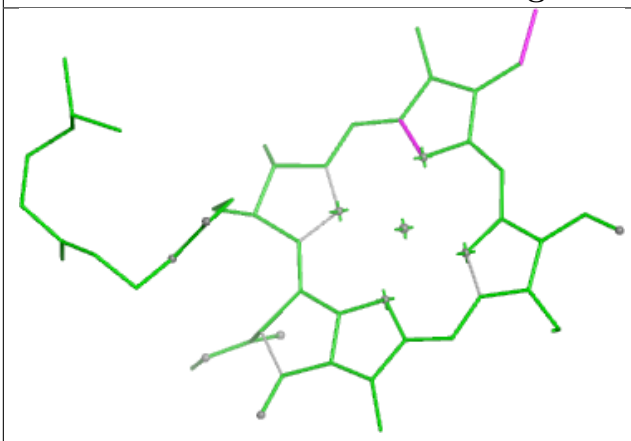


Ligand CHL 8 610



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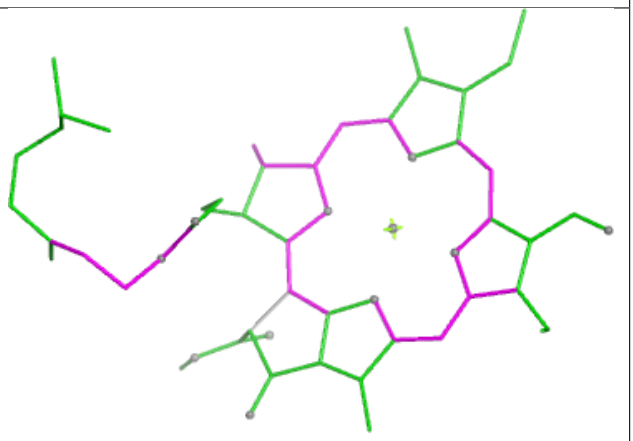
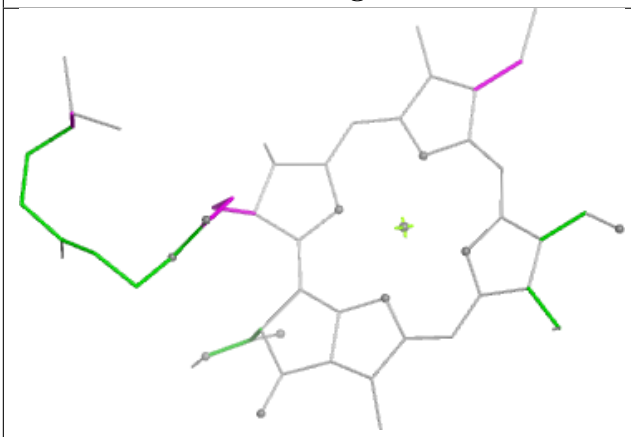


Bond angles



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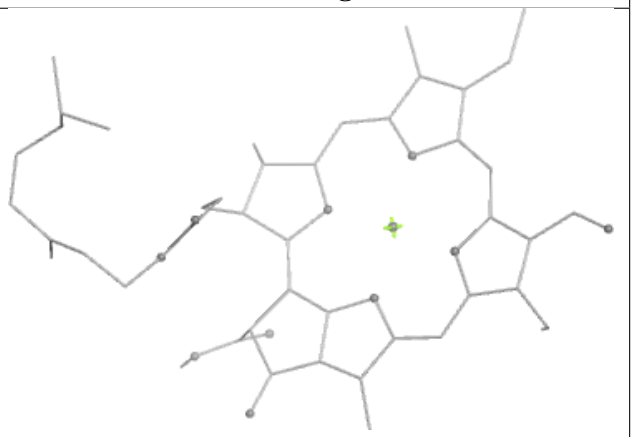
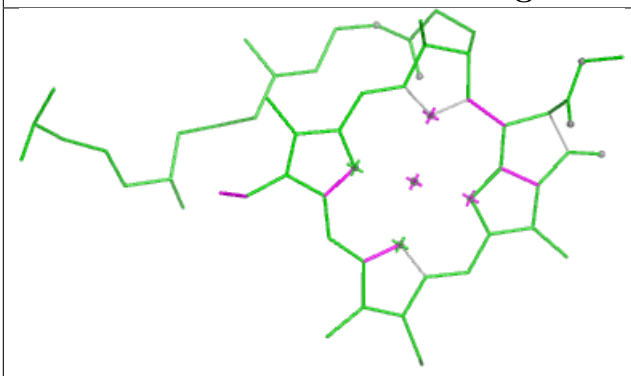


Rings

Ligand CLA B 1215



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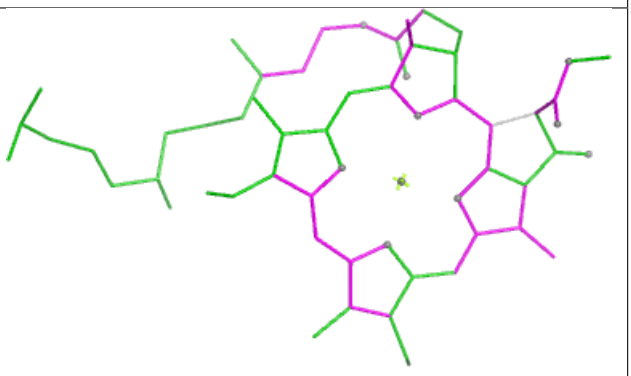
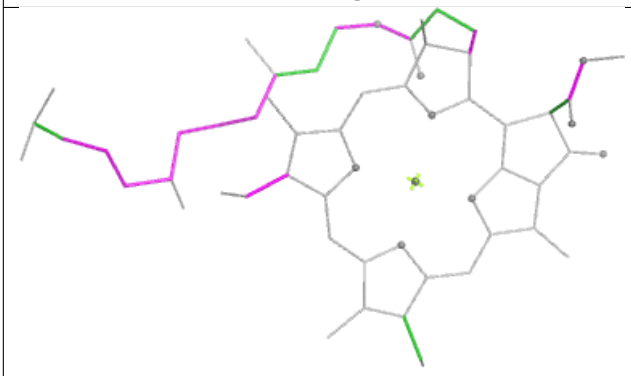


Bond angles



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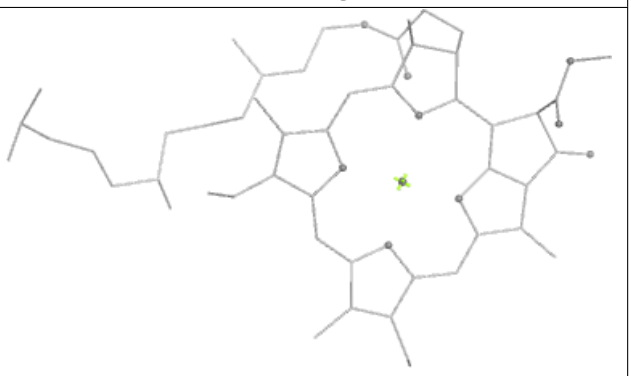


Rings

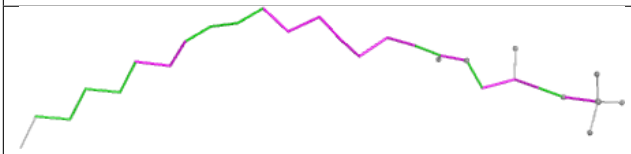
Ligand NKP 8 802



Bond lengths



Bond angles



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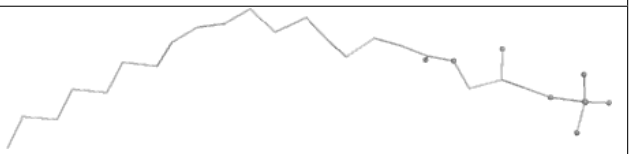
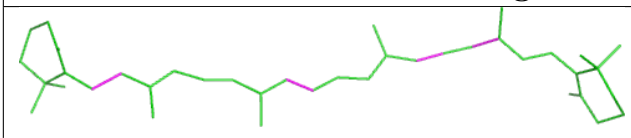


Rings

Ligand BCR A 4002



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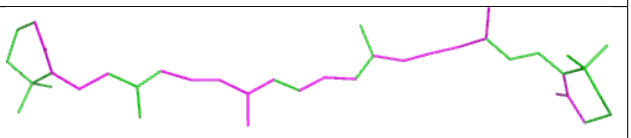
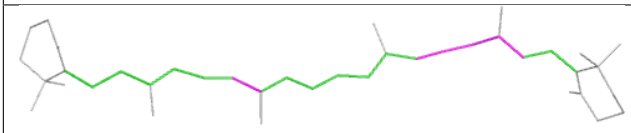


Bond angles



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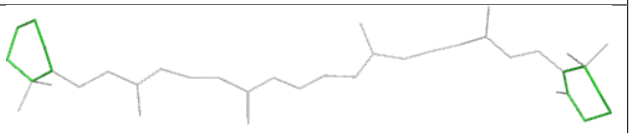
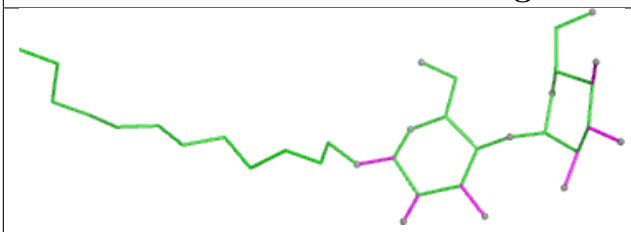


Rings

Ligand LMT F 5001



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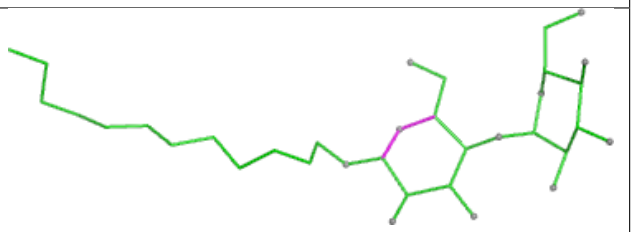
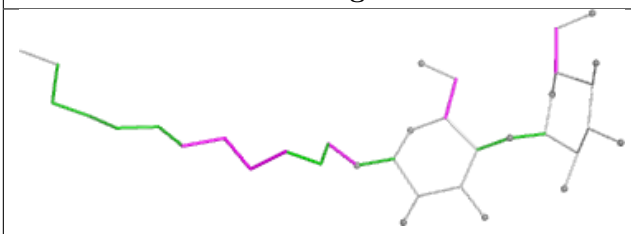


Bond angles



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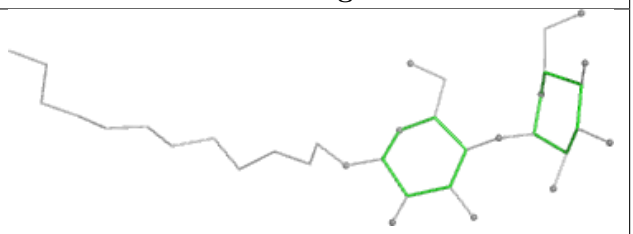
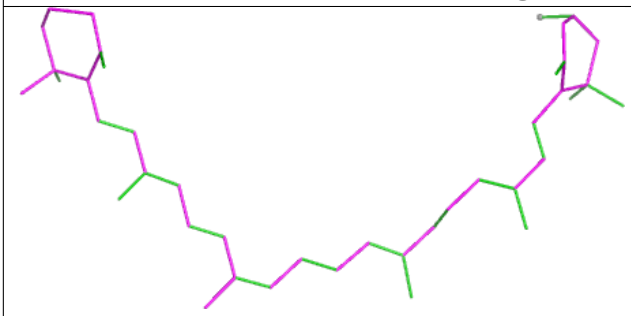


Rings

Ligand RRX F 4001



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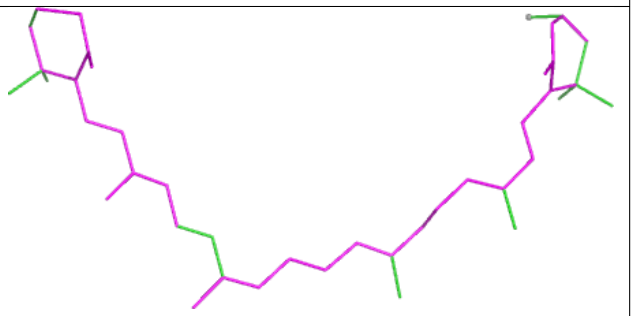
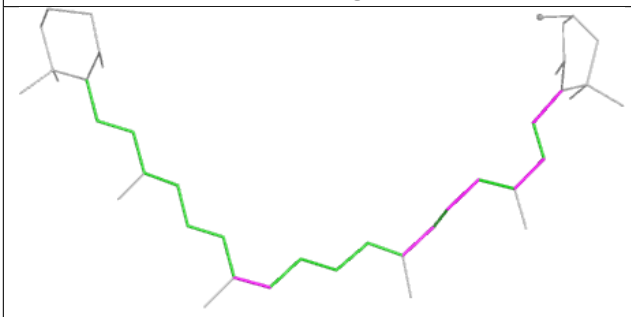


Bond angles



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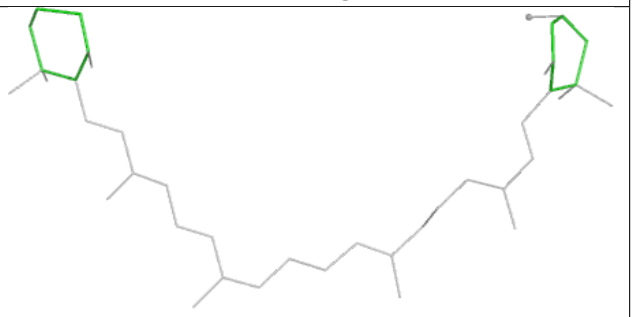
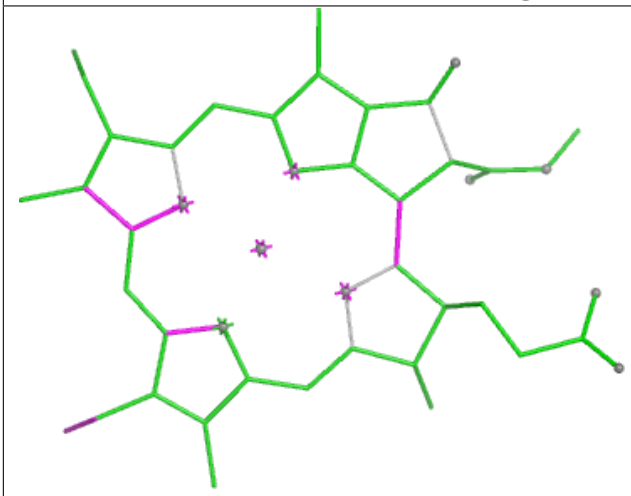


Rings

Ligand CLA F 1302



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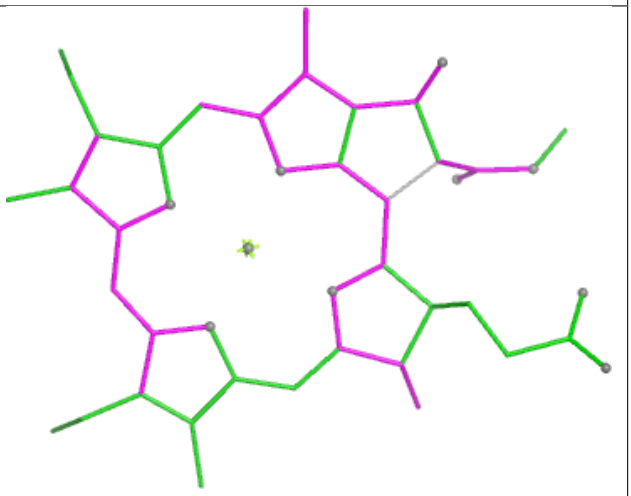
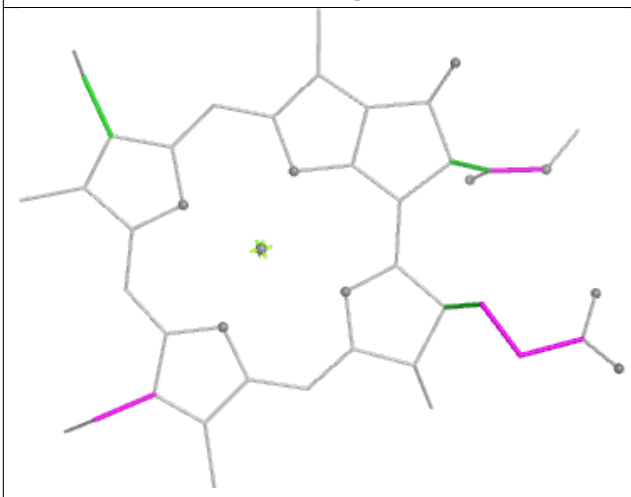


Bond angles



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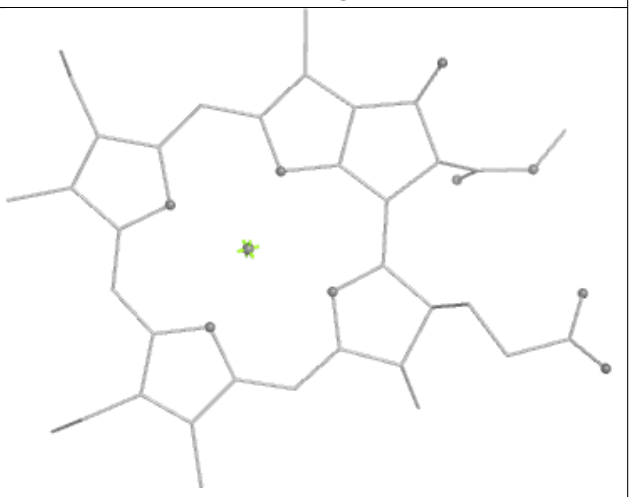
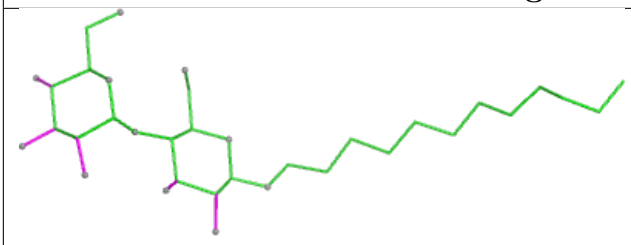
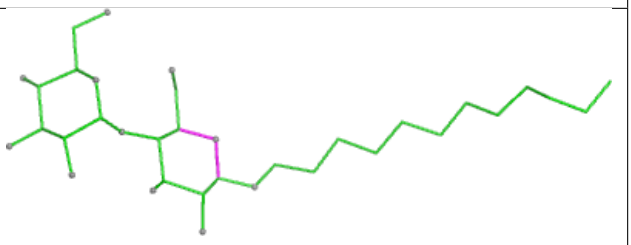


Rings

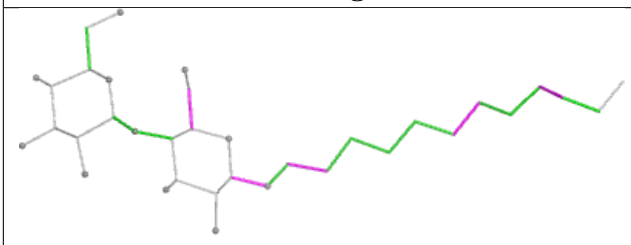
Ligand LMT 1 803



Bond lengths



Bond angles



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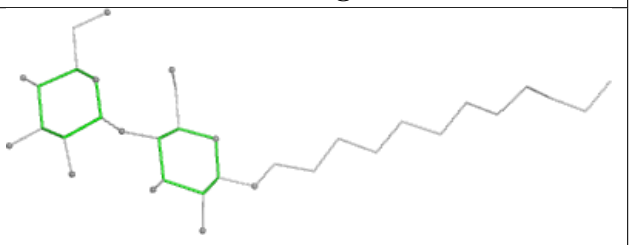
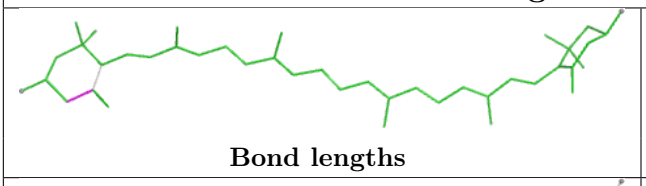
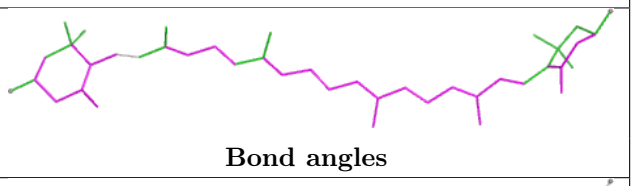


Rings

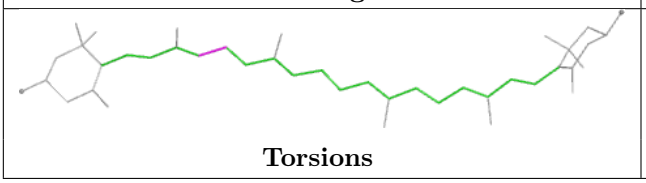
Ligand LUT 1 502



Bond lengths



Bond angles



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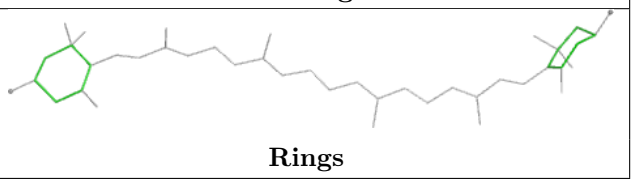
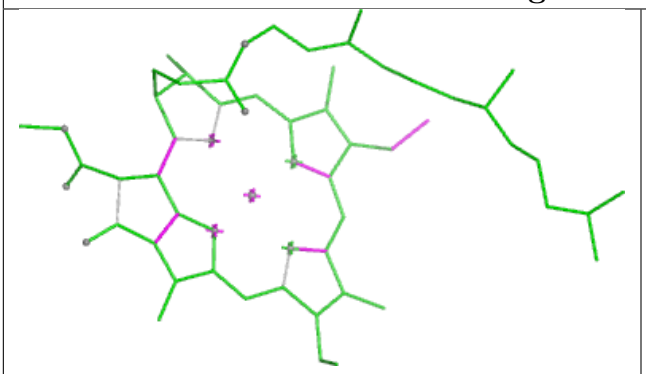
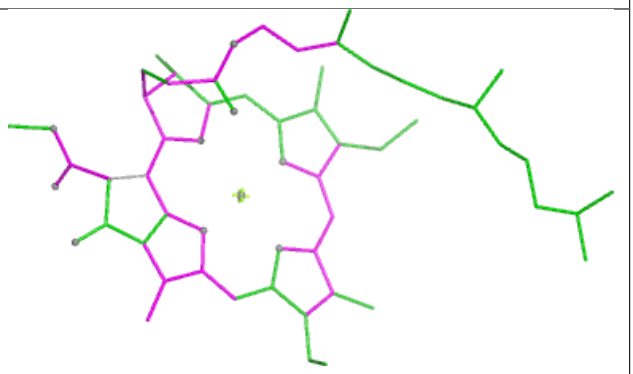


Rings

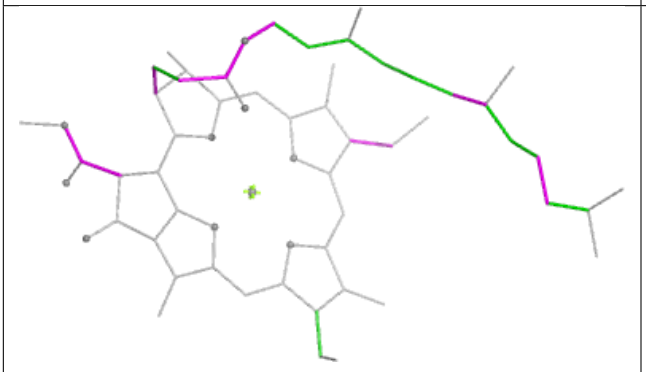
Ligand CLA 6 601



Bond lengths



Bond angles

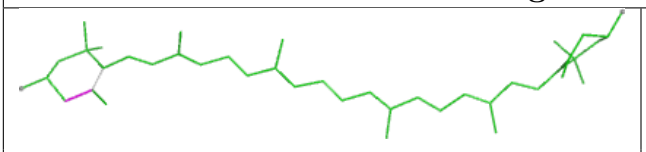


Torsions



Rings

Ligand LUT 4 502



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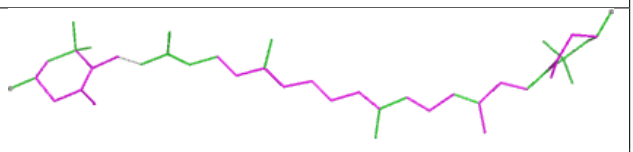

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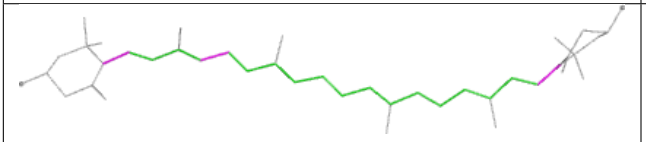

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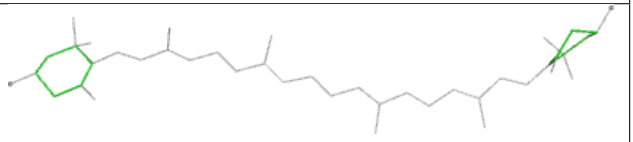
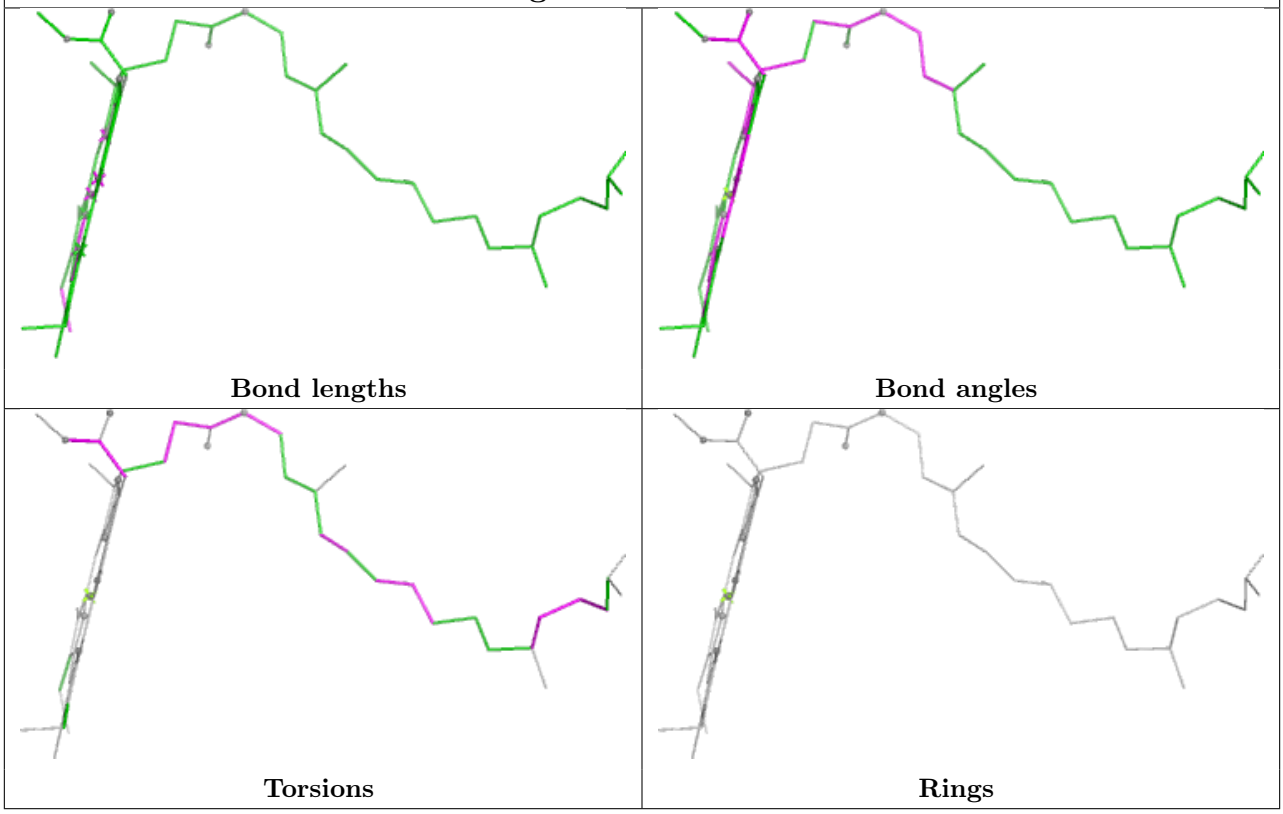
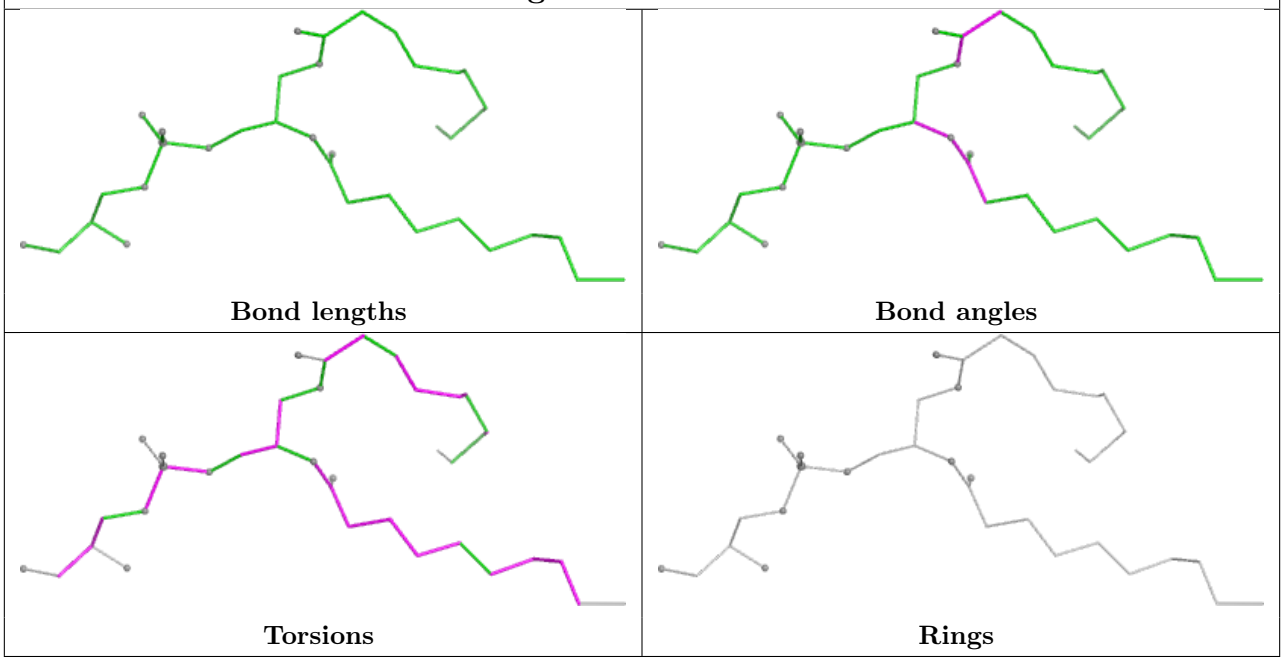


Rings

Ligand CLA 8 609



Ligand LHG 5 801



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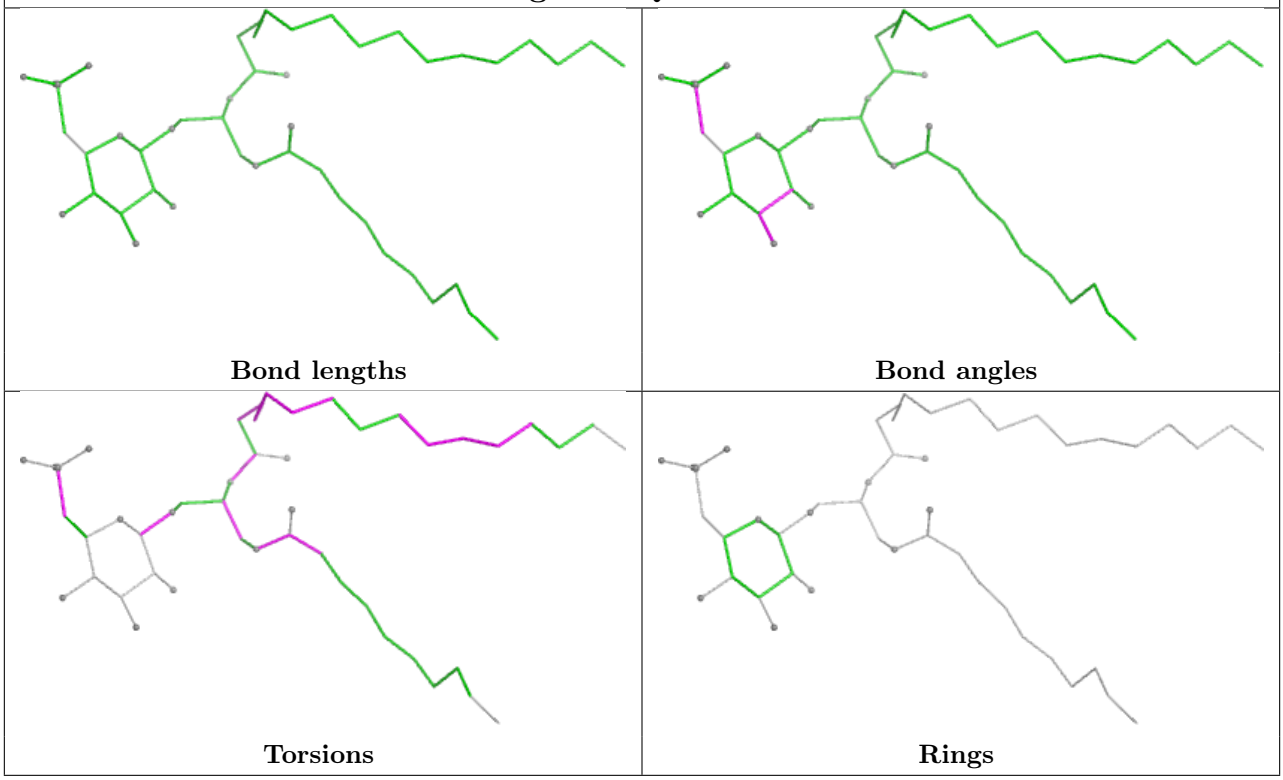

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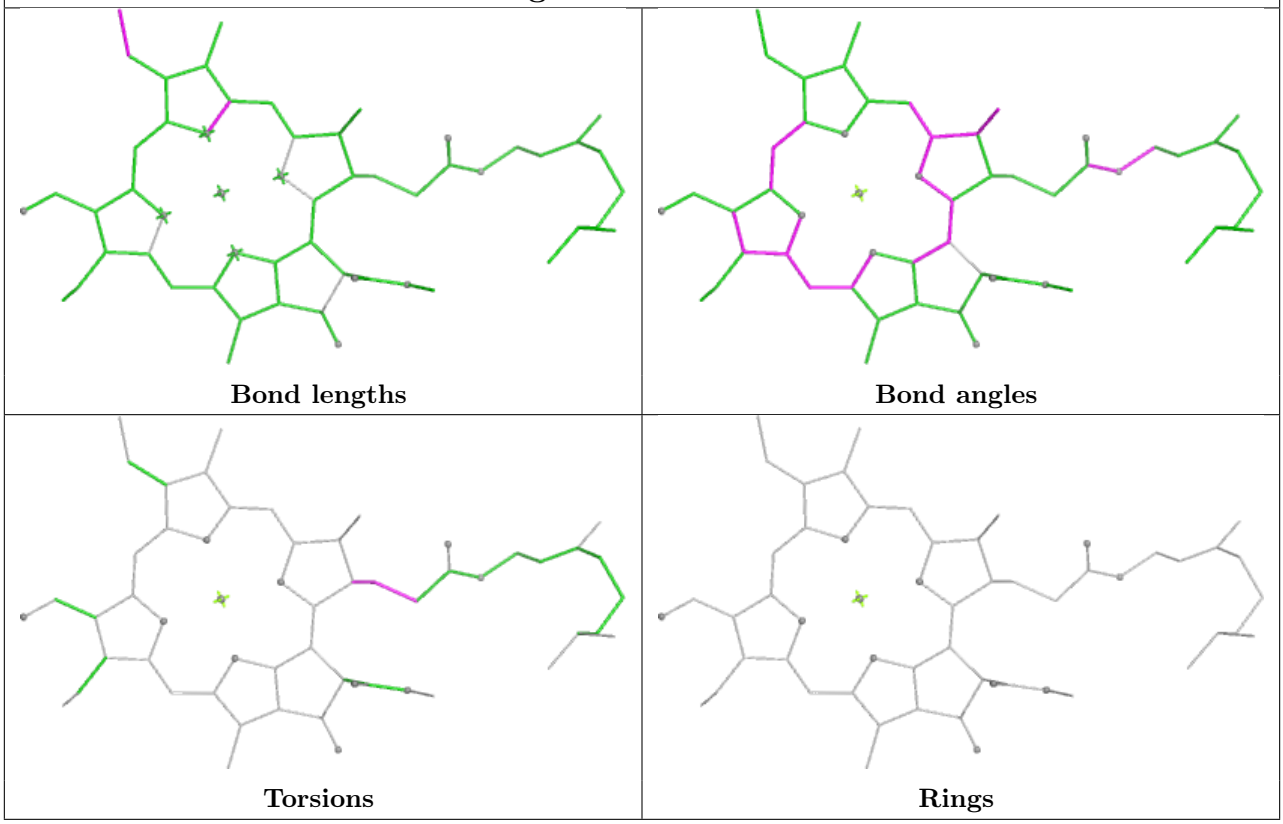

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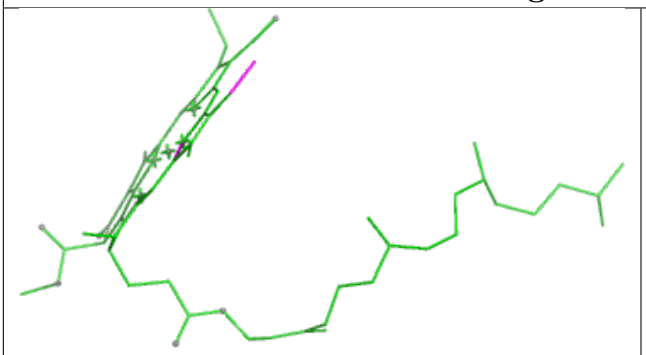

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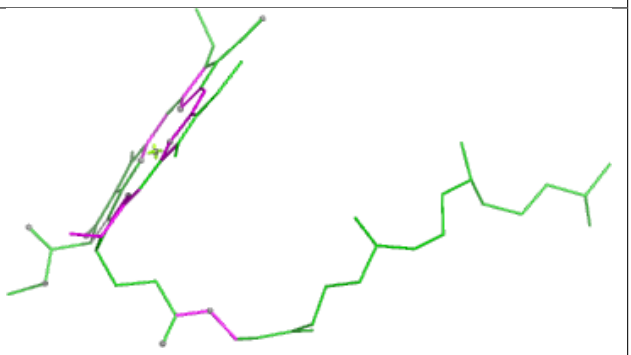

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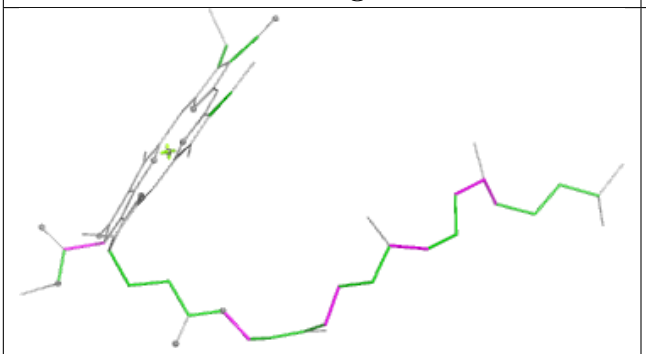
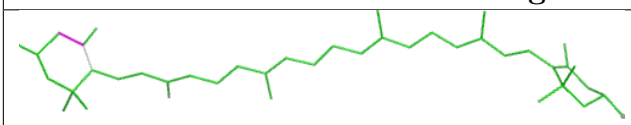


Torsions



Rings

Ligand LUT 7 502



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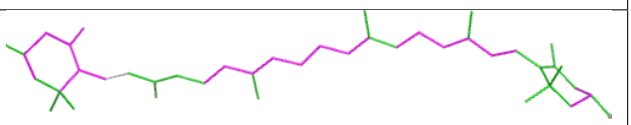
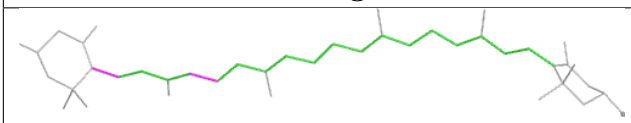
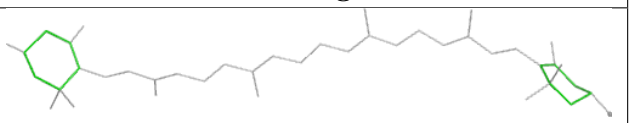


Bond angles

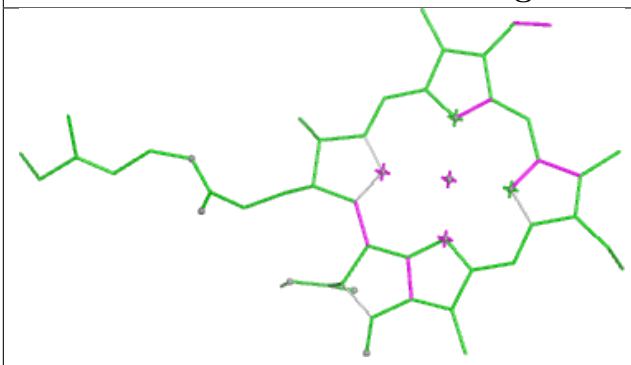


Torsions



Rings

Ligand CLA A 1135



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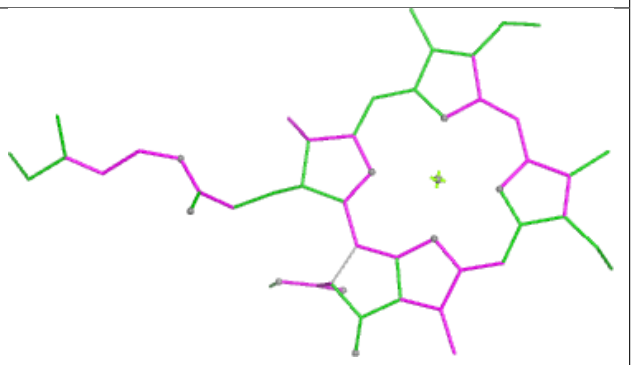

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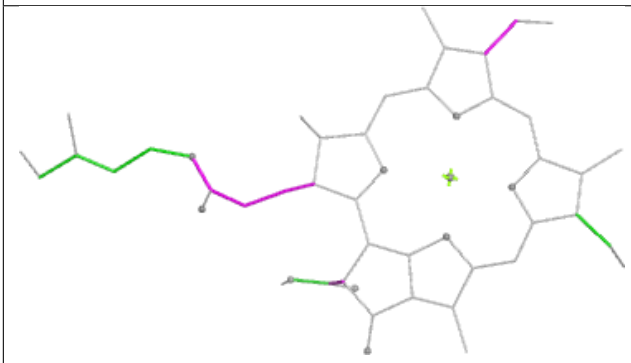

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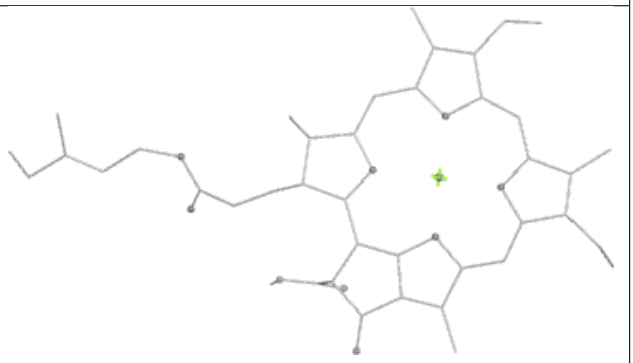
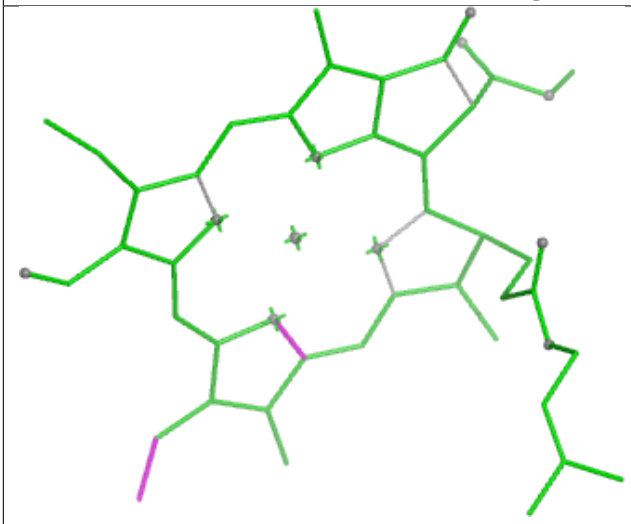


Rings

Ligand CHL 4 610



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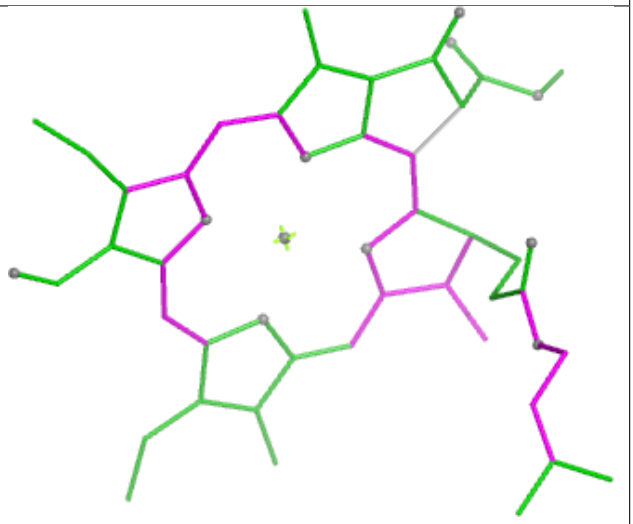
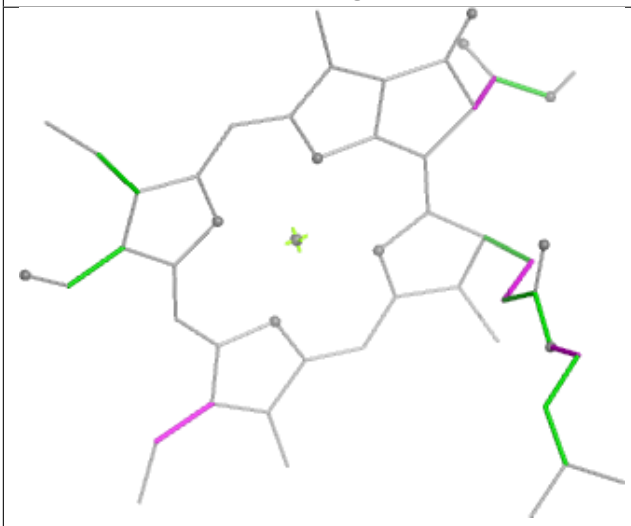


Bond angles



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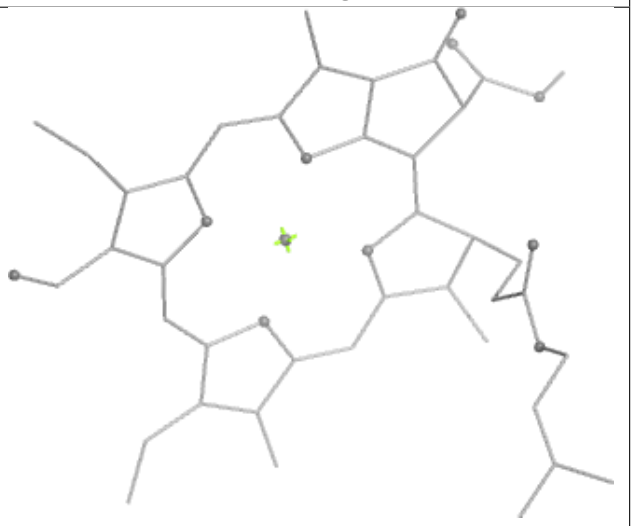
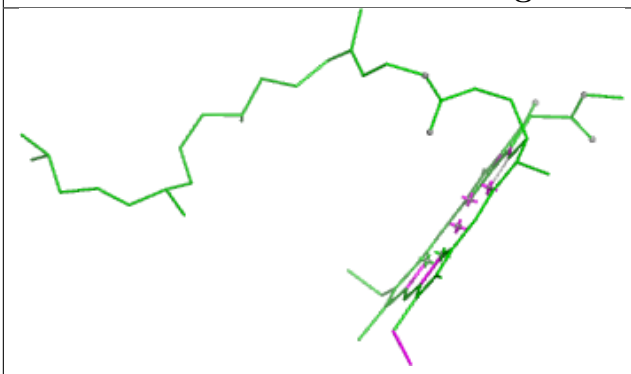


Rings

Ligand CLA A 1108



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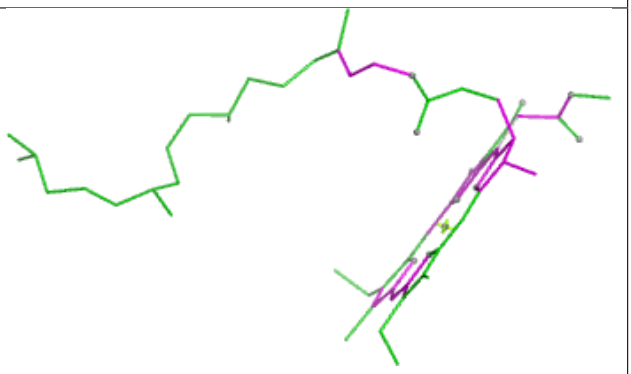
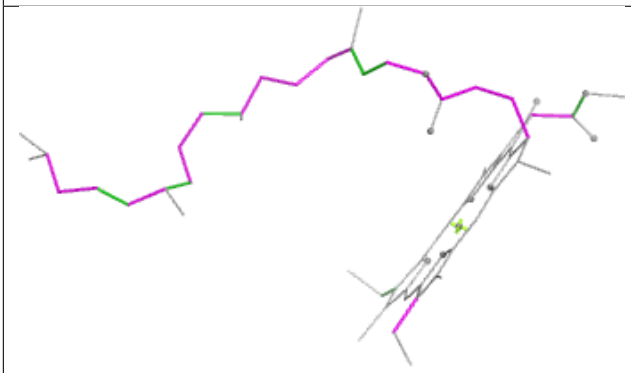


Bond angles

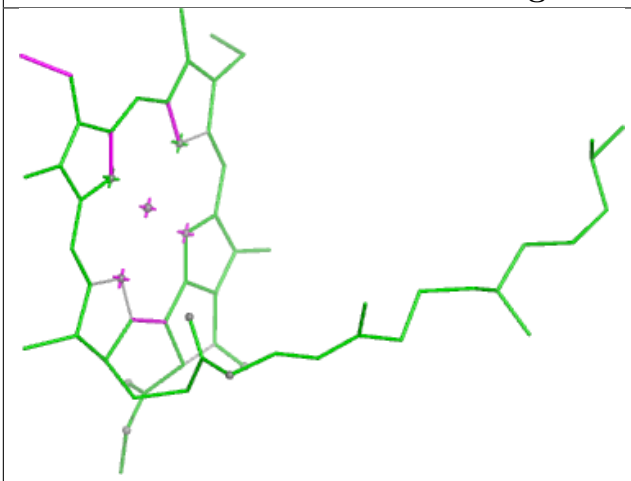


Torsions



Rings

Ligand CLA 1 607



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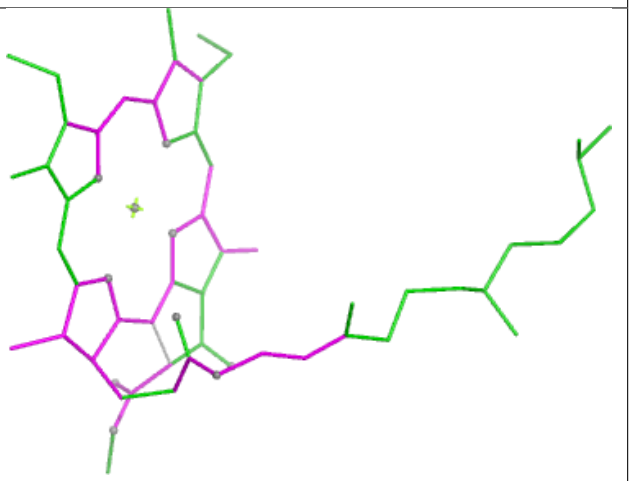

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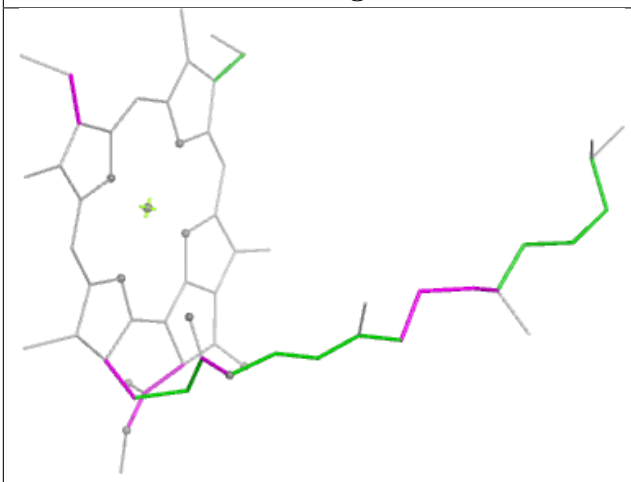

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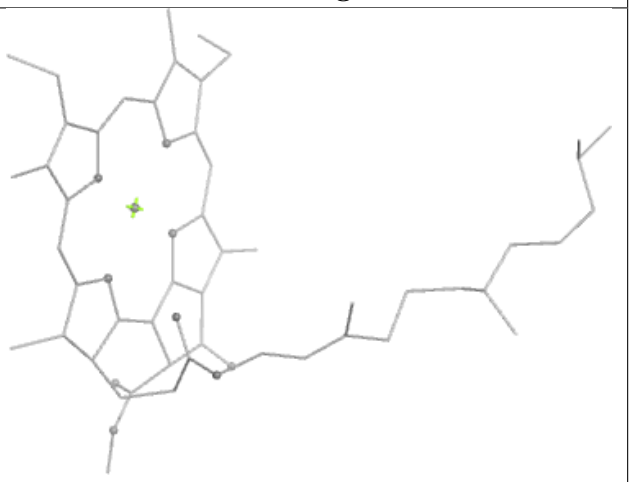
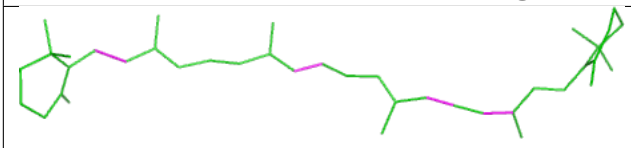


Rings

Ligand BCR B 4007



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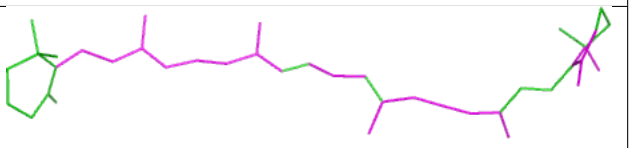
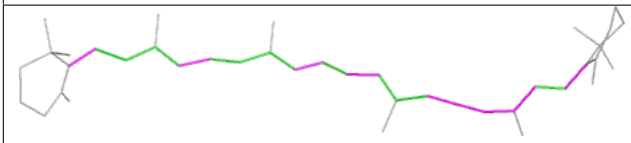


Bond angles



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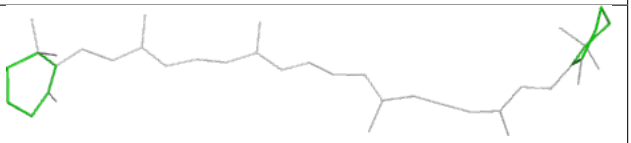
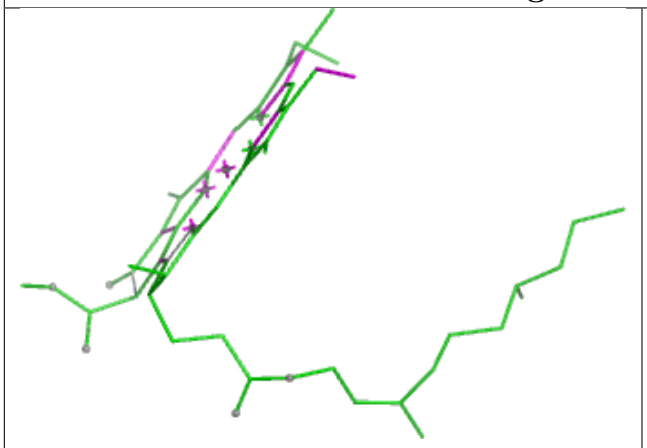


Rings

Ligand CLA Z 606



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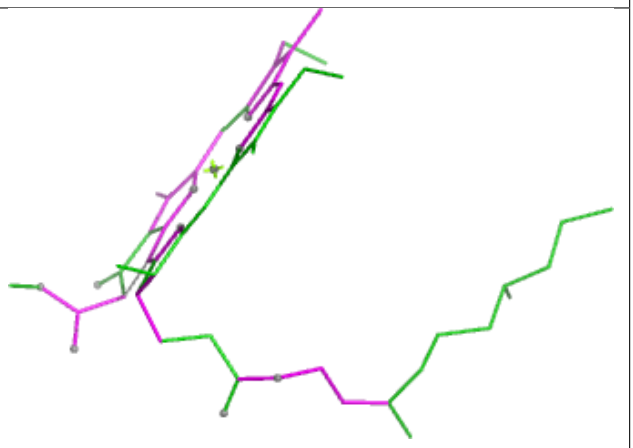
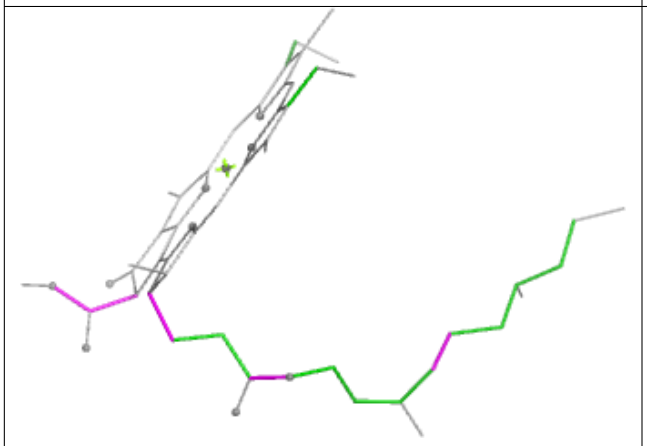


Bond angles



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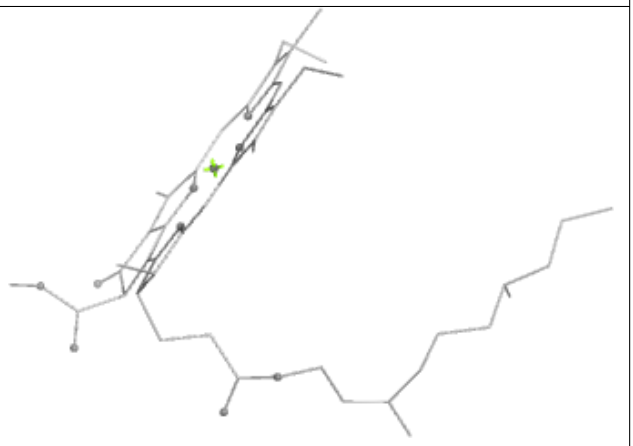
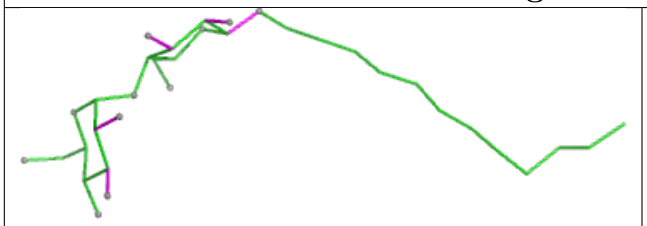


Rings

Ligand LMT 8 805



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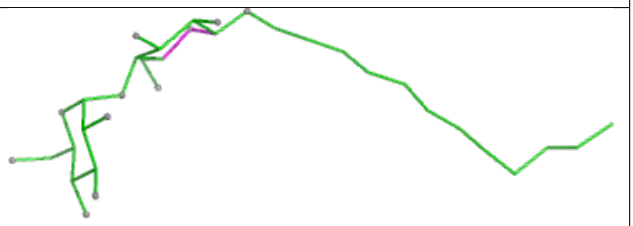
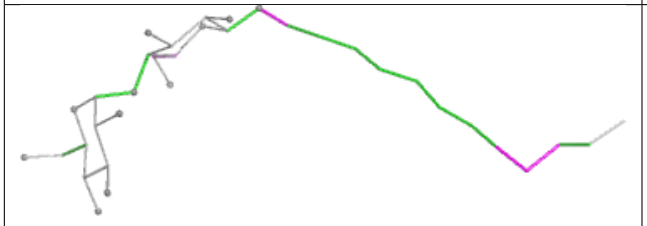


Bond angles

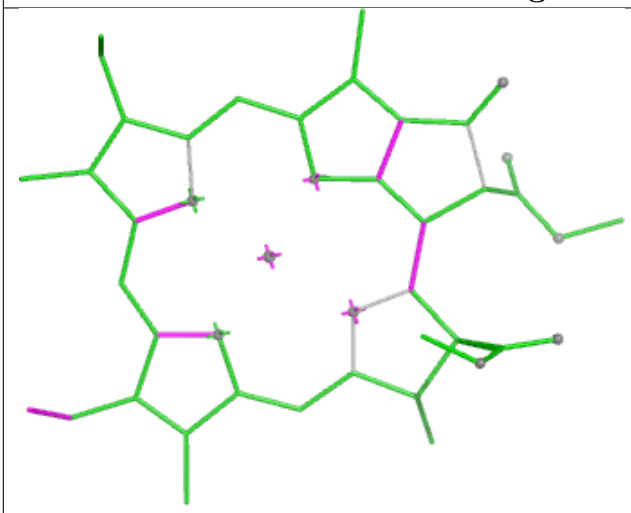


Torsions



Rings

Ligand CLA 8 615



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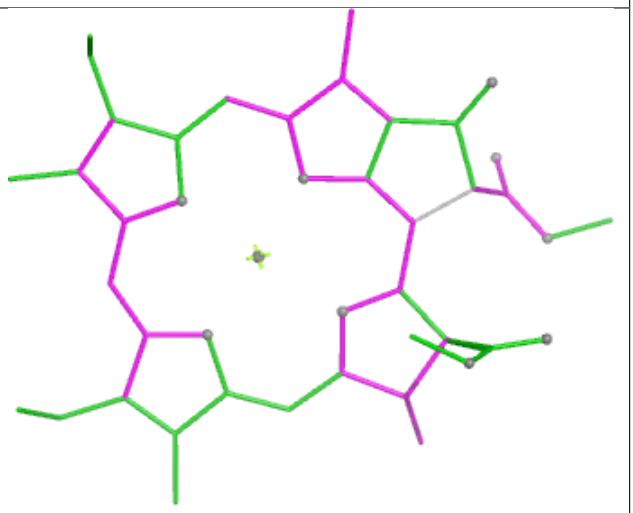

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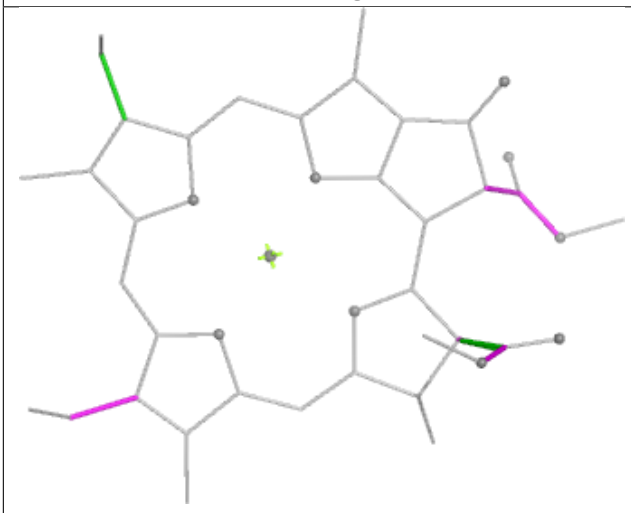

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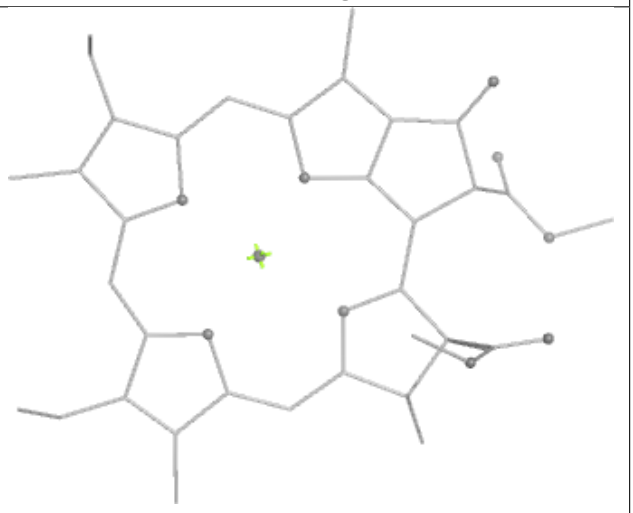
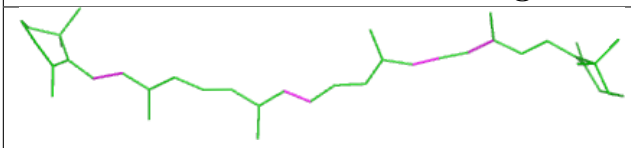


Rings

Ligand BCR B 4004



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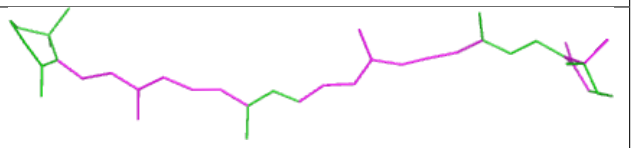
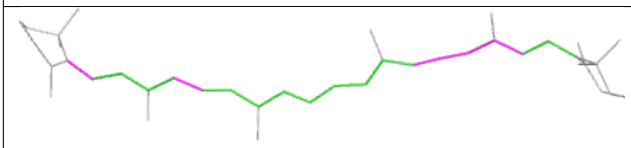


Bond angles



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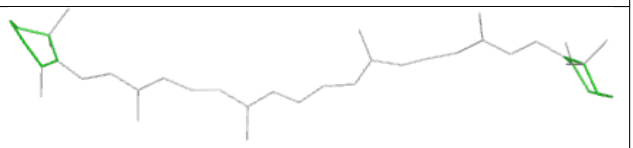
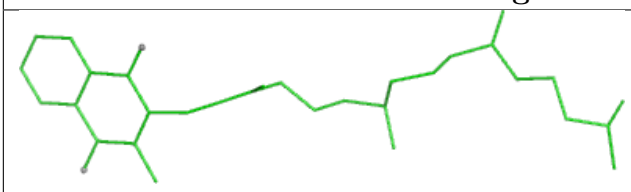


Rings

Ligand PQN A 2001



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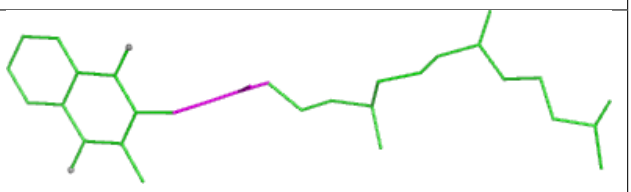
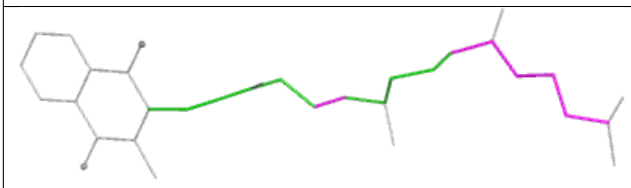


Bond angles



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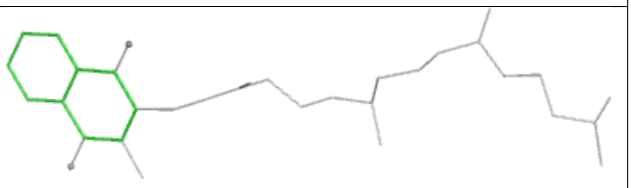
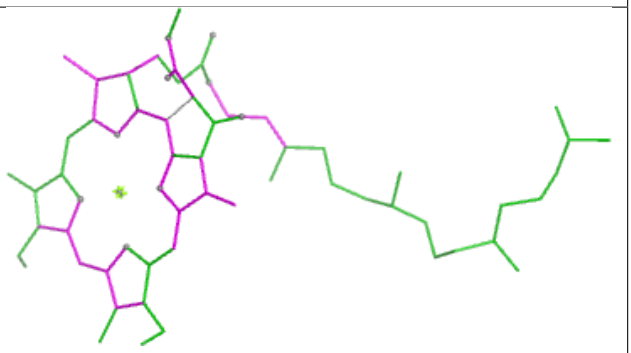


Rings

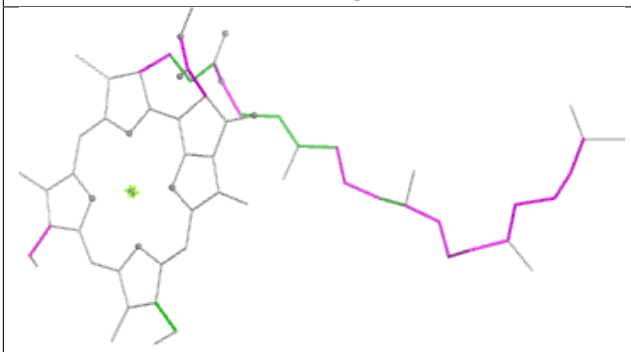
Ligand CLA 7 607



Bond lengths



Bond angles



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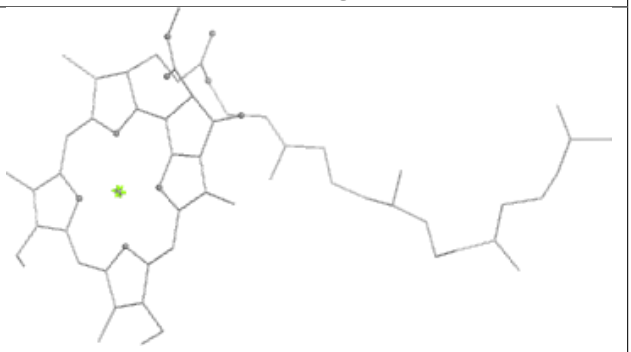


Rings

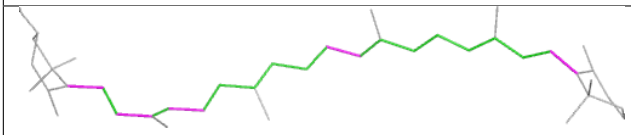
Ligand C7Z 1 503



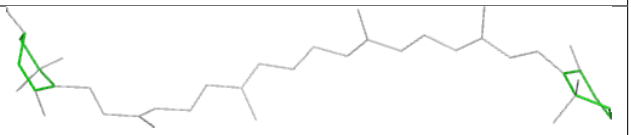
Bond lengths



Bond angles

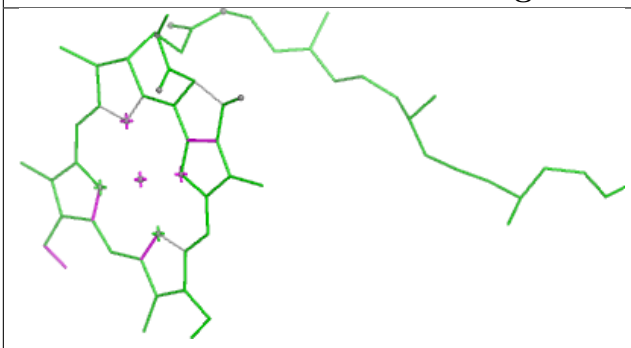


Torsions

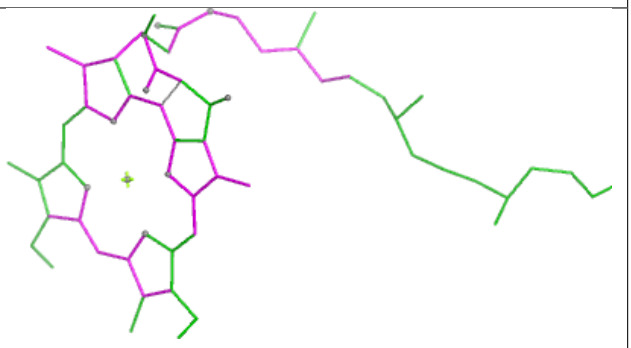


Rings

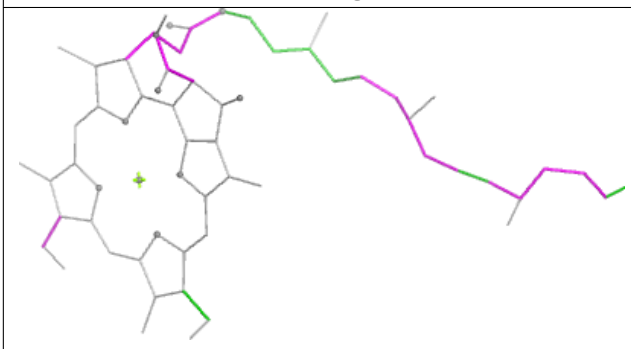
Ligand CLA A 1121



Bond lengths



Bond angles



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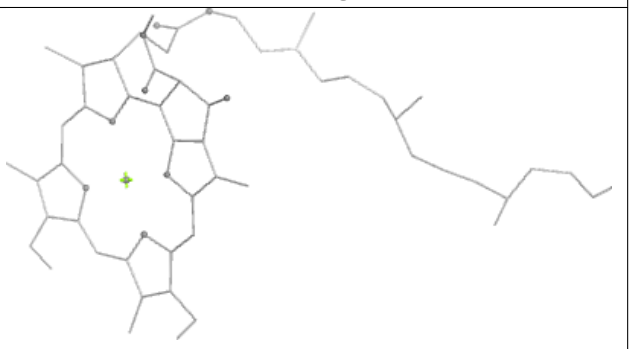
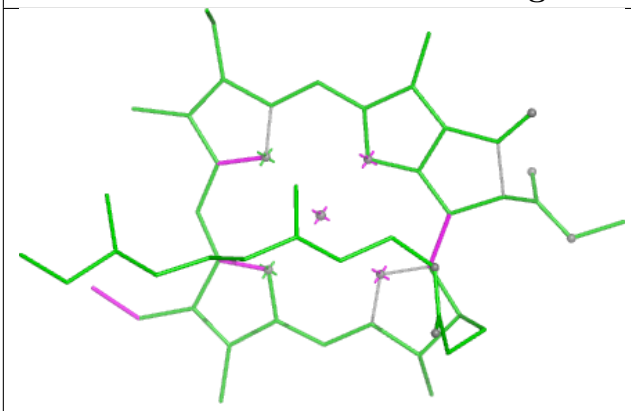


Rings

Ligand CLA 3 616



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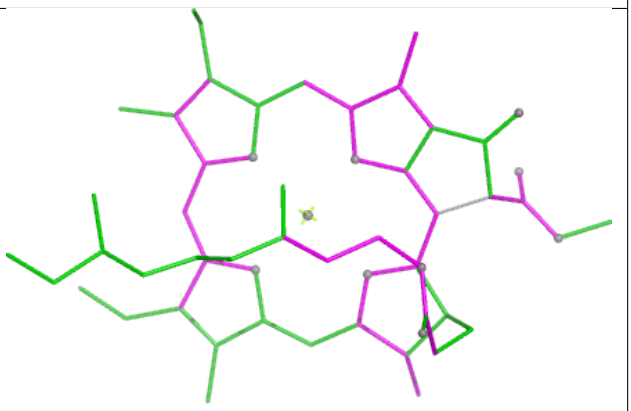
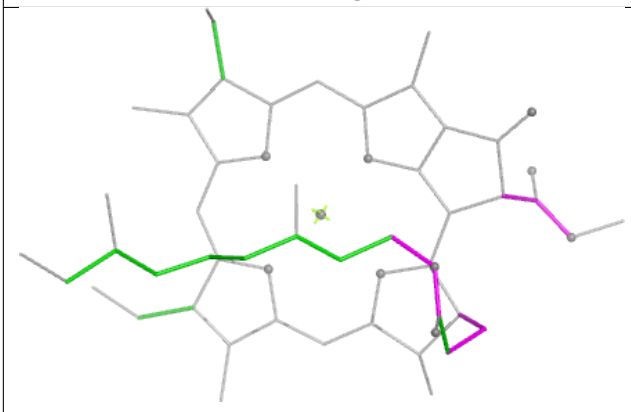


Bond angles

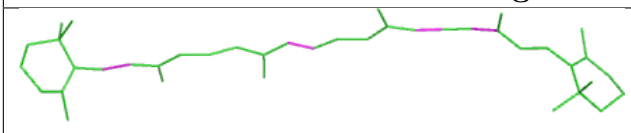


Torsions



Rings

Ligand BCR K 4002



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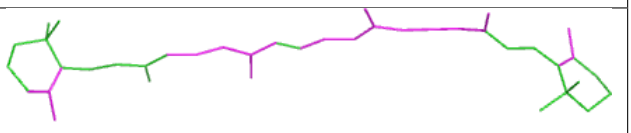

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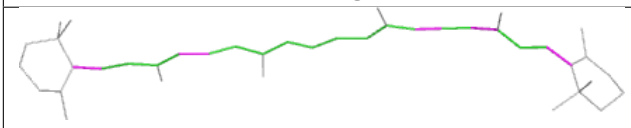
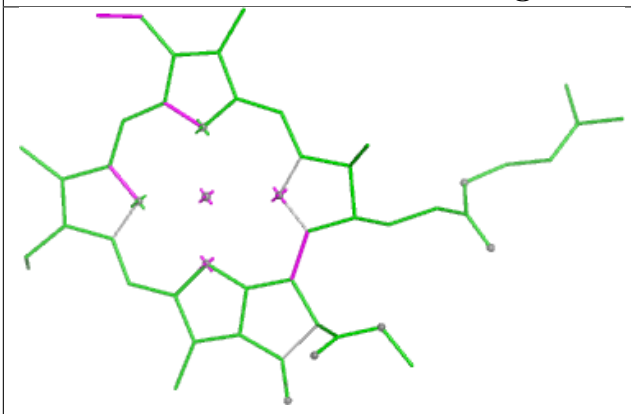


Torsions



Rings

Ligand CLA G 1601



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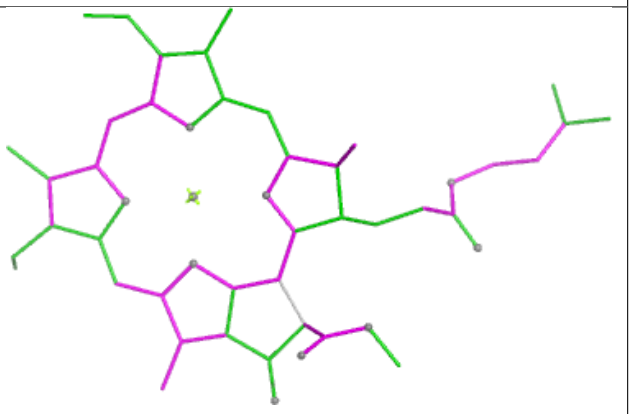

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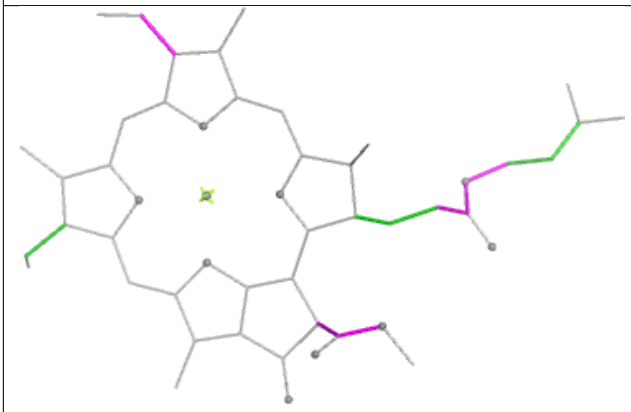

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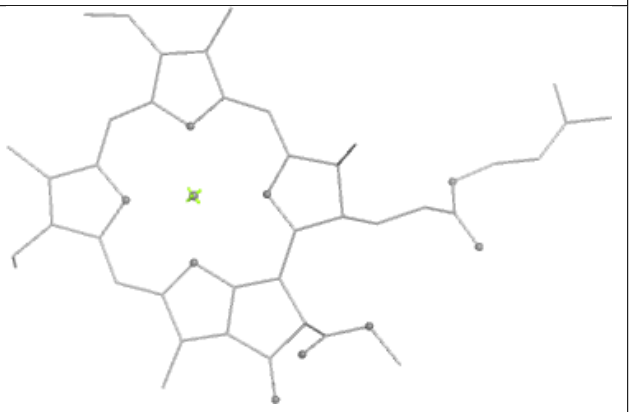

Rings

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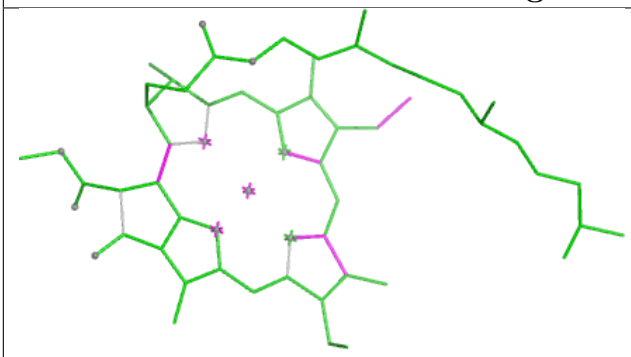

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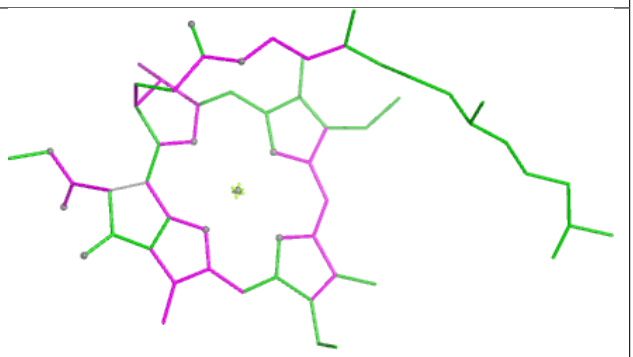
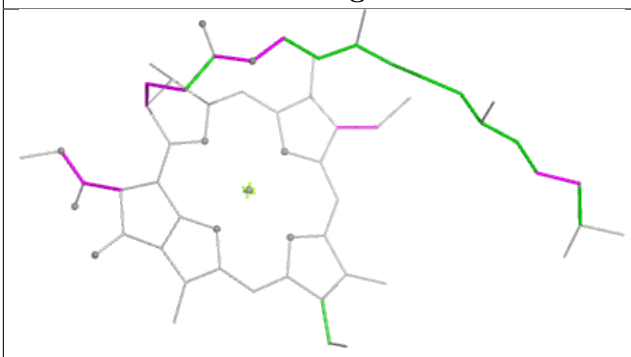


Bond angles



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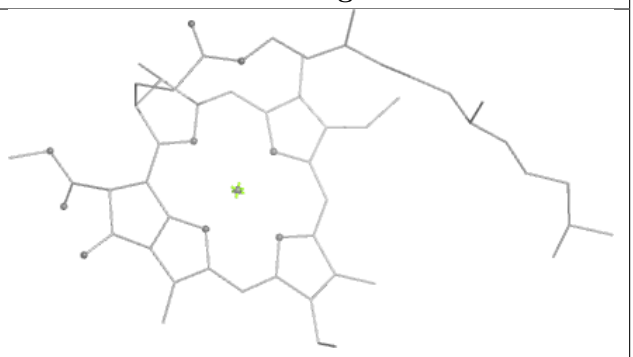
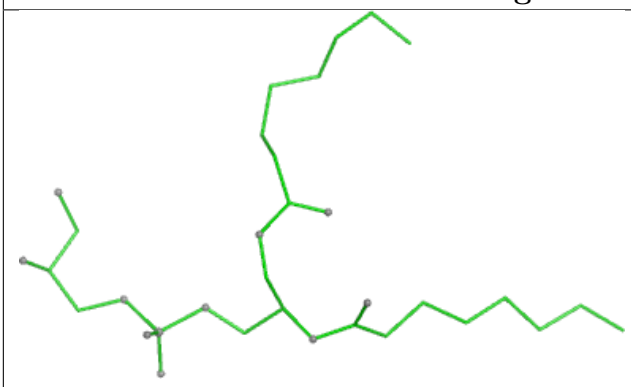


Rings

Ligand LHG B 5006



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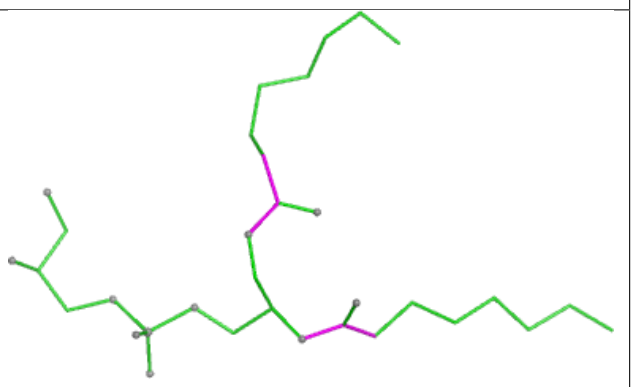

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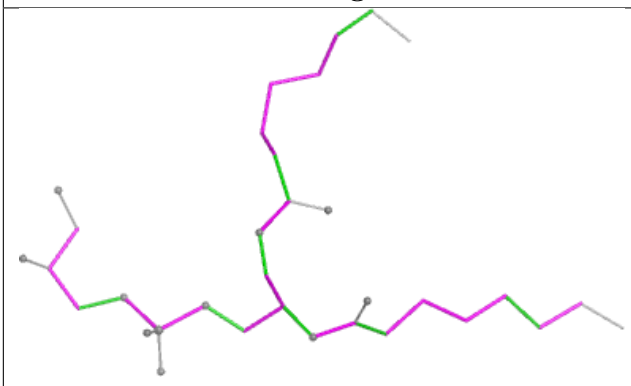

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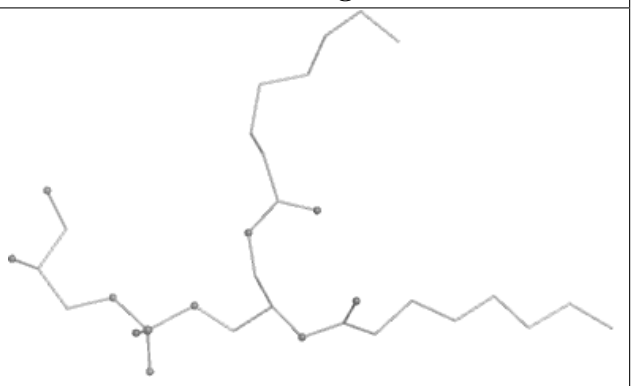
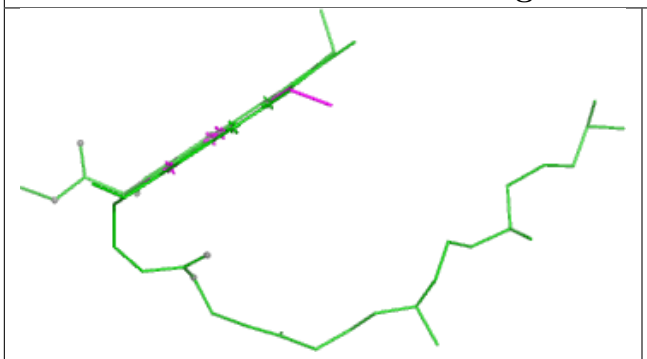


Rings

Ligand CLA A 1130



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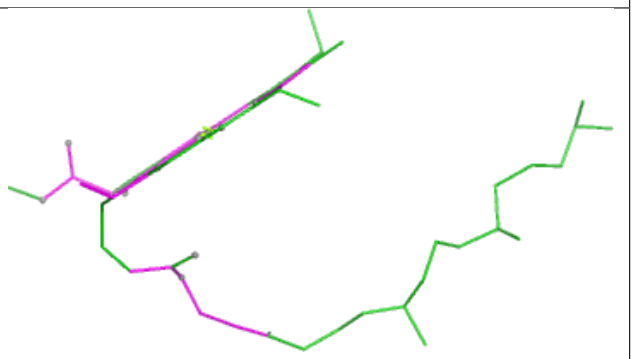


Bond angles

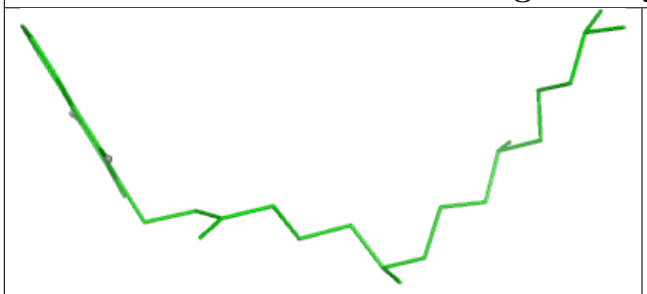


Torsions



Rings

Ligand PQN B 2002



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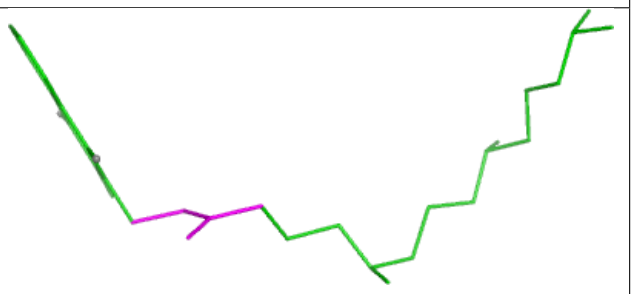
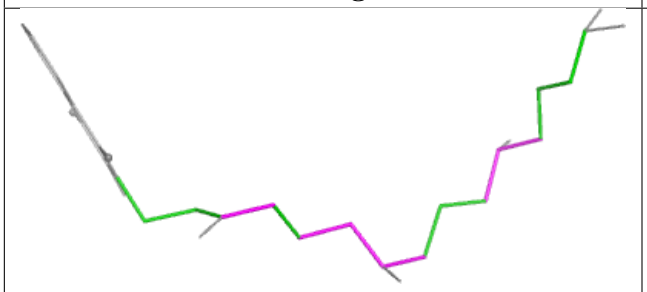


Bond angles



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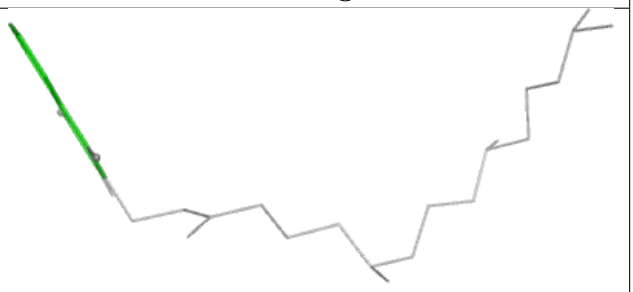
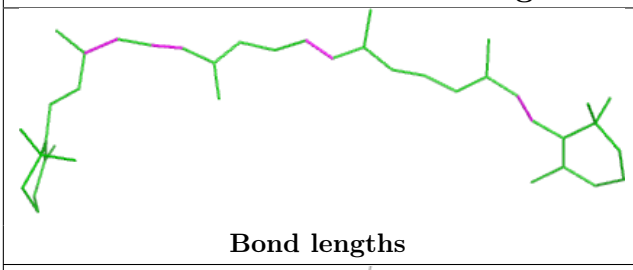


Rings

Ligand BCR L 4002



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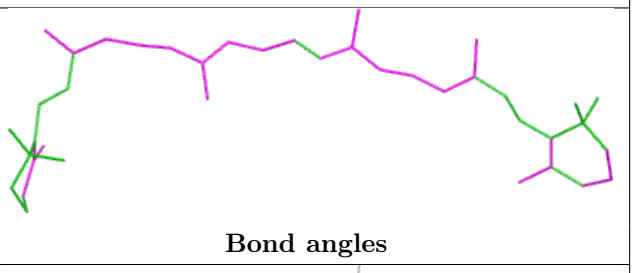
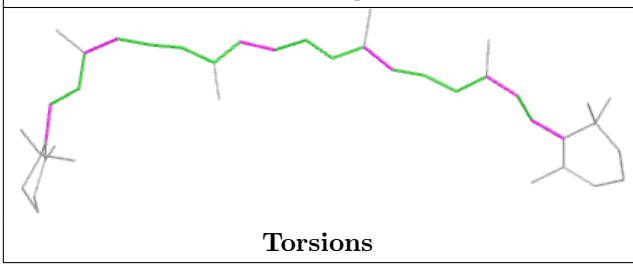


Bond angles



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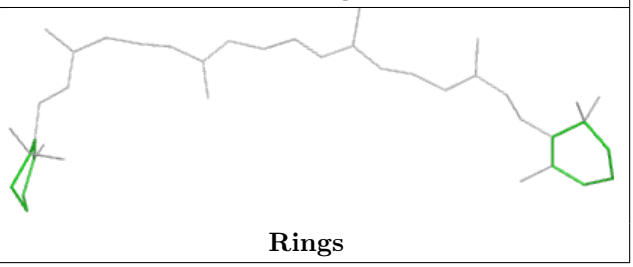
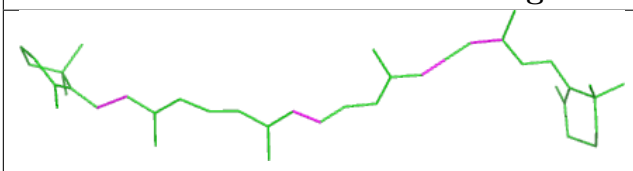


Rings

Ligand BCR 6 503



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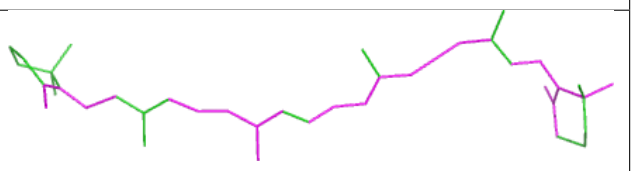
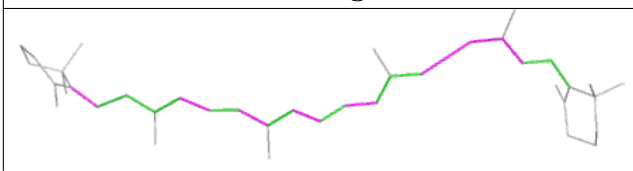


Bond angles



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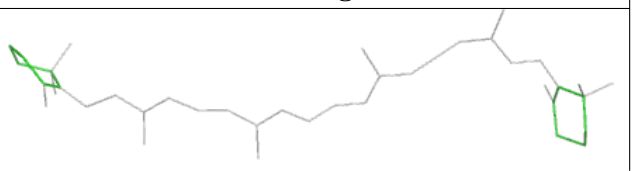
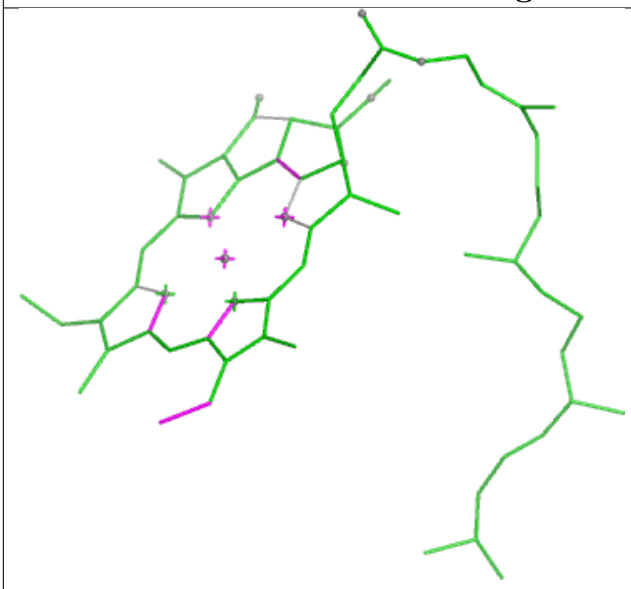


Rings

Ligand CLA B 1207



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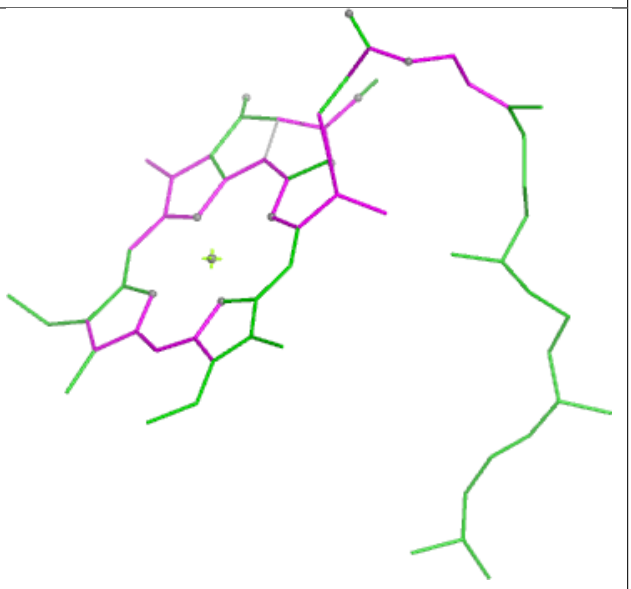

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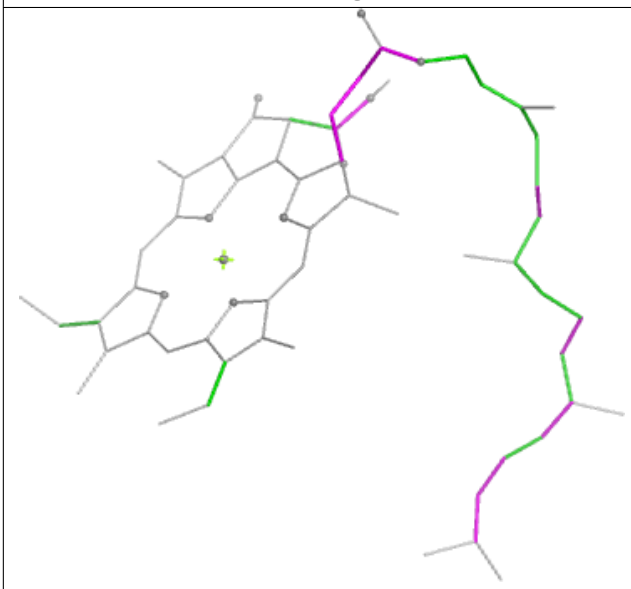
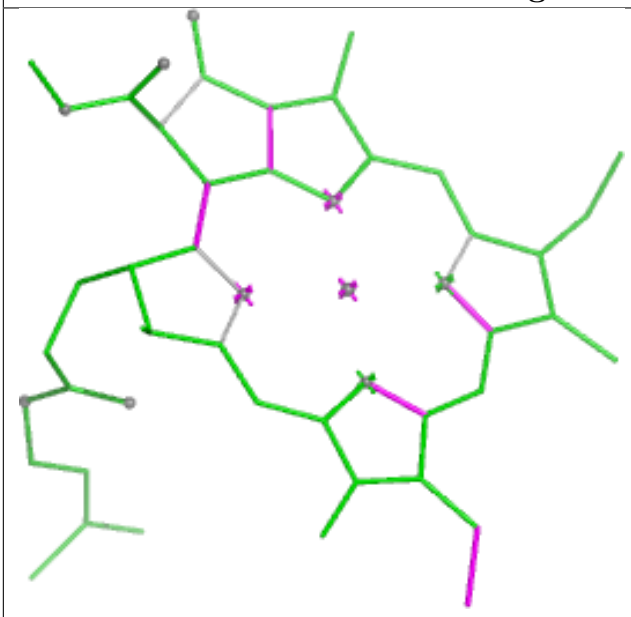


Torsions



Rings

Ligand CLA 7 612



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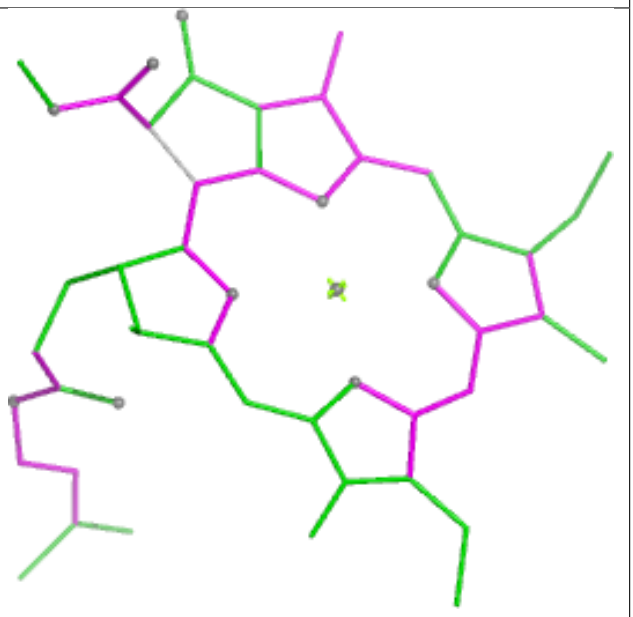
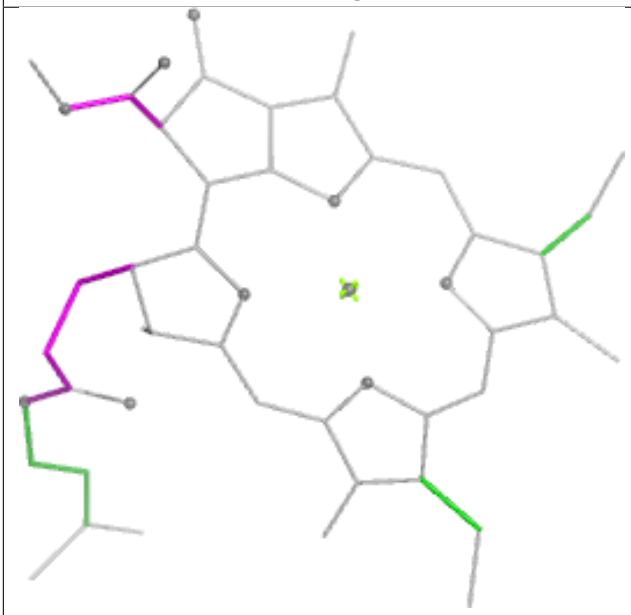


Bond angles



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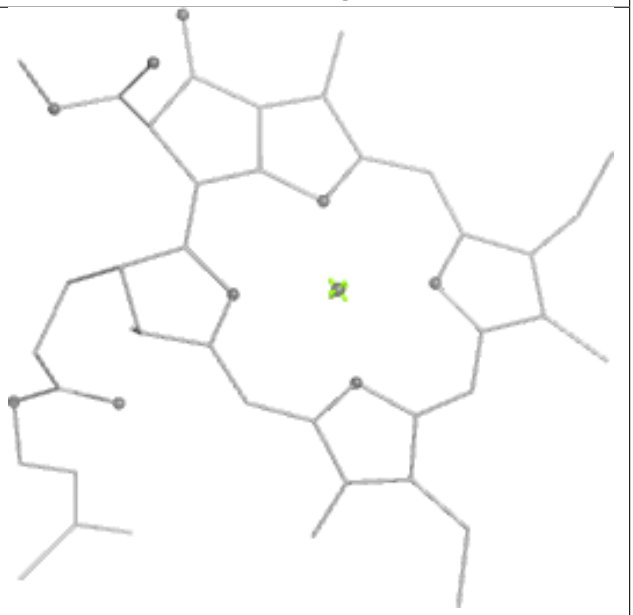
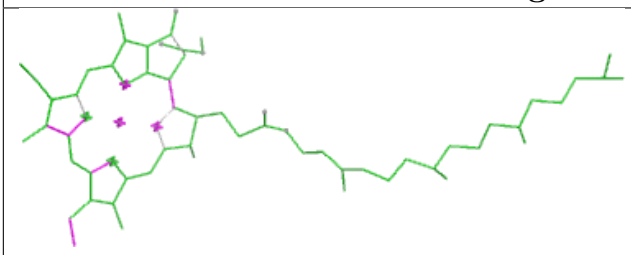
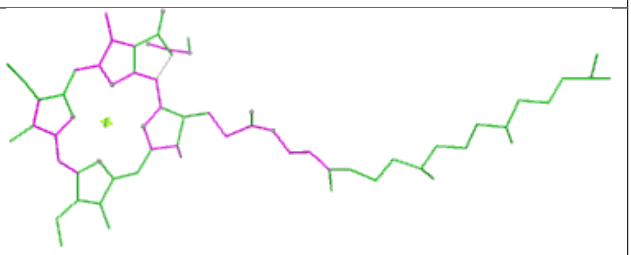


Rings

Ligand CLA 5 618	
	
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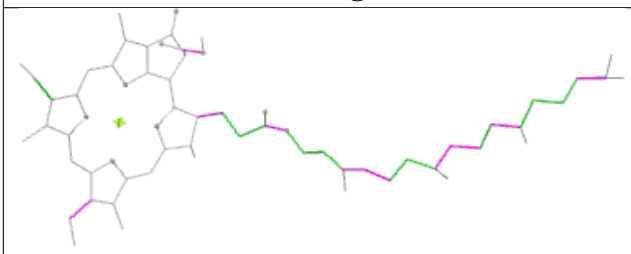
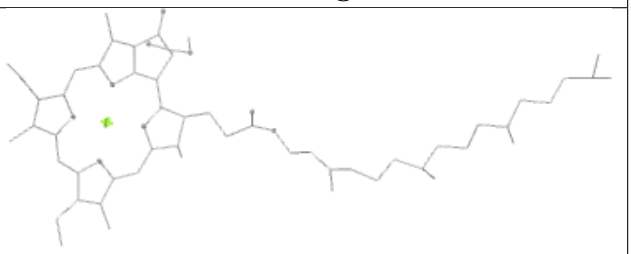
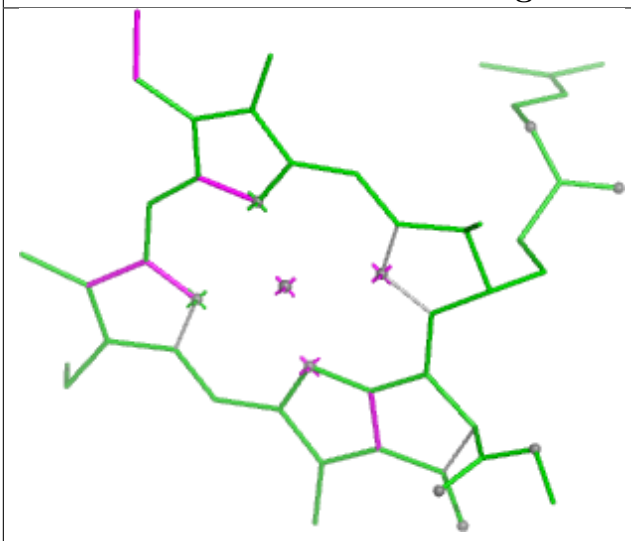
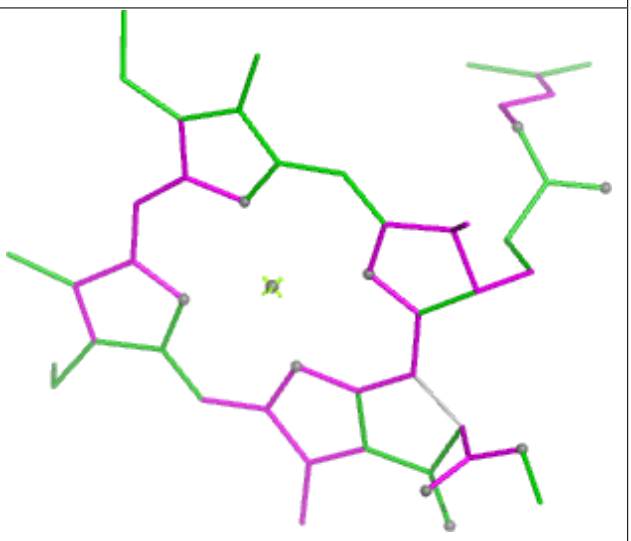
	
Torsions	**Rings**

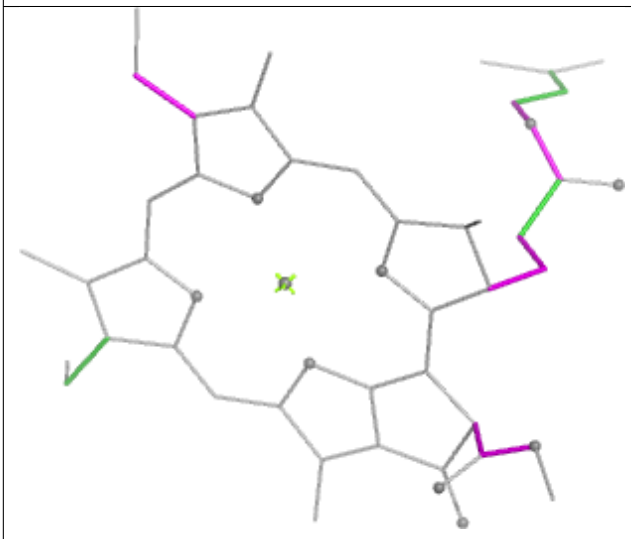
Ligand CLA B 1227



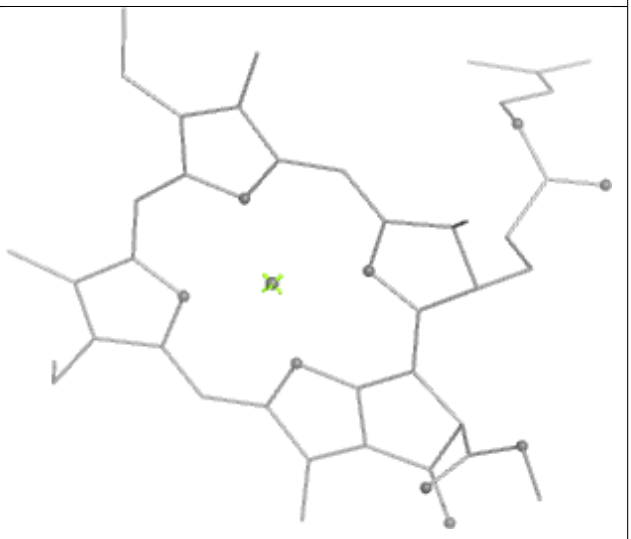
Bond lengths



Bond angles

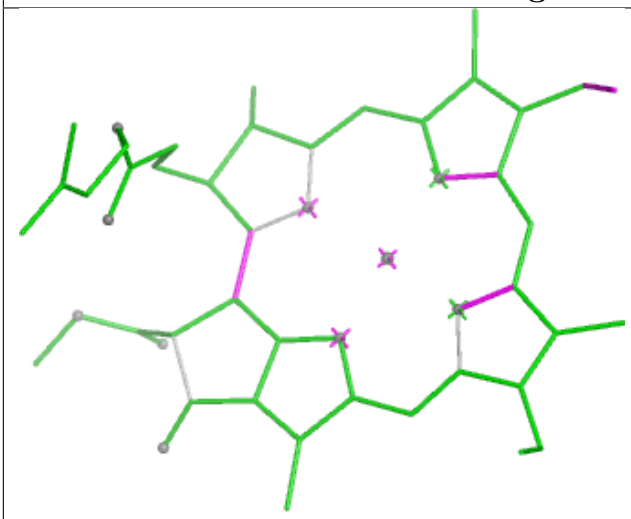


Torsions



Rings

Ligand CLA 5 615



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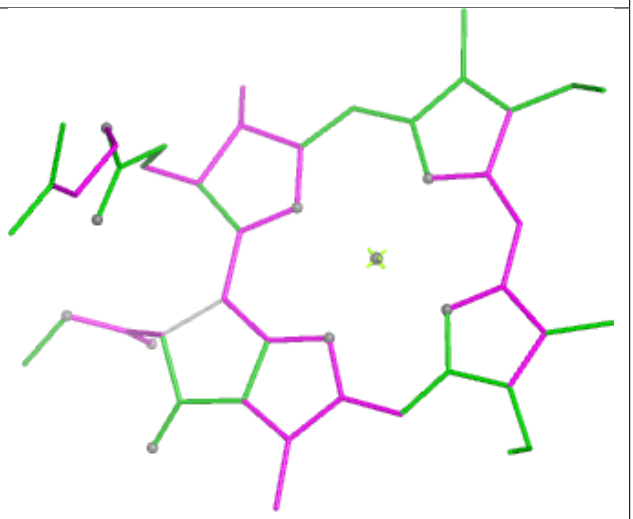
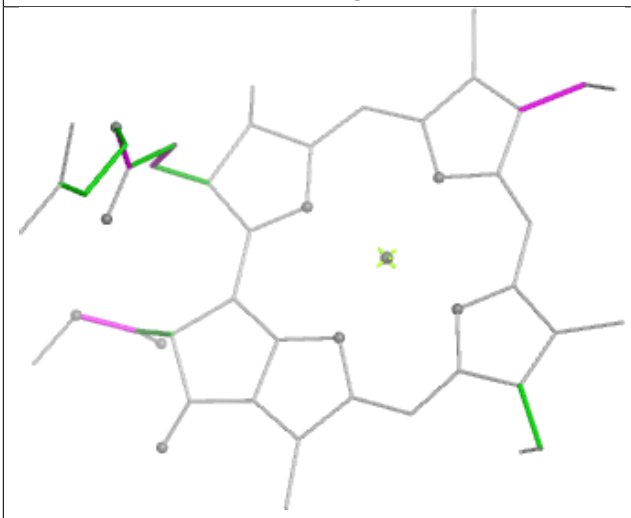


Bond angles



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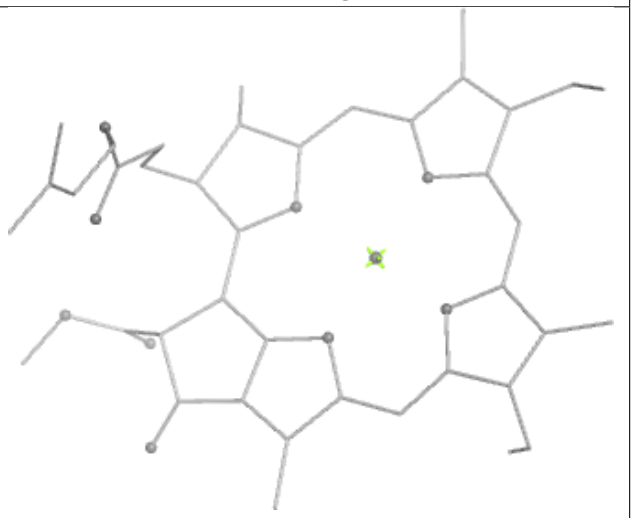
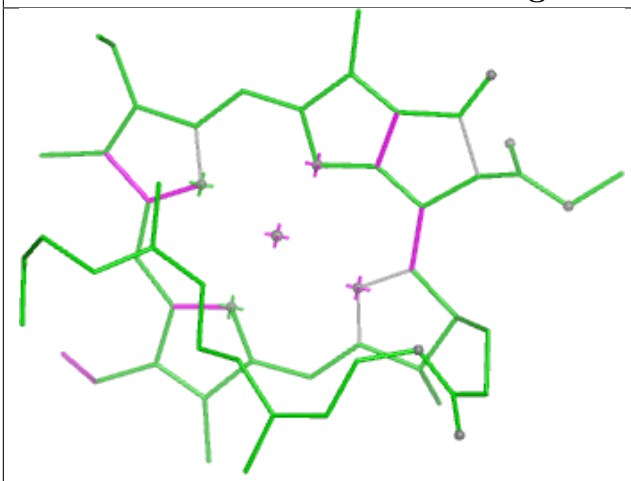


Rings

Ligand CLA 7 615



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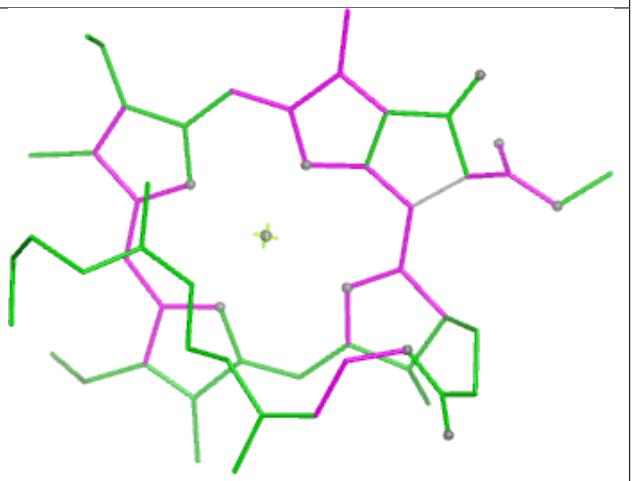
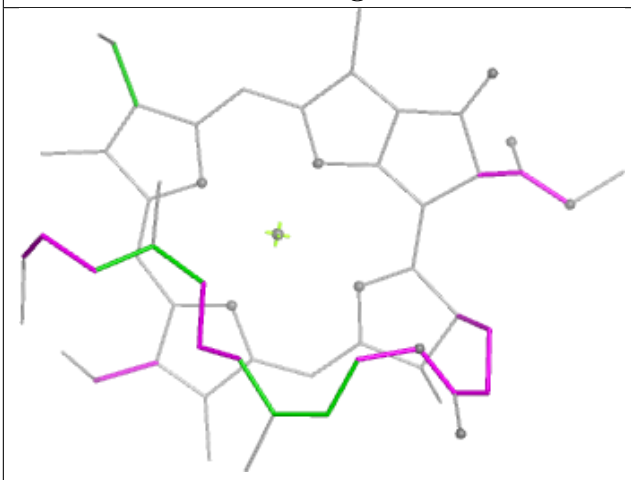
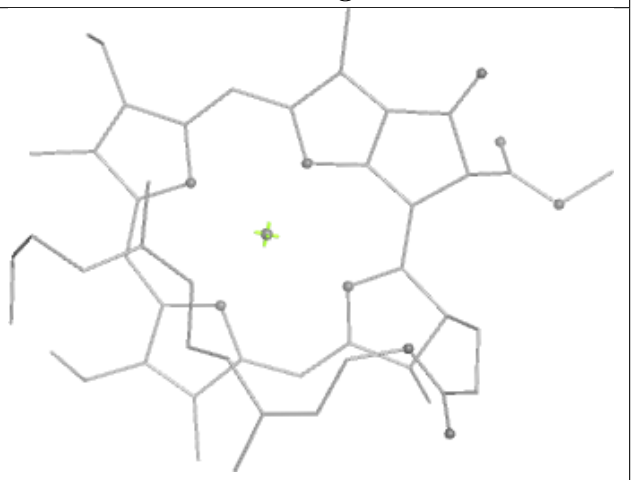


Bond angles

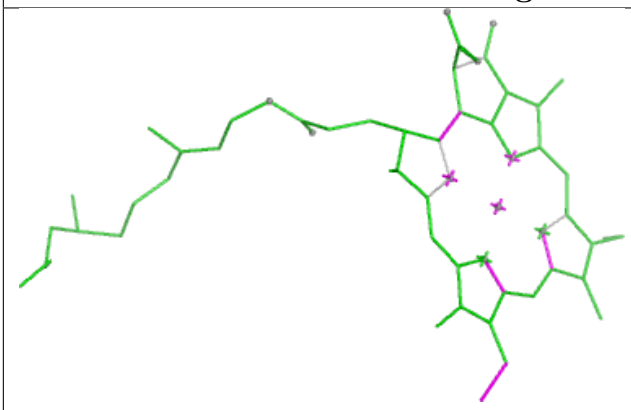


Torsions

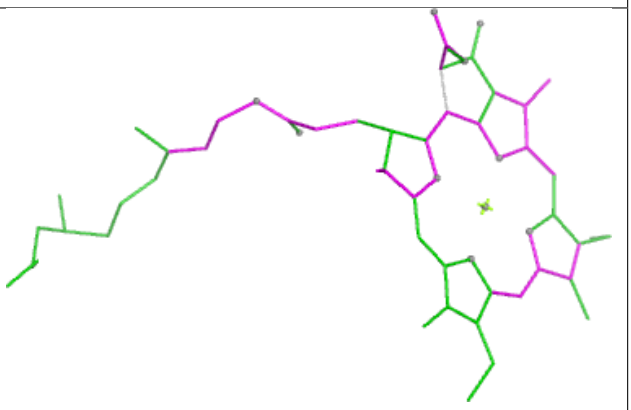


Rings

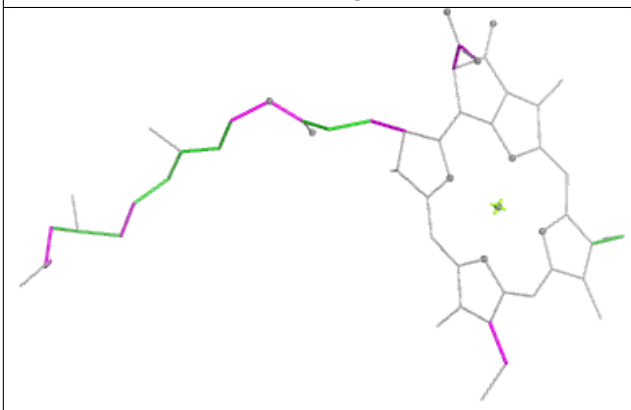
Ligand CLA B 1230



Bond lengths



Bond angles

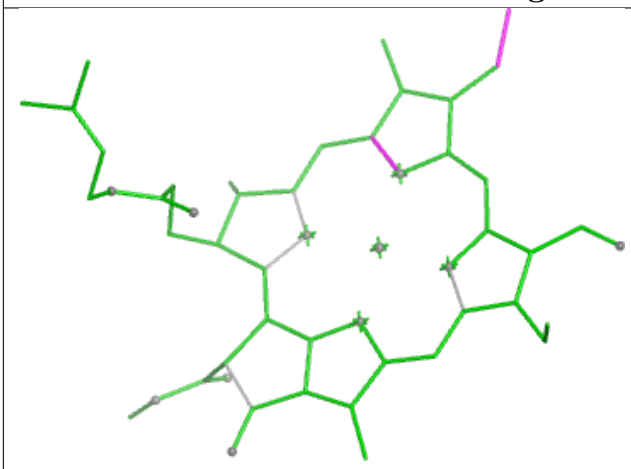


Torsions



Rings

Ligand CHL 4 611



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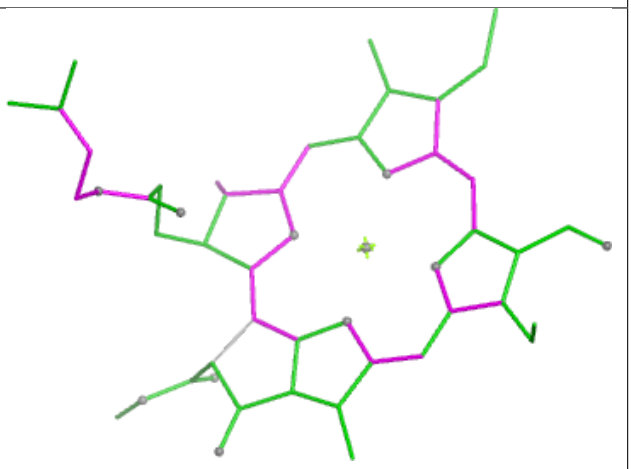
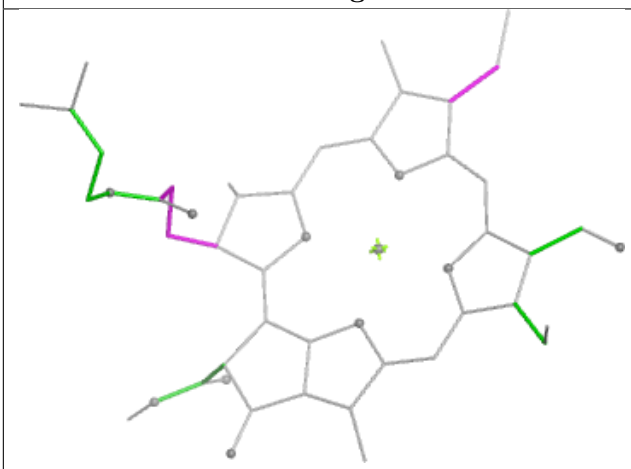


Bond angles



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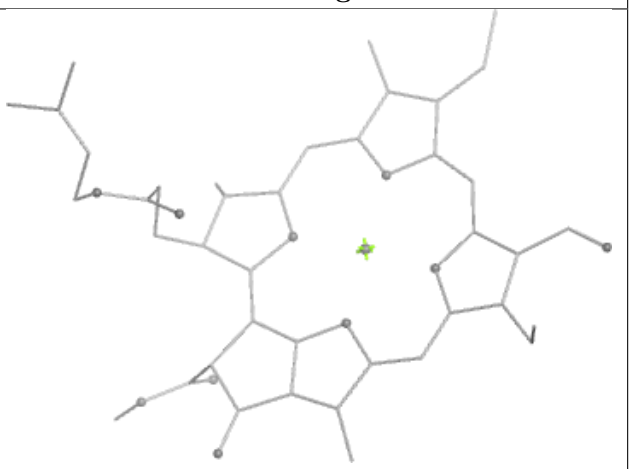
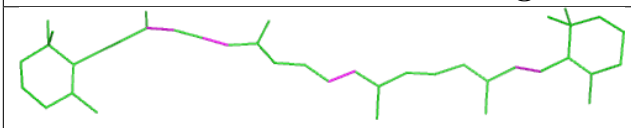


Rings

Ligand BCR L 4001



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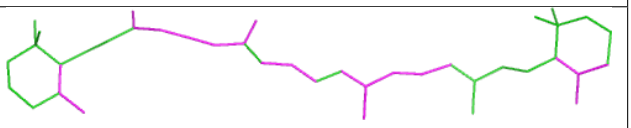
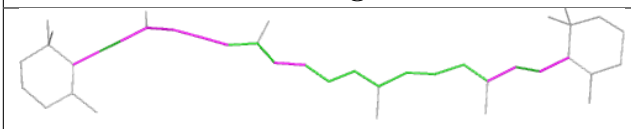


Bond angles



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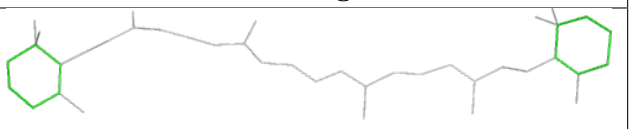
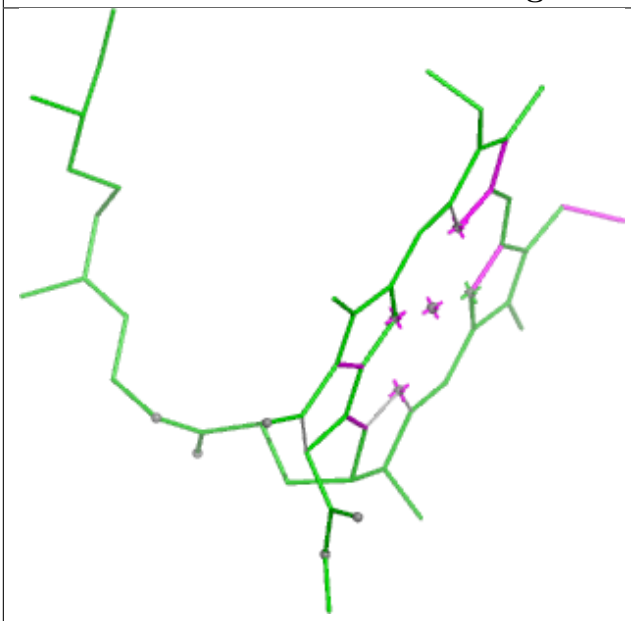


Rings

Ligand CLA Z 608



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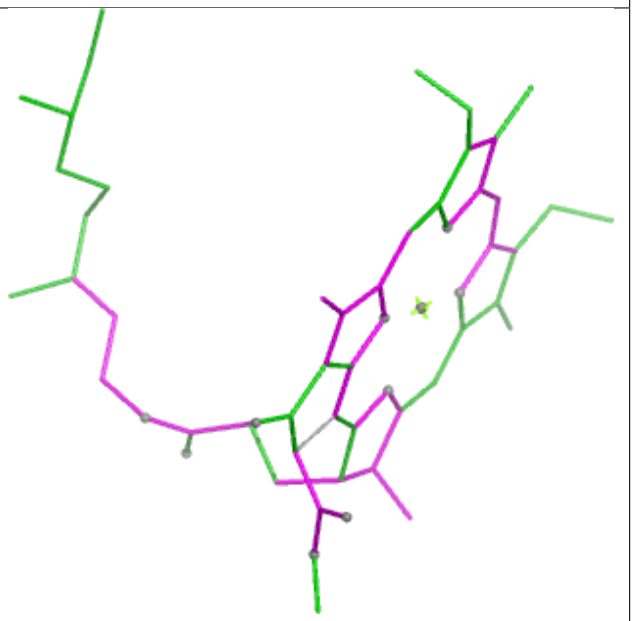
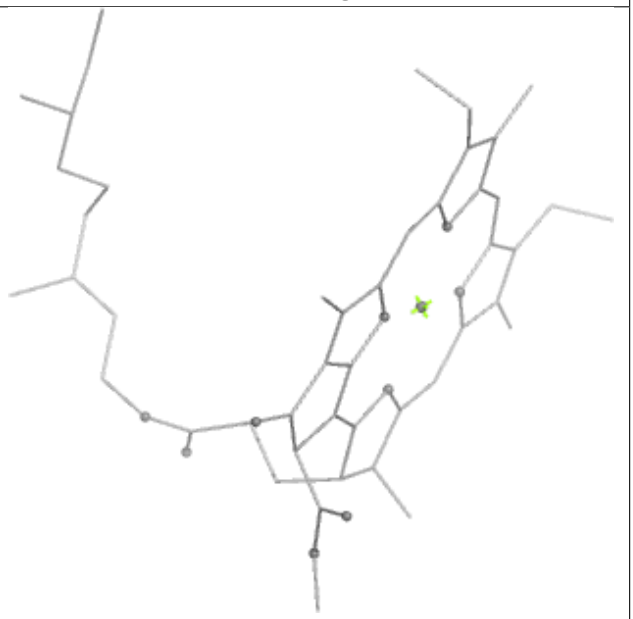


Bond angles

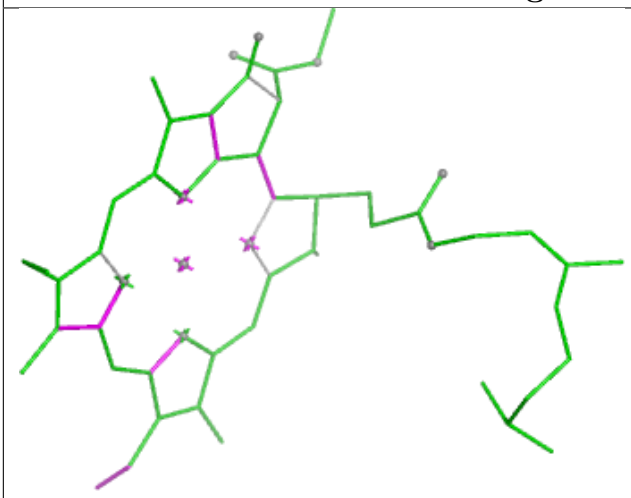


Torsions



Rings

Ligand CLA Z 611



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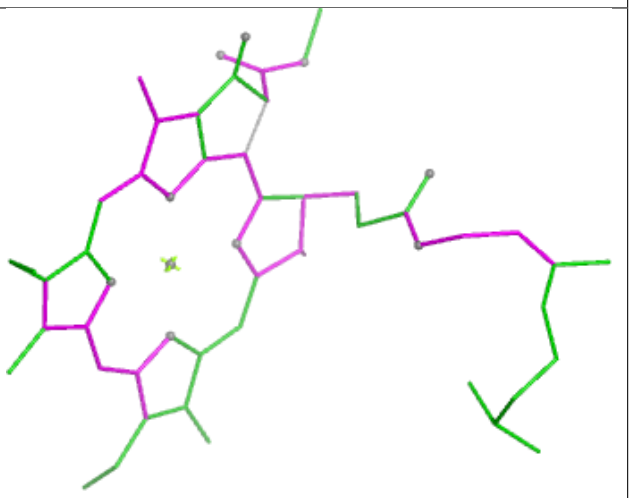
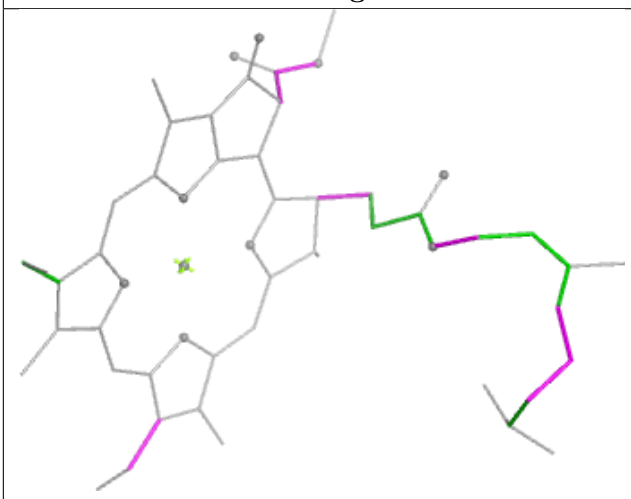


Bond angles



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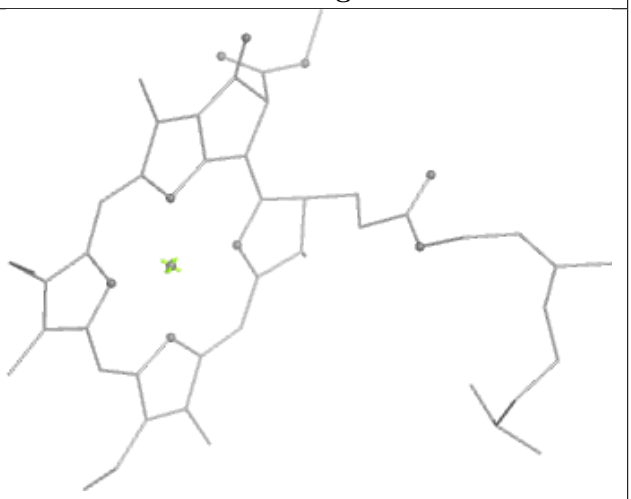
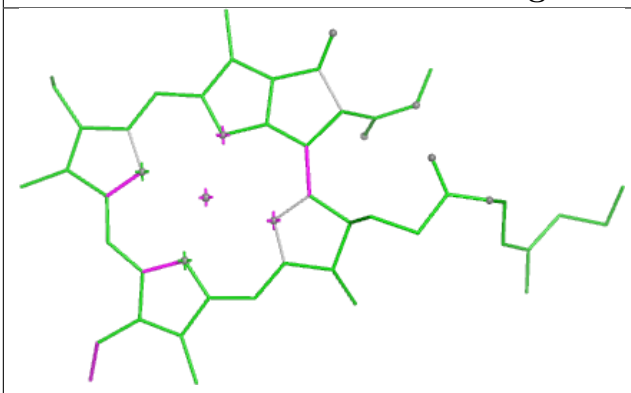


Rings

Ligand CLA 6 602



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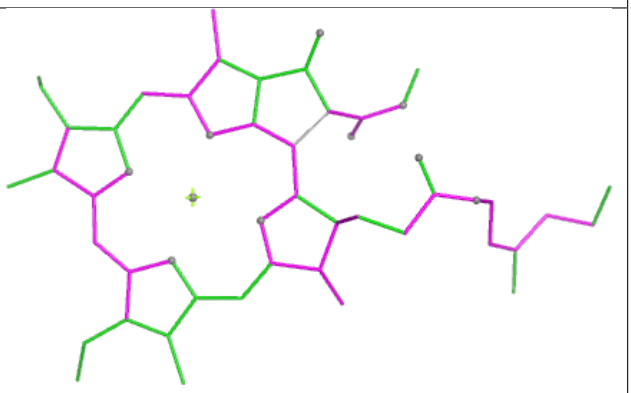
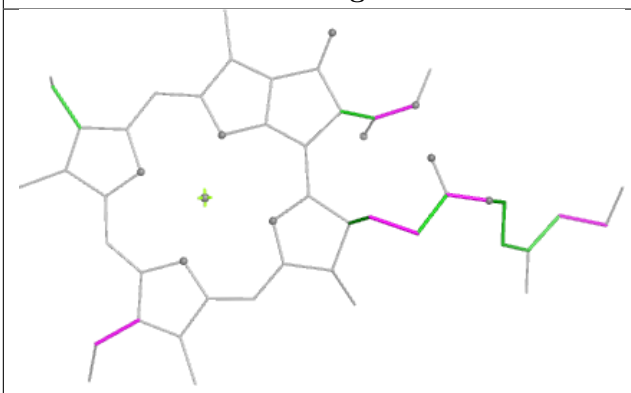


Bond angles



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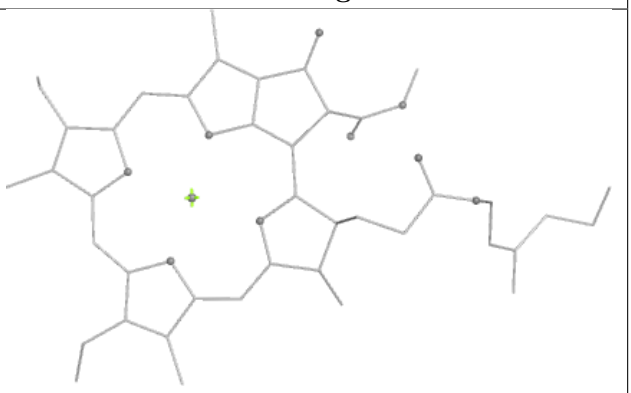
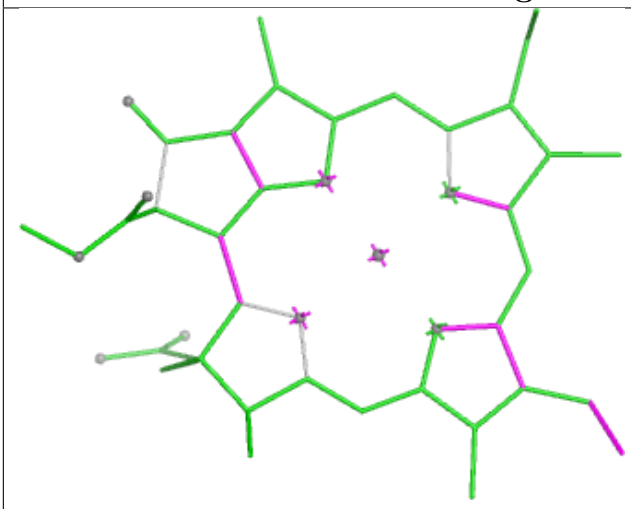


Rings

Ligand CLA B 1201



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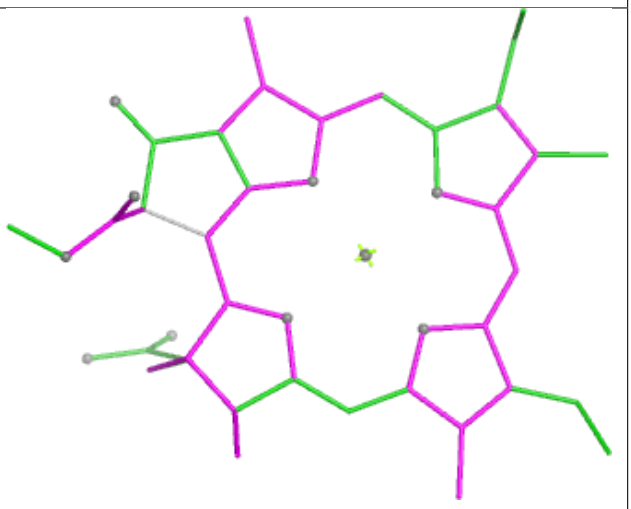
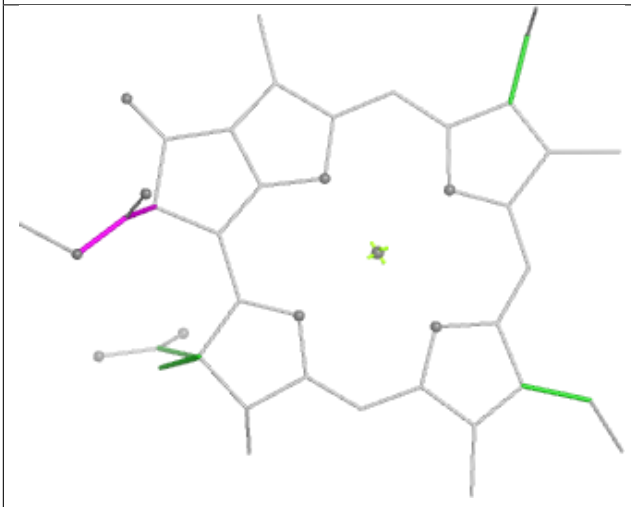


Bond angles



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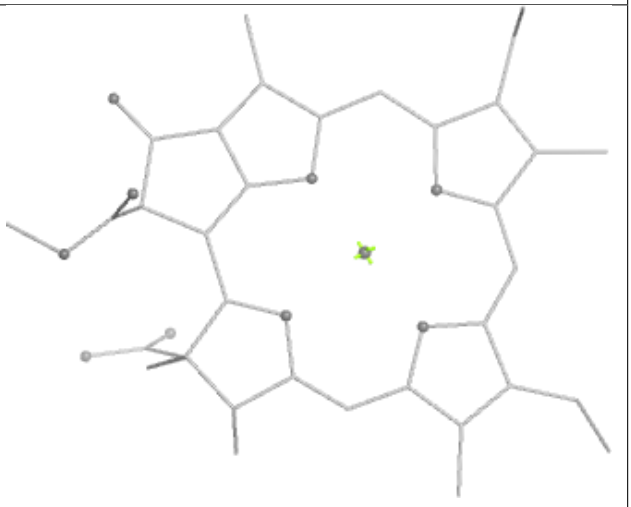
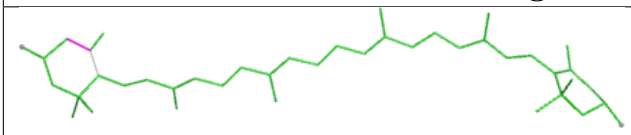


Rings

Ligand LUT 8 502



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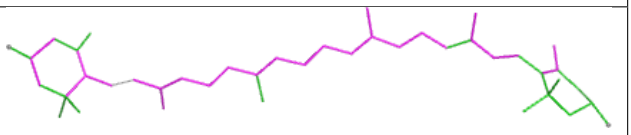
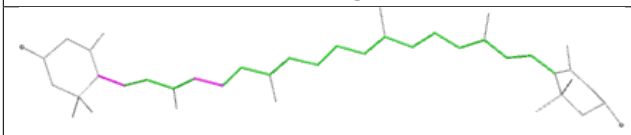


Bond angles



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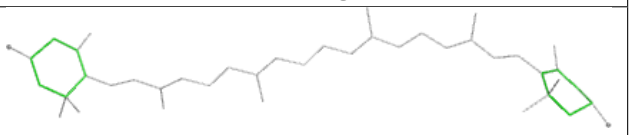
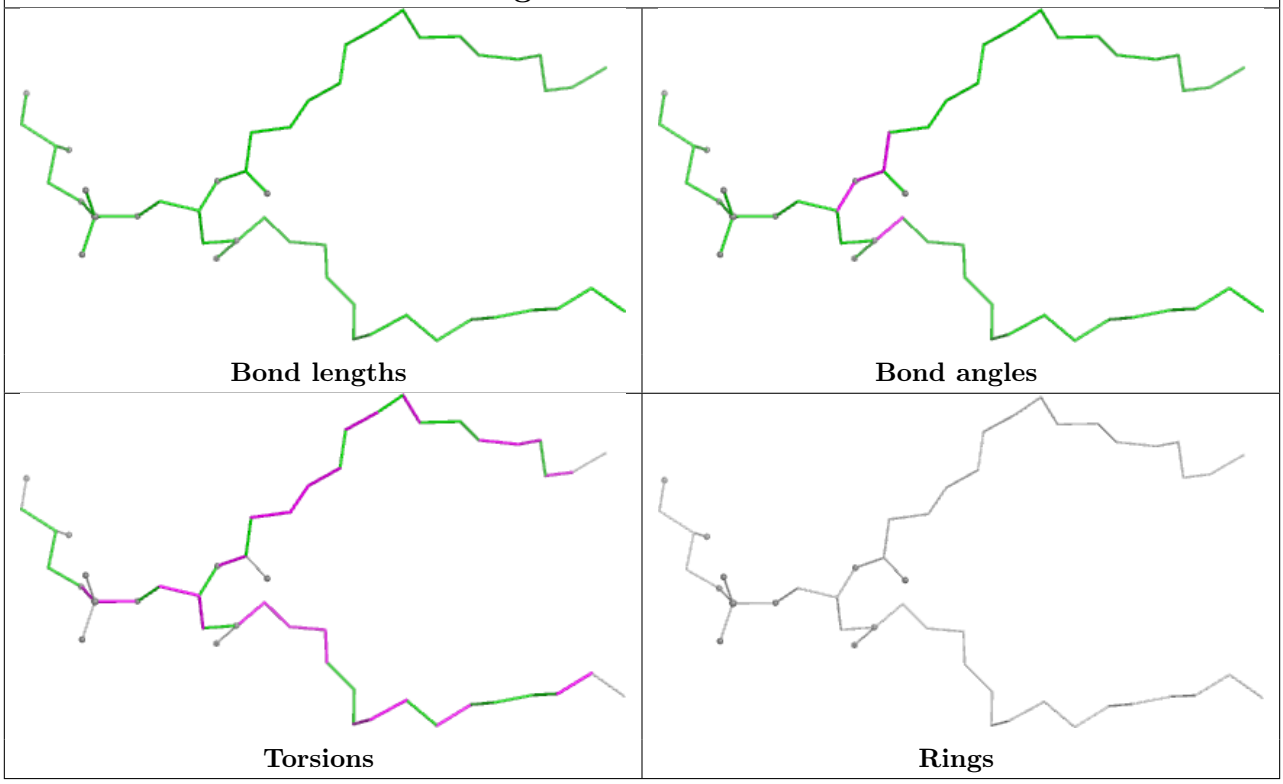
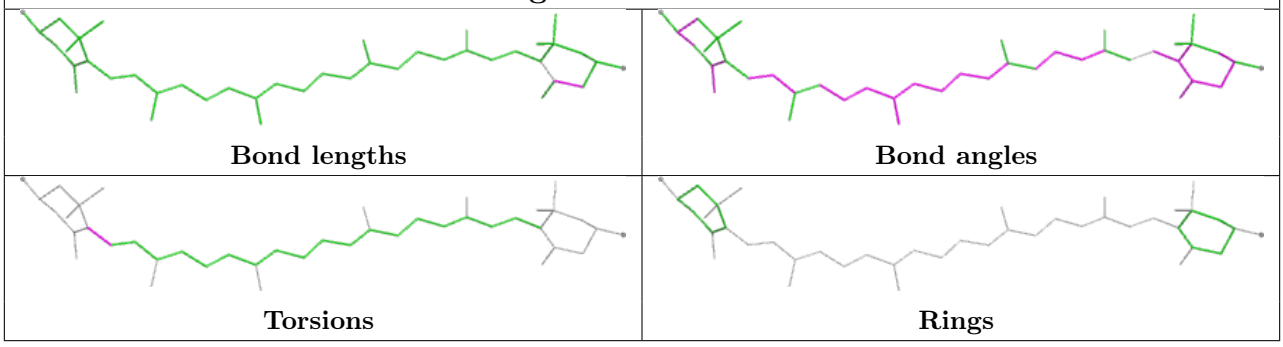


Rings

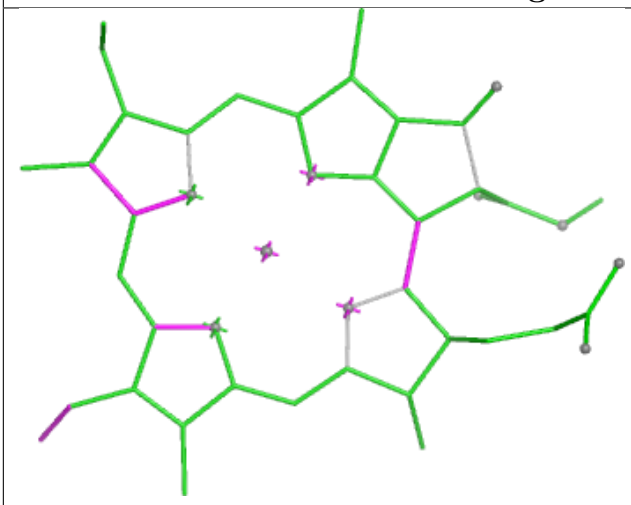
Ligand LHG A 5002



Ligand LUT 8 501



Ligand CLA 3 608



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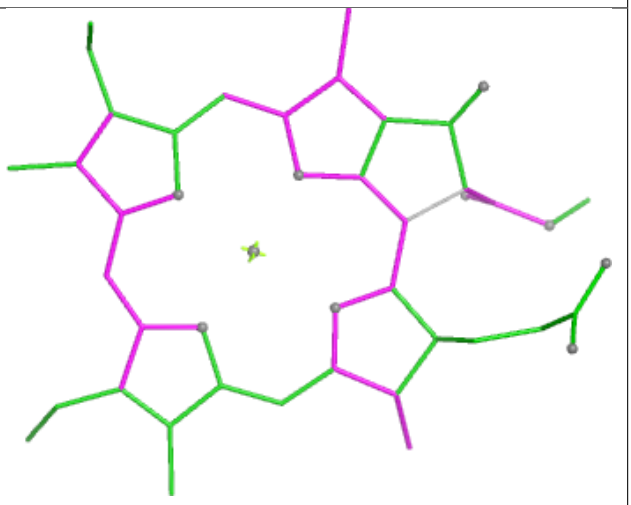
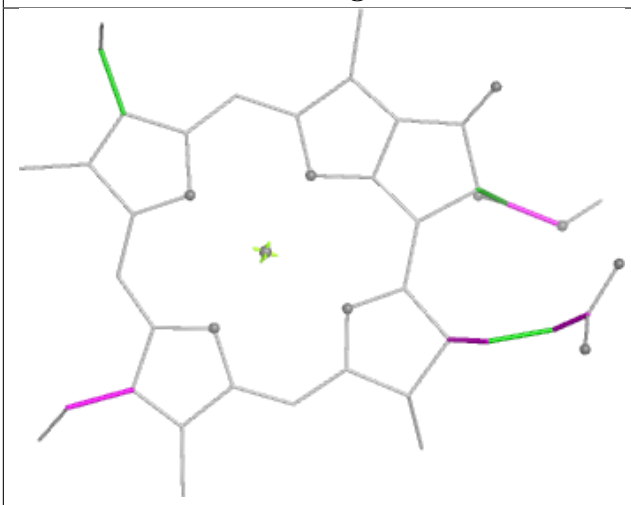


Bond angles



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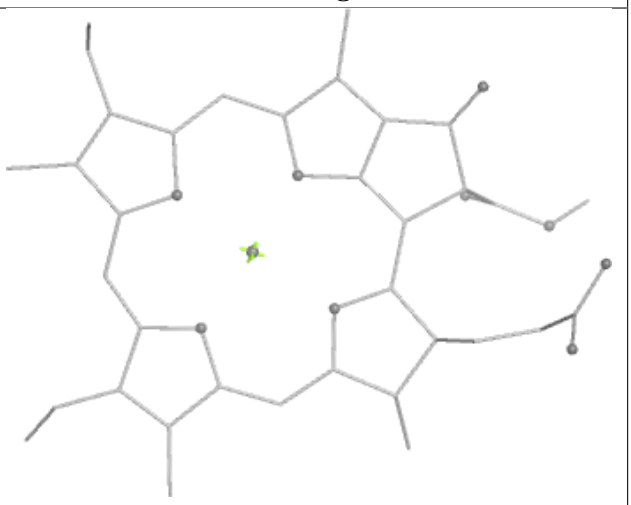
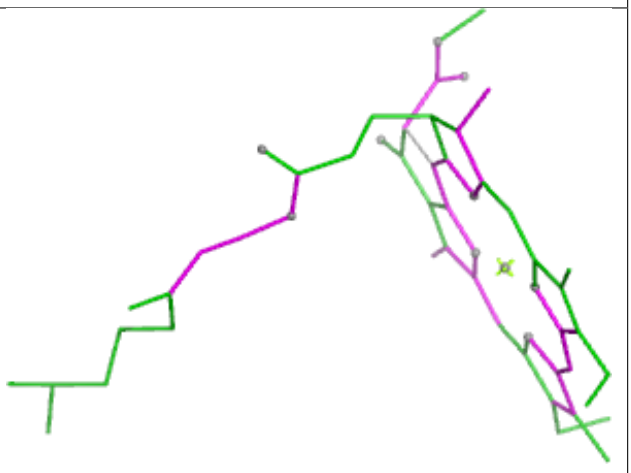


Rings

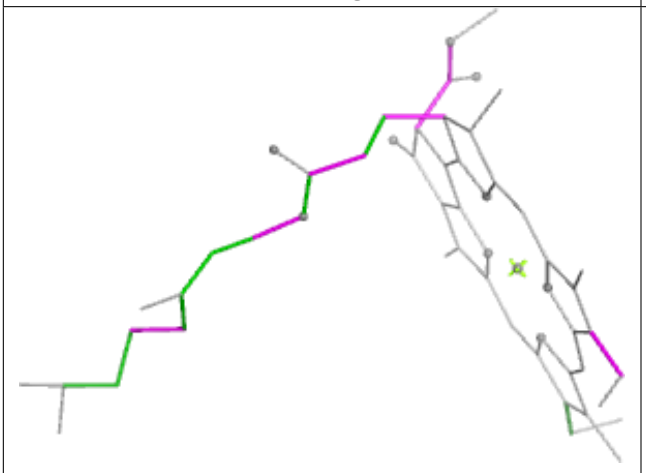
Ligand CLA A 1134



Bond lengths



Bond angles

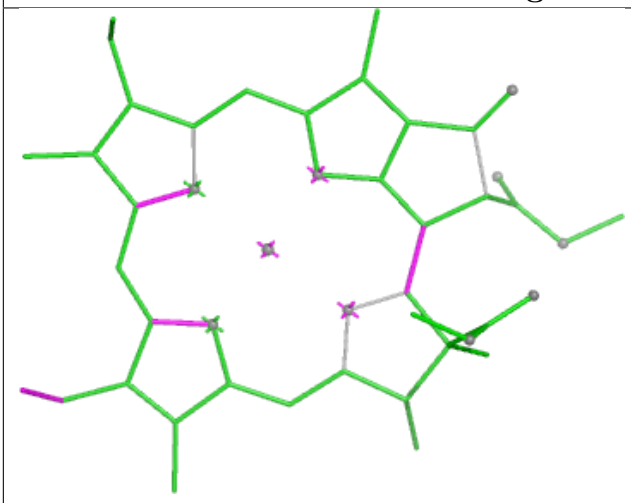


Torsions



Rings

Ligand CLA Z 615



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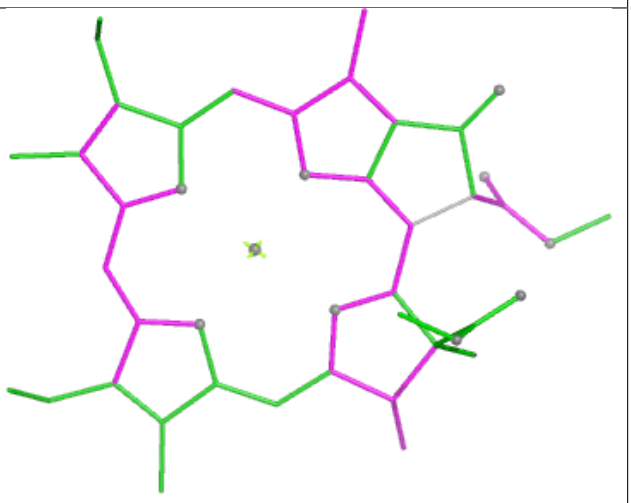
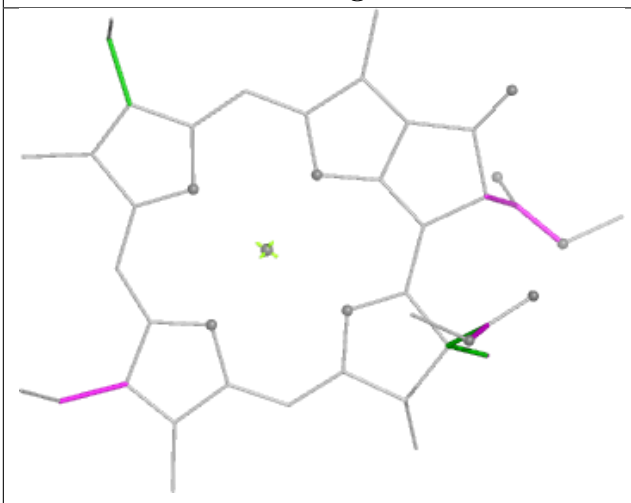


Bond angles



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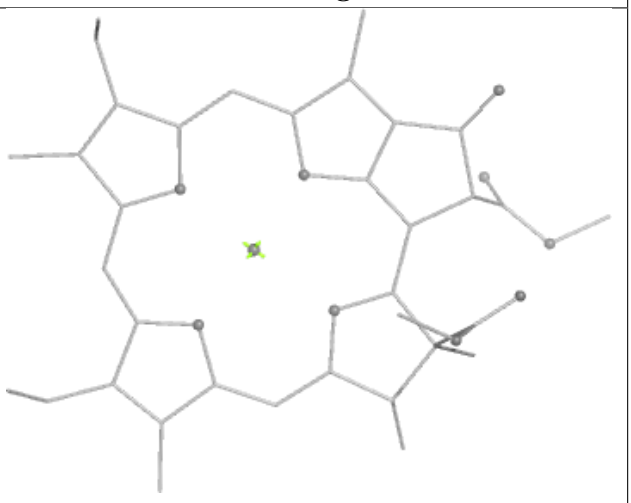
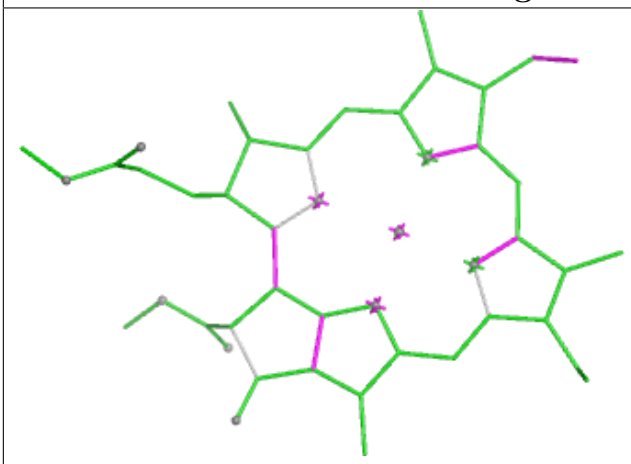


Rings

Ligand CLA K 1401



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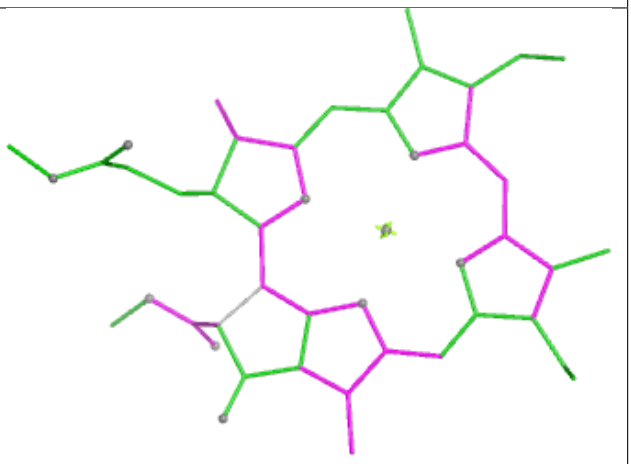
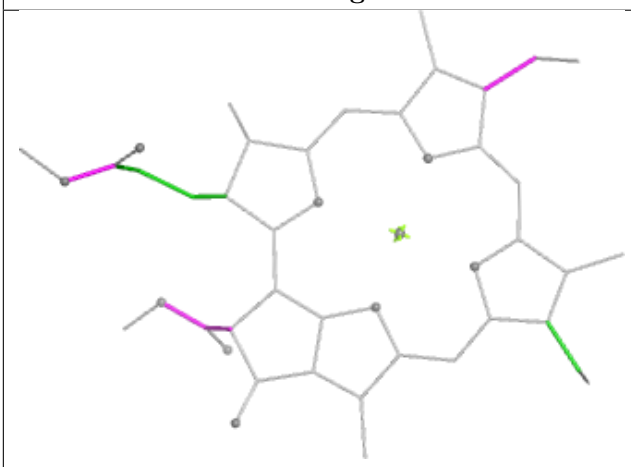


Bond angles



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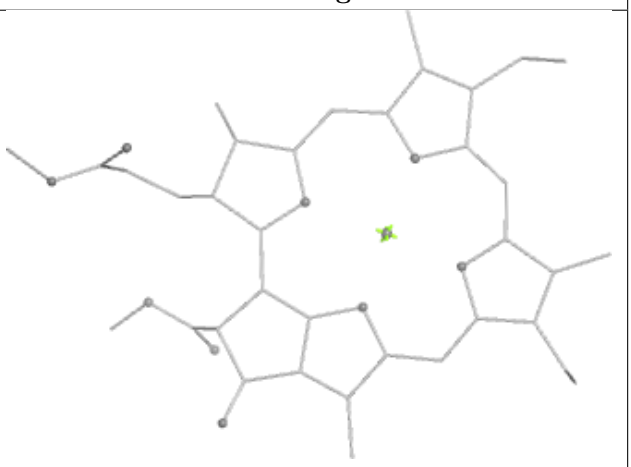
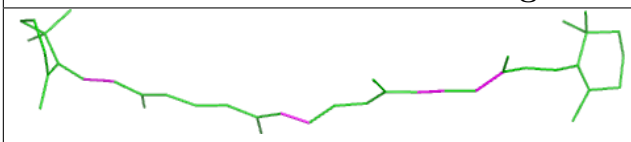


Rings

Ligand BCR I 4001



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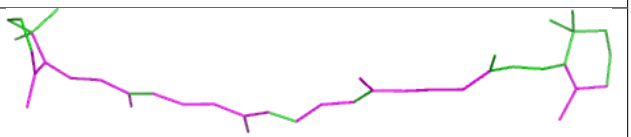
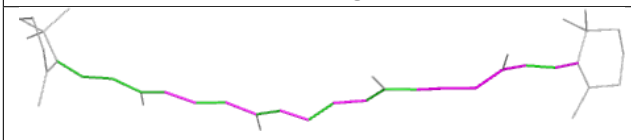


Bond angles



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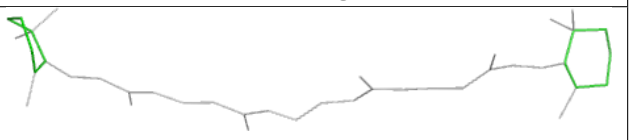
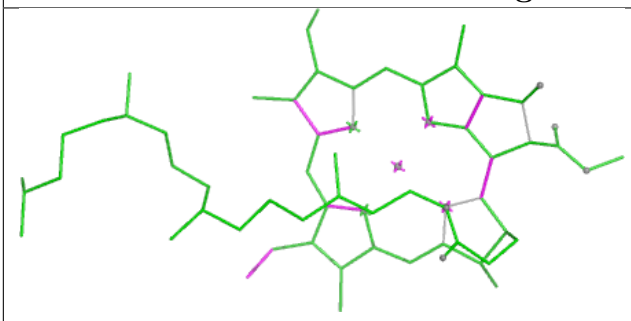


Rings

Ligand CLA B 1235



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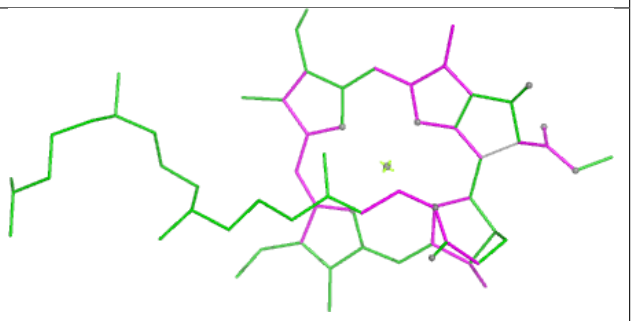
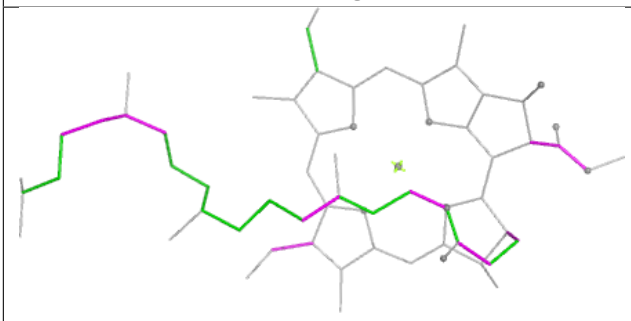


Bond angles



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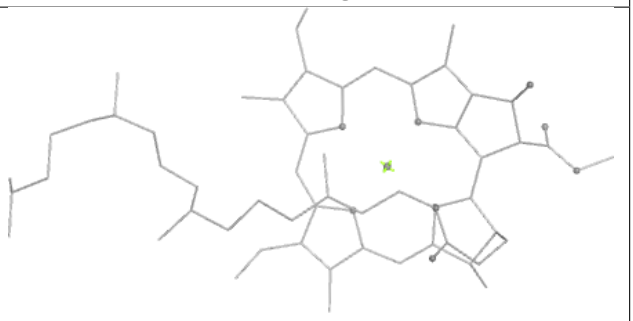
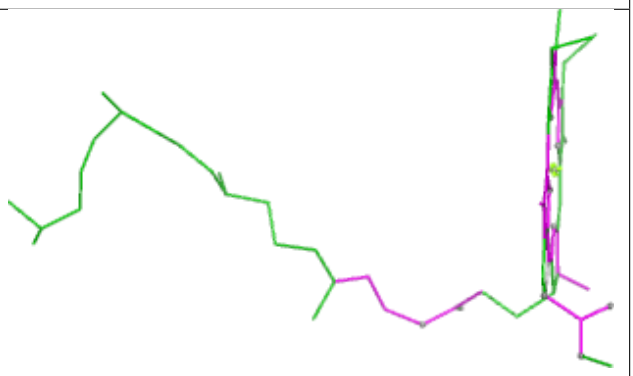


Rings

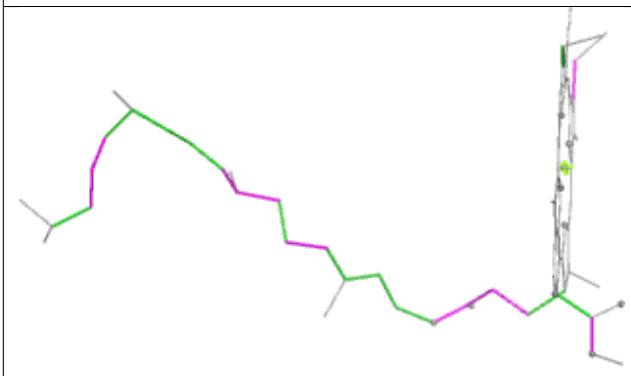
Ligand CLA B 1239



Bond lengths



Bond angles

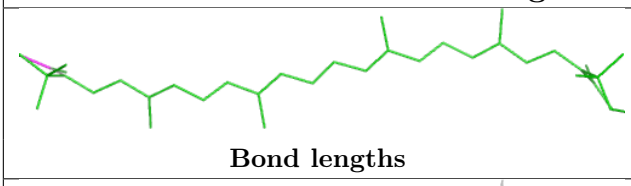


Torsions



Rings

Ligand LUT 3 502



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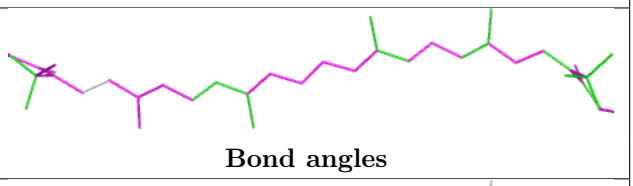

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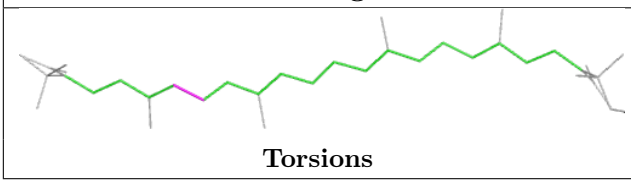

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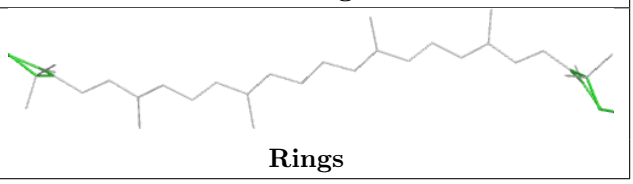
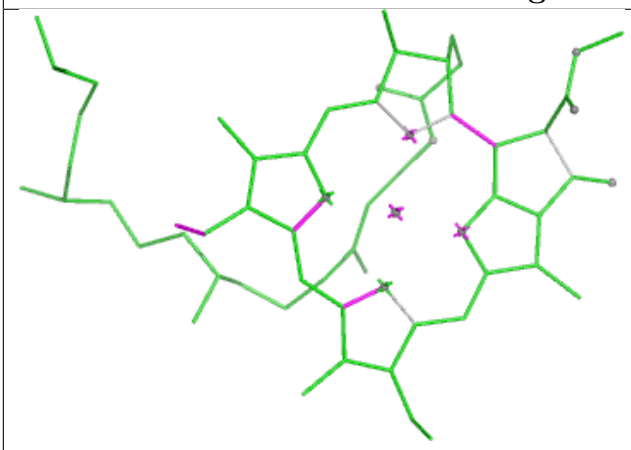


Rings

Ligand CLA 4 603



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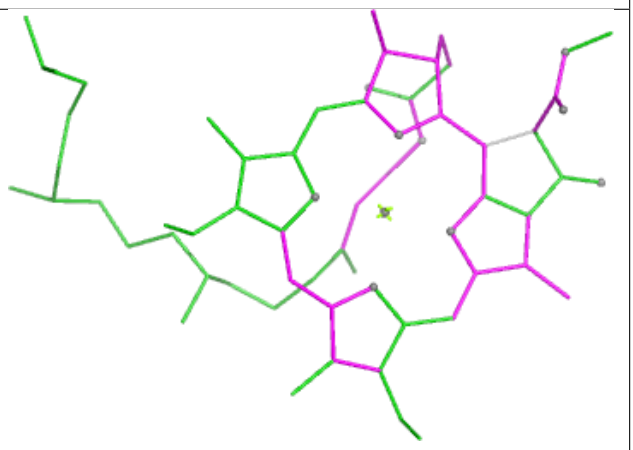

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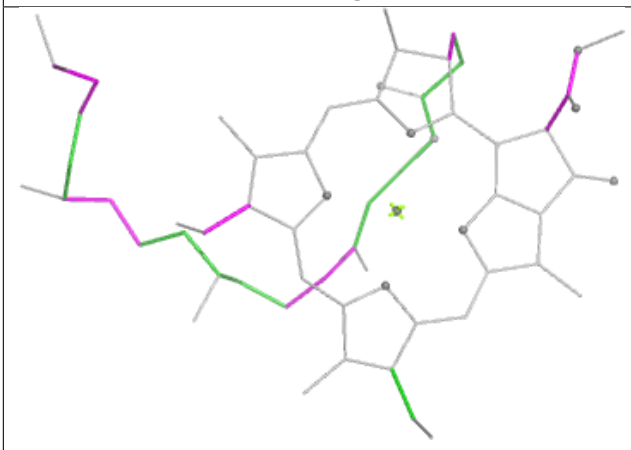

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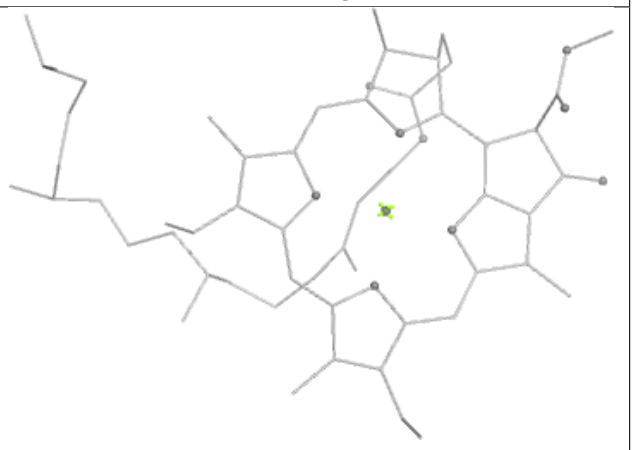
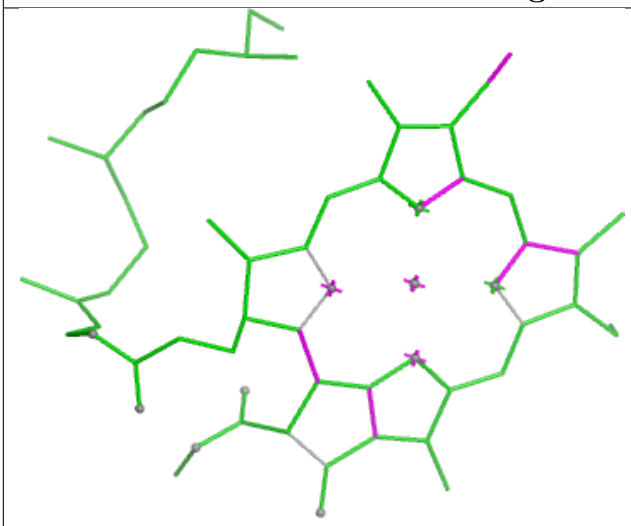


Rings

Ligand CLA 5 602



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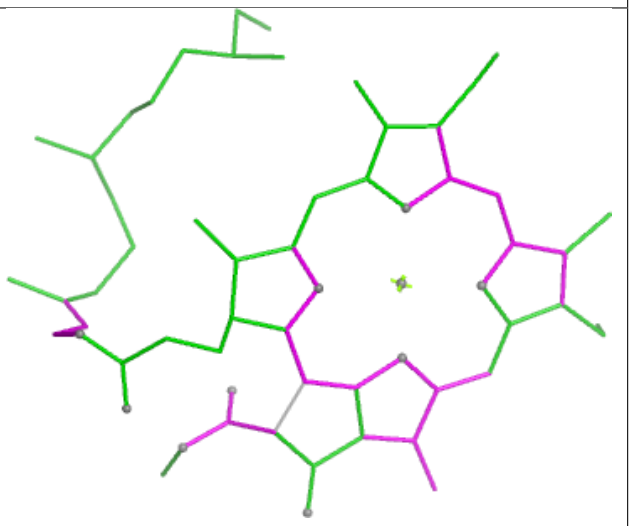

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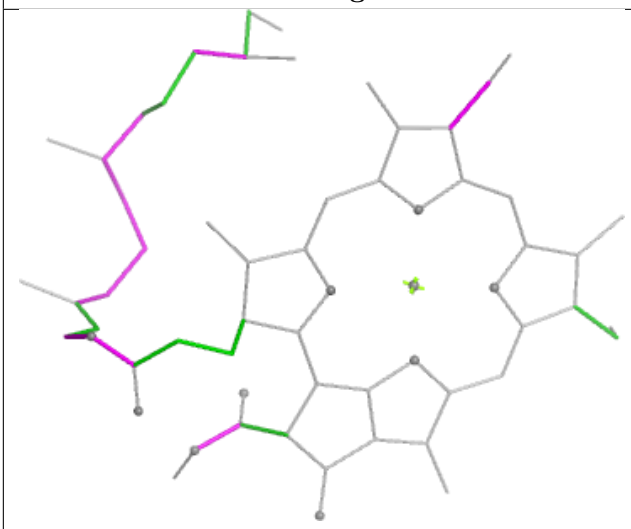

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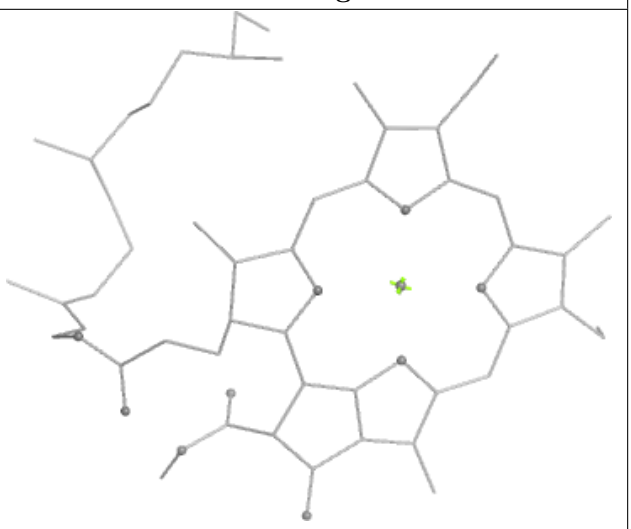
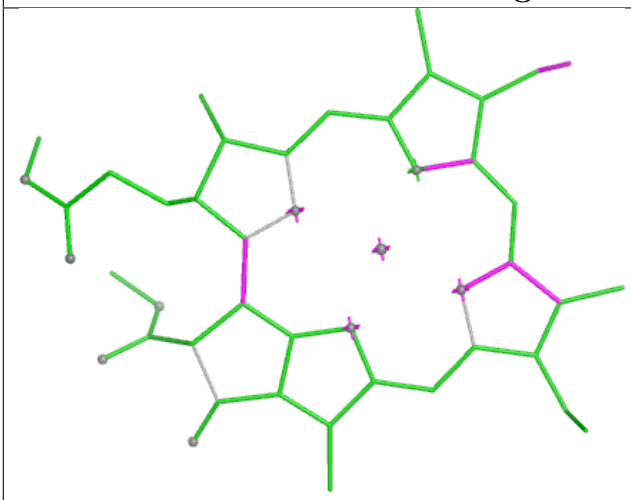


Rings

Ligand CLA G 1602



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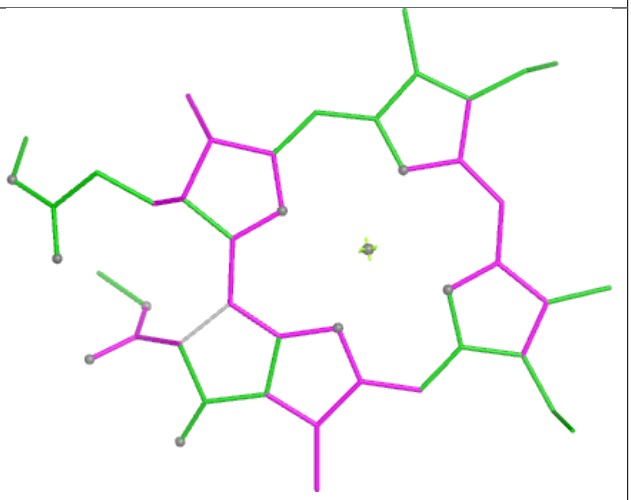

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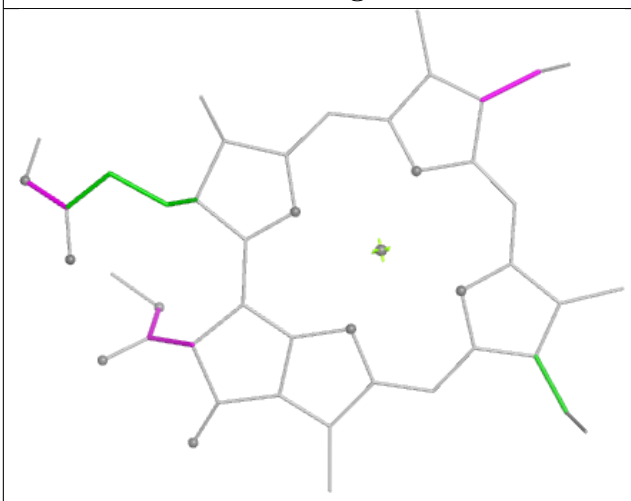

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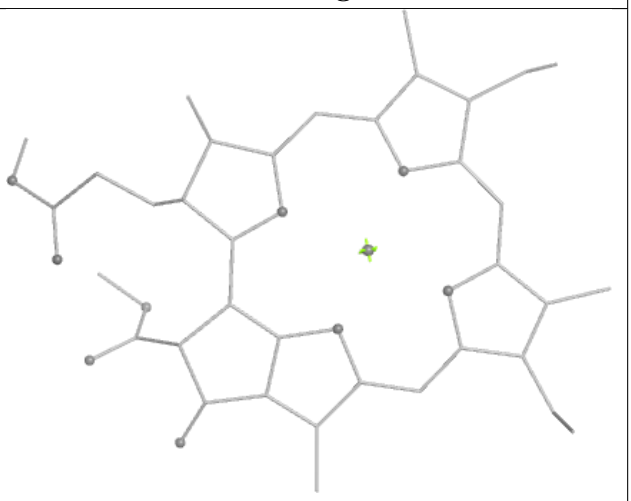
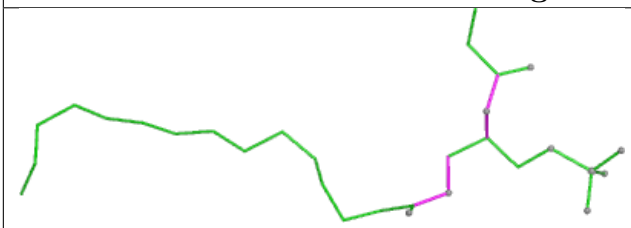


Rings

Ligand 3PH 8 806



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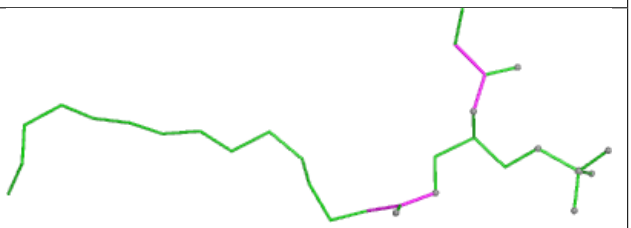

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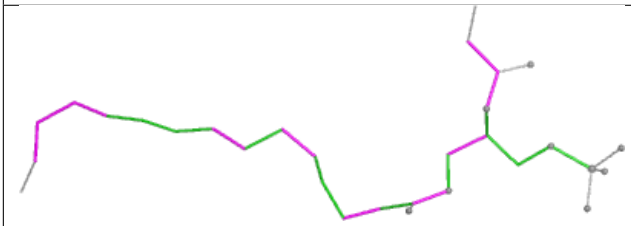

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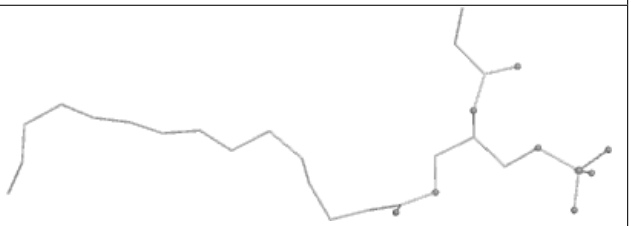
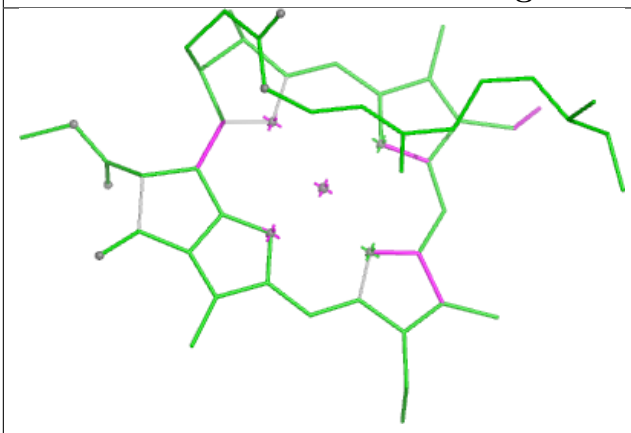


Rings

Ligand CLA B 1208



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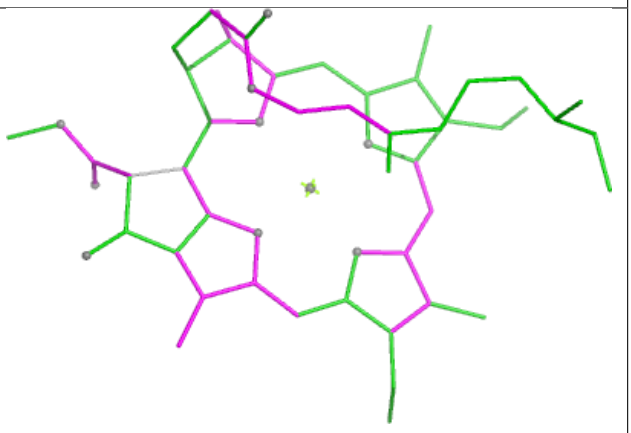

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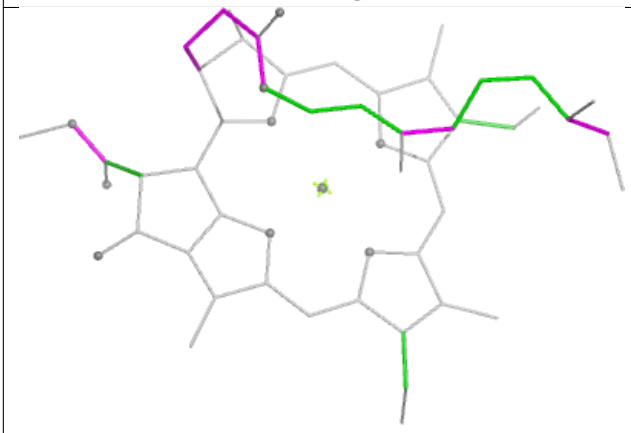

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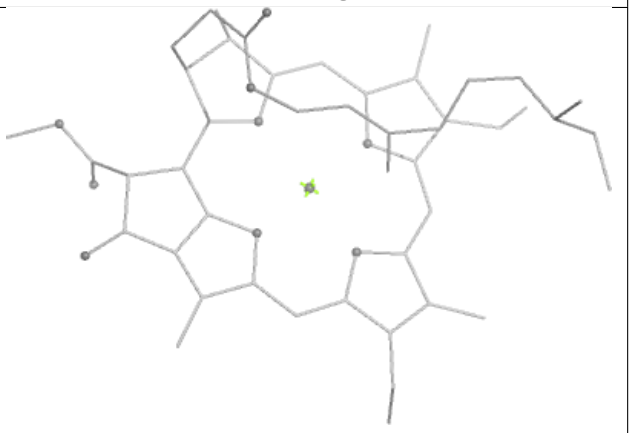
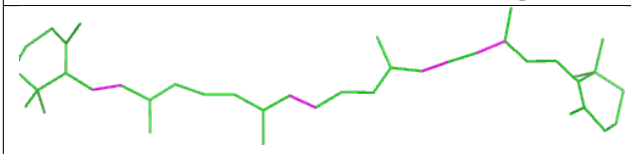


Rings

Ligand BCR B 4002



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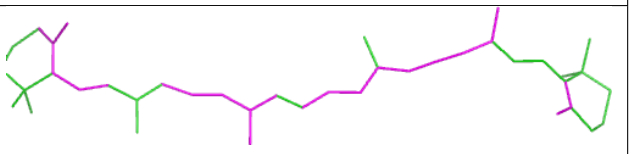

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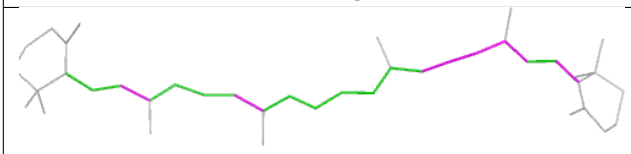

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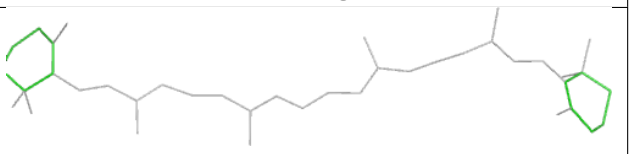
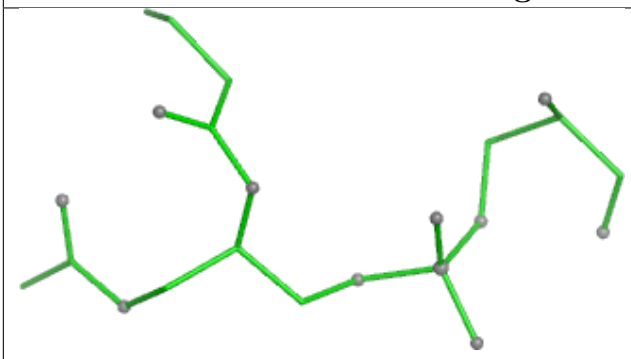


Rings

Ligand LHG B 5001



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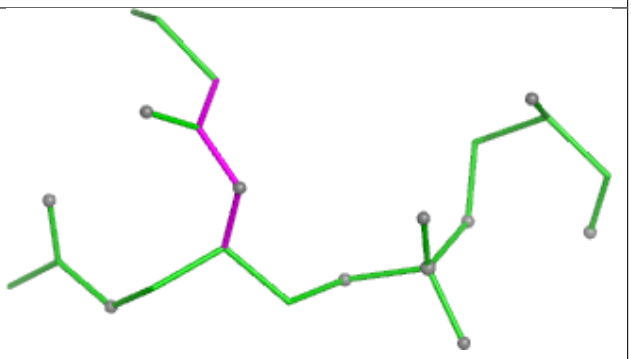

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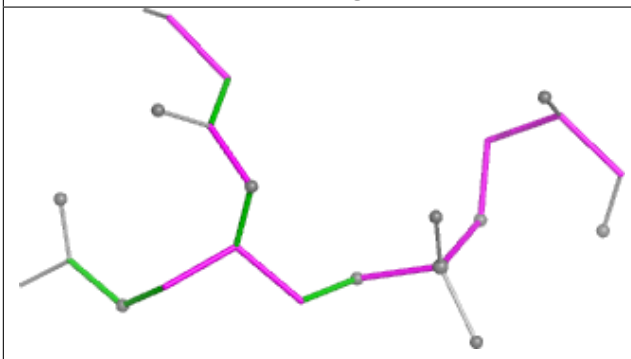

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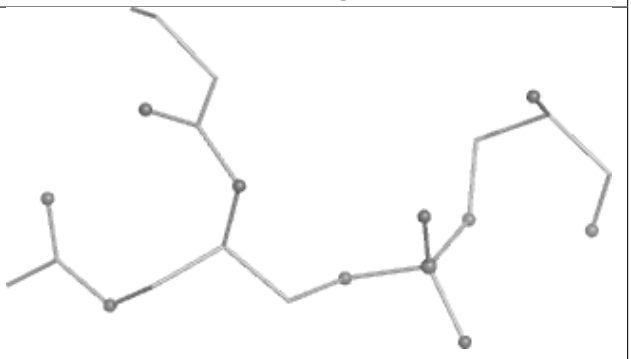
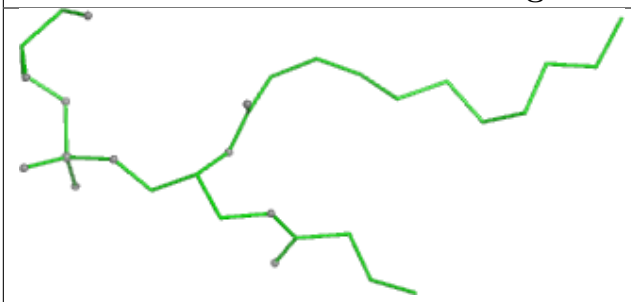


Rings

Ligand LHG 4 802



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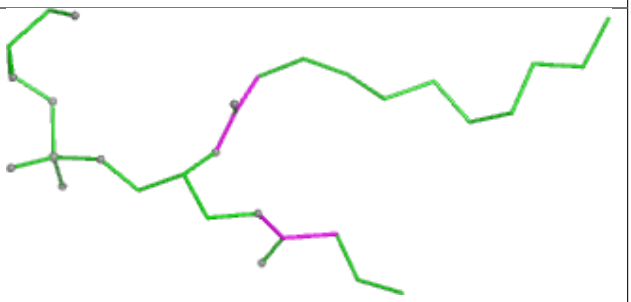

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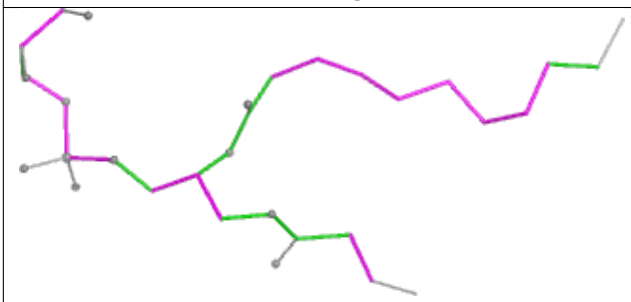

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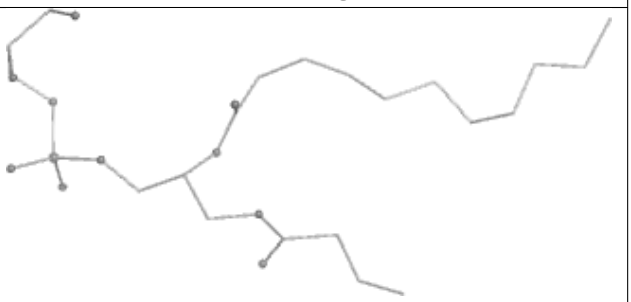
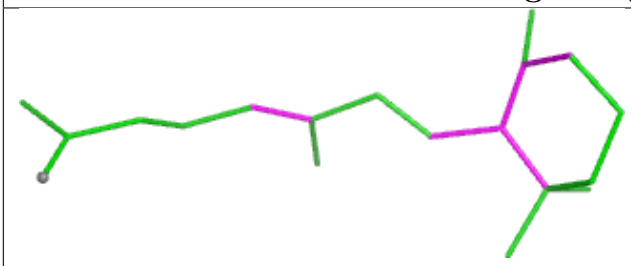


Rings

Ligand QTB Z 504



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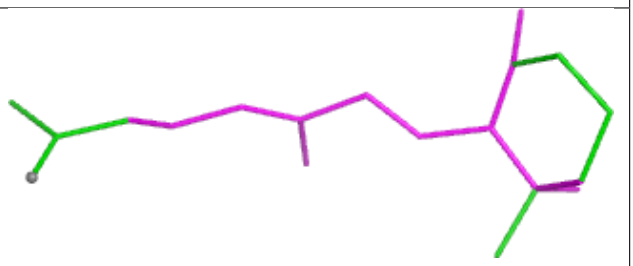

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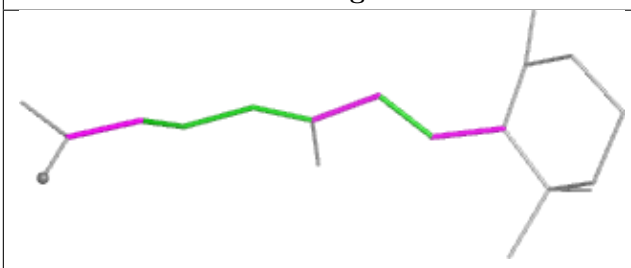

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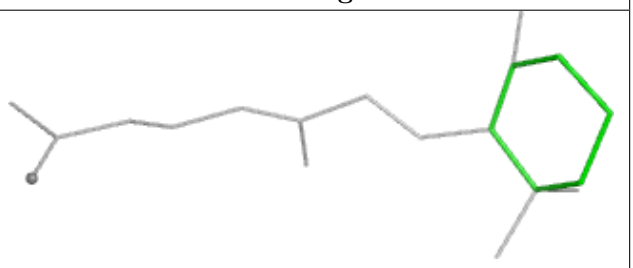
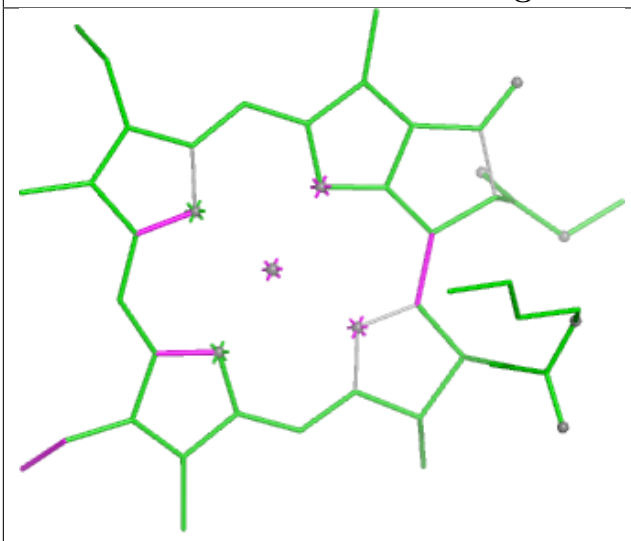


Rings

Ligand CLA K 1403



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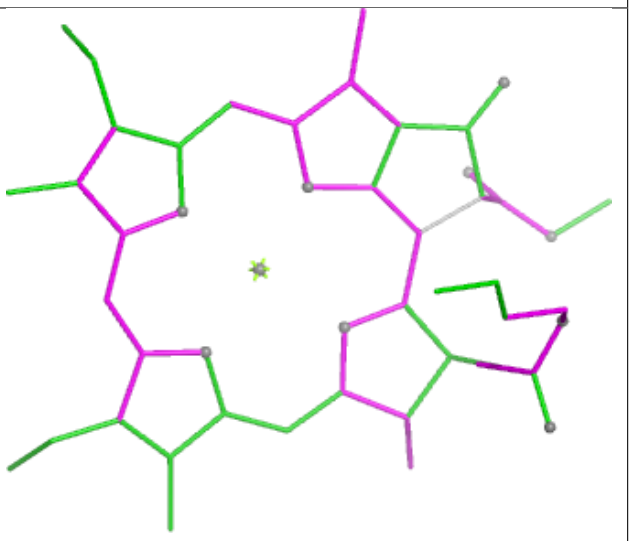

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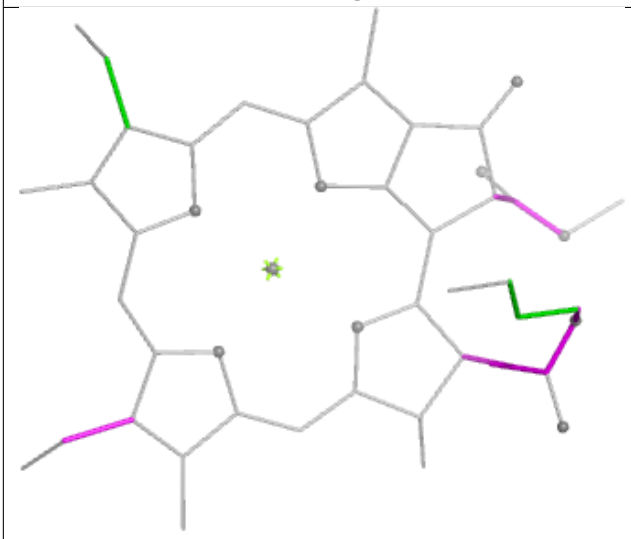

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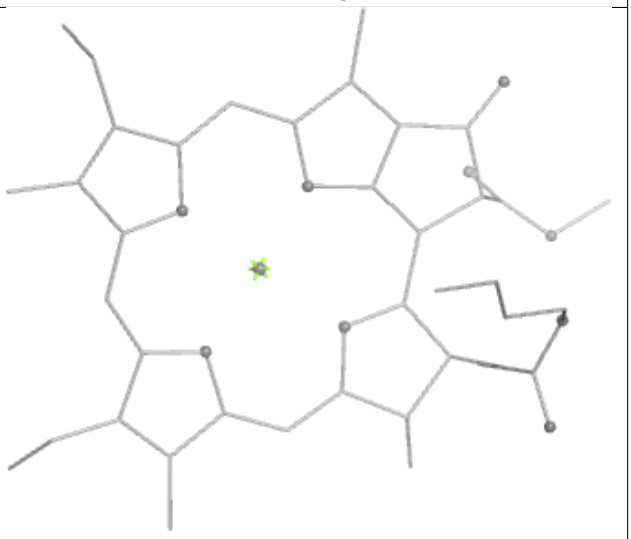
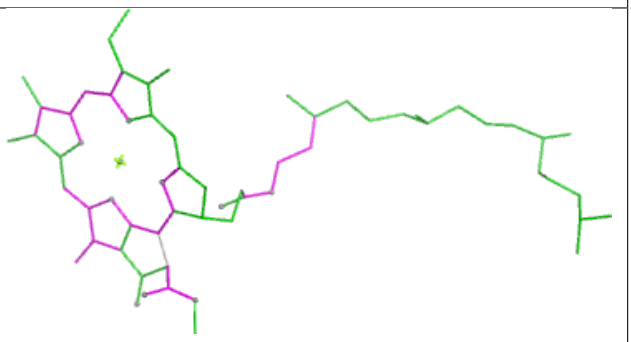


Rings

Ligand CLA A 1119



Bond lengths



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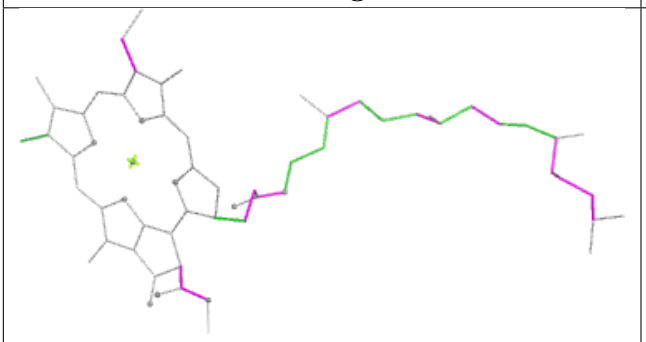

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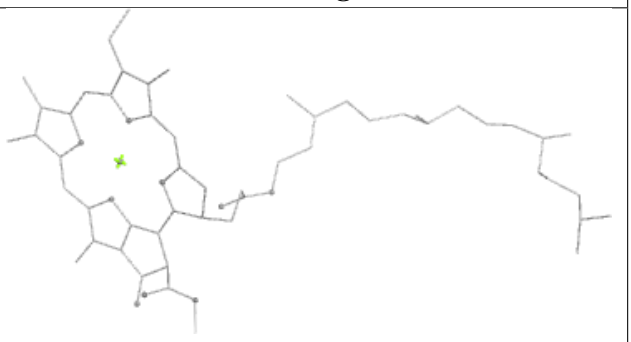


Rings

Ligand CLA 1 606



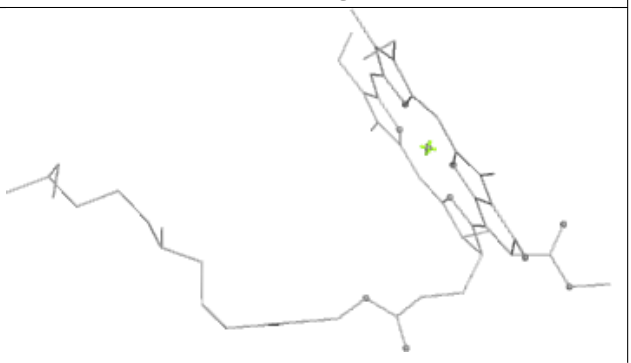
Bond lengths



Bond angles

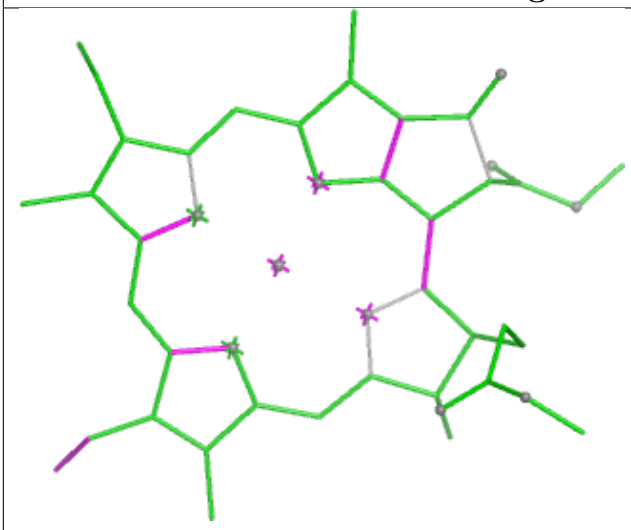


Torsions



Rings

Ligand CLA 3 618



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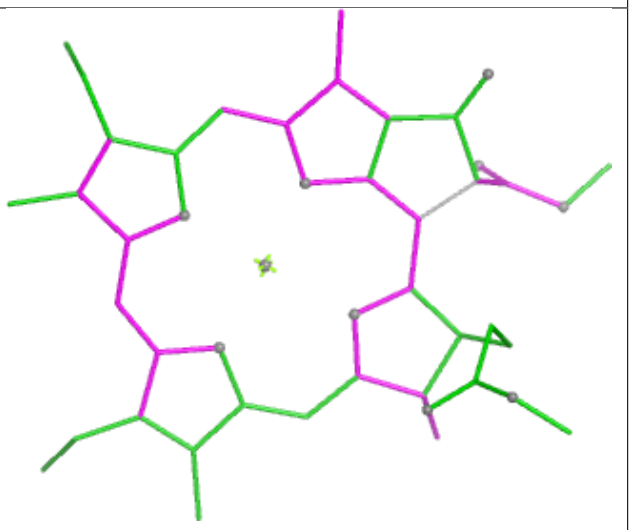
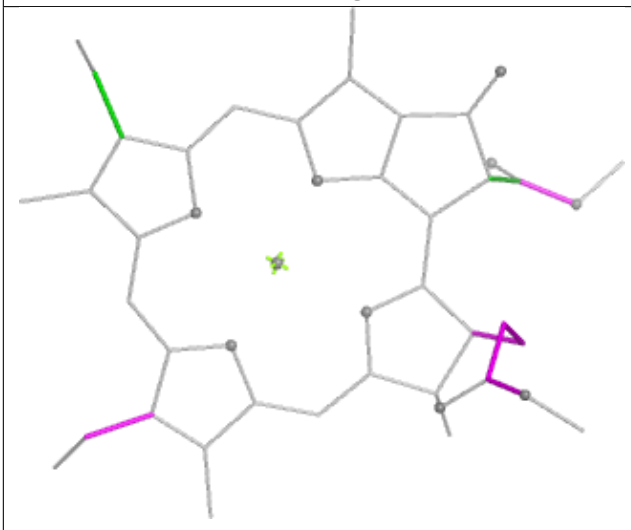


Bond angles



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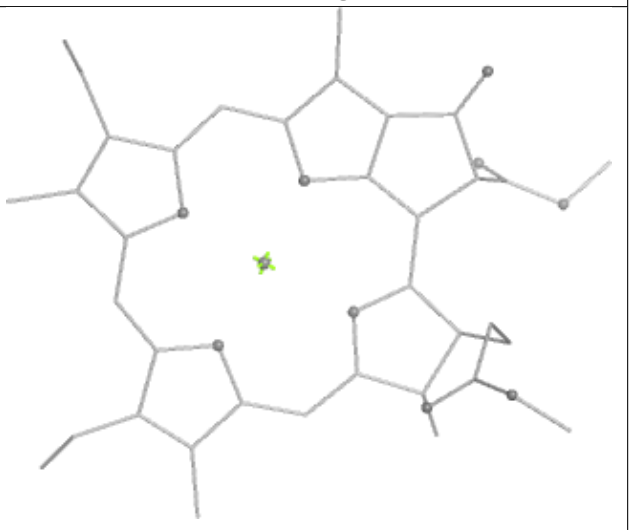
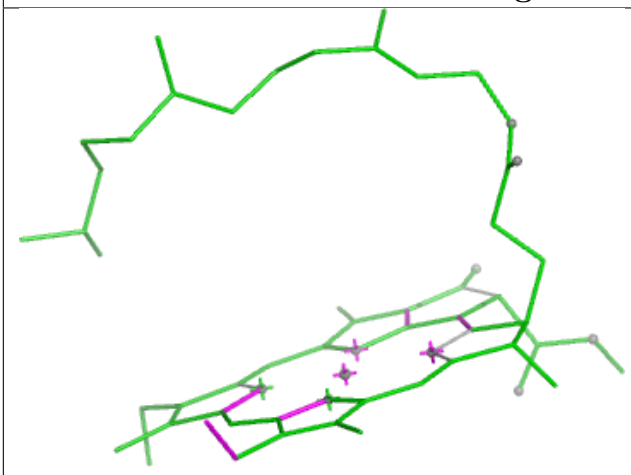


Rings

Ligand CLA A 1112



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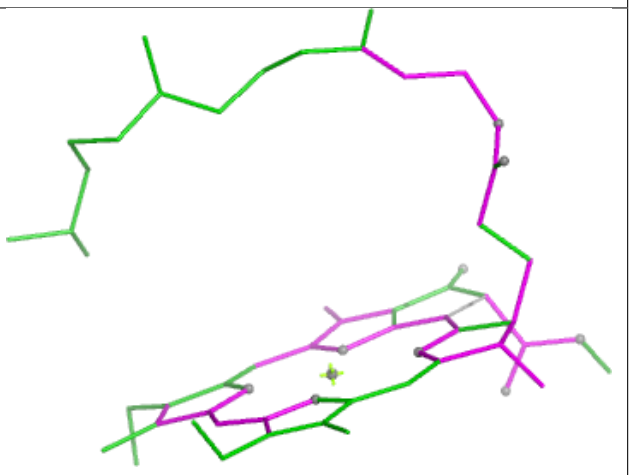
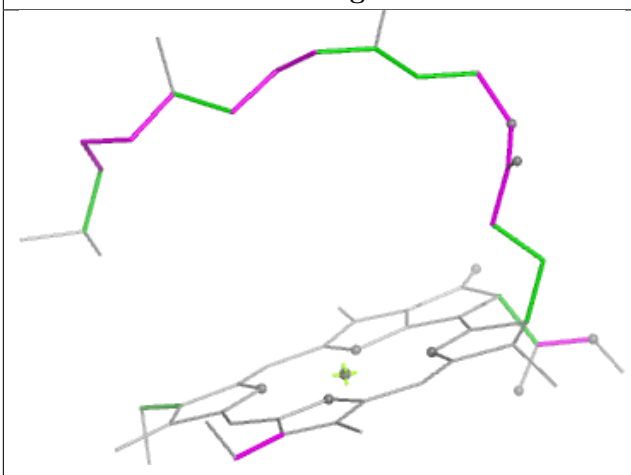


Bond angles



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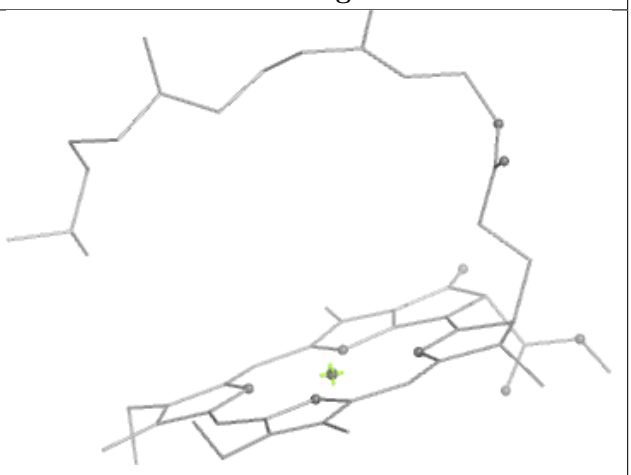
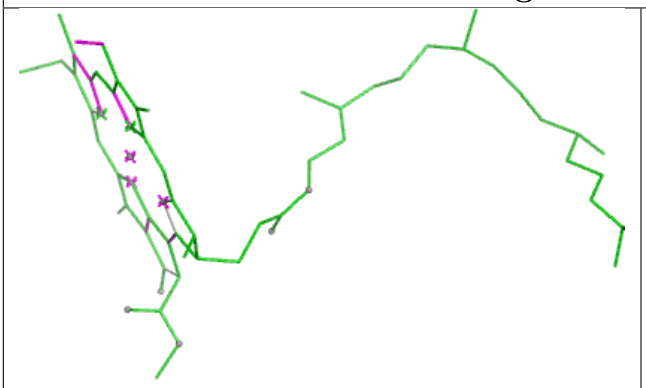


Rings

Ligand CLA B 1238



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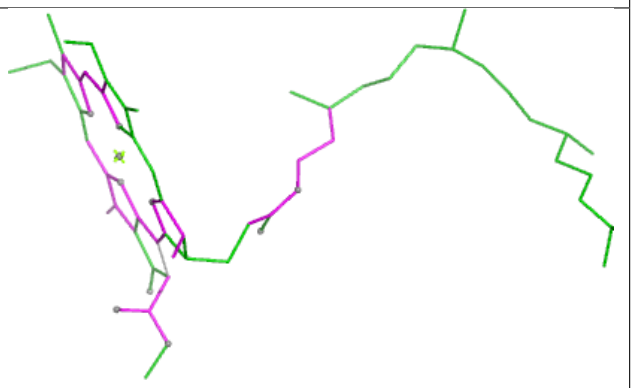
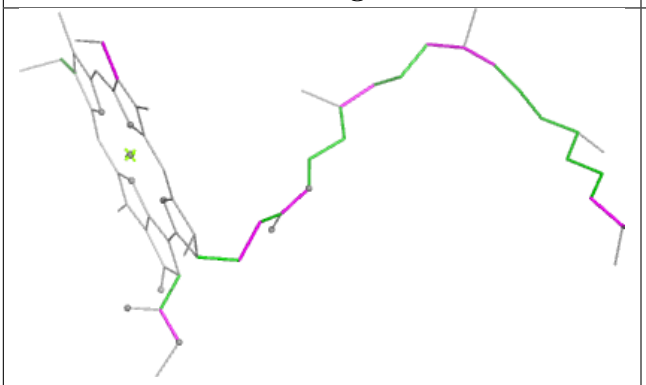


Bond angles

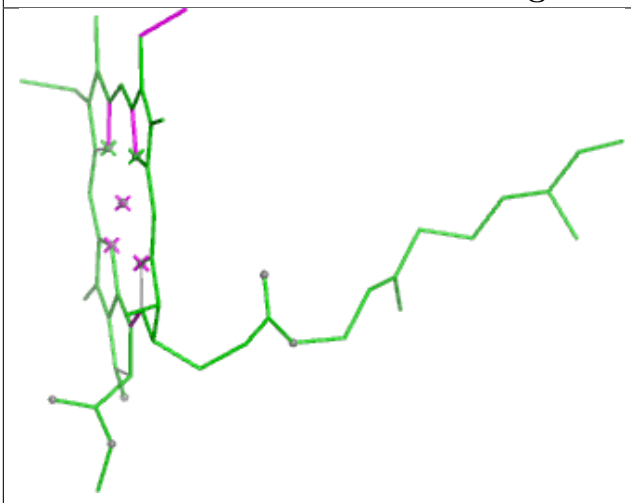


Torsions



Rings

Ligand CLA 7 606



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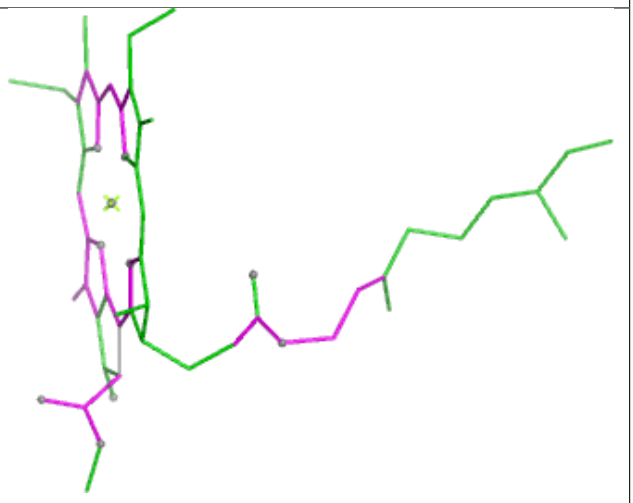

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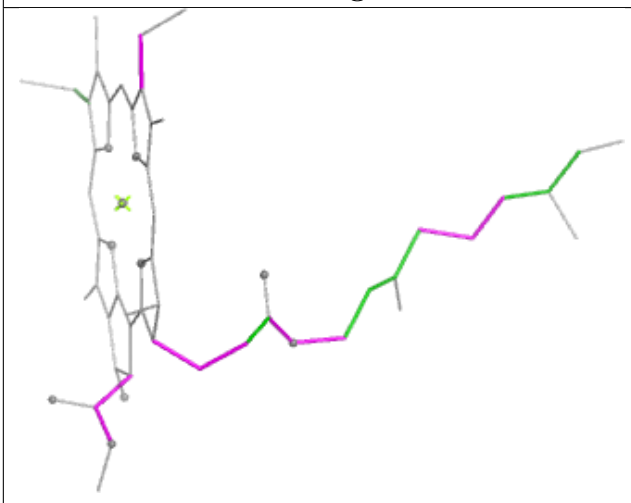
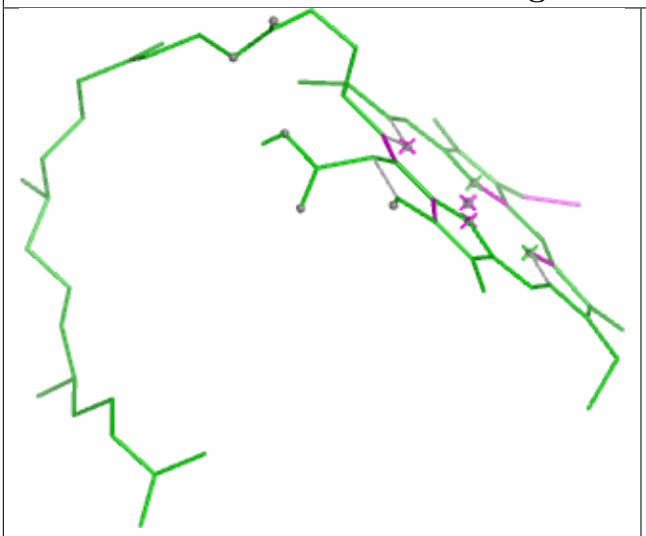


Torsions



Rings

Ligand CLA 4 605



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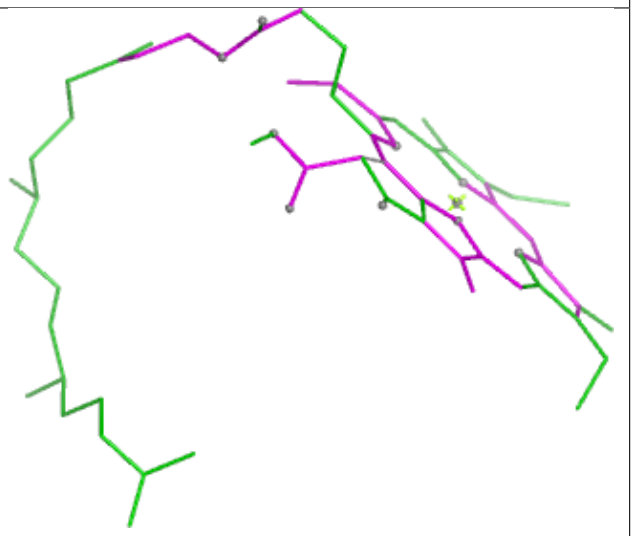

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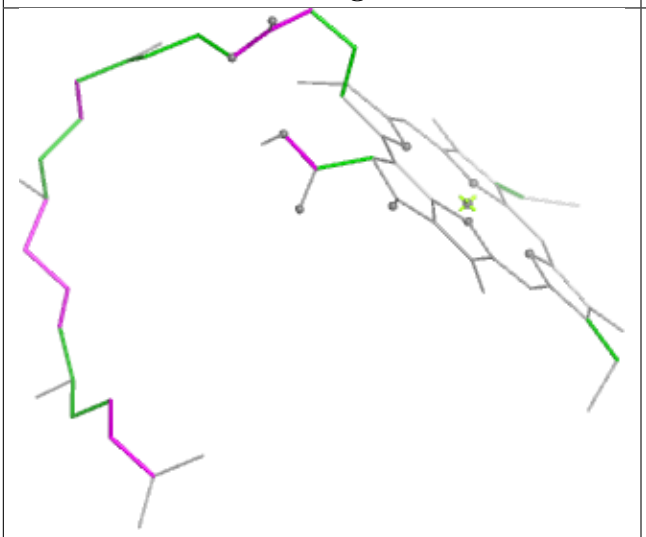

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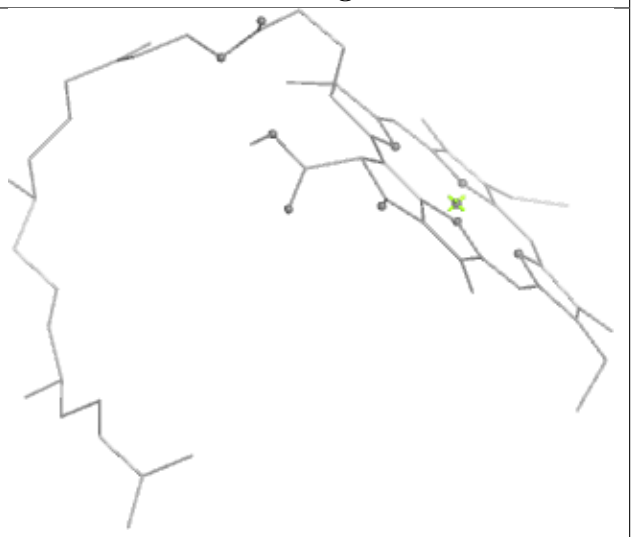
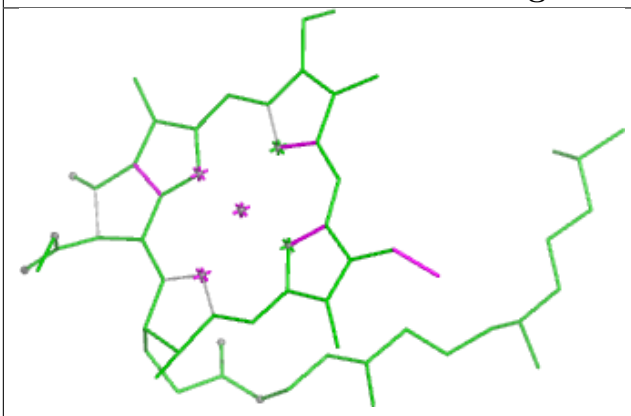


Rings

Ligand CLA 1 604



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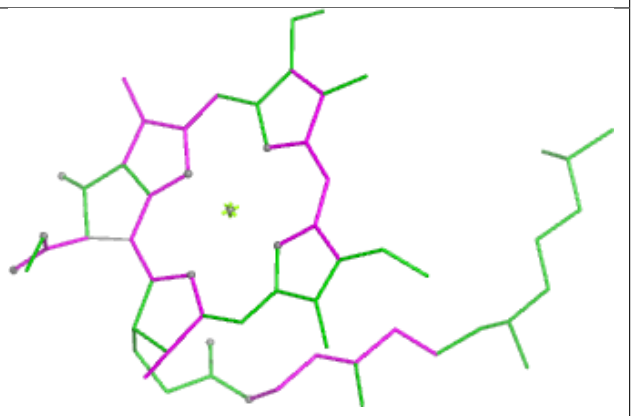

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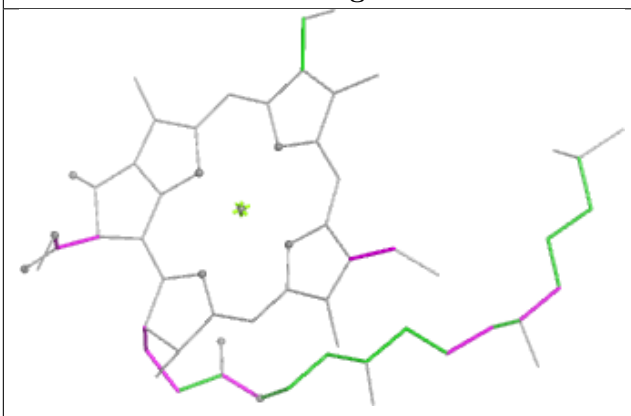

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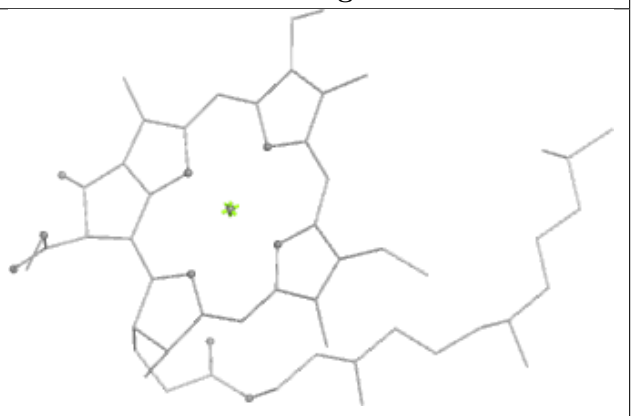
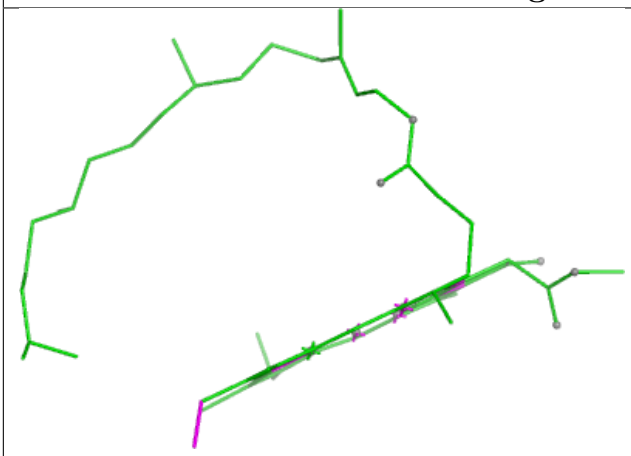


Rings

Ligand CLA 6 606



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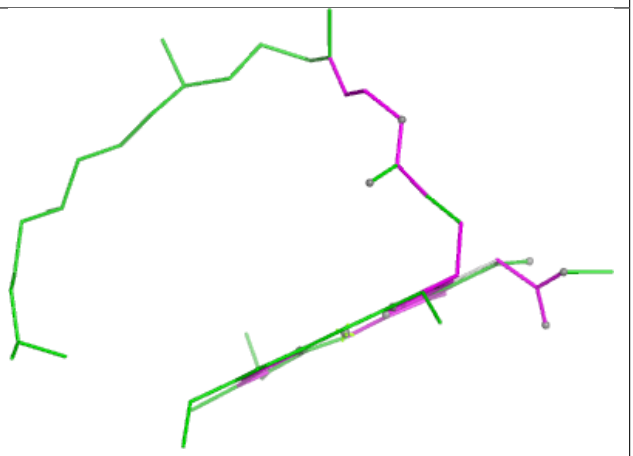

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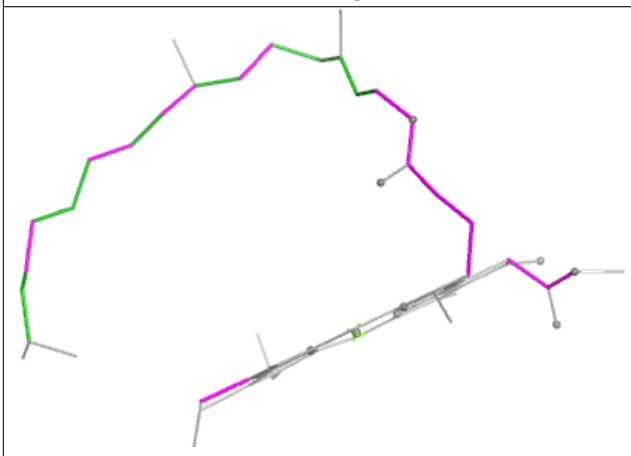

Torsions



Rings

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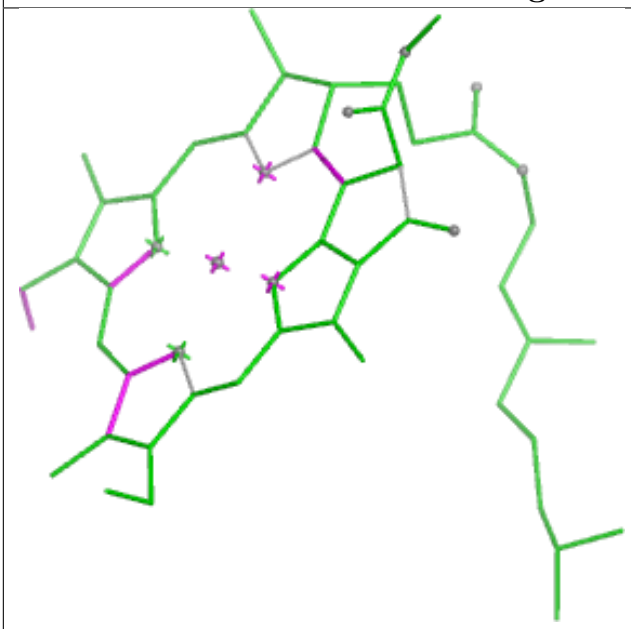

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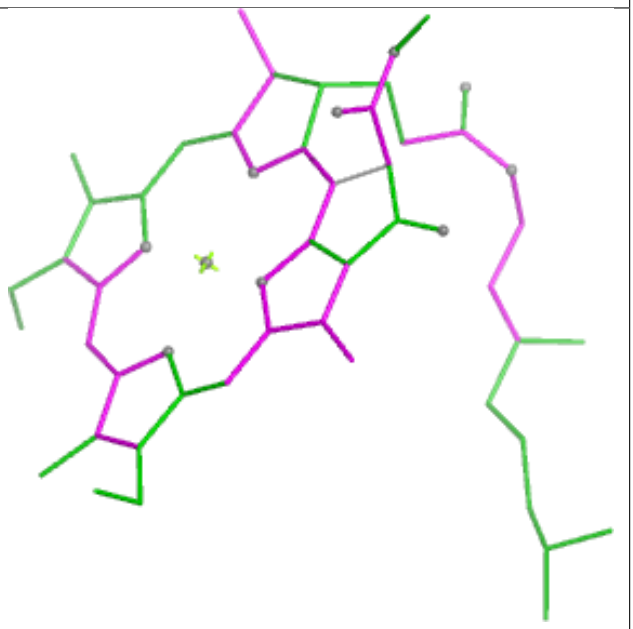

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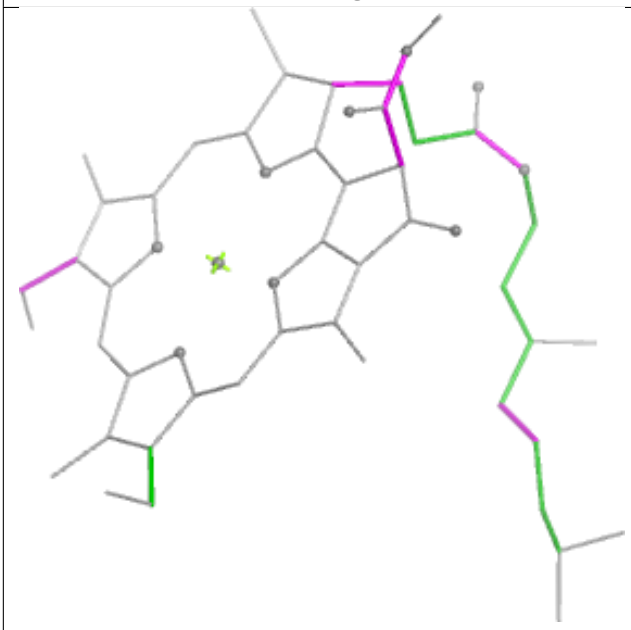

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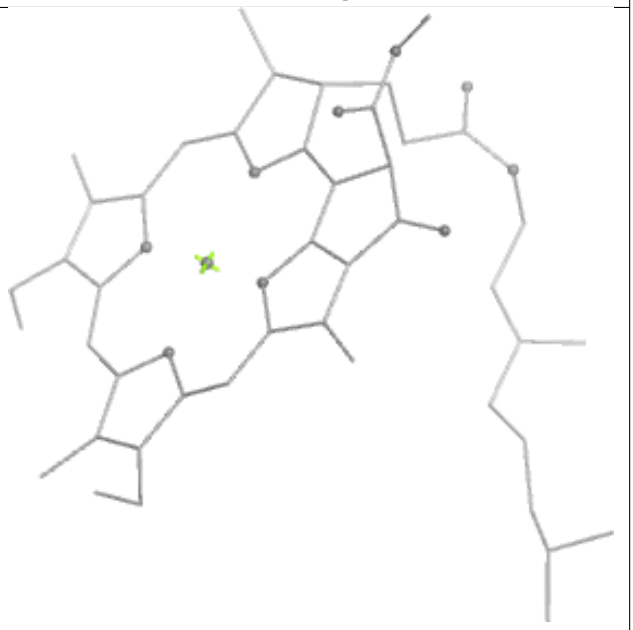

Rings

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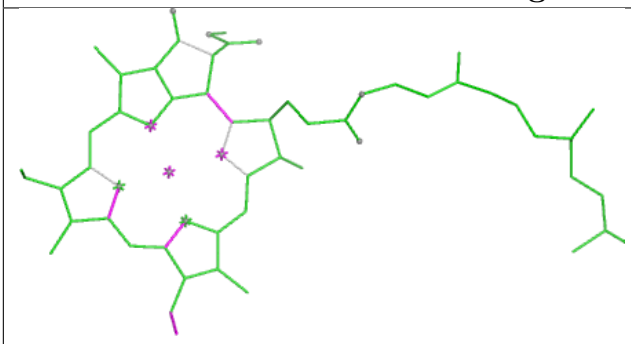

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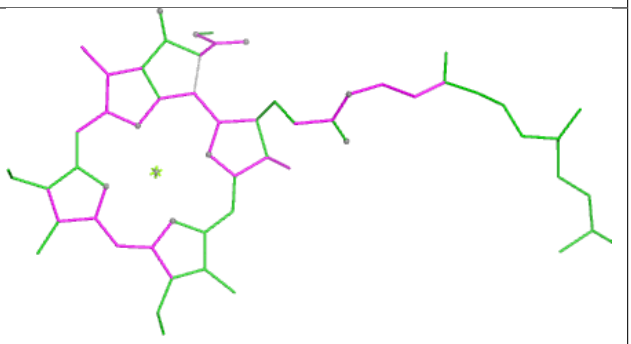

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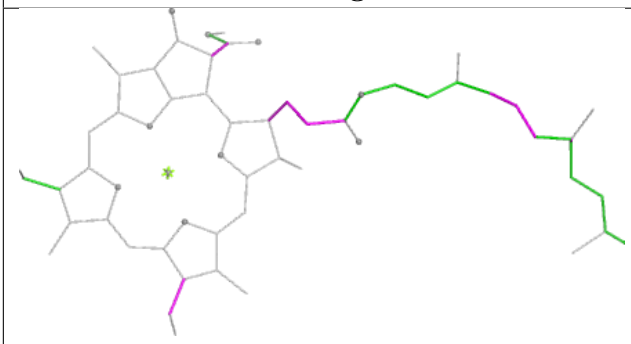

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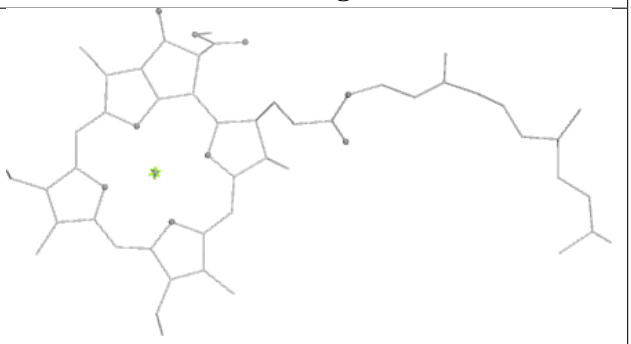
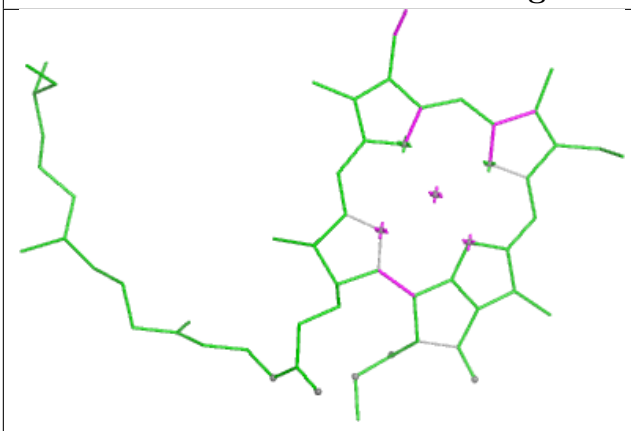


Rings

Ligand CLA 7 605



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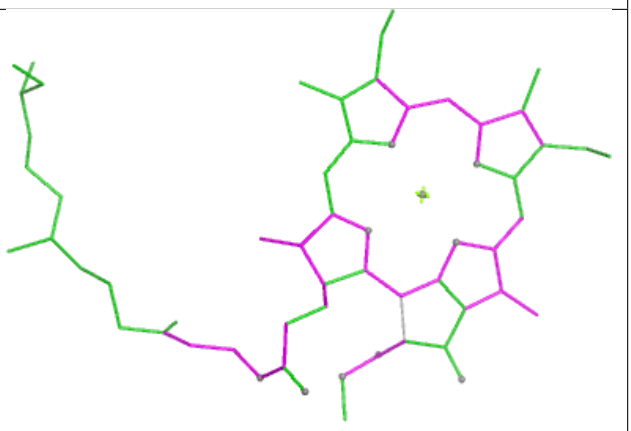

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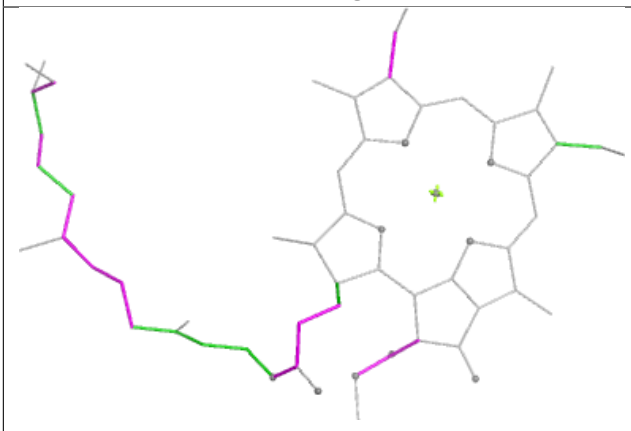

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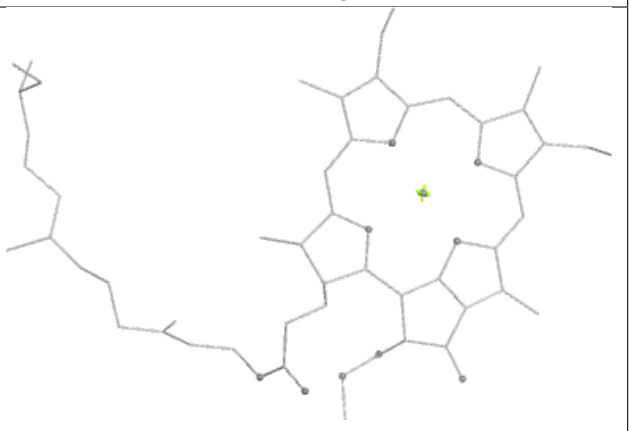

Rings

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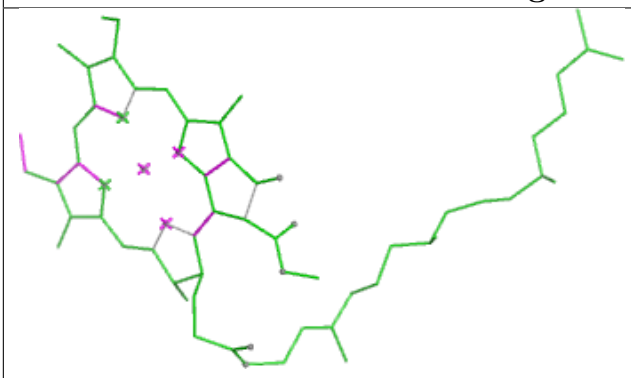

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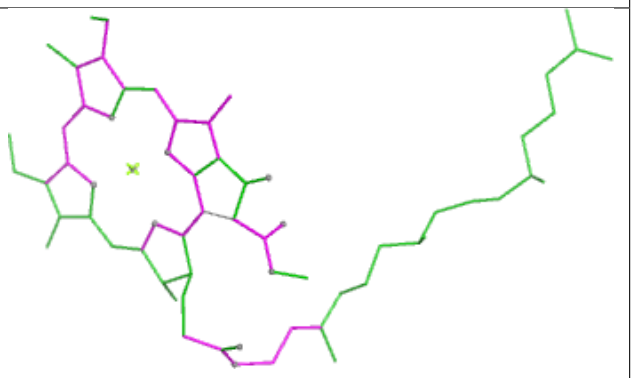

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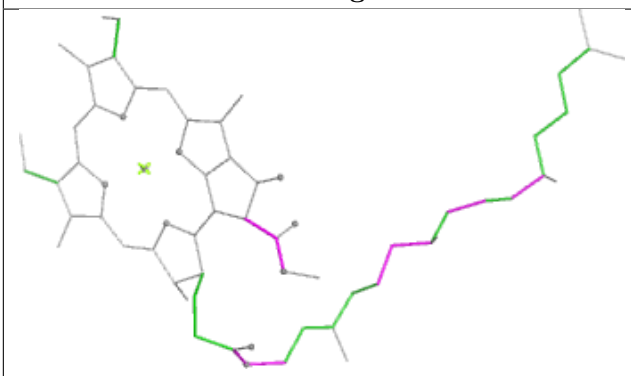

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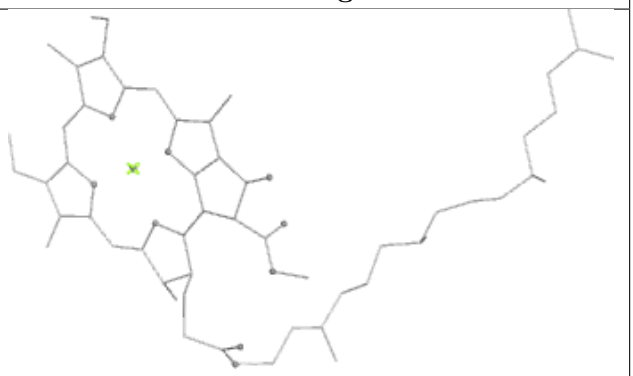
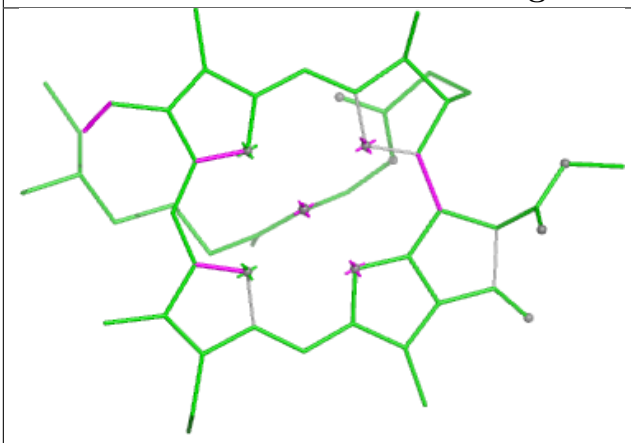


Rings

Ligand CLA 5 603



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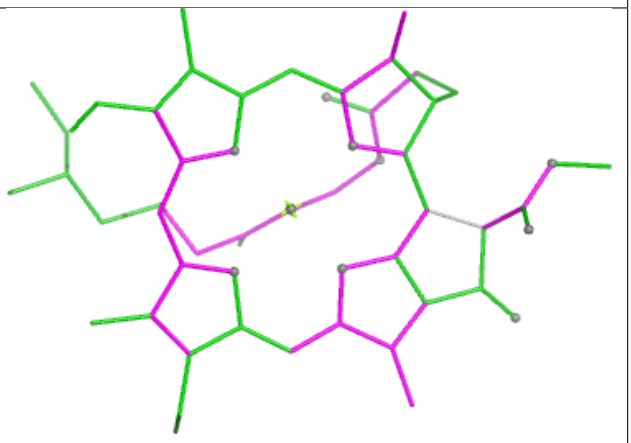

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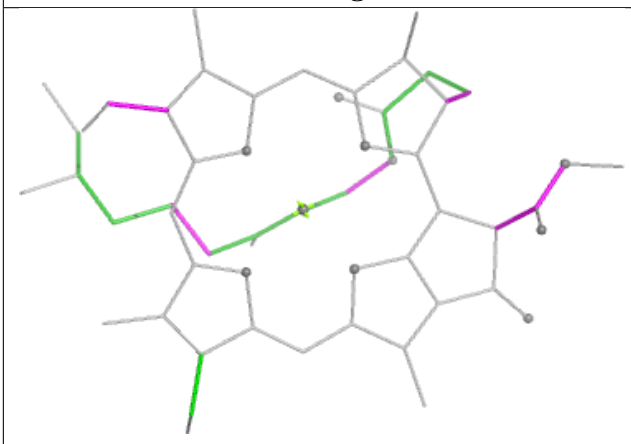

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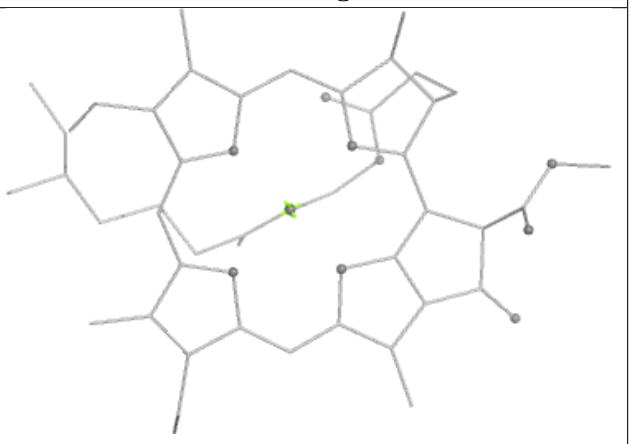
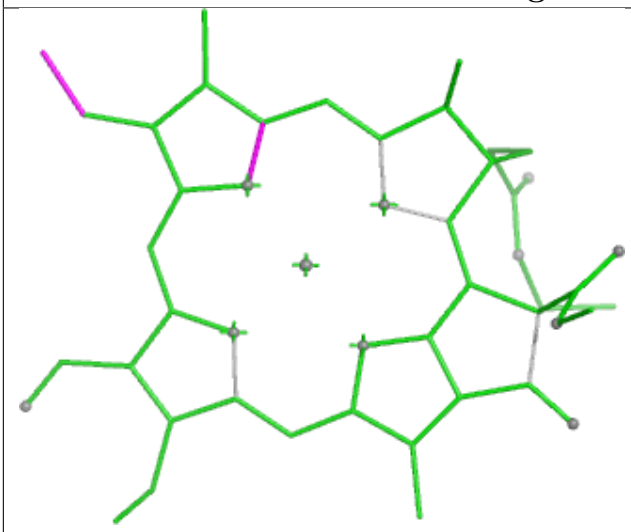


Rings

Ligand CHL 1 610



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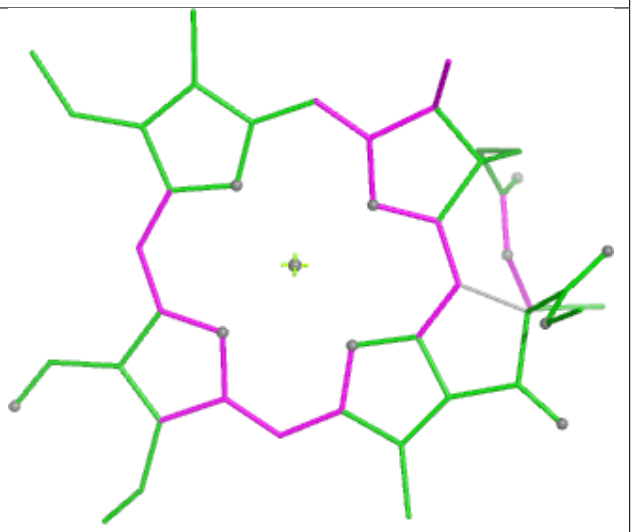

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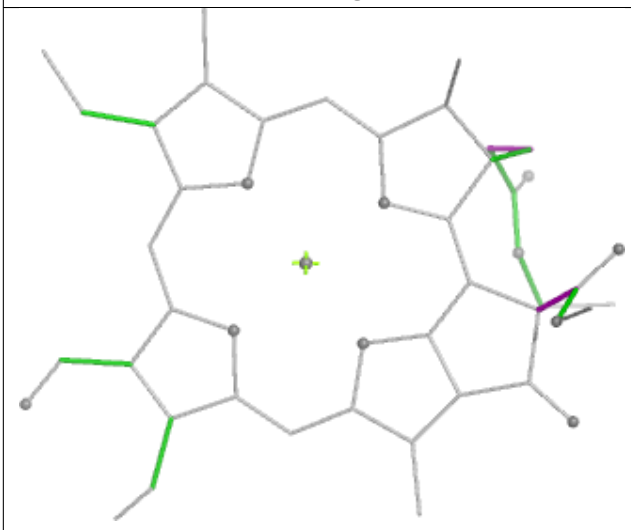

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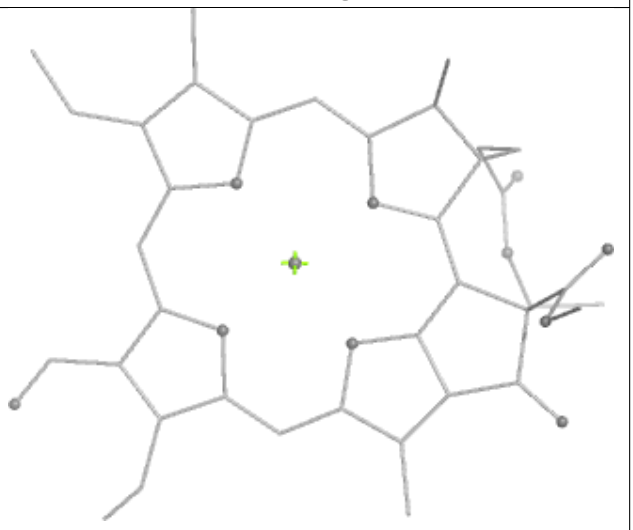

Rings

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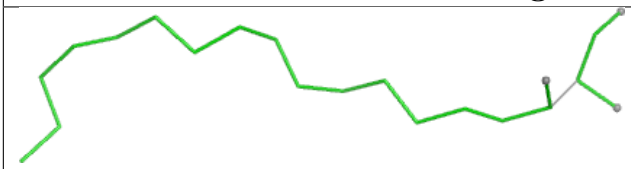
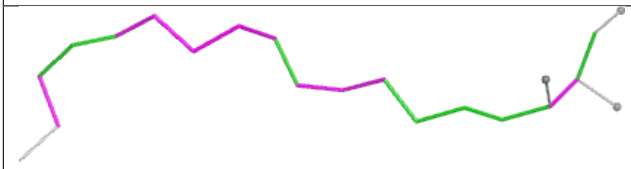


Bond lengths



Bond angles

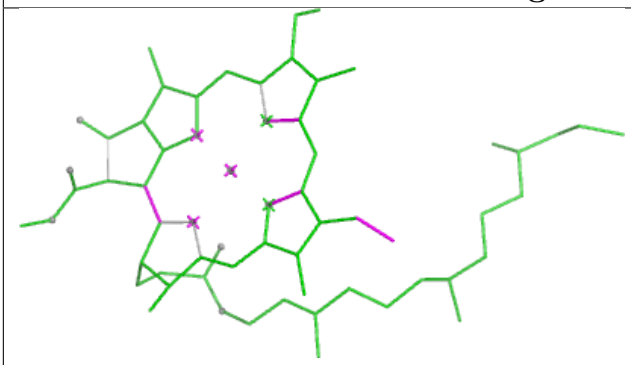


Torsions



Rings

Ligand CLA 8 604



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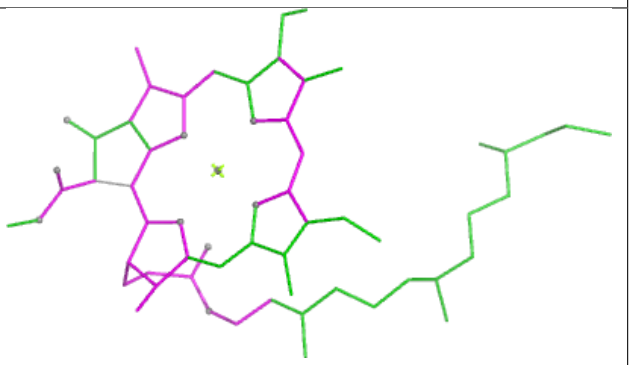

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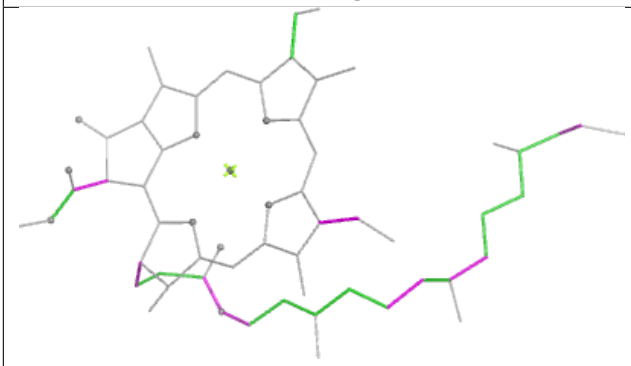
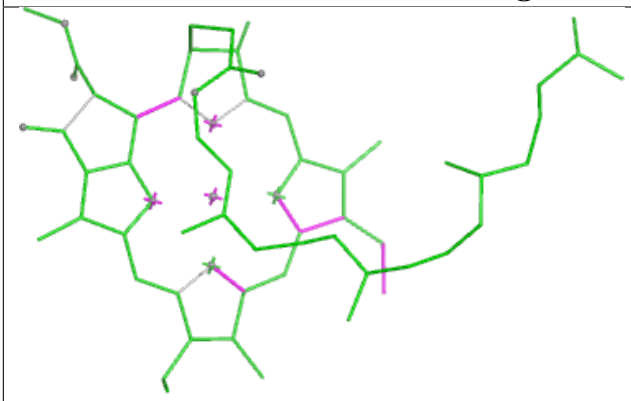


Torsions



Rings

Ligand CLA B 1209



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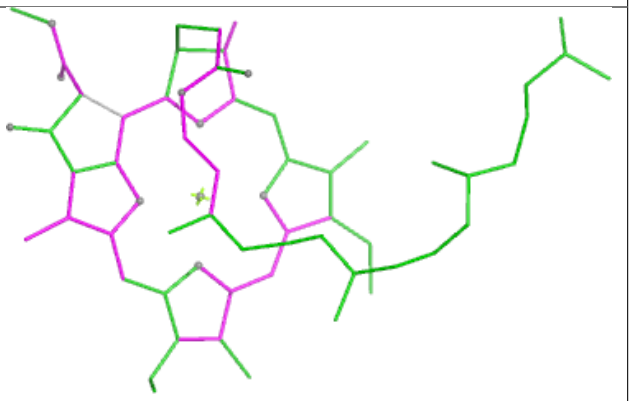

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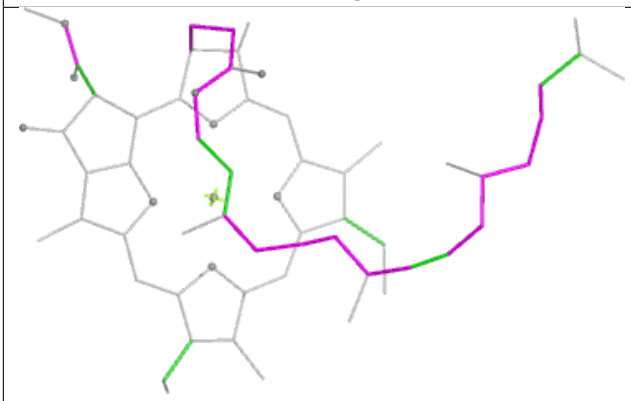

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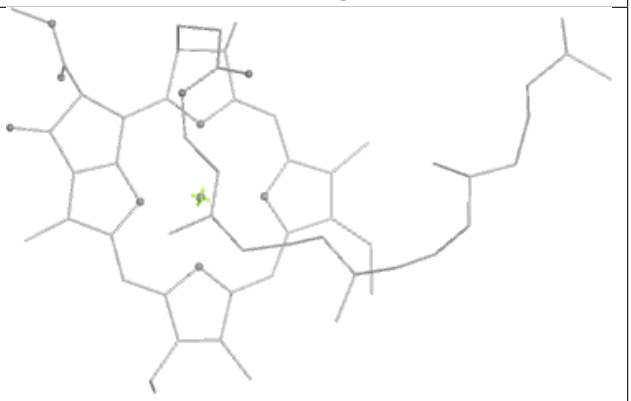
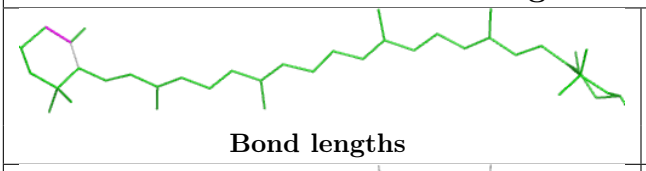


Rings

Ligand LUT 5 502



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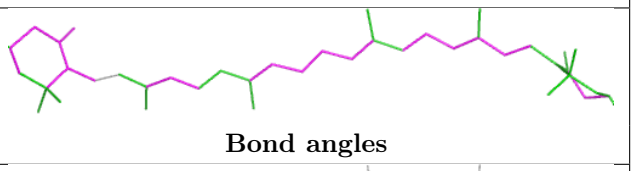
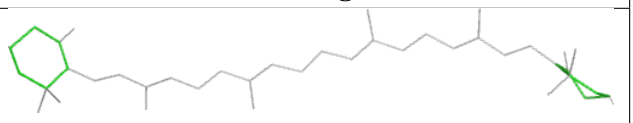


Bond angles

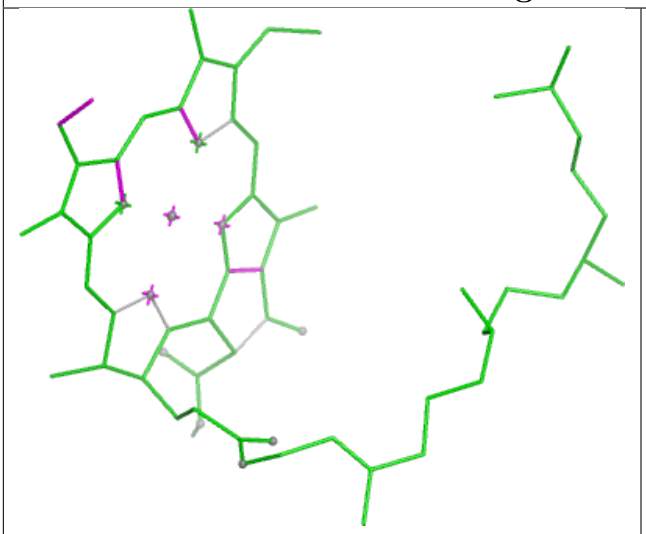


Torsions

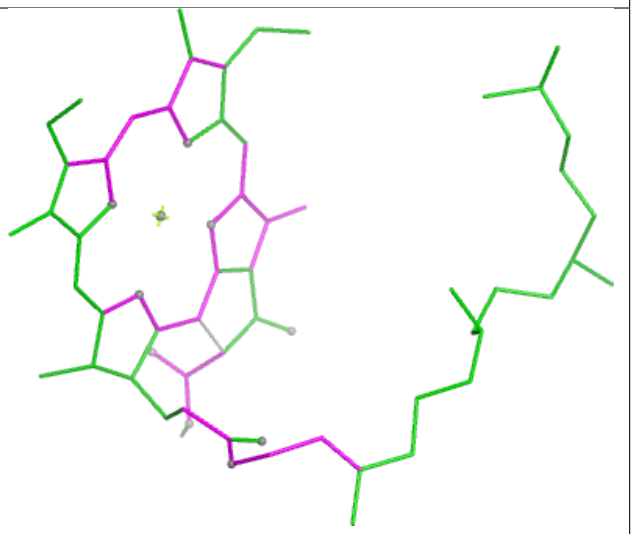


Rings

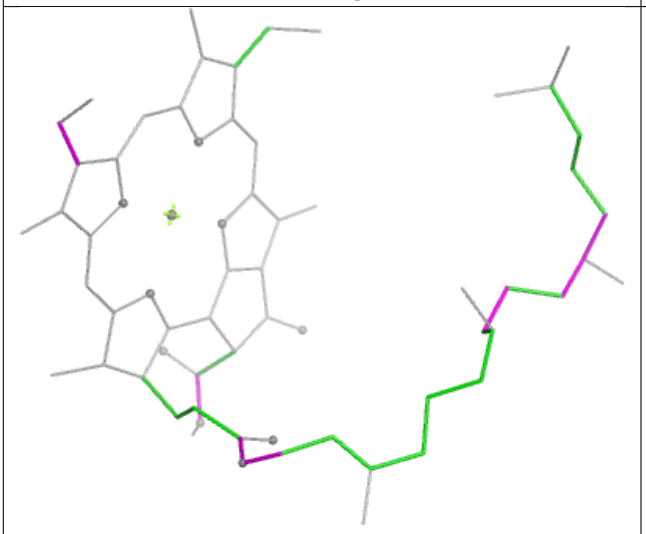
Ligand CLA B 1231



Bond lengths



Bond angles



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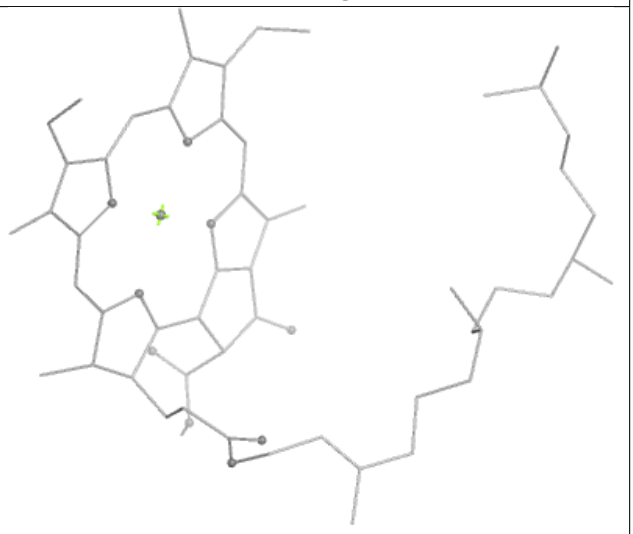
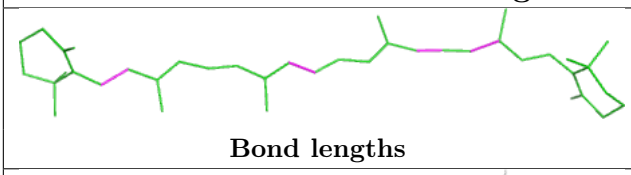


Rings

Ligand BCR A 4001



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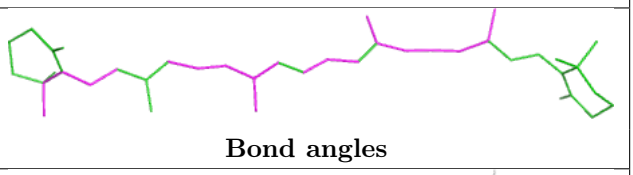
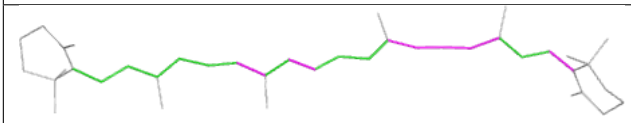


Bond angles



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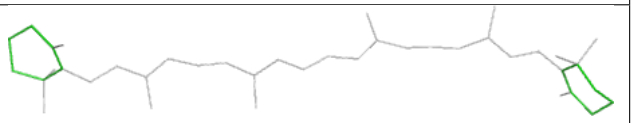
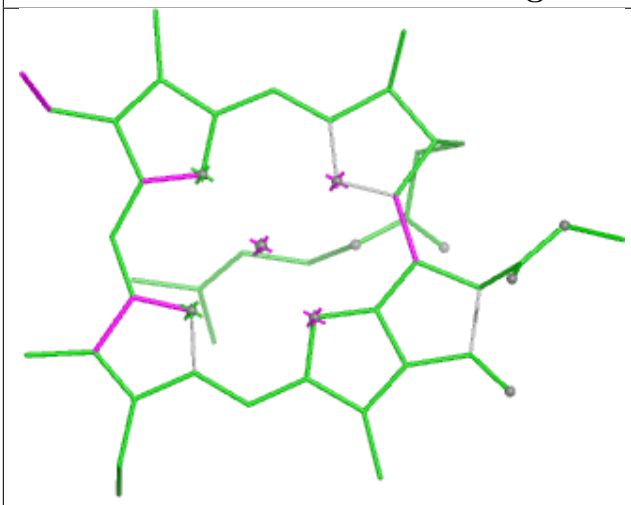
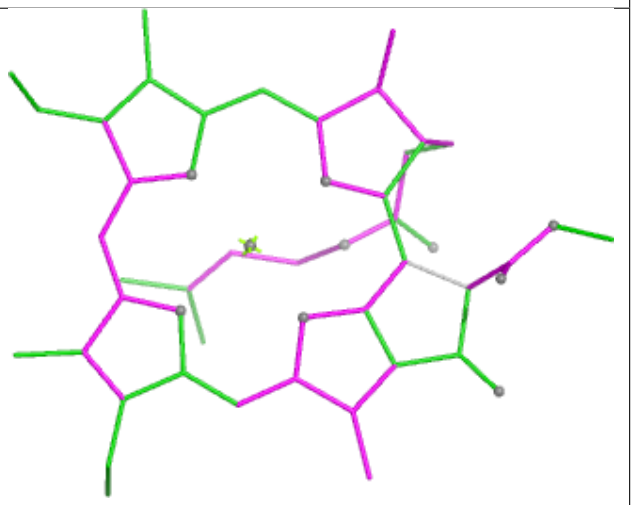


Rings

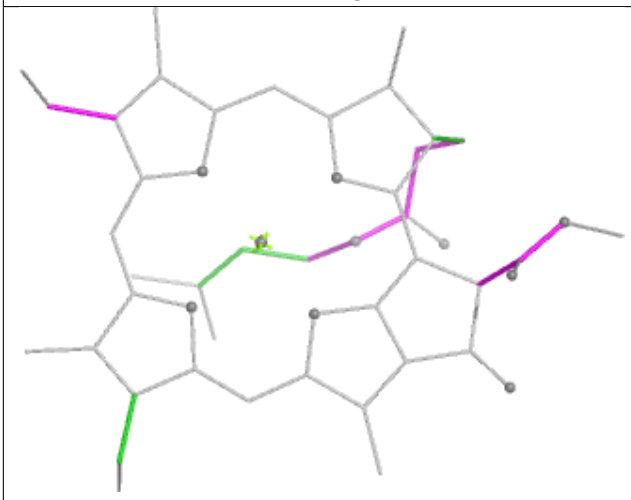
Ligand CLA Z 603



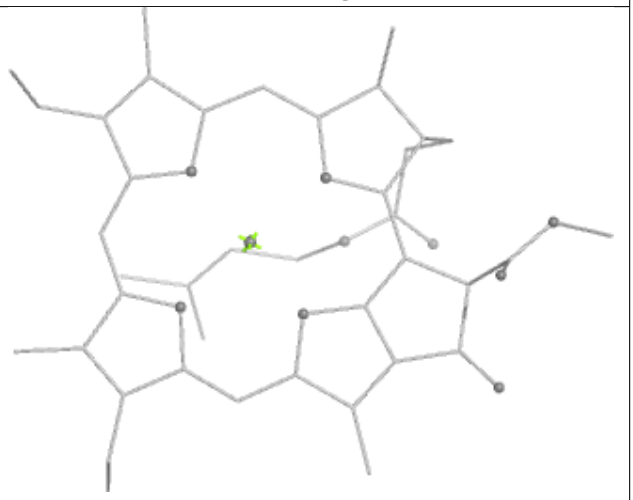
Bond lengths



Bond angles

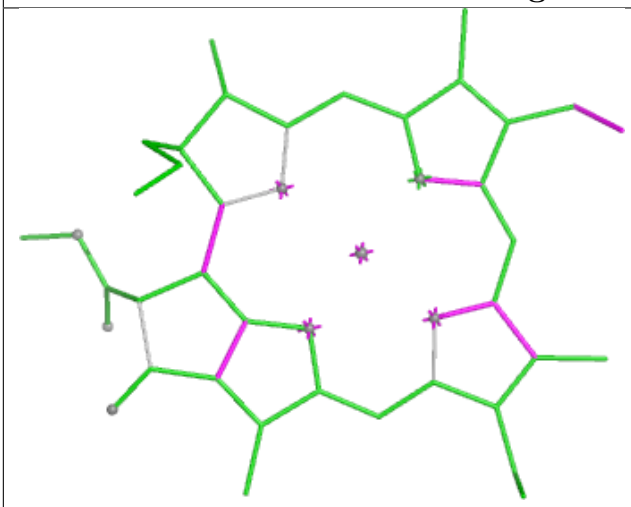


Torsions



Rings

Ligand CLA 7 608



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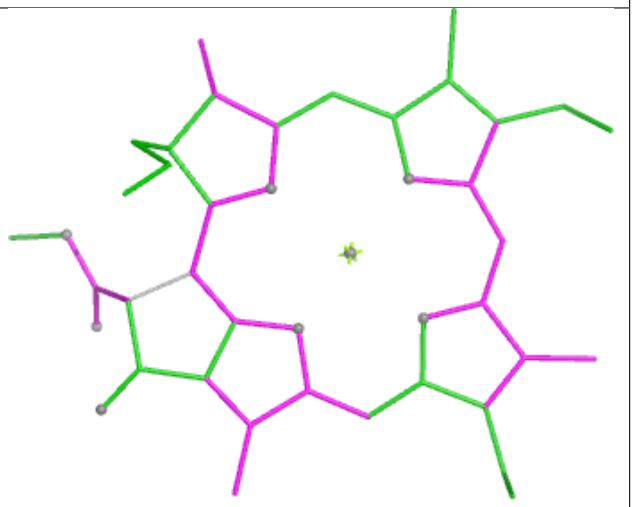
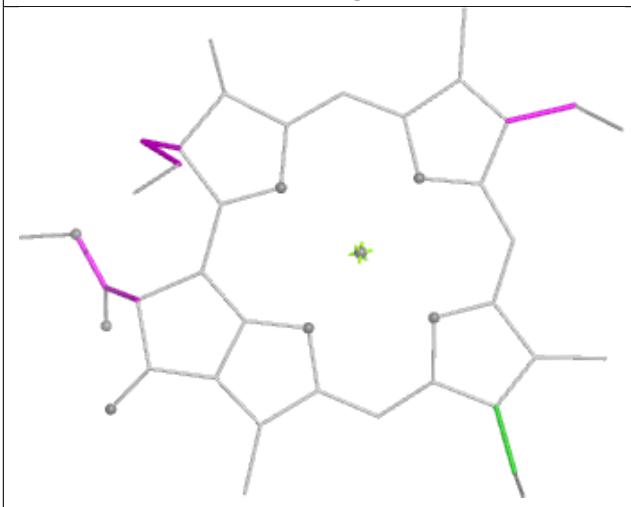


Bond angles



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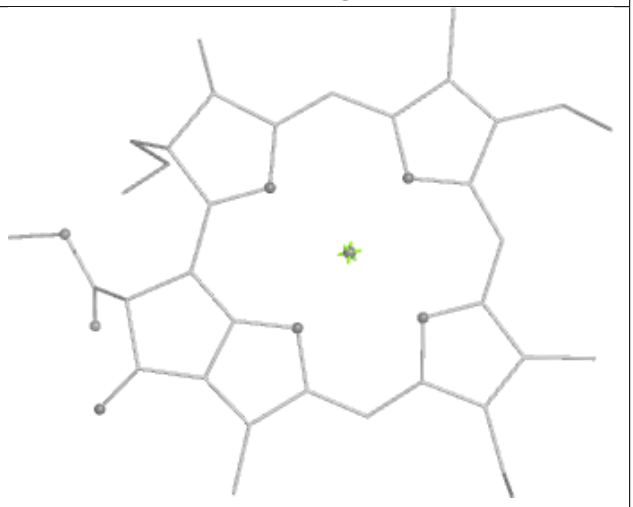
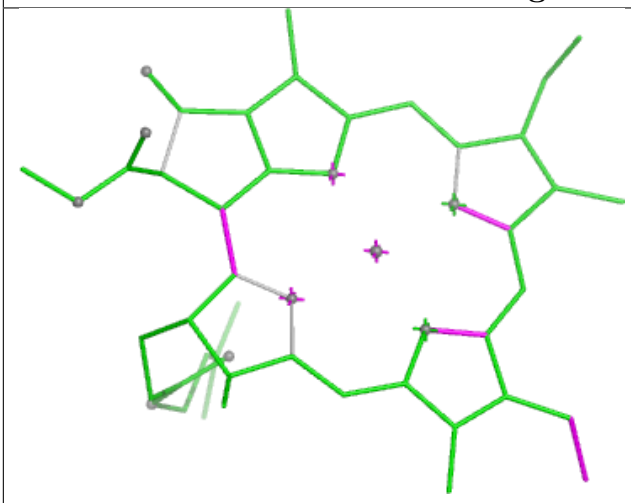


Rings

Ligand CLA 4 612



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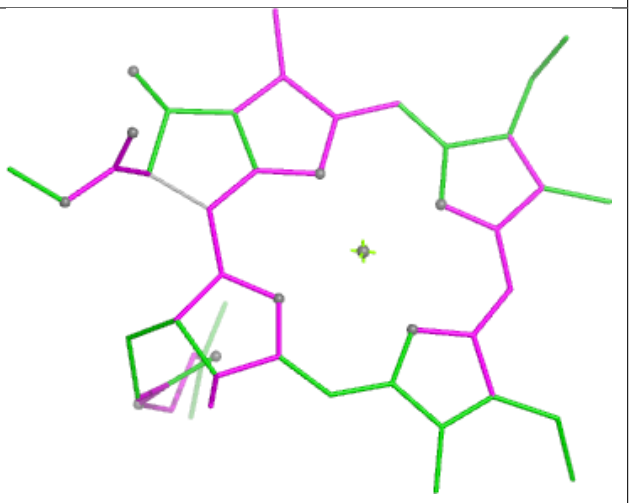

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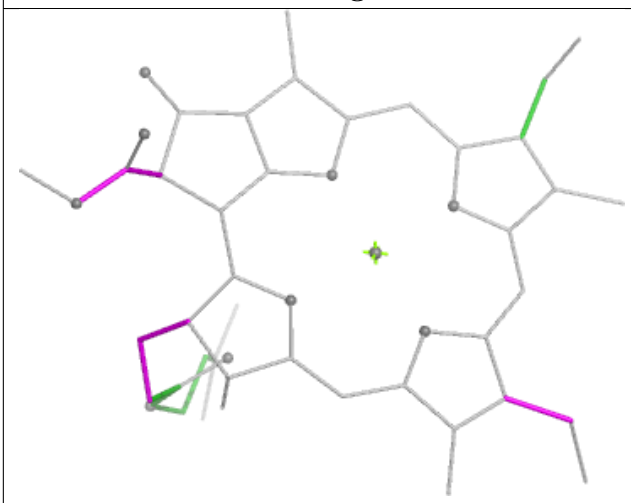

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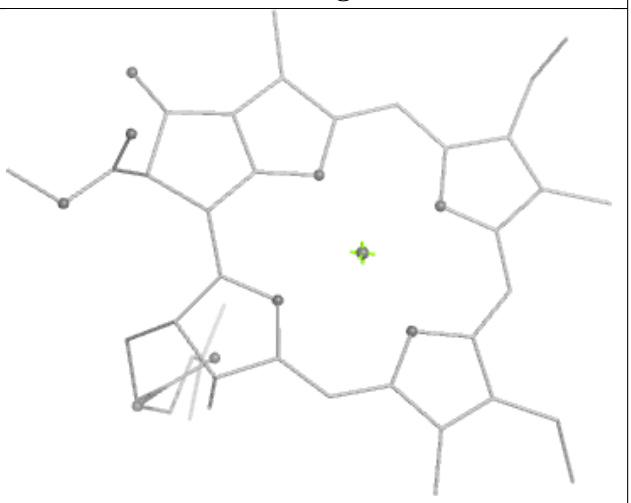
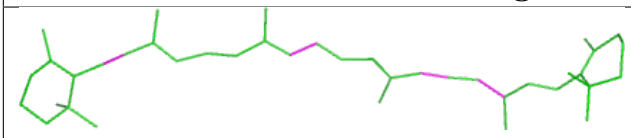


Rings

Ligand BCR A 4004



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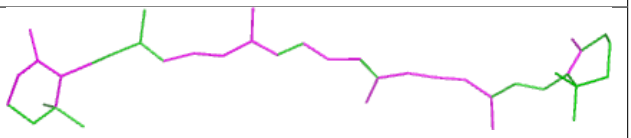

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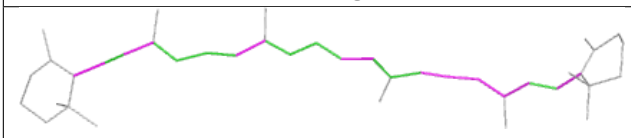

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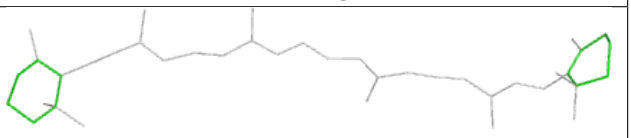
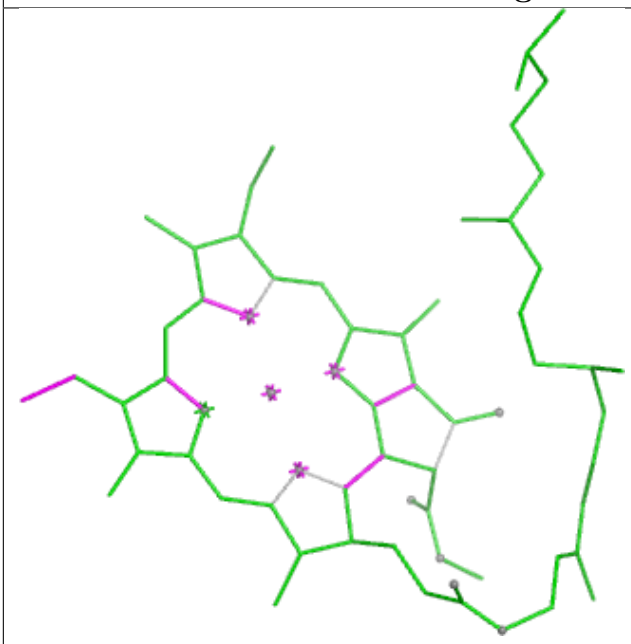


Rings

Ligand CLA A 1123



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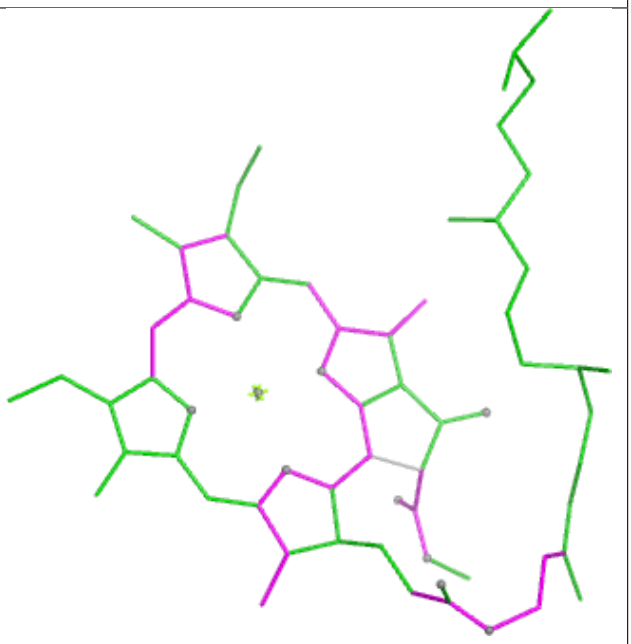

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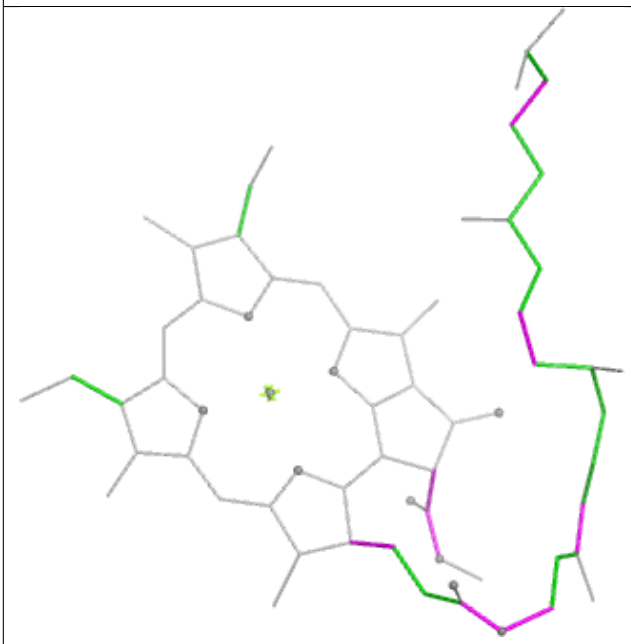
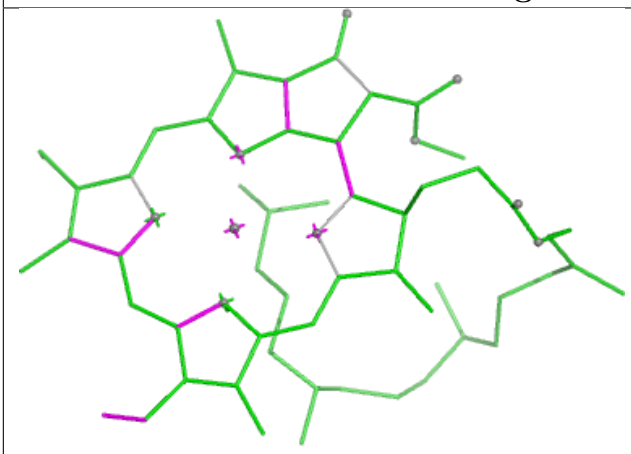


Torsions



Rings

Ligand CLA A 1104



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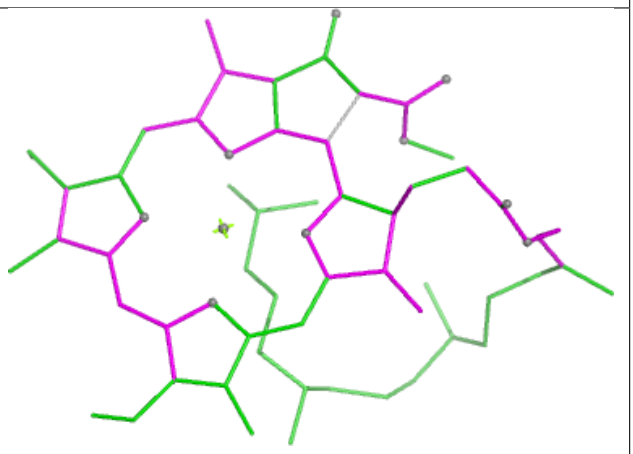
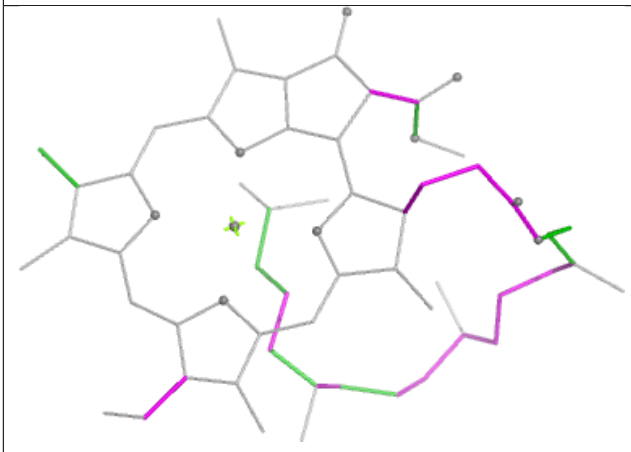


Bond angles



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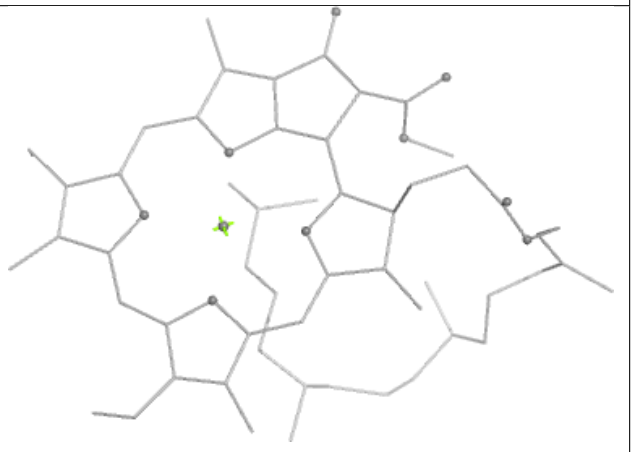
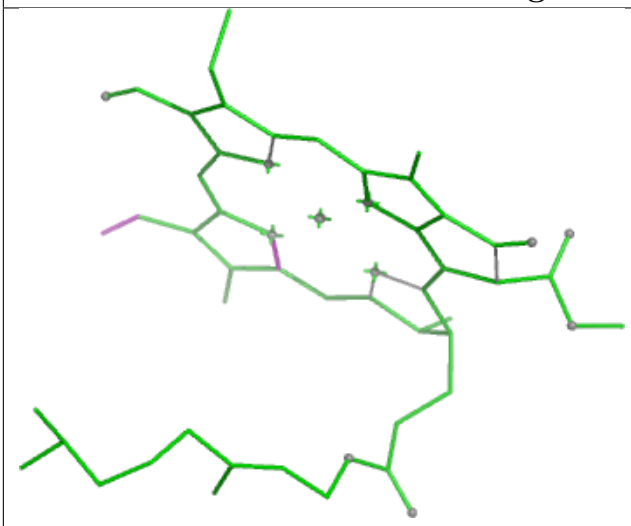


Rings

Ligand CHL 6 610



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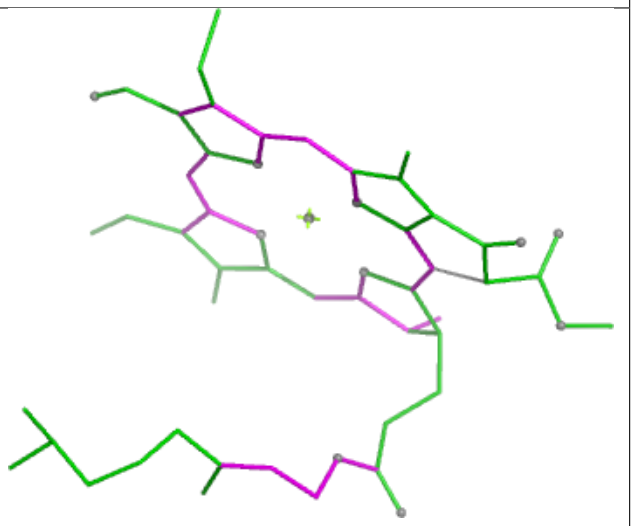
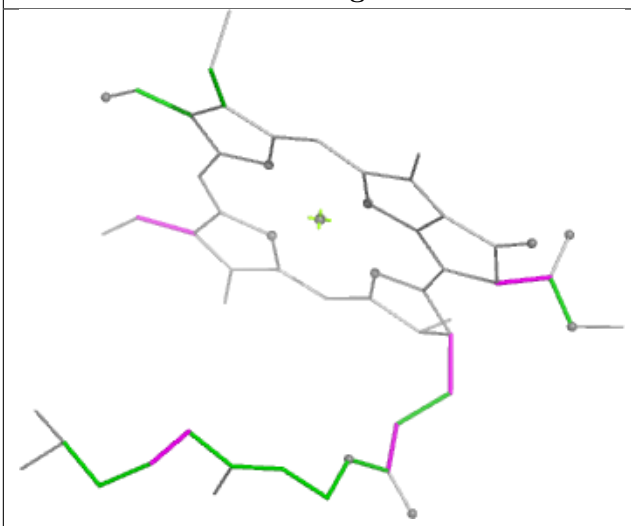


Bond angles



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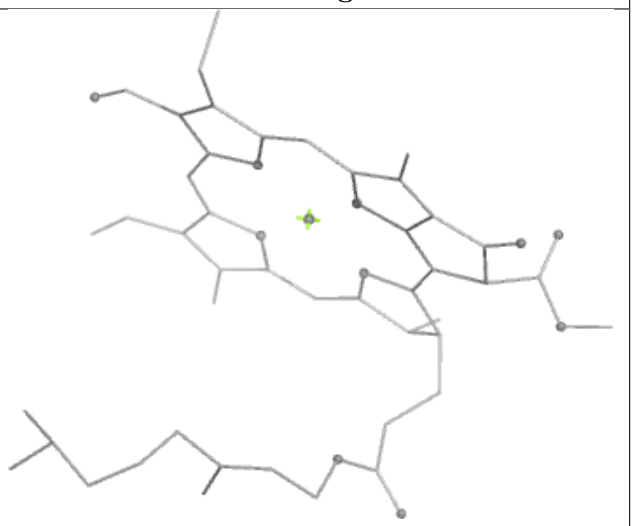
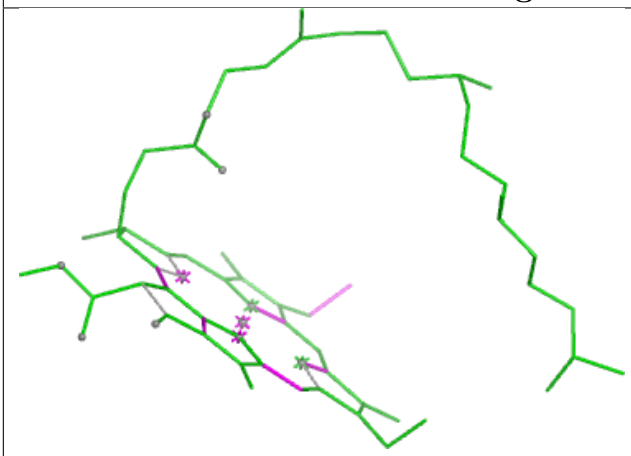


Rings

Ligand CLA B 1216



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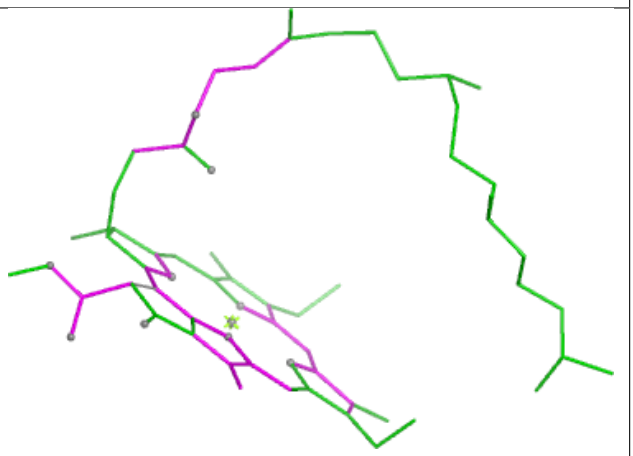
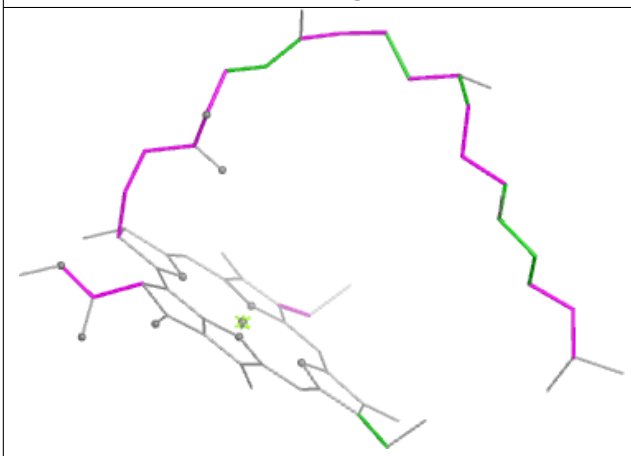


Bond angles

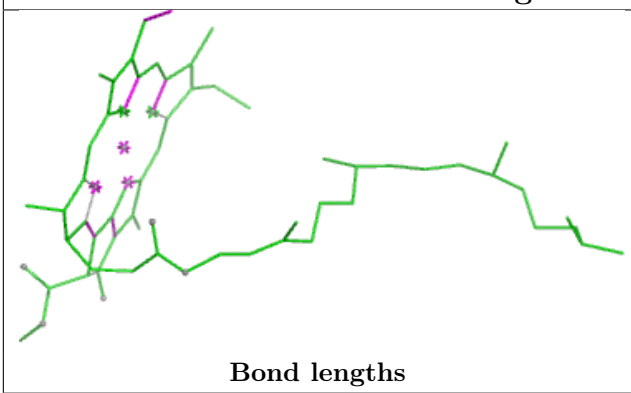


Torsions



Rings

Ligand CLA A 1109



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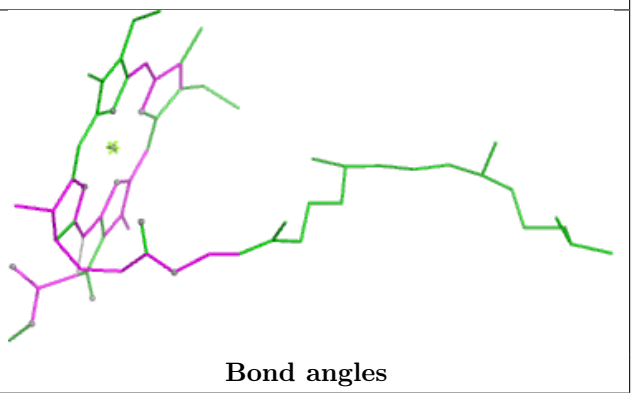
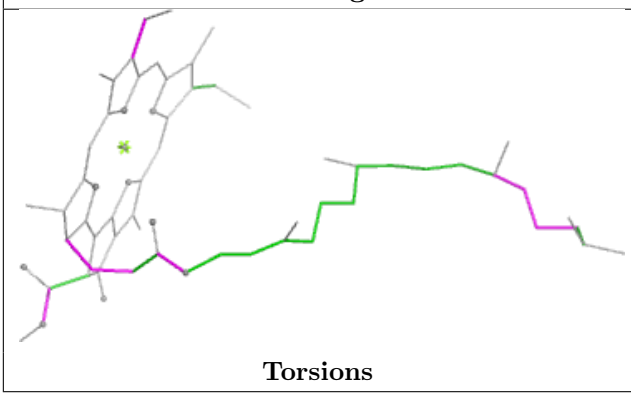


Bond angles



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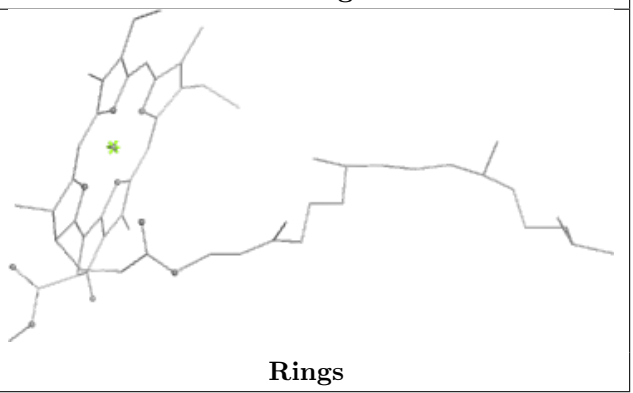
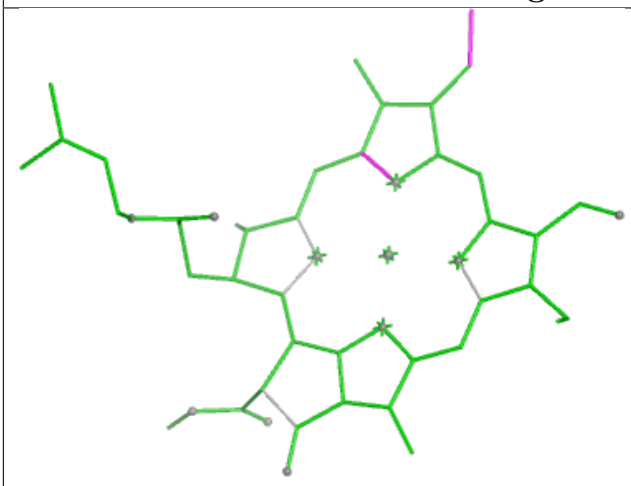


Rings

Ligand CHL 6 611



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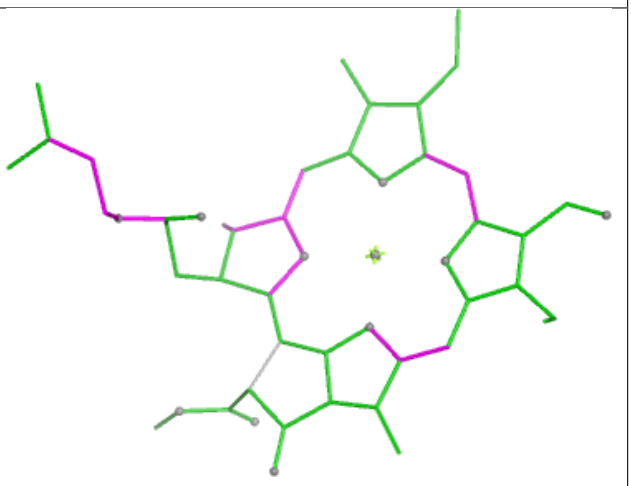
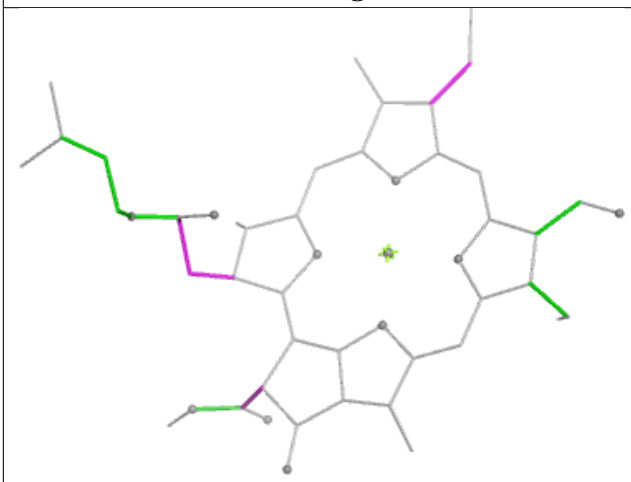


Bond angles



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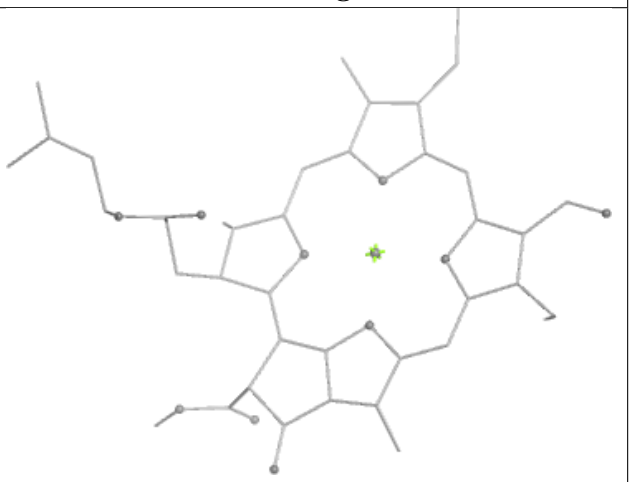
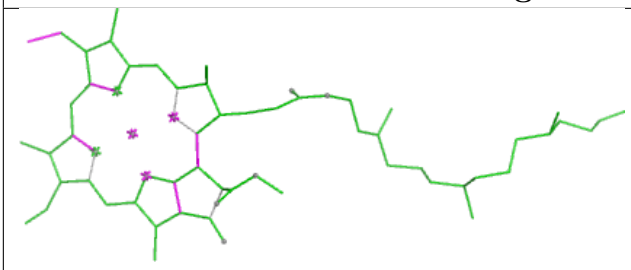


Rings

Ligand CLA A 1140



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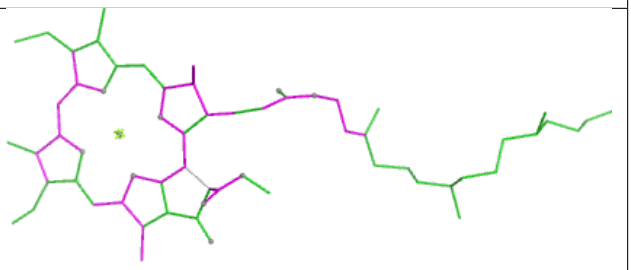
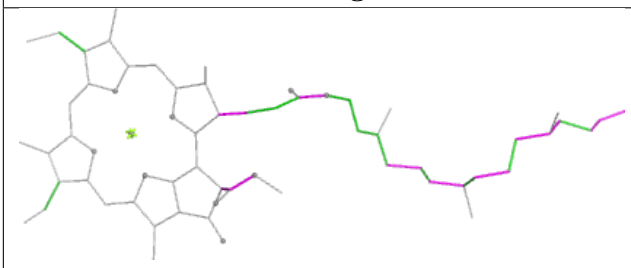


Bond angles



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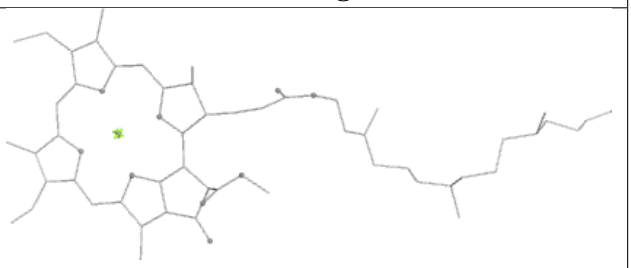
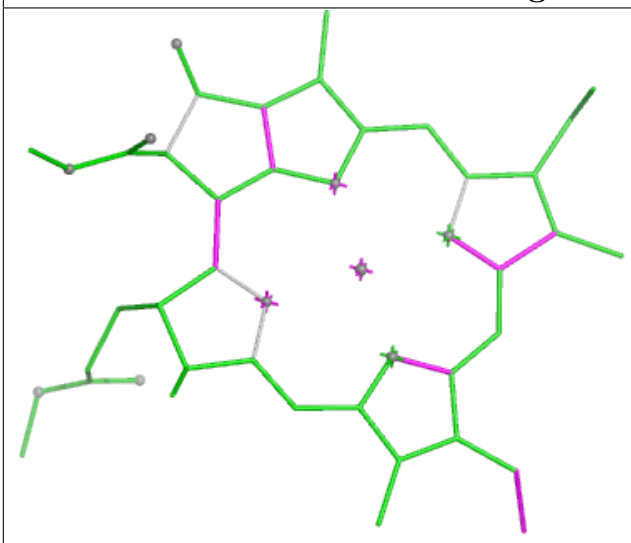


Rings

Ligand CLA 8 612



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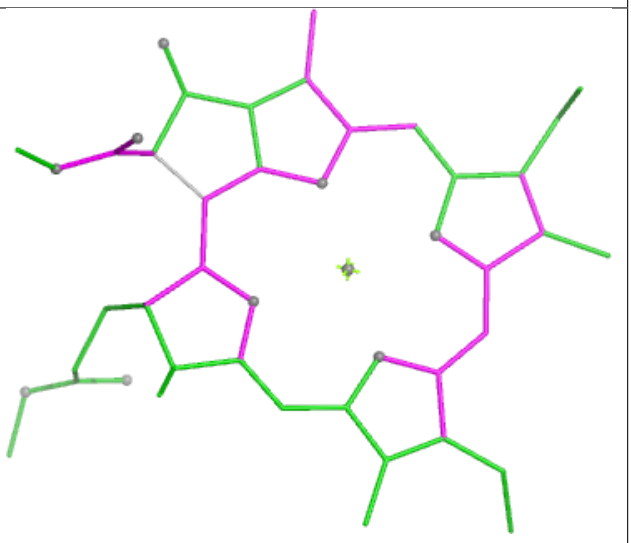
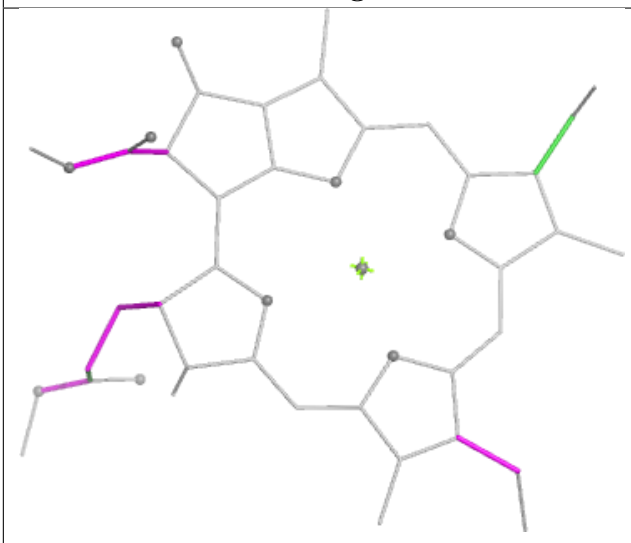


Bond angles



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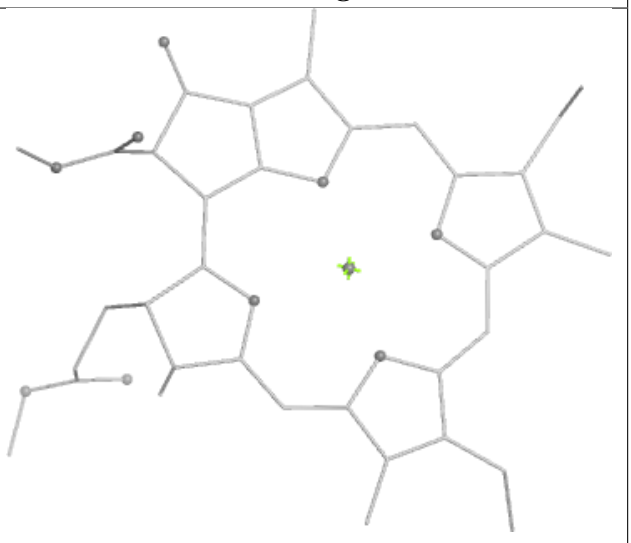

Rings

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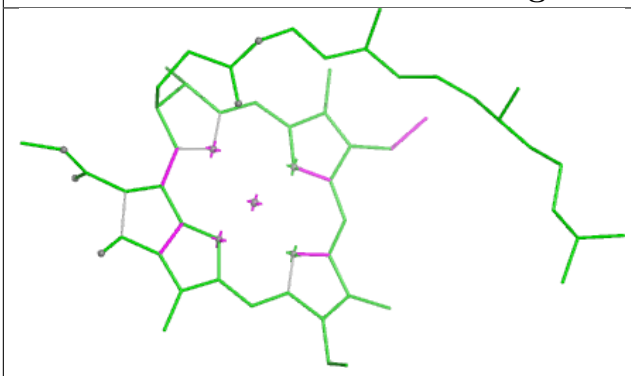

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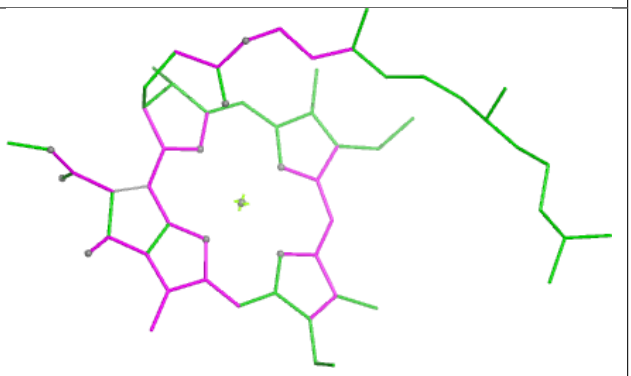
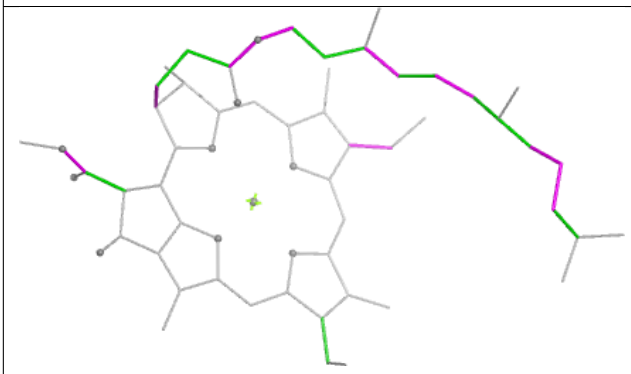


Bond angles



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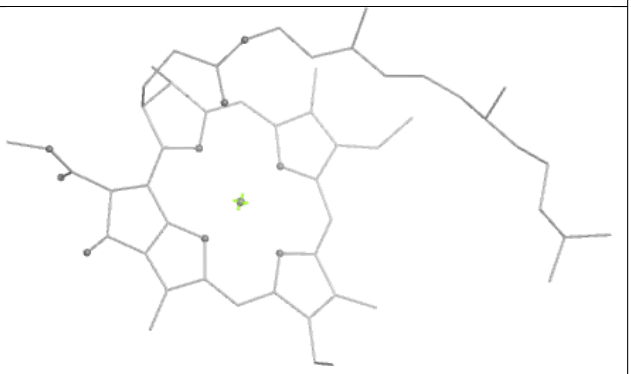
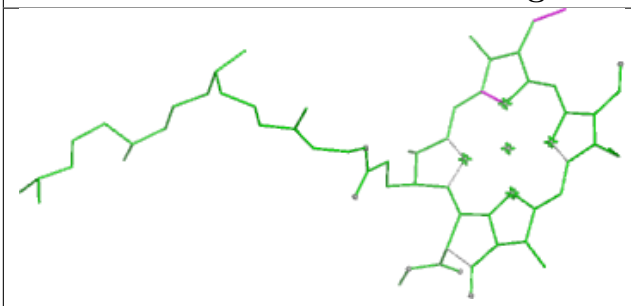


Rings

Ligand CHL 3 611



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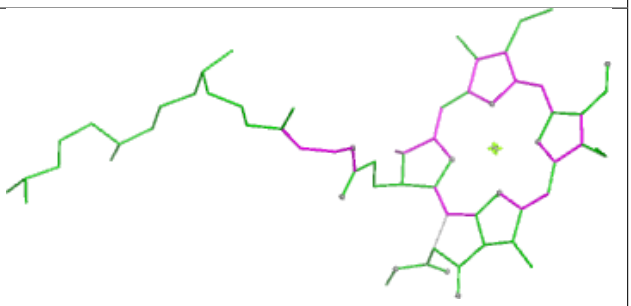
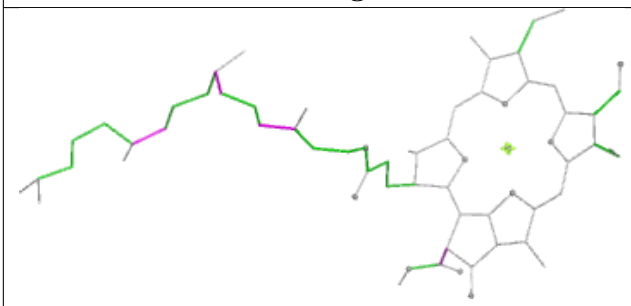


Bond angles



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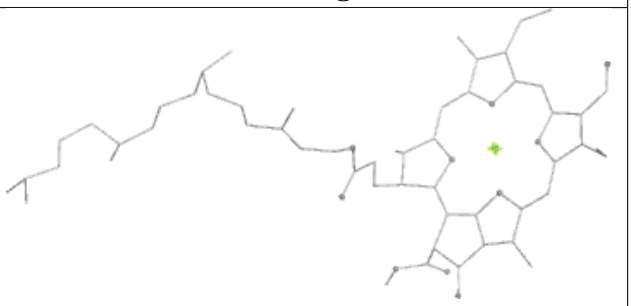


Rings

Ligand CLA B 1214



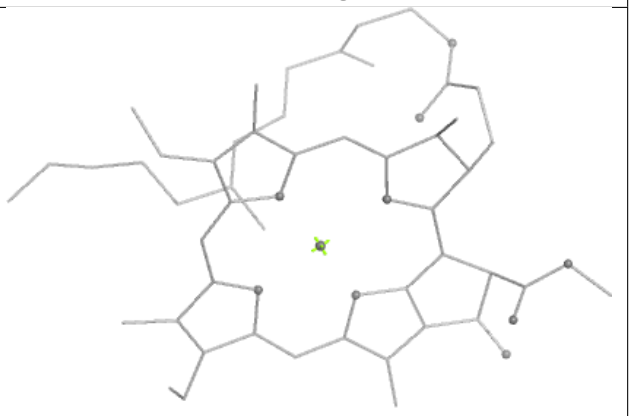
Bond lengths



Bond angles

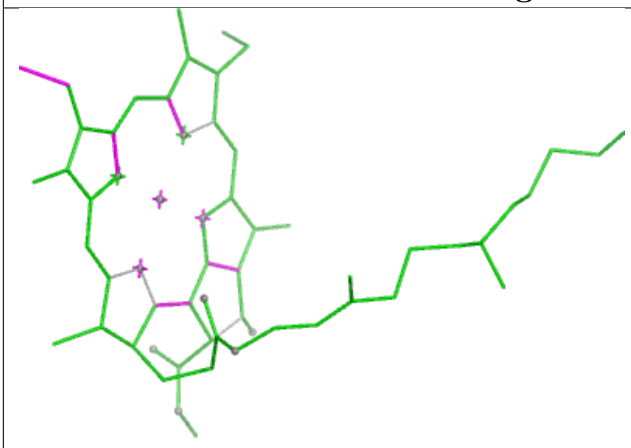


Torsions

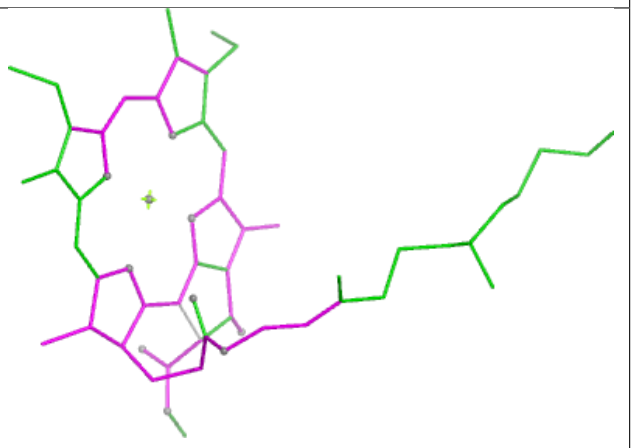


Rings

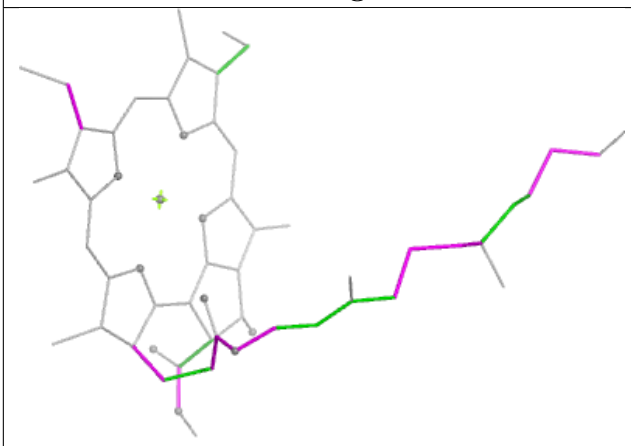
Ligand CLA B 1219



Bond lengths



Bond angles



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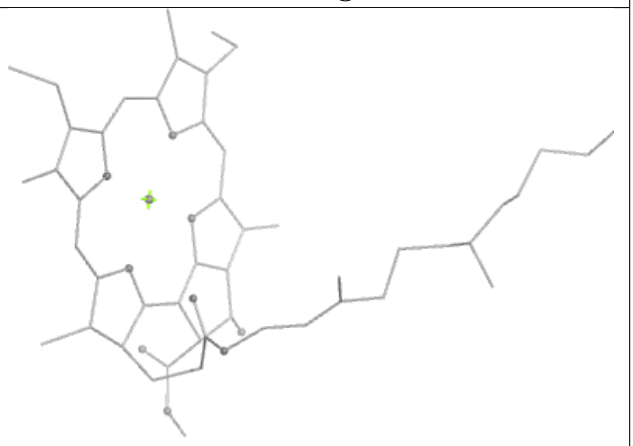
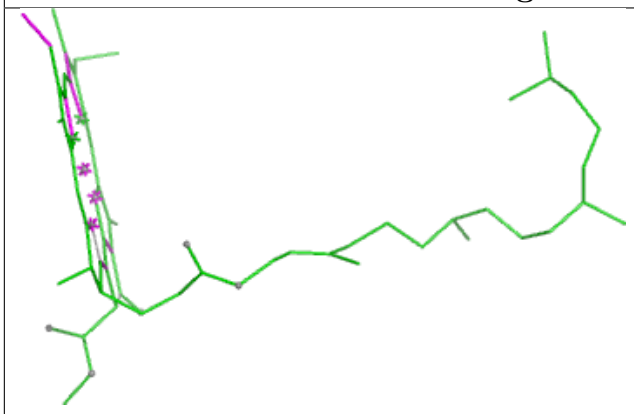
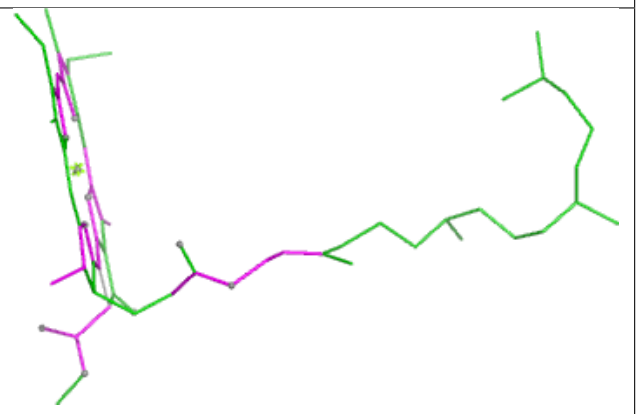


Rings

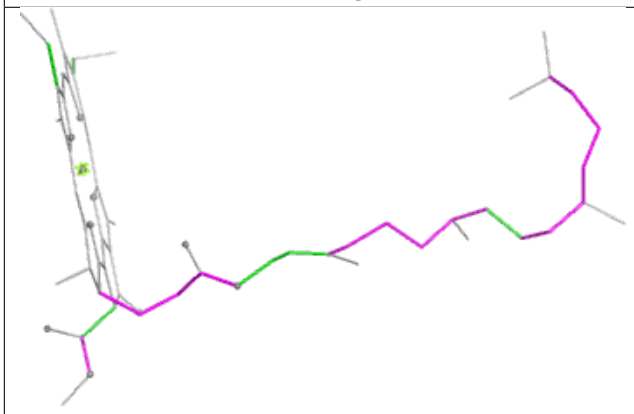
Ligand CLA B 1236



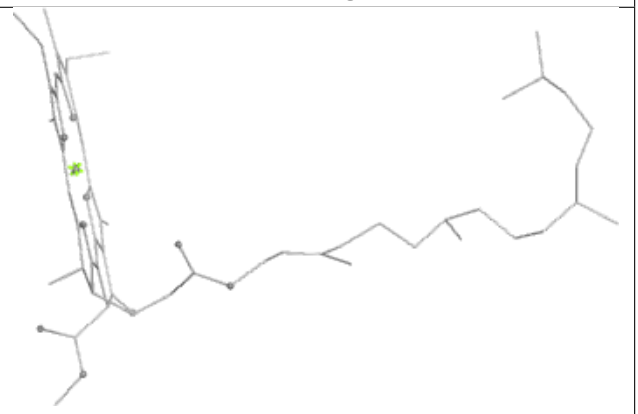
Bond lengths



Bond angles

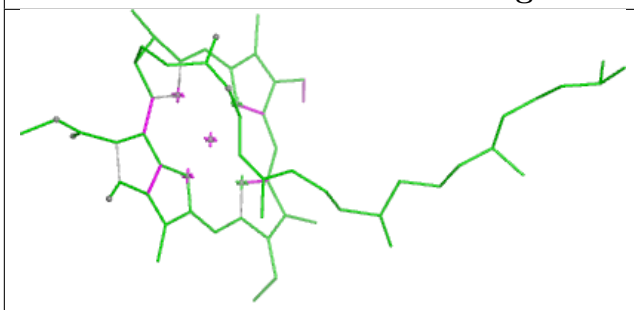


Torsions



Rings

Ligand CLA A 1139



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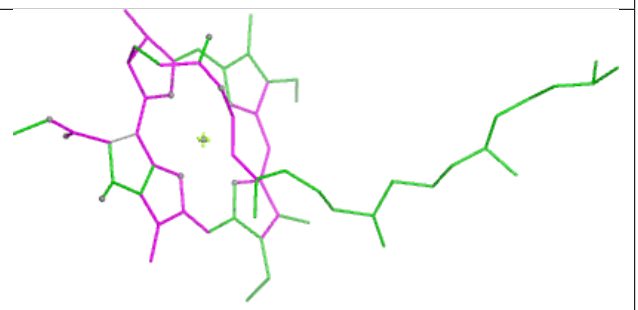
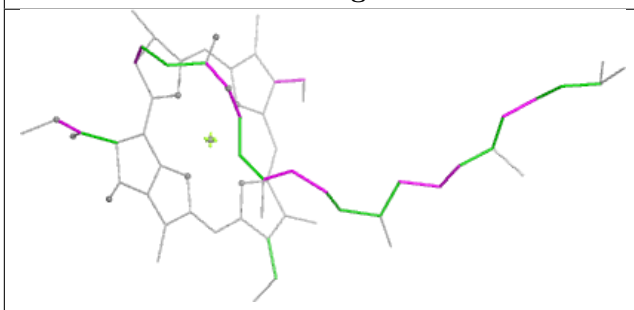


Bond angles

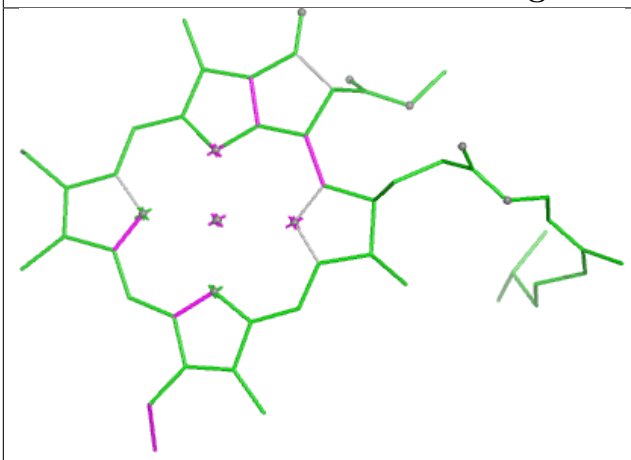


Torsions



Rings

Ligand CLA 5 605



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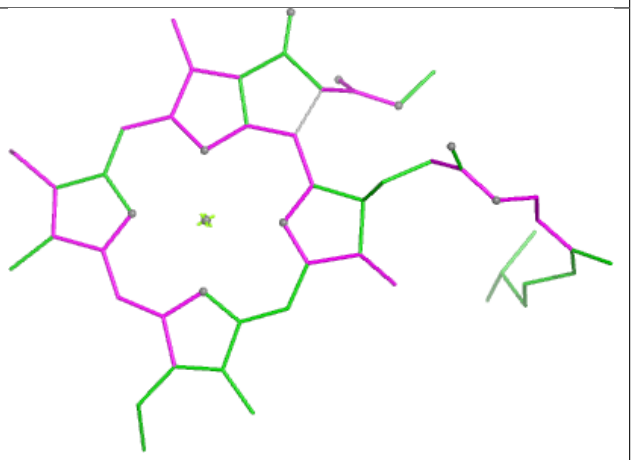
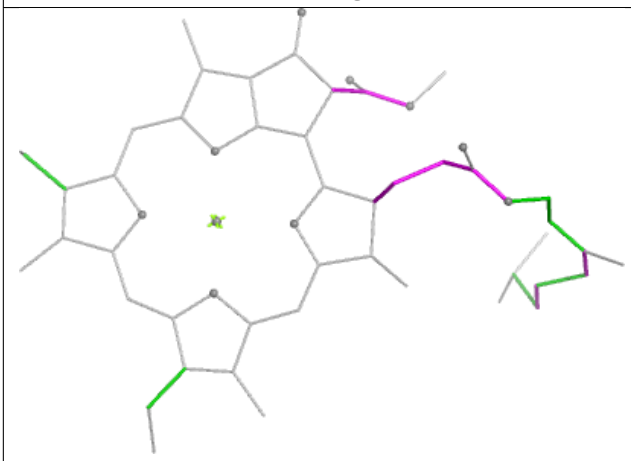


Bond angles



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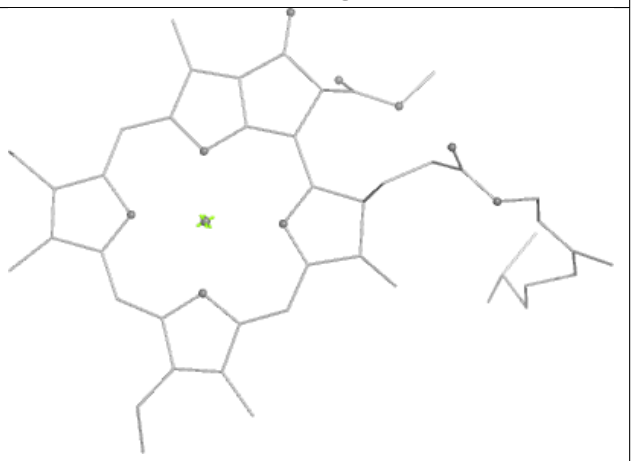
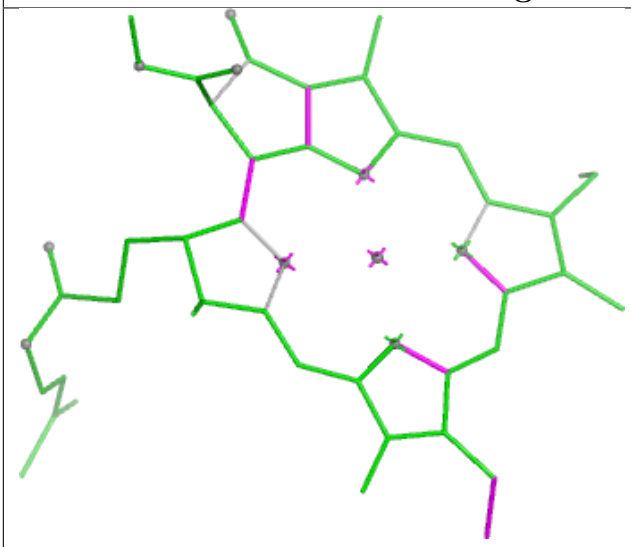


Rings

Ligand CLA A 1129



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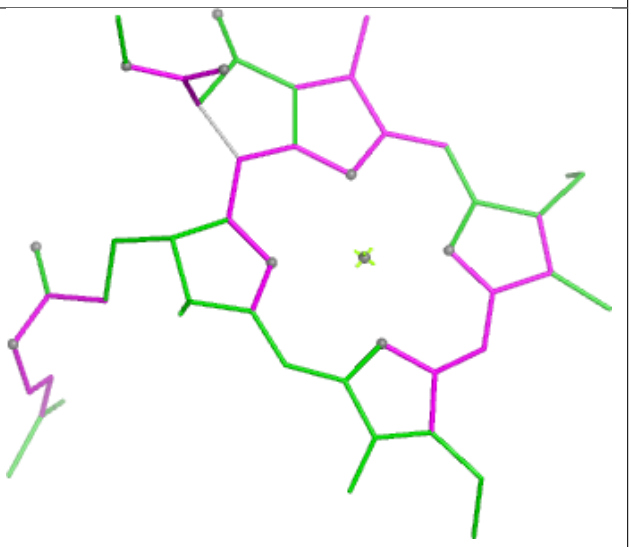
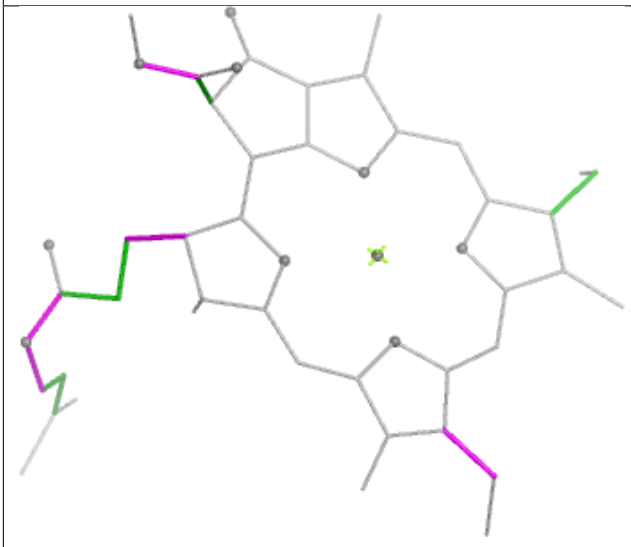


Bond angles



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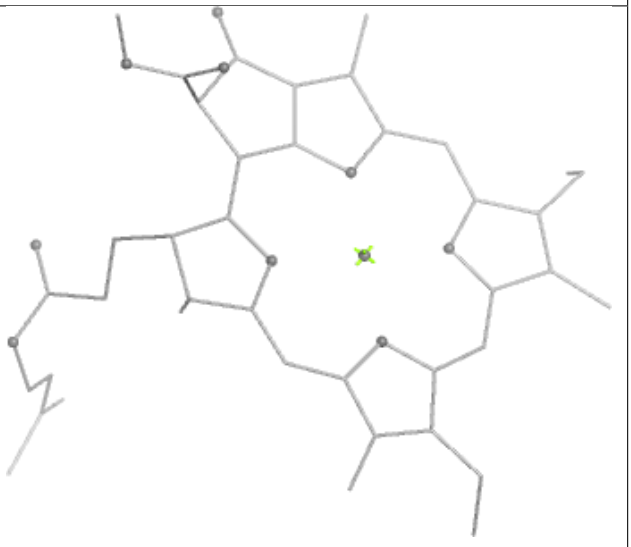
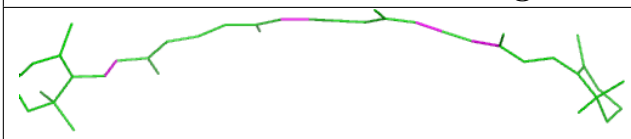


Rings

Ligand BCR B 4006



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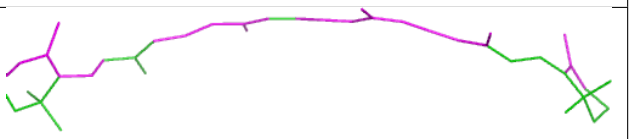
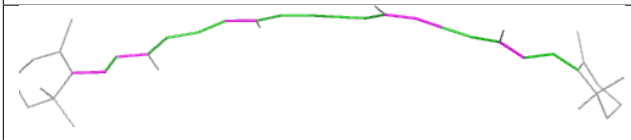


Bond angles

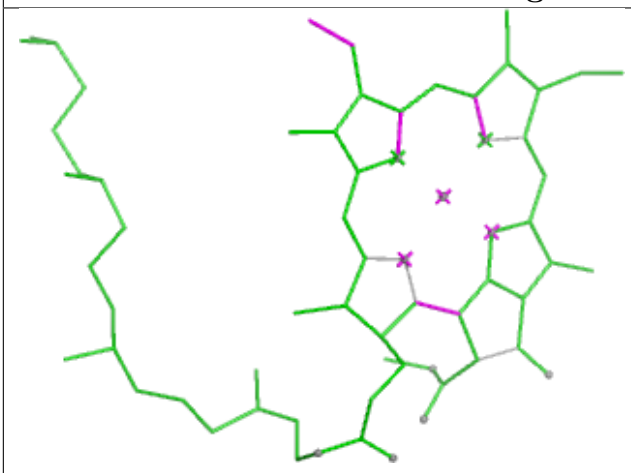


Torsions



Rings

Ligand CLA Z 605



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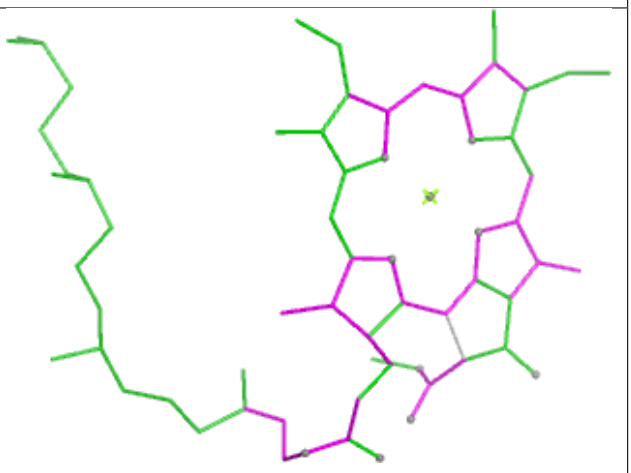

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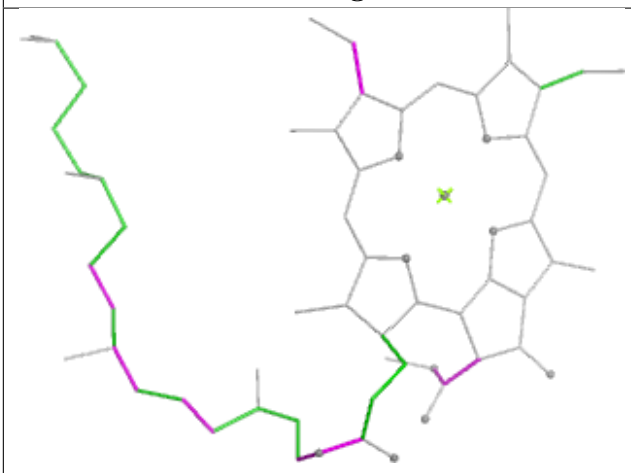

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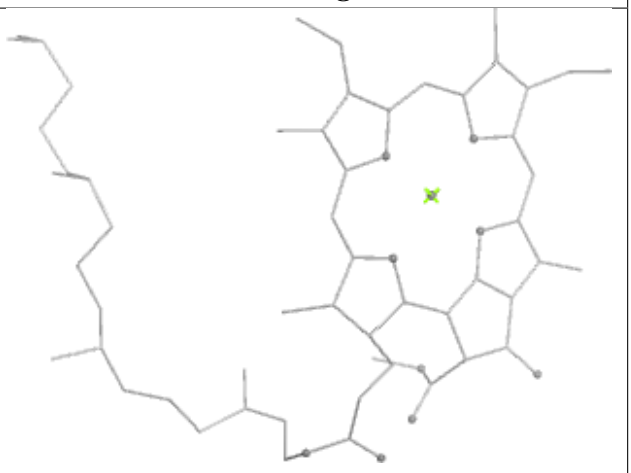
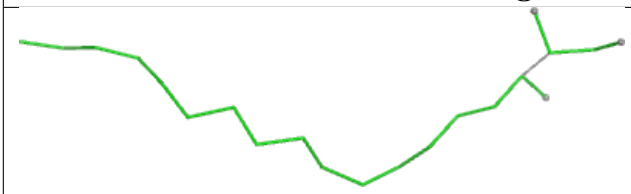


Rings

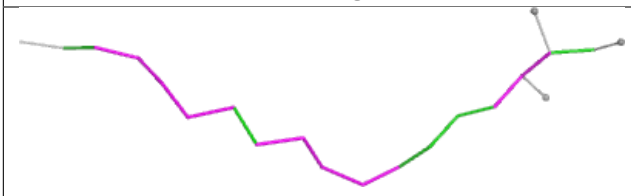
Ligand SPH K 5001



Bond lengths



Bond angles



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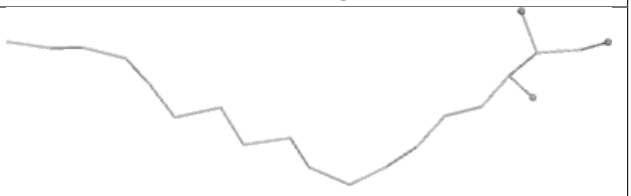
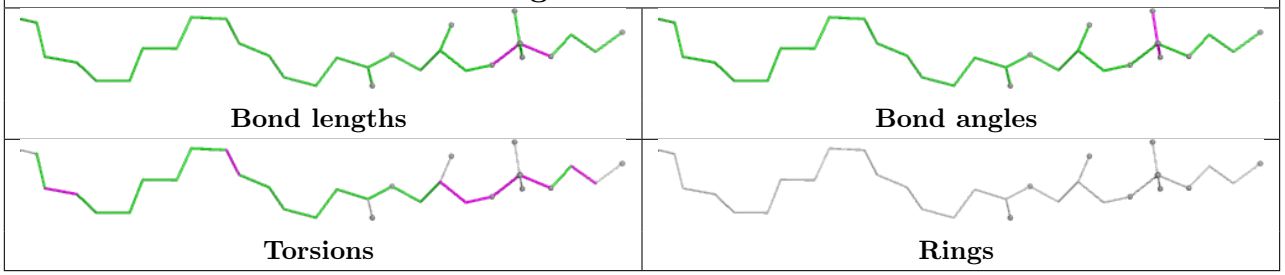
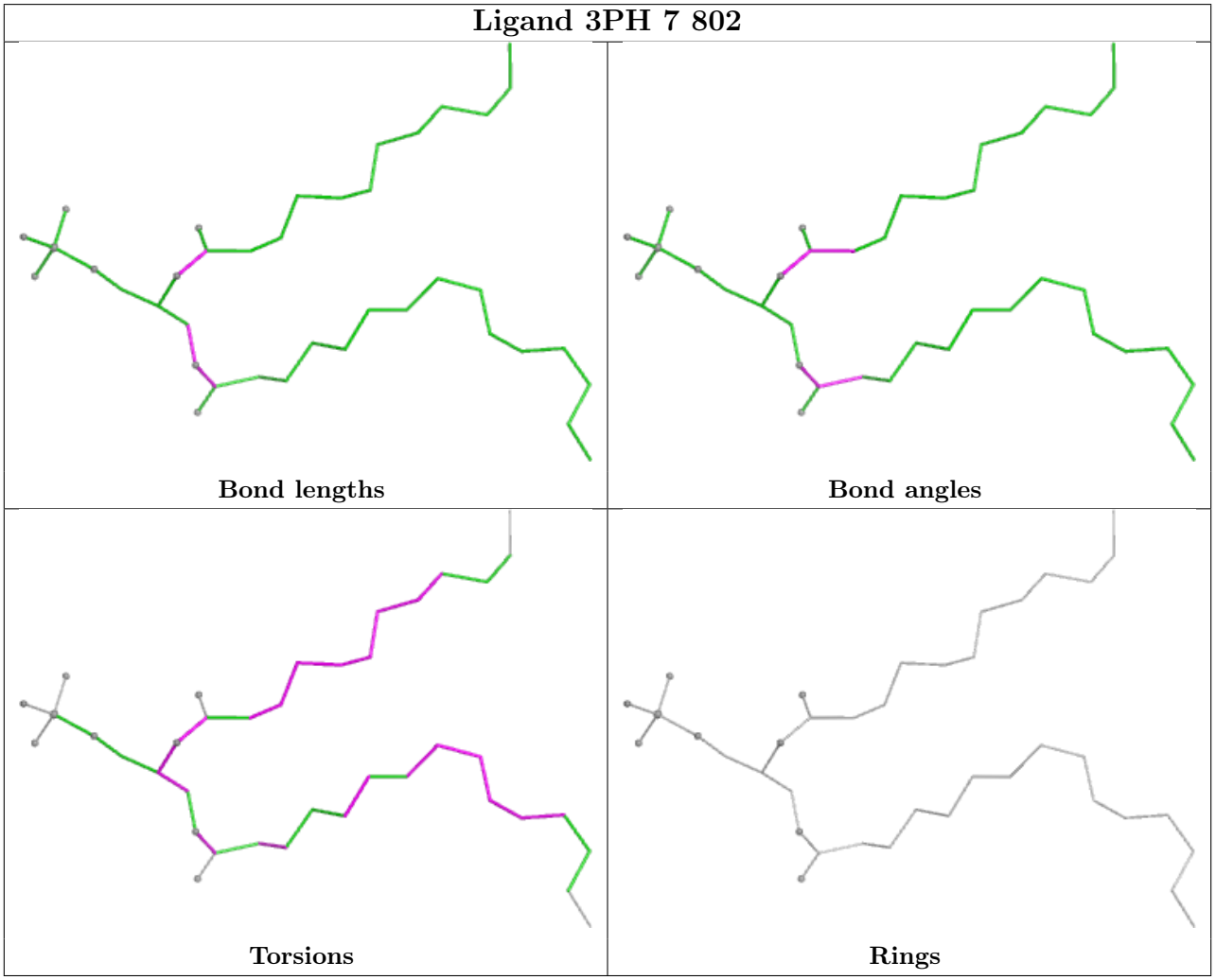


Rings

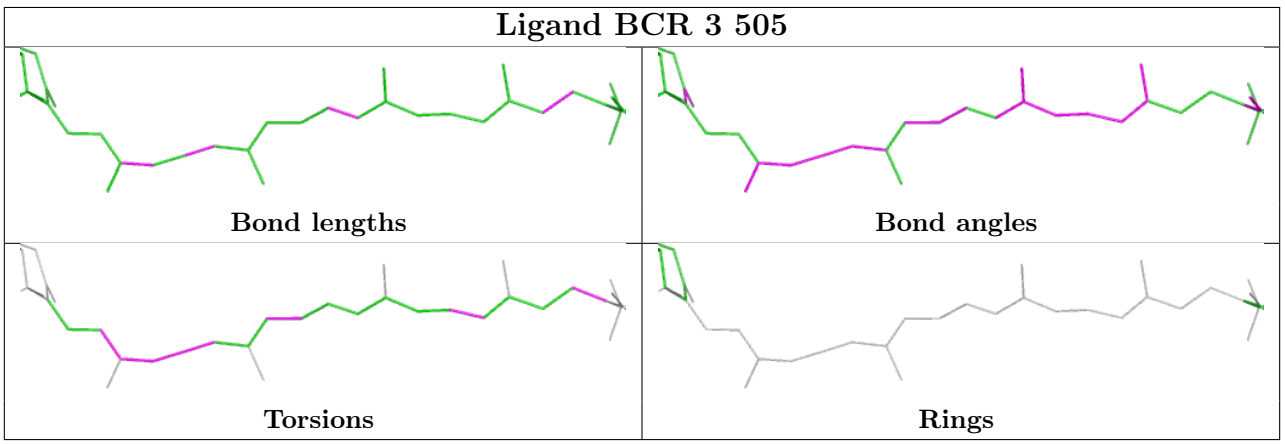
Ligand LPX 8 803



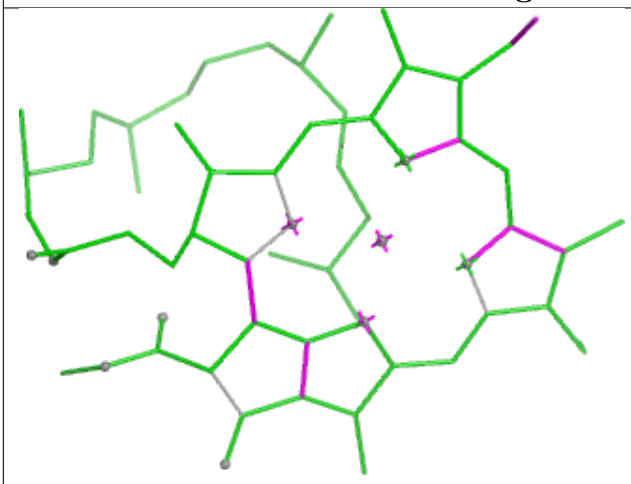
Ligand 3PH 7 802



Ligand BCR 3 505



Ligand CLA B 1203



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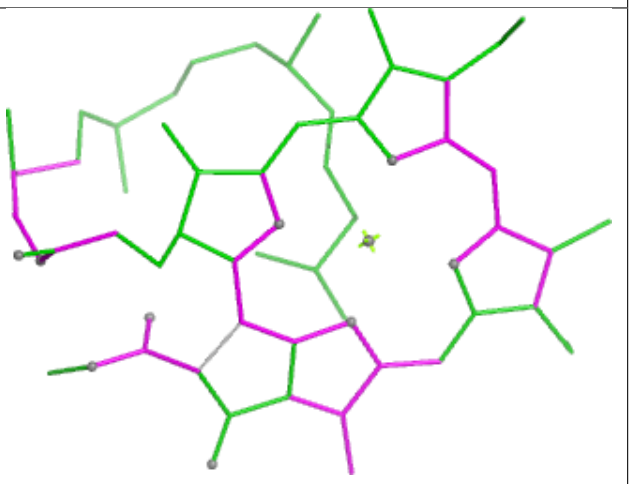
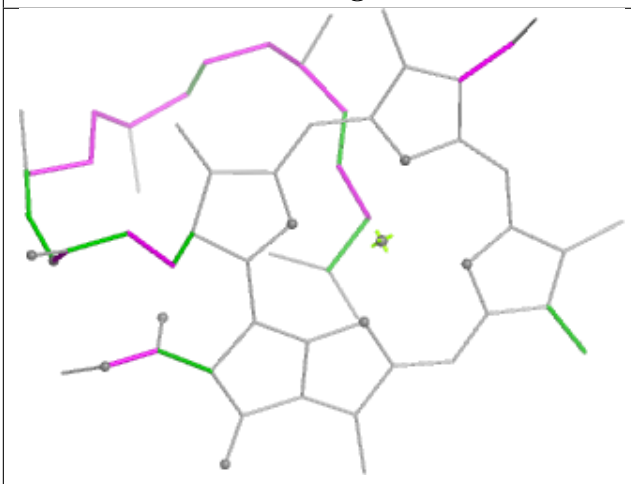


Bond angles

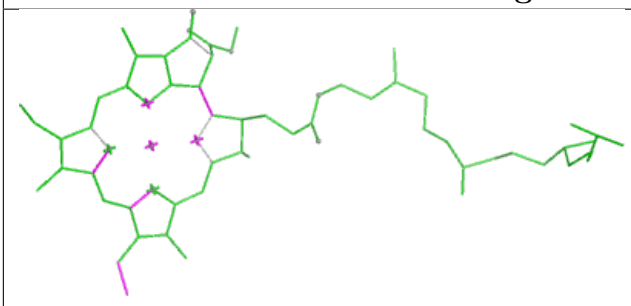


Torsions



Rings

Ligand CLA A 1103



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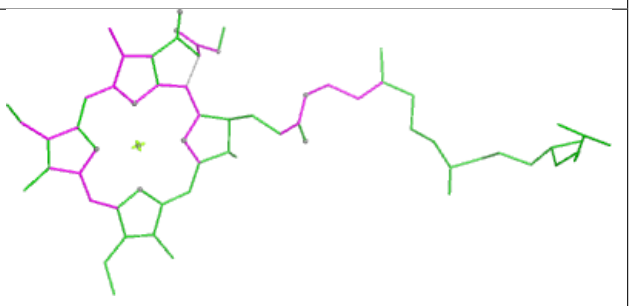
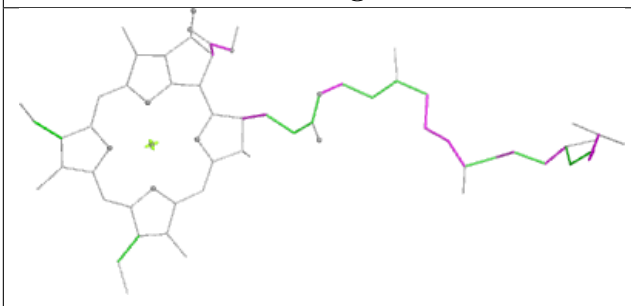


Bond angles



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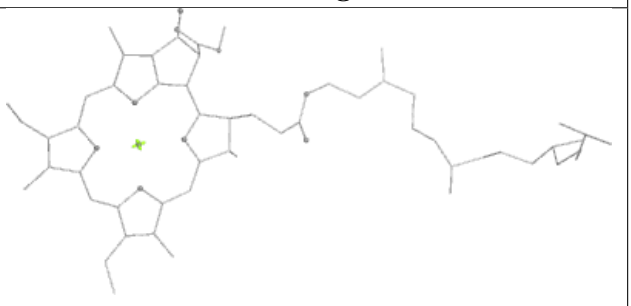
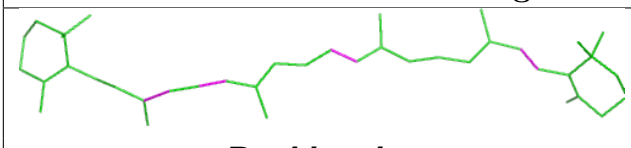


Rings

Ligand BCR A 4003



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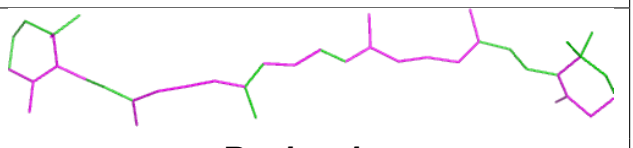
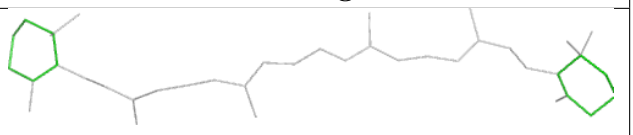


Bond angles

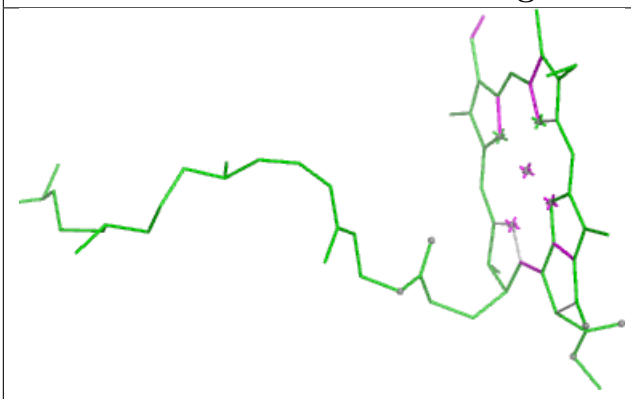


Torsions



Rings

Ligand CLA L 1502



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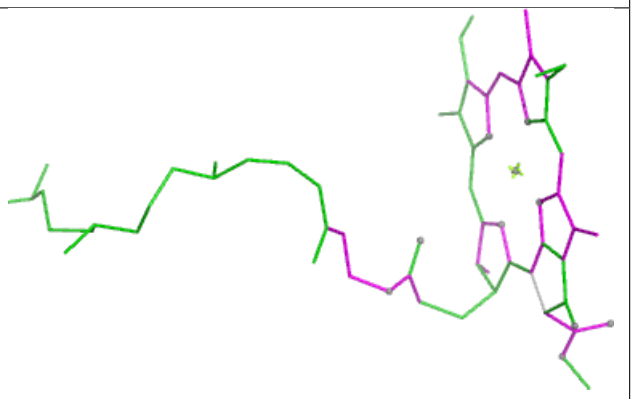
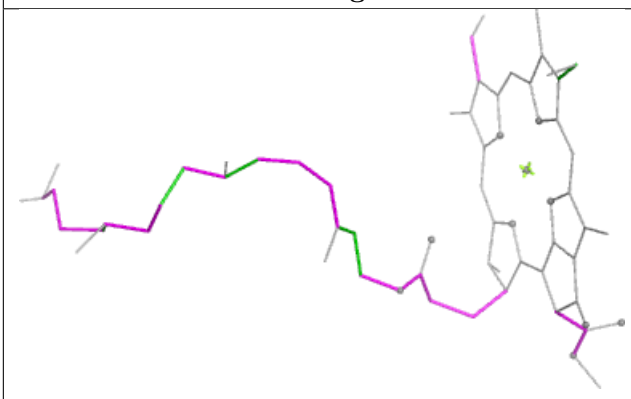


Bond angles



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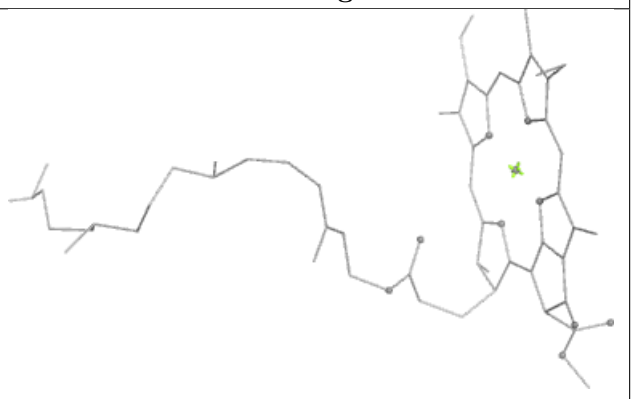
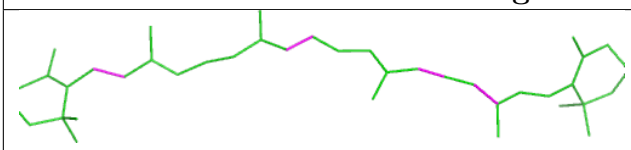


Rings

Ligand BCR K 4001



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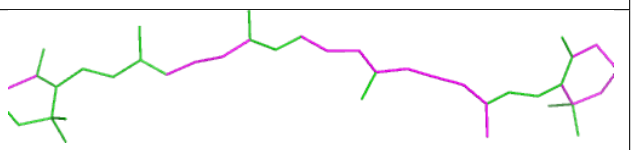
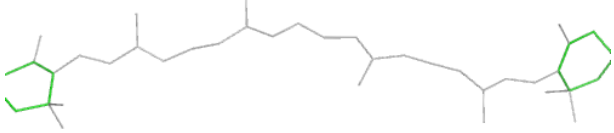


Bond angles

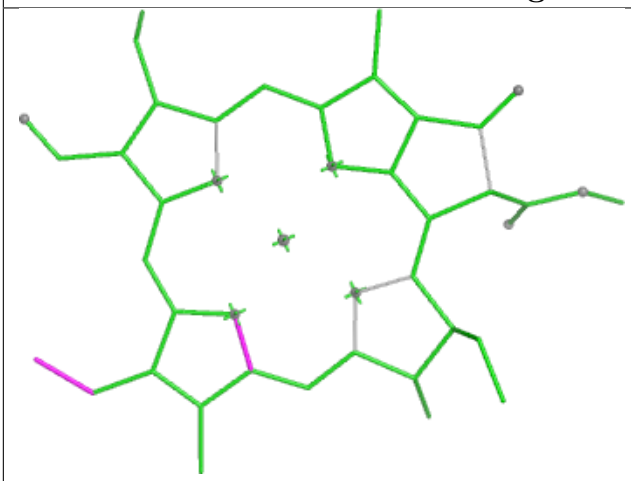


Torsions



Rings

Ligand CHL 4 617



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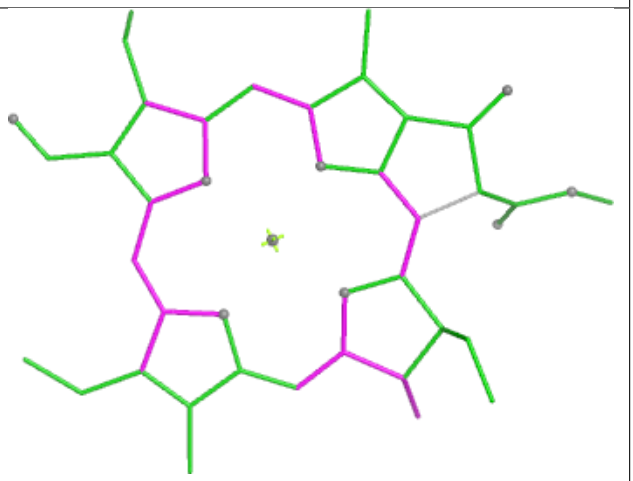
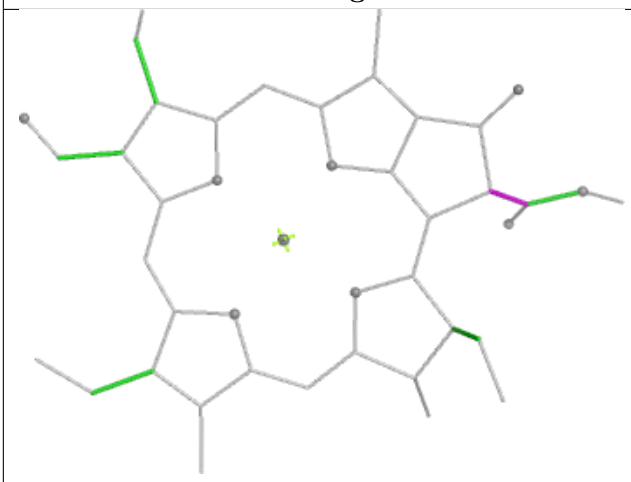


Bond angles



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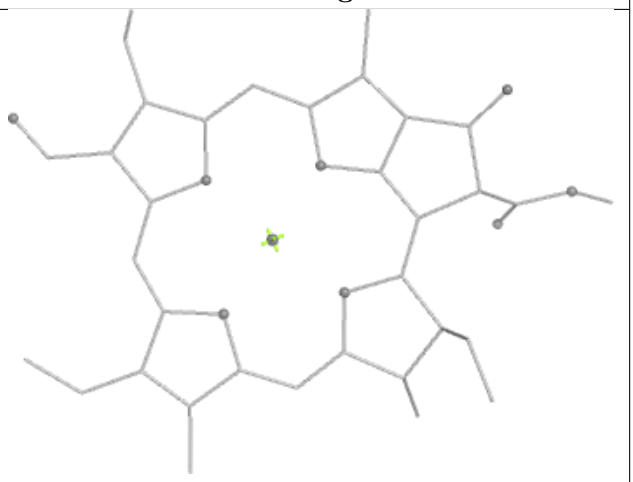
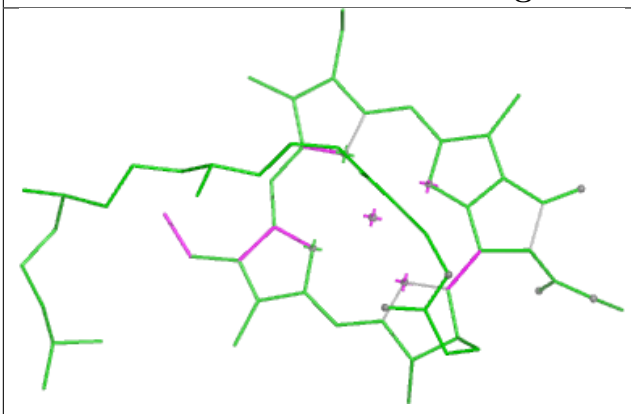
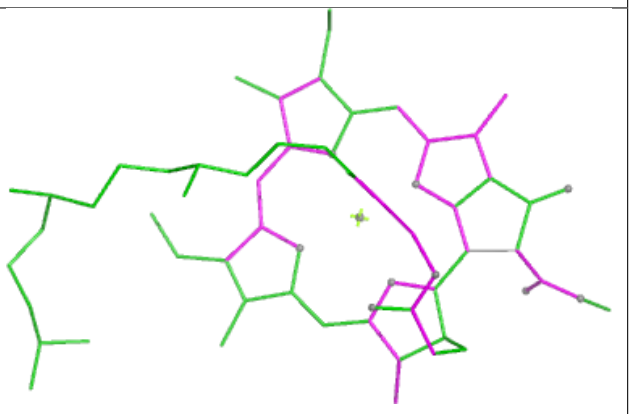


Rings

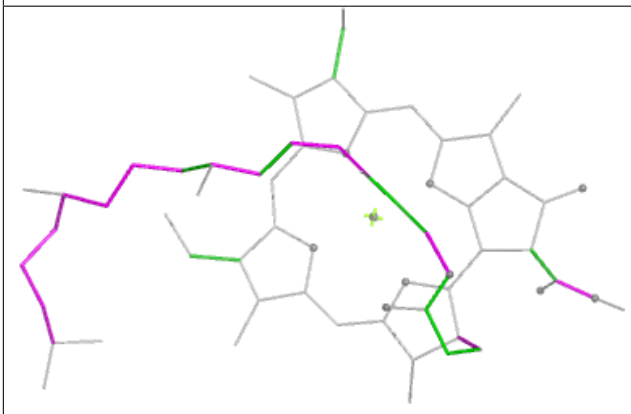
Ligand CLA A 1110



Bond lengths



Bond angles



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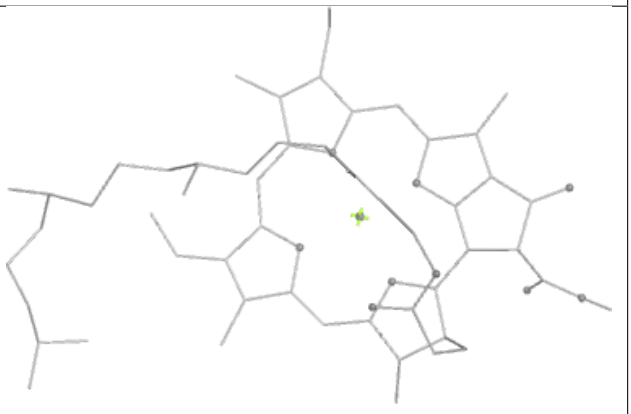
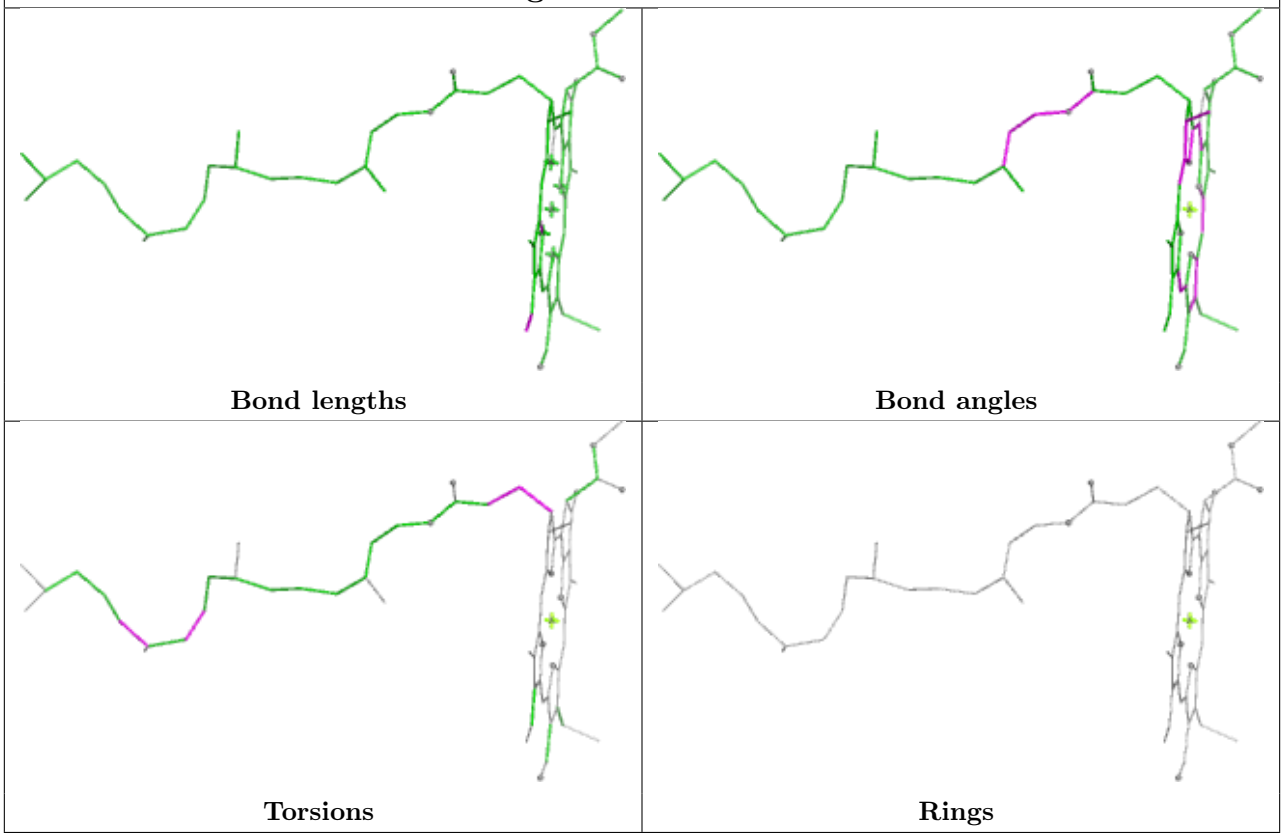
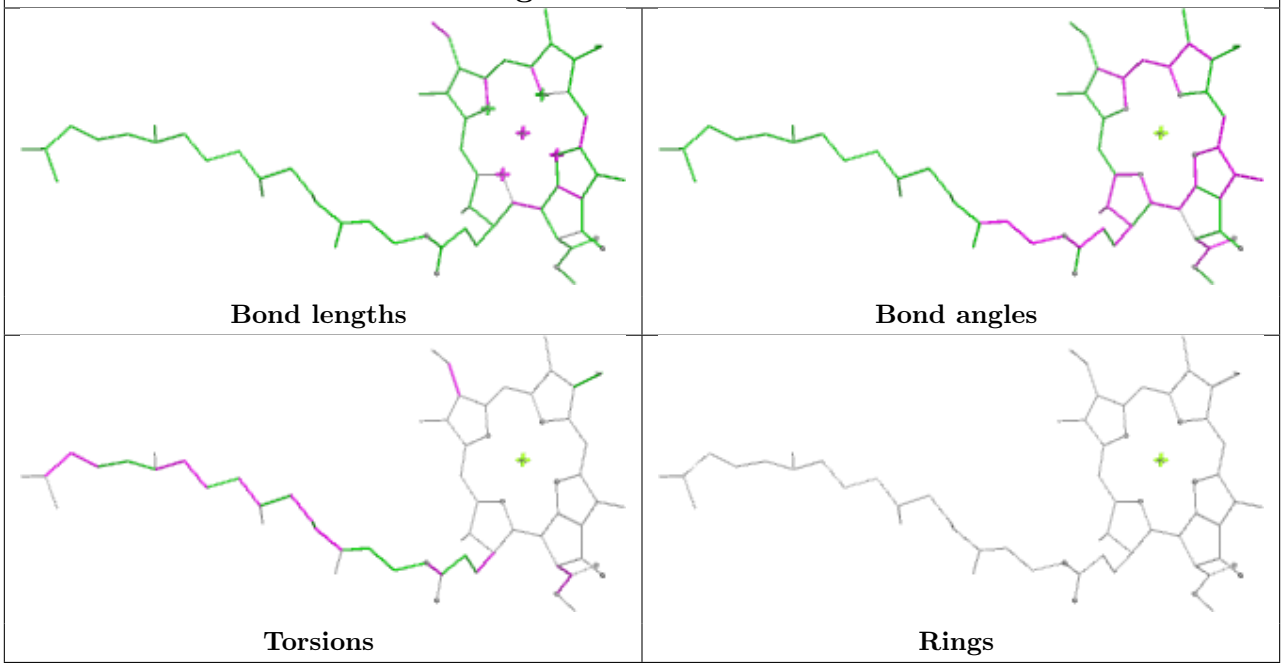


Rings

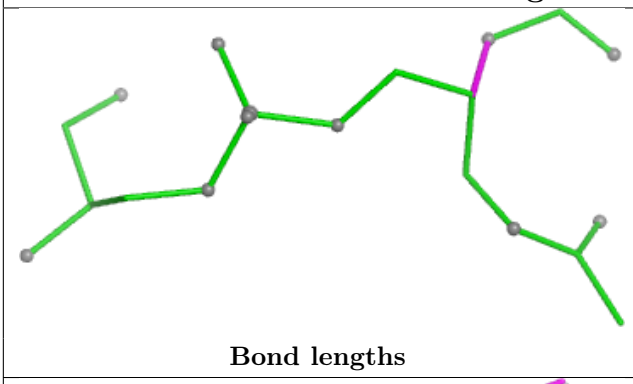
Ligand CHL Z 610



Ligand CLA A 1132



Ligand LHG 3 801



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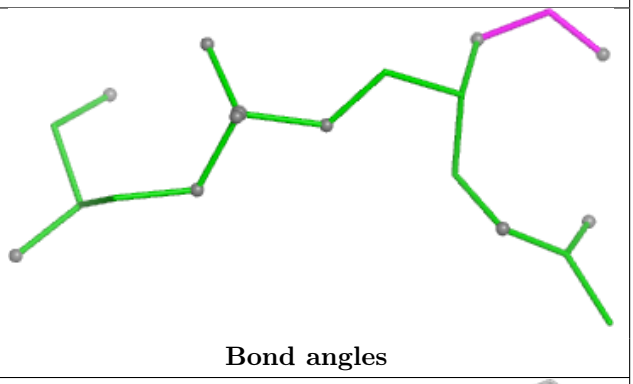
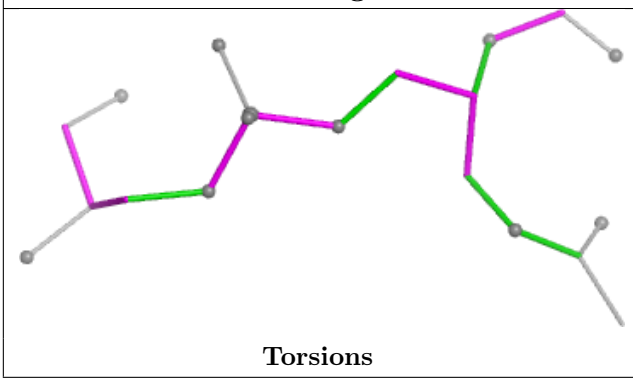


Bond angles



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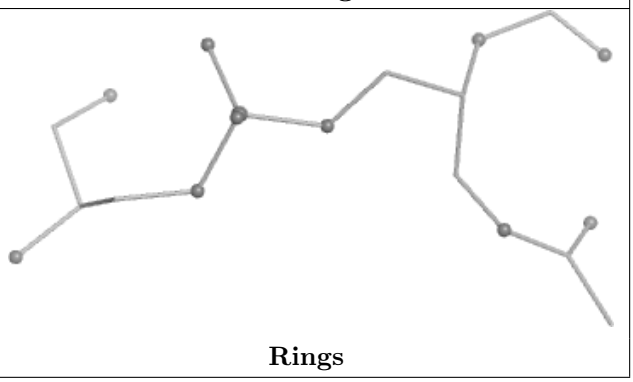
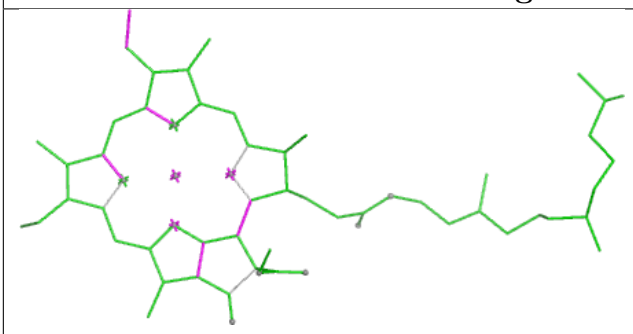


Rings

Ligand CLA B 1234



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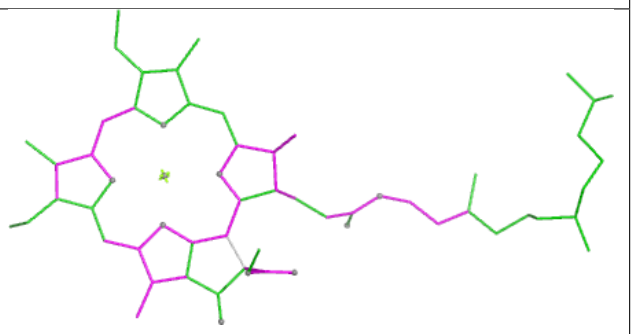
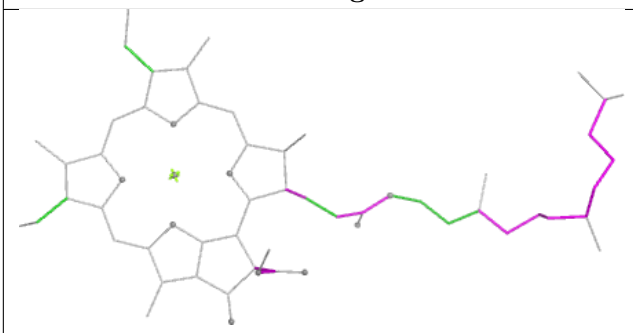
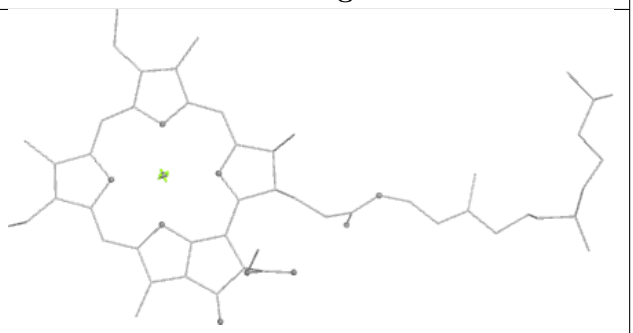


Bond angles

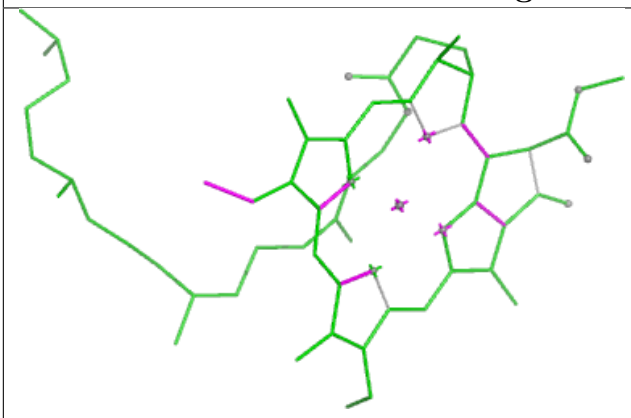


Torsions



Rings

Ligand CLA B 1204



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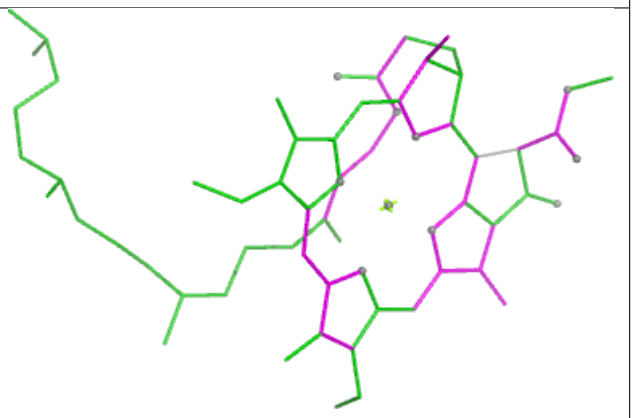

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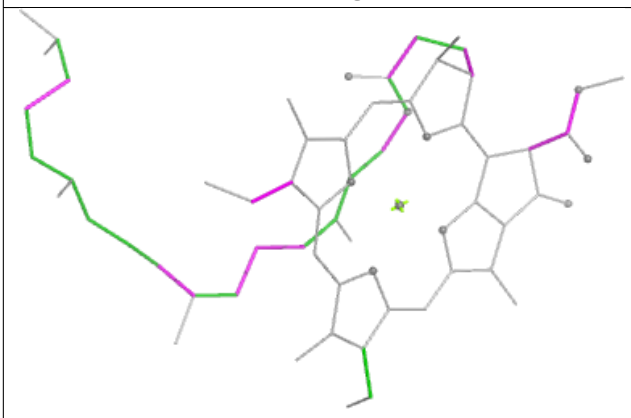
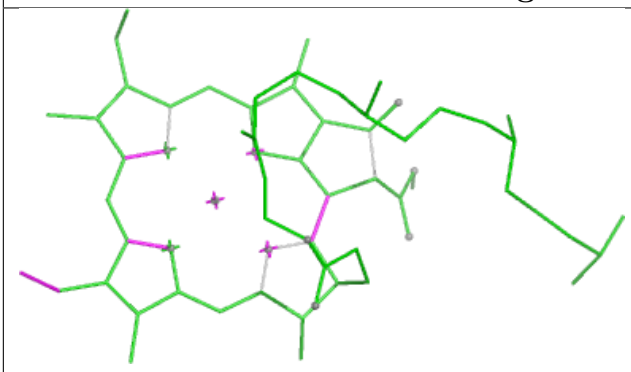


Torsions



Rings

Ligand CLA F 1301



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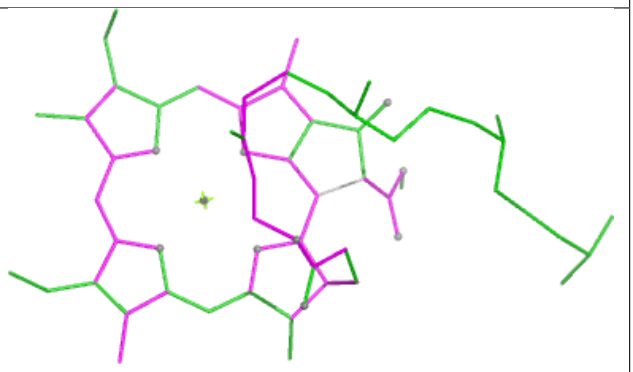

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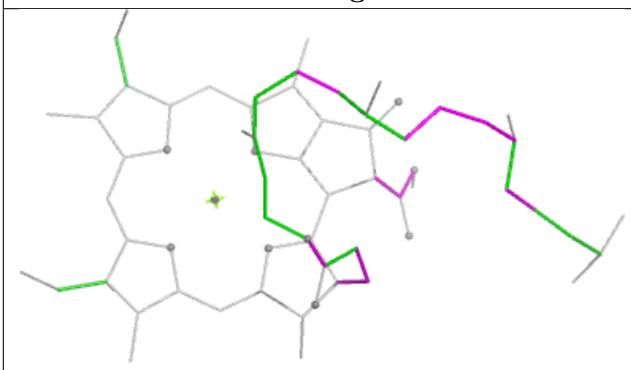

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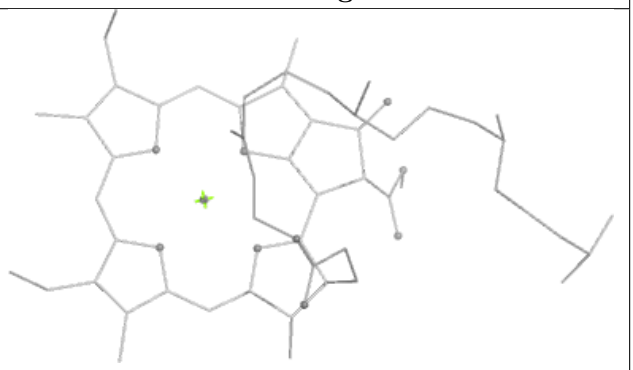
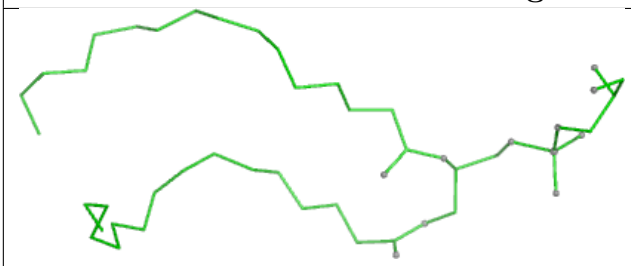


Rings

Ligand LHG 4 801



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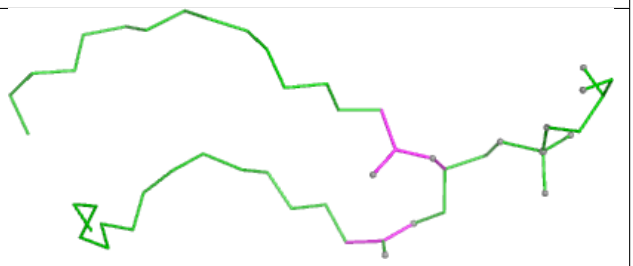

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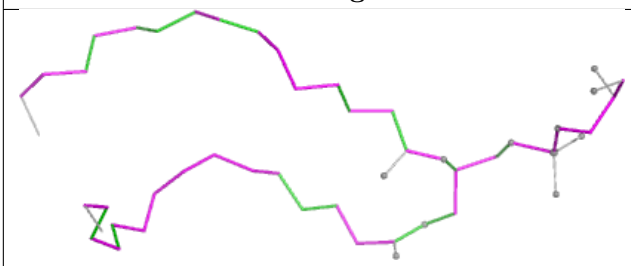
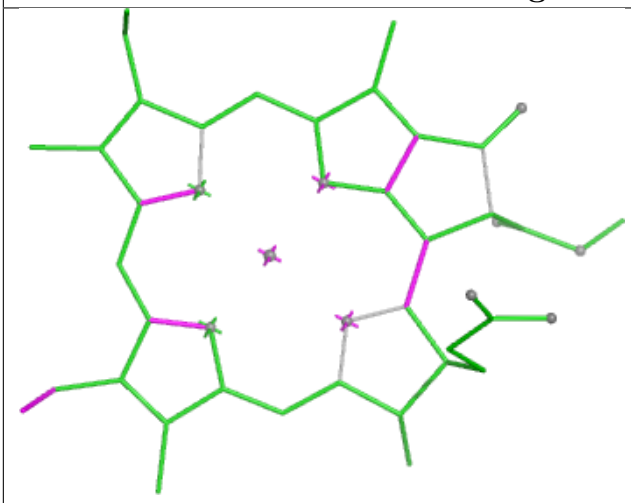


Torsions



Rings

Ligand CLA 5 608



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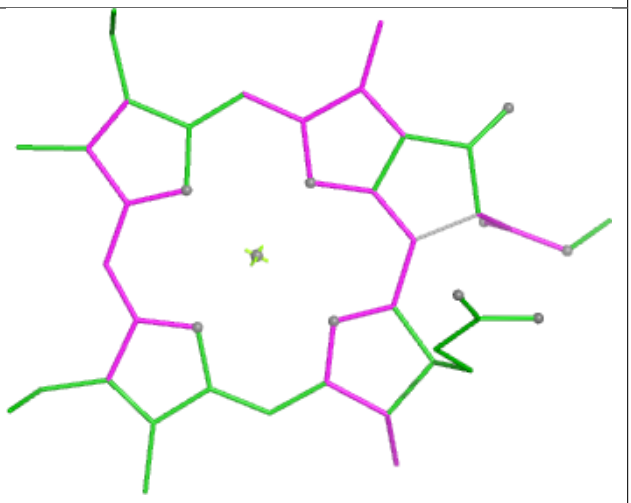

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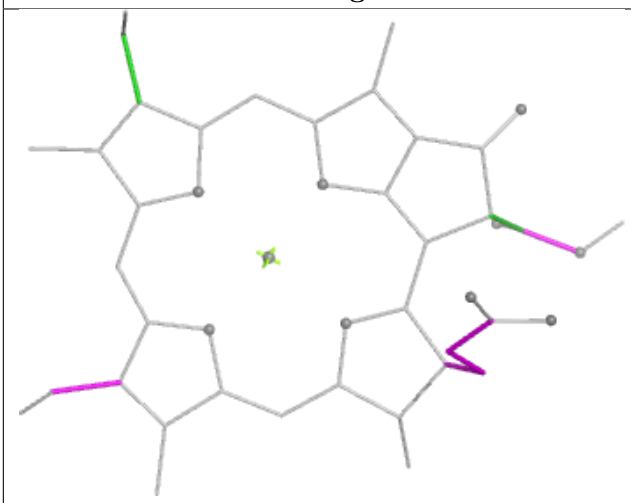

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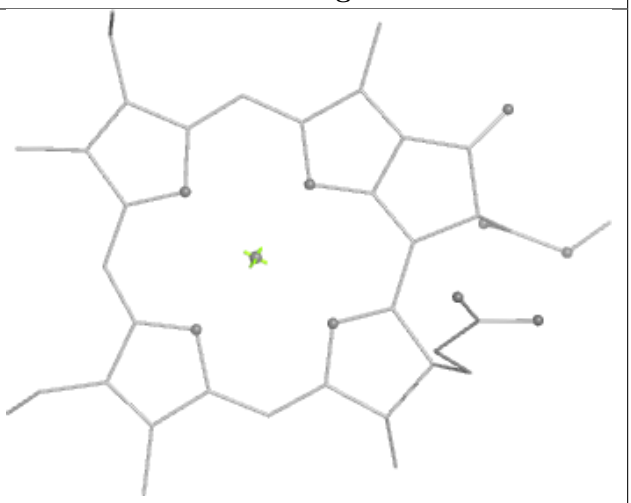
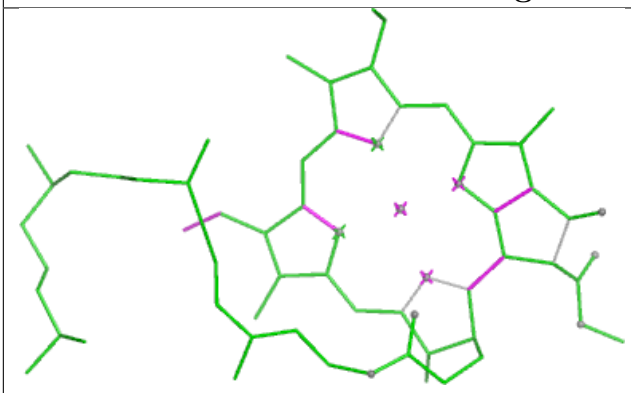


Rings

Ligand CLA A 1117



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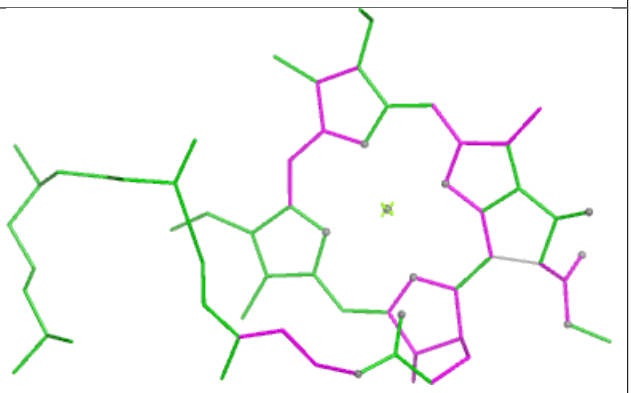

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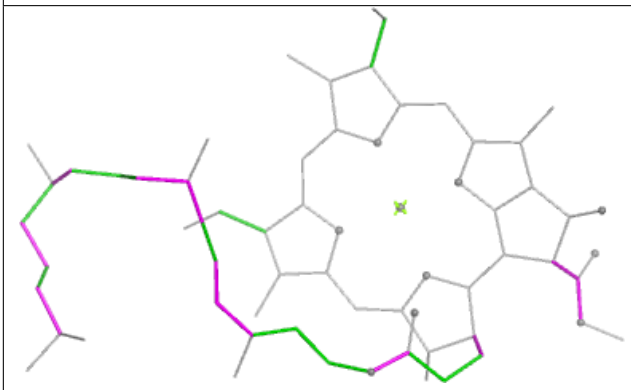

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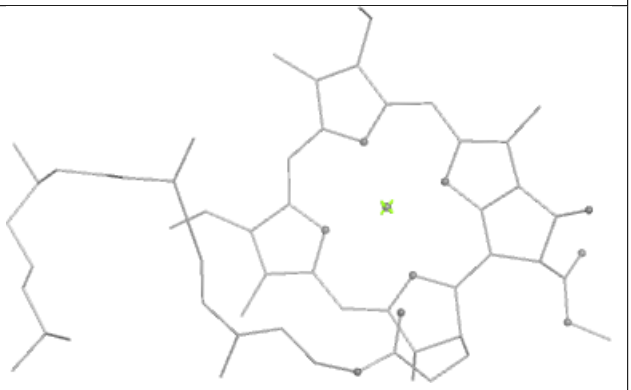
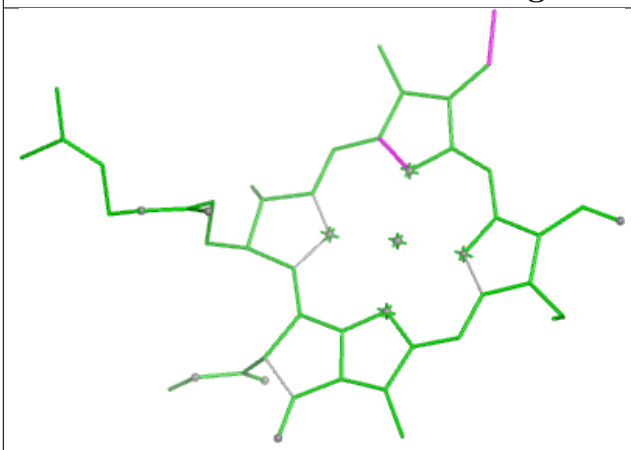


Rings

Ligand CHL 5 611



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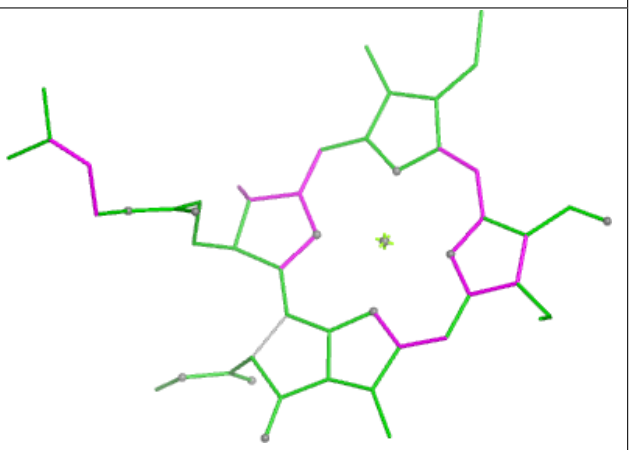

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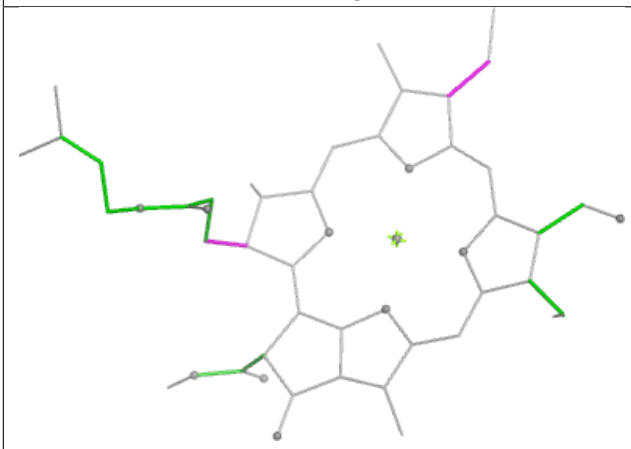
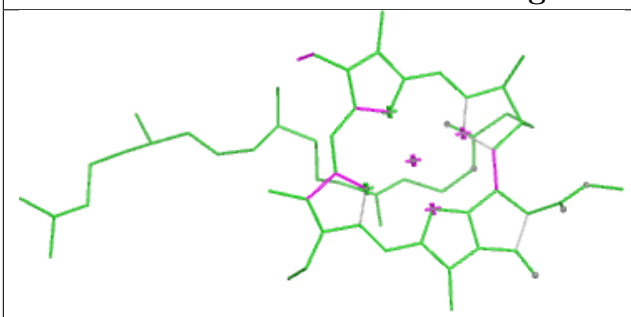


Torsions



Rings

Ligand CLA 3 603



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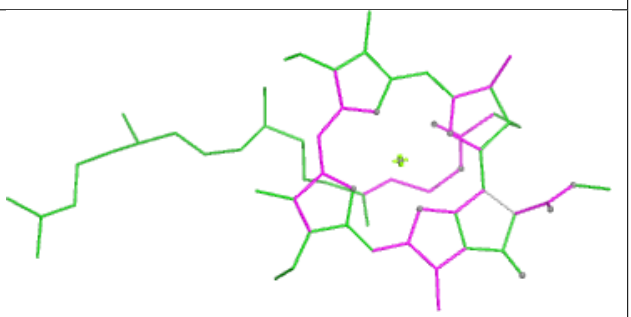

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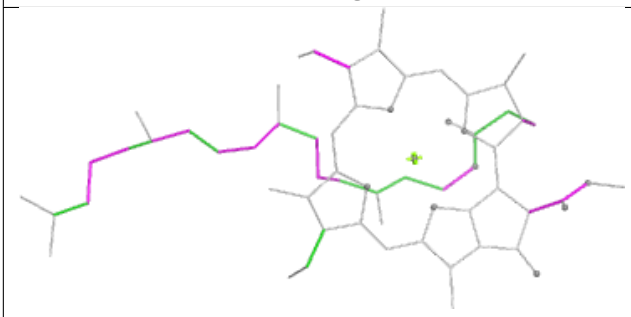

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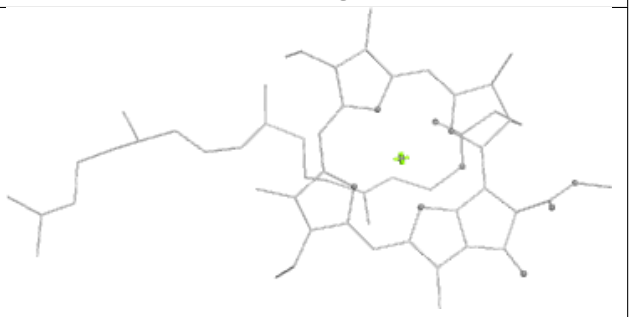
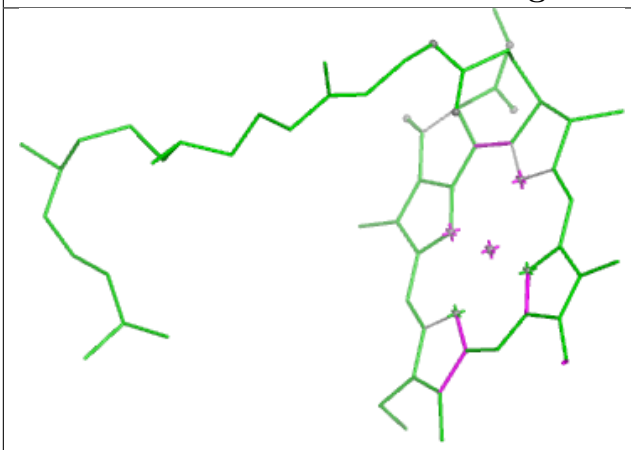


Rings

Ligand CLA 1 612



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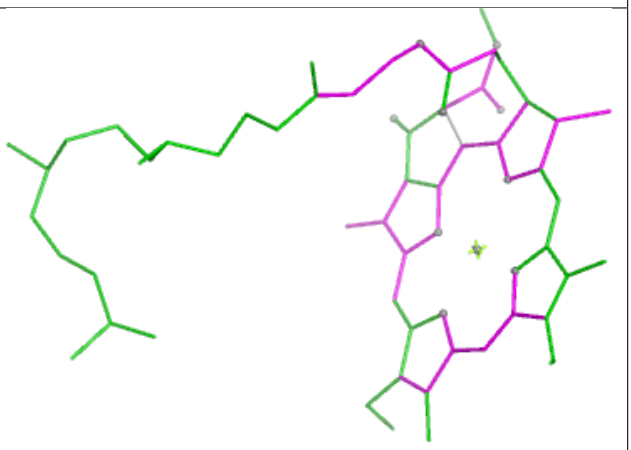

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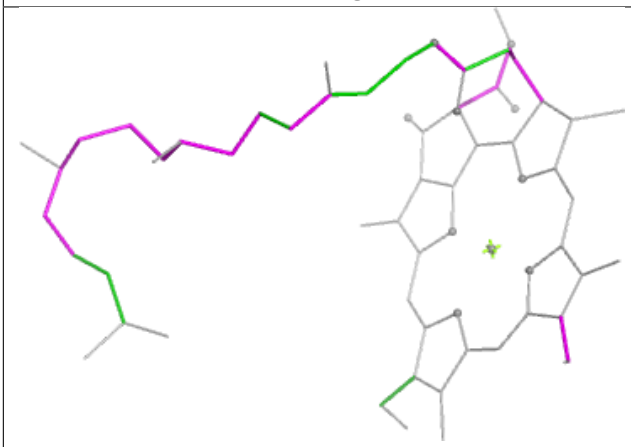
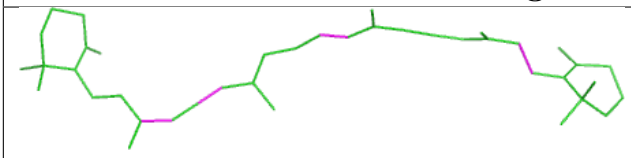


Torsions



Rings

Ligand BCR 7 504



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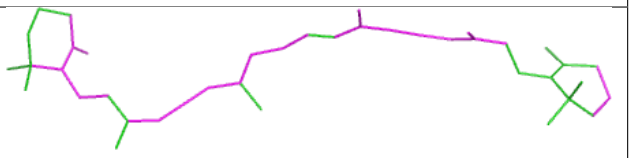

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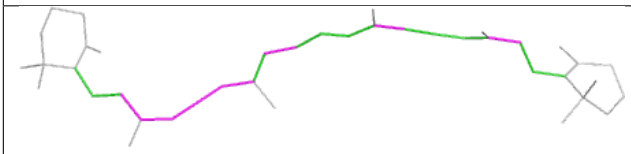

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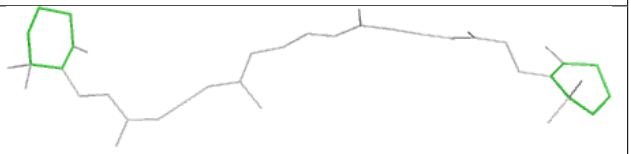
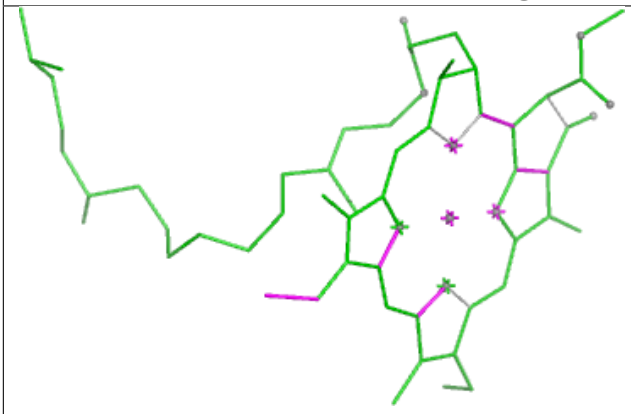


Rings

Ligand CLA B 1237



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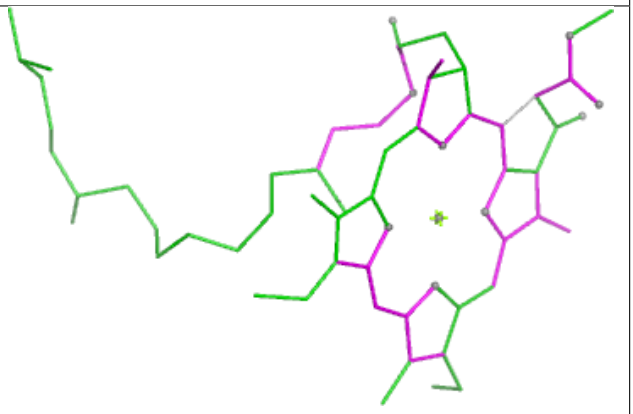

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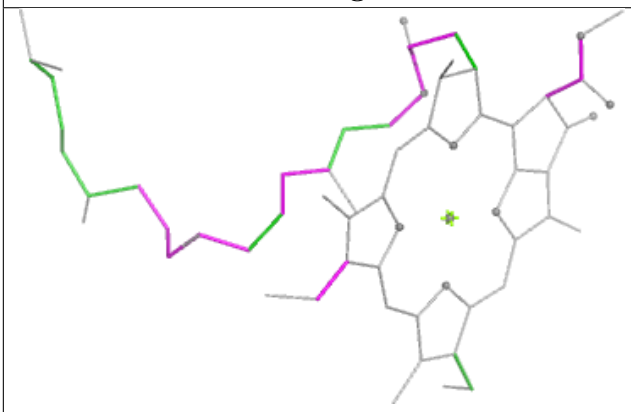

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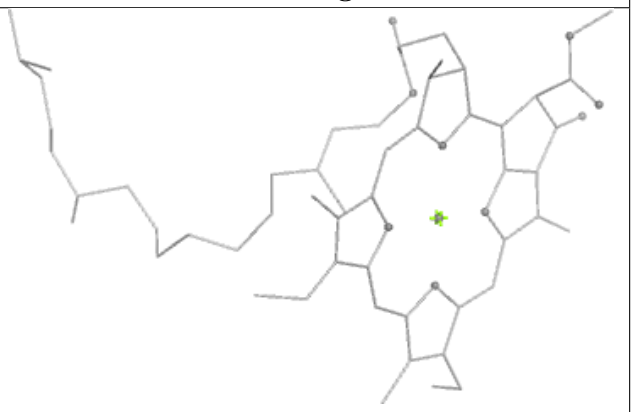
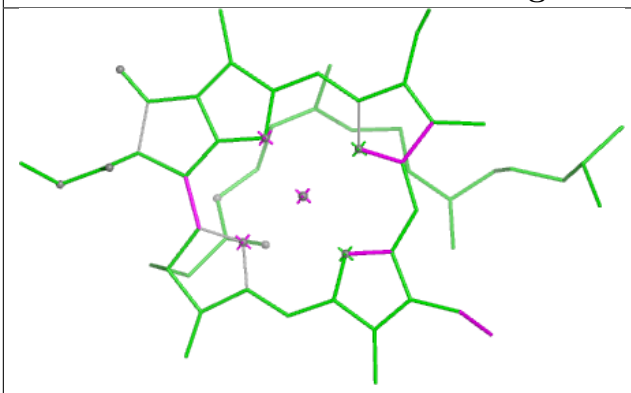


Rings

Ligand CLA 7 616



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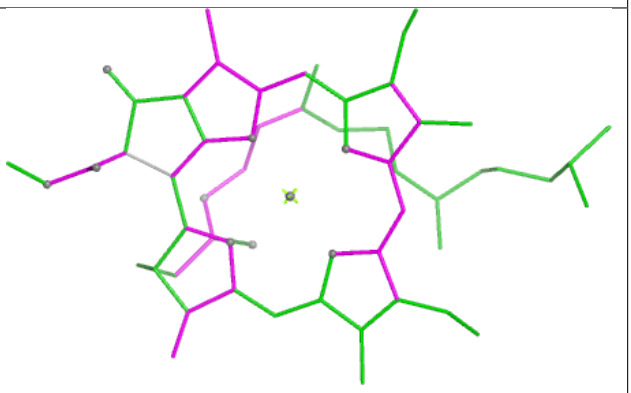

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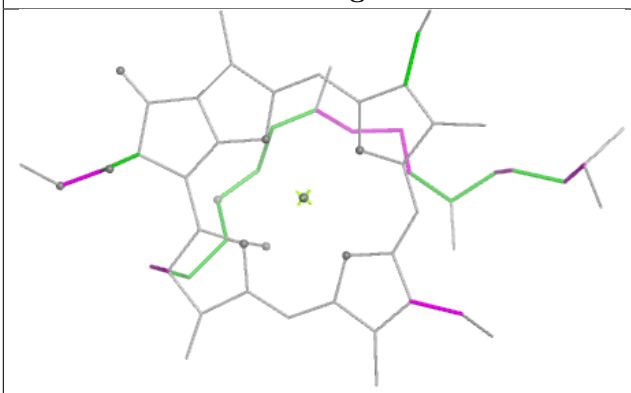

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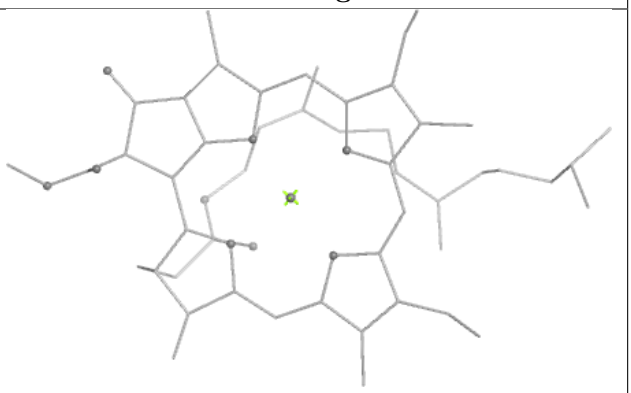
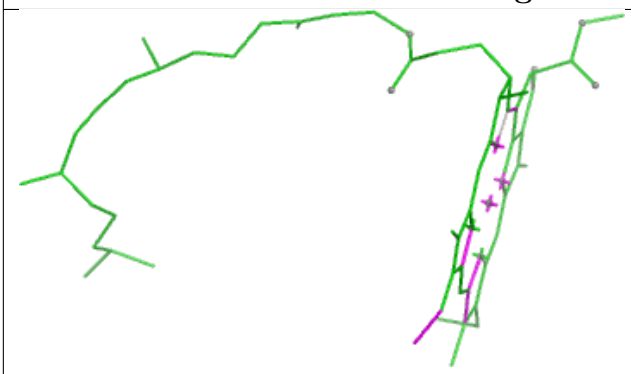


Rings

Ligand CLA A 1105



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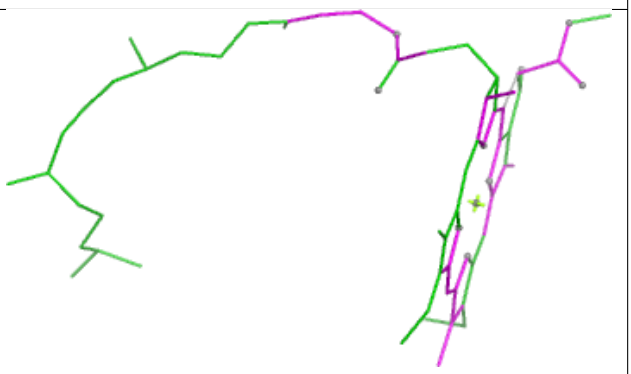

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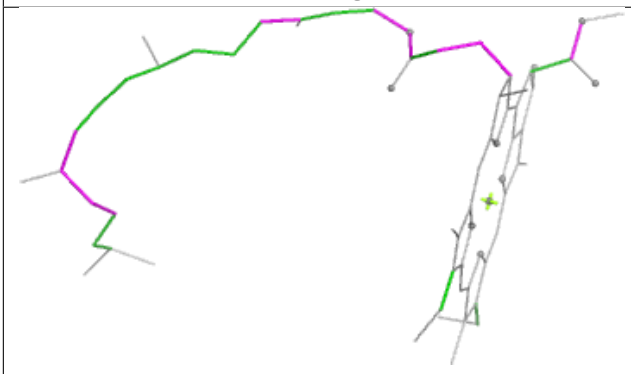
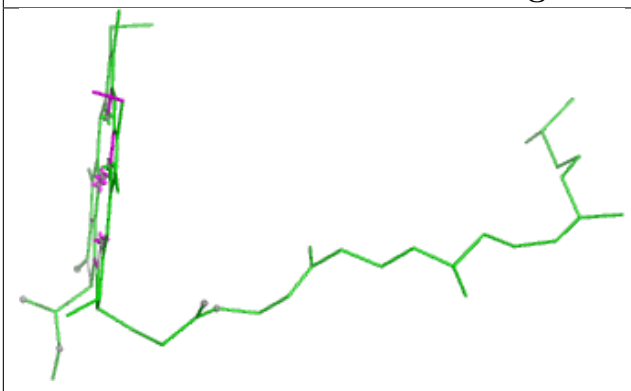


Torsions



Rings

Ligand CLA 3 606



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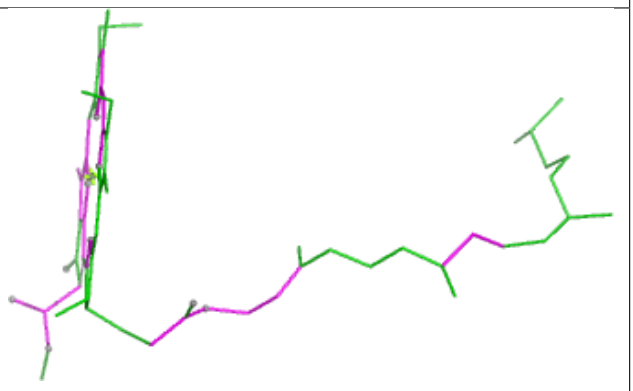
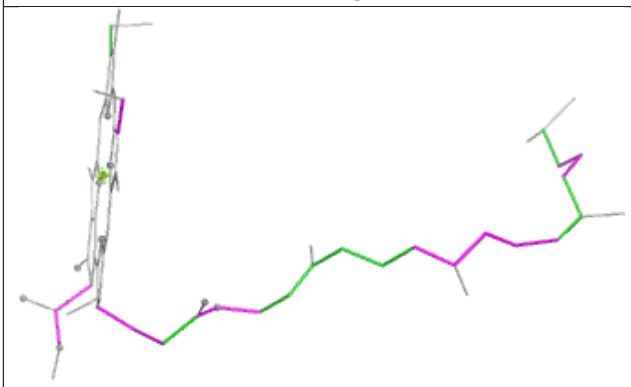


Bond angles



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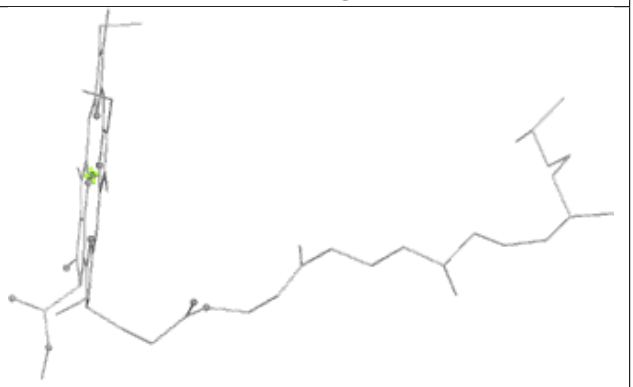
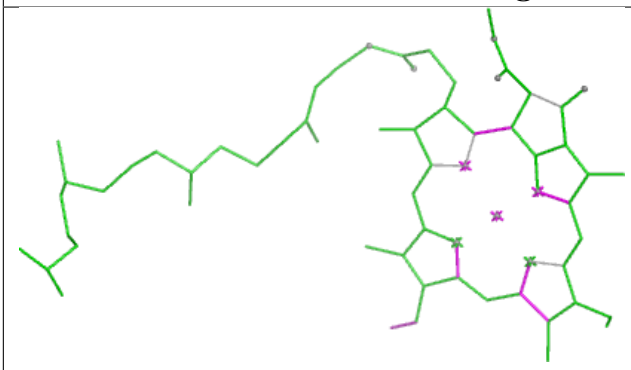


Rings

Ligand CLA A 1013



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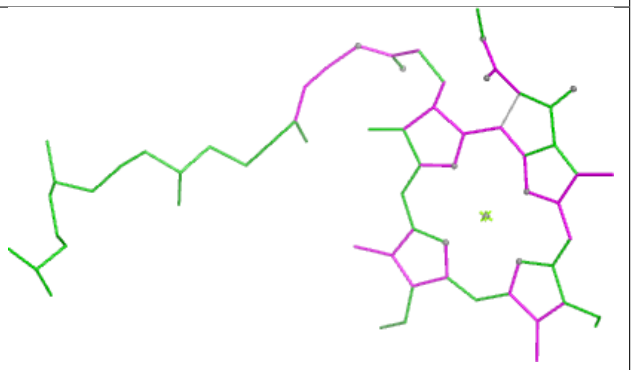
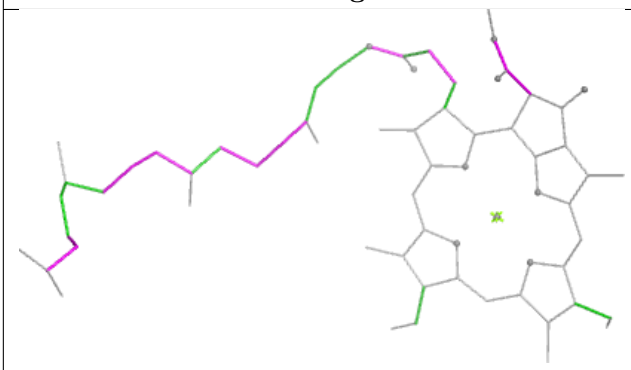


Bond angles



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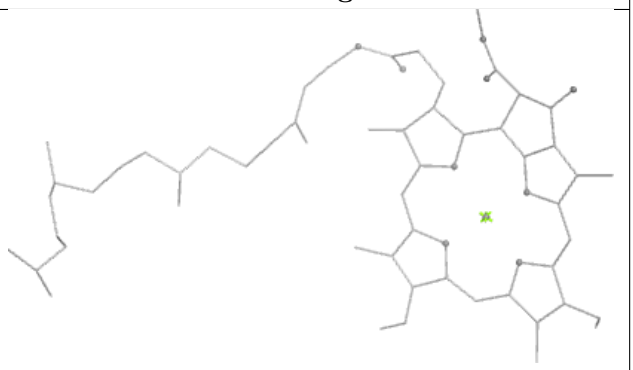
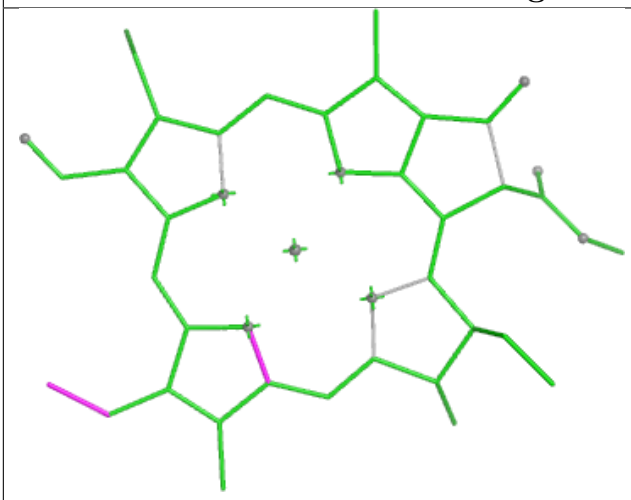


Rings

Ligand CHL 6 617



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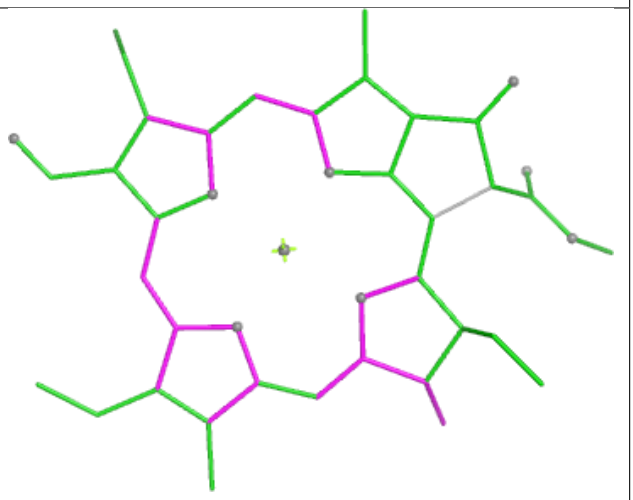
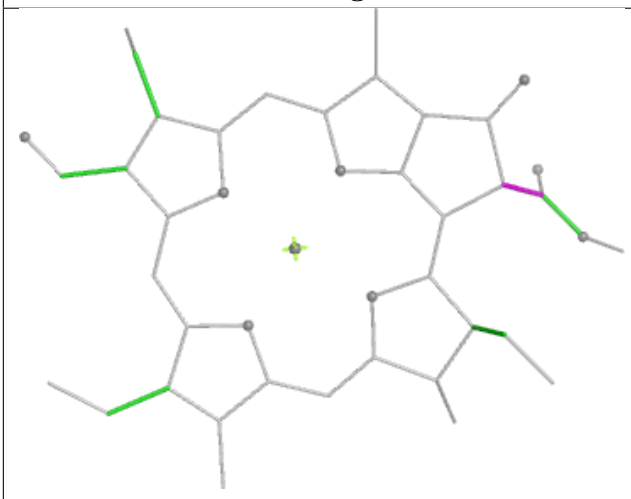


Bond angles



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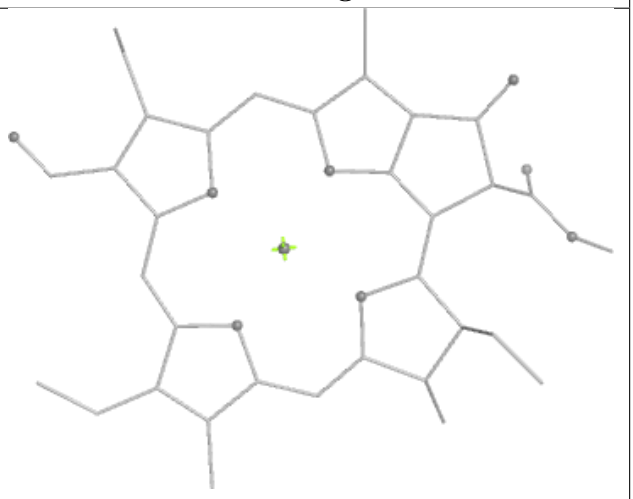
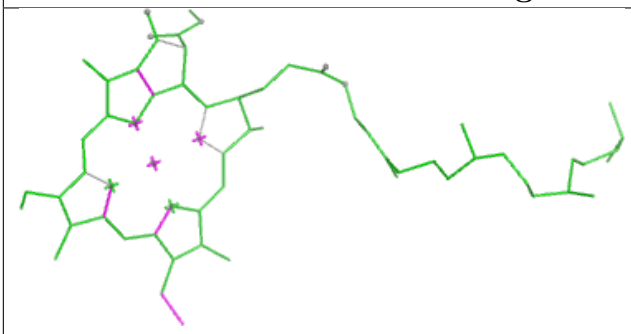
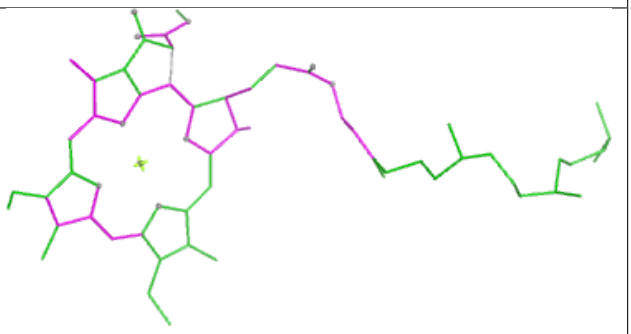


Rings

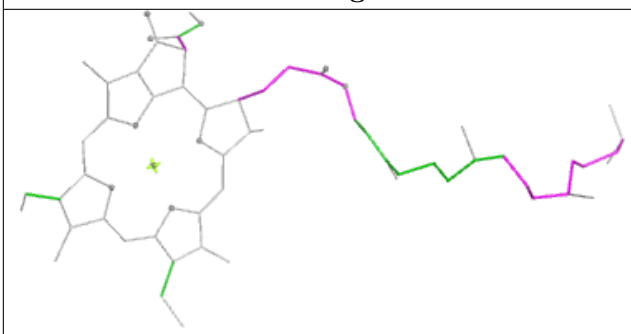
Ligand CLA B 1210



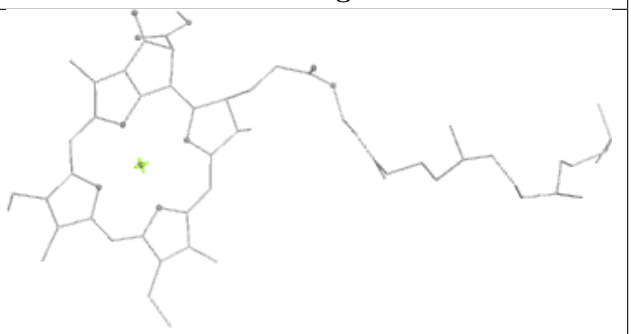
Bond lengths



Bond angles

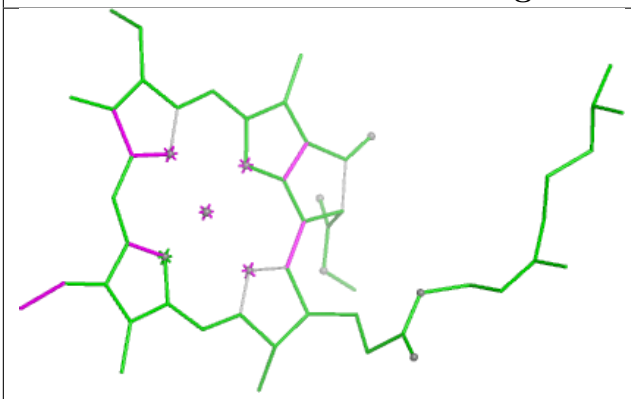


Torsions



Rings

Ligand CLA K 1402



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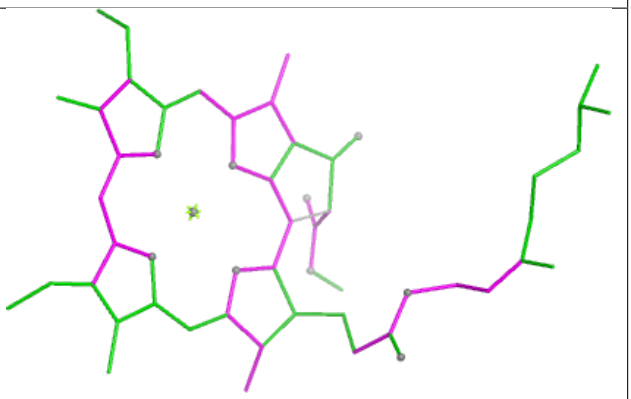

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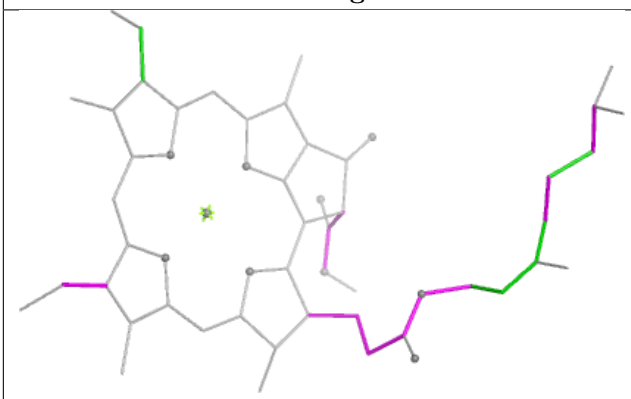

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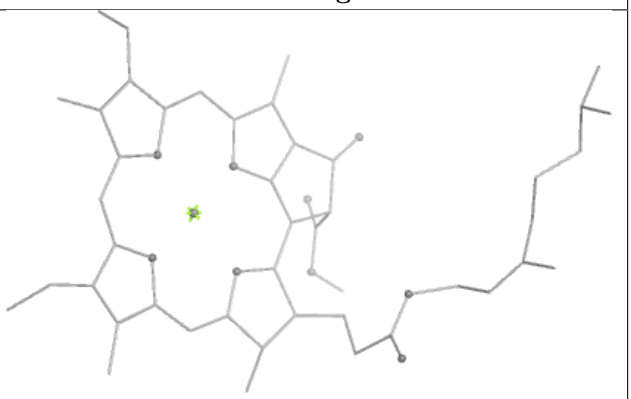
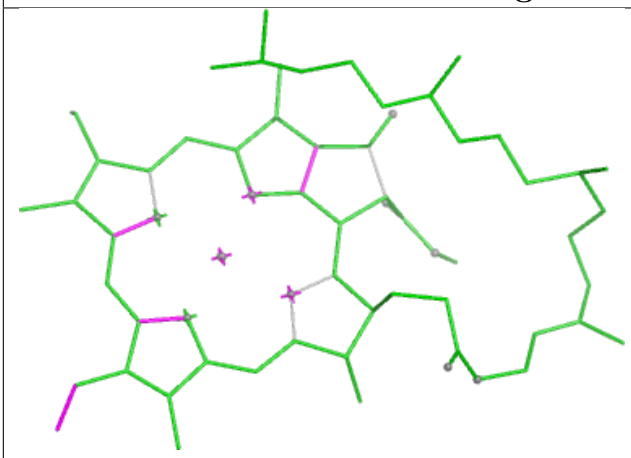


Rings

Ligand CLA B 1202



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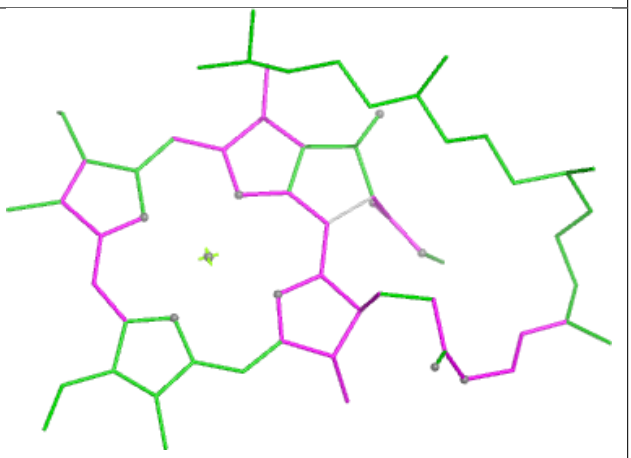
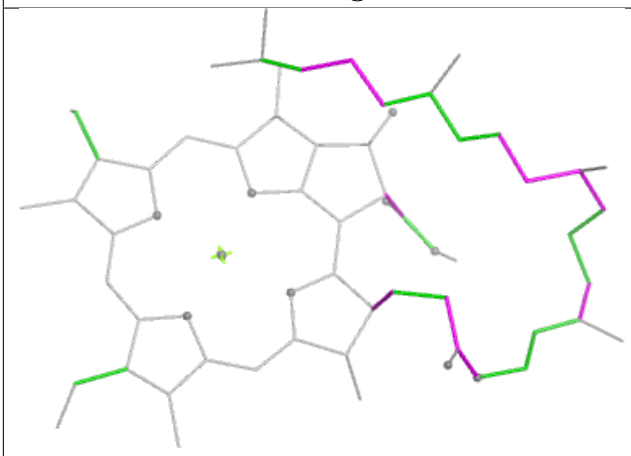


Bond angles



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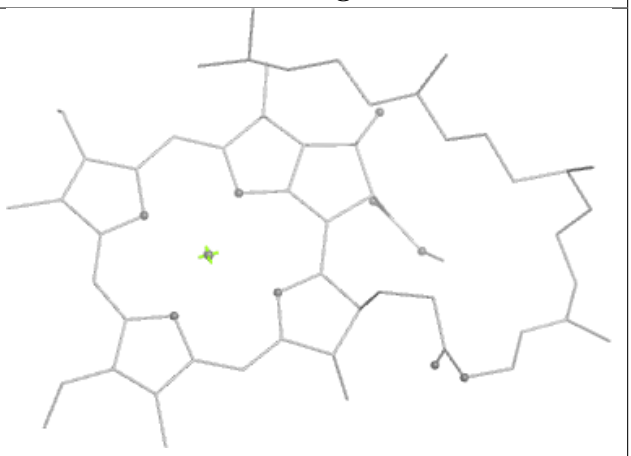
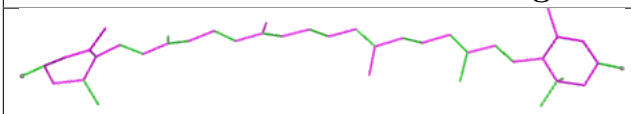


Rings

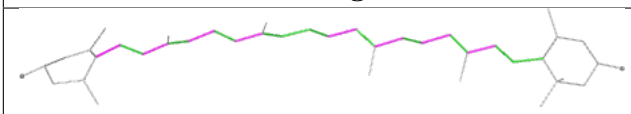
Ligand C7Z 5 505



Bond lengths



Bond angles



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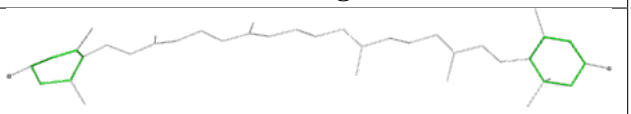
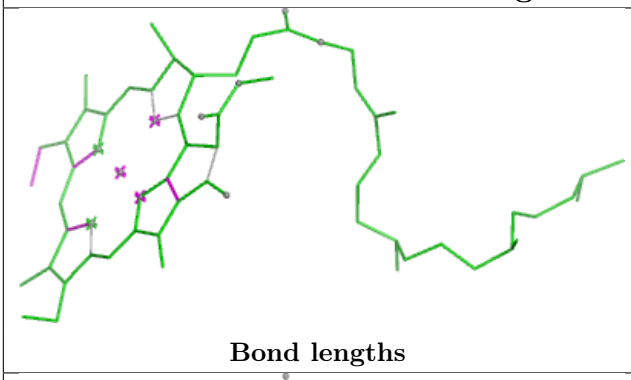
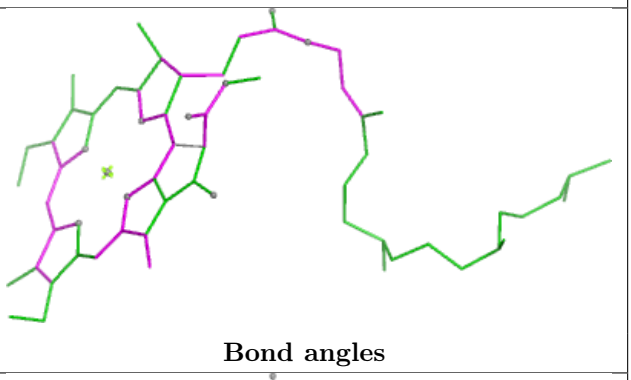


Rings

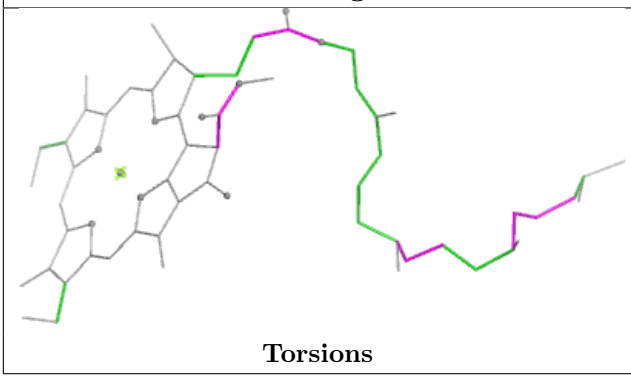
Ligand CLA B 1021



Bond lengths



Bond angles



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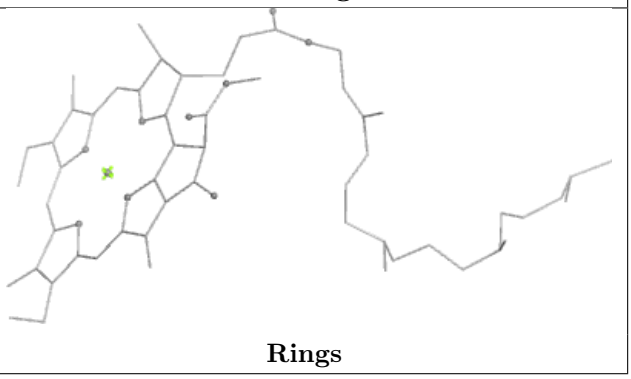


Rings

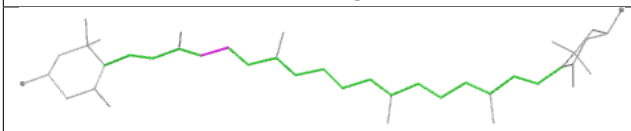
Ligand LUT Z 502



Bond lengths



Bond angles



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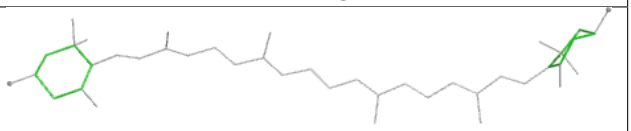
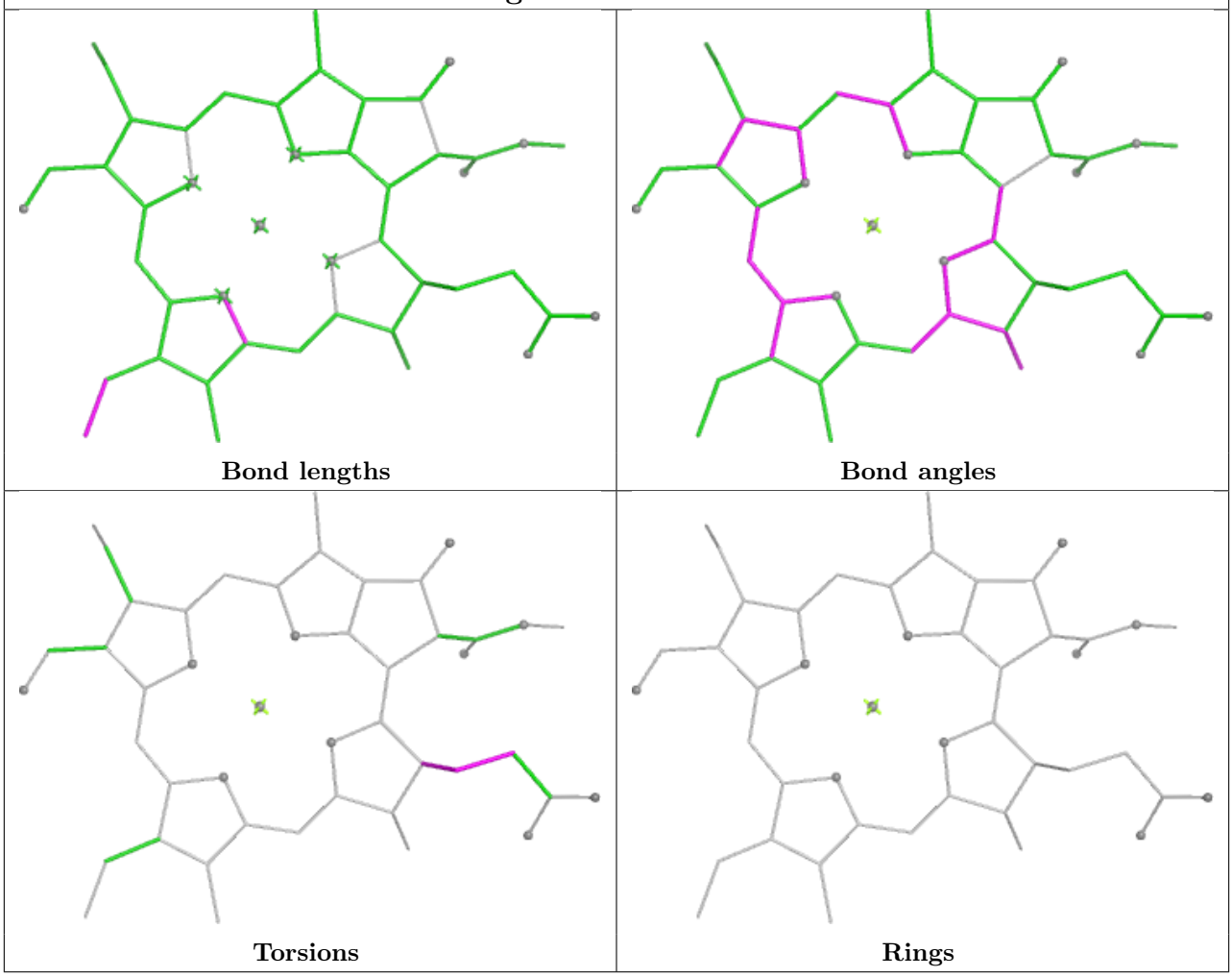


Rings

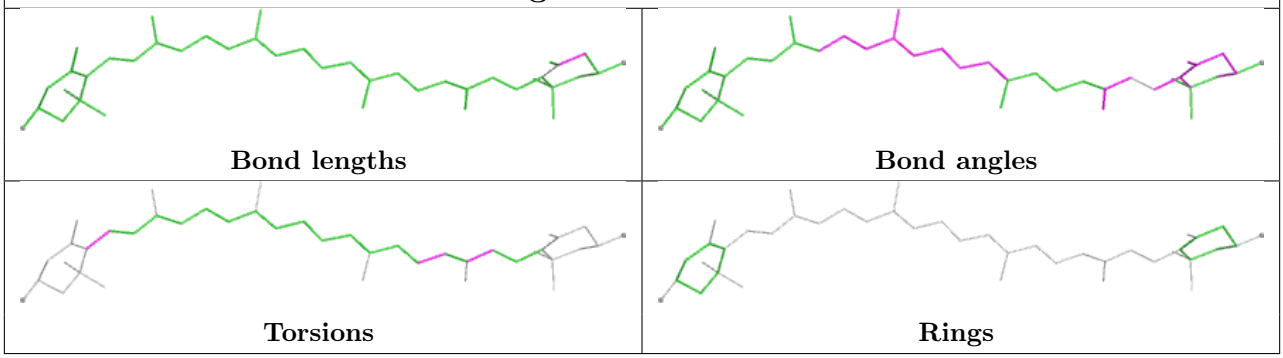
Ligand CHL Z 613



Bond lengths | Bond angles

Torsions | Rings

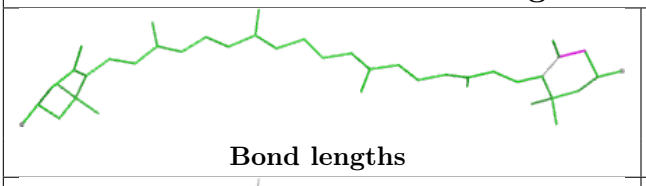
Ligand LUT 1 501



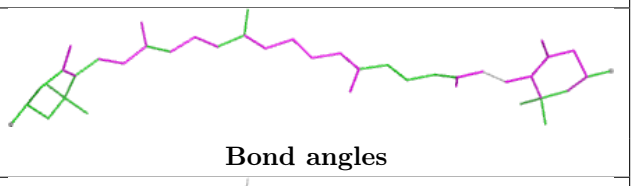
Bond lengths | Bond angles

Torsions | Rings

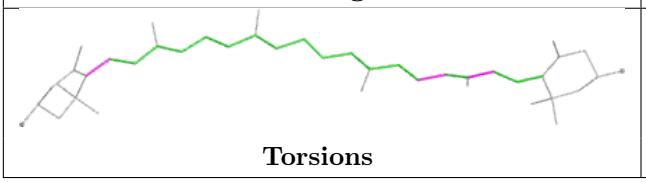
Ligand LUT 4 501



Bond lengths



Bond angles



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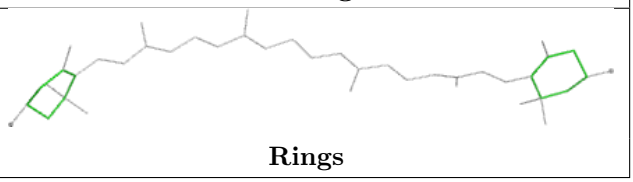
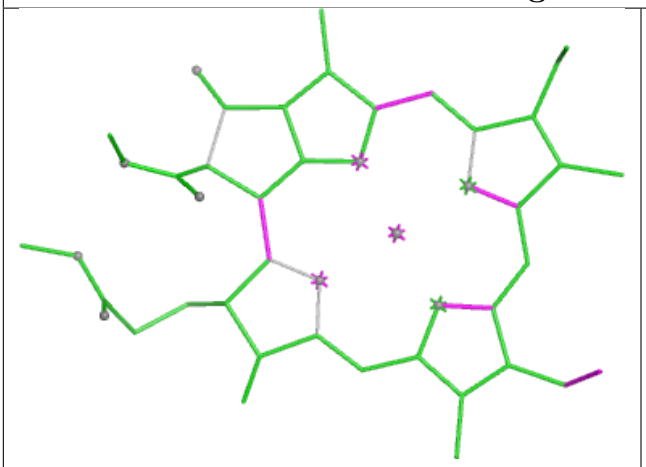
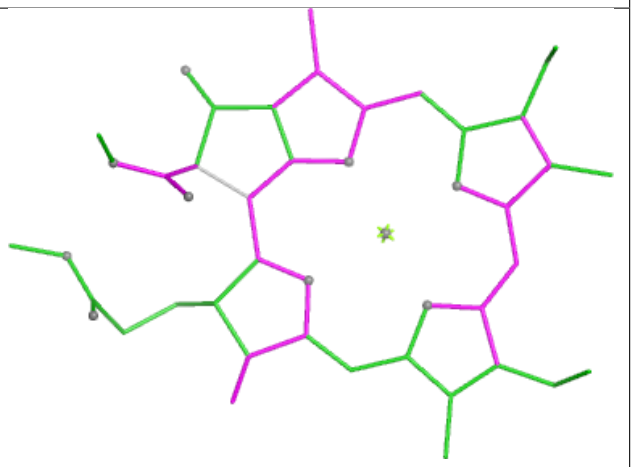


Rings

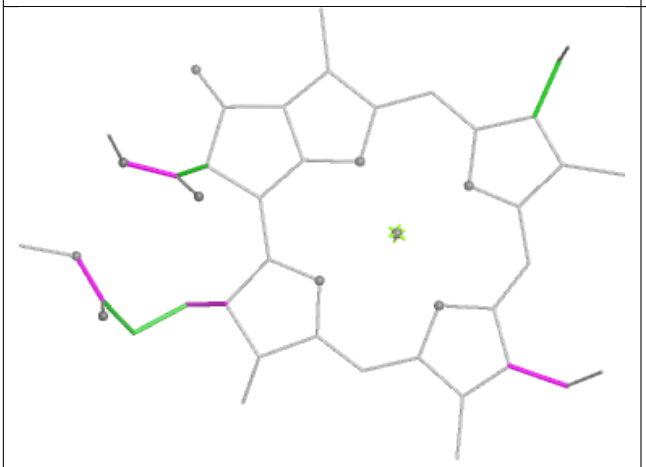
Ligand CLA 5 622



Bond lengths



Bond angles



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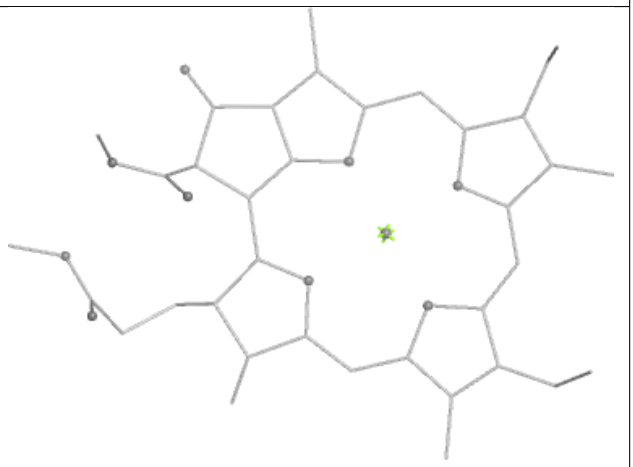
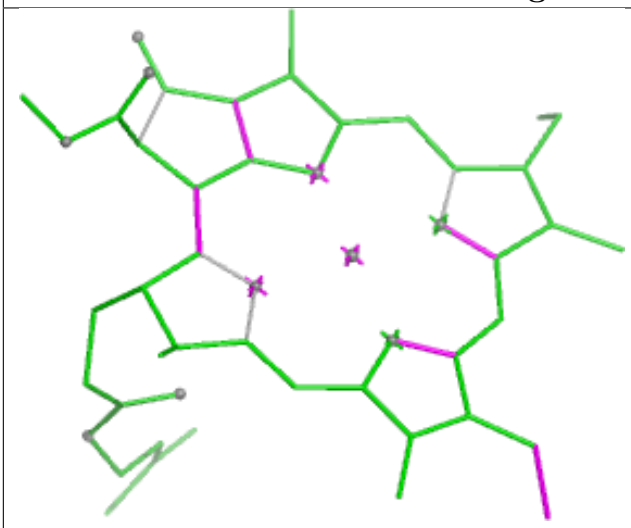


Rings

Ligand CLA 6 612



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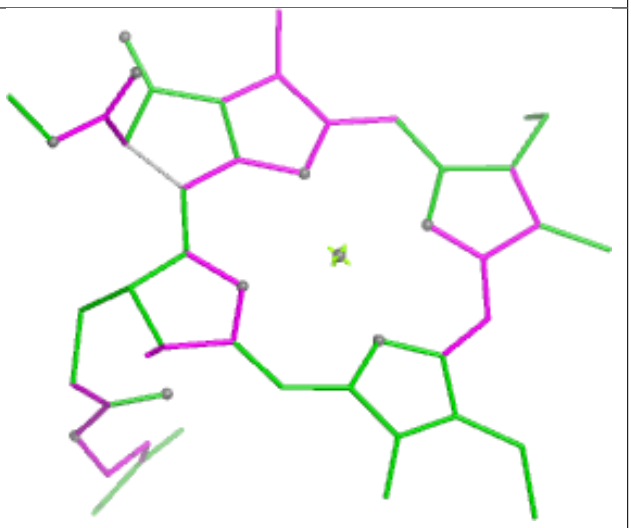
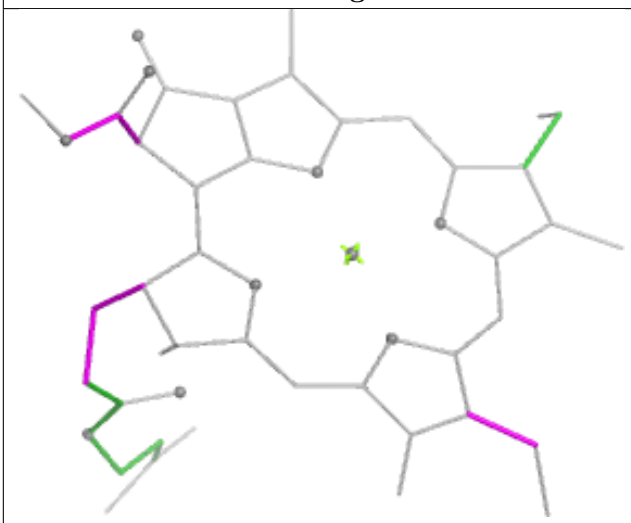


Bond angles



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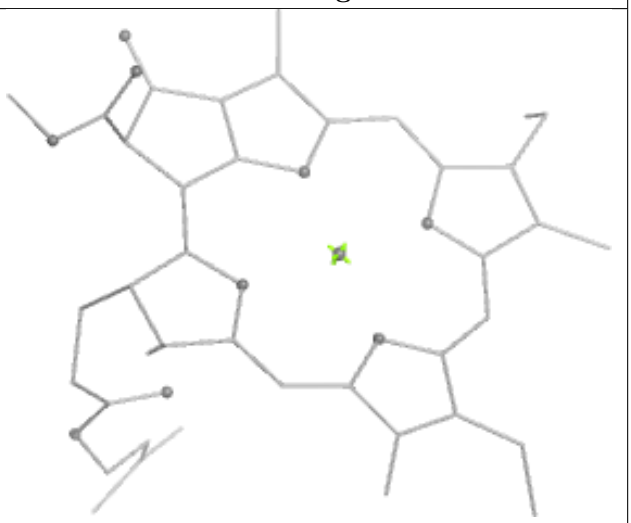
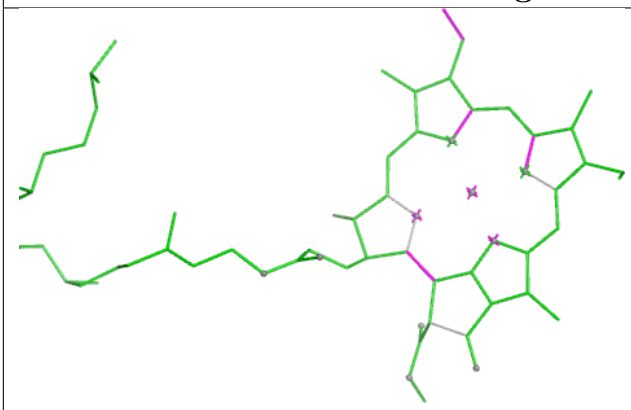
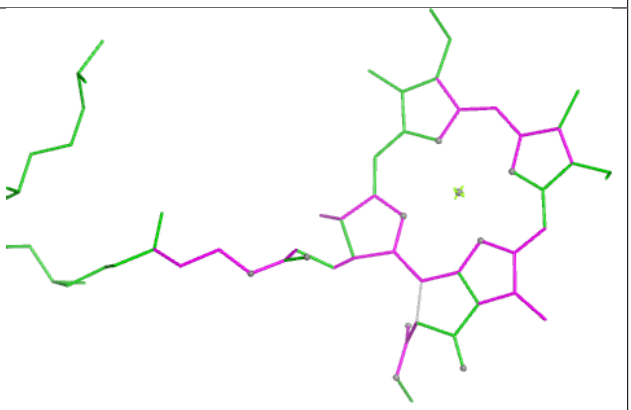


Rings

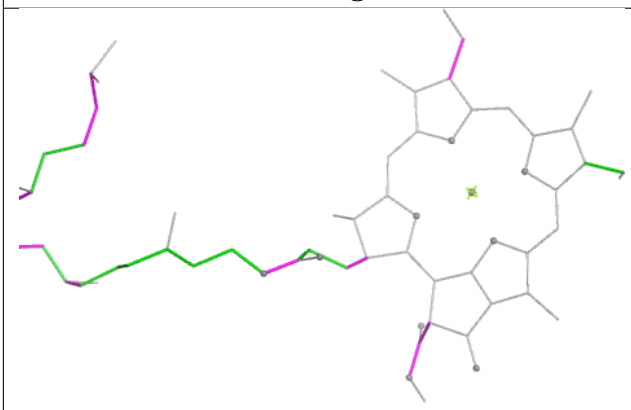
Ligand CLA A 1124



Bond lengths



Bond angles



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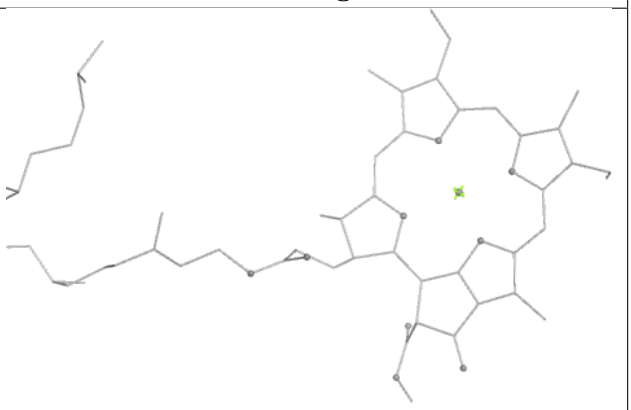
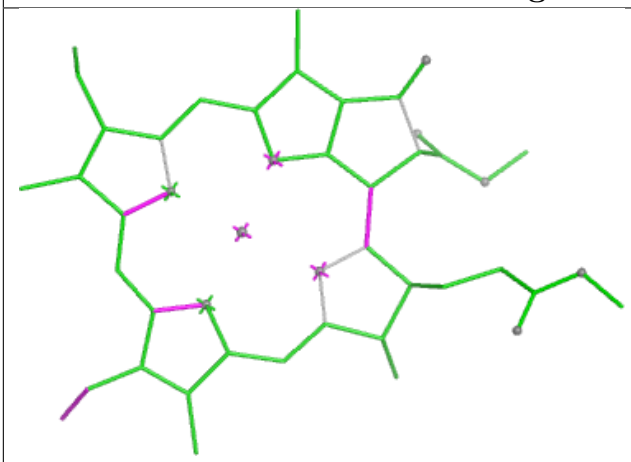


Rings

Ligand CLA 6 618



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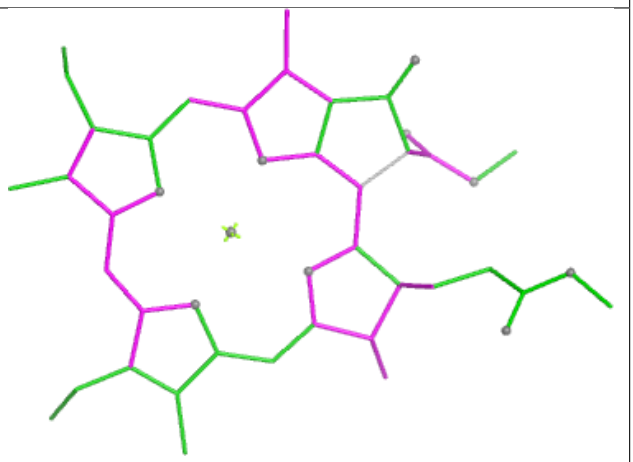
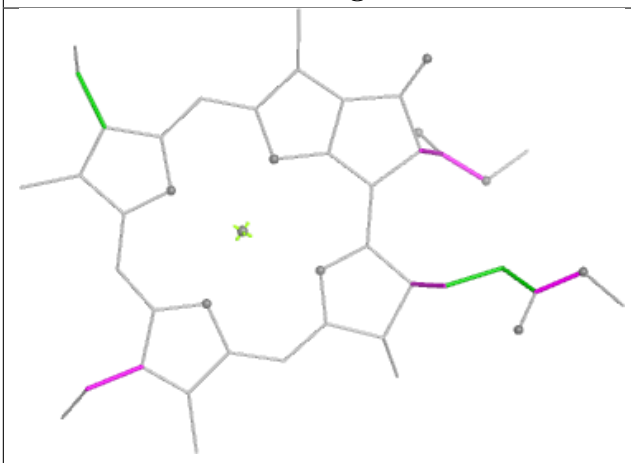


Bond angles



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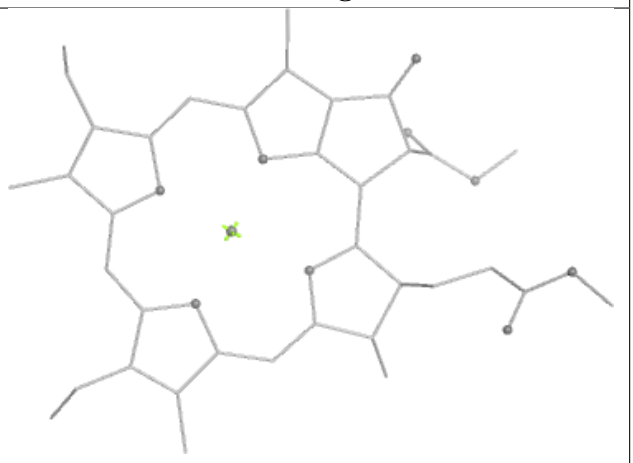
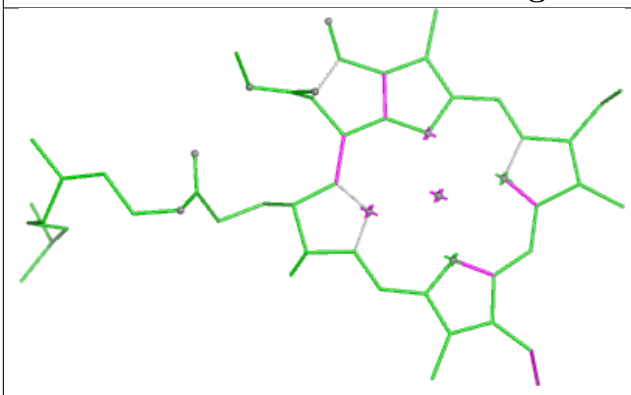


Rings

Ligand CLA 3 613



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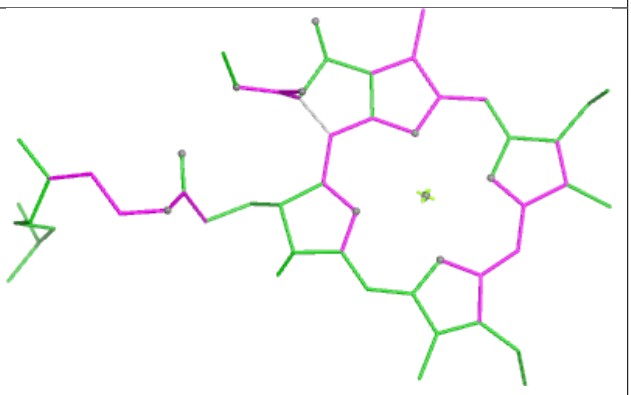
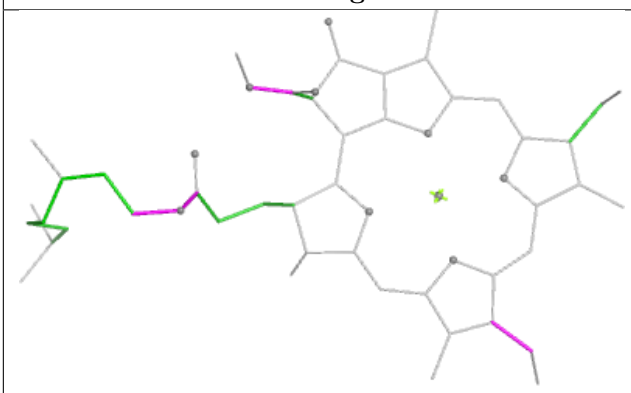


Bond angles



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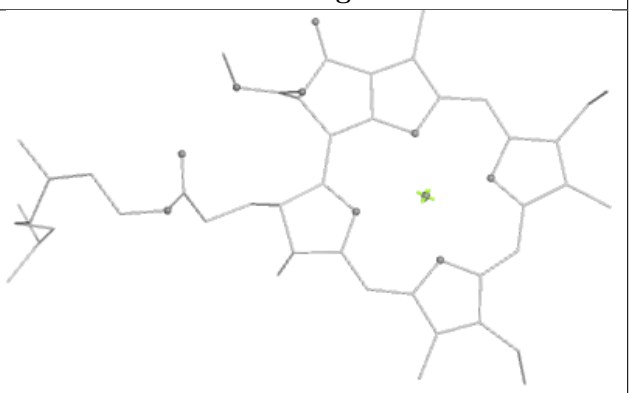
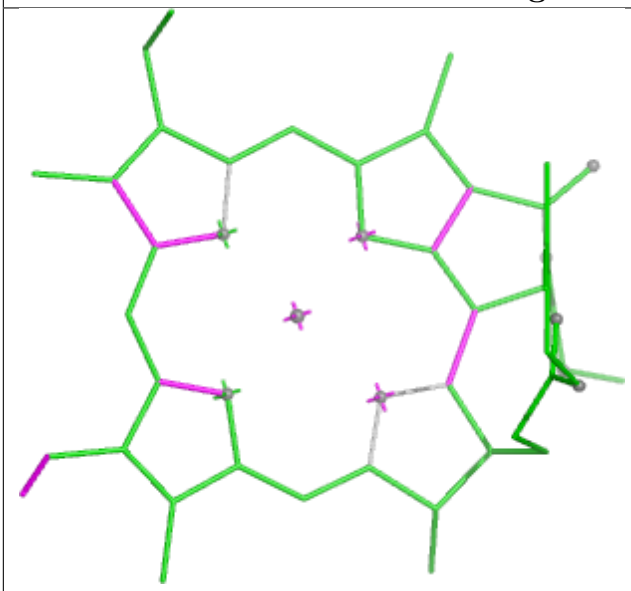


Rings

Ligand CLA 4 606



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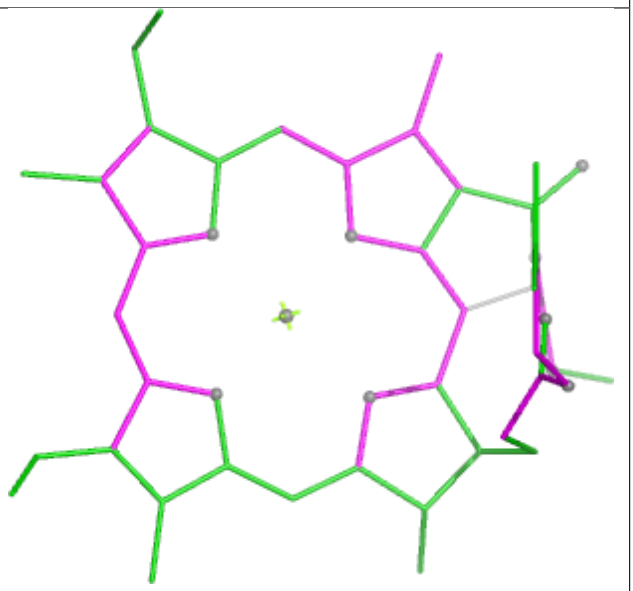
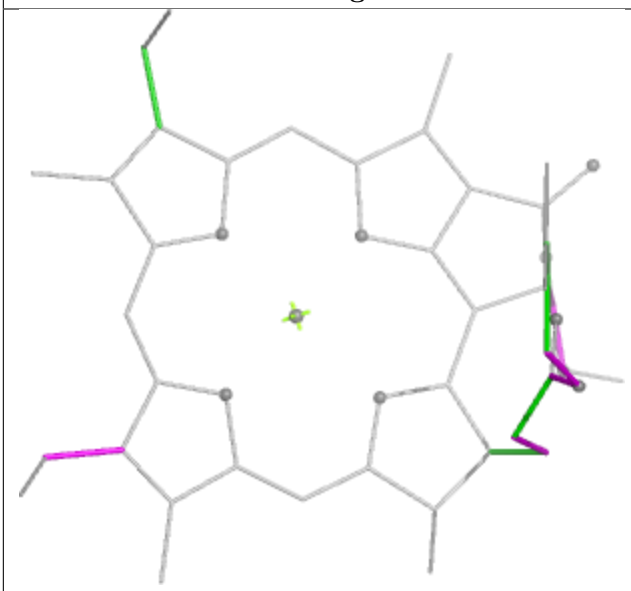


Bond angles



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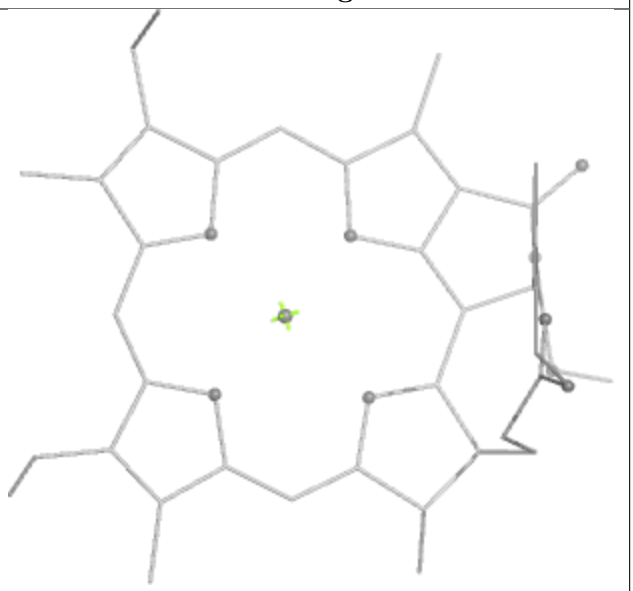
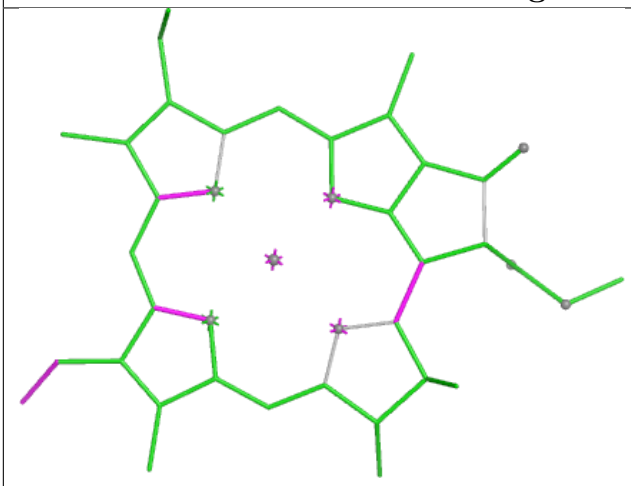


Rings

Ligand CLA 4 615



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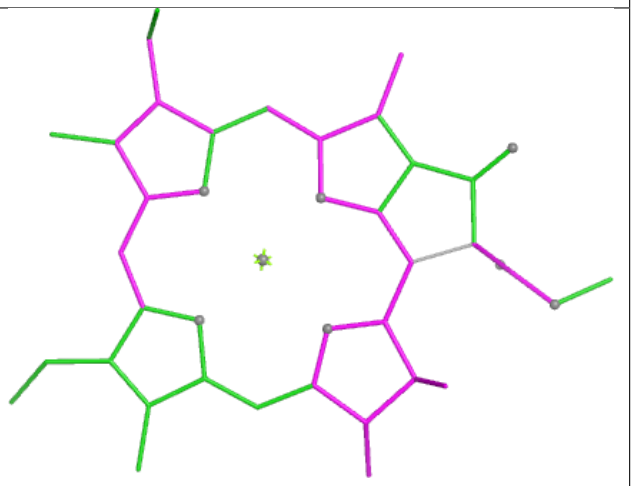
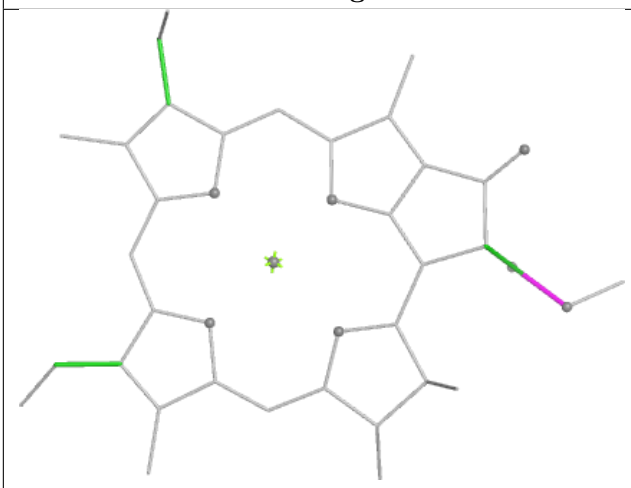


Bond angles



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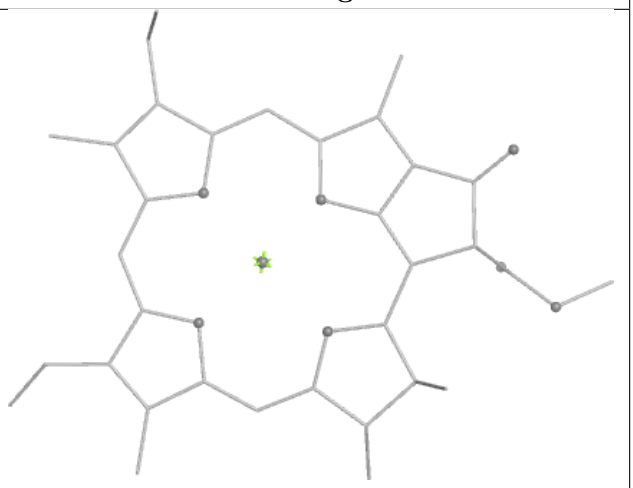
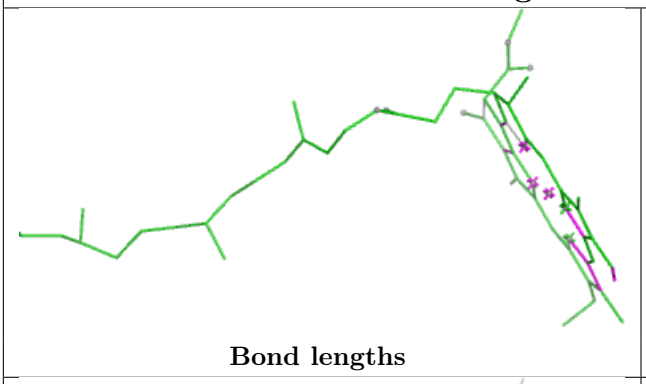
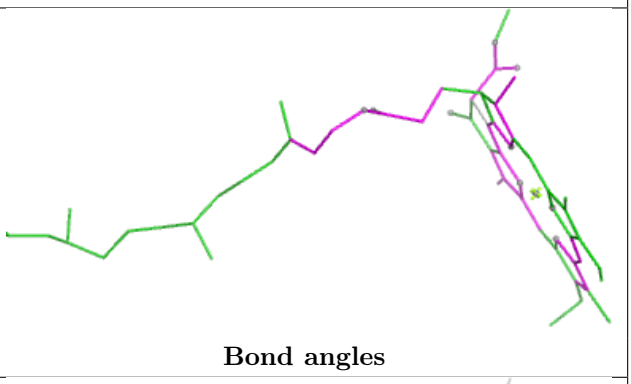


Rings

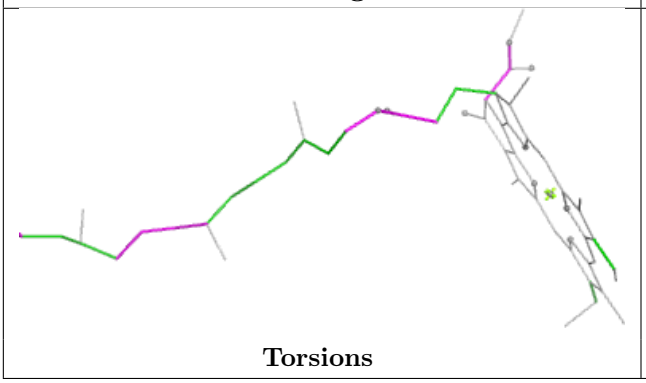
Ligand CLA A 1137



Bond lengths



Bond angles



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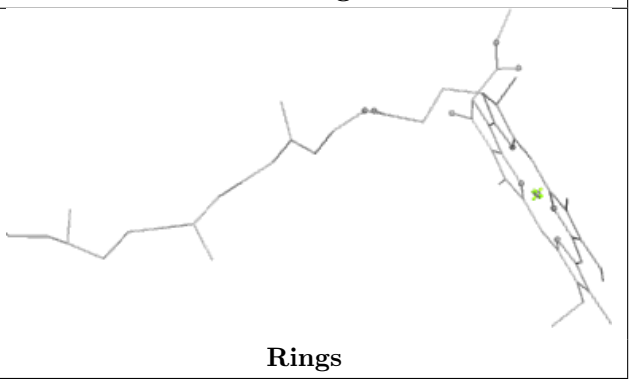
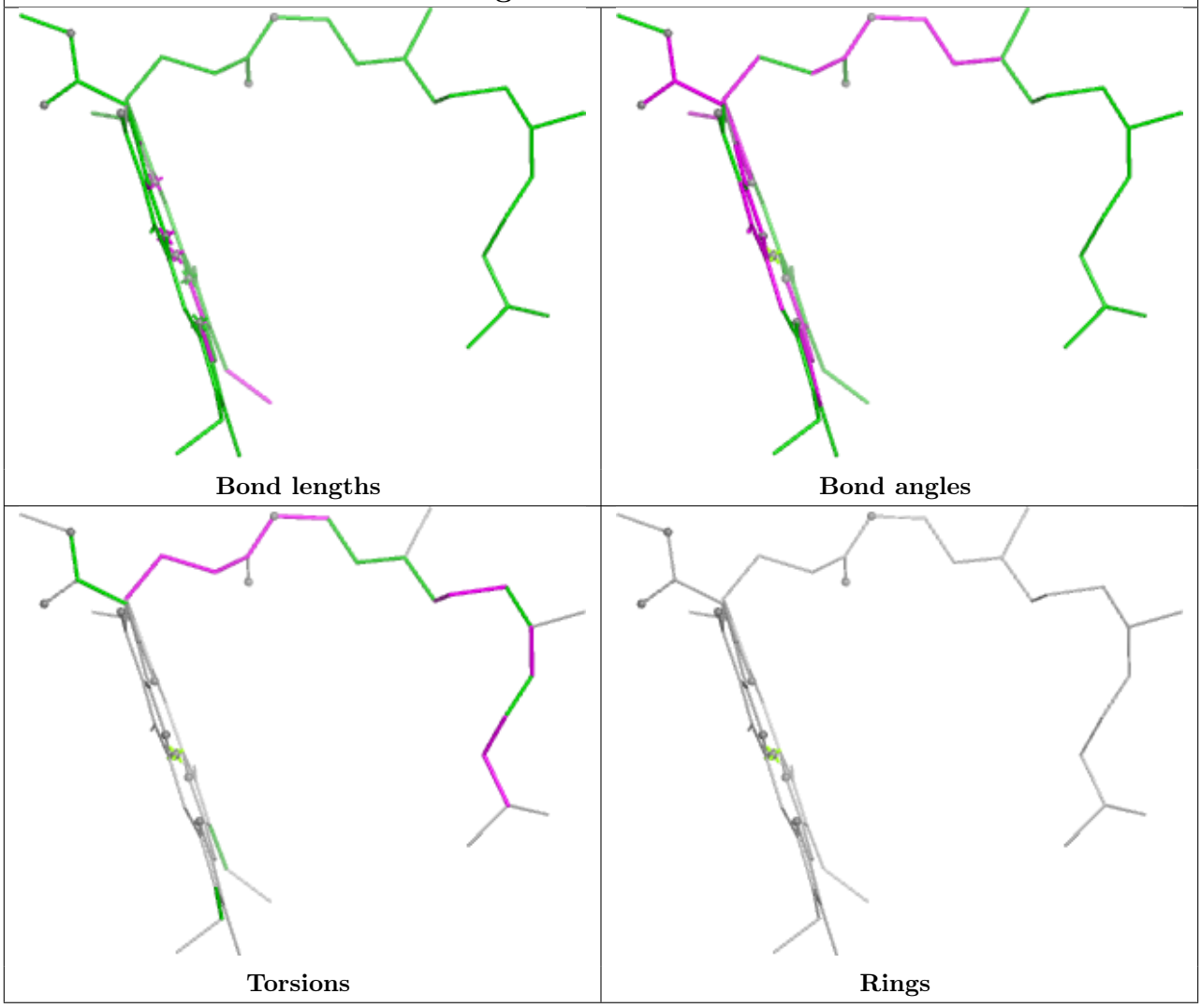


Rings

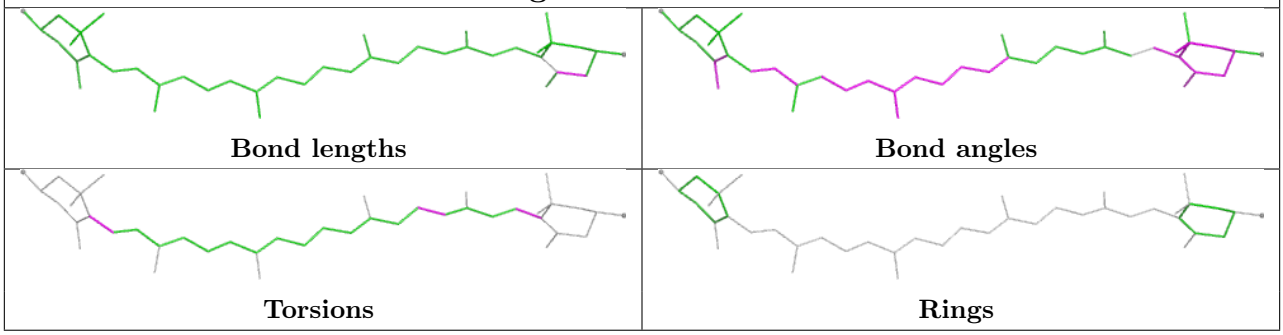
Ligand CLA 3 610



Bond lengths | Bond angles

Torsions | Rings

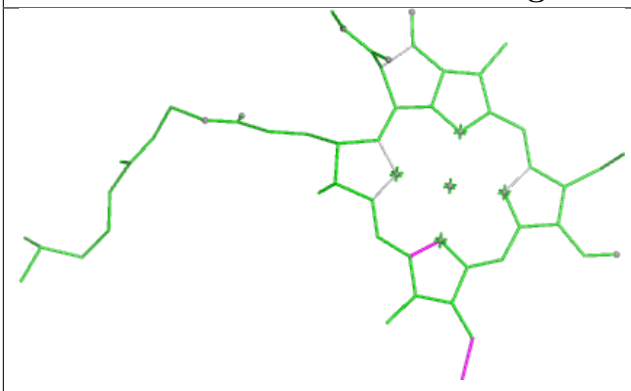
Ligand LUT 7 501



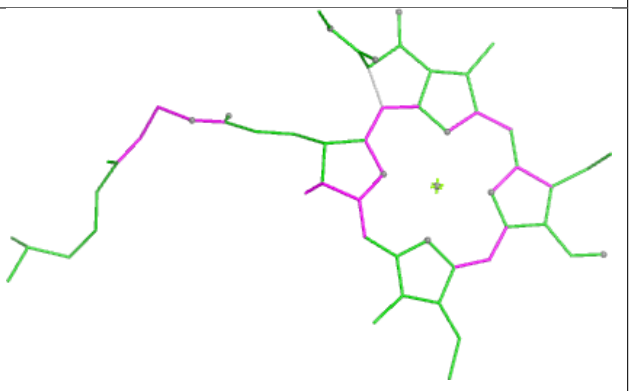
Bond lengths | Bond angles

Torsions | Rings

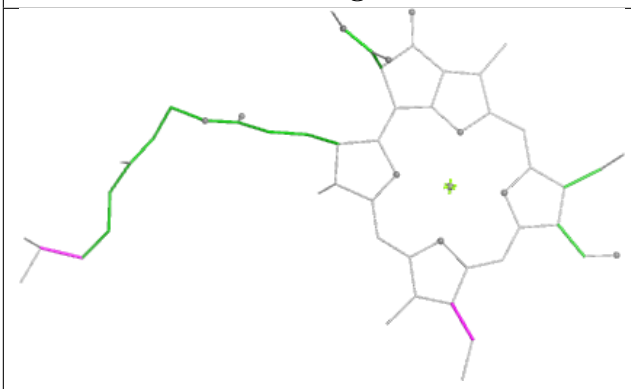
Ligand CHL 6 613



Bond lengths



Bond angles

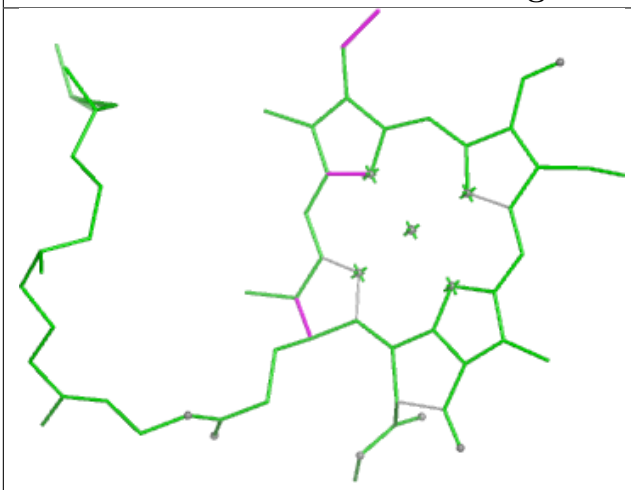


Torsions

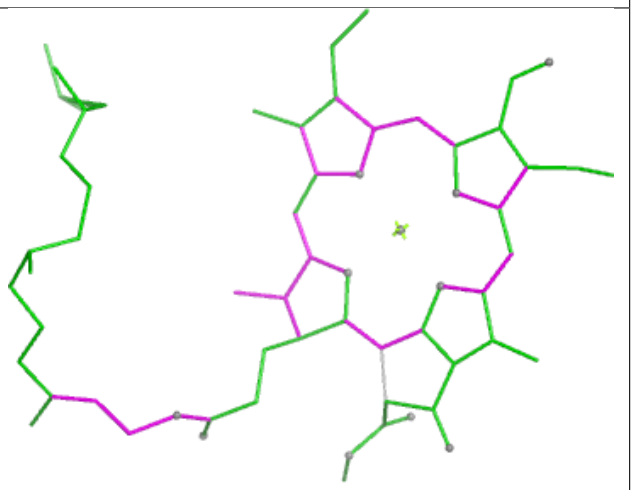


Rings

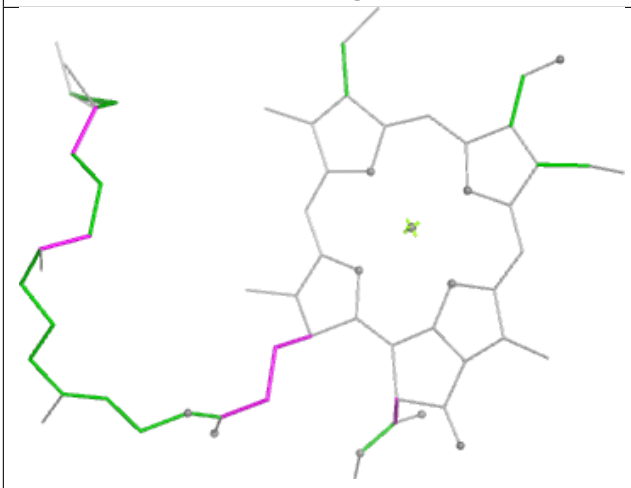
Ligand CHL 8 613



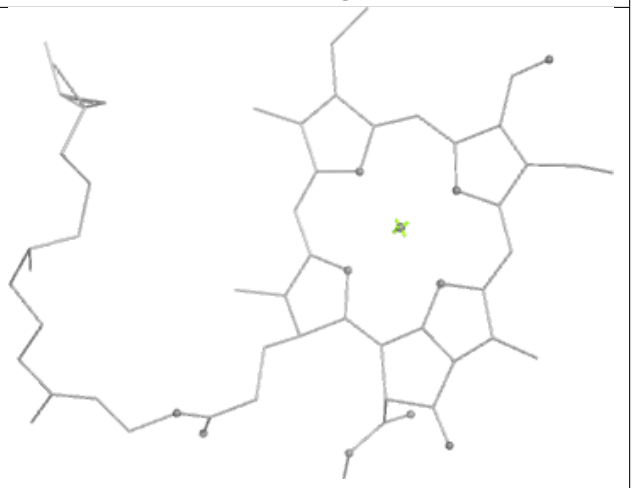
Bond lengths



Bond angles

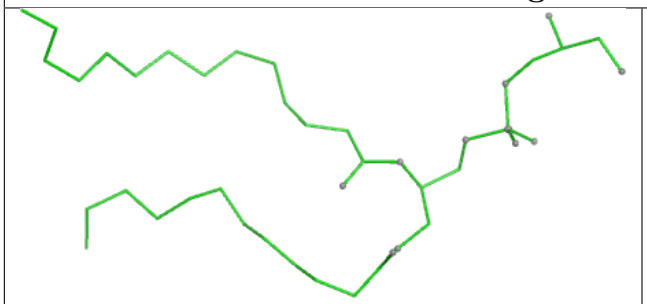


Torsions



Rings

Ligand LHG 1 801



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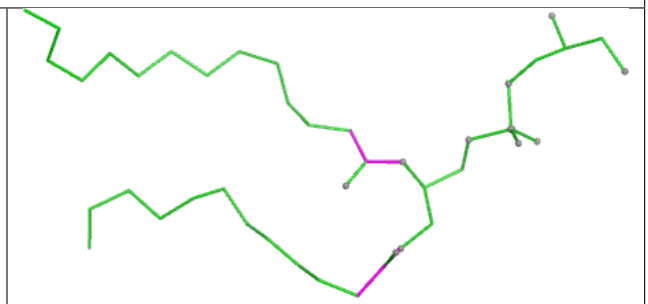
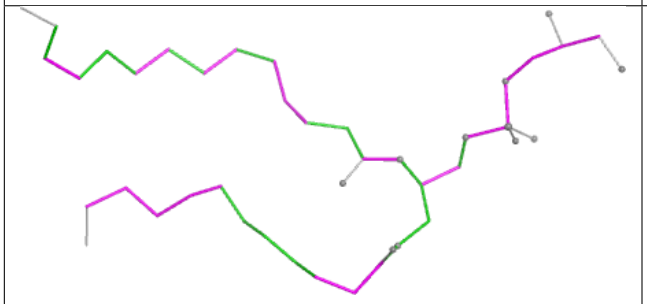
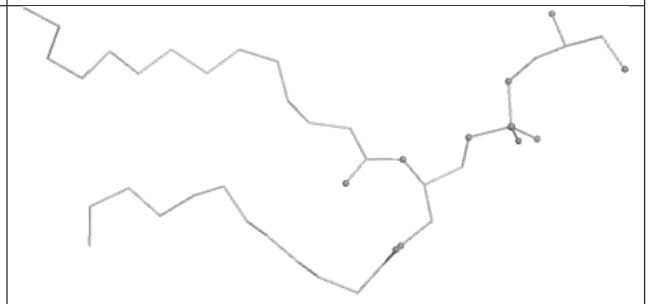


Bond angles

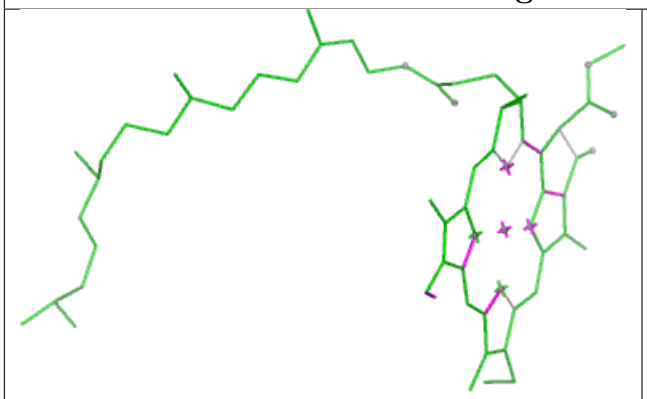


Torsions

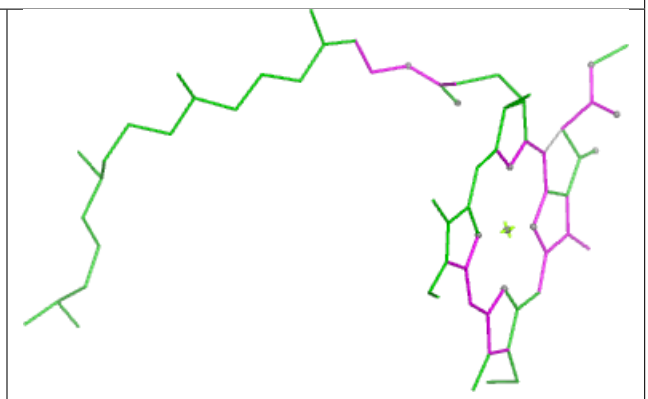


Rings

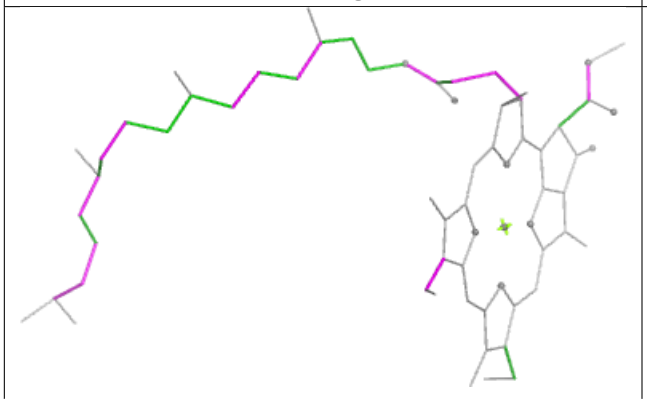
Ligand CLA A 1133



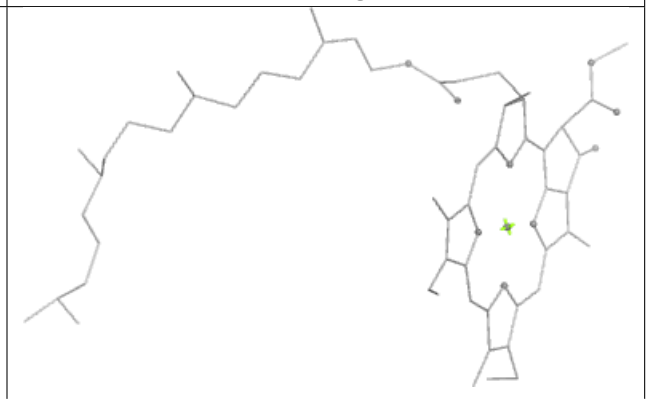
Bond lengths



Bond angles

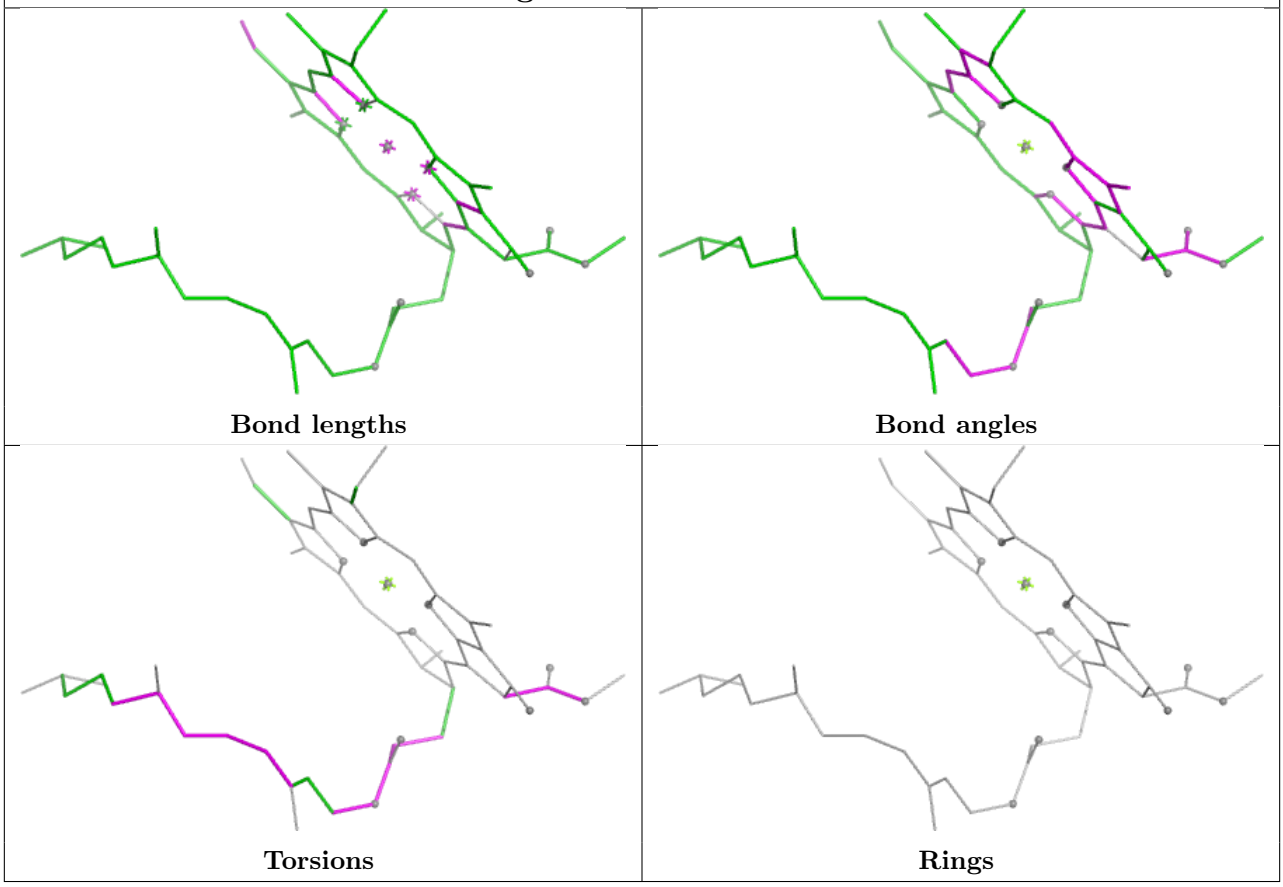


Torsions

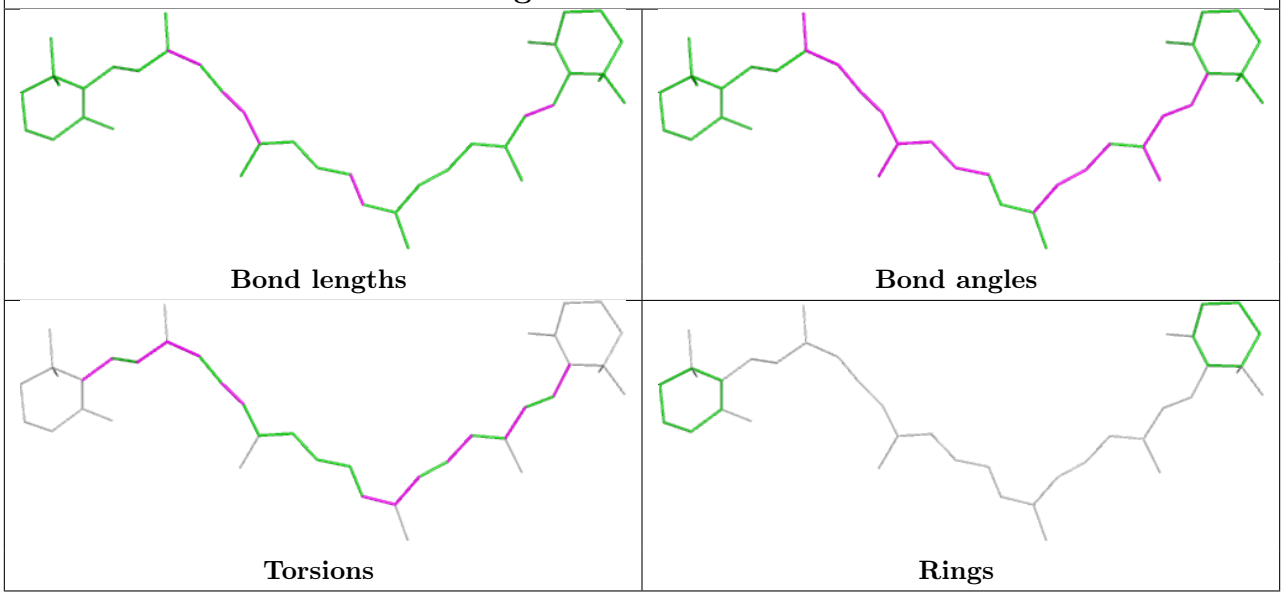


Rings

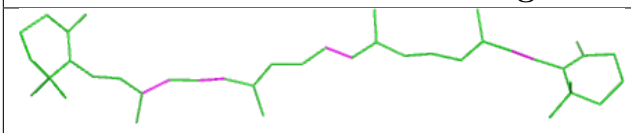
Ligand CLA B 1211



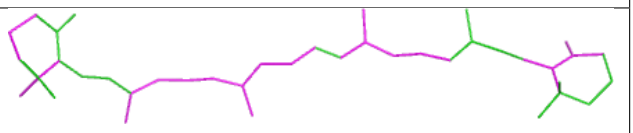
Ligand BCR A 4005



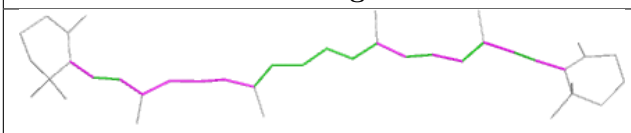
Ligand BCR J 4001



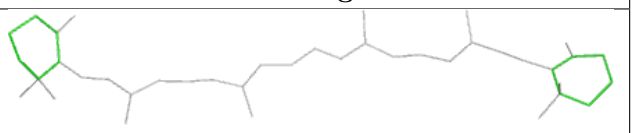
Bond lengths



Bond angles

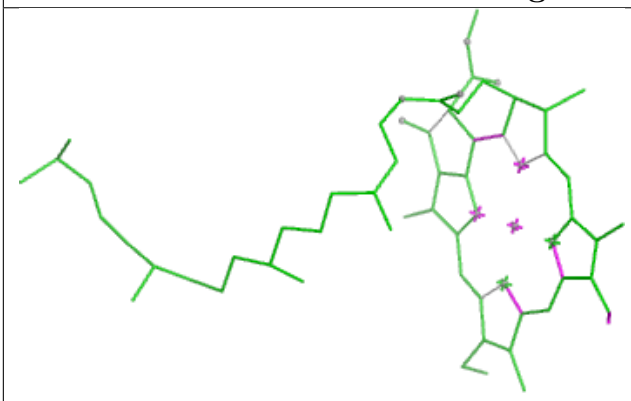


Torsions

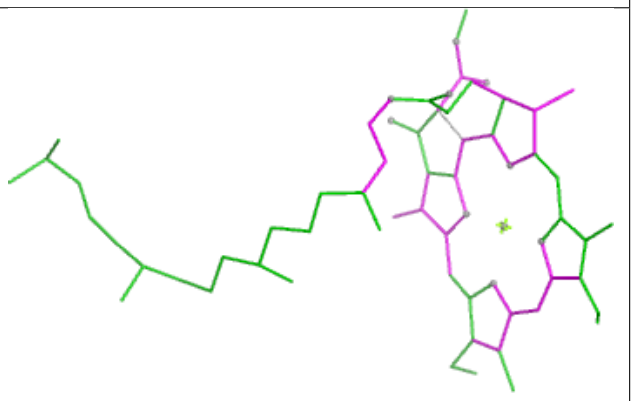


Rings

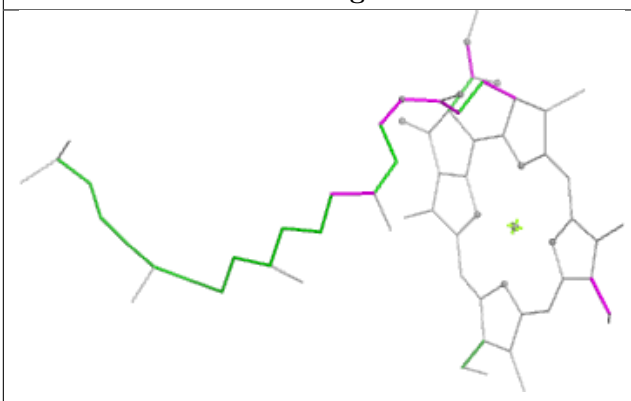
Ligand CLA 5 612



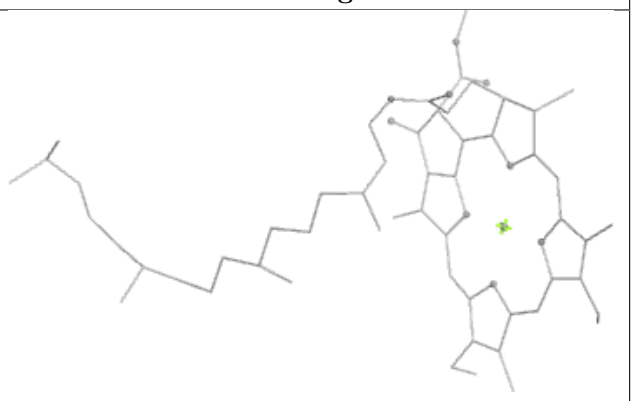
Bond lengths



Bond angles

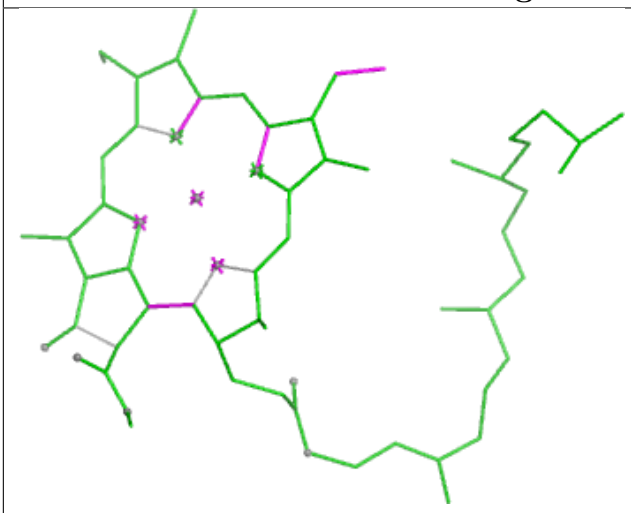


Torsions

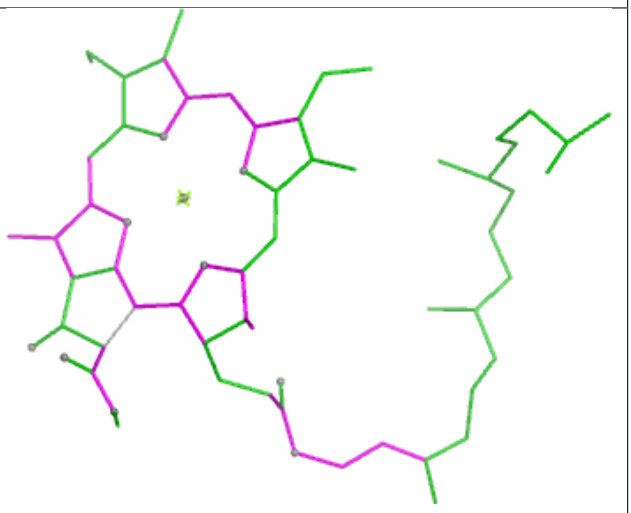


Rings

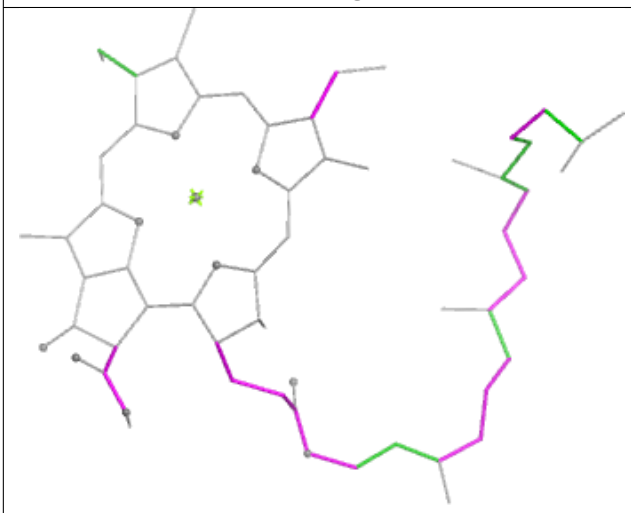
Ligand CLA B 1220



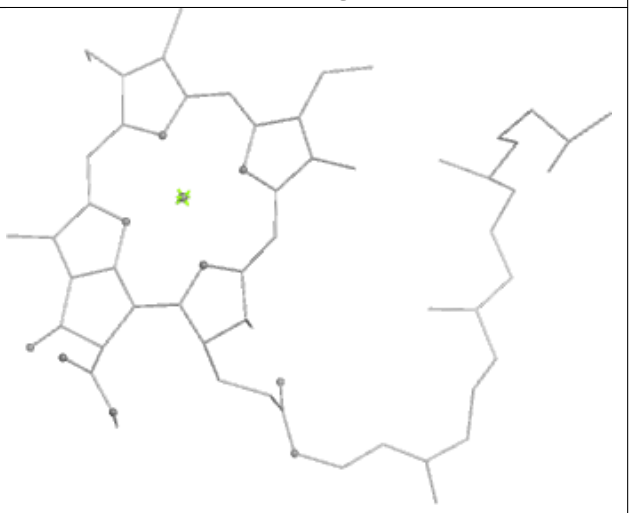
Bond lengths



Bond angles

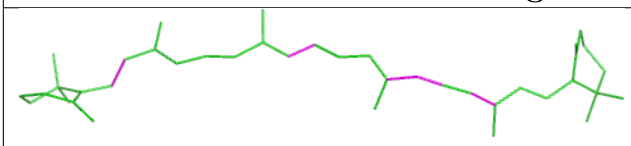


Torsions



Rings

Ligand BCR 3 504



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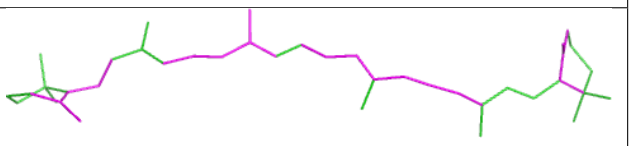
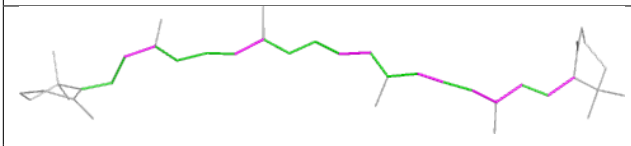
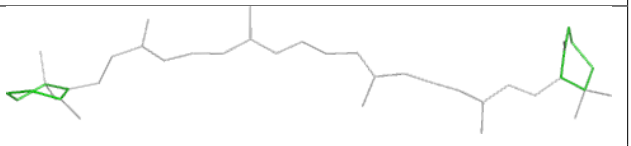


Bond angles

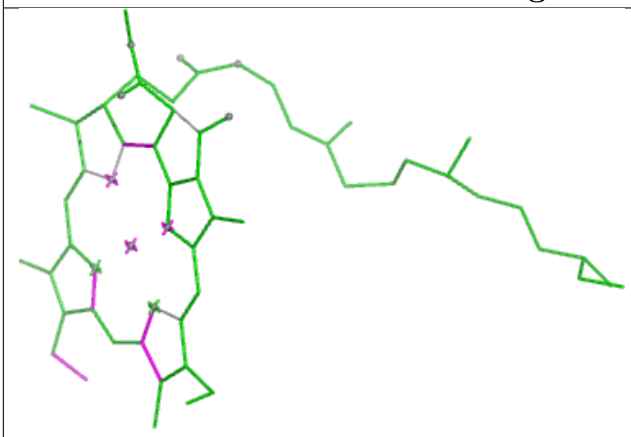


Torsions

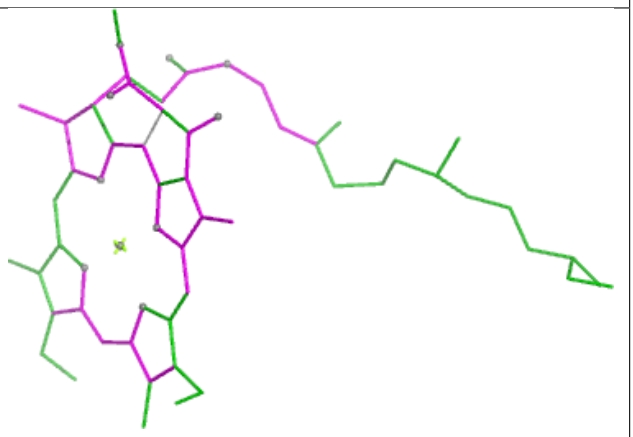


Rings

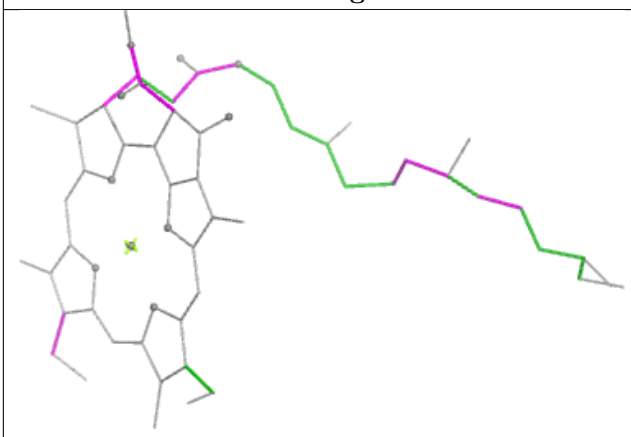
Ligand CLA 5 607



Bond lengths



Bond angles



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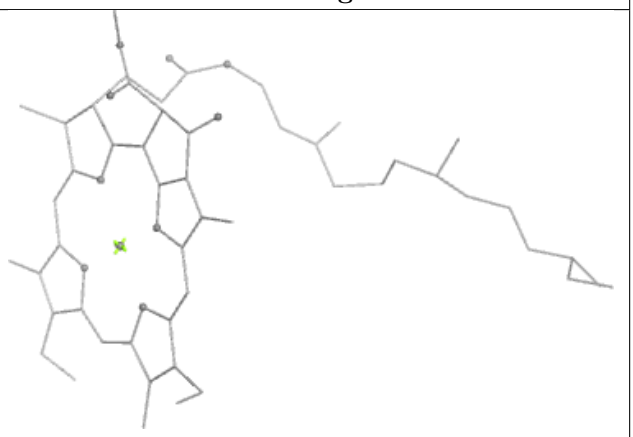
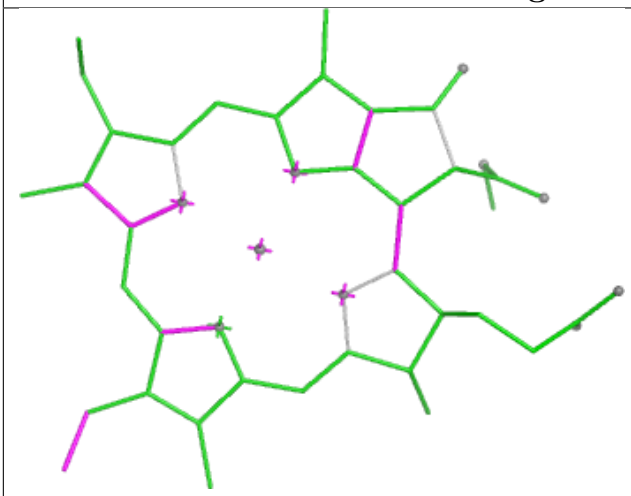
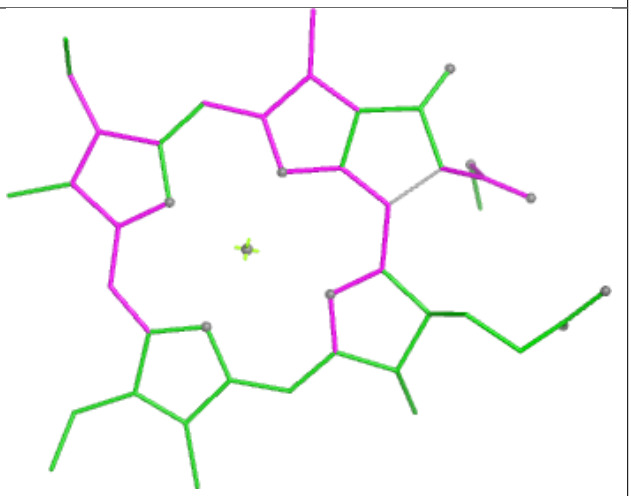


Rings

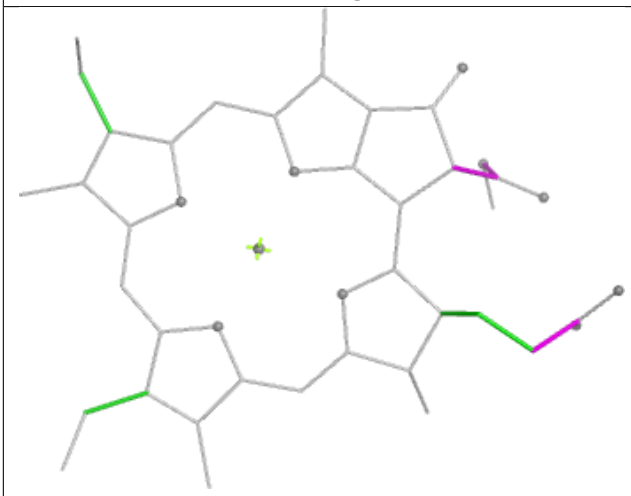
Ligand CLA 1 602



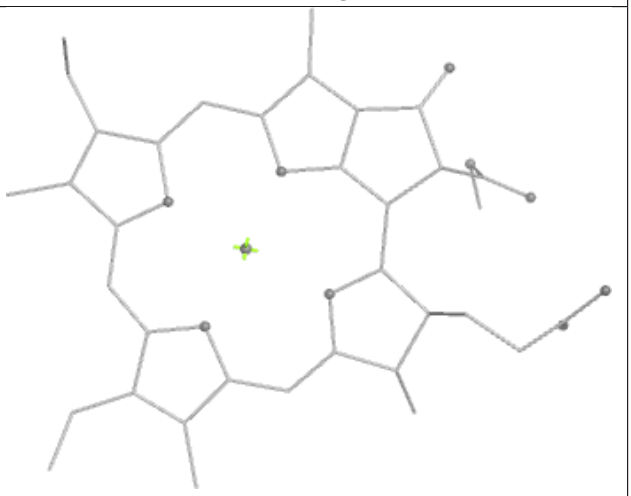
Bond lengths



Bond angles

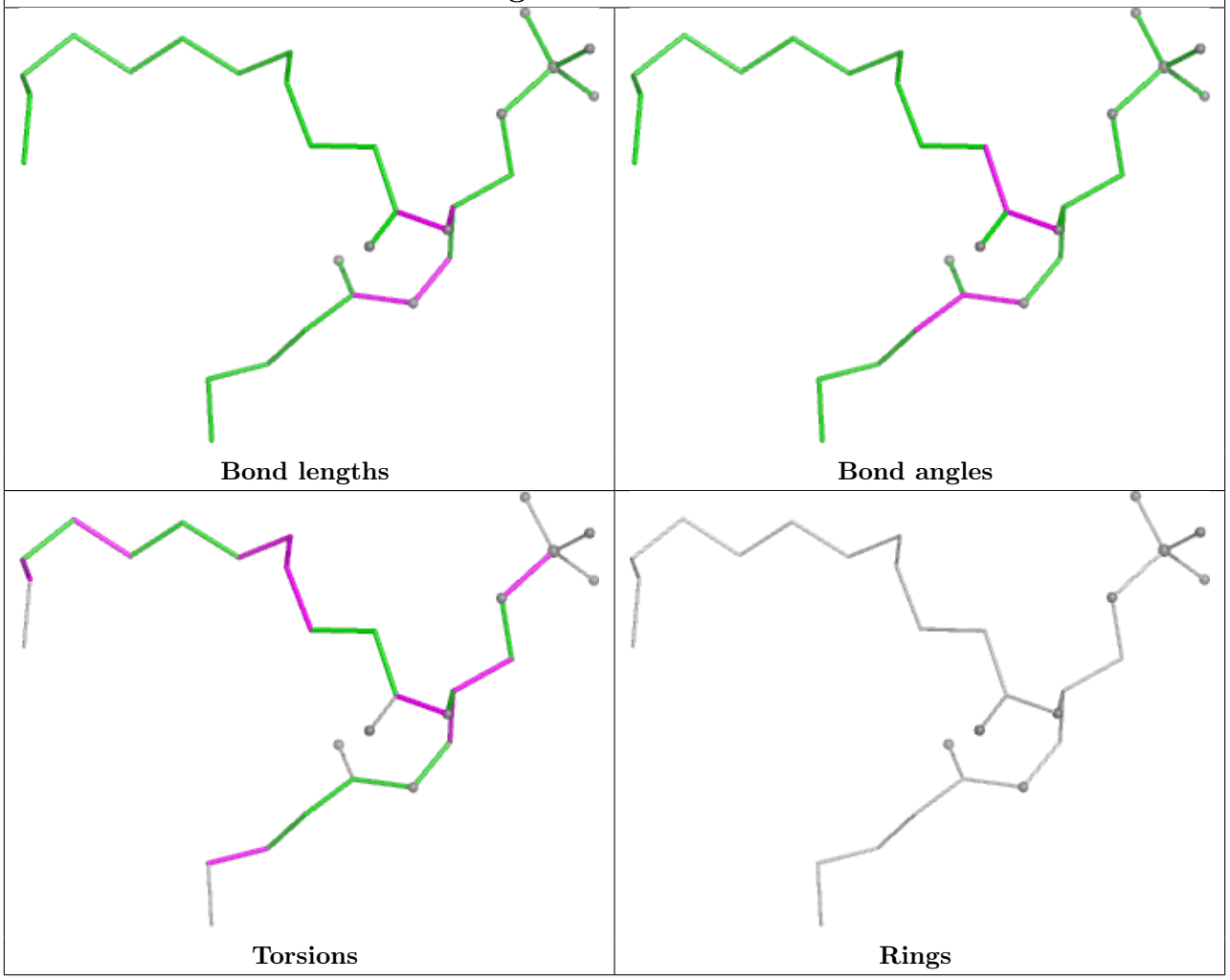


Torsions



Rings

Ligand 3PH 6 802



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	143:THR	C	156:VAL	N	16.29

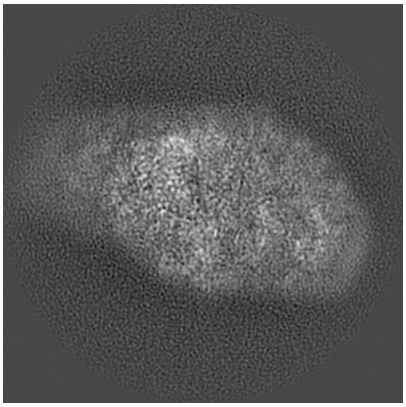
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12227. These allow visual inspection of the internal detail of the map and identification of artifacts.

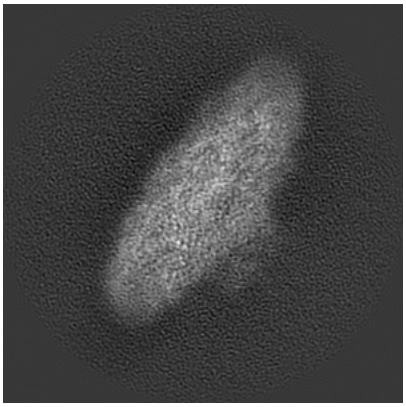
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

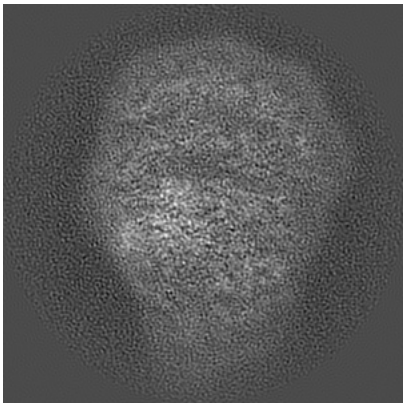
6.1.1 Primary map



X



Y

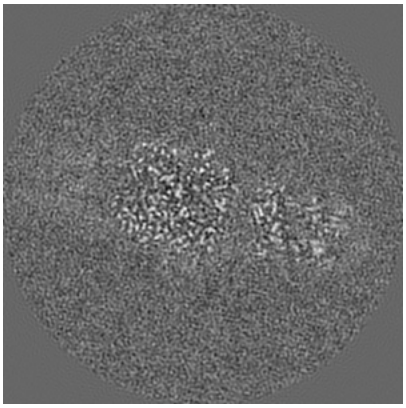


Z

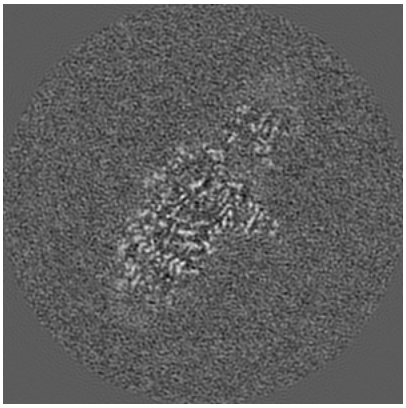
The images above show the map projected in three orthogonal directions.

6.2 Central slices

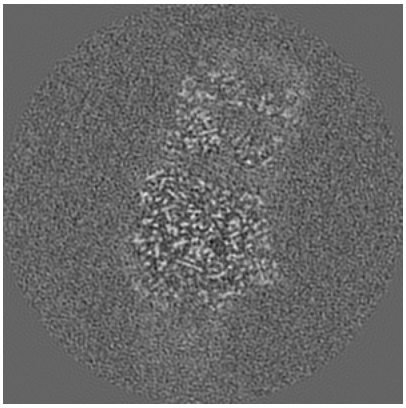
6.2.1 Primary map



X Index: 160



Y Index: 160

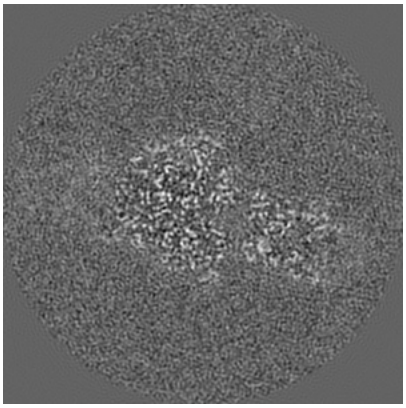


Z Index: 160

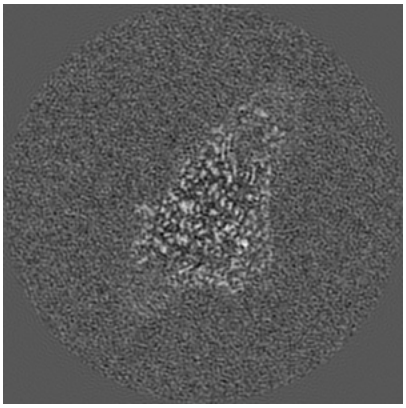
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

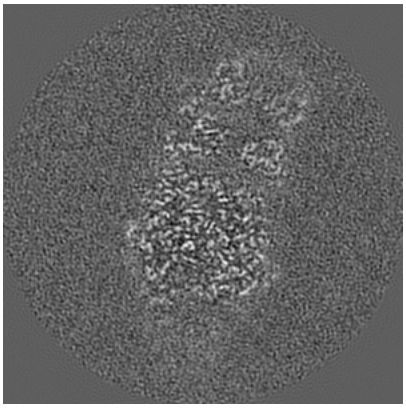
6.3.1 Primary map



X Index: 147



Y Index: 135

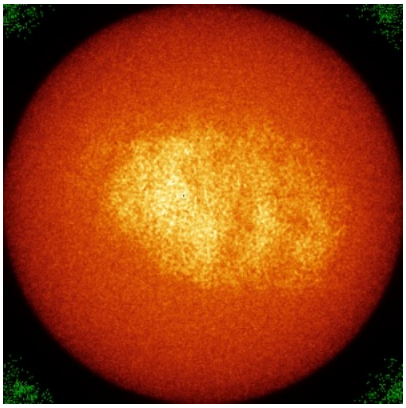


Z Index: 163

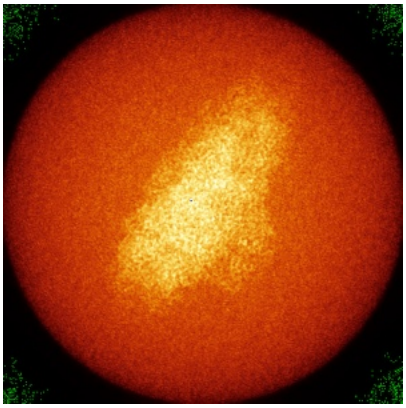
The images above show the largest variance slices of the map in three orthogonal directions.

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

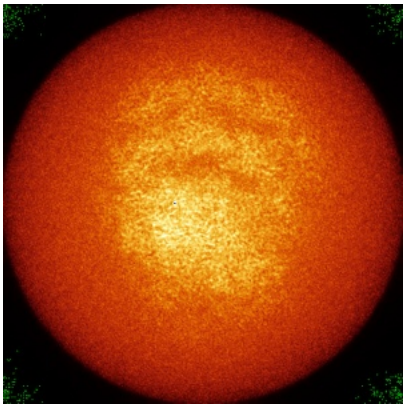
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

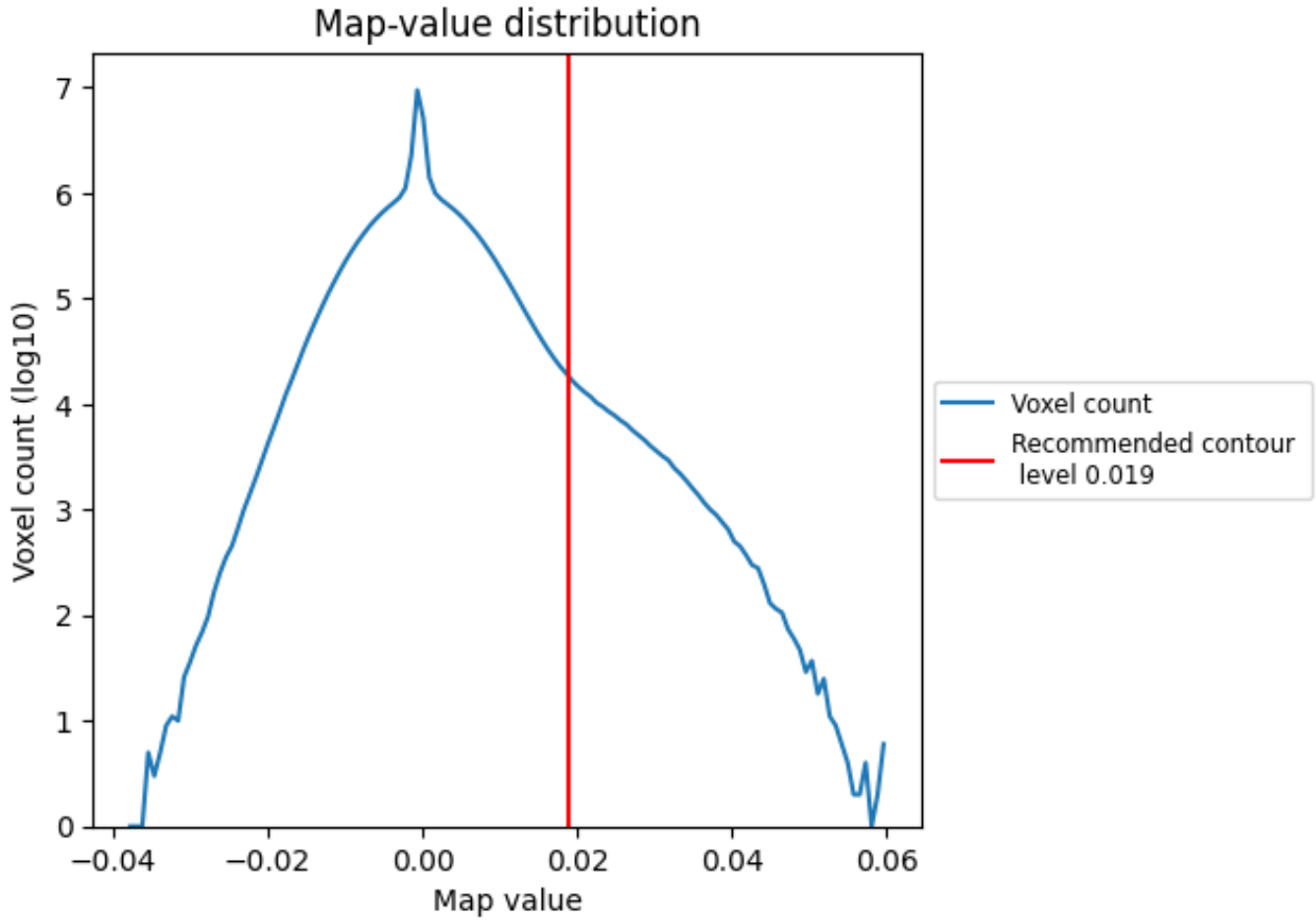
6.6 Mask visualisation (i)

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

7 Map analysis

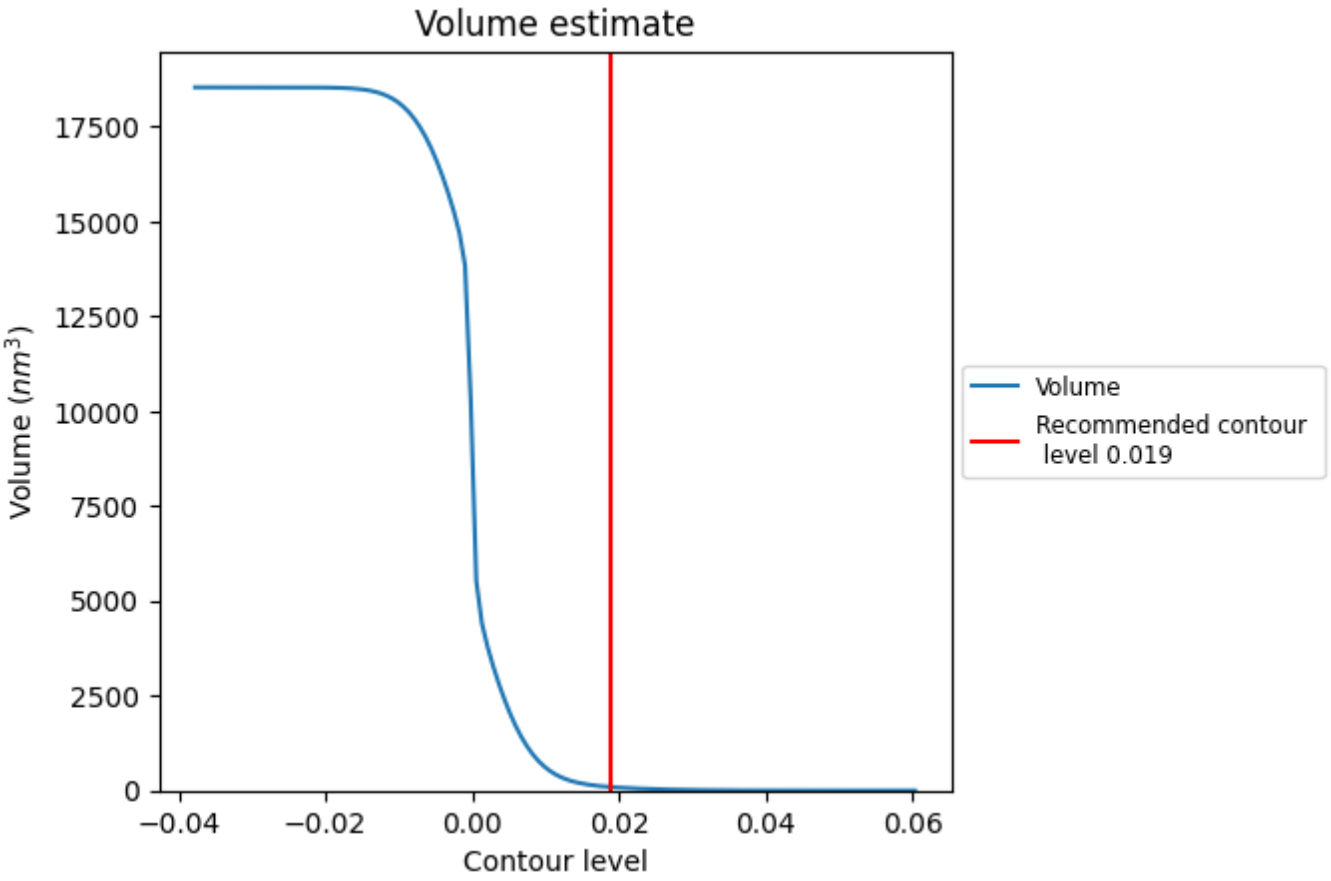
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

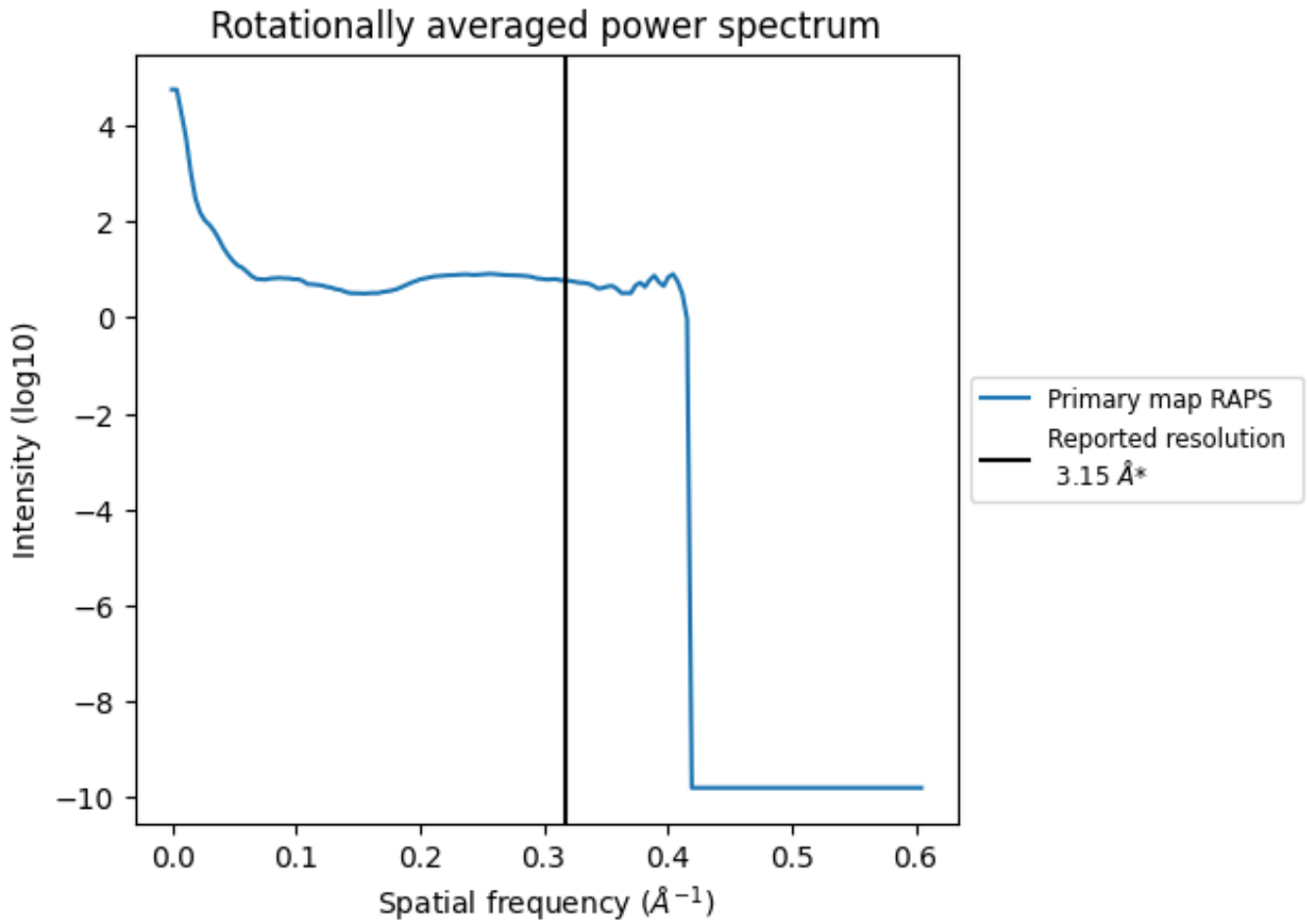
7.2 Volume estimate (i)



The volume at the recommended contour level is 91 nm^3; this corresponds to an approximate mass of 83 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)

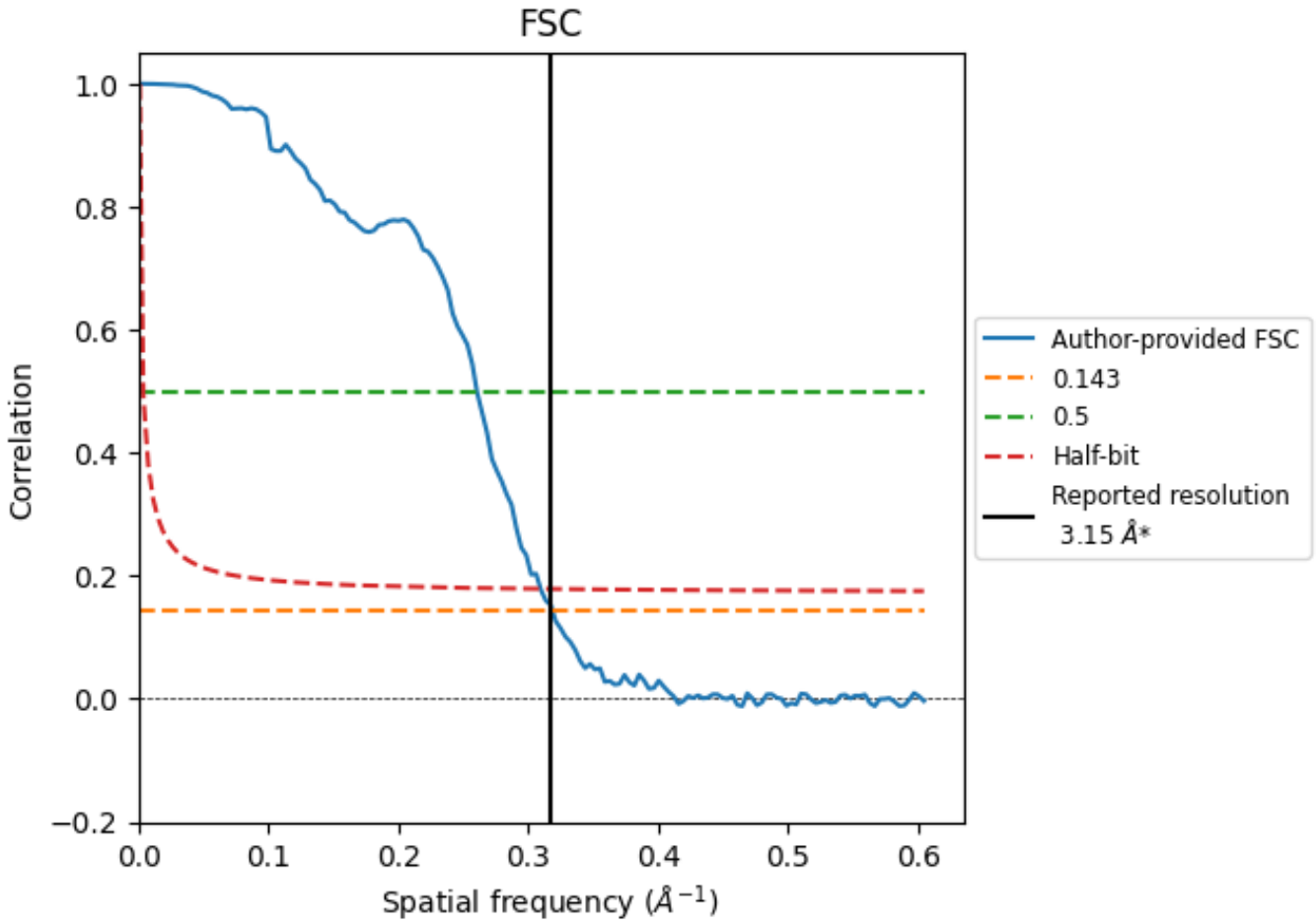


*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

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 0.317 Å^{-1}

8.2 Resolution estimates (i)

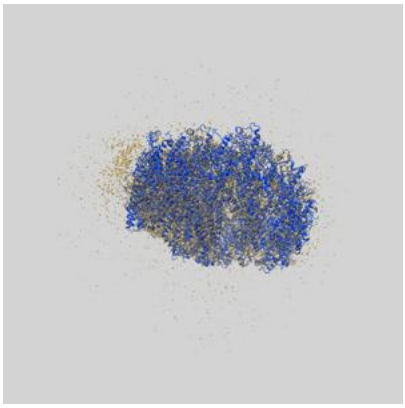
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.14	3.84	3.23
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

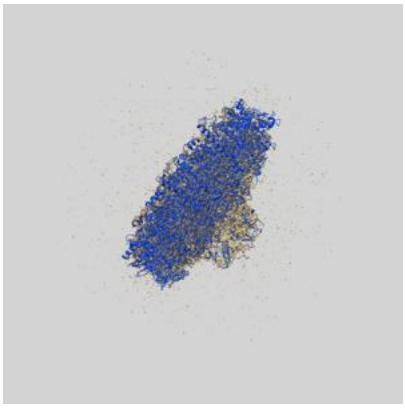
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12227 and PDB model 7BLX. Per-residue inclusion information can be found in section 3 on page 39.

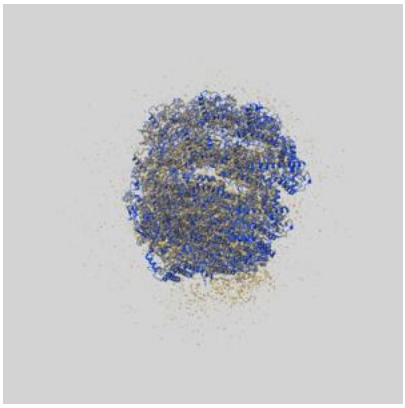
9.1 Map-model overlay



X



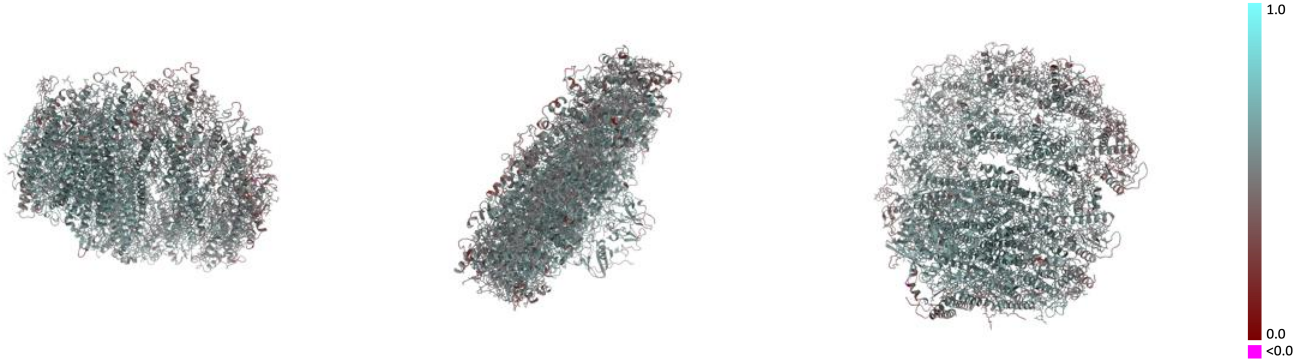
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

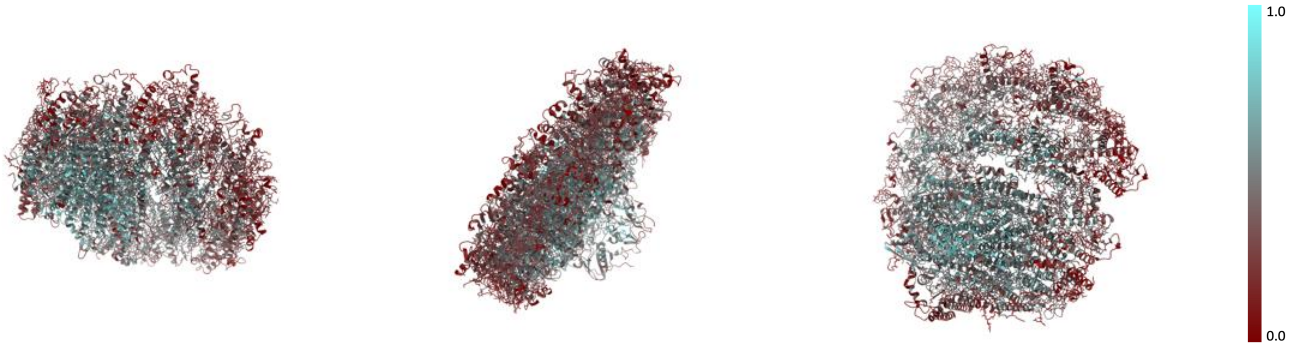
9.2 Q-score mapped to coordinate model



X Y Z

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

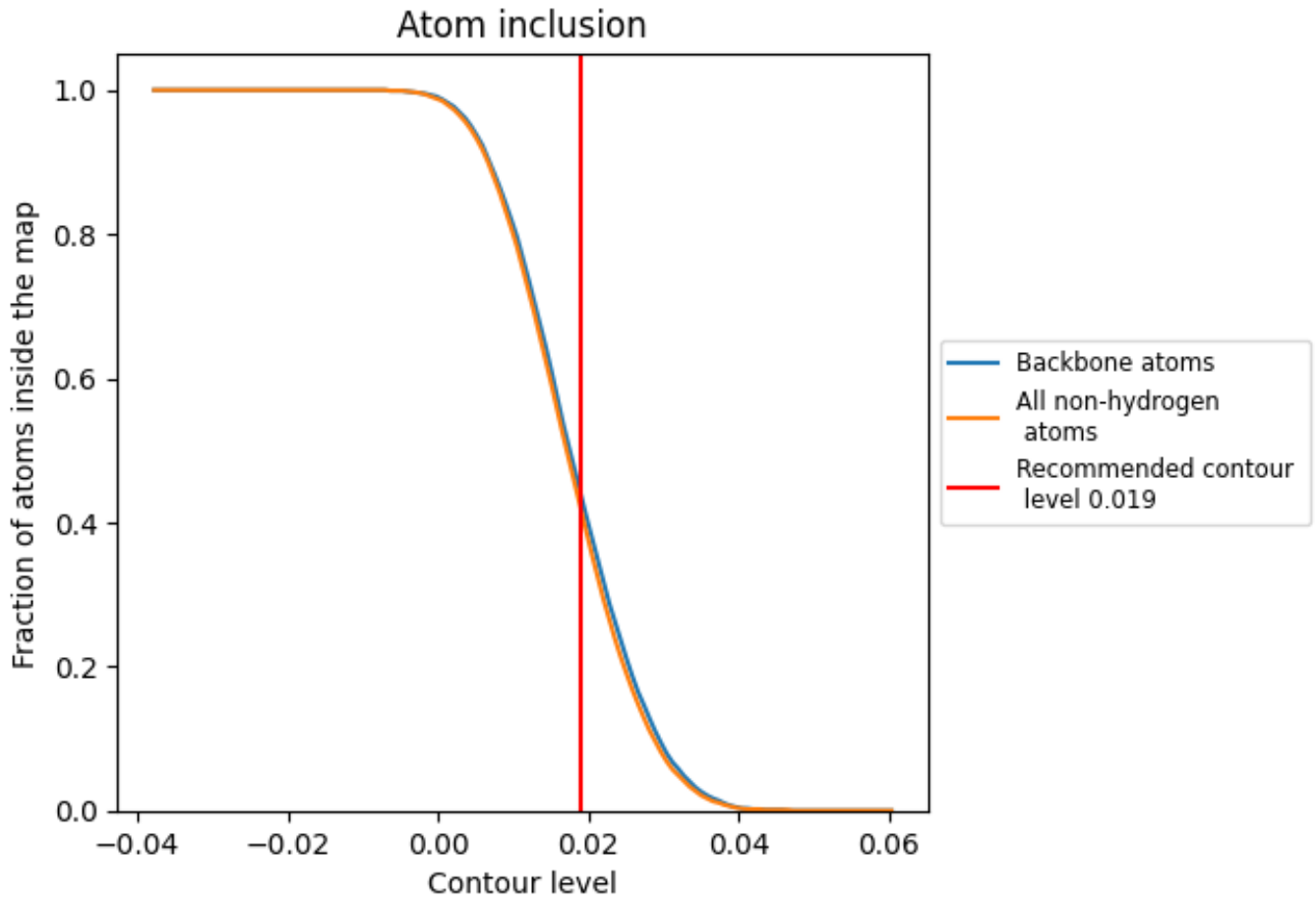
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 42% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4190	0.5360
1	0.3530	0.5190
3	0.3980	0.5260
4	0.2400	0.4710
5	0.2730	0.4920
6	0.2620	0.4830
7	0.4720	0.5520
8	0.4530	0.5500
A	0.5670	0.5860
B	0.5320	0.5780
C	0.5820	0.5690
D	0.4130	0.5350
E	0.4900	0.5270
F	0.4540	0.5500
G	0.1450	0.4470
I	0.2720	0.5160
J	0.4710	0.5680
K	0.1890	0.4500
L	0.1900	0.4460
Z	0.1980	0.4510

