wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 02:38 am BST

PDB ID	:	9I4T / pdb_00009i4t
EMDB ID	:	EMD-52620
Title	:	Photosystem II from Arabidopsis thaliana
Authors	:	Forsman, J.A.; Graca, A.T.; Hussein, R.; Hall, M.; Messinger, J.; Schroder, W.P.; Aydin, A.O.
Deposited on	:	2025-01-26
Resolution	:	2.44 Å(reported)
Based on initial model	:	3JCU

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

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

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

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

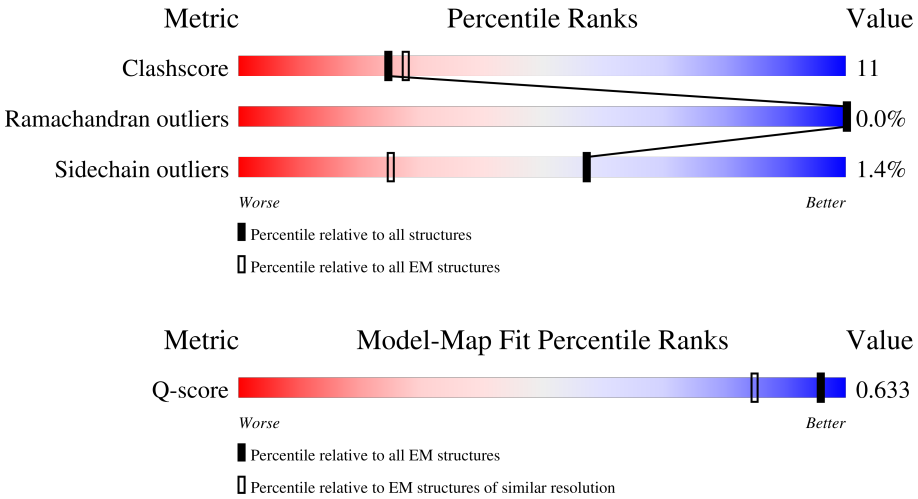
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.44 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	5856 (1.94 - 2.94)

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	353	68% 26% 5%
1	a	353	68% 27% 5%
2	B	508	80% 15% 5%
2	b	508	80% 16% 5%

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Mol	Chain	Length	Quality of chain
3	C	473	76% 18% • 5%
3	c	473	74% 20% • 5%
4	D	353	77% 20% •
4	d	353	78% 18% •
5	E	83	72% 17% 11%
5	e	83	73% 14% • 11%
6	F	39	72% 5% 23%
6	f	39	72% 5% 23%
7	G	267	63% 16% 21%
7	N	267	59% 17% 24%
7	g	267	62% 17% 21%
7	n	267	60% 16% 24%
8	H	73	71% 10% 19%
8	h	73	71% 10% 19%
9	I	36	86% 6% 8%
9	i	36	86% 6% 8%
10	J	40	82% 5% 12%
10	j	40	78% 10% 12%
11	K	61	46% 15% 39%
11	k	61	43% 18% 39%
12	L	38	76% 16% 8%
12	l	38	71% 21% 8%
13	M	34	68% 24% 9%
13	m	34	71% 21% 9%
14	O	332	• 57% 15% • 27%

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Mol	Chain	Length	Quality of chain
14	o	332	
15	P	263	
15	p	263	
16	Q	224	
16	q	224	
17	R	290	
17	r	290	
18	S	280	
18	s	280	
19	T	33	
19	t	33	
20	U	103	
20	u	103	
21	W	133	
21	w	133	
22	X	116	
22	x	116	
23	Y	265	
23	y	265	
24	Z	62	
24	z	62	

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 76824 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2613	1707	430	463	13		
1	a	334	Total	C	N	O	S	0	0
			2613	1707	430	463	13		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	485	Total	C	N	O	S	0	0
			3800	2489	642	657	12		
2	b	485	Total	C	N	O	S	0	0
			3800	2489	642	657	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	447	Total	C	N	O	S	0	0
			3468	2279	579	599	11		
3	c	447	Total	C	N	O	S	0	0
			3468	2279	579	599	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2713	1795	444	462	12		
4	d	341	Total	C	N	O	S	0	0
			2713	1795	444	462	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	74	Total 604	C 395	N 99	O 110	0	0
5	e	74	Total 604	C 395	N 99	O 110	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total 241	C 162	N 41	O 37	S 1	0	0
6	f	30	Total 241	C 162	N 41	O 37	S 1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	33	PHE	SER	variant	UNP P62095
f	33	PHE	SER	variant	UNP P62095

- Molecule 7 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	211	Total 1606	C 1037	N 264	O 300	S 5	0	0
7	N	202	Total 1536	C 994	N 251	O 286	S 5	0	0
7	g	211	Total 1606	C 1037	N 264	O 300	S 5	0	0
7	n	202	Total 1536	C 994	N 251	O 286	S 5	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total 438	C 289	N 68	O 79	S 2	0	0
8	h	59	Total 438	C 289	N 68	O 79	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			266	184	39	42	1		
9	i	33	Total	C	N	O	S	0	0
			266	184	39	42	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	35	Total	C	N	O	0	0
			255	174	39	42		
10	j	35	Total	C	N	O	0	0
			255	174	39	42		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			302	211	44	46	1		
11	k	37	Total	C	N	O	S	0	0
			302	211	44	46	1		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	35	Total	C	N	O	0	0
			293	195	45	53		
12	l	35	Total	C	N	O	0	0
			293	195	45	53		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			242	168	34	40		
13	m	31	Total	C	N	O	0	0
			242	168	34	40		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	241	Total	C	N	O	S	0	0
			1829	1157	297	371	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	241	Total	C	N	O	S	0	0
			1829	1157	297	371	4		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	171	Total	C	N	O	S	0	0
			1319	836	217	264	2		
15	p	171	Total	C	N	O	S	0	0
			1319	836	217	264	2		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	146	Total	C	N	O	0	0
			1139	726	193	220		
16	q	146	Total	C	N	O	0	0
			1139	726	193	220		

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	220	Total	C	N	O	S	0	0
			1710	1109	281	317	3		
17	r	220	Total	C	N	O	S	0	0
			1710	1109	281	317	3		

- Molecule 18 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		
18	s	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		

- Molecule 19 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	32	Total	C	N	O	S	0	0
			261	181	37	42	1		
19	t	32	Total	C	N	O	S	0	0
			261	181	37	42	1		

- Molecule 20 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	28	Total	C	N	O	S	0	0
			219	138	40	38	3		
20	u	28	Total	C	N	O	S	0	0
			219	138	40	38	3		

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total	C	N	O	S	0	0
			427	282	61	83	1		
21	w	54	Total	C	N	O	S	0	0
			427	282	61	83	1		

- Molecule 22 is a protein called Expressed protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	39	Total	C	N	O	0	0
			279	183	46	50		
22	x	39	Total	C	N	O	0	0
			279	183	46	50		

- Molecule 23 is a protein called Chlorophyll a-b binding protein 2.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	214	Total	C	N	O	S	0	0
			1652	1075	265	307	5		
23	y	214	Total	C	N	O	S	0	0
			1652	1075	265	307	5		

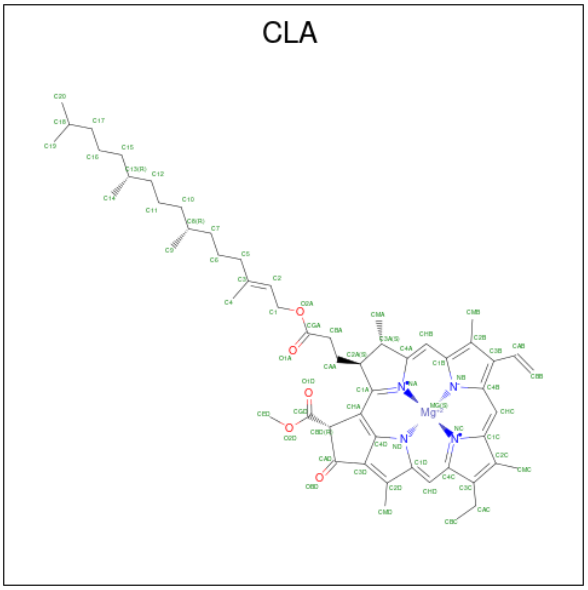
- Molecule 24 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	61	Total	C	N	O	0	0
			456	308	68	80		
24	z	61	Total	C	N	O	0	0
			456	308	68	80		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
25	A	2	Total Cl 2 2	0
25	a	2	Total Cl 2 2	0

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C Mg N O 65 55 1 4 5	0
26	A	1	Total C Mg N O 60 50 1 4 5	0
26	B	1	Total C Mg N O 65 55 1 4 5	0
26	B	1	Total C Mg N O 65 55 1 4 5	0
26	B	1	Total C Mg N O 65 55 1 4 5	0
26	B	1	Total C Mg N O 65 55 1 4 5	0
26	B	1	Total C Mg N O 65 55 1 4 5	0
26	B	1	Total C Mg N O 65 55 1 4 5	0
26	B	1	Total C Mg N O 65 55 1 4 5	0
26	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			64	55	1	3	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	Y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			64	55	1	3	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	d	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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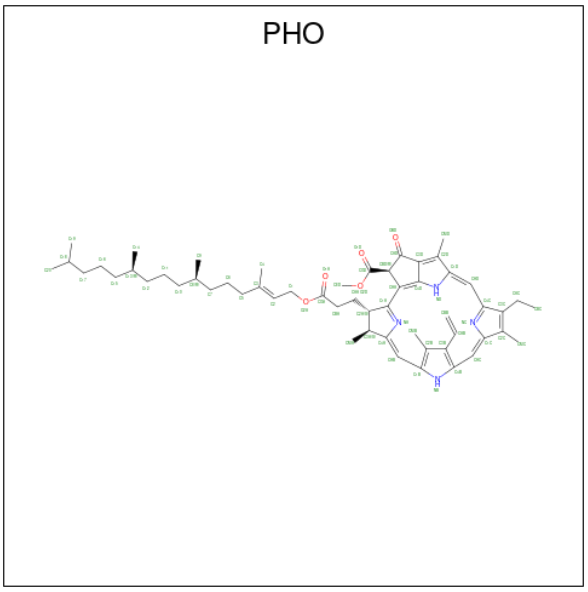
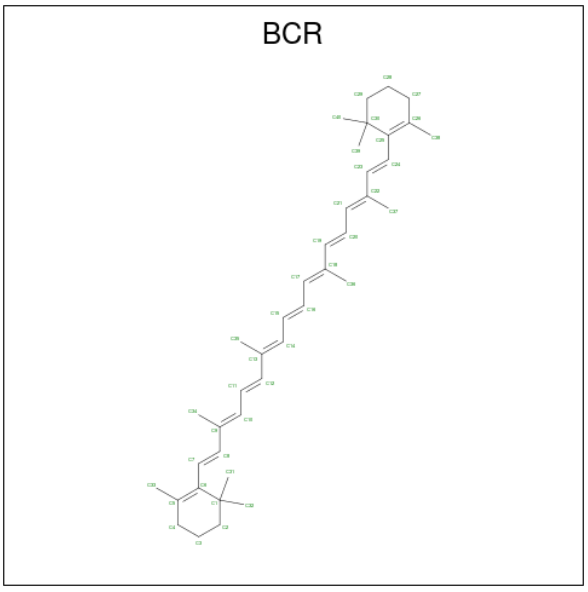
Mol	Chain	Residues	Atoms					AltConf
26	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



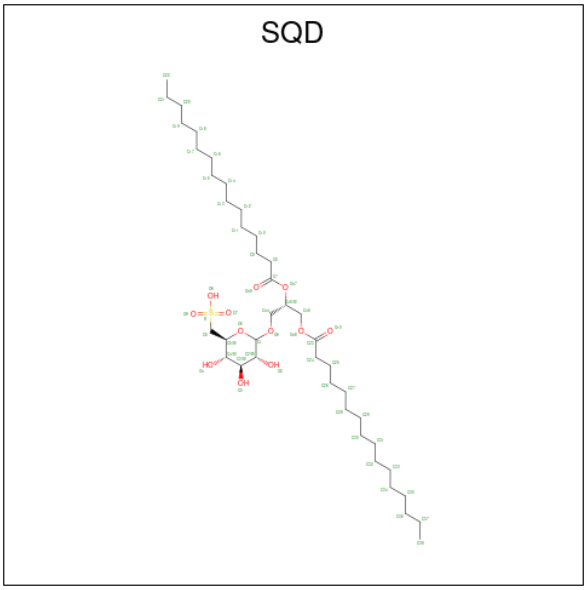
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	D	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	
27	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



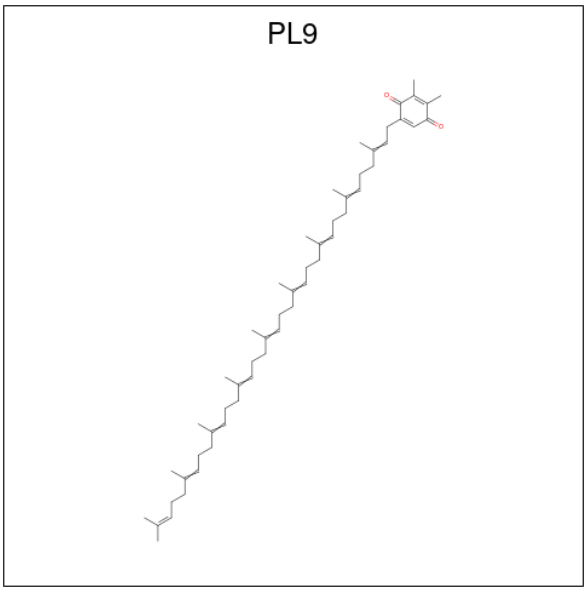
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	D	1	Total C 40 40	0
28	H	1	Total C 40 40	0
28	J	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	T	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	h	1	Total C 40 40	0
28	j	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	t	1	Total C 40 40	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	S	0
			54	41	12	1	
29	A	1	Total	C	O	S	0
			50	37	12	1	
29	B	1	Total	C	O	S	0
			54	41	12	1	
29	W	1	Total	C	O	S	0
			33	20	12	1	
29	a	1	Total	C	O	S	0
			54	41	12	1	
29	a	1	Total	C	O	S	0
			50	37	12	1	
29	b	1	Total	C	O	S	0
			54	41	12	1	
29	w	1	Total	C	O	S	0
			33	20	12	1	

- Molecule 30 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).

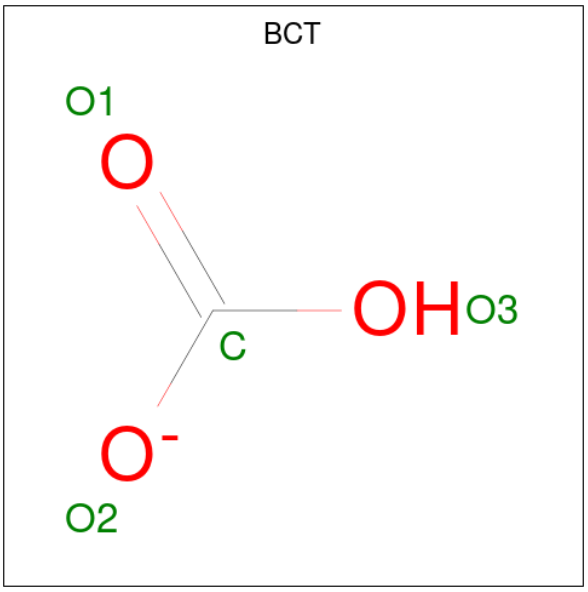


Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C O 22 20 2	0
30	D	1	Total C O 55 53 2	0
30	a	1	Total C O 22 20 2	0
30	d	1	Total C O 55 53 2	0

- Molecule 31 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

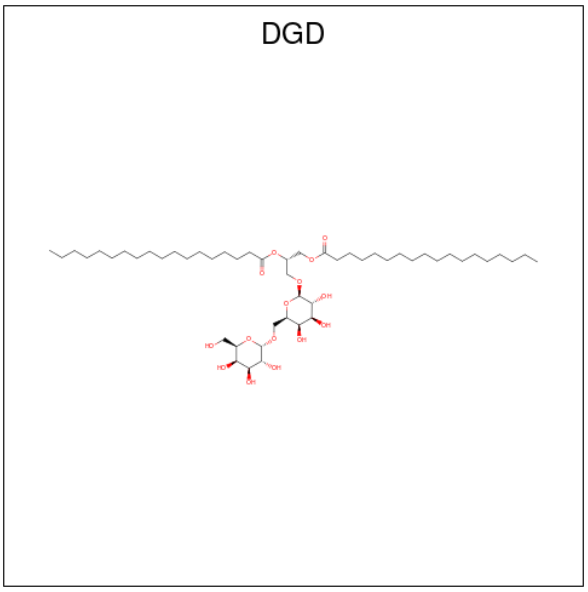
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Fe 1 1	0
31	a	1	Total Fe 1 1	0

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			4	1	3	
32	a	1	Total	C	O	0
			4	1	3	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			62	47	15	

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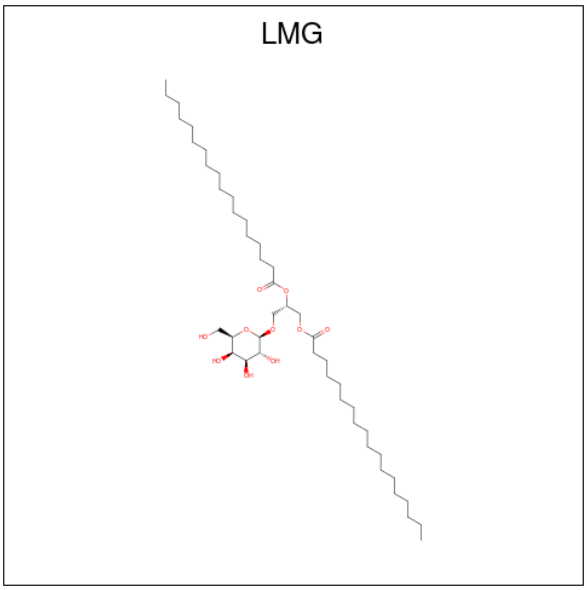
Mol	Chain	Residues	Atoms	AltConf
33	C	1	Total C O 55 40 15	0
33	C	1	Total C O 62 47 15	0
33	C	1	Total C O 62 47 15	0
33	Y	1	Total C O 43 28 15	0
33	b	1	Total C O 62 47 15	0
33	c	1	Total C O 62 47 15	0
33	c	1	Total C O 55 40 15	0
33	c	1	Total C O 62 47 15	0
33	y	1	Total C O 43 28 15	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
34	B	1	Total C O 51 41 10	0
34	C	1	Total C O 51 41 10	0

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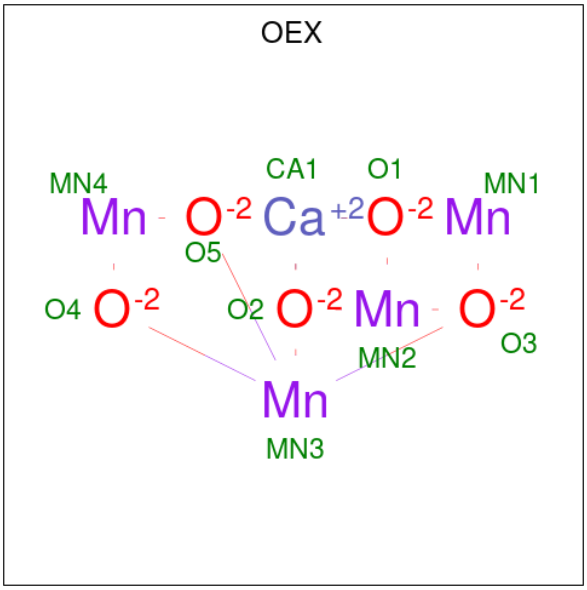
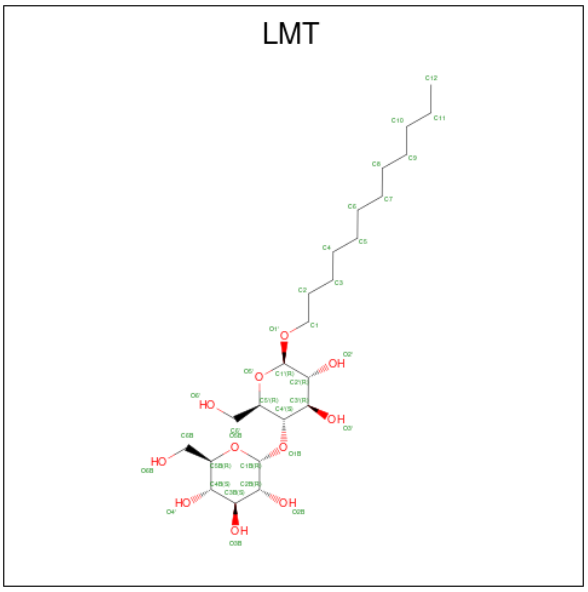
Mol	Chain	Residues	Atoms	AltConf
34	C	1	Total C O 51 41 10	0
34	D	1	Total C O 46 36 10	0
34	W	1	Total C O 48 38 10	0
34	b	1	Total C O 51 41 10	0
34	c	1	Total C O 51 41 10	0
34	c	1	Total C O 51 41 10	0
34	d	1	Total C O 46 36 10	0
34	w	1	Total C O 48 38 10	0

- Molecule 35 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



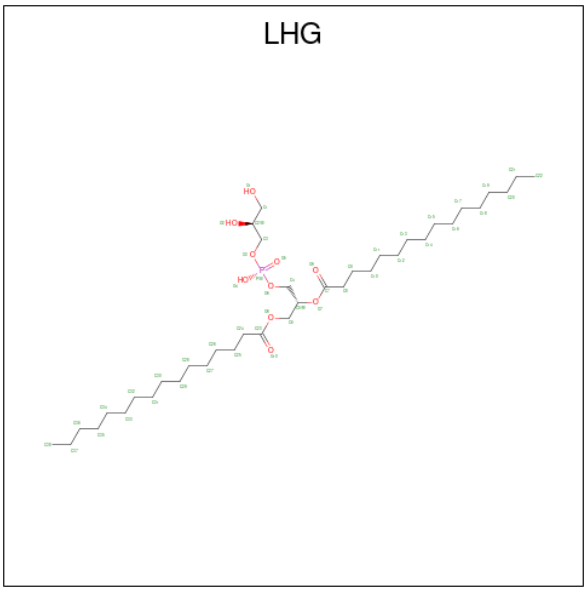
Mol	Chain	Residues	Atoms	AltConf
35	C	1	Total Ca Mn O 10 1 4 5	0
35	a	1	Total Ca Mn O 10 1 4 5	0

- Molecule 36 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			35	24	11	
36	d	1	Total	C	O	0
			35	24	11	

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
37	D	1	Total	C	O	P	0
			43	32	10	1	

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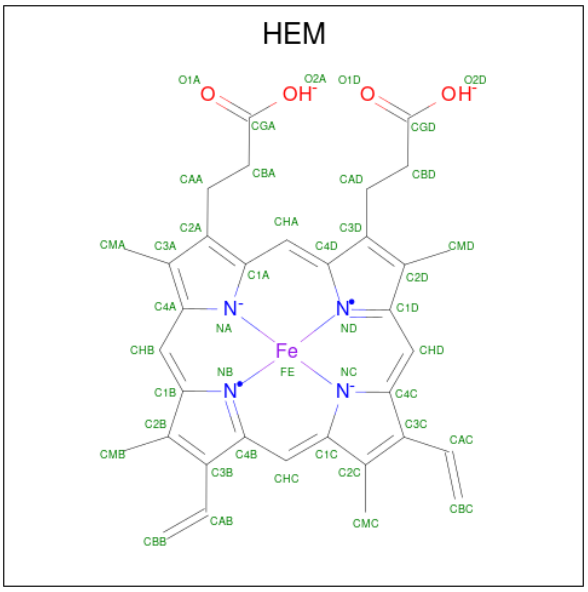
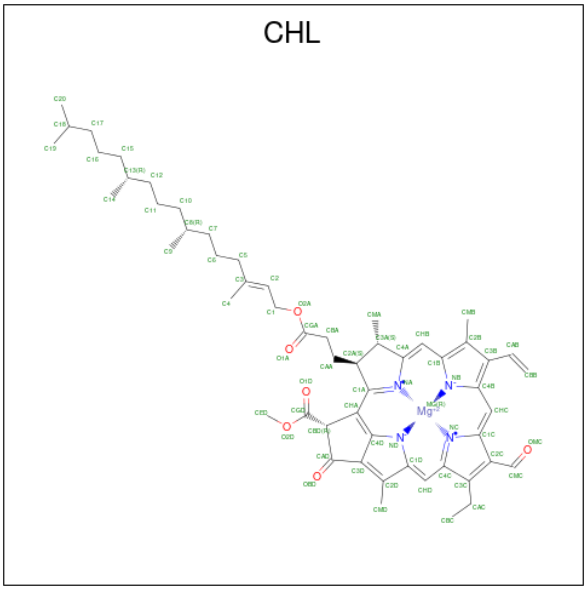
Mol	Chain	Residues	Atoms				AltConf
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			37	26	10	1	
37	G	1	Total	C	O	P	0
			49	38	10	1	
37	L	1	Total	C	O	P	0
			49	38	10	1	
37	N	1	Total	C	O	P	0
			49	38	10	1	
37	R	1	Total	C	O	P	0
			49	38	10	1	
37	S	1	Total	C	O	P	0
			49	38	10	1	
37	Y	1	Total	C	O	P	0
			49	38	10	1	
37	d	1	Total	C	O	P	0
			43	32	10	1	
37	d	1	Total	C	O	P	0
			49	38	10	1	
37	d	1	Total	C	O	P	0
			37	26	10	1	
37	g	1	Total	C	O	P	0
			49	38	10	1	
37	l	1	Total	C	O	P	0
			49	38	10	1	
37	n	1	Total	C	O	P	0
			49	38	10	1	
37	r	1	Total	C	O	P	0
			49	38	10	1	
37	s	1	Total	C	O	P	0
			49	38	10	1	
37	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
38	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
38	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	R	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	S	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	S	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
39	S	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	S	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
39	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
39	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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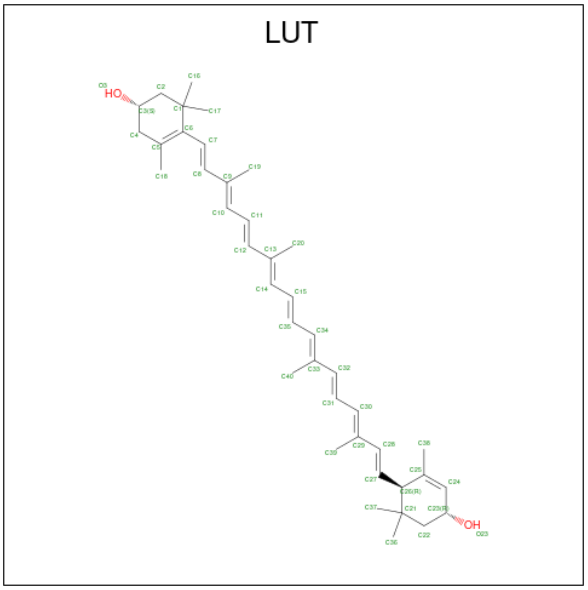
Mol	Chain	Residues	Atoms					AltConf
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 40 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
40	G	1	Total	C	O	0
			42	40	2	
40	G	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	R	1	Total	C	O	0
			42	40	2	

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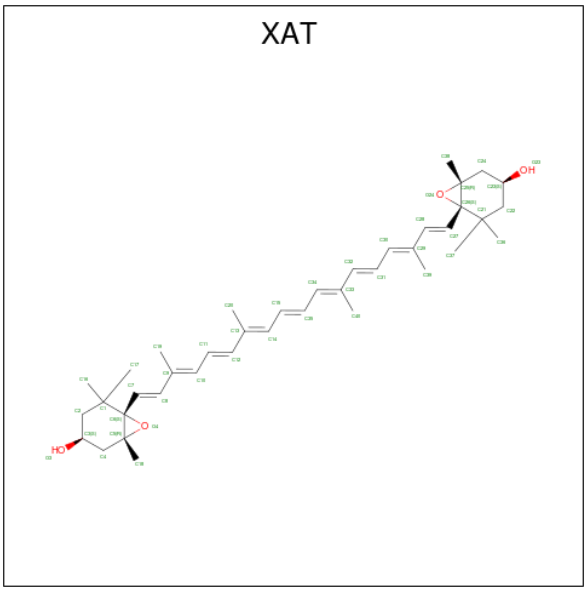
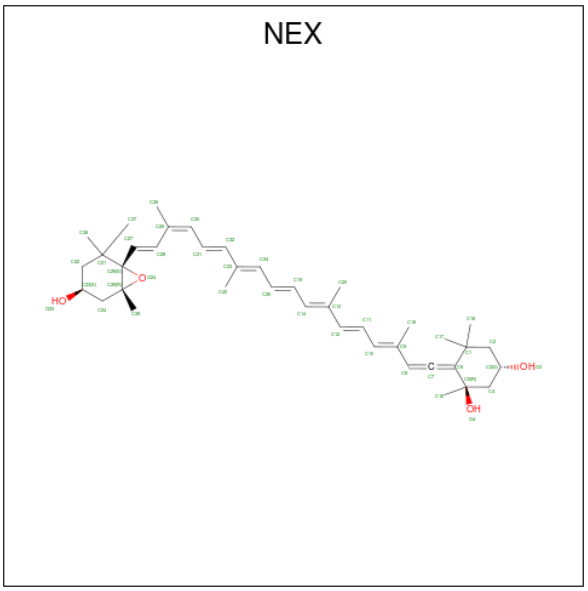
Mol	Chain	Residues	Atoms	AltConf
40	S	1	Total C O 42 40 2	0
40	S	1	Total C O 42 40 2	0
40	Y	1	Total C O 42 40 2	0
40	Y	1	Total C O 42 40 2	0
40	g	1	Total C O 42 40 2	0
40	g	1	Total C O 42 40 2	0
40	n	1	Total C O 42 40 2	0
40	n	1	Total C O 42 40 2	0
40	r	1	Total C O 42 40 2	0
40	s	1	Total C O 42 40 2	0
40	s	1	Total C O 42 40 2	0
40	y	1	Total C O 42 40 2	0
40	y	1	Total C O 42 40 2	0

- Molecule 41 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
41	G	1	Total	C	O	0
			44	40	4	
41	G	1	Total	C	O	0
			44	40	4	
41	N	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	g	1	Total	C	O	0
			44	40	4	
41	g	1	Total	C	O	0
			44	40	4	
41	n	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	

- Molecule 42 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
42	G	1	Total C O 44 40 4	0
42	N	1	Total C O 44 40 4	0
42	R	1	Total C O 44 40 4	0
42	S	1	Total C O 44 40 4	0
42	Y	1	Total C O 44 40 4	0
42	g	1	Total C O 44 40 4	0
42	n	1	Total C O 44 40 4	0
42	r	1	Total C O 44 40 4	0
42	s	1	Total C O 44 40 4	0
42	y	1	Total C O 44 40 4	0

- Molecule 43 is water.

Mol	Chain	Residues	Atoms	AltConf
43	A	82	Total O 82 82	0
43	B	115	Total O 115 115	0

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Mol	Chain	Residues	Atoms	AltConf
43	C	104	Total O 104 104	0
43	D	78	Total O 78 78	0
43	E	19	Total O 19 19	0
43	F	3	Total O 3 3	0
43	G	5	Total O 5 5	0
43	H	15	Total O 15 15	0
43	I	6	Total O 6 6	0
43	J	4	Total O 4 4	0
43	K	5	Total O 5 5	0
43	L	9	Total O 9 9	0
43	M	3	Total O 3 3	0
43	N	5	Total O 5 5	0
43	O	39	Total O 39 39	0
43	P	17	Total O 17 17	0
43	Q	1	Total O 1 1	0
43	R	19	Total O 19 19	0
43	S	5	Total O 5 5	0
43	T	7	Total O 7 7	0
43	U	1	Total O 1 1	0
43	W	18	Total O 18 18	0
43	X	5	Total O 5 5	0

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Mol	Chain	Residues	Atoms	AltConf
43	Y	36	Total O 36 36	0
43	Z	2	Total O 2 2	0
43	a	90	Total O 90 90	0
43	b	114	Total O 114 114	0
43	c	100	Total O 100 100	0
43	d	76	Total O 76 76	0
43	e	19	Total O 19 19	0
43	f	3	Total O 3 3	0
43	g	5	Total O 5 5	0
43	h	15	Total O 15 15	0
43	i	6	Total O 6 6	0
43	j	4	Total O 4 4	0
43	k	5	Total O 5 5	0
43	l	9	Total O 9 9	0
43	m	3	Total O 3 3	0
43	n	5	Total O 5 5	0
43	o	38	Total O 38 38	0
43	p	17	Total O 17 17	0
43	q	1	Total O 1 1	0
43	r	19	Total O 19 19	0
43	s	5	Total O 5 5	0

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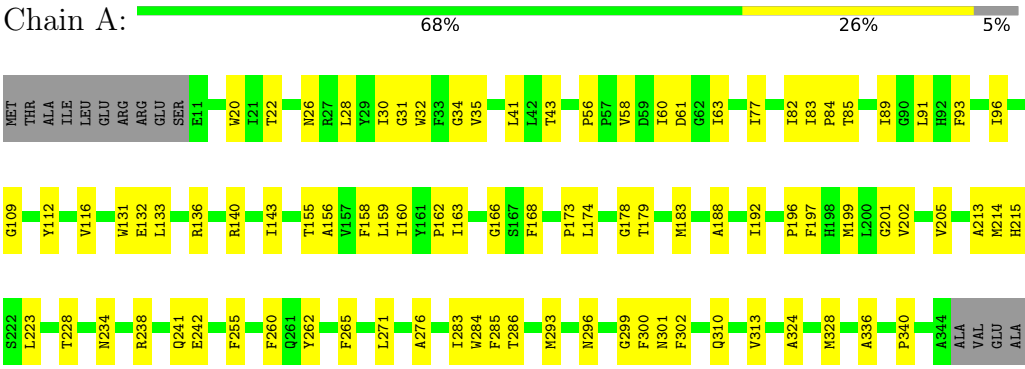
Mol	Chain	Residues	Atoms	AltConf
43	t	7	Total O 7 7	0
43	u	1	Total O 1 1	0
43	w	18	Total O 18 18	0
43	x	5	Total O 5 5	0
43	y	36	Total O 36 36	0
43	z	2	Total O 2 2	0

3 Residue-property plots (i)

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

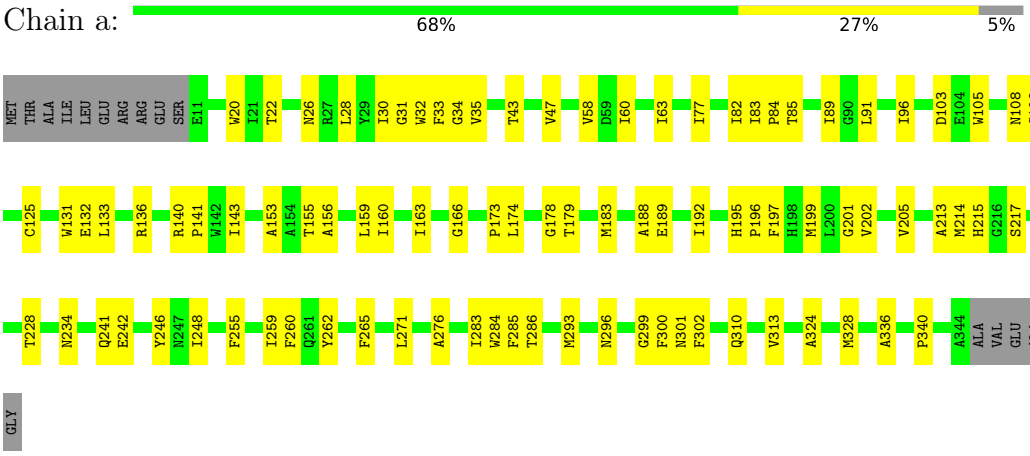
• Molecule 1: Photosystem II protein D1

Chain A:



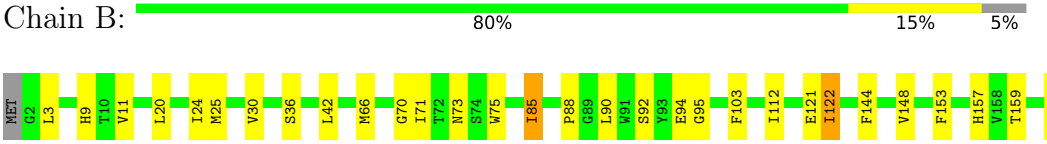
• Molecule 1: Photosystem II protein D1

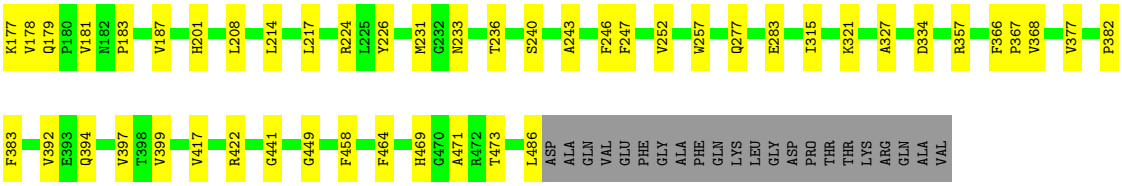
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

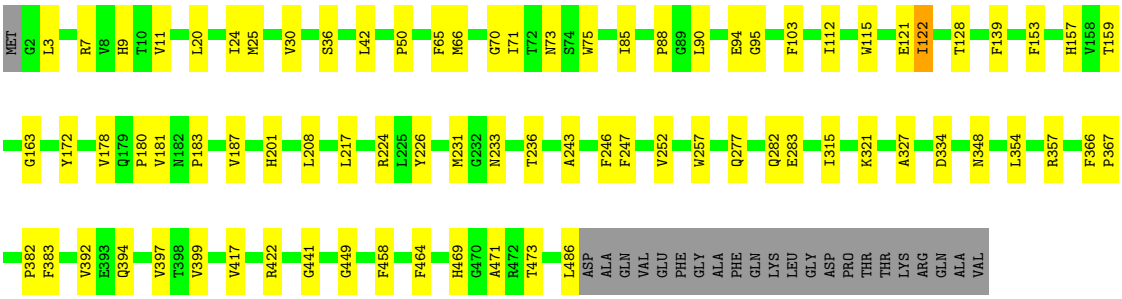
Chain B:





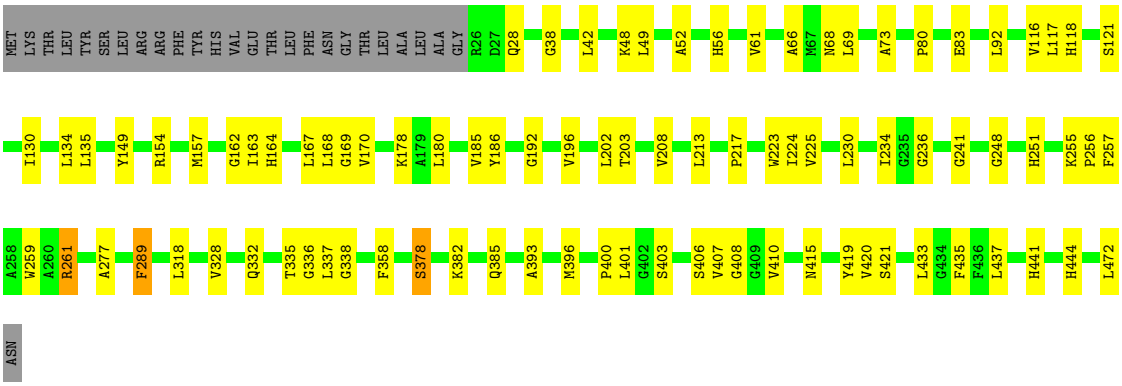
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



• Molecule 3: Photosystem II CP43 reaction center protein

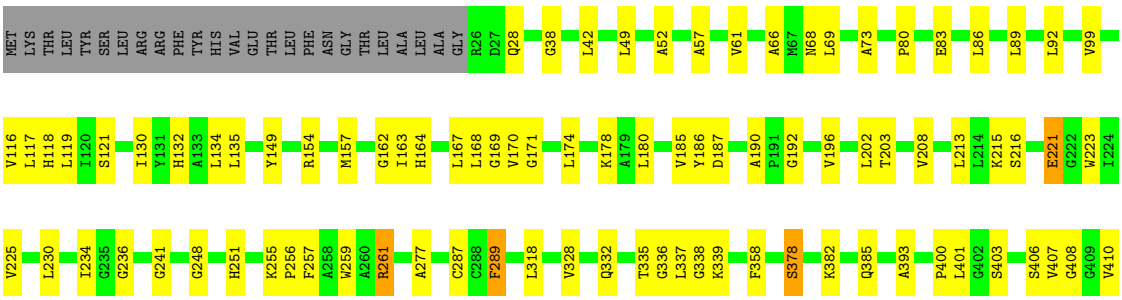
Chain C:



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



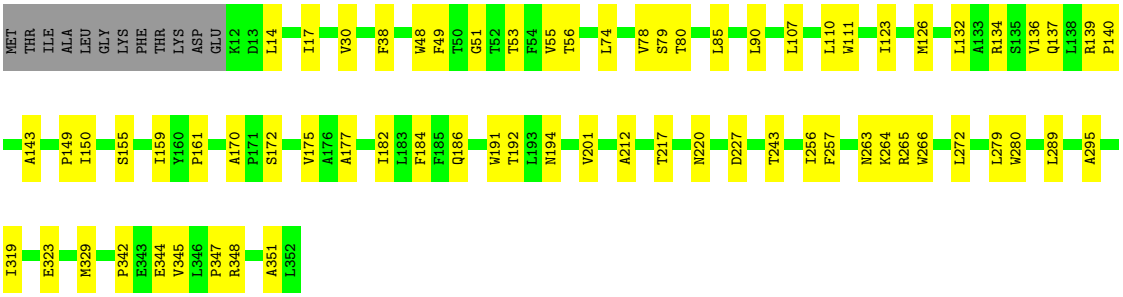




• Molecule 4: Photosystem II D2 protein

Chain D:





• Molecule 4: Photosystem II D2 protein

Chain d:

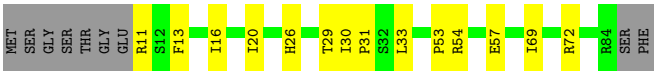




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:





• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

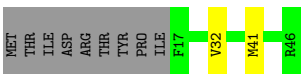




• Molecule 6: Cytochrome b559 subunit beta

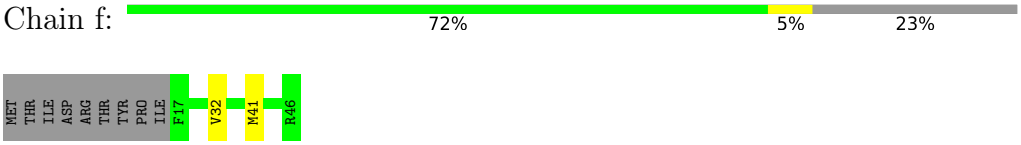
Chain F:





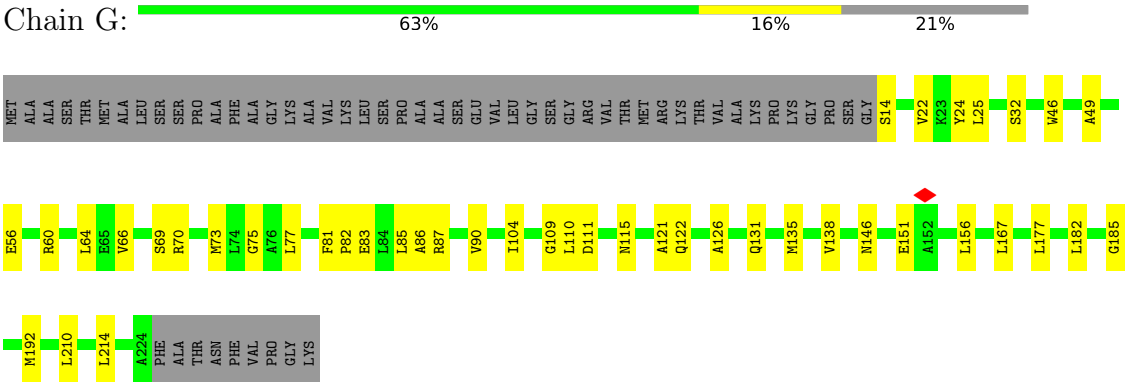
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



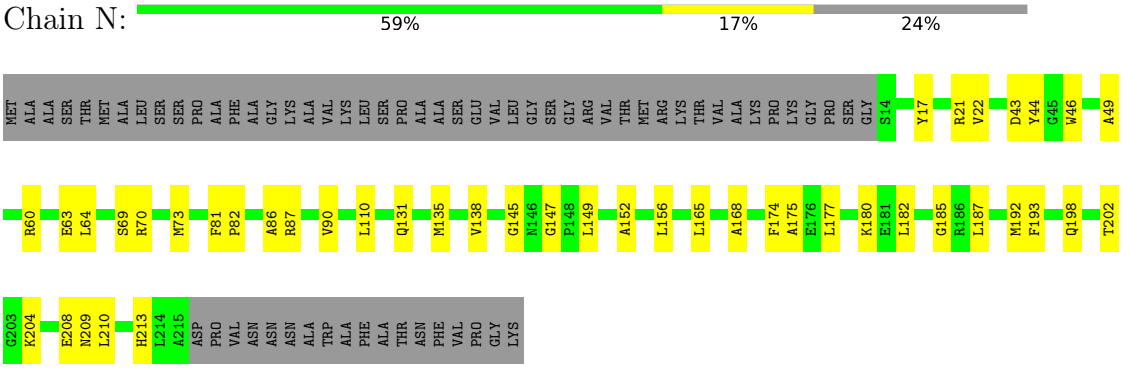
• Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain G:



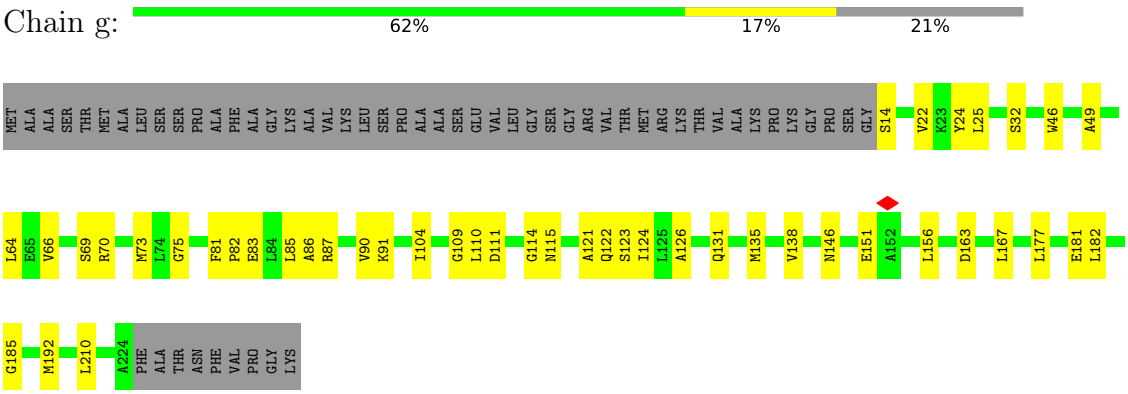
• Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain N:



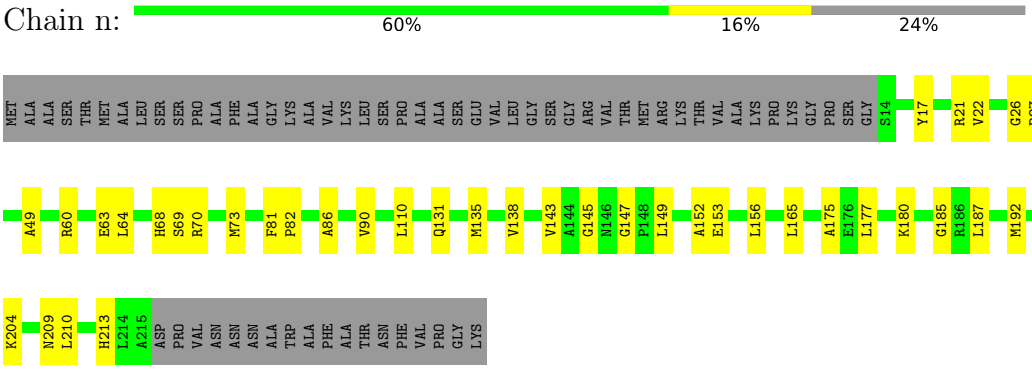
• Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain g:



• Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

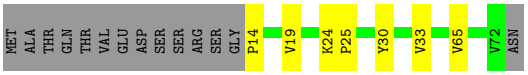
Chain n:



• Molecule 8: Photosystem II reaction center protein H

Chain H:

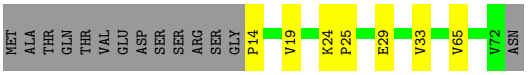




• Molecule 8: Photosystem II reaction center protein H

Chain h:

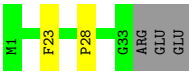




• Molecule 9: Photosystem II reaction center protein I

Chain I:





• Molecule 9: Photosystem II reaction center protein I

Chain i:

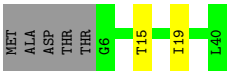




• Molecule 10: Photosystem II reaction center protein J

Chain J:





• Molecule 10: Photosystem II reaction center protein J

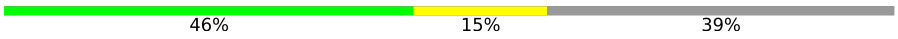
Chain j:

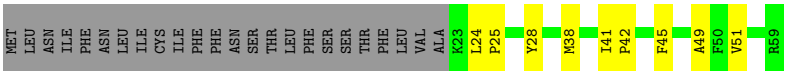




• Molecule 11: Photosystem II reaction center protein K

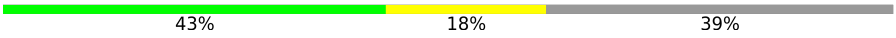
Chain K:

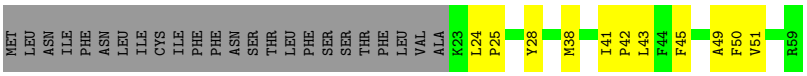




• Molecule 11: Photosystem II reaction center protein K

Chain k:





• Molecule 12: Photosystem II reaction center protein L

Chain L:

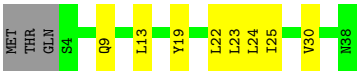




• Molecule 12: Photosystem II reaction center protein L

Chain l:

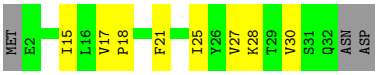




• Molecule 13: Photosystem II reaction center protein M

Chain M:

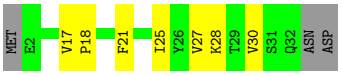




• Molecule 13: Photosystem II reaction center protein M

Chain m:

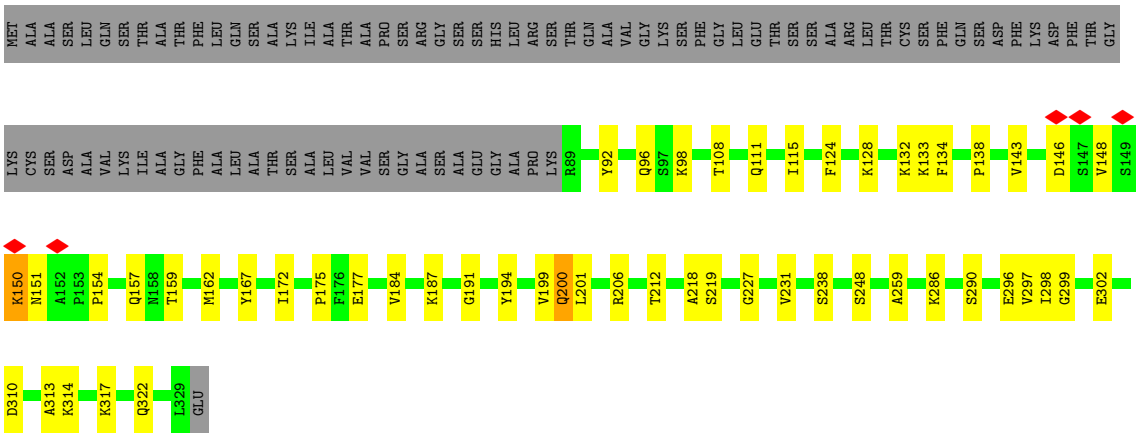


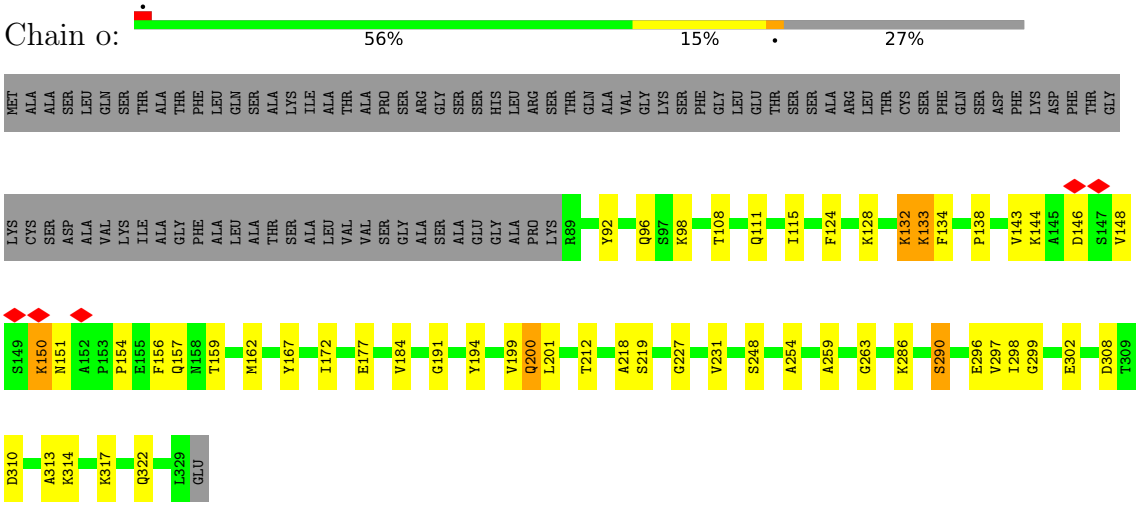


• Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain O:







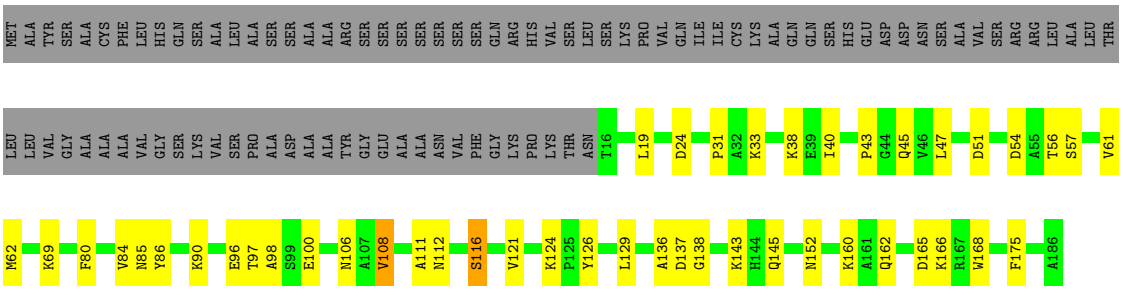
• Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain o:

• Molecule 15: Oxygen-evolving enhancer protein 2-1, chloroplastic

Chain P:

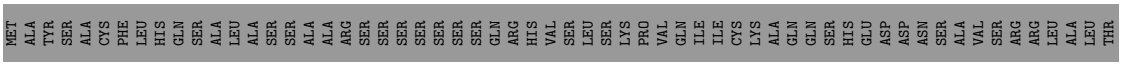


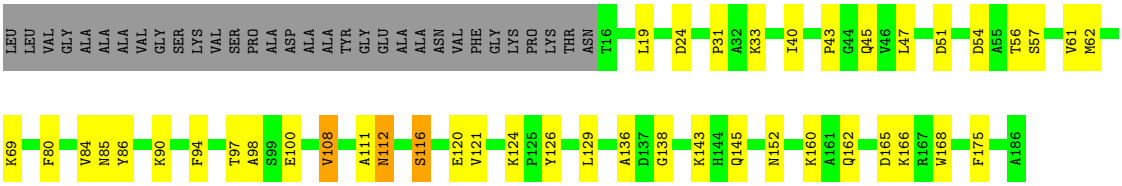


• Molecule 15: Oxygen-evolving enhancer protein 2-1, chloroplastic

Chain p:



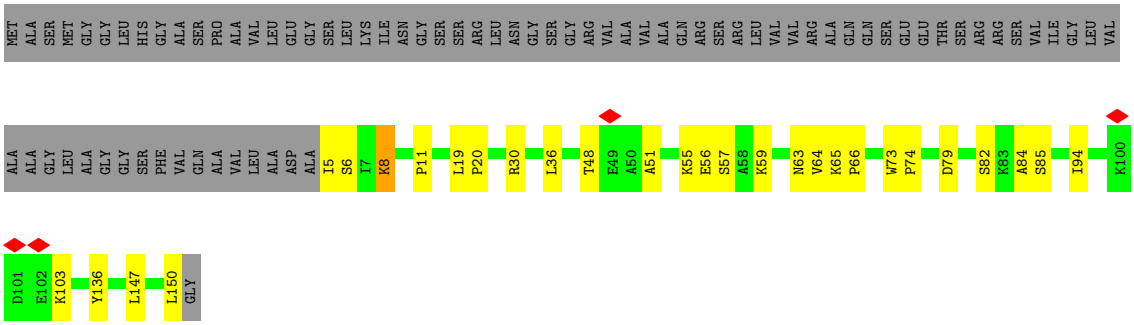




• Molecule 16: Oxygen-evolving enhancer protein 3-1, chloroplastic

Chain Q:

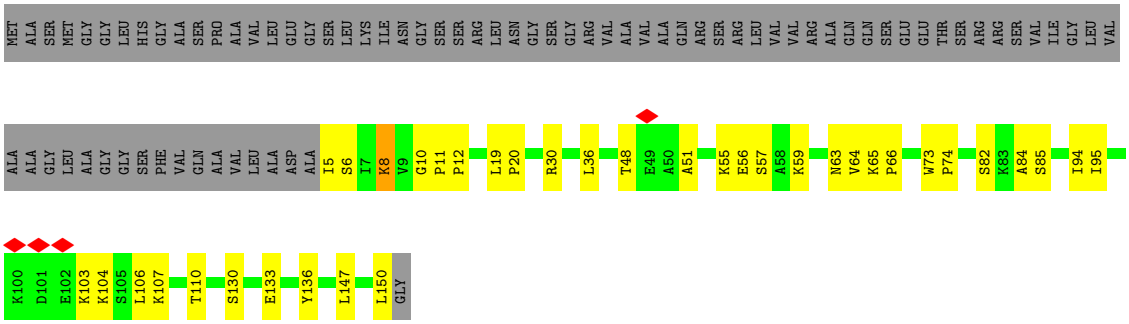




• Molecule 16: Oxygen-evolving enhancer protein 3-1, chloroplastic

Chain q:

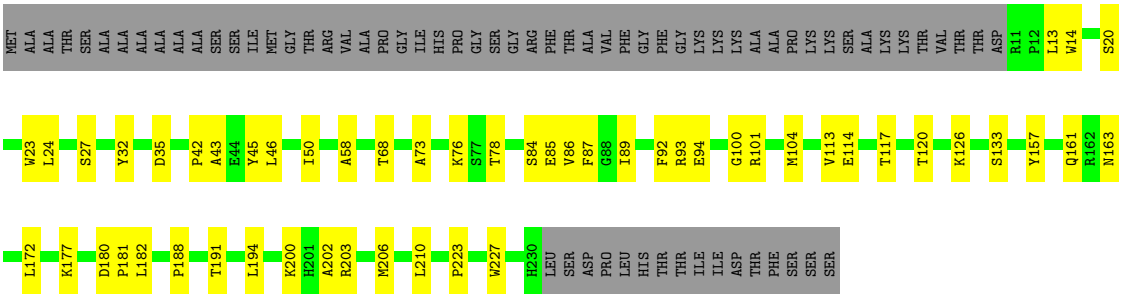




• Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain R:

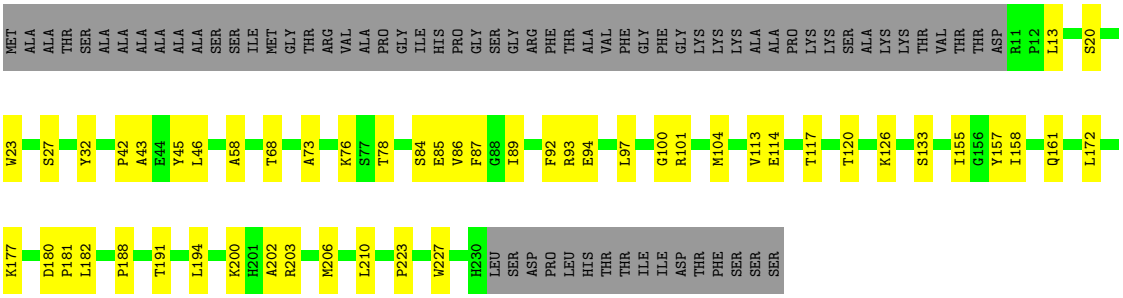




• Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain r:

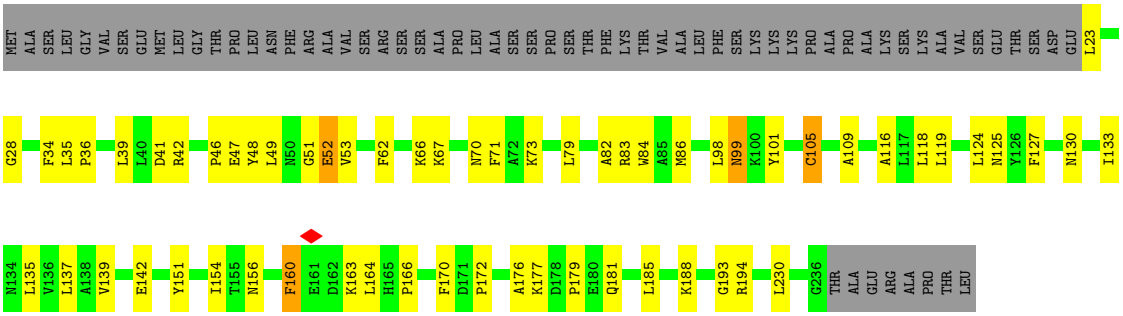




• Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

Chain S:

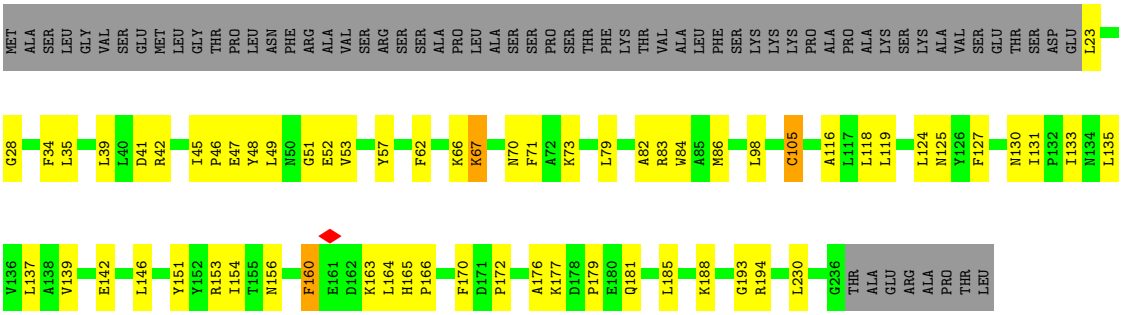




• Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

Chain s:

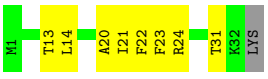




• Molecule 19: Photosystem II reaction center protein T

Chain T:

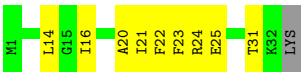




• Molecule 19: Photosystem II reaction center protein T

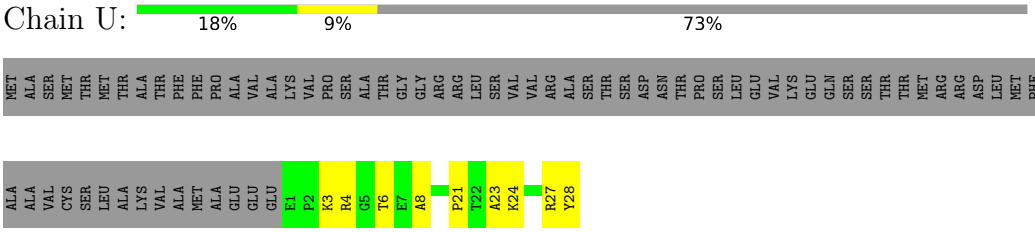
Chain t:





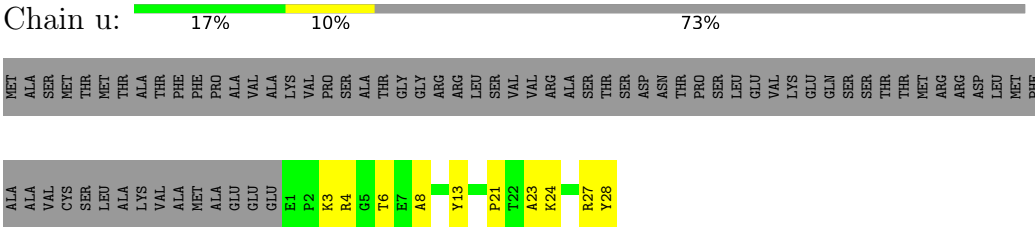
• Molecule 20: Photosystem II 5 kDa protein, chloroplastic

Chain U:



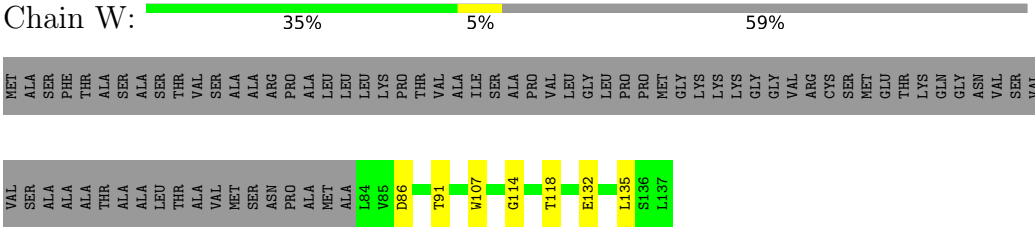
• Molecule 20: Photosystem II 5 kDa protein, chloroplastic

Chain u:



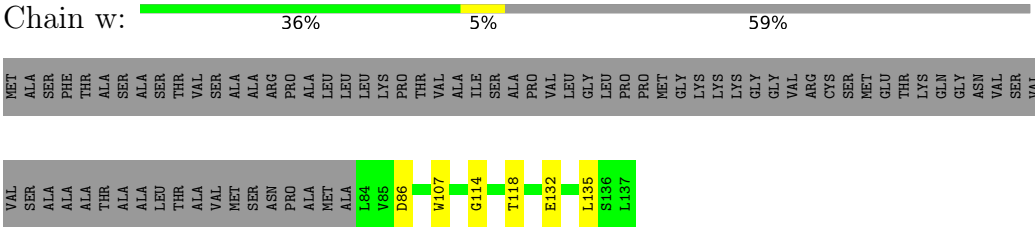
• Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain W:



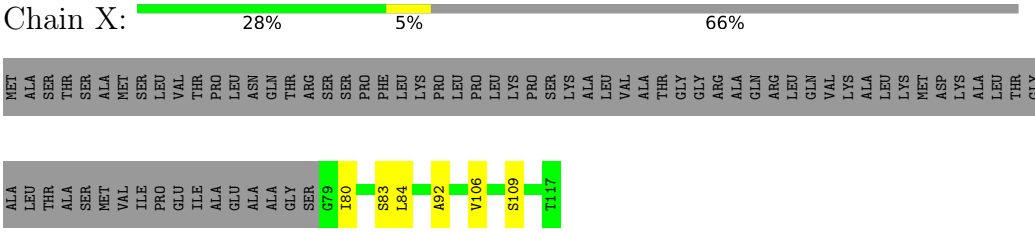
• Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain w:



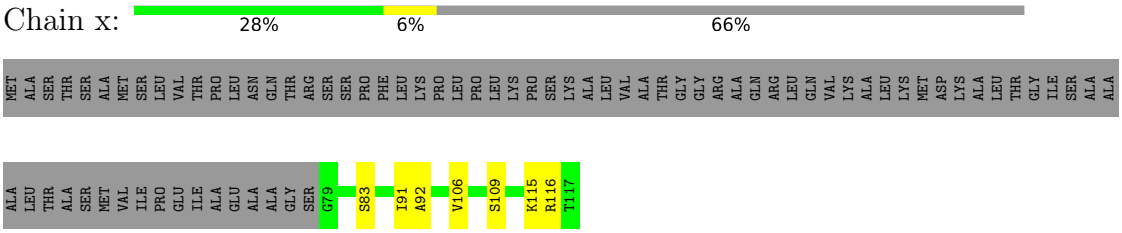
• Molecule 22: Expressed protein

Chain X:



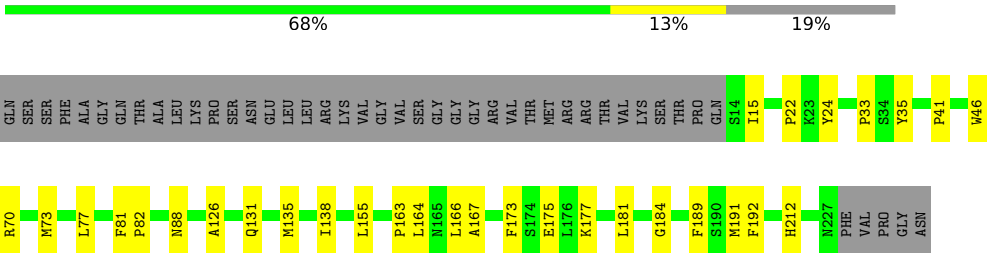
• Molecule 22: Expressed protein

Chain x:



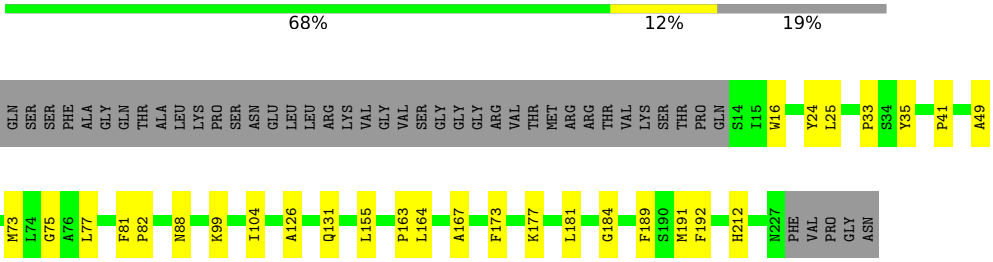
• Molecule 23: Chlorophyll a-b binding protein 2.1, chloroplastic

Chain Y:



• Molecule 23: Chlorophyll a-b binding protein 2.1, chloroplastic

Chain y:



• Molecule 24: Photosystem II reaction center protein Z

Chain Z:



• Molecule 24: Photosystem II reaction center protein Z

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	72301	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.641	Depositor
Minimum map value	-0.646	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.149	Depositor
Map size (Å)	560.952, 560.952, 560.952	wwPDB
Map dimensions	784, 784, 784	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71550006, 0.71550006, 0.71550006	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, FE2, BCT, LHG, HEM, SQD, DGD, CLA, PL9, LMT, BCR, LUT, XAT, OEX, CL, NEX, PHO, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/2694	0.36	0/3674
1	a	0.26	0/2694	0.36	0/3674
2	B	0.25	0/3930	0.33	0/5354
2	b	0.25	0/3930	0.34	0/5354
3	C	0.24	0/3583	0.33	0/4883
3	c	0.24	0/3583	0.33	0/4883
4	D	0.26	0/2806	0.35	0/3825
4	d	0.26	0/2806	0.35	0/3825
5	E	0.20	0/622	0.29	0/846
5	e	0.19	0/622	0.29	0/846
6	F	0.21	0/248	0.32	0/335
6	f	0.21	0/248	0.33	0/335
7	G	0.16	0/1653	0.29	0/2249
7	N	0.18	0/1580	0.31	0/2146
7	g	0.16	0/1653	0.28	0/2249
7	n	0.18	0/1580	0.31	0/2146
8	H	0.24	0/447	0.33	0/608
8	h	0.24	0/447	0.34	0/608
9	I	0.23	0/274	0.30	0/371
9	i	0.23	0/274	0.30	0/371
10	J	0.14	0/261	0.26	0/354
10	j	0.14	0/261	0.24	0/354
11	K	0.20	0/313	0.33	0/428
11	k	0.20	0/313	0.33	0/428
12	L	0.24	0/301	0.28	0/409
12	l	0.25	0/301	0.27	0/409
13	M	0.21	0/246	0.34	0/337
13	m	0.21	0/246	0.34	0/337
14	O	0.21	0/1867	0.37	0/2525
14	o	0.21	0/1867	0.37	0/2525
15	P	0.19	0/1349	0.34	0/1827

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	p	0.19	0/1349	0.35	0/1827
16	Q	0.18	0/1162	0.35	0/1575
16	q	0.18	0/1162	0.35	0/1575
17	R	0.19	0/1758	0.34	0/2395
17	r	0.19	0/1758	0.34	0/2395
18	S	0.18	0/1698	0.39	0/2305
18	s	0.18	0/1698	0.38	0/2305
19	T	0.20	0/268	0.28	0/362
19	t	0.21	0/268	0.28	0/362
20	U	0.18	0/222	0.37	0/296
20	u	0.17	0/222	0.39	0/296
21	W	0.20	0/438	0.37	0/594
21	w	0.20	0/438	0.36	0/594
22	X	0.19	0/282	0.32	0/383
22	x	0.19	0/282	0.32	0/383
23	Y	0.20	0/1704	0.32	0/2319
23	y	0.20	0/1704	0.32	0/2319
24	Z	0.17	0/466	0.37	0/639
24	z	0.18	0/466	0.33	0/639
All	All	0.22	0/60344	0.34	0/82078

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
24	z	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	z	3	ILE	Peptide

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	2613	0	2521	78	0
1	a	2613	0	2521	79	0
2	B	3800	0	3681	70	0
2	b	3800	0	3681	72	0
3	C	3468	0	3400	73	0
3	c	3468	0	3400	76	0
4	D	2713	0	2609	59	0
4	d	2713	0	2609	61	0
5	E	604	0	586	10	0
5	e	604	0	586	9	0
6	F	241	0	246	2	0
6	f	241	0	246	2	0
7	G	1606	0	1538	34	0
7	N	1536	0	1480	35	0
7	g	1606	0	1538	35	0
7	n	1536	0	1480	34	0
8	H	438	0	465	7	0
8	h	438	0	465	7	0
9	I	266	0	276	2	0
9	i	266	0	276	2	0
10	J	255	0	269	2	0
10	j	255	0	269	2	0
11	K	302	0	313	8	0
11	k	302	0	313	10	0
12	L	293	0	283	7	0
12	l	293	0	283	8	0
13	M	242	0	267	10	0
13	m	242	0	267	9	0
14	O	1829	0	1792	38	0
14	o	1829	0	1792	37	0
15	P	1319	0	1262	30	0
15	p	1319	0	1262	28	0
16	Q	1139	0	1171	21	0
16	q	1139	0	1171	27	0
17	R	1710	0	1668	41	0
17	r	1710	0	1668	38	0
18	S	1653	0	1639	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	s	1653	0	1639	54	0
19	T	261	0	280	9	0
19	t	261	0	280	9	0
20	U	219	0	235	6	0
20	u	219	0	235	7	0
21	W	427	0	405	5	0
21	w	427	0	405	4	0
22	X	279	0	307	5	0
22	x	279	0	307	7	0
23	Y	1652	0	1581	33	0
23	y	1652	0	1581	34	0
24	Z	456	0	483	8	0
24	z	456	0	483	7	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	125	0	131	3	0
26	B	1040	0	1152	60	0
26	C	828	0	903	42	0
26	D	244	0	255	15	0
26	G	424	0	378	17	0
26	N	424	0	378	15	0
26	R	522	0	456	21	0
26	S	441	0	351	21	0
26	Y	472	0	477	27	0
26	a	190	0	203	5	0
26	b	1040	0	1152	60	0
26	c	828	0	903	47	0
26	d	179	0	183	15	0
26	g	424	0	378	16	0
26	n	424	0	378	13	0
26	r	522	0	456	23	0
26	s	441	0	351	20	0
26	y	472	0	477	27	0
27	A	64	0	74	2	0
27	D	64	0	74	7	0
27	a	64	0	74	1	0
27	d	64	0	74	8	0
28	A	40	0	56	1	0
28	B	120	0	168	11	0
28	C	80	0	112	6	0
28	D	40	0	56	0	0
28	H	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	40	0	56	4	0
28	K	40	0	56	5	0
28	T	40	0	56	6	0
28	a	40	0	56	1	0
28	b	120	0	168	13	0
28	c	80	0	112	7	0
28	d	40	0	56	0	0
28	h	40	0	56	3	0
28	j	40	0	56	4	0
28	k	40	0	56	5	0
28	t	40	0	56	6	0
29	A	104	0	145	7	0
29	B	54	0	78	2	0
29	W	33	0	30	0	0
29	a	104	0	145	8	0
29	b	54	0	78	3	0
29	w	33	0	30	0	0
30	A	22	0	25	3	0
30	D	55	0	80	3	0
30	a	22	0	25	4	0
30	d	55	0	80	2	0
31	A	1	0	0	0	0
31	a	1	0	0	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	62	0	82	3	0
33	C	179	0	232	10	0
33	Y	43	0	44	3	0
33	b	62	0	82	3	0
33	c	179	0	232	8	0
33	y	43	0	44	2	0
34	B	51	0	72	2	0
34	C	102	0	144	3	0
34	D	46	0	62	1	0
34	W	48	0	66	3	0
34	b	51	0	72	3	0
34	c	102	0	144	2	0
34	d	46	0	62	2	0
34	w	48	0	66	2	0
35	C	10	0	0	2	0
35	a	10	0	0	3	0
36	D	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	d	35	0	46	0	0
37	D	129	0	177	11	0
37	G	49	0	74	6	0
37	L	49	0	74	2	0
37	N	49	0	74	5	0
37	R	49	0	74	0	0
37	S	49	0	74	2	0
37	Y	49	0	74	4	0
37	d	129	0	177	10	0
37	g	49	0	74	8	0
37	l	49	0	74	3	0
37	n	49	0	74	5	0
37	r	49	0	74	2	0
37	s	49	0	74	2	0
37	y	49	0	74	4	0
38	E	43	0	30	5	0
38	e	43	0	30	4	0
39	G	314	0	251	24	0
39	N	314	0	251	17	0
39	R	198	0	144	7	0
39	S	201	0	147	14	0
39	Y	282	0	251	17	0
39	g	314	0	251	26	0
39	n	314	0	251	19	0
39	r	198	0	144	8	0
39	s	201	0	147	15	0
39	y	282	0	251	16	0
40	G	84	0	112	5	0
40	N	84	0	112	7	0
40	R	42	0	56	5	0
40	S	84	0	112	6	0
40	Y	84	0	112	12	0
40	g	84	0	112	7	0
40	n	84	0	112	7	0
40	r	42	0	56	6	0
40	s	84	0	112	5	0
40	y	84	0	112	11	0
41	G	88	0	112	10	0
41	N	44	0	56	6	0
41	R	44	0	56	1	0
41	g	88	0	112	10	0
41	n	44	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	r	44	0	56	2	0
42	G	44	0	56	4	0
42	N	44	0	56	2	0
42	R	44	0	56	3	0
42	S	44	0	56	7	0
42	Y	44	0	56	3	0
42	g	44	0	56	4	0
42	n	44	0	56	1	0
42	r	44	0	56	4	0
42	s	44	0	56	6	0
42	y	44	0	56	3	0
43	A	82	0	0	0	0
43	B	115	0	0	0	0
43	C	104	0	0	0	0
43	D	78	0	0	1	0
43	E	19	0	0	1	0
43	F	3	0	0	0	0
43	G	5	0	0	0	0
43	H	15	0	0	1	0
43	I	6	0	0	0	0
43	J	4	0	0	0	0
43	K	5	0	0	0	0
43	L	9	0	0	0	0
43	M	3	0	0	0	0
43	N	5	0	0	0	0
43	O	39	0	0	0	0
43	P	17	0	0	0	0
43	Q	1	0	0	0	0
43	R	19	0	0	1	0
43	S	5	0	0	0	0
43	T	7	0	0	0	0
43	U	1	0	0	0	0
43	W	18	0	0	0	0
43	X	5	0	0	0	0
43	Y	36	0	0	0	0
43	Z	2	0	0	0	0
43	a	90	0	0	1	0
43	b	114	0	0	0	0
43	c	100	0	0	0	0
43	d	76	0	0	1	0
43	e	19	0	0	1	0
43	f	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	g	5	0	0	0	0
43	h	15	0	0	1	0
43	i	6	0	0	0	0
43	j	4	0	0	0	0
43	k	5	0	0	0	0
43	l	9	0	0	0	0
43	m	3	0	0	0	0
43	n	5	0	0	0	0
43	o	38	0	0	0	0
43	p	17	0	0	0	0
43	q	1	0	0	0	0
43	r	19	0	0	1	0
43	s	5	0	0	0	0
43	t	7	0	0	0	0
43	u	1	0	0	0	0
43	w	18	0	0	0	0
43	x	5	0	0	0	0
43	y	36	0	0	0	0
43	z	2	0	0	0	0
All	All	76824	0	75622	1602	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 11.

The worst 5 of 1602 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)
35:a:408:OEX:CA1	35:a:408:OEX:O1	1.31	1.05
35:C:501:OEX:O1	35:C:501:OEX:CA1	1.40	0.96
3:c:68:ASN:HD21	3:c:92:LEU:HD11	1.34	0.92
4:D:175:VAL:HG13	26:D:412:CLA:HED1	1.56	0.87
39:s:316:CHL:HBB2	39:s:317:CHL:HBB1	1.55	0.86

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	332/353 (94%)	328 (99%)	4 (1%)	0	100	100
1	a	332/353 (94%)	327 (98%)	5 (2%)	0	100	100
2	B	483/508 (95%)	476 (99%)	7 (1%)	0	100	100
2	b	483/508 (95%)	477 (99%)	6 (1%)	0	100	100
3	C	445/473 (94%)	437 (98%)	8 (2%)	0	100	100
3	c	445/473 (94%)	438 (98%)	7 (2%)	0	100	100
4	D	339/353 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	339/353 (96%)	332 (98%)	7 (2%)	0	100	100
5	E	72/83 (87%)	71 (99%)	1 (1%)	0	100	100
5	e	72/83 (87%)	71 (99%)	1 (1%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	0	100	100
6	f	28/39 (72%)	28 (100%)	0	0	100	100
7	G	209/267 (78%)	206 (99%)	3 (1%)	0	100	100
7	N	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
7	g	209/267 (78%)	206 (99%)	3 (1%)	0	100	100
7	n	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
9	I	31/36 (86%)	31 (100%)	0	0	100	100
9	i	31/36 (86%)	31 (100%)	0	0	100	100
10	J	33/40 (82%)	33 (100%)	0	0	100	100
10	j	33/40 (82%)	33 (100%)	0	0	100	100
11	K	35/61 (57%)	35 (100%)	0	0	100	100
11	k	35/61 (57%)	35 (100%)	0	0	100	100
12	L	33/38 (87%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	33/38 (87%)	33 (100%)	0	0	100	100
13	M	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
13	m	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
14	O	239/332 (72%)	228 (95%)	11 (5%)	0	100	100
14	o	239/332 (72%)	228 (95%)	11 (5%)	0	100	100
15	P	169/263 (64%)	161 (95%)	8 (5%)	0	100	100
15	p	169/263 (64%)	162 (96%)	7 (4%)	0	100	100
16	Q	144/224 (64%)	136 (94%)	8 (6%)	0	100	100
16	q	144/224 (64%)	136 (94%)	8 (6%)	0	100	100
17	R	218/290 (75%)	210 (96%)	8 (4%)	0	100	100
17	r	218/290 (75%)	211 (97%)	7 (3%)	0	100	100
18	S	212/280 (76%)	204 (96%)	8 (4%)	0	100	100
18	s	212/280 (76%)	203 (96%)	9 (4%)	0	100	100
19	T	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
19	t	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
20	U	26/103 (25%)	24 (92%)	2 (8%)	0	100	100
20	u	26/103 (25%)	23 (88%)	3 (12%)	0	100	100
21	W	52/133 (39%)	47 (90%)	4 (8%)	1 (2%)	6	4
21	w	52/133 (39%)	47 (90%)	4 (8%)	1 (2%)	6	4
22	X	37/116 (32%)	36 (97%)	1 (3%)	0	100	100
22	x	37/116 (32%)	36 (97%)	1 (3%)	0	100	100
23	Y	212/265 (80%)	206 (97%)	6 (3%)	0	100	100
23	y	212/265 (80%)	206 (97%)	6 (3%)	0	100	100
24	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
24	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	7448/9452 (79%)	7256 (97%)	190 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	W	86	ASP
21	w	86	ASP

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	270/285 (95%)	270 (100%)	0	100	100
1	a	270/285 (95%)	270 (100%)	0	100	100
2	B	384/402 (96%)	381 (99%)	3 (1%)	73	81
2	b	384/402 (96%)	381 (99%)	3 (1%)	73	81
3	C	351/373 (94%)	347 (99%)	4 (1%)	65	75
3	c	351/373 (94%)	344 (98%)	7 (2%)	48	62
4	D	273/283 (96%)	269 (98%)	4 (2%)	57	69
4	d	273/283 (96%)	271 (99%)	2 (1%)	76	83
5	E	66/73 (90%)	66 (100%)	0	100	100
5	e	66/73 (90%)	65 (98%)	1 (2%)	57	69
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	161/201 (80%)	159 (99%)	2 (1%)	63	74
7	N	154/201 (77%)	154 (100%)	0	100	100
7	g	161/201 (80%)	158 (98%)	3 (2%)	50	63
7	n	154/201 (77%)	153 (99%)	1 (1%)	78	85
8	H	49/61 (80%)	49 (100%)	0	100	100
8	h	49/61 (80%)	49 (100%)	0	100	100
9	I	30/33 (91%)	30 (100%)	0	100	100
9	i	30/33 (91%)	30 (100%)	0	100	100
10	J	26/30 (87%)	26 (100%)	0	100	100
10	j	26/30 (87%)	24 (92%)	2 (8%)	12	14
11	K	32/55 (58%)	32 (100%)	0	100	100
11	k	32/55 (58%)	32 (100%)	0	100	100
12	L	33/36 (92%)	33 (100%)	0	100	100
12	l	33/36 (92%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	27/30 (90%)	27 (100%)	0	100	100
13	m	27/30 (90%)	27 (100%)	0	100	100
14	O	200/268 (75%)	195 (98%)	5 (2%)	42	54
14	o	200/268 (75%)	194 (97%)	6 (3%)	36	48
15	P	139/210 (66%)	135 (97%)	4 (3%)	37	49
15	p	139/210 (66%)	134 (96%)	5 (4%)	31	42
16	Q	124/178 (70%)	121 (98%)	3 (2%)	43	56
16	q	124/178 (70%)	121 (98%)	3 (2%)	43	56
17	R	174/225 (77%)	170 (98%)	4 (2%)	44	57
17	r	174/225 (77%)	170 (98%)	4 (2%)	44	57
18	S	165/219 (75%)	160 (97%)	5 (3%)	36	48
18	s	165/219 (75%)	160 (97%)	5 (3%)	36	48
19	T	29/30 (97%)	29 (100%)	0	100	100
19	t	29/30 (97%)	28 (97%)	1 (3%)	32	45
20	U	23/82 (28%)	23 (100%)	0	100	100
20	u	23/82 (28%)	23 (100%)	0	100	100
21	W	47/102 (46%)	47 (100%)	0	100	100
21	w	47/102 (46%)	47 (100%)	0	100	100
22	X	33/92 (36%)	33 (100%)	0	100	100
22	x	33/92 (36%)	33 (100%)	0	100	100
23	Y	168/209 (80%)	166 (99%)	2 (1%)	63	74
23	y	168/209 (80%)	168 (100%)	0	100	100
24	Z	53/54 (98%)	51 (96%)	2 (4%)	29	41
24	z	53/54 (98%)	51 (96%)	2 (4%)	29	41
All	All	6072/7532 (81%)	5989 (99%)	83 (1%)	57	70

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	o	132	LYS
17	r	27	SER
14	o	150	LYS
15	p	112	ASN
18	s	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	234	ASN
4	d	263	ASN
1	a	304	GLN
3	c	332	GLN
6	f	45	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 332 ligands modelled in this entry, 6 are monoatomic - leaving 326 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	$\#\|Z\| > 2$
26	CLA	C	515	3	69,73,73	1.22	8 (11%)	83,113,113	1.27	8 (9%)
26	CLA	C	506	3	69,73,73	1.20	9 (13%)	83,113,113	1.22	6 (7%)
28	BCR	C	502	-	41,41,41	0.36	0	56,56,56	0.87	2 (3%)
37	LHG	N	301	26	48,48,48	0.52	0	51,54,54	0.47	0
26	CLA	N	319	37	53,57,73	1.40	8 (15%)	62,93,113	1.37	6 (9%)
42	NEX	G	315	-	38,46,46	1.55	8 (21%)	50,70,70	2.36	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	G	319	7	53,57,73	1.40	8 (15%)	62,93,113	1.36	6 (9%)
28	BCR	B	608	-	41,41,41	0.31	0	56,56,56	0.52	0
26	CLA	c	506	3	63,70,73	1.29	6 (9%)	73,103,113	0.98	3 (4%)
39	CHL	R	318	23,17	52,56,74	1.43	6 (11%)	58,92,114	2.08	13 (22%)
38	HEM	e	101	5,6	50,50,50	1.38	7 (14%)	66,82,82	1.26	7 (10%)
26	CLA	r	308	17	53,57,73	1.39	8 (15%)	62,93,113	1.32	6 (9%)
39	CHL	Y	314	43	54,58,74	1.44	6 (11%)	59,94,114	2.06	9 (15%)
26	CLA	Y	316	43	53,57,73	1.44	8 (15%)	62,93,113	1.29	8 (12%)
26	CLA	B	609	2	69,73,73	1.23	8 (11%)	83,113,113	1.26	8 (9%)
40	LUT	S	306	-	42,43,43	0.48	0	51,60,60	0.88	1 (1%)
29	SQD	a	413	-	49,50,54	0.79	1 (2%)	58,61,65	1.02	3 (5%)
41	XAT	g	309	-	39,47,47	1.14	4 (10%)	54,74,74	2.32	12 (22%)
42	NEX	y	307	-	38,46,46	1.59	9 (23%)	50,70,70	2.14	11 (22%)
28	BCR	b	619	-	41,41,41	0.33	0	56,56,56	0.56	0
26	CLA	S	308	37	53,57,73	1.38	9 (16%)	62,93,113	1.35	5 (8%)
40	LUT	n	317	-	42,43,43	0.48	0	51,60,60	0.84	1 (1%)
39	CHL	s	316	-	54,58,74	1.46	6 (11%)	59,94,114	1.99	11 (18%)
26	CLA	C	504	3	69,73,73	1.22	8 (11%)	83,113,113	1.31	5 (6%)
38	HEM	E	101	5,6	50,50,50	1.37	6 (12%)	66,82,82	1.25	7 (10%)
34	LMG	b	622	-	51,51,55	0.52	0	59,59,63	0.65	0
26	CLA	N	308	43	53,57,73	1.43	9 (16%)	62,93,113	1.27	7 (11%)
39	CHL	n	319	7	54,58,74	1.44	6 (11%)	59,94,114	2.04	10 (16%)
26	CLA	d	403	4	69,73,73	1.22	8 (11%)	83,113,113	1.24	7 (8%)
26	CLA	r	317	37	53,57,73	1.41	8 (15%)	62,93,113	1.39	6 (9%)
37	LHG	y	301	26	48,48,48	0.51	0	51,54,54	0.52	0
33	DGD	c	501	-	63,63,67	0.63	0	77,77,81	0.71	0
39	CHL	r	318	43	54,58,74	1.44	7 (12%)	59,94,114	2.04	14 (23%)
26	CLA	c	504	3	69,73,73	1.22	8 (11%)	83,113,113	1.28	9 (10%)
26	CLA	S	309	18	53,57,73	1.39	8 (15%)	62,93,113	1.41	6 (9%)
26	CLA	c	514	43	69,73,73	1.21	9 (13%)	83,113,113	1.23	9 (10%)
26	CLA	C	519	3	53,57,73	1.38	9 (16%)	62,93,113	1.38	7 (11%)
26	CLA	b	614	43	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
26	CLA	N	306	7	53,57,73	1.43	10 (18%)	62,93,113	1.40	6 (9%)
26	CLA	y	317	23	53,57,73	1.41	9 (16%)	62,93,113	1.29	6 (9%)
39	CHL	g	312	7	54,58,74	1.45	6 (11%)	59,94,114	2.05	10 (16%)
26	CLA	B	601	2	69,73,73	1.23	8 (11%)	83,113,113	1.18	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	XAT	R	304	-	39,47,47	1.16	4 (10%)	54,74,74	2.22	13 (24%)
26	CLA	y	316	23	69,73,73	1.23	8 (11%)	83,113,113	1.31	7 (8%)
26	CLA	R	307	17	53,57,73	2.71	11 (20%)	62,93,113	1.43	5 (8%)
26	CLA	n	304	7	53,57,73	1.41	10 (18%)	62,93,113	1.38	7 (11%)
26	CLA	G	317	7	53,57,73	1.39	9 (16%)	62,93,113	1.38	6 (9%)
26	CLA	b	602	2	69,73,73	1.21	8 (11%)	83,113,113	1.25	6 (7%)
39	CHL	S	313	-	54,58,74	1.45	6 (11%)	59,94,114	2.06	12 (20%)
39	CHL	G	318	7	70,74,74	1.32	6 (8%)	80,114,114	1.76	13 (16%)
26	CLA	R	306	17	69,73,73	1.21	9 (13%)	83,113,113	1.12	7 (8%)
26	CLA	r	314	17	69,73,73	1.21	8 (11%)	83,113,113	1.23	8 (9%)
39	CHL	n	308	7	52,56,74	1.46	6 (11%)	58,92,114	2.05	13 (22%)
41	XAT	G	320	-	39,47,47	1.13	5 (12%)	54,74,74	2.50	18 (33%)
26	CLA	b	605	2	69,73,73	1.22	8 (11%)	83,113,113	1.22	7 (8%)
28	BCR	c	511	-	41,41,41	0.34	0	56,56,56	0.83	2 (3%)
26	CLA	A	403	1	69,73,73	1.22	8 (11%)	83,113,113	1.16	7 (8%)
26	CLA	B	616	2	69,73,73	1.20	7 (10%)	83,113,113	1.31	6 (7%)
39	CHL	g	319	-	54,58,74	1.45	7 (12%)	59,94,114	2.06	11 (18%)
26	CLA	n	302	7	53,57,73	1.40	9 (16%)	62,93,113	1.41	5 (8%)
29	SQD	A	410	-	49,50,54	0.80	1 (2%)	58,61,65	1.03	3 (5%)
39	CHL	N	317	7	54,58,74	1.44	6 (11%)	59,94,114	2.03	11 (18%)
40	LUT	g	310	-	42,43,43	0.46	0	51,60,60	0.75	0
26	CLA	s	306	18	53,57,73	1.39	8 (15%)	62,93,113	1.30	6 (9%)
26	CLA	c	513	3	69,73,73	1.22	6 (8%)	83,113,113	1.27	7 (8%)
27	PHO	d	407	-	58,69,69	1.98	10 (17%)	56,99,99	1.55	6 (10%)
42	NEX	N	302	-	38,46,46	1.57	9 (23%)	50,70,70	2.26	11 (22%)
39	CHL	n	318	-	70,74,74	1.31	7 (10%)	80,114,114	1.83	13 (16%)
39	CHL	G	311	7	54,58,74	1.44	6 (11%)	59,94,114	2.05	10 (16%)
26	CLA	G	307	7	69,73,73	1.22	9 (13%)	83,113,113	1.11	7 (8%)
26	CLA	s	314	18	53,57,73	1.38	7 (13%)	62,93,113	1.36	8 (12%)
28	BCR	C	514	-	41,41,41	0.37	0	56,56,56	0.74	2 (3%)
37	LHG	D	407	-	42,42,48	0.56	0	45,48,54	0.50	0
39	CHL	N	304	43	54,58,74	1.45	6 (11%)	59,94,114	2.04	12 (20%)
34	LMG	c	512	-	51,51,55	0.48	0	59,59,63	0.64	0
28	BCR	H	101	-	41,41,41	0.33	0	56,56,56	0.69	0
26	CLA	y	313	43	53,57,73	1.45	8 (15%)	62,93,113	1.29	8 (12%)
37	LHG	r	312	26	48,48,48	0.51	0	51,54,54	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	B	617	2	69,73,73	1.21	8 (11%)	83,113,113	1.26	8 (9%)
26	CLA	G	314	7	69,73,73	1.26	10 (14%)	83,113,113	1.23	7 (8%)
37	LHG	L	101	-	48,48,48	0.52	0	51,54,54	0.55	0
26	CLA	N	313	7	53,57,73	1.40	9 (16%)	62,93,113	1.36	6 (9%)
37	LHG	d	410	-	36,36,48	0.61	0	39,42,54	0.59	0
41	XAT	g	320	-	39,47,47	1.13	4 (10%)	54,74,74	2.49	19 (35%)
26	CLA	r	305	17	53,57,73	1.41	7 (13%)	62,93,113	1.31	5 (8%)
39	CHL	R	315	43	54,58,74	1.45	7 (12%)	59,94,114	2.08	16 (27%)
40	LUT	y	311	-	42,43,43	0.48	0	51,60,60	0.86	0
26	CLA	R	314	37	53,57,73	1.41	8 (15%)	62,93,113	1.39	6 (9%)
26	CLA	S	311	18	53,57,73	1.37	8 (15%)	62,93,113	1.36	8 (12%)
26	CLA	y	304	37	69,73,73	1.24	7 (10%)	83,113,113	1.24	6 (7%)
26	CLA	n	310	37	53,57,73	1.42	8 (15%)	62,93,113	1.39	6 (9%)
26	CLA	B	618	2	69,73,73	1.22	8 (11%)	83,113,113	1.22	8 (9%)
26	CLA	C	511	3	69,73,73	1.18	8 (11%)	83,113,113	1.23	7 (8%)
26	CLA	Y	311	23	53,57,73	1.37	8 (15%)	62,93,113	1.45	6 (9%)
26	CLA	R	316	17	53,57,73	1.39	8 (15%)	62,93,113	1.30	5 (8%)
37	LHG	G	312	26	48,48,48	0.52	0	51,54,54	0.52	0
26	CLA	D	406	4	69,73,73	1.21	7 (10%)	83,113,113	1.24	6 (7%)
37	LHG	d	402	-	42,42,48	0.57	0	45,48,54	0.49	0
26	CLA	g	318	7	53,57,73	1.40	8 (15%)	62,93,113	1.38	7 (11%)
33	DGD	B	620	-	63,63,67	0.58	0	77,77,81	0.77	1 (1%)
28	BCR	c	507	-	41,41,41	0.36	0	56,56,56	0.75	2 (3%)
39	CHL	Y	302	23	70,74,74	1.30	6 (8%)	80,114,114	1.80	14 (17%)
39	CHL	R	301	43	54,58,74	1.44	6 (11%)	59,94,114	2.09	14 (23%)
42	NEX	R	305	-	38,46,46	1.57	9 (23%)	50,70,70	2.26	16 (32%)
26	CLA	b	604	-	69,73,73	1.25	8 (11%)	83,113,113	1.23	8 (9%)
26	CLA	N	307	7	69,73,73	1.22	7 (10%)	83,113,113	1.24	7 (8%)
26	CLA	N	318	7	53,57,73	1.39	9 (16%)	62,93,113	1.42	5 (8%)
40	LUT	R	311	-	42,43,43	0.53	0	51,60,60	1.04	3 (5%)
37	LHG	D	408	-	48,48,48	0.51	0	51,54,54	0.58	0
26	CLA	s	301	37	53,57,73	1.38	9 (16%)	62,93,113	1.36	5 (8%)
35	OEX	C	501	3,1,43	0,14,14	-	-	-		
33	DGD	b	620	-	63,63,67	0.58	0	77,77,81	0.79	1 (1%)
26	CLA	B	605	43	69,73,73	1.23	8 (11%)	83,113,113	1.27	5 (6%)
39	CHL	N	311	-	54,58,74	1.41	5 (9%)	59,94,114	2.08	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LMG	w	201	-	48,48,55	0.58	0	56,56,63	0.65	1 (1%)
32	BCT	A	411	31	2,3,3	1.16	0	2,3,3	1.79	1 (50%)
26	CLA	b	611	2	69,73,73	1.30	9 (13%)	83,113,113	1.46	10 (12%)
40	LUT	y	318	-	42,43,43	0.49	0	51,60,60	0.86	1 (1%)
26	CLA	B	607	43	69,73,73	1.21	8 (11%)	83,113,113	1.24	7 (8%)
34	LMG	W	201	-	48,48,55	0.57	0	56,56,63	0.63	1 (1%)
26	CLA	n	315	7	53,57,73	1.43	10 (18%)	62,93,113	1.39	6 (9%)
40	LUT	s	312	-	42,43,43	0.49	0	51,60,60	0.90	1 (1%)
39	CHL	G	305	-	54,58,74	1.45	6 (11%)	59,94,114	2.07	10 (16%)
26	CLA	c	510	3	53,57,73	1.37	9 (16%)	62,93,113	1.39	7 (11%)
40	LUT	G	308	-	42,43,43	0.47	0	51,60,60	0.74	0
39	CHL	y	305	43	54,58,74	1.43	5 (9%)	59,94,114	2.08	11 (18%)
39	CHL	N	310	7	52,56,74	1.45	6 (11%)	58,92,114	2.06	13 (22%)
39	CHL	G	309	7	52,56,74	1.49	7 (13%)	58,92,114	1.99	12 (20%)
26	CLA	Y	310	23	53,57,73	1.40	7 (13%)	62,93,113	1.28	6 (9%)
26	CLA	n	309	7	53,57,73	1.39	6 (11%)	62,93,113	1.33	5 (8%)
41	XAT	N	315	-	39,47,47	1.14	4 (10%)	54,74,74	2.32	15 (27%)
37	LHG	S	317	26	48,48,48	0.52	0	51,54,54	0.52	0
26	CLA	c	516	3	69,73,73	1.24	9 (13%)	83,113,113	1.24	9 (10%)
37	LHG	Y	306	26	48,48,48	0.51	0	51,54,54	0.52	0
40	LUT	N	314	-	42,43,43	0.47	0	51,60,60	0.84	0
26	CLA	g	303	7	69,73,73	1.26	10 (14%)	83,113,113	1.22	7 (8%)
26	CLA	R	310	17	53,57,73	1.34	6 (11%)	62,93,113	1.29	5 (8%)
26	CLA	R	313	17	69,73,73	1.21	8 (11%)	83,113,113	1.23	8 (9%)
26	CLA	c	518	3	69,73,73	1.22	7 (10%)	83,113,113	1.37	5 (6%)
42	NEX	r	302	-	38,46,46	1.56	9 (23%)	50,70,70	2.27	16 (32%)
33	DGD	C	513	-	63,63,67	0.63	0	77,77,81	0.70	0
26	CLA	r	306	17	69,73,73	1.20	9 (13%)	83,113,113	1.11	7 (8%)
26	CLA	s	305	18	53,57,73	1.38	7 (13%)	62,93,113	1.29	6 (9%)
26	CLA	y	306	23	69,73,73	1.21	6 (8%)	83,113,113	1.27	9 (10%)
34	LMG	C	503	-	51,51,55	0.48	0	59,59,63	0.64	0
26	CLA	G	306	7	53,57,73	1.42	9 (16%)	62,93,113	1.34	6 (9%)
29	SQD	a	403	-	53,54,54	0.78	1 (1%)	62,65,65	0.99	3 (4%)
40	LUT	r	307	-	42,43,43	0.53	0	51,60,60	1.05	3 (5%)
26	CLA	S	303	18	53,57,73	1.39	9 (16%)	62,93,113	1.32	6 (9%)
26	CLA	Y	308	23	69,73,73	1.21	6 (8%)	83,113,113	1.28	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	OEX	a	408	3,1,43	0,14,14	-	-	-		
33	DGD	y	308	-	44,44,67	0.69	0	58,58,81	0.88	2 (3%)
28	BCR	j	101	-	41,41,41	0.31	0	56,56,56	0.68	1 (1%)
26	CLA	y	310	23	69,73,73	1.24	7 (10%)	83,113,113	1.27	7 (8%)
39	CHL	r	301	23,17	52,56,74	1.43	6 (11%)	58,92,114	2.05	13 (22%)
26	CLA	Y	312	23	69,73,73	1.24	7 (10%)	83,113,113	1.26	7 (8%)
26	CLA	S	315	18	53,57,73	1.39	8 (15%)	62,93,113	1.30	6 (9%)
29	SQD	A	407	-	53,54,54	0.78	1 (1%)	62,65,65	0.99	4 (6%)
40	LUT	s	308	-	42,43,43	0.51	0	51,60,60	0.73	0
26	CLA	C	505	3	69,73,73	1.22	8 (11%)	83,113,113	1.22	7 (8%)
42	NEX	g	306	-	38,46,46	1.55	9 (23%)	50,70,70	2.36	14 (28%)
27	PHO	a	410	-	58,69,69	1.97	11 (18%)	56,99,99	1.47	8 (14%)
39	CHL	R	312	43	54,58,74	1.45	6 (11%)	59,94,114	2.01	11 (18%)
39	CHL	Y	318	-	54,58,74	1.43	7 (12%)	59,94,114	2.10	12 (20%)
26	CLA	s	307	18	53,57,73	1.39	8 (15%)	62,93,113	1.33	6 (9%)
39	CHL	r	316	43	54,58,74	1.44	6 (11%)	59,94,114	2.09	14 (23%)
41	XAT	n	316	-	39,47,47	1.14	4 (10%)	54,74,74	2.30	13 (24%)
26	CLA	b	607	2	69,73,73	1.23	9 (13%)	83,113,113	1.20	8 (9%)
26	CLA	b	609	2	69,73,73	1.19	7 (10%)	83,113,113	1.33	6 (7%)
40	LUT	G	316	-	42,43,43	0.49	0	51,60,60	0.96	0
26	CLA	c	508	43	69,73,73	1.25	9 (13%)	83,113,113	1.34	6 (7%)
28	BCR	K	101	-	41,41,41	0.33	0	56,56,56	0.87	3 (5%)
30	PL9	d	408	-	55,55,55	1.38	7 (12%)	68,69,69	1.51	10 (14%)
26	CLA	a	411	1	69,73,73	1.22	9 (13%)	83,113,113	1.17	7 (8%)
40	LUT	n	314	-	42,43,43	0.48	0	51,60,60	0.85	0
26	CLA	D	409	4	69,73,73	1.21	8 (11%)	83,113,113	1.16	5 (6%)
26	CLA	C	507	3	69,73,73	1.25	10 (14%)	83,113,113	1.29	7 (8%)
30	PL9	a	407	-	22,22,55	1.25	3 (13%)	28,29,69	1.51	6 (21%)
39	CHL	n	307	-	54,58,74	1.41	5 (9%)	59,94,114	2.08	11 (18%)
37	LHG	R	303	26	48,48,48	0.51	0	51,54,54	0.52	0
26	CLA	s	311	18	53,57,73	1.40	8 (15%)	62,93,113	1.26	7 (11%)
39	CHL	G	301	-	54,58,74	1.46	6 (11%)	59,94,114	2.02	10 (16%)
42	NEX	S	305	-	38,46,46	1.56	9 (23%)	50,70,70	2.34	16 (32%)
26	CLA	r	313	17	53,57,73	1.37	7 (13%)	62,93,113	1.56	12 (19%)
39	CHL	y	314	23	70,74,74	1.31	7 (10%)	80,114,114	1.79	12 (15%)
39	CHL	n	306	7	54,58,74	1.46	5 (9%)	59,94,114	2.00	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CHL	N	316	7	54,58,74	1.45	6 (11%)	59,94,114	2.00	16 (27%)
39	CHL	y	303	23	70,74,74	1.31	6 (8%)	80,114,114	1.80	12 (15%)
40	LUT	N	305	-	42,43,43	0.48	0	51,60,60	0.81	0
40	LUT	Y	309	-	42,43,43	0.50	0	51,60,60	0.86	1 (1%)
40	LUT	g	316	-	42,43,43	0.49	0	51,60,60	0.95	0
26	CLA	c	520	3	69,73,73	1.22	8 (11%)	83,113,113	1.23	8 (9%)
37	LHG	g	301	26	48,48,48	0.52	0	51,54,54	0.52	0
26	CLA	G	302	-	53,57,73	1.42	8 (15%)	62,93,113	1.33	6 (9%)
28	BCR	a	404	-	41,41,41	0.33	0	56,56,56	0.51	0
29	SQD	B	621	-	53,54,54	0.79	1 (1%)	62,65,65	0.85	2 (3%)
37	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.54	0
39	CHL	N	303	-	70,74,74	1.31	7 (10%)	80,114,114	1.82	13 (16%)
39	CHL	G	303	-	54,58,74	1.43	6 (11%)	59,94,114	1.99	13 (22%)
26	CLA	B	613	-	69,73,73	1.24	8 (11%)	83,113,113	1.23	7 (8%)
26	CLA	G	313	37	53,57,73	1.42	9 (16%)	62,93,113	1.39	7 (11%)
26	CLA	n	305	7	69,73,73	1.22	7 (10%)	83,113,113	1.24	7 (8%)
26	CLA	S	314	18	53,57,73	1.36	7 (13%)	62,93,113	1.16	5 (8%)
28	BCR	b	615	-	41,41,41	0.32	0	56,56,56	0.52	0
26	CLA	a	409	43	69,73,73	1.21	7 (10%)	83,113,113	1.20	6 (7%)
33	DGD	c	517	-	56,56,67	0.69	0	70,70,81	0.76	1 (1%)
26	CLA	r	315	17	53,57,73	1.37	8 (15%)	62,93,113	1.40	8 (12%)
26	CLA	R	302	17	53,57,73	1.38	8 (15%)	62,93,113	1.57	12 (19%)
34	LMG	D	404	-	46,46,55	0.60	0	54,54,63	0.69	1 (1%)
39	CHL	g	314	7	52,56,74	1.48	7 (13%)	58,92,114	1.97	12 (20%)
26	CLA	N	312	7	69,73,73	1.20	7 (10%)	83,113,113	1.08	7 (8%)
28	BCR	T	101	-	41,41,41	0.32	0	56,56,56	1.46	10 (17%)
34	LMG	c	509	-	51,51,55	0.52	0	59,59,63	0.60	0
30	PL9	D	411	-	55,55,55	1.37	7 (12%)	68,69,69	1.52	10 (14%)
39	CHL	g	307	-	54,58,74	1.43	6 (11%)	59,94,114	2.00	14 (23%)
39	CHL	Y	307	23	70,74,74	1.30	7 (10%)	80,114,114	1.79	12 (15%)
39	CHL	r	309	43	54,58,74	1.45	6 (11%)	59,94,114	2.01	11 (18%)
28	BCR	b	603	-	41,41,41	0.36	0	56,56,56	0.74	0
28	BCR	k	101	-	41,41,41	0.34	0	56,56,56	0.86	3 (5%)
26	CLA	B	610	2	69,73,73	1.20	9 (13%)	83,113,113	1.26	7 (8%)
26	CLA	y	315	23	53,57,73	1.36	8 (15%)	62,93,113	1.44	7 (11%)
37	LHG	s	309	26	48,48,48	0.52	0	51,54,54	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	BCR	t	101	-	41,41,41	0.32	0	56,56,56	1.40	10 (17%)
26	CLA	R	309	17	53,57,73	1.41	8 (15%)	62,93,113	1.31	7 (11%)
26	CLA	Y	305	23	69,73,73	1.22	8 (11%)	83,113,113	1.17	10 (12%)
34	LMG	C	518	-	51,51,55	0.52	0	59,59,63	0.59	0
26	CLA	B	615	2	69,73,73	1.30	8 (11%)	83,113,113	1.45	9 (10%)
40	LUT	S	301	-	42,43,43	0.51	0	51,60,60	0.74	0
41	XAT	G	310	-	39,47,47	1.14	4 (10%)	54,74,74	2.33	12 (22%)
33	DGD	c	519	-	63,63,67	0.62	0	77,77,81	0.70	0
26	CLA	g	305	7	53,57,73	1.42	9 (16%)	62,93,113	1.34	7 (11%)
29	SQD	W	202	-	32,33,54	1.03	2 (6%)	41,44,65	1.14	4 (9%)
42	NEX	n	313	-	38,46,46	1.55	9 (23%)	50,70,70	2.23	11 (22%)
26	CLA	c	503	3	69,73,73	1.18	8 (11%)	83,113,113	1.23	7 (8%)
36	LMT	d	406	-	36,36,36	0.57	0	47,47,47	0.68	0
26	CLA	R	308	43	53,57,73	1.41	9 (16%)	62,93,113	1.41	9 (14%)
26	CLA	C	517	3	69,73,73	1.23	7 (10%)	83,113,113	1.27	6 (7%)
26	CLA	B	604	2	69,73,73	1.27	9 (13%)	83,113,113	1.22	8 (9%)
39	CHL	s	303	18	56,60,74	1.46	7 (12%)	63,97,114	2.00	13 (20%)
37	LHG	n	301	26	48,48,48	0.51	0	51,54,54	0.47	0
28	BCR	B	619	-	41,41,41	0.37	0	56,56,56	0.73	0
27	PHO	D	403	-	58,69,69	1.97	10 (17%)	56,99,99	1.55	7 (12%)
26	CLA	d	411	43	53,57,73	1.43	9 (16%)	62,93,113	1.25	8 (12%)
26	CLA	C	516	43	69,73,73	1.24	7 (10%)	83,113,113	1.32	6 (7%)
39	CHL	s	317	-	54,58,74	1.44	6 (11%)	59,94,114	2.08	12 (20%)
26	CLA	B	606	2	69,73,73	1.21	8 (11%)	83,113,113	1.16	6 (7%)
26	CLA	g	315	37	53,57,73	1.41	9 (16%)	62,93,113	1.38	7 (11%)
26	CLA	s	304	18	53,57,73	1.39	8 (15%)	62,93,113	1.42	6 (9%)
28	BCR	A	406	-	41,41,41	0.32	0	56,56,56	0.51	0
26	CLA	S	304	18	53,57,73	1.38	7 (13%)	62,93,113	1.28	6 (9%)
33	DGD	Y	303	-	44,44,67	0.68	0	58,58,81	0.87	2 (3%)
39	CHL	S	302	-	54,58,74	1.46	6 (11%)	59,94,114	1.98	11 (18%)
39	CHL	g	311	7	70,74,74	1.32	6 (8%)	80,114,114	1.76	13 (16%)
26	CLA	D	401	43	69,73,73	1.21	8 (11%)	83,113,113	1.21	7 (8%)
28	BCR	J	101	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
26	CLA	r	303	17	53,57,73	1.40	9 (16%)	62,93,113	1.30	5 (8%)
36	LMT	D	402	-	36,36,36	0.57	0	47,47,47	0.68	0
39	CHL	y	312	43	54,58,74	1.44	6 (11%)	59,94,114	2.05	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	b	613	2	69,73,73	1.22	9 (13%)	83,113,113	1.24	8 (9%)
42	NEX	s	302	-	38,46,46	1.56	9 (23%)	50,70,70	2.28	16 (32%)
26	CLA	b	610	2	69,73,73	1.22	8 (11%)	83,113,113	1.24	8 (9%)
28	BCR	d	401	-	41,41,41	0.33	0	56,56,56	0.72	1 (1%)
26	CLA	a	402	1	64,68,73	1.25	9 (14%)	77,107,113	1.21	7 (9%)
26	CLA	B	612	43	69,73,73	1.23	8 (11%)	83,113,113	1.25	7 (8%)
26	CLA	c	515	3	69,73,73	1.20	7 (10%)	83,113,113	1.29	6 (7%)
39	CHL	g	313	-	54,58,74	1.47	6 (11%)	59,94,114	2.03	10 (16%)
26	CLA	b	601	2	69,73,73	1.21	8 (11%)	83,113,113	1.18	7 (8%)
42	NEX	Y	304	-	38,46,46	1.59	9 (23%)	50,70,70	2.15	11 (22%)
26	CLA	n	303	7	69,73,73	1.20	7 (10%)	83,113,113	1.08	7 (8%)
26	CLA	r	311	43	53,57,73	1.41	10 (18%)	62,93,113	1.42	9 (14%)
26	CLA	g	308	7	53,57,73	1.40	9 (16%)	62,93,113	1.38	6 (9%)
39	CHL	s	313	-	53,57,74	1.48	6 (11%)	59,93,114	2.18	16 (27%)
41	XAT	r	304	-	39,47,47	1.16	4 (10%)	54,74,74	2.20	12 (22%)
26	CLA	s	315	18	53,57,73	1.36	7 (13%)	62,93,113	1.16	5 (8%)
26	CLA	C	521	43	69,73,73	1.21	8 (11%)	83,113,113	1.23	7 (8%)
39	CHL	S	312	-	53,57,74	1.48	6 (11%)	59,93,114	2.19	15 (25%)
26	CLA	S	307	18	53,57,73	1.41	9 (16%)	62,93,113	1.26	7 (11%)
28	BCR	h	101	-	41,41,41	0.33	0	56,56,56	0.68	0
26	CLA	b	612	2	69,73,73	1.27	9 (13%)	83,113,113	1.22	9 (10%)
34	LMG	d	405	-	46,46,55	0.60	0	54,54,63	0.68	1 (1%)
26	CLA	G	304	7	53,57,73	1.40	7 (13%)	62,93,113	1.39	7 (11%)
34	LMG	B	622	-	51,51,55	0.52	0	59,59,63	0.65	0
26	CLA	B	602	2	69,73,73	1.21	9 (13%)	83,113,113	1.21	7 (8%)
26	CLA	d	404	4	69,73,73	1.21	8 (11%)	83,113,113	1.15	5 (6%)
29	SQD	w	202	-	32,33,54	1.02	2 (6%)	41,44,65	1.14	3 (7%)
26	CLA	C	508	3	69,73,73	1.23	8 (11%)	83,113,113	1.24	9 (10%)
33	DGD	C	510	-	63,63,67	0.63	0	77,77,81	0.69	0
26	CLA	C	512	3	69,73,73	1.20	7 (10%)	83,113,113	1.30	6 (7%)
40	LUT	Y	315	-	42,43,43	0.48	0	51,60,60	0.87	0
33	DGD	C	509	-	56,56,67	0.69	0	70,70,81	0.75	1 (1%)
26	CLA	N	309	7	53,57,73	1.39	6 (11%)	62,93,113	1.33	5 (8%)
26	CLA	g	317	7	69,73,73	1.22	9 (13%)	83,113,113	1.11	7 (8%)
26	CLA	B	603	2	69,73,73	1.20	8 (11%)	83,113,113	1.24	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	BCT	a	405	31	2,3,3	0.89	0	2,3,3	3.23	2 (100%)
26	CLA	r	310	17	53,57,73	1.34	6 (11%)	62,93,113	1.29	5 (8%)
26	CLA	A	405	1	64,68,73	1.25	7 (10%)	77,107,113	1.23	7 (9%)
26	CLA	b	616	43	69,73,73	1.21	7 (10%)	83,113,113	1.24	7 (8%)
26	CLA	D	412	43	53,57,73	1.43	9 (16%)	62,93,113	1.26	8 (12%)
26	CLA	g	304	7	53,57,73	1.40	8 (15%)	62,93,113	1.36	6 (9%)
26	CLA	R	317	17	53,57,73	1.37	8 (15%)	62,93,113	1.42	9 (14%)
39	CHL	Y	317	43	54,58,74	1.44	6 (11%)	59,94,114	2.09	11 (18%)
26	CLA	c	505	3	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
26	CLA	s	310	-	53,57,73	1.43	8 (15%)	62,93,113	1.30	7 (11%)
26	CLA	Y	313	23	69,73,73	1.20	9 (13%)	83,113,113	1.33	9 (10%)
26	CLA	C	520	3	63,70,73	1.29	6 (9%)	73,103,113	0.98	3 (4%)
26	CLA	b	606	2	69,73,73	1.24	8 (11%)	83,113,113	1.23	8 (9%)
26	CLA	g	302	-	53,57,73	1.42	9 (16%)	62,93,113	1.32	6 (9%)
30	PL9	A	408	-	22,22,55	1.24	3 (13%)	28,29,69	1.48	6 (21%)
26	CLA	S	310	-	53,57,73	1.44	9 (16%)	62,93,113	1.29	7 (11%)
39	CHL	S	316	18	56,60,74	1.46	6 (10%)	63,97,114	2.00	13 (20%)
26	CLA	b	608	43	69,73,73	1.23	8 (11%)	83,113,113	1.25	6 (7%)
28	BCR	B	614	-	41,41,41	0.33	0	56,56,56	0.55	0
37	LHG	D	410	-	36,36,48	0.61	0	39,42,54	0.59	0
26	CLA	b	617	2	69,73,73	1.20	9 (13%)	83,113,113	1.25	7 (8%)
26	CLA	B	611	2	69,73,73	1.23	9 (13%)	83,113,113	1.22	8 (9%)
39	CHL	y	302	-	54,58,74	1.43	7 (12%)	59,94,114	2.07	13 (22%)
26	CLA	y	309	23	69,73,73	1.22	8 (11%)	83,113,113	1.14	8 (9%)
26	CLA	c	502	3	69,73,73	1.21	8 (11%)	83,113,113	1.21	6 (7%)
27	PHO	A	404	-	58,69,69	1.98	11 (18%)	56,99,99	1.49	8 (14%)
39	CHL	n	311	43	54,58,74	1.44	6 (11%)	59,94,114	2.03	11 (18%)
26	CLA	Y	301	37	69,73,73	1.22	8 (11%)	83,113,113	1.26	6 (7%)
26	CLA	n	312	43	53,57,73	1.43	9 (16%)	62,93,113	1.27	7 (11%)
37	LHG	d	409	-	48,48,48	0.51	0	51,54,54	0.57	0
28	BCR	D	405	-	41,41,41	0.33	0	56,56,56	0.70	1 (1%)
29	SQD	b	621	-	53,54,54	0.78	1 (1%)	62,65,65	0.85	2 (3%)
26	CLA	b	618	2	69,73,73	1.23	8 (11%)	83,113,113	1.25	8 (9%)

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
26	CLA	C	515	3	-	8/39/115/115	-
26	CLA	C	506	3	-	13/39/115/115	-
28	BCR	C	502	-	-	1/29/63/63	0/2/2/2
37	LHG	N	301	26	-	14/53/53/53	-
26	CLA	N	319	37	-	12/20/96/115	-
42	NEX	G	315	-	-	2/27/83/83	0/3/3/3
26	CLA	G	319	7	-	11/20/96/115	-
28	BCR	B	608	-	-	1/29/63/63	0/2/2/2
26	CLA	c	506	3	-	15/51/101/115	-
39	CHL	R	318	23,17	-	8/20/96/117	-
38	HEM	e	101	5,6	-	2/14/54/54	-
26	CLA	r	308	17	-	7/20/96/115	-
39	CHL	Y	314	43	-	11/22/98/117	-
26	CLA	Y	316	43	-	7/20/96/115	-
26	CLA	B	609	2	-	11/39/115/115	-
40	LUT	S	306	-	-	2/29/67/67	0/2/2/2
29	SQD	a	413	-	-	17/45/65/69	0/1/1/1
41	XAT	g	309	-	-	0/31/93/93	0/4/4/4
42	NEX	y	307	-	-	2/27/83/83	0/3/3/3
28	BCR	b	619	-	-	5/29/63/63	0/2/2/2
26	CLA	S	308	37	-	11/20/96/115	-
40	LUT	n	317	-	-	3/29/67/67	0/2/2/2
39	CHL	s	316	-	-	15/22/98/117	-
26	CLA	C	504	3	-	8/39/115/115	-
38	HEM	E	101	5,6	-	2/14/54/54	-
34	LMG	b	622	-	-	16/46/66/70	0/1/1/1
26	CLA	N	308	43	-	7/20/96/115	-
39	CHL	n	319	7	-	5/22/98/117	-
26	CLA	d	403	4	-	12/39/115/115	-
26	CLA	r	317	37	-	10/20/96/115	-
37	LHG	y	301	26	-	28/53/53/53	-
33	DGD	c	501	-	-	18/51/91/95	0/2/2/2
39	CHL	r	318	43	-	6/22/98/117	-
26	CLA	c	504	3	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	S	309	18	-	7/20/96/115	-
26	CLA	c	514	43	-	9/39/115/115	-
26	CLA	C	519	3	-	6/20/96/115	-
26	CLA	b	614	43	-	5/39/115/115	-
26	CLA	N	306	7	-	11/20/96/115	-
26	CLA	y	317	23	-	11/20/96/115	-
39	CHL	g	312	7	-	6/22/98/117	-
26	CLA	B	601	2	-	14/39/115/115	-
41	XAT	R	304	-	-	1/31/93/93	0/4/4/4
26	CLA	y	316	23	-	14/39/115/115	-
26	CLA	R	307	17	-	7/20/96/115	-
26	CLA	n	304	7	-	9/20/96/115	-
26	CLA	G	317	7	-	9/20/96/115	-
26	CLA	b	602	2	-	10/39/115/115	-
39	CHL	S	313	-	-	8/22/98/117	-
39	CHL	G	318	7	-	18/41/117/117	-
26	CLA	R	306	17	-	6/39/115/115	-
26	CLA	r	314	17	-	13/39/115/115	-
39	CHL	n	308	7	-	6/20/96/117	-
41	XAT	G	320	-	-	4/31/93/93	0/4/4/4
26	CLA	b	605	2	-	14/39/115/115	-
28	BCR	c	511	-	-	3/29/63/63	0/2/2/2
26	CLA	A	403	1	-	8/39/115/115	-
26	CLA	B	616	2	-	10/39/115/115	-
39	CHL	g	319	-	-	7/22/98/117	-
26	CLA	n	302	7	-	8/20/96/115	-
29	SQD	A	410	-	-	17/45/65/69	0/1/1/1
39	CHL	N	317	7	-	6/22/98/117	-
40	LUT	g	310	-	-	2/29/67/67	0/2/2/2
26	CLA	s	306	18	-	10/20/96/115	-
26	CLA	c	513	3	-	4/39/115/115	-
27	PHO	d	407	-	-	13/37/103/103	0/5/6/6
42	NEX	N	302	-	-	2/27/83/83	0/3/3/3
39	CHL	n	318	-	-	14/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	G	311	7	-	6/22/98/117	-
26	CLA	G	307	7	-	12/39/115/115	-
26	CLA	s	314	18	-	11/20/96/115	-
28	BCR	C	514	-	-	4/29/63/63	0/2/2/2
37	LHG	D	407	-	-	15/47/47/53	-
39	CHL	N	304	43	-	10/22/98/117	-
34	LMG	c	512	-	-	19/46/66/70	0/1/1/1
28	BCR	H	101	-	-	2/29/63/63	0/2/2/2
26	CLA	y	313	43	-	6/20/96/115	-
37	LHG	r	312	26	-	16/53/53/53	-
26	CLA	B	617	2	-	8/39/115/115	-
26	CLA	G	314	7	-	7/39/115/115	-
37	LHG	L	101	-	-	11/53/53/53	-
26	CLA	N	313	7	-	9/20/96/115	-
37	LHG	d	410	-	-	10/41/41/53	-
41	XAT	g	320	-	-	3/31/93/93	0/4/4/4
26	CLA	r	305	17	-	11/20/96/115	-
39	CHL	R	315	43	-	7/22/98/117	-
40	LUT	y	311	-	-	0/29/67/67	0/2/2/2
26	CLA	R	314	37	-	10/20/96/115	-
26	CLA	S	311	18	-	8/20/96/115	-
26	CLA	y	304	37	-	12/39/115/115	-
26	CLA	n	310	37	-	12/20/96/115	-
26	CLA	B	618	2	-	12/39/115/115	-
26	CLA	C	511	3	-	14/39/115/115	-
26	CLA	Y	311	23	-	7/20/96/115	-
26	CLA	R	316	17	-	6/20/96/115	-
37	LHG	G	312	26	-	15/53/53/53	-
26	CLA	D	406	4	-	12/39/115/115	-
37	LHG	d	402	-	-	15/47/47/53	-
26	CLA	g	318	7	-	7/20/96/115	-
33	DGD	B	620	-	-	15/51/91/95	0/2/2/2
28	BCR	c	507	-	-	5/29/63/63	0/2/2/2
39	CHL	Y	302	23	-	13/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	R	301	43	-	13/22/98/117	-
42	NEX	R	305	-	-	2/27/83/83	0/3/3/3
26	CLA	b	604	-	-	10/39/115/115	-
26	CLA	N	307	7	-	5/39/115/115	-
26	CLA	N	318	7	-	8/20/96/115	-
40	LUT	R	311	-	-	8/29/67/67	0/2/2/2
37	LHG	D	408	-	-	14/53/53/53	-
26	CLA	s	301	37	-	11/20/96/115	-
33	DGD	b	620	-	-	18/51/91/95	0/2/2/2
26	CLA	B	605	43	-	19/39/115/115	-
39	CHL	N	311	-	-	11/22/98/117	-
34	LMG	w	201	-	-	14/43/63/70	0/1/1/1
26	CLA	b	611	2	-	19/39/115/115	-
40	LUT	y	318	-	-	3/29/67/67	0/2/2/2
26	CLA	B	607	43	-	11/39/115/115	-
34	LMG	W	201	-	-	13/43/63/70	0/1/1/1
26	CLA	n	315	7	-	11/20/96/115	-
40	LUT	s	312	-	-	2/29/67/67	0/2/2/2
39	CHL	G	305	-	-	7/22/98/117	-
26	CLA	c	510	3	-	6/20/96/115	-
40	LUT	G	308	-	-	1/29/67/67	0/2/2/2
39	CHL	y	305	43	-	8/22/98/117	-
39	CHL	N	310	7	-	6/20/96/117	-
39	CHL	G	309	7	-	11/20/96/117	-
26	CLA	Y	310	23	-	11/20/96/115	-
26	CLA	n	309	7	-	11/20/96/115	-
41	XAT	N	315	-	-	0/31/93/93	0/4/4/4
37	LHG	S	317	26	-	24/53/53/53	-
26	CLA	c	516	3	-	13/39/115/115	-
37	LHG	Y	306	26	-	29/53/53/53	-
40	LUT	N	314	-	-	1/29/67/67	0/2/2/2
26	CLA	g	303	7	-	8/39/115/115	-
26	CLA	R	310	17	-	10/20/96/115	-
26	CLA	R	313	17	-	11/39/115/115	-
26	CLA	c	518	3	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	NEX	r	302	-	-	2/27/83/83	0/3/3/3
33	DGD	C	513	-	-	17/51/91/95	0/2/2/2
26	CLA	r	306	17	-	6/39/115/115	-
26	CLA	s	305	18	-	6/20/96/115	-
26	CLA	y	306	23	-	10/39/115/115	-
34	LMG	C	503	-	-	19/46/66/70	0/1/1/1
26	CLA	G	306	7	-	10/20/96/115	-
29	SQD	a	403	-	-	21/49/69/69	0/1/1/1
40	LUT	r	307	-	-	8/29/67/67	0/2/2/2
26	CLA	S	303	18	-	6/20/96/115	-
26	CLA	Y	308	23	-	10/39/115/115	-
33	DGD	y	308	-	-	14/32/72/95	0/2/2/2
28	BCR	j	101	-	-	10/29/63/63	0/2/2/2
26	CLA	y	310	23	-	12/39/115/115	-
39	CHL	r	301	23,17	-	6/20/96/117	-
26	CLA	Y	312	23	-	12/39/115/115	-
26	CLA	S	315	18	-	10/20/96/115	-
29	SQD	A	407	-	-	22/49/69/69	0/1/1/1
40	LUT	s	308	-	-	4/29/67/67	0/2/2/2
26	CLA	C	505	3	-	11/39/115/115	-
42	NEX	g	306	-	-	2/27/83/83	0/3/3/3
27	PHO	a	410	-	-	10/37/103/103	0/5/6/6
39	CHL	R	312	43	-	10/22/98/117	-
39	CHL	Y	318	-	-	7/22/98/117	-
26	CLA	s	307	18	-	6/20/96/115	-
39	CHL	r	316	43	-	12/22/98/117	-
41	XAT	n	316	-	-	0/31/93/93	0/4/4/4
26	CLA	b	607	2	-	14/39/115/115	-
26	CLA	b	609	2	-	10/39/115/115	-
40	LUT	G	316	-	-	0/29/67/67	0/2/2/2
26	CLA	c	508	43	-	10/39/115/115	-
28	BCR	K	101	-	-	2/29/63/63	0/2/2/2
30	PL9	d	408	-	-	5/53/73/73	0/1/1/1
26	CLA	a	411	1	-	8/39/115/115	-
40	LUT	n	314	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	D	409	4	-	10/39/115/115	-
26	CLA	C	507	3	-	14/39/115/115	-
30	PL9	a	407	-	-	4/14/34/73	0/1/1/1
39	CHL	n	307	-	-	11/22/98/117	-
37	LHG	R	303	26	-	17/53/53/53	-
26	CLA	s	311	18	-	8/20/96/115	-
39	CHL	G	301	-	-	11/22/98/117	-
42	NEX	S	305	-	-	7/27/83/83	0/3/3/3
26	CLA	r	313	17	-	10/20/96/115	-
39	CHL	y	314	23	-	11/41/117/117	-
39	CHL	n	306	7	-	5/22/98/117	-
39	CHL	N	316	7	-	3/22/98/117	-
39	CHL	y	303	23	-	12/41/117/117	-
40	LUT	N	305	-	-	3/29/67/67	0/2/2/2
40	LUT	Y	309	-	-	3/29/67/67	0/2/2/2
40	LUT	g	316	-	-	1/29/67/67	0/2/2/2
26	CLA	c	520	3	-	10/39/115/115	-
37	LHG	g	301	26	-	18/53/53/53	-
26	CLA	G	302	-	-	10/20/96/115	-
28	BCR	a	404	-	-	2/29/63/63	0/2/2/2
29	SQD	B	621	-	-	25/49/69/69	0/1/1/1
37	LHG	l	101	-	-	13/53/53/53	-
39	CHL	N	303	-	-	12/41/117/117	-
39	CHL	G	303	-	-	8/22/98/117	-
26	CLA	B	613	-	-	10/39/115/115	-
26	CLA	G	313	37	-	6/20/96/115	-
26	CLA	n	305	7	-	5/39/115/115	-
26	CLA	S	314	18	-	6/20/96/115	-
28	BCR	b	615	-	-	1/29/63/63	0/2/2/2
26	CLA	a	409	43	-	3/39/115/115	-
33	DGD	c	517	-	-	17/44/84/95	0/2/2/2
26	CLA	r	315	17	-	4/20/96/115	-
26	CLA	R	302	17	-	10/20/96/115	-
34	LMG	D	404	-	-	10/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	g	314	7	-	10/20/96/117	-
26	CLA	N	312	7	-	9/39/115/115	-
28	BCR	T	101	-	-	16/29/63/63	0/2/2/2
34	LMG	c	509	-	-	19/46/66/70	0/1/1/1
30	PL9	D	411	-	-	6/53/73/73	0/1/1/1
39	CHL	g	307	-	-	7/22/98/117	-
39	CHL	Y	307	23	-	12/41/117/117	-
39	CHL	r	309	43	-	10/22/98/117	-
28	BCR	b	603	-	-	0/29/63/63	0/2/2/2
28	BCR	k	101	-	-	2/29/63/63	0/2/2/2
26	CLA	B	610	2	-	12/39/115/115	-
26	CLA	y	315	23	-	7/20/96/115	-
37	LHG	s	309	26	-	24/53/53/53	-
28	BCR	t	101	-	-	16/29/63/63	0/2/2/2
26	CLA	R	309	17	-	11/20/96/115	-
26	CLA	Y	305	23	-	12/39/115/115	-
34	LMG	C	518	-	-	19/46/66/70	0/1/1/1
26	CLA	B	615	2	-	17/39/115/115	-
40	LUT	S	301	-	-	3/29/67/67	0/2/2/2
41	XAT	G	310	-	-	0/31/93/93	0/4/4/4
33	DGD	c	519	-	-	18/51/91/95	0/2/2/2
26	CLA	g	305	7	-	11/20/96/115	-
29	SQD	W	202	-	-	12/28/48/69	0/1/1/1
42	NEX	n	313	-	-	3/27/83/83	0/3/3/3
26	CLA	c	503	3	-	16/39/115/115	-
36	LMT	d	406	-	-	7/21/61/61	0/2/2/2
26	CLA	R	308	43	-	12/20/96/115	-
26	CLA	C	517	3	-	4/39/115/115	-
26	CLA	B	604	2	-	3/39/115/115	-
39	CHL	s	303	18	-	7/25/101/117	-
37	LHG	n	301	26	-	14/53/53/53	-
28	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	PHO	D	403	-	-	13/37/103/103	0/5/6/6
26	CLA	d	411	43	-	9/20/96/115	-
26	CLA	C	516	43	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	s	317	-	-	7/22/98/117	-
26	CLA	B	606	2	-	16/39/115/115	-
26	CLA	g	315	37	-	6/20/96/115	-
26	CLA	s	304	18	-	7/20/96/115	-
28	BCR	A	406	-	-	2/29/63/63	0/2/2/2
26	CLA	S	304	18	-	7/20/96/115	-
33	DGD	Y	303	-	-	13/32/72/95	0/2/2/2
39	CHL	S	302	-	-	15/22/98/117	-
39	CHL	g	311	7	-	18/41/117/117	-
26	CLA	D	401	43	-	3/39/115/115	-
28	BCR	J	101	-	-	9/29/63/63	0/2/2/2
26	CLA	r	303	17	-	6/20/96/115	-
36	LMT	D	402	-	-	7/21/61/61	0/2/2/2
39	CHL	y	312	43	-	10/22/98/117	-
26	CLA	b	613	2	-	11/39/115/115	-
42	NEX	s	302	-	-	6/27/83/83	0/3/3/3
26	CLA	b	610	2	-	7/39/115/115	-
28	BCR	d	401	-	-	9/29/63/63	0/2/2/2
26	CLA	a	402	1	-	4/33/109/115	-
26	CLA	B	612	43	-	5/39/115/115	-
26	CLA	c	515	3	-	12/39/115/115	-
39	CHL	g	313	-	-	11/22/98/117	-
26	CLA	b	601	2	-	17/39/115/115	-
42	NEX	Y	304	-	-	2/27/83/83	0/3/3/3
26	CLA	n	303	7	-	10/39/115/115	-
26	CLA	r	311	43	-	12/20/96/115	-
26	CLA	g	308	7	-	9/20/96/115	-
39	CHL	s	313	-	-	9/21/97/117	-
41	XAT	r	304	-	-	1/31/93/93	0/4/4/4
26	CLA	s	315	18	-	6/20/96/115	-
26	CLA	C	521	43	-	9/39/115/115	-
39	CHL	S	312	-	-	9/21/97/117	-
26	CLA	S	307	18	-	7/20/96/115	-
28	BCR	h	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	612	2	-	4/39/115/115	-
34	LMG	d	405	-	-	9/41/61/70	0/1/1/1
26	CLA	G	304	7	-	7/20/96/115	-
34	LMG	B	622	-	-	17/46/66/70	0/1/1/1
26	CLA	B	602	2	-	14/39/115/115	-
26	CLA	d	404	4	-	10/39/115/115	-
29	SQD	w	202	-	-	12/28/48/69	0/1/1/1
26	CLA	C	508	3	-	13/39/115/115	-
33	DGD	C	510	-	-	14/51/91/95	0/2/2/2
26	CLA	C	512	3	-	12/39/115/115	-
40	LUT	Y	315	-	-	2/29/67/67	0/2/2/2
33	DGD	C	509	-	-	17/44/84/95	0/2/2/2
26	CLA	N	309	7	-	11/20/96/115	-
26	CLA	g	317	7	-	11/39/115/115	-
26	CLA	B	603	2	-	10/39/115/115	-
26	CLA	r	310	17	-	10/20/96/115	-
26	CLA	A	405	1	-	4/33/109/115	-
26	CLA	b	616	43	-	11/39/115/115	-
26	CLA	D	412	43	-	9/20/96/115	-
26	CLA	g	304	7	-	11/20/96/115	-
26	CLA	R	317	17	-	4/20/96/115	-
39	CHL	Y	317	43	-	8/22/98/117	-
26	CLA	c	505	3	-	14/39/115/115	-
26	CLA	s	310	-	-	15/20/96/115	-
26	CLA	Y	313	23	-	16/39/115/115	-
26	CLA	C	520	3	-	16/51/101/115	-
26	CLA	b	606	2	-	15/39/115/115	-
26	CLA	g	302	-	-	10/20/96/115	-
30	PL9	A	408	-	-	4/14/34/73	0/1/1/1
26	CLA	S	310	-	-	15/20/96/115	-
39	CHL	S	316	18	-	6/25/101/117	-
26	CLA	b	608	43	-	20/39/115/115	-
28	BCR	B	614	-	-	4/29/63/63	0/2/2/2
37	LHG	D	410	-	-	9/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	617	2	-	12/39/115/115	-
26	CLA	B	611	2	-	15/39/115/115	-
39	CHL	y	302	-	-	7/22/98/117	-
26	CLA	y	309	23	-	11/39/115/115	-
26	CLA	c	502	3	-	13/39/115/115	-
27	PHO	A	404	-	-	11/37/103/103	0/5/6/6
39	CHL	n	311	43	-	10/22/98/117	-
26	CLA	Y	301	37	-	12/39/115/115	-
26	CLA	n	312	43	-	7/20/96/115	-
37	LHG	d	409	-	-	13/53/53/53	-
28	BCR	D	405	-	-	9/29/63/63	0/2/2/2
29	SQD	b	621	-	-	26/49/69/69	0/1/1/1
26	CLA	b	618	2	-	12/39/115/115	-

The worst 5 of 1778 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	307	CLA	MG-NC	14.46	2.40	2.06
27	d	407	PHO	C1B-C2B	8.83	1.49	1.39
27	A	404	PHO	C1B-C2B	8.80	1.49	1.39
27	D	403	PHO	C1B-C2B	8.80	1.49	1.39
27	a	410	PHO	C1B-C2B	8.74	1.49	1.39

The worst 5 of 2094 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	S	312	CHL	C4A-NA-C1A	10.89	111.60	106.71
39	Y	314	CHL	C4A-NA-C1A	10.86	111.59	106.71
39	Y	317	CHL	C4A-NA-C1A	10.85	111.58	106.71
39	y	312	CHL	C4A-NA-C1A	10.84	111.58	106.71
39	R	301	CHL	C4A-NA-C1A	10.83	111.58	106.71

There are no chirality outliers.

5 of 3046 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	601	CLA	CHA-CBD-CGD-O1D
26	B	601	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	B	601	CLA	CAD-CBD-CGD-O1D
26	B	601	CLA	CAD-CBD-CGD-O2D
26	B	601	CLA	C2-C3-C5-C6

There are no ring outliers.

304 monomers are involved in 836 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	515	CLA	5	0
26	C	506	CLA	3	0
28	C	502	BCR	4	0
37	N	301	LHG	5	0
26	N	319	CLA	3	0
42	G	315	NEX	4	0
26	G	319	CLA	2	0
28	B	608	BCR	3	0
26	c	506	CLA	5	0
39	R	318	CHL	1	0
38	e	101	HEM	4	0
26	r	308	CLA	1	0
39	Y	314	CHL	1	0
26	Y	316	CLA	3	0
26	B	609	CLA	4	0
40	S	306	LUT	3	0
29	a	413	SQD	3	0
41	g	309	XAT	4	0
42	y	307	NEX	3	0
28	b	619	BCR	5	0
26	S	308	CLA	3	0
40	n	317	LUT	3	0
39	s	316	CHL	6	0
26	C	504	CLA	7	0
38	E	101	HEM	5	0
34	b	622	LMG	3	0
39	n	319	CHL	2	0
26	d	403	CLA	4	0
26	r	317	CLA	1	0
37	y	301	LHG	4	0
33	c	501	DGD	3	0
39	r	318	CHL	2	0
26	c	504	CLA	5	0
26	S	309	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	514	CLA	5	0
26	C	519	CLA	1	0
26	b	614	CLA	3	0
26	N	306	CLA	1	0
26	y	317	CLA	1	0
39	g	312	CHL	4	0
26	B	601	CLA	5	0
41	R	304	XAT	1	0
26	y	316	CLA	4	0
26	R	307	CLA	1	0
26	n	304	CLA	2	0
26	G	317	CLA	3	0
26	b	602	CLA	4	0
39	S	313	CHL	3	0
39	G	318	CHL	7	0
26	R	306	CLA	4	0
26	r	314	CLA	3	0
39	n	308	CHL	1	0
41	G	320	XAT	4	0
26	b	605	CLA	7	0
28	c	511	BCR	4	0
26	A	403	CLA	1	0
26	B	616	CLA	6	0
39	g	319	CHL	3	0
26	n	302	CLA	2	0
29	A	410	SQD	2	0
39	N	317	CHL	2	0
40	g	310	LUT	4	0
26	c	513	CLA	3	0
27	d	407	PHO	8	0
42	N	302	NEX	2	0
39	n	318	CHL	5	0
39	G	311	CHL	3	0
26	G	307	CLA	5	0
26	s	314	CLA	2	0
28	C	514	BCR	2	0
37	D	407	LHG	3	0
39	N	304	CHL	1	0
34	c	512	LMG	2	0
28	H	101	BCR	2	0
26	y	313	CLA	2	0
37	r	312	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	617	CLA	2	0
26	G	314	CLA	4	0
37	L	101	LHG	2	0
26	N	313	CLA	2	0
37	d	410	LHG	2	0
41	g	320	XAT	6	0
26	r	305	CLA	1	0
39	R	315	CHL	1	0
40	y	311	LUT	6	0
26	S	311	CLA	2	0
26	y	304	CLA	3	0
26	n	310	CLA	3	0
26	B	618	CLA	7	0
26	C	511	CLA	4	0
26	Y	311	CLA	1	0
26	R	316	CLA	1	0
37	G	312	LHG	6	0
26	D	406	CLA	1	0
37	d	402	LHG	4	0
33	B	620	DGD	3	0
28	c	507	BCR	3	0
39	Y	302	CHL	7	0
39	R	301	CHL	2	0
42	R	305	NEX	3	0
26	N	307	CLA	4	0
26	N	318	CLA	3	0
40	R	311	LUT	5	0
37	D	408	LHG	6	0
26	s	301	CLA	3	0
35	C	501	OEX	2	0
33	b	620	DGD	3	0
26	B	605	CLA	7	0
39	N	311	CHL	4	0
34	w	201	LMG	2	0
26	b	611	CLA	6	0
40	y	318	LUT	5	0
26	B	607	CLA	3	0
34	W	201	LMG	3	0
26	n	315	CLA	2	0
40	s	312	LUT	3	0
39	G	305	CHL	3	0
26	c	510	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	G	308	LUT	4	0
39	y	305	CHL	3	0
39	N	310	CHL	2	0
39	G	309	CHL	4	0
26	Y	310	CLA	1	0
41	N	315	XAT	6	0
37	S	317	LHG	2	0
26	c	516	CLA	2	0
37	Y	306	LHG	4	0
40	N	314	LUT	4	0
26	g	303	CLA	3	0
26	R	313	CLA	2	0
26	c	518	CLA	8	0
42	r	302	NEX	4	0
33	C	513	DGD	3	0
26	r	306	CLA	5	0
26	s	305	CLA	1	0
26	y	306	CLA	3	0
34	C	503	LMG	2	0
29	a	403	SQD	5	0
40	r	307	LUT	6	0
26	S	303	CLA	2	0
26	Y	308	CLA	4	0
35	a	408	OEX	3	0
33	y	308	DGD	2	0
28	j	101	BCR	4	0
26	y	310	CLA	6	0
39	r	301	CHL	2	0
26	Y	312	CLA	5	0
26	S	315	CLA	1	0
29	A	407	SQD	5	0
40	s	308	LUT	2	0
26	C	505	CLA	3	0
42	g	306	NEX	4	0
27	a	410	PHO	1	0
39	R	312	CHL	3	0
39	Y	318	CHL	3	0
26	s	307	CLA	2	0
39	r	316	CHL	1	0
41	n	316	XAT	4	0
26	b	607	CLA	5	0
26	b	609	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	G	316	LUT	1	0
26	c	508	CLA	3	0
28	K	101	BCR	5	0
30	d	408	PL9	2	0
26	a	411	CLA	3	0
40	n	314	LUT	4	0
26	D	409	CLA	9	0
26	C	507	CLA	5	0
30	a	407	PL9	4	0
39	n	307	CHL	4	0
26	s	311	CLA	4	0
39	G	301	CHL	5	0
42	S	305	NEX	7	0
26	r	313	CLA	7	0
39	y	314	CHL	3	0
39	n	306	CHL	6	0
39	N	316	CHL	5	0
39	y	303	CHL	6	0
40	N	305	LUT	3	0
40	Y	309	LUT	5	0
40	g	316	LUT	3	0
26	c	520	CLA	3	0
37	g	301	LHG	8	0
26	G	302	CLA	2	0
28	a	404	BCR	1	0
29	B	621	SQD	2	0
37	l	101	LHG	3	0
39	N	303	CHL	3	0
39	G	303	CHL	3	0
26	G	313	CLA	2	0
26	n	305	CLA	2	0
26	S	314	CLA	4	0
28	b	615	BCR	3	0
26	a	409	CLA	2	0
33	c	517	DGD	2	0
26	r	315	CLA	1	0
26	R	302	CLA	6	0
34	D	404	LMG	1	0
39	g	314	CHL	4	0
26	N	312	CLA	3	0
28	T	101	BCR	6	0
30	D	411	PL9	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	g	307	CHL	4	0
39	Y	307	CHL	3	0
39	r	309	CHL	3	0
28	b	603	BCR	5	0
28	k	101	BCR	5	0
26	B	610	CLA	7	0
26	y	315	CLA	2	0
37	s	309	LHG	2	0
28	t	101	BCR	6	0
26	R	309	CLA	2	0
26	Y	305	CLA	8	0
34	C	518	LMG	1	0
26	B	615	CLA	4	0
40	S	301	LUT	3	0
41	G	310	XAT	6	0
33	c	519	DGD	3	0
26	g	305	CLA	1	0
42	n	313	NEX	1	0
26	c	503	CLA	5	0
26	R	308	CLA	4	0
26	C	517	CLA	3	0
26	B	604	CLA	2	0
39	s	303	CHL	1	0
37	n	301	LHG	5	0
28	B	619	BCR	5	0
27	D	403	PHO	7	0
26	d	411	CLA	3	0
26	C	516	CLA	4	0
39	s	317	CHL	3	0
26	B	606	CLA	6	0
26	g	315	CLA	2	0
26	s	304	CLA	2	0
28	A	406	BCR	1	0
26	S	304	CLA	1	0
33	Y	303	DGD	3	0
39	S	302	CHL	6	0
39	g	311	CHL	7	0
26	D	401	CLA	3	0
28	J	101	BCR	4	0
26	r	303	CLA	1	0
39	y	312	CHL	2	0
26	b	613	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	s	302	NEX	6	0
26	b	610	CLA	4	0
26	a	402	CLA	1	0
26	B	612	CLA	2	0
26	c	515	CLA	4	0
39	g	313	CHL	5	0
26	b	601	CLA	6	0
42	Y	304	NEX	3	0
26	n	303	CLA	3	0
26	r	311	CLA	4	0
26	g	308	CLA	3	0
39	s	313	CHL	6	0
41	r	304	XAT	2	0
26	s	315	CLA	2	0
26	C	521	CLA	4	0
39	S	312	CHL	5	0
26	S	307	CLA	3	0
28	h	101	BCR	3	0
26	b	612	CLA	2	0
34	d	405	LMG	2	0
26	G	304	CLA	1	0
34	B	622	LMG	2	0
26	B	602	CLA	7	0
26	d	404	CLA	9	0
26	C	508	CLA	1	0
33	C	510	DGD	3	0
26	C	512	CLA	5	0
40	Y	315	LUT	7	0
33	C	509	DGD	4	0
26	g	317	CLA	6	0
26	B	603	CLA	4	0
26	A	405	CLA	2	0
26	b	616	CLA	1	0
26	D	412	CLA	3	0
26	g	304	CLA	1	0
26	R	317	CLA	2	0
39	Y	317	CHL	3	0
26	c	505	CLA	6	0
26	s	310	CLA	4	0
26	Y	313	CLA	3	0
26	C	520	CLA	5	0
26	b	606	CLA	3	0

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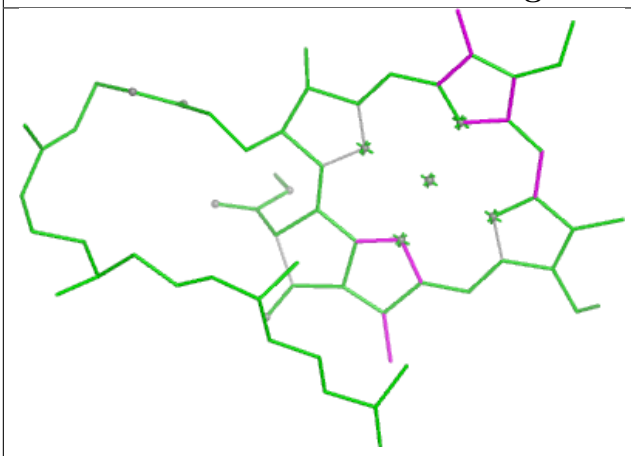
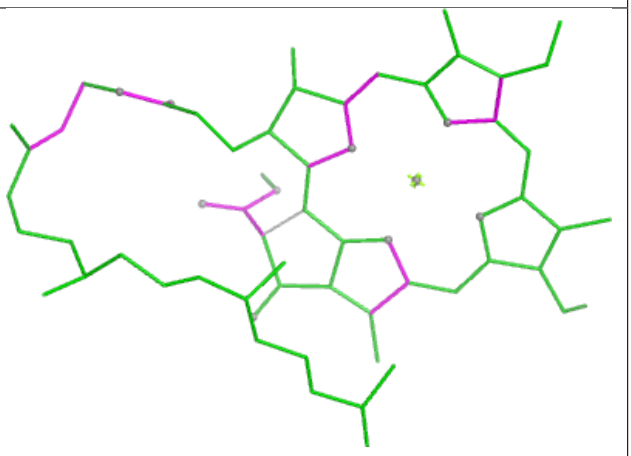
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	g	302	CLA	2	0
30	A	408	PL9	3	0
26	S	310	CLA	4	0
39	S	316	CHL	1	0
26	b	608	CLA	6	0
28	B	614	BCR	3	0
37	D	410	LHG	2	0
26	b	617	CLA	6	0
26	B	611	CLA	3	0
39	y	302	CHL	2	0
26	y	309	CLA	7	0
26	c	502	CLA	4	0
27	A	404	PHO	2	0
39	n	311	CHL	1	0
26	Y	301	CLA	3	0
37	d	409	LHG	4	0
29	b	621	SQD	3	0
26	b	618	CLA	3	0

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

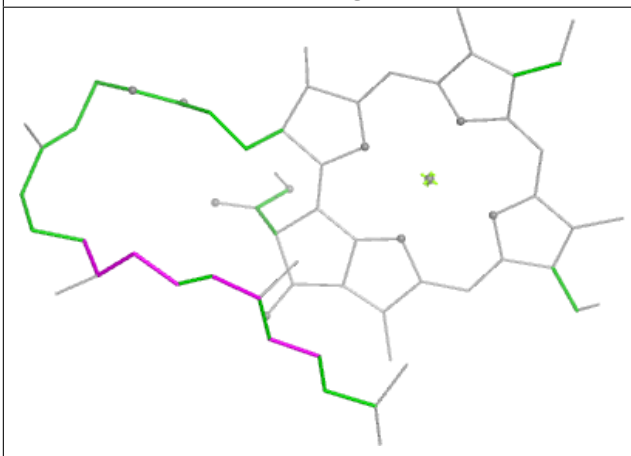
Ligand CLA C 515



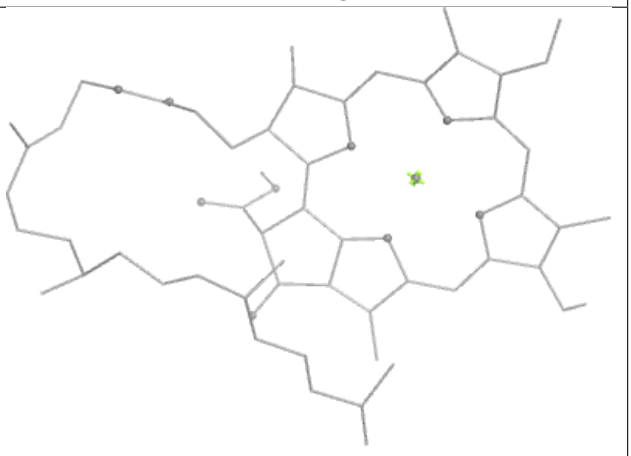
Bond lengths



Bond angles

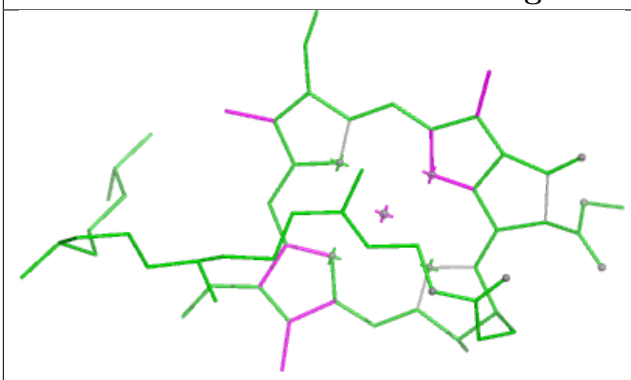


Torsions

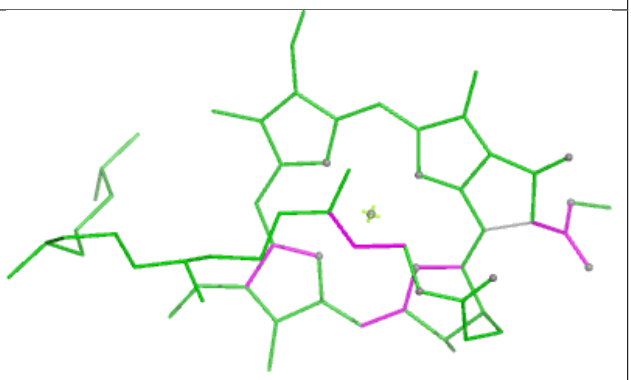


Rings

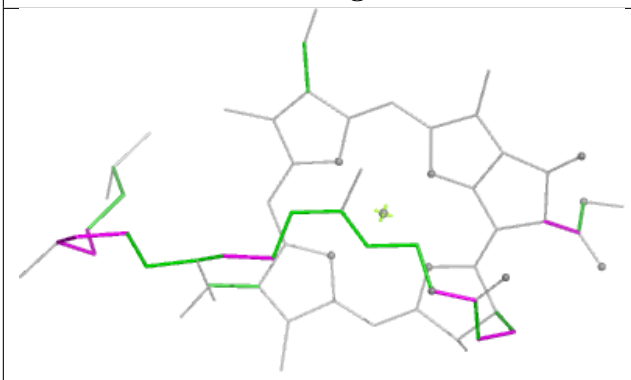
Ligand CLA C 506



Bond lengths



Bond angles



Torsions

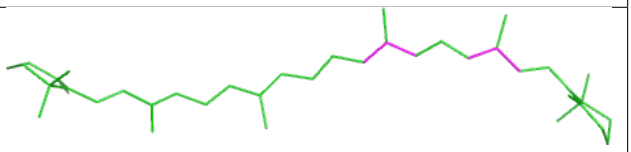


Rings

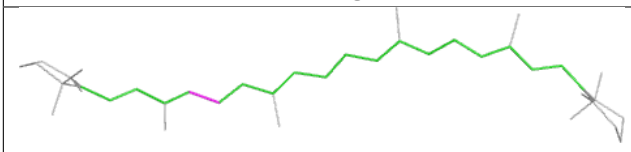
Ligand BCR C 502



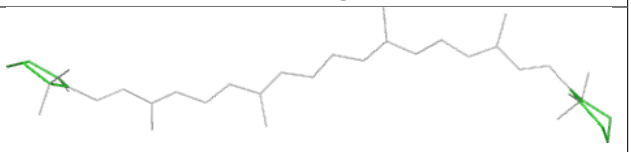
Bond lengths



Bond angles

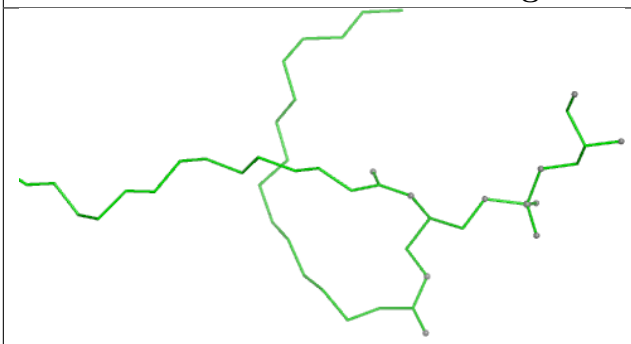


Torsions

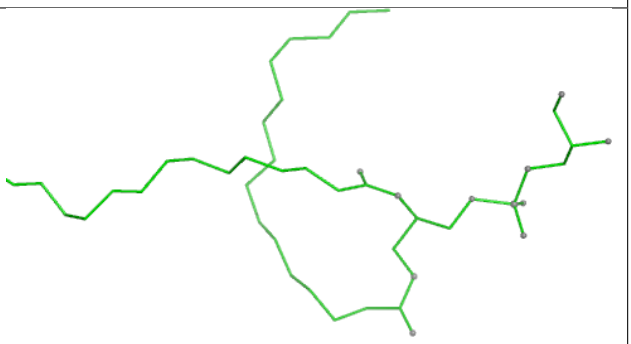


Rings

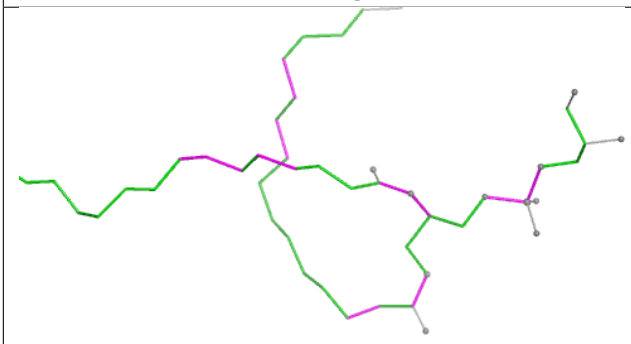
Ligand LHG N 301



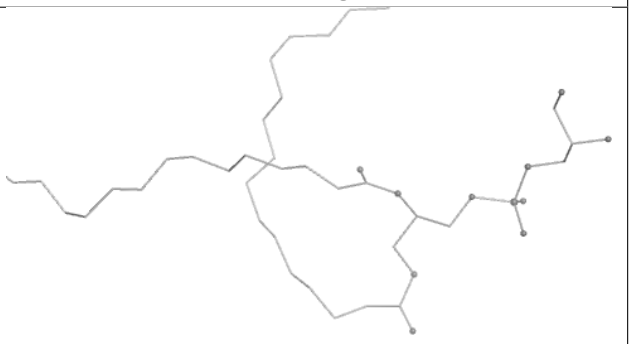
Bond lengths



Bond angles

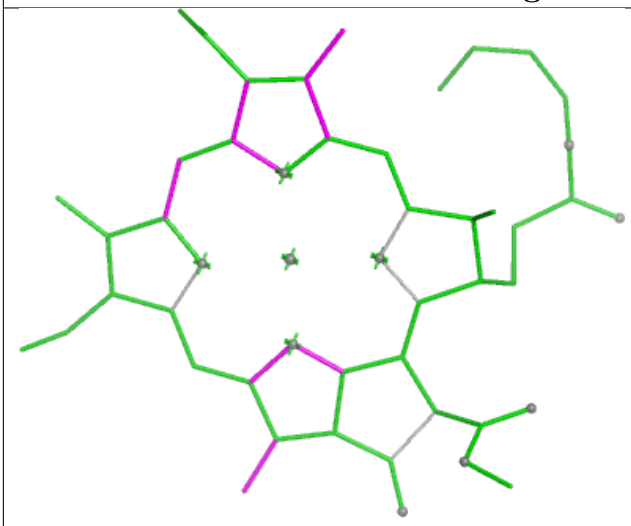


Torsions

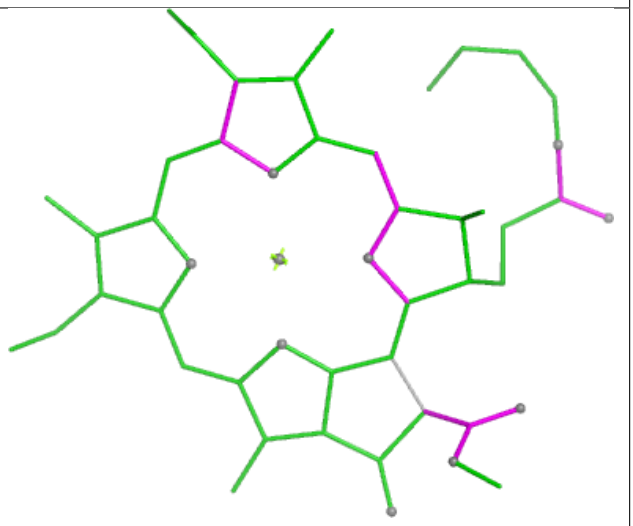


Rings

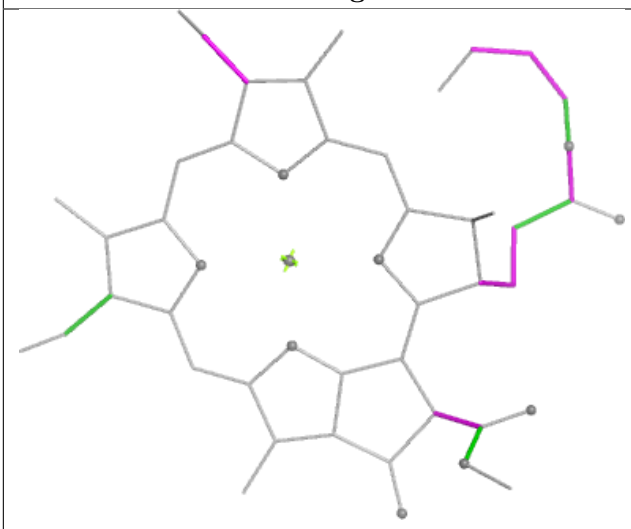
Ligand CLA N 319



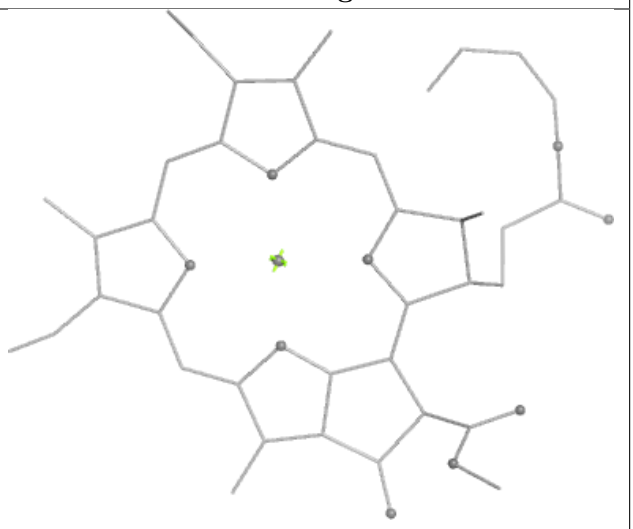
Bond lengths



Bond angles

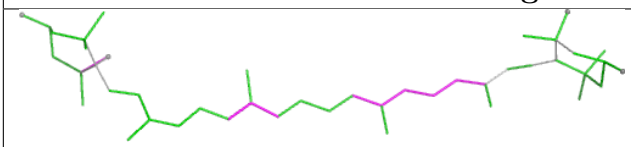


Torsions

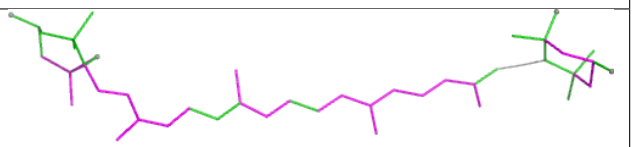


Rings

Ligand NEX G 315



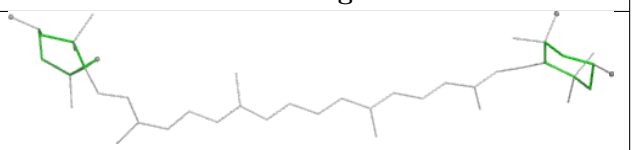
Bond lengths



Bond angles

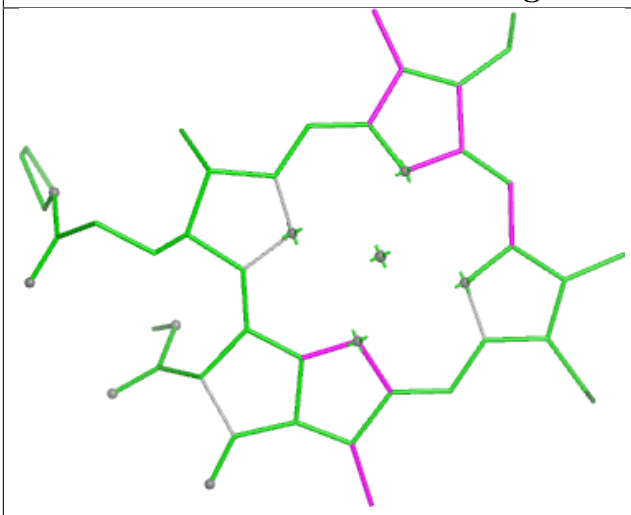


Torsions



Rings

Ligand CLA G 319



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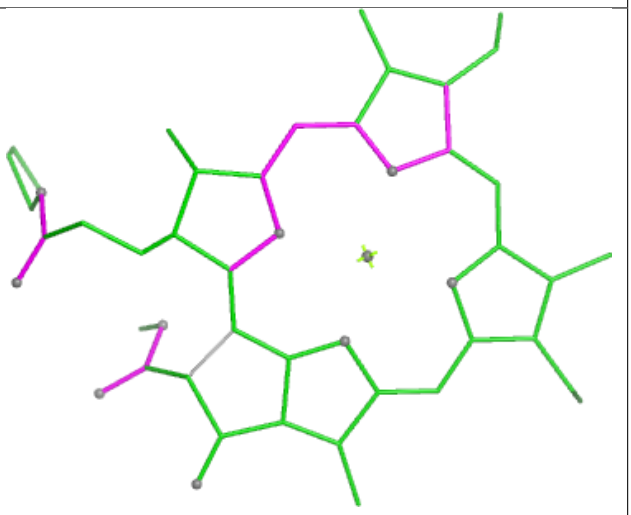
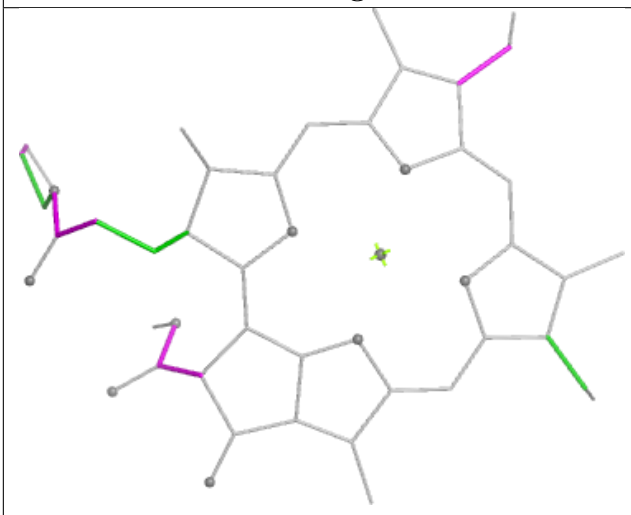


Bond angles



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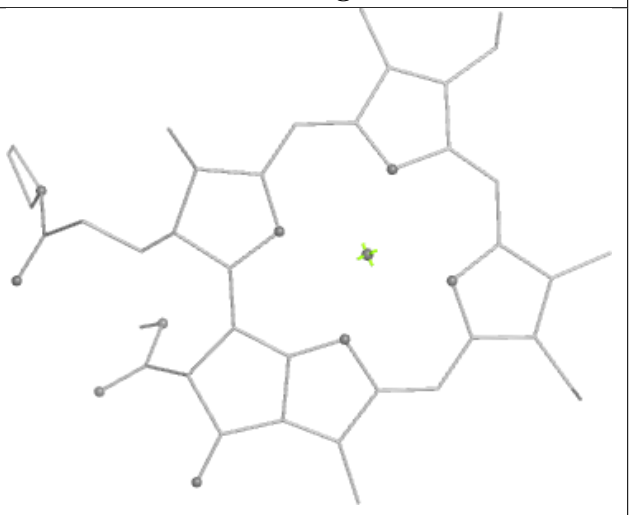


Rings

Ligand BCR B 608



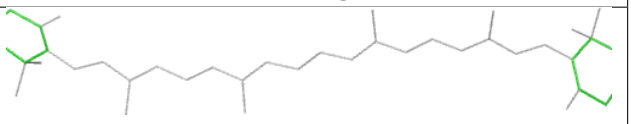
Bond lengths



Bond angles

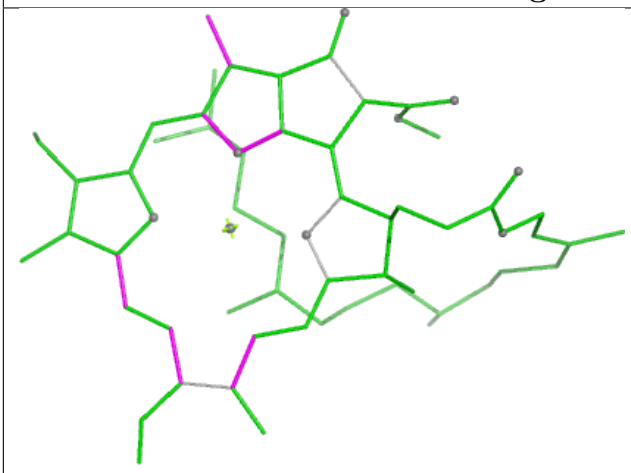


Torsions



Rings

Ligand CLA c 506



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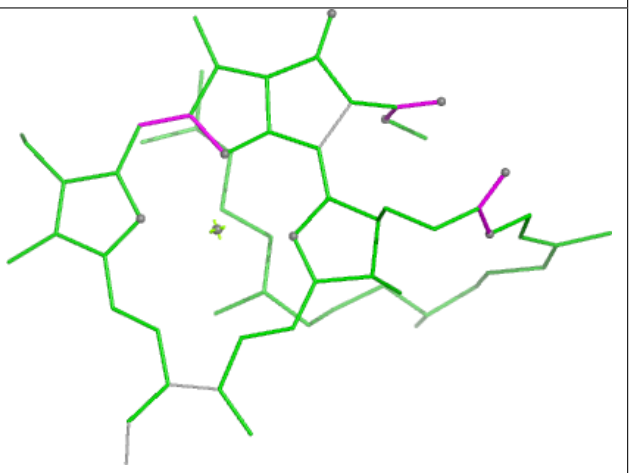
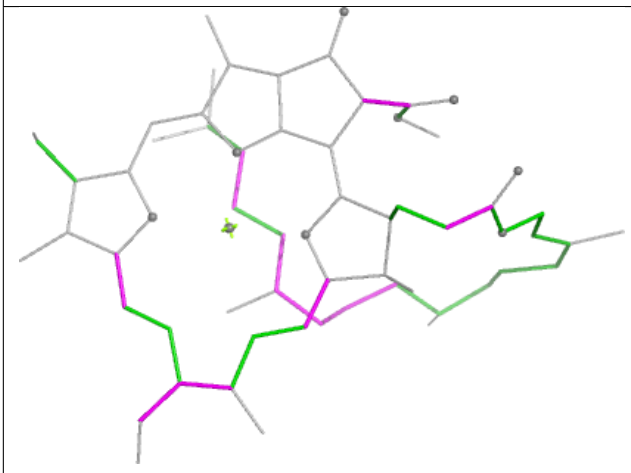


Bond angles



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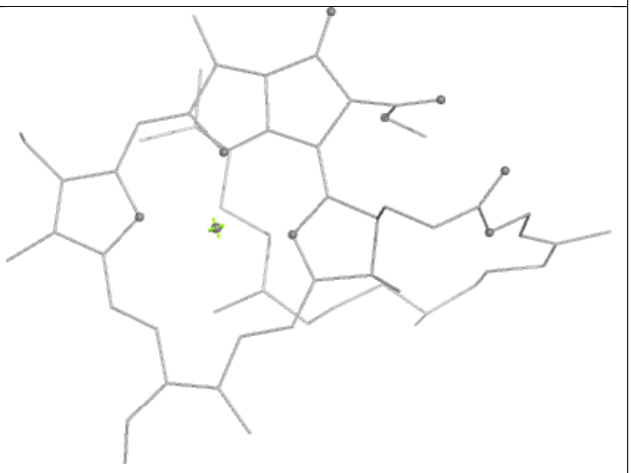
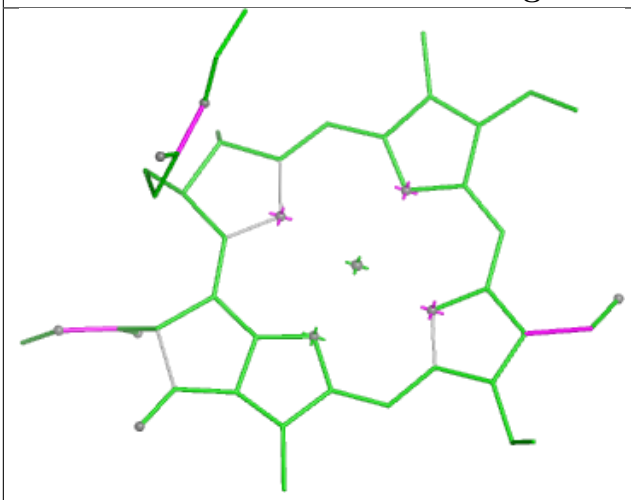


Rings

Ligand CHL R 318



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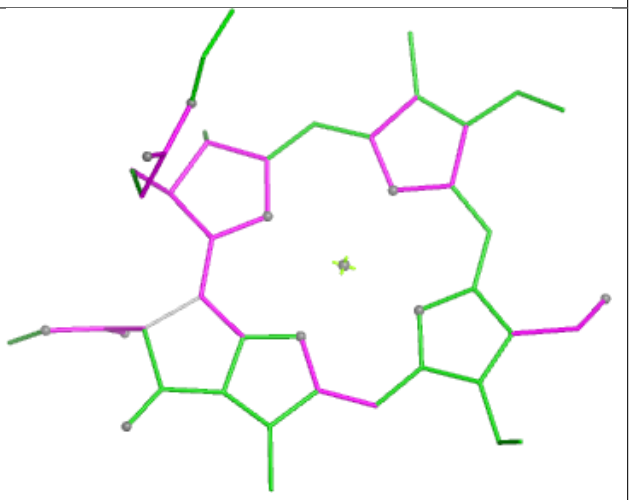
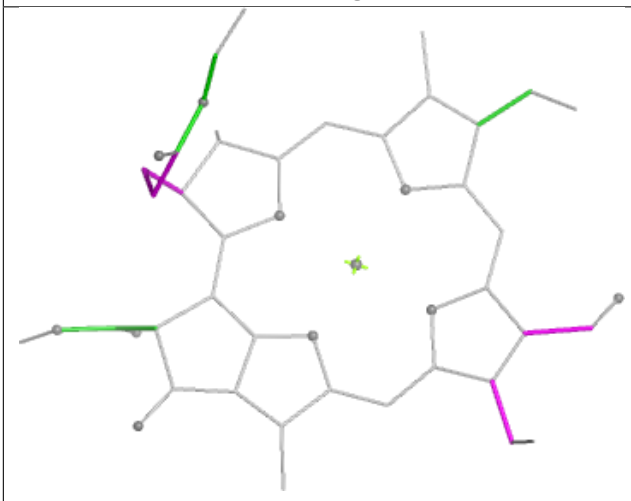


Bond angles



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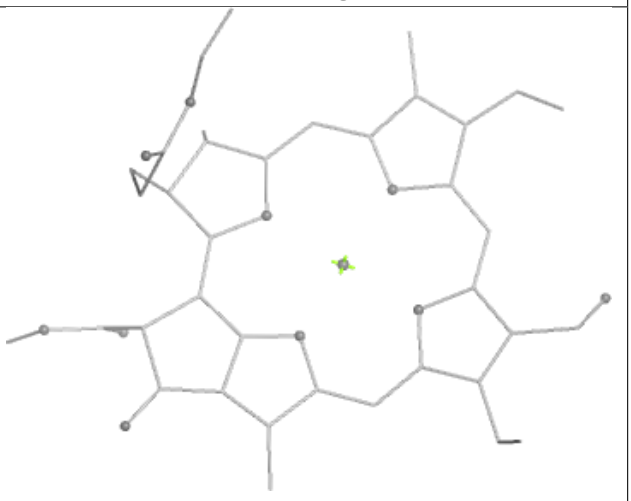
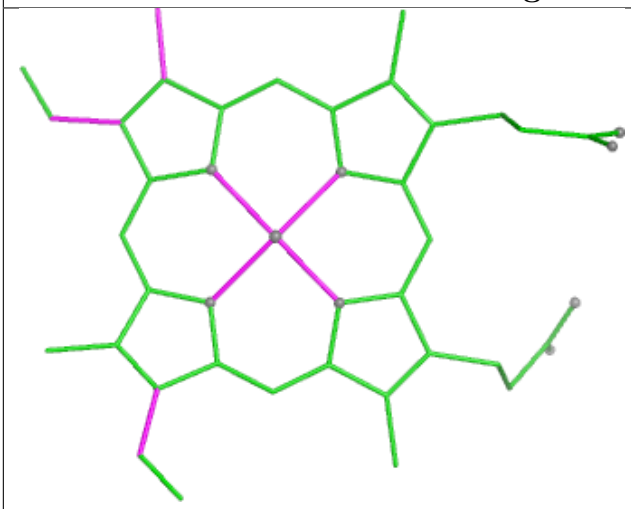


Rings

Ligand HEM e 101



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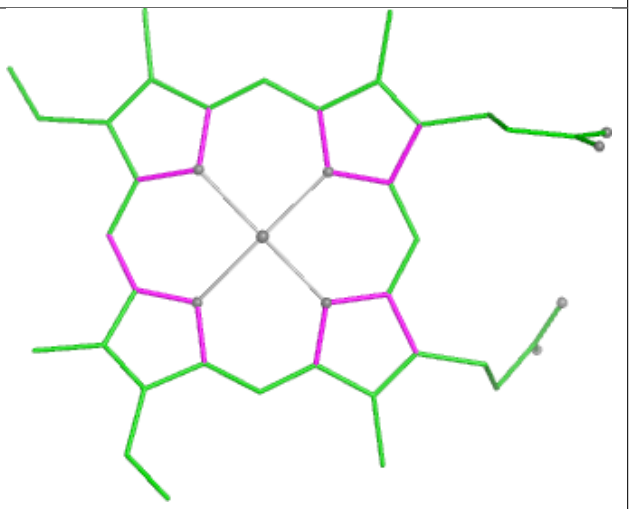
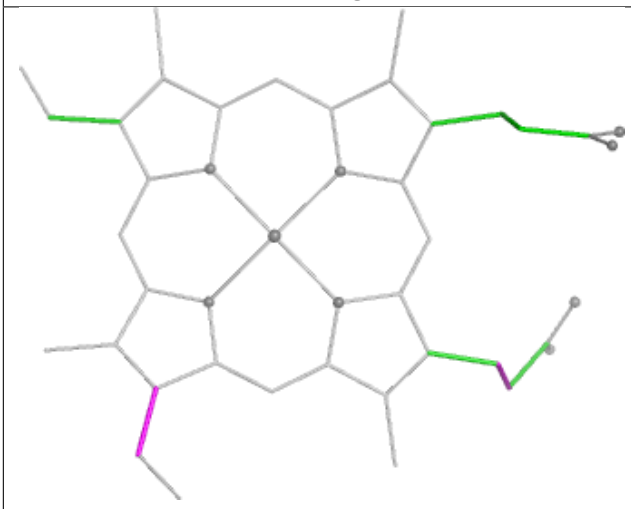


Bond angles



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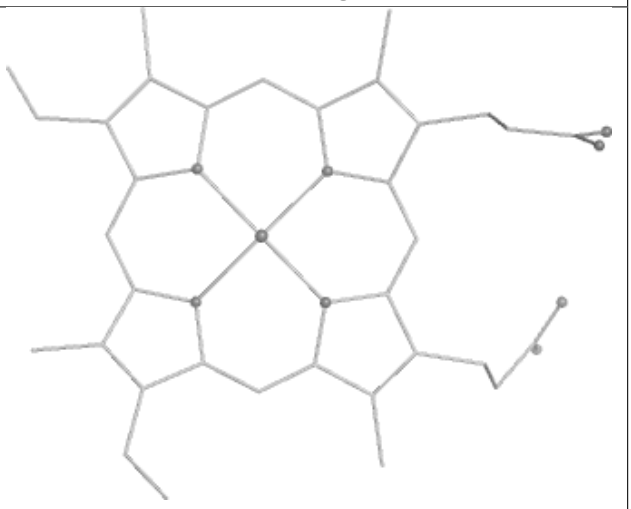
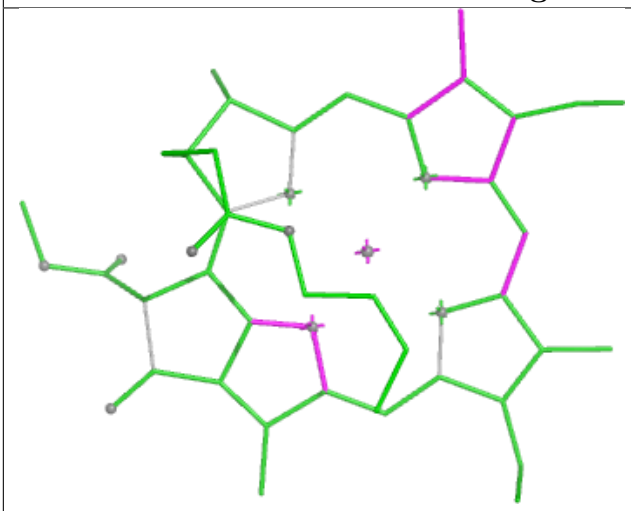


Rings

Ligand CLA r 308



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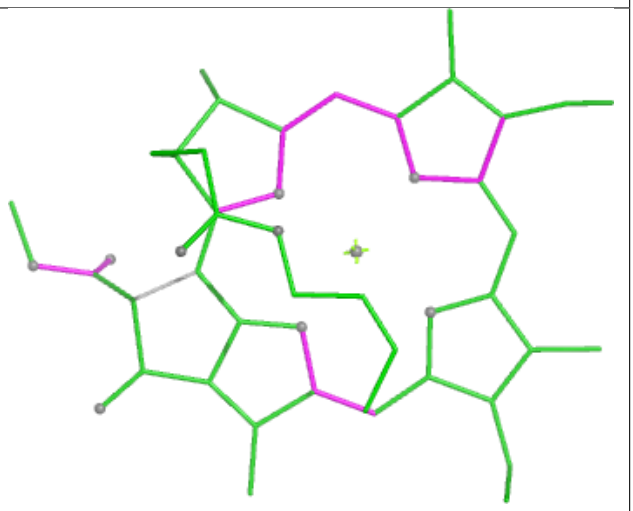
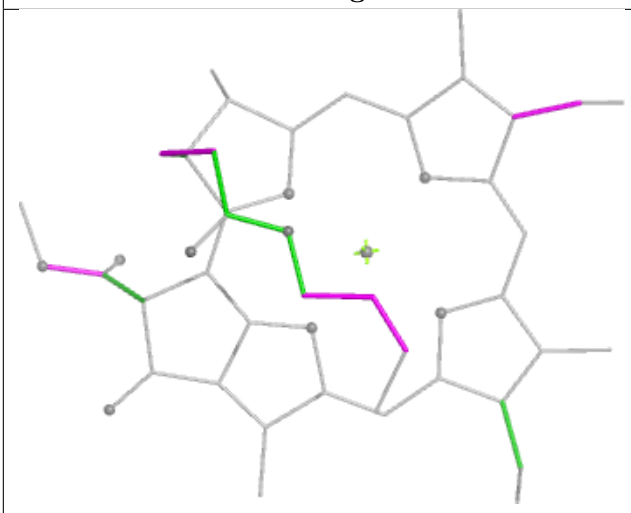


Bond angles



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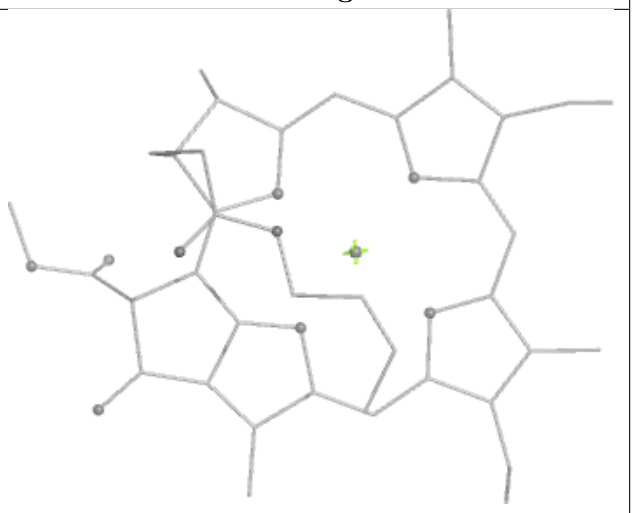
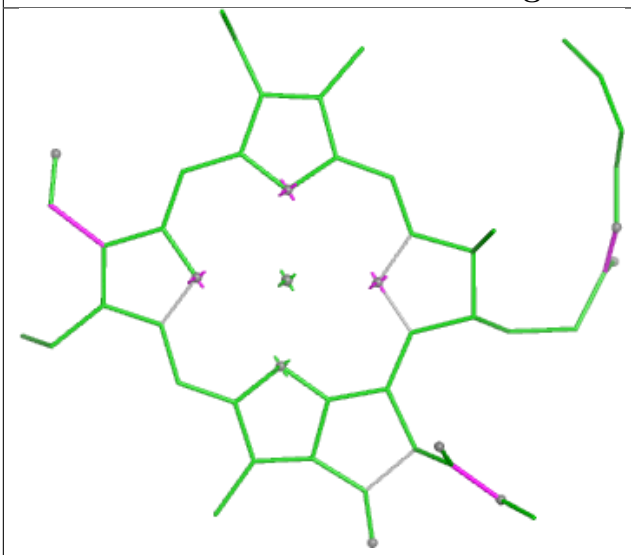


Rings

Ligand CHL Y 314



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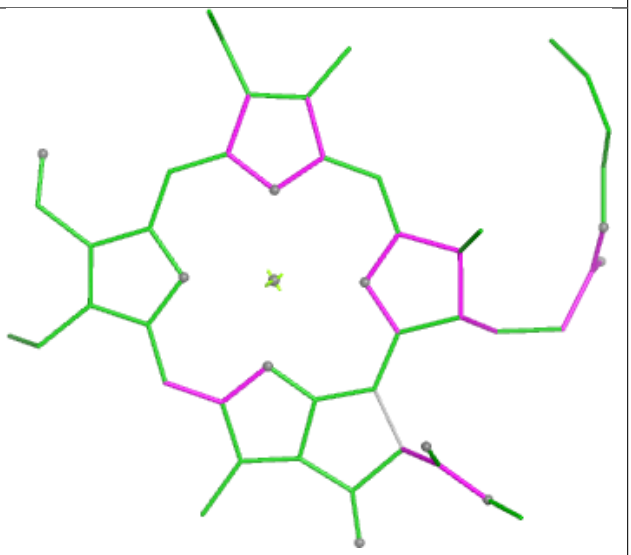
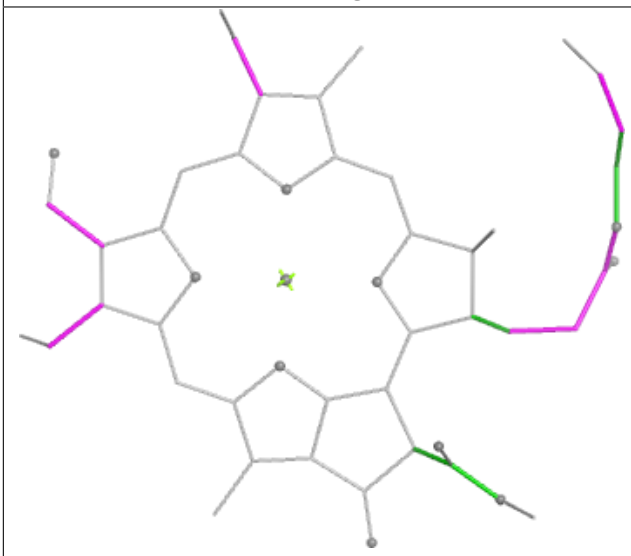


Bond angles



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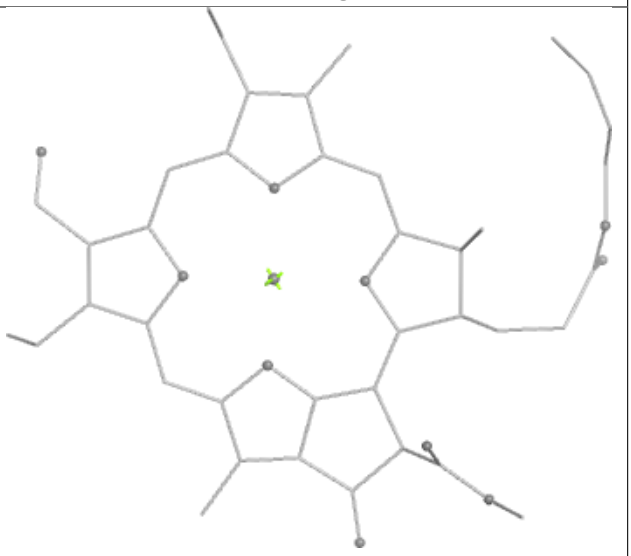
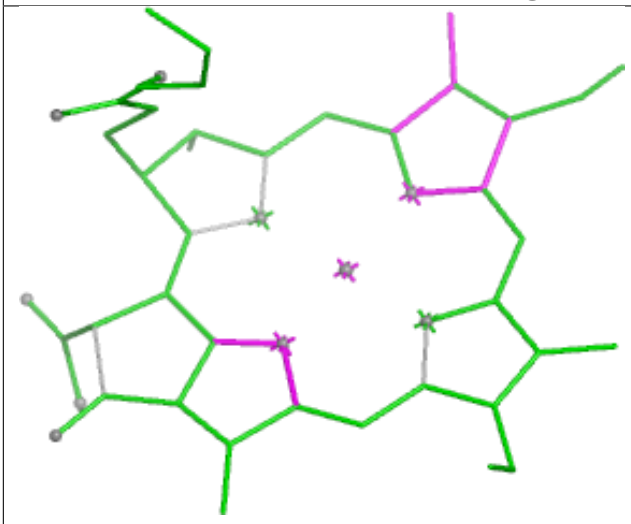


Rings

Ligand CLA Y 316



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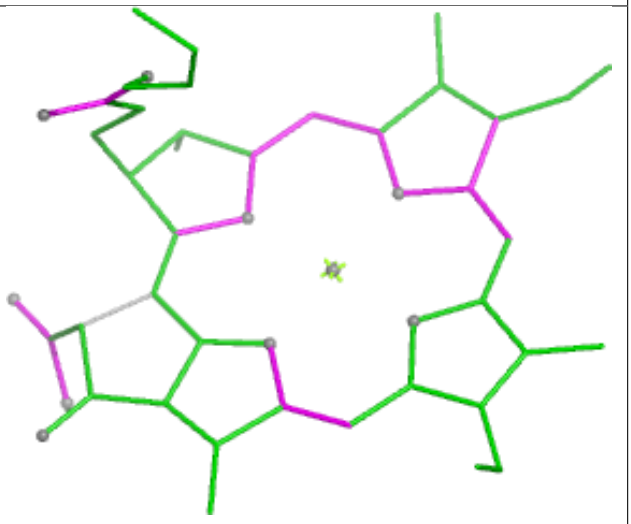
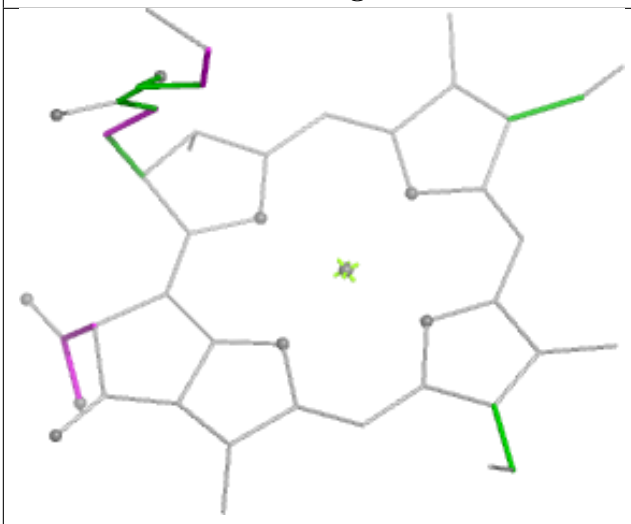


Bond angles

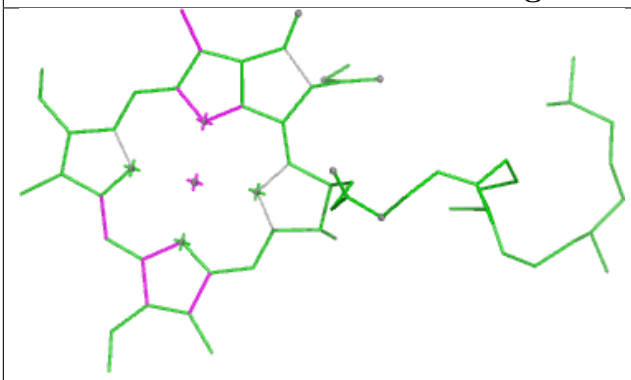


Torsions



Rings

Ligand CLA B 609



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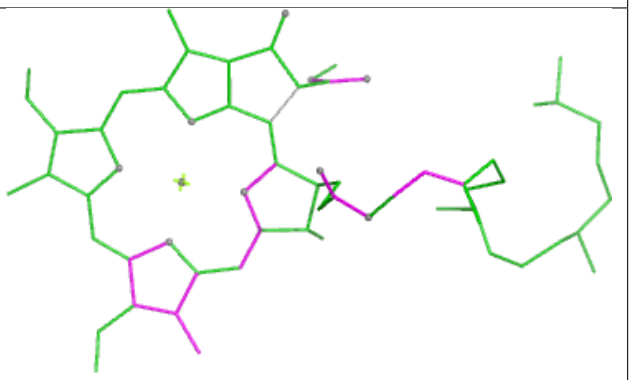
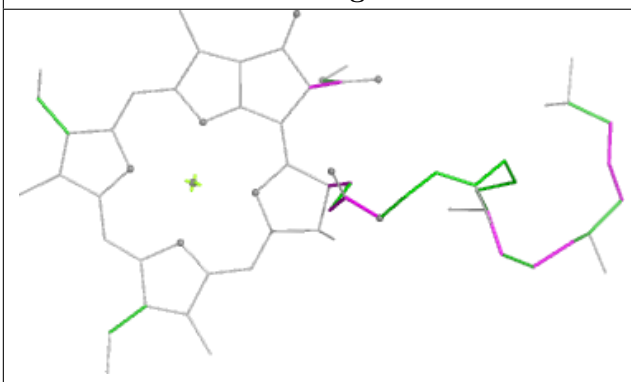


Bond angles



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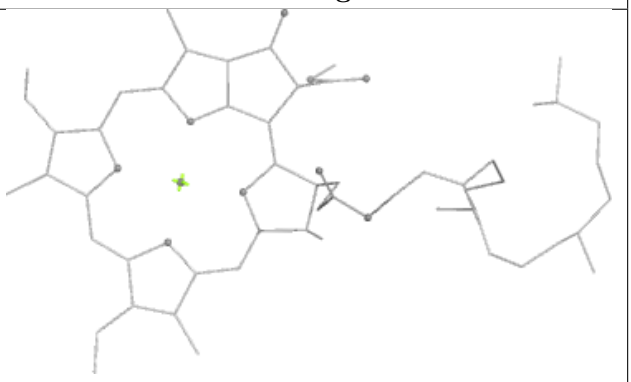


Rings

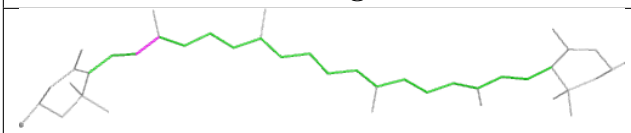
Ligand LUT S 306



Bond lengths



Bond angles

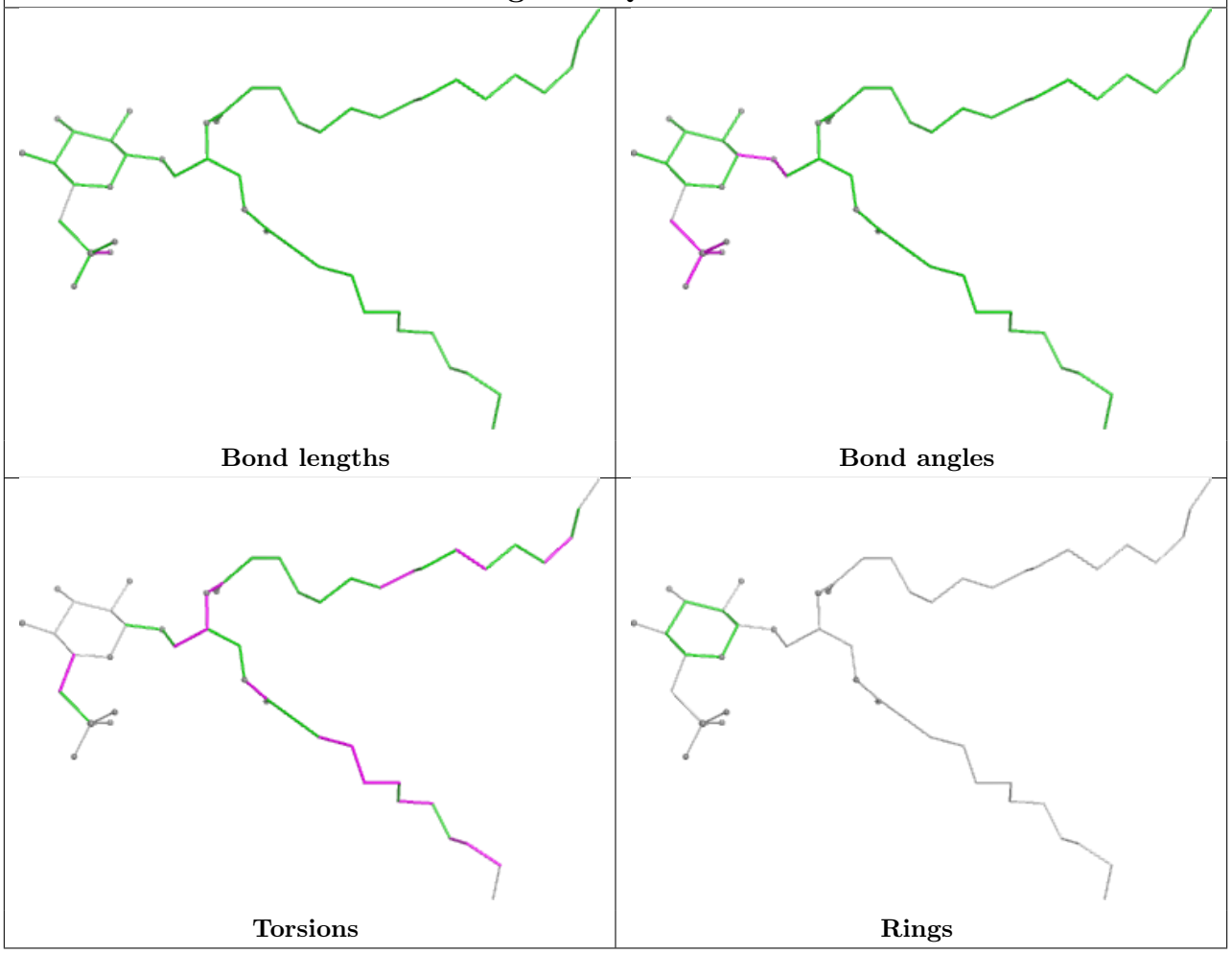


Torsions

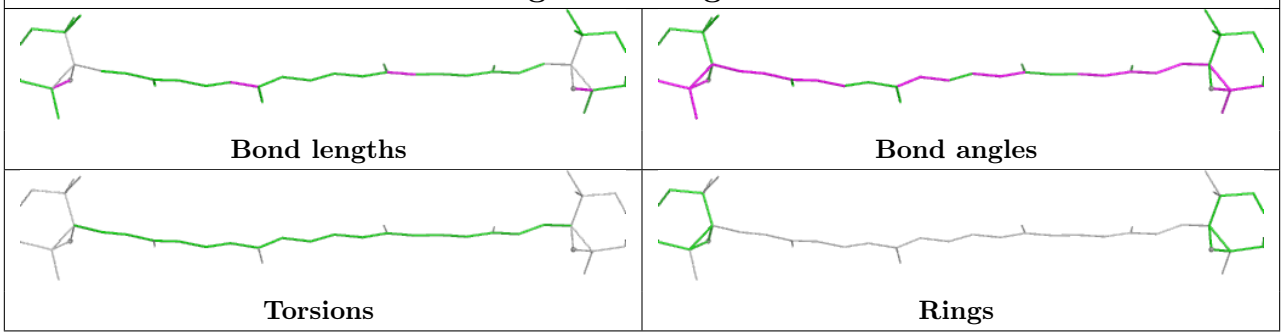


Rings

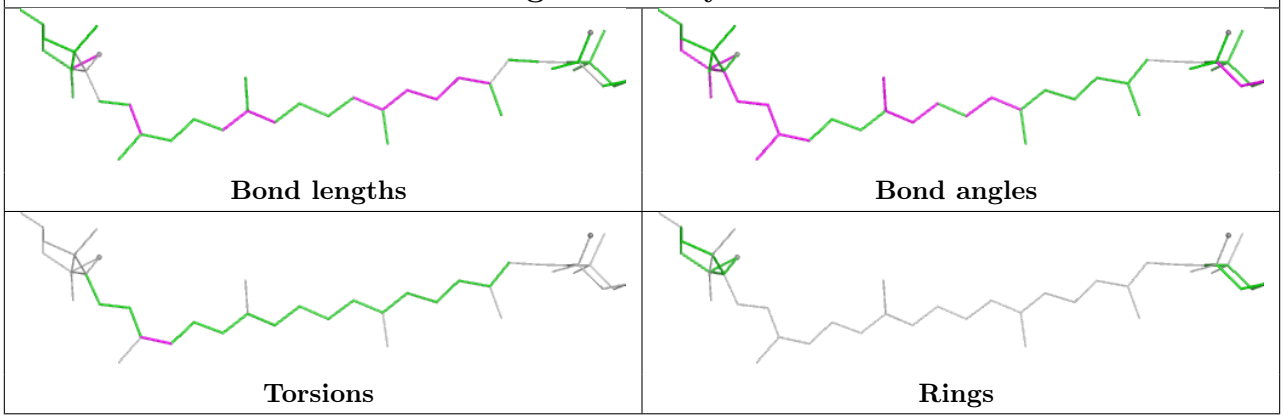
Ligand SQD a 413



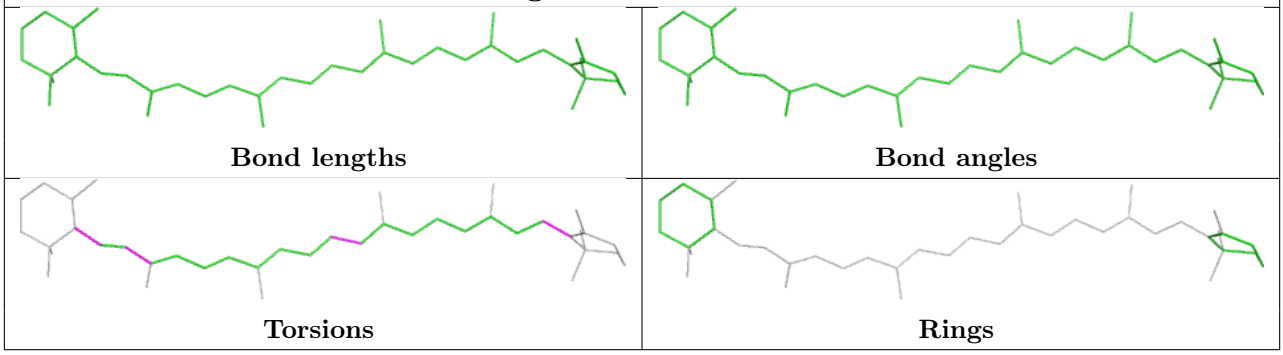
Ligand XAT g 309



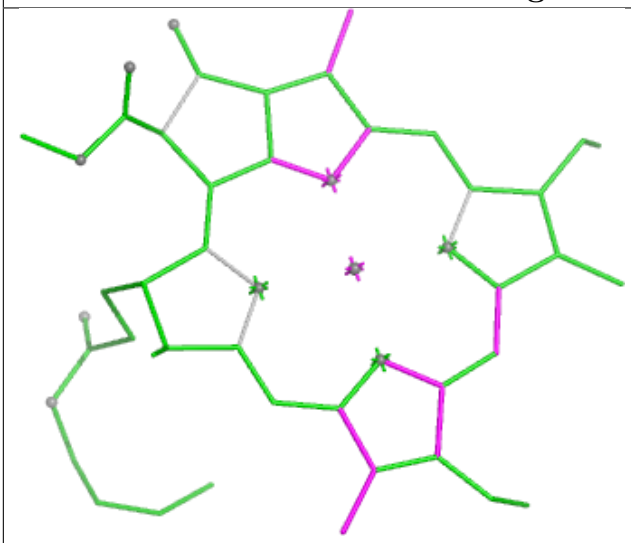
Ligand NEX y 307



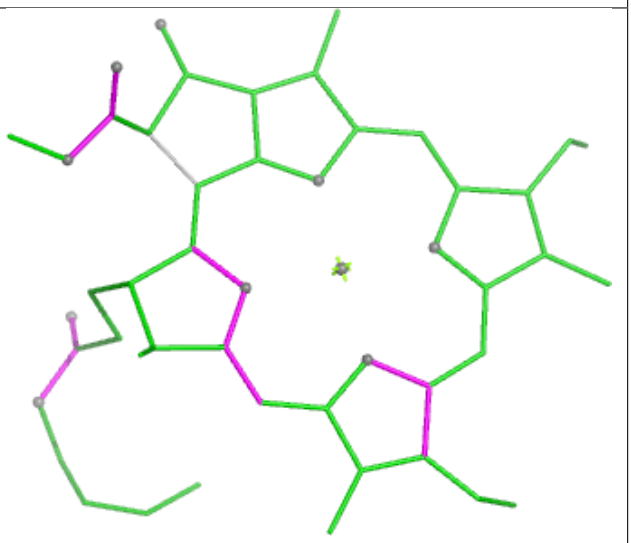
Ligand BCR b 619



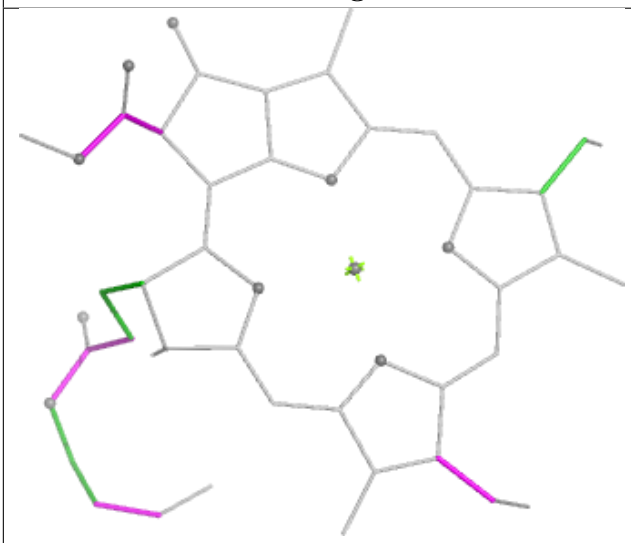
Ligand CLA S 308



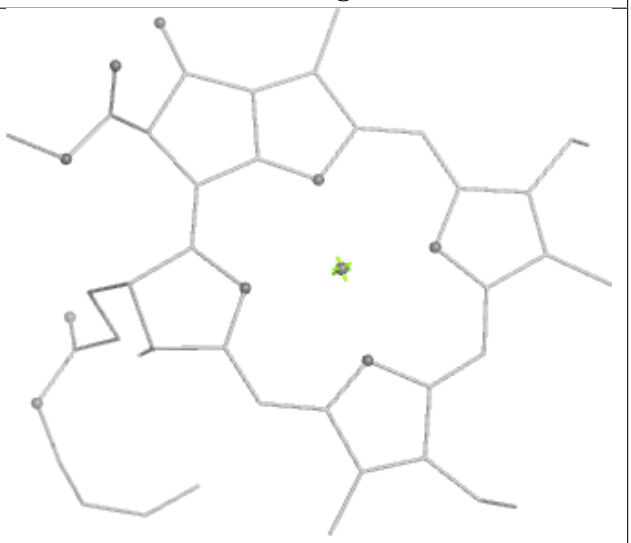
Bond lengths



Bond angles

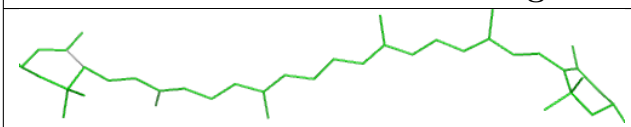


Torsions



Rings

Ligand LUT n 317



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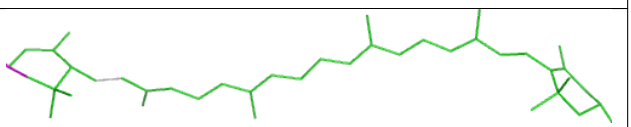
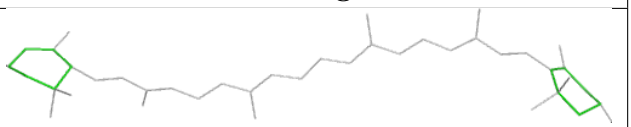


Bond angles

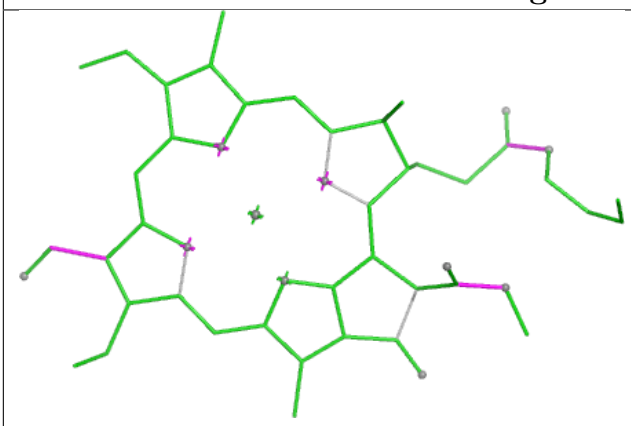


Torsions



Rings

Ligand CHL s 316



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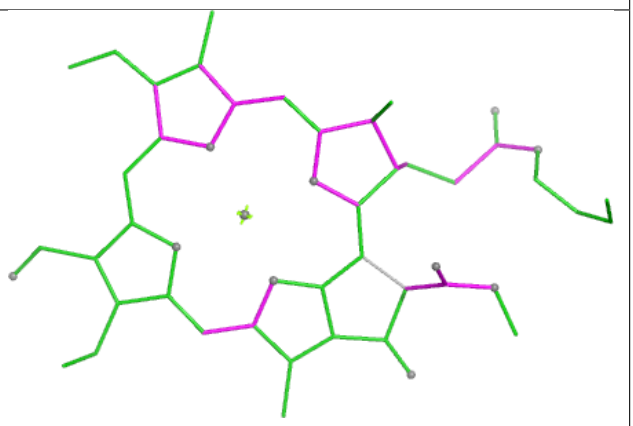
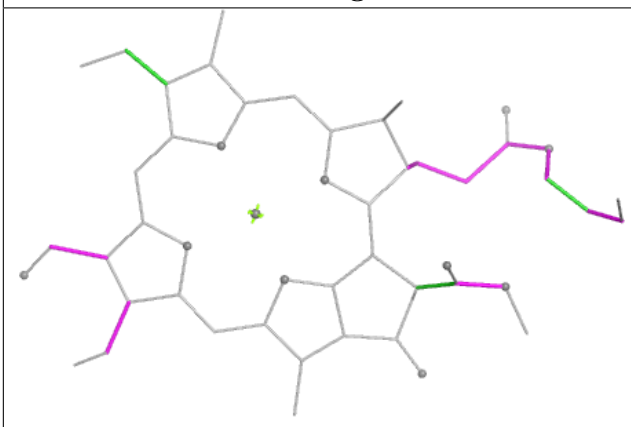


Bond angles



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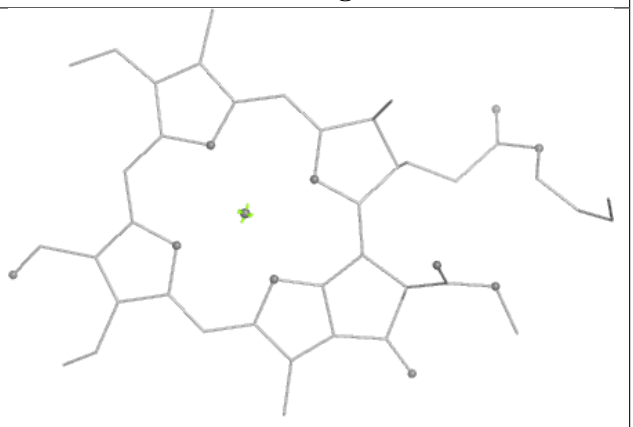
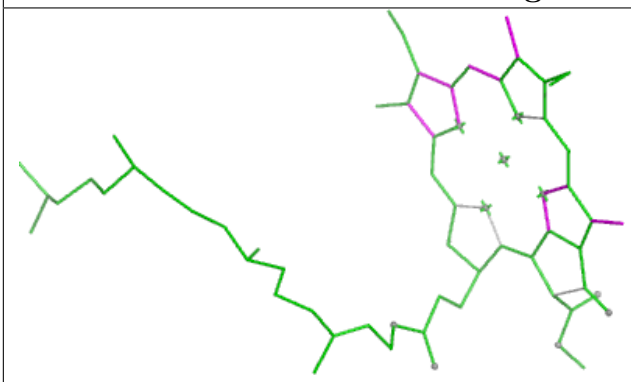


Rings

Ligand CLA C 504



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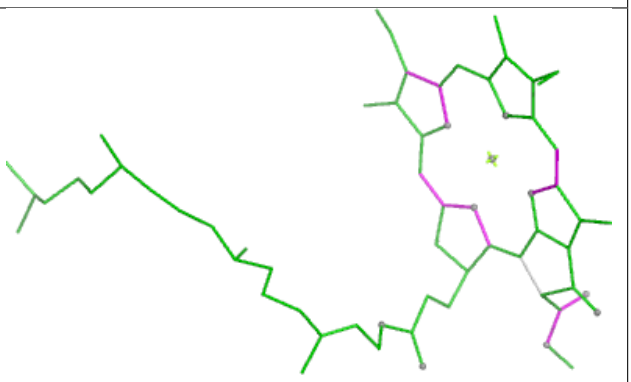
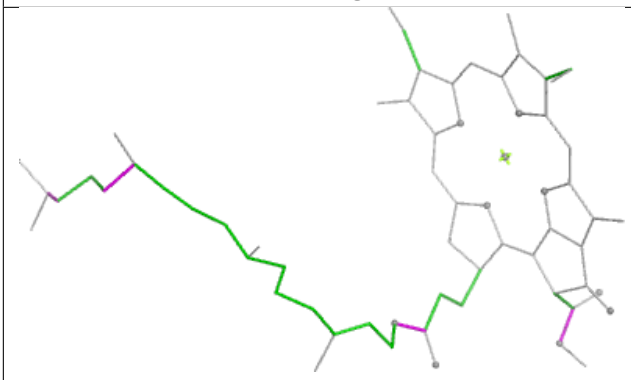


Bond angles

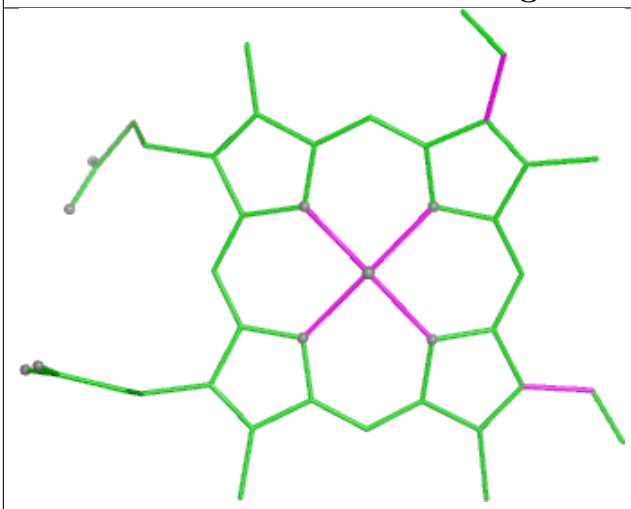


Torsions



Rings

Ligand HEM E 101



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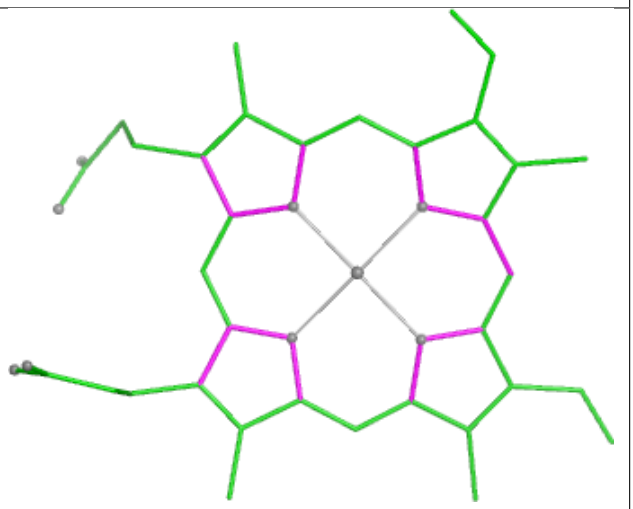
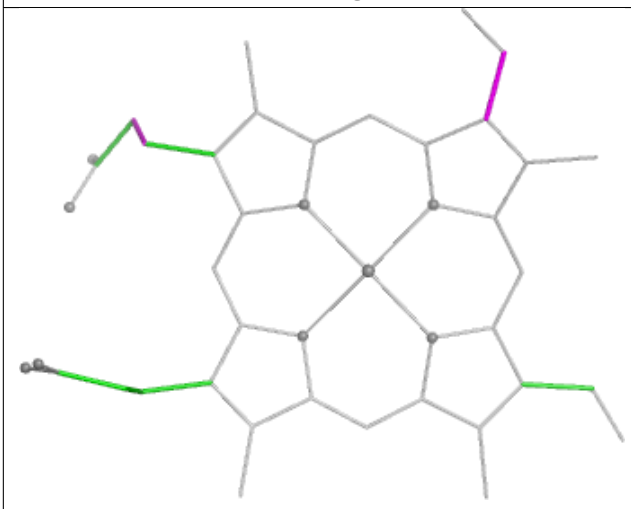
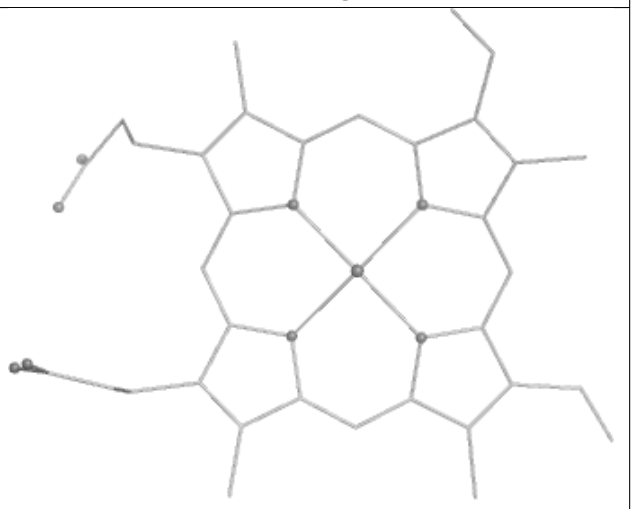


Bond angles



Torsions

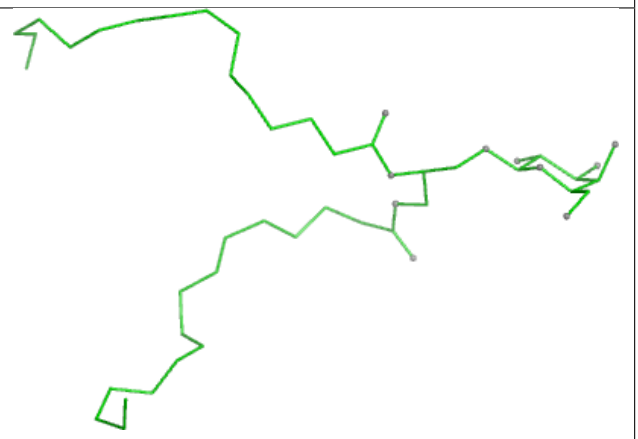


Rings

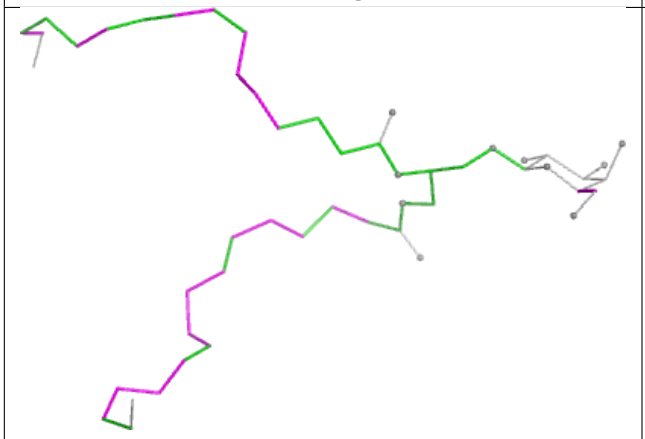
Ligand LMG b 622



Bond lengths



Bond angles

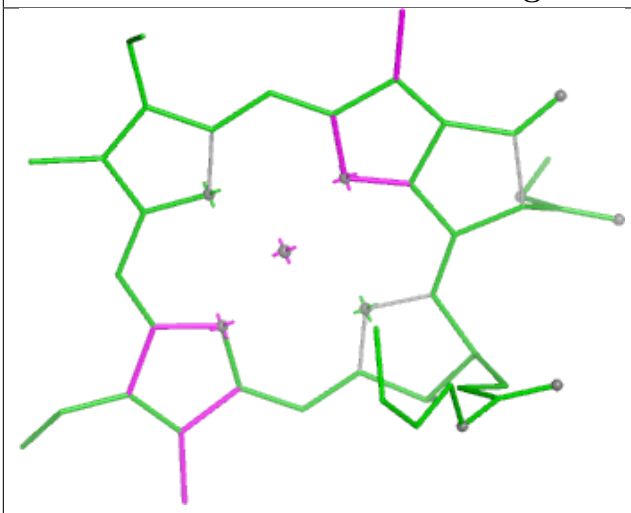


Torsions

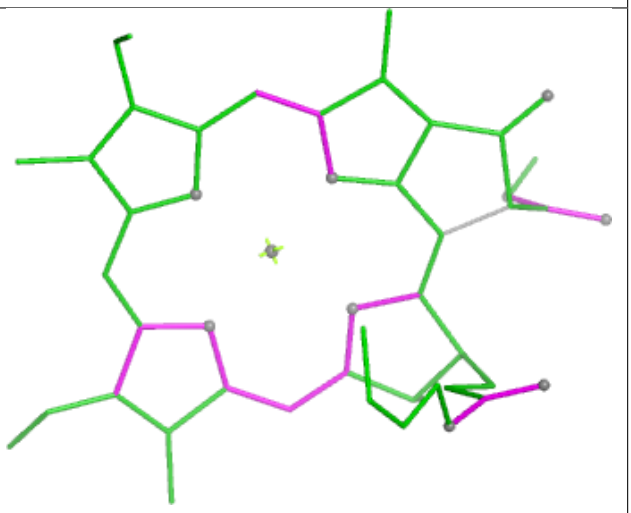


Rings

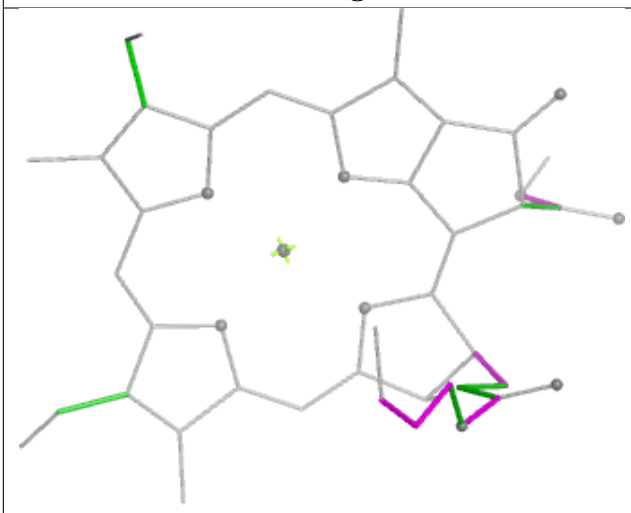
Ligand CLA N 308



Bond lengths



Bond angles



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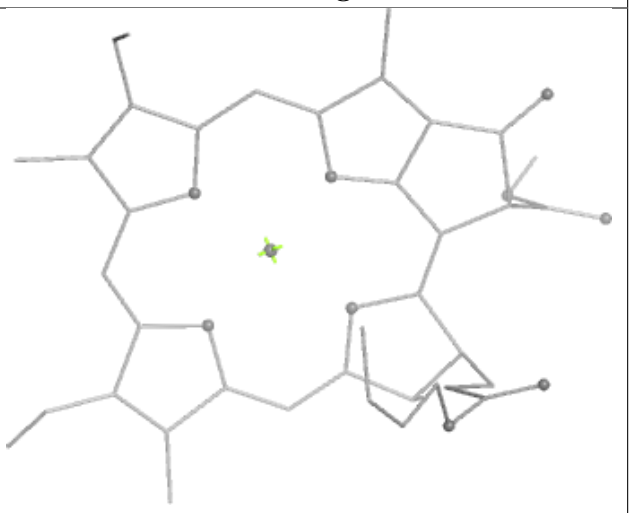
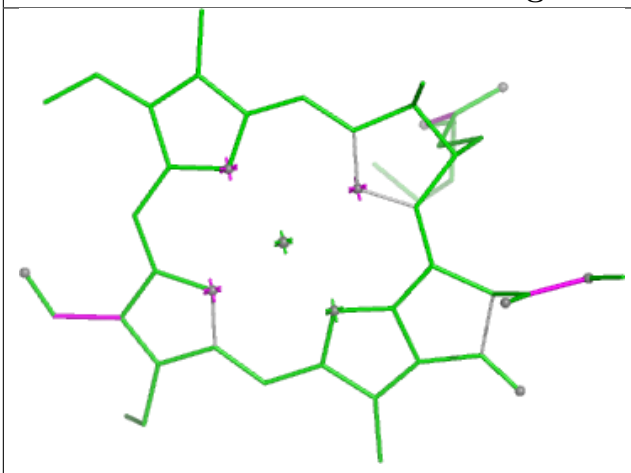
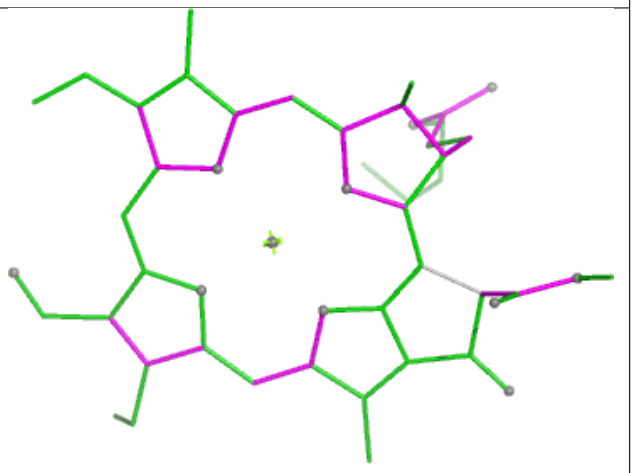


Rings

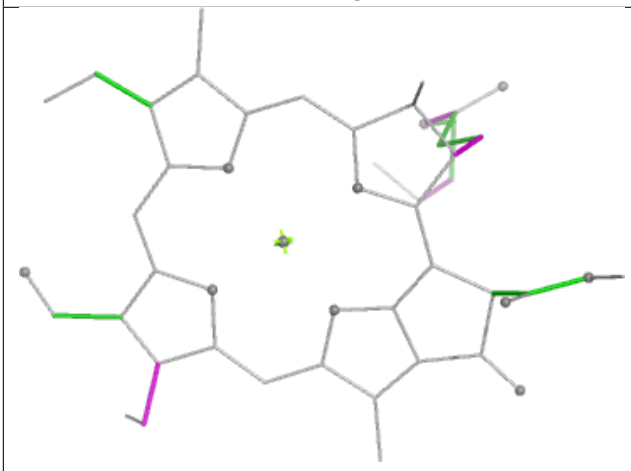
Ligand CHL n 319



Bond lengths



Bond angles



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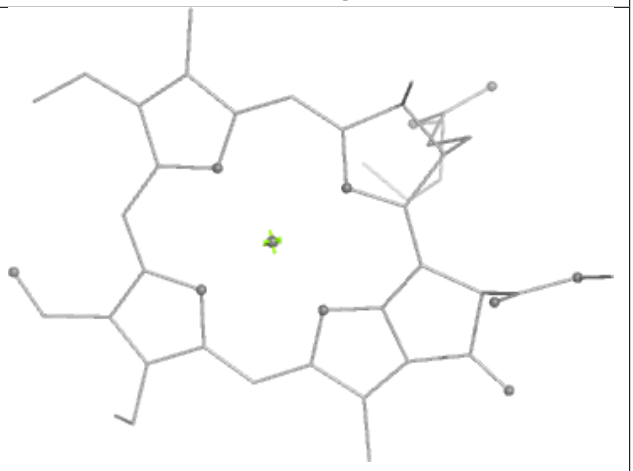
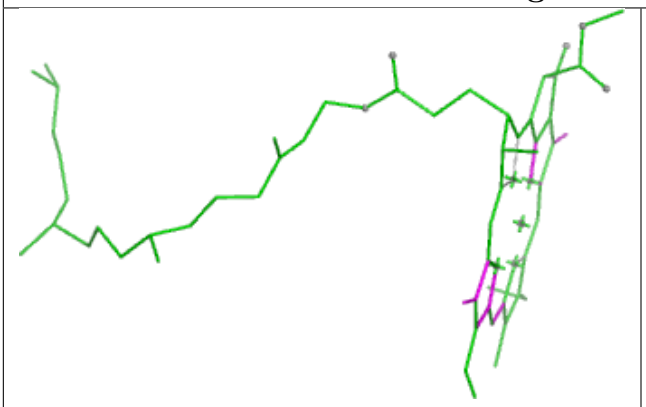
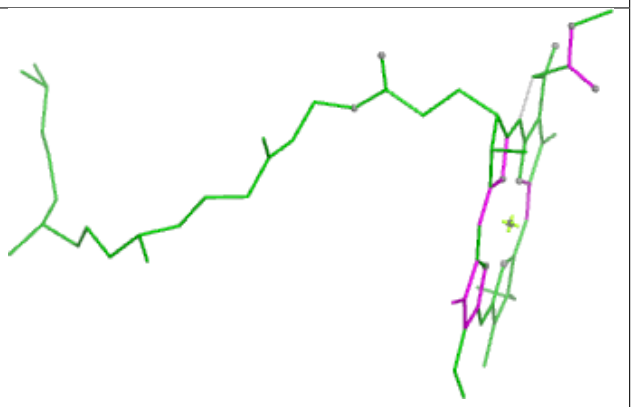


Rings

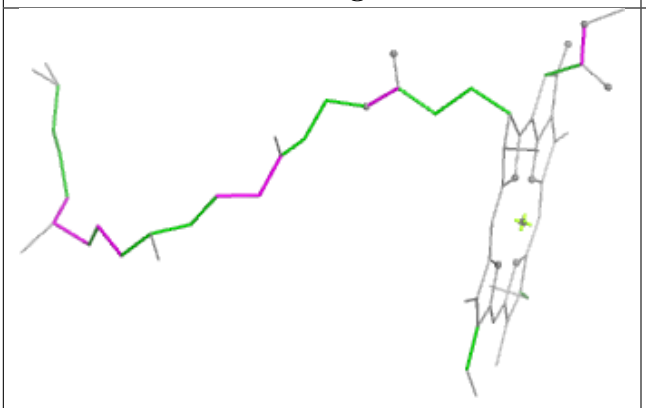
Ligand CLA d 403



Bond lengths



Bond angles



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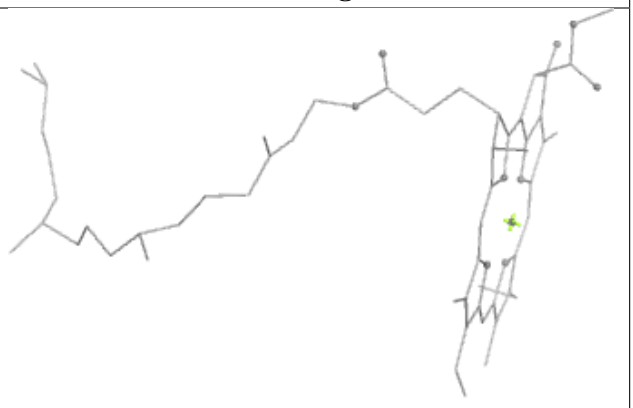
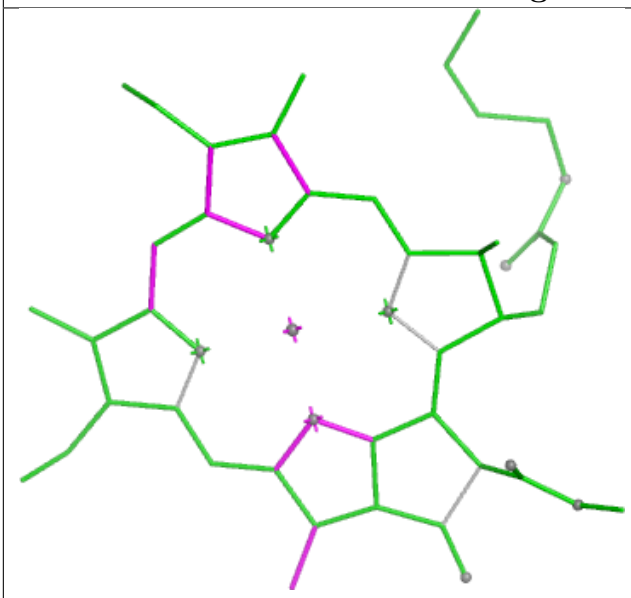


Rings

Ligand CLA r 317



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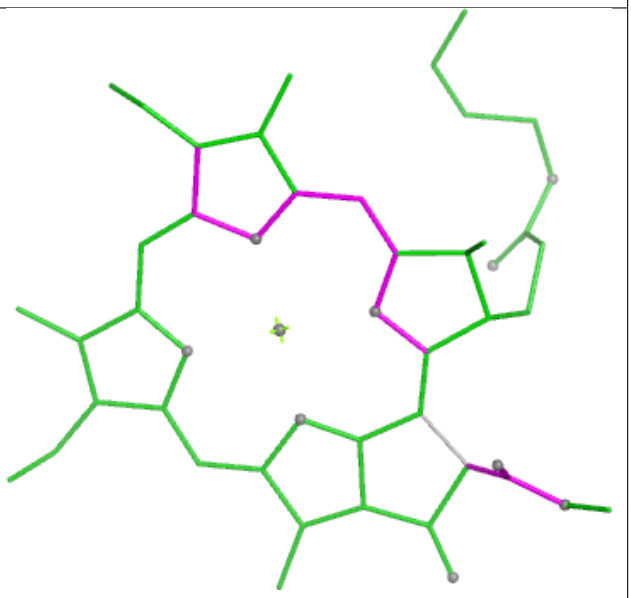
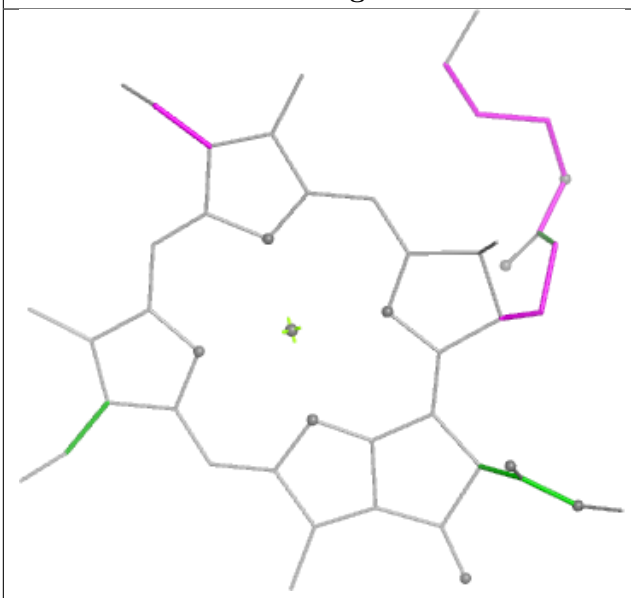


Bond angles



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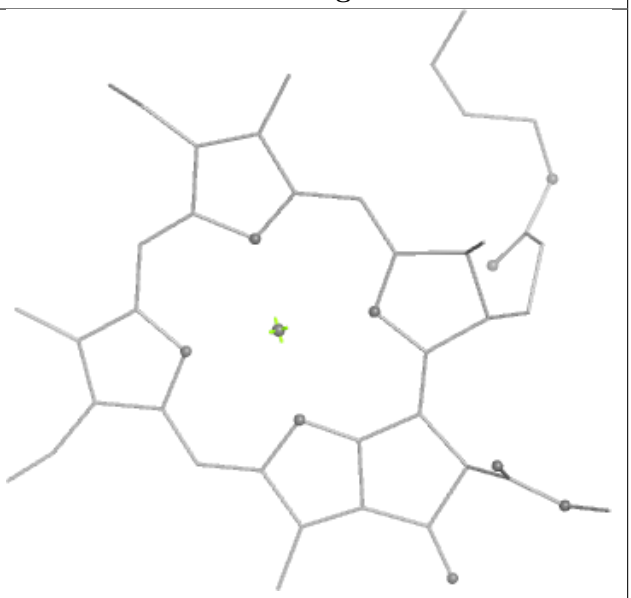
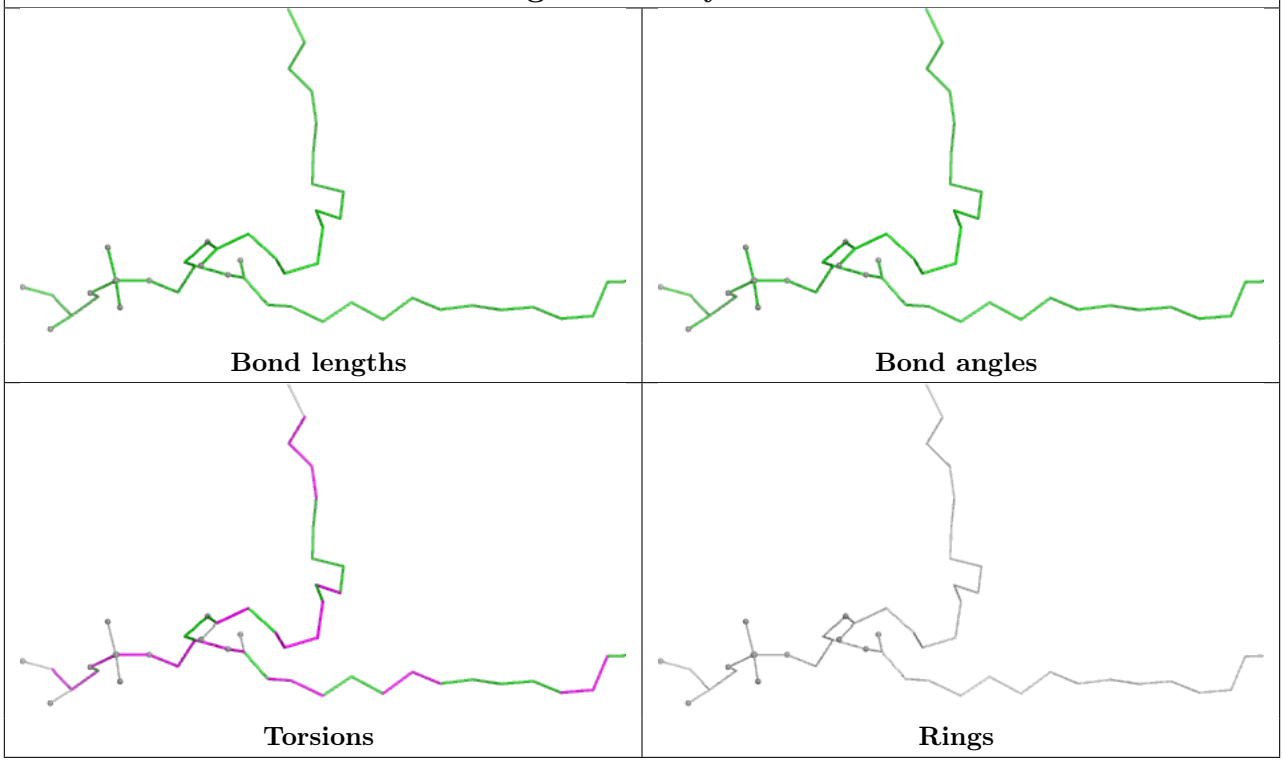
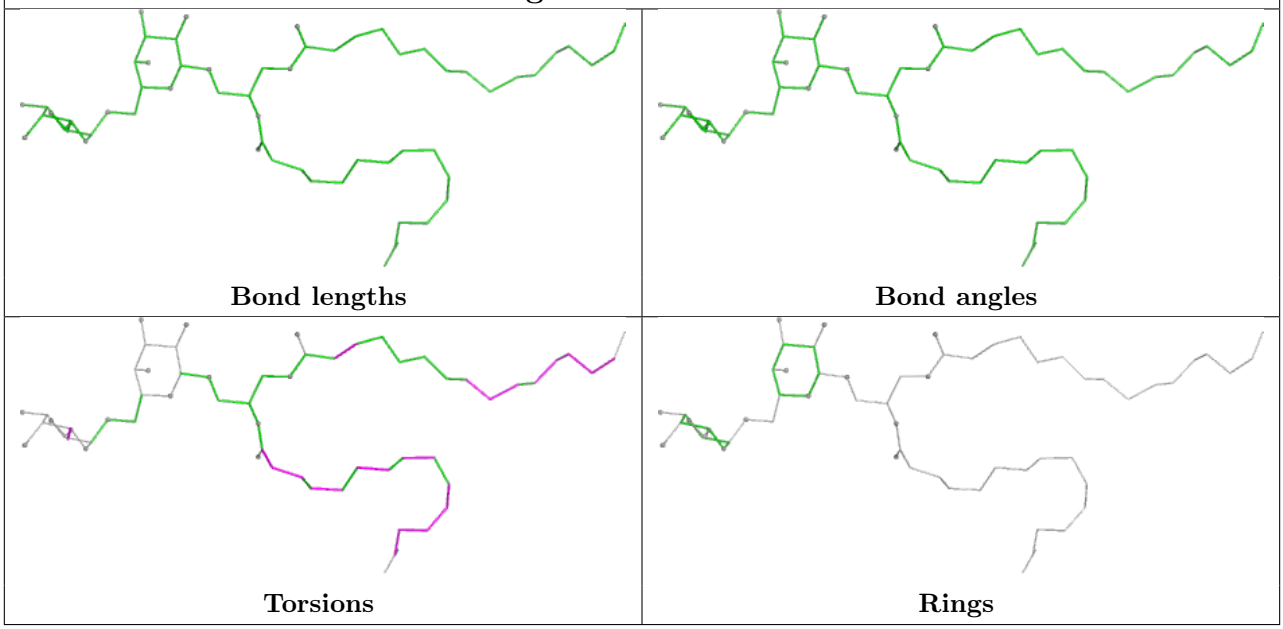


Rings

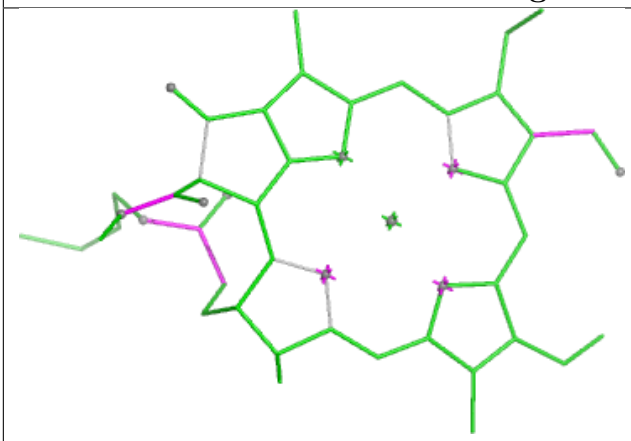
Ligand LHG y 301



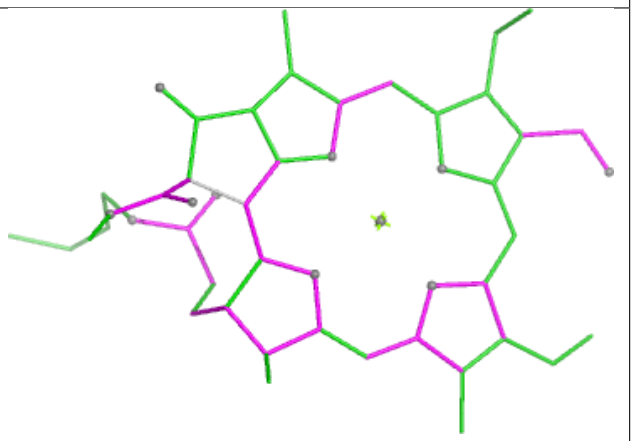
Ligand DGD c 501



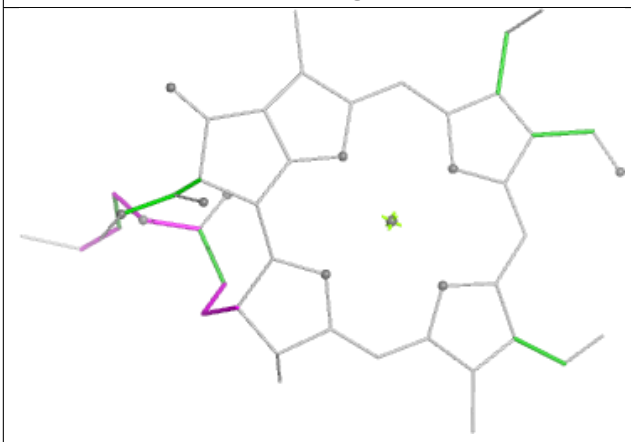
Ligand CHL r 318



Bond lengths



Bond angles



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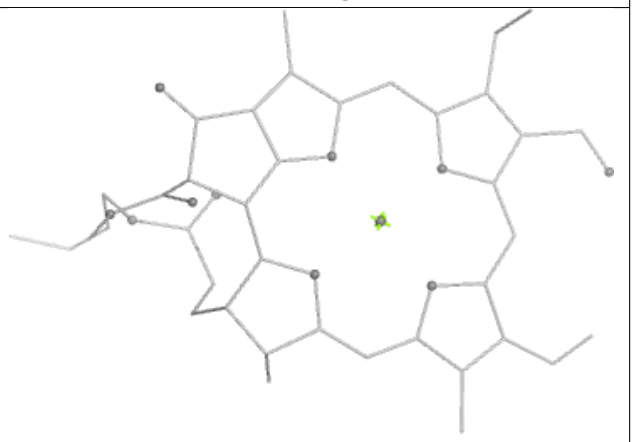
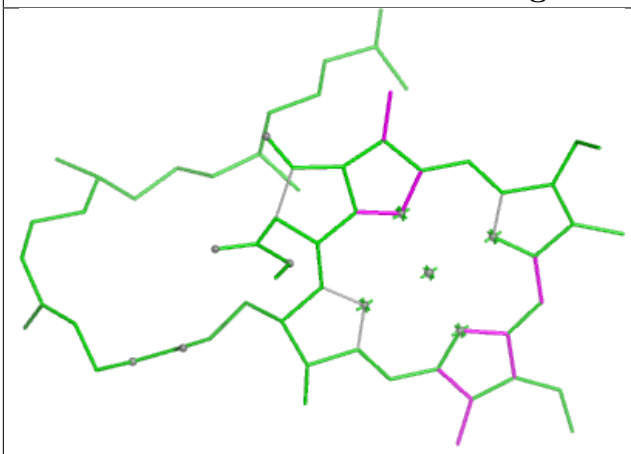


Rings

Ligand CLA c 504



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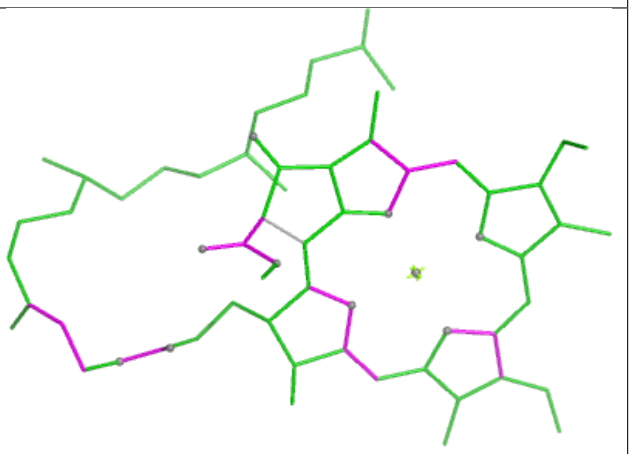
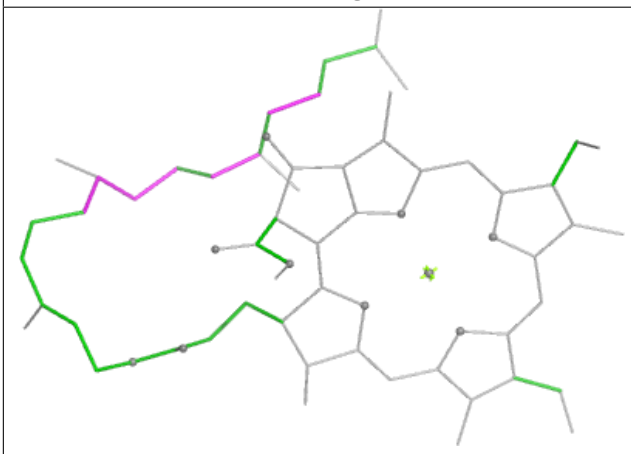


Bond angles



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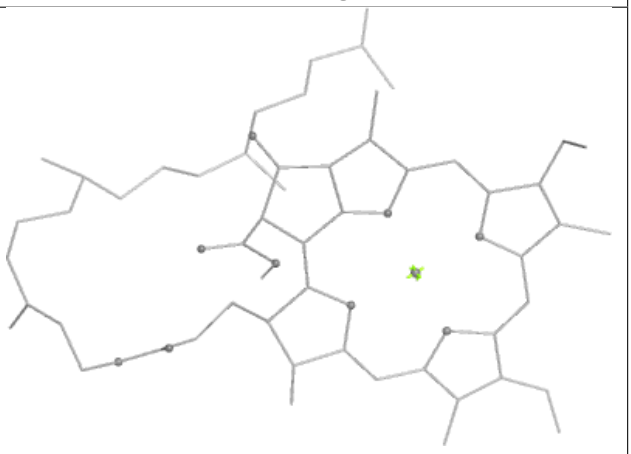
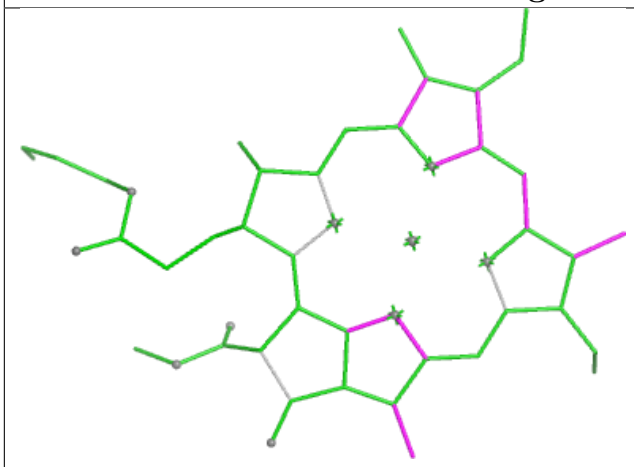


Rings

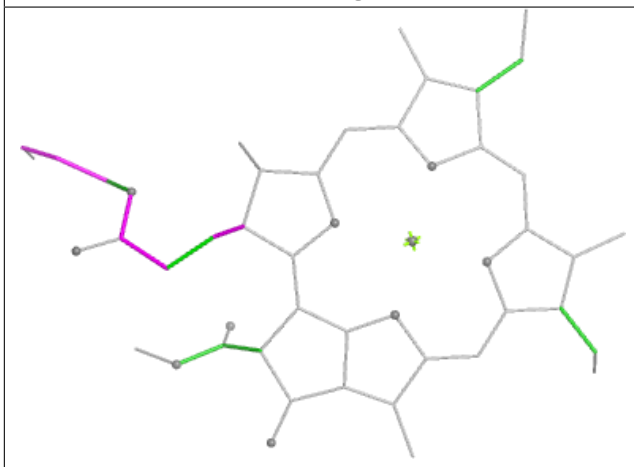
Ligand CLA S 309



Bond lengths



Bond angles

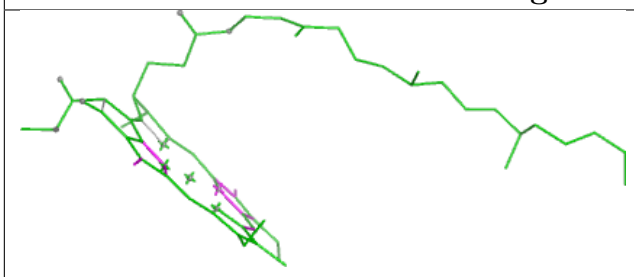


Torsions



Rings

Ligand CLA c 514



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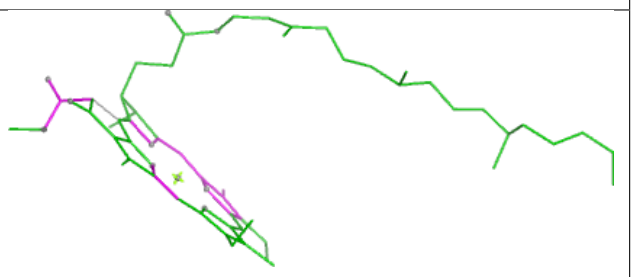
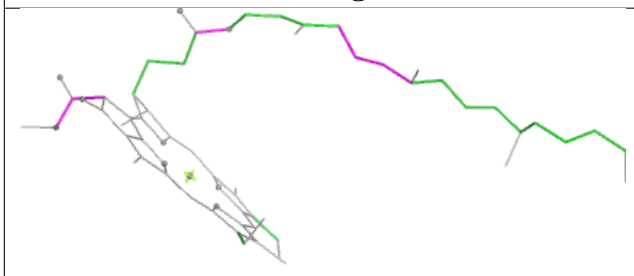


Bond angles

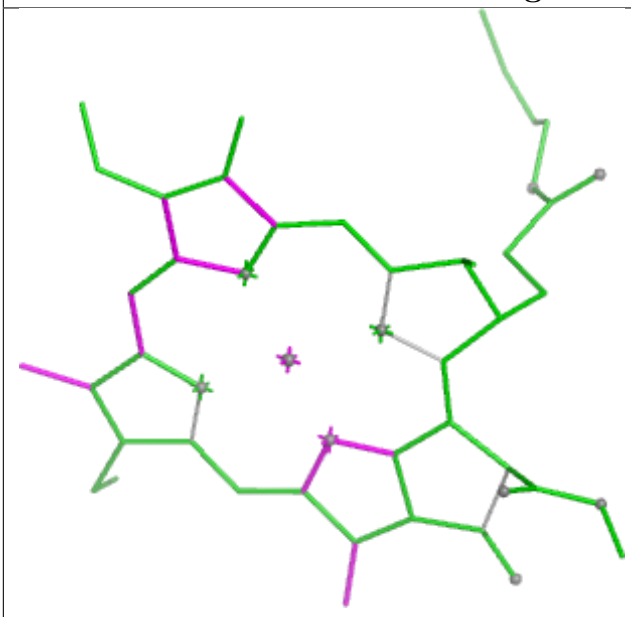


Torsions



Rings

Ligand CLA C 519



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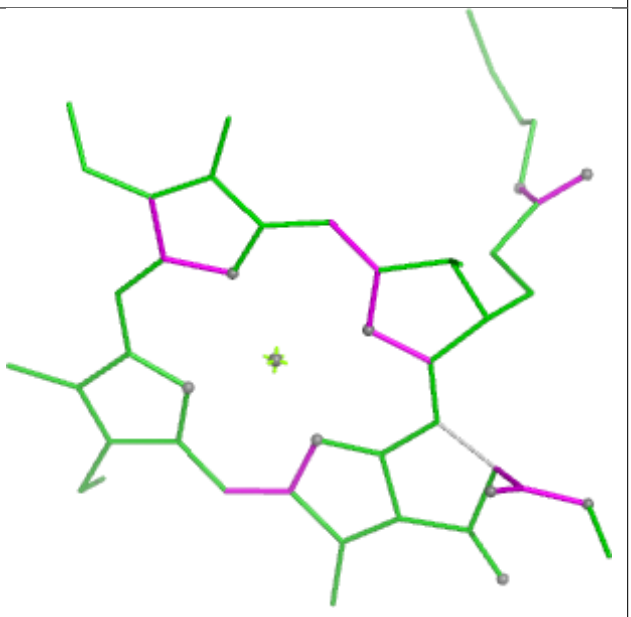
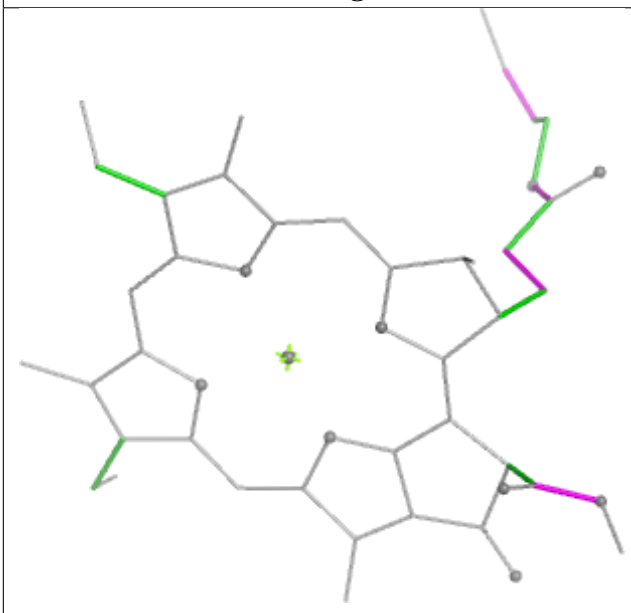


Bond angles



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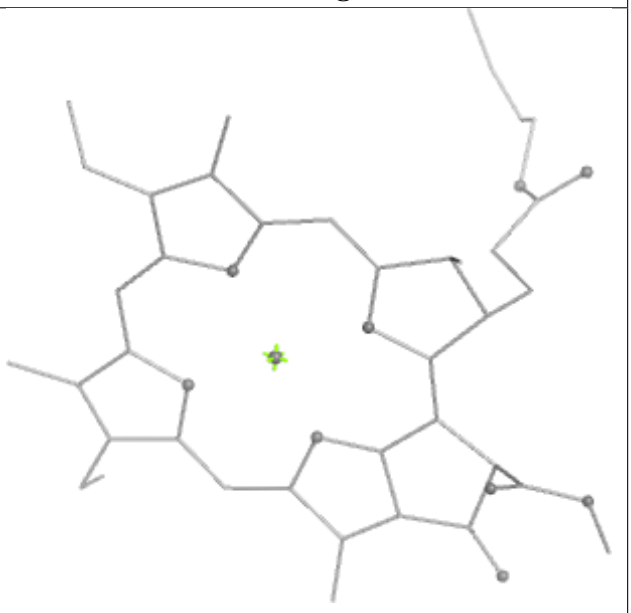
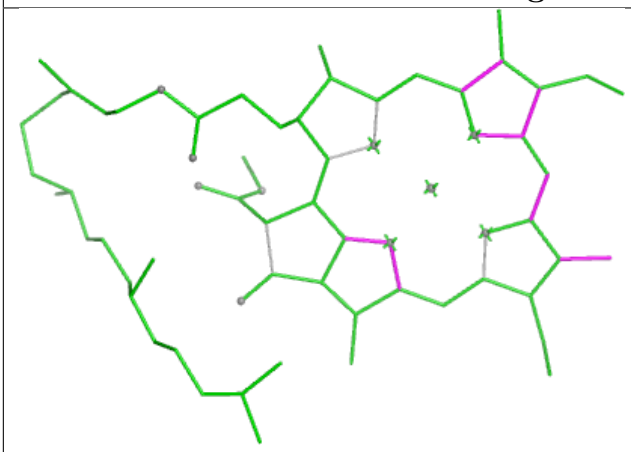


Rings

Ligand CLA b 614



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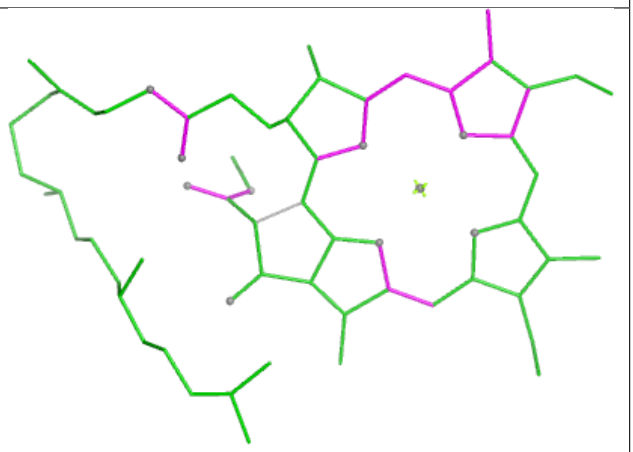
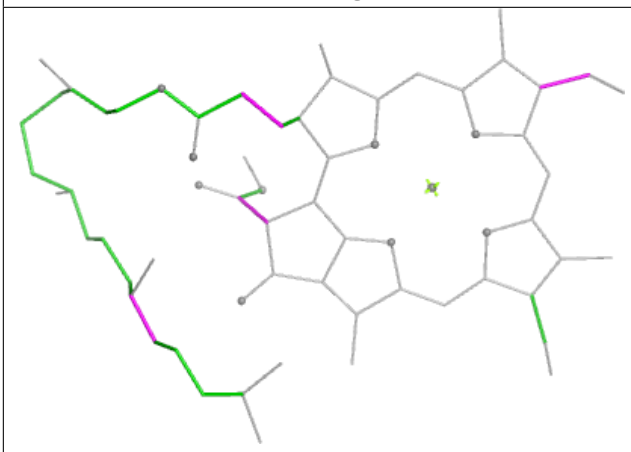


Bond angles



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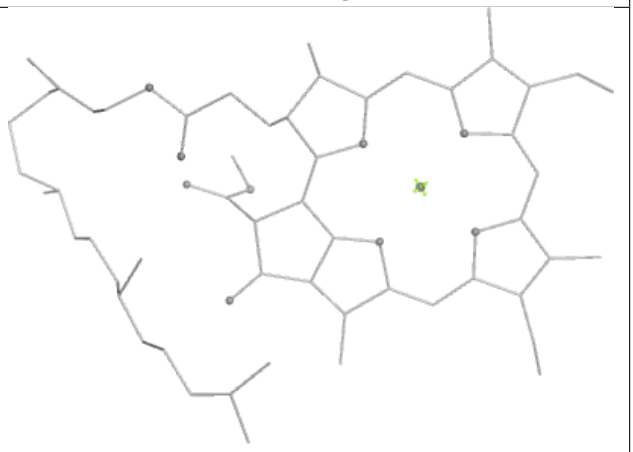
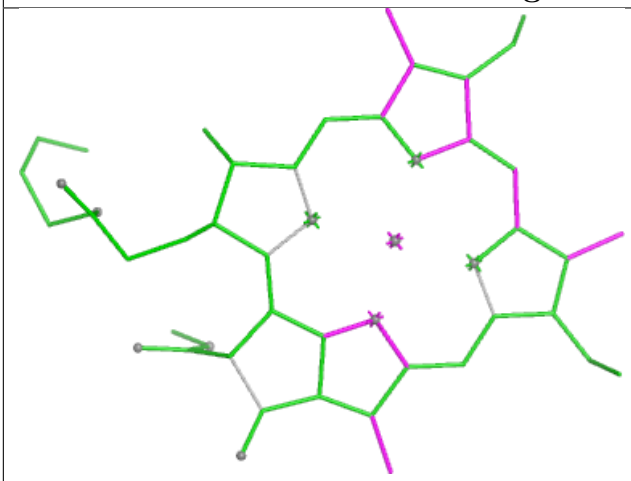


Rings

Ligand CLA N 306



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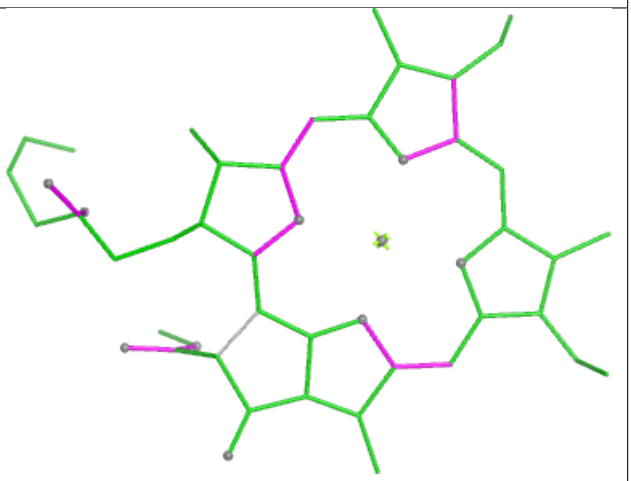
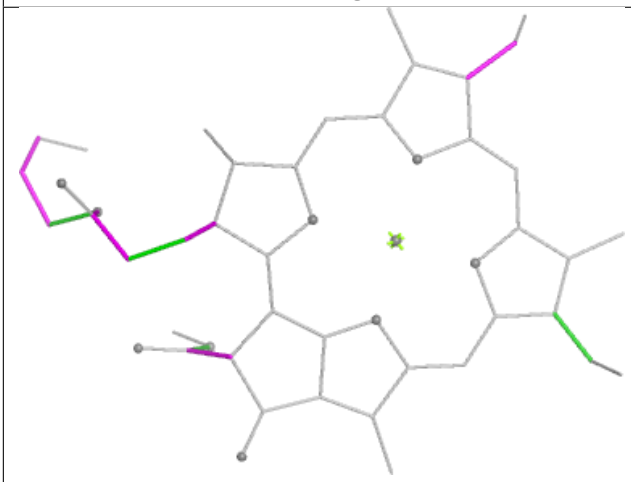


Bond angles

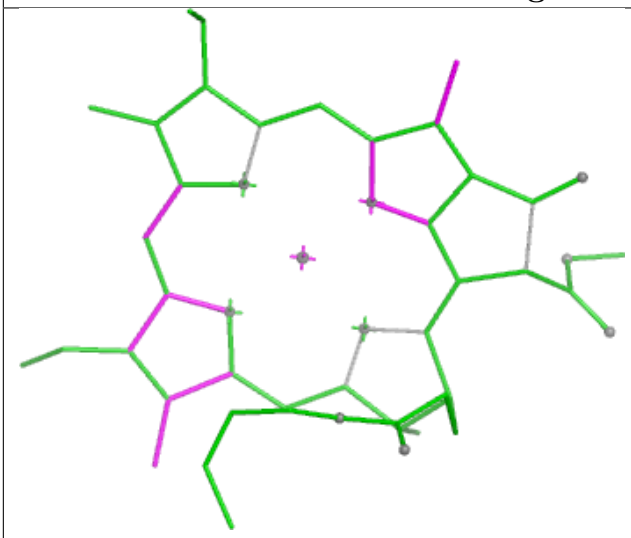


Torsions



Rings

Ligand CLA y 317



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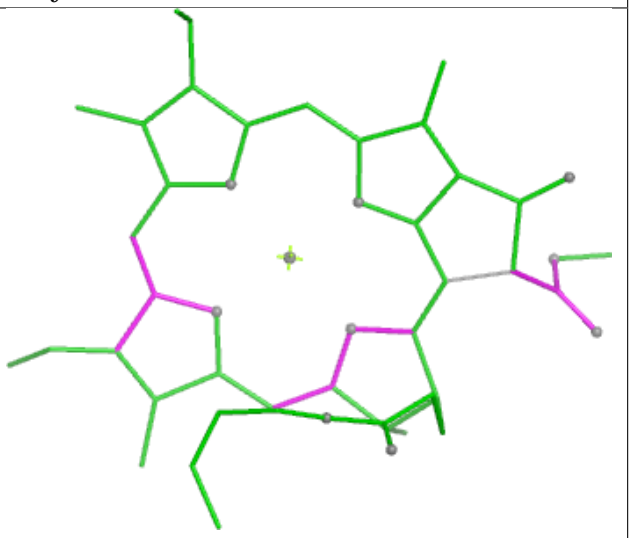
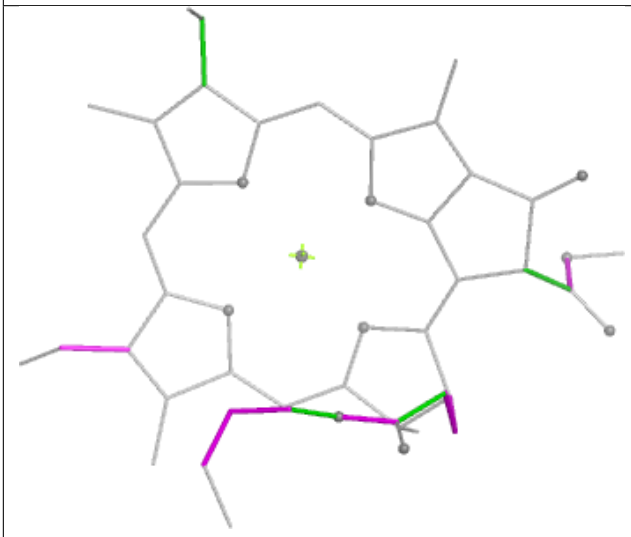


Bond angles



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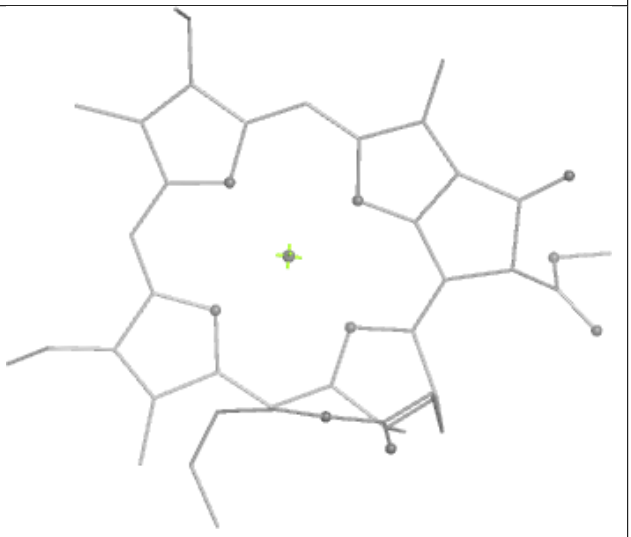
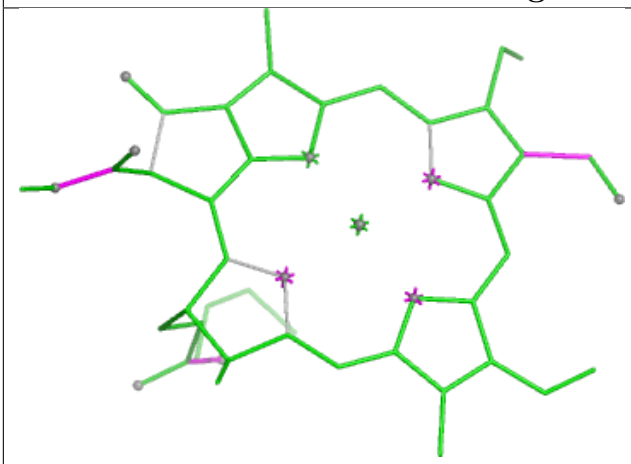
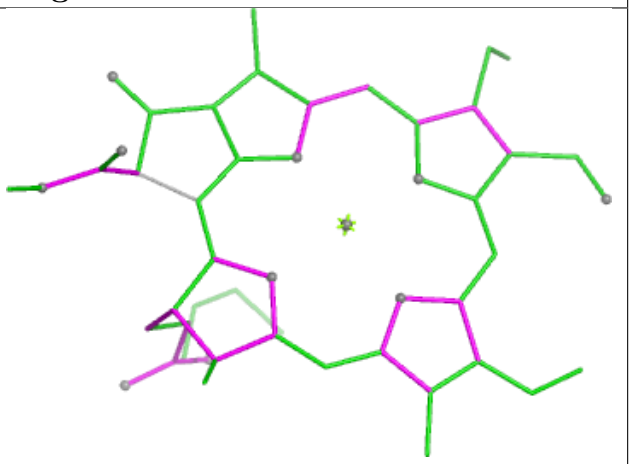


Rings

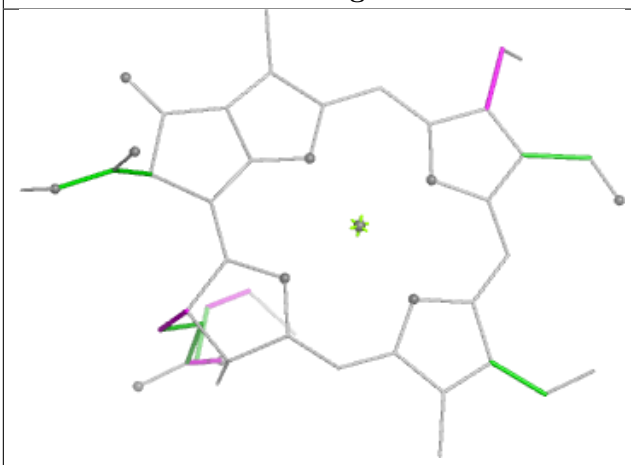
Ligand CHL g 312



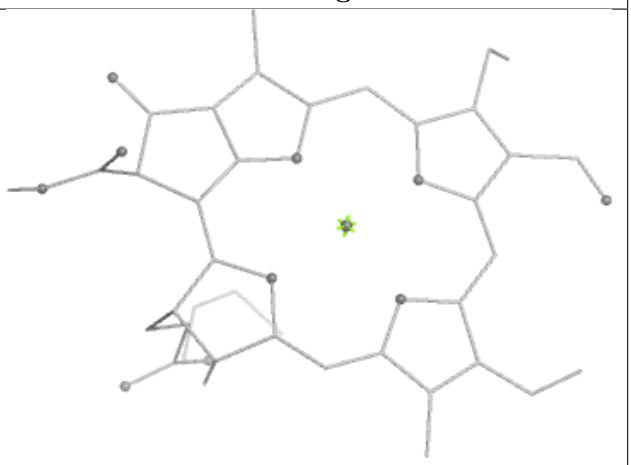
Bond lengths



Bond angles

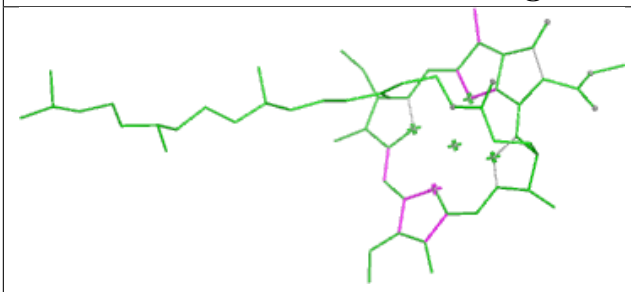


Torsions

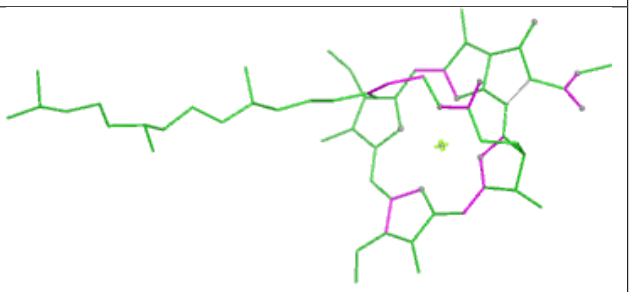


Rings

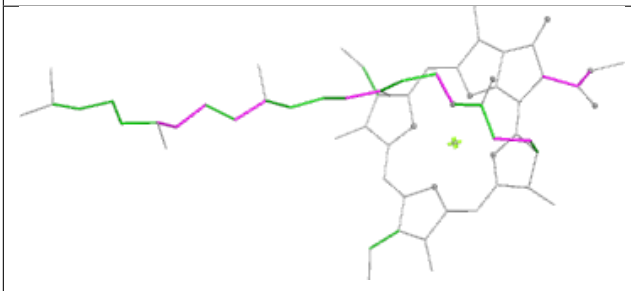
Ligand CLA B 601



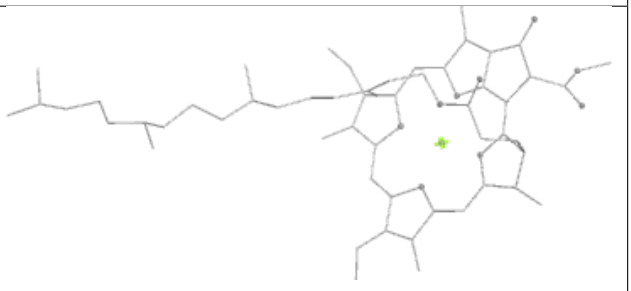
Bond lengths



Bond angles

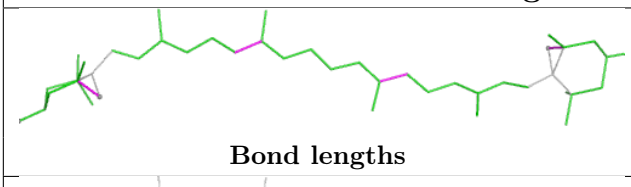


Torsions

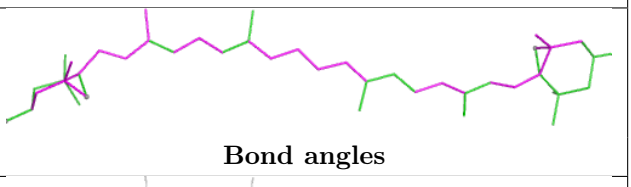


Rings

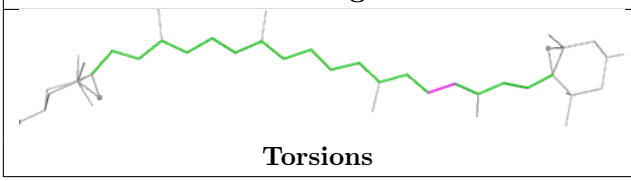
Ligand XAT R 304



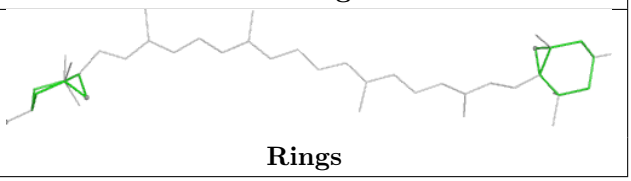
Bond lengths



Bond angles

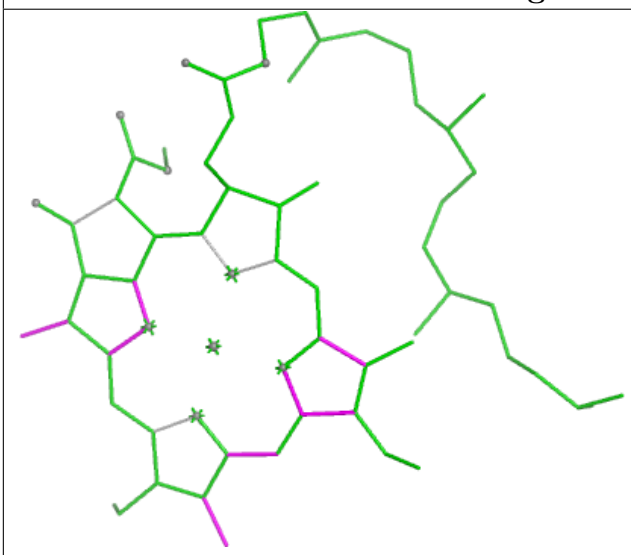


Torsions



Rings

Ligand CLA y 316



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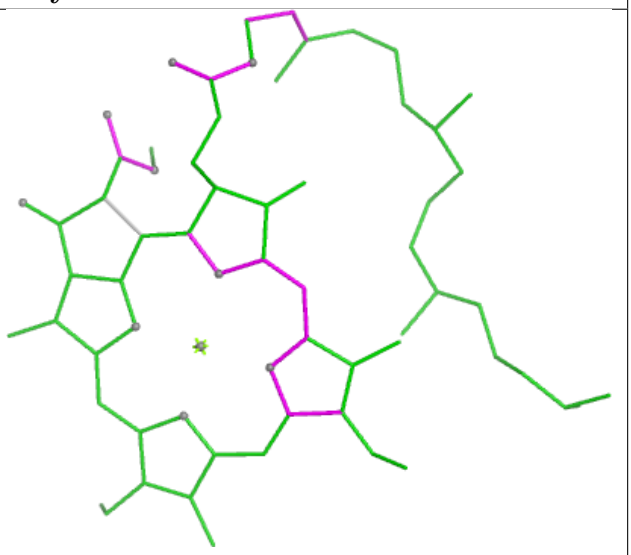
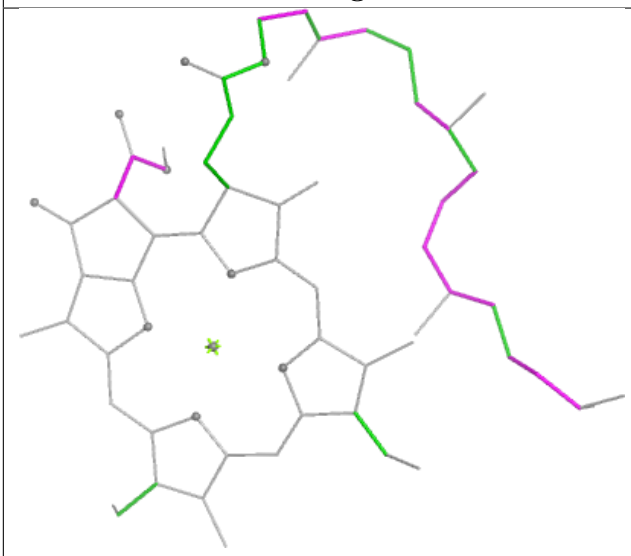


Bond angles

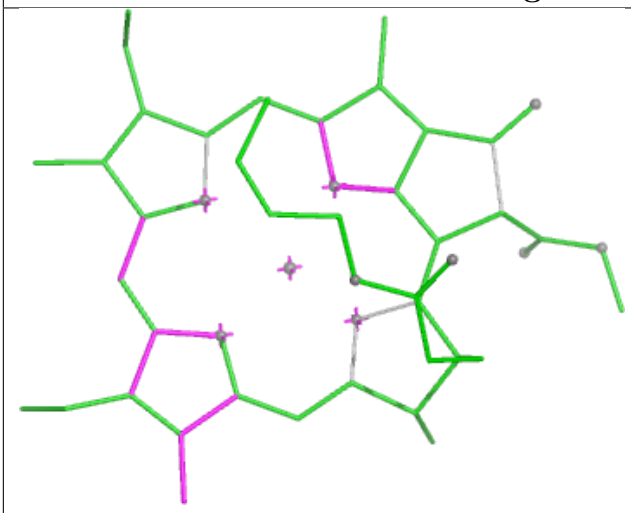


Torsions



Rings

Ligand CLA R 307



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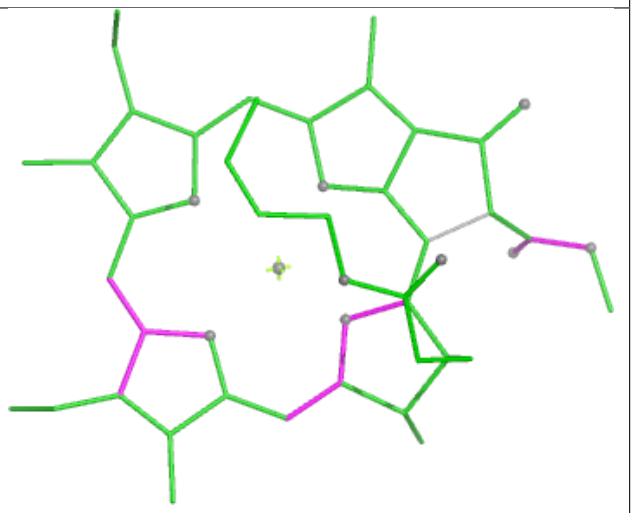
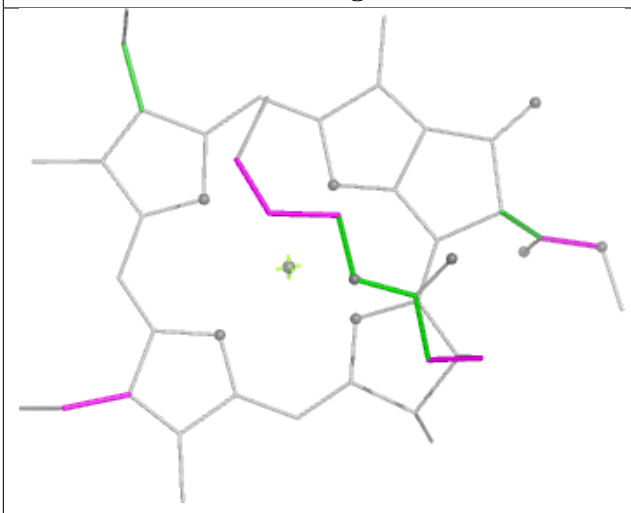


Bond angles



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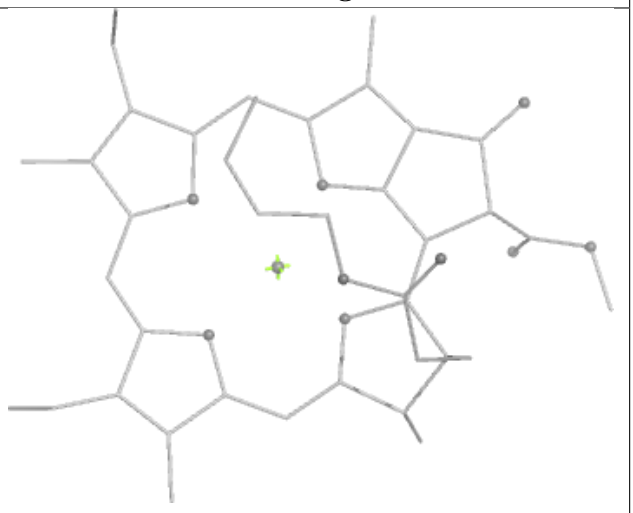
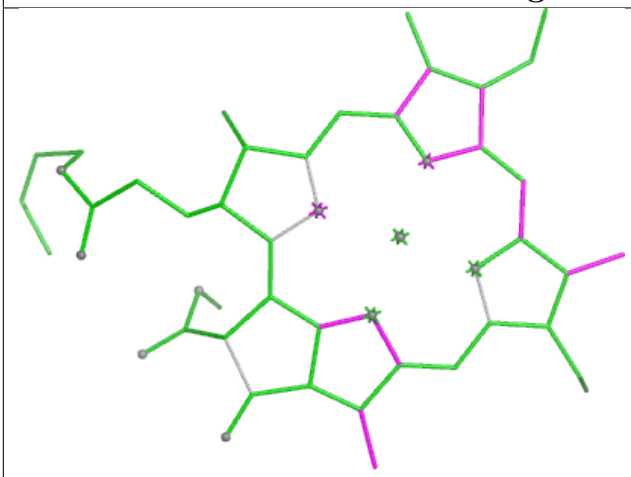


Rings

Ligand CLA n 304



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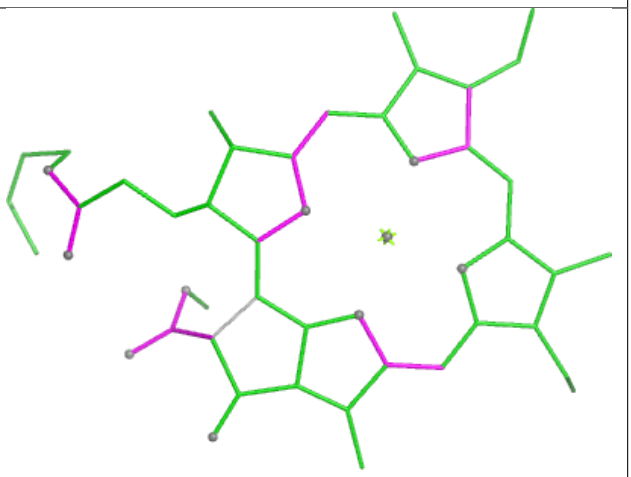
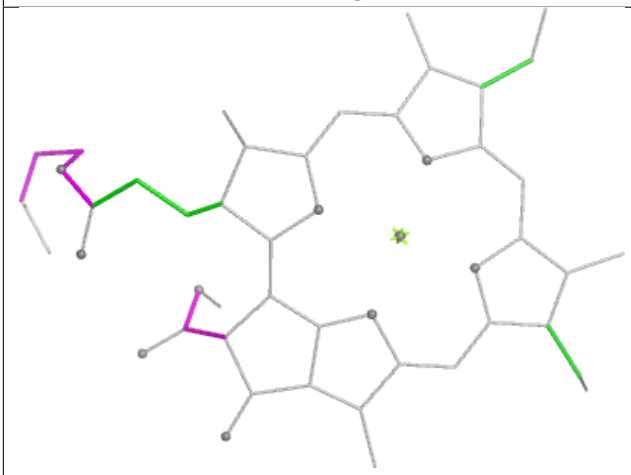


Bond angles

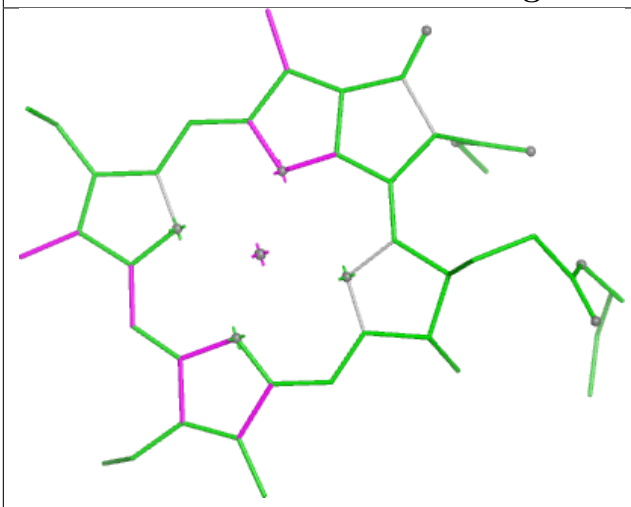


Torsions



Rings

Ligand CLA G 317



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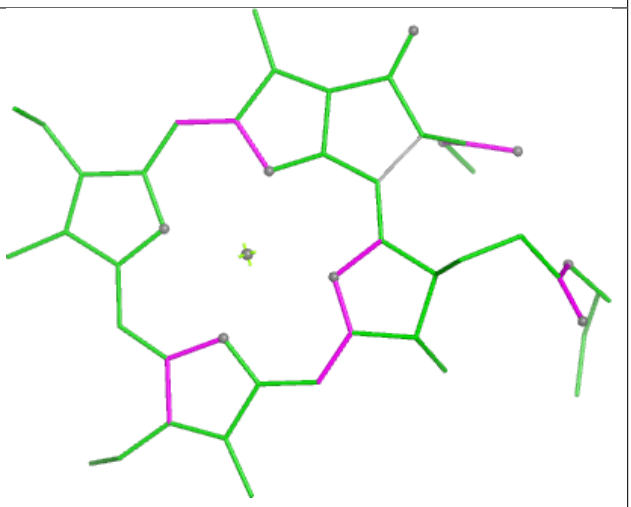
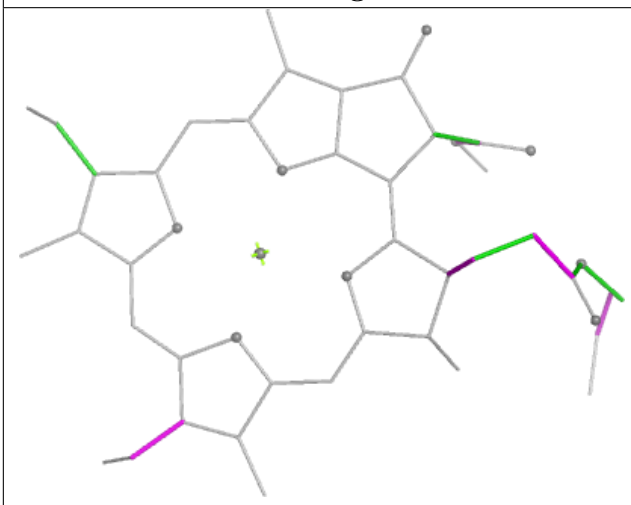
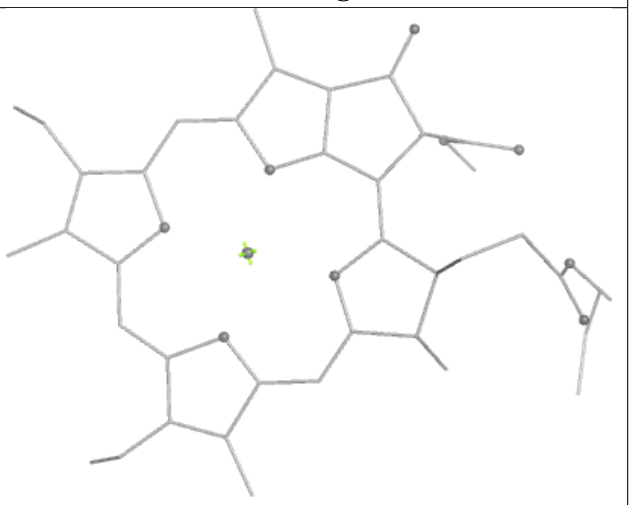


Bond angles

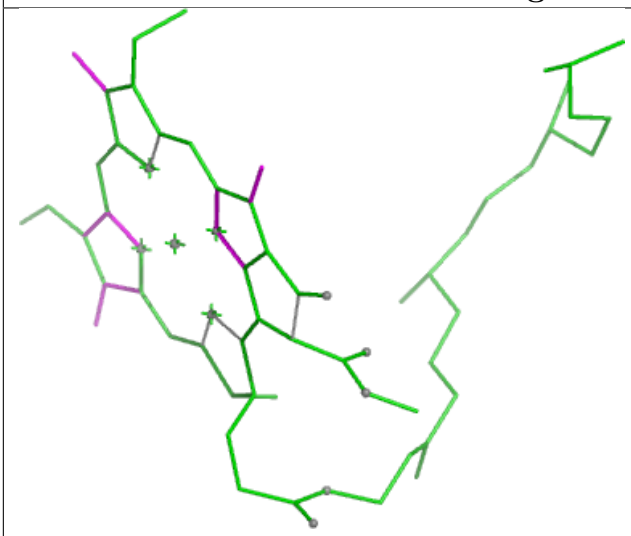


Torsions



Rings

Ligand CLA b 602



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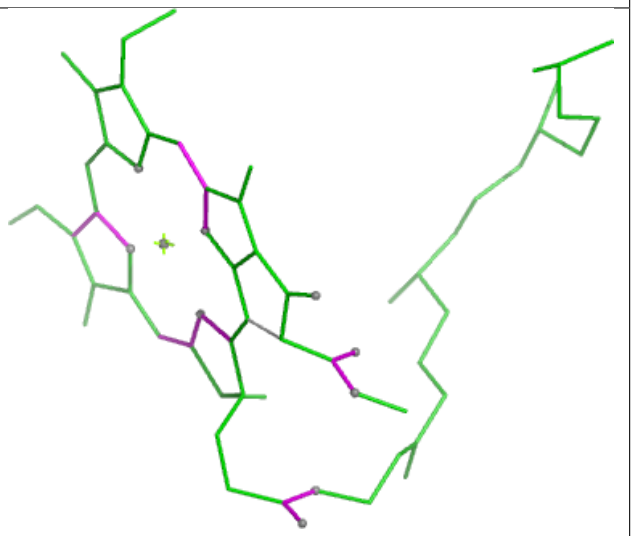
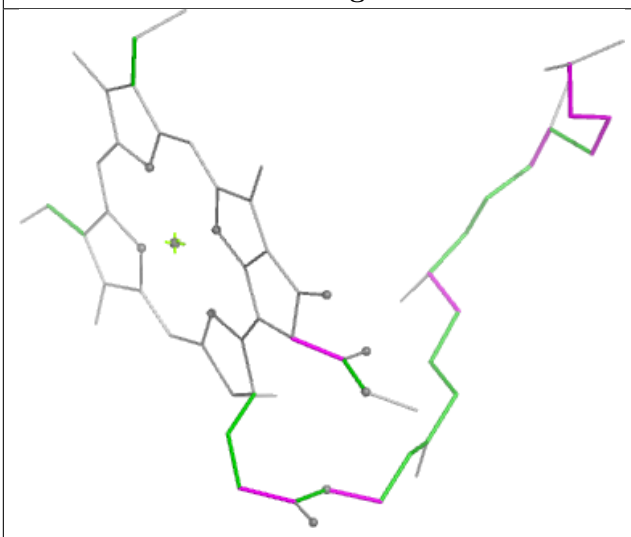


Bond angles



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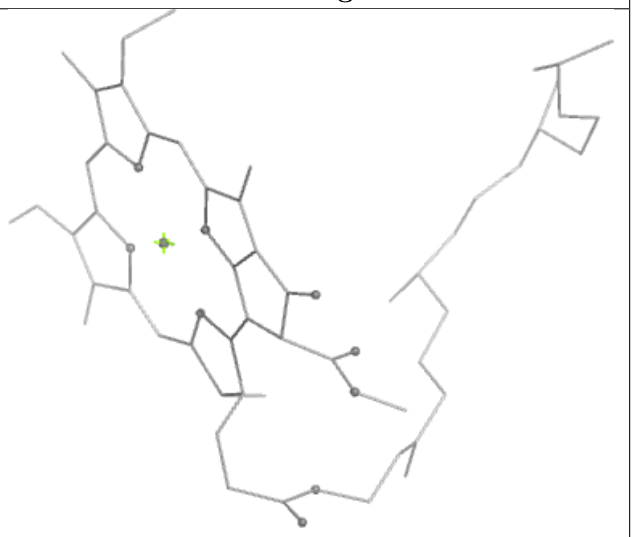
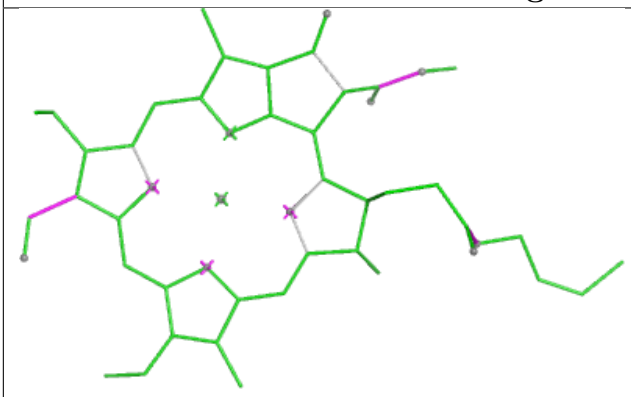
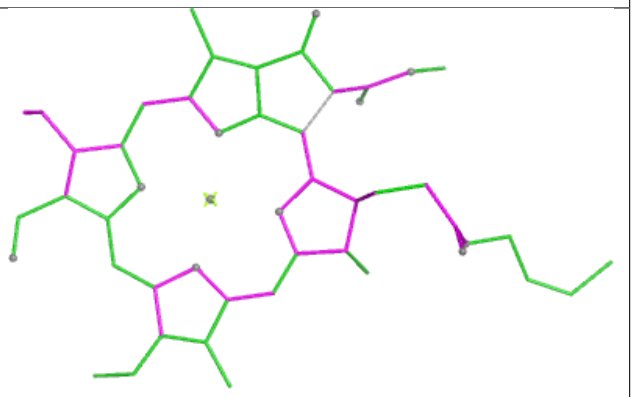


Rings

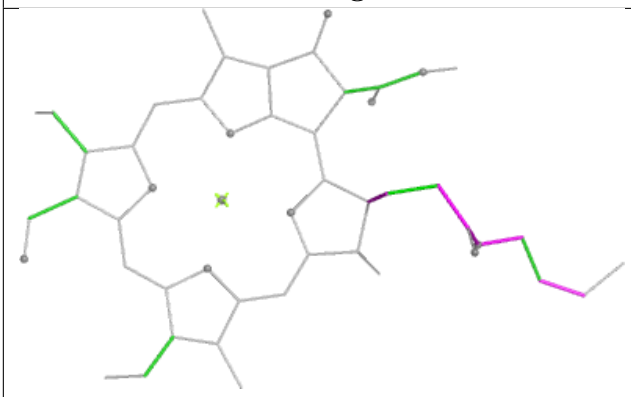
Ligand CHL S 313



Bond lengths



Bond angles

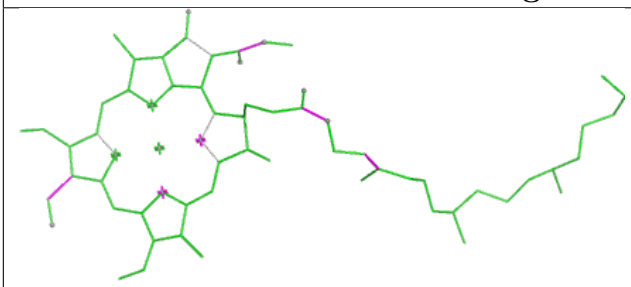


Torsions



Rings

Ligand CHL G 318



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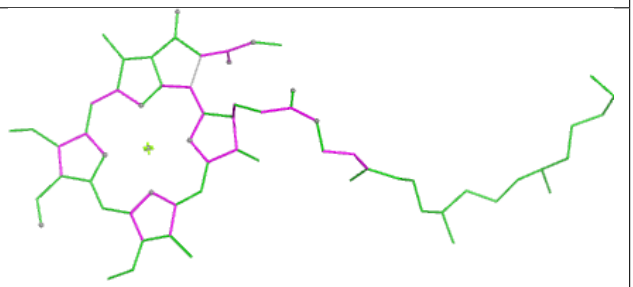
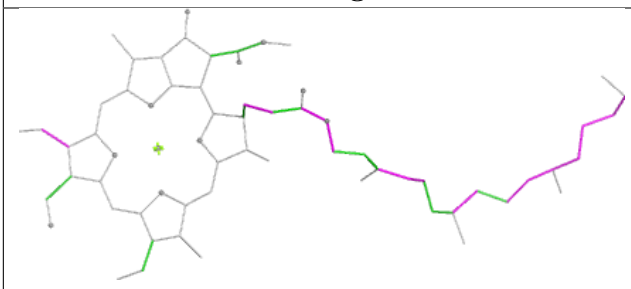


Bond angles



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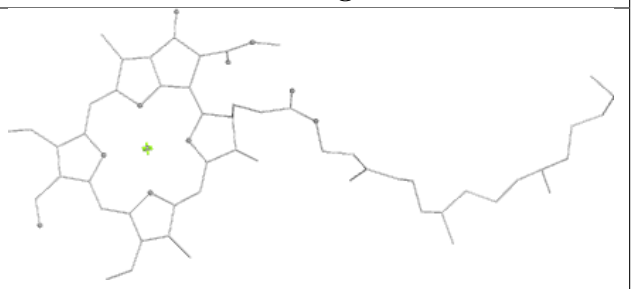
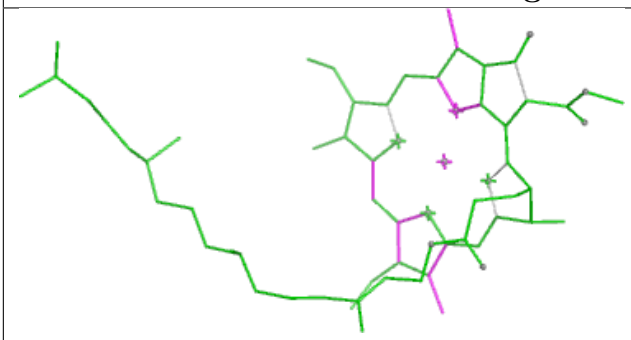


Rings

Ligand CLA R 306



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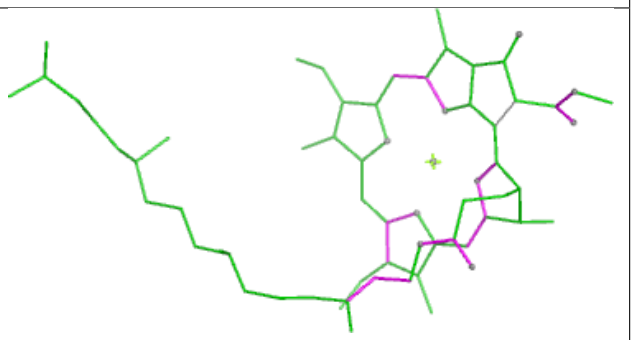
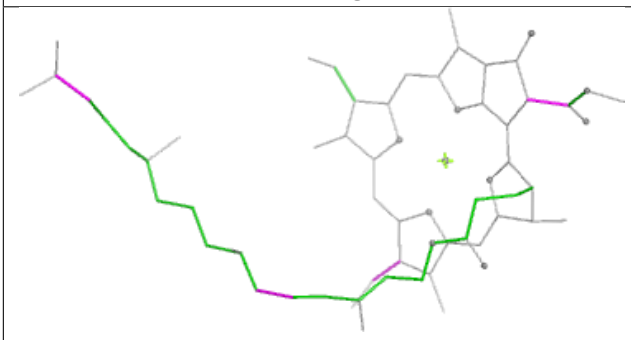


Bond angles

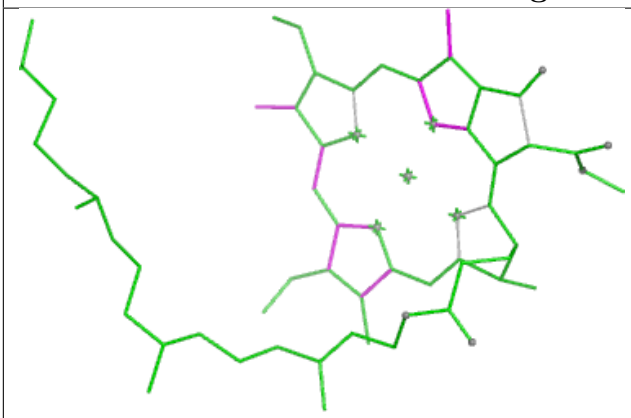


Torsions



Rings

Ligand CLA r 314



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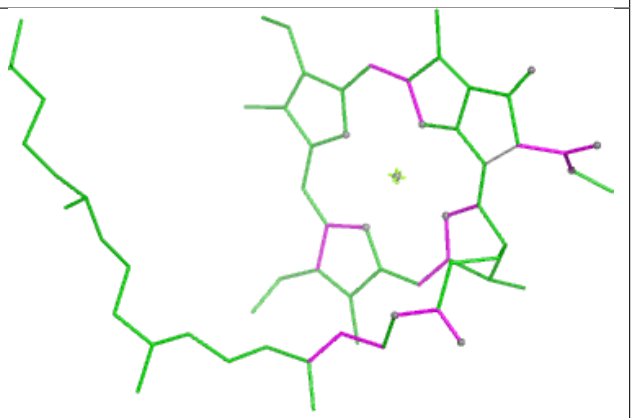
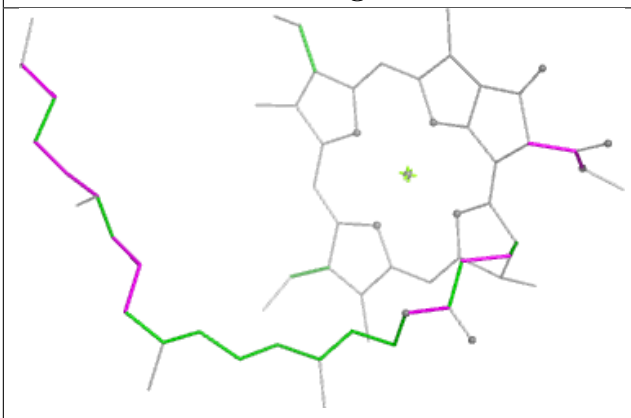


Bond angles



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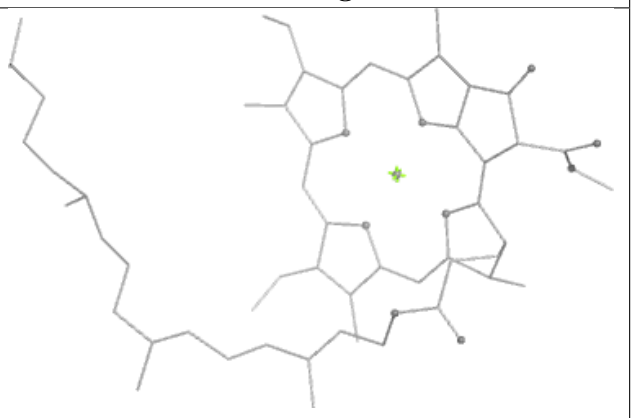
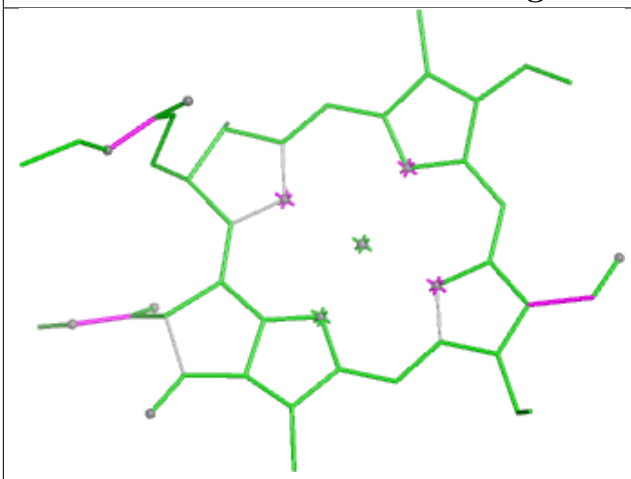


Rings

Ligand CHL n 308



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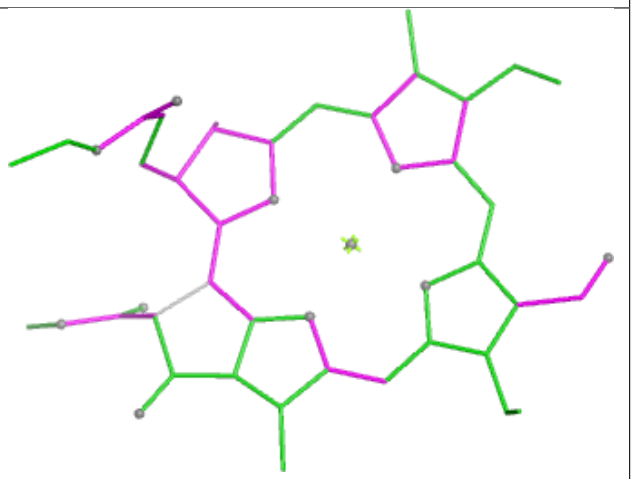
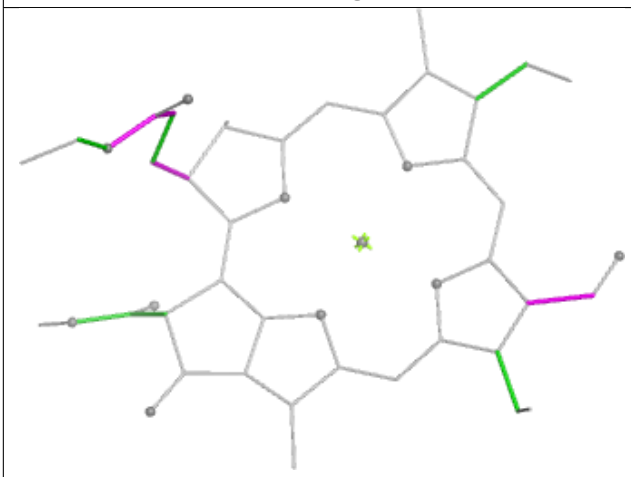


Bond angles



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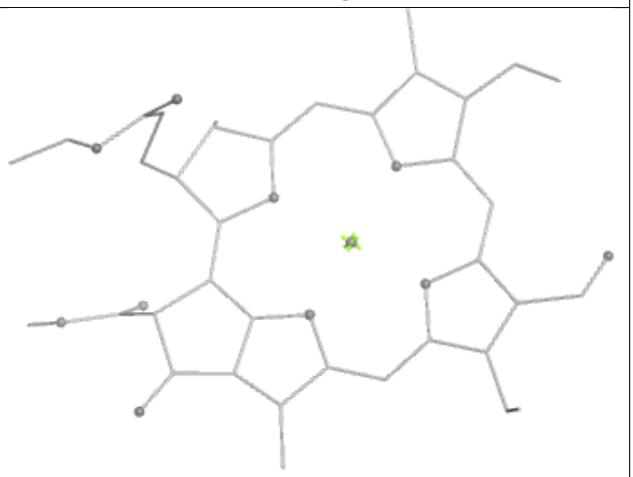
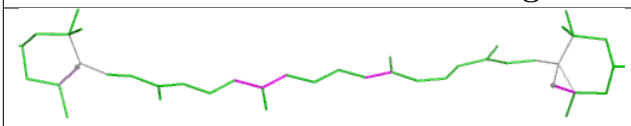
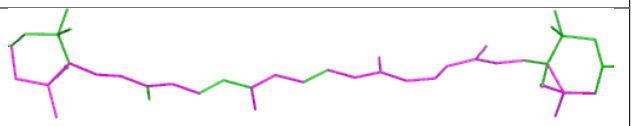


Rings

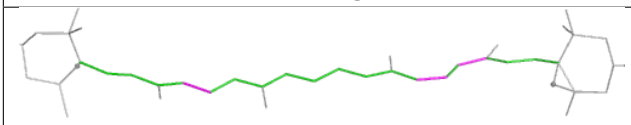
Ligand XAT G 320



Bond lengths



Bond angles



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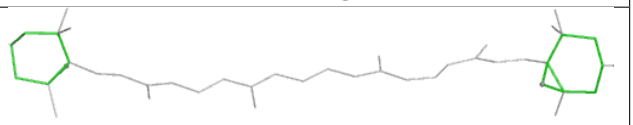
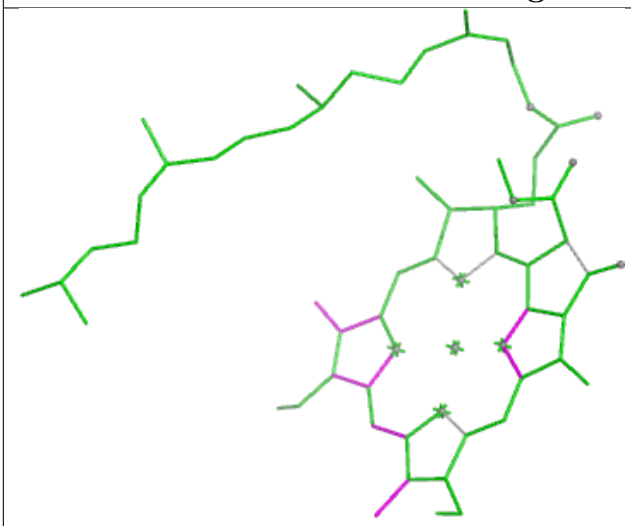


Rings

Ligand CLA b 605



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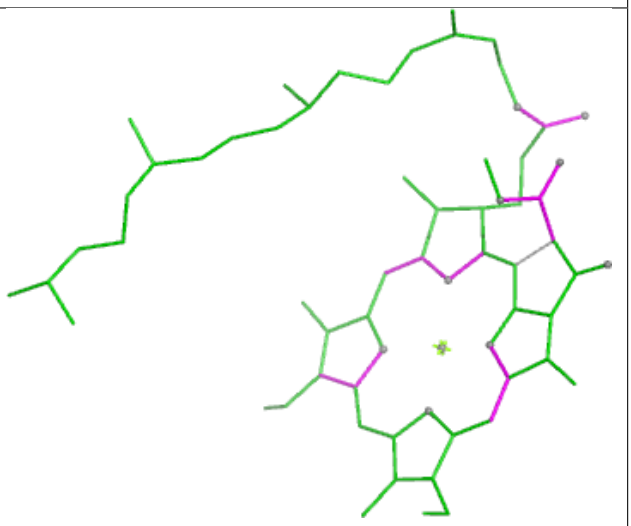
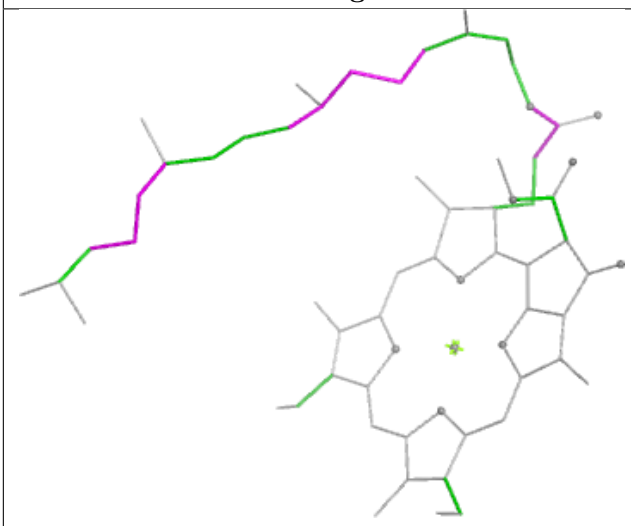


Bond angles



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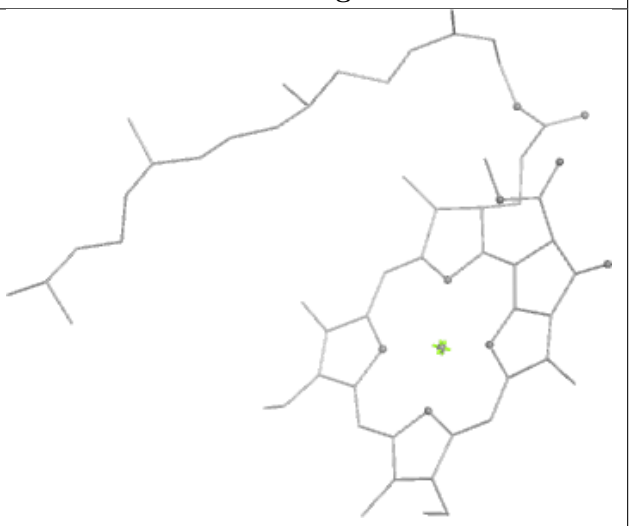
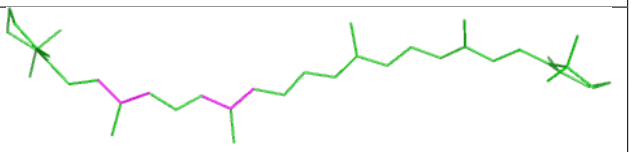


Rings

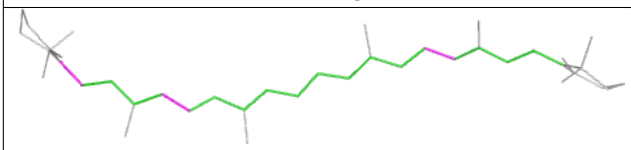
Ligand BCR c 511



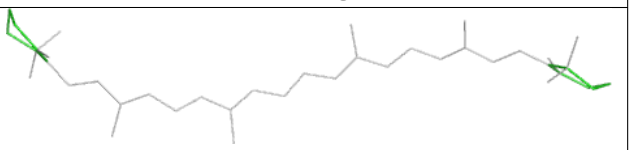
Bond lengths



Bond angles

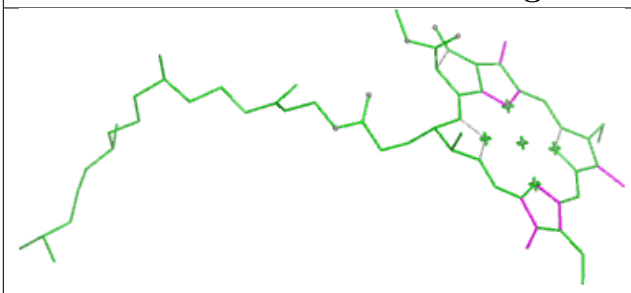


Torsions

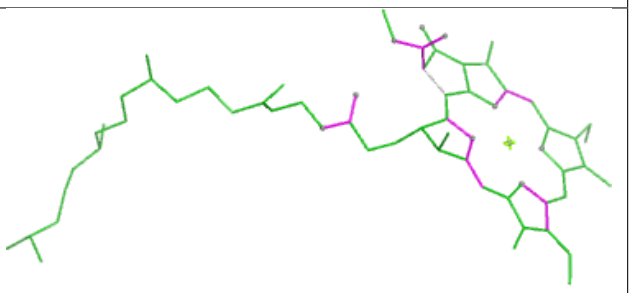


Rings

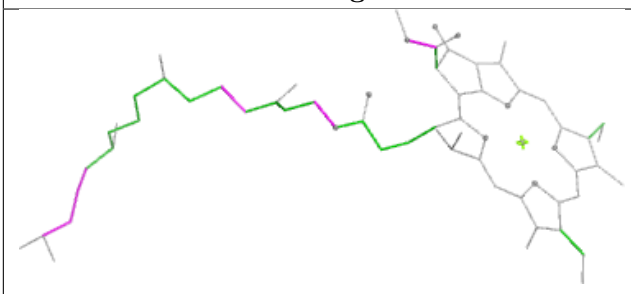
Ligand CLA A 403



Bond lengths



Bond angles



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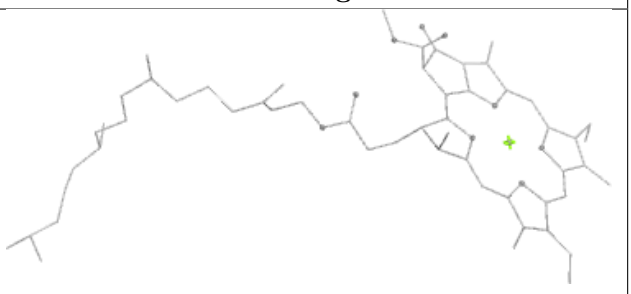
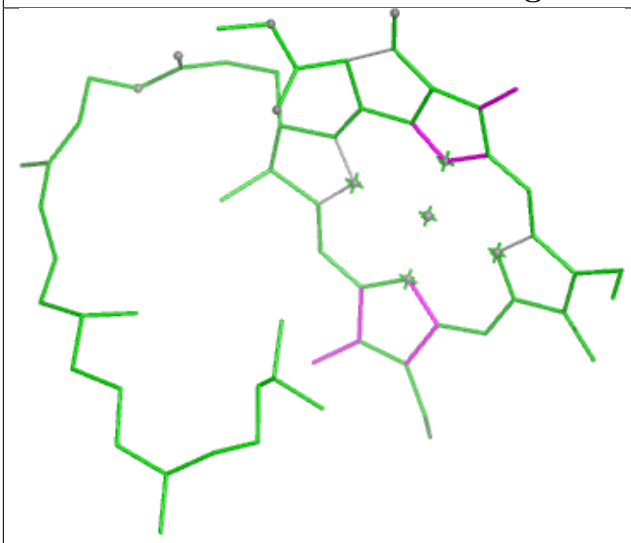
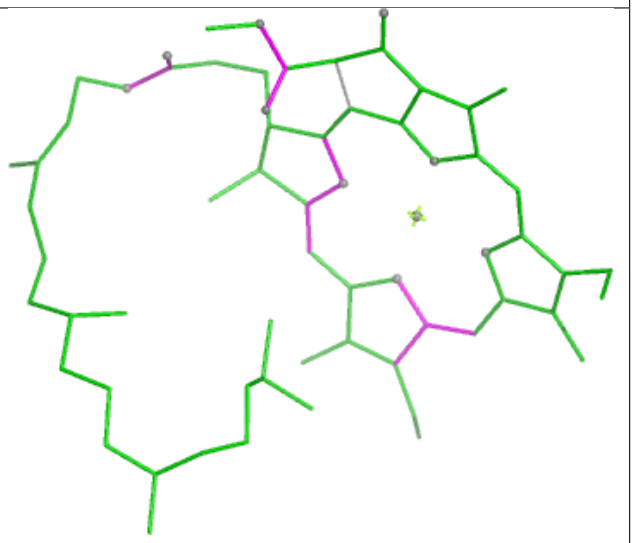


Rings

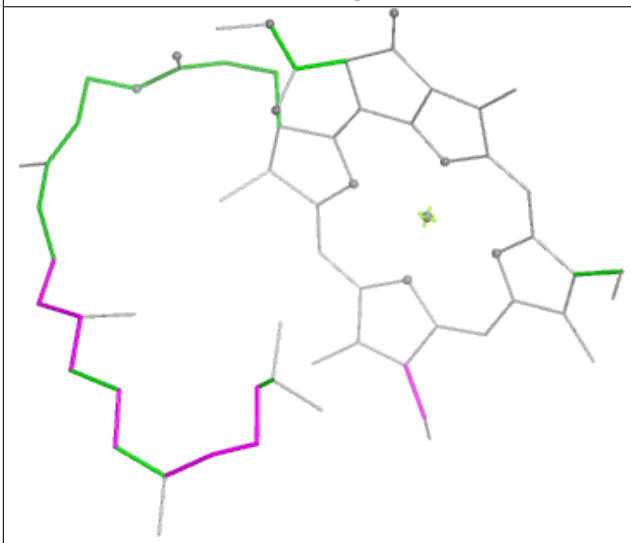
Ligand CLA B 616



Bond lengths



Bond angles



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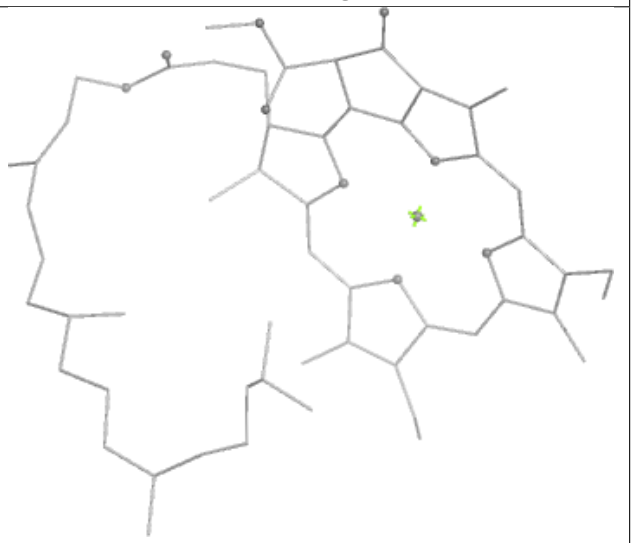
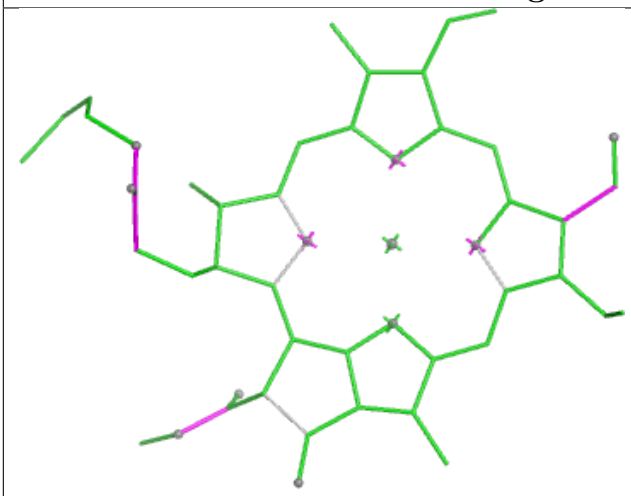
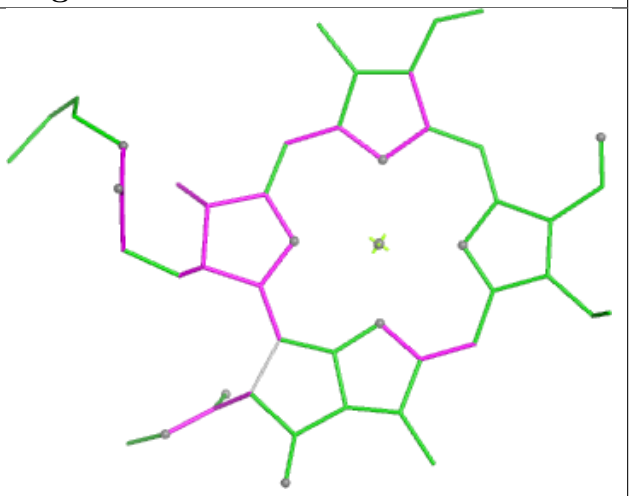


Rings

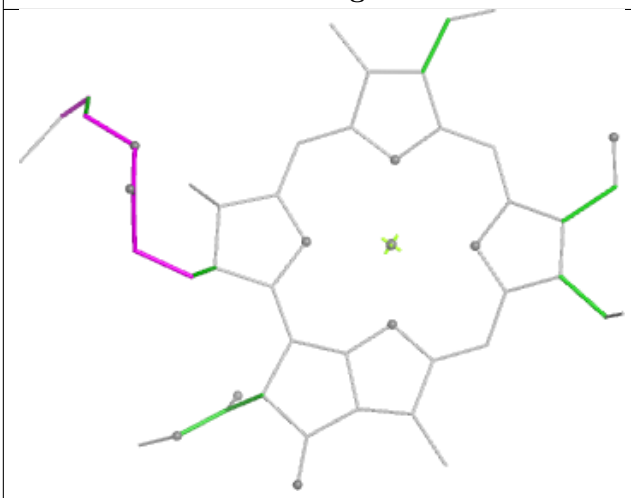
Ligand CHL g 319



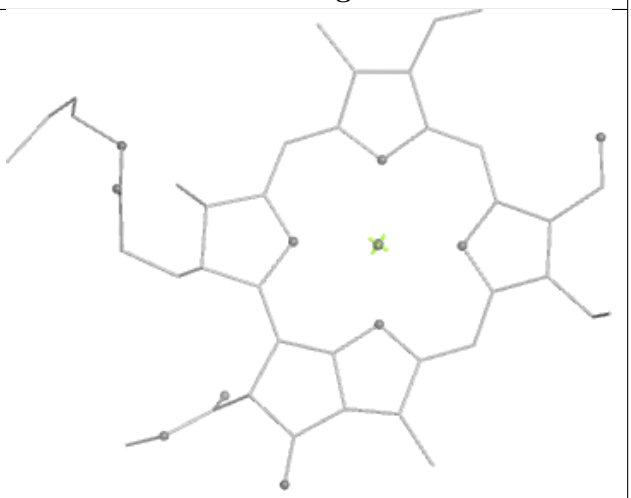
Bond lengths



Bond angles

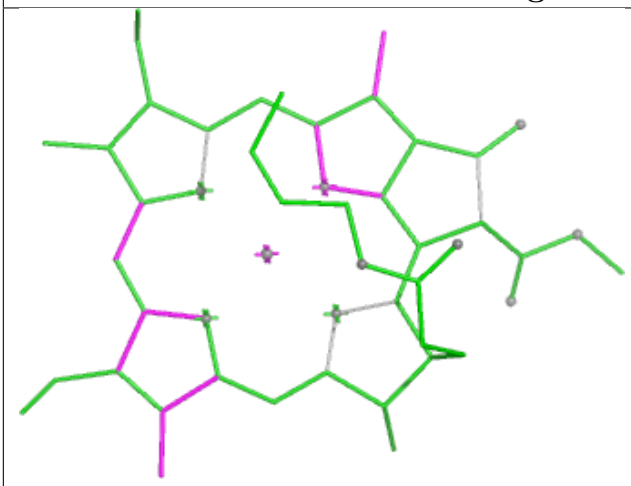


Torsions



Rings

Ligand CLA n 302



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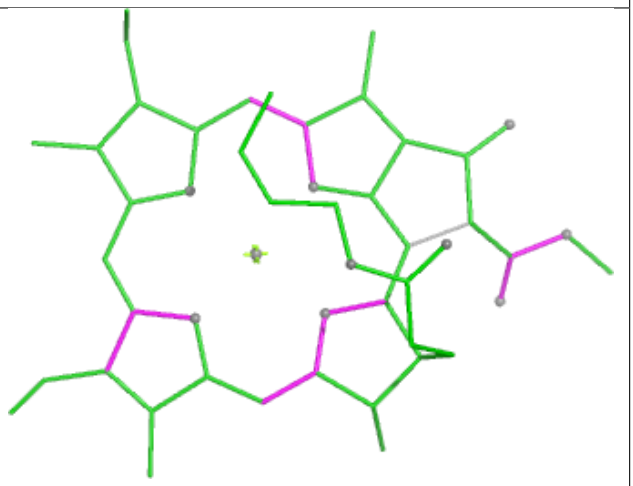
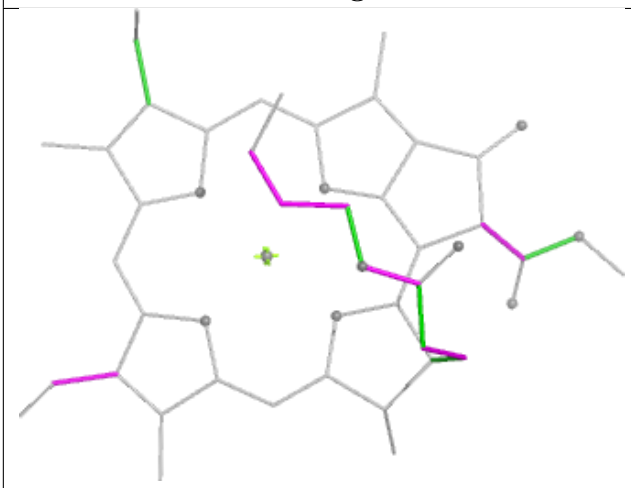


Bond angles



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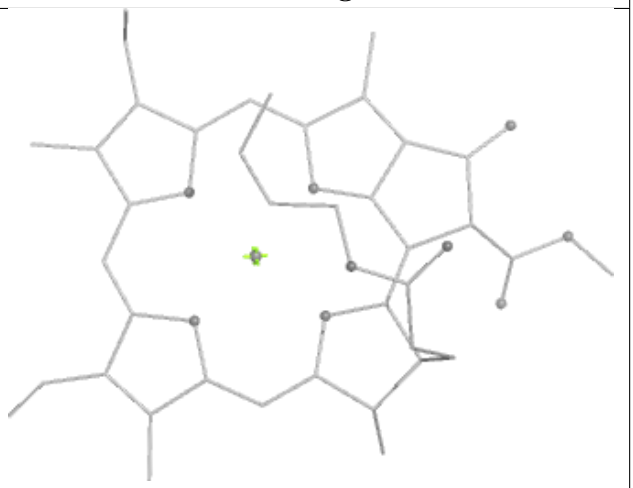
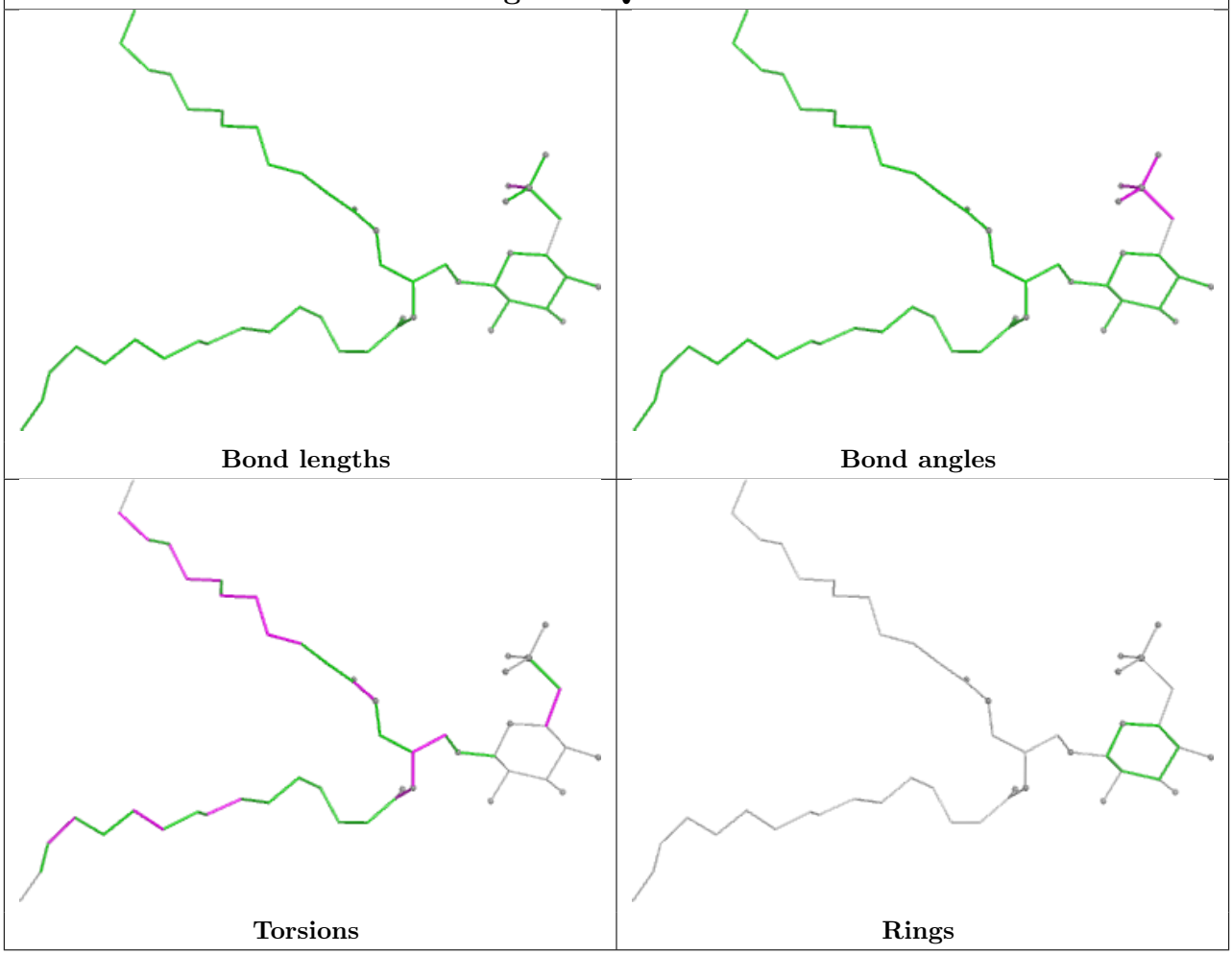
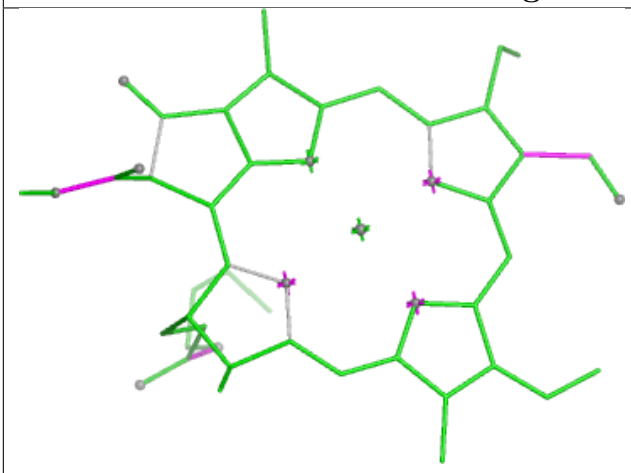


Rings

Ligand SQD A 410



Ligand CHL N 317



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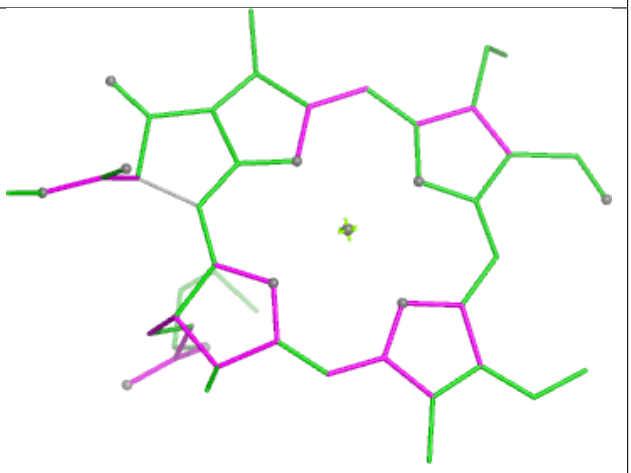
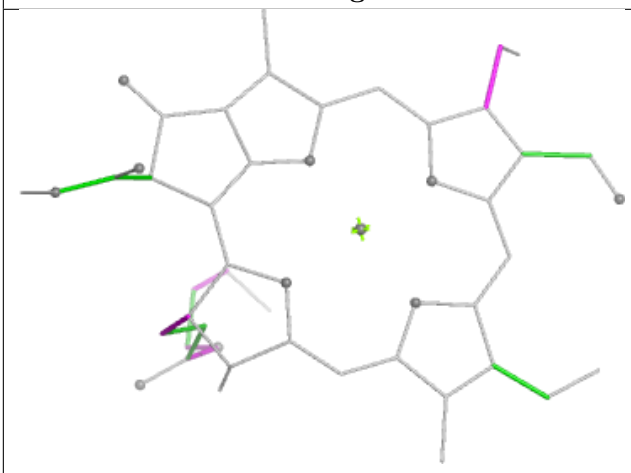


Bond angles



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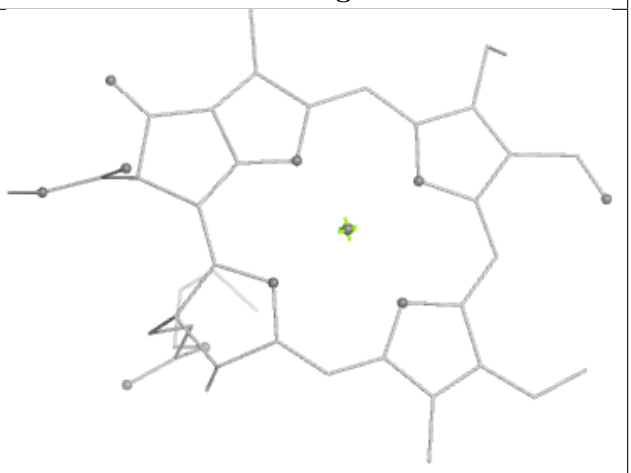
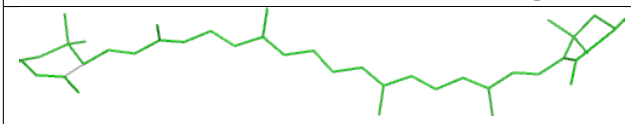


Rings

Ligand LUT g 310



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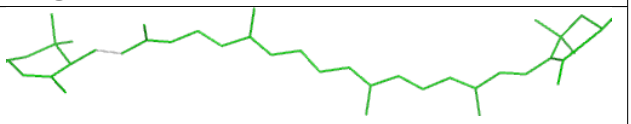

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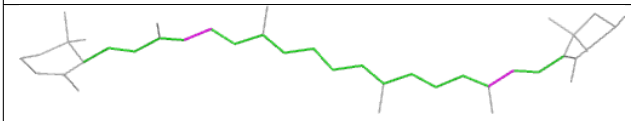

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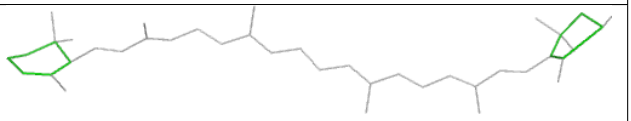
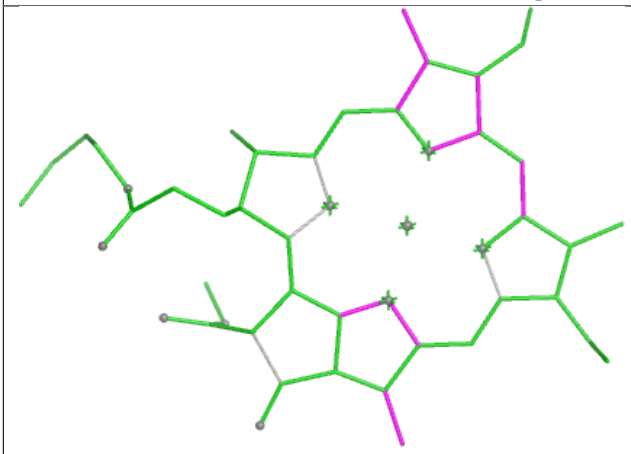


Rings

Ligand CLA s 306



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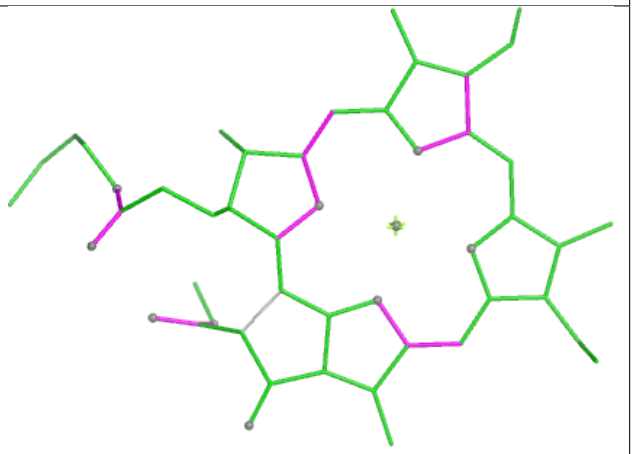
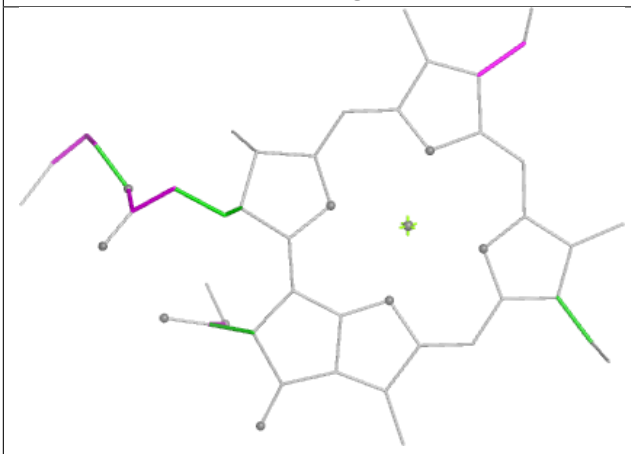


Bond angles



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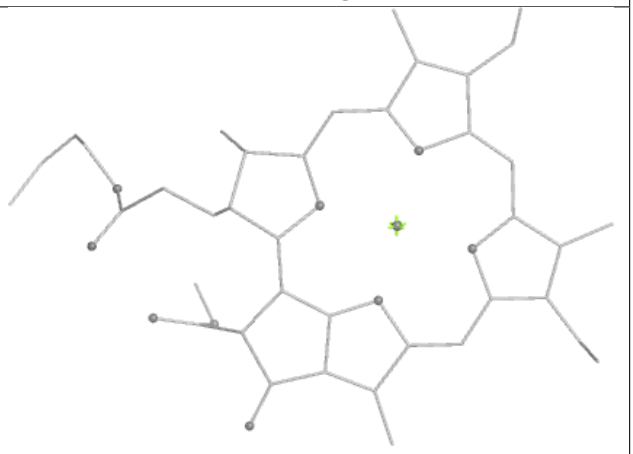
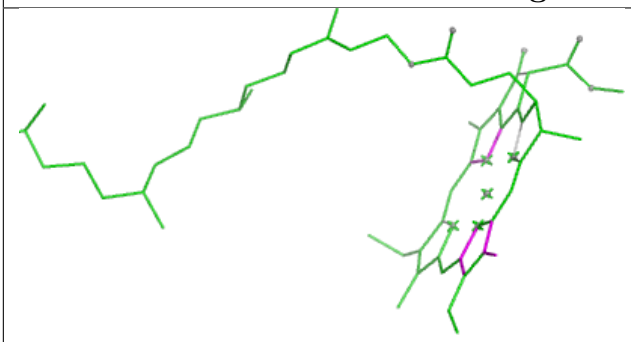


Rings

Ligand CLA c 513



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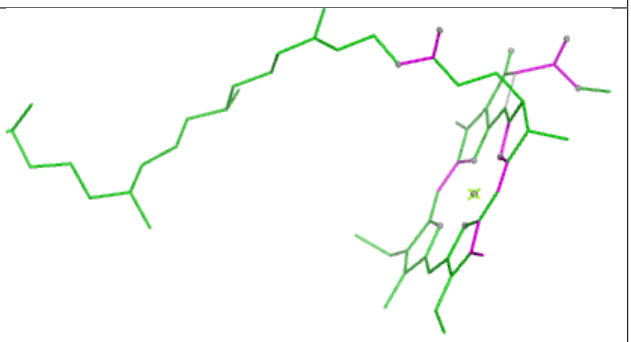
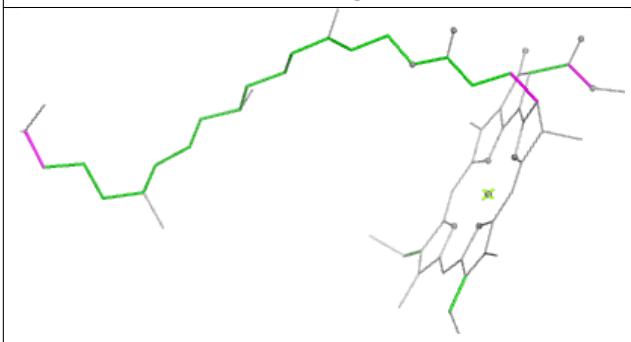


Bond angles

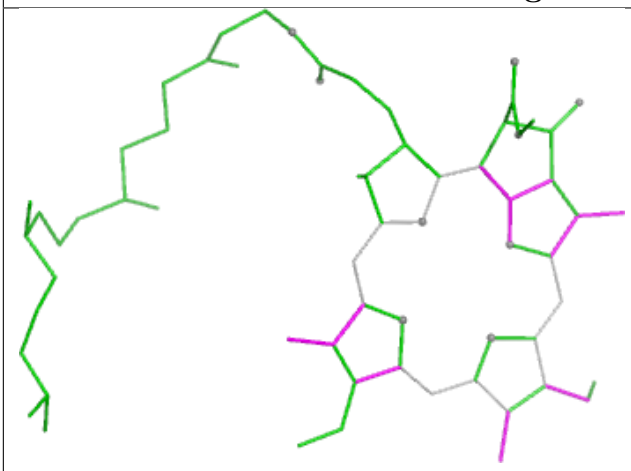


Torsions



Rings

Ligand PHO d 407



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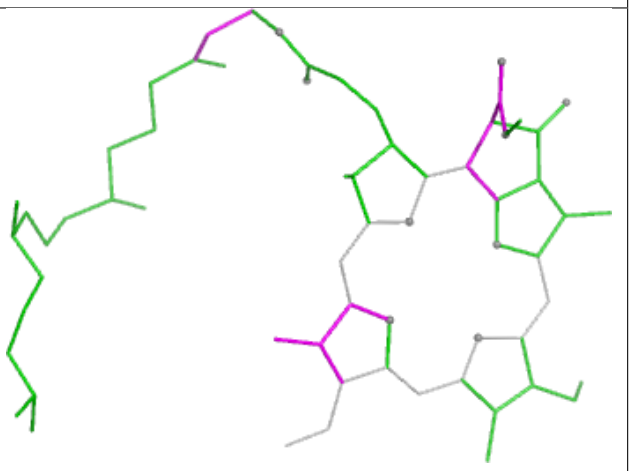
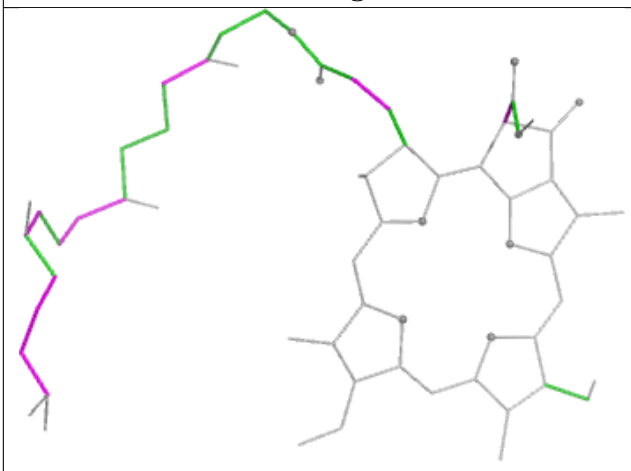


Bond angles



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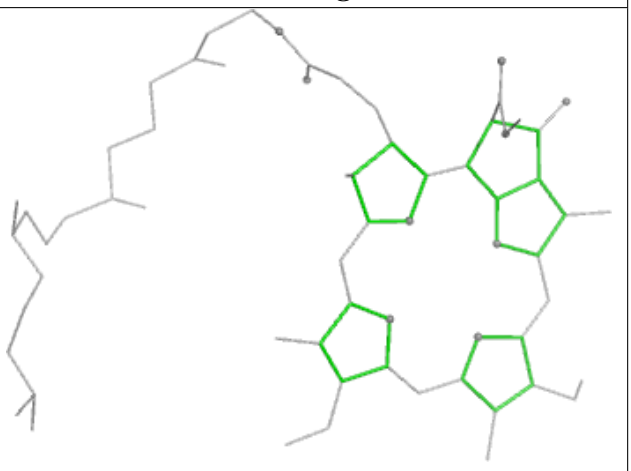
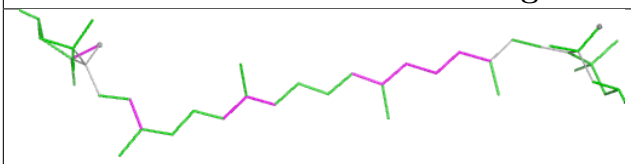


Rings

Ligand NEX N 302



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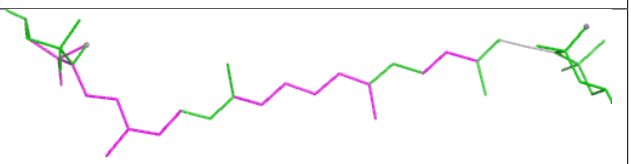

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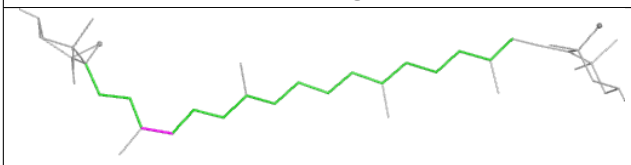

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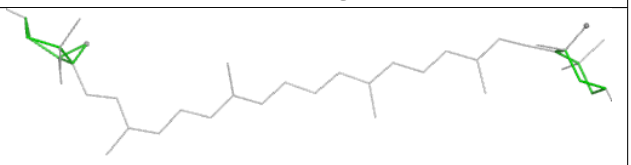
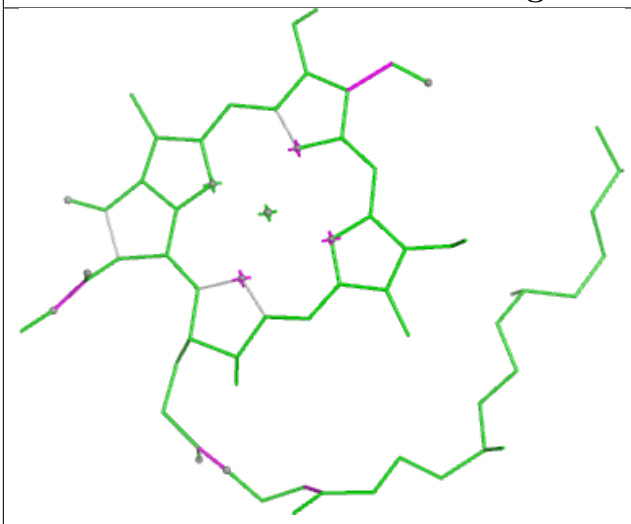


Rings

Ligand CHL n 318



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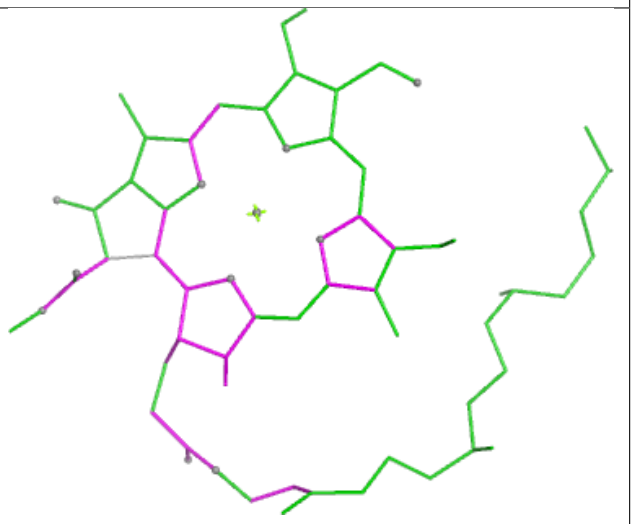
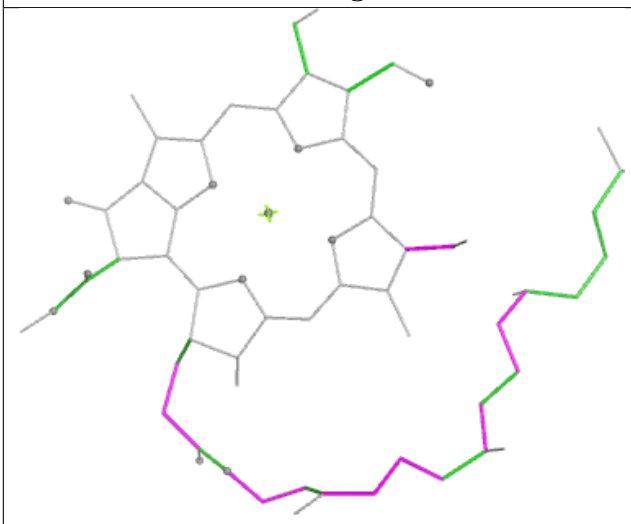


Bond angles



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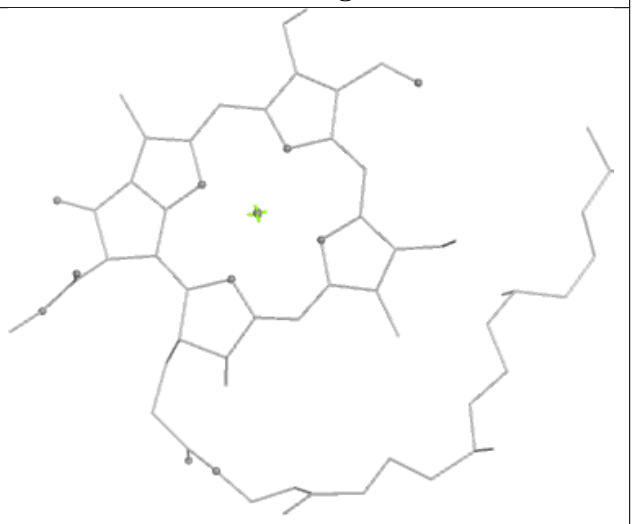
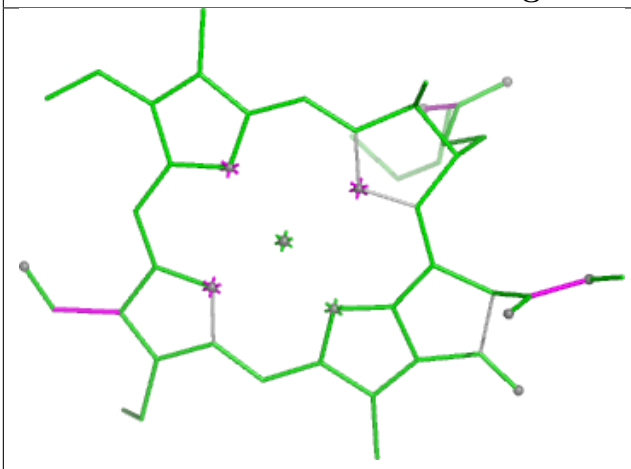


Rings

Ligand CHL G 311



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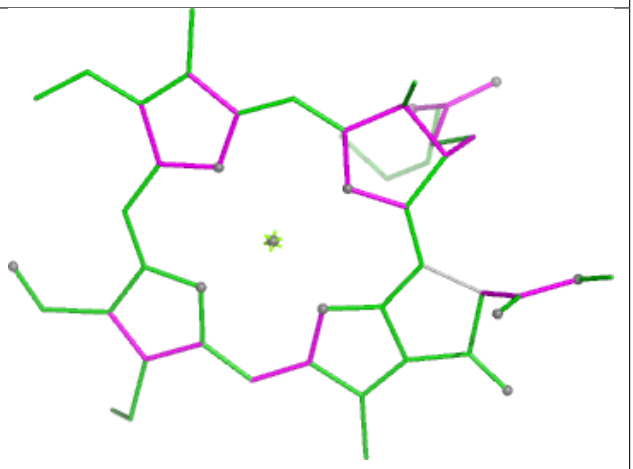

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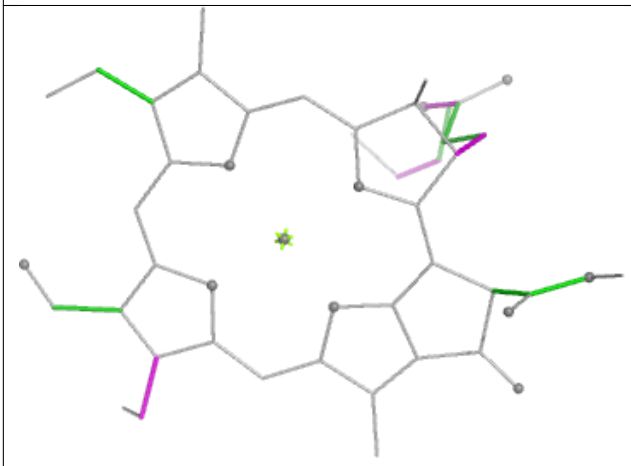

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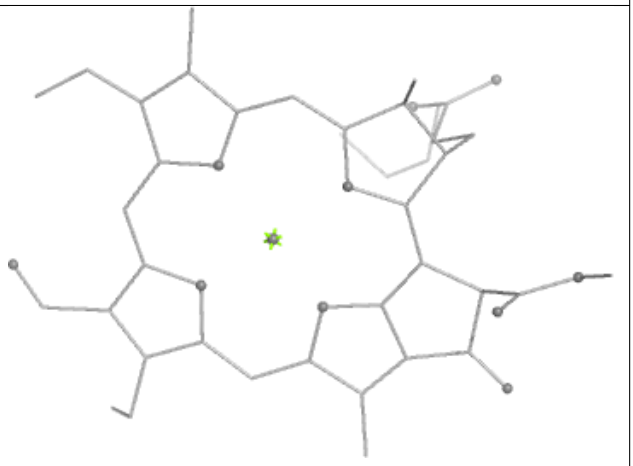
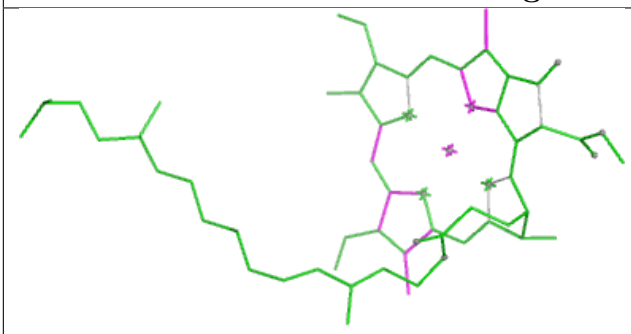


Rings

Ligand CLA G 307



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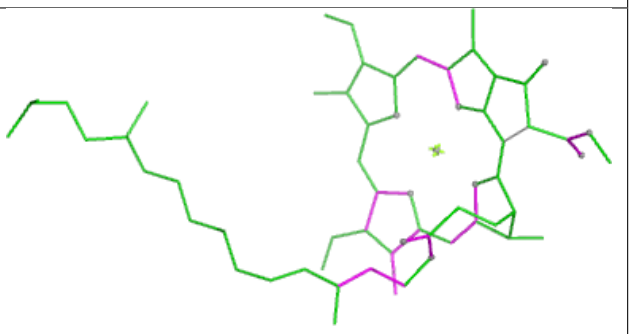
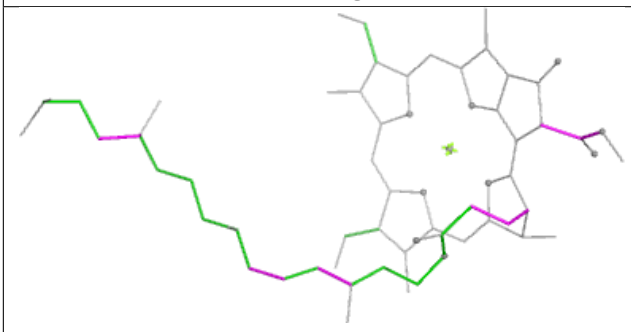


Bond angles



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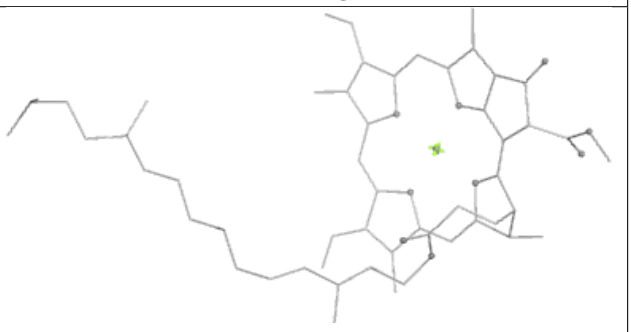
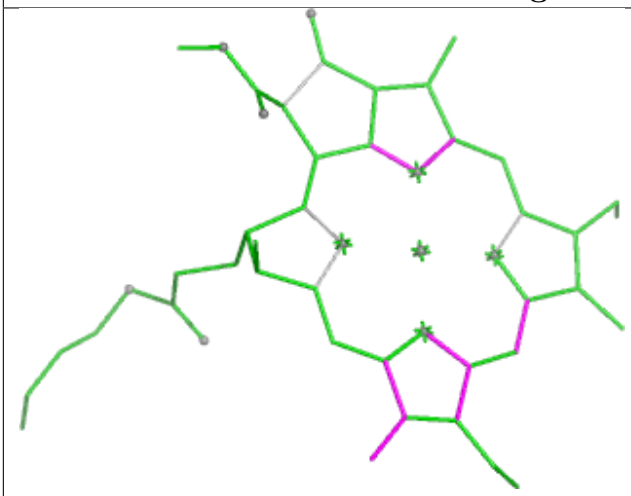


Rings

Ligand CLA s 314



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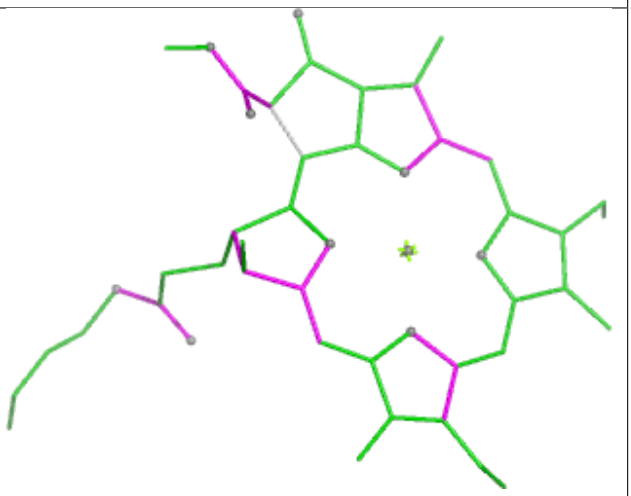
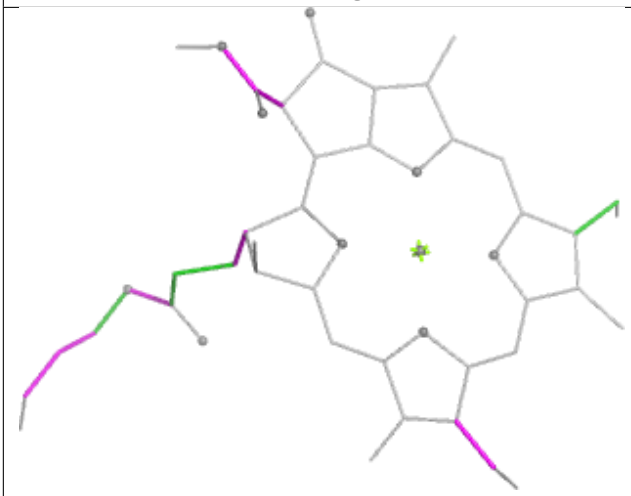


Bond angles



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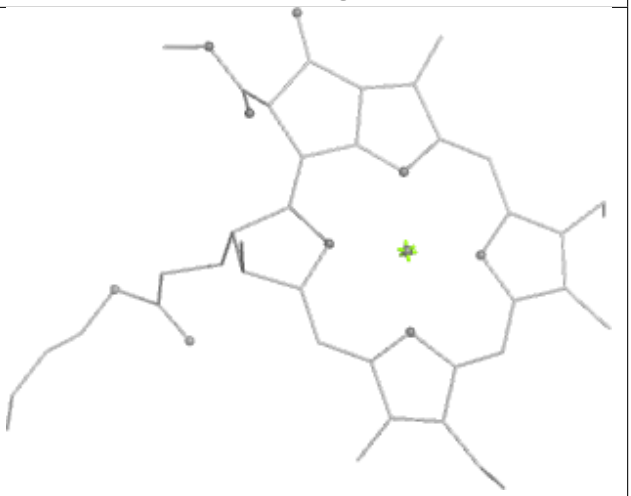
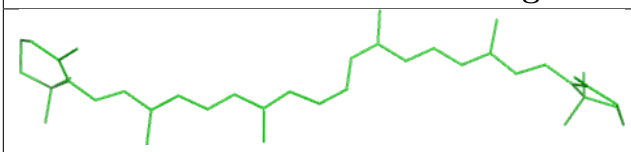


Rings

Ligand BCR C 514



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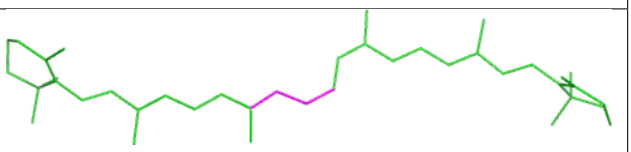
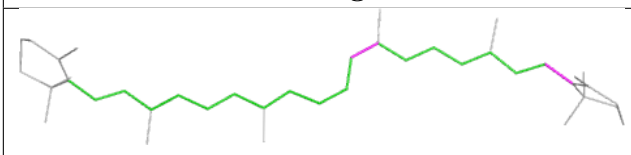


Bond angles



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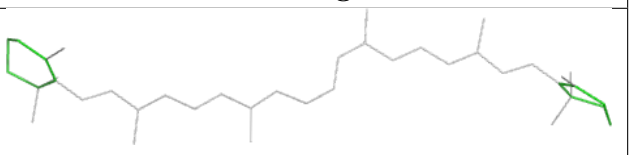
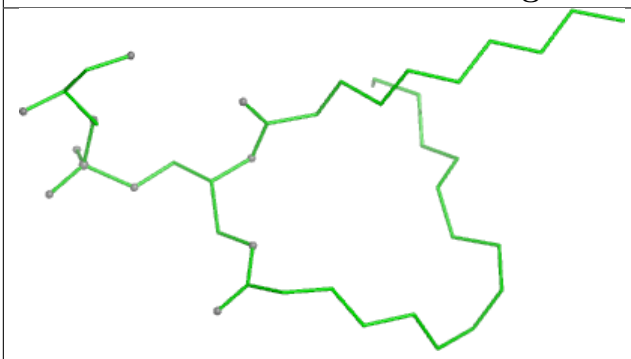
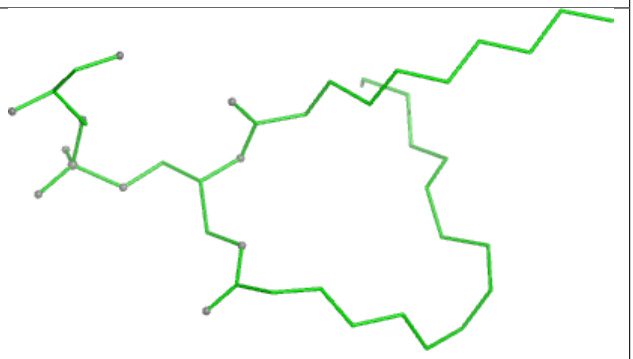


Rings

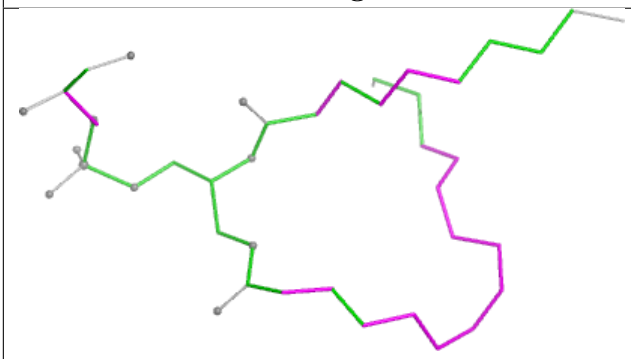
Ligand LHG D 407



Bond lengths



Bond angles



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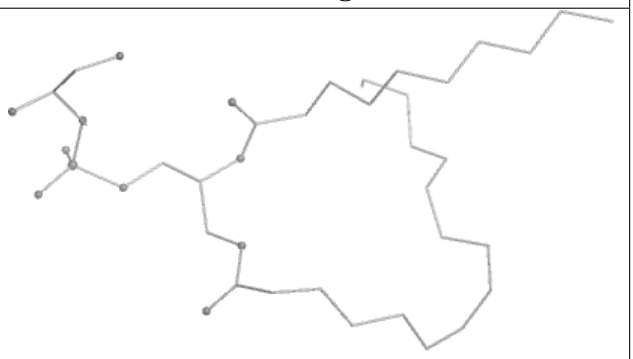
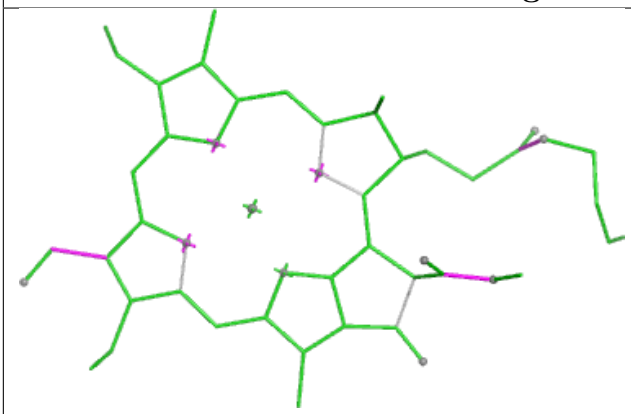


Rings

Ligand CHL N 304



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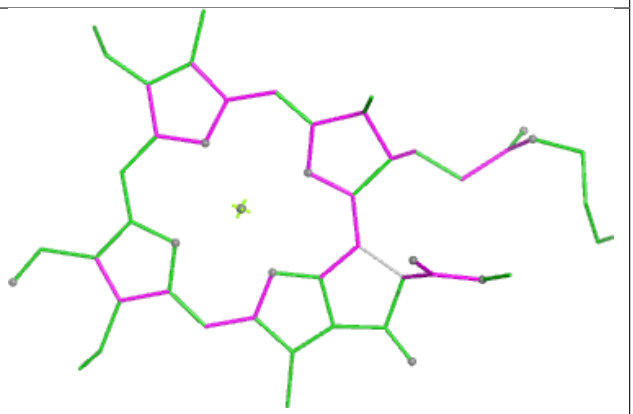
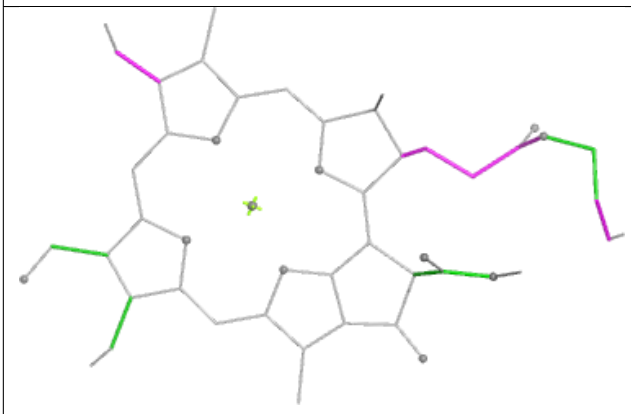
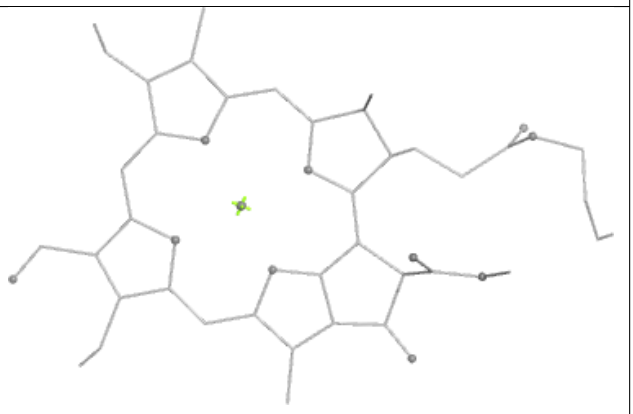


Bond angles

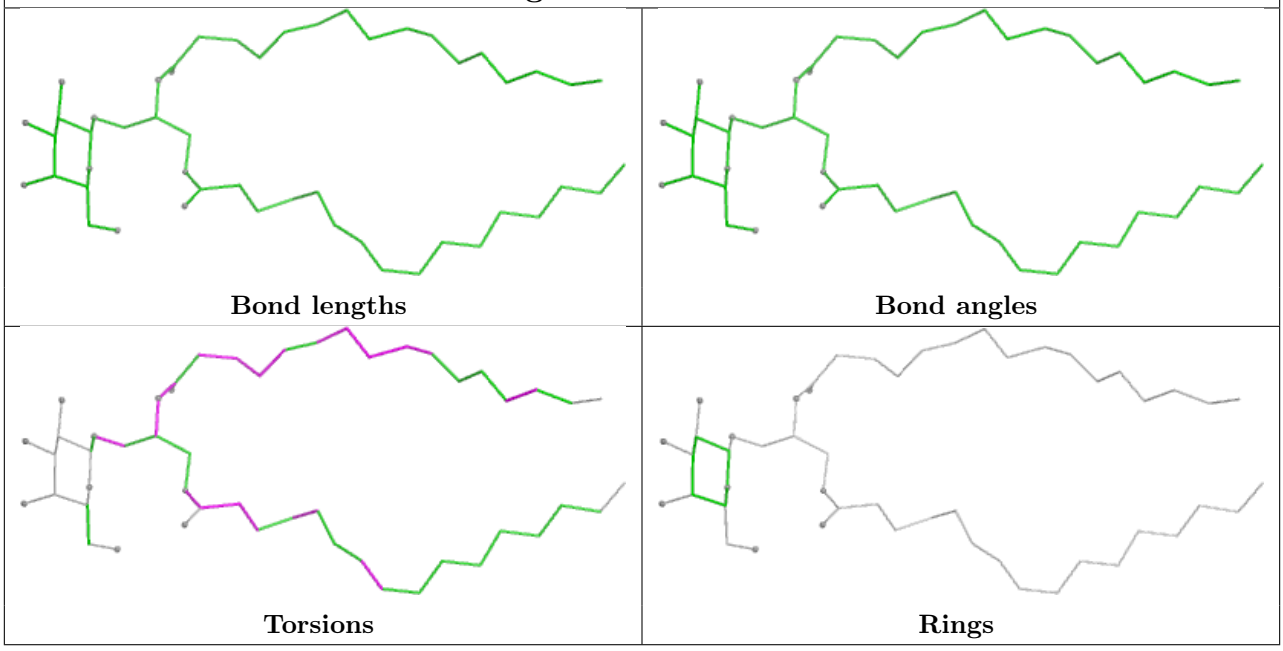


Torsions

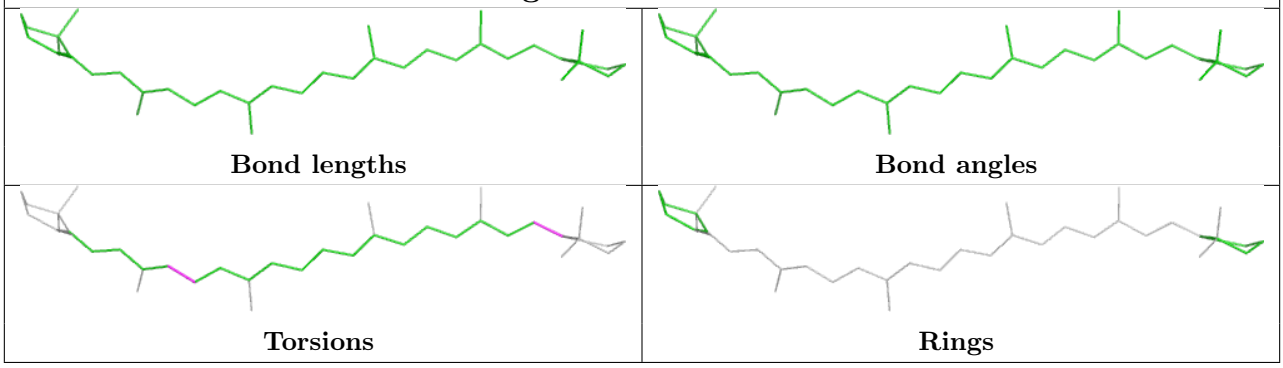


Rings

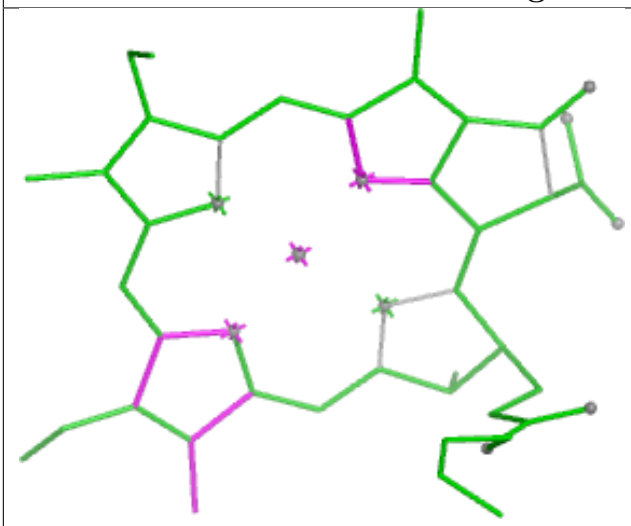
Ligand LMG c 512



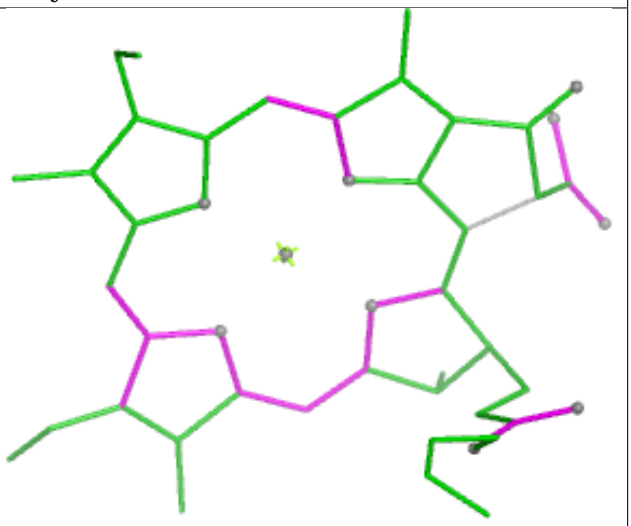
Ligand BCR H 101



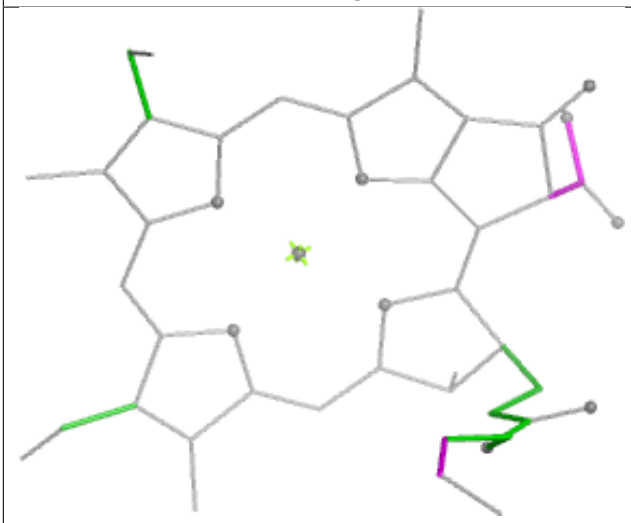
Ligand CLA y 313



Bond lengths



Bond angles



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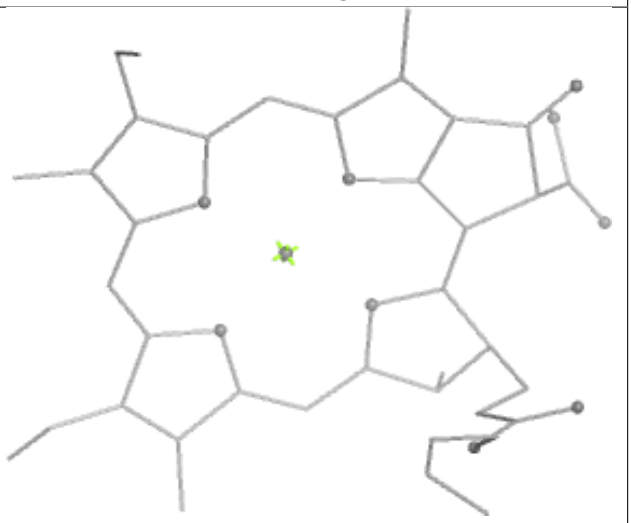
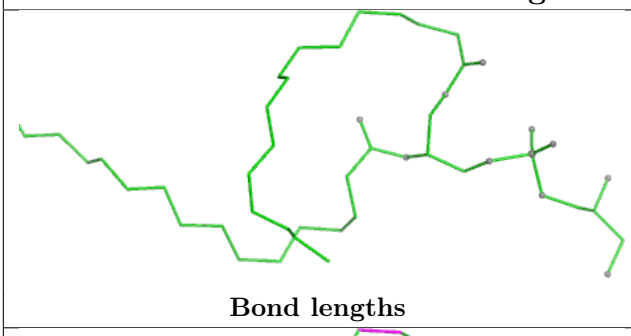


Rings

Ligand LHG r 312



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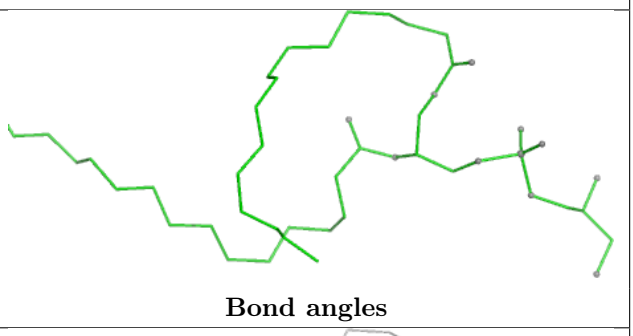
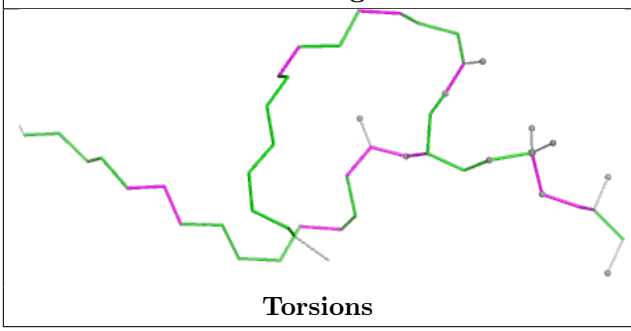


Bond angles



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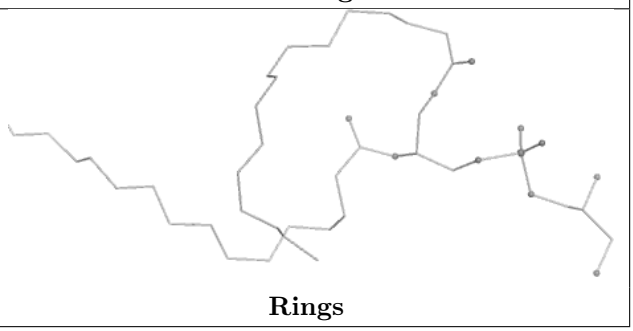
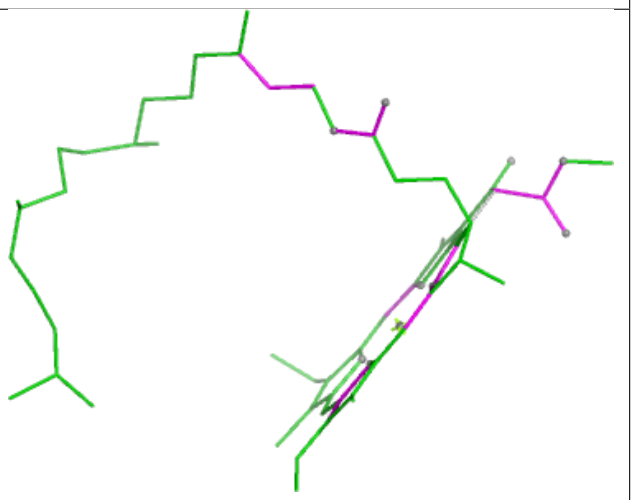


Rings

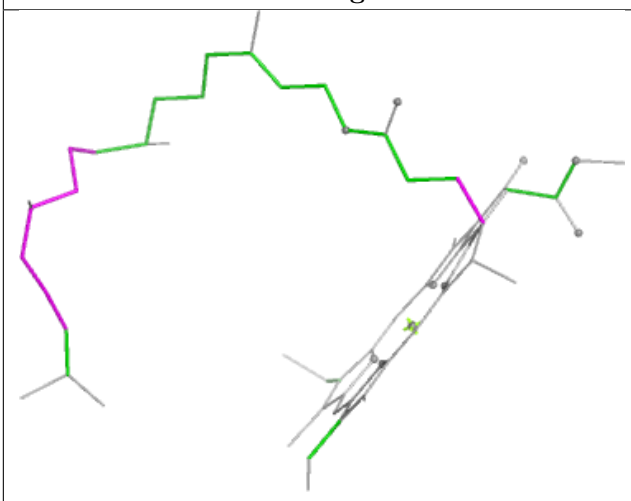
Ligand CLA B 617



Bond lengths



Bond angles



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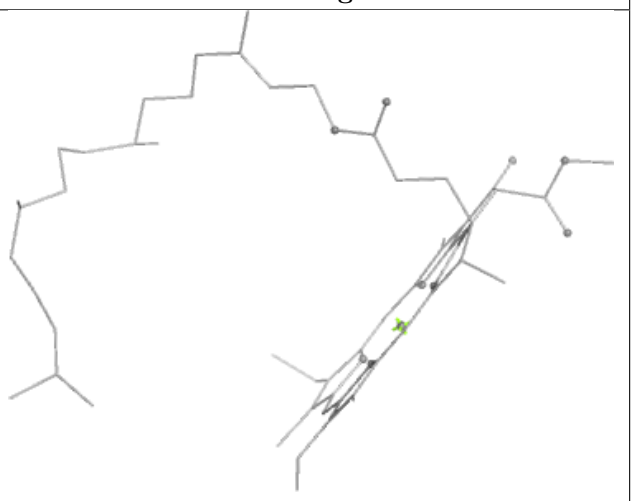
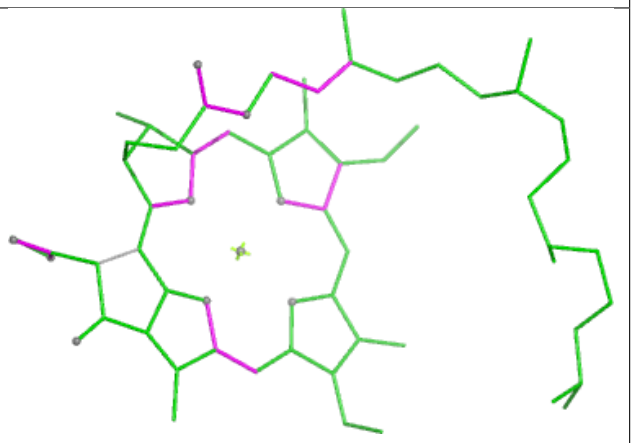


Rings

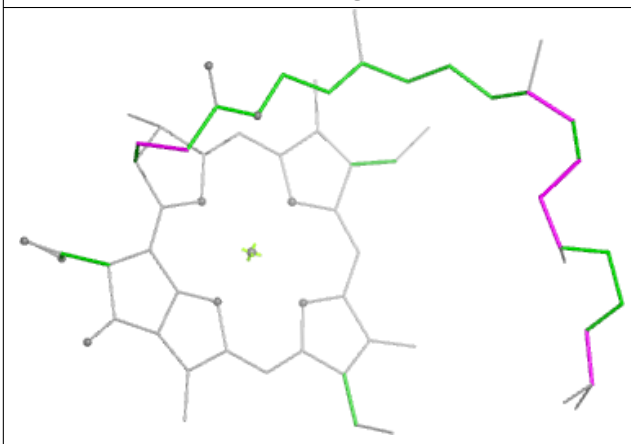
Ligand CLA G 314



Bond lengths



Bond angles



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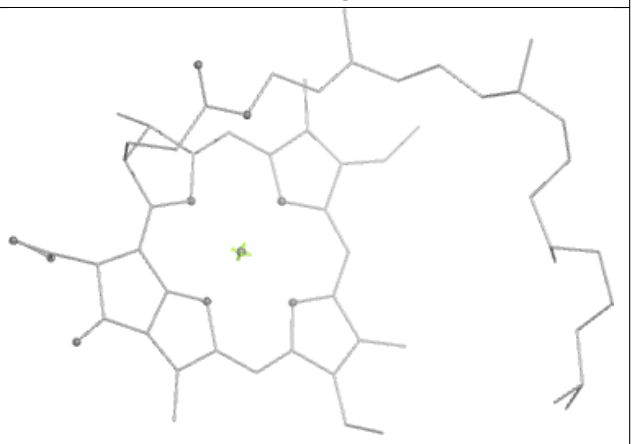


Rings

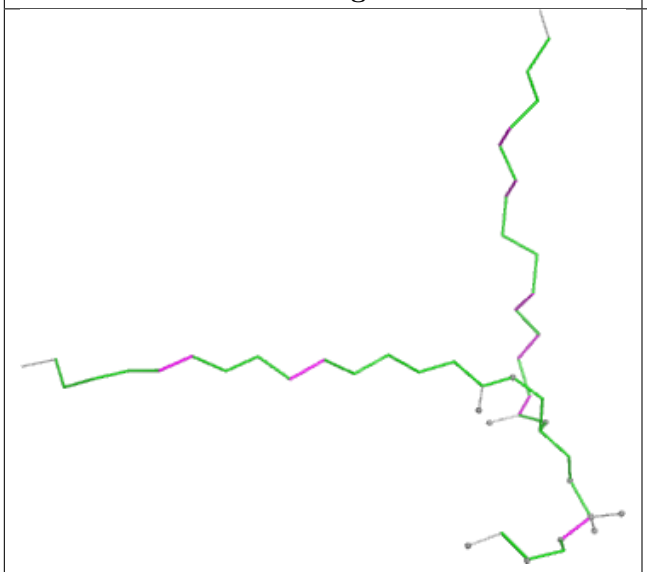
Ligand LHG L 101



Bond lengths



Bond angles

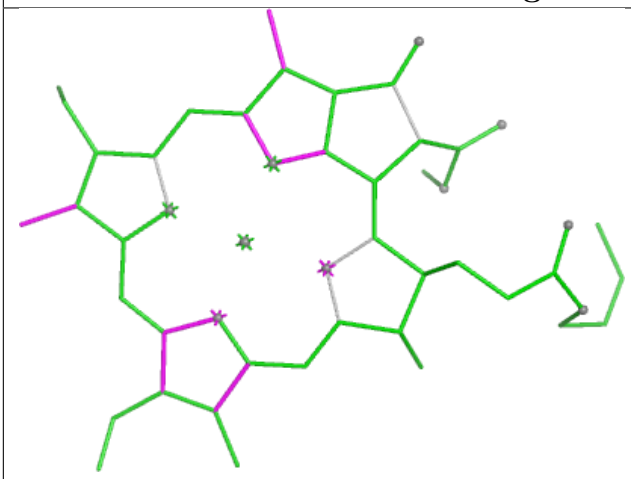


Torsions



Rings

Ligand CLA N 313



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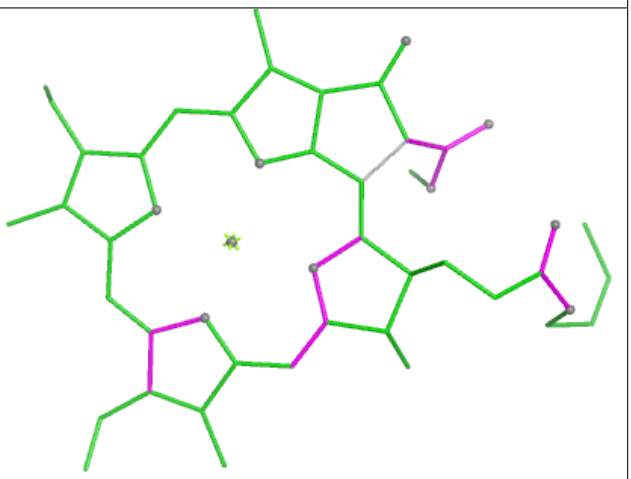
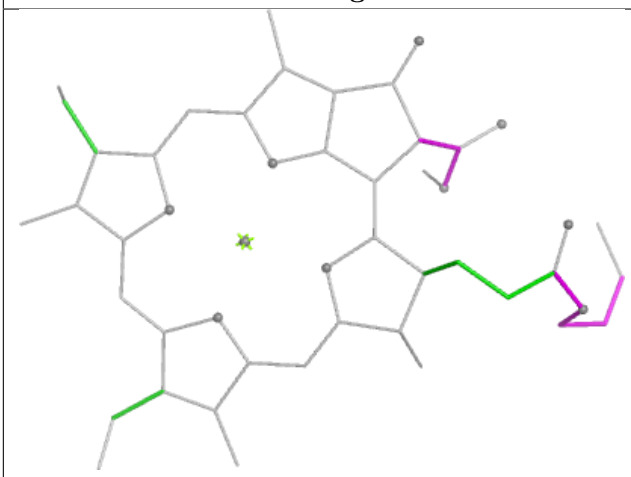


Bond angles



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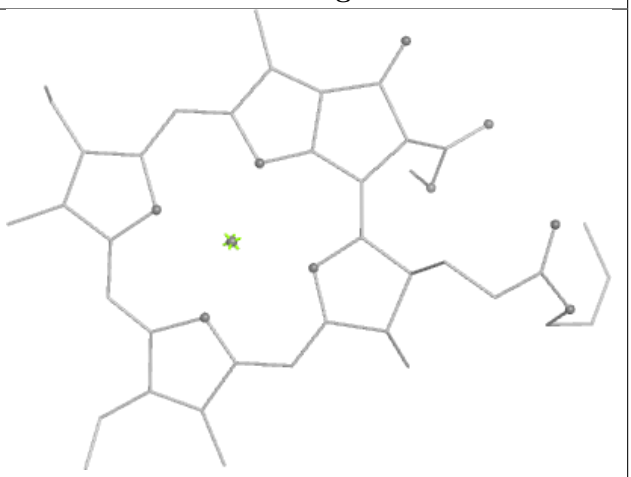
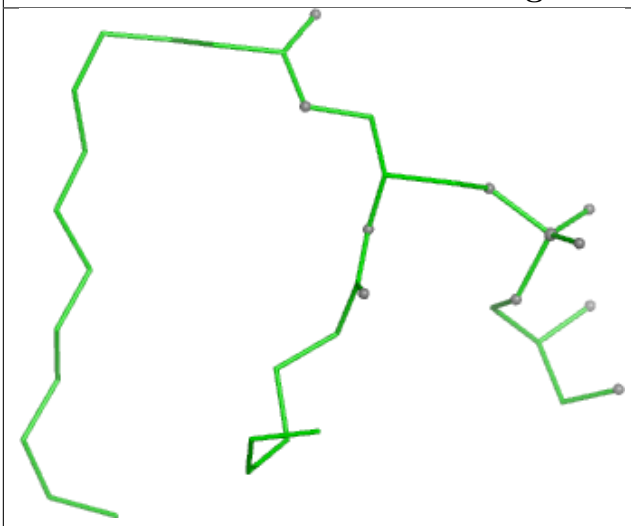


Rings

Ligand LHG d 410



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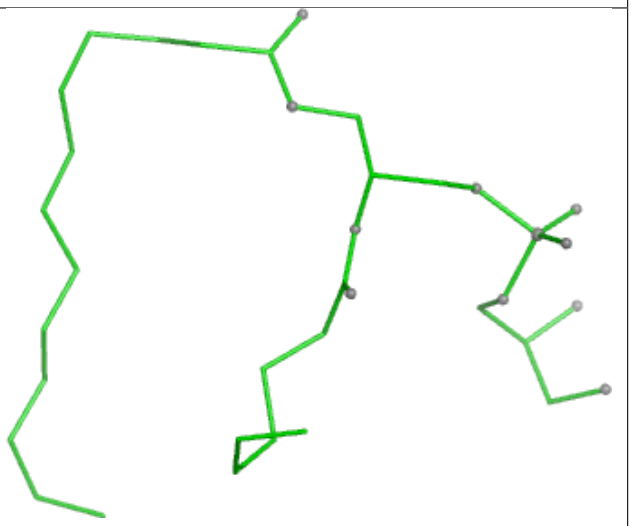
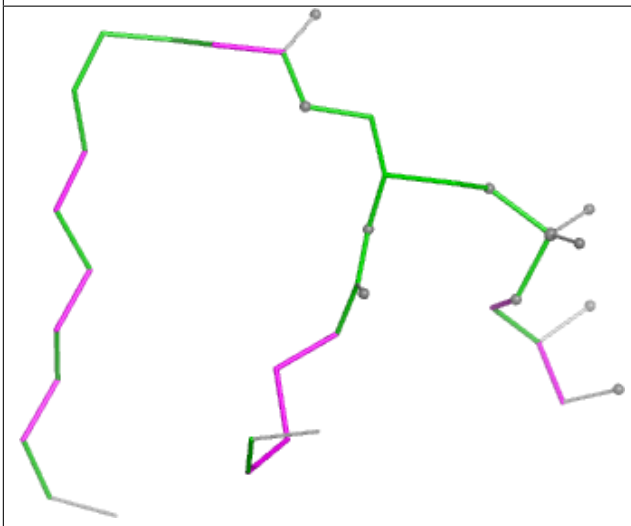


Bond angles



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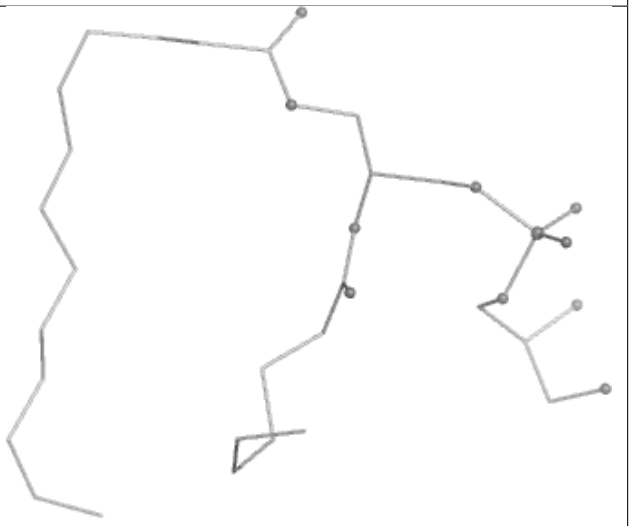
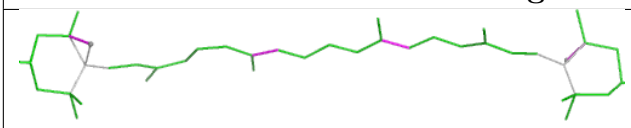


Rings

Ligand XAT g 320



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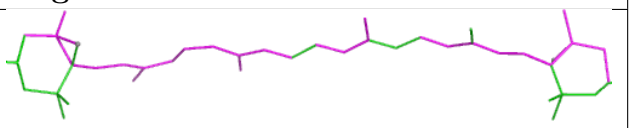
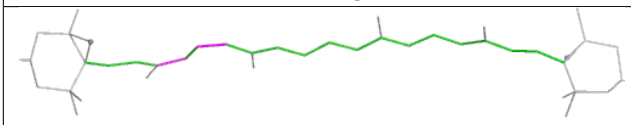


Bond angles



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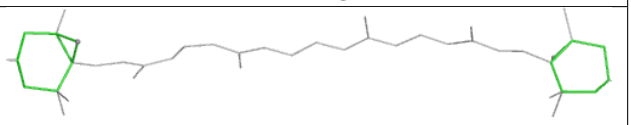
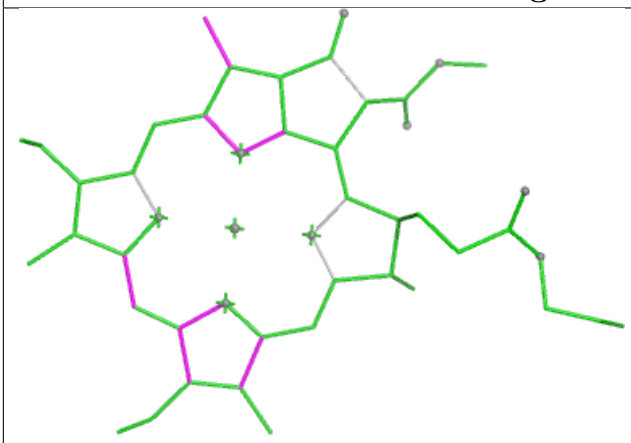


Rings

Ligand CLA r 305



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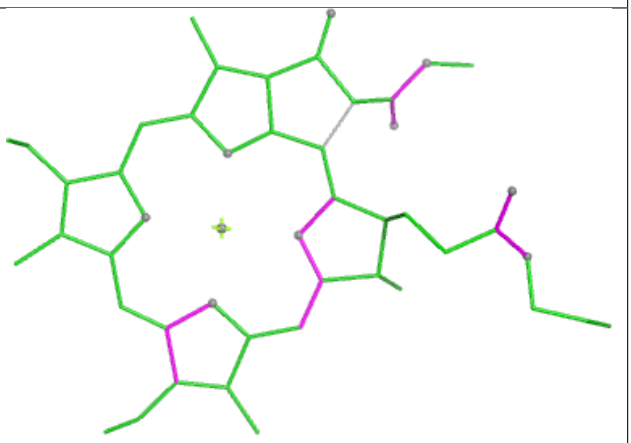
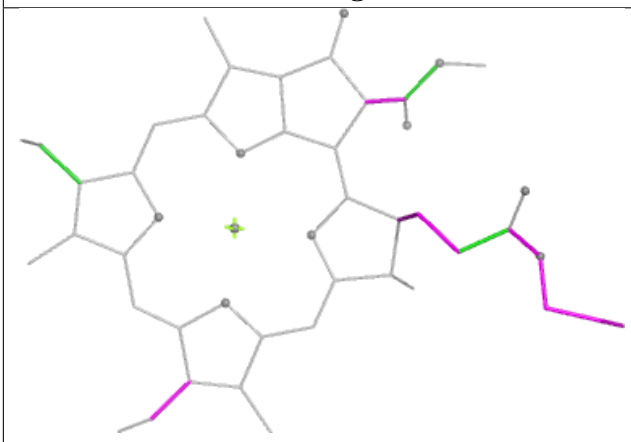


Bond angles



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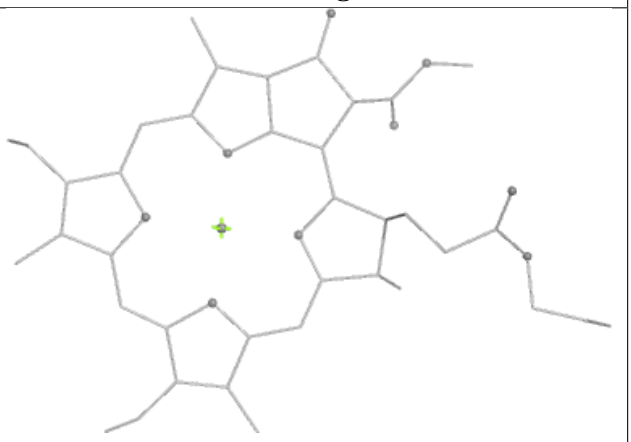
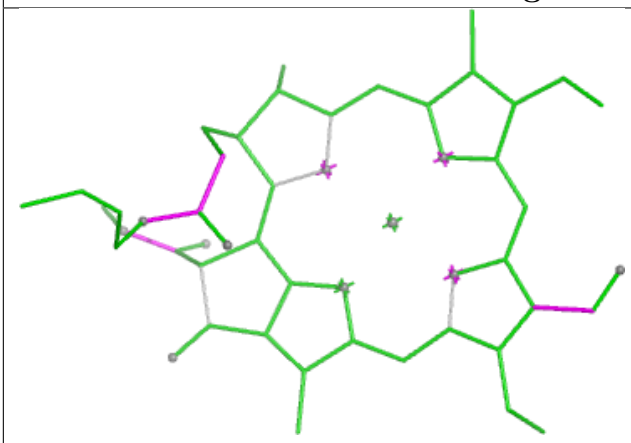


Rings

Ligand CHL R 315



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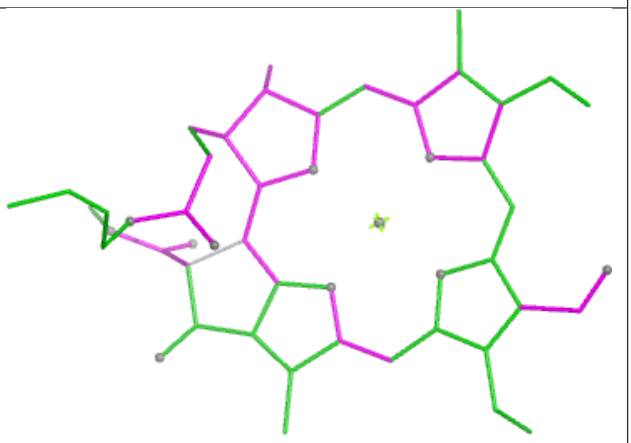

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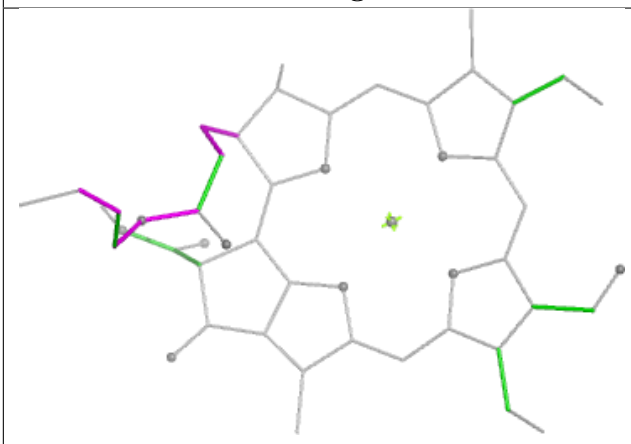

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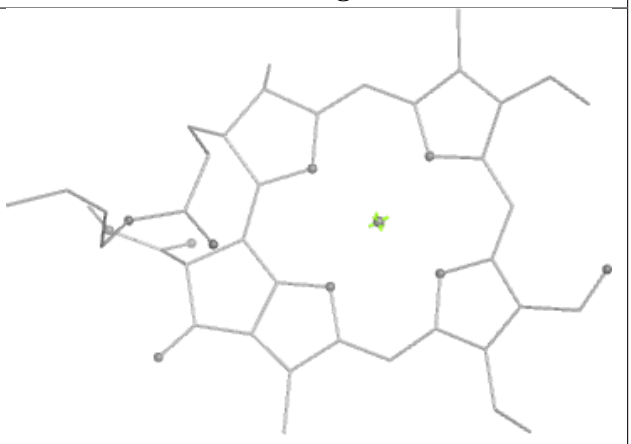
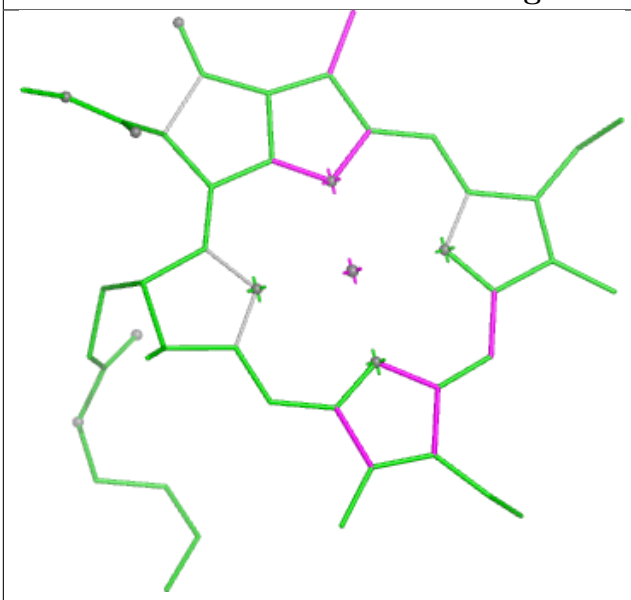


Rings

Ligand CLA R 314



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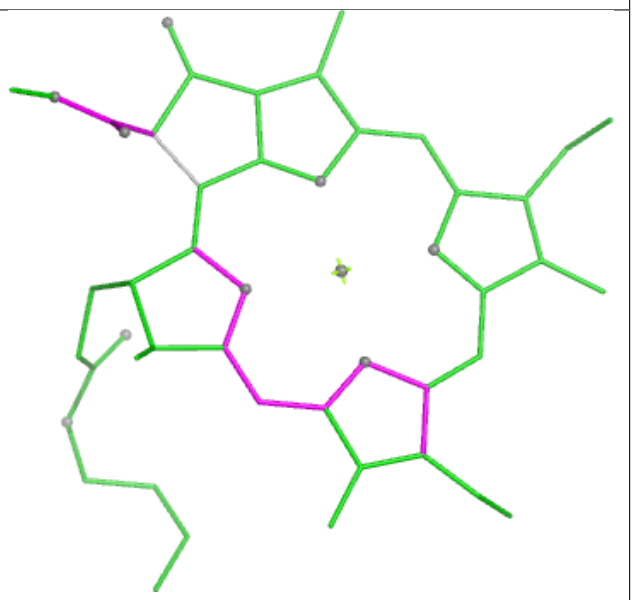
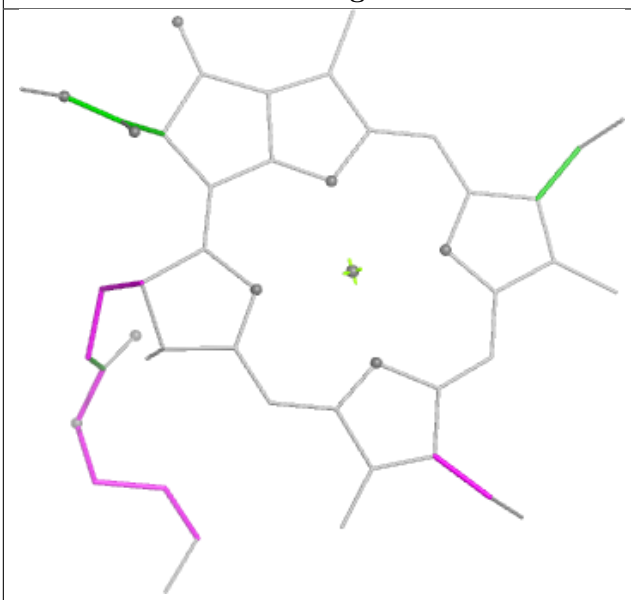


Bond angles



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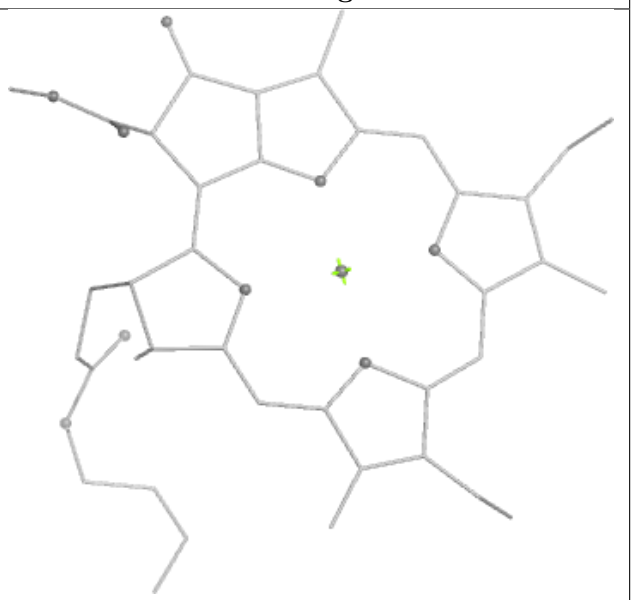
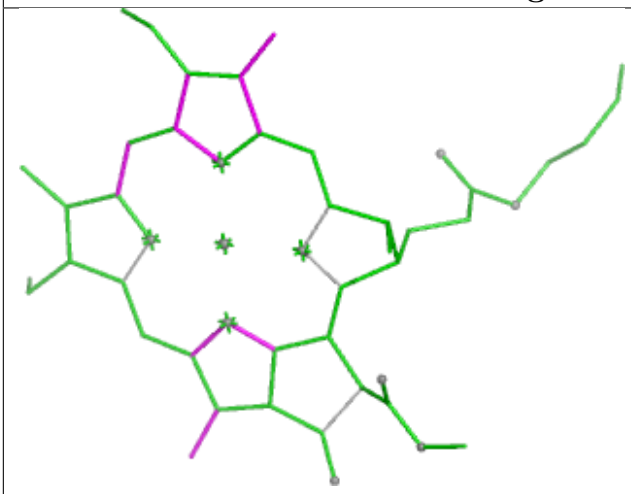


Rings

Ligand CLA S 311



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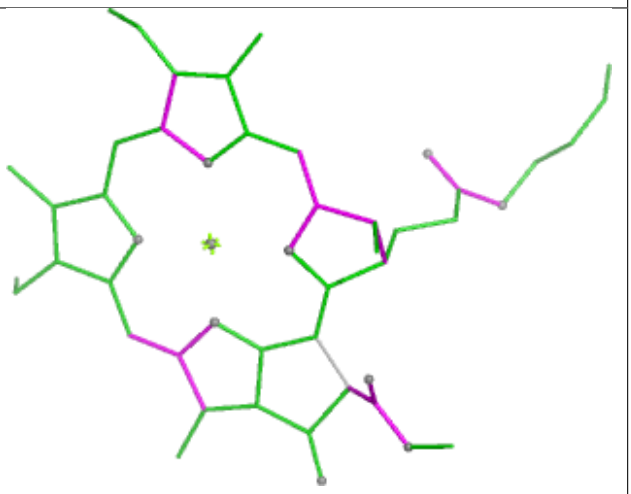
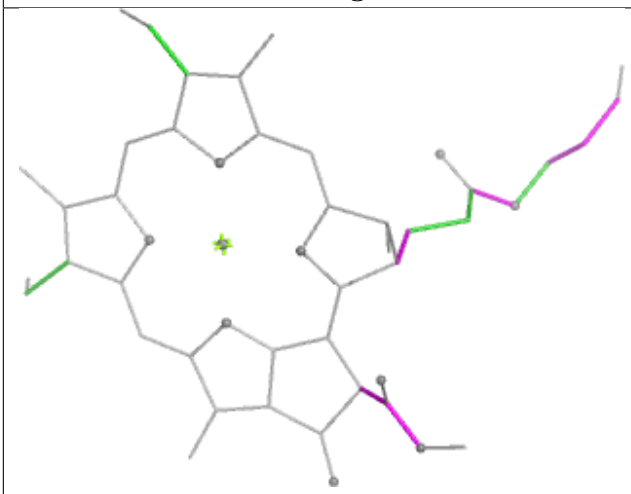


Bond angles



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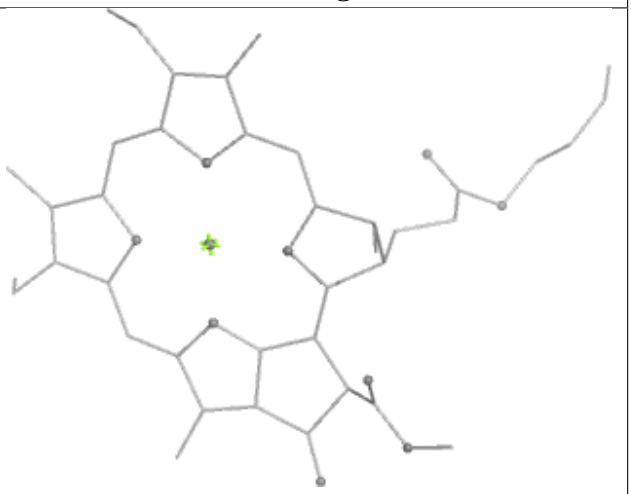
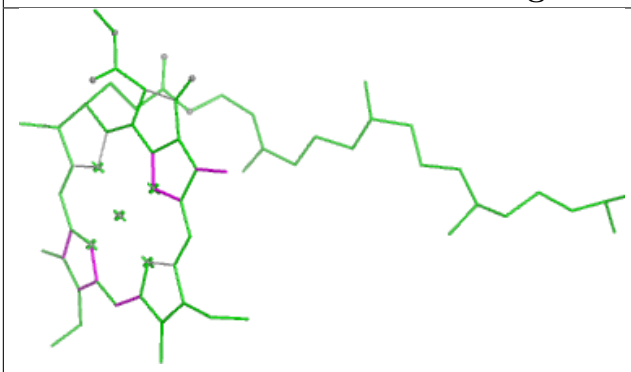


Rings

Ligand CLA y 304



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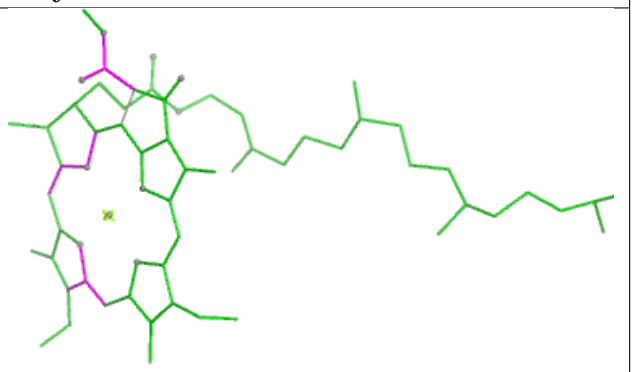
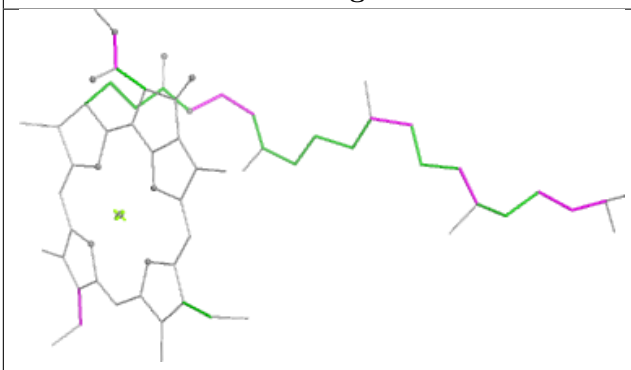


Bond angles



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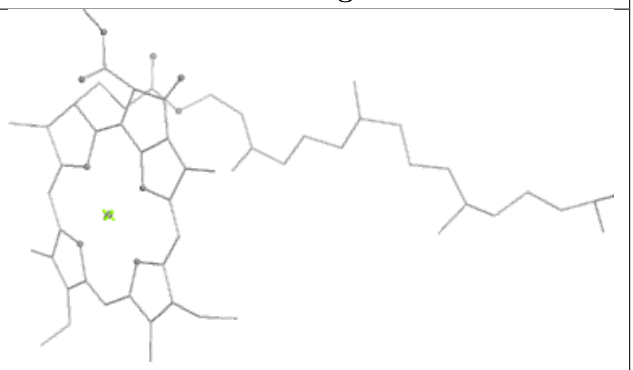
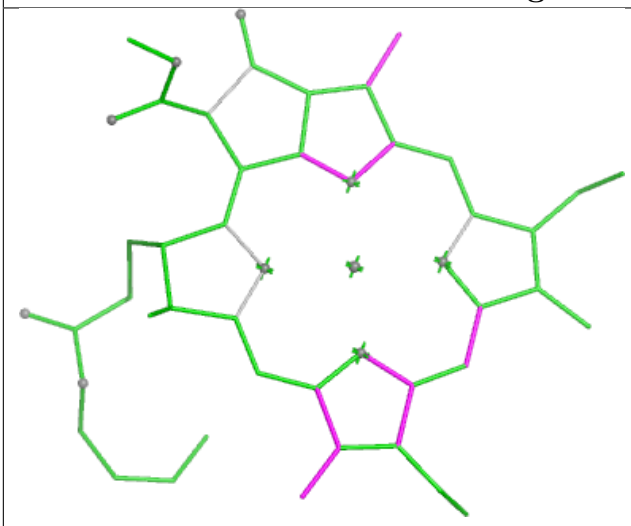


Rings

Ligand CLA n 310



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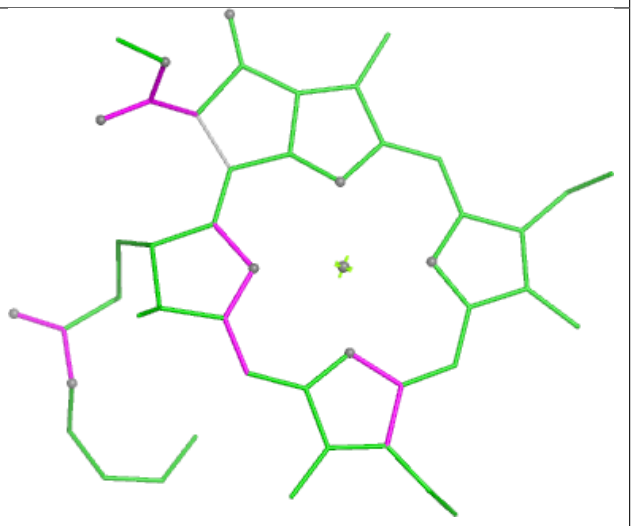
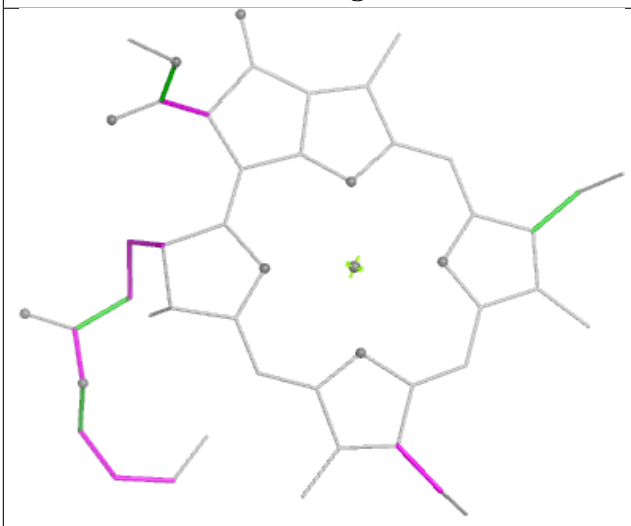


Bond angles



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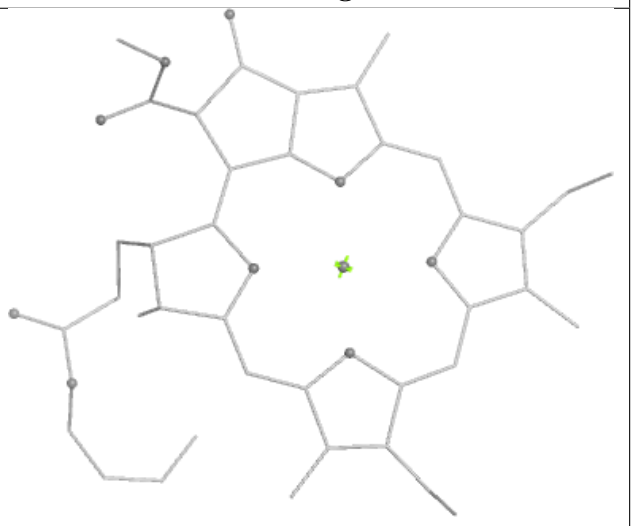
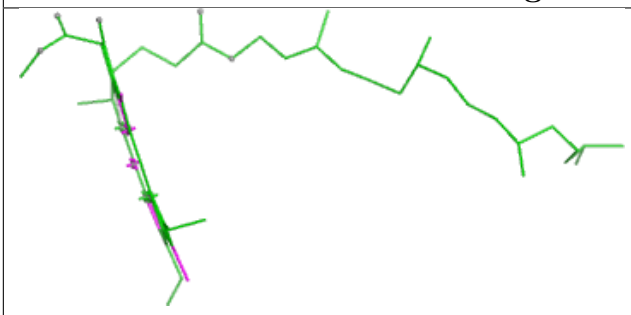
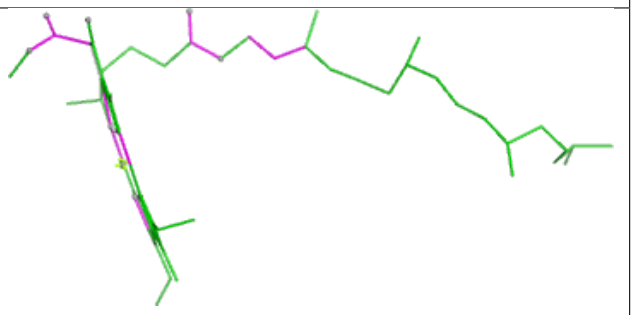


Rings

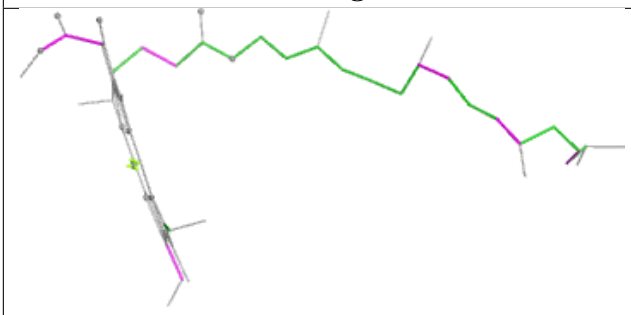
Ligand CLA B 618



Bond lengths



Bond angles



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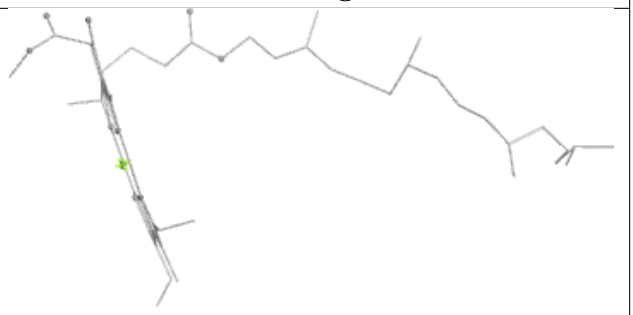
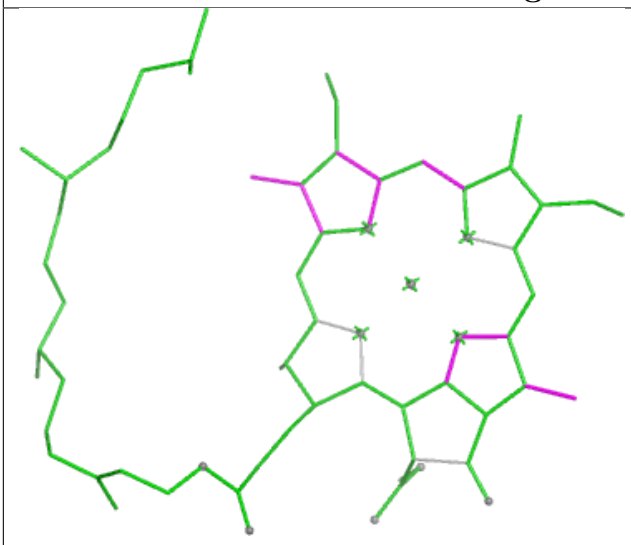
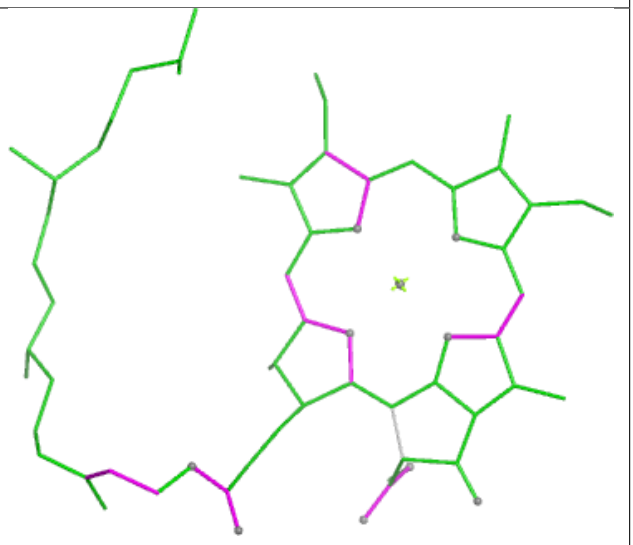


Rings

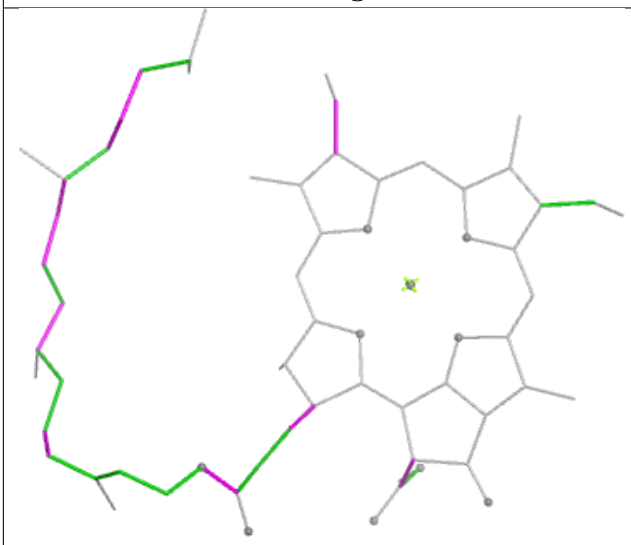
Ligand CLA C 511



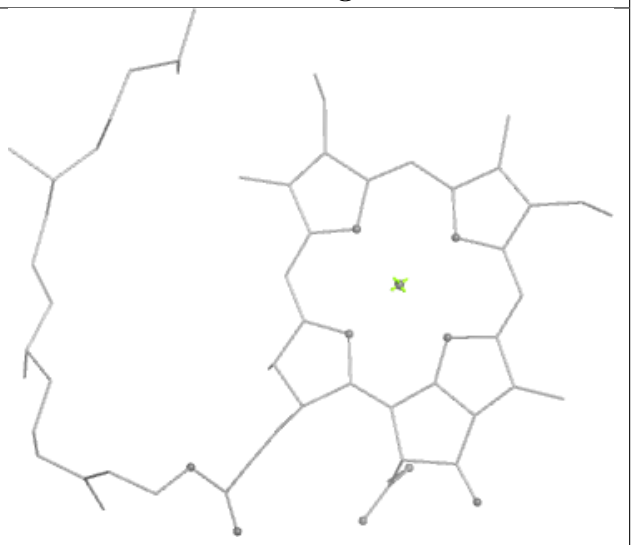
Bond lengths



Bond angles

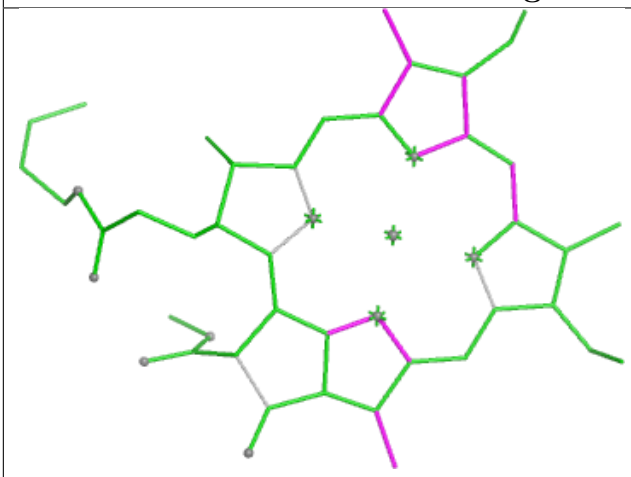


Torsions



Rings

Ligand CLA Y 311



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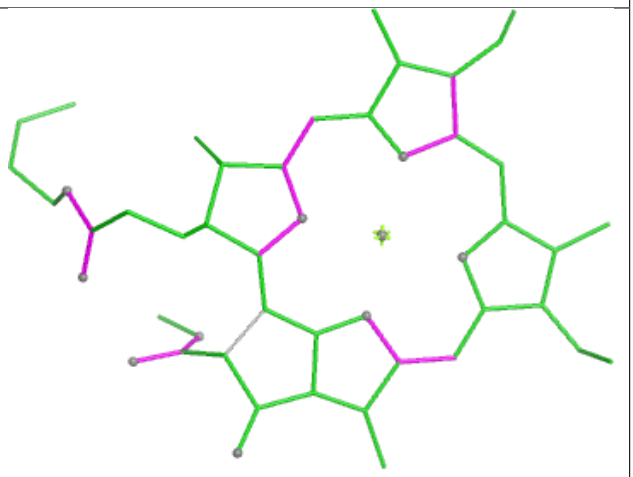
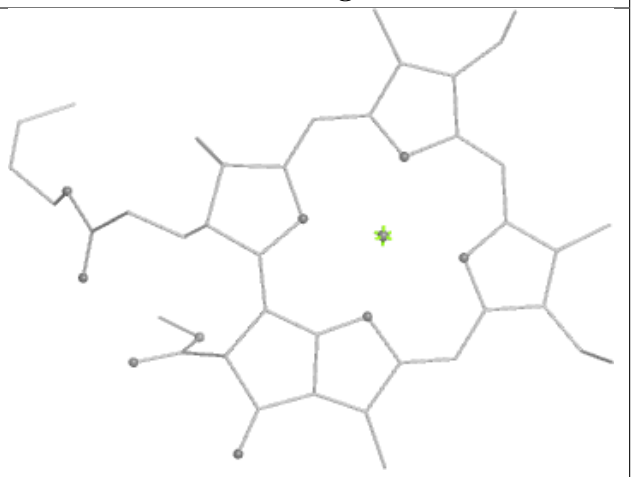


Bond angles

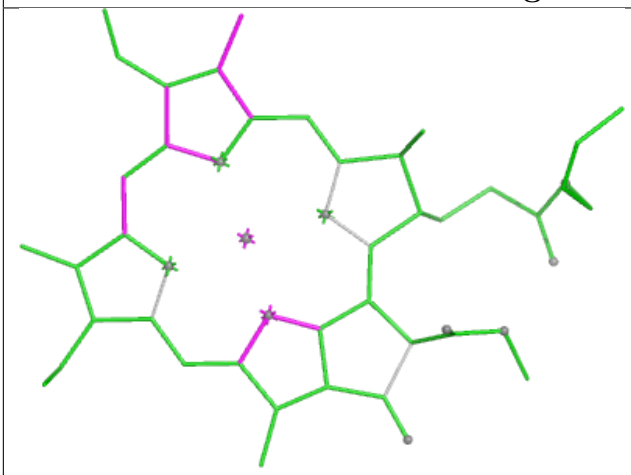


Torsions



Rings

Ligand CLA R 316



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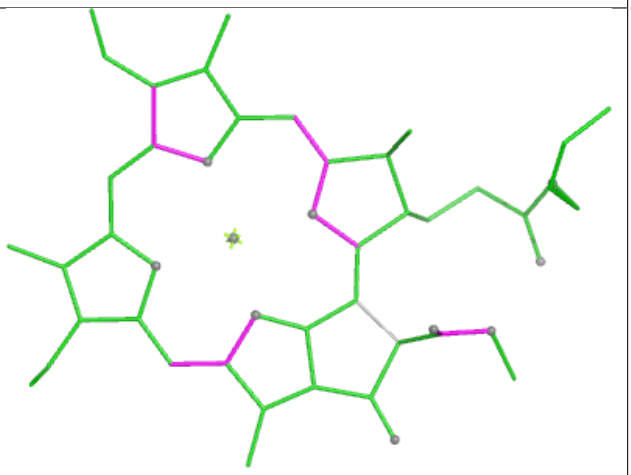
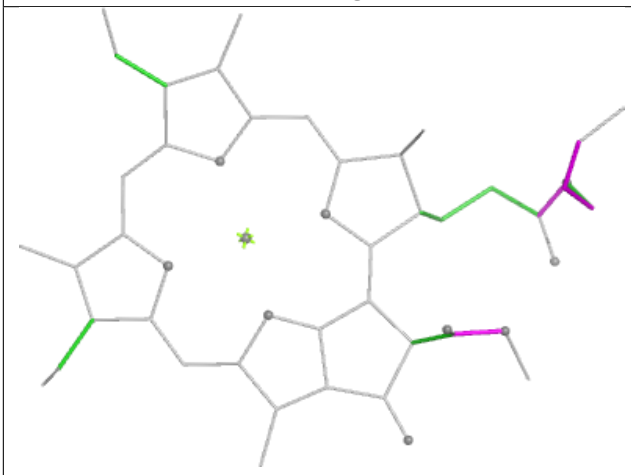


Bond angles



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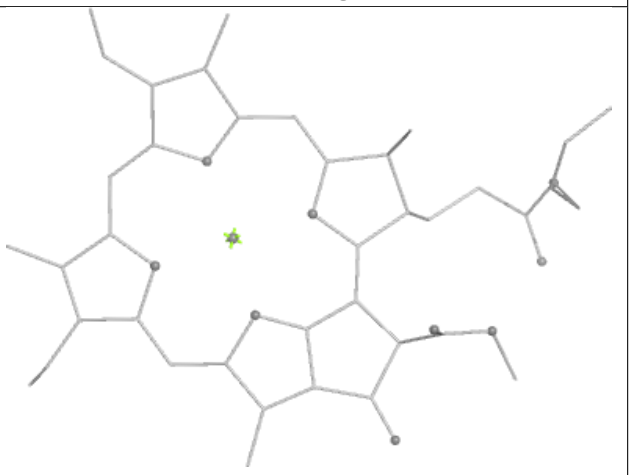
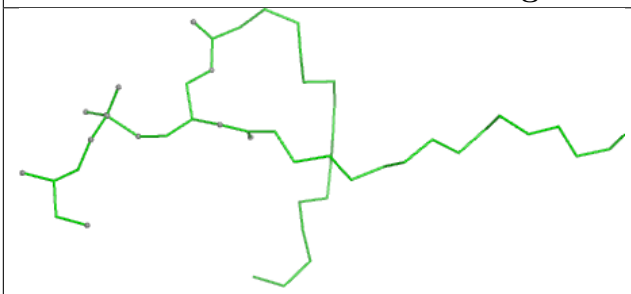


Rings

Ligand LHG G 312



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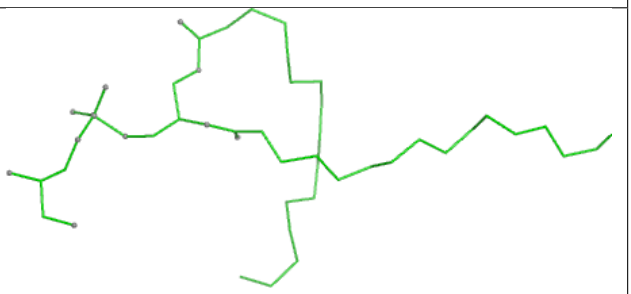
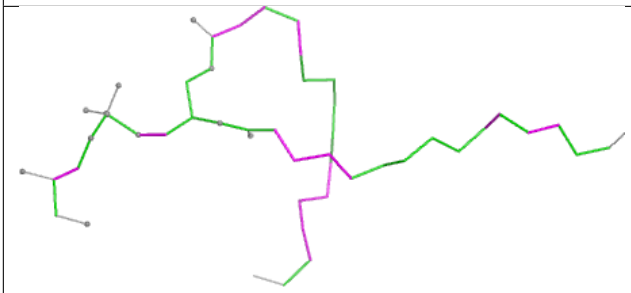


Bond angles



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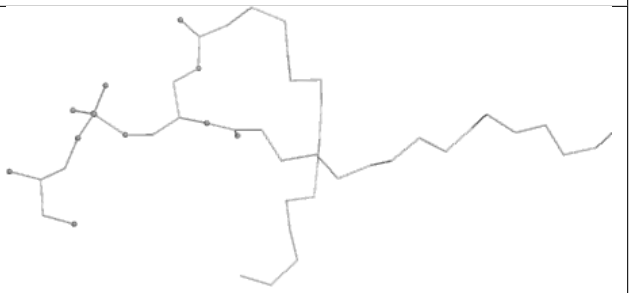
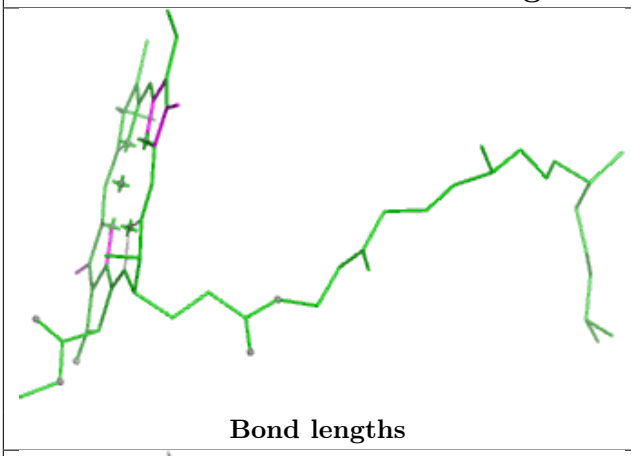
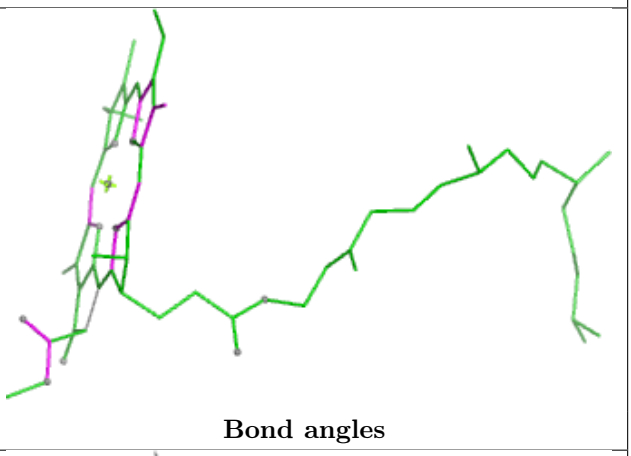


Rings

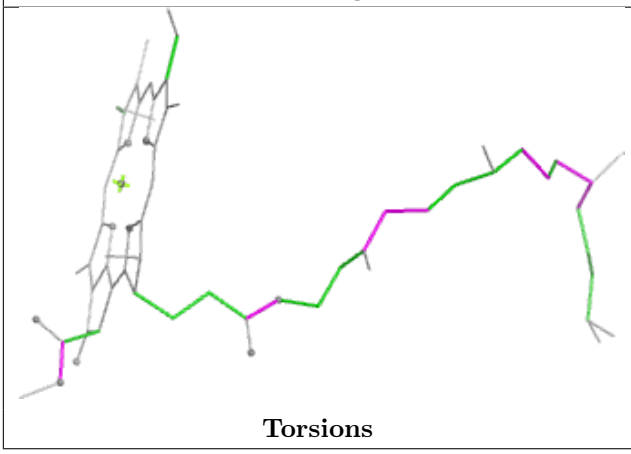
Ligand CLA D 406



Bond lengths



Bond angles

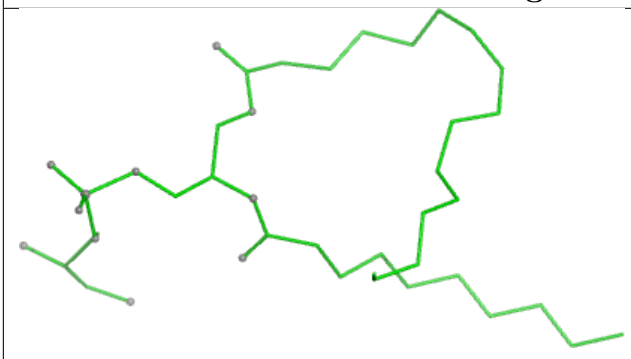


Torsions



Rings

Ligand LHG d 402



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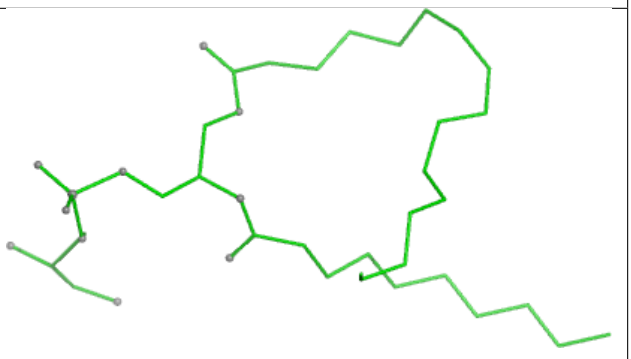
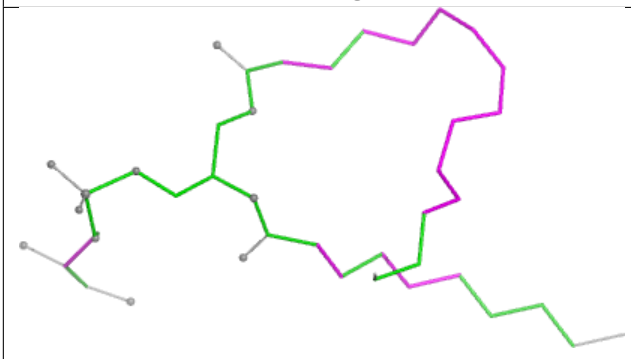


Bond angles



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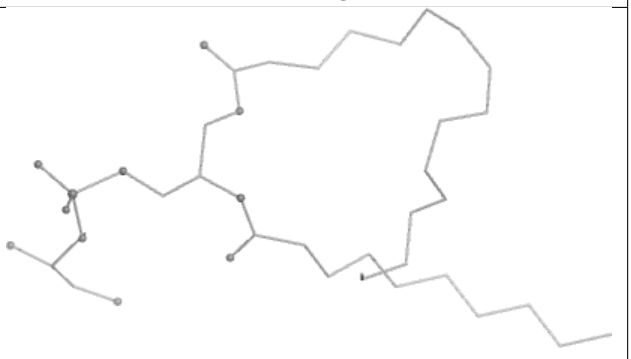
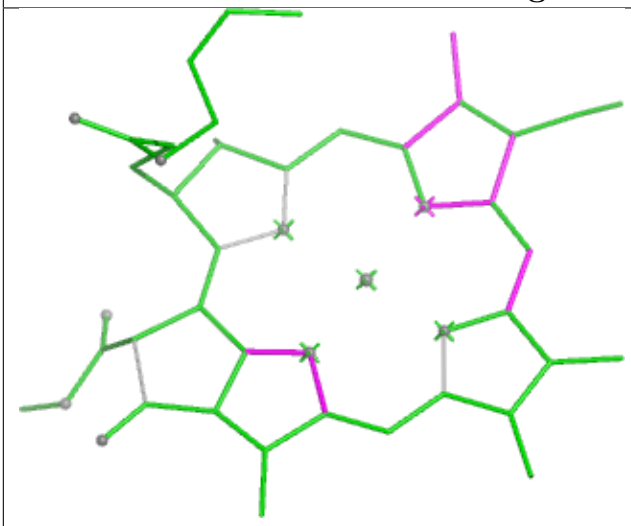


Rings

Ligand CLA g 318



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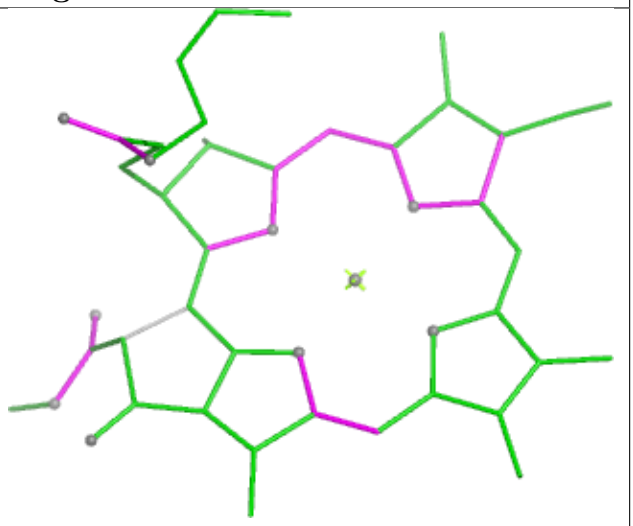
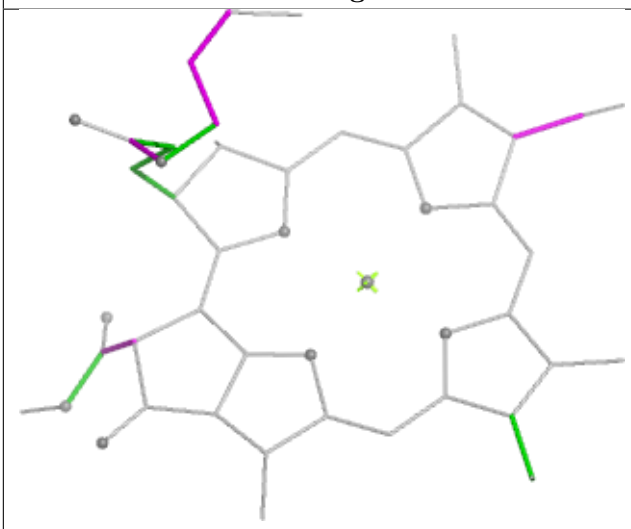


Bond angles



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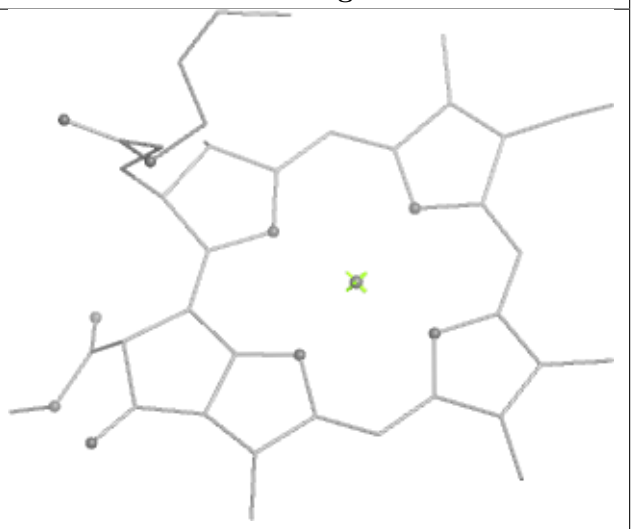
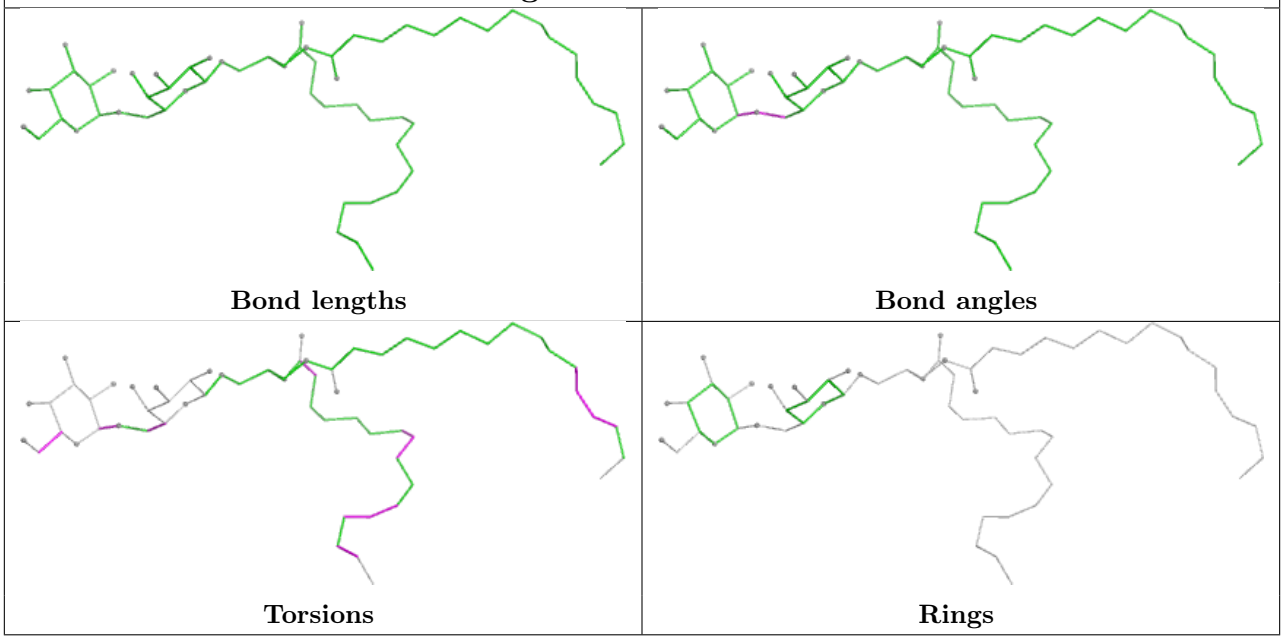


Rings

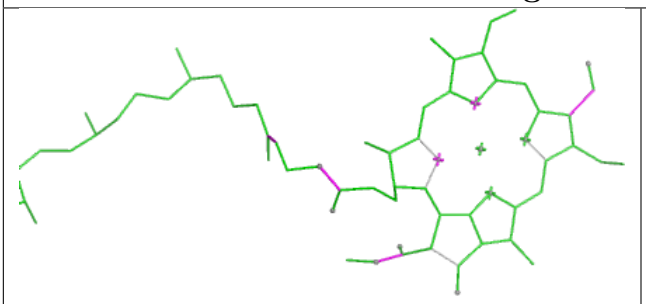
Ligand DGD B 620



Ligand BCR c 507



Ligand CHL Y 302



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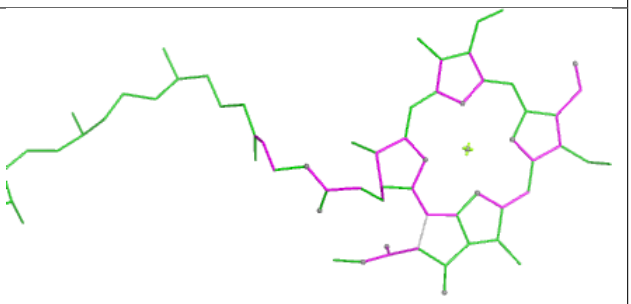
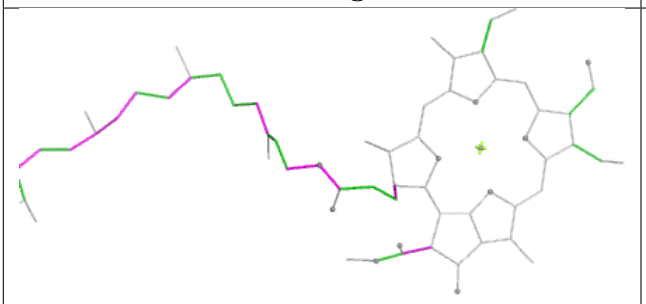


Bond angles



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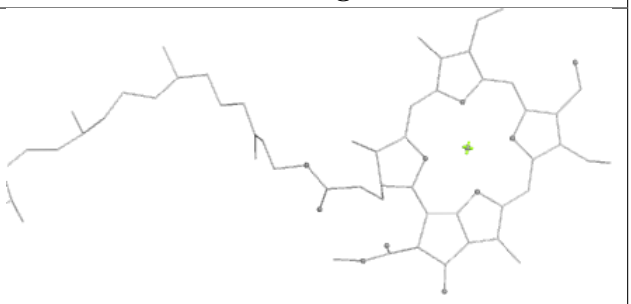
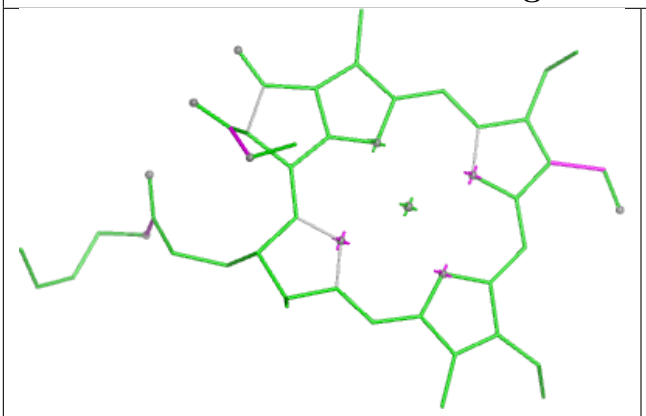


Rings

Ligand CHL R 301



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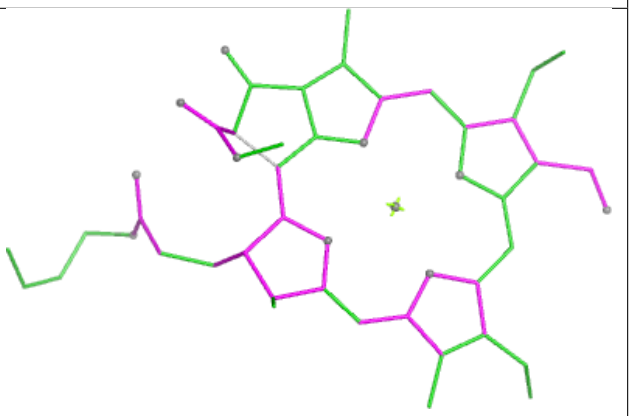
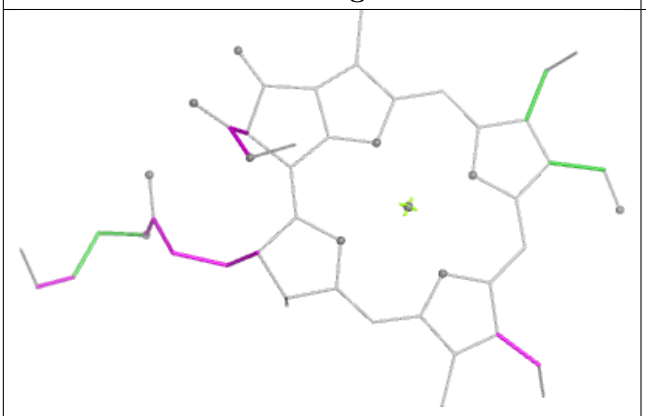


Bond angles



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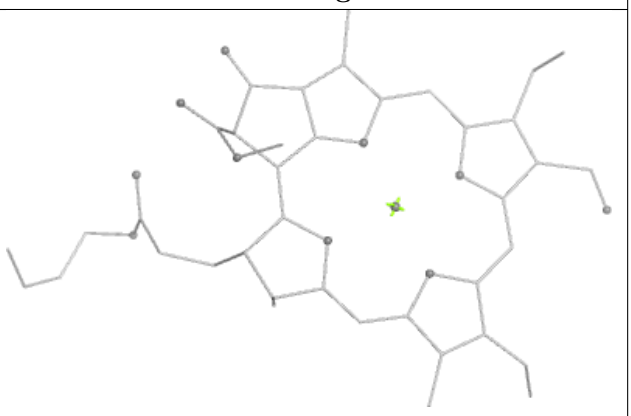
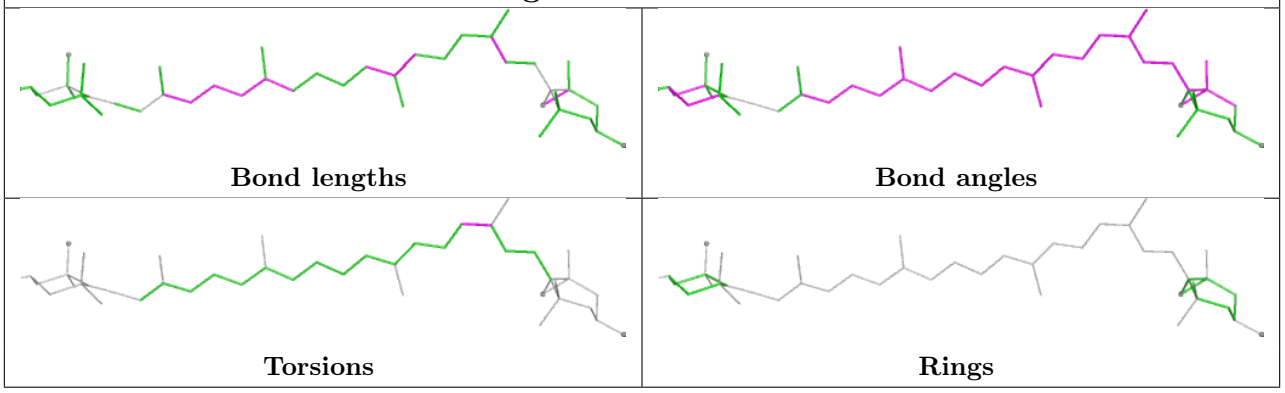
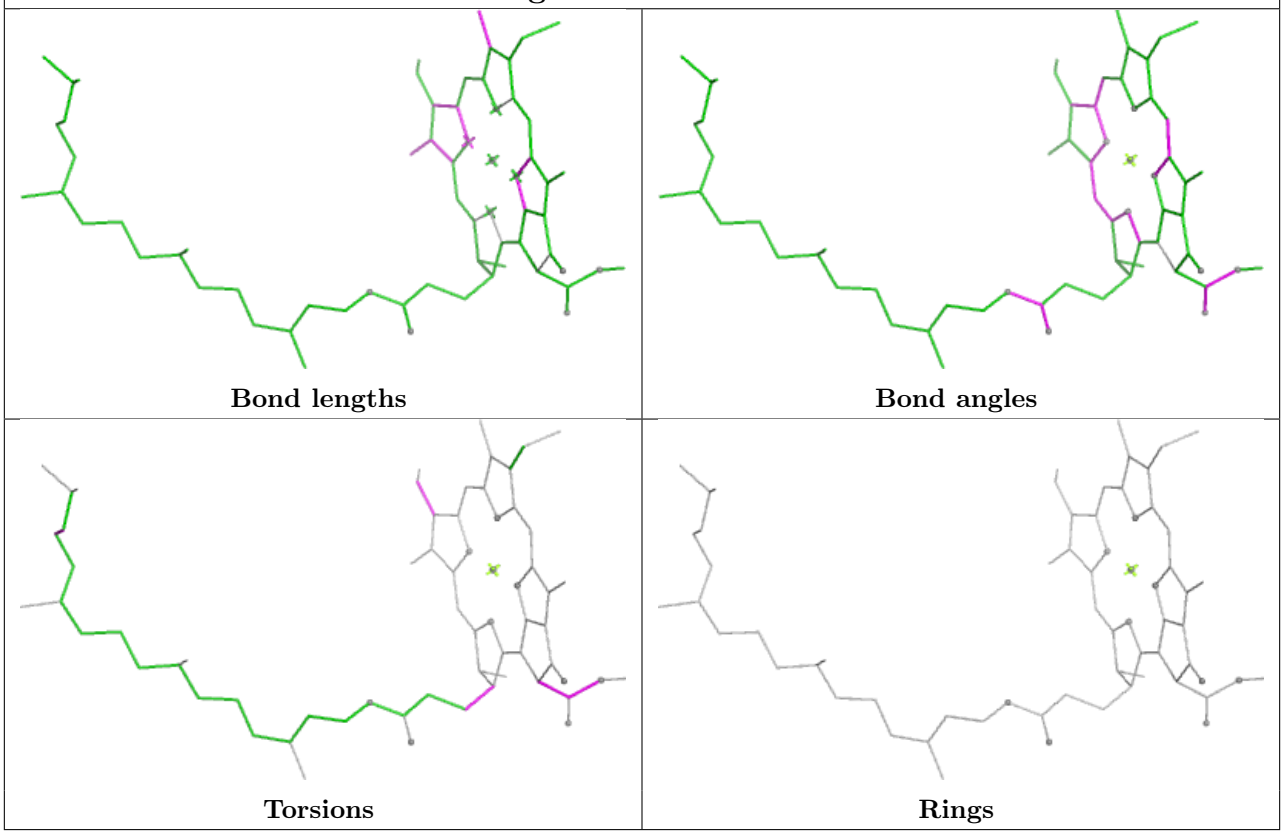


Rings

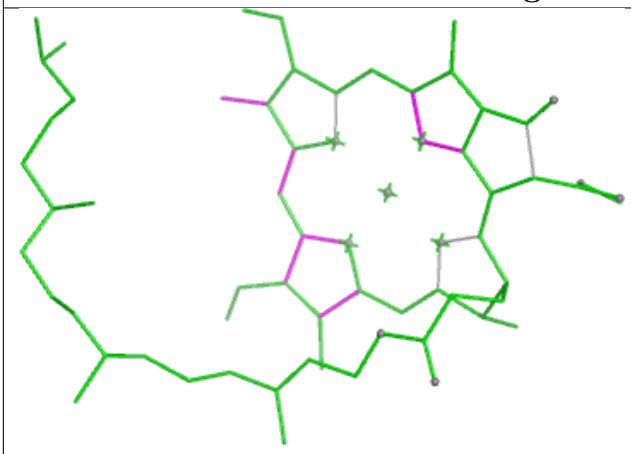
Ligand NEX R 305



Ligand CLA b 604



Ligand CLA N 307



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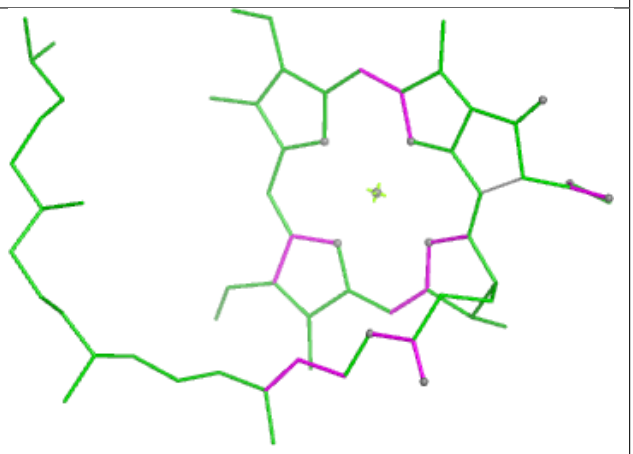
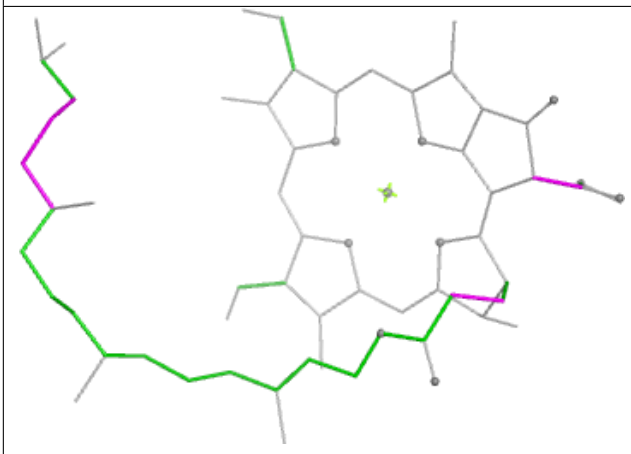


Bond angles



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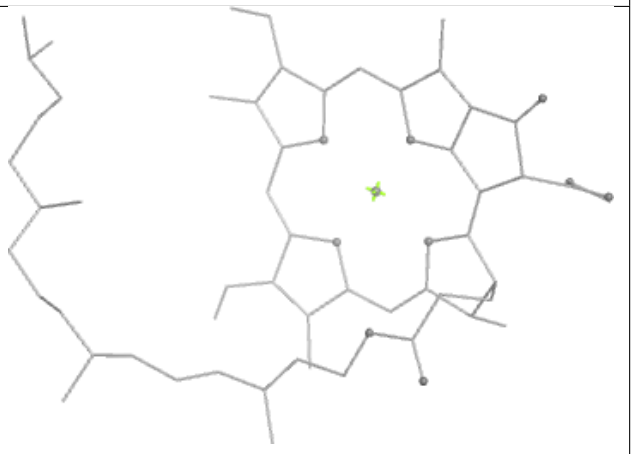
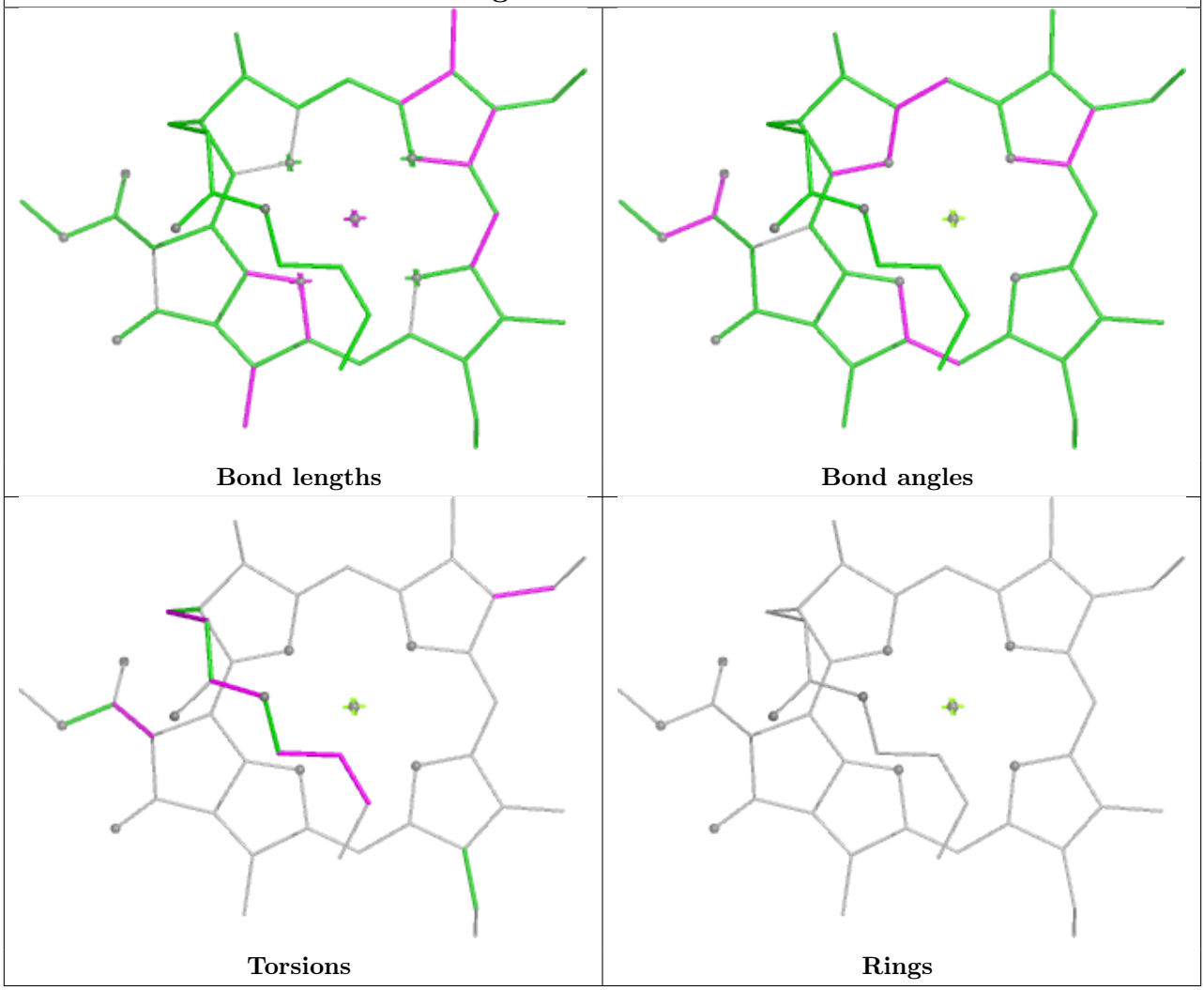
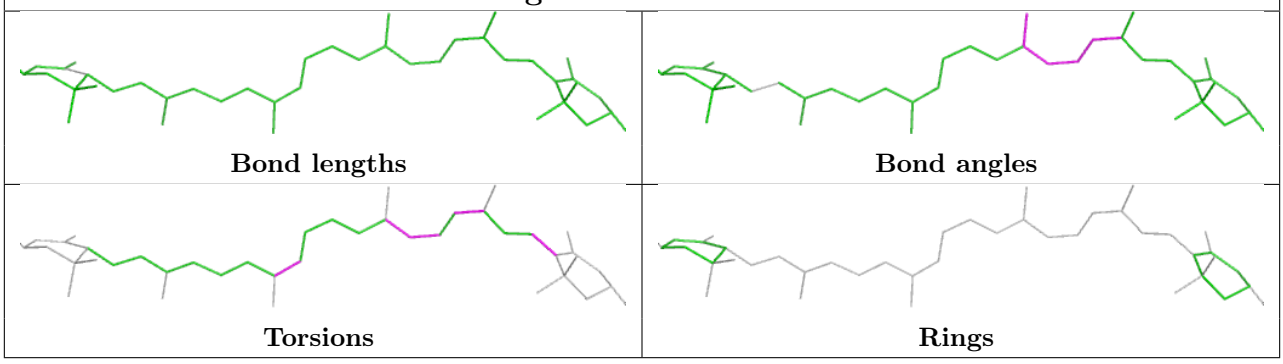


Rings

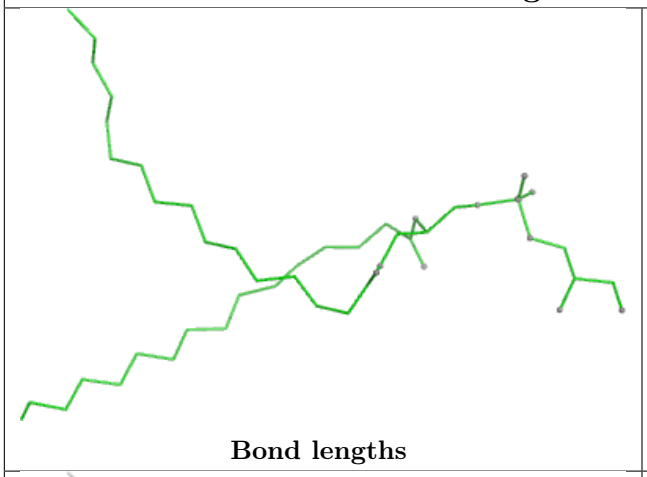
Ligand CLA N 318



Ligand LUT R 311



Ligand LHG D 408



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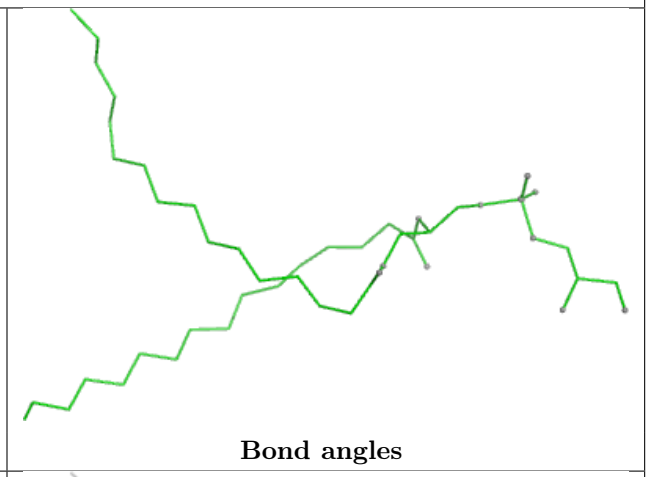
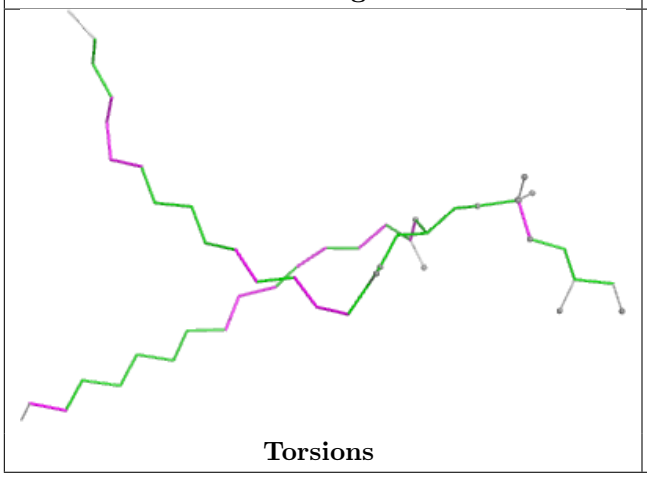
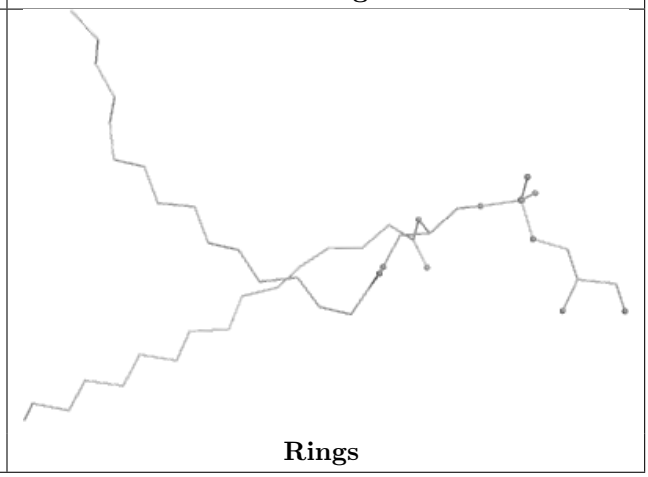


Bond angles

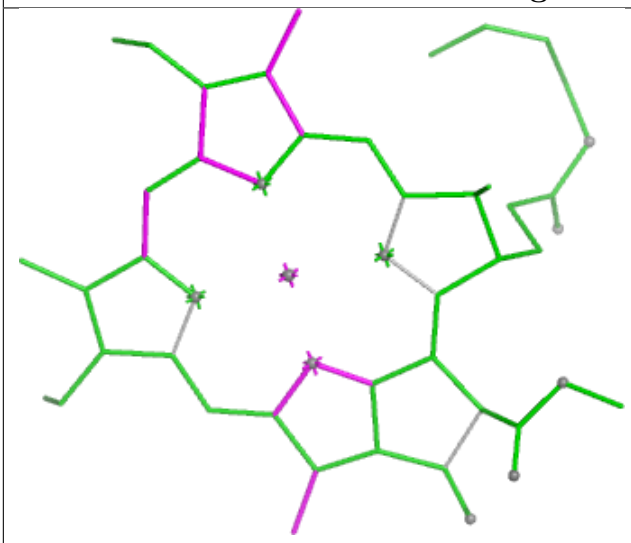


Torsions



Rings

Ligand CLA s 301



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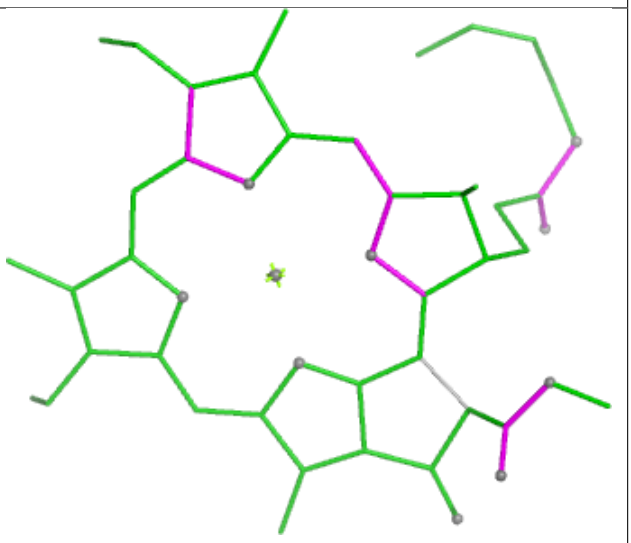
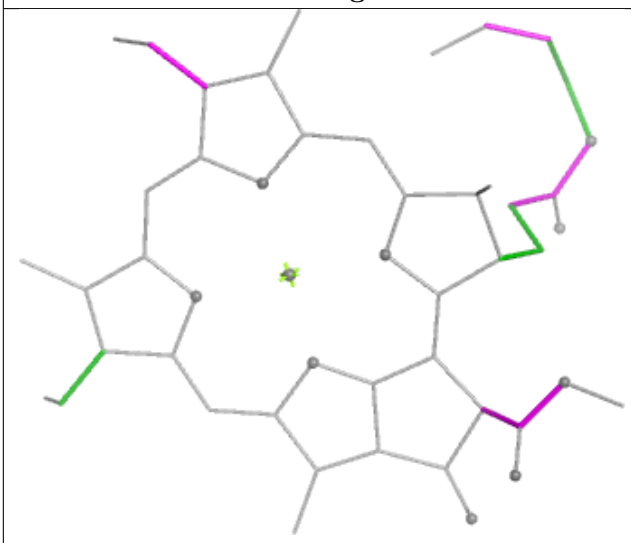
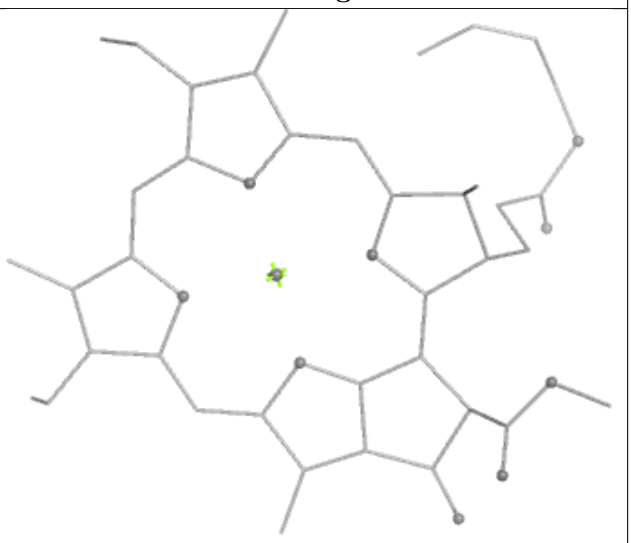


Bond angles

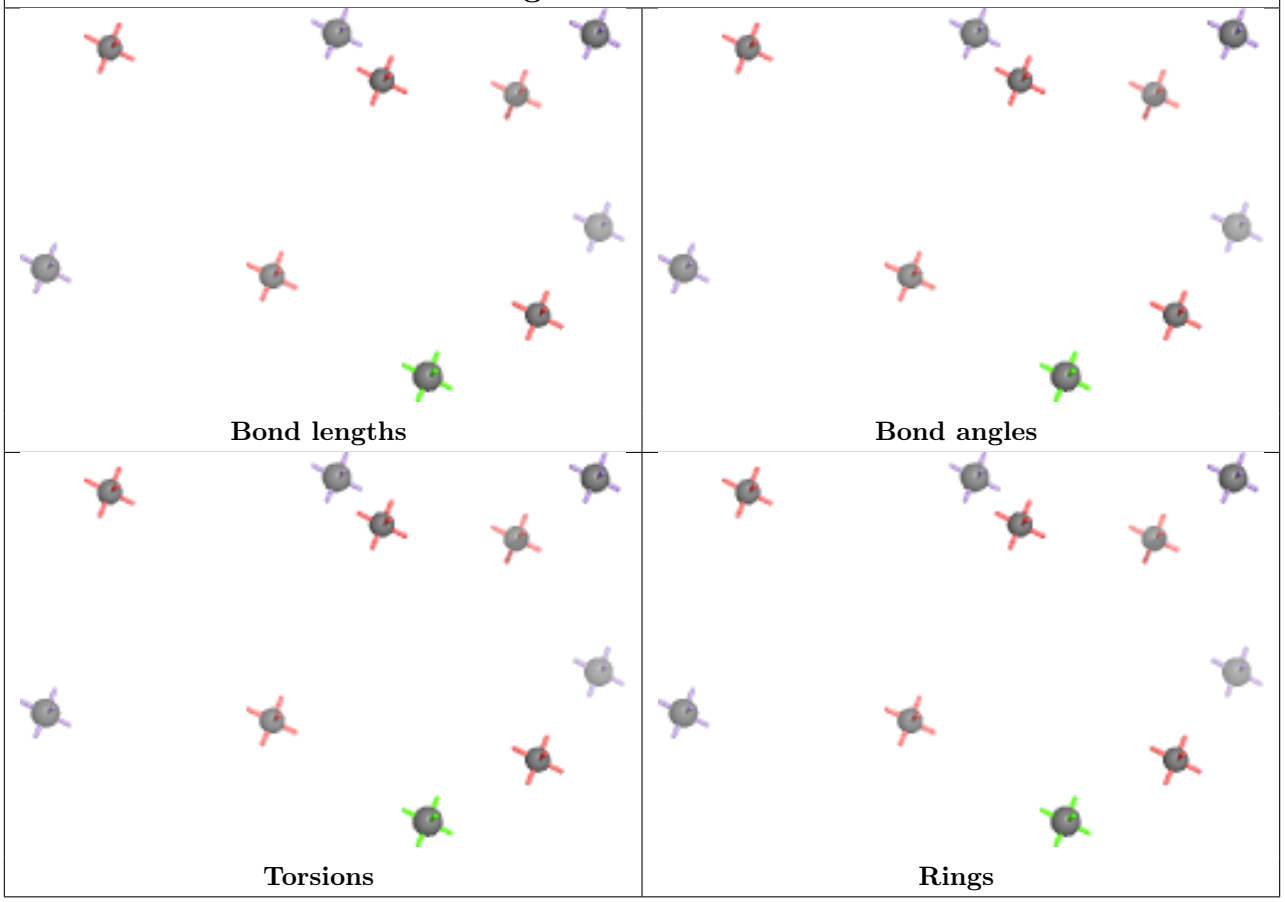


Torsions

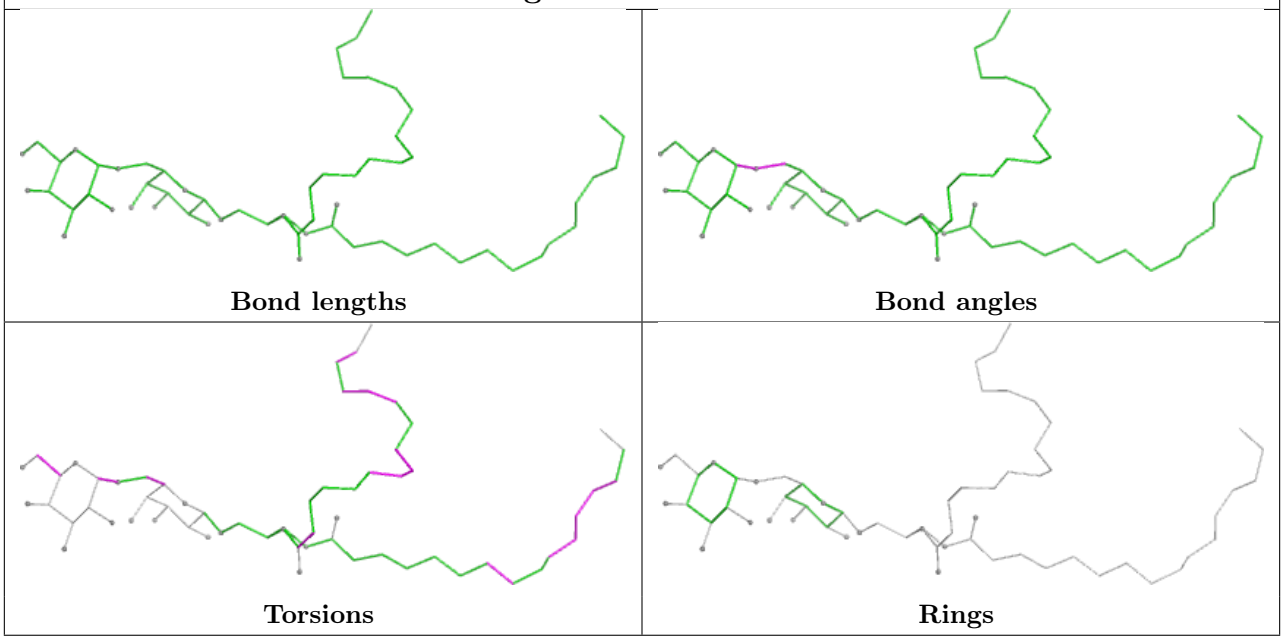


Rings

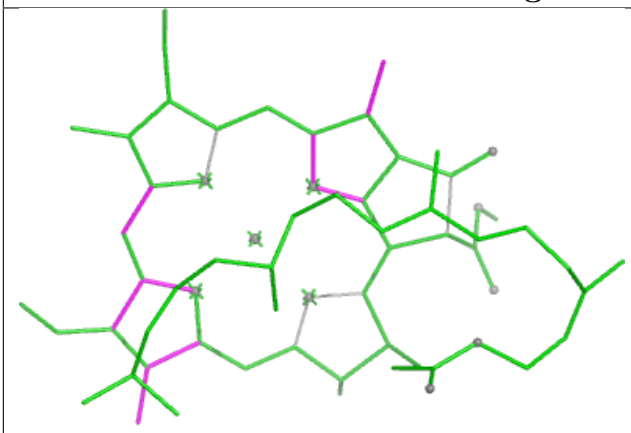
Ligand OEX C 501



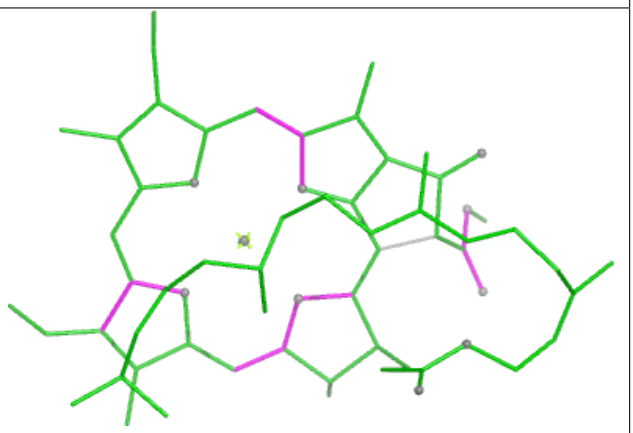
Ligand DGD b 620



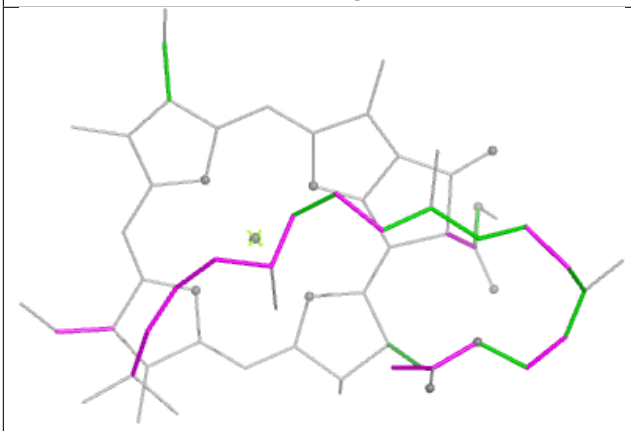
Ligand CLA B 605



Bond lengths



Bond angles



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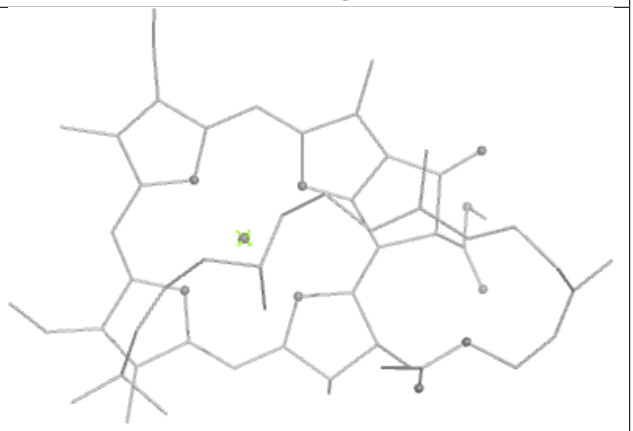
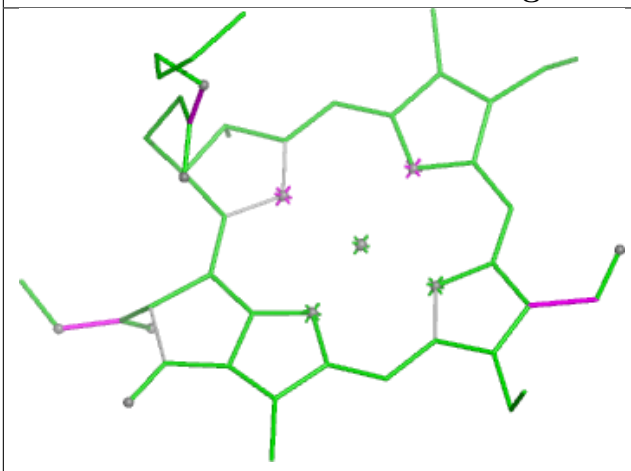
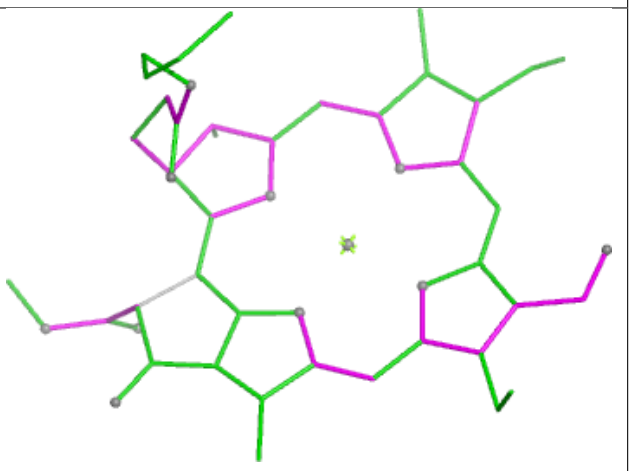


Rings

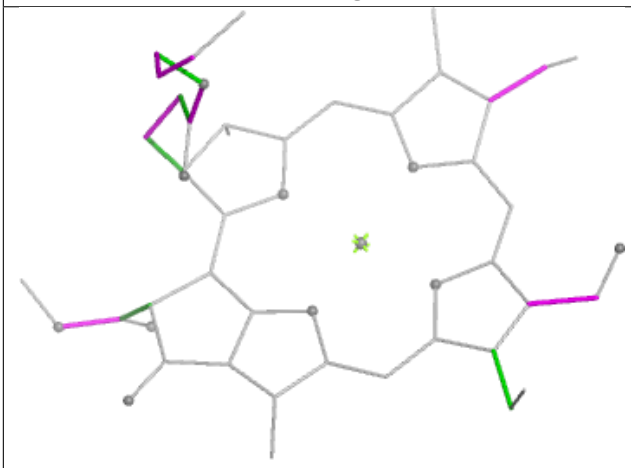
Ligand CHL N 311



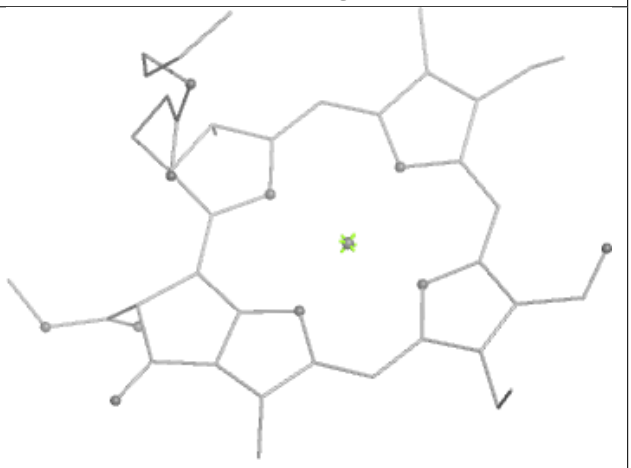
Bond lengths



Bond angles

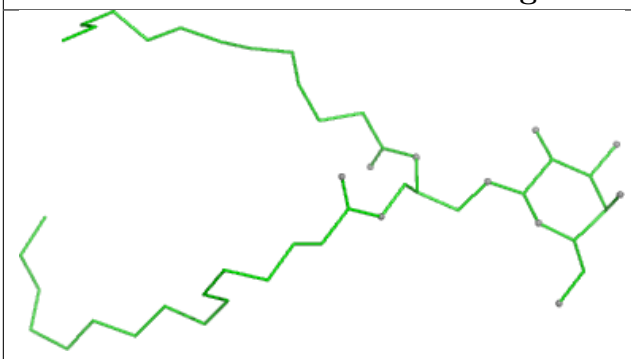


Torsions

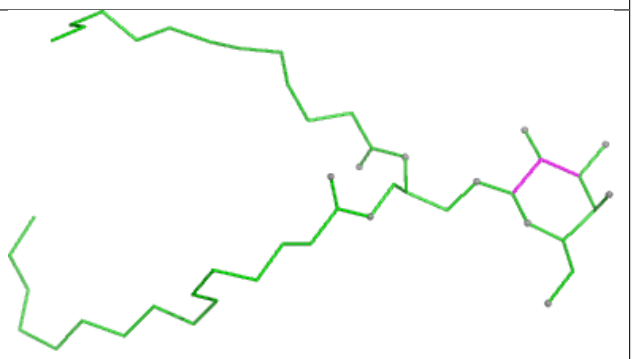


Rings

Ligand LMG w 201



Bond lengths



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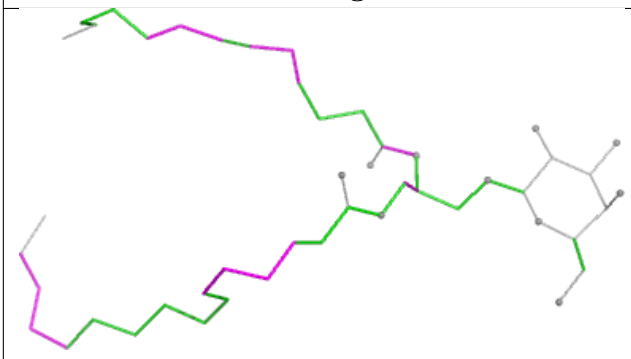

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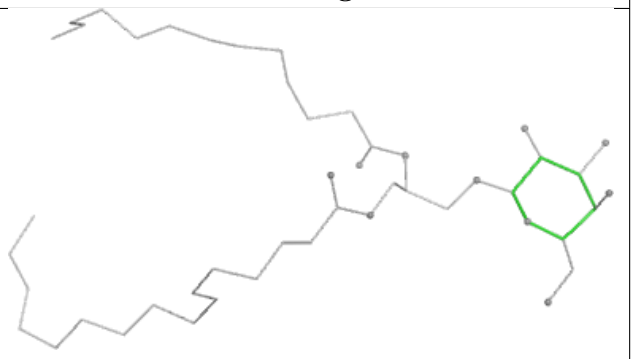
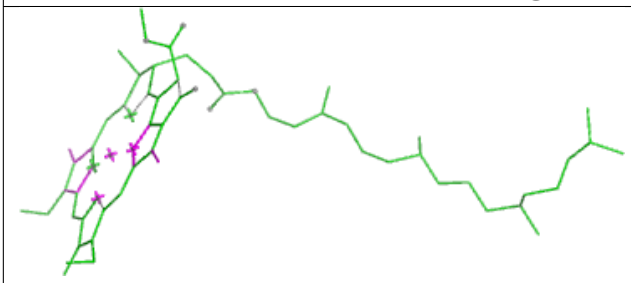
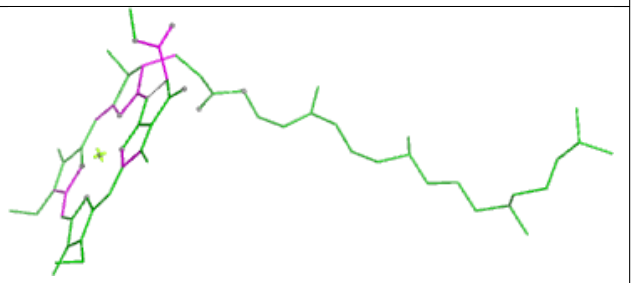


Rings

Ligand CLA b 611



Bond lengths



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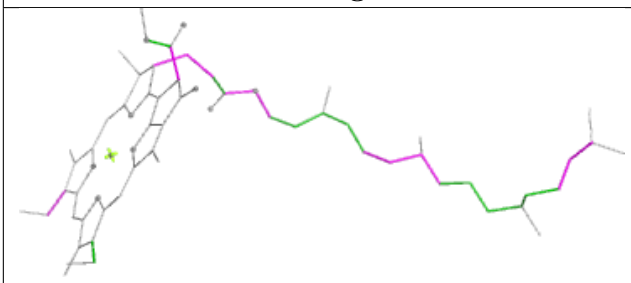

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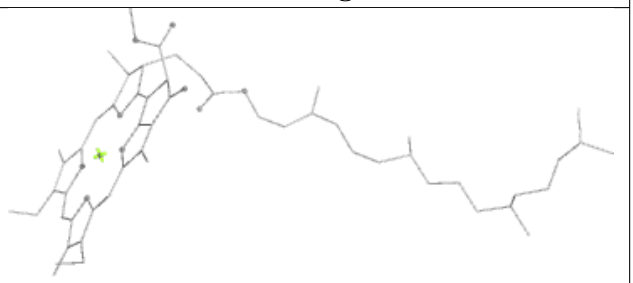
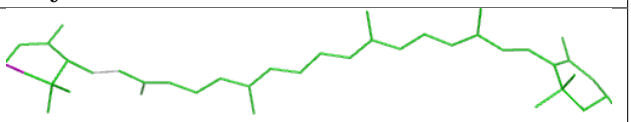
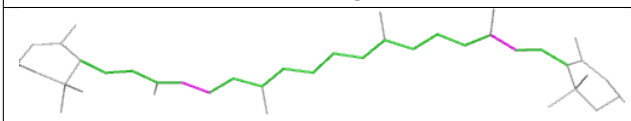
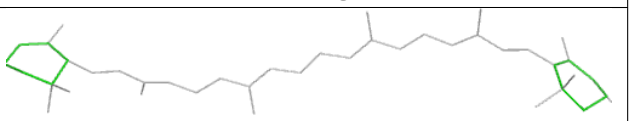
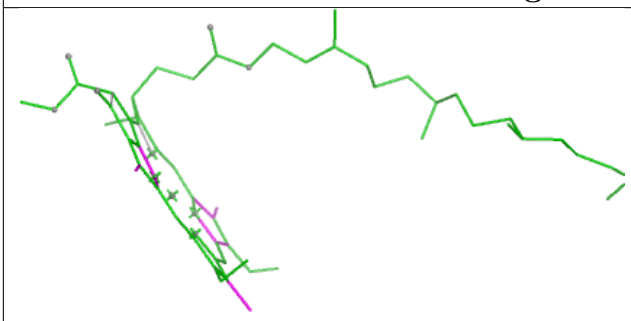
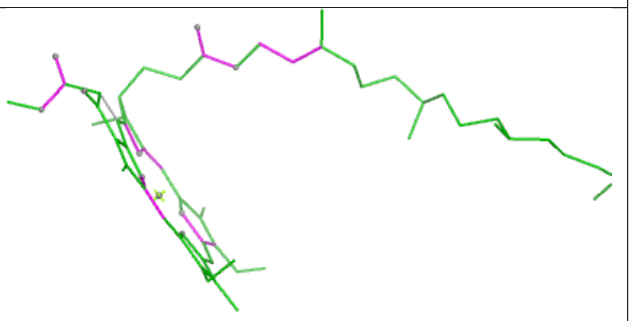
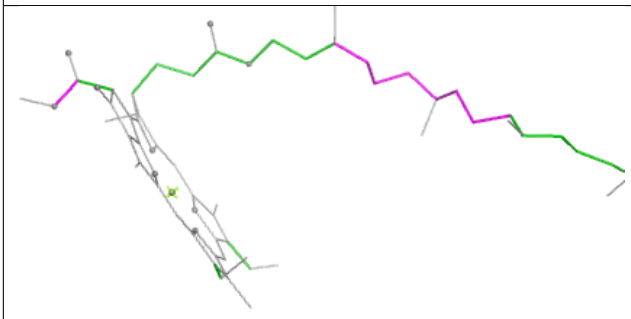
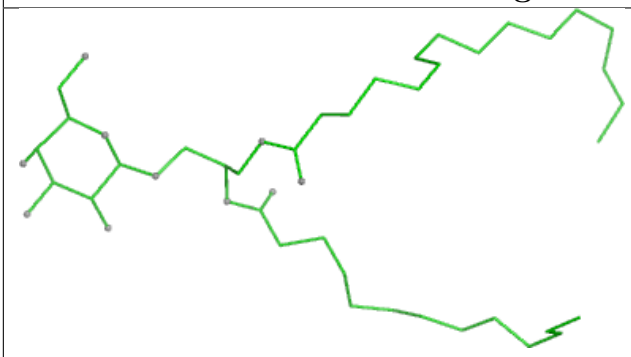


Rings

Ligand LUT y 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG W 201



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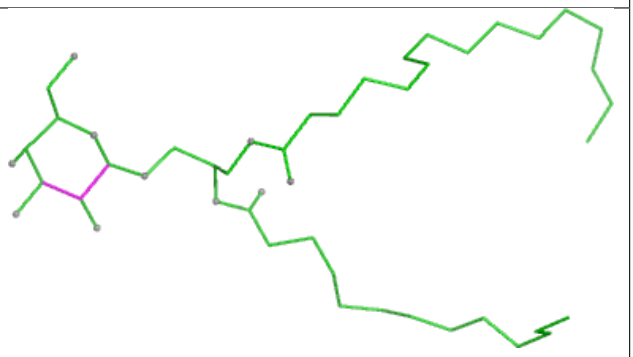

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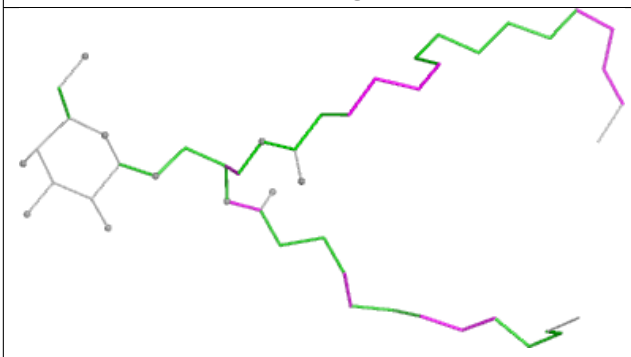

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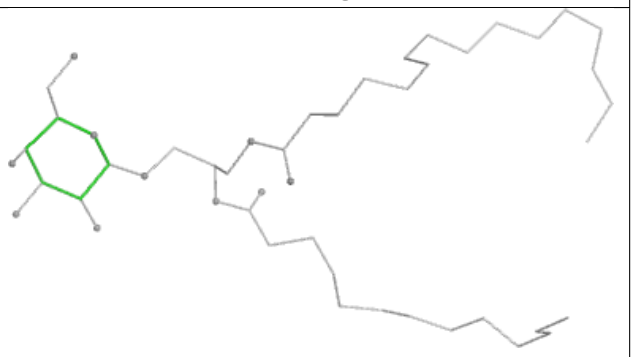
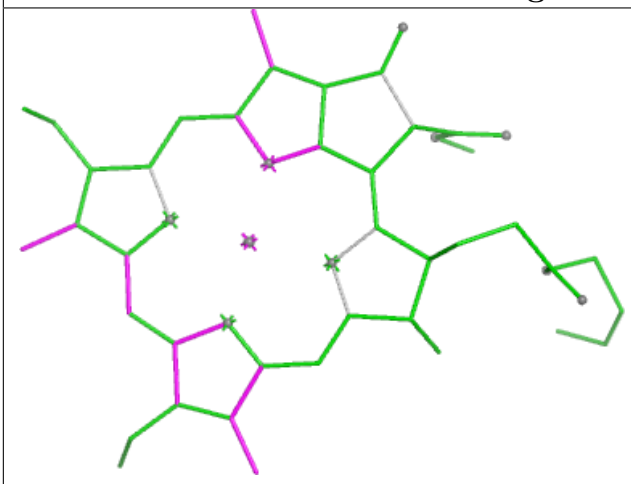


Rings

Ligand CLA n 315



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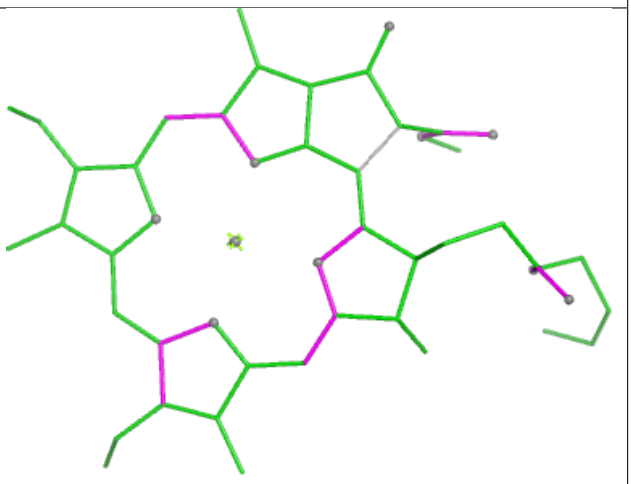
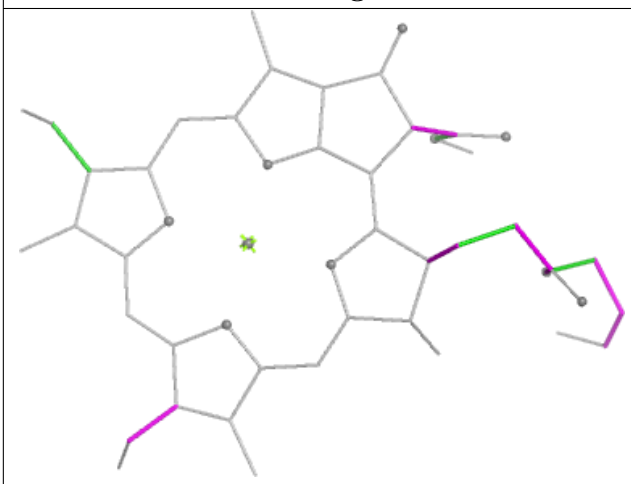


Bond angles



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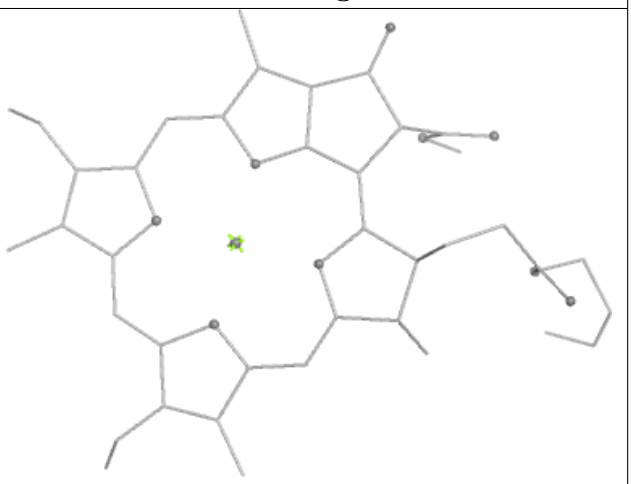
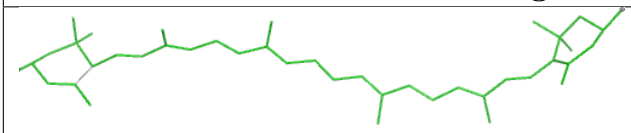


Rings

Ligand LUT s 312



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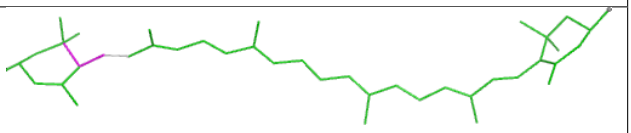
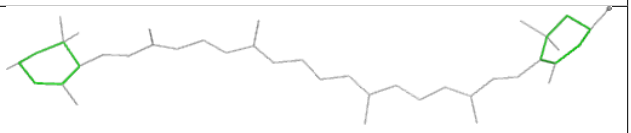


Bond angles

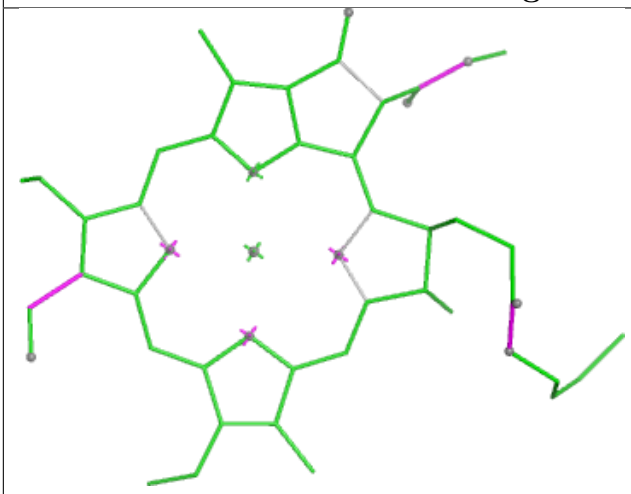


Torsions



Rings

Ligand CHL G 305



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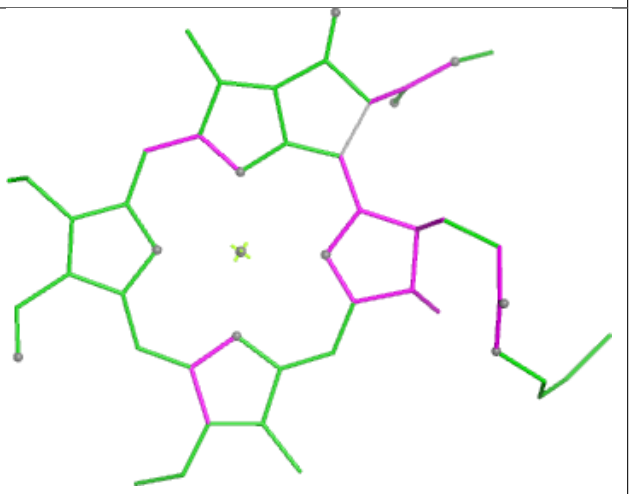

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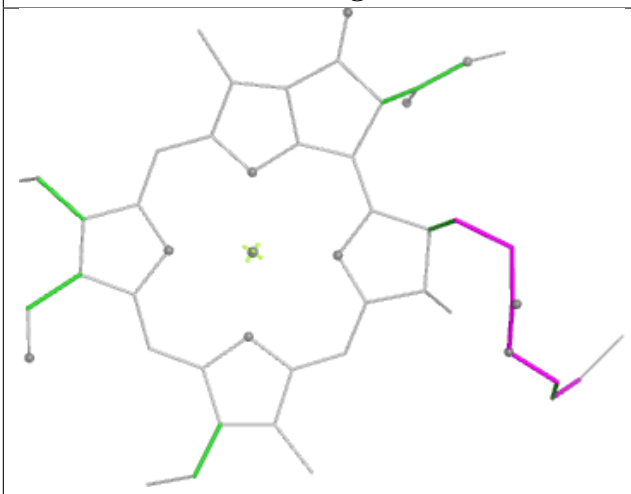

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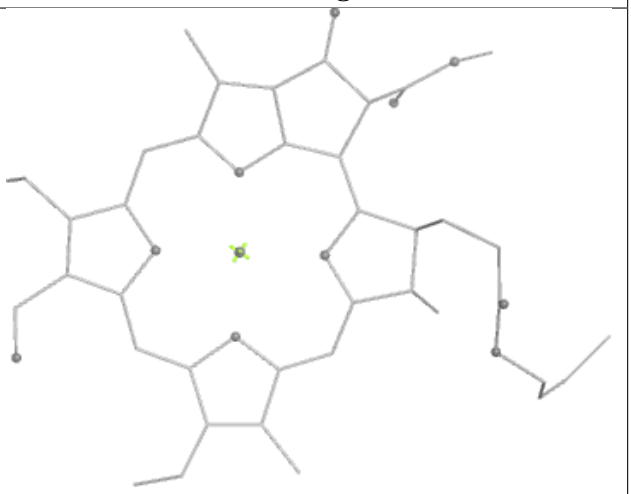
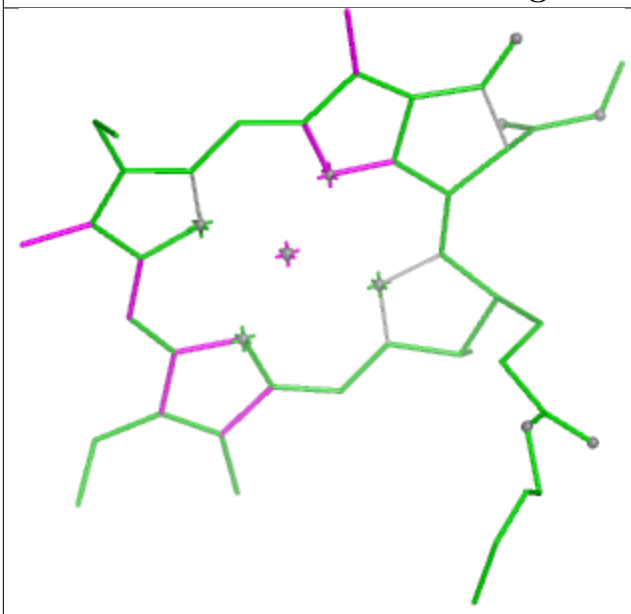


Rings

Ligand CLA c 510



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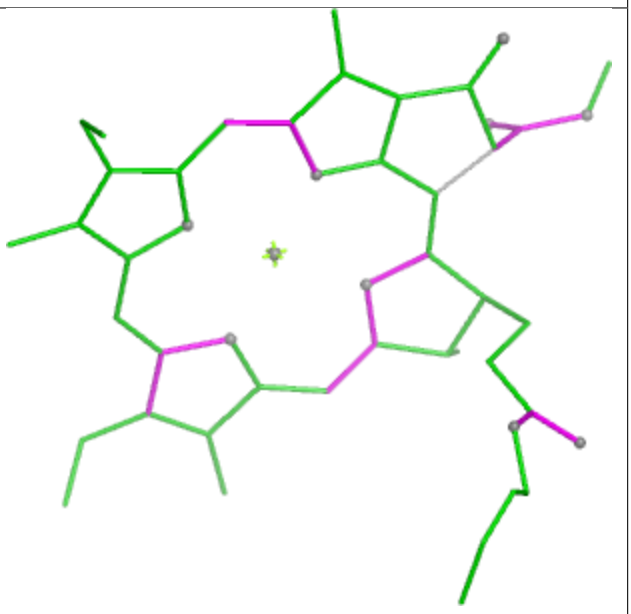
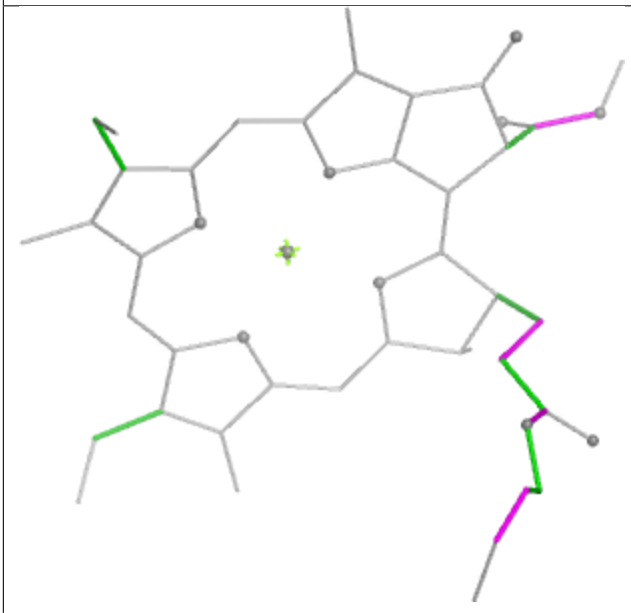


Bond angles



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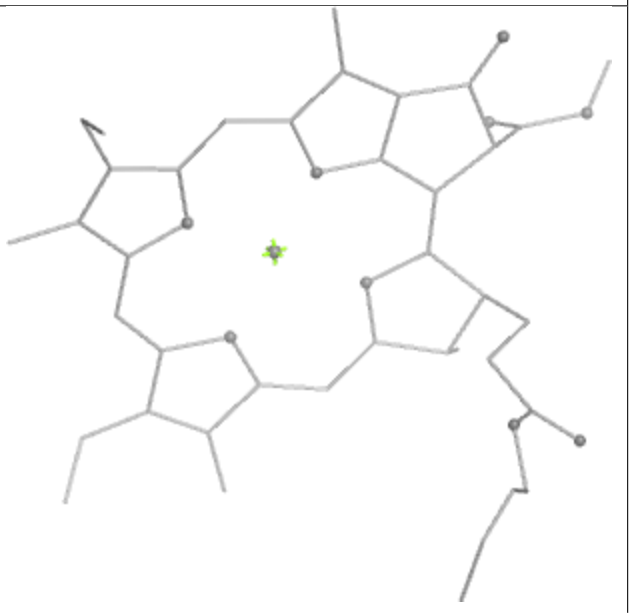


Rings

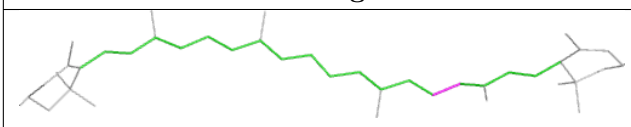
Ligand LUT G 308



Bond lengths



Bond angles



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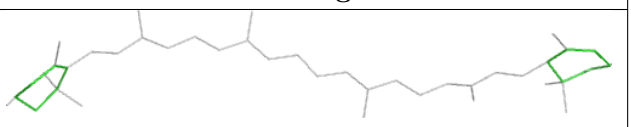
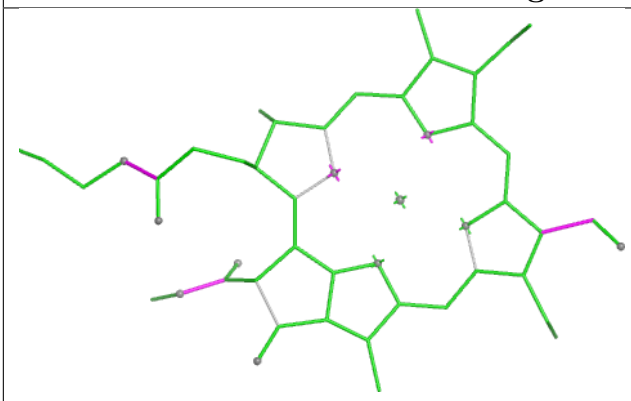
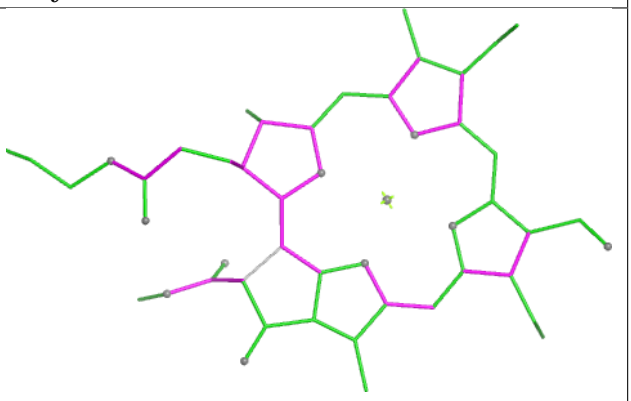


Rings

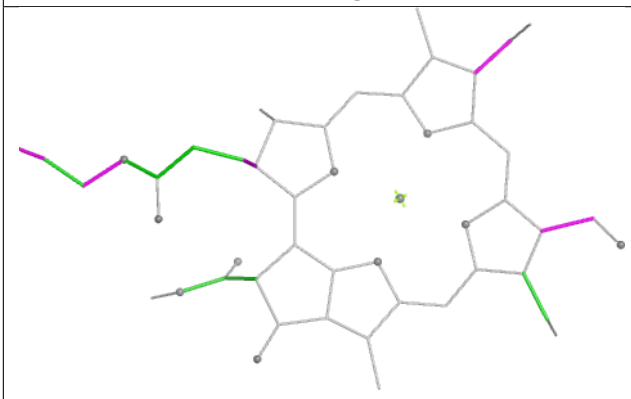
Ligand CHL y 305



Bond lengths



Bond angles



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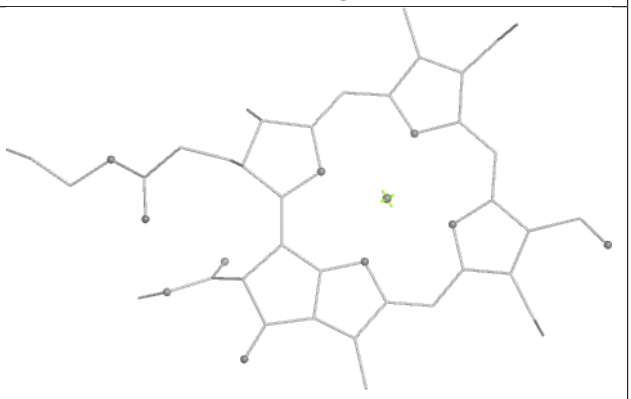
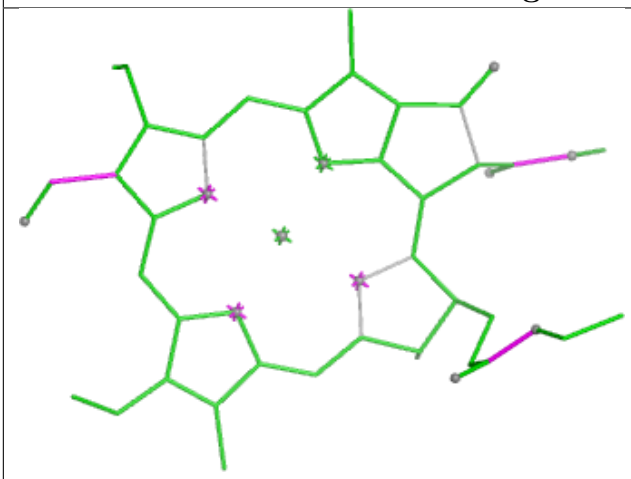


Rings

Ligand CHL N 310



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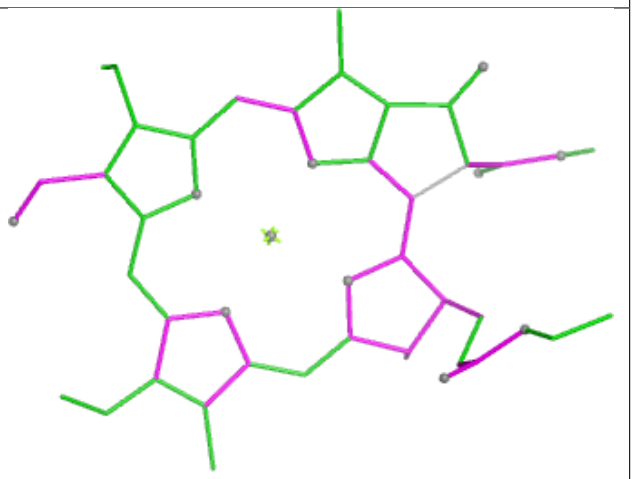

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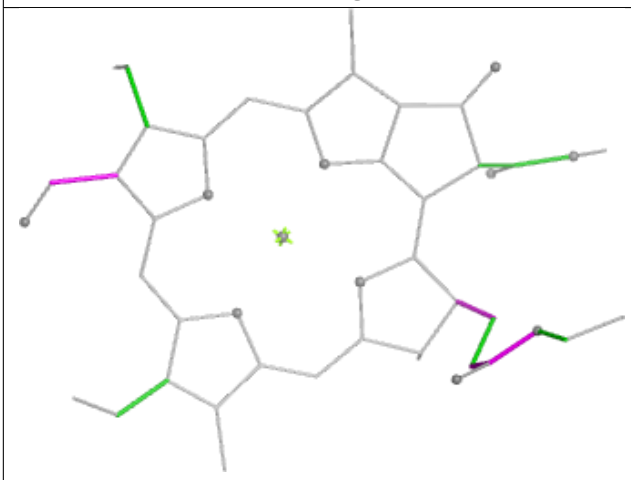

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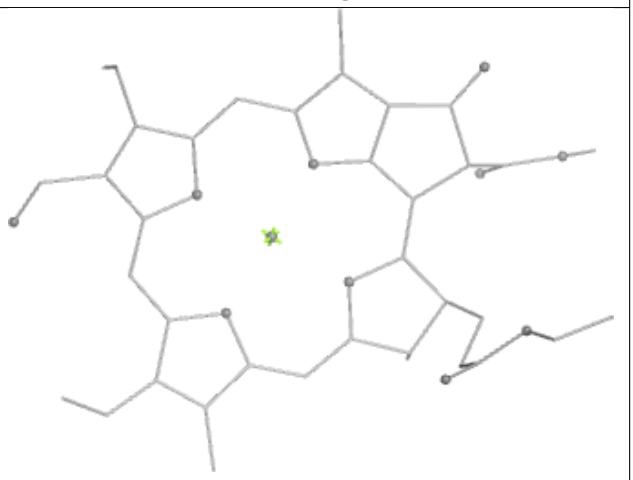
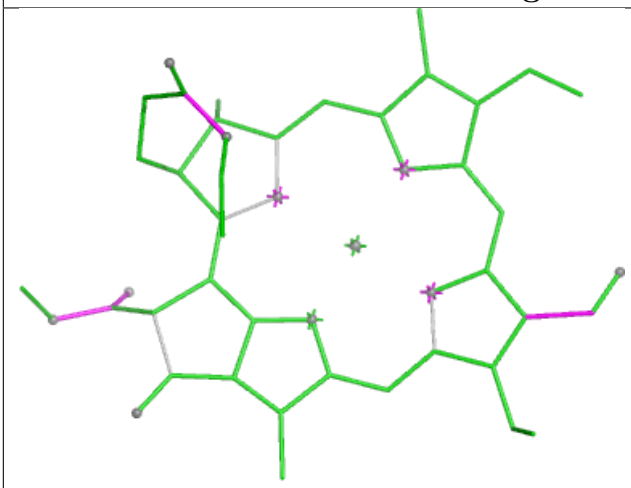


Rings

Ligand CHL G 309



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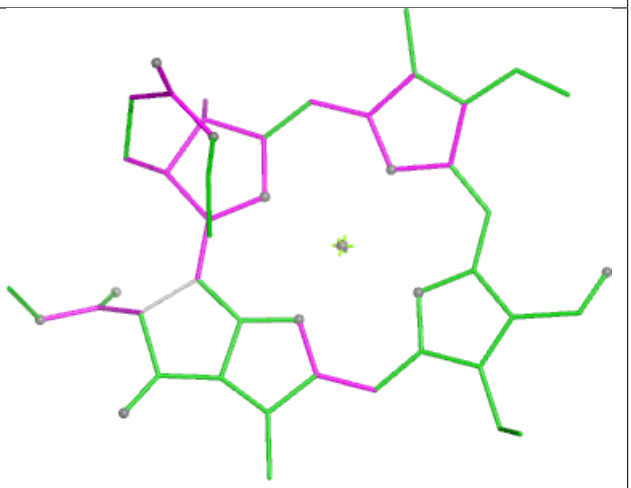
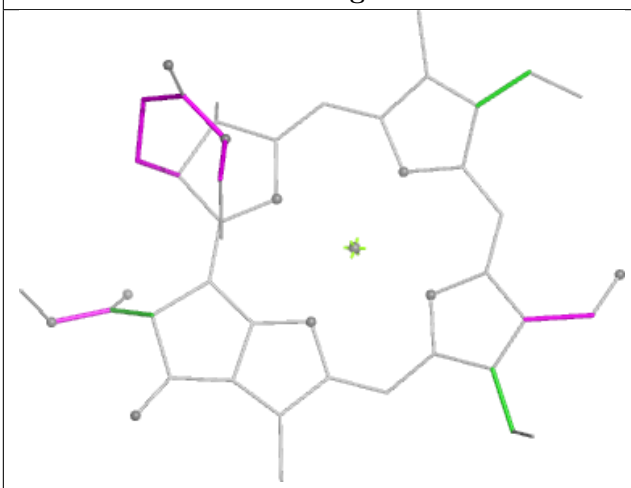


Bond angles



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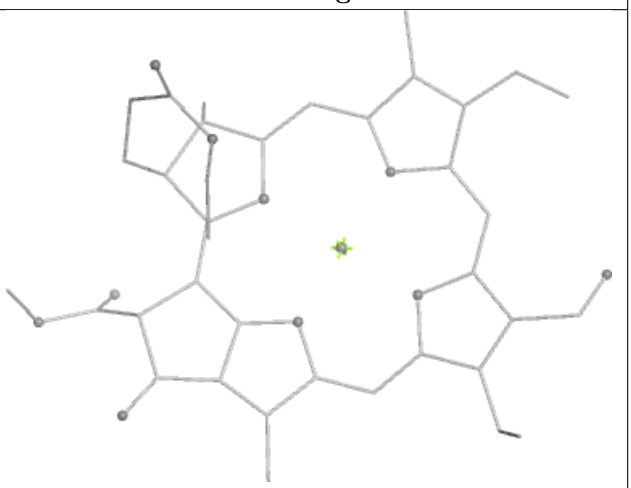
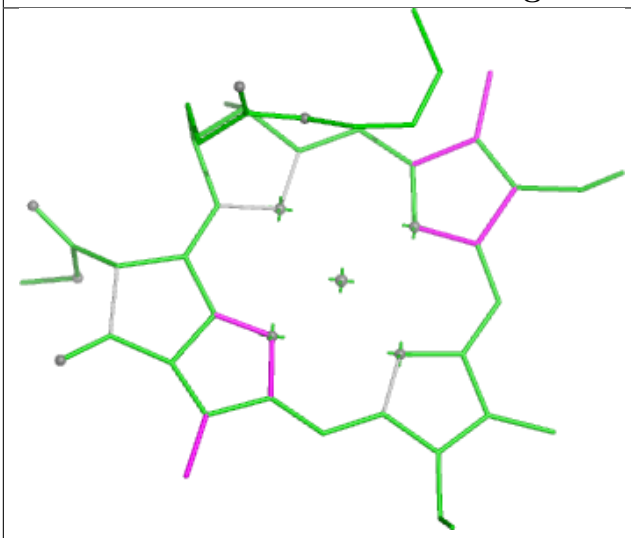


Rings

Ligand CLA Y 310



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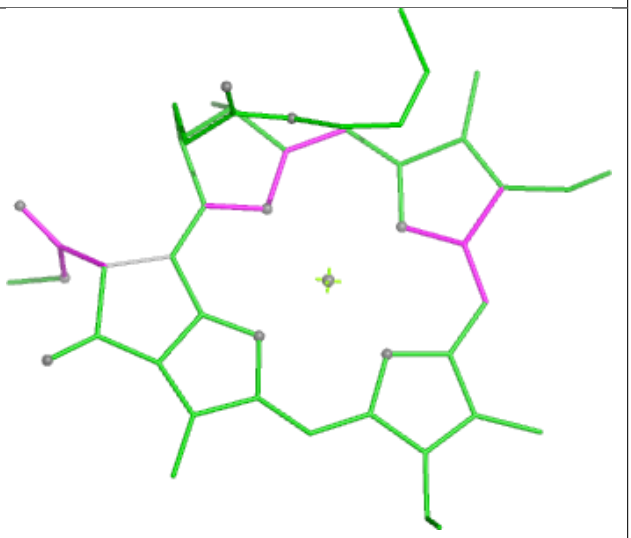
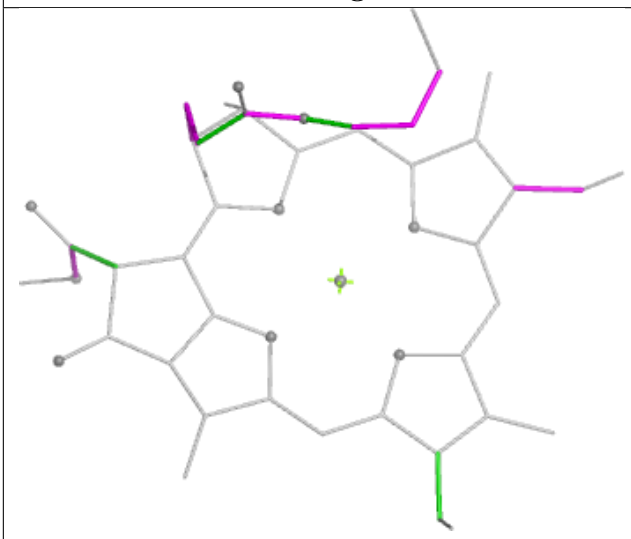


Bond angles



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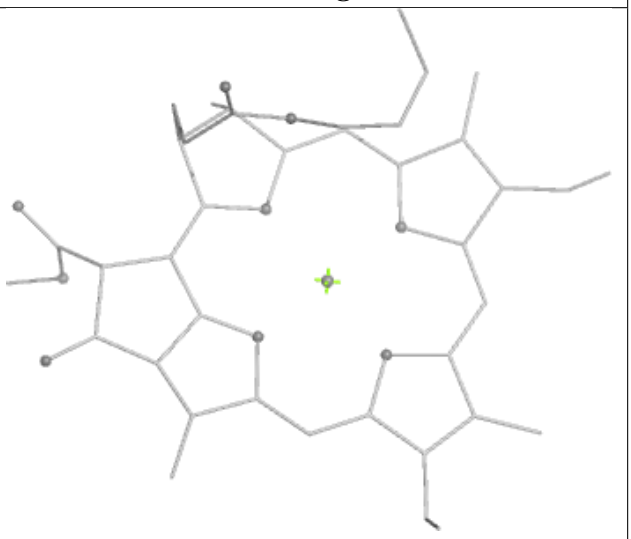

Rings

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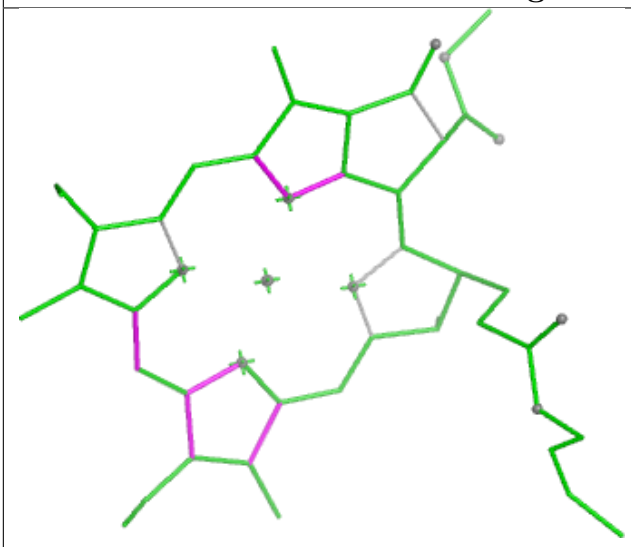

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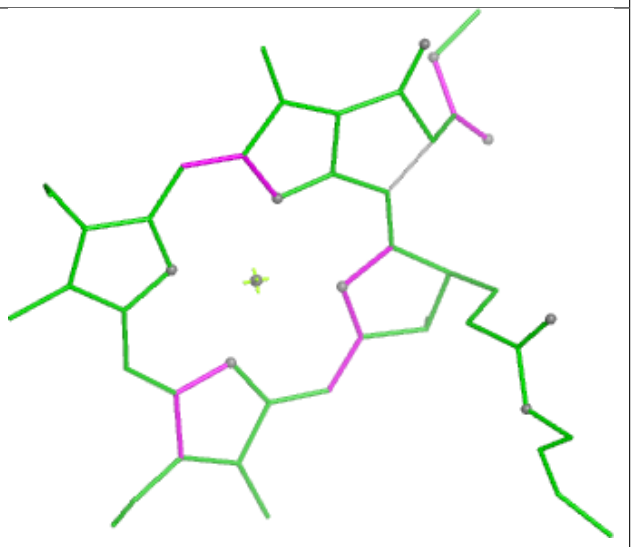
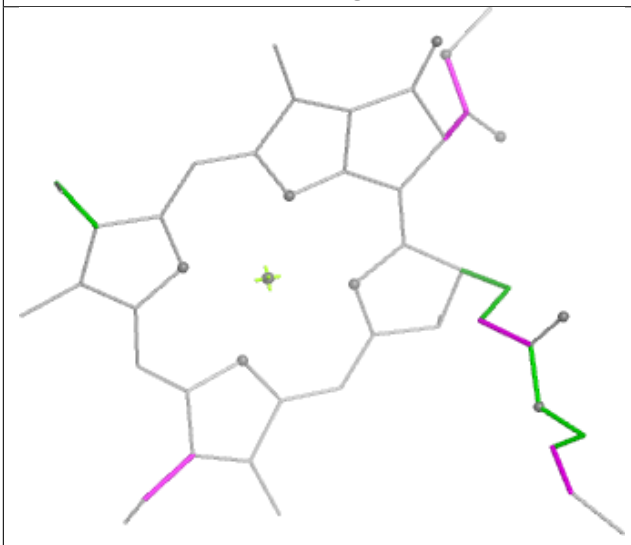


Bond angles



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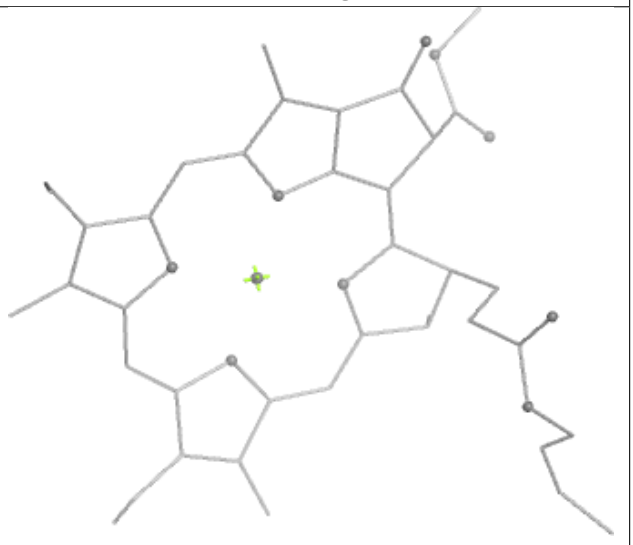
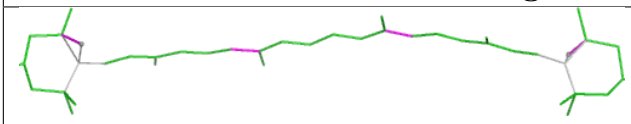
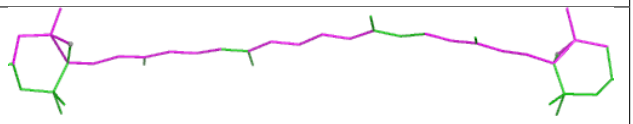


Rings

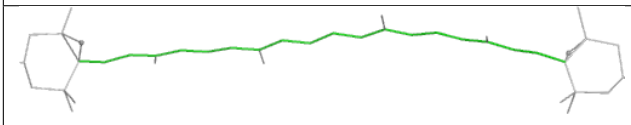
Ligand XAT N 315



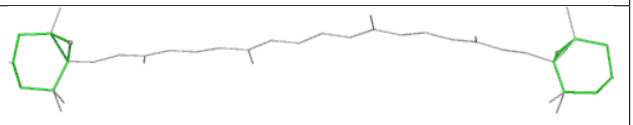
Bond lengths



Bond angles

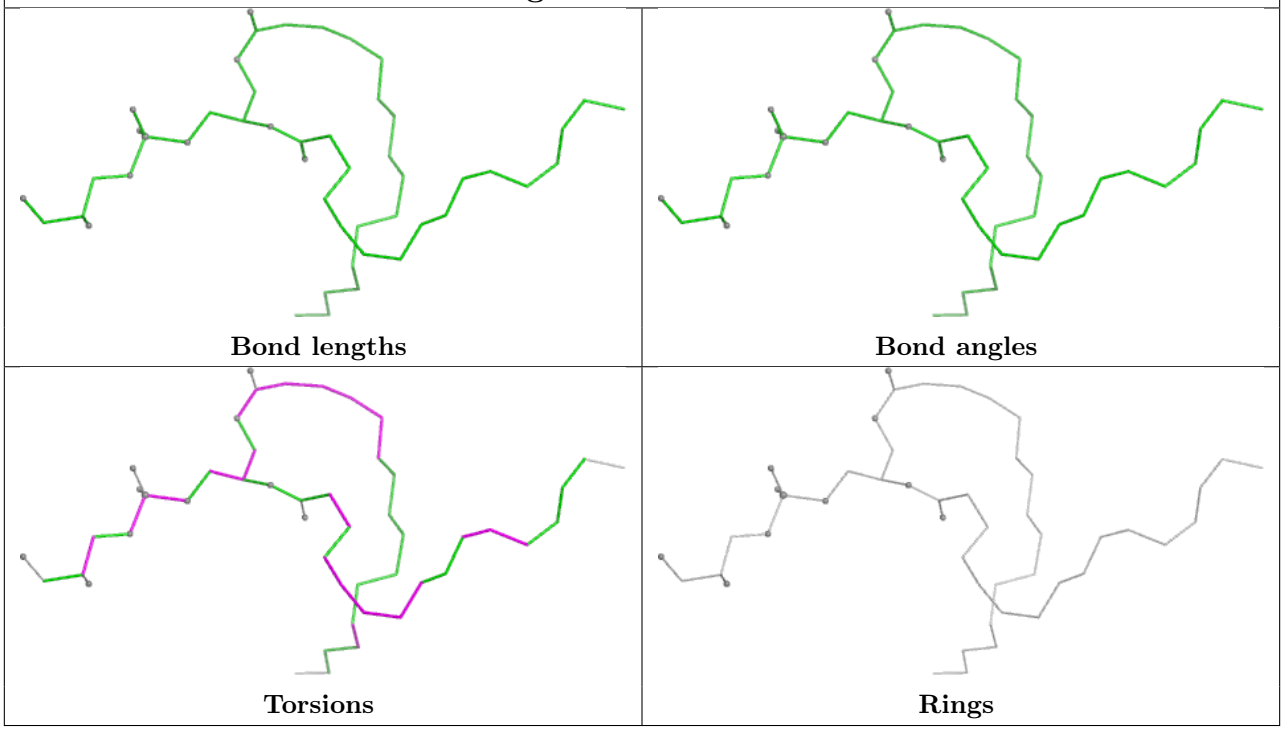


Torsions

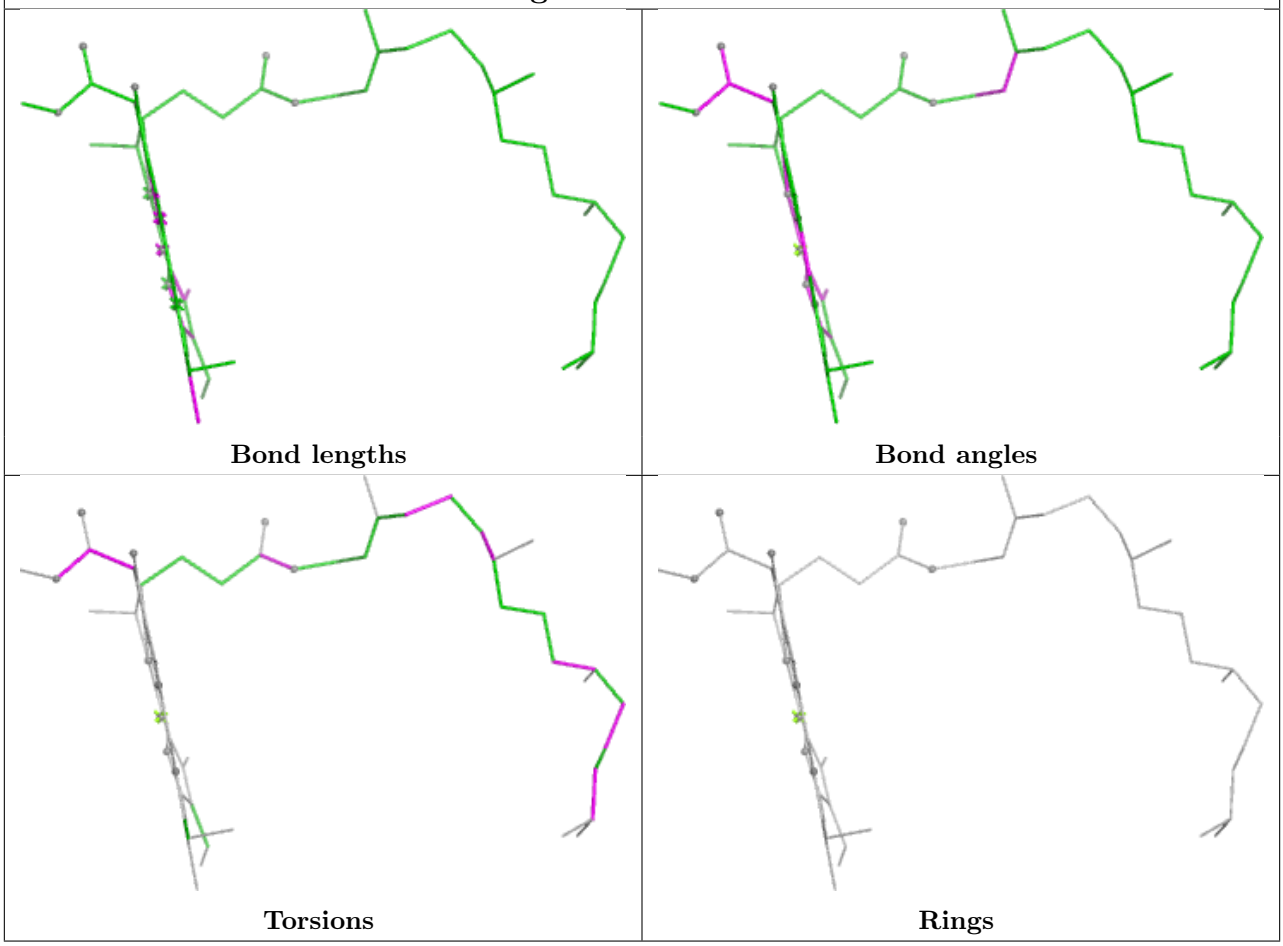


Rings

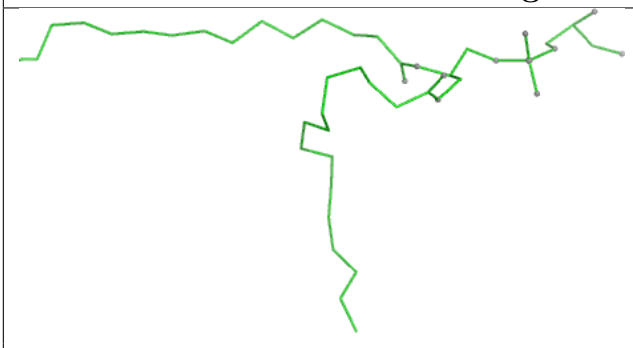
Ligand LHG S 317



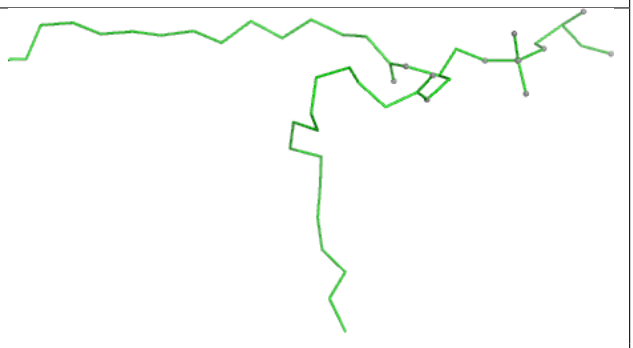
Ligand CLA c 516



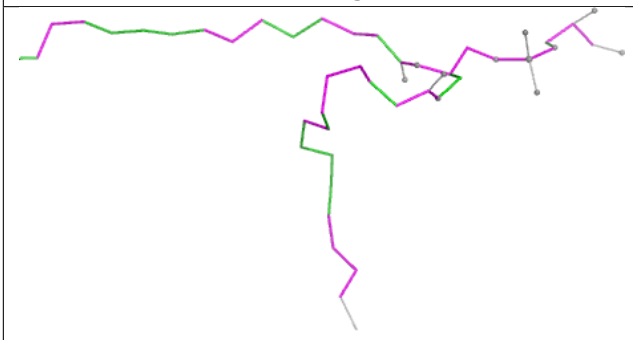
Ligand LHG Y 306



Bond lengths



Bond angles

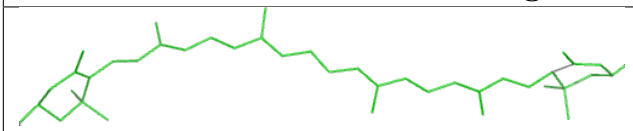


Torsions



Rings

Ligand LUT N 314



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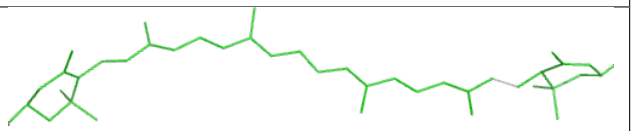
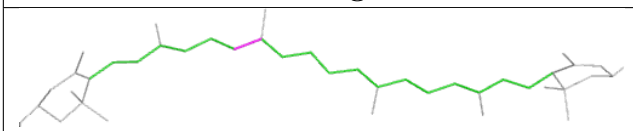
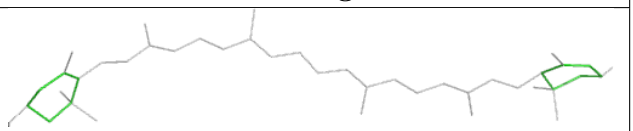


Bond angles

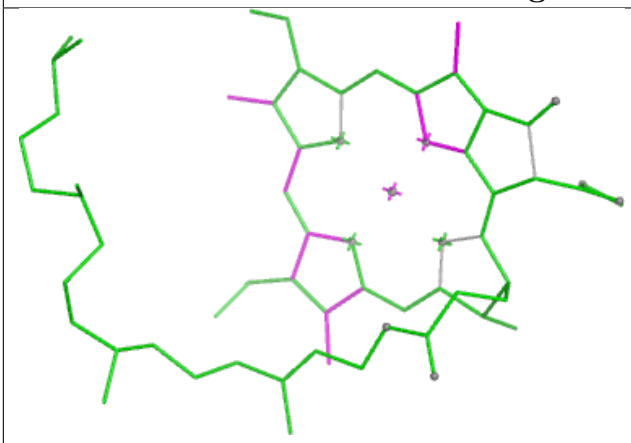


Torsions

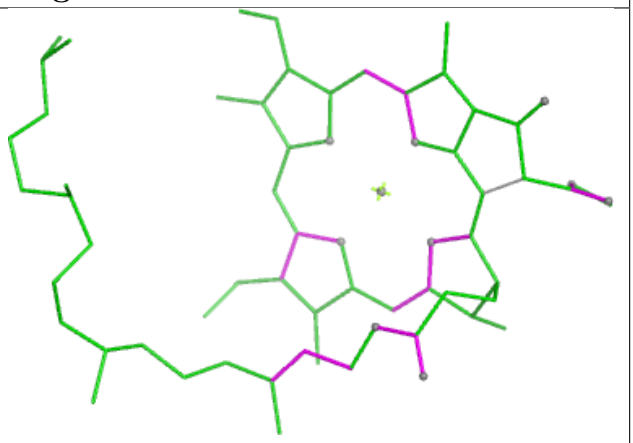


Rings

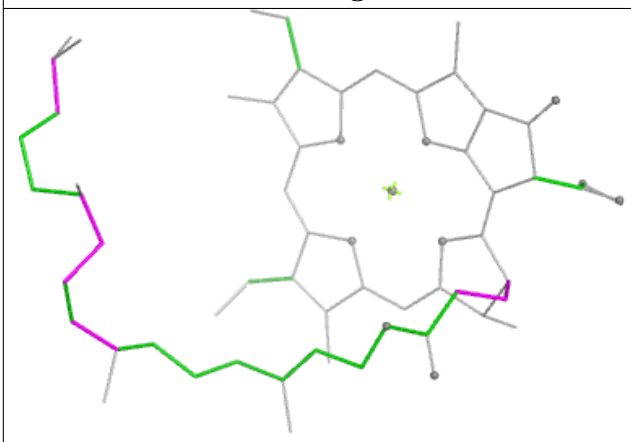
Ligand CLA g 303



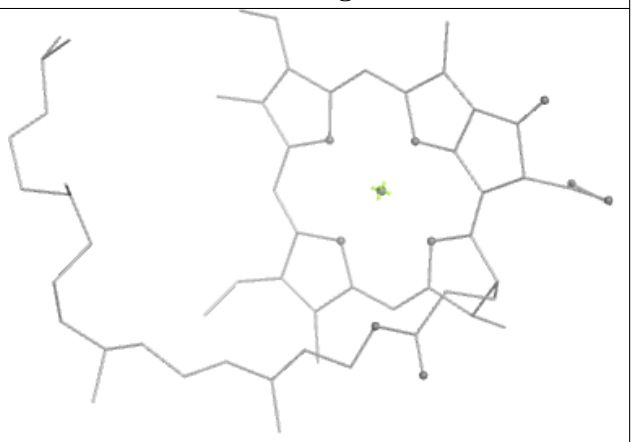
Bond lengths



Bond angles

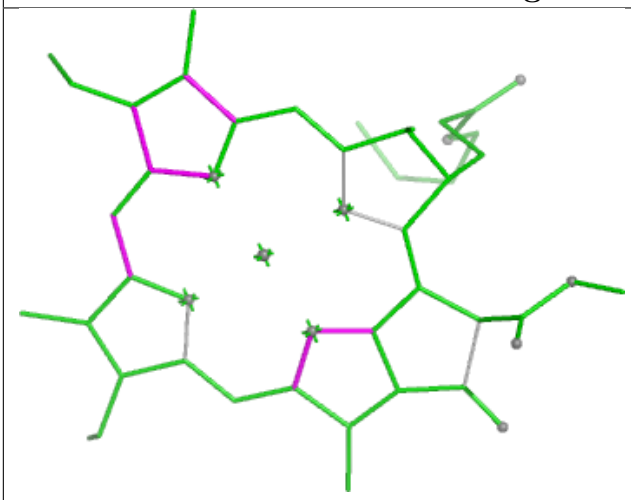


Torsions

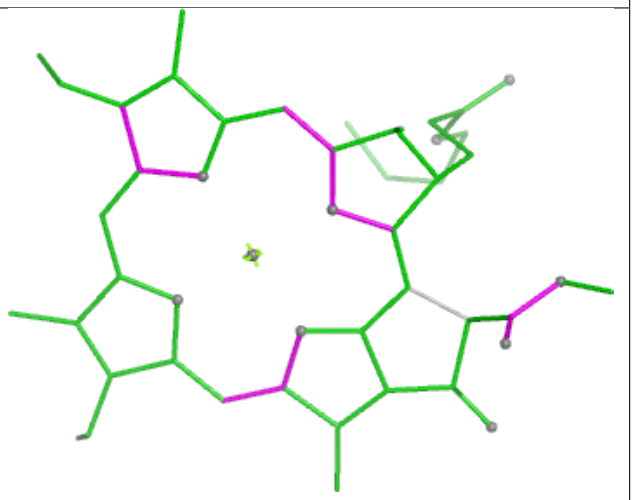


Rings

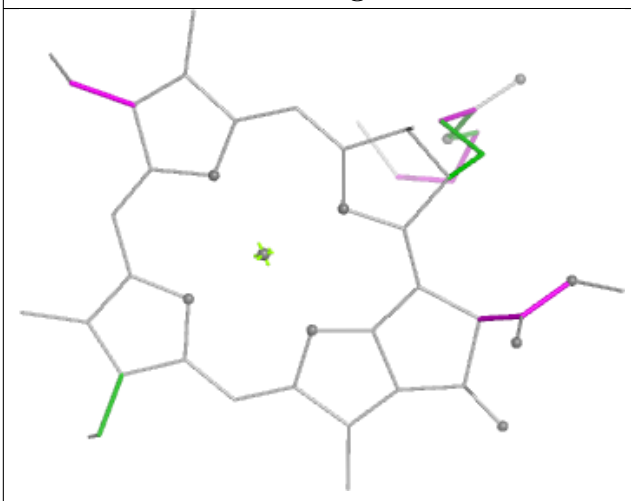
Ligand CLA R 310



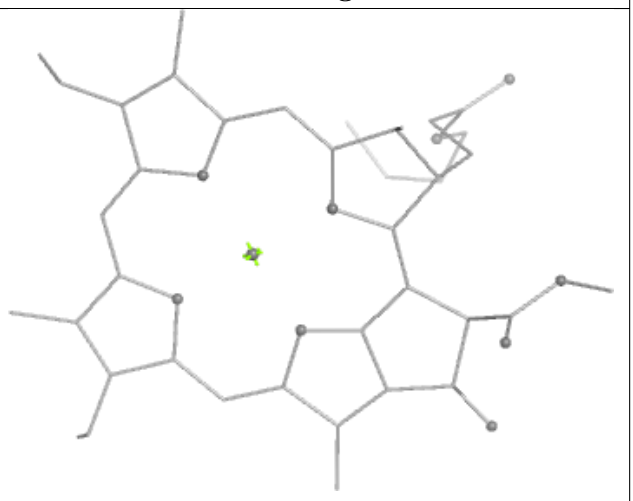
Bond lengths



Bond angles

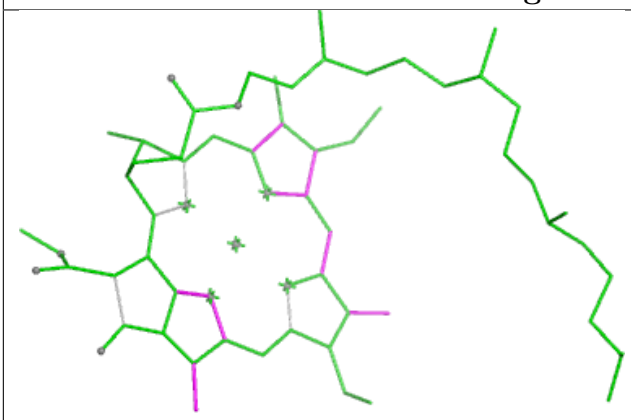


Torsions



Rings

Ligand CLA R 313



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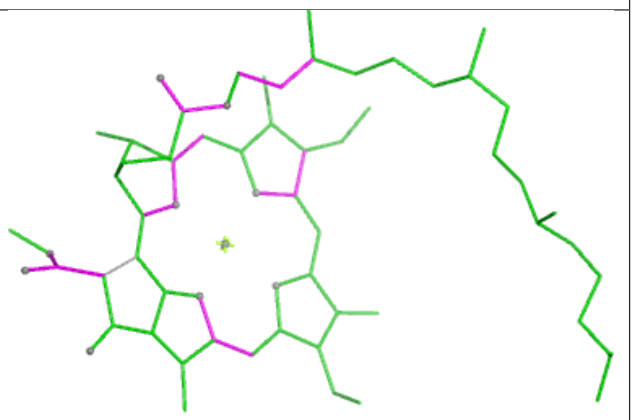
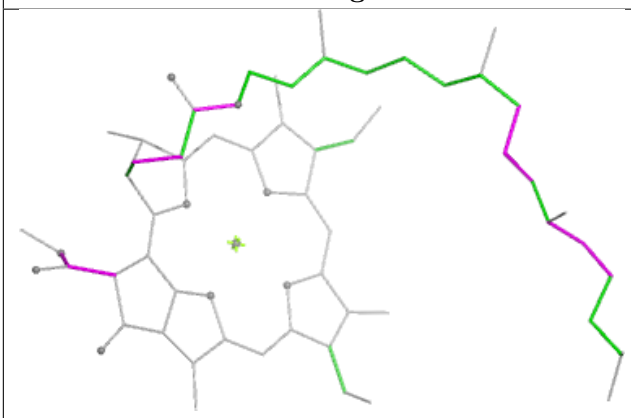
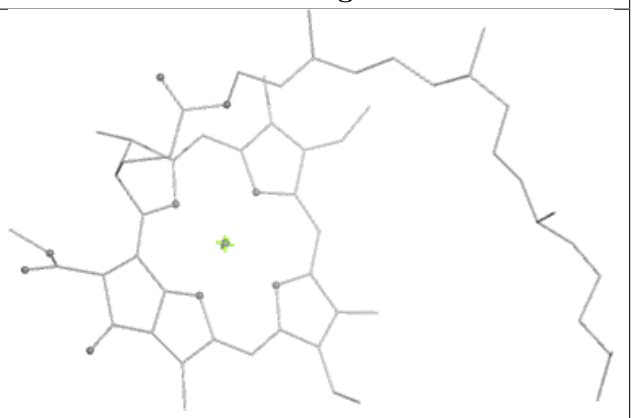


Bond angles

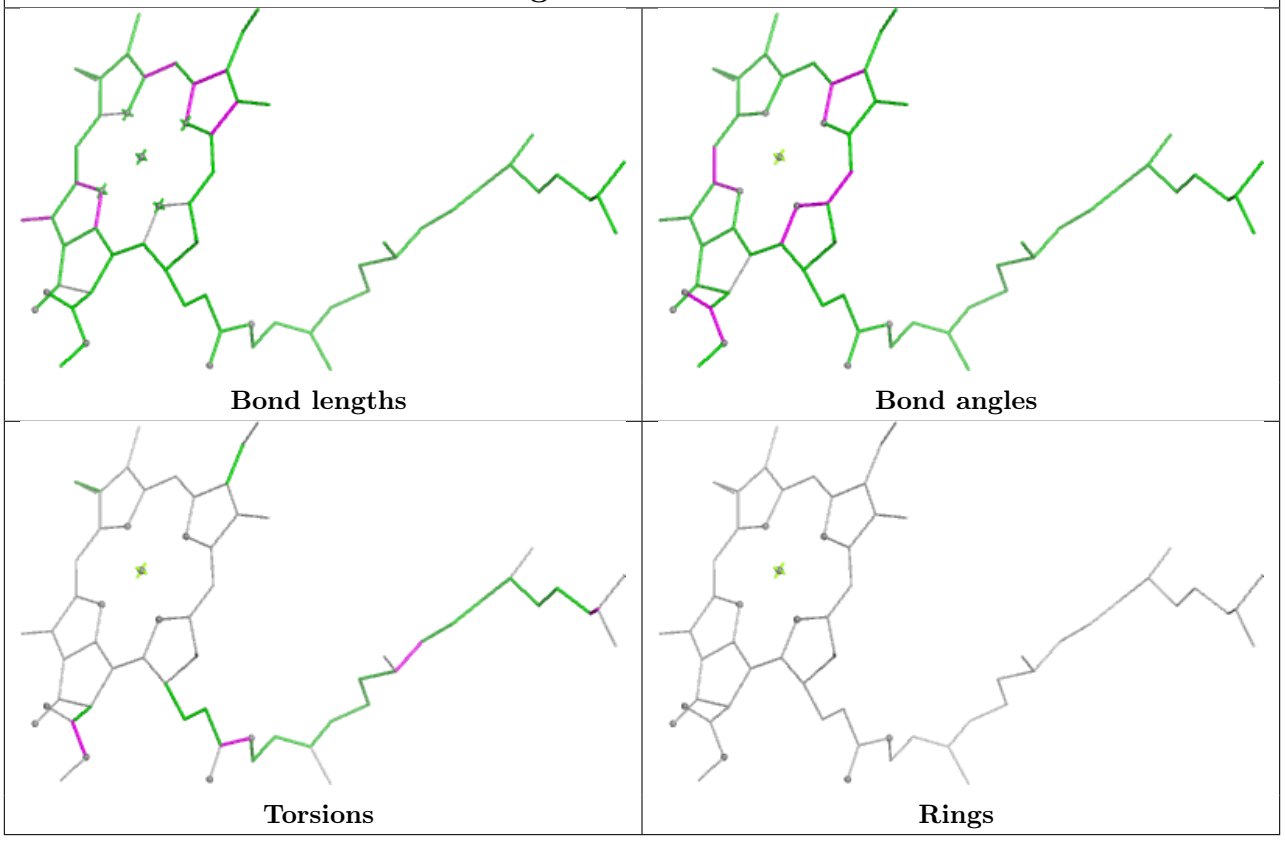


Torsions

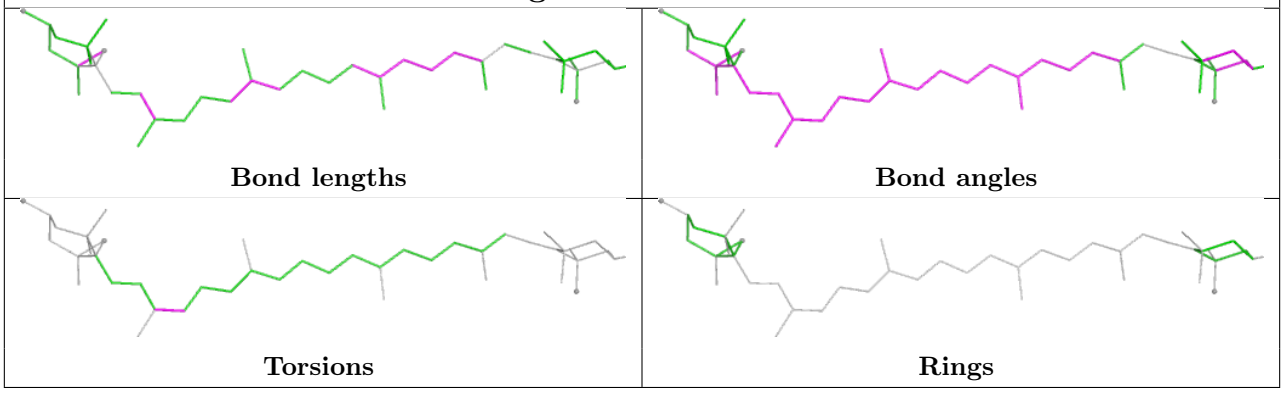


Rings

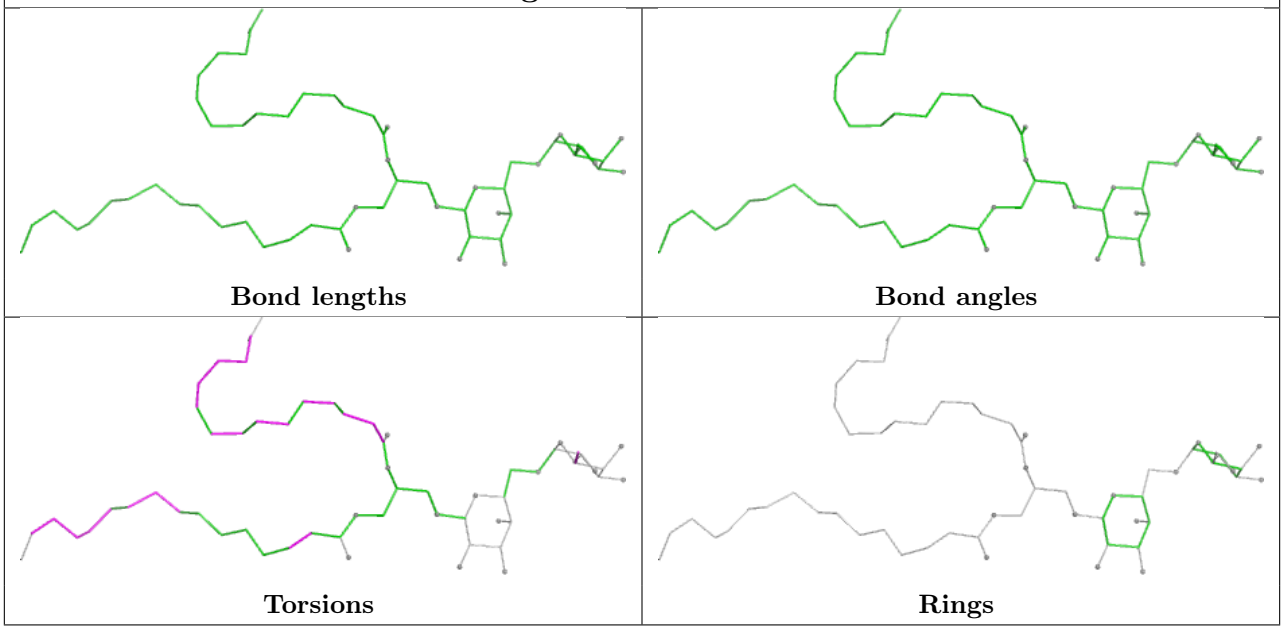
Ligand CLA c 518



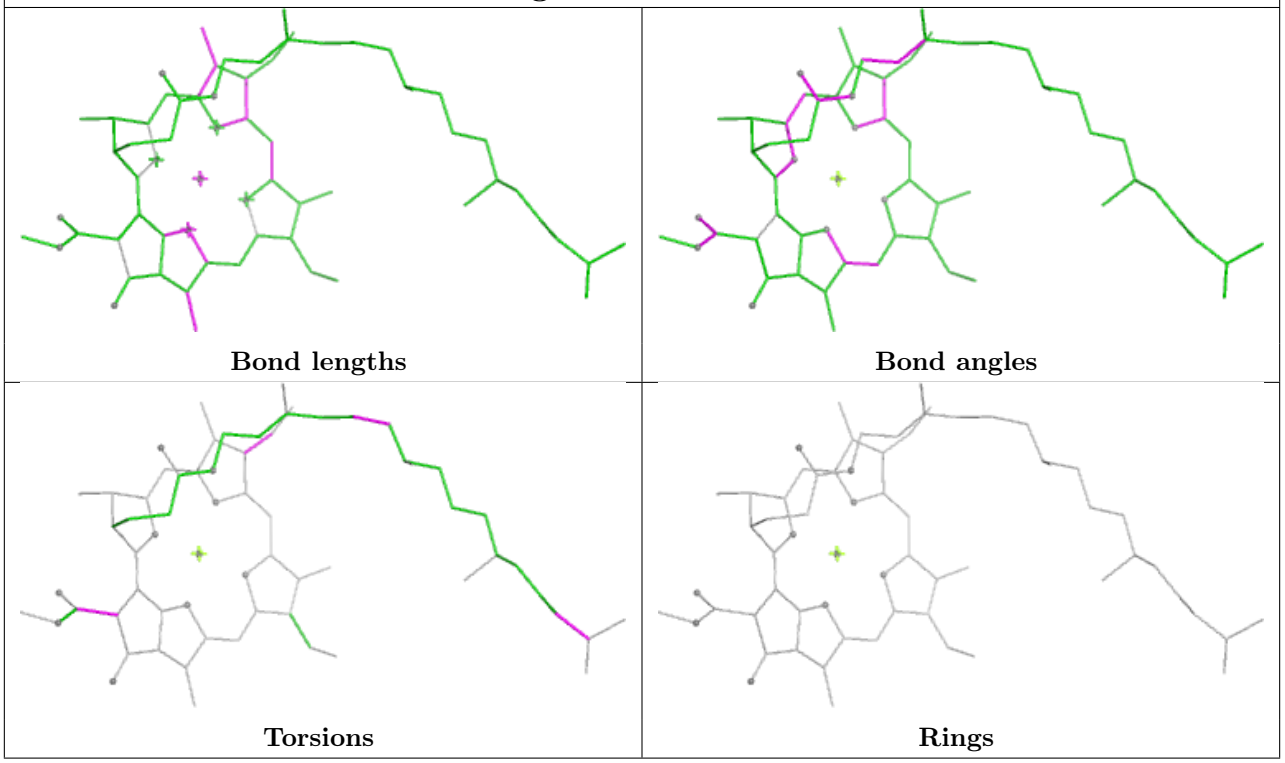
Ligand NEX r 302



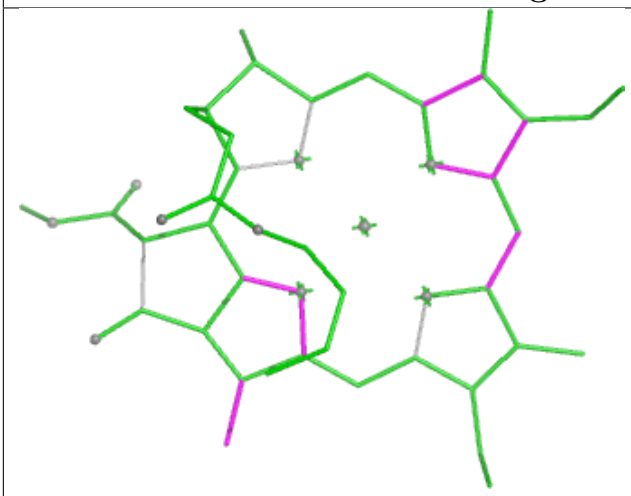
Ligand DGD C 513



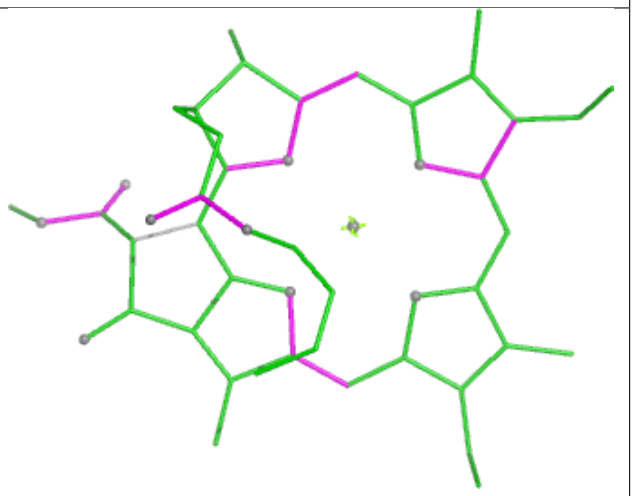
Ligand CLA r 306



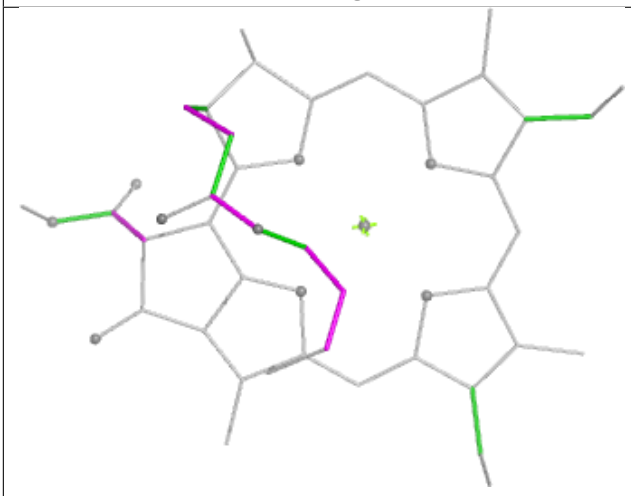
Ligand CLA s 305



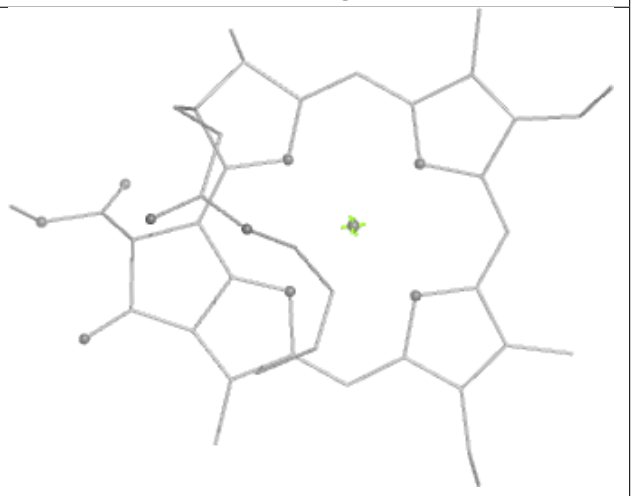
Bond lengths



Bond angles

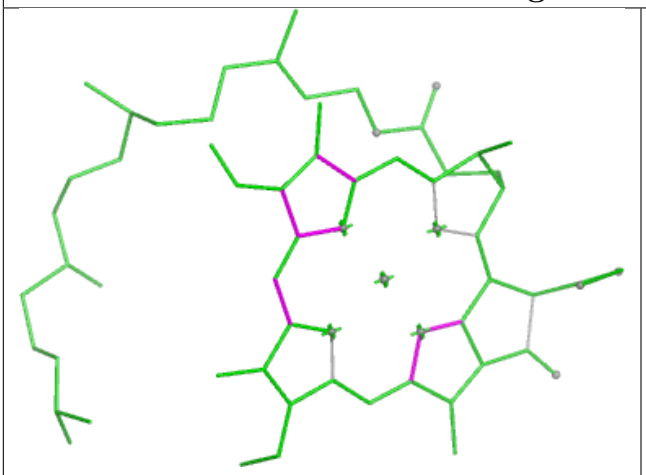


Torsions

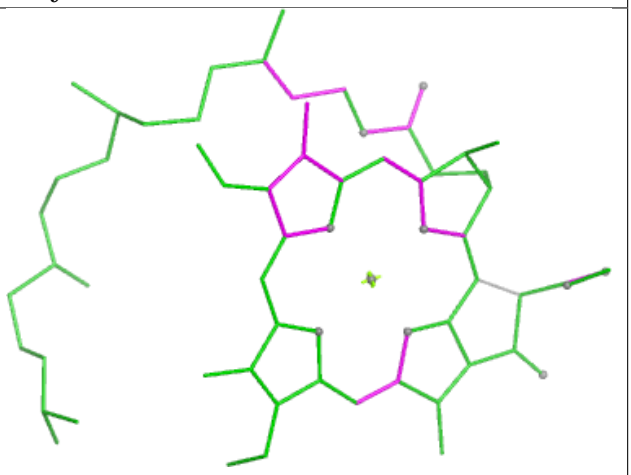


Rings

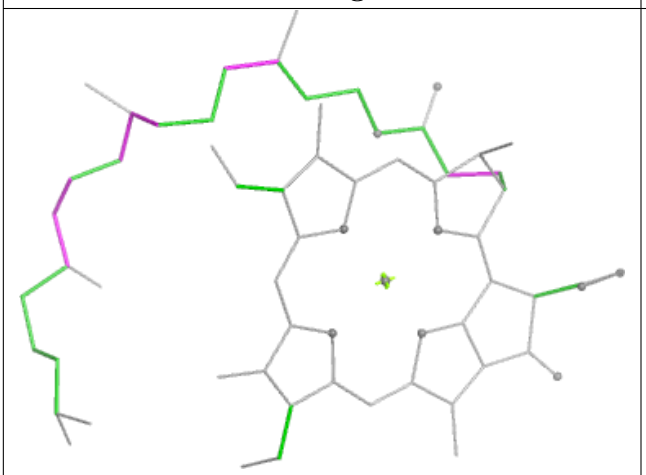
Ligand CLA y 306



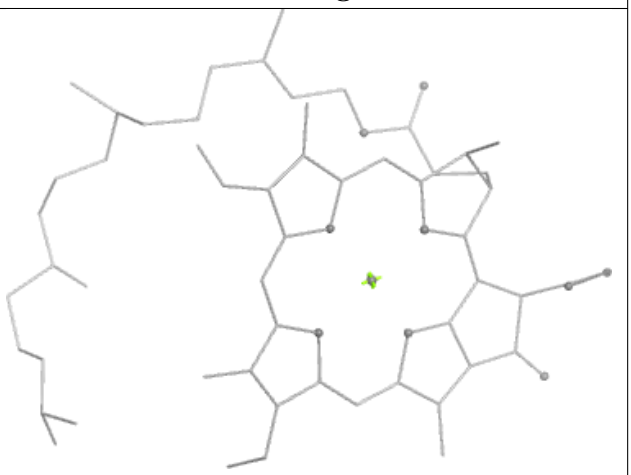
Bond lengths



Bond angles

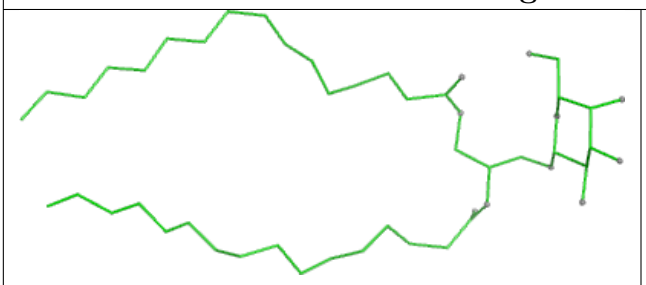


Torsions

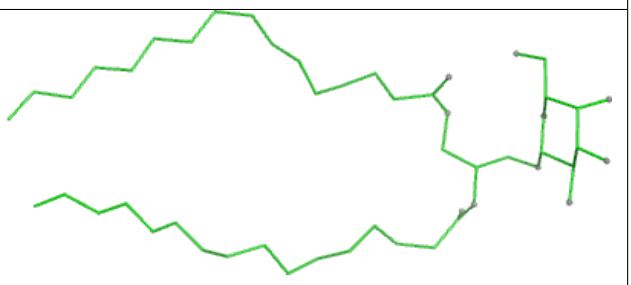


Rings

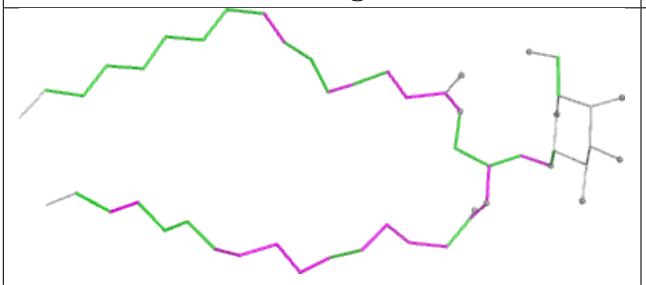
Ligand LMG C 503



Bond lengths



Bond angles

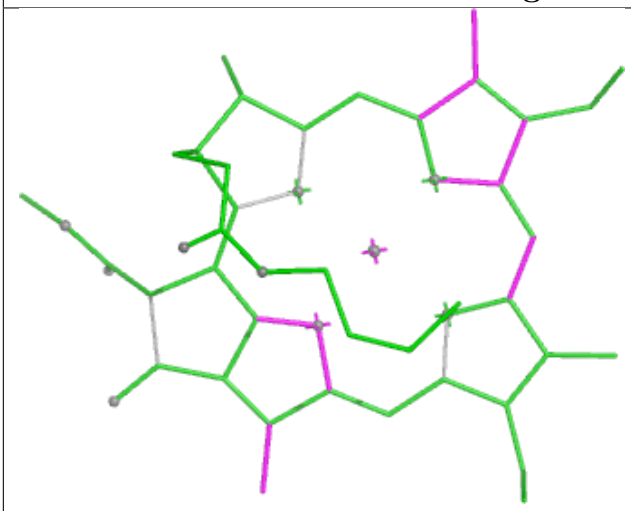


Torsions



Rings

Ligand CLA G 306



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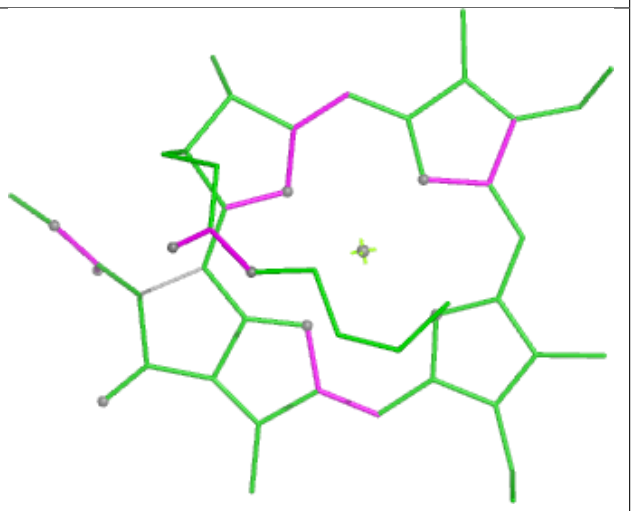
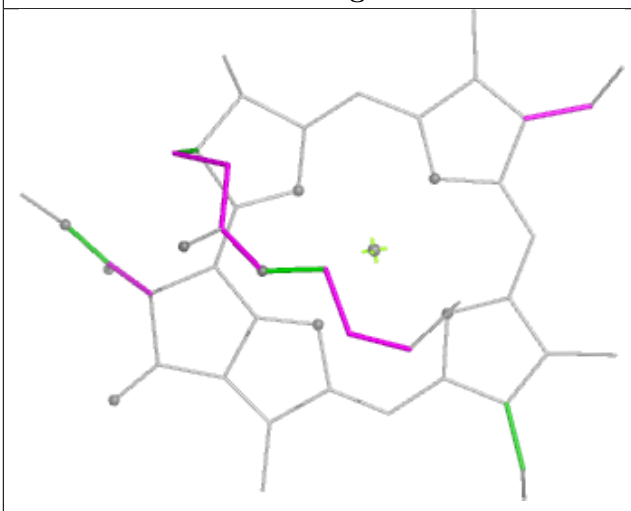


Bond angles



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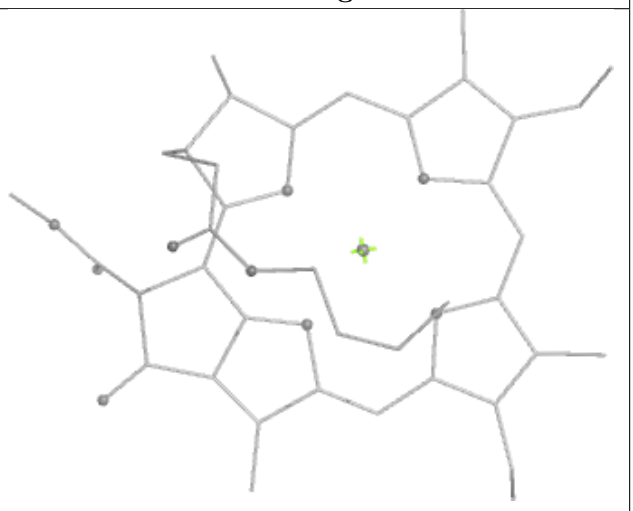
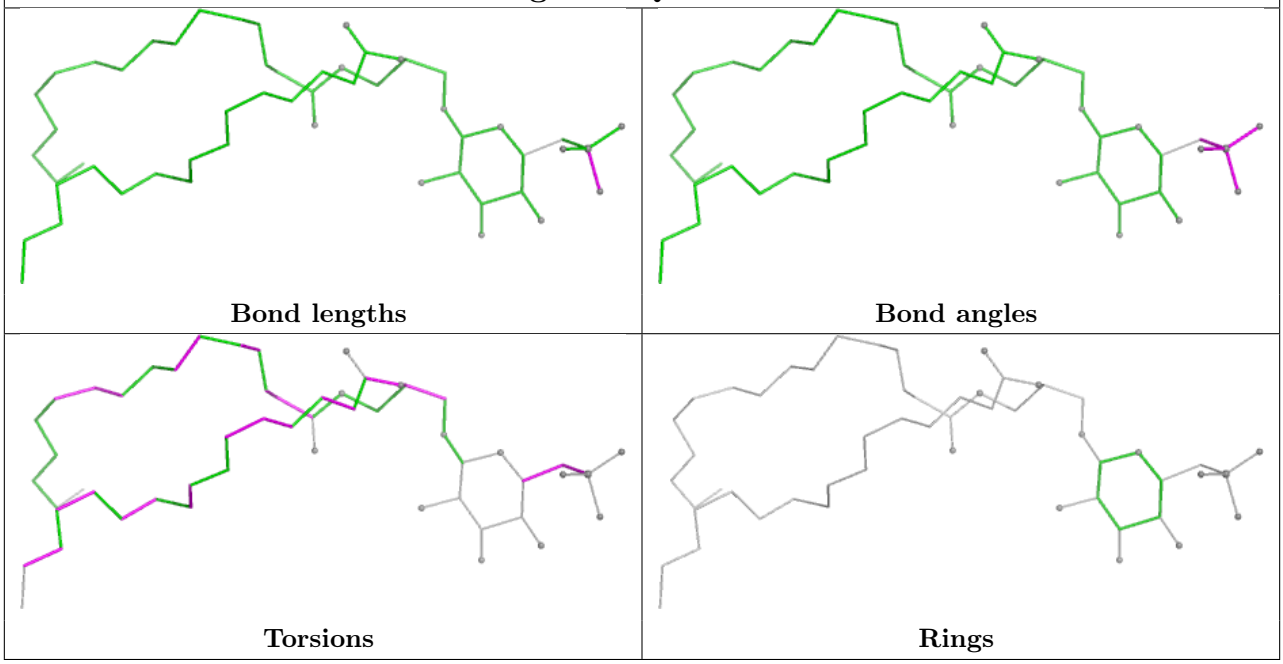
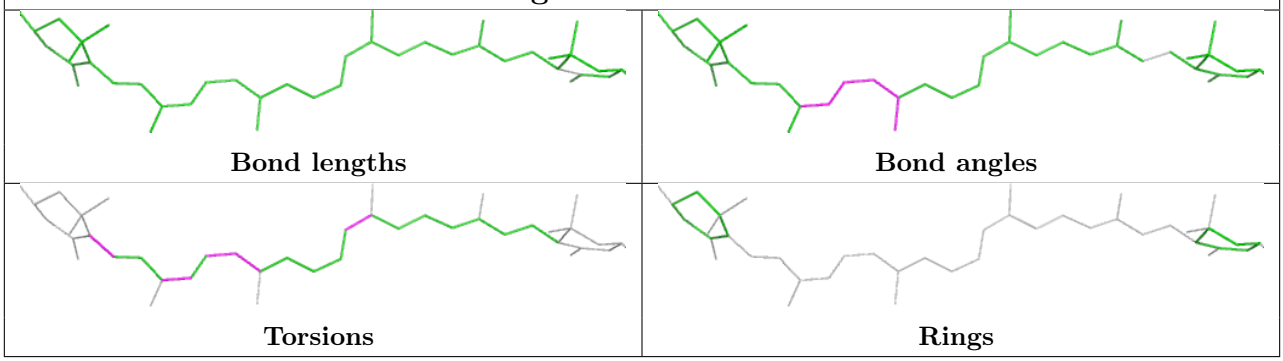


Rings

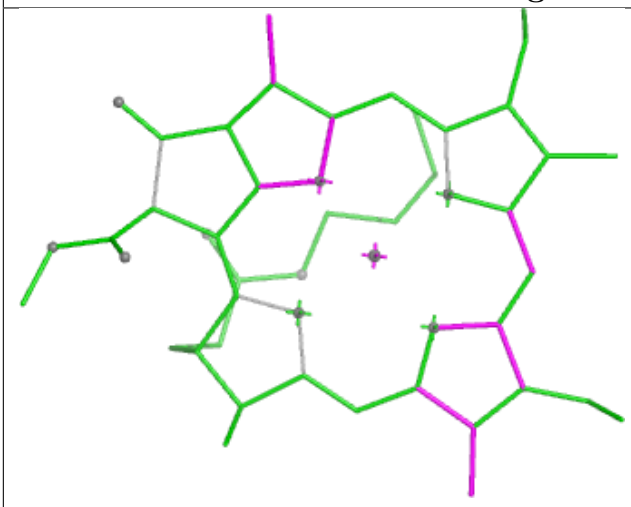
Ligand SQD a 403



Ligand LUT r 307



Ligand CLA S 303



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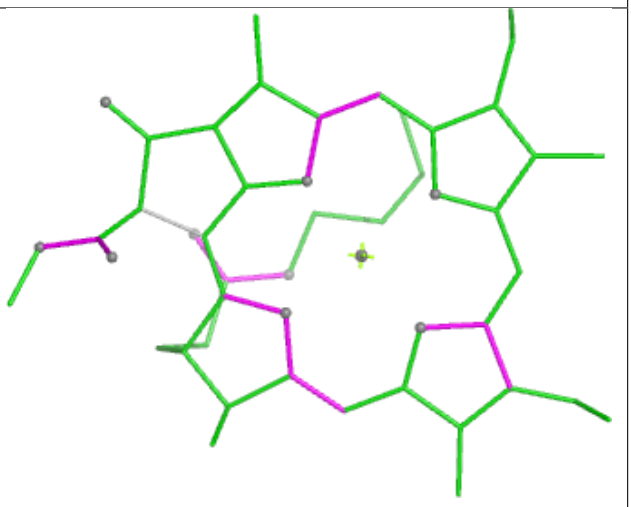
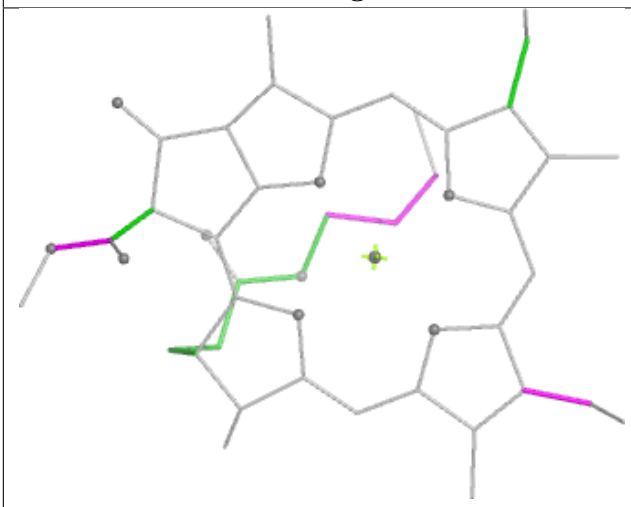


Bond angles



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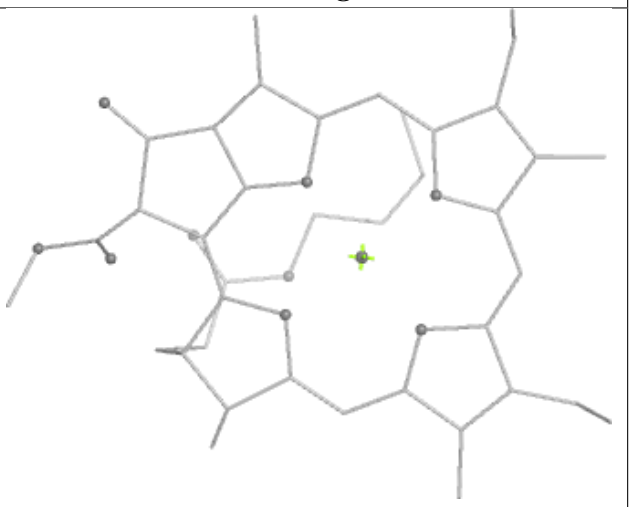
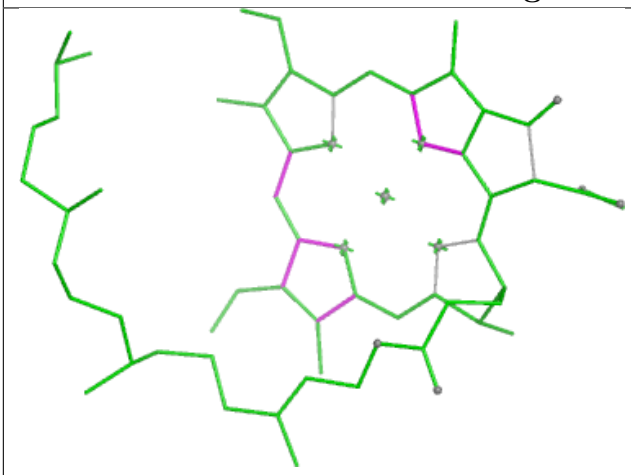
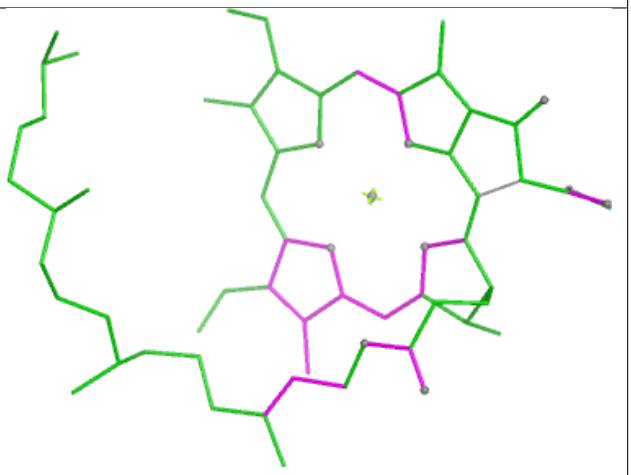


Rings

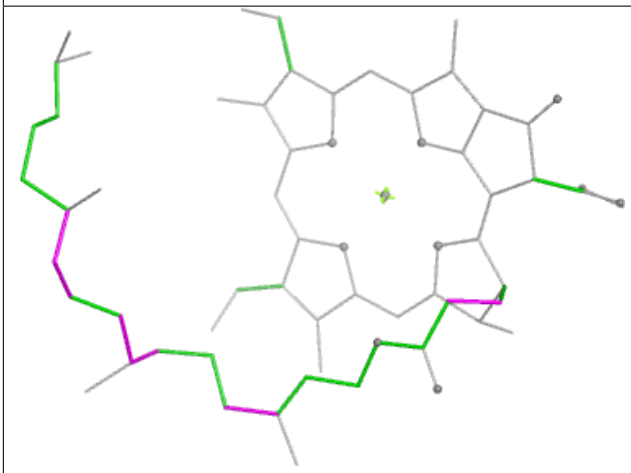
Ligand CLA Y 308



Bond lengths



Bond angles

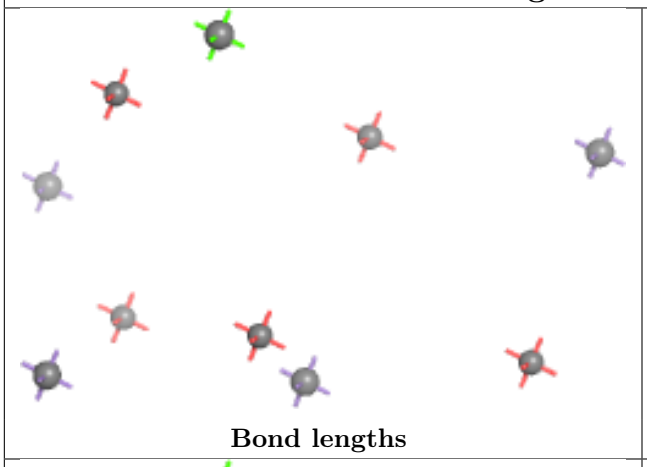


Torsions



Rings

Ligand OEX a 408



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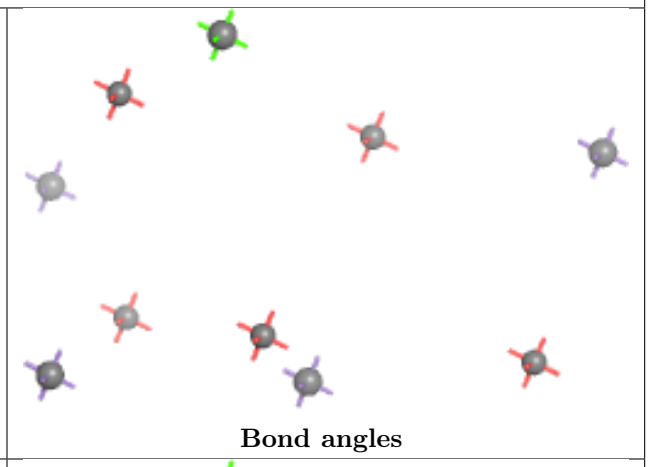
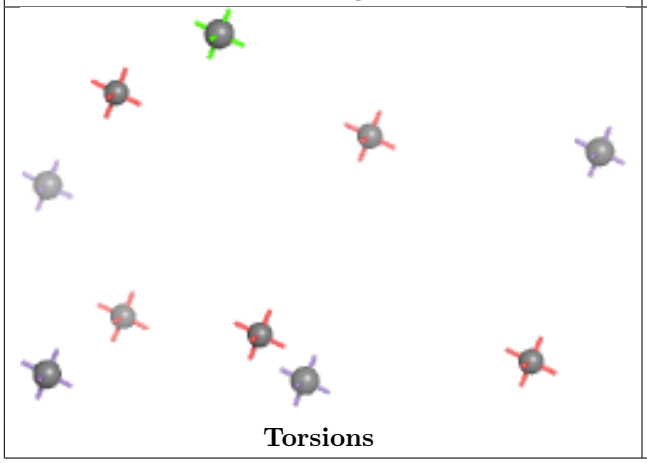
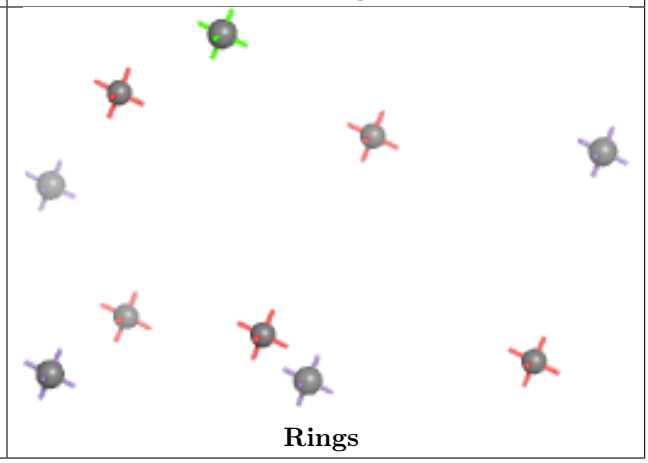


Bond angles

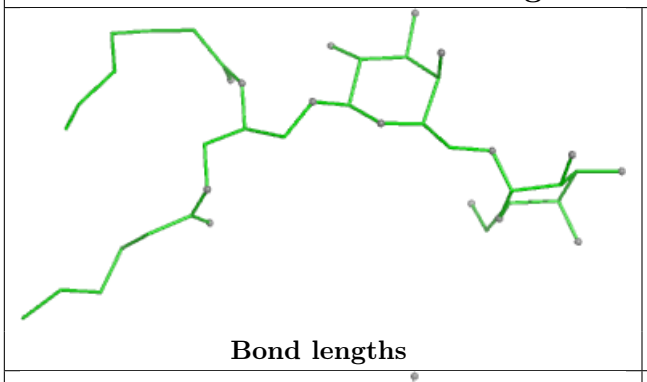


Torsions

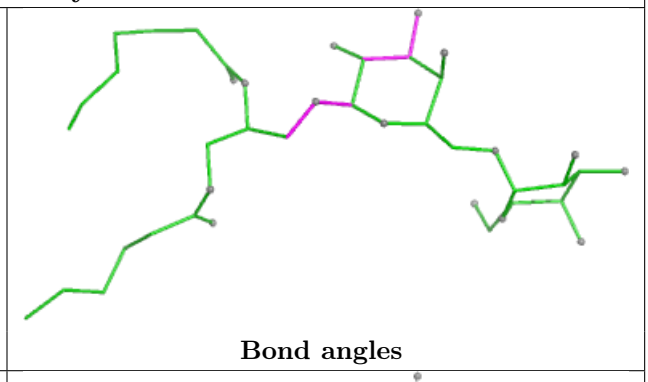


Rings

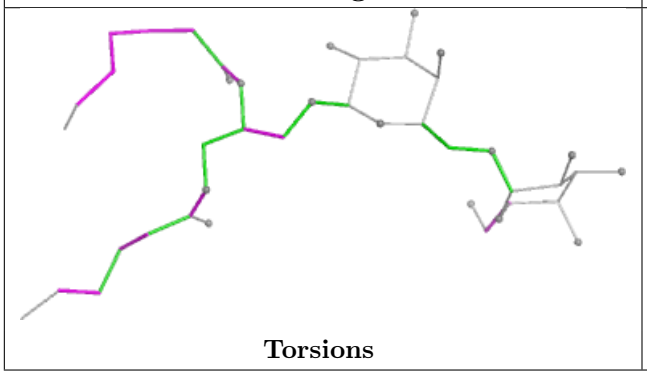
Ligand DGD y 308



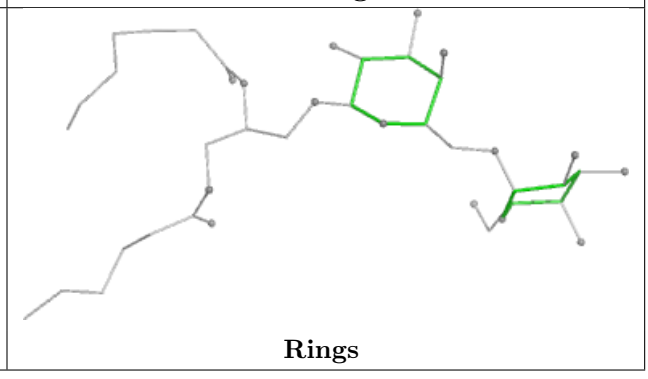
Bond lengths



Bond angles



Torsions

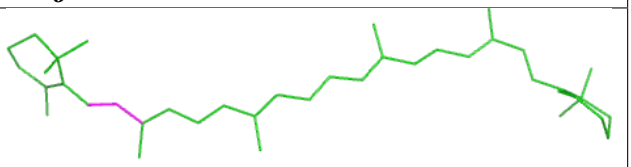


Rings

Ligand BCR j 101



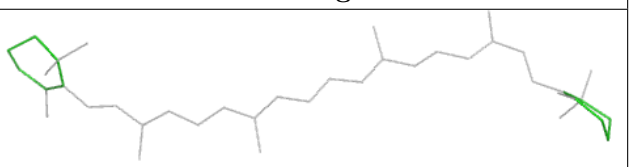
Bond lengths



Bond angles

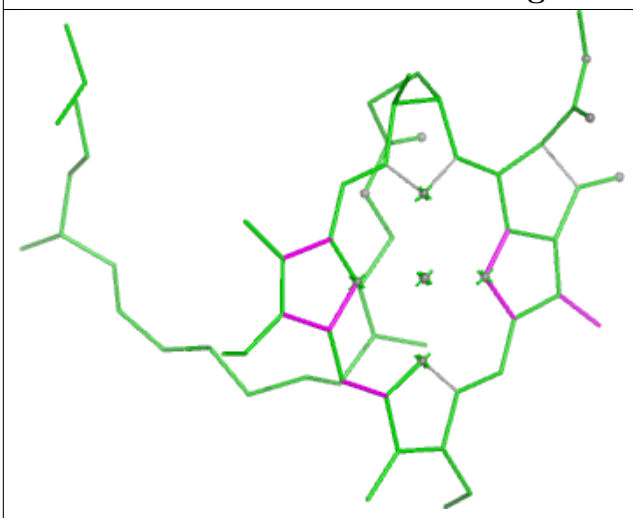


Torsions



Rings

Ligand CLA y 310



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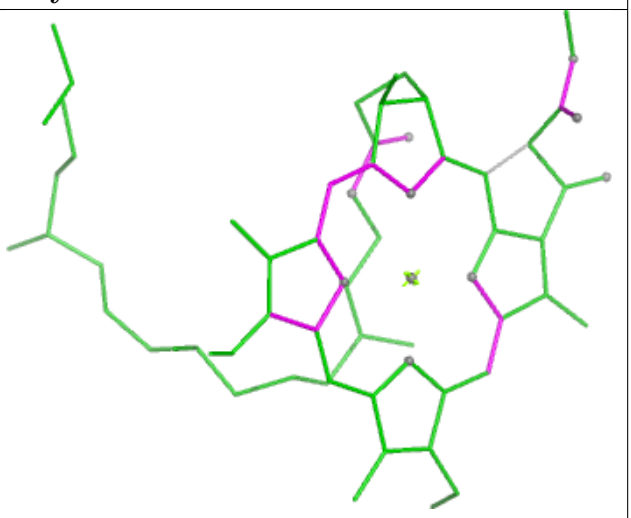
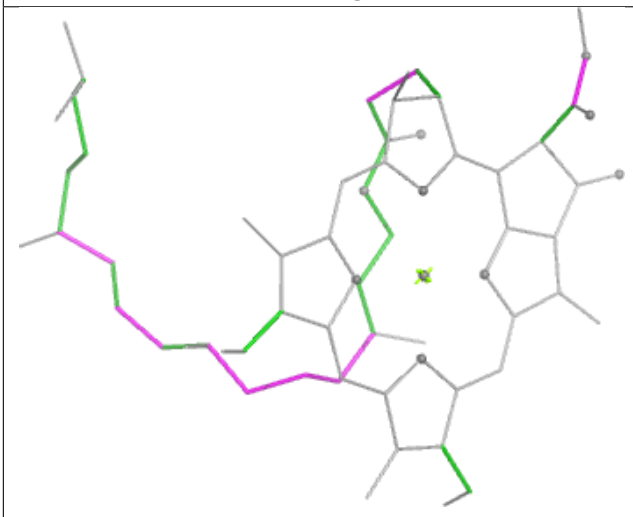


Bond angles



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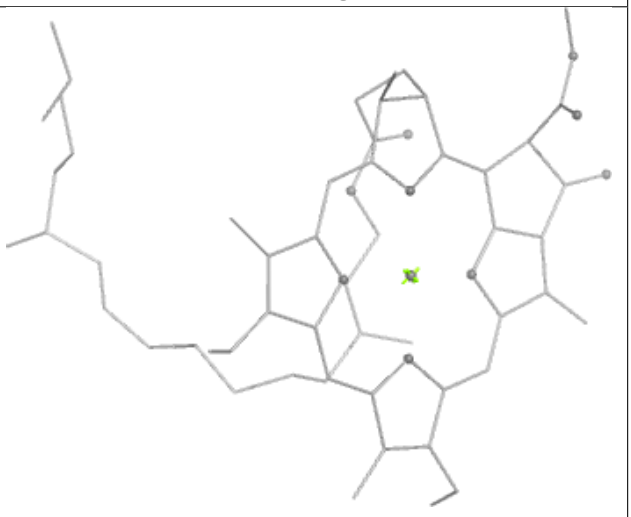
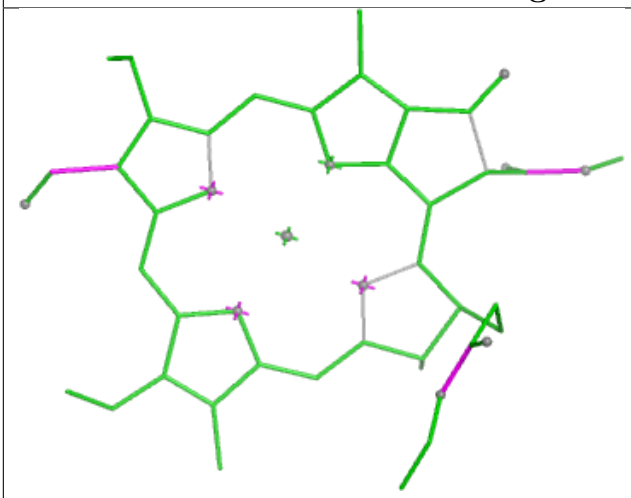


Rings

Ligand CHL r 301



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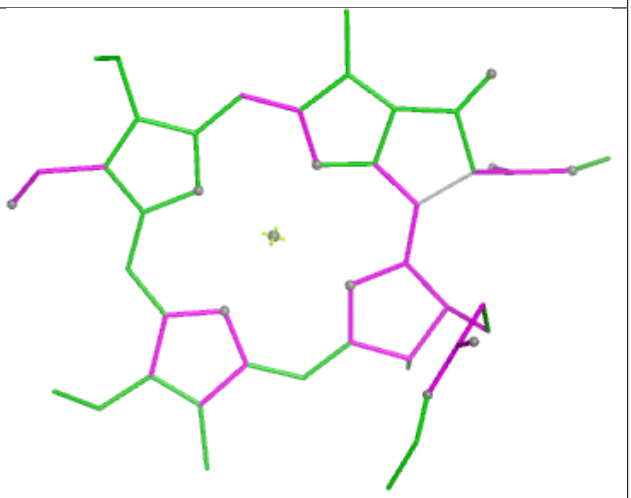

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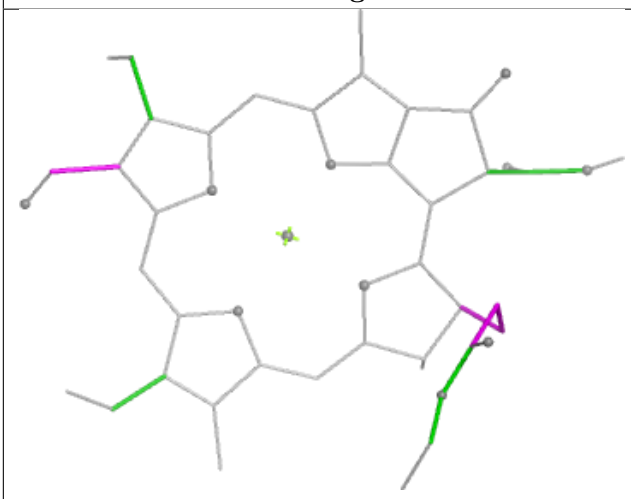

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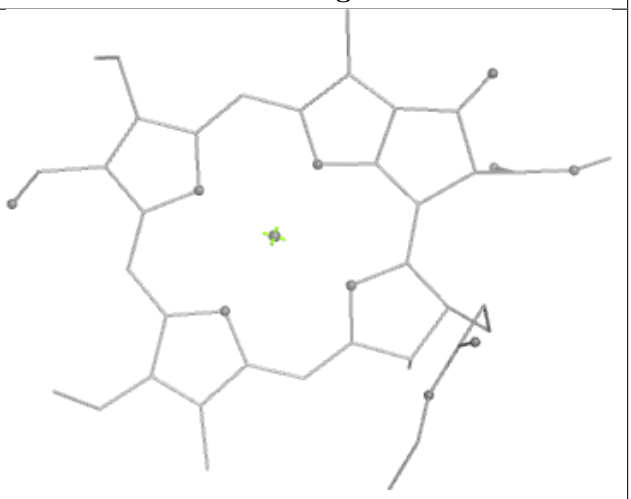
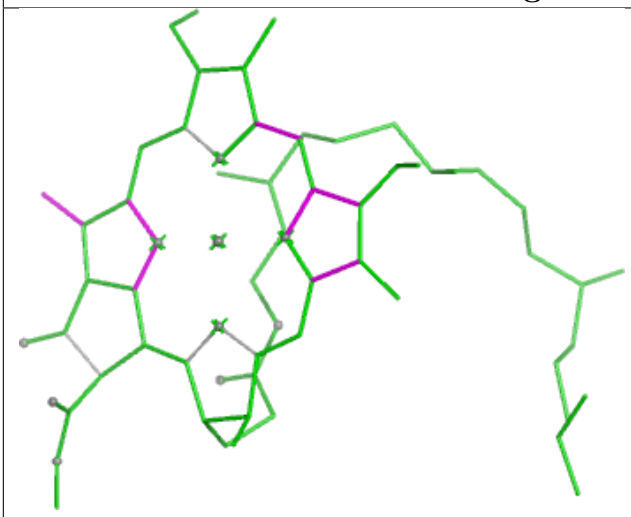


Rings

Ligand CLA Y 312



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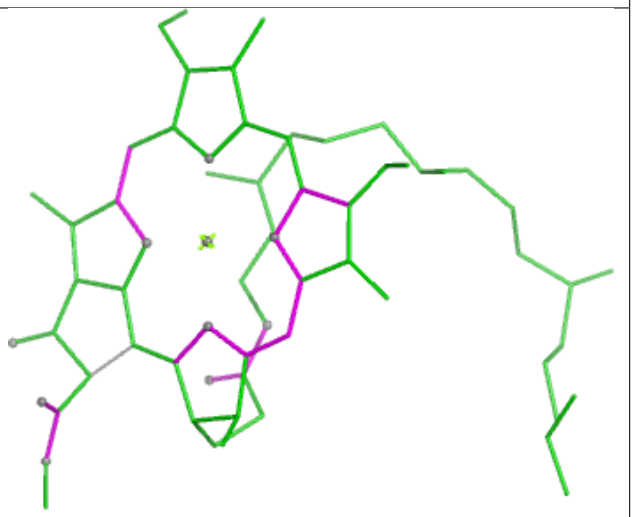

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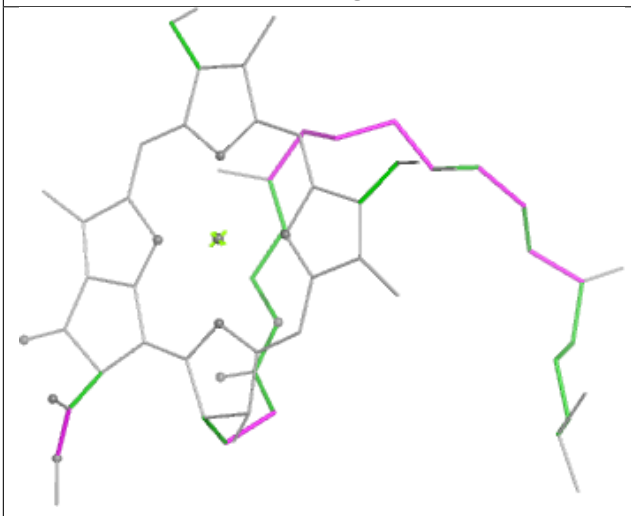

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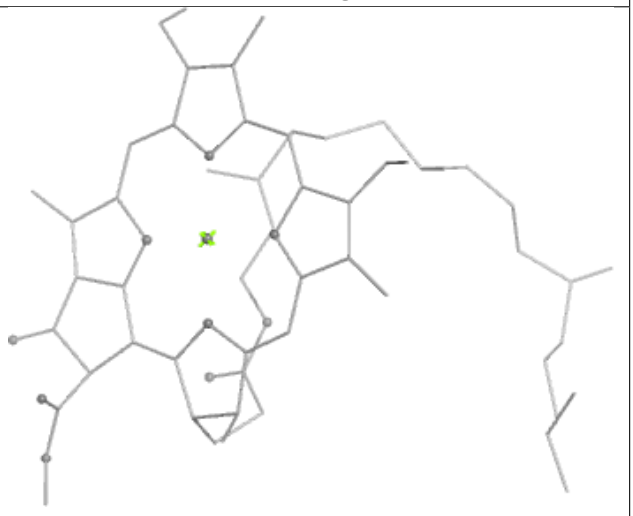
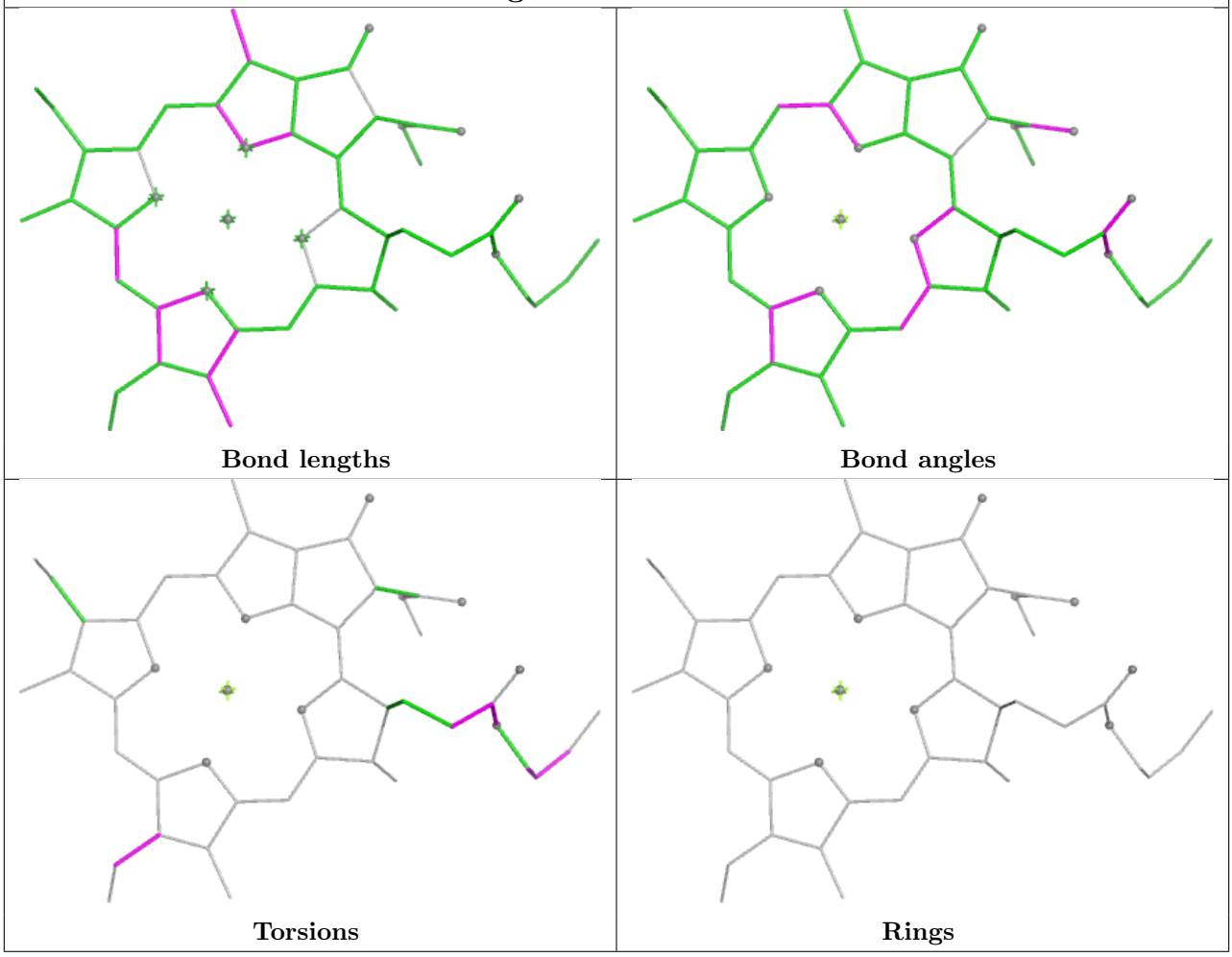
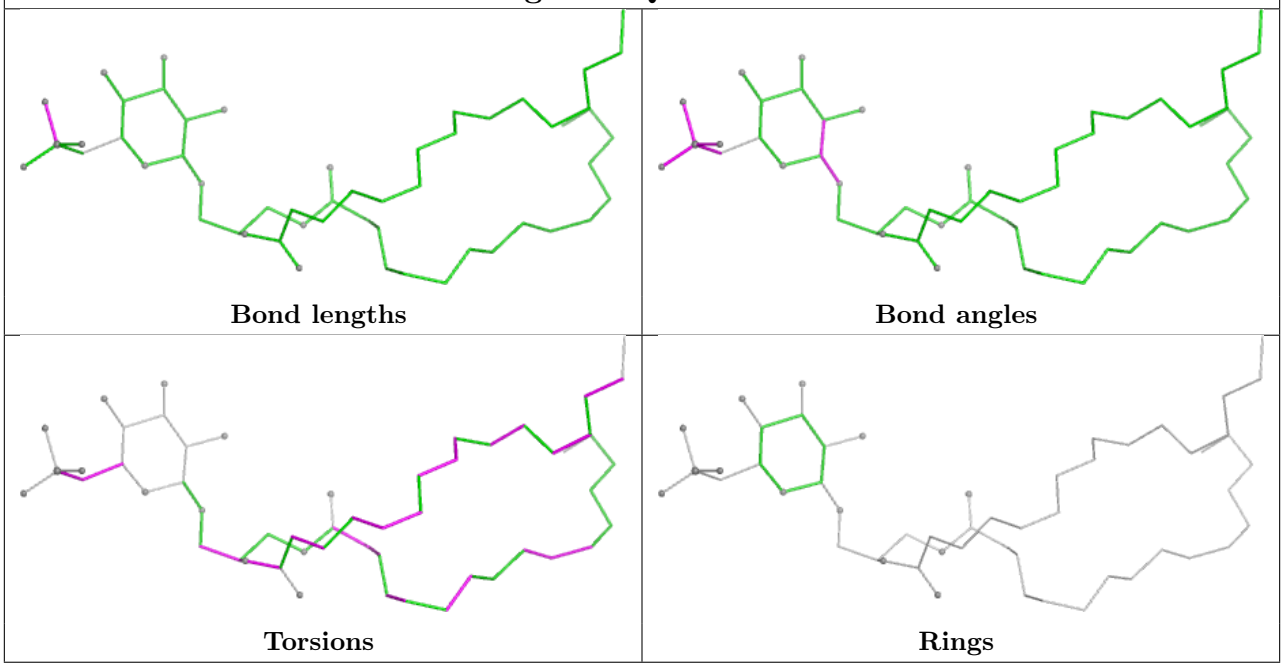


Rings

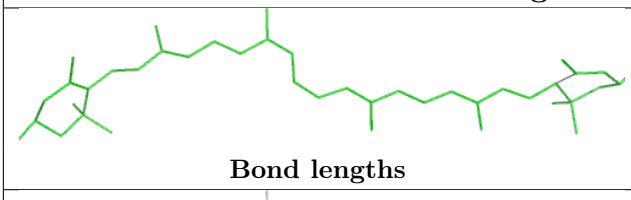
Ligand CLA S 315



Ligand SQD A 407



Ligand LUT s 308



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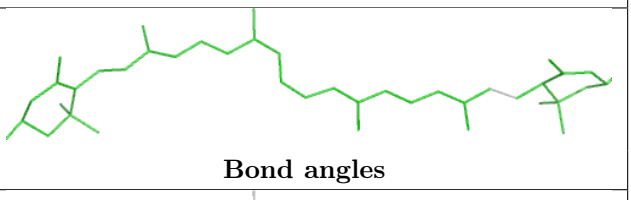

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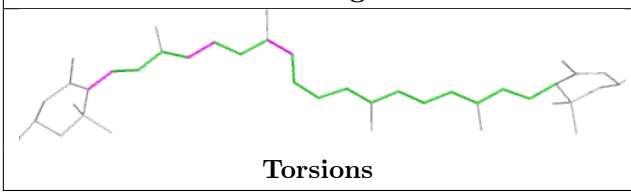

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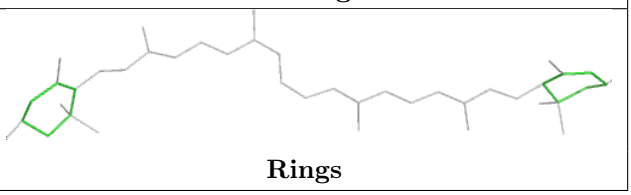
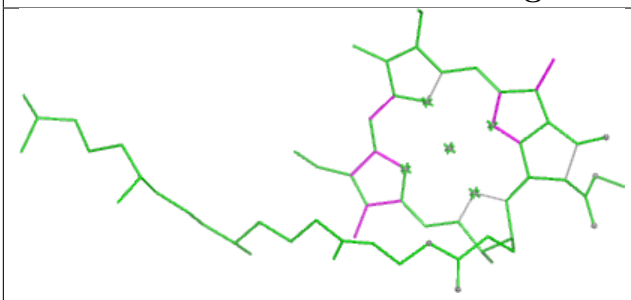


Rings

Ligand CLA C 505



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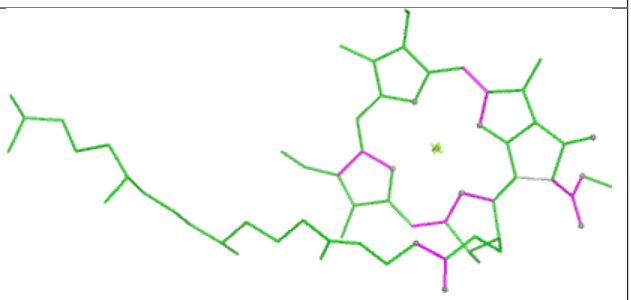

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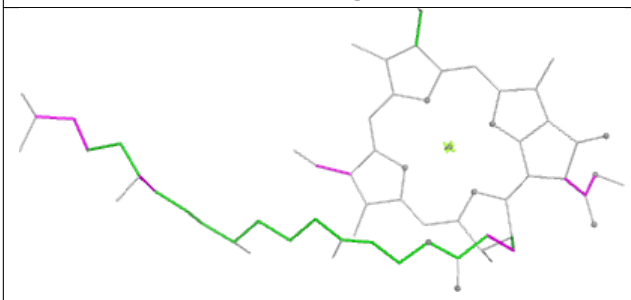

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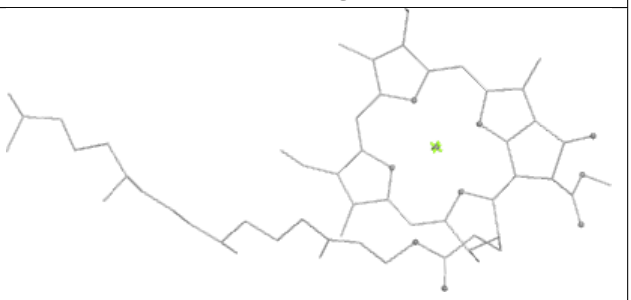
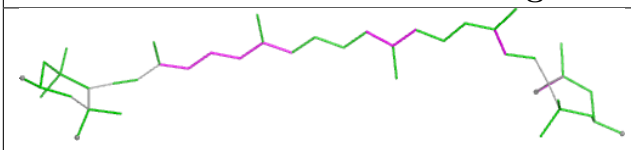


Rings

Ligand NEX g 306



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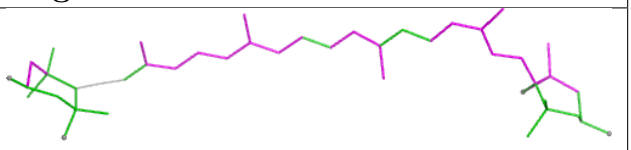

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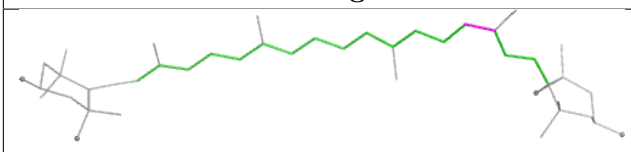

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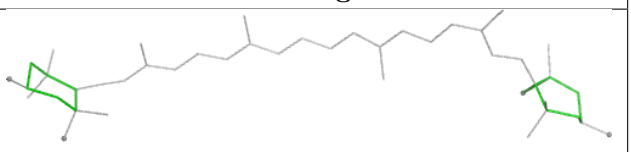
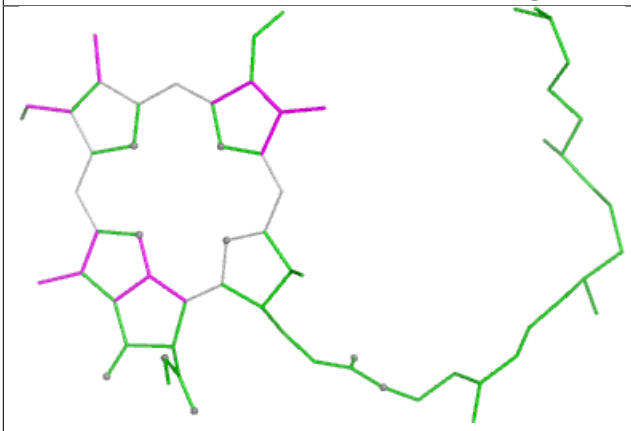


Rings

Ligand PHO a 410



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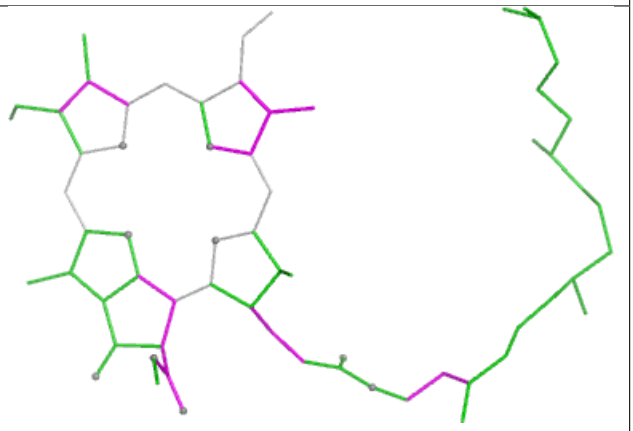
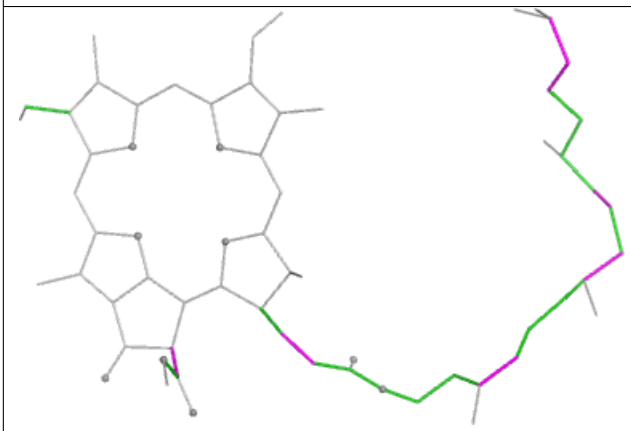


Bond angles



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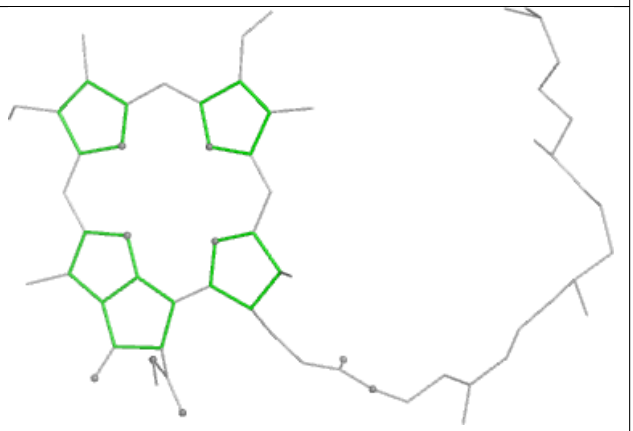
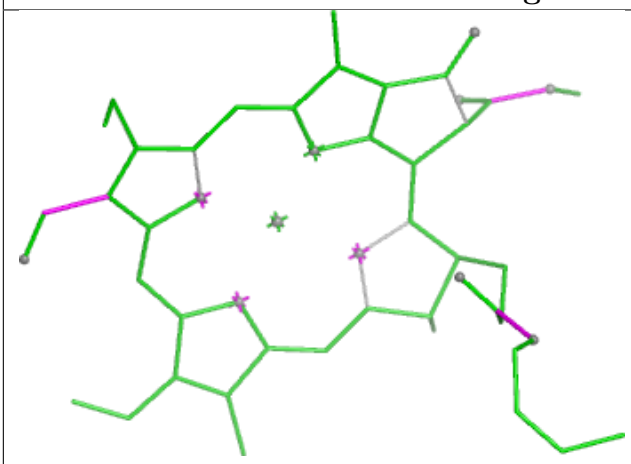


Rings

Ligand CHL R 312



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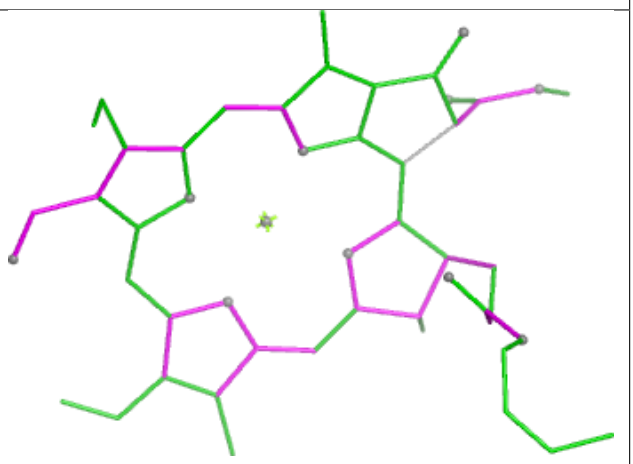
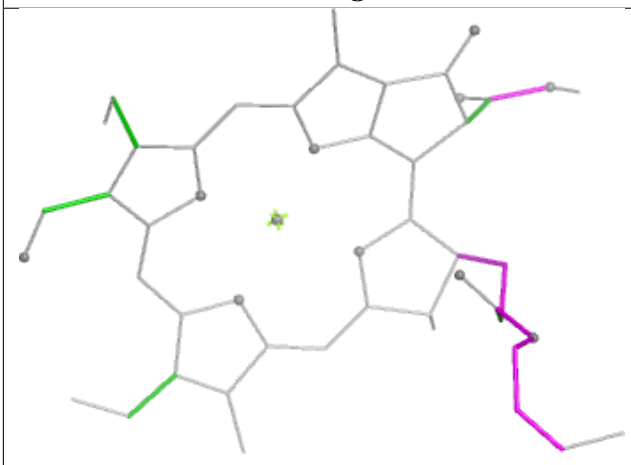


Bond angles



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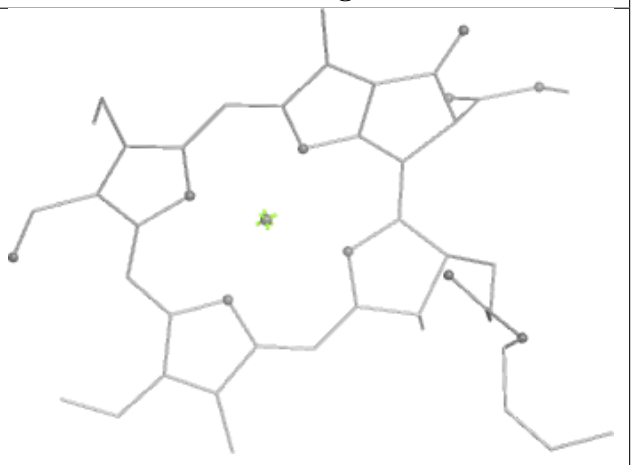
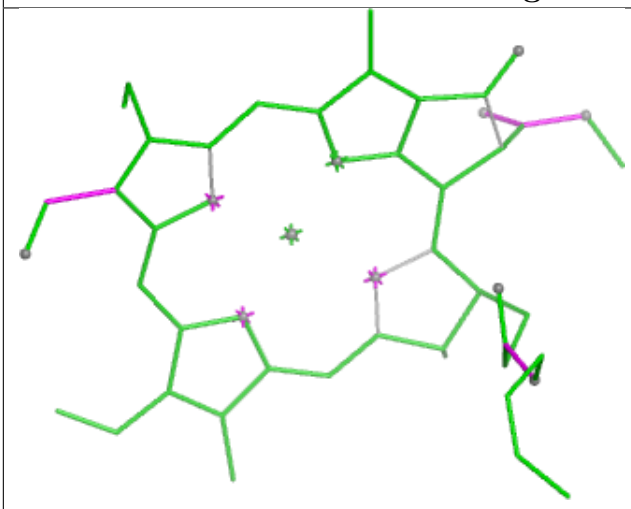


Rings

Ligand CHL Y 318



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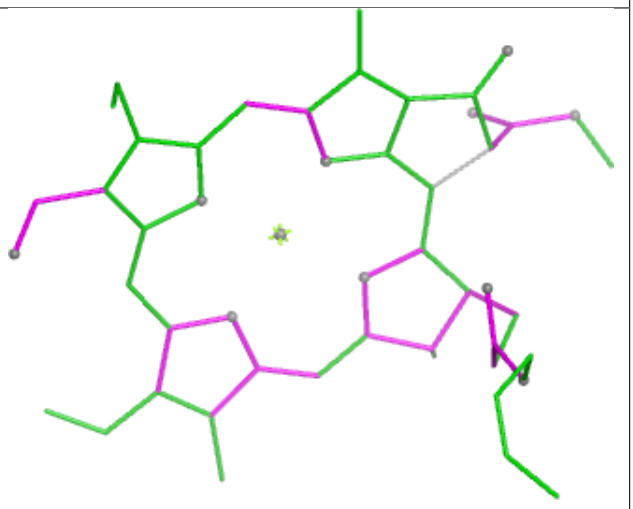
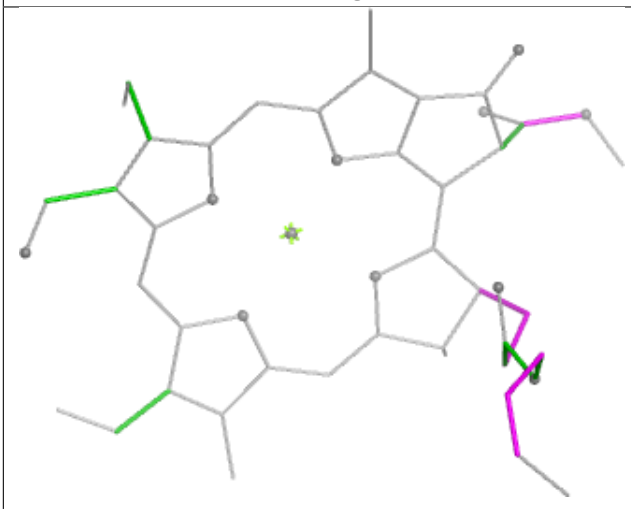


Bond angles



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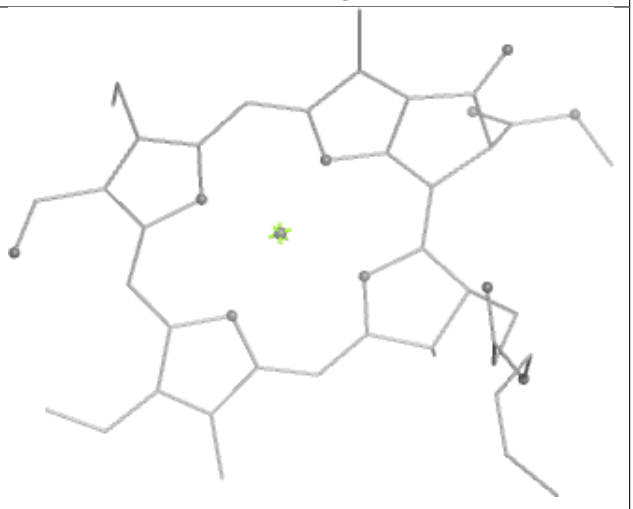
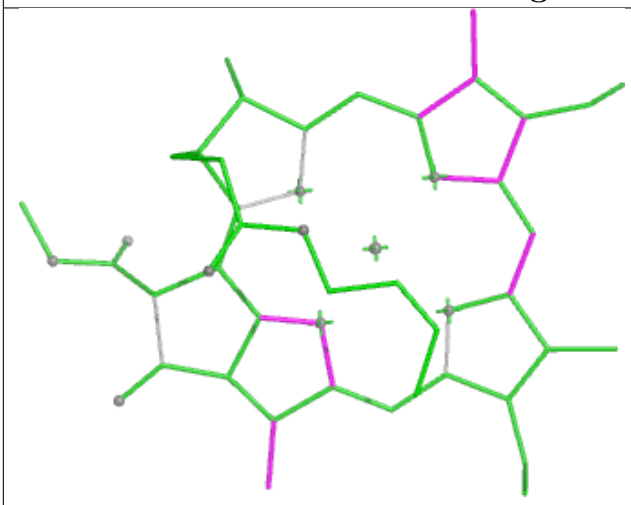


Rings

Ligand CLA s 307



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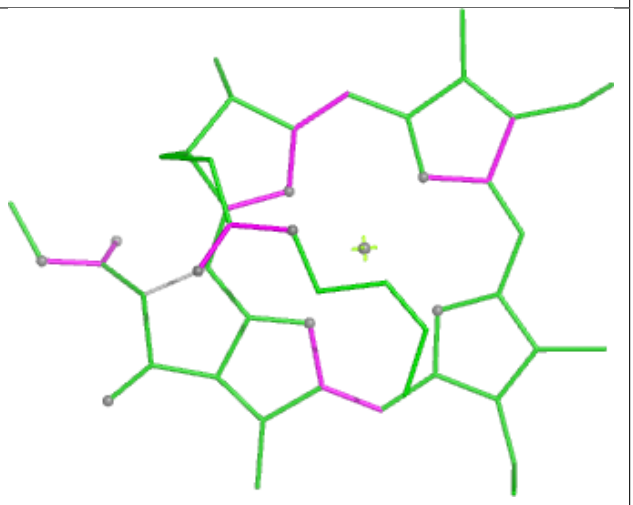

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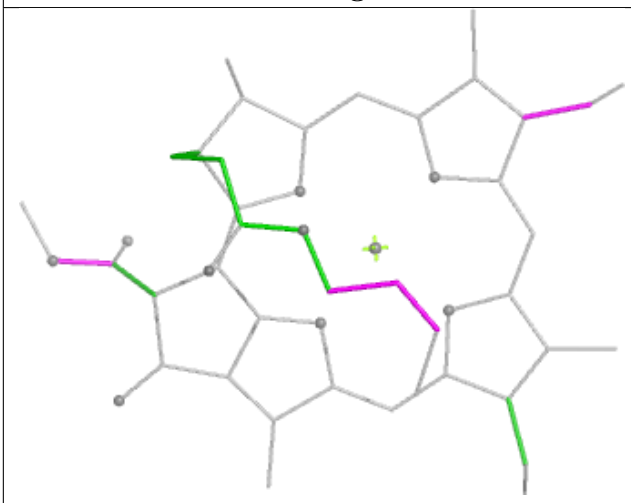

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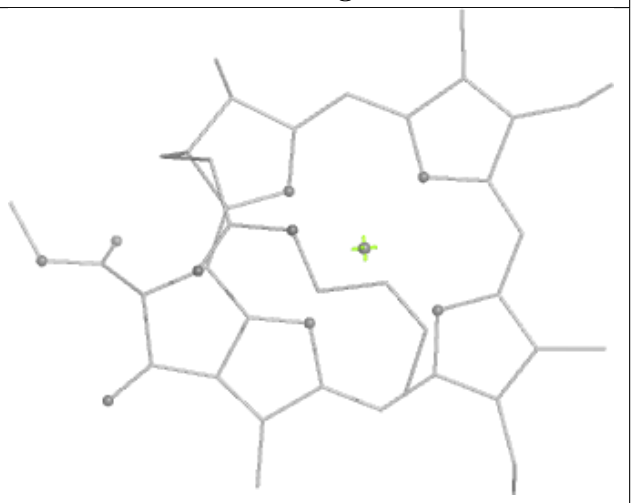
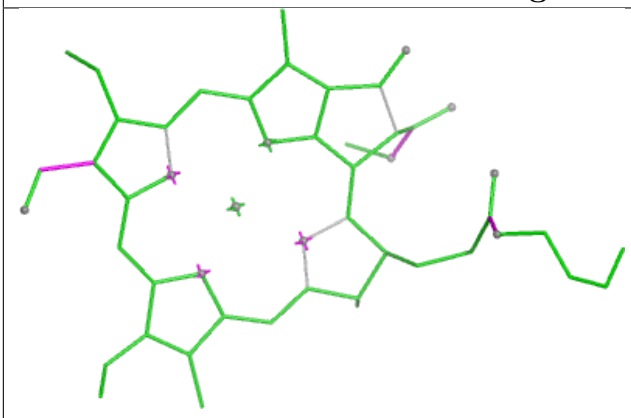


Rings

Ligand CHL r 316



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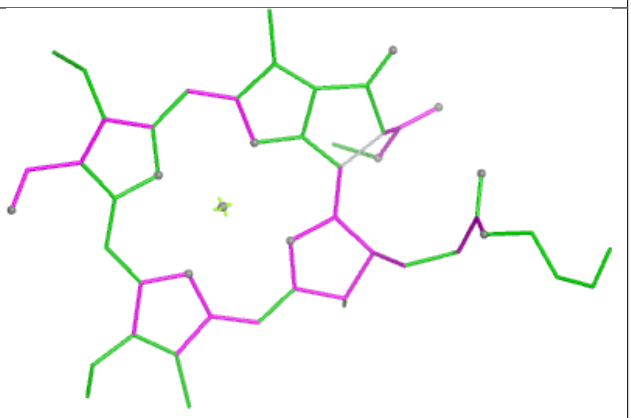
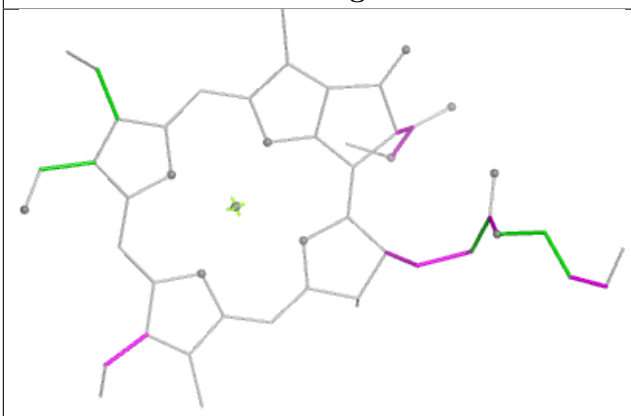


Bond angles



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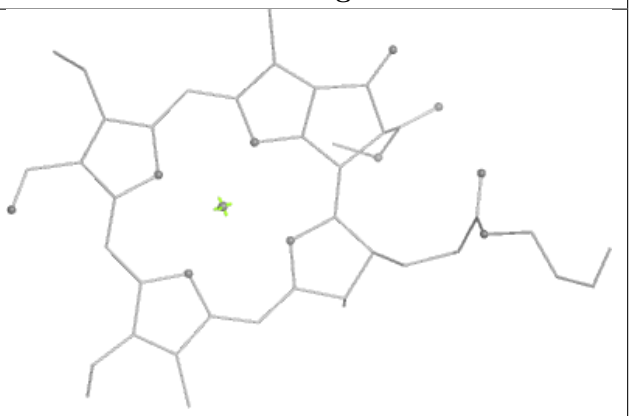
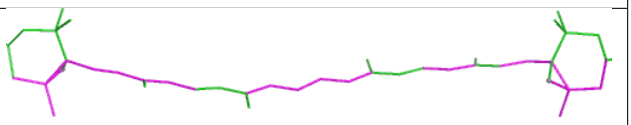


Rings

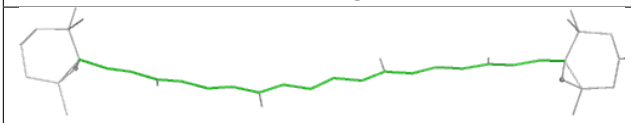
Ligand XAT n 316



Bond lengths



Bond angles



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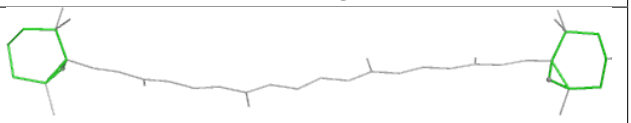
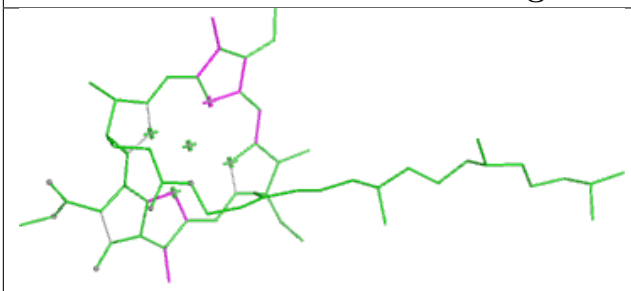


Rings

Ligand CLA b 607



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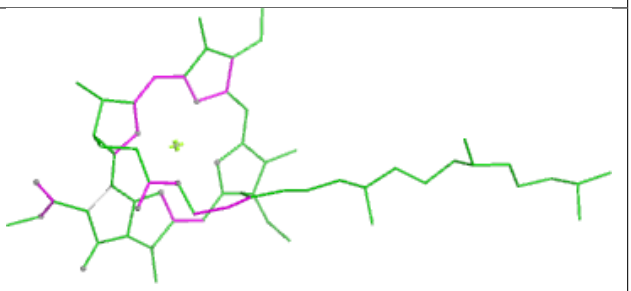
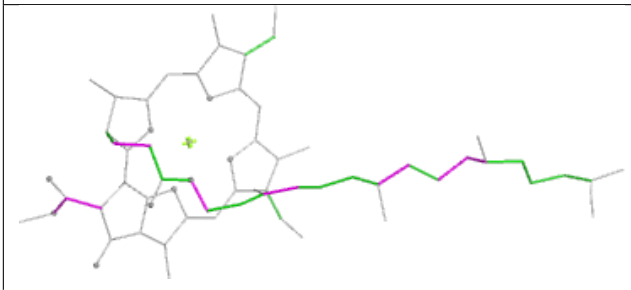


Bond angles

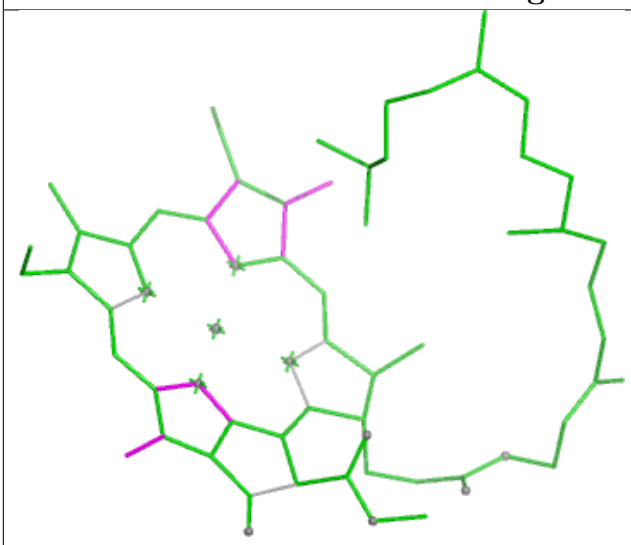


Torsions



Rings

Ligand CLA b 609



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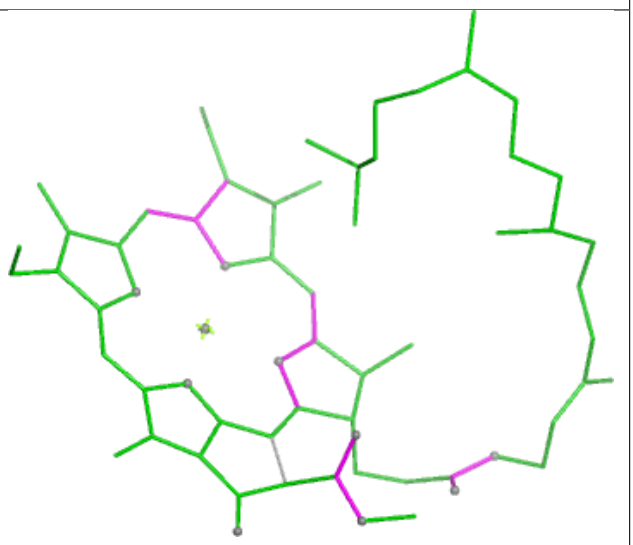
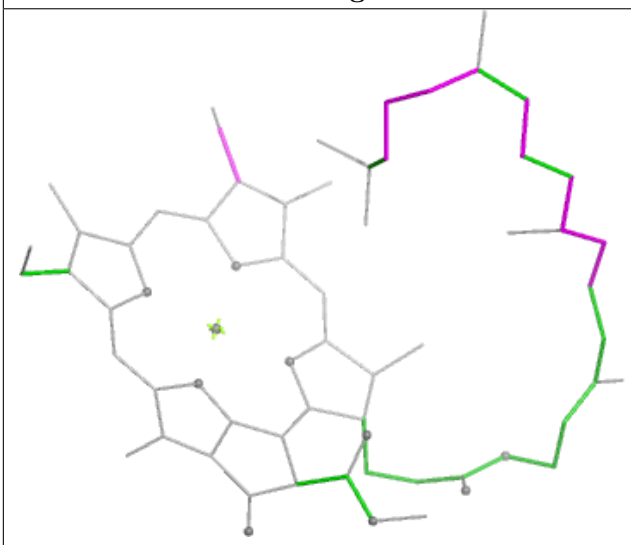
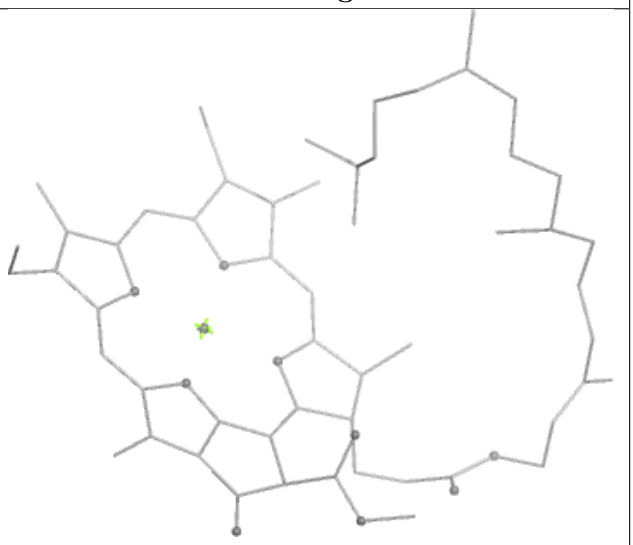


Bond angles

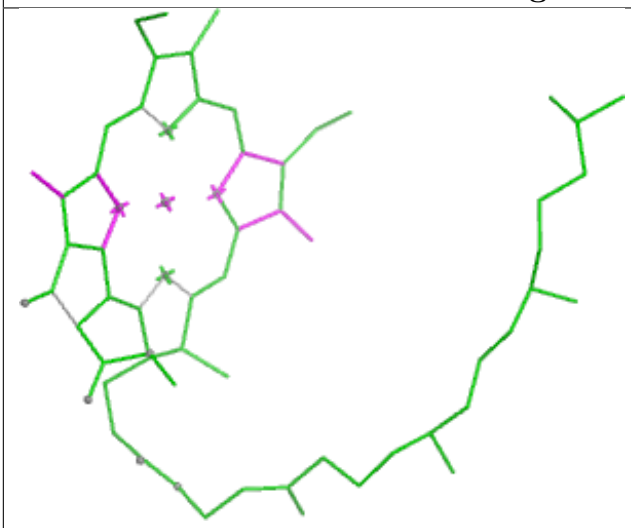


Torsions

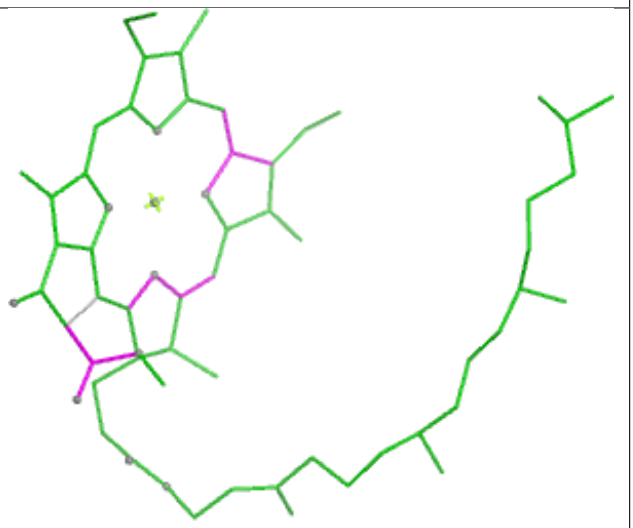


Rings

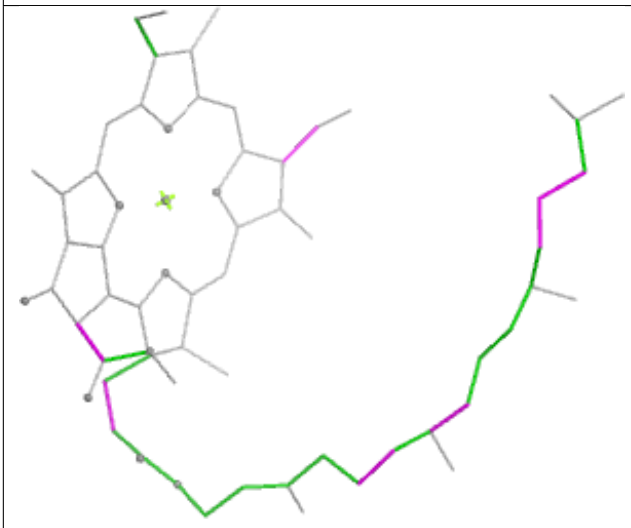
Ligand CLA c 508



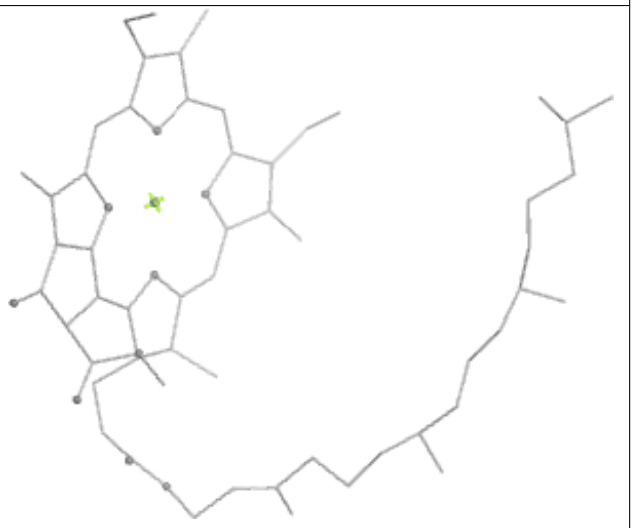
Bond lengths



Bond angles

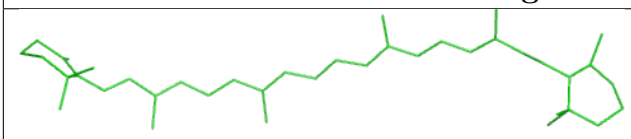


Torsions



Rings

Ligand BCR K 101



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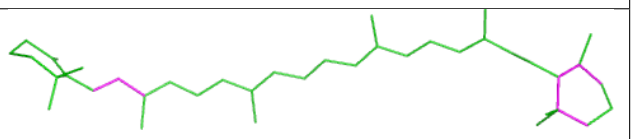
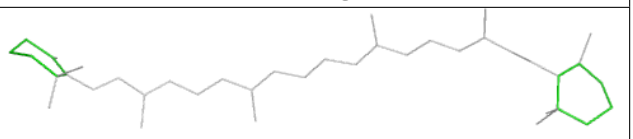


Bond angles

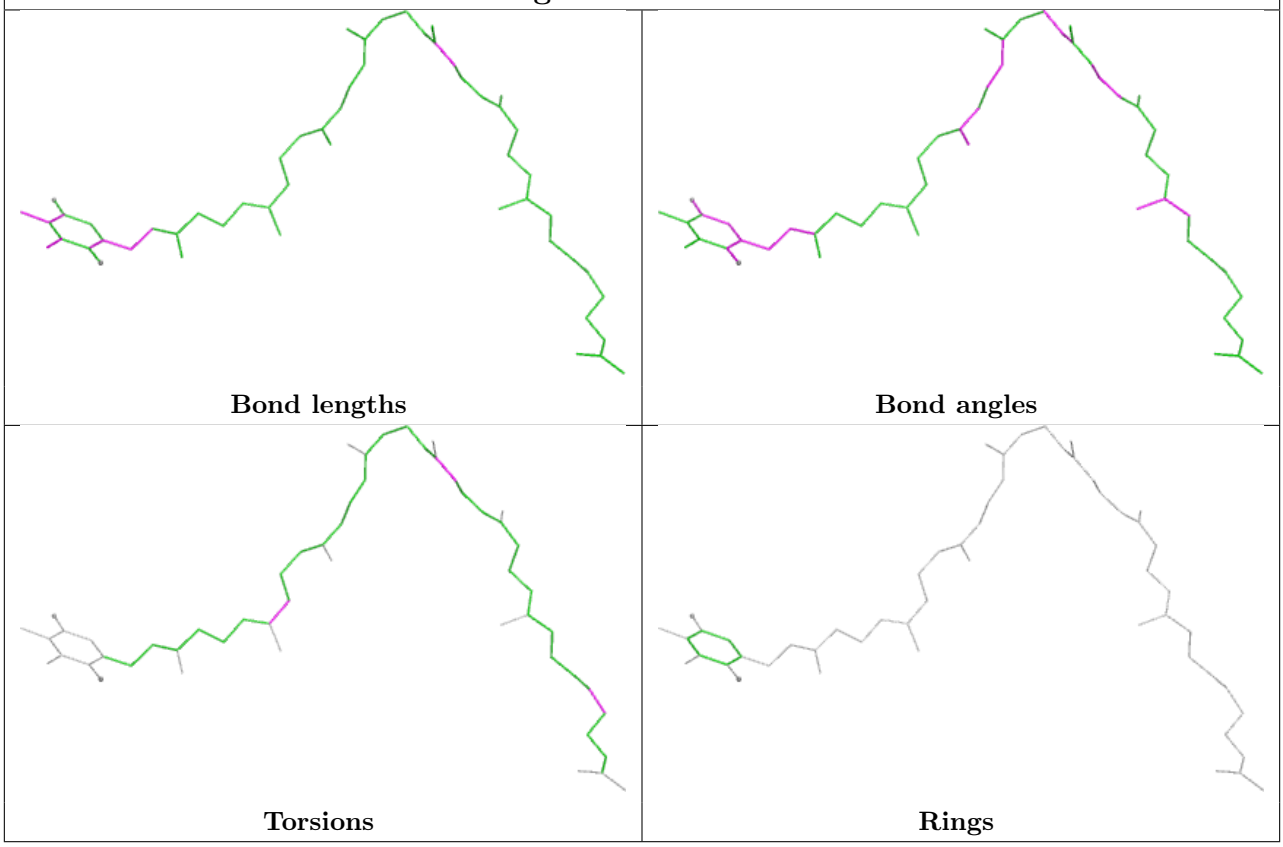


Torsions

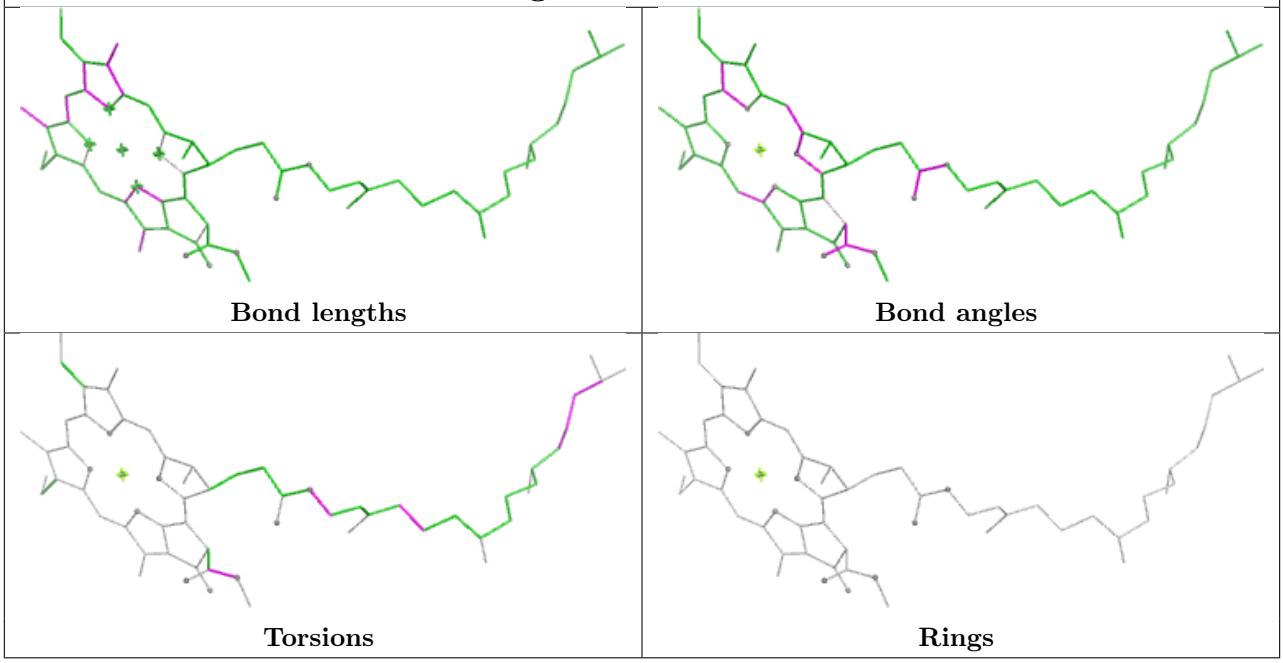


Rings

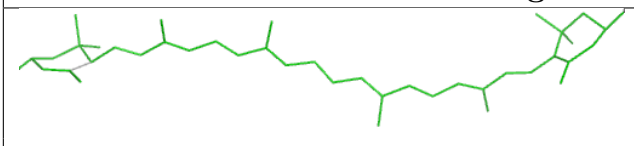
Ligand PL9 d 408



Ligand CLA a 411



Ligand LUT n 314



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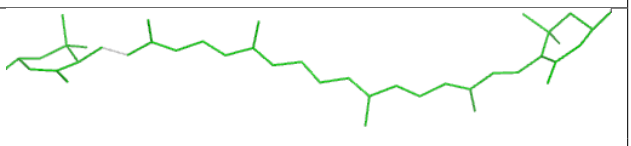
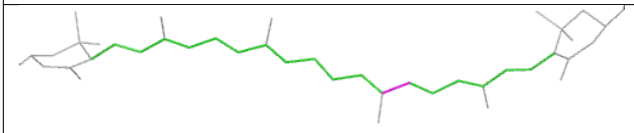


Bond angles



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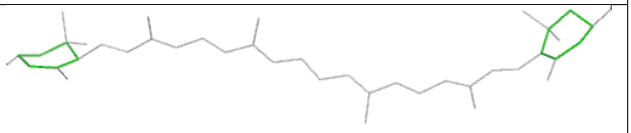
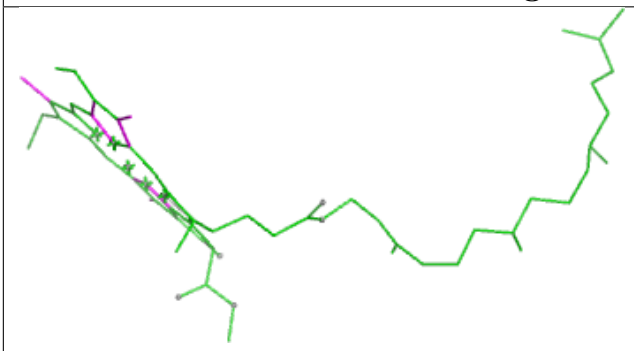


Rings

Ligand CLA D 409



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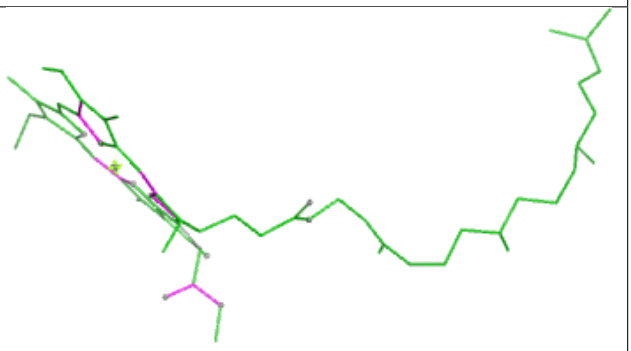
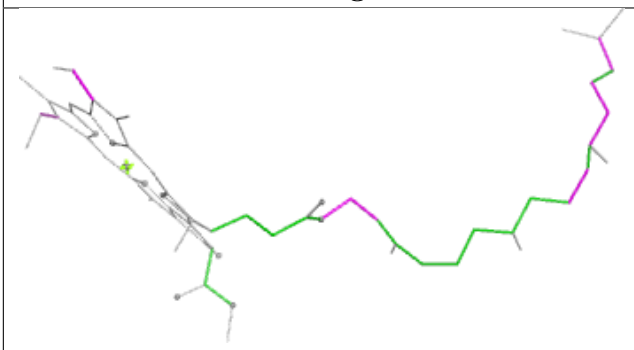


Bond angles



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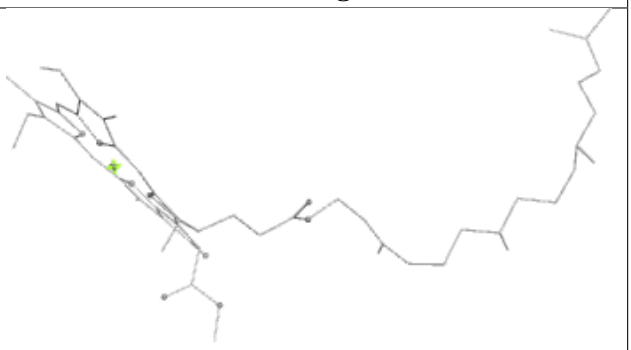
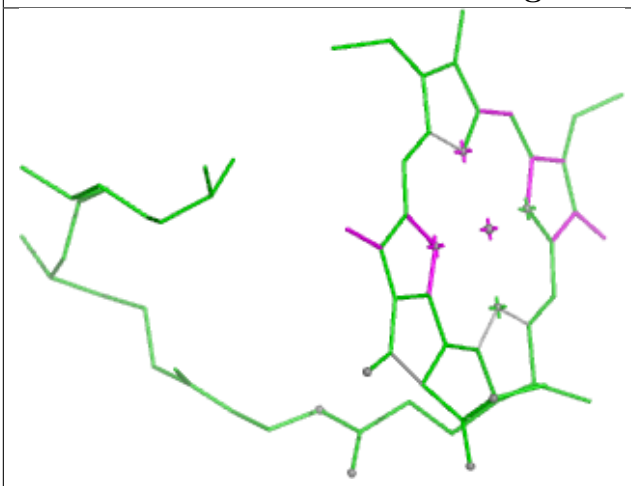


Rings

Ligand CLA C 507



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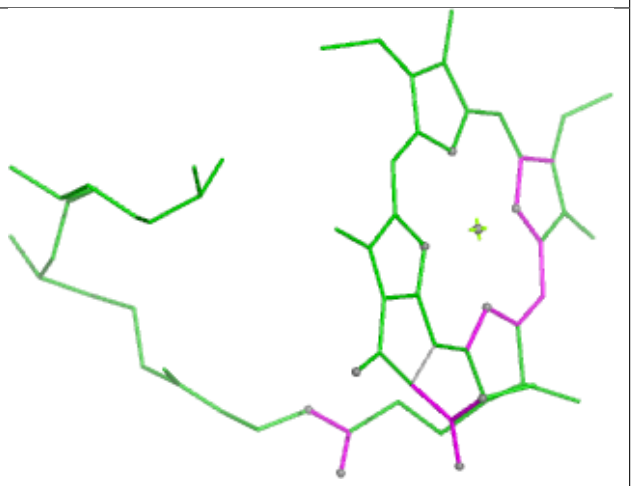
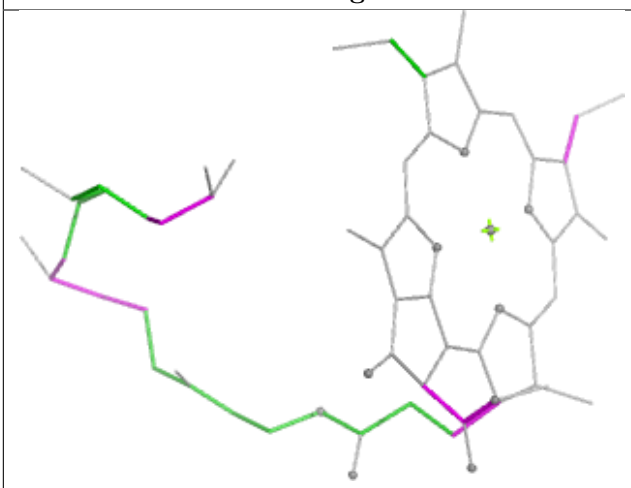


Bond angles



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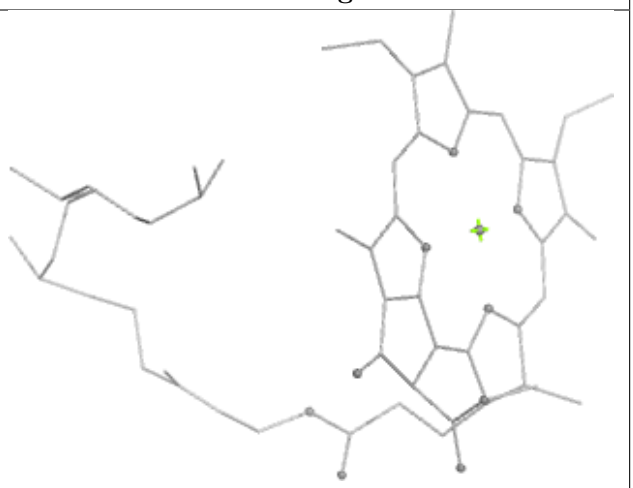
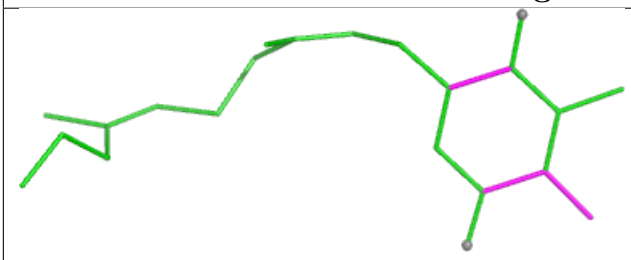


Rings

Ligand PL9 a 407



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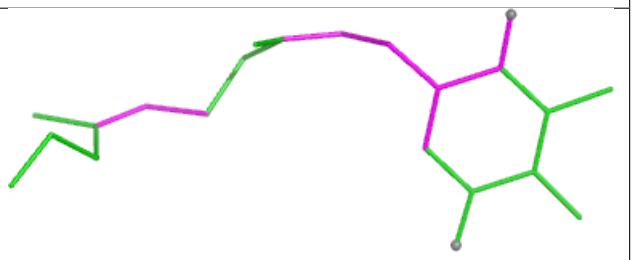
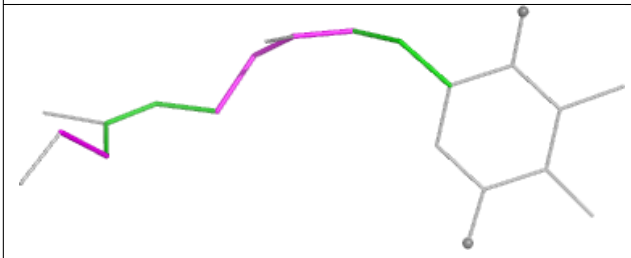


Bond angles



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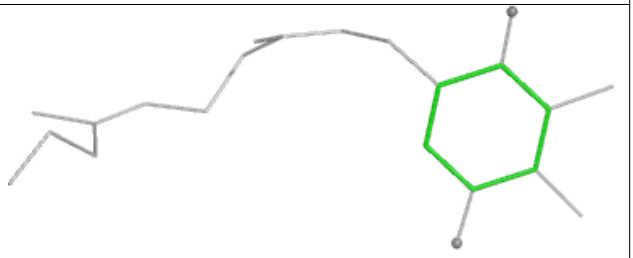
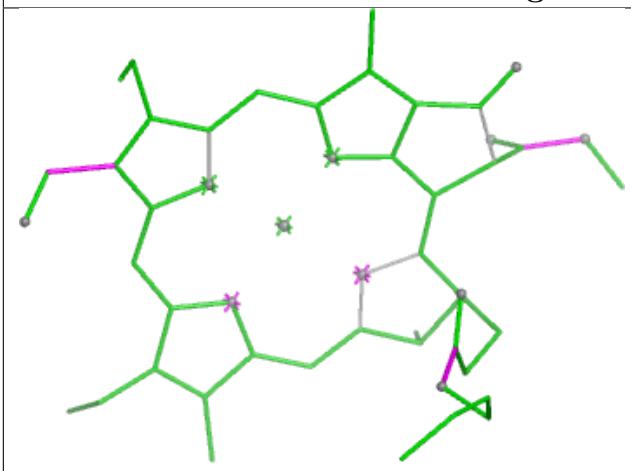


Rings

Ligand CHL n 307



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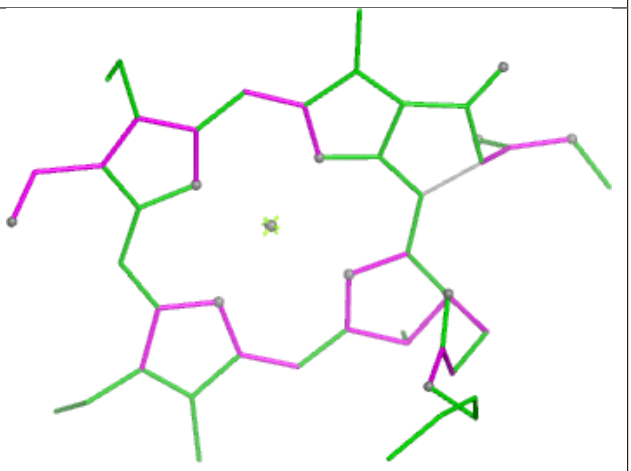
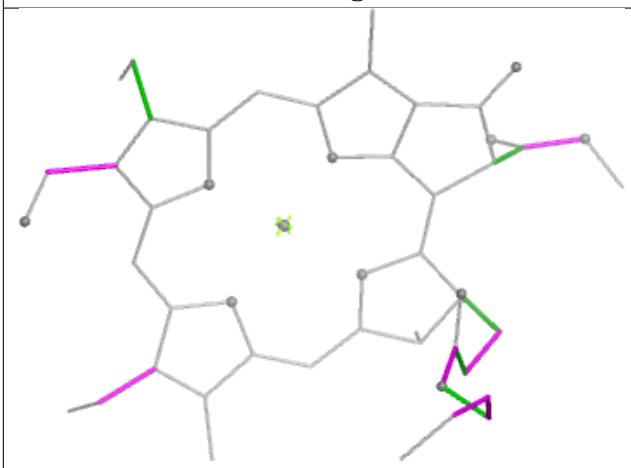


Bond angles



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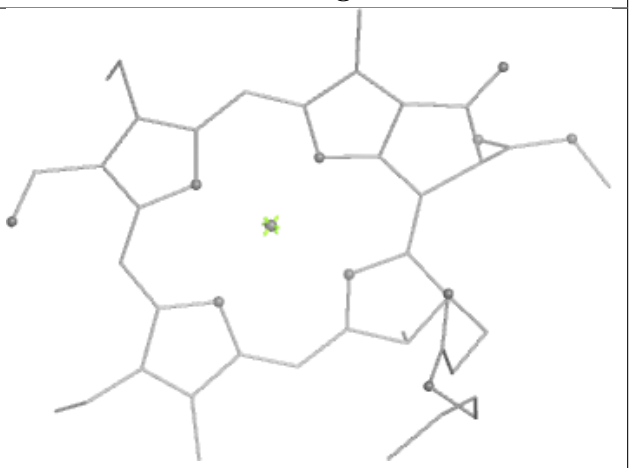
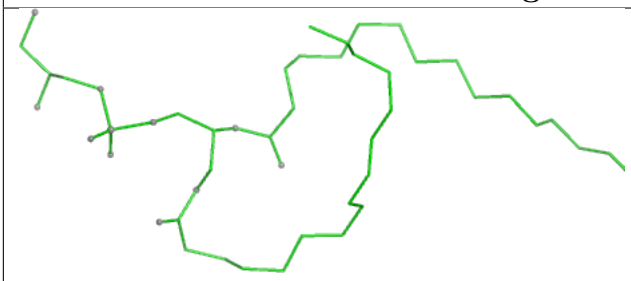


Rings

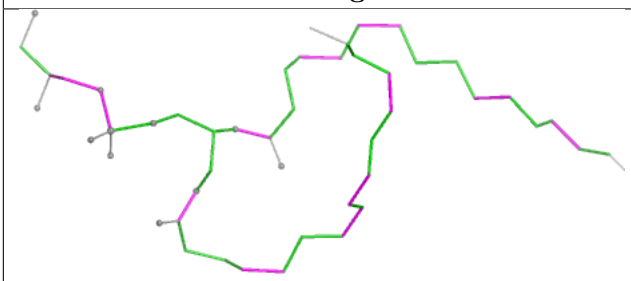
Ligand LHG R 303



Bond lengths



Bond angles

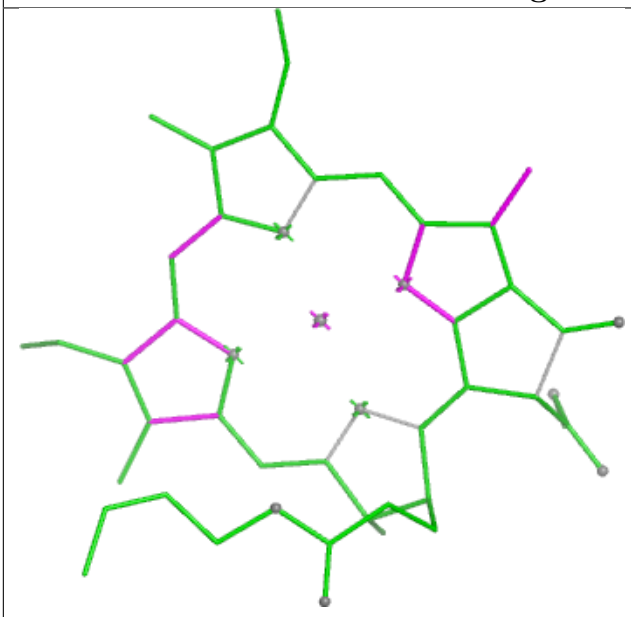


Torsions



Rings

Ligand CLA s 311



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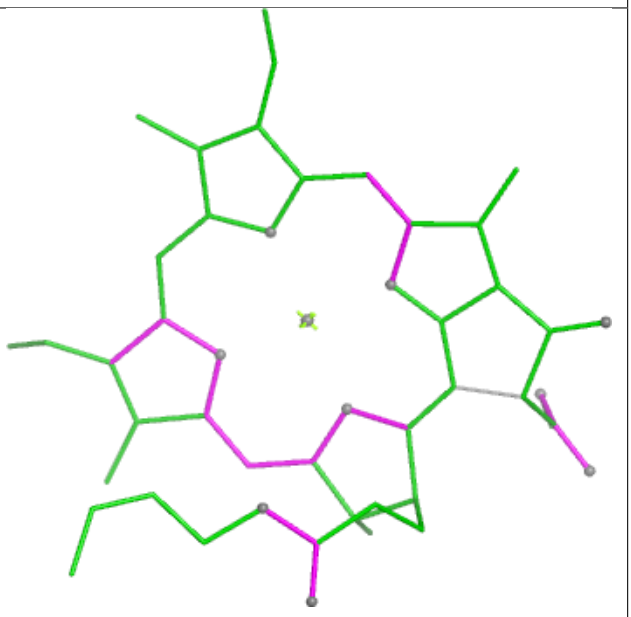
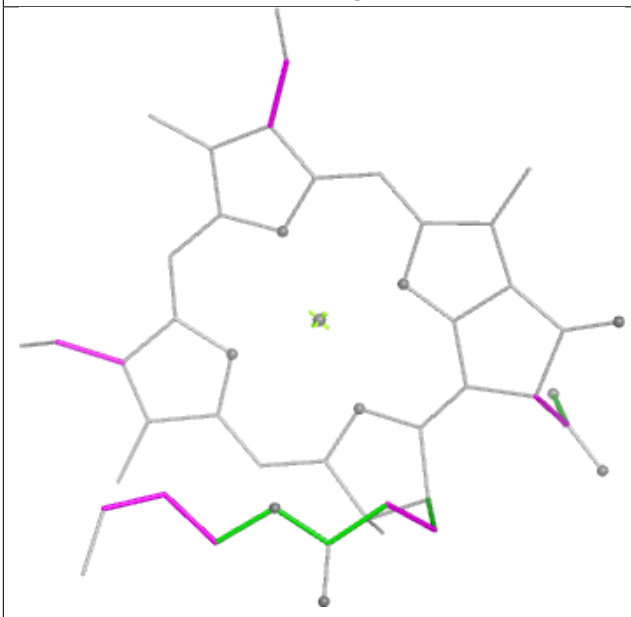


Bond angles



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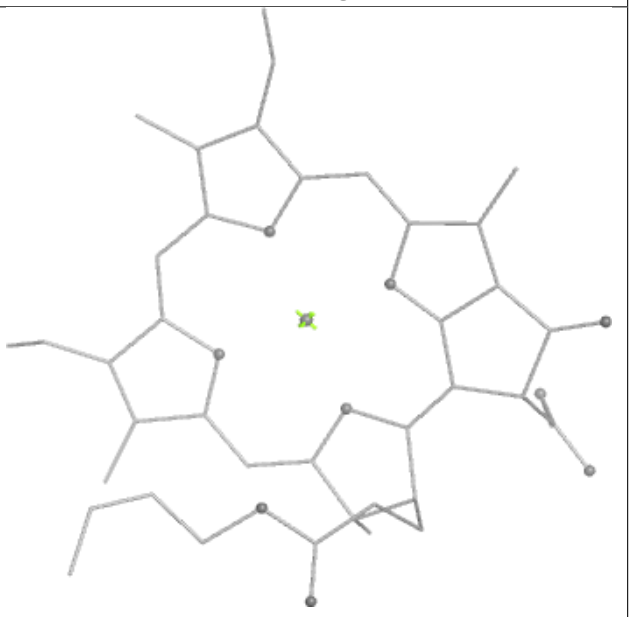
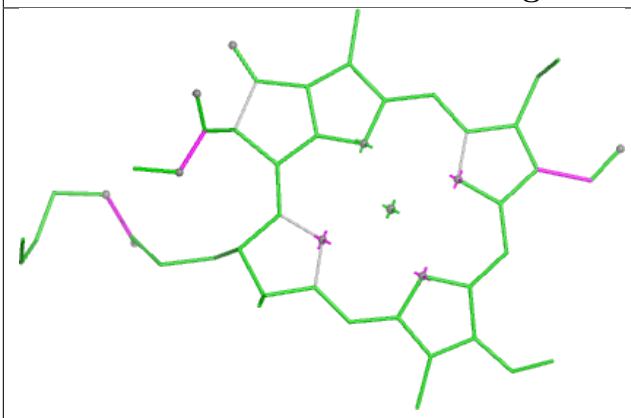


Rings

Ligand CHL G 301



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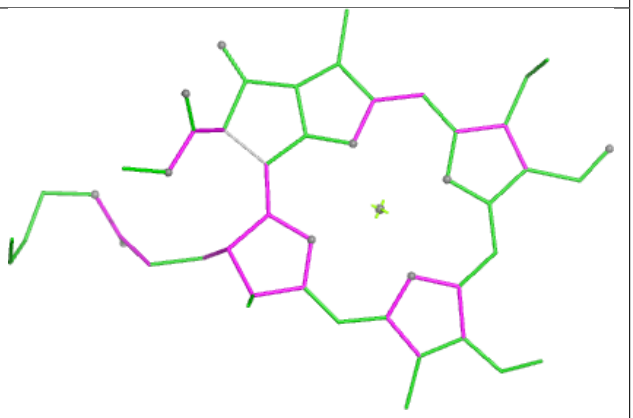
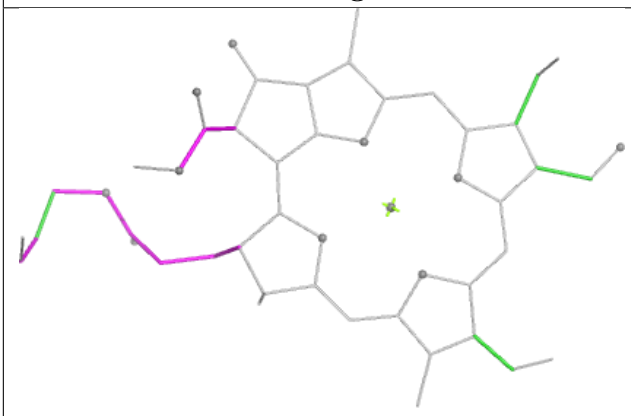


Bond angles



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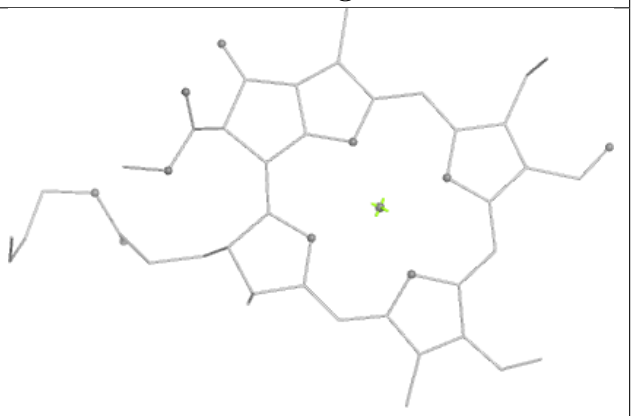
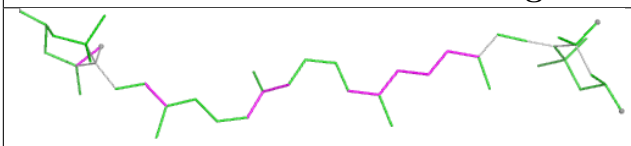


Rings

Ligand NEX S 305



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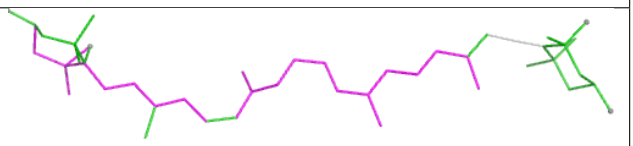
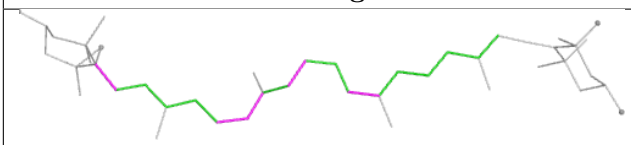


Bond angles



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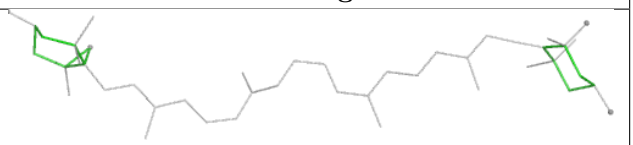
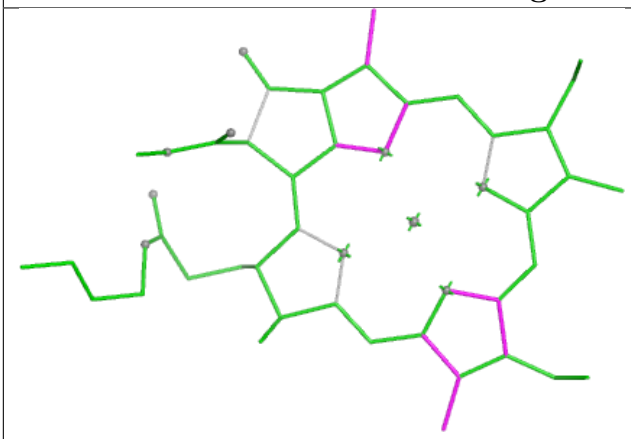


Rings

Ligand CLA r 313



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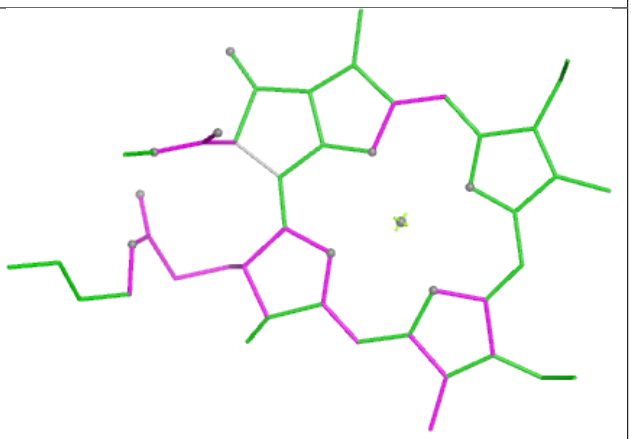
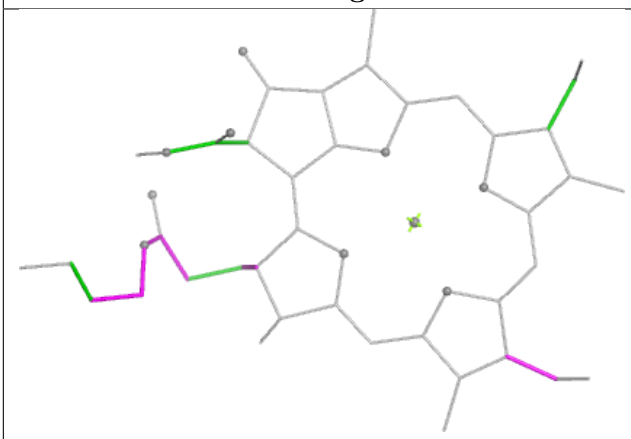


Bond angles



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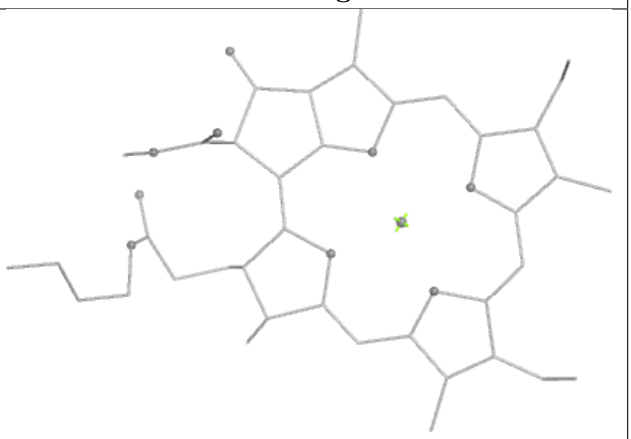
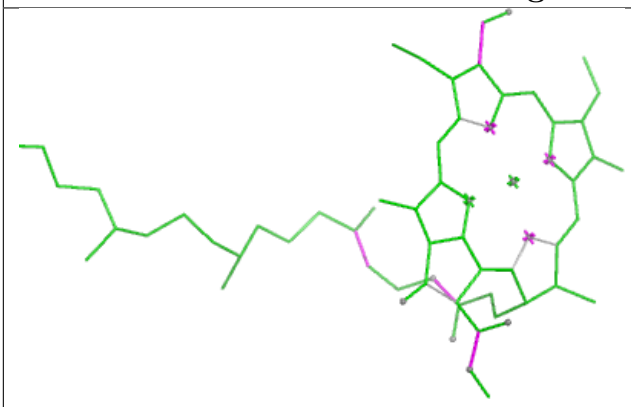


Rings

Ligand CHL y 314



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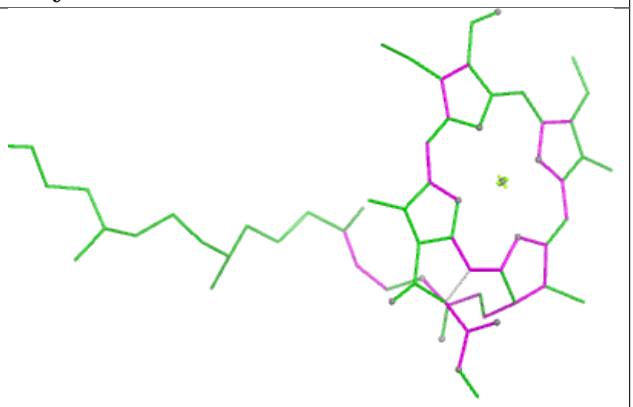
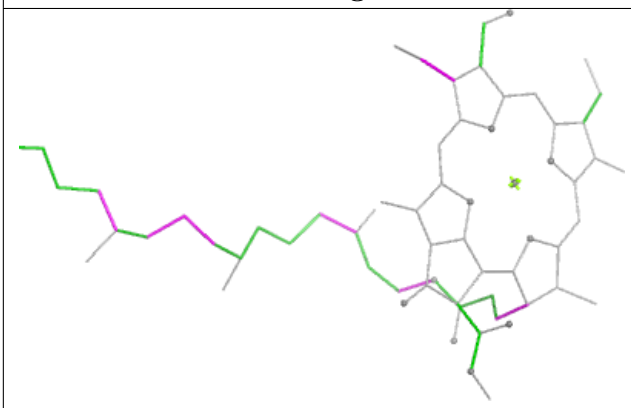


Bond angles

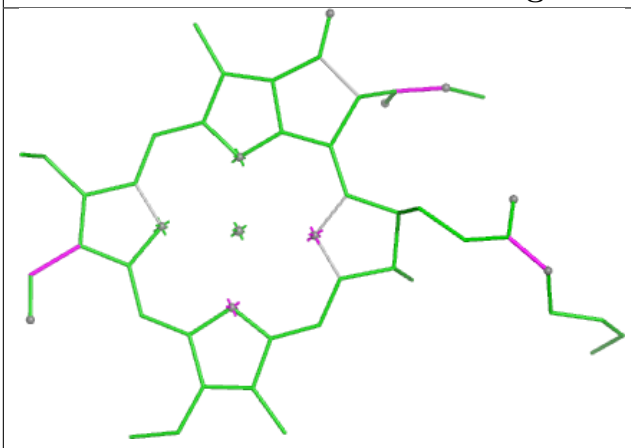


Torsions



Rings

Ligand CHL n 306



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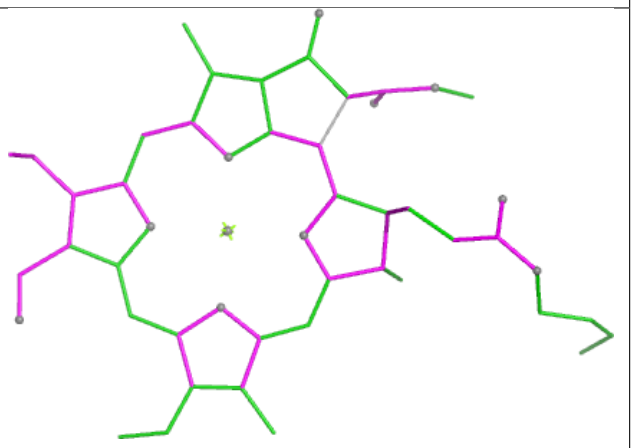
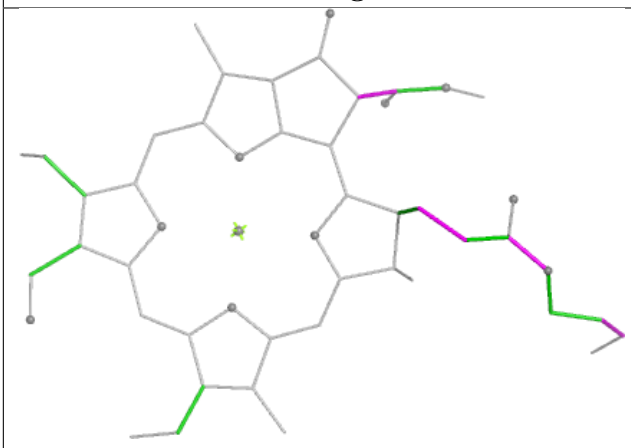


Bond angles



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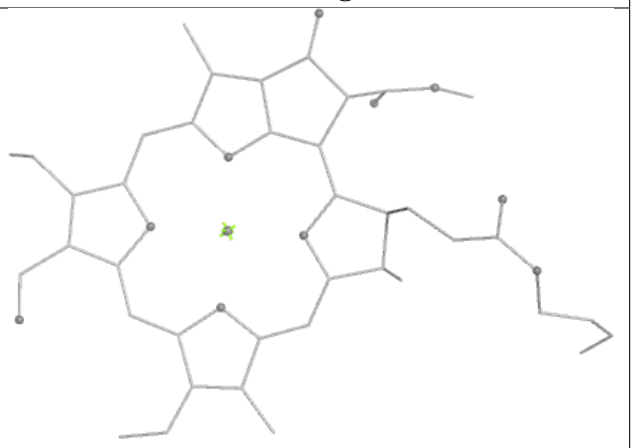
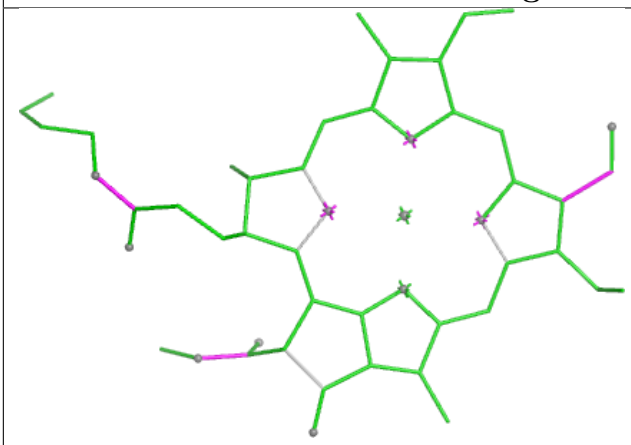


Rings

Ligand CHL N 316



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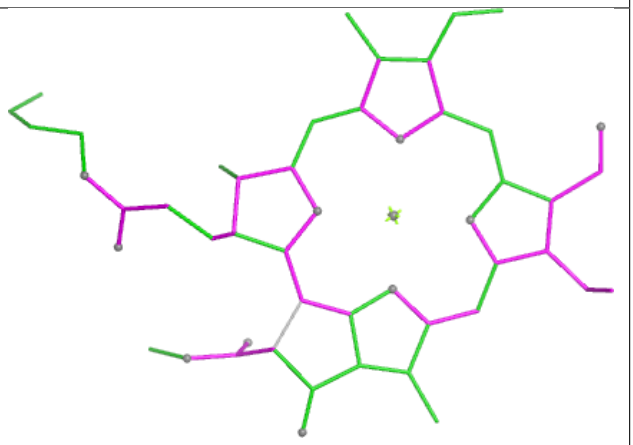
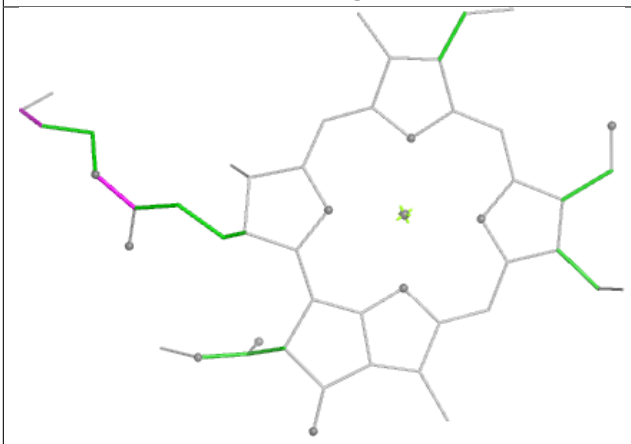
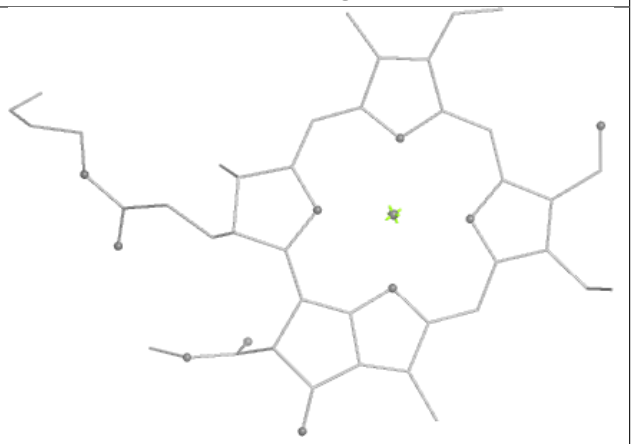


Bond angles

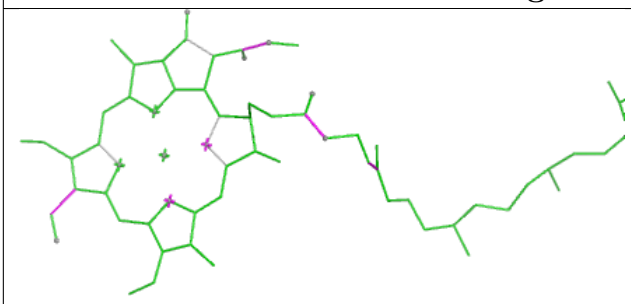


Torsions

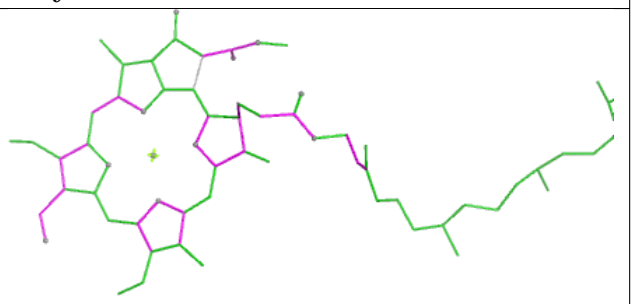


Rings

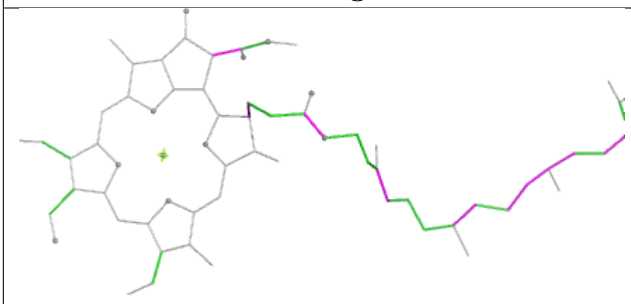
Ligand CHL y 303



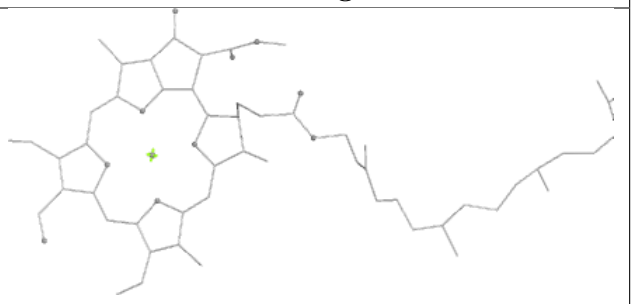
Bond lengths



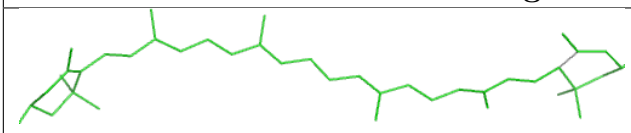
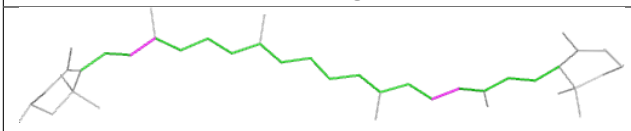
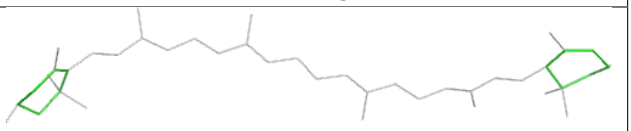
Bond angles

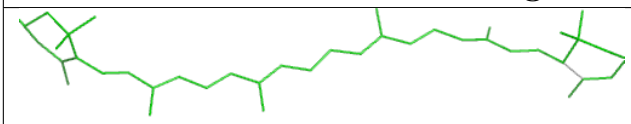
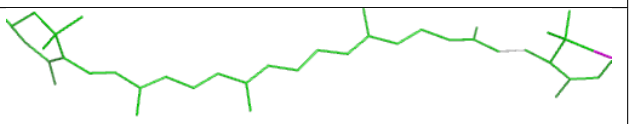
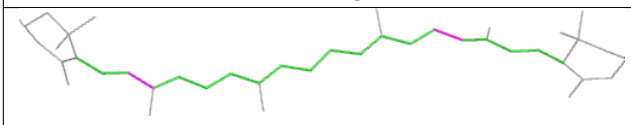
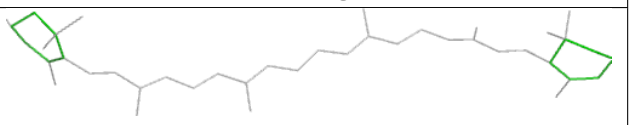


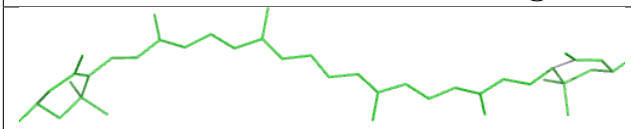
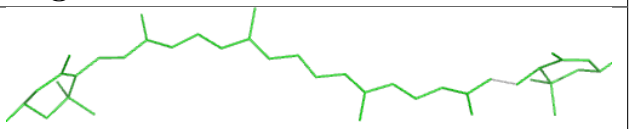
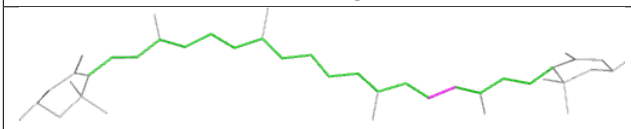
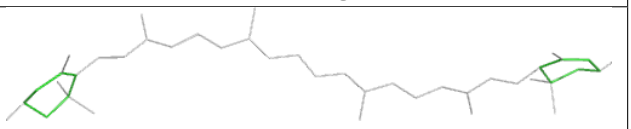
Torsions



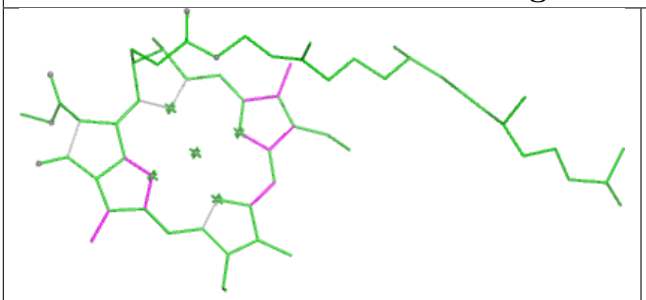
Rings

Ligand LUT N 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

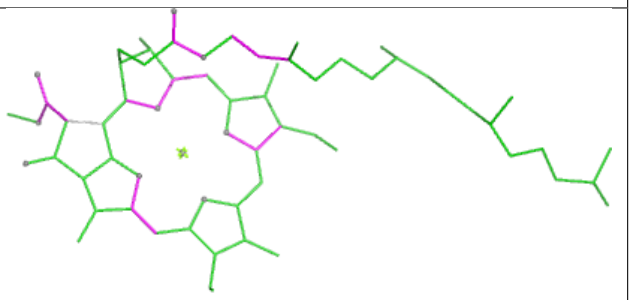
Ligand LUT Y 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT g 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

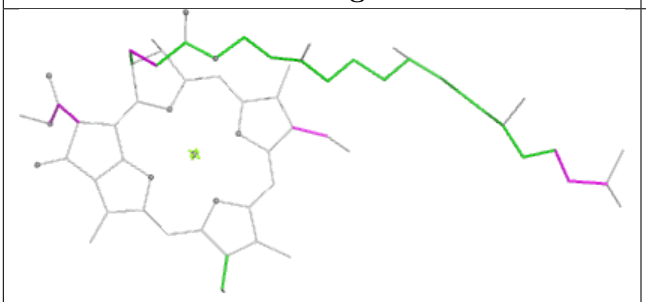
Ligand CLA c 520



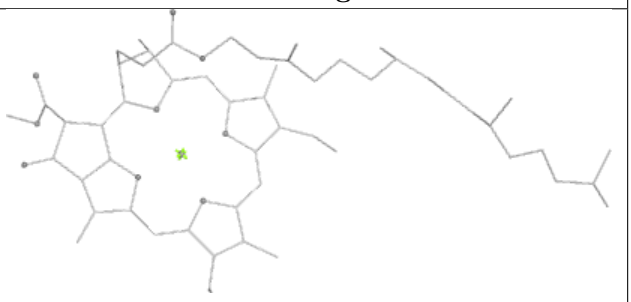
Bond lengths



Bond angles

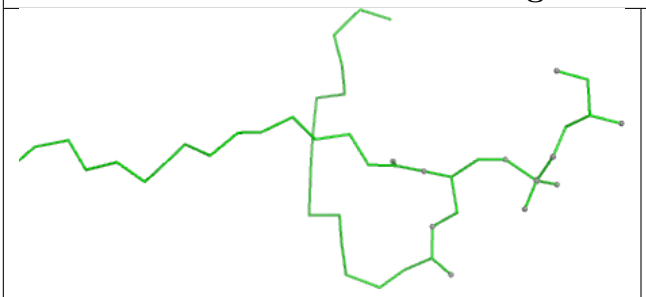


Torsions



Rings

Ligand LHG g 301



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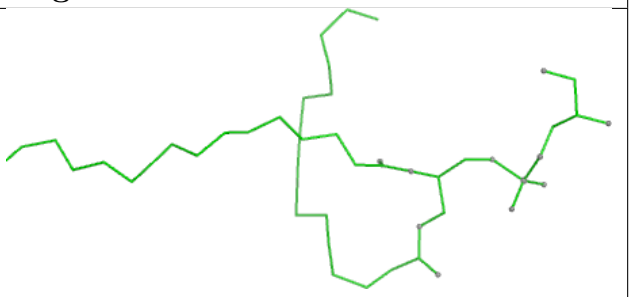
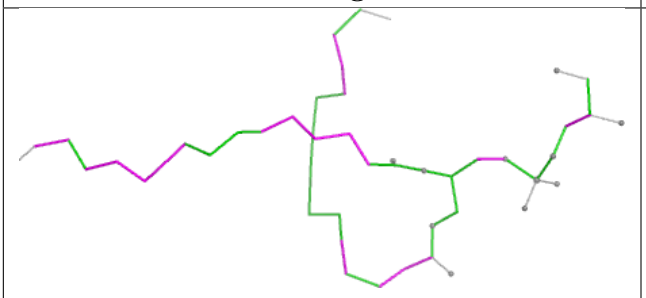
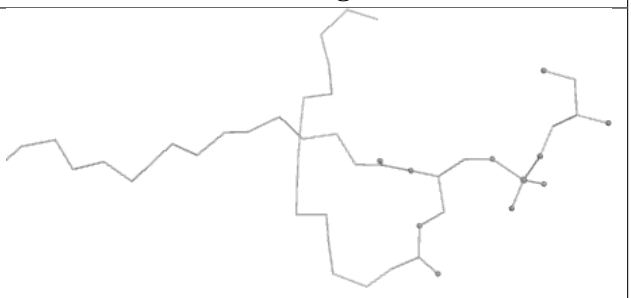


Bond angles

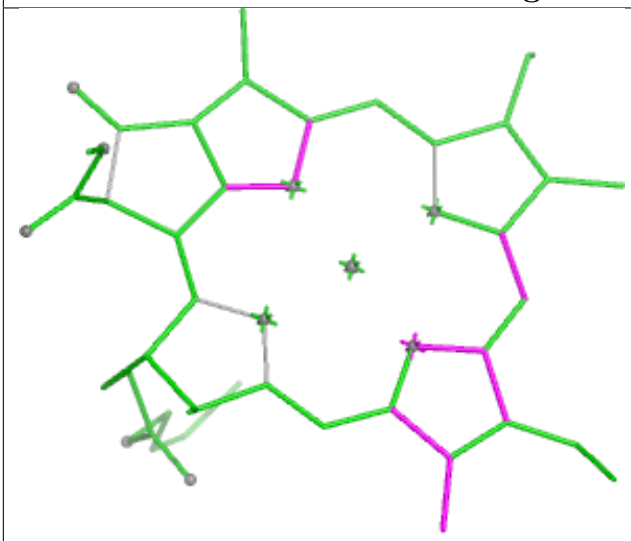


Torsions



Rings

Ligand CLA G 302



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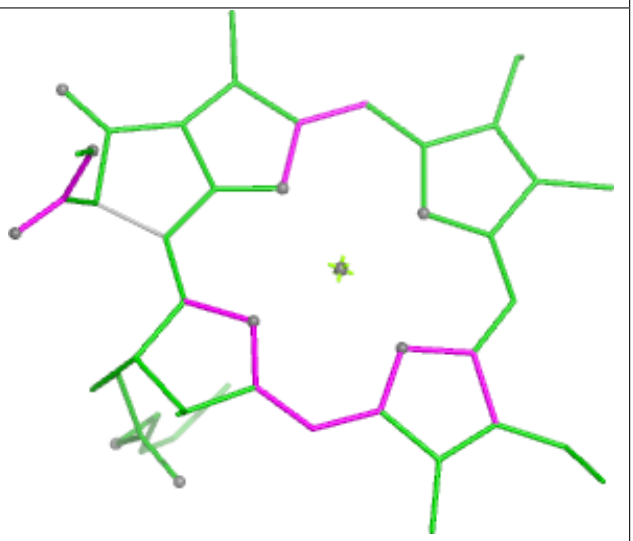
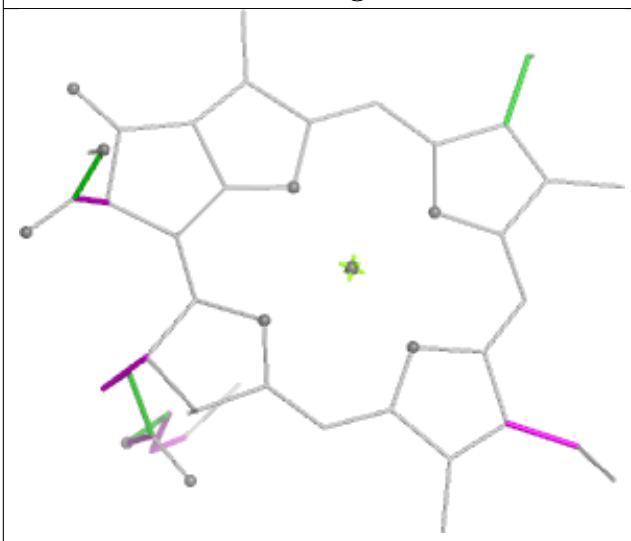


Bond angles



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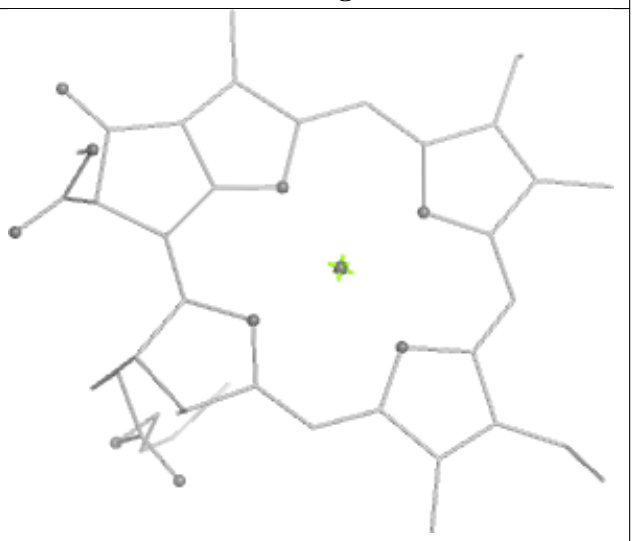
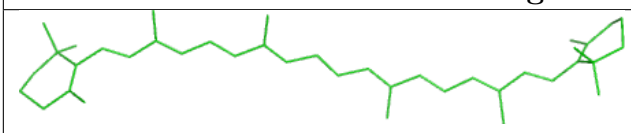


Rings

Ligand BCR a 404



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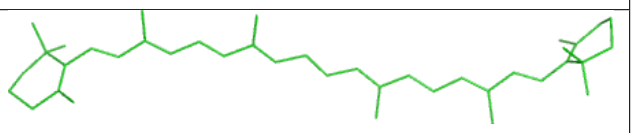
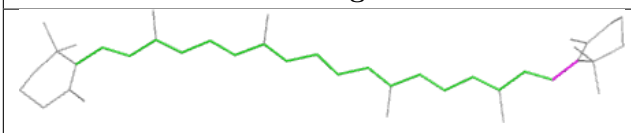


Bond angles



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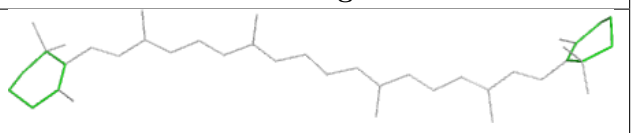
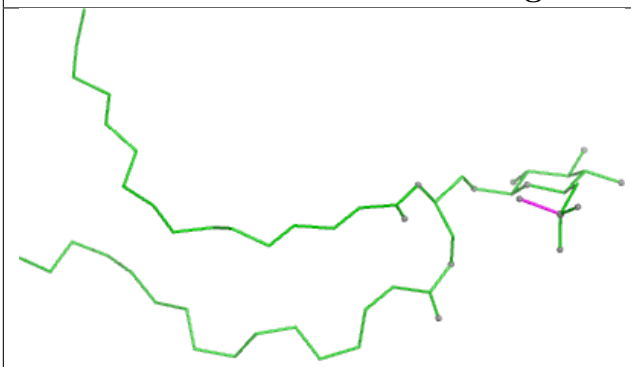


Rings

Ligand SQD B 621



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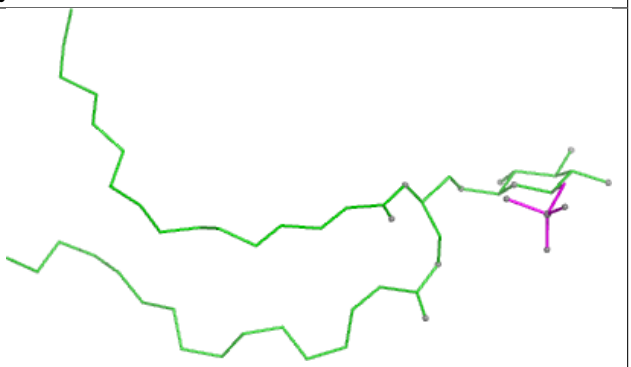
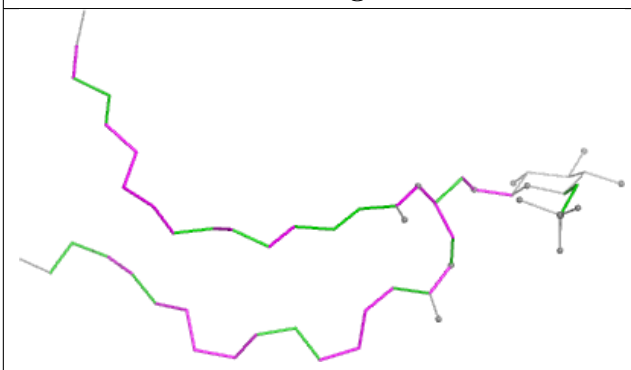
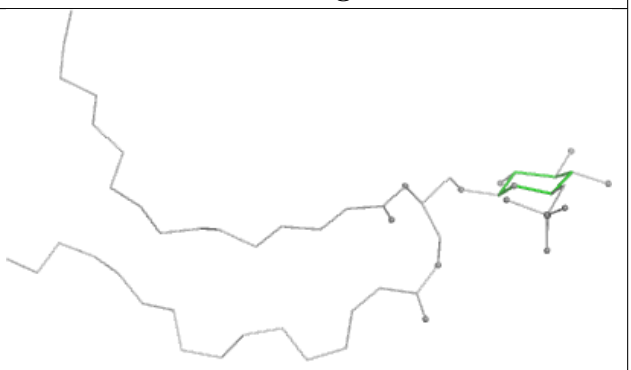


Bond angles



Torsions



Rings

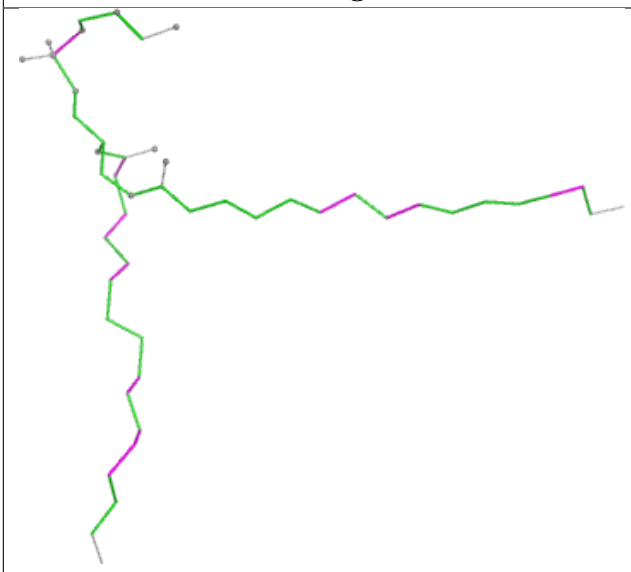
Ligand LHG l 101



Bond lengths



Bond angles

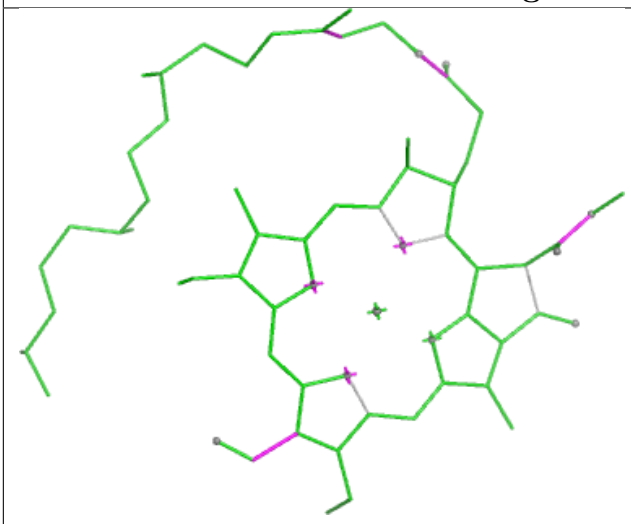


Torsions



Rings

Ligand CHL N 303



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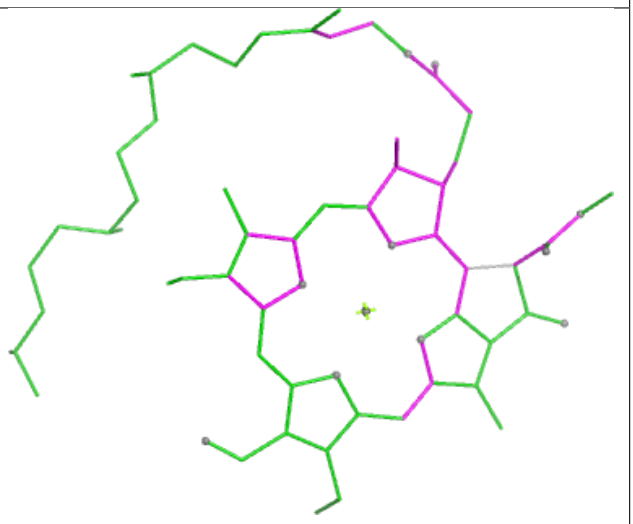
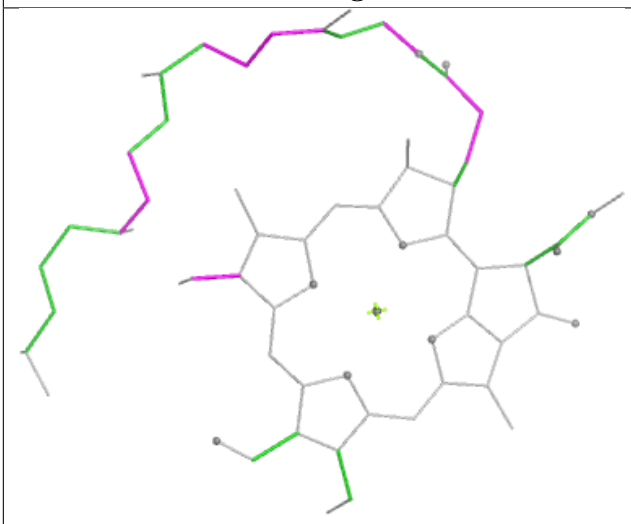


Bond angles



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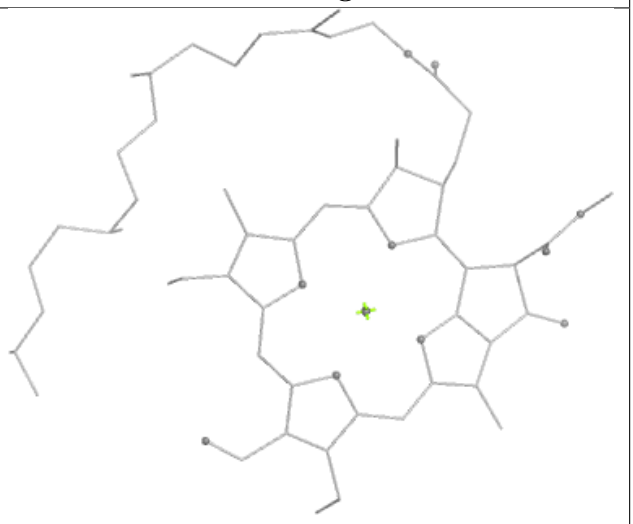
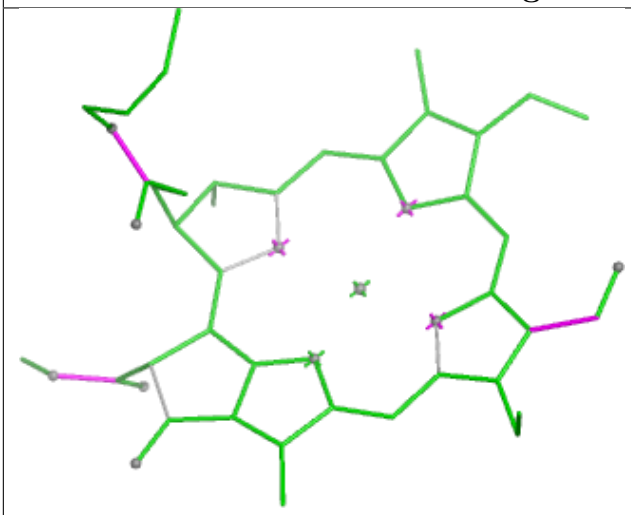


Rings

Ligand CHL G 303



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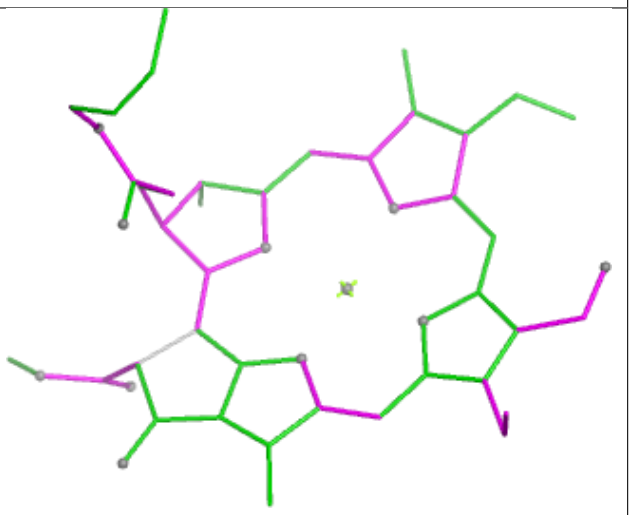
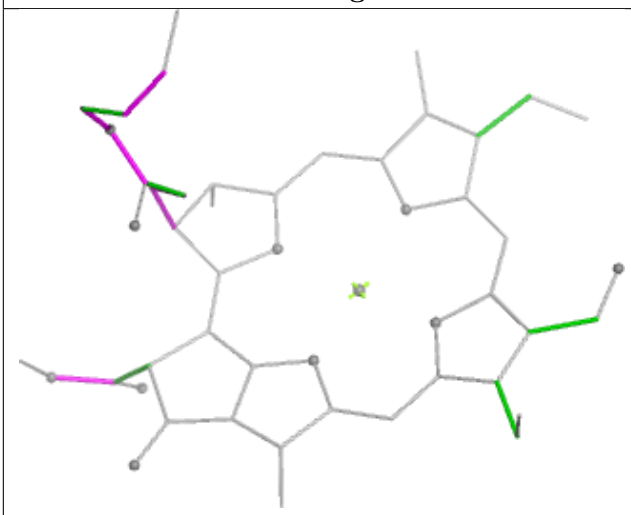


Bond angles



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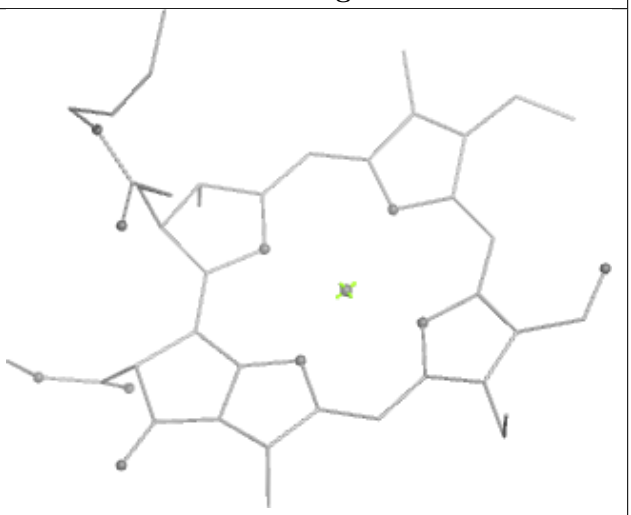
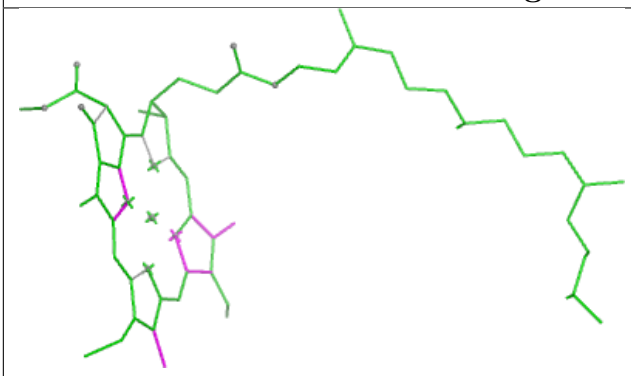


Rings

Ligand CLA B 613



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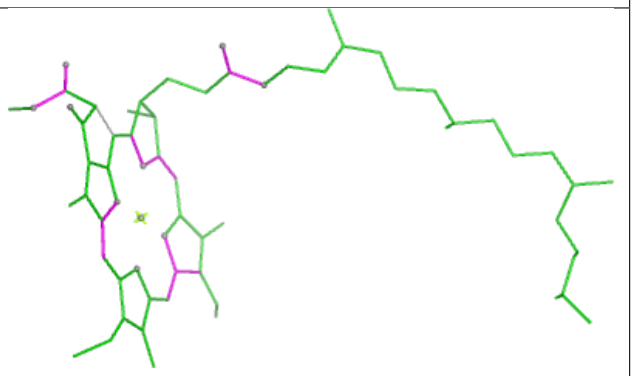
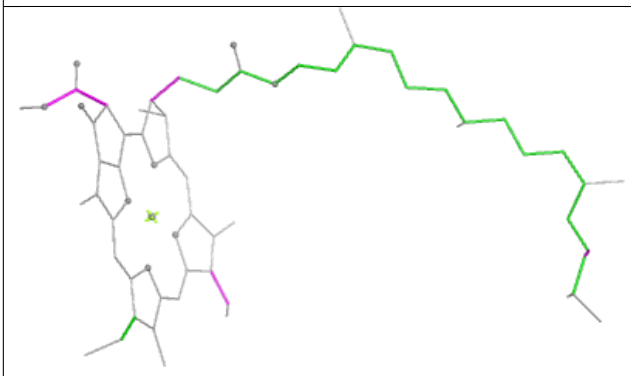


Bond angles



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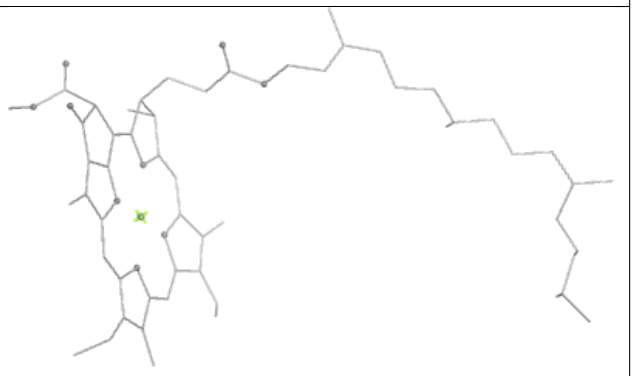
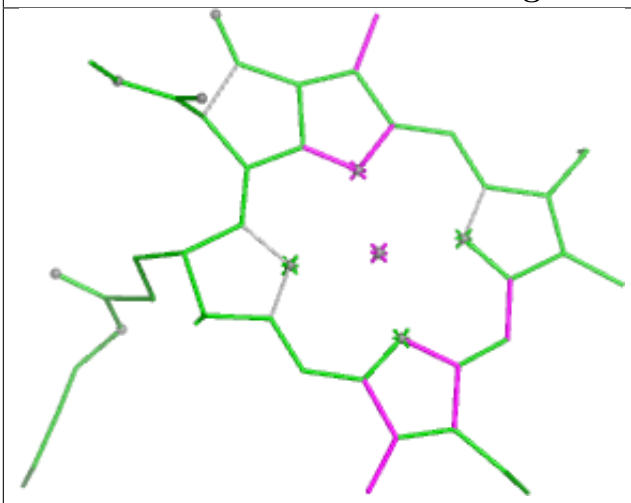


Rings

Ligand CLA G 313



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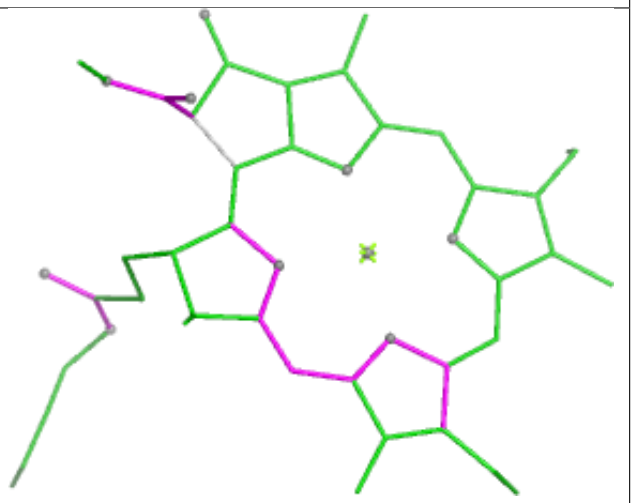
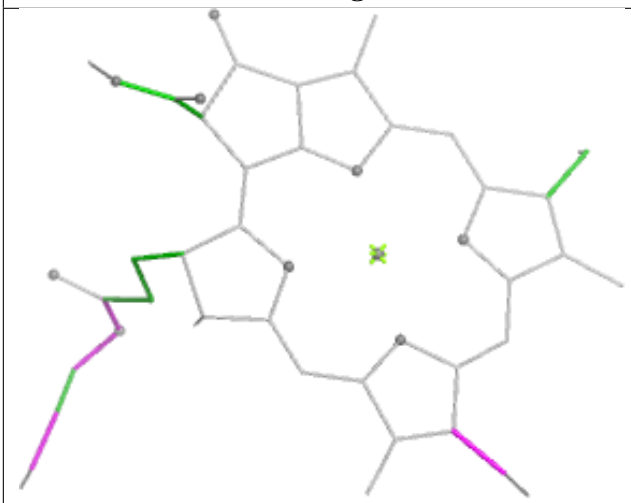


Bond angles

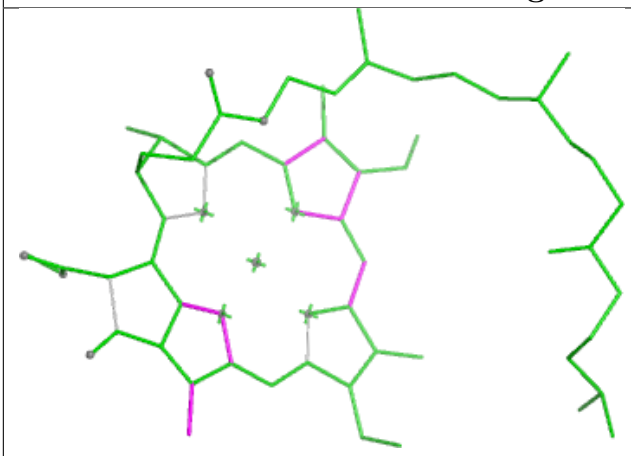


Torsions



Rings

Ligand CLA n 305



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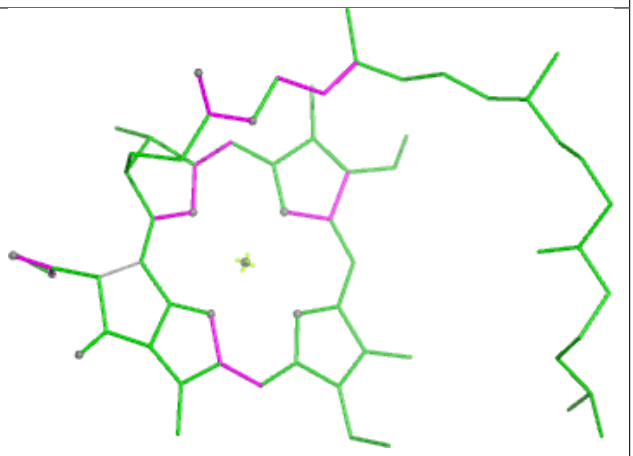
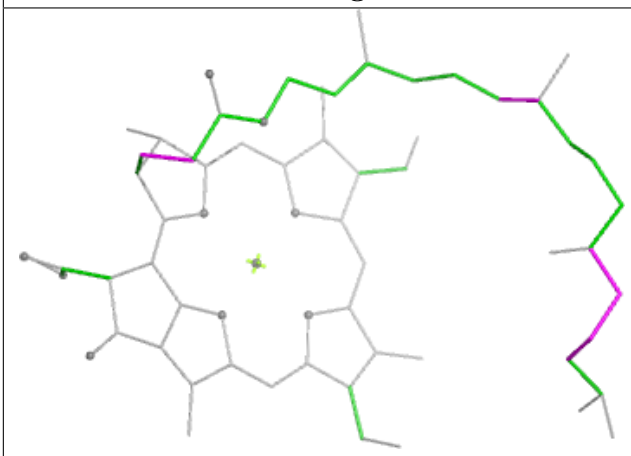


Bond angles



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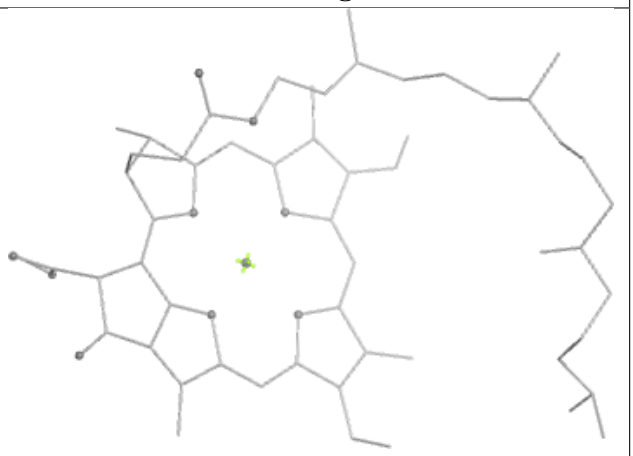
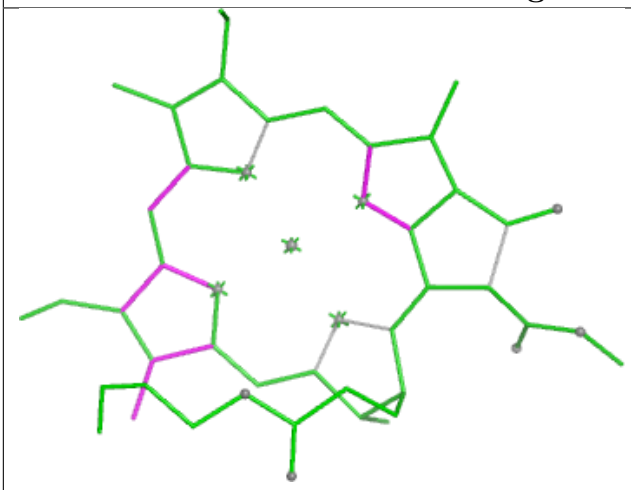
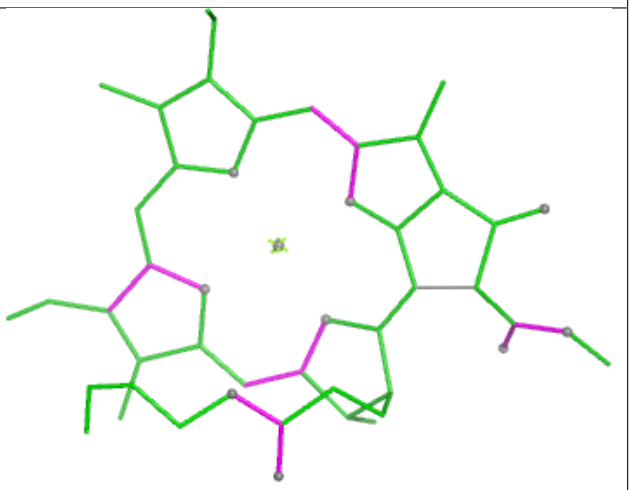


Rings

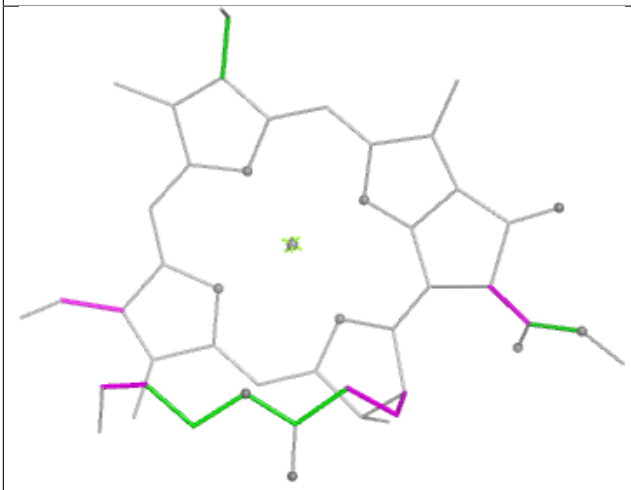
Ligand CLA S 314



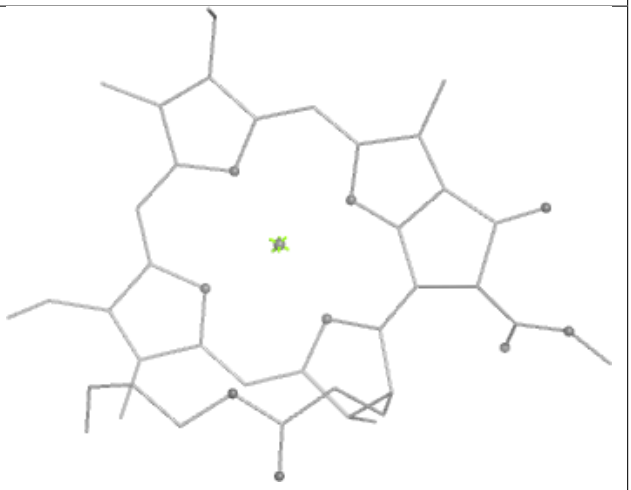
Bond lengths



Bond angles



Torsions



Rings

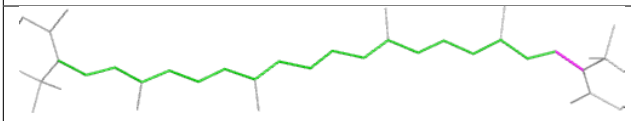
Ligand BCR b 615



Bond lengths



Bond angles



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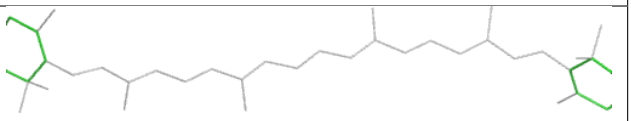
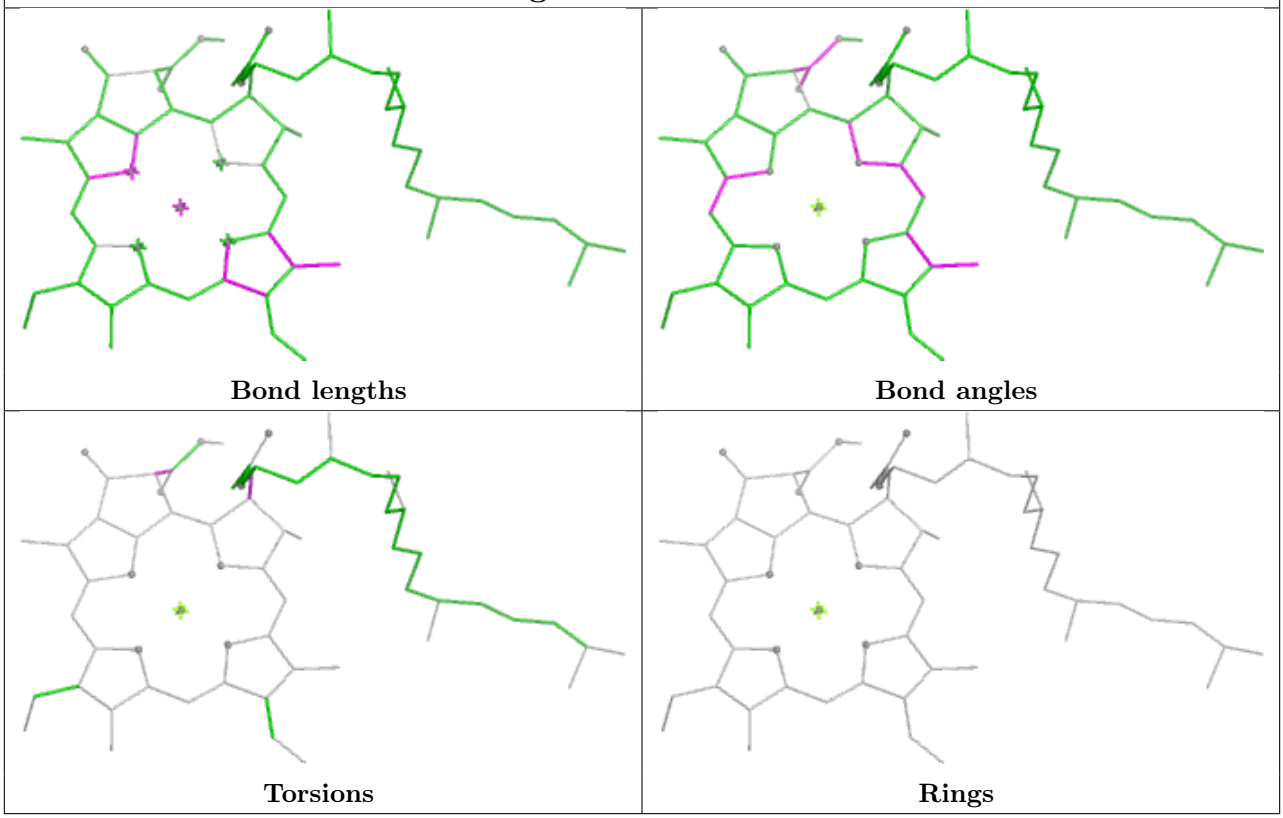


Rings

Ligand CLA a 409



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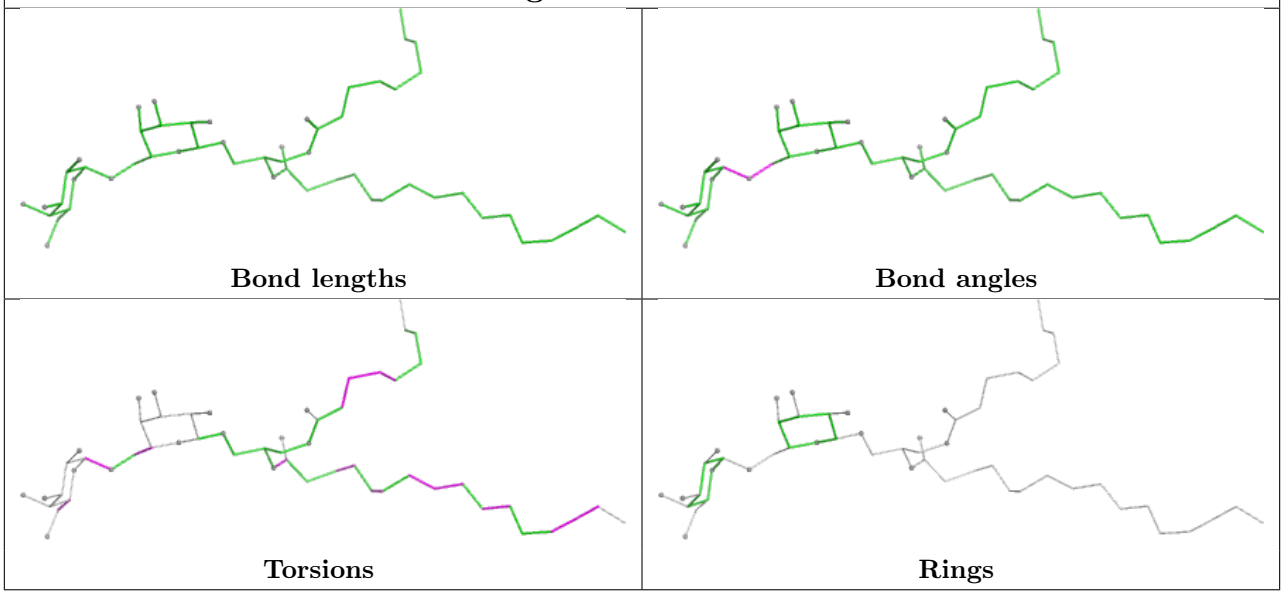
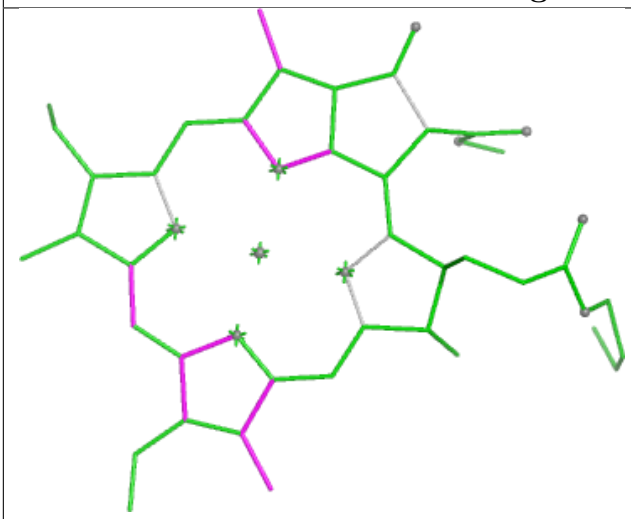
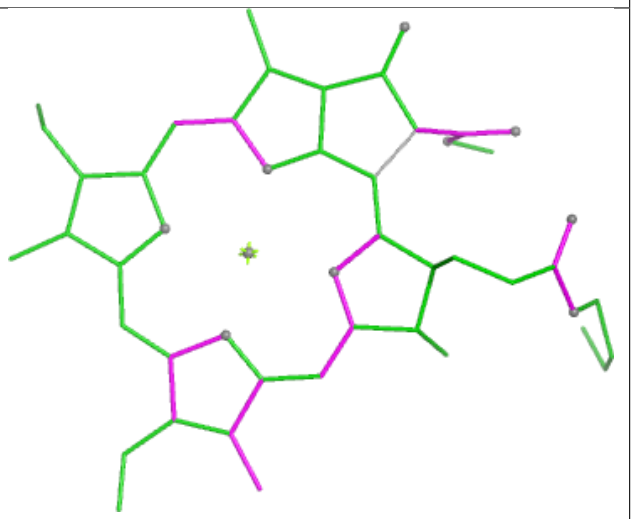


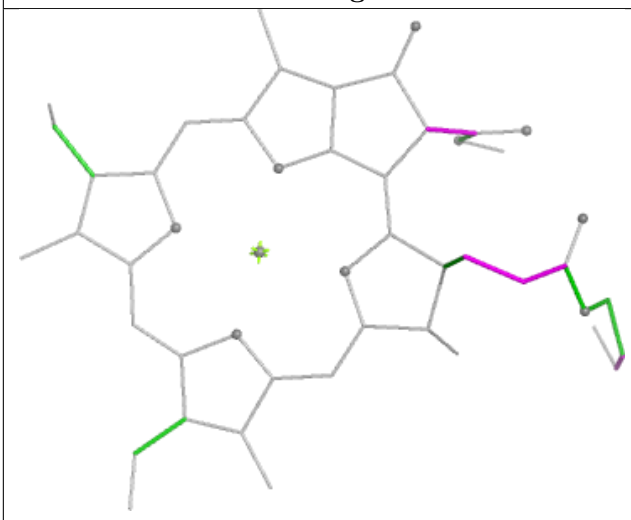
Ligand CLA r 315



Bond lengths



Bond angles



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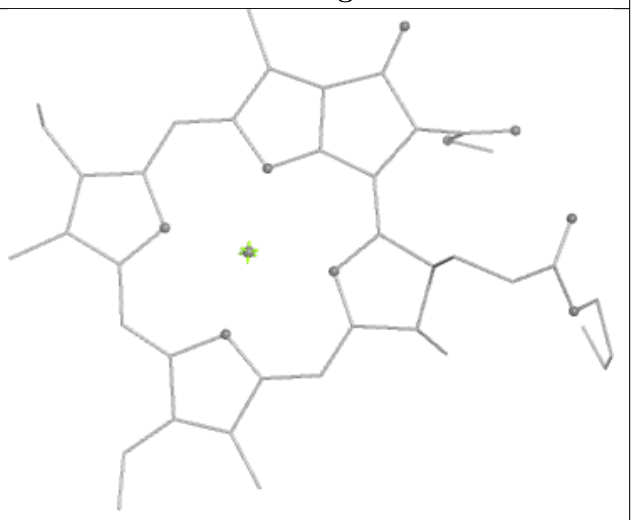
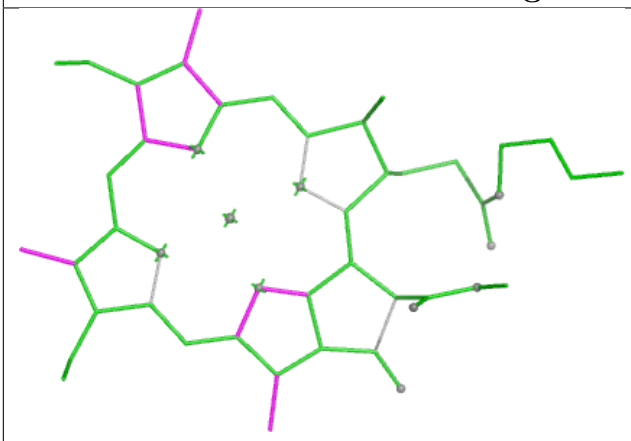


Rings

Ligand CLA R 302



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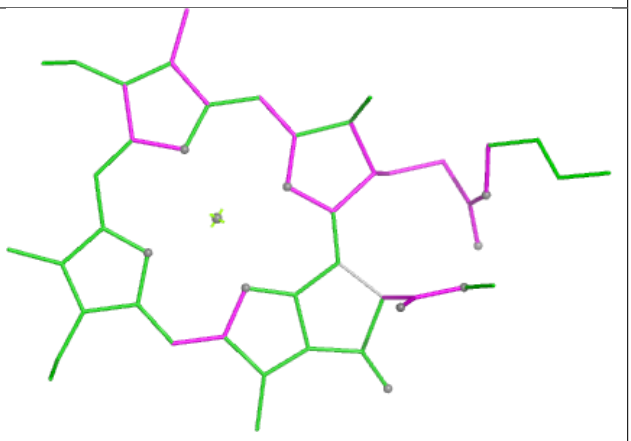
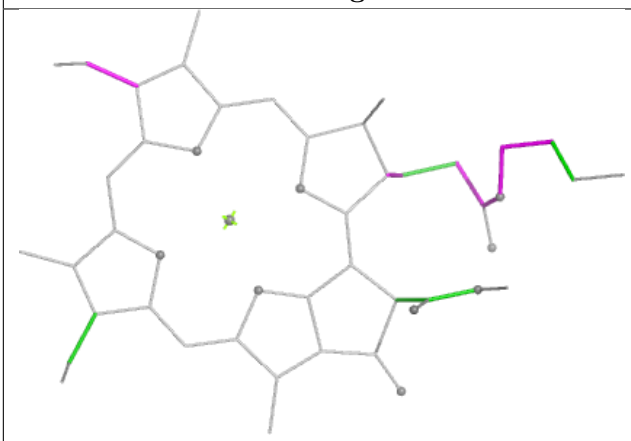


Bond angles



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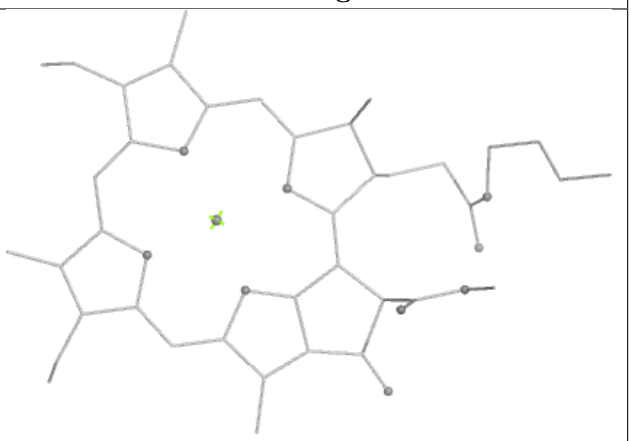
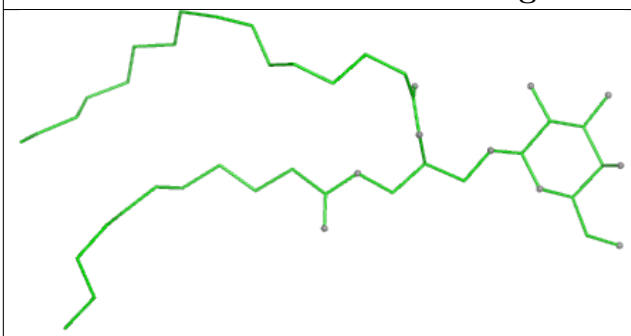


Rings

Ligand LMG D 404



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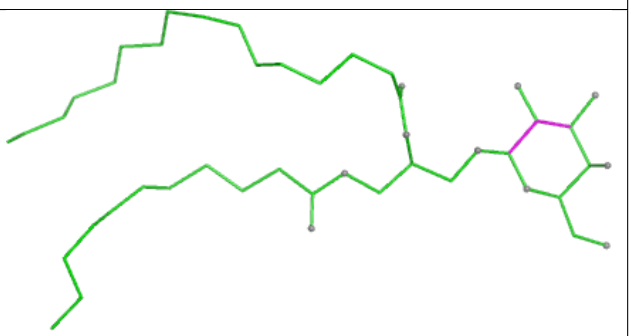
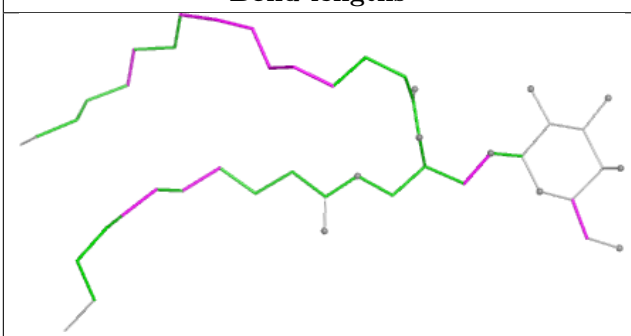


Bond angles



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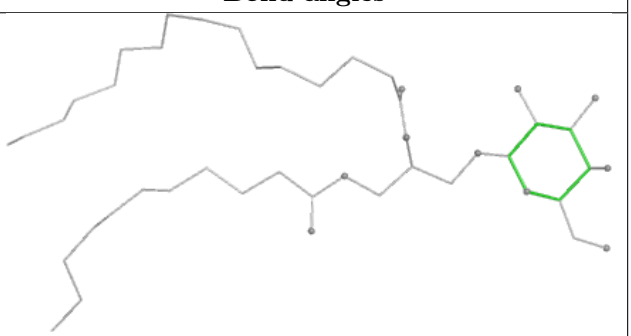
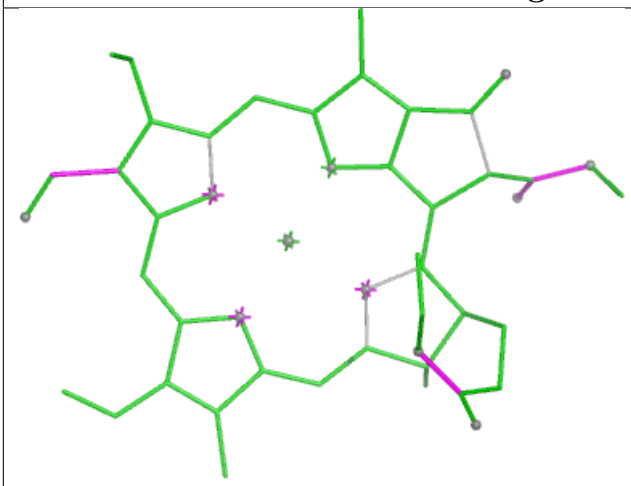


Rings

Ligand CHL g 314



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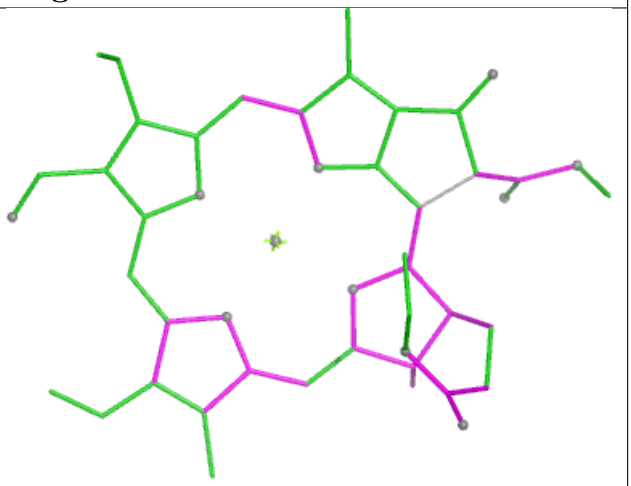
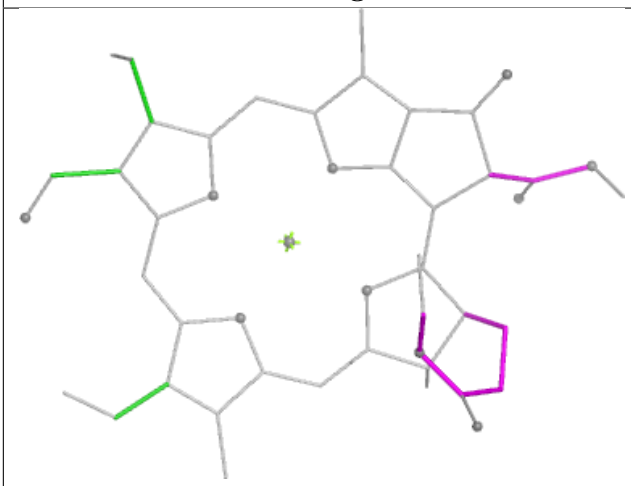


Bond angles



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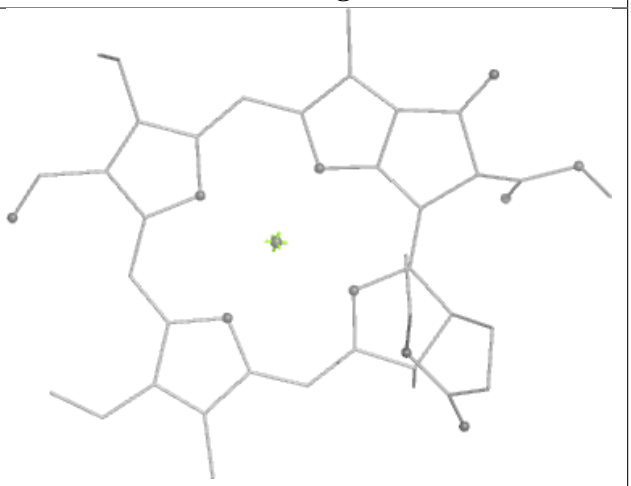
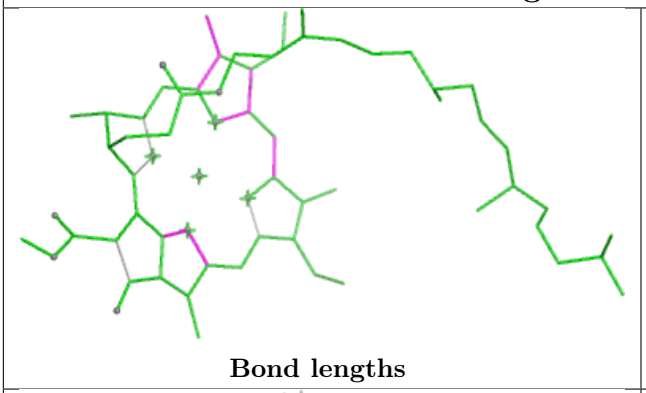


Rings

Ligand CLA N 312



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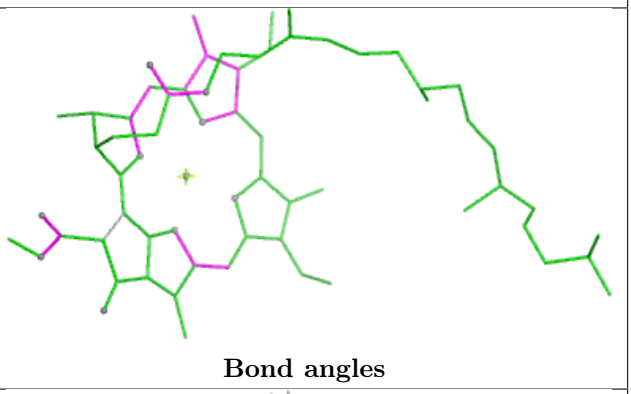
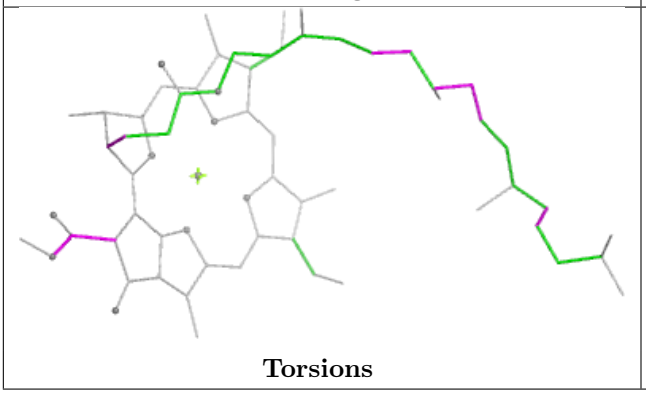


Bond angles



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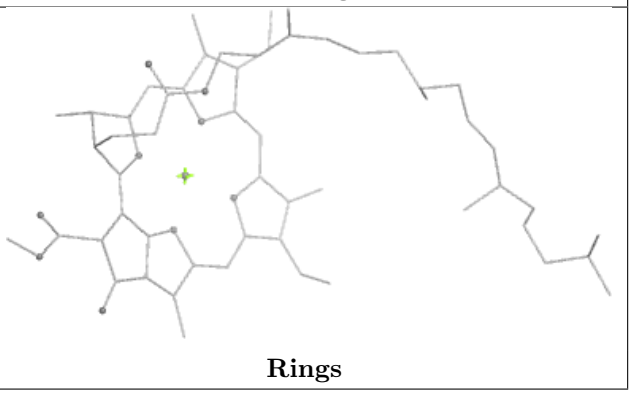
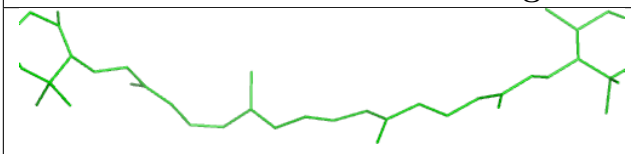


Rings

Ligand BCR T 101



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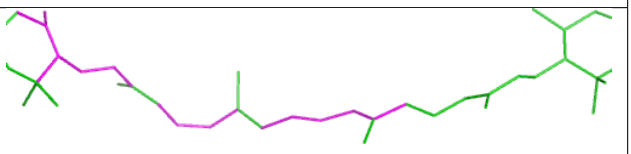

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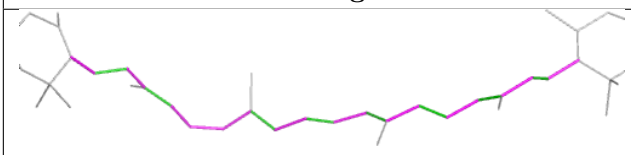

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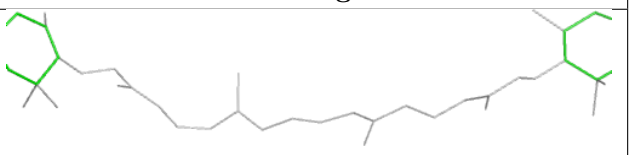
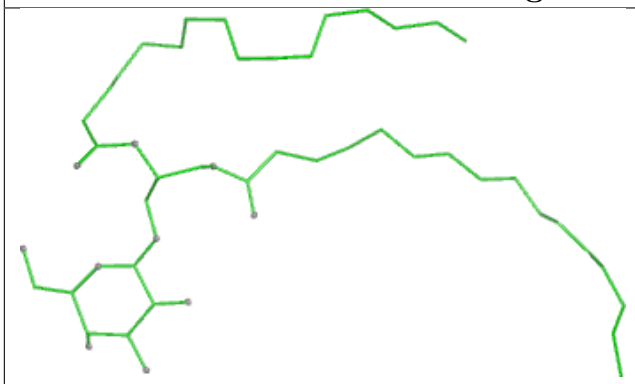


Rings

Ligand LMG c 509



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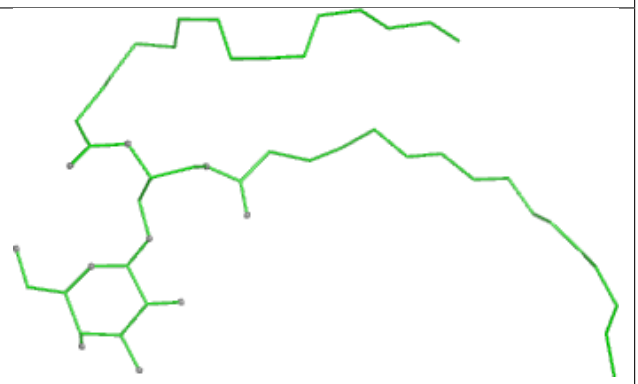
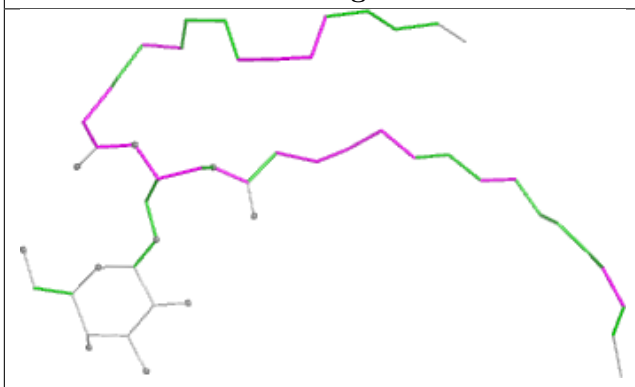


Bond angles

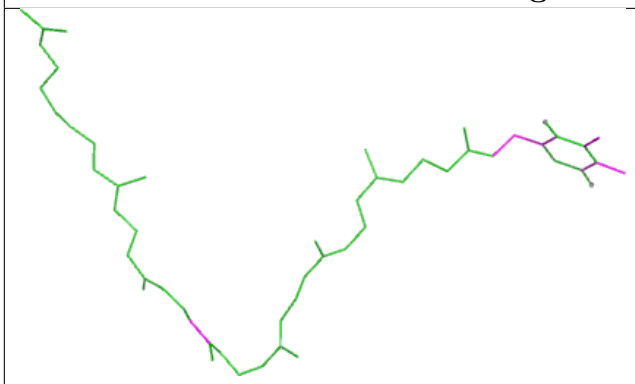


Torsions



Rings

Ligand PL9 D 411



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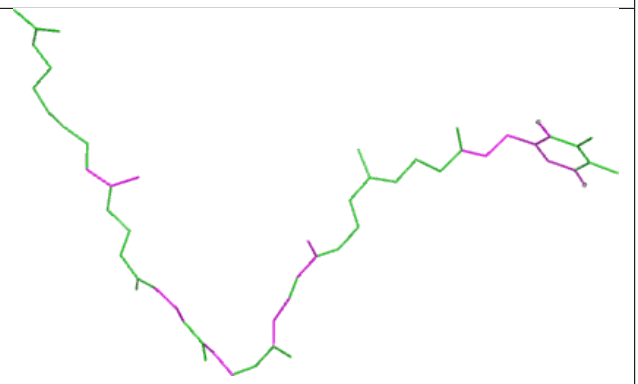

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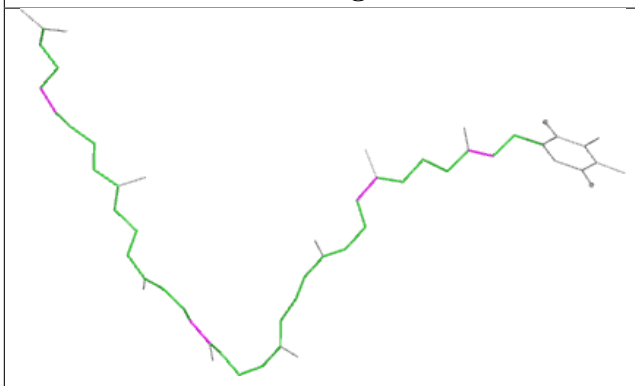

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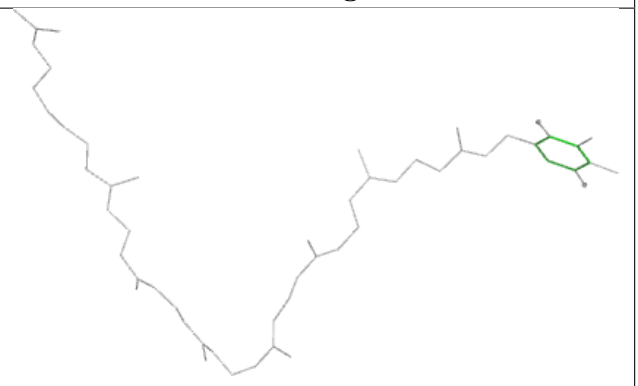
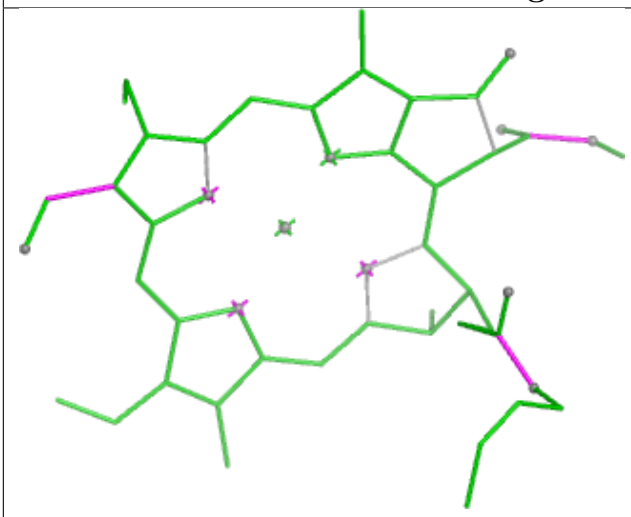


Rings

Ligand CHL g 307



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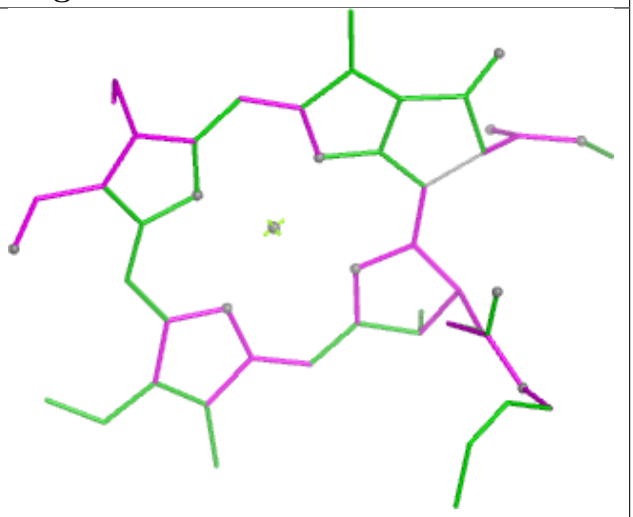
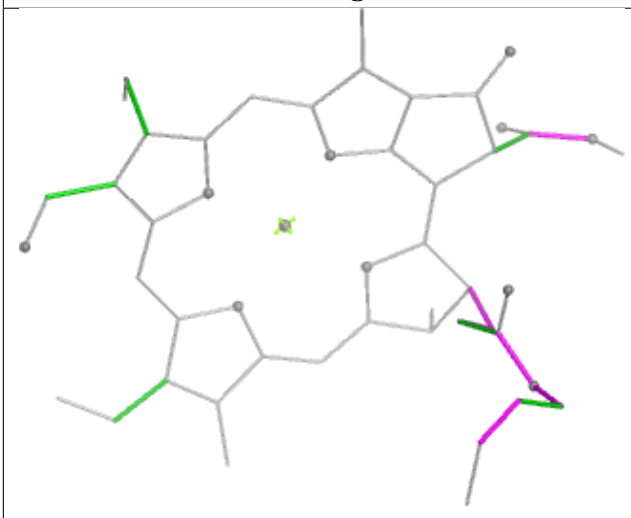


Bond angles

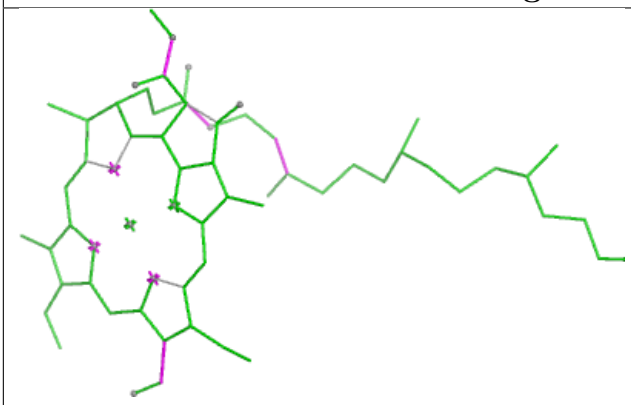


Torsions



Rings

Ligand CHL Y 307



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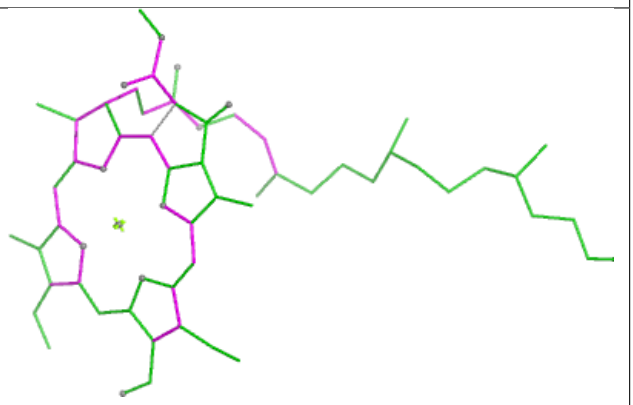
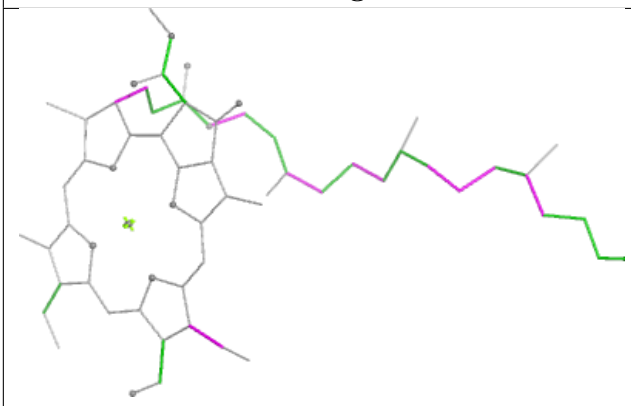


Bond angles



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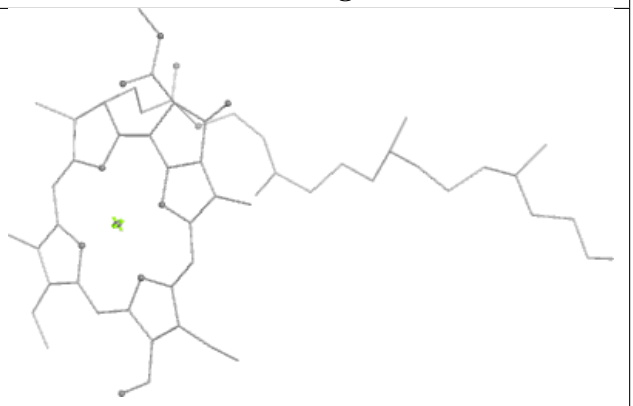
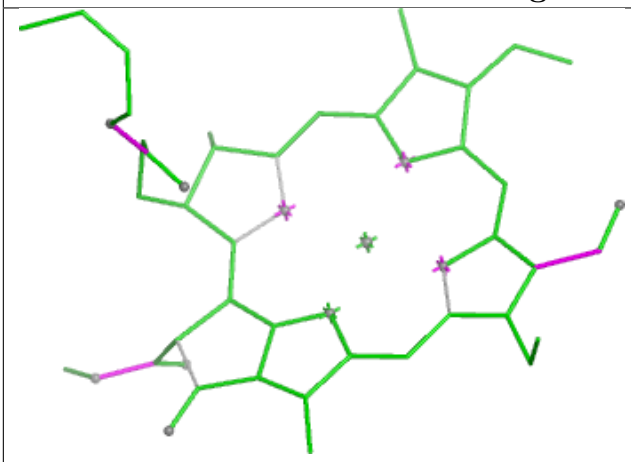


Rings

Ligand CHL r 309



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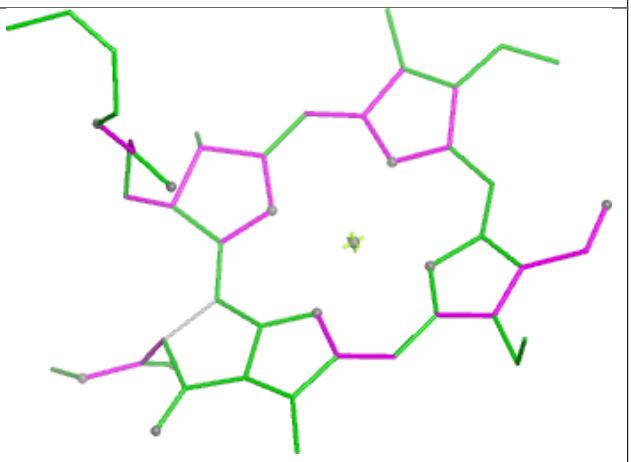
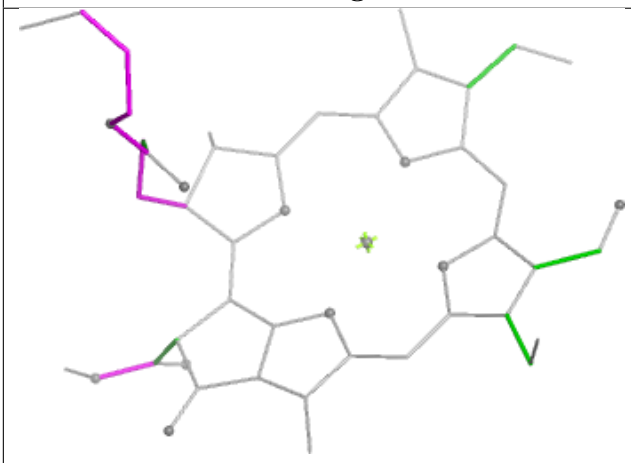


Bond angles



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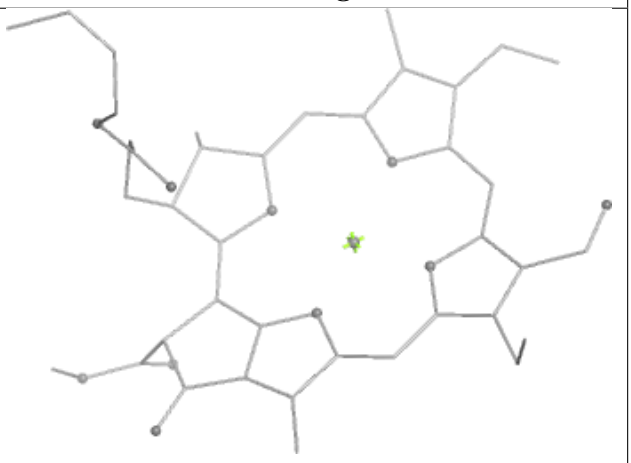
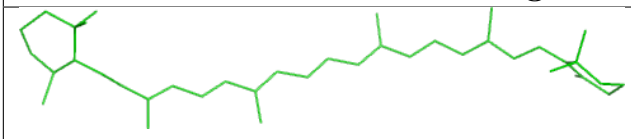


Rings

Ligand BCR k 101



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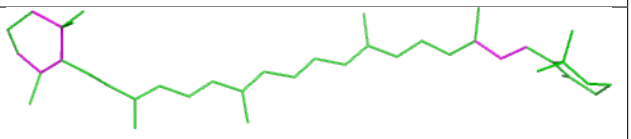
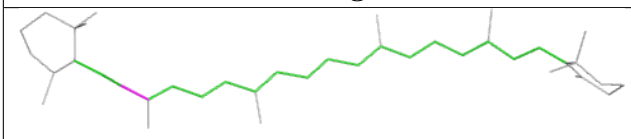


Bond angles



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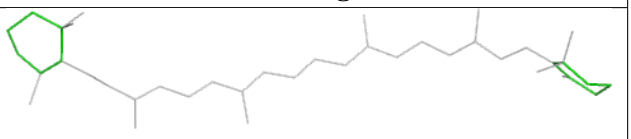
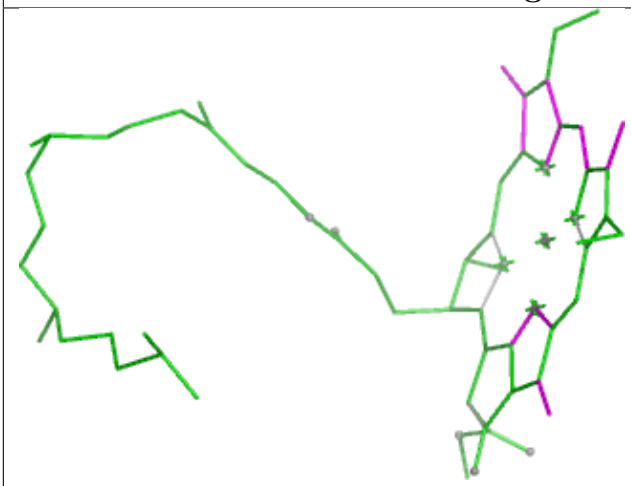


Rings

Ligand CLA B 610



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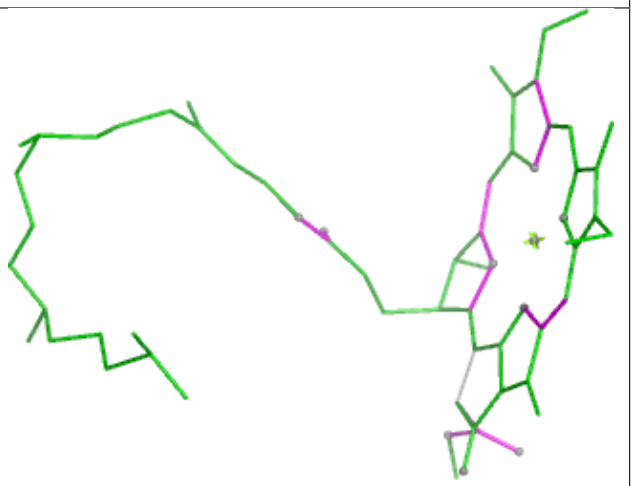
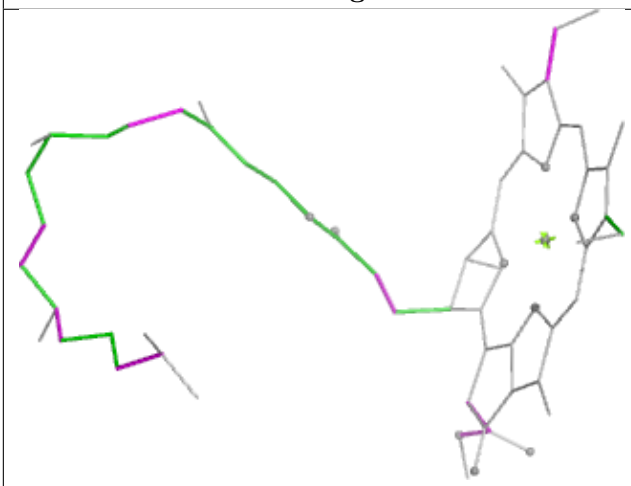


Bond angles

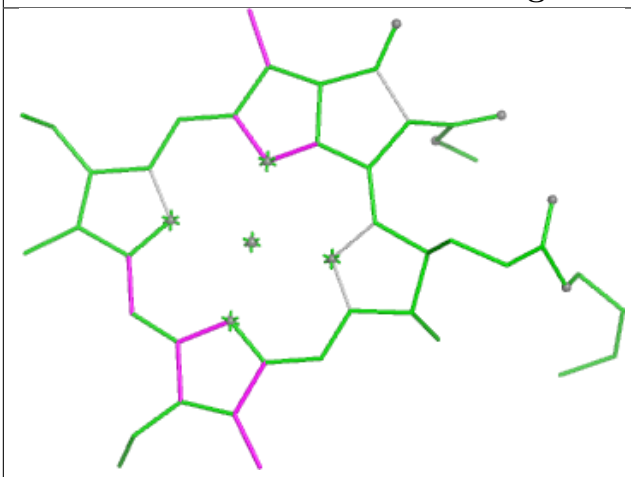


Torsions



Rings

Ligand CLA y 315



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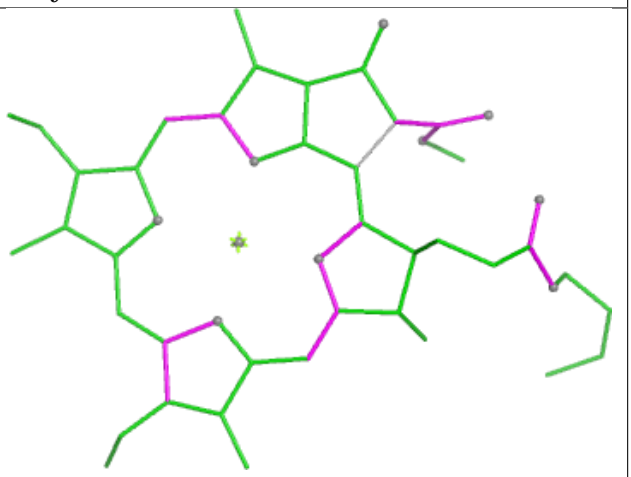
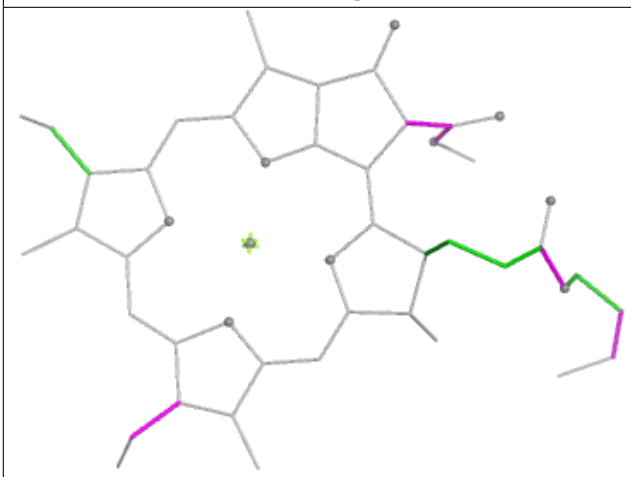
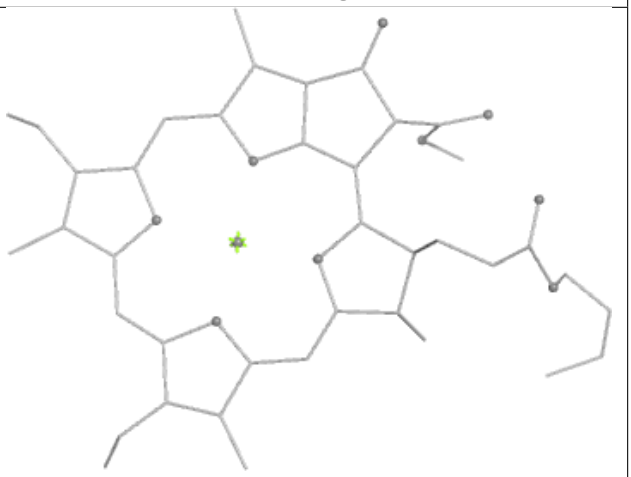


Bond angles

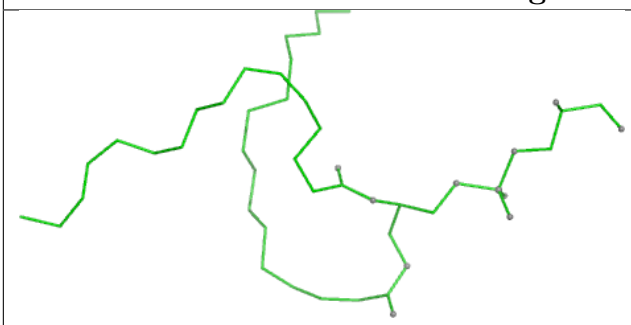


Torsions

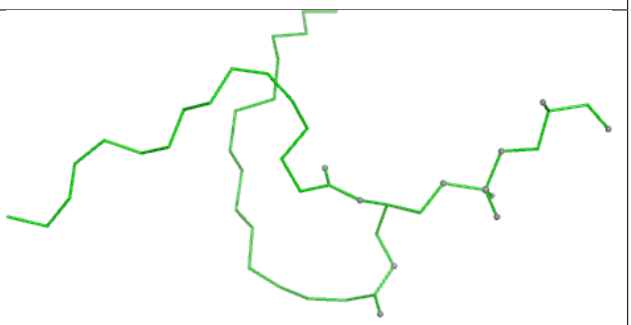


Rings

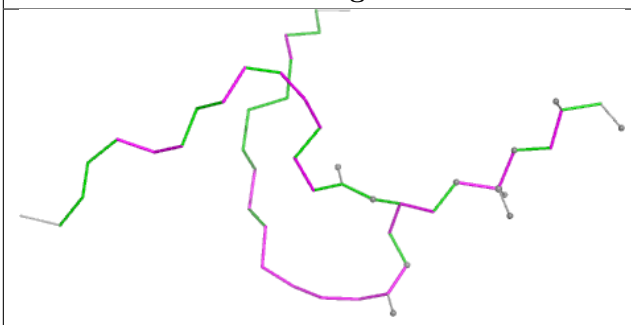
Ligand LHG s 309



Bond lengths



Bond angles



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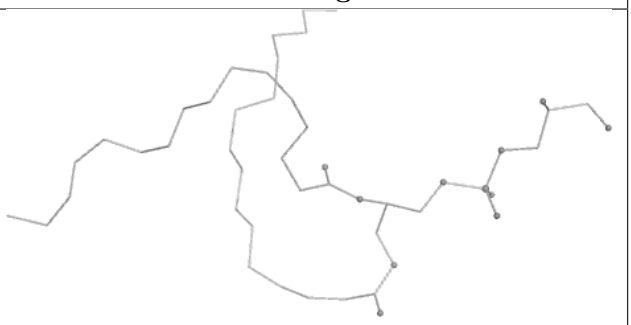
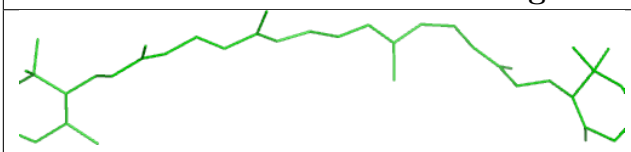


Rings

Ligand BCR t 101



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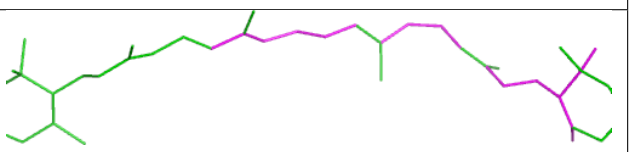

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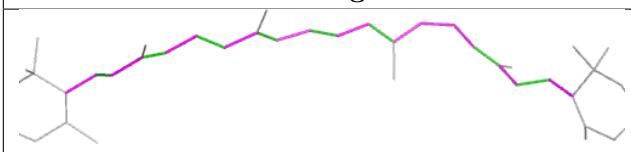

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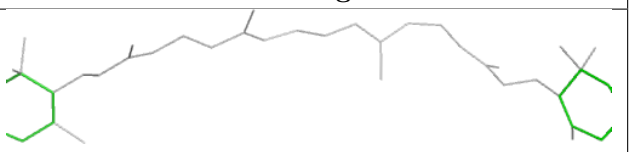
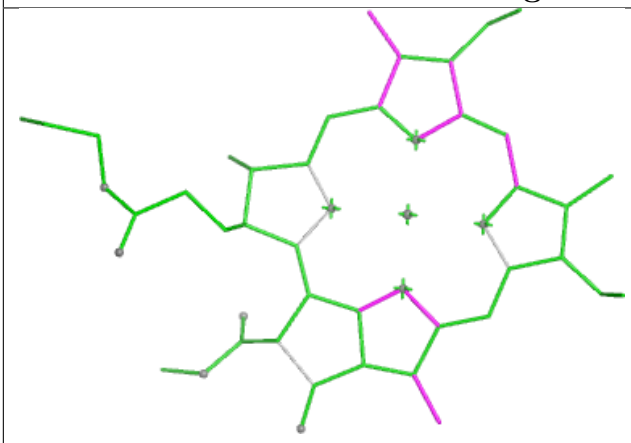


Rings

Ligand CLA R 309



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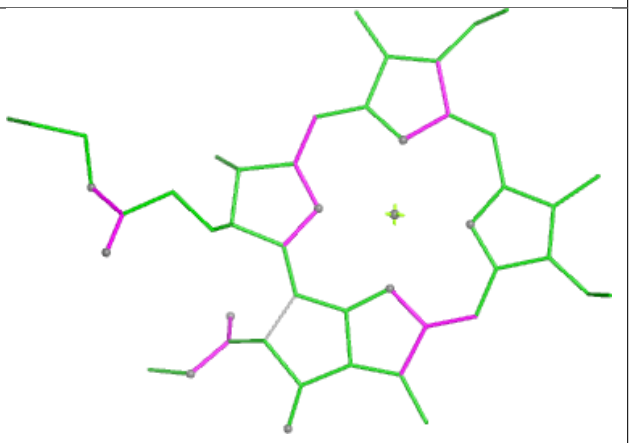
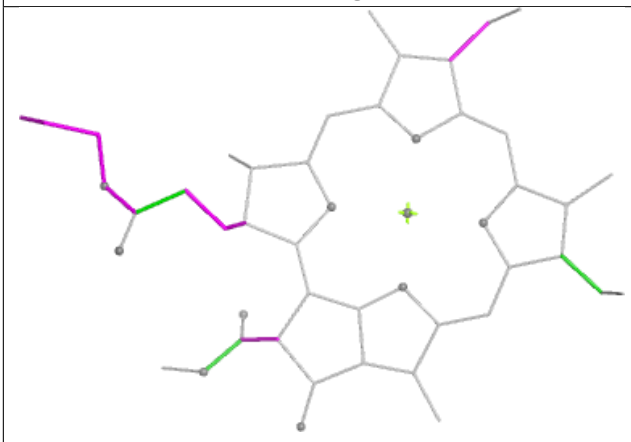


Bond angles



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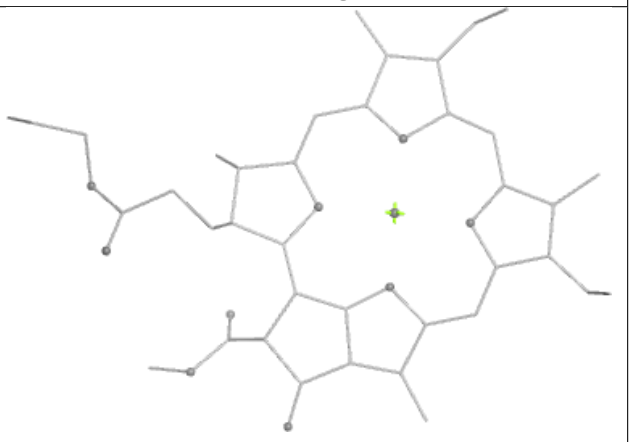
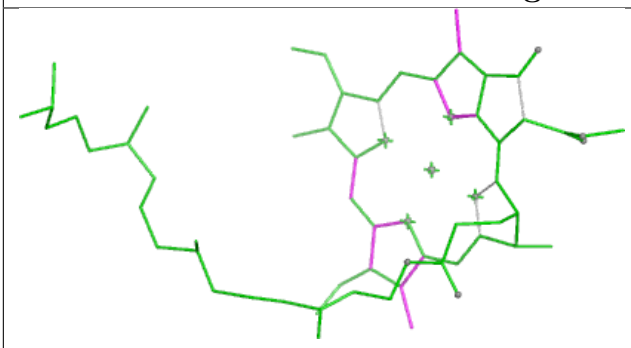


Rings

Ligand CLA Y 305



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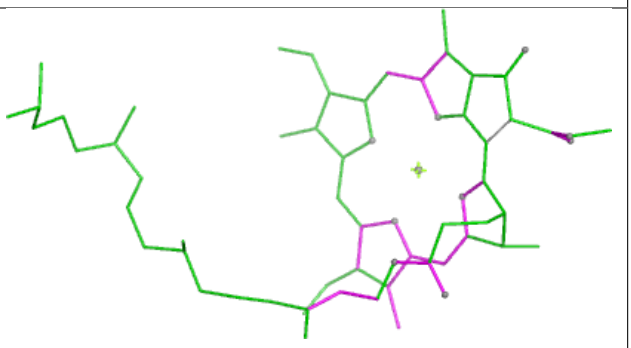
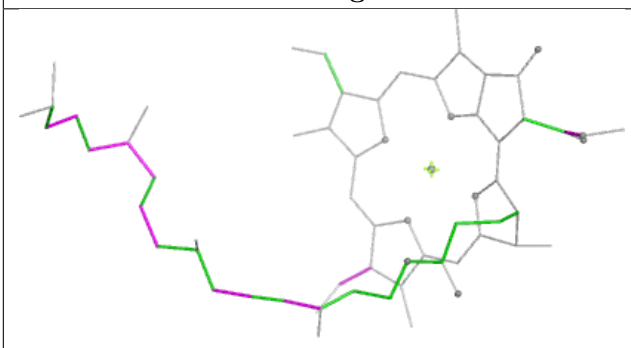


Bond angles



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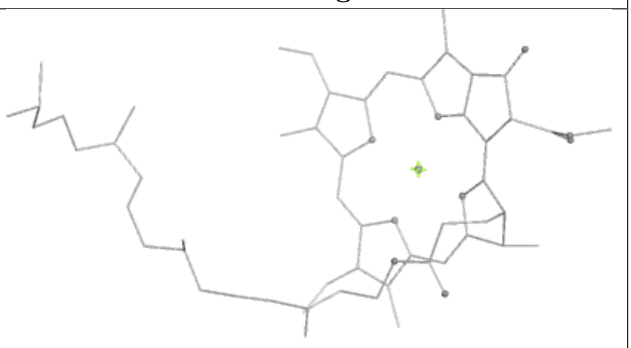
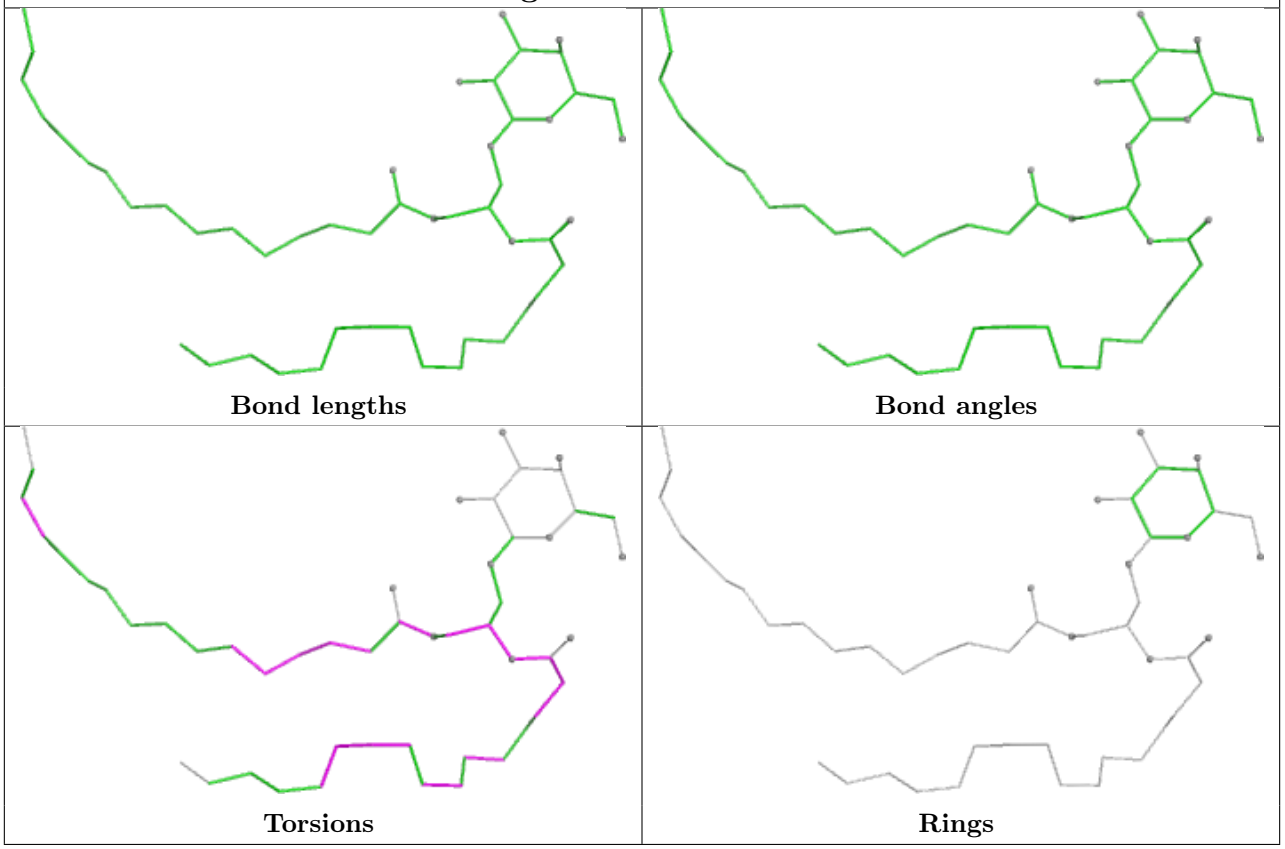
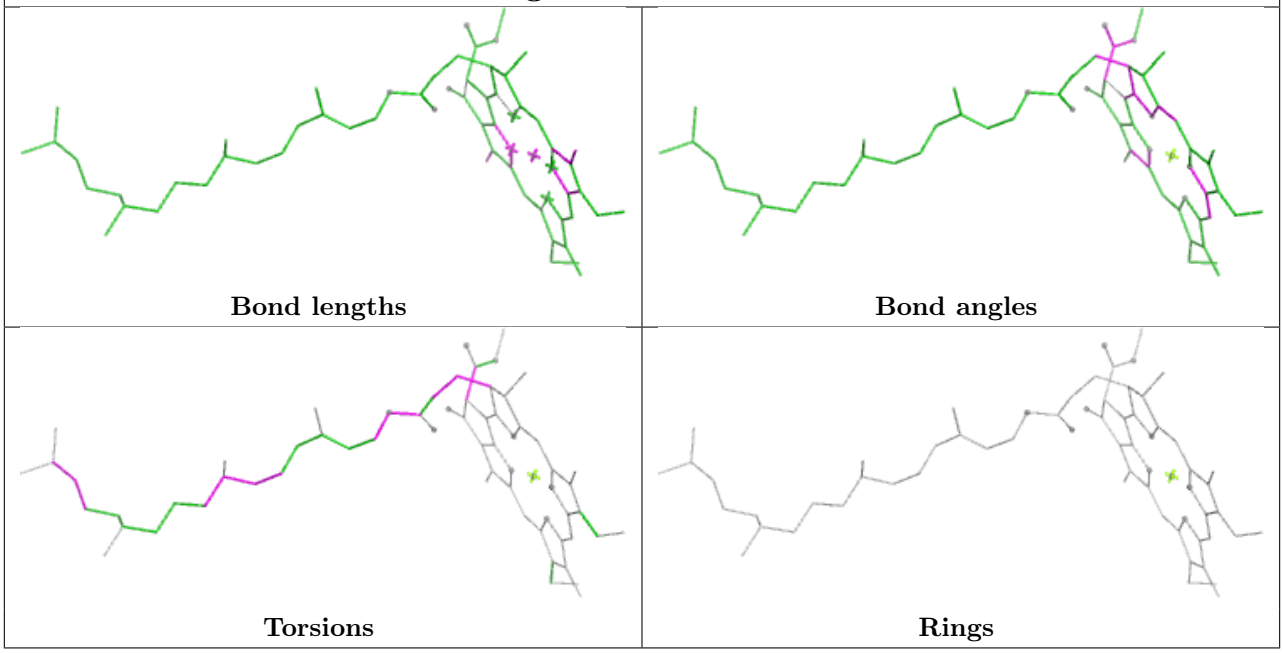


Rings

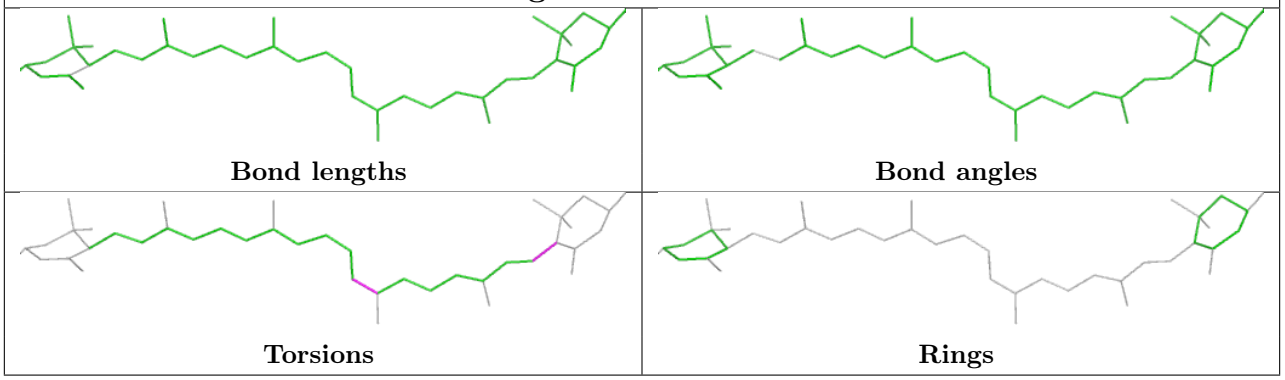
Ligand LMG C 518



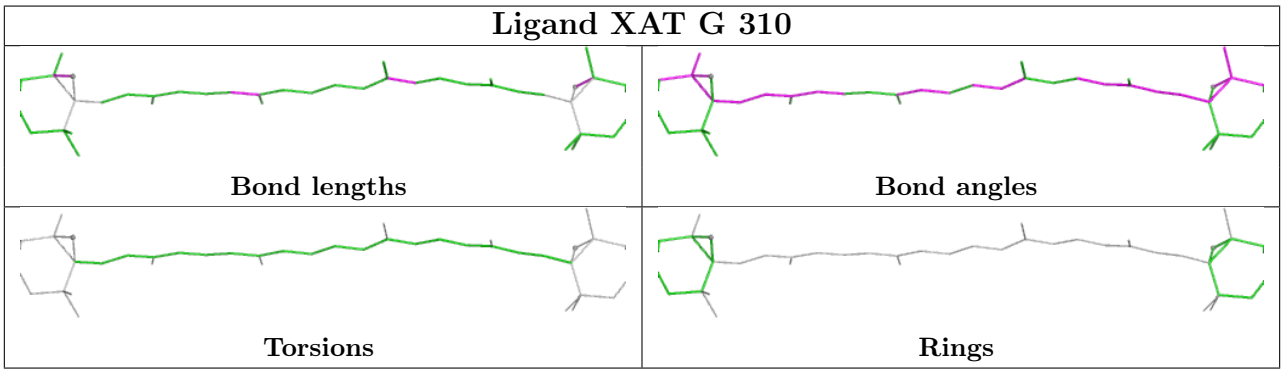
Ligand CLA B 615



Ligand LUT S 301



Ligand XAT G 310



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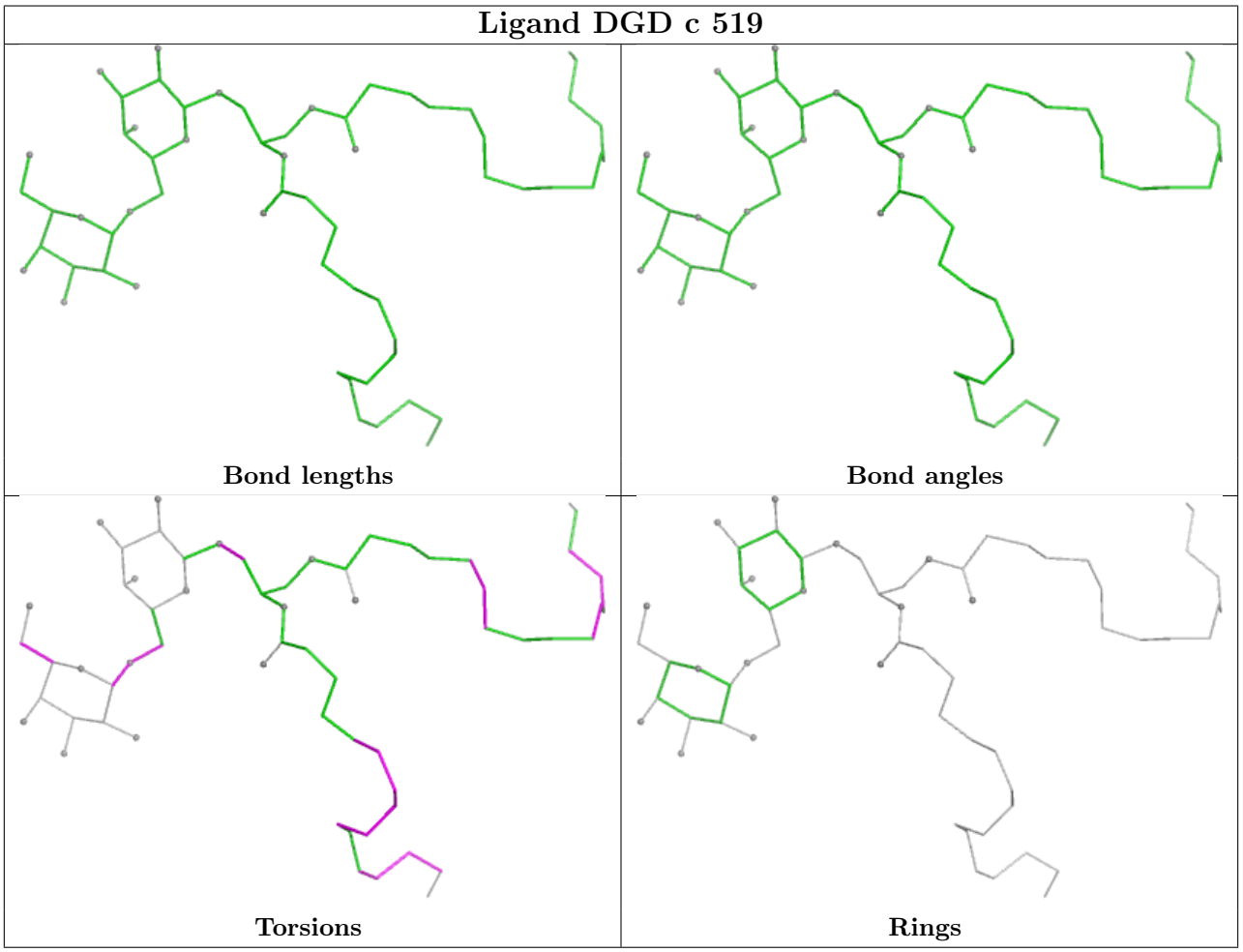

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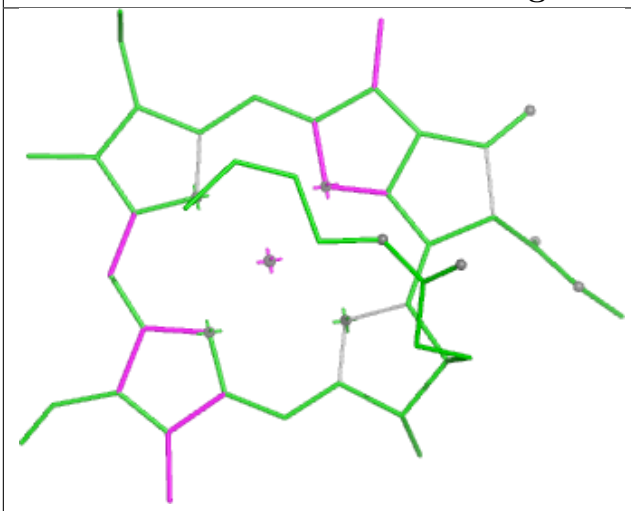
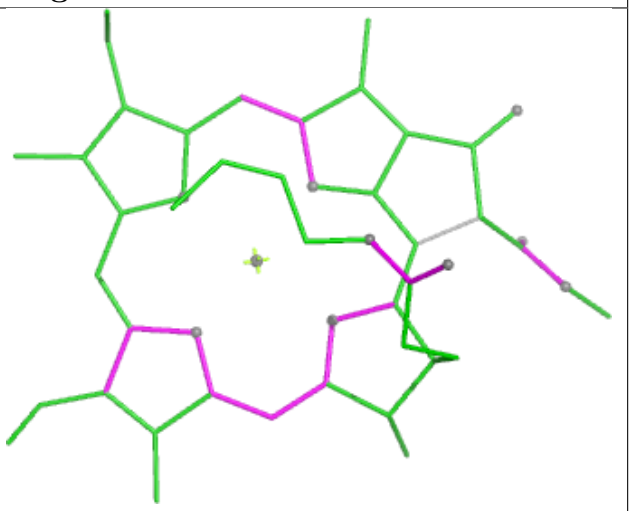
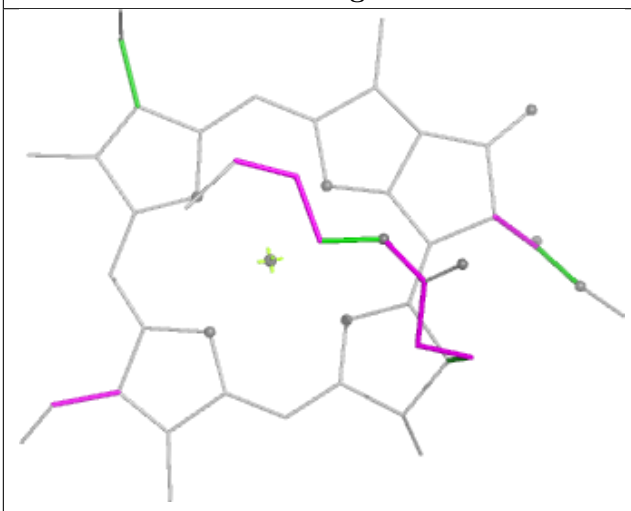


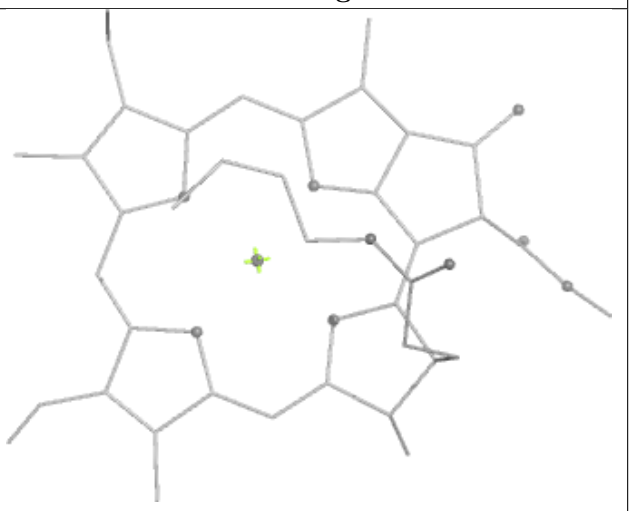
Bond lengths



Bond angles

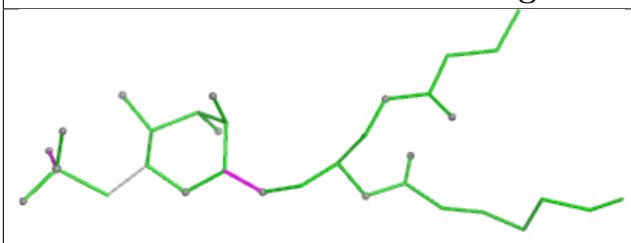


Torsions



Rings

Ligand SQD W 202



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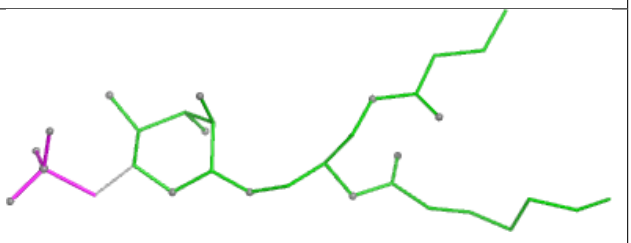
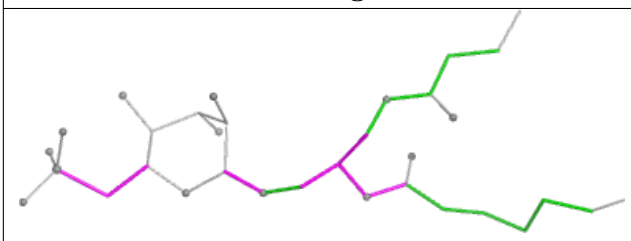


Bond angles



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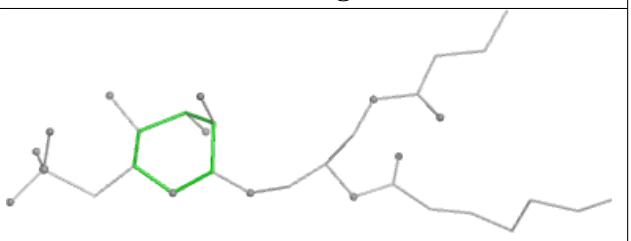
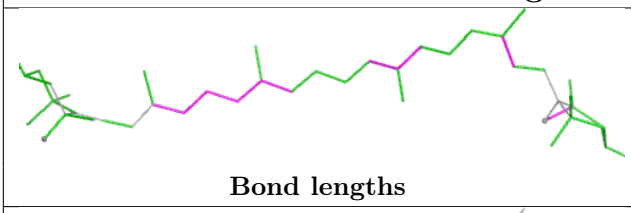


Rings

Ligand NEX n 313



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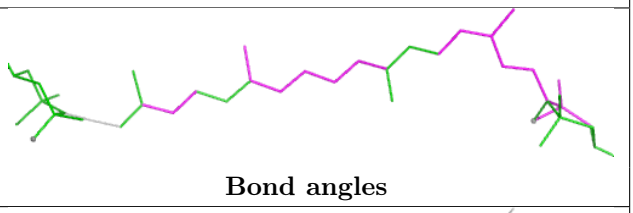
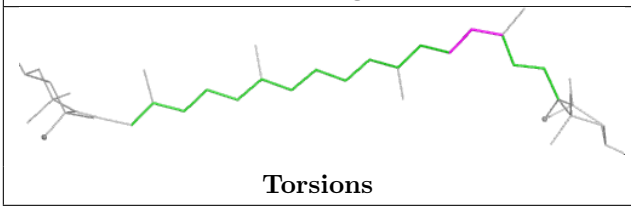


Bond angles



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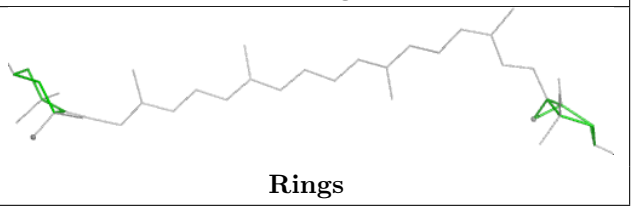
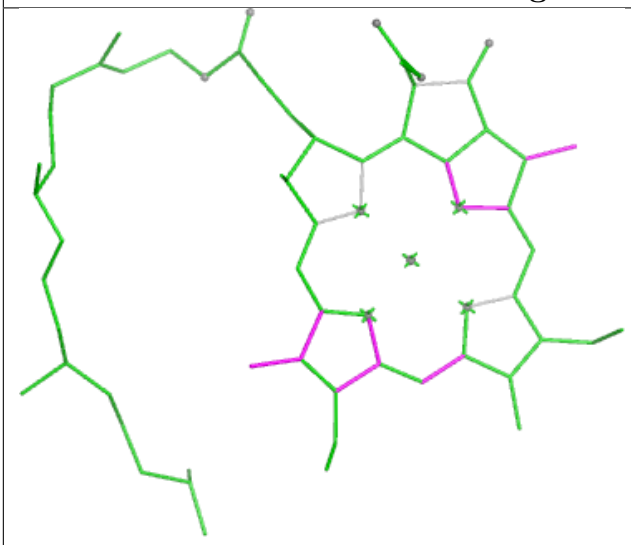


Rings

Ligand CLA c 503



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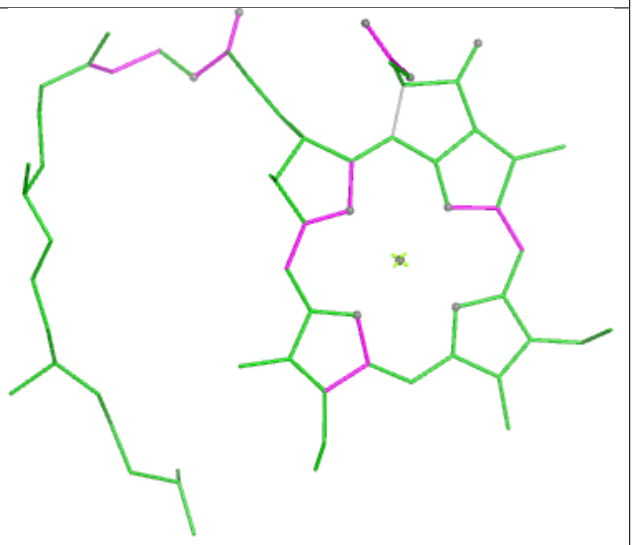
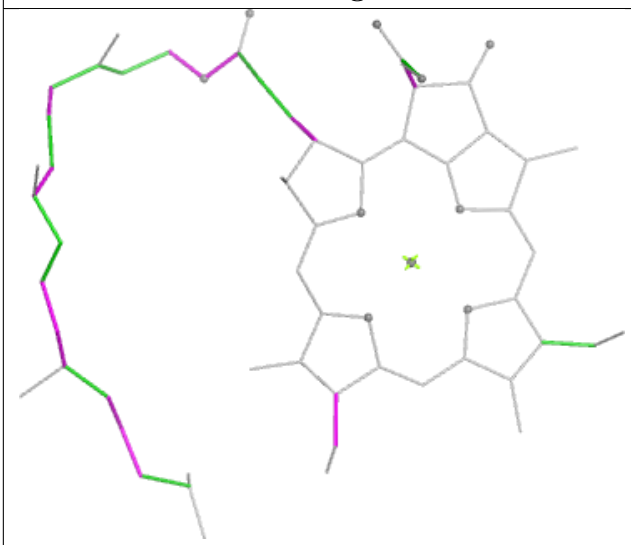


Bond angles



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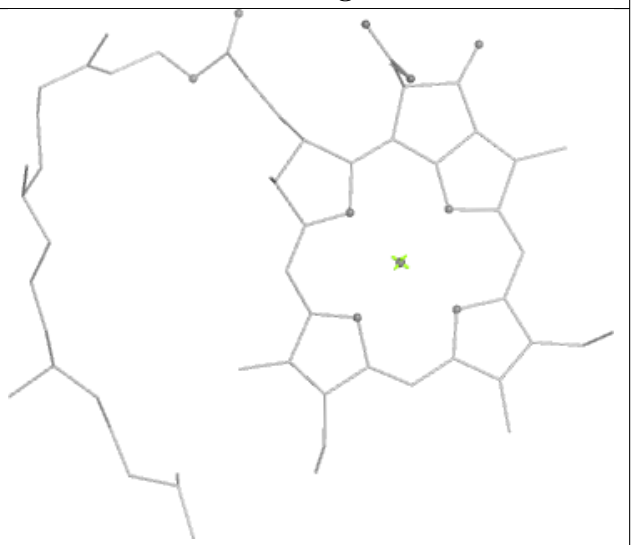
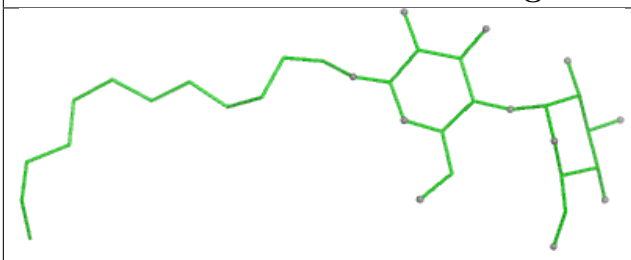


Rings

Ligand LMT d 406



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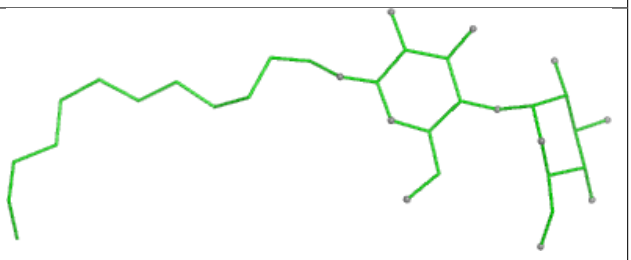
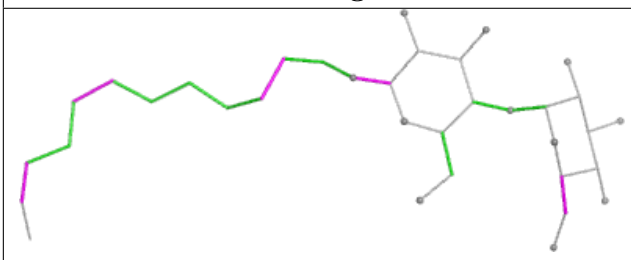


Bond angles



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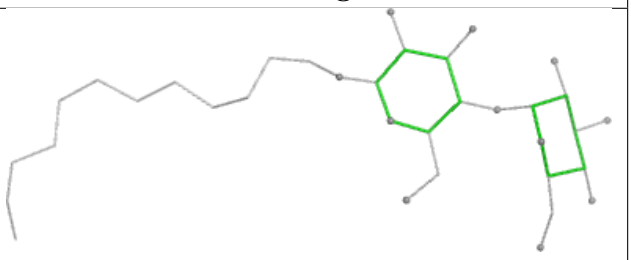
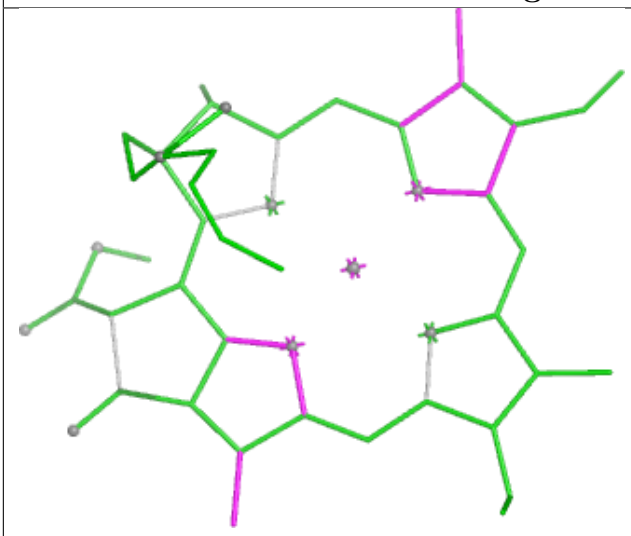


Rings

Ligand CLA R 308



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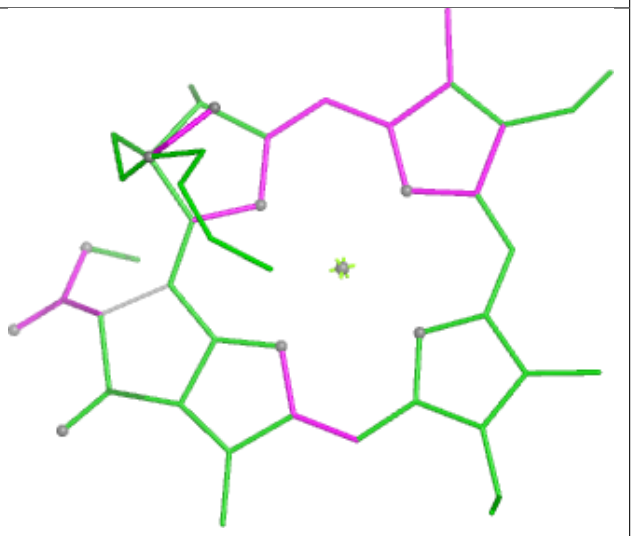
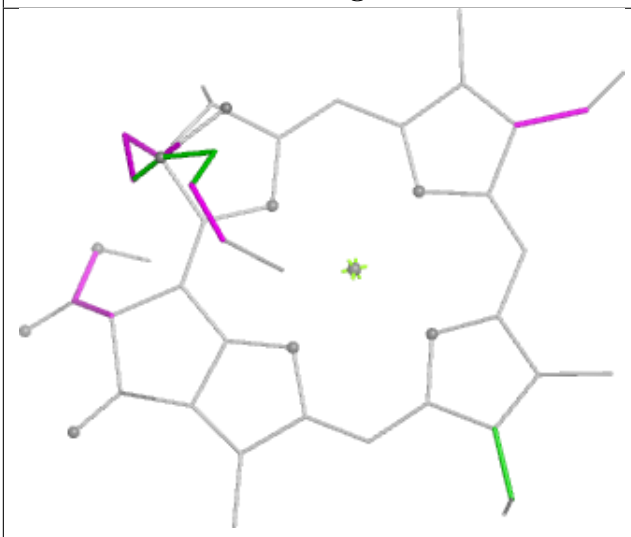


Bond angles



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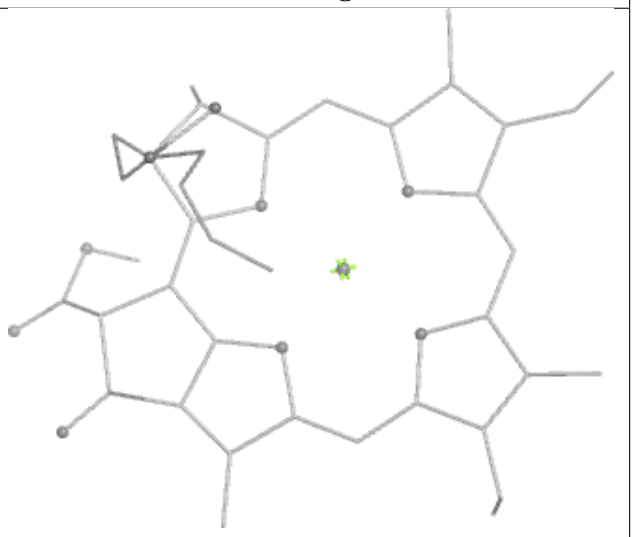
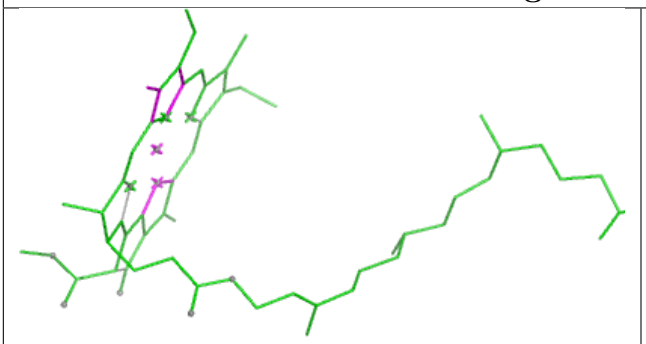


Rings

Ligand CLA C 517



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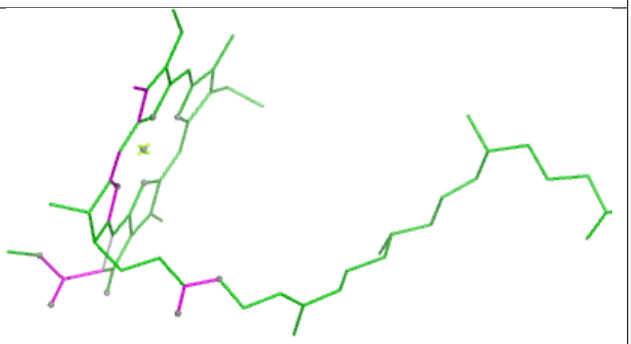
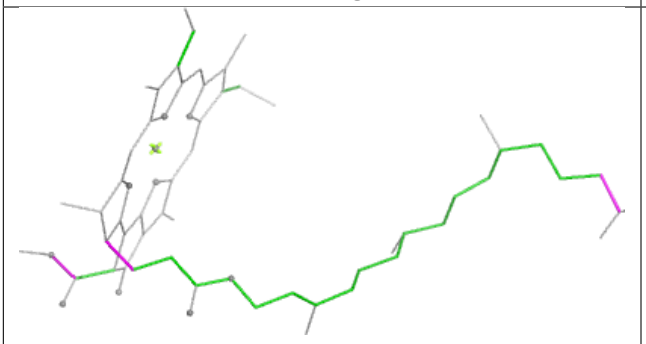


Bond angles



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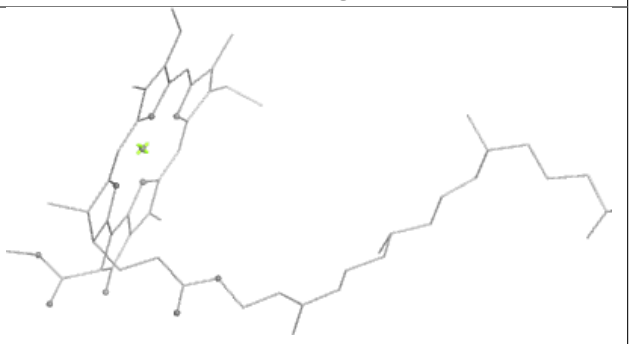
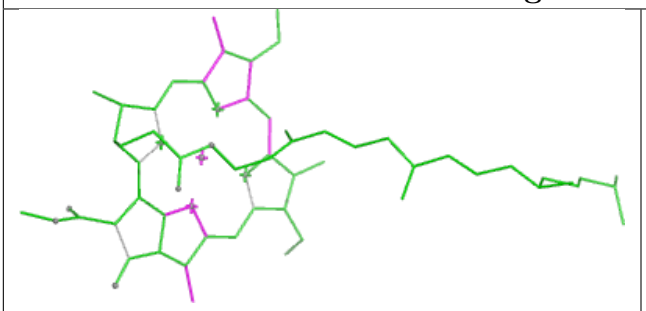


Rings

Ligand CLA B 604



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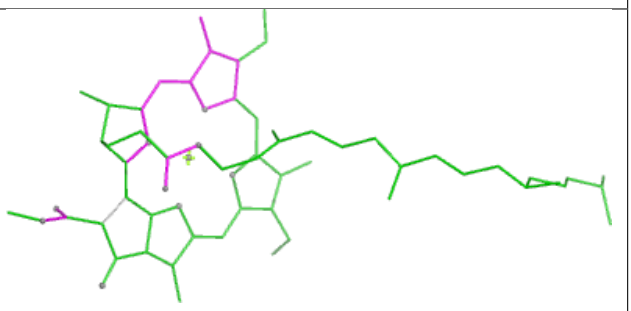
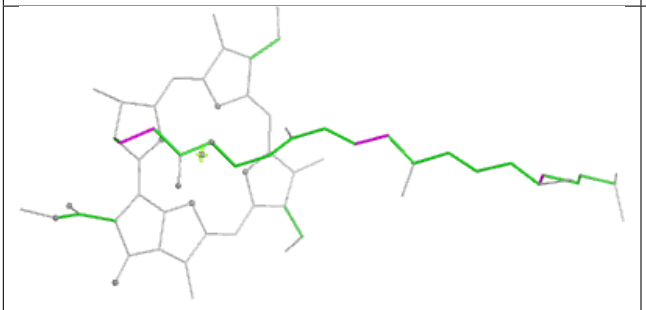


Bond angles



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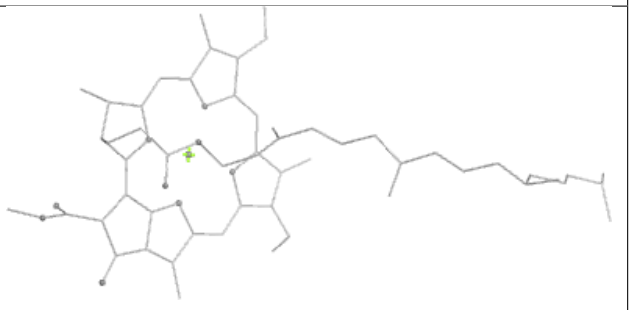
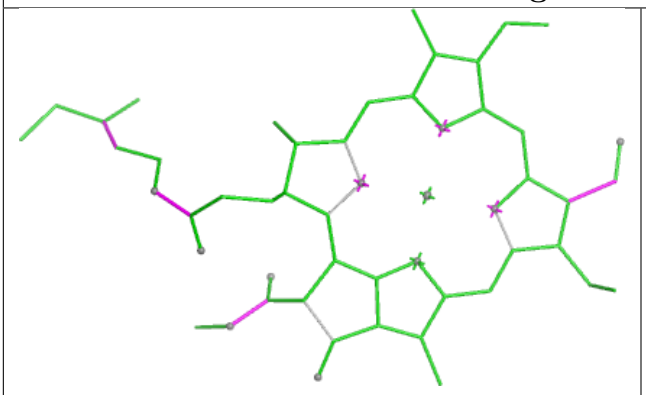


Rings

Ligand CHL s 303



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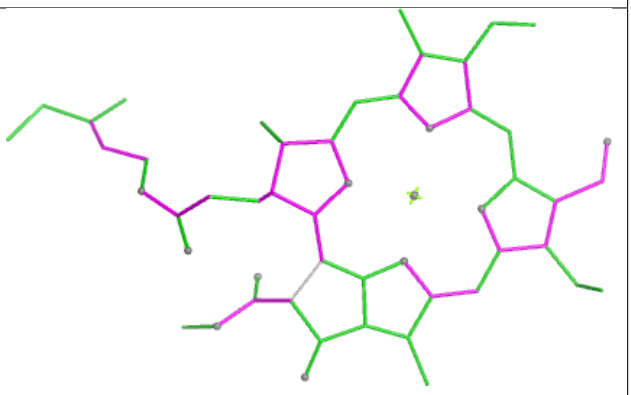
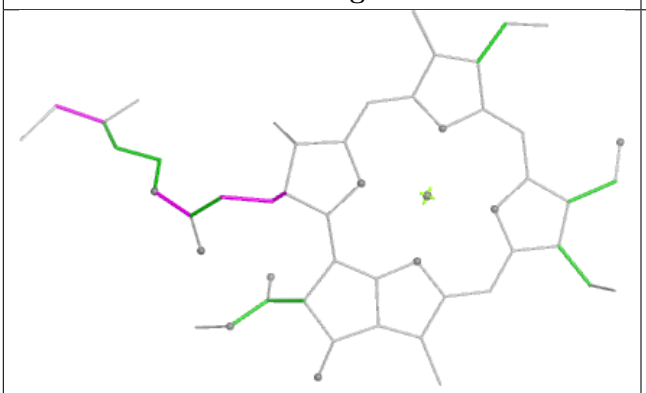


Bond angles



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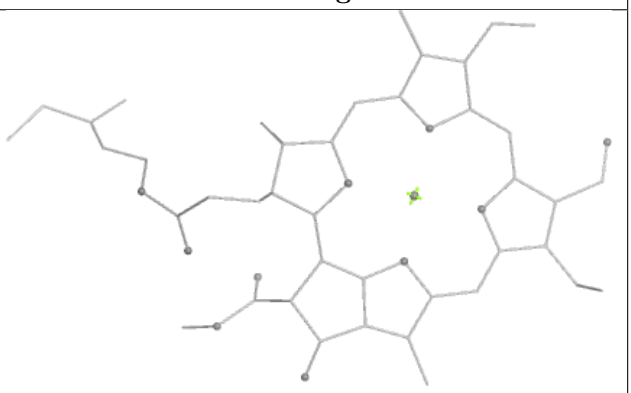
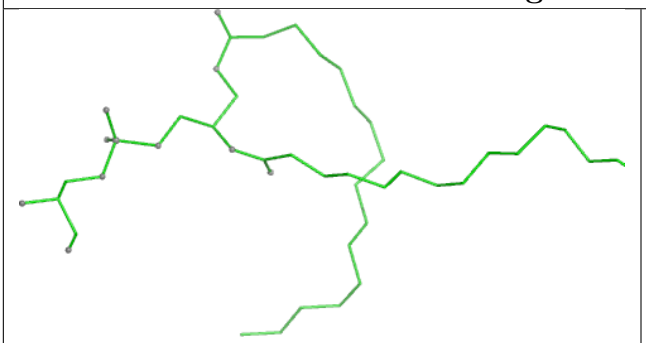
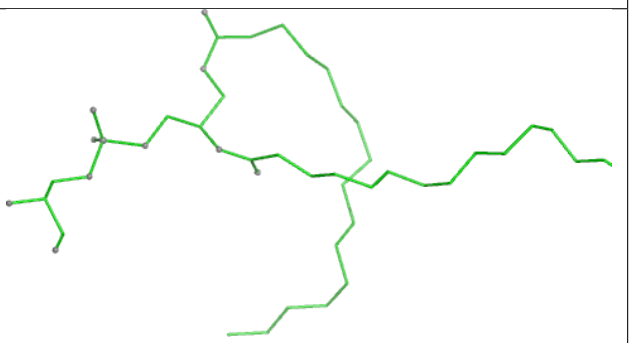


Rings

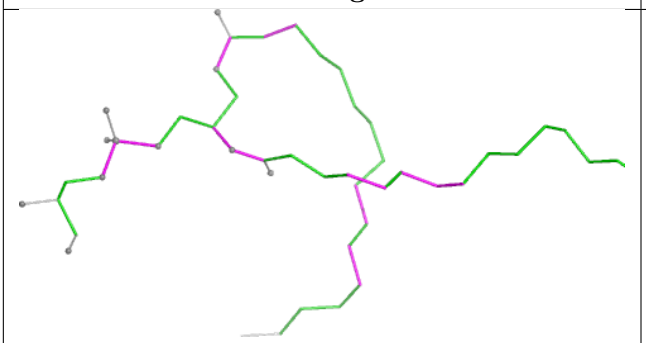
Ligand LHG n 301



Bond lengths



Bond angles

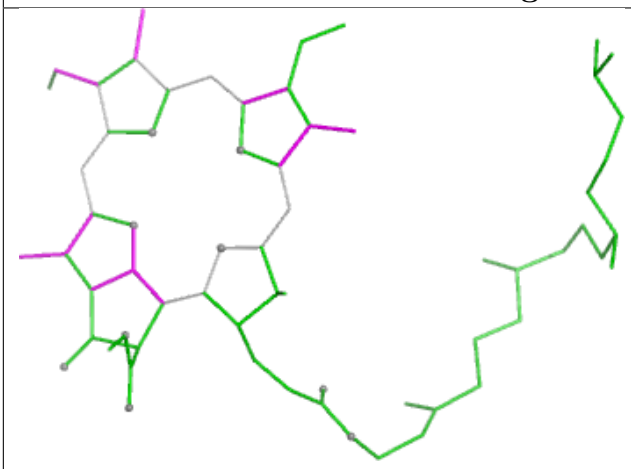


Torsions



Rings

Ligand PHO D 403



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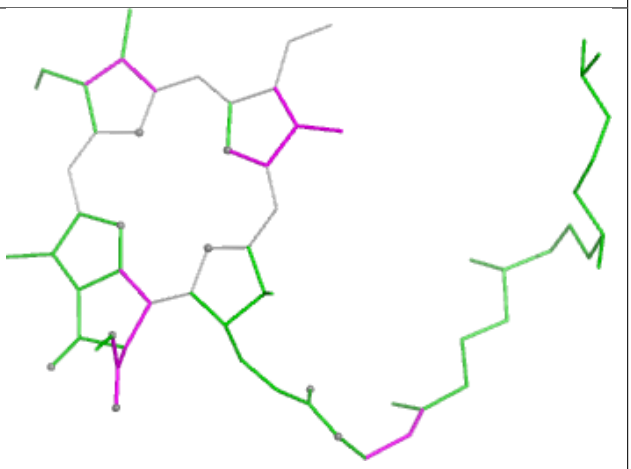

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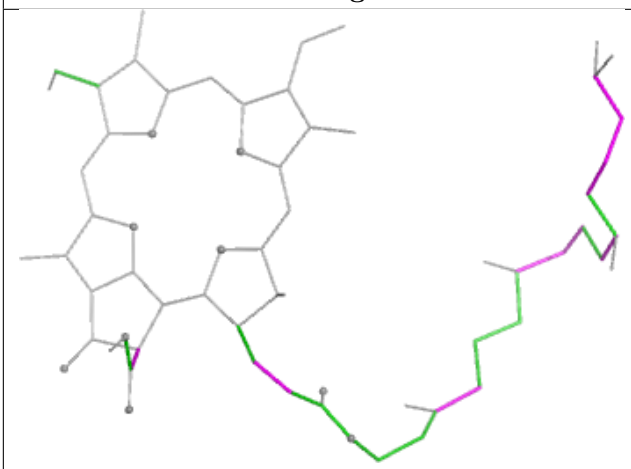
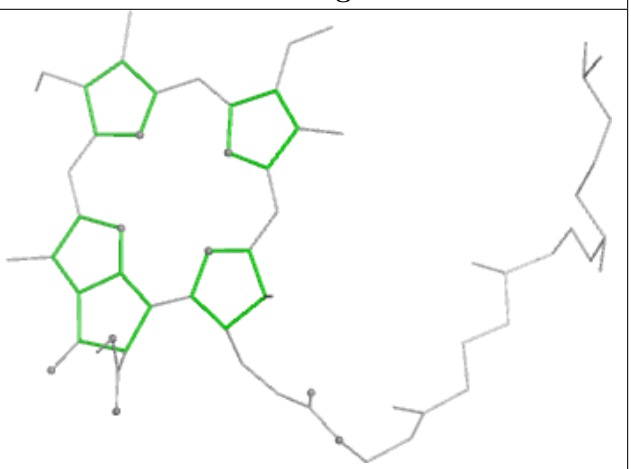
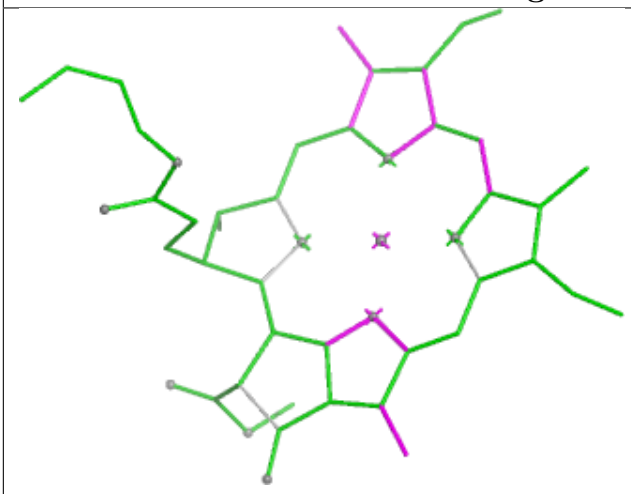


Torsions



Rings

Ligand CLA d 411



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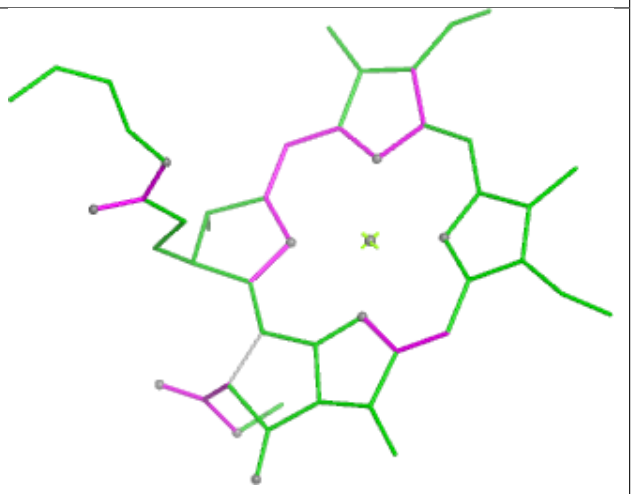

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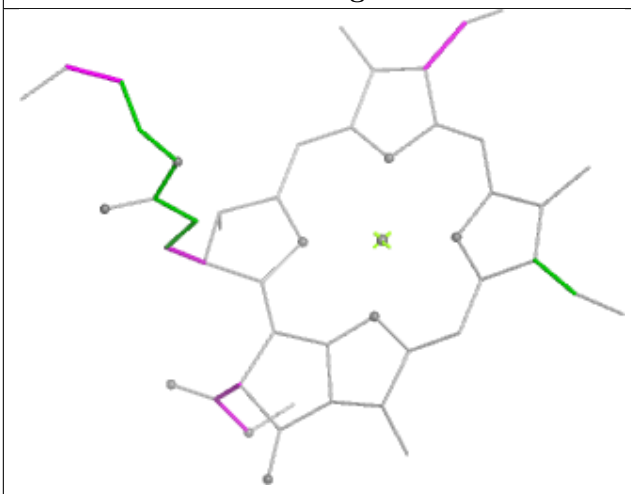

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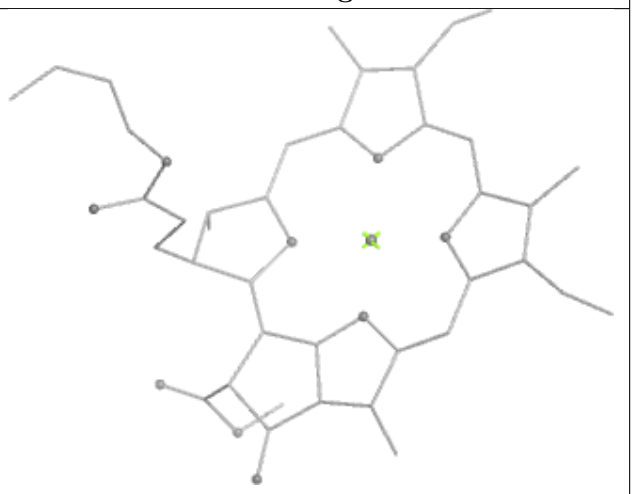
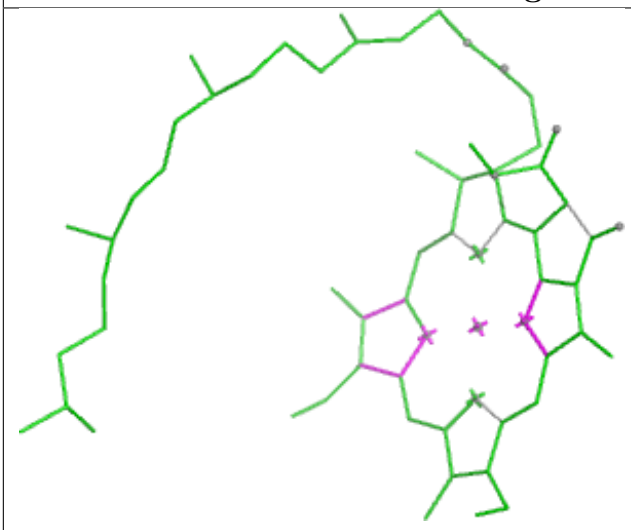


Rings

Ligand CLA C 516



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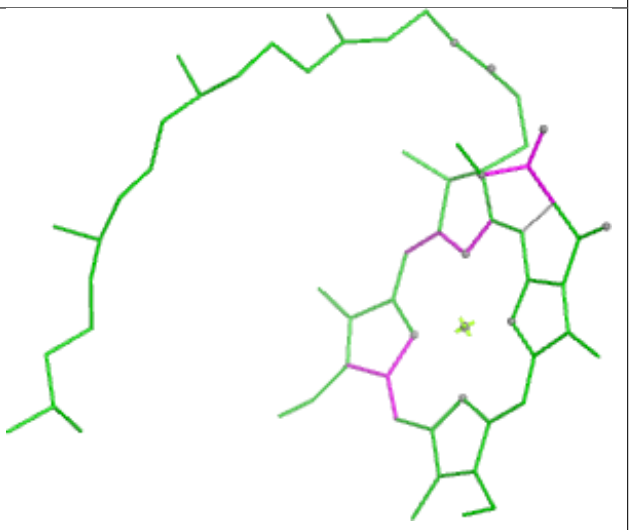

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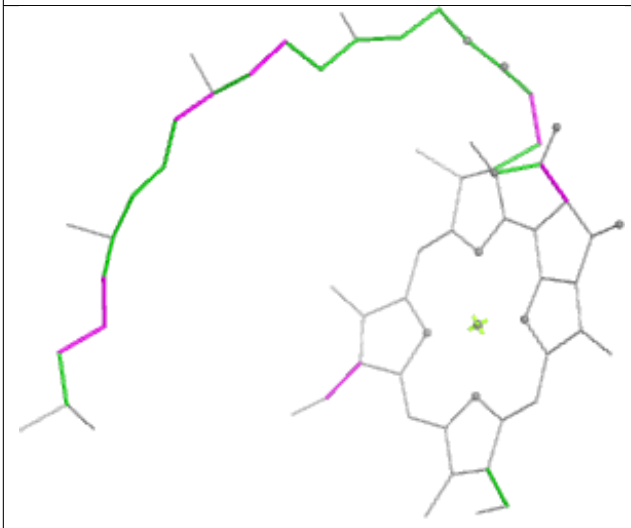

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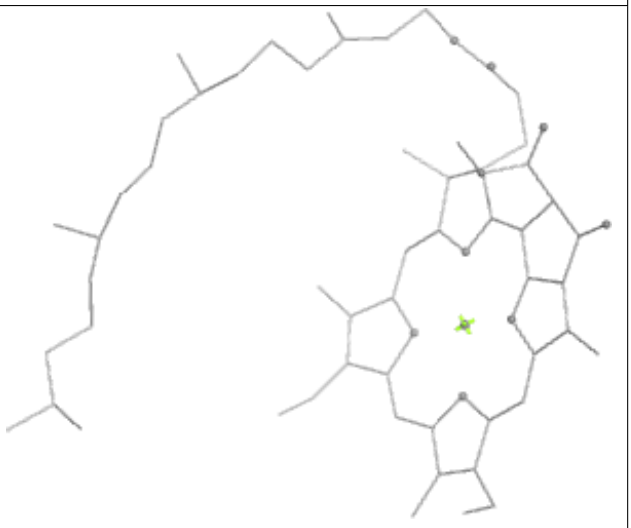
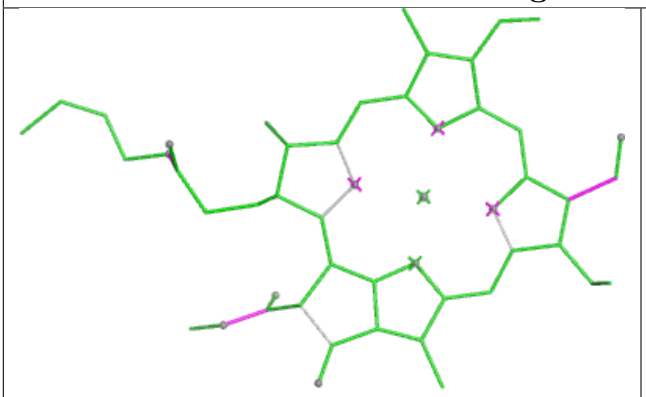


Rings

Ligand CHL s 317



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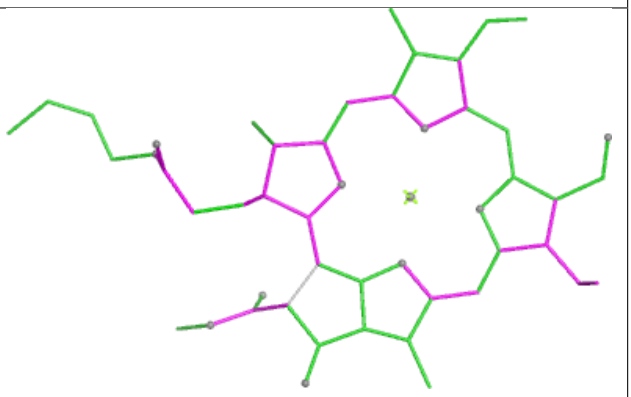
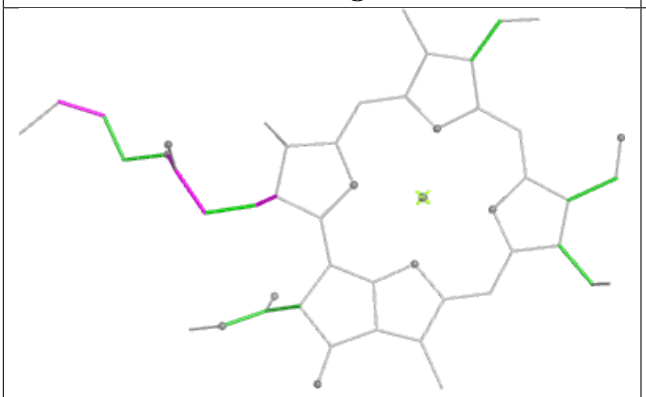


Bond angles



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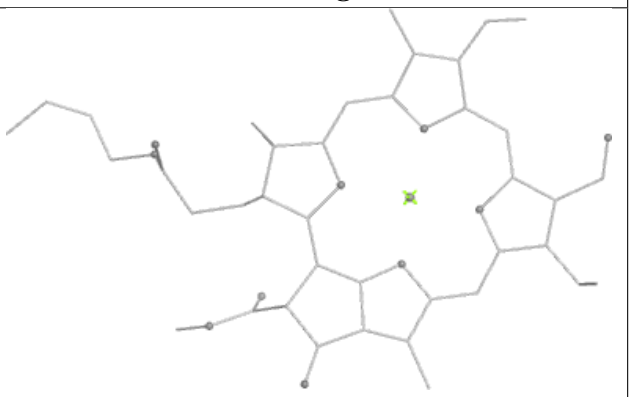
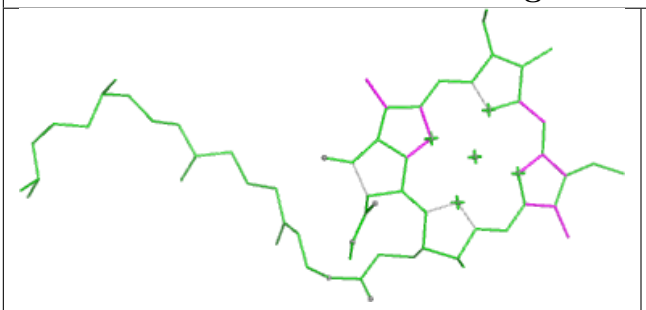


Rings

Ligand CLA B 606



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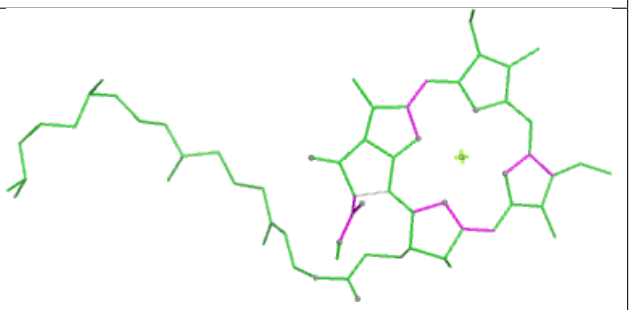
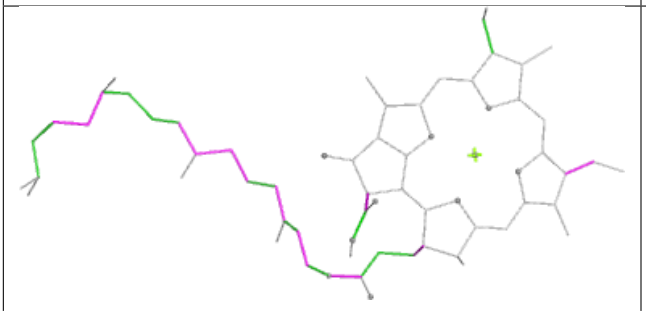


Bond angles



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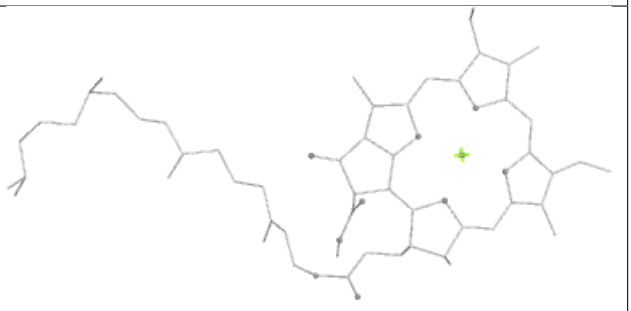
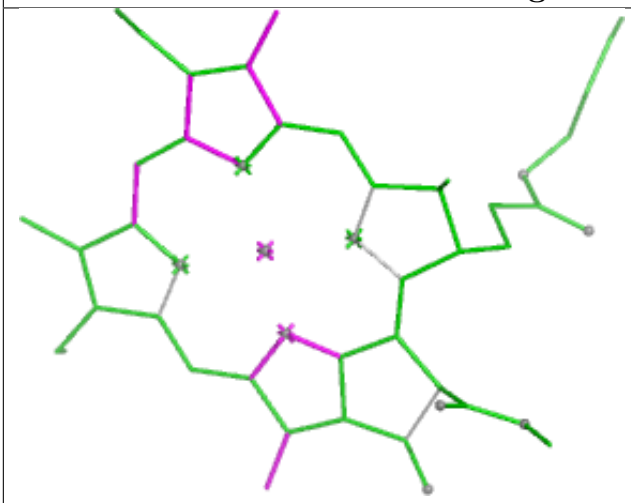


Rings

Ligand CLA g 315



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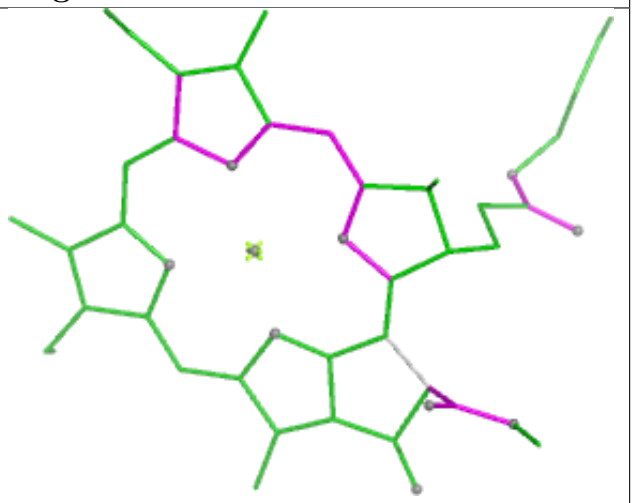
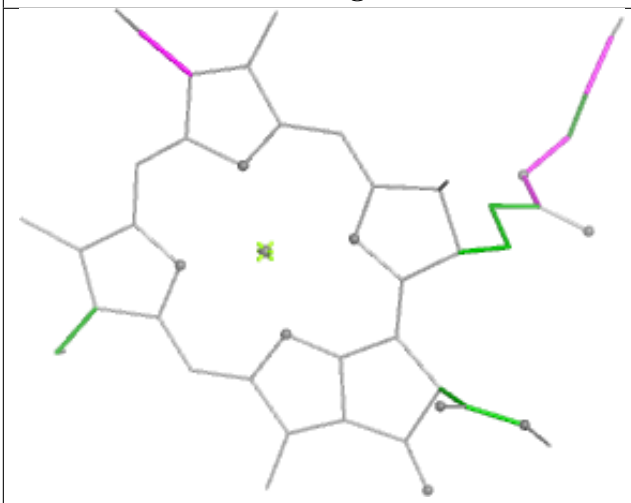


Bond angles



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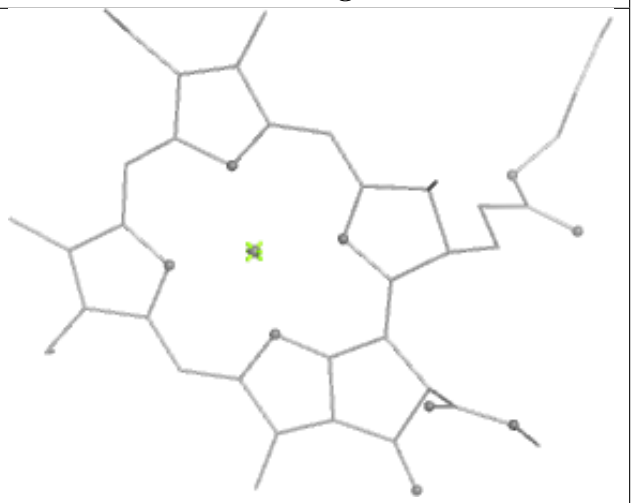
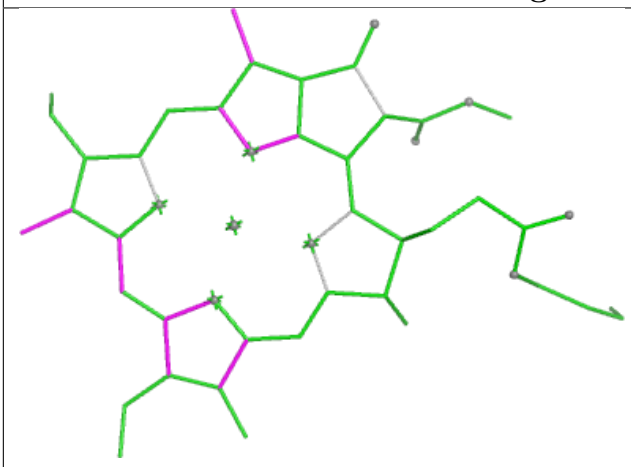


Rings

Ligand CLA s 304



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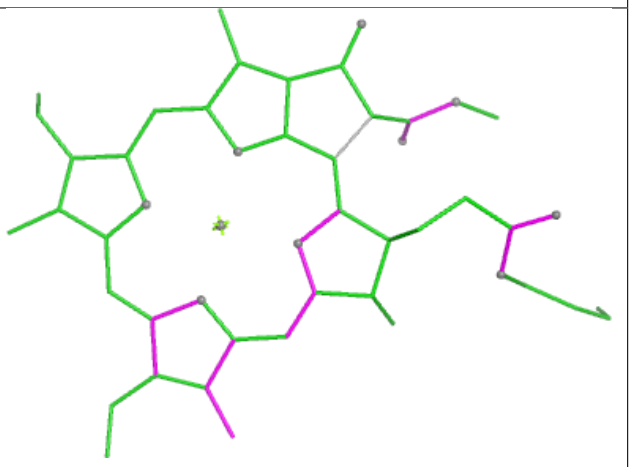
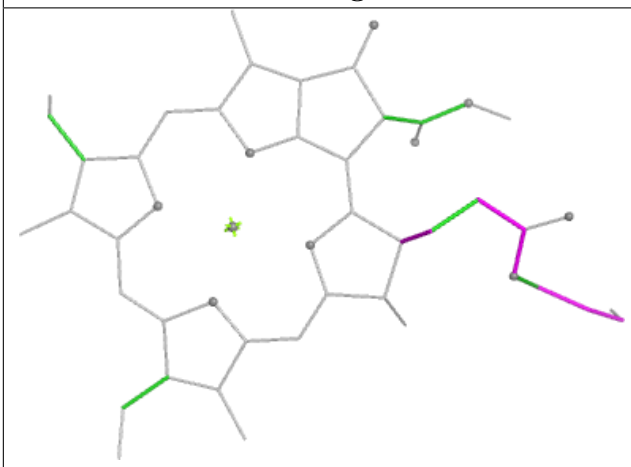


Bond angles



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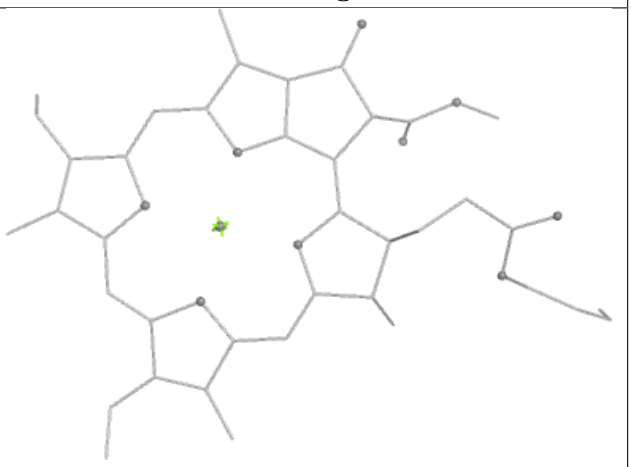
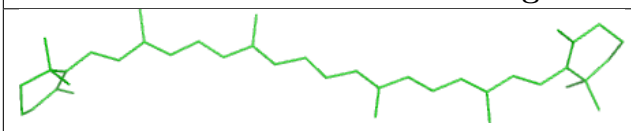


Rings

Ligand BCR A 406



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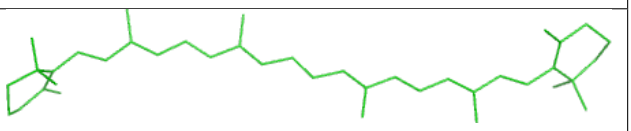
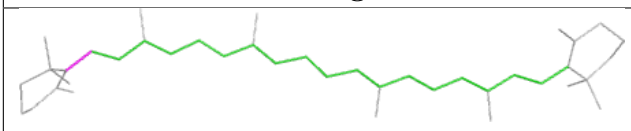


Bond angles



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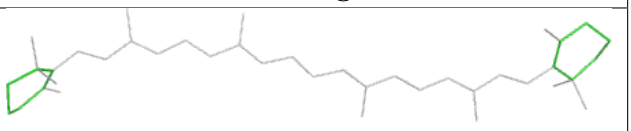
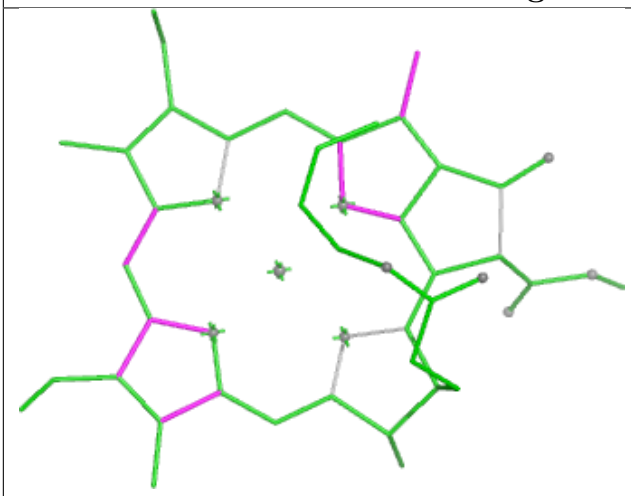


Rings

Ligand CLA S 304



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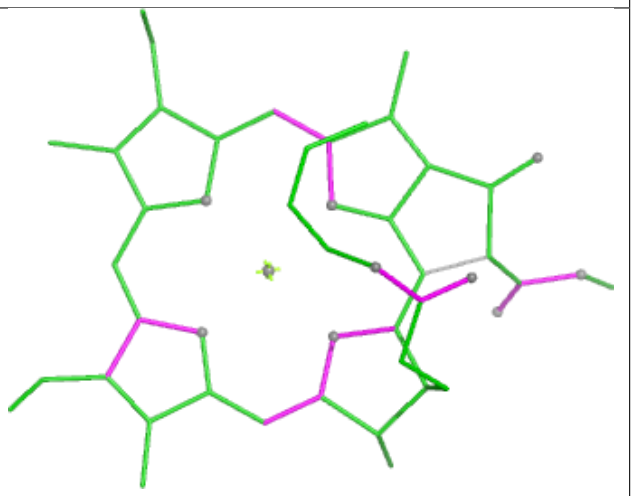
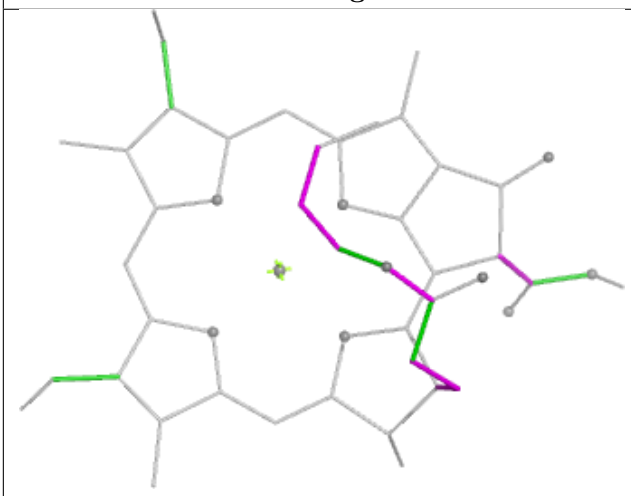


Bond angles



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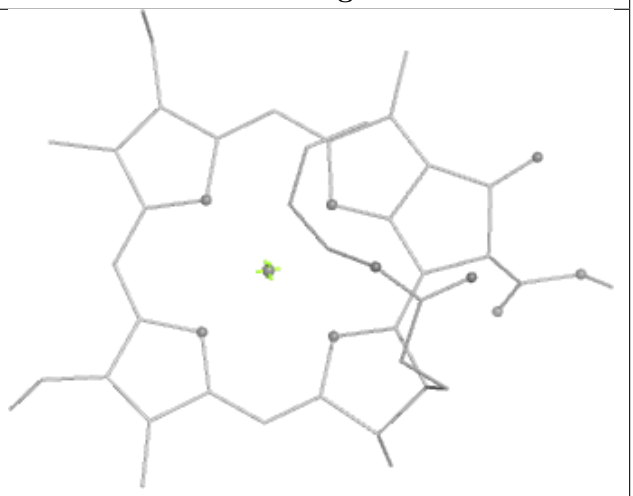
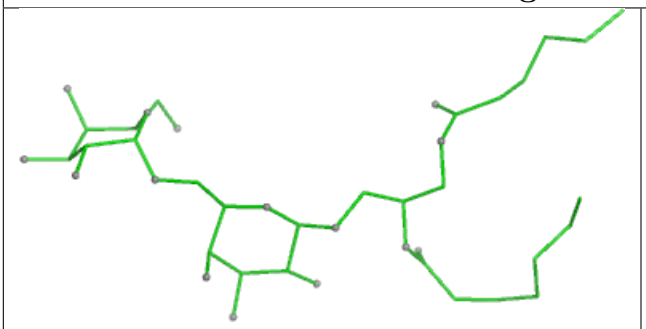


Rings

Ligand DGD Y 303



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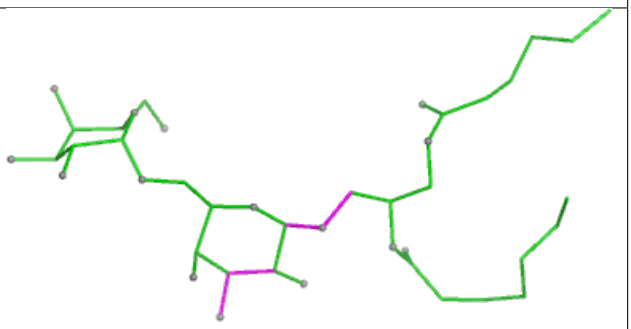
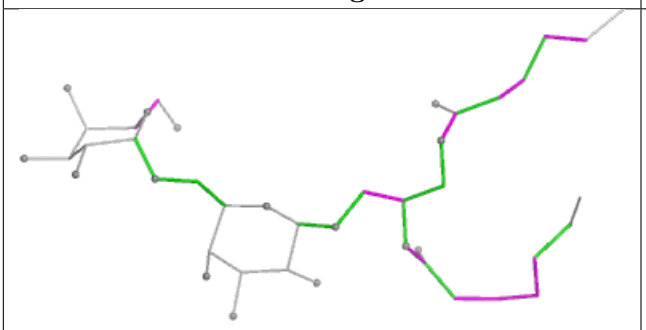


Bond angles



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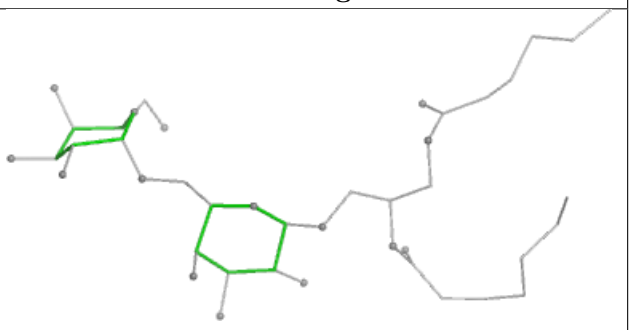
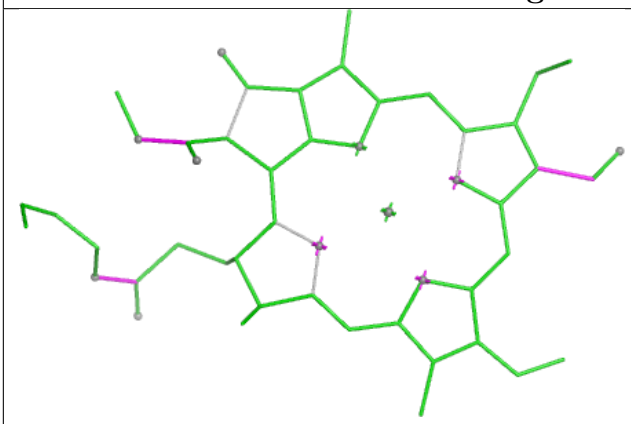


Rings

Ligand CHL S 302



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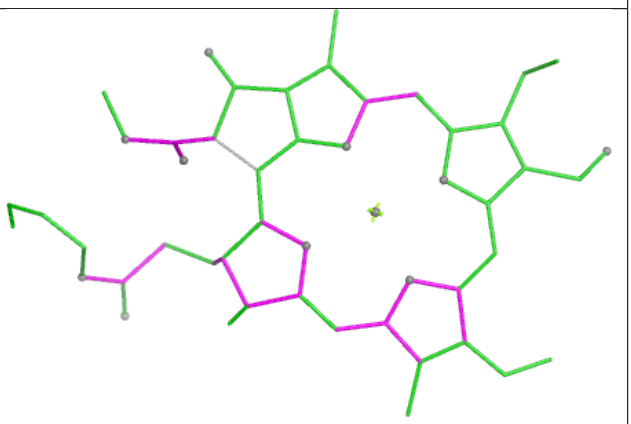
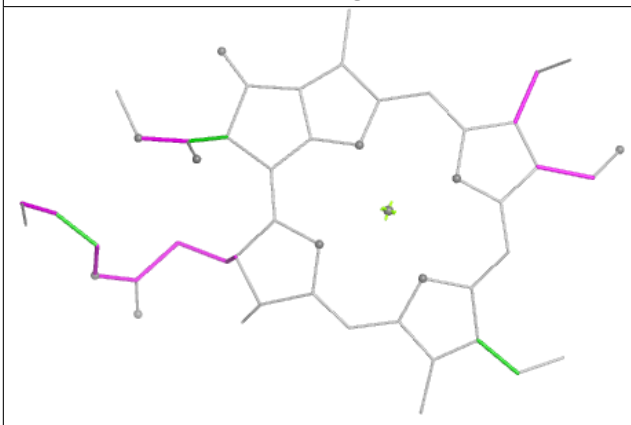


Bond angles



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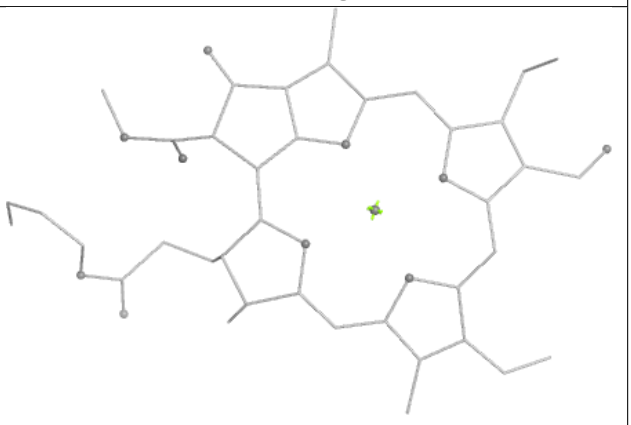
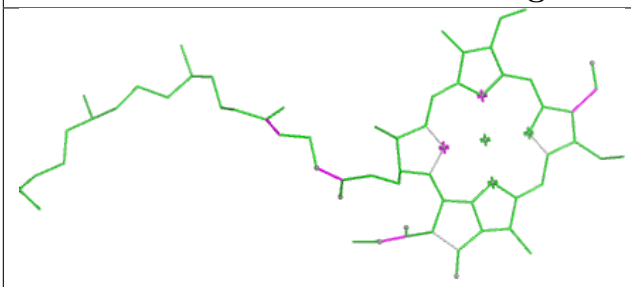


Rings

Ligand CHL g 311



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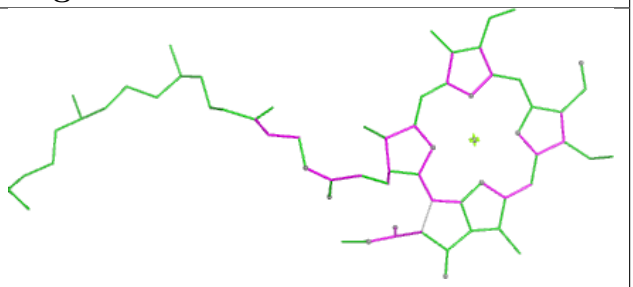
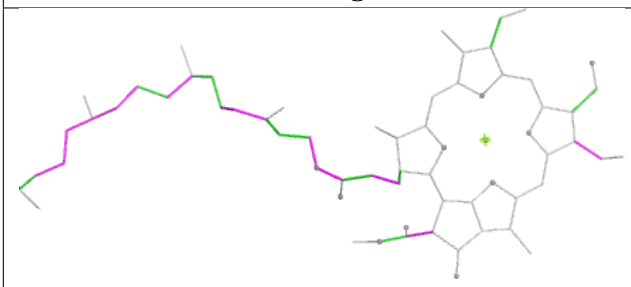


Bond angles



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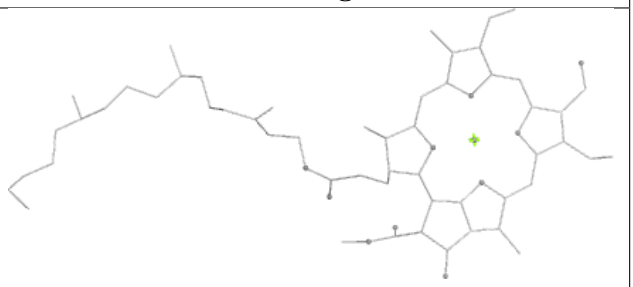
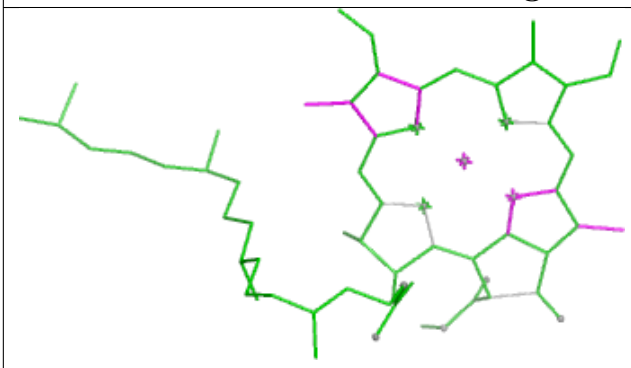


Rings

Ligand CLA D 401



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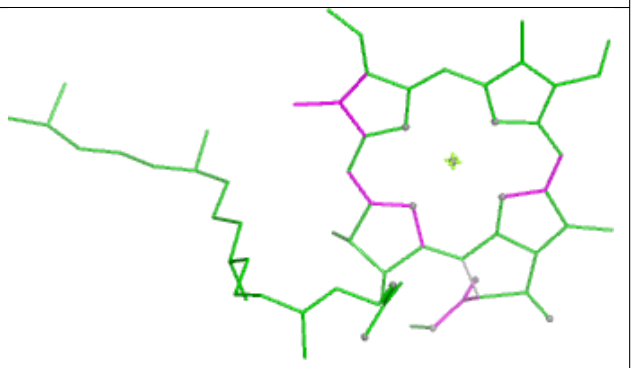
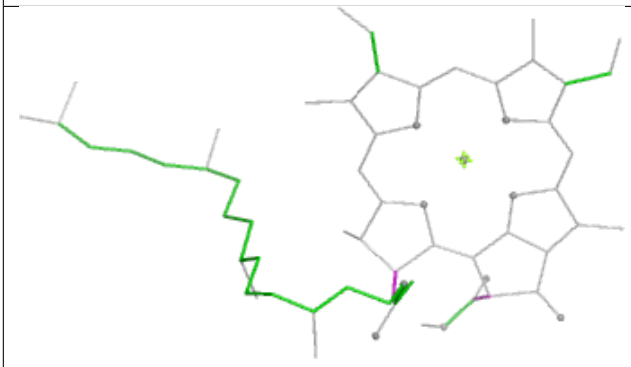


Bond angles

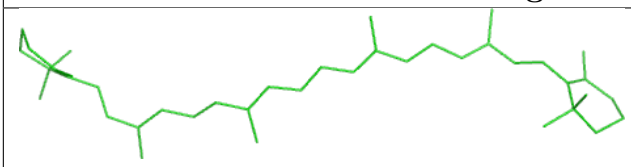


Torsions



Rings

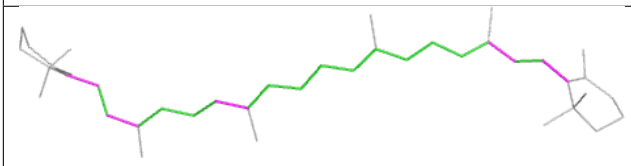
Ligand BCR J 101



Bond lengths



Bond angles



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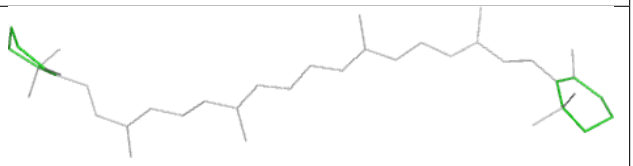
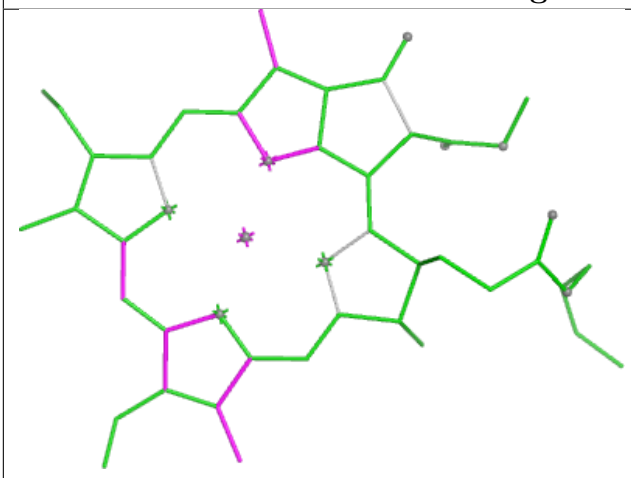
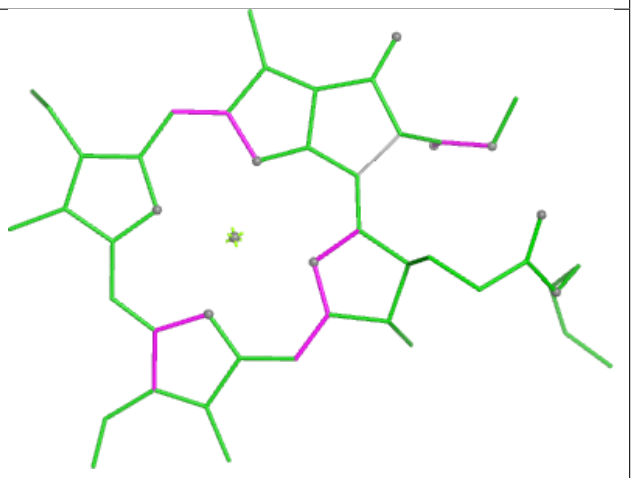


Rings

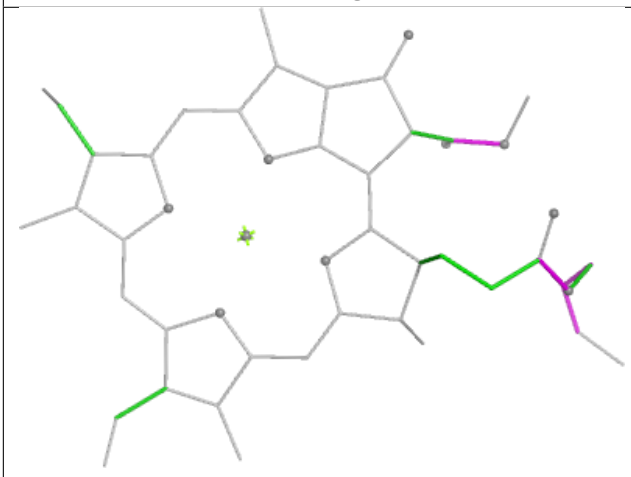
Ligand CLA r 303



Bond lengths



Bond angles

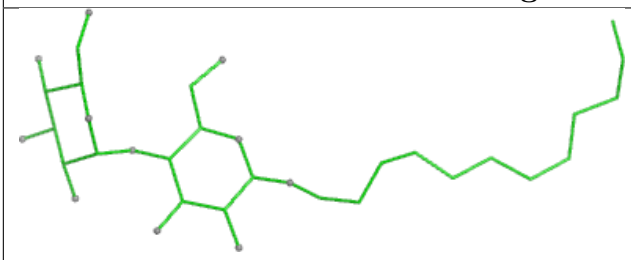


Torsions



Rings

Ligand LMT D 402



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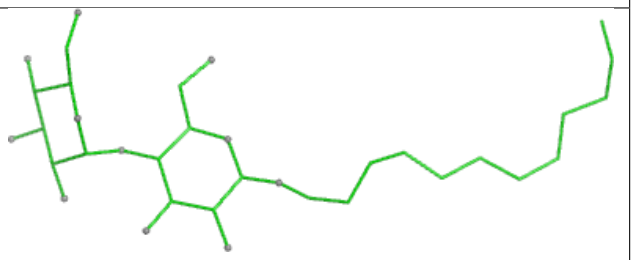

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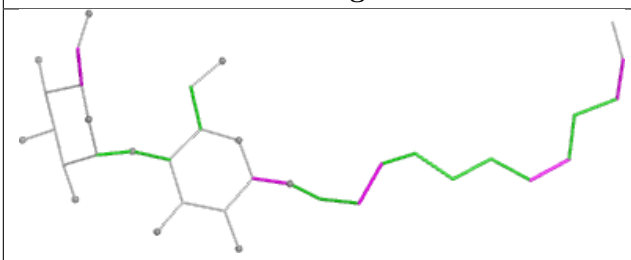
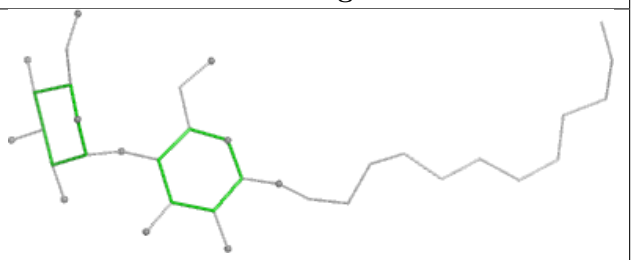
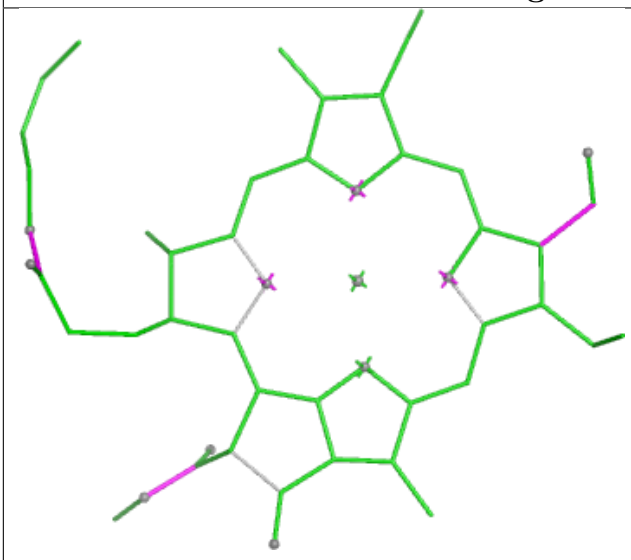


Torsions



Rings

Ligand CHL y 312



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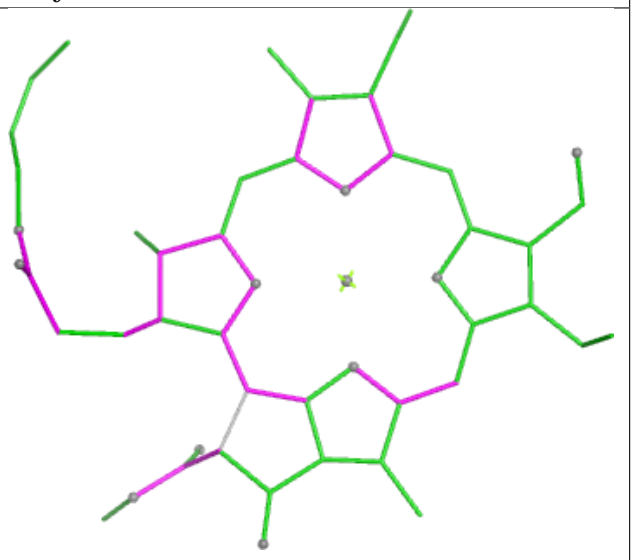

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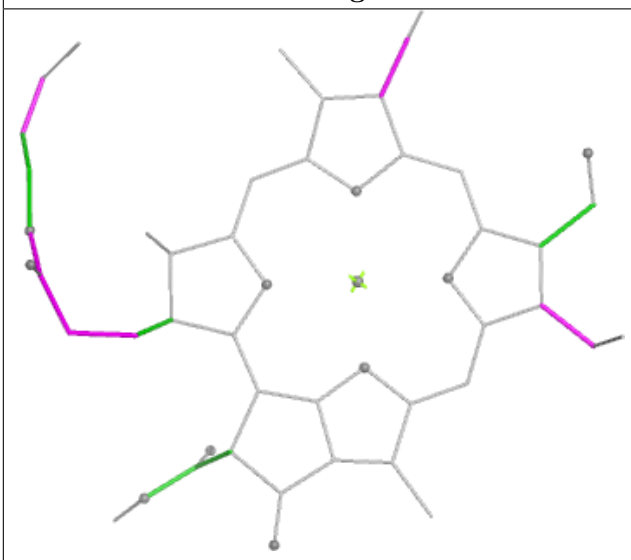

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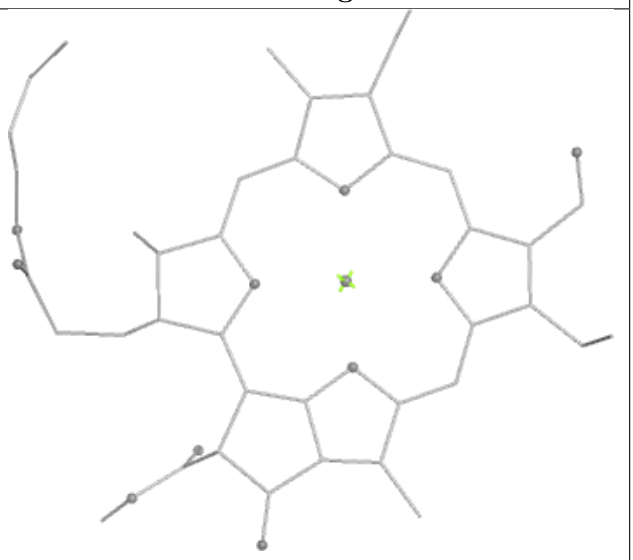
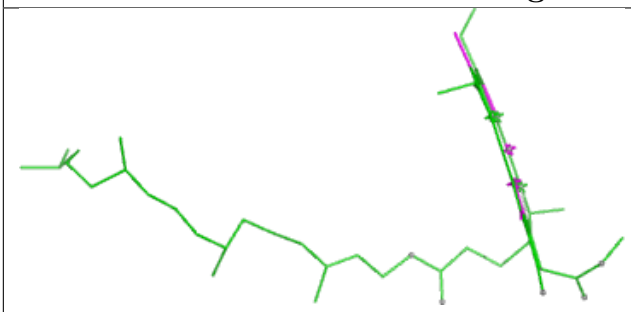


Rings

Ligand CLA b 613



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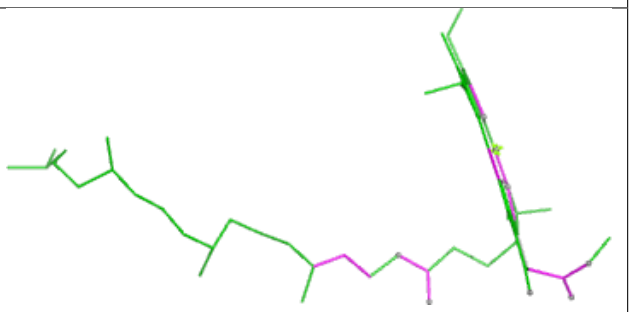

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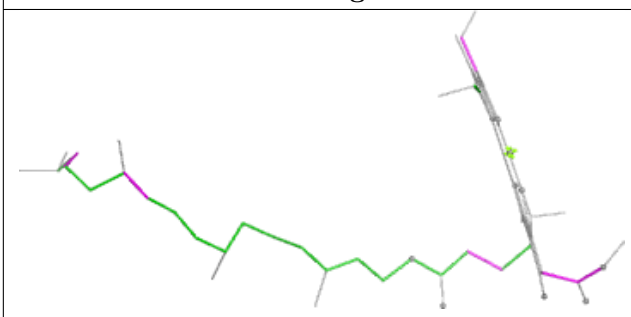

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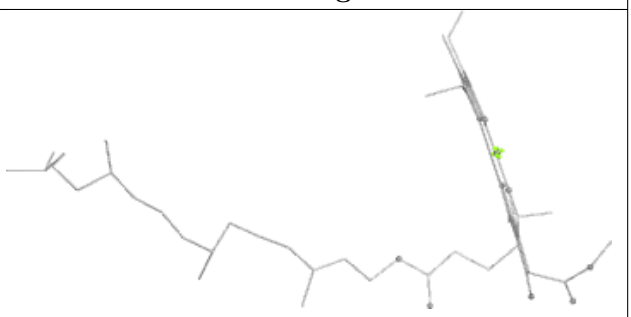
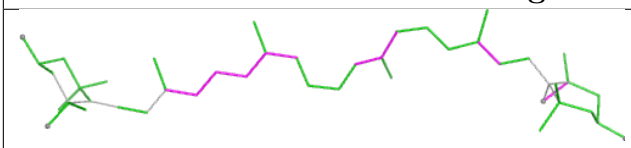


Rings

Ligand NEX s 302



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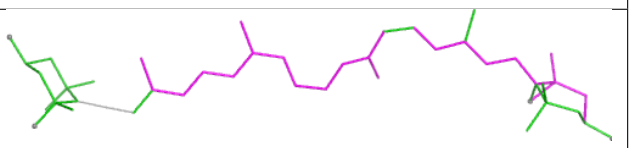

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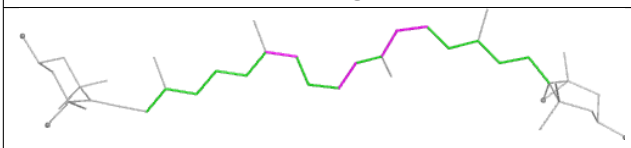

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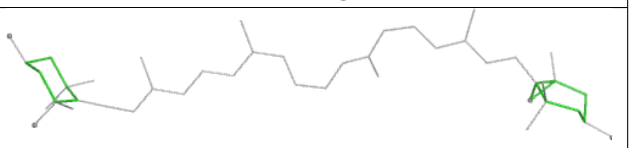
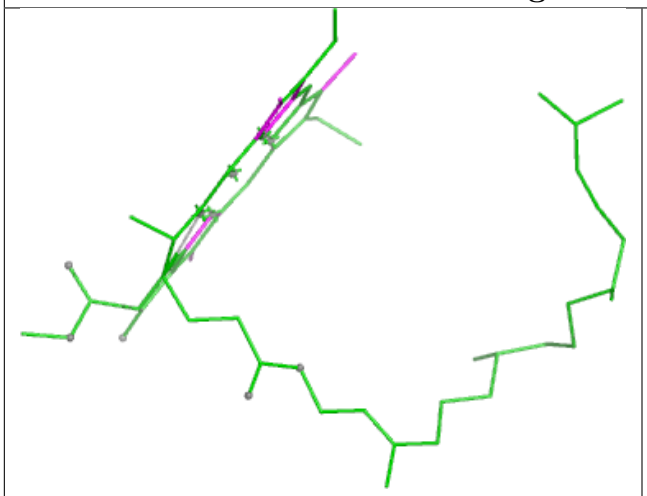


Rings

Ligand CLA b 610



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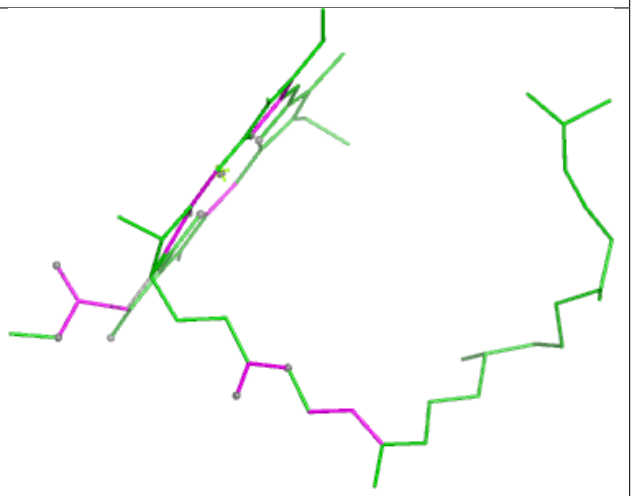

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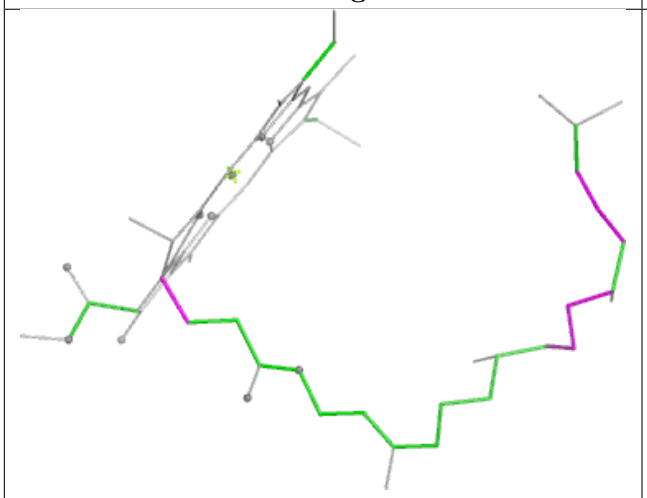

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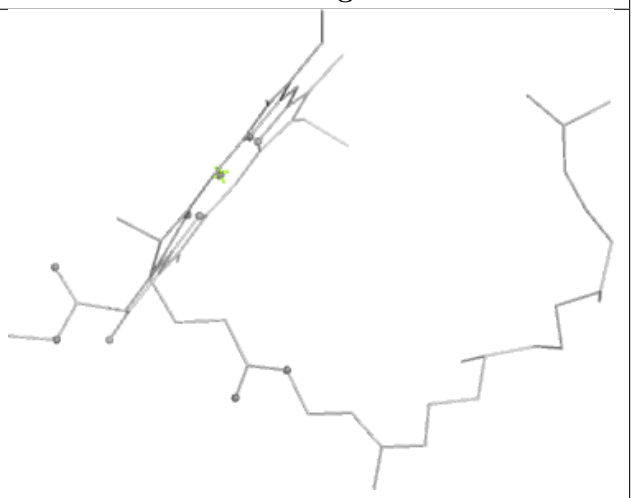
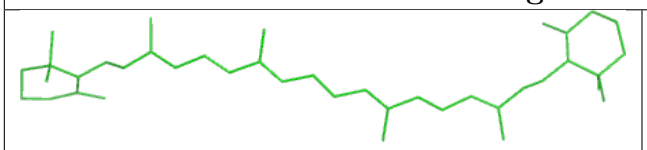


Rings

Ligand BCR d 401



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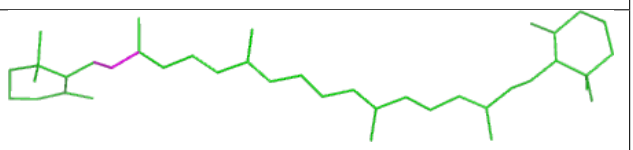

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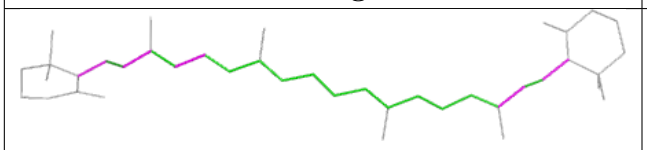

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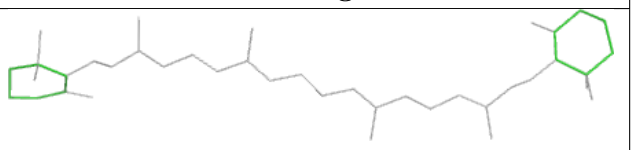
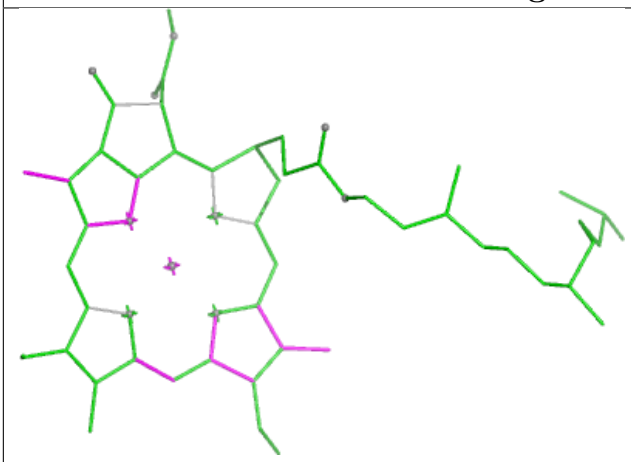


Rings

Ligand CLA a 402



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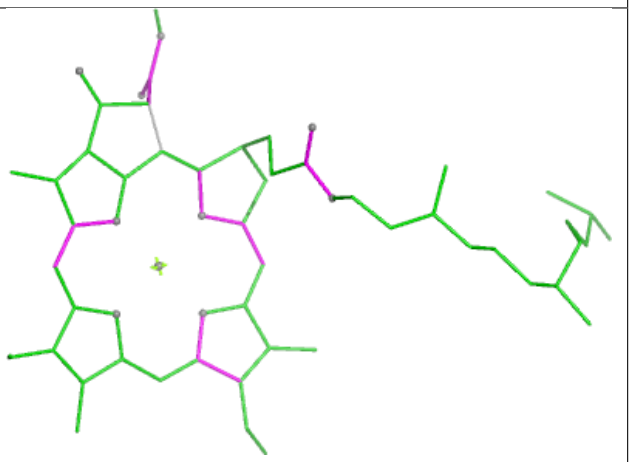

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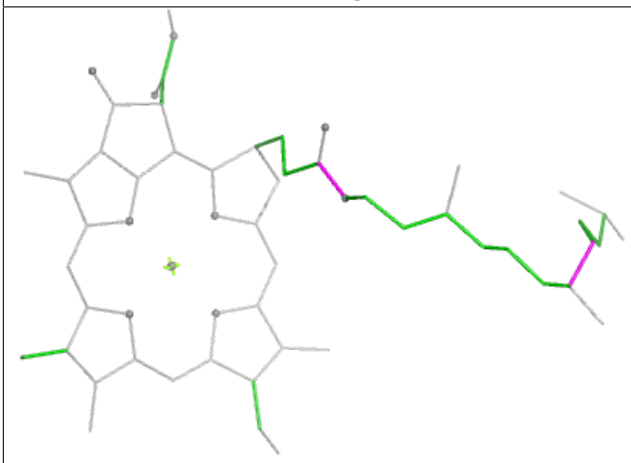
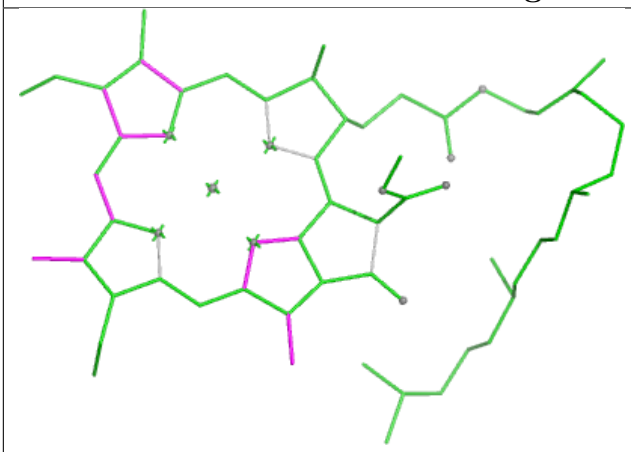


Torsions



Rings

Ligand CLA B 612



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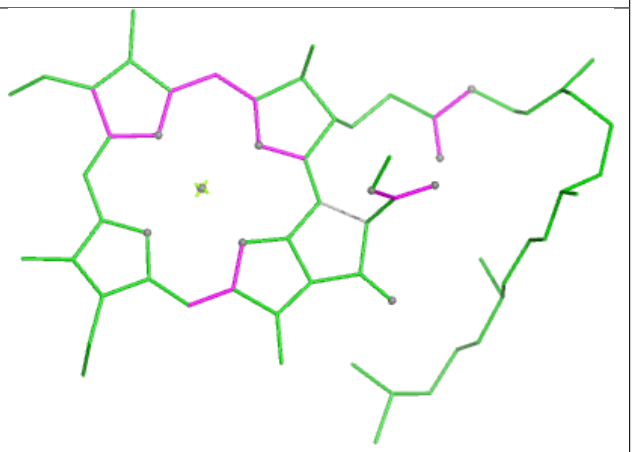

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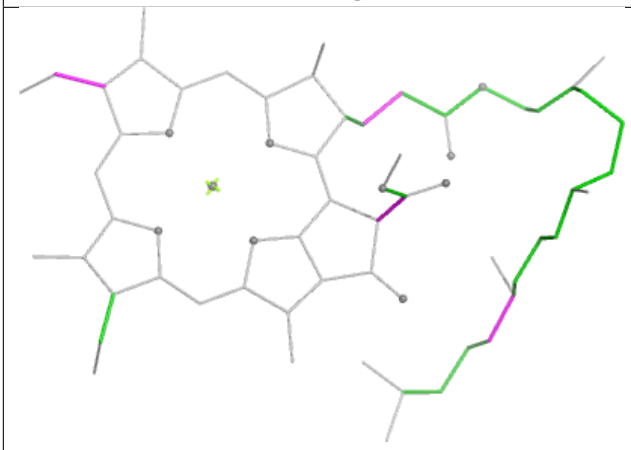

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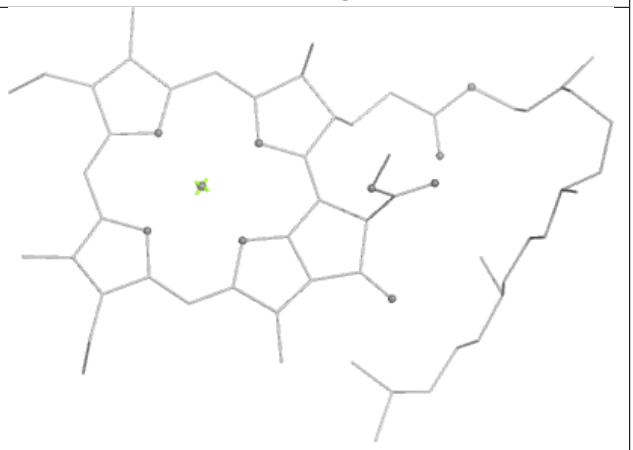
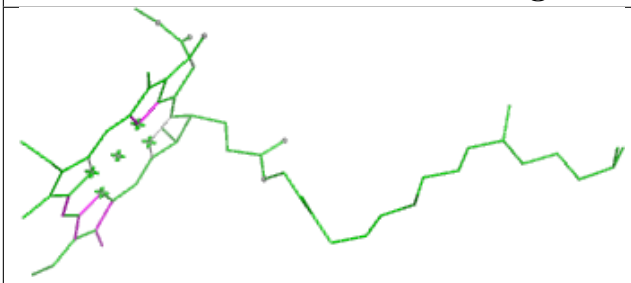


Rings

Ligand CLA c 515



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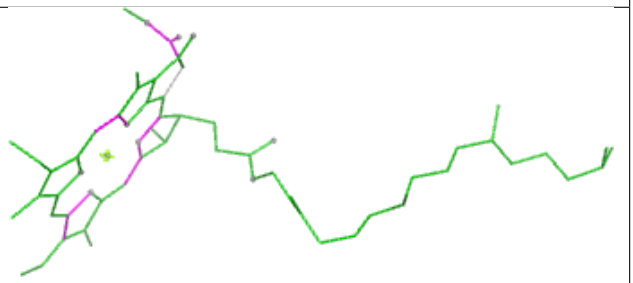
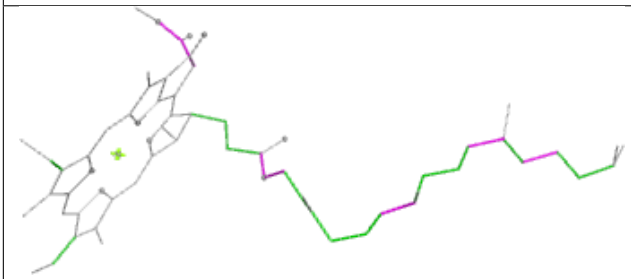


Bond angles



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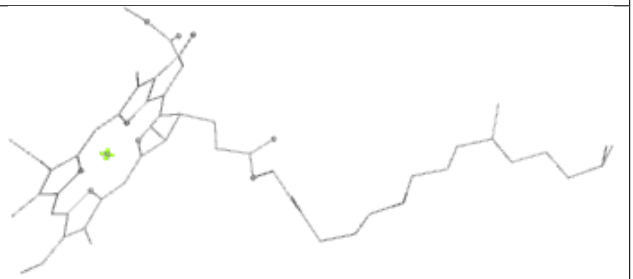
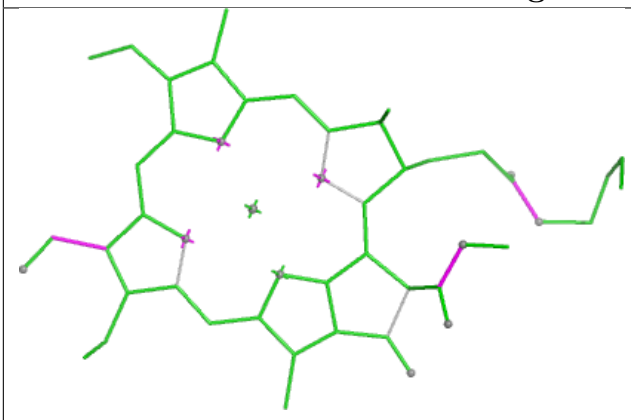


Rings

Ligand CHL g 313



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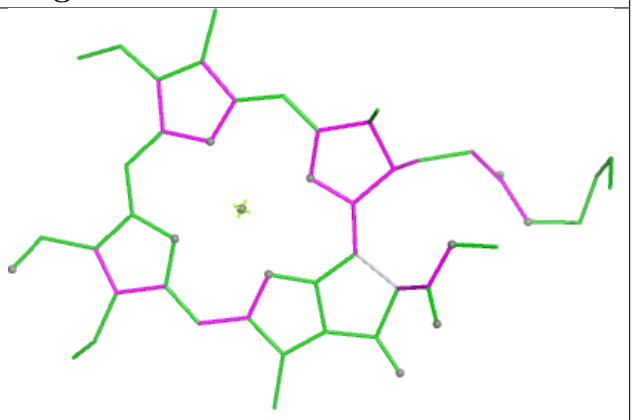

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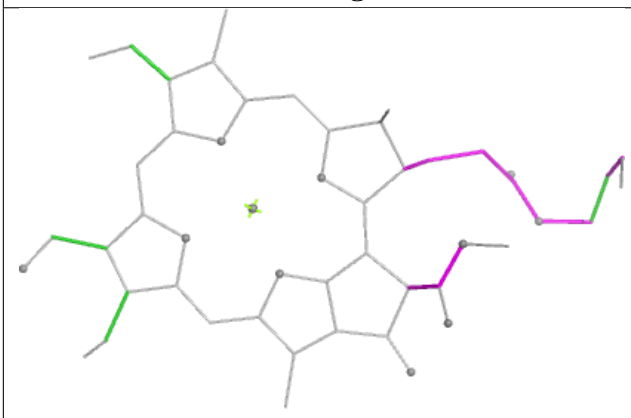

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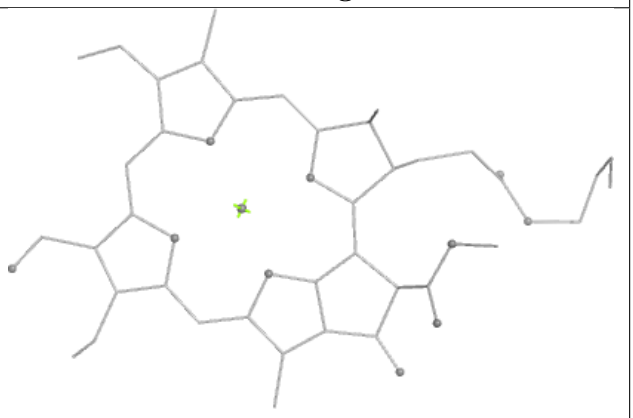
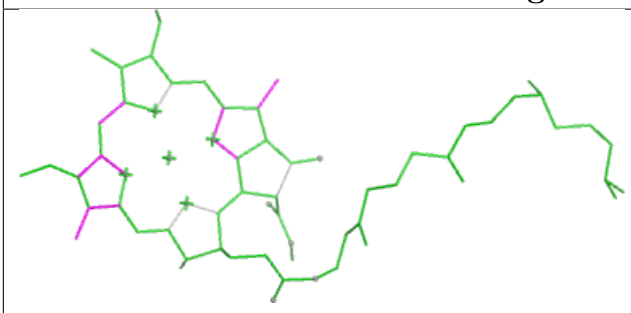


Rings

Ligand CLA b 601



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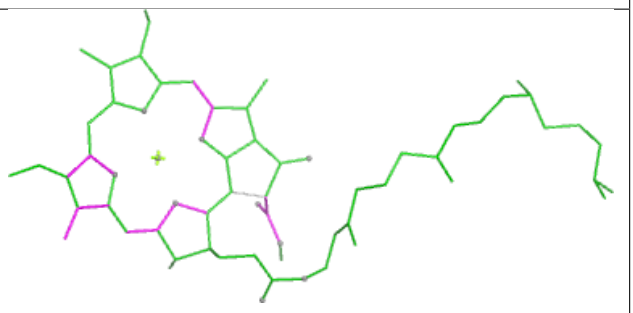
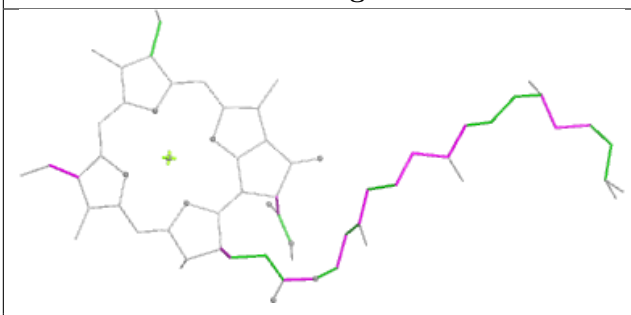


Bond angles



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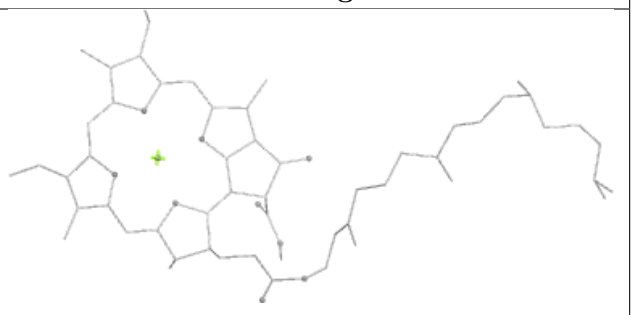
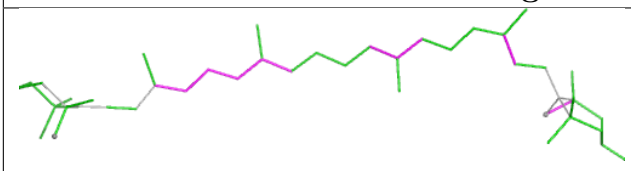


Rings

Ligand NEX Y 304



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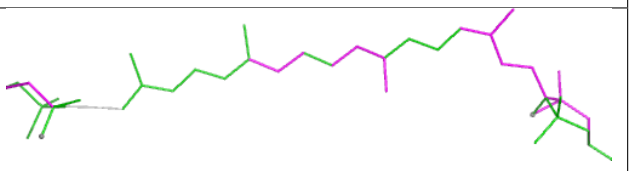
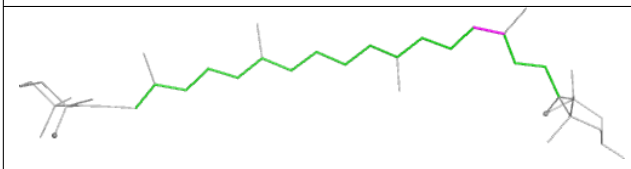


Bond angles



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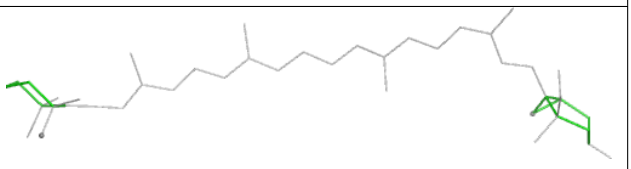
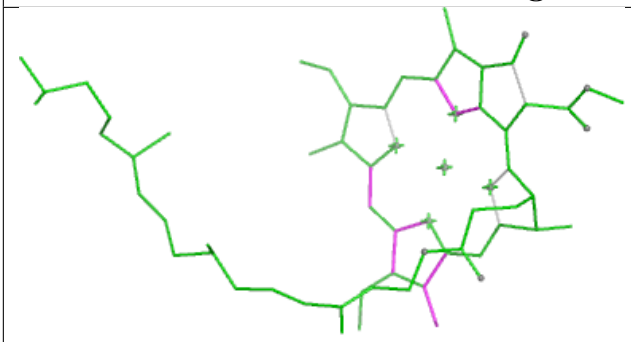


Rings

Ligand CLA n 303



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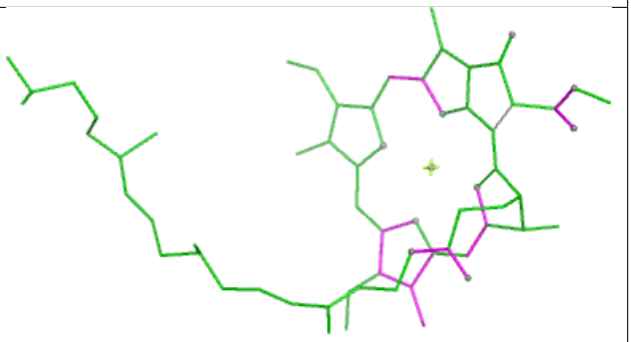
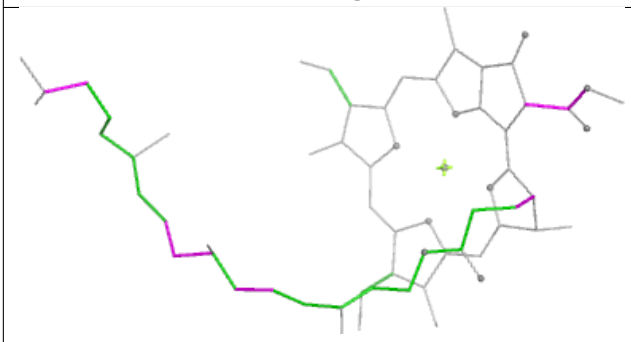


Bond angles

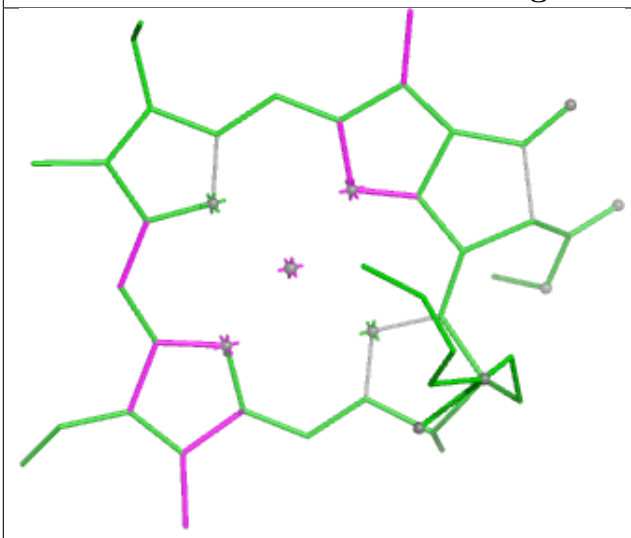


Torsions



Rings

Ligand CLA r 311



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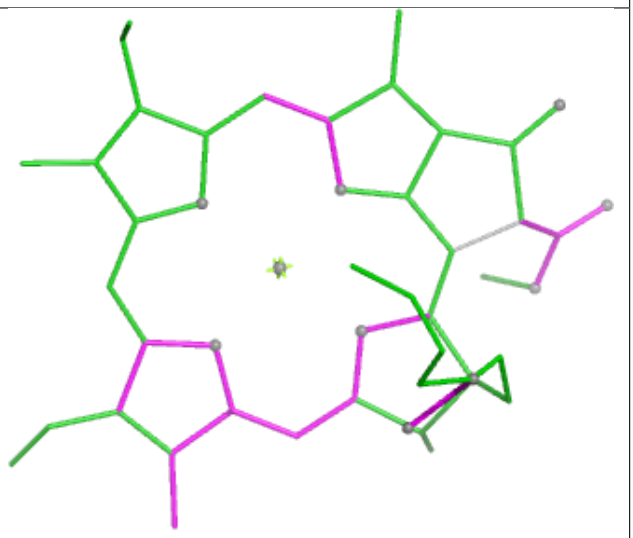
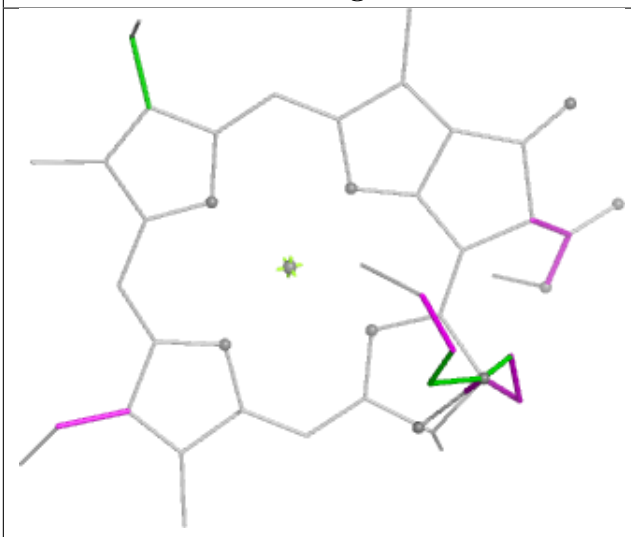


Bond angles



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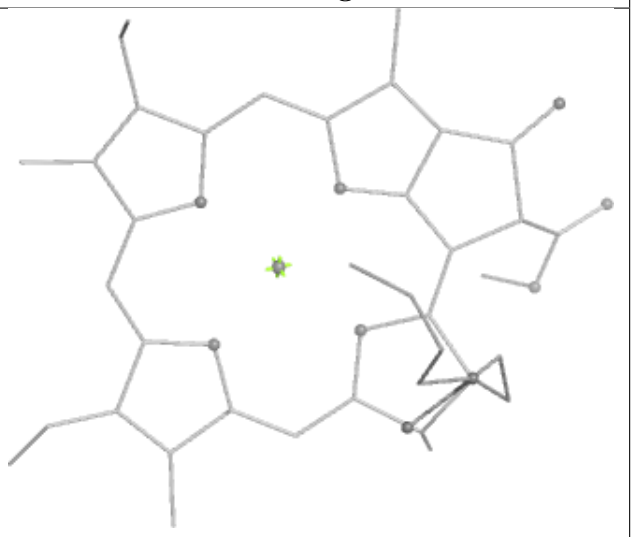
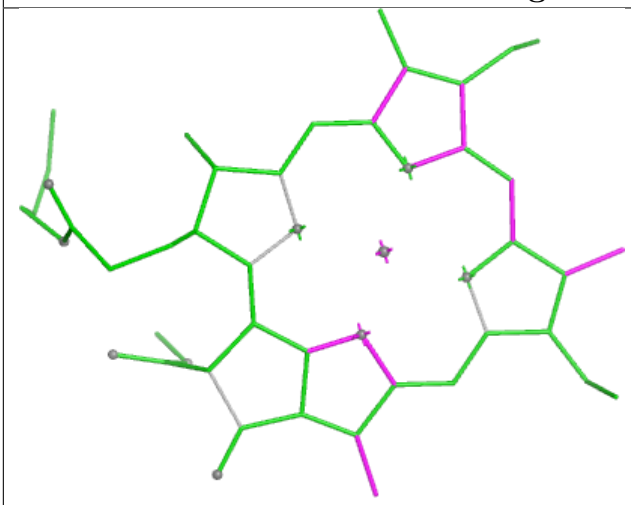


Rings

Ligand CLA g 308



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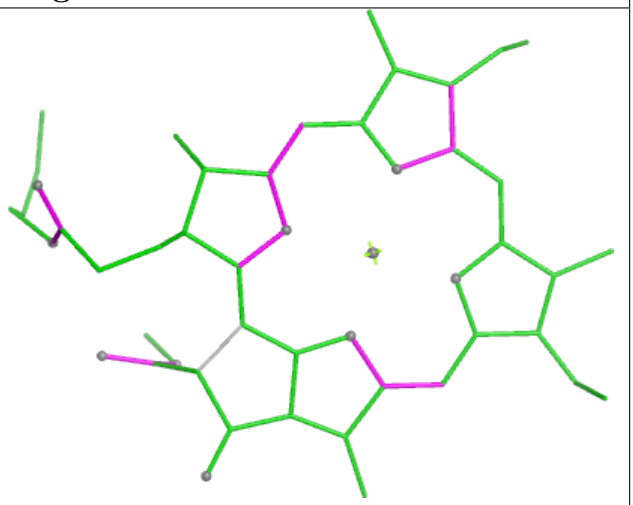
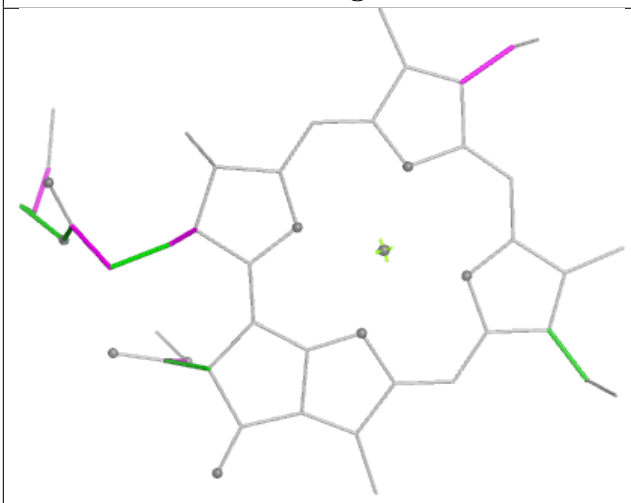
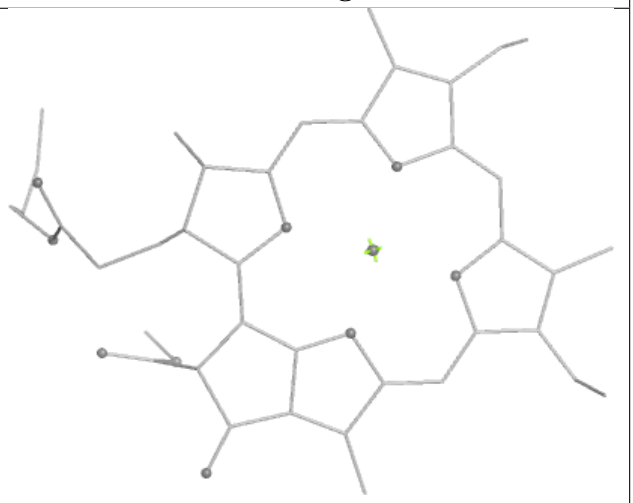


Bond angles

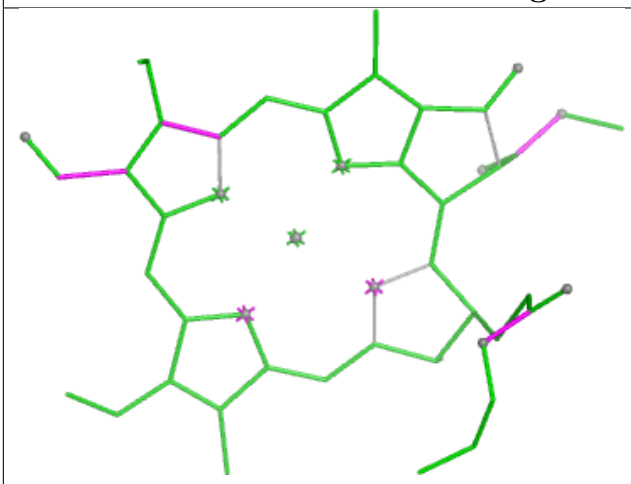


Torsions

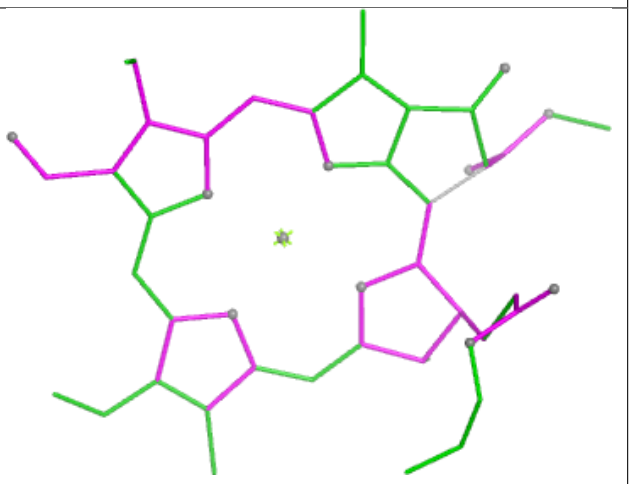


Rings

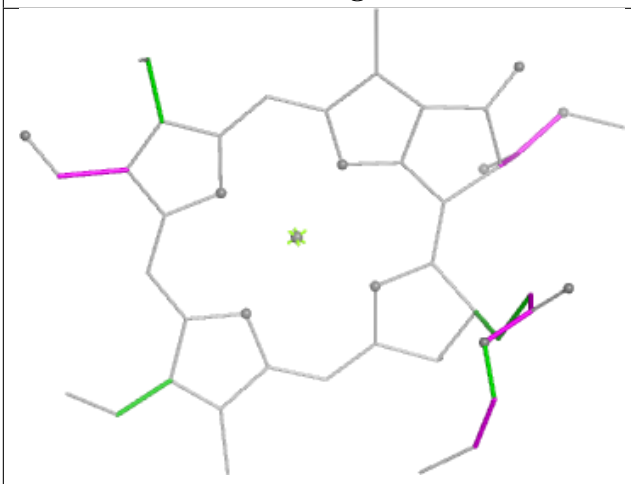
Ligand CHL s 313



Bond lengths



Bond angles



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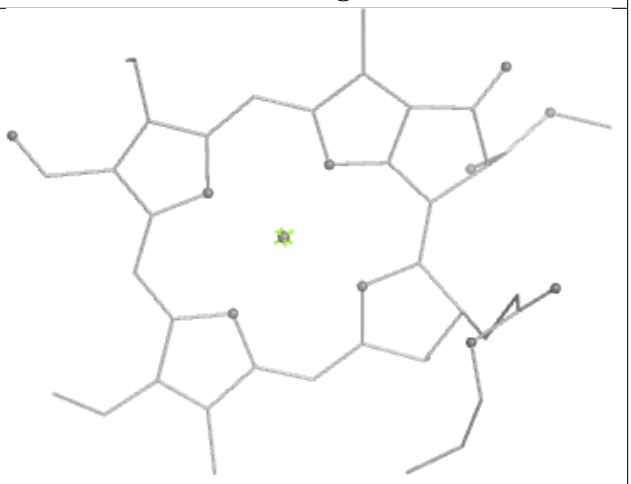
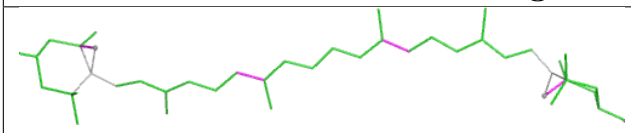


Rings

Ligand XAT r 304



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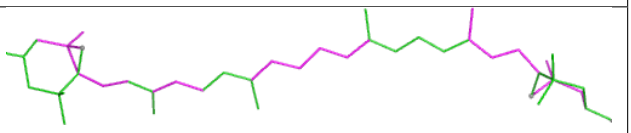
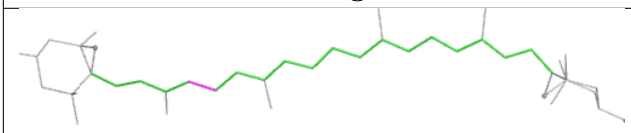
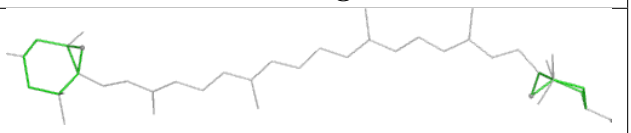


Bond angles

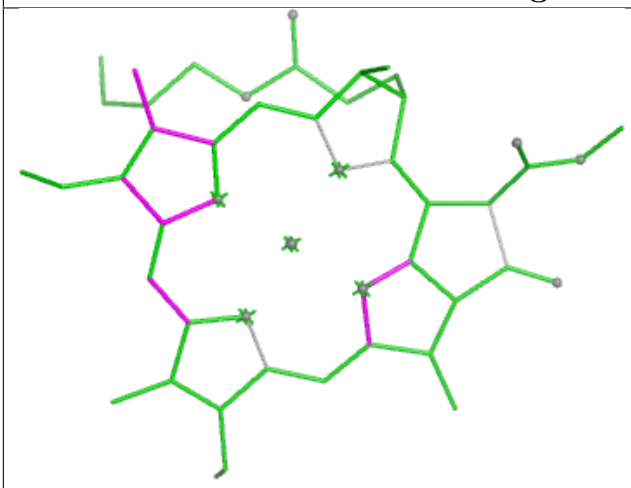


Torsions



Rings

Ligand CLA s 315



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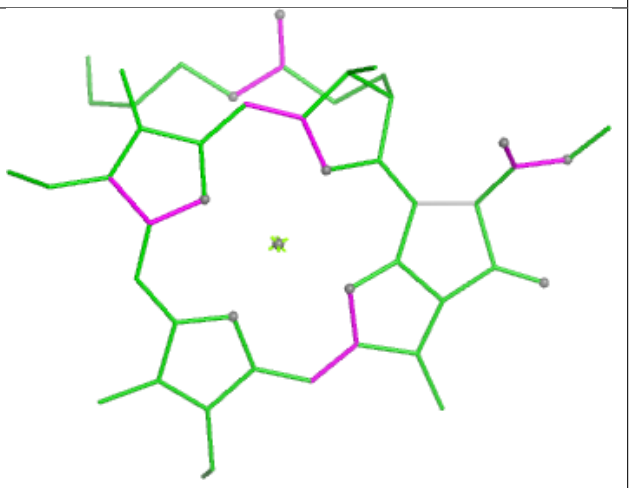
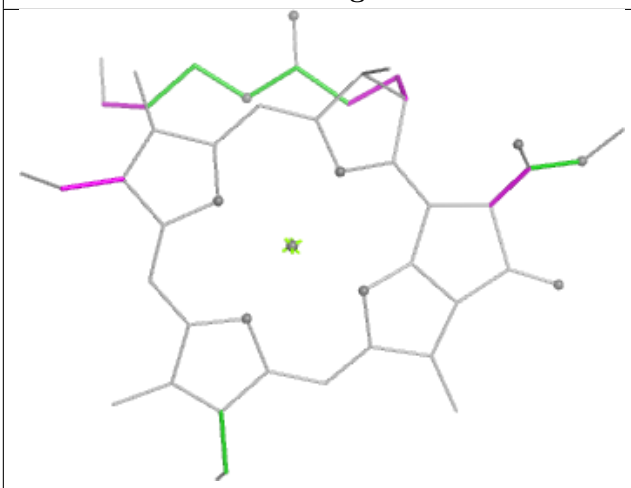


Bond angles



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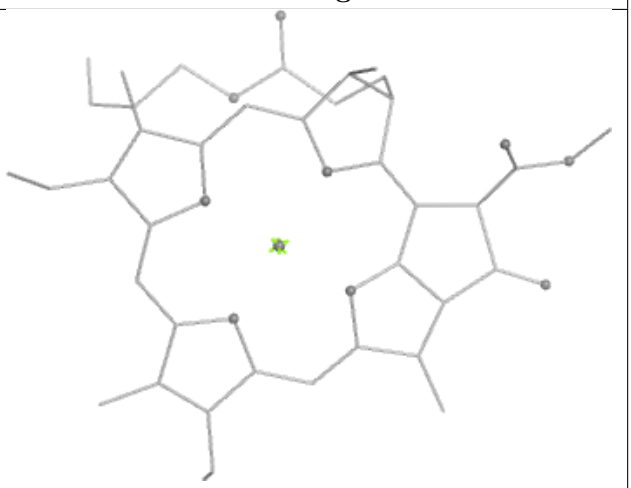
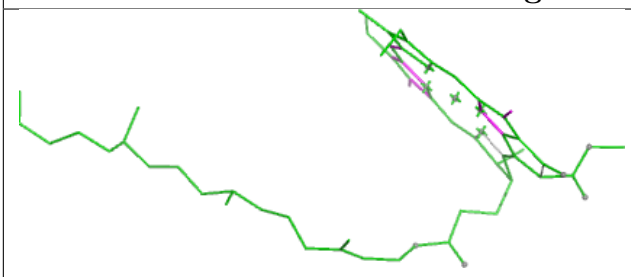


Rings

Ligand CLA C 521



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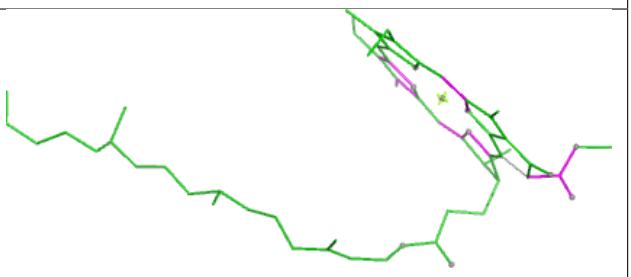
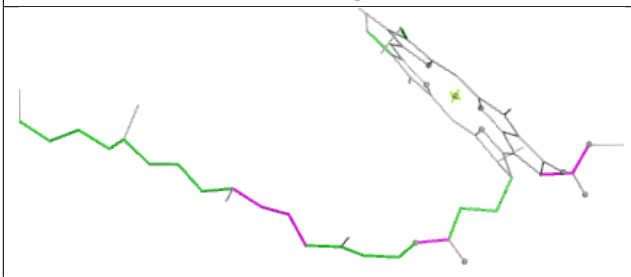


Bond angles



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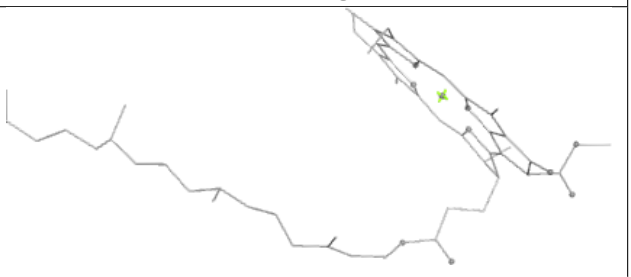
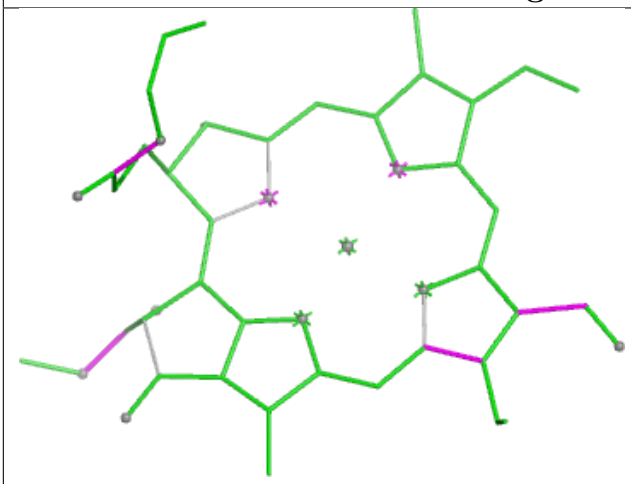


Rings

Ligand CHL S 312



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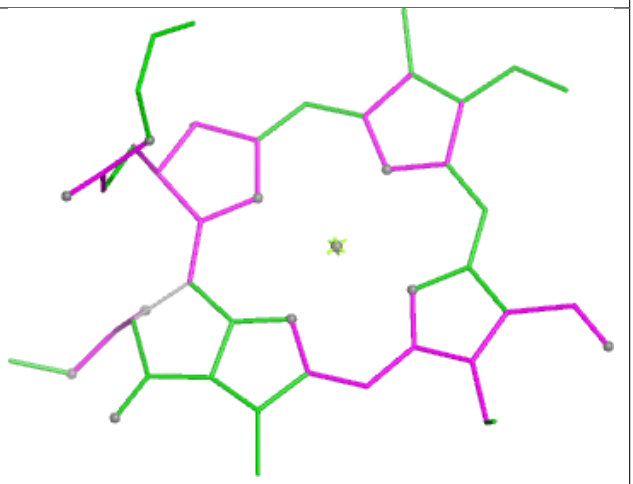
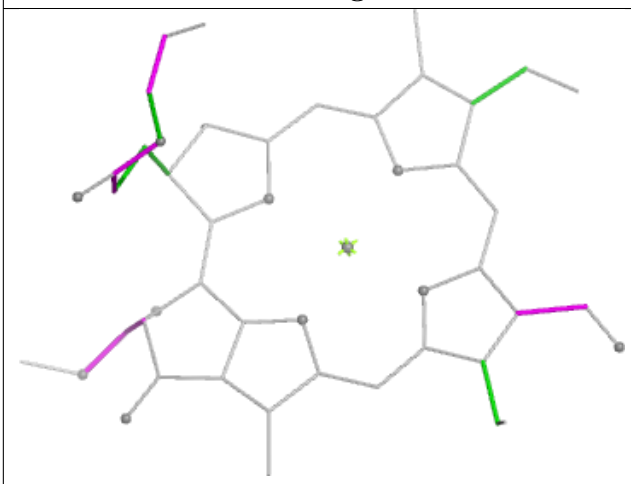


Bond angles



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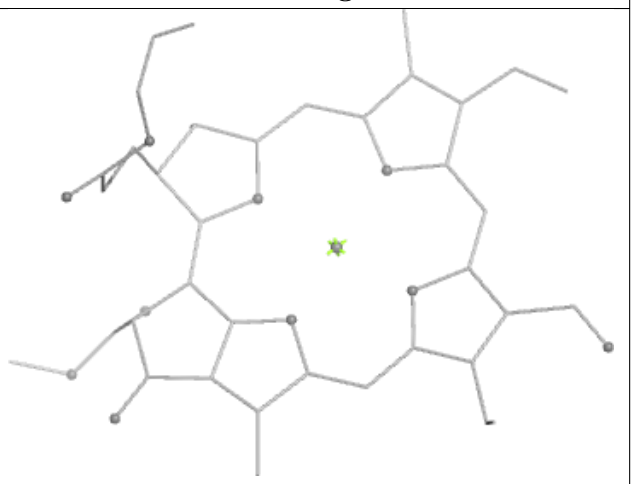
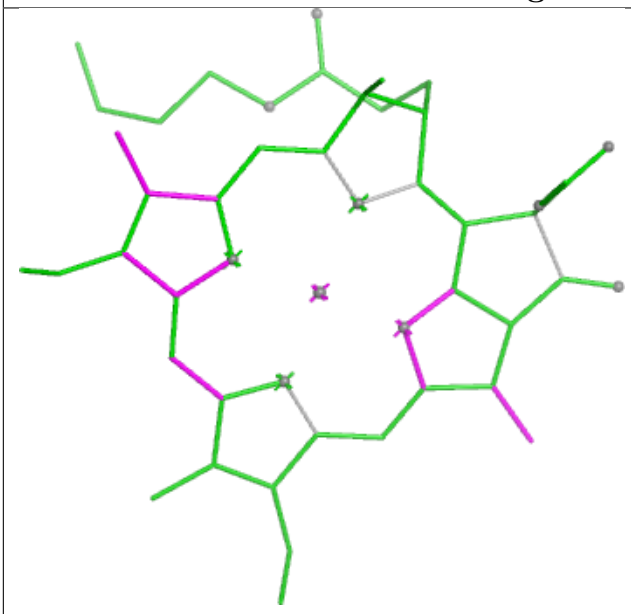


Rings

Ligand CLA S 307



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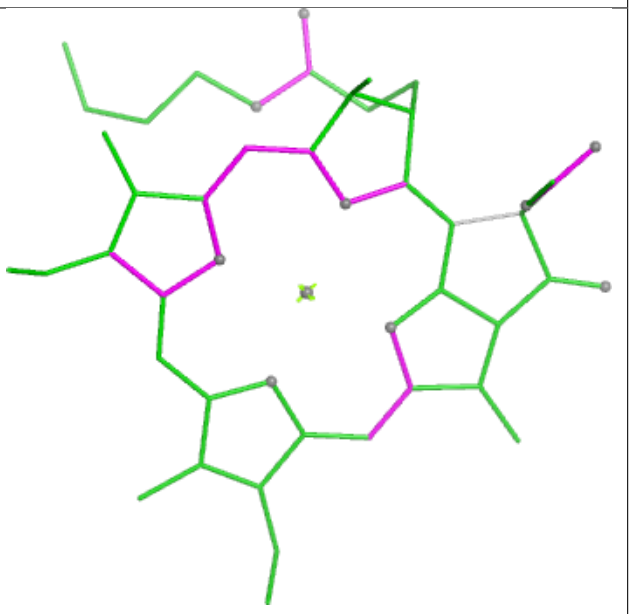
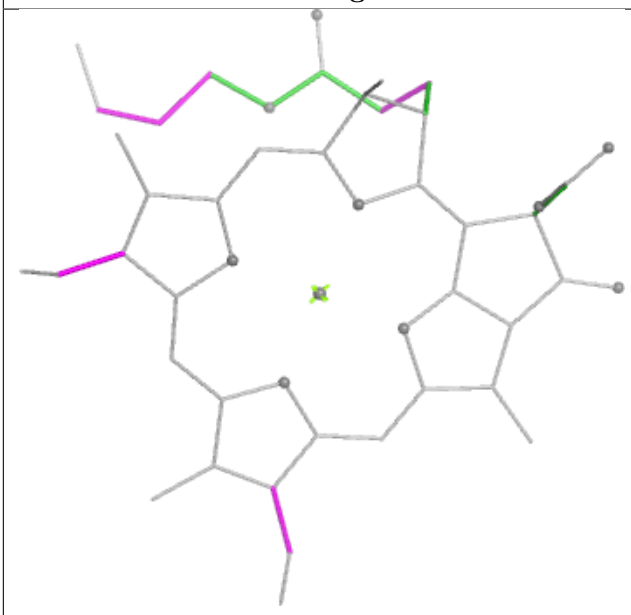


Bond angles



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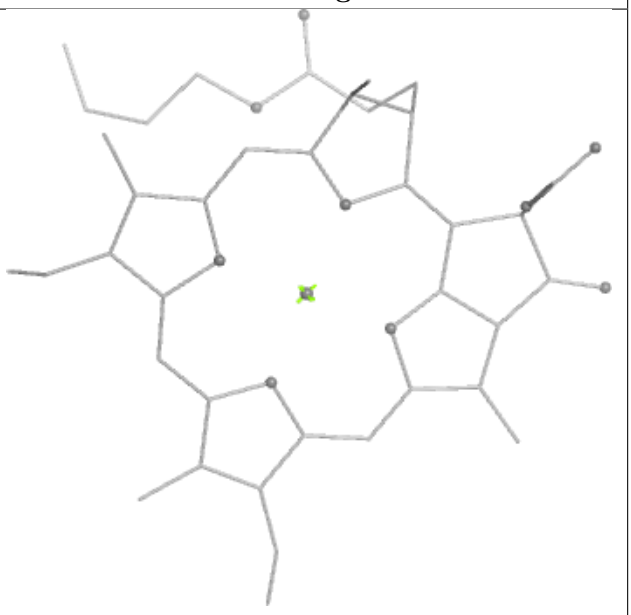
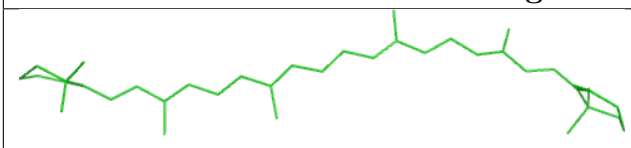


Rings

Ligand BCR h 101



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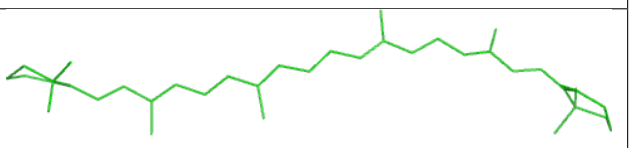
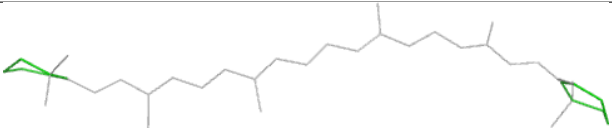


Bond angles

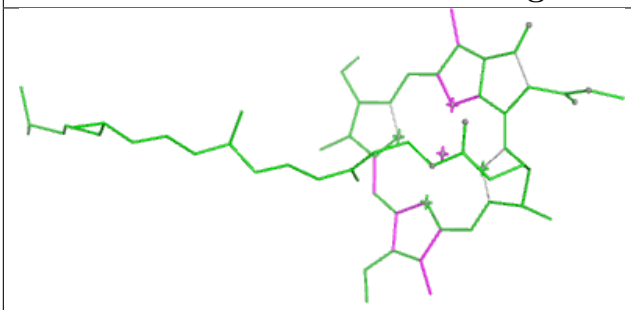


Torsions



Rings

Ligand CLA b 612



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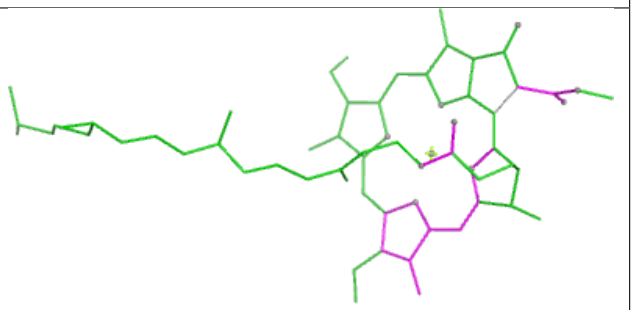
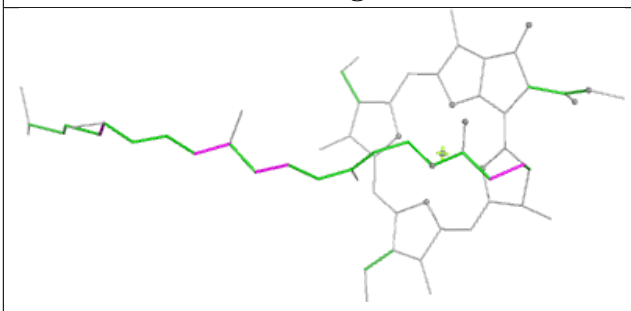


Bond angles



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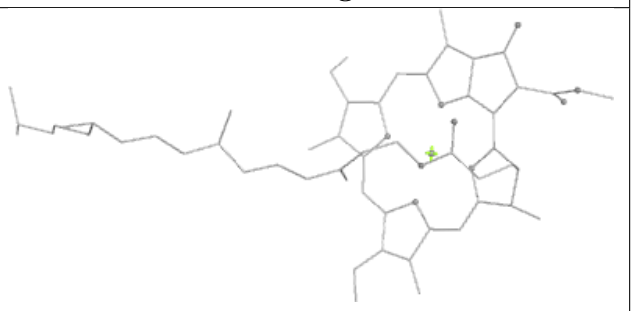
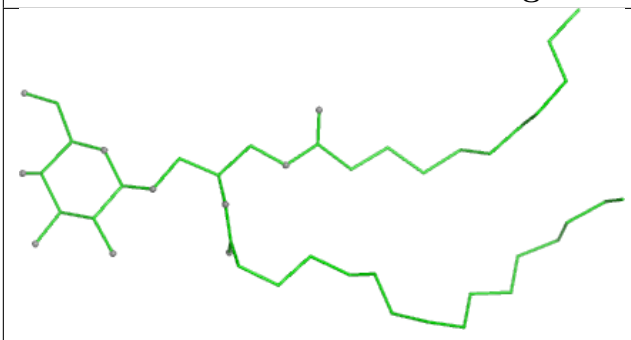


Rings

Ligand LMG d 405



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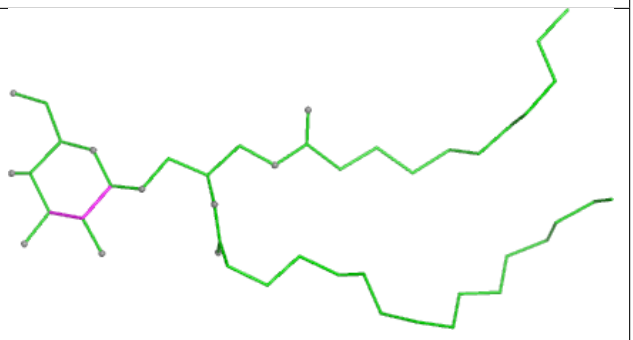
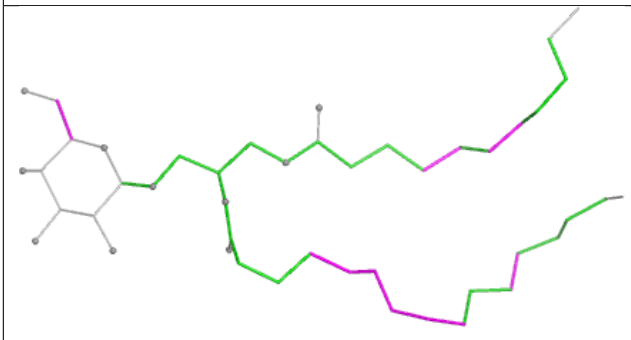


Bond angles



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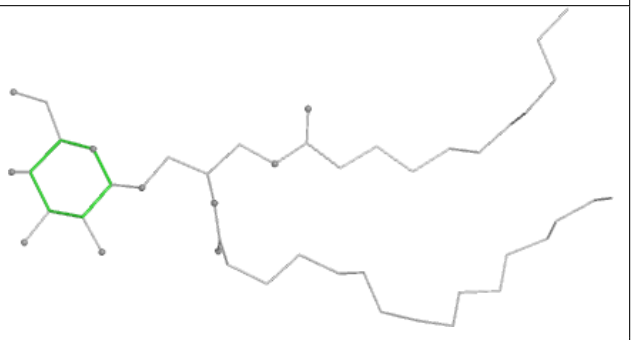
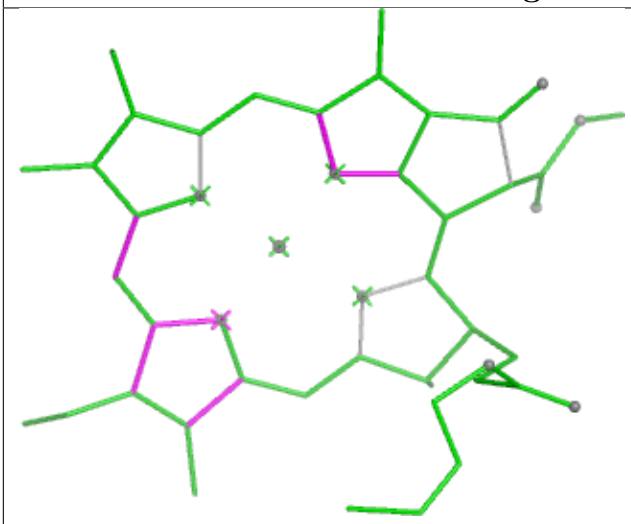


Rings

Ligand CLA G 304



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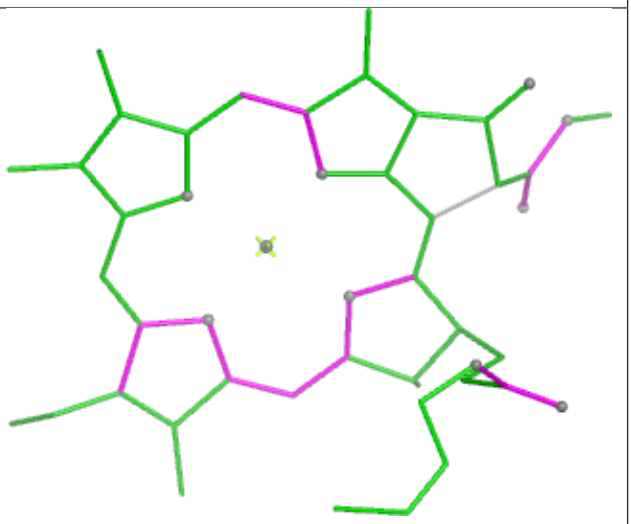
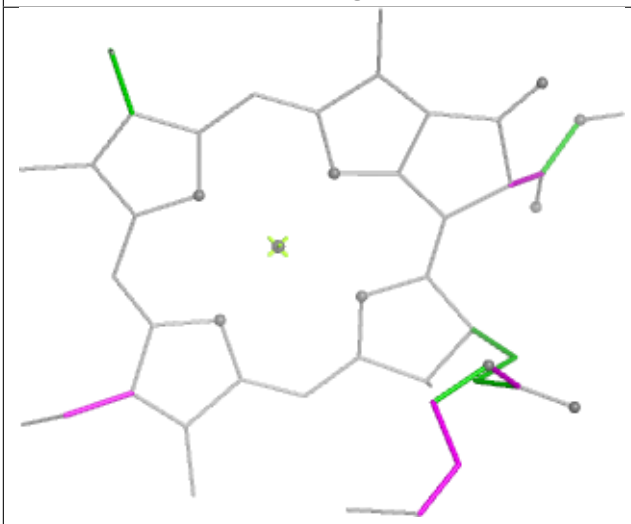


Bond angles



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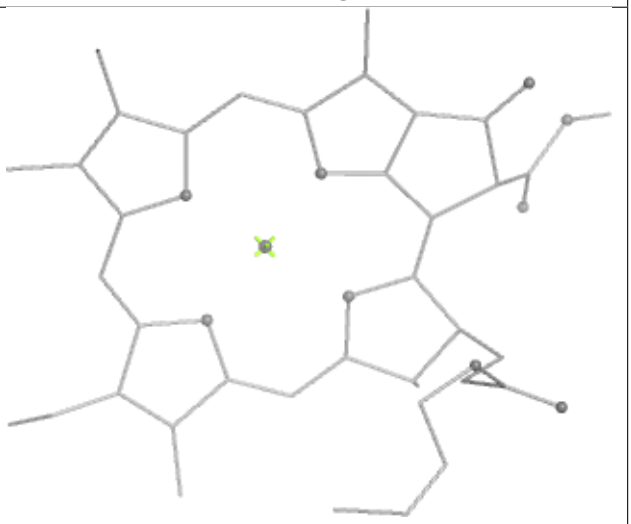
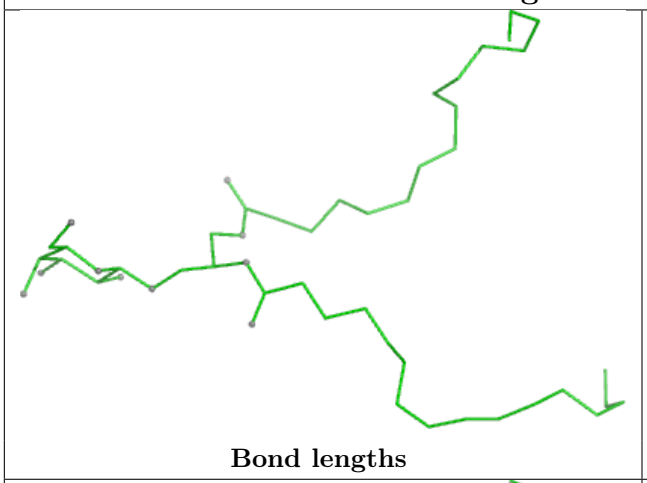


Rings

Ligand LMG B 622



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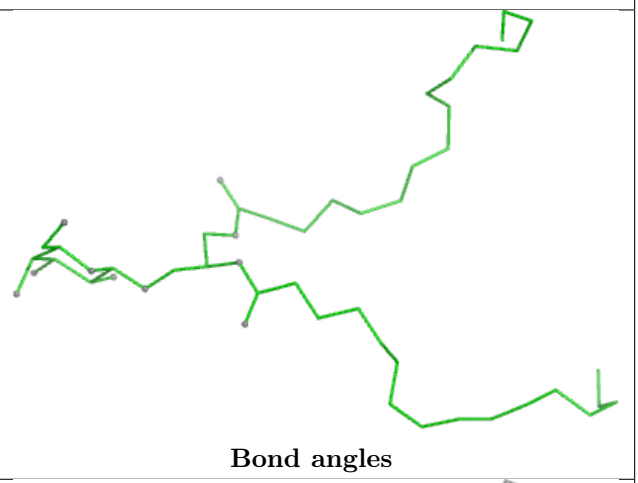
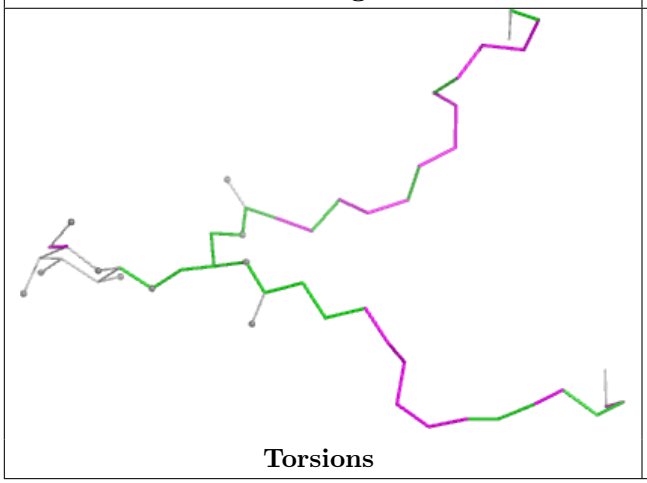


Bond angles



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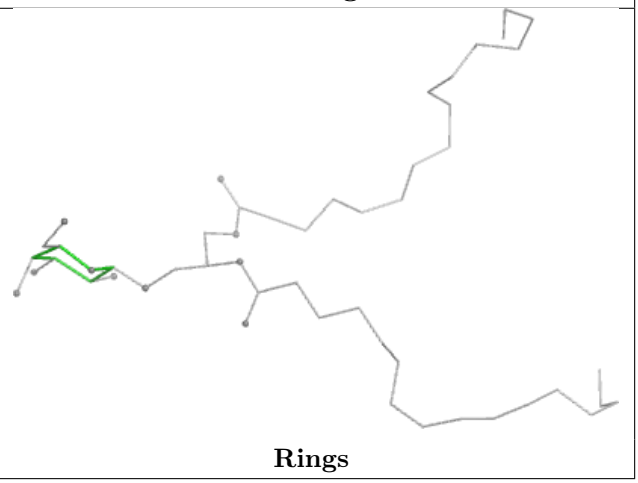
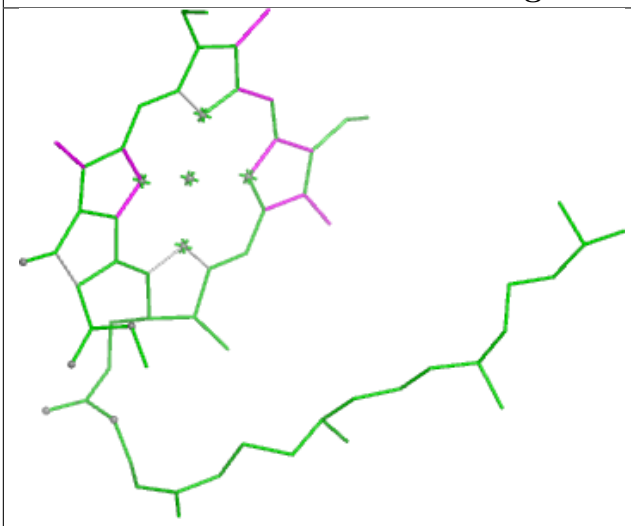


Rings

Ligand CLA B 602



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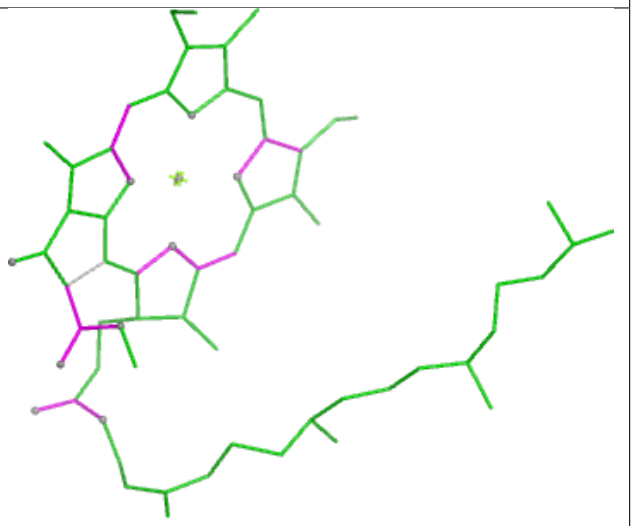
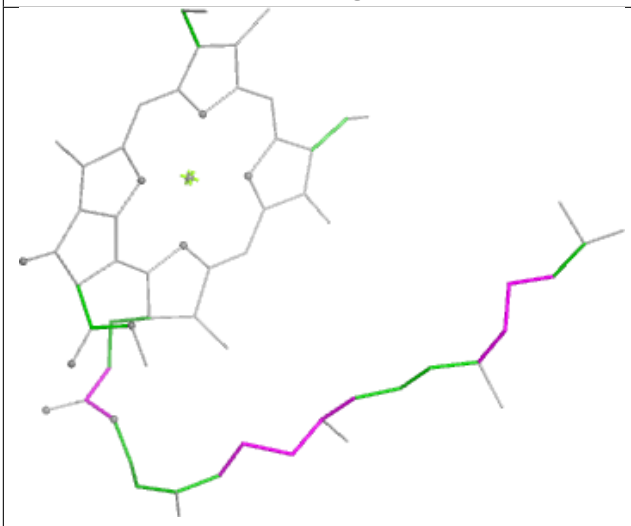


Bond angles

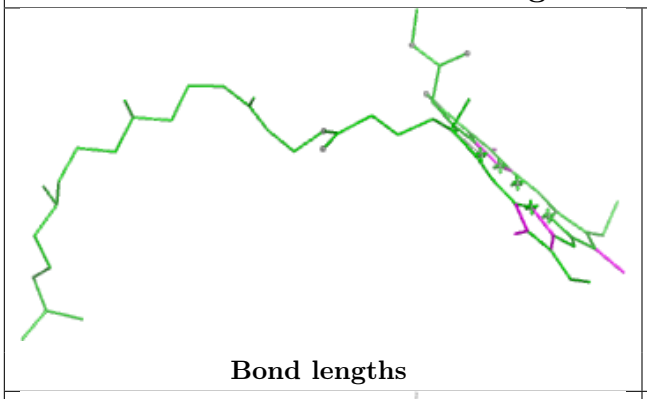


Torsions



Rings

Ligand CLA d 404



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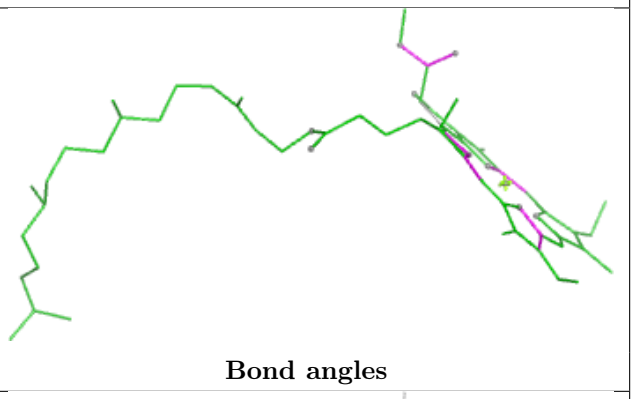
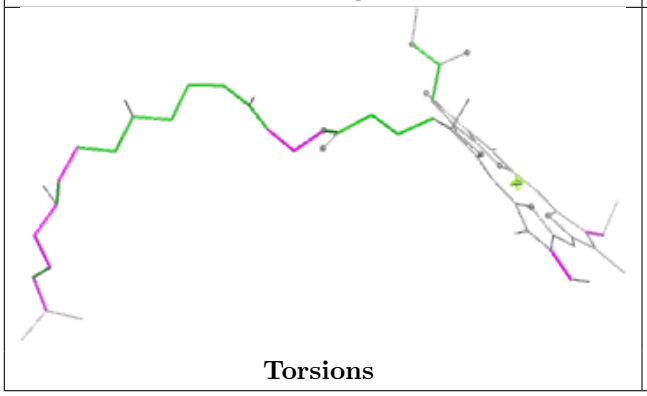


Bond angles

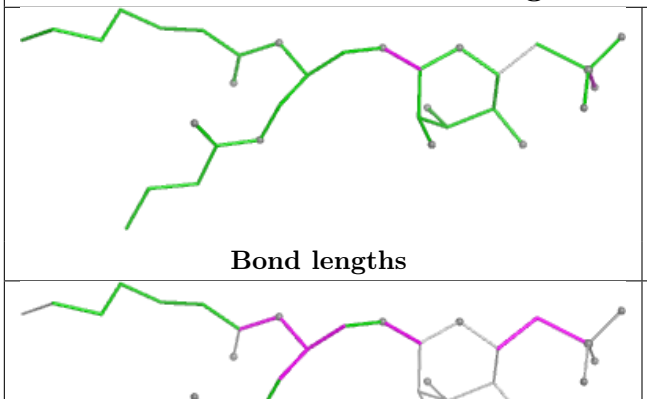


Torsions



Rings

Ligand SQD w 202



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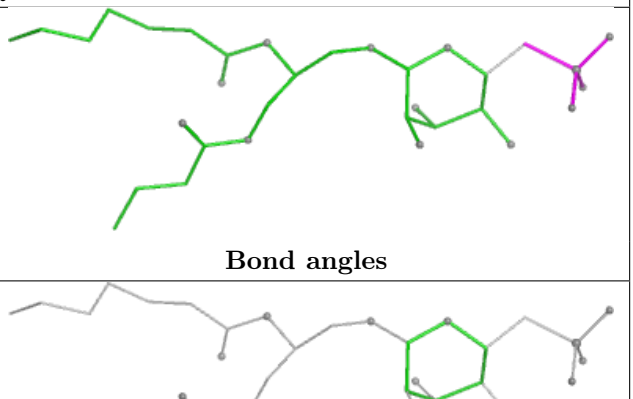
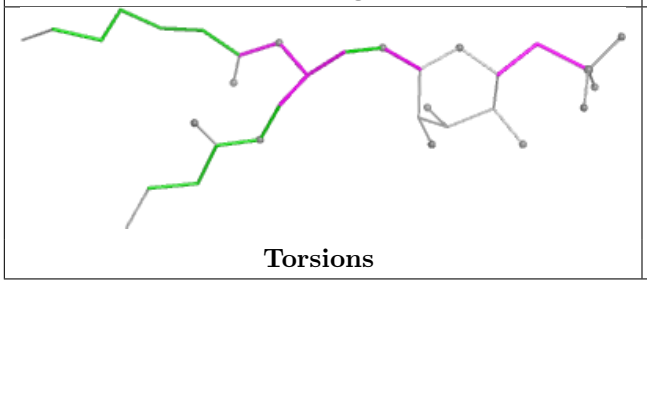


Bond angles



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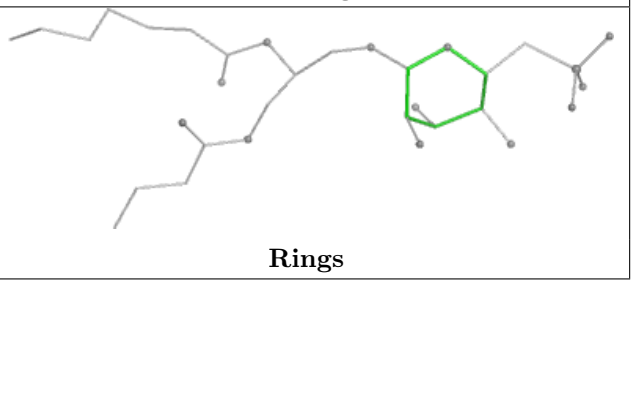
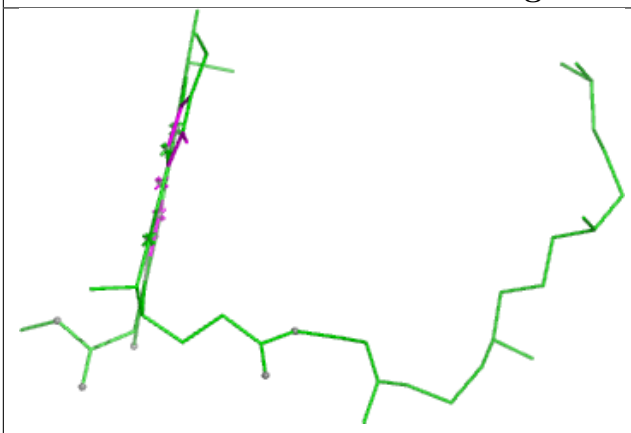


Rings

Ligand CLA C 508



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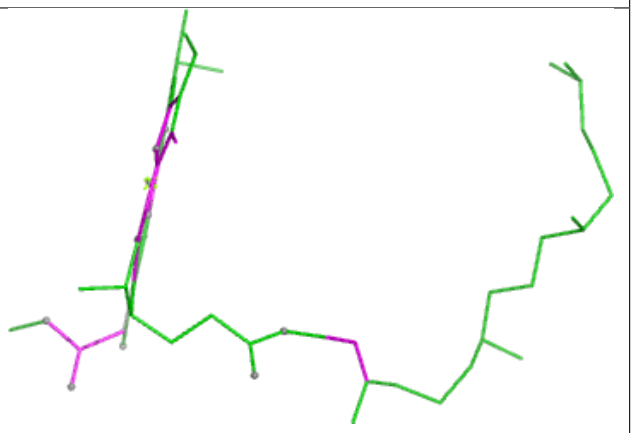
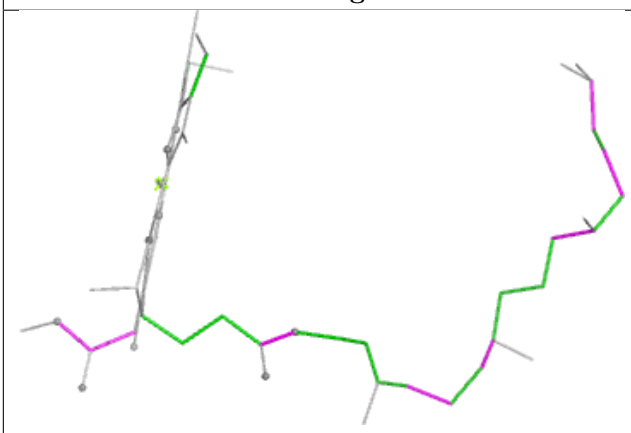


Bond angles

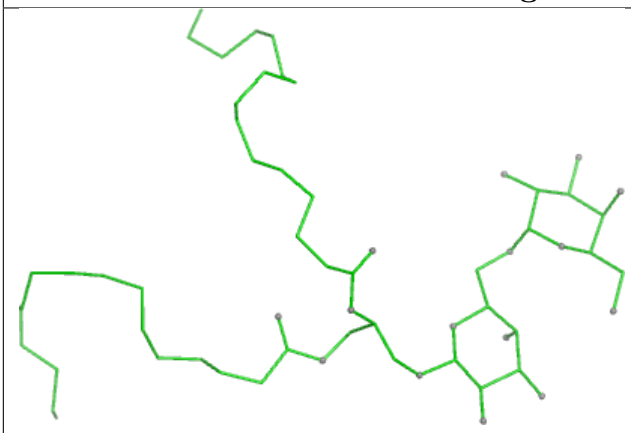


Torsions

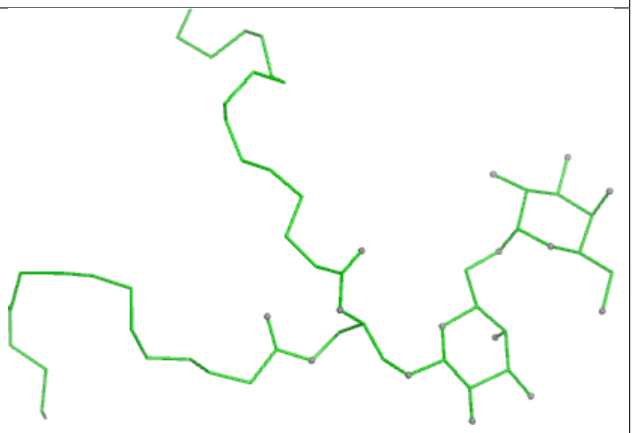


Rings

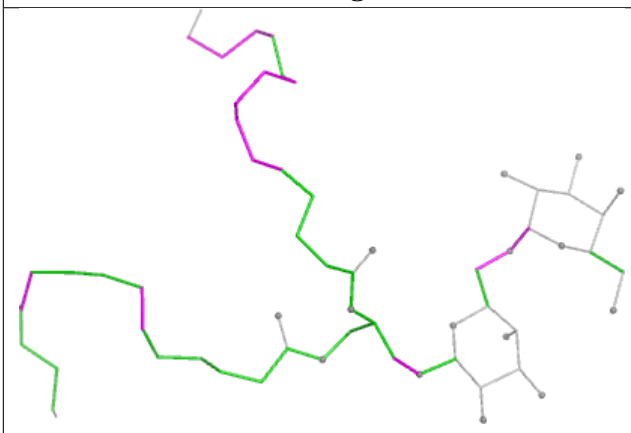
Ligand DGD C 510



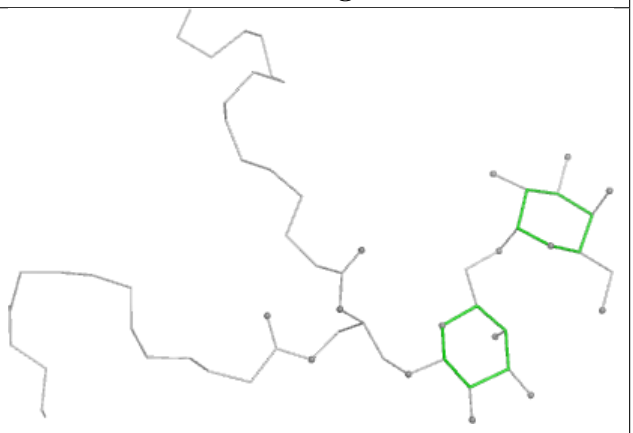
Bond lengths



Bond angles

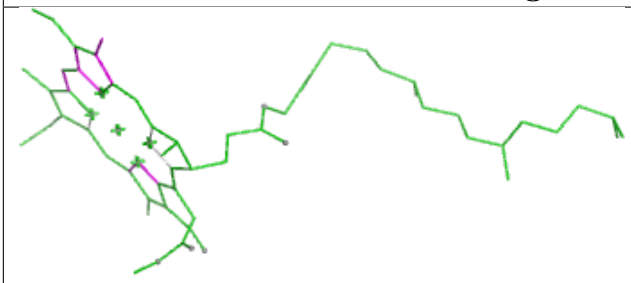


Torsions



Rings

Ligand CLA C 512



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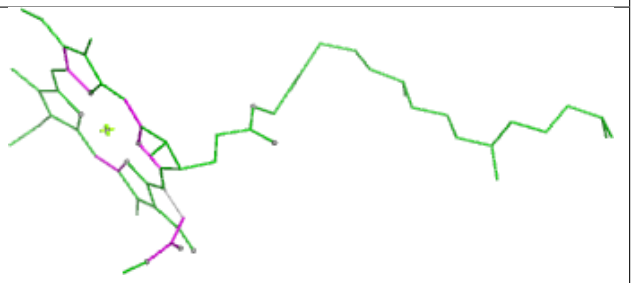

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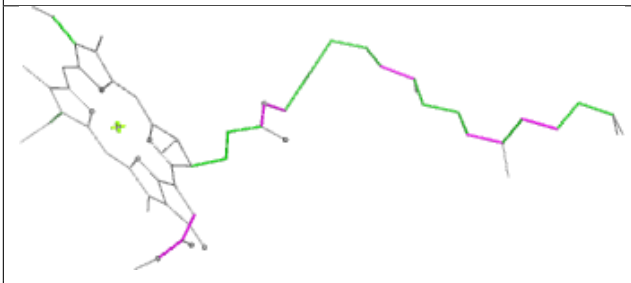

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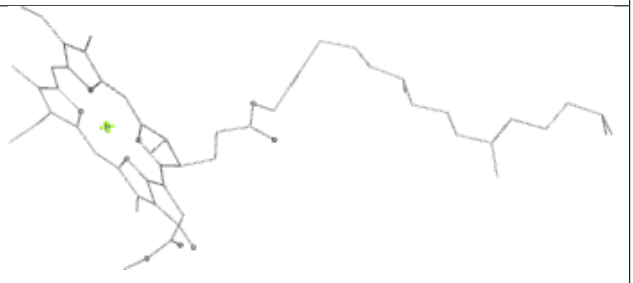
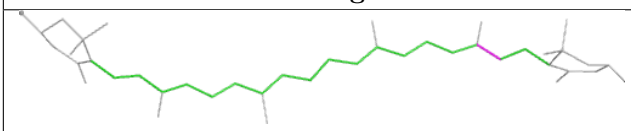
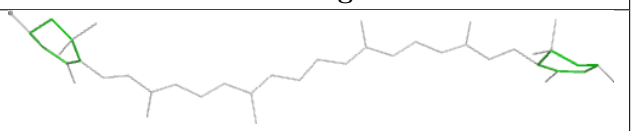


Rings

Ligand LUT Y 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

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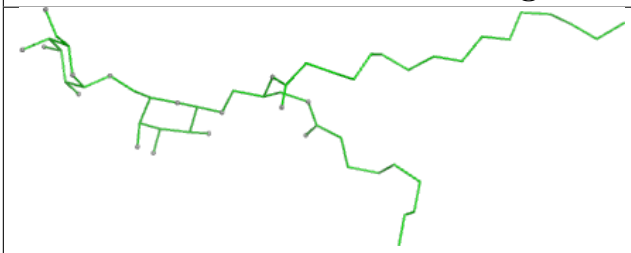
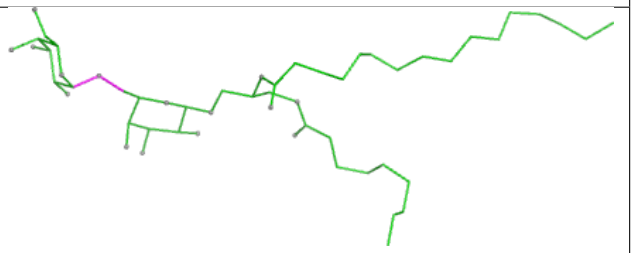
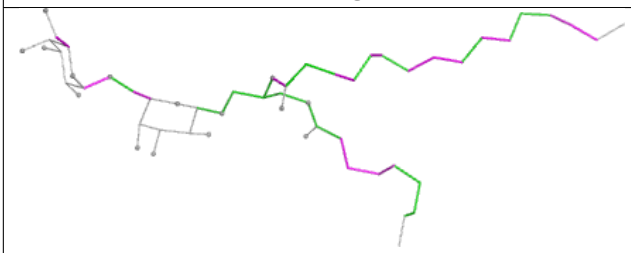
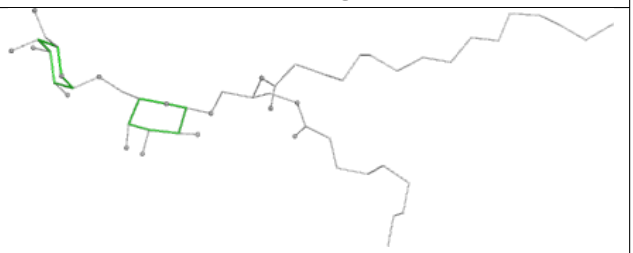
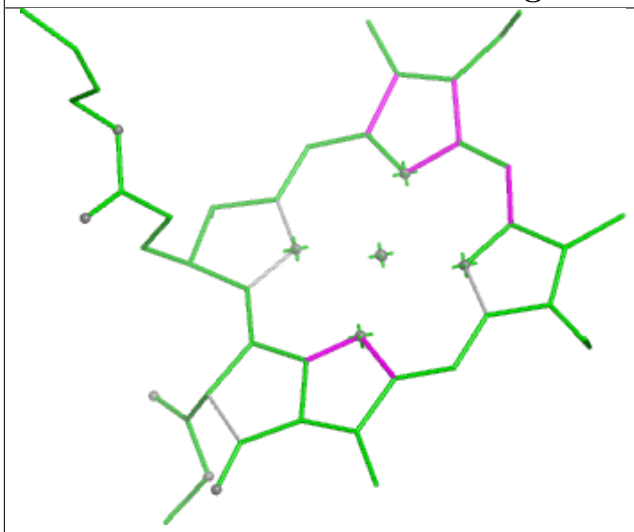
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 309



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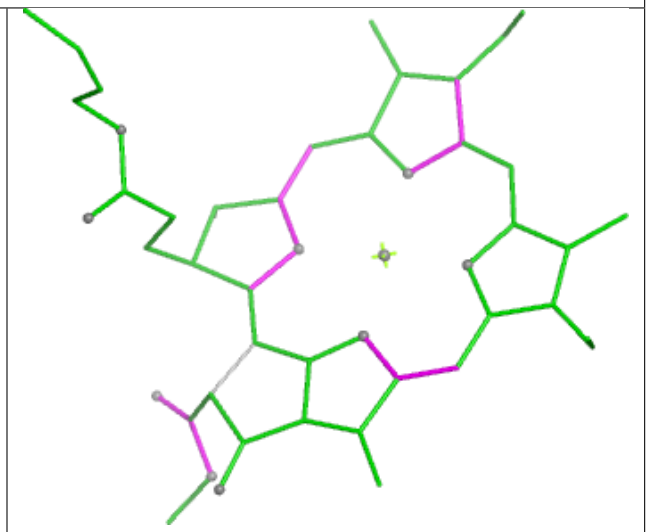

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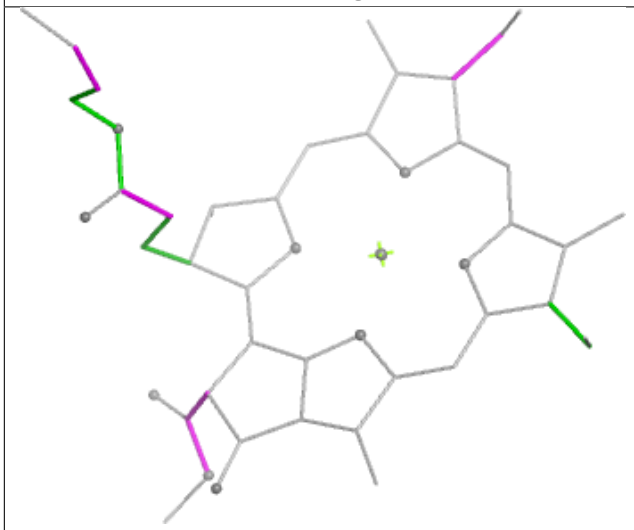

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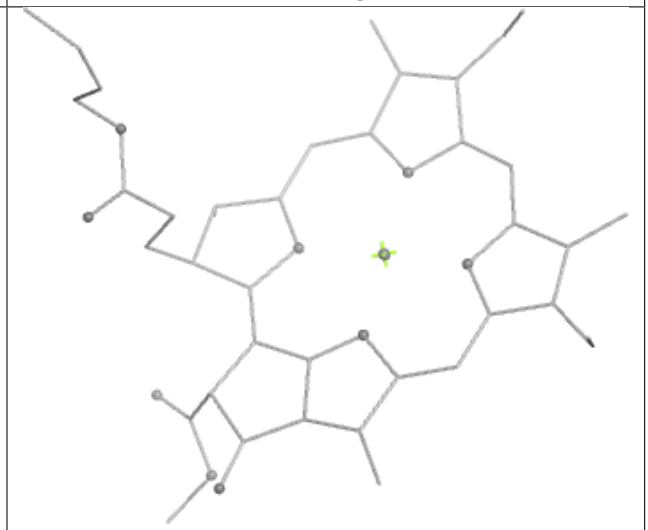
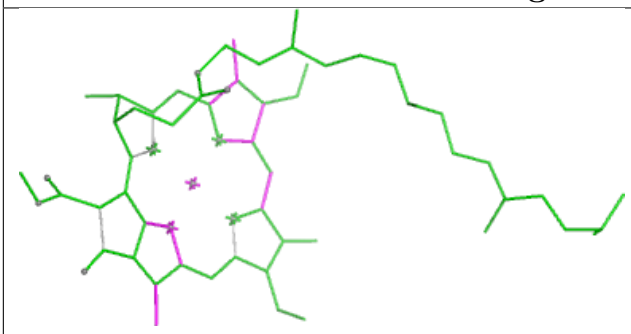


Rings

Ligand CLA g 317



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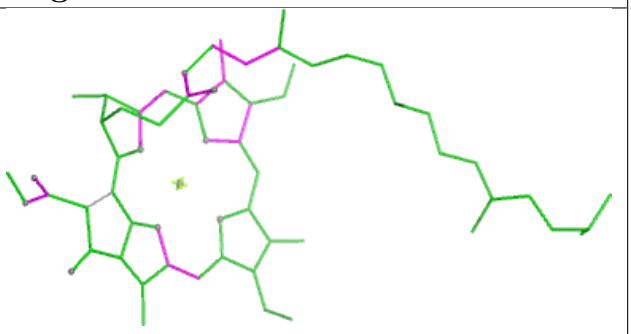

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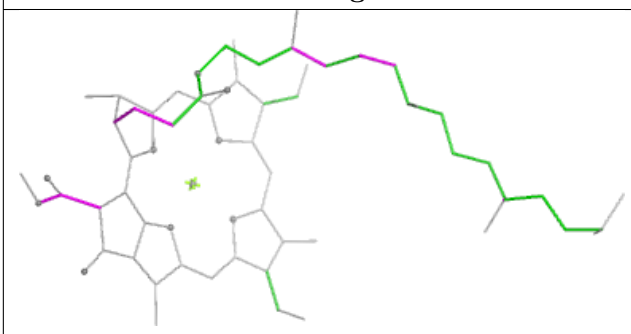

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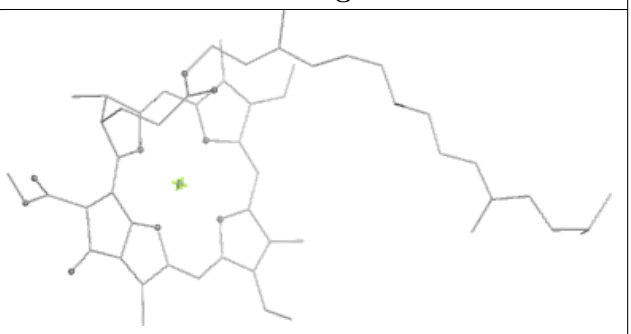
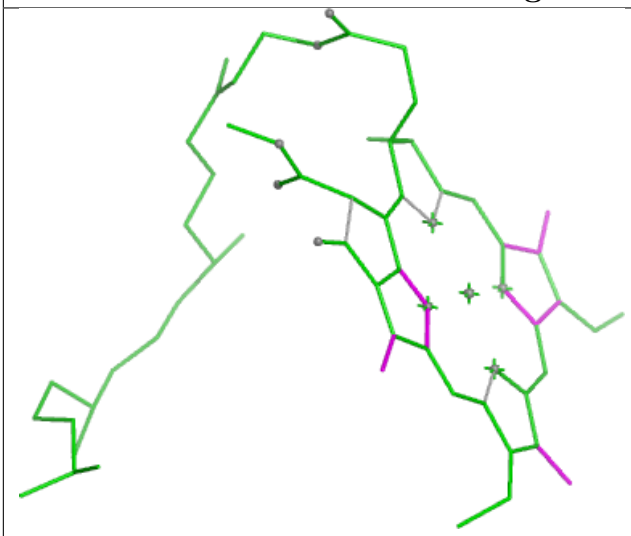


Rings

Ligand CLA B 603



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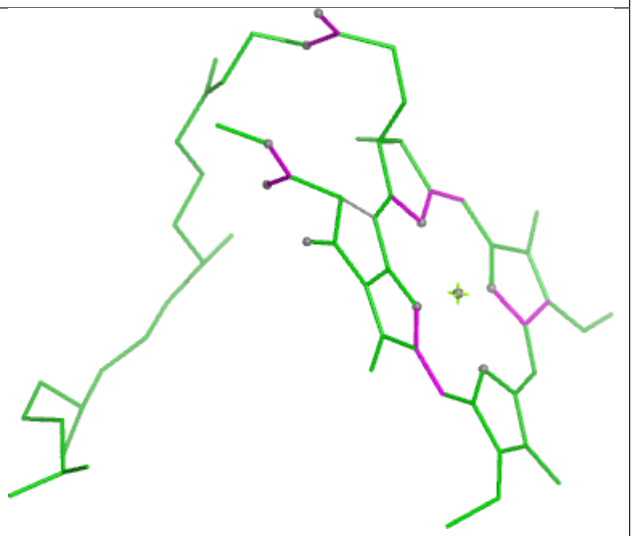

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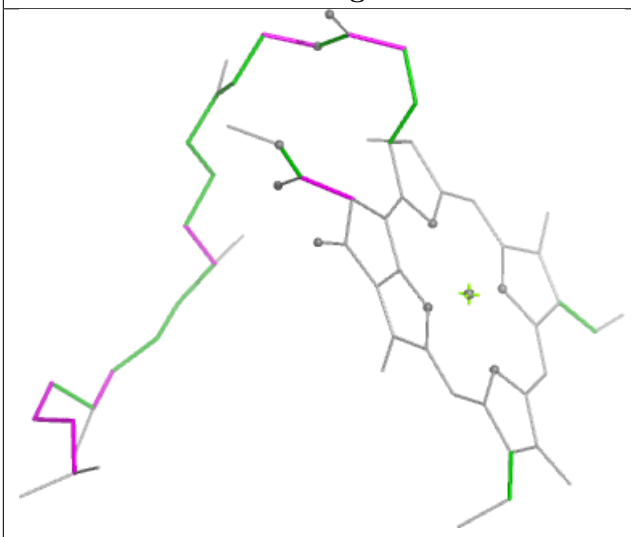

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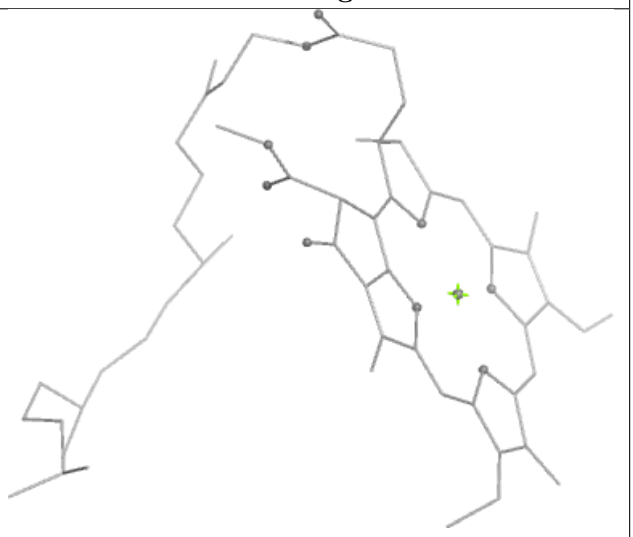
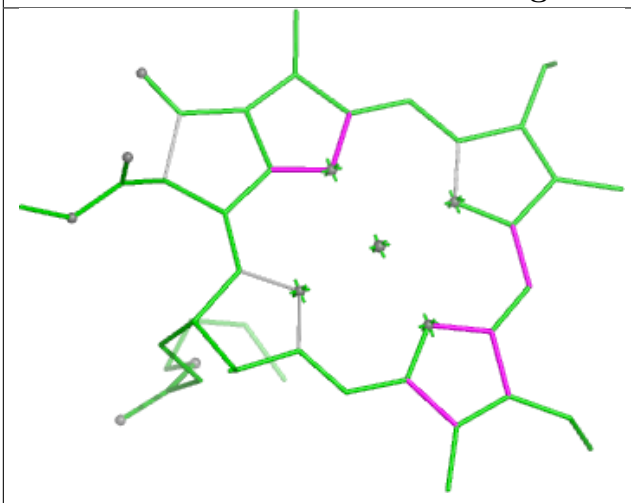


Rings

Ligand CLA r 310



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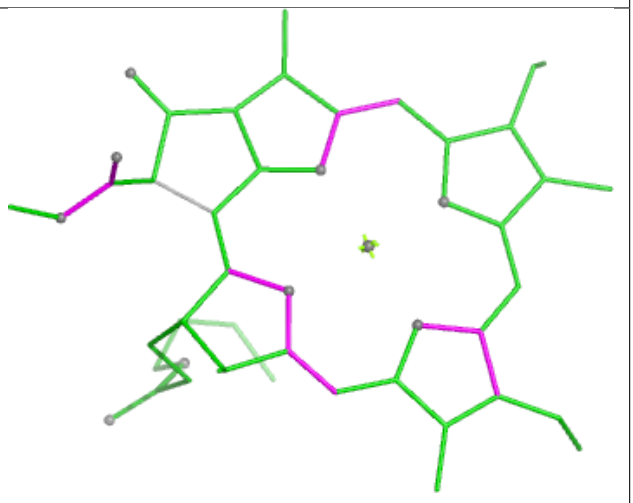

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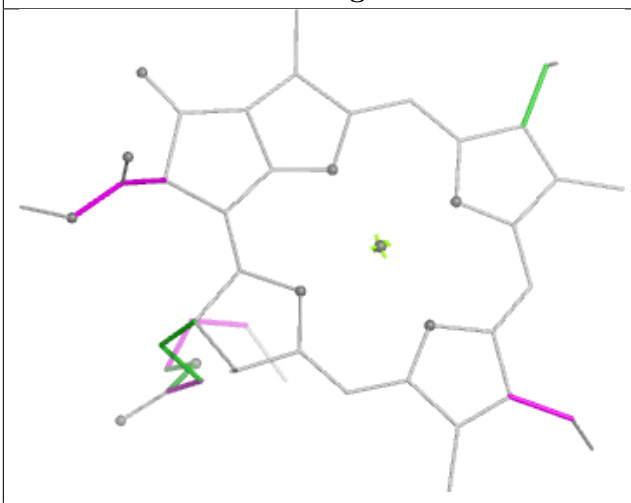

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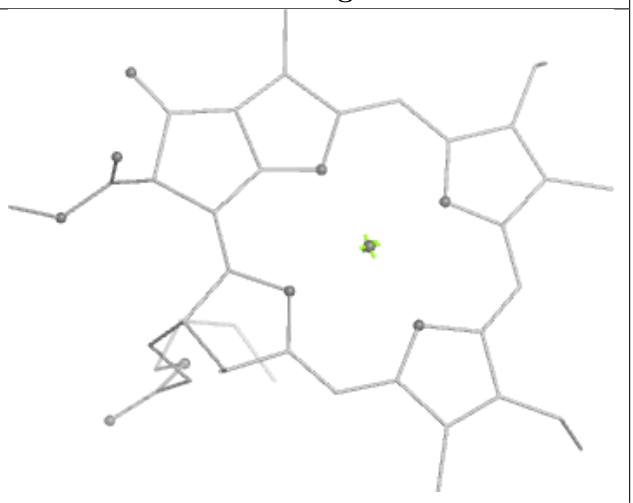
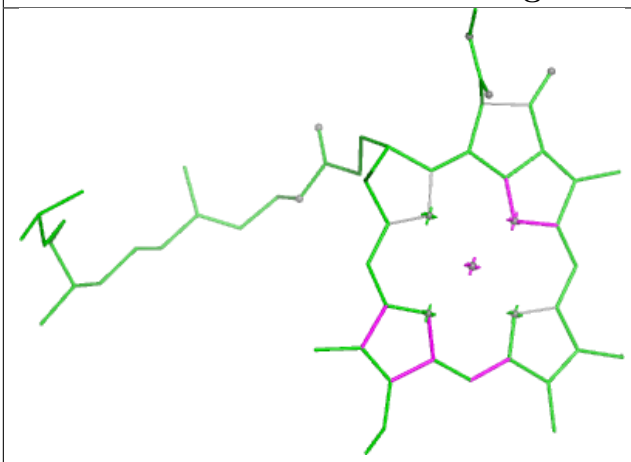


Rings

Ligand CLA A 405



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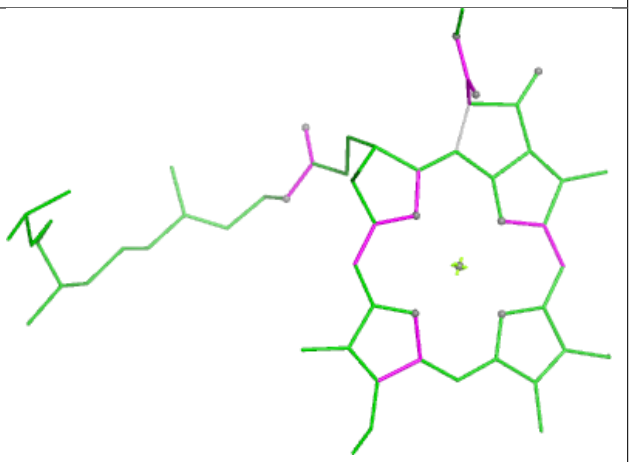

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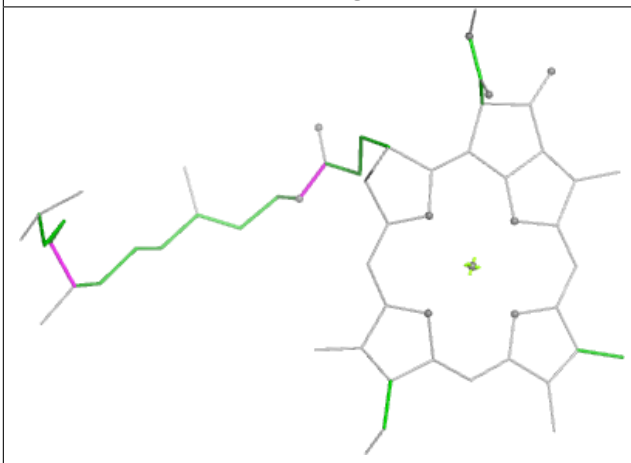
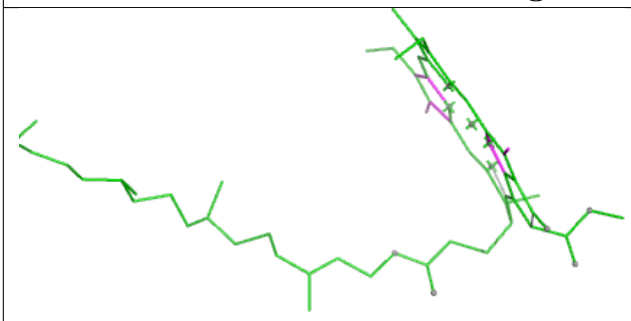


Torsions



Rings

Ligand CLA b 616



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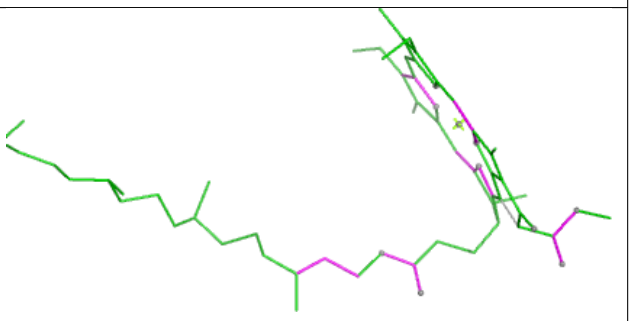

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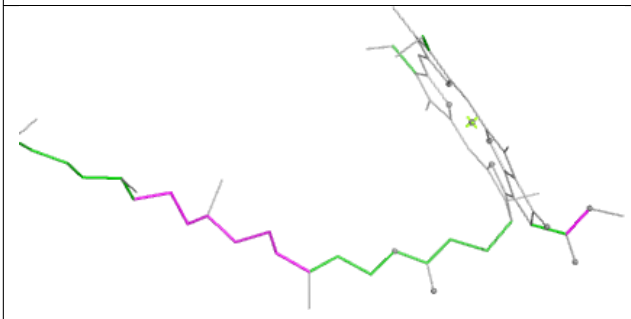

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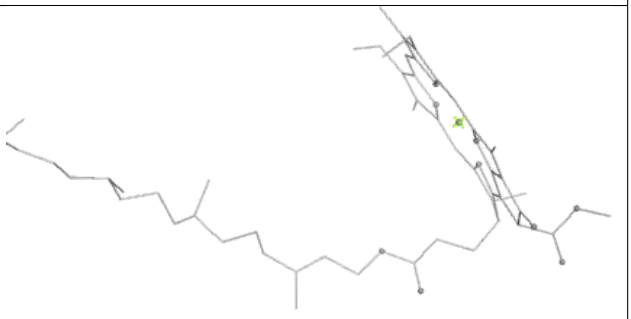
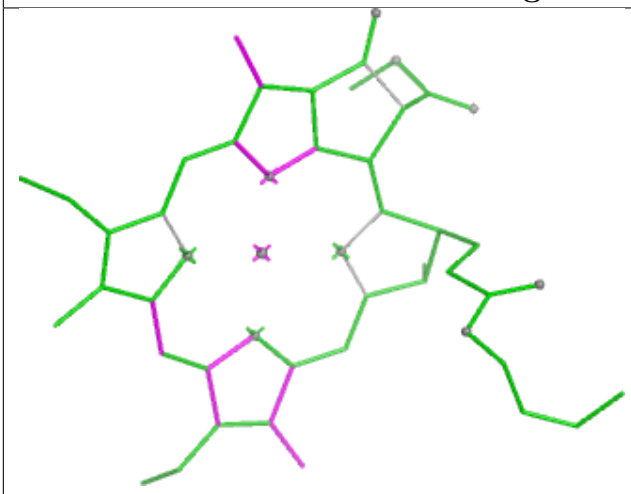


Rings

Ligand CLA D 412



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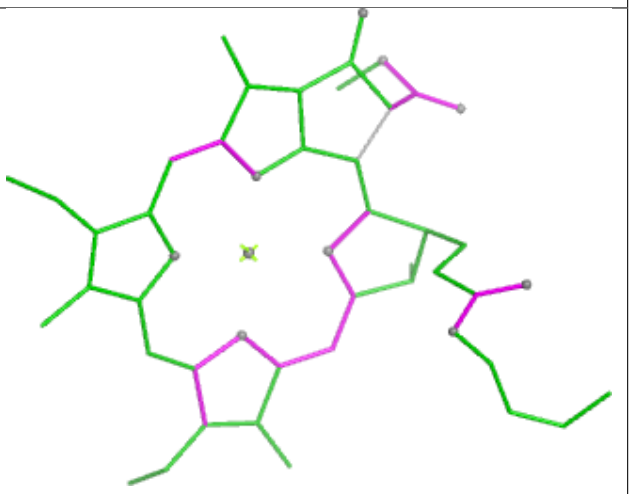
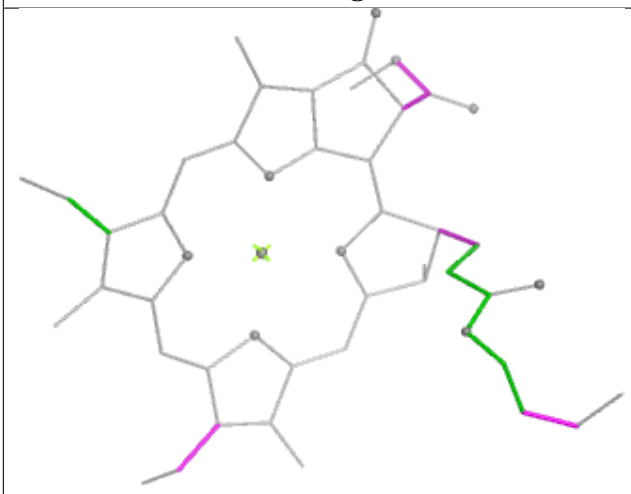


Bond angles



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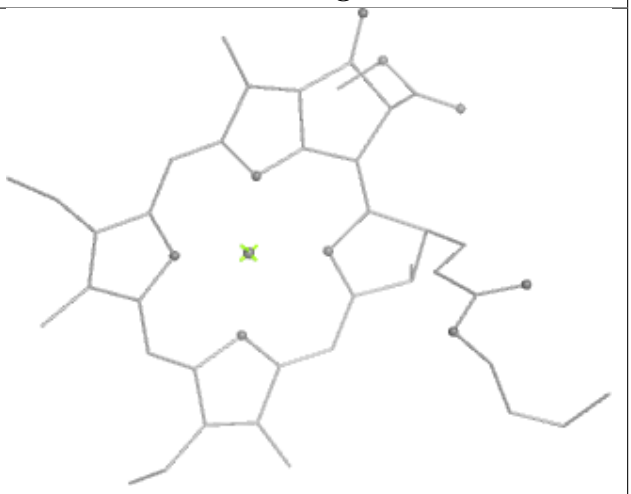
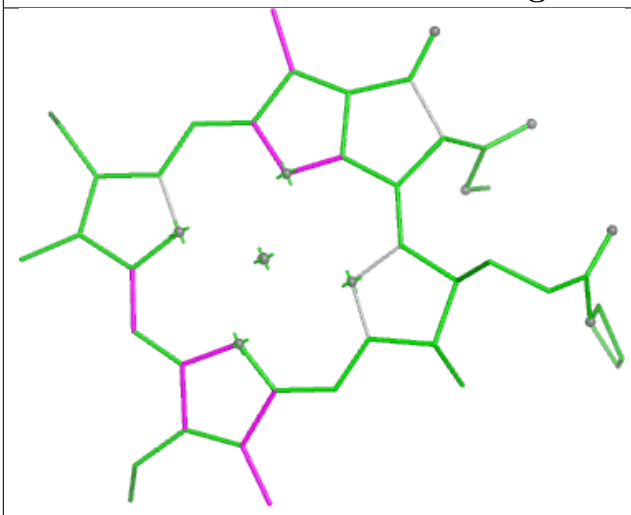


Rings

Ligand CLA g 304



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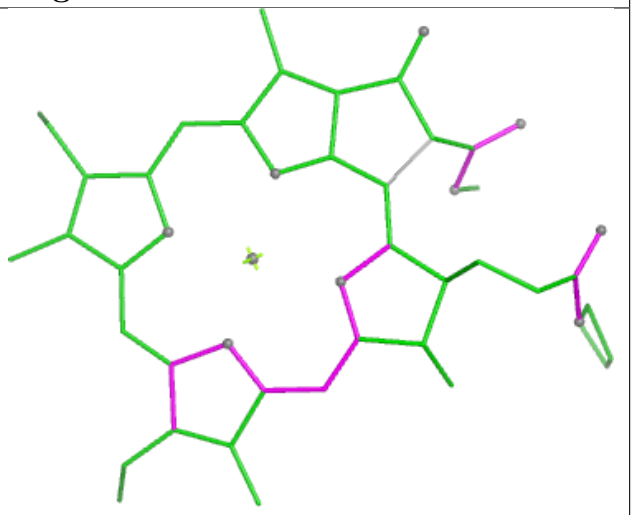

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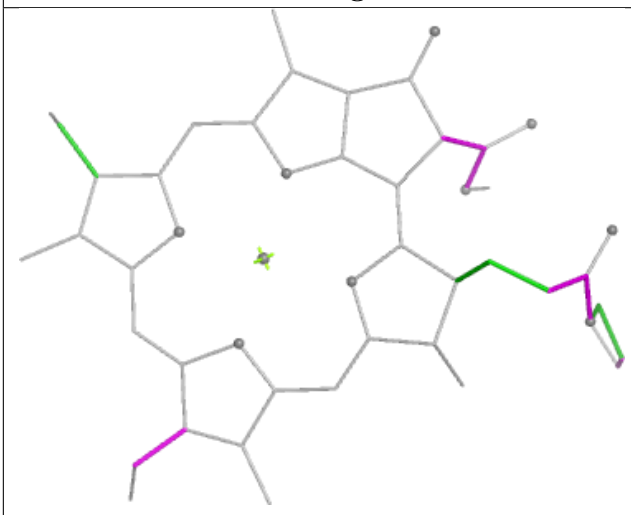

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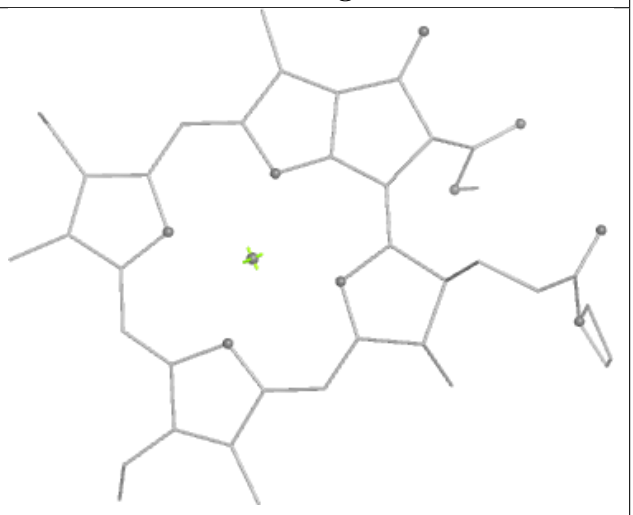
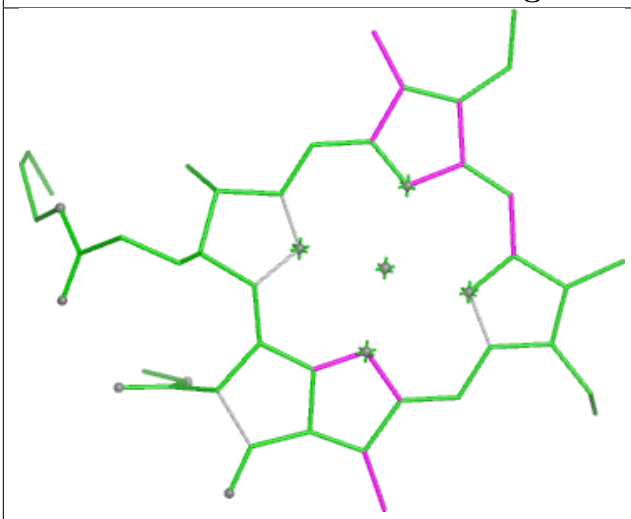


Rings

Ligand CLA R 317



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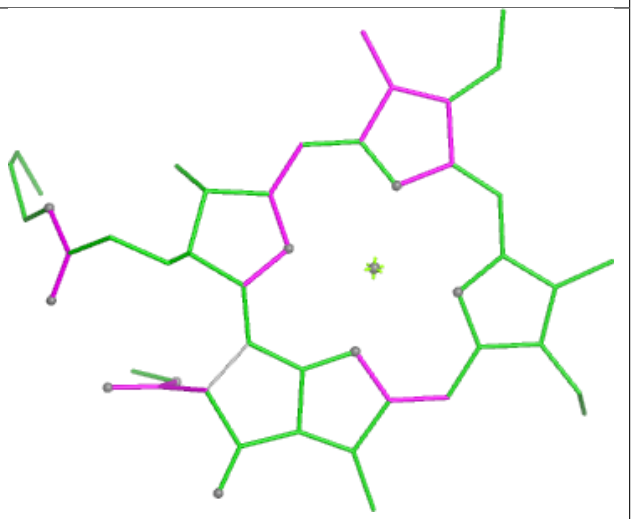
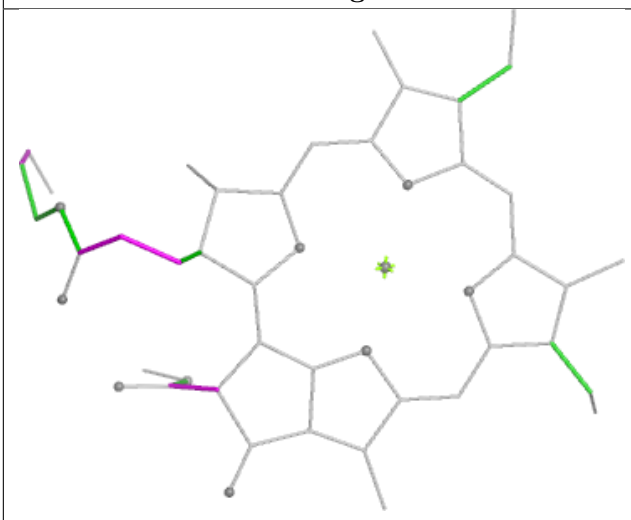


Bond angles



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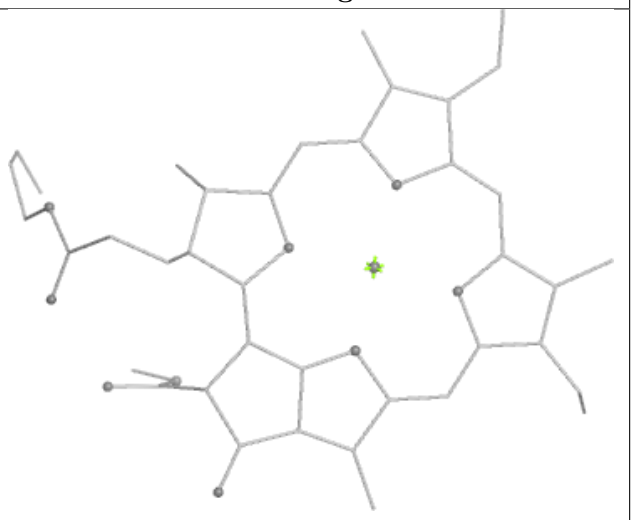
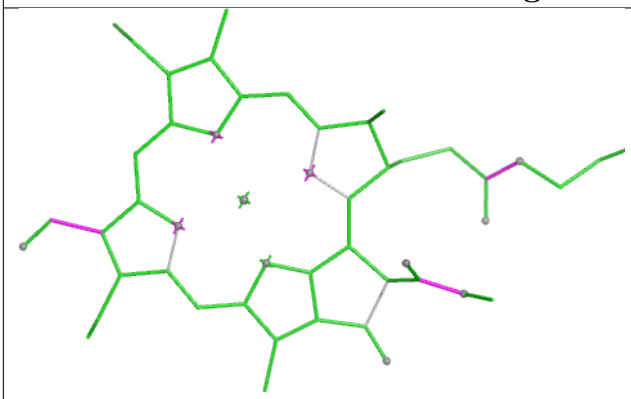


Rings

Ligand CHL Y 317



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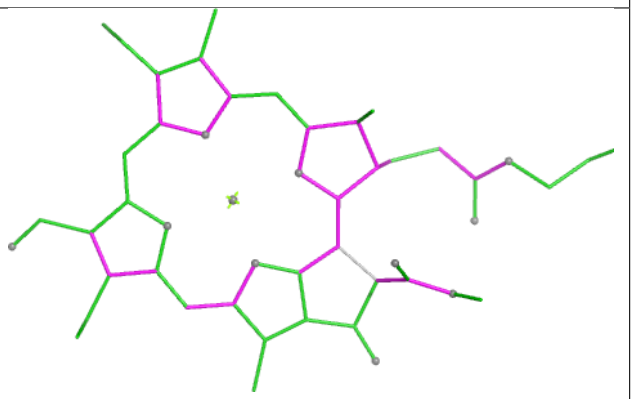
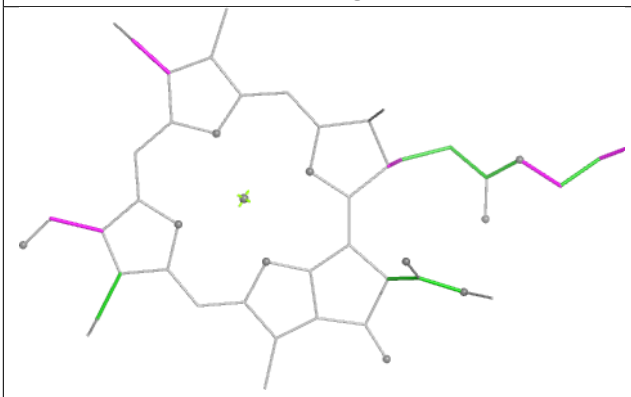


Bond angles



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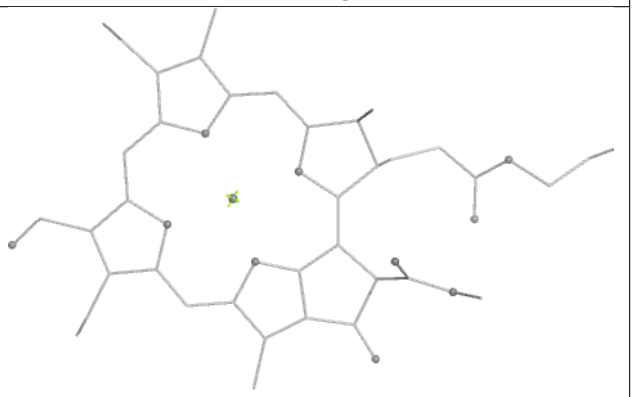
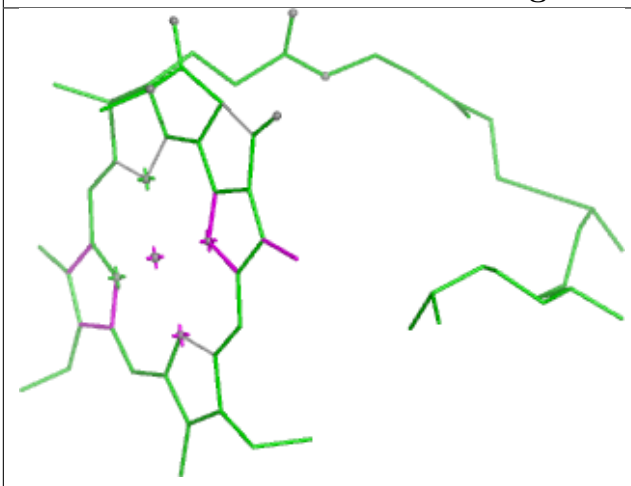


Rings

Ligand CLA c 505



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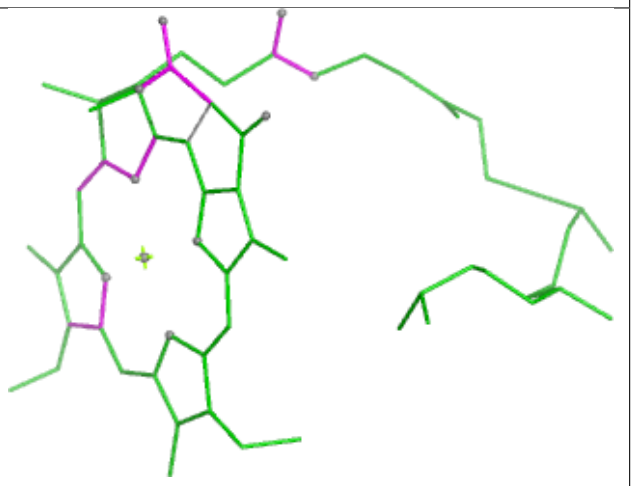
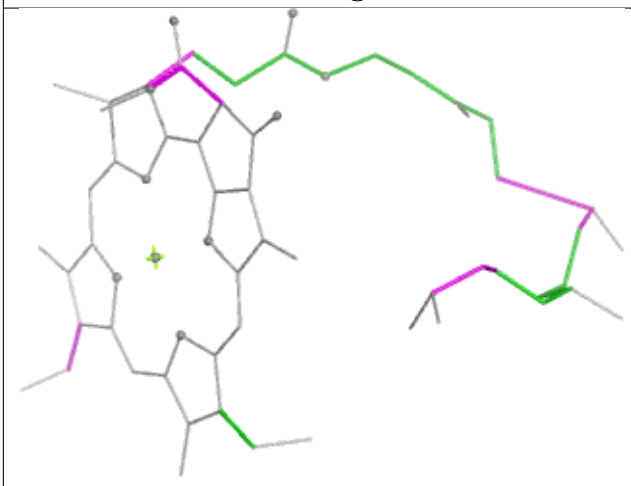


Bond angles



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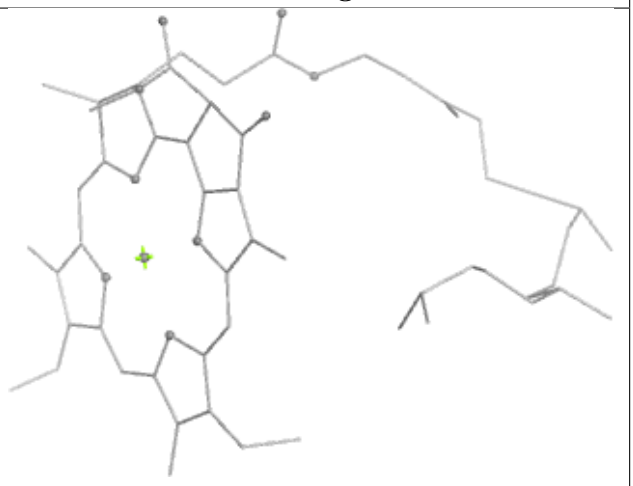
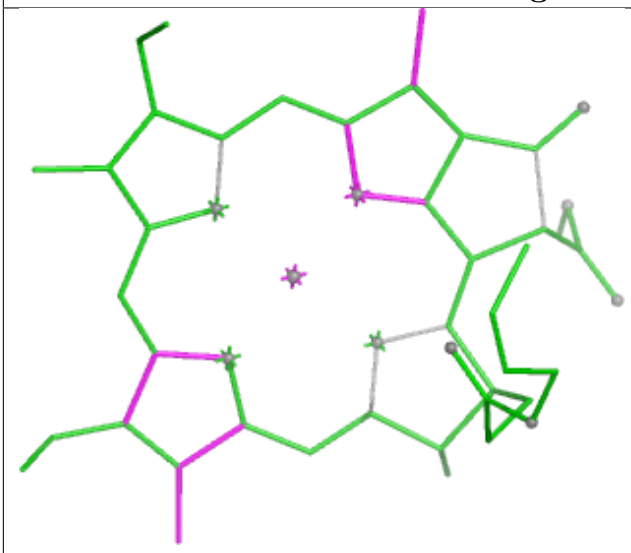


Rings

Ligand CLA s 310



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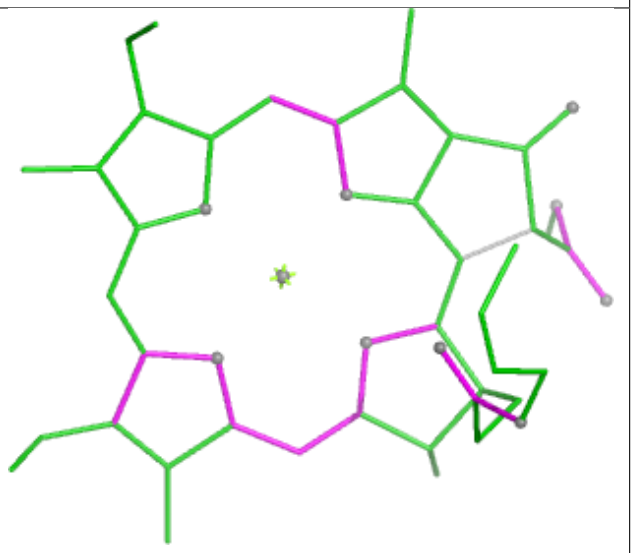
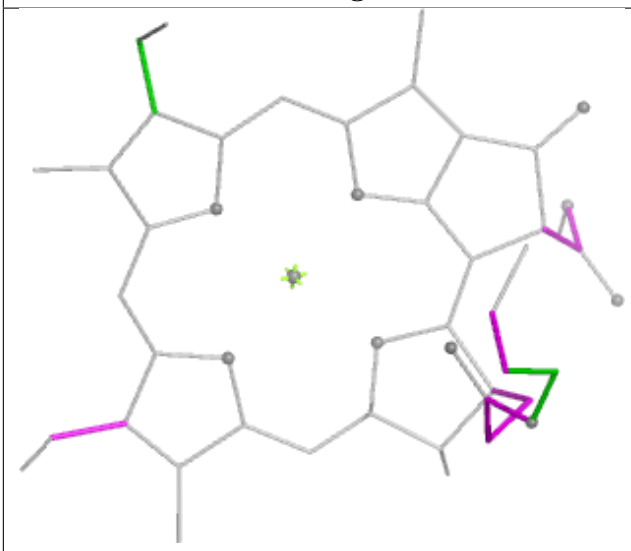
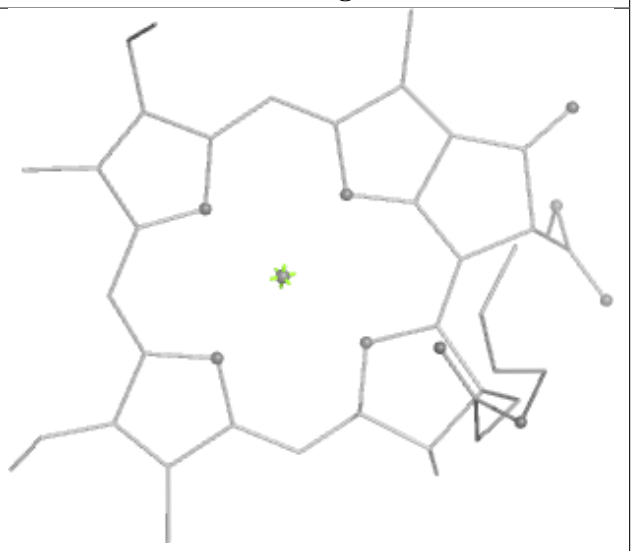


Bond angles

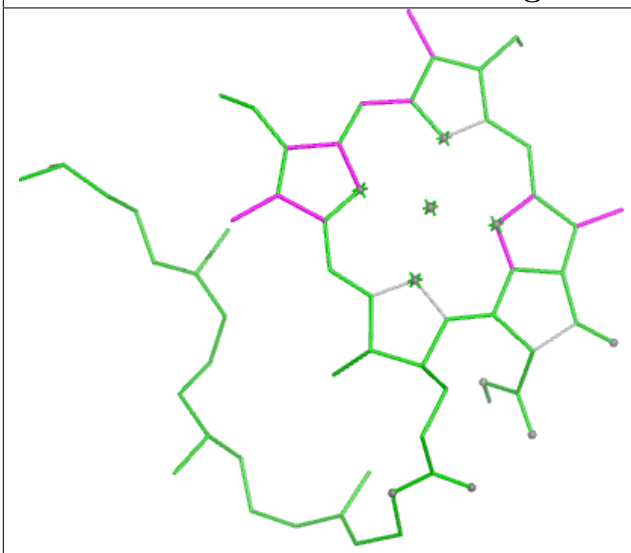


Torsions

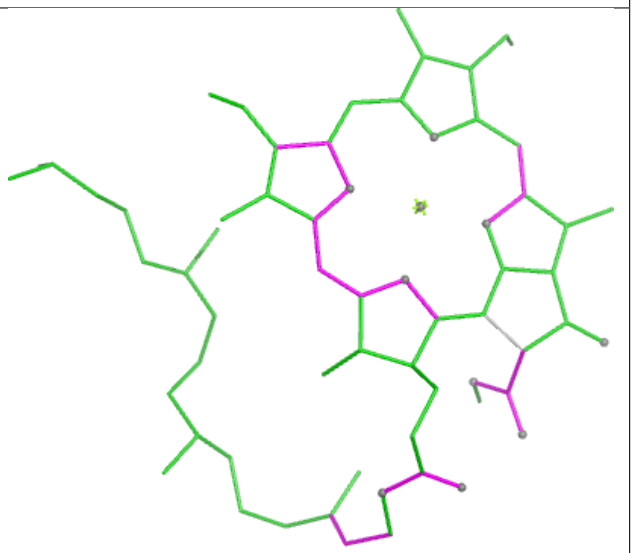


Rings

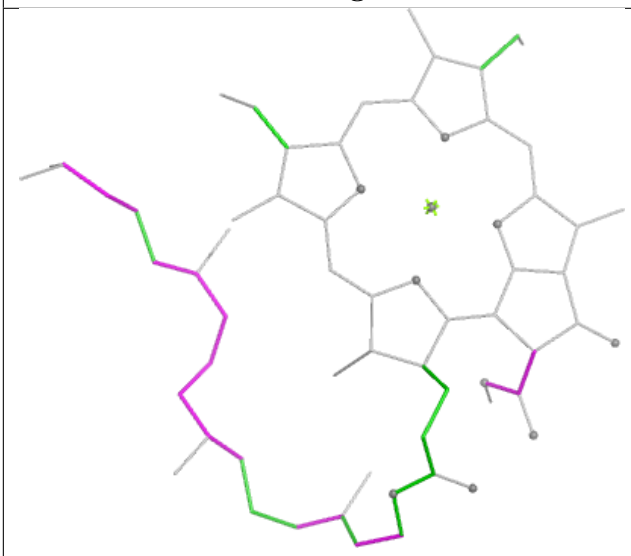
Ligand CLA Y 313



Bond lengths



Bond angles



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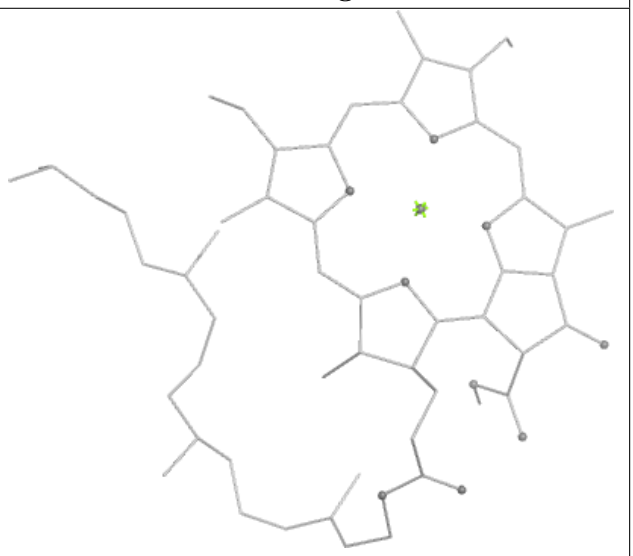
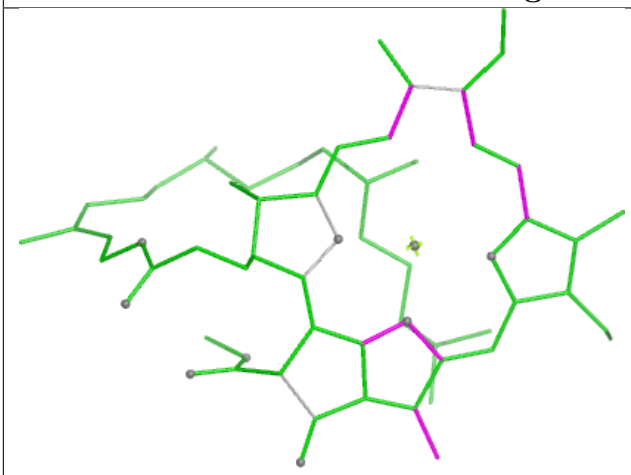


Rings

Ligand CLA C 520



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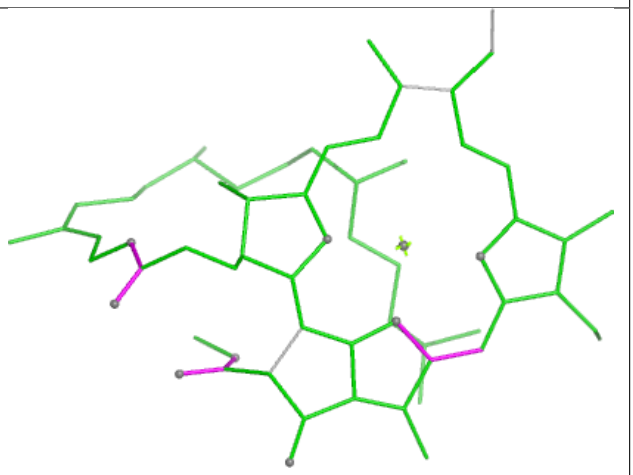
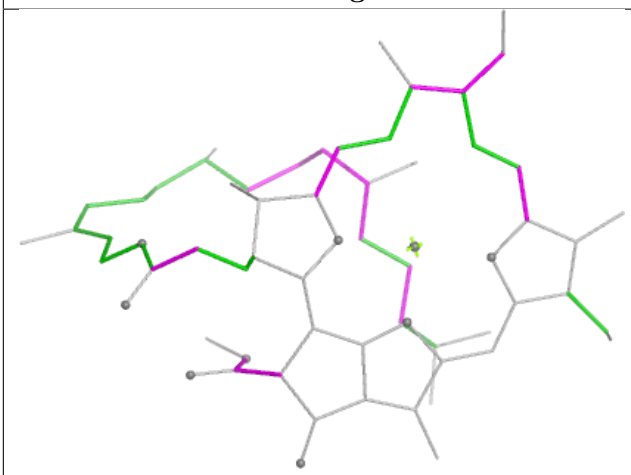


Bond angles



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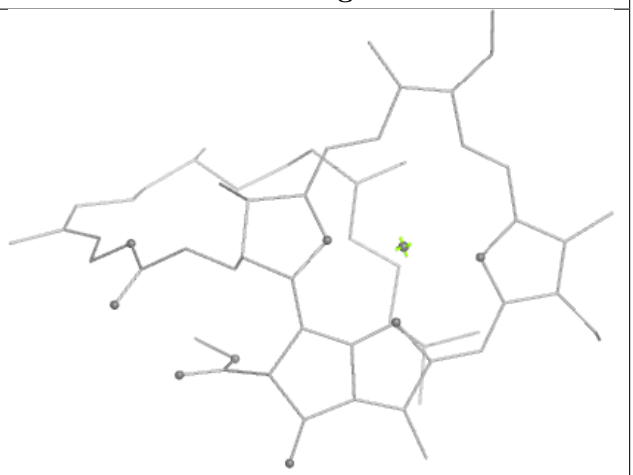
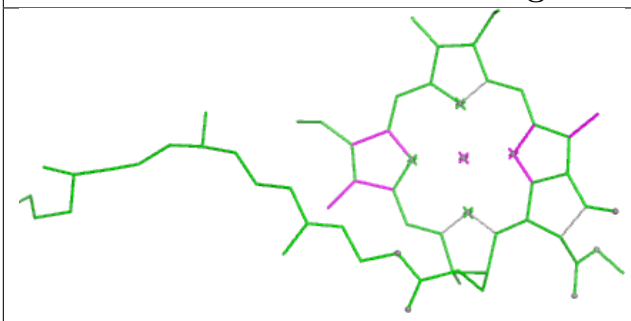


Rings

Ligand CLA b 606



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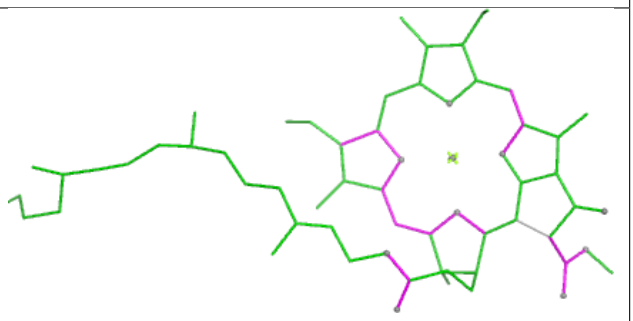
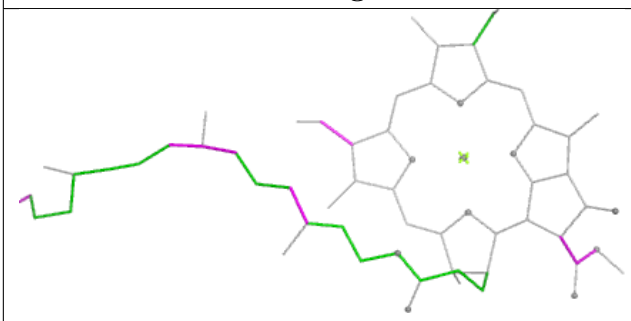


Bond angles



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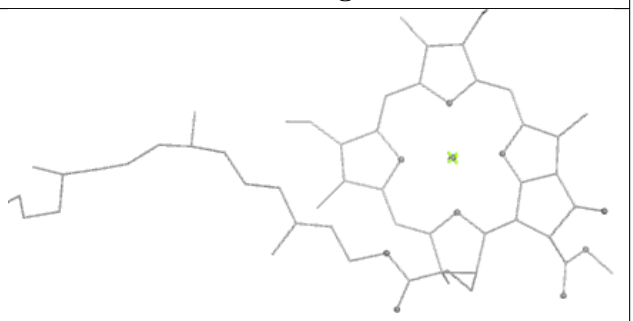
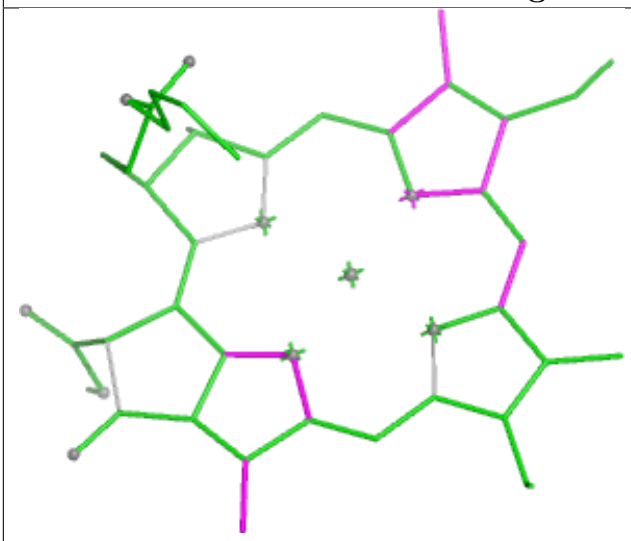


Rings

Ligand CLA g 302



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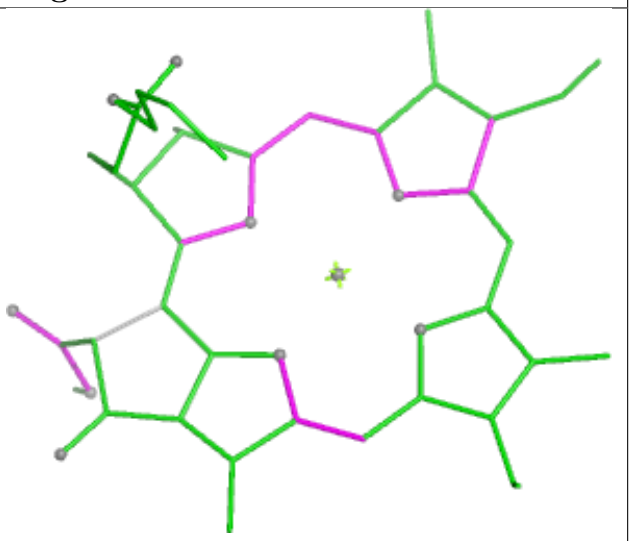

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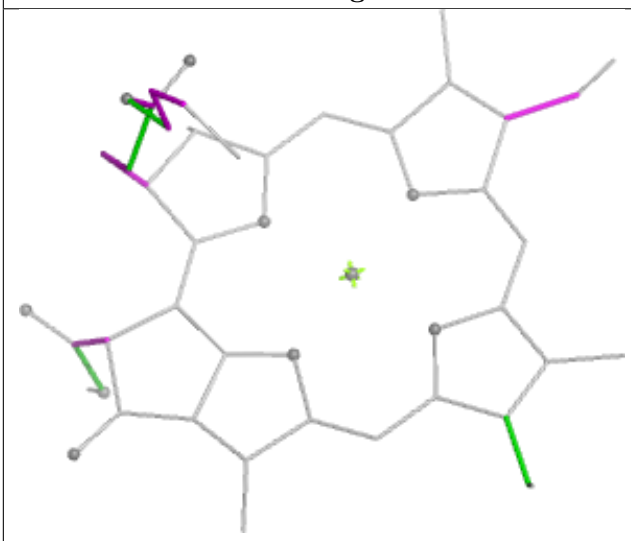

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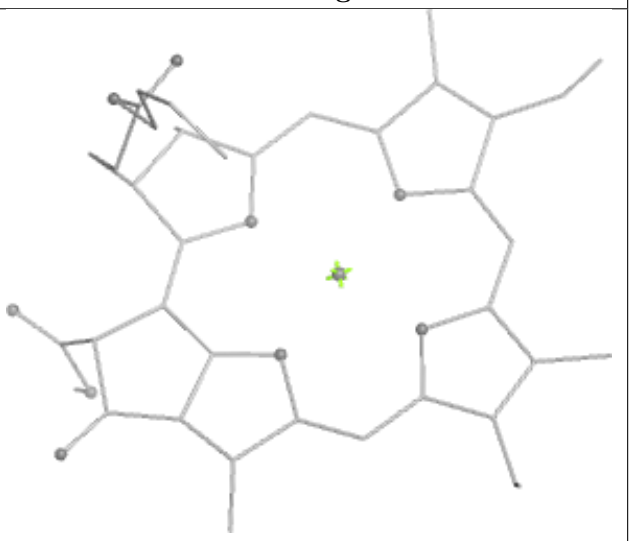
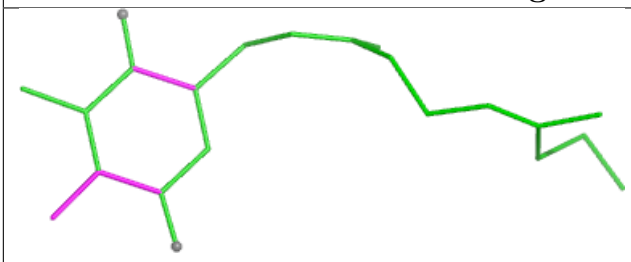


Rings

Ligand PL9 A 408



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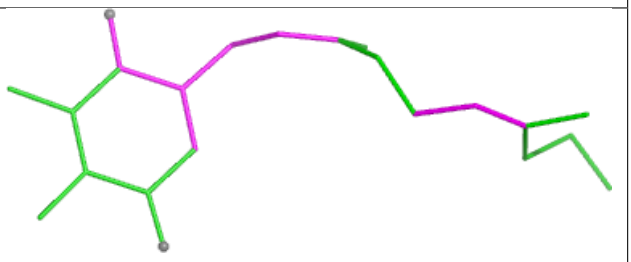

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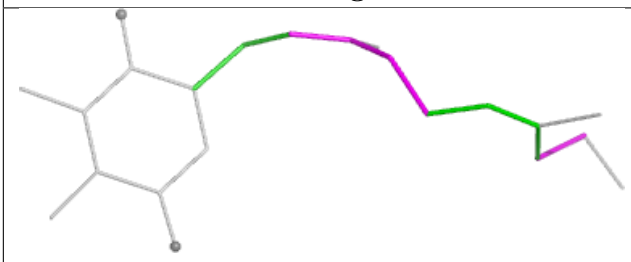

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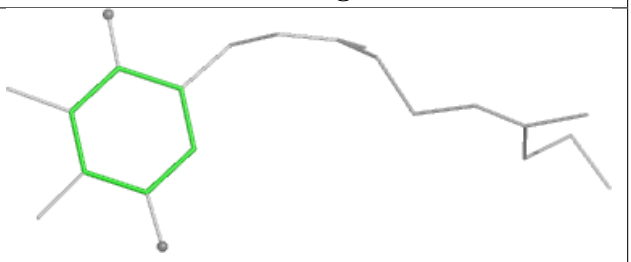
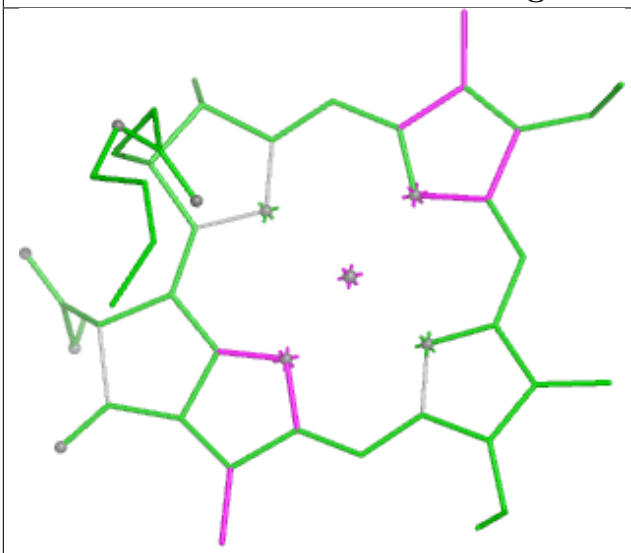


Rings

Ligand CLA S 310



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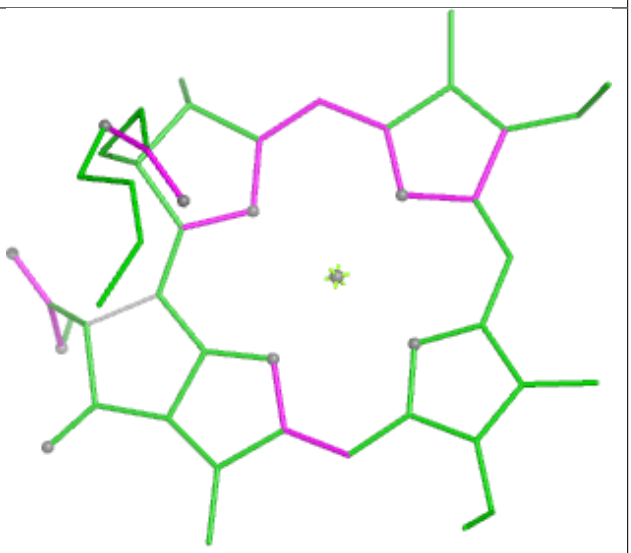
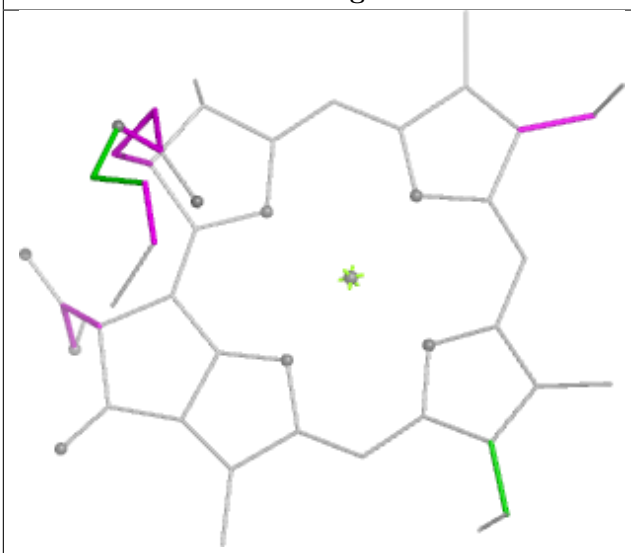


Bond angles



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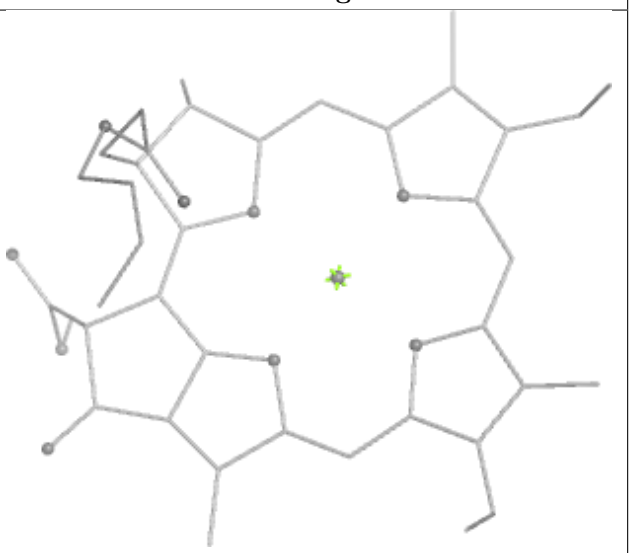
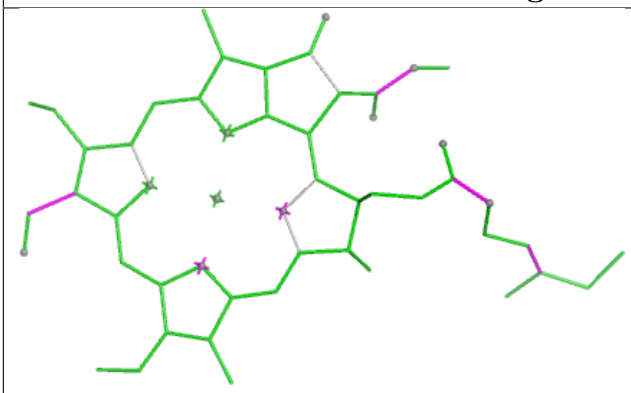


Rings

Ligand CHL S 316



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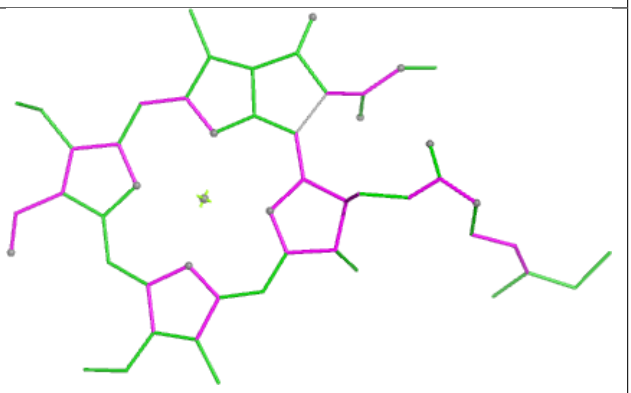
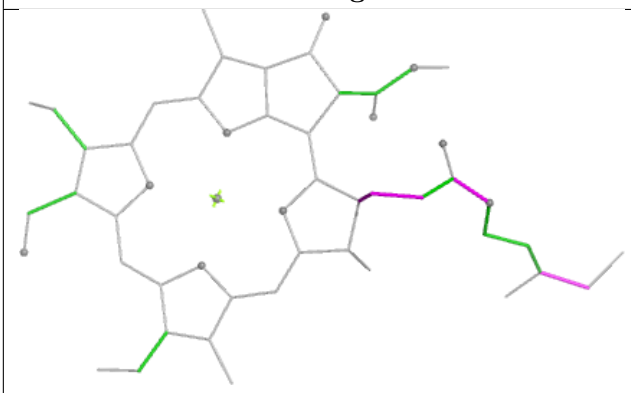


Bond angles

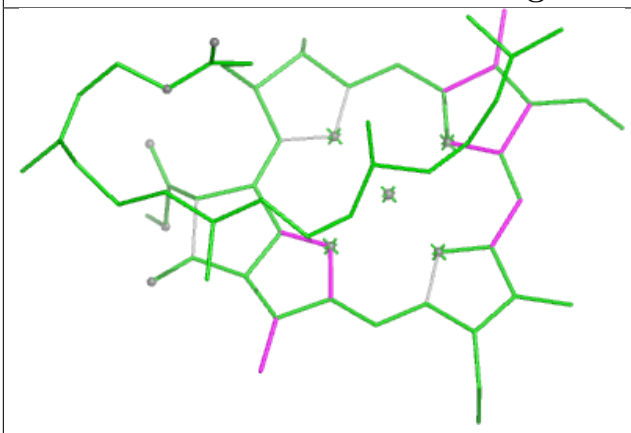


Torsions



Rings

Ligand CLA b 608



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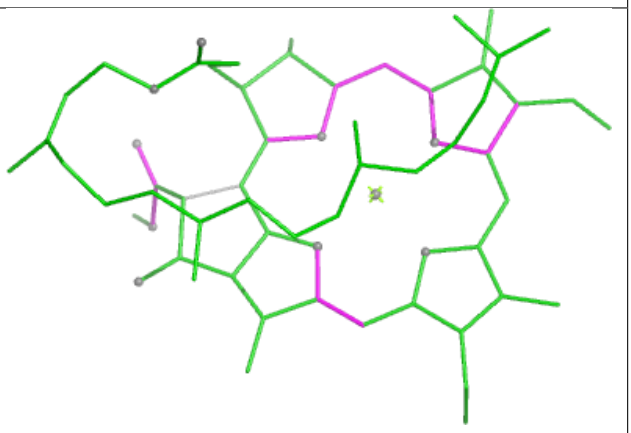
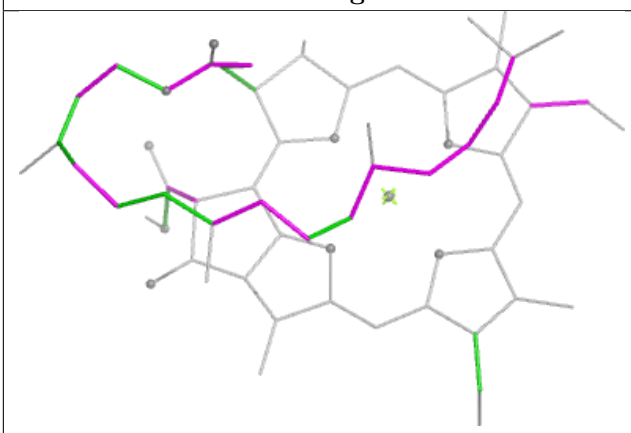


Bond angles



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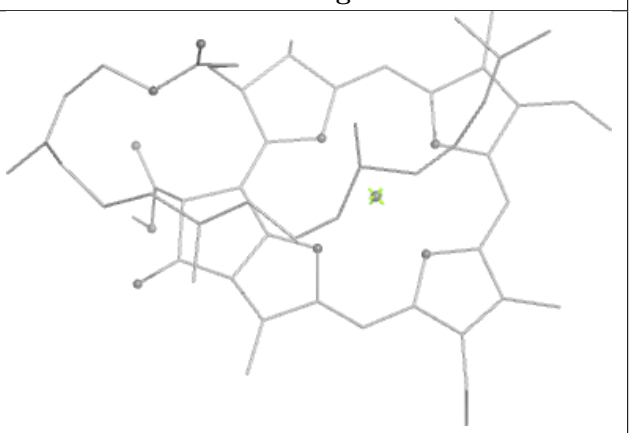
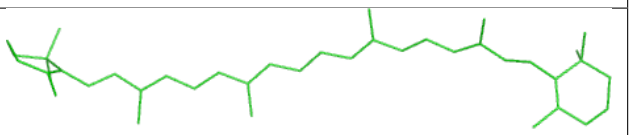


Rings

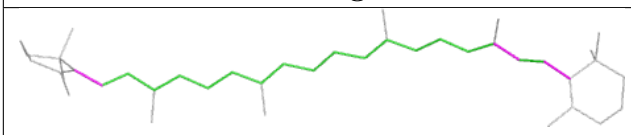
Ligand BCR B 614



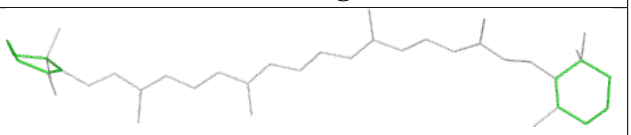
Bond lengths



Bond angles

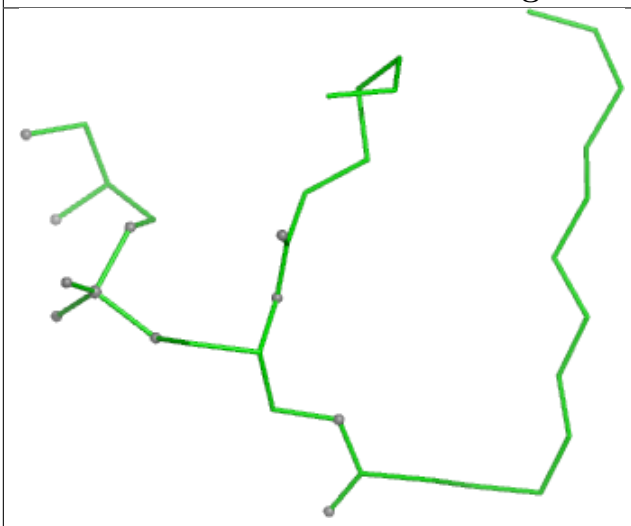


Torsions



Rings

Ligand LHG D 410



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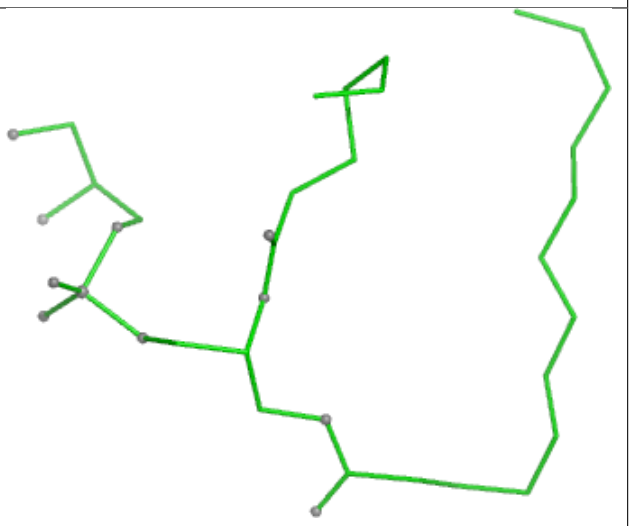
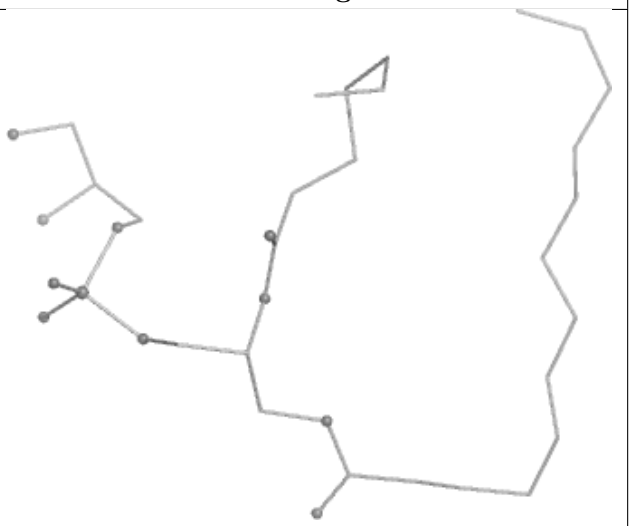


Bond angles

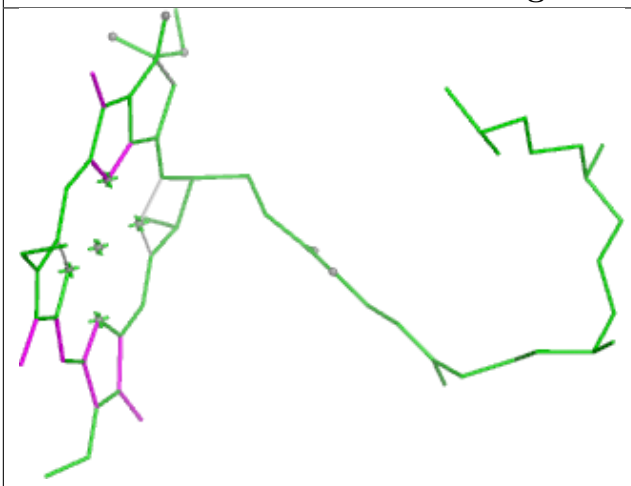


Torsions



Rings

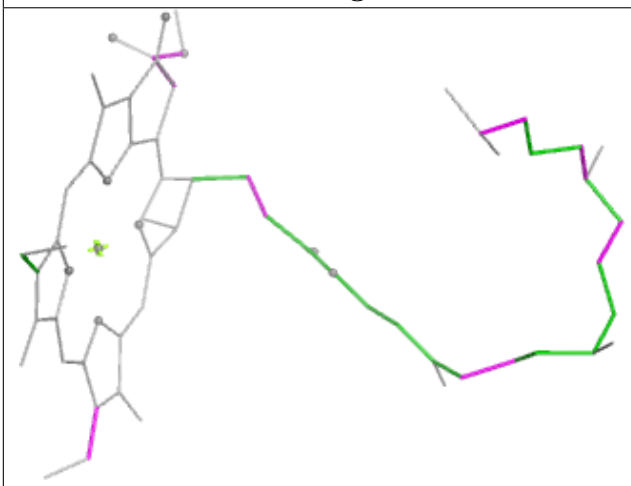
Ligand CLA b 617



Bond lengths



Bond angles



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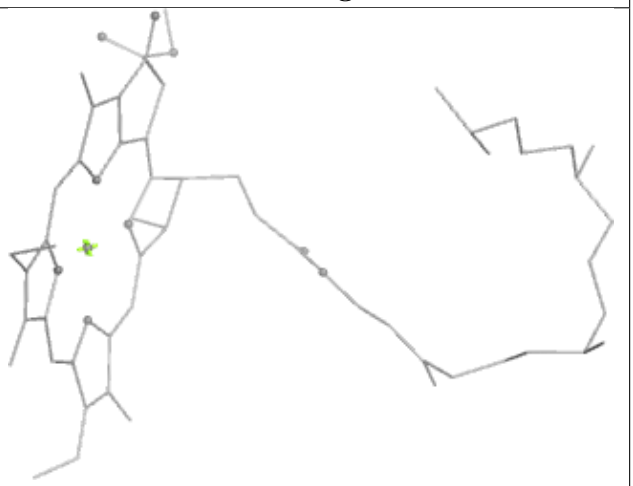
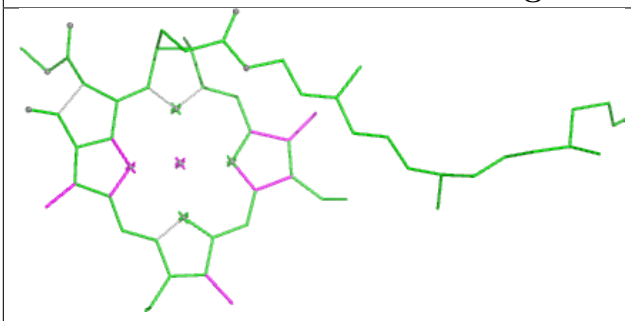


Rings

Ligand CLA B 611



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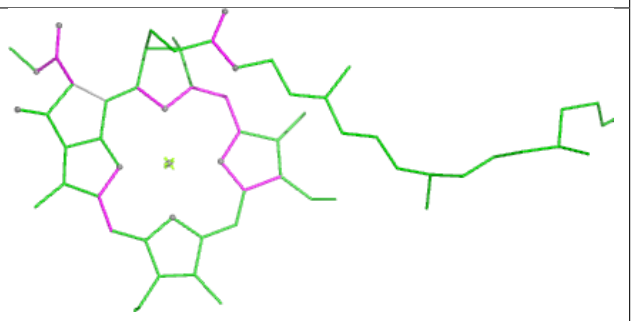
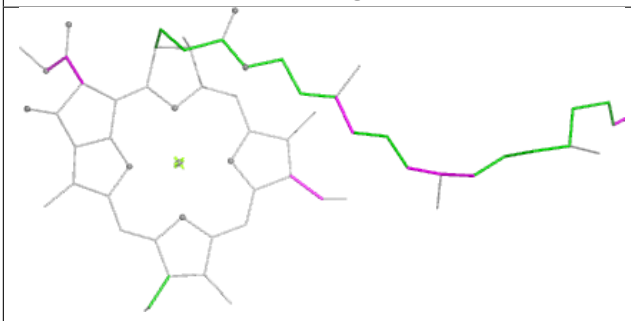


Bond angles



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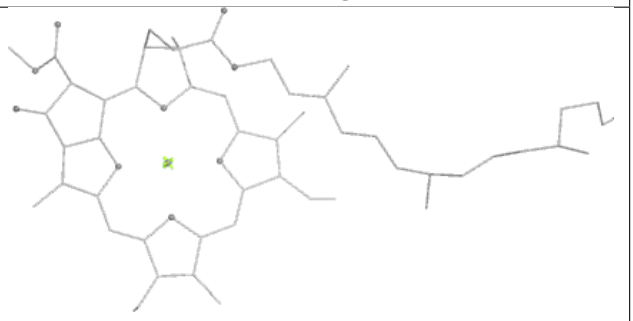
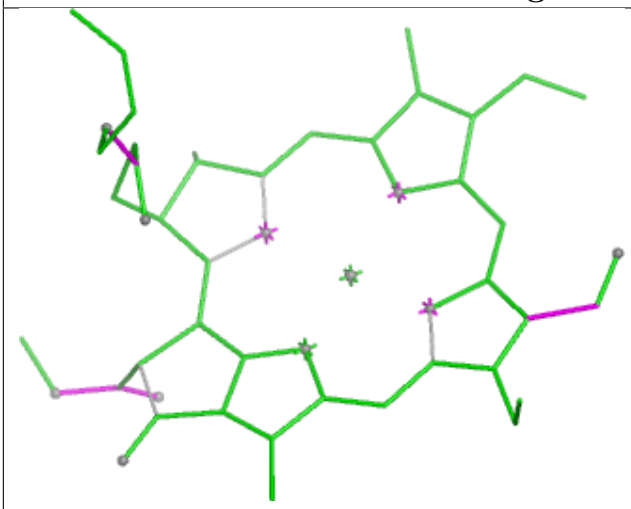


Rings

Ligand CHL y 302



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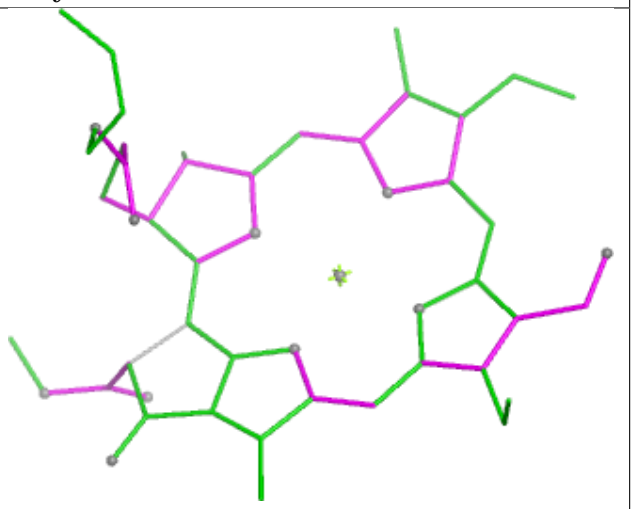
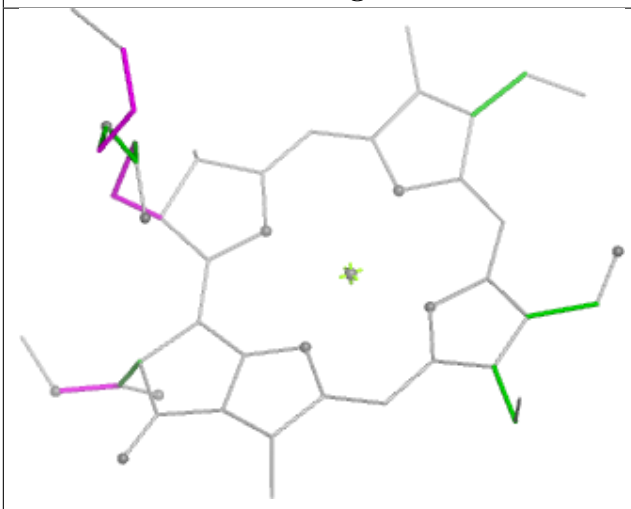


Bond angles



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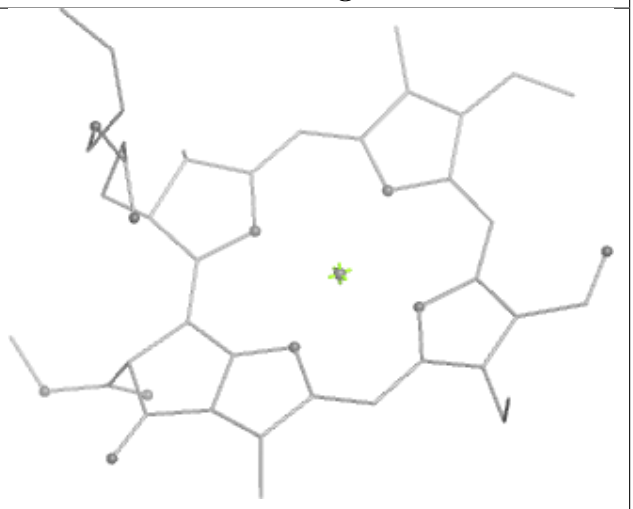
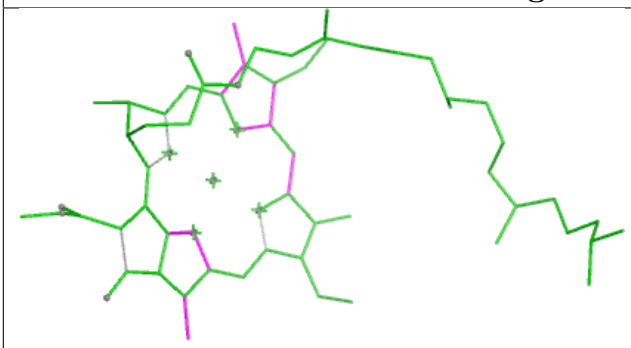
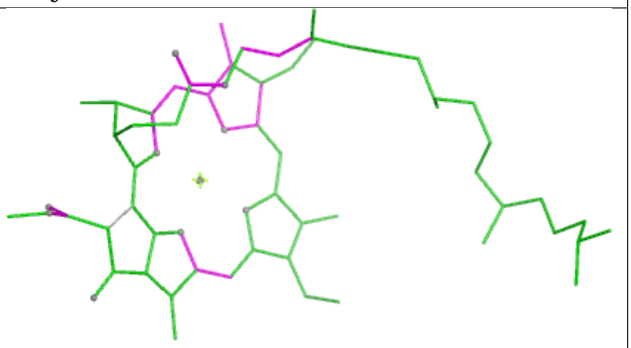


Rings

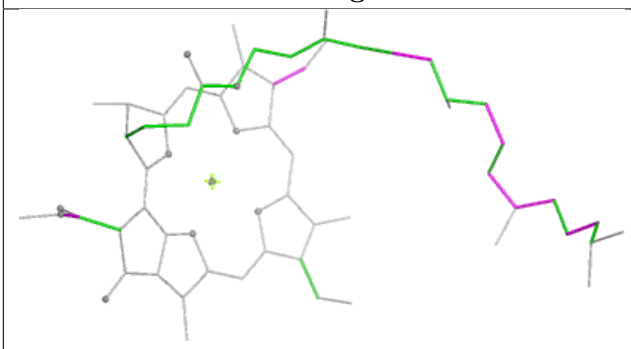
Ligand CLA y 309



Bond lengths



Bond angles



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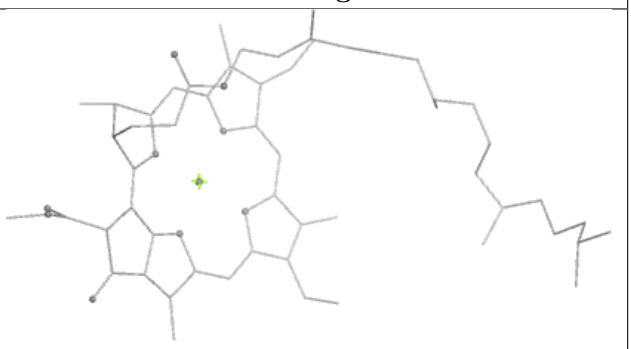
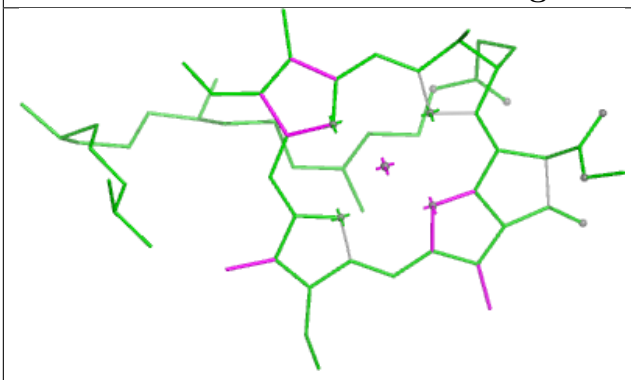


Rings

Ligand CLA c 502



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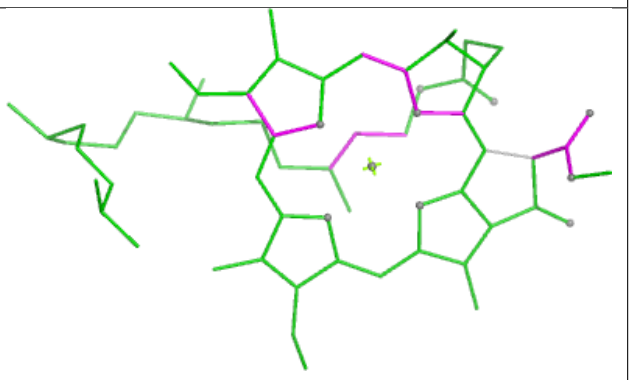


Bond angles

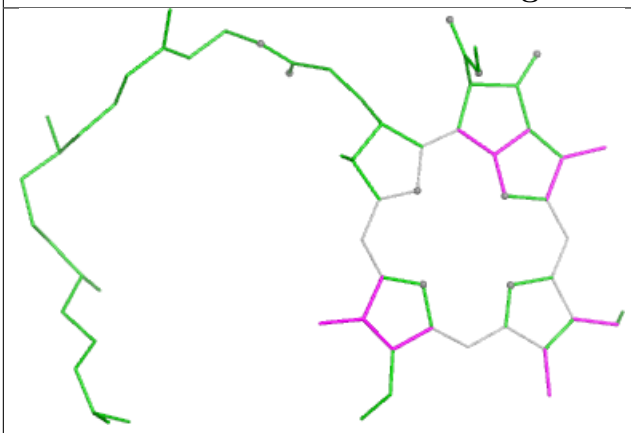


Torsions



Rings

Ligand PHO A 404



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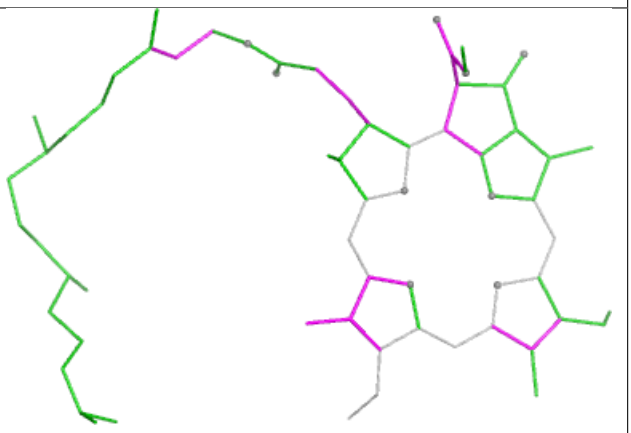
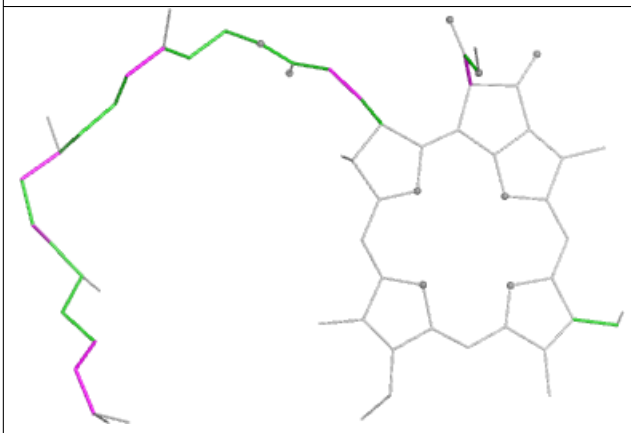
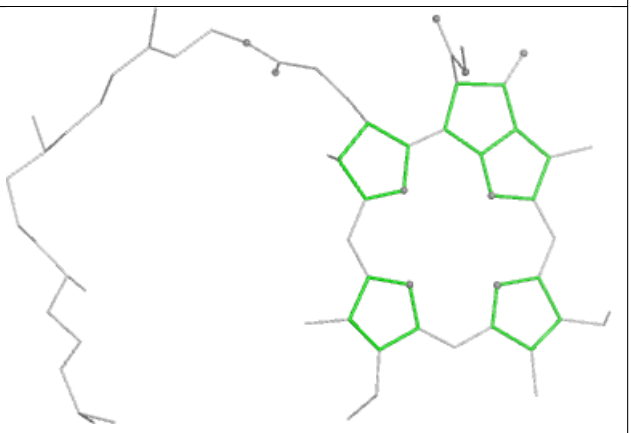


Bond angles

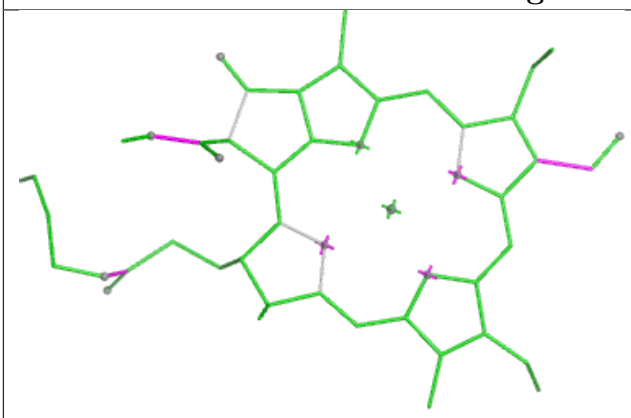


Torsions

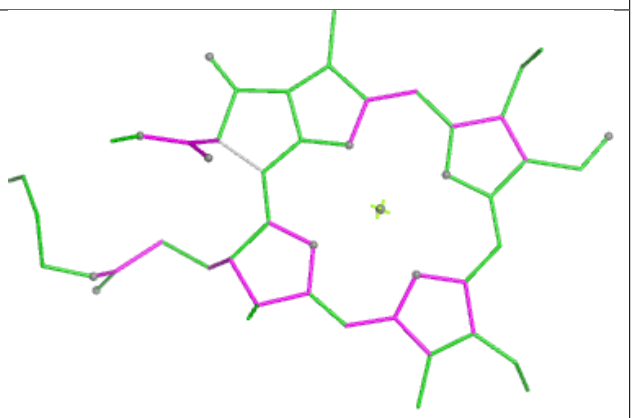


Rings

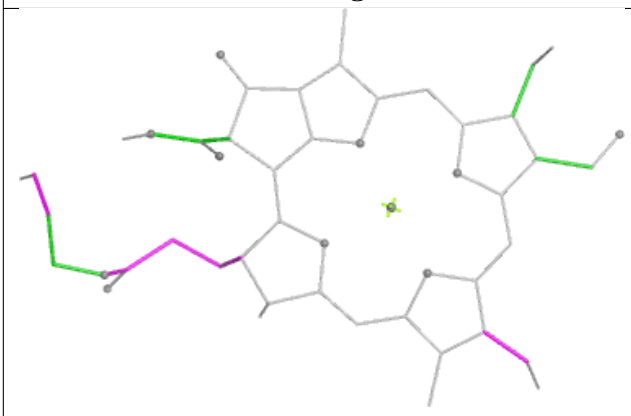
Ligand CHL n 311



Bond lengths



Bond angles

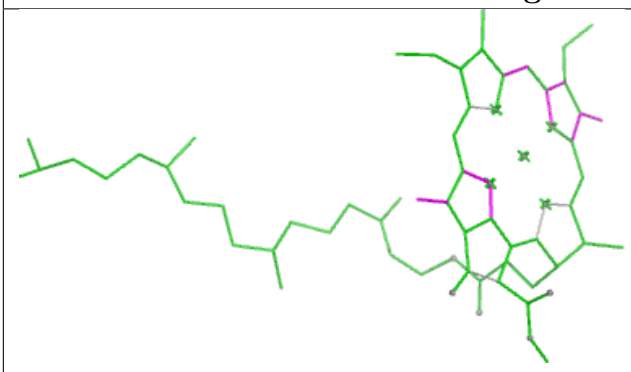


Torsions

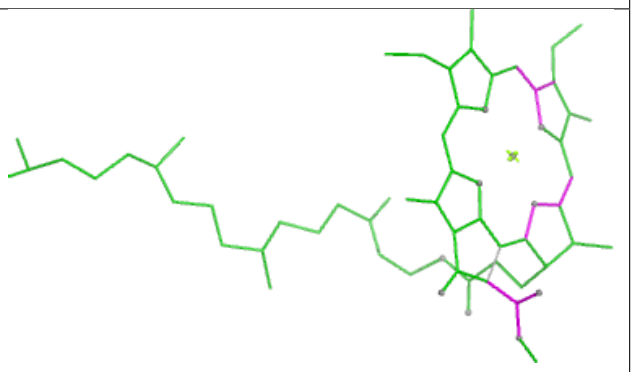


Rings

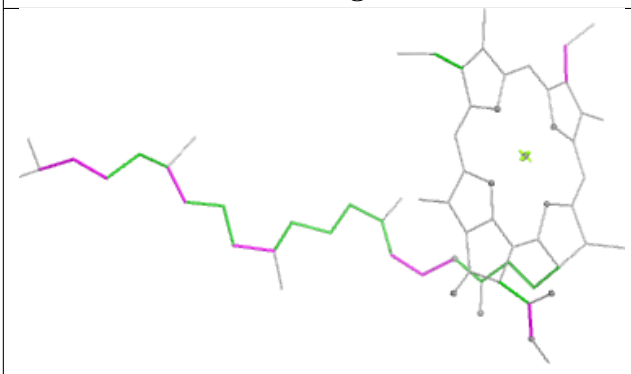
Ligand CLA Y 301



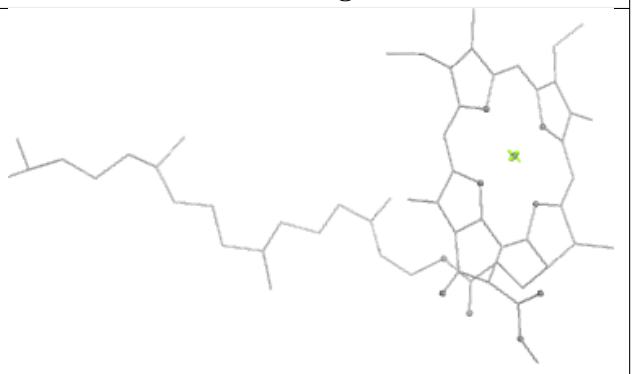
Bond lengths



Bond angles

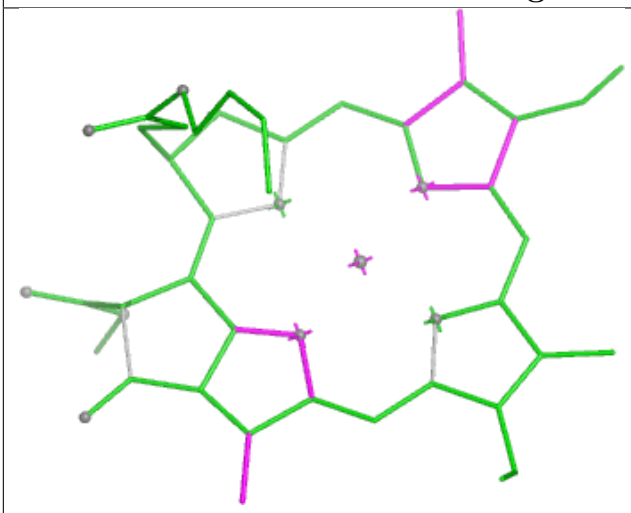


Torsions

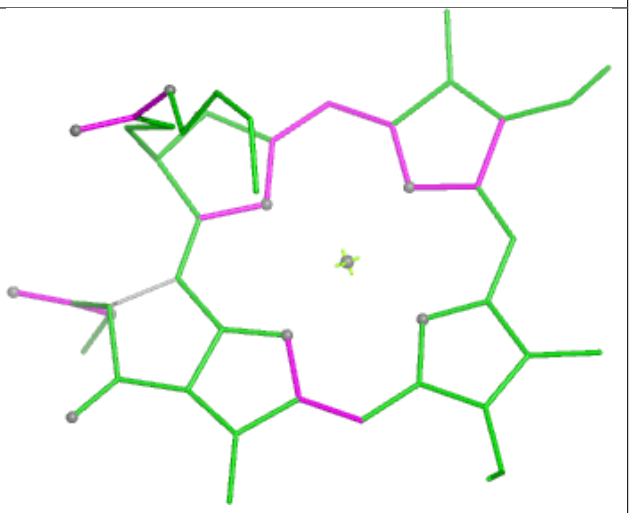


Rings

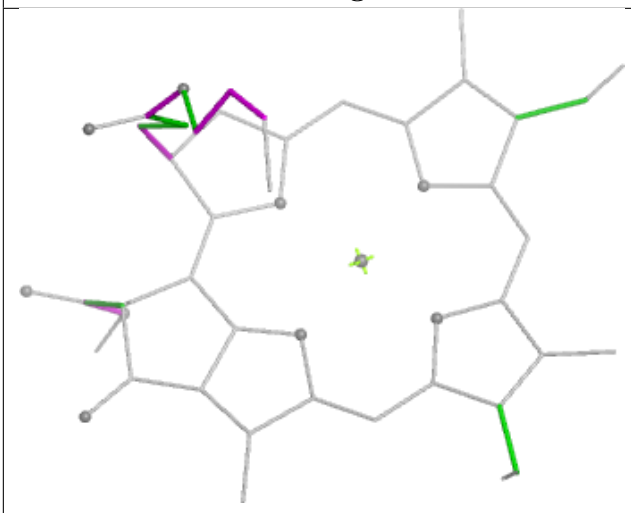
Ligand CLA n 312



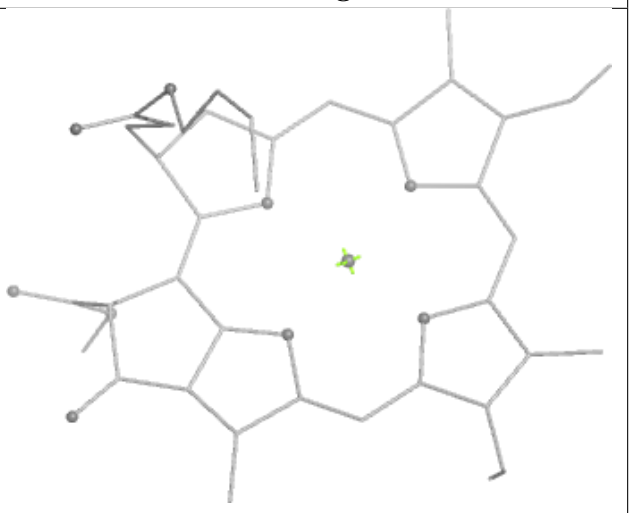
Bond lengths



Bond angles

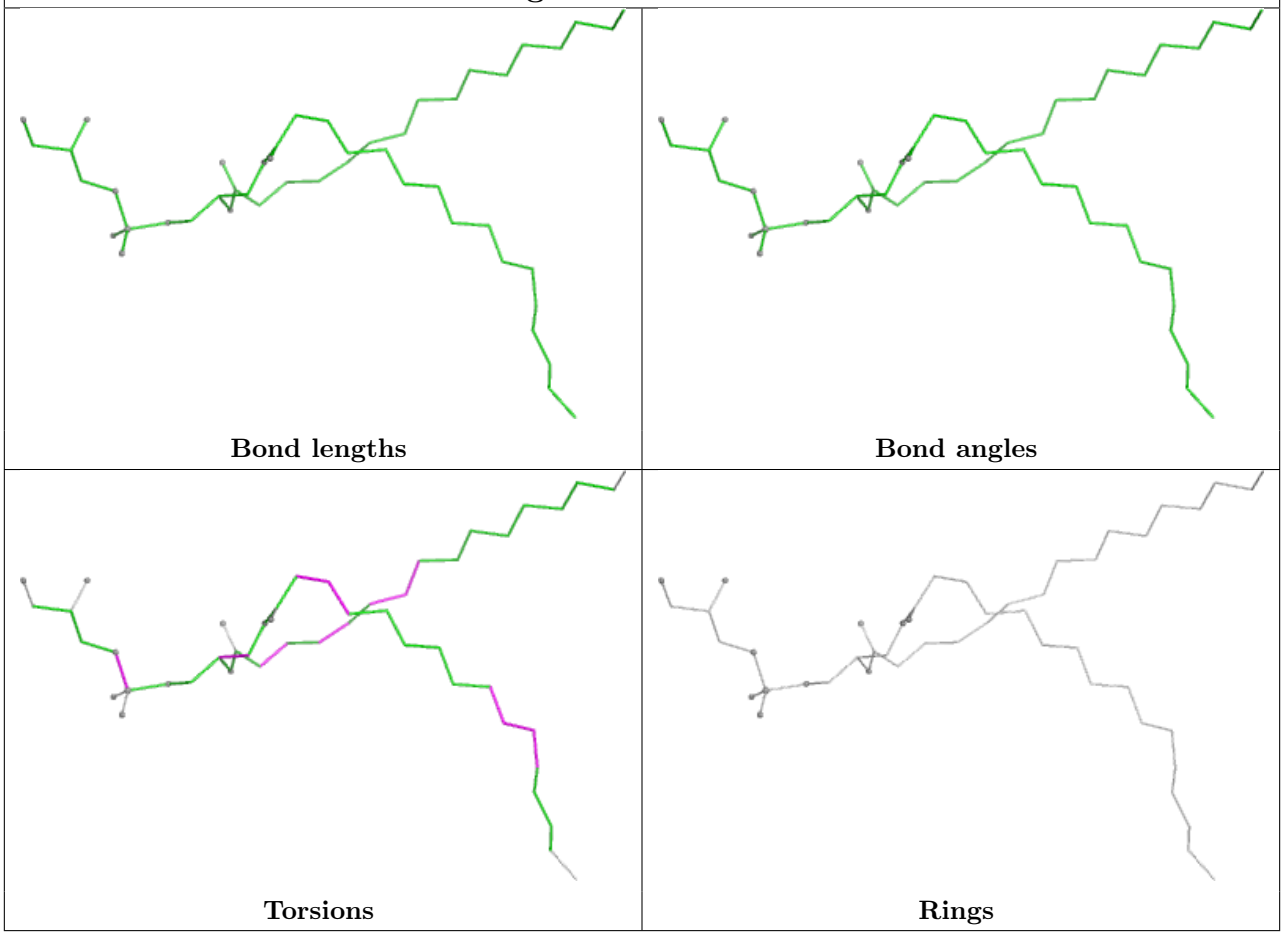


Torsions

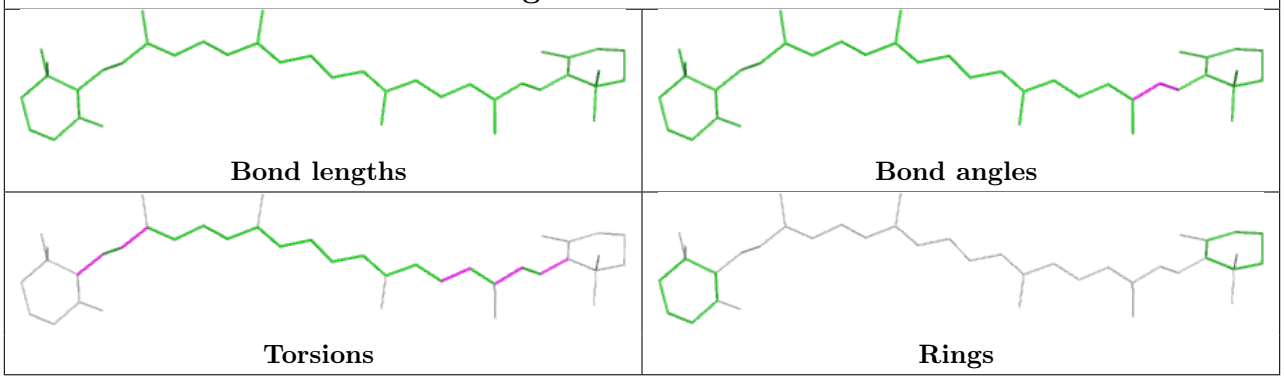


Rings

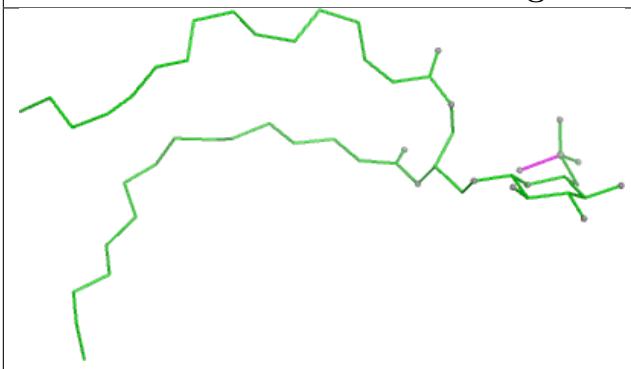
Ligand LHG d 409



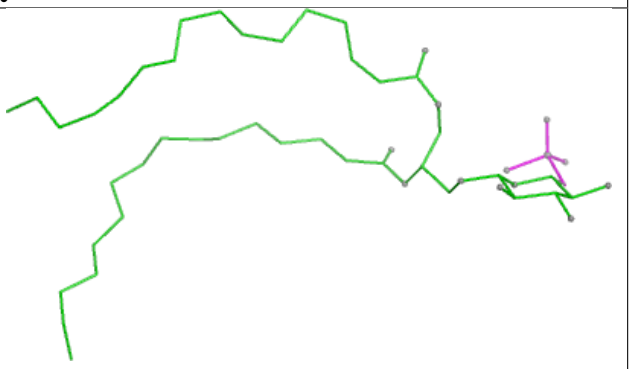
Ligand BCR D 405



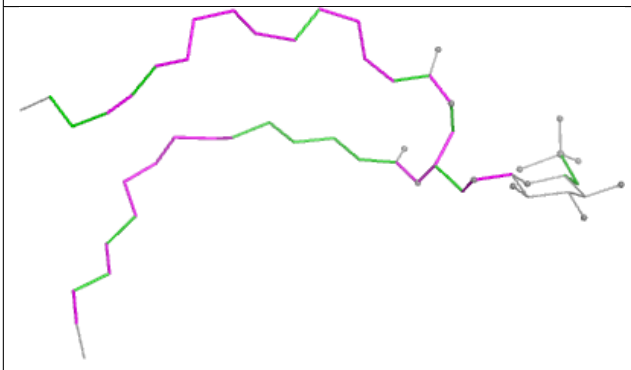
Ligand SQD b 621



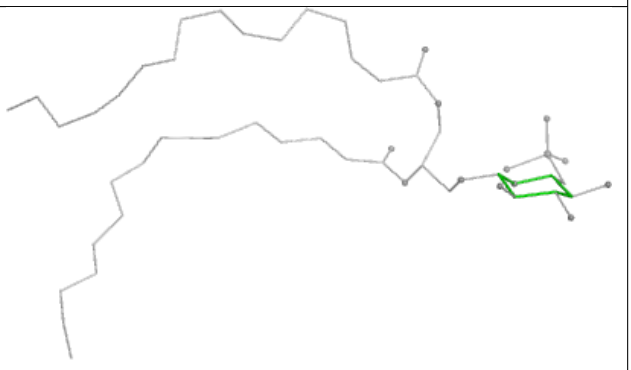
Bond lengths



Bond angles

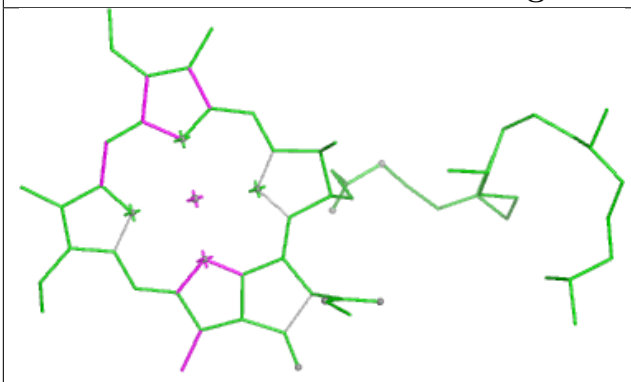


Torsions

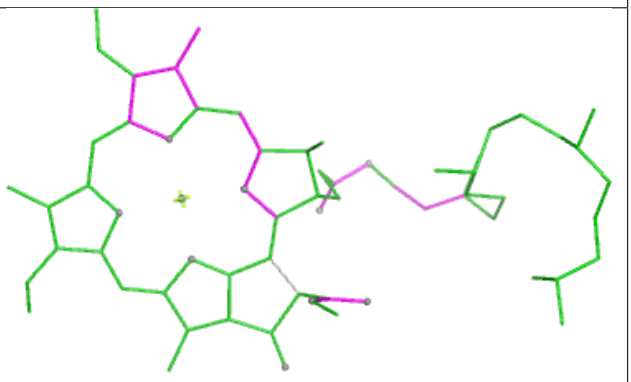


Rings

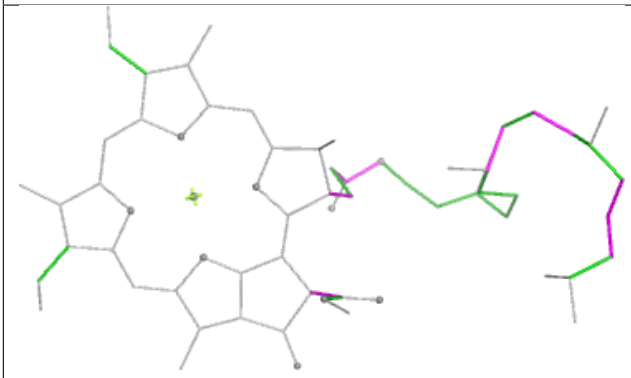
Ligand CLA b 618



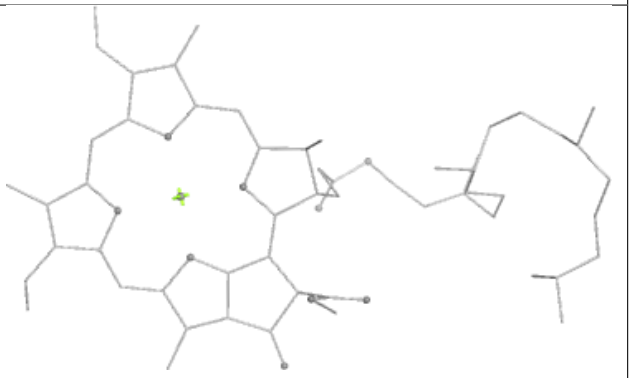
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

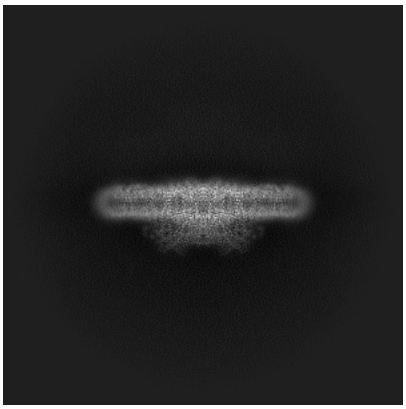
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52620. These allow visual inspection of the internal detail of the map and identification of artifacts.

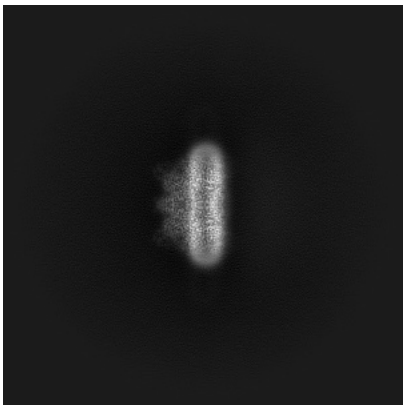
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

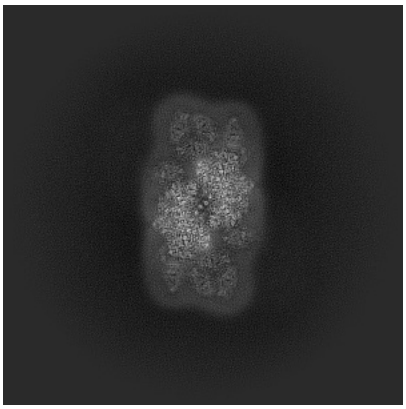
6.1.1 Primary map



X

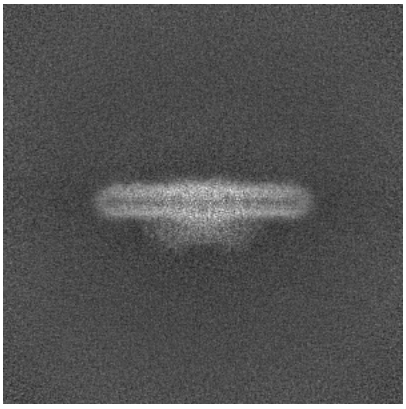


Y

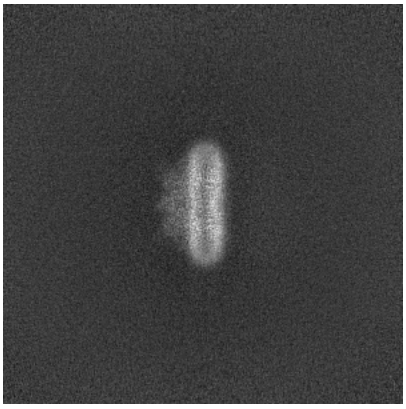


Z

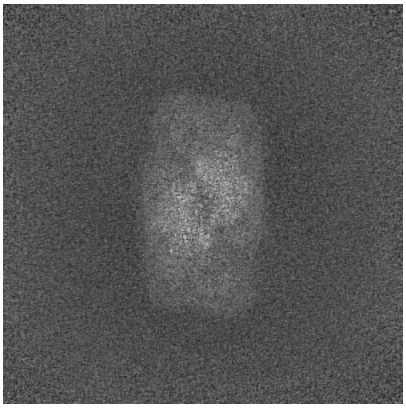
6.1.2 Raw map



X



Y

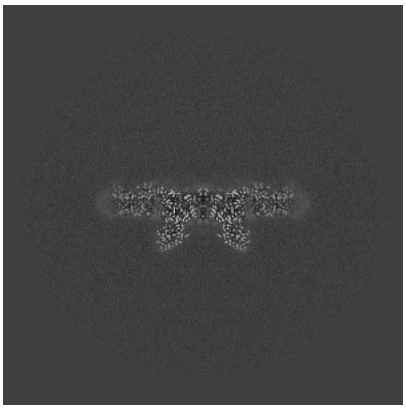


Z

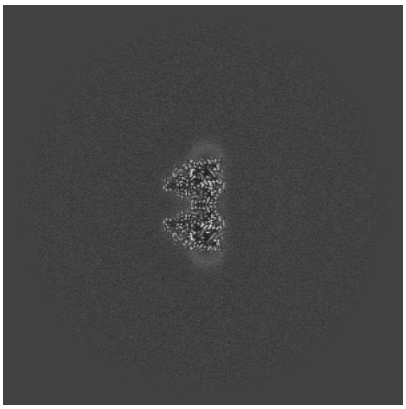
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

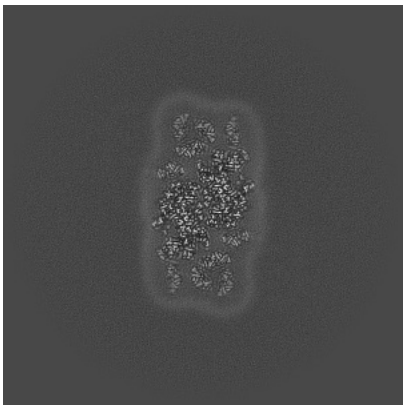
6.2.1 Primary map



X Index: 392

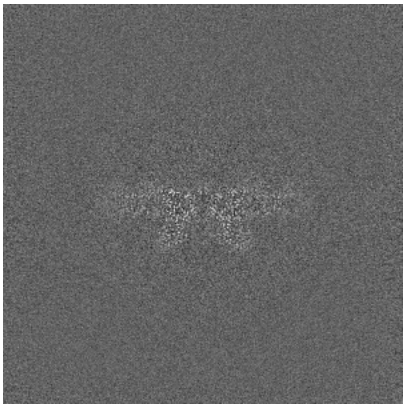


Y Index: 392

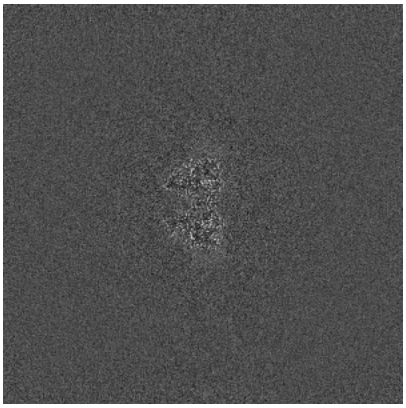


Z Index: 392

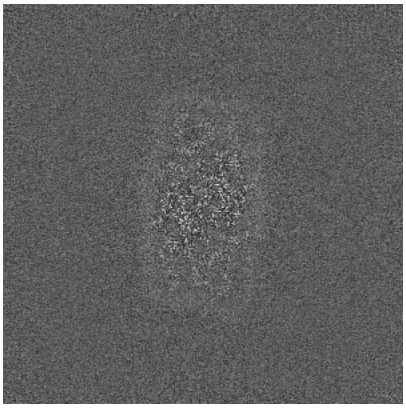
6.2.2 Raw map



X Index: 392



Y Index: 392

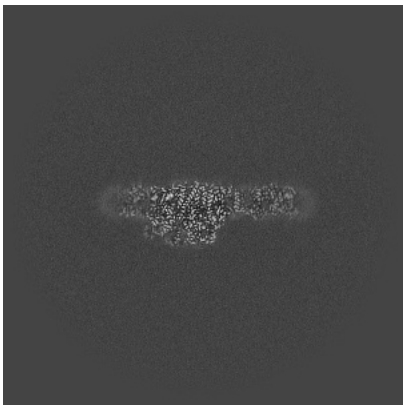


Z Index: 392

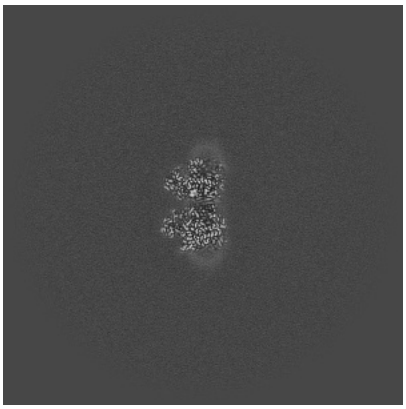
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

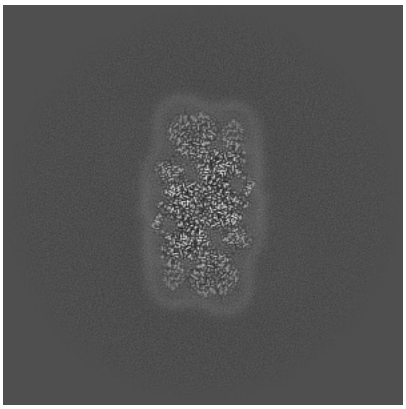
6.3.1 Primary map



X Index: 348

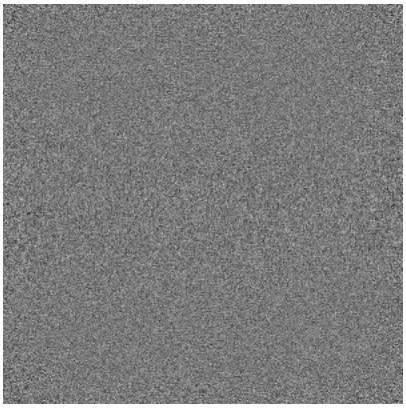


Y Index: 381

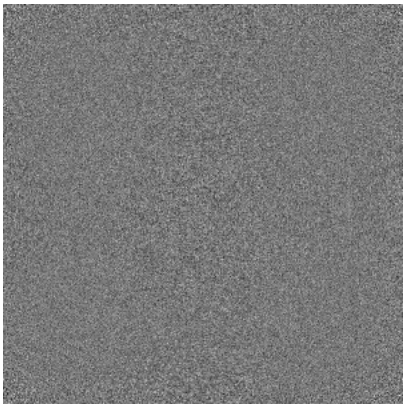


Z Index: 408

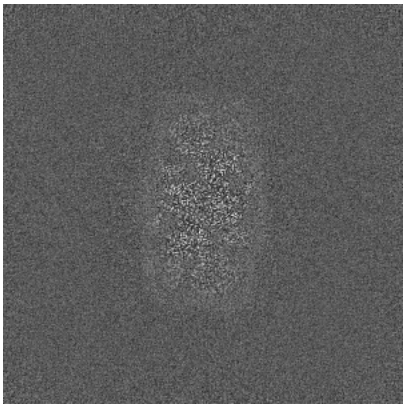
6.3.2 Raw map



X Index: 0



Y Index: 0

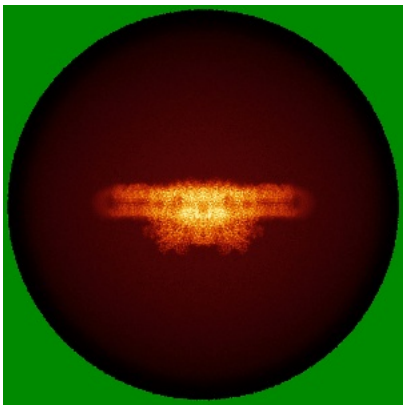


Z Index: 408

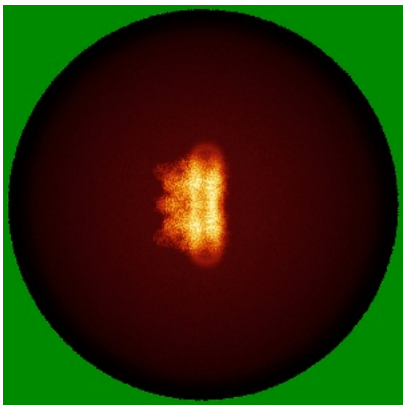
The images above show the largest variance slices of the map in three orthogonal directions.

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

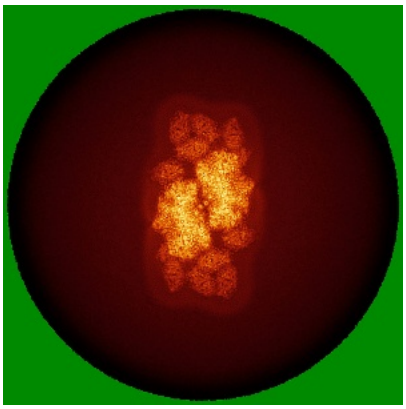
6.4.1 Primary map



X

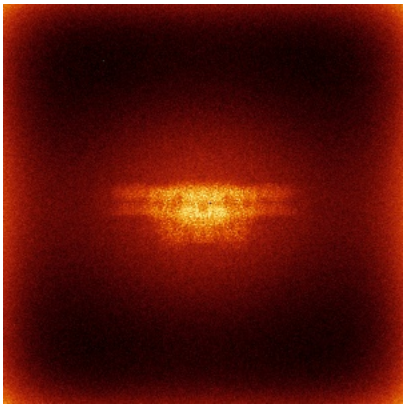


Y

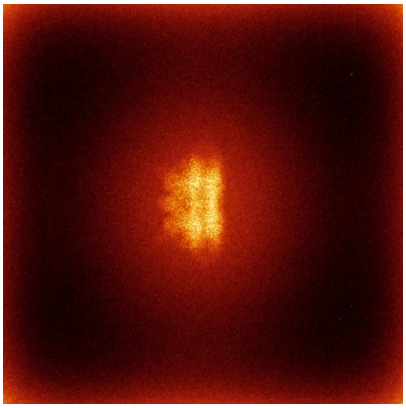


Z

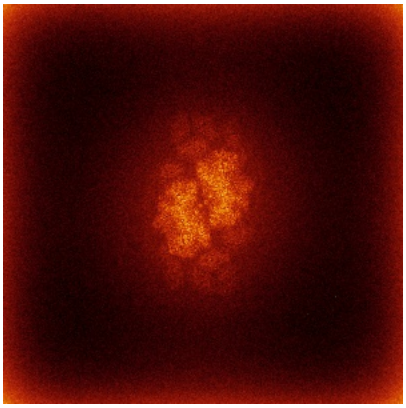
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

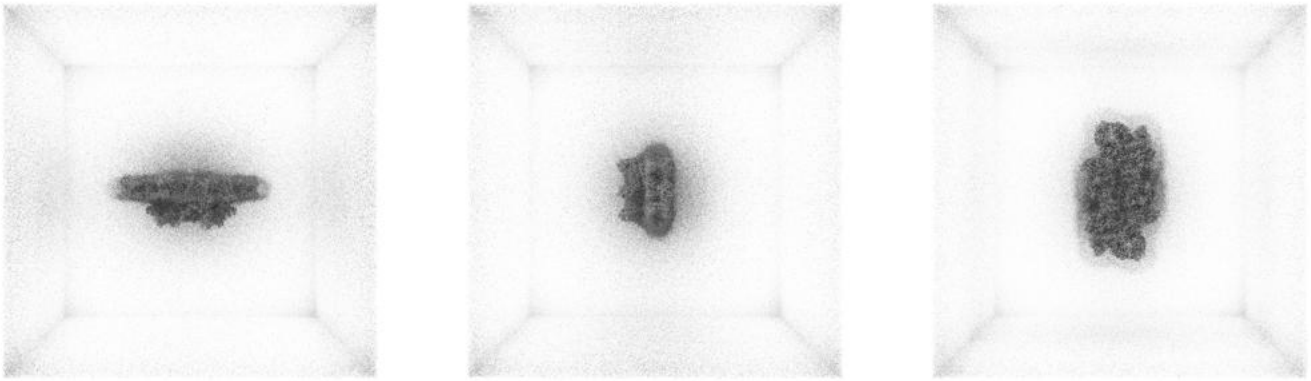
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

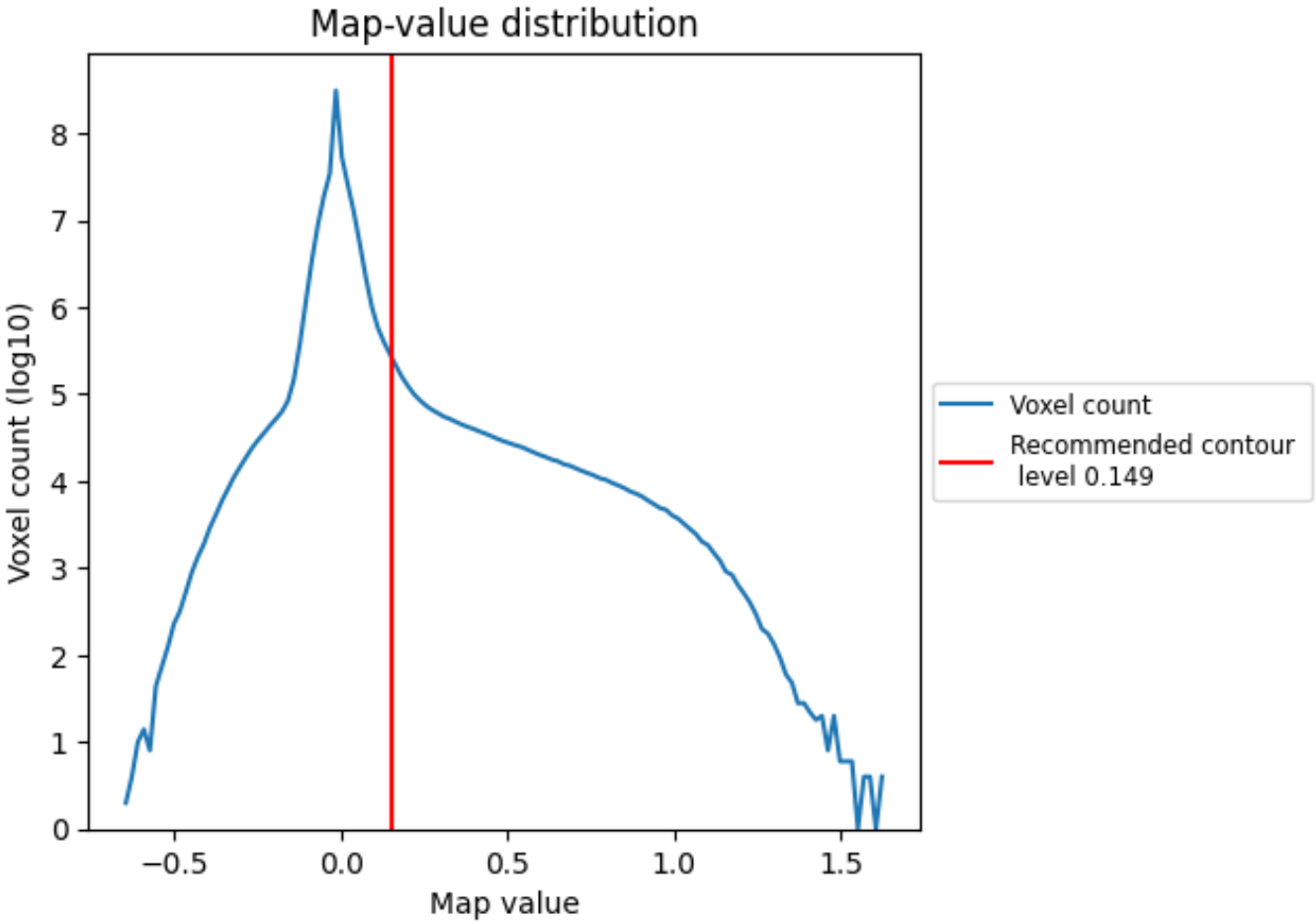
6.6 Mask visualisation (i)

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

7 Map analysis

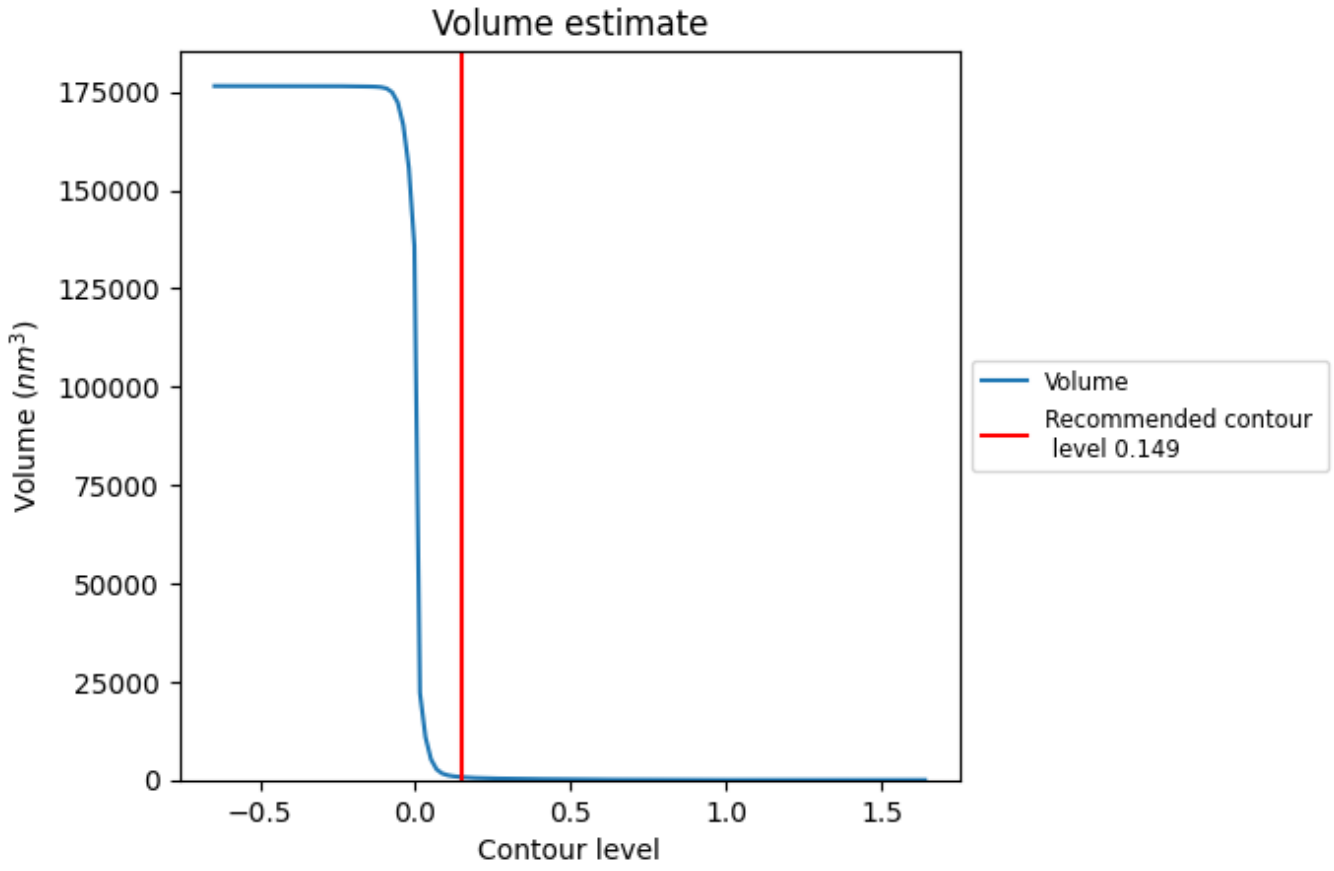
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

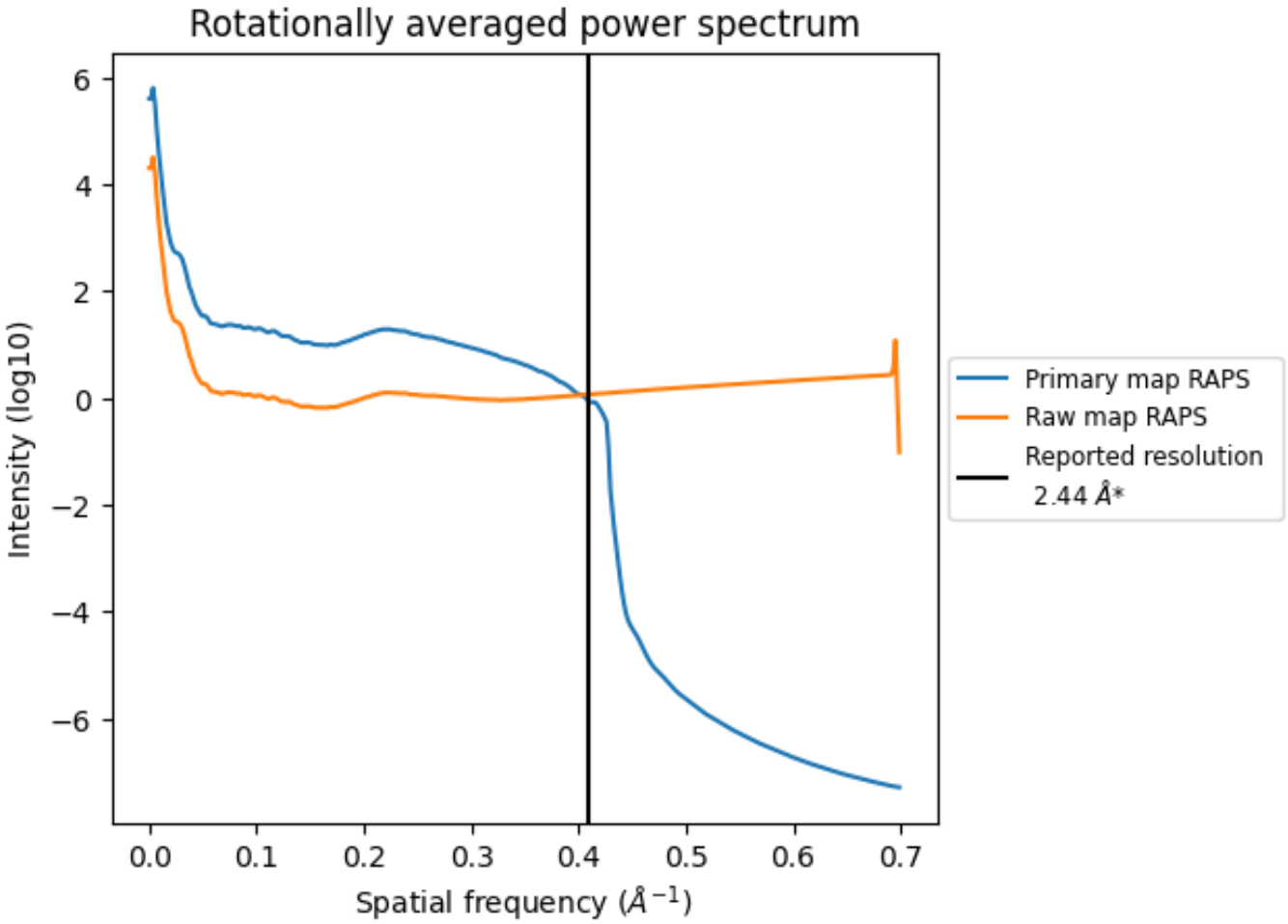
7.2 Volume estimate (i)



The volume at the recommended contour level is 724 nm^3; this corresponds to an approximate mass of 654 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)

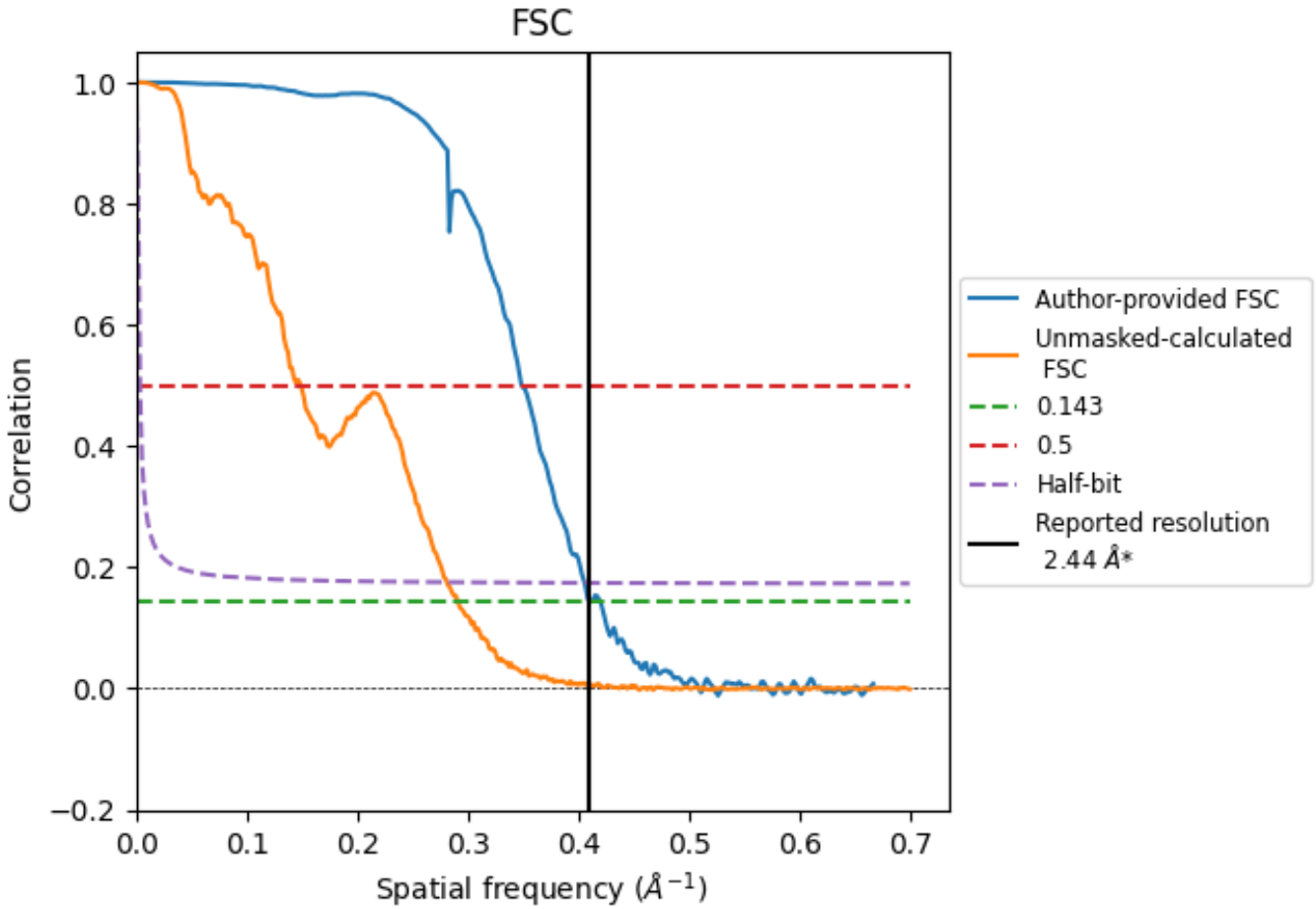


*Reported resolution corresponds to spatial frequency of 0.410 Å^{-1}

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 0.410 Å^{-1}

8.2 Resolution estimates (i)

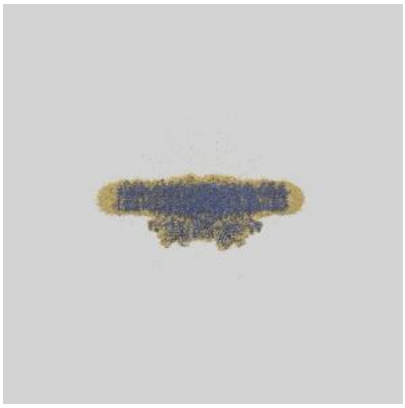
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.87	2.47
Unmasked-calculated*	3.44	6.72	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.44 by more than 10 %

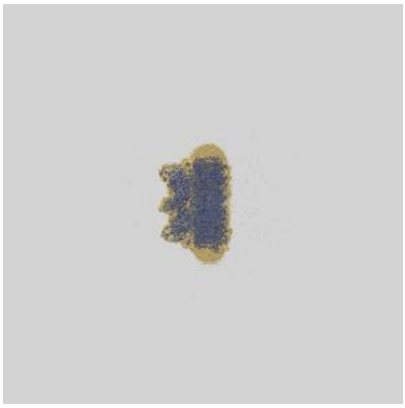
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52620 and PDB model 9I4T. Per-residue inclusion information can be found in section 3 on page 37.

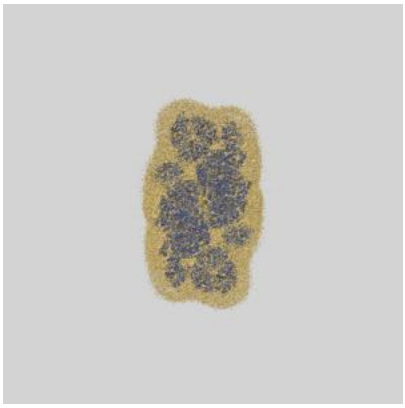
9.1 Map-model overlay



X



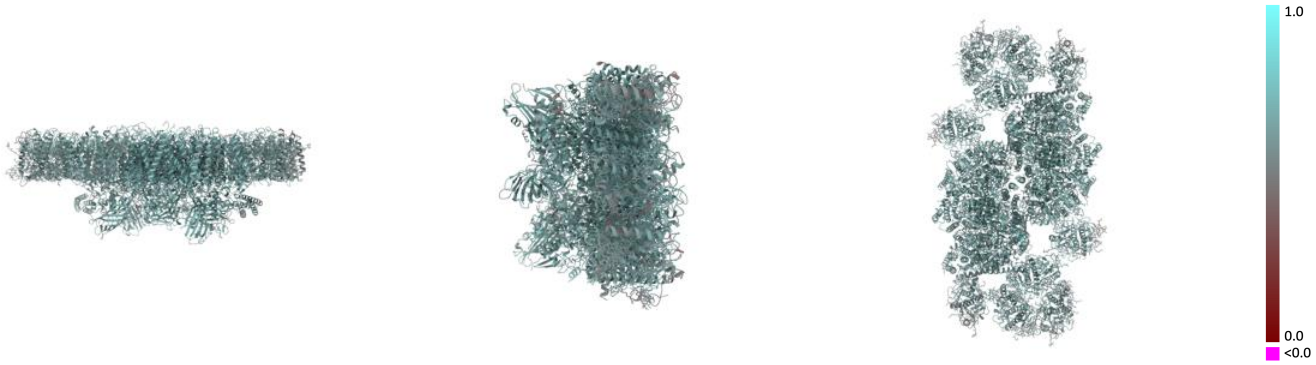
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

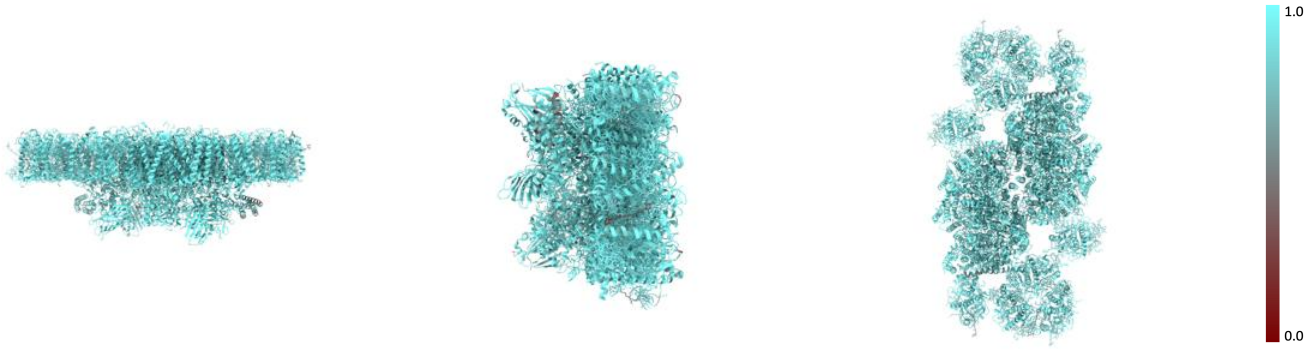
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

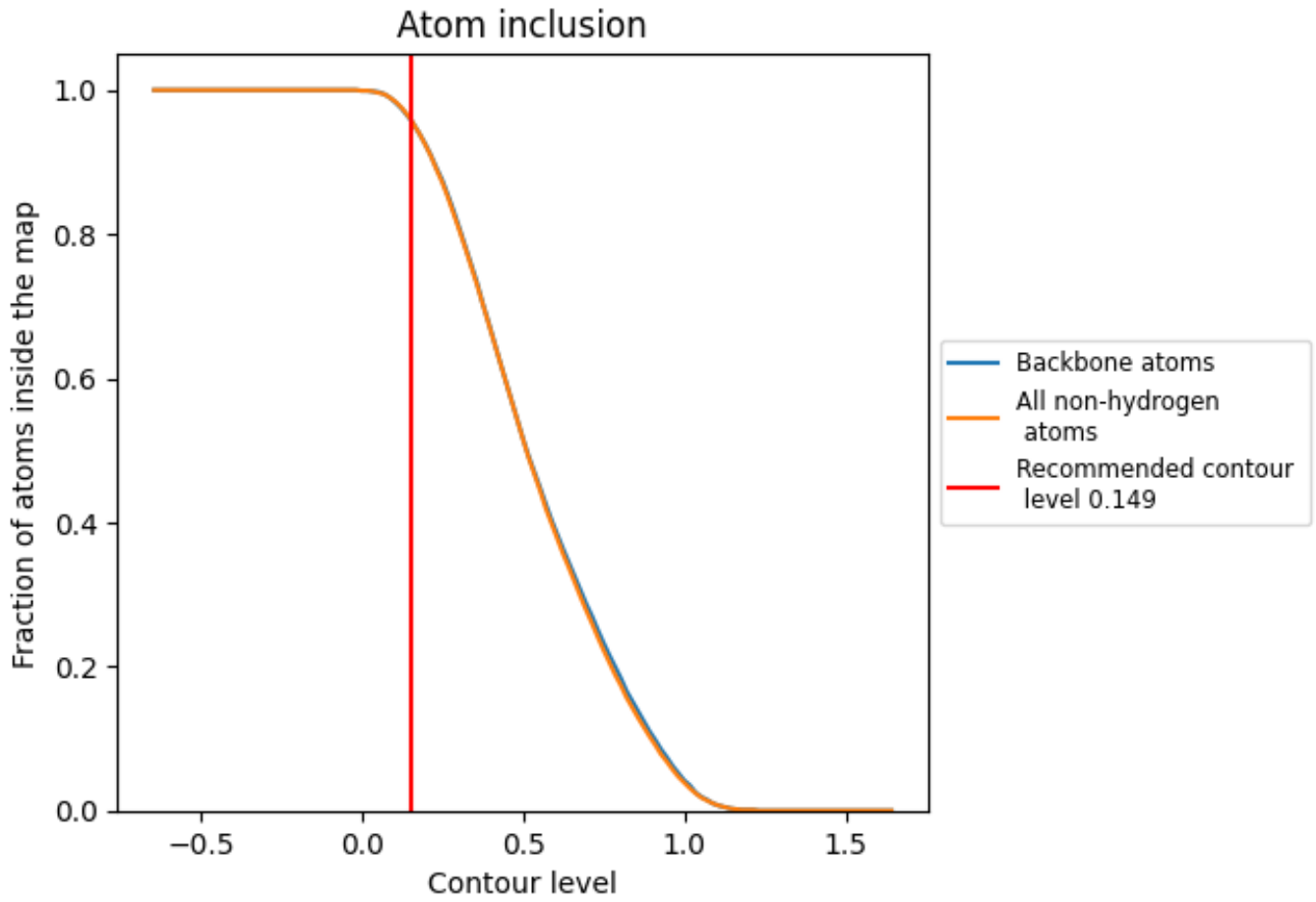
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.149).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9600	0.6330
A	0.9940	0.6680
B	0.9920	0.6650
C	0.9830	0.6550
D	0.9910	0.6720
E	0.9900	0.6360
F	0.9830	0.6340
G	0.8890	0.5710
H	0.9960	0.6570
I	1.0000	0.6690
J	0.9900	0.6260
K	0.9820	0.6380
L	0.9970	0.6720
M	0.9880	0.6430
N	0.9390	0.5990
O	0.9570	0.6270
P	0.9530	0.6390
Q	0.7890	0.5870
R	0.9490	0.6090
S	0.9120	0.5660
T	0.9530	0.6360
U	0.9480	0.6290
W	0.9600	0.6250
X	0.9780	0.6270
Y	0.9720	0.6380
Z	0.9630	0.5960
a	0.9940	0.6680
b	0.9910	0.6640
c	0.9830	0.6540
d	0.9910	0.6710
e	0.9890	0.6340
f	0.9790	0.6330
g	0.8900	0.5700
h	0.9940	0.6580
i	1.0000	0.6700



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Chain	Atom inclusion	Q-score
j	0.9830	0.6240
k	0.9820	0.6360
l	0.9970	0.6680
m	0.9880	0.6440
n	0.9400	0.5990
o	0.9550	0.6260
p	0.9520	0.6360
q	0.7920	0.5870
r	0.9480	0.6090
s	0.9110	0.5670
t	0.9560	0.6300
u	0.9480	0.6300
w	0.9620	0.6220
x	0.9780	0.6220
y	0.9720	0.6370
z	0.9600	0.5930