wwPDB EM Validation Summary Report

Sep 11, 2026 – 02:45 am BST

PDB ID	:	9IFM / pdb_00009ifm
EMDB ID	:	EMD-52846
Title	:	STRUCTURE OF UNSTACKED C2S2-TYPE PSII-LHCII SUPERCOMPLEX FROM PISUM SATIVUM
Authors	:	Klaiman, D.; Fadeeva, M.; Kandiah, E.; Nelson, N.
Deposited on	:	2025-02-18
Resolution	:	2.20 Å(reported)

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

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

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

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

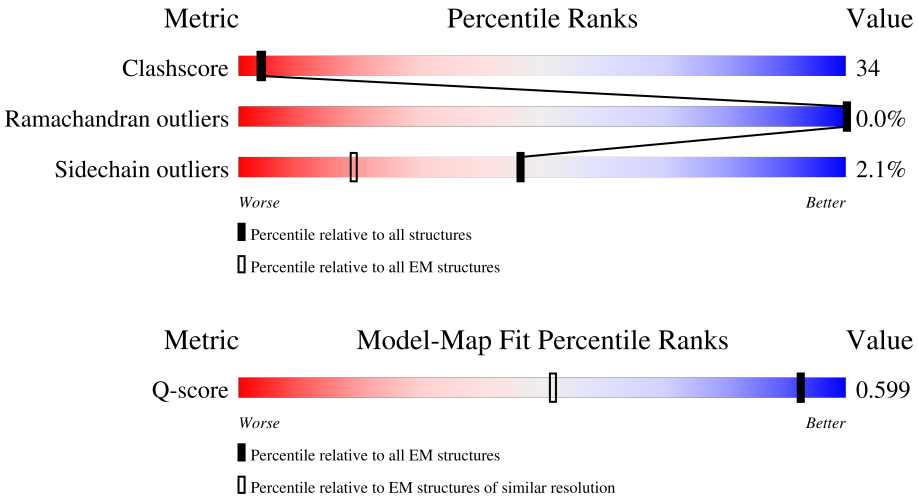
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	334	60% 40%
1	a	334	57% 40%
2	B	503	61% 39%
2	b	503	61% 38%

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Mol	Chain	Length	Quality of chain
3	C	450	58% 41%
3	c	450	58% 41%
4	D	352	59% 41%
4	d	352	63% 38%
5	E	75	64% 36%
5	e	75	51% 49%
6	F	30	37% 63%
6	f	30	53% 47%
7	G	216	6% 43% 56%
7	N	216	50% 48%
7	g	216	53% 46%
7	n	216	49% 49%
8	H	60	53% 45%
8	h	60	65% 35%
9	I	34	59% 41%
9	i	34	47% 53%
10	J	35	63% 34%
10	j	35	54% 40% 6%
11	K	37	35% 65%
11	k	37	32% 68%
12	L	36	50% 47%
12	l	36	64% 33%
13	M	33	12% 52% 48%
13	m	33	12% 55% 45%
14	O	248	59% 40%

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Mol	Chain	Length	Quality of chain
14	o	248	59% 40%
15	P	186	56% 41%
15	p	186	65% 33%
16	Q	148	45% 54%
16	q	148	54% 46%
17	R	224	52% 47%
17	r	224	47% 50%
18	S	218	6% 39% 59%
18	s	218	6% 39% 59%
19	T	31	71% 29%
19	t	31	52% 48%
20	W	54	6% 50% 44% 6%
20	w	54	6% 65% 35%
21	X	39	5% 59% 41%
21	x	39	8% 69% 31%
22	Y	219	52% 47%
22	y	219	55% 43%
23	Z	61	51% 46%
23	z	61	46% 49% 5%
24	U	28	54% 46%
24	u	28	7% 46% 46% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	B	603	-	-	X	-
28	CLA	C	506	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	C	507	-	-	X	-
28	CLA	G	610	-	-	X	-
28	CLA	G	613	-	-	X	-
28	CLA	N	602	-	-	X	-
28	CLA	S	303	-	-	X	-
28	CLA	S	310	-	-	X	-
28	CLA	n	603	-	-	X	-
28	CLA	n	610	-	-	X	-
28	CLA	y	304	-	-	X	-
30	BCR	B	619	-	-	X	-
30	BCR	C	514	-	X	-	-
30	BCR	C	516	-	-	X	-
30	BCR	a	410	-	-	X	-
30	BCR	t	101	-	X	-	-
35	LHG	S	317	-	-	X	-
36	DGD	C	518	-	-	X	-
38	CHL	Y	607	-	-	X	-
38	CHL	g	601	-	-	X	-
38	CHL	n	607	-	-	X	-
38	CHL	n	609	-	-	X	-
38	CHL	y	309	-	-	X	-
39	LUT	G	615	-	-	X	-
39	LUT	S	315	-	-	X	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 79416 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
			2616	1708	431	464	13		
1	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	503	Total	C	N	O	S	0	0
			3939	2577	665	685	12		
2	b	503	Total	C	N	O	S	0	0
			3939	2577	665	685	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
3	c	450	Total	C	N	O	S	0	0
			3496	2300	583	603	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	352	Total	C	N	O	S	0	0
			2797	1845	458	482	12		
4	d	352	Total	C	N	O	S	0	0
			2797	1845	458	482	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total 612	C 400	N 100	O 112	0	0
5	e	75	Total 612	C 400	N 100	O 112	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	26	PHE	SER	conflict	UNP P62096
f	26	PHE	SER	conflict	UNP P62096

- Molecule 7 is a protein called Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	216	Total 1650	C 1069	N 267	O 309	S 5	0	0
7	N	216	Total 1649	C 1068	N 267	O 309	S 5	0	0
7	g	216	Total 1650	C 1069	N 267	O 309	S 5	0	0
7	n	216	Total 1650	C 1069	N 267	O 309	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	60	Total 452	C 296	N 72	O 81	S 3	0	0
8	h	60	Total 452	C 296	N 72	O 81	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
9	i	34	Total	C	N	O	S	0	0
			278	191	43	43	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
			256	174	39	43		
10	j	35	Total	C	N	O	0	0
			256	174	39	43		

- 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
			306	215	44	46	1		
11	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total	C	N	O	0	0
			304	201	48	55		
12	l	36	Total	C	N	O	0	0
			304	201	48	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	33	Total	C	N	O	S	0	0
			256	176	36	43	1		
13	m	33	Total	C	N	O	S	0	0
			256	176	36	43	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	248	Total 1870	C 1179	N 306	O 382	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	186	Total 1434	C 909	N 238	O 286	S 1	0	0
15	p	186	Total 1434	C 909	N 238	O 286	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	148	Total 1157	C 742	N 197	O 218	0	0
16	q	148	Total 1157	C 742	N 197	O 218	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	224	Total 1755	C 1142	N 285	O 325	S 3	0	0
17	r	224	Total 1755	C 1142	N 285	O 325	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	218	Total 1688	C 1105	N 271	O 308	S 4	0	0
18	s	218	Total 1688	C 1105	N 271	O 308	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	31	Total 252	C 176	N 35	O 40	S 1	0	0
19	t	31	Total 252	C 176	N 35	O 40	S 1	0	0

- Molecule 20 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
20	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

- Molecule 21 is a protein called Ultraviolet-B-repressible protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	39	Total	C	N	O	0	0
			276	180	46	50		
21	x	39	Total	C	N	O	0	0
			276	180	46	50		

- Molecule 22 is a protein called Chlorophyll a-b binding protein AB80, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	219	Total	C	N	O	S	0	0
			1667	1081	270	311	5		
22	y	219	Total	C	N	O	S	0	0
			1667	1081	270	311	5		

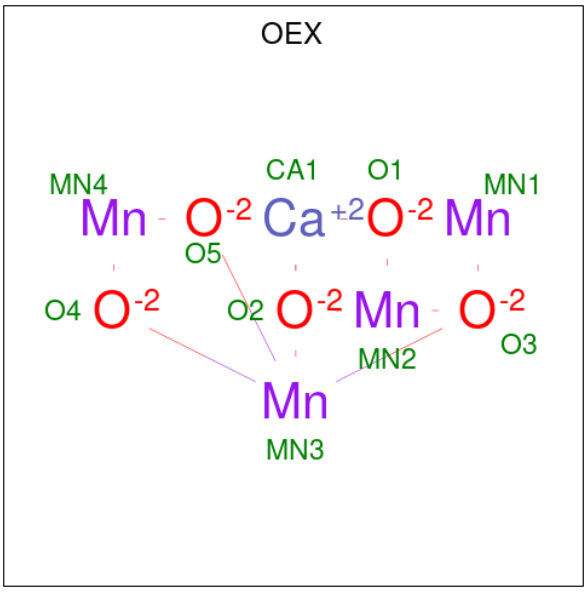
- Molecule 23 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	61	Total	C	N	O	S	0	0
			457	309	68	79	1		
23	z	61	Total	C	N	O	S	0	0
			457	309	68	79	1		

- Molecule 24 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	28	Total	C	N	O	S	0	0
			212	131	41	37	3		
24	u	28	Total	C	N	O	S	0	0
			212	131	41	37	3		

- Molecule 25 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
25	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

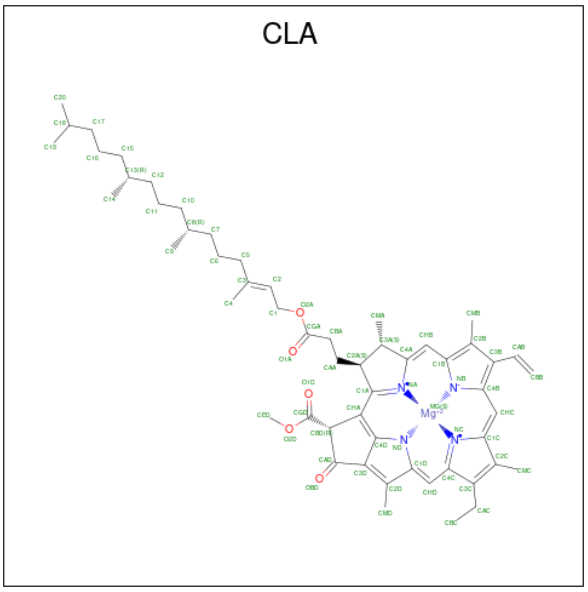
- Molecule 26 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 27 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	g	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	s	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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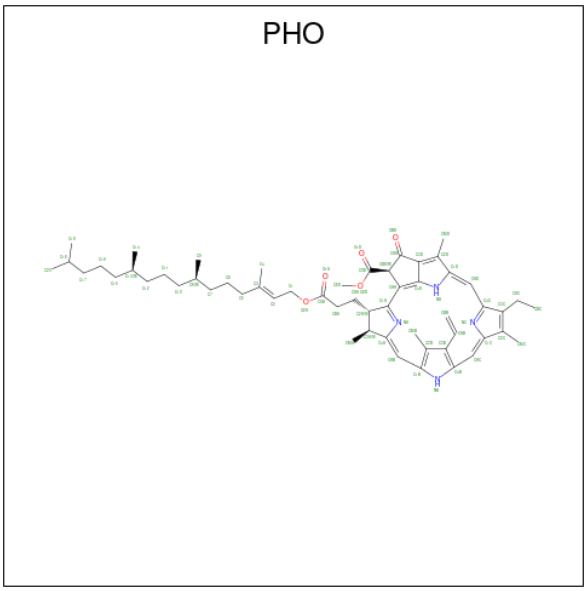
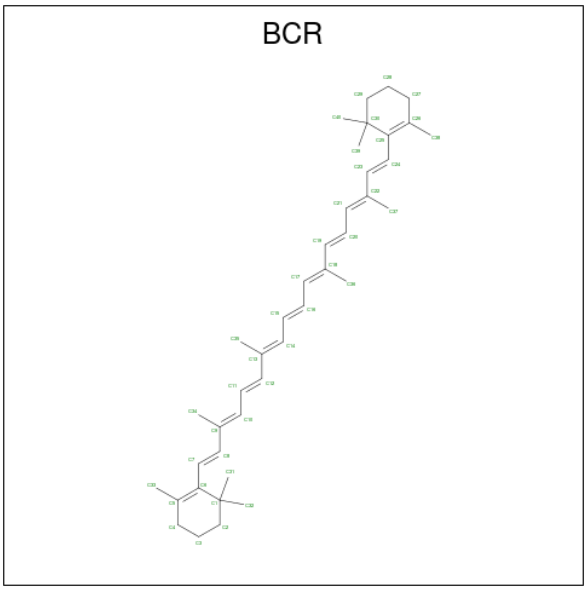
Mol	Chain	Residues	Atoms					AltConf
28	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 48	C 38	Mg 1	N 4	O 5	0

- Molecule 29 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



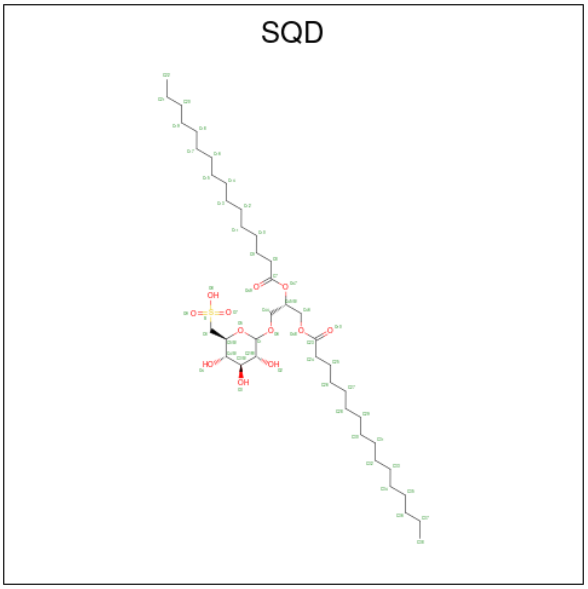
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	N	O	0
			64	55	4	5	
29	D	1	Total	C	N	O	0
			64	55	4	5	
29	a	1	Total	C	N	O	0
			64	55	4	5	
29	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



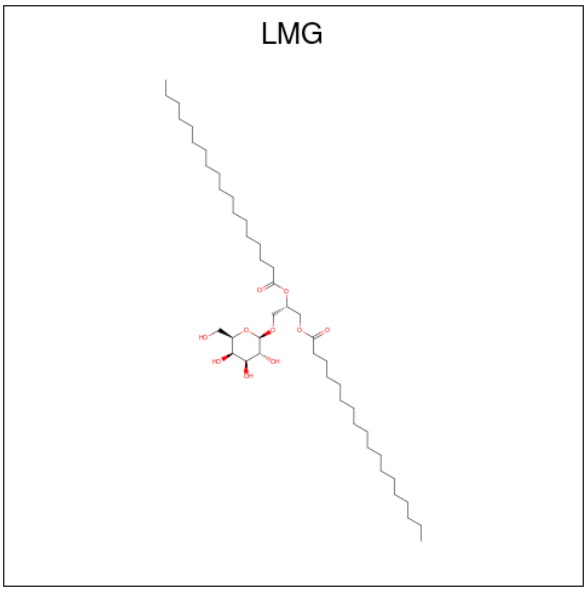
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	T	1	Total C 40 40	0
30	a	1	Total C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

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



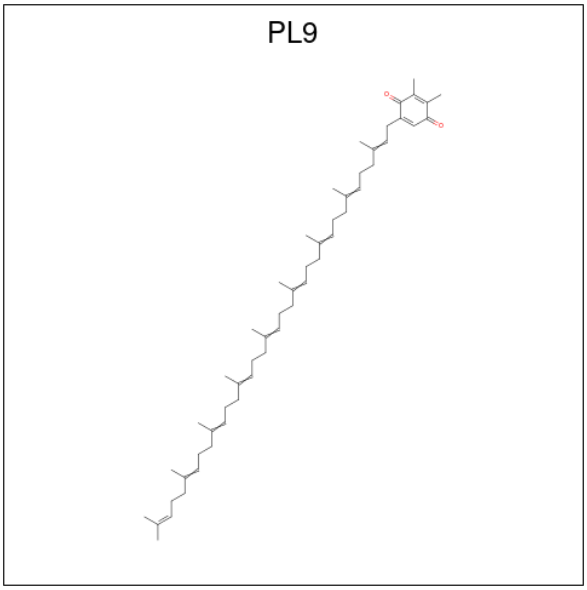
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	S	0
			50	37	12	1	
31	A	1	Total	C	O	S	0
			54	41	12	1	
31	B	1	Total	C	O	S	0
			54	41	12	1	
31	L	1	Total	C	O	S	0
			42	29	12	1	
31	L	1	Total	C	O	S	0
			54	41	12	1	
31	M	1	Total	C	O	S	0
			42	29	12	1	
31	a	1	Total	C	O	S	0
			50	37	12	1	
31	a	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



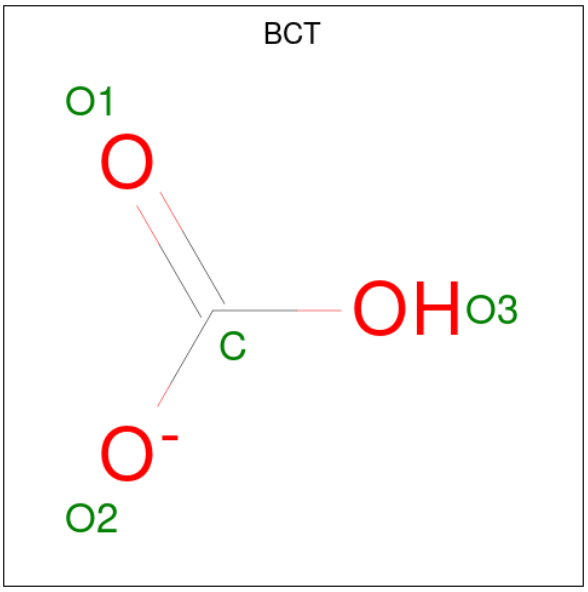
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C O 48 38 10	0
32	A	1	Total C O 40 30 10	0
32	B	1	Total C O 51 41 10	0
32	B	1	Total C O 31 21 10	0
32	C	1	Total C O 51 41 10	0
32	C	1	Total C O 44 34 10	0
32	D	1	Total C O 46 36 10	0
32	a	1	Total C O 40 30 10	0
32	b	1	Total C O 51 41 10	0
32	b	1	Total C O 50 40 10	0
32	c	1	Total C O 51 41 10	0
32	d	1	Total C O 46 36 10	0
32	k	1	Total C O 51 41 10	0
32	w	1	Total C O 48 38 10	0

- Molecule 33 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: $C_{53}H_{80}O_2$).



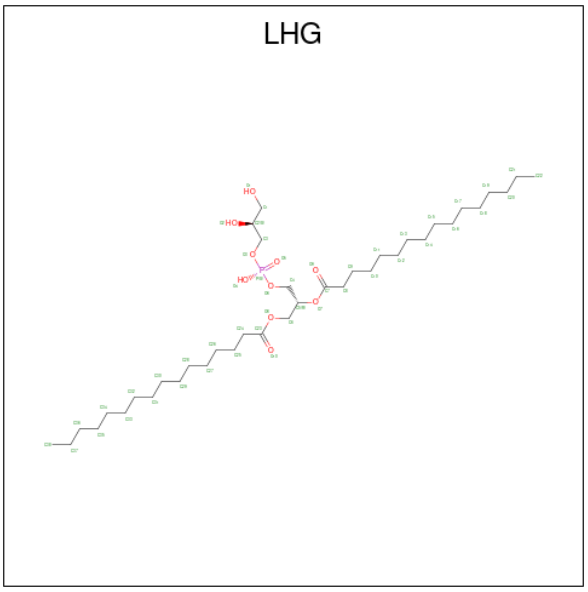
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			13	11	2	
33	D	1	Total	C	O	0
			55	53	2	
33	a	1	Total	C	O	0
			13	11	2	
33	d	1	Total	C	O	0
			55	53	2	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			4	1	3	
34	d	1	Total	C	O	0
			4	1	3	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			43	32	10	1	

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Mol	Chain	Residues	Atoms				AltConf
35	B	1	Total	C	O	P	0
			30	19	10	1	
35	B	1	Total	C	O	P	0
			41	30	10	1	
35	B	1	Total	C	O	P	0
			46	35	10	1	
35	C	1	Total	C	O	P	0
			49	38	10	1	
35	D	1	Total	C	O	P	0
			49	38	10	1	
35	G	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	N	1	Total	C	O	P	0
			31	20	10	1	
35	R	1	Total	C	O	P	0
			25	14	10	1	
35	S	1	Total	C	O	P	0
			34	23	10	1	
35	S	1	Total	C	O	P	0
			43	32	10	1	
35	W	1	Total	C	O	P	0
			49	38	10	1	
35	Y	1	Total	C	O	P	0
			49	38	10	1	
35	a	1	Total	C	O	P	0
			43	32	10	1	
35	b	1	Total	C	O	P	0
			34	23	10	1	
35	b	1	Total	C	O	P	0
			41	30	10	1	
35	b	1	Total	C	O	P	0
			46	35	10	1	
35	c	1	Total	C	O	P	0
			32	21	10	1	
35	c	1	Total	C	O	P	0
			40	29	10	1	
35	d	1	Total	C	O	P	0
			49	38	10	1	
35	g	1	Total	C	O	P	0
			41	30	10	1	

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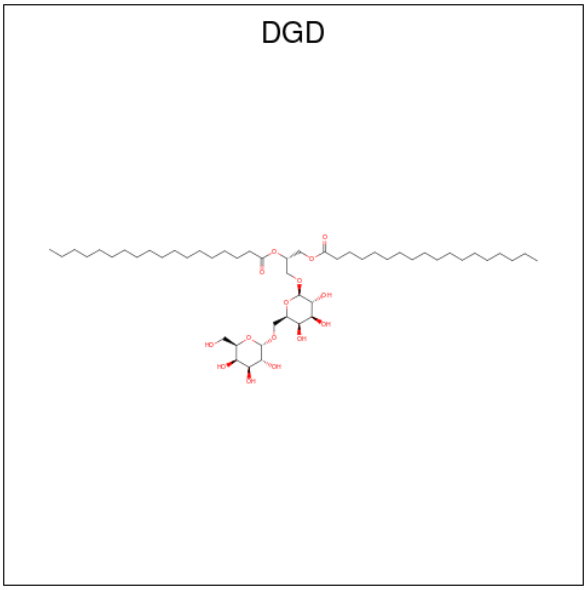
Mol	Chain	Residues	Atoms				AltConf
35	l	1	Total	C	O	P	0
			49	38	10	1	
35	n	1	Total	C	O	P	0
			32	21	10	1	
35	r	1	Total	C	O	P	0
			30	19	10	1	
35	s	1	Total	C	O	P	0
			49	38	10	1	
35	w	1	Total	C	O	P	0
			39	28	10	1	
35	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			59	44	15	
36	B	1	Total	C	O	0
			62	47	15	
36	C	1	Total	C	O	0
			55	40	15	
36	C	1	Total	C	O	0
			62	47	15	
36	C	1	Total	C	O	0
			60	45	15	

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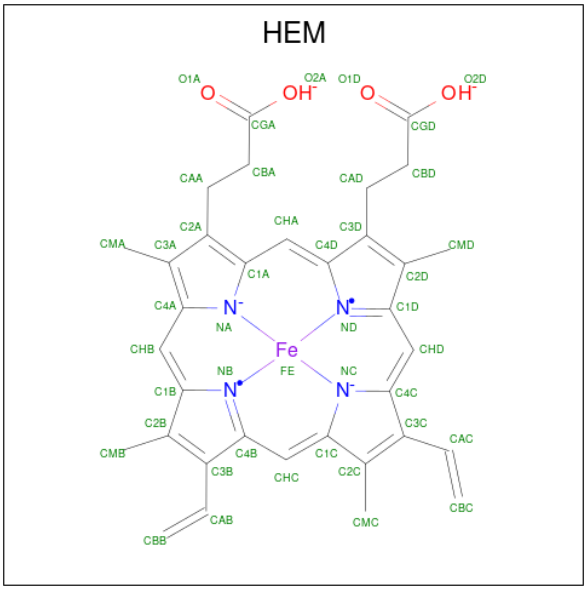
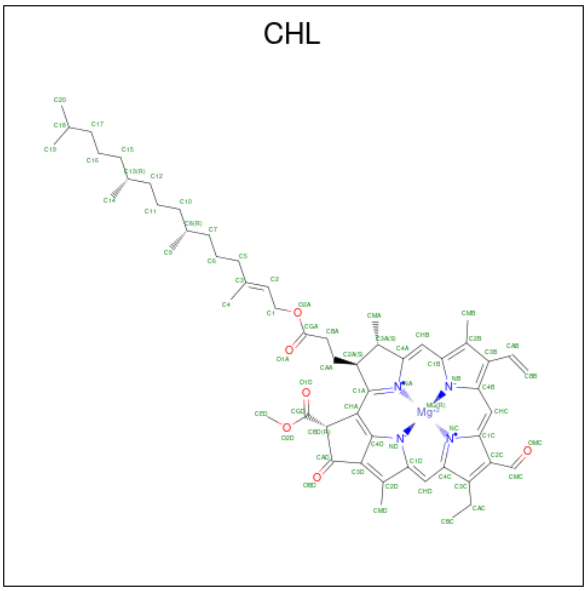
Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C O 59 44 15	0
36	b	1	Total C O 62 47 15	0
36	c	1	Total C O 55 40 15	0
36	c	1	Total C O 54 39 15	0
36	c	1	Total C O 59 44 15	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 38 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
38	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	G	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	N	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
38	R	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
38	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
38	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
38	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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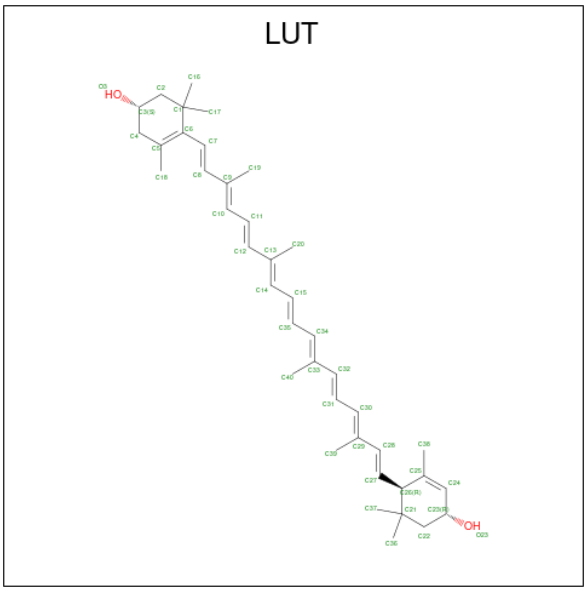
Mol	Chain	Residues	Atoms					AltConf
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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



Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	R	1	Total	C	O	0
			42	40	2	
39	S	1	Total	C	O	0
			42	40	2	
39	S	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	n	1	Total	C	O	0
			42	40	2	
39	n	1	Total	C	O	0
			42	40	2	
39	r	1	Total	C	O	0
			42	40	2	

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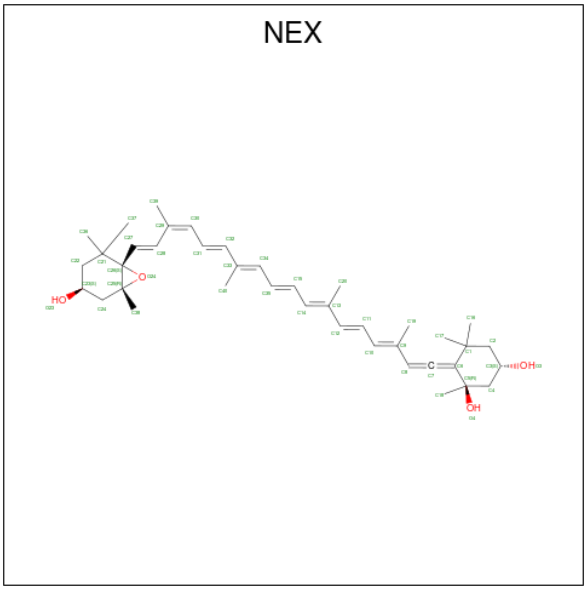
Mol	Chain	Residues	Atoms	AltConf
39	s	1	Total C O 42 40 2	0
39	s	1	Total C O 42 40 2	0
39	y	1	Total C O 42 40 2	0
39	y	1	Total C O 42 40 2	0

- Molecule 40 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
40	G	1	Total C O 44 40 4	0
40	N	1	Total C O 44 40 4	0
40	Y	1	Total C O 44 40 4	0
40	g	1	Total C O 44 40 4	0
40	n	1	Total C O 44 40 4	0
40	r	1	Total C O 44 40 4	0

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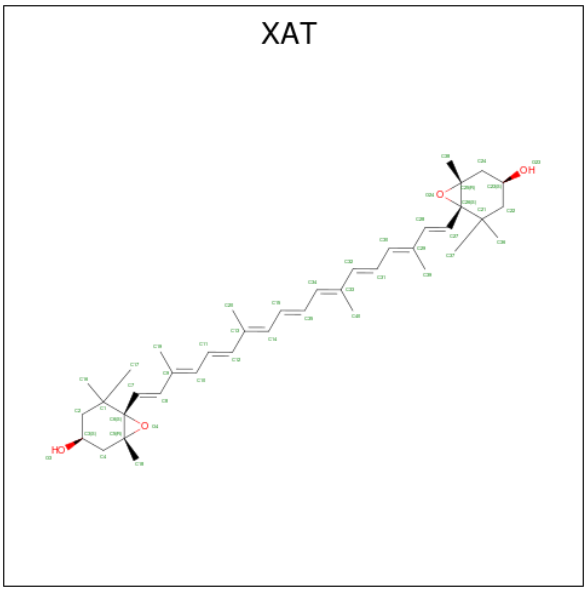
Mol	Chain	Residues	Atoms	AltConf
40	s	1	Total C O 44 40 4	0
40	y	1	Total C O 44 40 4	0
40	y	1	Total C O 44 40 4	0

- 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	R	1	Total C O 44 40 4	0
41	Y	1	Total C O 44 40 4	0
41	r	1	Total C O 44 40 4	0
41	y	1	Total C O 44 40 4	0

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	AltConf
42	A	92	Total O 92 92	0
42	B	151	Total O 151 151	0

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Mol	Chain	Residues	Atoms	AltConf
42	C	134	Total O 134 134	0
42	D	101	Total O 101 101	0
42	E	14	Total O 14 14	0
42	F	6	Total O 6 6	0
42	G	26	Total O 26 26	0
42	H	16	Total O 16 16	0
42	I	3	Total O 3 3	0
42	J	5	Total O 5 5	0
42	K	6	Total O 6 6	0
42	L	8	Total O 8 8	0
42	M	6	Total O 6 6	0
42	N	28	Total O 28 28	0
42	O	69	Total O 69 69	0
42	P	52	Total O 52 52	0
42	Q	28	Total O 28 28	0
42	R	40	Total O 40 40	0
42	S	24	Total O 24 24	0
42	T	7	Total O 7 7	0
42	W	11	Total O 11 11	0
42	X	10	Total O 10 10	0
42	Y	45	Total O 45 45	0

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Mol	Chain	Residues	Atoms	AltConf
42	Z	6	Total O 6 6	0
42	U	1	Total O 1 1	0
42	a	100	Total O 100 100	0
42	b	167	Total O 167 167	0
42	c	128	Total O 128 128	0
42	d	85	Total O 85 85	0
42	e	21	Total O 21 21	0
42	f	3	Total O 3 3	0
42	g	23	Total O 23 23	0
42	h	14	Total O 14 14	0
42	i	2	Total O 2 2	0
42	j	4	Total O 4 4	0
42	k	4	Total O 4 4	0
42	l	8	Total O 8 8	0
42	m	2	Total O 2 2	0
42	n	23	Total O 23 23	0
42	o	67	Total O 67 67	0
42	p	43	Total O 43 43	0
42	q	18	Total O 18 18	0
42	r	33	Total O 33 33	0
42	s	19	Total O 19 19	0

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Mol	Chain	Residues	Atoms	AltConf
42	t	3	Total O 3 3	0
42	w	11	Total O 11 11	0
42	x	7	Total O 7 7	0
42	y	31	Total O 31 31	0
42	z	2	Total O 2 2	0
42	u	4	Total O 4 4	0

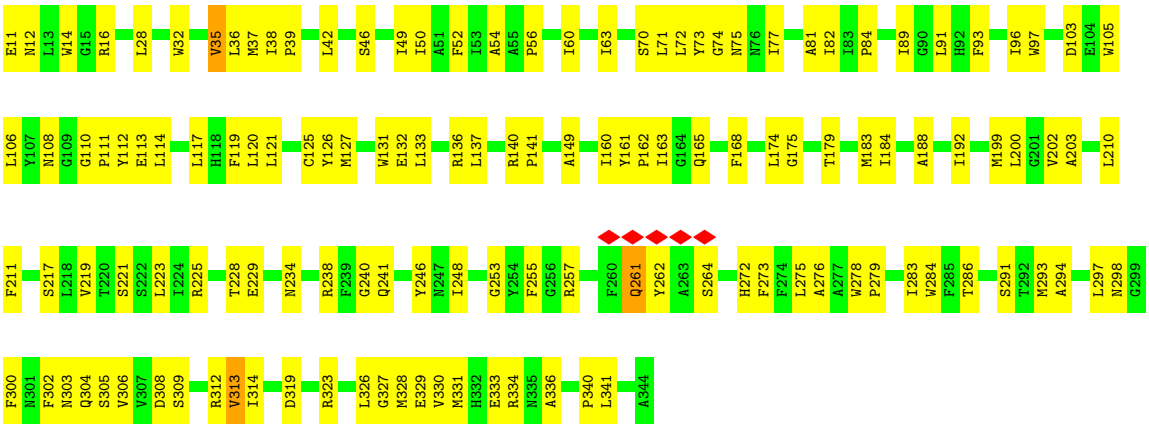
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

Chain A:

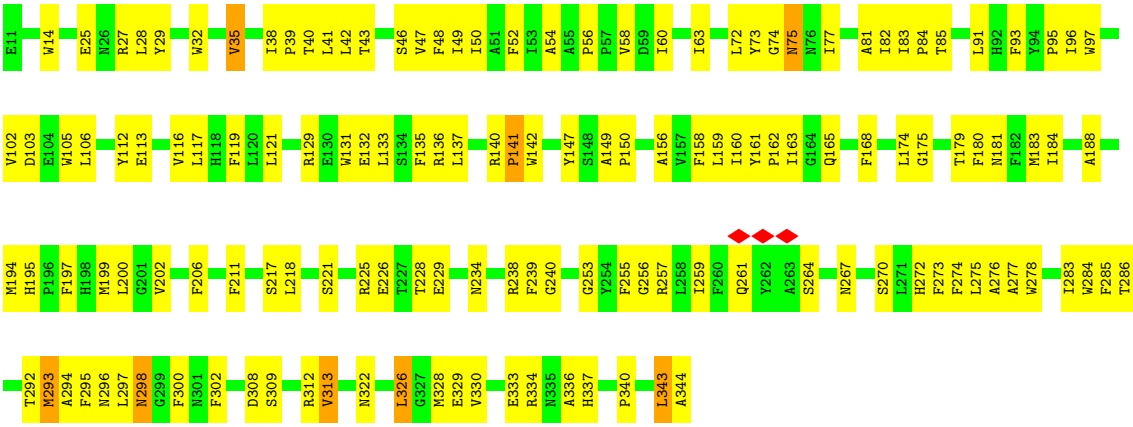




• Molecule 1: Photosystem II protein D1

Chain a:

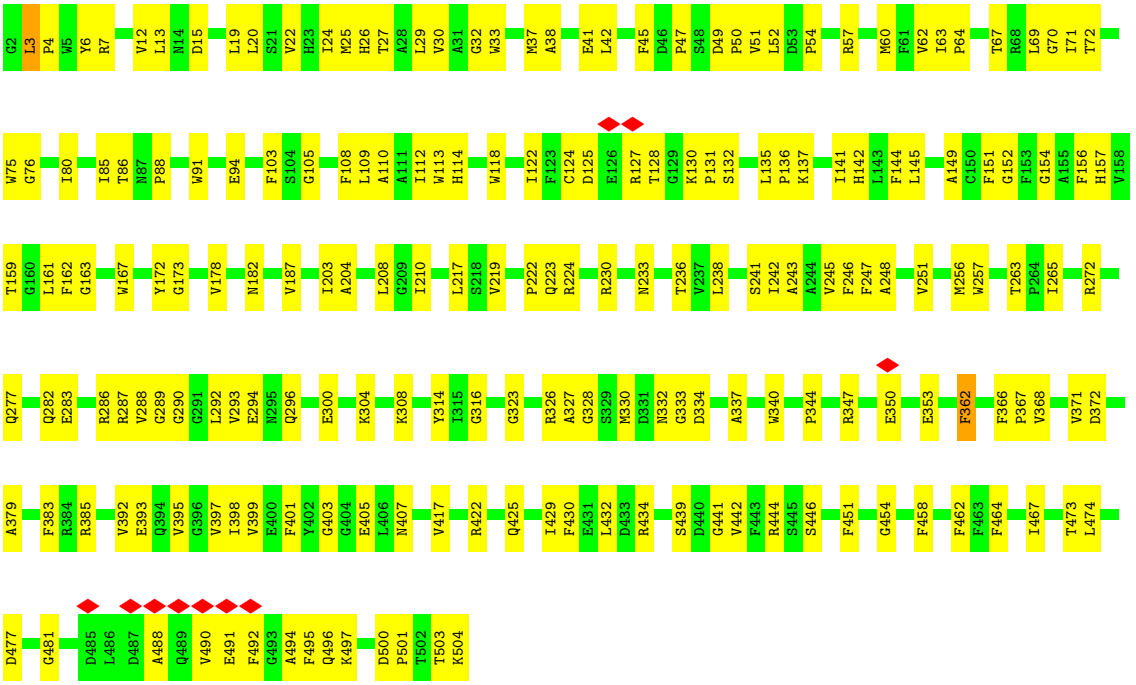




• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:

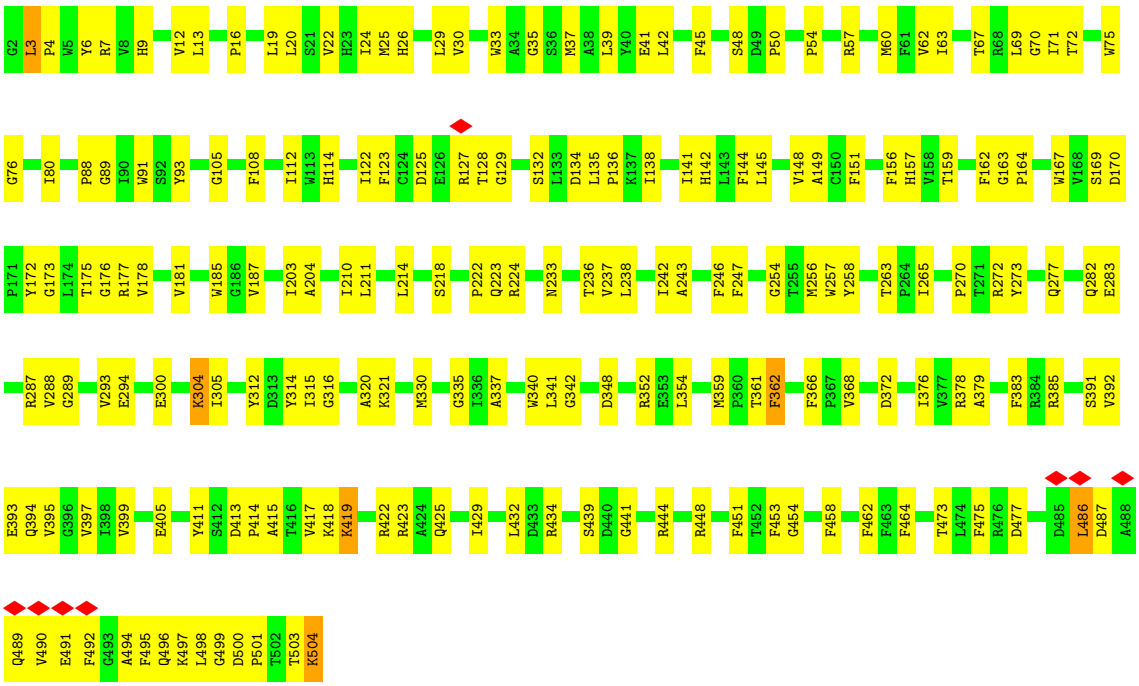




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

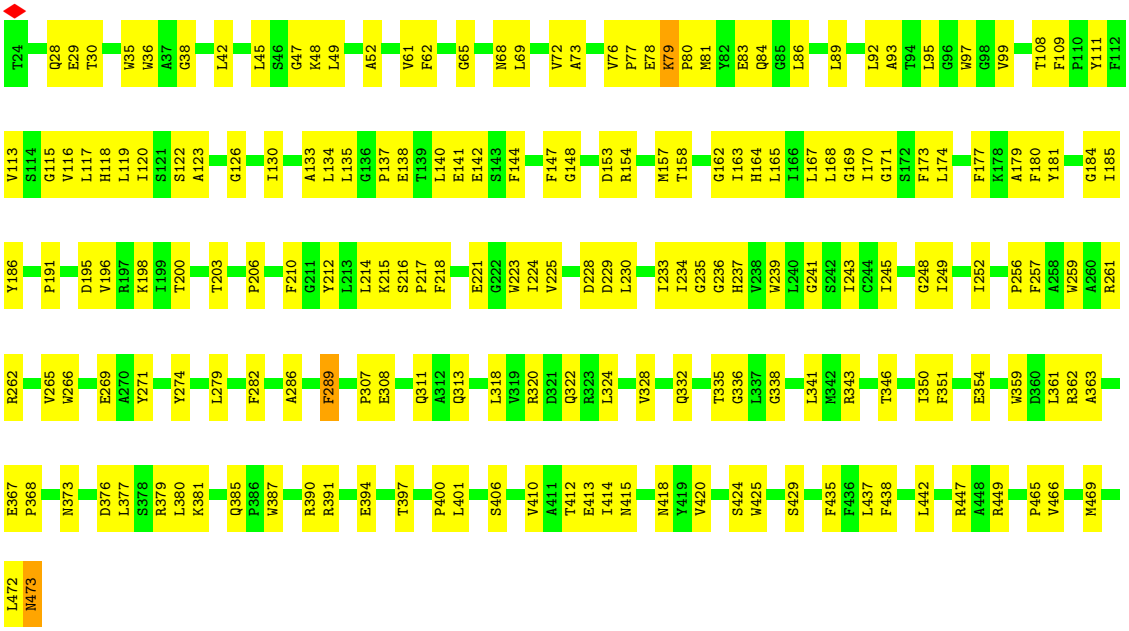




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

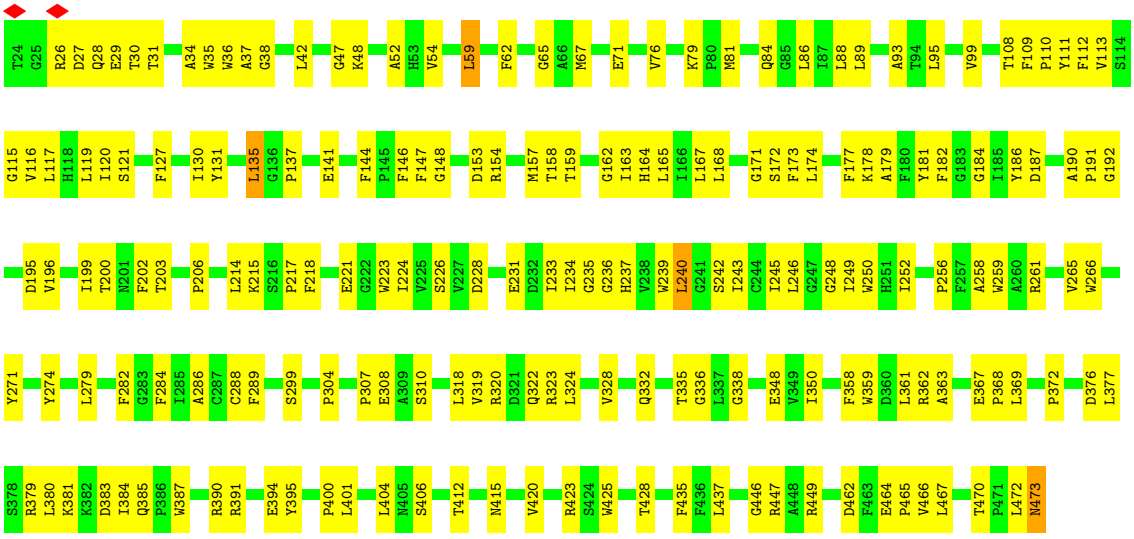




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

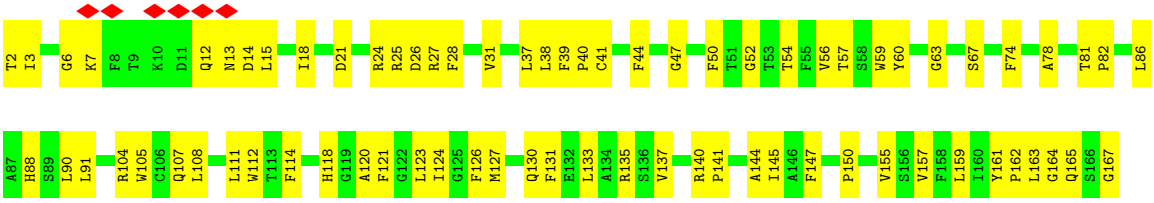




• Molecule 4: Photosystem II D2 protein

Chain D:



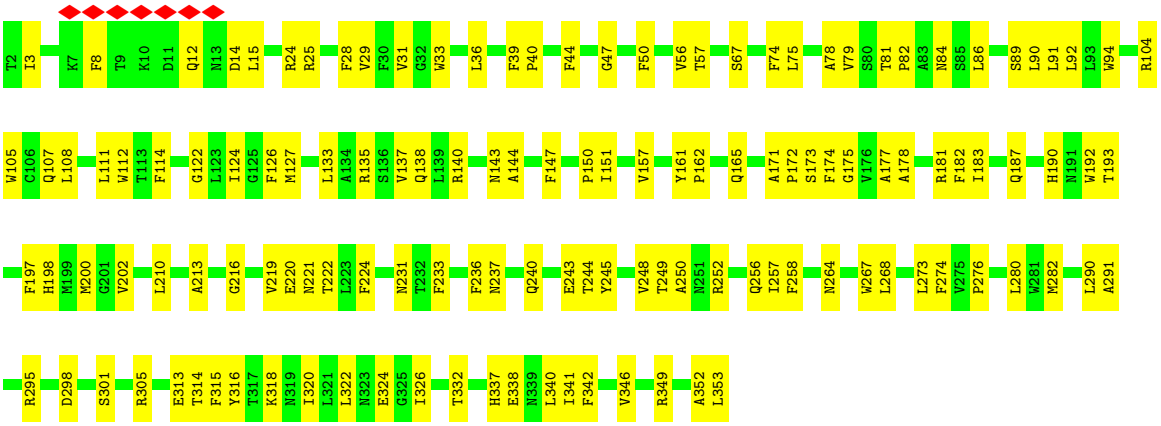




• Molecule 4: Photosystem II D2 protein

Chain d:

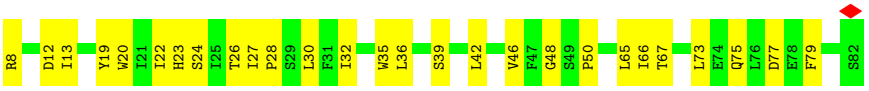




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

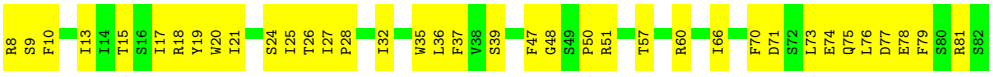




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

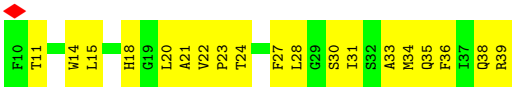




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

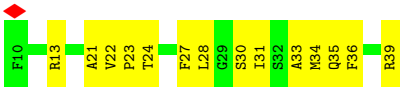




• Molecule 6: Cytochrome b559 subunit beta

Chain f:

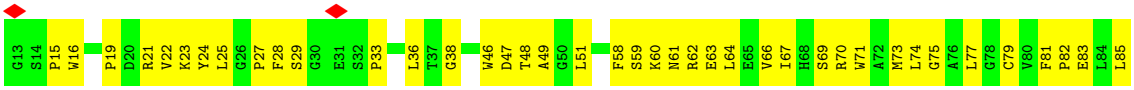




• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain G:





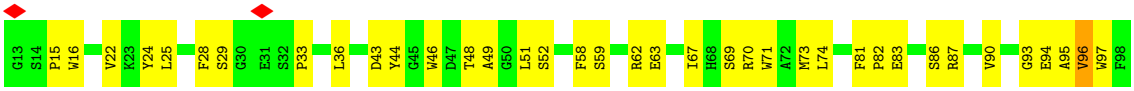


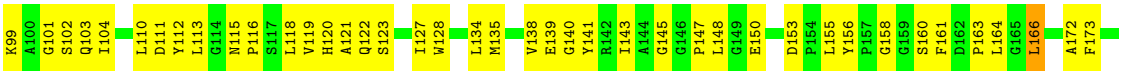


• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain N:





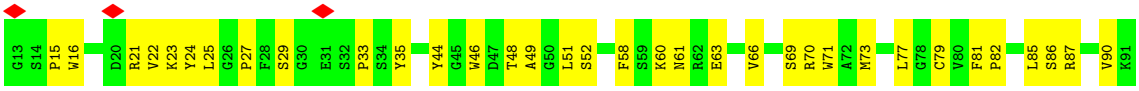


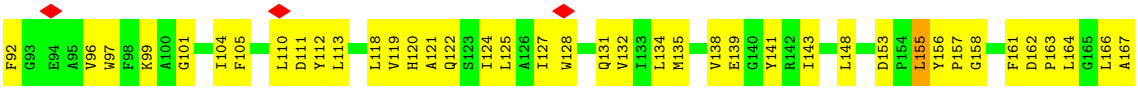


• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain g:



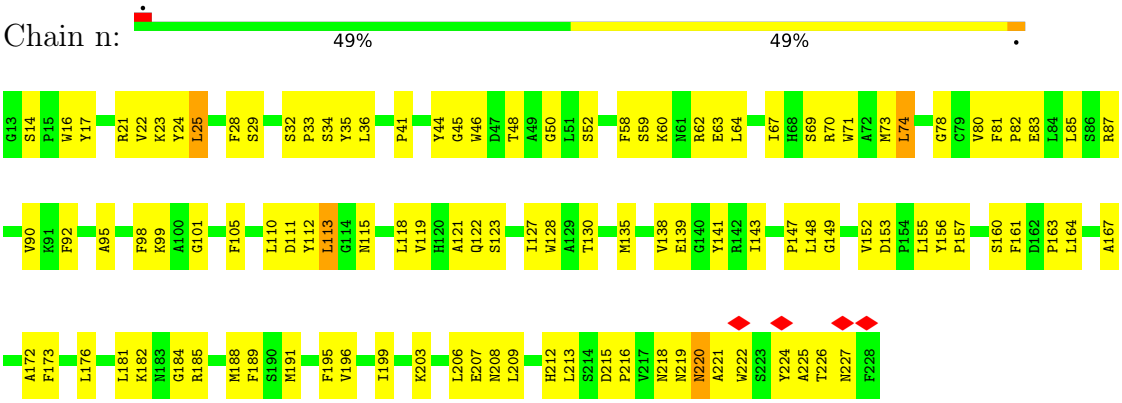






• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

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:



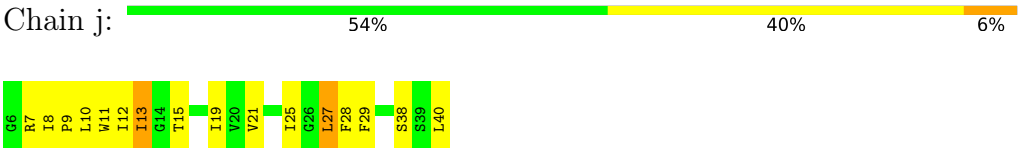
• Molecule 10: Photosystem II reaction center protein J

Chain J:



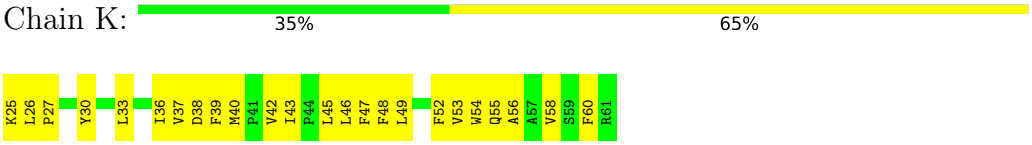
• Molecule 10: Photosystem II reaction center protein J

Chain j:



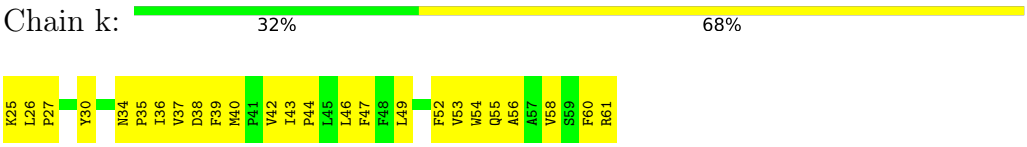
• Molecule 11: Photosystem II reaction center protein K

Chain K:



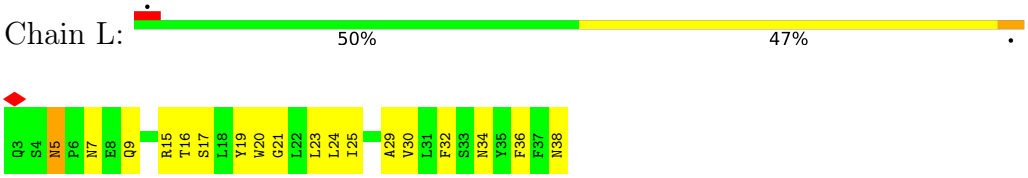
• Molecule 11: Photosystem II reaction center protein K

Chain k:



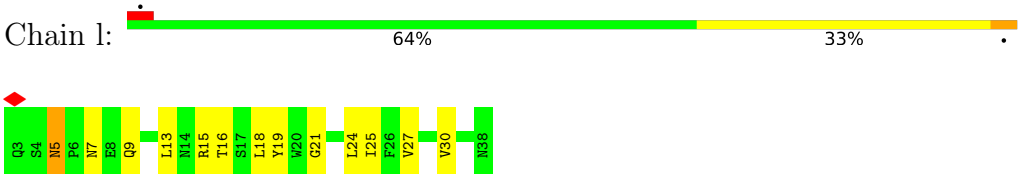
• Molecule 12: Photosystem II reaction center protein L

Chain L:



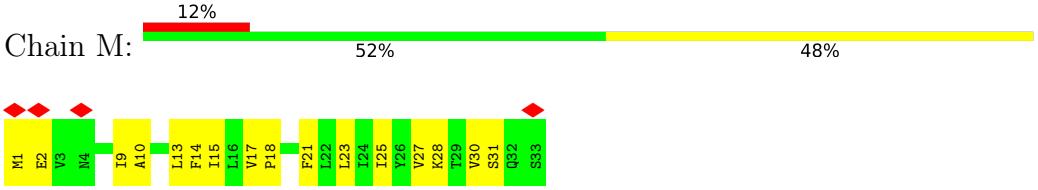
• Molecule 12: Photosystem II reaction center protein L

Chain l:



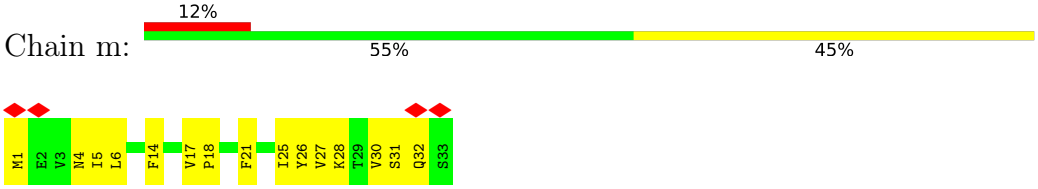
• Molecule 13: Photosystem II reaction center protein M

Chain M:



• Molecule 13: Photosystem II reaction center protein M

Chain m:



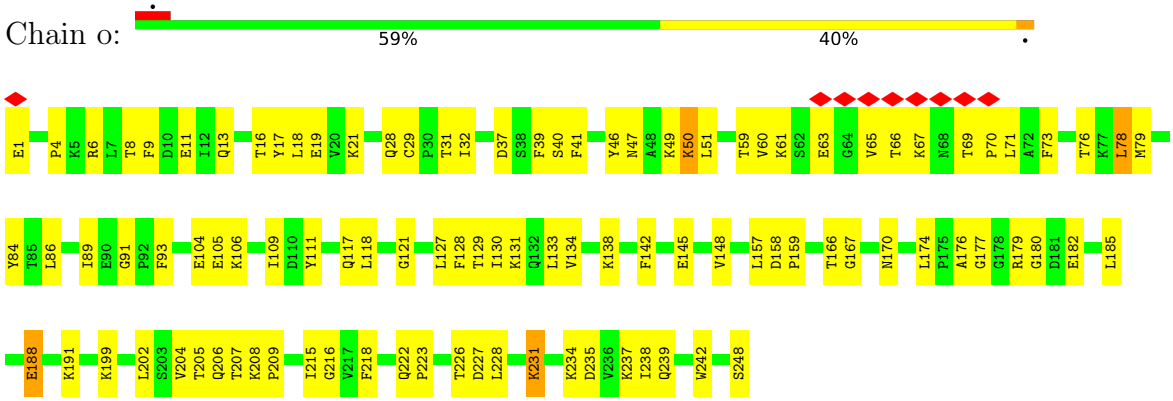
• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:



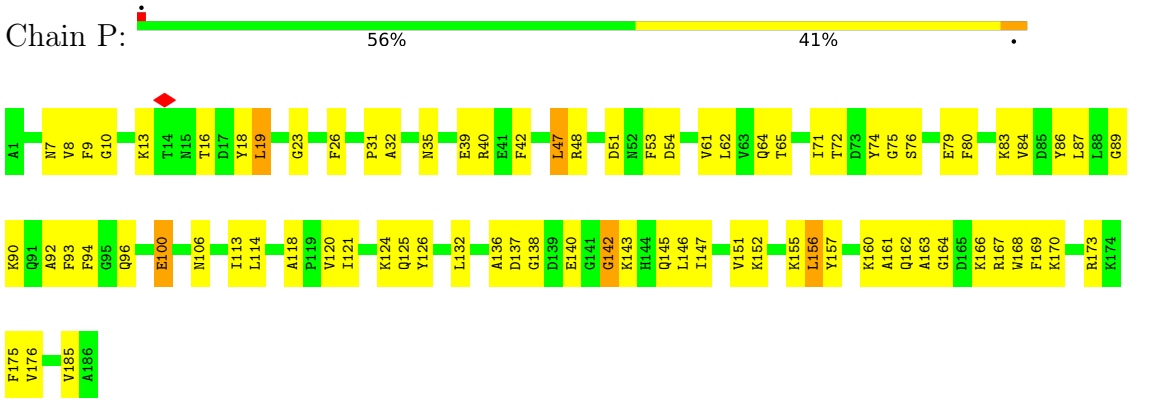
• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:



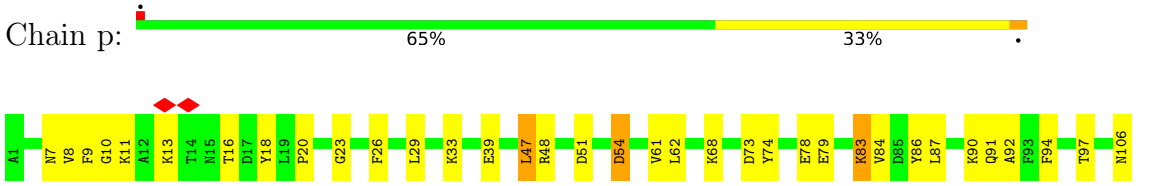
• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

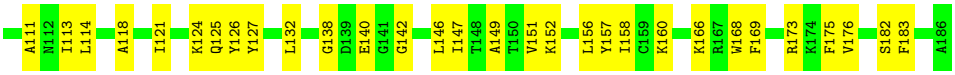
Chain P:



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

Chain p:

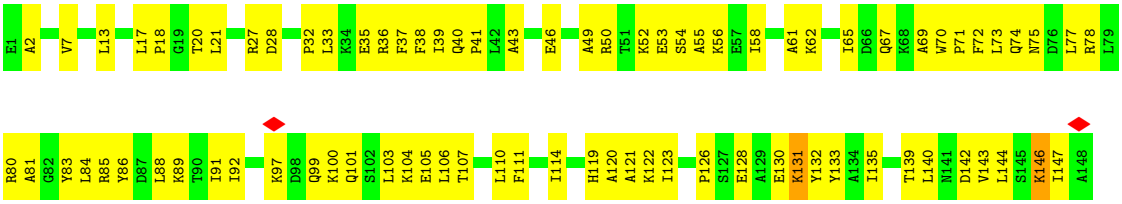




• Molecule 16: Oxygen-evolving enhancer protein 3

Chain Q:

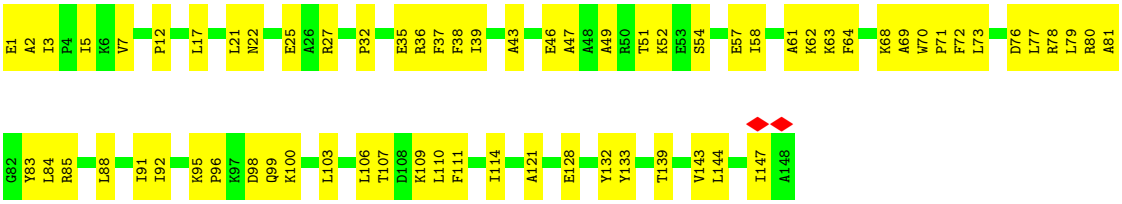




• Molecule 16: Oxygen-evolving enhancer protein 3

Chain q:

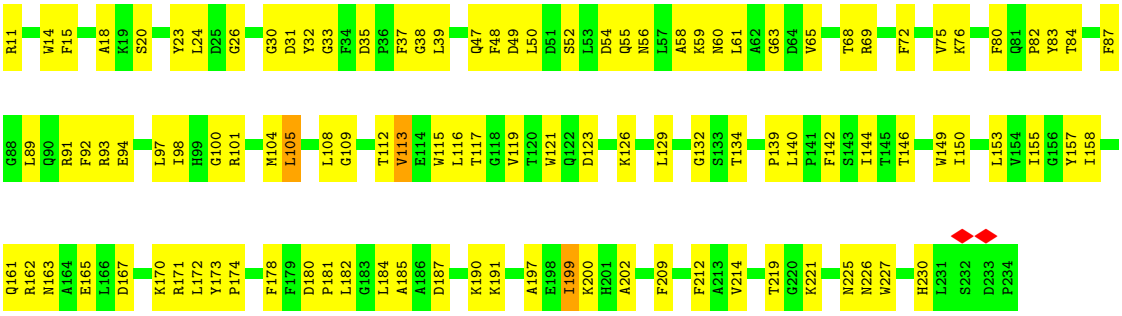




• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain R:



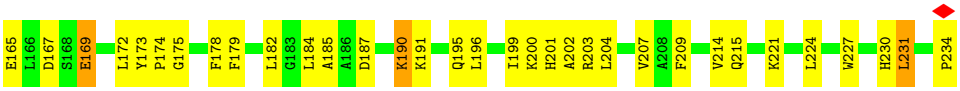


• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain r:

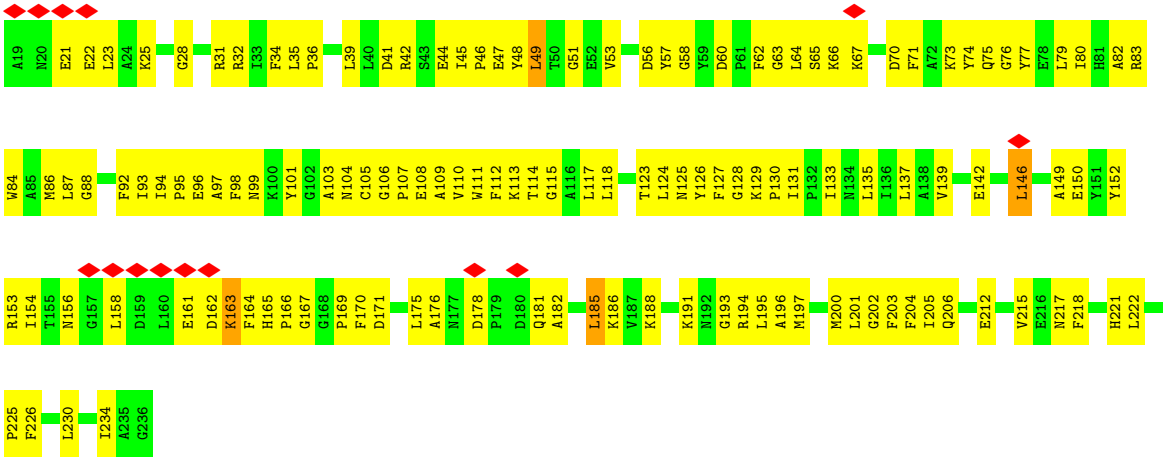






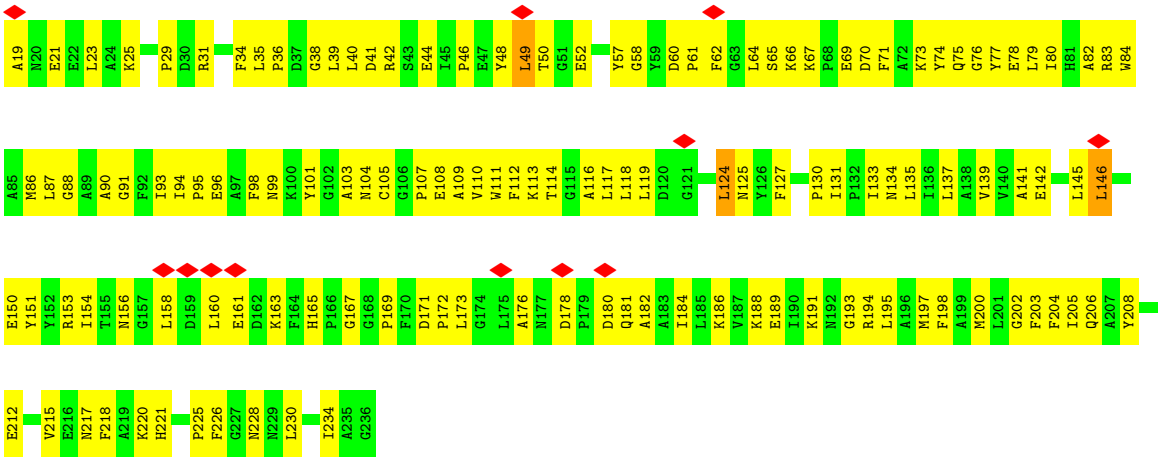
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic





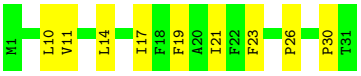
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic





• Molecule 19: Photosystem II reaction center protein T





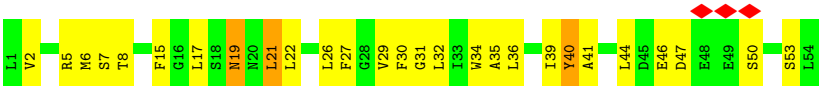
• Molecule 19: Photosystem II reaction center protein T





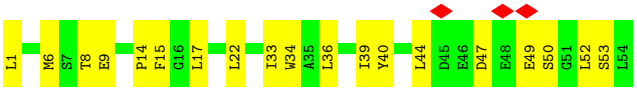
• Molecule 20: Photosystem II reaction center protein W





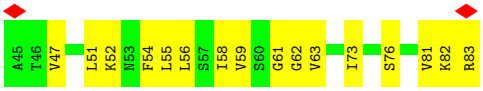
• Molecule 20: Photosystem II reaction center protein W





• Molecule 21: Ultraviolet-B-repressible protein





• Molecule 21: Ultraviolet-B-repressible protein





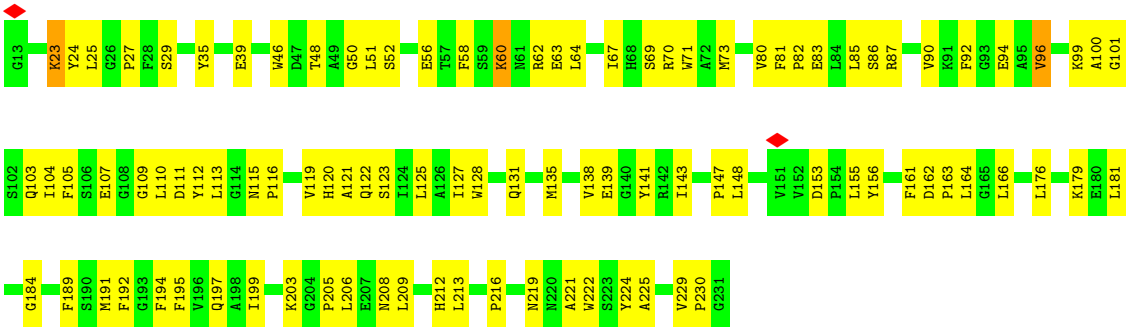
• Molecule 22: Chlorophyll a-b binding protein AB80, chloroplastic





• Molecule 22: Chlorophyll a-b binding protein AB80, chloroplastic

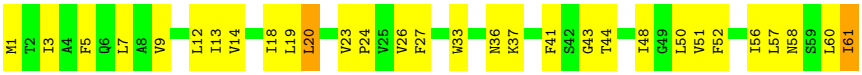




• Molecule 23: Photosystem II reaction center protein Z

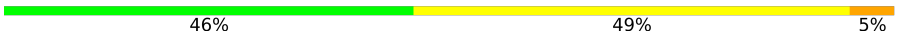
Chain Z:

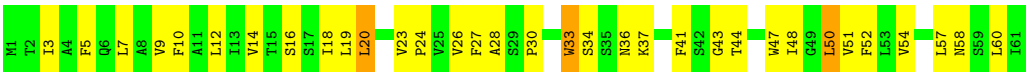




• Molecule 23: Photosystem II reaction center protein Z

Chain z:

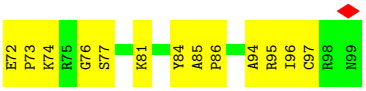




• Molecule 24: Photosystem II 5 kDa protein, chloroplastic

Chain U:

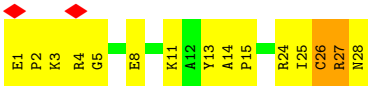




• Molecule 24: Photosystem II 5 kDa protein, chloroplastic

Chain u:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	200827	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.95	0/2697	1.13	0/3677
1	a	0.95	0/2697	1.12	1/3677 (0.0%)
2	B	0.95	0/4071	1.13	0/5542
2	b	0.95	0/4071	1.13	2/5542 (0.0%)
3	C	0.94	1/3614 (0.0%)	1.13	0/4922
3	c	0.94	0/3613	1.12	0/4920
4	D	0.92	0/2890	1.12	0/3938
4	d	0.92	0/2890	1.12	0/3938
5	E	0.93	0/630	1.13	0/857
5	e	0.92	0/630	1.14	0/857
6	F	0.92	0/248	1.14	0/335
6	f	0.92	0/248	1.14	0/335
7	G	0.93	0/1701	1.17	0/2315
7	N	0.93	0/1700	1.16	2/2313 (0.1%)
7	g	0.93	0/1701	1.16	0/2315
7	n	0.93	0/1701	1.18	1/2315 (0.0%)
8	H	0.97	0/461	1.18	0/626
8	h	0.96	0/461	1.15	0/626
9	I	0.91	0/286	1.13	0/386
9	i	0.91	0/286	1.14	0/386
10	J	0.95	0/262	1.19	0/354
10	j	0.94	0/262	1.20	0/354
11	K	0.90	0/318	1.05	0/434
11	k	0.90	0/318	1.06	0/434
12	L	0.89	0/312	1.06	0/424
12	l	0.90	0/312	1.05	0/424
13	M	0.94	0/260	1.18	0/355
13	m	0.94	0/260	1.14	0/355
14	O	0.99	0/1906	1.09	0/2575
14	o	0.99	0/1906	1.10	0/2575
15	P	0.97	0/1464	1.08	2/1978 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	p	0.98	0/1464	1.08	1/1978 (0.1%)
16	Q	0.95	0/1179	1.17	0/1591
16	q	0.96	0/1179	1.18	0/1591
17	R	0.93	0/1804	1.14	1/2456 (0.0%)
17	r	0.92	0/1804	1.15	0/2456
18	S	0.93	0/1737	1.14	0/2361
18	s	0.91	0/1737	1.15	0/2361
19	T	0.90	0/260	1.10	0/354
19	t	0.89	0/260	1.12	0/354
20	W	0.92	0/429	1.11	0/581
20	w	0.92	0/429	1.13	0/581
21	X	0.97	0/279	1.28	0/380
21	x	0.98	0/279	1.27	0/380
22	Y	0.93	0/1719	1.17	0/2341
22	y	0.94	0/1719	1.16	0/2341
23	Z	0.97	0/467	1.23	0/640
23	z	0.96	0/467	1.22	0/640
24	U	0.94	0/216	1.21	0/291
24	u	0.94	0/216	1.17	0/291
All	All	0.94	1/61820 (0.0%)	1.14	10/84052 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	76	VAL	N-CA	5.10	1.49	1.45

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	145	GLY	CA-C-O	-6.09	118.03	122.23
15	P	89	GLY	CA-C-O	-5.92	118.05	122.37
2	b	89	GLY	CA-C-O	-5.92	118.15	122.23
17	R	132	GLY	CA-C-O	-5.89	118.17	122.23
15	p	142	GLY	CA-C-O	-5.85	118.19	122.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2522	138	0
1	a	2616	0	2522	178	0
2	B	3939	0	3814	208	0
2	b	3939	0	3814	180	0
3	C	3497	0	3422	198	0
3	c	3496	0	3422	208	0
4	D	2797	0	2695	152	0
4	d	2797	0	2695	134	0
5	E	612	0	595	33	0
5	e	612	0	595	38	0
6	F	241	0	246	22	0
6	f	241	0	246	18	0
7	G	1650	0	1577	168	0
7	N	1649	0	1573	135	0
7	g	1650	0	1577	137	0
7	n	1650	0	1577	136	0
8	H	452	0	473	34	0
8	h	452	0	473	31	0
9	I	278	0	291	16	0
9	i	278	0	291	17	0
10	J	256	0	269	11	0
10	j	256	0	269	15	0
11	K	306	0	313	41	0
11	k	306	0	313	32	0
12	L	304	0	292	24	0
12	l	304	0	292	12	0
13	M	256	0	284	23	0
13	m	256	0	284	22	0
14	O	1870	0	1849	86	0
14	o	1870	0	1851	92	0
15	P	1434	0	1392	80	0
15	p	1434	0	1392	51	0
16	Q	1157	0	1210	77	0
16	q	1157	0	1210	63	0
17	R	1755	0	1722	110	0
17	r	1755	0	1722	121	0
18	S	1688	0	1652	188	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	s	1688	0	1652	148	0
19	T	252	0	267	13	0
19	t	252	0	267	24	0
20	W	419	0	402	34	0
20	w	419	0	402	28	0
21	X	276	0	301	23	0
21	x	276	0	301	17	0
22	Y	1667	0	1596	120	0
22	y	1667	0	1596	110	0
23	Z	457	0	488	31	0
23	z	457	0	488	40	0
24	U	212	0	220	8	0
24	u	212	0	223	16	0
25	A	10	0	0	0	0
25	a	10	0	0	0	0
26	A	1	0	0	0	0
26	a	1	0	0	0	0
27	A	2	0	0	0	0
27	a	2	0	0	1	0
28	A	175	0	168	31	0
28	B	1040	0	1142	177	0
28	C	837	0	908	164	0
28	D	195	0	214	23	0
28	G	465	0	443	105	0
28	N	456	0	426	88	0
28	R	554	0	507	99	0
28	S	465	0	387	113	0
28	Y	463	0	440	79	0
28	a	175	0	169	32	0
28	b	1040	0	1144	176	0
28	c	808	0	837	127	0
28	d	195	0	214	34	0
28	g	440	0	402	81	0
28	n	465	0	450	97	0
28	r	563	0	524	107	0
28	s	465	0	387	84	0
28	y	473	0	463	88	0
29	A	64	0	74	9	0
29	D	64	0	74	9	0
29	a	64	0	74	12	0
29	d	64	0	74	12	0
30	A	40	0	56	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	120	0	168	51	0
30	C	120	0	168	50	0
30	D	40	0	56	11	0
30	H	40	0	56	14	0
30	K	40	0	56	13	0
30	T	40	0	56	13	0
30	a	40	0	56	22	0
30	b	120	0	168	34	0
30	c	80	0	112	30	0
30	d	40	0	56	20	0
30	h	40	0	56	19	0
30	i	40	0	56	8	0
30	k	40	0	56	16	0
30	t	40	0	56	10	0
31	A	104	0	143	23	0
31	B	54	0	77	12	0
31	L	96	0	124	21	0
31	M	42	0	47	5	0
31	a	104	0	143	30	0
32	A	88	0	116	31	0
32	B	82	0	104	23	0
32	C	95	0	130	24	0
32	D	46	0	62	15	0
32	a	40	0	50	14	0
32	b	101	0	145	22	0
32	c	51	0	72	15	0
32	d	46	0	62	20	0
32	k	51	0	72	15	0
32	w	48	0	66	13	0
33	A	13	0	7	0	0
33	D	55	0	80	8	0
33	a	13	0	7	0	0
33	d	55	0	80	6	0
34	A	4	0	0	0	0
34	d	4	0	0	0	0
35	A	43	0	56	4	0
35	B	117	0	150	30	0
35	C	49	0	74	11	0
35	D	49	0	74	13	0
35	G	49	0	74	7	0
35	L	49	0	74	6	0
35	N	31	0	32	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	R	25	0	20	5	0
35	S	77	0	97	26	0
35	W	49	0	74	20	0
35	Y	49	0	74	5	0
35	a	43	0	56	10	0
35	b	121	0	158	23	0
35	c	72	0	83	14	0
35	d	49	0	74	12	0
35	g	41	0	55	9	0
35	l	49	0	74	5	0
35	n	32	0	34	6	0
35	r	30	0	30	5	0
35	s	49	0	74	16	0
35	w	39	0	51	8	0
35	y	49	0	74	6	0
36	A	59	0	76	10	0
36	B	62	0	82	11	0
36	C	177	0	228	48	0
36	a	59	0	76	17	0
36	b	62	0	82	11	0
36	c	168	0	210	45	0
37	E	43	0	30	7	0
37	f	43	0	30	6	0
38	G	339	0	295	75	0
38	N	347	0	310	78	0
38	R	154	0	116	25	0
38	S	196	0	140	47	0
38	Y	362	0	345	93	0
38	g	412	0	378	99	0
38	n	350	0	317	86	0
38	r	183	0	171	37	0
38	s	196	0	140	36	0
38	y	296	0	276	67	0
39	G	84	0	112	39	0
39	N	84	0	112	27	0
39	R	42	0	56	14	0
39	S	84	0	112	43	0
39	Y	84	0	112	15	0
39	g	84	0	112	36	0
39	n	84	0	112	21	0
39	r	42	0	56	15	0
39	s	84	0	112	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	y	84	0	112	17	0
40	G	44	0	54	11	0
40	N	44	0	54	9	0
40	Y	44	0	54	9	0
40	g	44	0	55	9	0
40	n	44	0	54	8	0
40	r	44	0	54	13	0
40	s	44	0	54	7	0
40	y	88	0	108	10	0
41	R	44	0	56	13	0
41	Y	44	0	56	17	0
41	r	44	0	56	9	0
41	y	44	0	56	11	0
42	A	92	0	0	4	0
42	B	151	0	0	2	0
42	C	134	0	0	0	0
42	D	101	0	0	2	0
42	E	14	0	0	0	0
42	F	6	0	0	0	0
42	G	26	0	0	2	0
42	H	16	0	0	2	0
42	I	3	0	0	0	0
42	J	5	0	0	0	0
42	K	6	0	0	0	0
42	L	8	0	0	0	0
42	M	6	0	0	0	0
42	N	28	0	0	1	0
42	O	69	0	0	1	0
42	P	52	0	0	2	0
42	Q	28	0	0	2	0
42	R	40	0	0	3	0
42	S	24	0	0	3	0
42	T	7	0	0	2	0
42	U	1	0	0	0	0
42	W	11	0	0	0	0
42	X	10	0	0	0	0
42	Y	45	0	0	1	0
42	Z	6	0	0	0	0
42	a	100	0	0	5	0
42	b	167	0	0	1	0
42	c	128	0	0	2	0
42	d	85	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	e	21	0	0	1	0
42	f	3	0	0	0	0
42	g	23	0	0	0	0
42	h	14	0	0	0	0
42	i	2	0	0	0	0
42	j	4	0	0	0	0
42	k	4	0	0	1	0
42	l	8	0	0	0	0
42	m	2	0	0	0	0
42	n	23	0	0	2	0
42	o	67	0	0	0	0
42	p	43	0	0	1	0
42	q	18	0	0	0	0
42	r	33	0	0	1	0
42	s	19	0	0	1	0
42	t	3	0	0	0	0
42	u	4	0	0	0	0
42	w	11	0	0	0	0
42	x	7	0	0	0	0
42	y	31	0	0	1	0
42	z	2	0	0	0	0
All	All	79416	0	77862	5285	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 34.

The worst 5 of 5285 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)
28:B:601:CLA:H152	30:H:101:BCR:H17C	1.34	1.09
16:Q:13:LEU:HD22	16:Q:18:PRO:HA	1.40	1.04
1:a:42:LEU:HB3	30:a:410:BCR:H353	1.38	1.04
36:a:401:DGD:HA92	32:a:413:LMG:H352	1.39	1.04
14:O:65:VAL:HA	14:O:71:LEU:HD21	1.39	1.03

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	332/334 (99%)	321 (97%)	10 (3%)	1 (0%)	36	42
1	a	332/334 (99%)	317 (96%)	14 (4%)	1 (0%)	36	42
2	B	501/503 (100%)	489 (98%)	12 (2%)	0	100	100
2	b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
3	C	448/450 (100%)	432 (96%)	16 (4%)	0	100	100
3	c	448/450 (100%)	429 (96%)	19 (4%)	0	100	100
4	D	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
4	d	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
5	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
5	e	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
6	F	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
6	f	28/30 (93%)	28 (100%)	0	0	100	100
7	G	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
7	N	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
7	g	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
7	n	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
8	H	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
8	h	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
10	J	33/35 (94%)	33 (100%)	0	0	100	100
10	j	33/35 (94%)	33 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	L	34/36 (94%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	34/36 (94%)	34 (100%)	0	0	100	100
13	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
13	m	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
14	O	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
14	o	246/248 (99%)	234 (95%)	12 (5%)	0	100	100
15	P	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
15	p	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
16	Q	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
16	q	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
17	R	222/224 (99%)	215 (97%)	7 (3%)	0	100	100
17	r	222/224 (99%)	216 (97%)	6 (3%)	0	100	100
18	S	216/218 (99%)	204 (94%)	11 (5%)	1 (0%)	24	27
18	s	216/218 (99%)	202 (94%)	14 (6%)	0	100	100
19	T	29/31 (94%)	29 (100%)	0	0	100	100
19	t	29/31 (94%)	29 (100%)	0	0	100	100
20	W	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
20	w	52/54 (96%)	52 (100%)	0	0	100	100
21	X	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
21	x	37/39 (95%)	37 (100%)	0	0	100	100
22	Y	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
22	y	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
23	Z	59/61 (97%)	59 (100%)	0	0	100	100
23	z	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
24	U	26/28 (93%)	26 (100%)	0	0	100	100
24	u	26/28 (93%)	26 (100%)	0	0	100	100
All	All	7634/7734 (99%)	7353 (96%)	278 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	S	161	GLU
1	a	141	PRO
1	A	141	PRO

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	270/270 (100%)	265 (98%)	5 (2%)	50 66
1	a	270/270 (100%)	262 (97%)	8 (3%)	36 49
2	B	399/399 (100%)	396 (99%)	3 (1%)	73 85
2	b	399/399 (100%)	391 (98%)	8 (2%)	48 64
3	C	352/352 (100%)	348 (99%)	4 (1%)	65 79
3	c	352/352 (100%)	345 (98%)	7 (2%)	48 64
4	D	284/284 (100%)	281 (99%)	3 (1%)	65 79
4	d	284/284 (100%)	281 (99%)	3 (1%)	65 79
5	E	67/67 (100%)	67 (100%)	0	100 100
5	e	67/67 (100%)	67 (100%)	0	100 100
6	F	25/25 (100%)	25 (100%)	0	100 100
6	f	25/25 (100%)	25 (100%)	0	100 100
7	G	169/169 (100%)	166 (98%)	3 (2%)	51 68
7	N	168/169 (99%)	162 (96%)	6 (4%)	31 42
7	g	169/169 (100%)	166 (98%)	3 (2%)	51 68
7	n	169/169 (100%)	161 (95%)	8 (5%)	23 31
8	H	49/49 (100%)	46 (94%)	3 (6%)	17 20
8	h	49/49 (100%)	49 (100%)	0	100 100
9	I	31/31 (100%)	31 (100%)	0	100 100
9	i	31/31 (100%)	30 (97%)	1 (3%)	34 47
10	J	26/26 (100%)	25 (96%)	1 (4%)	29 40
10	j	26/26 (100%)	24 (92%)	2 (8%)	12 13
11	K	32/32 (100%)	31 (97%)	1 (3%)	35 48
11	k	32/32 (100%)	32 (100%)	0	100 100
12	L	34/34 (100%)	33 (97%)	1 (3%)	37 51
12	l	34/34 (100%)	33 (97%)	1 (3%)	37 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	M	29/29 (100%)	29 (100%)	0	100 100
13	m	29/29 (100%)	29 (100%)	0	100 100
14	O	204/204 (100%)	201 (98%)	3 (2%)	57 73
14	o	204/204 (100%)	200 (98%)	4 (2%)	48 64
15	P	150/150 (100%)	145 (97%)	5 (3%)	33 45
15	p	150/150 (100%)	147 (98%)	3 (2%)	48 64
16	Q	125/125 (100%)	122 (98%)	3 (2%)	43 58
16	q	125/125 (100%)	124 (99%)	1 (1%)	73 85
17	R	181/181 (100%)	178 (98%)	3 (2%)	53 69
17	r	181/181 (100%)	174 (96%)	7 (4%)	28 39
18	S	169/169 (100%)	165 (98%)	4 (2%)	43 58
18	s	169/169 (100%)	164 (97%)	5 (3%)	36 49
19	T	28/28 (100%)	28 (100%)	0	100 100
19	t	28/28 (100%)	28 (100%)	0	100 100
20	W	44/44 (100%)	41 (93%)	3 (7%)	14 17
20	w	44/44 (100%)	43 (98%)	1 (2%)	44 59
21	X	32/32 (100%)	32 (100%)	0	100 100
21	x	32/32 (100%)	32 (100%)	0	100 100
22	Y	170/170 (100%)	166 (98%)	4 (2%)	43 58
22	y	170/170 (100%)	165 (97%)	5 (3%)	37 51
23	Z	53/53 (100%)	51 (96%)	2 (4%)	29 40
23	z	53/53 (100%)	50 (94%)	3 (6%)	18 23
24	U	23/23 (100%)	23 (100%)	0	100 100
24	u	23/23 (100%)	21 (91%)	2 (9%)	9 10
All	All	6229/6230 (100%)	6100 (98%)	129 (2%)	46 63

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	s	124	LEU
22	y	23	LYS
20	W	19	ASN
18	S	185	LEU
22	y	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
13	m	32	GLN
22	y	88	ASN
7	n	208	ASN
16	q	112	GLN
7	N	220	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 339 ligands modelled in this entry, 6 are monoatomic - leaving 333 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	$\#\|Z\| > 2$
28	CLA	r	612	17	64,68,73	1.40	7 (10%)	77,107,113	2.02	18 (23%)
30	BCR	K	101	-	41,41,41	4.77	27 (65%)	56,56,56	2.41	21 (37%)
38	CHL	R	607	42	65,69,74	0.80	2 (3%)	74,108,114	1.33	14 (18%)
32	LMG	A	413	-	40,40,55	0.92	3 (7%)	48,48,63	1.11	3 (6%)
38	CHL	N	609	7	68,72,74	0.80	2 (2%)	77,111,114	1.30	11 (14%)
36	DGD	B	626	-	63,63,67	1.13	6 (9%)	77,77,81	0.94	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LHG	l	101	-	48,48,48	0.42	0	51,54,54	1.09	2 (3%)
30	BCR	a	410	-	41,41,41	4.79	27 (65%)	56,56,56	2.31	21 (37%)
30	BCR	A	409	-	41,41,41	4.79	27 (65%)	56,56,56	2.23	18 (32%)
28	CLA	Y	602	22	69,73,73	1.43	7 (10%)	83,113,113	1.90	22 (26%)
28	CLA	s	603	18	49,53,73	1.60	7 (14%)	59,89,113	2.07	16 (27%)
28	CLA	G	610	7	68,72,73	1.36	6 (8%)	81,111,113	1.98	19 (23%)
33	PL9	a	412	-	13,13,55	1.47	1 (7%)	17,17,69	1.04	0
38	CHL	g	608	42	70,74,74	0.80	2 (2%)	80,114,114	1.35	14 (17%)
30	BCR	k	101	-	41,41,41	4.80	27 (65%)	56,56,56	2.31	19 (33%)
35	LHG	Y	619	28	48,48,48	0.47	1 (2%)	51,54,54	1.07	2 (3%)
28	CLA	d	405	4	69,73,73	1.36	6 (8%)	83,113,113	1.96	18 (21%)
28	CLA	C	513	3	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
28	CLA	s	604	42	54,58,73	1.52	6 (11%)	65,95,113	2.15	17 (26%)
28	CLA	B	606	2	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)
28	CLA	S	311	35	60,64,73	1.44	6 (10%)	72,102,113	2.09	20 (27%)
28	CLA	g	610	7	62,66,73	1.43	6 (9%)	74,104,113	2.26	22 (29%)
28	CLA	n	611	35	64,68,73	1.43	6 (9%)	77,107,113	2.03	22 (28%)
33	PL9	A	412	-	13,13,55	1.49	1 (7%)	17,17,69	1.02	0
38	CHL	r	605	42	70,74,74	0.81	2 (2%)	80,114,114	1.31	12 (15%)
28	CLA	b	616	2	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)
36	DGD	a	401	-	60,60,67	1.06	6 (10%)	74,74,81	0.92	2 (2%)
28	CLA	r	604	42,40	52,56,73	1.55	7 (13%)	62,92,113	2.12	17 (27%)
28	CLA	r	602	17	64,68,73	1.40	6 (9%)	77,107,113	1.98	20 (25%)
38	CHL	N	607	42	70,74,74	0.78	2 (2%)	80,114,114	1.26	13 (16%)
38	CHL	y	308	42	70,74,74	0.79	2 (2%)	80,114,114	1.30	14 (17%)
28	CLA	N	612	7	64,68,73	1.41	7 (10%)	77,107,113	1.97	19 (24%)
31	SQD	A	410	-	49,50,54	0.81	0	58,61,65	0.94	2 (3%)
28	CLA	G	614	7	52,56,73	1.55	6 (11%)	62,92,113	2.08	18 (29%)
28	CLA	b	603	-	69,73,73	1.35	6 (8%)	83,113,113	1.94	18 (21%)
28	CLA	d	401	42	69,73,73	1.36	6 (8%)	83,113,113	1.89	19 (22%)
38	CHL	n	601	7	58,62,74	0.86	2 (3%)	65,99,114	1.47	14 (21%)
28	CLA	s	602	18	65,69,73	1.39	7 (10%)	78,108,113	2.00	19 (24%)
28	CLA	G	604	40	54,58,73	1.53	7 (12%)	65,95,113	2.14	18 (27%)
37	HEM	E	101	5,6	50,50,50	1.56	8 (16%)	66,82,82	1.77	13 (19%)
41	XAT	y	317	-	39,47,47	0.67	0	54,74,74	1.87	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMG	A	411	-	48,48,55	0.99	5 (10%)	56,56,63	1.16	4 (7%)
39	LUT	S	315	-	42,43,43	6.07	27 (64%)	51,60,60	1.87	13 (25%)
36	DGD	A	417	-	60,60,67	1.07	6 (10%)	74,74,81	1.03	5 (6%)
35	LHG	a	415	-	42,42,48	0.40	0	45,48,54	1.09	3 (6%)
35	LHG	d	408	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
38	CHL	G	607	42	60,64,74	0.83	1 (1%)	68,102,114	1.35	14 (20%)
38	CHL	r	606	42	60,64,74	0.87	2 (3%)	68,102,114	1.39	13 (19%)
35	LHG	R	616	28	24,24,48	0.51	0	27,30,54	1.21	2 (7%)
38	CHL	N	605	7	52,56,74	0.90	2 (3%)	58,92,114	1.42	13 (22%)
35	LHG	G	618	28	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
30	BCR	B	617	-	41,41,41	4.80	27 (65%)	56,56,56	2.20	19 (33%)
31	SQD	L	103	-	53,54,54	0.79	0	62,65,65	0.92	3 (4%)
28	CLA	C	505	3	69,73,73	1.36	7 (10%)	83,113,113	1.90	18 (21%)
28	CLA	G	602	7	69,73,73	1.36	6 (8%)	83,113,113	1.96	21 (25%)
28	CLA	R	610	35	53,57,73	1.53	6 (11%)	62,93,113	2.17	16 (25%)
28	CLA	Y	611	35	64,68,73	1.40	6 (9%)	77,107,113	2.00	18 (23%)
28	CLA	B	608	2	69,73,73	1.35	7 (10%)	83,113,113	1.89	18 (21%)
38	CHL	s	606	42	62,66,74	0.82	1 (1%)	70,104,114	1.40	14 (20%)
28	CLA	G	611	35	64,68,73	1.40	6 (9%)	77,107,113	1.96	17 (22%)
28	CLA	G	613	-	69,73,73	1.35	7 (10%)	83,113,113	1.99	18 (21%)
28	CLA	b	608	2	69,73,73	1.35	7 (10%)	83,113,113	1.93	18 (21%)
31	SQD	B	620	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
36	DGD	C	517	-	56,56,67	1.00	4 (7%)	70,70,81	1.00	3 (4%)
32	LMG	C	522	-	44,44,55	0.86	3 (6%)	52,52,63	1.10	2 (3%)
28	CLA	g	602	7	69,73,73	1.34	6 (8%)	83,113,113	1.94	20 (24%)
28	CLA	c	513	3	61,65,73	1.44	6 (9%)	73,103,113	2.05	19 (26%)
38	CHL	Y	608	42	70,74,74	0.79	2 (2%)	80,114,114	1.29	13 (16%)
39	LUT	g	616	-	42,43,43	6.04	28 (66%)	51,60,60	2.02	14 (27%)
28	CLA	y	304	22	69,73,73	1.35	6 (8%)	83,113,113	1.98	20 (24%)
28	CLA	a	406	1	69,73,73	1.35	6 (8%)	83,113,113	1.89	18 (21%)
28	CLA	Y	604	42,40	54,58,73	1.53	7 (12%)	65,95,113	2.14	17 (26%)
32	LMG	k	102	-	51,51,55	1.07	5 (9%)	59,59,63	1.08	3 (5%)
30	BCR	b	617	-	41,41,41	4.80	27 (65%)	56,56,56	2.25	19 (33%)
35	LHG	b	621	-	33,33,48	0.45	0	36,39,54	1.13	3 (8%)
38	CHL	Y	605	22	52,56,74	0.90	1 (1%)	58,92,114	1.42	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LHG	D	407	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
38	CHL	G	605	7	50,54,74	0.91	2 (4%)	56,90,114	1.46	13 (23%)
35	LHG	g	618	28	40,40,48	0.41	0	43,46,54	1.14	3 (6%)
38	CHL	g	607	42	61,65,74	0.84	1 (1%)	69,103,114	1.35	14 (20%)
39	LUT	s	615	-	42,43,43	6.04	27 (64%)	51,60,60	2.18	15 (29%)
31	SQD	L	101	-	41,42,54	0.88	0	50,53,65	0.98	2 (4%)
28	CLA	B	610	42	69,73,73	1.35	6 (8%)	83,113,113	1.91	19 (22%)
32	LMG	C	520	-	51,51,55	1.07	6 (11%)	59,59,63	1.11	3 (5%)
32	LMG	c	521	-	51,51,55	1.07	6 (11%)	59,59,63	1.04	3 (5%)
40	NEX	N	617	28	38,46,46	3.37	11 (28%)	50,70,70	1.54	10 (20%)
28	CLA	r	603	17	64,68,73	1.41	7 (10%)	77,107,113	1.97	18 (23%)
28	CLA	b	610	42	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
38	CHL	r	607	42	65,69,74	0.80	2 (3%)	74,108,114	1.30	13 (17%)
32	LMG	D	408	-	46,46,55	0.93	4 (8%)	54,54,63	1.02	2 (3%)
28	CLA	B	615	2	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
31	SQD	a	411	-	49,50,54	0.81	0	58,61,65	0.96	2 (3%)
30	BCR	C	514	-	41,41,41	4.78	27 (65%)	56,56,56	3.63	27 (48%)
28	CLA	Y	603	22	59,63,73	1.45	7 (11%)	71,101,113	2.11	20 (28%)
28	CLA	c	501	3	69,73,73	1.36	6 (8%)	83,113,113	1.90	19 (22%)
28	CLA	G	603	7	57,61,73	1.49	7 (12%)	68,98,113	2.11	19 (27%)
35	LHG	b	624	-	45,45,48	0.40	0	48,51,54	1.12	4 (8%)
35	LHG	A	416	-	42,42,48	0.41	0	45,48,54	1.09	3 (6%)
38	CHL	G	608	42	70,74,74	0.80	2 (2%)	80,114,114	1.31	14 (17%)
28	CLA	r	613	17	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
30	BCR	b	619	-	41,41,41	4.72	26 (63%)	56,56,56	2.42	24 (42%)
28	CLA	B	614	2	69,73,73	1.35	7 (10%)	83,113,113	1.93	19 (22%)
28	CLA	C	507	42	69,73,73	1.36	6 (8%)	83,113,113	1.95	20 (24%)
28	CLA	s	612	18	59,63,73	1.45	6 (10%)	71,101,113	2.00	18 (25%)
40	NEX	G	617	28	38,46,46	3.50	11 (28%)	50,70,70	1.99	10 (20%)
28	CLA	a	409	1	64,68,73	1.40	6 (9%)	77,107,113	2.03	18 (23%)
28	CLA	b	605	2	69,73,73	1.40	6 (8%)	83,113,113	2.01	18 (21%)
28	CLA	b	614	2	69,73,73	1.35	7 (10%)	83,113,113	1.96	18 (21%)
28	CLA	R	609	17	69,73,73	1.35	7 (10%)	83,113,113	1.92	18 (21%)
28	CLA	n	604	42,40	54,58,73	1.54	7 (12%)	65,95,113	2.18	18 (27%)
28	CLA	y	312	22	64,68,73	1.40	7 (10%)	77,107,113	2.00	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	NEX	s	616	-	38,46,46	3.38	11 (28%)	50,70,70	1.58	9 (18%)
28	CLA	N	614	7	52,56,73	1.55	6 (11%)	62,92,113	2.09	18 (29%)
39	LUT	Y	615	-	42,43,43	5.92	29 (69%)	51,60,60	2.13	21 (41%)
28	CLA	s	611	-	53,57,73	1.54	7 (13%)	62,93,113	2.11	17 (27%)
39	LUT	G	615	-	42,43,43	6.09	27 (64%)	51,60,60	2.68	16 (31%)
35	LHG	N	618	28	30,30,48	0.48	0	33,36,54	1.38	4 (12%)
38	CHL	n	607	42	70,74,74	0.77	2 (2%)	80,114,114	1.20	14 (17%)
34	BCT	A	415	26	2,3,3	0.98	0	2,3,3	1.65	1 (50%)
28	CLA	C	504	42	69,73,73	1.35	6 (8%)	83,113,113	1.95	18 (21%)
35	LHG	S	317	28	42,42,48	0.41	0	45,48,54	1.09	3 (6%)
28	CLA	c	512	3	61,65,73	1.44	6 (9%)	73,103,113	2.08	19 (26%)
28	CLA	N	602	7	69,73,73	1.36	7 (10%)	83,113,113	1.97	19 (22%)
30	BCR	d	406	-	41,41,41	4.77	27 (65%)	56,56,56	2.52	20 (35%)
38	CHL	s	607	-	50,54,74	0.92	1 (2%)	56,90,114	1.48	11 (19%)
28	CLA	c	510	3	69,73,73	1.35	7 (10%)	83,113,113	1.95	17 (20%)
30	BCR	h	101	-	41,41,41	4.83	27 (65%)	56,56,56	2.25	19 (33%)
28	CLA	C	511	3	69,73,73	1.35	6 (8%)	83,113,113	1.99	21 (25%)
28	CLA	r	601	17	53,57,73	1.54	7 (13%)	62,93,113	2.13	17 (27%)
28	CLA	B	602	2	69,73,73	1.35	7 (10%)	83,113,113	1.96	17 (20%)
38	CHL	n	609	7	70,74,74	0.78	1 (1%)	80,114,114	1.31	14 (17%)
28	CLA	y	303	22	69,73,73	1.36	6 (8%)	83,113,113	1.95	22 (26%)
28	CLA	b	606	2	69,73,73	1.35	7 (10%)	83,113,113	1.89	20 (24%)
40	NEX	y	301	-	38,46,46	3.46	11 (28%)	50,70,70	1.48	8 (16%)
28	CLA	b	602	2	69,73,73	1.35	7 (10%)	83,113,113	1.92	18 (21%)
28	CLA	C	502	-	69,73,73	1.35	7 (10%)	83,113,113	1.96	20 (24%)
28	CLA	B	613	2	69,73,73	1.35	6 (8%)	83,113,113	1.91	17 (20%)
38	CHL	S	308	-	50,54,74	0.92	2 (4%)	56,90,114	1.52	12 (21%)
28	CLA	R	613	17	69,73,73	1.34	6 (8%)	83,113,113	1.91	19 (22%)
38	CHL	g	601	7	70,74,74	0.76	2 (2%)	80,114,114	1.33	14 (17%)
40	NEX	g	617	-	38,46,46	3.42	11 (28%)	50,70,70	1.57	8 (16%)
35	LHG	B	622	-	29,29,48	0.48	0	32,35,54	1.20	3 (9%)
28	CLA	D	403	4	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
35	LHG	y	319	28	48,48,48	0.48	1 (2%)	51,54,54	1.12	3 (5%)
35	LHG	b	622	-	40,40,48	0.41	0	43,46,54	1.11	3 (6%)
28	CLA	c	511	3	69,73,73	1.35	6 (8%)	83,113,113	1.95	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	r	610	35	53,57,73	1.54	6 (11%)	62,93,113	2.16	17 (27%)
37	HEM	f	101	5,6	50,50,50	1.56	8 (16%)	66,82,82	1.71	12 (18%)
28	CLA	a	407	42	54,58,73	1.52	6 (11%)	65,95,113	2.13	18 (27%)
36	DGD	c	516	-	56,56,67	0.99	4 (7%)	70,70,81	0.97	3 (4%)
28	CLA	y	305	42	54,58,73	1.53	7 (12%)	65,95,113	2.13	17 (26%)
28	CLA	B	607	42	69,73,73	1.35	6 (8%)	83,113,113	1.94	17 (20%)
30	BCR	B	619	-	41,41,41	4.80	27 (65%)	56,56,56	2.43	19 (33%)
35	LHG	S	301	-	33,33,48	0.46	0	36,39,54	1.13	3 (8%)
38	CHL	N	601	7	56,60,74	0.86	2 (3%)	63,97,114	1.49	14 (22%)
28	CLA	b	607	42	69,73,73	1.36	7 (10%)	83,113,113	1.94	20 (24%)
38	CHL	y	306	22	52,56,74	0.89	2 (3%)	58,92,114	1.39	12 (20%)
30	BCR	D	405	-	41,41,41	4.76	27 (65%)	56,56,56	2.51	20 (35%)
38	CHL	Y	607	42	70,74,74	0.80	3 (4%)	80,114,114	1.22	12 (15%)
28	CLA	Y	612	22	64,68,73	1.40	7 (10%)	77,107,113	1.98	18 (23%)
38	CHL	S	306	42	50,54,74	0.94	1 (2%)	56,90,114	1.47	12 (21%)
28	CLA	N	613	7	57,61,73	1.49	7 (12%)	68,98,113	2.07	18 (26%)
25	OEX	A	401	42,1,3	0,14,14	-	-	-		
38	CHL	g	606	42	54,58,74	0.95	1 (1%)	59,94,114	1.40	9 (15%)
38	CHL	y	307	42	54,58,74	0.90	1 (1%)	59,94,114	1.43	11 (18%)
28	CLA	S	303	18	65,69,73	1.39	7 (10%)	78,108,113	2.00	18 (23%)
28	CLA	G	612	-	64,68,73	1.40	6 (9%)	77,107,113	2.04	19 (24%)
38	CHL	R	605	42	51,55,74	0.94	1 (1%)	57,91,114	1.43	11 (19%)
28	CLA	c	504	42	63,67,73	1.42	6 (9%)	75,105,113	1.96	20 (26%)
39	LUT	g	615	-	42,43,43	6.08	28 (66%)	51,60,60	1.94	12 (23%)
32	LMG	b	620	-	51,51,55	1.07	6 (11%)	59,59,63	1.04	3 (5%)
25	OEX	a	402	42,1,3	0,14,14	-	-	-		
28	CLA	C	512	3	61,65,73	1.43	6 (9%)	73,103,113	2.02	20 (27%)
28	CLA	N	604	42,40	54,58,73	1.52	5 (9%)	65,95,113	2.18	18 (27%)
30	BCR	c	515	-	41,41,41	4.81	27 (65%)	56,56,56	2.26	20 (35%)
29	PHO	A	407	-	58,69,69	0.79	2 (3%)	56,99,99	0.95	3 (5%)
38	CHL	S	302	18	50,54,74	0.95	2 (4%)	56,90,114	1.46	12 (21%)
28	CLA	g	614	7	49,53,73	1.60	7 (14%)	59,89,113	2.12	16 (27%)
35	LHG	C	521	-	48,48,48	0.38	0	51,54,54	1.09	3 (5%)
28	CLA	A	405	1	69,73,73	1.35	6 (8%)	83,113,113	1.88	18 (21%)
39	LUT	N	615	-	42,43,43	6.06	28 (66%)	51,60,60	1.92	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LUT	y	315	-	42,43,43	6.09	28 (66%)	51,60,60	1.79	15 (29%)
36	DGD	C	518	-	63,63,67	1.12	7 (11%)	77,77,81	0.91	3 (3%)
38	CHL	y	309	22	70,74,74	0.80	2 (2%)	80,114,114	1.33	13 (16%)
39	LUT	G	616	-	42,43,43	6.01	27 (64%)	51,60,60	2.15	13 (25%)
28	CLA	r	608	17	62,66,73	1.42	6 (9%)	74,104,113	2.05	17 (22%)
41	XAT	R	615	-	39,47,47	0.65	0	54,74,74	1.89	15 (27%)
28	CLA	Y	610	22	64,68,73	1.44	6 (9%)	77,107,113	1.97	20 (25%)
39	LUT	r	614	-	42,43,43	6.08	28 (66%)	51,60,60	3.37	21 (41%)
30	BCR	t	101	-	41,41,41	4.78	27 (65%)	56,56,56	2.56	23 (41%)
28	CLA	B	604	2	69,73,73	1.36	7 (10%)	83,113,113	1.96	19 (22%)
35	LHG	r	617	28	29,29,48	0.48	0	32,35,54	1.35	4 (12%)
28	CLA	n	612	7	64,68,73	1.42	6 (9%)	77,107,113	1.99	18 (23%)
30	BCR	C	515	-	41,41,41	4.81	27 (65%)	56,56,56	2.30	20 (35%)
30	BCR	i	101	-	41,41,41	4.81	27 (65%)	56,56,56	2.43	22 (39%)
32	LMG	a	413	-	40,40,55	0.91	3 (7%)	48,48,63	1.09	4 (8%)
31	SQD	A	414	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
29	PHO	d	402	-	58,69,69	0.78	2 (3%)	56,99,99	0.97	3 (5%)
28	CLA	g	613	7	56,60,73	1.49	5 (8%)	67,97,113	2.20	19 (28%)
38	CHL	G	609	7	59,63,74	0.86	2 (3%)	66,100,114	1.47	13 (19%)
38	CHL	g	619	42	70,74,74	0.79	2 (2%)	80,114,114	1.28	14 (17%)
33	PL9	d	407	-	55,55,55	0.69	1 (1%)	68,69,69	0.61	1 (1%)
36	DGD	C	519	-	61,61,67	1.08	6 (9%)	75,75,81	0.93	3 (4%)
40	NEX	Y	618	28	38,46,46	3.33	11 (28%)	50,70,70	1.53	9 (18%)
35	LHG	B	625	-	45,45,48	0.41	0	48,51,54	1.01	3 (6%)
38	CHL	R	606	42	50,54,74	0.93	1 (2%)	56,90,114	1.49	11 (19%)
28	CLA	A	406	42	54,58,73	1.53	6 (11%)	65,95,113	2.14	18 (27%)
28	CLA	s	608	-	49,53,73	1.60	6 (12%)	59,89,113	2.07	16 (27%)
38	CHL	n	608	42	70,74,74	0.78	2 (2%)	80,114,114	1.33	14 (17%)
39	LUT	R	614	-	42,43,43	6.05	28 (66%)	51,60,60	2.26	19 (37%)
28	CLA	C	503	-	69,73,73	1.35	6 (8%)	83,113,113	1.96	19 (22%)
35	LHG	s	617	28	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
28	CLA	n	610	7	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
28	CLA	s	613	18	53,57,73	1.54	6 (11%)	62,93,113	2.15	18 (29%)
32	LMG	b	623	-	50,50,55	1.03	5 (10%)	58,58,63	0.96	2 (3%)
28	CLA	N	610	7	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	S	312	18	53,57,73	1.54	7 (13%)	62,93,113	2.14	16 (25%)
28	CLA	Y	614	22	52,56,73	1.55	5 (9%)	62,92,113	2.10	17 (27%)
35	LHG	L	102	-	48,48,48	0.38	0	51,54,54	0.98	2 (3%)
38	CHL	Y	606	42	54,58,74	0.91	1 (1%)	59,94,114	1.43	12 (20%)
28	CLA	R	603	17	64,68,73	1.44	6 (9%)	77,107,113	1.98	19 (24%)
35	LHG	n	618	28	31,31,48	0.50	0	34,37,54	1.18	2 (5%)
39	LUT	S	316	-	42,43,43	6.11	28 (66%)	51,60,60	2.07	13 (25%)
38	CHL	N	608	42	70,74,74	0.79	2 (2%)	80,114,114	1.31	14 (17%)
28	CLA	R	612	17	59,63,73	1.47	7 (11%)	71,101,113	2.09	19 (26%)
28	CLA	S	310	18	59,63,73	1.47	7 (11%)	71,101,113	2.09	21 (29%)
38	CHL	g	609	-	65,69,74	0.82	2 (3%)	74,108,114	1.41	14 (18%)
28	CLA	r	611	17	53,57,73	1.61	5 (9%)	62,93,113	2.27	18 (29%)
28	CLA	N	611	35	64,68,73	1.40	7 (10%)	77,107,113	1.95	18 (23%)
28	CLA	y	314	22	52,56,73	1.55	7 (13%)	62,92,113	2.08	17 (27%)
38	CHL	g	605	7	50,54,74	0.91	2 (4%)	56,90,114	1.44	12 (21%)
28	CLA	d	404	4	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
28	CLA	R	611	17	53,57,73	1.54	6 (11%)	62,93,113	2.19	18 (29%)
28	CLA	R	601	17	49,53,73	1.61	6 (12%)	59,89,113	2.12	15 (25%)
28	CLA	S	304	18	49,53,73	1.59	6 (12%)	59,89,113	2.11	17 (28%)
28	CLA	C	501	3	69,73,73	1.36	6 (8%)	83,113,113	1.89	19 (22%)
39	LUT	y	316	-	42,43,43	6.09	28 (66%)	51,60,60	1.94	14 (27%)
28	CLA	b	615	2	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
28	CLA	B	603	2	69,73,73	1.35	6 (8%)	83,113,113	1.89	18 (21%)
29	PHO	D	402	-	58,69,69	0.78	3 (5%)	56,99,99	0.96	3 (5%)
29	PHO	a	408	-	58,69,69	0.79	2 (3%)	56,99,99	0.96	3 (5%)
28	CLA	B	612	2	69,73,73	1.35	6 (8%)	83,113,113	1.94	18 (21%)
28	CLA	B	616	2	69,73,73	1.36	7 (10%)	83,113,113	1.92	19 (22%)
38	CHL	s	605	42	50,54,74	0.93	1 (2%)	56,90,114	1.49	12 (21%)
35	LHG	c	519	-	30,30,48	0.47	0	32,35,54	1.26	3 (9%)
28	CLA	Y	613	22	69,73,73	1.35	7 (10%)	83,113,113	1.89	19 (22%)
34	BCT	d	403	26	2,3,3	0.98	0	2,3,3	1.67	1 (50%)
28	CLA	g	603	7	69,73,73	1.36	6 (8%)	83,113,113	1.91	18 (21%)
38	CHL	s	601	18	50,54,74	0.93	2 (4%)	56,90,114	1.44	12 (21%)
28	CLA	S	314	18	53,57,73	1.54	7 (13%)	62,93,113	2.15	17 (27%)
30	BCR	C	516	-	41,41,41	4.80	27 (65%)	56,56,56	2.44	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	B	611	2	69,73,73	1.36	6 (8%)	83,113,113	1.94	19 (22%)
32	LMG	w	101	-	48,48,55	0.99	5 (10%)	56,56,63	1.17	3 (5%)
35	LHG	w	102	-	38,38,48	0.43	0	41,44,54	1.04	3 (7%)
35	LHG	W	101	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
28	CLA	b	611	2	69,73,73	1.36	6 (8%)	83,113,113	1.94	20 (24%)
30	BCR	c	514	-	41,41,41	4.77	27 (65%)	56,56,56	2.54	21 (37%)
28	CLA	c	503	3	69,73,73	1.36	6 (8%)	83,113,113	1.91	19 (22%)
41	XAT	Y	617	-	39,47,47	0.66	0	54,74,74	1.99	13 (24%)
41	XAT	r	615	-	39,47,47	0.64	0	54,74,74	1.90	15 (27%)
28	CLA	S	309	18	49,53,73	1.60	5 (10%)	59,89,113	2.11	16 (27%)
33	PL9	D	406	-	55,55,55	0.69	1 (1%)	68,69,69	0.60	1 (1%)
28	CLA	c	508	3	69,73,73	1.37	6 (8%)	83,113,113	1.94	19 (22%)
28	CLA	N	603	7	59,63,73	1.45	7 (11%)	71,101,113	2.07	17 (23%)
28	CLA	S	313	18	59,63,73	1.46	6 (10%)	71,101,113	2.01	18 (25%)
28	CLA	n	603	7	69,73,73	1.35	7 (10%)	83,113,113	2.01	19 (22%)
28	CLA	c	509	3	69,73,73	1.38	6 (8%)	83,113,113	1.99	18 (21%)
38	CHL	G	606	42	54,58,74	0.93	2 (3%)	59,94,114	1.42	10 (16%)
28	CLA	B	605	2	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
28	CLA	b	612	2	69,73,73	1.34	6 (8%)	83,113,113	1.98	18 (21%)
28	CLA	R	604	42	52,56,73	1.60	9 (17%)	62,92,113	2.16	18 (29%)
28	CLA	R	602	17	64,68,73	1.45	6 (9%)	77,107,113	1.98	20 (25%)
28	CLA	b	609	-	69,73,73	1.35	6 (8%)	83,113,113	1.97	17 (20%)
31	SQD	M	101	-	41,42,54	0.86	0	50,53,65	0.97	2 (4%)
28	CLA	B	601	42	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
30	BCR	T	101	-	41,41,41	4.76	26 (63%)	56,56,56	2.58	20 (35%)
39	LUT	Y	616	-	42,43,43	6.09	28 (66%)	51,60,60	1.82	12 (23%)
40	NEX	n	617	28	38,46,46	3.44	11 (28%)	50,70,70	1.74	9 (18%)
28	CLA	D	404	4	69,73,73	1.35	6 (8%)	83,113,113	2.00	19 (22%)
28	CLA	y	313	22	69,73,73	1.35	7 (10%)	83,113,113	1.95	18 (21%)
28	CLA	b	613	2	69,73,73	1.36	6 (8%)	83,113,113	1.90	18 (21%)
28	CLA	n	613	7	59,63,73	1.48	6 (10%)	71,101,113	2.14	17 (23%)
28	CLA	r	609	17	69,73,73	1.35	7 (10%)	83,113,113	1.96	20 (24%)
38	CHL	Y	601	22	70,74,74	0.79	2 (2%)	80,114,114	1.34	13 (16%)
28	CLA	y	310	22	64,68,73	1.40	6 (9%)	77,107,113	2.01	20 (25%)
28	CLA	y	311	35	64,68,73	1.40	6 (9%)	77,107,113	1.98	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	S	305	42	54,58,73	1.56	6 (11%)	65,95,113	2.17	21 (32%)
39	LUT	n	615	-	42,43,43	6.08	28 (66%)	51,60,60	2.00	17 (33%)
28	CLA	c	505	3	61,65,73	1.44	7 (11%)	73,103,113	2.00	18 (24%)
28	CLA	b	604	2	69,73,73	1.36	7 (10%)	83,113,113	2.00	19 (22%)
38	CHL	G	601	7	70,74,74	0.76	2 (2%)	80,114,114	1.28	15 (18%)
32	LMG	d	409	-	46,46,55	0.92	3 (6%)	54,54,63	1.03	3 (5%)
31	SQD	a	414	-	53,54,54	0.78	0	62,65,65	0.91	2 (3%)
28	CLA	B	609	2	69,73,73	1.35	6 (8%)	83,113,113	1.95	18 (21%)
35	LHG	c	520	-	39,39,48	0.42	0	42,45,54	1.19	3 (7%)
30	BCR	b	618	-	41,41,41	4.81	27 (65%)	56,56,56	2.22	19 (33%)
28	CLA	b	601	42	69,73,73	1.35	6 (8%)	83,113,113	1.96	20 (24%)
28	CLA	g	604	42	54,58,73	1.58	7 (12%)	65,95,113	2.20	18 (27%)
28	CLA	g	612	7	49,53,73	1.60	7 (14%)	59,89,113	2.08	17 (28%)
38	CHL	Y	609	22	70,74,74	0.80	2 (2%)	80,114,114	1.35	14 (17%)
28	CLA	c	502	3	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
36	DGD	c	518	-	60,60,67	4.56	7 (11%)	74,74,81	1.17	4 (5%)
32	LMG	B	621	-	51,51,55	1.07	6 (11%)	59,59,63	1.23	4 (6%)
28	CLA	g	611	35	64,68,73	1.43	6 (9%)	77,107,113	2.00	17 (22%)
32	LMG	B	624	-	31,31,55	0.53	0	39,39,63	1.29	3 (7%)
39	LUT	N	616	-	42,43,43	6.01	29 (69%)	51,60,60	2.12	17 (33%)
38	CHL	n	606	42	54,58,74	0.90	2 (3%)	59,94,114	1.43	13 (22%)
28	CLA	c	506	3	60,64,73	1.45	7 (11%)	72,102,113	2.03	19 (26%)
28	CLA	C	506	3	69,73,73	1.36	6 (8%)	83,113,113	1.93	18 (21%)
39	LUT	s	614	-	42,43,43	6.07	27 (64%)	51,60,60	2.08	15 (29%)
38	CHL	y	302	22	70,74,74	0.78	2 (2%)	80,114,114	1.30	14 (17%)
28	CLA	A	408	1	64,68,73	1.40	6 (9%)	77,107,113	1.97	16 (20%)
38	CHL	N	606	42	54,58,74	0.92	2 (3%)	59,94,114	1.46	11 (18%)
30	BCR	H	101	-	41,41,41	4.80	27 (65%)	56,56,56	2.42	21 (37%)
40	NEX	y	318	-	38,46,46	3.29	11 (28%)	50,70,70	1.73	11 (22%)
28	CLA	c	507	42	69,73,73	1.35	6 (8%)	83,113,113	1.98	18 (21%)
28	CLA	C	508	3	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
38	CHL	n	605	7	52,56,74	0.89	2 (3%)	58,92,114	1.42	13 (22%)
28	CLA	n	602	7	69,73,73	1.35	6 (8%)	83,113,113	1.94	19 (22%)
28	CLA	D	401	42	69,73,73	1.35	6 (8%)	83,113,113	1.89	20 (24%)
28	CLA	C	509	3	69,73,73	1.36	6 (8%)	83,113,113	1.92	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	s	609	18	59,63,73	1.47	6 (10%)	71,101,113	2.04	18 (25%)
30	BCR	B	618	-	41,41,41	4.81	27 (65%)	56,56,56	2.25	21 (37%)
40	NEX	r	616	28	38,46,46	3.35	11 (28%)	50,70,70	1.58	9 (18%)
28	CLA	C	510	3	69,73,73	1.34	6 (8%)	83,113,113	1.91	18 (21%)
28	CLA	s	610	35	60,64,73	1.45	6 (10%)	72,102,113	2.03	18 (25%)
39	LUT	n	616	-	42,43,43	5.99	28 (66%)	51,60,60	2.12	17 (33%)
36	DGD	b	625	-	63,63,67	1.12	6 (9%)	77,77,81	0.96	2 (2%)
36	DGD	c	517	-	55,55,67	1.00	3 (5%)	69,69,81	1.00	4 (5%)
28	CLA	n	614	7	49,53,73	1.60	6 (12%)	59,89,113	2.05	16 (27%)
28	CLA	R	608	17	62,66,73	1.42	5 (8%)	74,104,113	2.04	18 (24%)
35	LHG	B	623	-	40,40,48	0.42	0	43,46,54	1.09	3 (6%)
38	CHL	S	307	42	62,66,74	0.82	2 (3%)	70,104,114	1.35	14 (20%)

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
28	CLA	r	612	17	-	19/33/109/115	-
30	BCR	K	101	-	-	14/29/63/63	0/2/2/2
38	CHL	R	607	42	-	11/35/111/117	-
32	LMG	A	413	-	-	7/35/55/70	0/1/1/1
38	CHL	N	609	7	-	14/35/111/117	-
36	DGD	B	626	-	-	9/51/91/95	0/2/2/2
35	LHG	l	101	-	-	25/53/53/53	-
30	BCR	a	410	-	-	15/29/63/63	0/2/2/2
30	BCR	A	409	-	-	14/29/63/63	0/2/2/2
28	CLA	Y	602	22	-	12/39/115/115	-
28	CLA	s	603	18	-	7/15/91/115	-
28	CLA	G	610	7	-	13/38/114/115	-
33	PL9	a	412	-	-	0/5/18/73	0/1/1/1
38	CHL	g	608	42	-	14/41/117/117	-
30	BCR	k	101	-	-	13/29/63/63	0/2/2/2
35	LHG	Y	619	28	-	33/53/53/53	-
28	CLA	d	405	4	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	C	513	3	-	11/39/115/115	-
28	CLA	s	604	42	-	8/21/97/115	-
28	CLA	B	606	2	-	13/39/115/115	-
28	CLA	S	311	35	-	15/29/105/115	-
28	CLA	g	610	7	-	11/31/107/115	-
28	CLA	n	611	35	-	16/33/109/115	-
33	PL9	A	412	-	-	0/5/18/73	0/1/1/1
38	CHL	r	605	42	-	7/41/117/117	-
28	CLA	b	616	2	-	17/39/115/115	-
36	DGD	a	401	-	-	10/48/88/95	0/2/2/2
28	CLA	r	604	42,40	-	10/19/95/115	-
28	CLA	r	602	17	-	12/33/109/115	-
38	CHL	N	607	42	-	10/41/117/117	-
38	CHL	y	308	42	-	14/41/117/117	-
28	CLA	N	612	7	-	13/33/109/115	-
31	SQD	A	410	-	-	9/45/65/69	0/1/1/1
28	CLA	G	614	7	-	7/19/95/115	-
28	CLA	b	603	-	-	14/39/115/115	-
28	CLA	d	401	42	-	15/39/115/115	-
38	CHL	n	601	7	-	4/27/103/117	-
28	CLA	s	602	18	-	15/35/111/115	-
28	CLA	G	604	40	-	11/21/97/115	-
37	HEM	E	101	5,6	-	7/14/54/54	-
41	XAT	y	317	-	-	2/31/93/93	0/4/4/4
32	LMG	A	411	-	-	6/43/63/70	0/1/1/1
39	LUT	S	315	-	-	7/29/67/67	0/2/2/2
36	DGD	A	417	-	-	14/48/88/95	0/2/2/2
35	LHG	a	415	-	-	30/47/47/53	-
35	LHG	d	408	-	-	30/53/53/53	-
38	CHL	G	607	42	-	8/29/105/117	-
38	CHL	r	606	42	-	7/29/105/117	-
35	LHG	R	616	28	-	18/29/29/53	-
38	CHL	N	605	7	-	6/20/96/117	-
35	LHG	G	618	28	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	B	617	-	-	14/29/63/63	0/2/2/2
31	SQD	L	103	-	-	8/49/69/69	0/1/1/1
28	CLA	C	505	3	-	11/39/115/115	-
28	CLA	G	602	7	-	16/39/115/115	-
28	CLA	R	610	35	-	12/20/96/115	-
28	CLA	Y	611	35	-	12/33/109/115	-
28	CLA	B	608	2	-	13/39/115/115	-
38	CHL	s	606	42	-	6/32/108/117	-
28	CLA	G	611	35	-	15/33/109/115	-
28	CLA	G	613	-	-	20/39/115/115	-
28	CLA	b	608	2	-	9/39/115/115	-
31	SQD	B	620	-	-	8/49/69/69	0/1/1/1
36	DGD	C	517	-	-	4/44/84/95	0/2/2/2
32	LMG	C	522	-	-	14/39/59/70	0/1/1/1
28	CLA	g	602	7	-	18/39/115/115	-
28	CLA	c	513	3	-	8/30/106/115	-
38	CHL	Y	608	42	-	12/41/117/117	-
39	LUT	g	616	-	-	7/29/67/67	0/2/2/2
28	CLA	y	304	22	-	11/39/115/115	-
28	CLA	a	406	1	-	13/39/115/115	-
28	CLA	Y	604	42,40	-	8/21/97/115	-
32	LMG	k	102	-	-	9/46/66/70	0/1/1/1
30	BCR	b	617	-	-	14/29/63/63	0/2/2/2
35	LHG	b	621	-	-	23/38/38/53	-
38	CHL	Y	605	22	-	2/20/96/117	-
35	LHG	D	407	-	-	37/53/53/53	-
38	CHL	G	605	7	-	8/17/93/117	-
35	LHG	g	618	28	-	29/45/45/53	-
38	CHL	g	607	42	-	10/31/107/117	-
39	LUT	s	615	-	-	6/29/67/67	0/2/2/2
31	SQD	L	101	-	-	5/37/57/69	0/1/1/1
28	CLA	B	610	42	-	18/39/115/115	-
32	LMG	C	520	-	-	13/46/66/70	0/1/1/1
32	LMG	c	521	-	-	13/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	NEX	N	617	28	-	5/27/83/83	0/3/3/3
28	CLA	r	603	17	-	18/33/109/115	-
28	CLA	b	610	42	-	4/39/115/115	-
38	CHL	r	607	42	-	14/35/111/117	-
32	LMG	D	408	-	-	8/41/61/70	0/1/1/1
28	CLA	B	615	2	-	17/39/115/115	-
31	SQD	a	411	-	-	12/45/65/69	0/1/1/1
30	BCR	C	514	-	-	14/29/63/63	0/2/2/2
28	CLA	Y	603	22	-	12/27/103/115	-
28	CLA	c	501	3	-	12/39/115/115	-
28	CLA	G	603	7	-	10/25/101/115	-
35	LHG	b	624	-	-	31/50/50/53	-
35	LHG	A	416	-	-	31/47/47/53	-
38	CHL	G	608	42	-	7/41/117/117	-
28	CLA	r	613	17	-	14/39/115/115	-
30	BCR	b	619	-	-	5/29/63/63	0/2/2/2
28	CLA	B	614	2	-	16/39/115/115	-
28	CLA	C	507	42	-	15/39/115/115	-
28	CLA	s	612	18	-	10/27/103/115	-
40	NEX	G	617	28	-	8/27/83/83	0/3/3/3
28	CLA	a	409	1	-	13/33/109/115	-
28	CLA	b	605	2	-	10/39/115/115	-
28	CLA	b	614	2	-	13/39/115/115	-
28	CLA	R	609	17	-	12/39/115/115	-
28	CLA	n	604	42,40	-	11/21/97/115	-
28	CLA	y	312	22	-	14/33/109/115	-
40	NEX	s	616	-	-	8/27/83/83	0/3/3/3
28	CLA	N	614	7	-	10/19/95/115	-
39	LUT	Y	615	-	-	3/29/67/67	0/2/2/2
28	CLA	s	611	-	-	7/20/96/115	-
39	LUT	G	615	-	-	10/29/67/67	0/2/2/2
35	LHG	N	618	28	-	23/35/35/53	-
38	CHL	n	607	42	-	11/41/117/117	-
28	CLA	C	504	42	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	S	317	28	-	29/47/47/53	-
28	CLA	c	512	3	-	19/30/106/115	-
28	CLA	N	602	7	-	16/39/115/115	-
30	BCR	d	406	-	-	10/29/63/63	0/2/2/2
38	CHL	s	607	-	-	4/17/93/117	-
28	CLA	c	510	3	-	16/39/115/115	-
30	BCR	h	101	-	-	13/29/63/63	0/2/2/2
28	CLA	C	511	3	-	15/39/115/115	-
28	CLA	r	601	17	-	8/20/96/115	-
28	CLA	B	602	2	-	16/39/115/115	-
38	CHL	n	609	7	-	10/41/117/117	-
28	CLA	y	303	22	-	13/39/115/115	-
28	CLA	b	606	2	-	15/39/115/115	-
40	NEX	y	301	-	-	13/27/83/83	0/3/3/3
28	CLA	b	602	2	-	20/39/115/115	-
28	CLA	C	502	-	-	18/39/115/115	-
28	CLA	B	613	2	-	13/39/115/115	-
38	CHL	S	308	-	-	5/17/93/117	-
28	CLA	R	613	17	-	13/39/115/115	-
38	CHL	g	601	7	-	10/41/117/117	-
40	NEX	g	617	-	-	18/27/83/83	0/3/3/3
35	LHG	B	622	-	-	28/34/34/53	-
28	CLA	D	403	4	-	13/39/115/115	-
35	LHG	y	319	28	-	34/53/53/53	-
35	LHG	b	622	-	-	28/45/45/53	-
28	CLA	c	511	3	-	16/39/115/115	-
28	CLA	r	610	35	-	13/20/96/115	-
37	HEM	f	101	5,6	-	6/14/54/54	-
28	CLA	a	407	42	-	5/21/97/115	-
36	DGD	c	516	-	-	6/44/84/95	0/2/2/2
28	CLA	y	305	42	-	10/21/97/115	-
28	CLA	B	607	42	-	20/39/115/115	-
30	BCR	B	619	-	-	14/29/63/63	0/2/2/2
35	LHG	S	301	-	-	27/38/38/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	N	601	7	-	4/25/101/117	-
28	CLA	b	607	42	-	20/39/115/115	-
38	CHL	y	306	22	-	2/20/96/117	-
30	BCR	D	405	-	-	15/29/63/63	0/2/2/2
38	CHL	Y	607	42	-	17/41/117/117	-
28	CLA	Y	612	22	-	11/33/109/115	-
38	CHL	S	306	42	-	3/17/93/117	-
28	CLA	N	613	7	-	8/25/101/115	-
38	CHL	g	606	42	-	7/22/98/117	-
38	CHL	y	307	42	-	3/22/98/117	-
28	CLA	S	303	18	-	16/35/111/115	-
28	CLA	G	612	-	-	12/33/109/115	-
38	CHL	R	605	42	-	2/19/95/117	-
28	CLA	c	504	42	-	15/29/105/115	-
39	LUT	g	615	-	-	5/29/67/67	0/2/2/2
32	LMG	b	620	-	-	12/46/66/70	0/1/1/1
28	CLA	C	512	3	-	19/30/106/115	-
28	CLA	N	604	42,40	-	9/21/97/115	-
30	BCR	c	515	-	-	13/29/63/63	0/2/2/2
29	PHO	A	407	-	-	6/37/103/103	0/5/6/6
38	CHL	S	302	18	-	2/17/93/117	-
28	CLA	g	614	7	-	6/15/91/115	-
35	LHG	C	521	-	-	35/53/53/53	-
28	CLA	A	405	1	-	13/39/115/115	-
39	LUT	N	615	-	-	5/29/67/67	0/2/2/2
39	LUT	y	315	-	-	5/29/67/67	0/2/2/2
36	DGD	C	518	-	-	13/51/91/95	0/2/2/2
38	CHL	y	309	22	-	7/41/117/117	-
39	LUT	G	616	-	-	5/29/67/67	0/2/2/2
28	CLA	r	608	17	-	14/31/107/115	-
41	XAT	R	615	-	-	7/31/93/93	0/4/4/4
28	CLA	Y	610	22	-	13/33/109/115	-
39	LUT	r	614	-	-	8/29/67/67	0/2/2/2
30	BCR	t	101	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	604	2	-	17/39/115/115	-
35	LHG	r	617	28	-	23/34/34/53	-
28	CLA	n	612	7	-	12/33/109/115	-
30	BCR	C	515	-	-	14/29/63/63	0/2/2/2
30	BCR	i	101	-	-	14/29/63/63	0/2/2/2
32	LMG	a	413	-	-	5/35/55/70	0/1/1/1
31	SQD	A	414	-	-	12/49/69/69	0/1/1/1
29	PHO	d	402	-	-	2/37/103/103	0/5/6/6
28	CLA	g	613	7	-	10/24/100/115	-
38	CHL	G	609	7	-	5/28/104/117	-
38	CHL	g	619	42	-	16/41/117/117	-
33	PL9	d	407	-	-	7/53/73/73	0/1/1/1
36	DGD	C	519	-	-	11/49/89/95	0/2/2/2
40	NEX	Y	618	28	-	4/27/83/83	0/3/3/3
35	LHG	B	625	-	-	33/50/50/53	-
38	CHL	R	606	42	-	4/17/93/117	-
28	CLA	A	406	42	-	11/21/97/115	-
28	CLA	s	608	-	-	6/15/91/115	-
38	CHL	n	608	42	-	15/41/117/117	-
39	LUT	R	614	-	-	5/29/67/67	0/2/2/2
28	CLA	C	503	-	-	18/39/115/115	-
35	LHG	s	617	28	-	35/53/53/53	-
28	CLA	n	610	7	-	22/39/115/115	-
28	CLA	s	613	18	-	8/20/96/115	-
32	LMG	b	623	-	-	13/45/65/70	0/1/1/1
28	CLA	N	610	7	-	20/39/115/115	-
28	CLA	S	312	18	-	9/20/96/115	-
28	CLA	Y	614	22	-	8/19/95/115	-
35	LHG	L	102	-	-	30/53/53/53	-
38	CHL	Y	606	42	-	2/22/98/117	-
28	CLA	R	603	17	-	14/33/109/115	-
35	LHG	n	618	28	-	22/36/36/53	-
39	LUT	S	316	-	-	6/29/67/67	0/2/2/2
38	CHL	N	608	42	-	11/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	R	612	17	-	10/27/103/115	-
28	CLA	S	310	18	-	12/27/103/115	-
38	CHL	g	609	-	-	15/35/111/117	-
28	CLA	r	611	17	-	9/20/96/115	-
28	CLA	N	611	35	-	17/33/109/115	-
28	CLA	y	314	22	-	9/19/95/115	-
38	CHL	g	605	7	-	6/17/93/117	-
28	CLA	d	404	4	-	12/39/115/115	-
28	CLA	R	611	17	-	8/20/96/115	-
28	CLA	R	601	17	-	8/15/91/115	-
28	CLA	S	304	18	-	8/15/91/115	-
28	CLA	C	501	3	-	10/39/115/115	-
39	LUT	y	316	-	-	7/29/67/67	0/2/2/2
28	CLA	b	615	2	-	11/39/115/115	-
28	CLA	B	603	2	-	13/39/115/115	-
29	PHO	D	402	-	-	4/37/103/103	0/5/6/6
29	PHO	a	408	-	-	5/37/103/103	0/5/6/6
28	CLA	B	612	2	-	15/39/115/115	-
28	CLA	B	616	2	-	14/39/115/115	-
38	CHL	s	605	42	-	7/17/93/117	-
35	LHG	c	519	-	-	24/34/34/53	-
28	CLA	Y	613	22	-	11/39/115/115	-
28	CLA	g	603	7	-	11/39/115/115	-
38	CHL	s	601	18	-	5/17/93/117	-
28	CLA	S	314	18	-	4/20/96/115	-
30	BCR	C	516	-	-	16/29/63/63	0/2/2/2
28	CLA	B	611	2	-	16/39/115/115	-
32	LMG	w	101	-	-	7/43/63/70	0/1/1/1
35	LHG	w	102	-	-	28/43/43/53	-
35	LHG	W	101	-	-	35/53/53/53	-
28	CLA	b	611	2	-	17/39/115/115	-
30	BCR	c	514	-	-	12/29/63/63	0/2/2/2
28	CLA	c	503	3	-	18/39/115/115	-
41	XAT	Y	617	-	-	4/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	XAT	r	615	-	-	7/31/93/93	0/4/4/4
28	CLA	S	309	18	-	8/15/91/115	-
33	PL9	D	406	-	-	8/53/73/73	0/1/1/1
28	CLA	c	508	3	-	16/39/115/115	-
28	CLA	N	603	7	-	11/27/103/115	-
28	CLA	S	313	18	-	9/27/103/115	-
28	CLA	n	603	7	-	18/39/115/115	-
28	CLA	c	509	3	-	11/39/115/115	-
38	CHL	G	606	42	-	5/22/98/117	-
28	CLA	B	605	2	-	17/39/115/115	-
28	CLA	b	612	2	-	20/39/115/115	-
28	CLA	R	604	42	-	8/19/95/115	-
28	CLA	R	602	17	-	11/33/109/115	-
28	CLA	b	609	-	-	14/39/115/115	-
31	SQD	M	101	-	-	12/37/57/69	0/1/1/1
28	CLA	B	601	42	-	12/39/115/115	-
30	BCR	T	101	-	-	9/29/63/63	0/2/2/2
39	LUT	Y	616	-	-	2/29/67/67	0/2/2/2
40	NEX	n	617	28	-	12/27/83/83	0/3/3/3
28	CLA	D	404	4	-	12/39/115/115	-
28	CLA	y	313	22	-	11/39/115/115	-
28	CLA	b	613	2	-	9/39/115/115	-
28	CLA	n	613	7	-	5/27/103/115	-
28	CLA	r	609	17	-	15/39/115/115	-
38	CHL	Y	601	22	-	11/41/117/117	-
28	CLA	y	310	22	-	14/33/109/115	-
28	CLA	y	311	35	-	12/33/109/115	-
28	CLA	S	305	42	-	11/21/97/115	-
39	LUT	n	615	-	-	7/29/67/67	0/2/2/2
28	CLA	c	505	3	-	14/30/106/115	-
28	CLA	b	604	2	-	14/39/115/115	-
38	CHL	G	601	7	-	11/41/117/117	-
32	LMG	d	409	-	-	4/41/61/70	0/1/1/1
31	SQD	a	414	-	-	10/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	609	2	-	17/39/115/115	-
35	LHG	c	520	-	-	27/44/44/53	-
30	BCR	b	618	-	-	15/29/63/63	0/2/2/2
28	CLA	b	601	42	-	14/39/115/115	-
28	CLA	g	604	42	-	6/21/97/115	-
28	CLA	g	612	7	-	6/15/91/115	-
38	CHL	Y	609	22	-	7/41/117/117	-
28	CLA	c	502	3	-	18/39/115/115	-
36	DGD	c	518	-	-	13/48/88/95	0/2/2/2
32	LMG	B	621	-	-	10/46/66/70	0/1/1/1
28	CLA	g	611	35	-	16/33/109/115	-
32	LMG	B	624	-	-	14/26/46/70	0/1/1/1
39	LUT	N	616	-	-	4/29/67/67	0/2/2/2
38	CHL	n	606	42	-	6/22/98/117	-
28	CLA	c	506	3	-	11/29/105/115	-
28	CLA	C	506	3	-	16/39/115/115	-
39	LUT	s	614	-	-	9/29/67/67	0/2/2/2
38	CHL	y	302	22	-	17/41/117/117	-
28	CLA	A	408	1	-	18/33/109/115	-
38	CHL	N	606	42	-	2/22/98/117	-
30	BCR	H	101	-	-	13/29/63/63	0/2/2/2
40	NEX	y	318	-	-	8/27/83/83	0/3/3/3
28	CLA	c	507	42	-	10/39/115/115	-
28	CLA	C	508	3	-	12/39/115/115	-
38	CHL	n	605	7	-	8/20/96/117	-
28	CLA	n	602	7	-	20/39/115/115	-
28	CLA	D	401	42	-	16/39/115/115	-
28	CLA	C	509	3	-	15/39/115/115	-
28	CLA	s	609	18	-	11/27/103/115	-
30	BCR	B	618	-	-	14/29/63/63	0/2/2/2
40	NEX	r	616	28	-	6/27/83/83	0/3/3/3
28	CLA	C	510	3	-	17/39/115/115	-
28	CLA	s	610	35	-	11/29/105/115	-
39	LUT	n	616	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	b	625	-	-	6/51/91/95	0/2/2/2
36	DGD	c	517	-	-	13/43/83/95	0/2/2/2
28	CLA	n	614	7	-	5/15/91/115	-
28	CLA	R	608	17	-	13/31/107/115	-
35	LHG	B	623	-	-	25/45/45/53	-
38	CHL	S	307	42	-	13/32/108/117	-

The worst 5 of 2412 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	518	DGD	C6B-C5B	34.31	3.44	1.51
39	S	316	LUT	C24-C25	23.38	1.62	1.33
39	n	615	LUT	C24-C25	23.19	1.62	1.33
39	y	315	LUT	C24-C25	23.19	1.62	1.33
39	g	615	LUT	C24-C25	23.18	1.62	1.33

The worst 5 of 4591 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	r	614	LUT	C15-C14-C13	-13.17	108.51	127.31
28	r	611	CLA	C4A-NA-C1A	10.37	111.37	106.71
30	C	514	BCR	C16-C17-C18	-9.95	113.12	127.31
30	C	514	BCR	C15-C14-C13	-9.81	113.30	127.31
39	G	615	LUT	C31-C30-C29	-9.61	113.59	127.31

There are no chirality outliers.

5 of 4063 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	405	CLA	CBD-CGD-O2D-CED
28	A	405	CLA	C6-C7-C8-C9
28	A	406	CLA	C1A-C2A-CAA-CBA
28	A	408	CLA	O2A-C1-C2-C3
28	B	601	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

327 monomers are involved in 3043 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	r	612	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	K	101	BCR	13	0
38	R	607	CHL	4	0
32	A	413	LMG	11	0
38	N	609	CHL	19	0
36	B	626	DGD	11	0
35	l	101	LHG	5	0
30	a	410	BCR	22	0
30	A	409	BCR	12	0
28	Y	602	CLA	11	0
28	s	603	CLA	7	0
28	G	610	CLA	30	0
38	g	608	CHL	14	0
30	k	101	BCR	16	0
35	Y	619	LHG	5	0
28	d	405	CLA	9	0
28	C	513	CLA	13	0
28	s	604	CLA	11	0
28	B	606	CLA	16	0
28	S	311	CLA	16	0
28	g	610	CLA	15	0
28	n	611	CLA	13	0
38	r	605	CHL	17	0
28	b	616	CLA	16	0
36	a	401	DGD	17	0
28	r	604	CLA	11	0
28	r	602	CLA	7	0
38	N	607	CHL	13	0
38	y	308	CHL	13	0
28	N	612	CLA	17	0
31	A	410	SQD	9	0
28	G	614	CLA	9	0
28	b	603	CLA	14	0
28	d	401	CLA	16	0
38	n	601	CHL	11	0
28	s	602	CLA	16	0
28	G	604	CLA	7	0
37	E	101	HEM	7	0
41	y	317	XAT	11	0
32	A	411	LMG	20	0
39	S	315	LUT	24	0
36	A	417	DGD	10	0
35	a	415	LHG	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	d	408	LHG	12	0
38	G	607	CHL	11	0
38	r	606	CHL	11	0
35	R	616	LHG	5	0
38	N	605	CHL	10	0
35	G	618	LHG	7	0
30	B	617	BCR	16	0
31	L	103	SQD	10	0
28	C	505	CLA	15	0
28	G	602	CLA	10	0
28	R	610	CLA	9	0
28	Y	611	CLA	12	0
28	B	608	CLA	11	0
38	s	606	CHL	10	0
28	G	611	CLA	13	0
28	G	613	CLA	23	0
28	b	608	CLA	18	0
31	B	620	SQD	12	0
36	C	517	DGD	7	0
32	C	522	LMG	7	0
28	g	602	CLA	18	0
28	c	513	CLA	12	0
38	Y	608	CHL	12	0
39	g	616	LUT	18	0
28	y	304	CLA	28	0
28	a	406	CLA	13	0
28	Y	604	CLA	14	0
32	k	102	LMG	15	0
30	b	617	BCR	9	0
35	b	621	LHG	3	0
38	Y	605	CHL	11	0
35	D	407	LHG	13	0
38	G	605	CHL	10	0
35	g	618	LHG	9	0
38	g	607	CHL	5	0
39	s	615	LUT	17	0
31	L	101	SQD	11	0
28	B	610	CLA	5	0
32	C	520	LMG	17	0
32	c	521	LMG	15	0
40	N	617	NEX	9	0
28	r	603	CLA	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	610	CLA	13	0
38	r	607	CHL	13	0
32	D	408	LMG	15	0
28	B	615	CLA	12	0
31	a	411	SQD	20	0
30	C	514	BCR	18	0
28	Y	603	CLA	16	0
28	c	501	CLA	15	0
28	G	603	CLA	10	0
35	b	624	LHG	10	0
35	A	416	LHG	4	0
38	G	608	CHL	19	0
28	r	613	CLA	19	0
30	b	619	BCR	10	0
28	B	614	CLA	15	0
28	C	507	CLA	21	0
28	s	612	CLA	10	0
40	G	617	NEX	11	0
28	a	409	CLA	11	0
28	b	605	CLA	14	0
28	b	614	CLA	12	0
28	R	609	CLA	14	0
28	n	604	CLA	6	0
28	y	312	CLA	16	0
40	s	616	NEX	7	0
28	N	614	CLA	6	0
39	Y	615	LUT	8	0
28	s	611	CLA	8	0
39	G	615	LUT	28	0
35	N	618	LHG	8	0
38	n	607	CHL	21	0
28	C	504	CLA	10	0
35	S	317	LHG	21	0
28	c	512	CLA	10	0
28	N	602	CLA	21	0
30	d	406	BCR	20	0
38	s	607	CHL	5	0
28	c	510	CLA	11	0
30	h	101	BCR	19	0
28	C	511	CLA	16	0
28	r	601	CLA	9	0
28	B	602	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	n	609	CHL	21	0
28	y	303	CLA	7	0
28	b	606	CLA	17	0
40	y	301	NEX	4	0
28	b	602	CLA	8	0
28	C	502	CLA	11	0
28	B	613	CLA	16	0
38	S	308	CHL	9	0
28	R	613	CLA	15	0
38	g	601	CHL	23	0
40	g	617	NEX	9	0
35	B	622	LHG	8	0
28	D	403	CLA	7	0
35	y	319	LHG	6	0
35	b	622	LHG	10	0
28	c	511	CLA	17	0
28	r	610	CLA	8	0
37	f	101	HEM	6	0
28	a	407	CLA	8	0
36	c	516	DGD	12	0
28	y	305	CLA	6	0
28	B	607	CLA	8	0
30	B	619	BCR	21	0
35	S	301	LHG	5	0
38	N	601	CHL	13	0
28	b	607	CLA	8	0
38	y	306	CHL	8	0
30	D	405	BCR	11	0
38	Y	607	CHL	31	0
28	Y	612	CLA	13	0
38	S	306	CHL	11	0
28	N	613	CLA	7	0
38	g	606	CHL	18	0
38	y	307	CHL	10	0
28	S	303	CLA	23	0
28	G	612	CLA	19	0
38	R	605	CHL	11	0
28	c	504	CLA	16	0
39	g	615	LUT	18	0
32	b	620	LMG	14	0
28	C	512	CLA	17	0
28	N	604	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	c	515	BCR	11	0
29	A	407	PHO	9	0
38	S	302	CHL	15	0
28	g	614	CLA	7	0
35	C	521	LHG	11	0
28	A	405	CLA	6	0
39	N	615	LUT	10	0
39	y	315	LUT	11	0
36	C	518	DGD	28	0
38	y	309	CHL	24	0
39	G	616	LUT	11	0
28	r	608	CLA	19	0
41	R	615	XAT	13	0
28	Y	610	CLA	6	0
39	r	614	LUT	15	0
30	t	101	BCR	10	0
28	B	604	CLA	7	0
35	r	617	LHG	5	0
28	n	612	CLA	15	0
30	C	515	BCR	10	0
30	i	101	BCR	8	0
32	a	413	LMG	14	0
31	A	414	SQD	14	0
29	d	402	PHO	12	0
28	g	613	CLA	8	0
38	G	609	CHL	15	0
38	g	619	CHL	20	0
33	d	407	PL9	6	0
36	C	519	DGD	20	0
40	Y	618	NEX	9	0
35	B	625	LHG	8	0
38	R	606	CHL	12	0
28	A	406	CLA	9	0
28	s	608	CLA	8	0
38	n	608	CHL	13	0
39	R	614	LUT	14	0
28	C	503	CLA	9	0
35	s	617	LHG	16	0
28	n	610	CLA	24	0
28	s	613	CLA	5	0
32	b	623	LMG	8	0
28	N	610	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	S	312	CLA	12	0
28	Y	614	CLA	7	0
35	L	102	LHG	6	0
38	Y	606	CHL	10	0
28	R	603	CLA	9	0
35	n	618	LHG	6	0
39	S	316	LUT	19	0
38	N	608	CHL	16	0
28	R	612	CLA	12	0
28	S	310	CLA	26	0
38	g	609	CHL	14	0
28	r	611	CLA	5	0
28	N	611	CLA	13	0
28	y	314	CLA	6	0
38	g	605	CHL	11	0
28	d	404	CLA	9	0
28	R	611	CLA	5	0
28	R	601	CLA	12	0
28	S	304	CLA	11	0
28	C	501	CLA	13	0
39	y	316	LUT	6	0
28	b	615	CLA	17	0
28	B	603	CLA	21	0
29	D	402	PHO	9	0
29	a	408	PHO	12	0
28	B	612	CLA	10	0
28	B	616	CLA	16	0
38	s	605	CHL	9	0
35	c	519	LHG	5	0
28	Y	613	CLA	13	0
28	g	603	CLA	9	0
38	s	601	CHL	14	0
28	S	314	CLA	6	0
30	C	516	BCR	22	0
28	B	611	CLA	15	0
32	w	101	LMG	13	0
35	w	102	LHG	8	0
35	W	101	LHG	20	0
28	b	611	CLA	15	0
30	c	514	BCR	19	0
28	c	503	CLA	9	0
41	Y	617	XAT	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	r	615	XAT	9	0
28	S	309	CLA	13	0
33	D	406	PL9	8	0
28	c	508	CLA	11	0
28	N	603	CLA	10	0
28	S	313	CLA	9	0
28	n	603	CLA	23	0
28	c	509	CLA	7	0
38	G	606	CHL	11	0
28	B	605	CLA	19	0
28	b	612	CLA	15	0
28	R	604	CLA	11	0
28	R	602	CLA	9	0
28	b	609	CLA	12	0
31	M	101	SQD	5	0
28	B	601	CLA	14	0
30	T	101	BCR	13	0
39	Y	616	LUT	7	0
40	n	617	NEX	8	0
28	D	404	CLA	9	0
28	y	313	CLA	10	0
28	b	613	CLA	12	0
28	n	613	CLA	12	0
28	r	609	CLA	19	0
38	Y	601	CHL	16	0
28	y	310	CLA	11	0
28	y	311	CLA	12	0
28	S	305	CLA	8	0
39	n	615	LUT	14	0
28	c	505	CLA	10	0
28	b	604	CLA	15	0
38	G	601	CHL	12	0
32	d	409	LMG	20	0
31	a	414	SQD	10	0
28	B	609	CLA	13	0
35	c	520	LHG	9	0
30	b	618	BCR	15	0
28	b	601	CLA	16	0
28	g	604	CLA	14	0
28	g	612	CLA	10	0
38	Y	609	CHL	15	0
28	c	502	CLA	6	0

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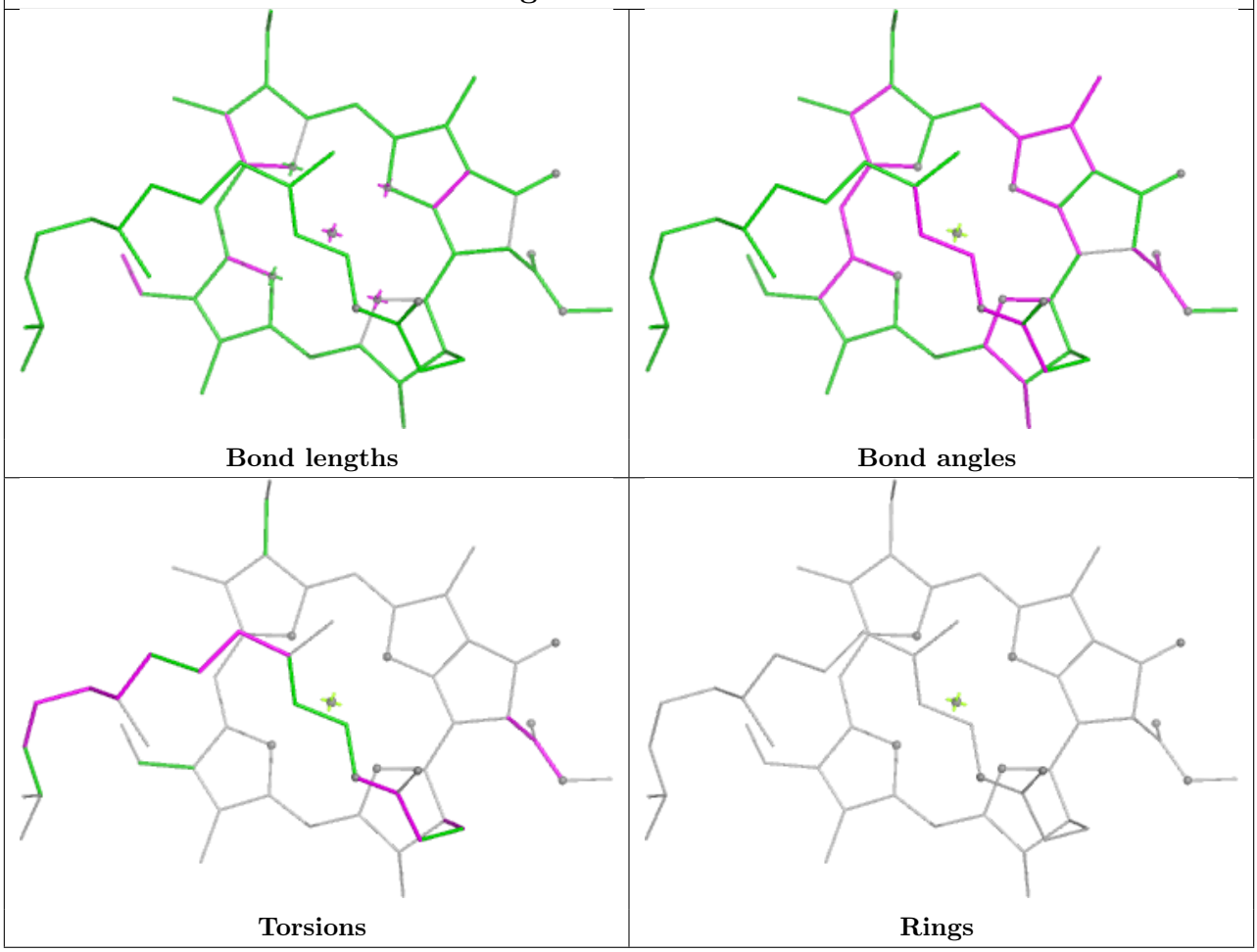
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	c	518	DGD	15	0
32	B	621	LMG	18	0
28	g	611	CLA	5	0
32	B	624	LMG	5	0
39	N	616	LUT	17	0
38	n	606	CHL	12	0
28	c	506	CLA	12	0
28	C	506	CLA	23	0
39	s	614	LUT	16	0
38	y	302	CHL	13	0
28	A	408	CLA	16	0
38	N	606	CHL	11	0
30	H	101	BCR	14	0
40	y	318	NEX	6	0
28	c	507	CLA	15	0
28	C	508	CLA	18	0
38	n	605	CHL	12	0
28	n	602	CLA	15	0
28	D	401	CLA	7	0
28	C	509	CLA	13	0
28	s	609	CLA	18	0
30	B	618	BCR	14	0
40	r	616	NEX	13	0
28	C	510	CLA	16	0
28	s	610	CLA	7	0
39	n	616	LUT	7	0
36	b	625	DGD	11	0
36	c	517	DGD	18	0
28	n	614	CLA	3	0
28	R	608	CLA	20	0
35	B	623	LHG	14	0
38	S	307	CHL	14	0

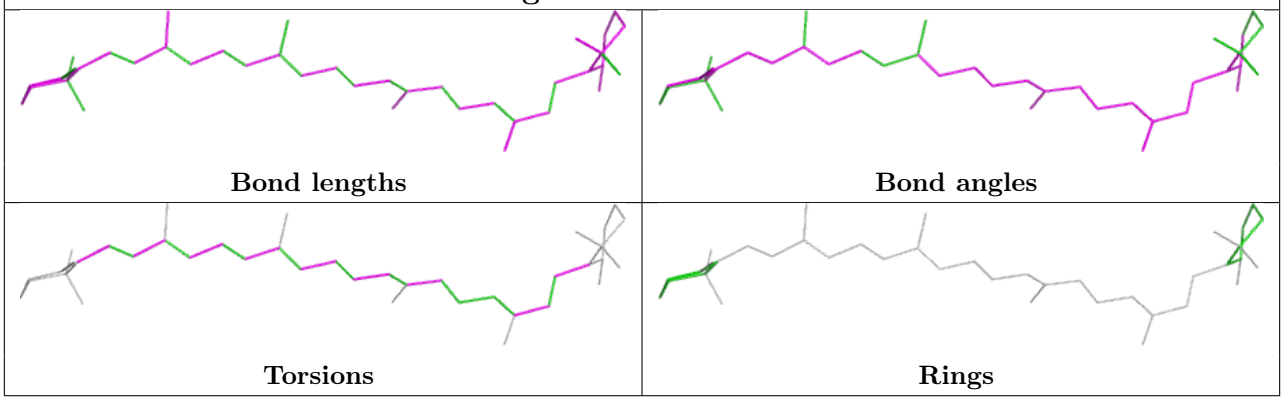
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

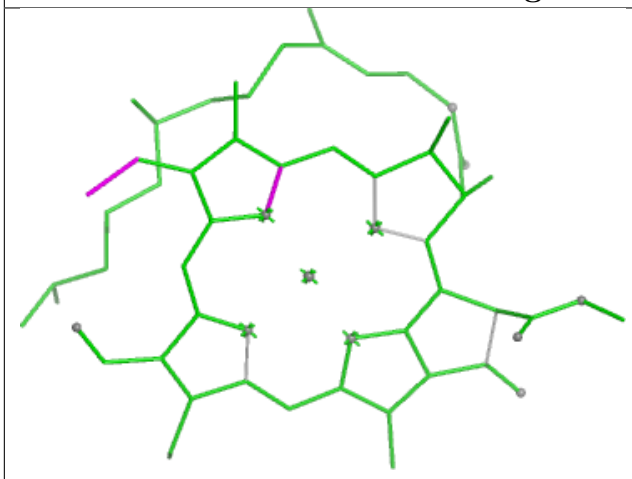
Ligand CLA r 612



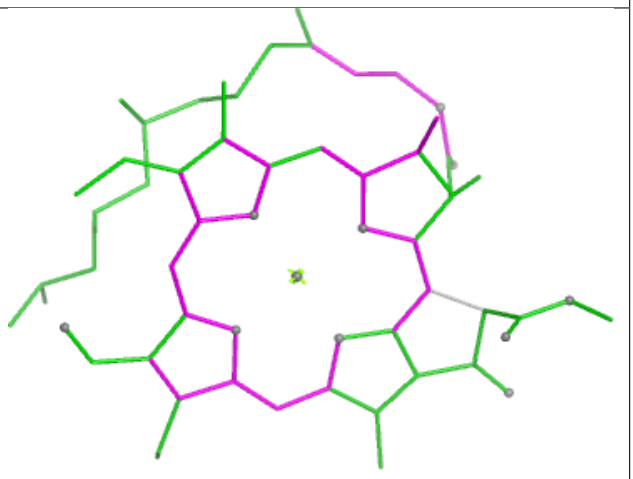
Ligand BCR K 101



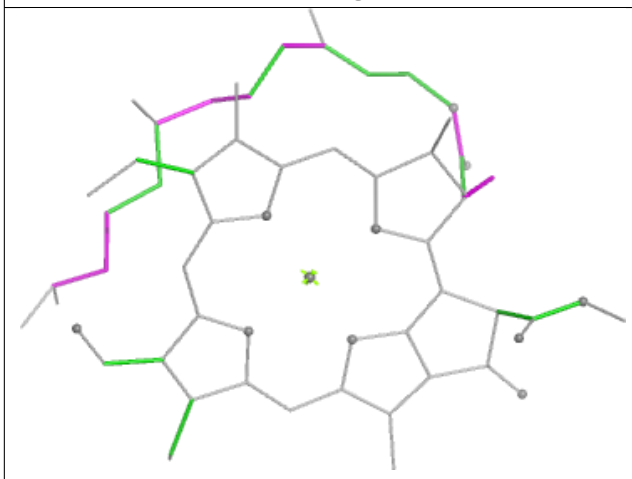
Ligand CHL R 607



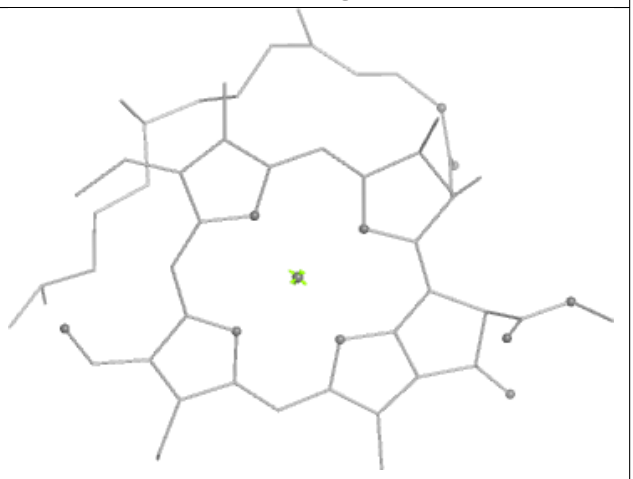
Bond lengths



Bond angles

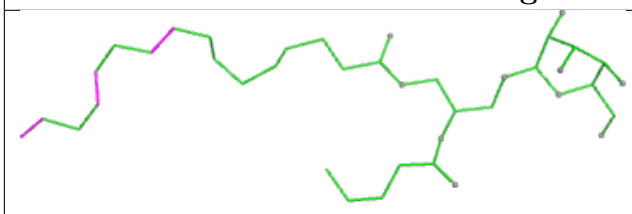


Torsions



Rings

Ligand LMG A 413



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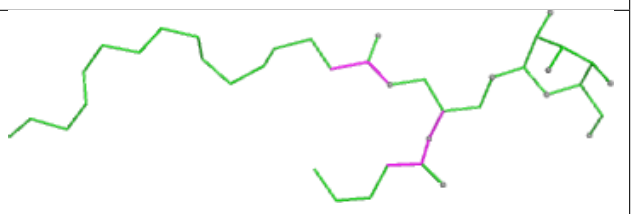

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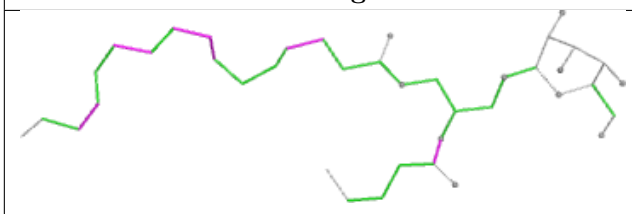
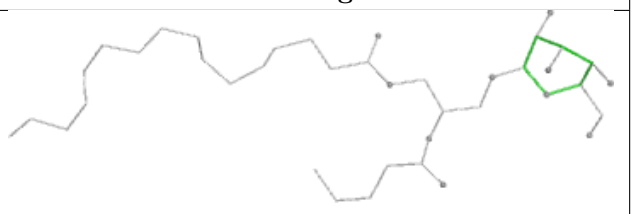
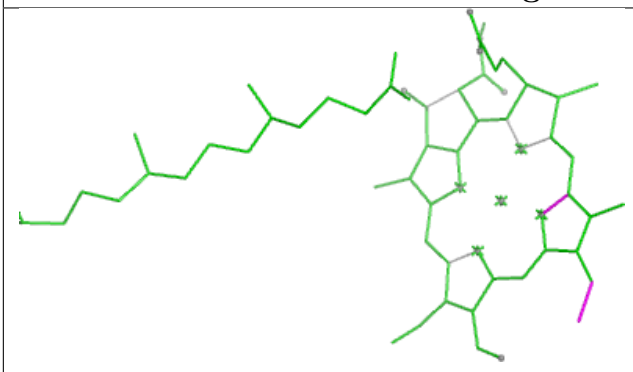


Torsions



Rings

Ligand CHL N 609



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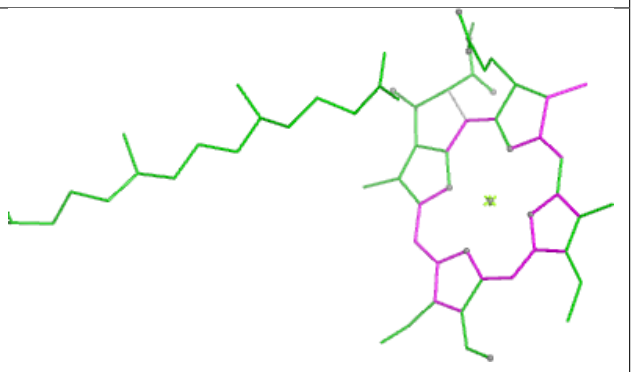

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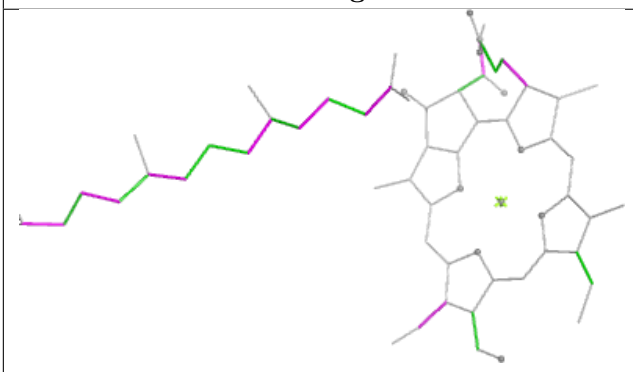

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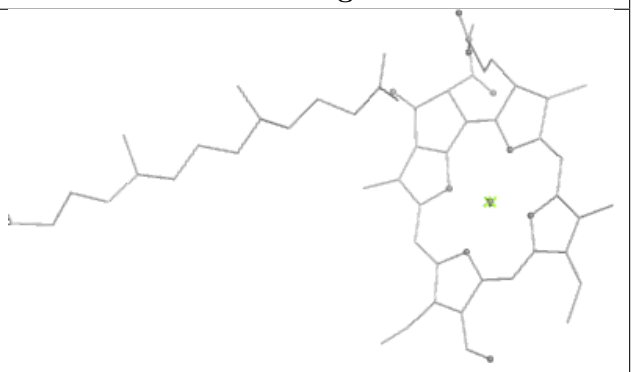
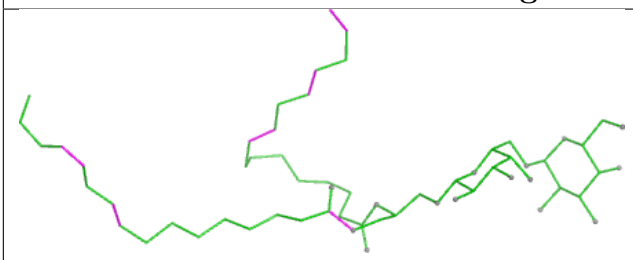


Rings

Ligand DGD B 626



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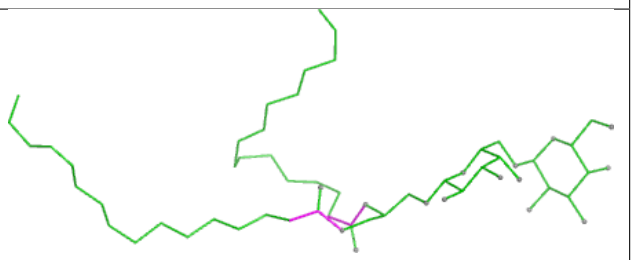

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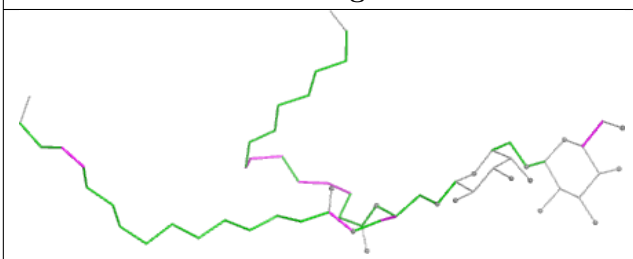

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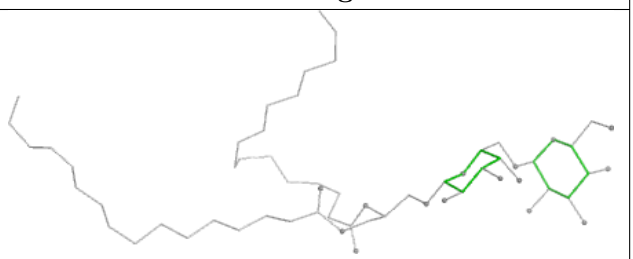
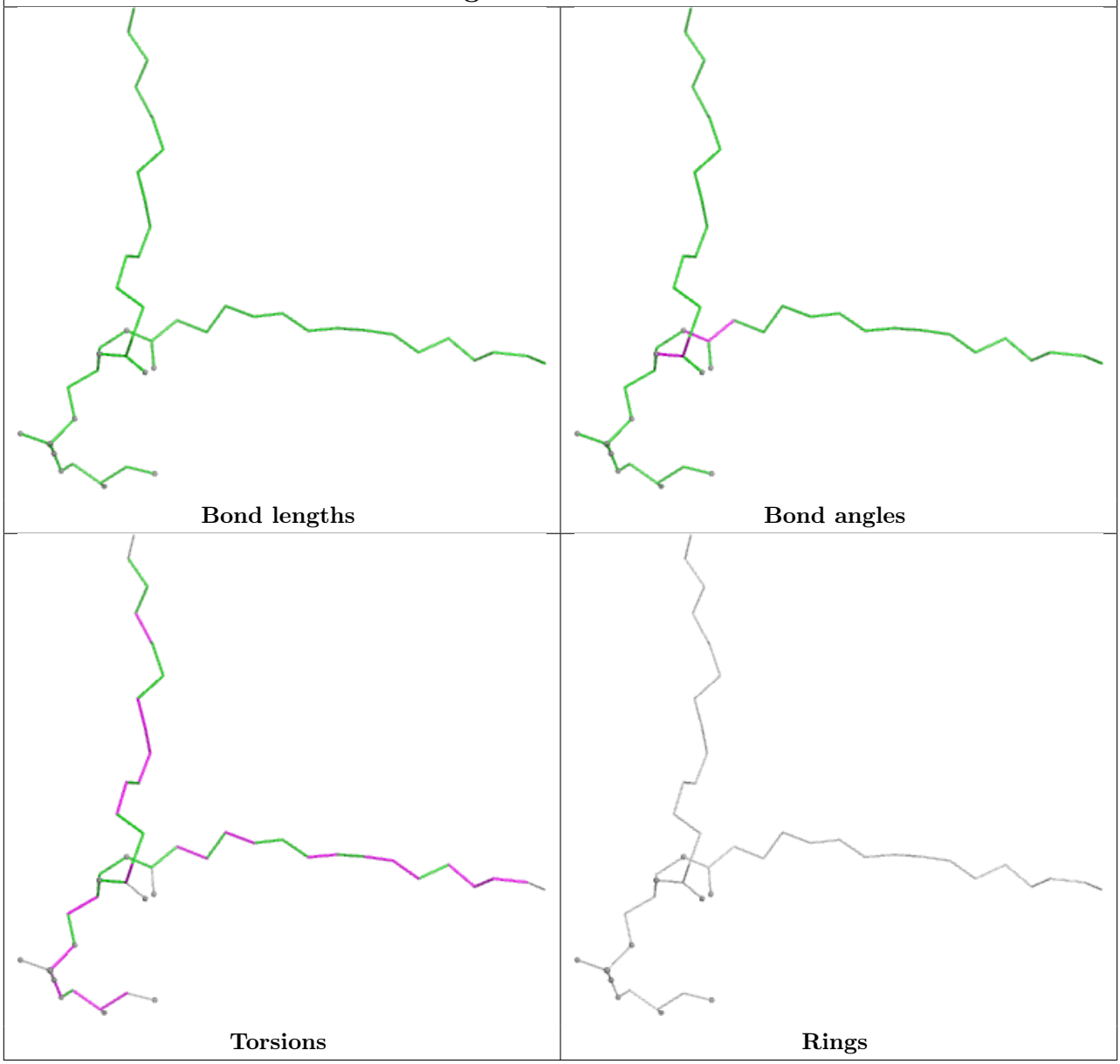
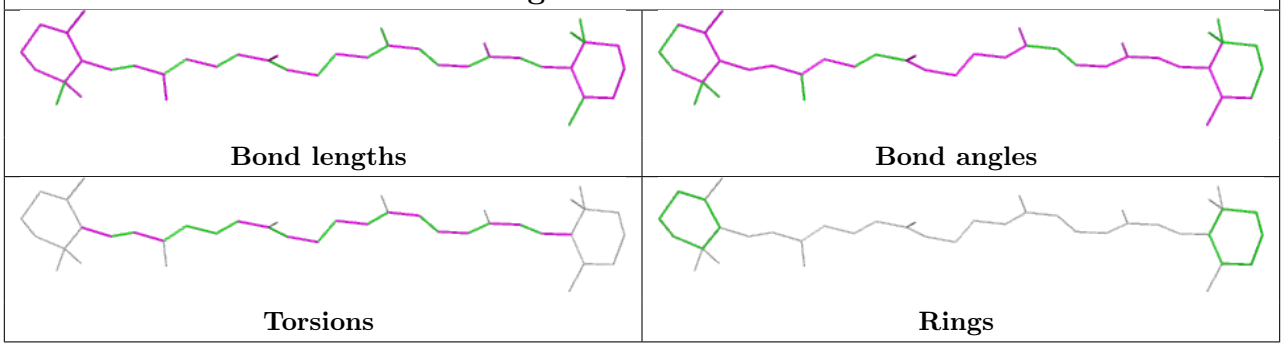


Rings

Ligand LHG l 101



Ligand BCR a 410



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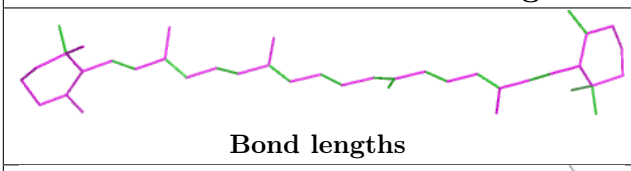

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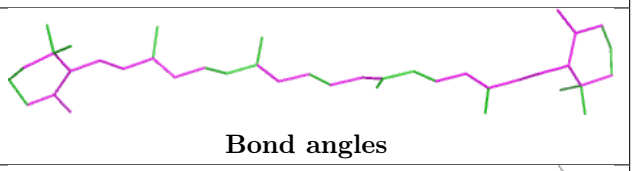

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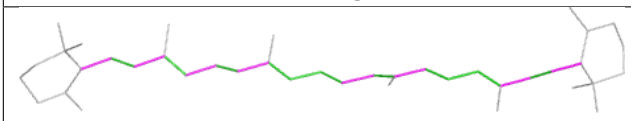

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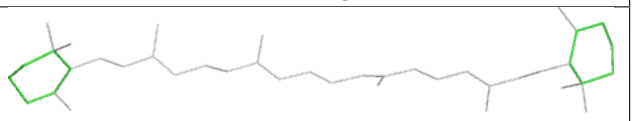
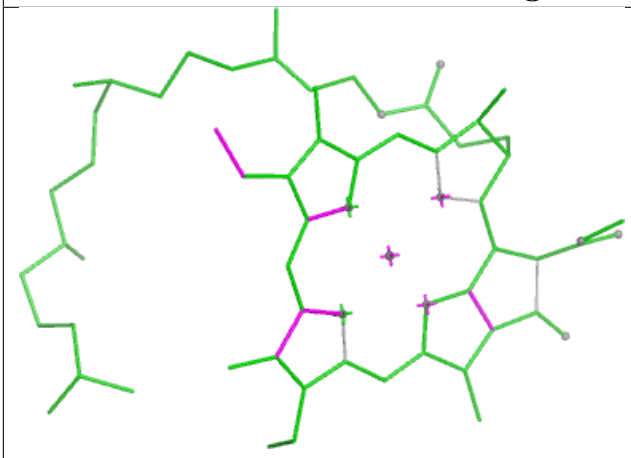


Rings

Ligand CLA Y 602



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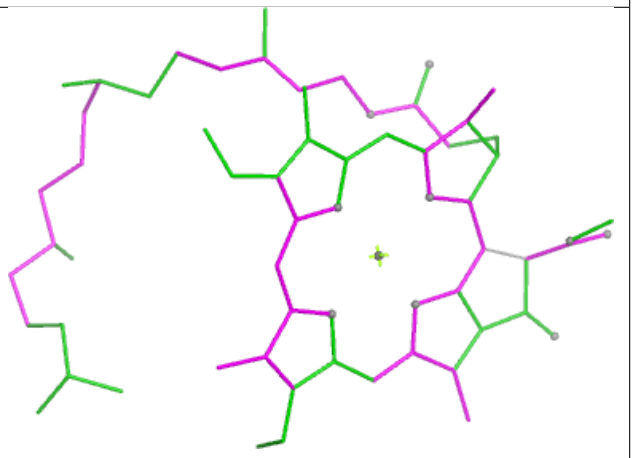
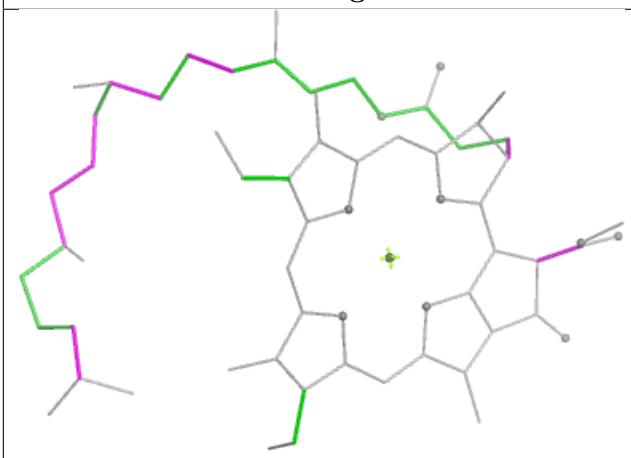


Bond angles



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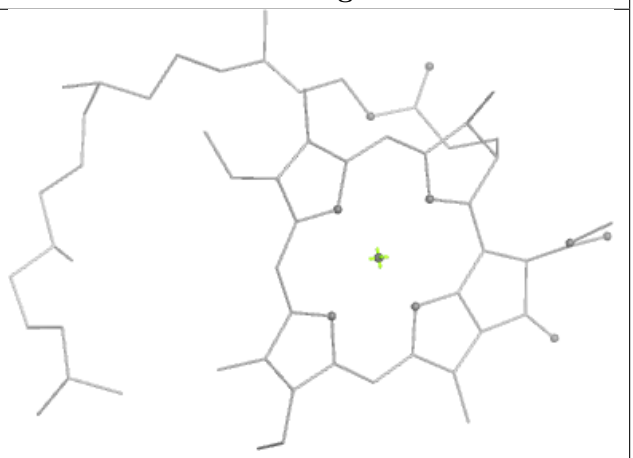
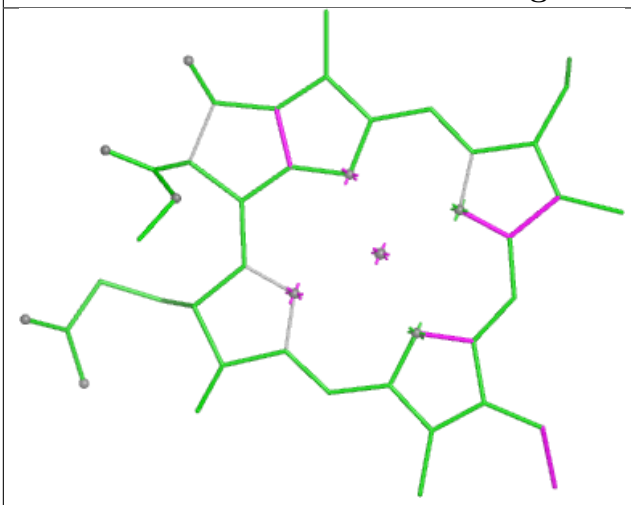


Rings

Ligand CLA s 603



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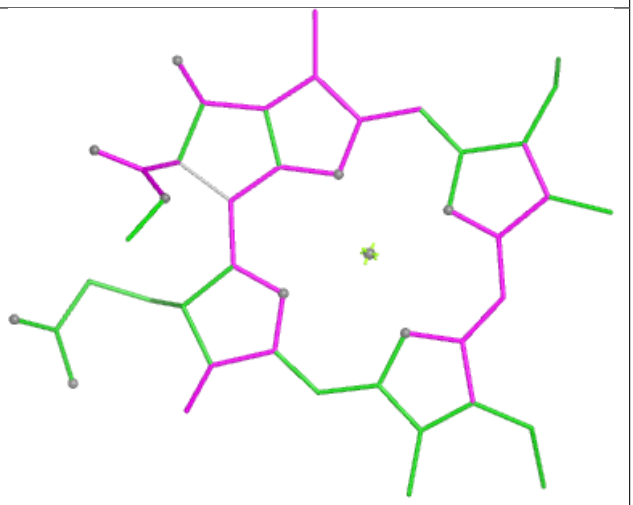

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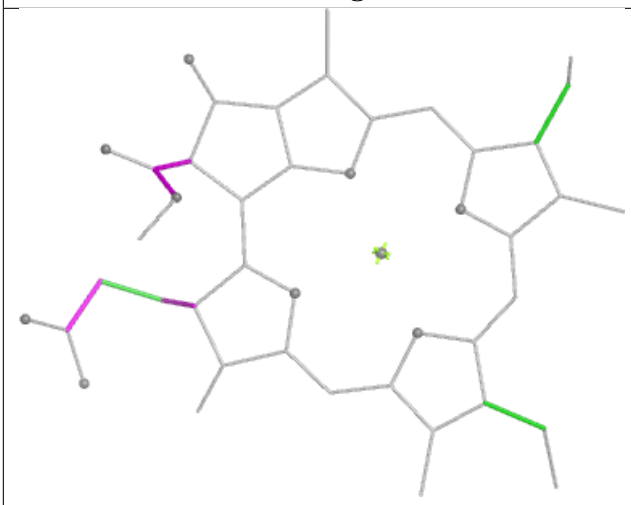

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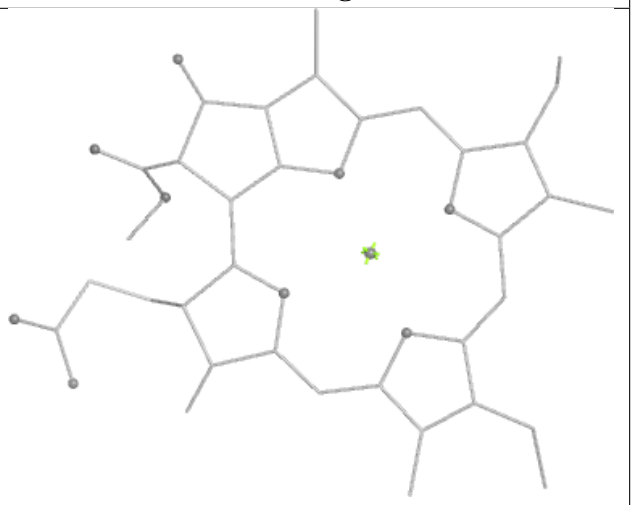

Rings

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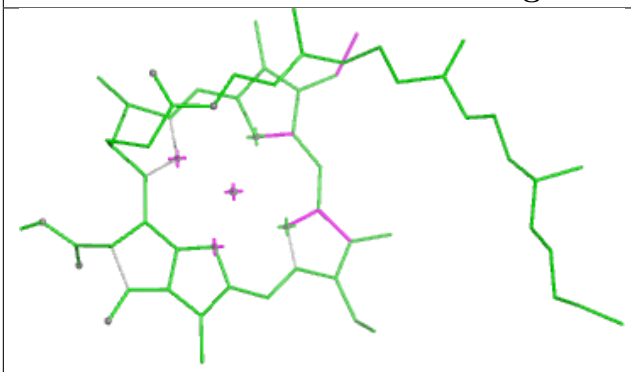

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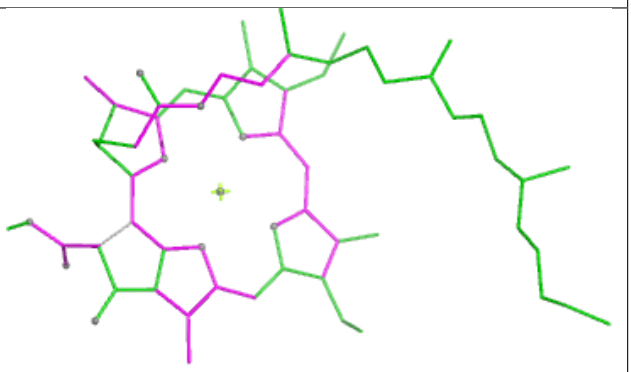

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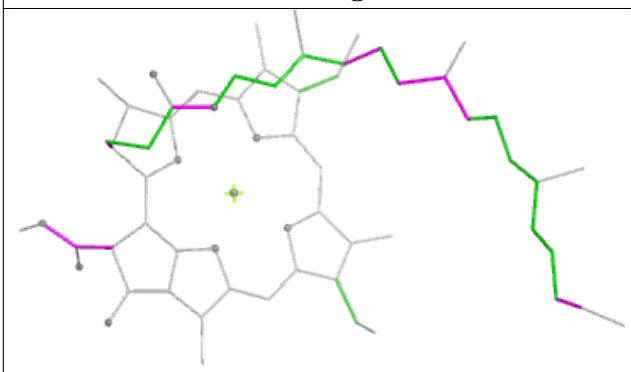

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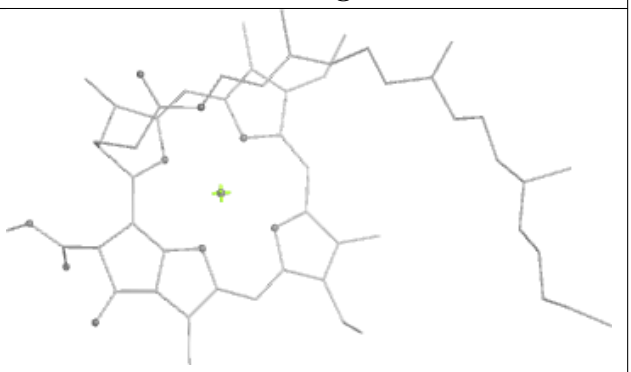
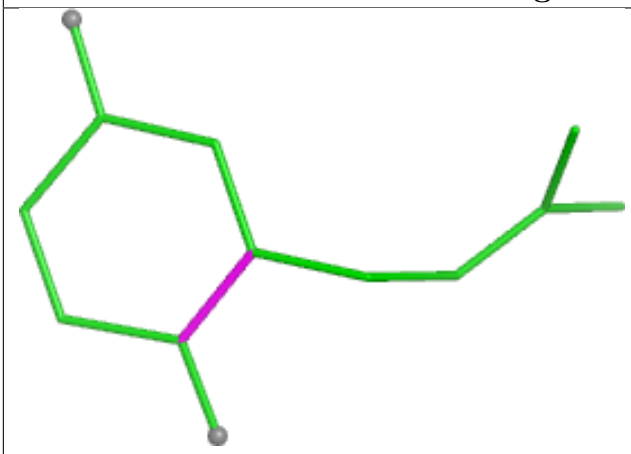


Rings

Ligand PL9 a 412



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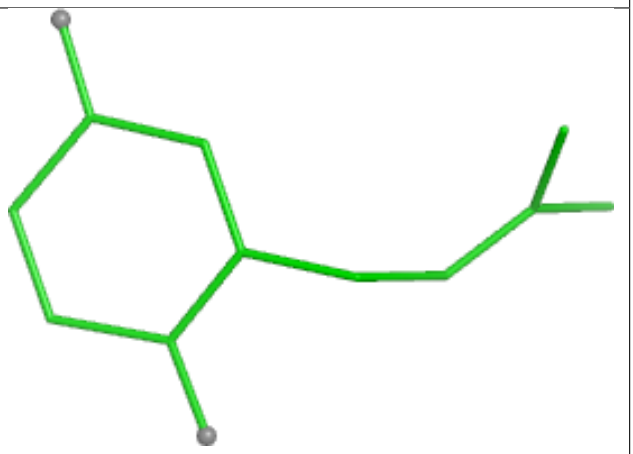

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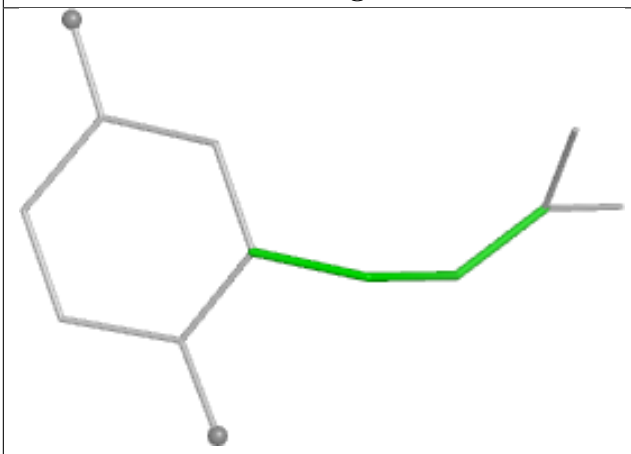

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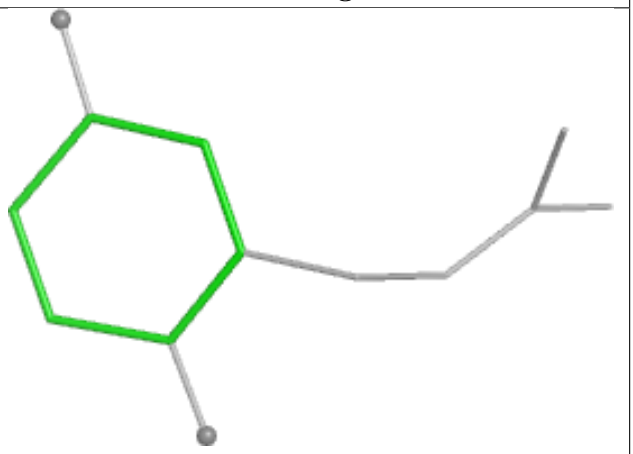
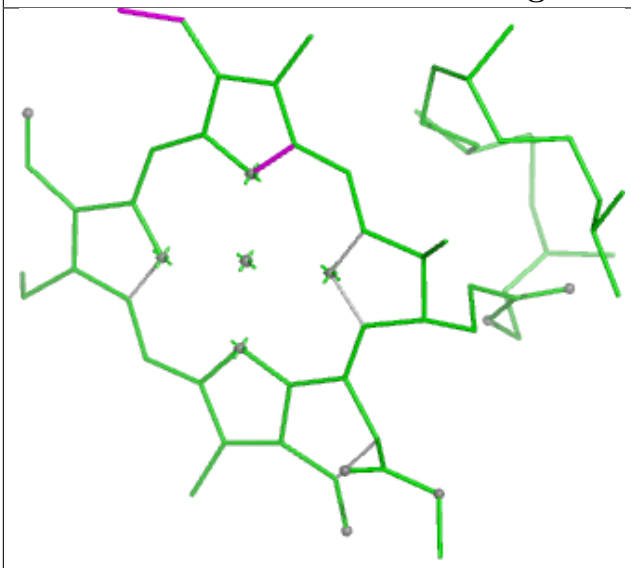


Rings

Ligand CHL g 608



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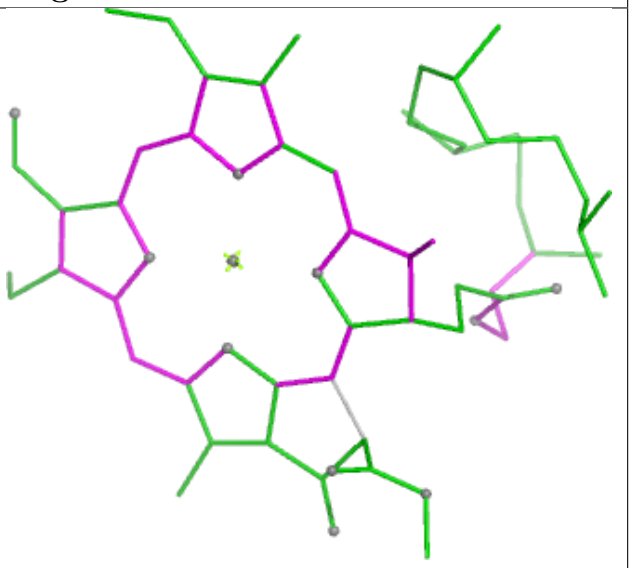

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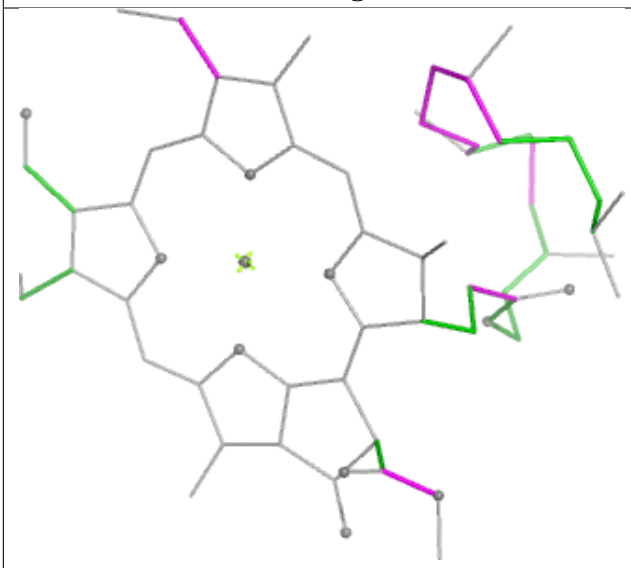

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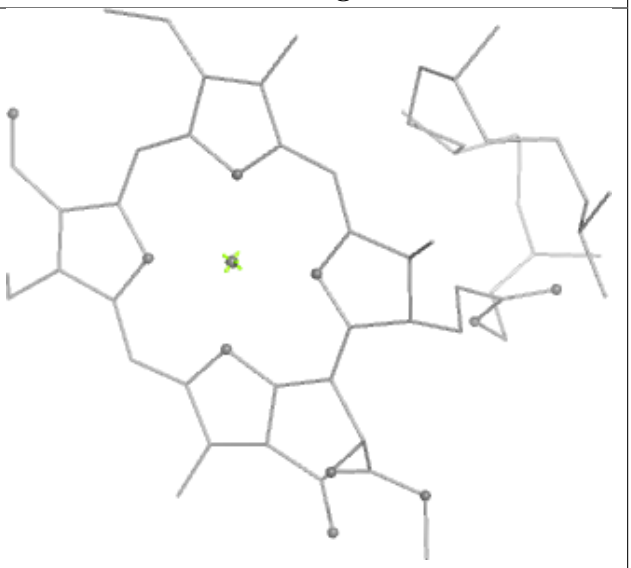
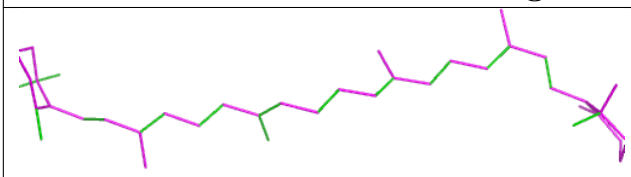


Rings

Ligand BCR k 101



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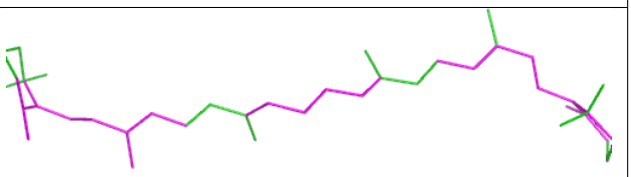

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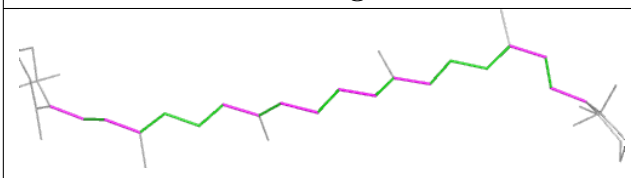

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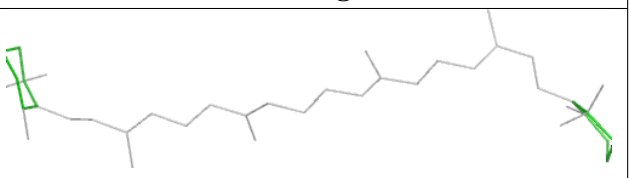
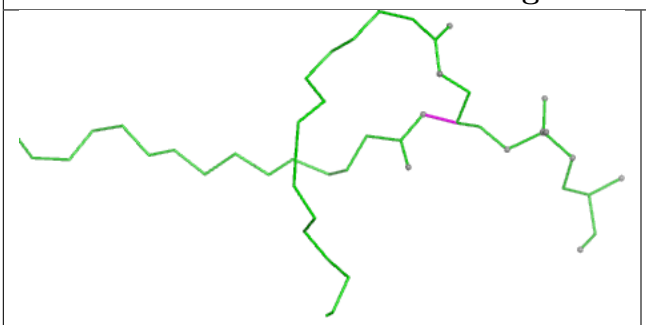


Rings

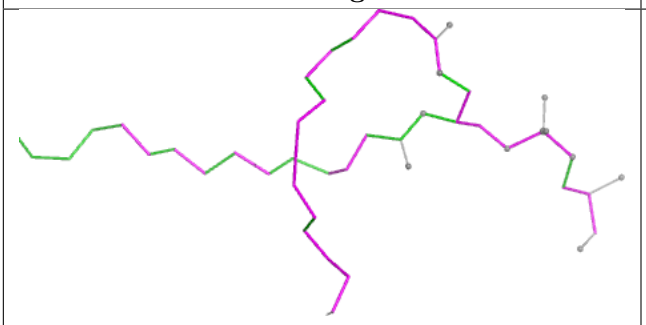
Ligand LHG Y 619



Bond lengths



Bond angles

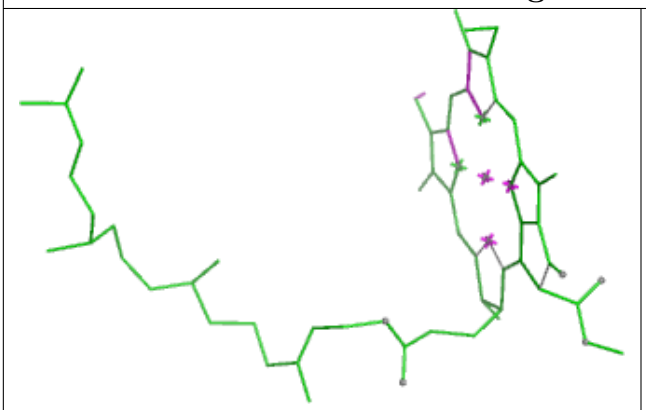


Torsions



Rings

Ligand CLA d 405



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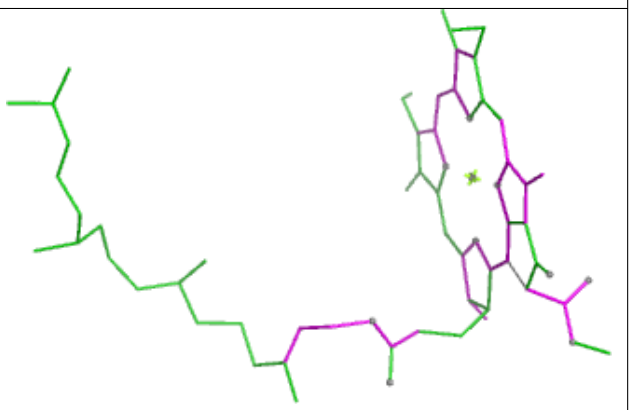

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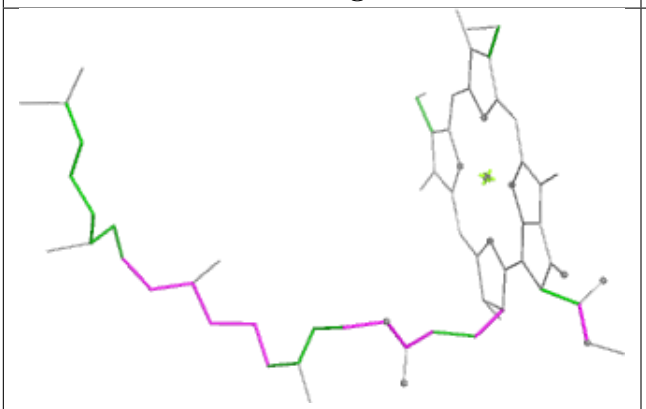

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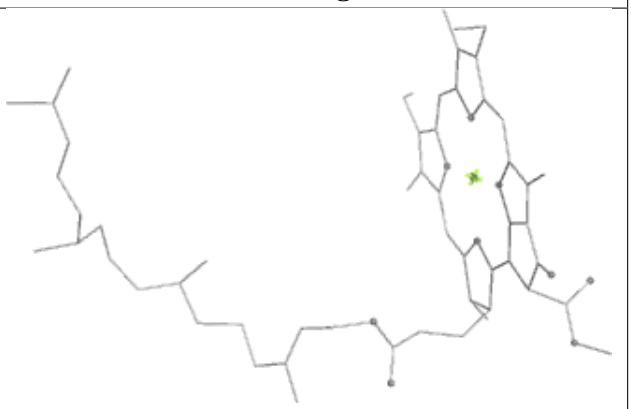
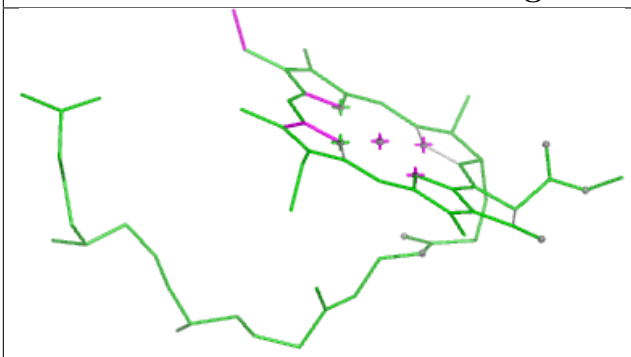


Rings

Ligand CLA C 513



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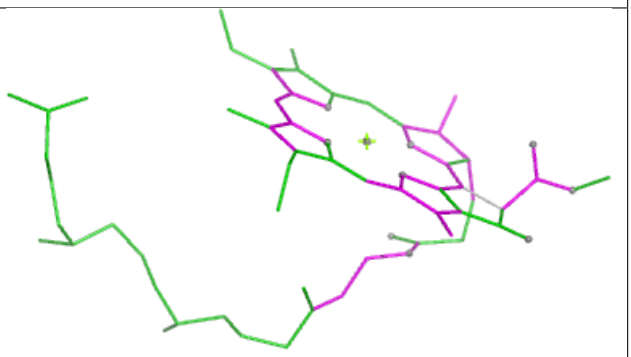
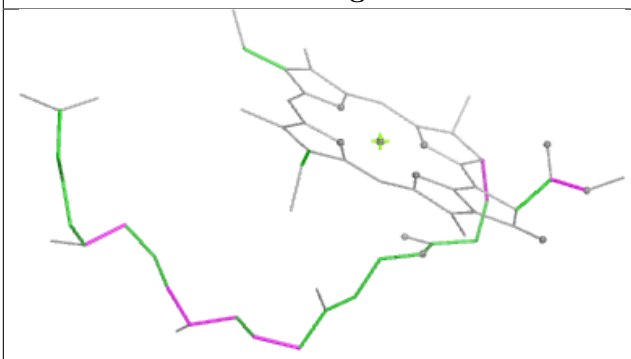


Bond angles



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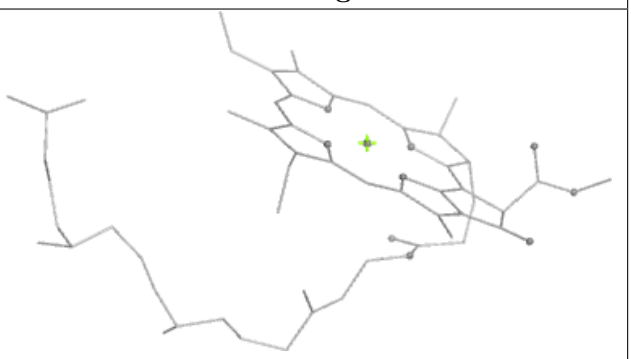
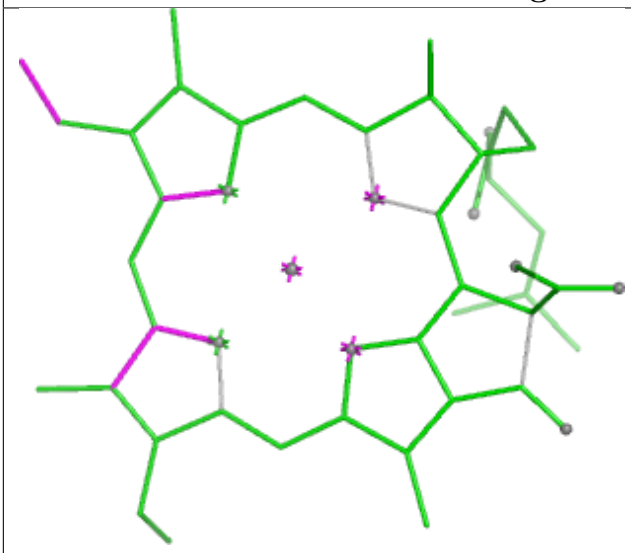


Rings

Ligand CLA s 604



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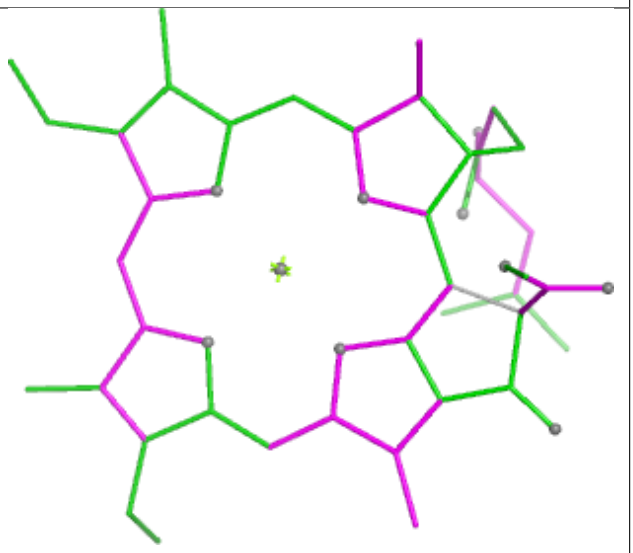
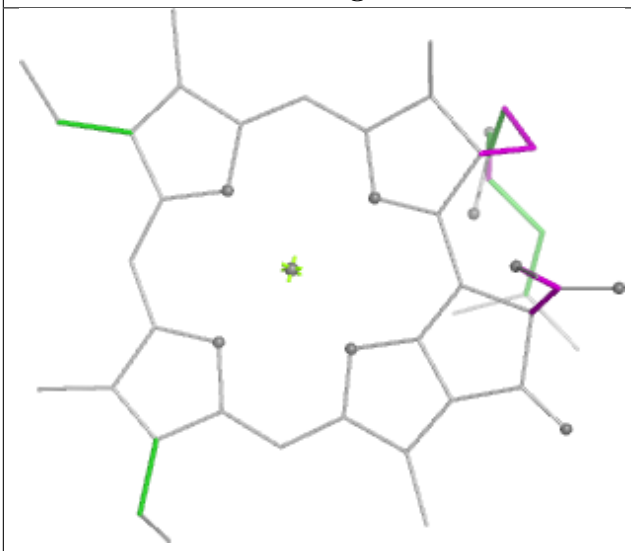


Bond angles



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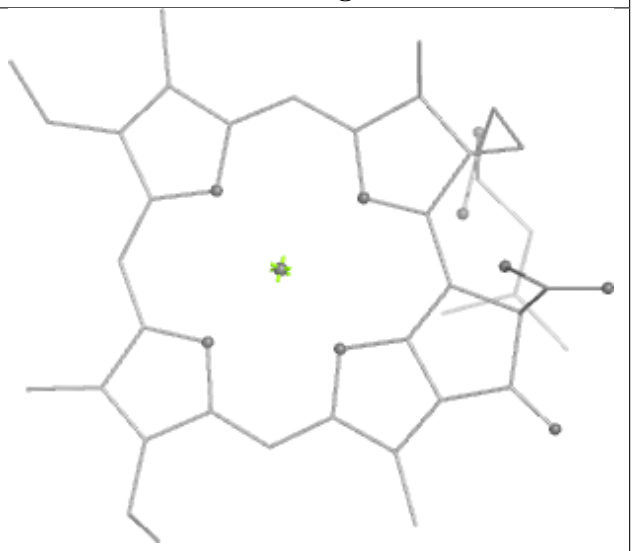
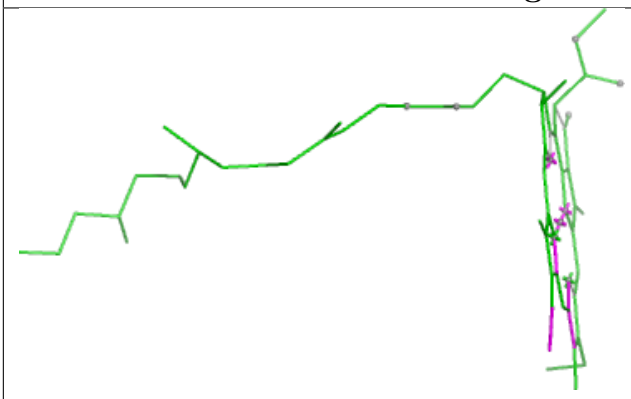
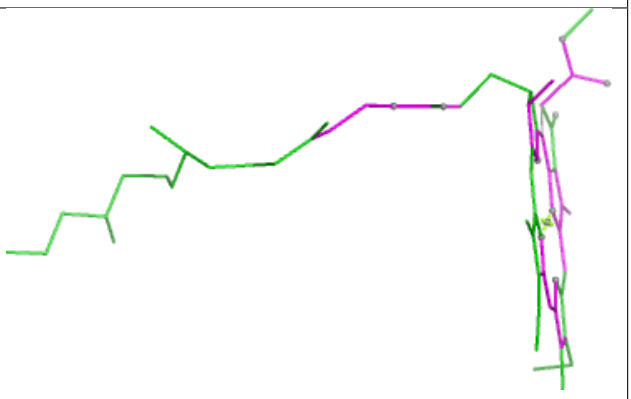


Rings

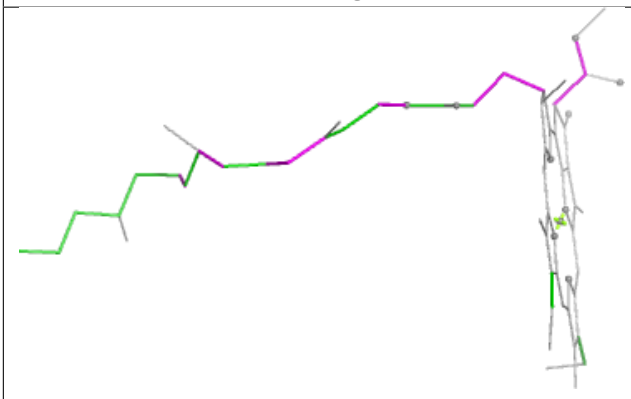
Ligand CLA B 606



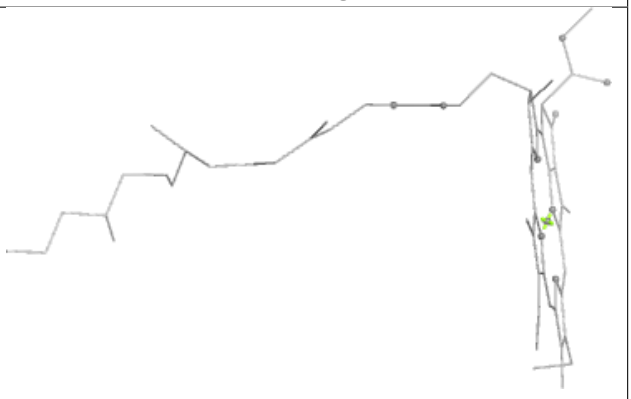
Bond lengths



Bond angles

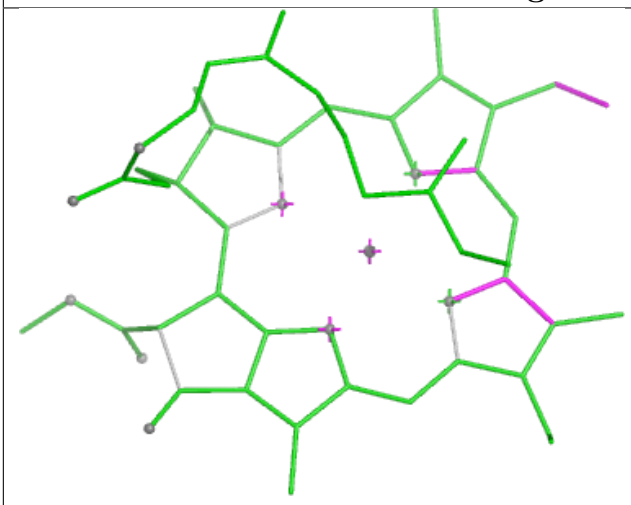


Torsions



Rings

Ligand CLA S 311



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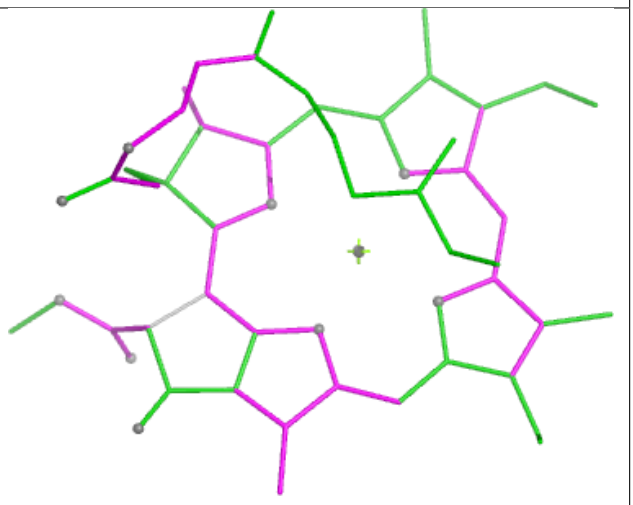
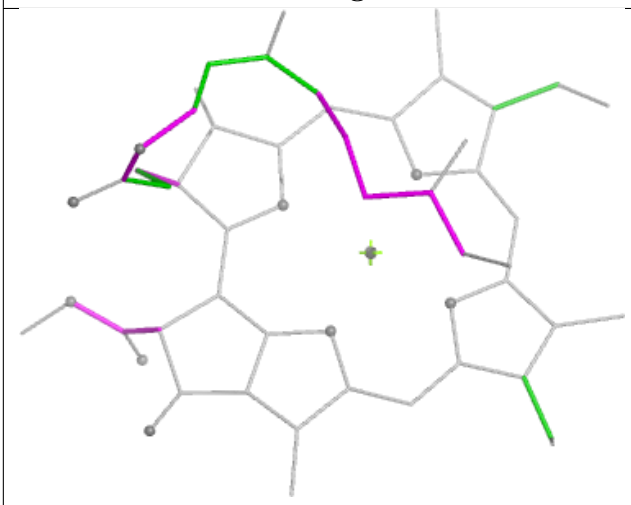


Bond angles



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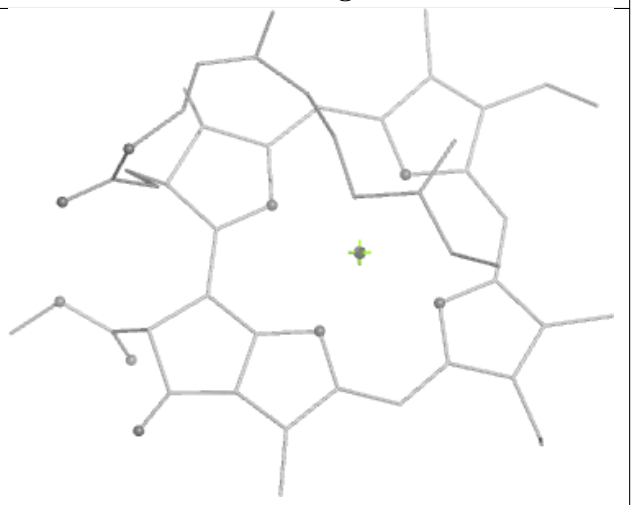
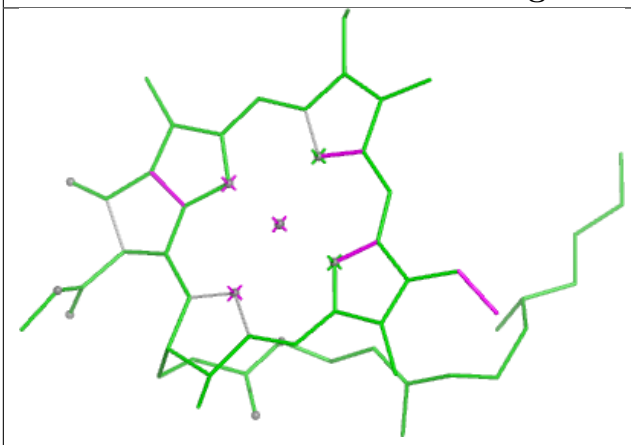


Rings

Ligand CLA g 610



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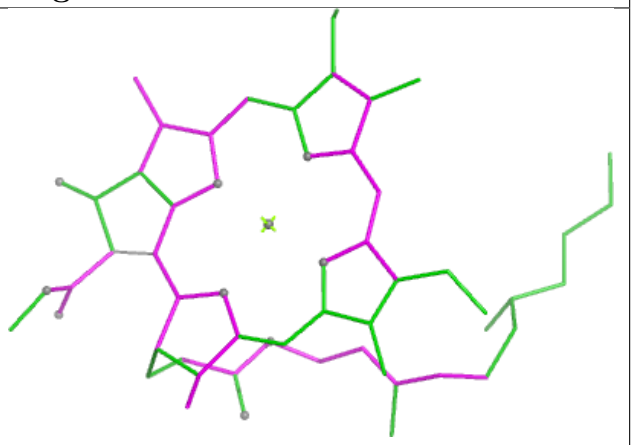

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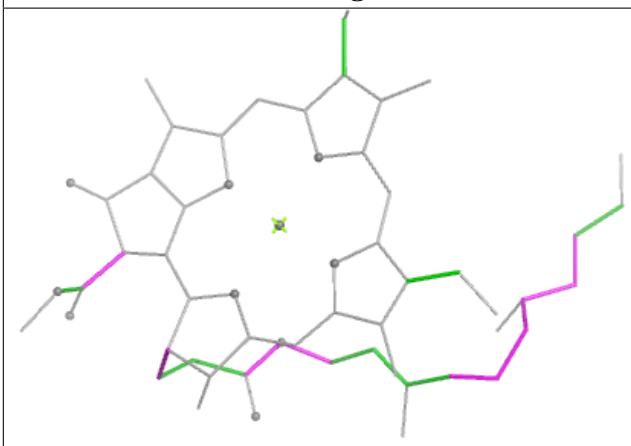

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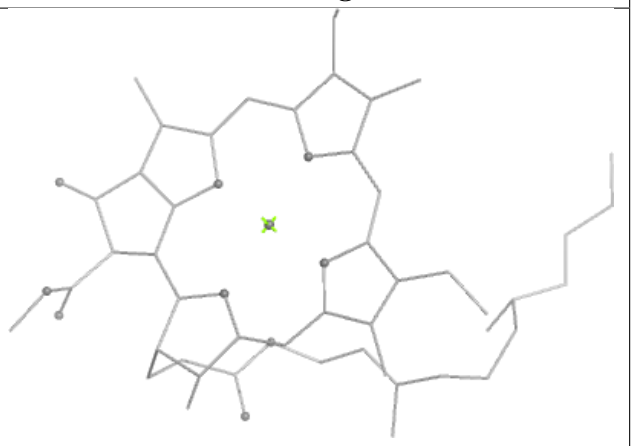
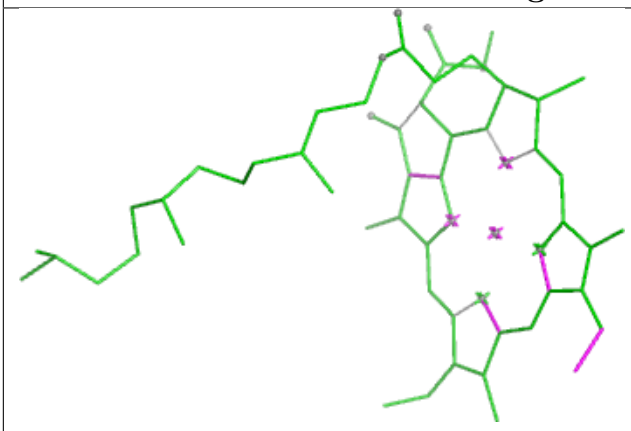


Rings

Ligand CLA n 611



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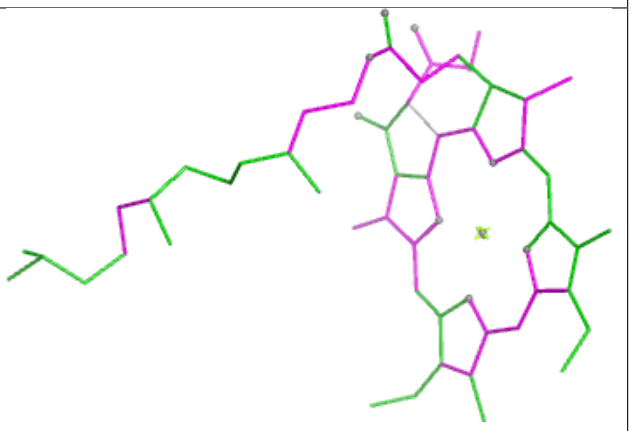
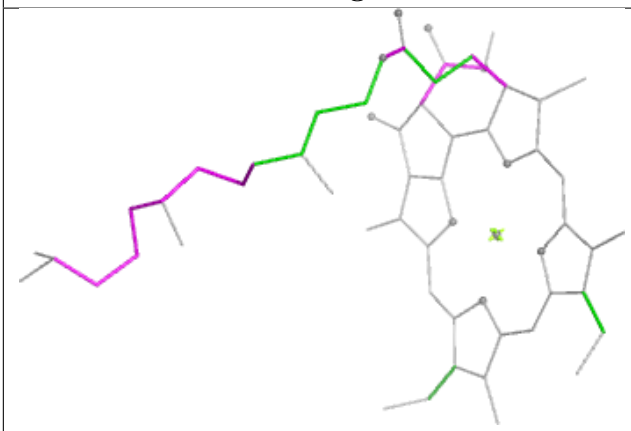


Bond angles



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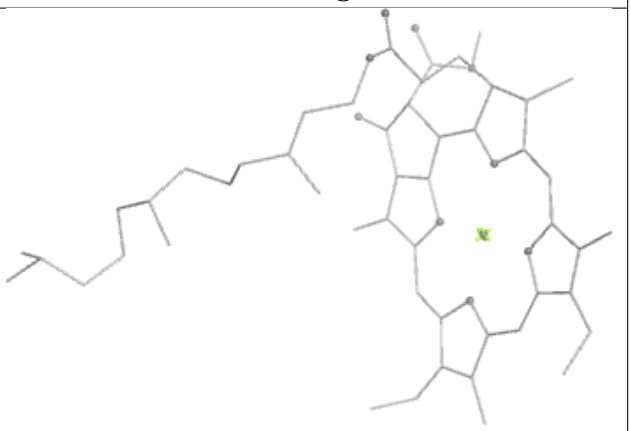
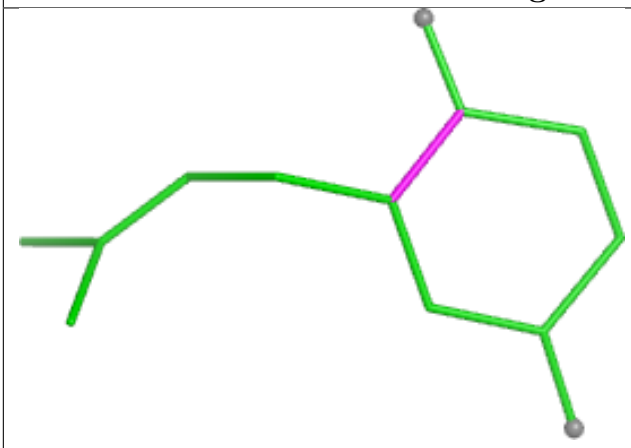


Rings

Ligand PL9 A 412



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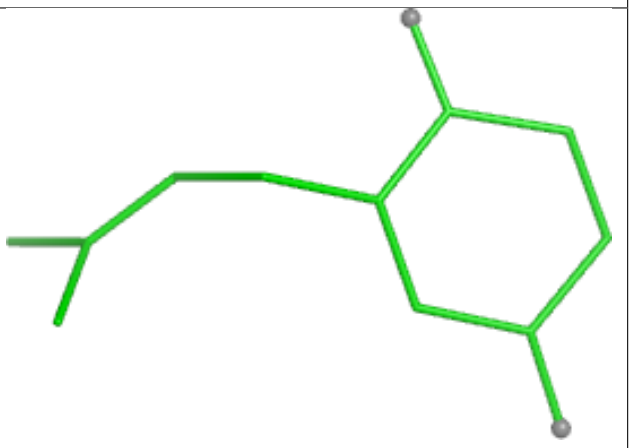

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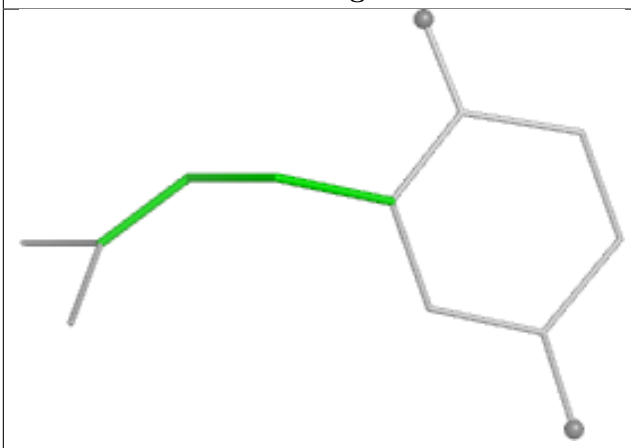

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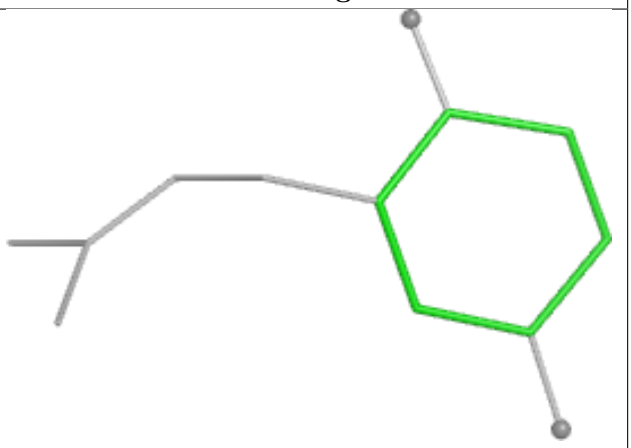
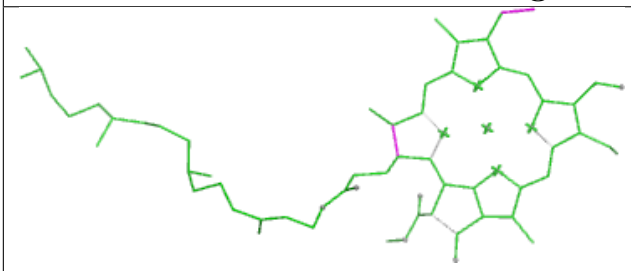


Rings

Ligand CHL r 605



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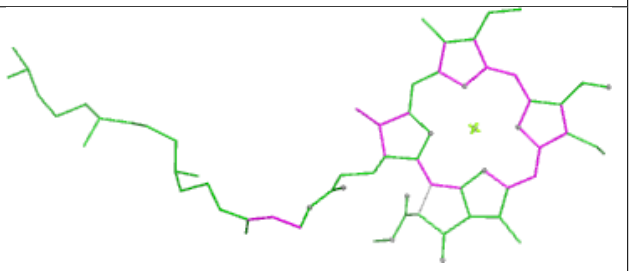

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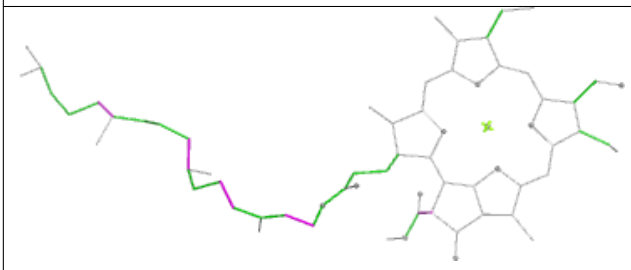

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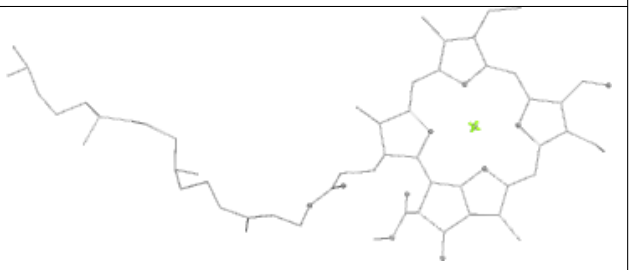
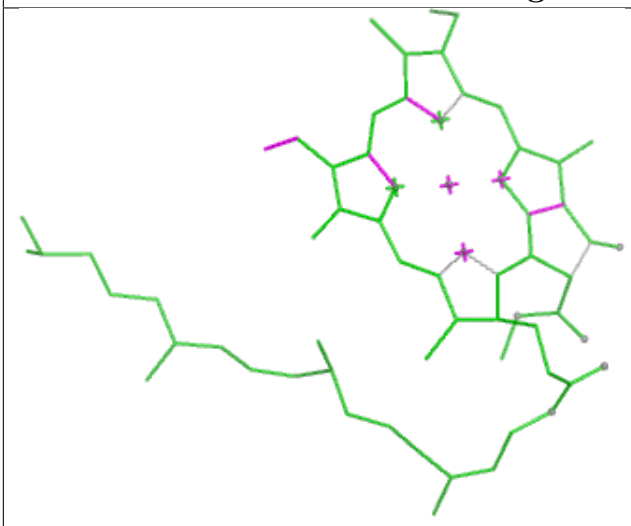


Rings

Ligand CLA b 616



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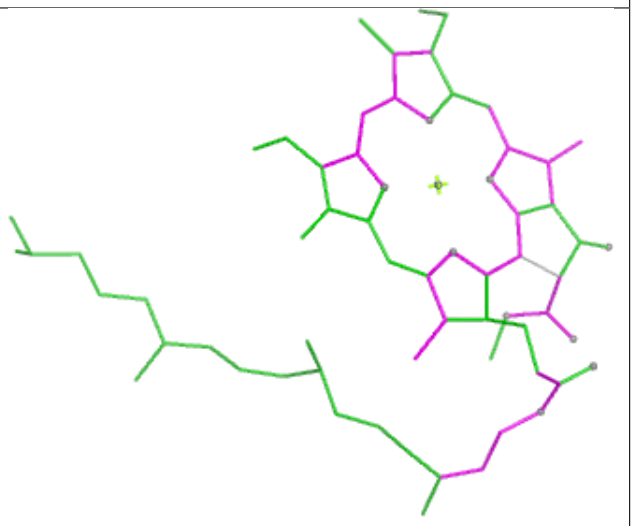
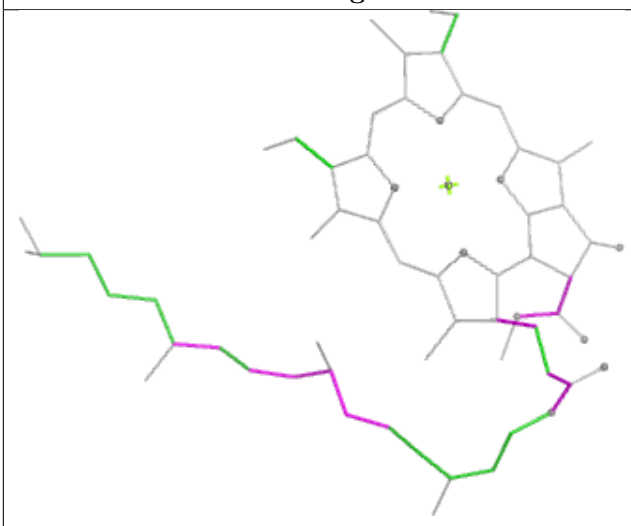


Bond angles



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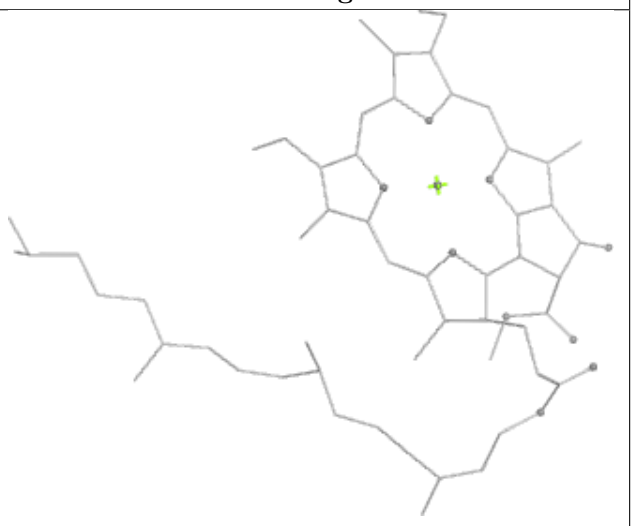
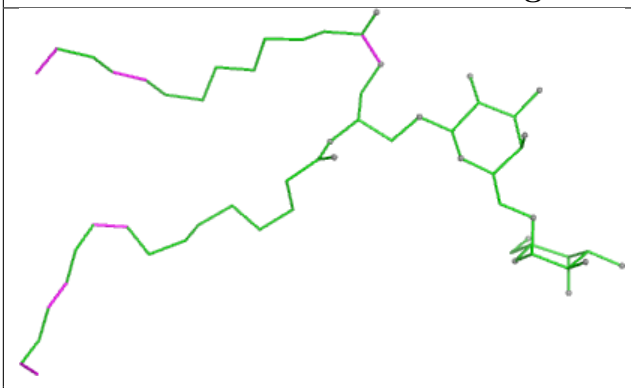


Rings

Ligand DGD a 401



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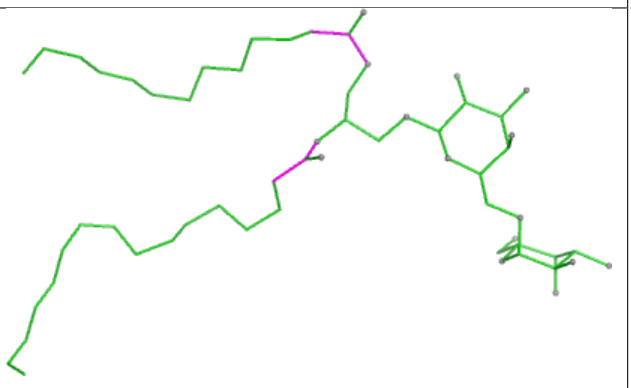
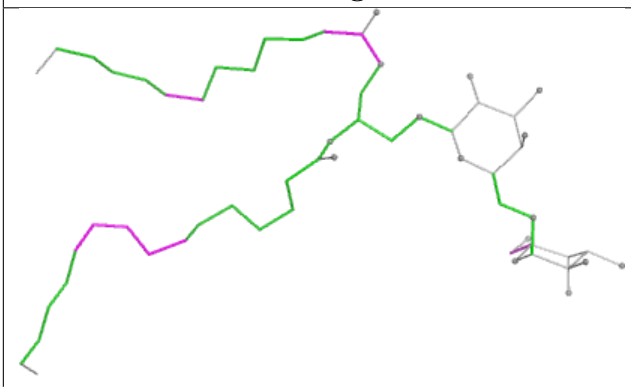


Bond angles



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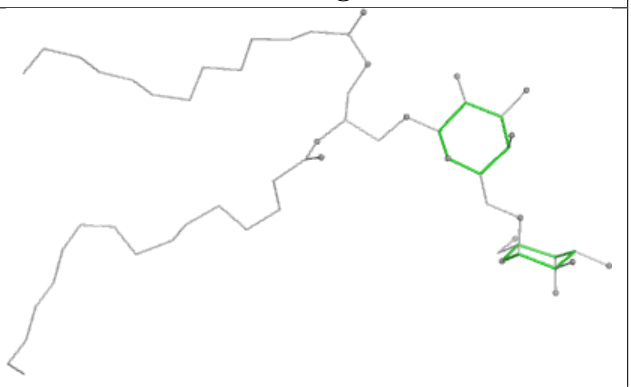
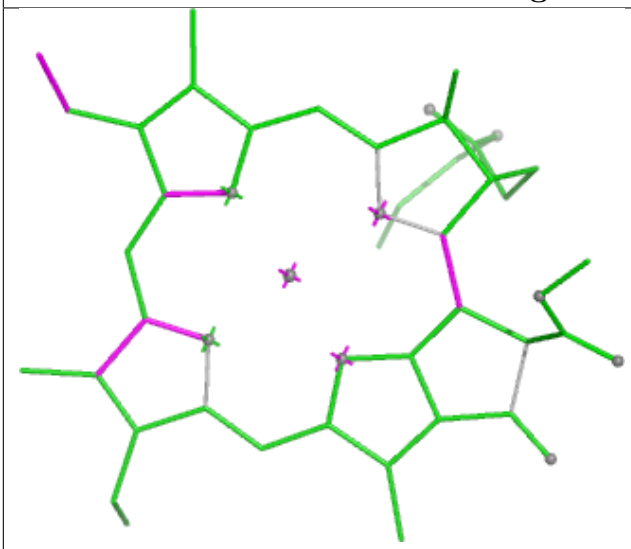


Rings

Ligand CLA r 604



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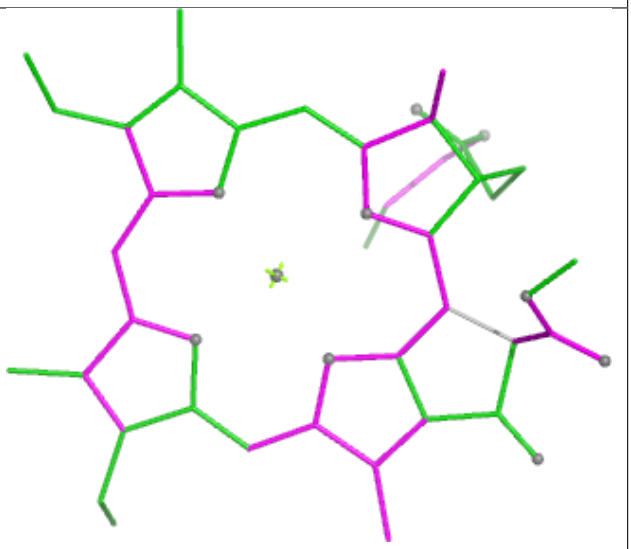
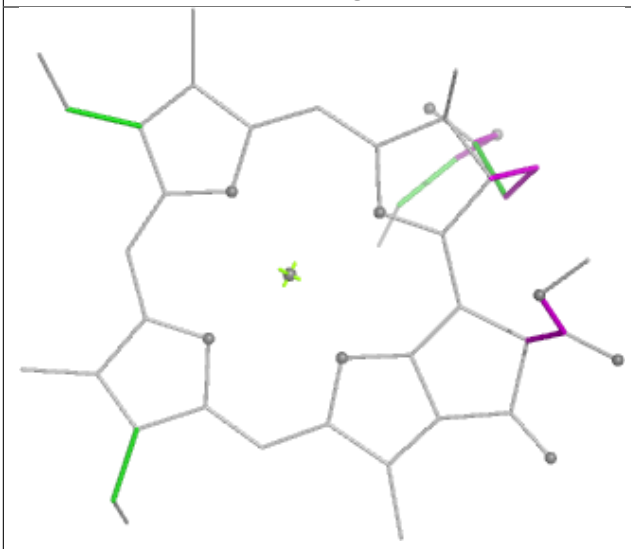


Bond angles



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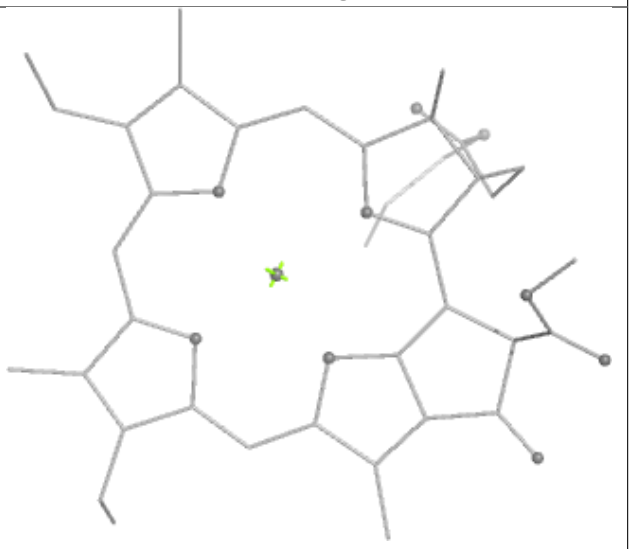
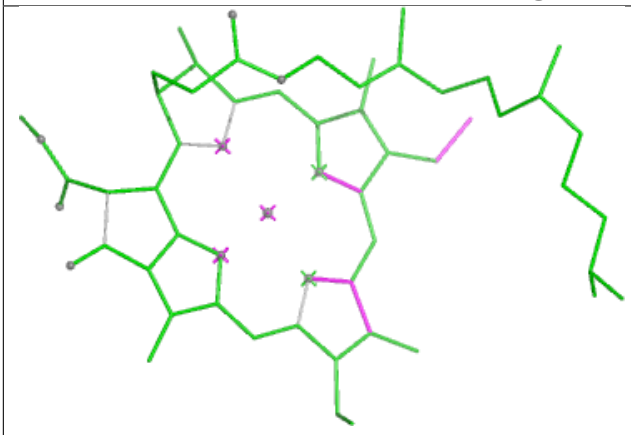


Rings

Ligand CLA r 602



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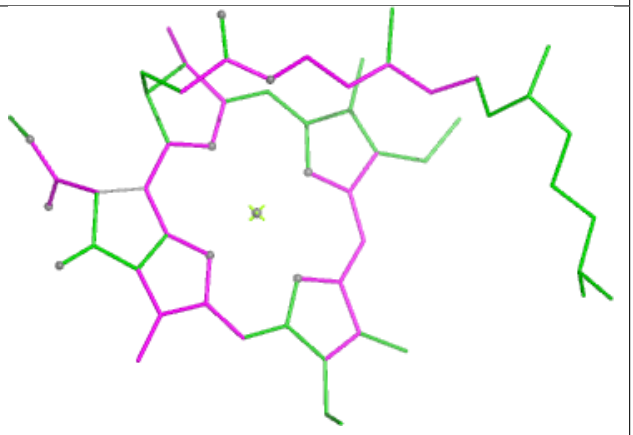

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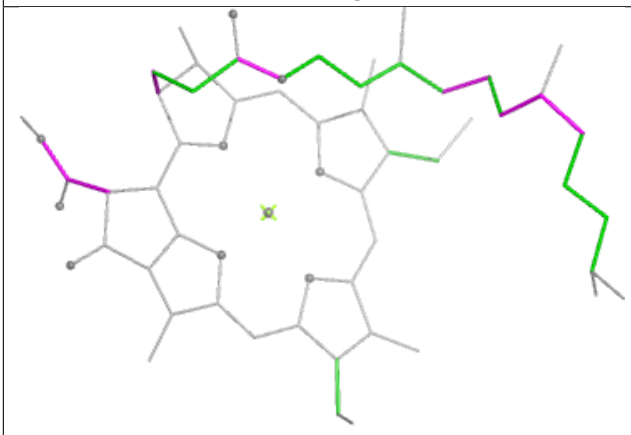

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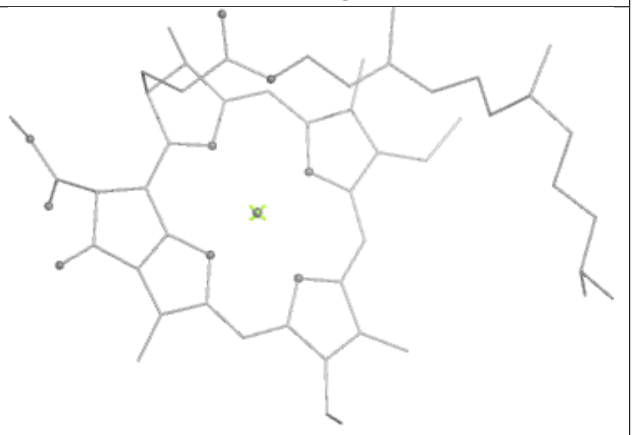
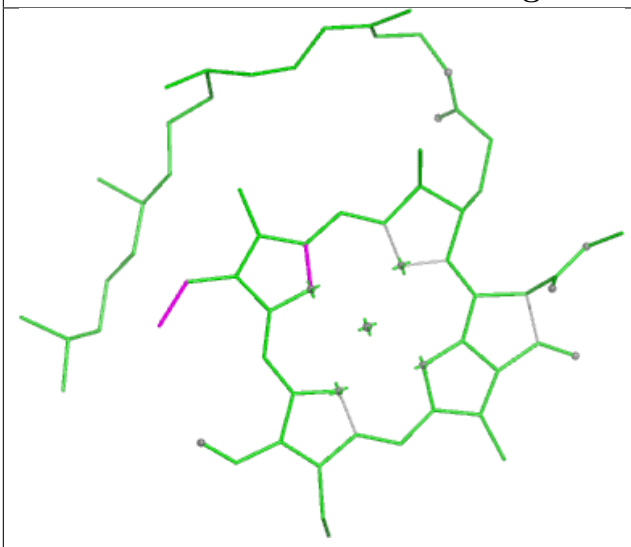


Rings

Ligand CHL N 607



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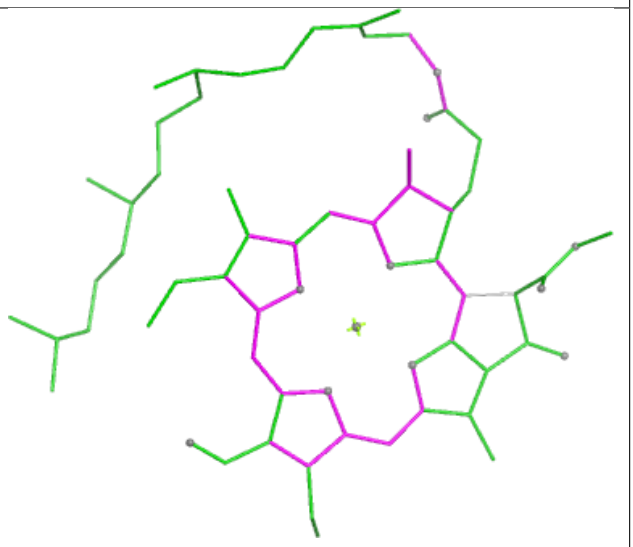
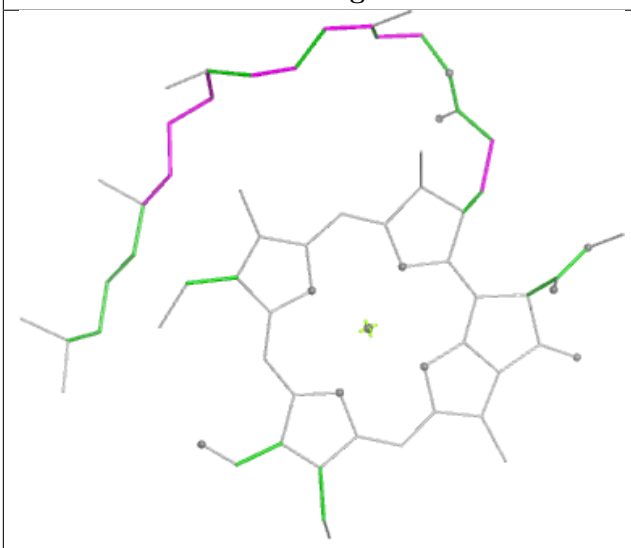


Bond angles



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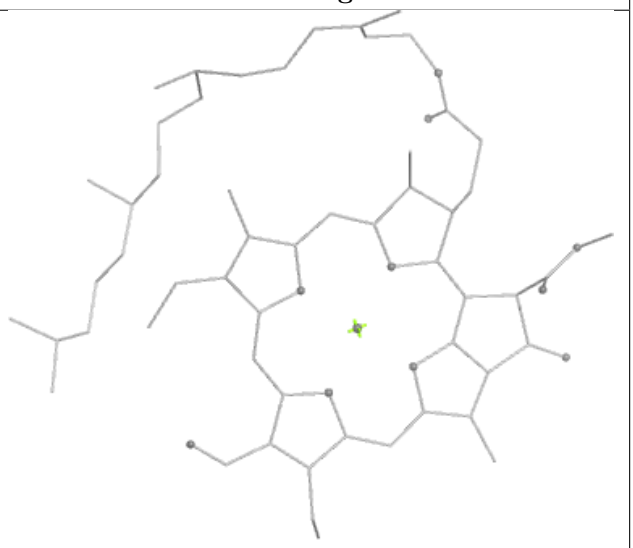
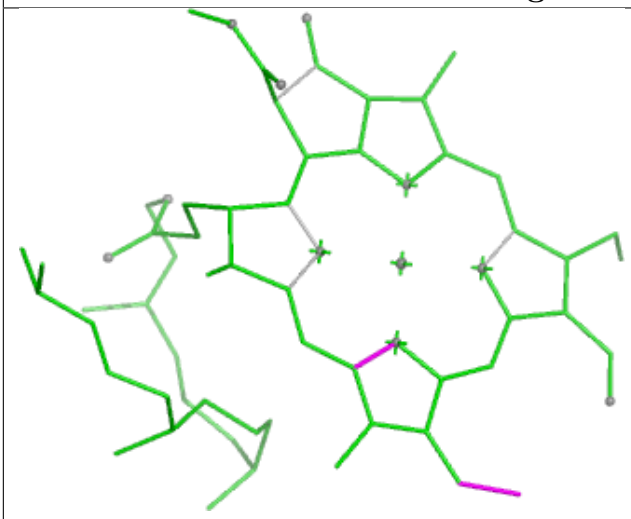


Rings

Ligand CHL y 308



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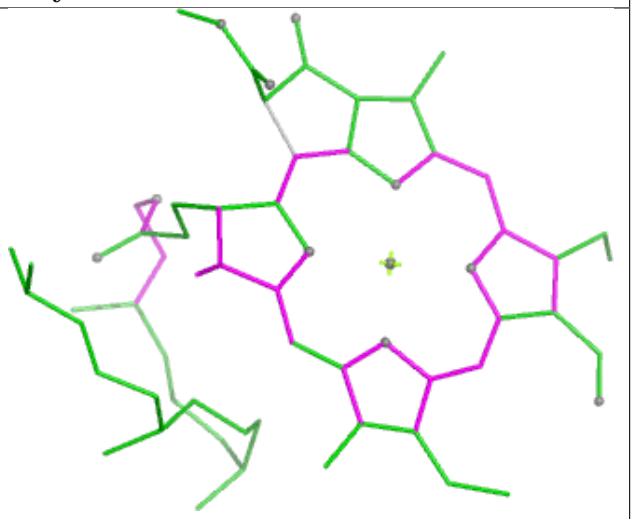

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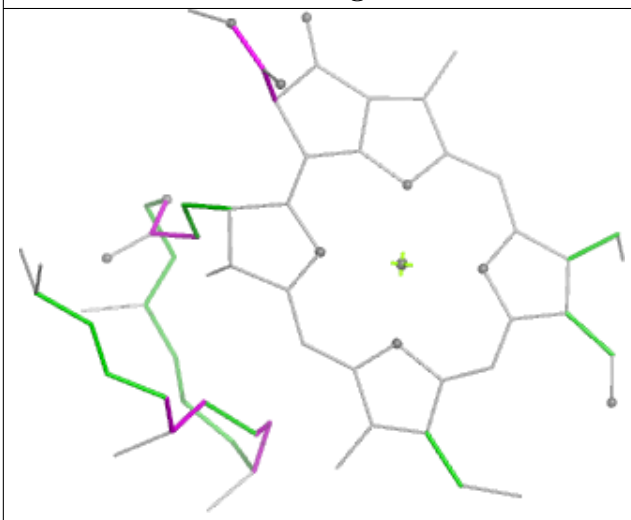

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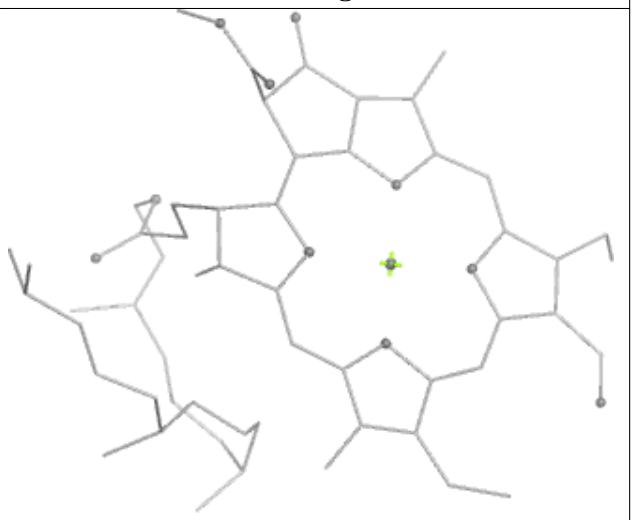
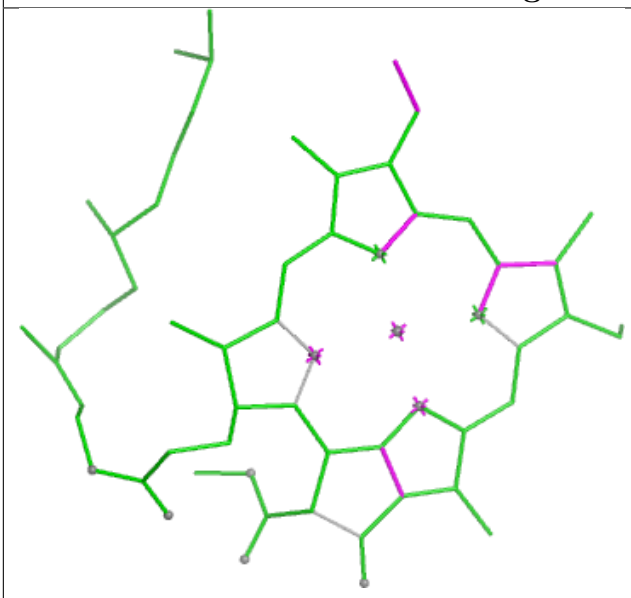


Rings

Ligand CLA N 612



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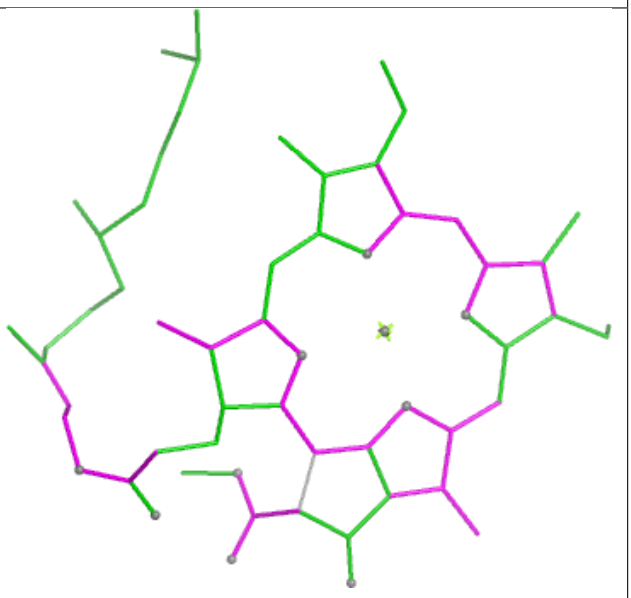
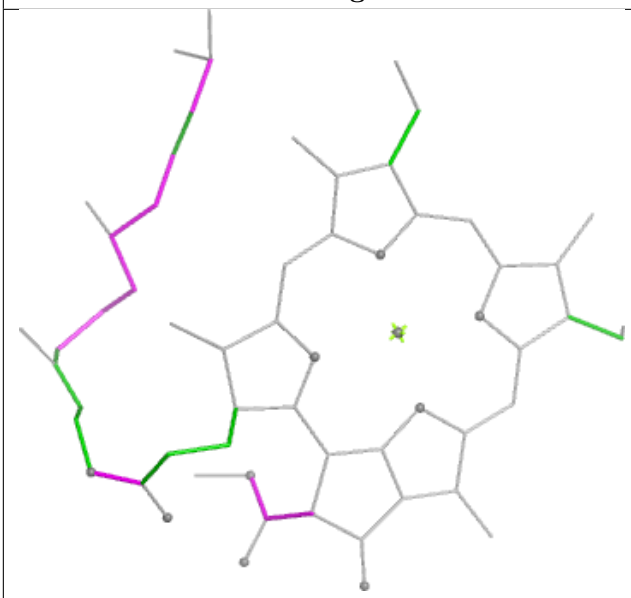


Bond angles



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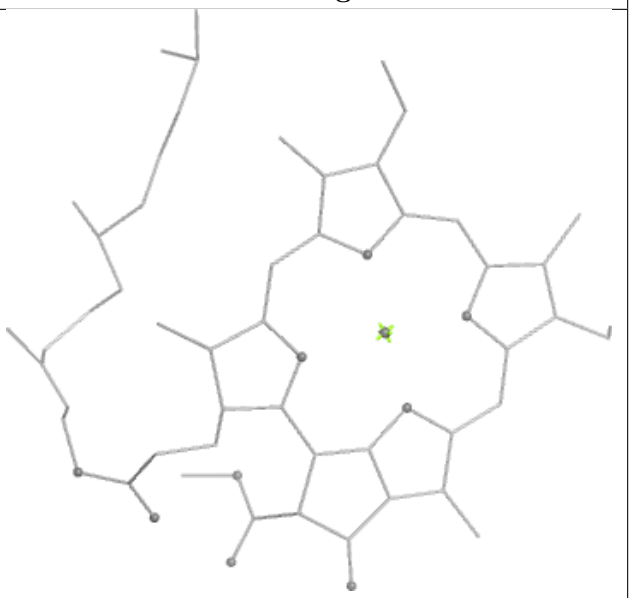
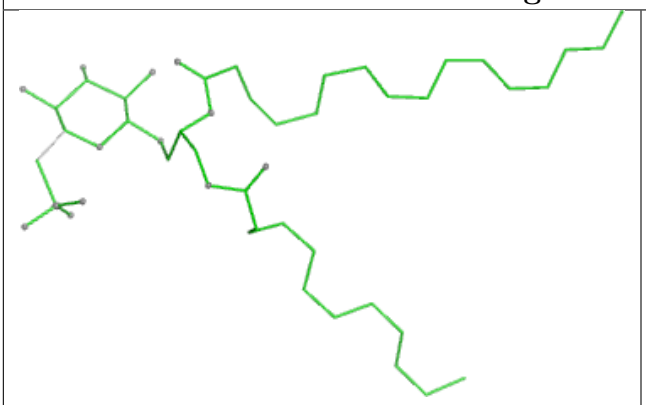


Rings

Ligand SQD A 410



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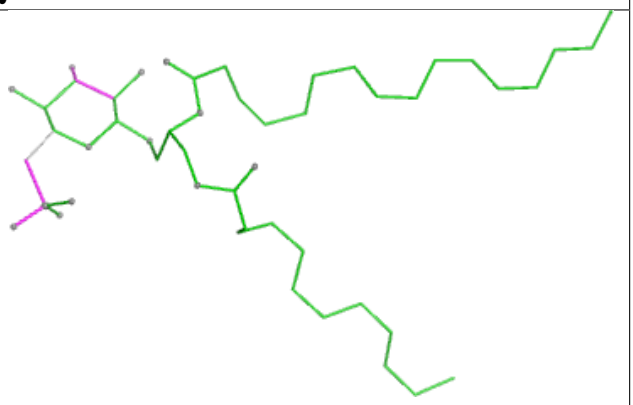
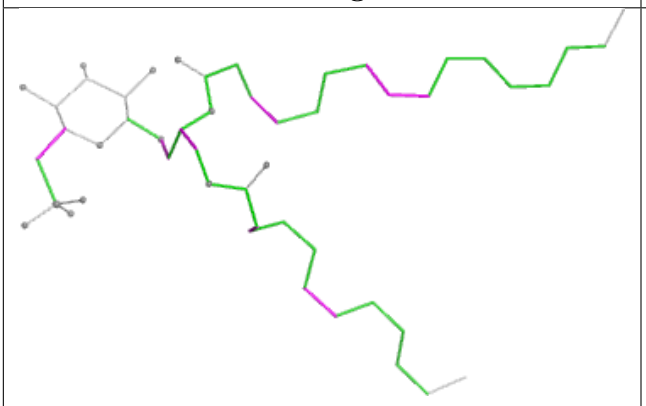


Bond angles



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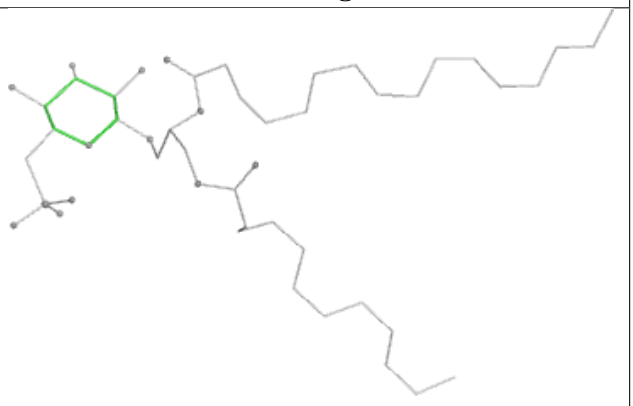
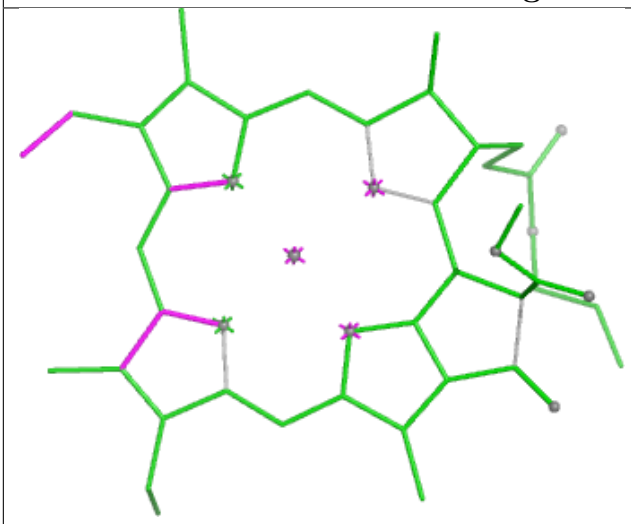


Rings

Ligand CLA G 614



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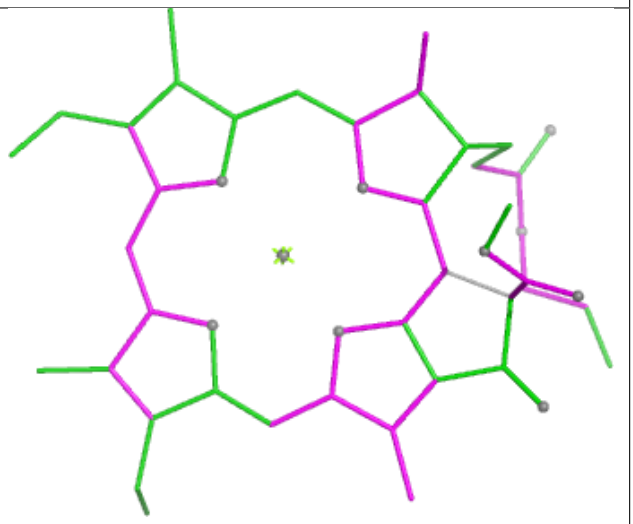
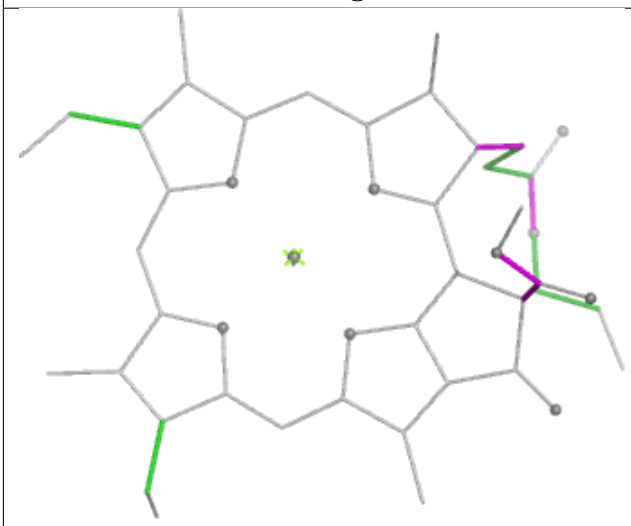


Bond angles



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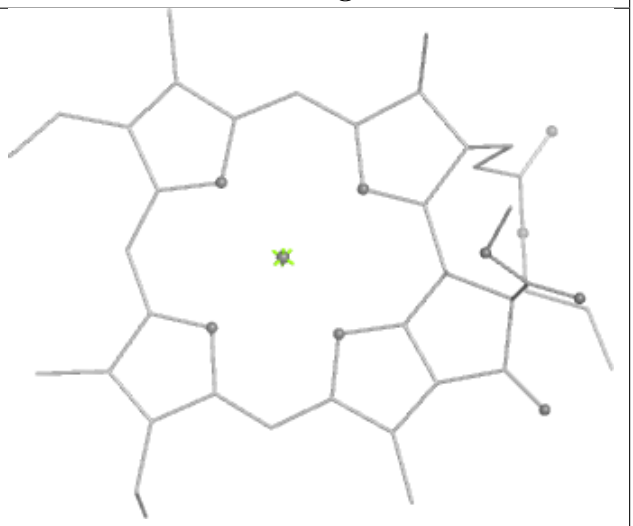
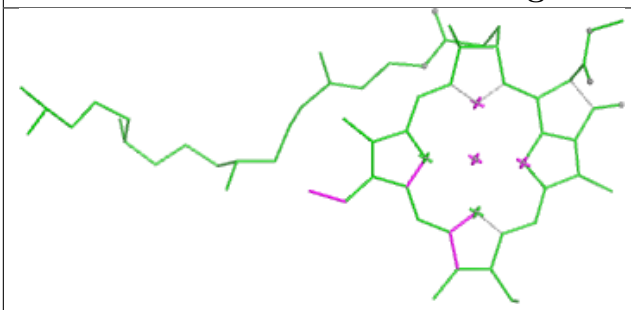


Rings

Ligand CLA b 603



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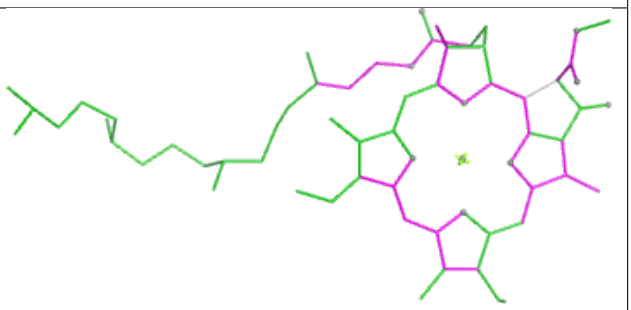
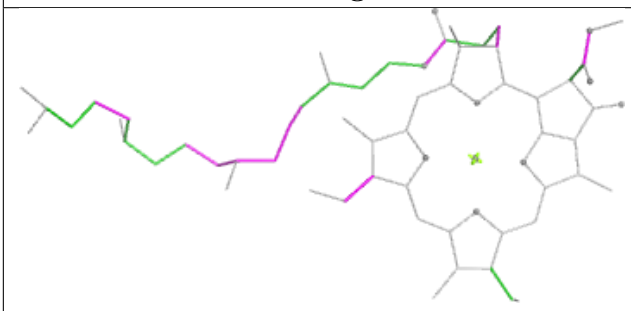


Bond angles

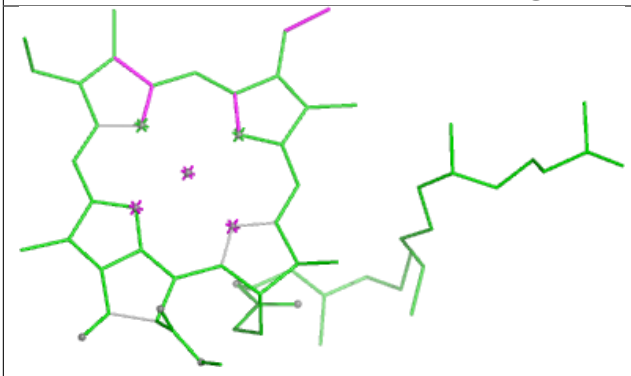


Torsions



Rings

Ligand CLA d 401



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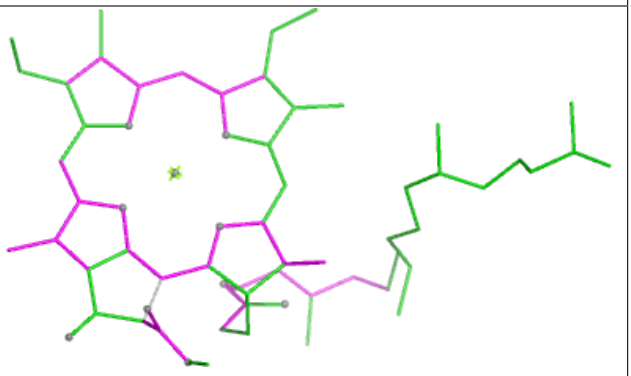
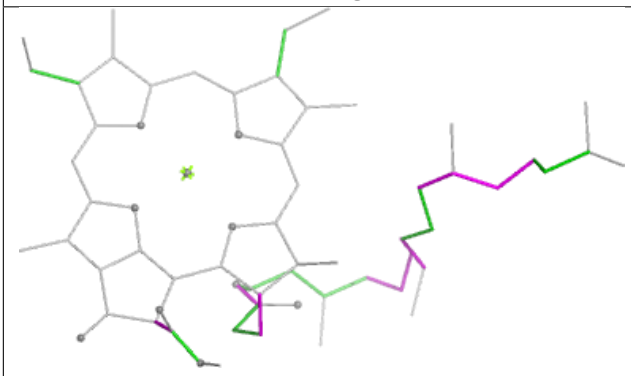
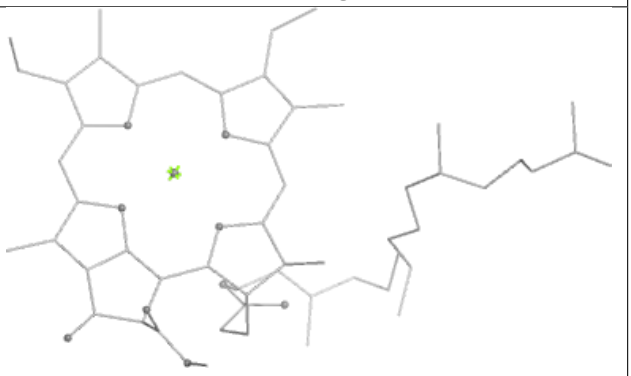


Bond angles

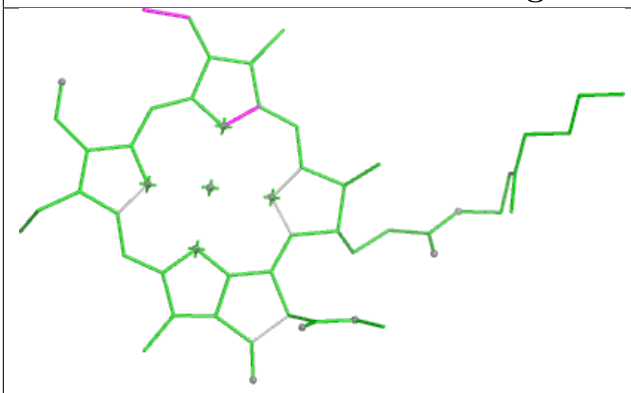


Torsions



Rings

Ligand CHL n 601



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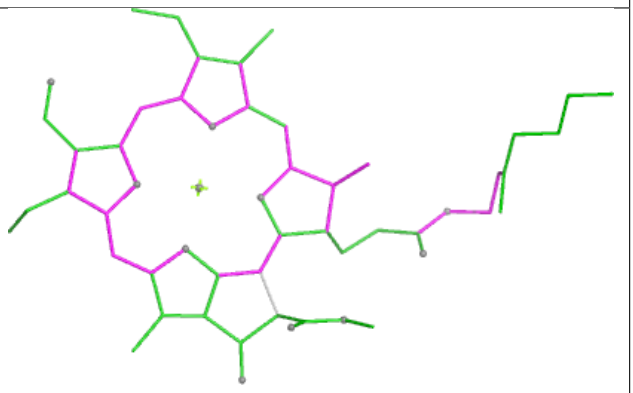

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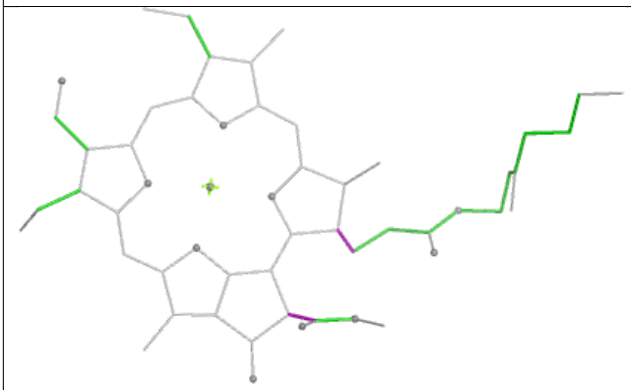

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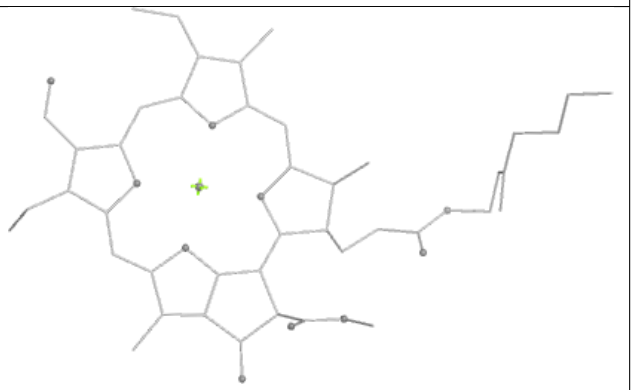
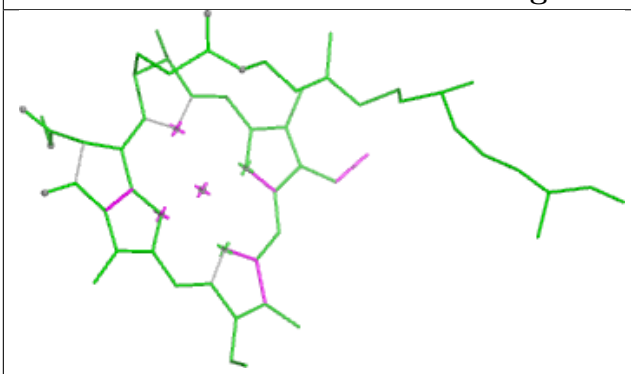


Rings

Ligand CLA s 602



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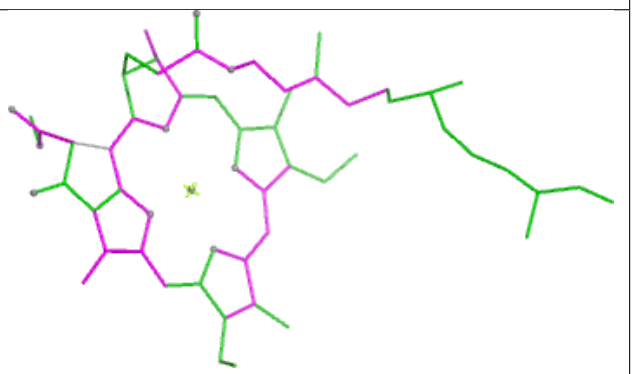

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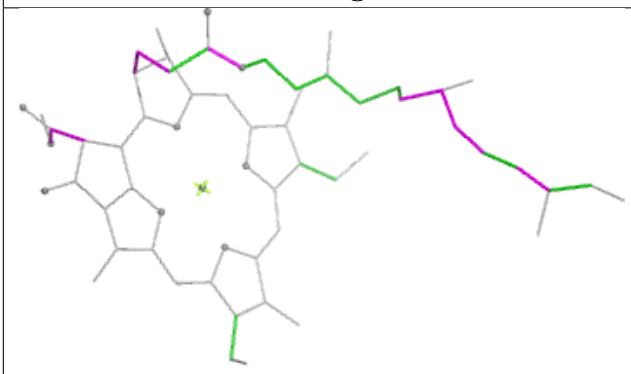
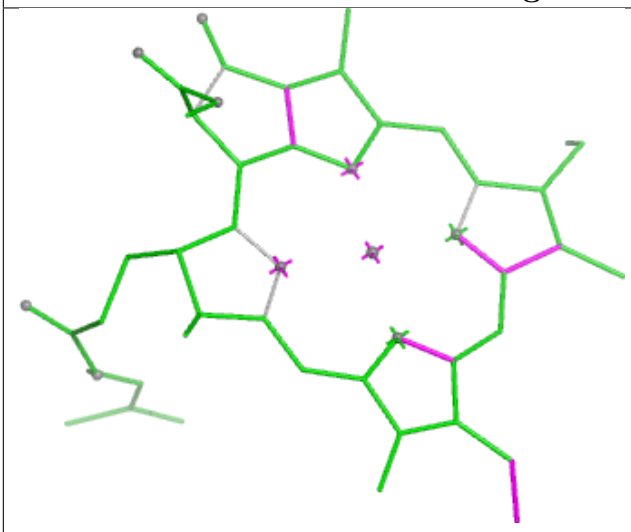


Torsions



Rings

Ligand CLA G 604



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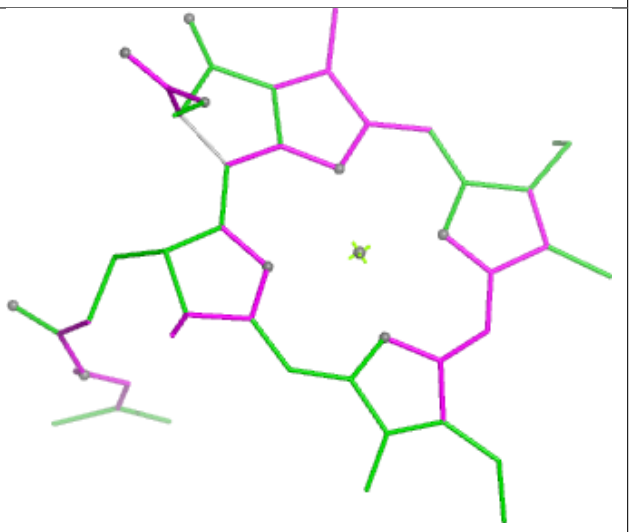
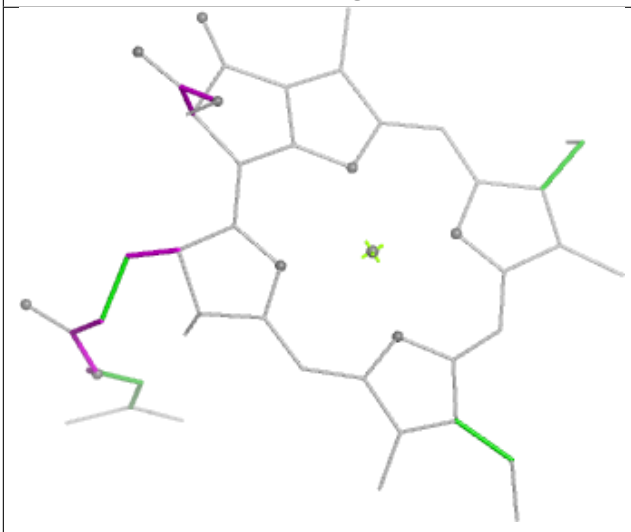


Bond angles



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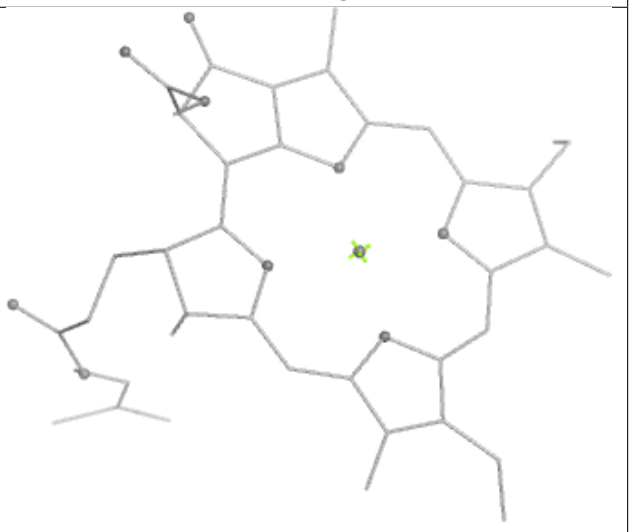
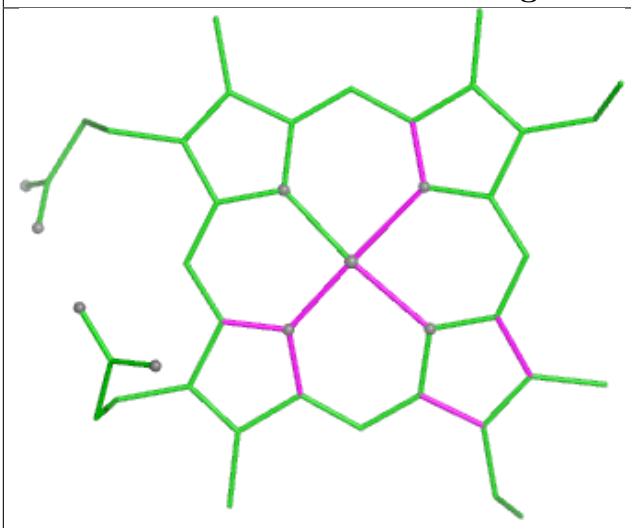


Rings

Ligand HEM E 101



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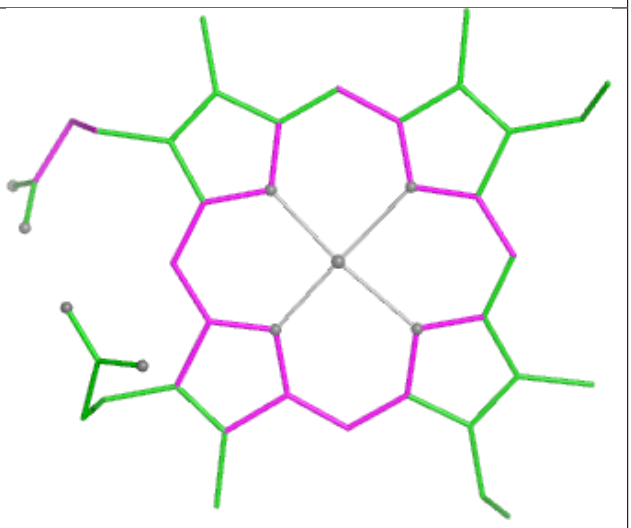
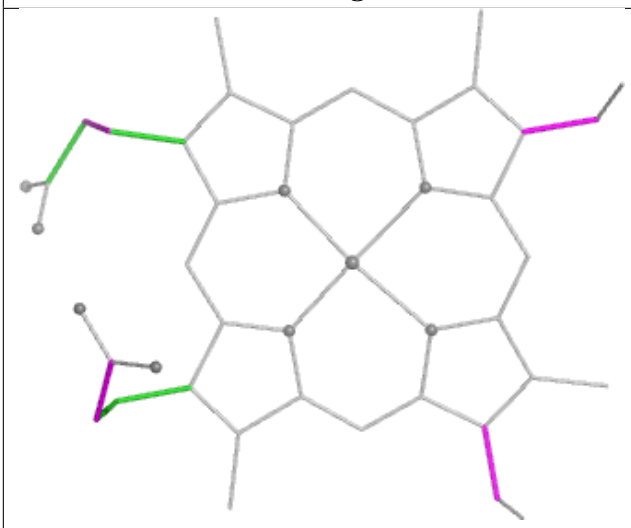


Bond angles



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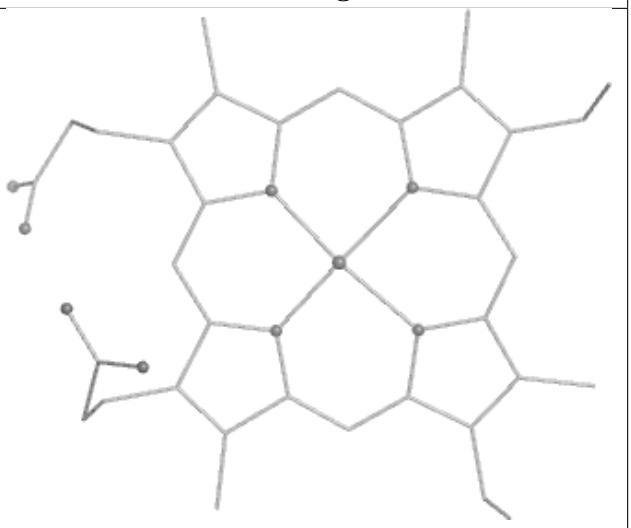
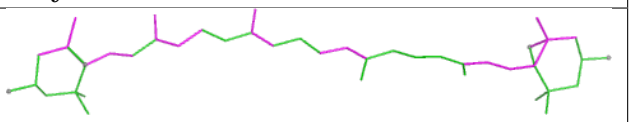


Rings

Ligand XAT y 317



Bond lengths



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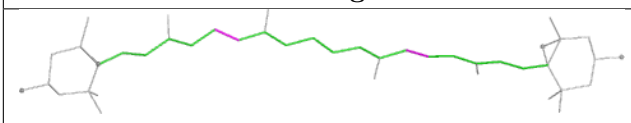

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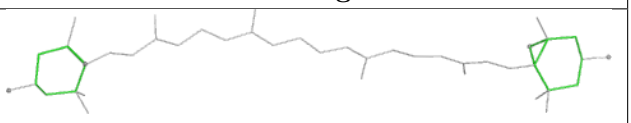
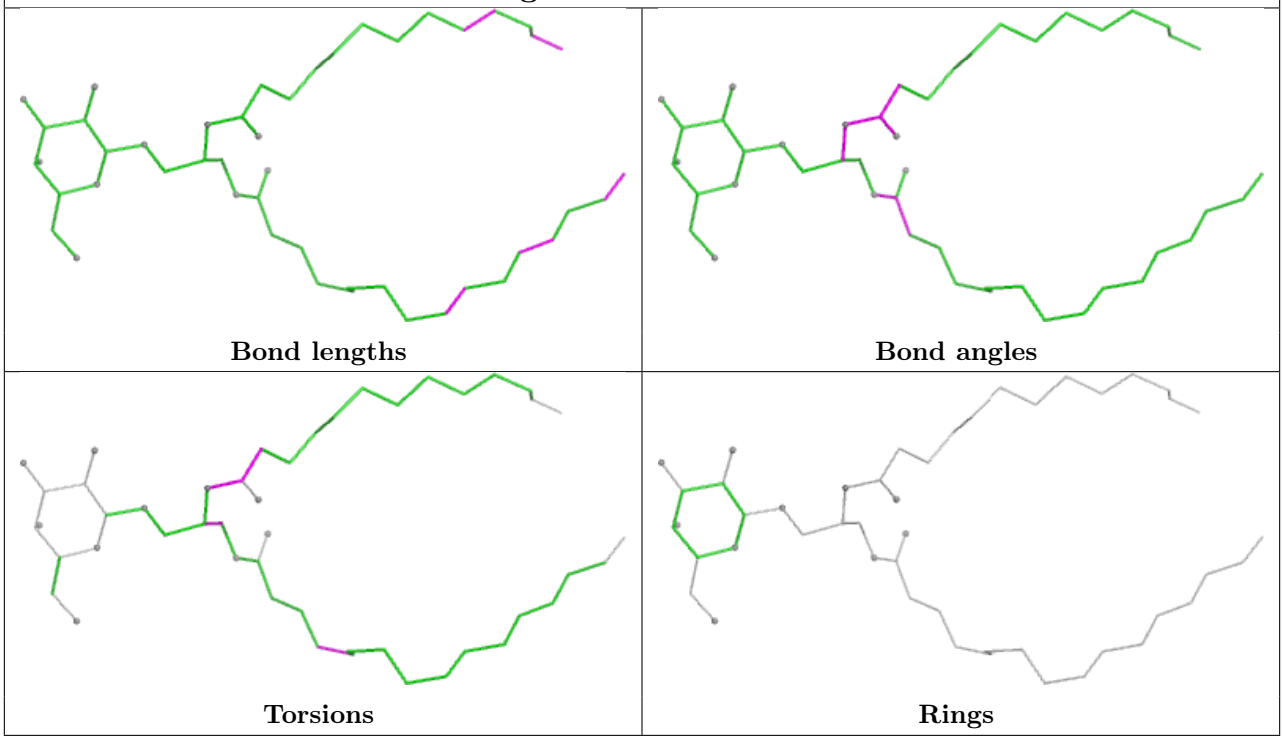
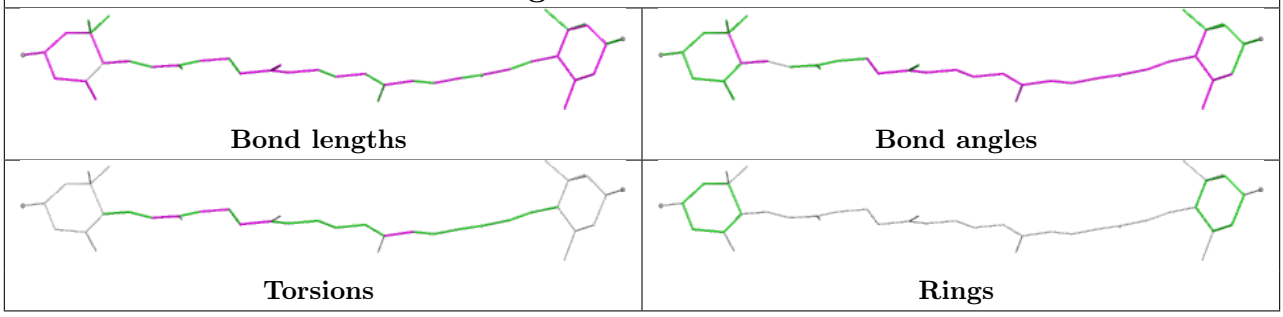


Rings

Ligand LMG A 411



Ligand LUT S 315



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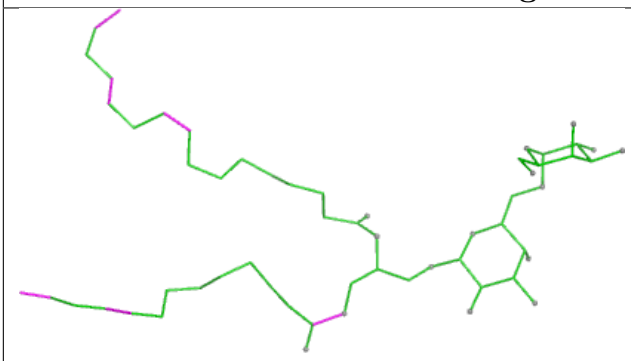

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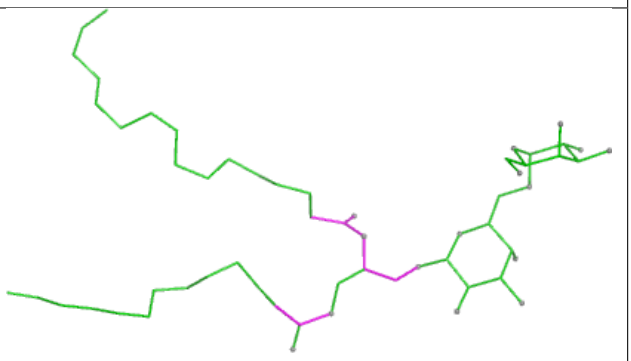
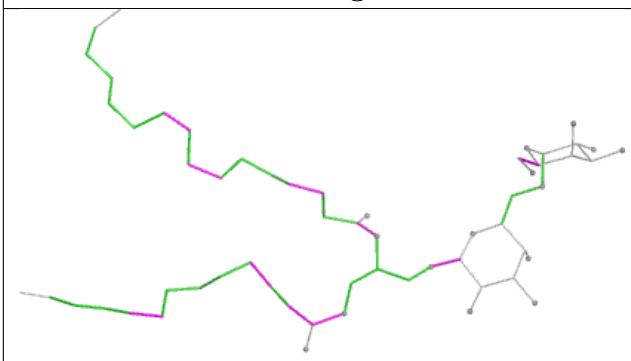


Bond angles



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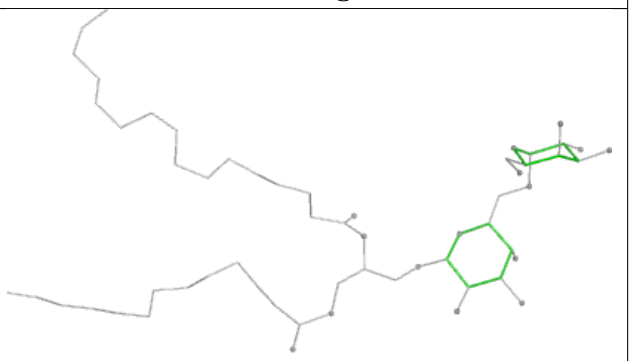
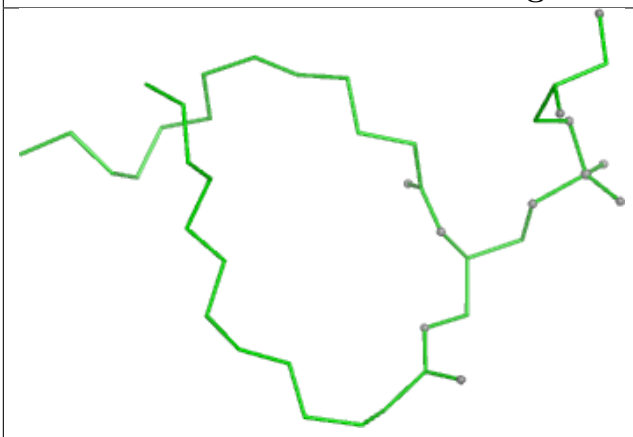


Rings

Ligand LHG a 415



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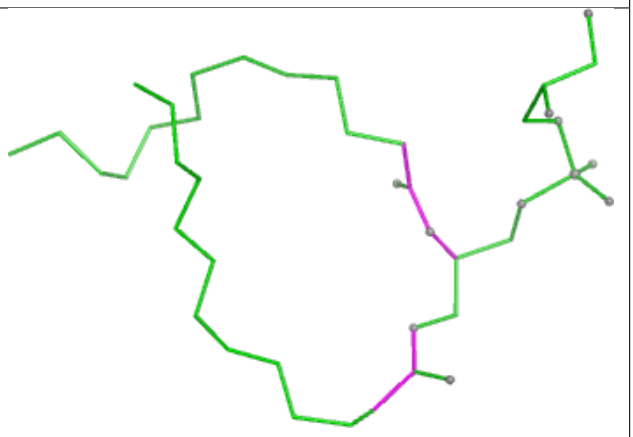
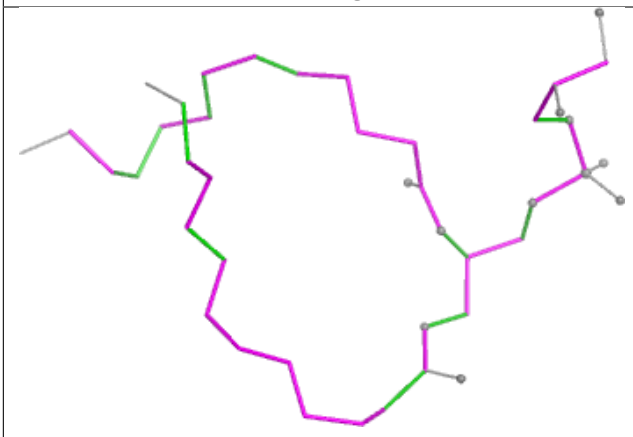


Bond angles



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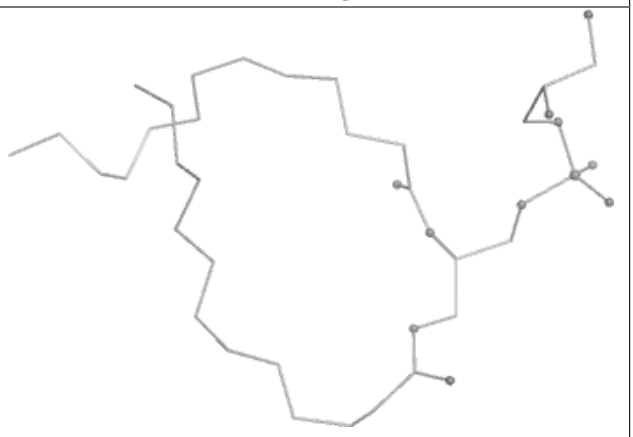
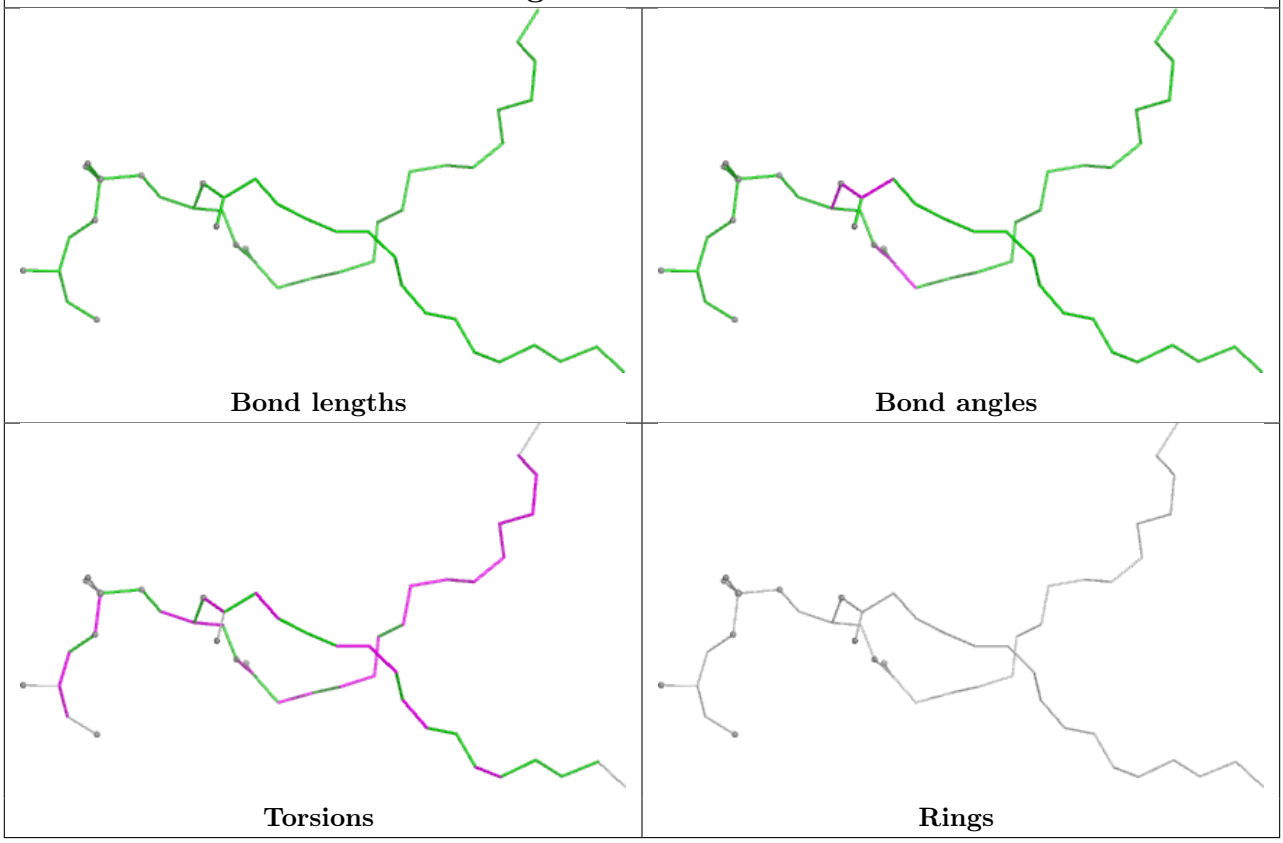
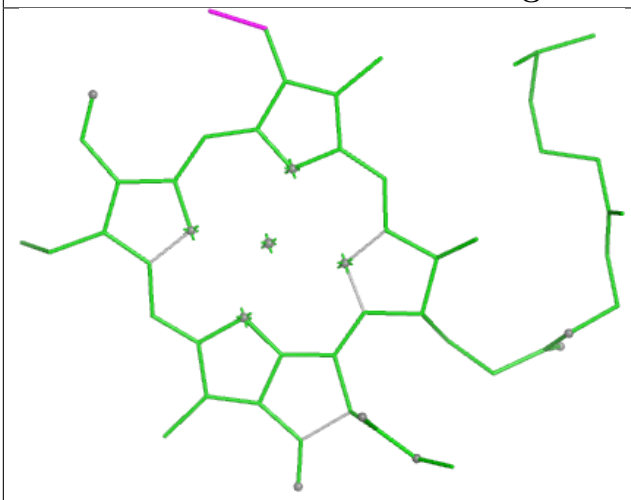


Rings

Ligand LHG d 408



Ligand CHL G 607



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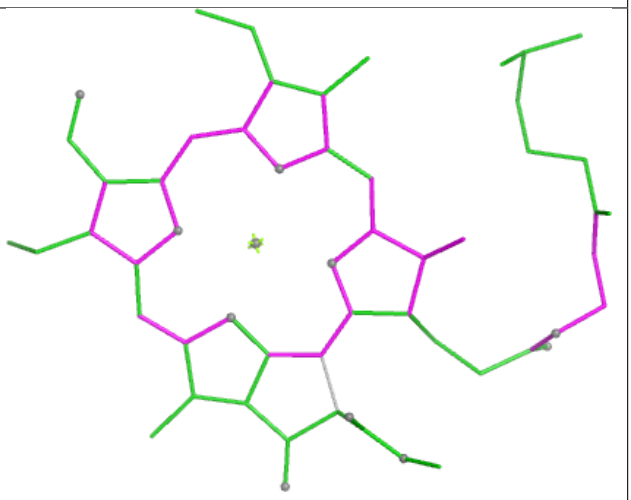
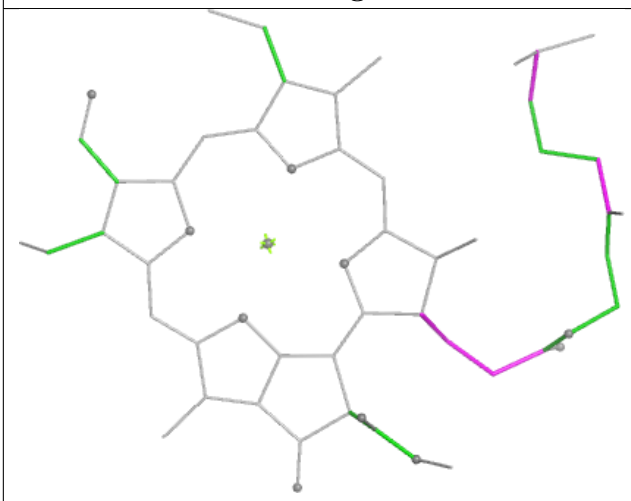


Bond angles



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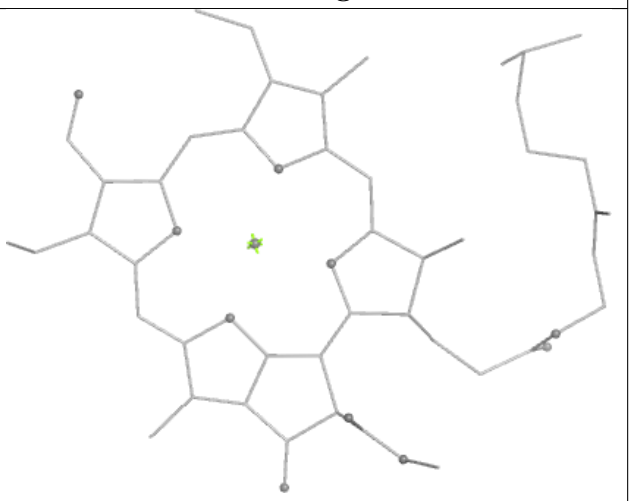
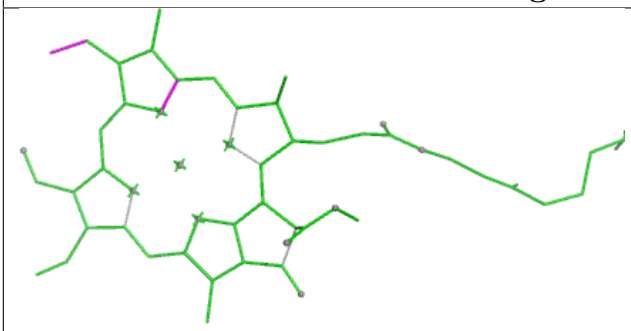


Rings

Ligand CHL r 606



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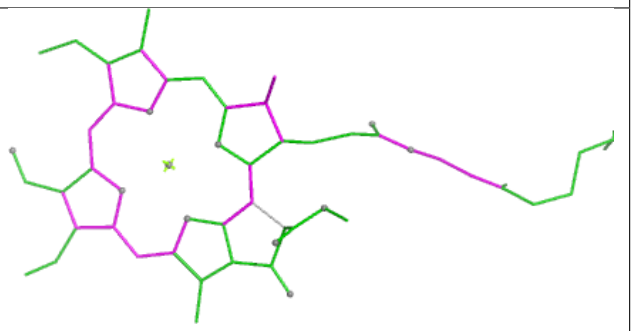
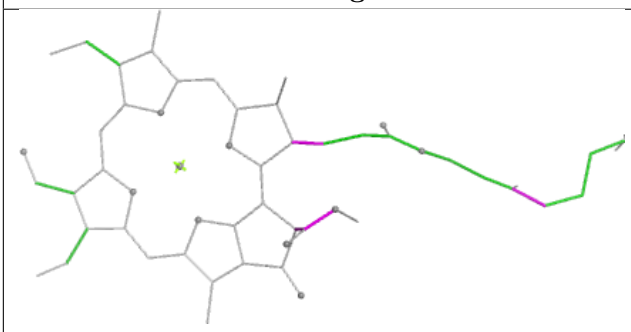


Bond angles



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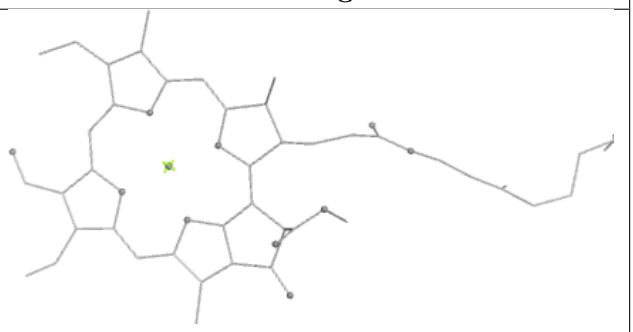
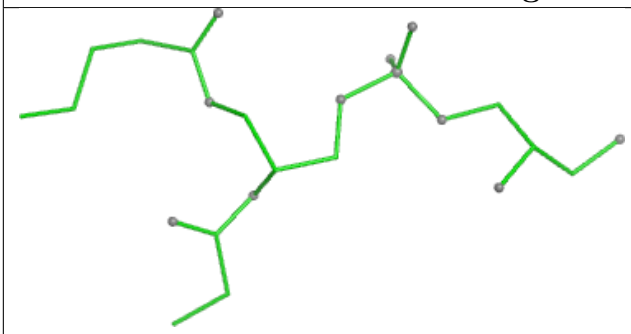


Rings

Ligand LHG R 616



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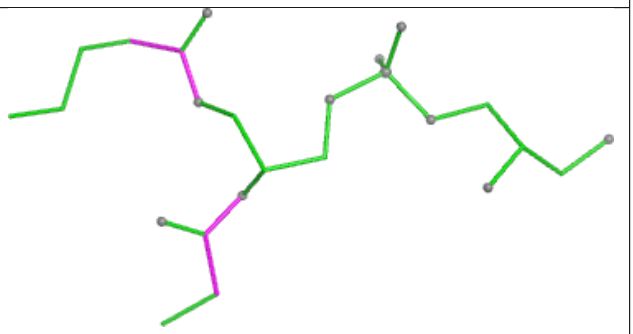
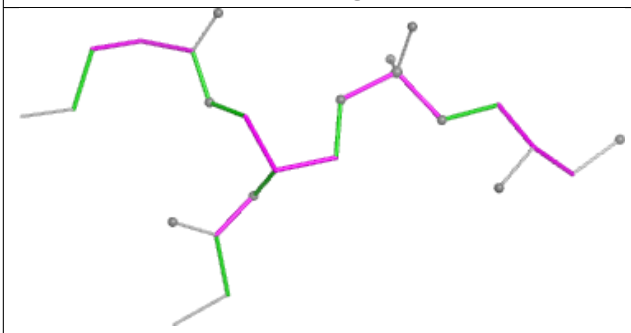


Bond angles



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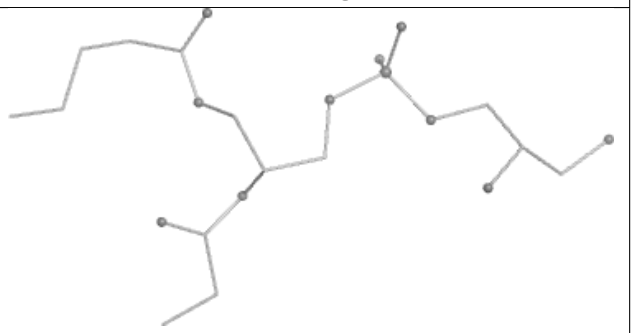
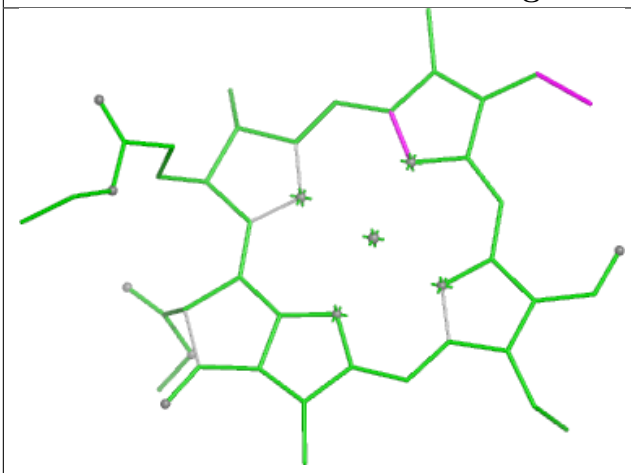


Rings

Ligand CHL N 605



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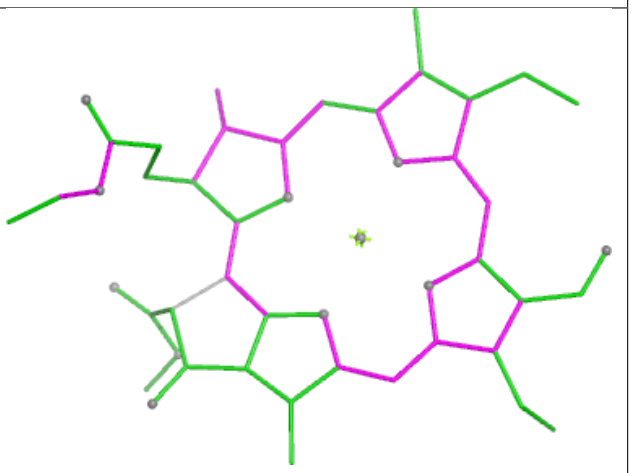
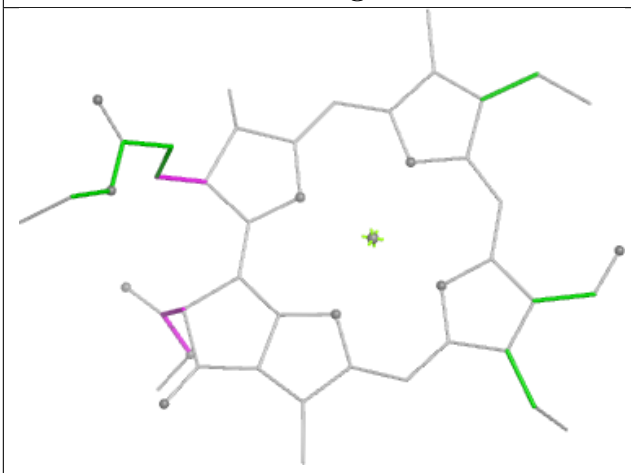


Bond angles



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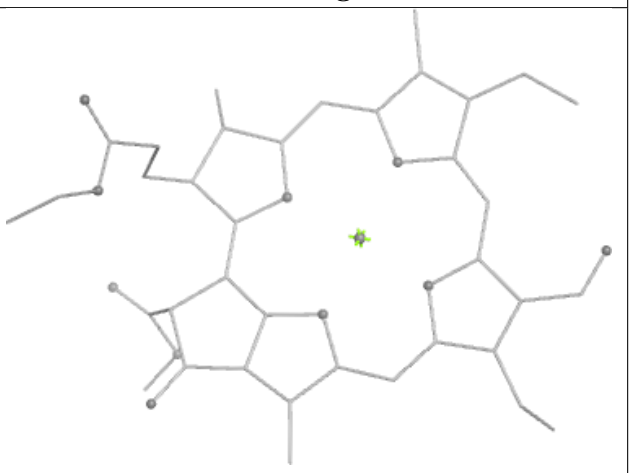
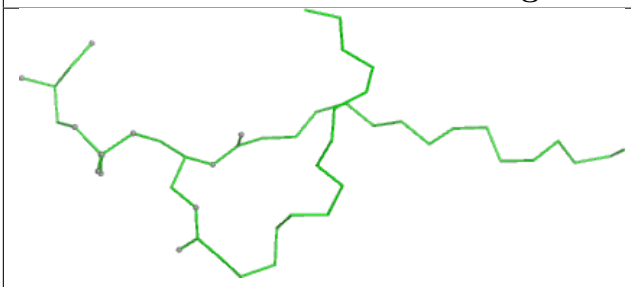
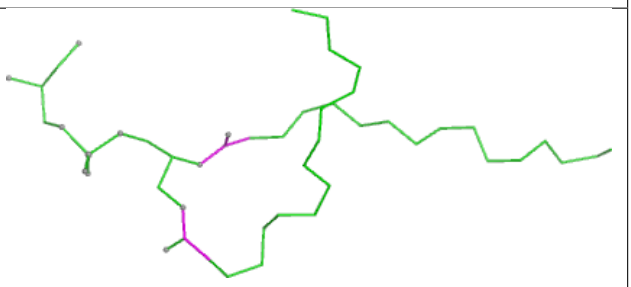


Rings

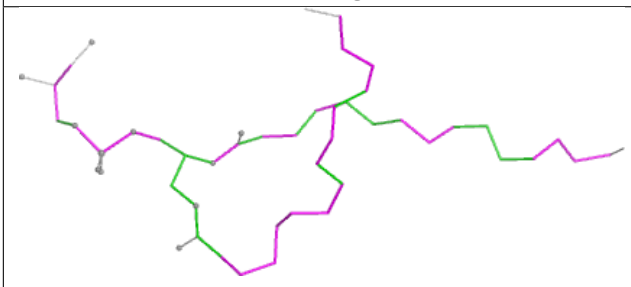
Ligand LHG G 618



Bond lengths



Bond angles

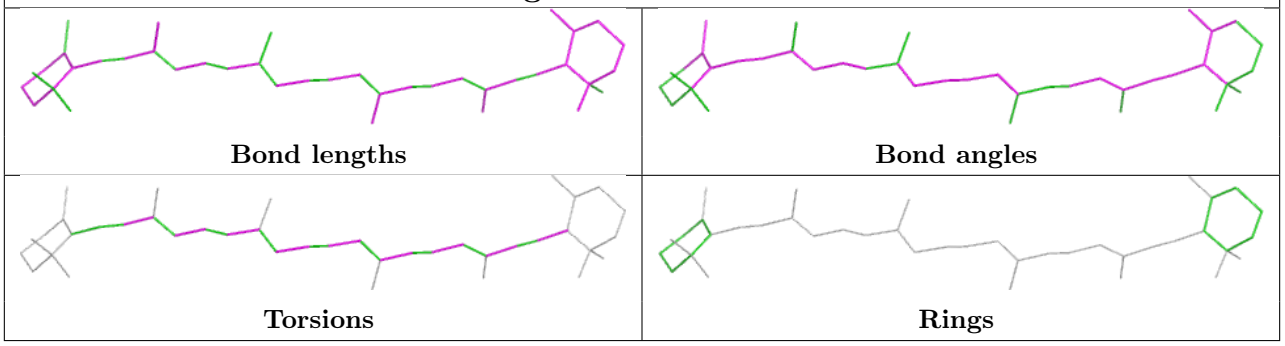


Torsions

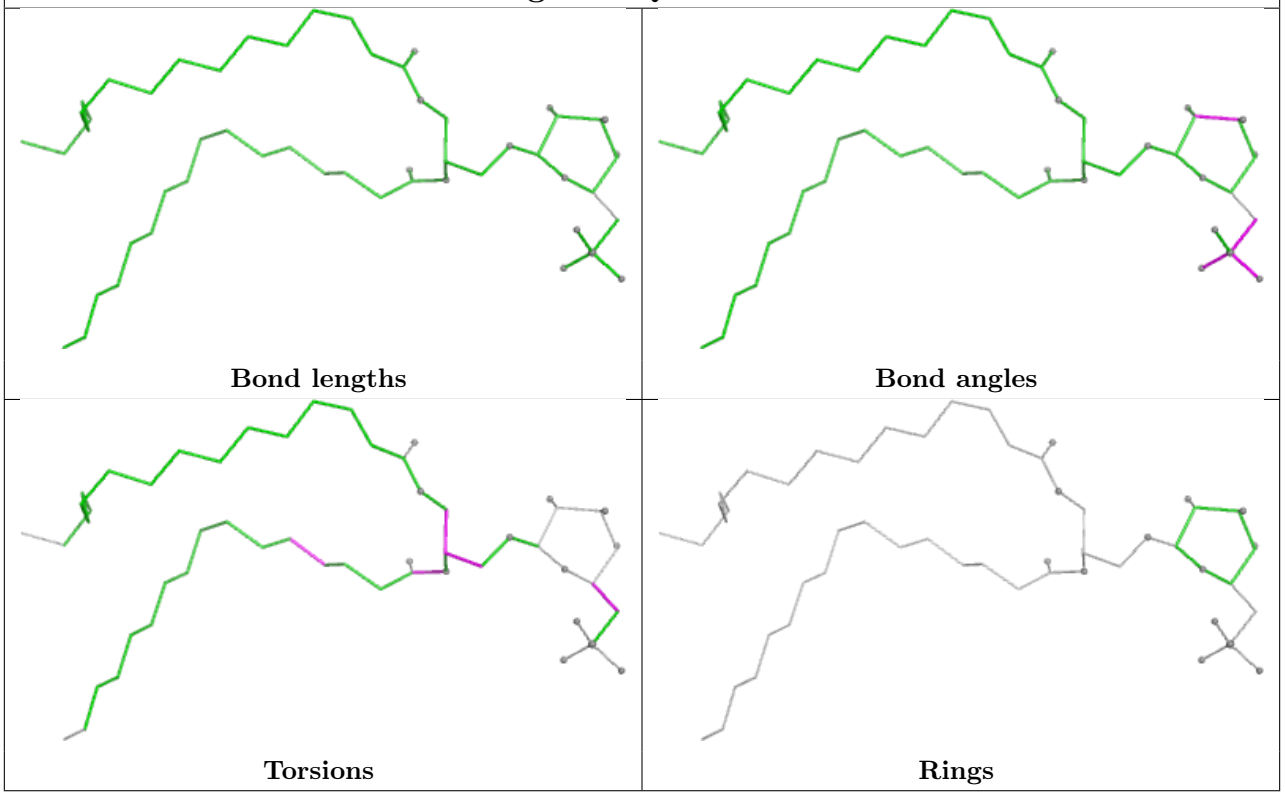


Rings

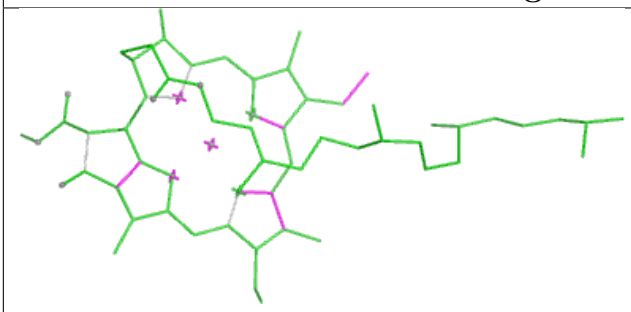
Ligand BCR B 617



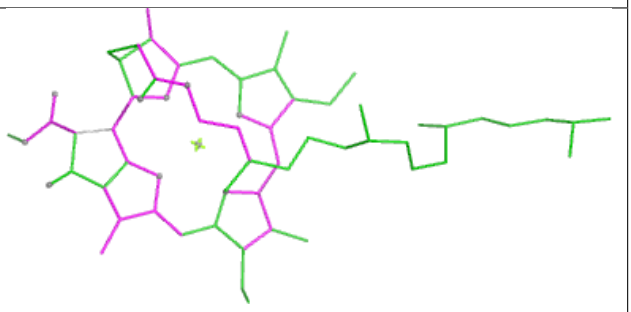
Ligand SQD L 103



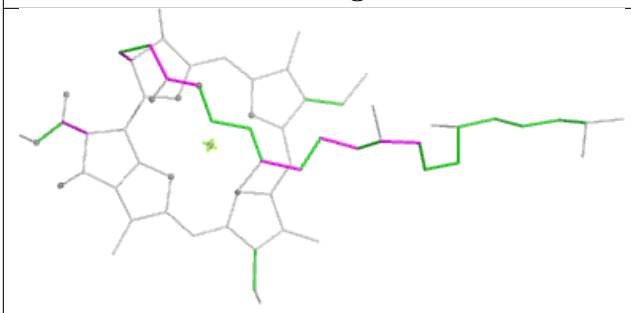
Ligand CLA C 505



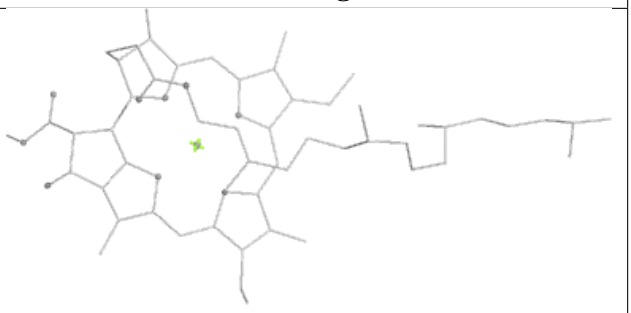
Bond lengths



Bond angles

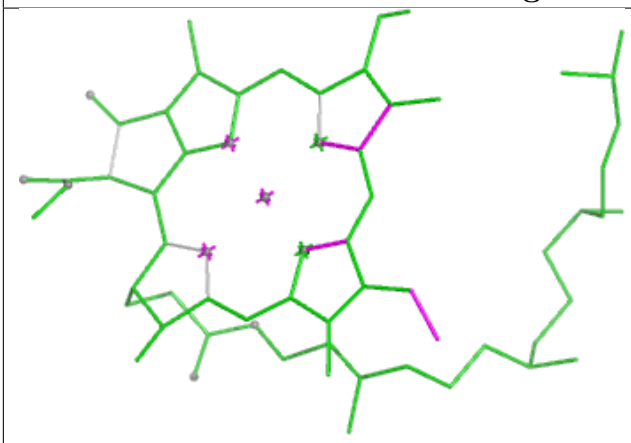


Torsions



Rings

Ligand CLA G 602



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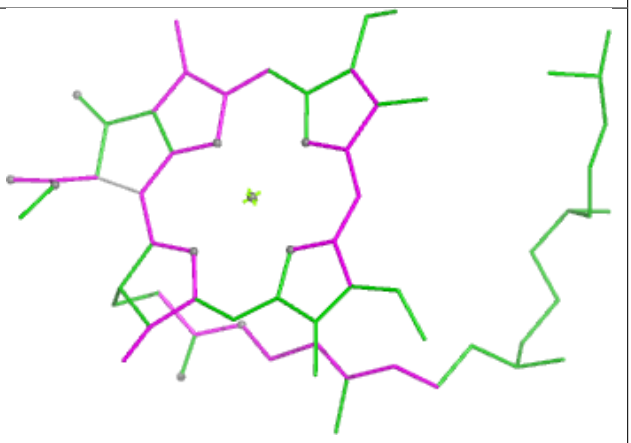
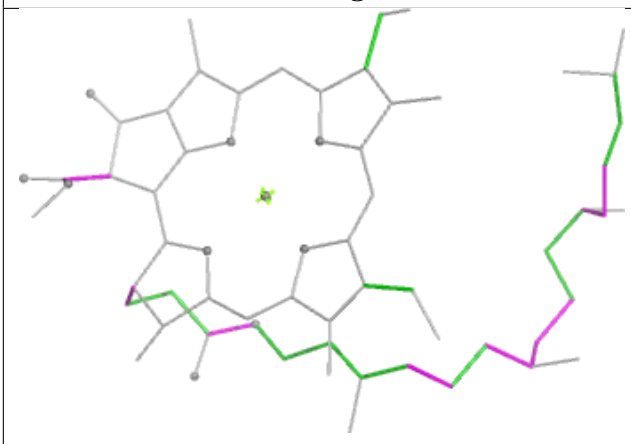


Bond angles



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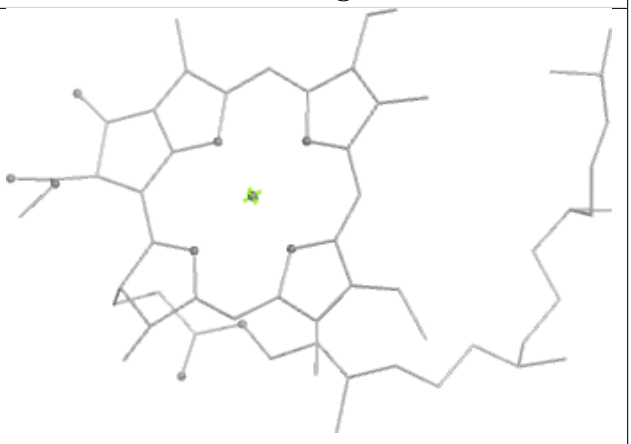
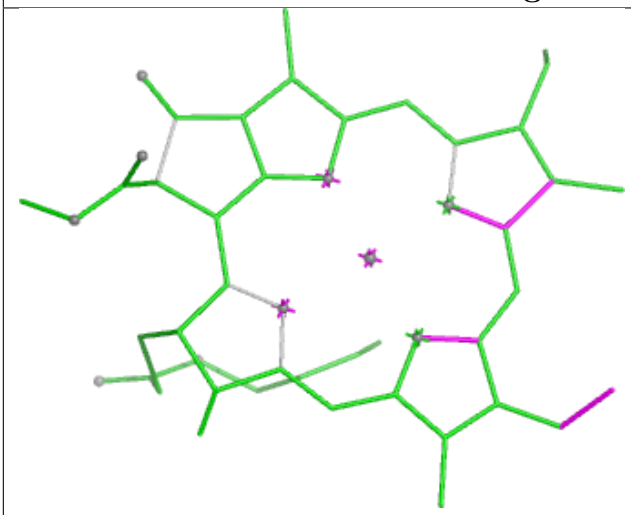


Rings

Ligand CLA R 610



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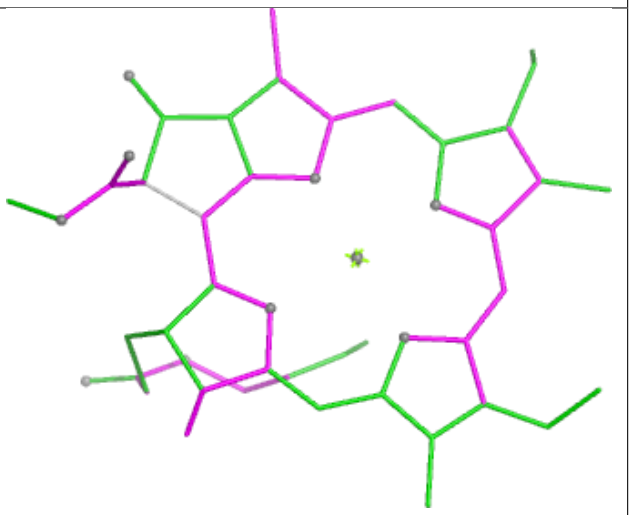

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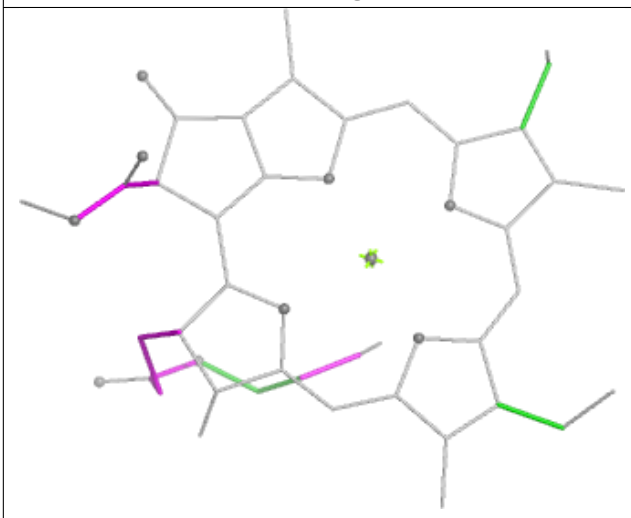

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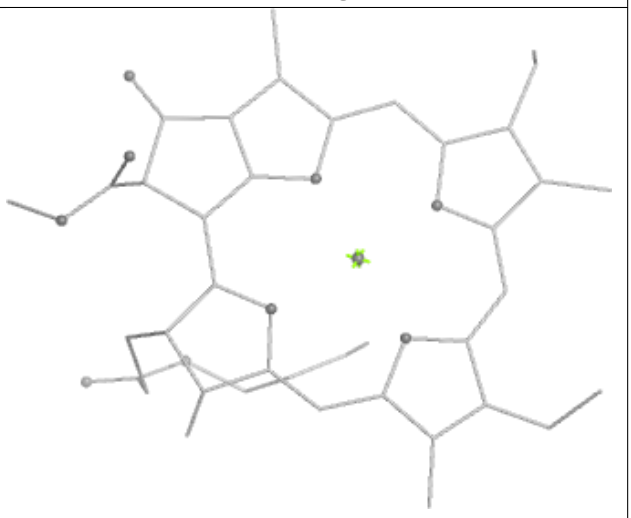
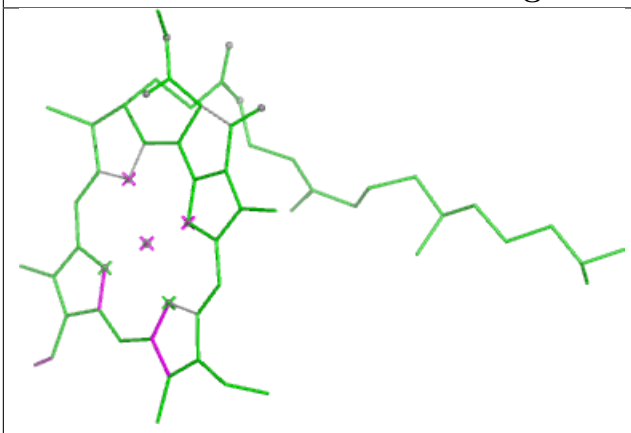


Rings

Ligand CLA Y 611



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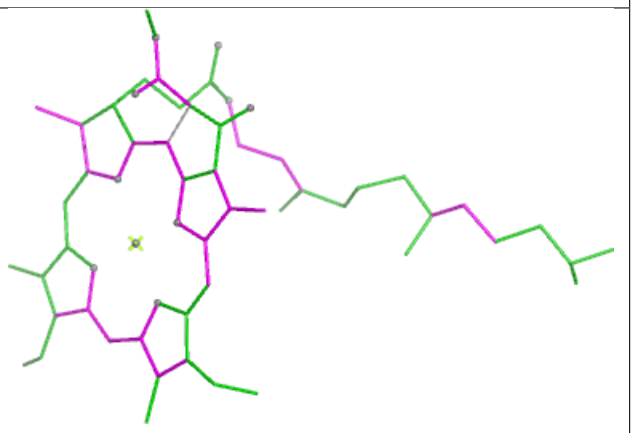

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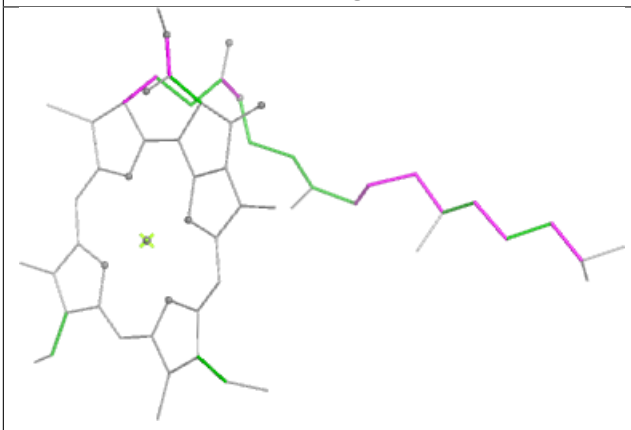

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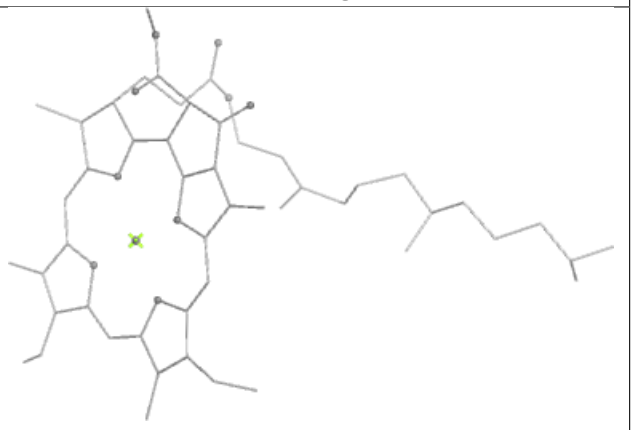
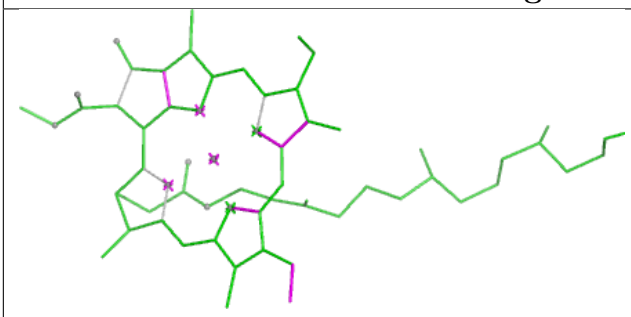


Rings

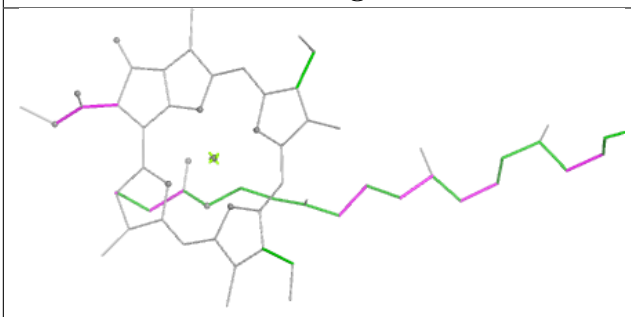
Ligand CLA B 608



Bond lengths



Bond angles



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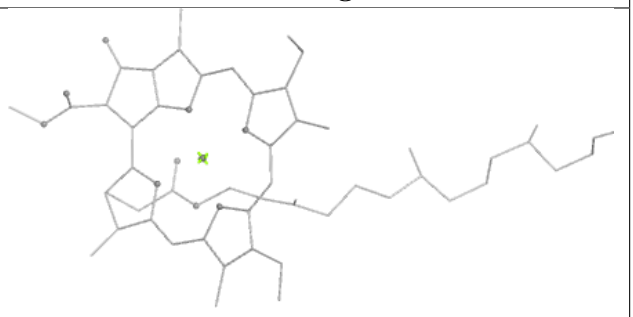
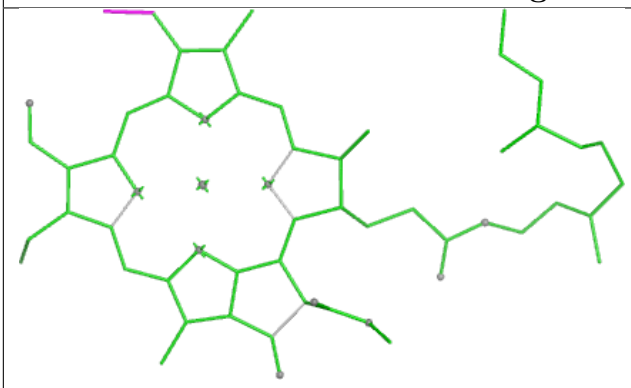


Rings

Ligand CHL s 606



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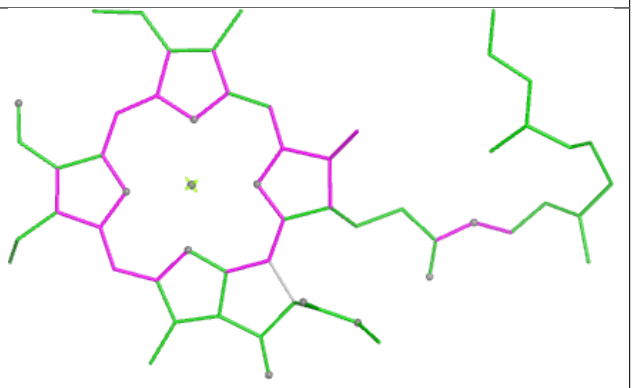
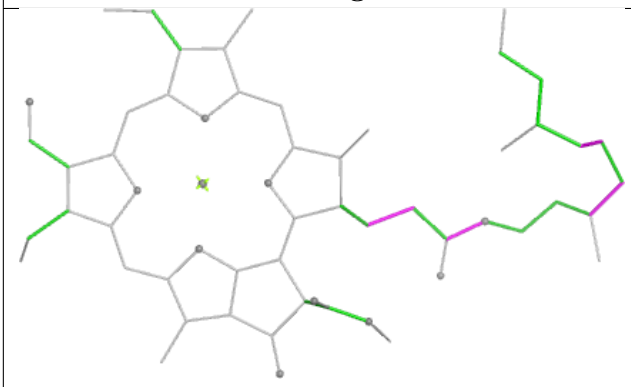


Bond angles

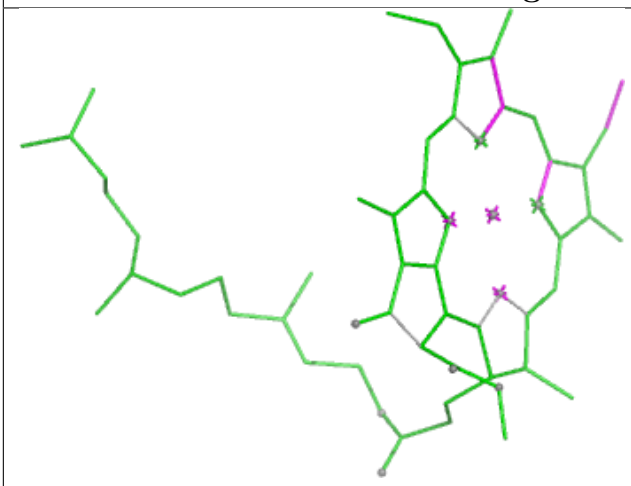


Torsions



Rings

Ligand CLA G 611



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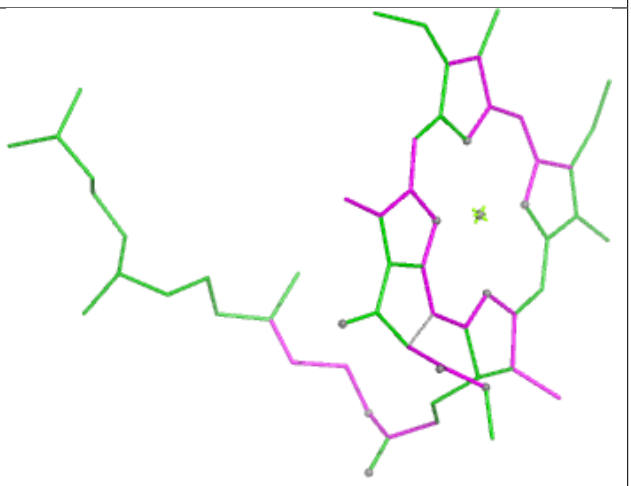
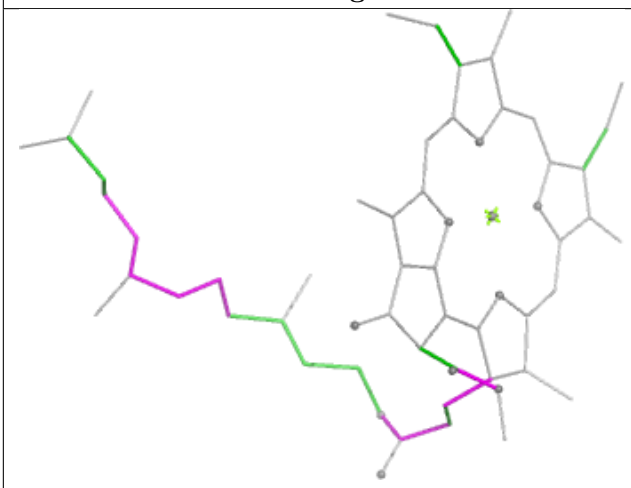


Bond angles



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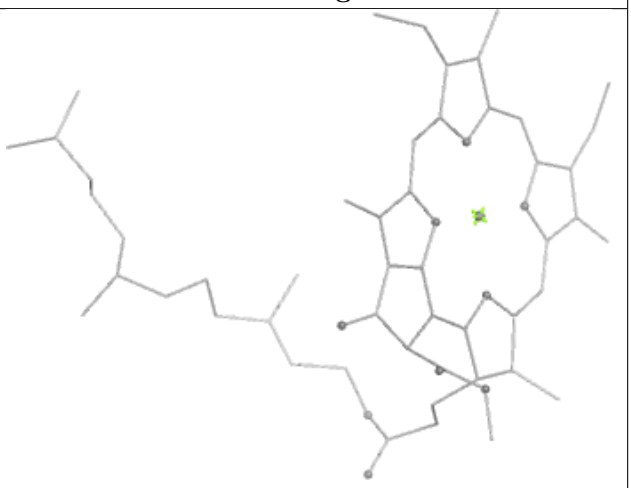
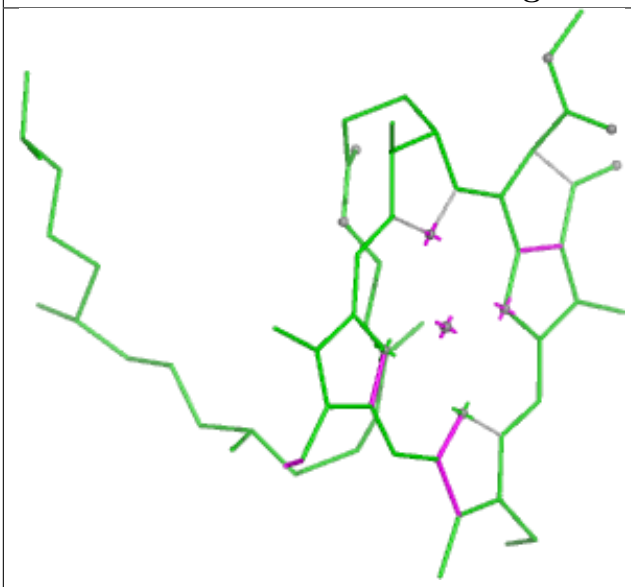


Rings

Ligand CLA G 613



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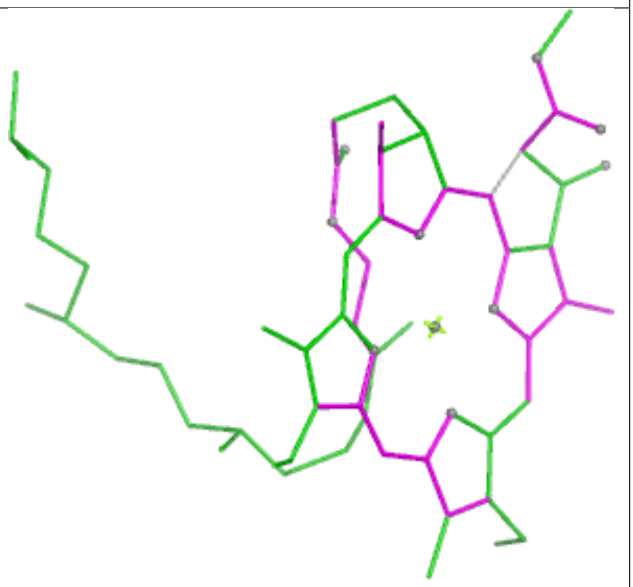
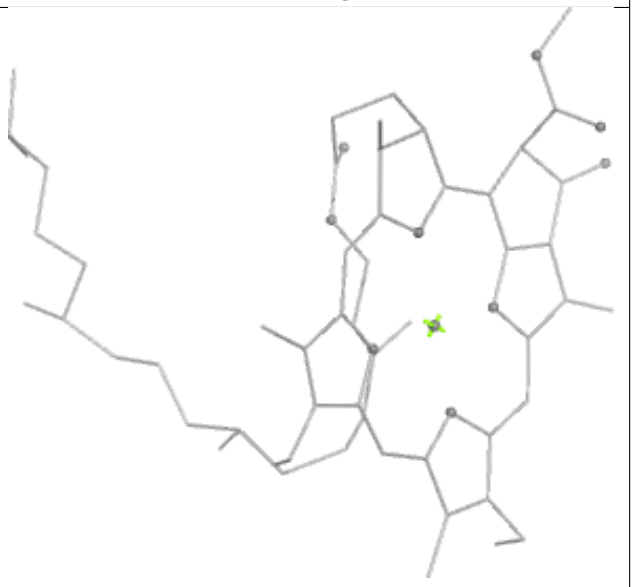


Bond angles

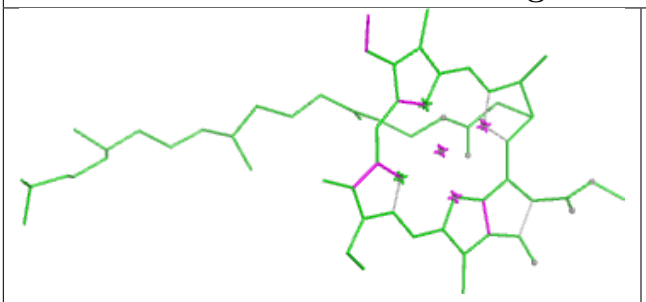


Torsions



Rings

Ligand CLA b 608



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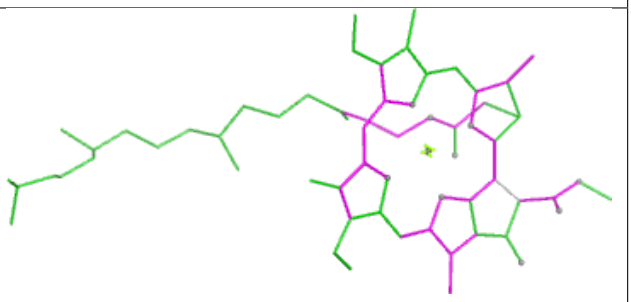
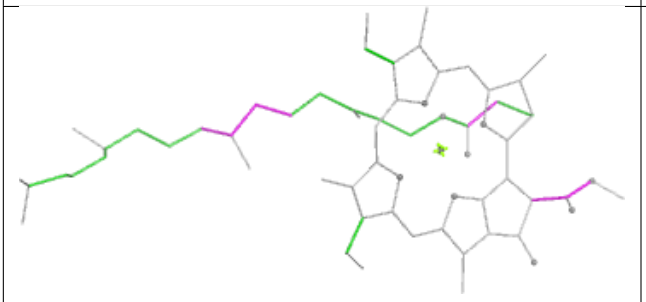


Bond angles

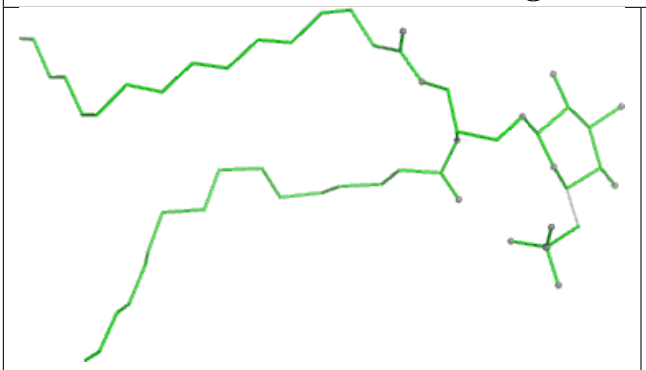


Torsions



Rings

Ligand SQD B 620



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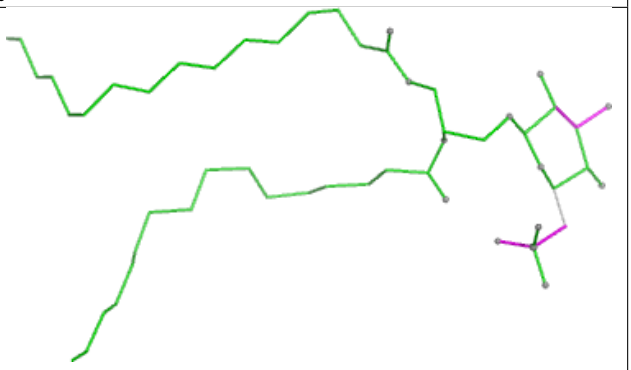
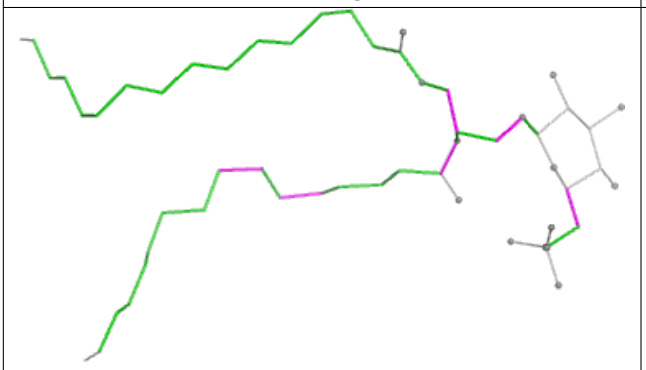


Bond angles

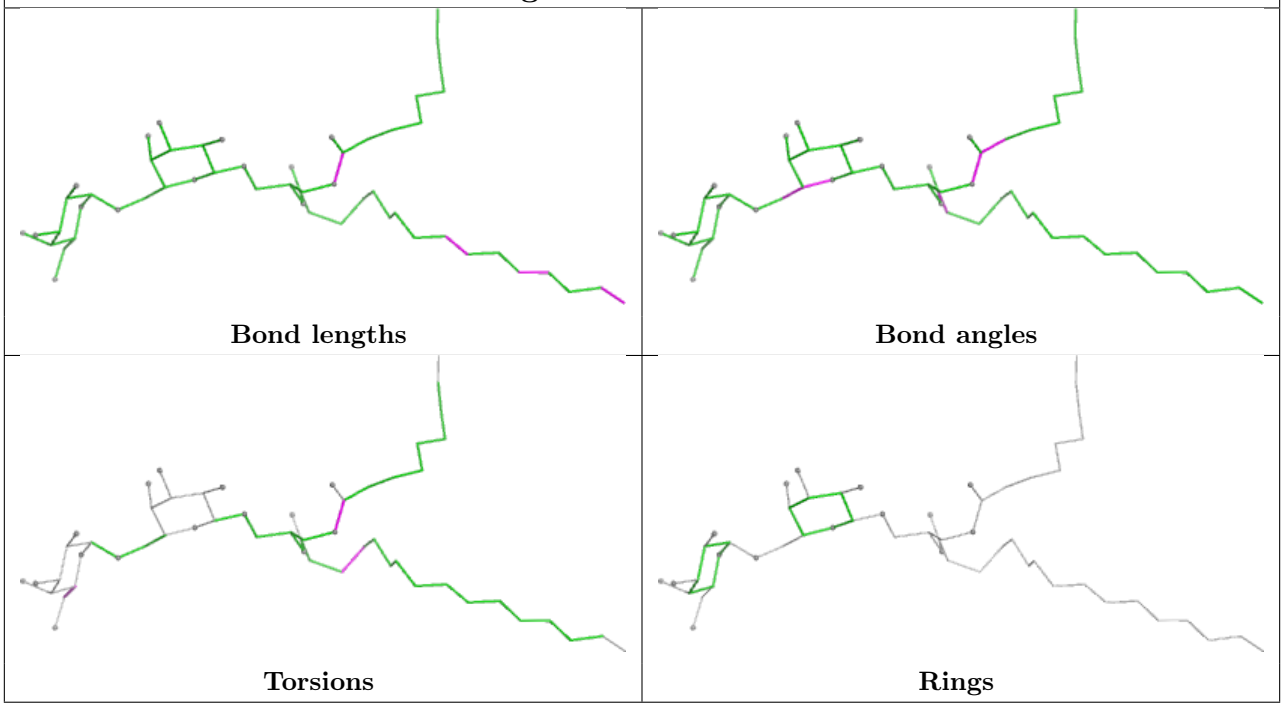


Torsions

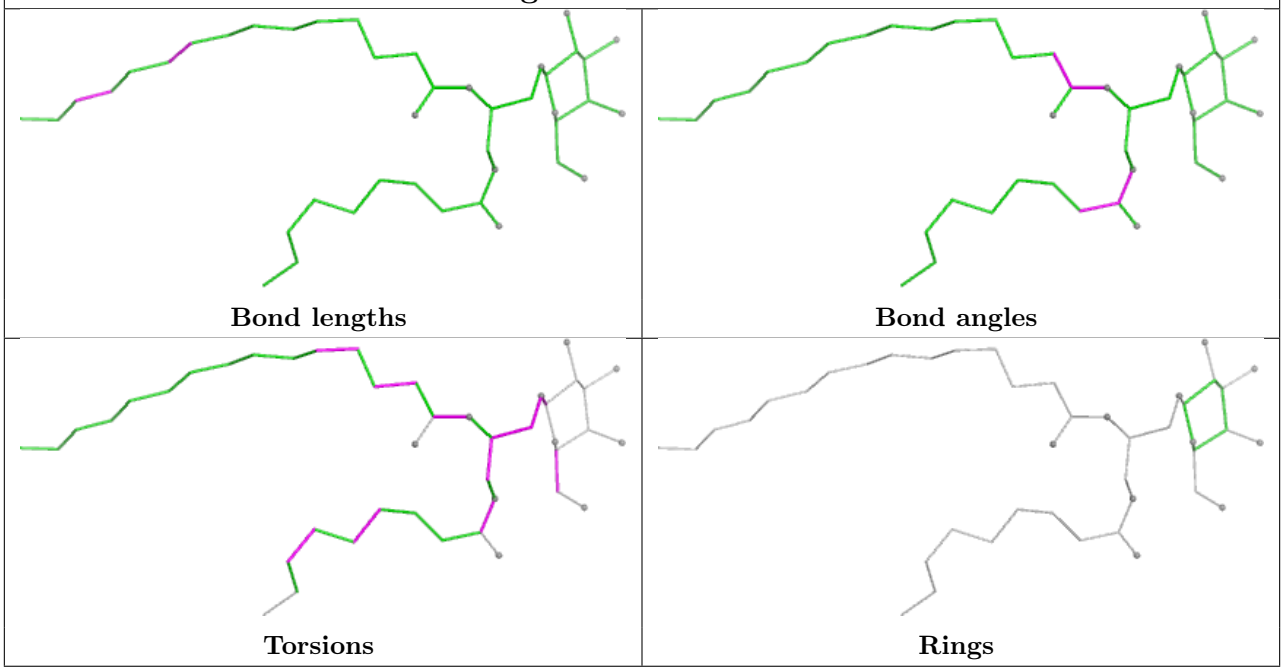


Rings

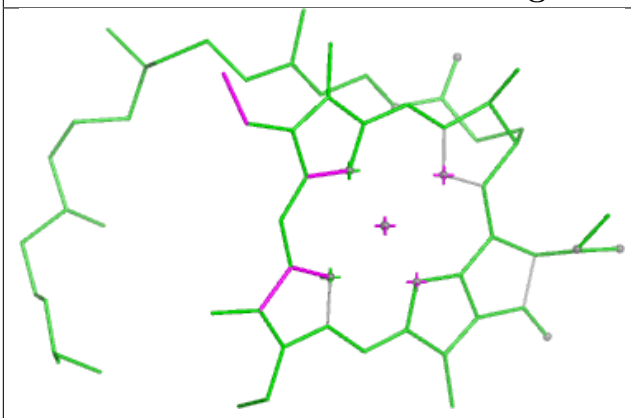
Ligand DGD C 517



Ligand LMG C 522



Ligand CLA g 602



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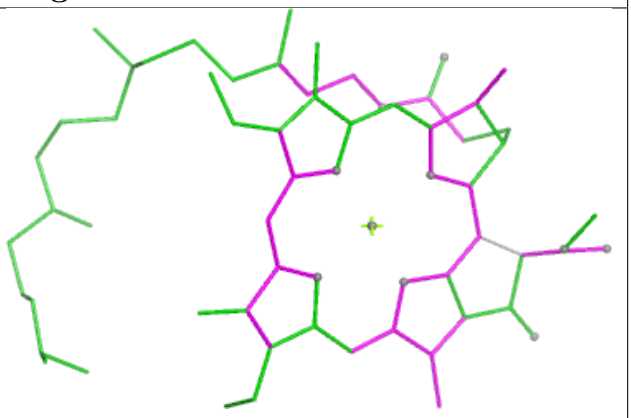
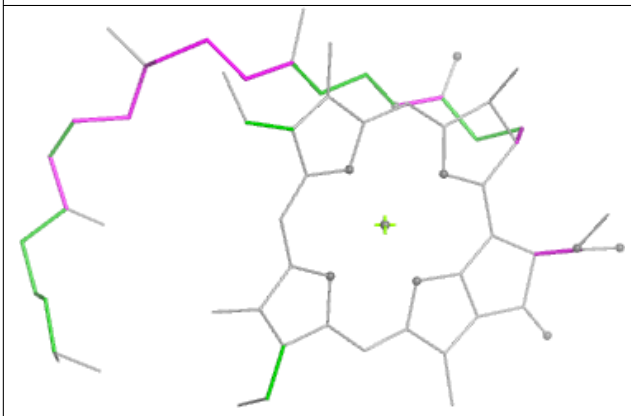


Bond angles



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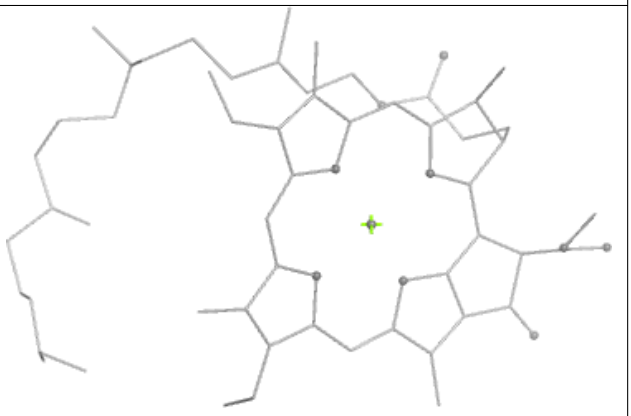
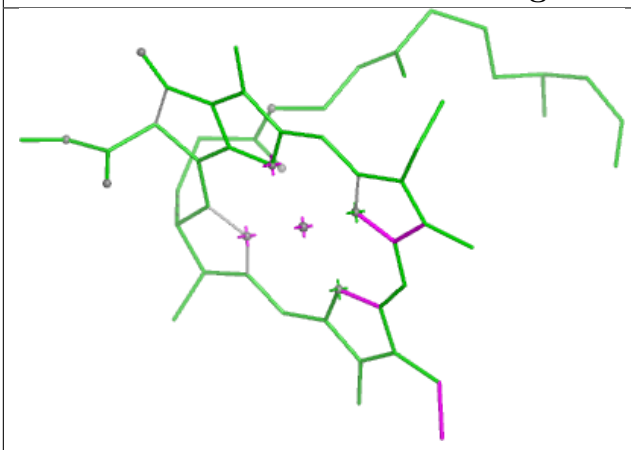


Rings

Ligand CLA c 513



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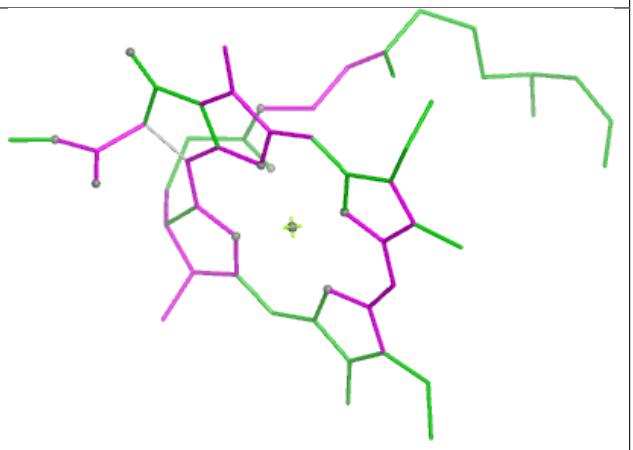
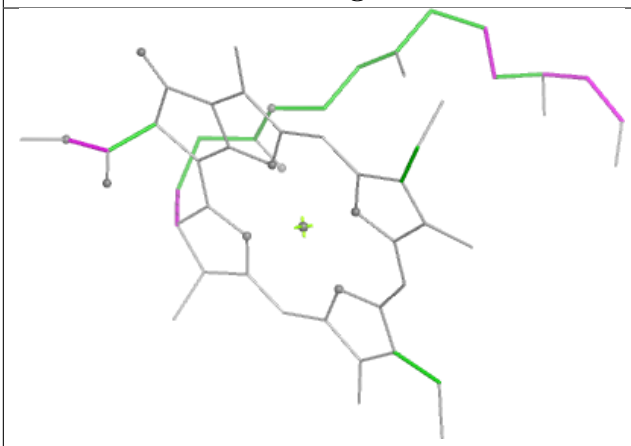


Bond angles



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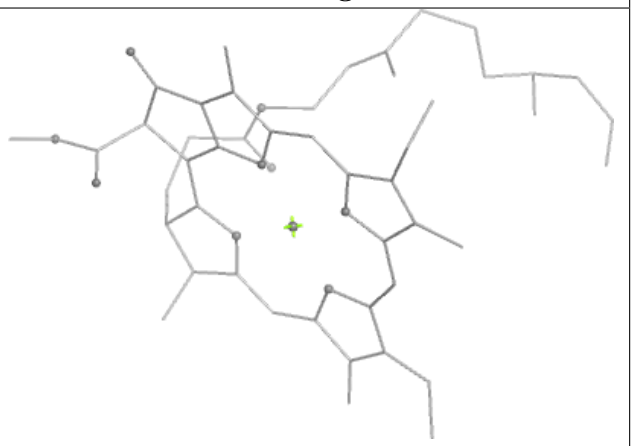
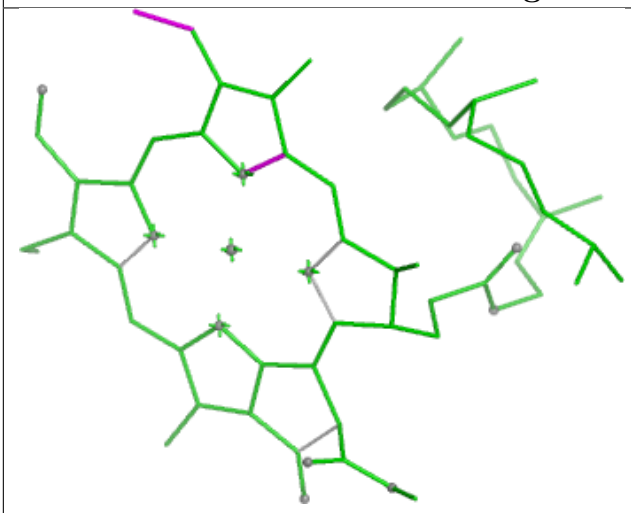


Rings

Ligand CHL Y 608



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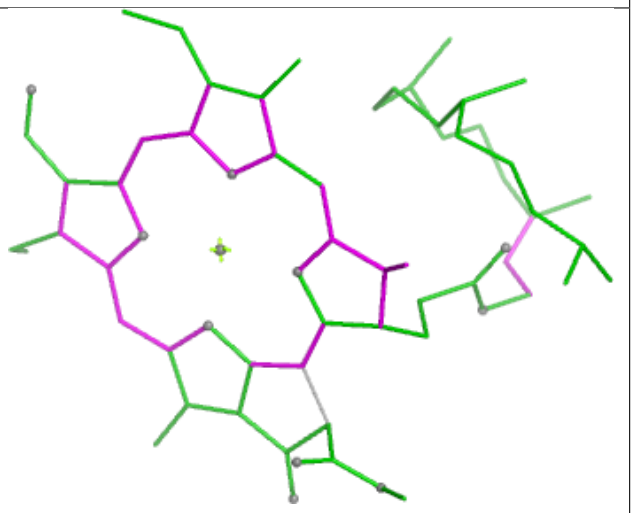

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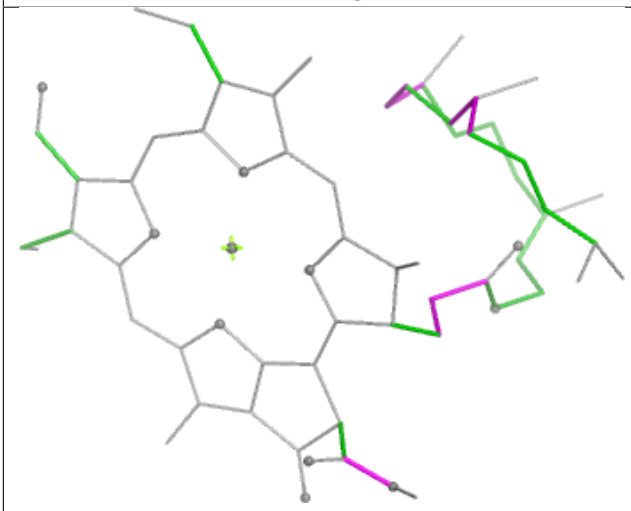

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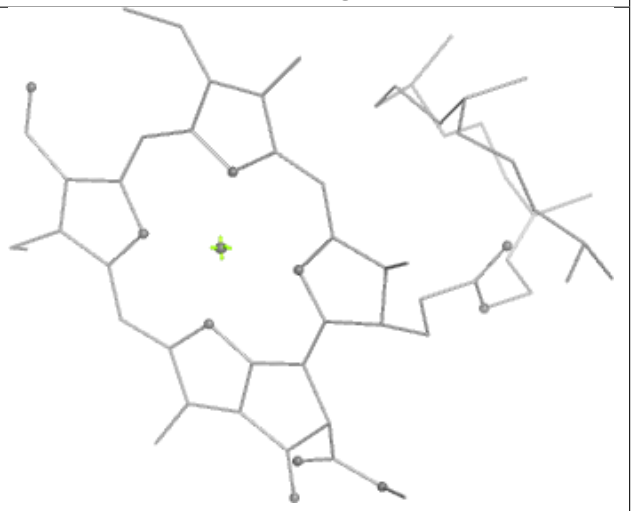
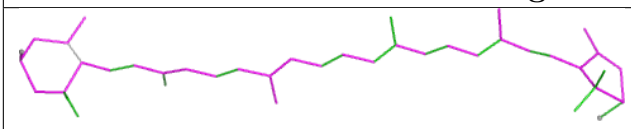


Rings

Ligand LUT g 616



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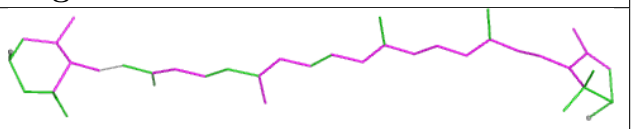
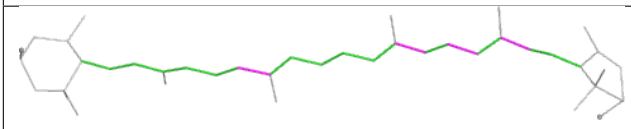


Bond angles



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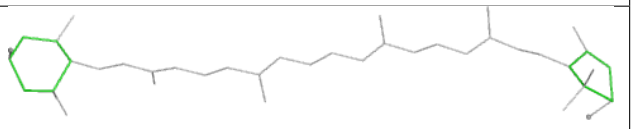
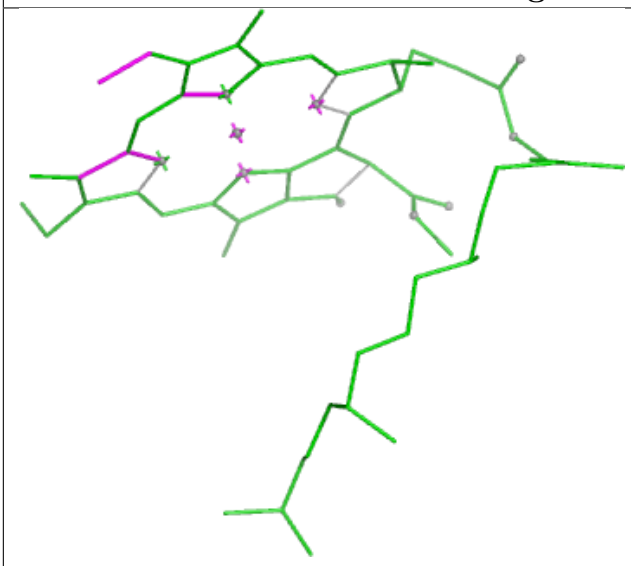


Rings

Ligand CLA y 304



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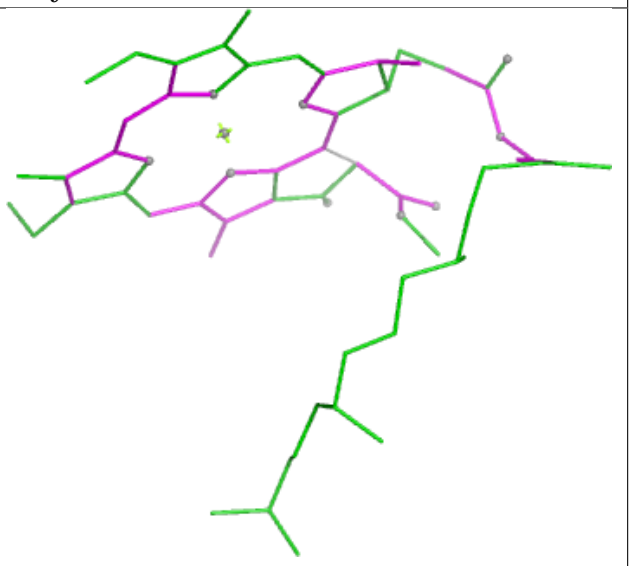
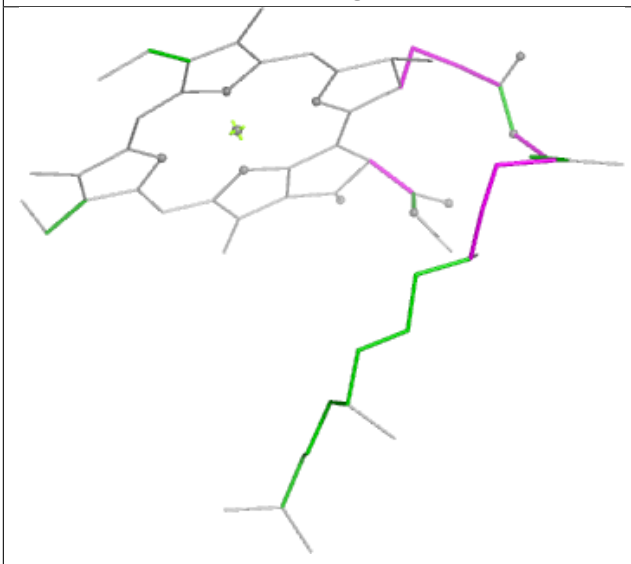


Bond angles



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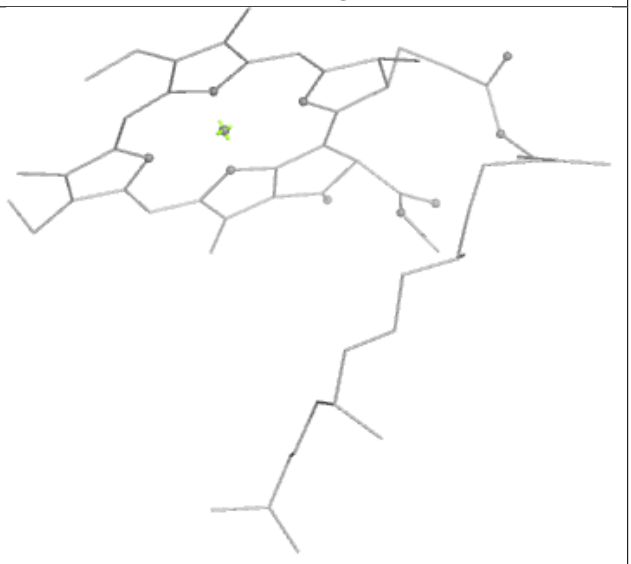
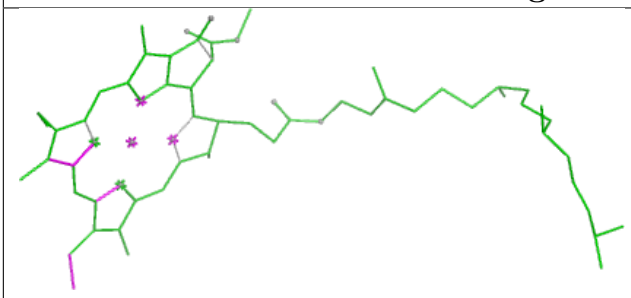


Rings

Ligand CLA a 406



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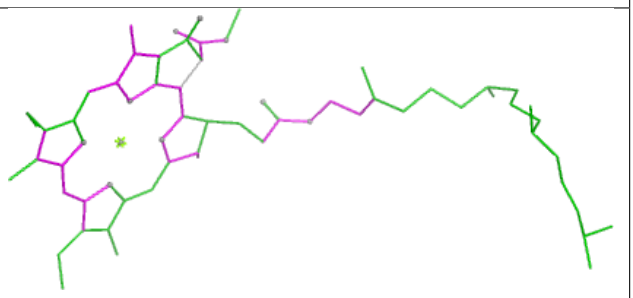
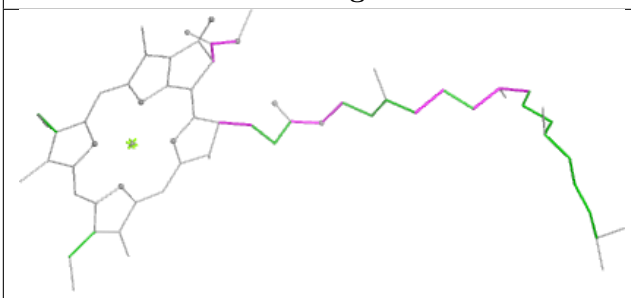


Bond angles



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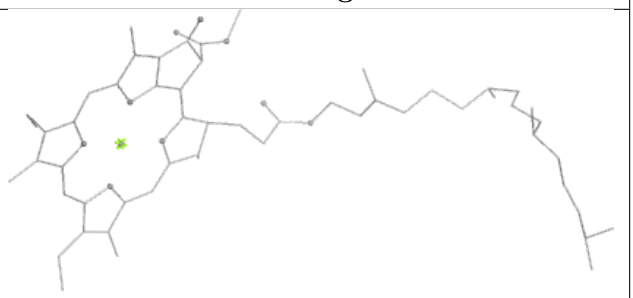
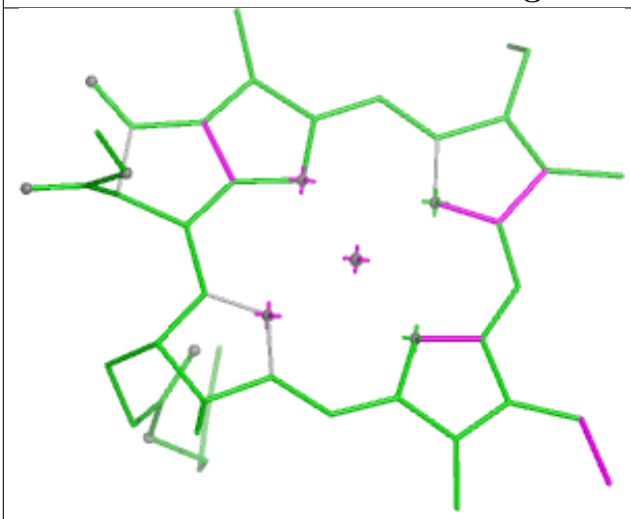
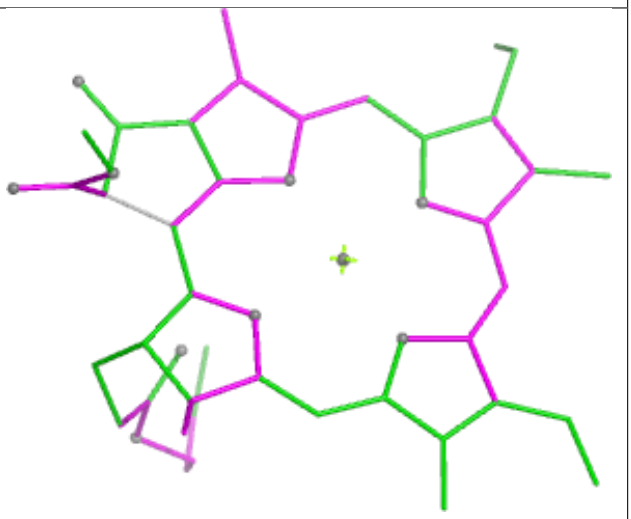


Rings

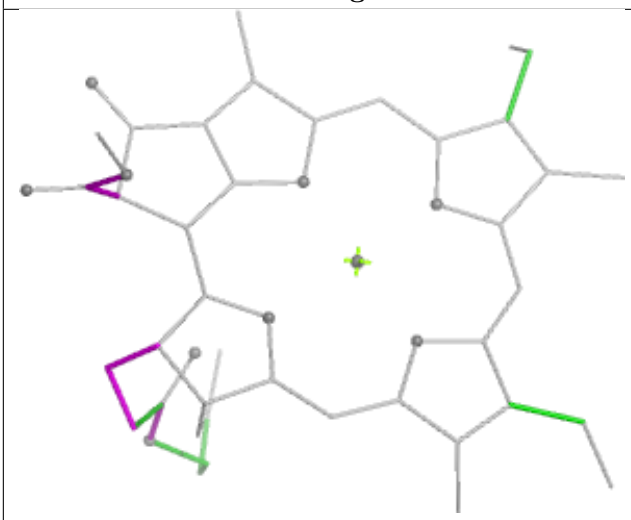
Ligand CLA Y 604



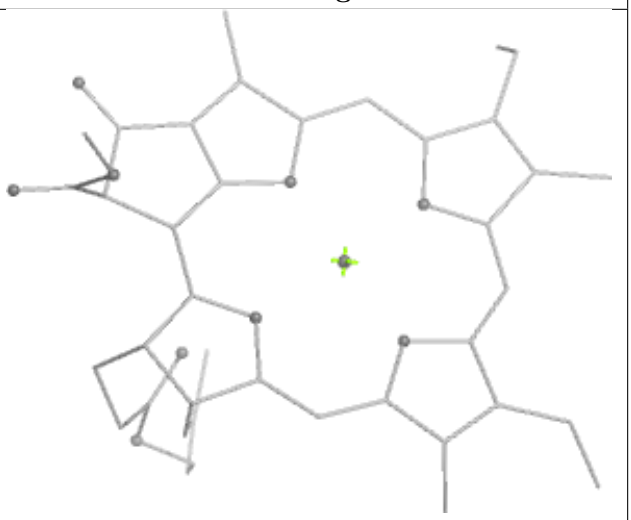
Bond lengths



Bond angles

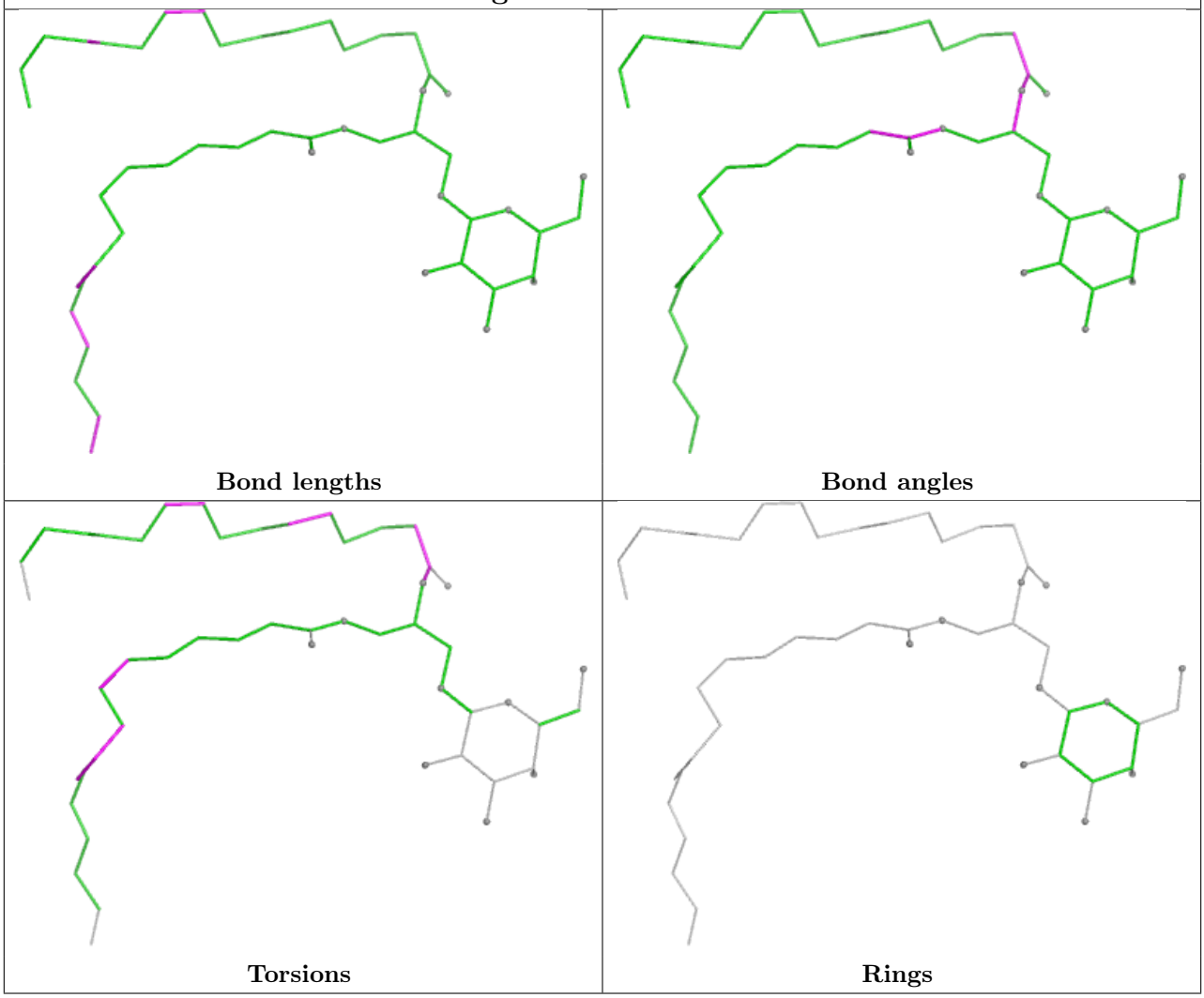


Torsions

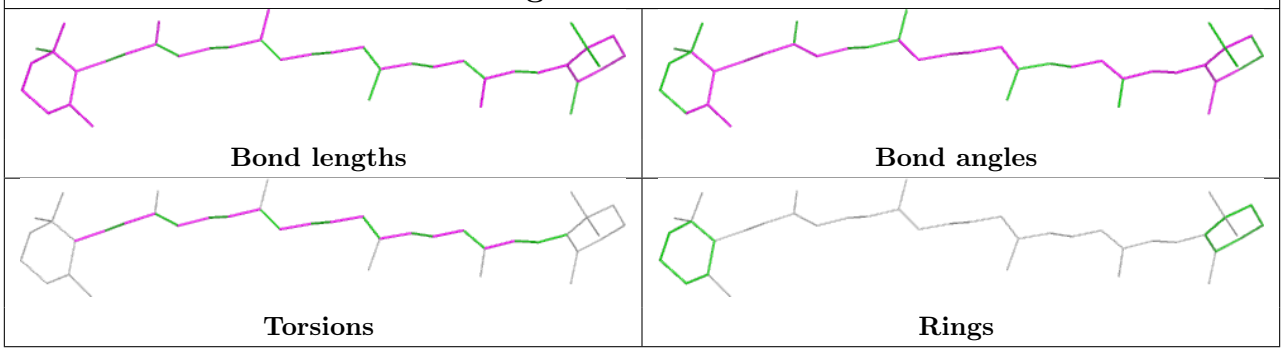


Rings

Ligand LMG k 102



Ligand BCR b 617



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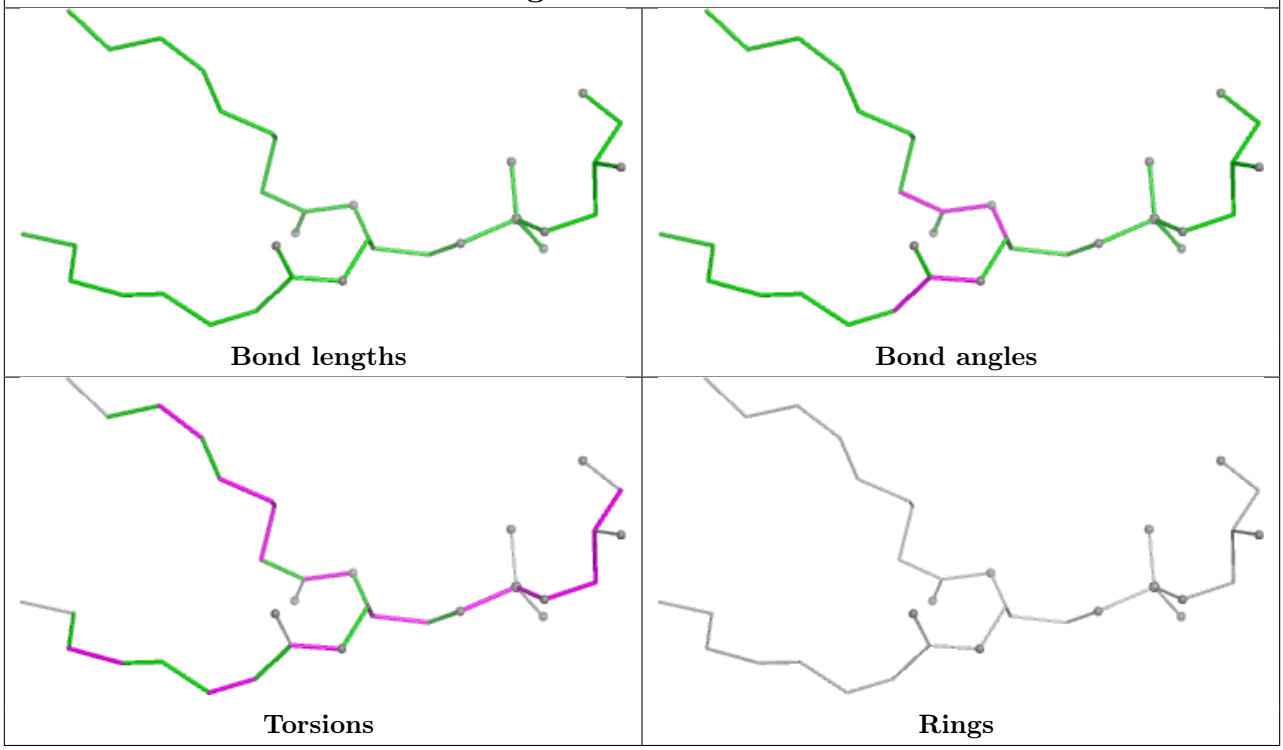
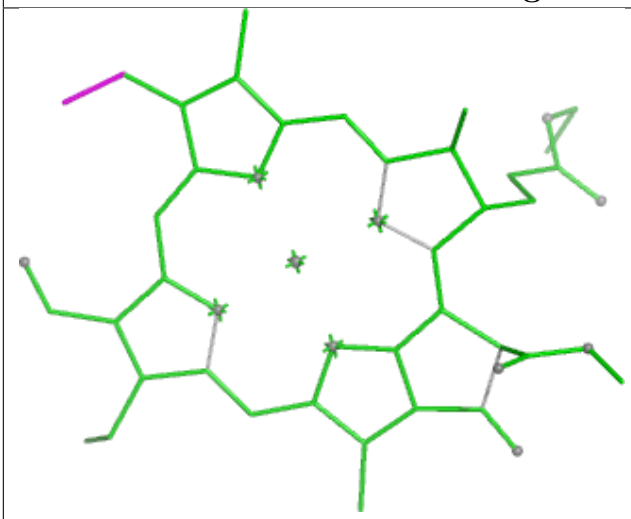


Ligand CHL Y 605



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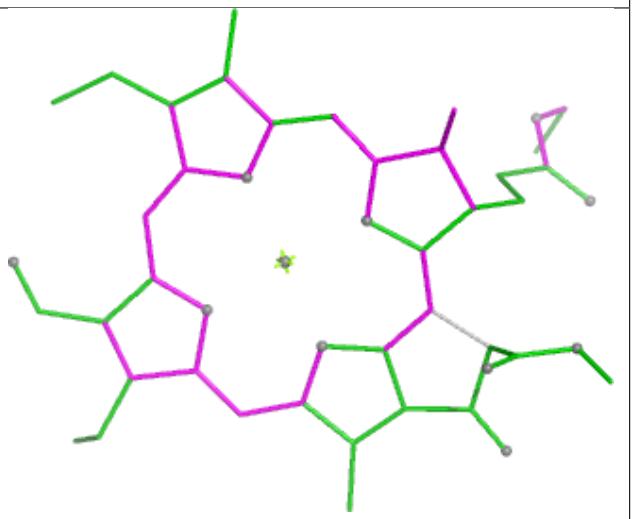
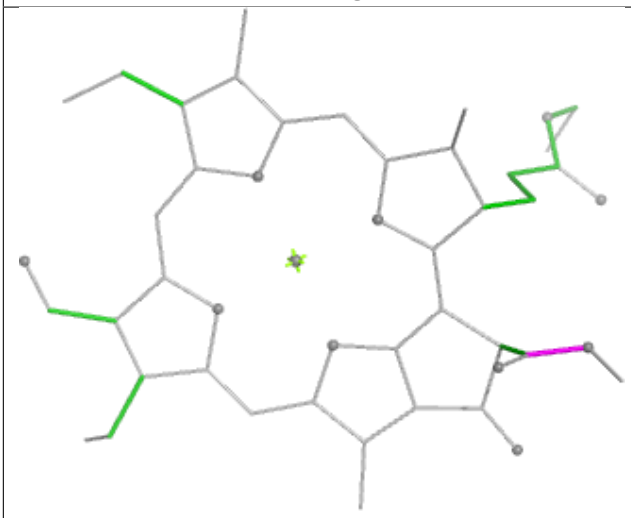


Bond angles



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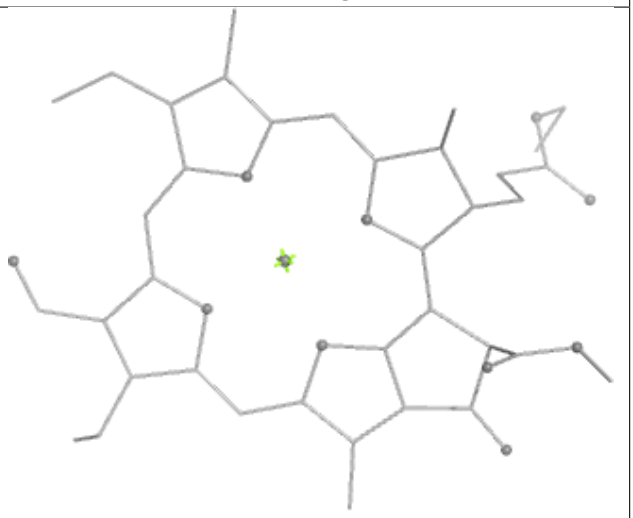
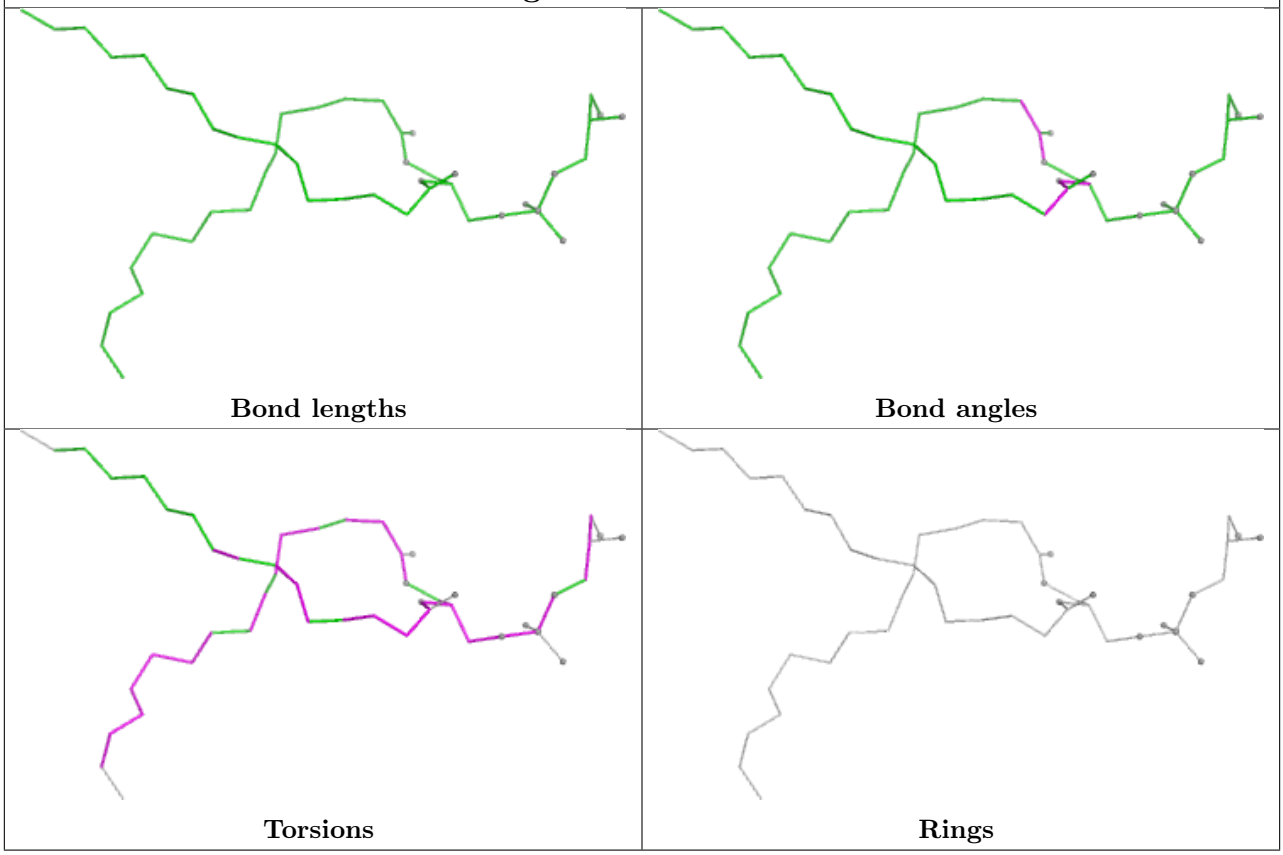
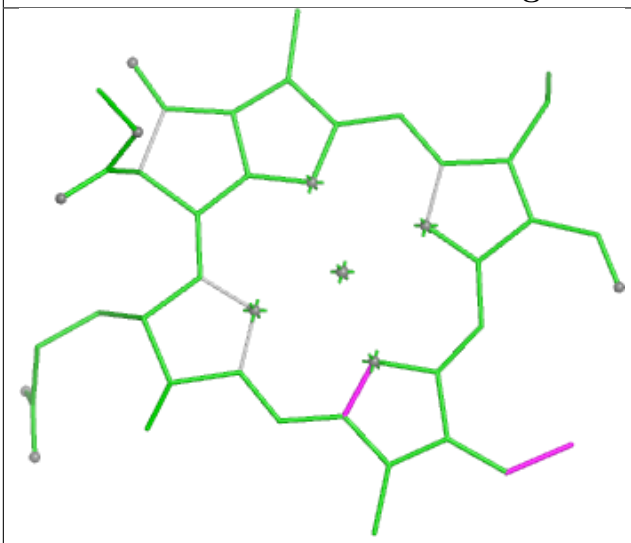


Rings

Ligand LHG D 407



Ligand CHL G 605



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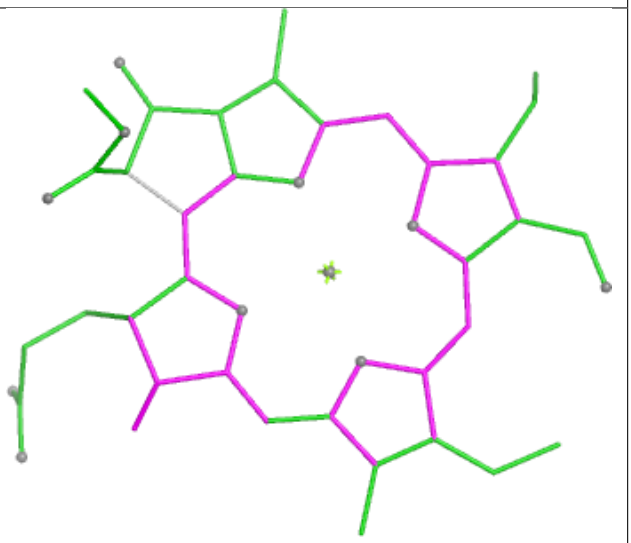
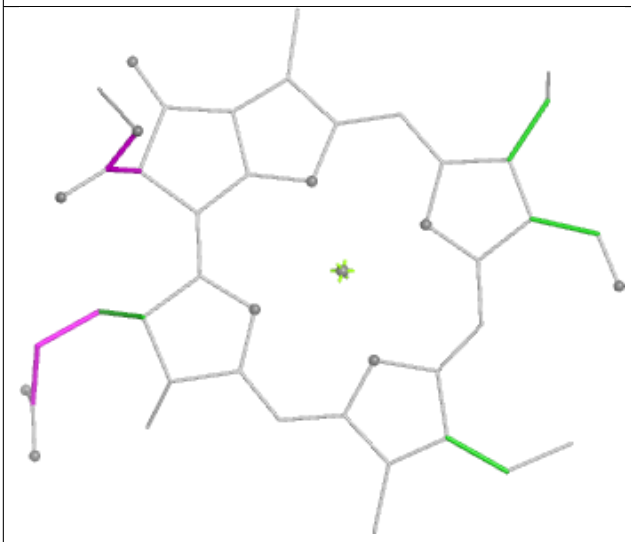


Bond angles



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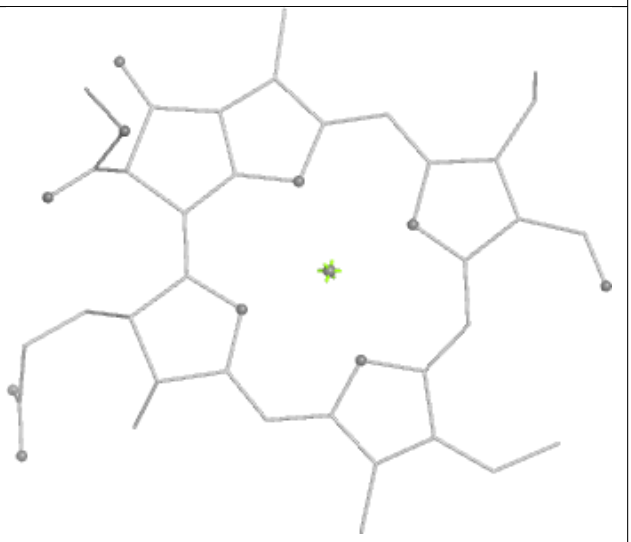
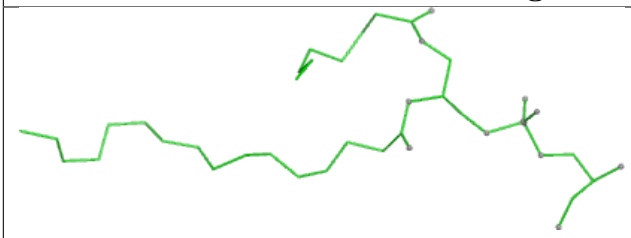


Rings

Ligand LHG g 618



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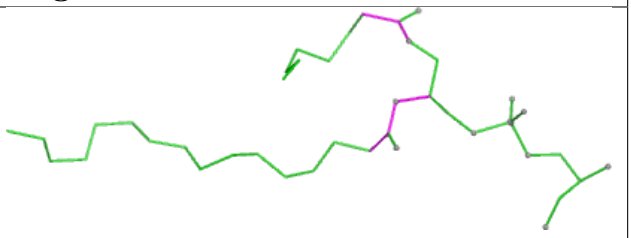

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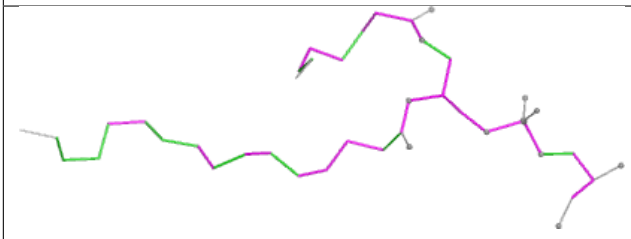

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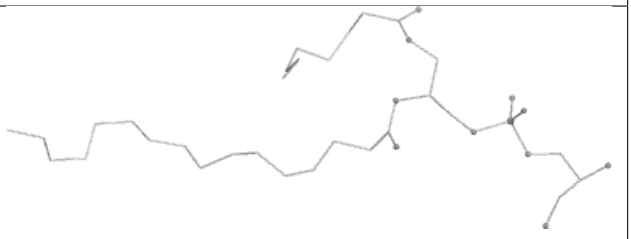
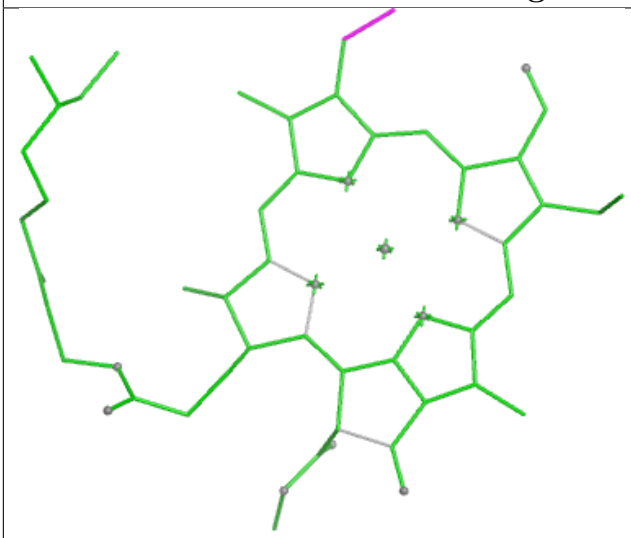


Rings

Ligand CHL g 607



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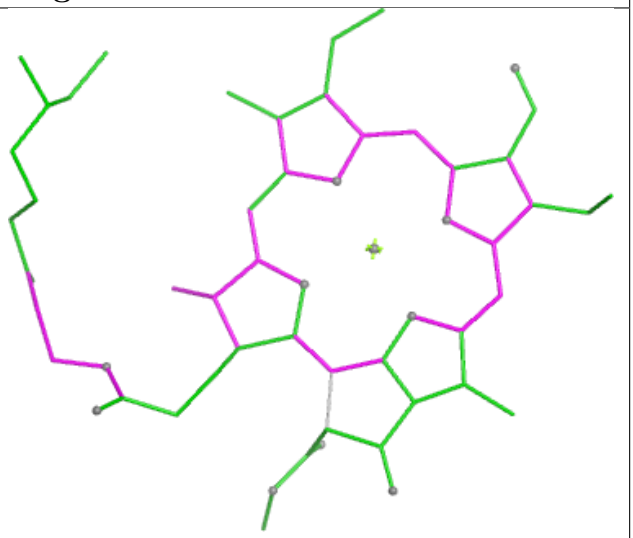

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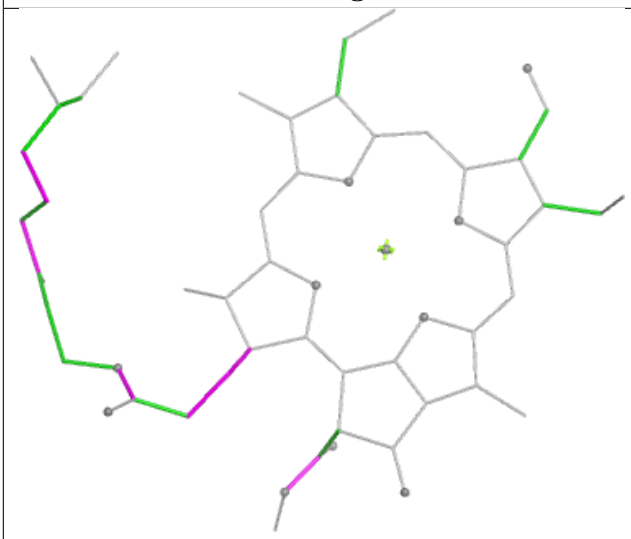
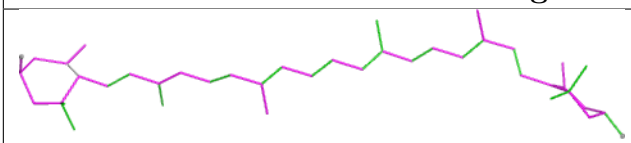


Torsions



Rings

Ligand LUT s 615



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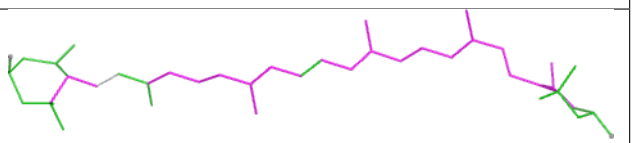
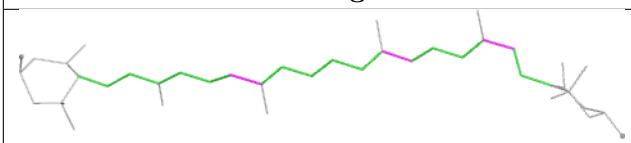


Bond angles



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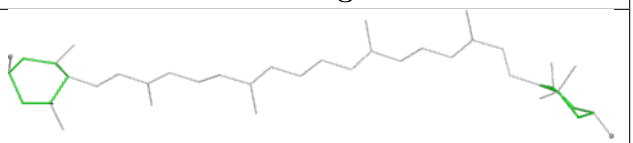
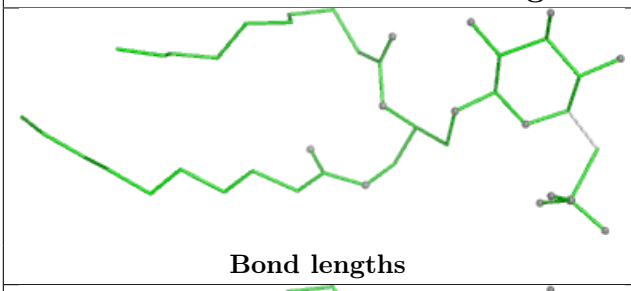


Rings

Ligand SQD L 101



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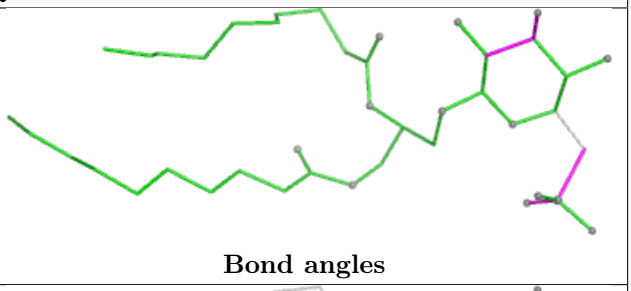
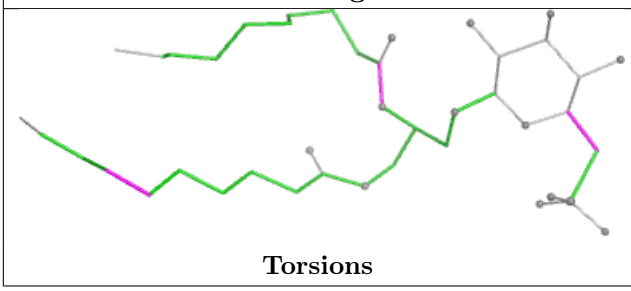


Bond angles



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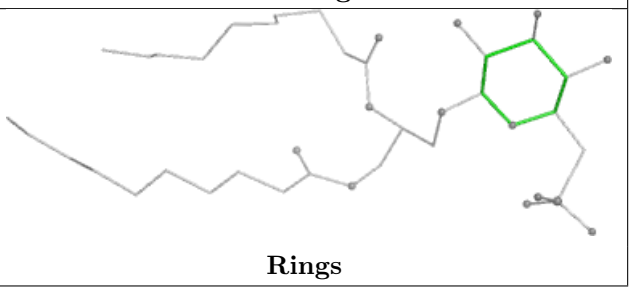
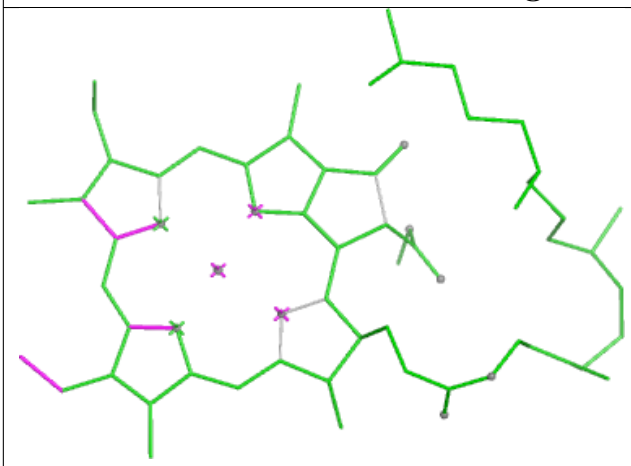


Rings

Ligand CLA B 610



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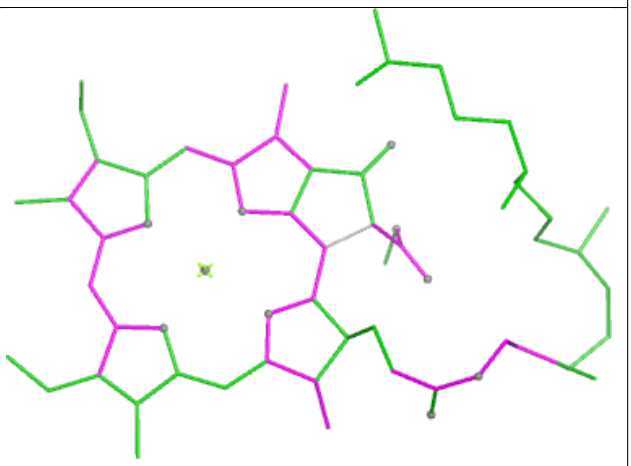
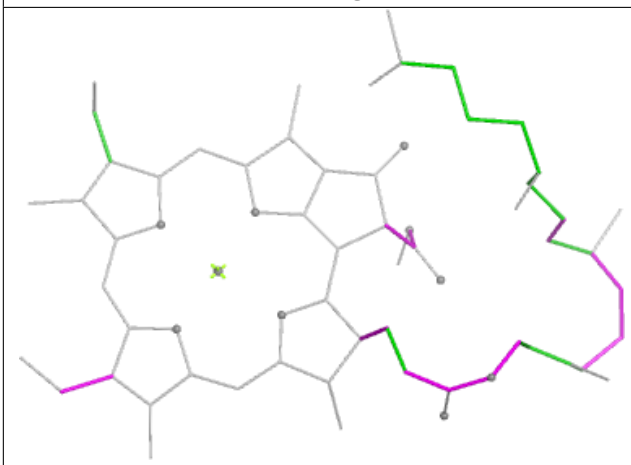


Bond angles



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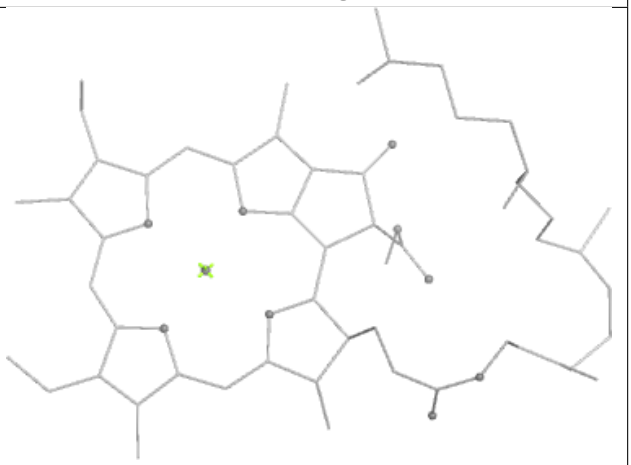
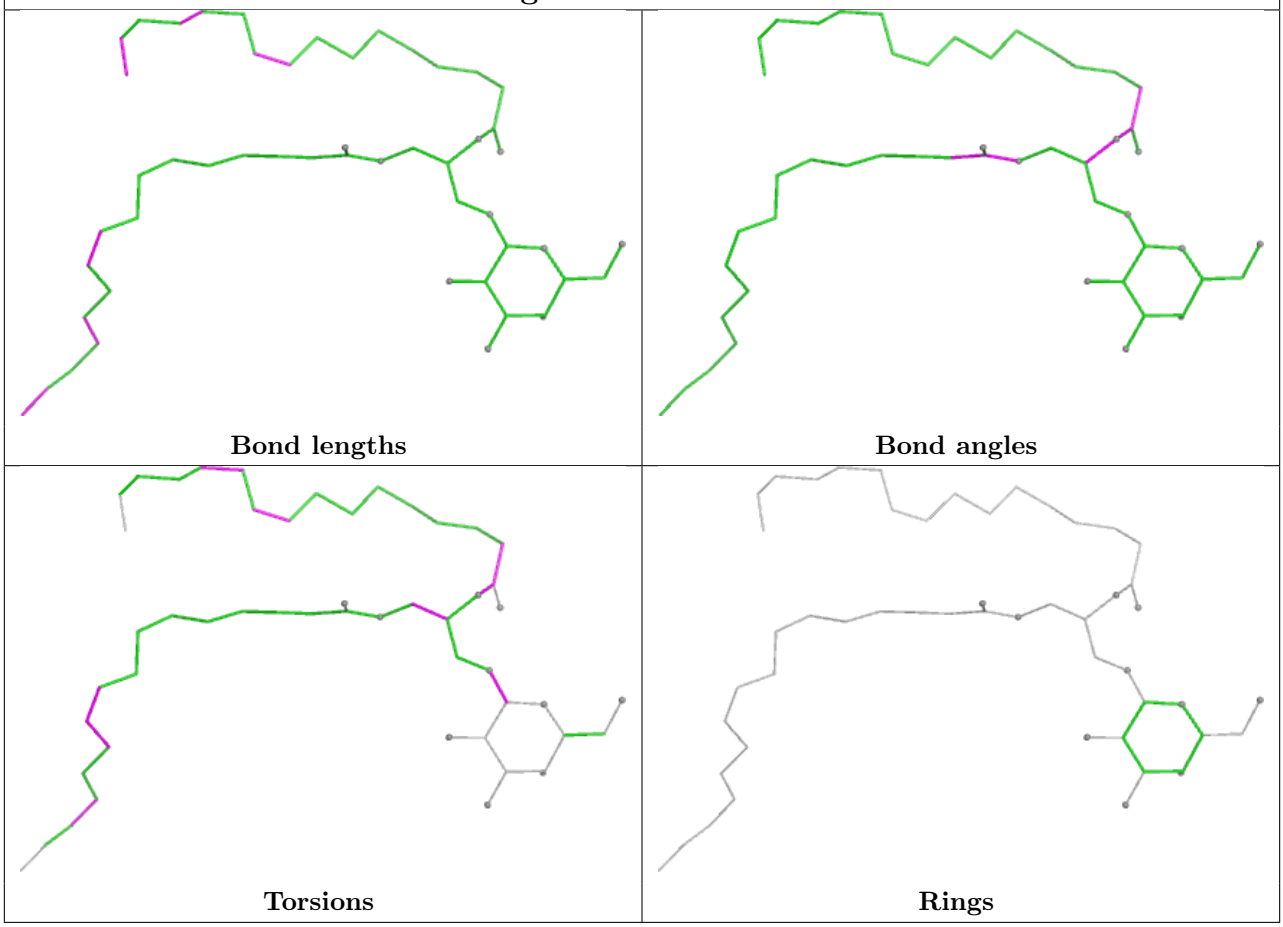


Rings

Ligand LMG C 520



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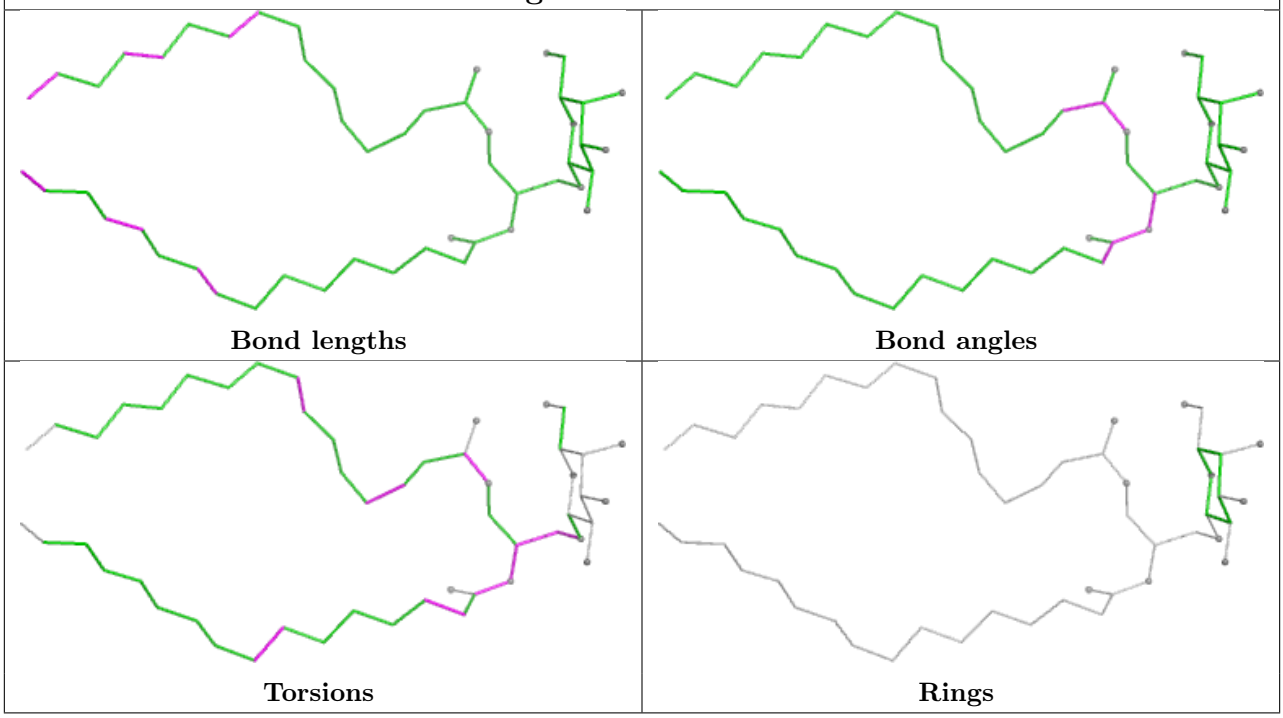
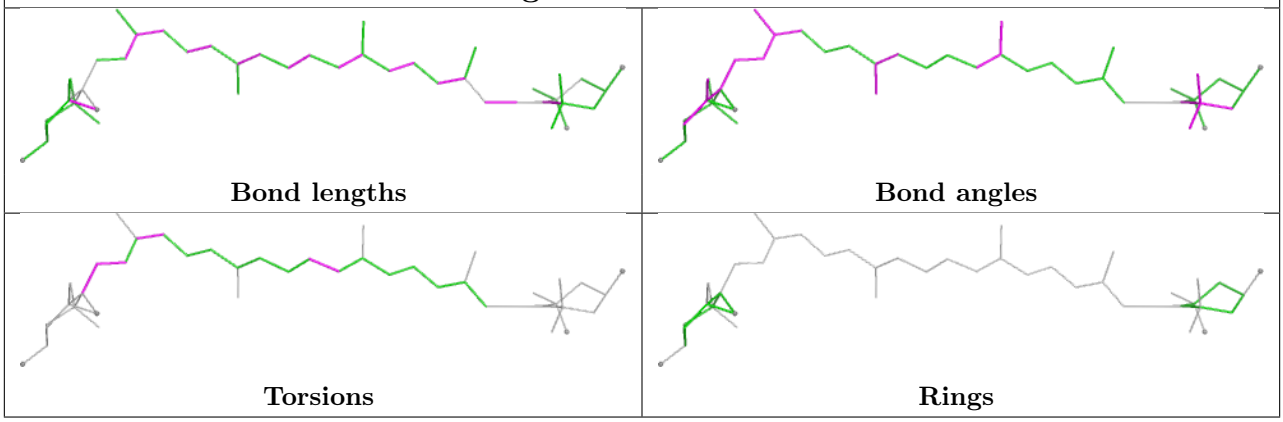


Ligand NEX N 617



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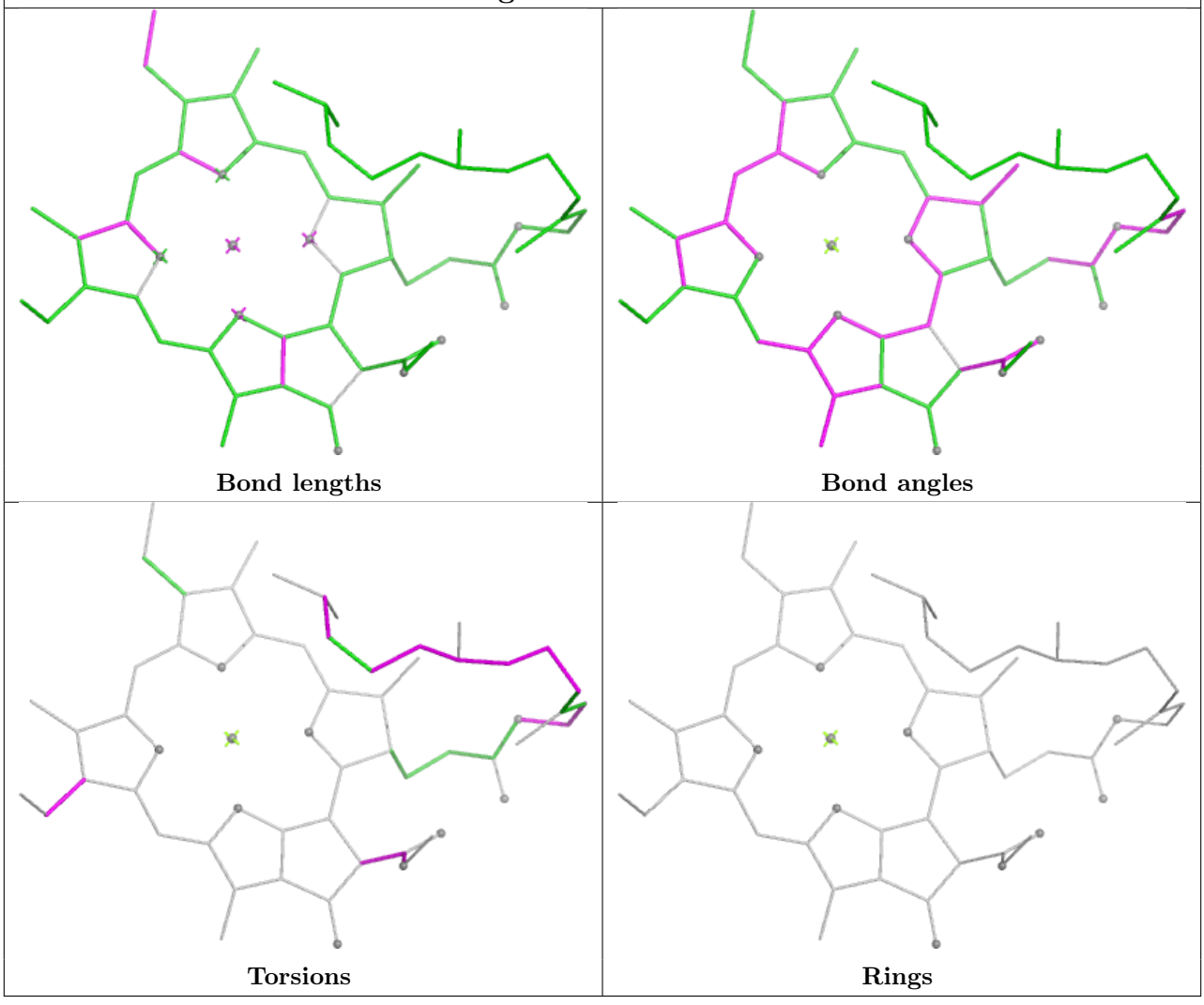

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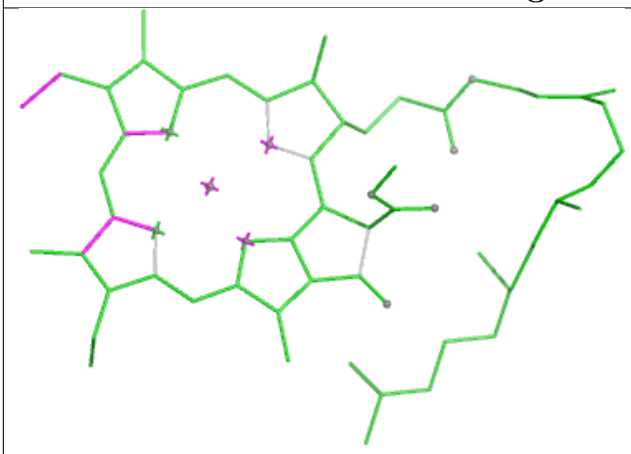
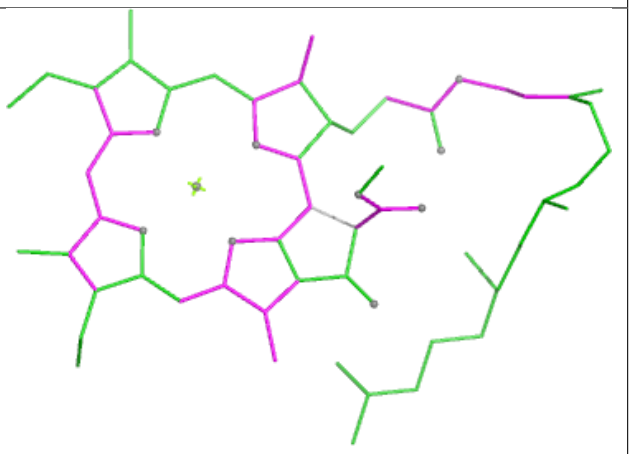
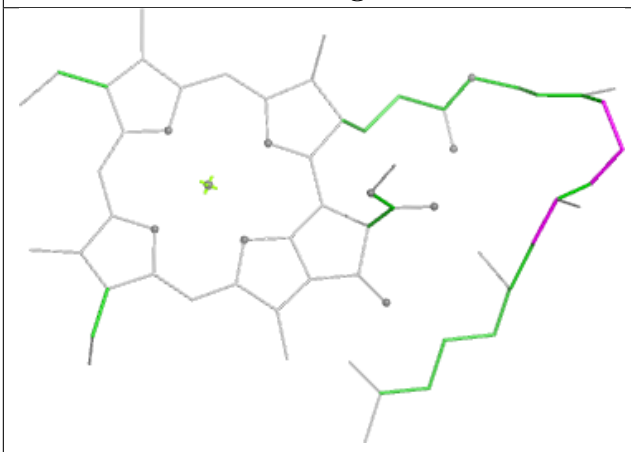


Bond lengths



Bond angles



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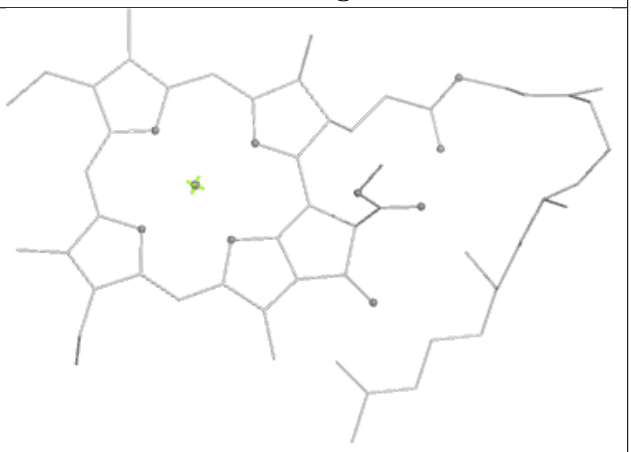
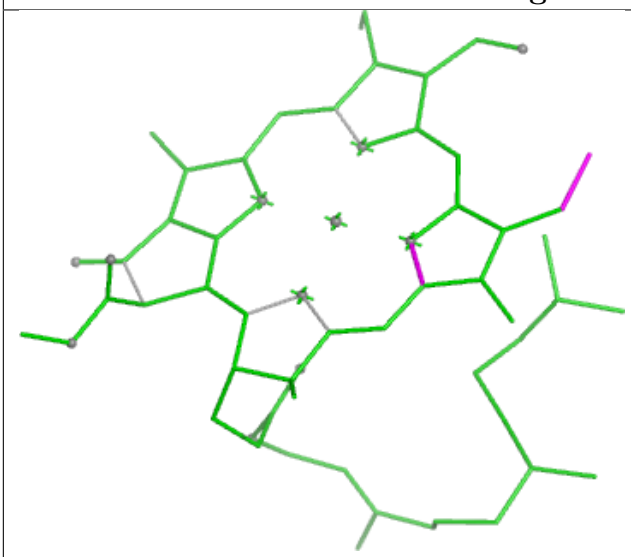


Rings

Ligand CHL r 607



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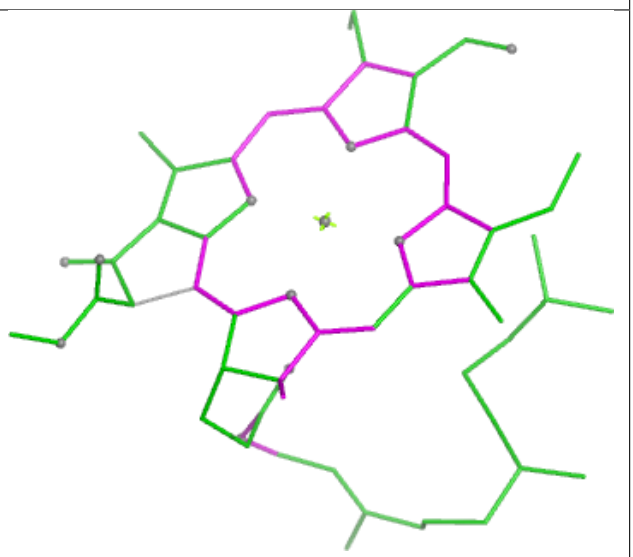
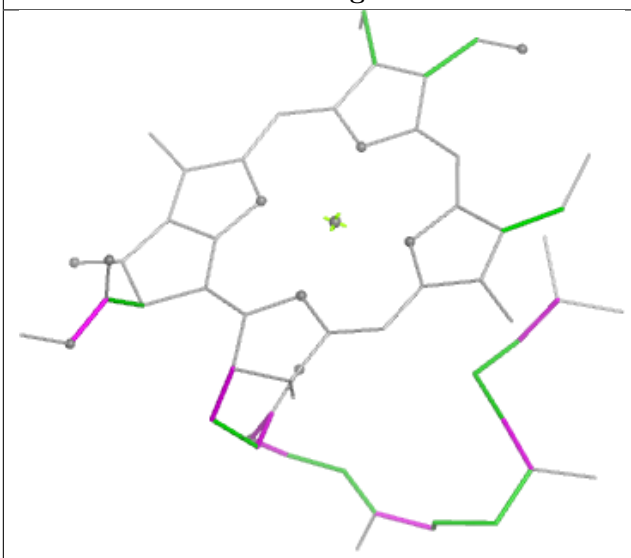


Bond angles



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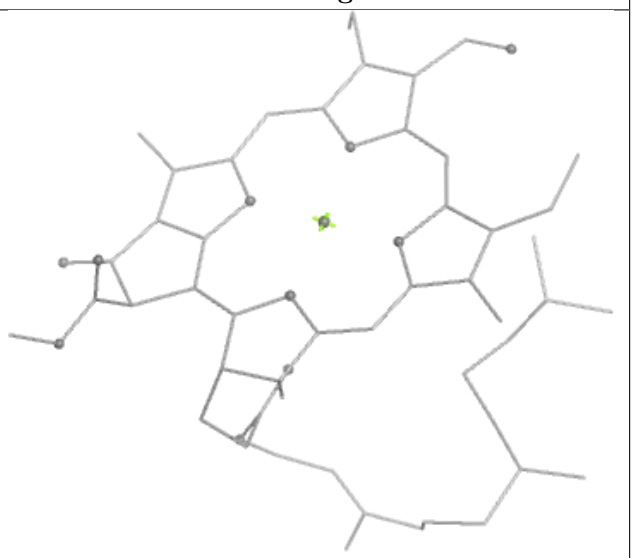
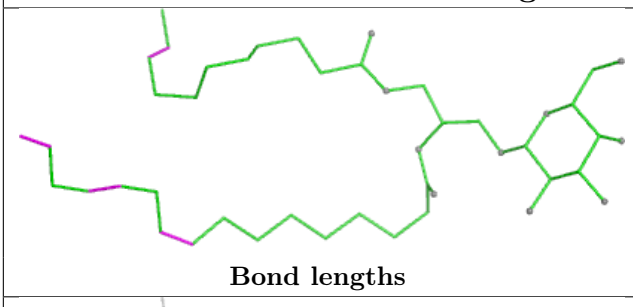


Rings

Ligand LMG D 408



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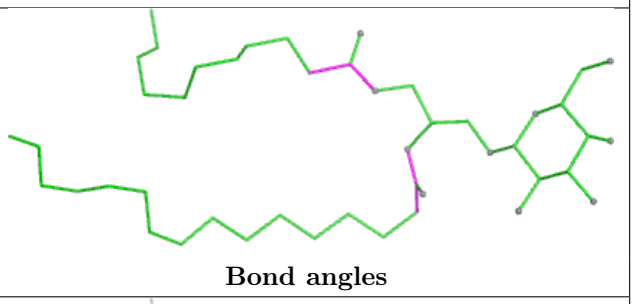
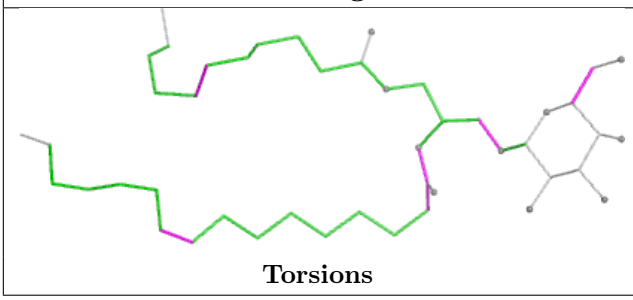


Bond angles



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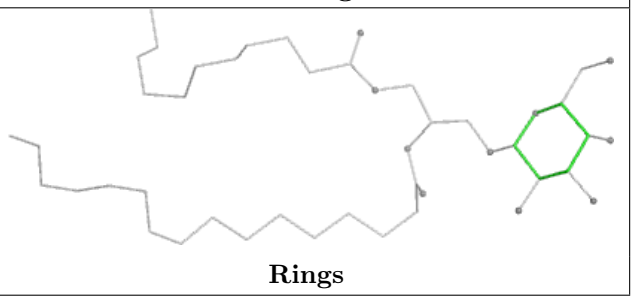
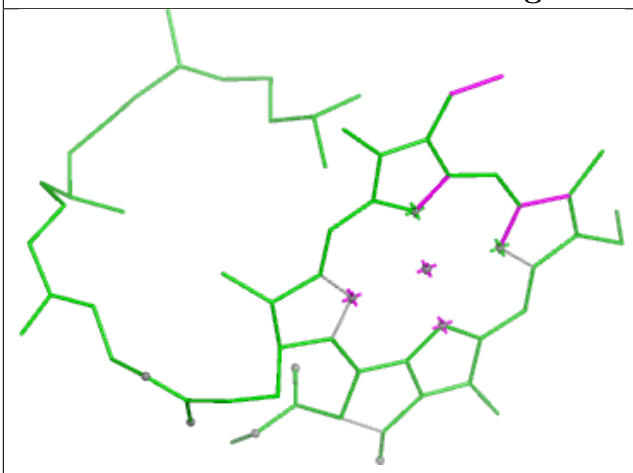


Rings

Ligand CLA B 615



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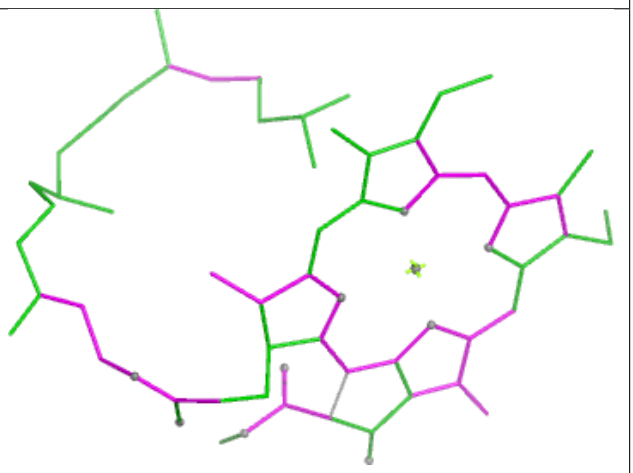
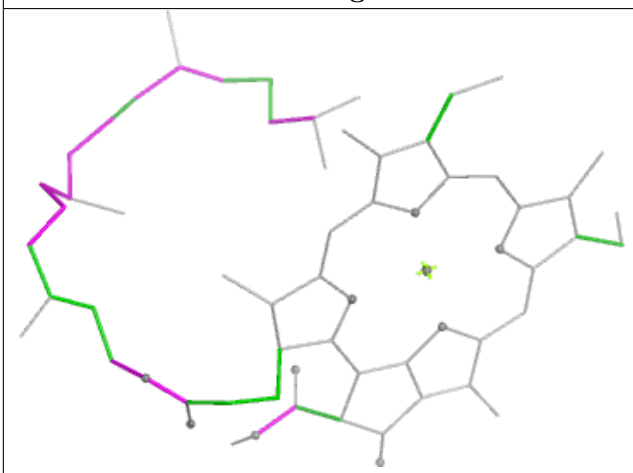


Bond angles



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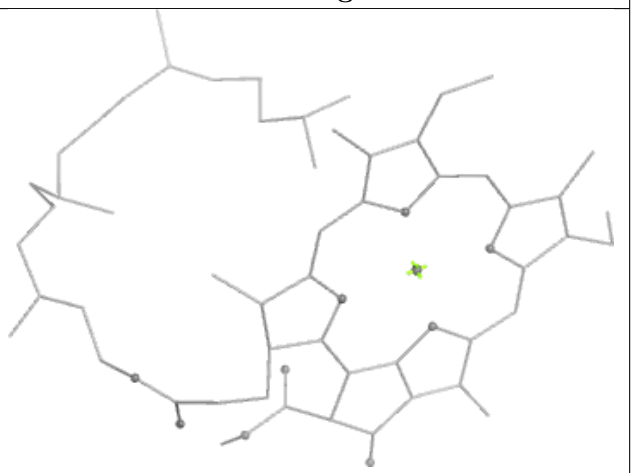
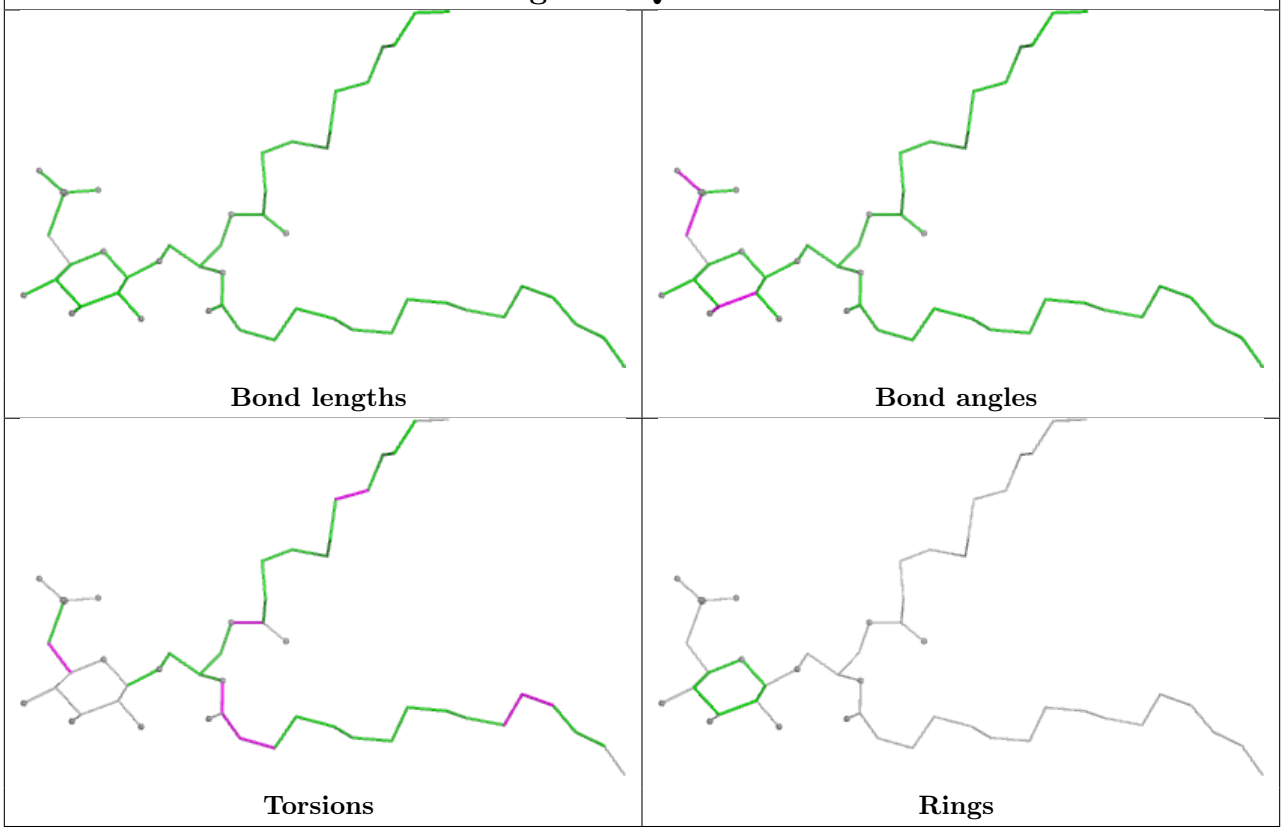
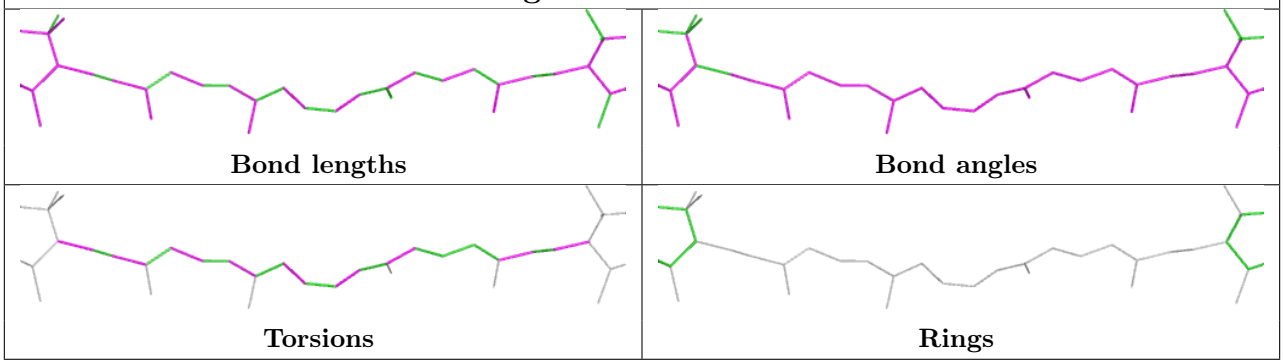


Rings

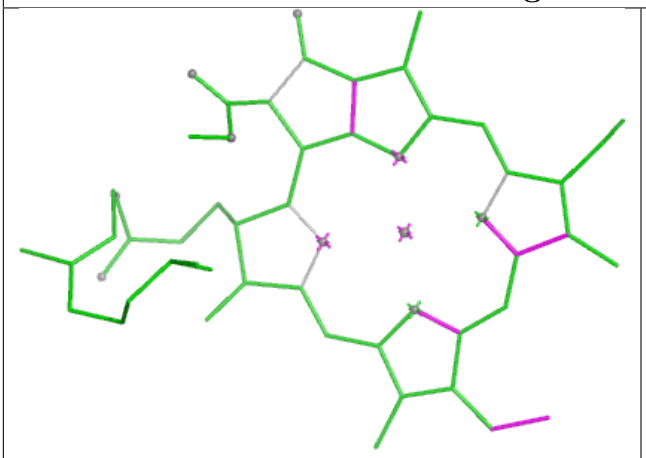
Ligand SQD a 411



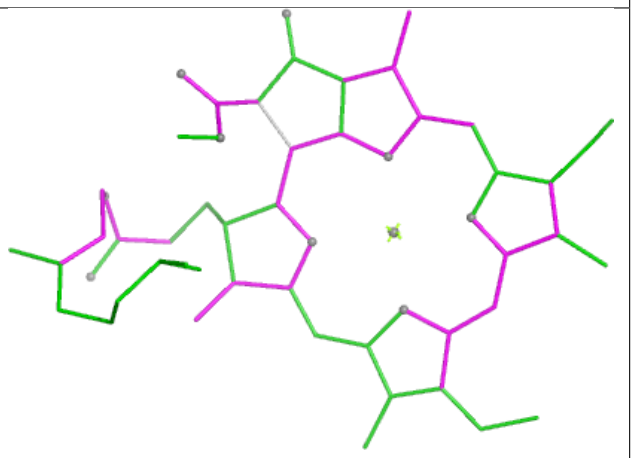
Ligand BCR C 514



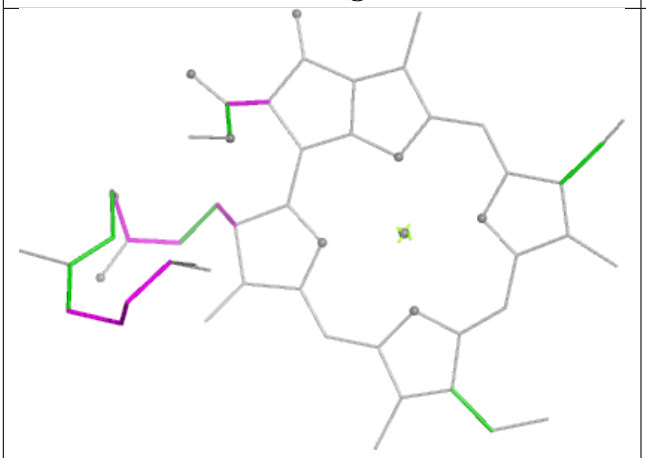
Ligand CLA Y 603



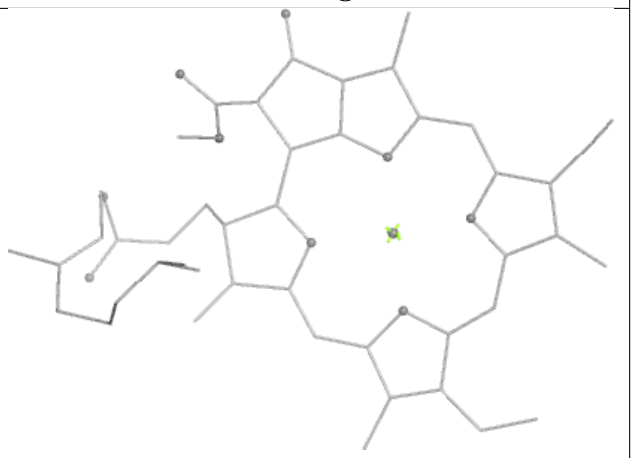
Bond lengths



Bond angles

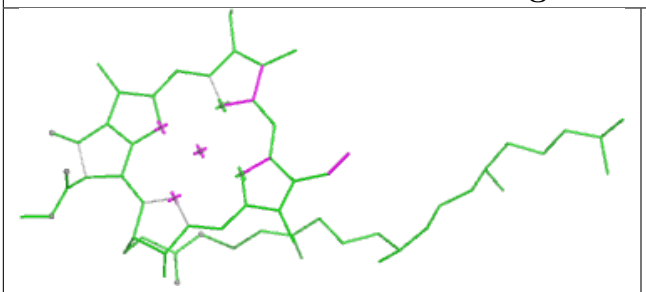


Torsions

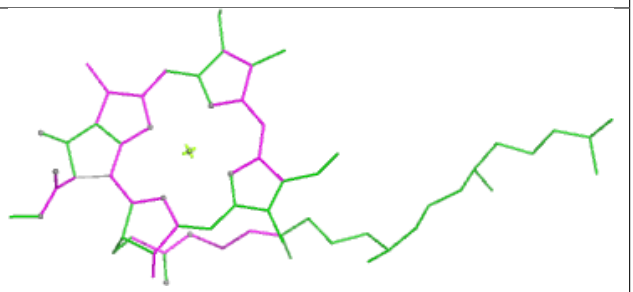


Rings

Ligand CLA c 501



Bond lengths



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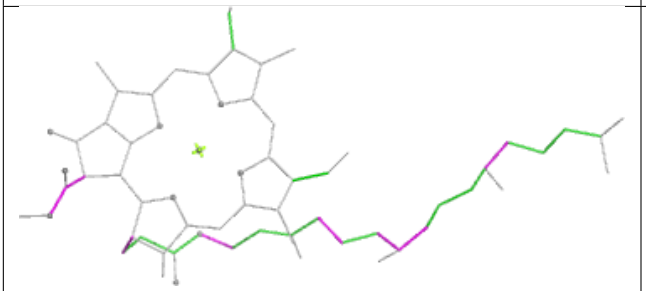
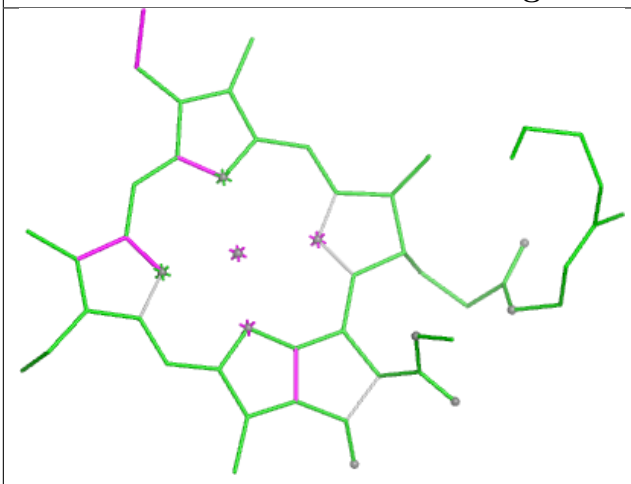


Torsions



Rings

Ligand CLA G 603



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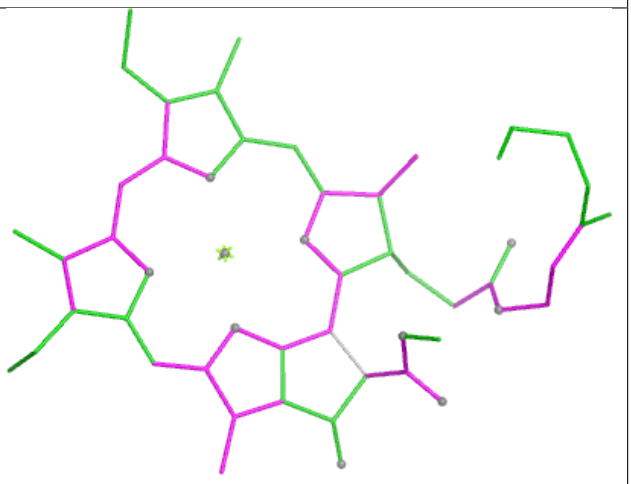
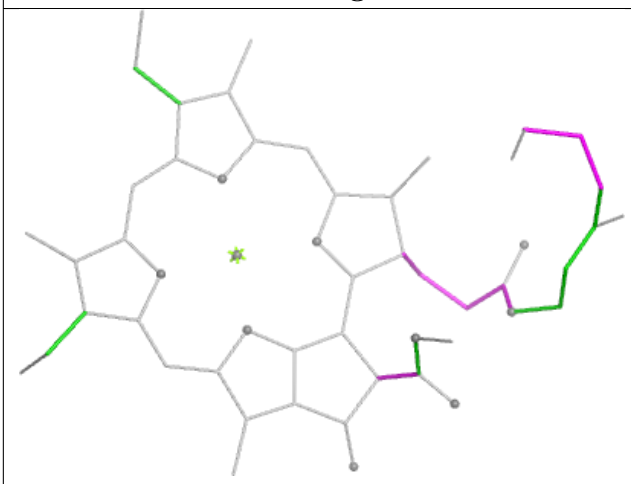


Bond angles



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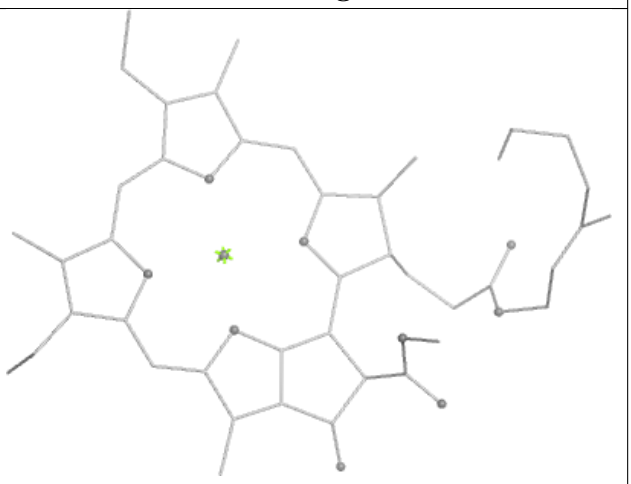
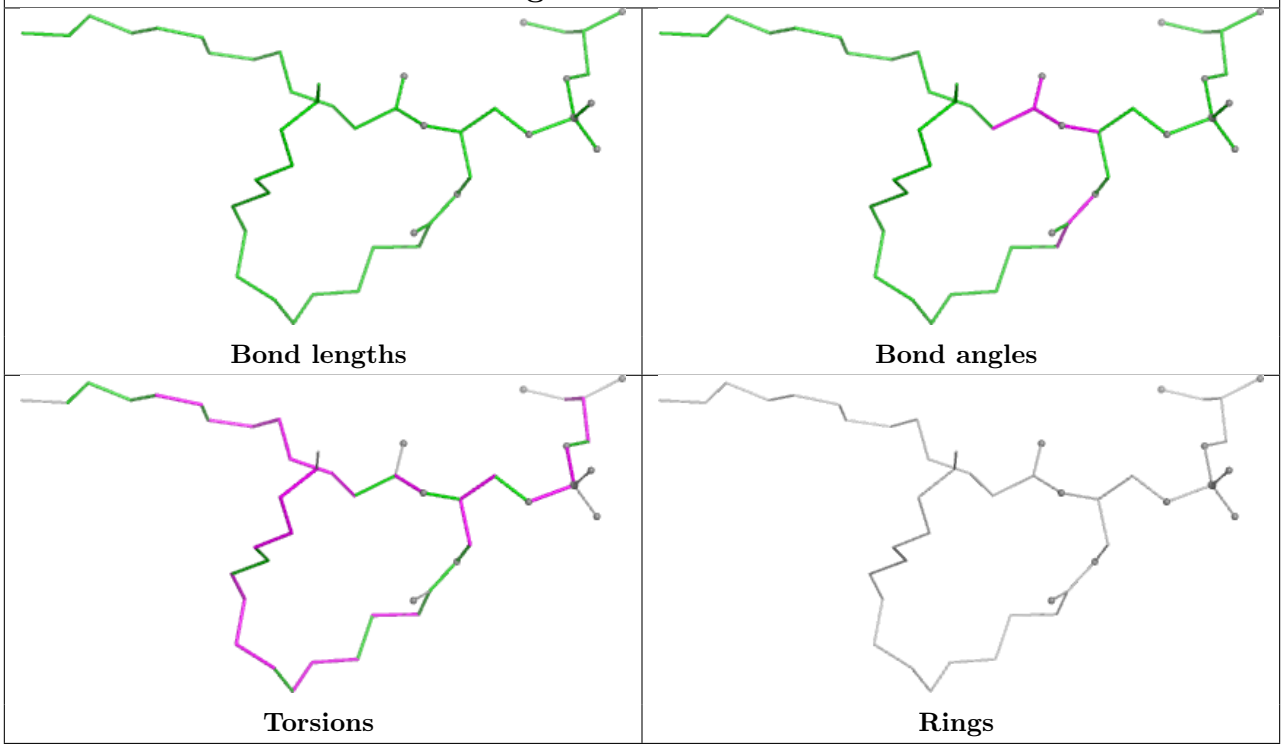
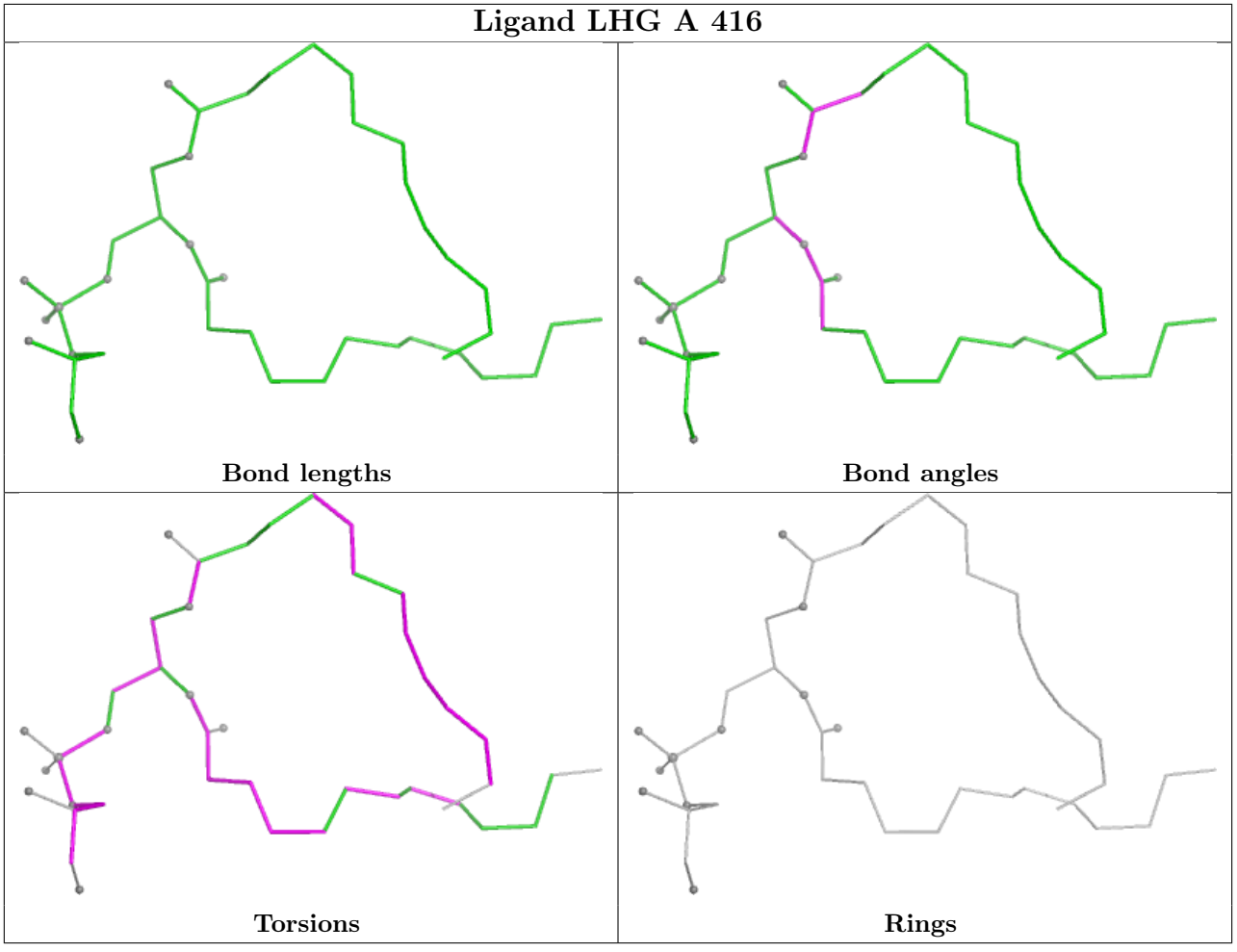


Rings

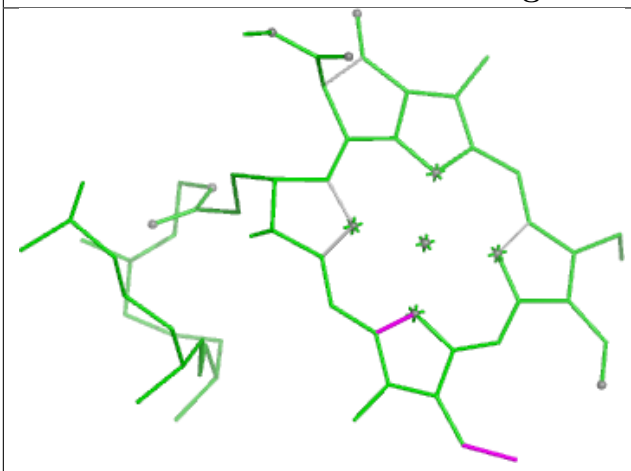
Ligand LHG b 624



Ligand LHG A 416



Ligand CHL G 608



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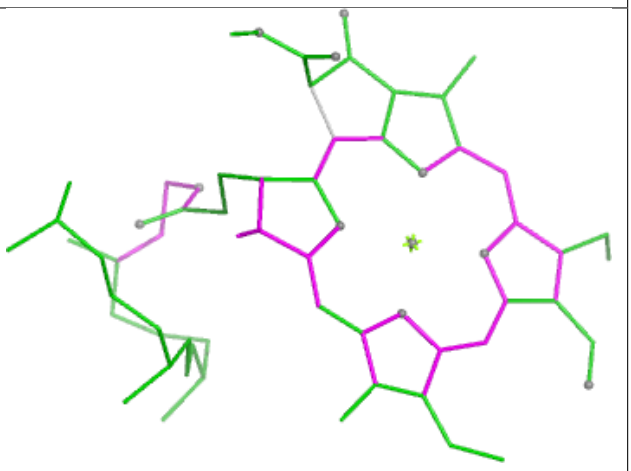
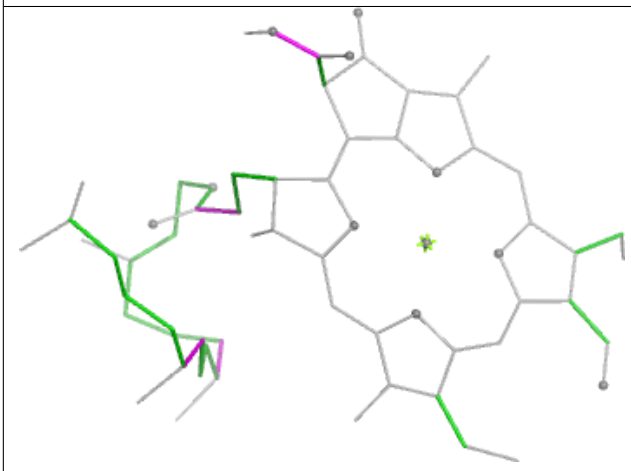


Bond angles

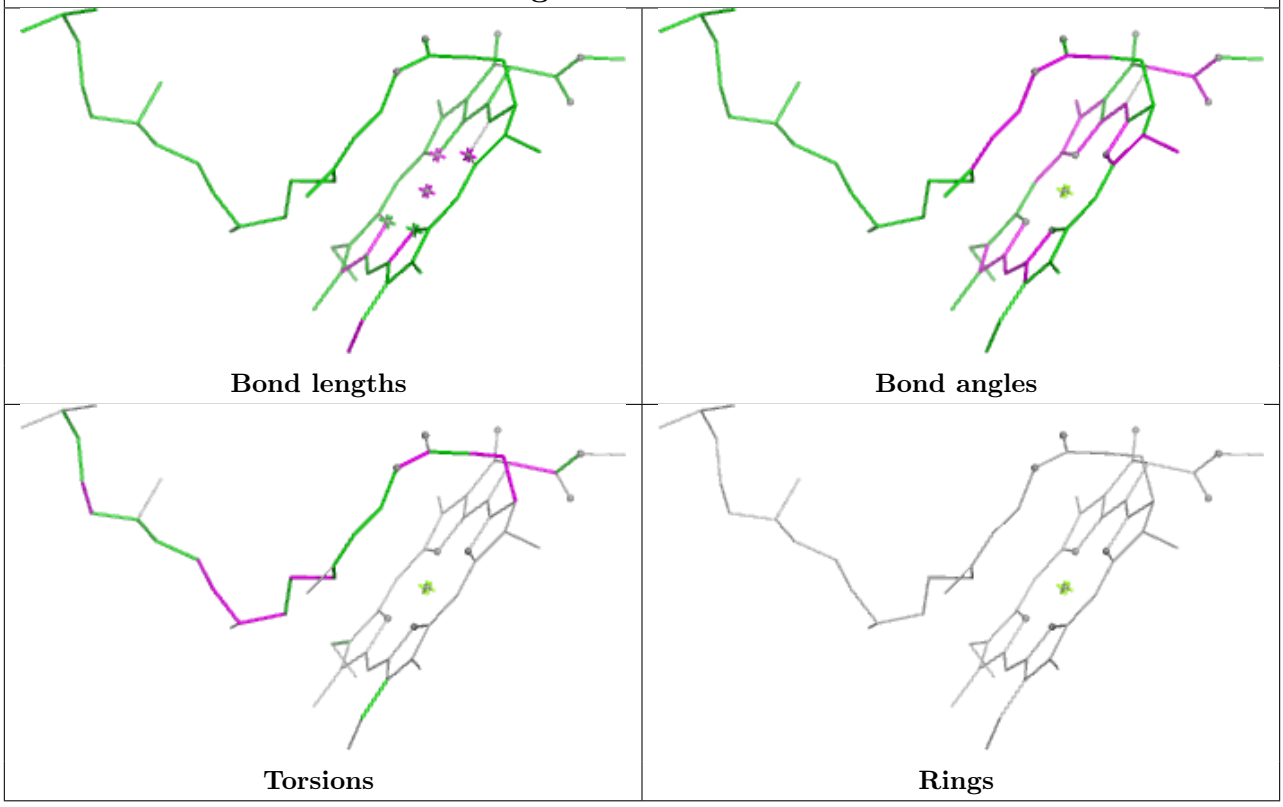


Torsions



Rings

Ligand CLA r 613



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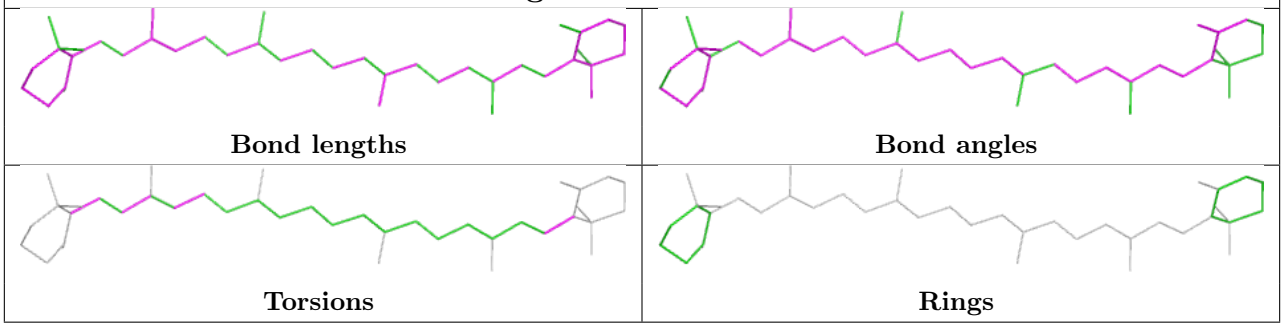

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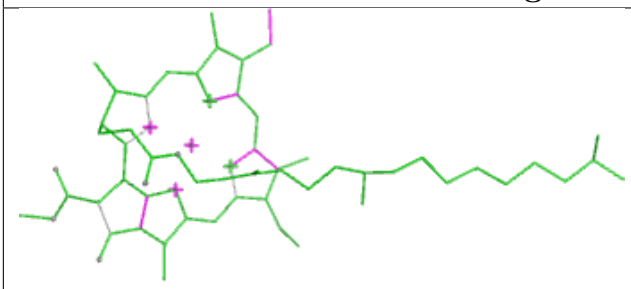

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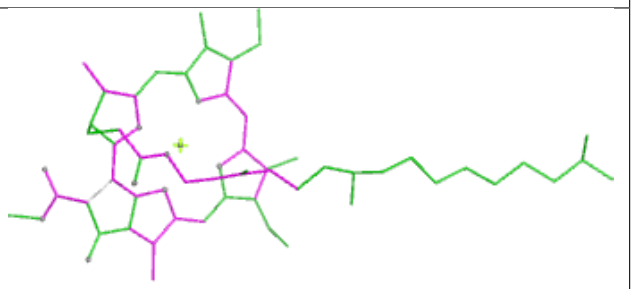
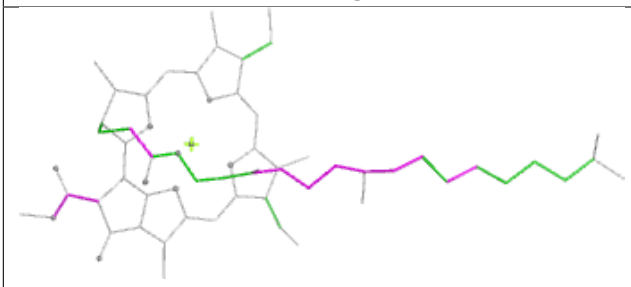


Bond angles



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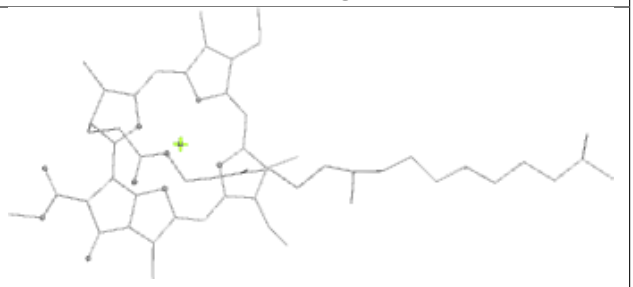
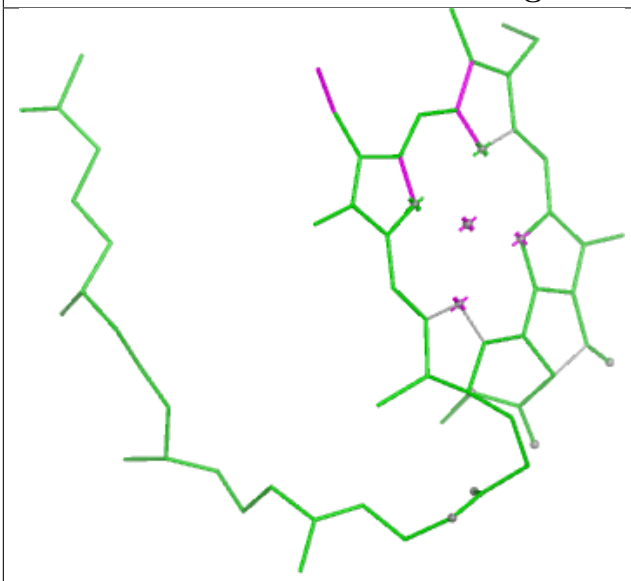


Rings

Ligand CLA C 507



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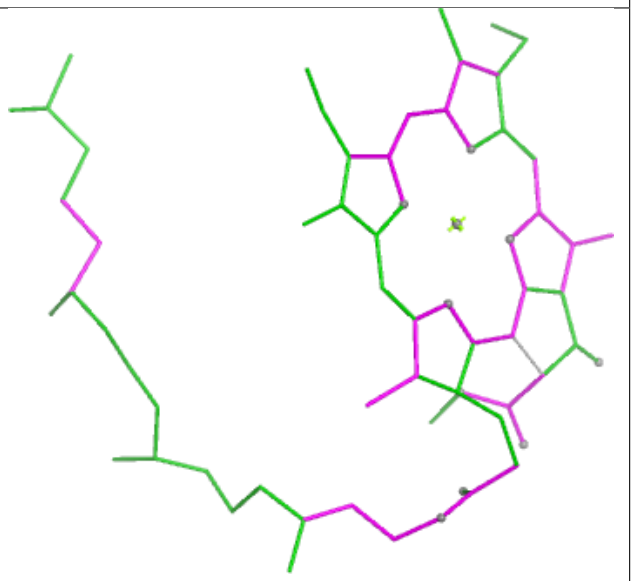
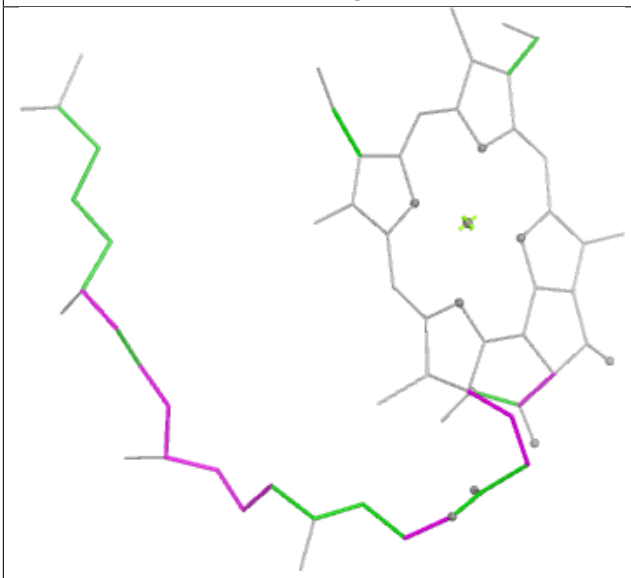


Bond angles



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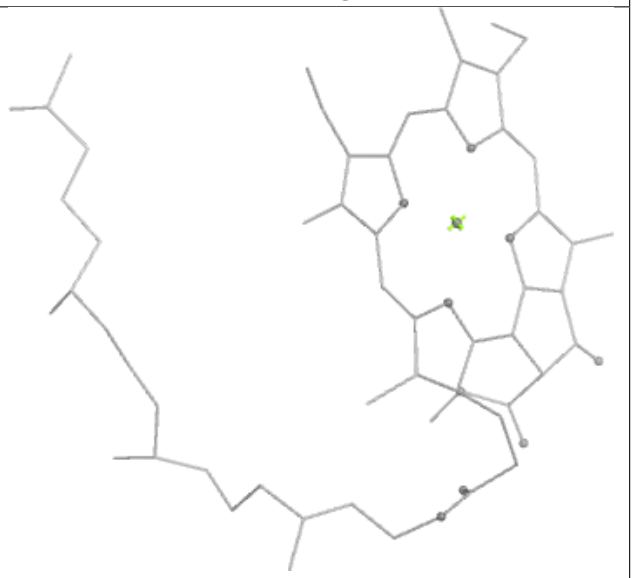
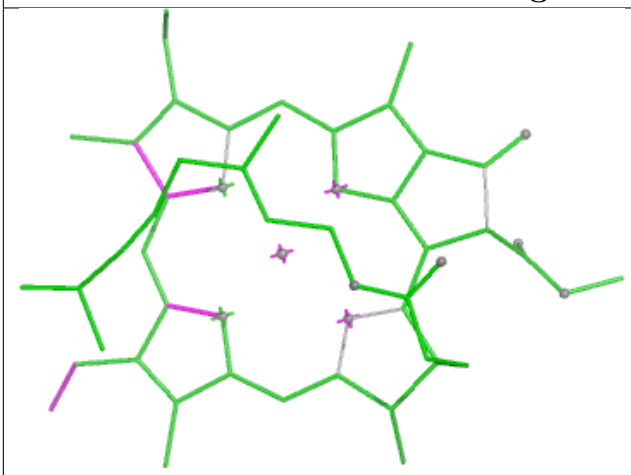


Rings

Ligand CLA s 612



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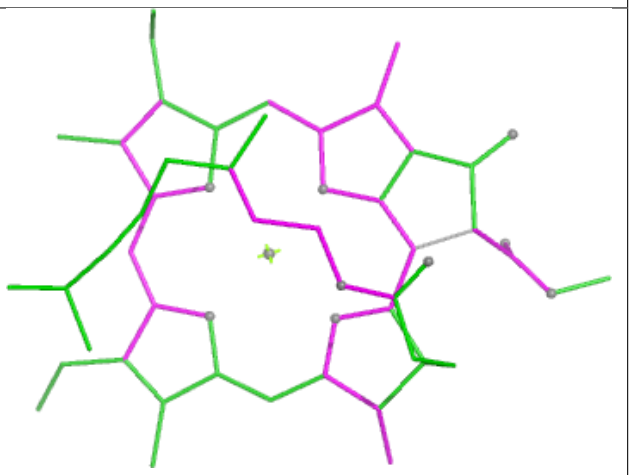
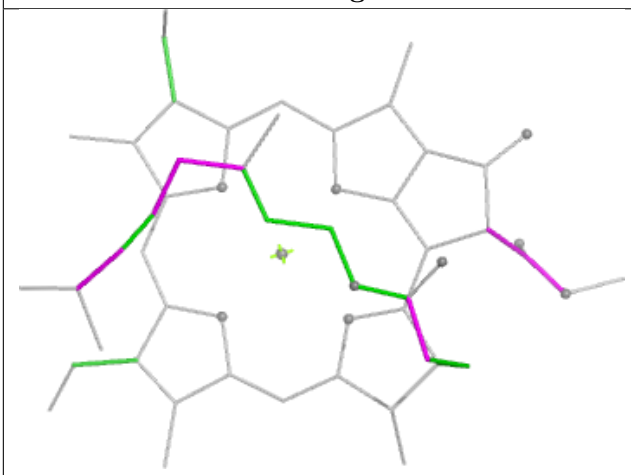


Bond angles



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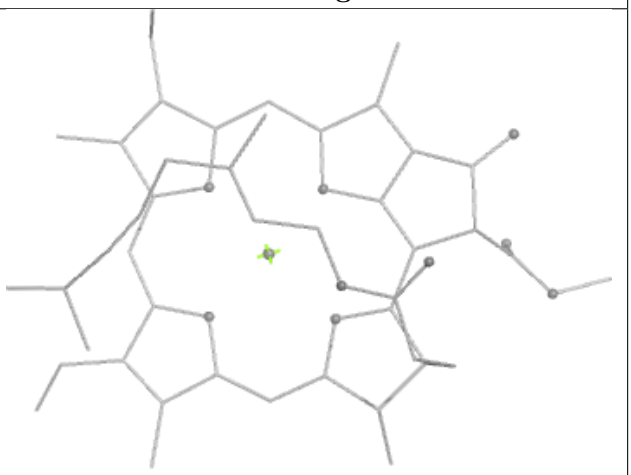
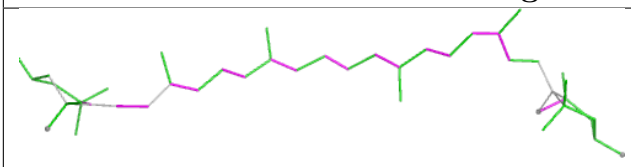


Rings

Ligand NEX G 617



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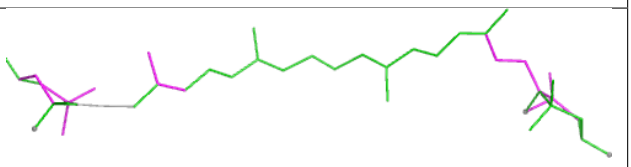
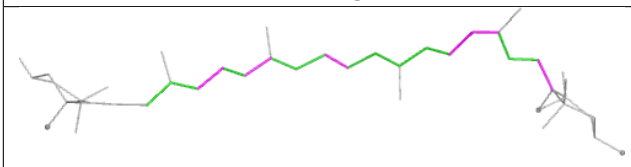


Bond angles



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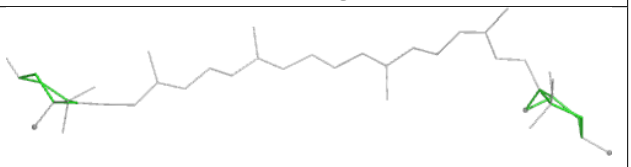
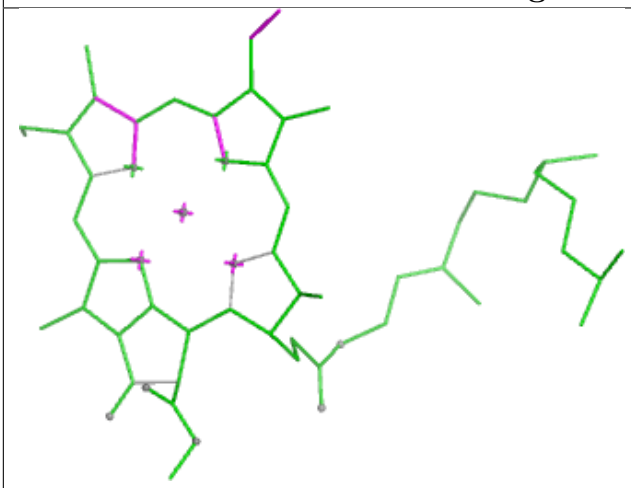


Rings

Ligand CLA a 409



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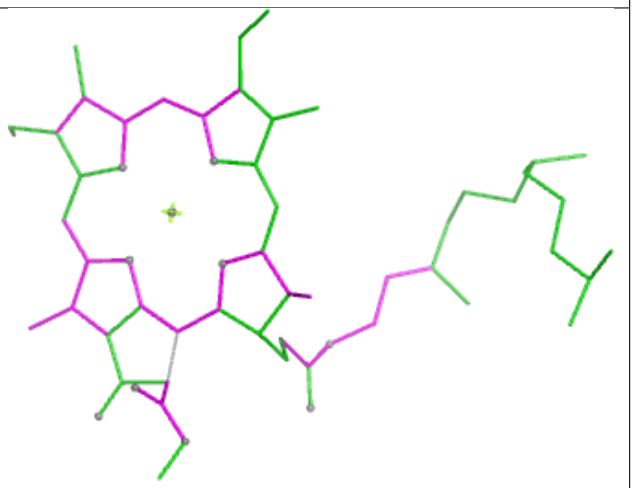
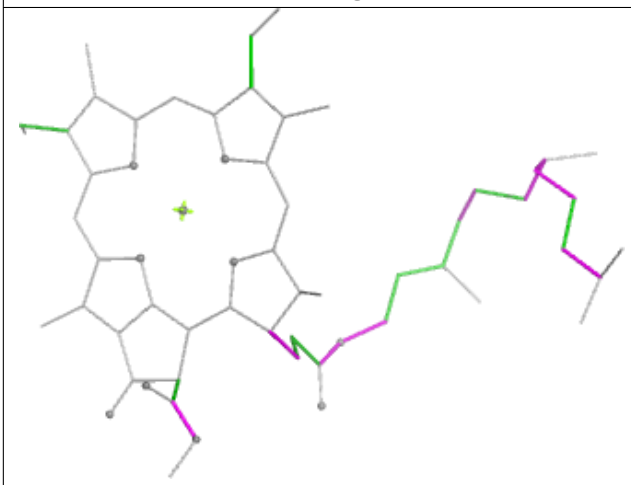


Bond angles



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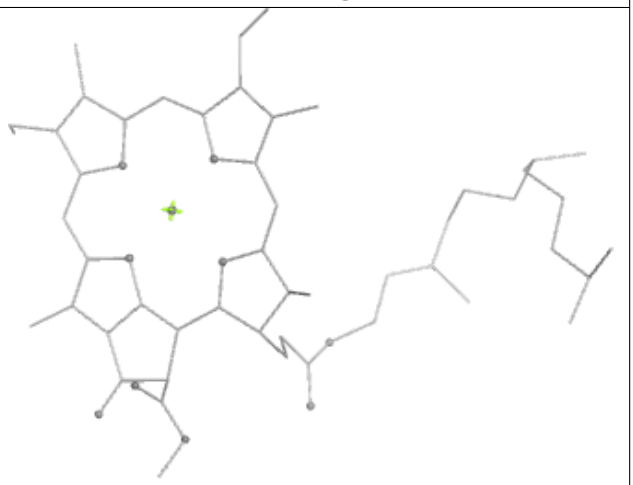
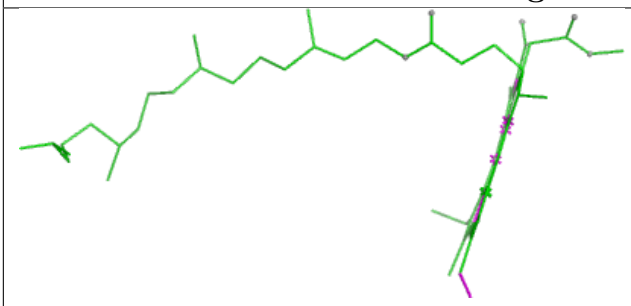


Rings

Ligand CLA b 605



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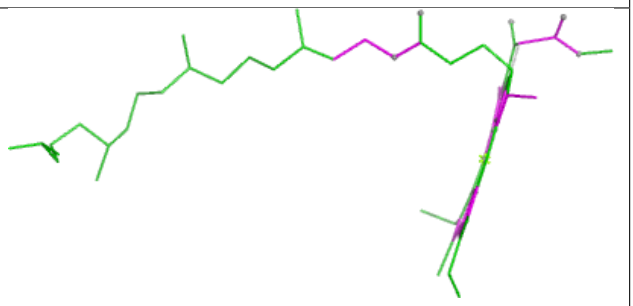
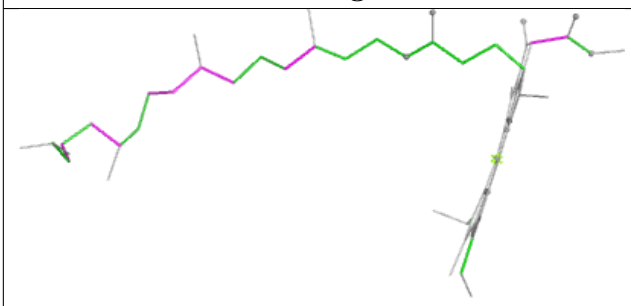


Bond angles



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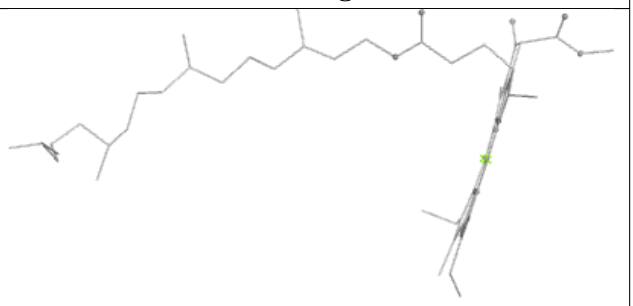
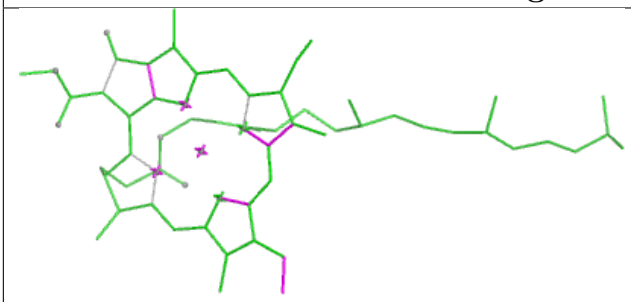


Rings

Ligand CLA b 614



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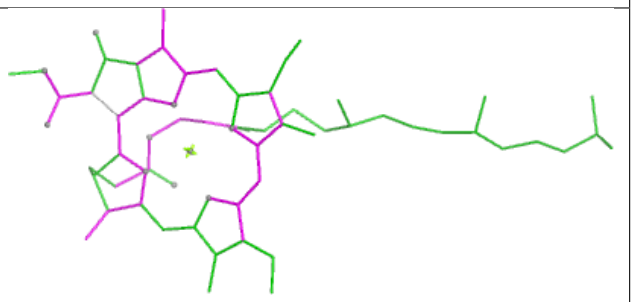
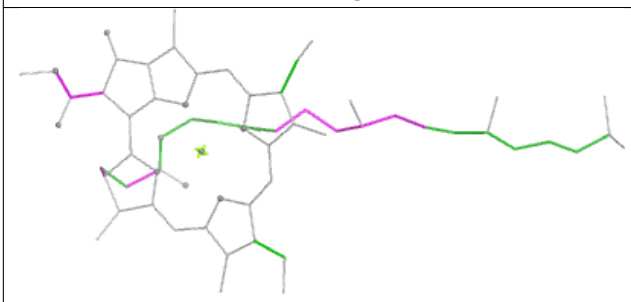


Bond angles

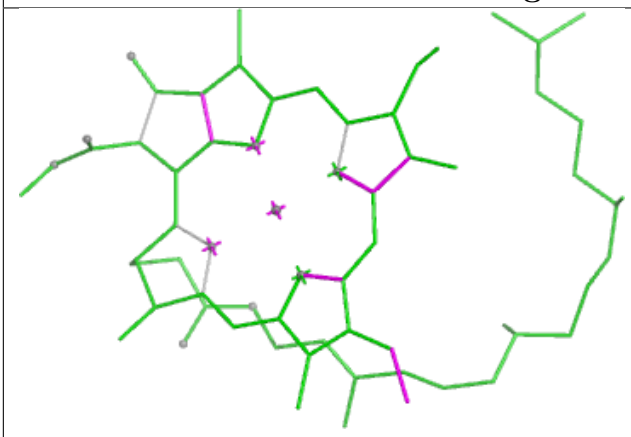


Torsions



Rings

Ligand CLA R 609



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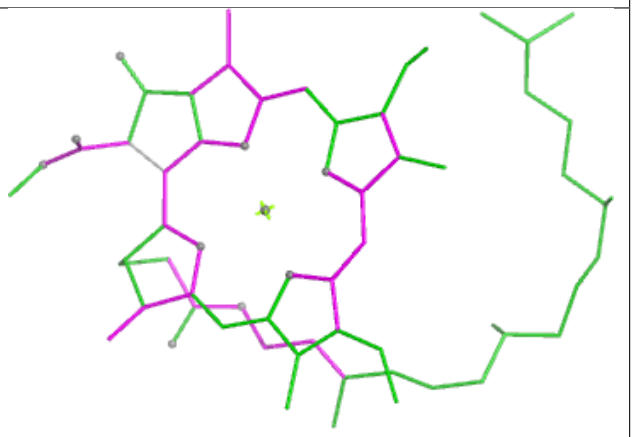
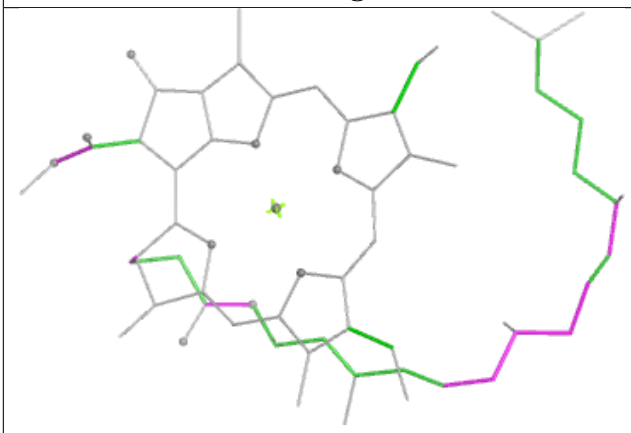


Bond angles



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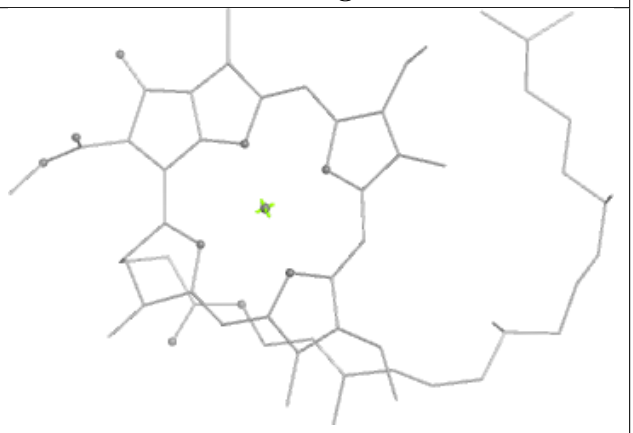
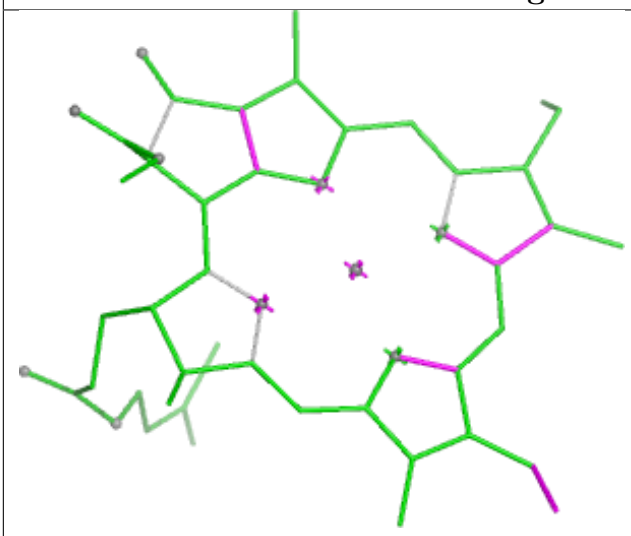


Rings

Ligand CLA n 604



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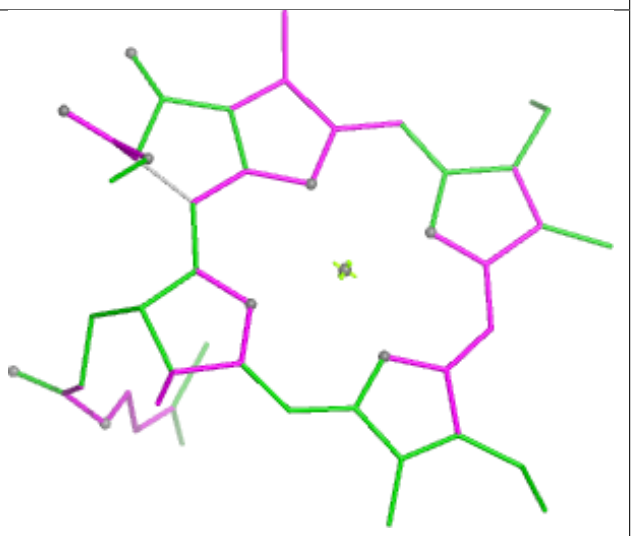
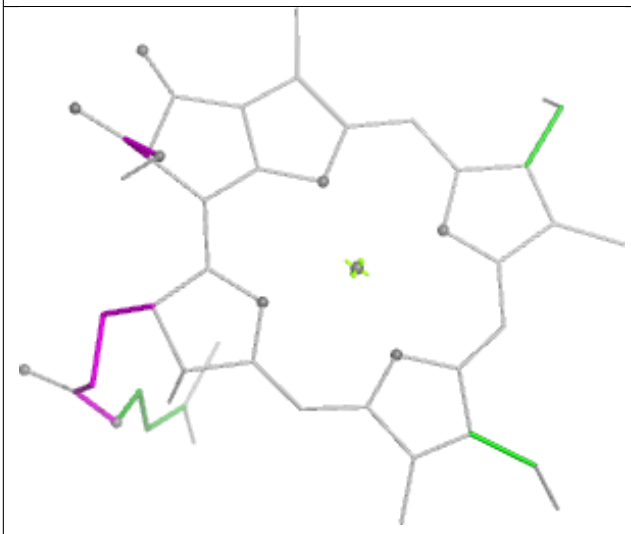


Bond angles



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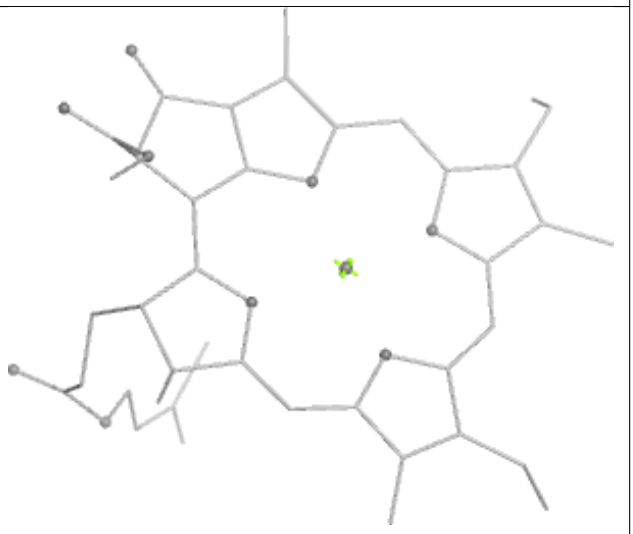
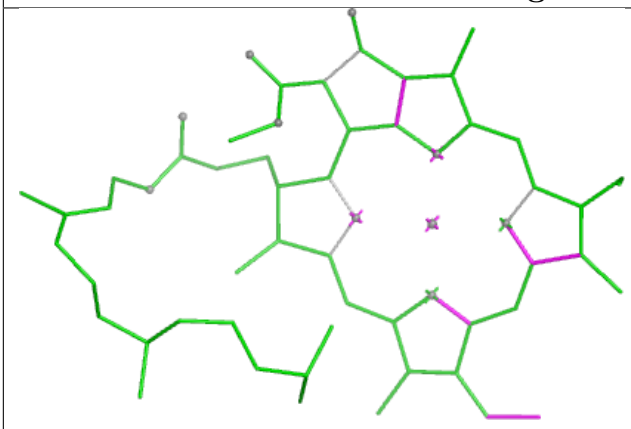


Rings

Ligand CLA y 312



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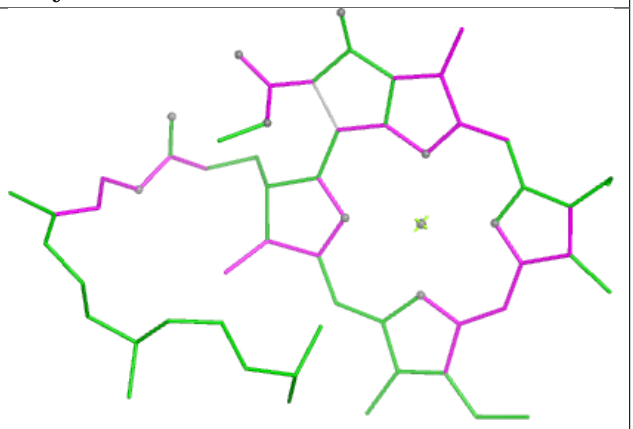
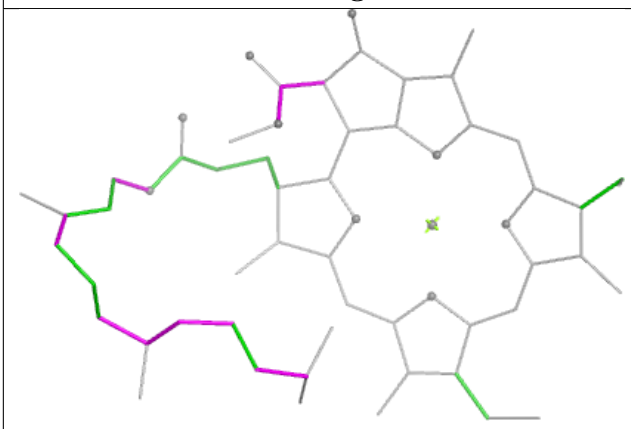


Bond angles



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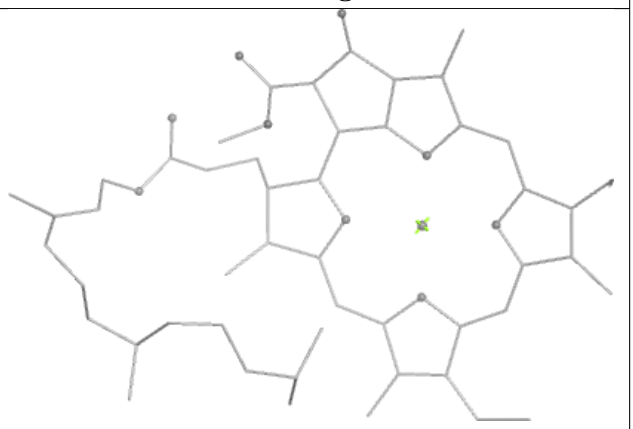
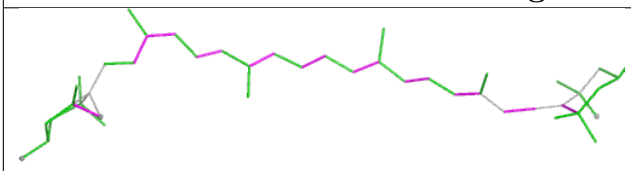


Rings

Ligand NEX s 616



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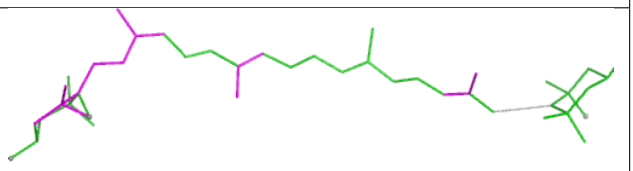
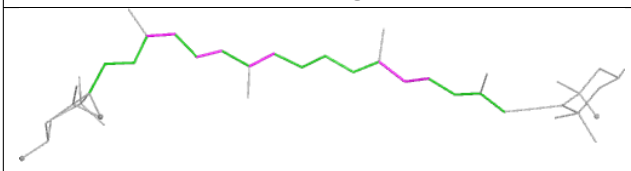
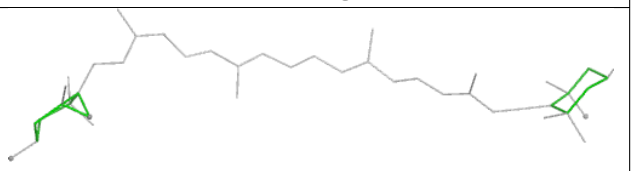


Bond angles

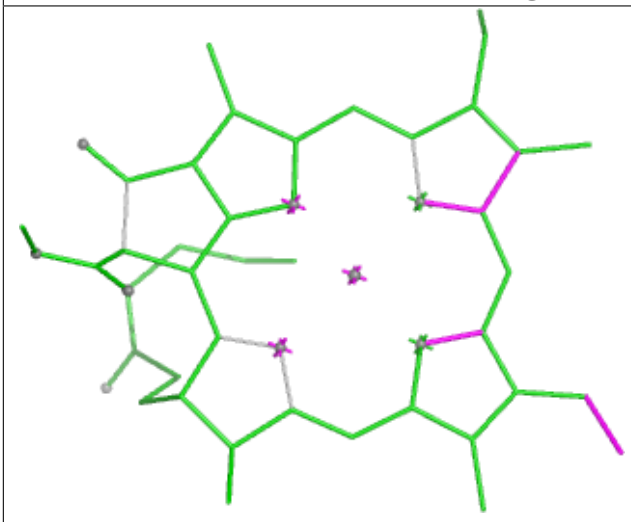


Torsions

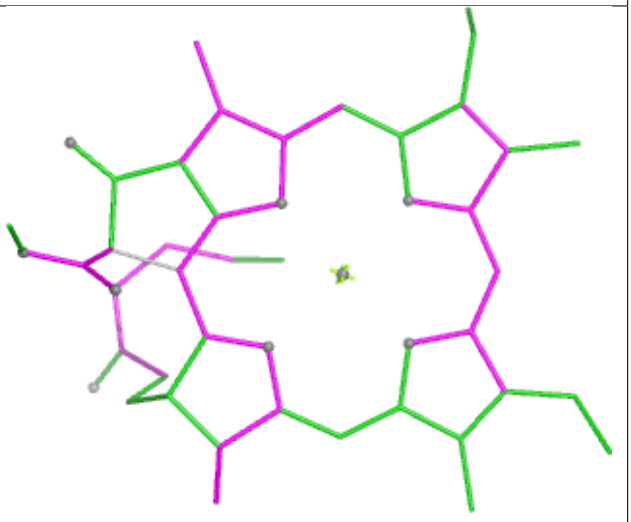


Rings

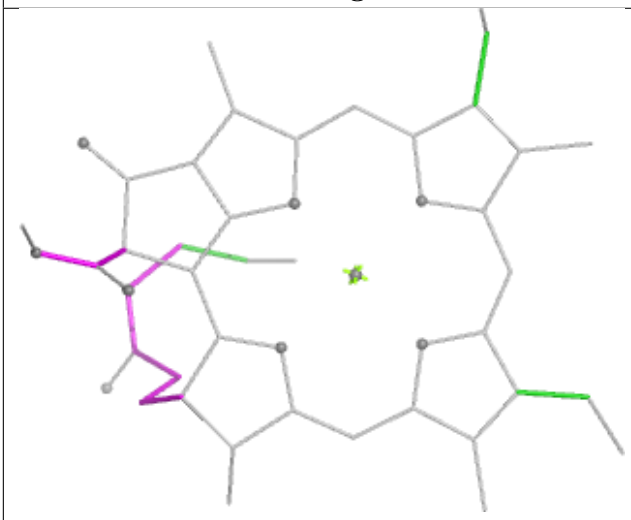
Ligand CLA N 614



Bond lengths



Bond angles



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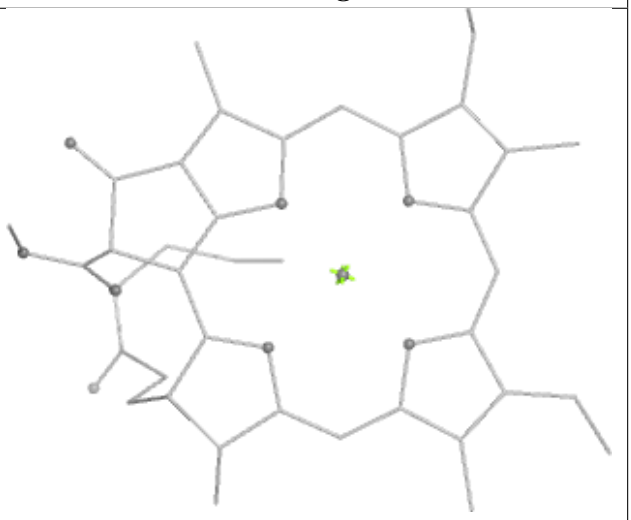
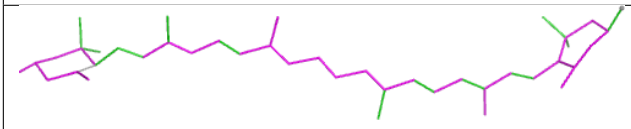


Rings

Ligand LUT Y 615



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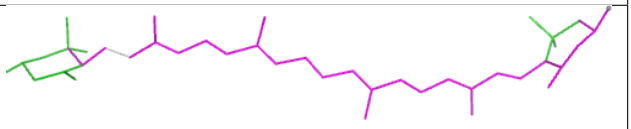
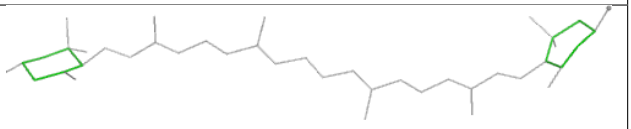


Bond angles

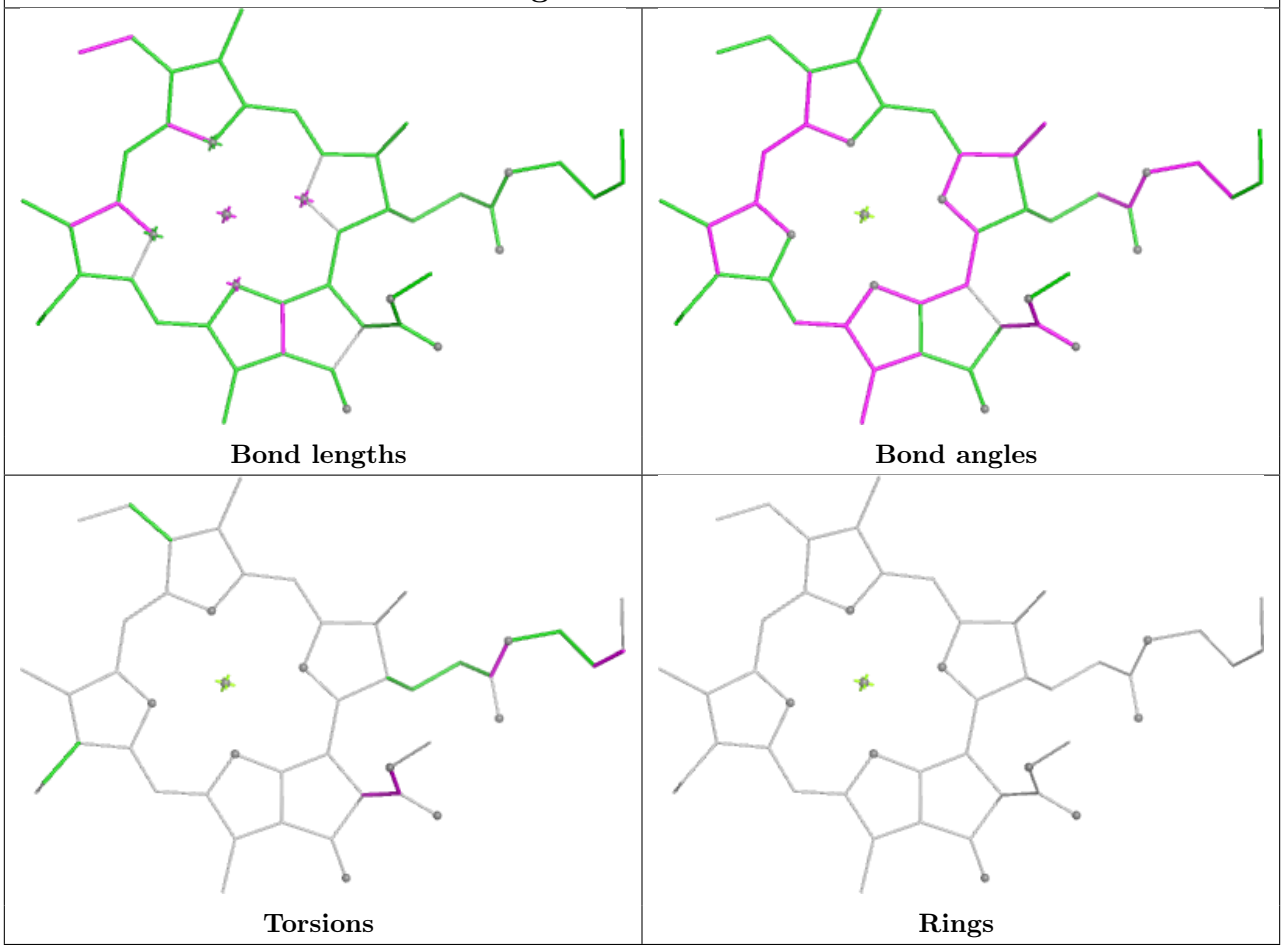


Torsions



Rings

Ligand CLA s 611



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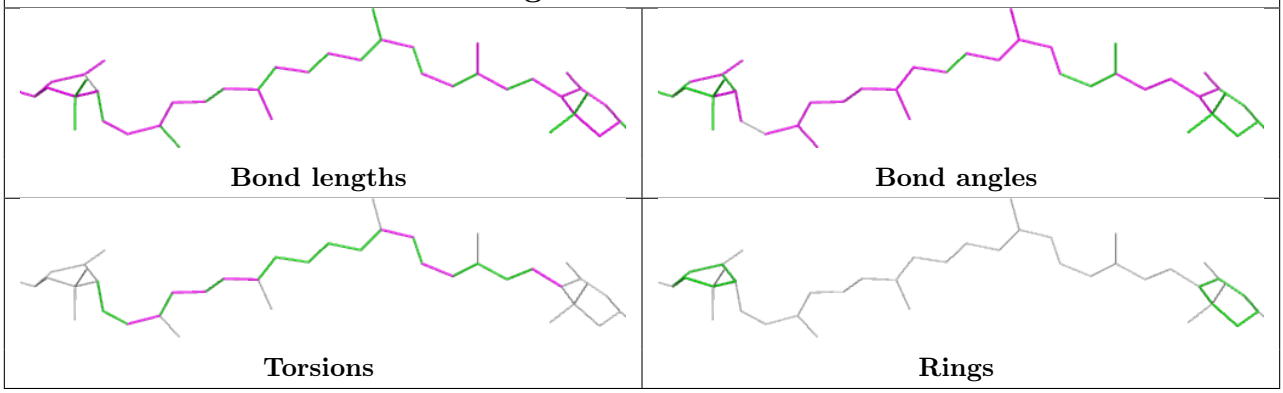

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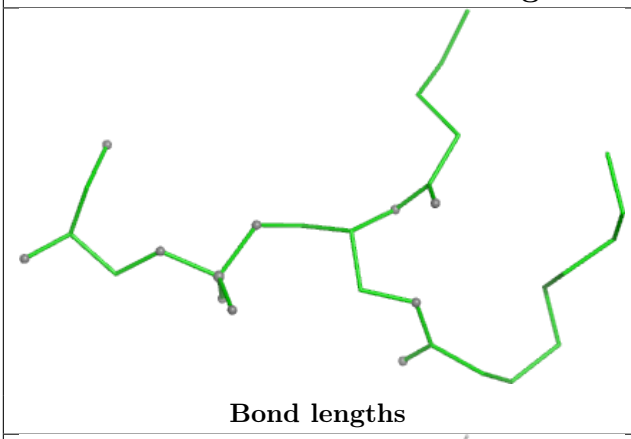

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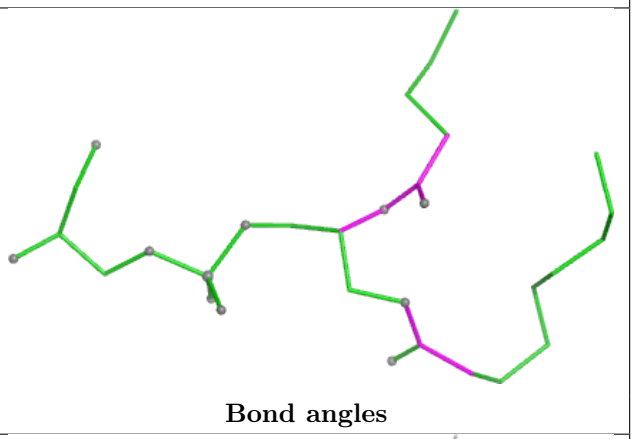
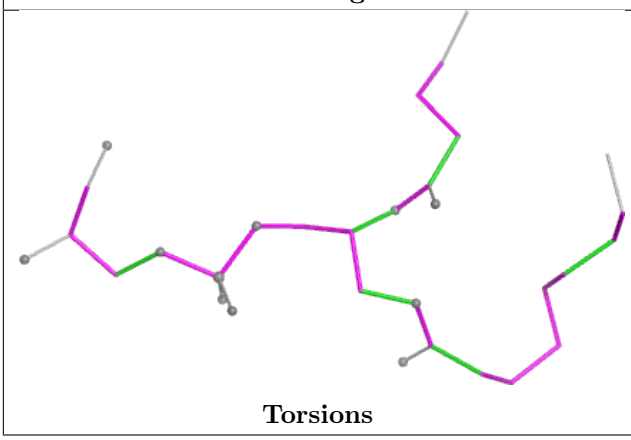


Bond angles



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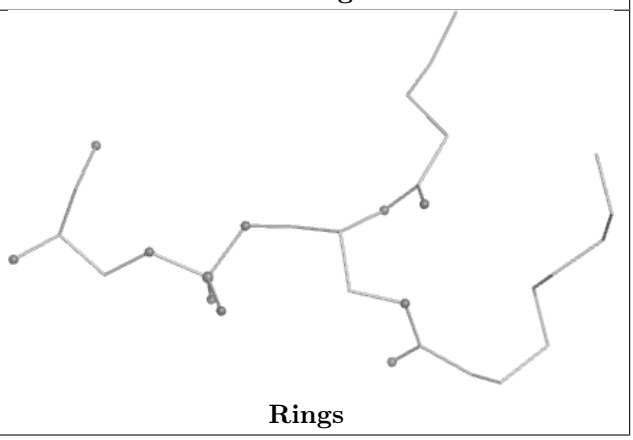
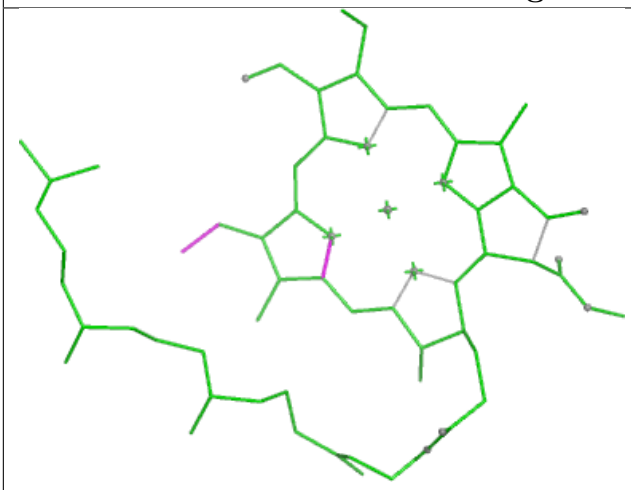


Rings

Ligand CHL n 607



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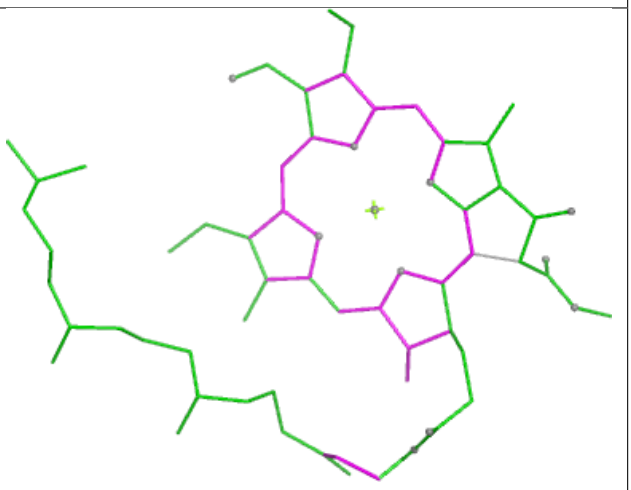

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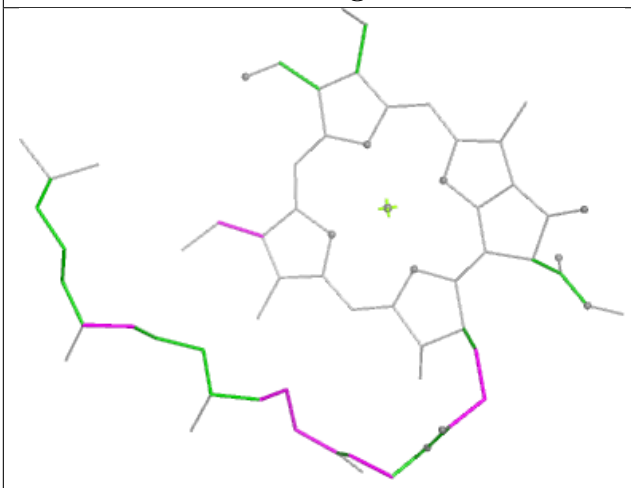

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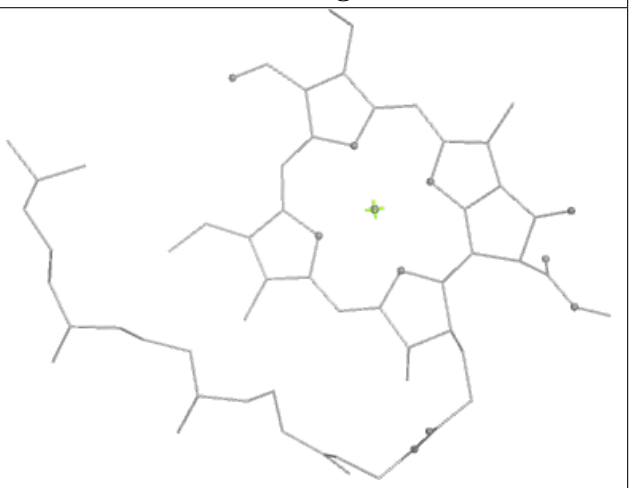
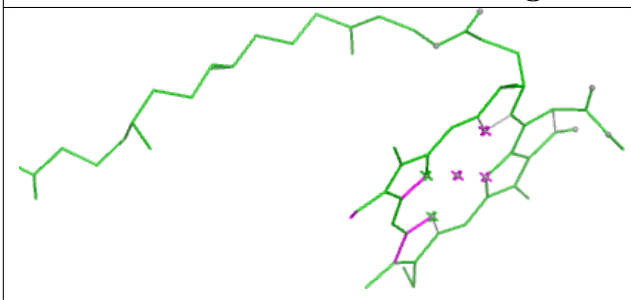


Rings

Ligand CLA C 504



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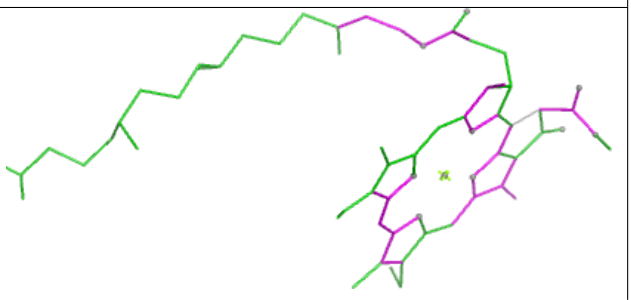

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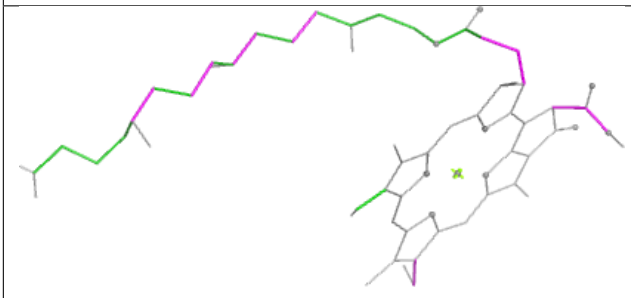
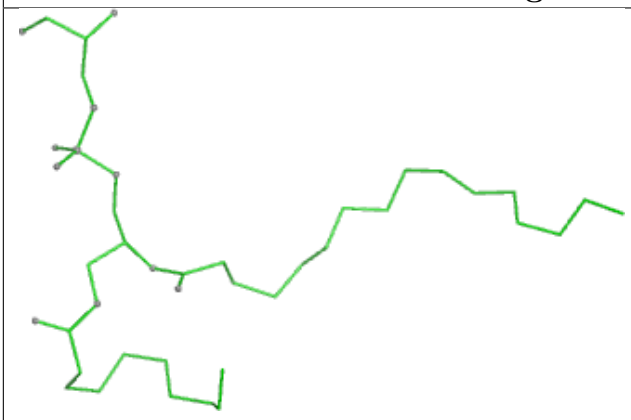


Torsions



Rings

Ligand LHG S 317



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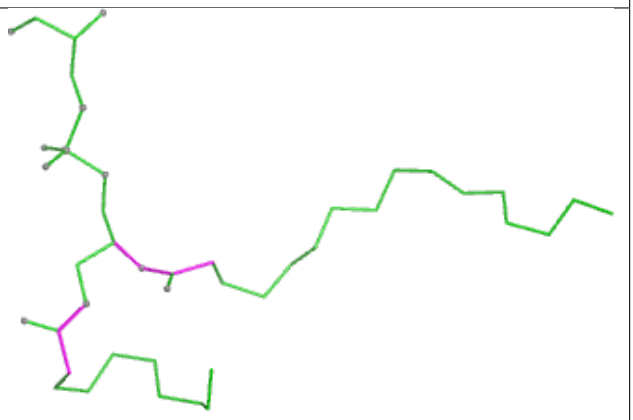
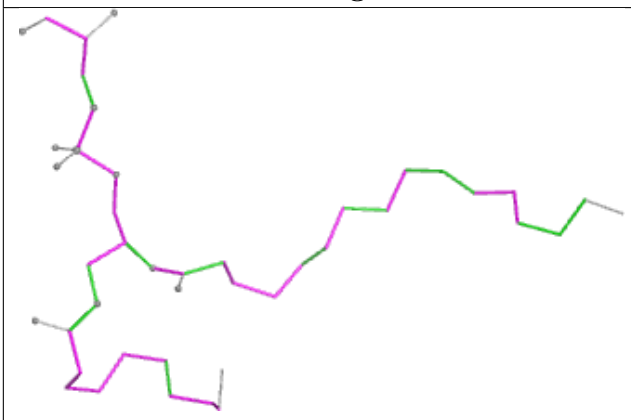


Bond angles

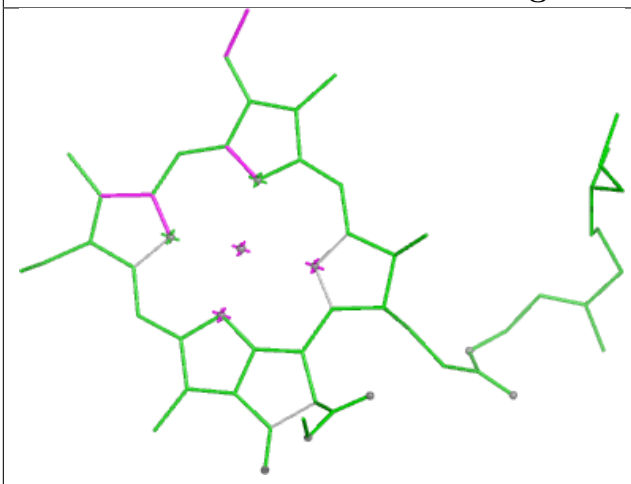


Torsions



Rings

Ligand CLA c 512



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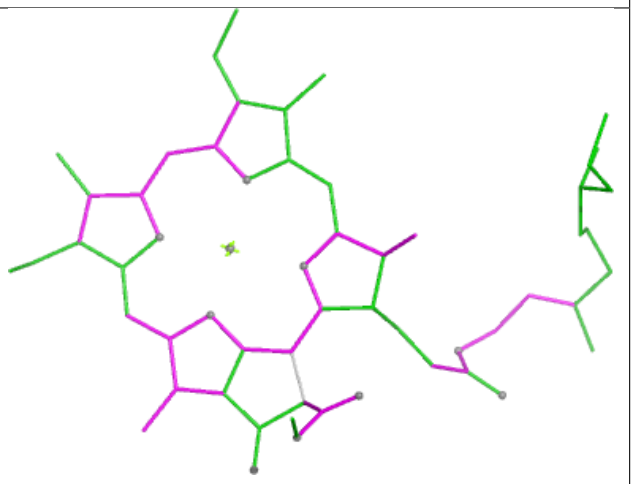

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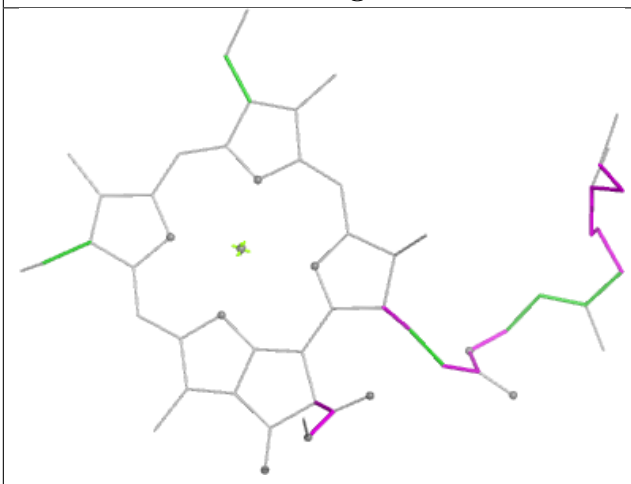

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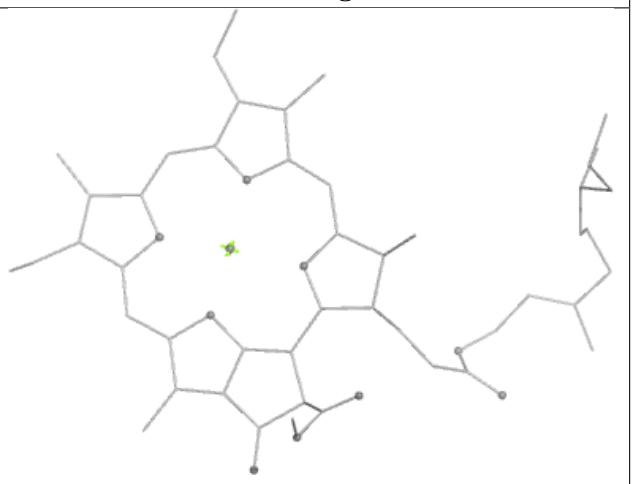
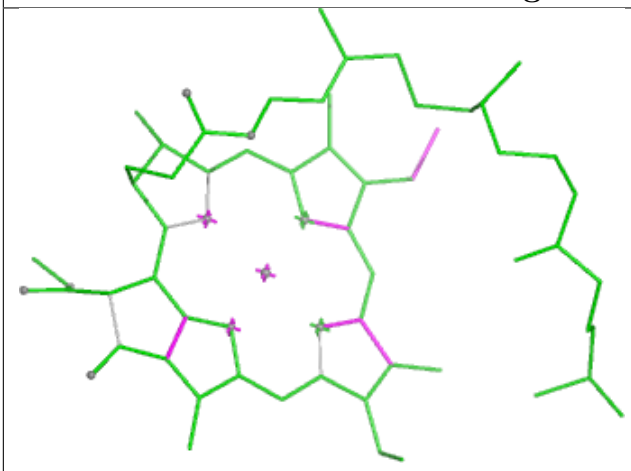


Rings

Ligand CLA N 602



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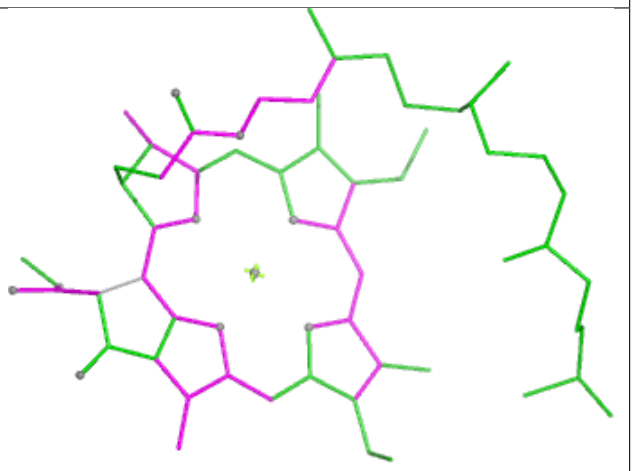
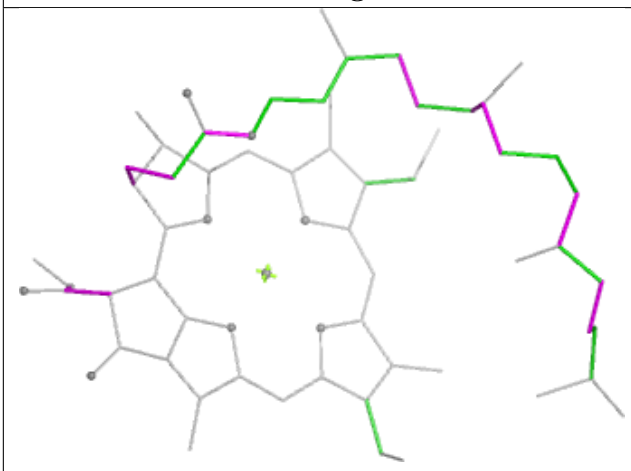


Bond angles



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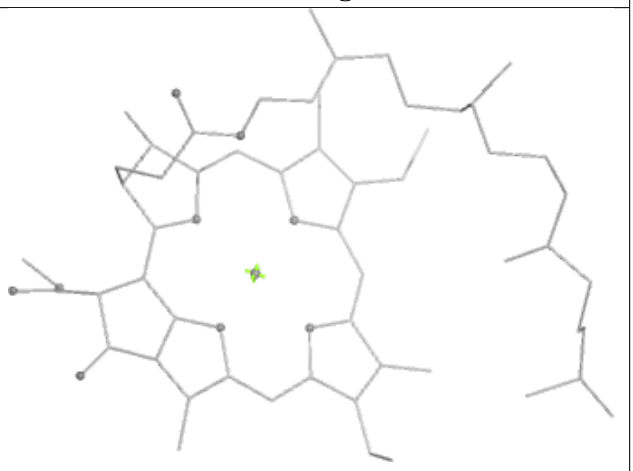


Rings

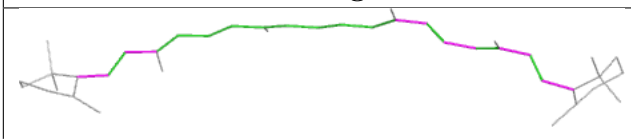
Ligand BCR d 406



Bond lengths



Bond angles

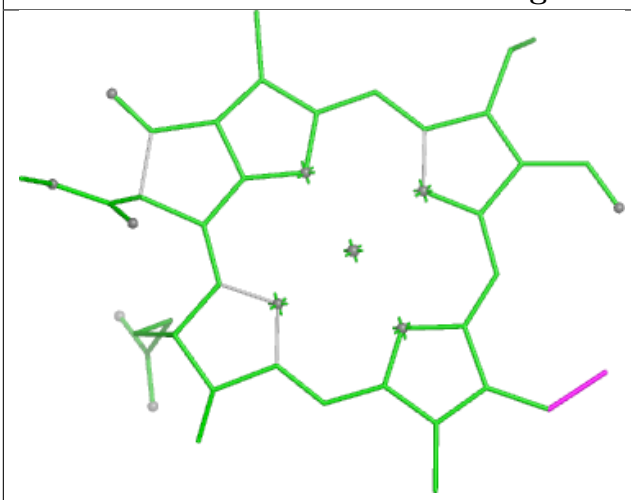


Torsions



Rings

Ligand CHL s 607



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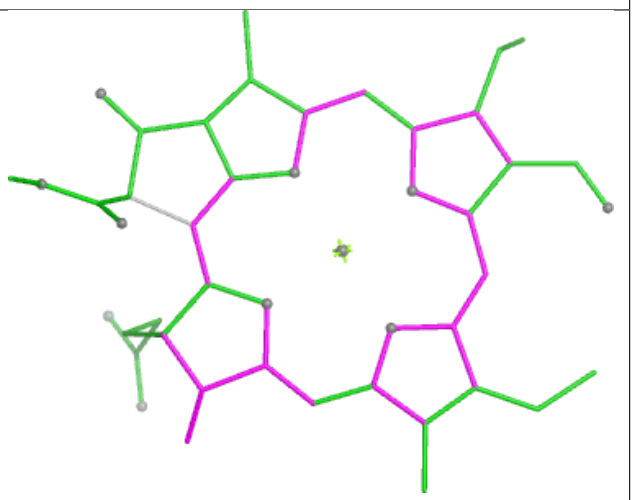
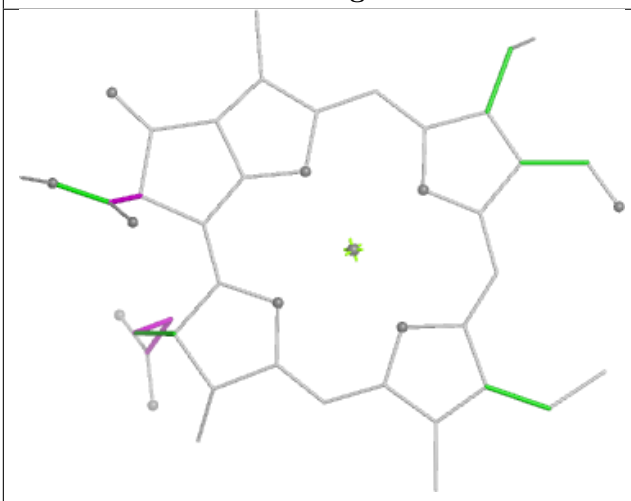


Bond angles



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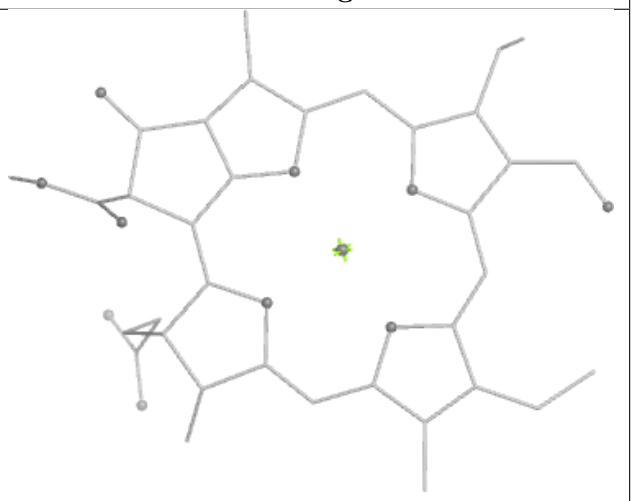
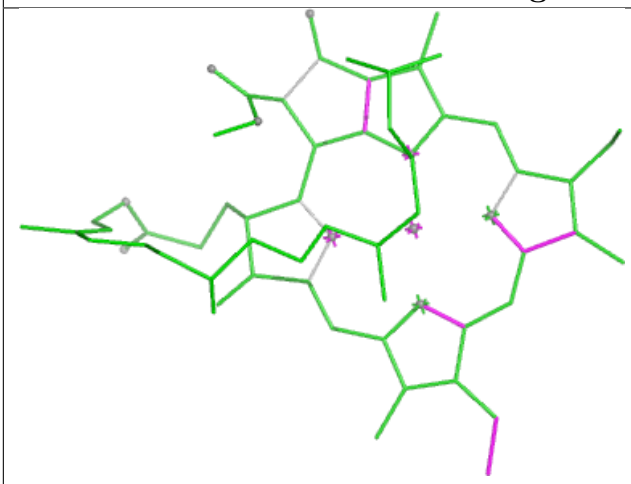


Rings

Ligand CLA c 510



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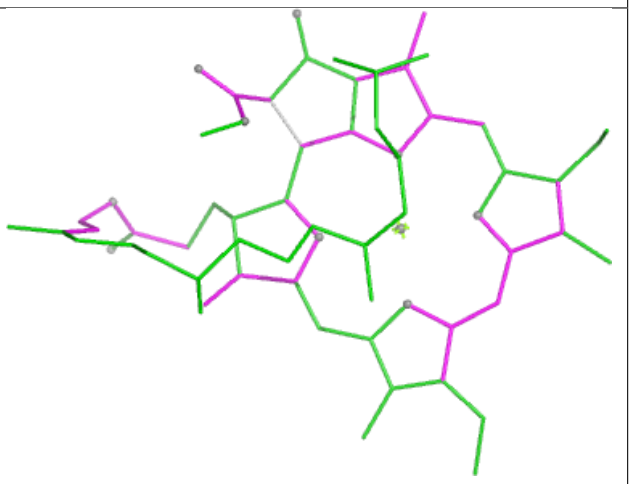
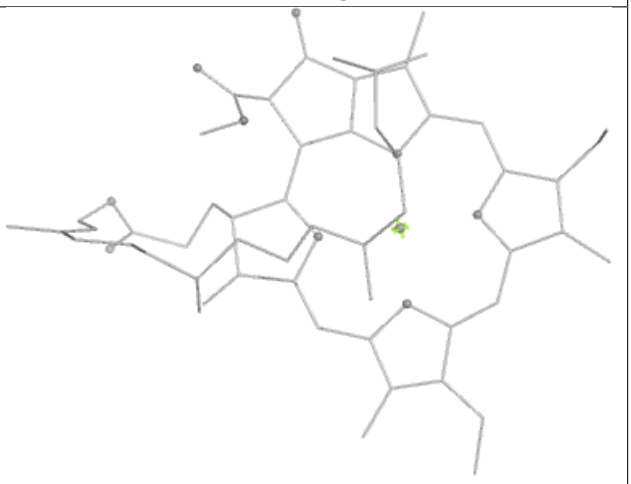


Bond angles

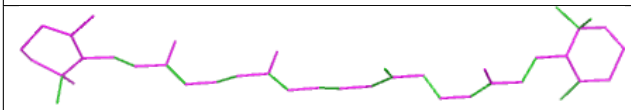


Torsions



Rings

Ligand BCR h 101



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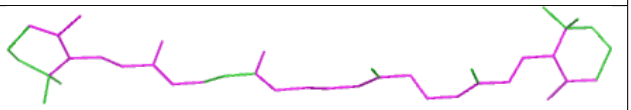
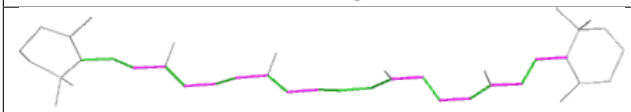


Bond angles



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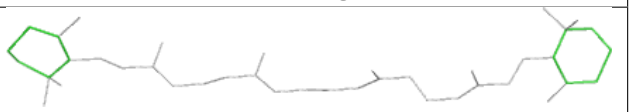
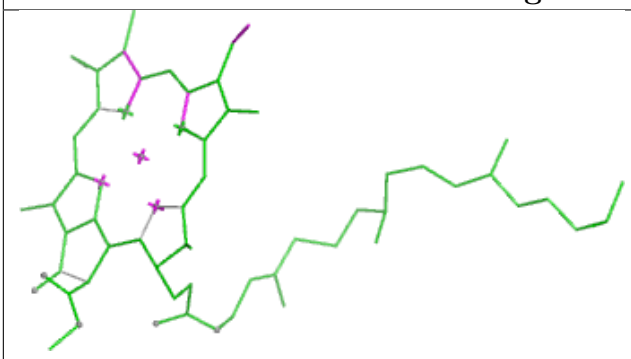


Rings

Ligand CLA C 511



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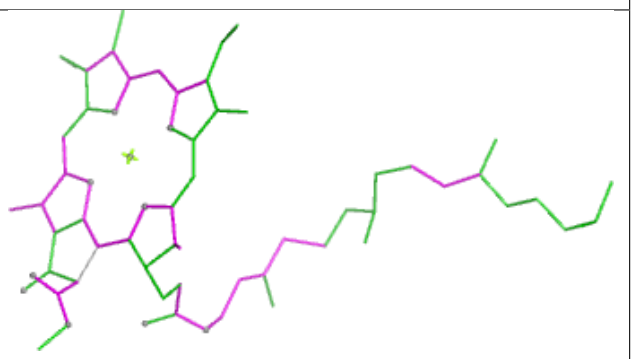
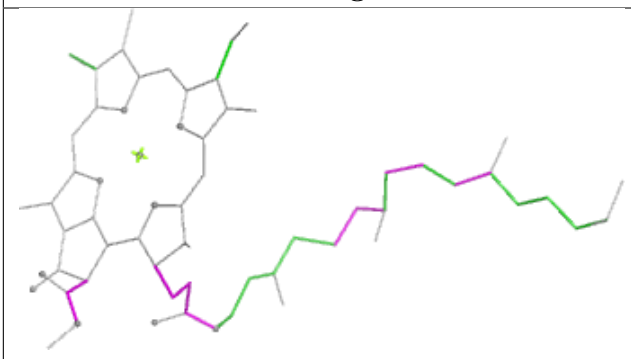


Bond angles



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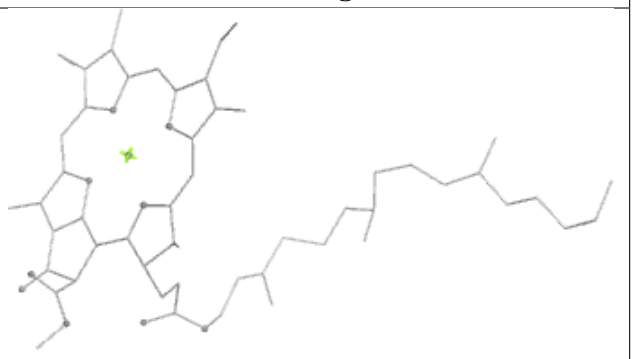
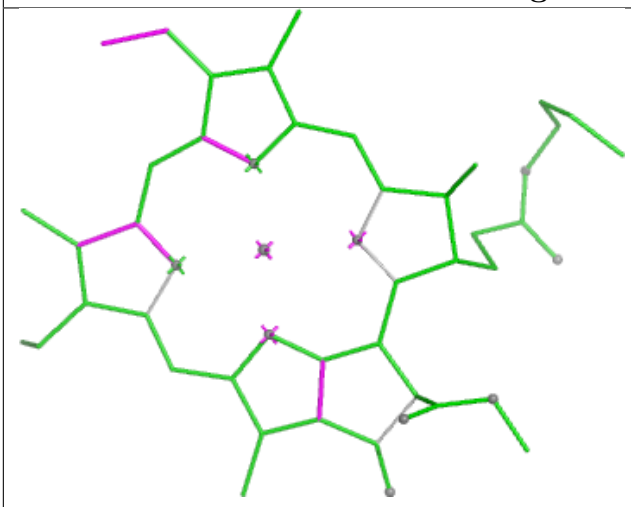


Rings

Ligand CLA r 601



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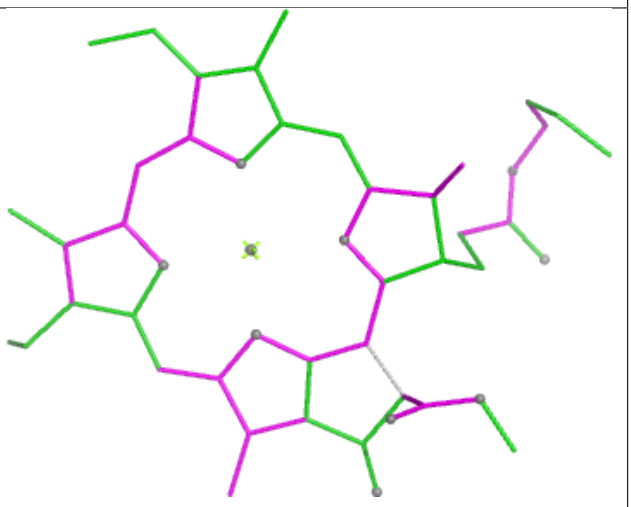
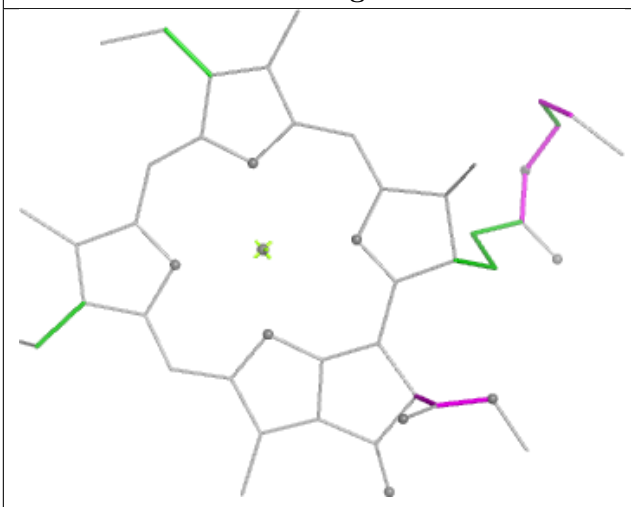


Bond angles



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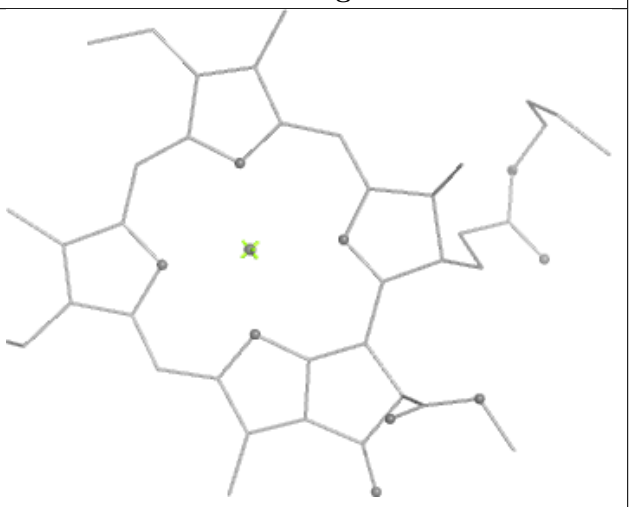
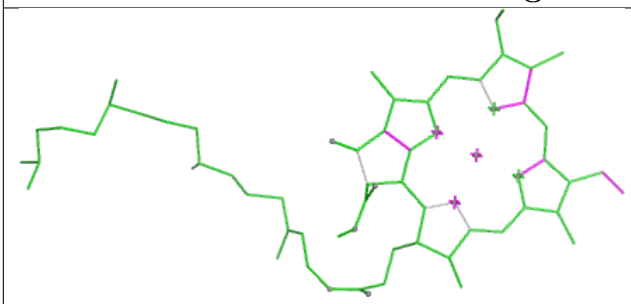


Rings

Ligand CLA B 602



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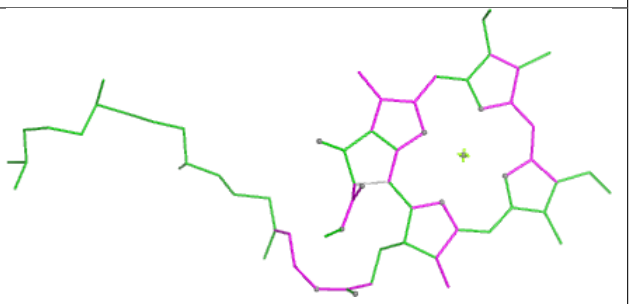
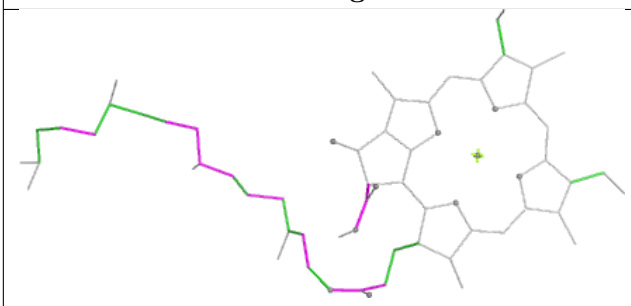


Bond angles



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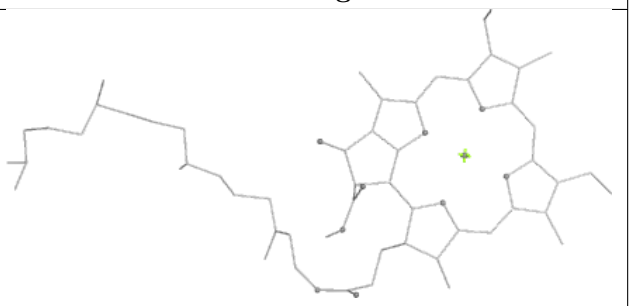
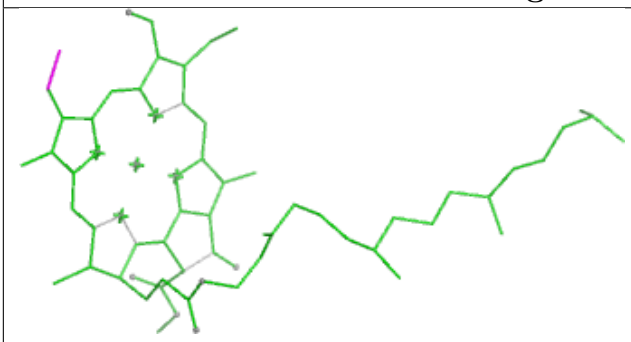


Rings

Ligand CHL n 609



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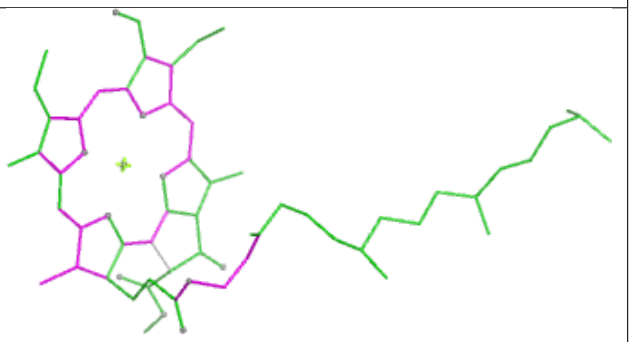
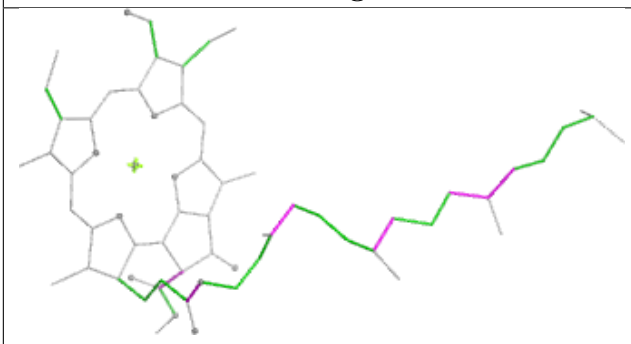
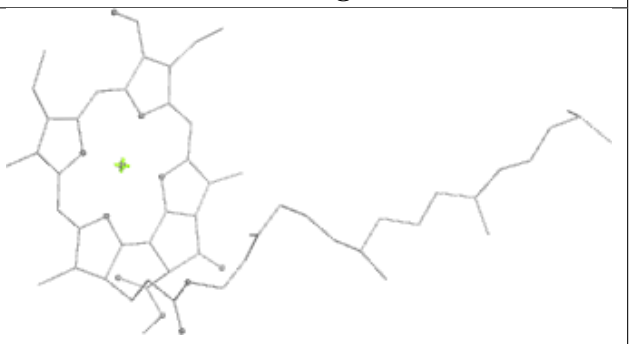


Bond angles

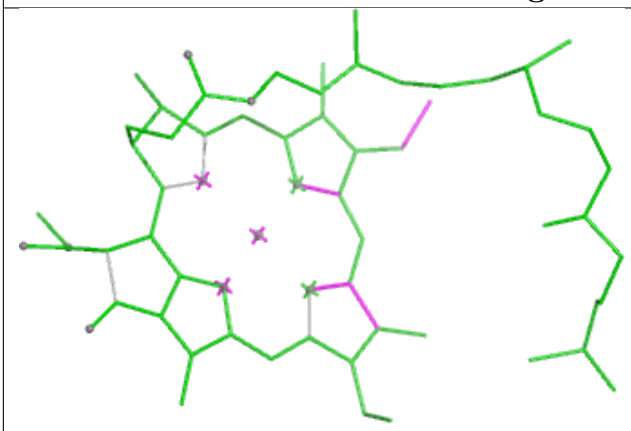


Torsions

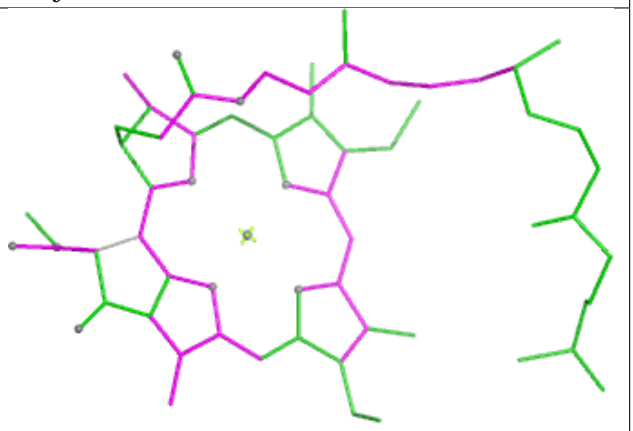


Rings

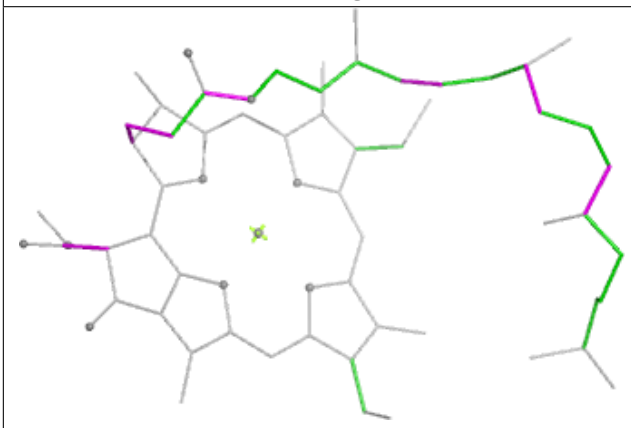
Ligand CLA y 303



Bond lengths



Bond angles



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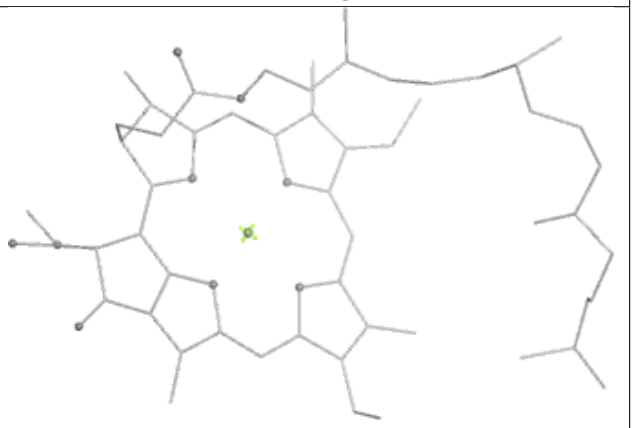
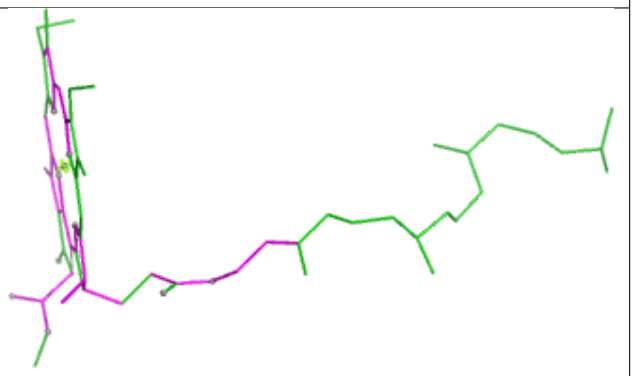


Rings

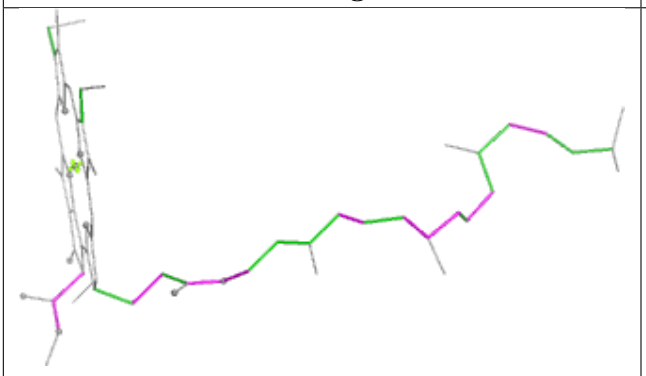
Ligand CLA b 606



Bond lengths



Bond angles



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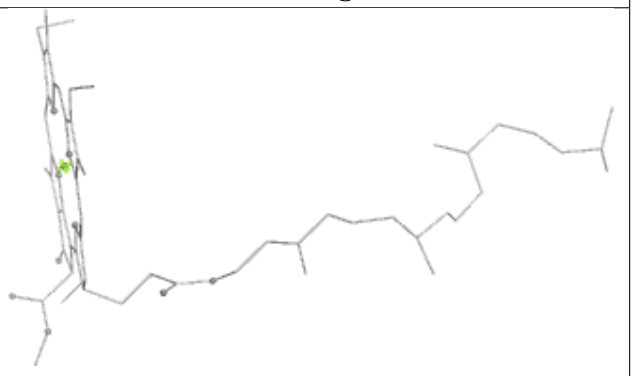
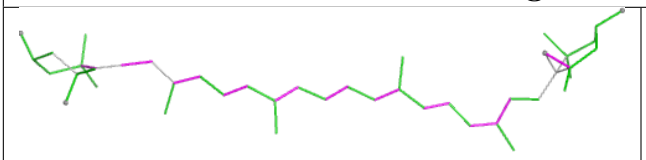


Rings

Ligand NEX y 301



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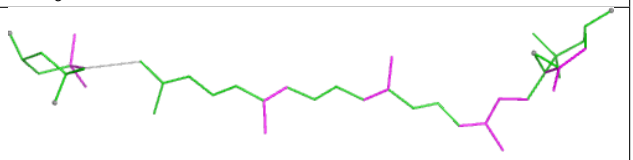
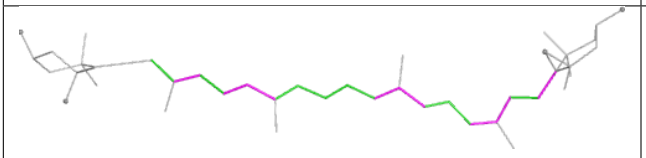


Bond angles



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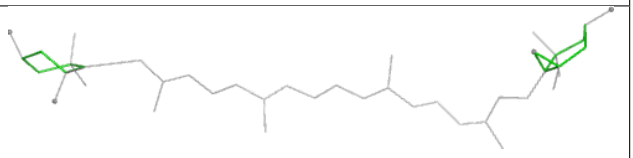
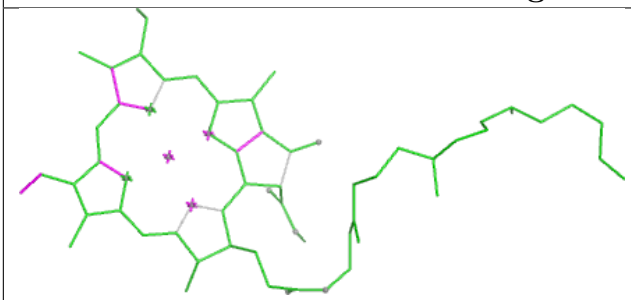


Rings

Ligand CLA b 602



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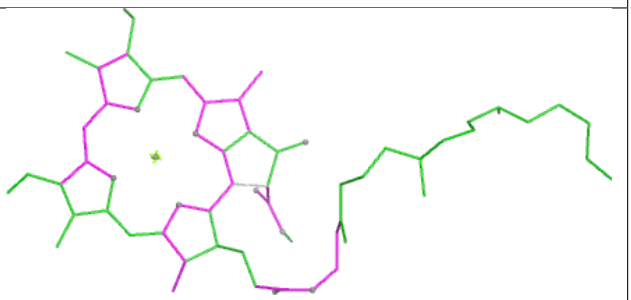
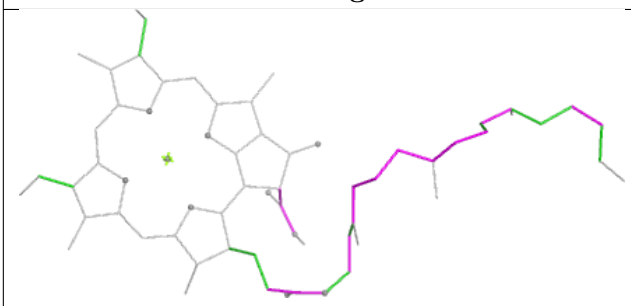


Bond angles



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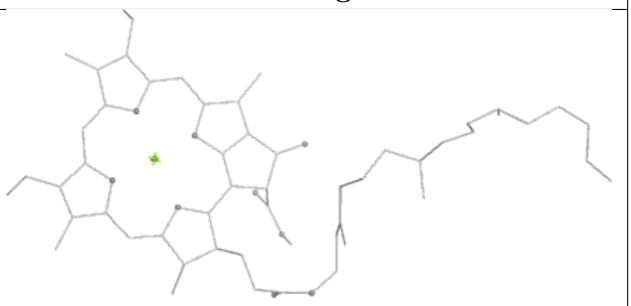
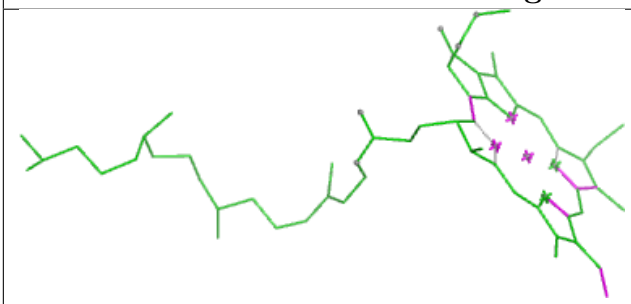


Rings

Ligand CLA C 502



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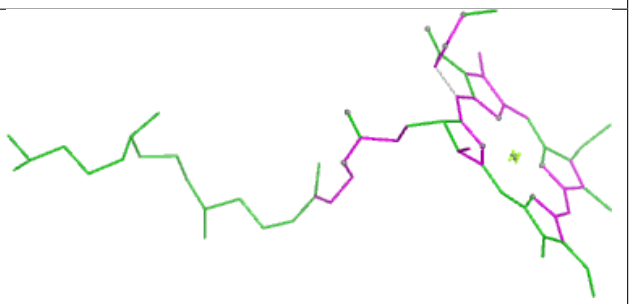
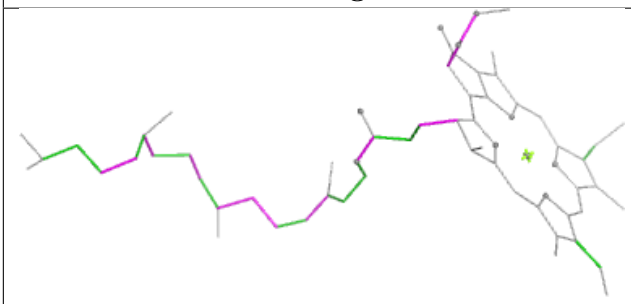


Bond angles



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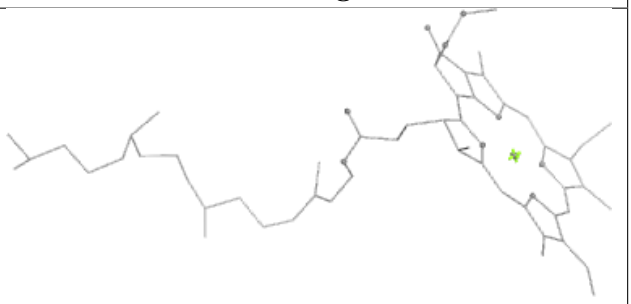
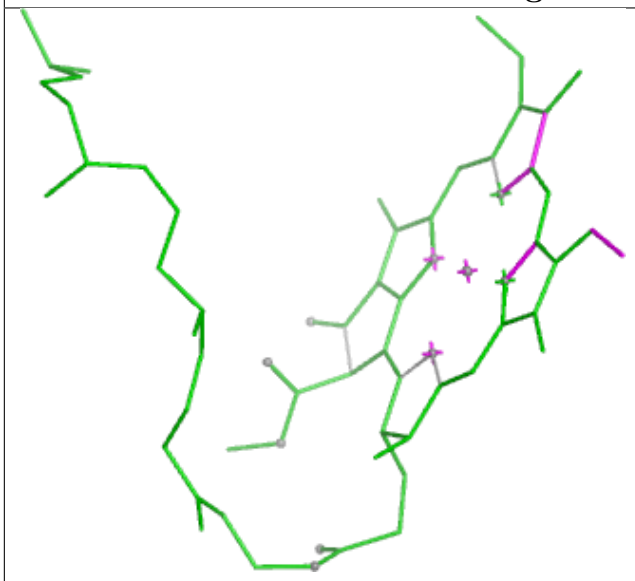


Rings

Ligand CLA B 613



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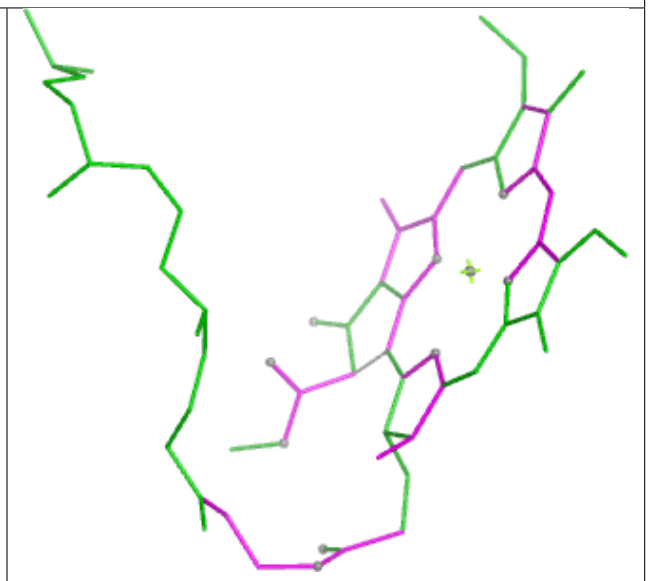
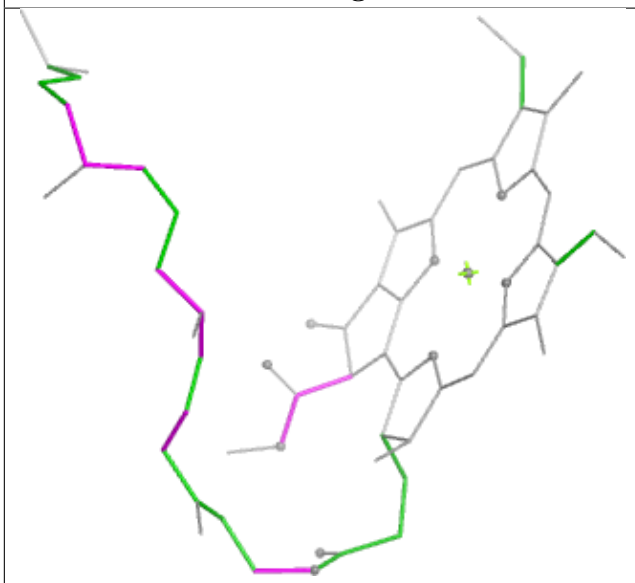


Bond angles

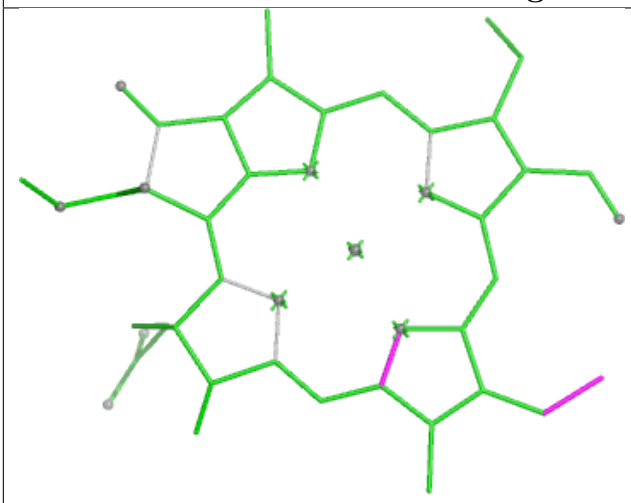


Torsions



Rings

Ligand CHL S 308



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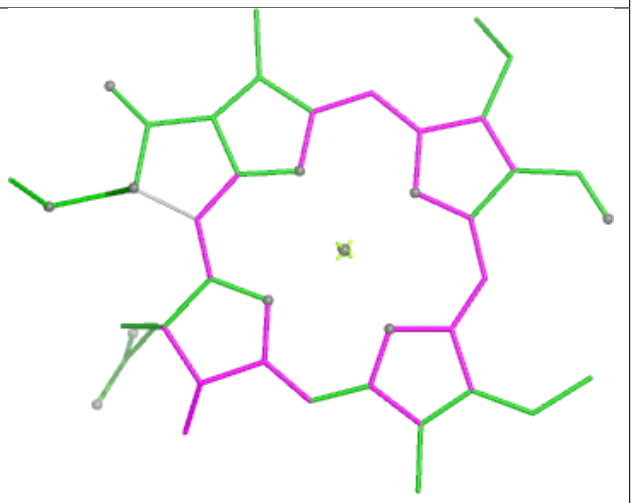
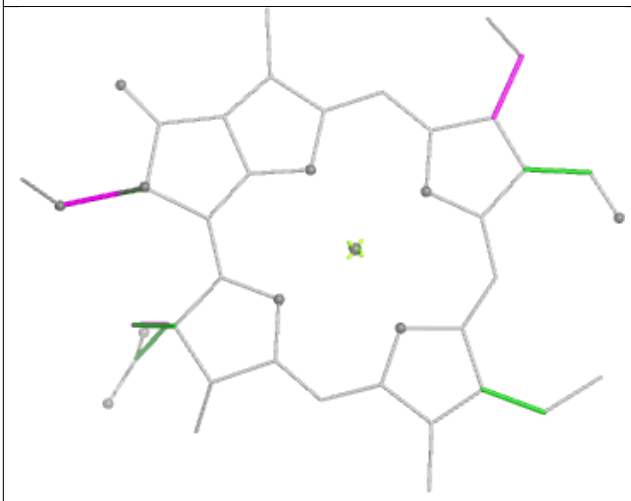


Bond angles



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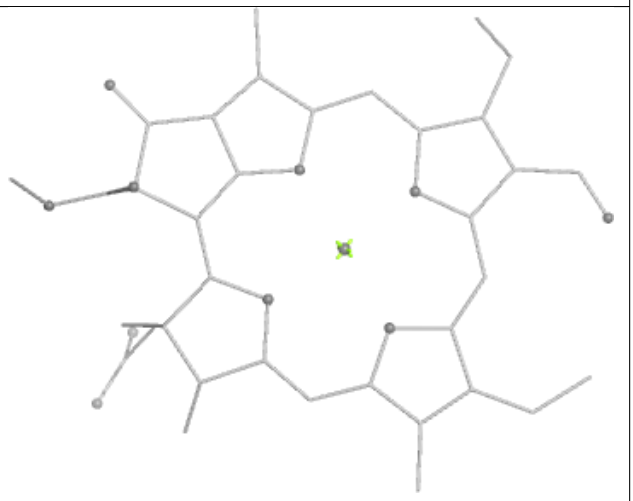
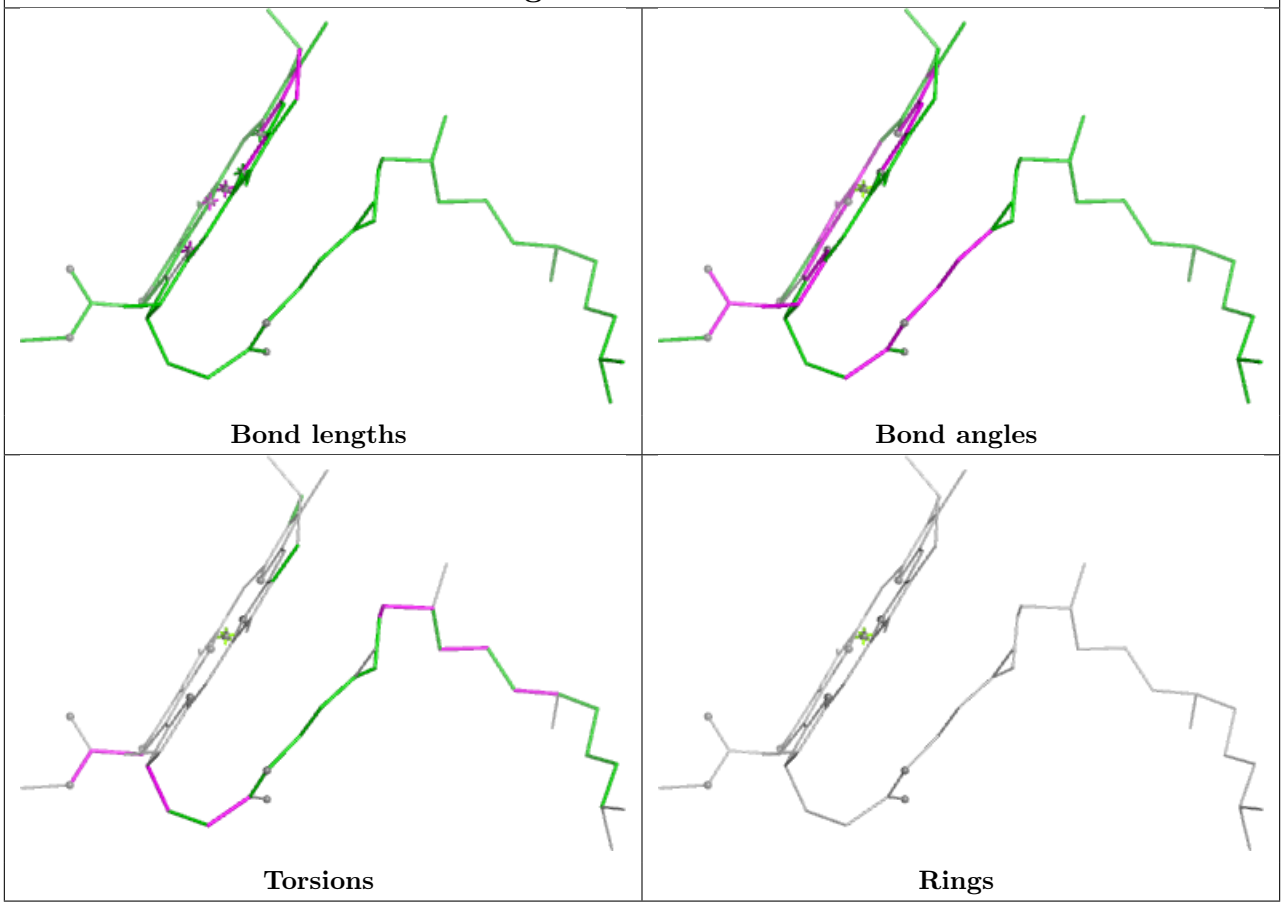
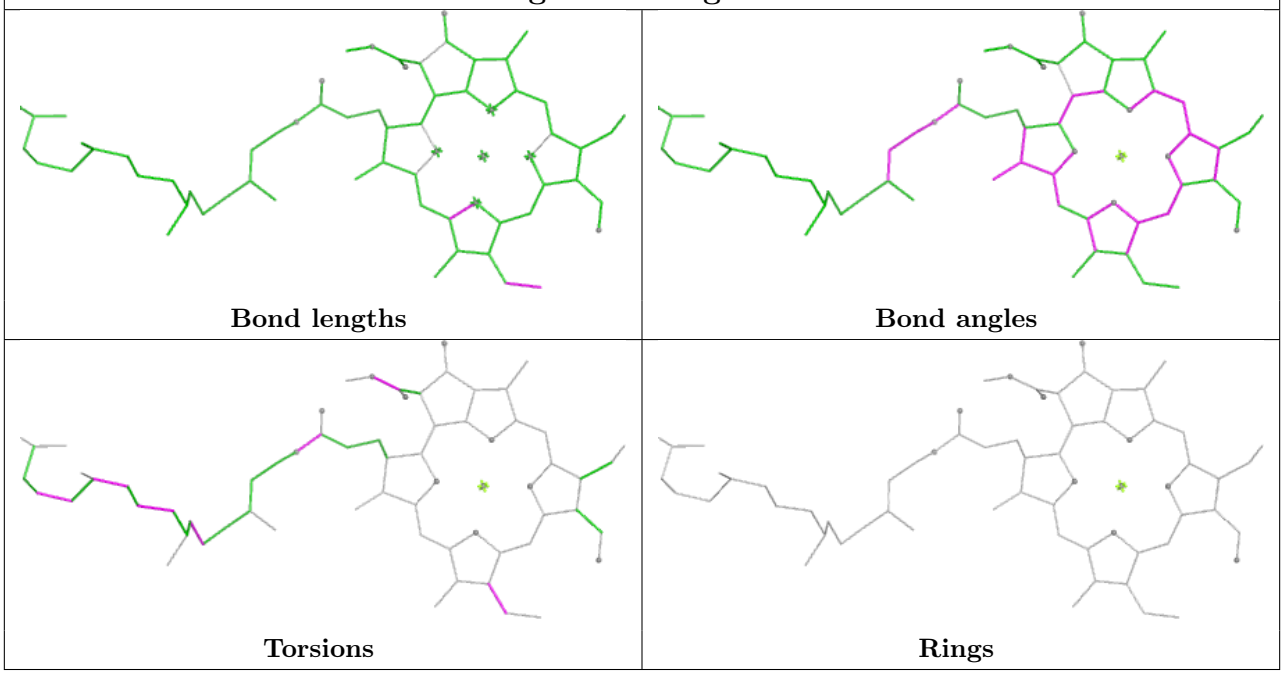


Rings

Ligand CLA R 613



Ligand CHL g 601



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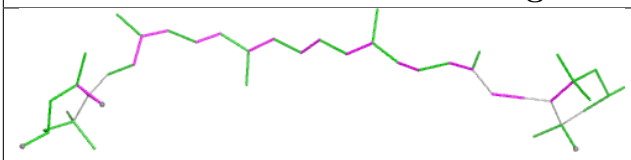

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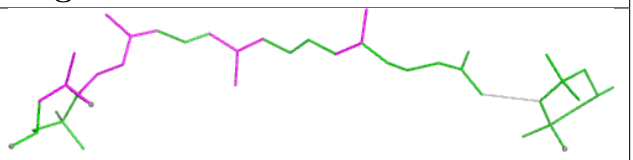
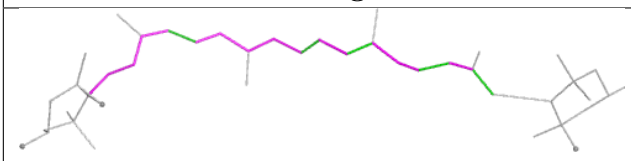


Bond angles



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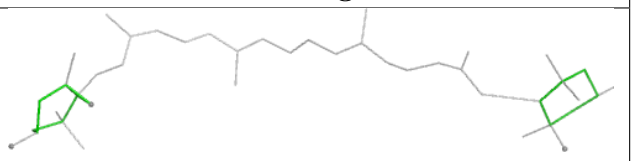
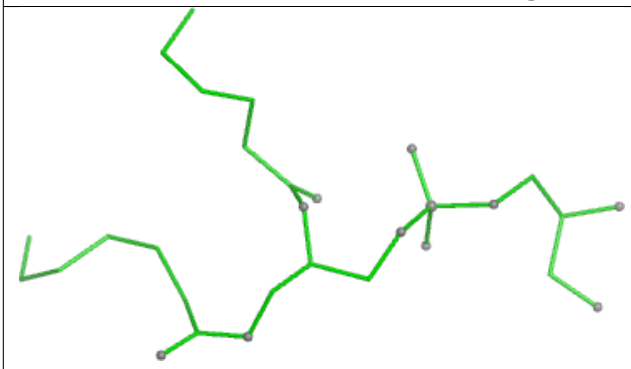


Rings

Ligand LHG B 622



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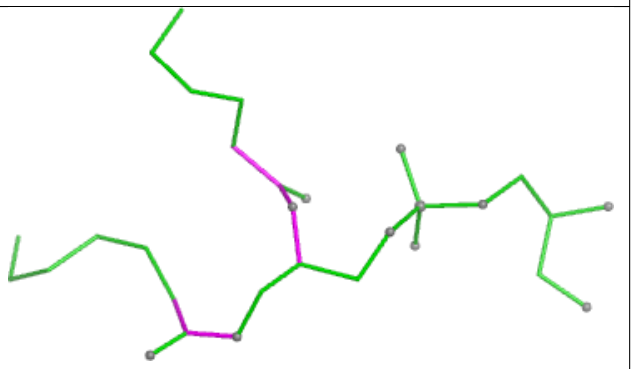
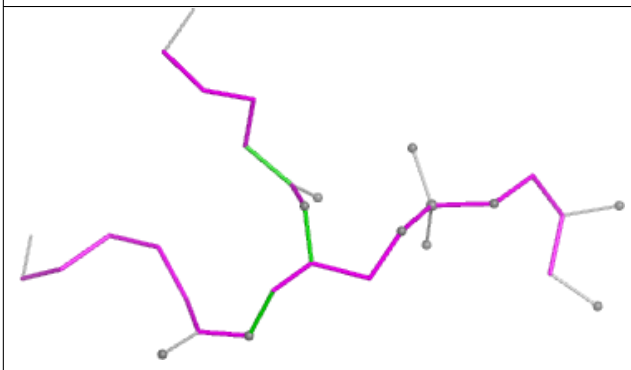


Bond angles



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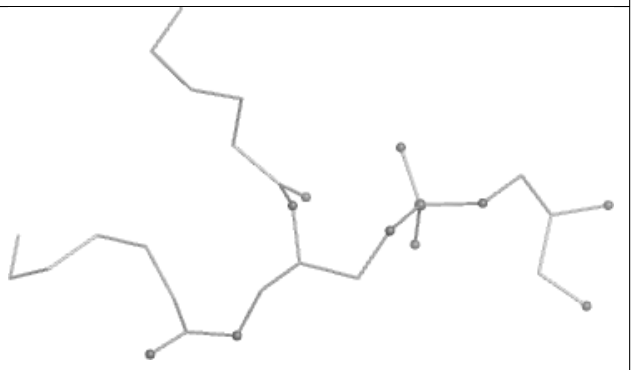
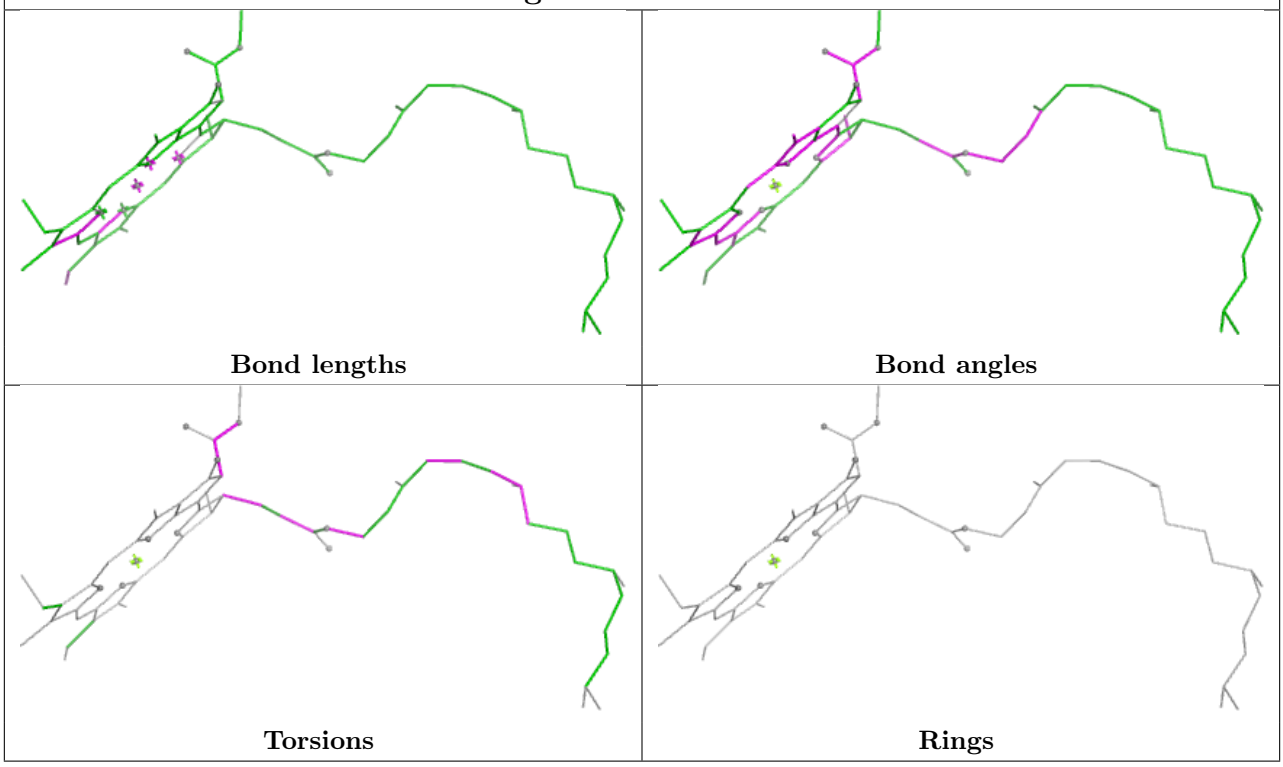
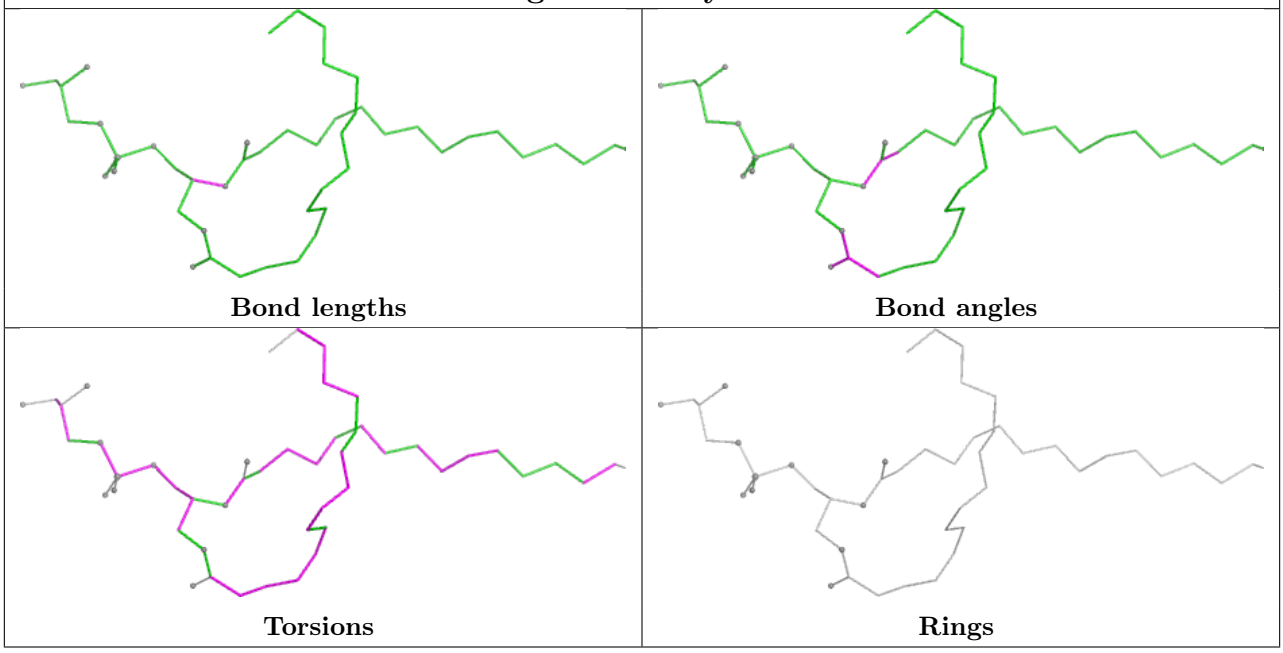


Rings

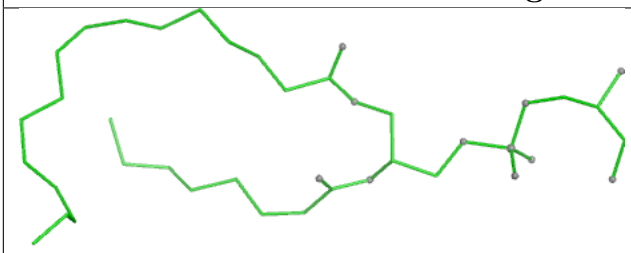
Ligand CLA D 403



Ligand LHG y 319



Ligand LHG b 622



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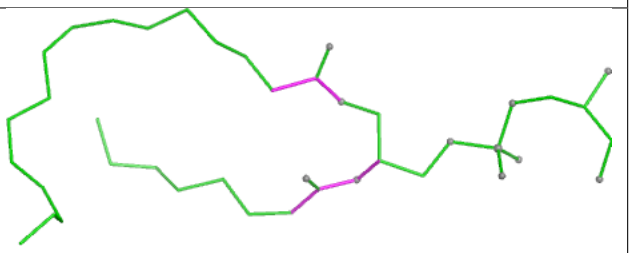
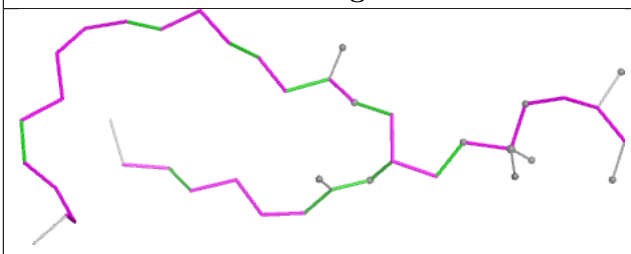


Bond angles



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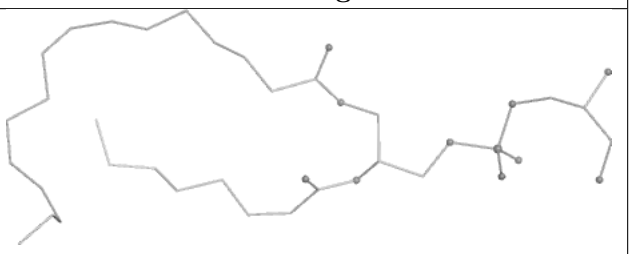
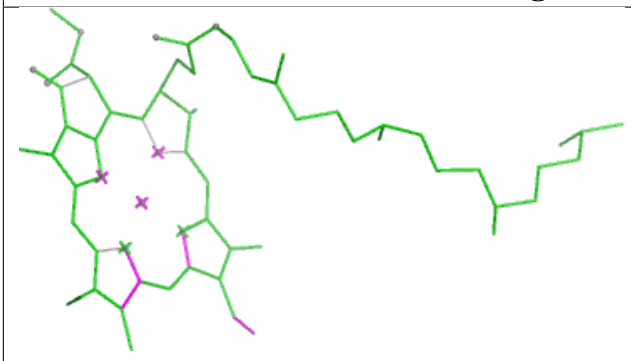


Rings

Ligand CLA c 511



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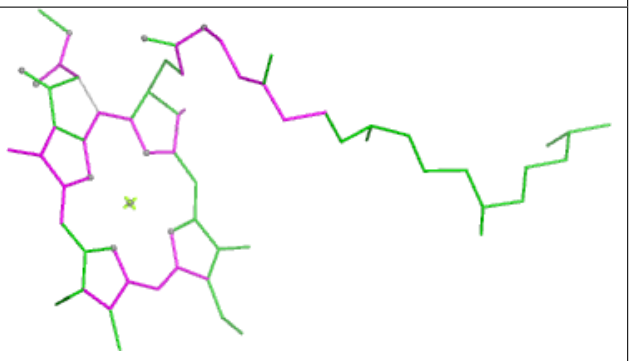
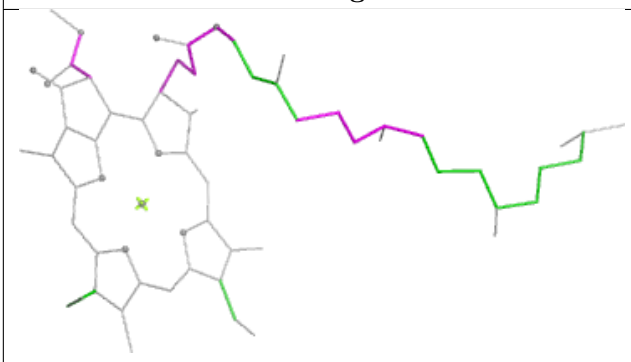


Bond angles



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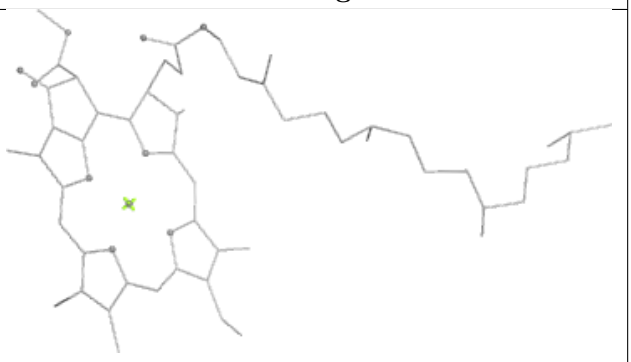
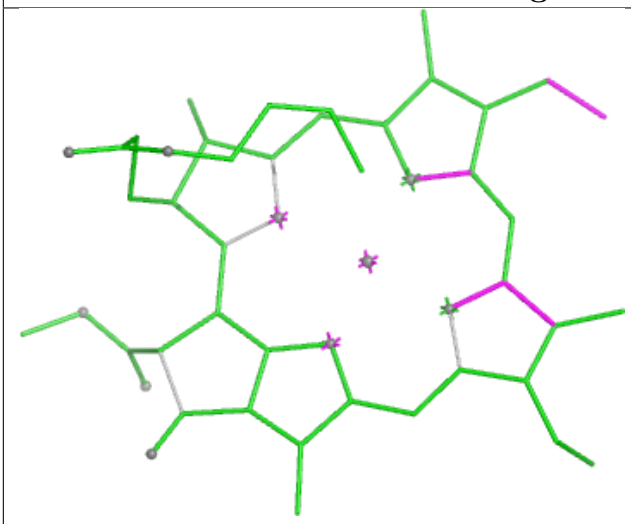
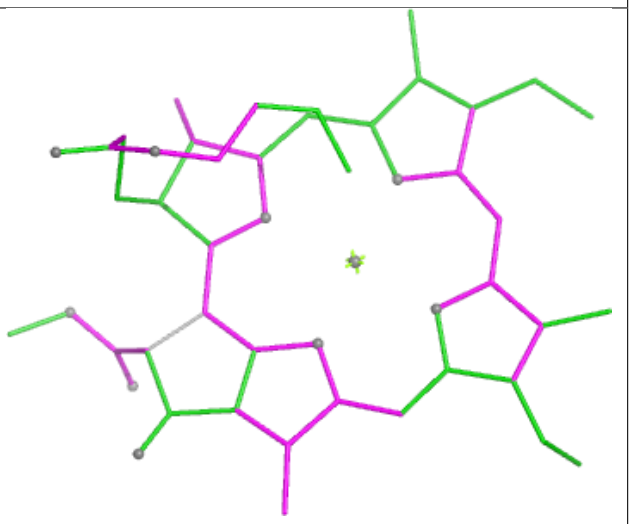


Rings

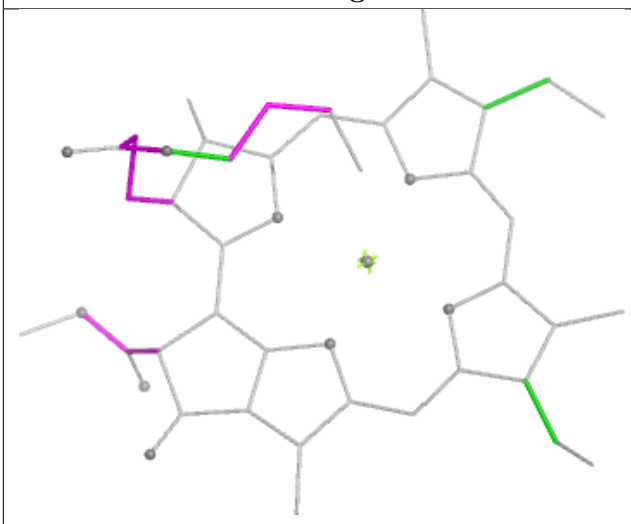
Ligand CLA r 610



Bond lengths



Bond angles



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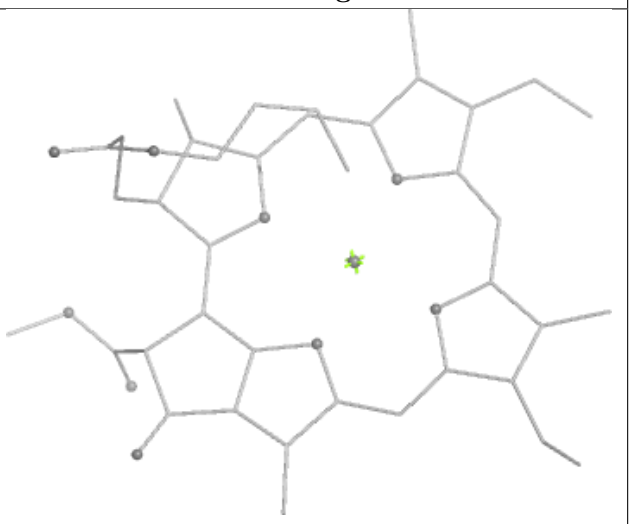
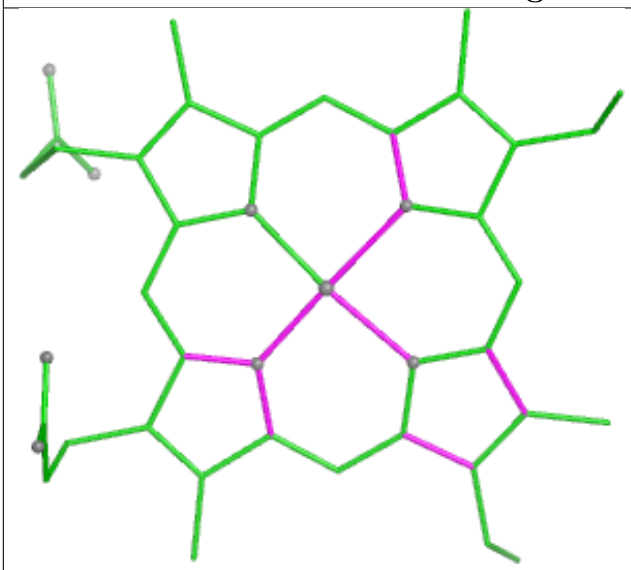


Rings

Ligand HEM f 101



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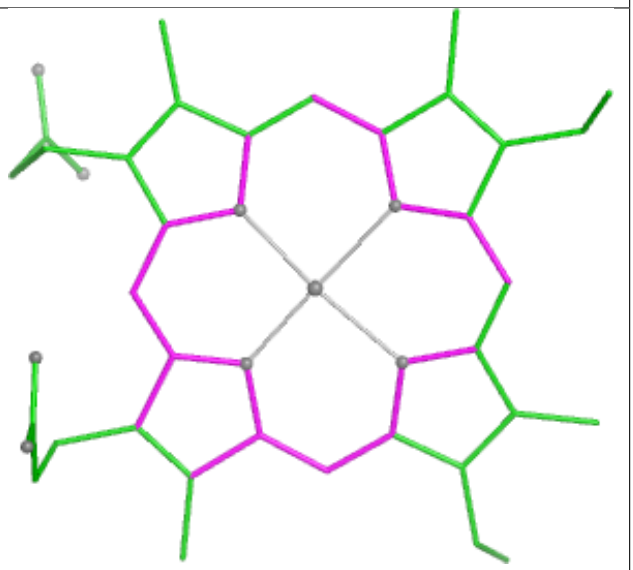
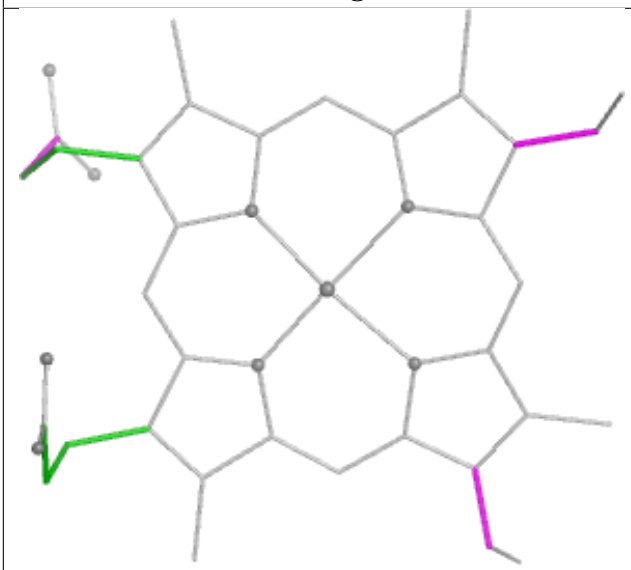


Bond angles



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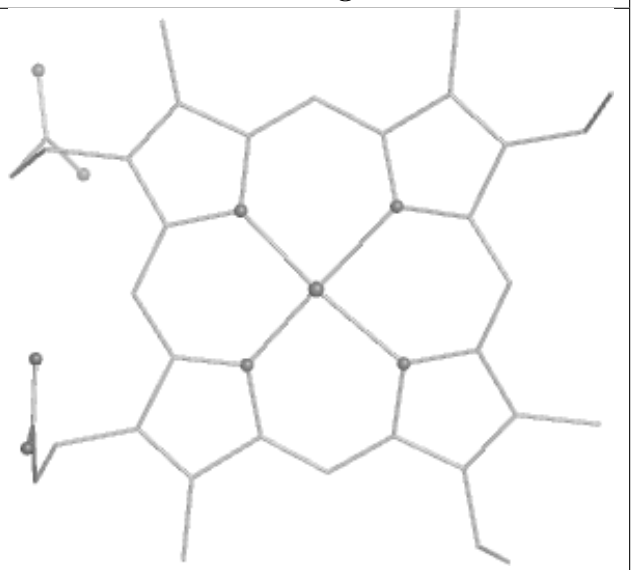
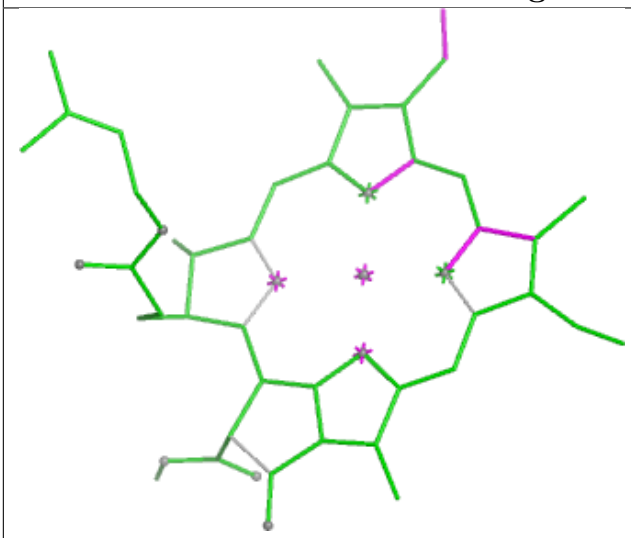
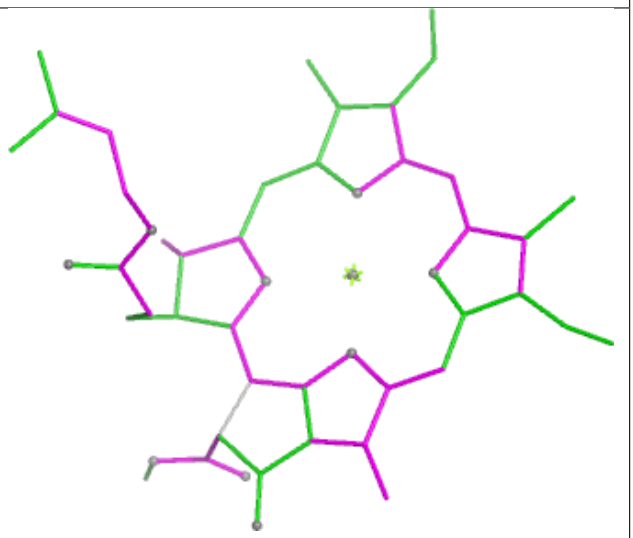


Rings

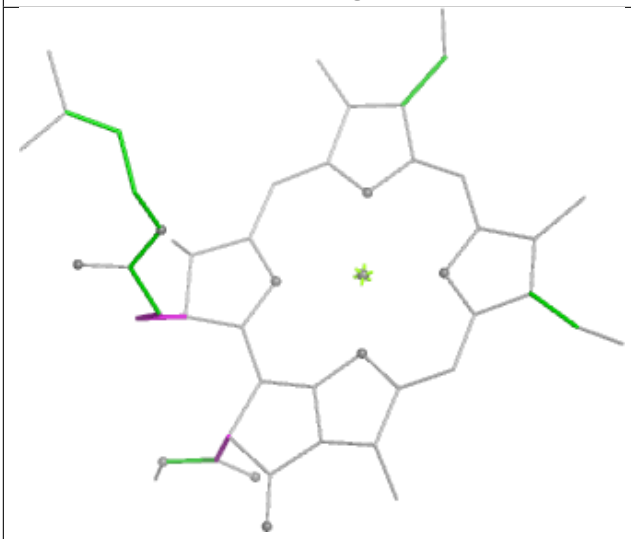
Ligand CLA a 407



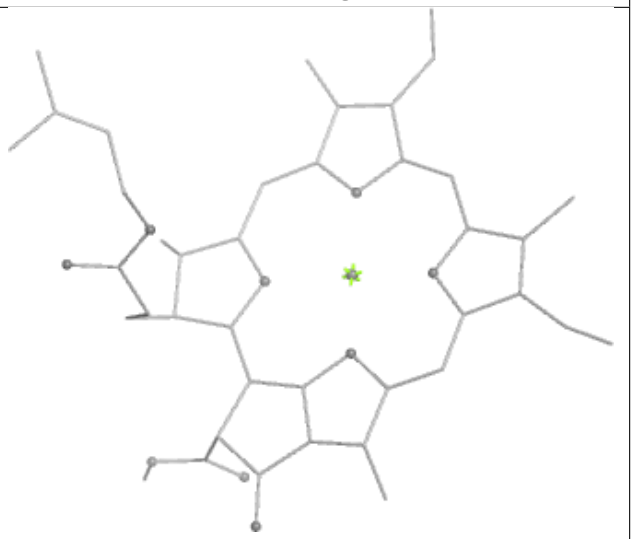
Bond lengths



Bond angles

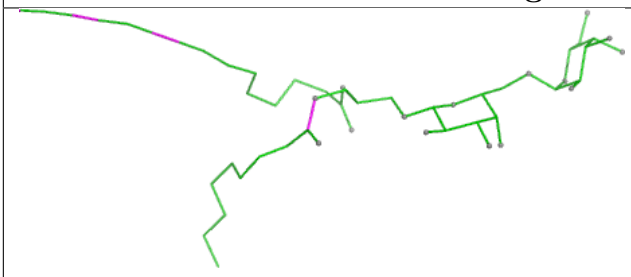


Torsions



Rings

Ligand DGD c 516



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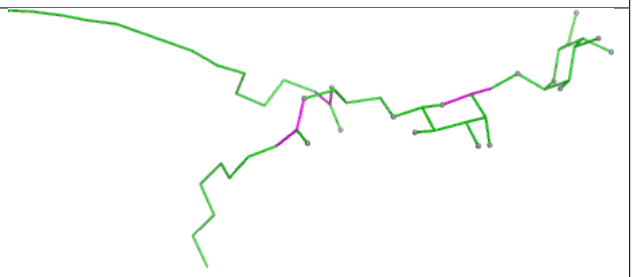
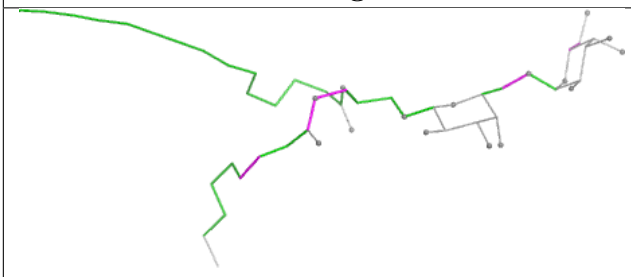


Bond angles



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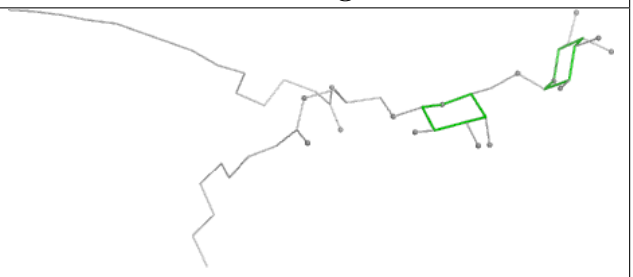
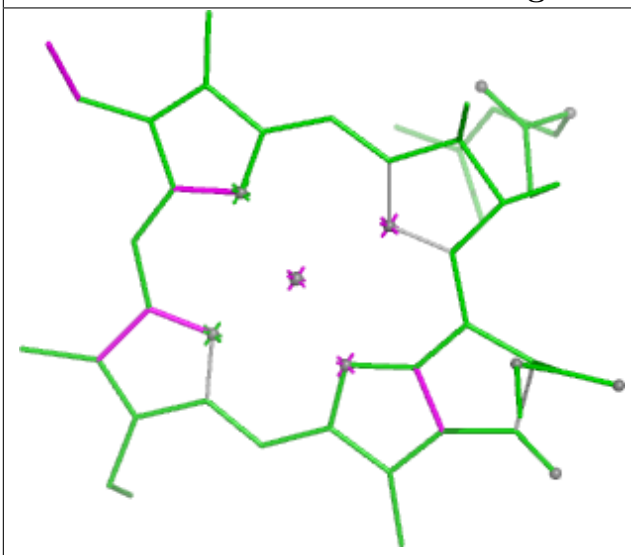


Rings

Ligand CLA y 305



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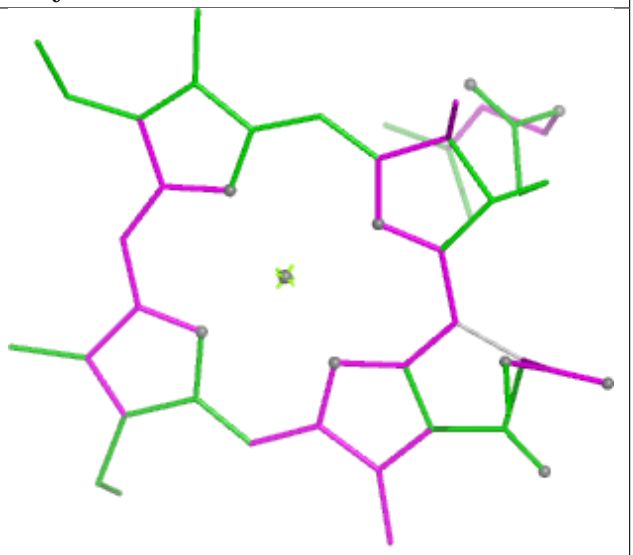
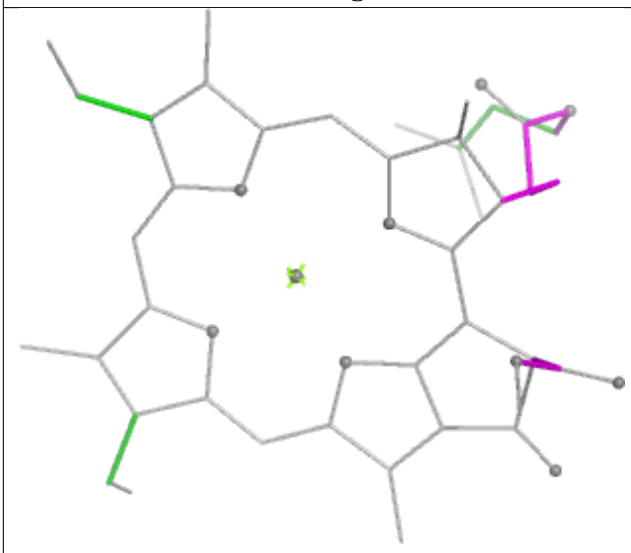


Bond angles



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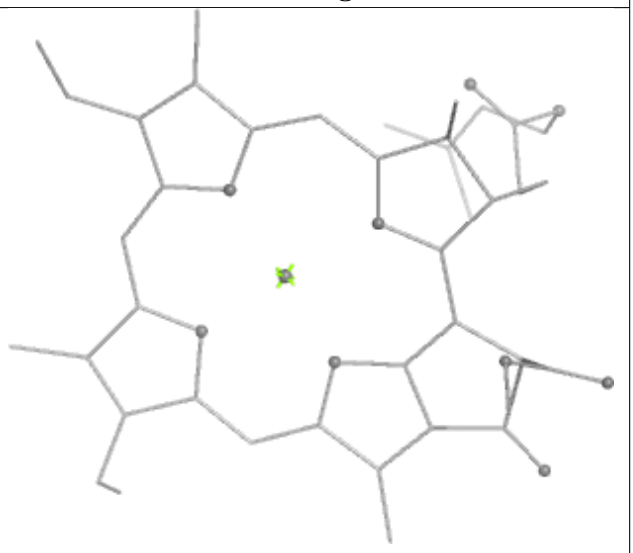
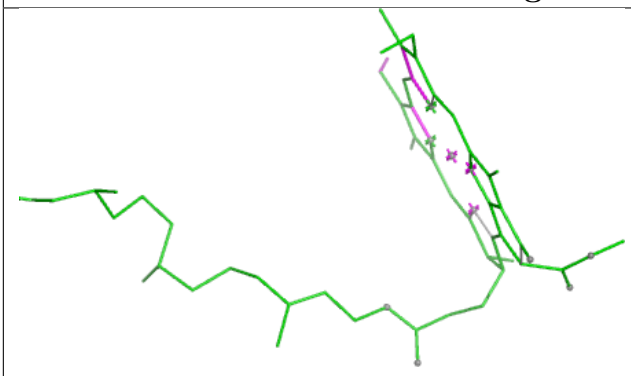


Rings

Ligand CLA B 607



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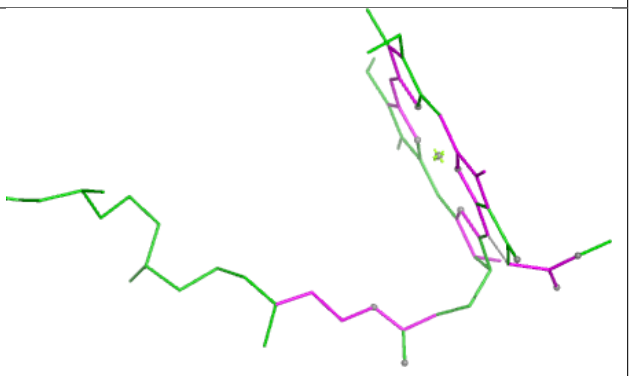

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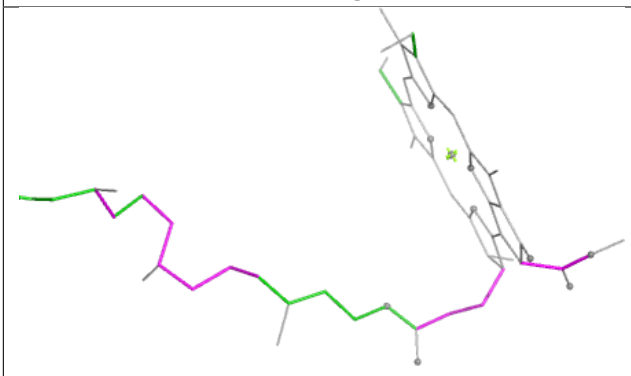
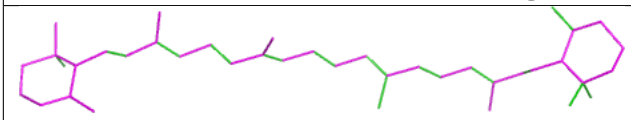


Torsions



Rings

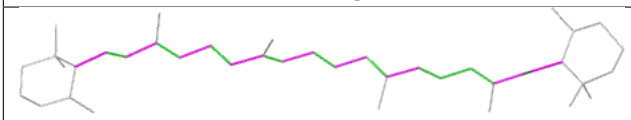
Ligand BCR B 619



Bond lengths



Bond angles



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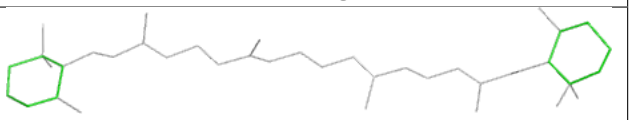
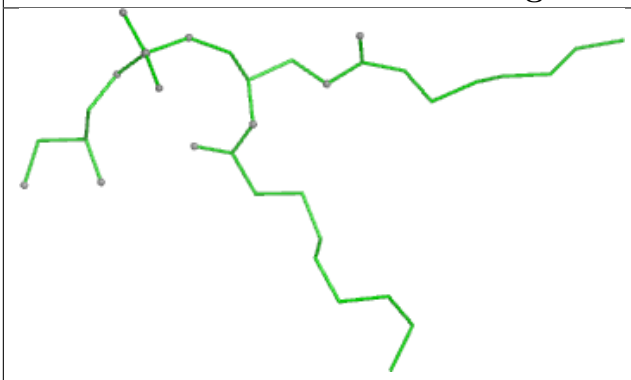


Rings

Ligand LHG S 301



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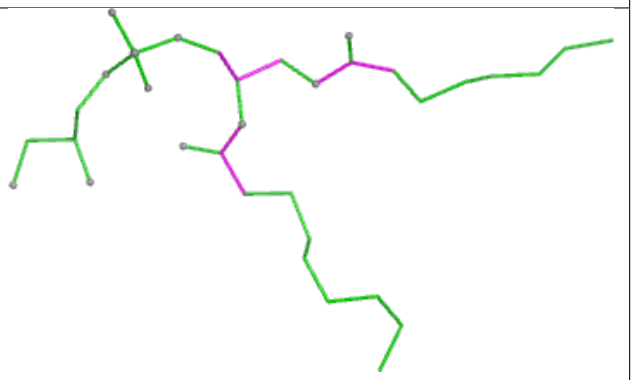
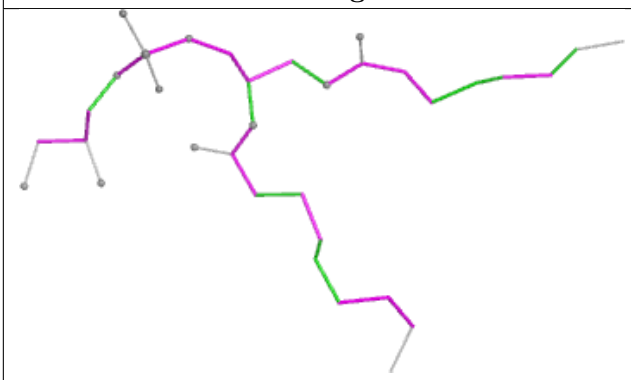


Bond angles

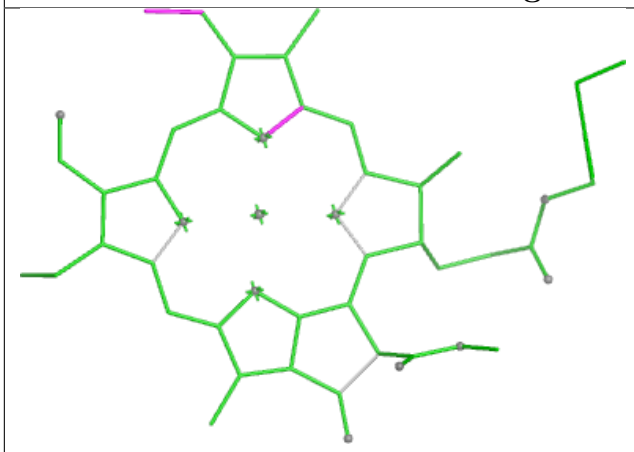


Torsions



Rings

Ligand CHL N 601



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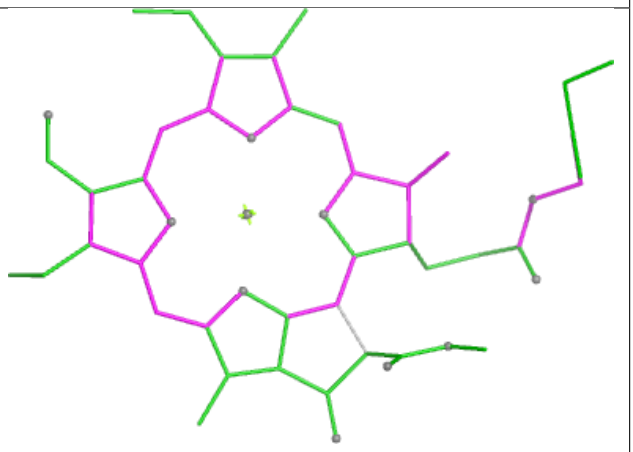
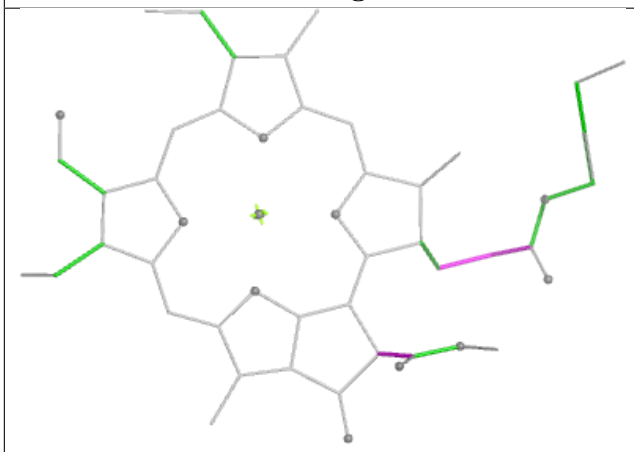


Bond angles



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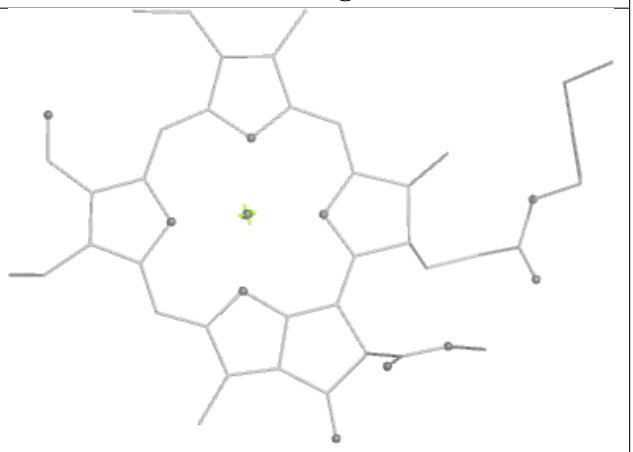
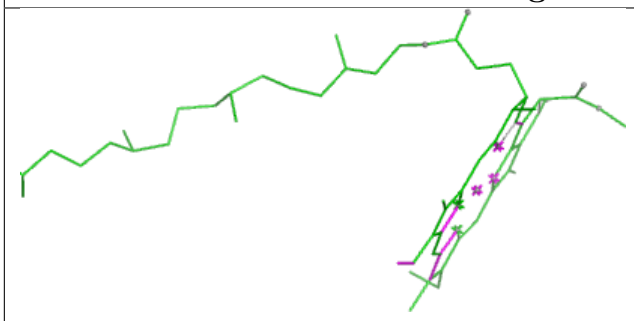


Rings

Ligand CLA b 607



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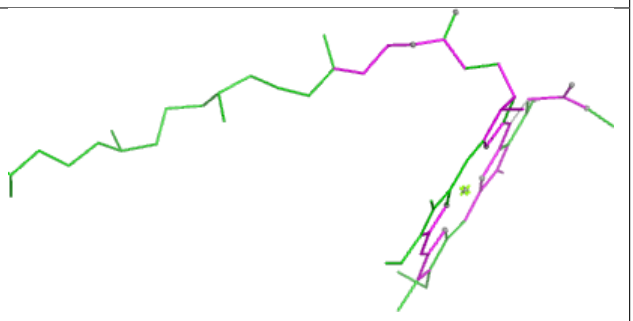
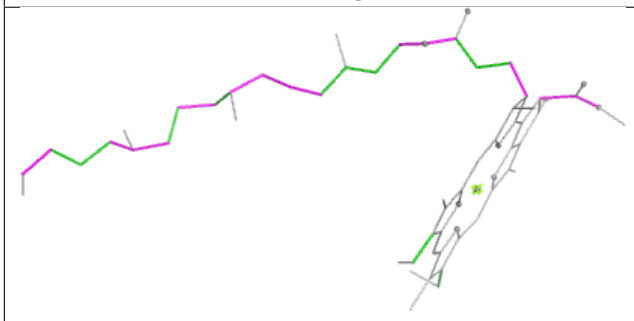


Bond angles

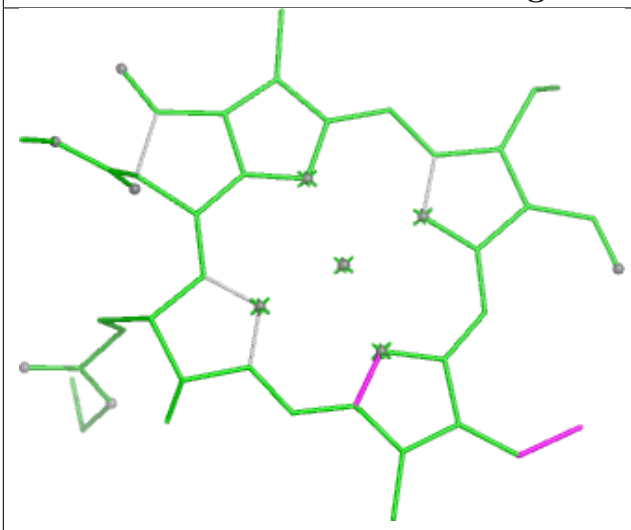


Torsions



Rings

Ligand CHL y 306



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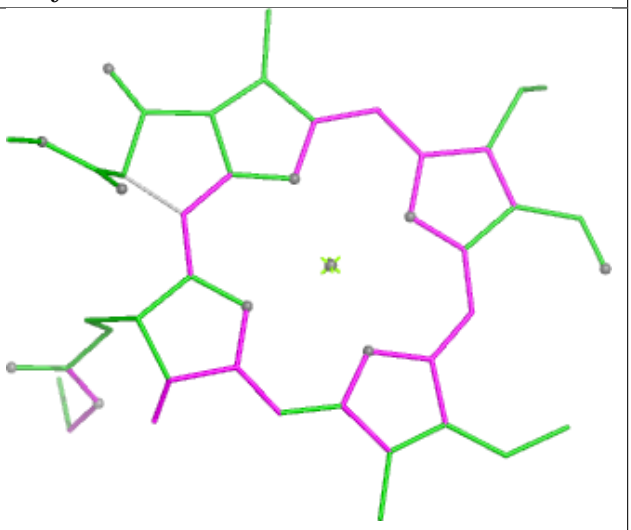
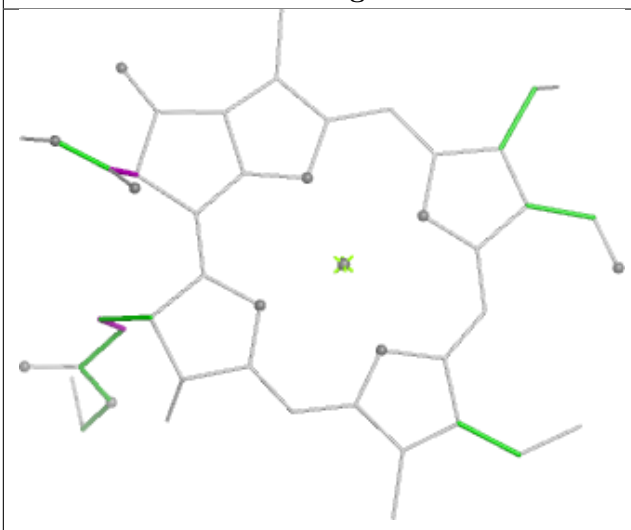


Bond angles



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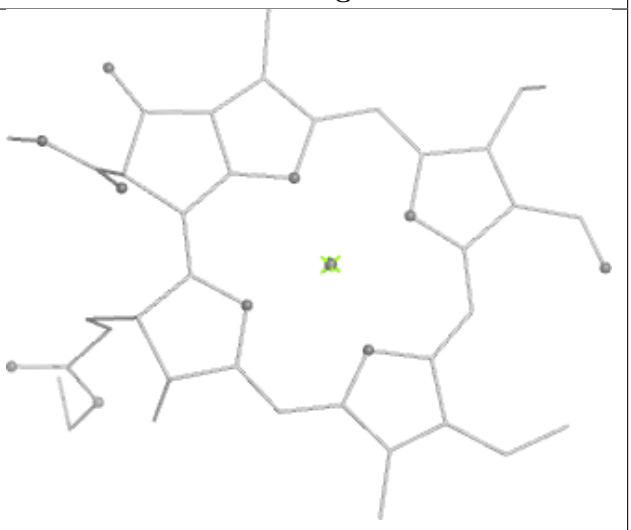
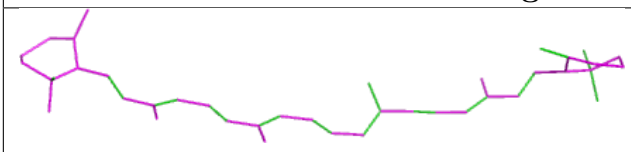


Rings

Ligand BCR D 405



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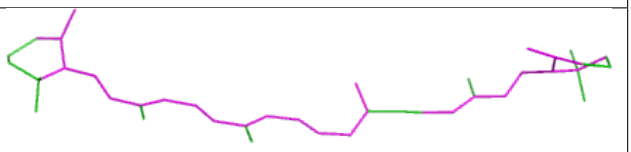
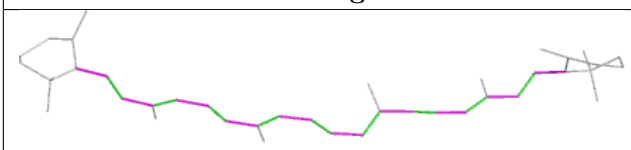


Bond angles



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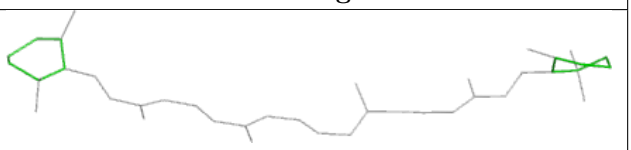
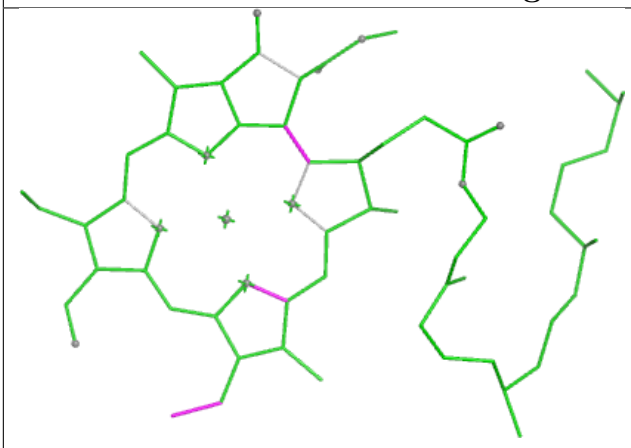


Rings

Ligand CHL Y 607



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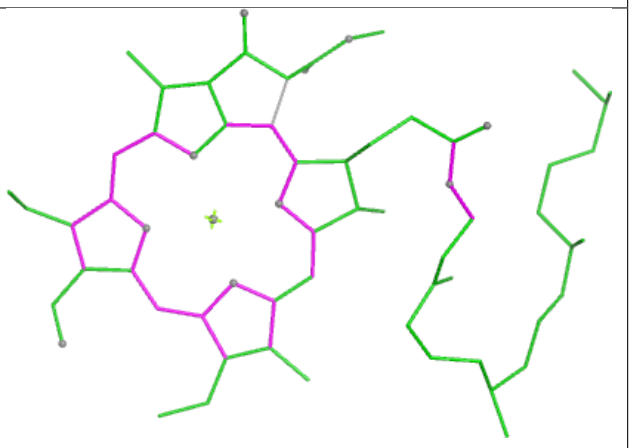
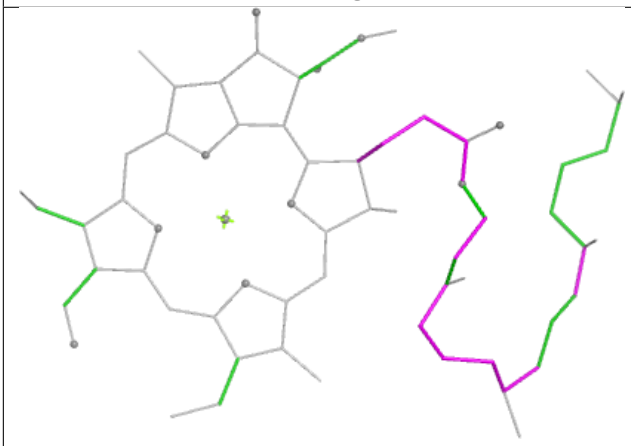


Bond angles



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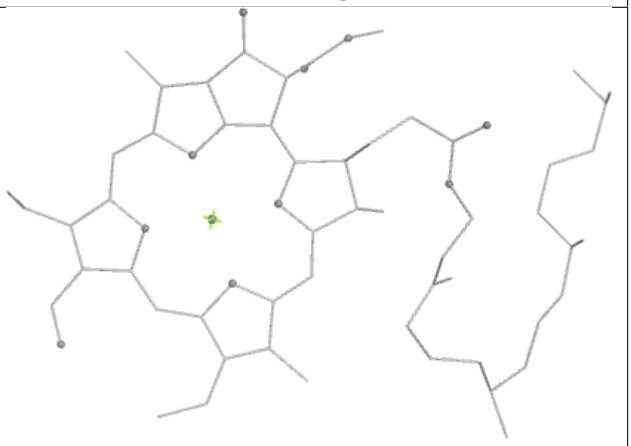
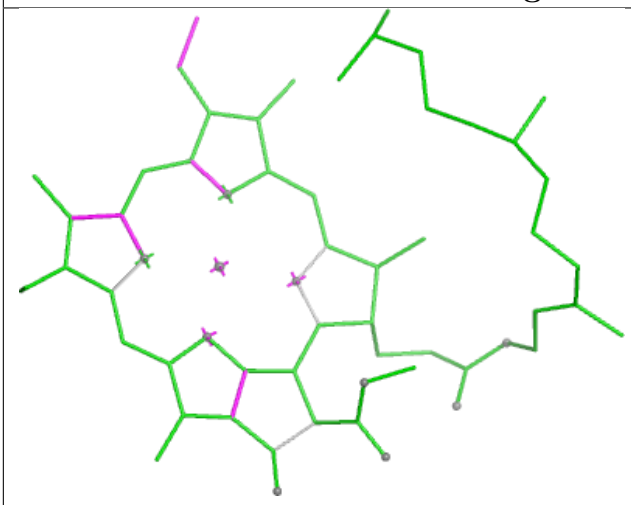


Rings

Ligand CLA Y 612



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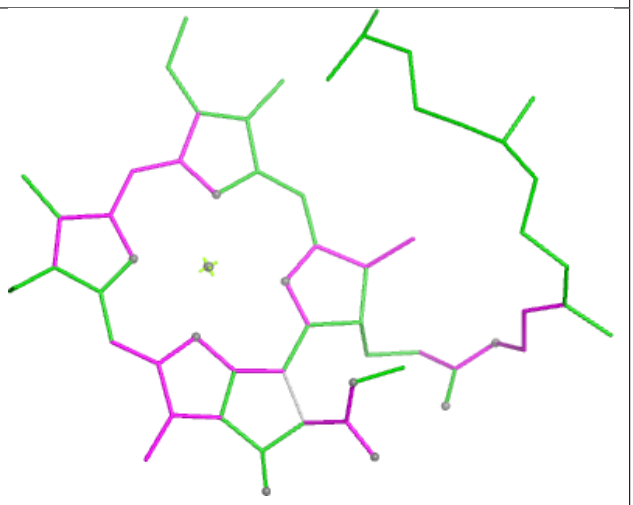
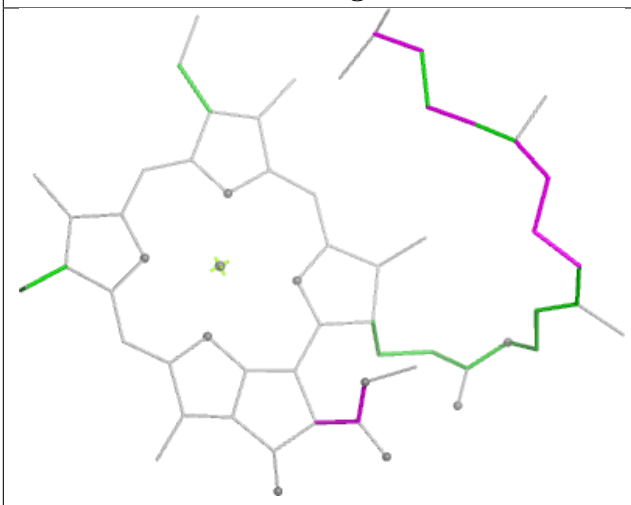


Bond angles



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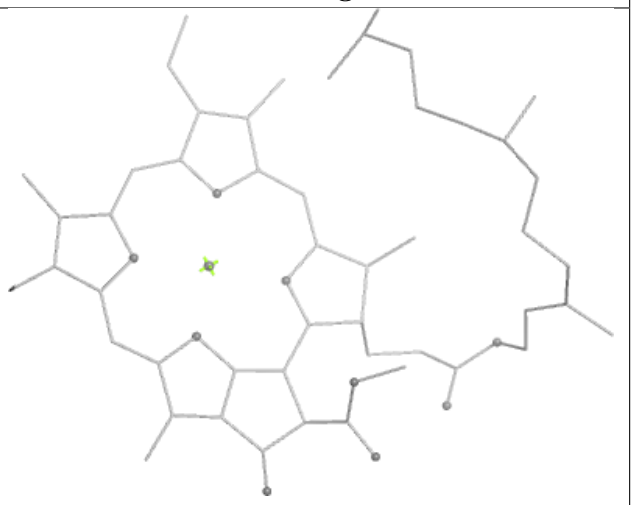
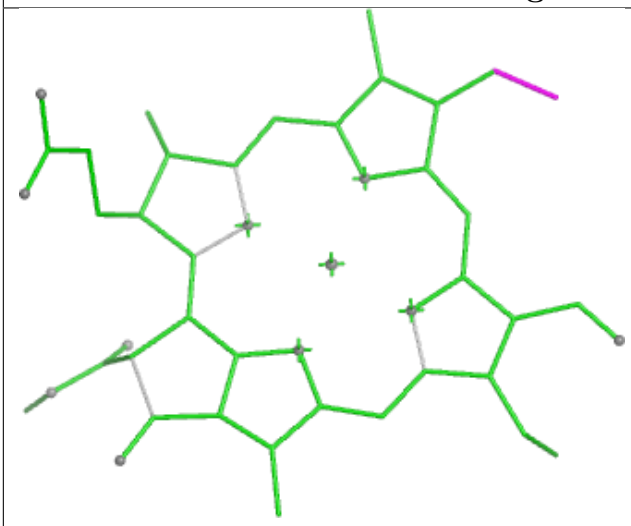


Rings

Ligand CHL S 306



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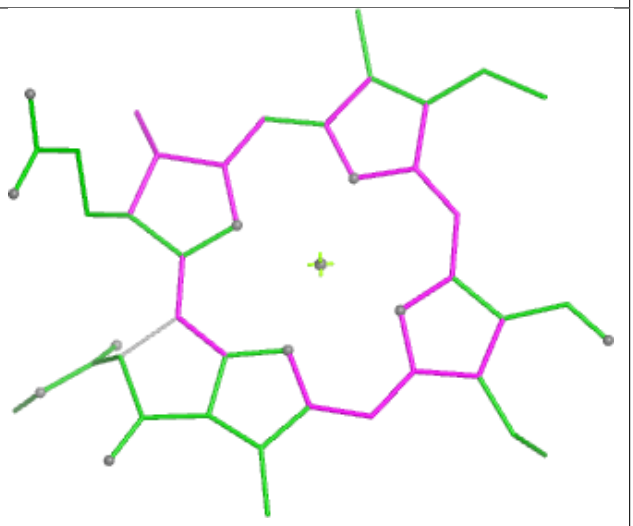
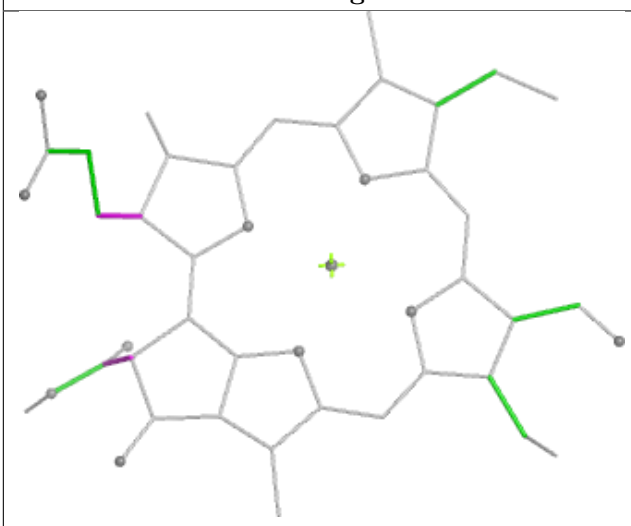


Bond angles



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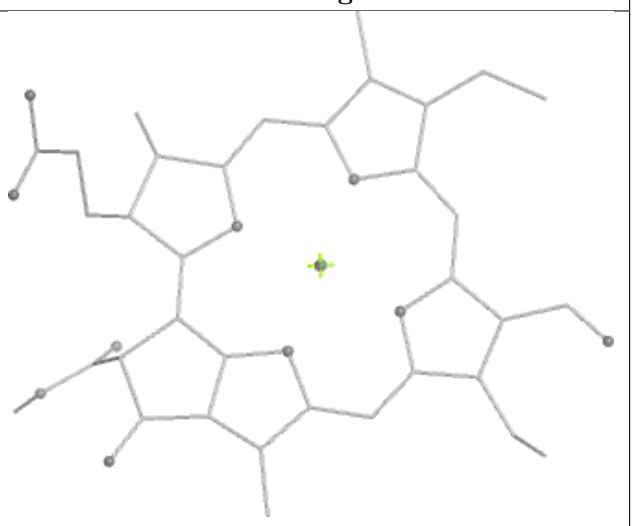
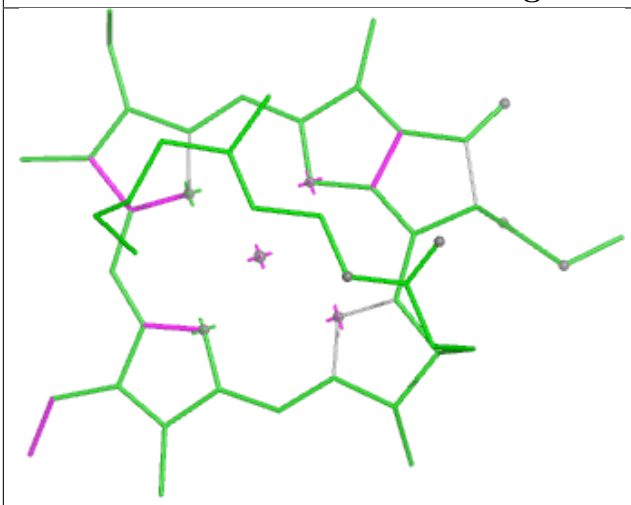


Rings

Ligand CLA N 613



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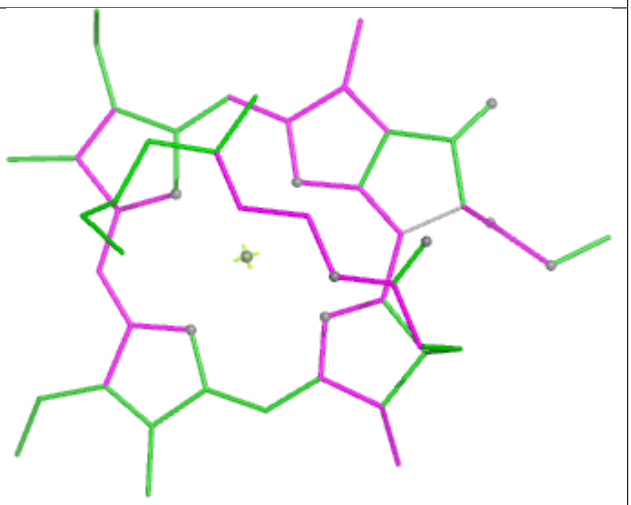
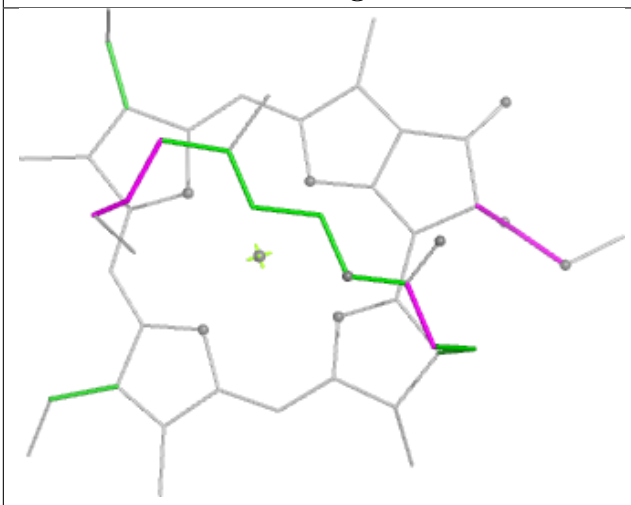


Bond angles



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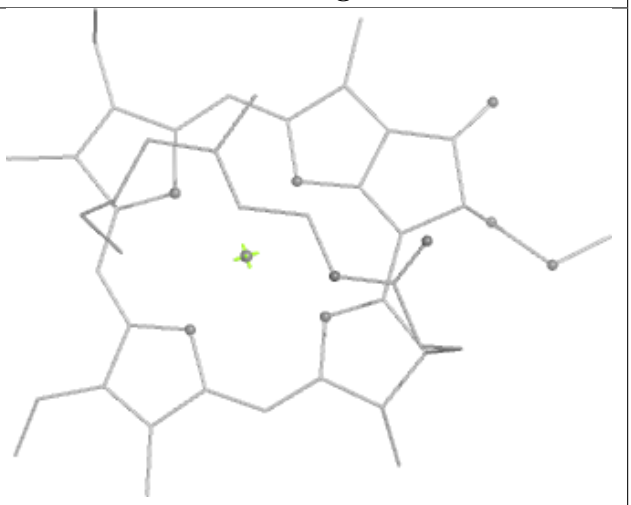
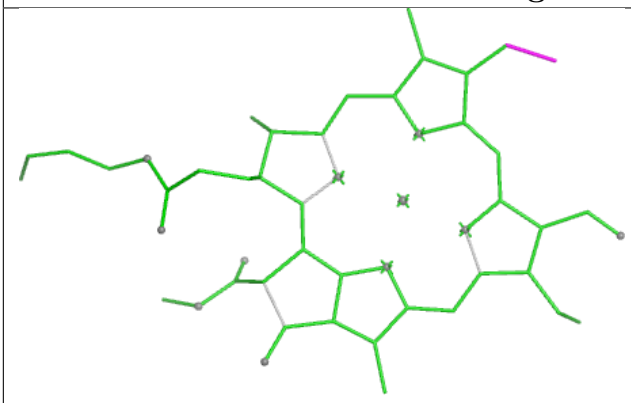


Rings

Ligand CHL g 606



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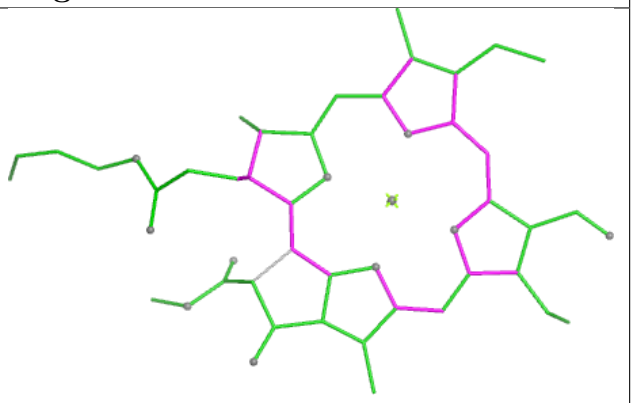
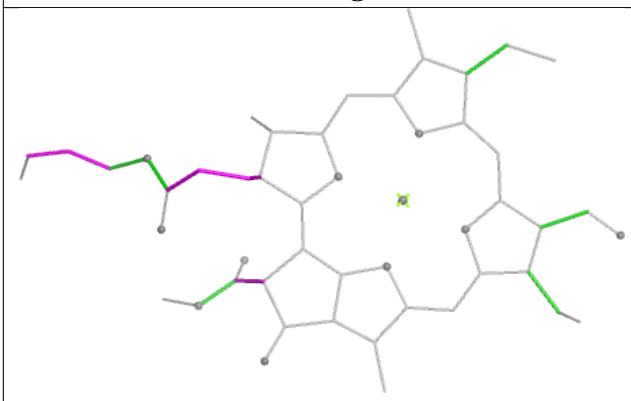


Bond angles



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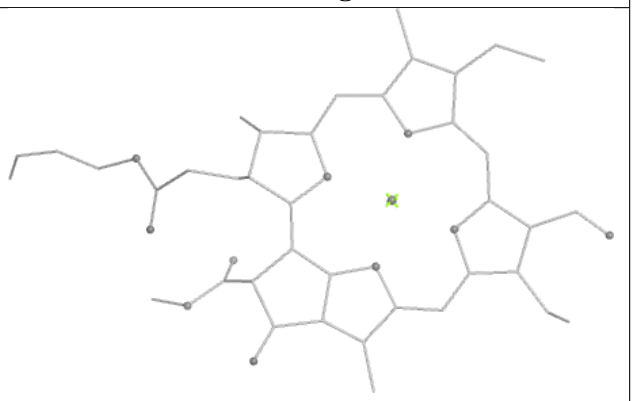
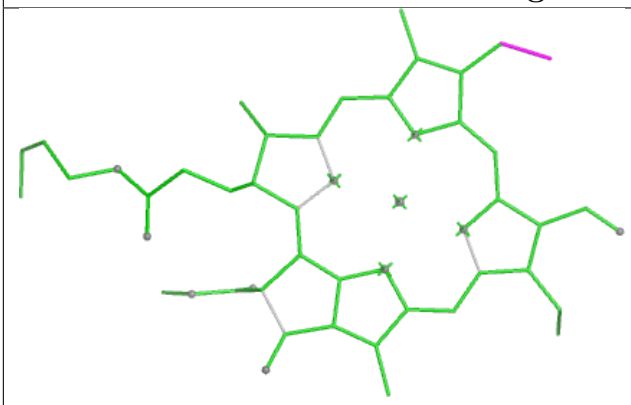
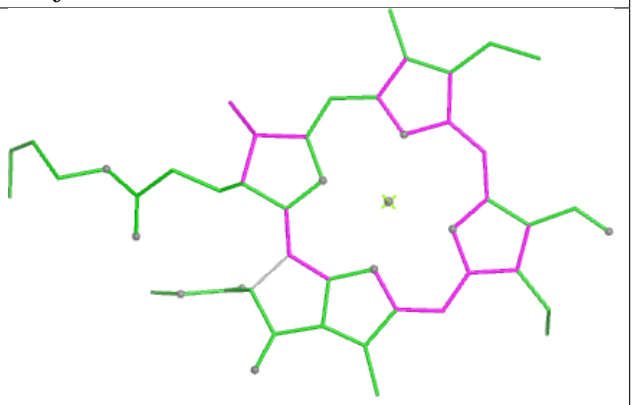


Rings

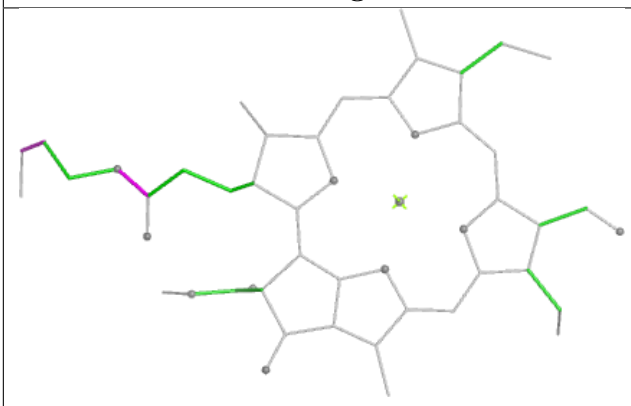
Ligand CHL y 307



Bond lengths



Bond angles



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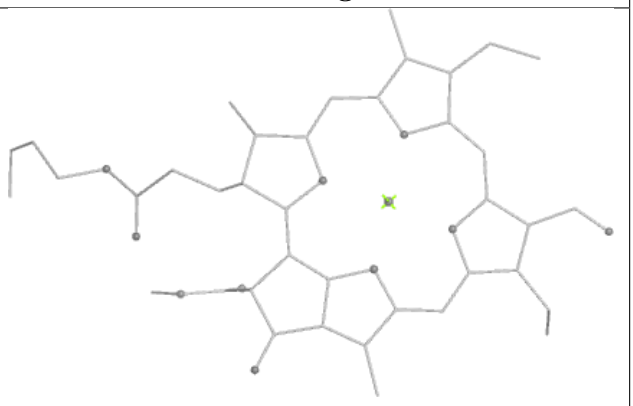
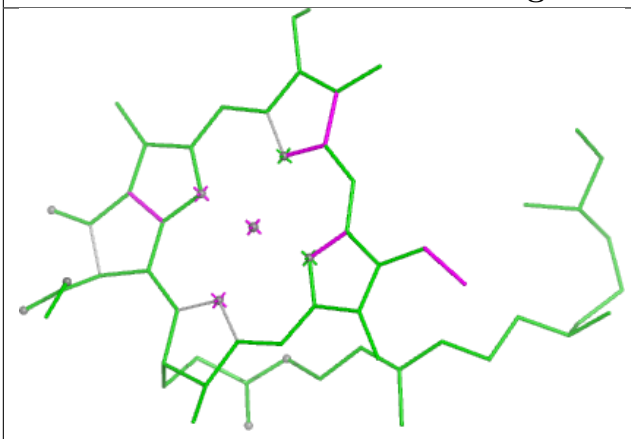
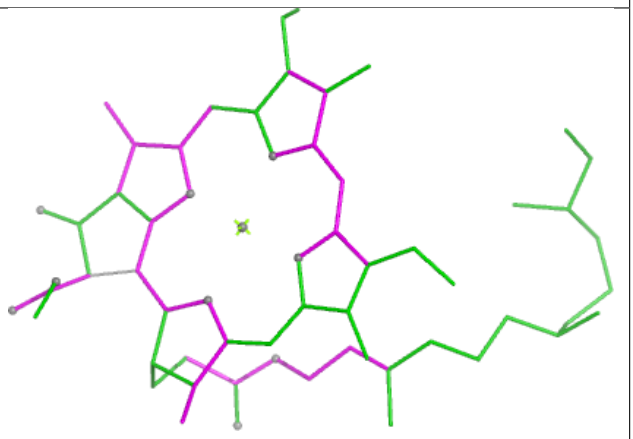


Rings

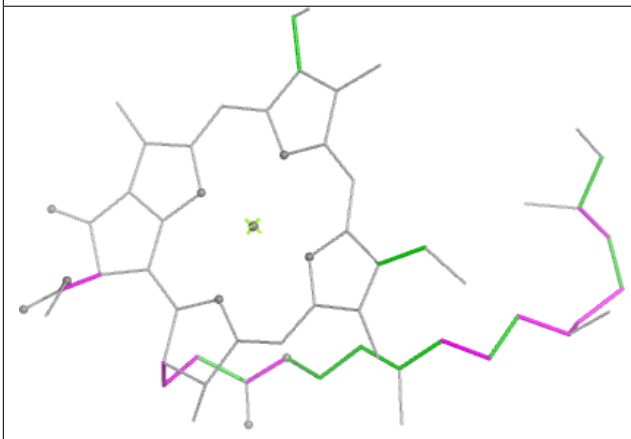
Ligand CLA S 303



Bond lengths



Bond angles

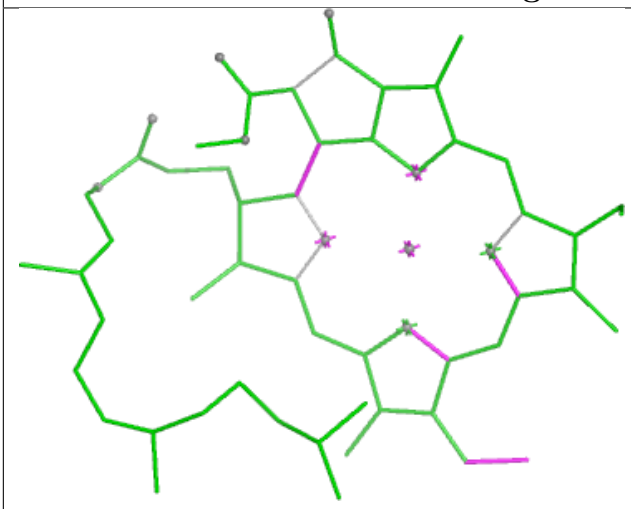


Torsions



Rings

Ligand CLA G 612



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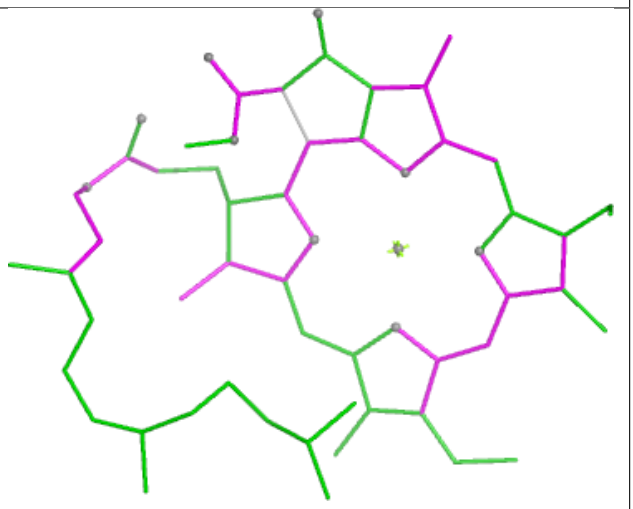
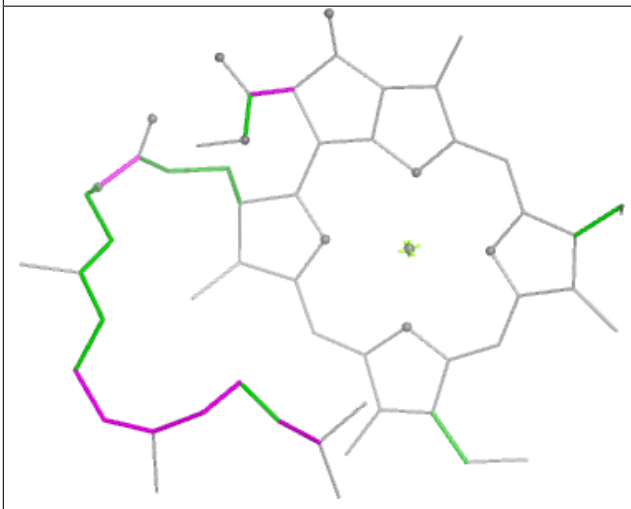
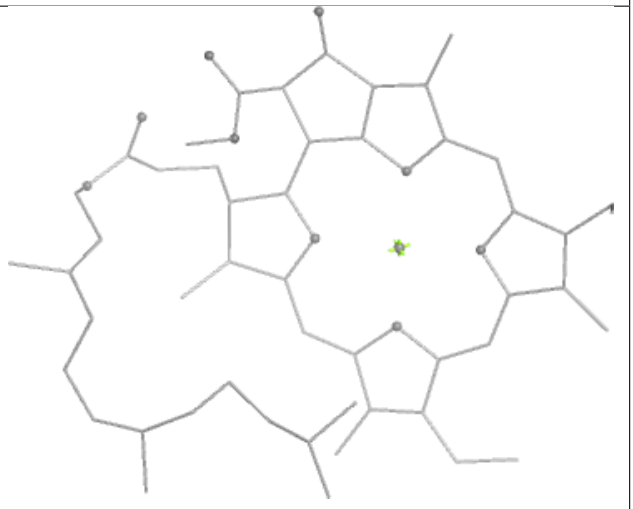


Bond angles

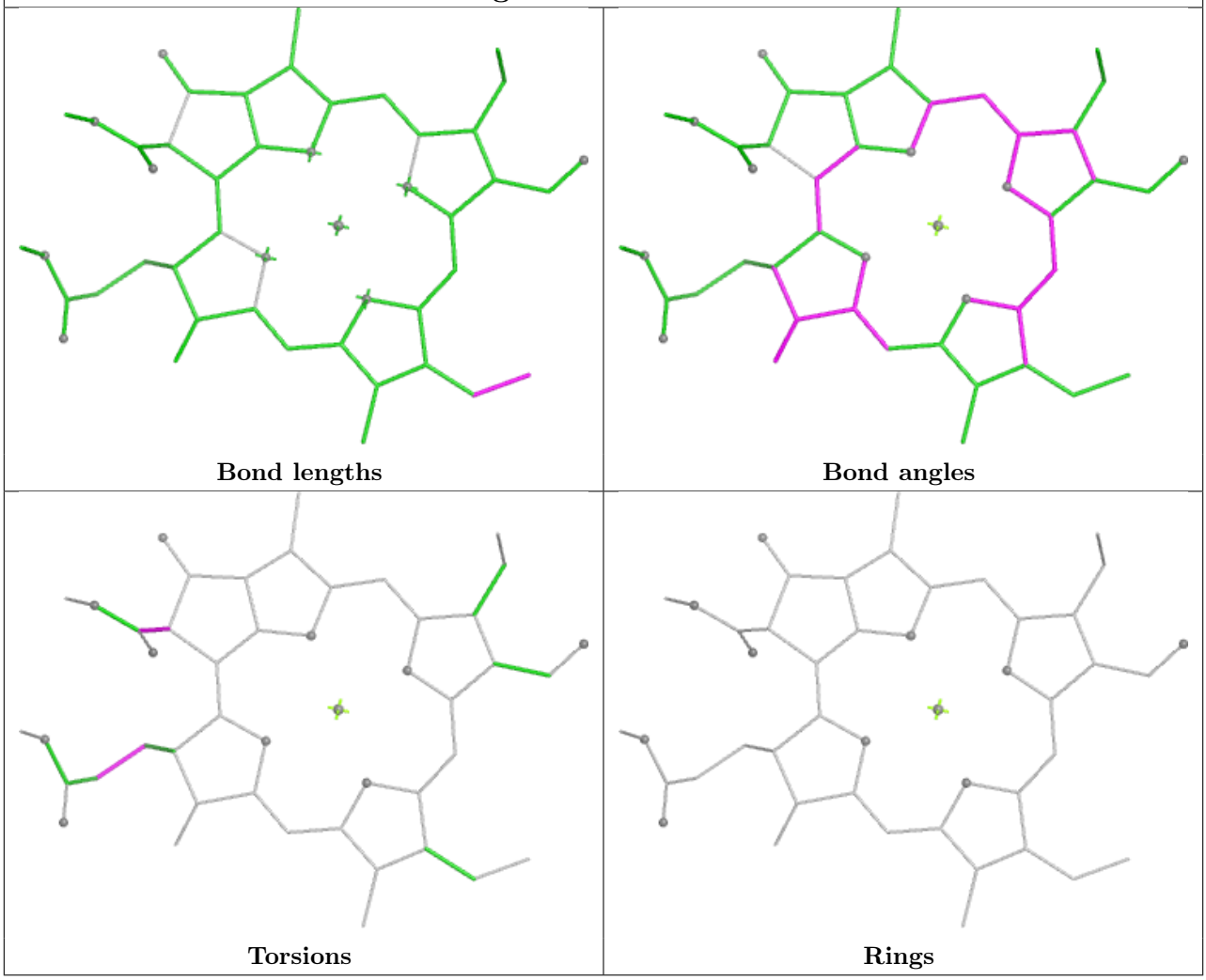


Torsions

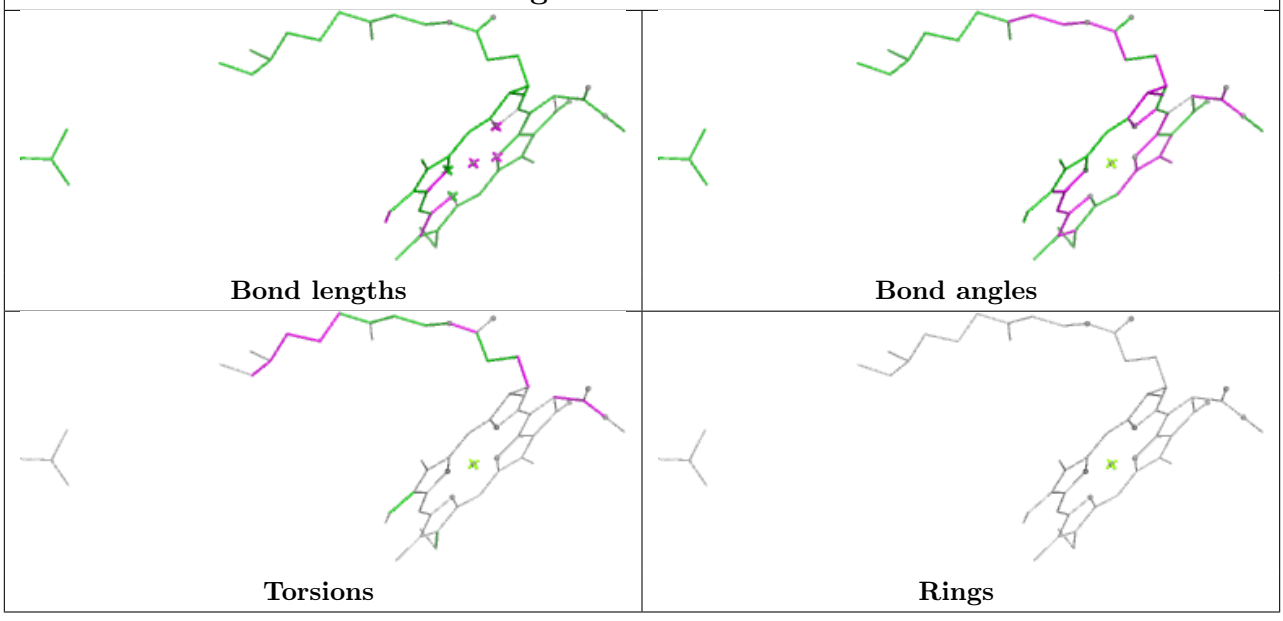


Rings

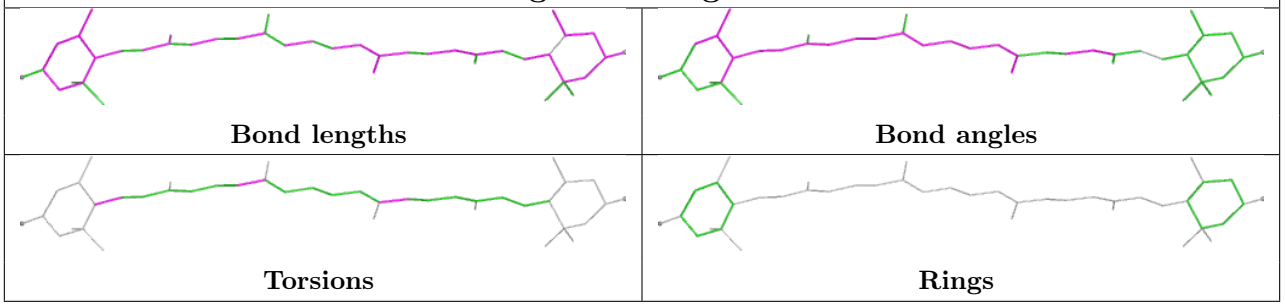
Ligand CHL R 605



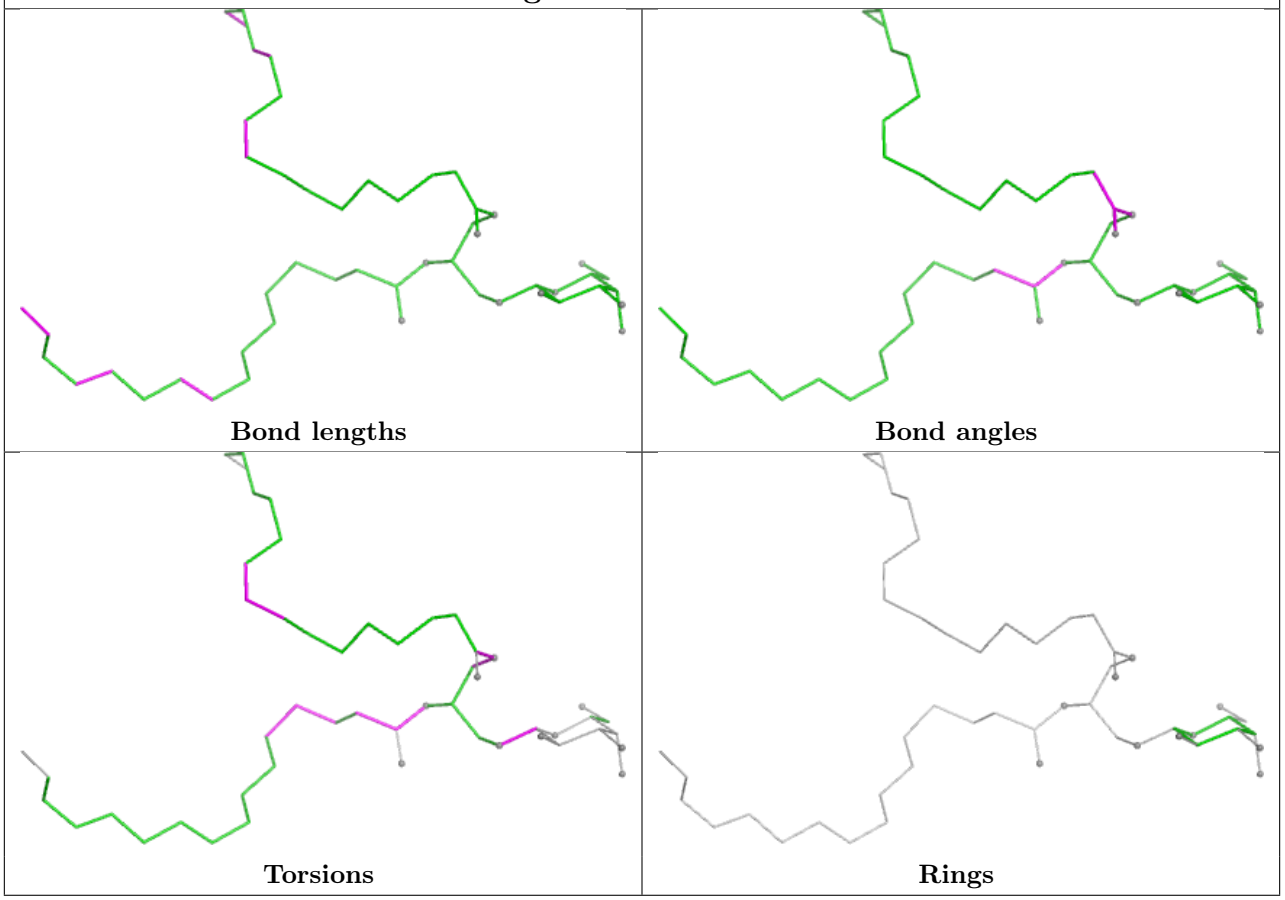
Ligand CLA c 504



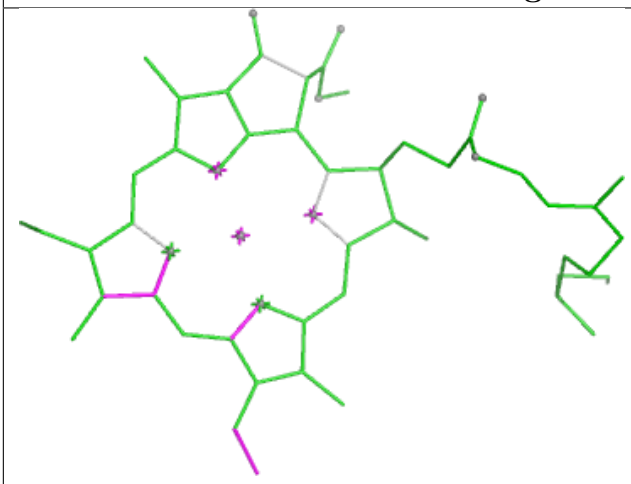
Ligand LUT g 615



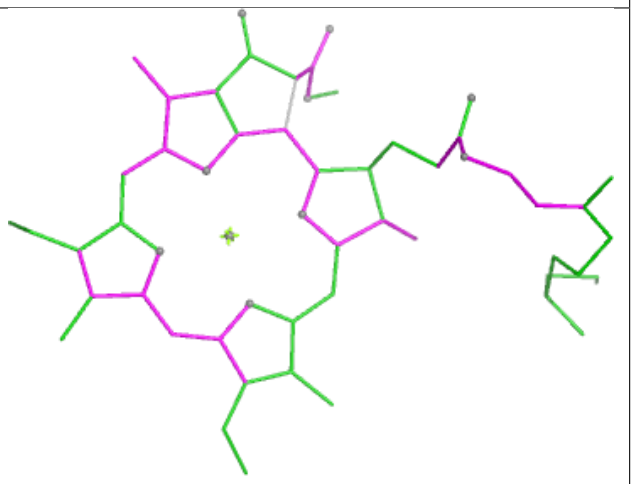
Ligand LMG b 620



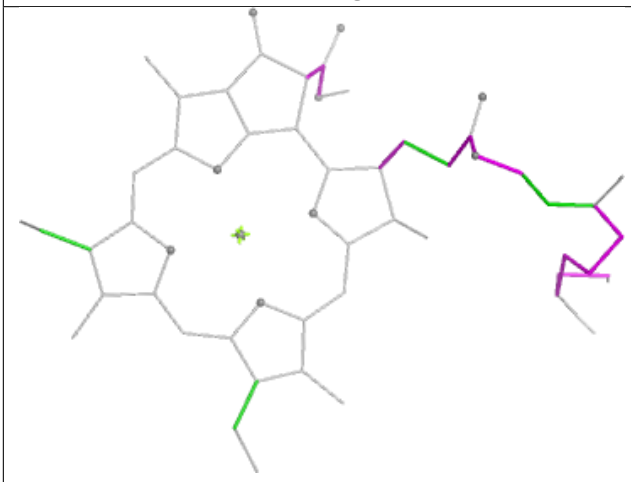
Ligand CLA C 512



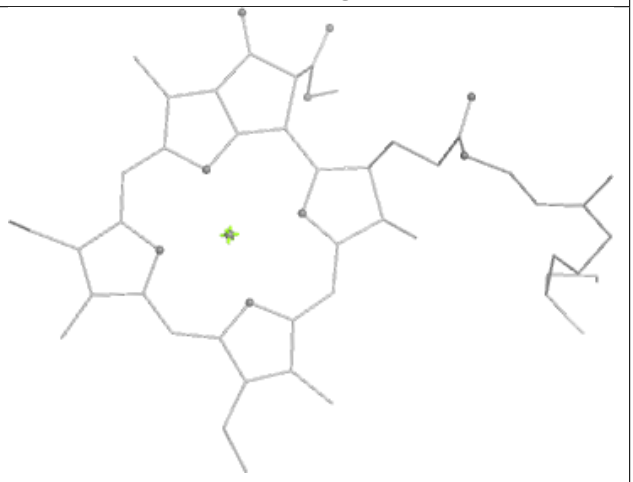
Bond lengths



Bond angles

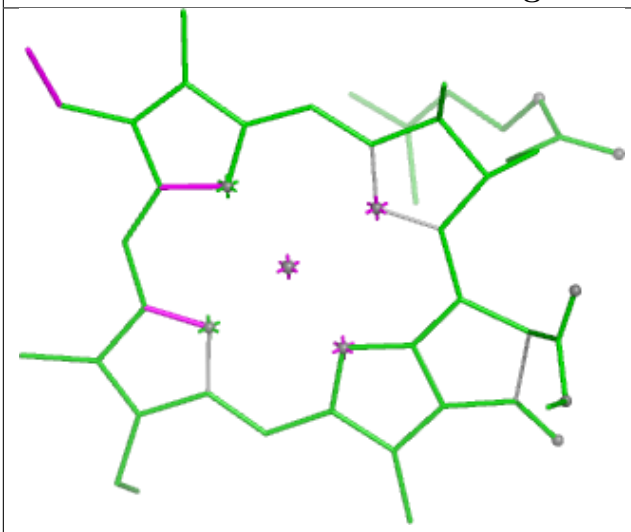


Torsions



Rings

Ligand CLA N 604



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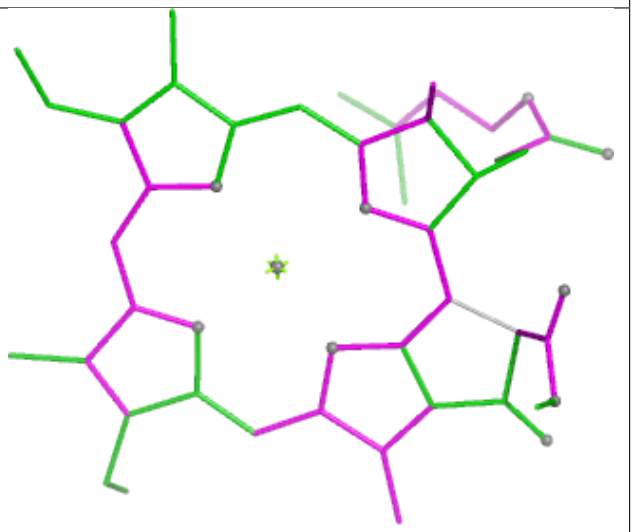
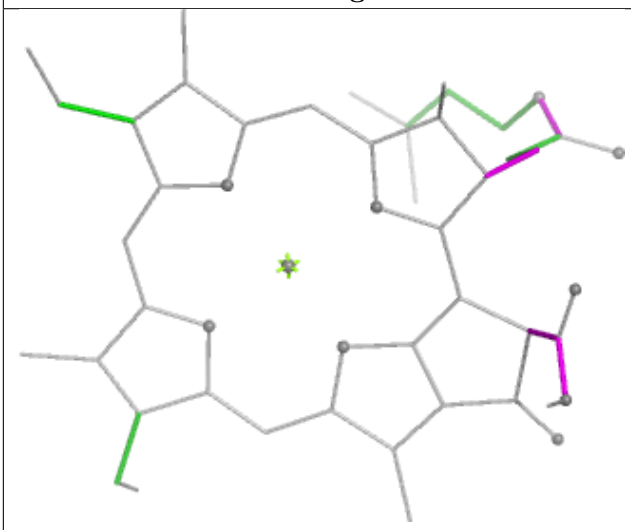


Bond angles



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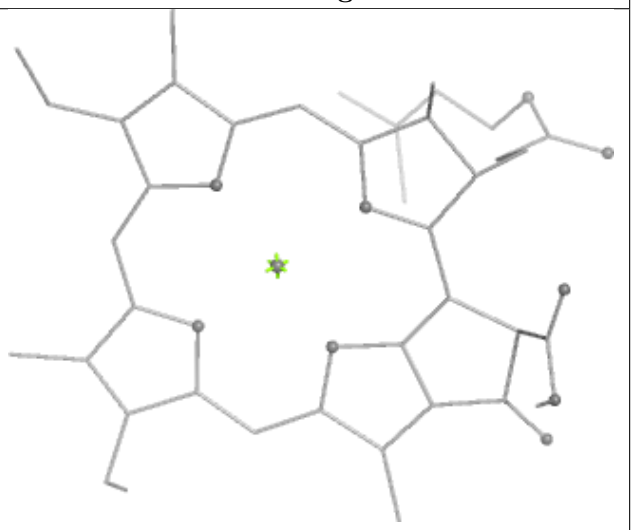
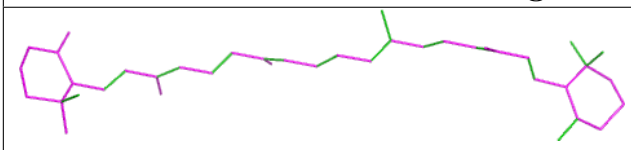


Rings

Ligand BCR c 515



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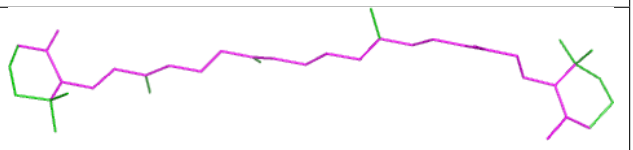

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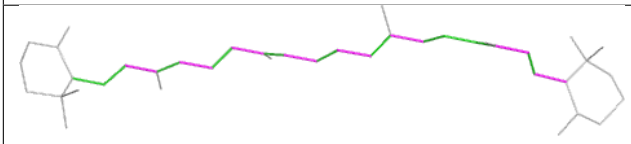
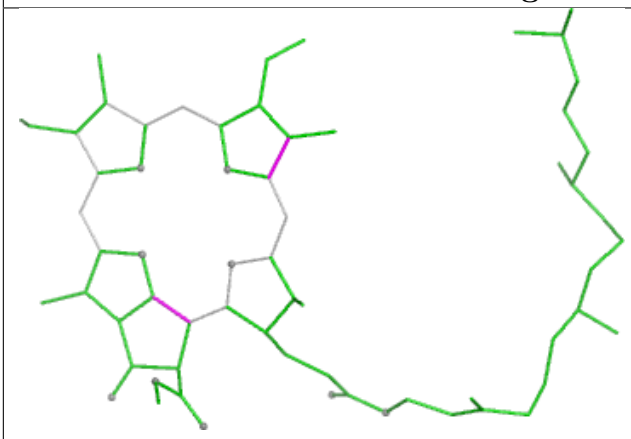


Torsions



Rings

Ligand PHO A 407



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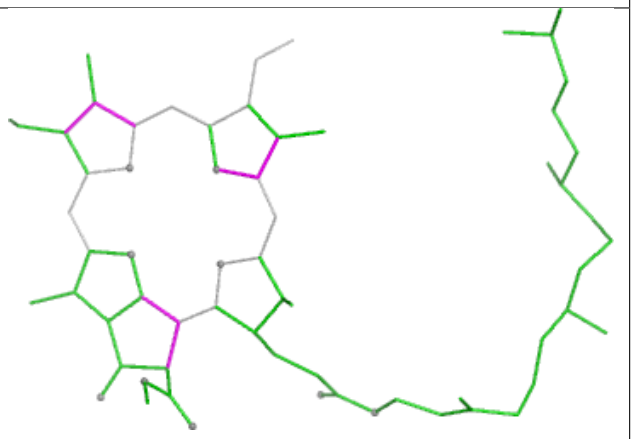
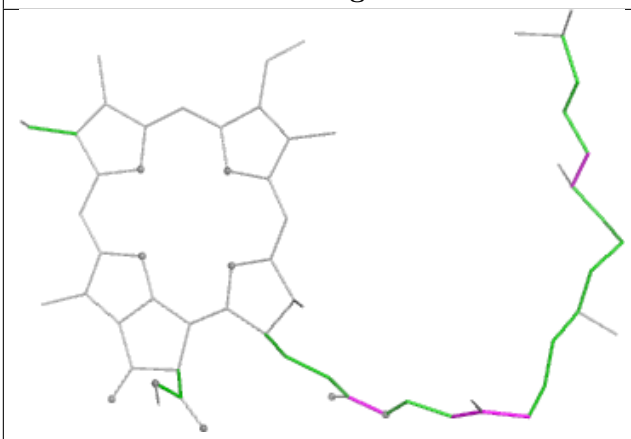


Bond angles



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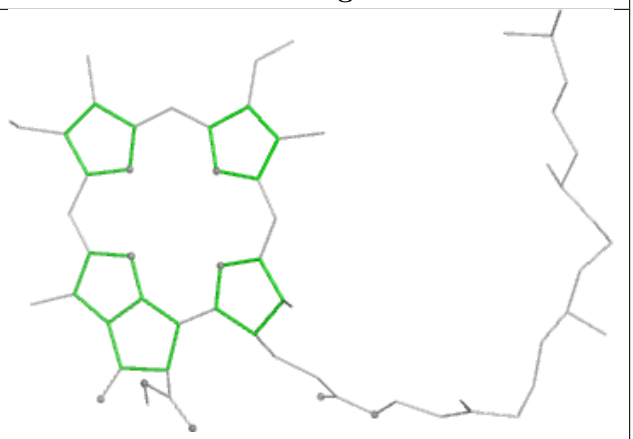
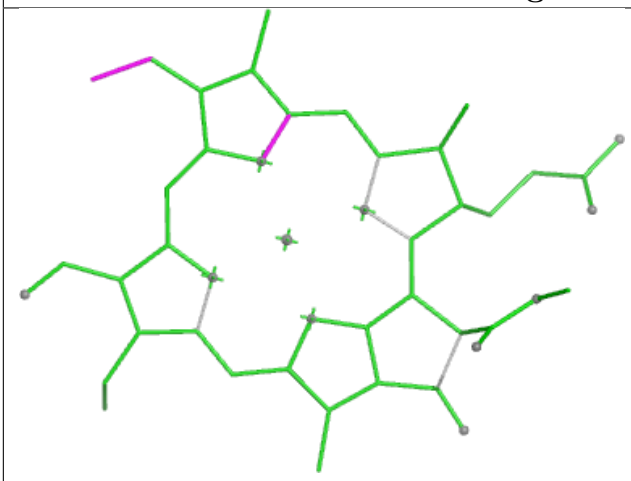


Rings

Ligand CHL S 302



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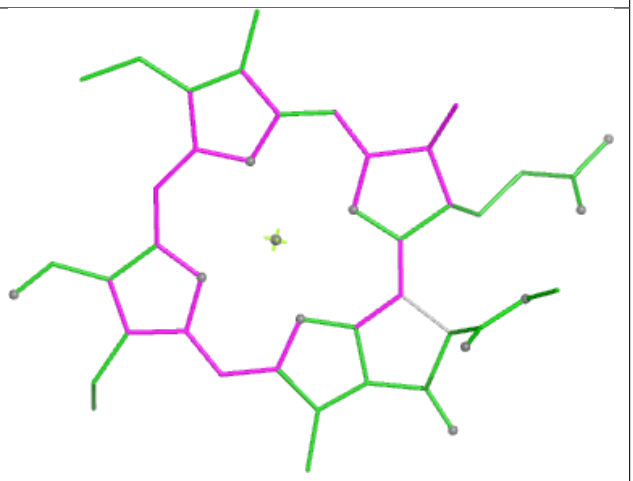
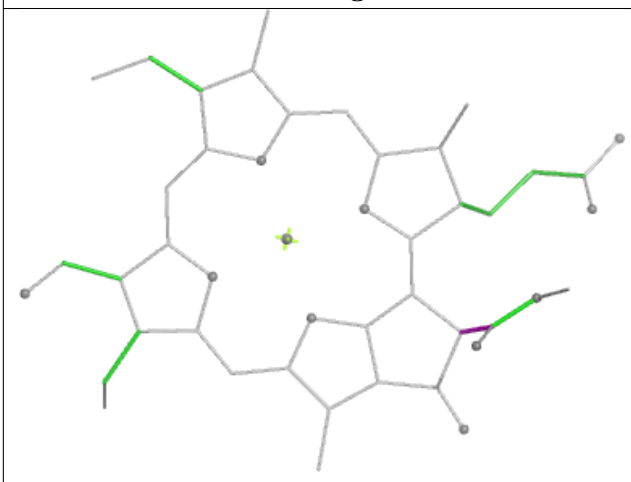


Bond angles



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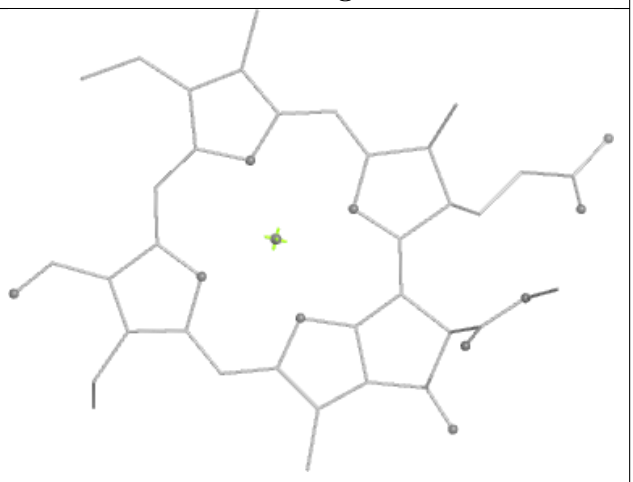
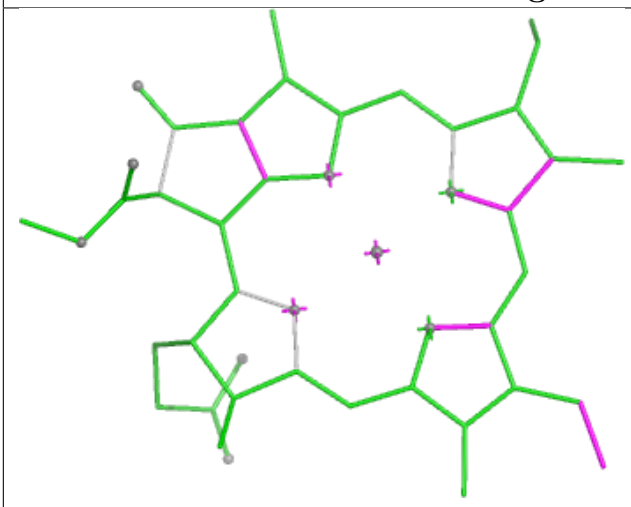


Rings

Ligand CLA g 614



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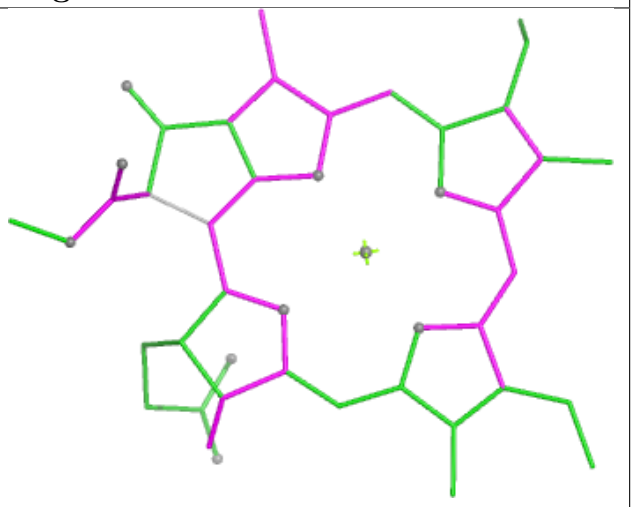
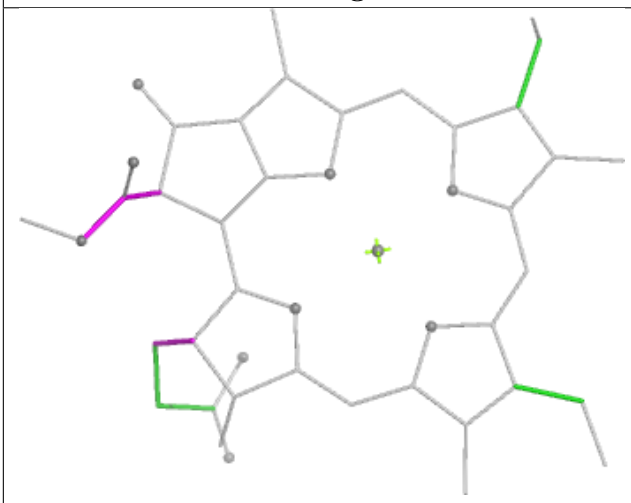


Bond angles



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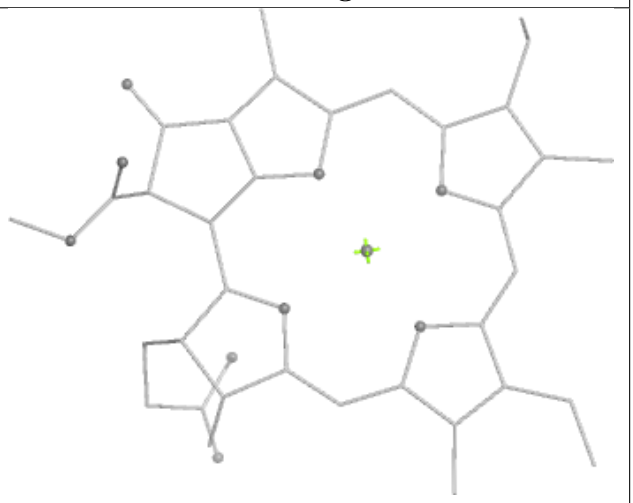
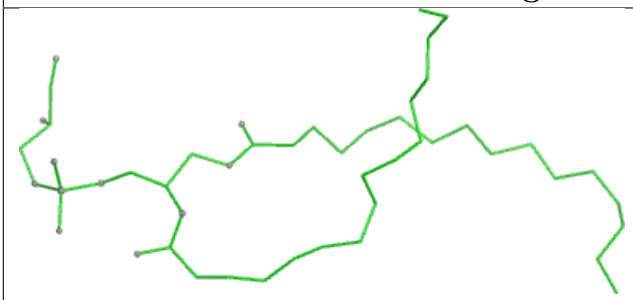


Rings

Ligand LHG C 521



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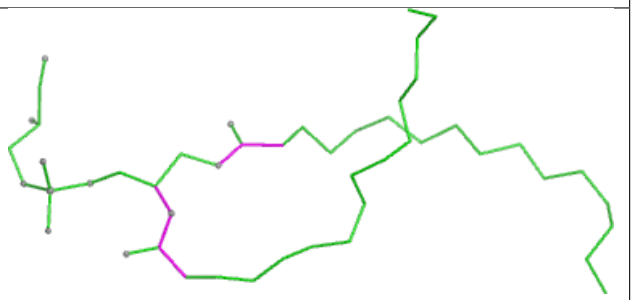
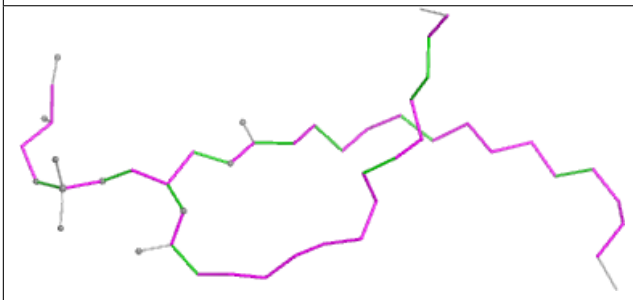


Bond angles



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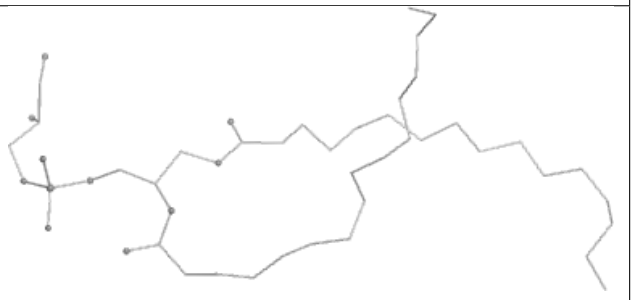
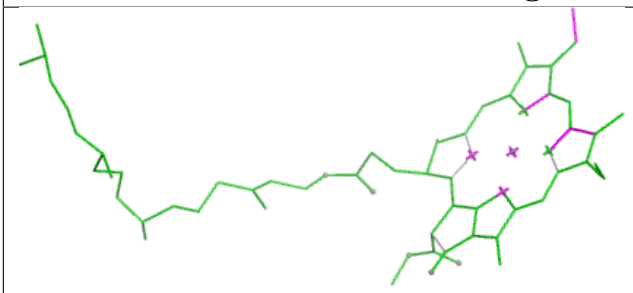


Rings

Ligand CLA A 405



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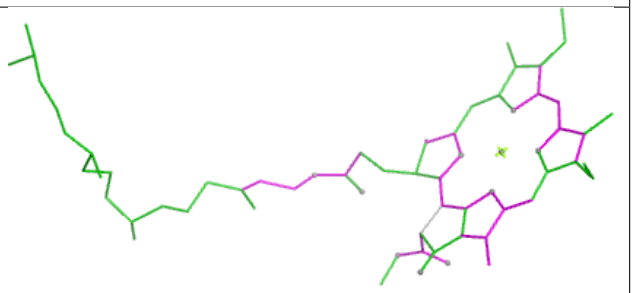
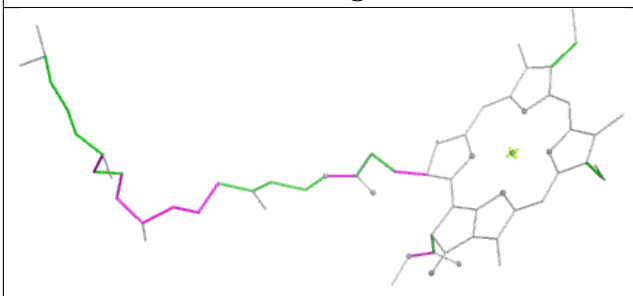


Bond angles



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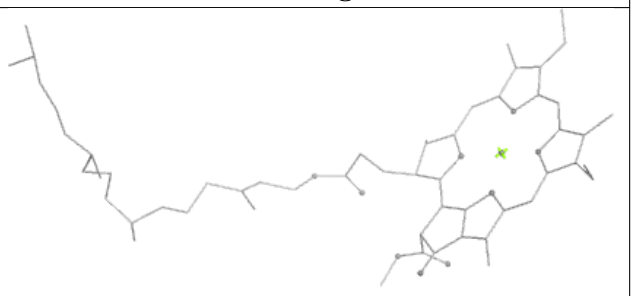
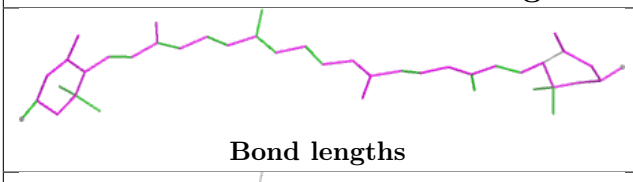


Rings

Ligand LUT N 615



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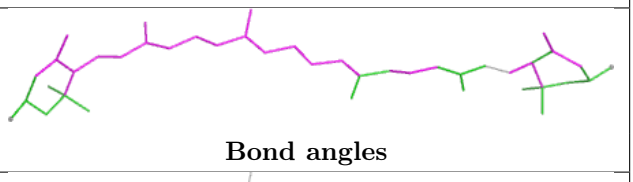
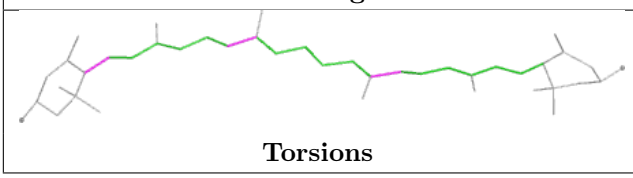


Bond angles



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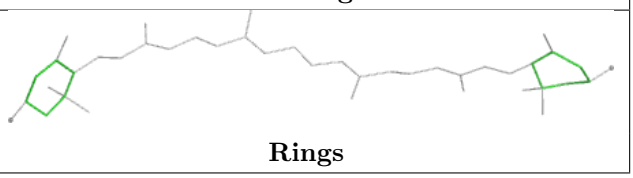
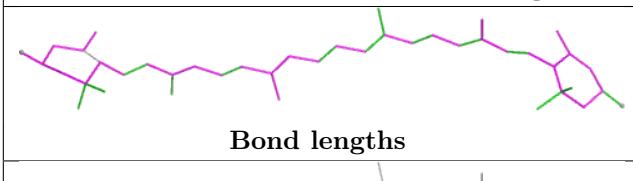


Rings

Ligand LUT y 315



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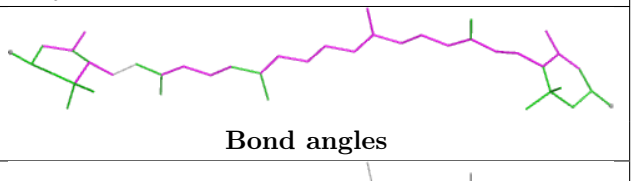
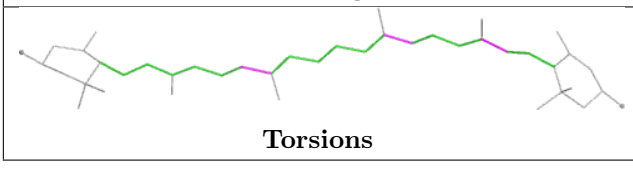


Bond angles



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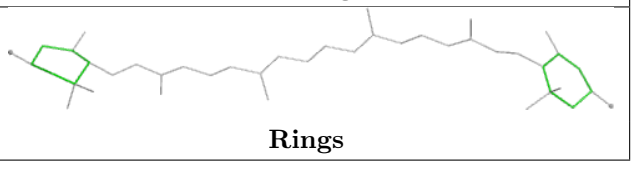
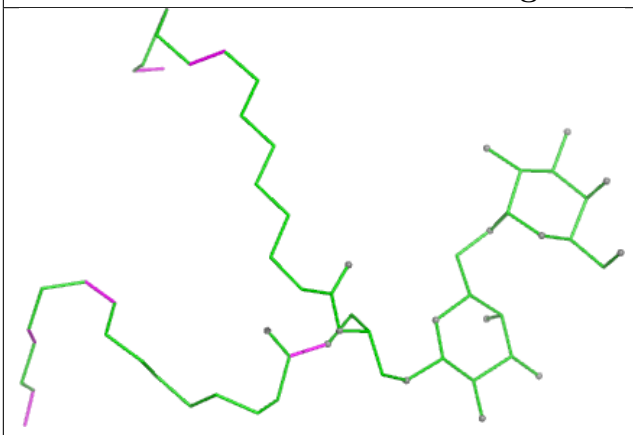
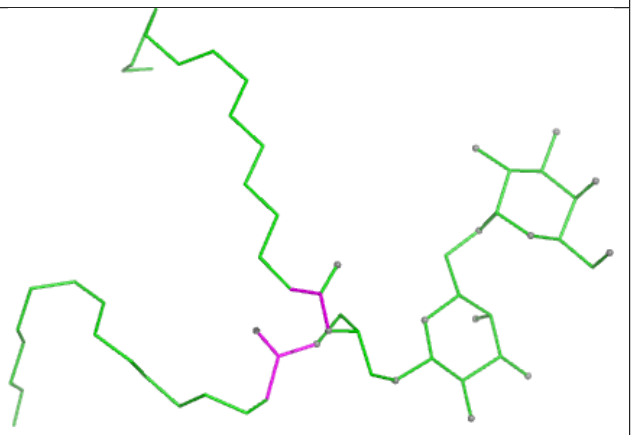


Rings

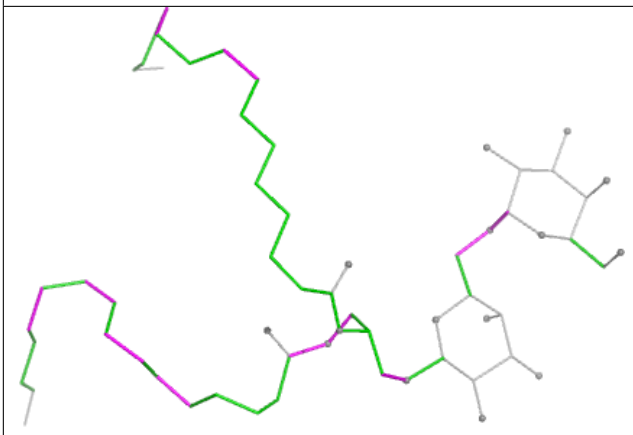
Ligand DGD C 518



Bond lengths



Bond angles



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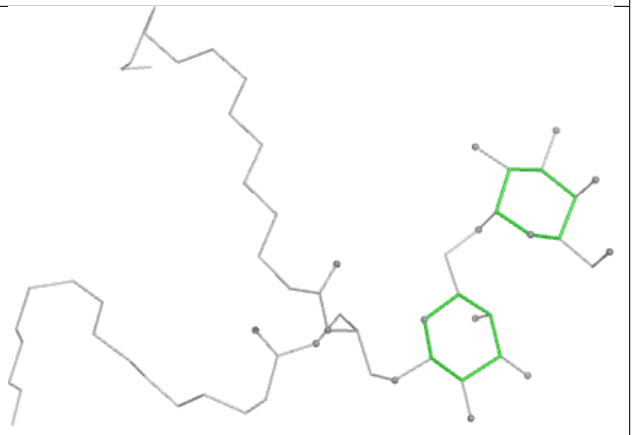
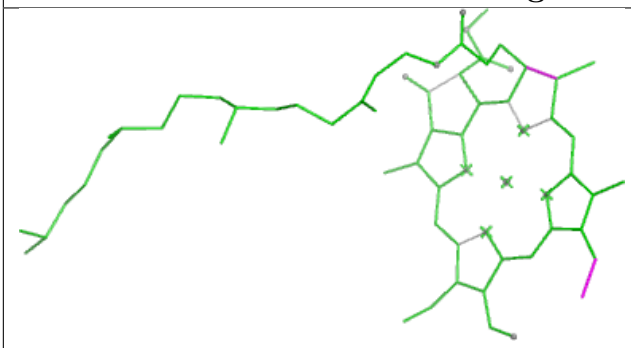


Rings

Ligand CHL y 309



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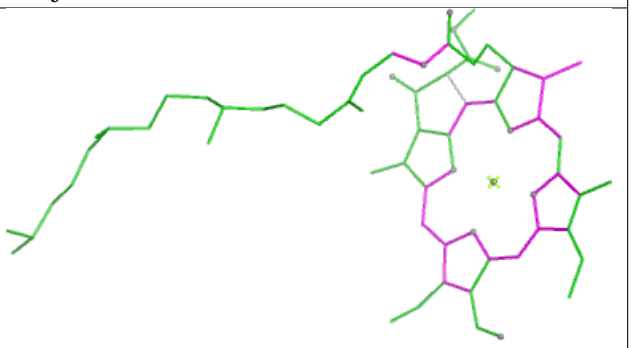
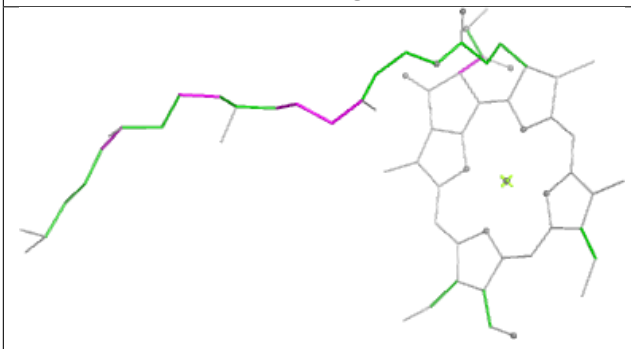


Bond angles

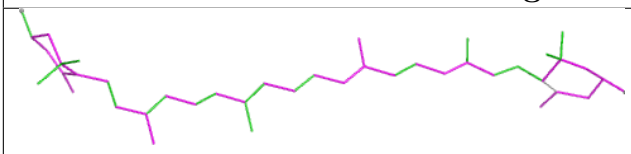


Torsions



Rings

Ligand LUT G 616



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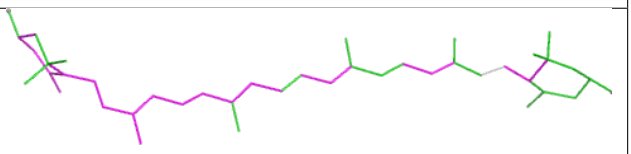
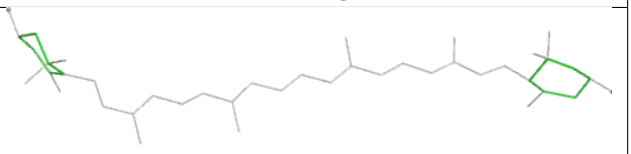


Bond angles

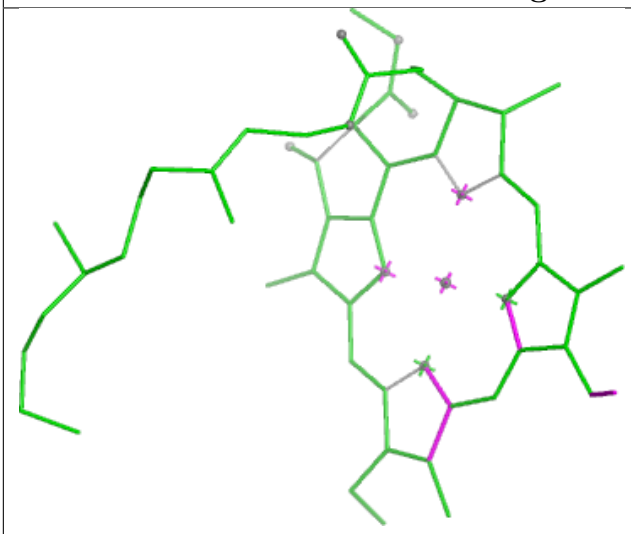


Torsions

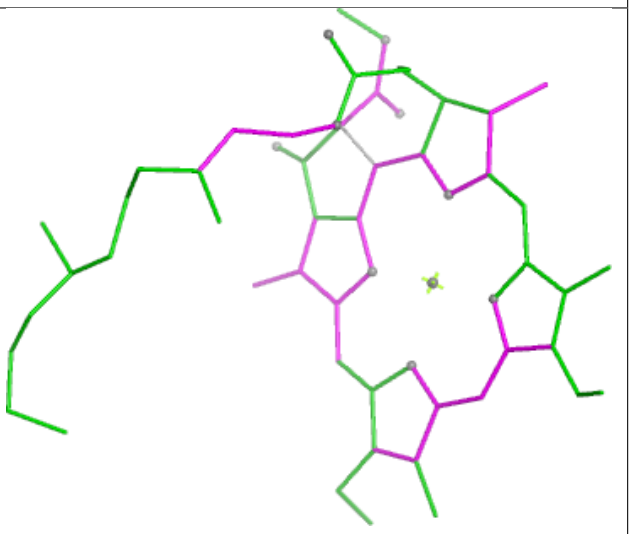


Rings

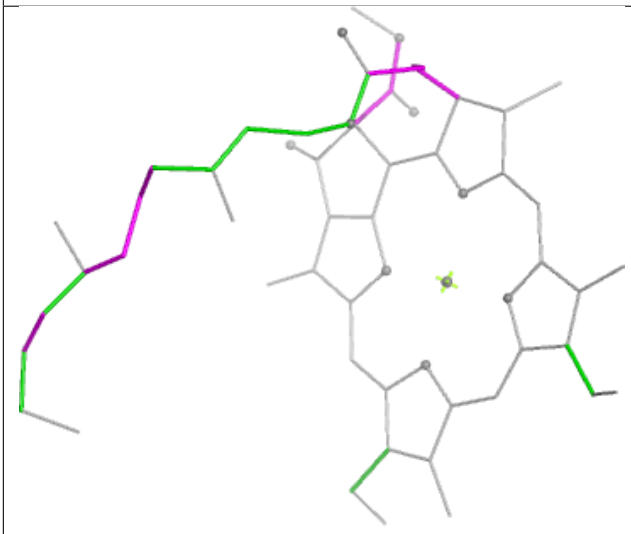
Ligand CLA r 608



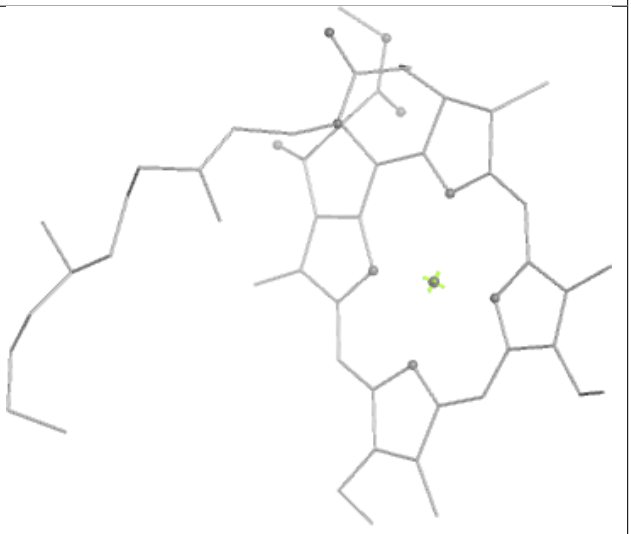
Bond lengths



Bond angles

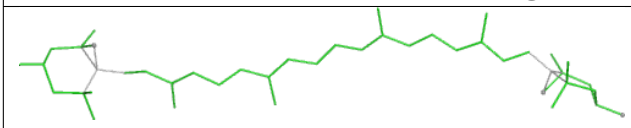


Torsions



Rings

Ligand XAT R 615



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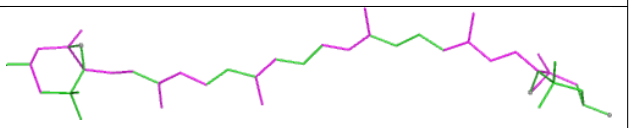

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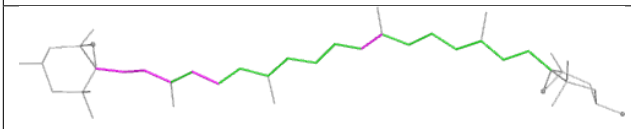

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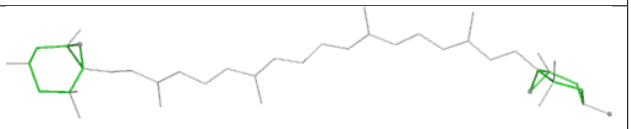
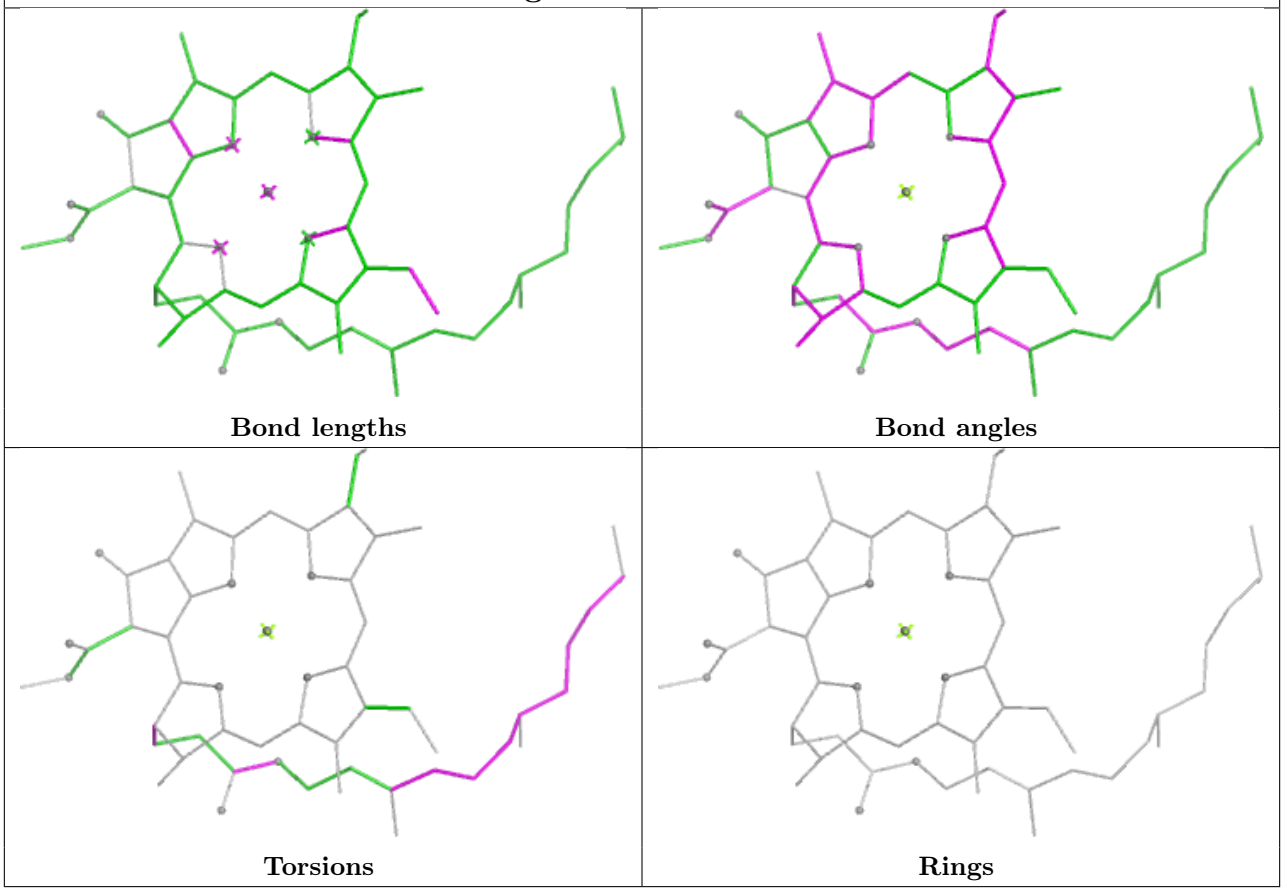


Rings

Ligand CLA Y 610



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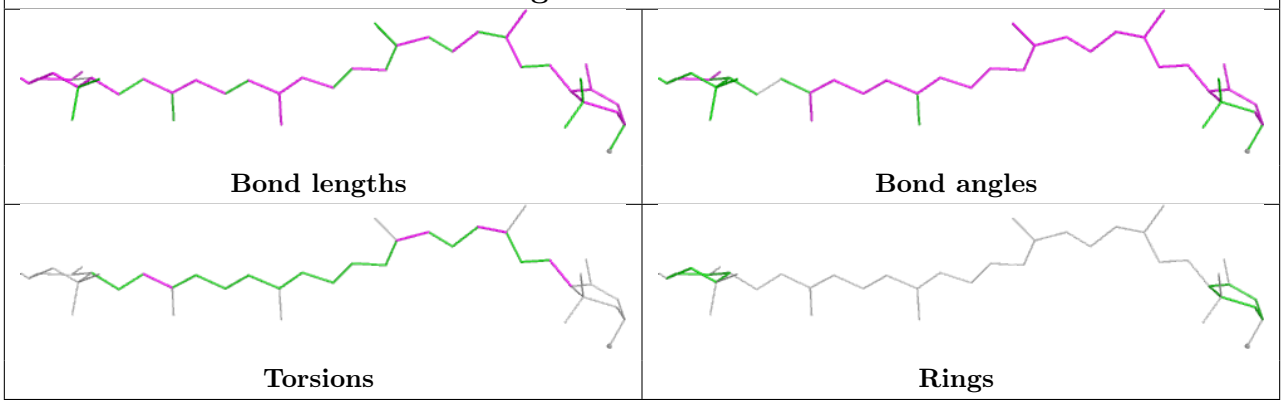
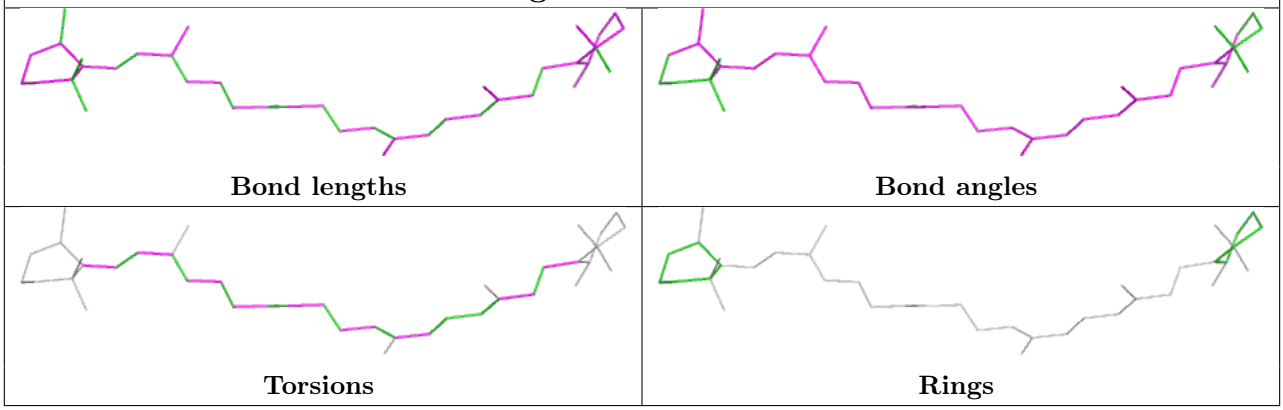


Ligand BCR t 101



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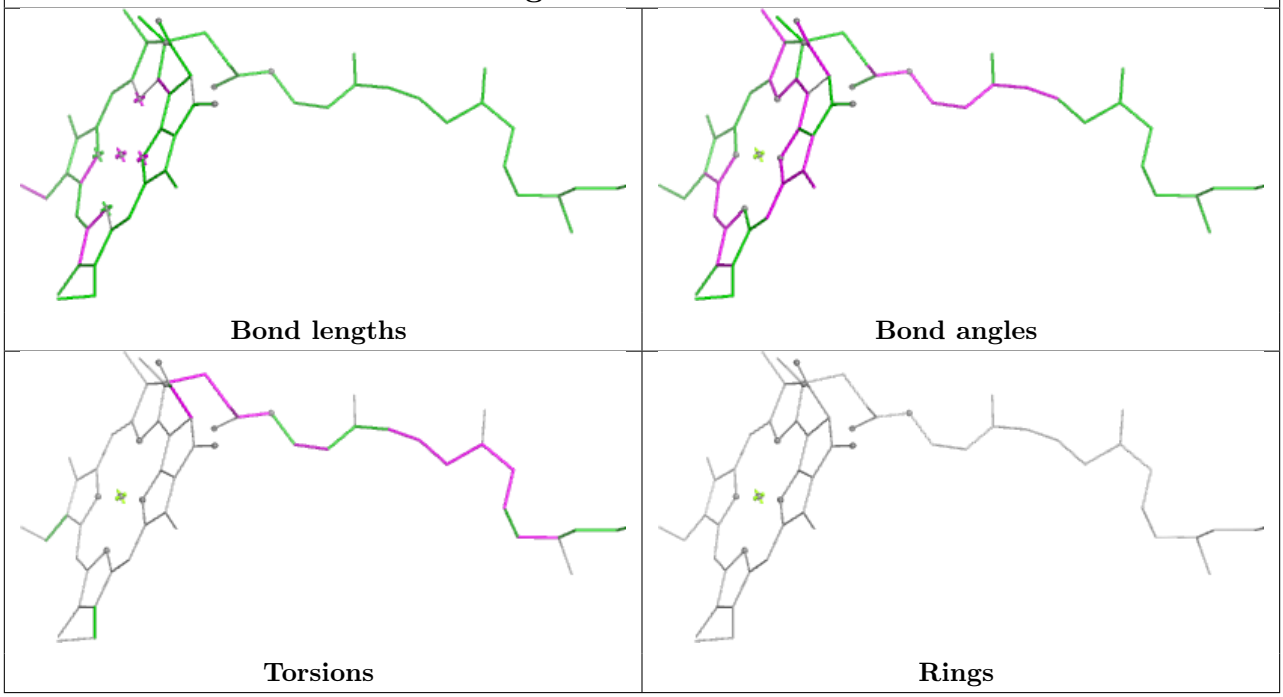

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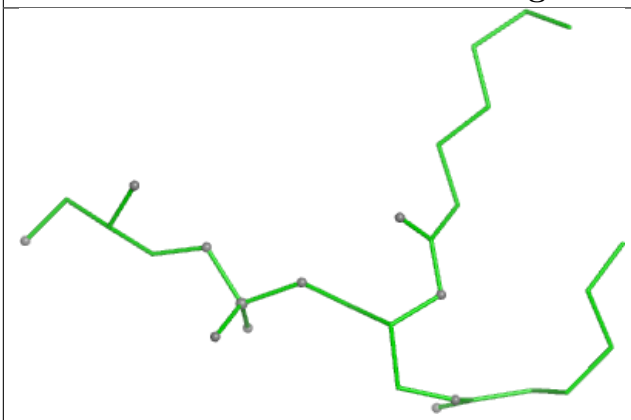
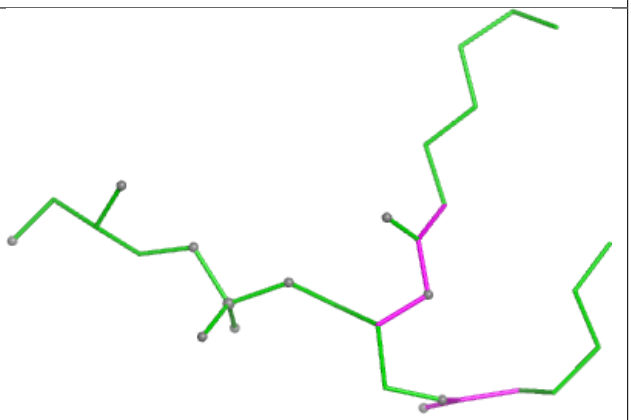
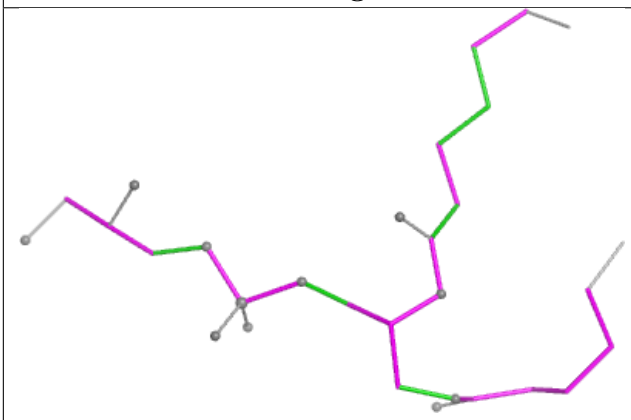


Bond lengths



Bond angles



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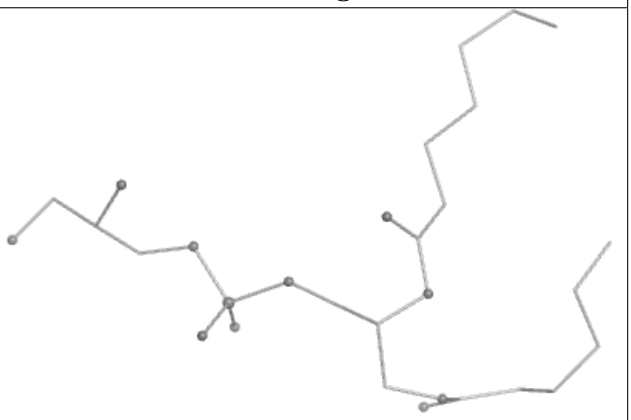
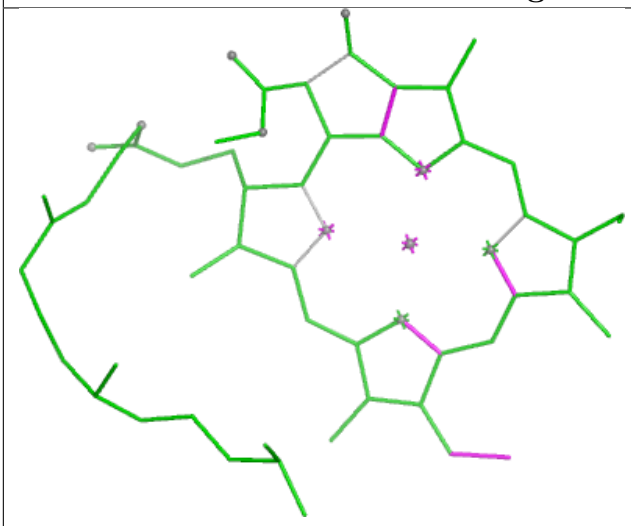


Rings

Ligand CLA n 612



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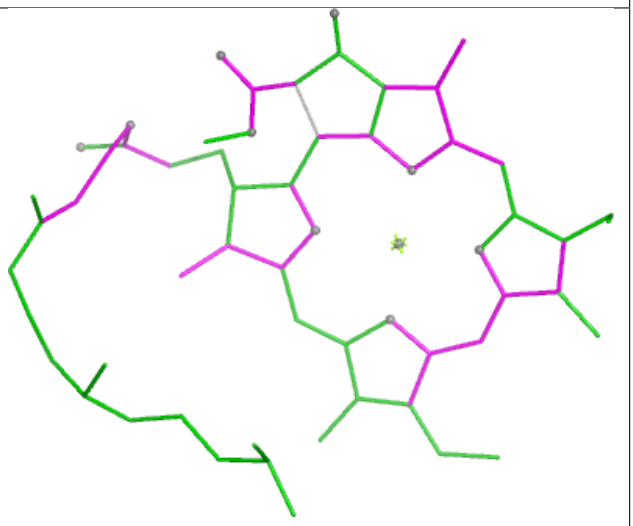
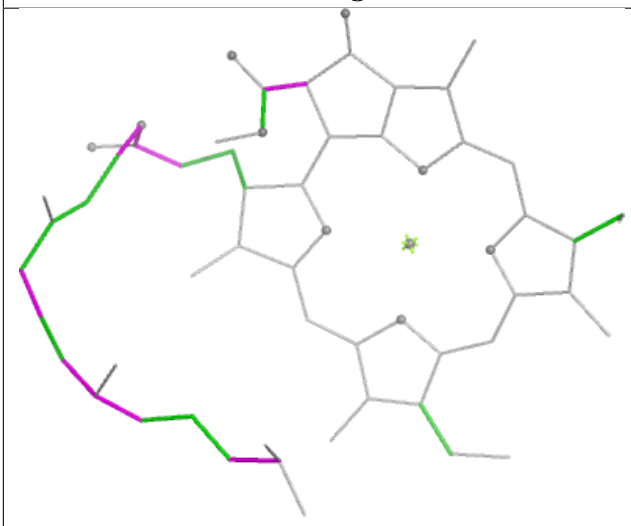


Bond angles



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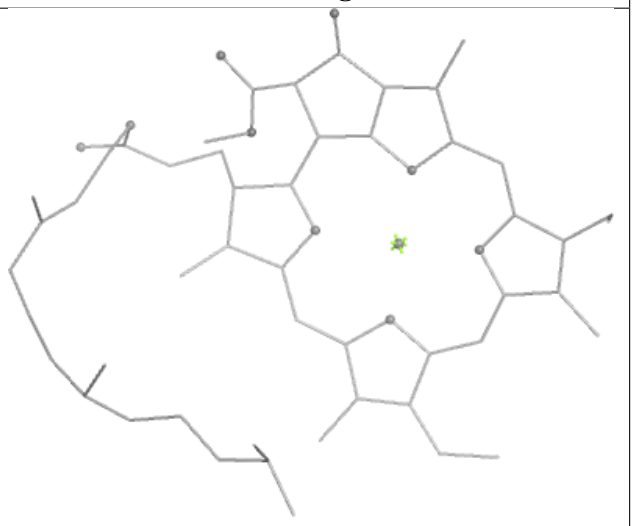
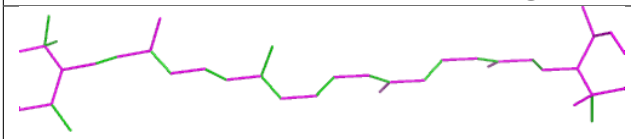


Rings

Ligand BCR C 515



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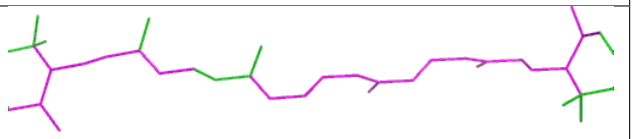

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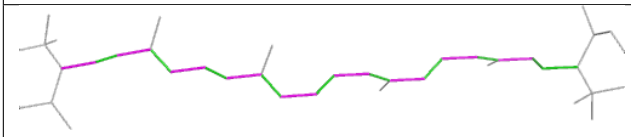

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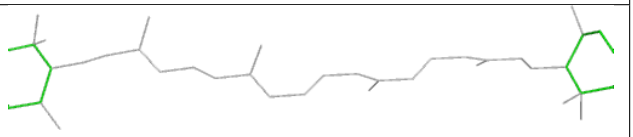
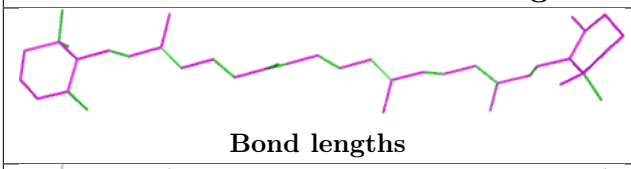


Rings

Ligand BCR i 101



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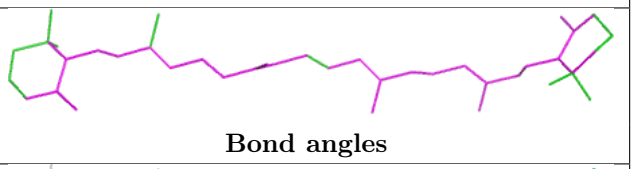

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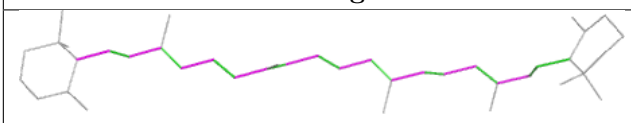

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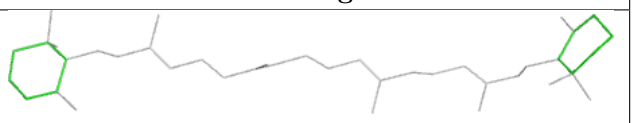
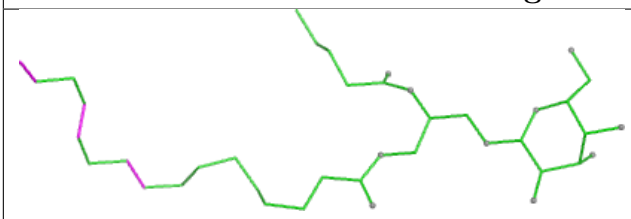


Rings

Ligand LMG a 413



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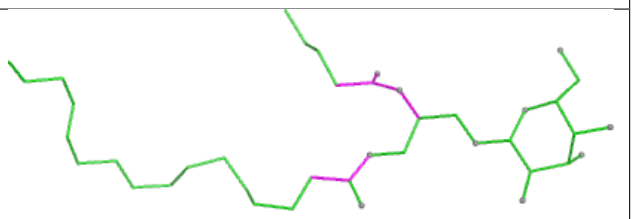
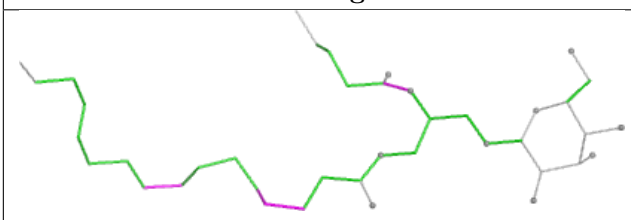


Bond angles



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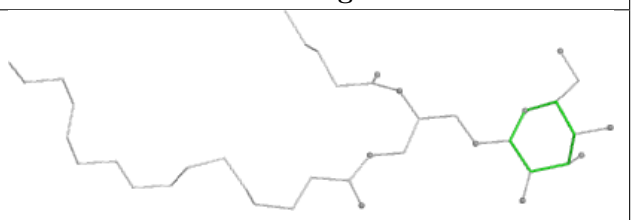
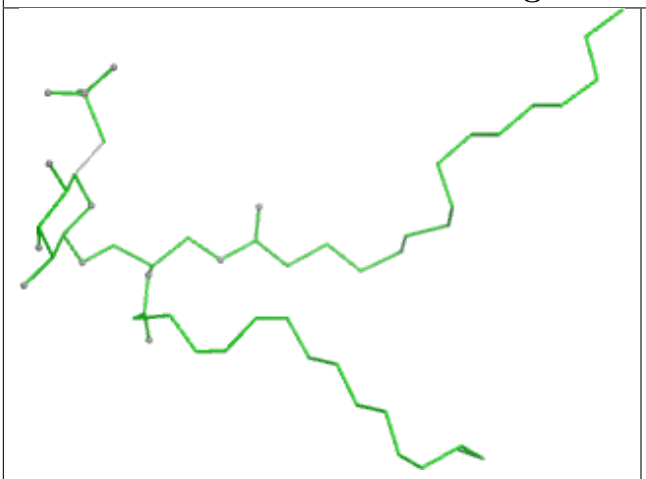


Rings

Ligand SQD A 414



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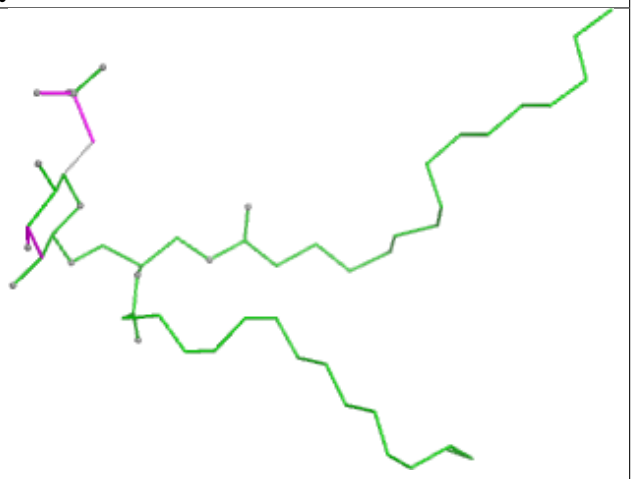
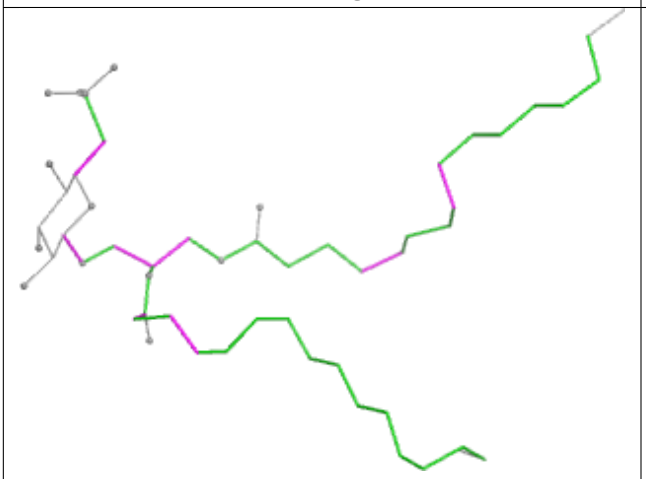


Bond angles



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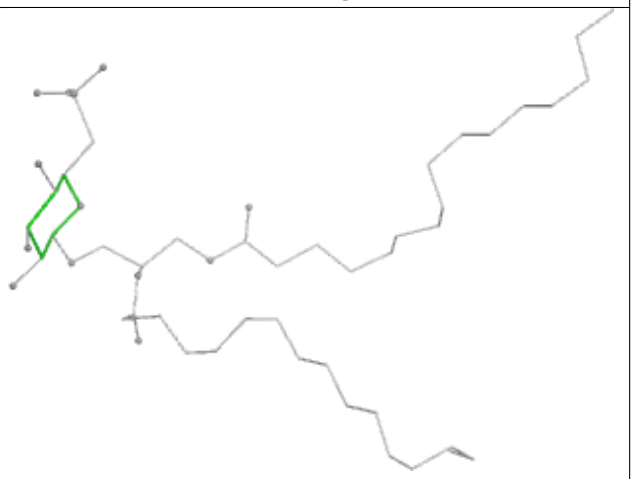
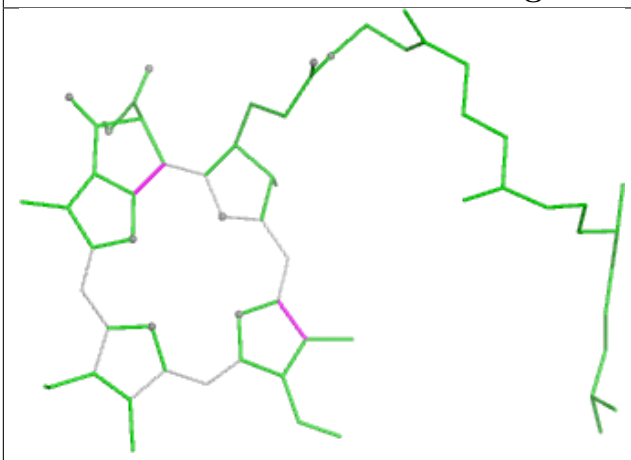


Rings

Ligand PHO d 402



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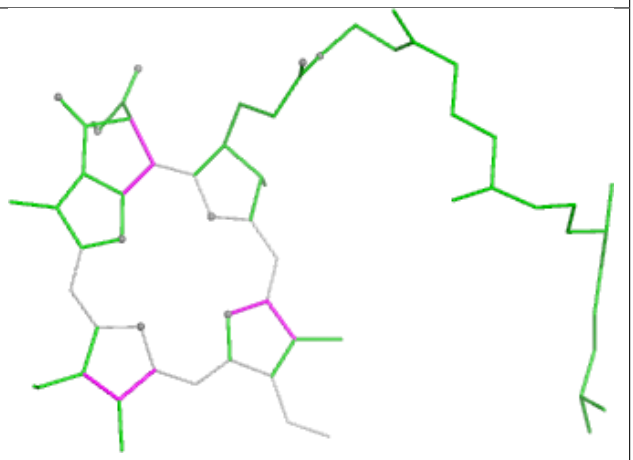
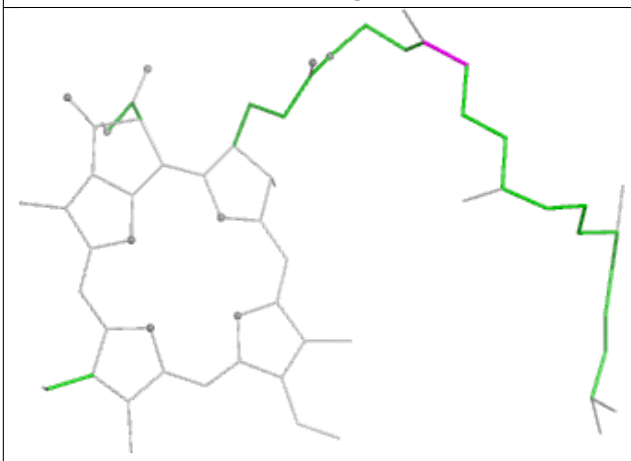


Bond angles



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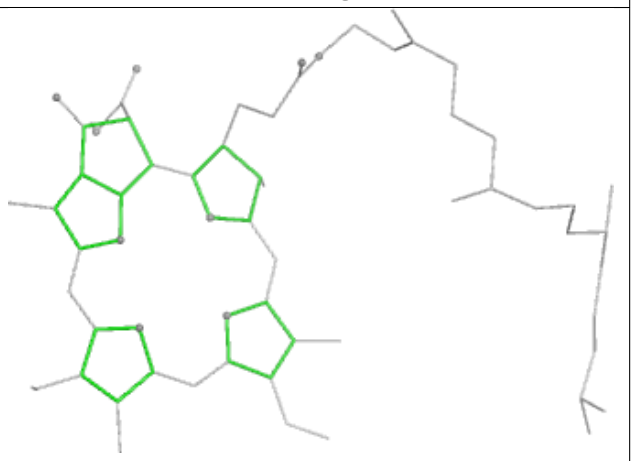
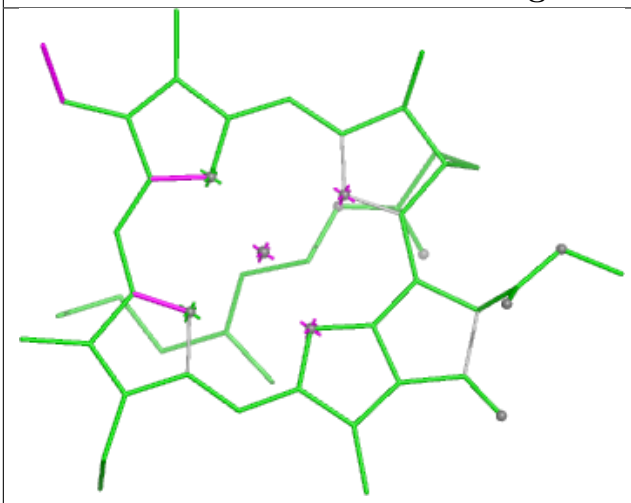


Rings

Ligand CLA g 613



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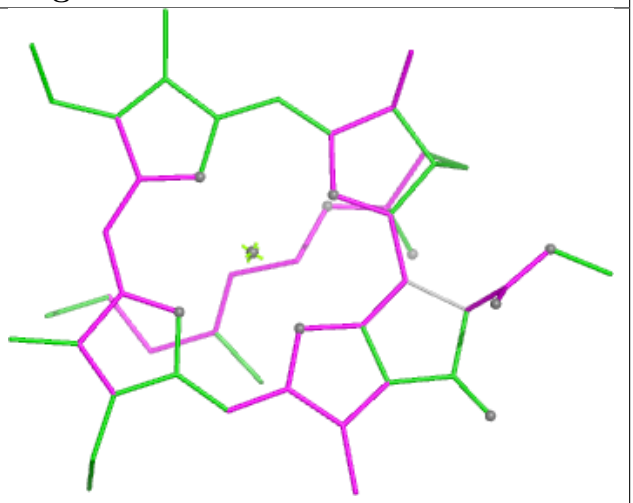
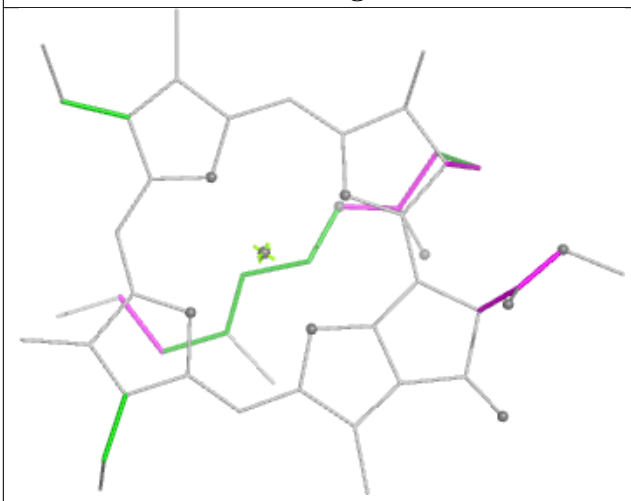


Bond angles



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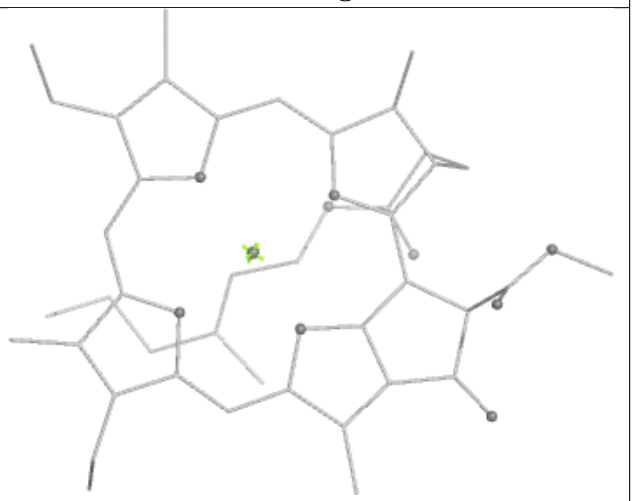
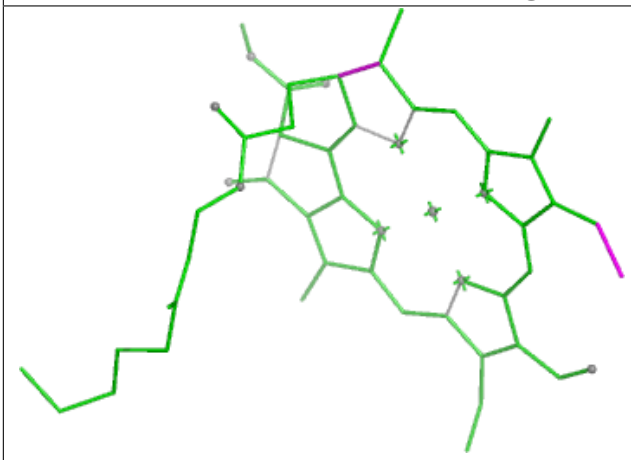


Rings

Ligand CHL G 609



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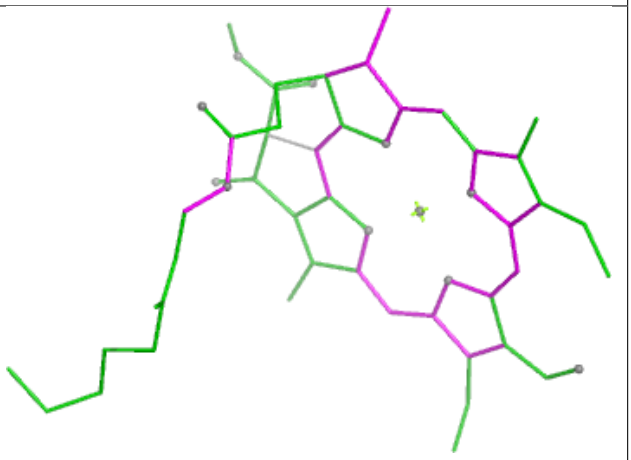
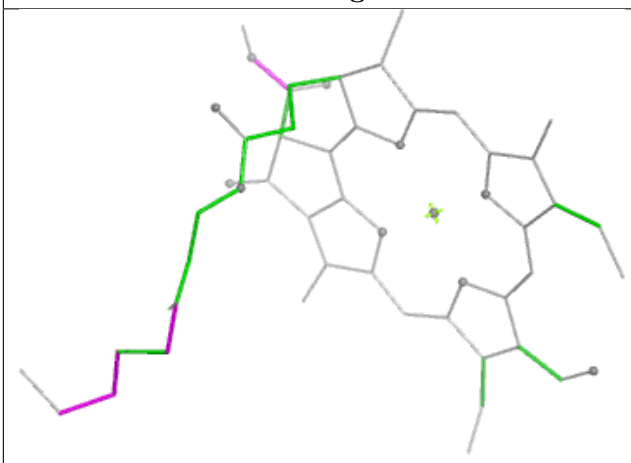


Bond angles



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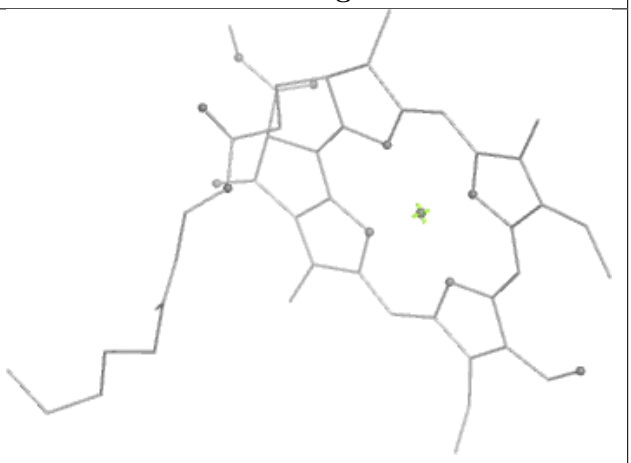
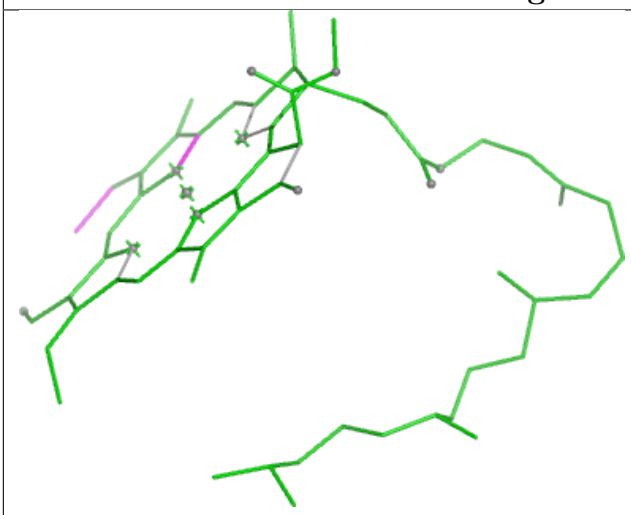
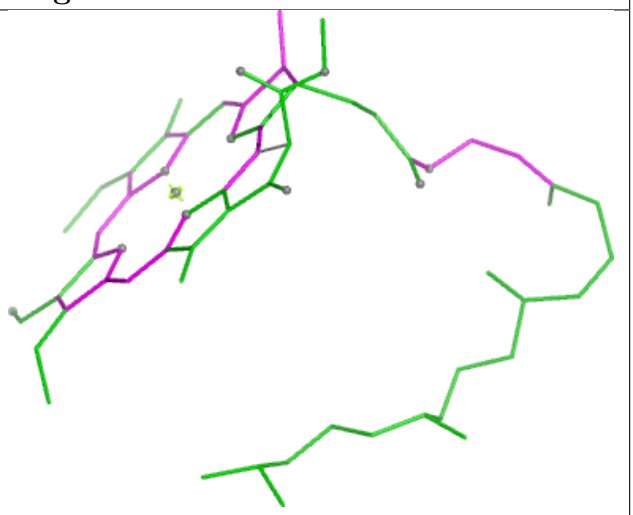


Rings

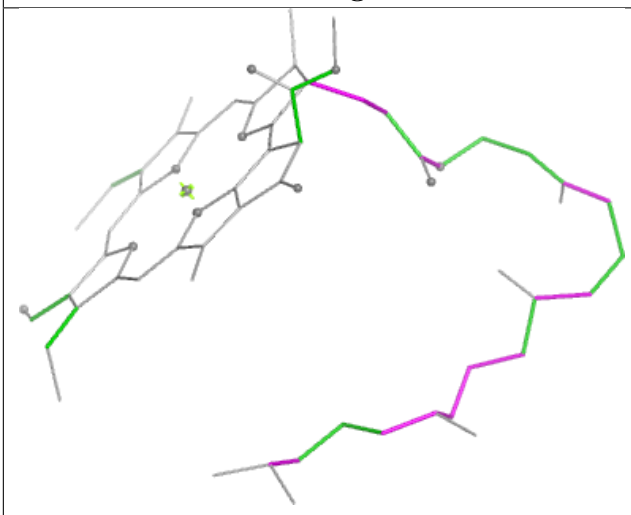
Ligand CHL g 619



Bond lengths



Bond angles



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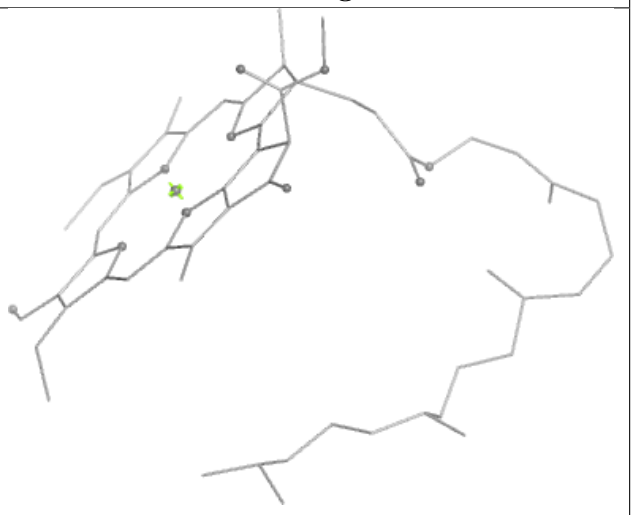
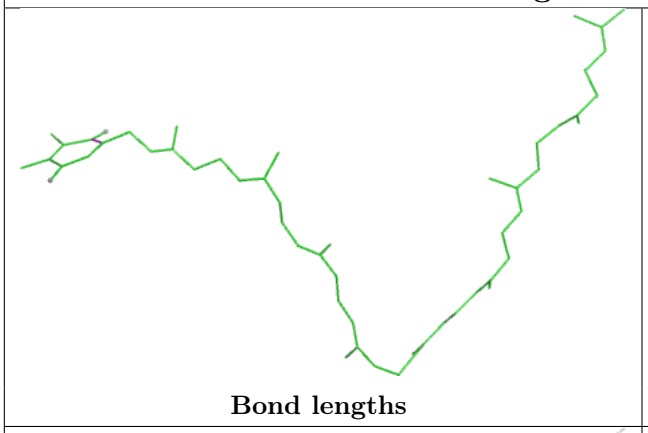
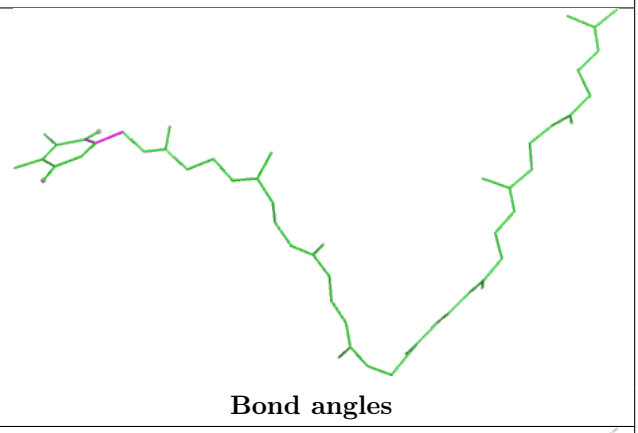


Rings

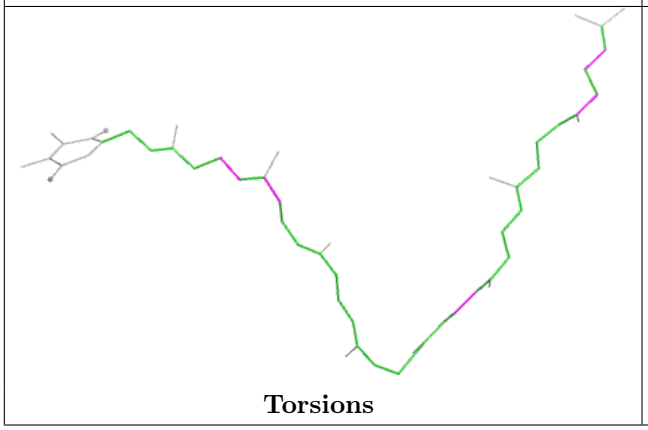
Ligand PL9 d 407



Bond lengths



Bond angles



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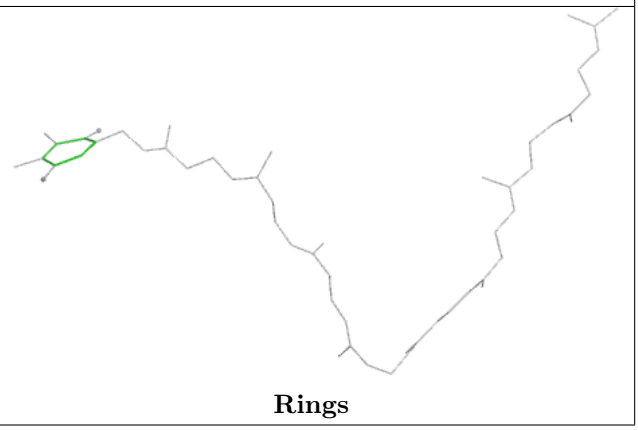
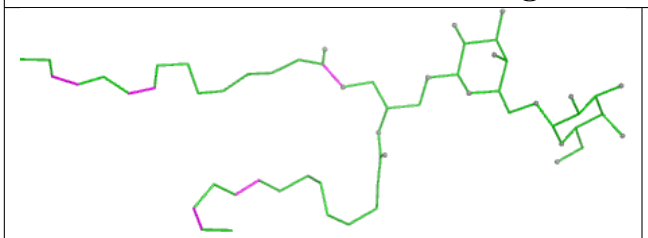
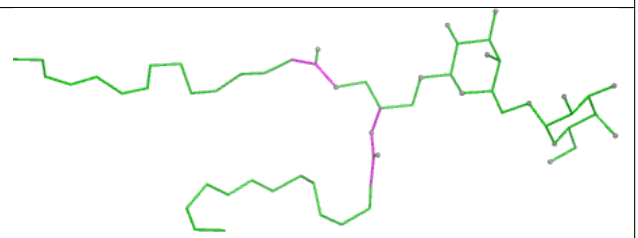


Rings

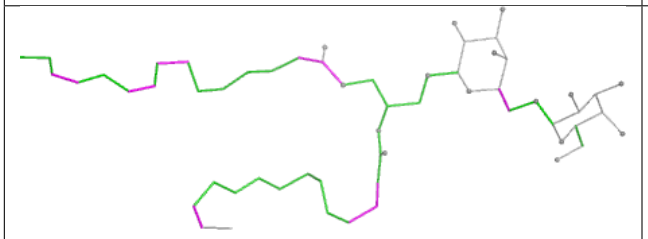
Ligand DGD C 519



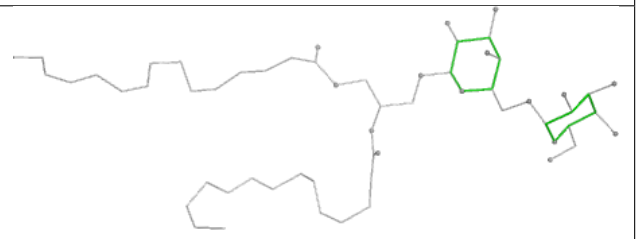
Bond lengths



Bond angles

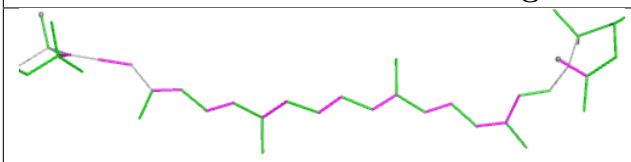


Torsions

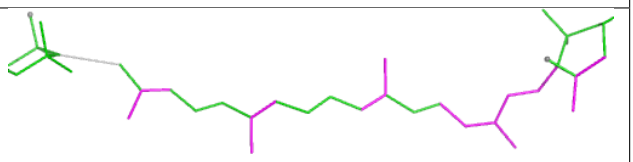


Rings

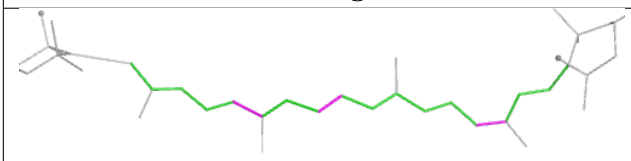
Ligand NEX Y 618



Bond lengths



Bond angles



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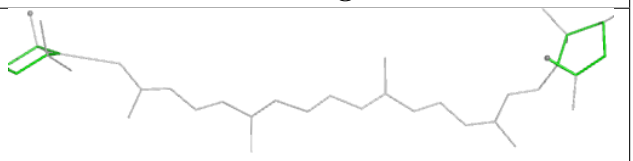
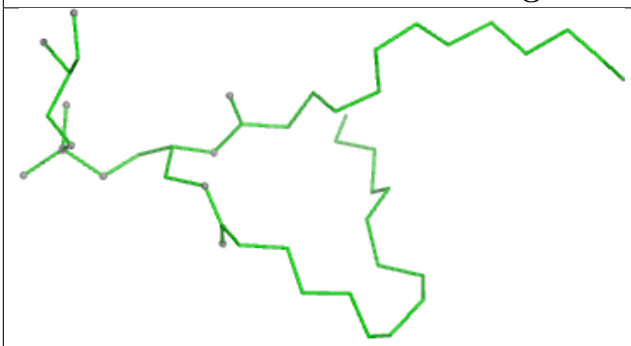


Rings

Ligand LHG B 625



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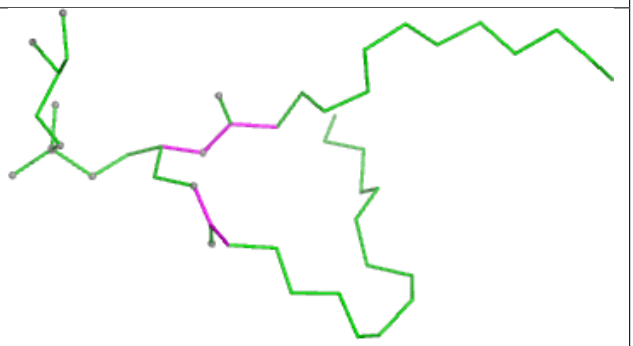
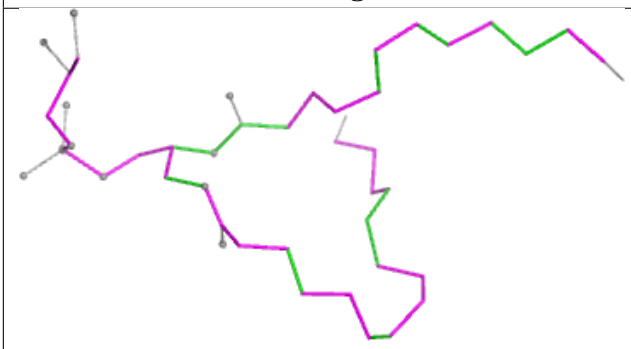


Bond angles



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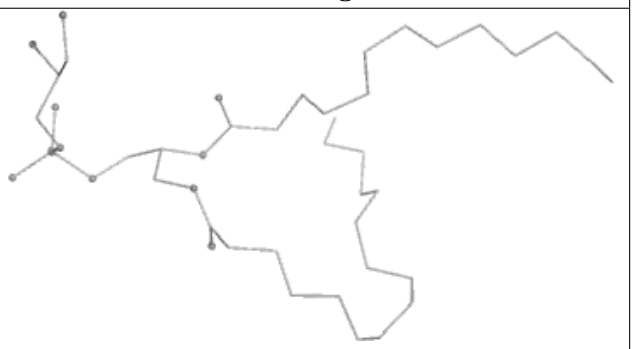
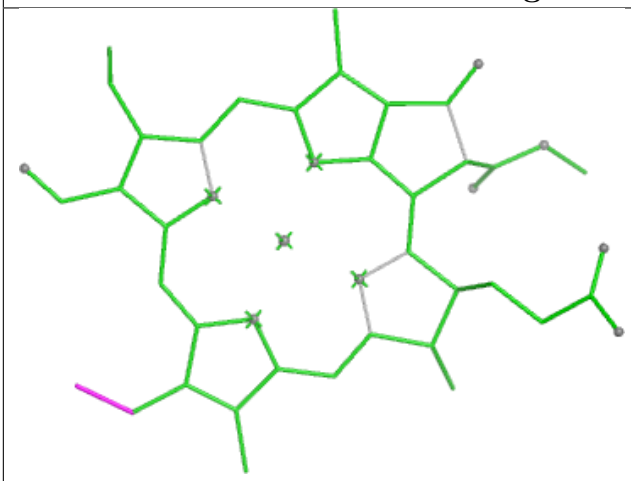


Rings

Ligand CHL R 606



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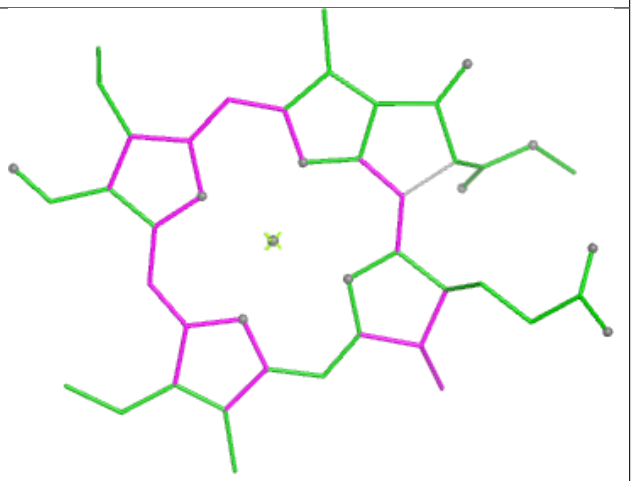
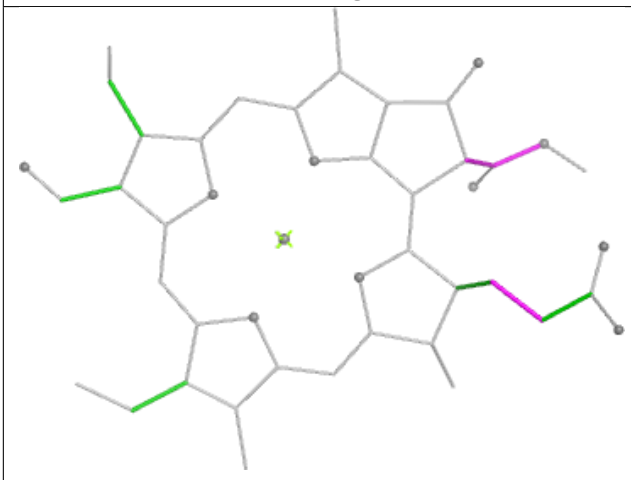


Bond angles



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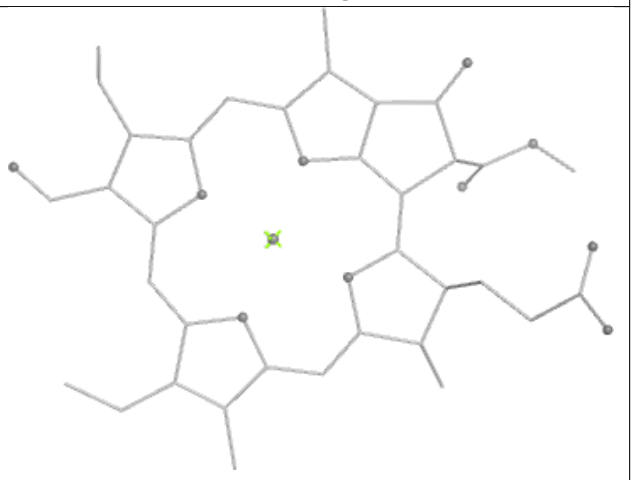
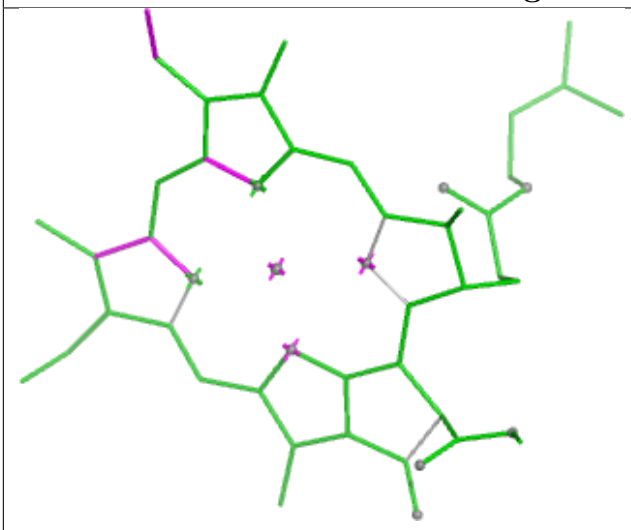


Rings

Ligand CLA A 406



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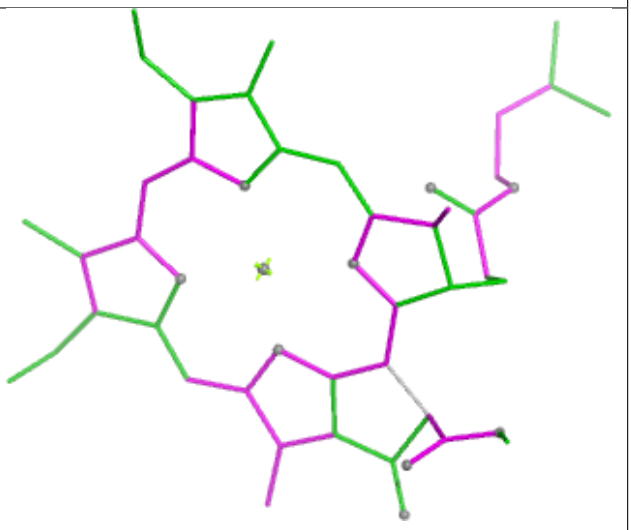
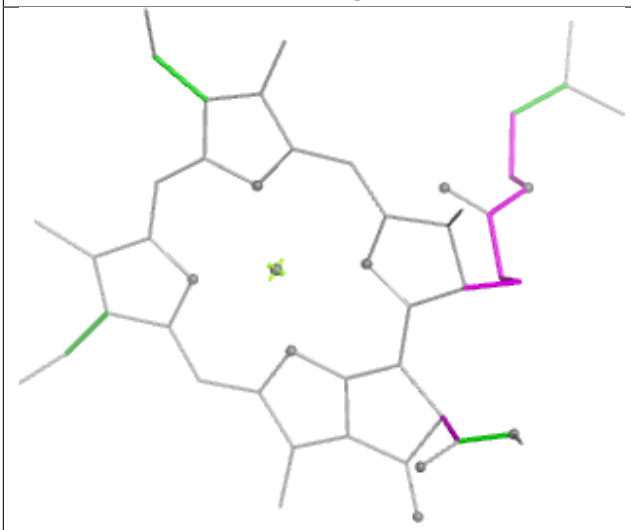


Bond angles



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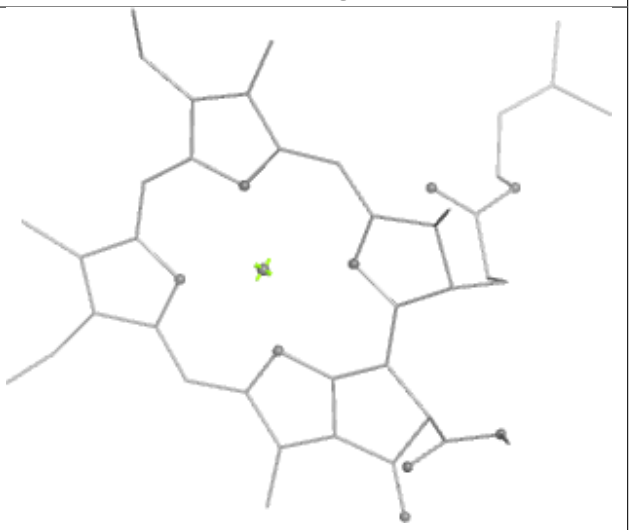
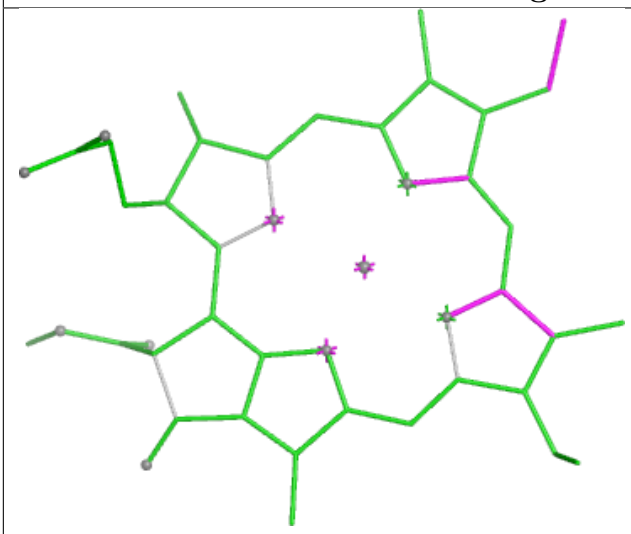


Rings

Ligand CLA s 608



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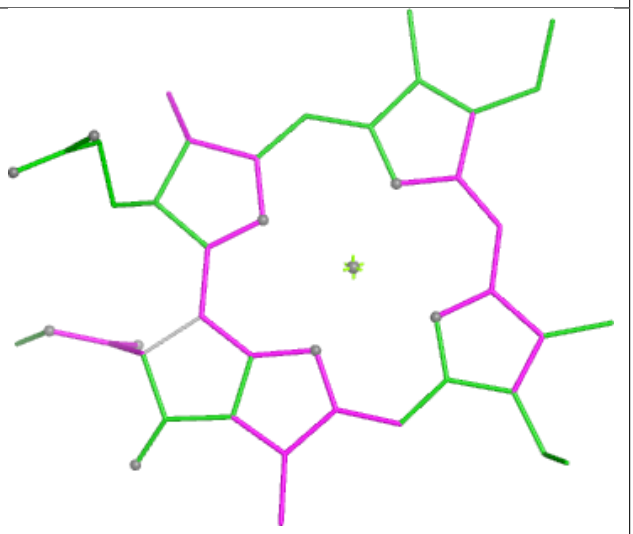
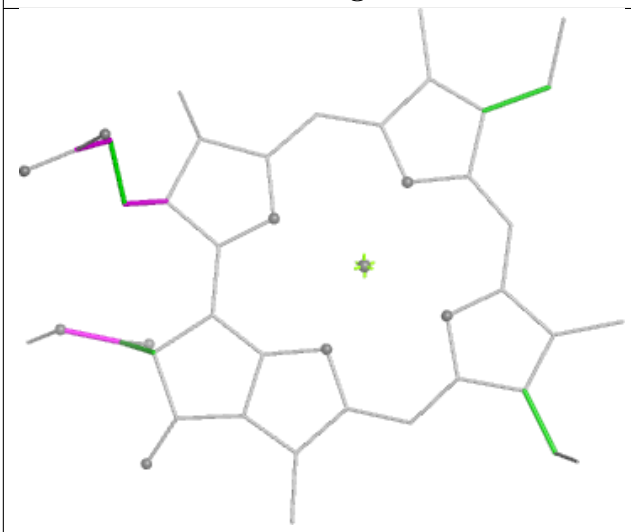


Bond angles



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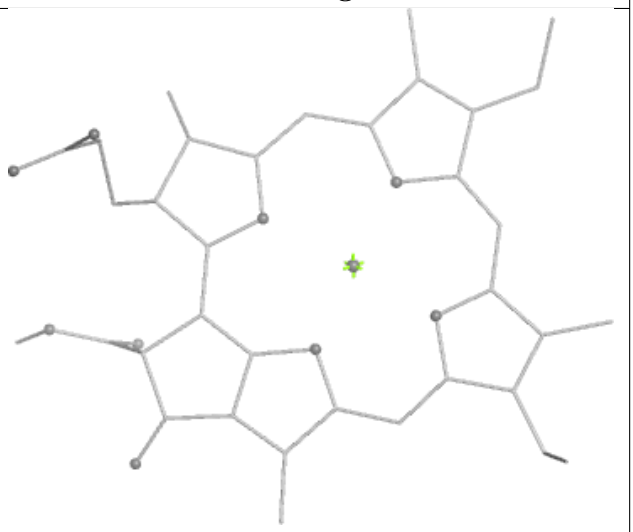
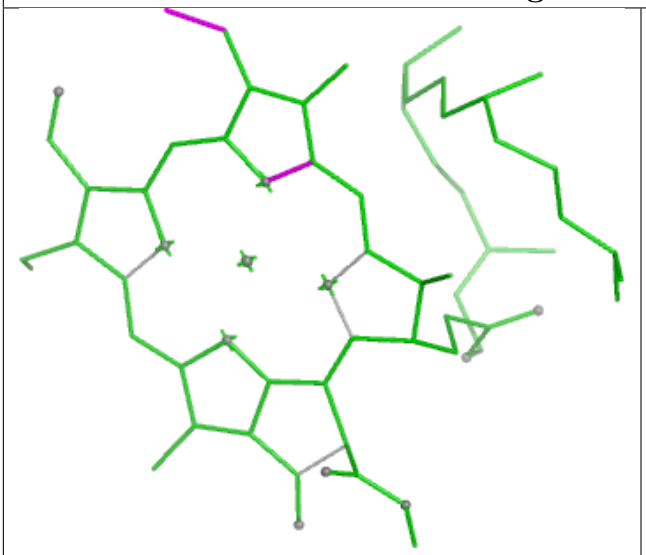


Rings

Ligand CHL n 608



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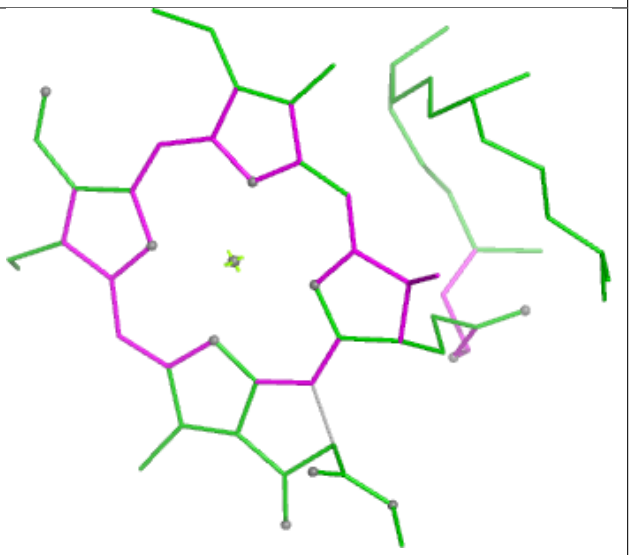
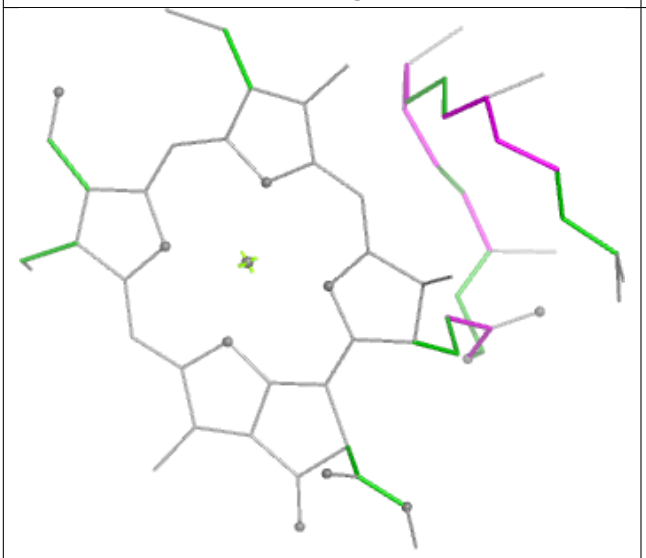


Bond angles



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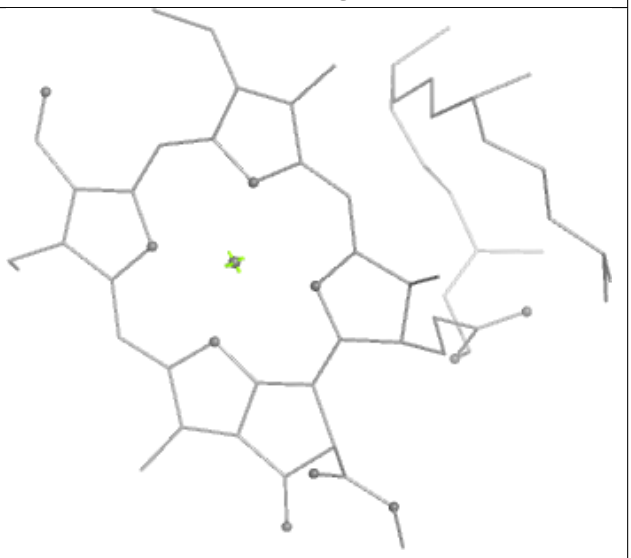
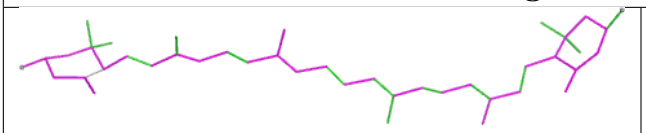


Rings

Ligand LUT R 614



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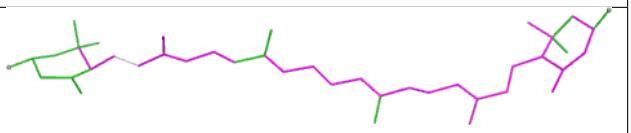
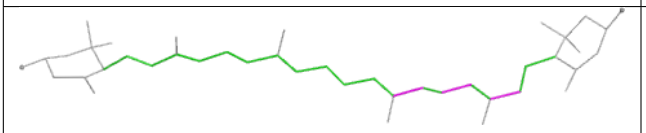


Bond angles



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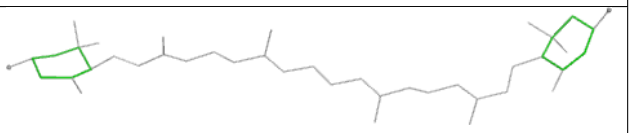
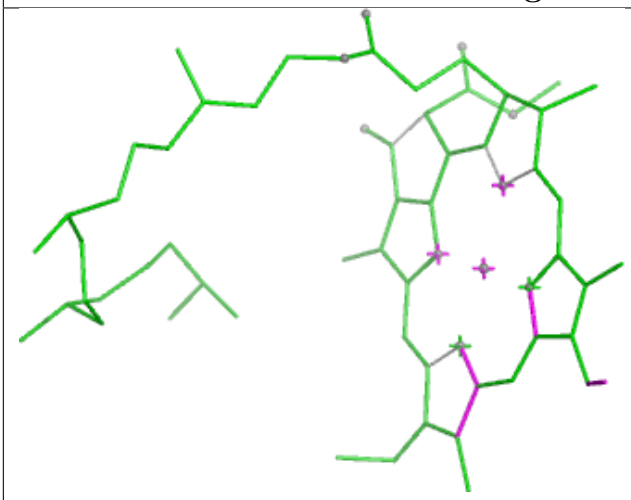


Rings

Ligand CLA C 503



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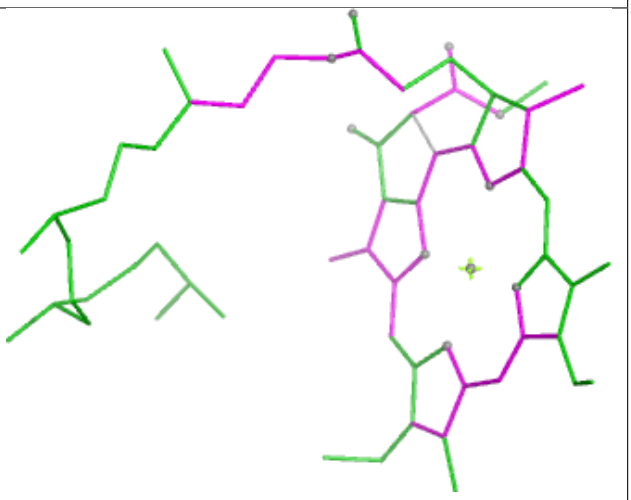
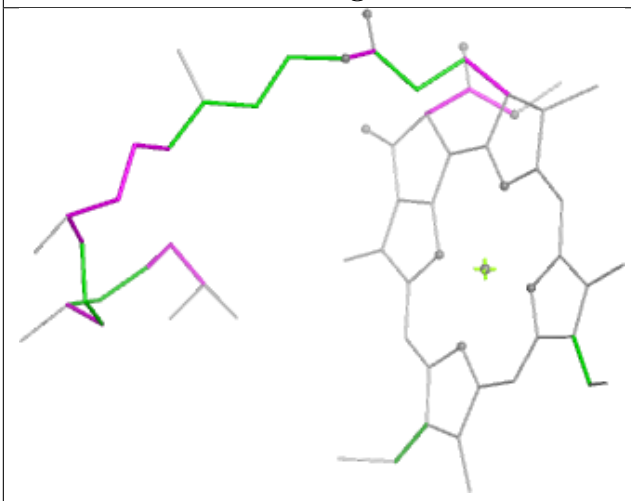


Bond angles



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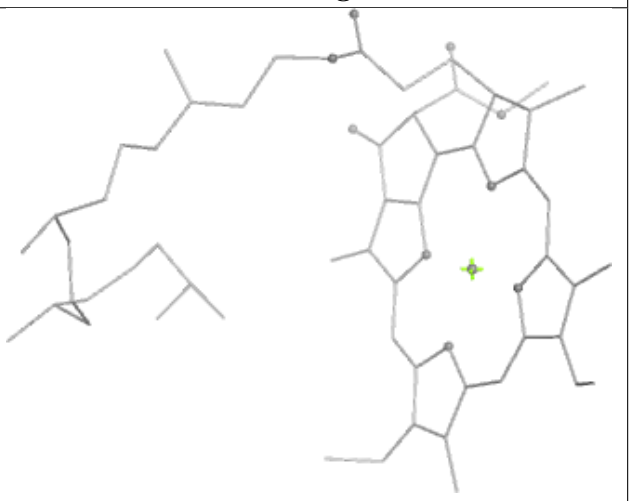
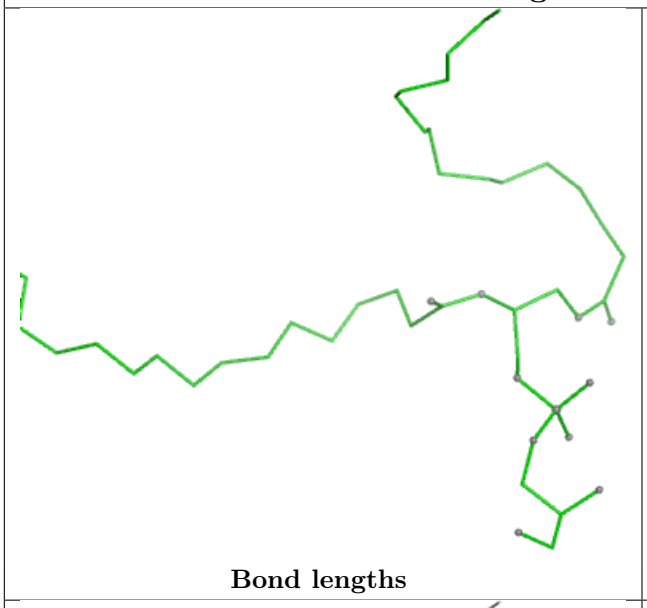


Rings

Ligand LHG s 617



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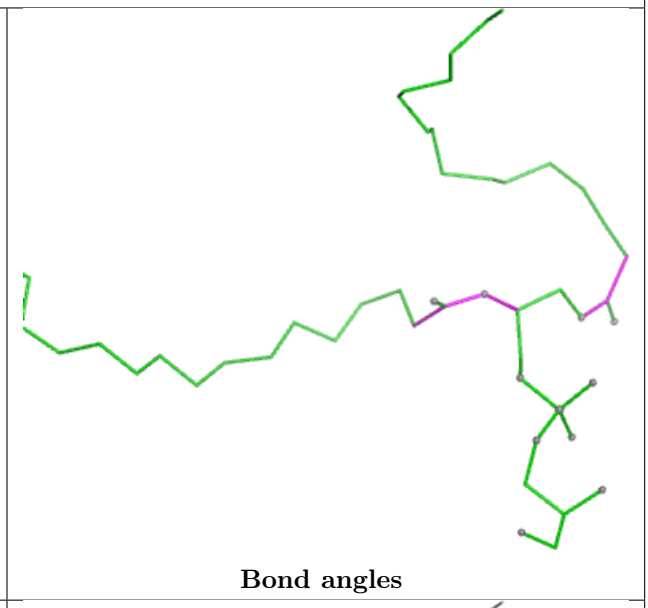
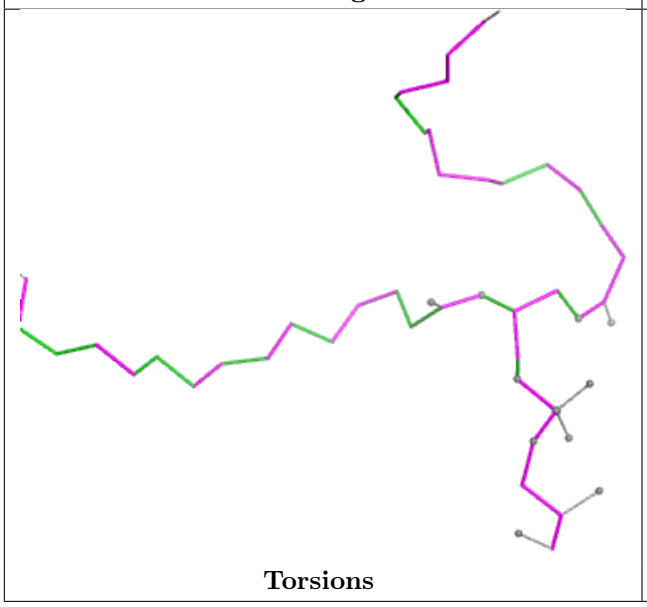


Bond angles



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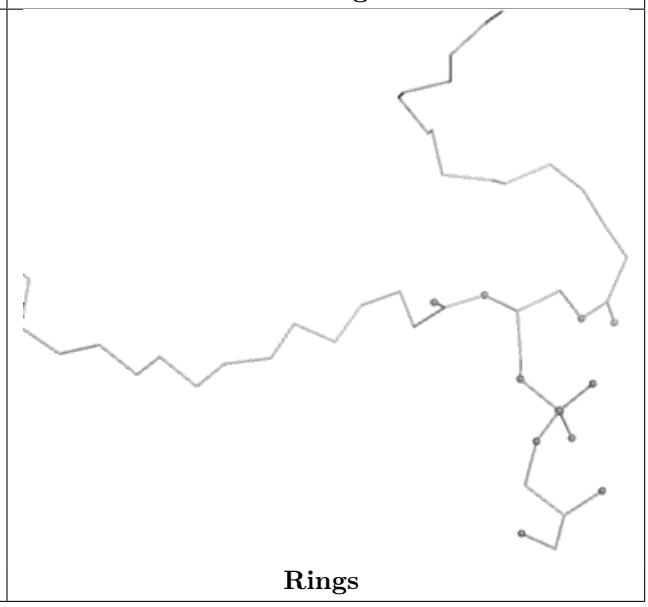
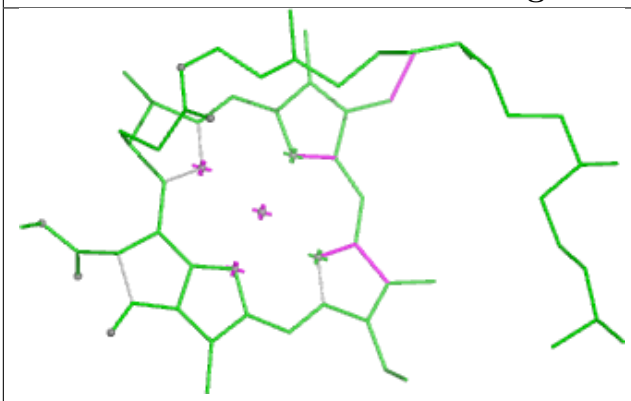


Rings

Ligand CLA n 610



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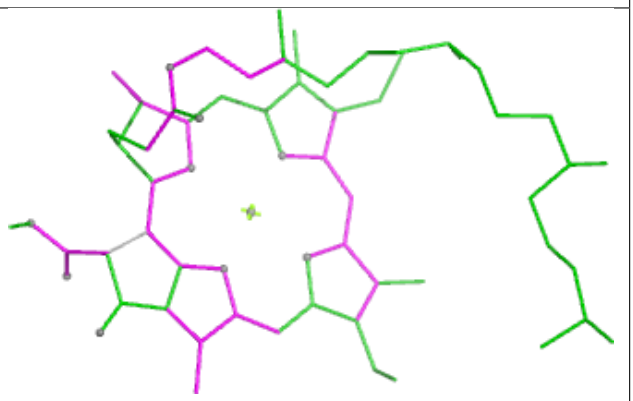
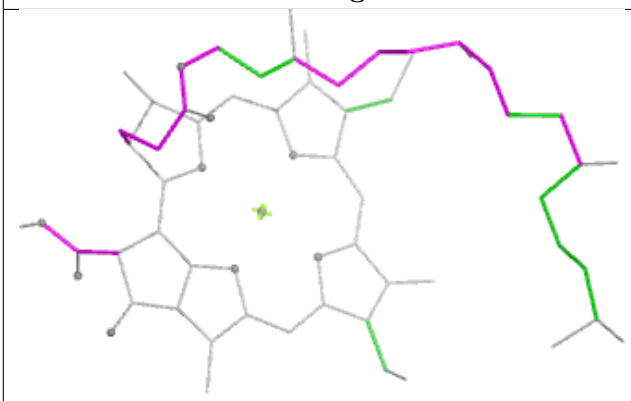


Bond angles

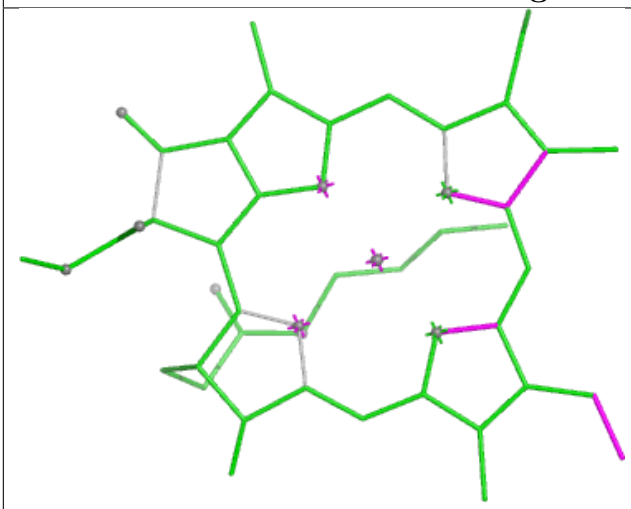


Torsions



Rings

Ligand CLA s 613



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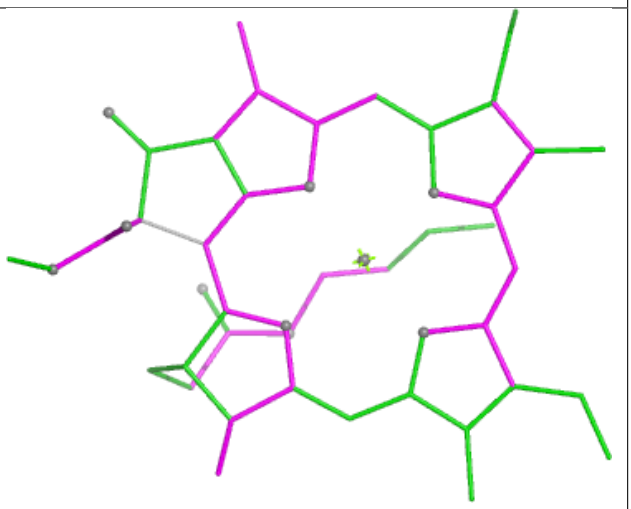
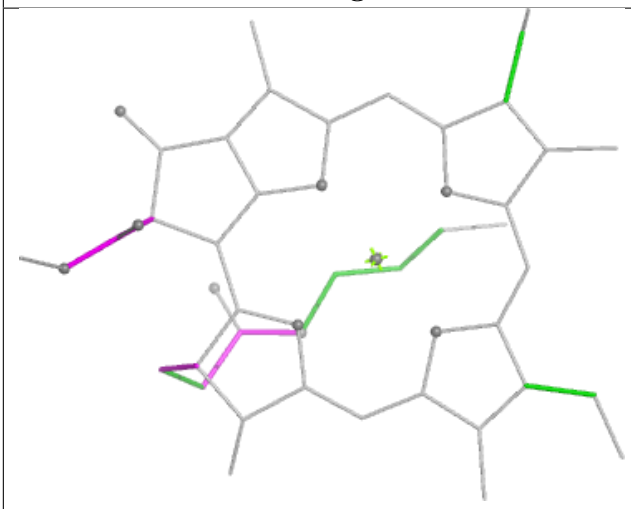


Bond angles



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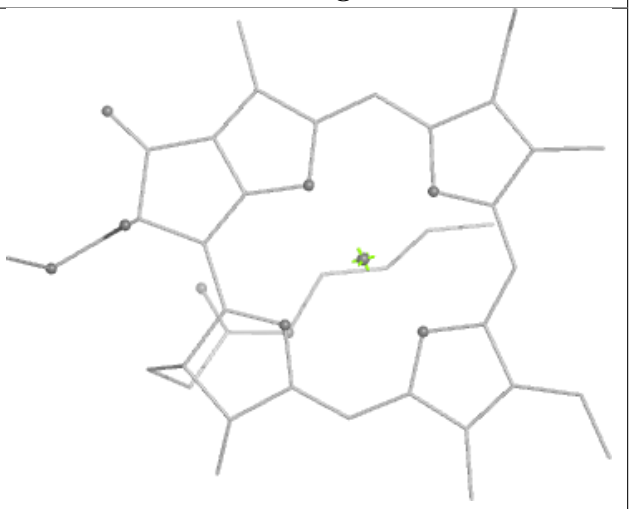
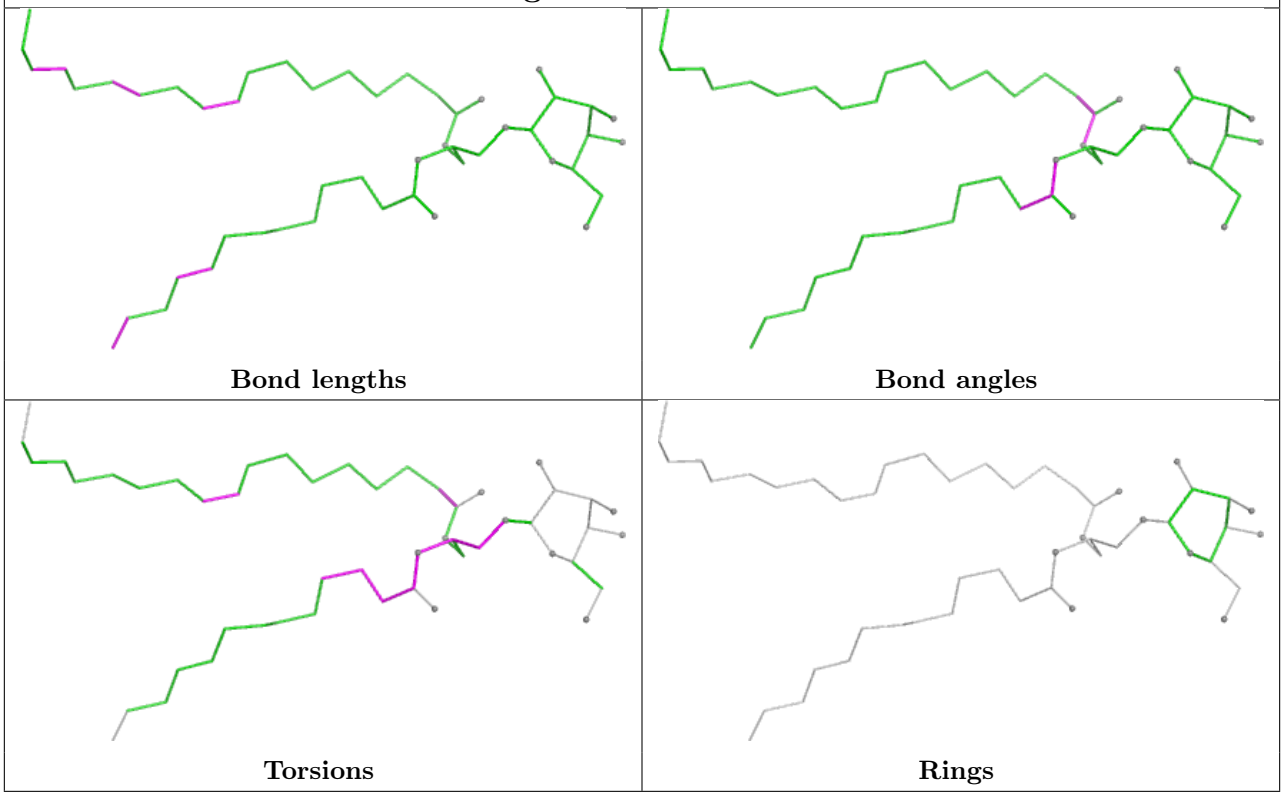
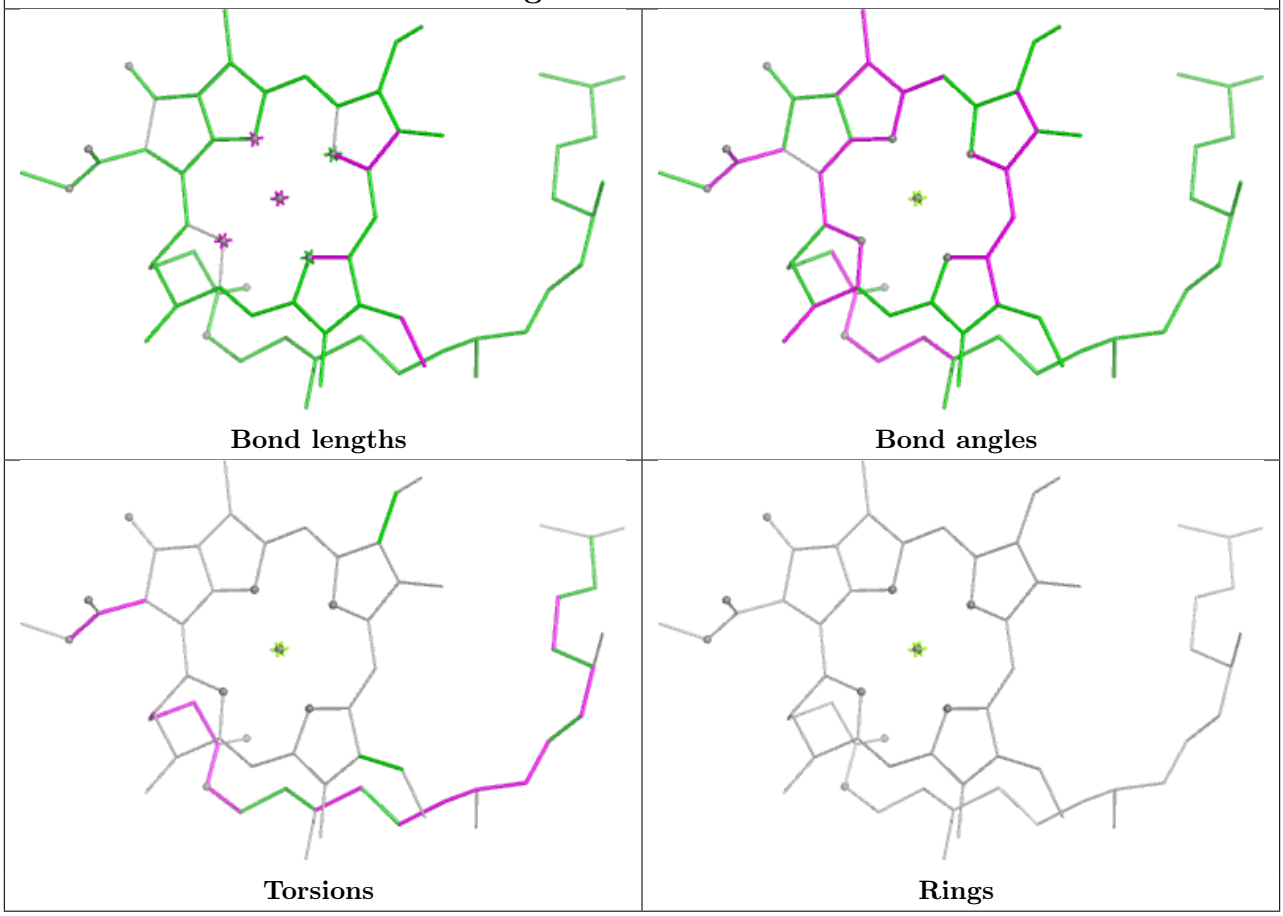


Rings

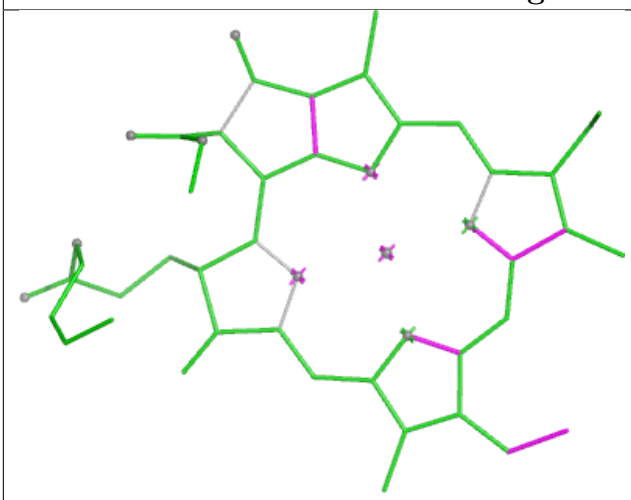
Ligand LMG b 623



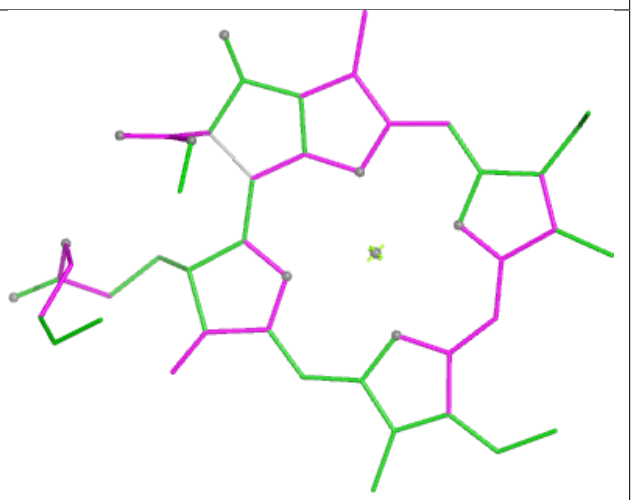
Ligand CLA N 610



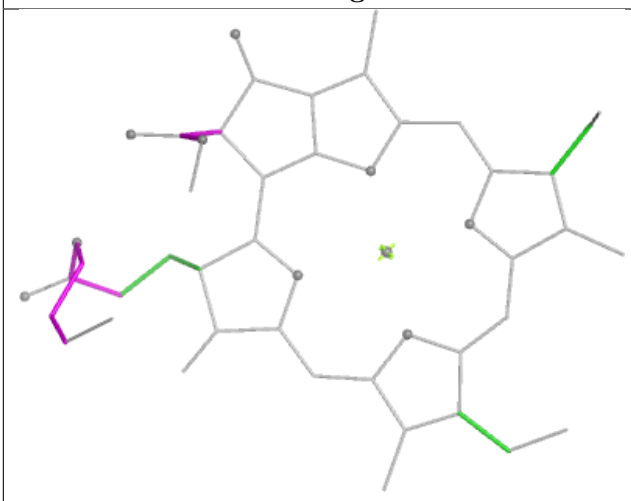
Ligand CLA S 312



Bond lengths



Bond angles



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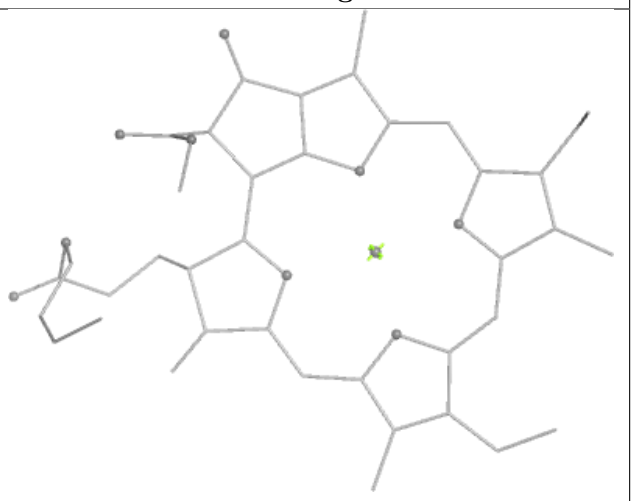
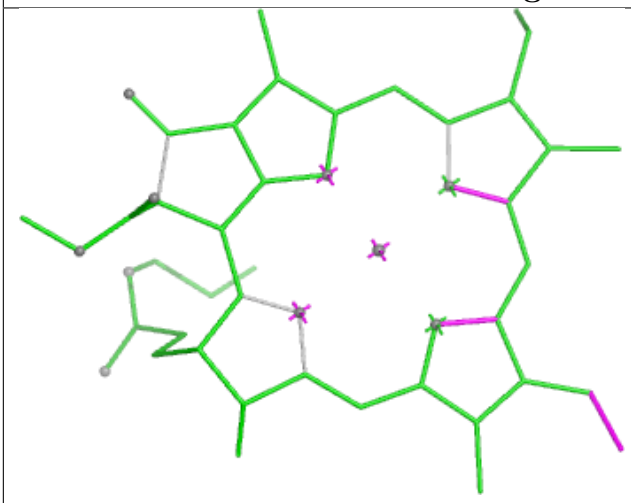


Rings

Ligand CLA Y 614



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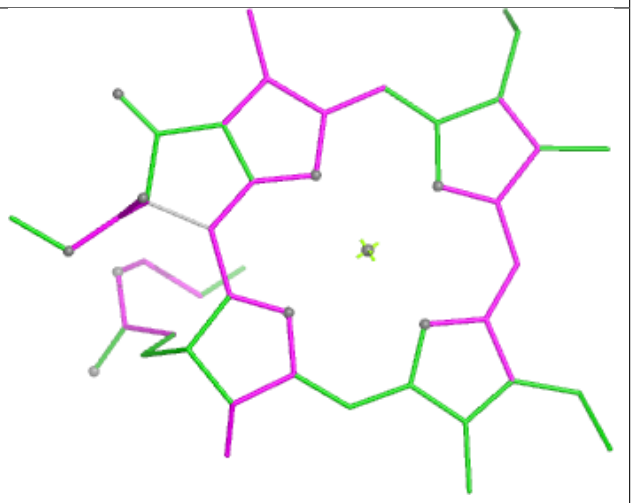
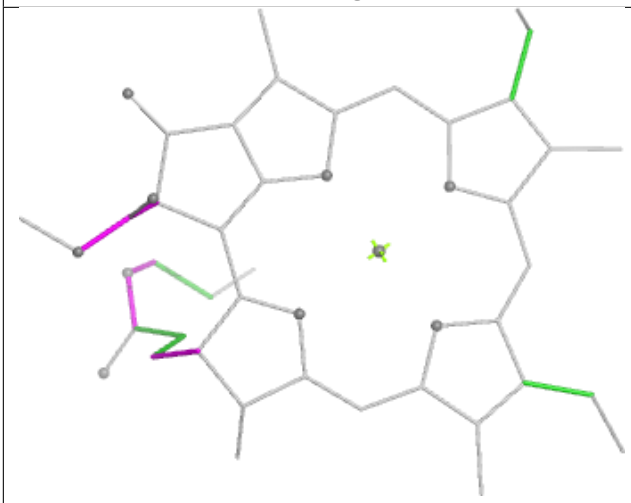


Bond angles



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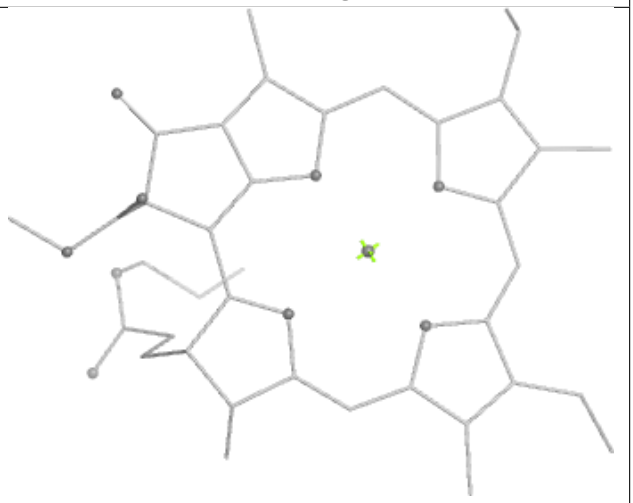
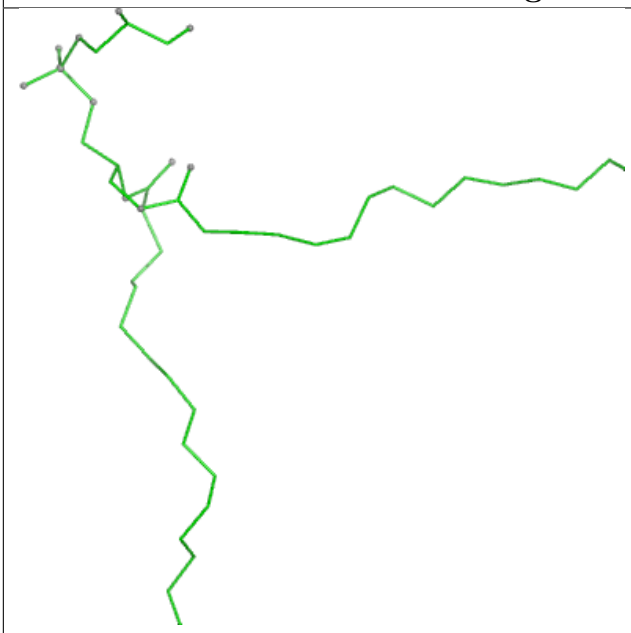


Rings

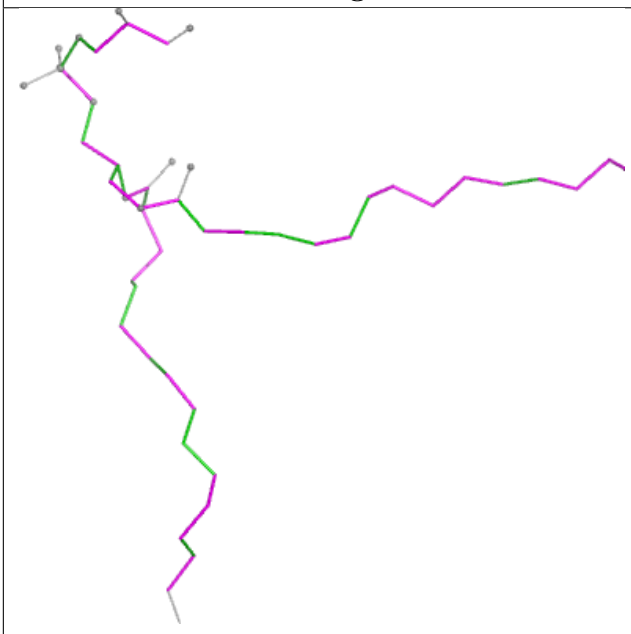
Ligand LHG L 102



Bond lengths



Bond angles

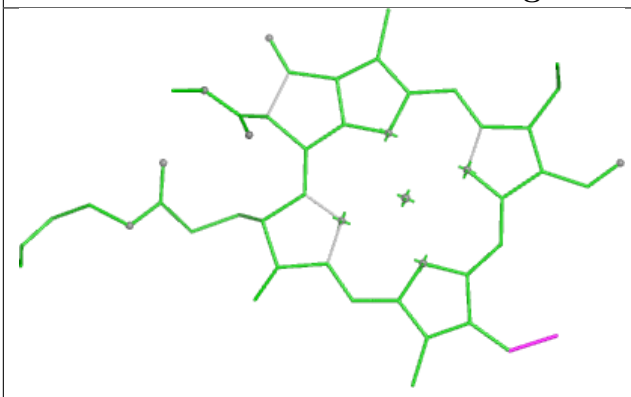


Torsions

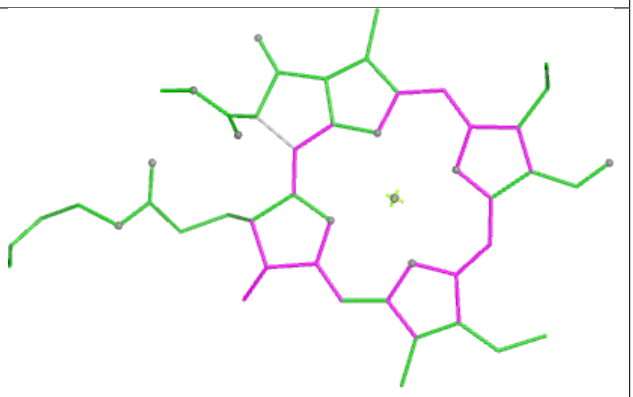


Rings

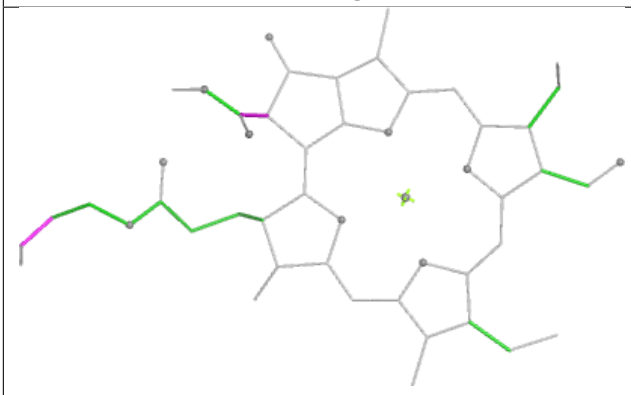
Ligand CHL Y 606



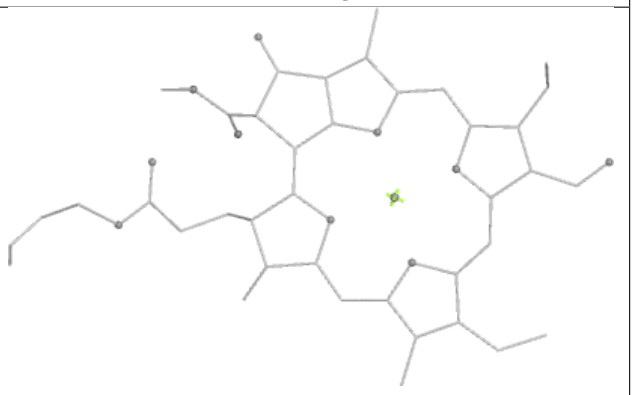
Bond lengths



Bond angles

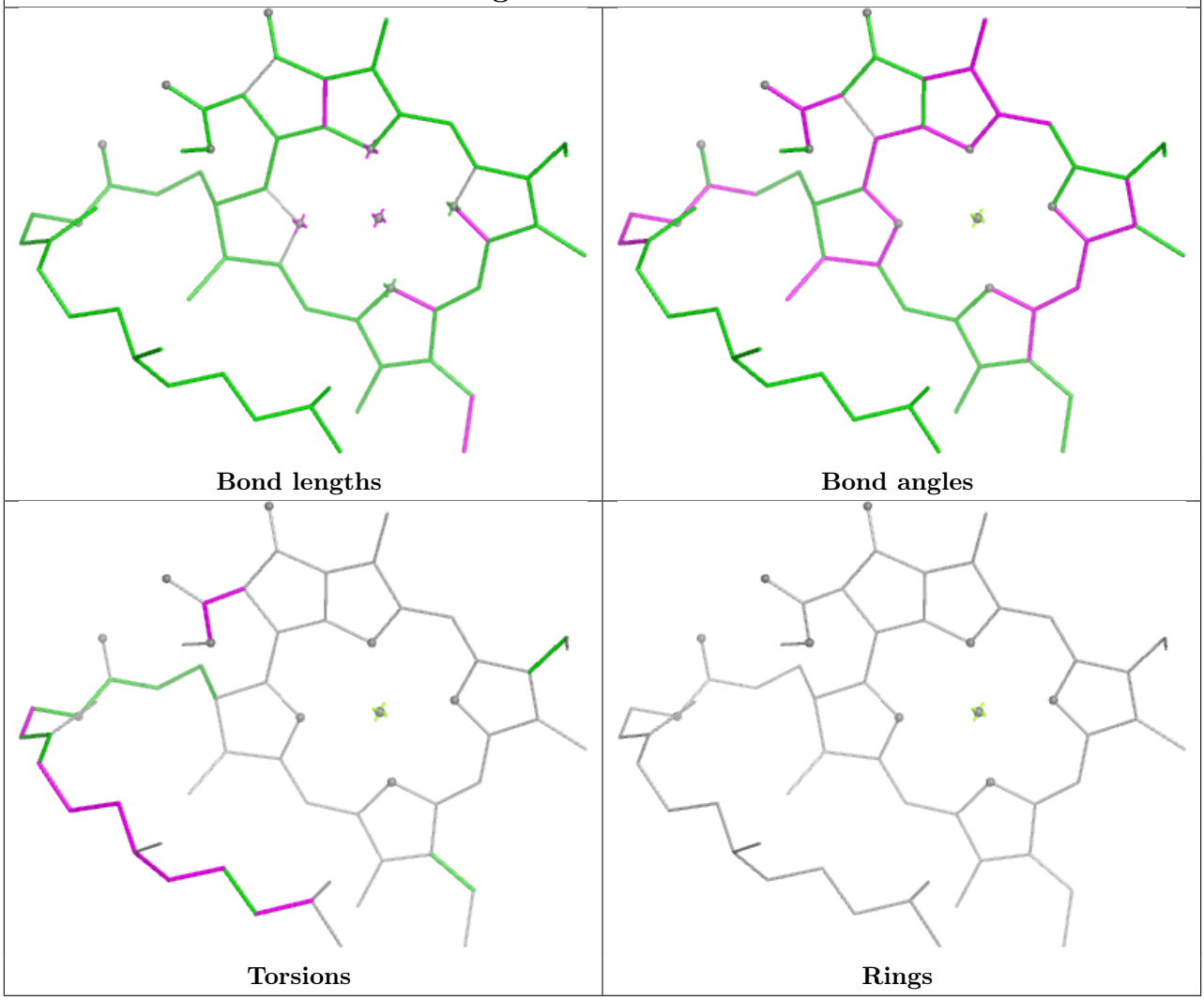


Torsions

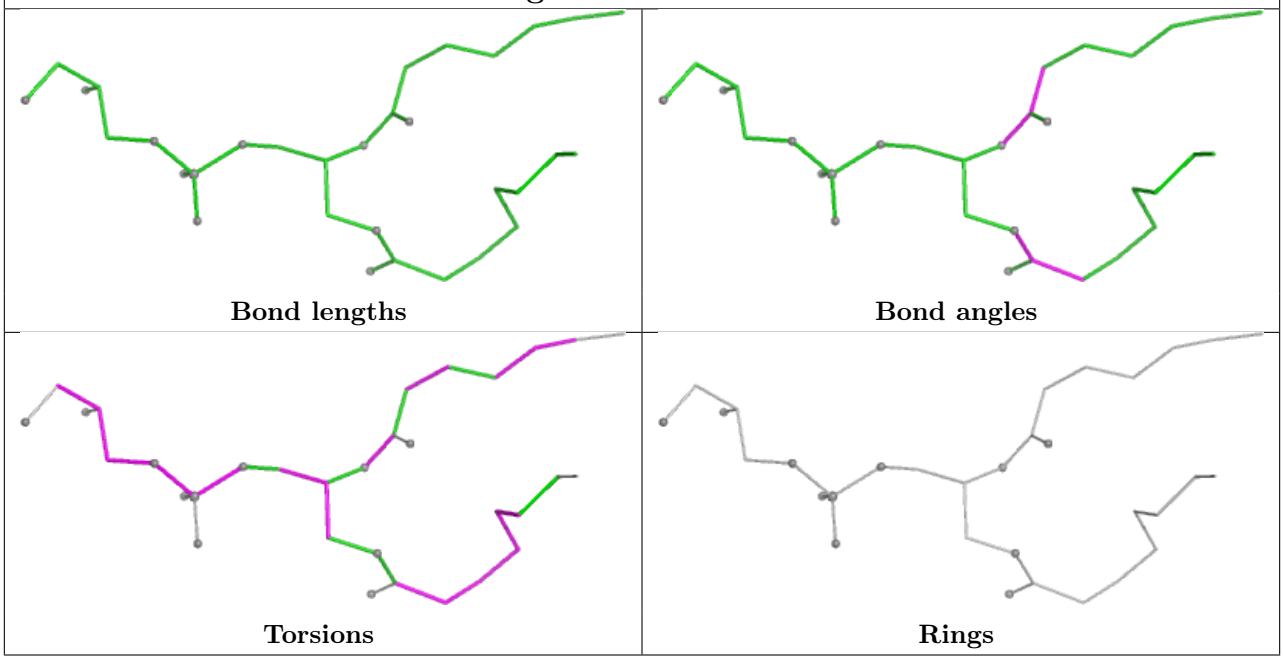


Rings

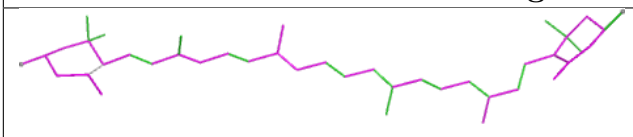
Ligand CLA R 603



Ligand LHG n 618



Ligand LUT S 316



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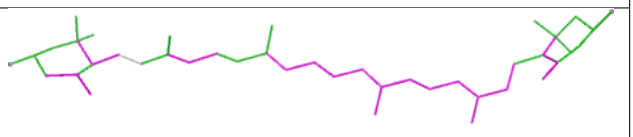
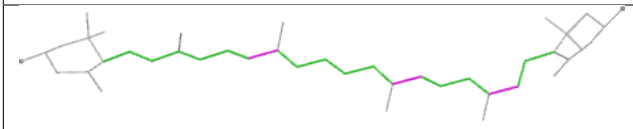


Bond angles



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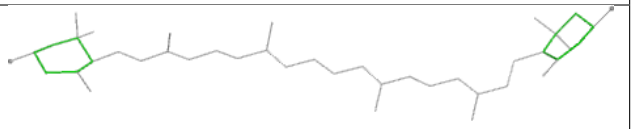
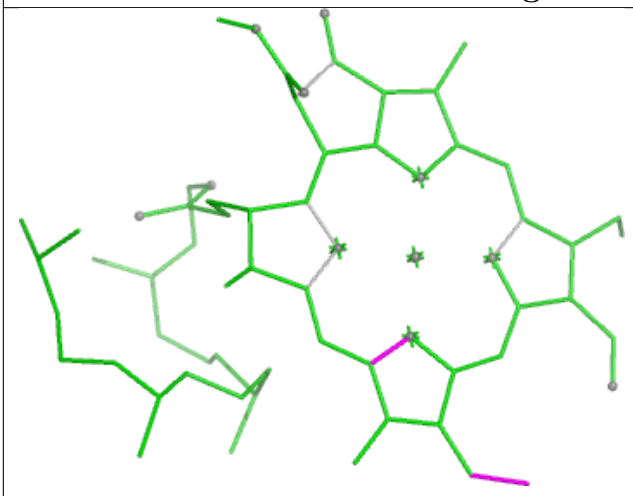


Rings

Ligand CHL N 608



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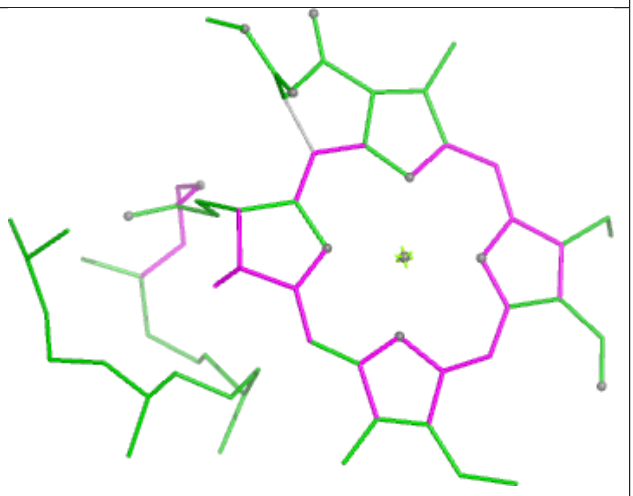
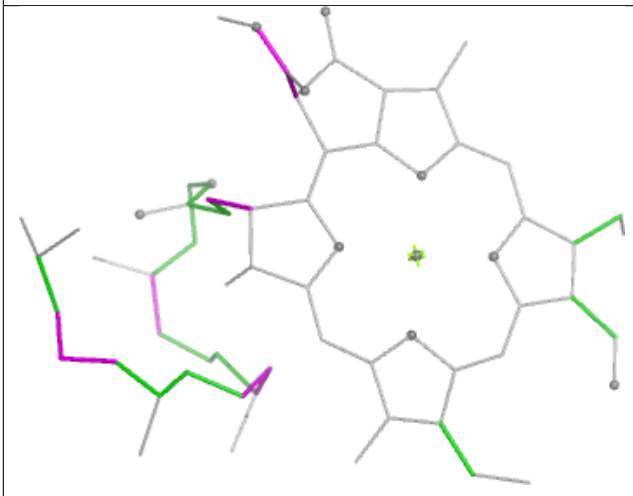


Bond angles



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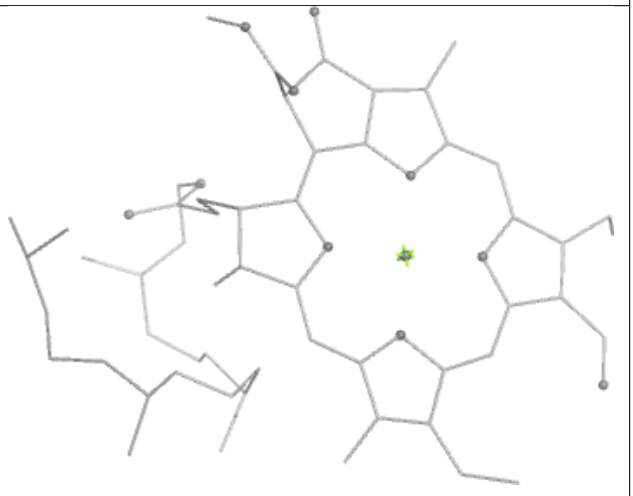
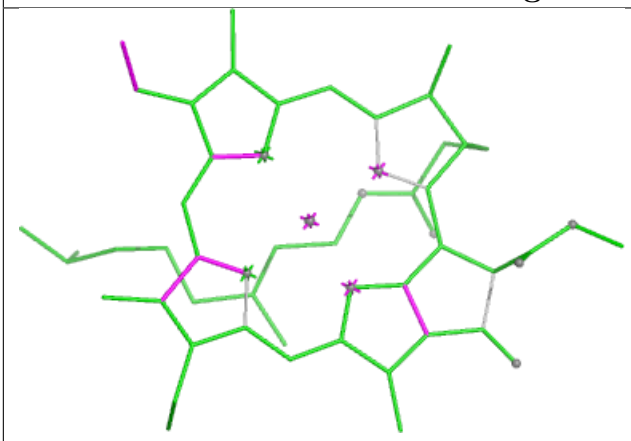


Rings

Ligand CLA R 612



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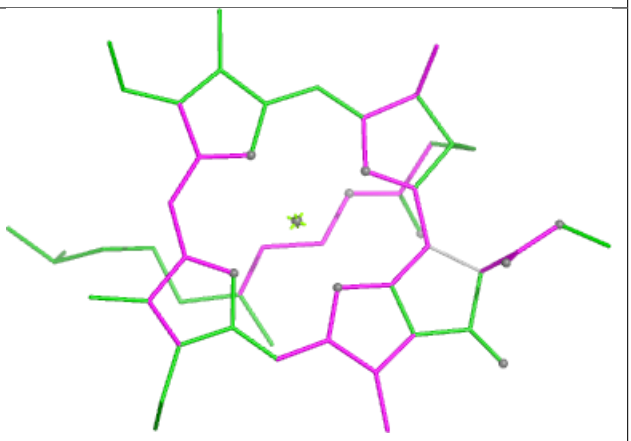
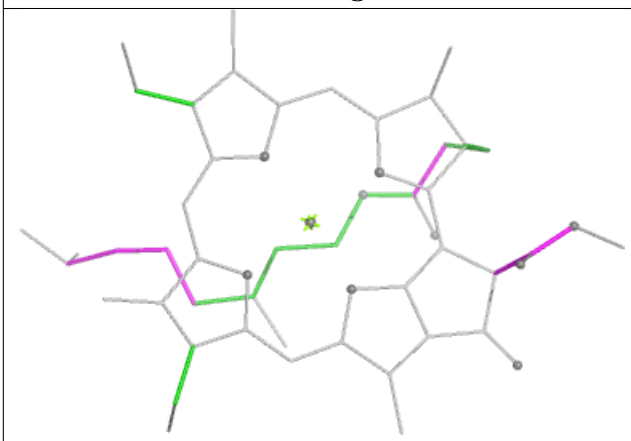


Bond angles



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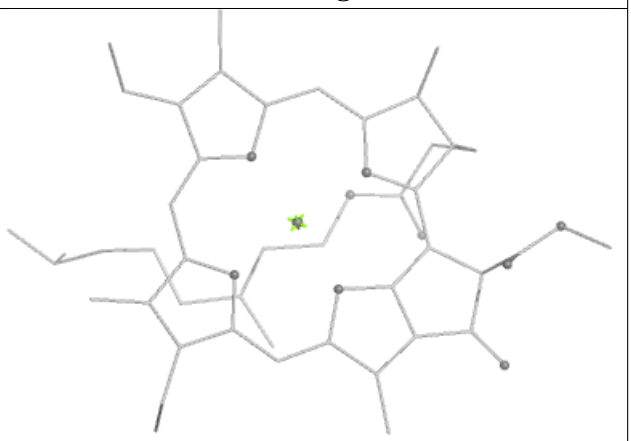
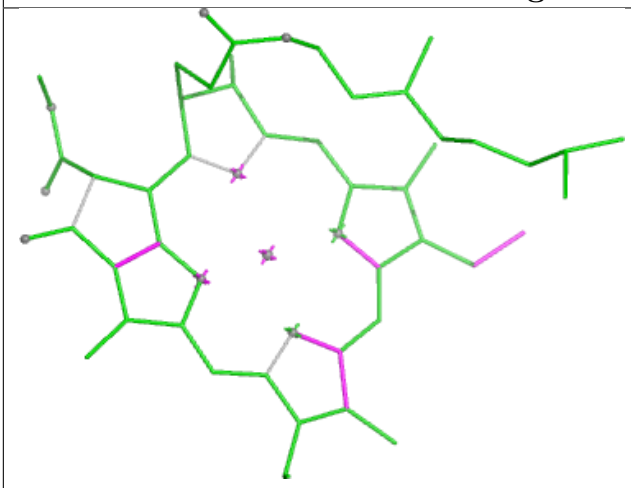


Rings

Ligand CLA S 310



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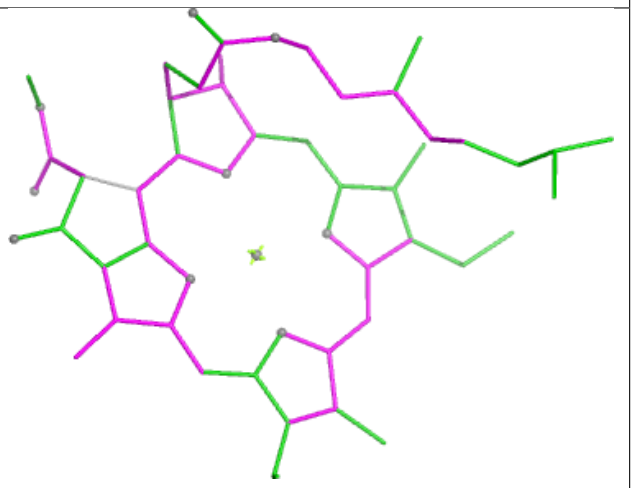

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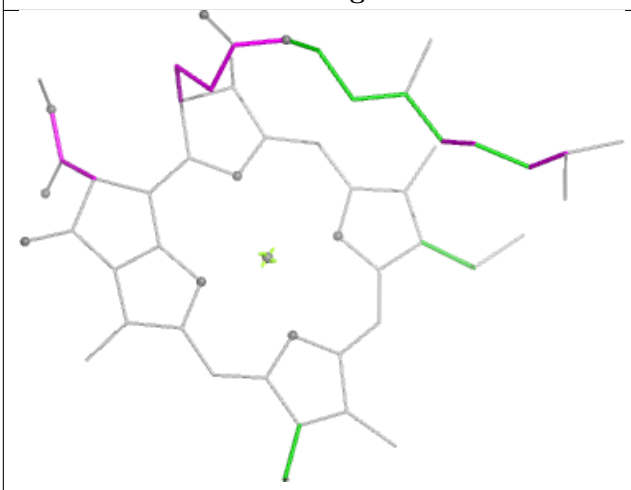

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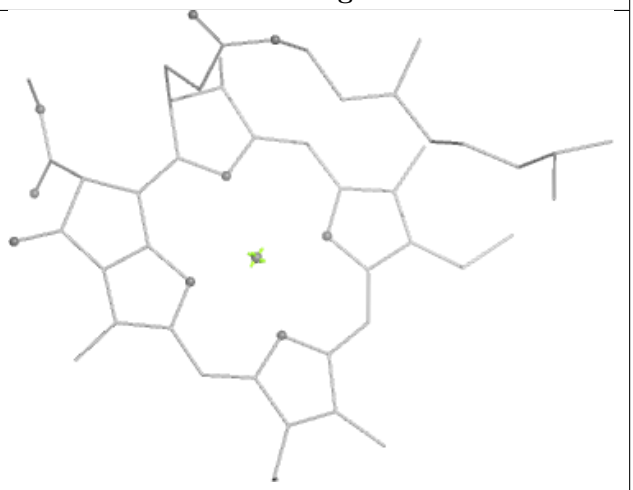
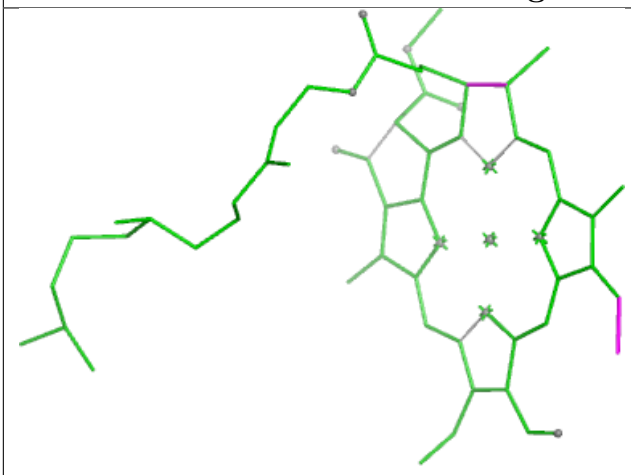


Rings

Ligand CHL g 609



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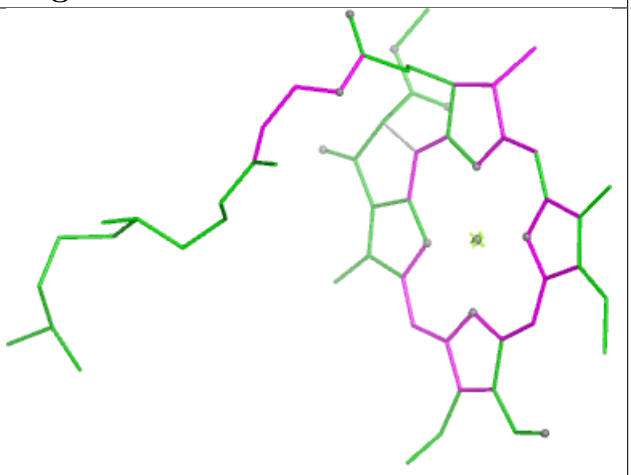
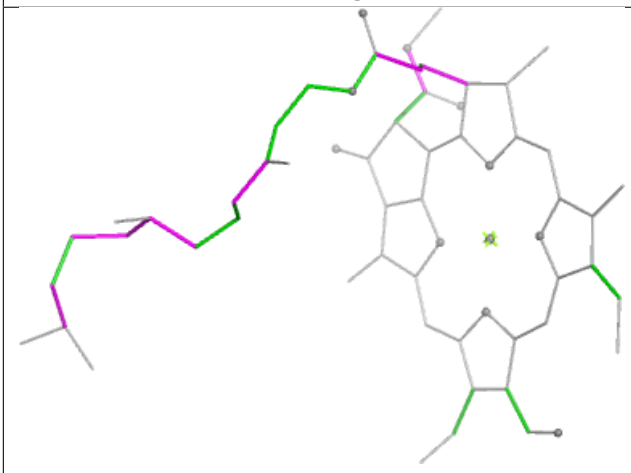


Bond angles

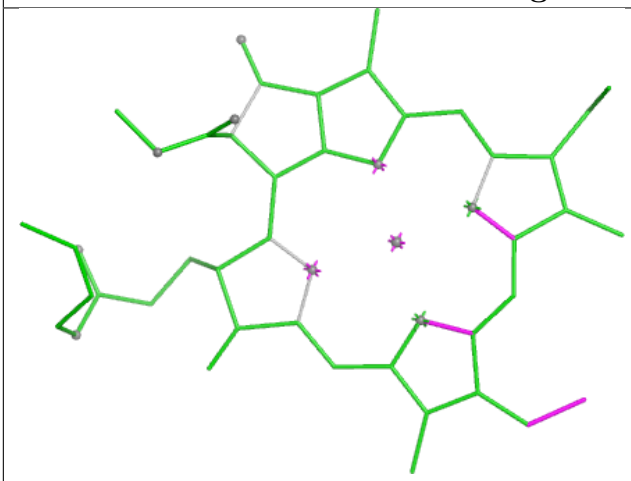


Torsions



Rings

Ligand CLA r 611



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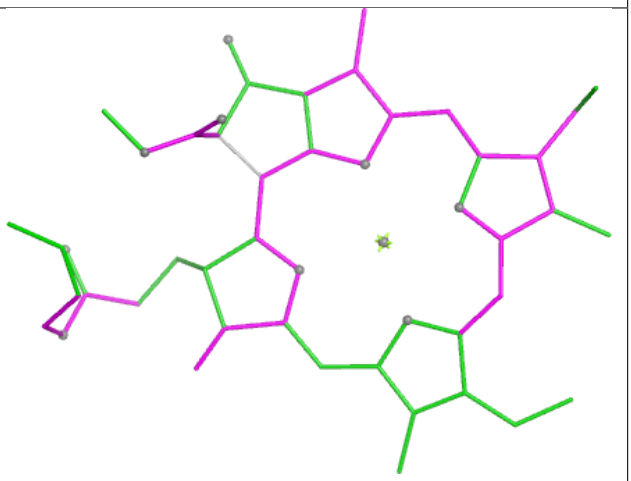

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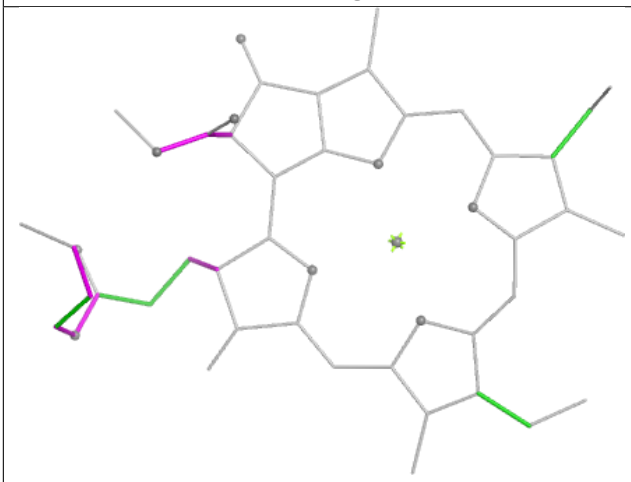
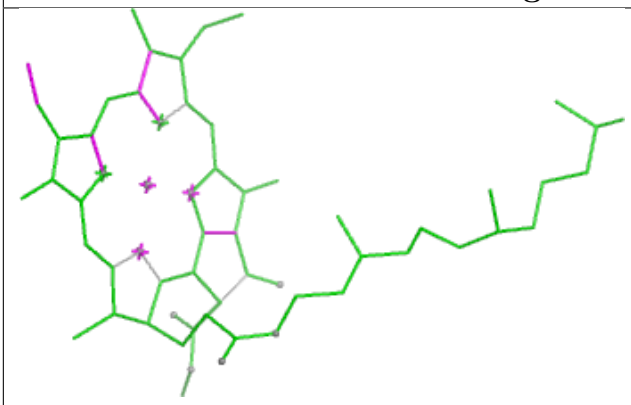


Torsions



Rings

Ligand CLA N 611



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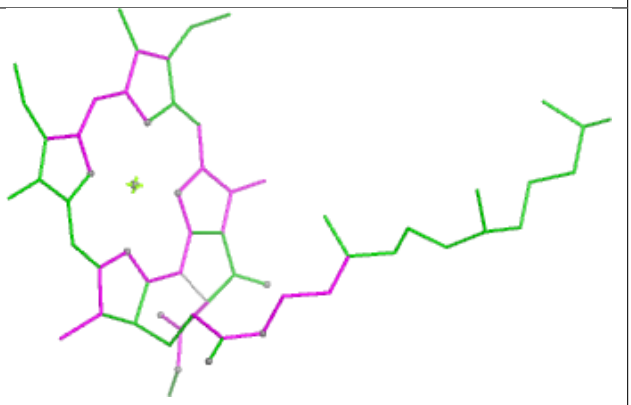

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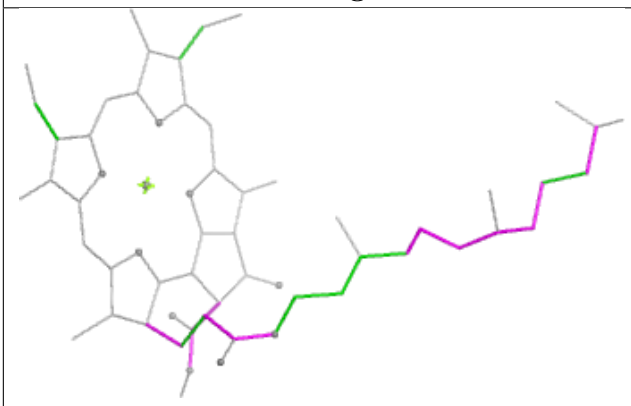

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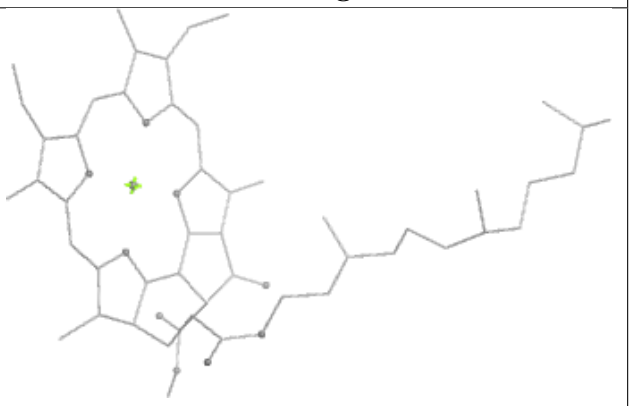
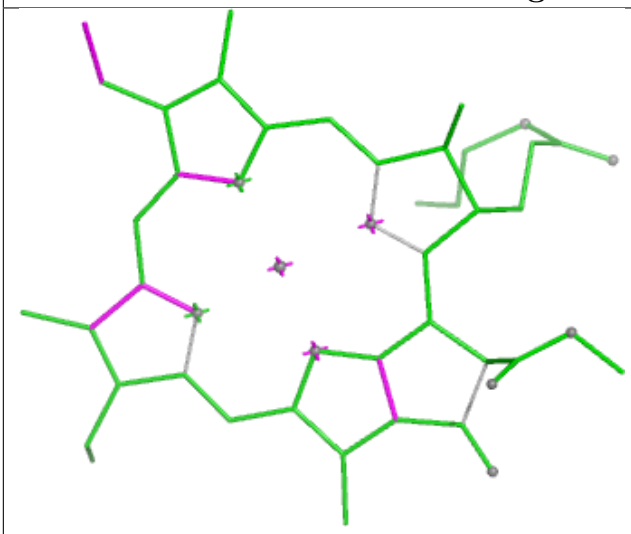


Rings

Ligand CLA y 314



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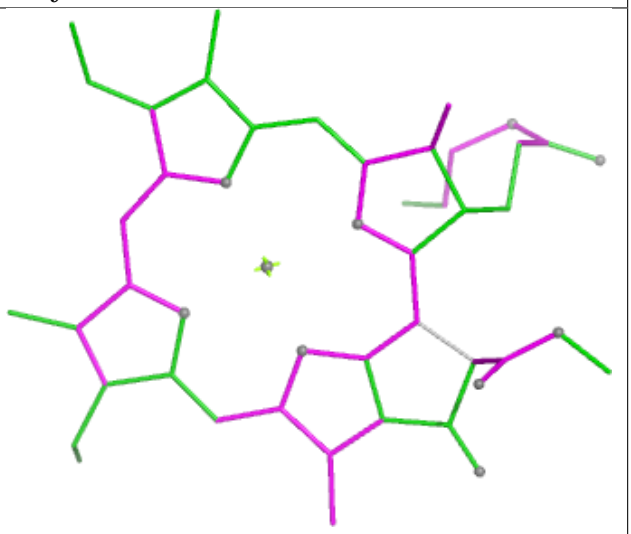

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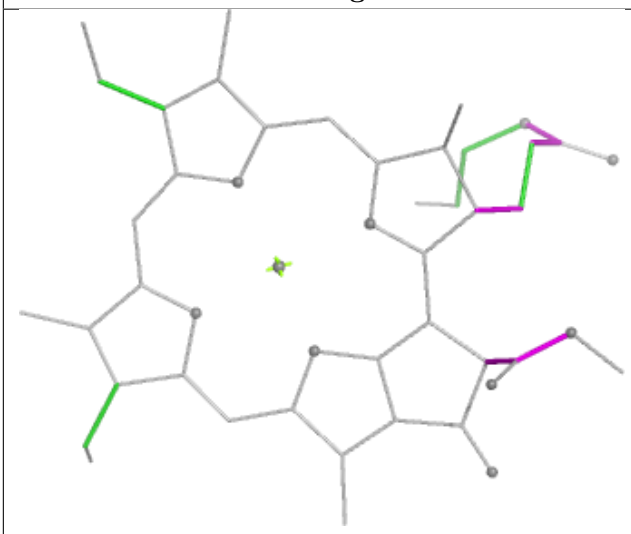

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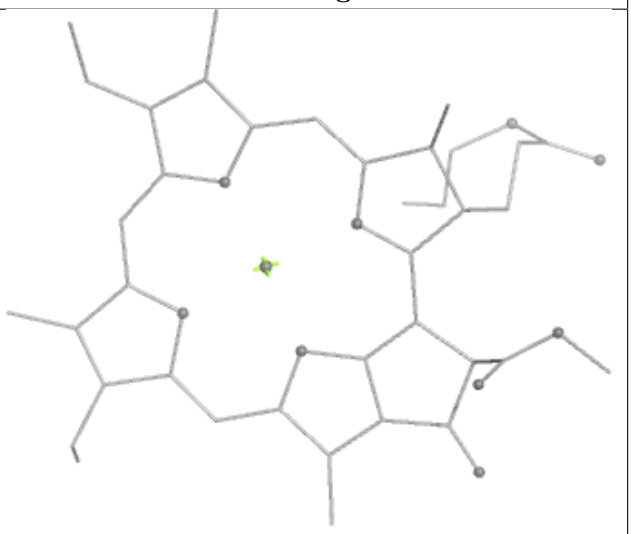
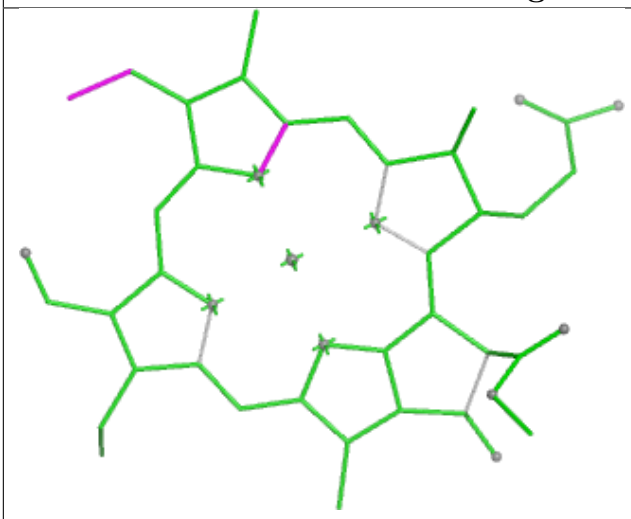


Rings

Ligand CHL g 605



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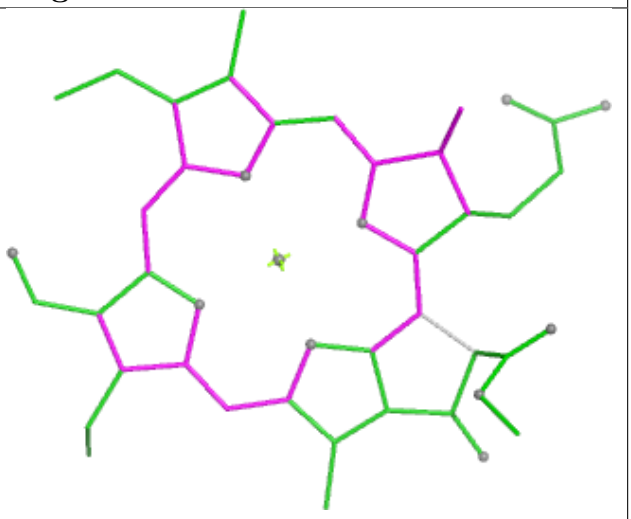

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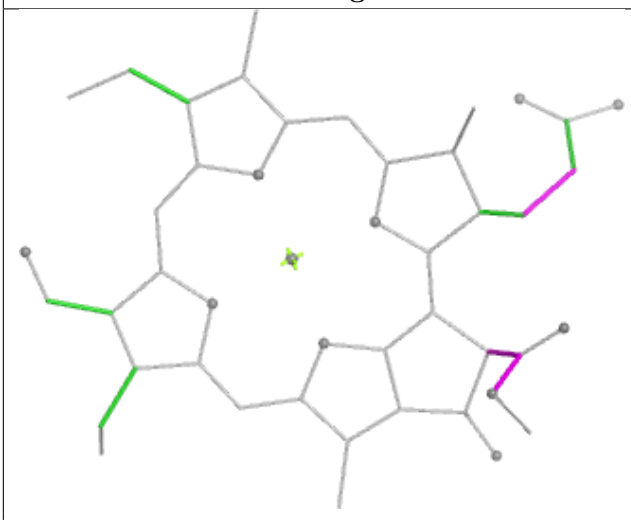

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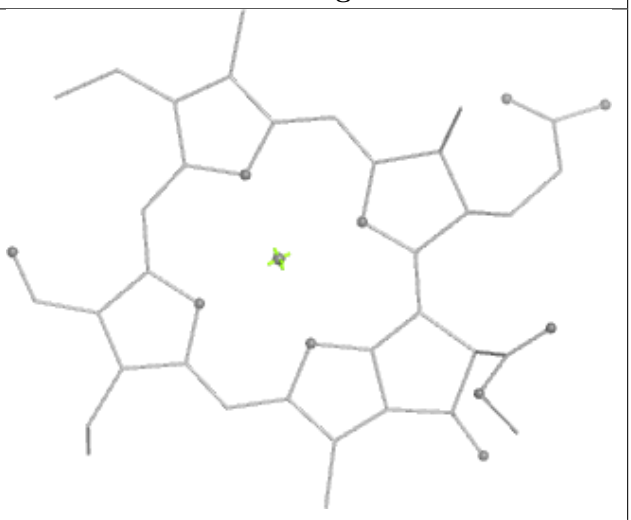
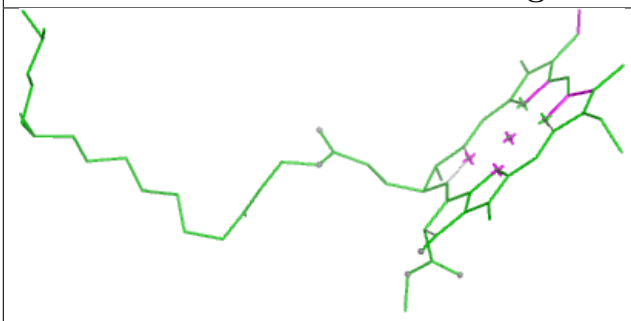


Rings

Ligand CLA d 404



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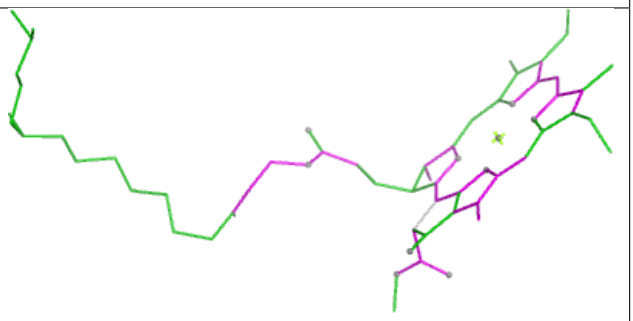
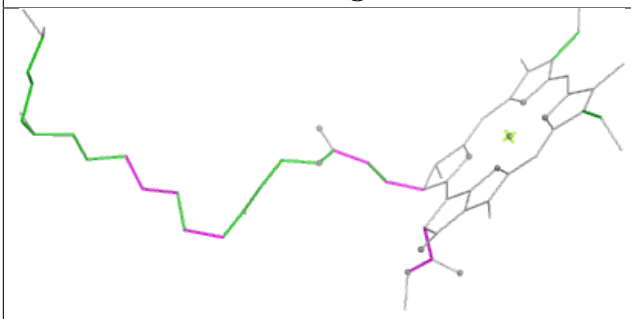


Bond angles



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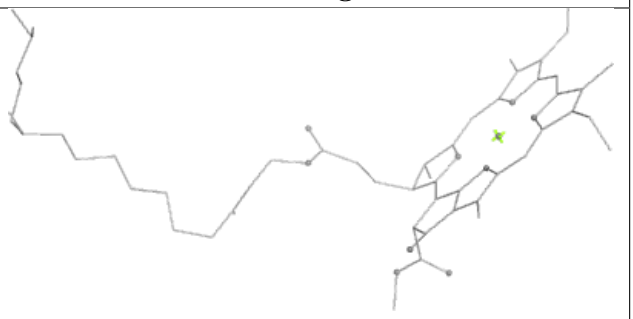
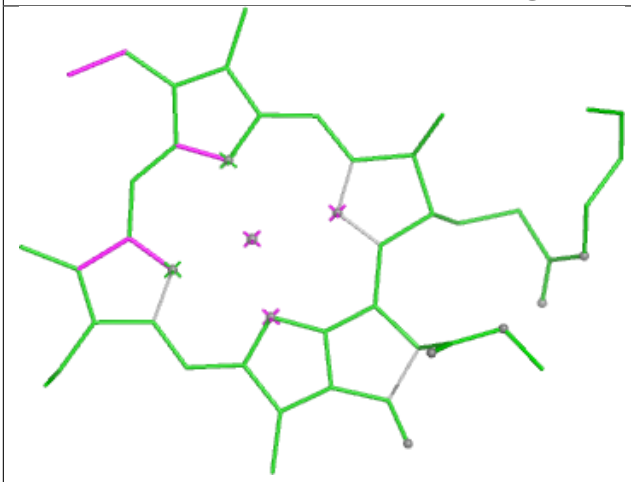


Rings

Ligand CLA R 611



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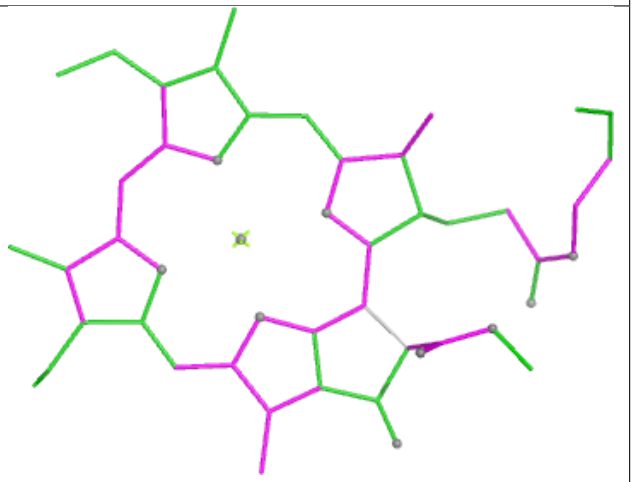
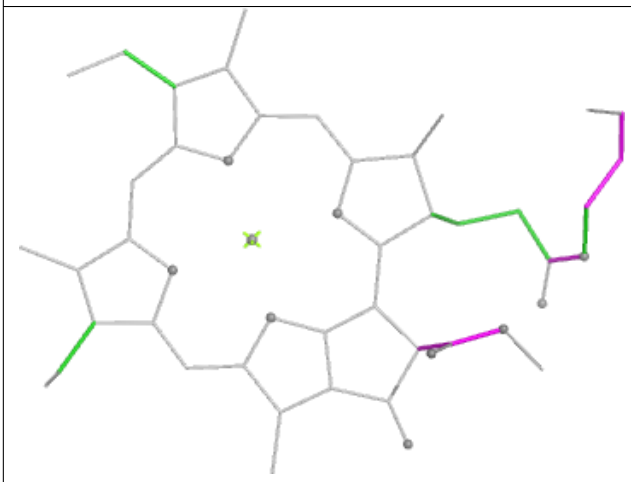


Bond angles



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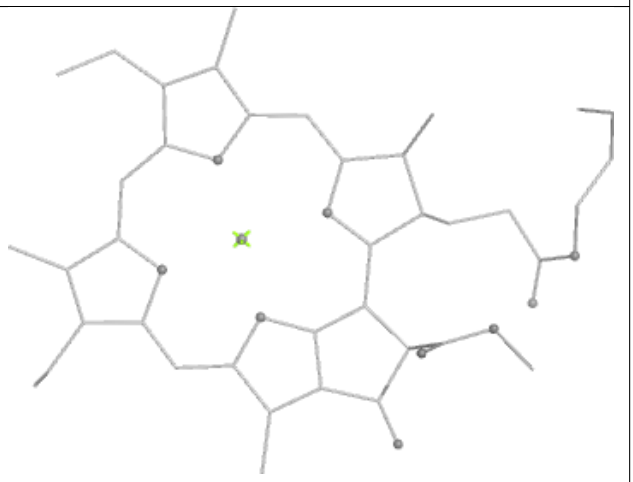
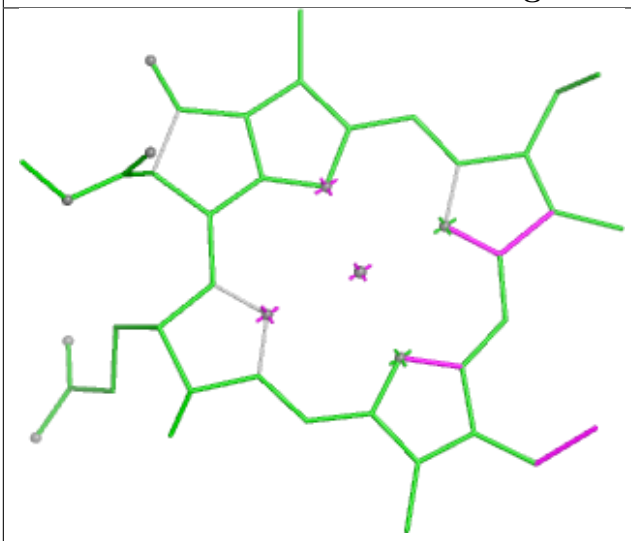


Rings

Ligand CLA R 601



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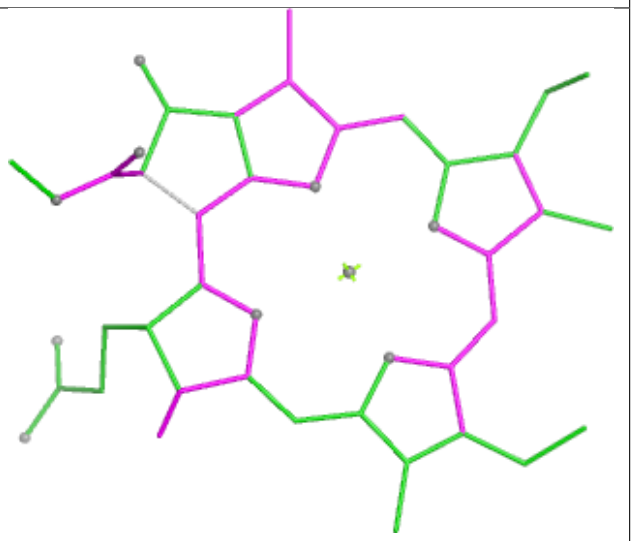
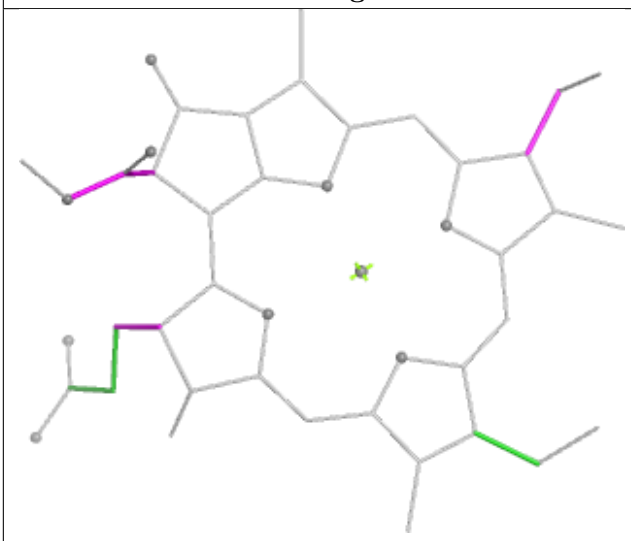


Bond angles



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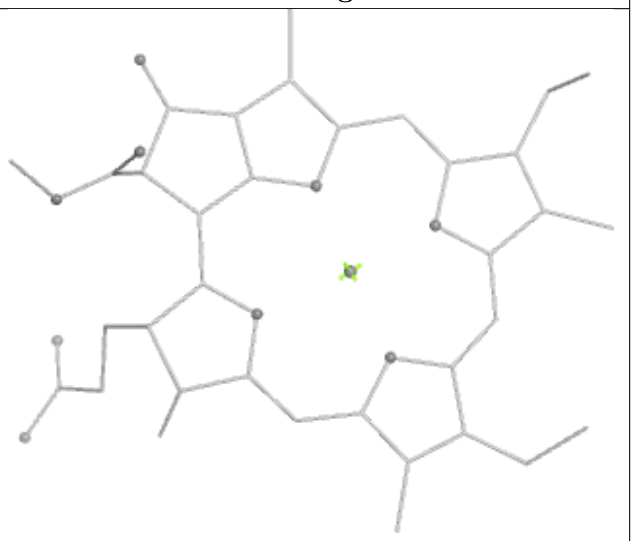
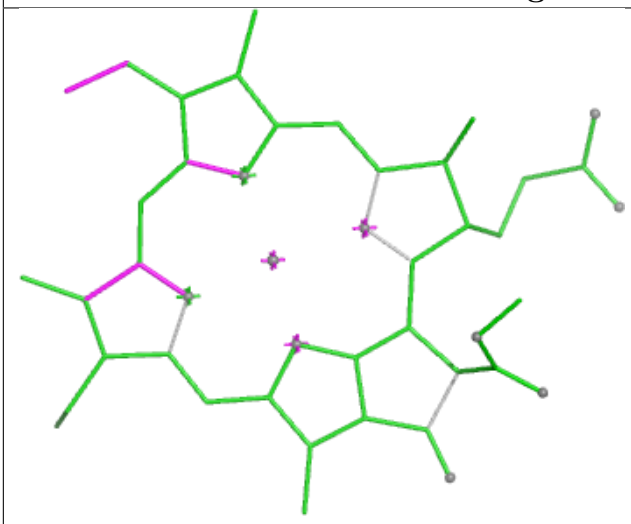
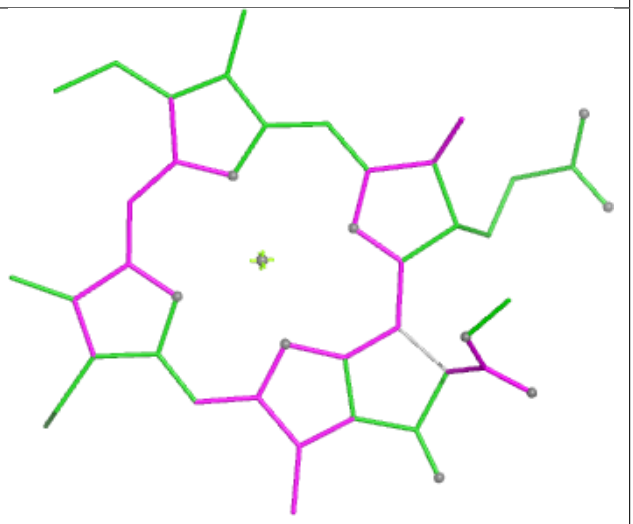


Rings

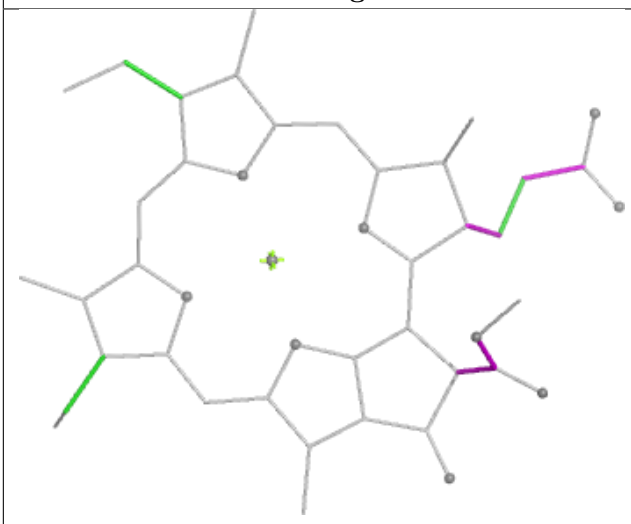
Ligand CLA S 304



Bond lengths



Bond angles



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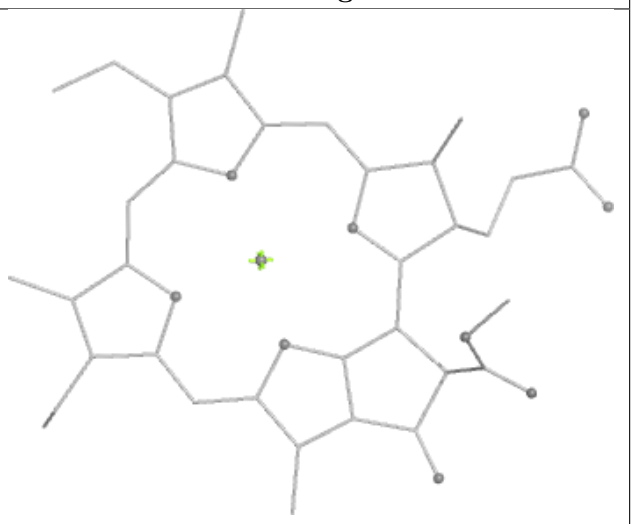
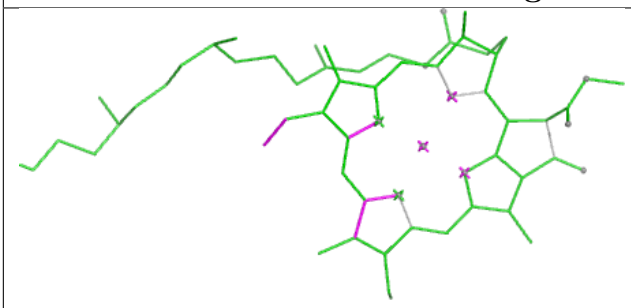
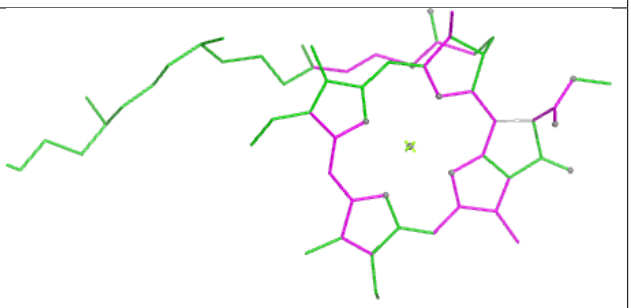


Rings

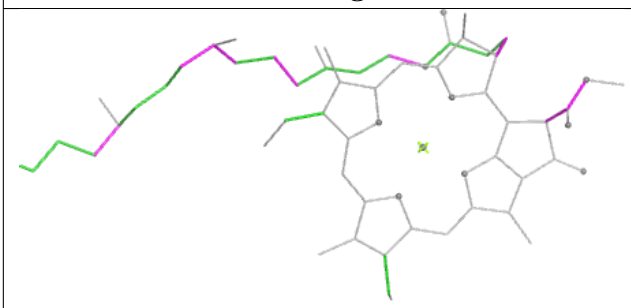
Ligand CLA C 501



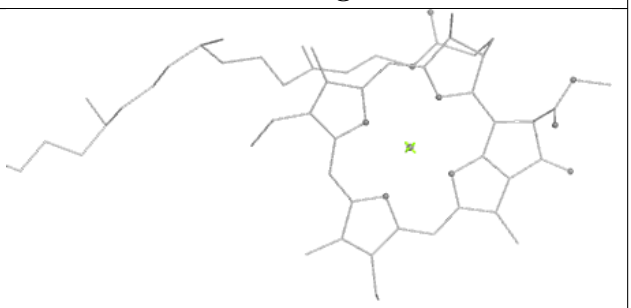
Bond lengths



Bond angles

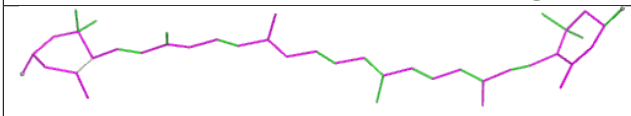


Torsions

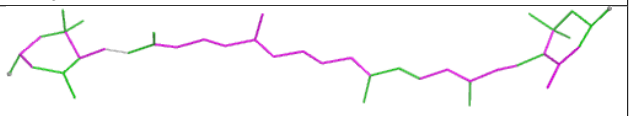


Rings

Ligand LUT y 316



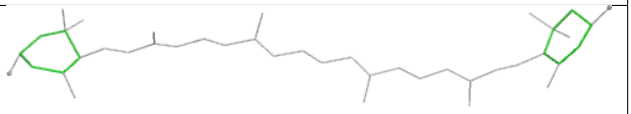
Bond lengths



Bond angles

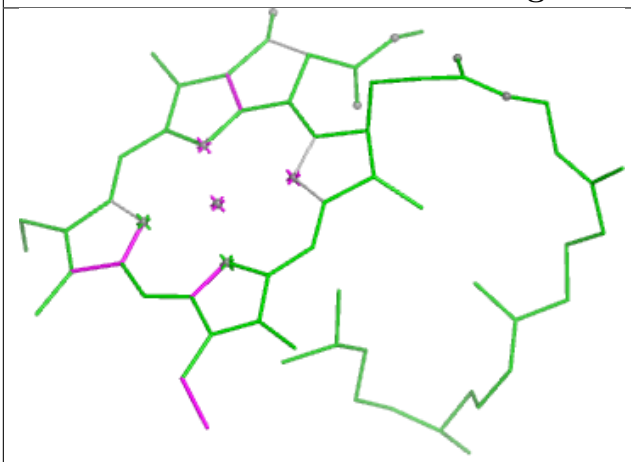


Torsions



Rings

Ligand CLA b 615



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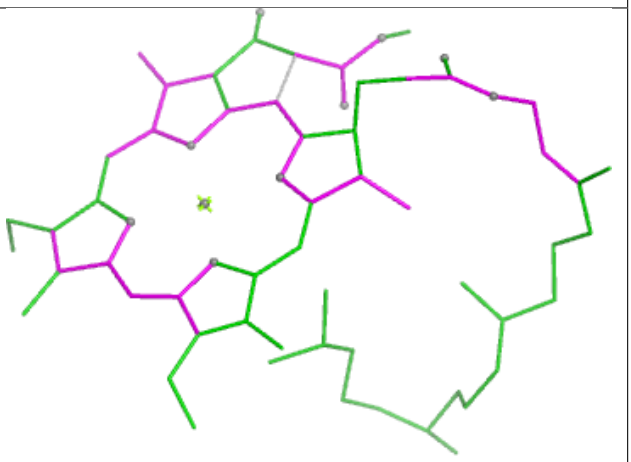
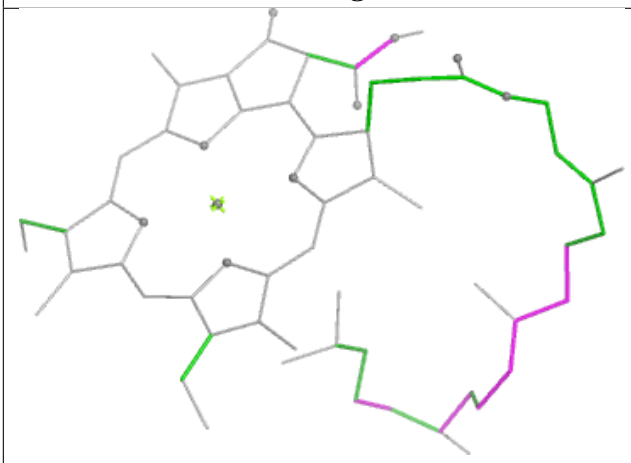


Bond angles



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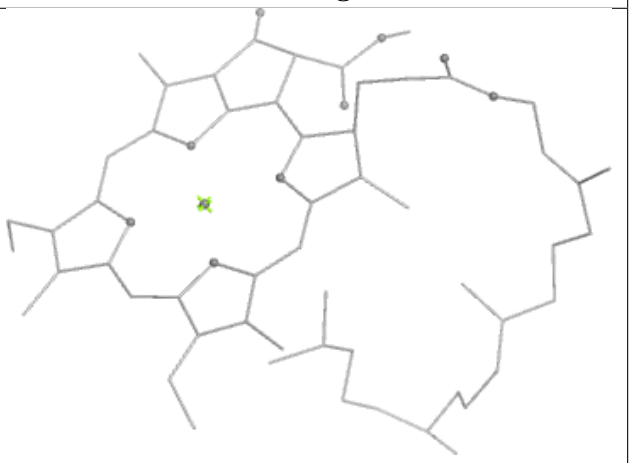
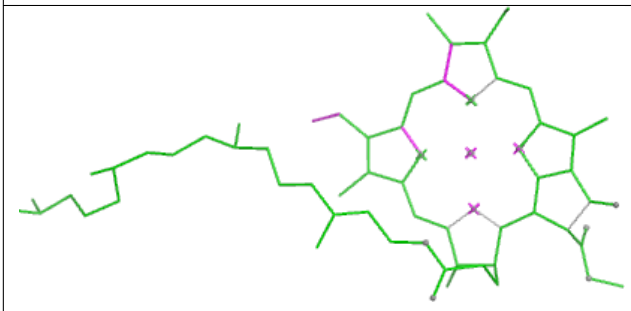


Rings

Ligand CLA B 603



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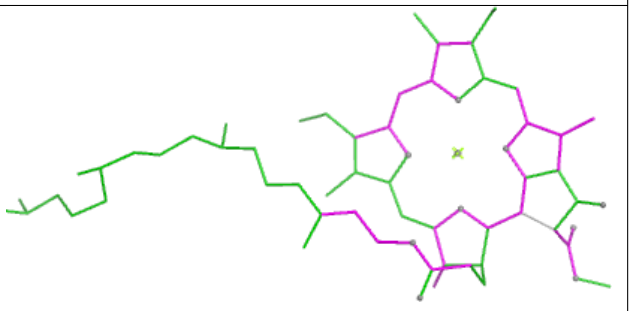
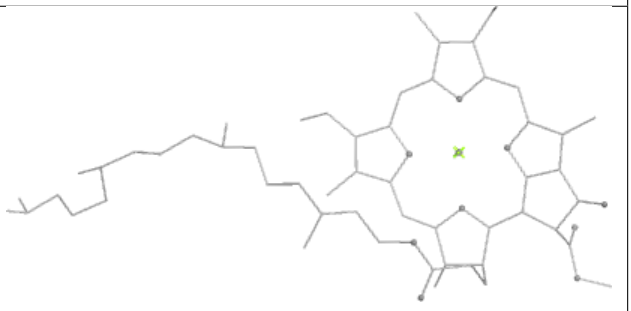


Bond angles

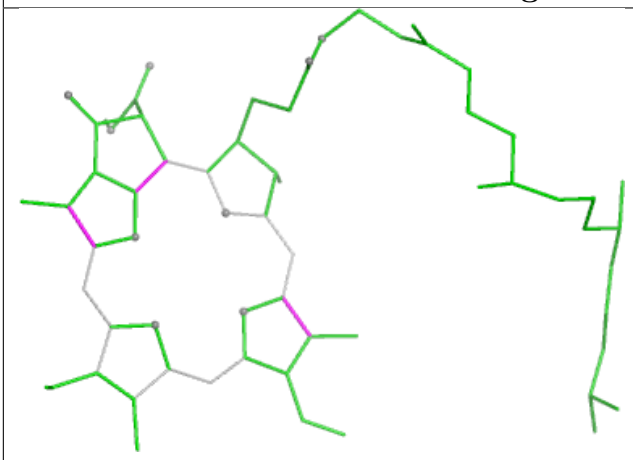


Torsions



Rings

Ligand PHO D 402



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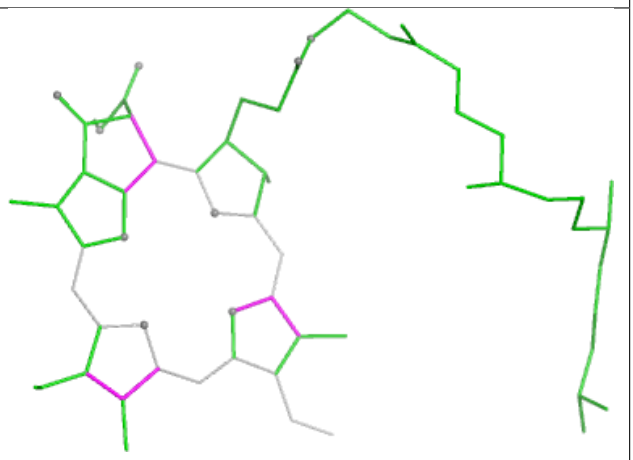
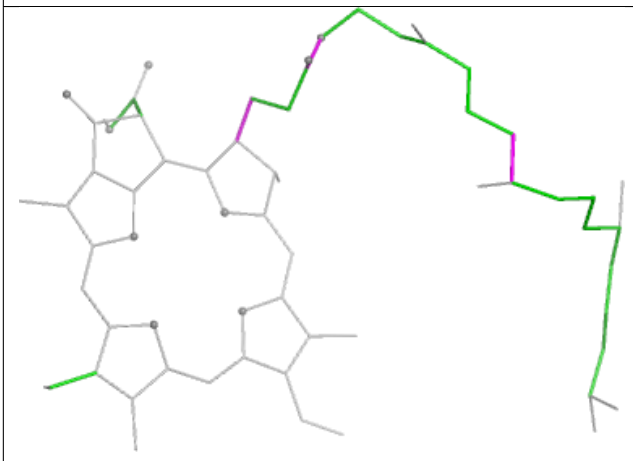


Bond angles



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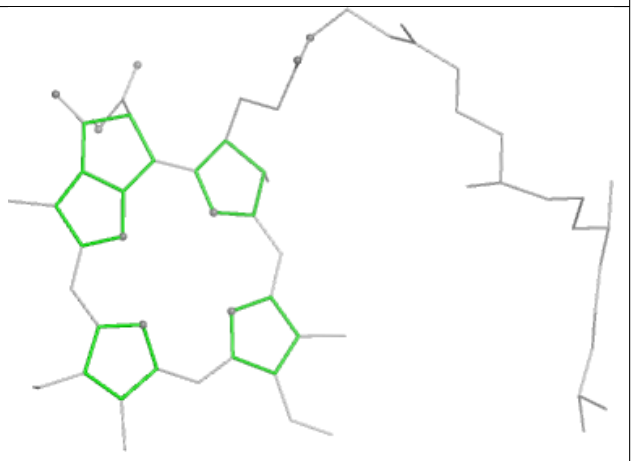
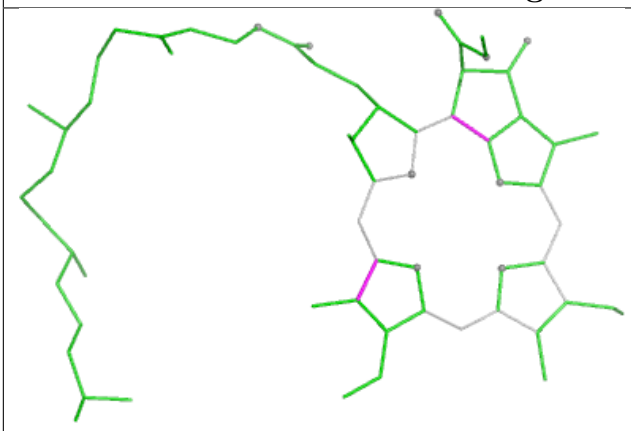


Rings

Ligand PHO a 408



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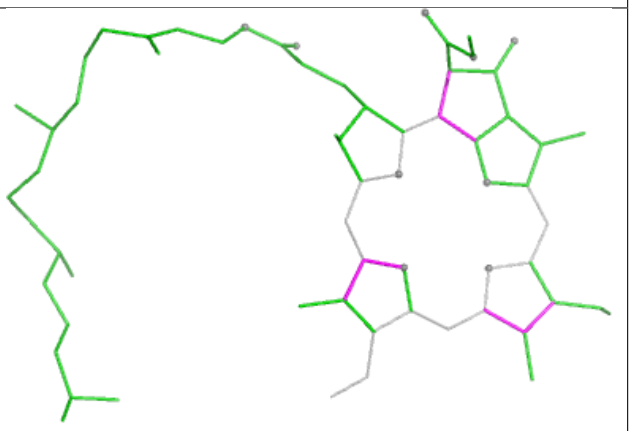
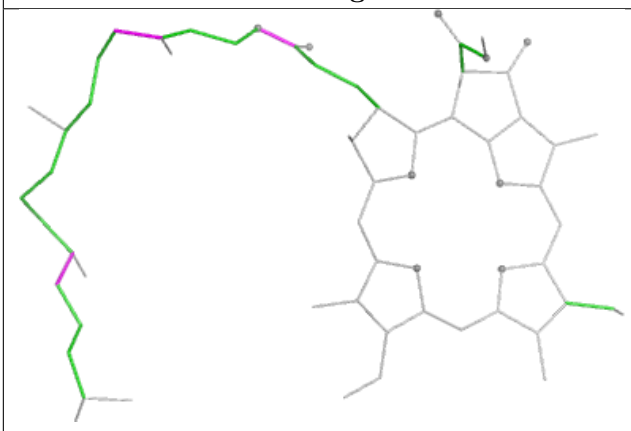


Bond angles



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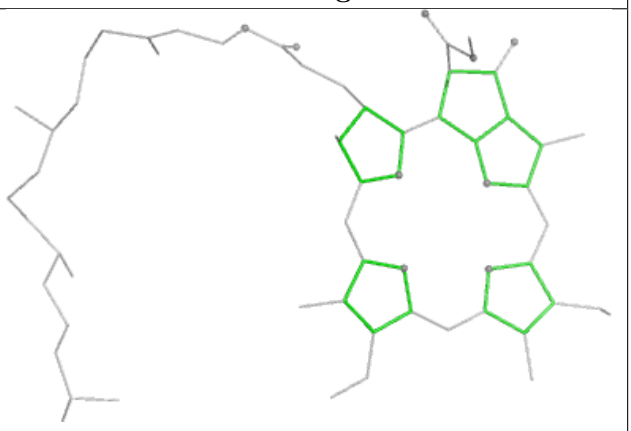
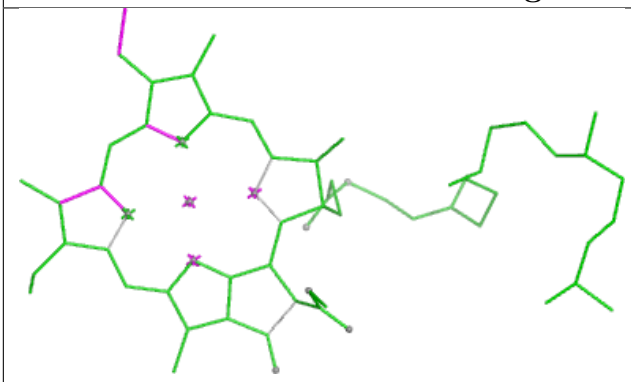


Rings

Ligand CLA B 612



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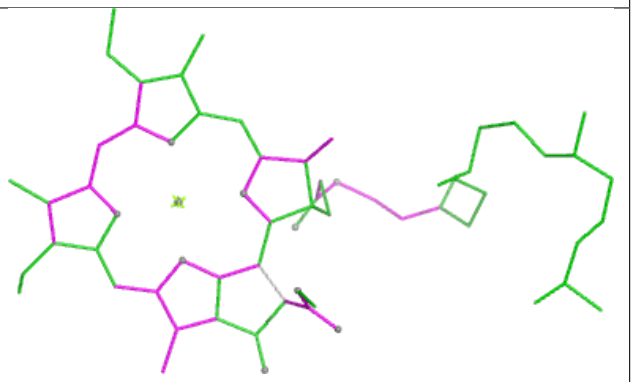
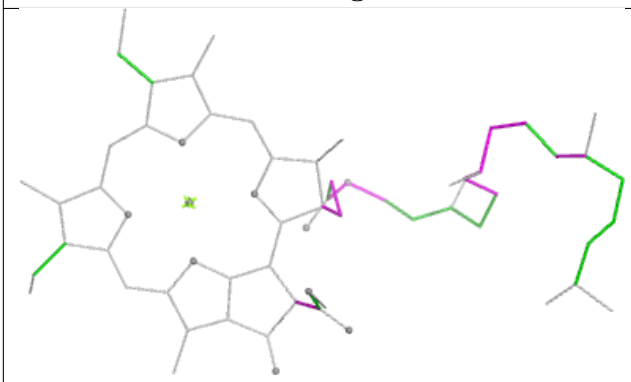


Bond angles



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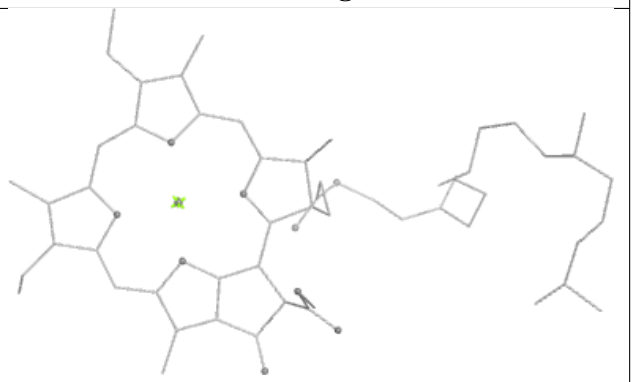
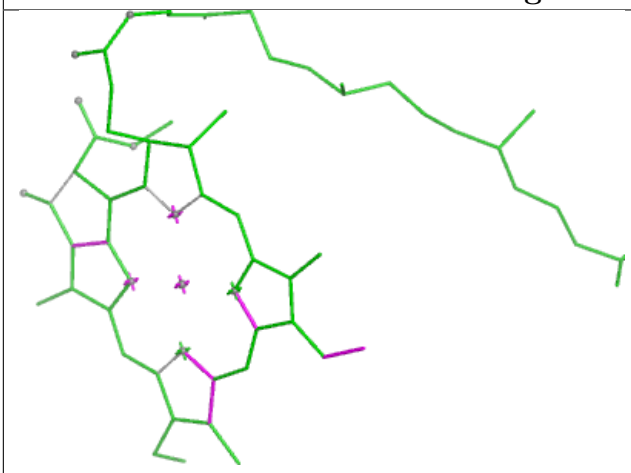


Rings

Ligand CLA B 616



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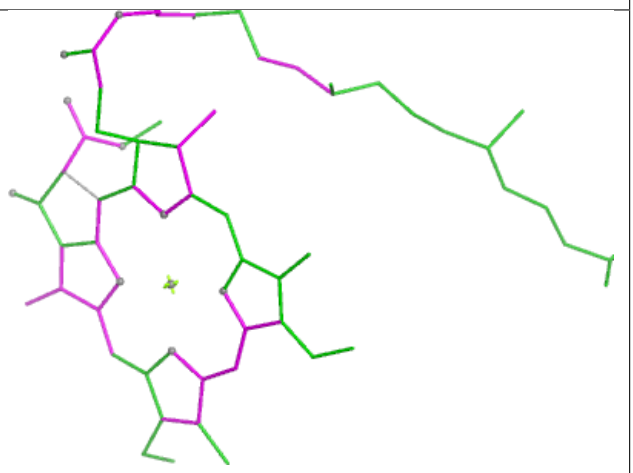
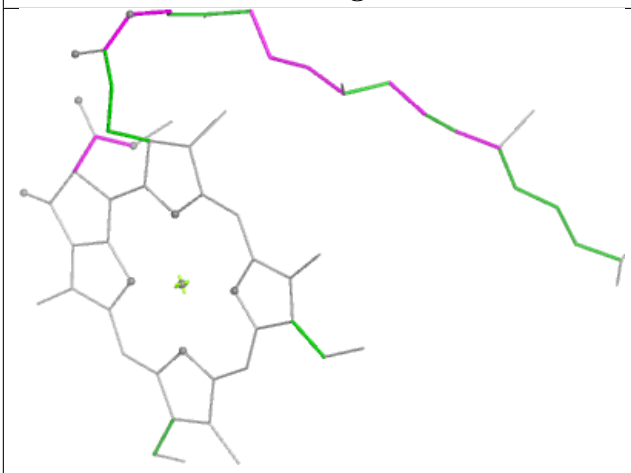


Bond angles



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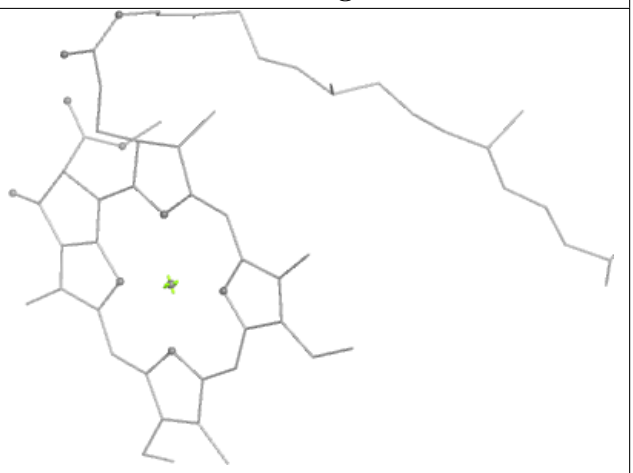
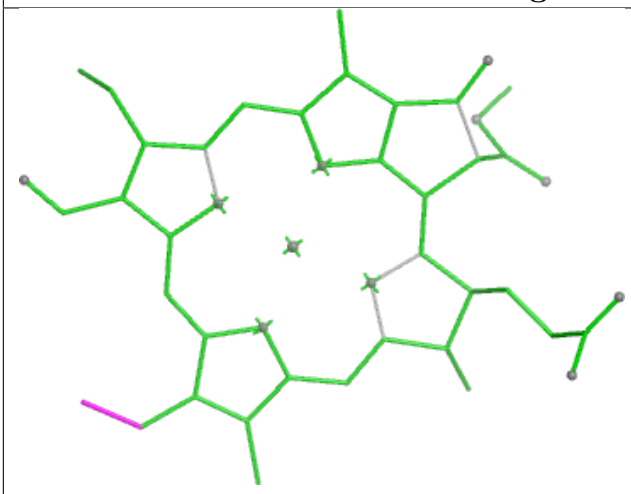


Rings

Ligand CHL s 605



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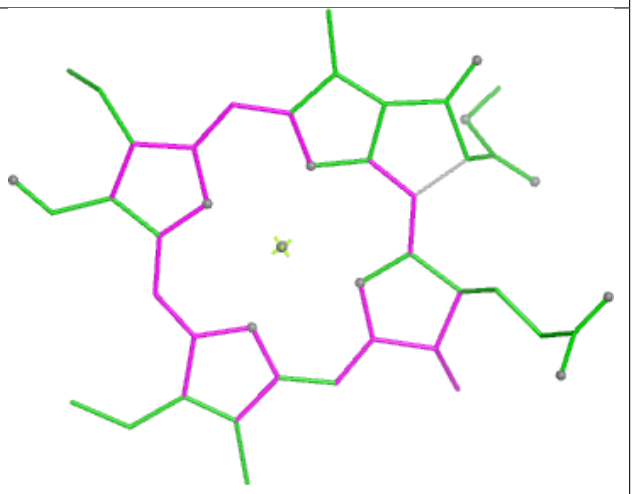
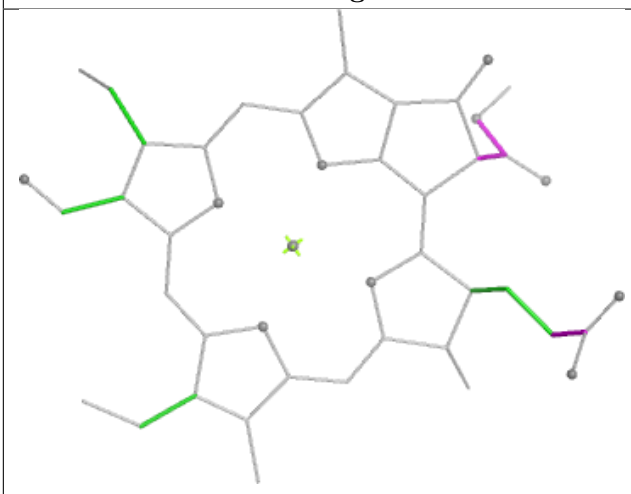


Bond angles



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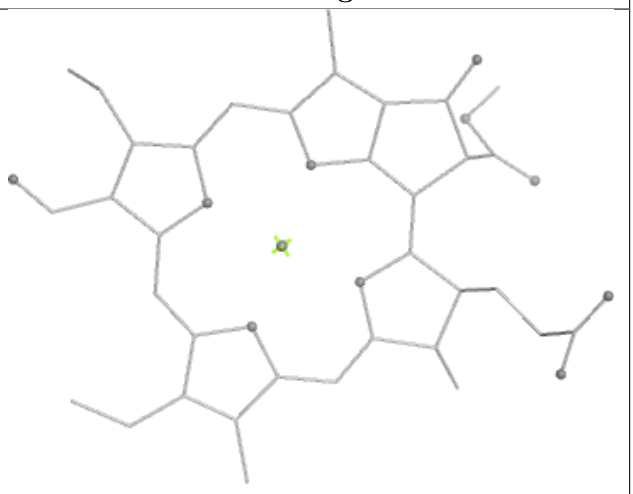
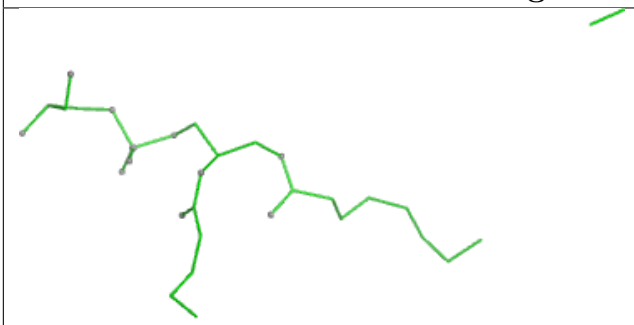


Rings

Ligand LHG c 519



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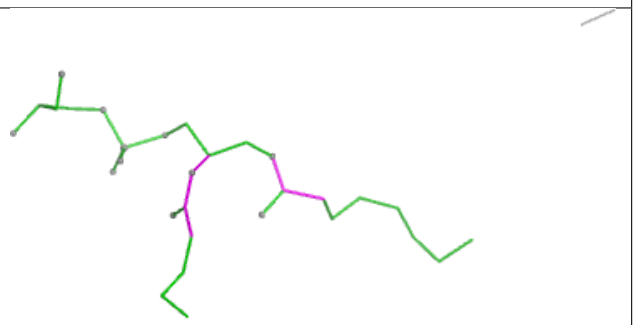
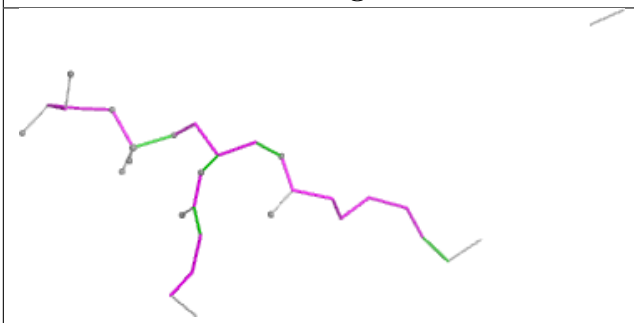


Bond angles



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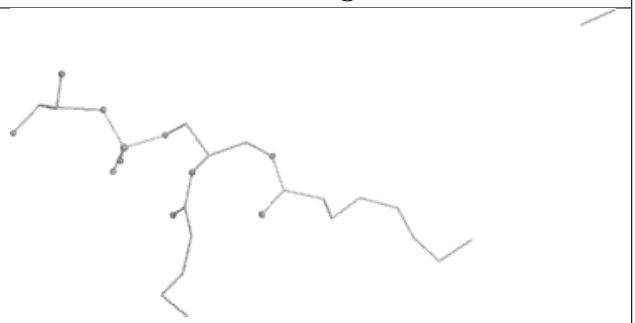
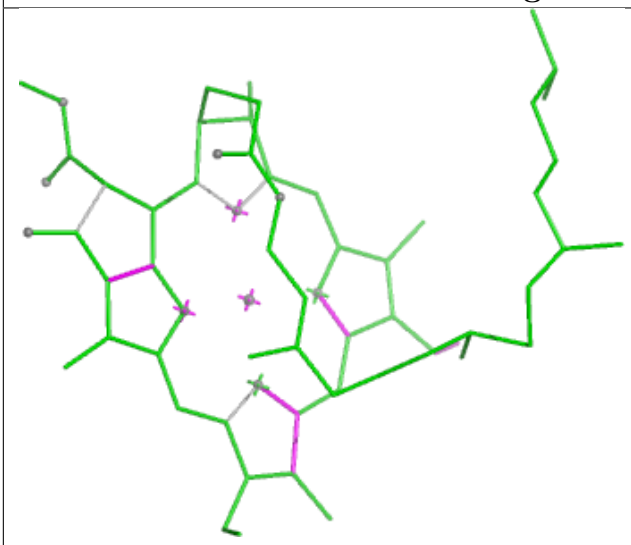


Rings

Ligand CLA Y 613



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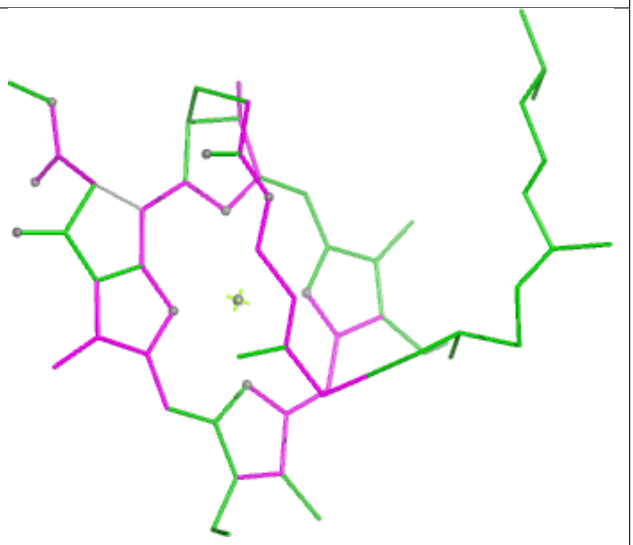

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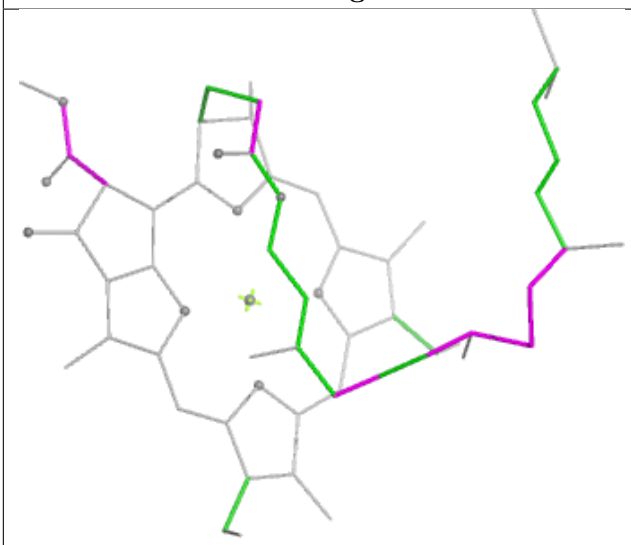

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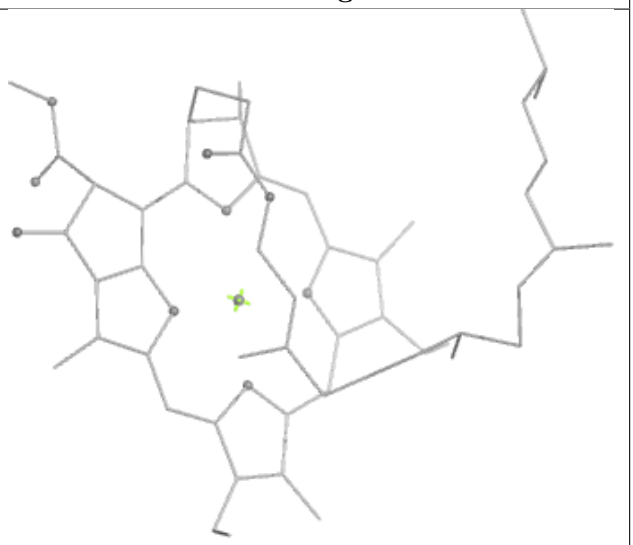
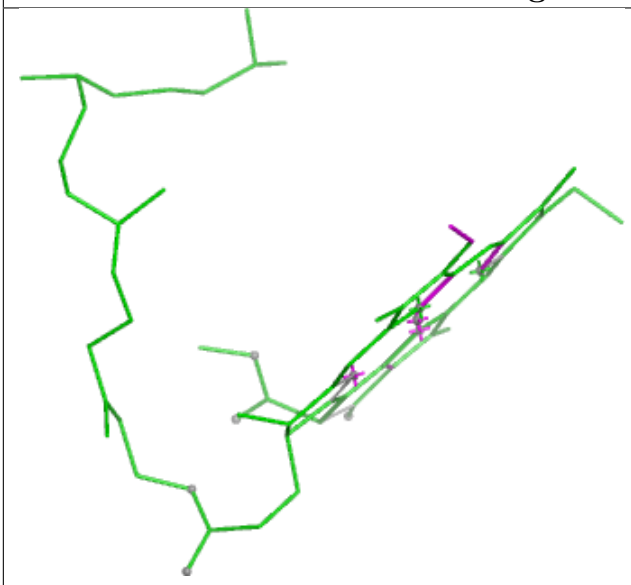


Rings

Ligand CLA g 603



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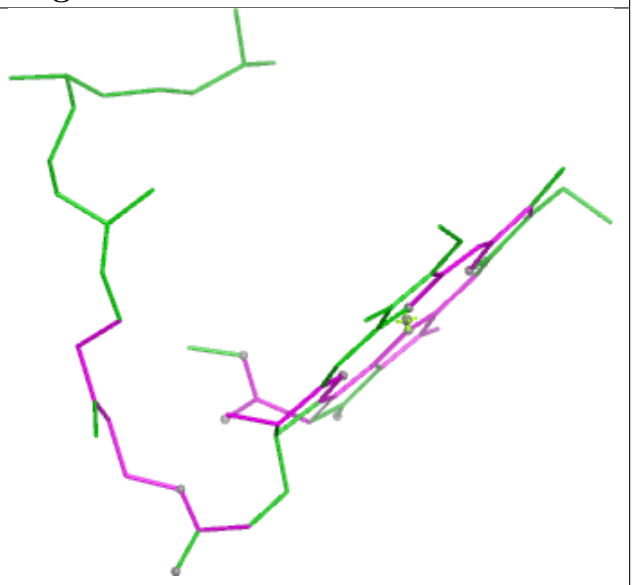
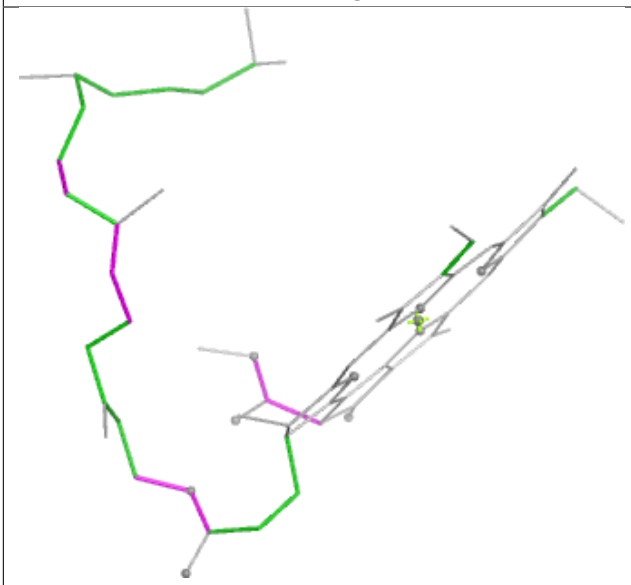


Bond angles

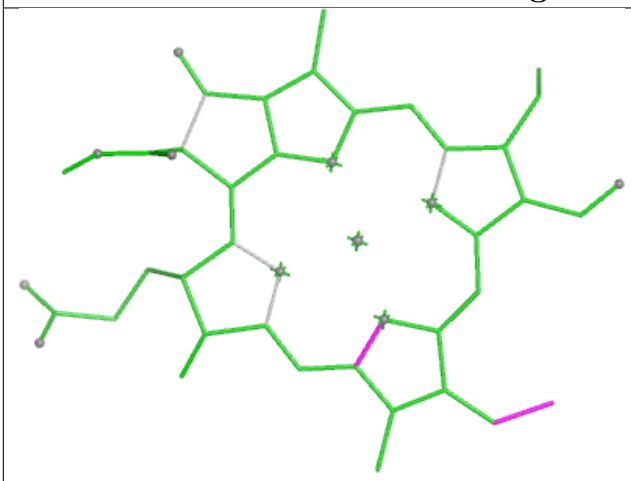


Torsions



Rings

Ligand CHL s 601



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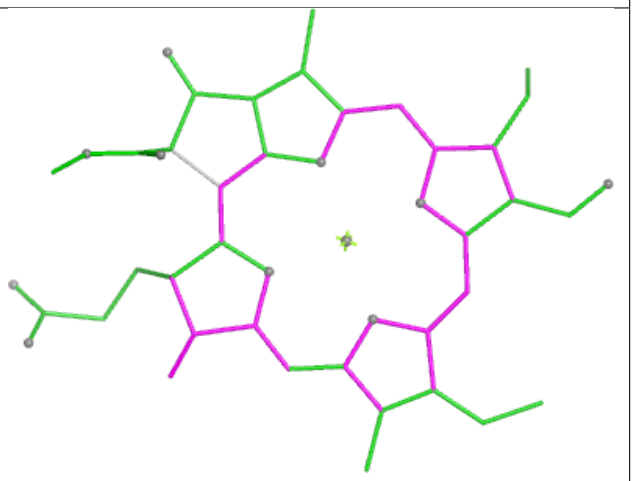
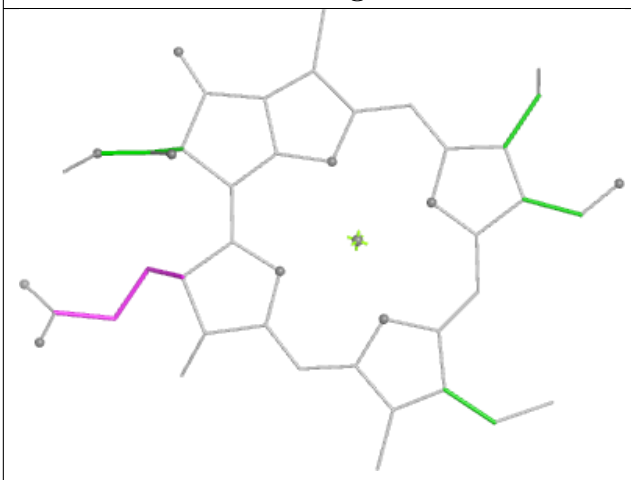


Bond angles



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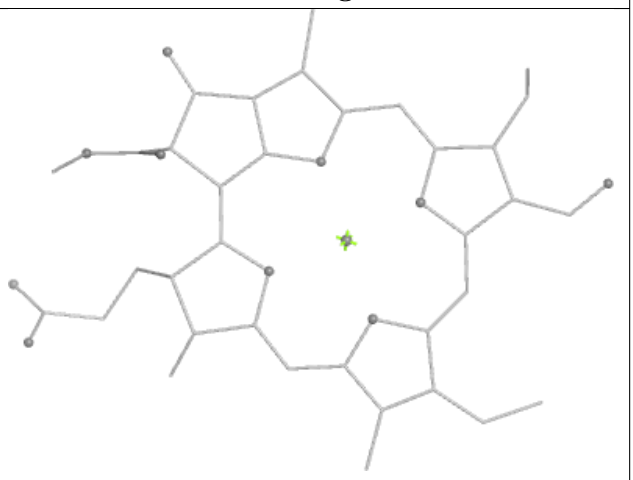
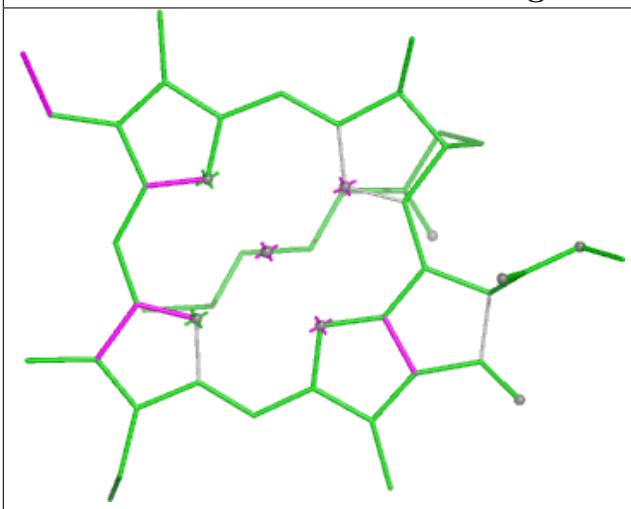


Rings

Ligand CLA S 314



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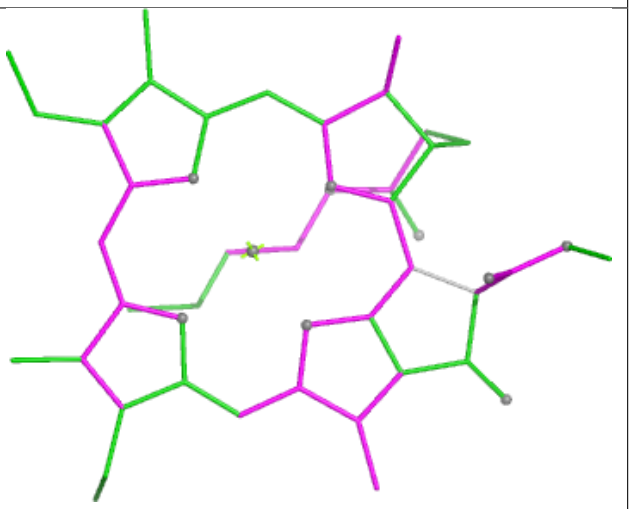
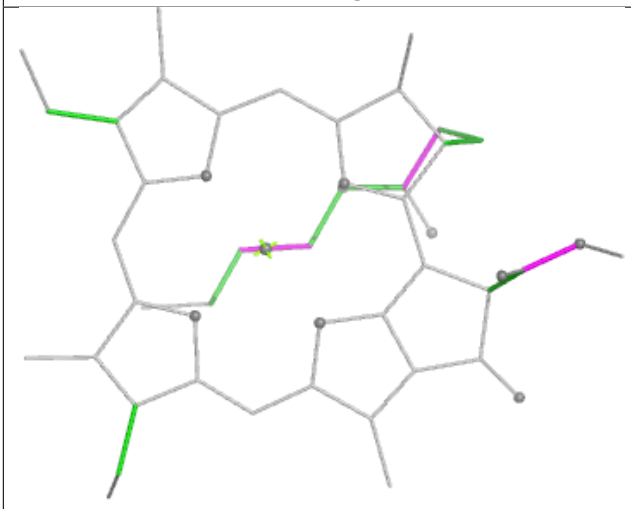


Bond angles



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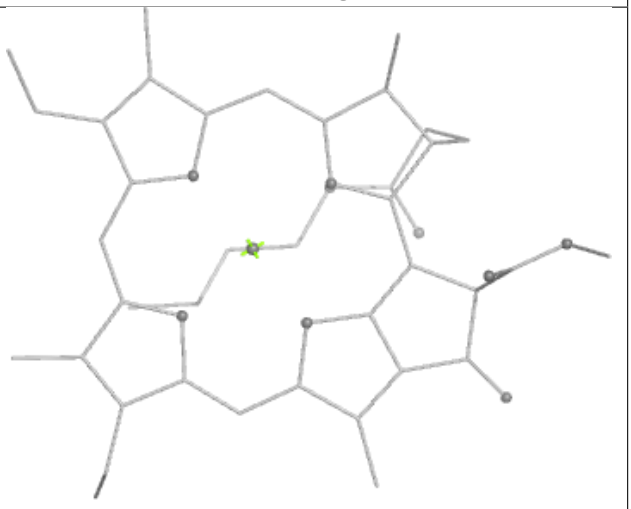
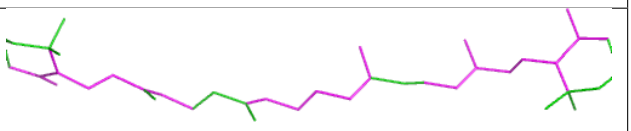


Rings

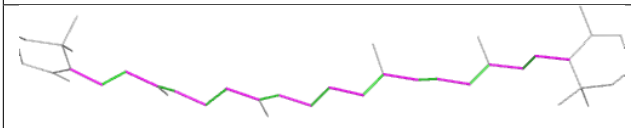
Ligand BCR C 516



Bond lengths



Bond angles



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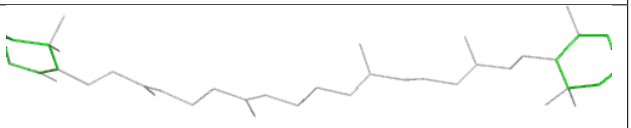
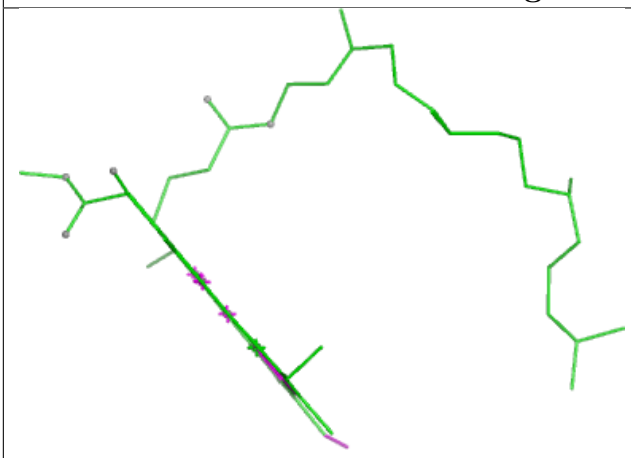


Rings

Ligand CLA B 611



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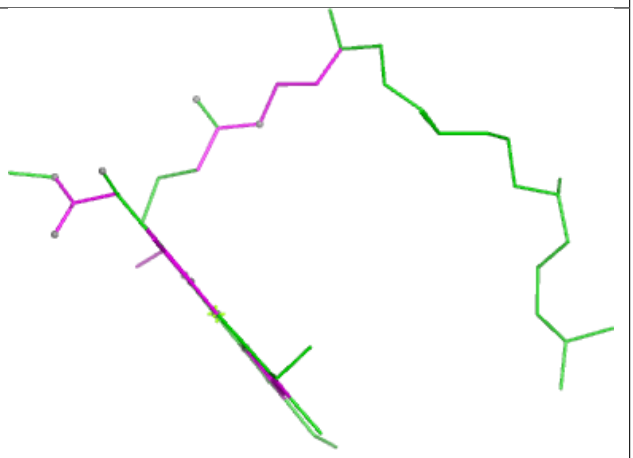


Bond angles

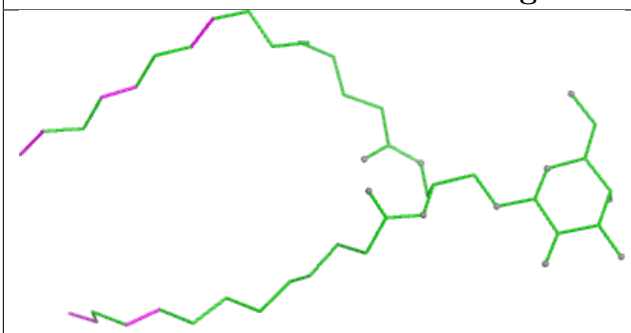


Torsions

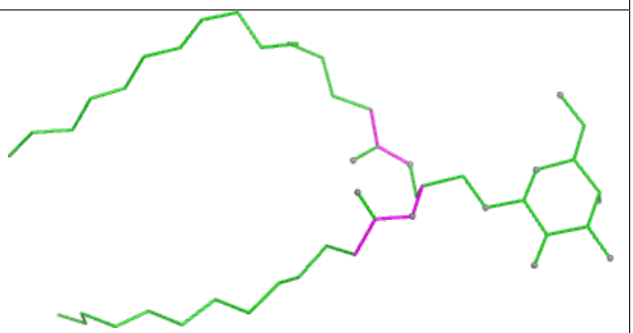


Rings

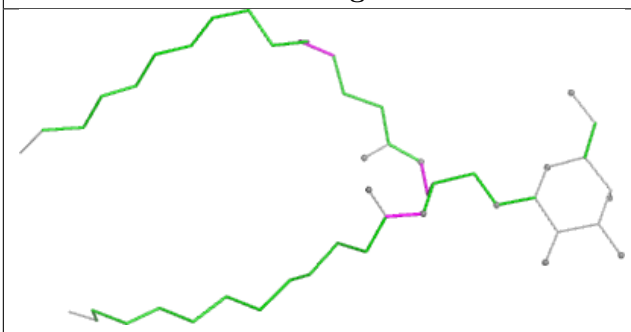
Ligand LMG w 101



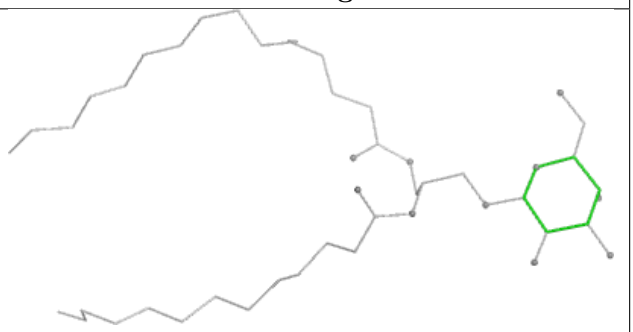
Bond lengths



Bond angles

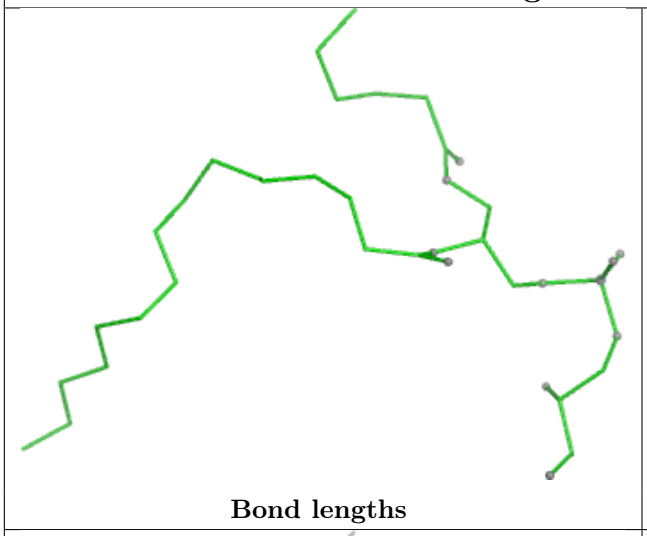


Torsions

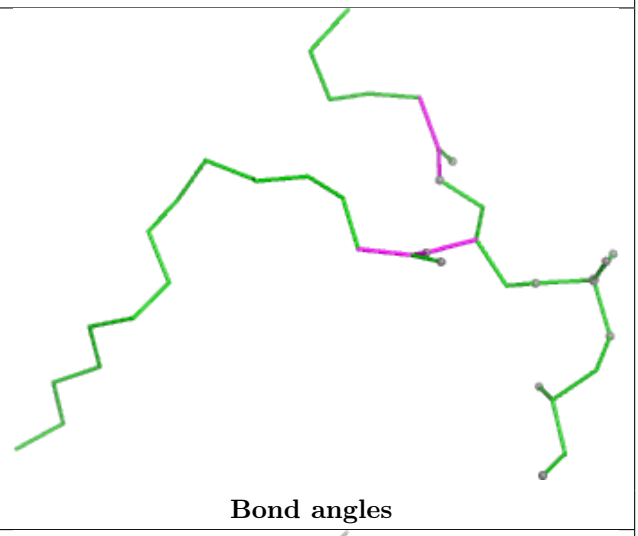


Rings

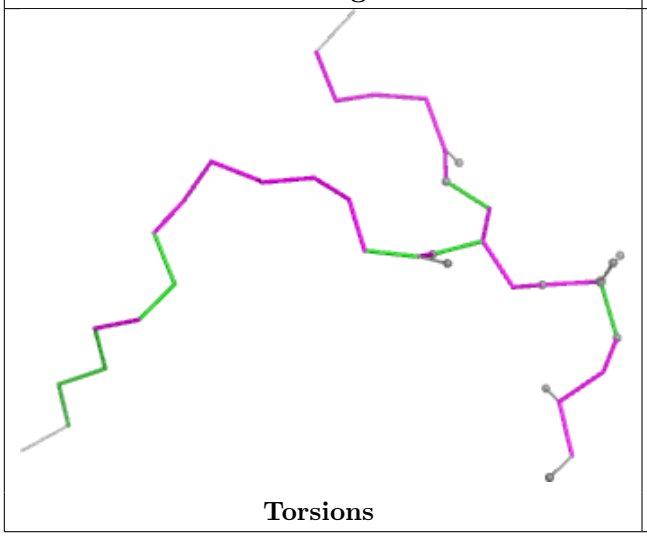
Ligand LHG w 102



Bond lengths



Bond angles



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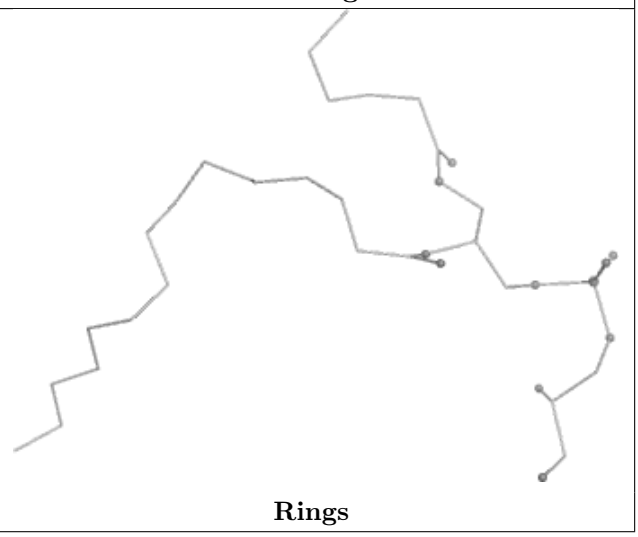
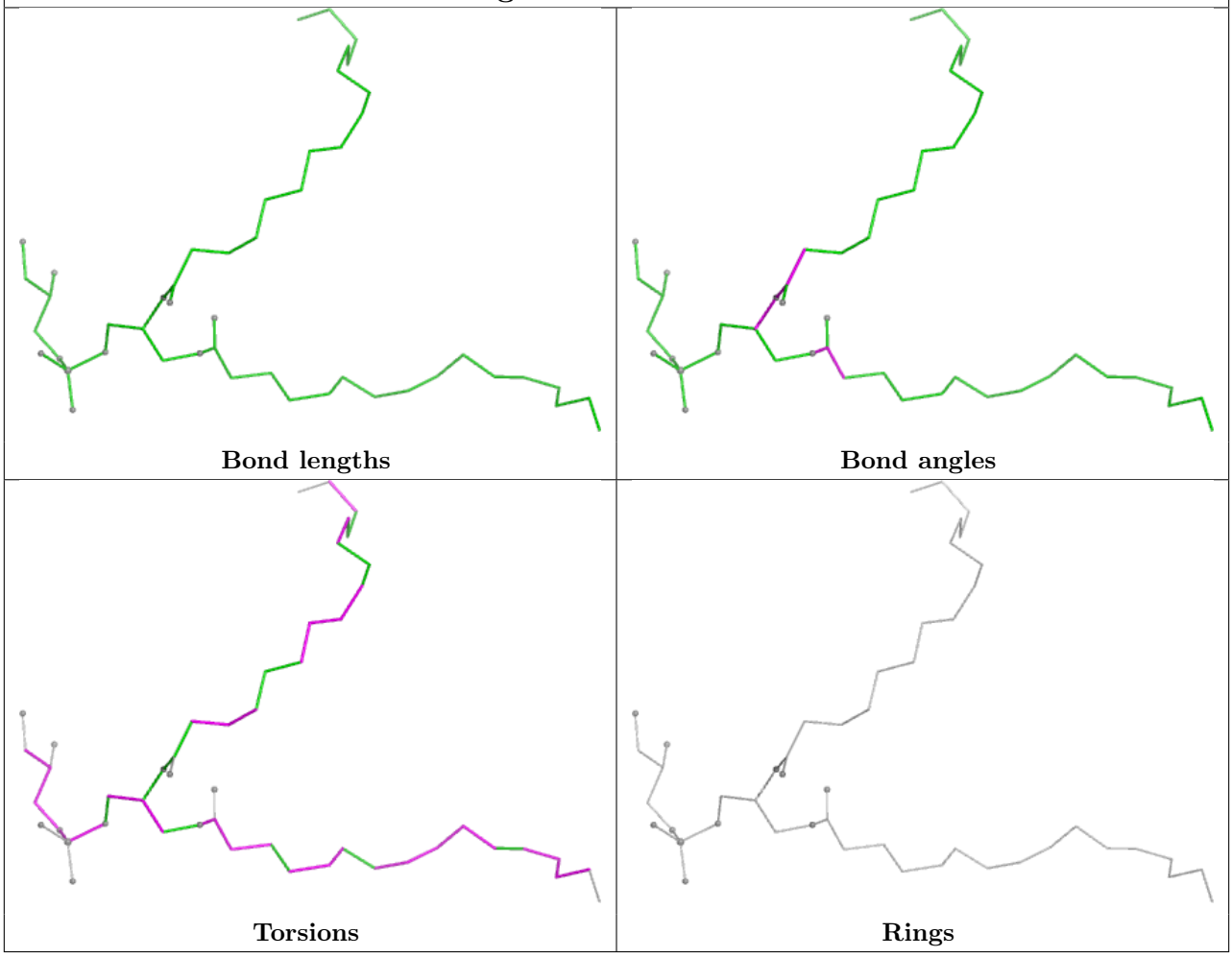
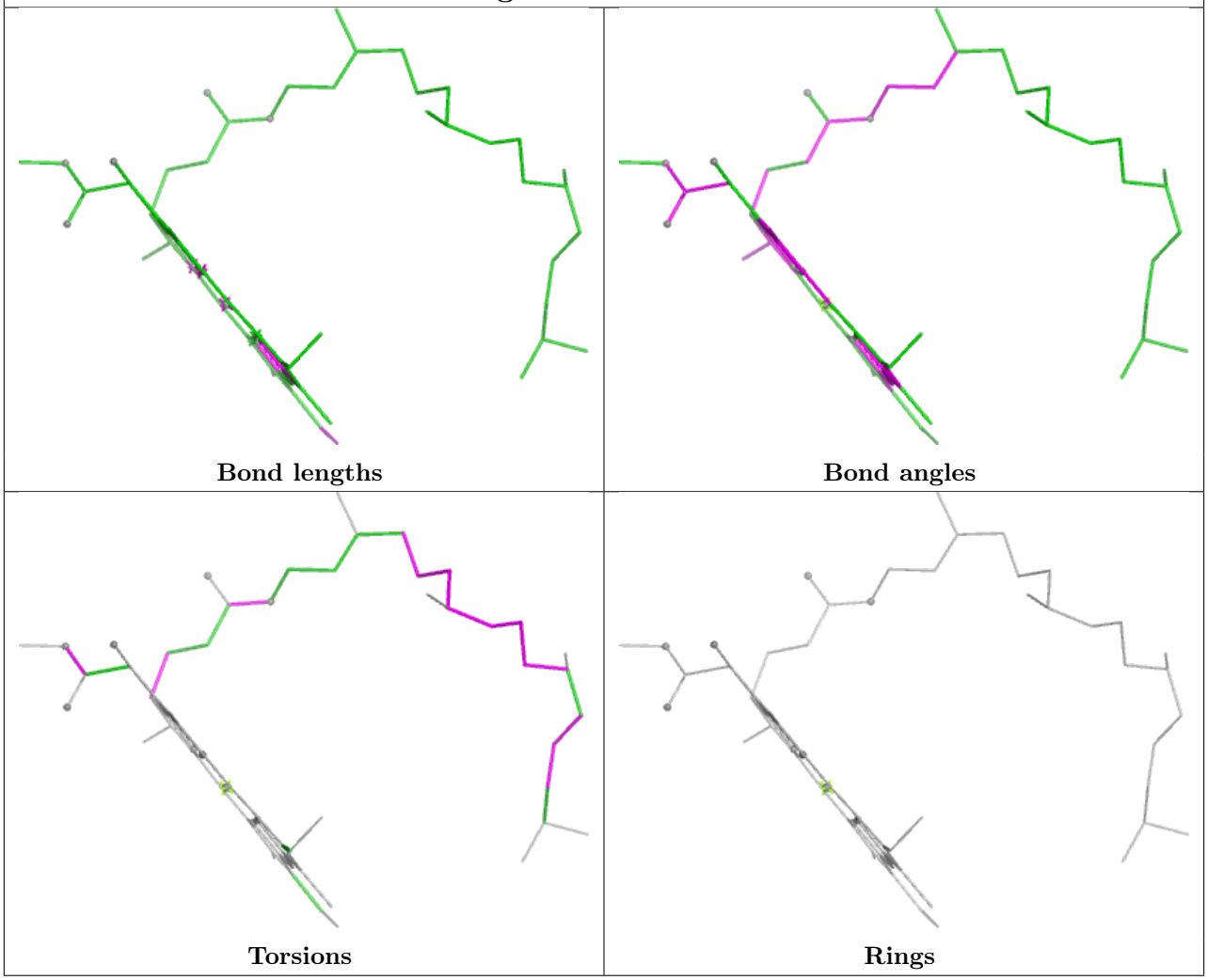


Rings

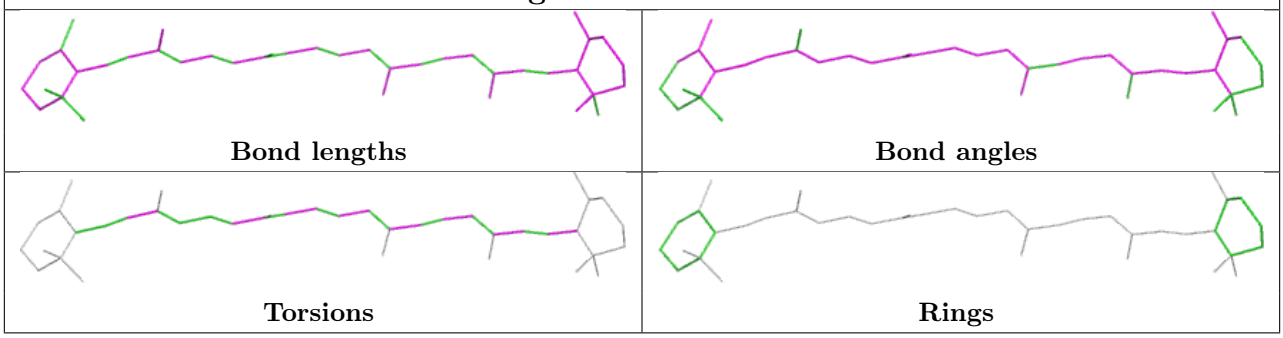
Ligand LHG W 101



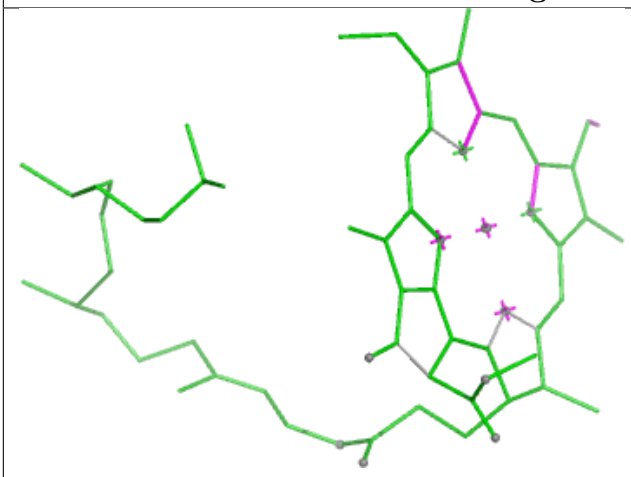
Ligand CLA b 611



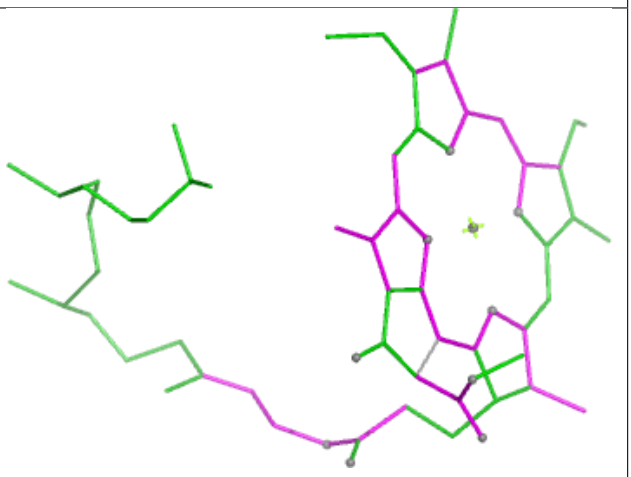
Ligand BCR c 514



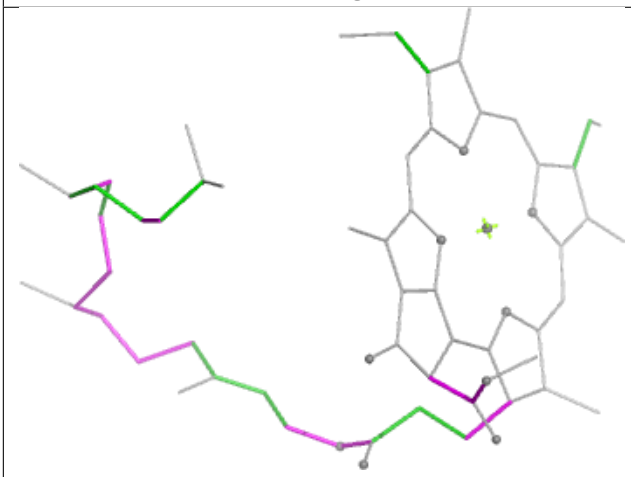
Ligand CLA c 503



Bond lengths



Bond angles



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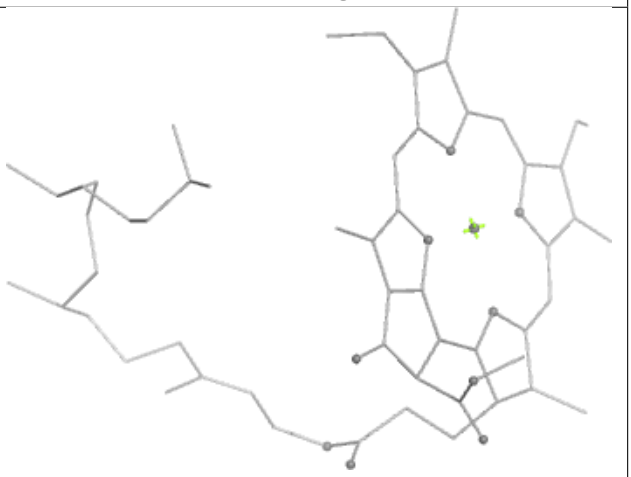
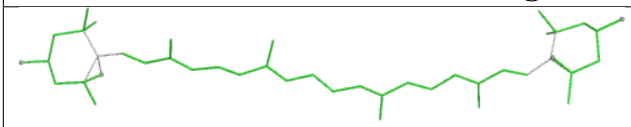


Rings

Ligand XAT Y 617



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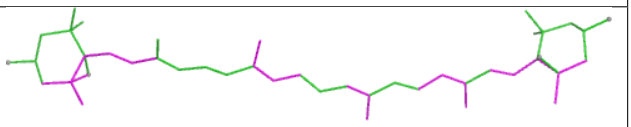
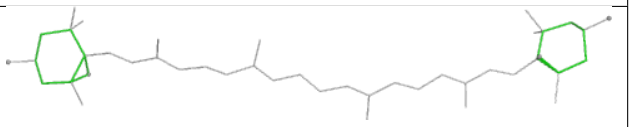


Bond angles



Torsions

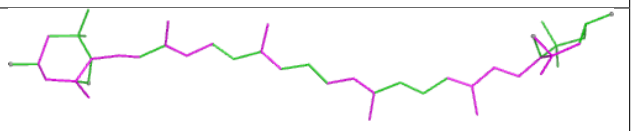


Rings

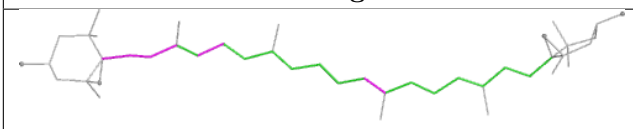
Ligand XAT r 615



Bond lengths



Bond angles



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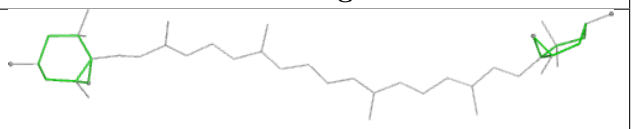
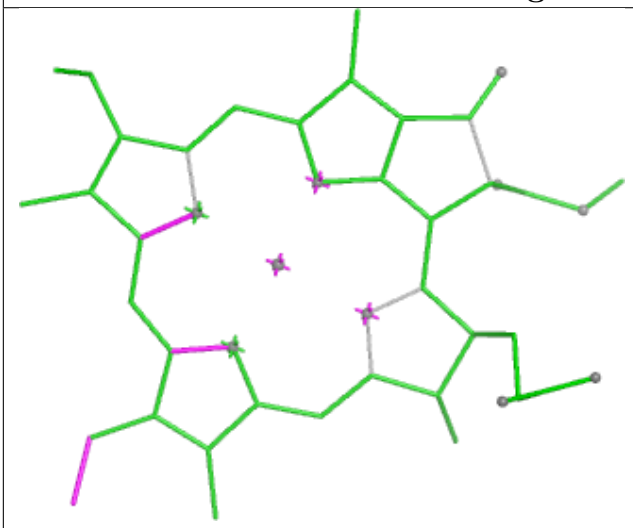


Rings

Ligand CLA S 309



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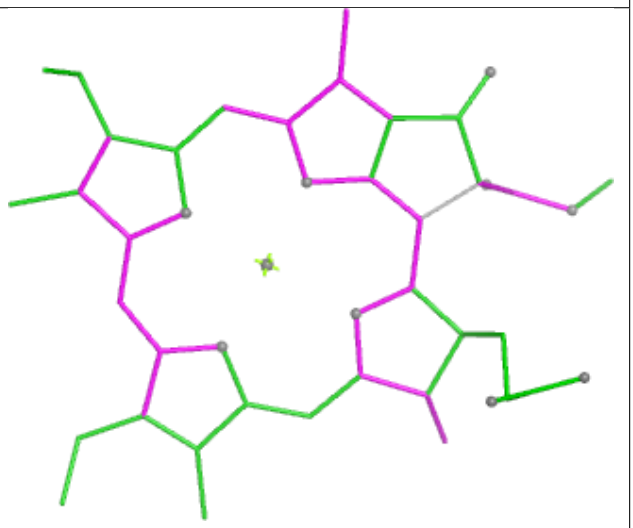
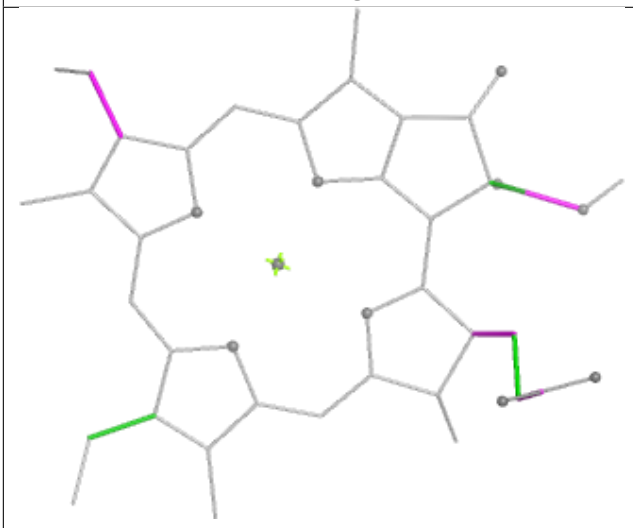


Bond angles



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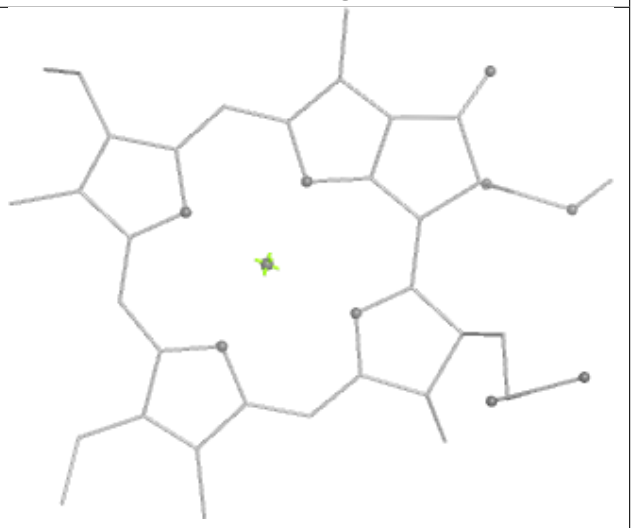
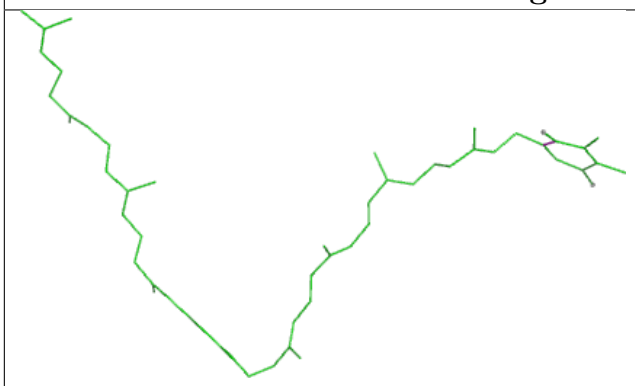


Rings

Ligand PL9 D 406



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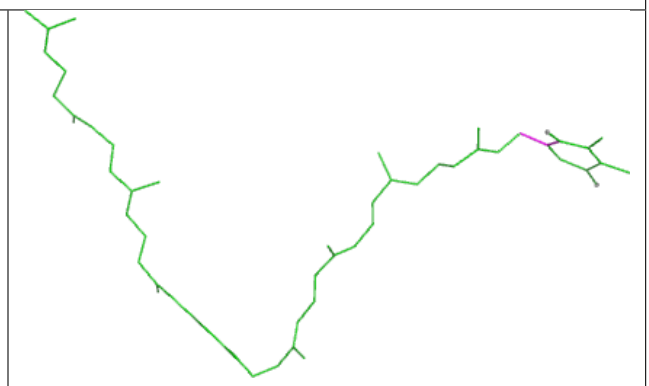

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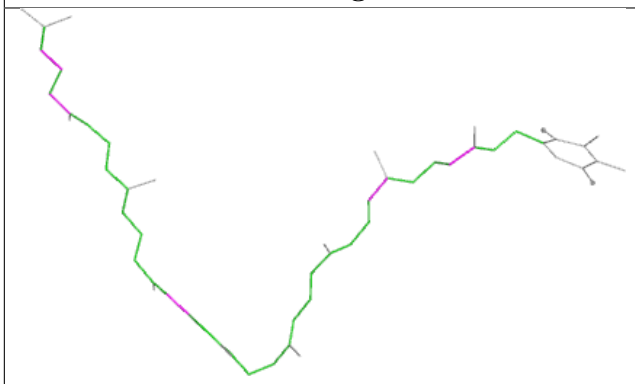

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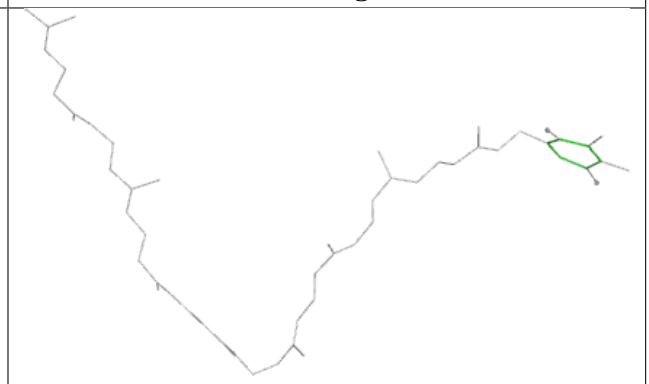
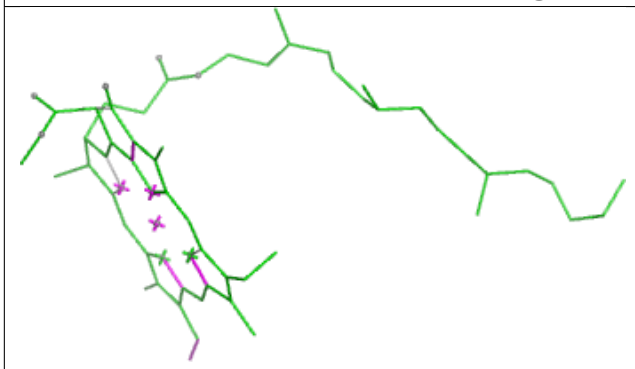


Rings

Ligand CLA c 508



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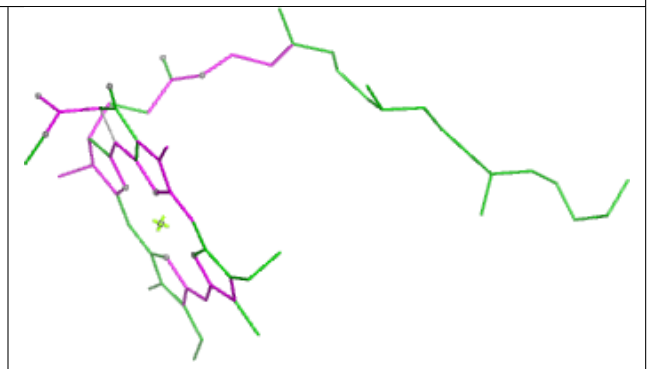
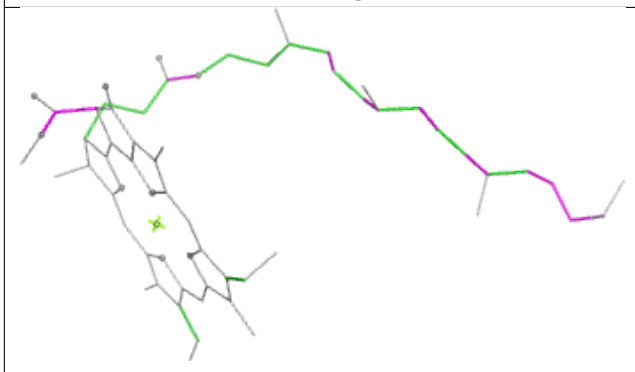


Bond angles



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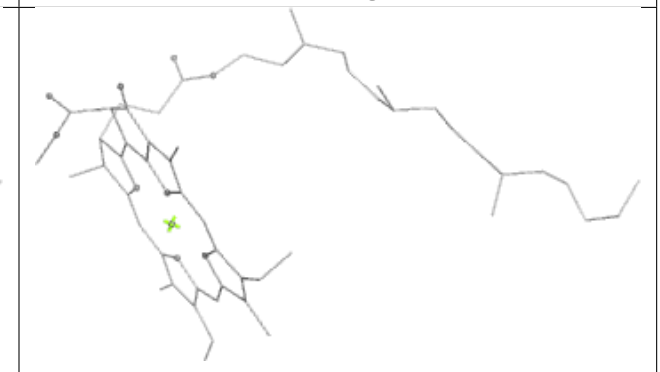
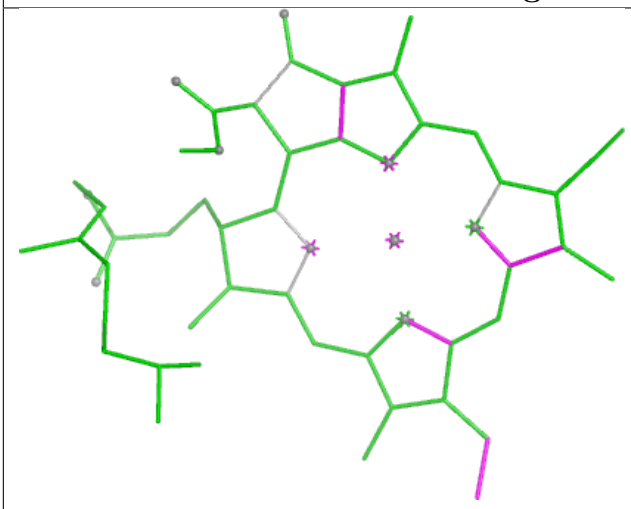


Rings

Ligand CLA N 603



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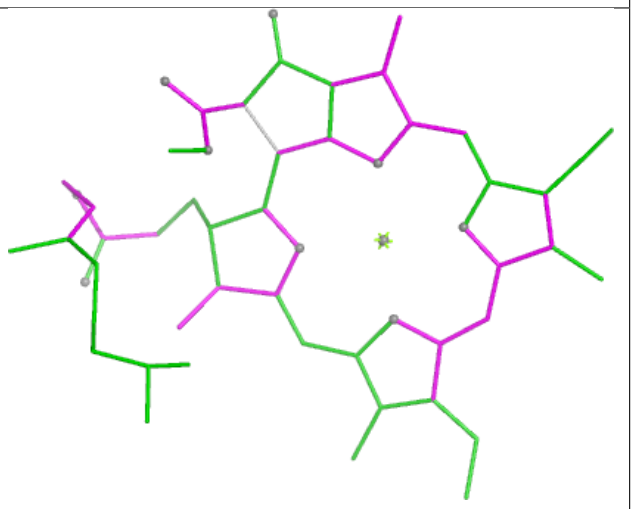
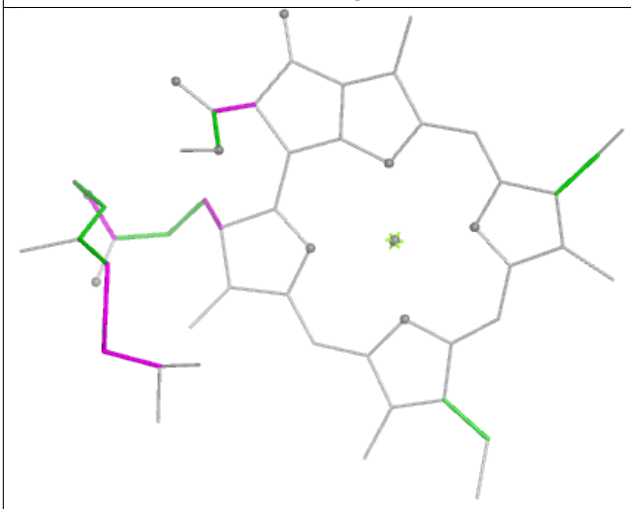


Bond angles



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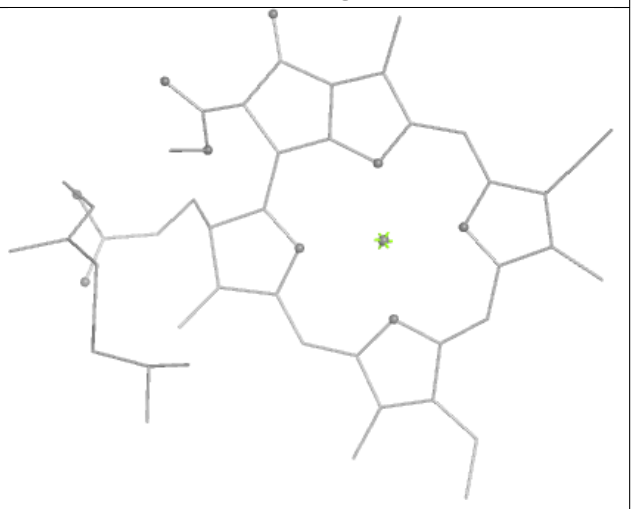
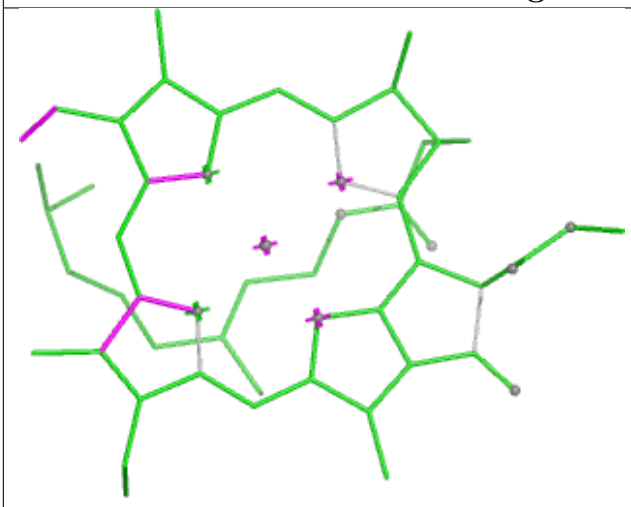


Rings

Ligand CLA S 313



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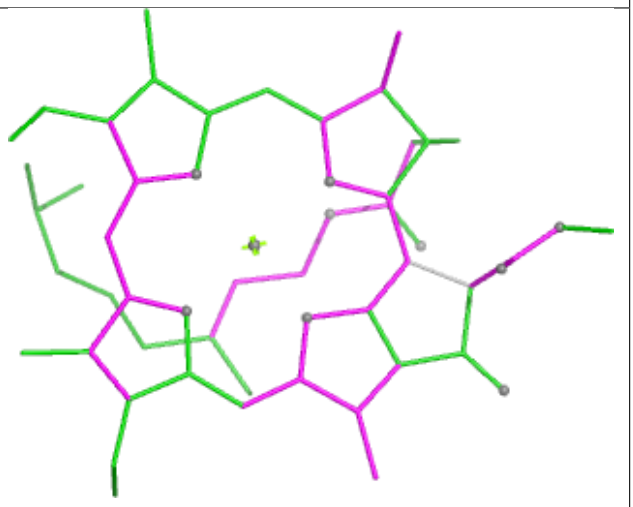

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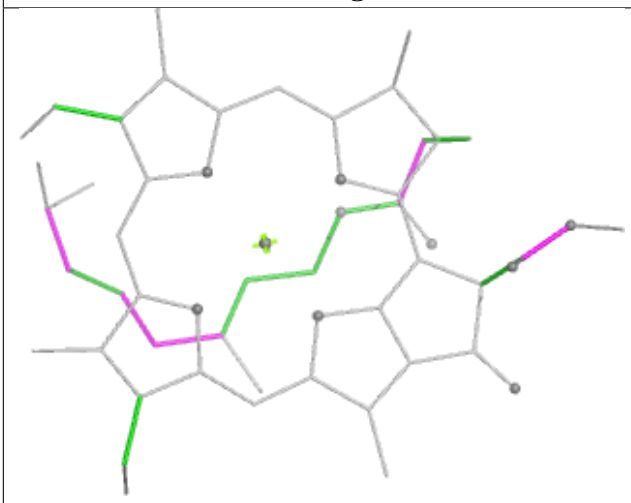

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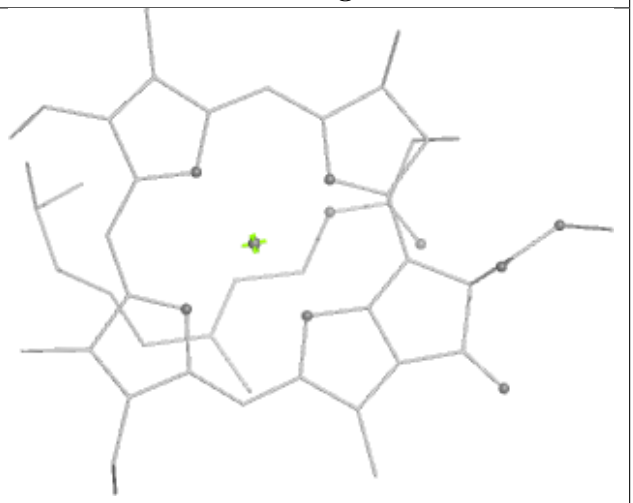
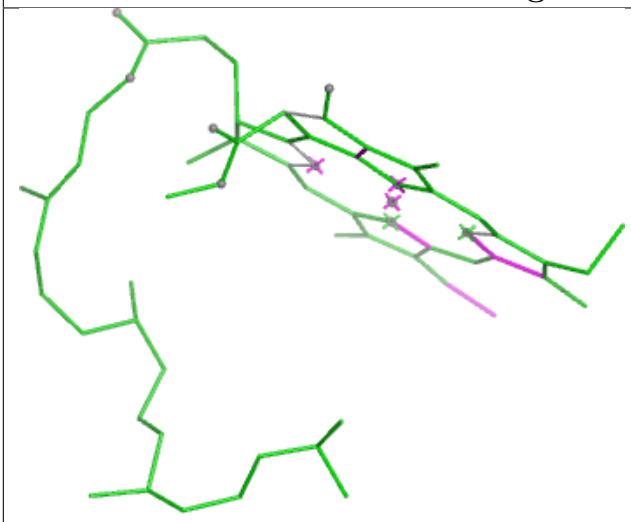


Rings

Ligand CLA n 603



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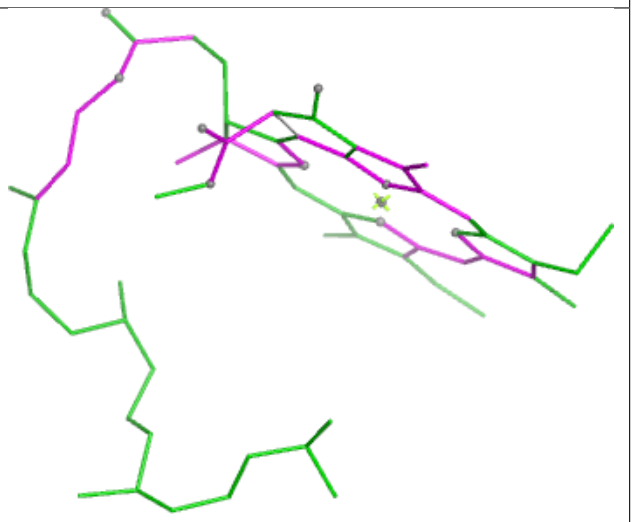

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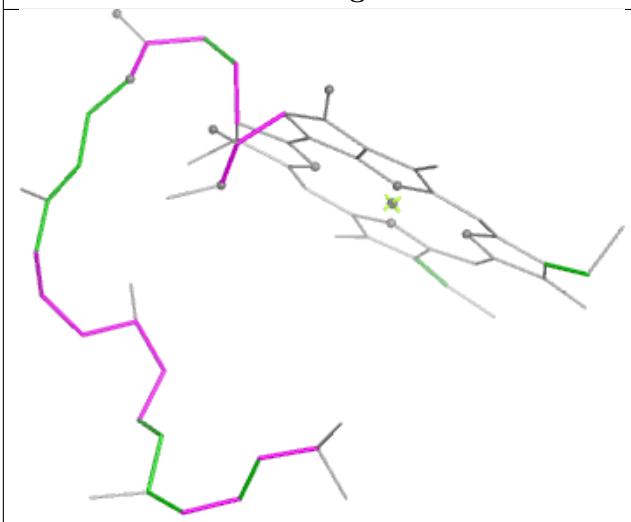

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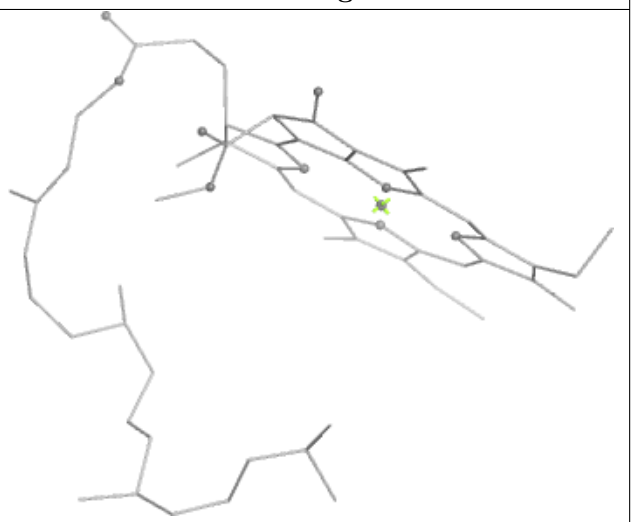
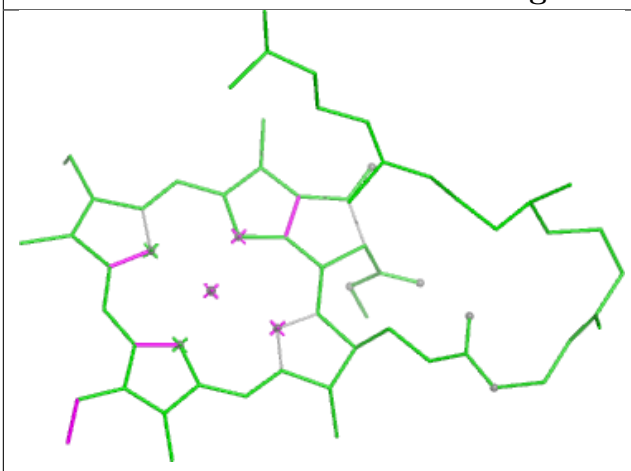


Rings

Ligand CLA c 509



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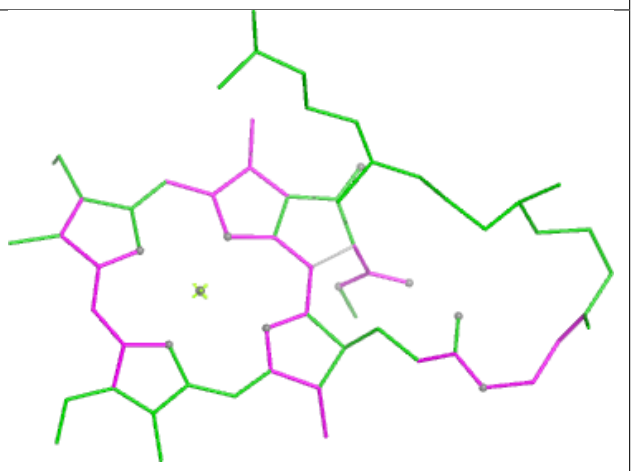
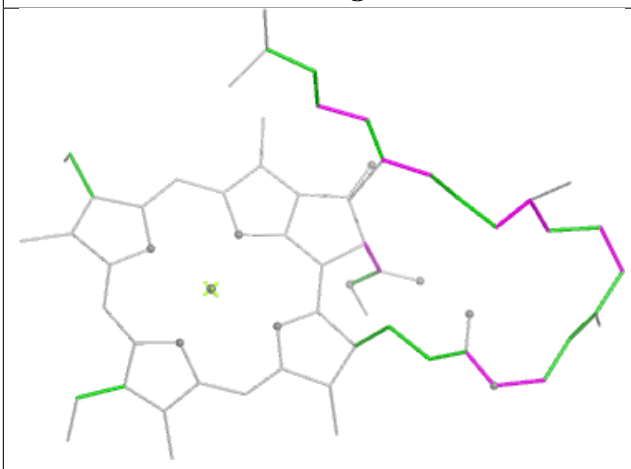


Bond angles



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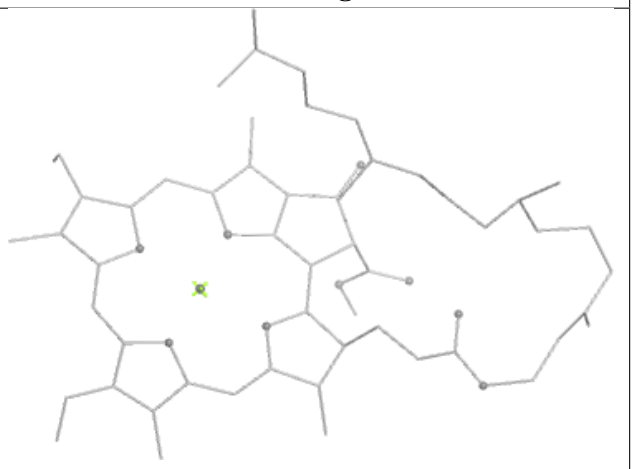
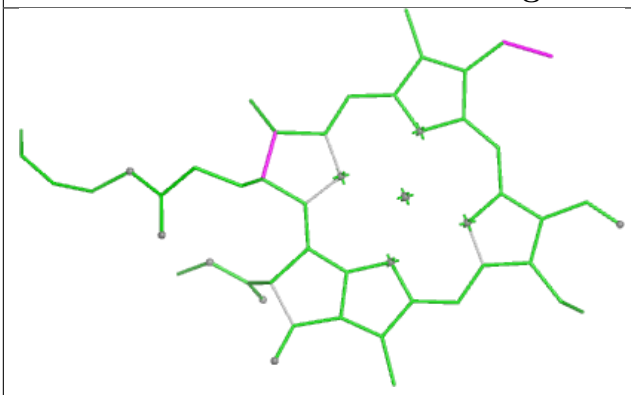


Rings

Ligand CHL G 606



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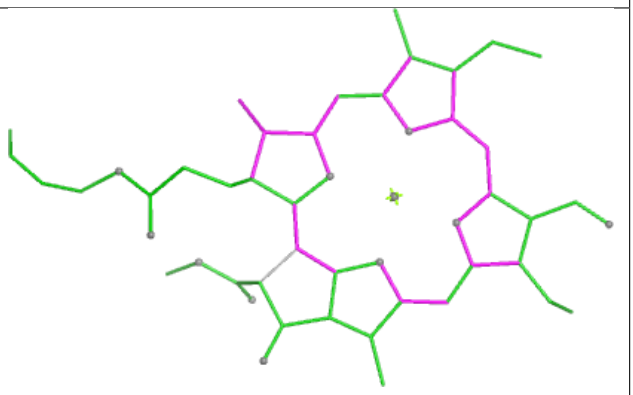

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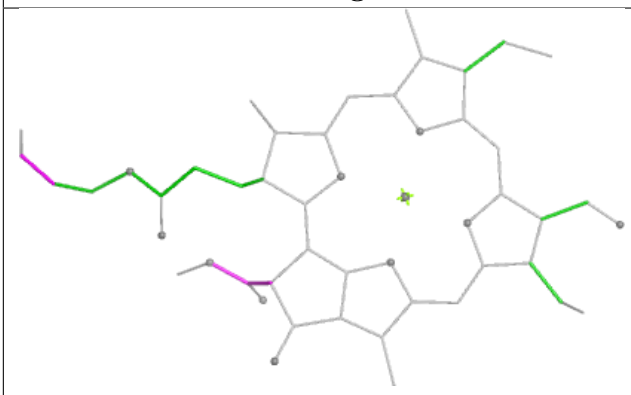

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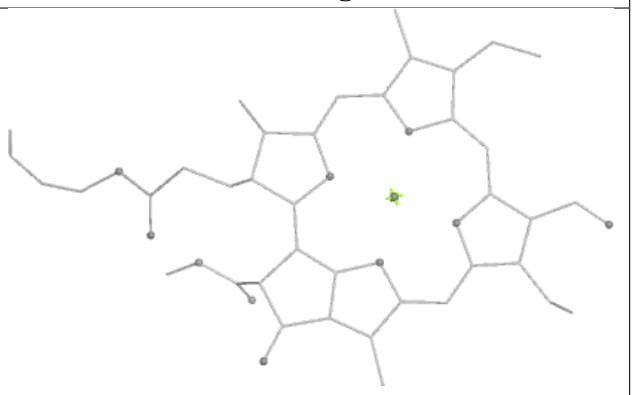
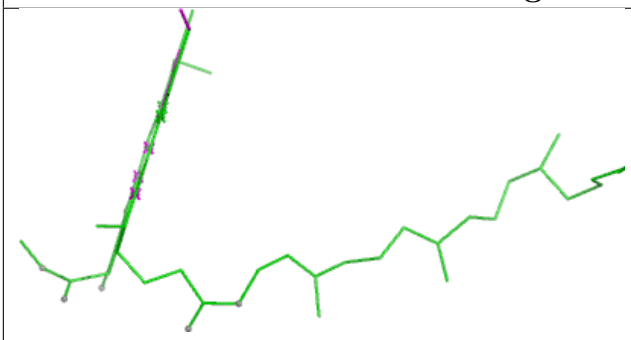


Rings

Ligand CLA B 605



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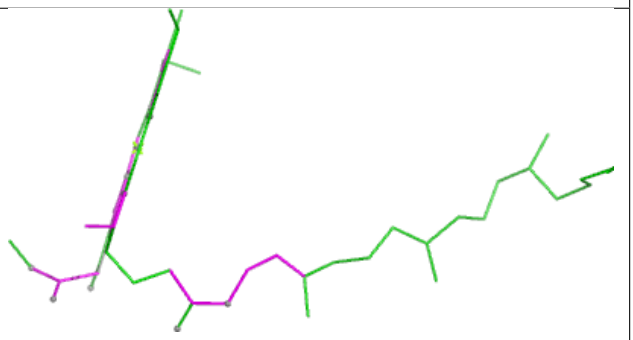
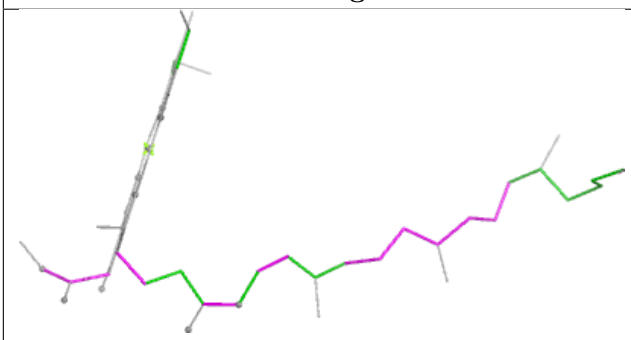


Bond angles



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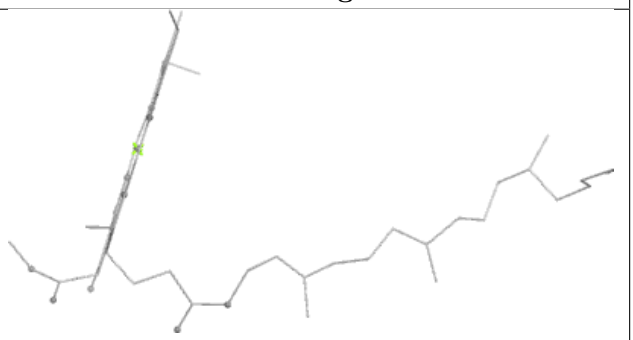
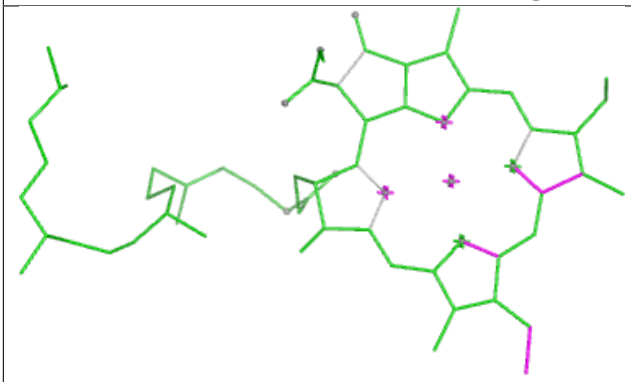


Rings

Ligand CLA b 612



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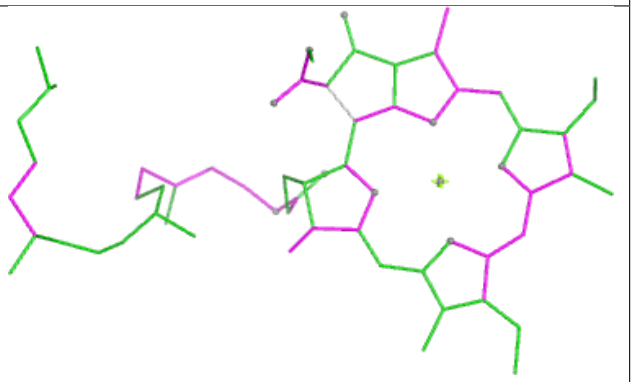
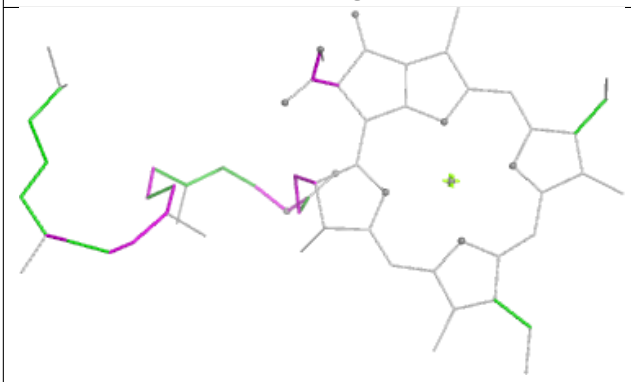


Bond angles



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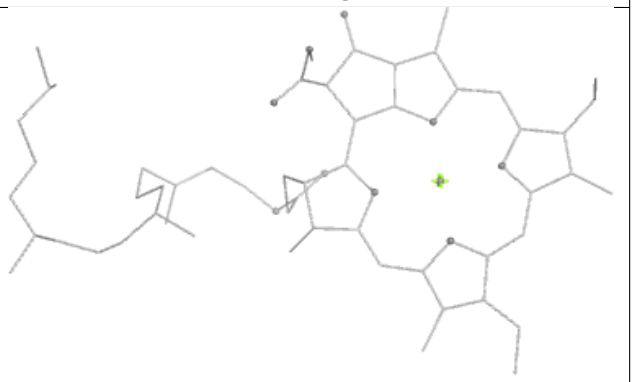
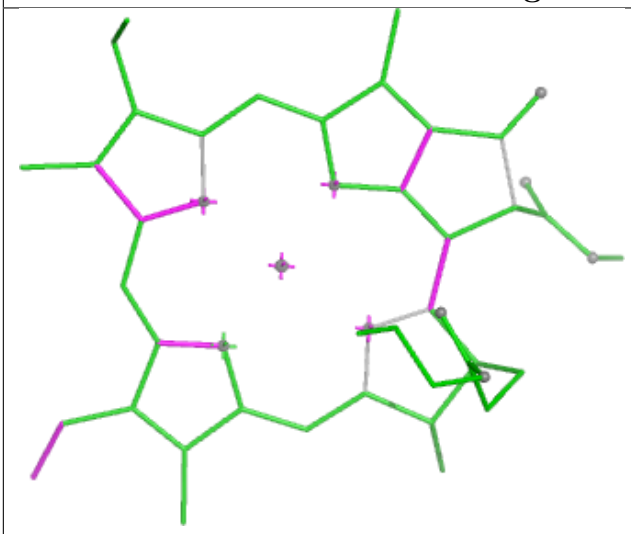
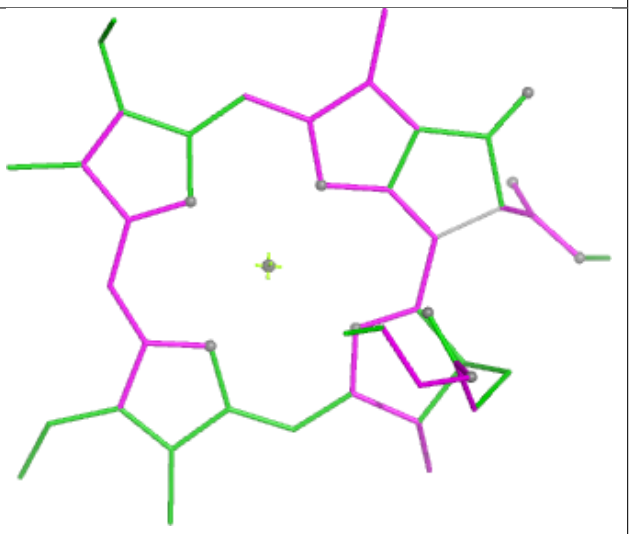


Rings

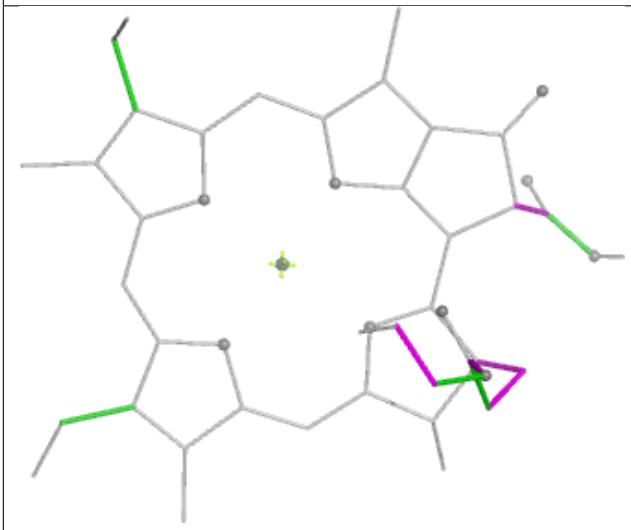
Ligand CLA R 604



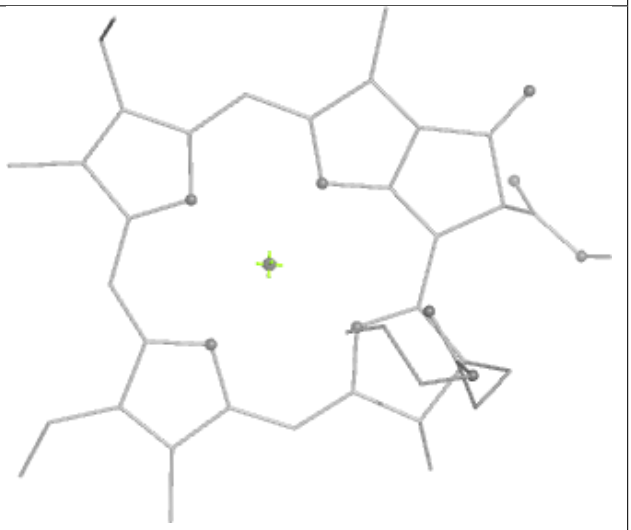
Bond lengths



Bond angles

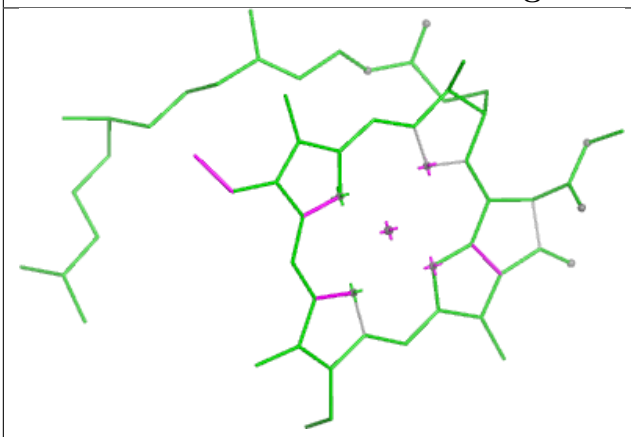


Torsions



Rings

Ligand CLA R 602



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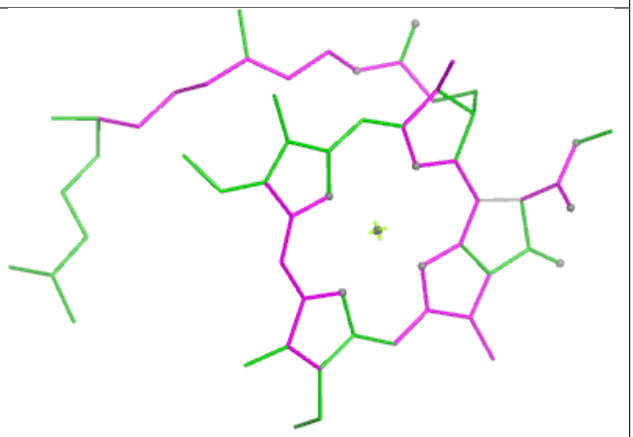

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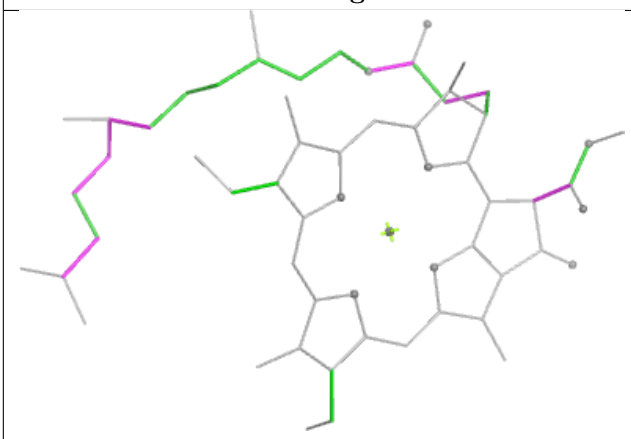

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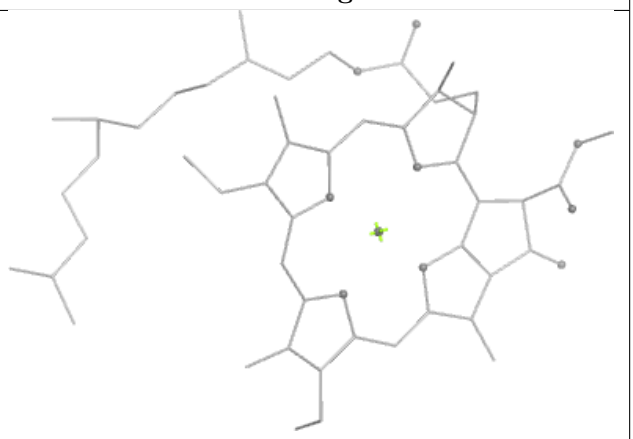
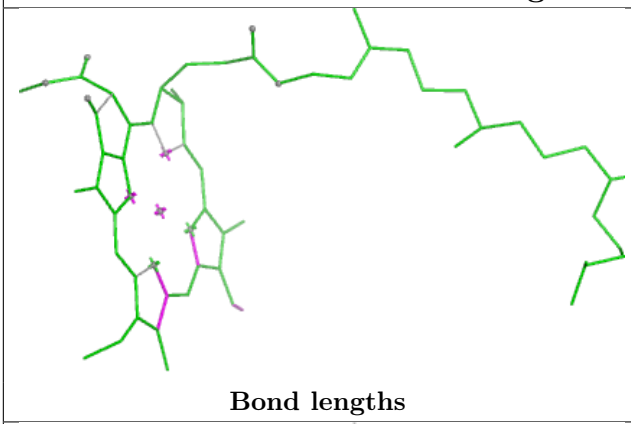


Rings

Ligand CLA b 609



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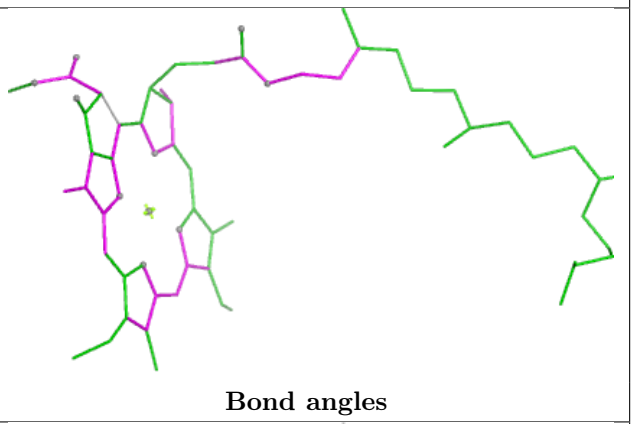

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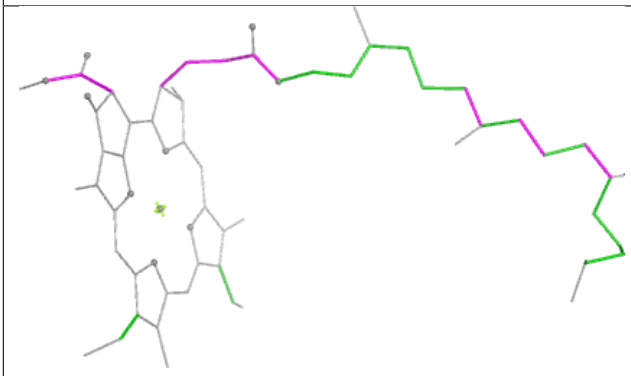
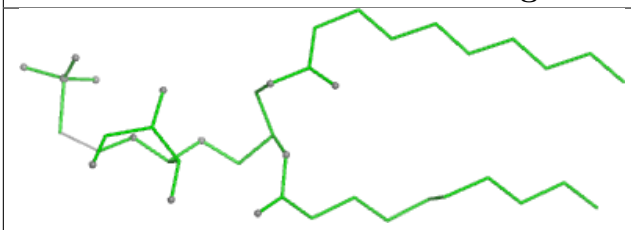


Torsions



Rings

Ligand SQD M 101



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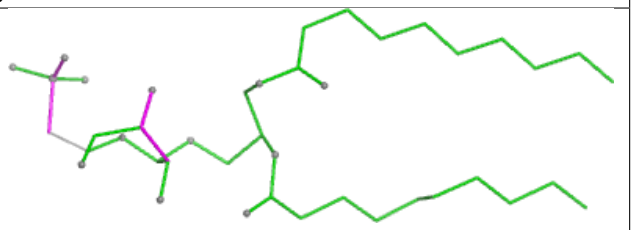
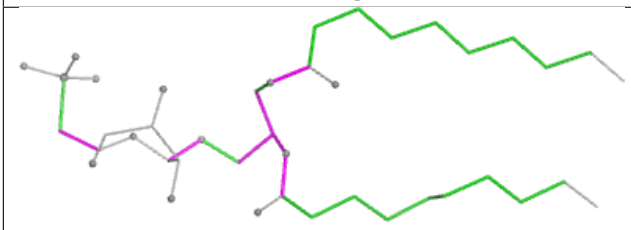


Bond angles



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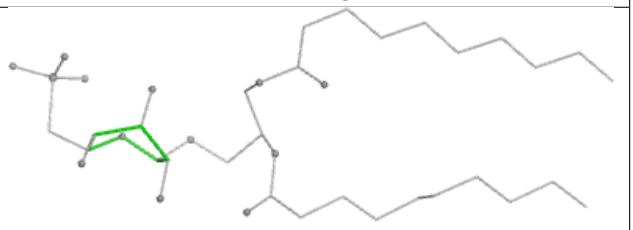
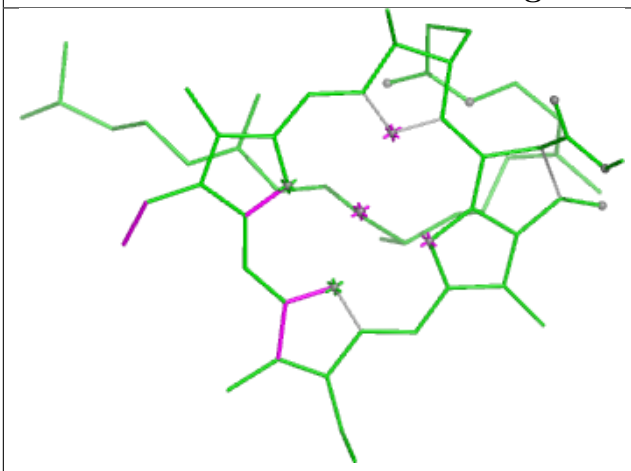


Rings

Ligand CLA B 601



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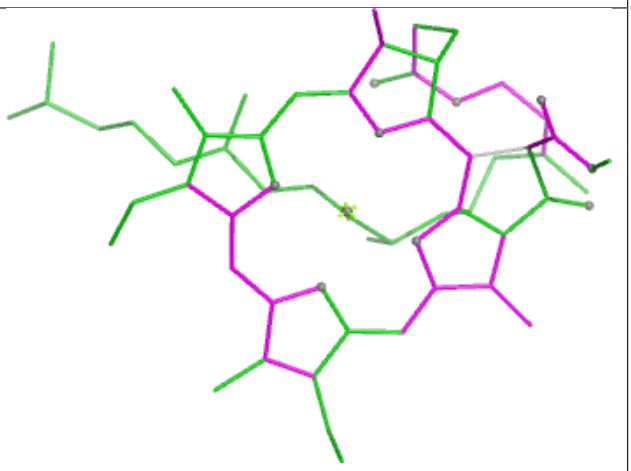
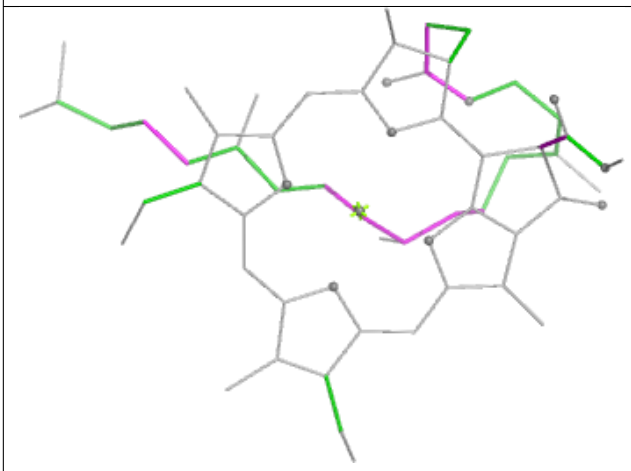


Bond angles



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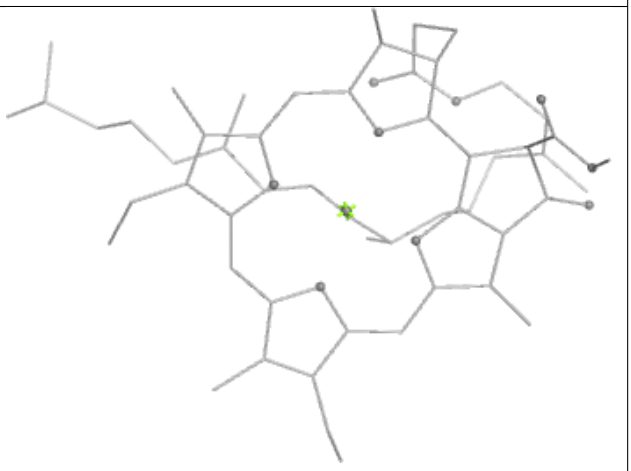
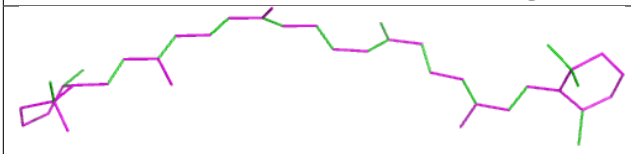


Rings

Ligand BCR T 101



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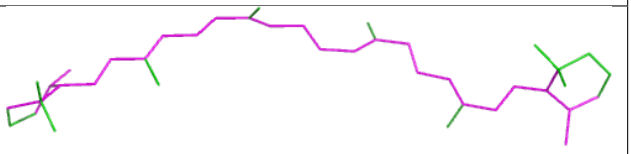

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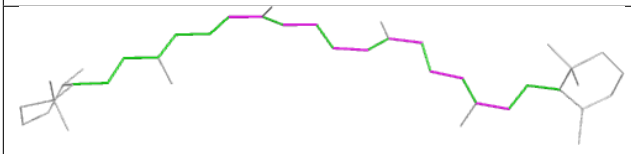

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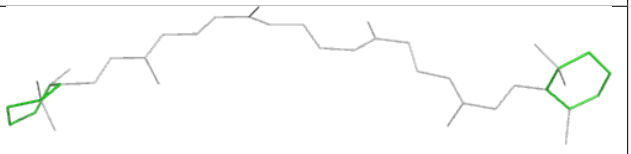
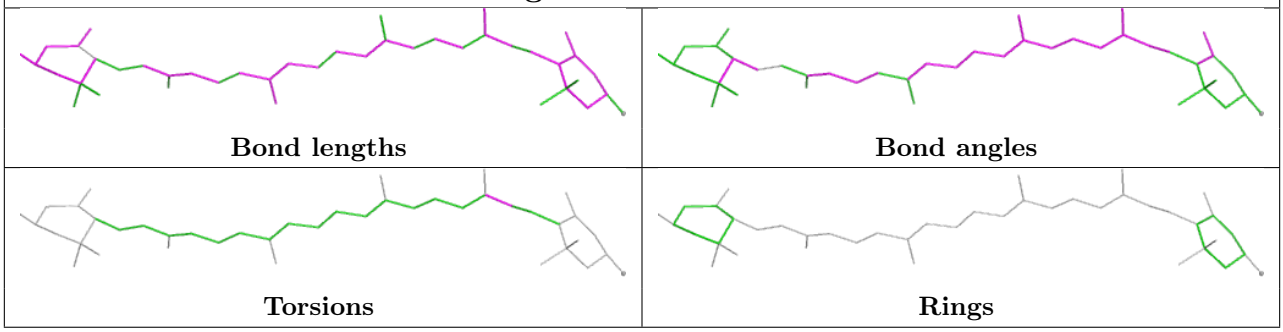
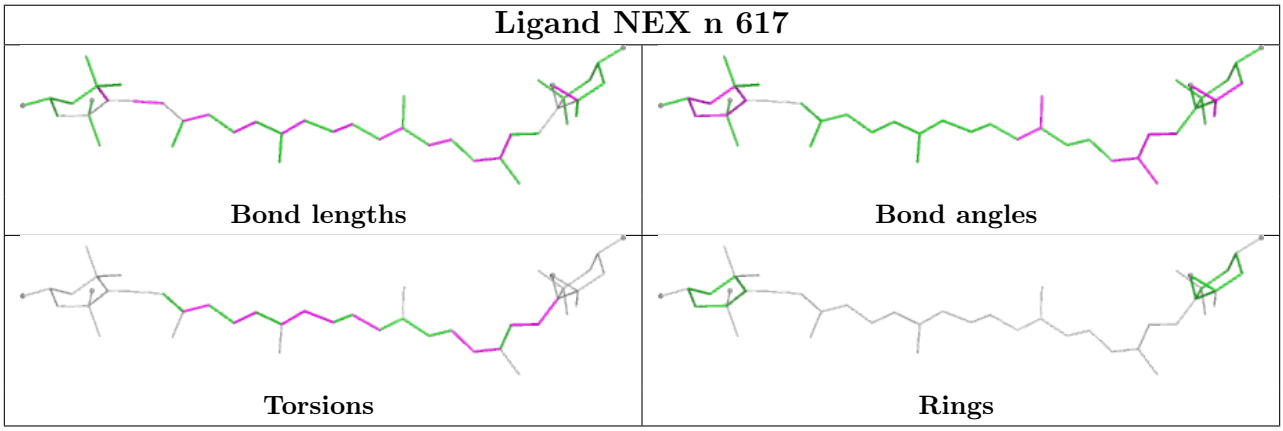


Rings

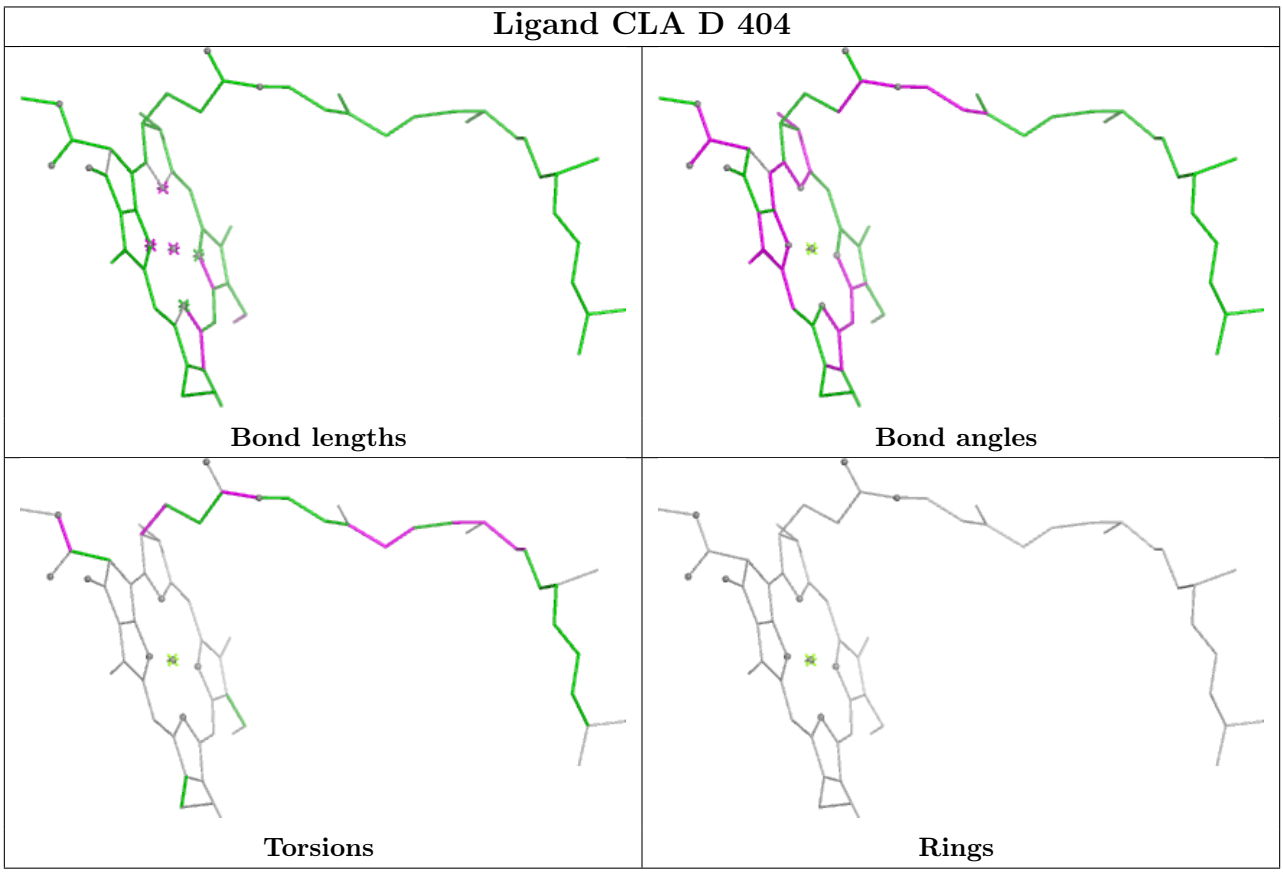
Ligand LUT Y 616



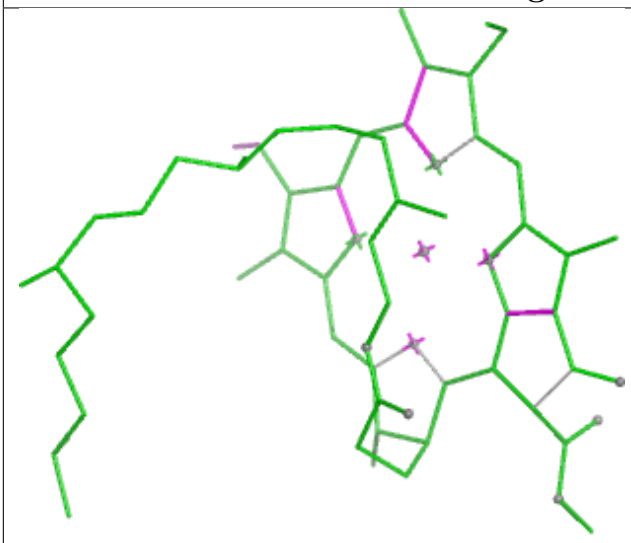
Ligand NEX n 617



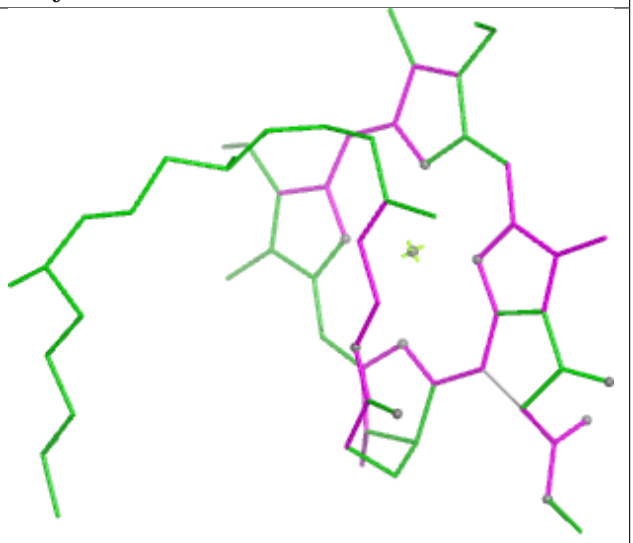
Ligand CLA D 404



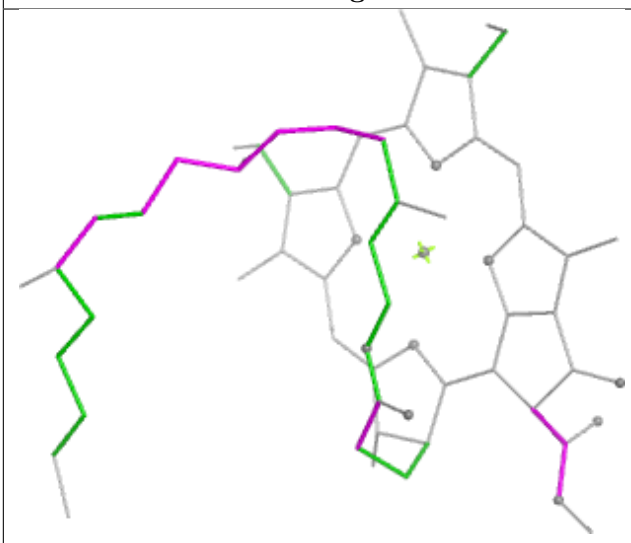
Ligand CLA y 313



Bond lengths



Bond angles



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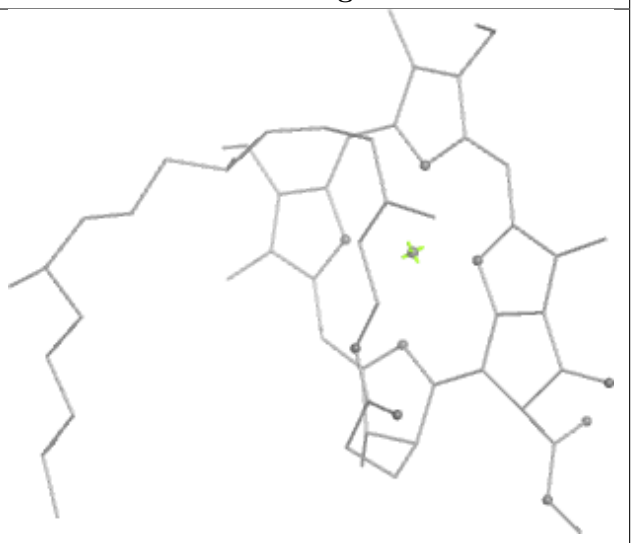
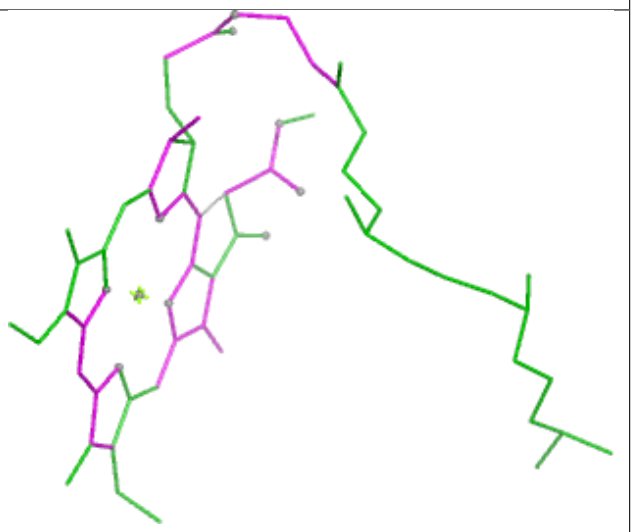


Rings

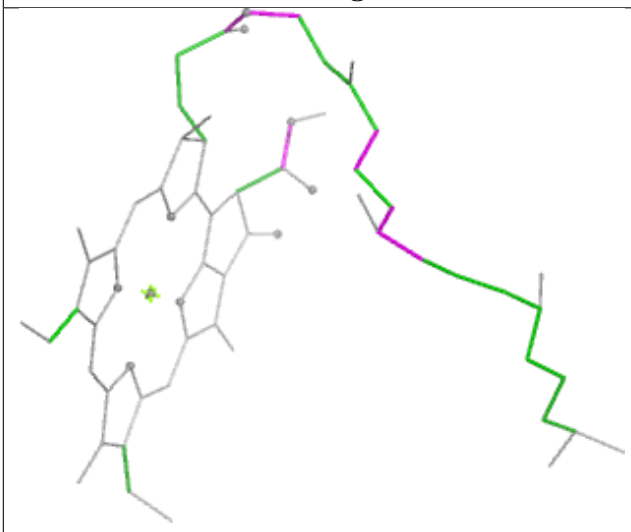
Ligand CLA b 613



Bond lengths



Bond angles



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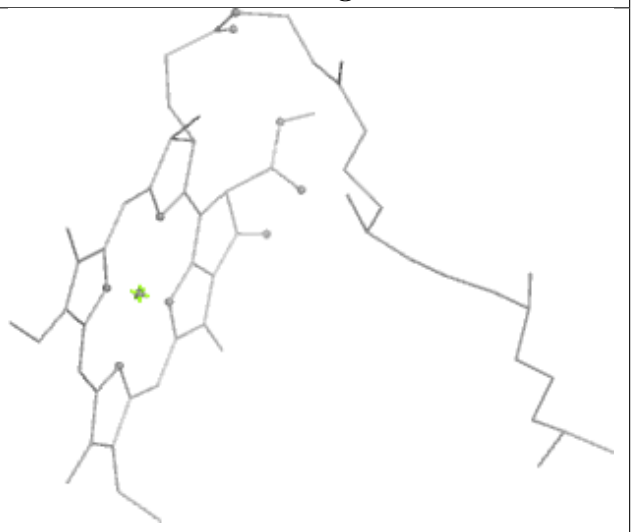
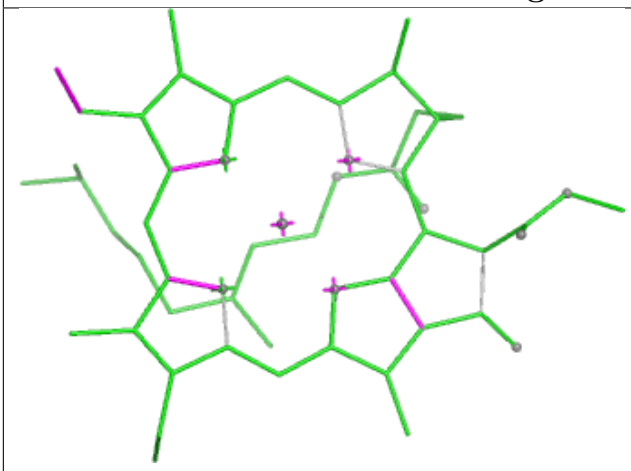


Rings

Ligand CLA n 613



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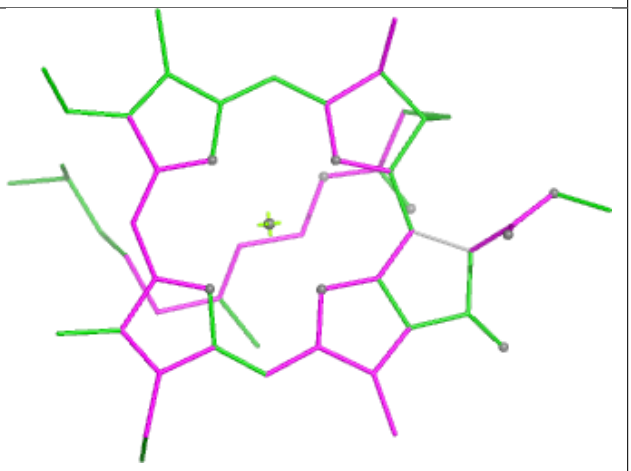
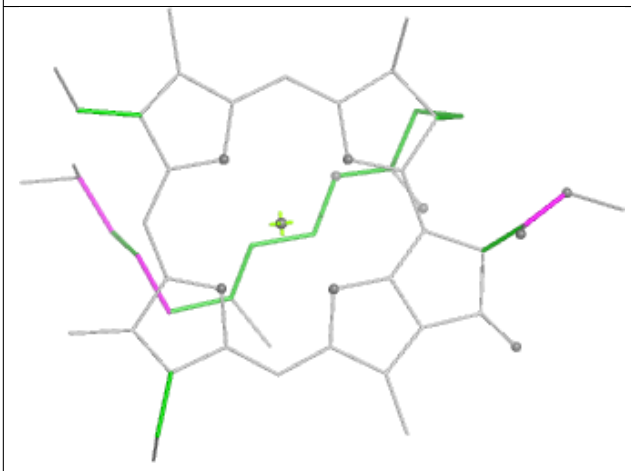


Bond angles



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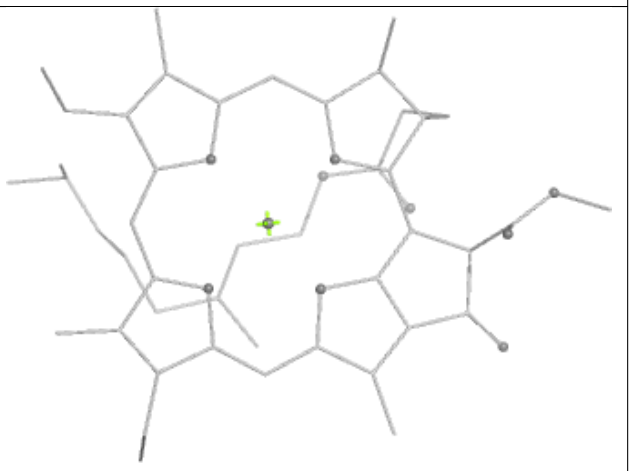
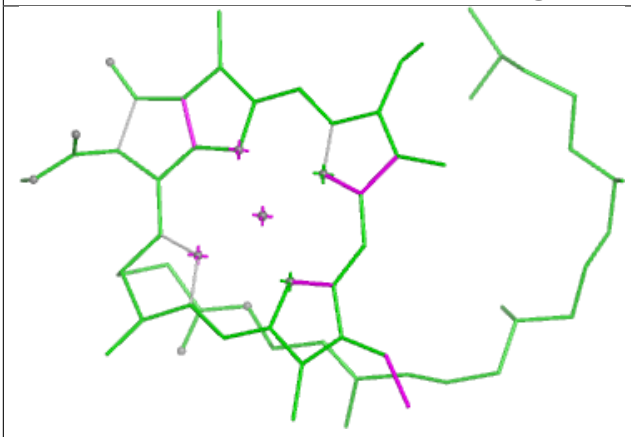


Rings

Ligand CLA r 609



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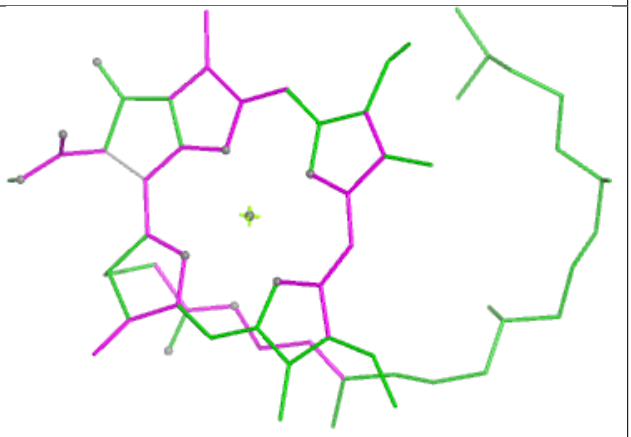

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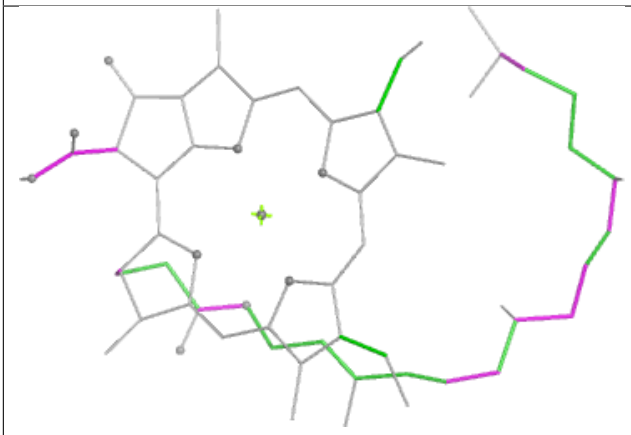

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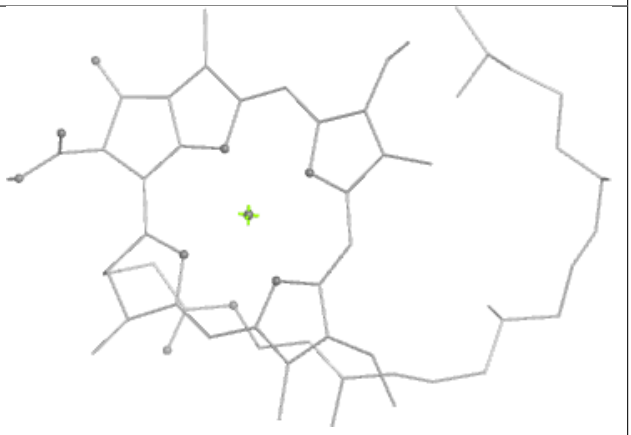
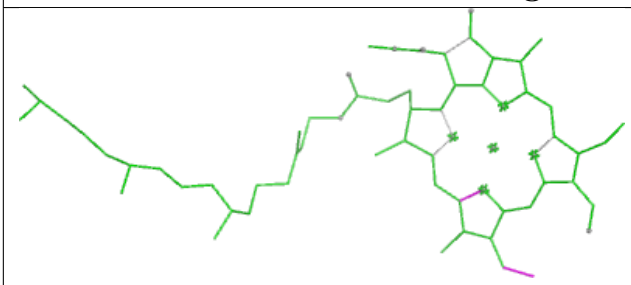


Rings

Ligand CHL Y 601



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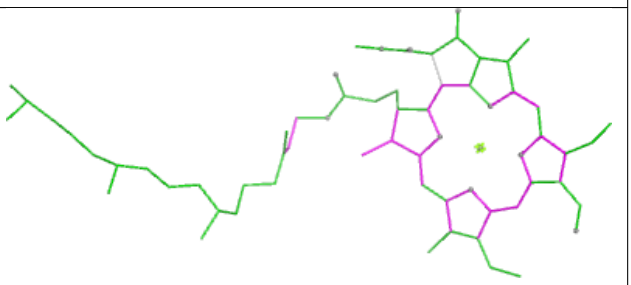
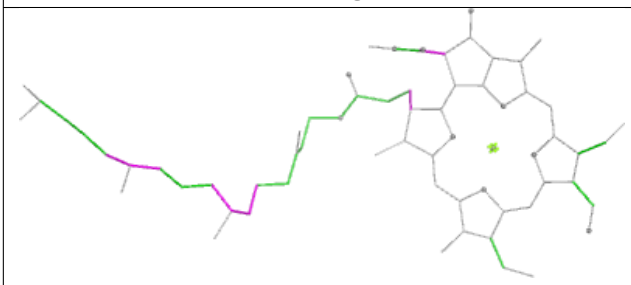


Bond angles



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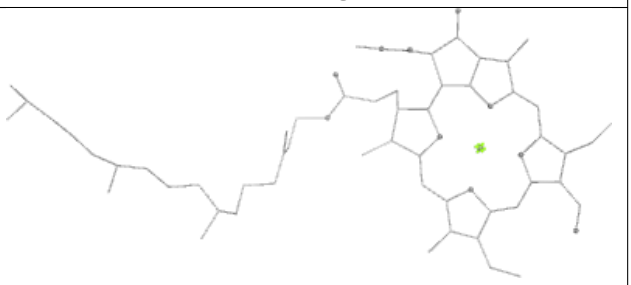
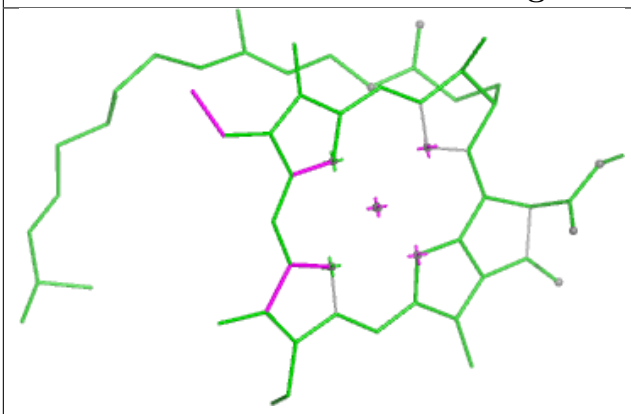


Rings

Ligand CLA y 310



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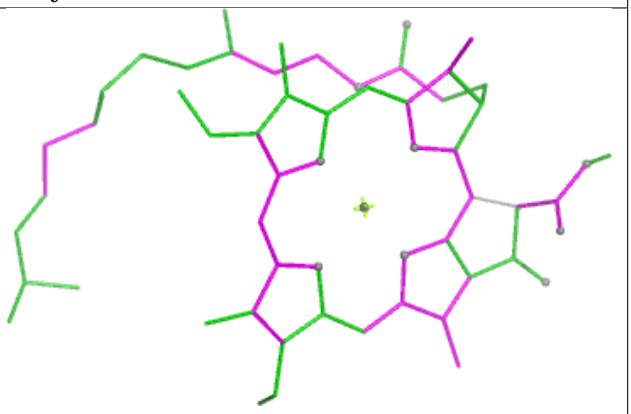
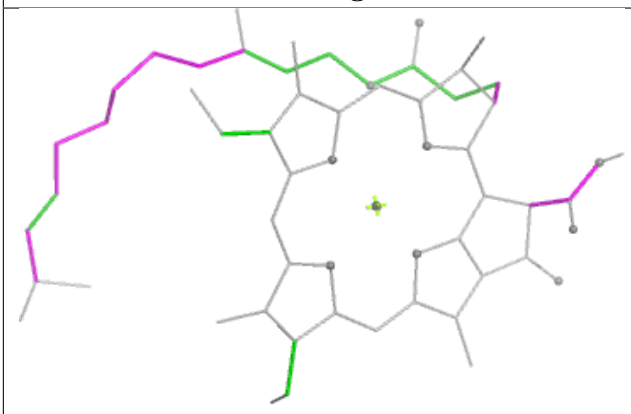


Bond angles



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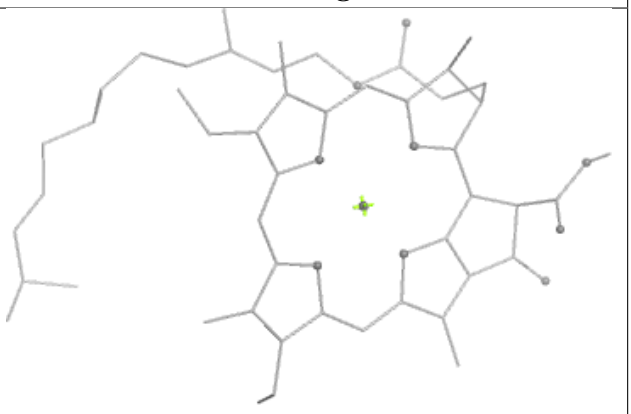
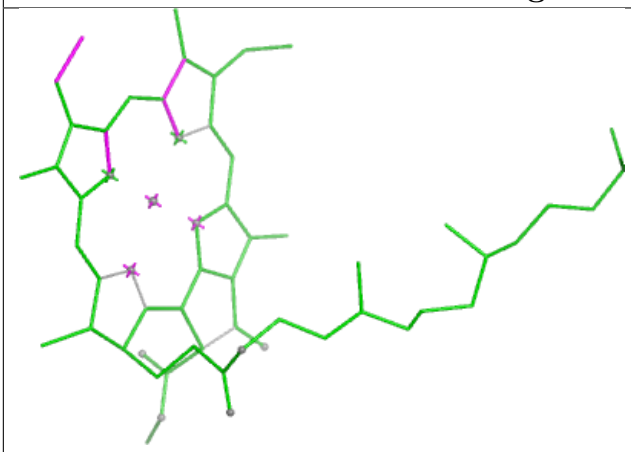


Rings

Ligand CLA y 311



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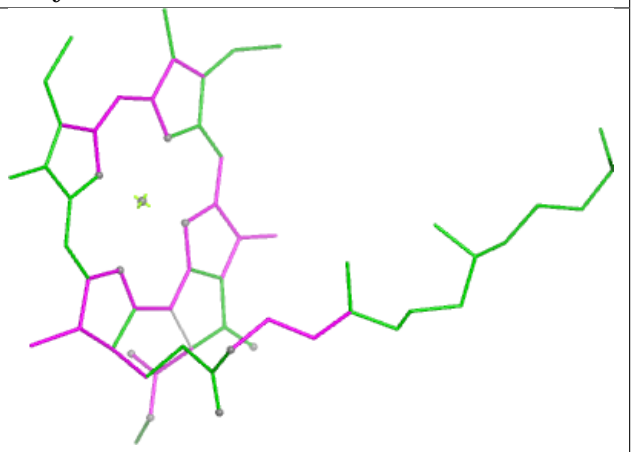
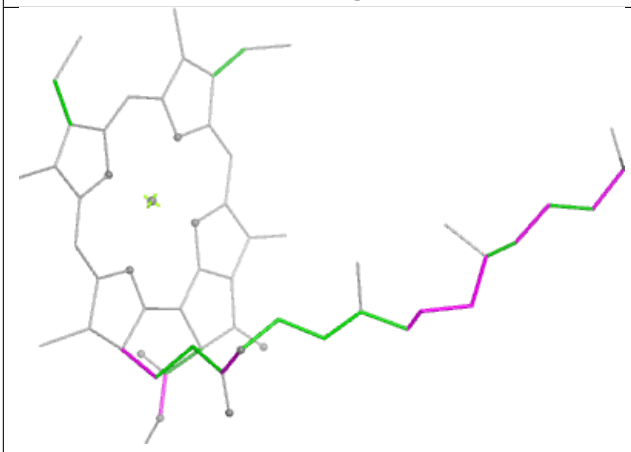


Bond angles



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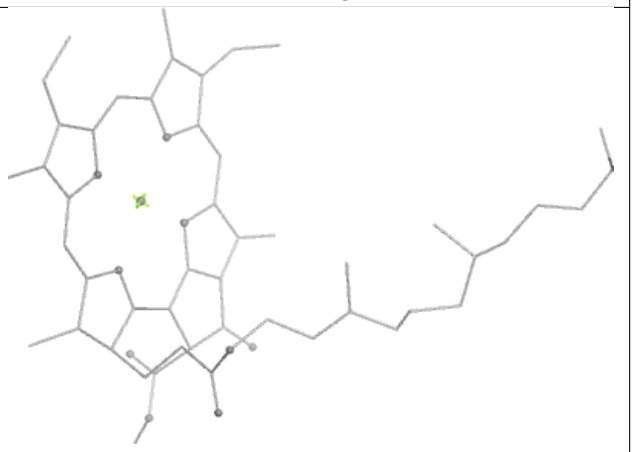
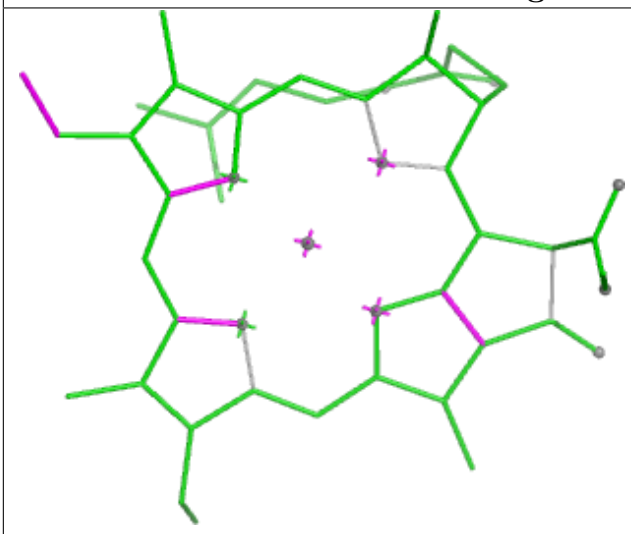


Rings

Ligand CLA S 305



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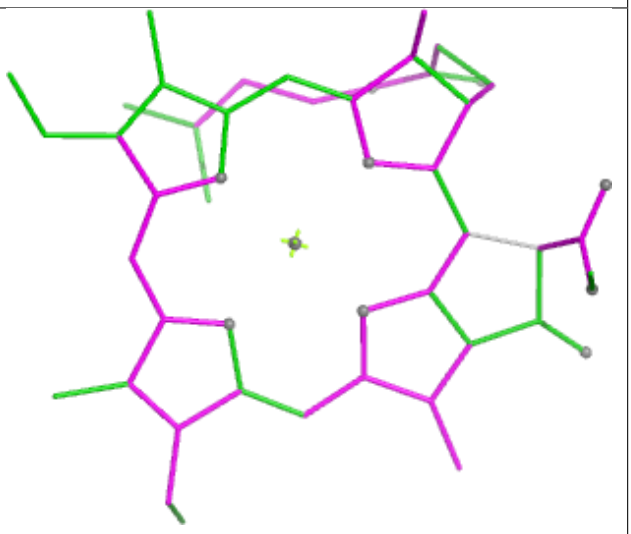

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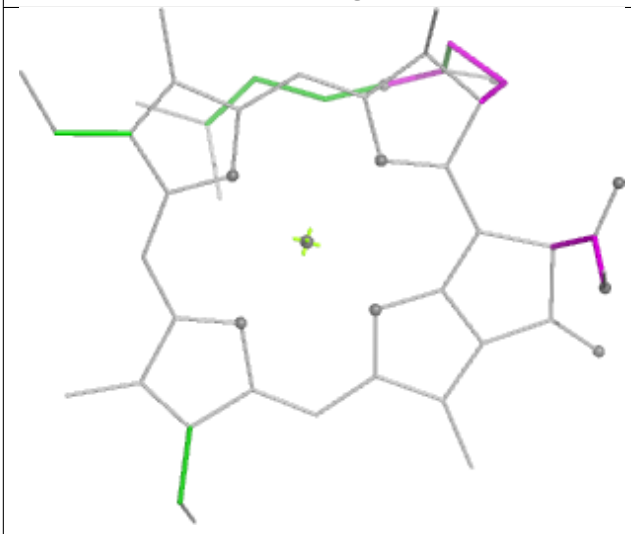

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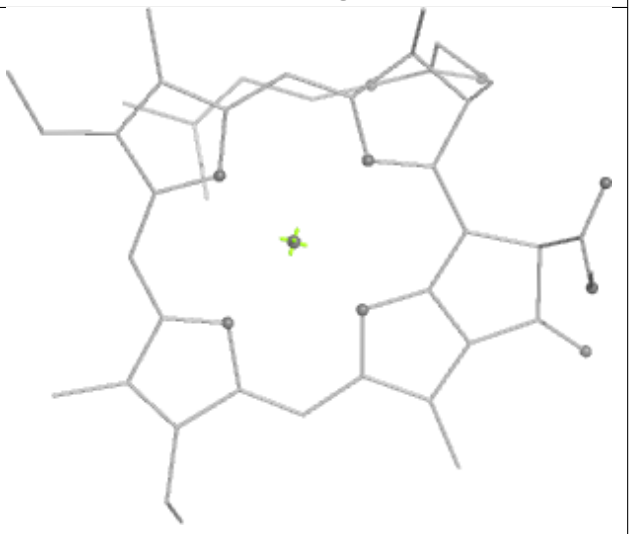
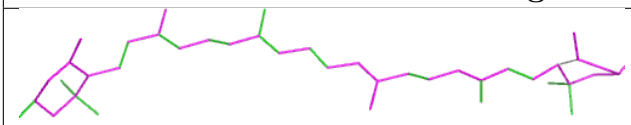


Rings

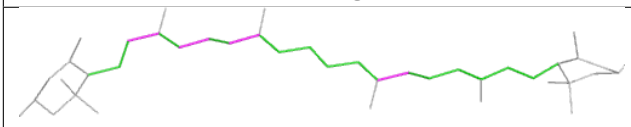
Ligand LUT n 615



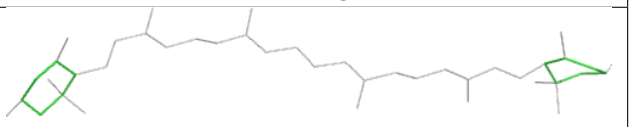
Bond lengths



Bond angles

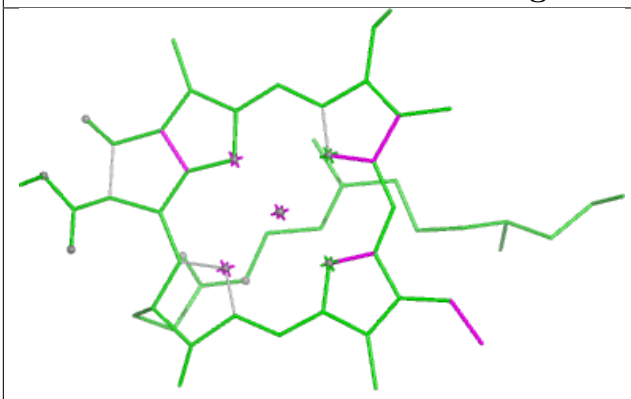


Torsions

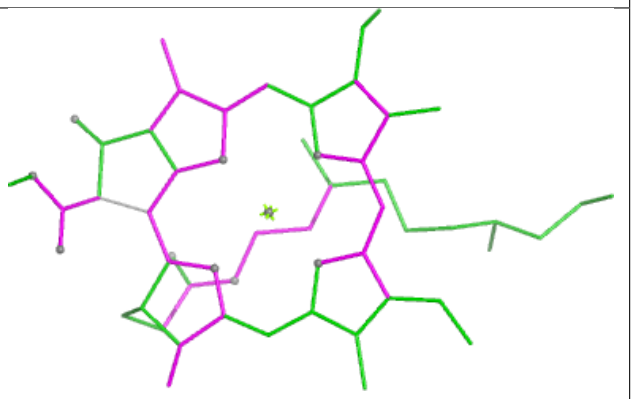


Rings

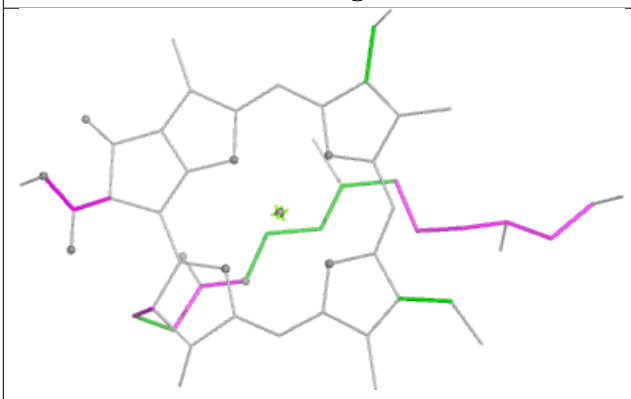
Ligand CLA c 505



Bond lengths



Bond angles



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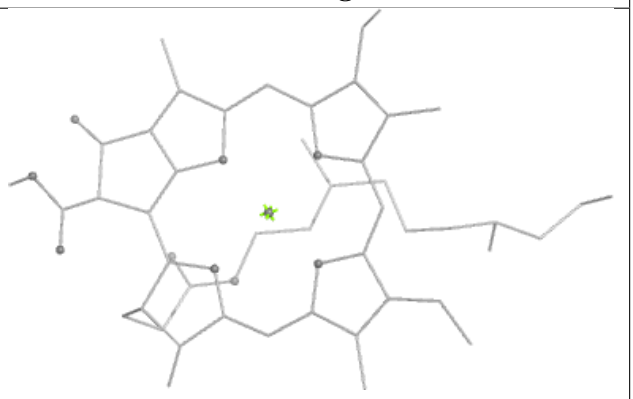
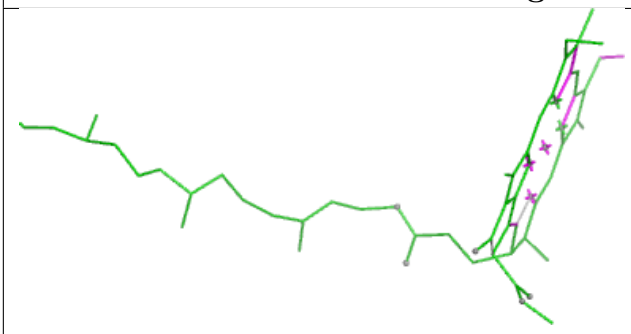


Rings

Ligand CLA b 604



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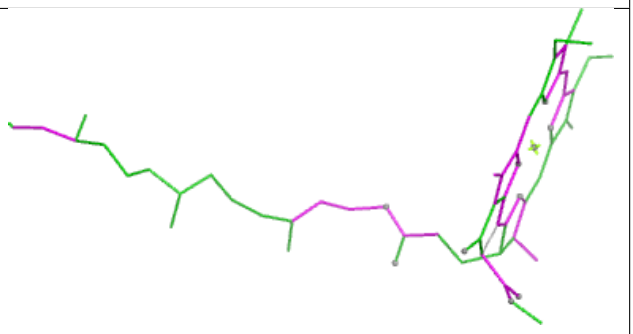
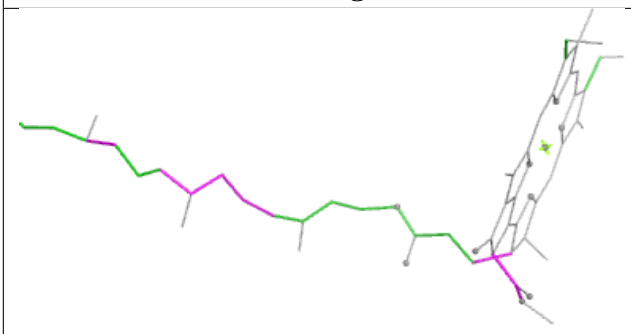


Bond angles



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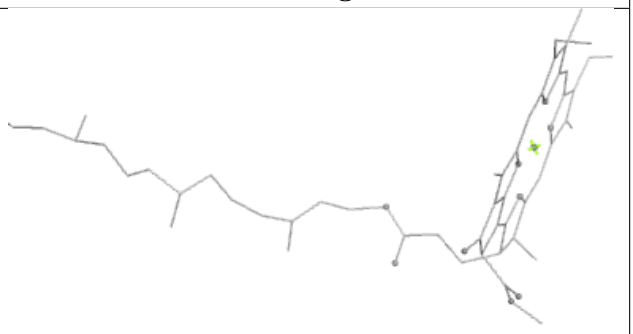
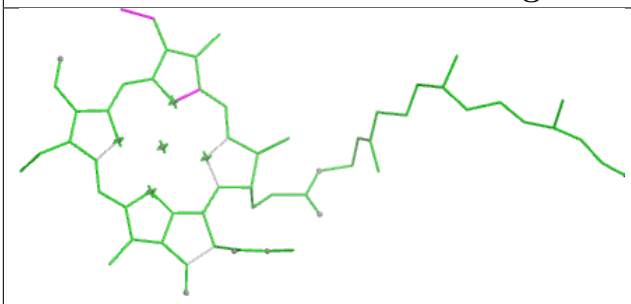


Rings

Ligand CHL G 601



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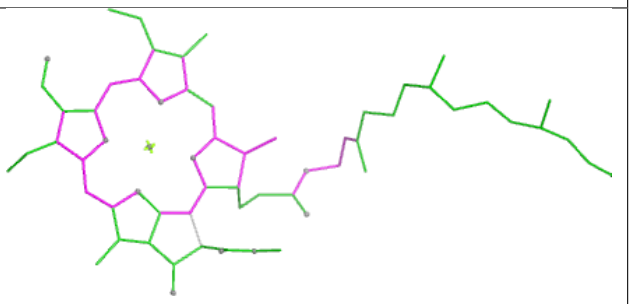
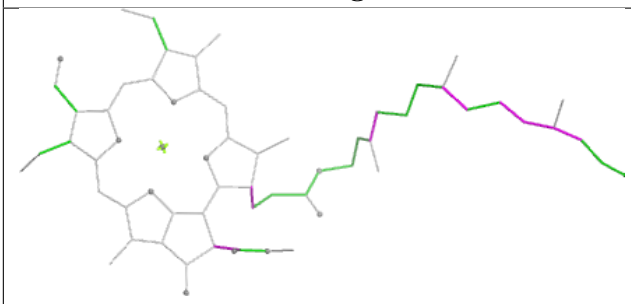


Bond angles



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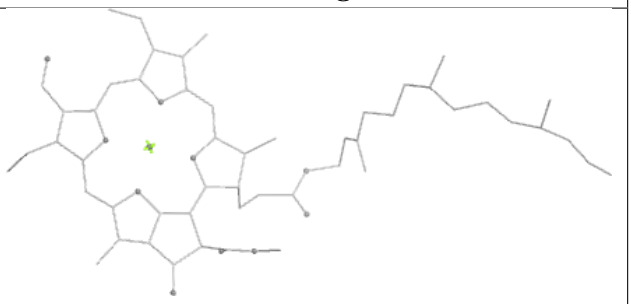
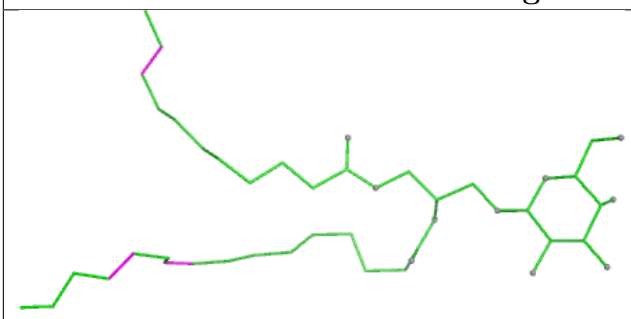


Rings

Ligand LMG d 409



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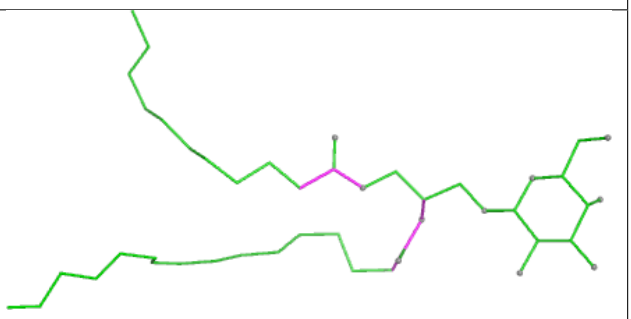
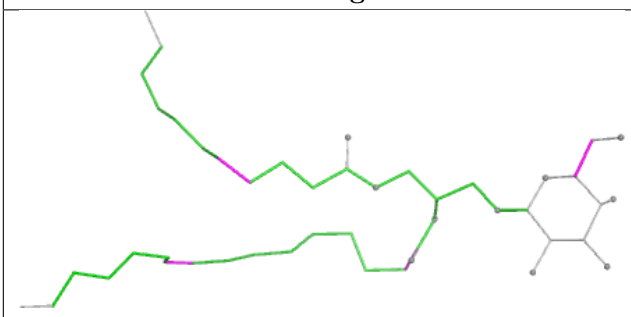
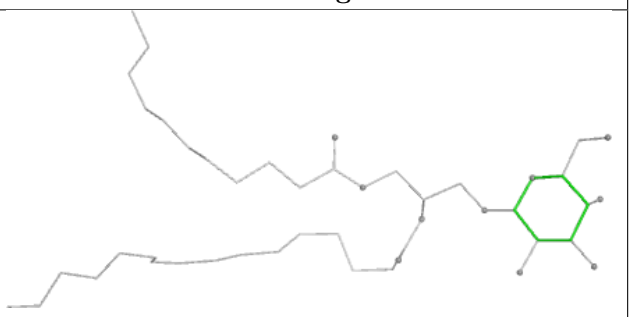


Bond angles

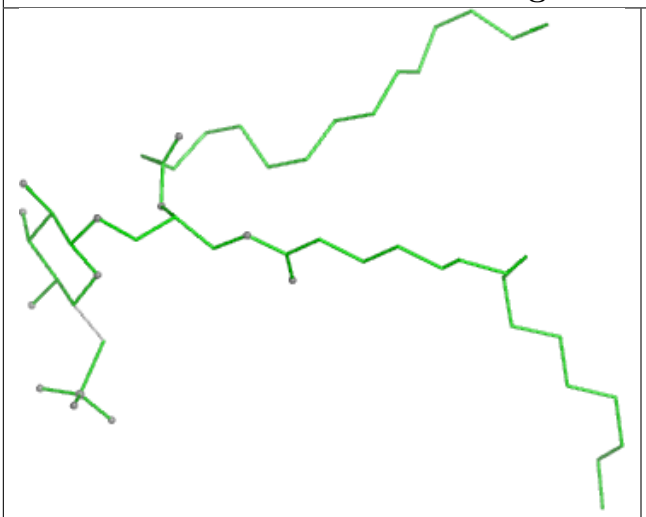


Torsions



Rings

Ligand SQD a 414



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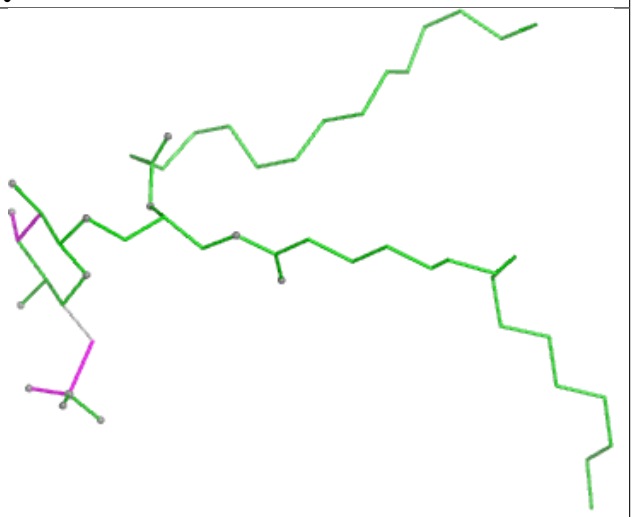
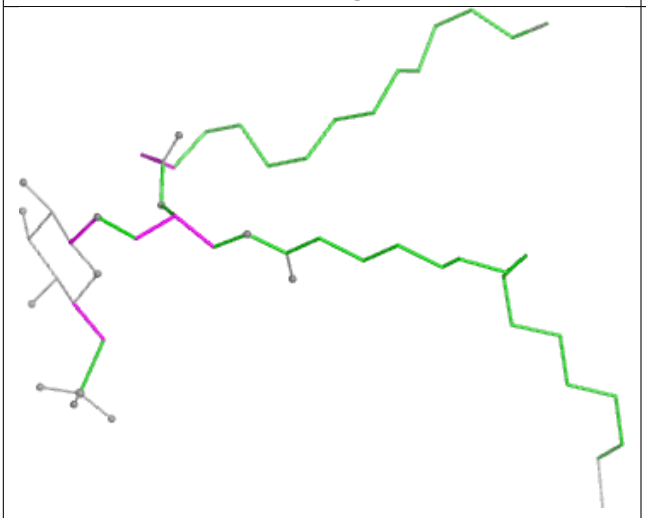


Bond angles



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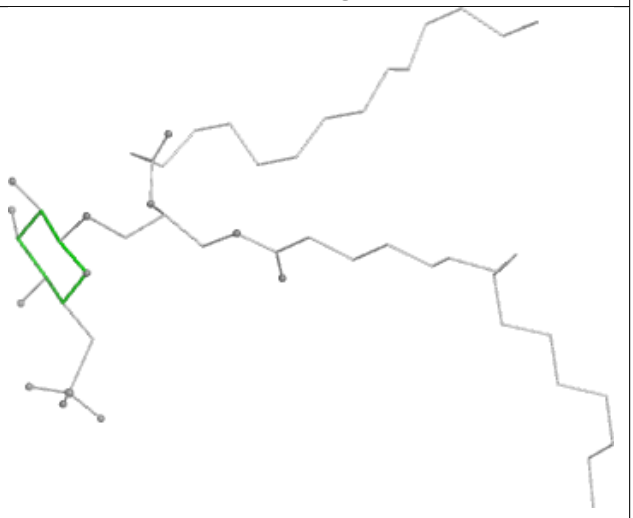
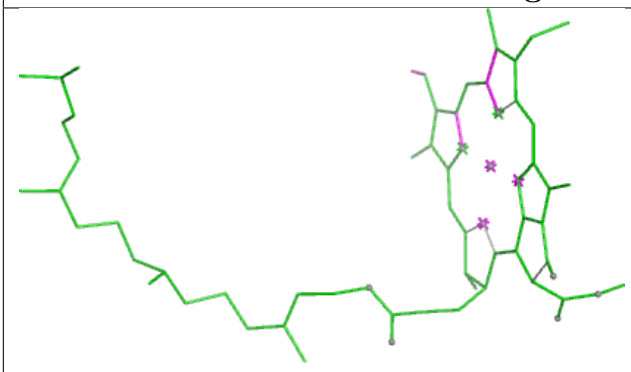


Rings

Ligand CLA B 609



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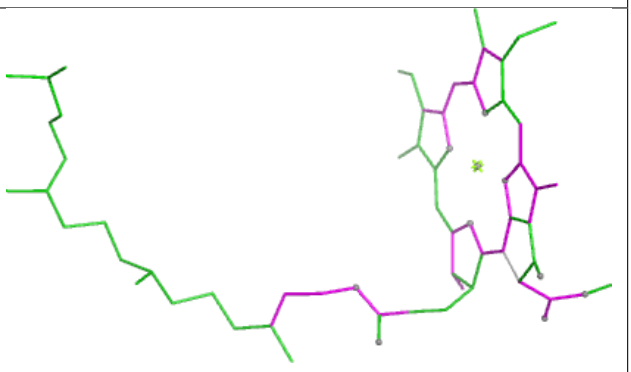
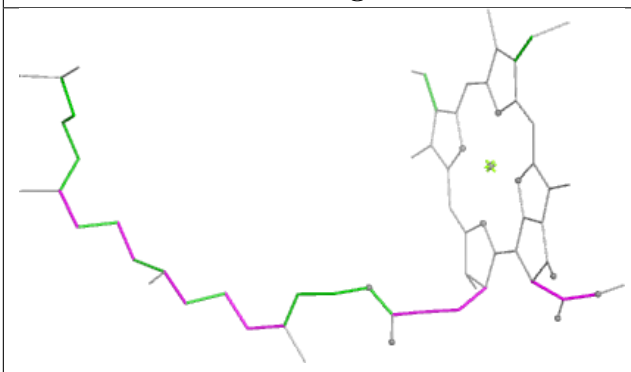


Bond angles

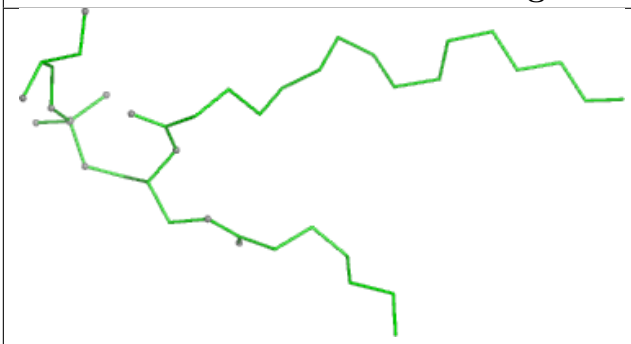


Torsions



Rings

Ligand LHG c 520



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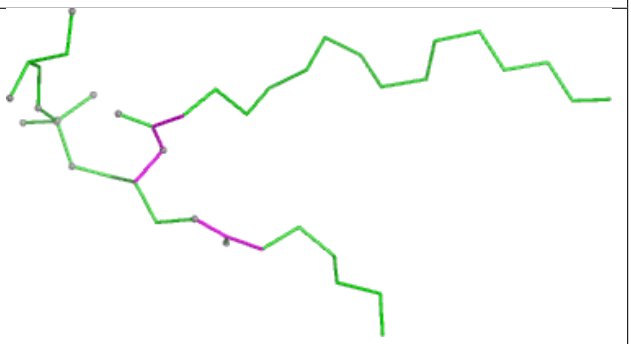
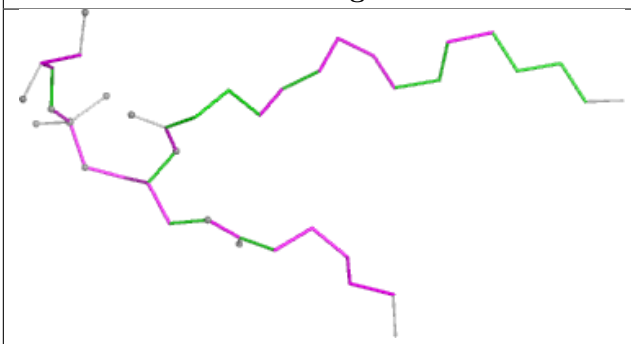


Bond angles



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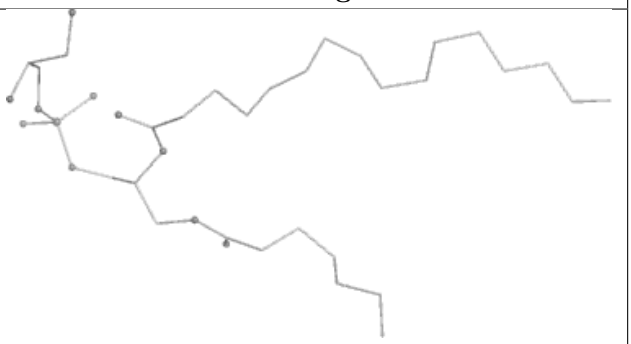
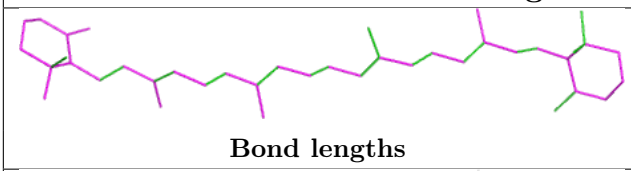


Rings

Ligand BCR b 618



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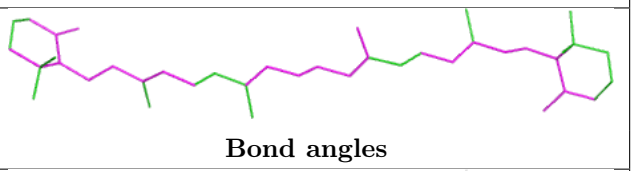
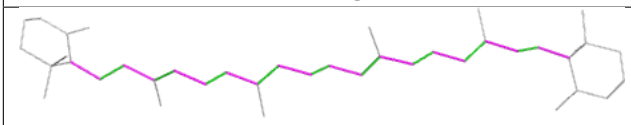


Bond angles



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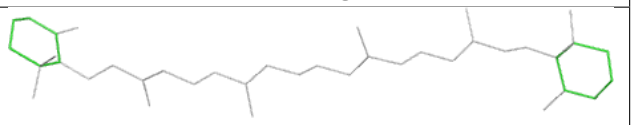
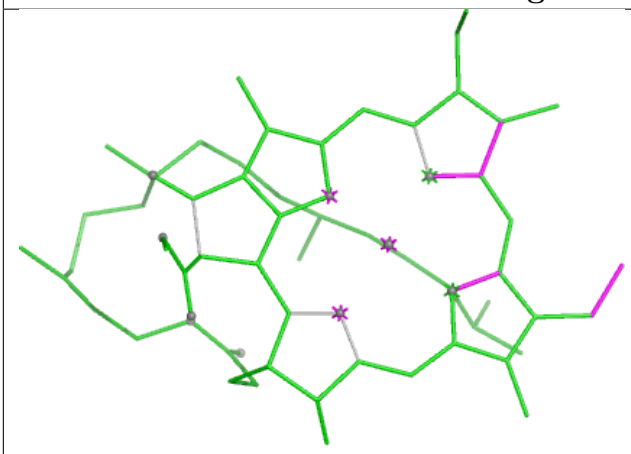


Rings

Ligand CLA b 601



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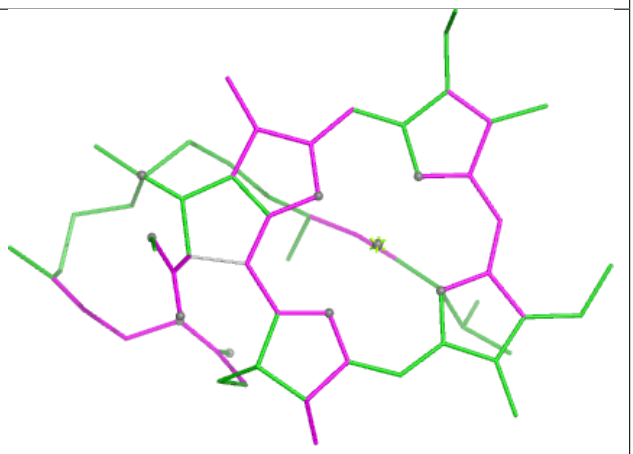
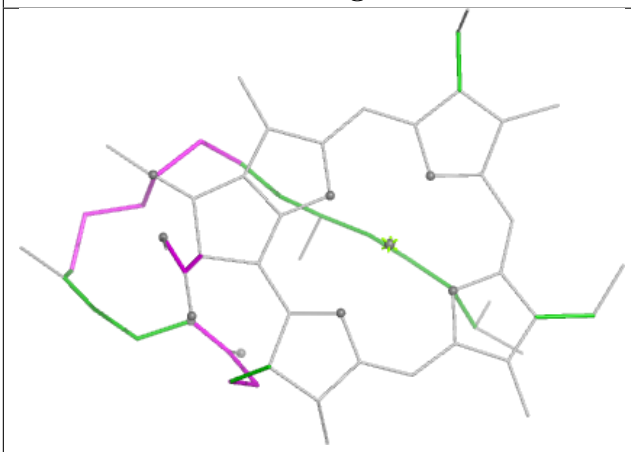


Bond angles



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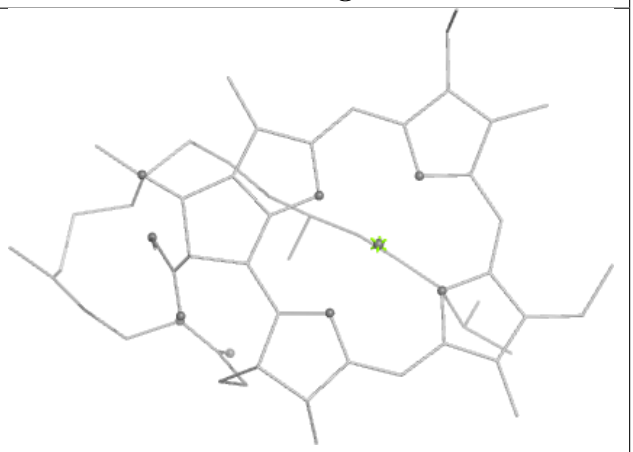
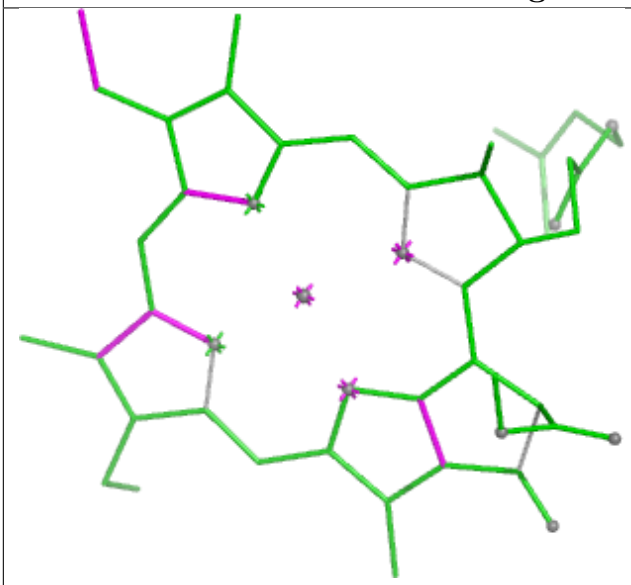


Rings

Ligand CLA g 604



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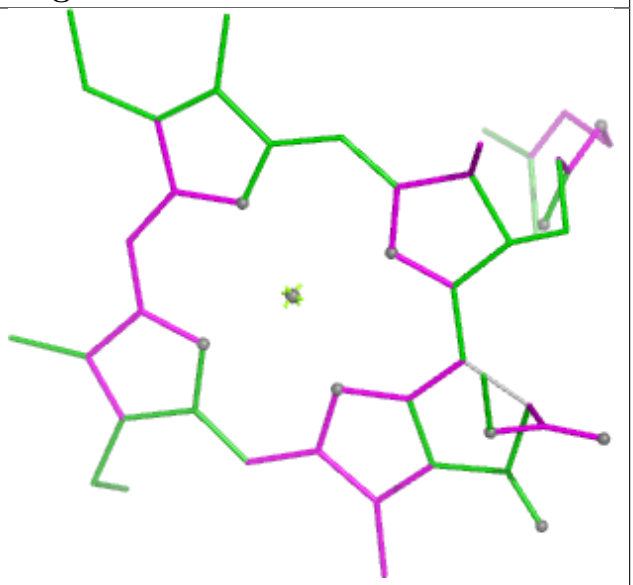
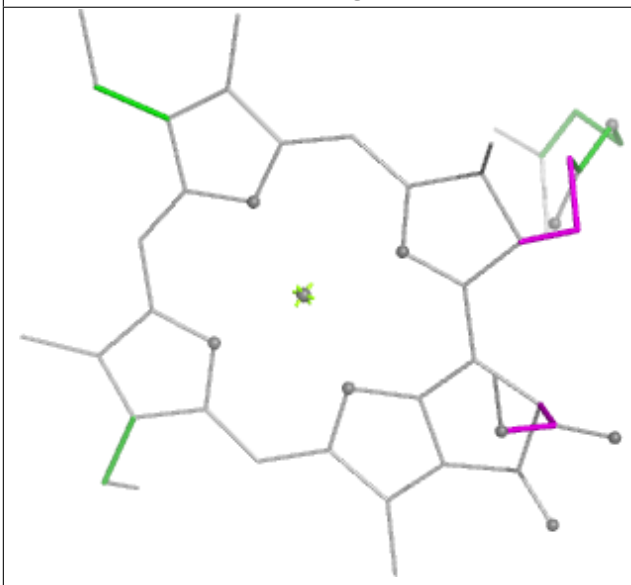


Bond angles



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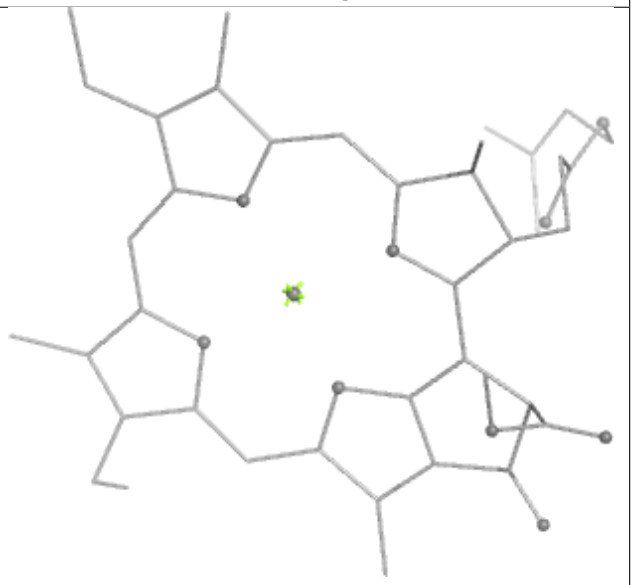
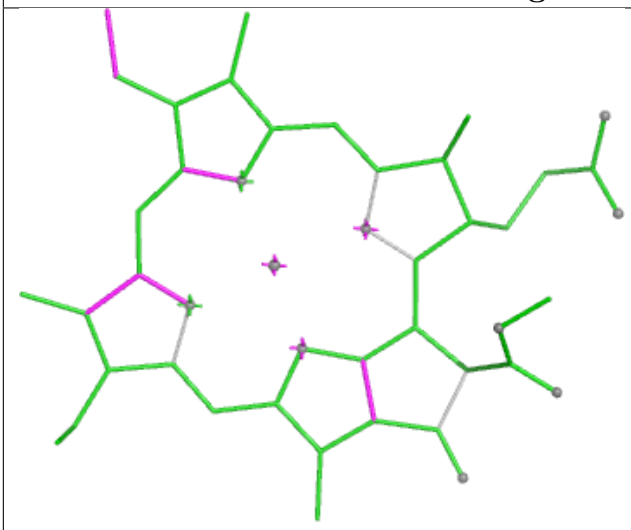
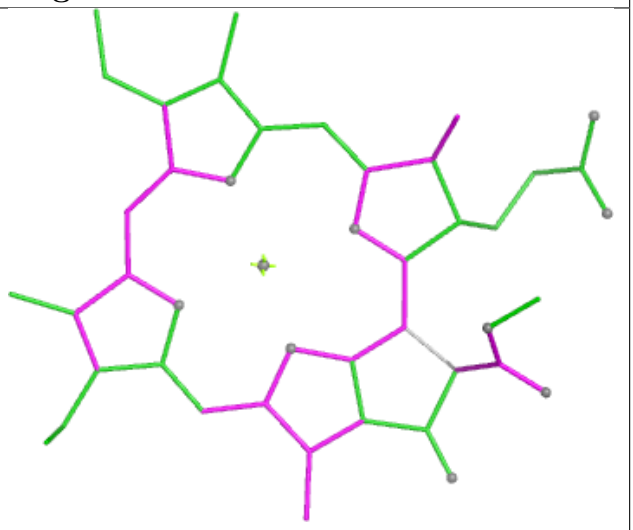


Rings

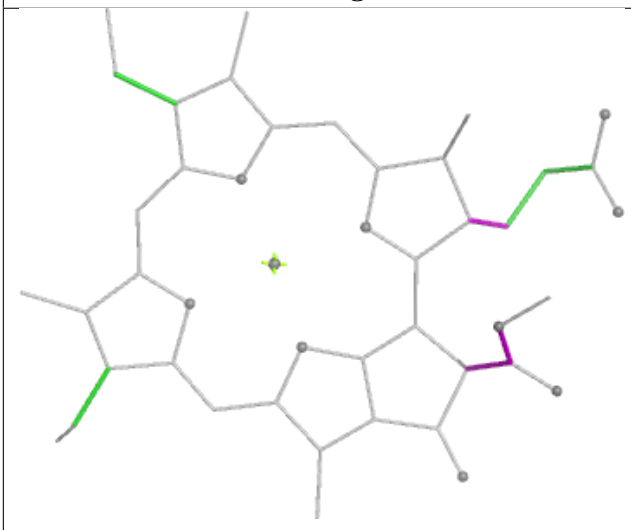
Ligand CLA g 612



Bond lengths



Bond angles



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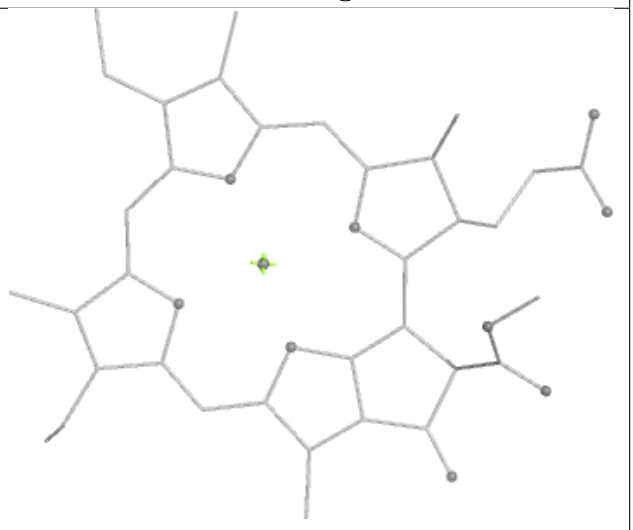
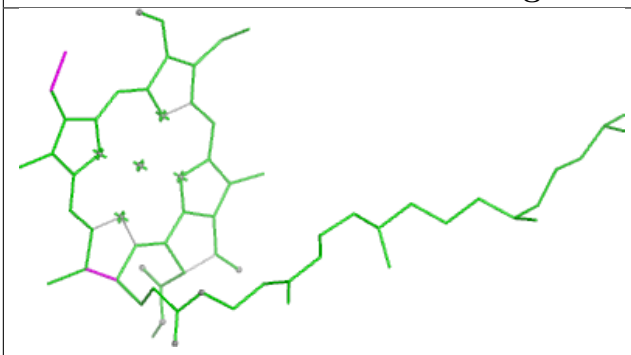


Rings

Ligand CHL Y 609



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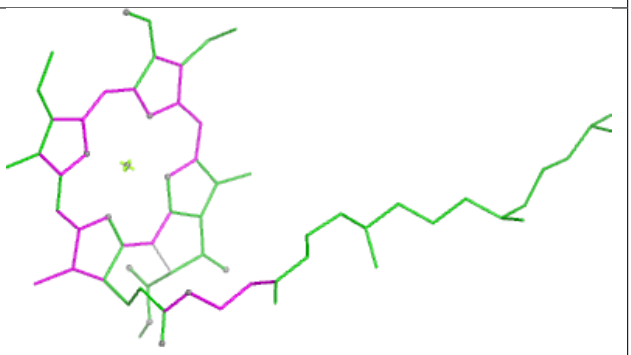
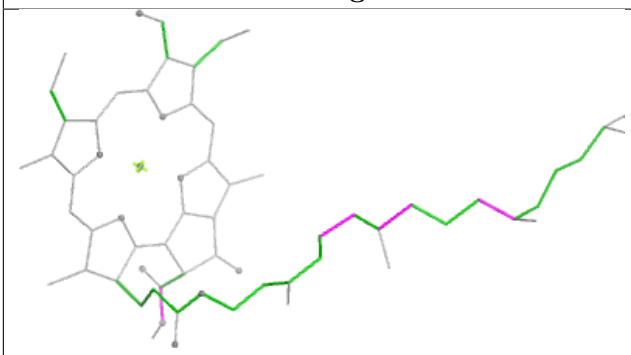


Bond angles



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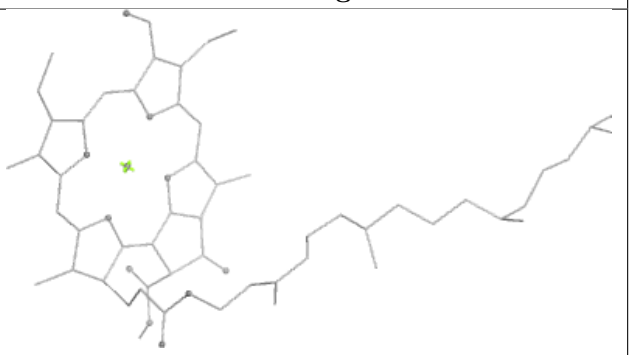
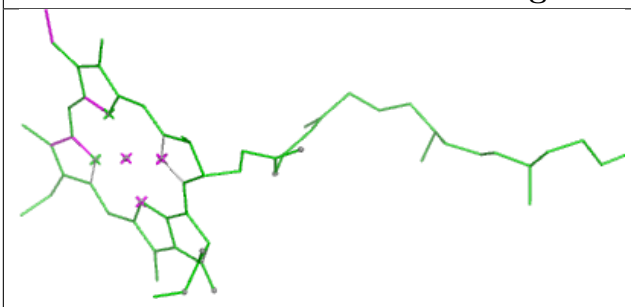
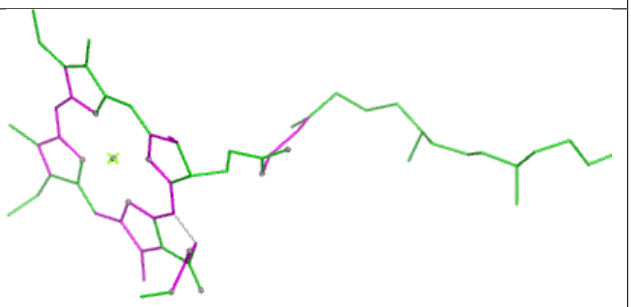


Rings

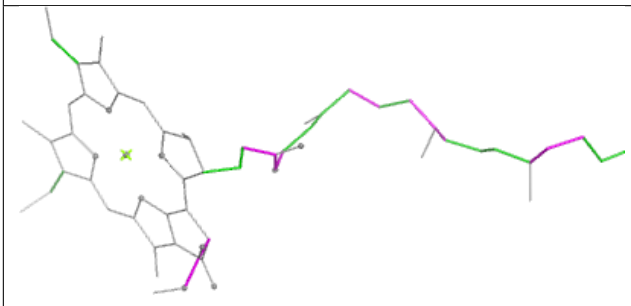
Ligand CLA c 502



Bond lengths



Bond angles



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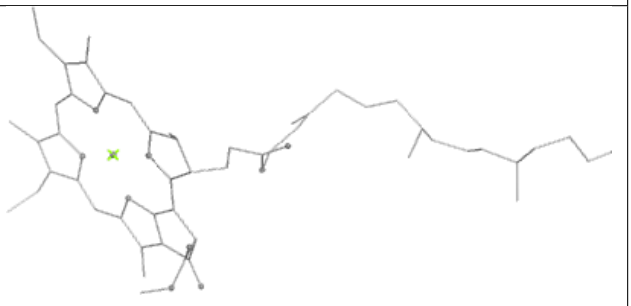
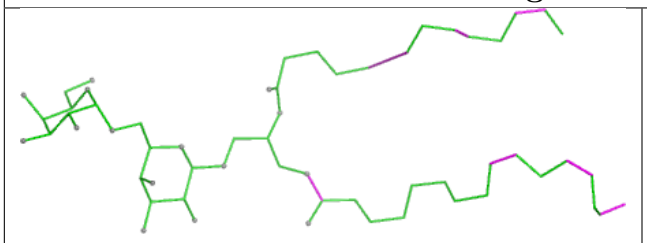
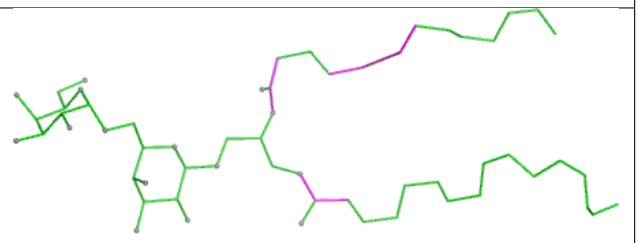


Rings

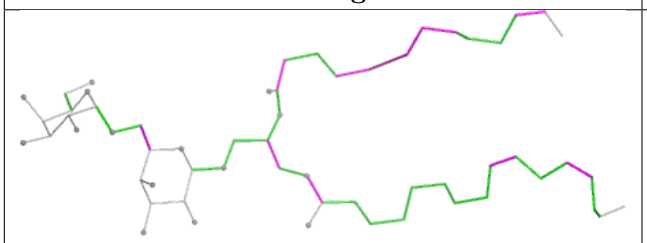
Ligand DGD c 518



Bond lengths



Bond angles



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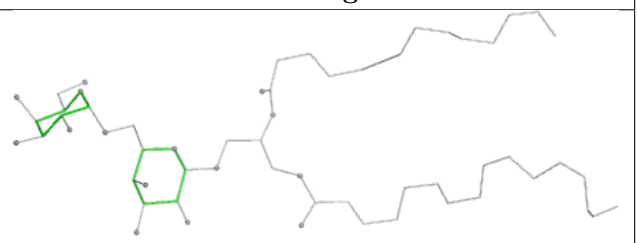
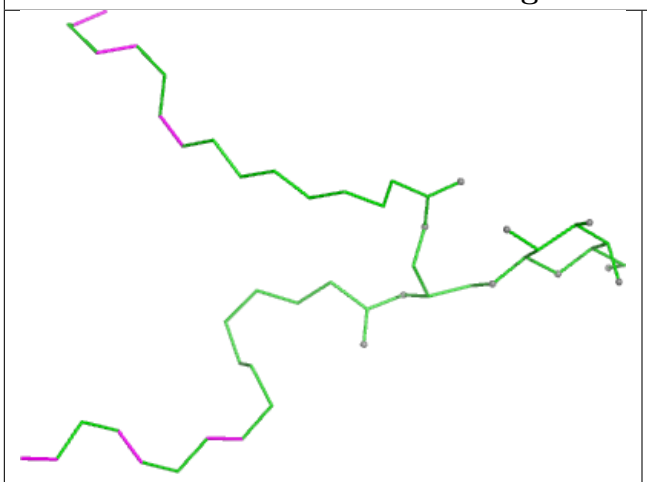
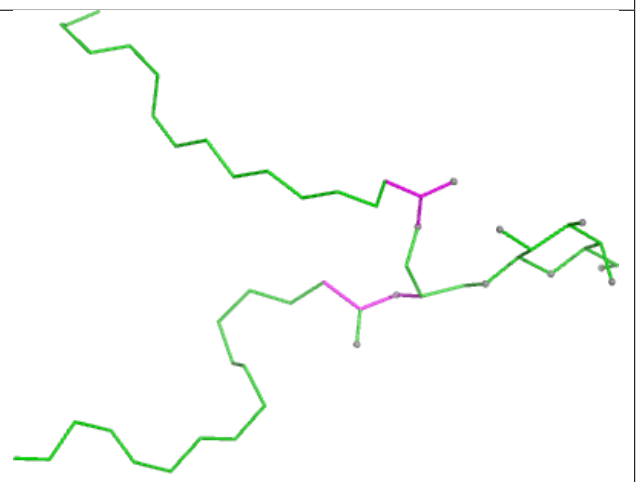


Rings

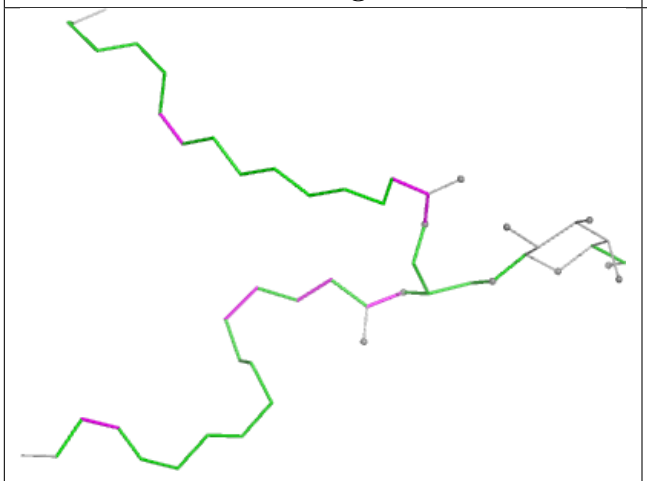
Ligand LMG B 621



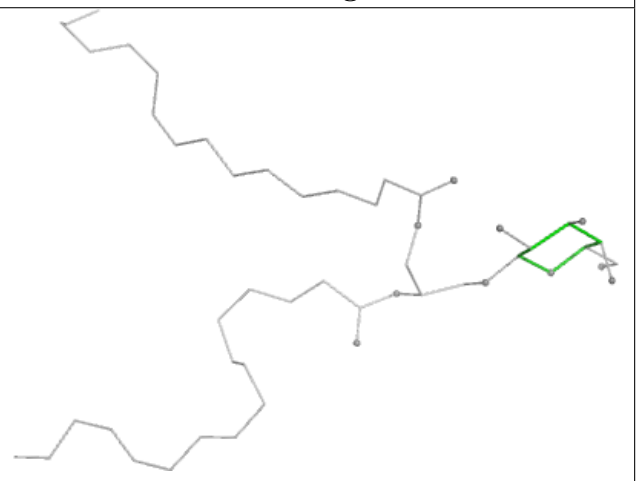
Bond lengths



Bond angles

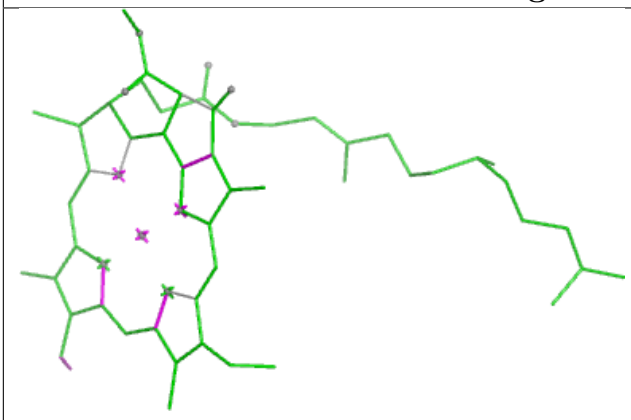


Torsions

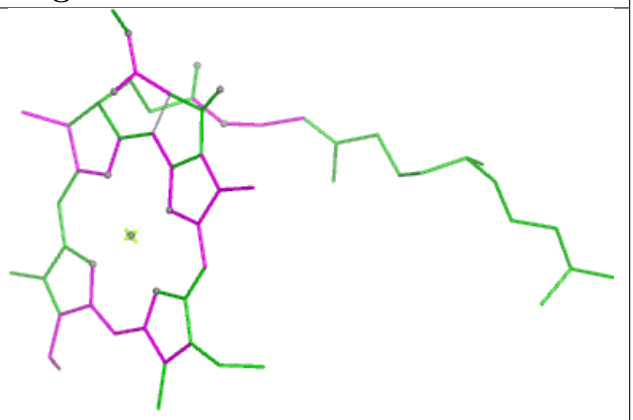


Rings

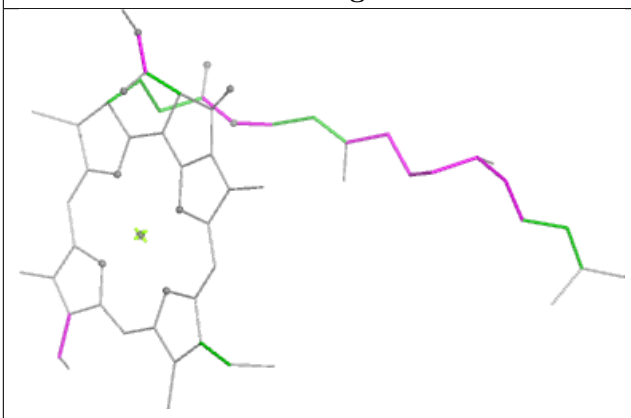
Ligand CLA g 611



Bond lengths



Bond angles



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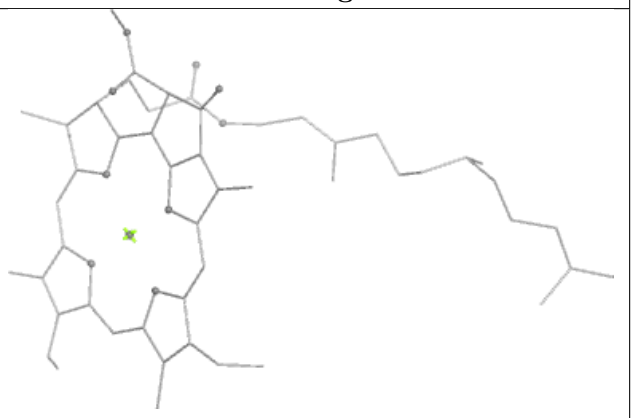
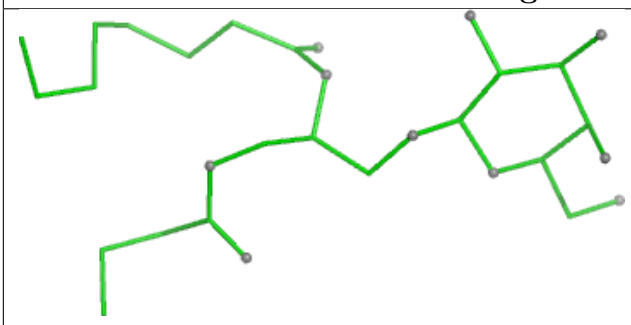


Rings

Ligand LMG B 624



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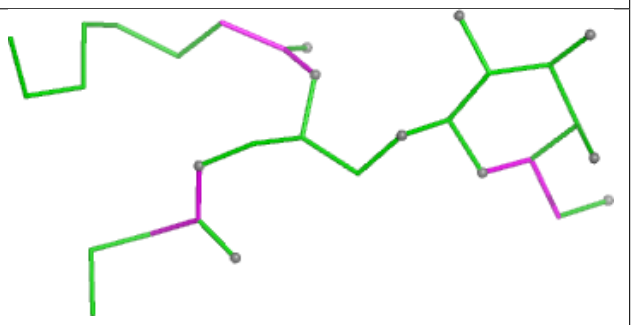
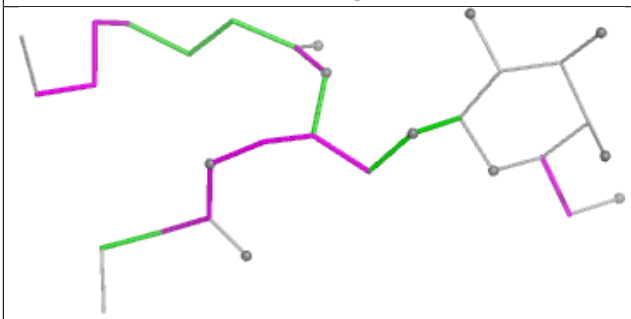


Bond angles



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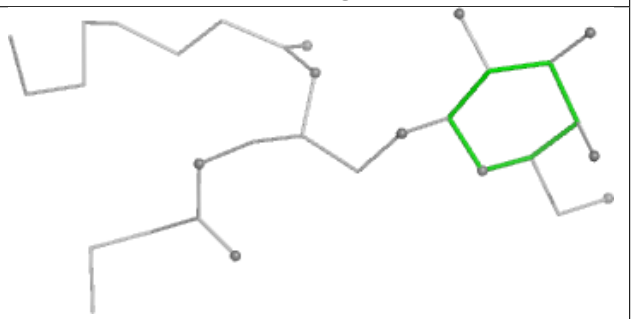
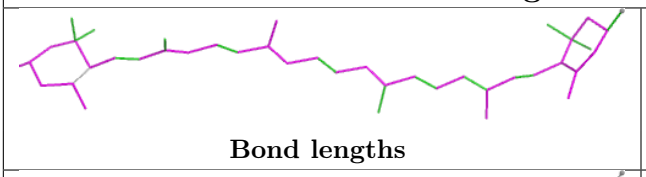


Rings

Ligand LUT N 616



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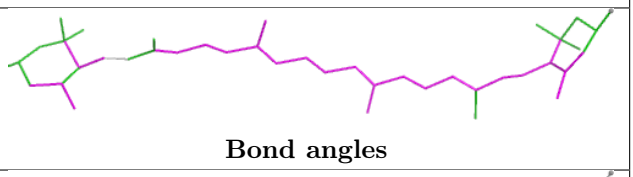
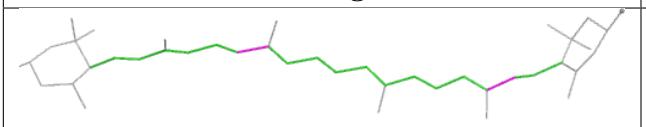


Bond angles



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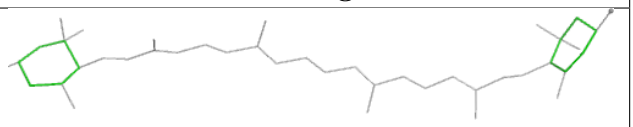
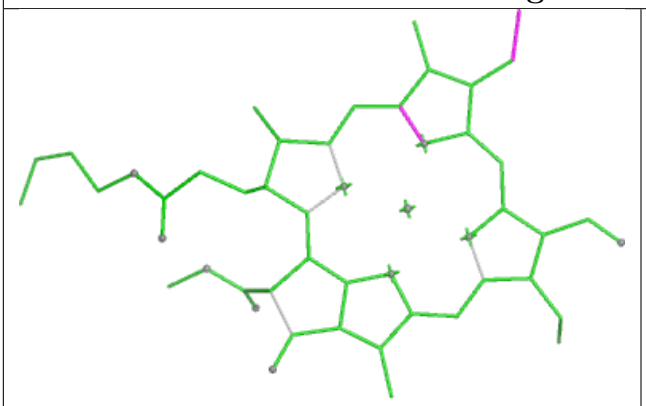


Rings

Ligand CHL n 606



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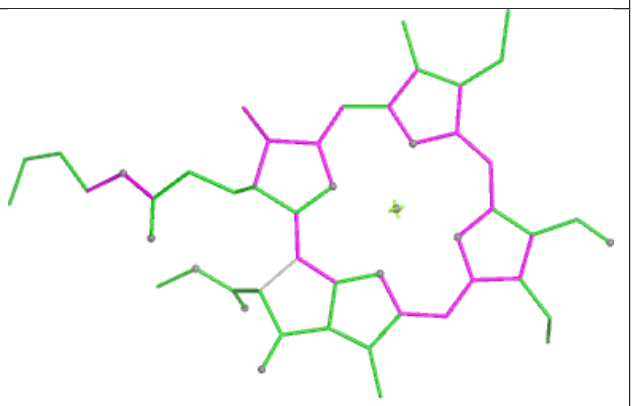
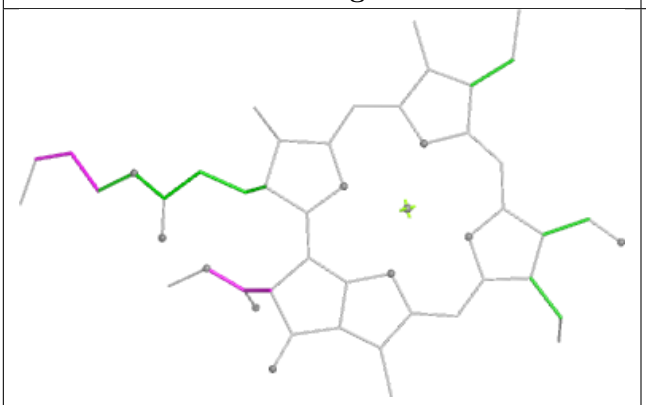


Bond angles



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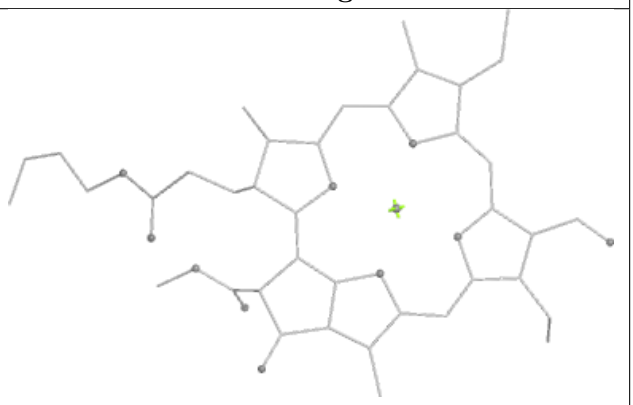
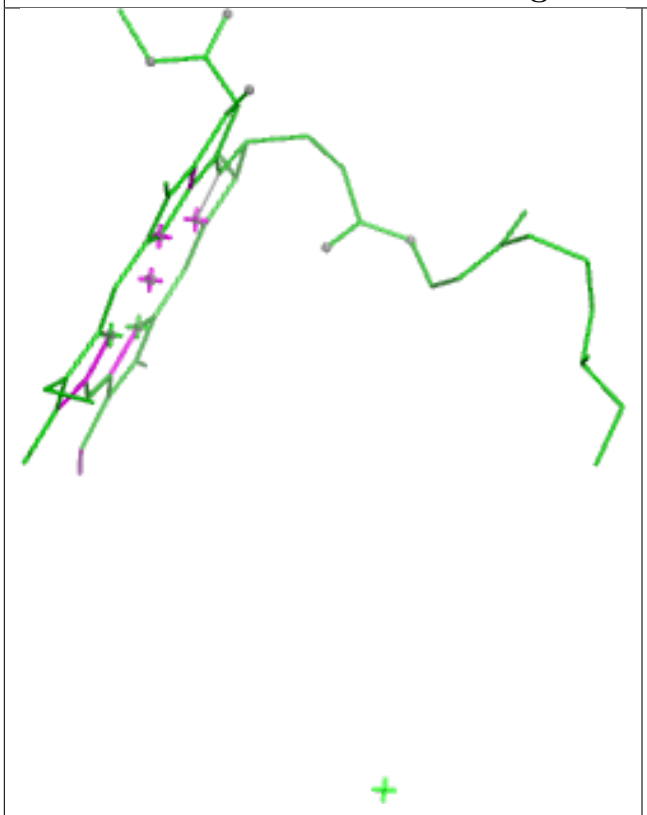


Rings

Ligand CLA c 506



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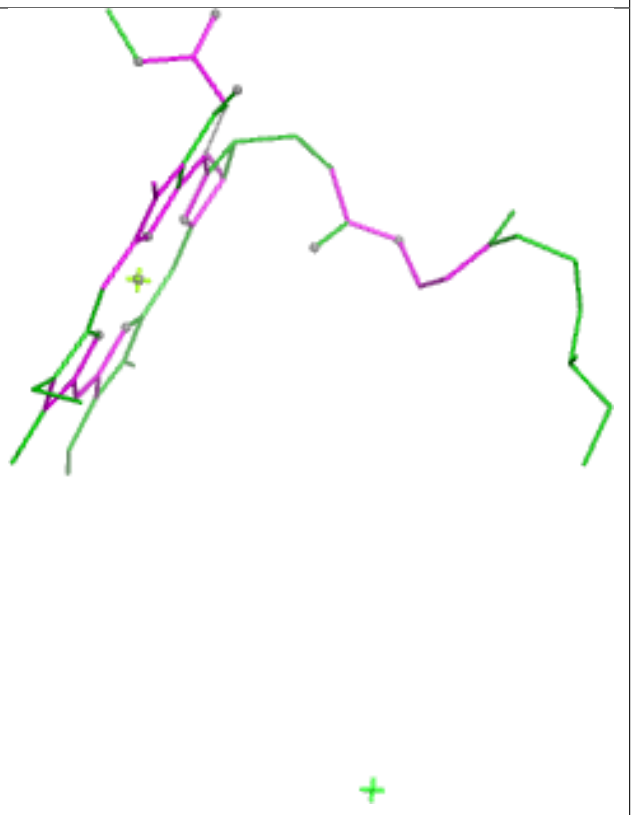


Bond angles

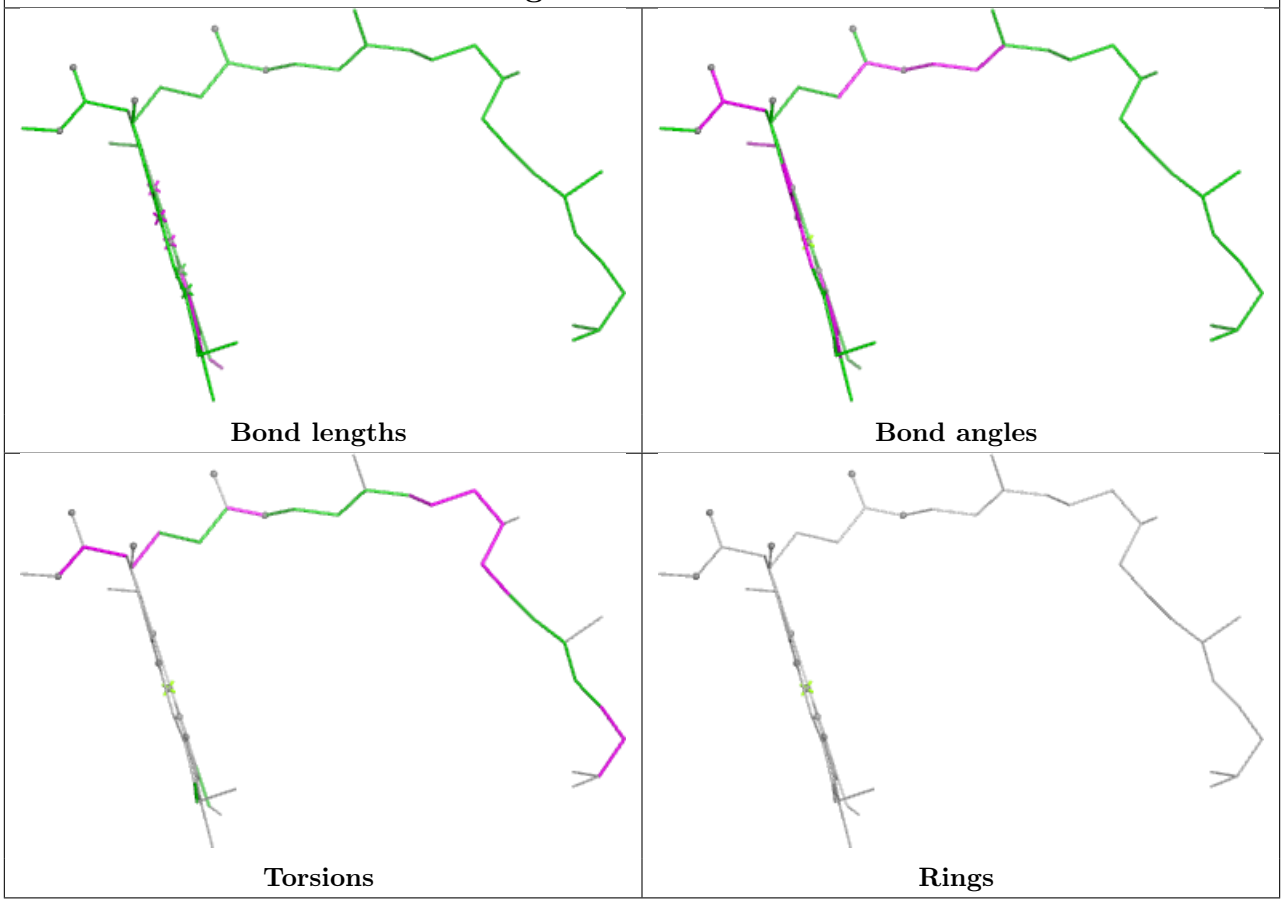


Torsions

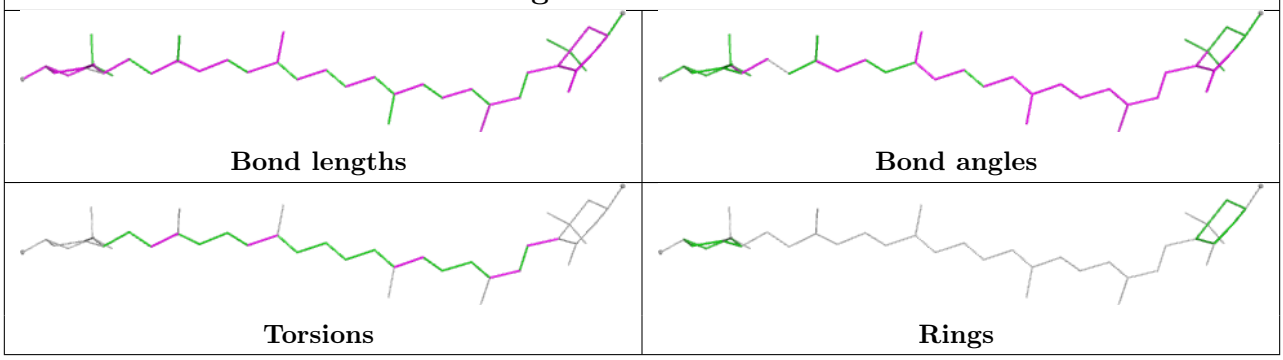


Rings

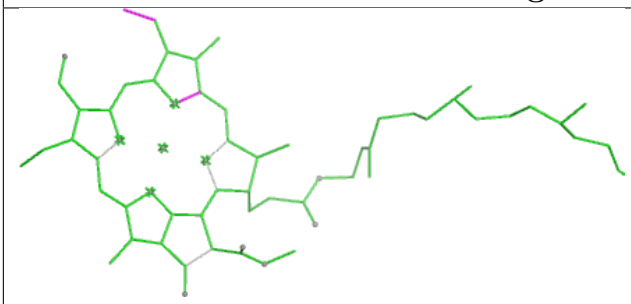
Ligand CLA C 506



Ligand LUT s 614



Ligand CHL y 302



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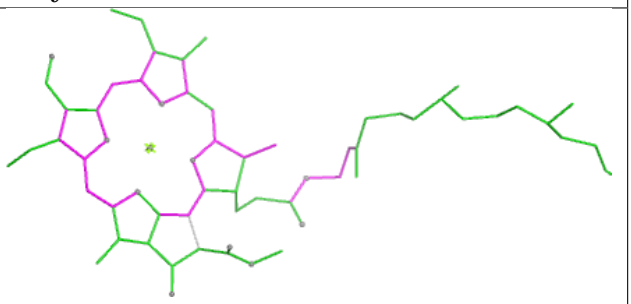
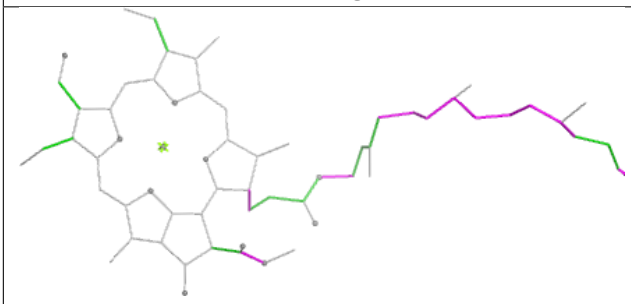


Bond angles



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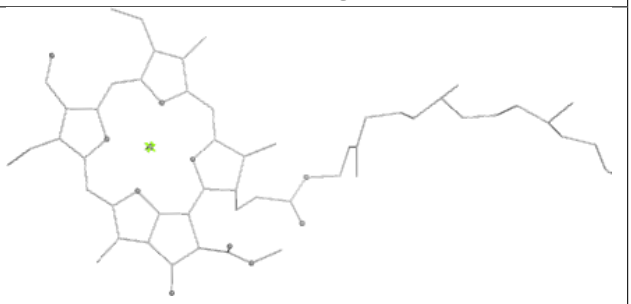
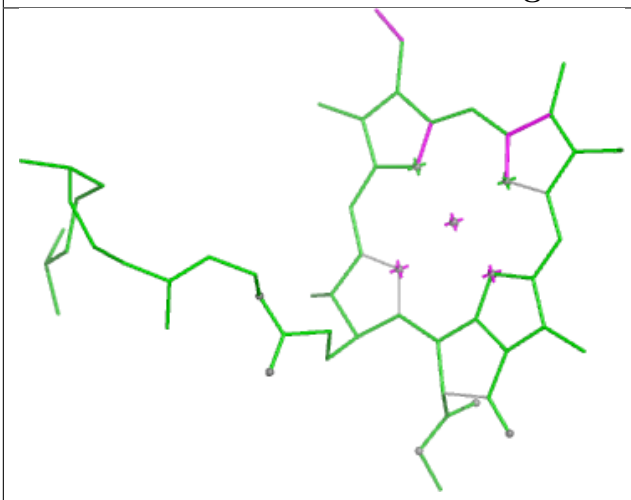


Rings

Ligand CLA A 408



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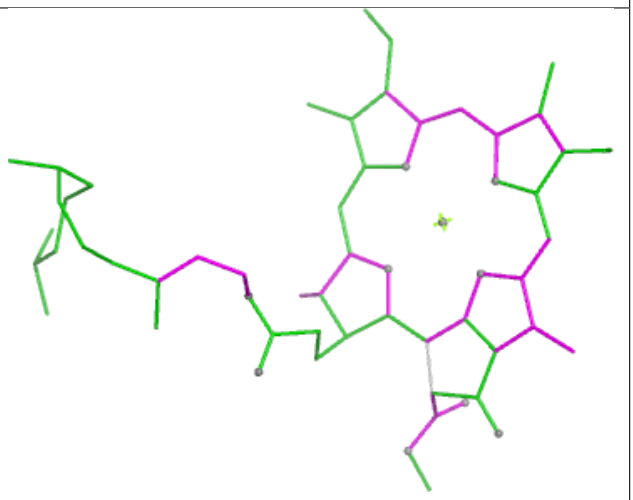
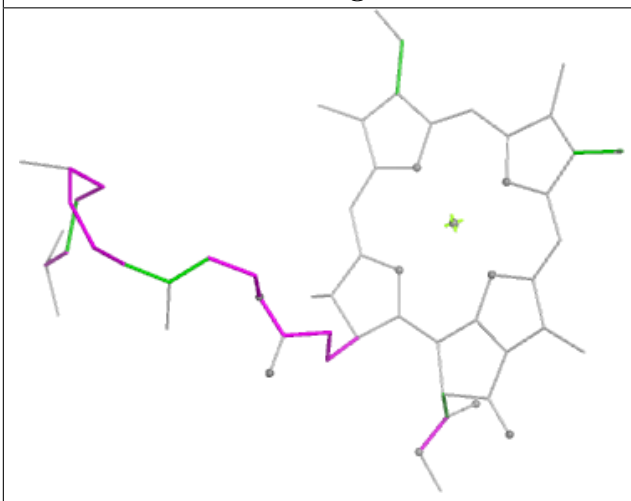


Bond angles



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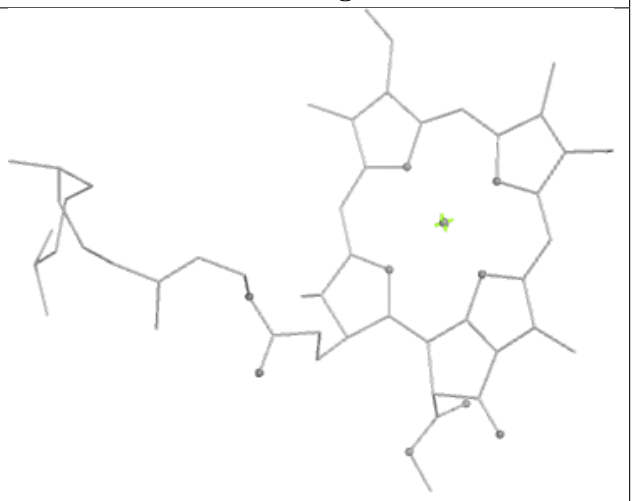
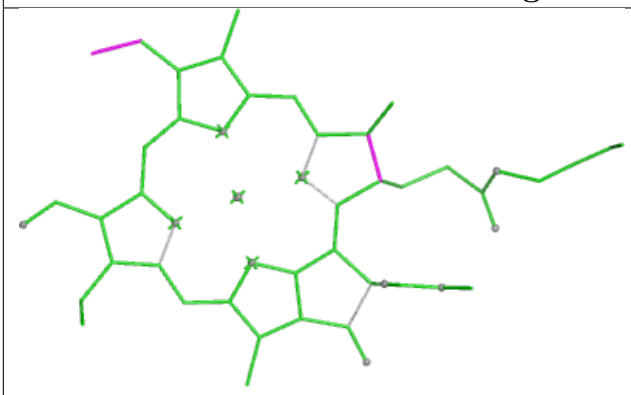


Rings

Ligand CHL N 606



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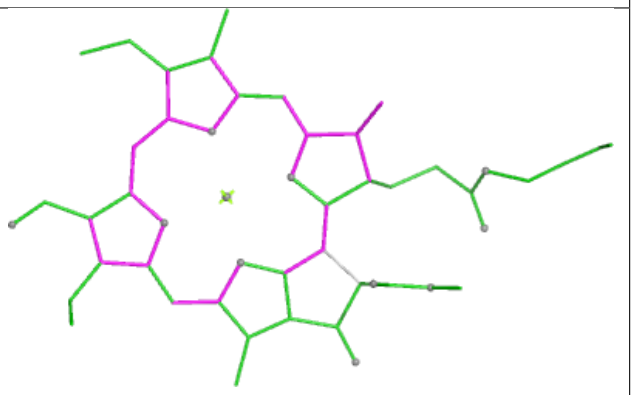
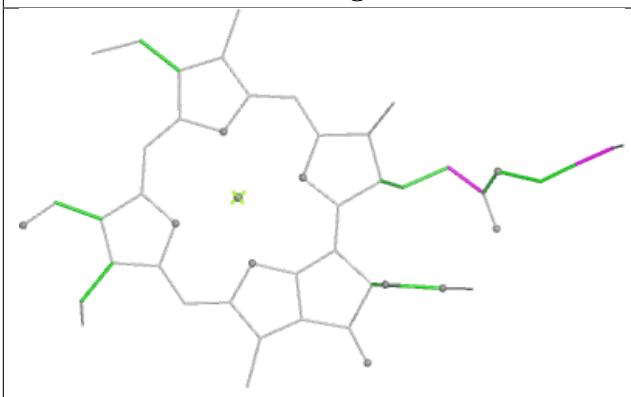


Bond angles



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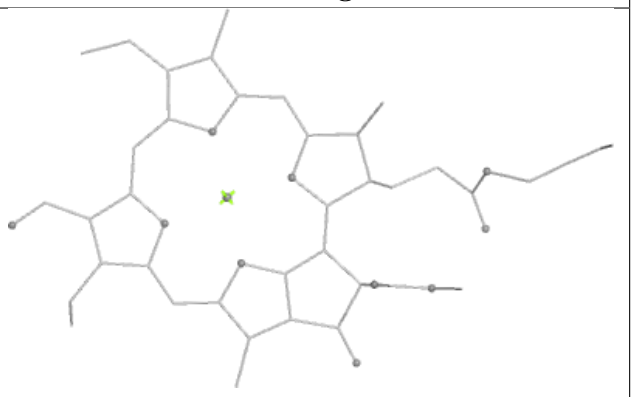
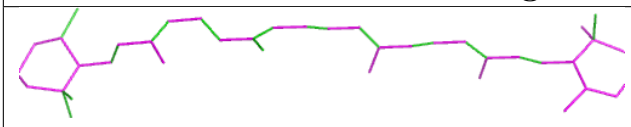


Rings

Ligand BCR H 101



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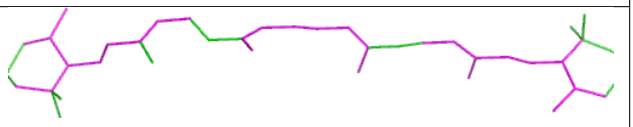
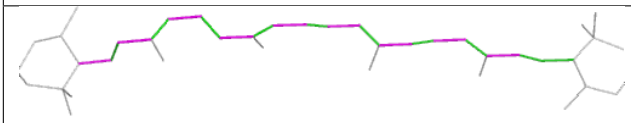


Bond angles



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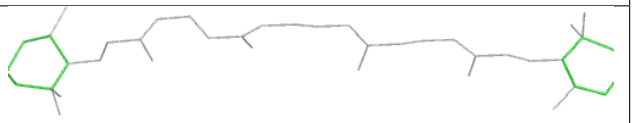
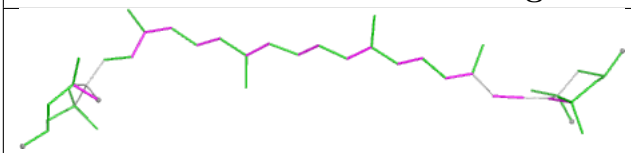


Rings

Ligand NEX y 318



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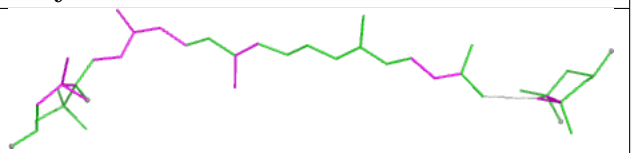
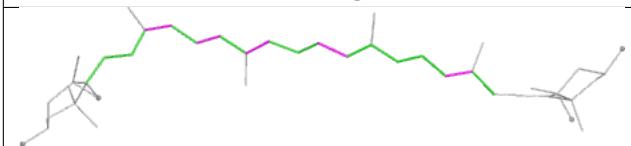


Bond angles



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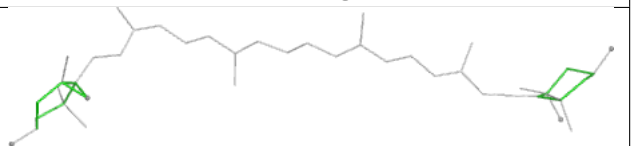
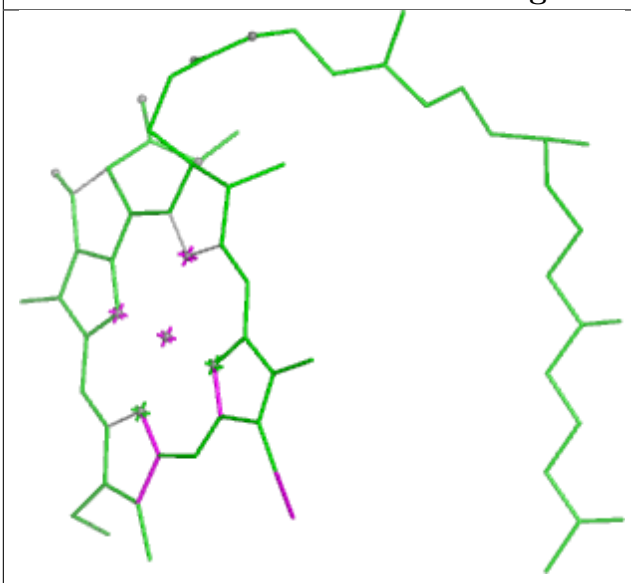


Rings

Ligand CLA c 507



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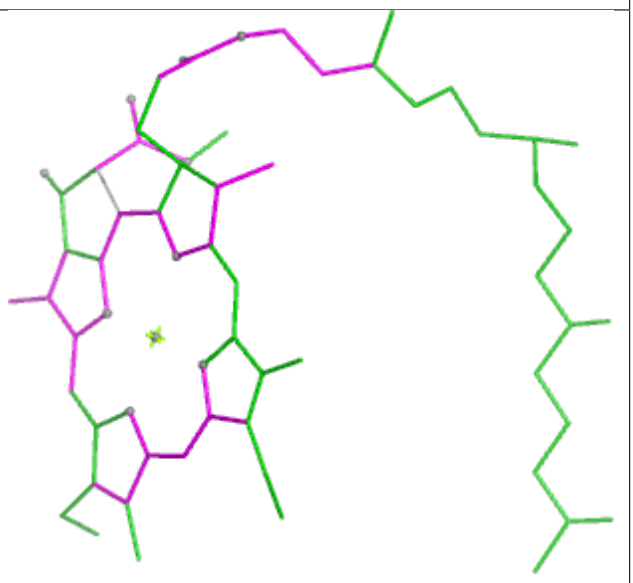
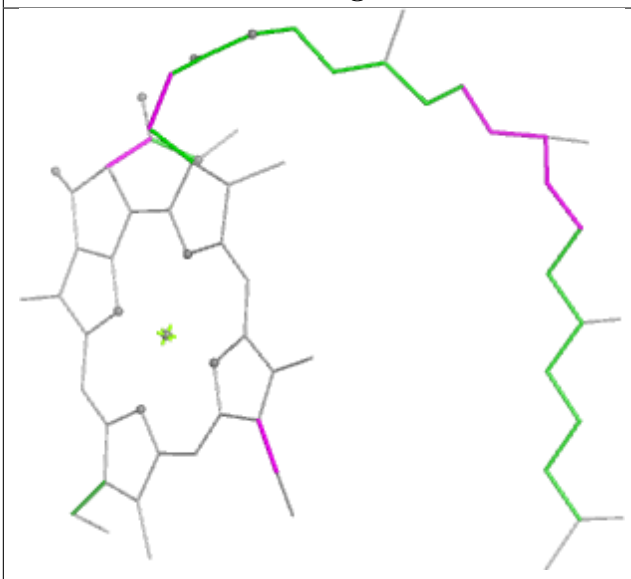


Bond angles



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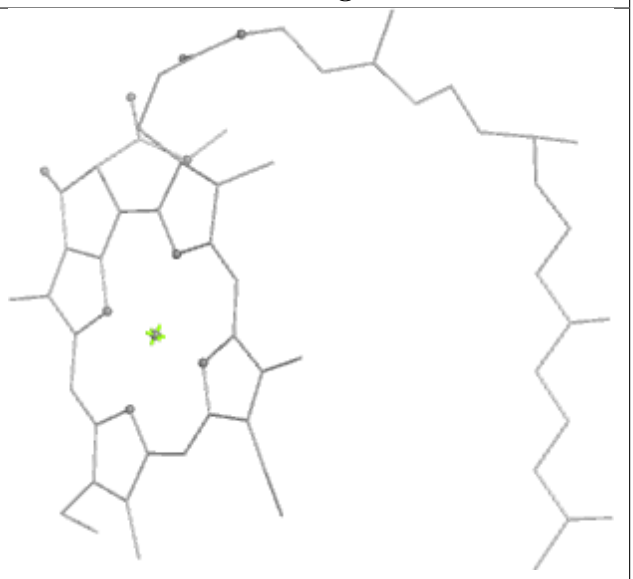
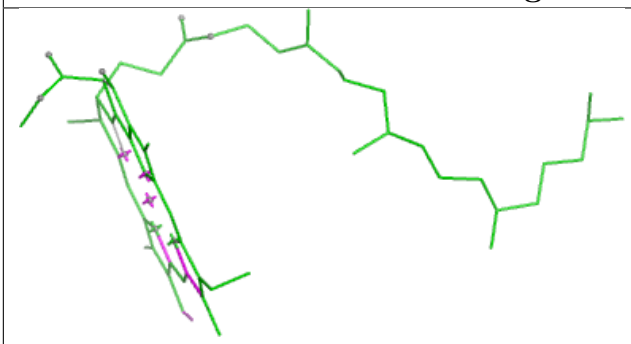


Rings

Ligand CLA C 508



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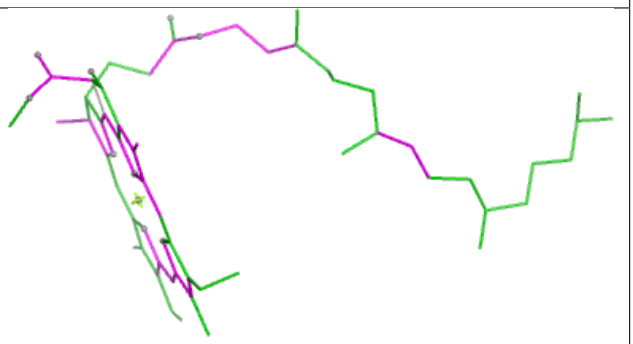
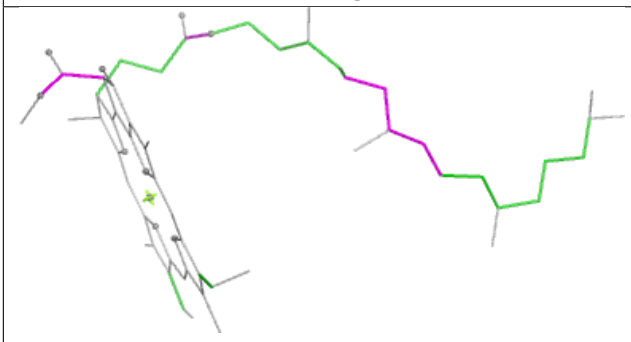


Bond angles

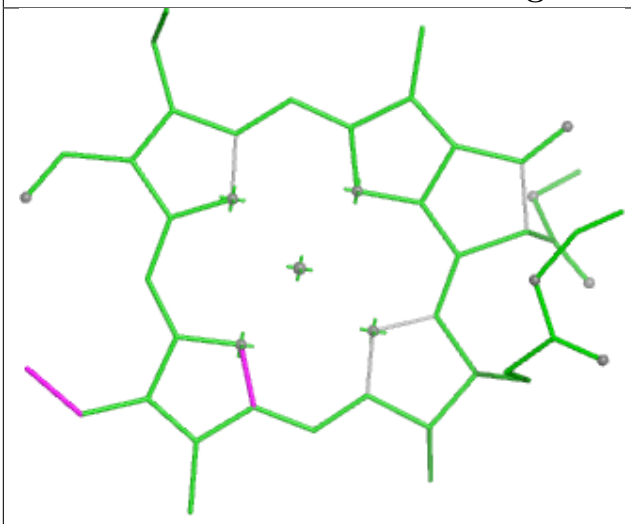


Torsions



Rings

Ligand CHL n 605



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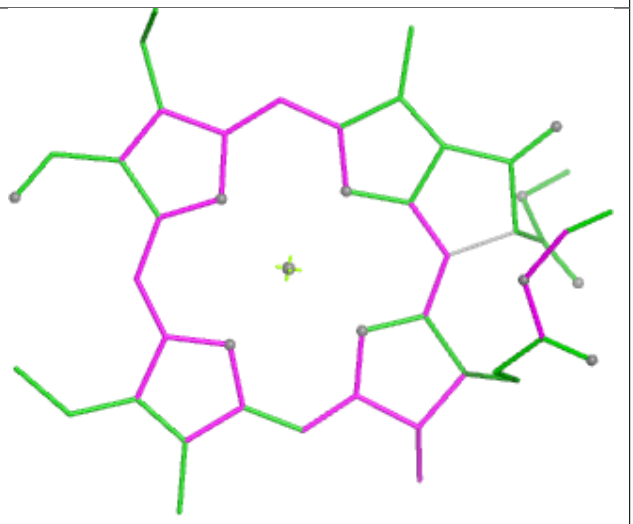
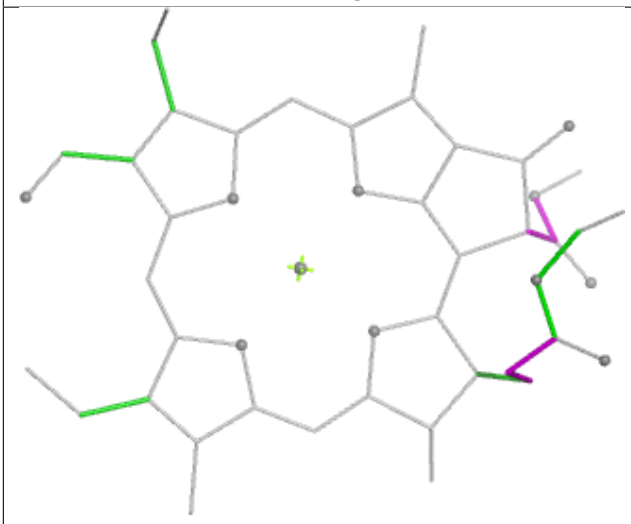


Bond angles



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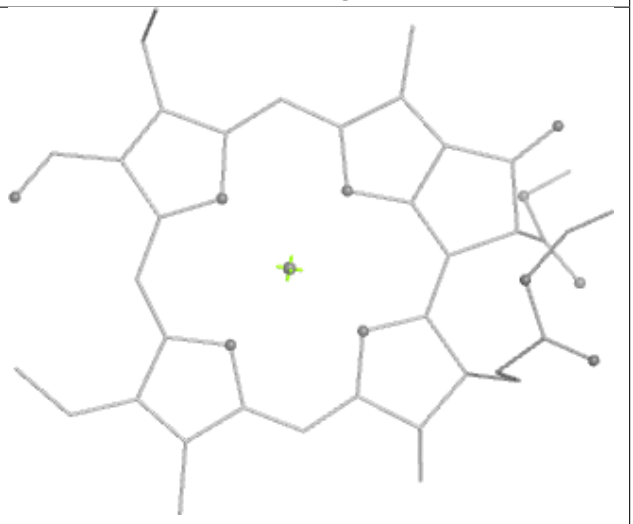
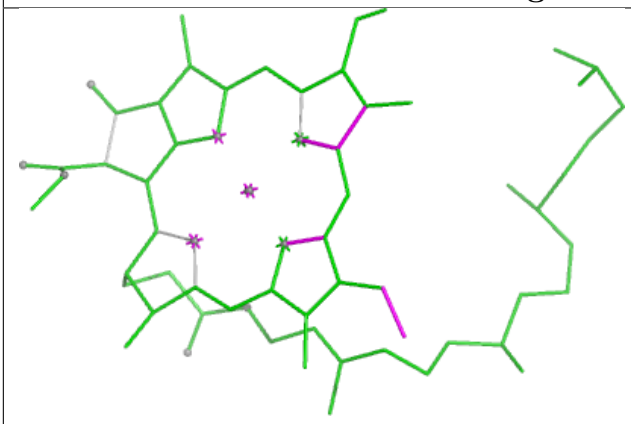


Rings

Ligand CLA n 602



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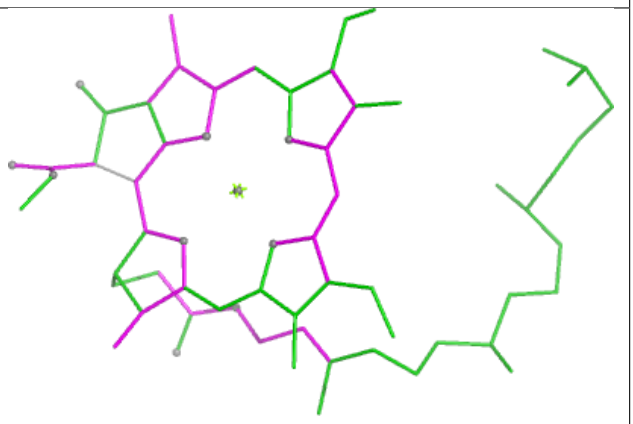
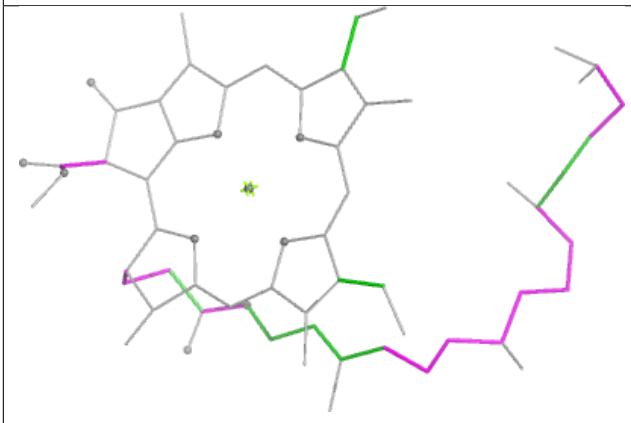


Bond angles



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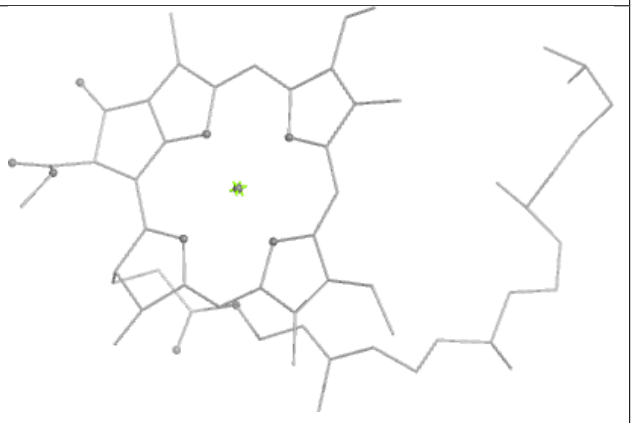
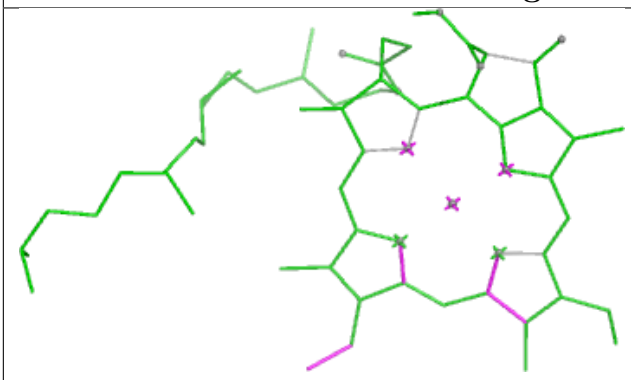
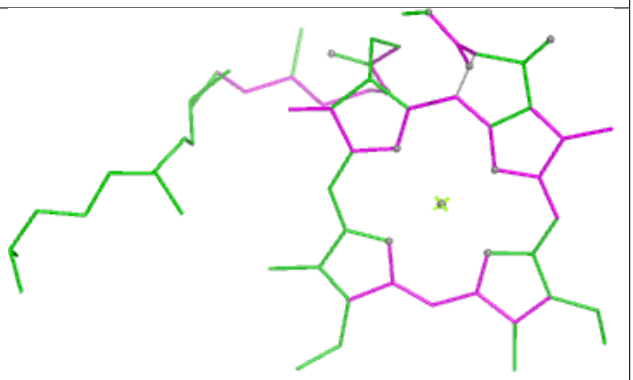


Rings

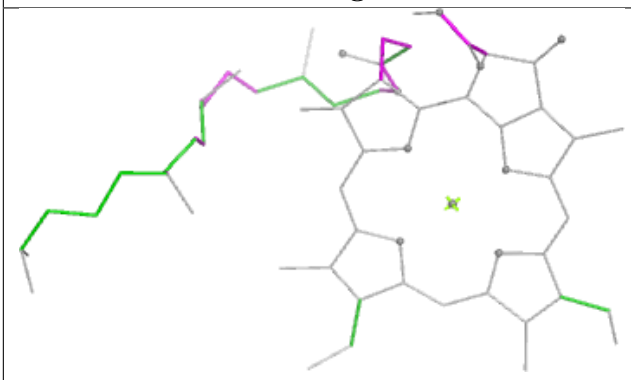
Ligand CLA D 401



Bond lengths



Bond angles

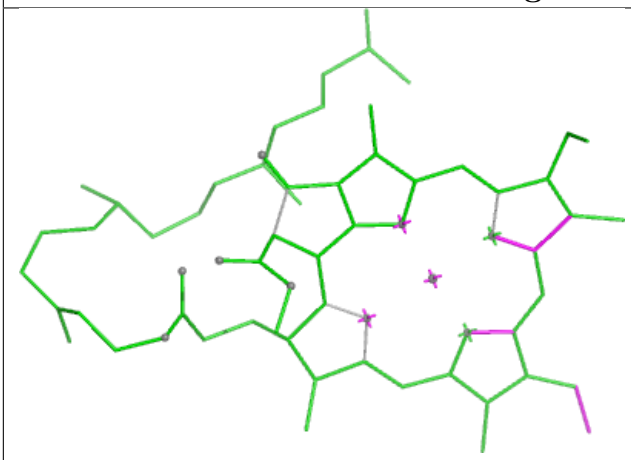


Torsions



Rings

Ligand CLA C 509



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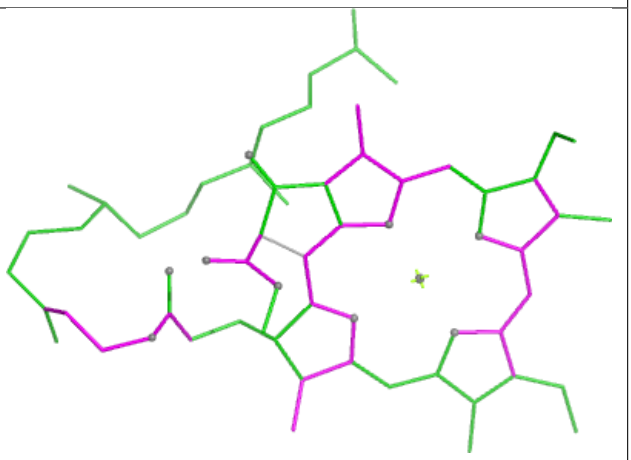
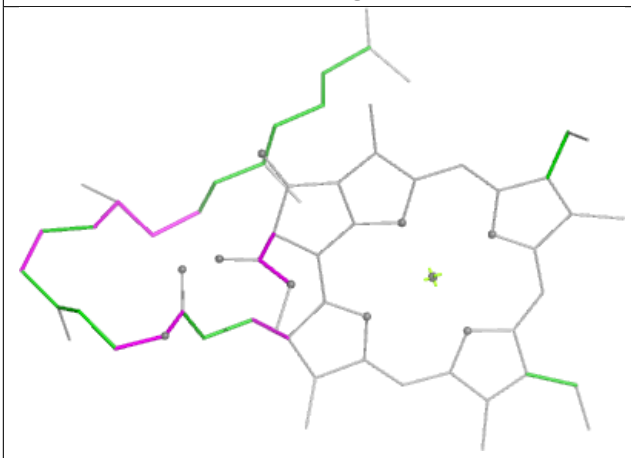


Bond angles



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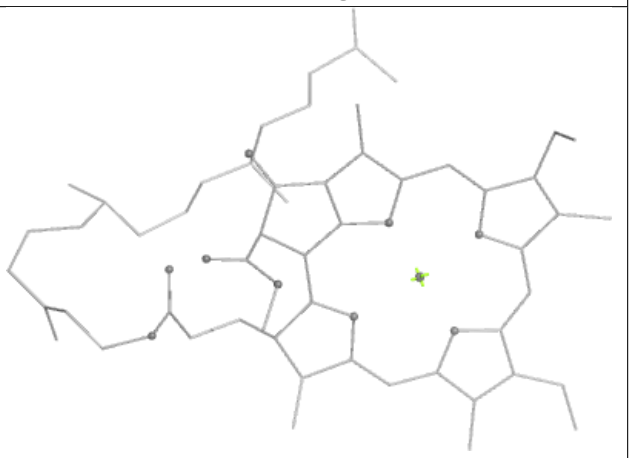
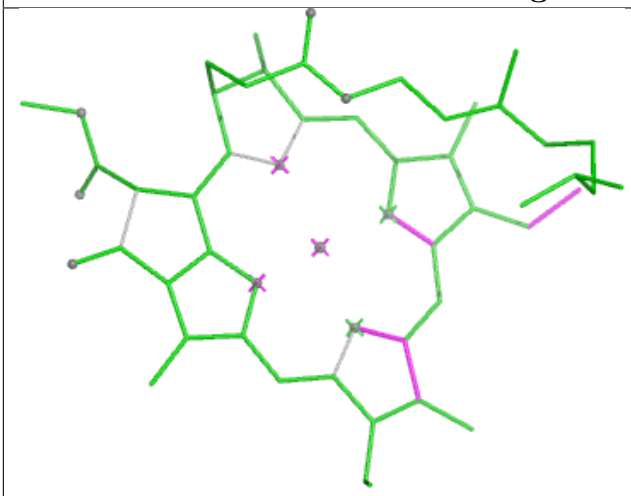


Rings

Ligand CLA s 609



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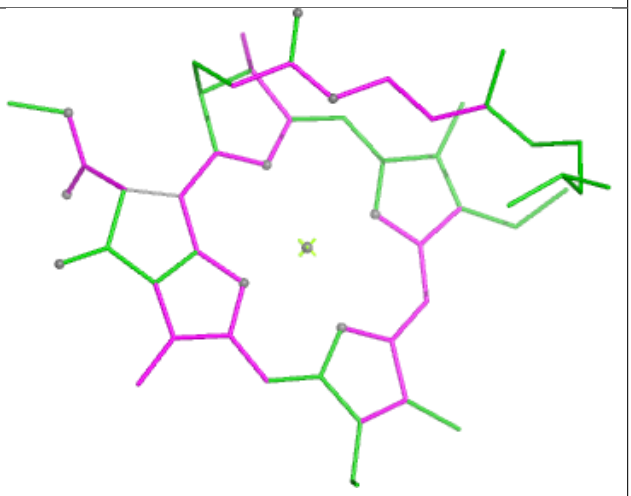
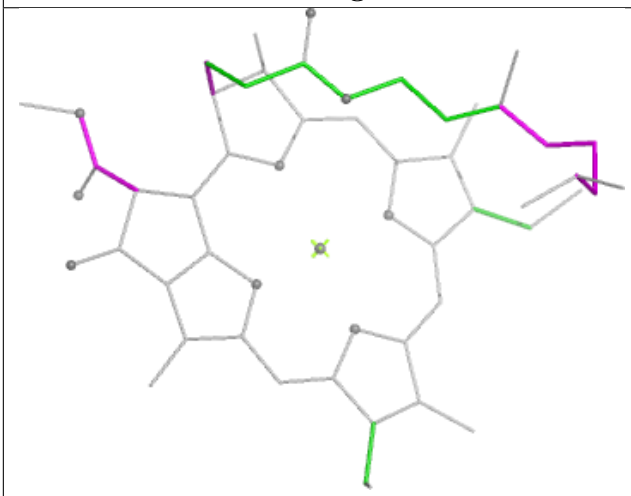


Bond angles



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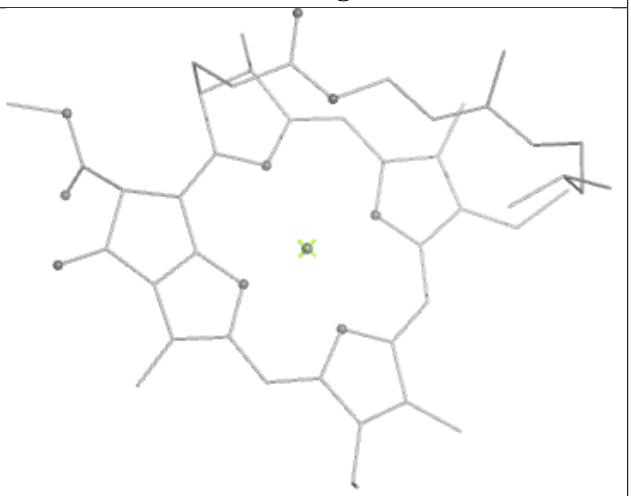
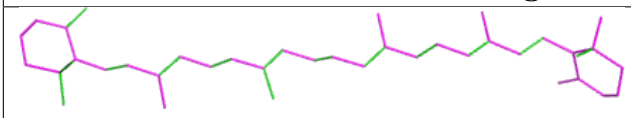


Rings

Ligand BCR B 618



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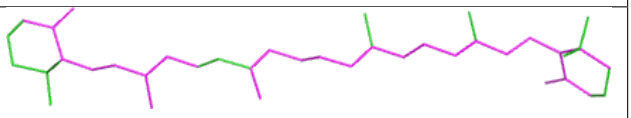

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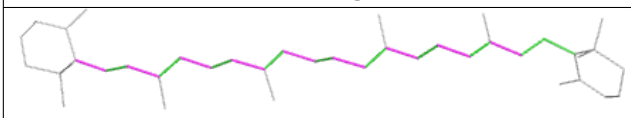

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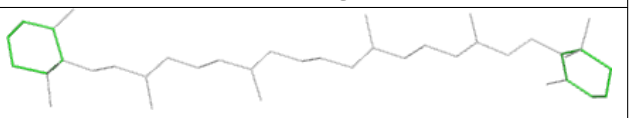
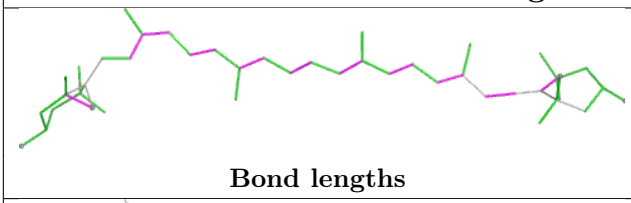


Rings

Ligand NEX r 616



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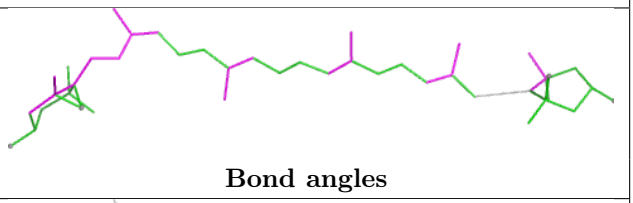
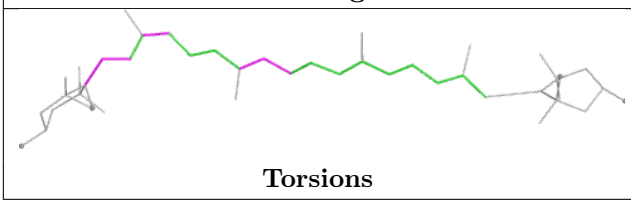


Bond angles



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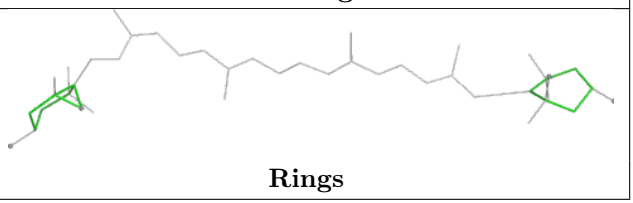
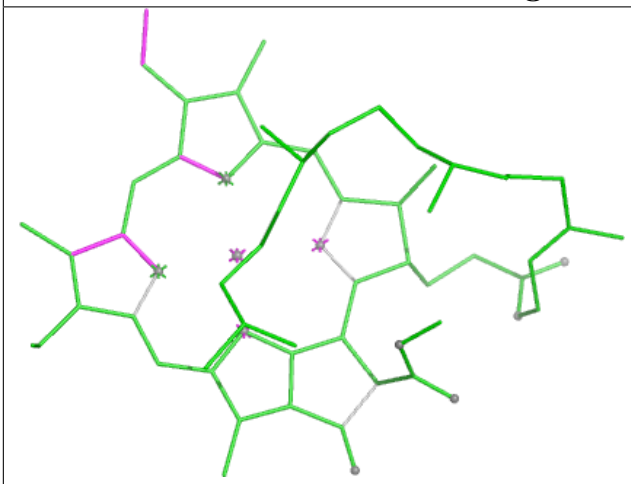


Rings

Ligand CLA C 510



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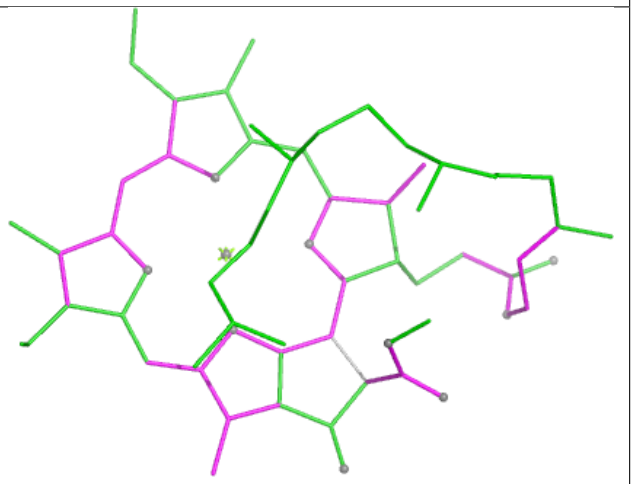
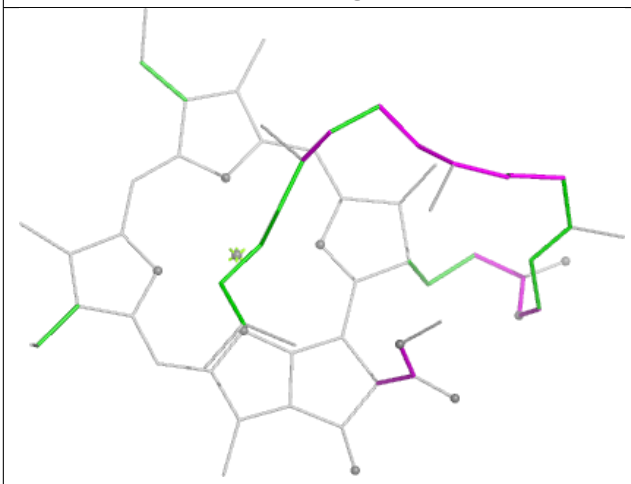


Bond angles



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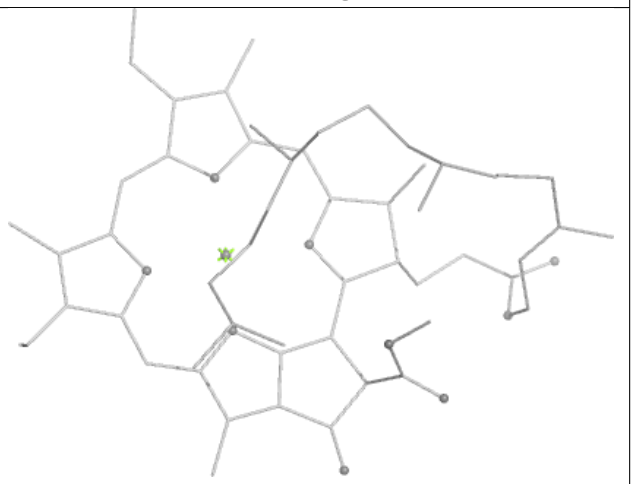
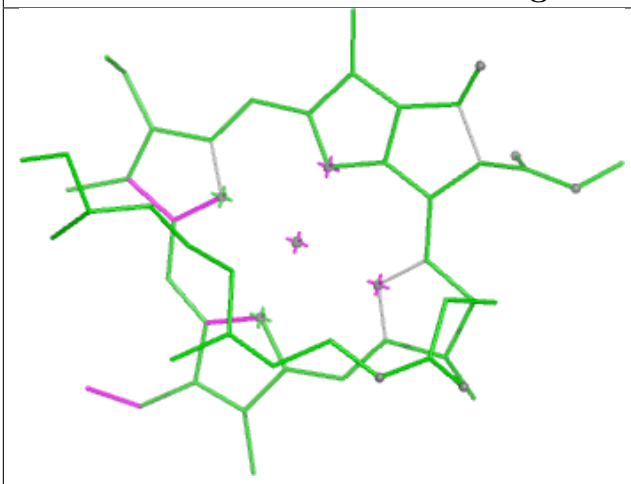


Rings

Ligand CLA s 610



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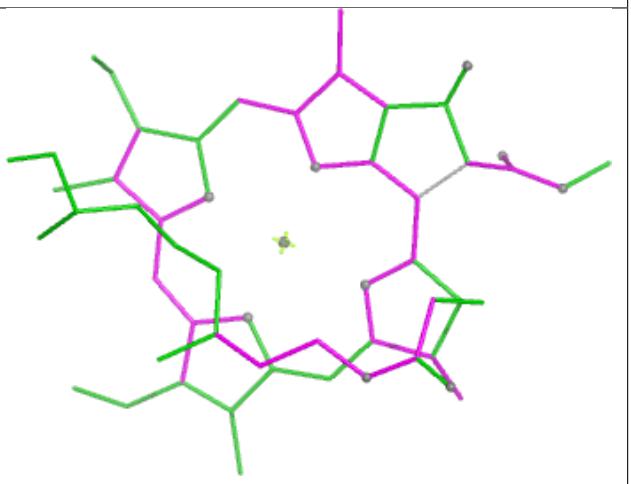
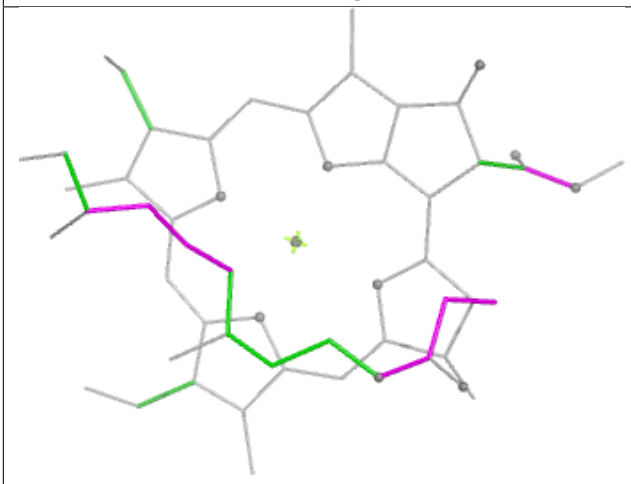


Bond angles



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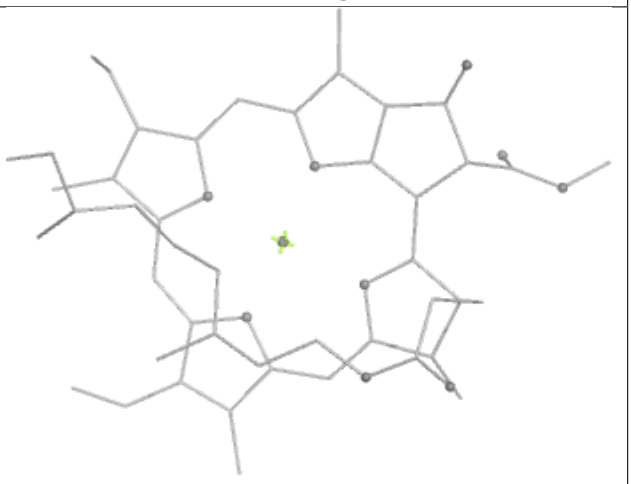
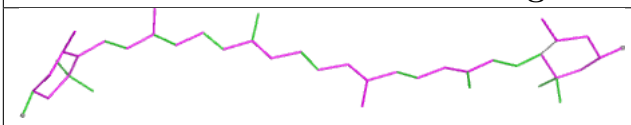


Rings

Ligand LUT n 616



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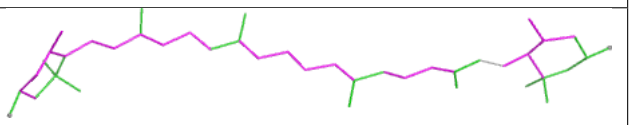


Bond angles

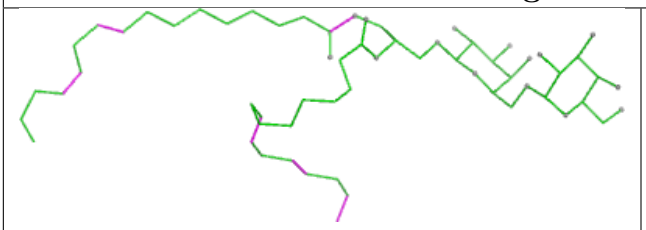


Torsions



Rings

Ligand DGD b 625



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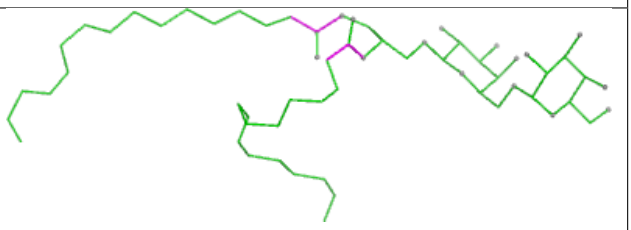
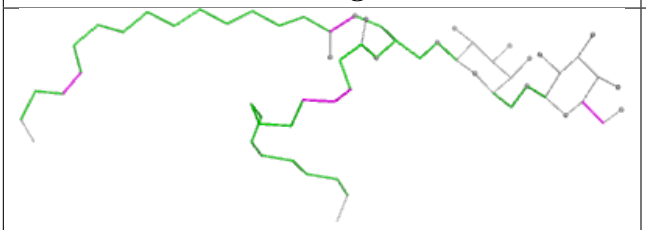


Bond angles



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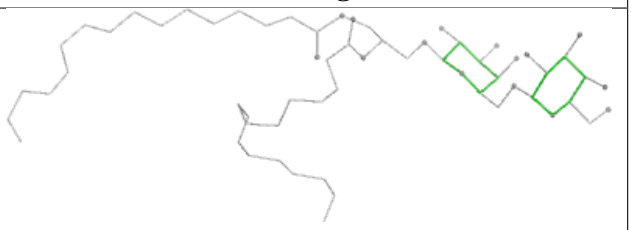

Rings

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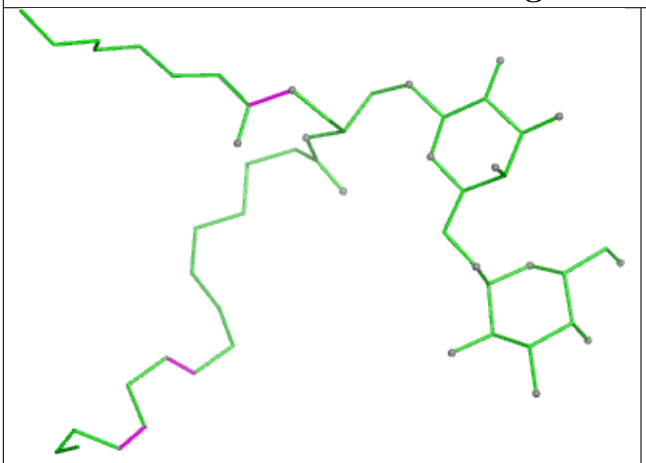

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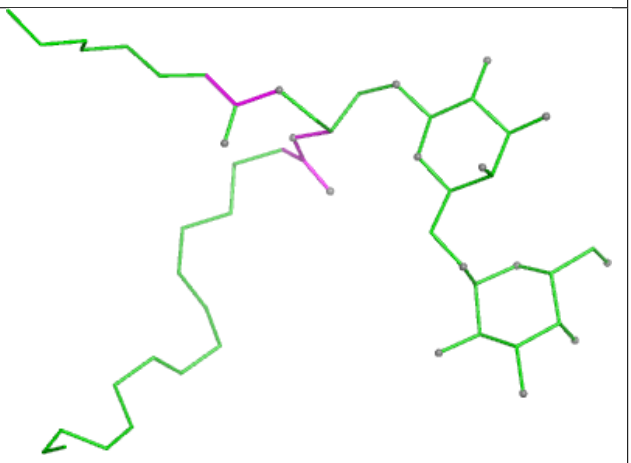
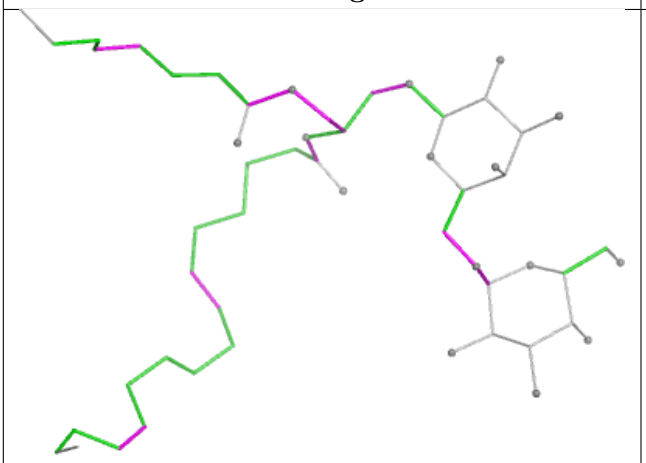


Bond angles



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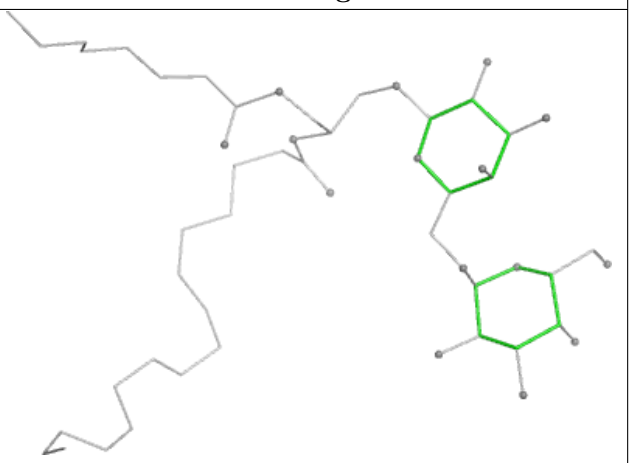
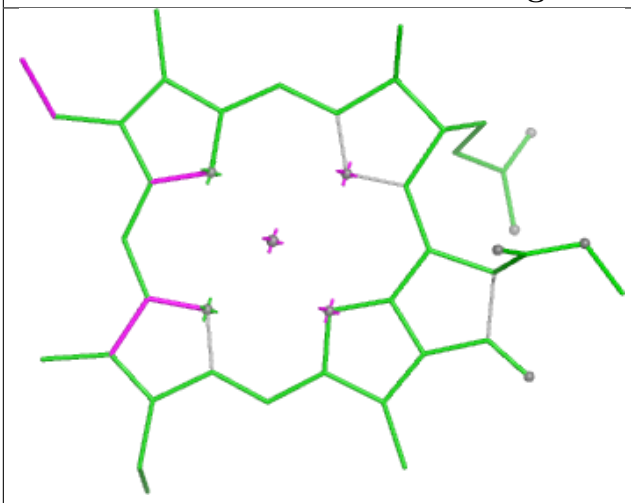


Rings

Ligand CLA n 614



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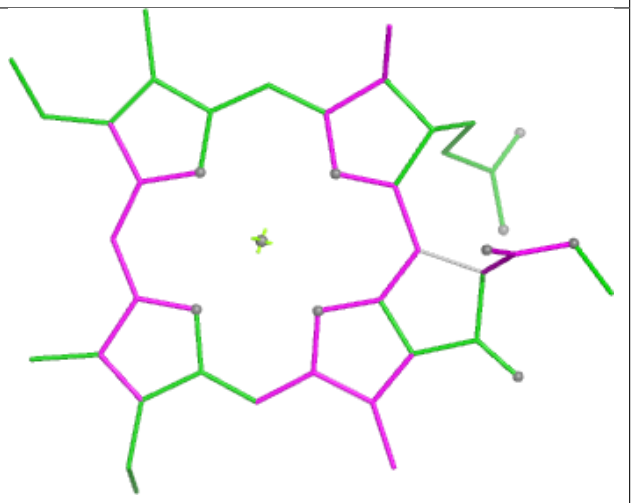
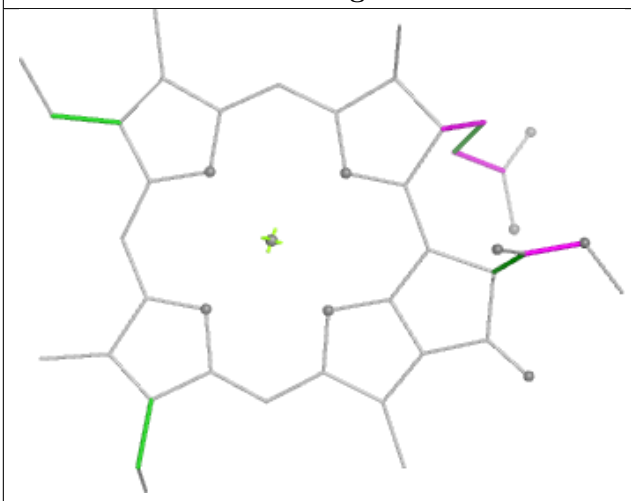


Bond angles



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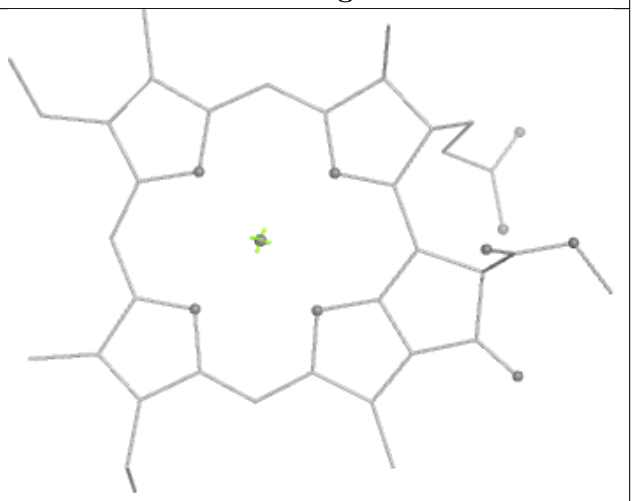
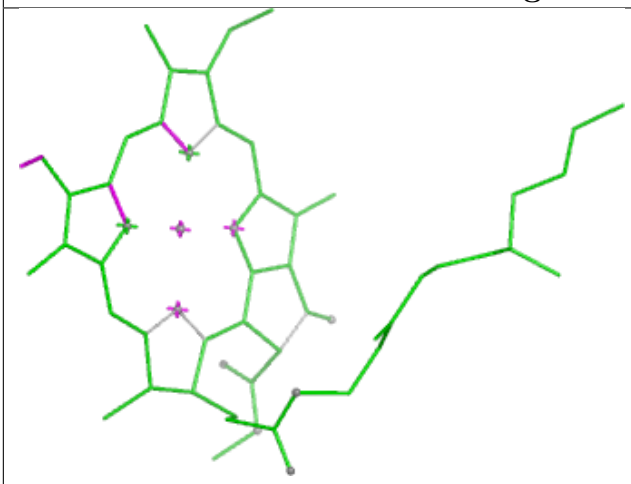


Rings

Ligand CLA R 608



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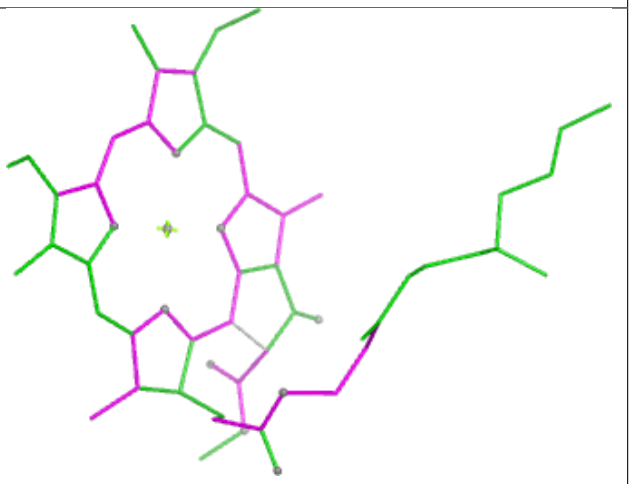
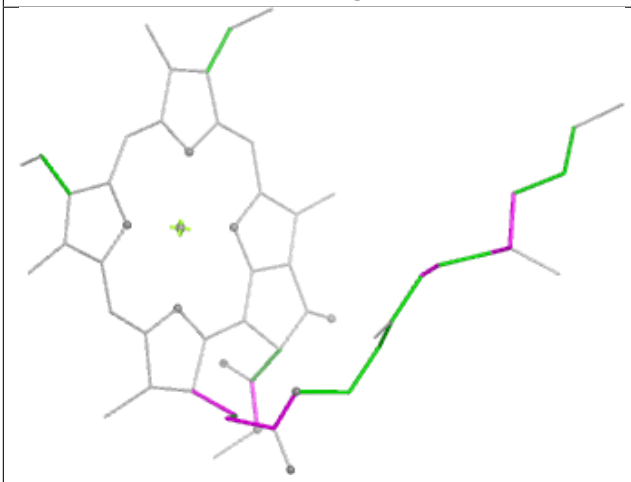


Bond angles



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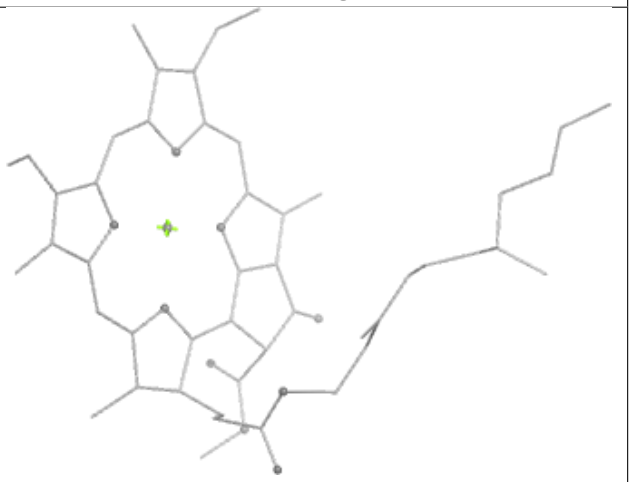
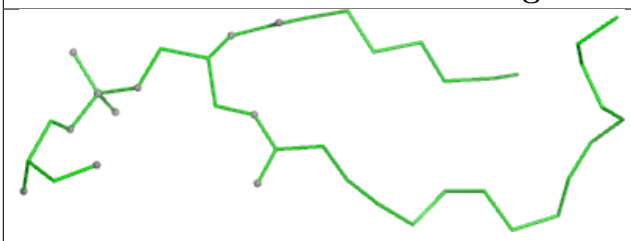


Rings

Ligand LHG B 623



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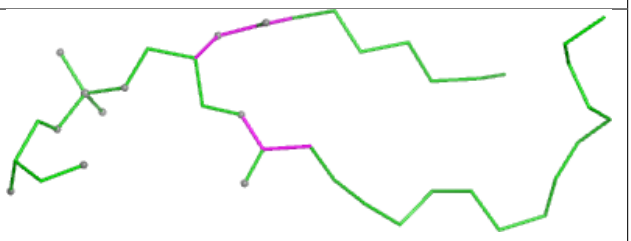
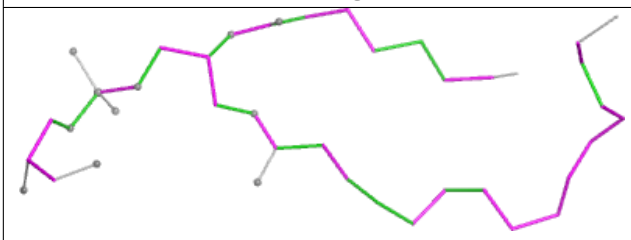


Bond angles

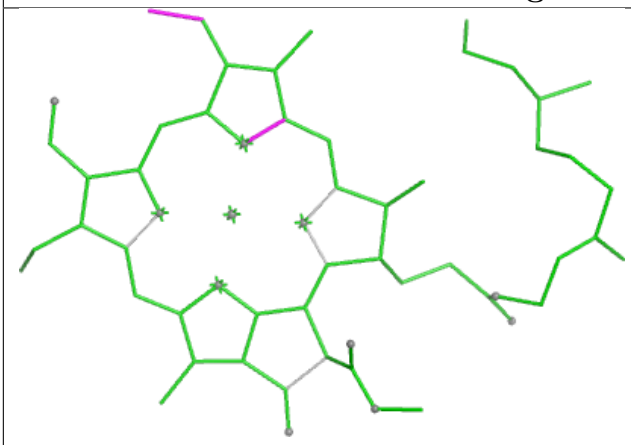


Torsions



Rings

Ligand CHL S 307



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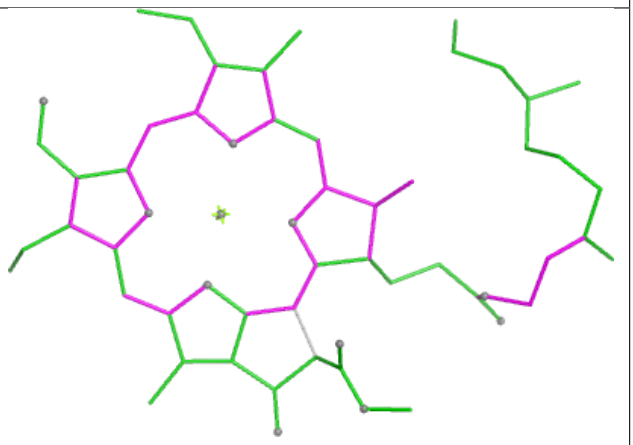
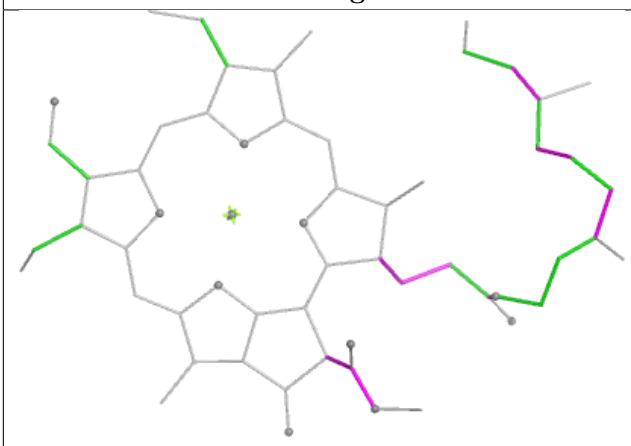
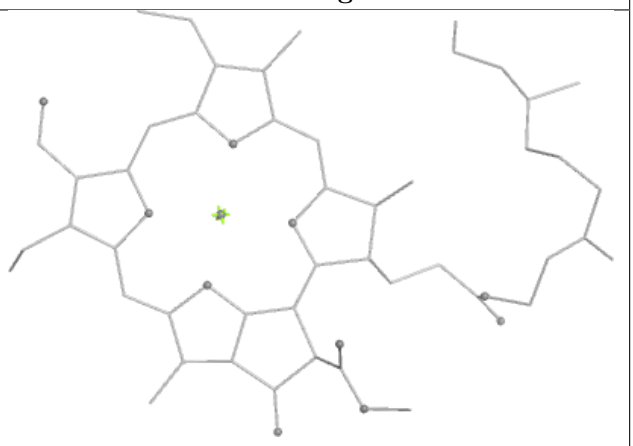


Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

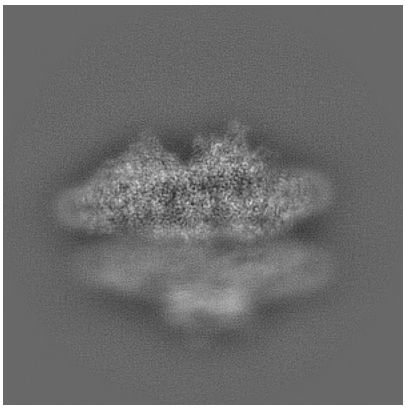
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52846. These allow visual inspection of the internal detail of the map and identification of artifacts.

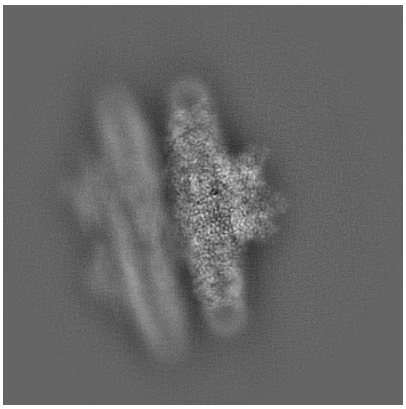
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

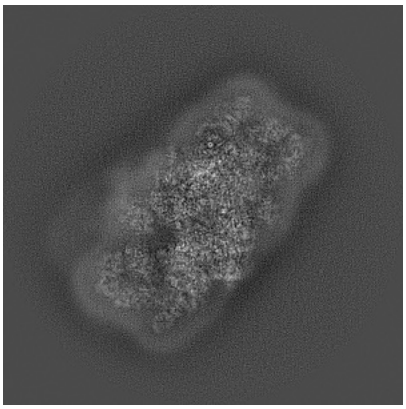
6.1.1 Primary map



X

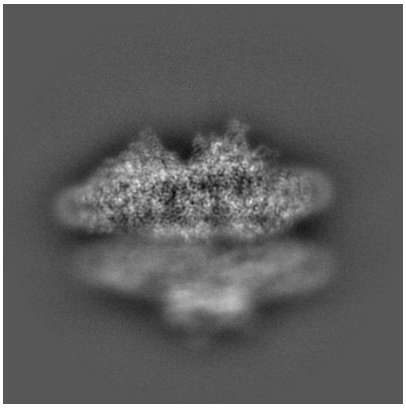


Y

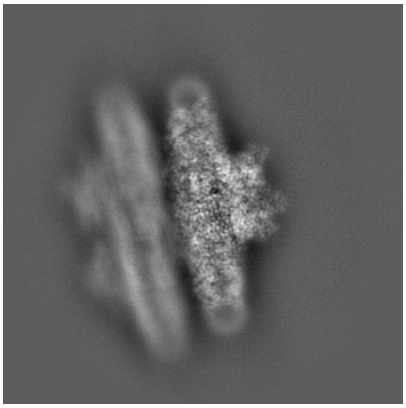


Z

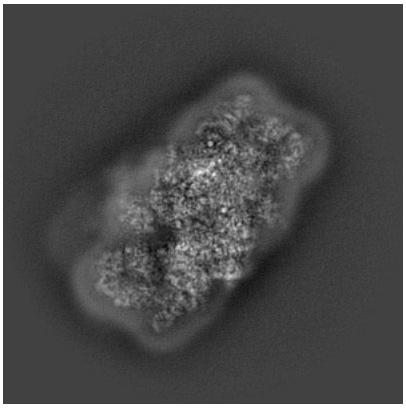
6.1.2 Raw map



X



Y

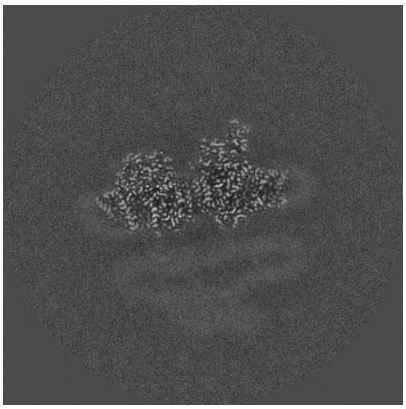


Z

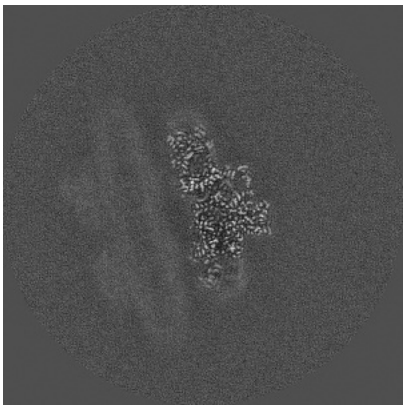
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

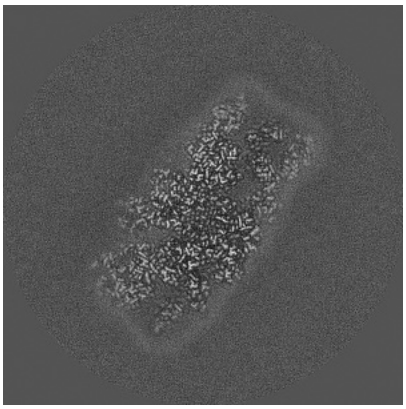
6.2.1 Primary map



X Index: 250

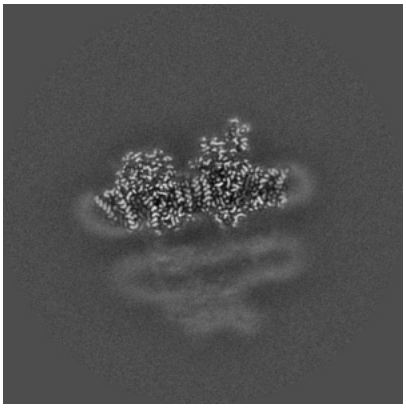


Y Index: 250

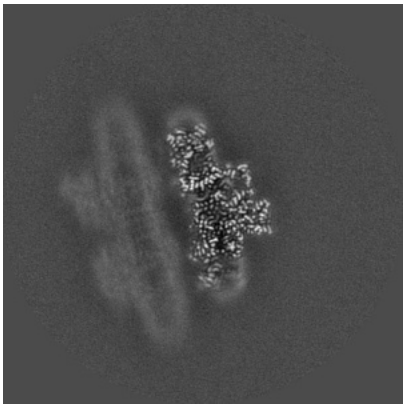


Z Index: 250

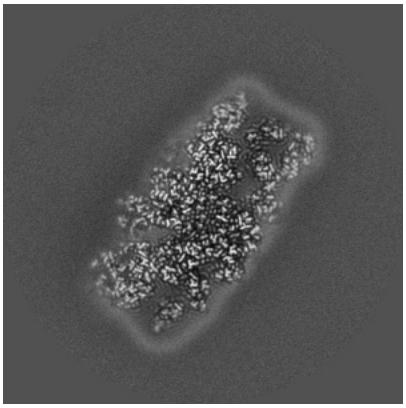
6.2.2 Raw map



X Index: 250



Y Index: 250

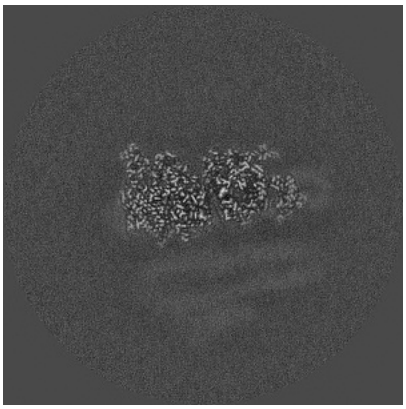


Z Index: 250

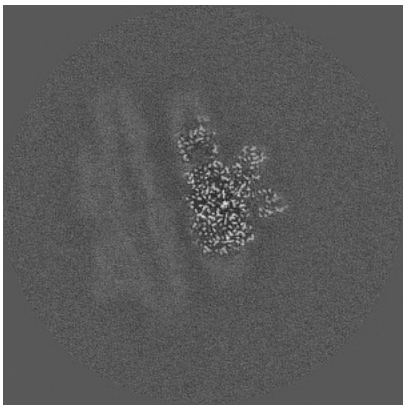
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

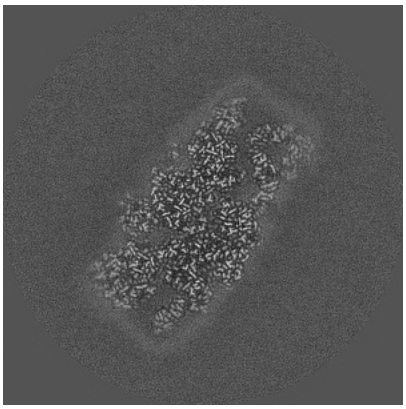
6.3.1 Primary map



X Index: 283

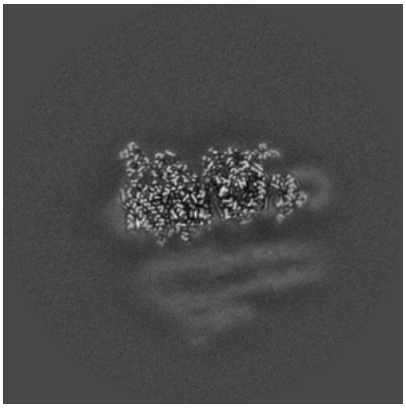


Y Index: 282

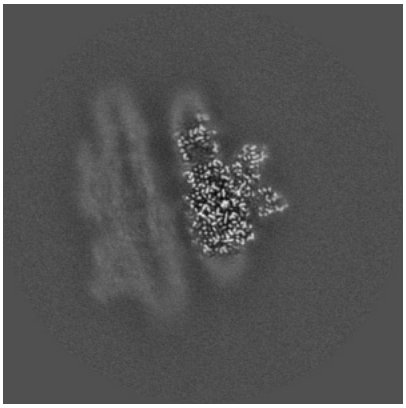


Z Index: 254

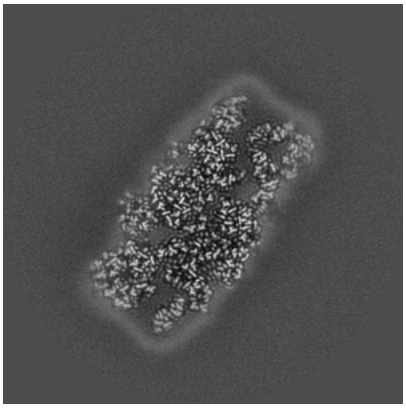
6.3.2 Raw map



X Index: 283



Y Index: 282

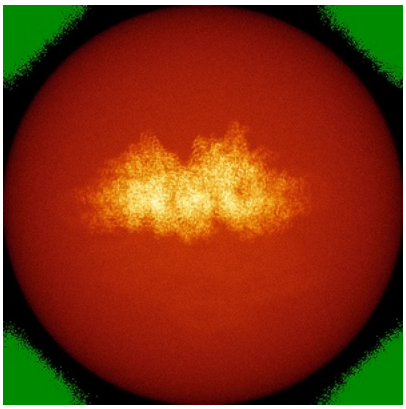


Z Index: 254

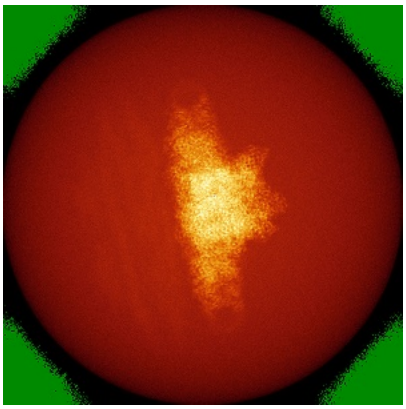
The images above show the largest variance slices of the map in three orthogonal directions.

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

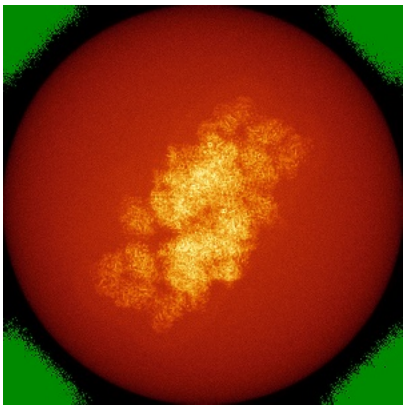
6.4.1 Primary map



X

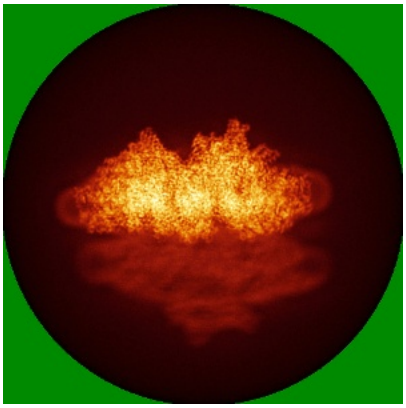


Y

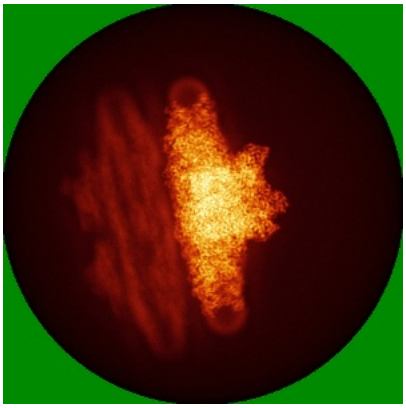


Z

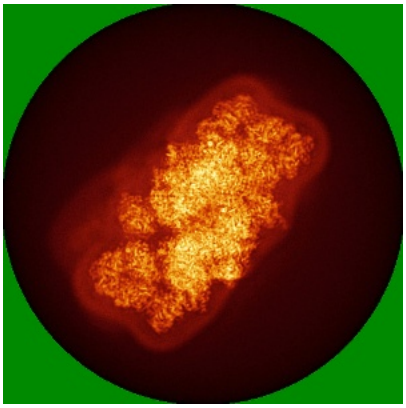
6.4.2 Raw map



X



Y

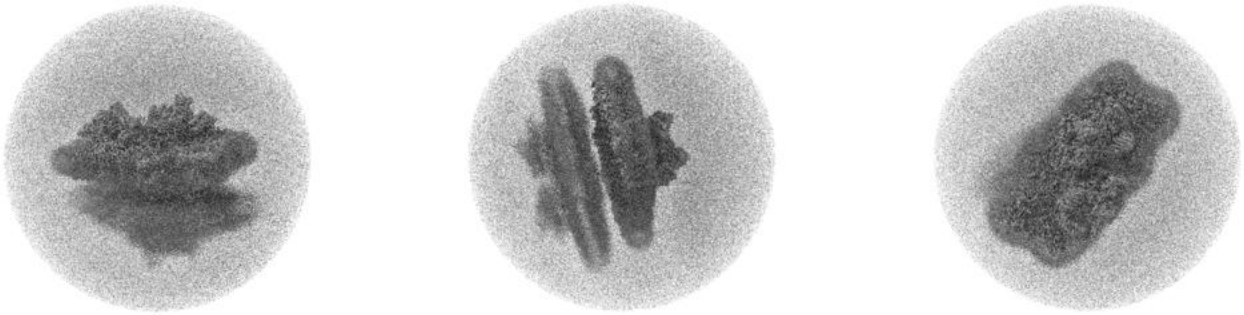


Z

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)

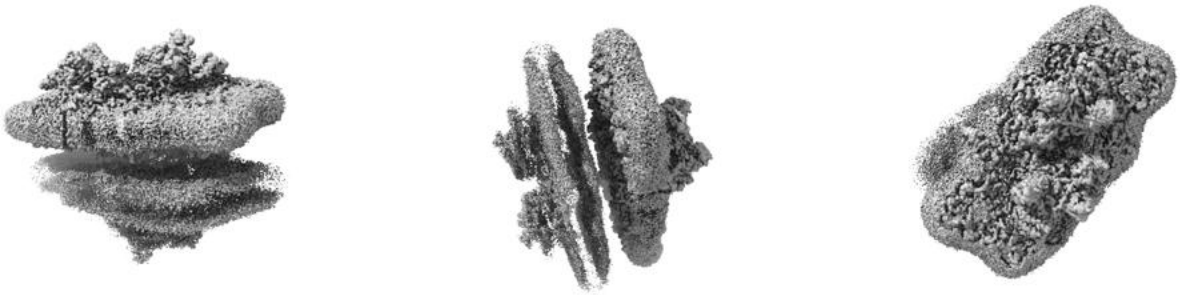
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

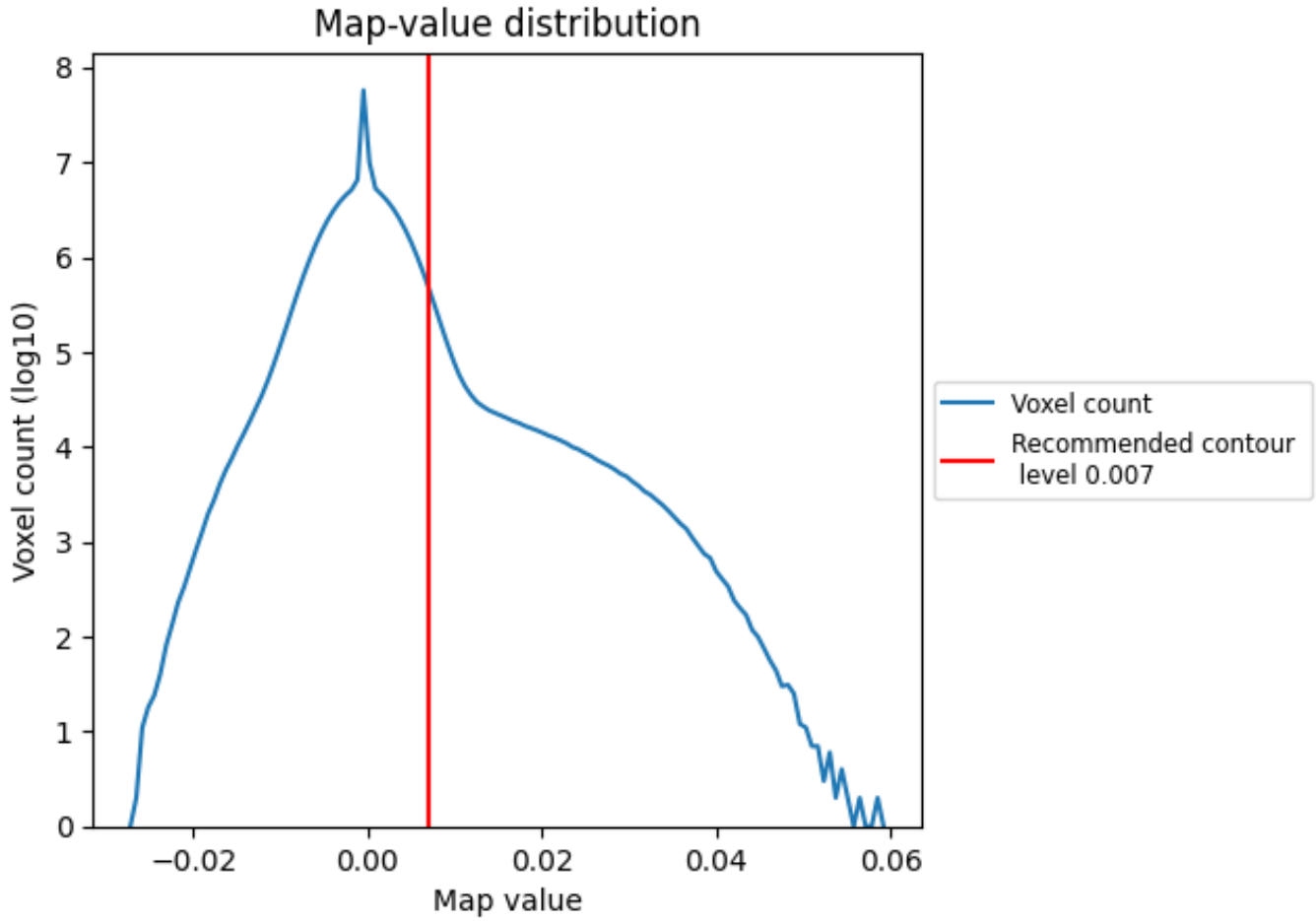
6.6 Mask visualisation (i)

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

7 Map analysis

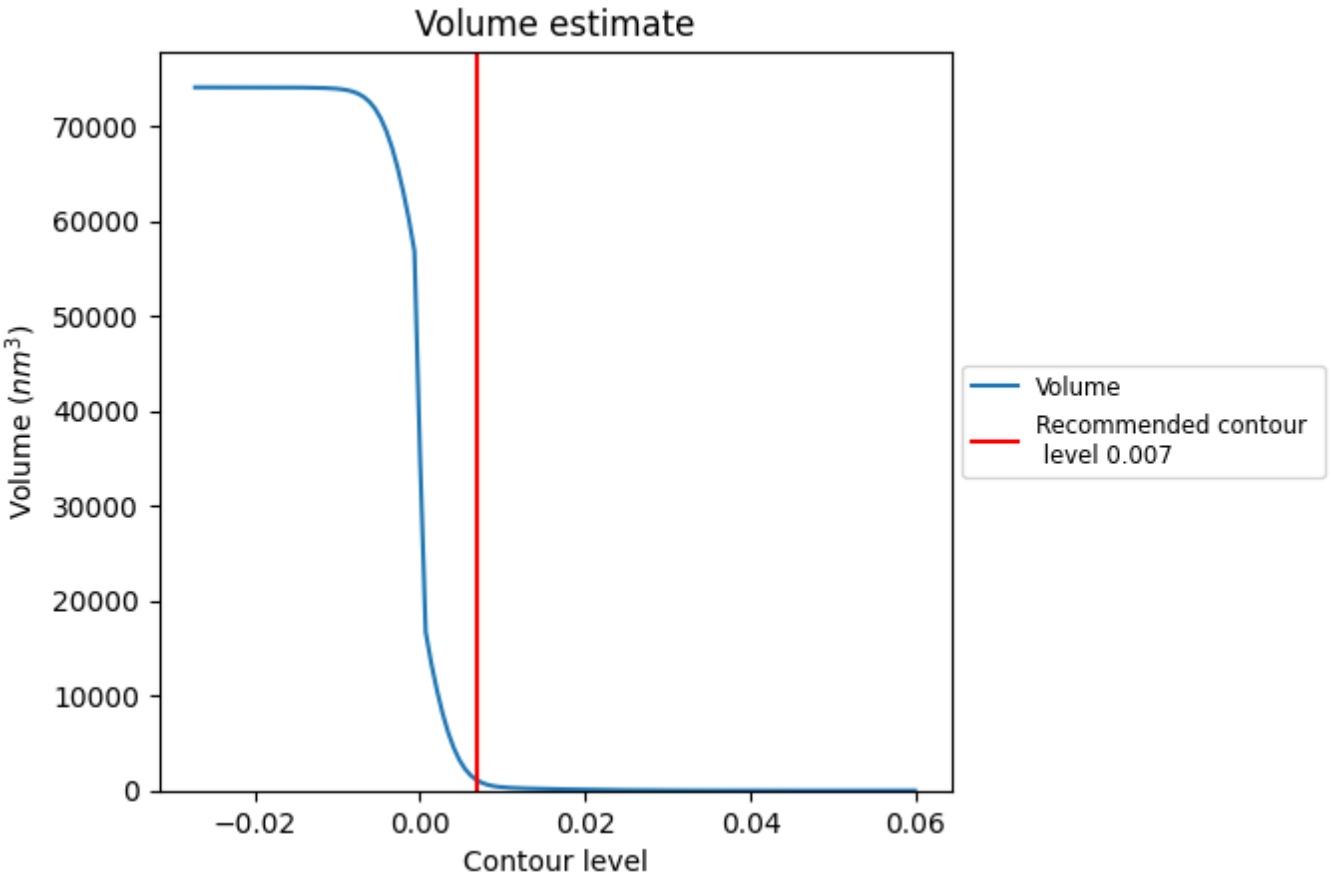
This section contains the results of statistical analysis of the map.

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.

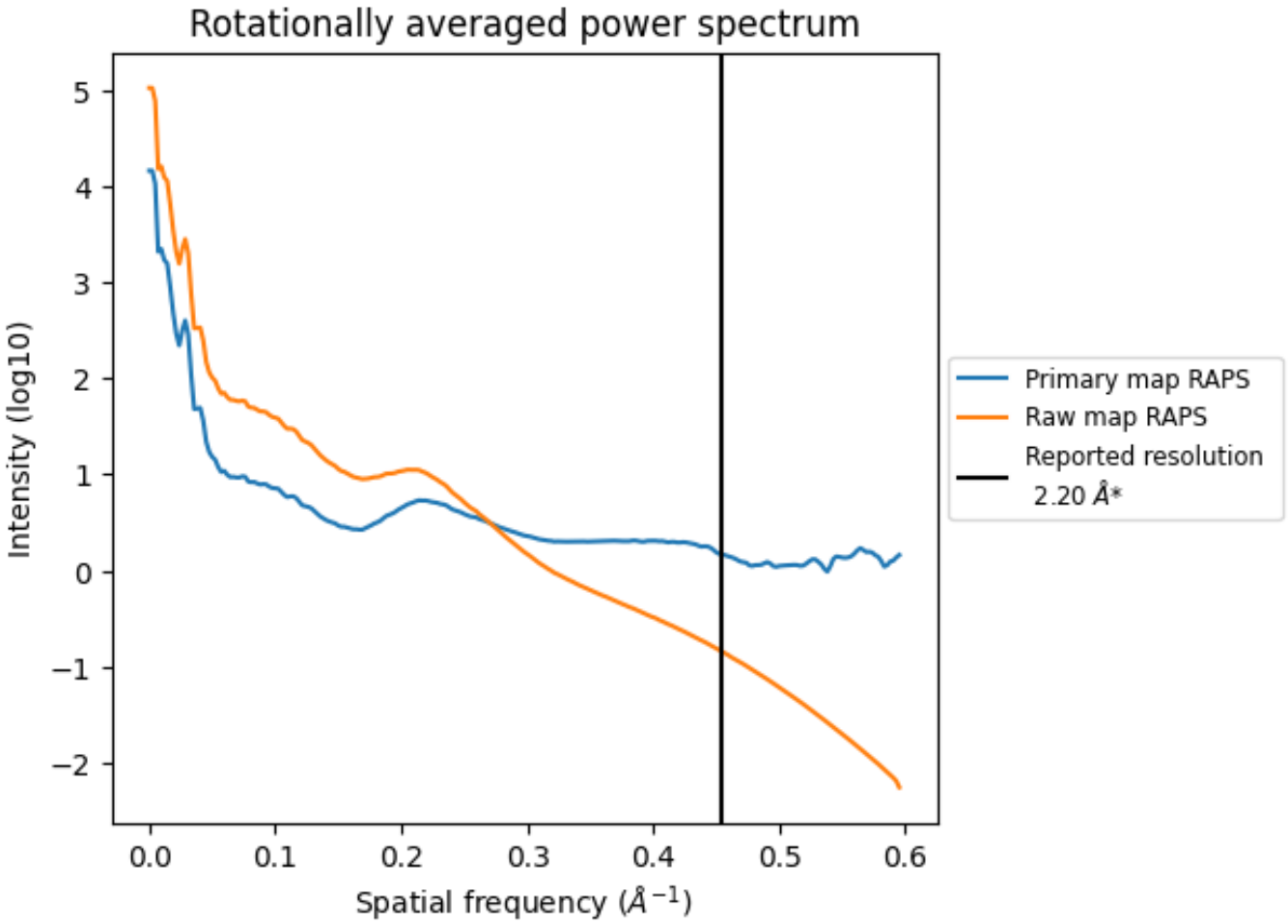
7.2 Volume estimate (i)



The volume at the recommended contour level is 1052 nm^3; this corresponds to an approximate mass of 950 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)

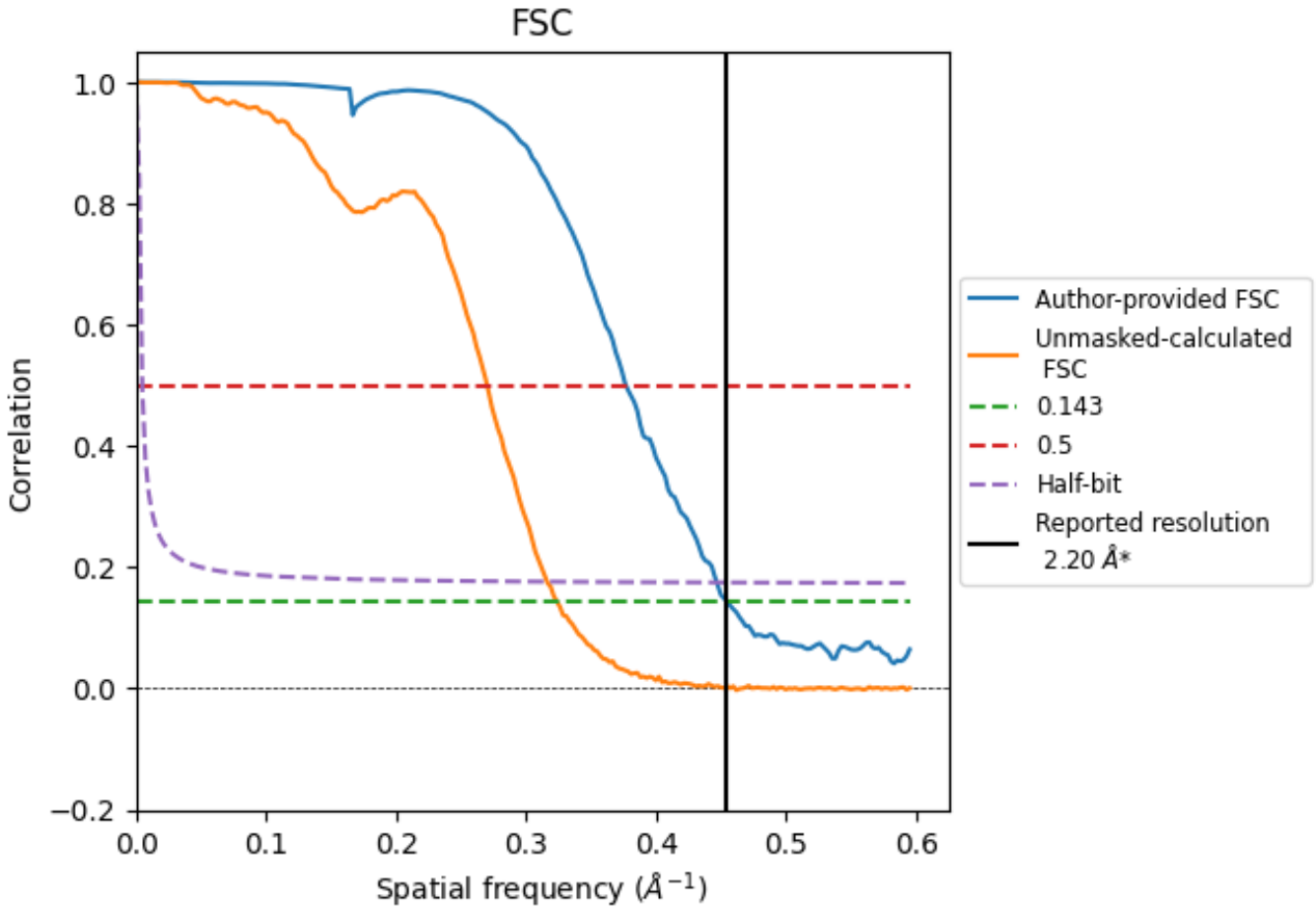


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

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 0.455 Å^{-1}

8.2 Resolution estimates (i)

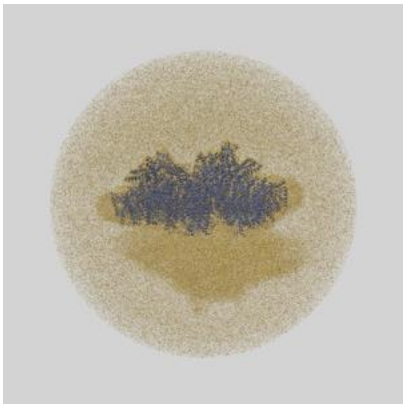
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.65	2.24
Unmasked-calculated*	3.09	3.70	3.16

*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 3.09 differs from the reported value 2.2 by more than 10 %

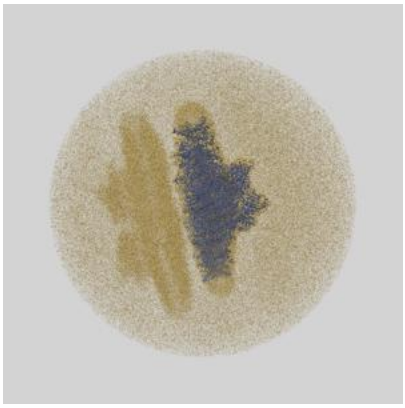
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52846 and PDB model 9IFM. Per-residue inclusion information can be found in section 3 on page 38.

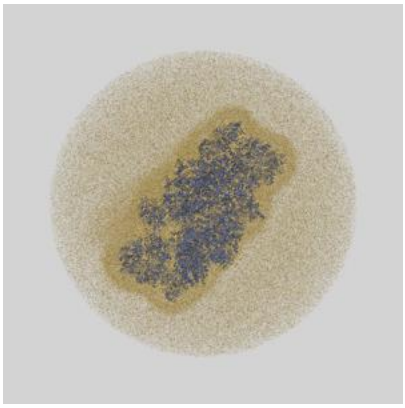
9.1 Map-model overlay



X



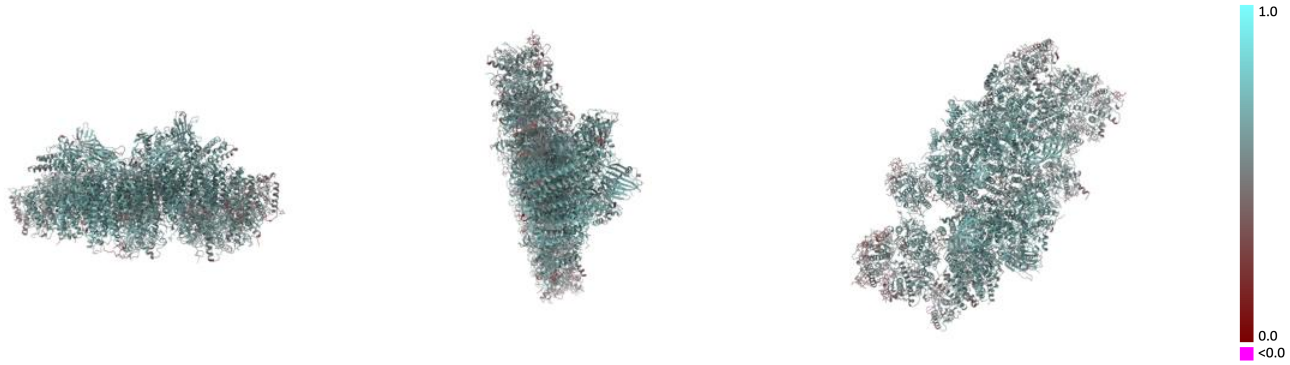
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

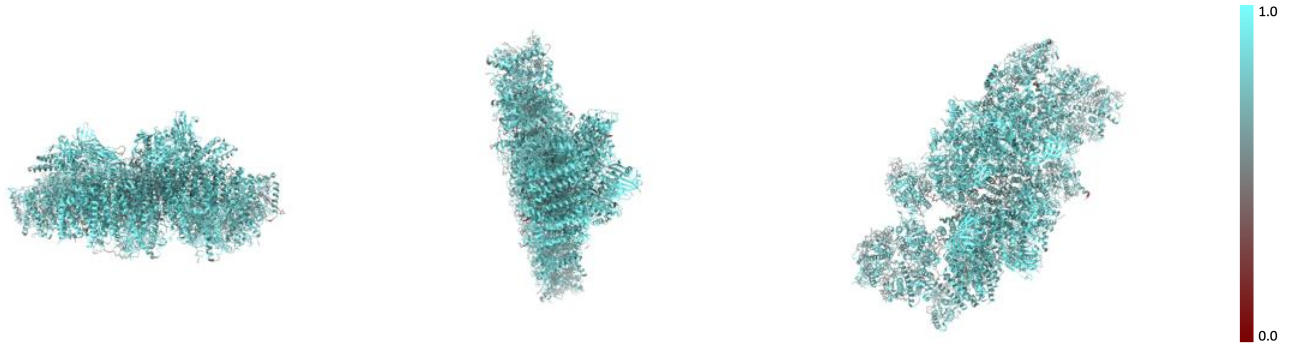
9.2 Q-score mapped to coordinate model (i)



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.

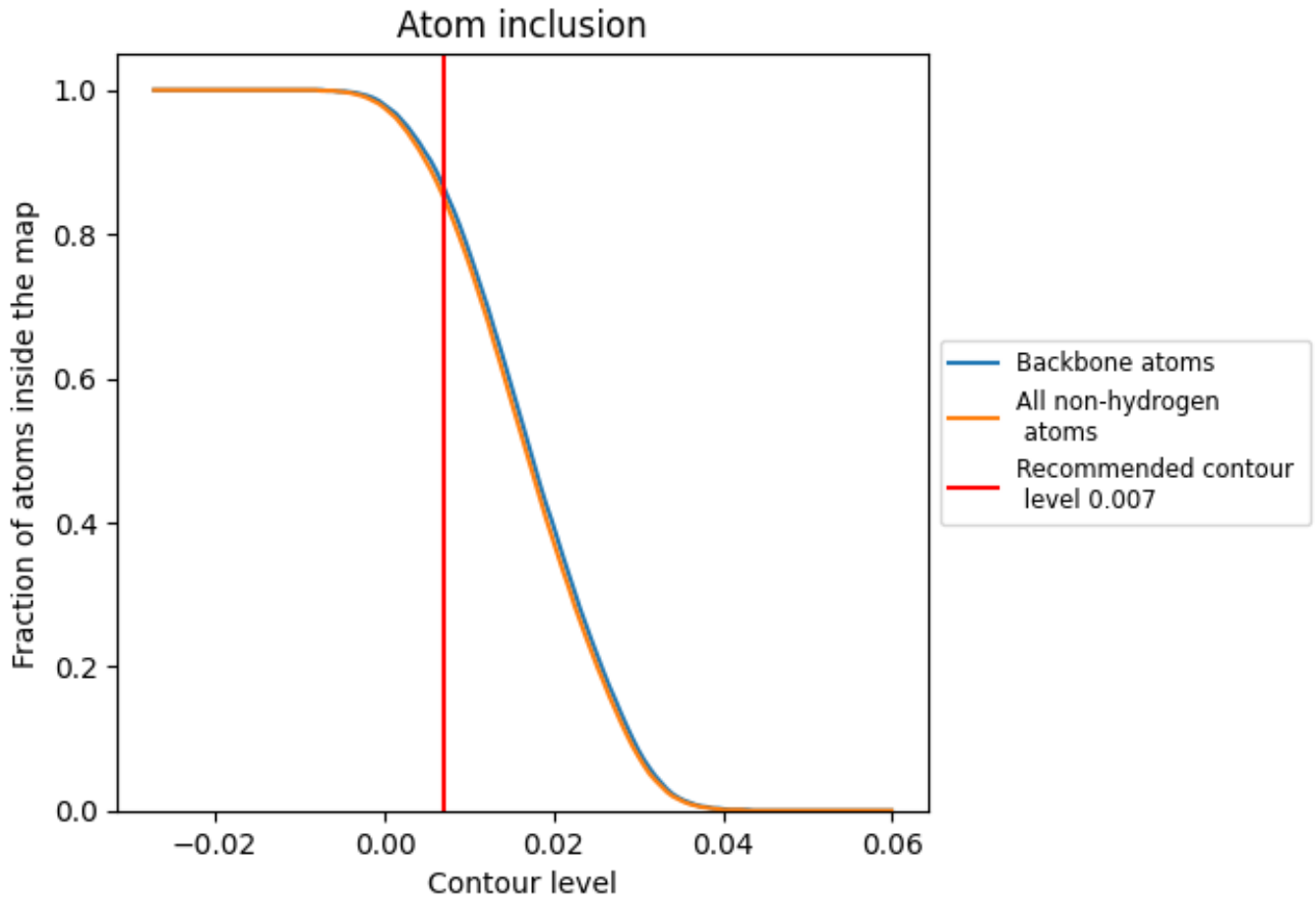
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.5990
A	0.9000	0.6540
B	0.8850	0.6340
C	0.8900	0.6310
D	0.9200	0.6580
E	0.8960	0.6110
F	0.9150	0.6340
G	0.7160	0.4780
H	0.9220	0.6500
I	0.9340	0.6660
J	0.8370	0.6090
K	0.8300	0.6090
L	0.7790	0.6010
M	0.7140	0.5630
N	0.7700	0.5190
O	0.8690	0.6070
P	0.8720	0.6040
Q	0.8090	0.5690
R	0.8240	0.5660
S	0.7490	0.4950
T	0.8480	0.6410
U	0.7800	0.5290
W	0.7900	0.5670
X	0.8390	0.5890
Y	0.8580	0.5970
Z	0.7800	0.5590
a	0.9030	0.6500
b	0.9000	0.6400
c	0.9070	0.6470
d	0.9200	0.6610
e	0.9090	0.6080
f	0.8980	0.6340
g	0.7540	0.5090
h	0.9260	0.6400
i	0.9390	0.6610



Continued on next page...

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Chain	Atom inclusion	Q-score
j	0.8490	0.6150
k	0.7760	0.5710
l	0.9170	0.6630
m	0.7800	0.6070
n	0.7870	0.5420
o	0.8690	0.6110
p	0.8870	0.6100
q	0.8160	0.5660
r	0.8070	0.5620
s	0.7410	0.4970
t	0.8300	0.6340
u	0.7710	0.5200
w	0.8060	0.5830
x	0.8290	0.5910
y	0.8670	0.6060
z	0.7520	0.5530