wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 07:59 am BST

PDB ID	:	9T5T / pdb_00009t5t
EMDB ID	:	EMD-55593
Title	:	Chlorophyll f-containing dimeric far-red Photosystem II from Chroococcidiopsis thermalis PCC 7203
Authors	:	Leong, H.F.; Consoli, G.; Murray, J.W.; Fantuzzi, A.; Rutherford, A.W.
Deposited on	:	2025-11-05
Resolution	:	2.17 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 (i) symbol.

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

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

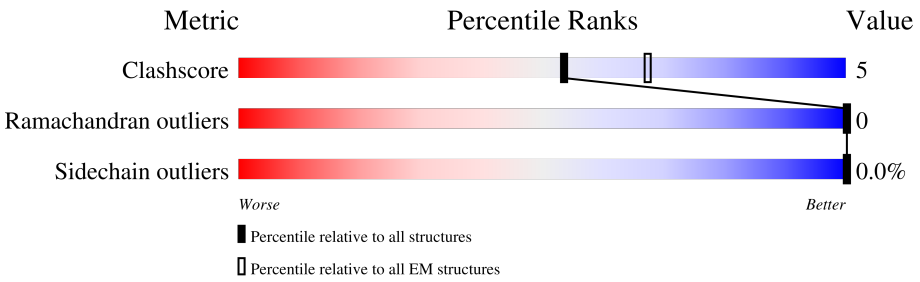
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

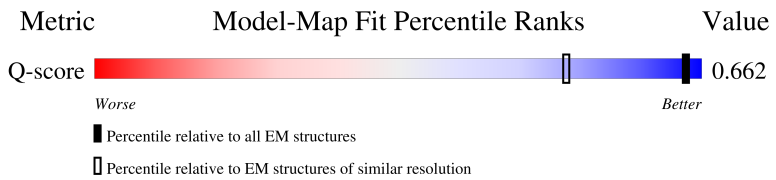
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.17 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	2651 (1.67 - 2.67)

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	369	79% 11% 9%
1	a	369	78% 12% 9%
2	B	520	89% 8% •
2	b	520	88% 9% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	466	88% 8% •
3	c	466	88% 9% •
4	D	352	89% 7% •
4	d	352	90% 7% •
5	E	82	• 85% 10% 5%
5	e	82	• 85% 10% 5%
6	F	44	5% 75% 7% 18%
6	f	44	5% 75% 7% 18%
7	G	48	79% • 17%
7	g	48	81% • 17%
8	H	69	96% • •
8	h	69	96% • •
9	I	38	84% 5% 11%
9	i	38	82% 8% 11%
10	J	39	• 90% • 8%
10	j	39	• 90% • 8%
11	K	60	53% 8% 38%
11	k	60	55% 7% 38%
12	L	41	80% 7% 12%
12	l	41	80% 7% 12%
13	M	37	78% 14% 8%
13	m	37	78% 14% 8%
14	O	274	• 82% 7% 11%
14	o	274	• 82% 7% 11%
15	R	41	22% 61% 20% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	r	41	22% 61% 20% 20%
16	T	32	72% 22% 6%
16	t	32	72% 22% 6%
17	U	153	58% 5% 37%
17	u	153	58% 5% 37%
18	V	163	77% 7% 16%
18	v	163	77% 7% 16%
19	X	39	95%
19	x	39	95%
20	Y	43	72% 26%
20	y	43	72% 26%
21	Z	63	87% 11%
21	z	63	90% 8%

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
26	CL7	A	406	X	-	-	-
26	CL7	a	406	X	-	-	-
34	F6C	B	608	X	-	-	-
34	F6C	B	614	X	-	-	-
34	F6C	B	617	X	-	-	-
34	F6C	C	507	X	-	-	-
34	F6C	b	608	X	-	-	-
34	F6C	b	614	X	-	-	-
34	F6C	b	617	X	-	-	-
34	F6C	c	507	X	-	-	-
38	HEC	V	201	X	-	-	-
38	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 52226 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
			Total	C	N	O	S		
1	A	334	2616	1708	430	460	18	0	0
1	a	334	2616	1708	430	460	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	504	3970	2597	669	688	16	0	0
2	b	504	3970	2597	669	688	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	450	3475	2267	591	606	11	0	0
3	c	450	3475	2267	591	606	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	340	2733	1812	443	465	13	0	0
4	d	340	2733	1812	443	465	13	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	78	639	418	104	117	0	0
5	e	78	639	418	104	117	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	36	293	200	48	44	1	0	0
6	f	36	293	200	48	44	1	0	0

- Molecule 7 is a protein called PsbH2'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	40	301	198	47	55	1	0	0
7	g	40	301	198	47	55	1	0	0

- Molecule 8 is a protein called Photosystem II phosphoprotein PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	67	535	361	87	84	3	0	0
8	h	67	535	361	87	84	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	34	274	187	43	43	1	0	0
9	i	34	274	187	43	43	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	36	266	178	42	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	j	36	266	178	42	46	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	37	299	209	43	47	0	0
11	k	37	299	209	43	47	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	36	294	196	46	52	0	0
12	l	36	294	196	46	52	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	34	266	178	40	47	1	0	0
13	m	34	266	178	40	47	1	0	0

- Molecule 14 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	243	1832	1151	308	369	4	0	0
14	o	243	1832	1151	308	369	4	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	R	33	252	170	43	39	0	0
15	r	33	252	170	43	39	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	T	30	239	162	36	40	1	0	0
16	t	30	239	162	36	40	1	0	0

- Molecule 17 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	U	97	765	474	136	153	2	0	0
17	u	97	765	474	136	153	2	0	0

- Molecule 18 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	V	137	1048	652	180	211	5	0	0
18	v	137	1048	652	180	211	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	X	38	297	199	46	50	2	0	0
19	x	38	297	199	46	50	2	0	0

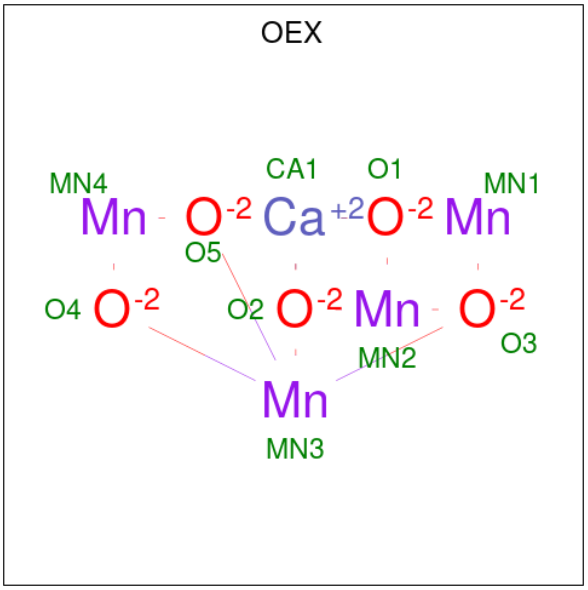
- Molecule 20 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Y	32	250	168	39	42	1	0	0
20	y	32	250	168	39	42	1	0	0

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	62	Total 482	C 334	N 73	O 74	S 1	0	0
21	z	62	Total 482	C 334	N 73	O 74	S 1	0	0

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

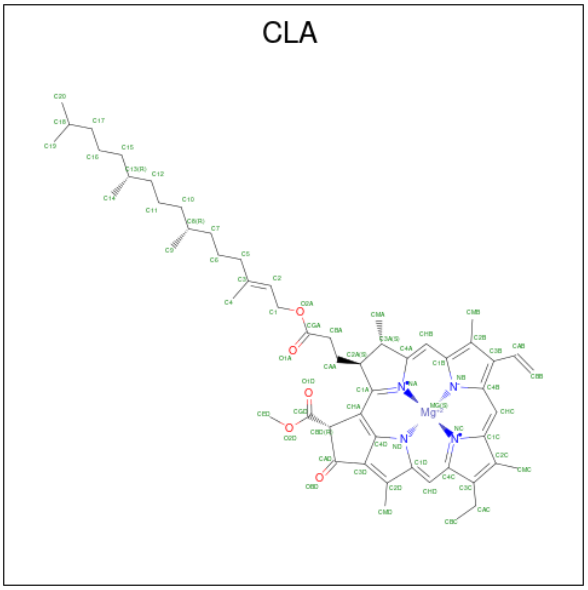
Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total 2	Cl 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
24	a	2	2	2	0

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
25	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	a	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

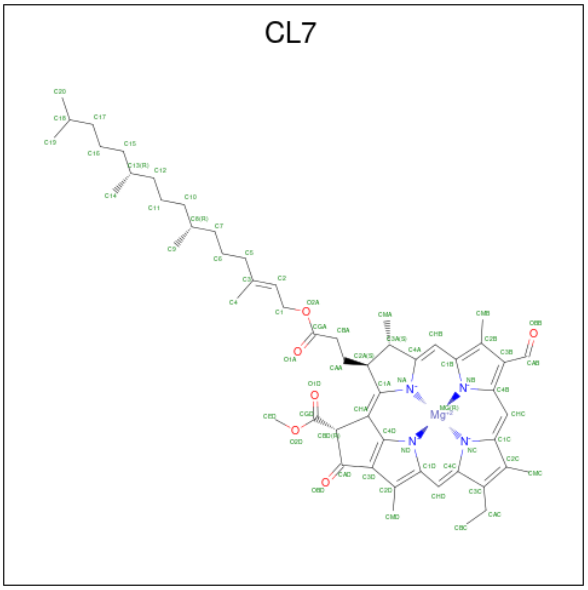
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	c	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
25	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	d	1	65	55	1	4	5	0

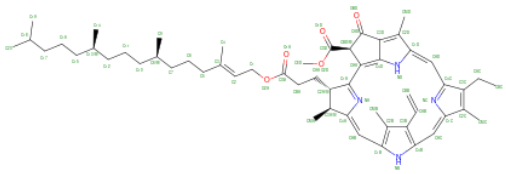
- Molecule 26 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	A	1	65	54	1	4	6	0
			Total	C	Mg	N	O	
26	a	1	65	54	1	4	6	0

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

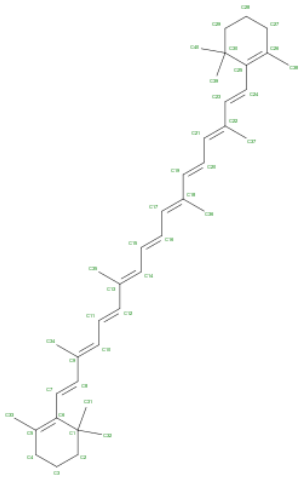
PHO



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

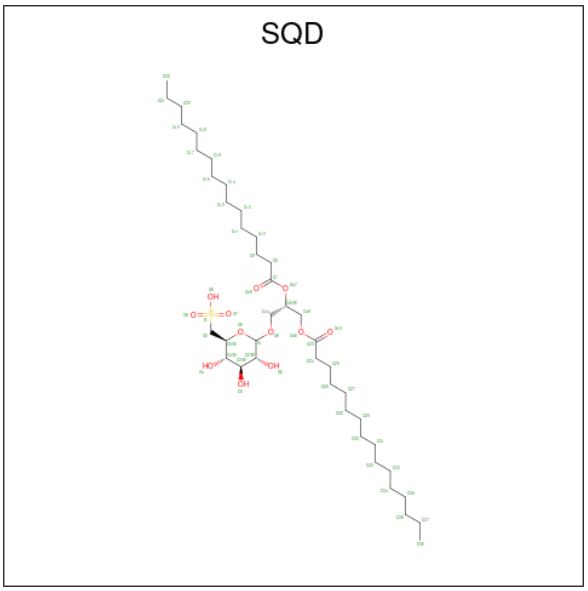
- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

BCR



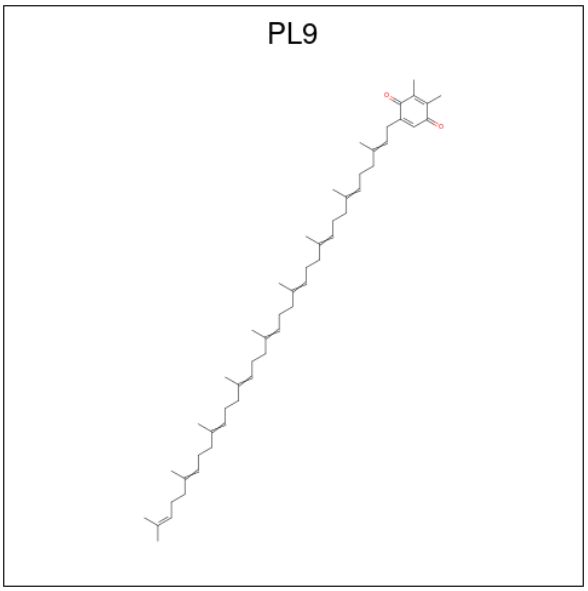
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
28	A	1	40	40	0
28	B	1	40	40	0
28	B	1	40	40	0
28	B	1	40	40	0
28	B	1	40	40	0
28	C	1	40	40	0
28	C	1	40	40	0
28	D	1	40	40	0
28	K	1	40	40	0
28	K	1	40	40	0
28	a	1	40	40	0
28	b	1	40	40	0
28	b	1	40	40	0
28	b	1	40	40	0
28	b	1	40	40	0
28	c	1	40	40	0
28	c	1	40	40	0
28	d	1	40	40	0
28	k	1	40	40	0
28	k	1	40	40	0

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



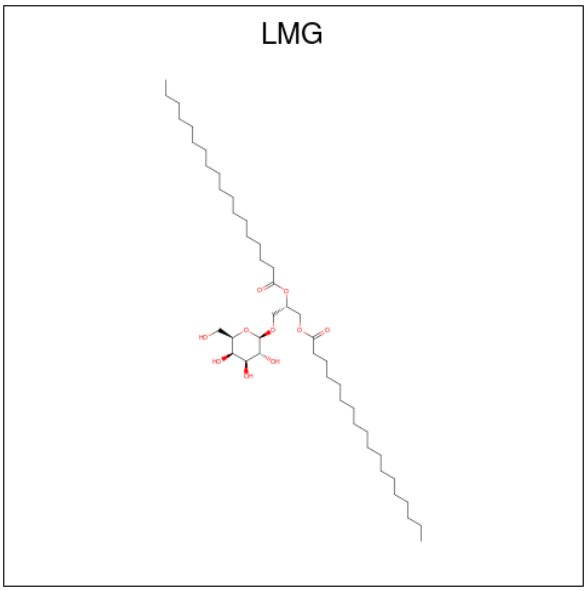
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
29	A	1	54	41	12	1	0
			Total	C	O	S	
29	A	1	54	41	12	1	0
			Total	C	O	S	
29	B	1	54	41	12	1	0
			Total	C	O	S	
29	C	1	38	25	12	1	0
			Total	C	O	S	
29	D	1	45	32	12	1	0
			Total	C	O	S	
29	H	1	54	41	12	1	0
			Total	C	O	S	
29	a	1	54	41	12	1	0
			Total	C	O	S	
29	a	1	54	41	12	1	0
			Total	C	O	S	
29	b	1	54	41	12	1	0
			Total	C	O	S	
29	c	1	38	25	12	1	0
			Total	C	O	S	
29	d	1	45	32	12	1	0
			Total	C	O	S	
29	h	1	54	41	12	1	0

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



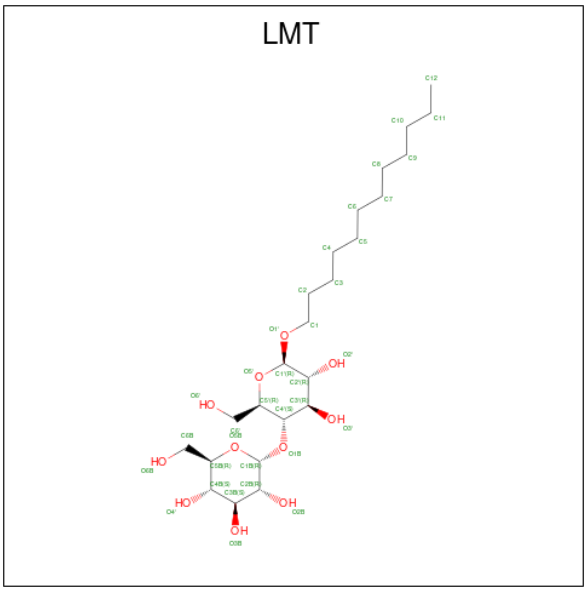
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	A	1	55	53	2	0
30	D	1	55	53	2	0
30	a	1	55	53	2	0
30	d	1	55	53	2	0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	A	1	48	38	10	0
31	B	1	55	45	10	0
31	C	1	51	41	10	0
31	C	1	53	43	10	0
31	D	1	51	41	10	0
31	L	1	55	45	10	0
31	a	1	48	38	10	0
31	b	1	55	45	10	0
31	c	1	51	41	10	0
31	c	1	53	43	10	0
31	d	1	51	41	10	0
31	l	1	55	45	10	0
31	P	1	47	37	10	0
31	p	1	47	37	10	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



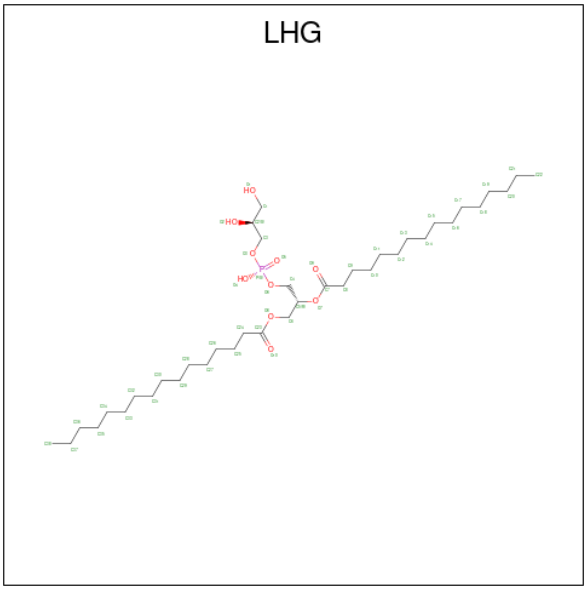
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total 32	C 21	O 11	0
32	A	1	Total 35	C 24	O 11	0
32	B	1	Total 25	C 19	O 6	0
32	C	1	Total 32	C 21	O 11	0
32	F	1	Total 35	C 24	O 11	0
32	G	1	Total 35	C 24	O 11	0
32	L	1	Total 35	C 24	O 11	0
32	L	1	Total 35	C 24	O 11	0
32	M	1	Total 35	C 24	O 11	0
32	Z	1	Total 35	C 24	O 11	0
32	a	1	Total 32	C 21	O 11	0
32	a	1	Total 35	C 24	O 11	0
32	b	1	Total 25	C 19	O 6	0
32	c	1	Total 32	C 21	O 11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	f	1	35	24	11	0
32	g	1	35	24	11	0
32	l	1	35	24	11	0
32	l	1	35	24	11	0
32	m	1	35	24	11	0
32	z	1	35	24	11	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	A	1	49	38	10	1	0
33	A	1	49	38	10	1	0
33	D	1	49	38	10	1	0
33	D	1	49	38	10	1	0
33	D	1	41	30	10	1	0

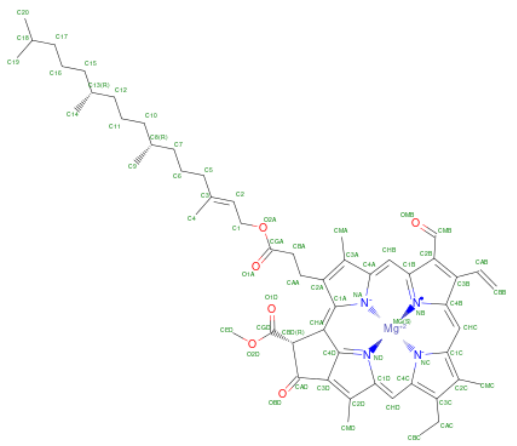
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	E	1	49	38	10	1	0
33	E	1	49	38	10	1	0
33	J	1	49	38	10	1	0
33	L	1	49	38	10	1	0
33	a	1	49	38	10	1	0
33	a	1	49	38	10	1	0
33	d	1	49	38	10	1	0
33	d	1	49	38	10	1	0
33	d	1	41	30	10	1	0
33	e	1	49	38	10	1	0
33	e	1	49	38	10	1	0
33	j	1	49	38	10	1	0
33	l	1	49	38	10	1	0
33	P	1	49	38	10	1	0
33	p	1	49	38	10	1	0

- Molecule 34 is Chlorophyll F (CCD ID: F6C) (formula: $C_{55}H_{68}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).

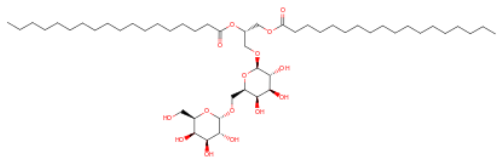
F6C



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
34	B	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
34	B	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
34	B	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
34	C	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
34	b	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
34	b	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
34	b	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
34	c	1	66	55	1	4	6	0

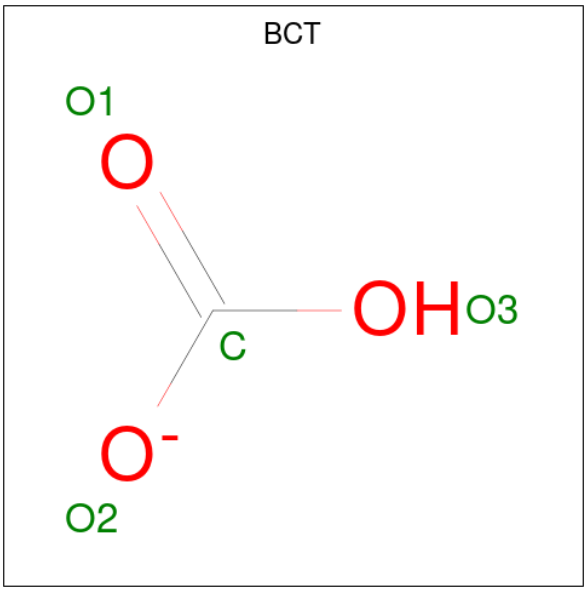
- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



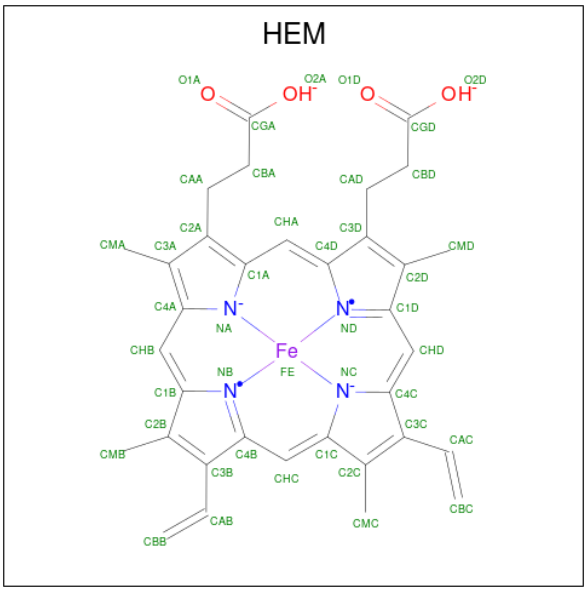
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	C	1	62	47	15	0
35	C	1	62	47	15	0
35	C	1	62	47	15	0
35	c	1	62	47	15	0
35	c	1	62	47	15	0
35	c	1	62	47	15	0

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				AltConf
36	D	1	Total	C	O		0
			4	1	3		
36	d	1	Total	C	O		0
			4	1	3		

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



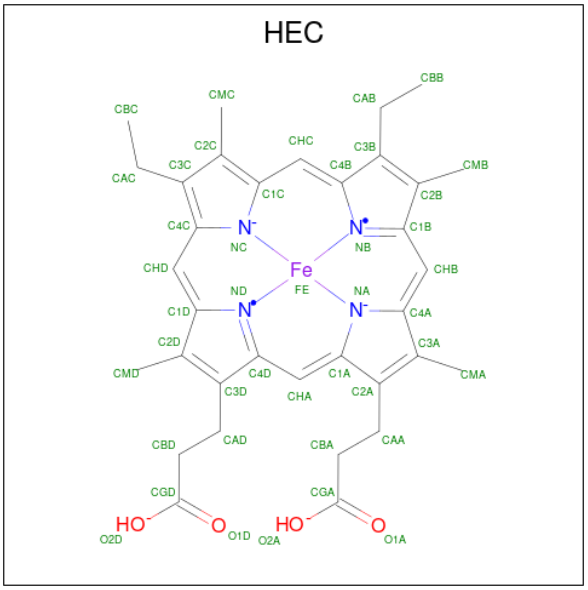
Mol	Chain	Residues	Atoms					AltConf
37	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

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

- Molecule 38 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	A	27	27	27	0
39	A	24	24	24	0
39	A	5	5	5	0
39	A	1	1	1	0
39	A	1	1	1	0
39	A	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	A	1	1	1	0
			Total	O	
39	A	1	1	1	0
			Total	O	
39	A	1	1	1	0
			Total	O	
39	A	1	1	1	0
			Total	O	
39	A	1	1	1	0
			Total	O	
39	B	18	18	18	0
			Total	O	
39	B	3	3	3	0
			Total	O	
39	B	16	16	16	0
			Total	O	
39	B	1	1	1	0
			Total	O	
39	B	38	38	38	0
			Total	O	
39	B	1	1	1	0
			Total	O	
39	B	1	1	1	0
			Total	O	
39	B	1	1	1	0
			Total	O	
39	B	1	1	1	0
			Total	O	
39	B	1	1	1	0
			Total	O	
39	C	16	16	16	0
			Total	O	
39	C	8	8	8	0
			Total	O	
39	C	12	12	12	0
			Total	O	
39	C	2	2	2	0
			Total	O	
39	C	5	5	5	0
			Total	O	
39	C	3	3	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	C	11	11	11	0
			Total	O	
39	C	5	5	5	0
			Total	O	
39	C	1	1	1	0
			Total	O	
39	C	1	1	1	0
			Total	O	
39	C	1	1	1	0
			Total	O	
39	C	1	1	1	0
			Total	O	
39	C	1	1	1	0
			Total	O	
39	C	1	1	1	0
			Total	O	
39	D	1	1	1	0
			Total	O	
39	D	1	1	1	0
			Total	O	
39	D	1	1	1	0
			Total	O	
39	D	1	1	1	0
			Total	O	
39	D	1	1	1	0
			Total	O	
39	D	15	15	15	0
			Total	O	
39	D	1	1	1	0
			Total	O	
39	D	3	3	3	0
			Total	O	
39	D	5	5	5	0
			Total	O	
39	D	4	4	4	0
			Total	O	
39	D	17	17	17	0
			Total	O	
39	D	5	5	5	0
			Total	O	
39	E	4	4	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	F	1	1	1	0
39	G	1	1	1	0
39	G	1	1	1	0
39	H	1	1	1	0
39	H	1	1	1	0
39	H	1	1	1	0
39	H	1	1	1	0
39	H	3	3	3	0
39	H	1	1	1	0
39	L	3	3	3	0
39	O	1	1	1	0
39	O	1	1	1	0
39	O	1	1	1	0
39	O	6	6	6	0
39	O	11	11	11	0
39	T	1	1	1	0
39	U	5	5	5	0
39	U	1	1	1	0
39	U	1	1	1	0
39	U	1	1	1	0
39	V	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	V	1	1	1	0
			Total	O	
39	V	1	1	1	0
			Total	O	
39	V	1	1	1	0
			Total	O	
39	V	2	2	2	0
			Total	O	
39	V	3	3	3	0
			Total	O	
39	V	5	5	5	0
			Total	O	
39	X	1	1	1	0
			Total	O	
39	a	27	27	27	0
			Total	O	
39	a	24	24	24	0
			Total	O	
39	a	5	5	5	0
			Total	O	
39	a	1	1	1	0
			Total	O	
39	a	1	1	1	0
			Total	O	
39	a	1	1	1	0
			Total	O	
39	a	1	1	1	0
			Total	O	
39	a	1	1	1	0
			Total	O	
39	a	1	1	1	0
			Total	O	
39	a	1	1	1	0
			Total	O	
39	a	1	1	1	0
			Total	O	
39	b	18	18	18	0
			Total	O	
39	b	2	2	2	0
			Total	O	
39	b	17	17	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	b	1	1	1	0
			Total	O	
39	b	38	38	38	0
			Total	O	
39	b	1	1	1	0
			Total	O	
39	b	1	1	1	0
			Total	O	
39	b	1	1	1	0
			Total	O	
39	b	1	1	1	0
			Total	O	
39	b	1	1	1	0
			Total	O	
39	c	16	16	16	0
			Total	O	
39	c	8	8	8	0
			Total	O	
39	c	12	12	12	0
			Total	O	
39	c	2	2	2	0
			Total	O	
39	c	5	5	5	0
			Total	O	
39	c	3	3	3	0
			Total	O	
39	c	11	11	11	0
			Total	O	
39	c	5	5	5	0
			Total	O	
39	c	1	1	1	0
			Total	O	
39	c	1	1	1	0
			Total	O	
39	c	1	1	1	0
			Total	O	
39	c	1	1	1	0
			Total	O	
39	c	1	1	1	0
			Total	O	
39	c	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	d	1	1	1	0
			Total	O	
39	d	1	1	1	0
			Total	O	
39	d	1	1	1	0
			Total	O	
39	d	1	1	1	0
			Total	O	
39	d	1	1	1	0
			Total	O	
39	d	15	15	15	0
			Total	O	
39	d	1	1	1	0
			Total	O	
39	d	3	3	3	0
			Total	O	
39	d	5	5	5	0
			Total	O	
39	d	4	4	4	0
			Total	O	
39	d	17	17	17	0
			Total	O	
39	d	5	5	5	0
			Total	O	
39	e	4	4	4	0
			Total	O	
39	f	1	1	1	0
			Total	O	
39	g	1	1	1	0
			Total	O	
39	g	1	1	1	0
			Total	O	
39	h	1	1	1	0
			Total	O	
39	h	1	1	1	0
			Total	O	
39	h	1	1	1	0
			Total	O	
39	h	1	1	1	0
			Total	O	
39	h	3	3	3	0

Continued on next page...

Continued from previous page...

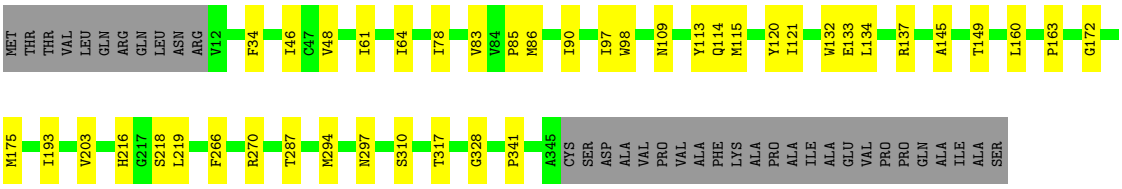
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
39	h	1	1	1	0
			Total	O	
39	l	3	3	3	0
			Total	O	
39	o	1	1	1	0
			Total	O	
39	o	1	1	1	0
			Total	O	
39	o	1	1	1	0
			Total	O	
39	o	6	6	6	0
			Total	O	
39	o	11	11	11	0
			Total	O	
39	t	1	1	1	0
			Total	O	
39	u	5	5	5	0
			Total	O	
39	u	1	1	1	0
			Total	O	
39	u	1	1	1	0
			Total	O	
39	u	1	1	1	0
			Total	O	
39	v	1	1	1	0
			Total	O	
39	v	1	1	1	0
			Total	O	
39	v	1	1	1	0
			Total	O	
39	v	1	1	1	0
			Total	O	
39	v	2	2	2	0
			Total	O	
39	v	3	3	3	0
			Total	O	
39	v	5	5	5	0
			Total	O	
39	x	1	1	1	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.

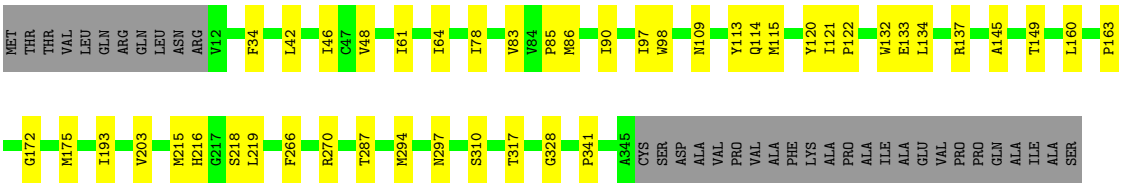
• Molecule 1: Photosystem II protein D1

Chain A: 79% 11% 9%



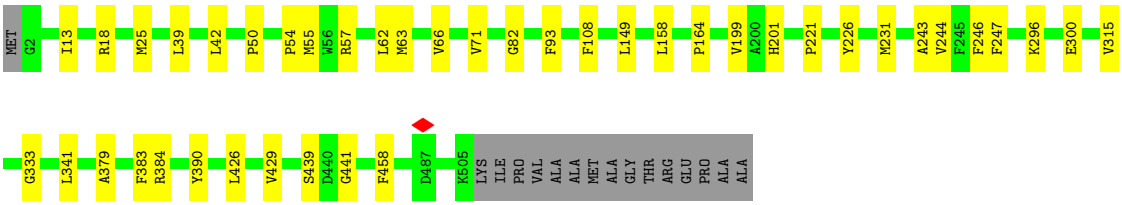
• Molecule 1: Photosystem II protein D1

Chain a: 78% 12% 9%



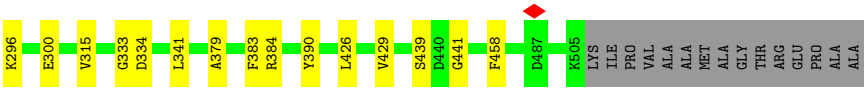
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 89% 8% •



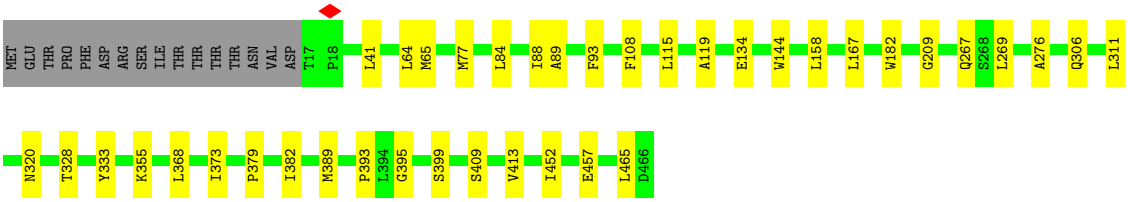
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 88% 9% •



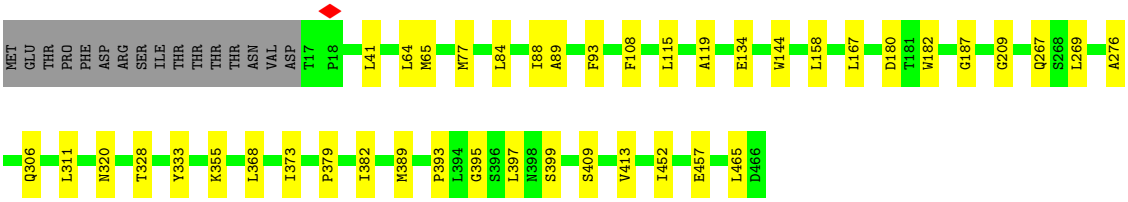
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



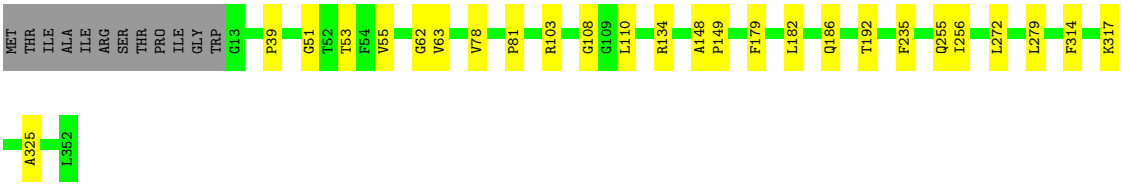
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



• Molecule 4: Photosystem II D2 protein

Chain D:

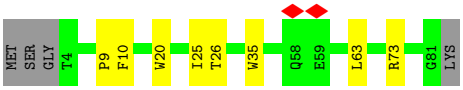


• Molecule 4: Photosystem II D2 protein

Chain d:

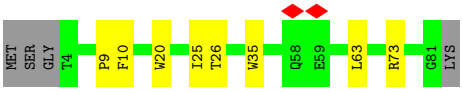
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



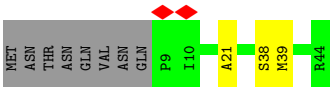
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:



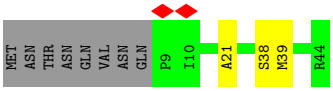
- Molecule 6: Cytochrome b559 subunit beta

Chain F:



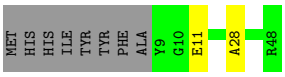
- Molecule 6: Cytochrome b559 subunit beta

Chain f:



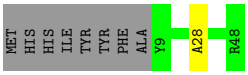
- Molecule 7: PsbH2'

Chain G:



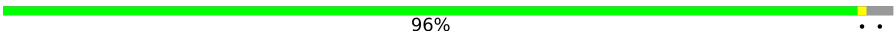
- Molecule 7: PsbH2'

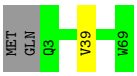
Chain g:



- Molecule 8: Photosystem II phosphoprotein PsbH

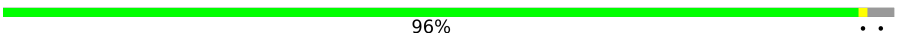
Chain H:

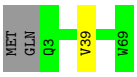




- Molecule 8: Photosystem II phosphoprotein PsbH

Chain h:





• Molecule 9: Photosystem II reaction center protein I

Chain I: 84% 5% 11%

M1 V7 R34 ARG ASP LEU ASP

• Molecule 9: Photosystem II reaction center protein I

Chain i: 82% 8% 11%

M1 L4 V7 R34 ARG ASP LEU ASP

• Molecule 10: Photosystem II reaction center protein J

Chain J: 90% 8%

MET SER GLY S4 I7 L39

• Molecule 10: Photosystem II reaction center protein J

Chain j: 90% 8%

MET SER GLY S4 I7 L39

• Molecule 11: Photosystem II reaction center protein K

Chain K: 53% 8% 38%

MET HIS VAL ASN SER GLU SER CYS VAL GLU LYS GLU ASN LEU SER MET GLU ALA ALA LEU LEU LEU ALA K24 L32 P40 P43 L44 F45 F46 R60

• Molecule 11: Photosystem II reaction center protein K

Chain k: 55% 7% 38%

MET HIS VAL ASN SER GLU SER CYS VAL GLU LYS GLU ASN LEU SER MET GLU ALA ALA LEU LEU LEU ALA K24 L32 P43 L44 F45 F46 R60

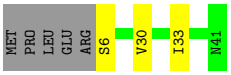
• Molecule 12: Photosystem II reaction center protein L

Chain L: 80% 7% 12%

MET PRO LEU GLU ARG S6 V30 I33 M41

• Molecule 12: Photosystem II reaction center protein L

Chain l:



• Molecule 13: Photosystem II reaction center protein M

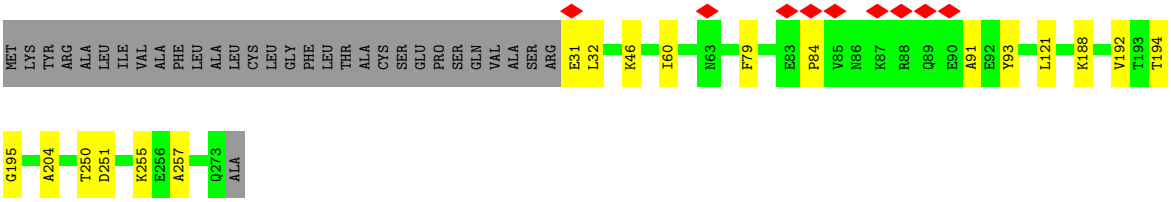
Chain M:

• Molecule 13: Photosystem II reaction center protein M

Chain m:

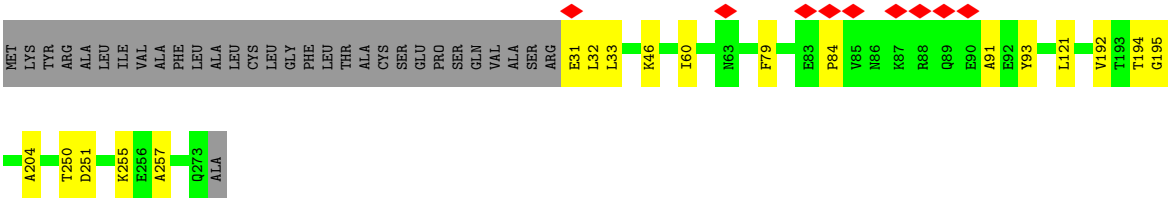
• Molecule 14: Photosystem II extrinsic protein O

Chain O:



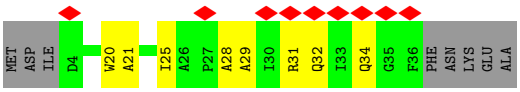
• Molecule 14: Photosystem II extrinsic protein O

Chain o:



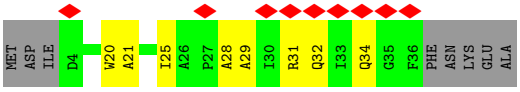
• Molecule 15: Photosystem II reaction center protein Y

Chain R:



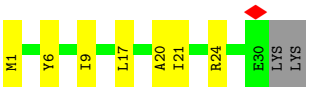
• Molecule 15: Photosystem II reaction center protein Y

Chain r:



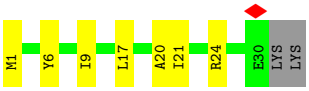
• Molecule 16: Photosystem II reaction center protein T

Chain T:



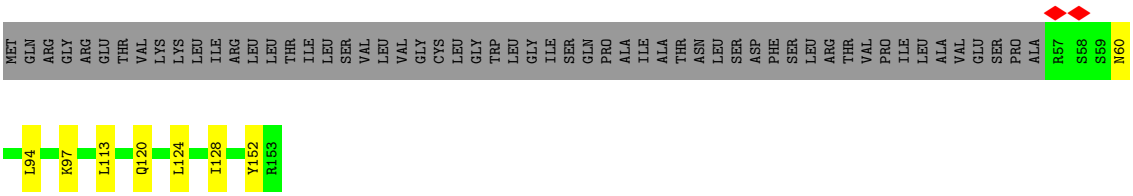
• Molecule 16: Photosystem II reaction center protein T

Chain t:



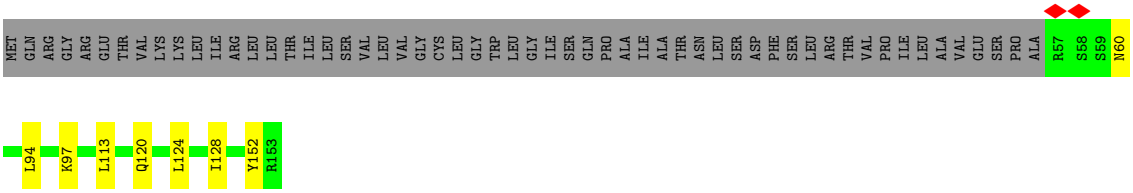
• Molecule 17: Photosystem II extrinsic protein U

Chain U:



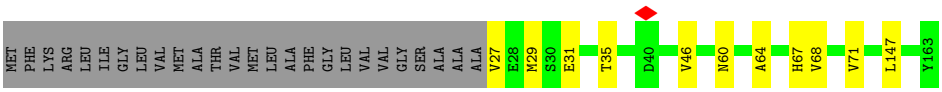
• Molecule 17: Photosystem II extrinsic protein U

Chain u:



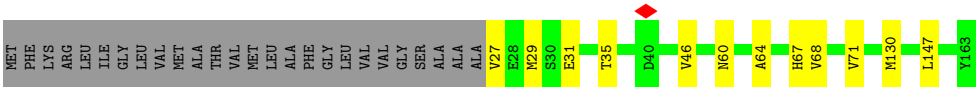
• Molecule 18: Photosystem II extrinsic protein V

Chain V:



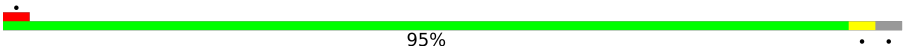
- Molecule 18: Photosystem II extrinsic protein V

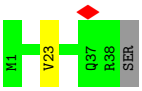
Chain v:



- Molecule 19: Photosystem II reaction center protein X

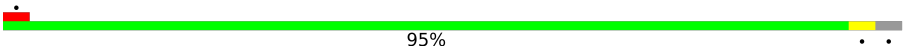
Chain X:

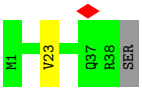




- Molecule 19: Photosystem II reaction center protein X

Chain x:





- Molecule 20: Photosystem II reaction center protein Psb30

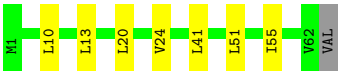
Chain Y:

- Molecule 20: Photosystem II reaction center protein Psb30

Chain y:

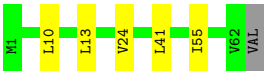
- Molecule 21: Photosystem II reaction center protein Z

Chain Z:



- Molecule 21: Photosystem II reaction center protein Z

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	49763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.357	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	469.94998, 469.94998, 469.94998	wwPDB
Map dimensions	650, 650, 650	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.723, 0.723, 0.723	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: OEX, BCR, SQD, HEC, CL, DGD, FE2, CLA, PHO, BCT, FME, LMG, HEM, CL7, LHG, F6C, LMT, PL9

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	0.25	0/2702	0.33	0/3688
1	a	0.25	0/2702	0.33	0/3688
2	B	0.24	0/4103	0.30	0/5580
2	b	0.24	0/4103	0.30	0/5580
3	C	0.22	0/3586	0.29	0/4882
3	c	0.23	0/3586	0.29	0/4882
4	D	0.25	0/2832	0.32	0/3857
4	d	0.25	0/2832	0.32	0/3857
5	E	0.21	0/659	0.28	0/899
5	e	0.21	0/659	0.28	0/899
6	F	0.22	0/303	0.31	0/414
6	f	0.22	0/303	0.31	0/414
7	G	0.17	0/307	0.18	0/416
7	g	0.17	0/307	0.18	0/416
8	H	0.21	0/552	0.27	0/749
8	h	0.21	0/552	0.27	0/749
9	I	0.20	0/271	0.27	0/368
9	i	0.20	0/271	0.27	0/368
10	J	0.17	0/273	0.27	0/372
10	j	0.17	0/273	0.27	0/372
11	K	0.22	0/309	0.34	0/423
11	k	0.22	0/309	0.34	0/423
12	L	0.21	0/301	0.26	0/407
12	l	0.22	0/301	0.26	0/407
13	M	0.22	0/260	0.37	0/354
13	m	0.22	0/260	0.37	0/354
14	O	0.19	0/1863	0.31	0/2529
14	o	0.19	0/1863	0.31	0/2529
15	R	0.16	0/258	0.30	0/353
15	r	0.16	0/258	0.30	0/353
16	T	0.20	0/234	0.26	0/318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	t	0.20	0/234	0.27	0/318
17	U	0.17	0/777	0.26	0/1051
17	u	0.17	0/777	0.26	0/1051
18	V	0.20	0/1066	0.26	0/1444
18	v	0.20	0/1066	0.26	0/1444
19	X	0.18	0/292	0.25	0/396
19	x	0.18	0/292	0.25	0/396
20	Y	0.14	0/255	0.28	0/346
20	y	0.14	0/255	0.28	0/346
21	Z	0.16	0/495	0.23	0/679
21	z	0.16	0/495	0.23	0/679
All	All	0.22	0/43396	0.30	0/59050

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2508	34	0
1	a	2616	0	2508	37	0
2	B	3970	0	3820	32	0
2	b	3970	0	3820	34	0
3	C	3475	0	3382	28	0
3	c	3475	0	3382	30	0
4	D	2733	0	2617	20	0
4	d	2733	0	2617	19	0
5	E	639	0	617	10	0
5	e	639	0	617	10	0
6	F	293	0	304	3	0
6	f	293	0	304	3	0
7	G	301	0	302	2	0
7	g	301	0	302	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	535	0	554	2	0
8	h	535	0	554	2	0
9	I	274	0	288	2	0
9	i	274	0	288	3	0
10	J	266	0	272	1	0
10	j	266	0	272	1	0
11	K	299	0	315	4	0
11	k	299	0	315	3	0
12	L	294	0	298	3	0
12	l	294	0	298	3	0
13	M	266	0	280	6	0
13	m	266	0	280	6	0
14	O	1832	0	1791	12	0
14	o	1832	0	1791	13	0
15	R	252	0	265	6	0
15	r	252	0	265	6	0
16	T	239	0	252	7	0
16	t	239	0	252	7	0
17	U	765	0	739	5	0
17	u	765	0	739	5	0
18	V	1048	0	1027	8	0
18	v	1048	0	1027	9	0
19	X	297	0	320	1	0
19	x	297	0	320	1	0
20	Y	250	0	259	1	0
20	y	250	0	259	1	0
21	Z	482	0	520	5	0
21	z	482	0	520	3	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	195	0	216	7	0
25	B	845	0	936	34	0
25	C	771	0	843	40	0
25	D	130	0	144	5	0
25	a	195	0	216	8	0
25	b	845	0	936	34	0
25	c	771	0	843	38	0
25	d	130	0	144	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	65	0	70	1	0
26	a	65	0	70	1	0
27	A	128	0	148	6	0
27	a	128	0	148	6	0
28	A	40	0	56	2	0
28	B	160	0	224	9	0
28	C	80	0	112	1	0
28	D	40	0	56	3	0
28	K	80	0	112	6	0
28	a	40	0	56	0	0
28	b	160	0	224	7	0
28	c	80	0	112	2	0
28	d	40	0	56	2	0
28	k	80	0	112	5	0
29	A	108	0	156	8	0
29	B	54	0	78	3	0
29	C	38	0	40	1	0
29	D	45	0	57	1	0
29	H	54	0	78	1	0
29	a	108	0	156	7	0
29	b	54	0	78	3	0
29	c	38	0	40	1	0
29	d	45	0	57	1	0
29	h	54	0	78	2	0
30	A	55	0	80	6	0
30	D	55	0	80	0	0
30	a	55	0	80	6	0
30	d	55	0	80	0	0
31	A	48	0	69	2	0
31	B	55	0	86	3	0
31	C	104	0	151	8	0
31	D	51	0	72	1	0
31	L	55	0	86	2	0
31	P	47	0	67	1	0
31	a	48	0	69	2	0
31	b	55	0	86	2	0
31	c	104	0	151	8	0
31	d	51	0	72	2	0
31	l	55	0	86	2	0
31	p	47	0	67	1	0
32	A	67	0	83	3	0
32	B	25	0	35	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	C	32	0	37	0	0
32	F	35	0	46	0	0
32	G	35	0	46	0	0
32	L	70	0	92	2	0
32	M	35	0	46	3	0
32	Z	35	0	46	1	0
32	a	67	0	83	3	0
32	b	25	0	35	0	0
32	c	32	0	37	0	0
32	f	35	0	46	0	0
32	g	35	0	46	0	0
32	l	70	0	92	1	0
32	m	35	0	46	3	0
32	z	35	0	46	1	0
33	A	98	0	148	6	0
33	D	139	0	203	2	0
33	E	98	0	148	4	0
33	J	49	0	74	4	0
33	L	49	0	74	1	0
33	P	49	0	74	3	0
33	a	98	0	148	7	0
33	d	139	0	203	2	0
33	e	98	0	148	4	0
33	j	49	0	74	3	0
33	l	49	0	74	1	0
33	p	49	0	74	3	0
34	B	183	0	0	1	0
34	C	66	0	0	0	0
34	b	183	0	0	1	0
34	c	66	0	0	0	0
35	C	186	0	246	7	0
35	c	186	0	246	6	0
36	D	4	0	0	0	0
36	d	4	0	0	0	0
37	F	43	0	30	5	0
37	f	43	0	30	5	0
38	V	43	0	30	0	0
38	v	43	0	30	0	0
39	A	64	0	0	0	0
39	B	81	0	0	0	0
39	C	68	0	0	0	0
39	D	55	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	E	4	0	0	0	0
39	F	1	0	0	0	0
39	G	2	0	0	0	0
39	H	8	0	0	0	0
39	L	3	0	0	0	0
39	O	20	0	0	0	0
39	T	1	0	0	0	0
39	U	8	0	0	0	0
39	V	14	0	0	0	0
39	X	1	0	0	0	0
39	a	64	0	0	0	0
39	b	81	0	0	0	0
39	c	68	0	0	0	0
39	d	55	0	0	0	0
39	e	4	0	0	0	0
39	f	1	0	0	0	0
39	g	2	0	0	0	0
39	h	8	0	0	0	0
39	l	3	0	0	0	0
39	o	20	0	0	0	0
39	t	1	0	0	0	0
39	u	8	0	0	0	0
39	v	14	0	0	0	0
39	x	1	0	0	0	0
All	All	52226	0	52410	540	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 5.

The worst 5 of 540 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)
11:k:32:LEU:HD13	28:k:102:BCR:H312	1.70	0.73
2:b:50:PRO:HG2	2:b:82:GLY:HA2	1.71	0.73
11:K:32:LEU:HD13	28:K:102:BCR:H312	1.70	0.73
2:B:50:PRO:HG2	2:B:82:GLY:HA2	1.71	0.72
2:B:149:LEU:HD11	25:B:606:CLA:H151	1.73	0.71

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	332/369 (90%)	326 (98%)	6 (2%)	0	100	100
1	a	332/369 (90%)	326 (98%)	6 (2%)	0	100	100
2	B	502/520 (96%)	499 (99%)	3 (1%)	0	100	100
2	b	502/520 (96%)	499 (99%)	3 (1%)	0	100	100
3	C	448/466 (96%)	443 (99%)	5 (1%)	0	100	100
3	c	448/466 (96%)	443 (99%)	5 (1%)	0	100	100
4	D	338/352 (96%)	332 (98%)	6 (2%)	0	100	100
4	d	338/352 (96%)	332 (98%)	6 (2%)	0	100	100
5	E	76/82 (93%)	75 (99%)	1 (1%)	0	100	100
5	e	76/82 (93%)	75 (99%)	1 (1%)	0	100	100
6	F	34/44 (77%)	34 (100%)	0	0	100	100
6	f	34/44 (77%)	34 (100%)	0	0	100	100
7	G	38/48 (79%)	38 (100%)	0	0	100	100
7	g	38/48 (79%)	38 (100%)	0	0	100	100
8	H	65/69 (94%)	64 (98%)	1 (2%)	0	100	100
8	h	65/69 (94%)	64 (98%)	1 (2%)	0	100	100
9	I	32/38 (84%)	30 (94%)	2 (6%)	0	100	100
9	i	32/38 (84%)	30 (94%)	2 (6%)	0	100	100
10	J	34/39 (87%)	32 (94%)	2 (6%)	0	100	100
10	j	34/39 (87%)	32 (94%)	2 (6%)	0	100	100
11	K	35/60 (58%)	35 (100%)	0	0	100	100
11	k	35/60 (58%)	35 (100%)	0	0	100	100
12	L	34/41 (83%)	34 (100%)	0	0	100	100
12	l	34/41 (83%)	34 (100%)	0	0	100	100
13	M	32/37 (86%)	31 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	32/37 (86%)	31 (97%)	1 (3%)	0	100	100
14	O	241/274 (88%)	234 (97%)	7 (3%)	0	100	100
14	o	241/274 (88%)	234 (97%)	7 (3%)	0	100	100
15	R	31/41 (76%)	31 (100%)	0	0	100	100
15	r	31/41 (76%)	31 (100%)	0	0	100	100
16	T	28/32 (88%)	28 (100%)	0	0	100	100
16	t	28/32 (88%)	28 (100%)	0	0	100	100
17	U	95/153 (62%)	92 (97%)	3 (3%)	0	100	100
17	u	95/153 (62%)	92 (97%)	3 (3%)	0	100	100
18	V	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
18	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
19	X	36/39 (92%)	36 (100%)	0	0	100	100
19	x	36/39 (92%)	36 (100%)	0	0	100	100
20	Y	30/43 (70%)	30 (100%)	0	0	100	100
20	y	30/43 (70%)	30 (100%)	0	0	100	100
21	Z	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
21	z	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
All	All	5312/5946 (89%)	5224 (98%)	88 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/301 (91%)	273 (100%)	0	100	100
1	a	273/301 (91%)	273 (100%)	0	100	100
2	B	402/412 (98%)	402 (100%)	0	100	100
2	b	402/412 (98%)	402 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	341/357 (96%)	340 (100%)	1 (0%)	86	92
3	c	341/357 (96%)	340 (100%)	1 (0%)	86	92
4	D	281/291 (97%)	281 (100%)	0	100	100
4	d	281/291 (97%)	281 (100%)	0	100	100
5	E	69/73 (94%)	69 (100%)	0	100	100
5	e	69/73 (94%)	69 (100%)	0	100	100
6	F	31/39 (80%)	31 (100%)	0	100	100
6	f	31/39 (80%)	31 (100%)	0	100	100
7	G	30/37 (81%)	30 (100%)	0	100	100
7	g	30/37 (81%)	30 (100%)	0	100	100
8	H	56/58 (97%)	56 (100%)	0	100	100
8	h	56/58 (97%)	56 (100%)	0	100	100
9	I	29/33 (88%)	29 (100%)	0	100	100
9	i	29/33 (88%)	29 (100%)	0	100	100
10	J	28/30 (93%)	28 (100%)	0	100	100
10	j	28/30 (93%)	28 (100%)	0	100	100
11	K	32/52 (62%)	32 (100%)	0	100	100
11	k	32/52 (62%)	32 (100%)	0	100	100
12	L	34/39 (87%)	34 (100%)	0	100	100
12	l	34/39 (87%)	34 (100%)	0	100	100
13	M	29/32 (91%)	29 (100%)	0	100	100
13	m	29/32 (91%)	29 (100%)	0	100	100
14	O	196/228 (86%)	196 (100%)	0	100	100
14	o	196/228 (86%)	196 (100%)	0	100	100
15	R	24/31 (77%)	24 (100%)	0	100	100
15	r	24/31 (77%)	24 (100%)	0	100	100
16	T	23/25 (92%)	23 (100%)	0	100	100
16	t	23/25 (92%)	23 (100%)	0	100	100
17	U	80/129 (62%)	80 (100%)	0	100	100
17	u	80/129 (62%)	80 (100%)	0	100	100
18	V	114/132 (86%)	114 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	v	114/132 (86%)	114 (100%)	0	100	100
19	X	33/34 (97%)	33 (100%)	0	100	100
19	x	33/34 (97%)	33 (100%)	0	100	100
20	Y	26/34 (76%)	26 (100%)	0	100	100
20	y	26/34 (76%)	26 (100%)	0	100	100
21	Z	51/52 (98%)	51 (100%)	0	100	100
21	z	51/52 (98%)	51 (100%)	0	100	100
All	All	4364/4838 (90%)	4362 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	320	ASN
3	c	320	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	309	ASN
4	d	350	ASN
14	o	221	ASN
14	o	183	ASN
4	D	350	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)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	FME	m	1	13	8,9,10	0.35	0	7,9,11	0.91	0
16	FME	T	1	16	8,9,10	0.35	0	7,9,11	0.95	0
19	FME	X	1	19	8,9,10	0.35	0	7,9,11	0.90	0
13	FME	M	1	13	8,9,10	0.35	0	7,9,11	0.91	0
16	FME	t	1	16	8,9,10	0.35	0	7,9,11	0.95	0
19	FME	x	1	19	8,9,10	0.35	0	7,9,11	0.90	0
9	FME	I	1	9	8,9,10	0.34	0	7,9,11	0.99	0
9	FME	i	1	9	8,9,10	0.34	0	7,9,11	0.99	0

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
13	FME	m	1	13	-	2/7/9/11	-
16	FME	T	1	16	-	2/7/9/11	-
19	FME	X	1	19	-	0/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
16	FME	t	1	16	-	2/7/9/11	-
19	FME	x	1	19	-	0/7/9/11	-
9	FME	I	1	9	-	4/7/9/11	-
9	FME	i	1	9	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	1	FME	N-CA-CB-CG
9	I	1	FME	C-CA-CB-CG
9	i	1	FME	N-CA-CB-CG
9	i	1	FME	C-CA-CB-CG
9	I	1	FME	CA-CB-CG-SD

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	1	FME	2	0
16	t	1	FME	2	0
9	I	1	FME	1	0
9	i	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 184 ligands modelled in this entry, 6 are monoatomic - leaving 178 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	$\#\|Z\| > 2$
31	LMG	c	519	-	51,51,55	0.55	0	59,59,63	0.68	1 (1%)
25	CLA	a	405	1	69,73,73	1.18	7 (10%)	83,113,113	0.96	4 (4%)
25	CLA	b	616	2	69,73,73	1.23	8 (11%)	83,113,113	1.00	4 (4%)
25	CLA	C	504	39	69,73,73	1.20	7 (10%)	83,113,113	0.93	5 (6%)
33	LHG	E	101	-	48,48,48	0.52	0	51,54,54	0.49	0
25	CLA	C	509	3	69,73,73	1.20	8 (11%)	83,113,113	0.96	5 (6%)
32	LMT	g	104	-	36,36,36	0.57	0	47,47,47	0.64	0
28	BCR	K	102	-	41,41,41	0.34	0	56,56,56	0.84	1 (1%)
28	BCR	B	619	-	41,41,41	0.35	0	56,56,56	0.69	1 (1%)
25	CLA	D	403	4	69,73,73	1.19	7 (10%)	83,113,113	0.94	4 (4%)
25	CLA	c	511	3	69,73,73	1.22	8 (11%)	83,113,113	0.94	4 (4%)
31	LMG	l	212	-	55,55,55	0.51	0	63,63,63	0.66	0
33	LHG	d	410	-	40,40,48	0.58	0	43,46,54	0.54	0
33	LHG	P	629	-	48,48,48	0.49	0	51,54,54	0.63	1 (1%)
25	CLA	C	510	3	69,73,73	1.18	7 (10%)	83,113,113	0.95	4 (4%)
25	CLA	b	603	2	69,73,73	1.18	6 (8%)	83,113,113	0.94	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	LHG	d	409	-	48,48,48	0.52	0	51,54,54	0.49	0
33	LHG	D	410	-	40,40,48	0.58	0	43,46,54	0.54	0
32	LMT	L	213	-	36,36,36	0.54	0	47,47,47	0.78	1 (2%)
35	DGD	c	517	-	63,63,67	0.64	0	77,77,81	0.71	0
32	LMT	c	904	-	33,33,36	0.61	0	44,44,47	0.63	0
25	CLA	c	509	3	69,73,73	1.20	8 (11%)	83,113,113	0.96	5 (6%)
32	LMT	l	210	-	36,36,36	0.53	0	47,47,47	1.01	1 (2%)
25	CLA	C	506	3	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
25	CLA	B	602	39	69,73,73	1.18	7 (10%)	83,113,113	0.98	4 (4%)
31	LMG	D	411	-	51,51,55	0.59	0	59,59,63	0.65	1 (1%)
33	LHG	D	408	-	48,48,48	0.53	0	51,54,54	0.53	0
32	LMT	A	675	-	33,33,36	0.59	0	44,44,47	0.80	1 (2%)
25	CLA	c	510	3	69,73,73	1.18	7 (10%)	83,113,113	0.95	4 (4%)
25	CLA	c	506	3	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
31	LMG	A	415	-	48,48,55	0.59	0	56,56,63	0.69	0
25	CLA	C	505	3	69,73,73	1.21	8 (11%)	83,113,113	0.92	4 (4%)
38	HEC	V	201	18	50,50,50	1.42	6 (12%)	68,82,82	1.26	8 (11%)
27	PHO	a	408	-	58,69,69	1.95	10 (17%)	56,99,99	1.54	7 (12%)
25	CLA	c	502	3	69,73,73	1.19	8 (11%)	83,113,113	0.99	5 (6%)
33	LHG	e	244	-	48,48,48	0.51	0	51,54,54	0.50	0
25	CLA	C	501	3	69,73,73	1.19	7 (10%)	83,113,113	1.00	5 (6%)
35	DGD	C	516	-	63,63,67	0.66	0	77,77,81	0.69	1 (1%)
28	BCR	d	404	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
29	SQD	d	407	-	44,45,54	1.57	5 (11%)	53,56,65	1.61	8 (15%)
25	CLA	B	611	39	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
35	DGD	c	516	-	63,63,67	0.66	0	77,77,81	0.69	1 (1%)
34	F6C	b	614	2	72,74,74	1.67	10 (13%)	81,114,114	2.02	15 (18%)
38	HEC	v	201	18	50,50,50	1.42	6 (12%)	68,82,82	1.27	8 (11%)
29	SQD	B	622	-	53,54,54	1.49	6 (11%)	62,65,65	1.57	9 (14%)
25	CLA	A	410	1	69,73,73	1.18	8 (11%)	83,113,113	0.97	4 (4%)
29	SQD	a	412	-	53,54,54	1.52	9 (16%)	62,65,65	1.42	7 (11%)
25	CLA	c	505	3	69,73,73	1.21	8 (11%)	83,113,113	0.92	4 (4%)
25	CLA	a	410	1	69,73,73	1.18	8 (11%)	83,113,113	0.97	4 (4%)
25	CLA	c	501	3	69,73,73	1.19	7 (10%)	83,113,113	1.00	5 (6%)
25	CLA	B	609	2	69,73,73	1.19	7 (10%)	83,113,113	0.94	4 (4%)
27	PHO	a	409	-	58,69,69	1.97	9 (15%)	56,99,99	1.58	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	LHG	d	408	-	48,48,48	0.53	0	51,54,54	0.53	0
33	LHG	j	101	-	48,48,48	0.50	0	51,54,54	0.49	0
32	LMT	Z	102	-	36,36,36	0.54	0	47,47,47	1.00	2 (4%)
25	CLA	B	603	2	69,73,73	1.18	6 (8%)	83,113,113	0.94	4 (4%)
25	CLA	c	508	3	69,73,73	1.20	8 (11%)	83,113,113	0.93	4 (4%)
25	CLA	a	407	39	69,73,73	1.17	6 (8%)	83,113,113	1.00	4 (4%)
31	LMG	L	212	-	55,55,55	0.51	0	63,63,63	0.66	0
32	LMT	z	102	-	36,36,36	0.54	0	47,47,47	1.00	2 (4%)
25	CLA	B	607	2	69,73,73	1.23	8 (11%)	83,113,113	0.93	4 (4%)
32	LMT	G	104	-	36,36,36	0.57	0	47,47,47	0.64	0
34	F6C	B	617	2	57,59,74	1.85	11 (19%)	63,96,114	2.31	16 (25%)
28	BCR	D	404	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
25	CLA	B	606	2	69,73,73	1.20	6 (8%)	83,113,113	1.13	5 (6%)
33	LHG	J	101	-	48,48,48	0.50	0	51,54,54	0.49	0
28	BCR	k	102	-	41,41,41	0.34	0	56,56,56	0.84	1 (1%)
29	SQD	c	903	-	37,38,54	1.67	7 (18%)	46,49,65	1.54	8 (17%)
32	LMT	C	904	-	33,33,36	0.61	0	44,44,47	0.63	0
28	BCR	B	618	-	41,41,41	0.32	0	56,56,56	0.79	1 (1%)
25	CLA	B	605	2	69,73,73	1.25	8 (11%)	83,113,113	0.88	4 (4%)
25	CLA	C	513	3	60,64,73	1.26	7 (11%)	72,102,113	0.97	4 (5%)
28	BCR	C	514	-	41,41,41	0.31	0	56,56,56	0.59	0
34	F6C	C	507	39	72,74,74	1.67	11 (15%)	81,114,114	2.08	16 (19%)
25	CLA	c	504	39	69,73,73	1.20	7 (10%)	83,113,113	0.93	5 (6%)
25	CLA	b	611	39	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
26	CL7	a	406	39	71,73,73	1.16	5 (7%)	80,113,113	0.87	3 (3%)
25	CLA	c	512	3	69,73,73	1.19	6 (8%)	83,113,113	0.97	4 (4%)
29	SQD	b	622	-	53,54,54	1.49	6 (11%)	62,65,65	1.57	9 (14%)
35	DGD	C	518	-	63,63,67	0.65	0	77,77,81	0.69	1 (1%)
25	CLA	C	502	3	69,73,73	1.19	8 (11%)	83,113,113	0.99	5 (6%)
31	LMG	B	628	-	55,55,55	0.52	0	63,63,63	0.59	0
25	CLA	b	609	2	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)
25	CLA	C	511	3	69,73,73	1.22	8 (11%)	83,113,113	0.94	4 (4%)
29	SQD	a	417	-	53,54,54	1.47	7 (13%)	62,65,65	1.49	8 (12%)
34	F6C	b	608	39	72,74,74	1.67	11 (15%)	81,114,114	2.02	14 (17%)
29	SQD	A	412	-	53,54,54	1.52	9 (16%)	62,65,65	1.42	7 (11%)
31	LMG	c	902	-	53,53,55	0.46	0	61,61,63	0.61	0
28	BCR	A	411	-	41,41,41	0.33	0	56,56,56	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	CLA	d	403	4	69,73,73	1.19	7 (10%)	83,113,113	0.94	5 (6%)
28	BCR	b	619	-	41,41,41	0.35	0	56,56,56	0.69	1 (1%)
32	LMT	L	210	-	36,36,36	0.53	0	47,47,47	1.01	1 (2%)
31	LMG	C	519	-	51,51,55	0.55	0	59,59,63	0.68	1 (1%)
33	LHG	E	244	-	48,48,48	0.50	0	51,54,54	0.50	0
22	OEX	a	401	1,3	0,14,14	-	-	-		
30	PL9	a	414	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
34	F6C	b	617	2	57,59,74	1.85	11 (19%)	63,96,114	2.31	16 (25%)
35	DGD	c	518	-	63,63,67	0.65	0	77,77,81	0.69	1 (1%)
32	LMT	a	674	-	36,36,36	0.56	0	47,47,47	0.76	0
28	BCR	B	627	-	41,41,41	0.32	0	56,56,56	0.92	2 (3%)
28	BCR	C	515	-	41,41,41	0.37	0	56,56,56	0.69	1 (1%)
25	CLA	b	602	39	69,73,73	1.18	7 (10%)	83,113,113	0.98	4 (4%)
32	LMT	F	102	-	36,36,36	0.55	0	47,47,47	0.65	0
25	CLA	b	605	2	69,73,73	1.25	8 (11%)	83,113,113	0.88	4 (4%)
25	CLA	C	512	3	69,73,73	1.19	6 (8%)	83,113,113	0.97	4 (4%)
25	CLA	B	613	2	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
31	LMG	b	628	-	55,55,55	0.52	0	63,63,63	0.60	0
33	LHG	a	419	-	48,48,48	0.51	0	51,54,54	0.50	0
27	PHO	A	408	-	58,69,69	1.95	10 (17%)	56,99,99	1.54	7 (12%)
34	F6C	c	507	39	72,74,74	1.67	11 (15%)	81,114,114	2.08	16 (19%)
32	LMT	l	213	-	36,36,36	0.54	0	47,47,47	0.78	1 (2%)
29	SQD	A	417	-	53,54,54	1.47	7 (13%)	62,65,65	1.49	8 (12%)
29	SQD	D	407	-	44,45,54	1.57	5 (11%)	53,56,65	1.61	8 (15%)
28	BCR	B	620	-	41,41,41	0.35	0	56,56,56	0.70	0
33	LHG	A	419	-	48,48,48	0.51	0	51,54,54	0.50	0
36	BCT	d	401	23	2,3,3	0.89	0	2,3,3	3.27	2 (100%)
29	SQD	C	903	-	37,38,54	1.67	7 (18%)	46,49,65	1.54	8 (17%)
25	CLA	B	616	2	69,73,73	1.23	8 (11%)	83,113,113	1.00	4 (4%)
28	BCR	k	101	-	41,41,41	0.33	0	56,56,56	0.83	0
30	PL9	A	414	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
32	LMT	m	101	-	36,36,36	0.57	0	47,47,47	0.64	0
28	BCR	c	515	-	41,41,41	0.37	0	56,56,56	0.69	1 (1%)
25	CLA	b	612	2	69,73,73	1.21	7 (10%)	83,113,113	1.00	4 (4%)
25	CLA	b	615	2	69,73,73	1.19	7 (10%)	83,113,113	0.99	4 (4%)
25	CLA	C	503	3	69,73,73	1.21	8 (11%)	83,113,113	0.99	5 (6%)
29	SQD	H	102	-	53,54,54	1.46	5 (9%)	62,65,65	1.60	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
29	SQD	h	102	-	53,54,54	1.46	5 (9%)	62,65,65	1.60	8 (12%)
28	BCR	b	618	-	41,41,41	0.32	0	56,56,56	0.79	1 (1%)
28	BCR	b	627	-	41,41,41	0.32	0	56,56,56	0.92	2 (3%)
32	LMT	A	674	-	36,36,36	0.56	0	47,47,47	0.76	0
33	LHG	D	409	-	48,48,48	0.52	0	51,54,54	0.49	0
33	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.52	0
25	CLA	c	513	3	60,64,73	1.26	7 (11%)	72,102,113	0.97	4 (5%)
25	CLA	b	607	2	69,73,73	1.23	8 (11%)	83,113,113	0.93	4 (4%)
32	LMT	M	101	-	36,36,36	0.57	0	47,47,47	0.64	0
25	CLA	C	508	3	69,73,73	1.20	8 (11%)	83,113,113	0.93	4 (4%)
37	HEM	F	101	5,6	50,50,50	1.38	7 (14%)	66,82,82	1.08	4 (6%)
25	CLA	b	604	2	69,73,73	1.20	8 (11%)	83,113,113	0.90	3 (3%)
25	CLA	B	610	2	69,73,73	1.20	8 (11%)	83,113,113	1.03	5 (6%)
25	CLA	b	613	2	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
25	CLA	B	615	2	69,73,73	1.19	7 (10%)	83,113,113	0.99	4 (4%)
25	CLA	b	606	2	69,73,73	1.20	6 (8%)	83,113,113	1.13	5 (6%)
33	LHG	A	416	-	48,48,48	0.51	0	51,54,54	0.51	0
25	CLA	c	503	3	69,73,73	1.21	8 (11%)	83,113,113	0.99	5 (6%)
28	BCR	b	620	-	41,41,41	0.35	0	56,56,56	0.70	0
32	LMT	B	675	-	25,25,36	0.53	0	30,30,47	0.68	0
26	CL7	A	406	39	71,73,73	1.16	5 (7%)	80,113,113	0.87	3 (3%)
36	BCT	D	401	23	2,3,3	0.88	0	2,3,3	3.27	2 (100%)
30	PL9	D	405	-	55,55,55	1.46	7 (12%)	68,69,69	1.52	12 (17%)
25	CLA	A	407	39	69,73,73	1.18	6 (8%)	83,113,113	1.00	4 (4%)
22	OEX	A	401	1,3	0,14,14	-	-	-		
25	CLA	B	604	2	69,73,73	1.20	8 (11%)	83,113,113	0.90	3 (3%)
31	LMG	d	411	-	51,51,55	0.59	0	59,59,63	0.65	1 (1%)
37	HEM	f	101	5,6	50,50,50	1.38	7 (14%)	66,82,82	1.08	4 (6%)
34	F6C	B	614	2	72,74,74	1.67	10 (13%)	81,114,114	2.02	15 (18%)
32	LMT	a	675	-	33,33,36	0.59	0	44,44,47	0.80	1 (2%)
25	CLA	B	612	2	69,73,73	1.21	7 (10%)	83,113,113	1.00	4 (4%)
31	LMG	a	415	-	48,48,55	0.59	0	56,56,63	0.69	0
35	DGD	C	517	-	63,63,67	0.64	0	77,77,81	0.71	0
27	PHO	A	409	-	58,69,69	1.97	9 (15%)	56,99,99	1.58	7 (12%)
33	LHG	e	101	-	48,48,48	0.52	0	51,54,54	0.49	0
25	CLA	A	405	1	69,73,73	1.18	7 (10%)	83,113,113	0.96	4 (4%)
25	CLA	d	402	4	69,73,73	1.21	8 (11%)	83,113,113	0.94	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	LMG	P	628	-	47,47,55	0.50	0	55,55,63	0.61	0
25	CLA	b	610	2	69,73,73	1.19	8 (11%)	83,113,113	1.03	5 (6%)
28	BCR	c	514	-	41,41,41	0.31	0	56,56,56	0.59	0
25	CLA	D	402	4	69,73,73	1.20	8 (11%)	83,113,113	0.94	4 (4%)
30	PL9	d	405	-	55,55,55	1.46	7 (12%)	68,69,69	1.52	12 (17%)
28	BCR	a	411	-	41,41,41	0.34	0	56,56,56	0.49	0
33	LHG	L	101	-	48,48,48	0.53	0	51,54,54	0.52	0
33	LHG	p	629	-	48,48,48	0.49	0	51,54,54	0.63	1 (1%)
28	BCR	K	101	-	41,41,41	0.33	0	56,56,56	0.83	0
31	LMG	p	628	-	47,47,55	0.50	0	55,55,63	0.61	0
34	F6C	B	608	39	72,74,74	1.67	11 (15%)	81,114,114	2.02	14 (17%)
32	LMT	b	675	-	25,25,36	0.53	0	30,30,47	0.68	0
32	LMT	f	102	-	36,36,36	0.55	0	47,47,47	0.65	0
33	LHG	a	416	-	48,48,48	0.51	0	51,54,54	0.51	0
31	LMG	C	902	-	53,53,55	0.46	0	61,61,63	0.61	0

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
31	LMG	c	519	-	-	12/46/66/70	0/1/1/1
25	CLA	a	405	1	-	4/39/115/115	-
25	CLA	b	616	2	-	6/39/115/115	-
25	CLA	C	504	39	-	2/39/115/115	-
33	LHG	E	101	-	-	27/53/53/53	-
25	CLA	C	509	3	-	5/39/115/115	-
32	LMT	g	104	-	-	8/21/61/61	0/2/2/2
28	BCR	K	102	-	-	3/29/63/63	0/2/2/2
28	BCR	B	619	-	-	7/29/63/63	0/2/2/2
25	CLA	D	403	4	-	2/39/115/115	-
25	CLA	c	511	3	-	0/39/115/115	-
31	LMG	l	212	-	-	21/50/70/70	0/1/1/1
33	LHG	d	410	-	-	26/45/45/53	-
33	LHG	P	629	-	-	21/53/53/53	-
25	CLA	C	510	3	-	3/39/115/115	-
25	CLA	b	603	2	-	3/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	d	409	-	-	12/53/53/53	-
33	LHG	D	410	-	-	26/45/45/53	-
32	LMT	L	213	-	-	6/21/61/61	0/2/2/2
35	DGD	c	517	-	-	17/51/91/95	0/2/2/2
32	LMT	c	904	-	-	3/18/58/61	0/2/2/2
25	CLA	c	509	3	-	5/39/115/115	-
32	LMT	l	210	-	-	10/21/61/61	0/2/2/2
25	CLA	C	506	3	-	1/39/115/115	-
25	CLA	B	602	39	-	9/39/115/115	-
31	LMG	D	411	-	-	6/46/66/70	0/1/1/1
33	LHG	D	408	-	-	15/53/53/53	-
32	LMT	A	675	-	-	1/18/58/61	0/2/2/2
25	CLA	c	510	3	-	3/39/115/115	-
25	CLA	c	506	3	-	1/39/115/115	-
31	LMG	A	415	-	-	12/43/63/70	0/1/1/1
38	HEC	V	201	18	1/1/3/7	4/14/54/54	-
25	CLA	C	505	3	-	1/39/115/115	-
27	PHO	a	408	-	-	4/37/103/103	0/5/6/6
25	CLA	c	502	3	-	10/39/115/115	-
33	LHG	e	244	-	-	24/53/53/53	-
25	CLA	C	501	3	-	3/39/115/115	-
35	DGD	C	516	-	-	20/51/91/95	0/2/2/2
28	BCR	d	404	-	-	8/29/63/63	0/2/2/2
29	SQD	d	407	-	-	17/40/60/69	0/1/1/1
25	CLA	B	611	39	-	1/39/115/115	-
35	DGD	c	516	-	-	20/51/91/95	0/2/2/2
34	F6C	b	614	2	1/1/10/16	21/41/97/97	-
38	HEC	v	201	18	1/1/3/7	4/14/54/54	-
29	SQD	B	622	-	-	18/49/69/69	0/1/1/1
25	CLA	A	410	1	-	5/39/115/115	-
29	SQD	a	412	-	-	25/49/69/69	0/1/1/1
25	CLA	c	505	3	-	1/39/115/115	-
25	CLA	a	410	1	-	5/39/115/115	-
25	CLA	c	501	3	-	3/39/115/115	-
25	CLA	B	609	2	-	1/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PHO	a	409	-	-	3/37/103/103	0/5/6/6
33	LHG	d	408	-	-	15/53/53/53	-
33	LHG	j	101	-	-	29/53/53/53	-
32	LMT	Z	102	-	-	10/21/61/61	0/2/2/2
25	CLA	B	603	2	-	3/39/115/115	-
25	CLA	c	508	3	-	3/39/115/115	-
25	CLA	a	407	39	-	2/39/115/115	-
31	LMG	L	212	-	-	21/50/70/70	0/1/1/1
32	LMT	z	102	-	-	10/21/61/61	0/2/2/2
25	CLA	B	607	2	-	5/39/115/115	-
32	LMT	G	104	-	-	8/21/61/61	0/2/2/2
34	F6C	B	617	2	1/1/7/16	6/23/79/97	-
28	BCR	D	404	-	-	8/29/63/63	0/2/2/2
25	CLA	B	606	2	-	6/39/115/115	-
33	LHG	J	101	-	-	29/53/53/53	-
28	BCR	k	102	-	-	3/29/63/63	0/2/2/2
29	SQD	c	903	-	-	21/33/53/69	0/1/1/1
32	LMT	C	904	-	-	3/18/58/61	0/2/2/2
28	BCR	B	618	-	-	4/29/63/63	0/2/2/2
34	F6C	C	507	39	1/1/10/16	17/41/97/97	-
25	CLA	B	605	2	-	2/39/115/115	-
25	CLA	C	513	3	-	3/29/105/115	-
28	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	CLA	c	504	39	-	2/39/115/115	-
25	CLA	b	611	39	-	1/39/115/115	-
26	CL7	a	406	39	2/2/15/20	2/39/115/115	-
25	CLA	c	512	3	-	6/39/115/115	-
29	SQD	b	622	-	-	18/49/69/69	0/1/1/1
35	DGD	C	518	-	-	16/51/91/95	0/2/2/2
25	CLA	C	502	3	-	10/39/115/115	-
31	LMG	B	628	-	-	18/50/70/70	0/1/1/1
25	CLA	b	609	2	-	1/39/115/115	-
25	CLA	C	511	3	-	0/39/115/115	-
29	SQD	a	417	-	-	31/49/69/69	0/1/1/1
34	F6C	b	608	39	1/1/10/16	10/41/97/97	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	A	412	-	-	25/49/69/69	0/1/1/1
31	LMG	c	902	-	-	18/48/68/70	0/1/1/1
28	BCR	A	411	-	-	2/29/63/63	0/2/2/2
25	CLA	d	403	4	-	2/39/115/115	-
28	BCR	b	619	-	-	7/29/63/63	0/2/2/2
32	LMT	L	210	-	-	10/21/61/61	0/2/2/2
31	LMG	C	519	-	-	12/46/66/70	0/1/1/1
33	LHG	E	244	-	-	24/53/53/53	-
30	PL9	a	414	-	-	18/53/73/73	0/1/1/1
34	F6C	b	617	2	1/1/7/16	6/23/79/97	-
35	DGD	c	518	-	-	16/51/91/95	0/2/2/2
32	LMT	a	674	-	-	6/21/61/61	0/2/2/2
28	BCR	B	627	-	-	7/29/63/63	0/2/2/2
28	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	CLA	b	602	39	-	9/39/115/115	-
32	LMT	F	102	-	-	5/21/61/61	0/2/2/2
25	CLA	b	605	2	-	2/39/115/115	-
25	CLA	C	512	3	-	6/39/115/115	-
25	CLA	B	613	2	-	4/39/115/115	-
31	LMG	b	628	-	-	18/50/70/70	0/1/1/1
33	LHG	a	419	-	-	15/53/53/53	-
27	PHO	A	408	-	-	4/37/103/103	0/5/6/6
34	F6C	c	507	39	1/1/10/16	17/41/97/97	-
32	LMT	l	213	-	-	6/21/61/61	0/2/2/2
29	SQD	A	417	-	-	31/49/69/69	0/1/1/1
29	SQD	D	407	-	-	17/40/60/69	0/1/1/1
28	BCR	B	620	-	-	4/29/63/63	0/2/2/2
33	LHG	A	419	-	-	15/53/53/53	-
29	SQD	C	903	-	-	21/33/53/69	0/1/1/1
25	CLA	B	616	2	-	6/39/115/115	-
28	BCR	k	101	-	-	6/29/63/63	0/2/2/2
30	PL9	A	414	-	-	18/53/73/73	0/1/1/1
32	LMT	m	101	-	-	7/21/61/61	0/2/2/2
28	BCR	c	515	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	612	2	-	0/39/115/115	-
25	CLA	b	615	2	-	6/39/115/115	-
25	CLA	C	503	3	-	2/39/115/115	-
29	SQD	H	102	-	-	19/49/69/69	0/1/1/1
29	SQD	h	102	-	-	19/49/69/69	0/1/1/1
28	BCR	b	618	-	-	4/29/63/63	0/2/2/2
28	BCR	b	627	-	-	7/29/63/63	0/2/2/2
32	LMT	A	674	-	-	6/21/61/61	0/2/2/2
33	LHG	D	409	-	-	12/53/53/53	-
33	LHG	l	101	-	-	11/53/53/53	-
25	CLA	c	513	3	-	3/29/105/115	-
25	CLA	b	607	2	-	5/39/115/115	-
32	LMT	M	101	-	-	7/21/61/61	0/2/2/2
25	CLA	C	508	3	-	3/39/115/115	-
37	HEM	F	101	5,6	-	1/14/54/54	-
25	CLA	b	604	2	-	3/39/115/115	-
25	CLA	B	610	2	-	3/39/115/115	-
25	CLA	b	613	2	-	4/39/115/115	-
25	CLA	B	615	2	-	6/39/115/115	-
25	CLA	b	606	2	-	6/39/115/115	-
33	LHG	A	416	-	-	24/53/53/53	-
25	CLA	c	503	3	-	2/39/115/115	-
28	BCR	b	620	-	-	4/29/63/63	0/2/2/2
32	LMT	B	675	-	-	10/17/37/61	0/1/1/2
26	CL7	A	406	39	2/2/15/20	2/39/115/115	-
30	PL9	D	405	-	-	15/53/73/73	0/1/1/1
25	CLA	A	407	39	-	2/39/115/115	-
25	CLA	B	604	2	-	3/39/115/115	-
31	LMG	d	411	-	-	6/46/66/70	0/1/1/1
37	HEM	f	101	5,6	-	1/14/54/54	-
34	F6C	B	614	2	1/1/10/16	21/41/97/97	-
32	LMT	a	675	-	-	1/18/58/61	0/2/2/2
25	CLA	B	612	2	-	0/39/115/115	-
31	LMG	a	415	-	-	12/43/63/70	0/1/1/1
35	DGD	C	517	-	-	17/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PHO	A	409	-	-	3/37/103/103	0/5/6/6
33	LHG	e	101	-	-	27/53/53/53	-
25	CLA	A	405	1	-	4/39/115/115	-
25	CLA	d	402	4	-	3/39/115/115	-
31	LMG	P	628	-	-	19/42/62/70	0/1/1/1
25	CLA	b	610	2	-	3/39/115/115	-
28	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	CLA	D	402	4	-	3/39/115/115	-
30	PL9	d	405	-	-	15/53/73/73	0/1/1/1
28	BCR	a	411	-	-	2/29/63/63	0/2/2/2
33	LHG	L	101	-	-	11/53/53/53	-
33	LHG	p	629	-	-	21/53/53/53	-
28	BCR	K	101	-	-	6/29/63/63	0/2/2/2
31	LMG	p	628	-	-	19/42/62/70	0/1/1/1
34	F6C	B	608	39	1/1/10/16	10/41/97/97	-
32	LMT	b	675	-	-	10/17/37/61	0/1/1/2
32	LMT	f	102	-	-	5/21/61/61	0/2/2/2
33	LHG	a	416	-	-	24/53/53/53	-
31	LMG	C	902	-	-	18/48/68/70	0/1/1/1

The worst 5 of 698 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	409	PHO	C1B-C2B	9.01	1.49	1.39
27	A	409	PHO	C1B-C2B	9.01	1.49	1.39
27	A	408	PHO	C1B-C2B	8.77	1.49	1.39
27	a	408	PHO	C1B-C2B	8.77	1.49	1.39
34	c	507	F6C	C2A-C3A	8.60	1.55	1.36

The worst 5 of 617 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	507	F6C	CAA-C2A-C3A	-9.25	110.65	127.88
34	c	507	F6C	CAA-C2A-C3A	-9.24	110.66	127.88
34	B	617	F6C	CAA-C2A-C3A	-8.81	111.48	127.88
34	b	617	F6C	CAA-C2A-C3A	-8.81	111.48	127.88
34	b	614	F6C	CAA-C2A-C3A	-8.52	112.02	127.88

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	406	CL7	NA
26	A	406	CL7	NC
26	a	406	CL7	NA
26	a	406	CL7	NC
34	B	608	F6C	NA

5 of 1620 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	407	CLA	CHA-CBD-CGD-O1D
25	A	407	CLA	CHA-CBD-CGD-O2D
25	A	410	CLA	C2-C3-C5-C6
25	A	410	CLA	C4-C3-C5-C6
25	B	602	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

146 monomers are involved in 328 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	519	LMG	3	0
25	a	405	CLA	2	0
25	b	616	CLA	6	0
25	C	504	CLA	2	0
33	E	101	LHG	3	0
25	C	509	CLA	3	0
28	K	102	BCR	5	0
28	B	619	BCR	4	0
25	D	403	CLA	1	0
25	c	511	CLA	2	0
31	l	212	LMG	2	0
33	P	629	LHG	3	0
25	C	510	CLA	5	0
25	b	603	CLA	5	0
33	d	409	LHG	2	0
32	L	213	LMT	1	0
35	c	517	DGD	3	0
25	c	509	CLA	3	0
32	l	210	LMT	1	0
25	C	506	CLA	3	0
25	B	602	CLA	2	0
31	D	411	LMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	510	CLA	4	0
25	c	506	CLA	3	0
31	A	415	LMG	2	0
25	C	505	CLA	5	0
27	a	408	PHO	3	0
25	c	502	CLA	6	0
33	e	244	LHG	1	0
25	C	501	CLA	5	0
35	C	516	DGD	1	0
28	d	404	BCR	2	0
29	d	407	SQD	1	0
25	B	611	CLA	3	0
35	c	516	DGD	2	0
29	B	622	SQD	3	0
25	A	410	CLA	2	0
29	a	412	SQD	4	0
25	c	505	CLA	4	0
25	a	410	CLA	2	0
25	c	501	CLA	5	0
25	B	609	CLA	1	0
27	a	409	PHO	3	0
33	j	101	LHG	3	0
32	Z	102	LMT	1	0
25	B	603	CLA	5	0
25	c	508	CLA	6	0
25	a	407	CLA	4	0
31	L	212	LMG	2	0
32	z	102	LMT	1	0
25	B	607	CLA	2	0
34	B	617	F6C	1	0
28	D	404	BCR	3	0
25	B	606	CLA	6	0
33	J	101	LHG	4	0
28	k	102	BCR	4	0
29	c	903	SQD	1	0
28	B	618	BCR	2	0
25	B	605	CLA	5	0
25	C	513	CLA	1	0
28	C	514	BCR	1	0
25	c	504	CLA	2	0
25	b	611	CLA	3	0
26	a	406	CL7	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	512	CLA	3	0
29	b	622	SQD	3	0
35	C	518	DGD	1	0
25	C	502	CLA	6	0
31	B	628	LMG	3	0
25	b	609	CLA	1	0
25	C	511	CLA	2	0
29	a	417	SQD	3	0
29	A	412	SQD	4	0
31	c	902	LMG	5	0
28	A	411	BCR	2	0
25	d	403	CLA	1	0
28	b	619	BCR	3	0
32	L	210	LMT	1	0
31	C	519	LMG	3	0
33	E	244	LHG	1	0
30	a	414	PL9	6	0
34	b	617	F6C	1	0
35	c	518	DGD	1	0
32	a	674	LMT	3	0
28	B	627	BCR	1	0
25	b	602	CLA	2	0
25	b	605	CLA	5	0
25	C	512	CLA	3	0
25	B	613	CLA	2	0
31	b	628	LMG	2	0
33	a	419	LHG	1	0
27	A	408	PHO	4	0
29	A	417	SQD	4	0
29	D	407	SQD	1	0
28	B	620	BCR	2	0
33	A	419	LHG	1	0
29	C	903	SQD	1	0
25	B	616	CLA	6	0
28	k	101	BCR	1	0
30	A	414	PL9	6	0
32	m	101	LMT	3	0
25	b	612	CLA	1	0
25	b	615	CLA	2	0
25	C	503	CLA	5	0
29	H	102	SQD	1	0
29	h	102	SQD	2	0

Continued on next page...

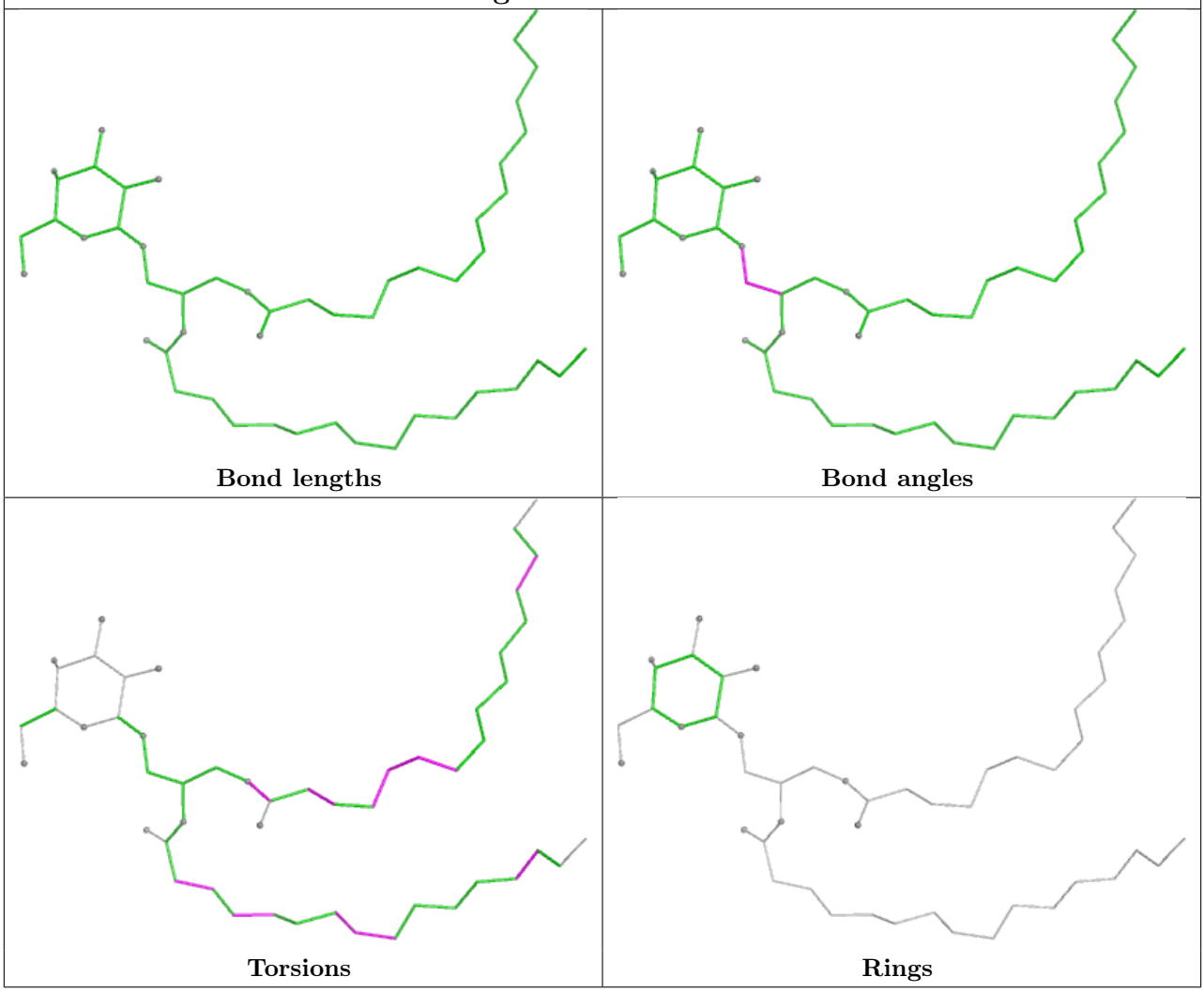
Continued from previous page...

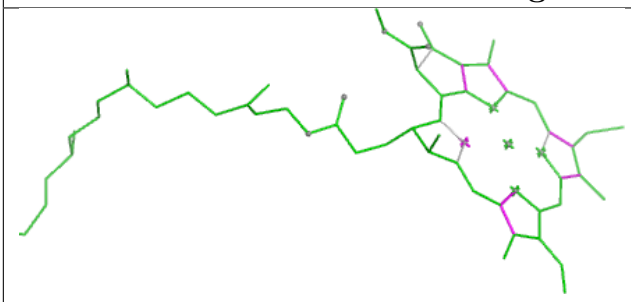
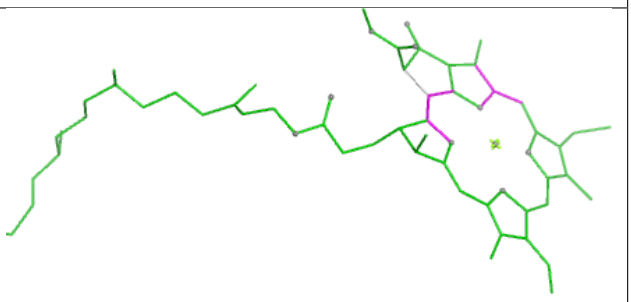
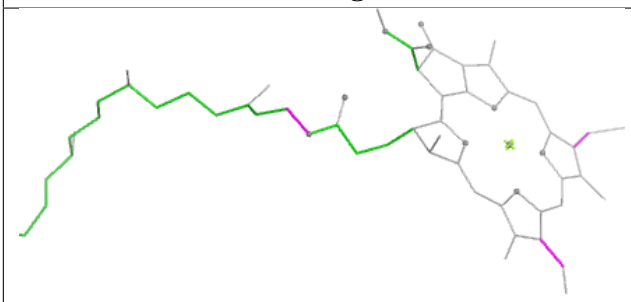
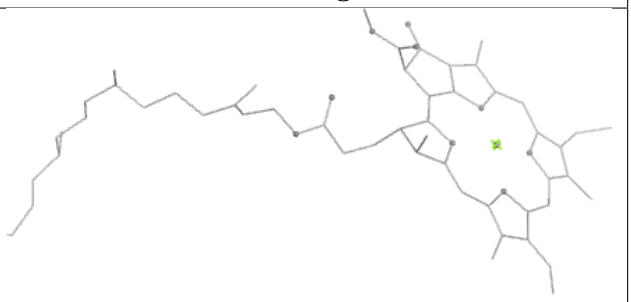
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	618	BCR	2	0
28	b	627	BCR	1	0
32	A	674	LMT	3	0
33	D	409	LHG	2	0
33	l	101	LHG	1	0
25	c	513	CLA	1	0
25	b	607	CLA	2	0
32	M	101	LMT	3	0
25	C	508	CLA	7	0
37	F	101	HEM	5	0
25	b	604	CLA	2	0
25	B	610	CLA	3	0
25	b	613	CLA	2	0
25	B	615	CLA	1	0
25	b	606	CLA	6	0
33	A	416	LHG	5	0
25	c	503	CLA	5	0
28	b	620	BCR	1	0
26	A	406	CL7	1	0
25	A	407	CLA	3	0
25	B	604	CLA	2	0
31	d	411	LMG	2	0
37	f	101	HEM	5	0
25	B	612	CLA	1	0
31	a	415	LMG	2	0
35	C	517	DGD	5	0
27	A	409	PHO	2	0
33	e	101	LHG	3	0
25	A	405	CLA	2	0
25	d	402	CLA	4	0
31	P	628	LMG	1	0
25	b	610	CLA	3	0
28	c	514	BCR	2	0
25	D	402	CLA	4	0
33	L	101	LHG	1	0
33	p	629	LHG	3	0
28	K	101	BCR	1	0
31	p	628	LMG	1	0
33	a	416	LHG	6	0
31	C	902	LMG	5	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

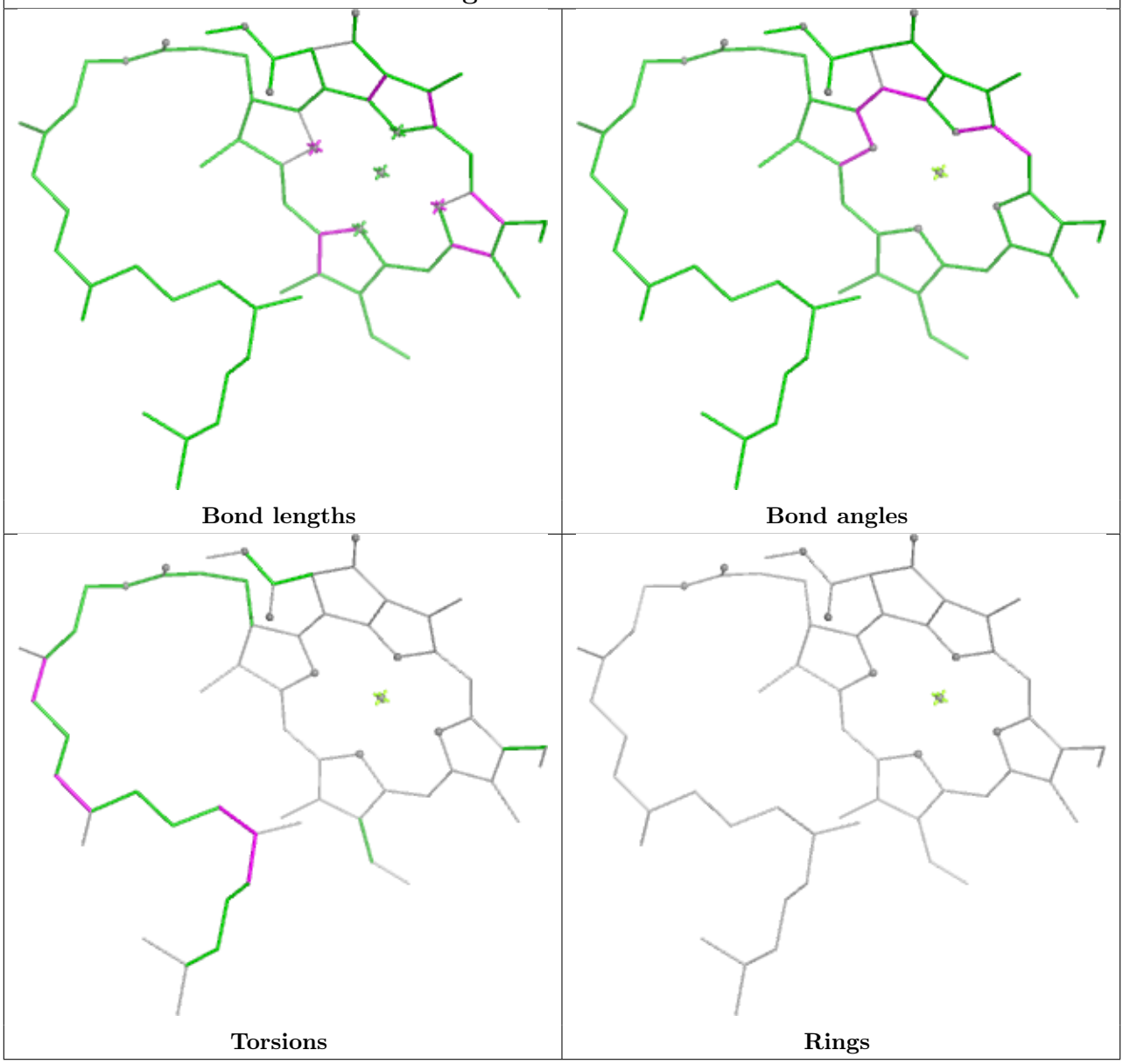
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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 LMG c 519

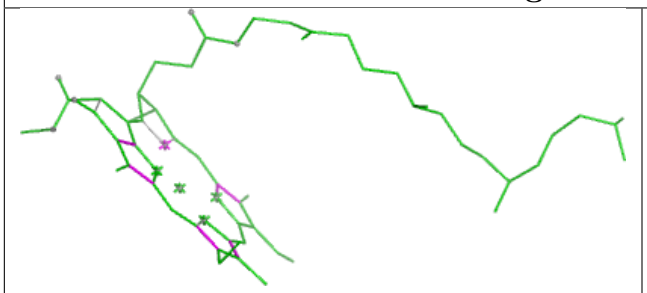


Ligand CLA a 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

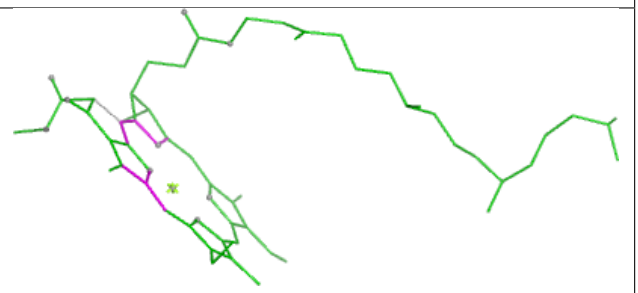
Ligand CLA b 616



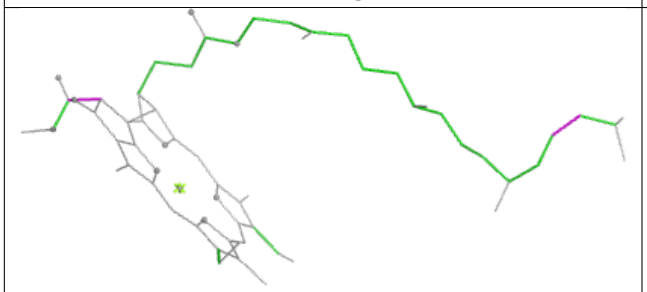
Ligand CLA C 504



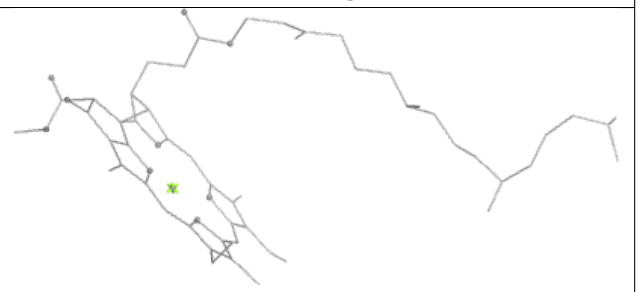
Bond lengths



Bond angles

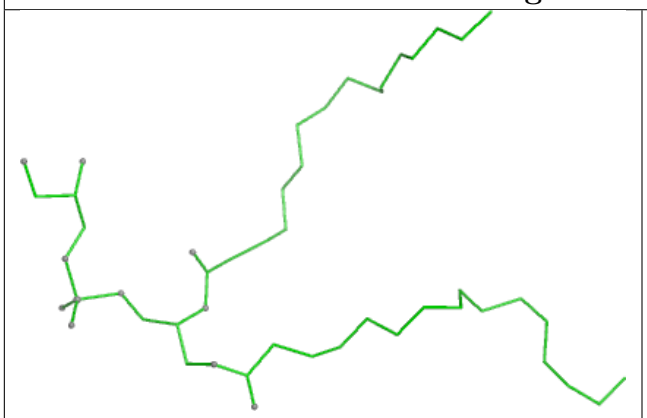


Torsions

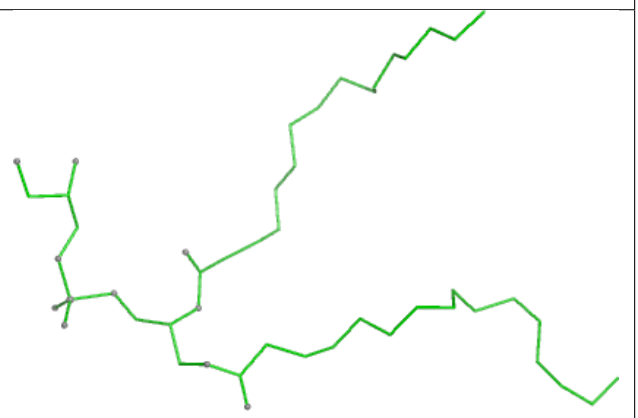


Rings

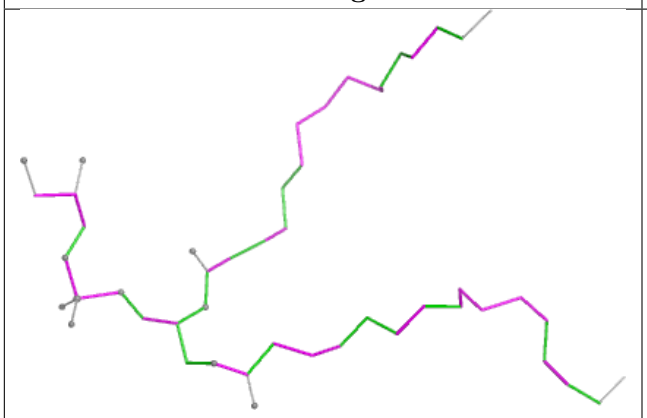
Ligand LHG E 101



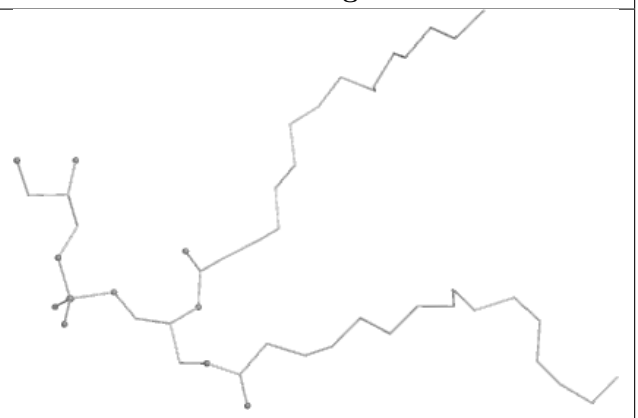
Bond lengths



Bond angles

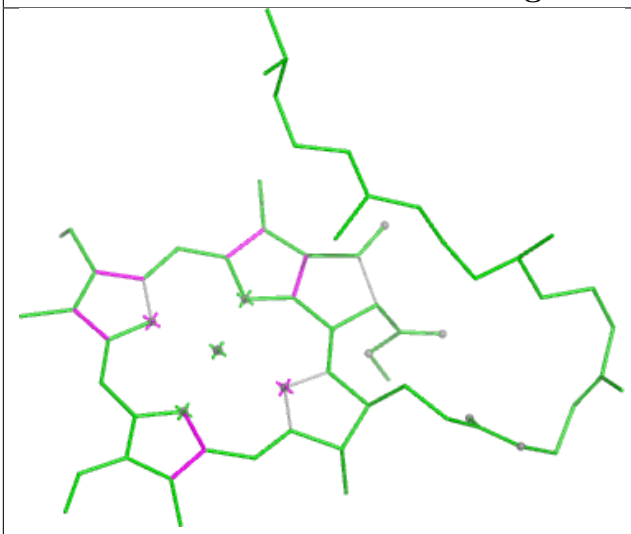


Torsions

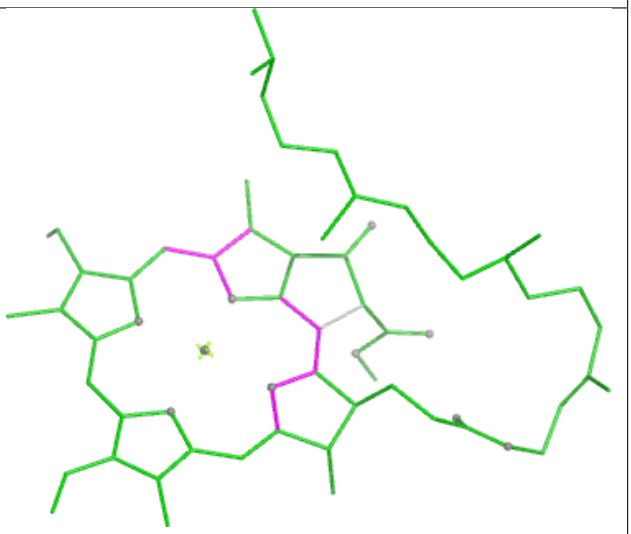


Rings

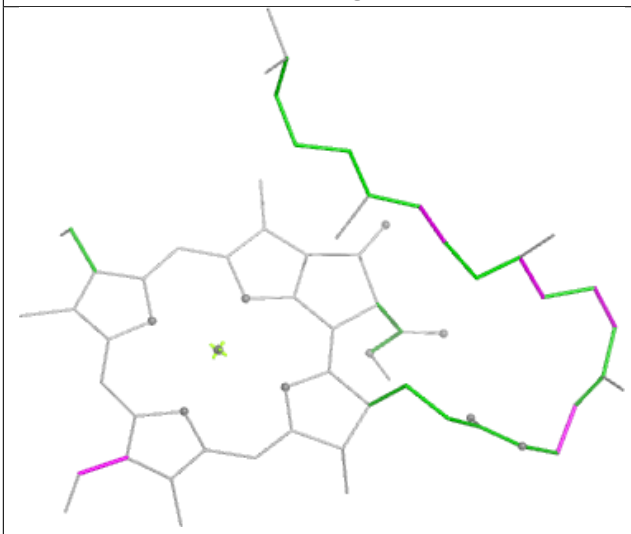
Ligand CLA C 509



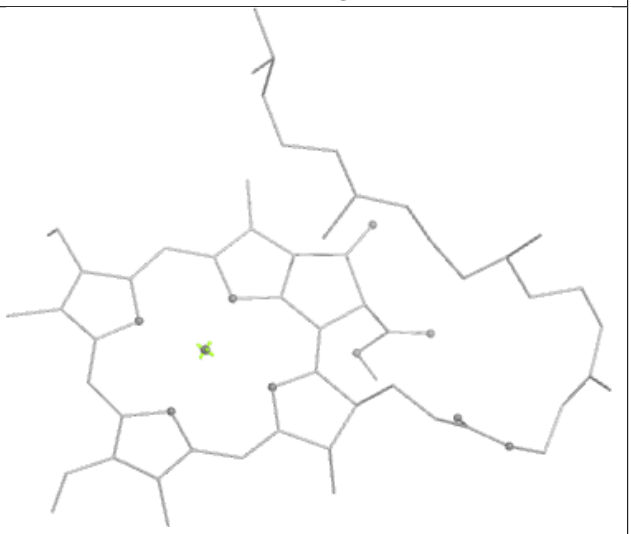
Bond lengths



Bond angles

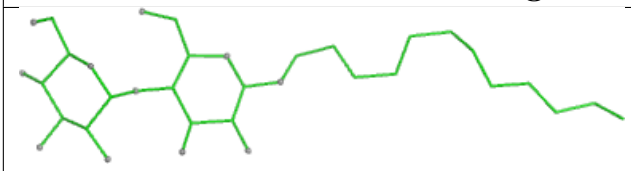


Torsions



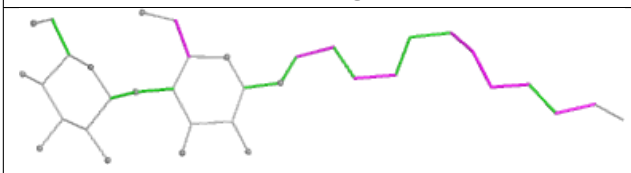
Rings

Ligand LMT g 104

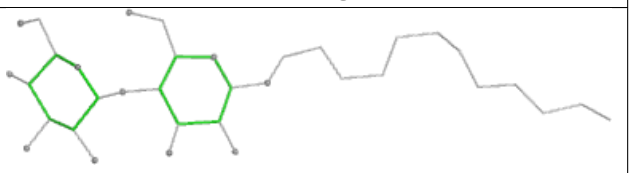


Bond lengths

Bond angles

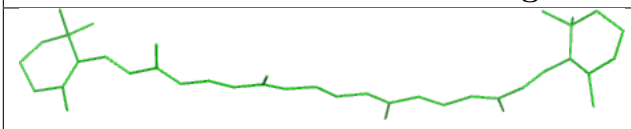


Torsions

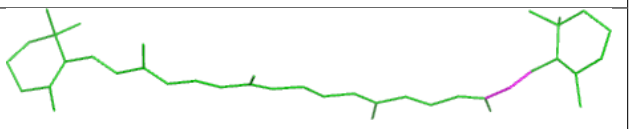


Rings

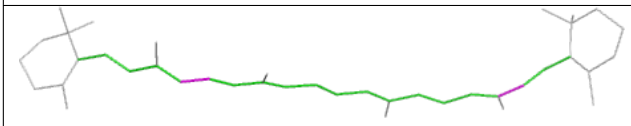
Ligand BCR K 102



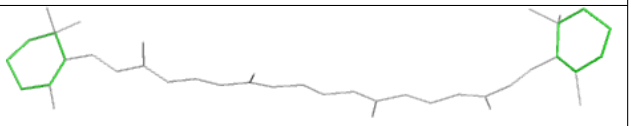
Bond lengths



Bond angles

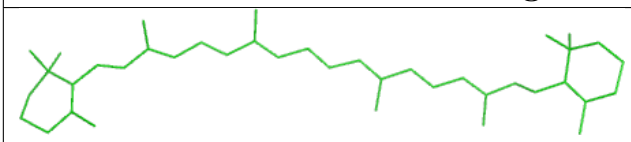


Torsions

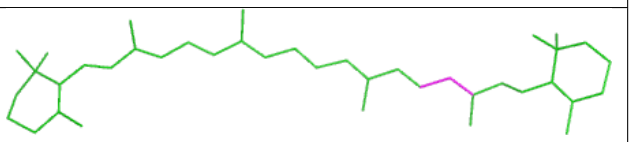


Rings

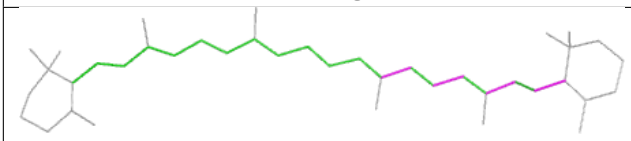
Ligand BCR B 619



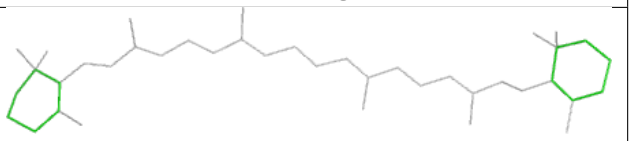
Bond lengths



Bond angles



Torsions

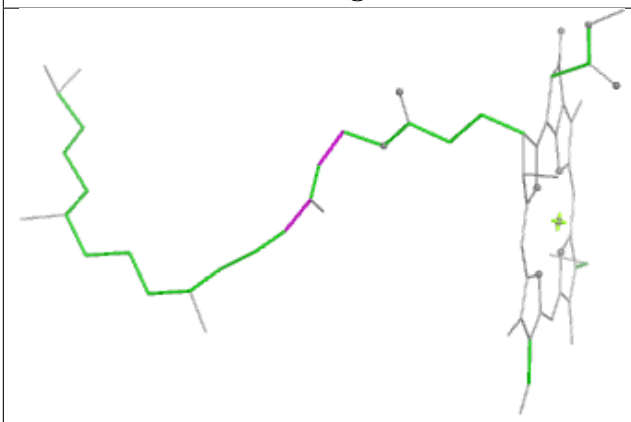


Rings

Ligand CLA D 403

Bond lengths

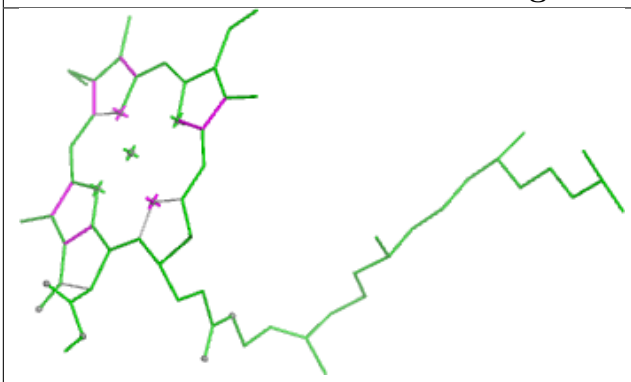
Bond angles



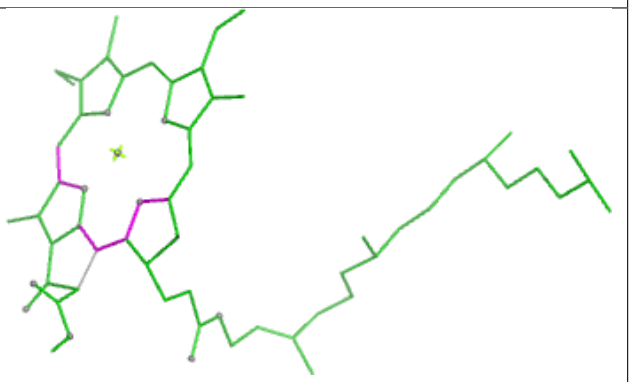
Torsions

Rings

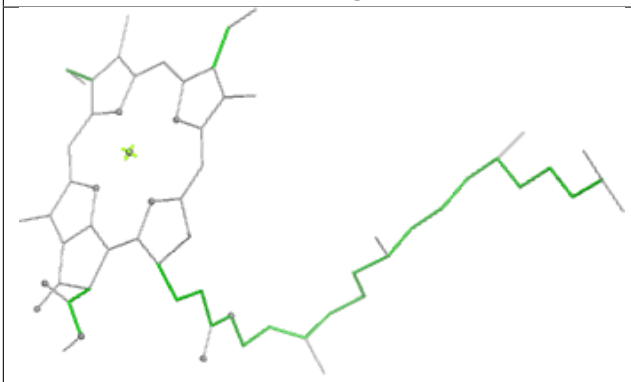
Ligand CLA c 511



Bond lengths



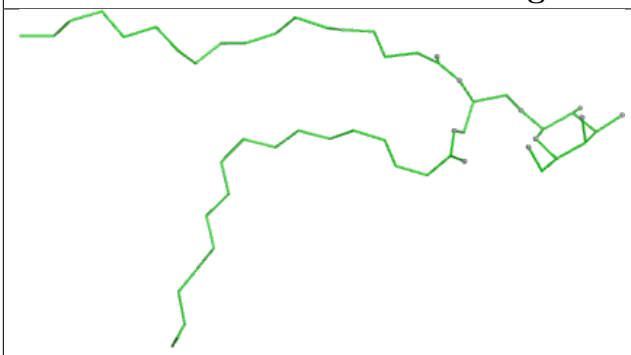
Bond angles



Torsions

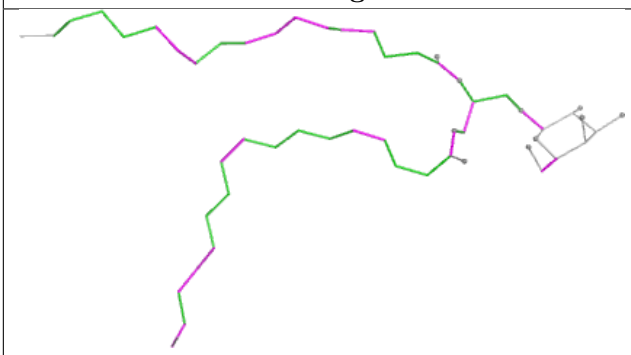
Rings

Ligand LMG l 212



Bond lengths

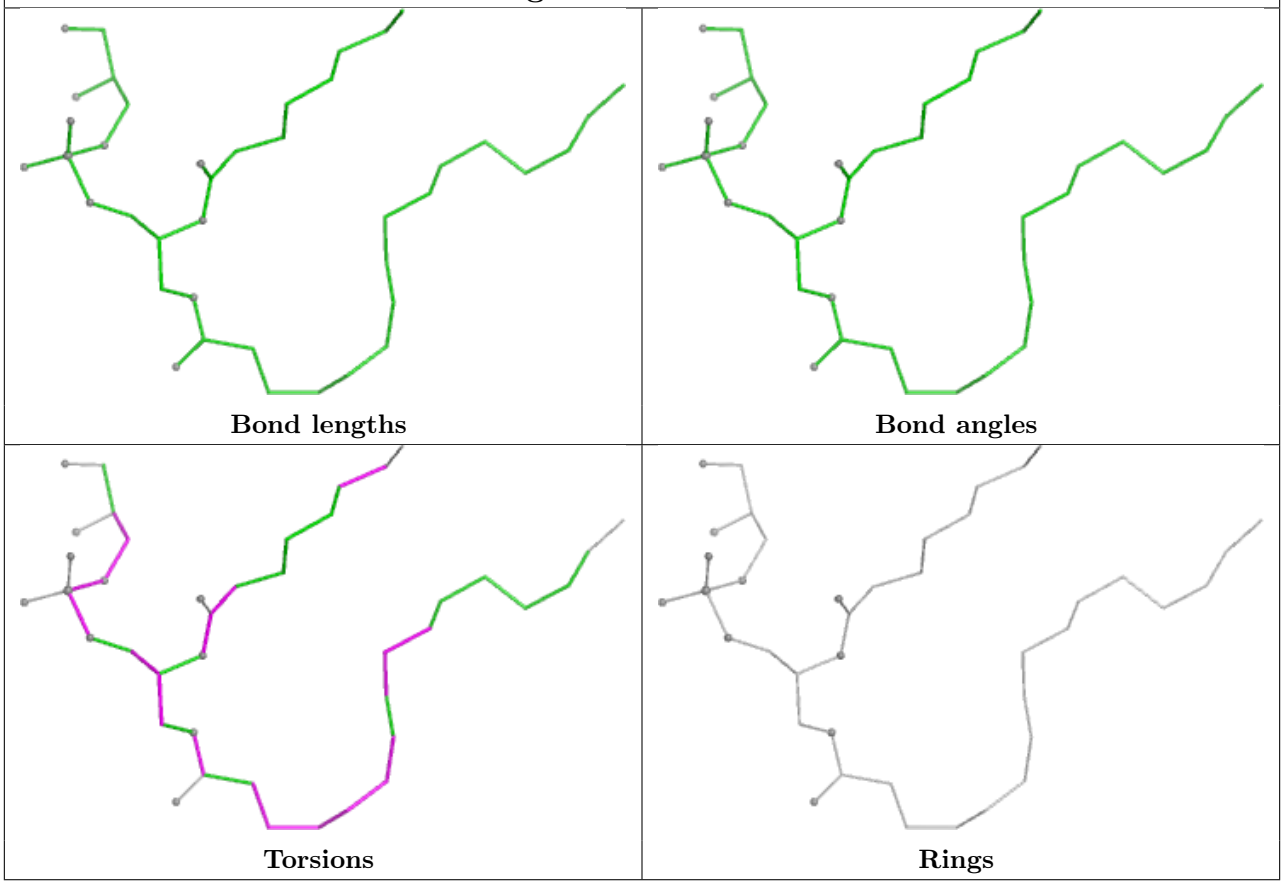
Bond angles



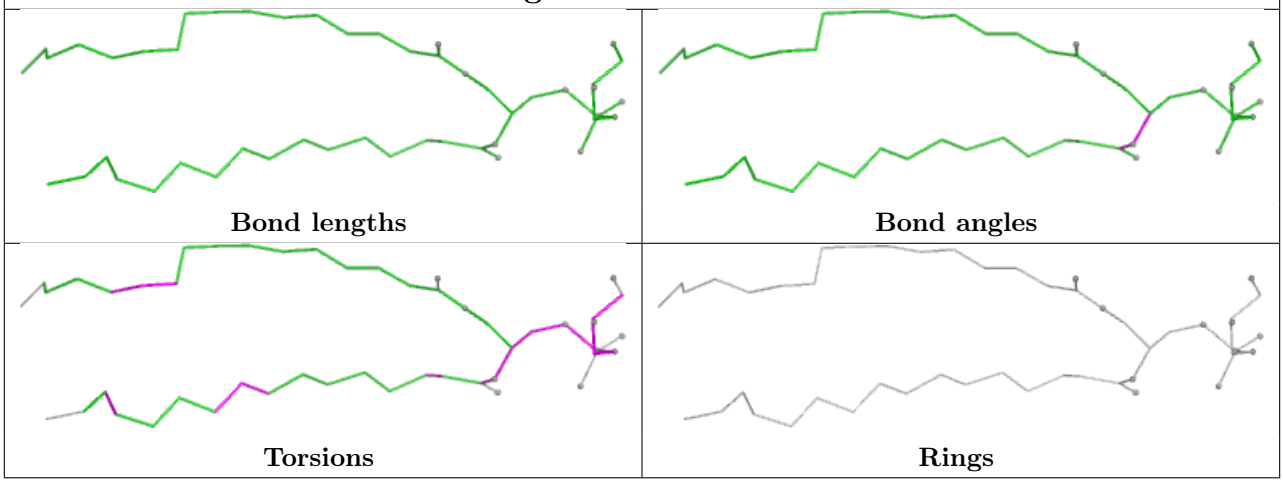
Torsions

Rings

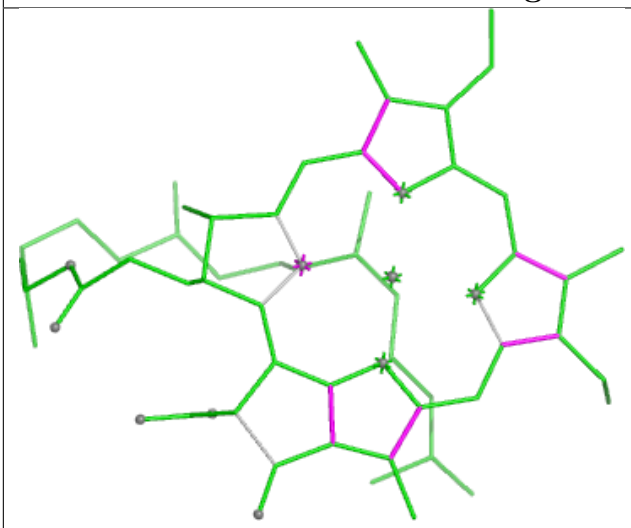
Ligand LHG d 410



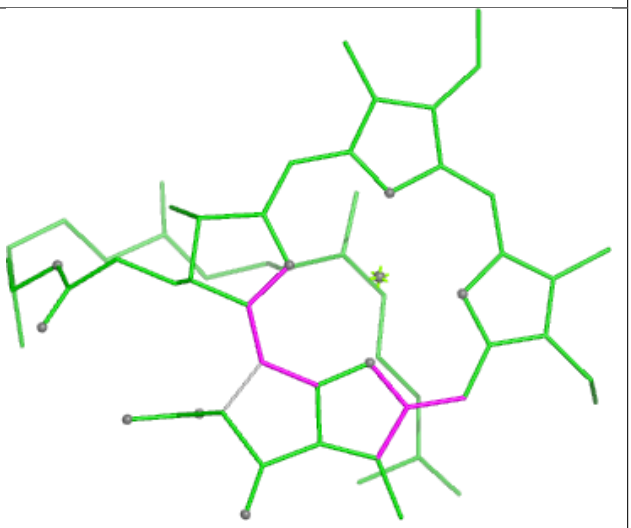
Ligand LHG P 629



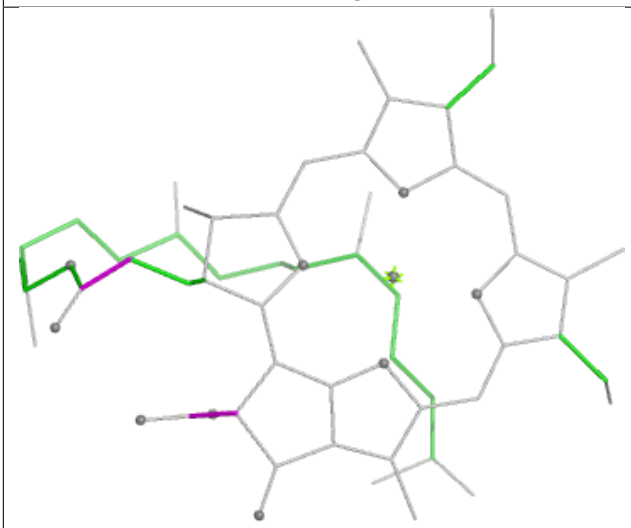
Ligand CLA C 510



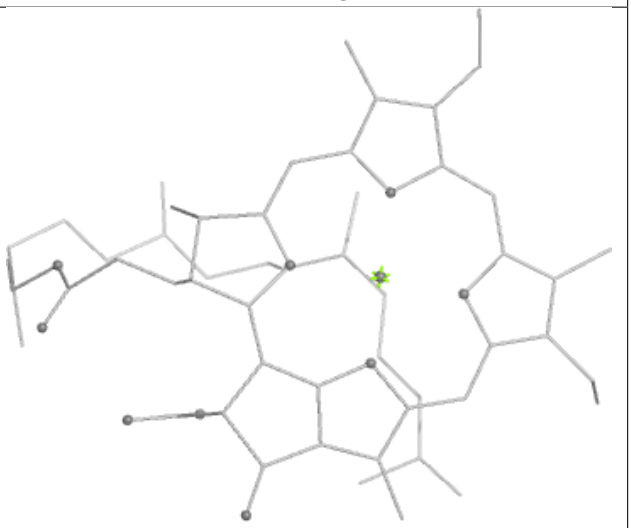
Bond lengths



Bond angles

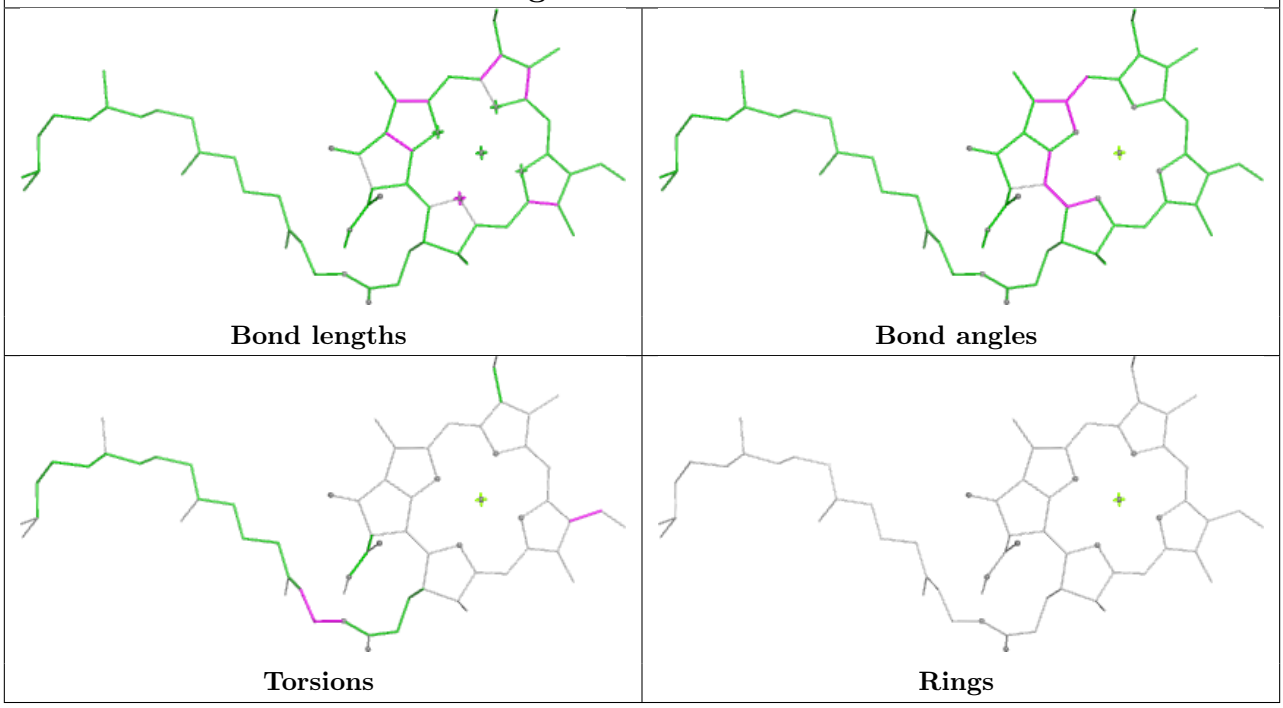


Torsions

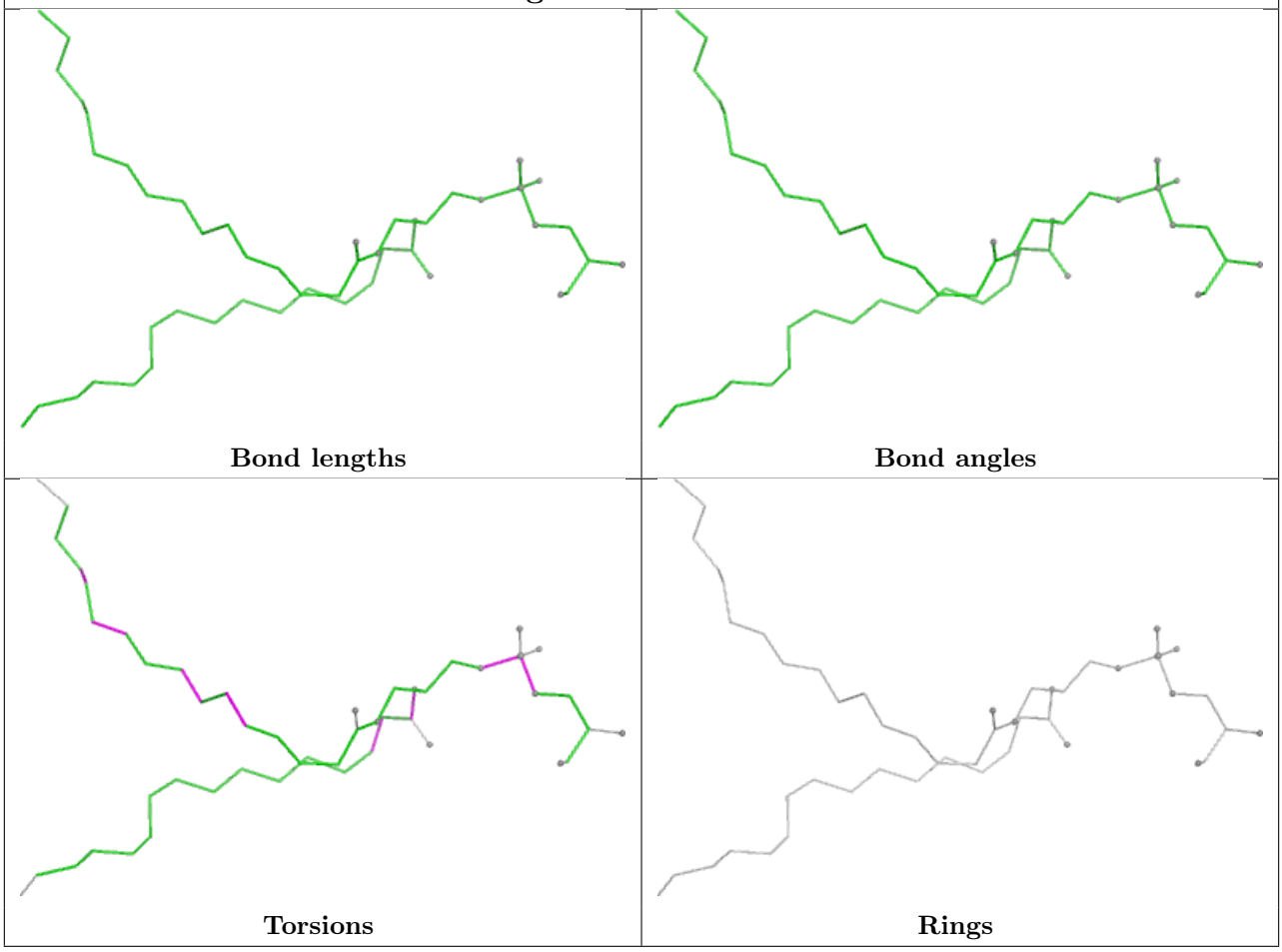


Rings

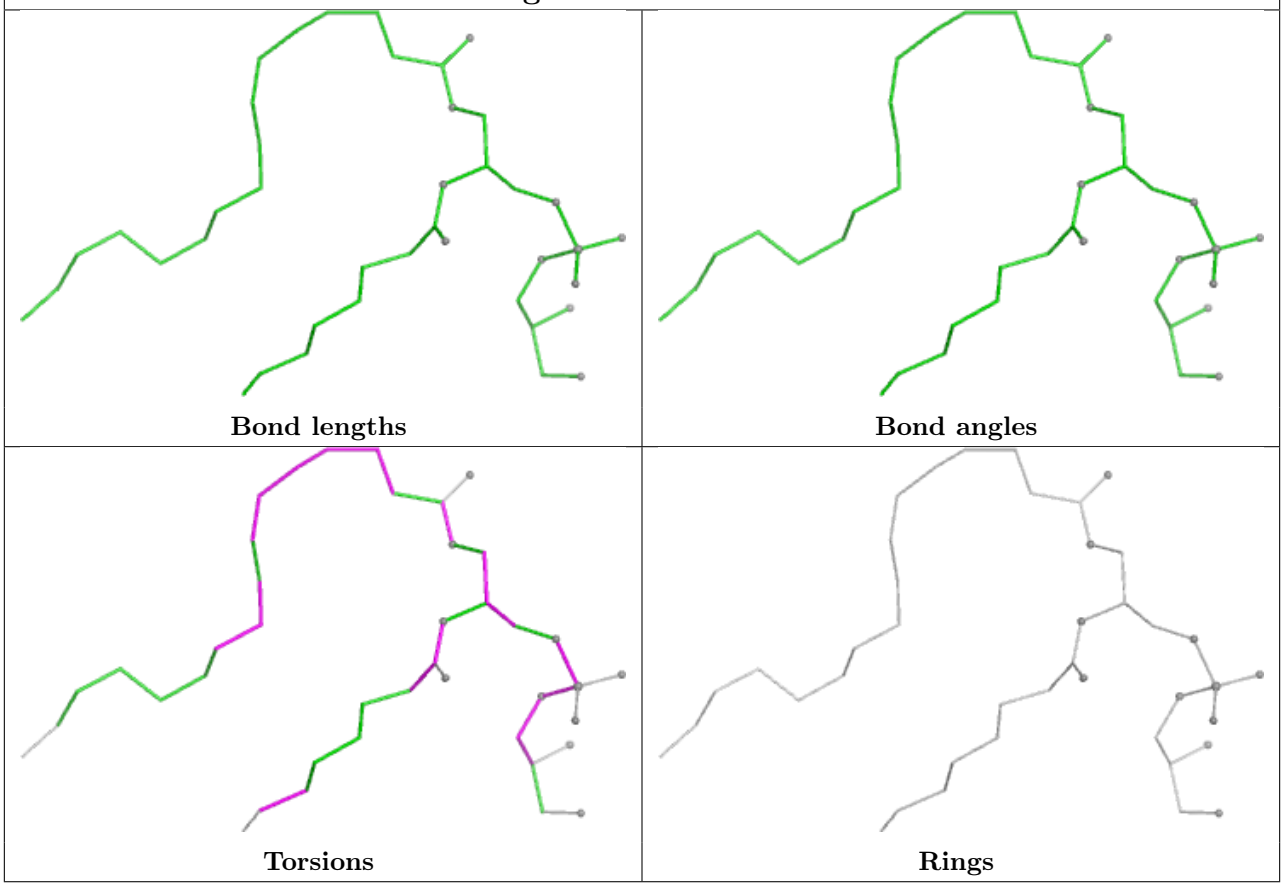
Ligand CLA b 603



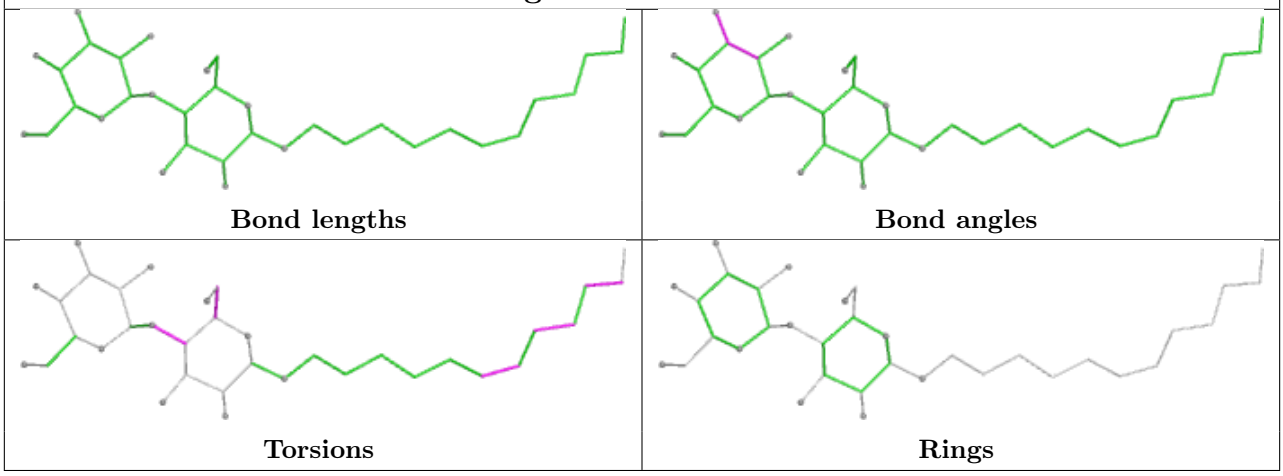
Ligand LHG d 409



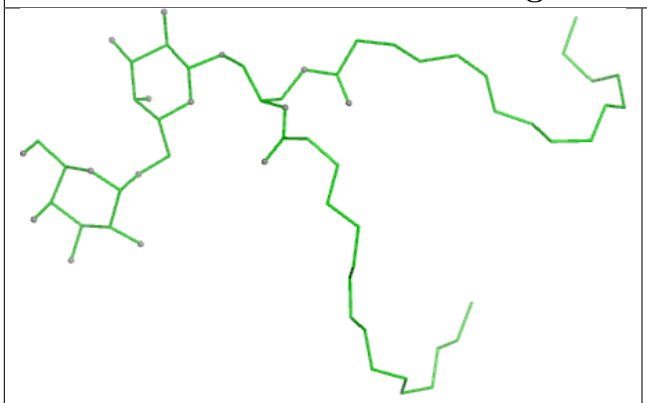
Ligand LHG D 410



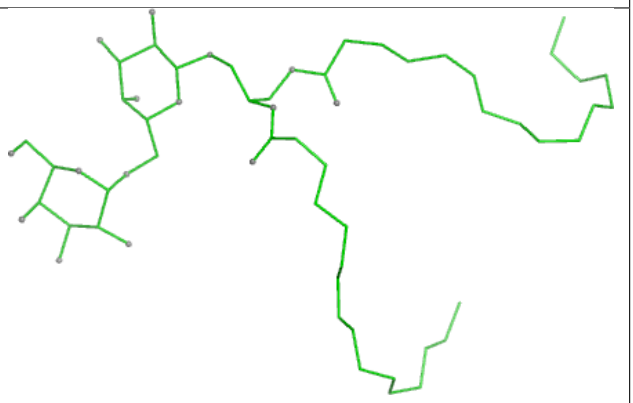
Ligand LMT L 213



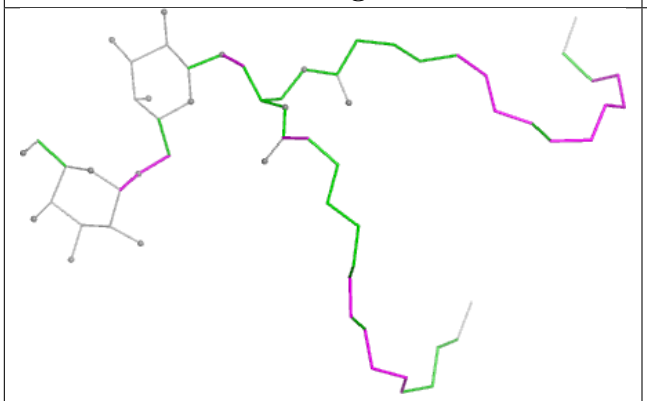
Ligand DGD c 517



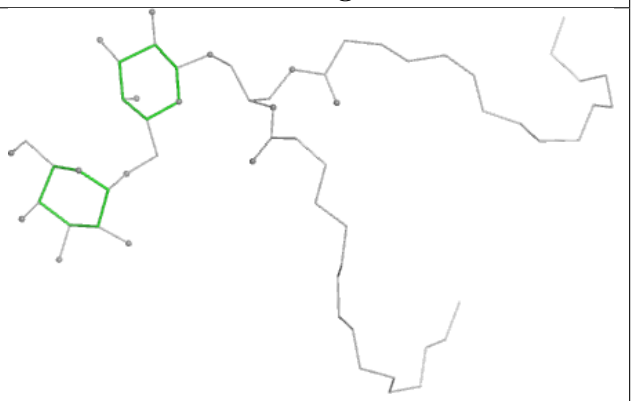
Bond lengths



Bond angles

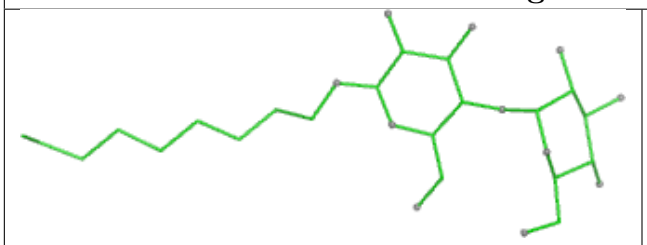


Torsions

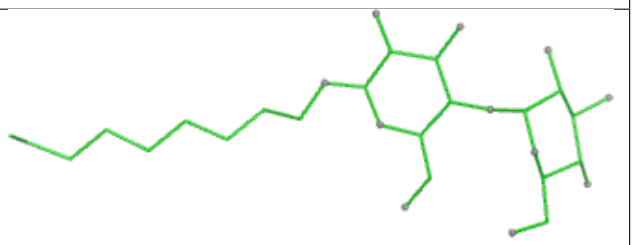


Rings

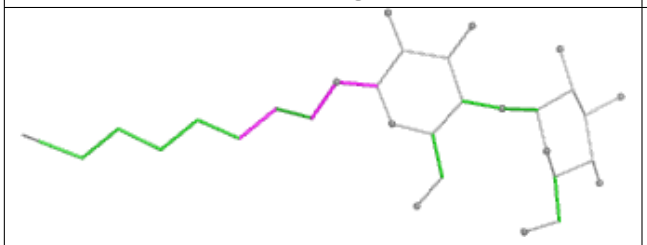
Ligand LMT c 904



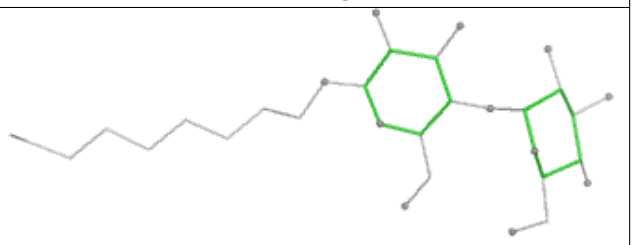
Bond lengths



Bond angles

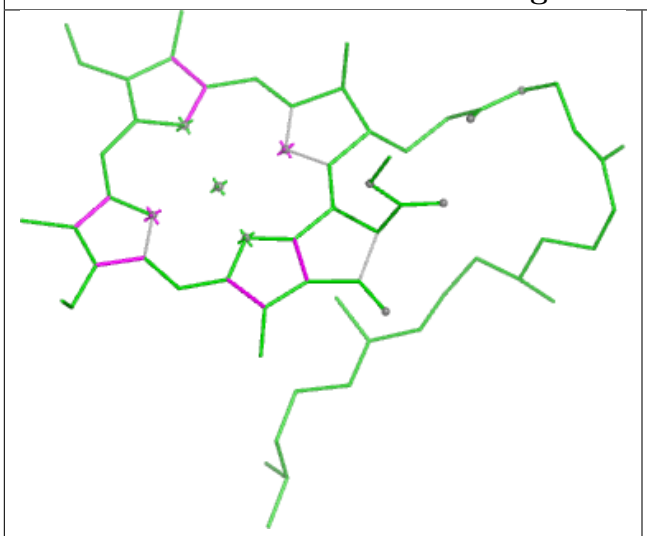


Torsions

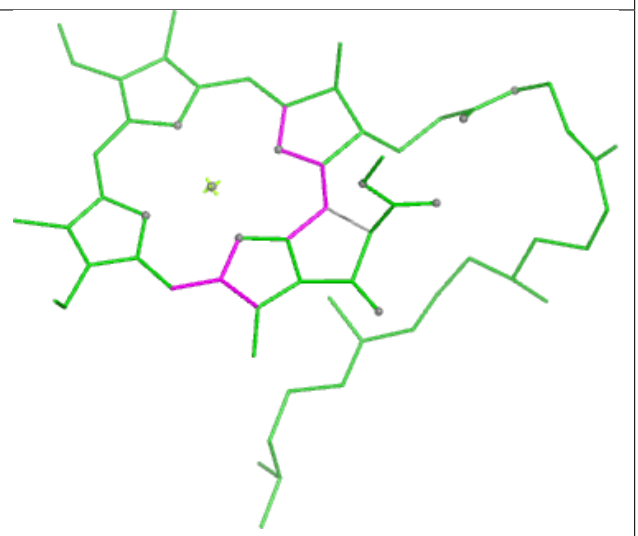


Rings

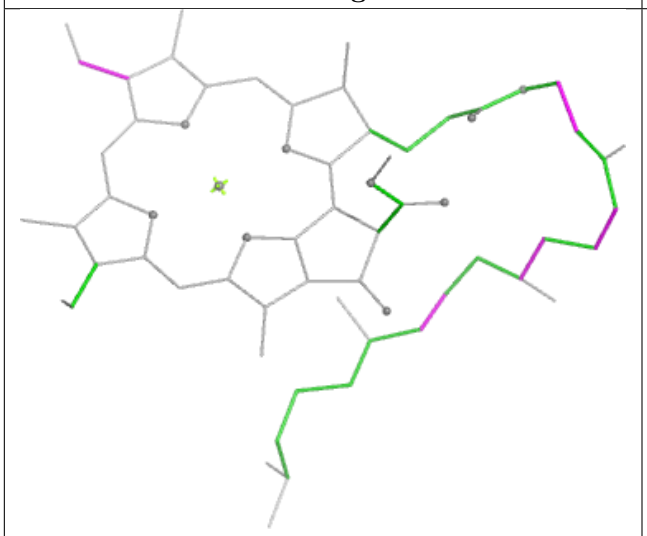
Ligand CLA c 509



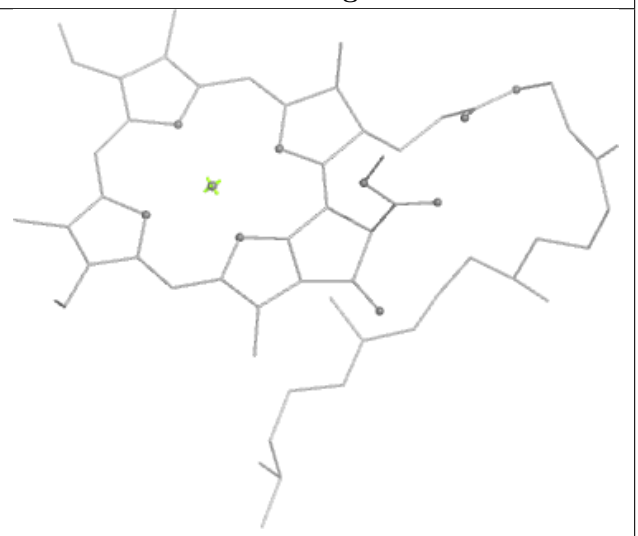
Bond lengths



Bond angles

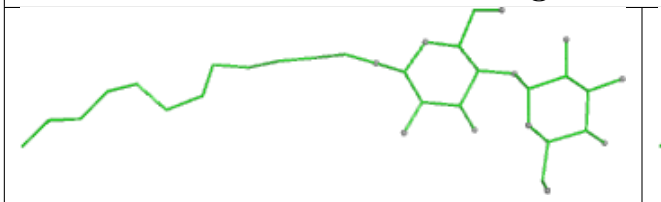


Torsions

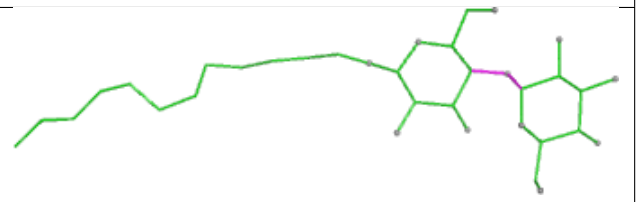


Rings

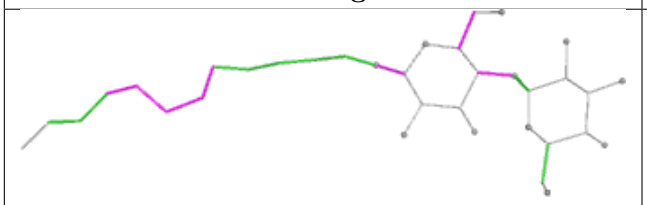
Ligand LMT l 210



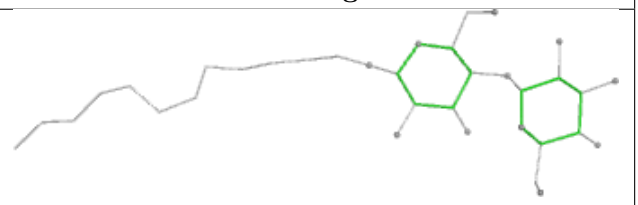
Bond lengths



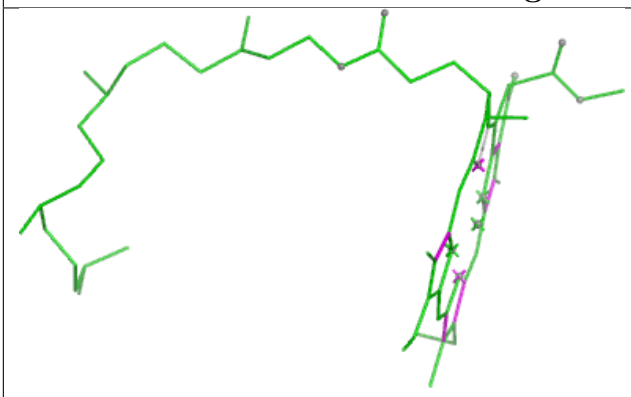
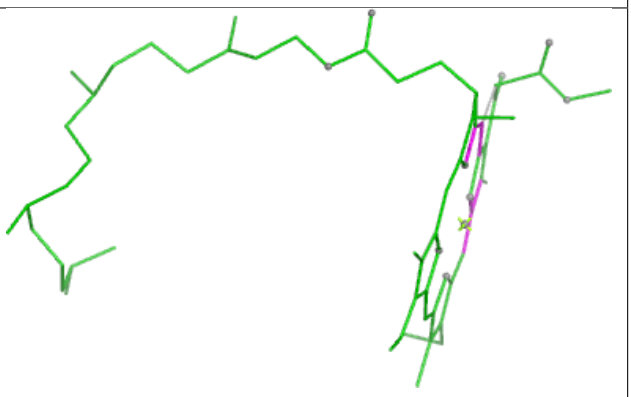
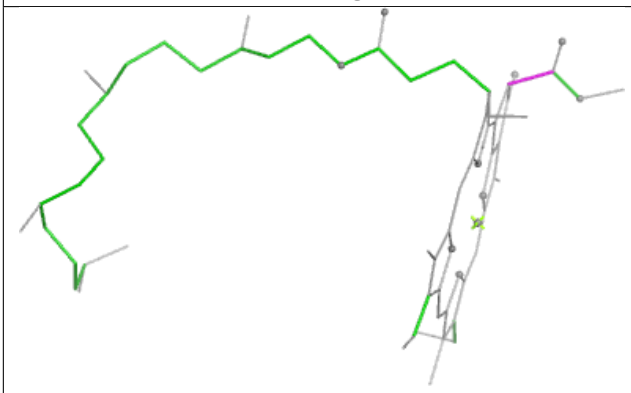
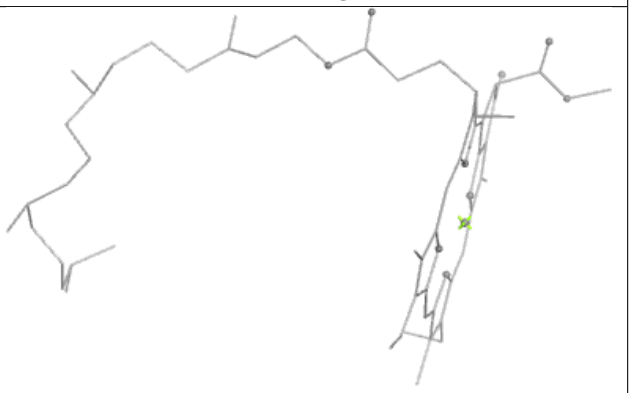
Bond angles



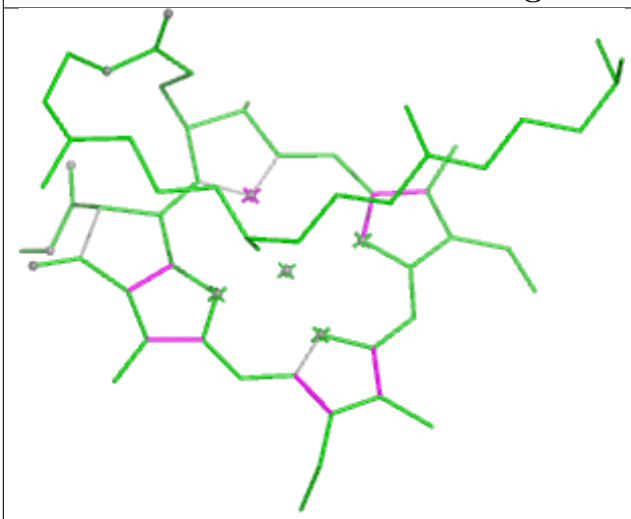
Torsions



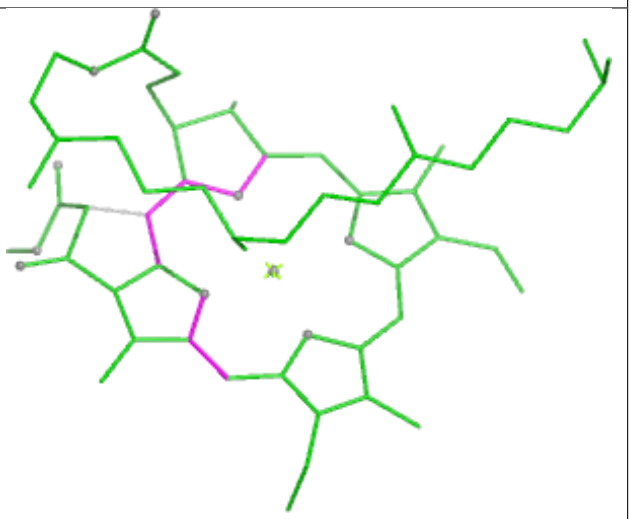
Rings

Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

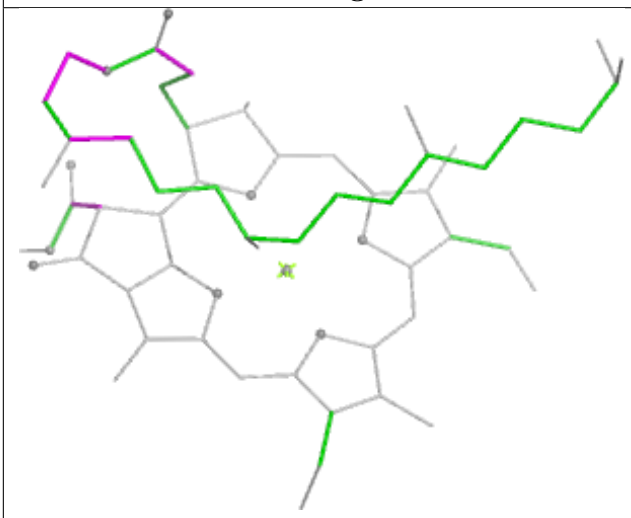
Ligand CLA B 602



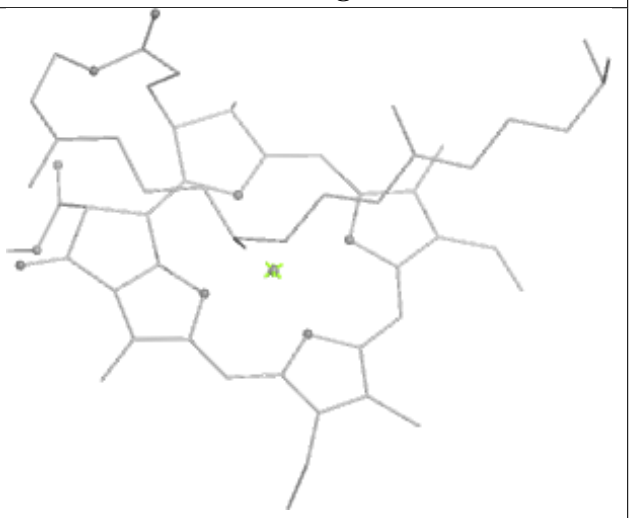
Bond lengths



Bond angles

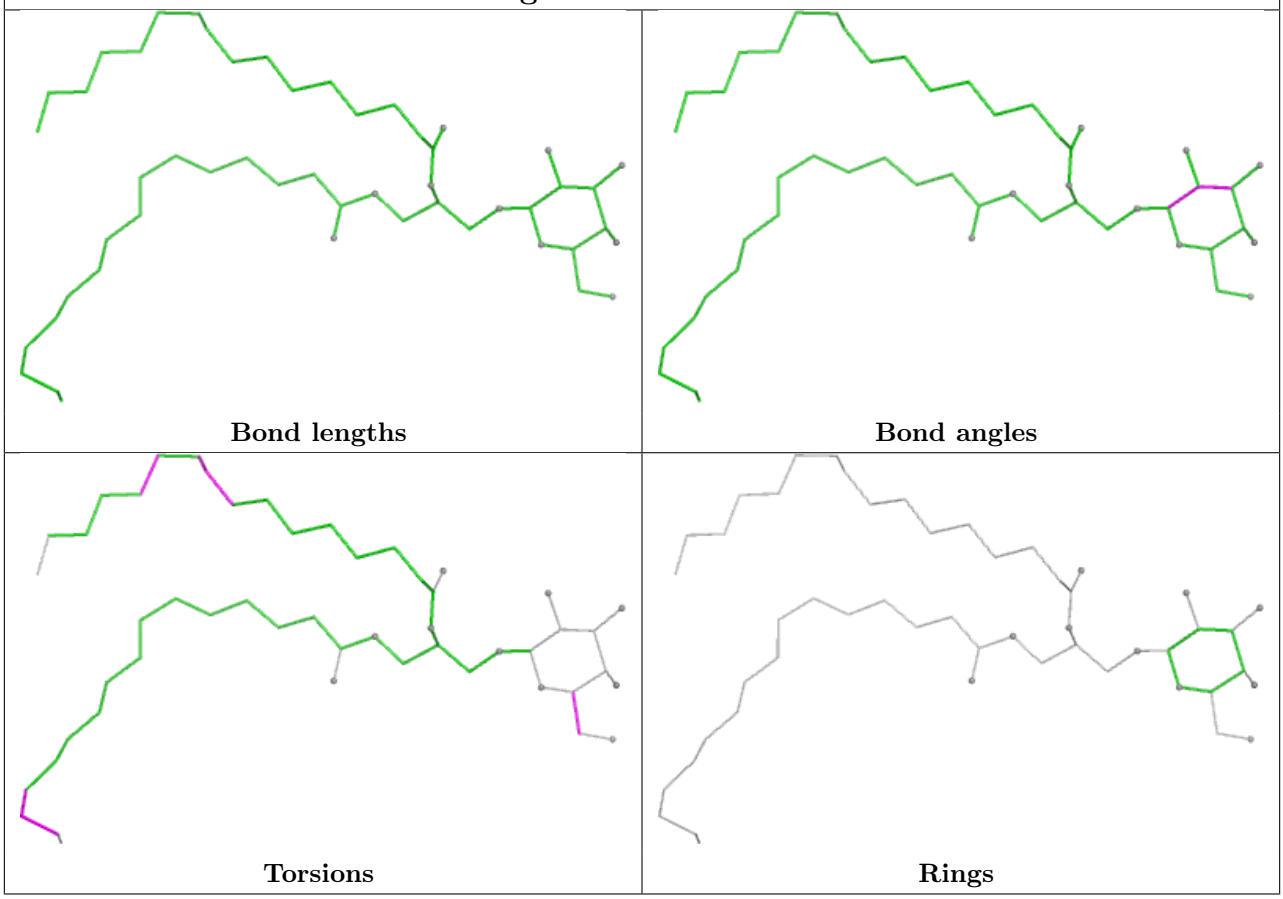


Torsions

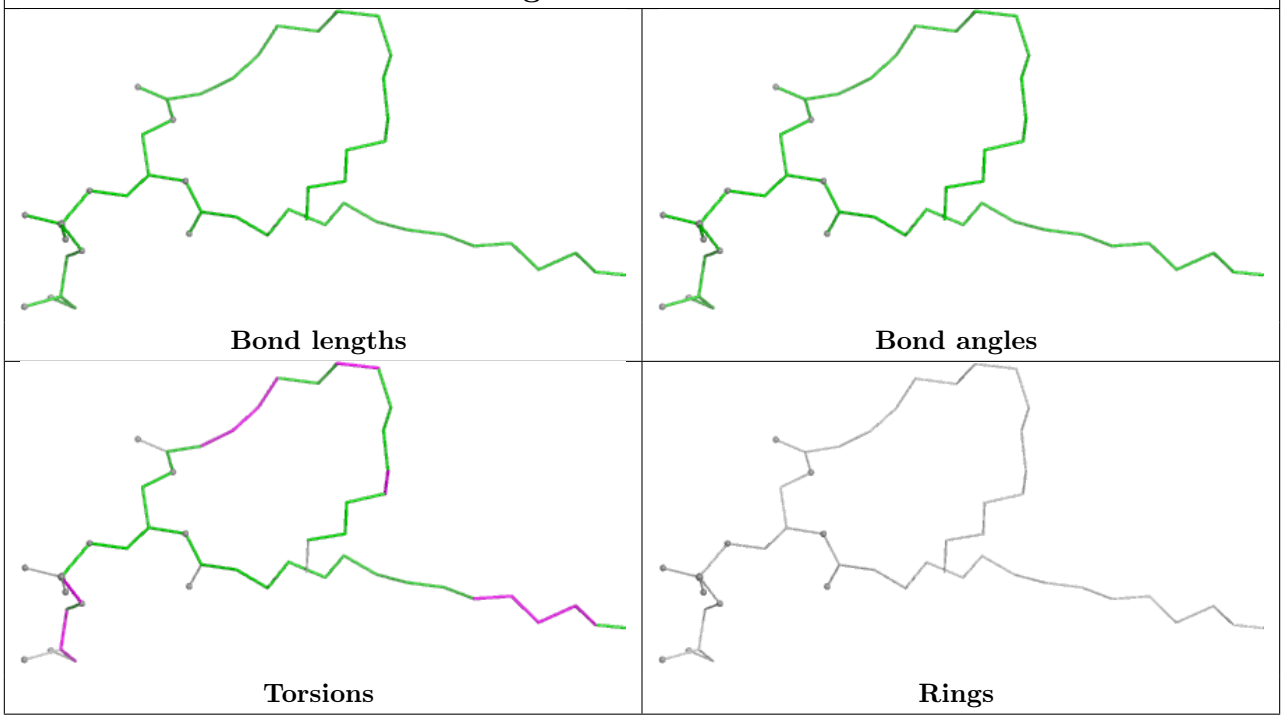


Rings

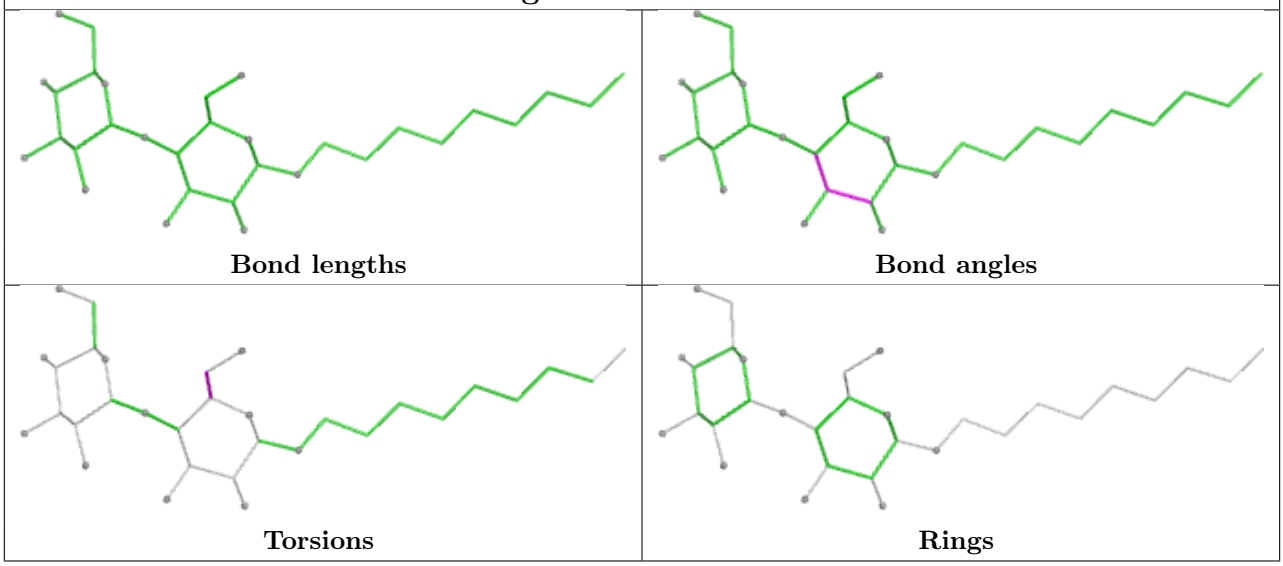
Ligand LMG D 411



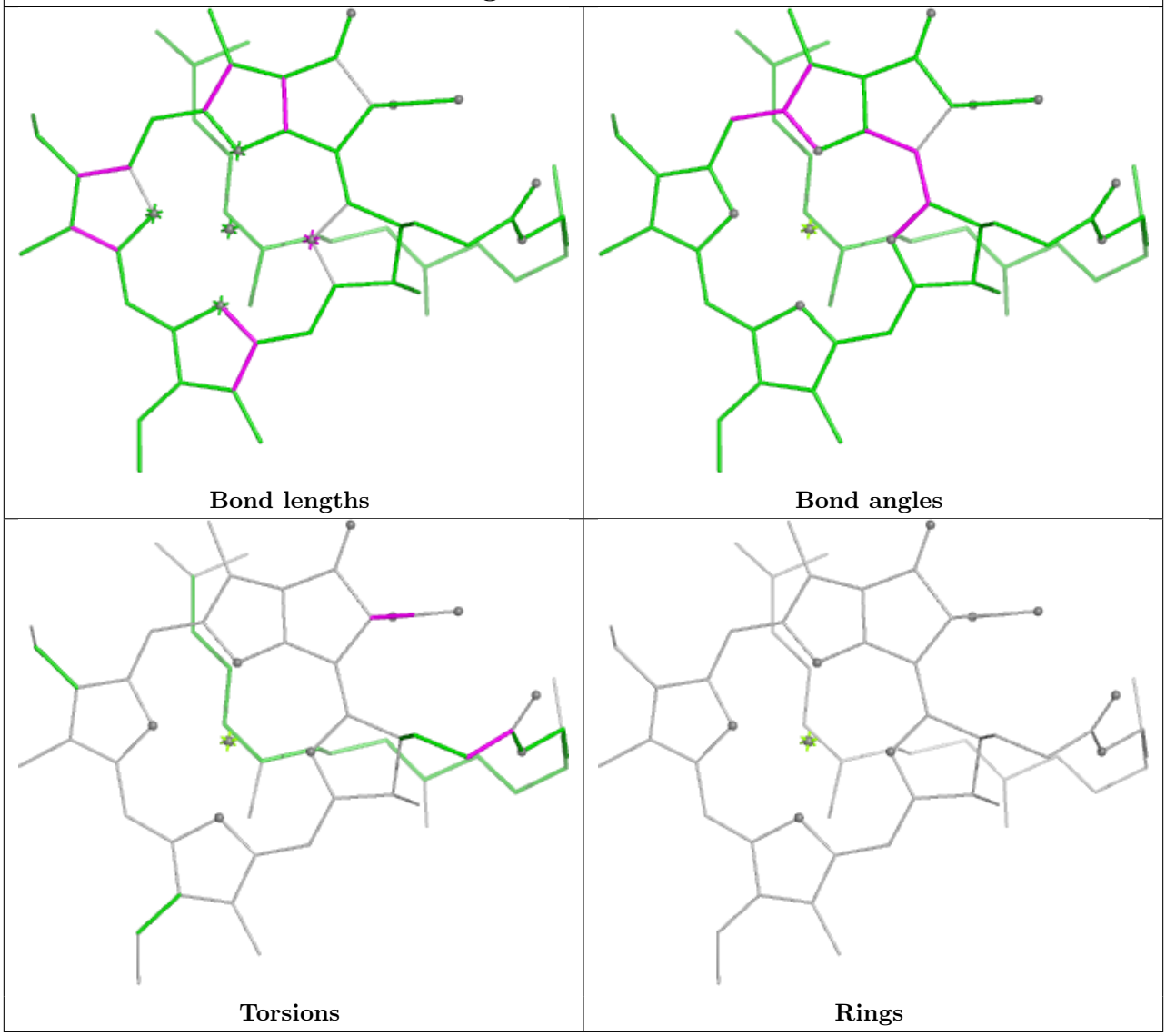
Ligand LHG D 408



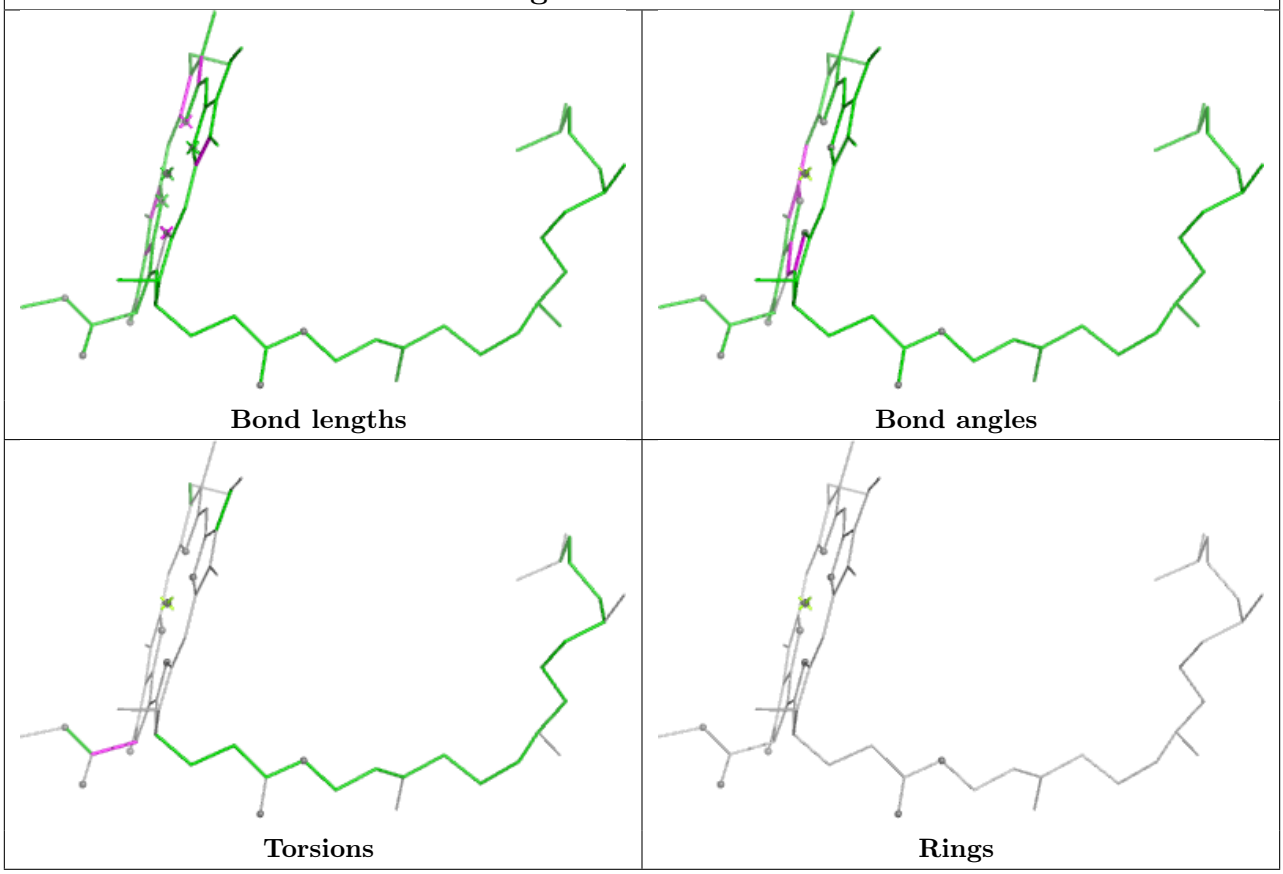
Ligand LMT A 675



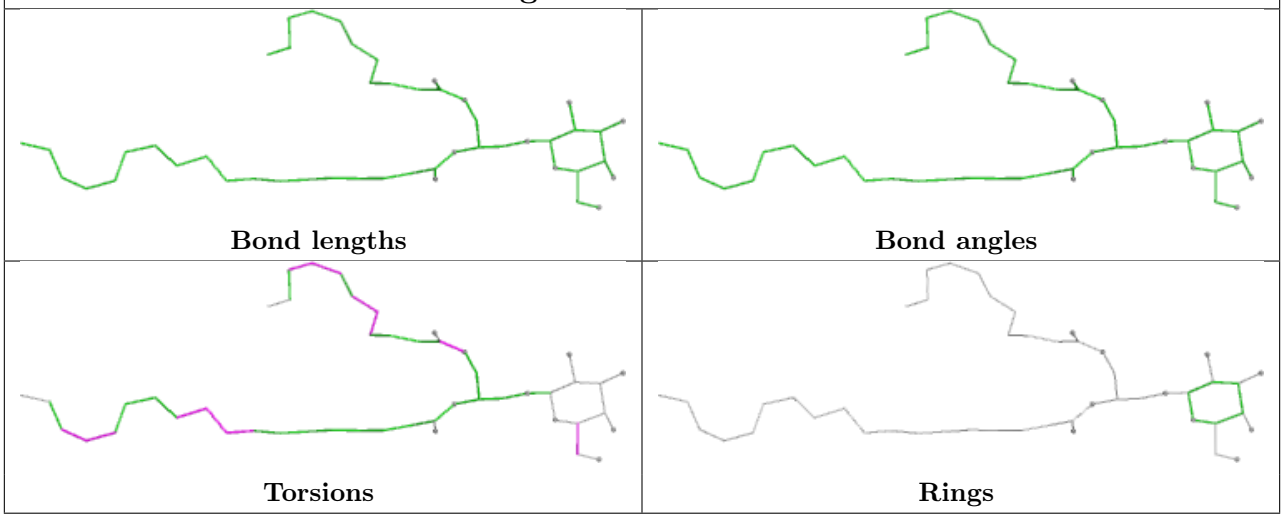
Ligand CLA c 510

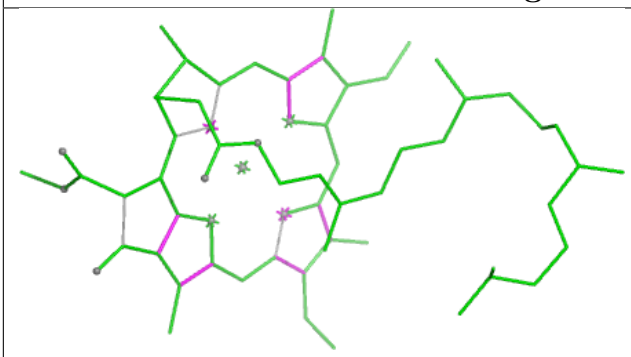
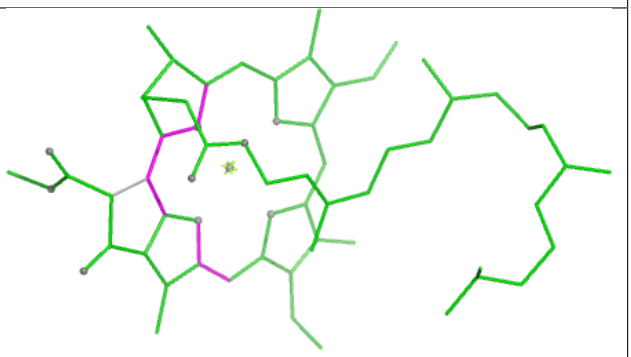
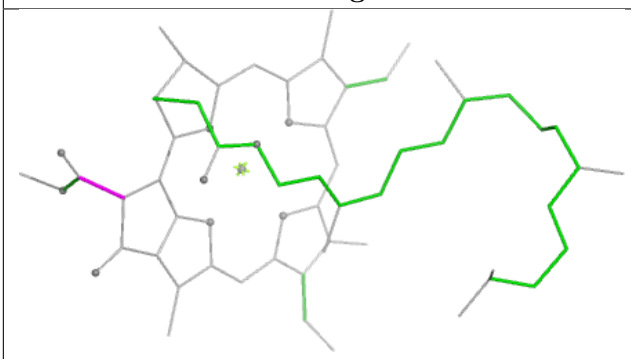
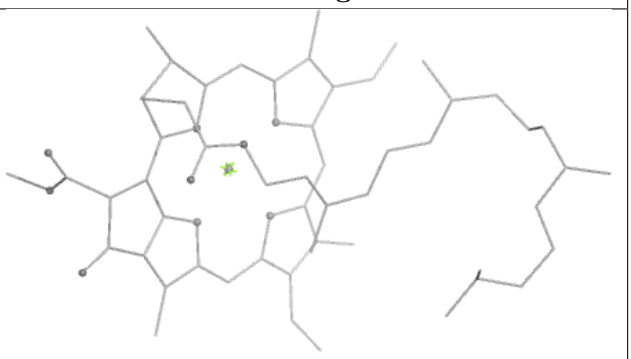


Ligand CLA c 506

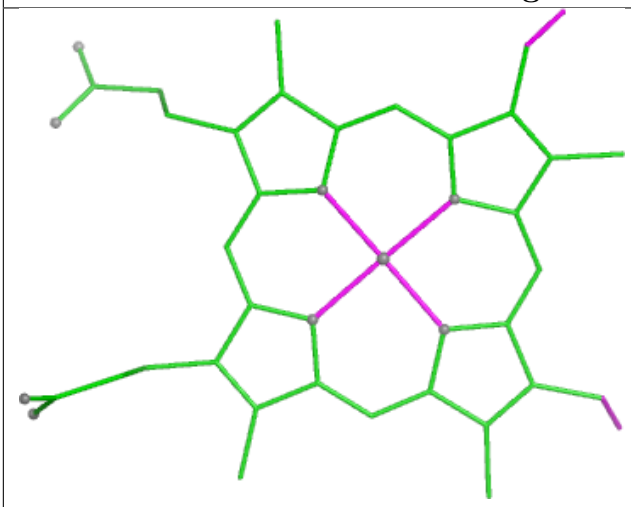


Ligand LMG A 415

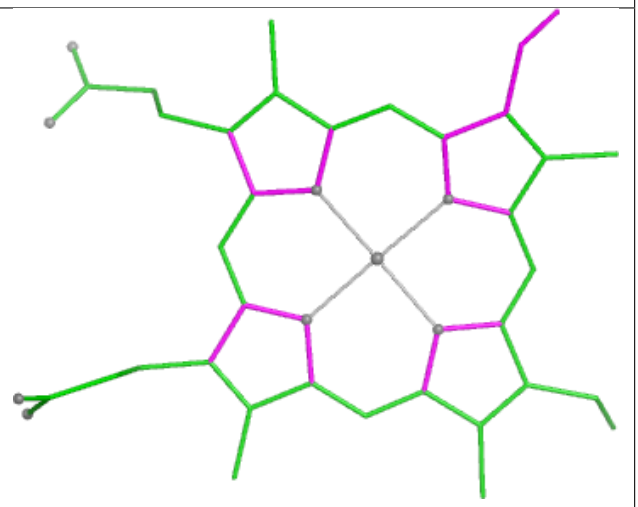


Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

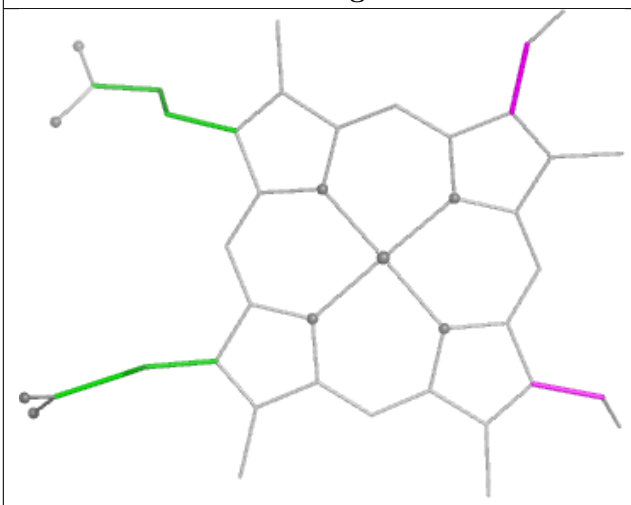
Ligand HEC V 201



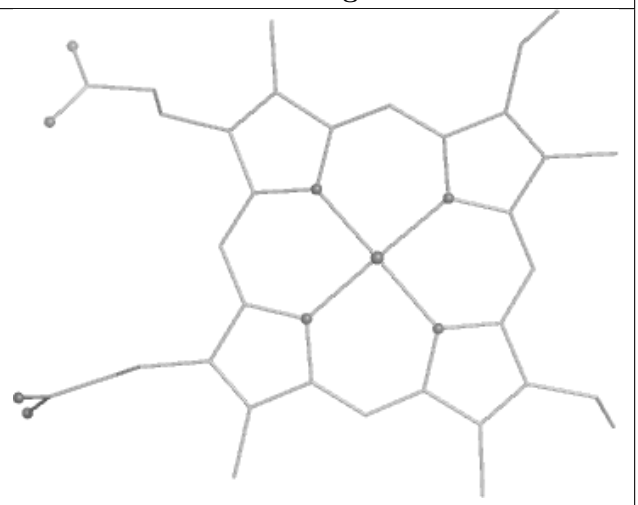
Bond lengths



Bond angles

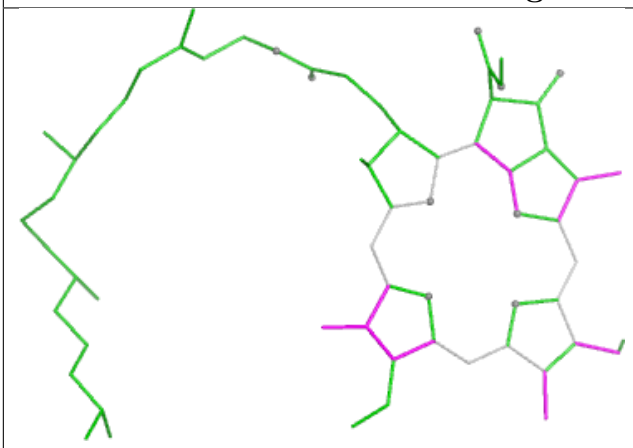


Torsions

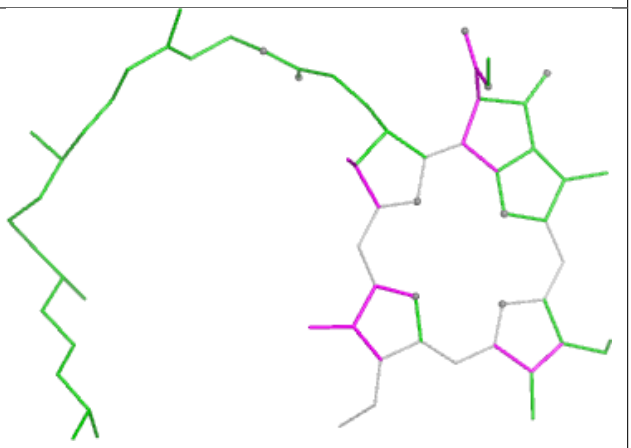


Rings

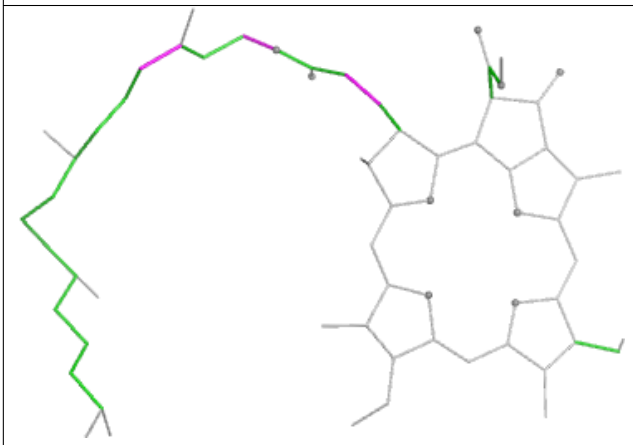
Ligand PHO a 408



Bond lengths



Bond angles

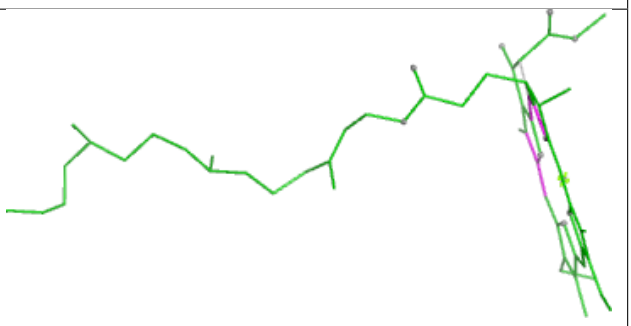


Torsions

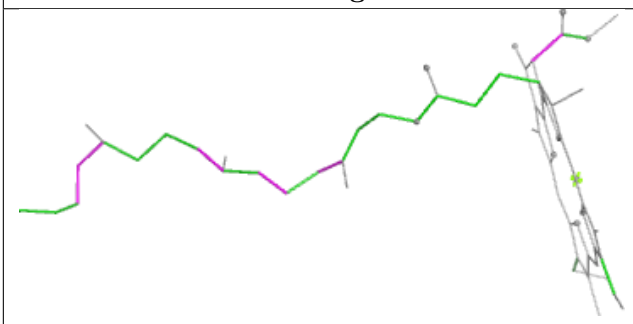
Rings

Ligand CLA c 502

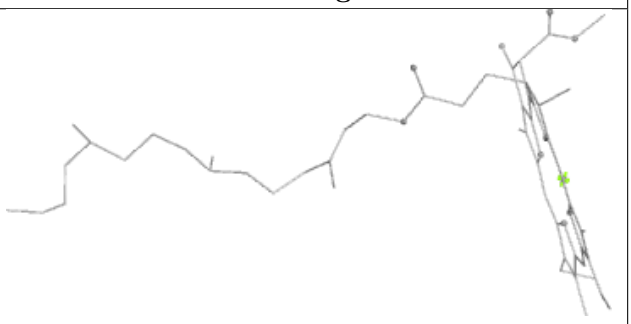
Bond lengths



Bond angles

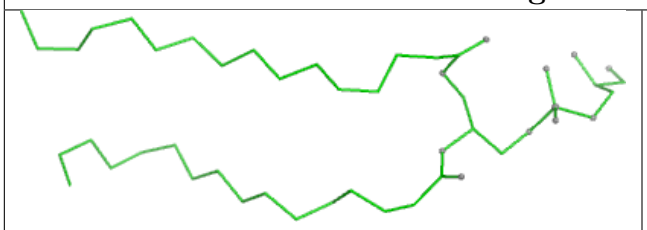


Torsions

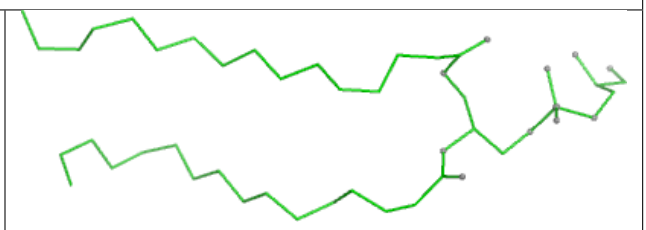


Rings

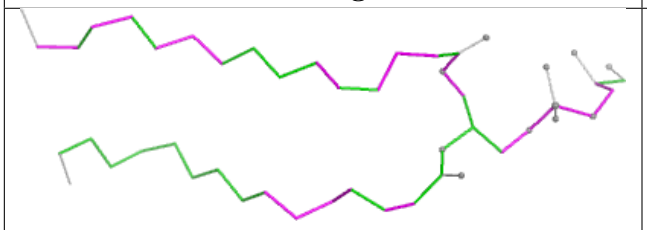
Ligand LHG e 244



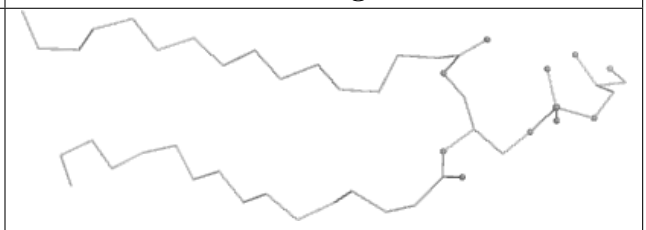
Bond lengths



Bond angles

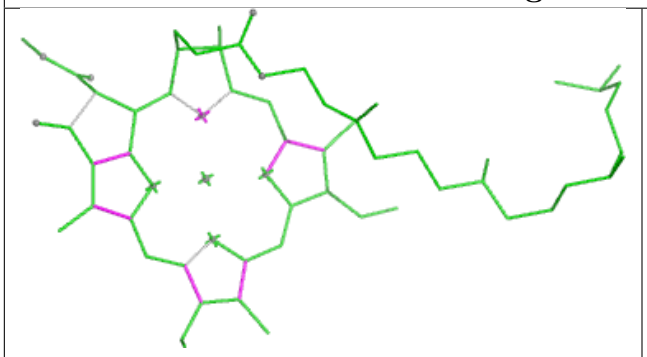


Torsions

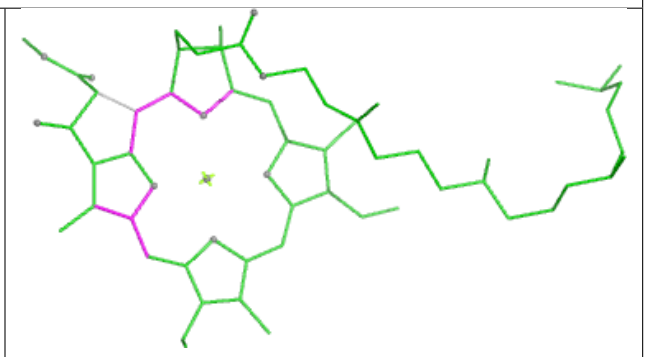


Rings

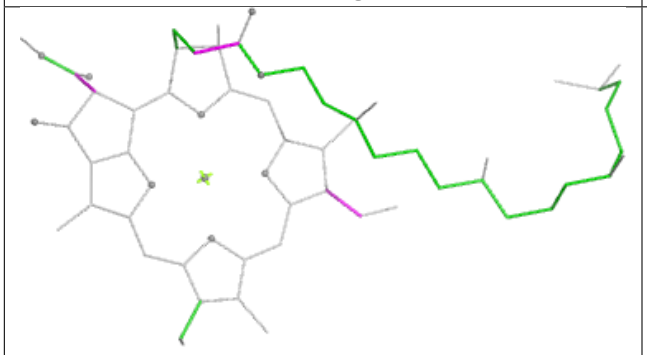
Ligand CLA C 501



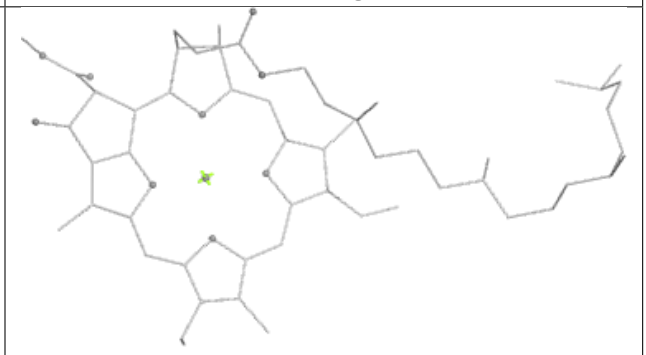
Bond lengths



Bond angles



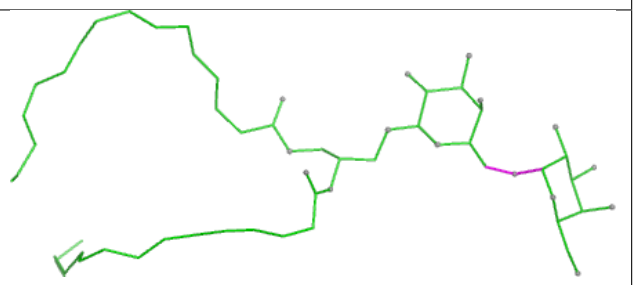
Torsions



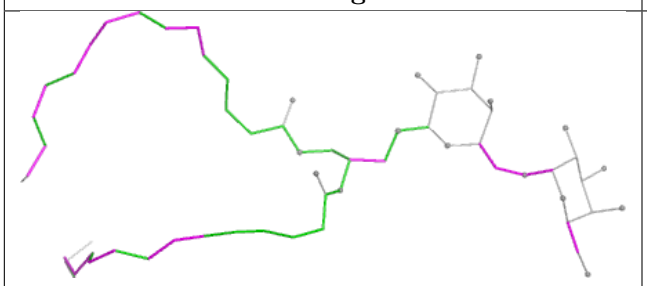
Rings

Ligand DGD C 516

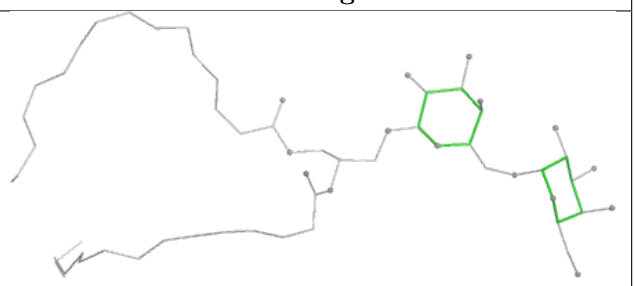
Bond lengths



Bond angles

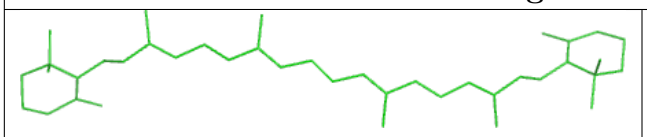


Torsions



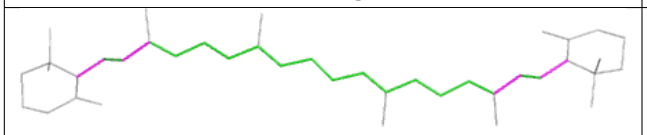
Rings

Ligand BCR d 404

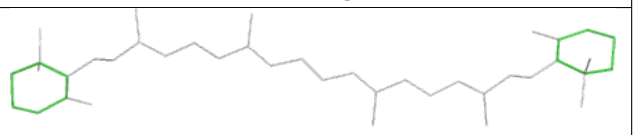


Bond lengths

Bond angles

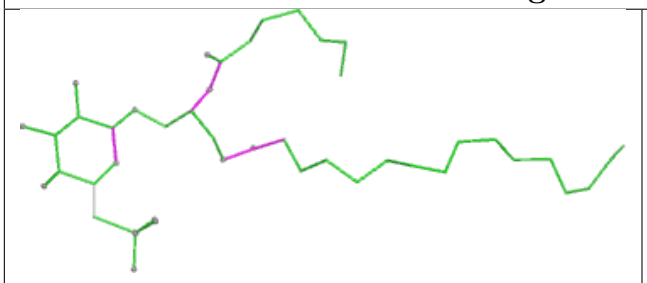


Torsions

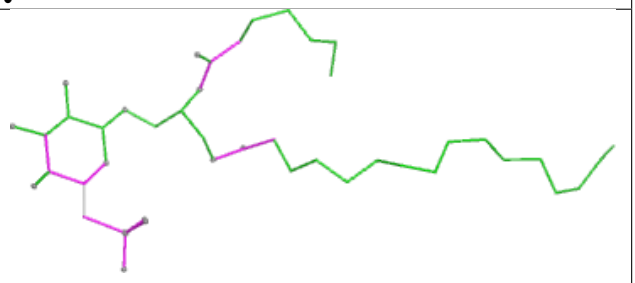


Rings

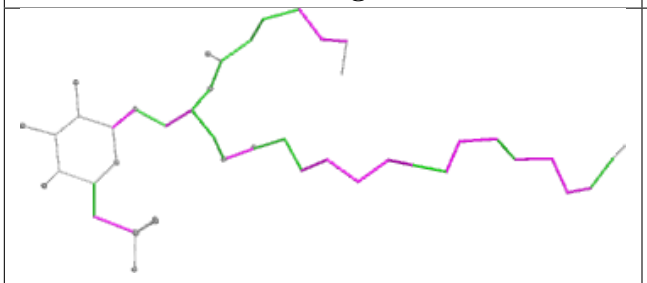
Ligand SQD d 407



Bond lengths



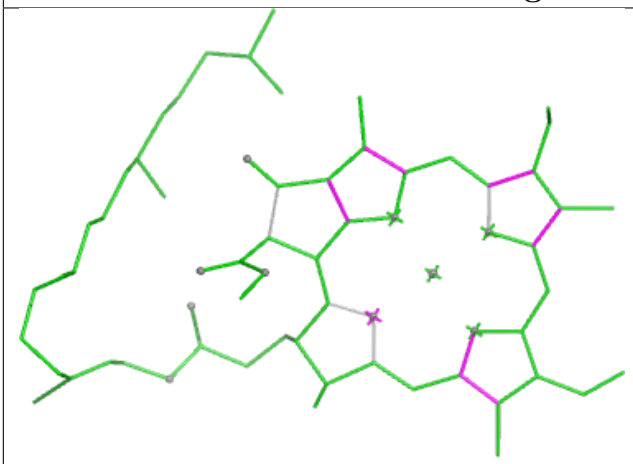
Bond angles



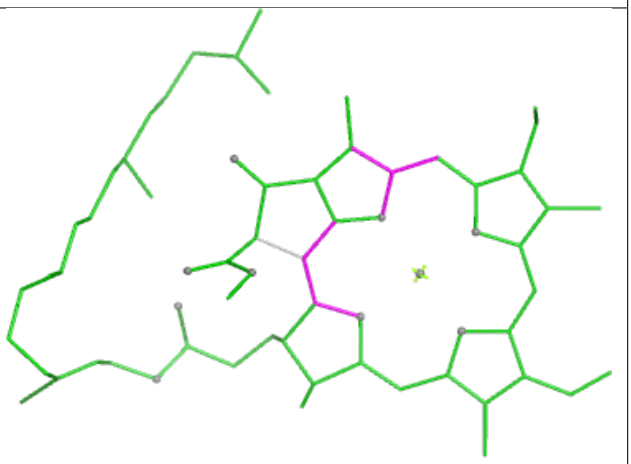
Torsions

Rings

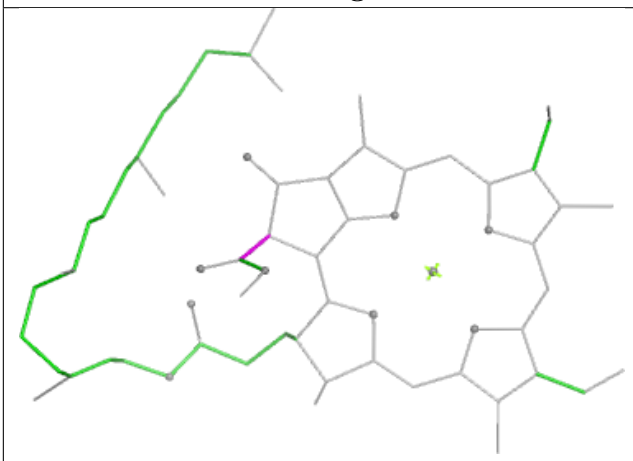
Ligand CLA B 611



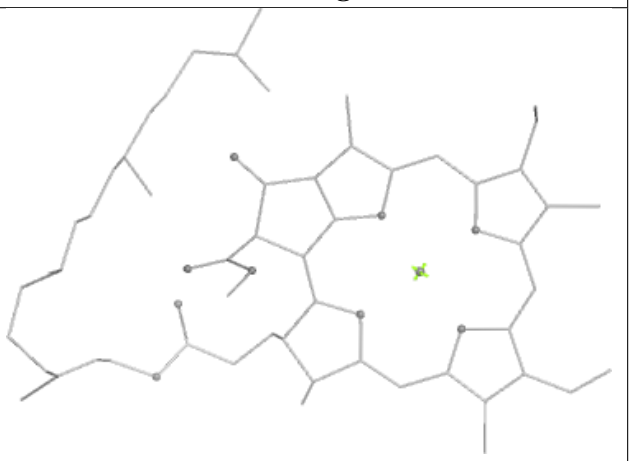
Bond lengths



Bond angles

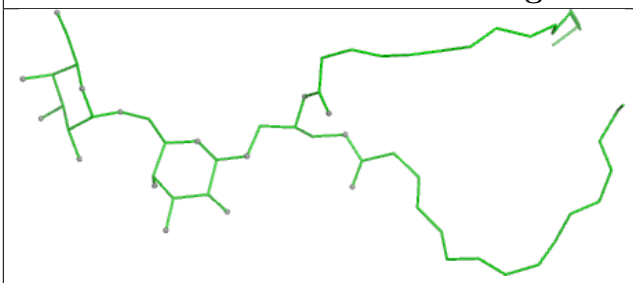


Torsions

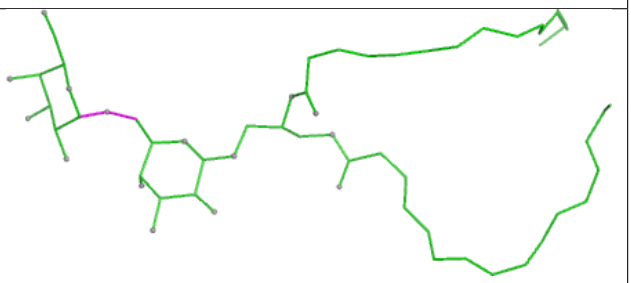


Rings

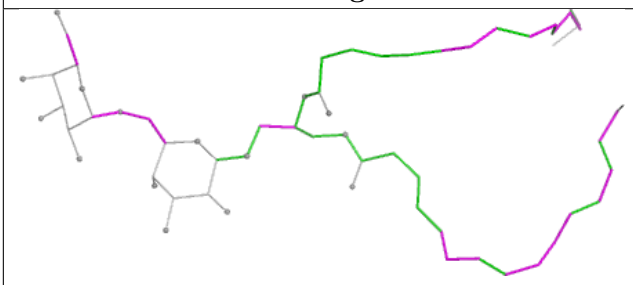
Ligand DGD c 516



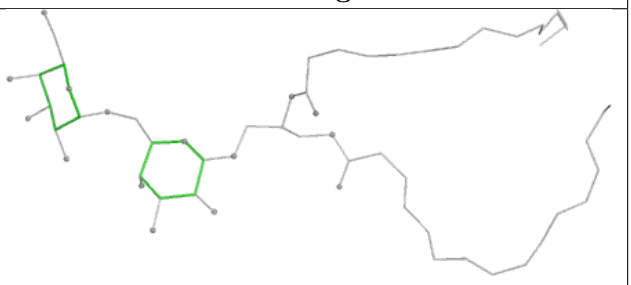
Bond lengths



Bond angles

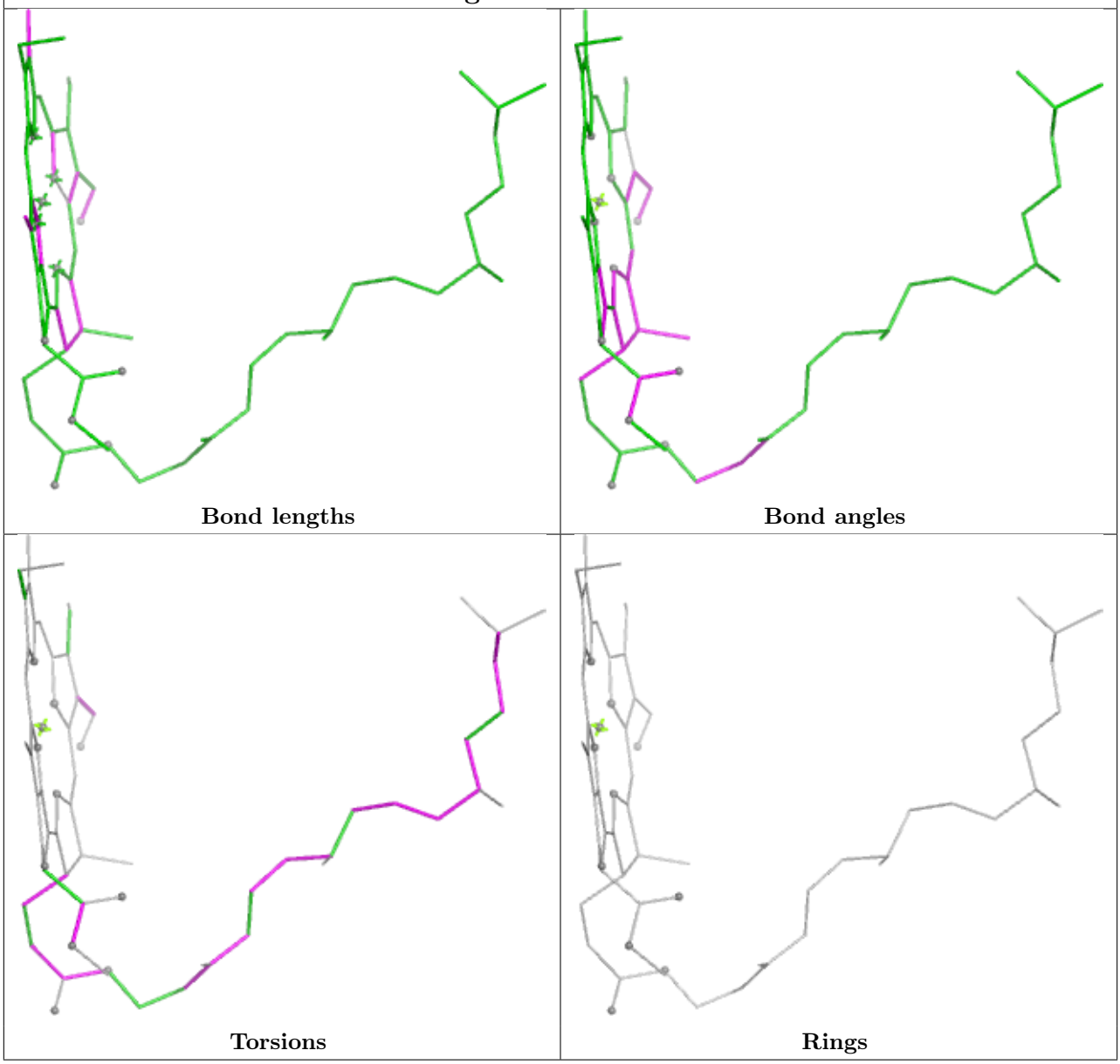


Torsions

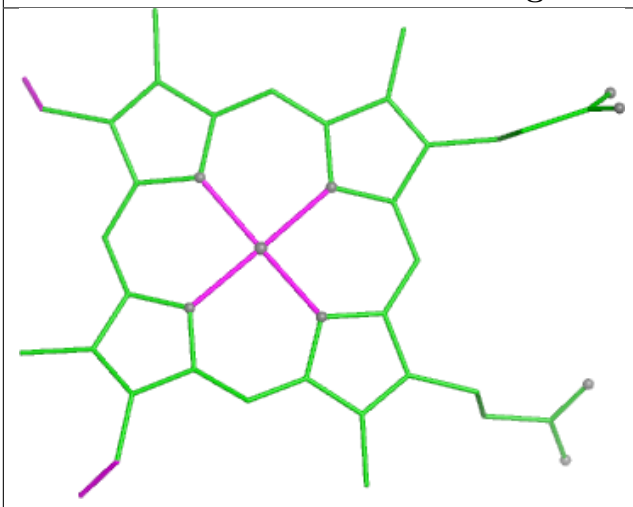


Rings

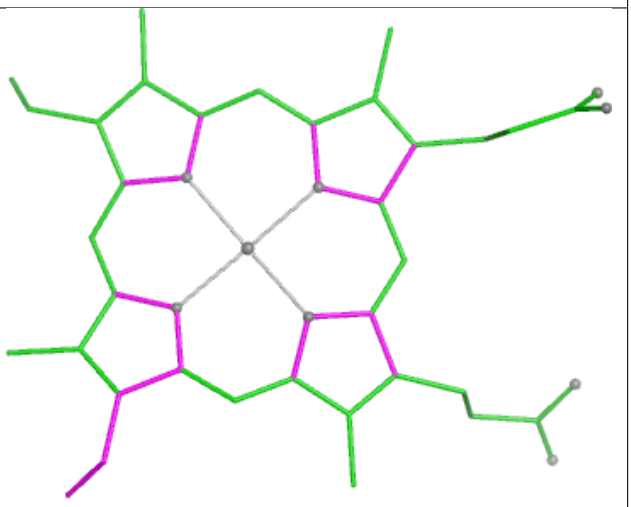
Ligand F6C b 614



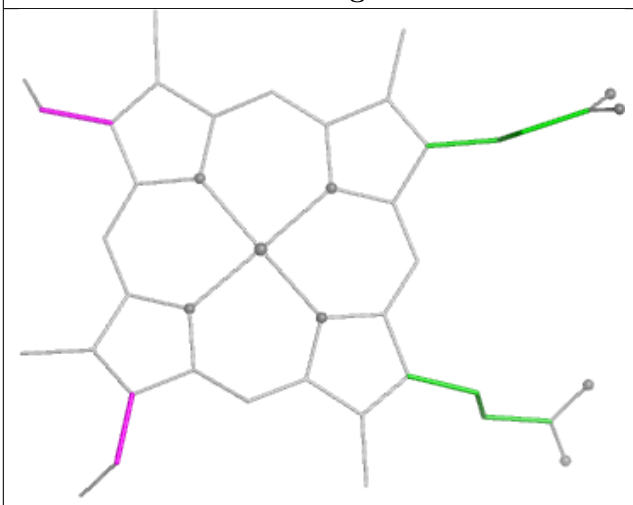
Ligand HEC v 201



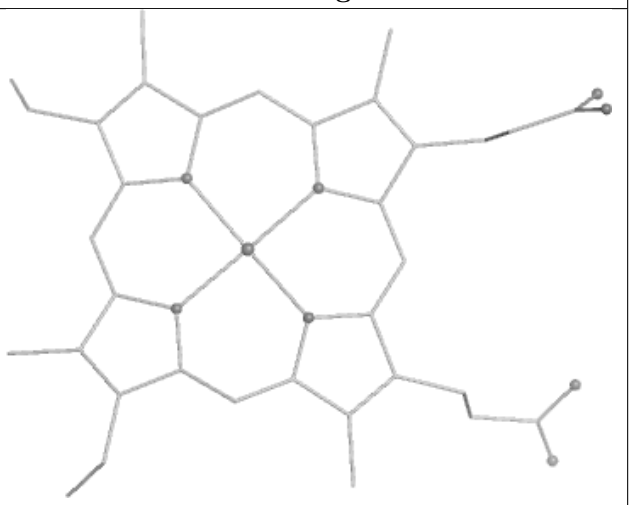
Bond lengths



Bond angles

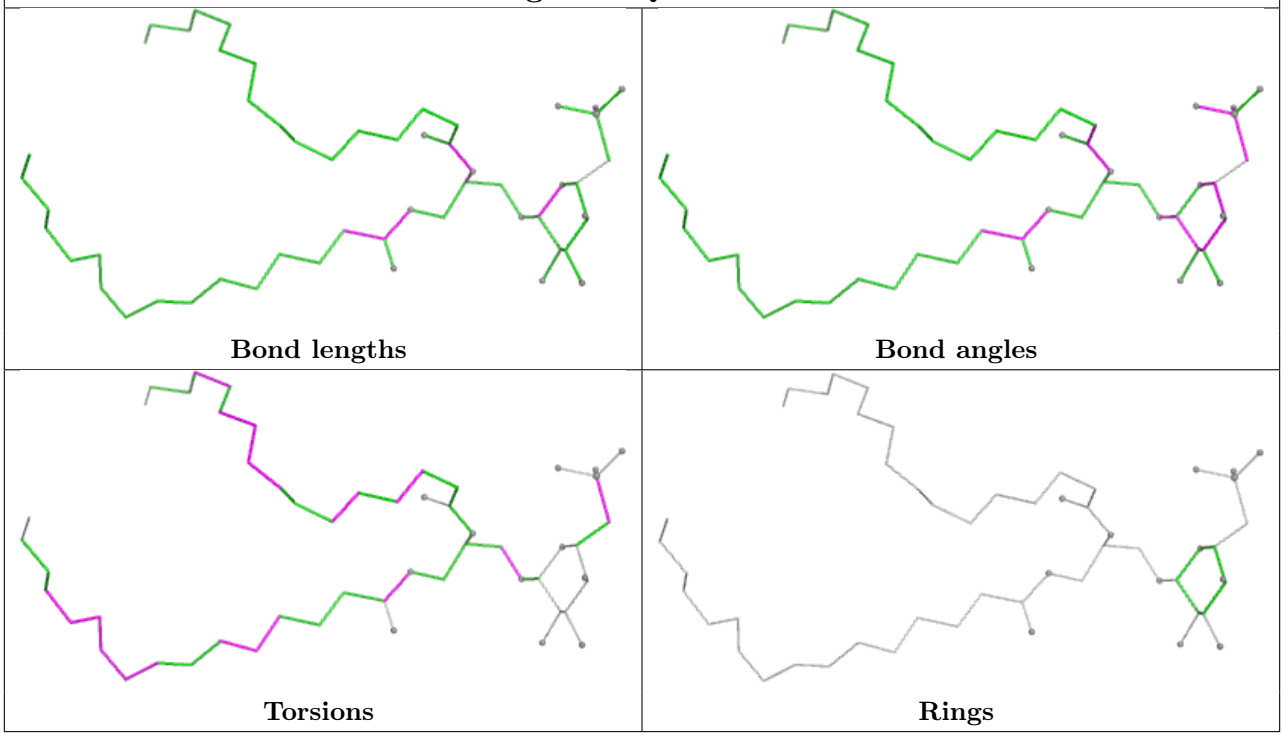


Torsions

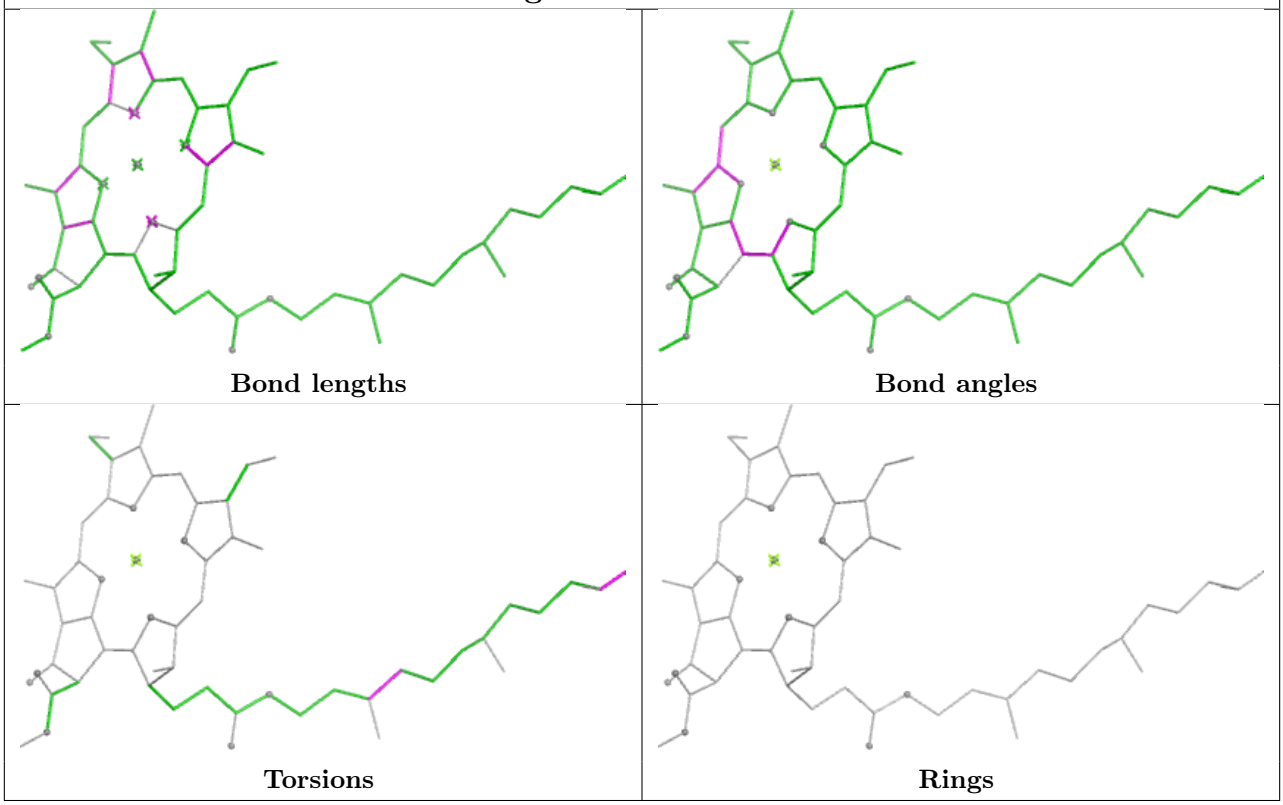


Rings

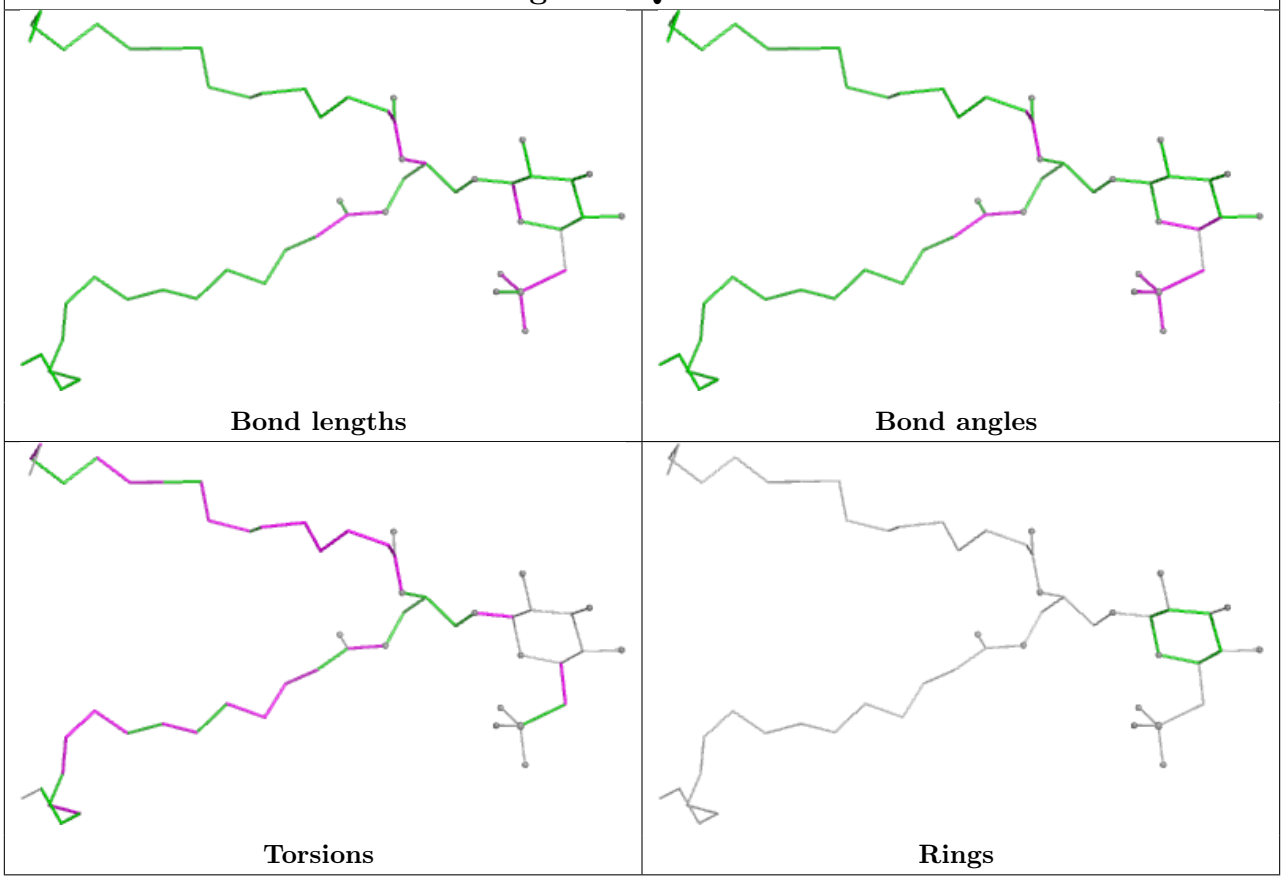
Ligand SQD B 622



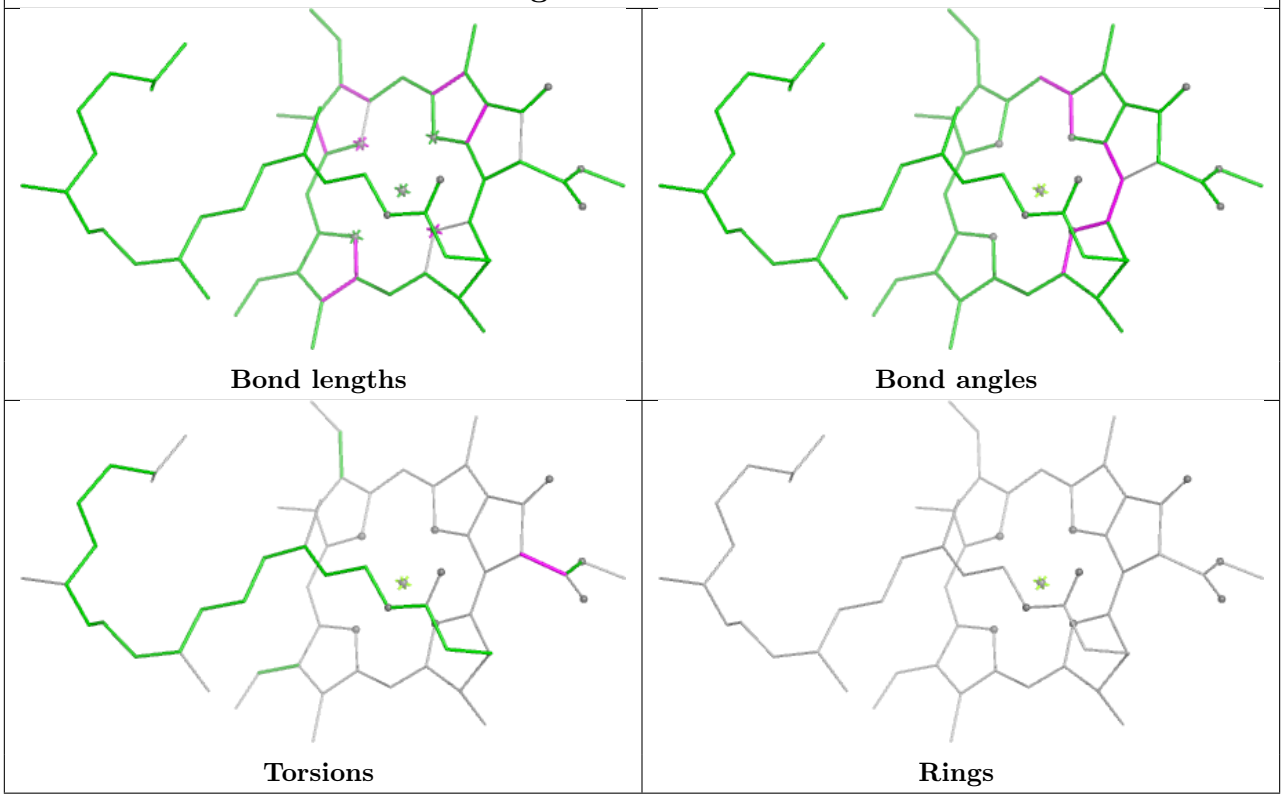
Ligand CLA A 410



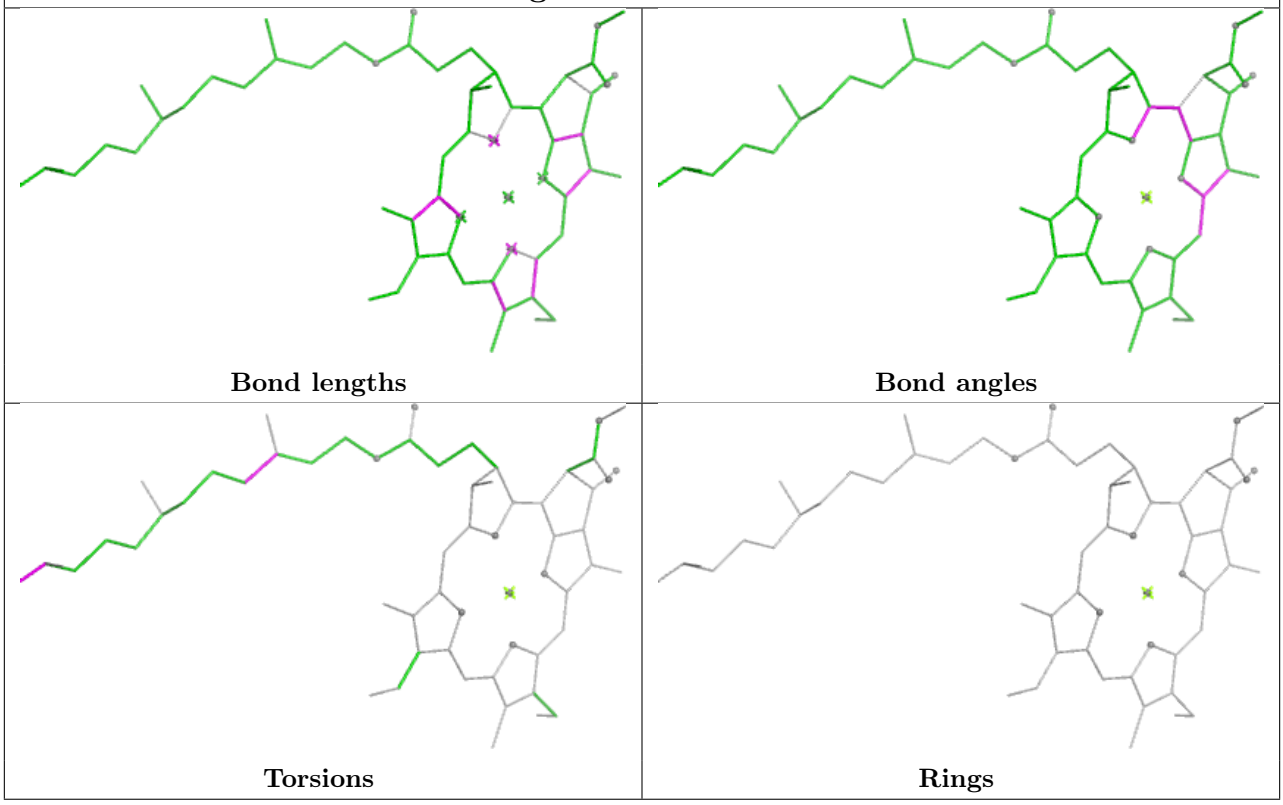
Ligand SQD a 412



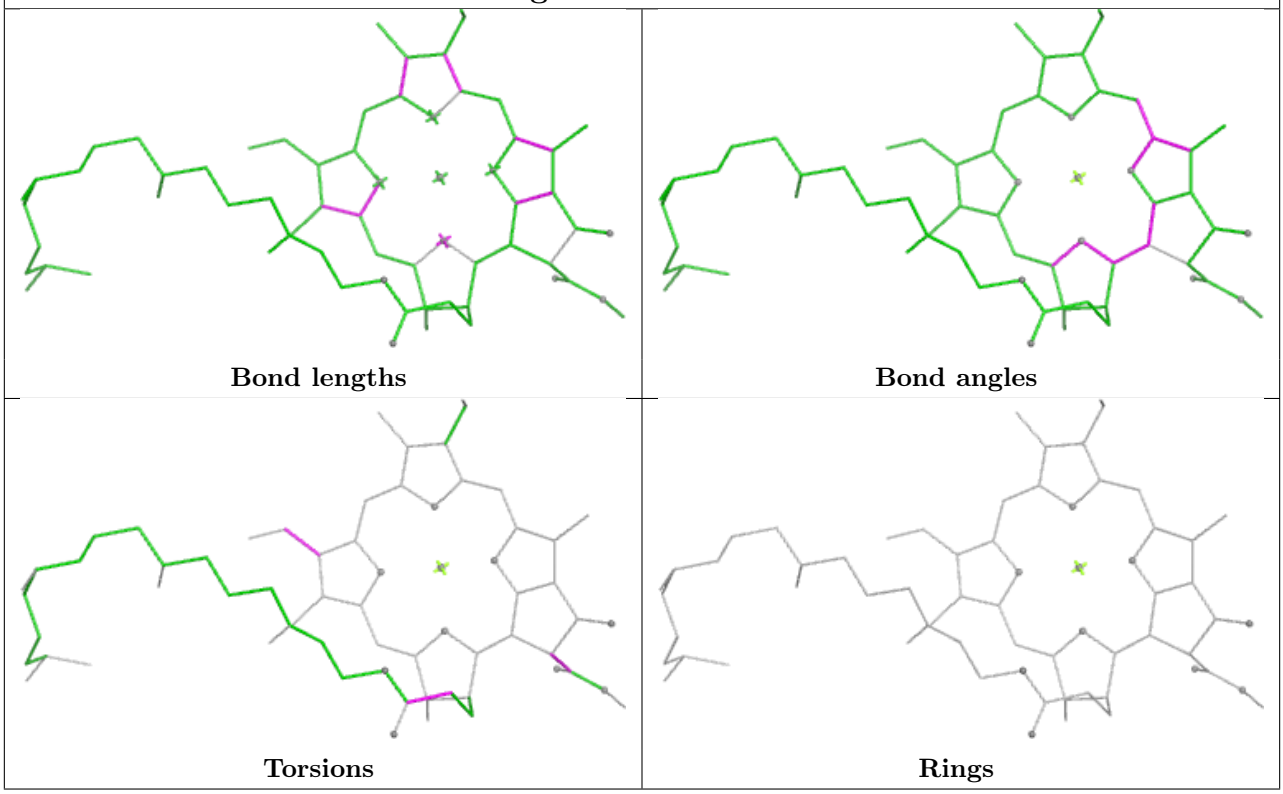
Ligand CLA c 505



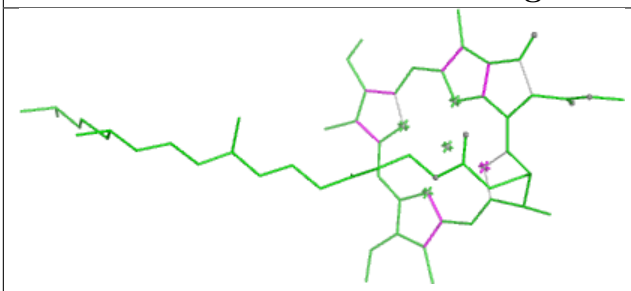
Ligand CLA a 410



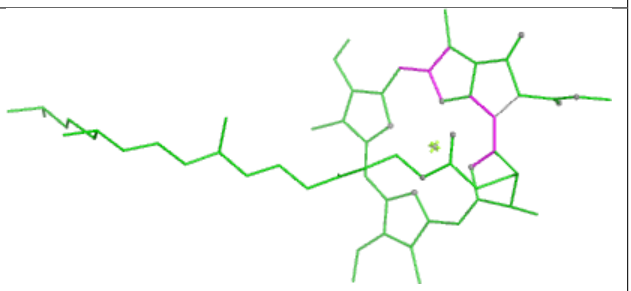
Ligand CLA c 501



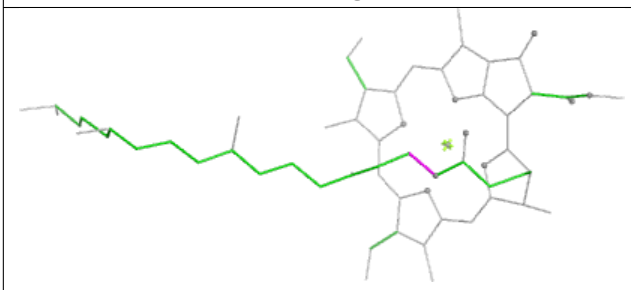
Ligand CLA B 609



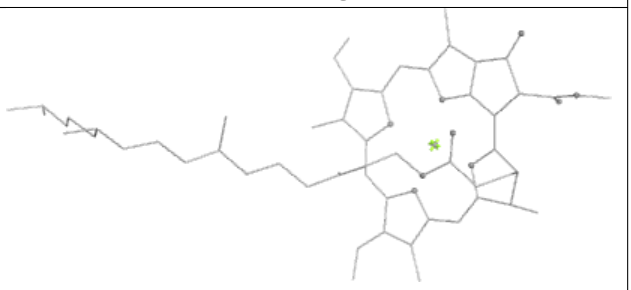
Bond lengths



Bond angles

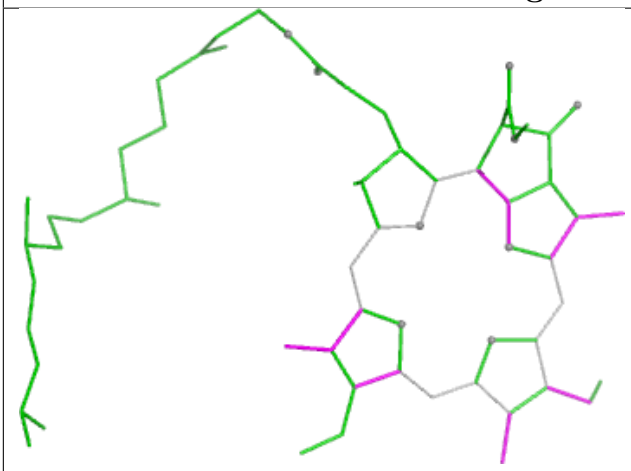


Torsions

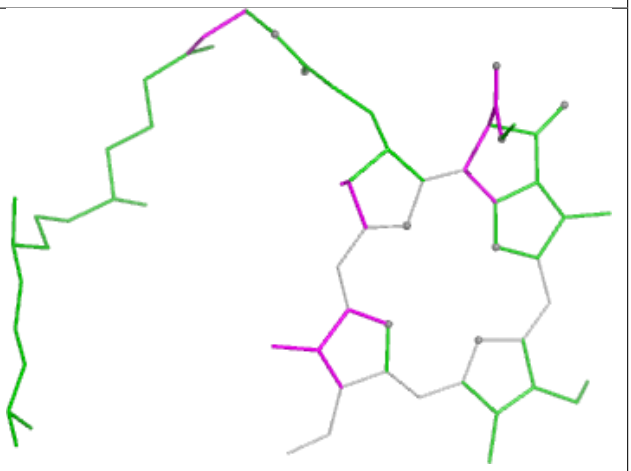


Rings

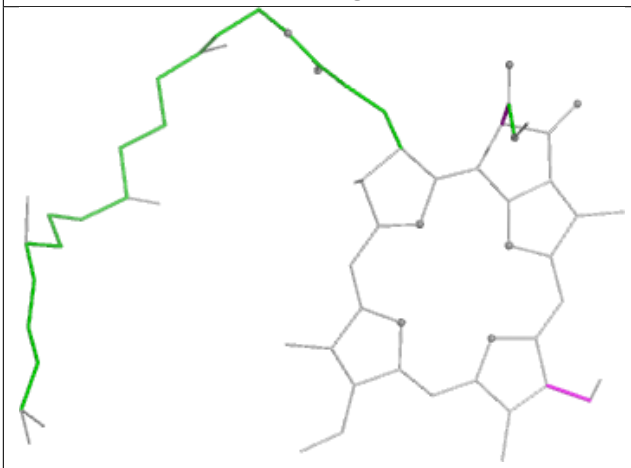
Ligand PHO a 409



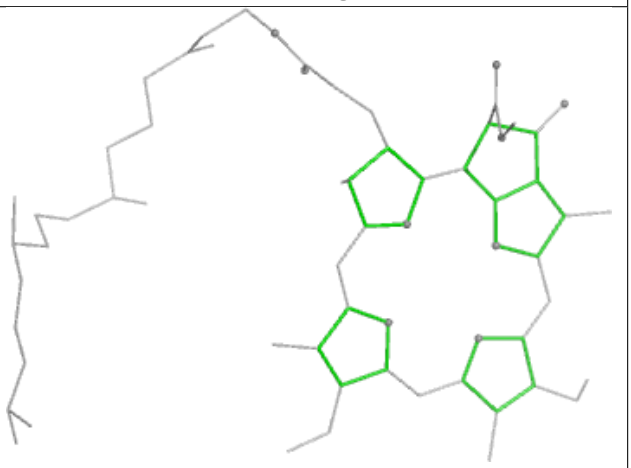
Bond lengths



Bond angles

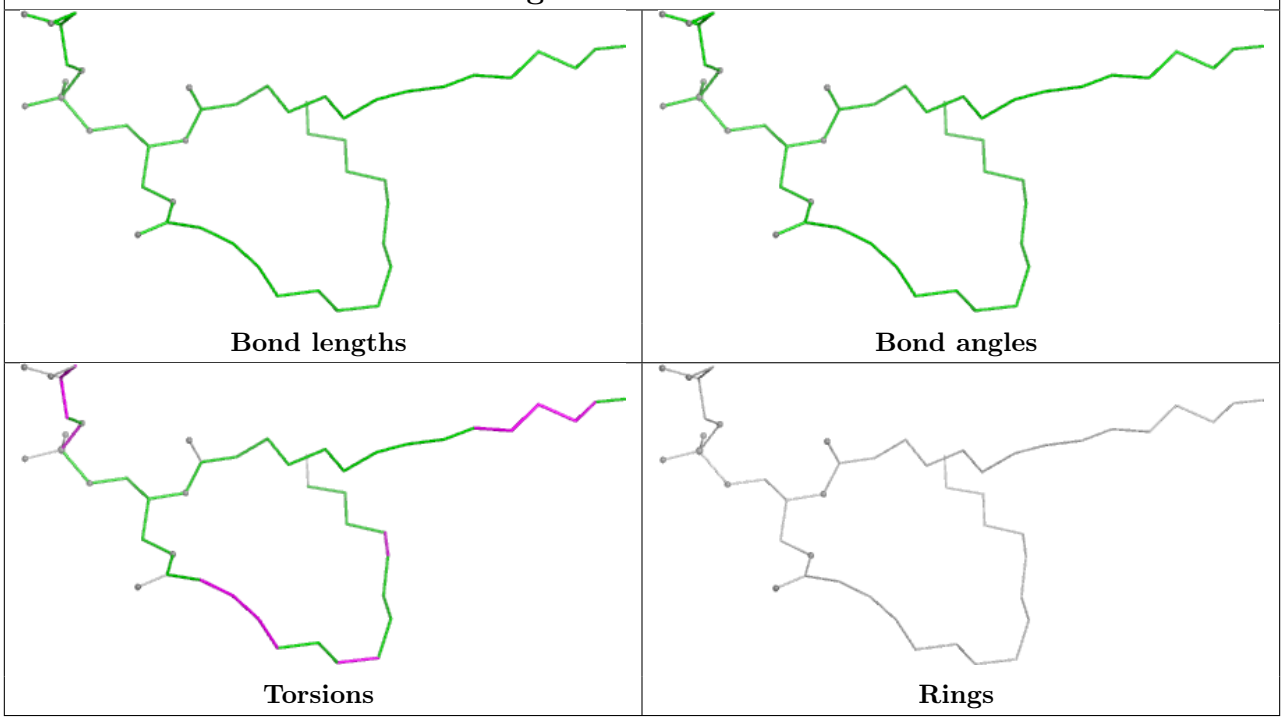


Torsions

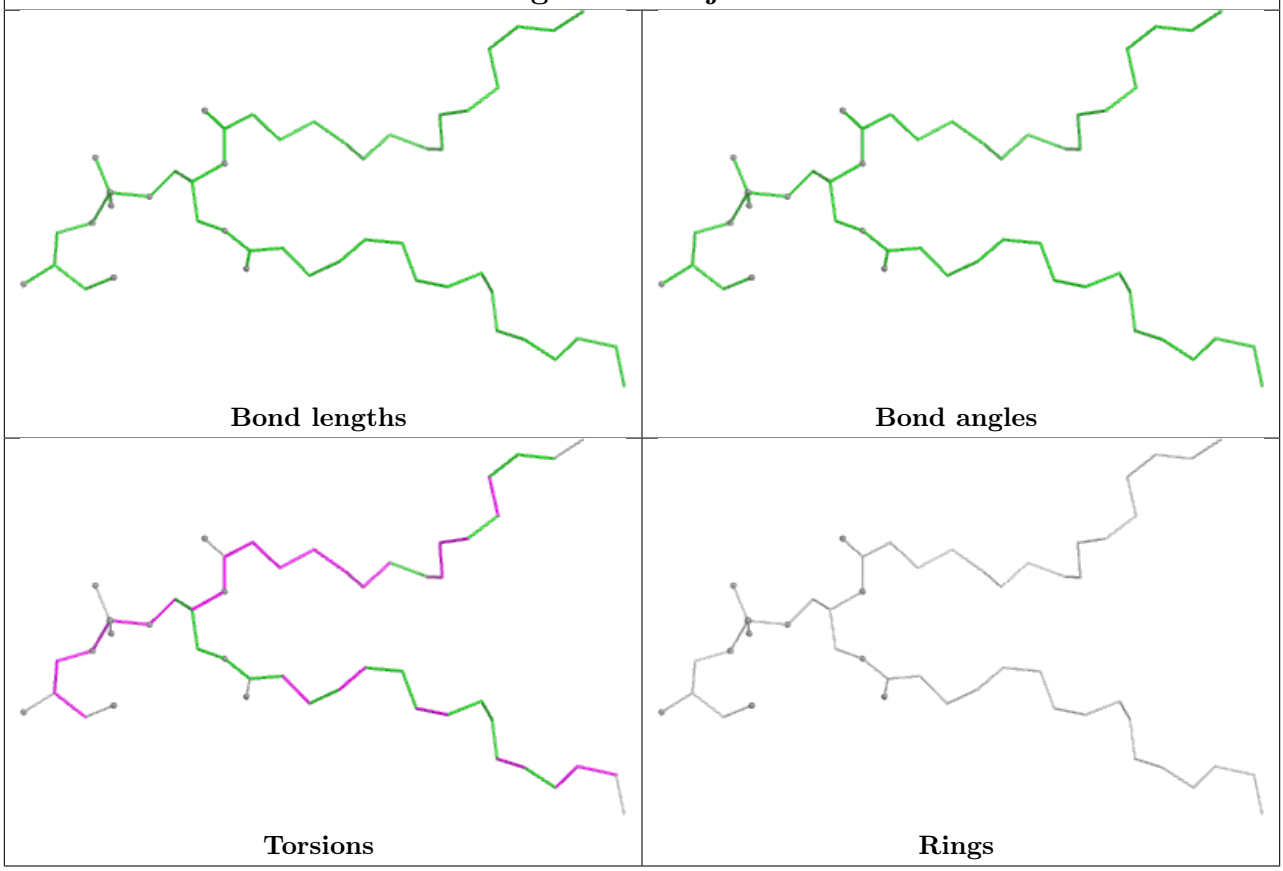


Rings

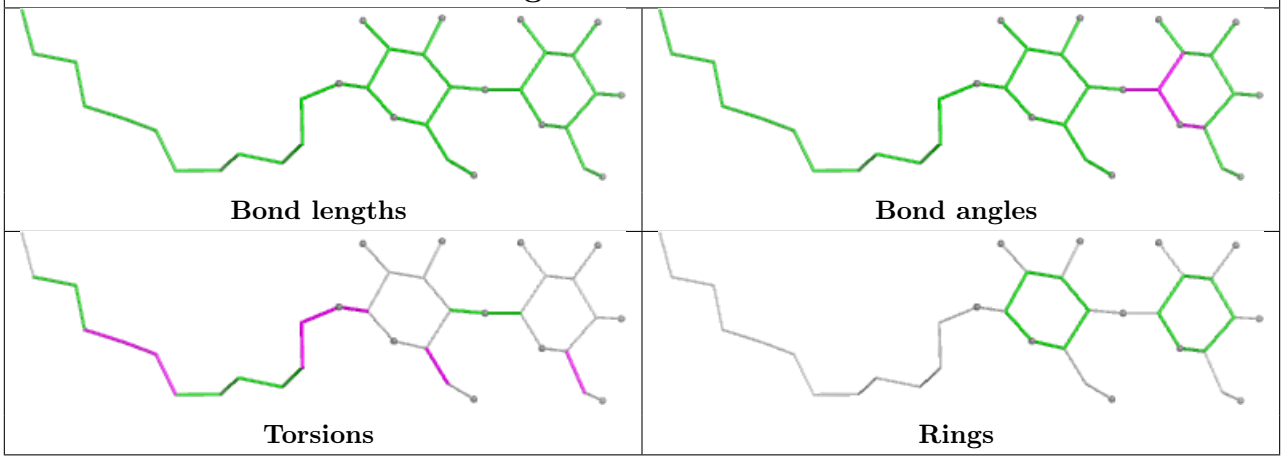
Ligand LHG d 408



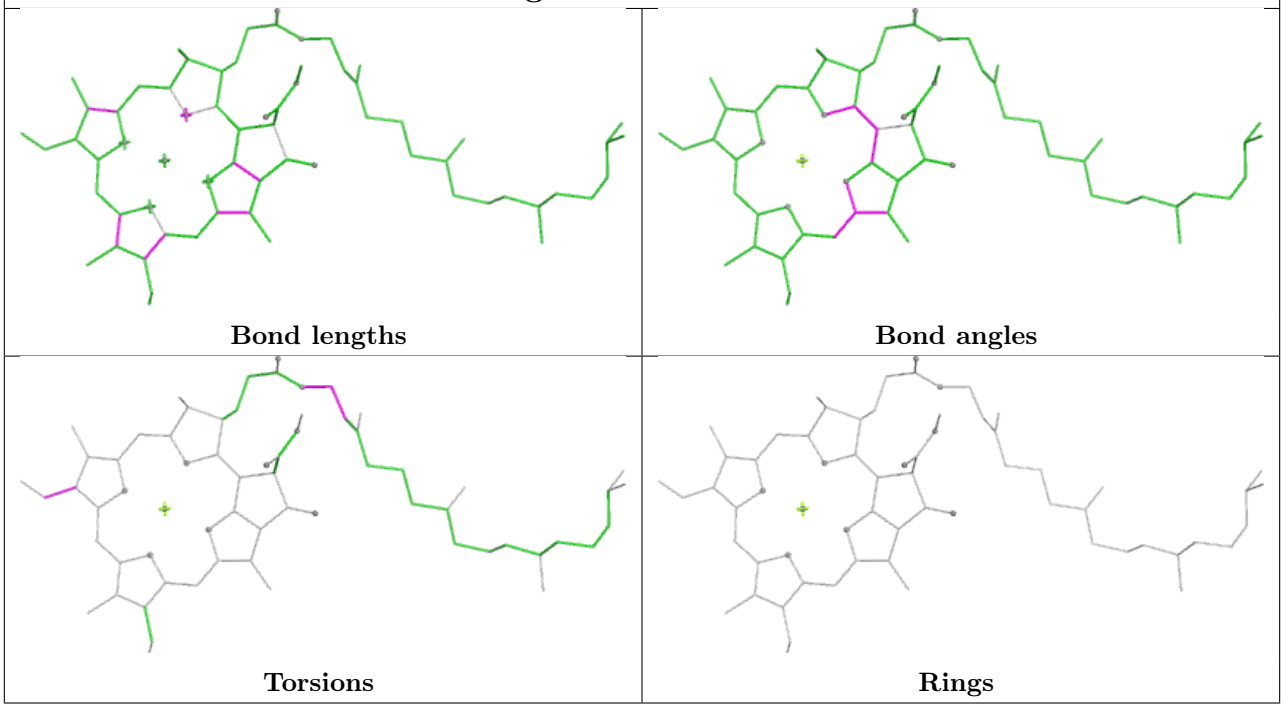
Ligand LHG j 101



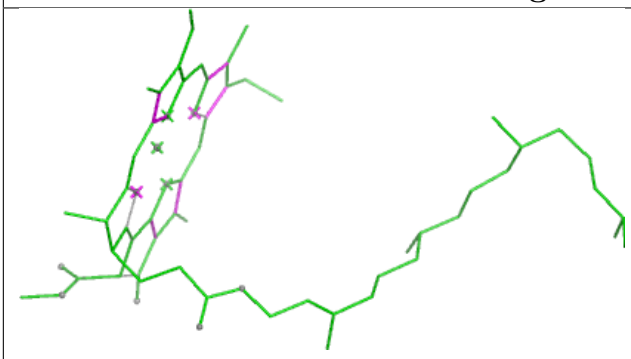
Ligand LMT Z 102



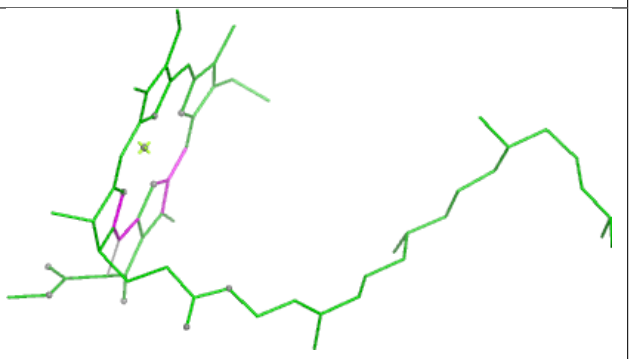
Ligand CLA B 603



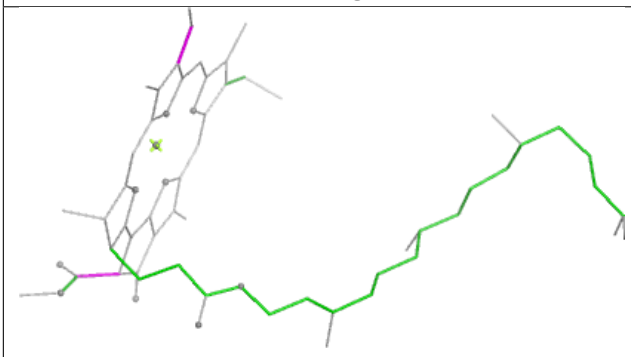
Ligand CLA c 508



Bond lengths



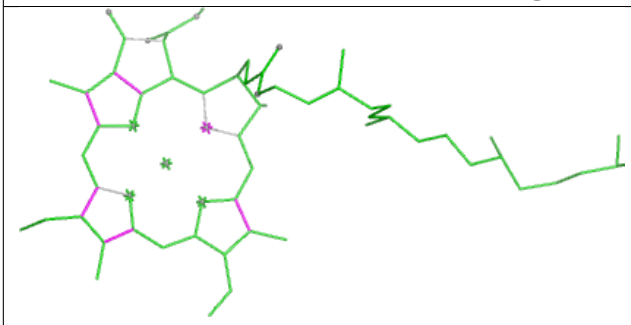
Bond angles



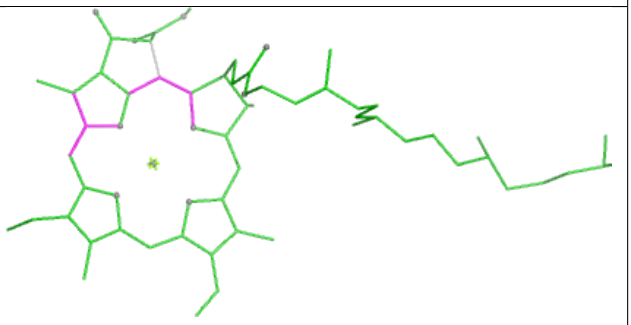
Torsions

Rings

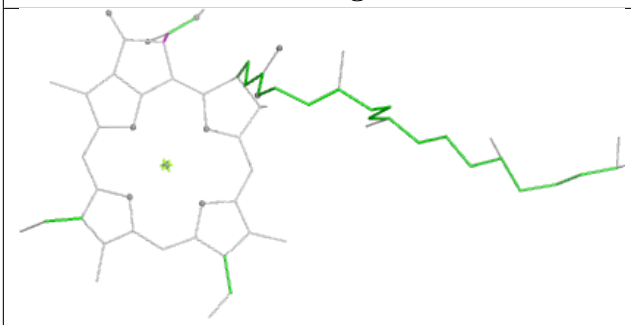
Ligand CLA a 407



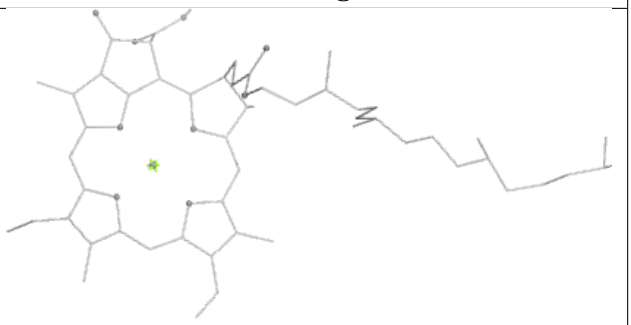
Bond lengths



Bond angles

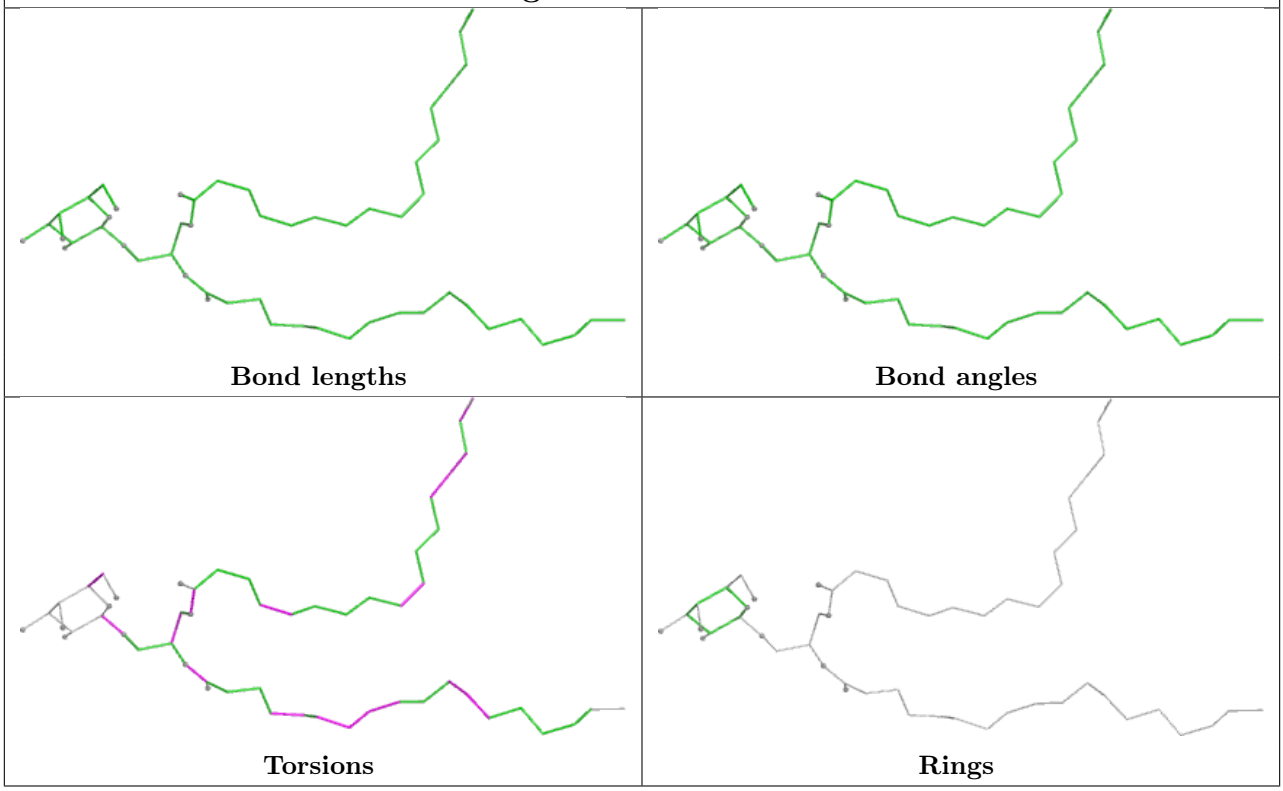


Torsions

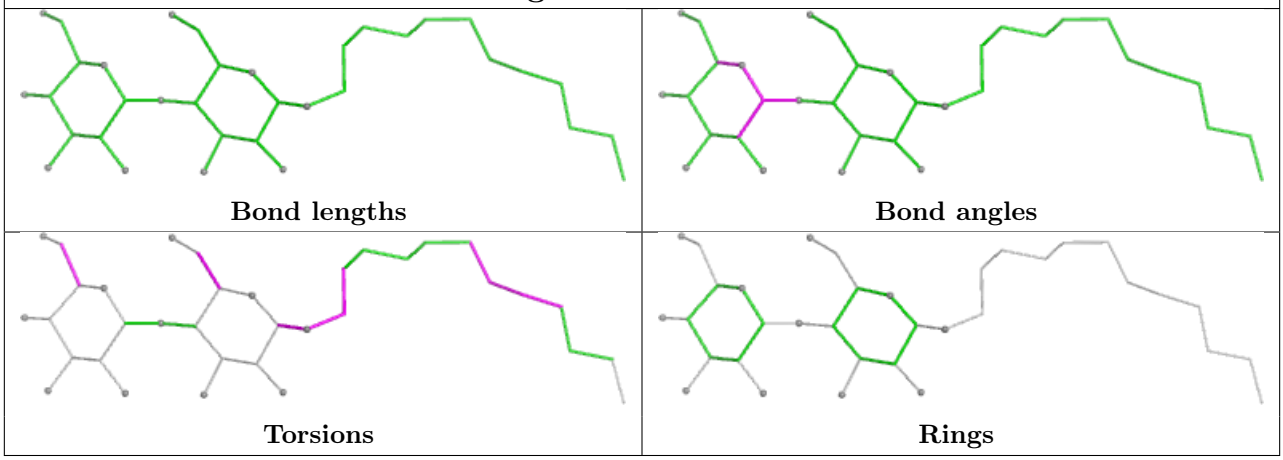


Rings

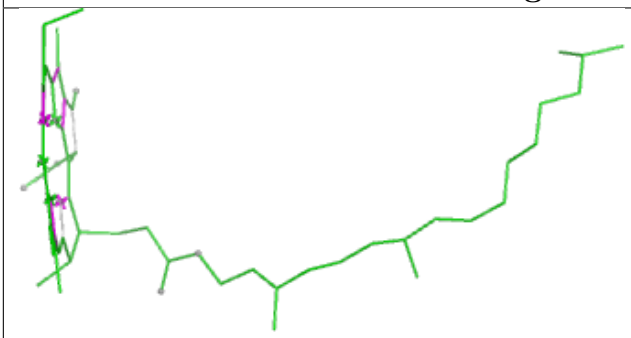
Ligand LMG L 212



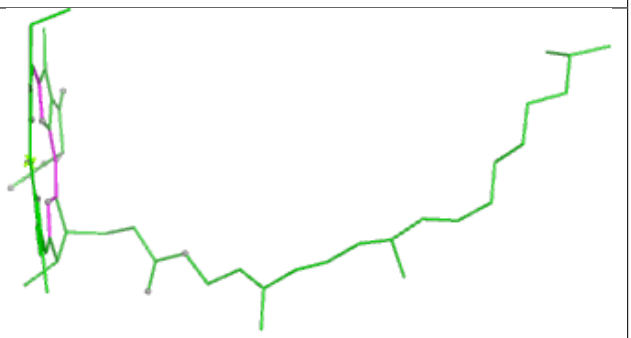
Ligand LMT z 102



Ligand CLA B 607



Bond lengths

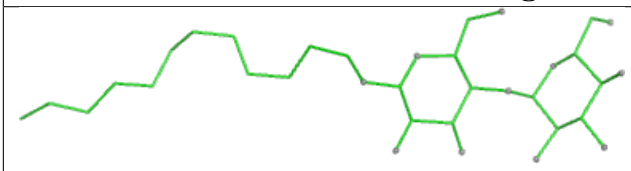


Bond angles

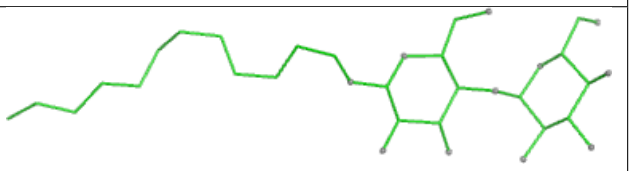
Torsions

Rings

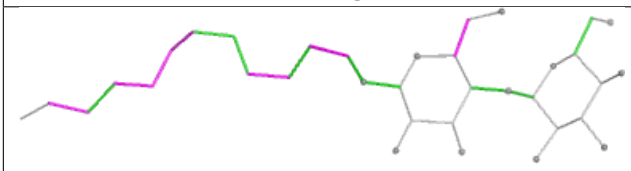
Ligand LMT G 104



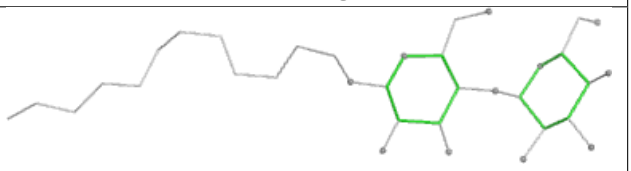
Bond lengths



Bond angles

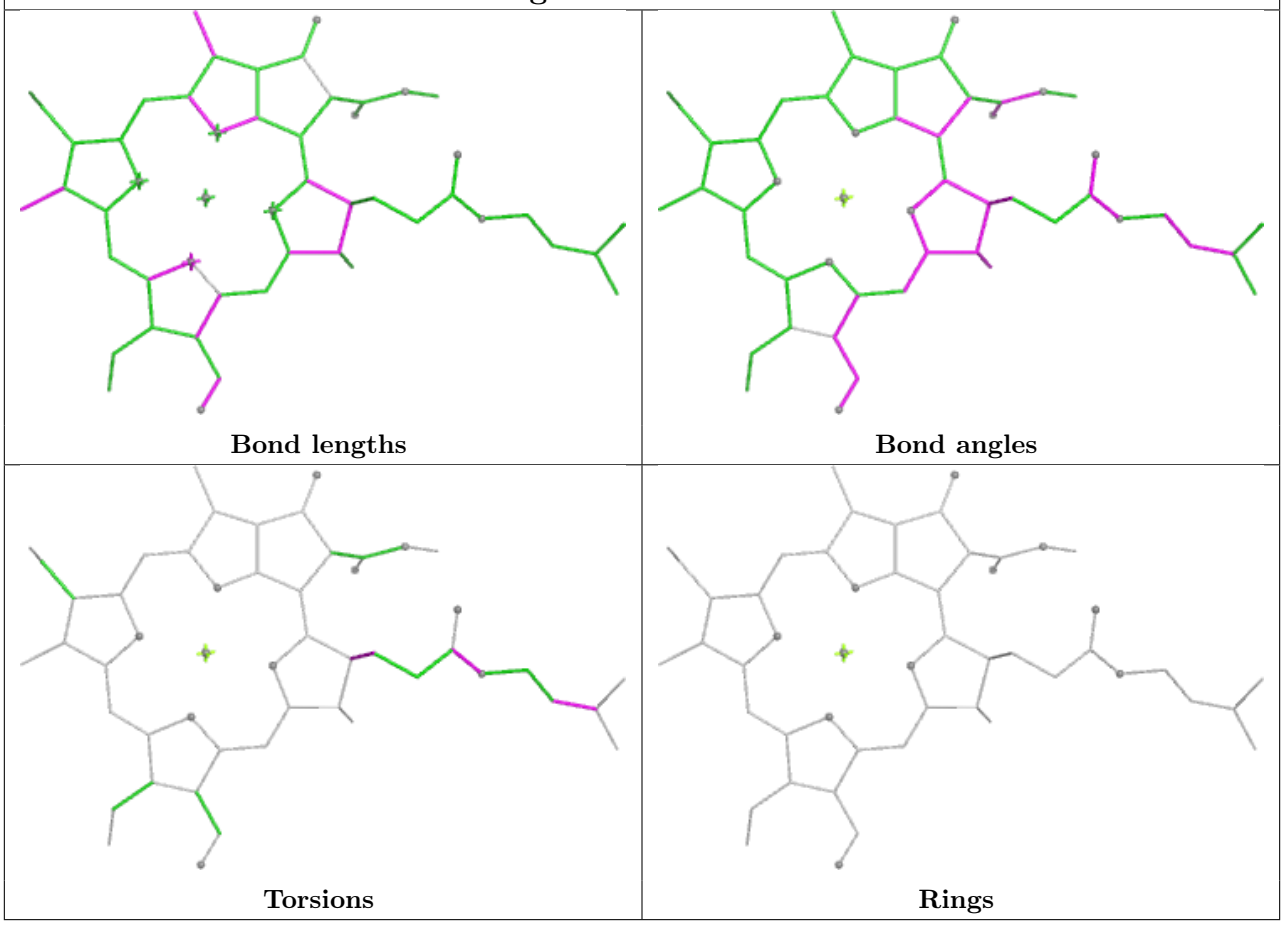


Torsions

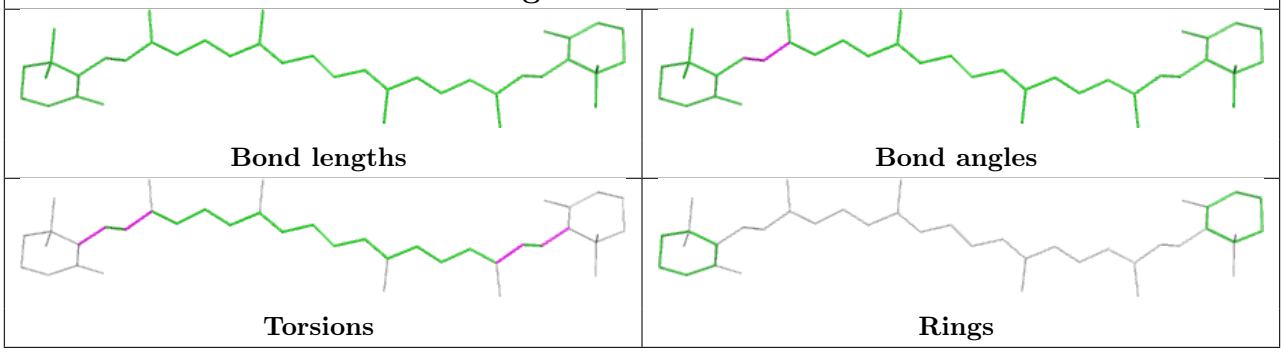


Rings

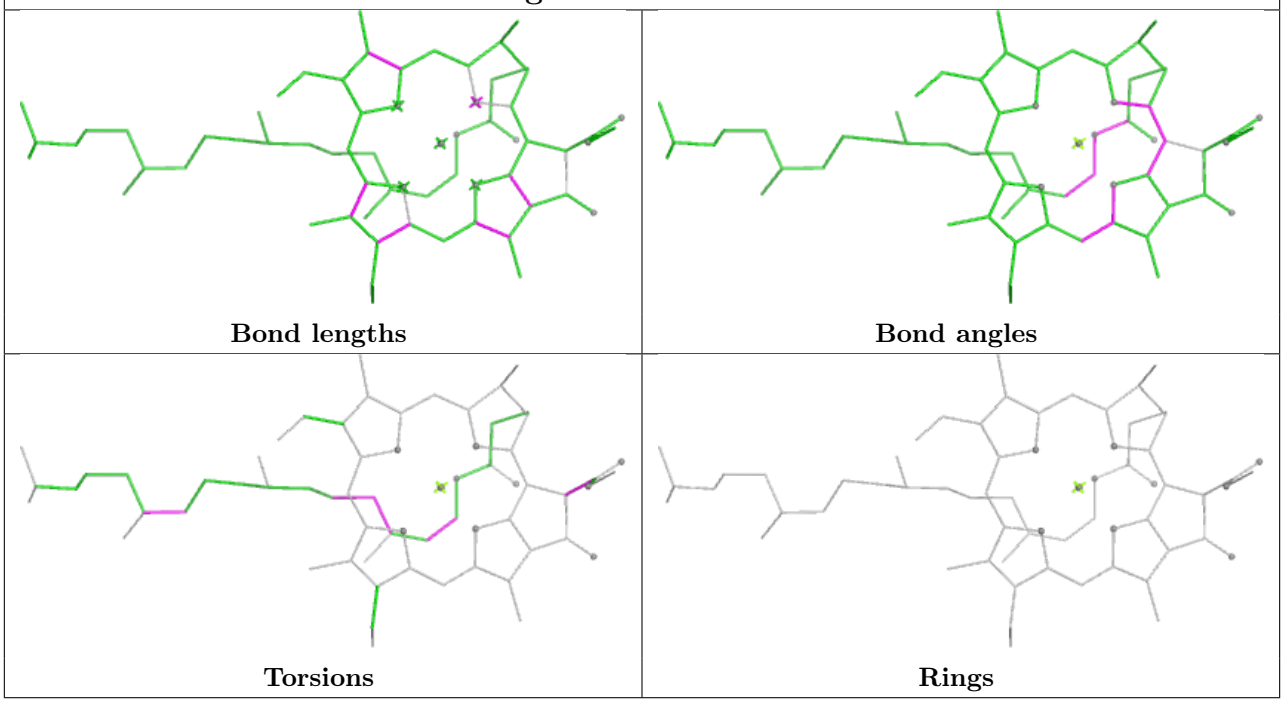
Ligand F6C B 617



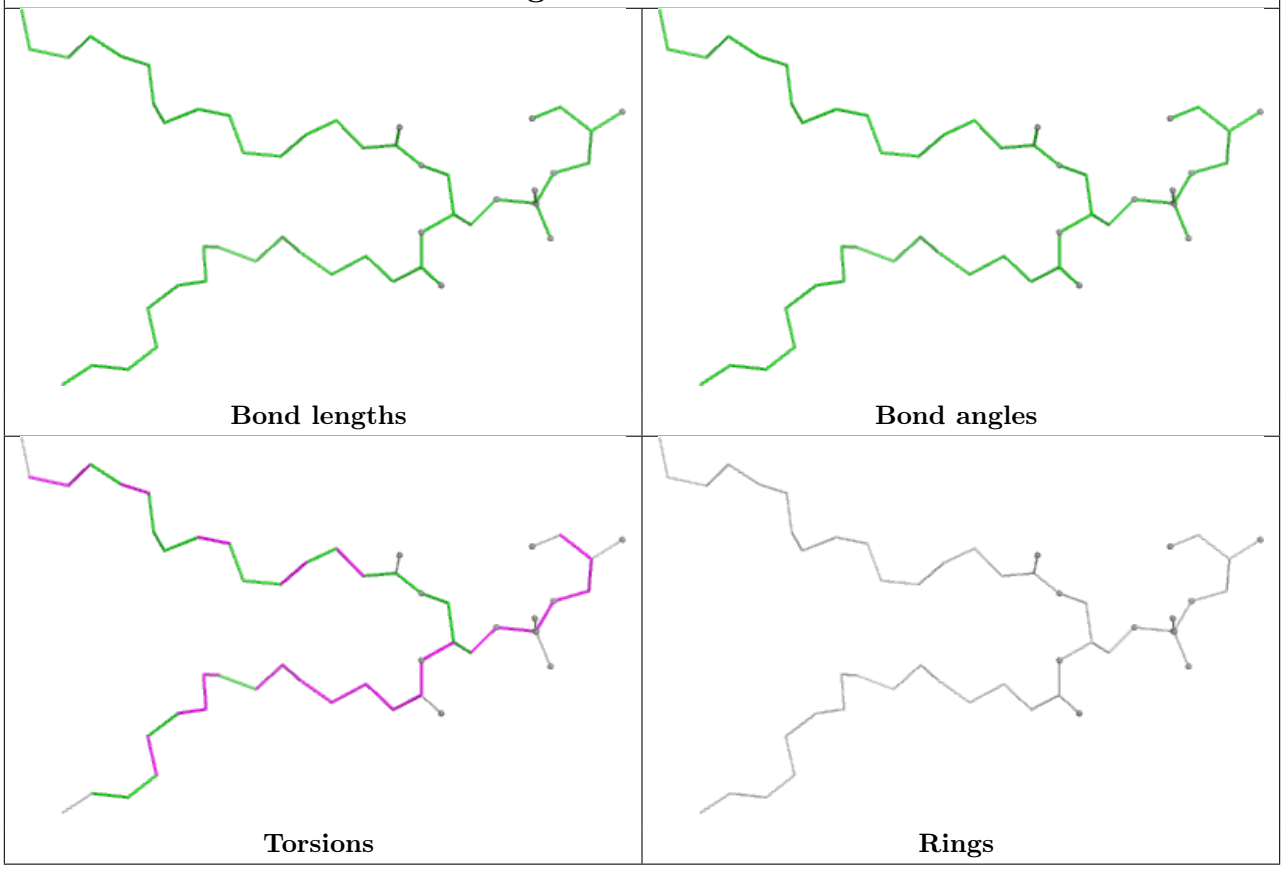
Ligand BCR D 404

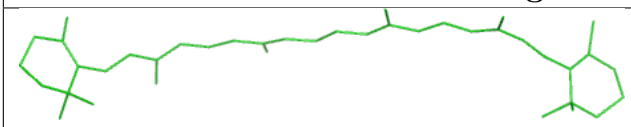
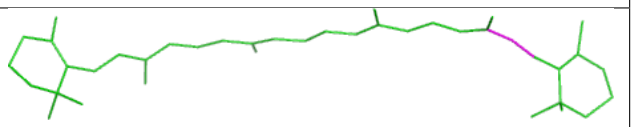
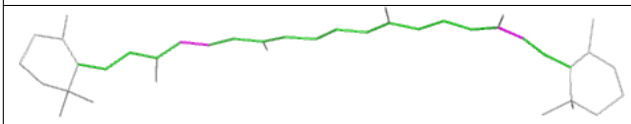
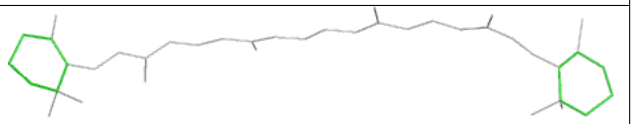


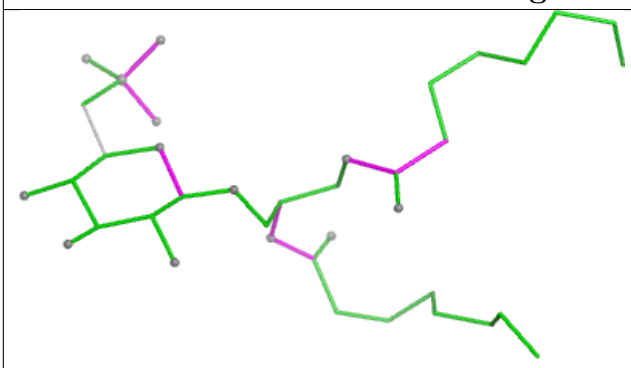
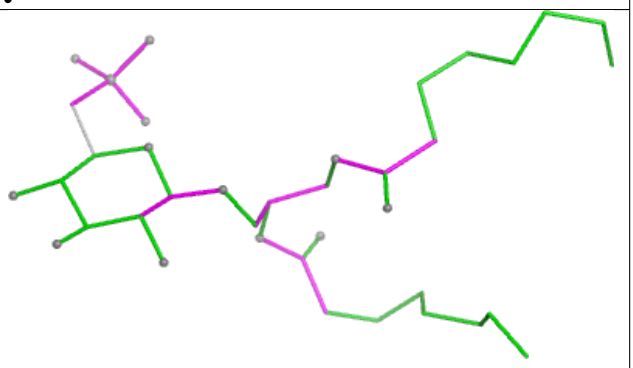
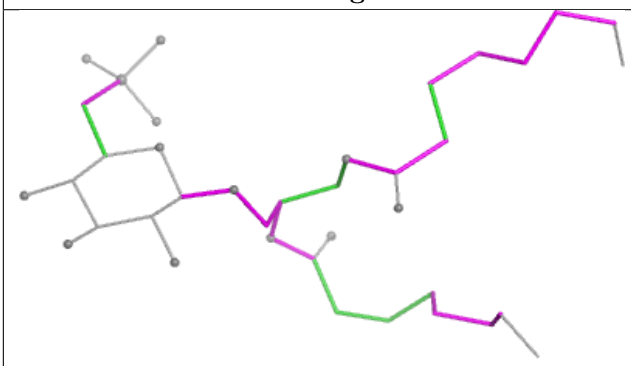
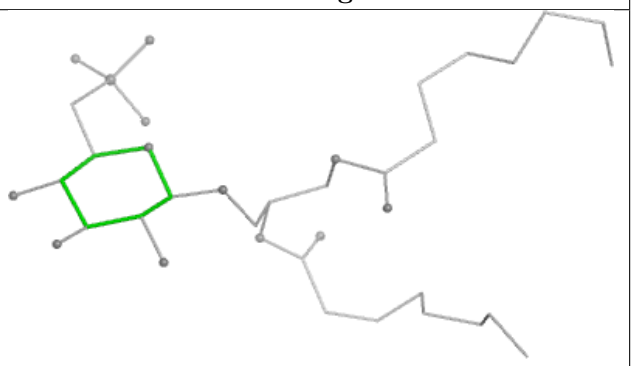
Ligand CLA B 606



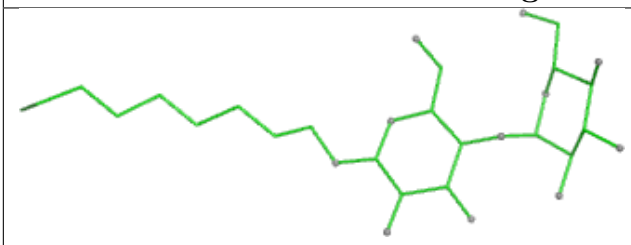
Ligand LHG J 101



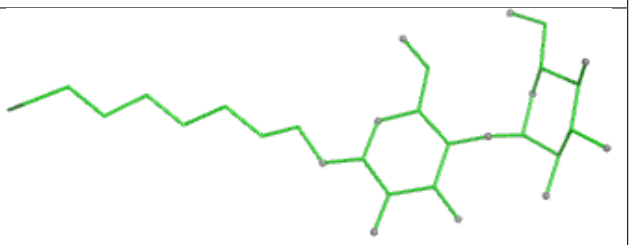
Ligand BCR k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD c 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

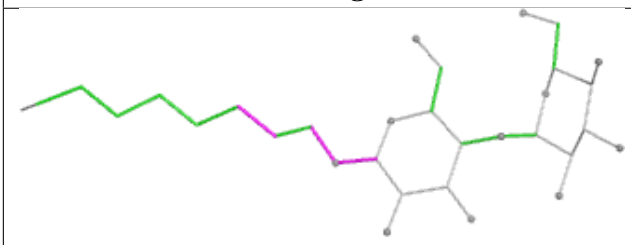
Ligand LMT C 904



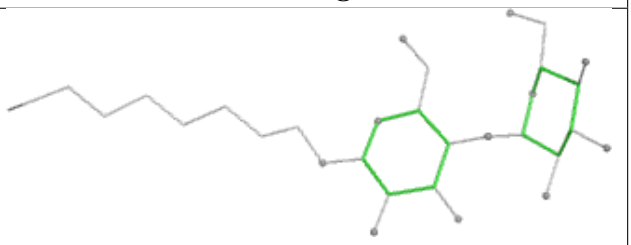
Bond lengths



Bond angles

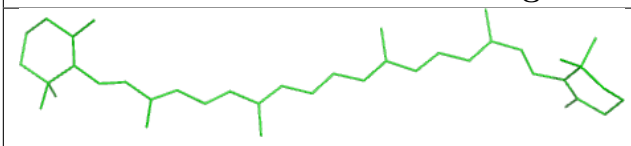


Torsions

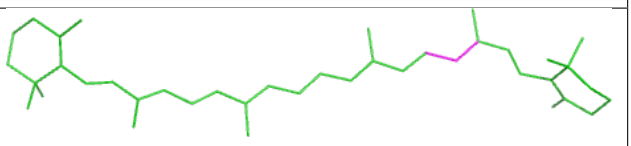


Rings

Ligand BCR B 618

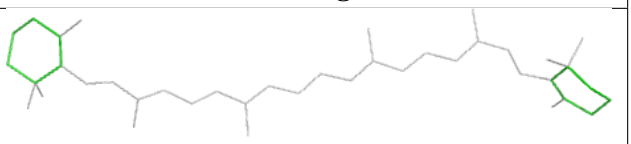


Bond lengths



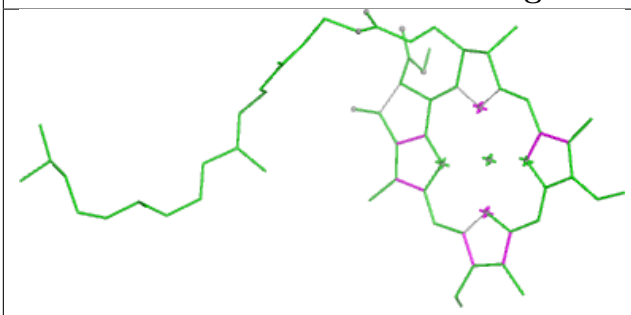
Bond angles

Torsions

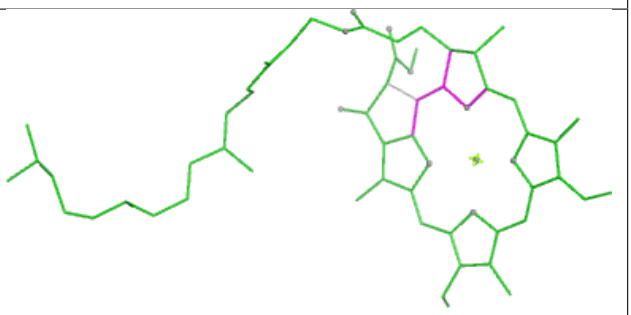


Rings

Ligand CLA B 605

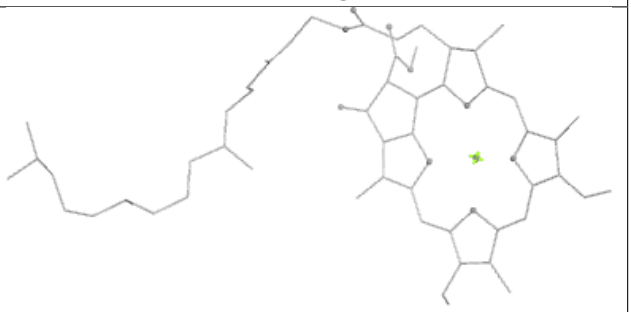


Bond lengths

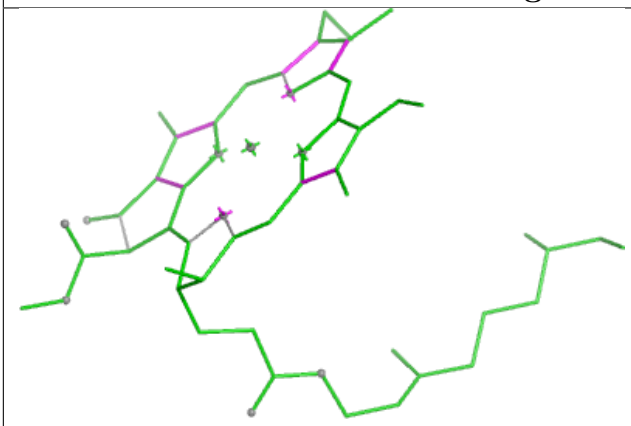
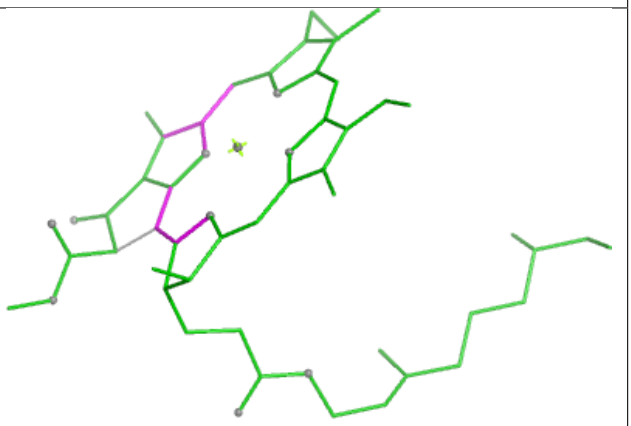
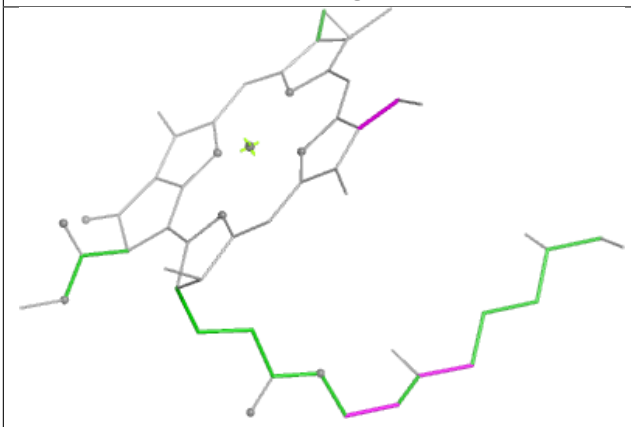
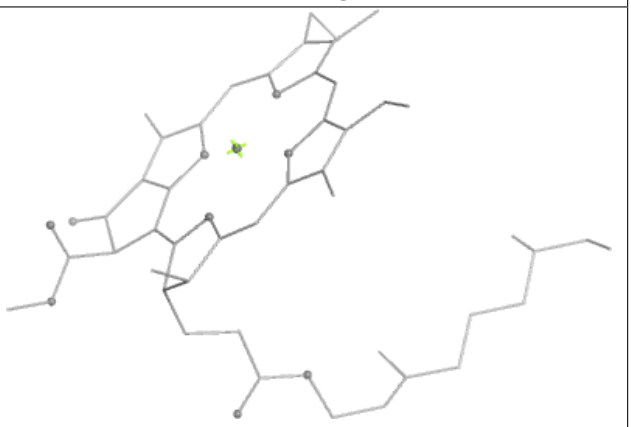


Bond angles

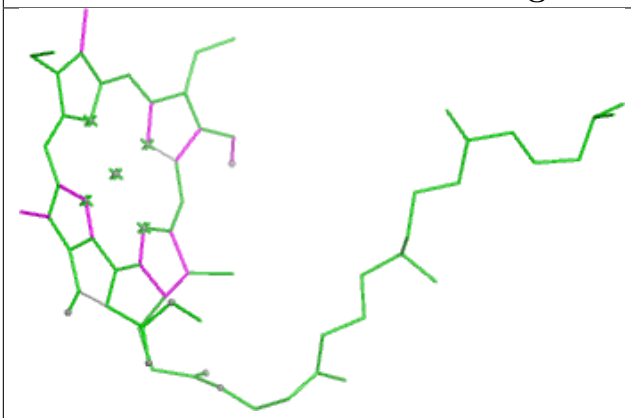
Torsions



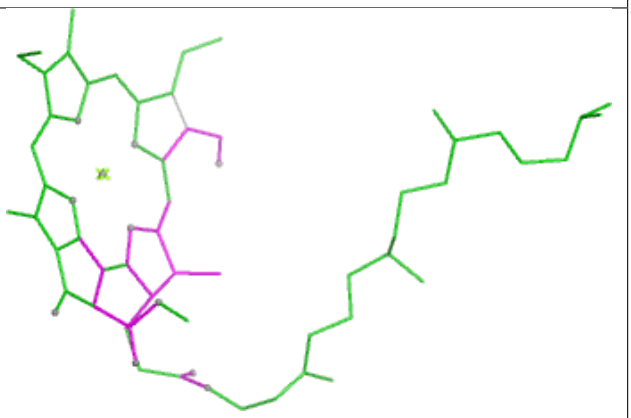
Rings

Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

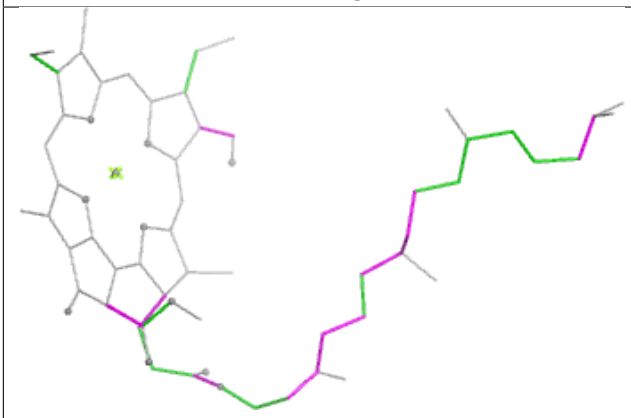
Ligand F6C C 507



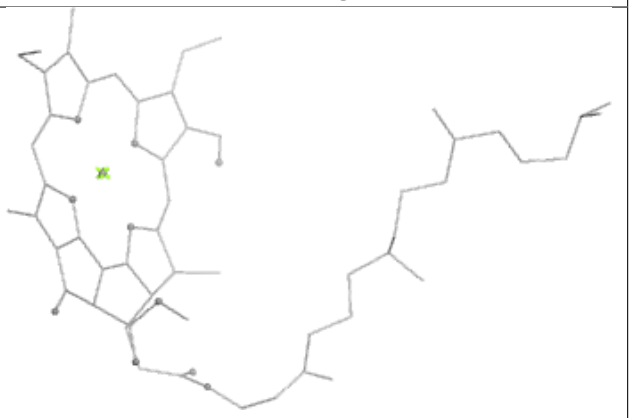
Bond lengths



Bond angles

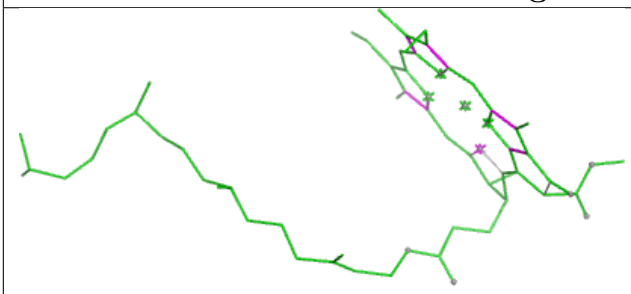


Torsions

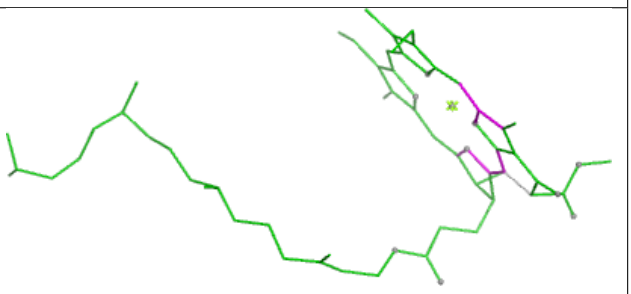


Rings

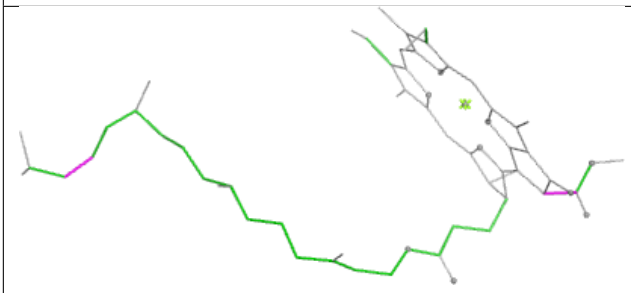
Ligand CLA c 504



Bond lengths

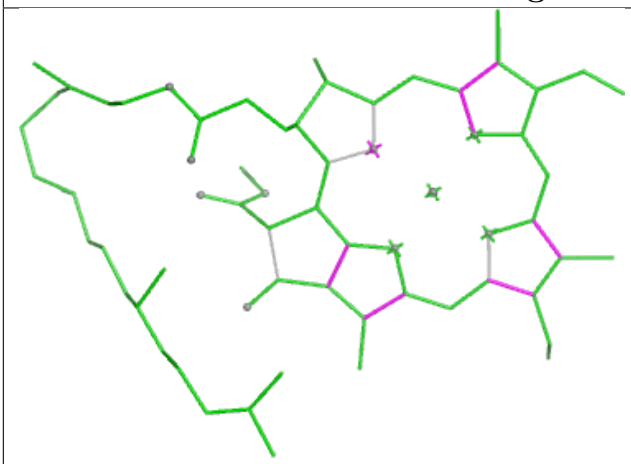
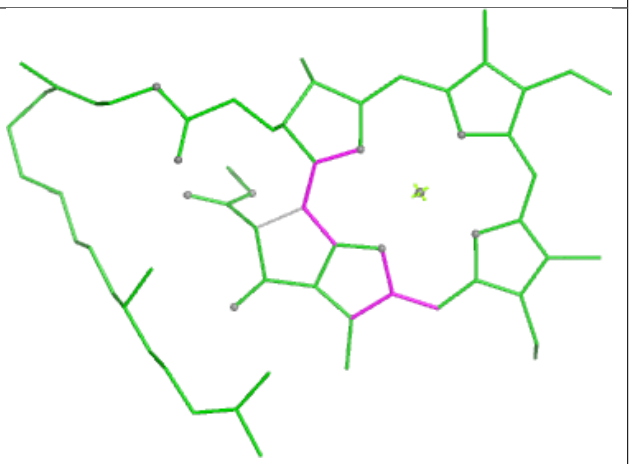
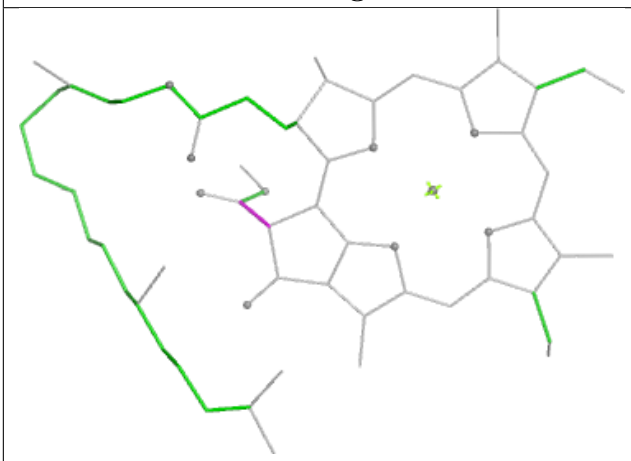
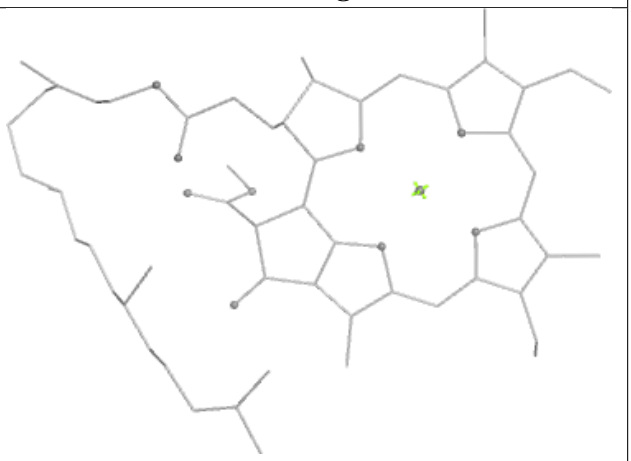


Bond angles

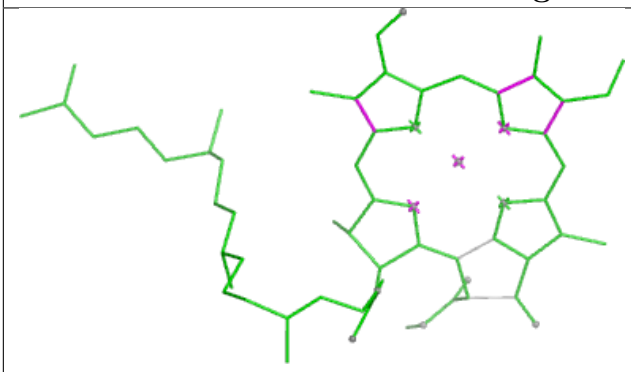


Torsions

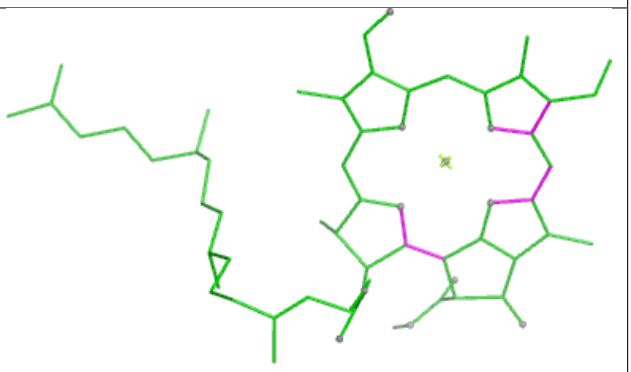
Rings

Ligand CLA b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

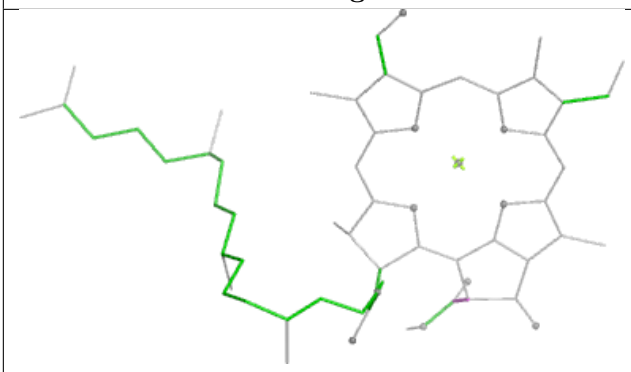
Ligand CL7 a 406



Bond lengths



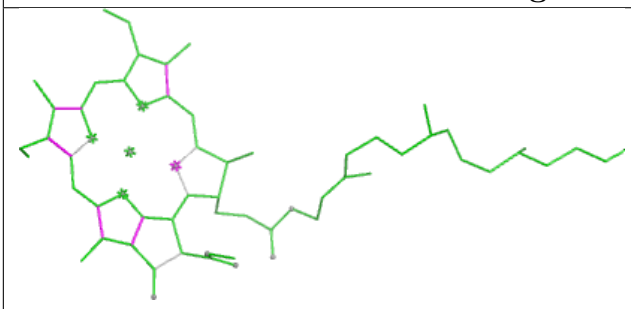
Bond angles



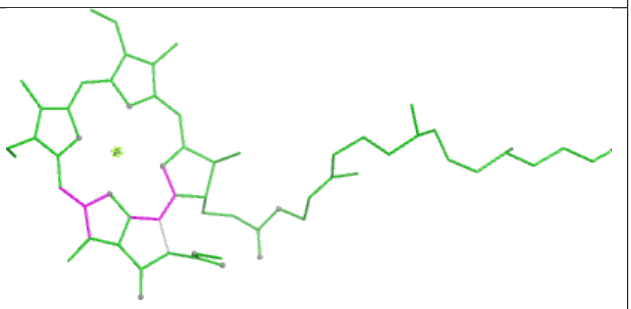
Torsions

Rings

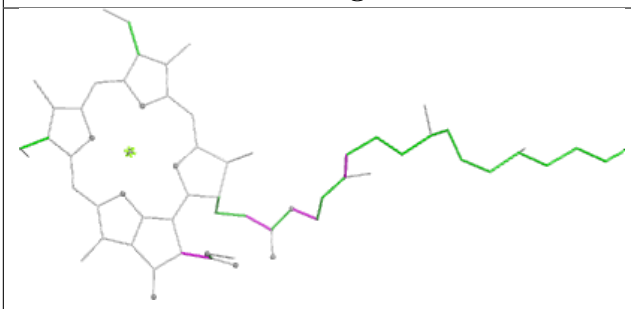
Ligand CLA c 512



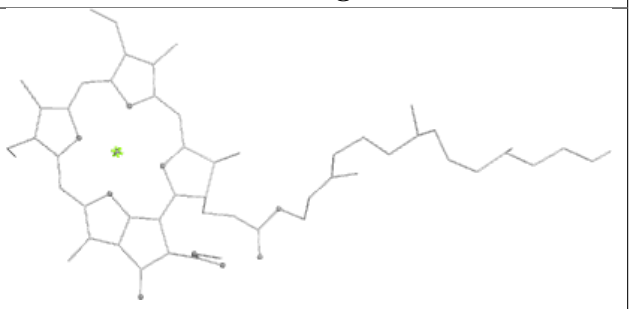
Bond lengths



Bond angles

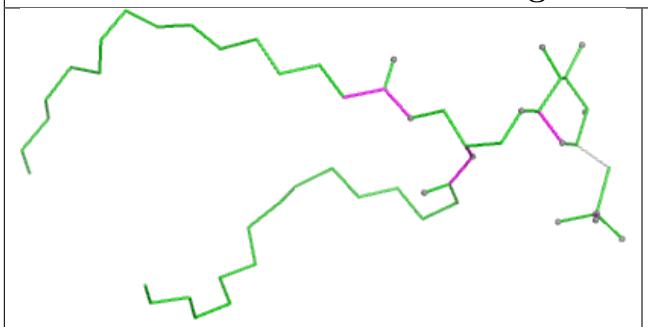


Torsions

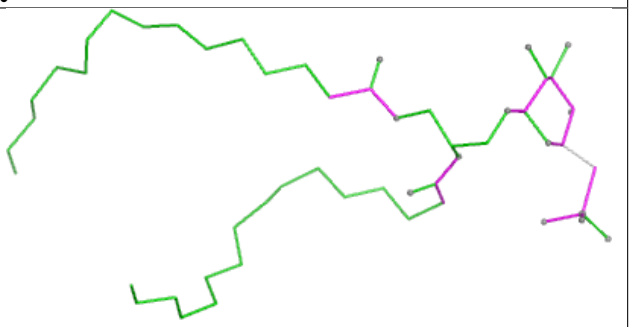


Rings

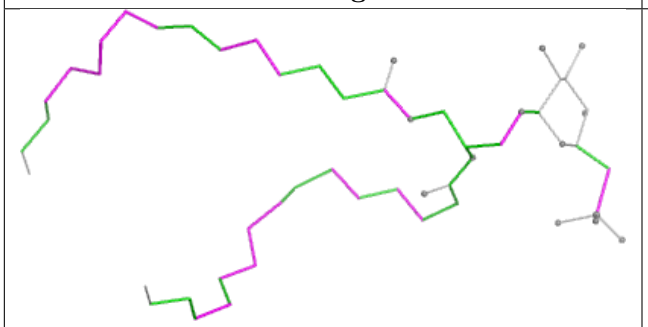
Ligand SQD b 622



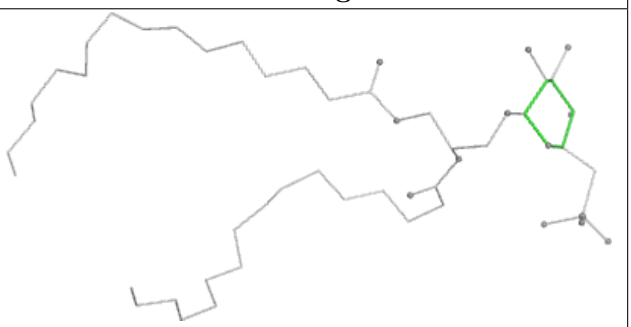
Bond lengths



Bond angles

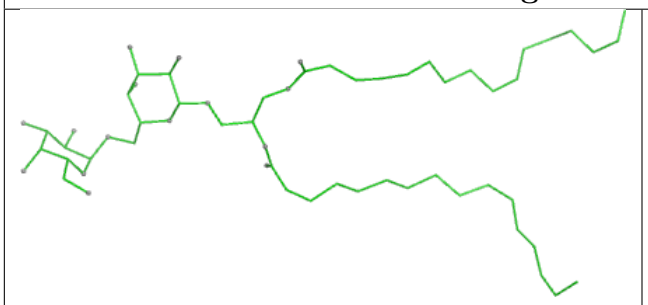


Torsions

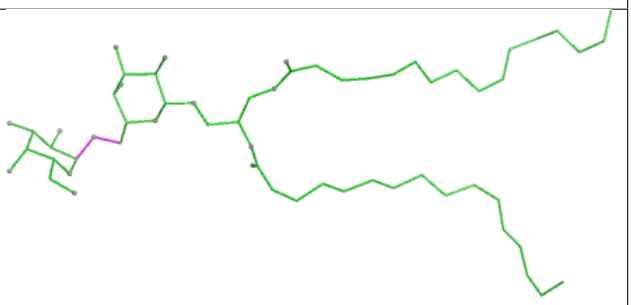


Rings

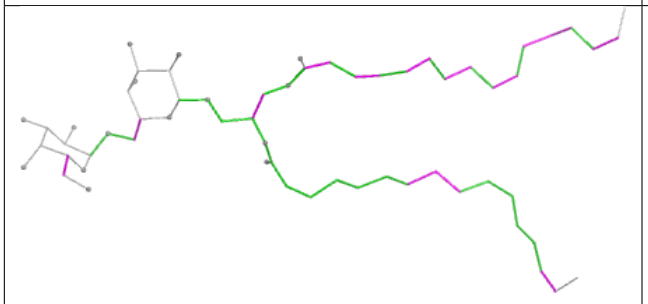
Ligand DGD C 518



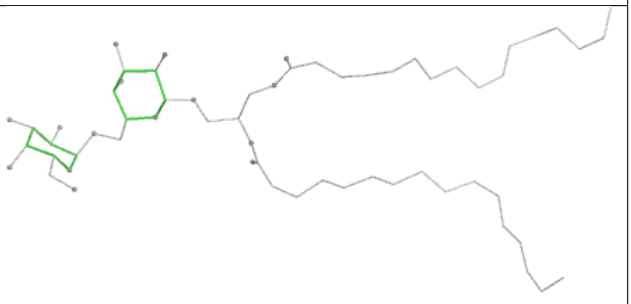
Bond lengths



Bond angles

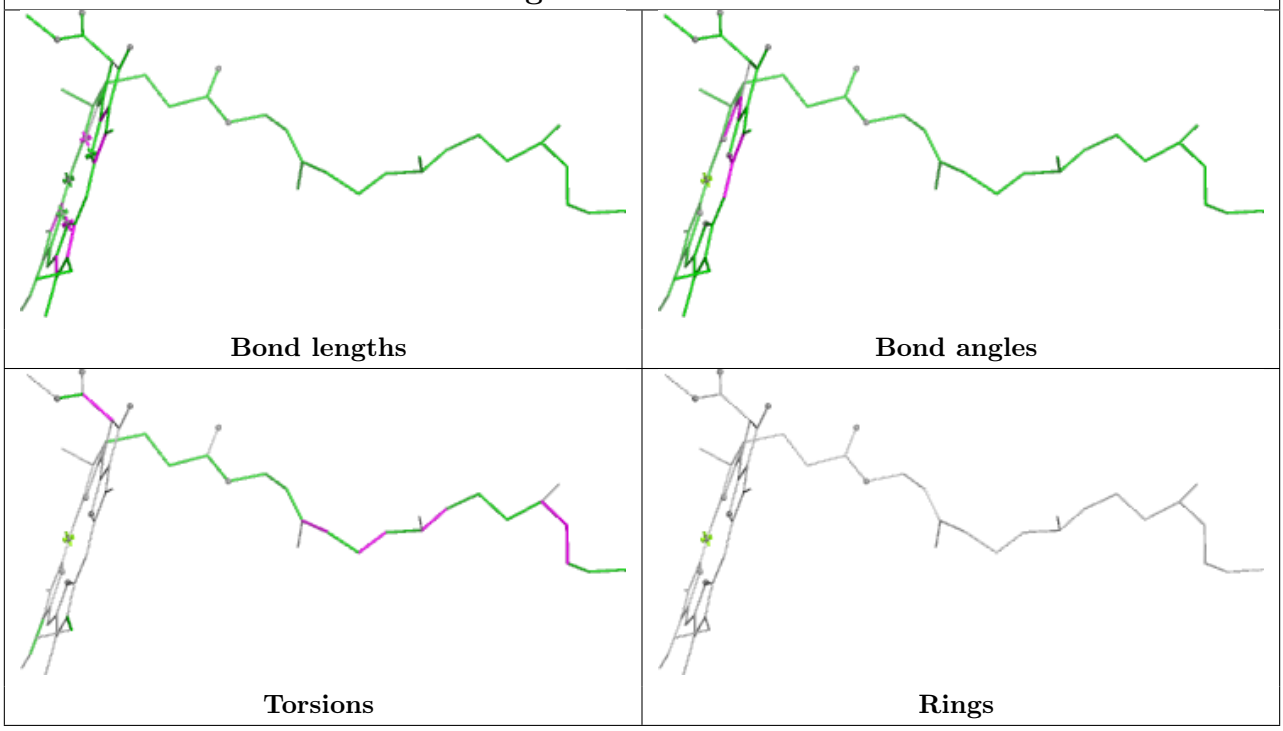


Torsions

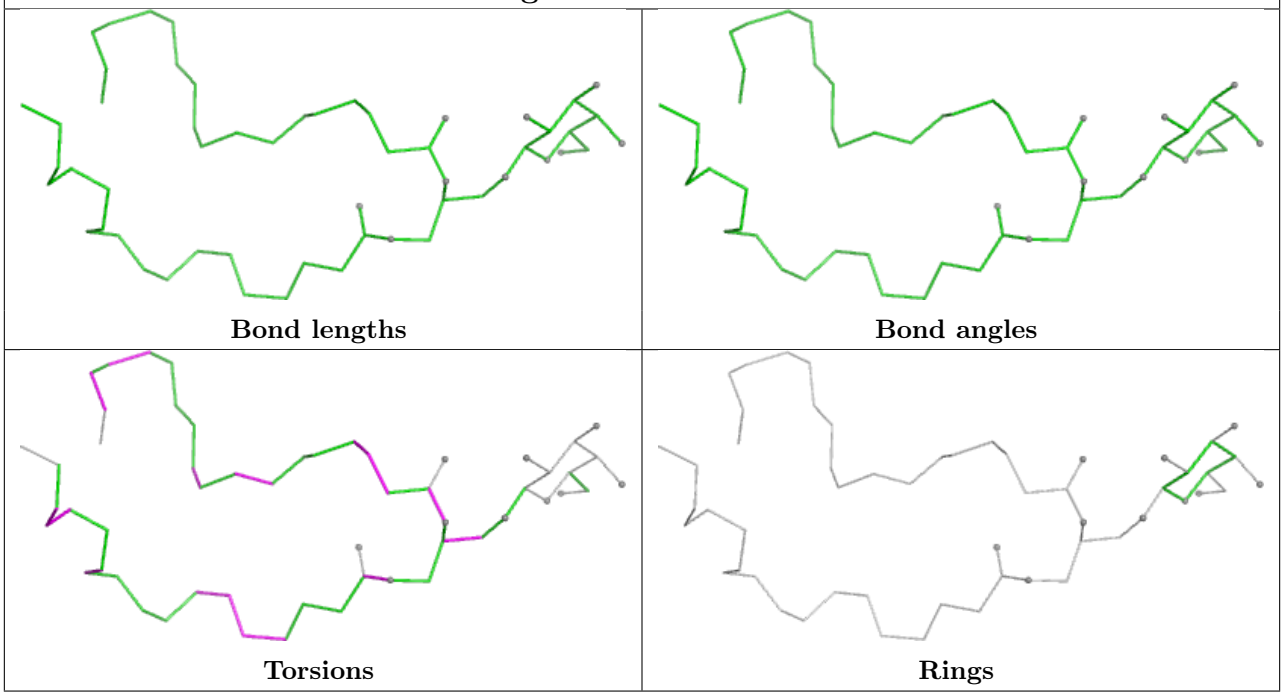


Rings

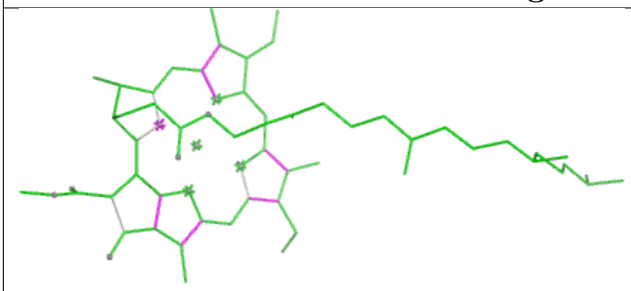
Ligand CLA C 502



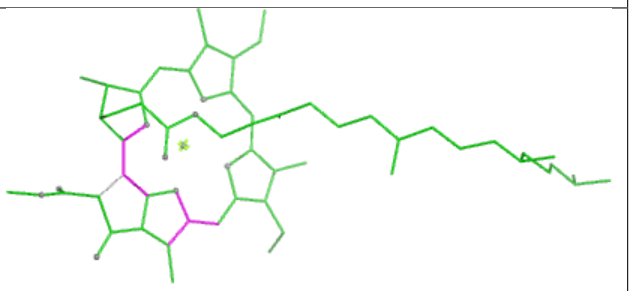
Ligand LMG B 628



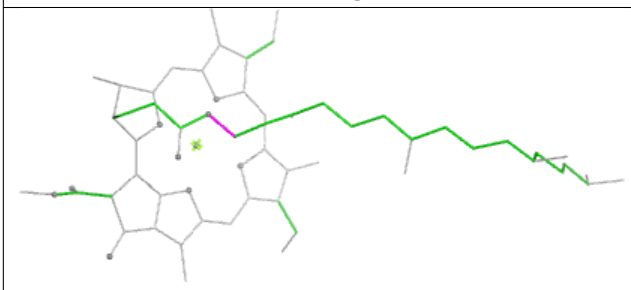
Ligand CLA b 609



Bond lengths



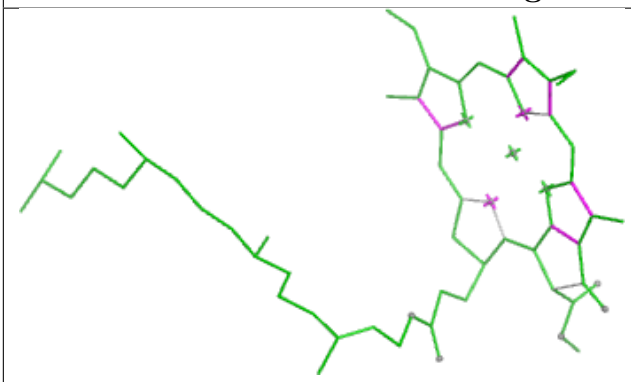
Bond angles



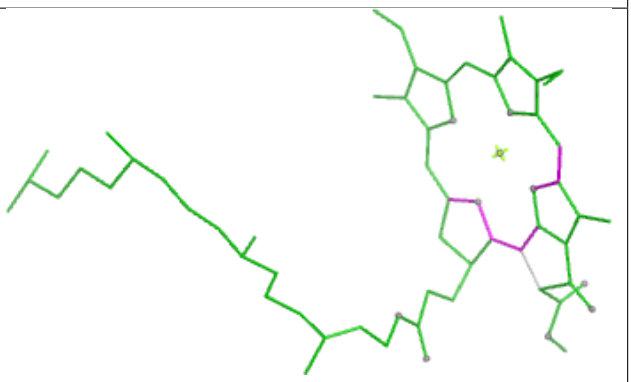
Torsions

Rings

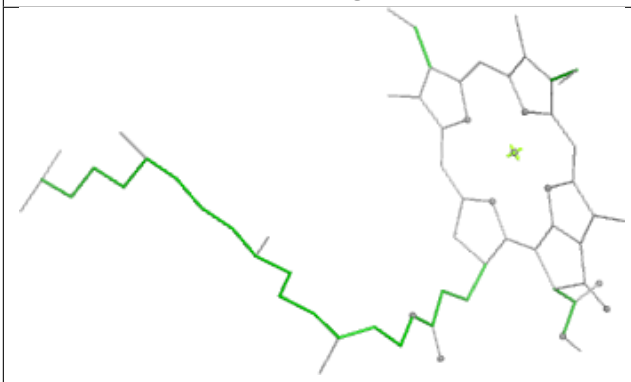
Ligand CLA C 511



Bond lengths



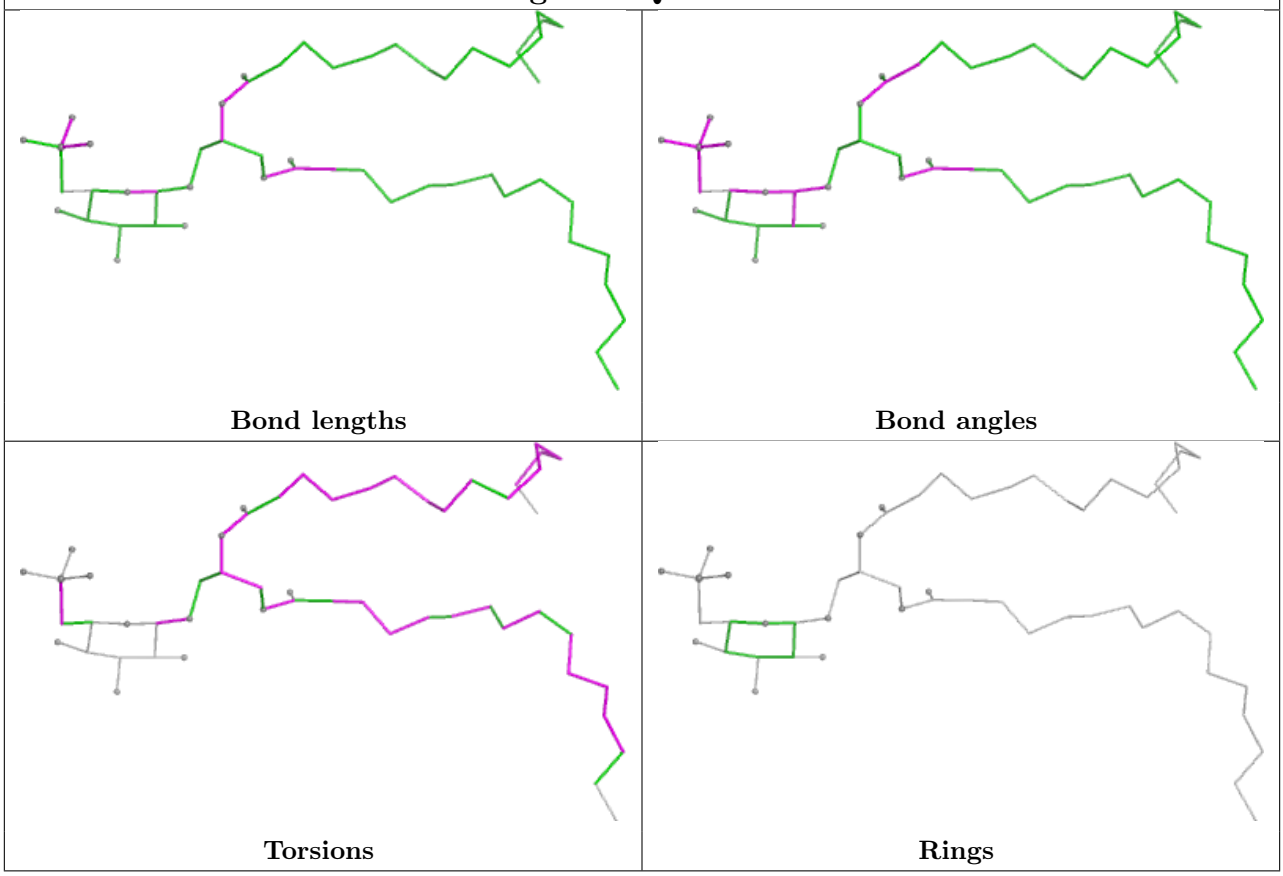
Bond angles



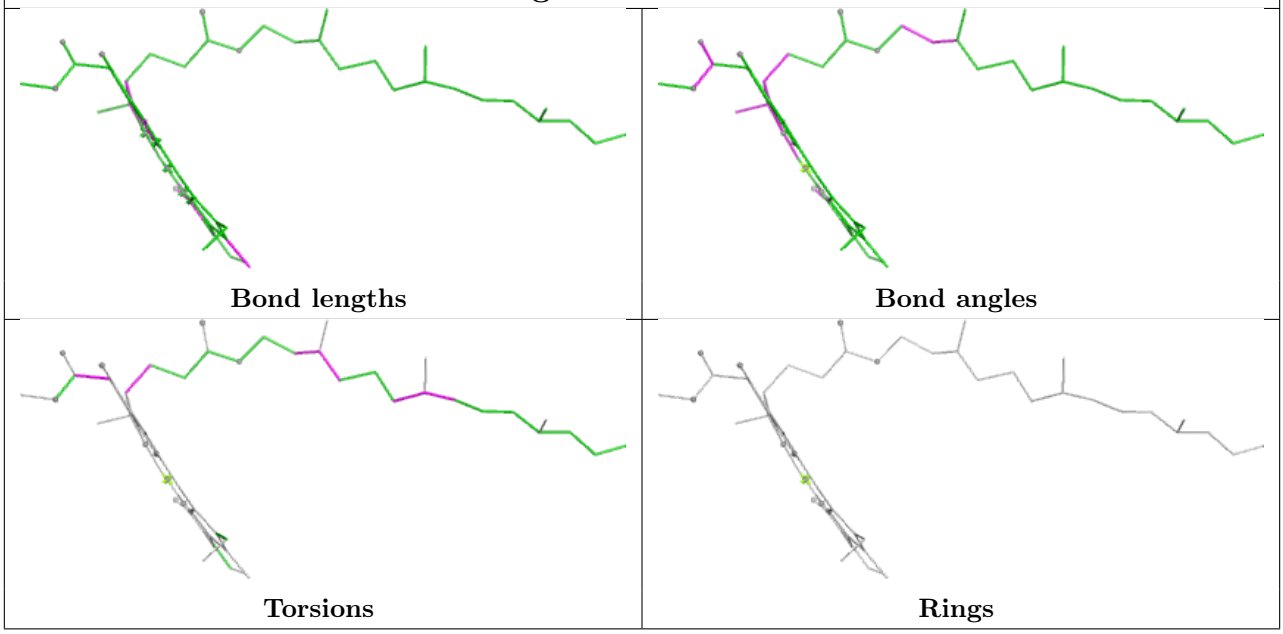
Torsions

Rings

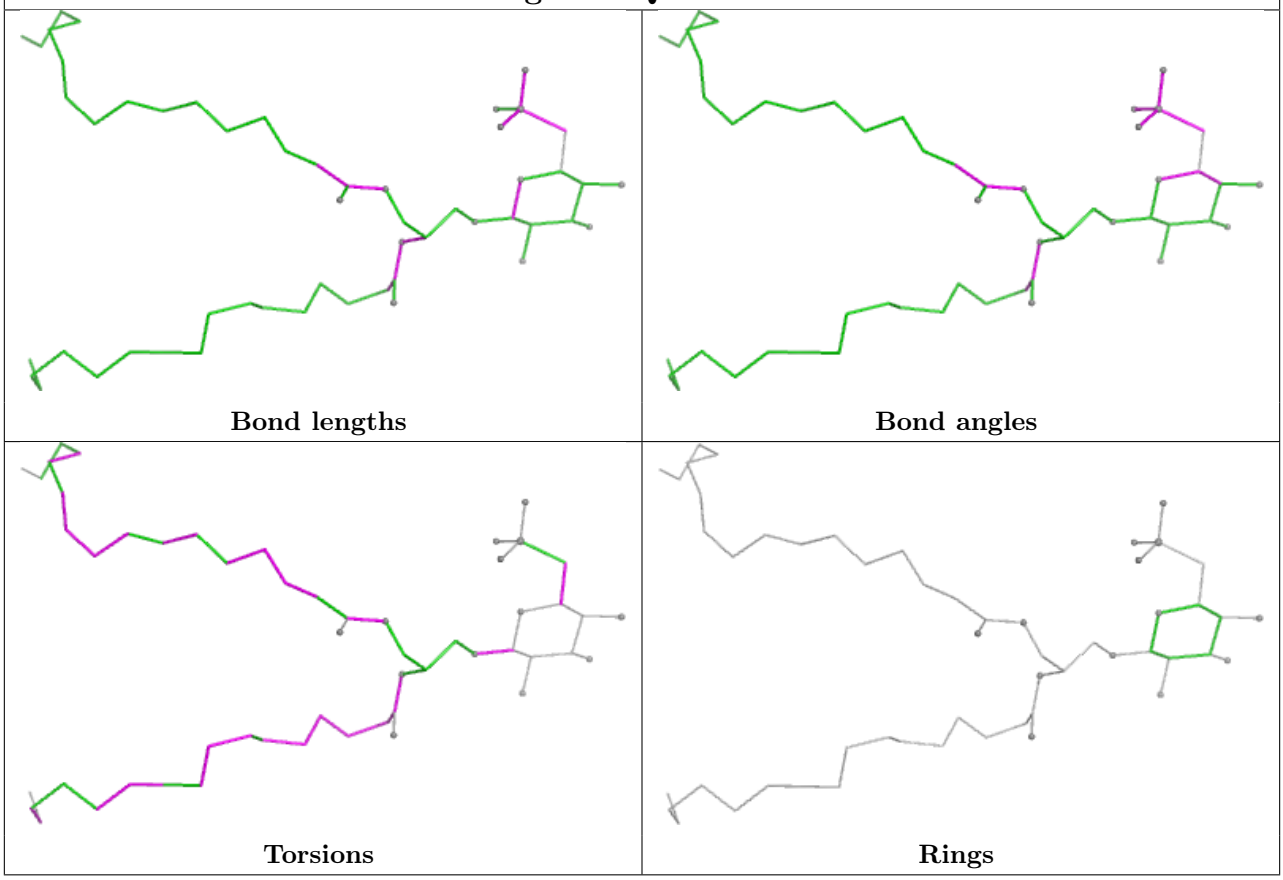
Ligand SQD a 417



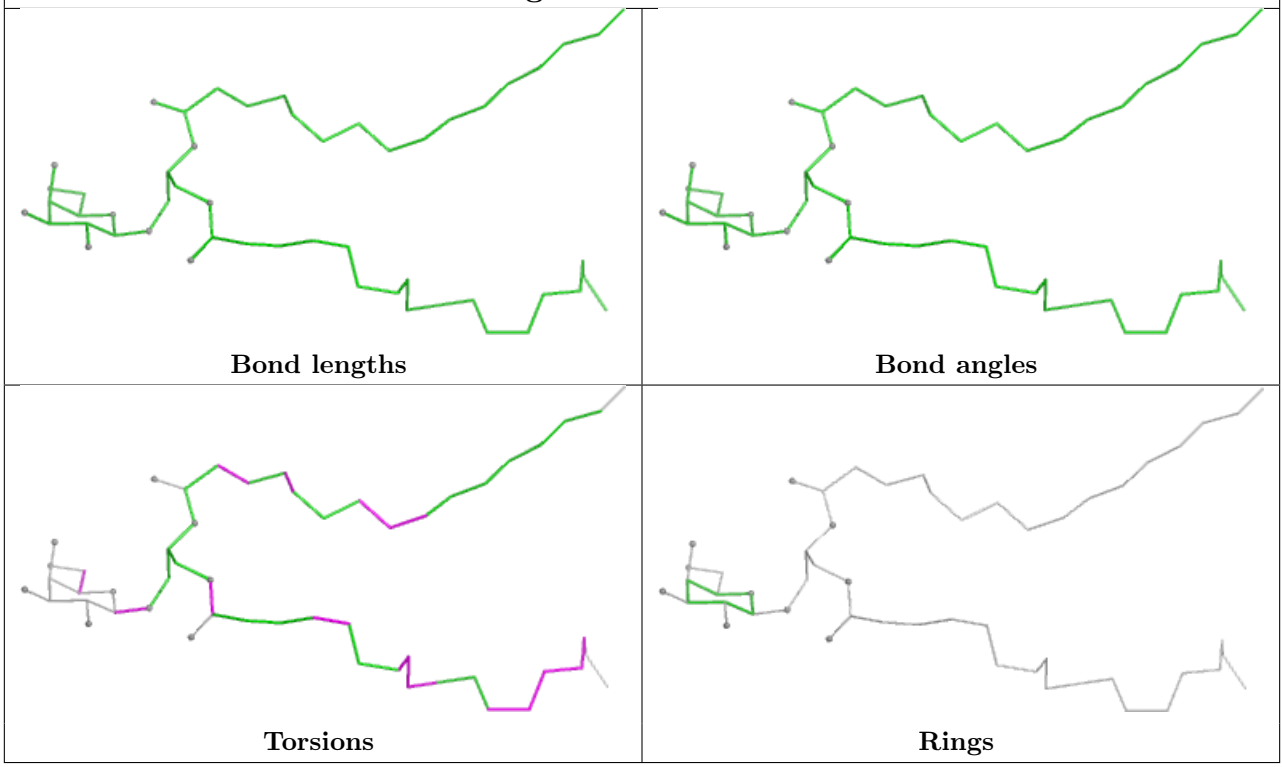
Ligand F6C b 608



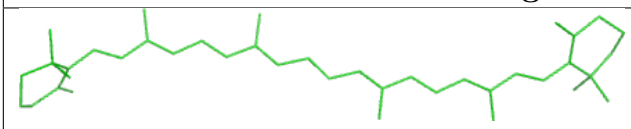
Ligand SQD A 412



Ligand LMG c 902

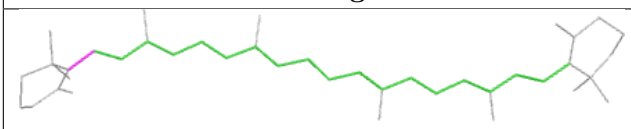


Ligand BCR A 411

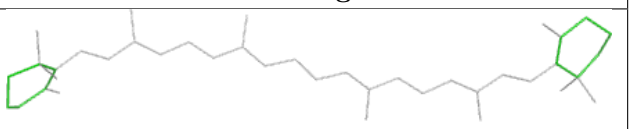


Bond lengths

Bond angles



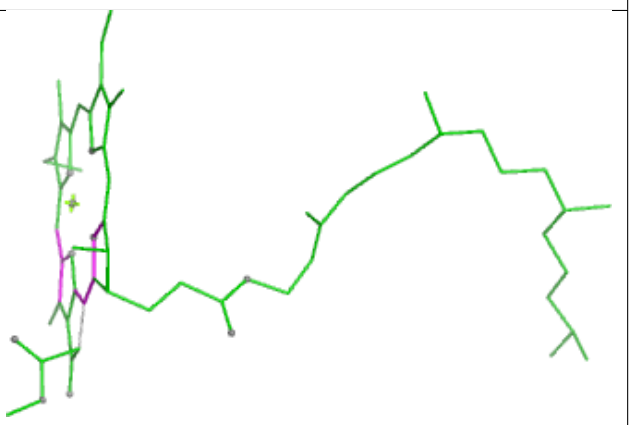
Torsions



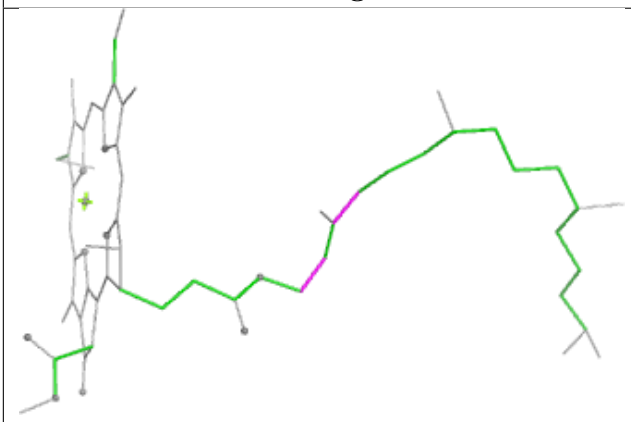
Rings

Ligand CLA d 403

Bond lengths



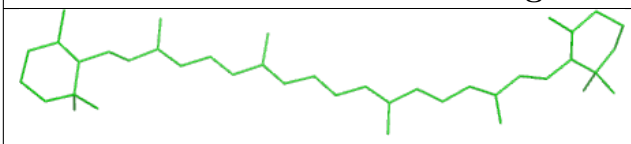
Bond angles



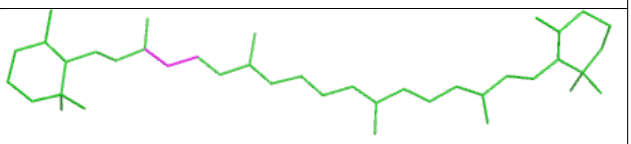
Torsions

Rings

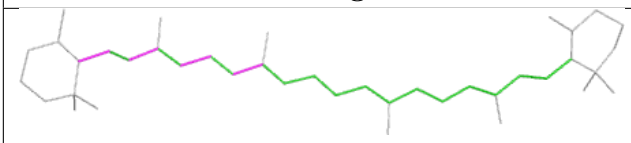
Ligand BCR b 619



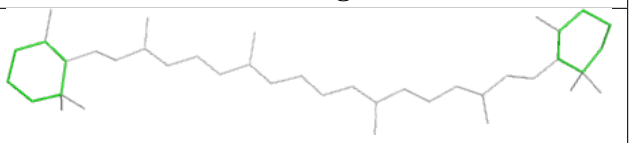
Bond lengths



Bond angles

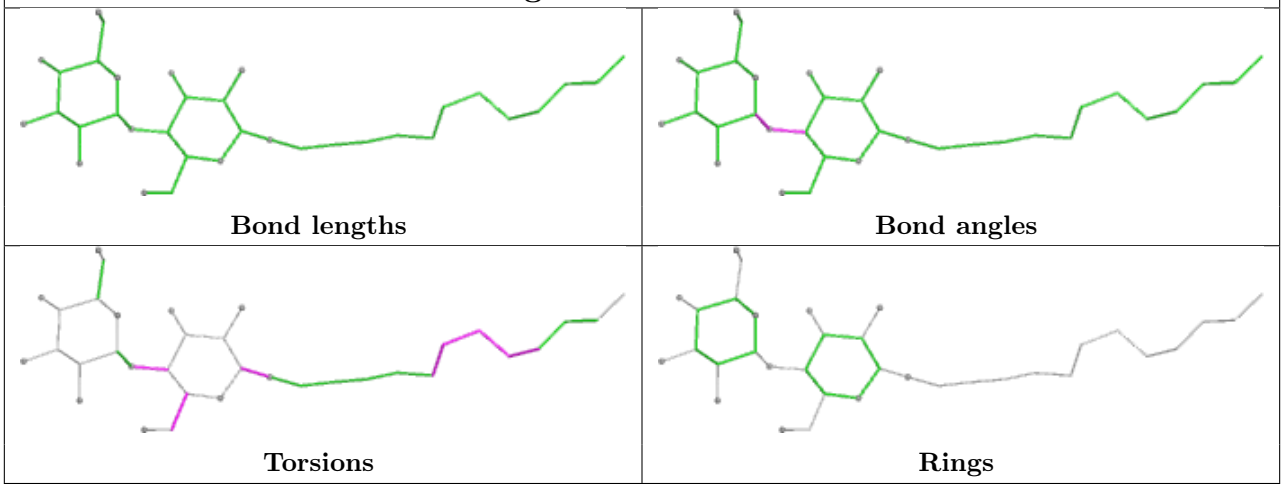


Torsions

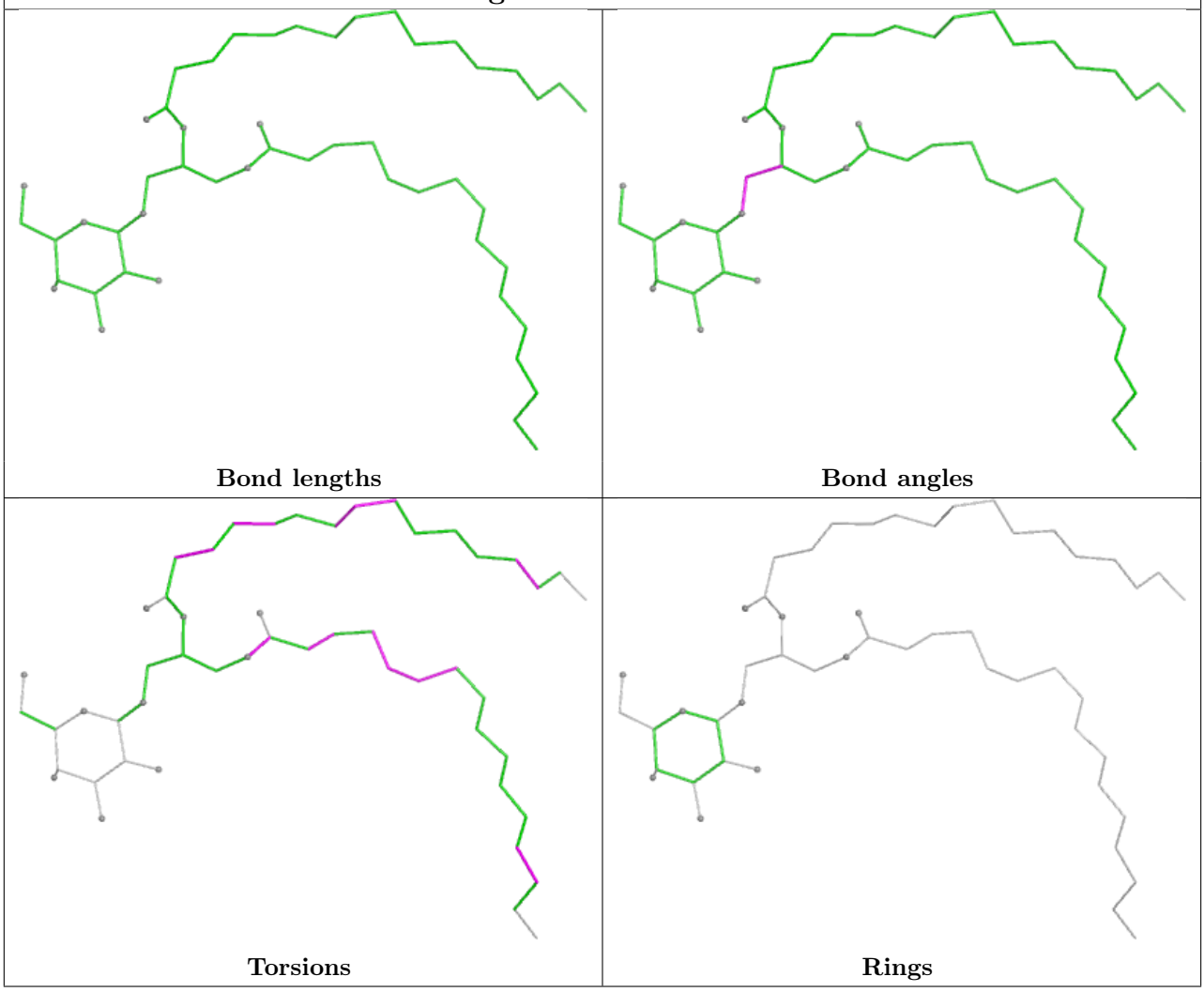


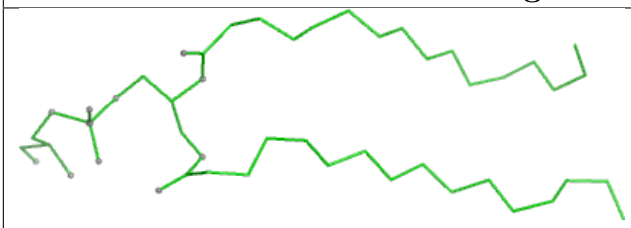
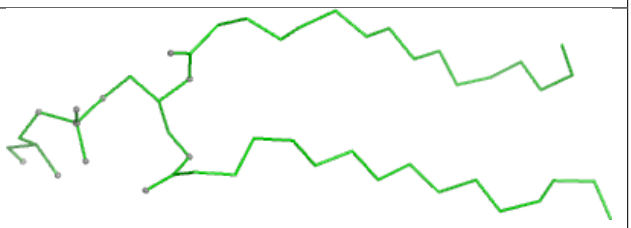
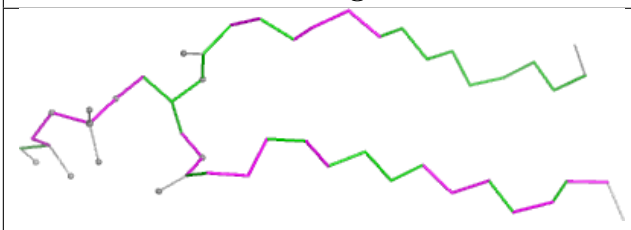
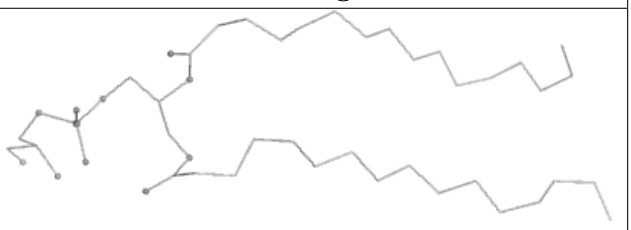
Rings

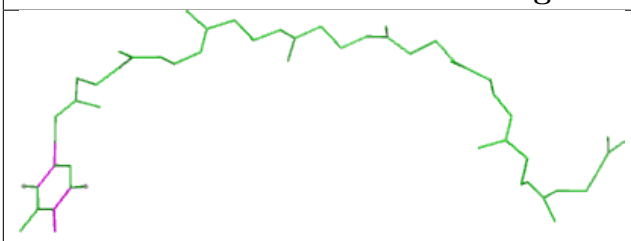
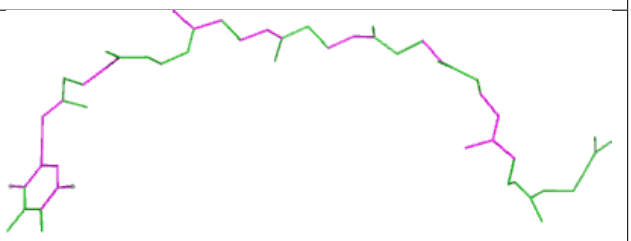
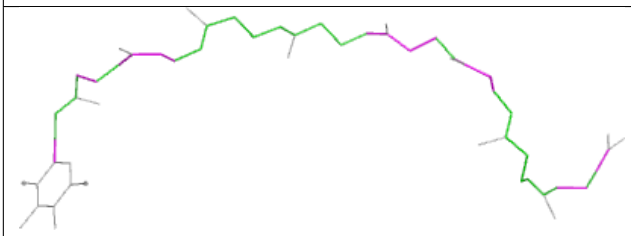
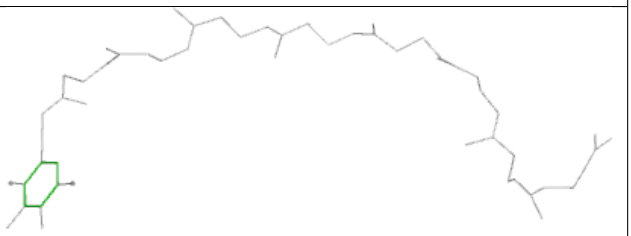
Ligand LMT L 210



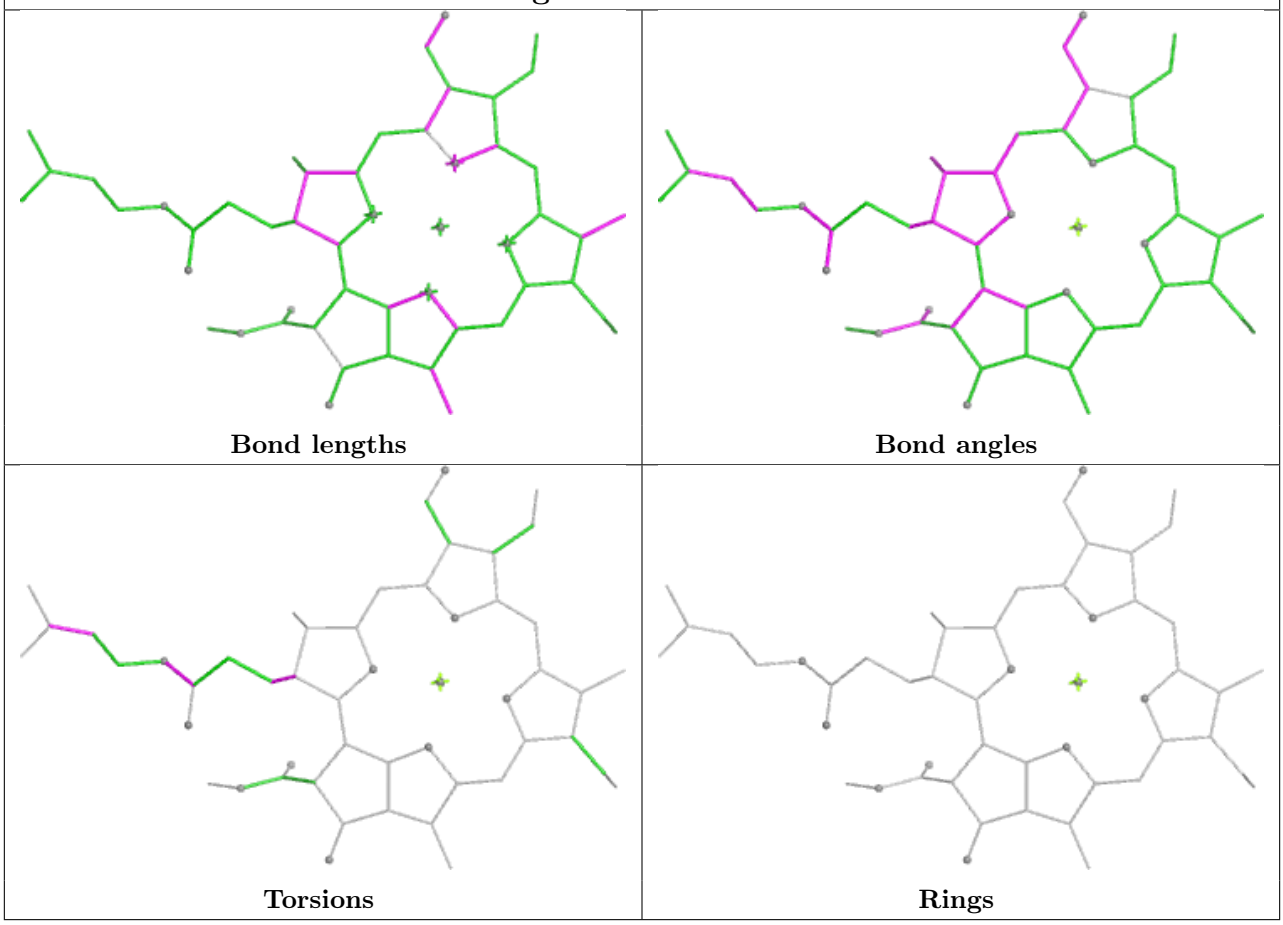
Ligand LMG C 519



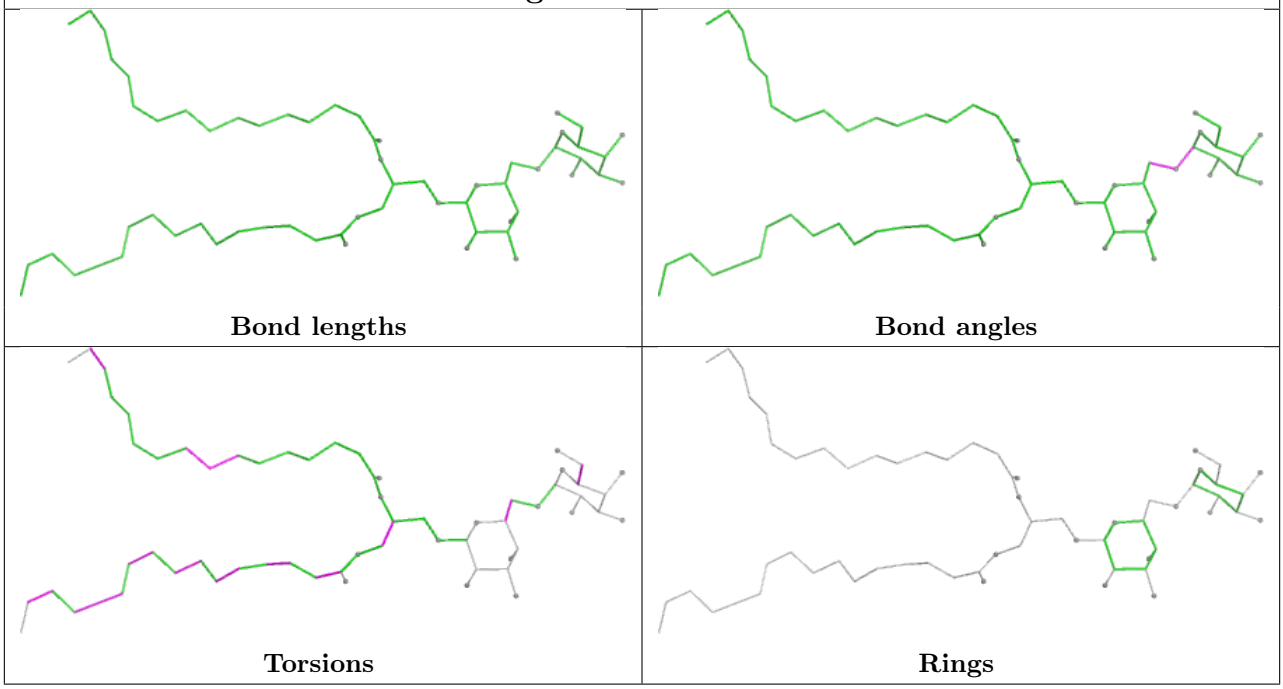
Ligand LHG E 244	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 a 414	
 Bond lengths	 Bond angles
 Torsions	 Rings

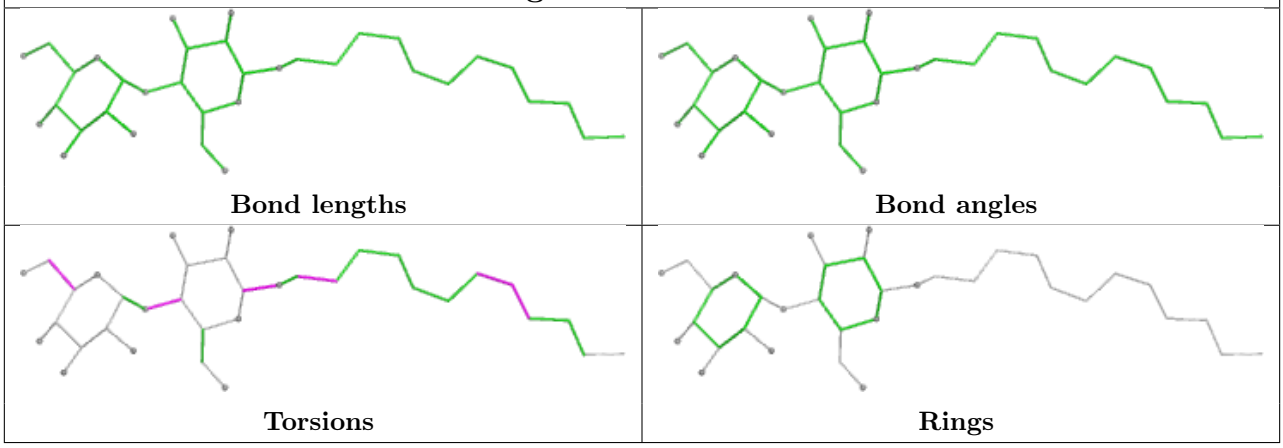
Ligand F6C b 617



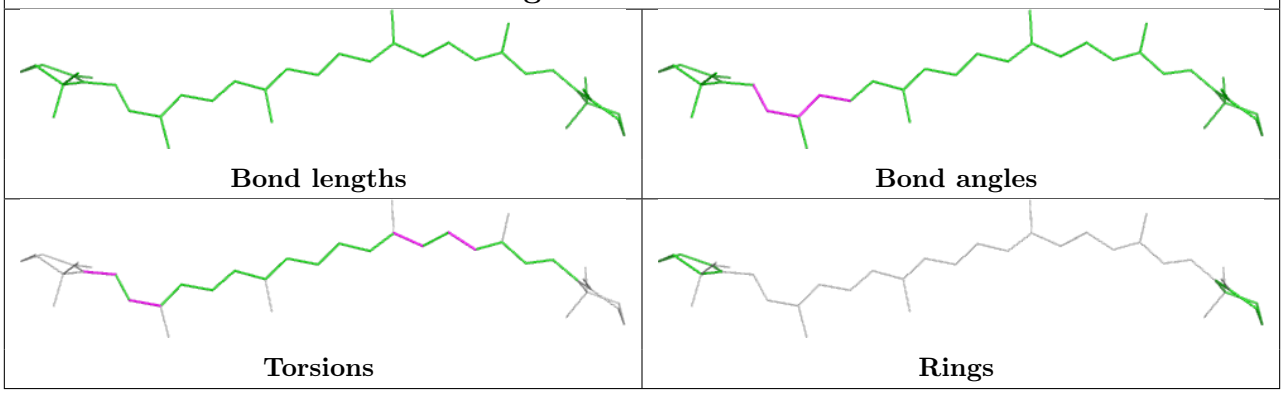
Ligand DGD c 518



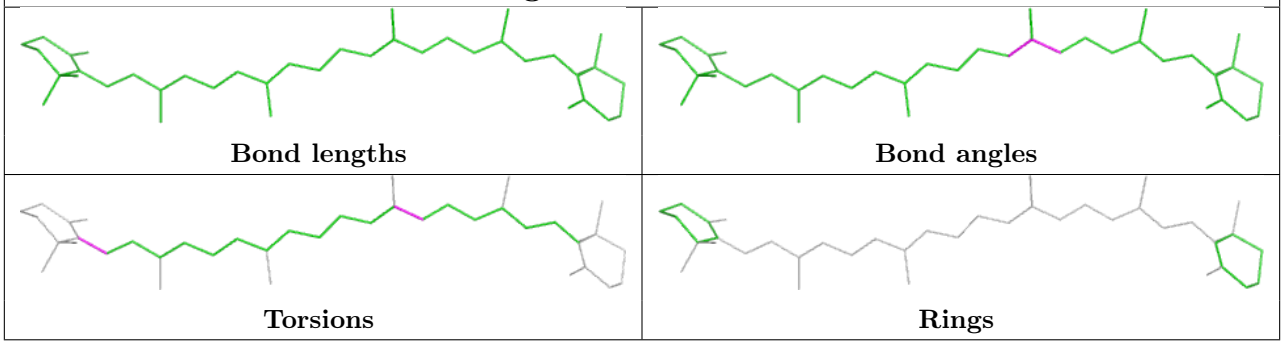
Ligand LMT a 674



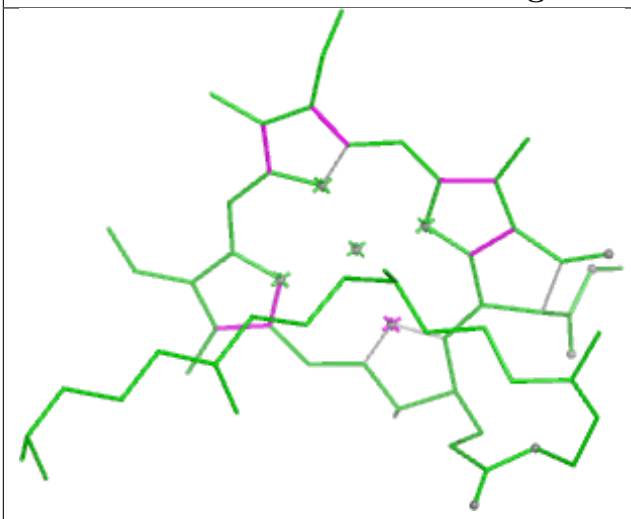
Ligand BCR B 627



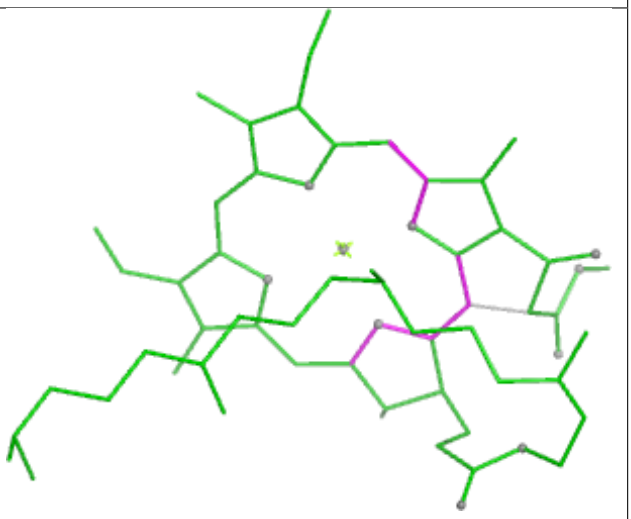
Ligand BCR C 515



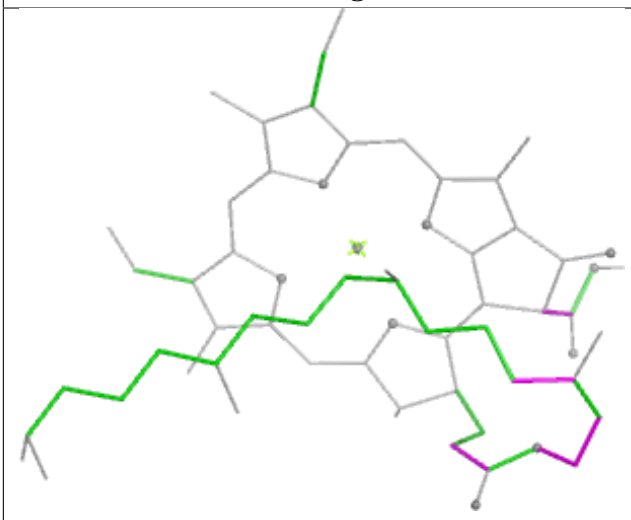
Ligand CLA b 602



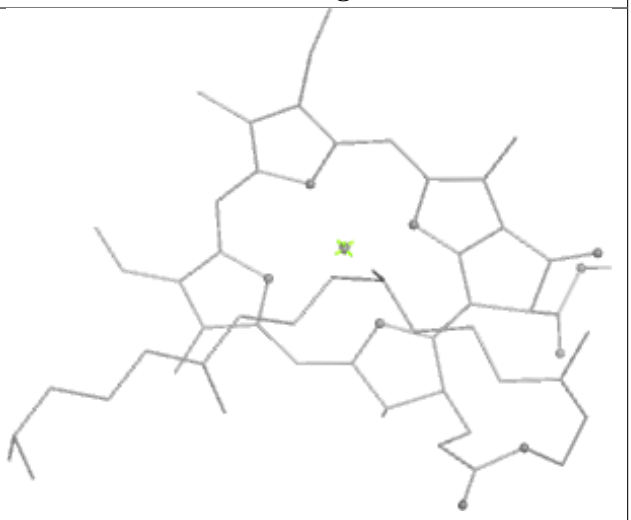
Bond lengths



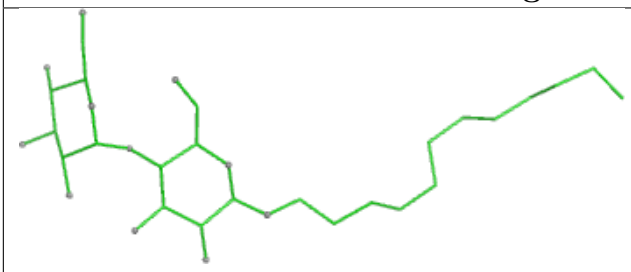
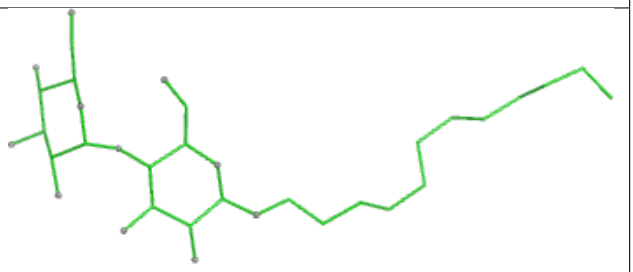
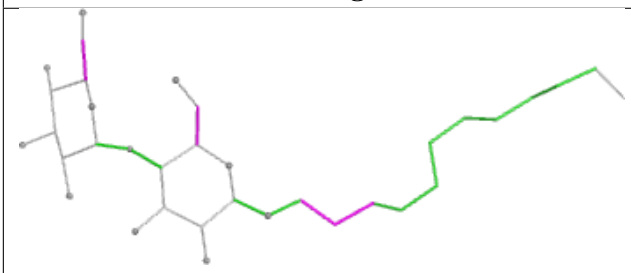
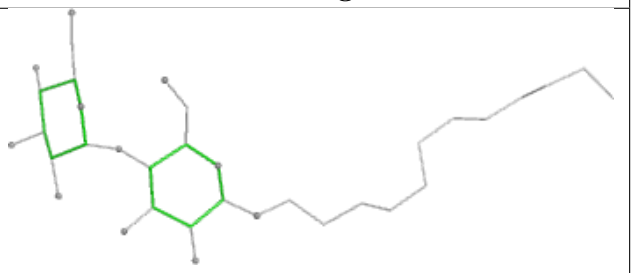
Bond angles

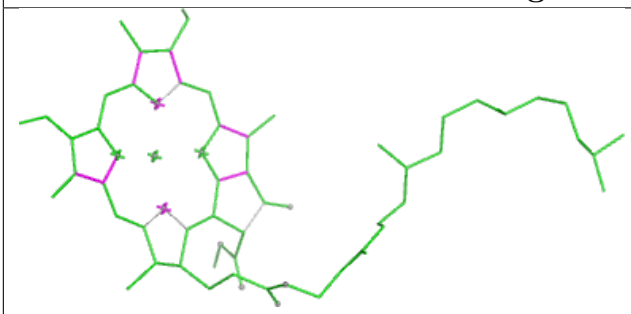
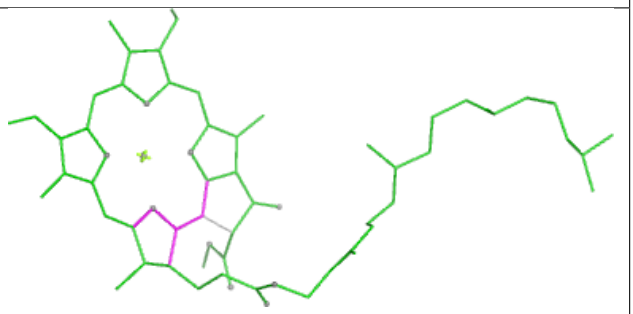
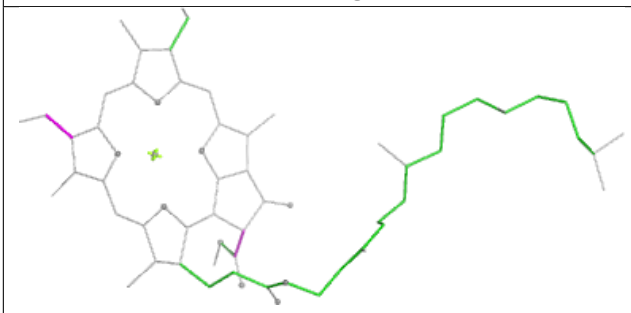
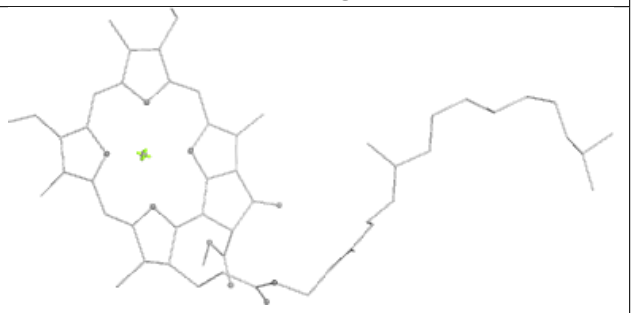


Torsions

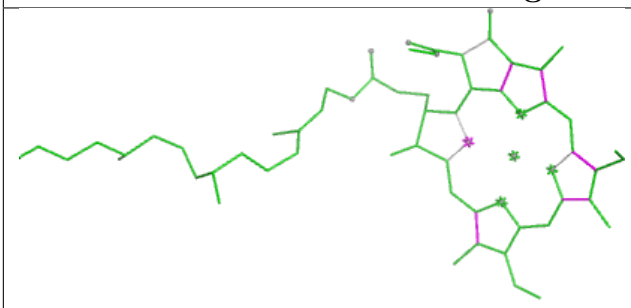


Rings

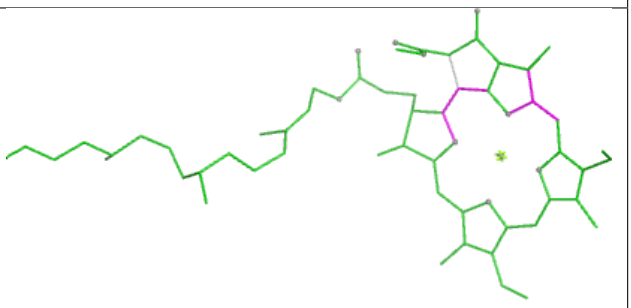
Ligand LMT F 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

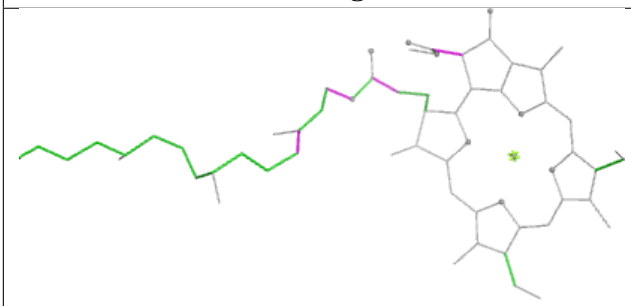
Ligand CLA C 512



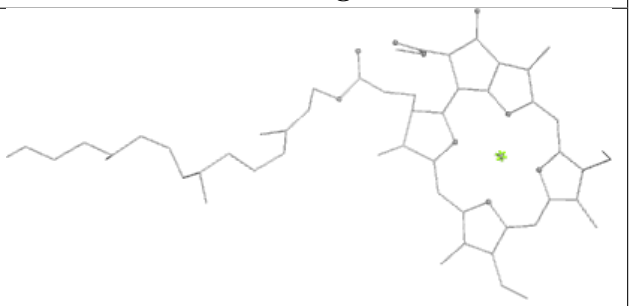
Bond lengths



Bond angles

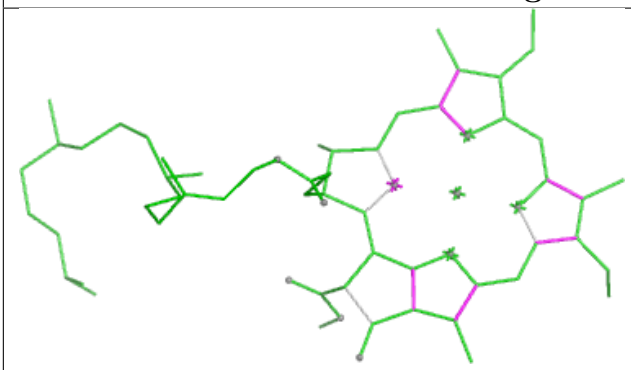


Torsions

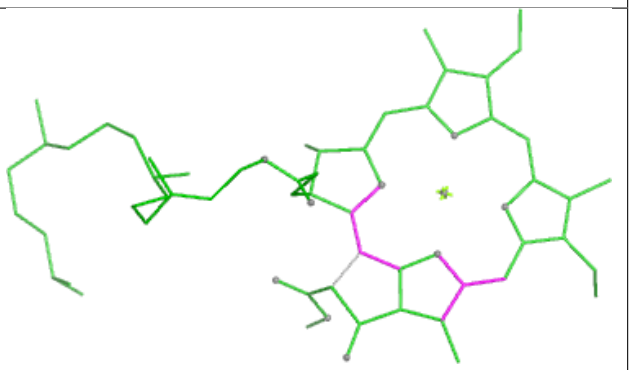


Rings

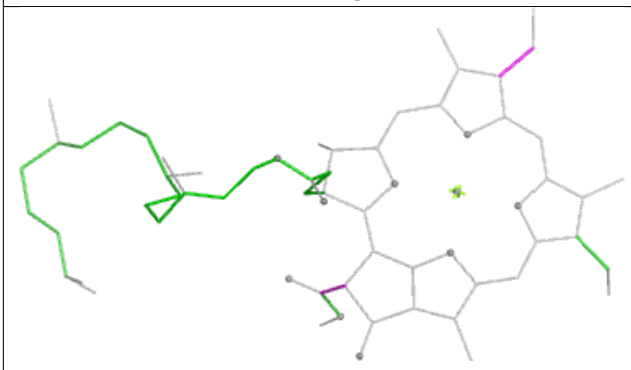
Ligand CLA B 613



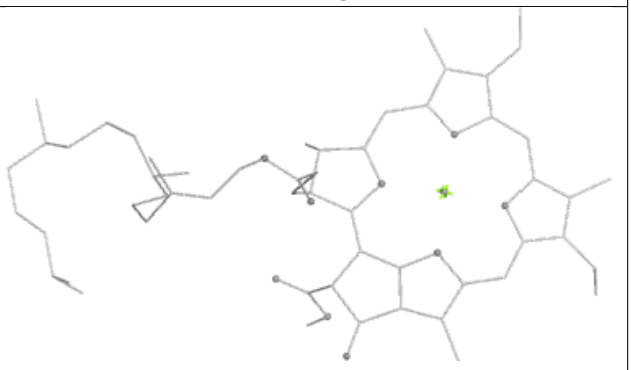
Bond lengths



Bond angles

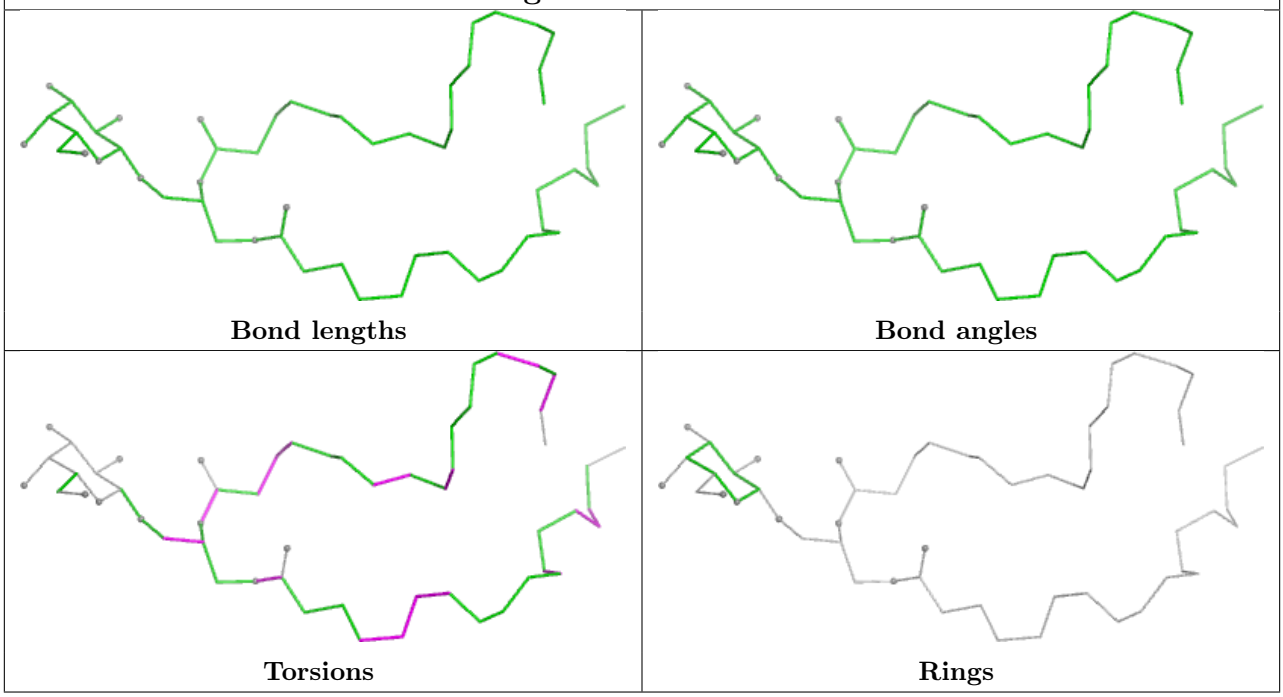


Torsions

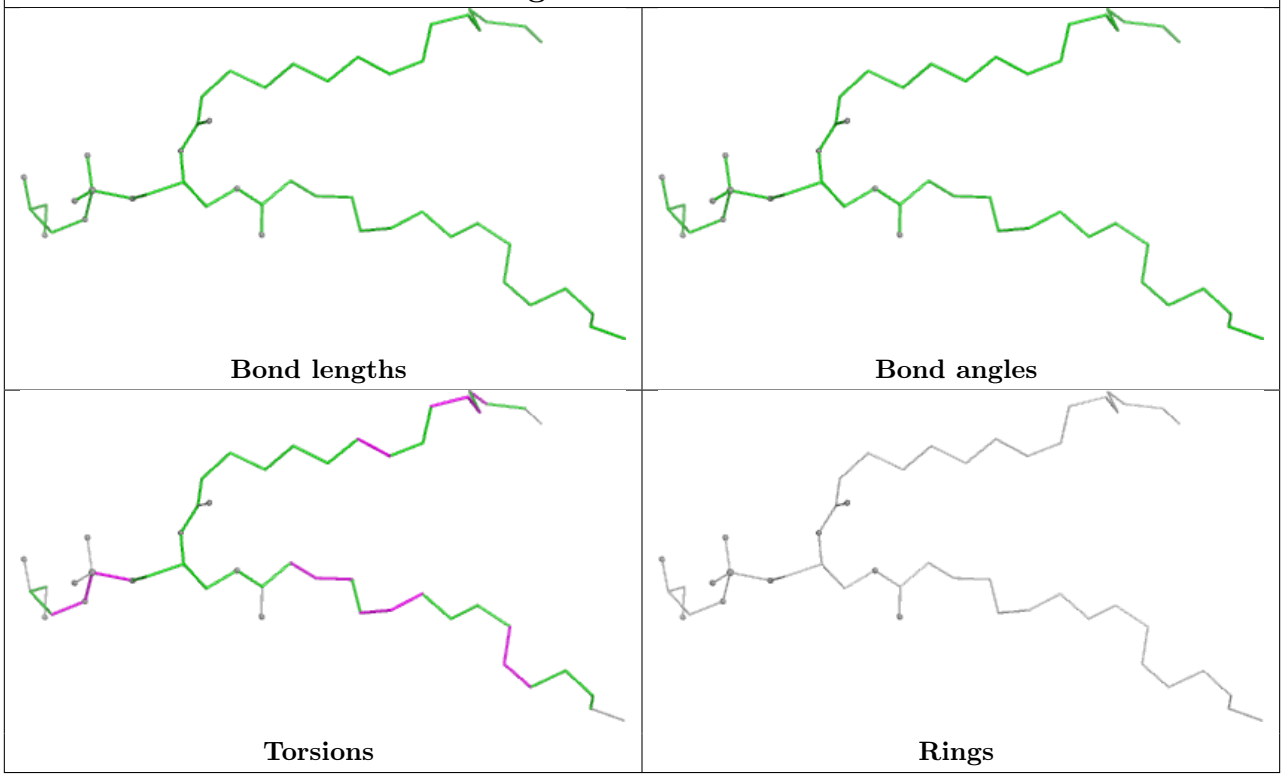


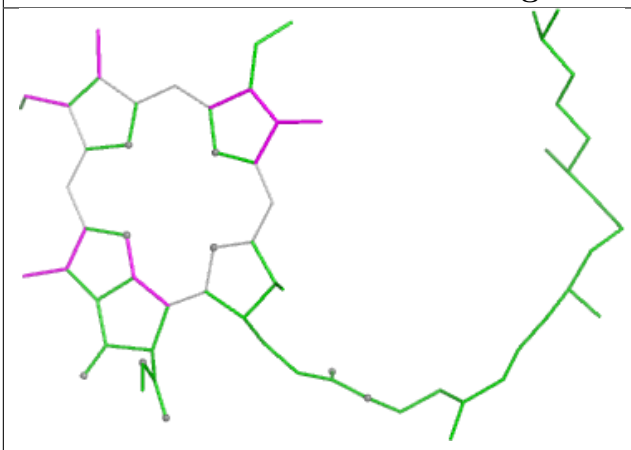
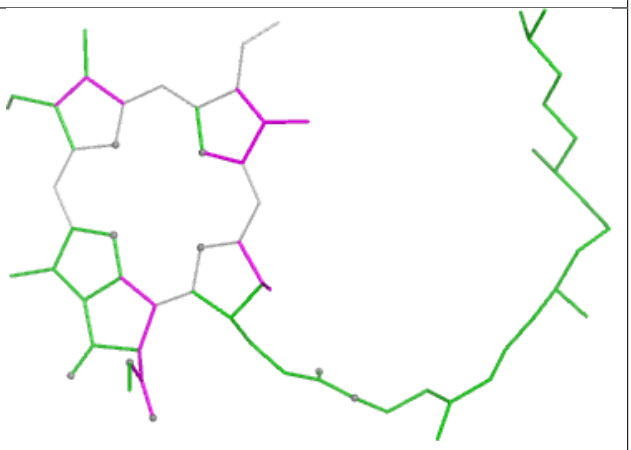
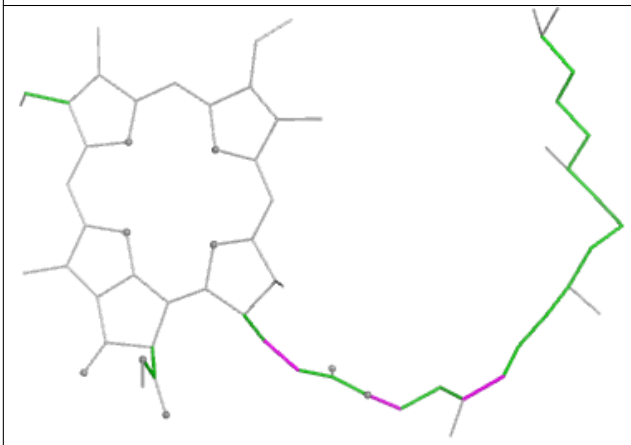
Rings

Ligand LMG b 628

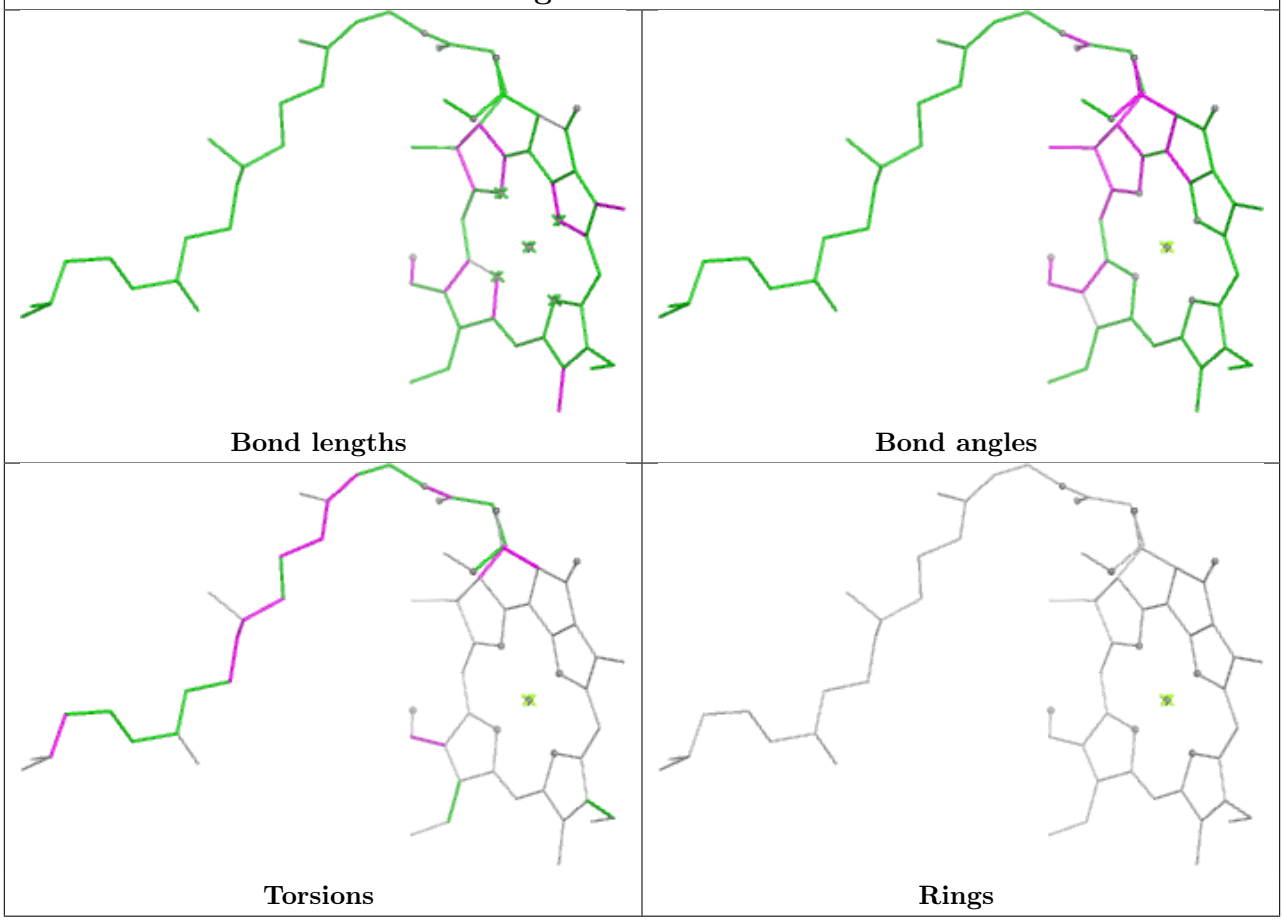


Ligand LHG a 419

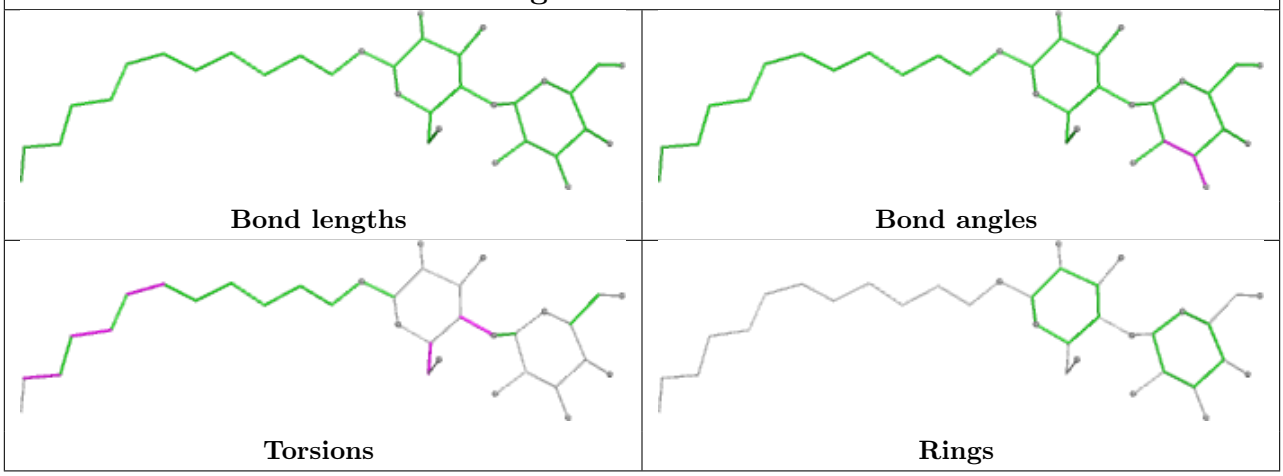


Ligand PHO A 408	
 Bond lengths	 Bond angles
 Torsions	Rings

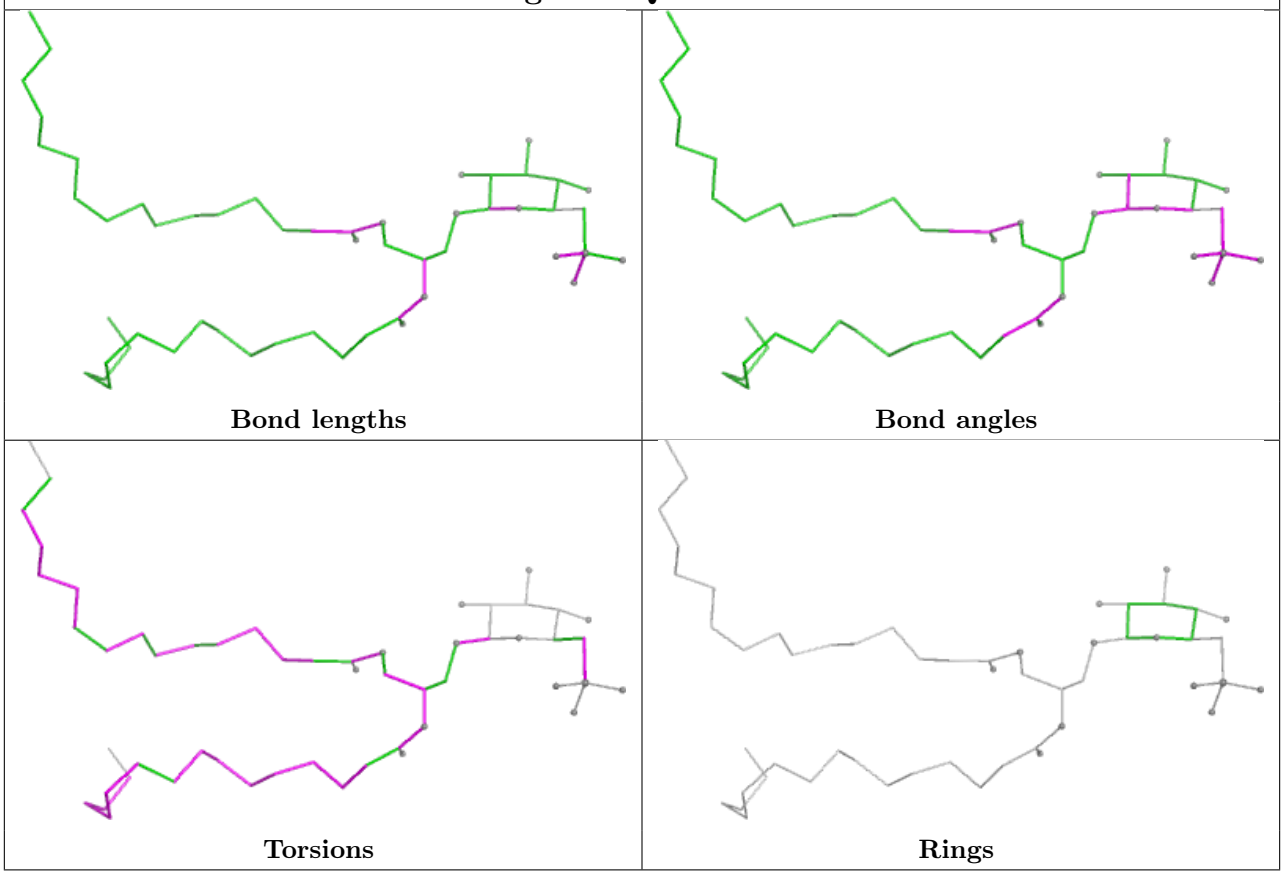
Ligand F6C c 507



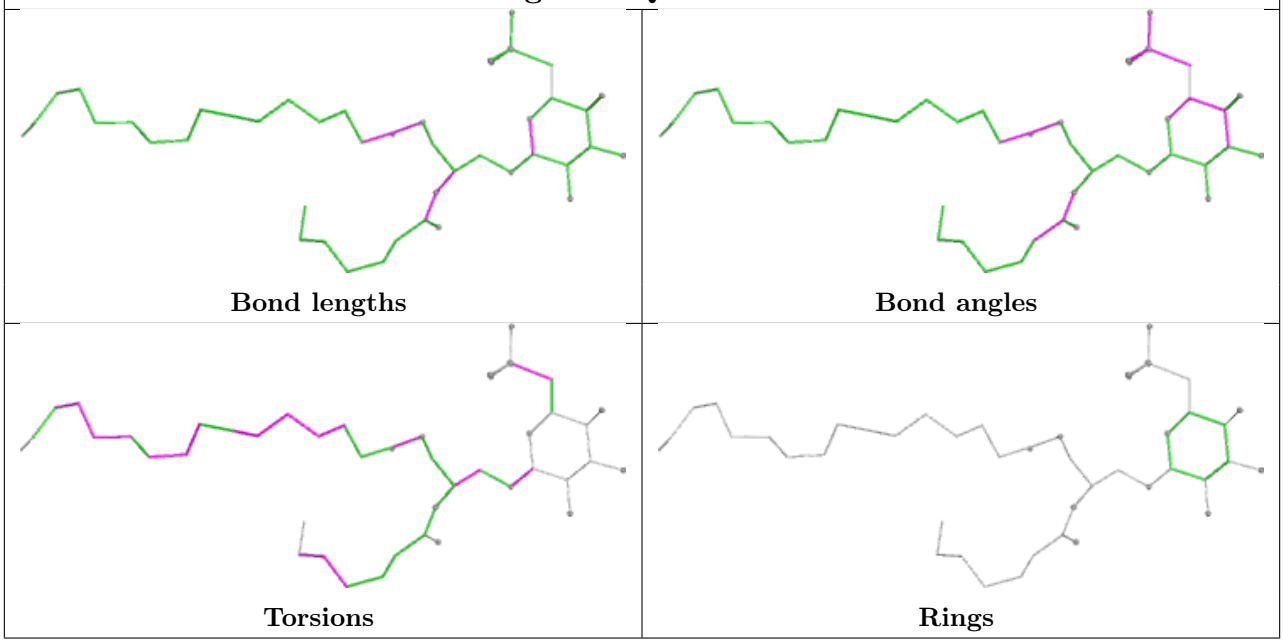
Ligand LMT l 213

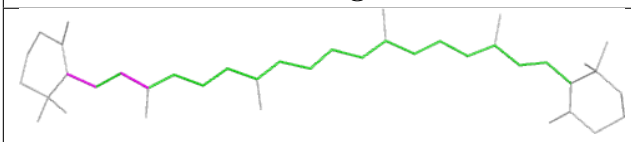
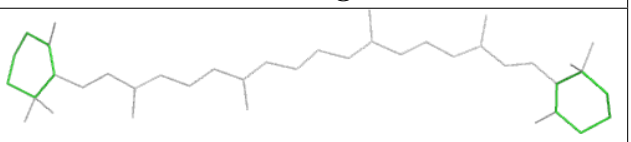


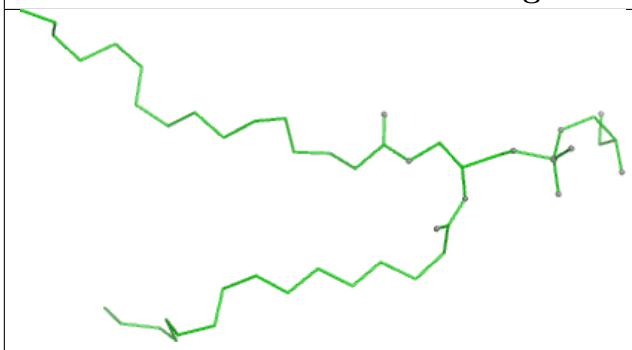
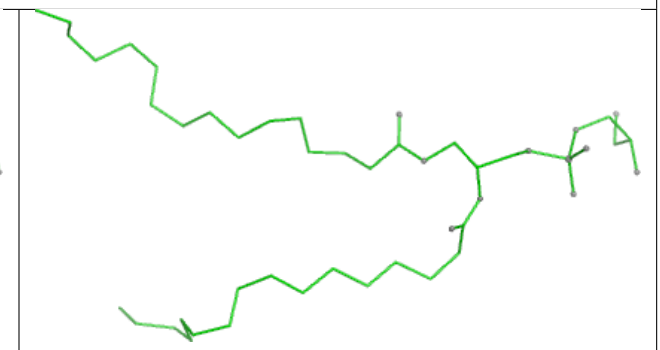
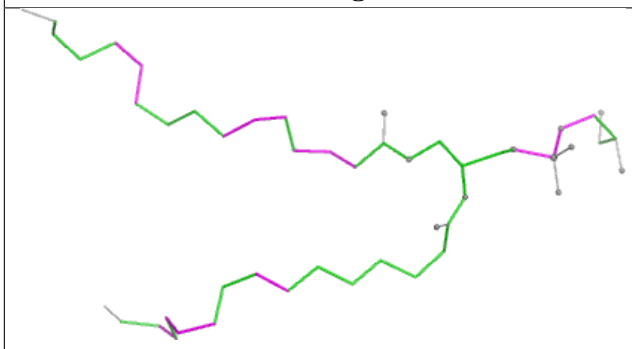
Ligand SQD A 417



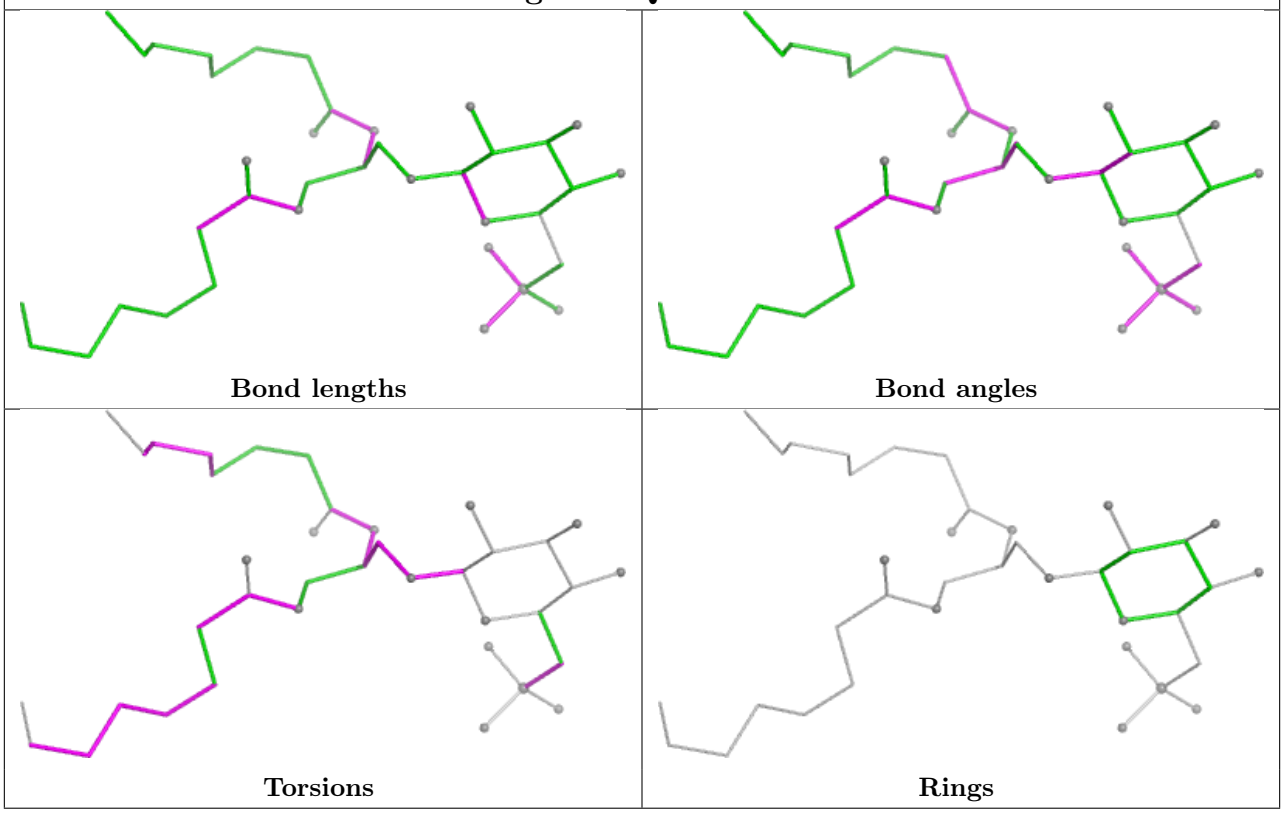
Ligand SQD D 407



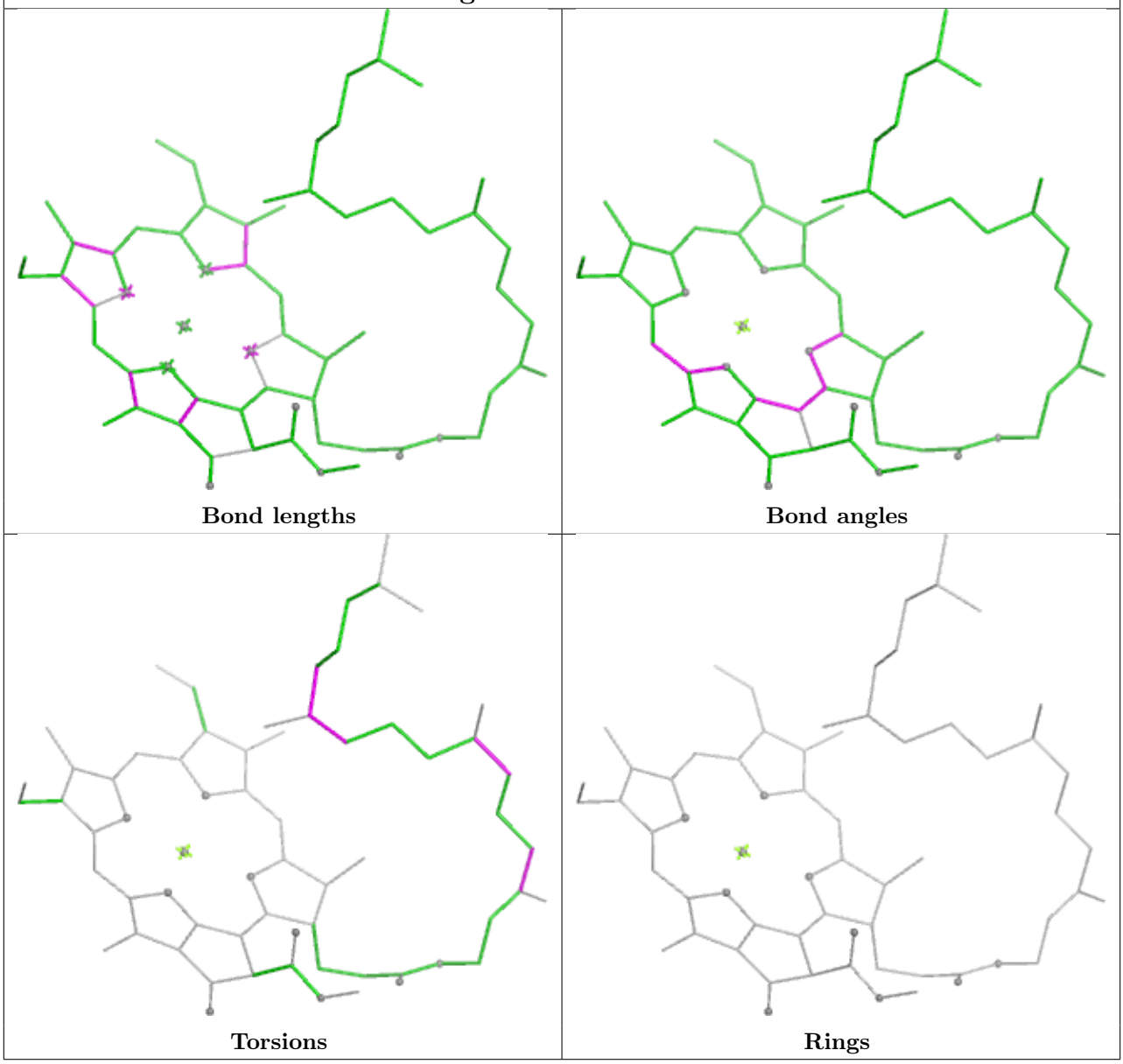
Ligand BCR B 620	
Bond lengths	Bond angles
 Torsions	 Rings

Ligand LHG A 419	
 Bond lengths	 Bond angles
 Torsions	Rings

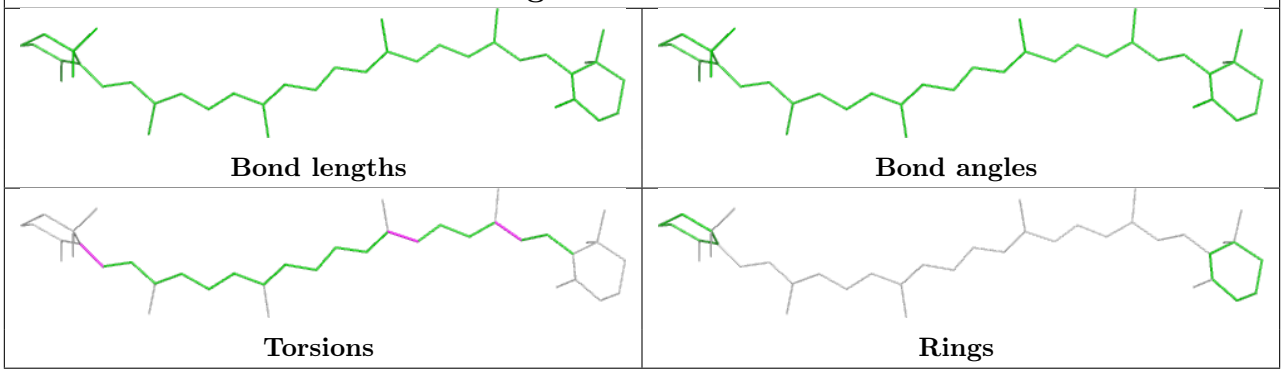
Ligand SQD C 903



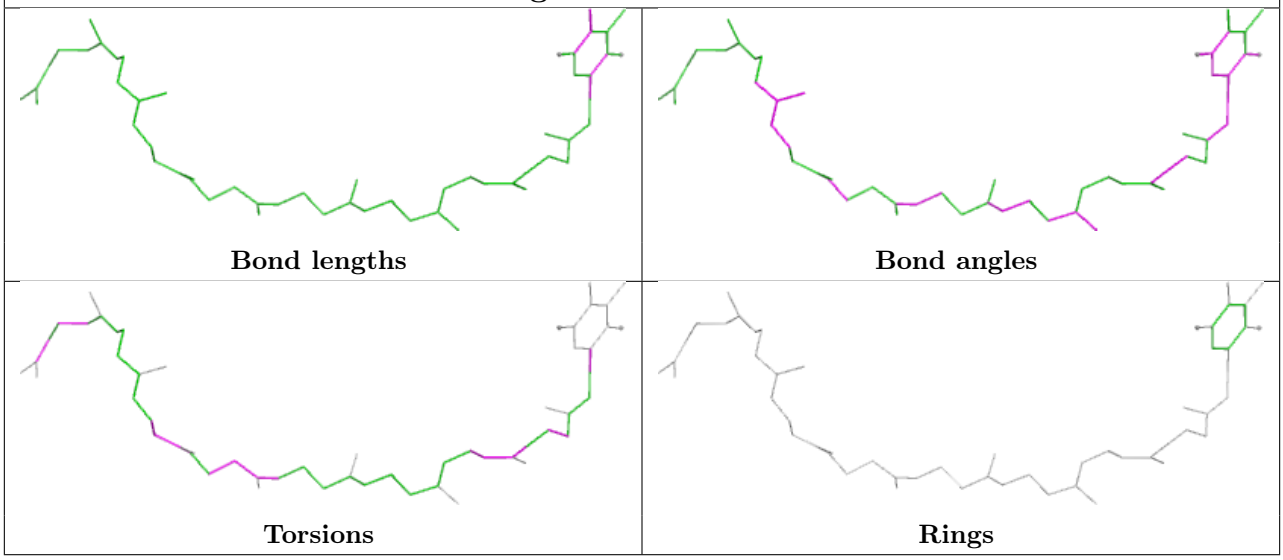
Ligand CLA B 616



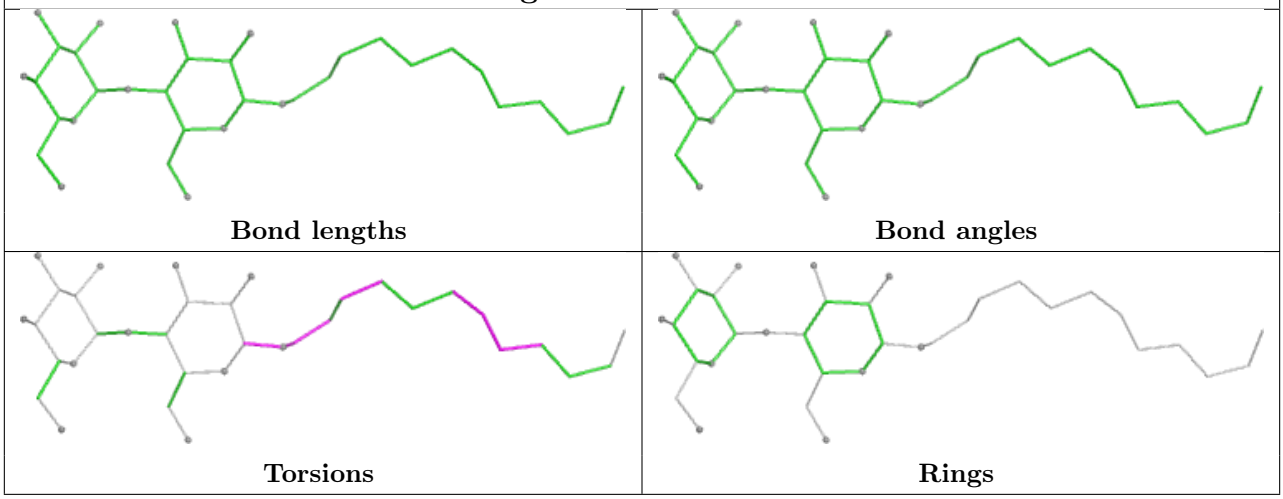
Ligand BCR k 101



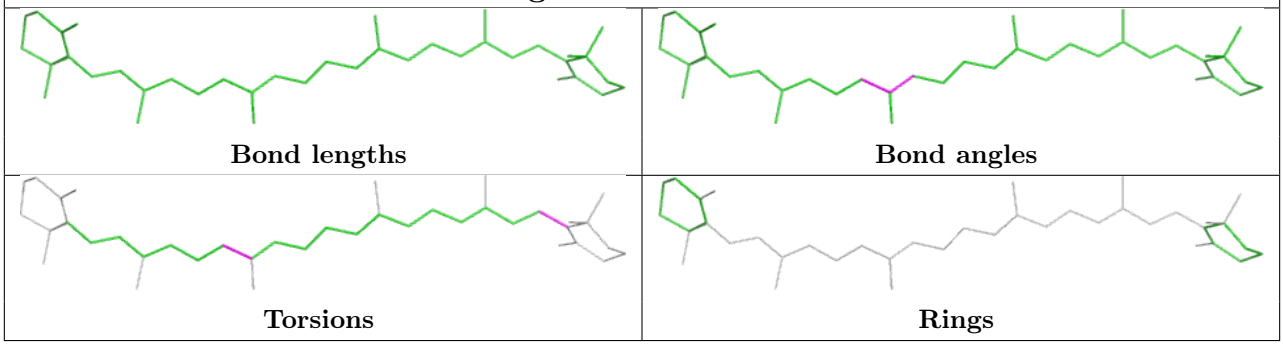
Ligand PL9 A 414



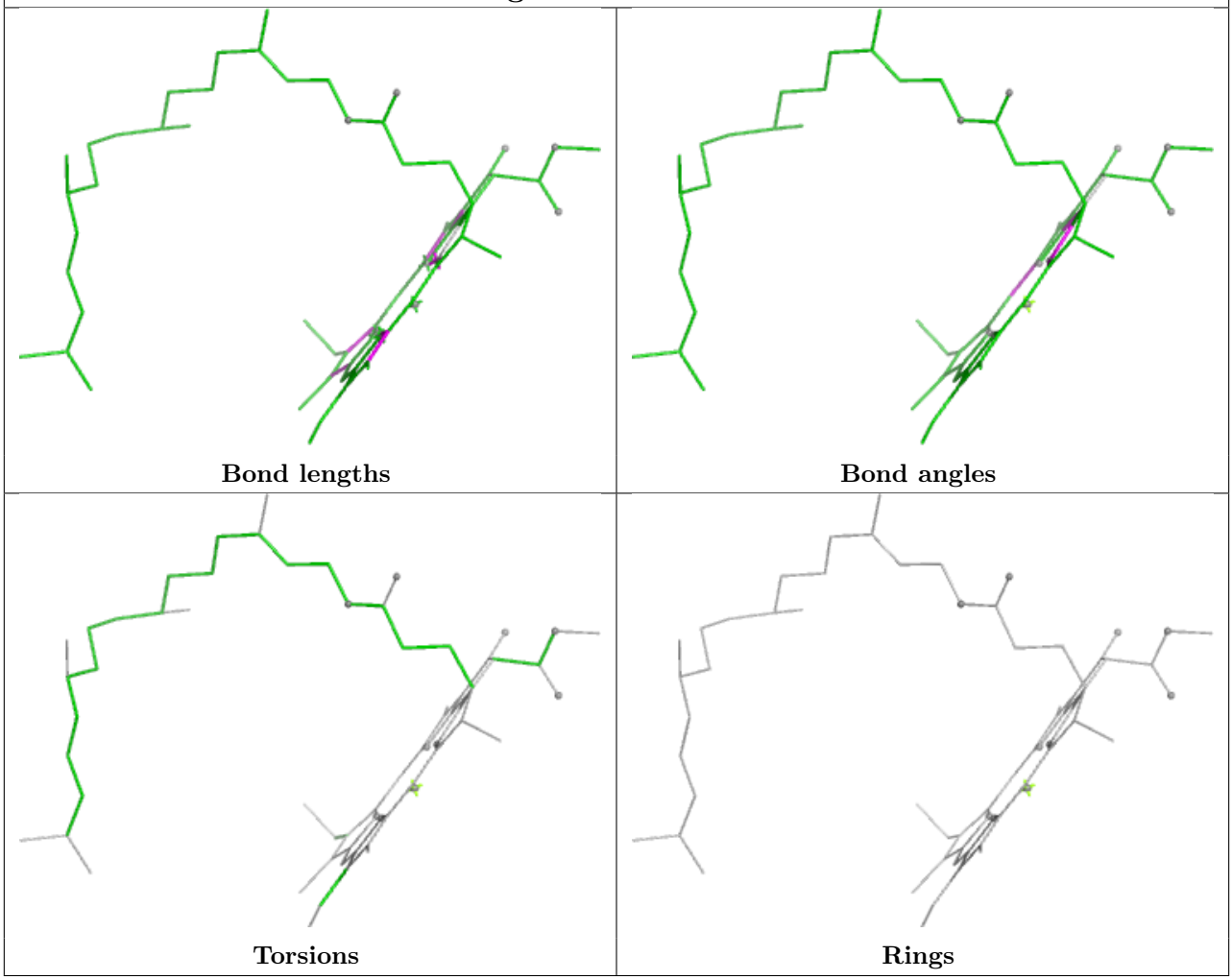
Ligand LMT m 101



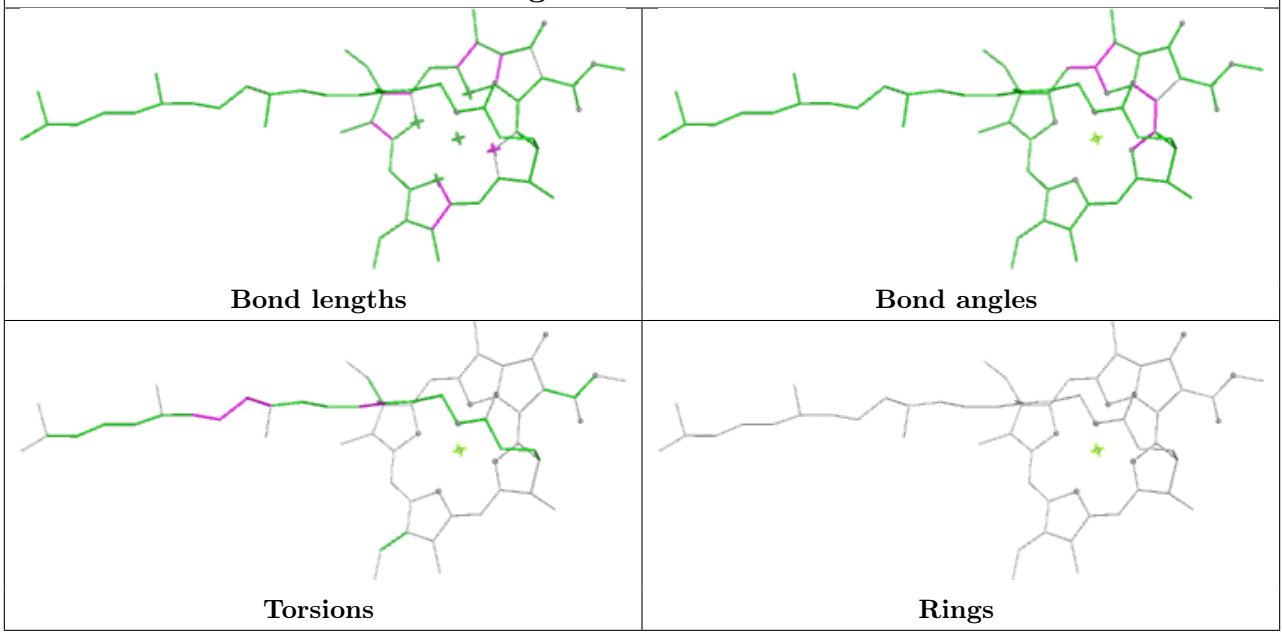
Ligand BCR c 515



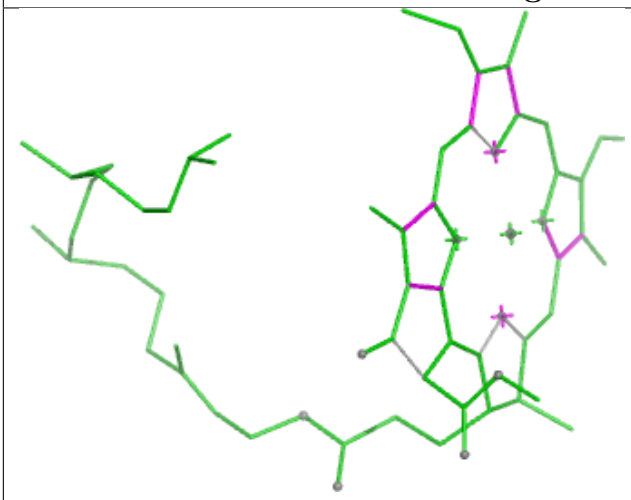
Ligand CLA b 612



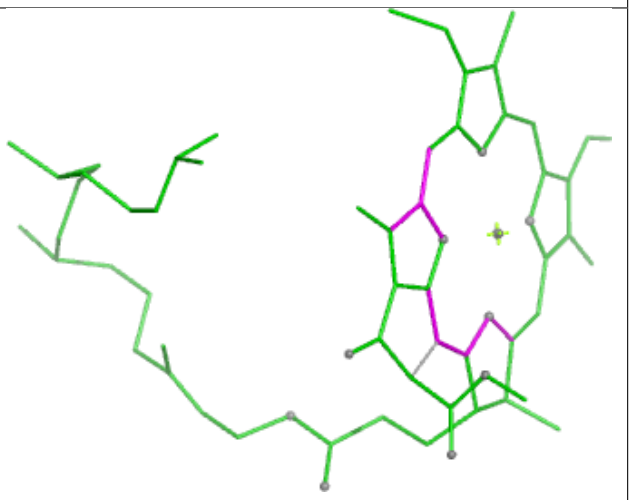
Ligand CLA b 615



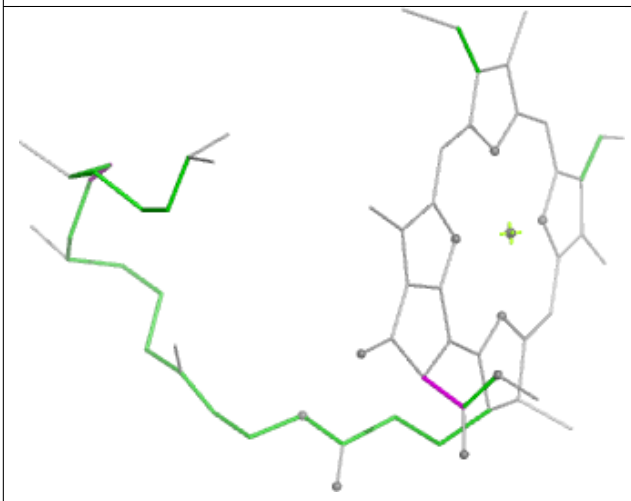
Ligand CLA C 503



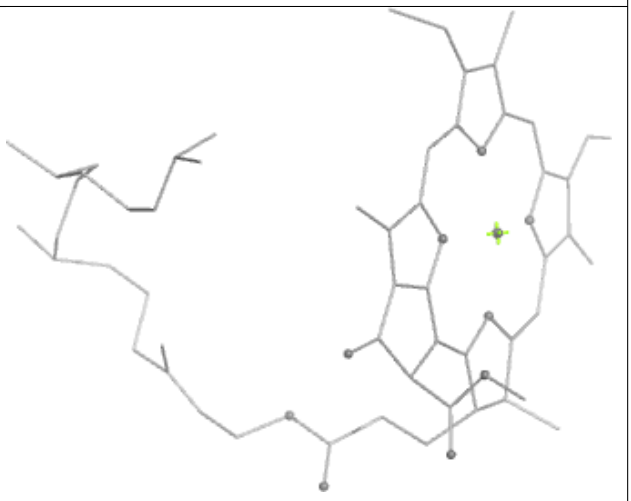
Bond lengths



Bond angles

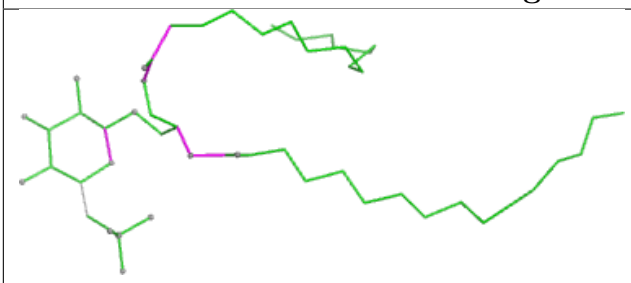


Torsions

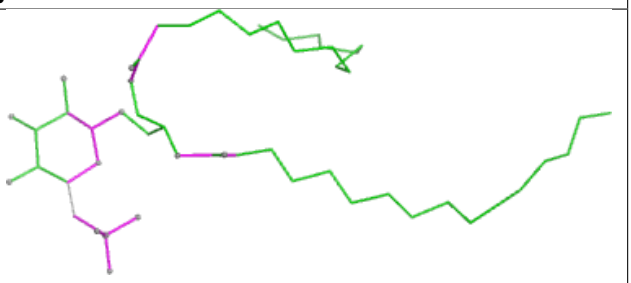


Rings

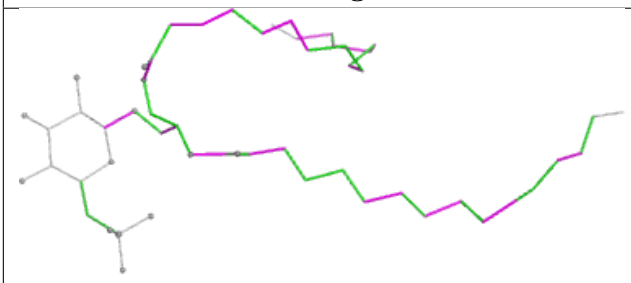
Ligand SQD H 102



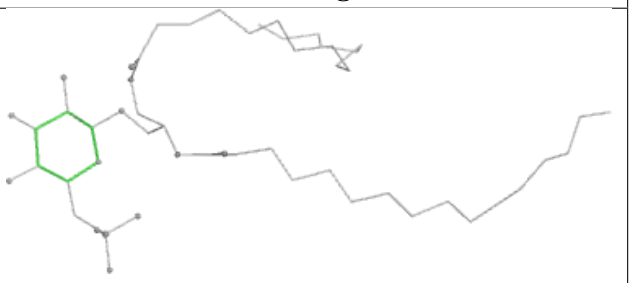
Bond lengths



Bond angles

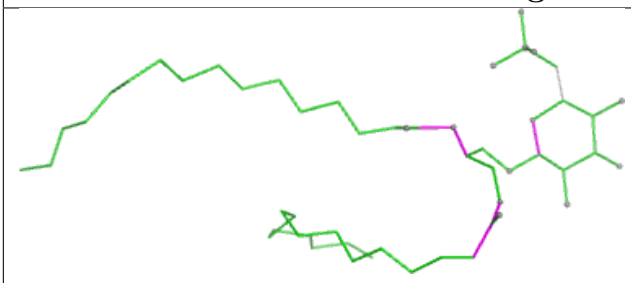


Torsions

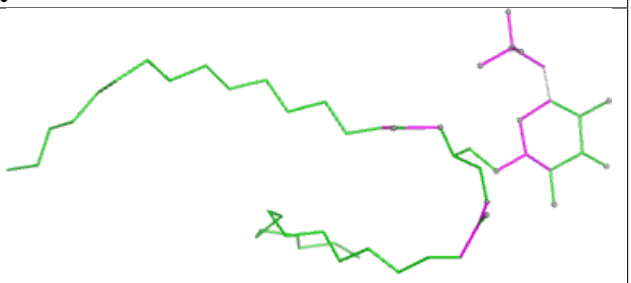


Rings

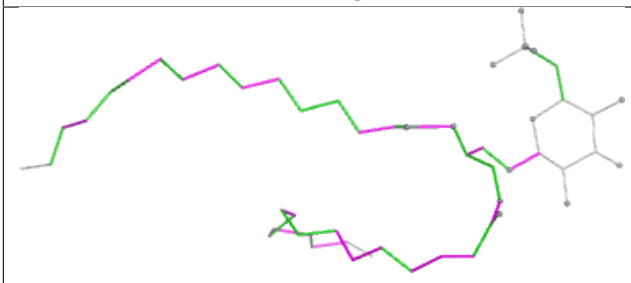
Ligand SQD h 102



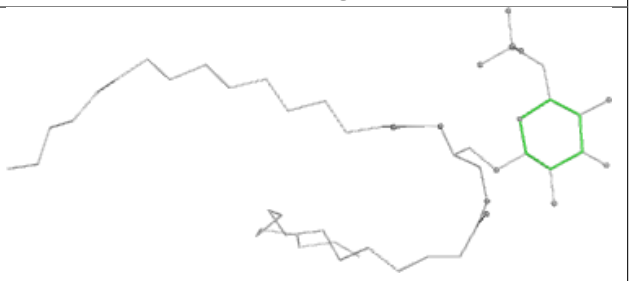
Bond lengths



Bond angles

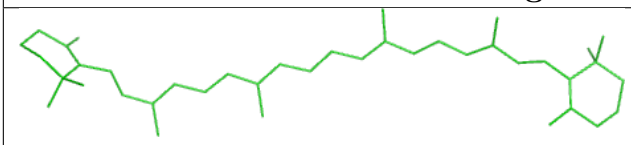


Torsions

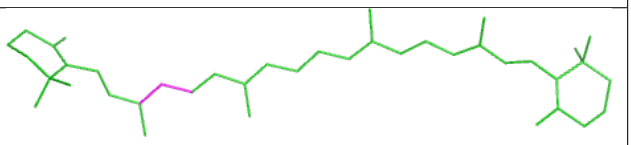


Rings

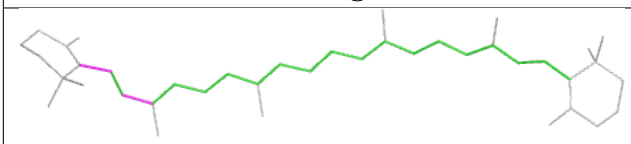
Ligand BCR b 618



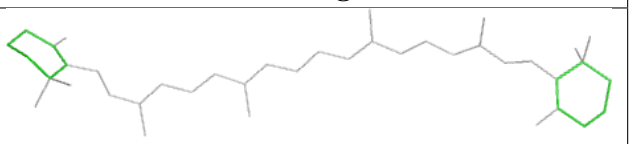
Bond lengths



Bond angles

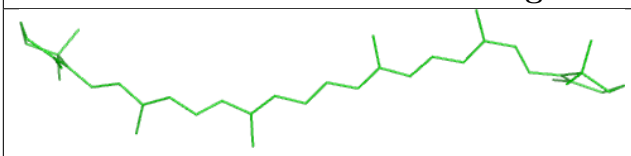


Torsions

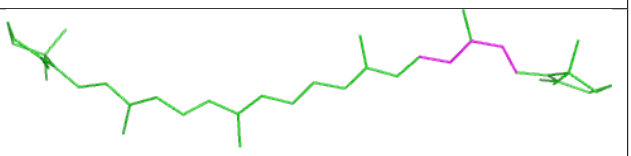


Rings

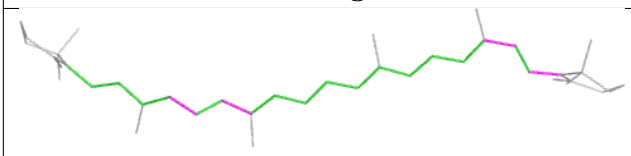
Ligand BCR b 627



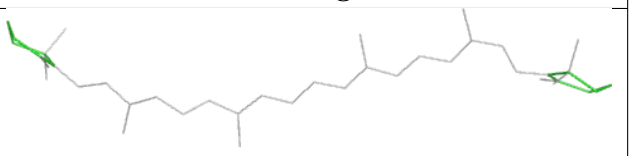
Bond lengths



Bond angles



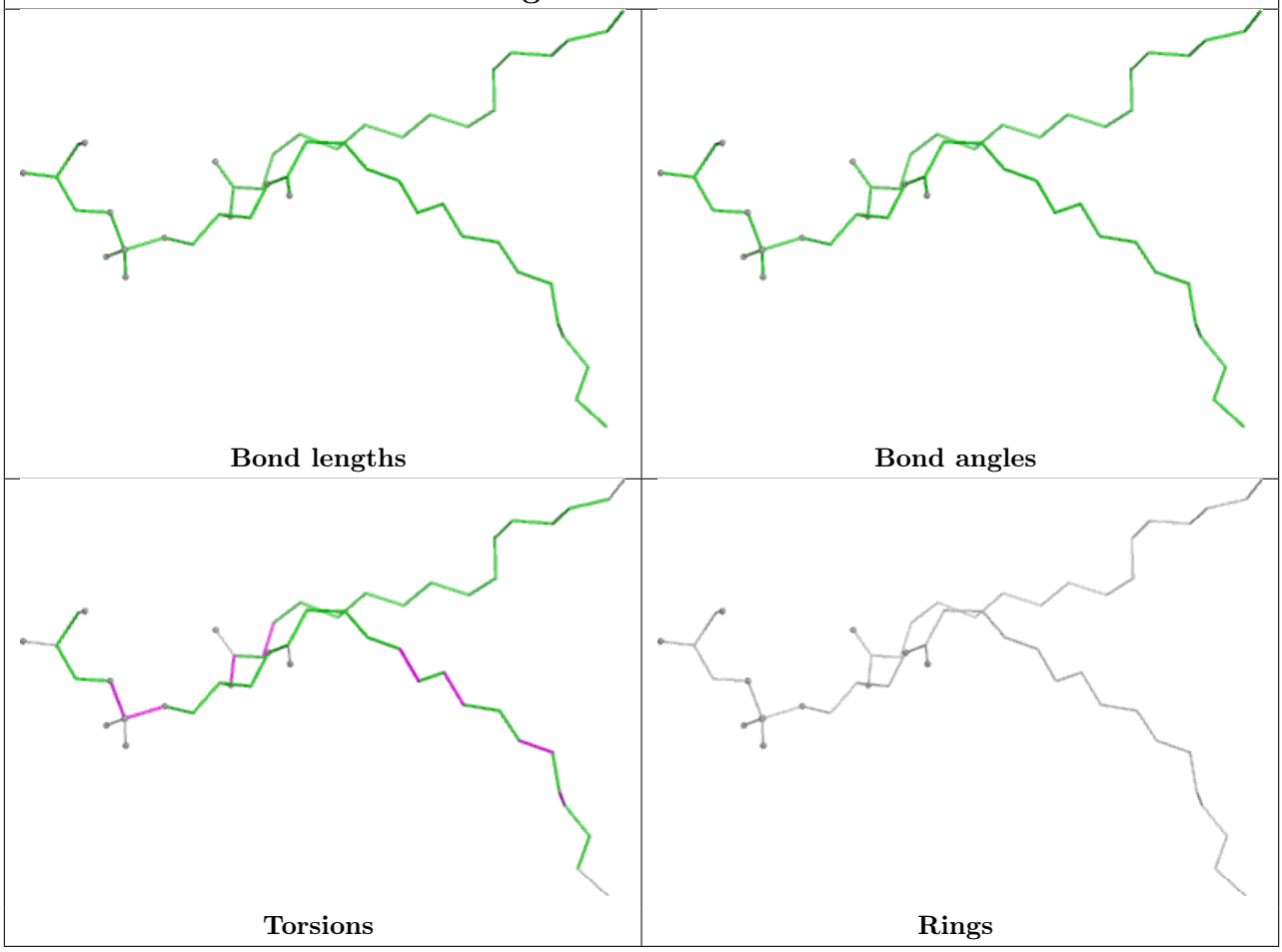
Torsions



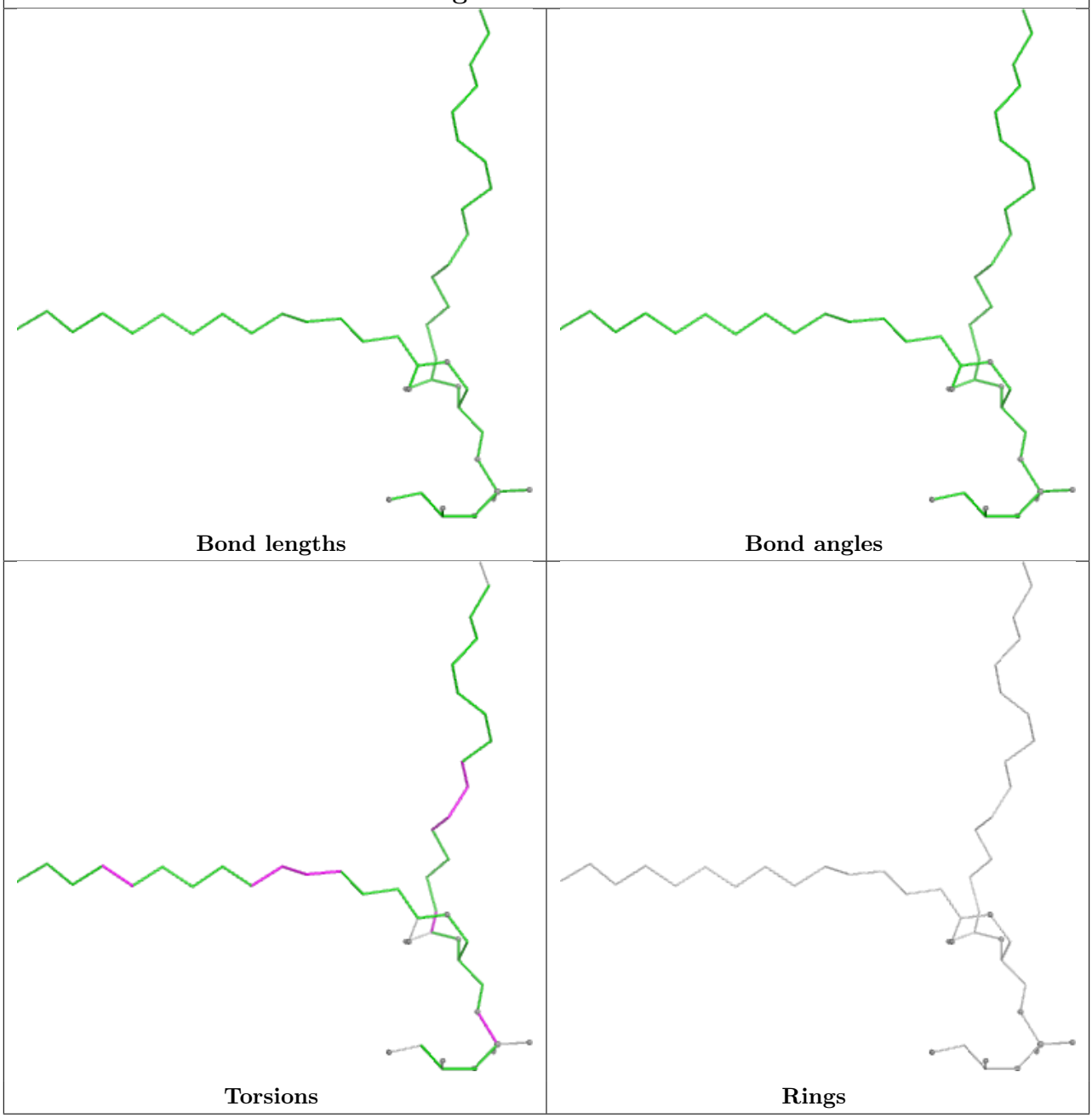
Rings

Ligand LMT A 674

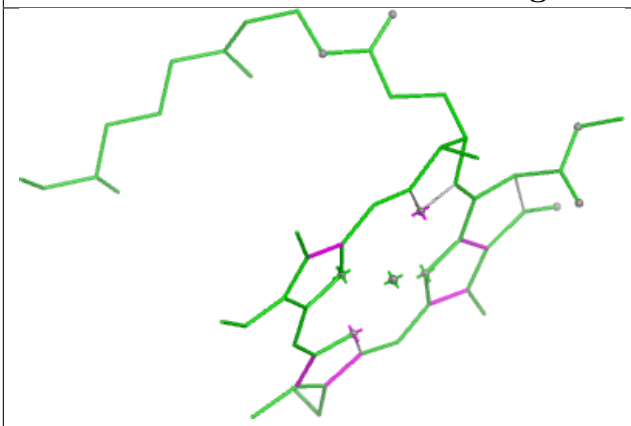
Ligand LHG D 409



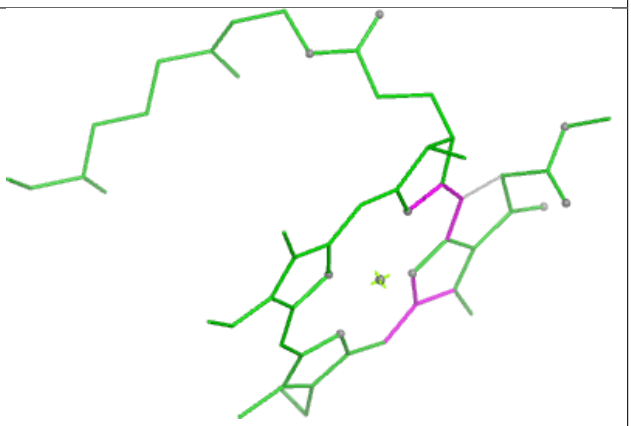
Ligand LHG l 101



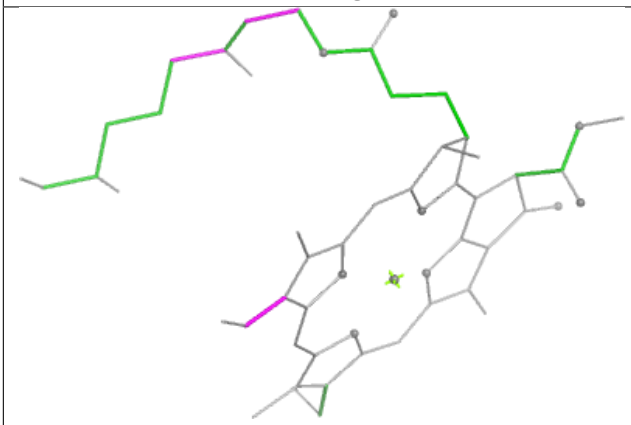
Ligand CLA c 513



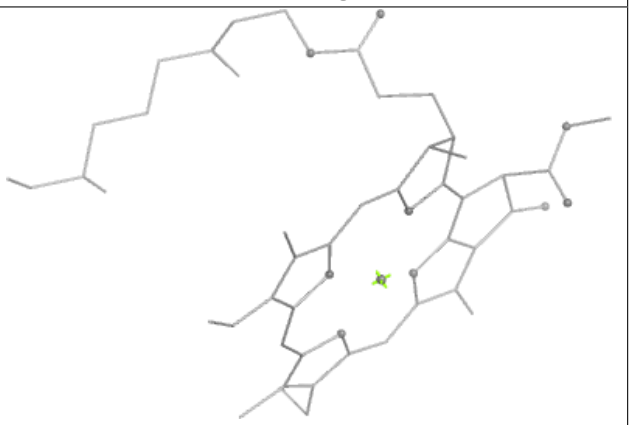
Bond lengths



Bond angles

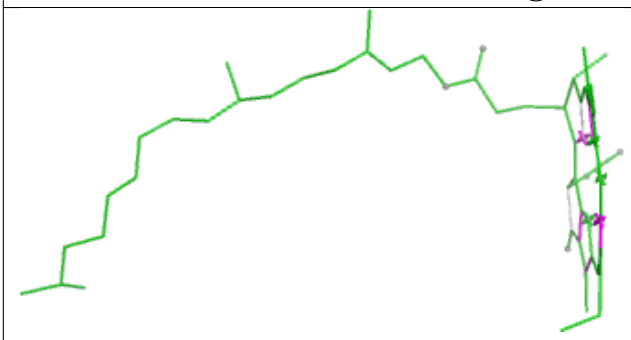


Torsions

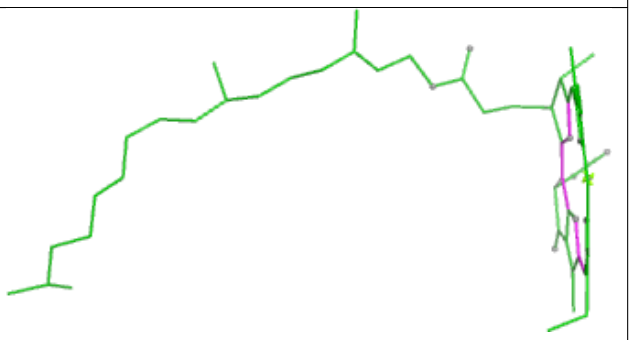


Rings

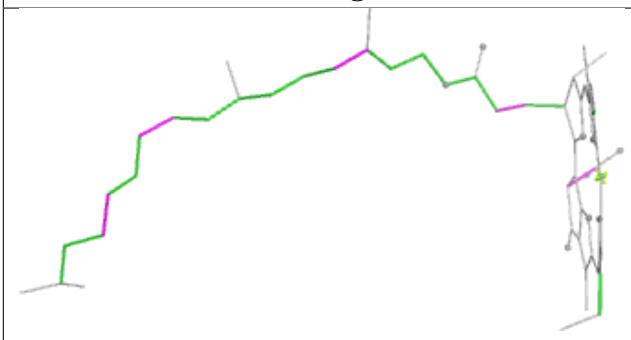
Ligand CLA b 607



Bond lengths



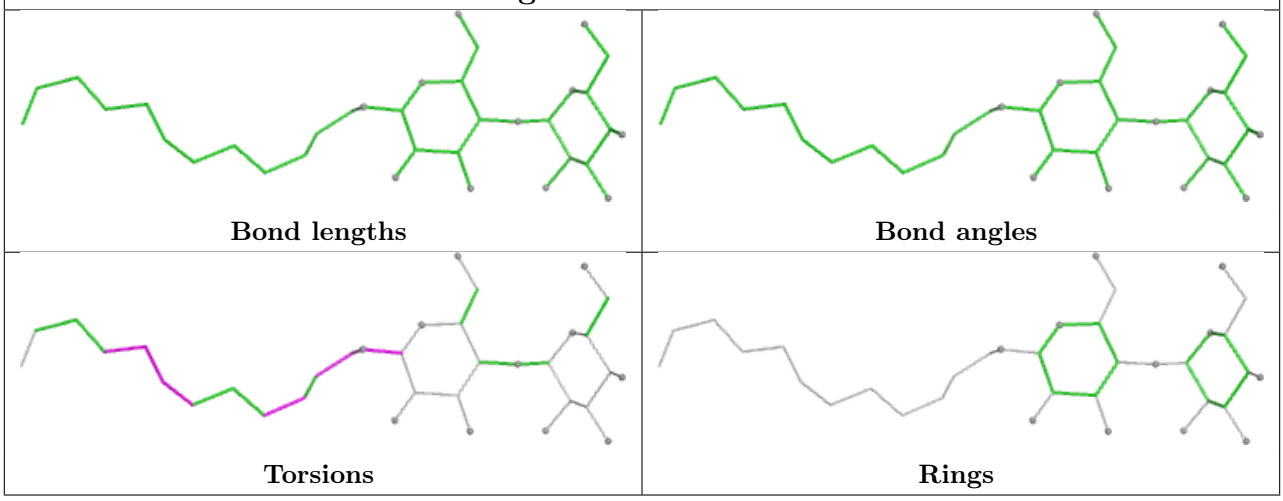
Bond angles



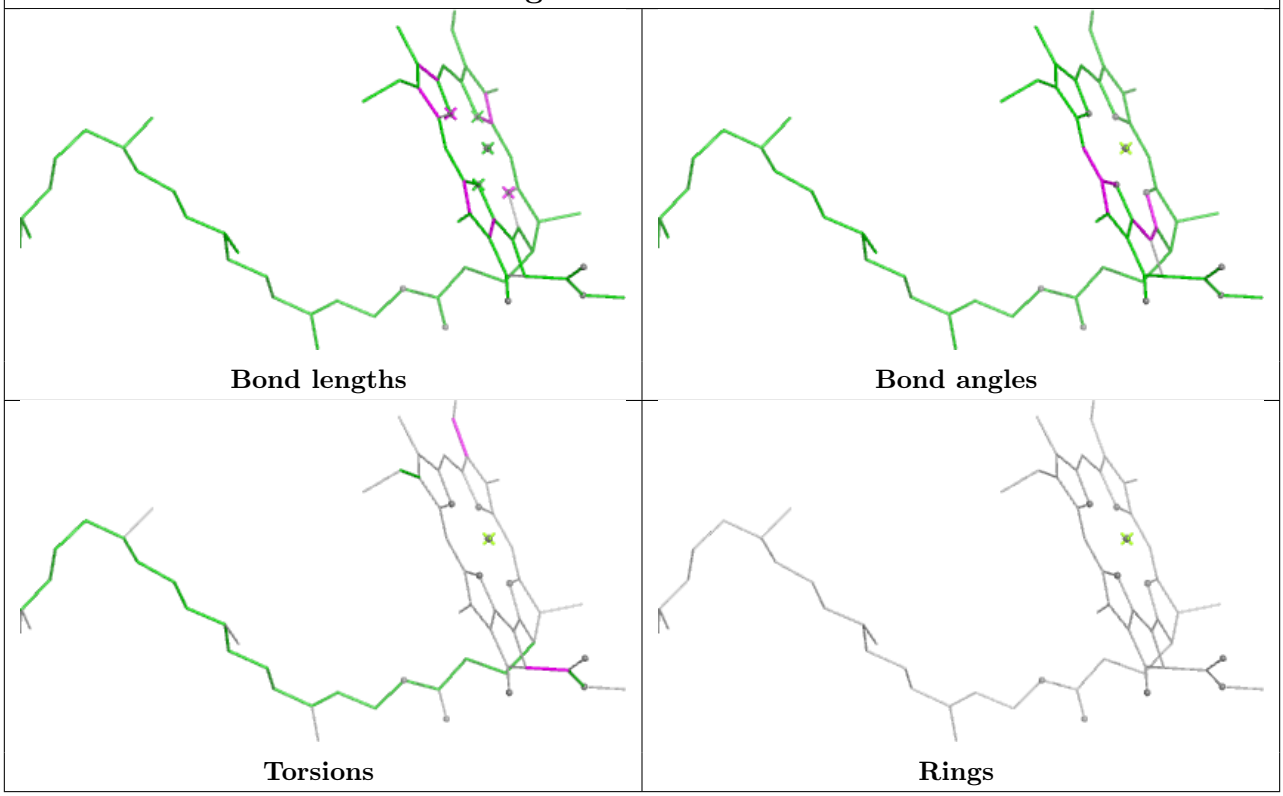
Torsions

Rings

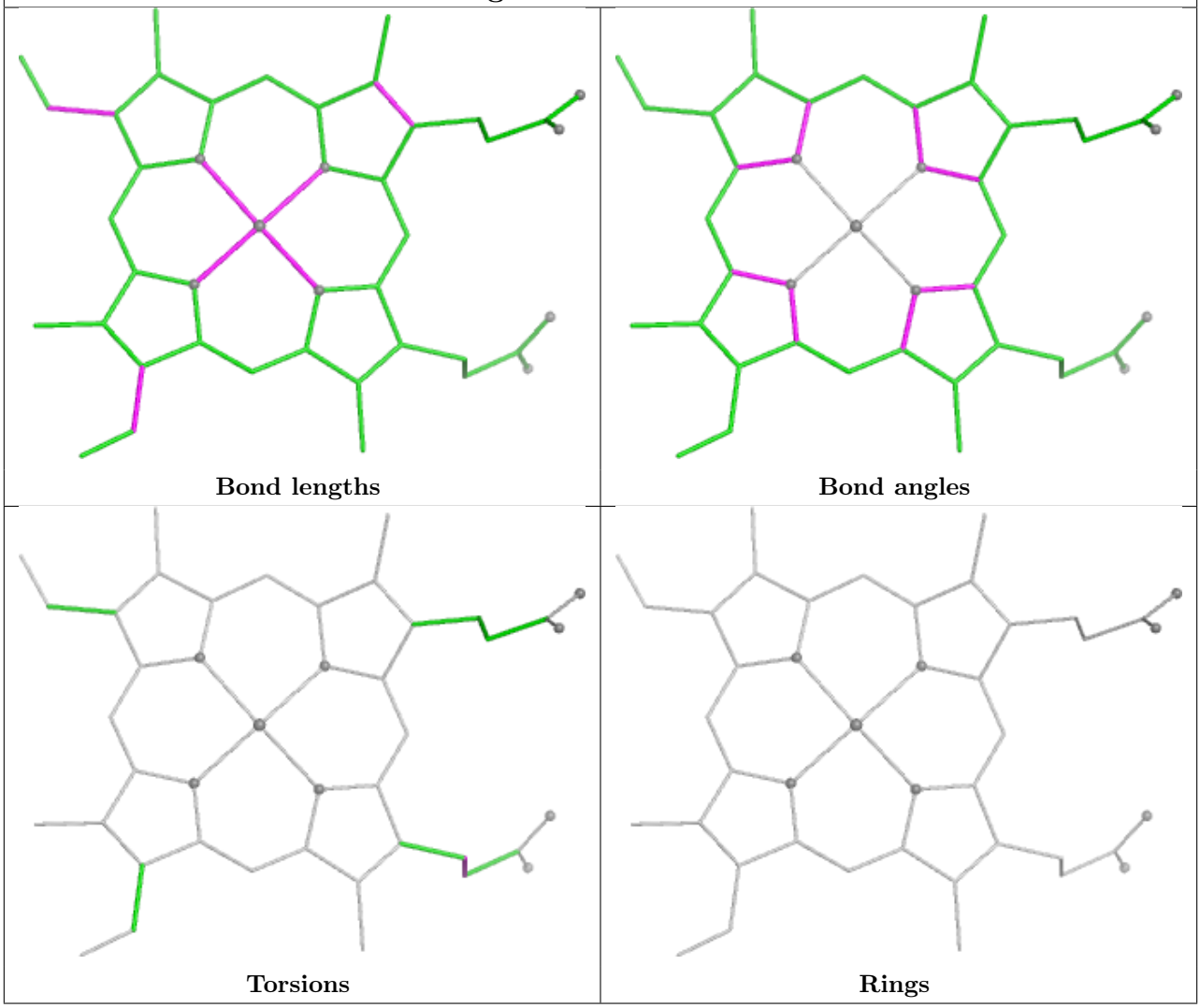
Ligand LMT M 101



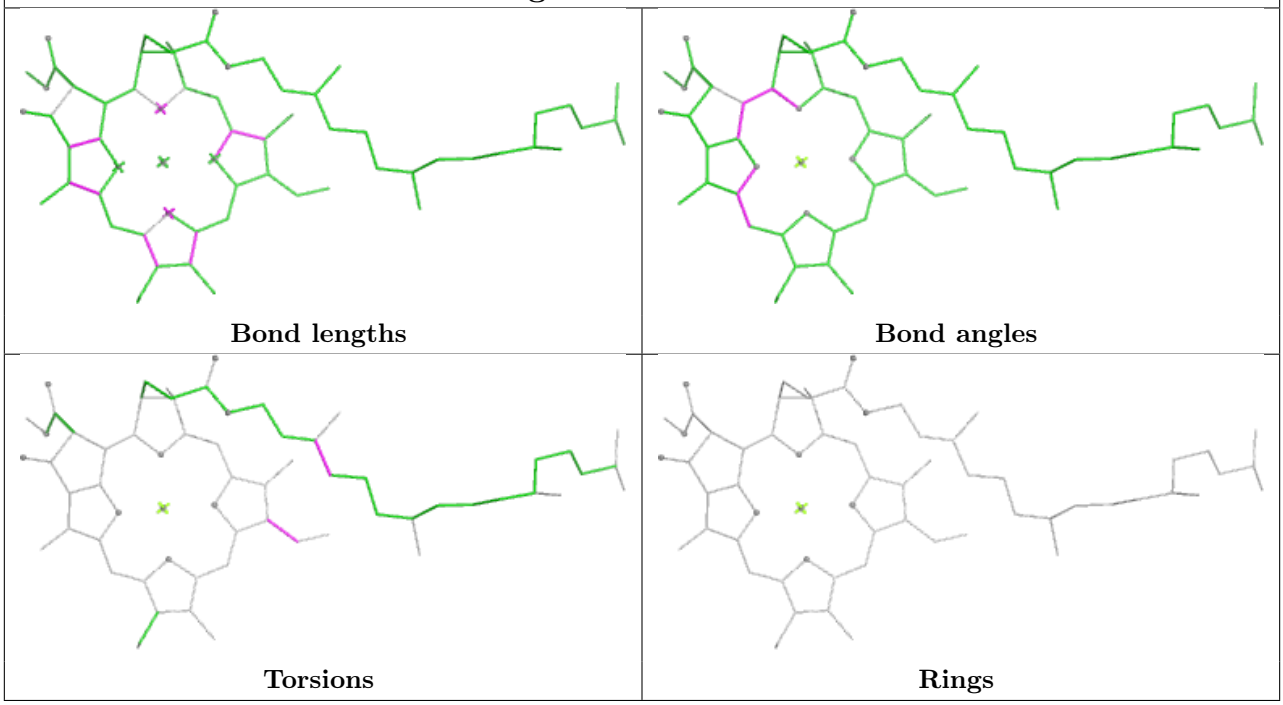
Ligand CLA C 508



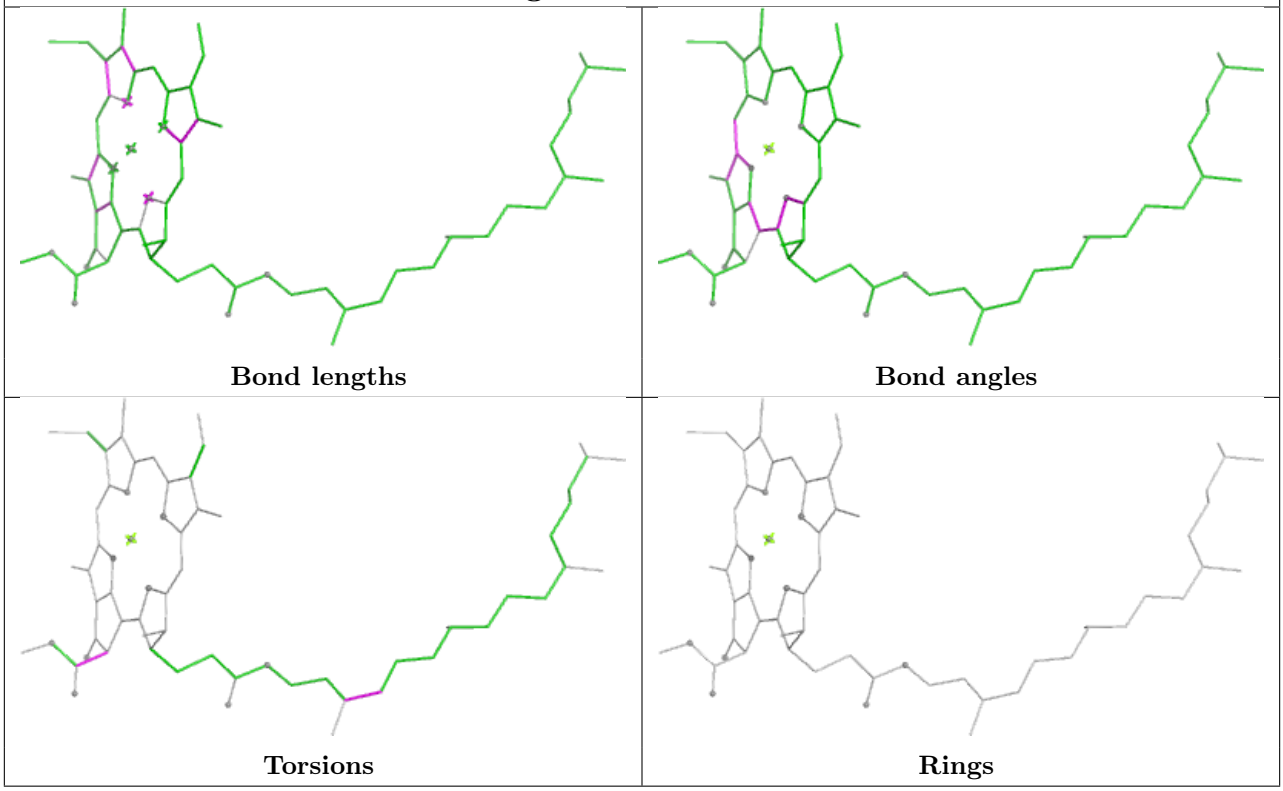
Ligand HEM F 101



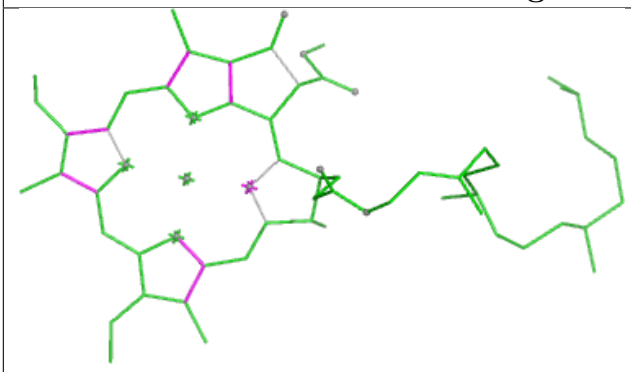
Ligand CLA b 604



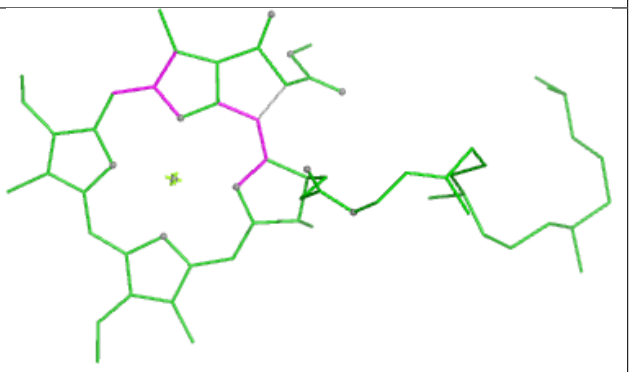
Ligand CLA B 610



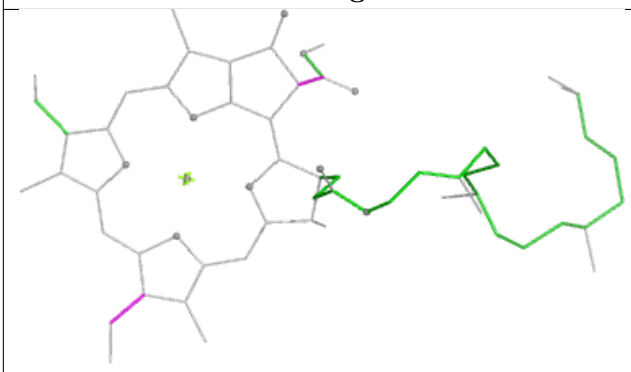
Ligand CLA b 613



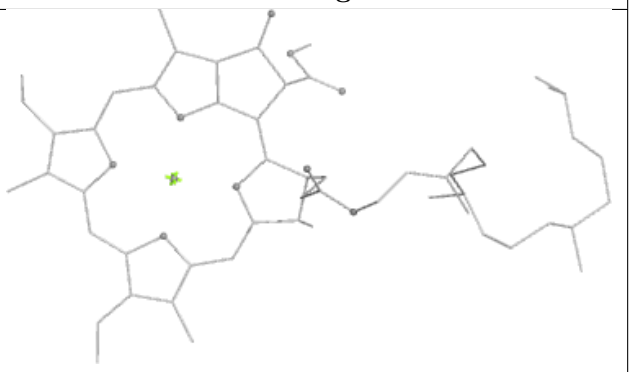
Bond lengths



Bond angles

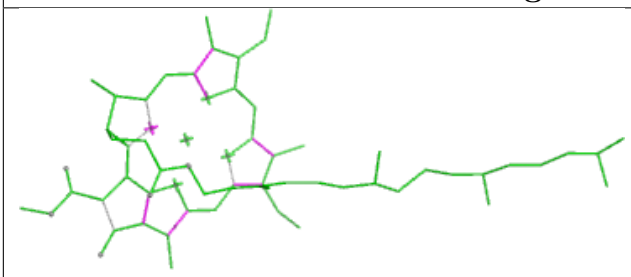


Torsions

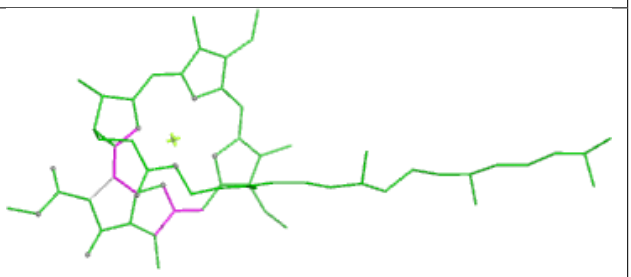


Rings

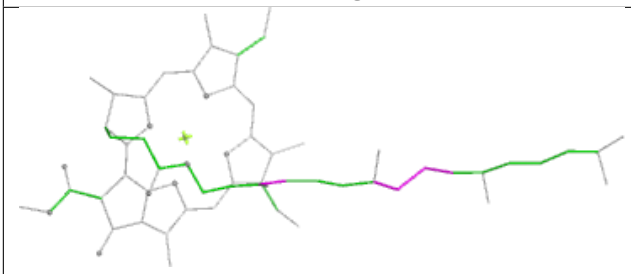
Ligand CLA B 615



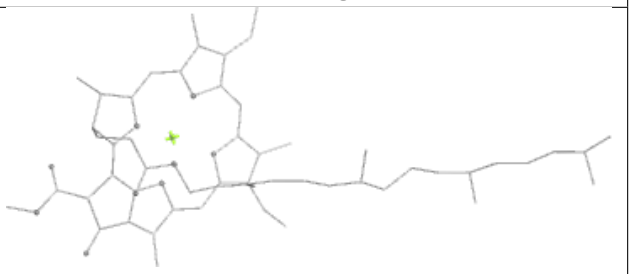
Bond lengths



Bond angles

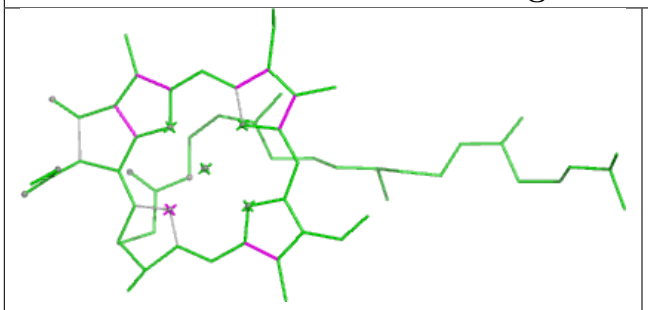


Torsions

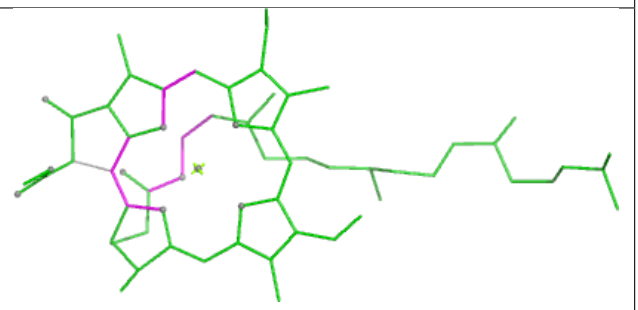


Rings

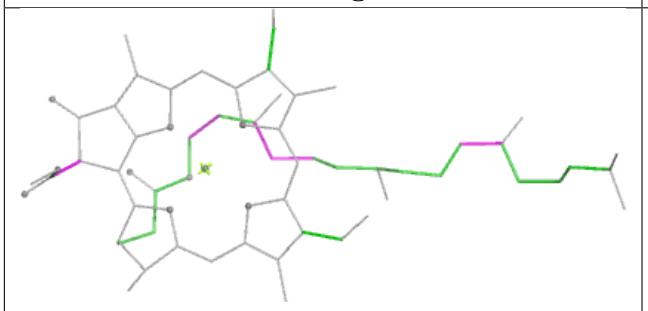
Ligand CLA b 606



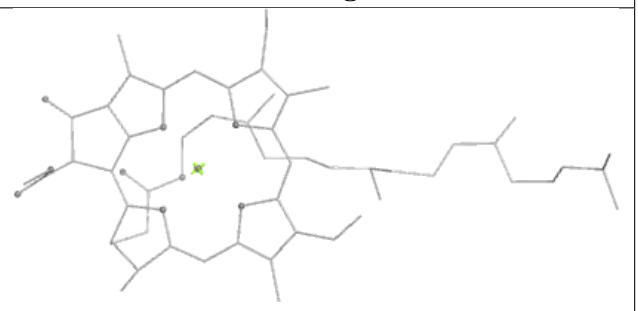
Bond lengths



Bond angles

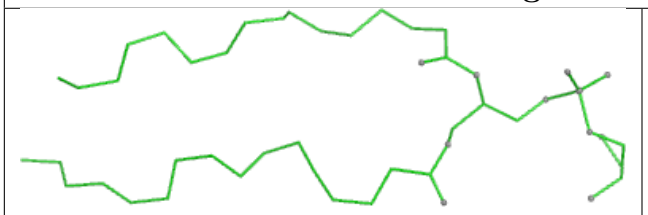


Torsions

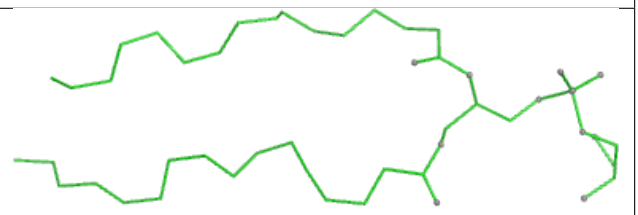


Rings

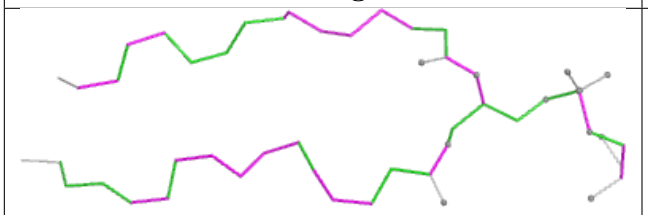
Ligand LHG A 416



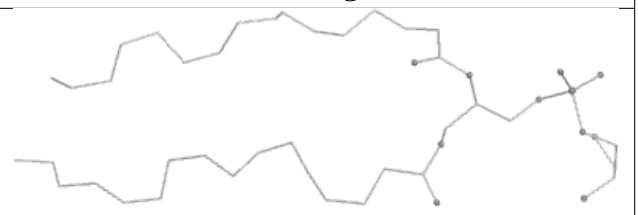
Bond lengths



Bond angles

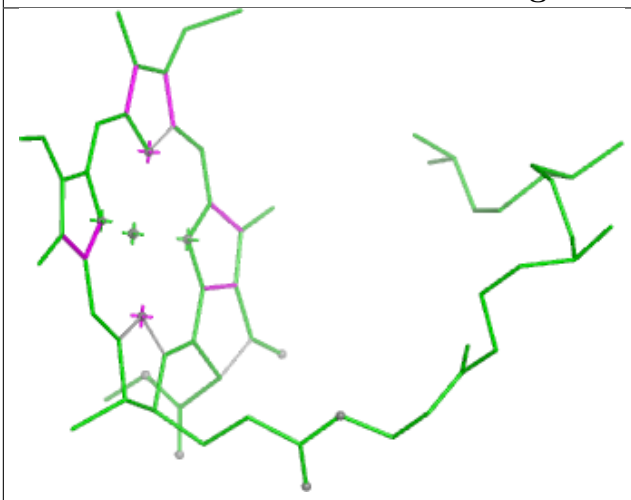


Torsions

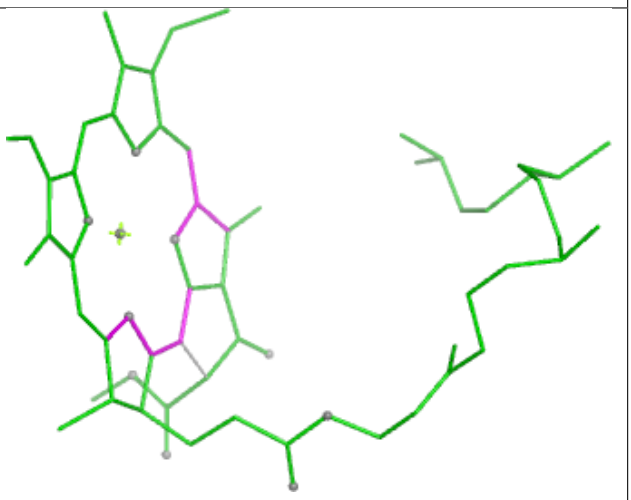


Rings

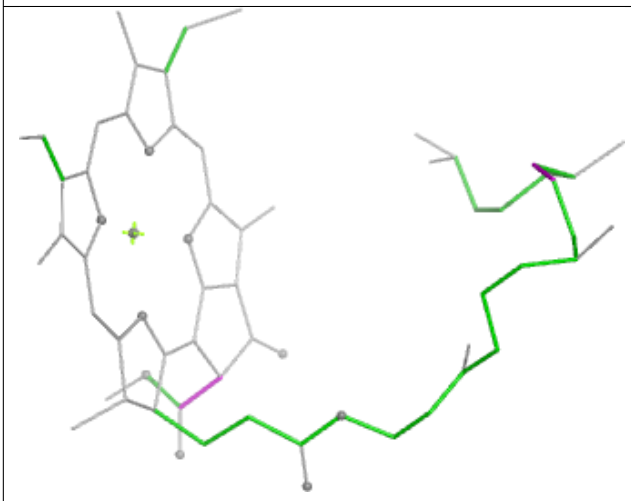
Ligand CLA c 503



Bond lengths



Bond angles



Torsions

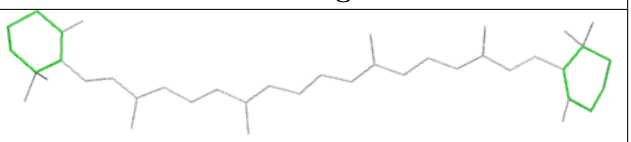
Rings

Ligand BCR b 620

Bond lengths

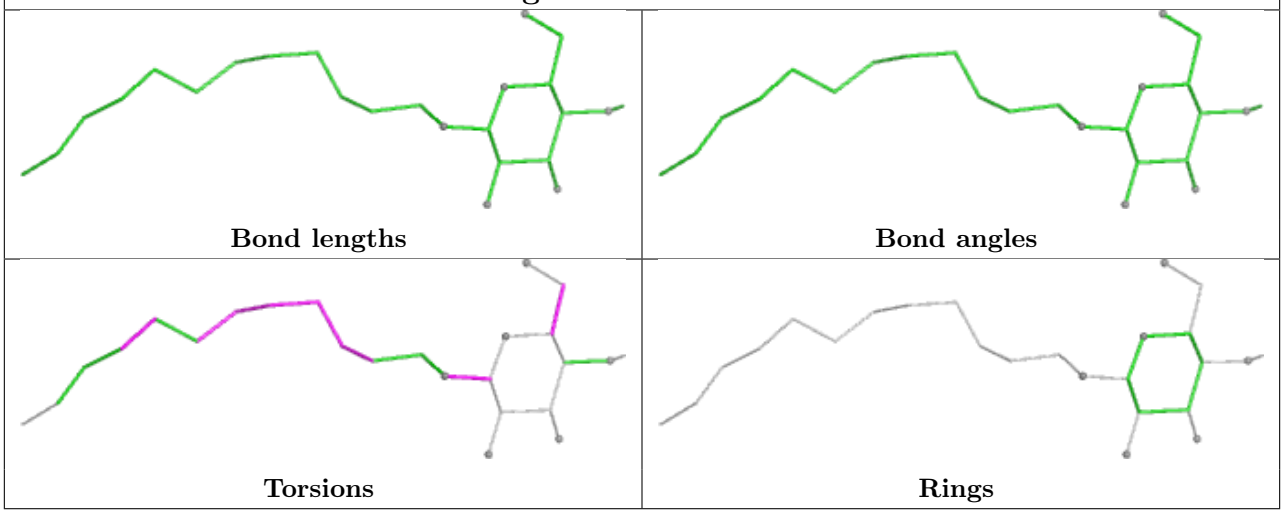
Bond angles

Torsions

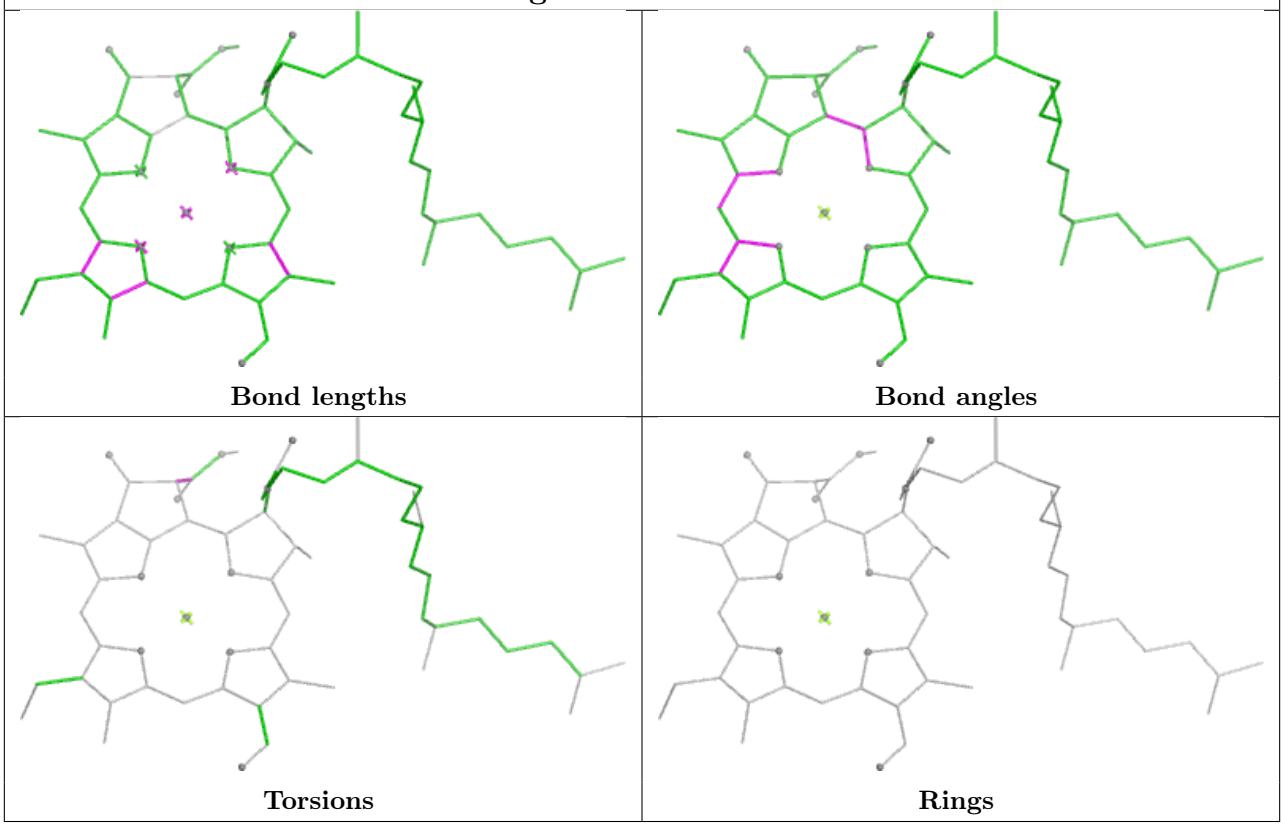


Rings

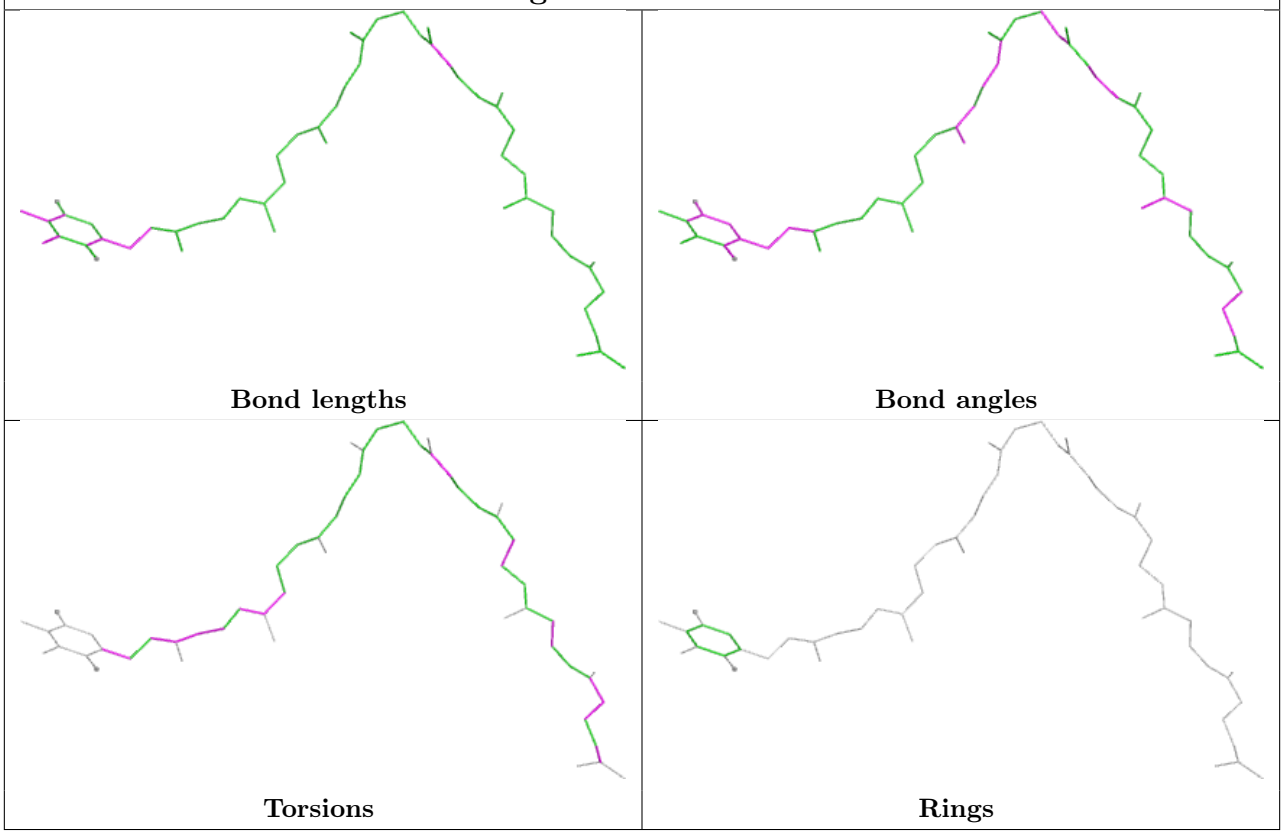
Ligand LMT B 675



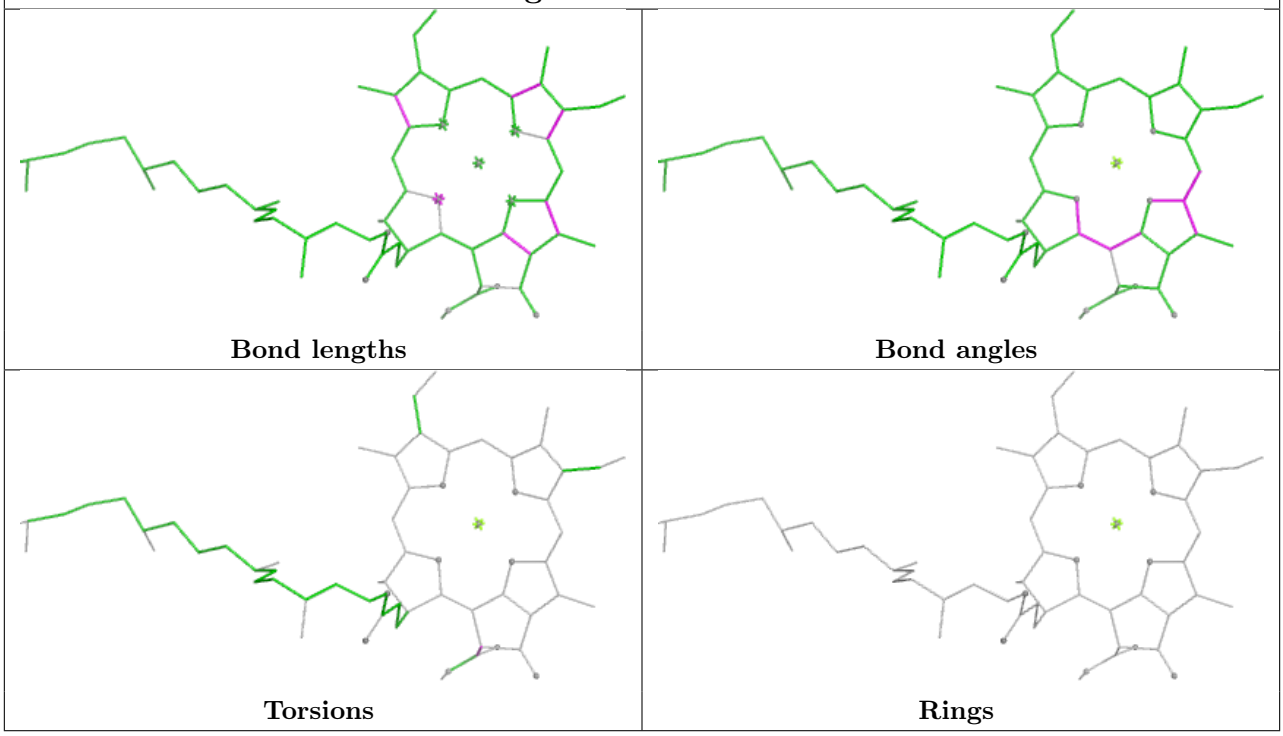
Ligand CL7 A 406



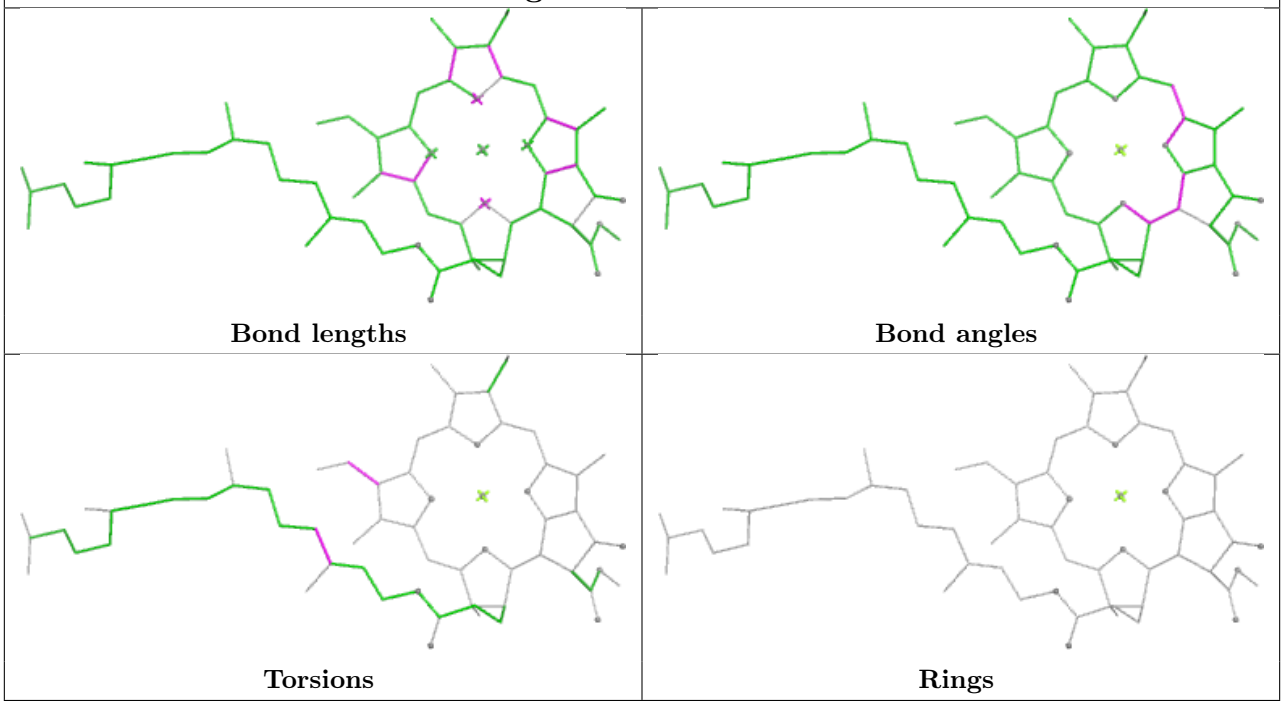
Ligand PL9 D 405



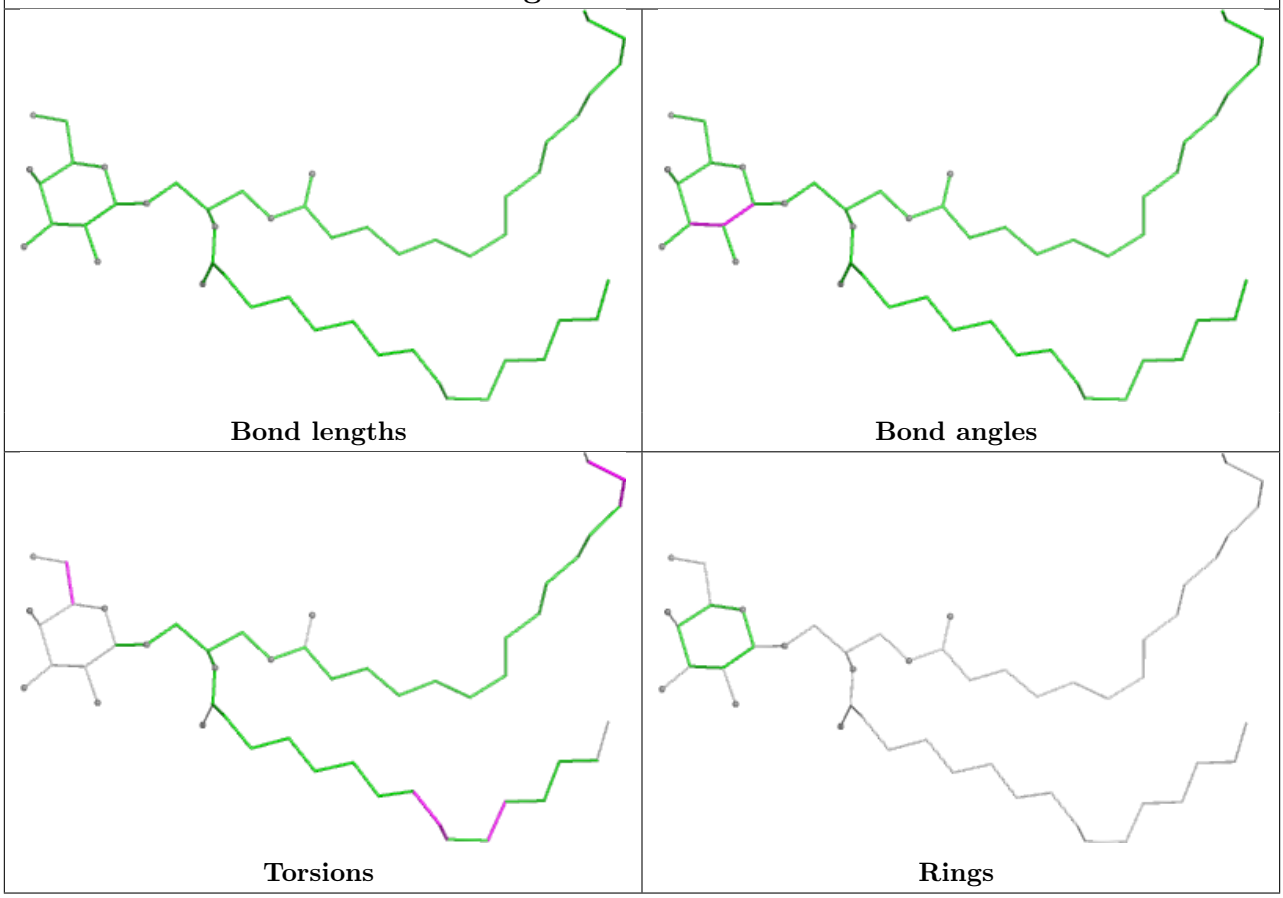
Ligand CLA A 407



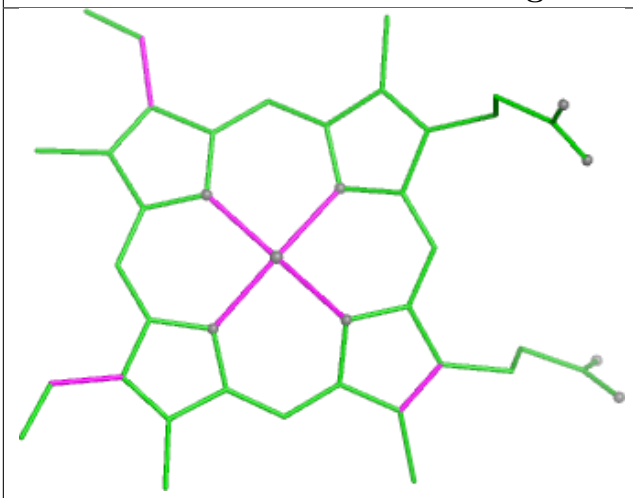
Ligand CLA B 604



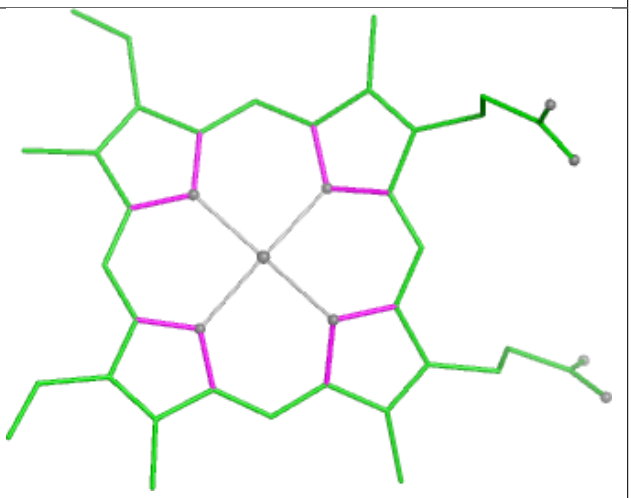
Ligand LMG d 411



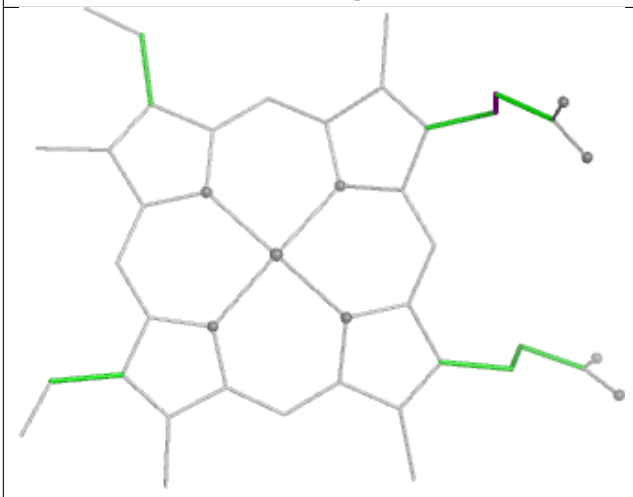
Ligand HEM f 101



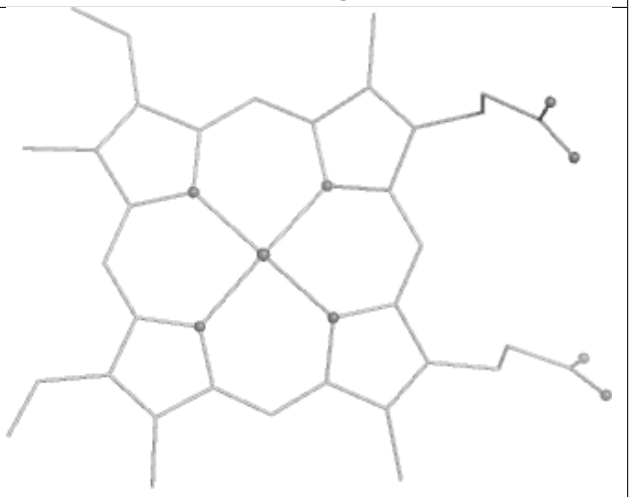
Bond lengths



Bond angles

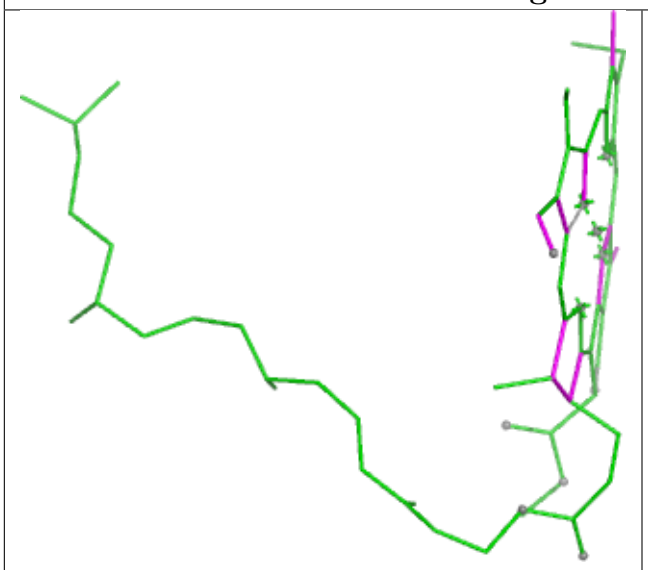


Torsions

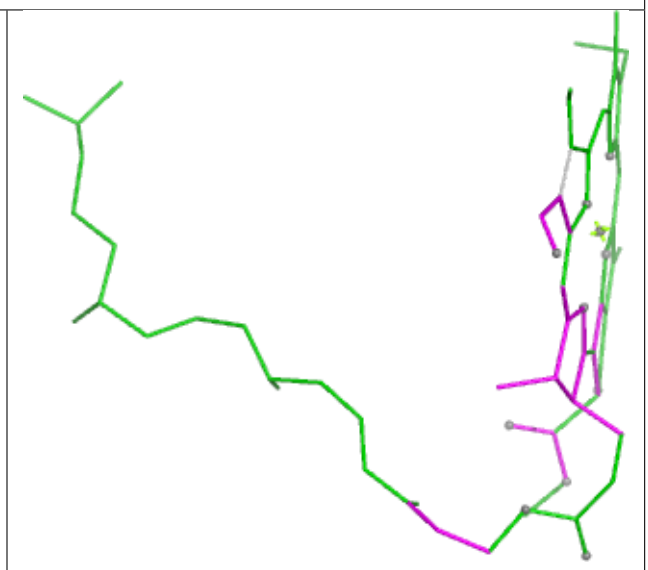


Rings

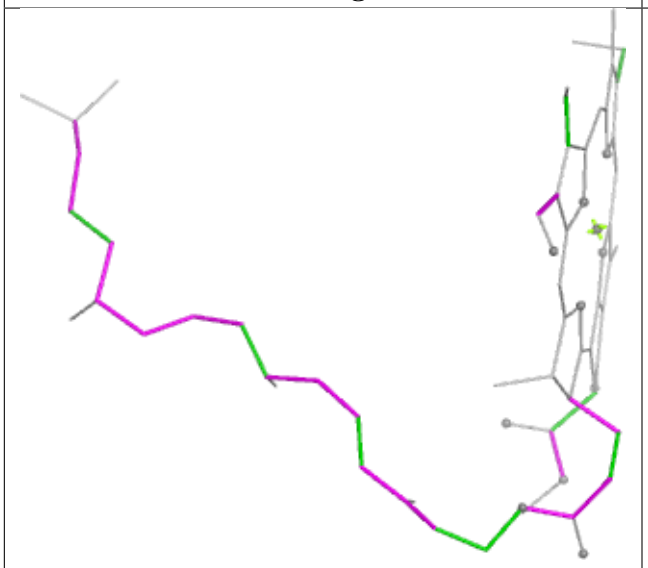
Ligand F6C B 614



Bond lengths



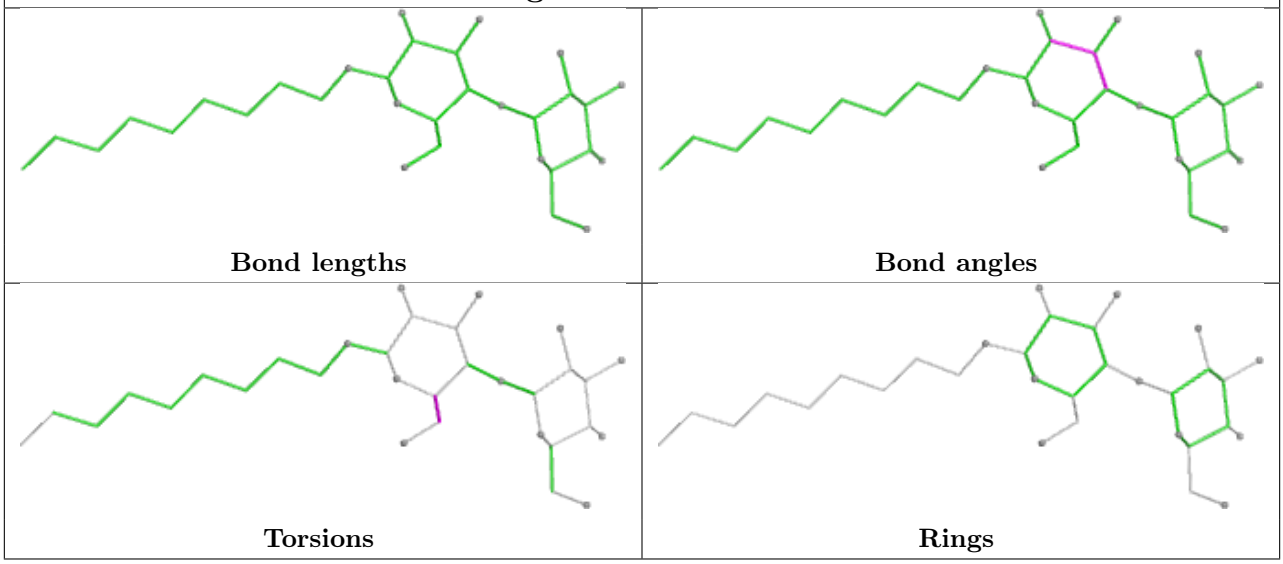
Bond angles



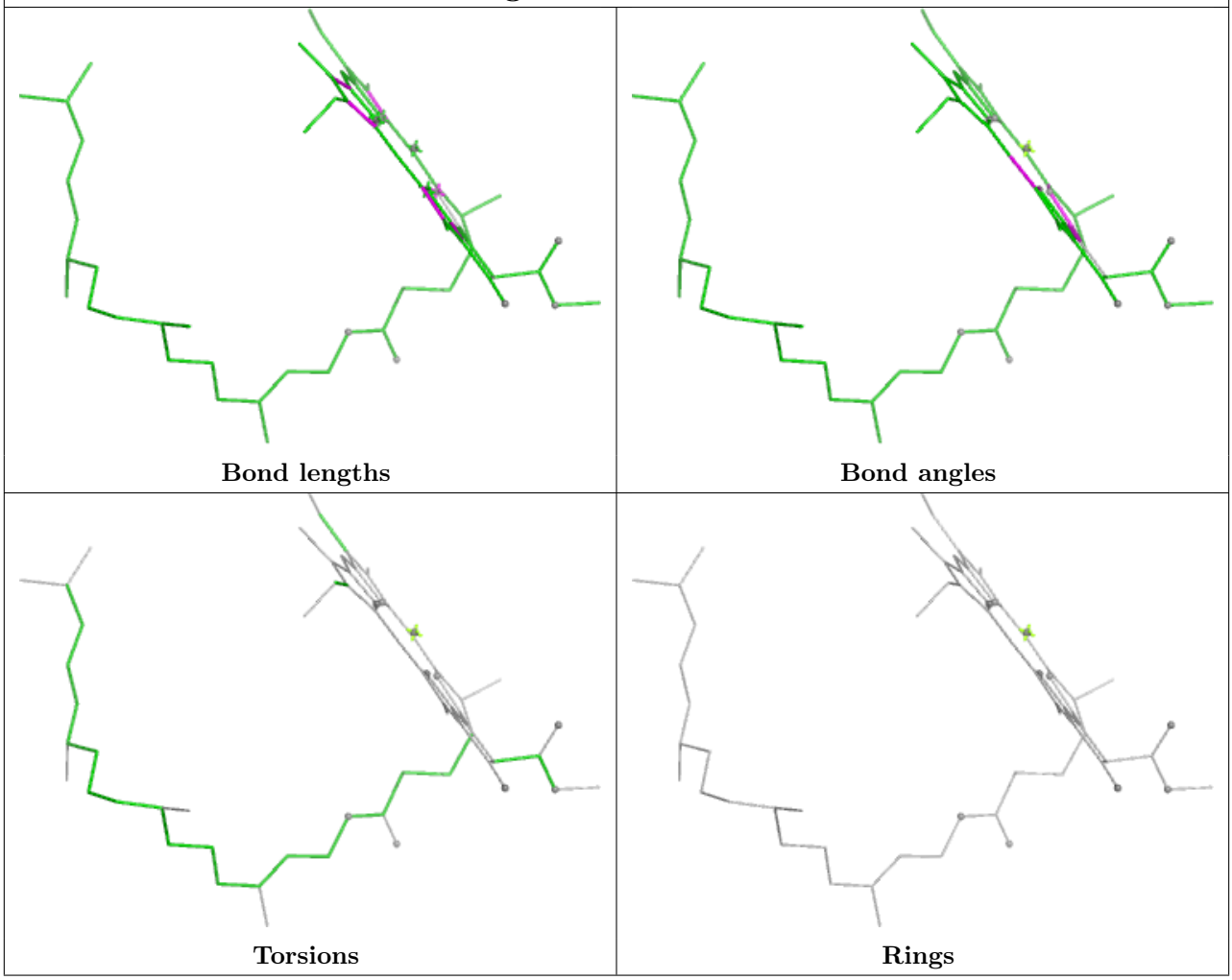
Torsions

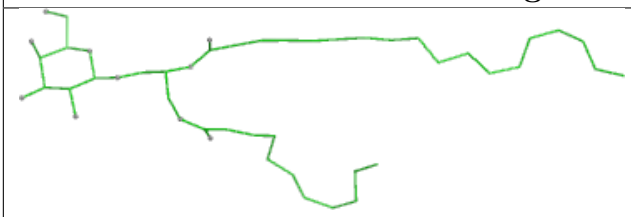
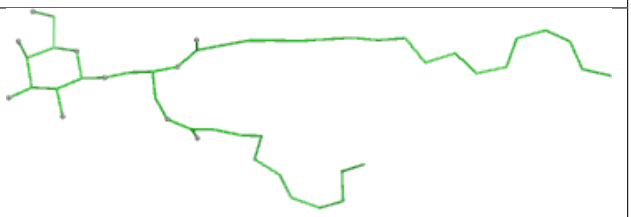
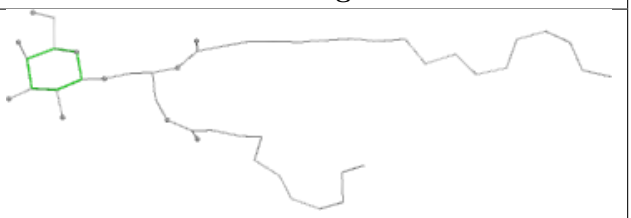
Rings

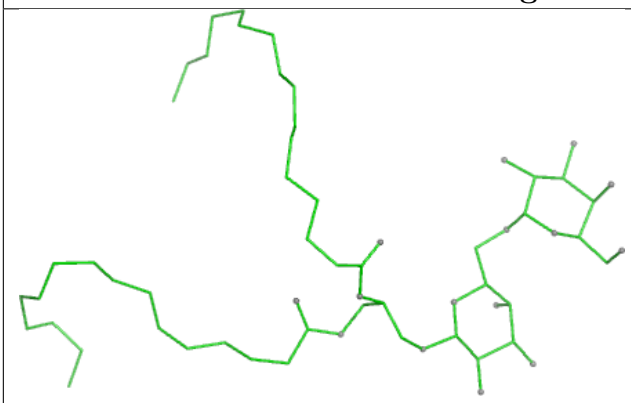
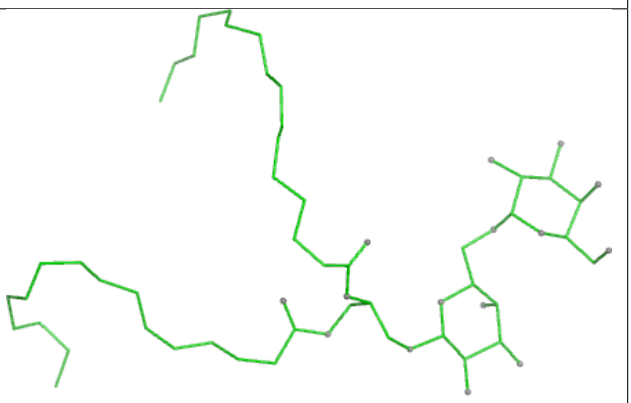
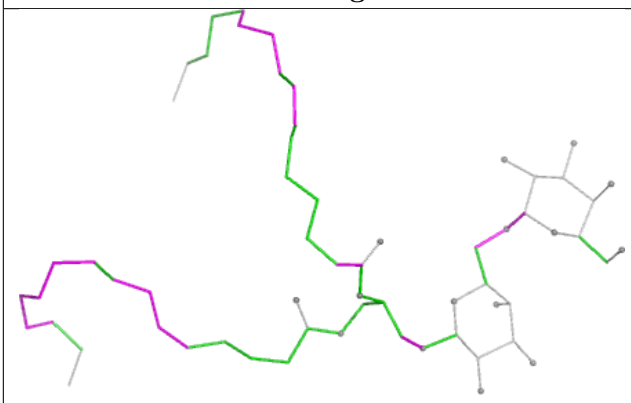
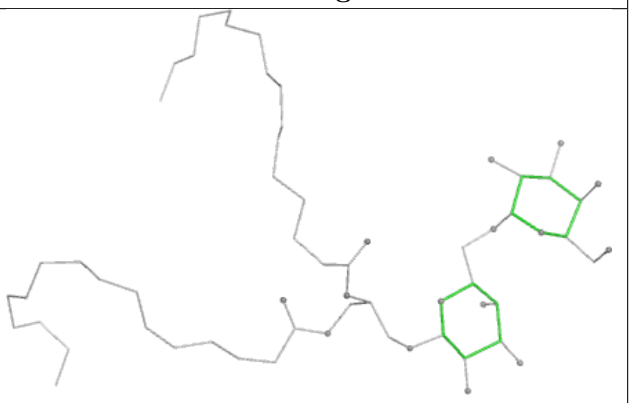
Ligand LMT a 675

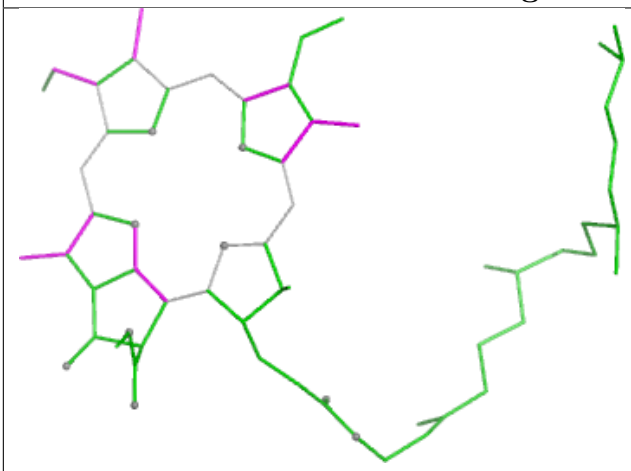
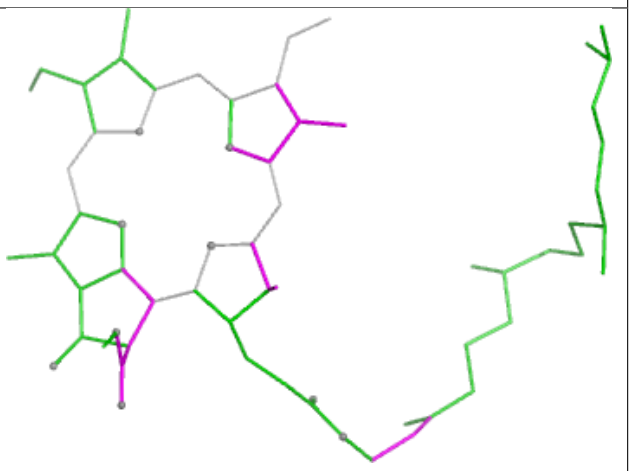
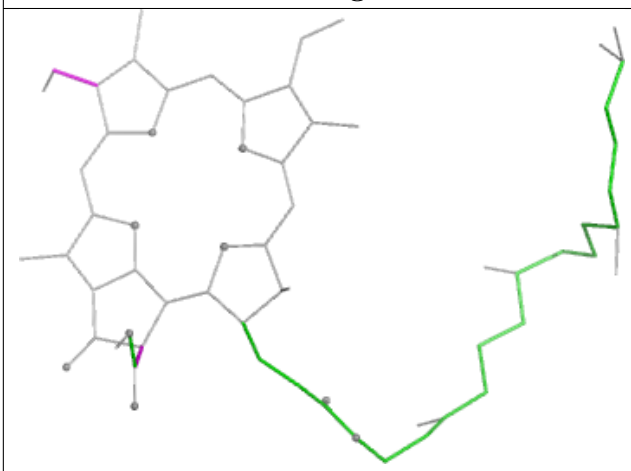
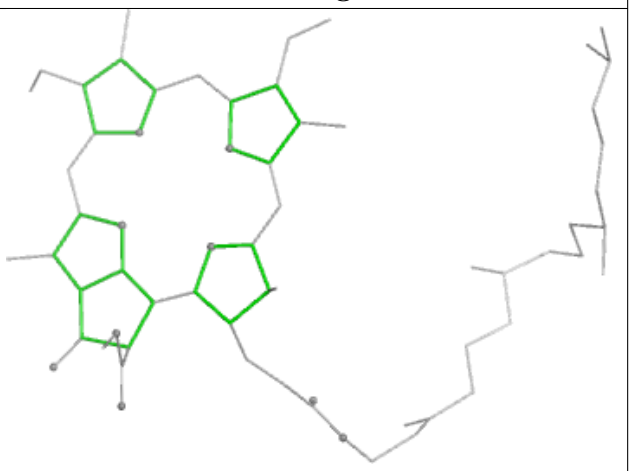


Ligand CLA B 612

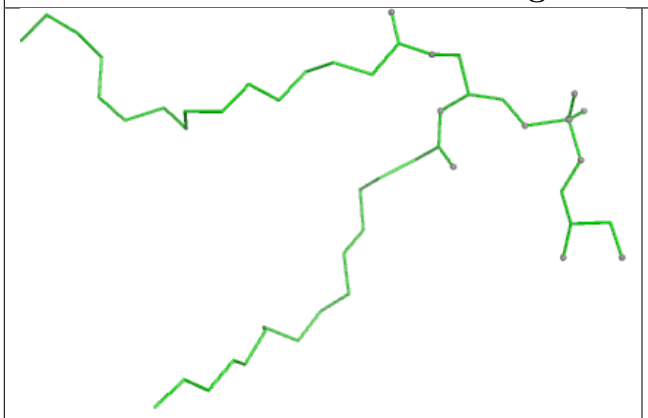


Ligand LMG a 415	
 Bond lengths	 Bond angles
Torsions	 Rings

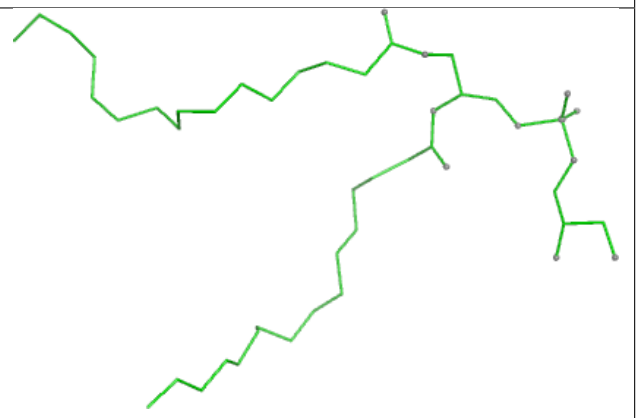
Ligand DGD C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

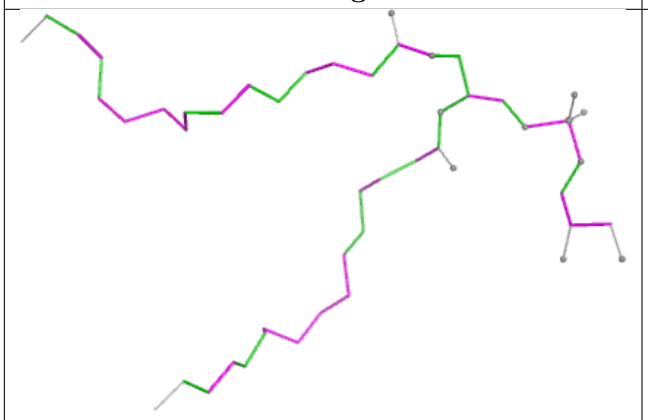
Ligand LHG e 101



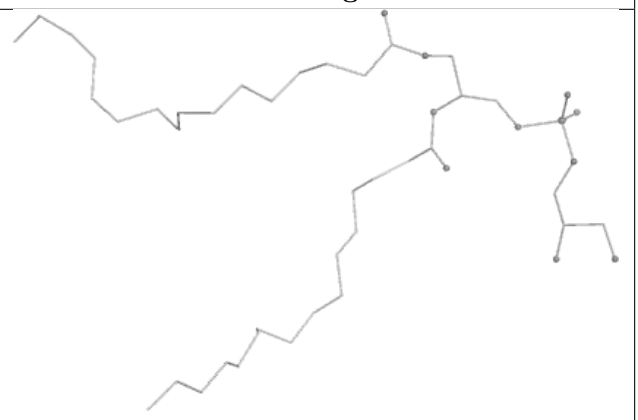
Bond lengths



Bond angles

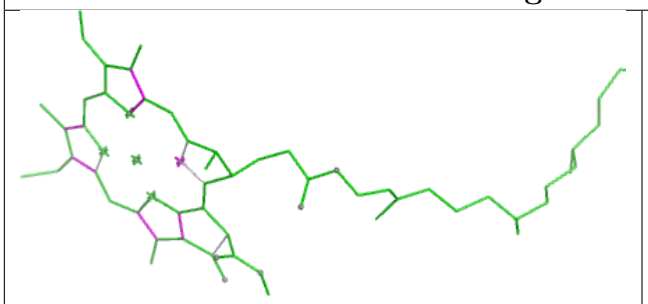


Torsions

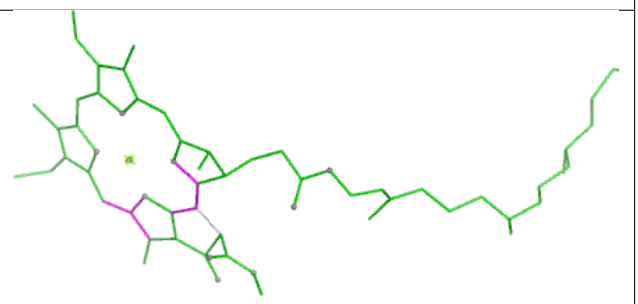


Rings

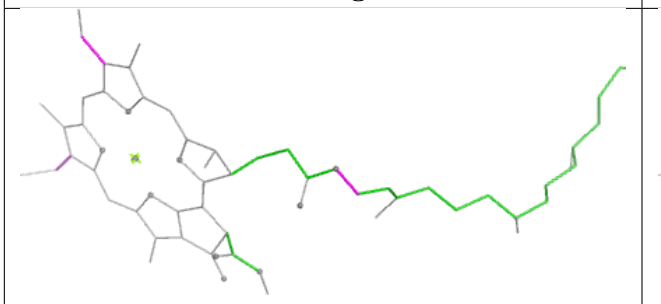
Ligand CLA A 405



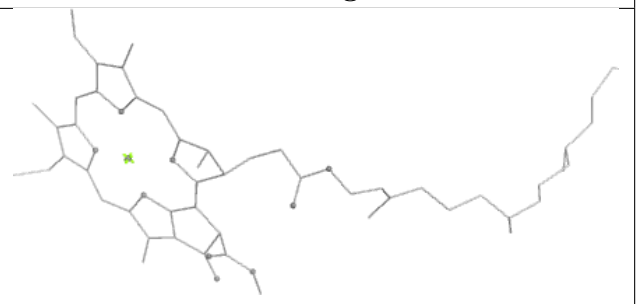
Bond lengths



Bond angles

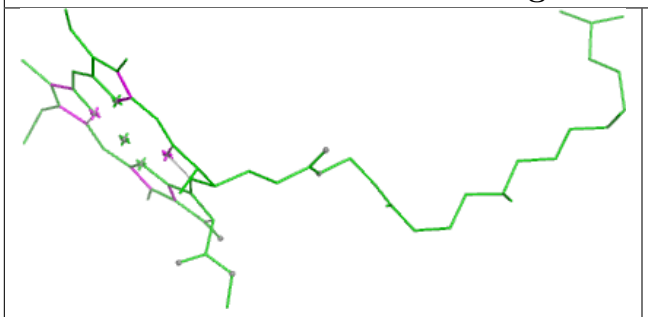


Torsions

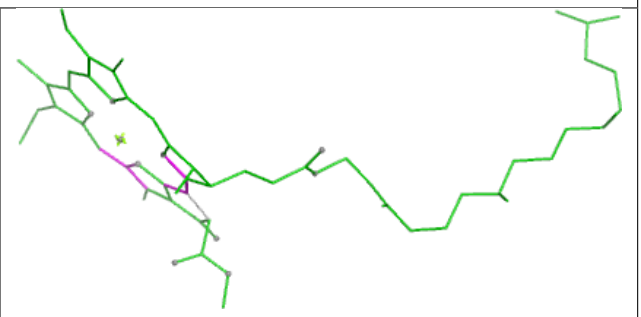


Rings

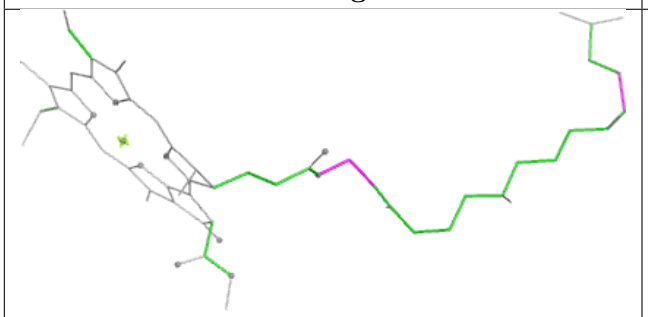
Ligand CLA d 402



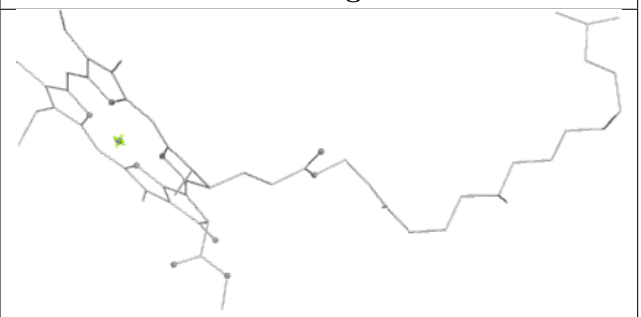
Bond lengths



Bond angles

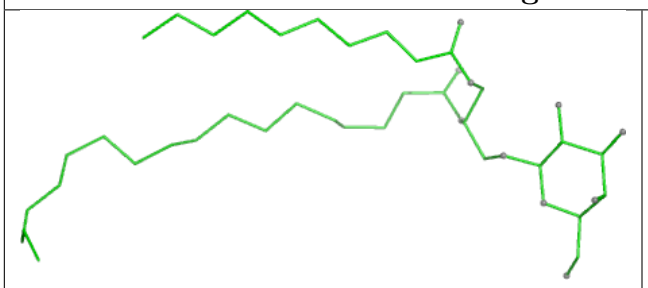


Torsions

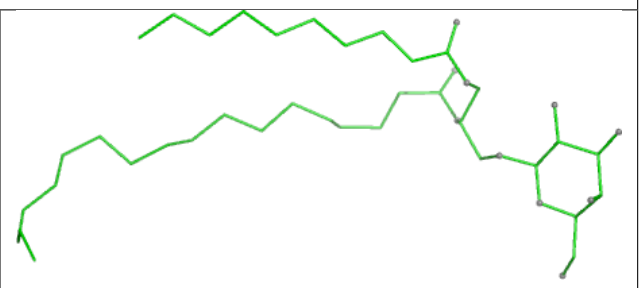


Rings

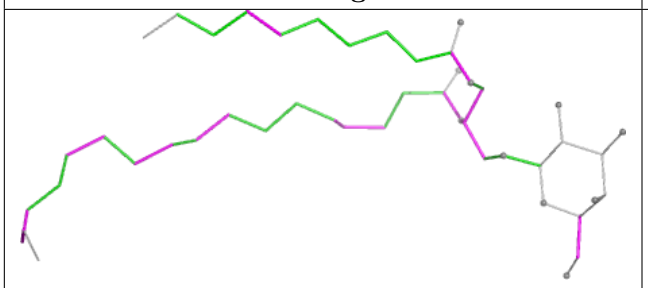
Ligand LMG P 628



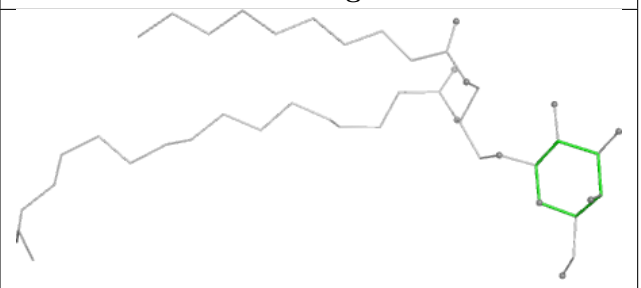
Bond lengths



Bond angles

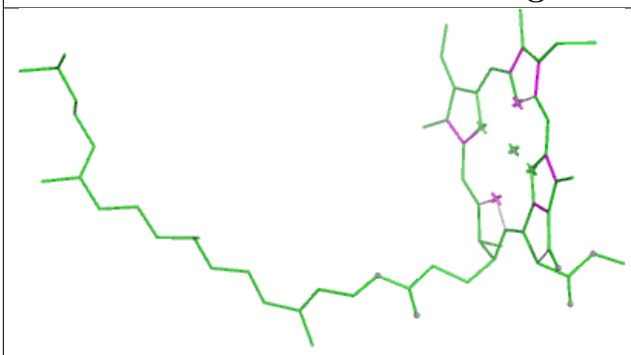


Torsions

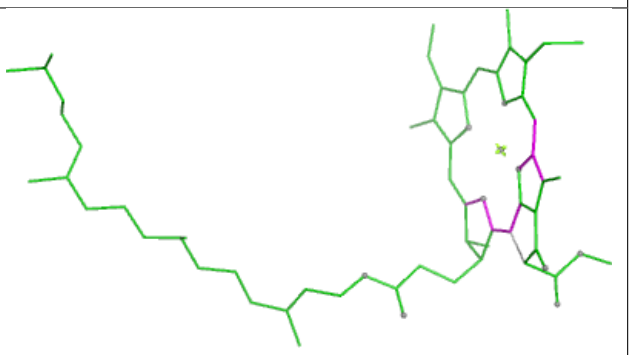


Rings

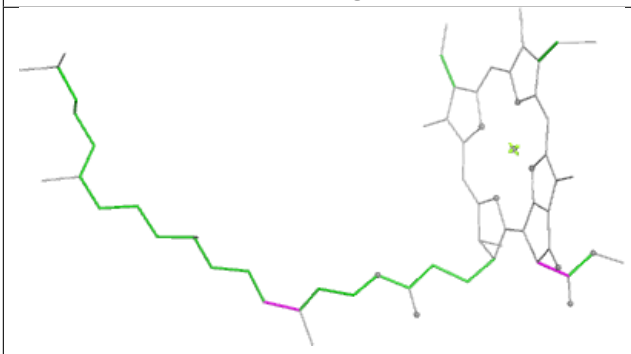
Ligand CLA b 610



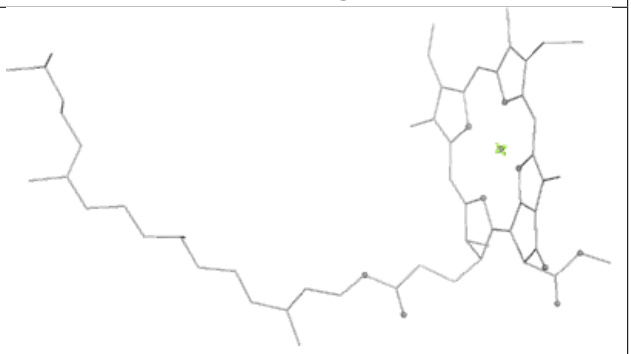
Bond lengths



Bond angles

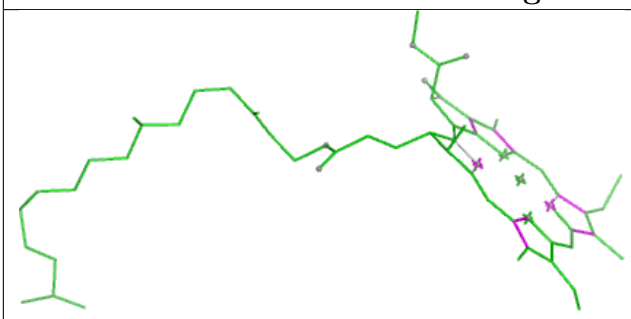


Torsions

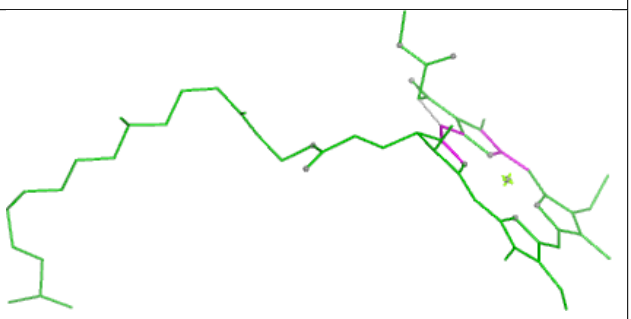


Rings

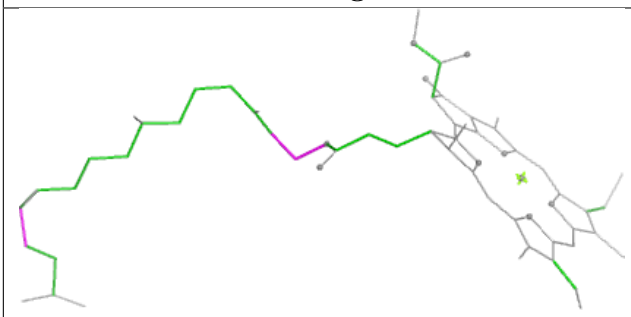
Ligand CLA D 402



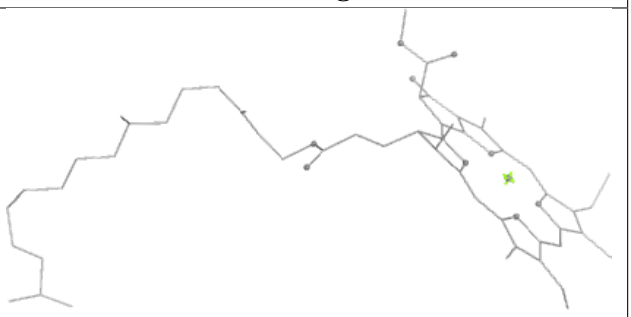
Bond lengths



Bond angles

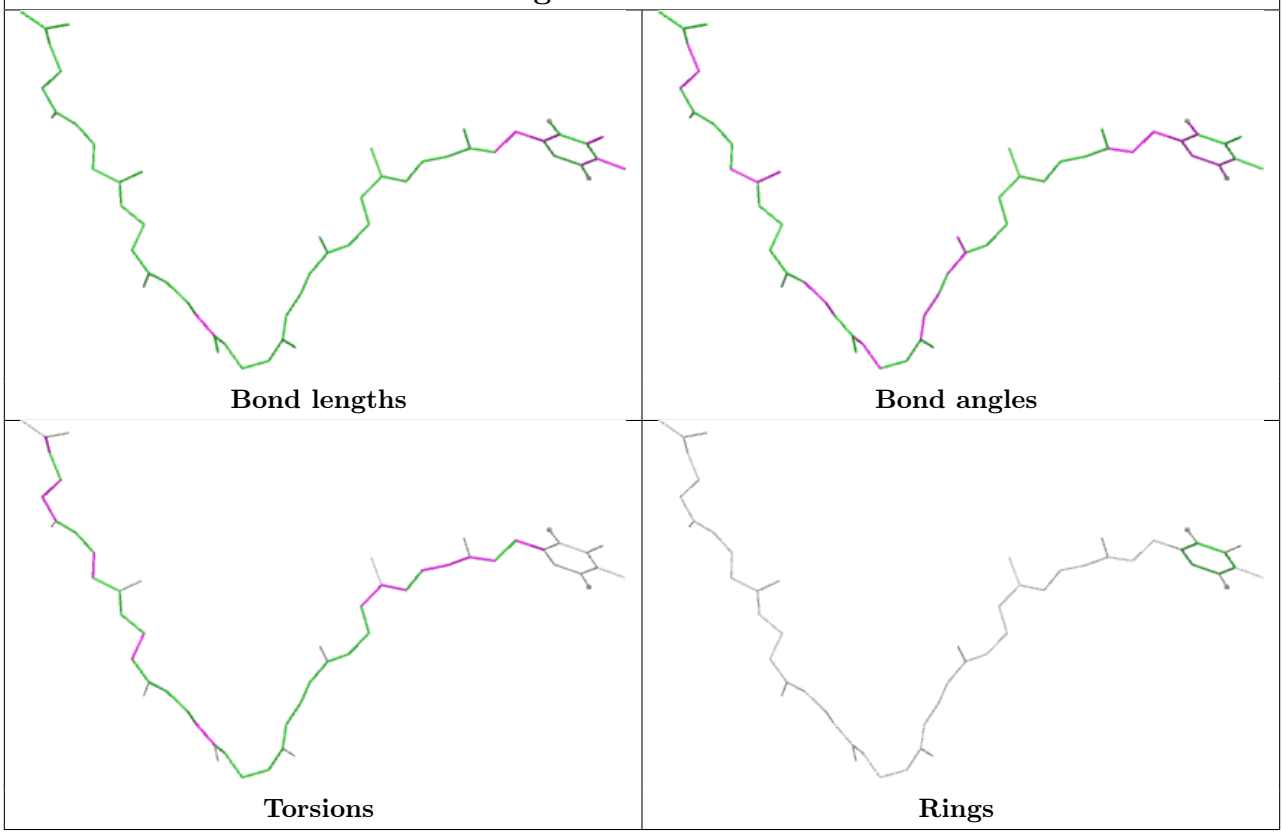


Torsions

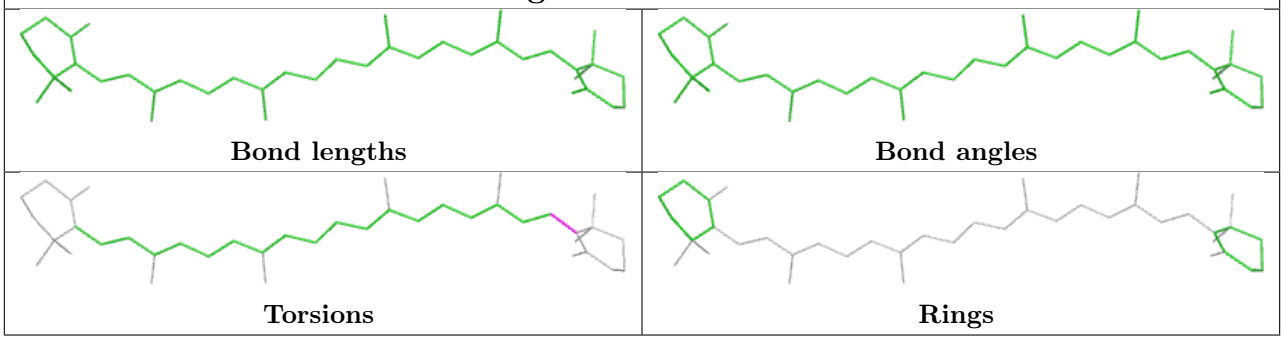


Rings

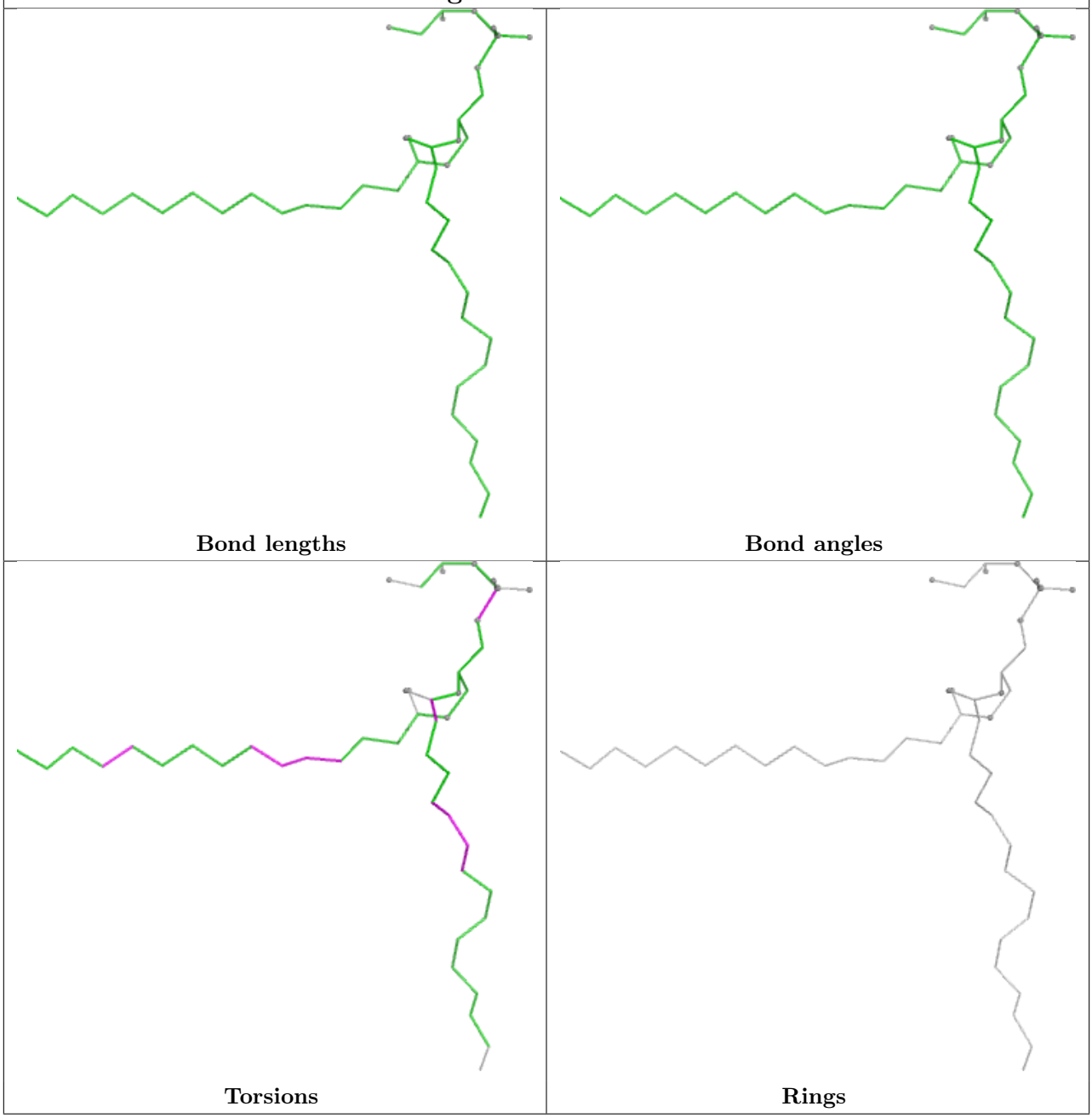
Ligand PL9 d 405

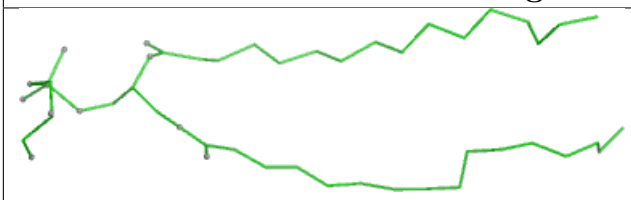
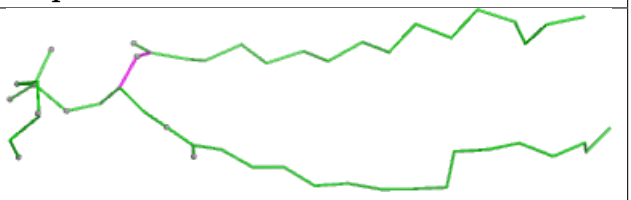
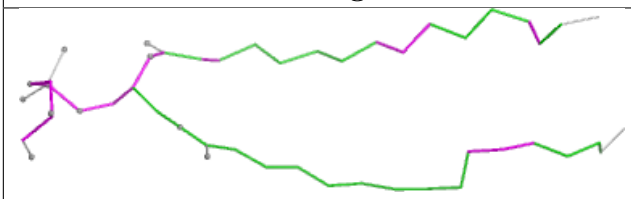
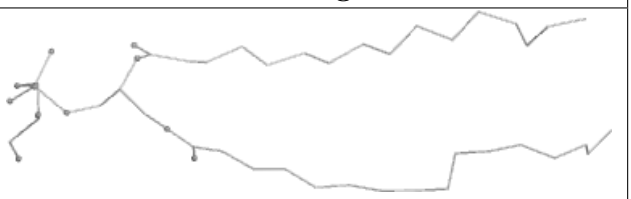


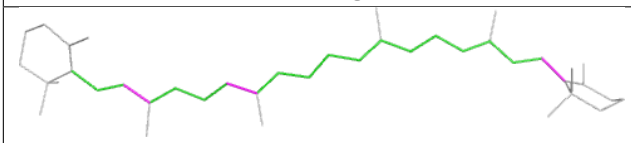
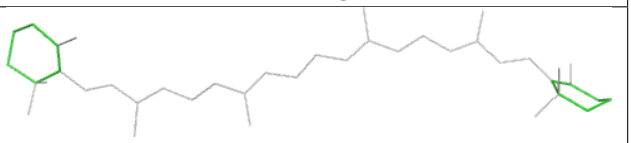
Ligand BCR a 411

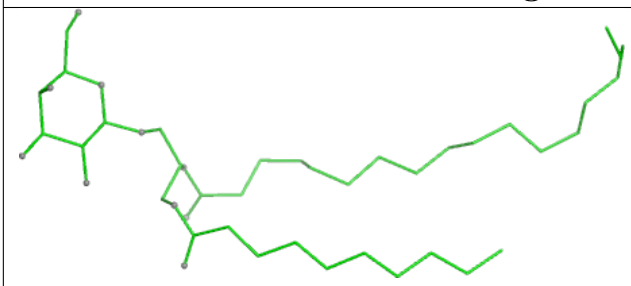
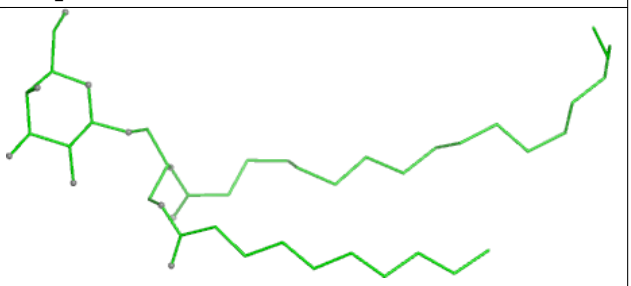
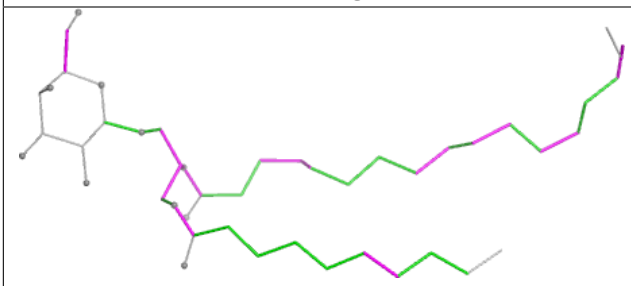
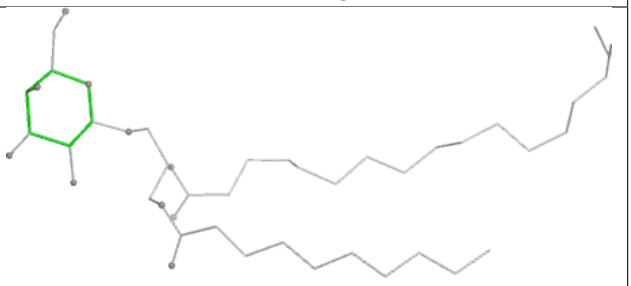


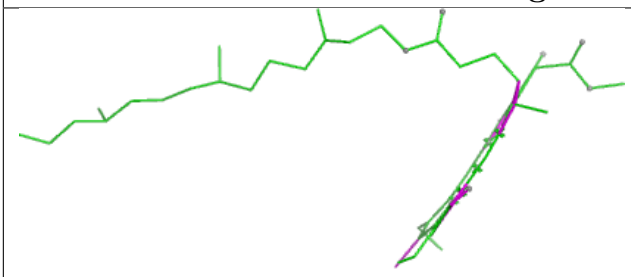
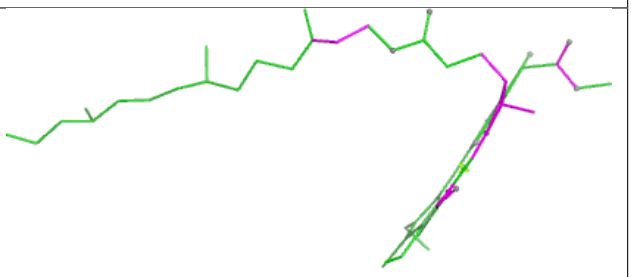
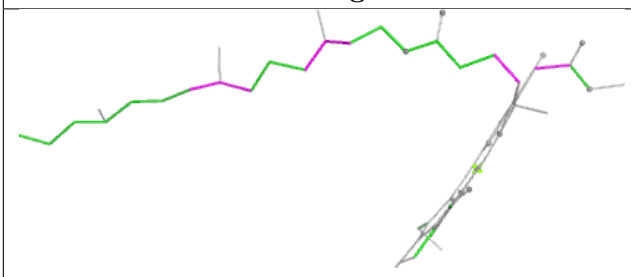
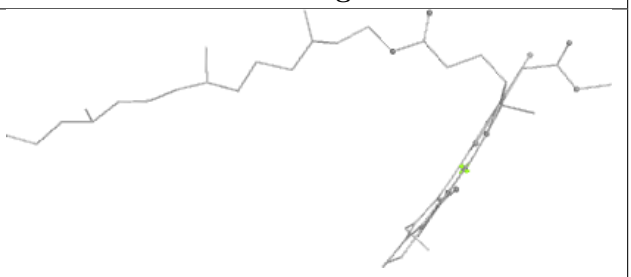
Ligand LHG L 101

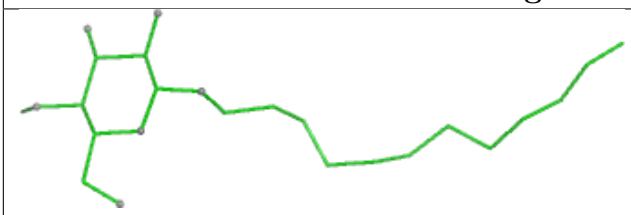
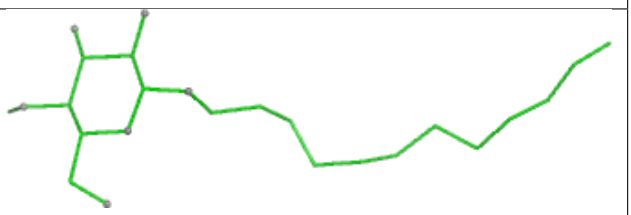
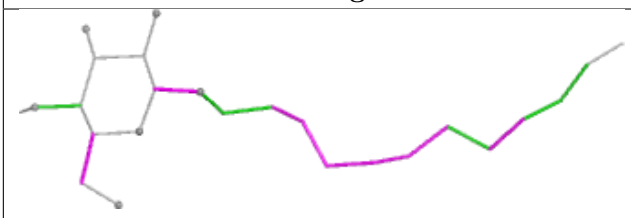
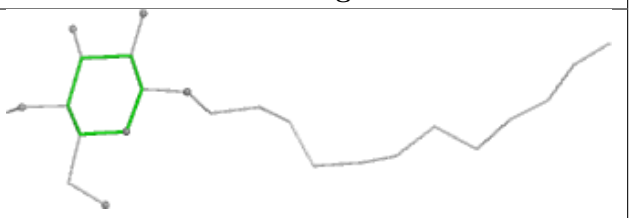


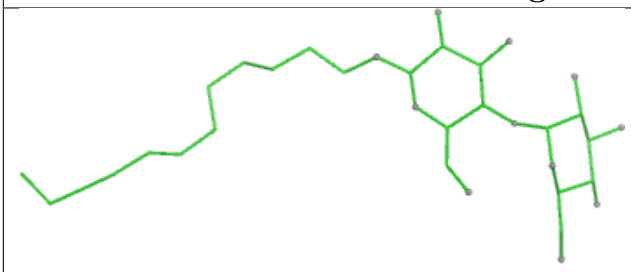
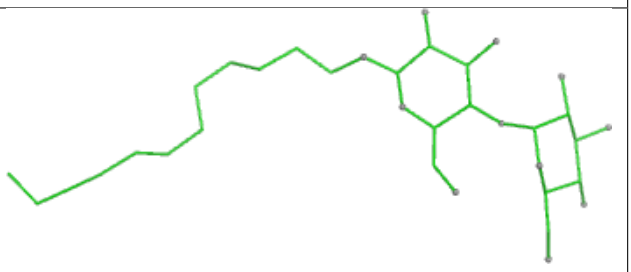
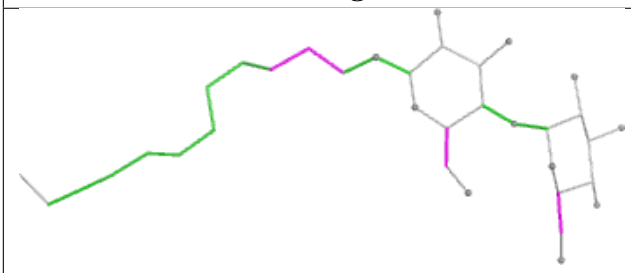
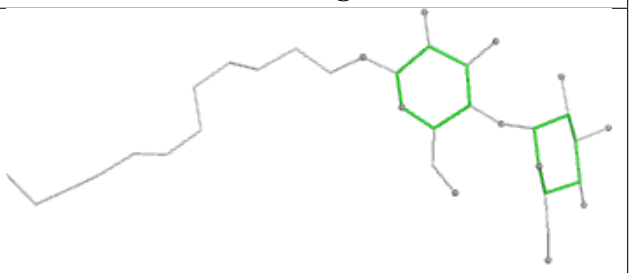
Ligand LHG p 629	
 Bond lengths	 Bond angles
 Torsions	 Rings

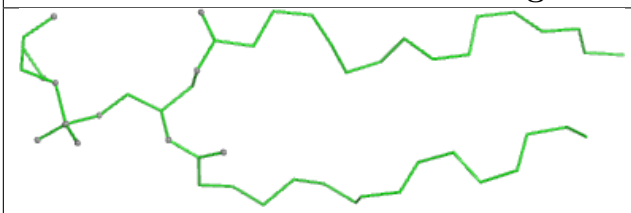
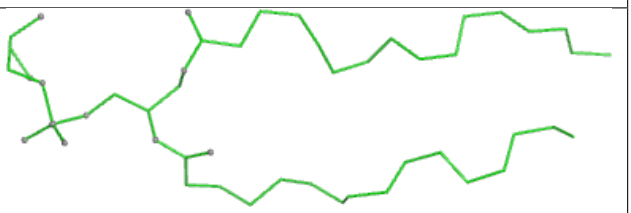
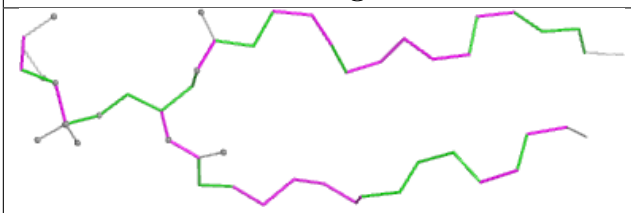
Ligand BCR K 101	
Bond lengths	Bond angles
 Torsions	 Rings

Ligand LMG p 628	
 Bond lengths	 Bond angles
 Torsions	 Rings

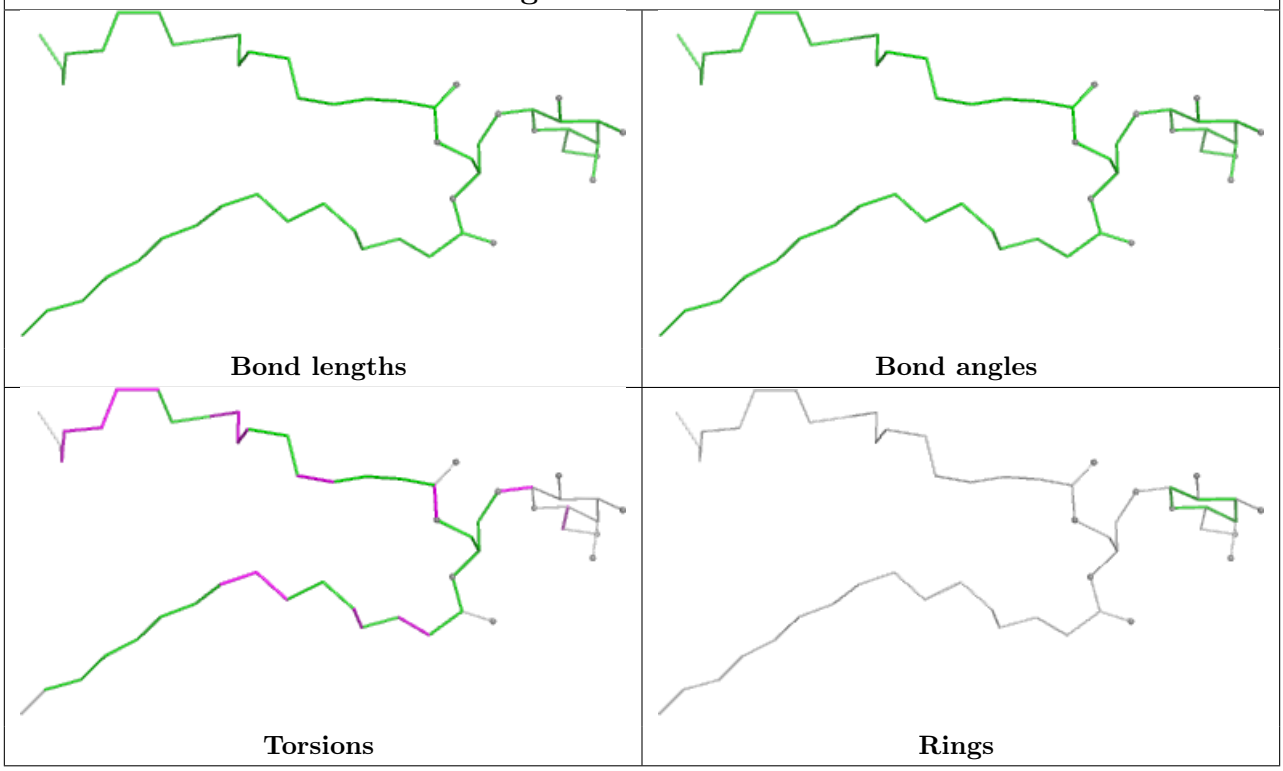
Ligand F6C B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT b 675	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT f 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG a 416	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LMG C 902



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

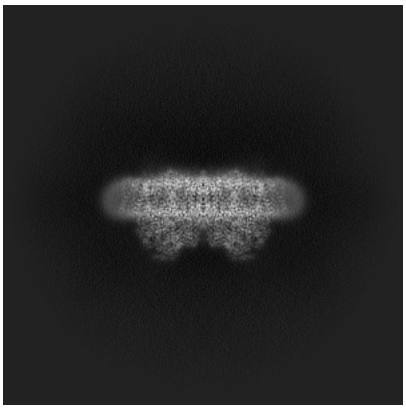
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55593. These allow visual inspection of the internal detail of the map and identification of artifacts.

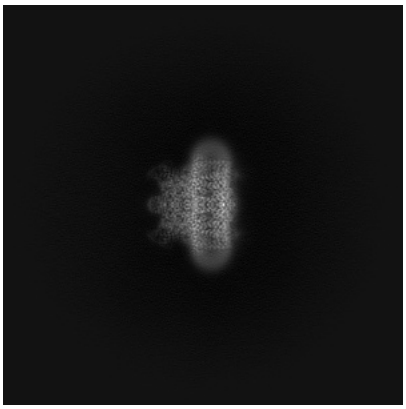
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

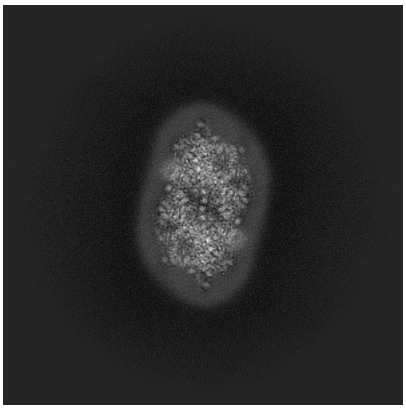
6.1.1 Primary map



X

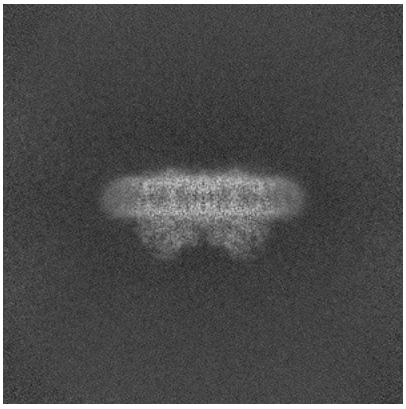


Y

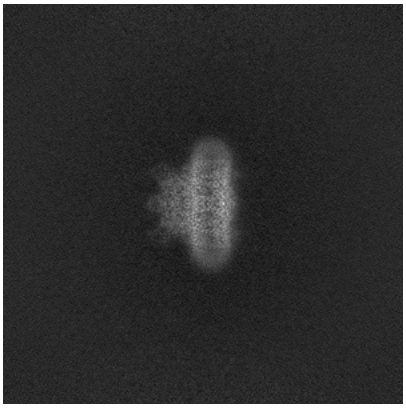


Z

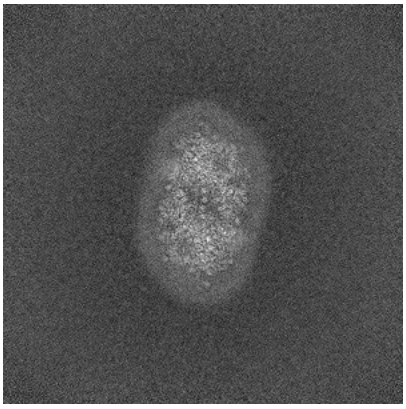
6.1.2 Raw map



X



Y

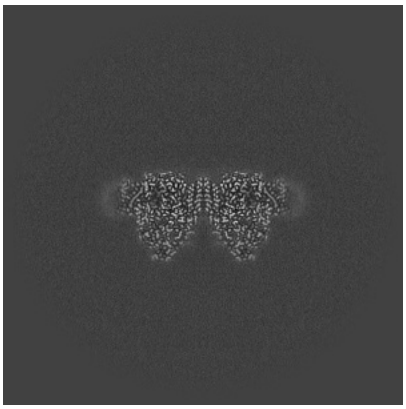


Z

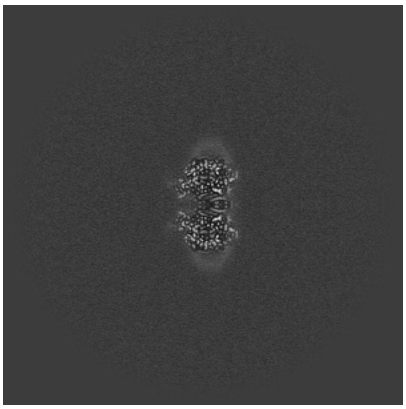
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

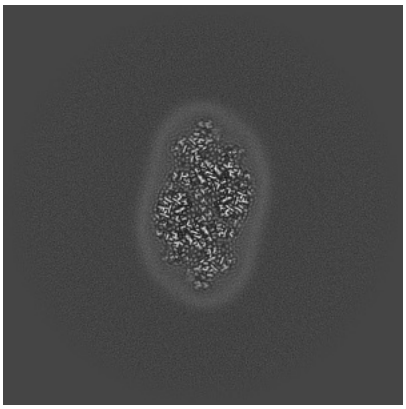
6.2.1 Primary map



X Index: 325

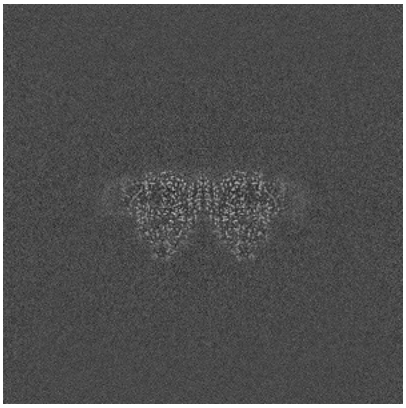


Y Index: 325

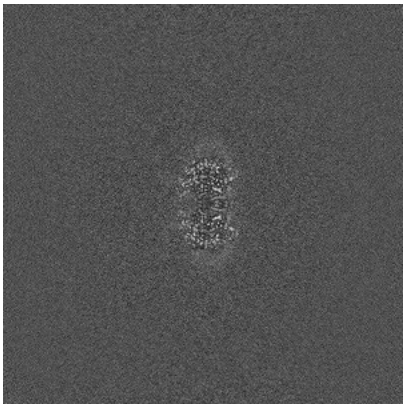


Z Index: 325

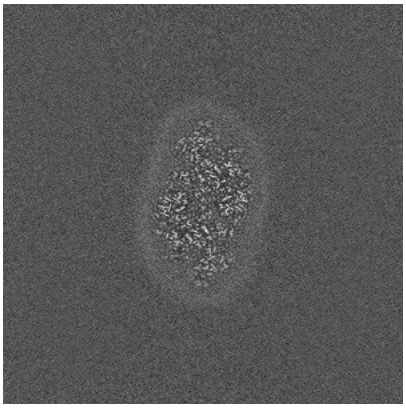
6.2.2 Raw map



X Index: 325



Y Index: 325

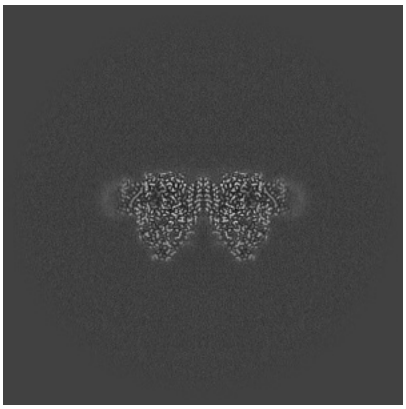


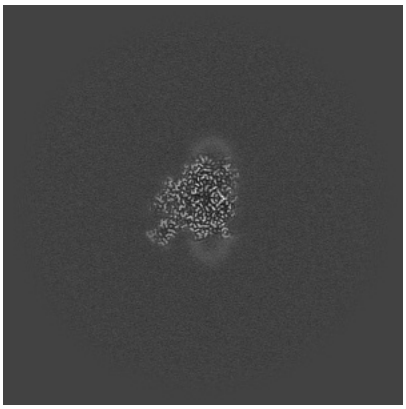
Z Index: 325

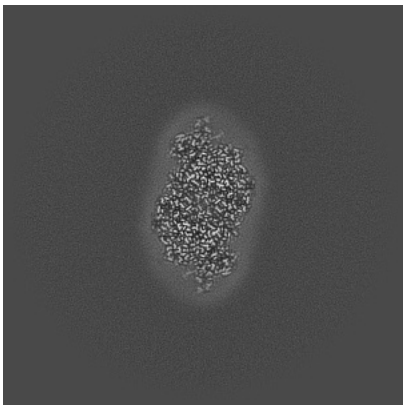
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

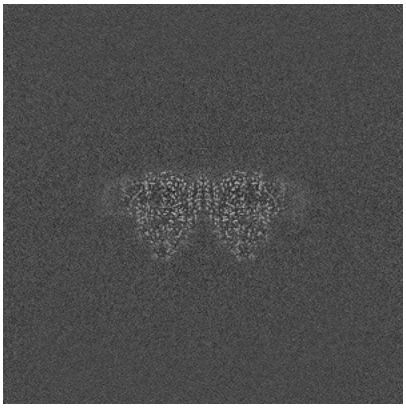
6.3.1 Primary map

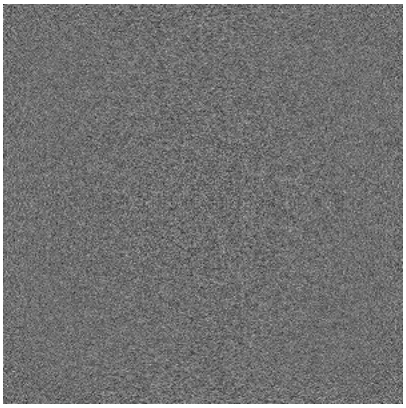

X Index: 325

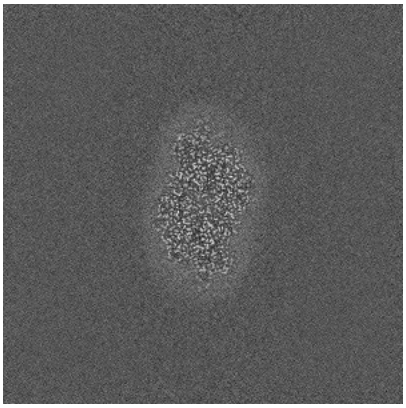

Y Index: 373


Z Index: 313

6.3.2 Raw map


X Index: 325

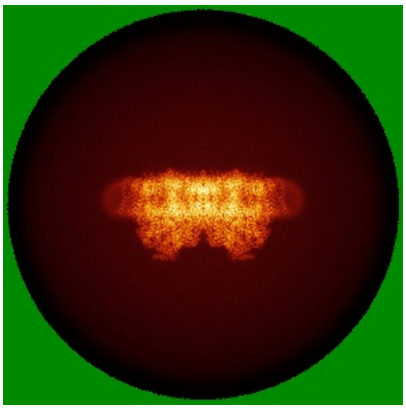

Y Index: 0

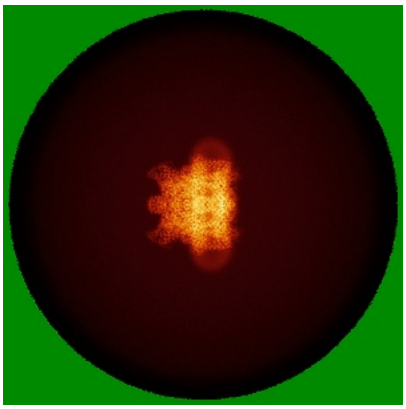

Z Index: 312

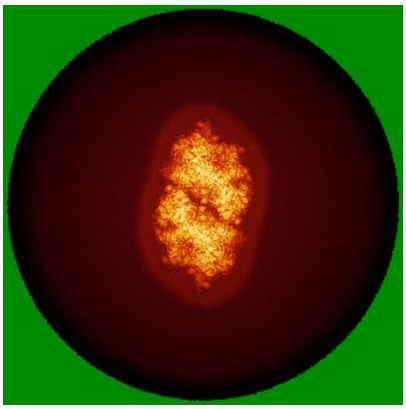
The images above show the largest variance slices of the map in three orthogonal directions.

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

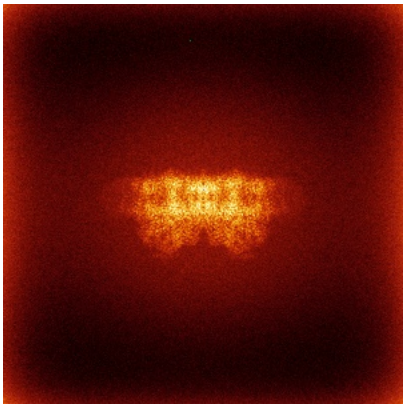
6.4.1 Primary map

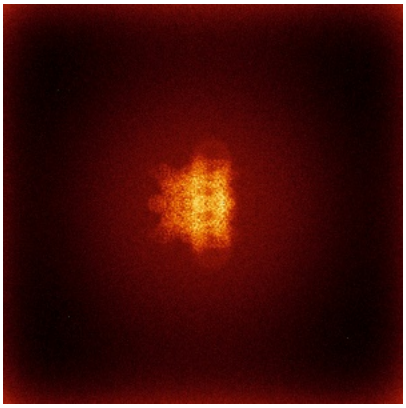

X

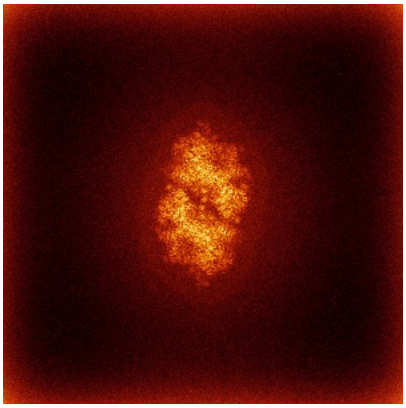

Y


Z

6.4.2 Raw map


X

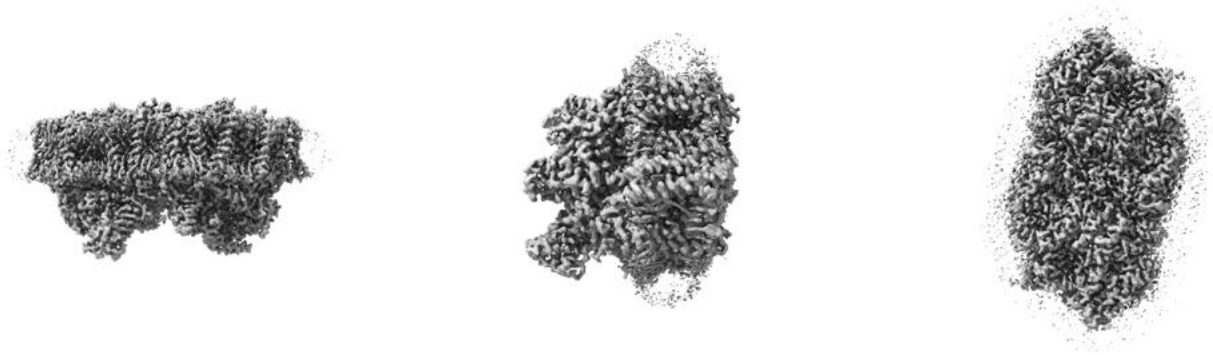

Y


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 0.05. 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.

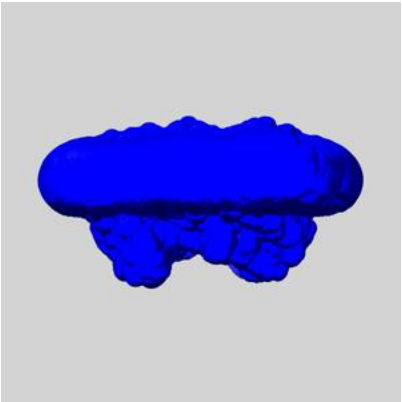
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

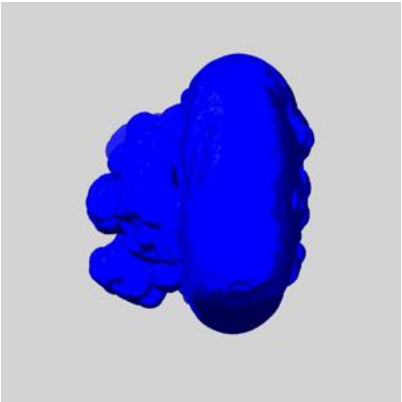
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

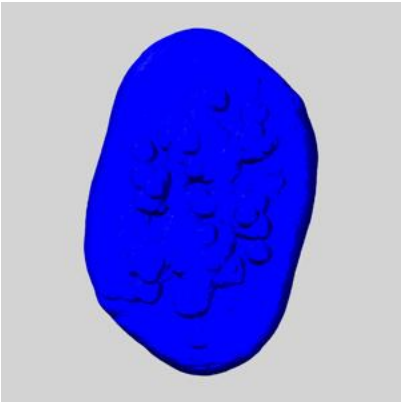
6.6.1 emd_55593_msk_1.map (i)



X



Y

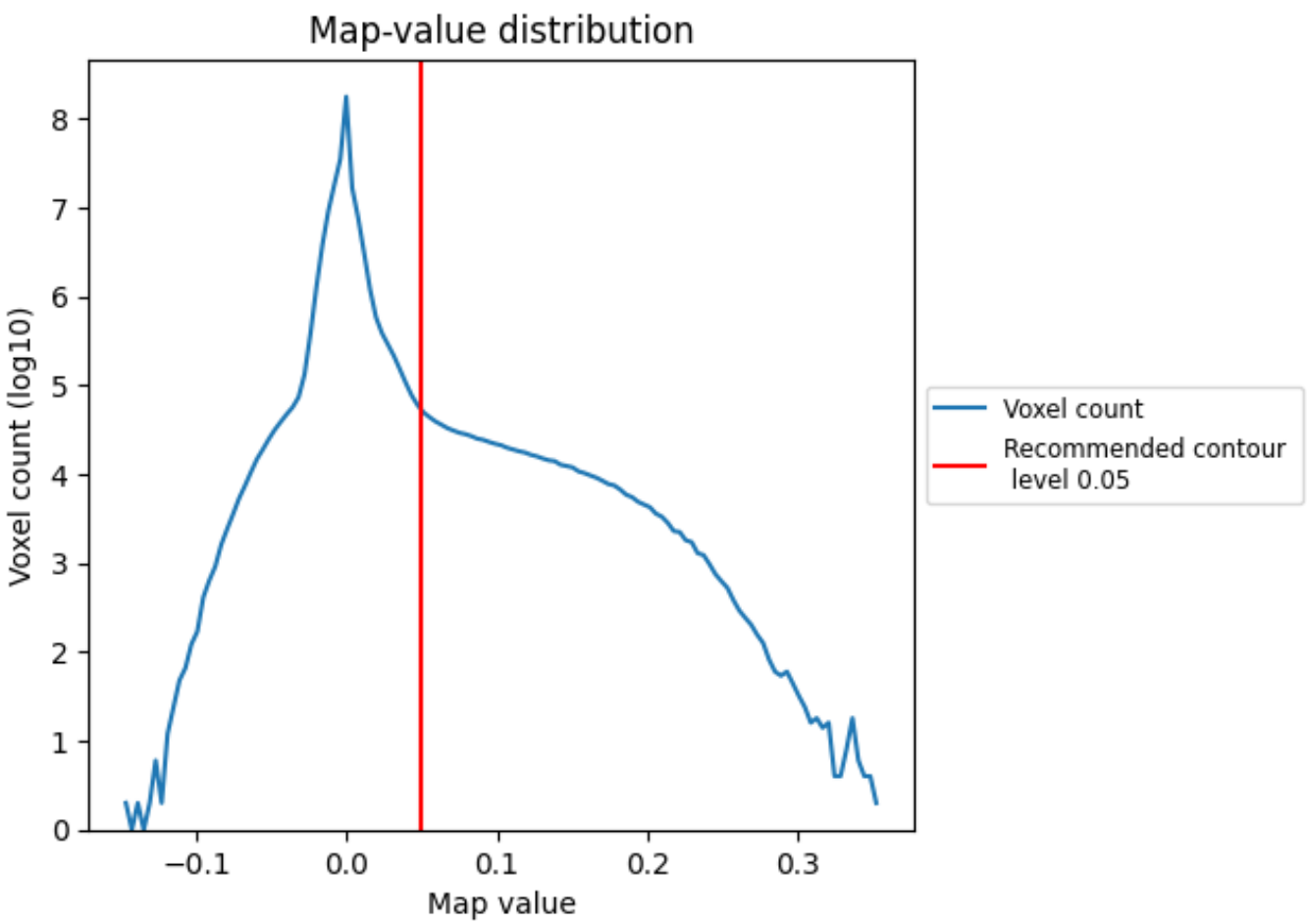


Z

7 Map analysis (i)

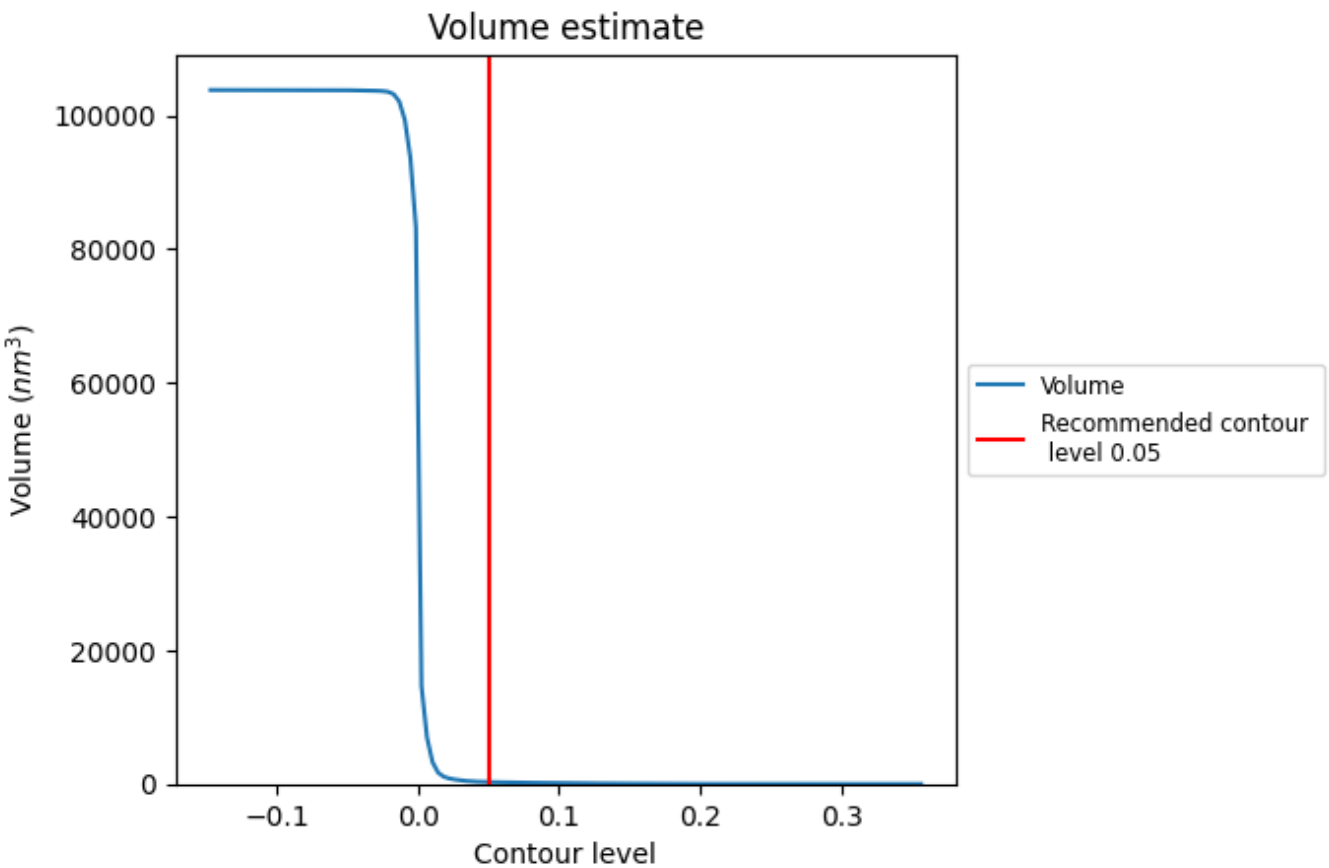
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

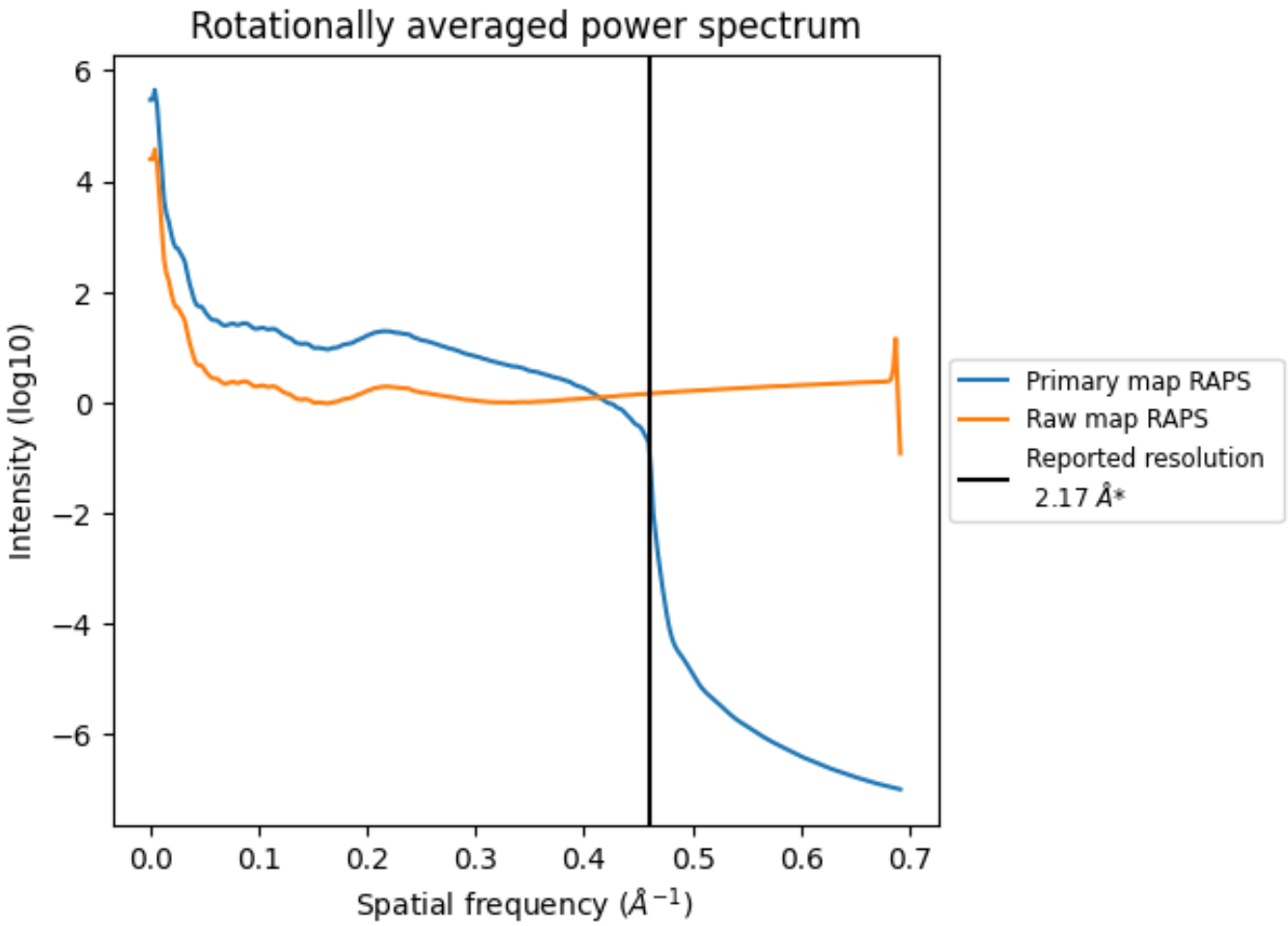
7.2 Volume estimate (i)



The volume at the recommended contour level is 285 nm^3; this corresponds to an approximate mass of 258 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)

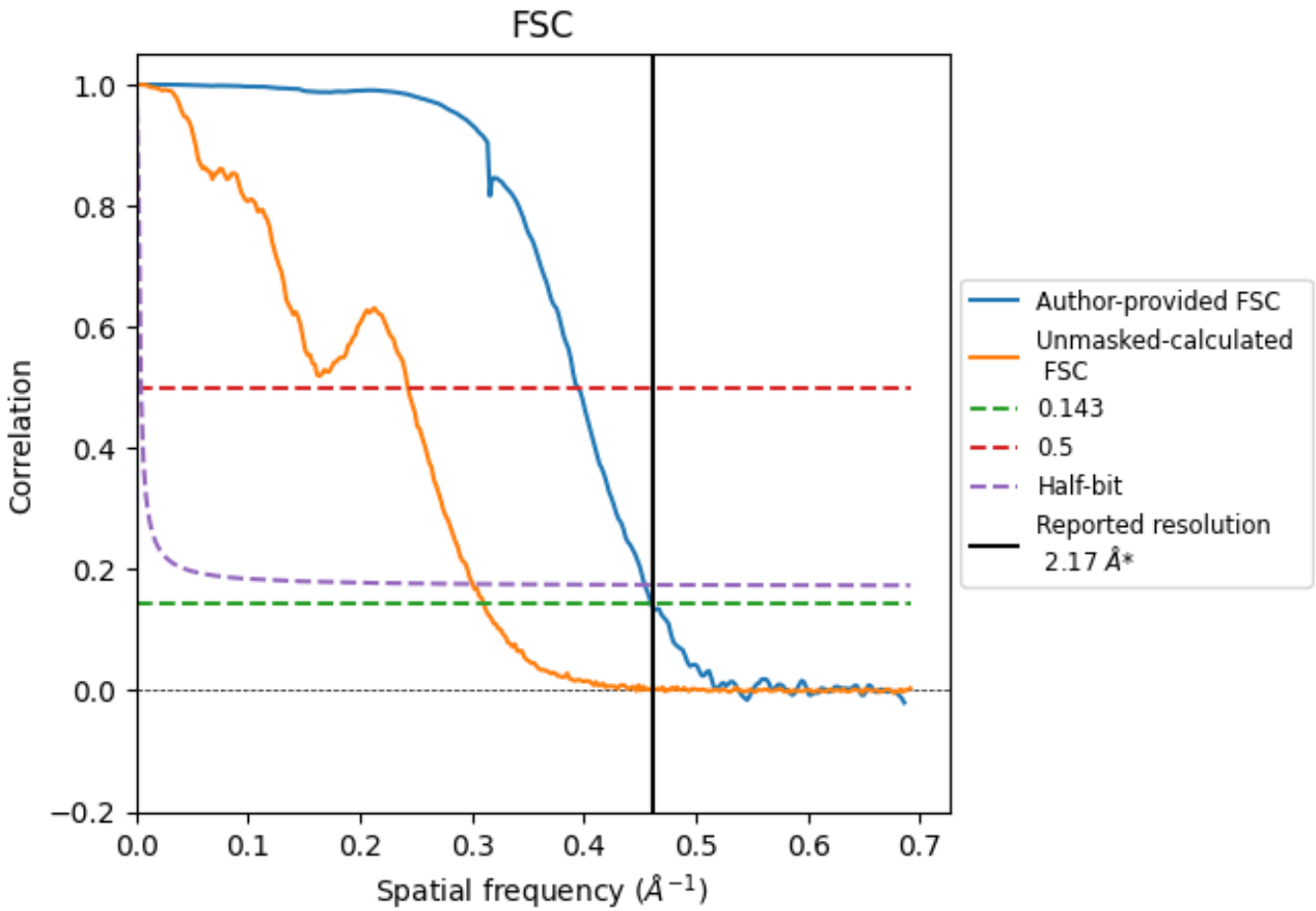


*Reported resolution corresponds to spatial frequency of 0.461 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.461 Å^{-1}

8.2 Resolution estimates (i)

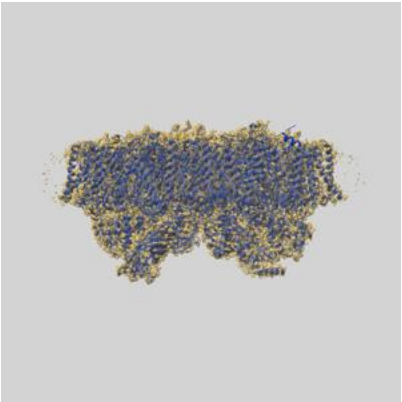
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.53	2.20
Unmasked-calculated*	3.22	4.12	3.33

*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 3.22 differs from the reported value 2.17 by more than 10 %

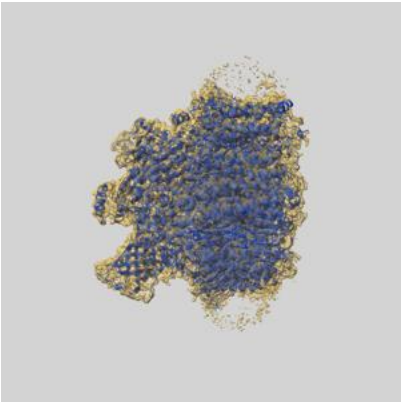
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55593 and PDB model 9T5T. Per-residue inclusion information can be found in section 3 on page 33.

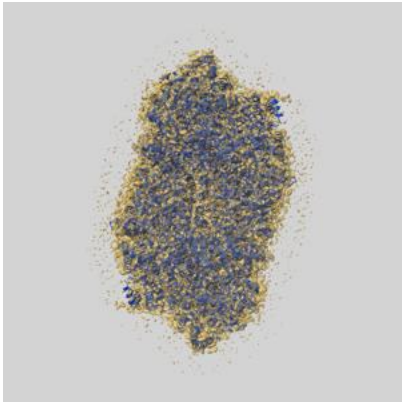
9.1 Map-model overlay (i)



X



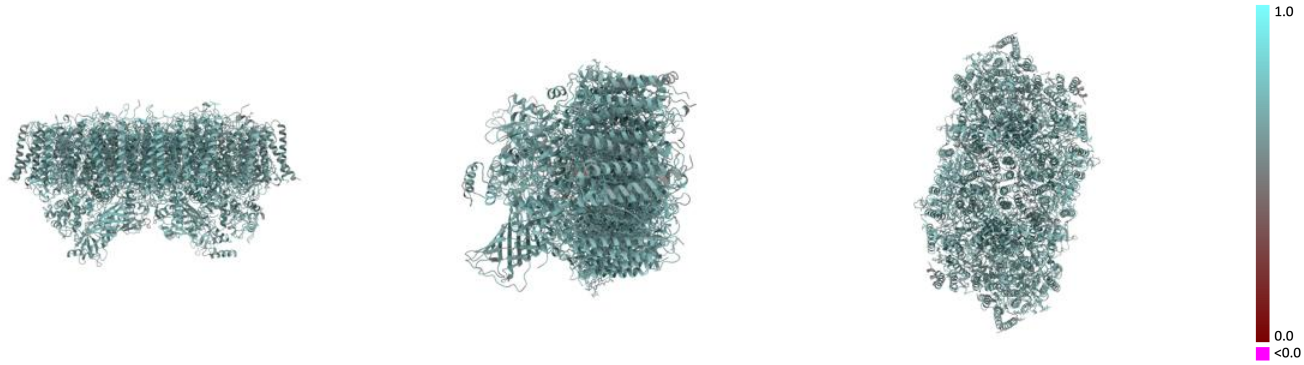
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

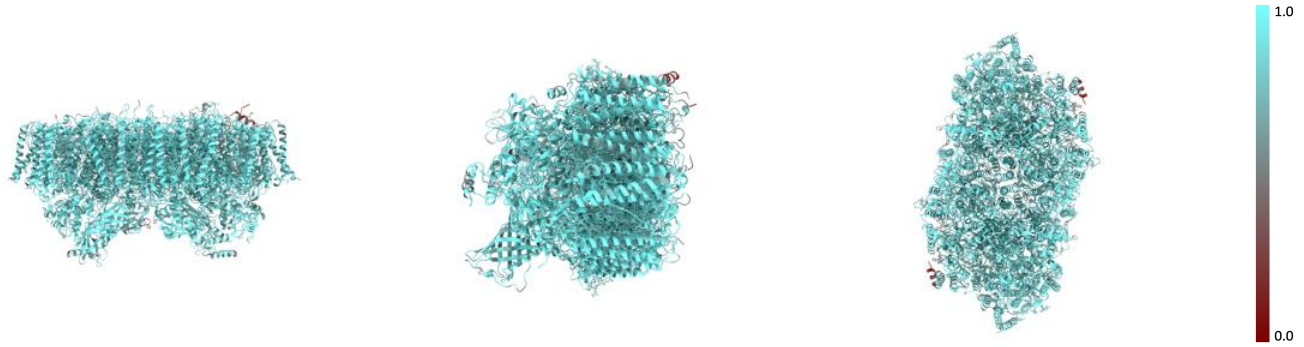
9.2 Q-score mapped to coordinate model (i)



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.

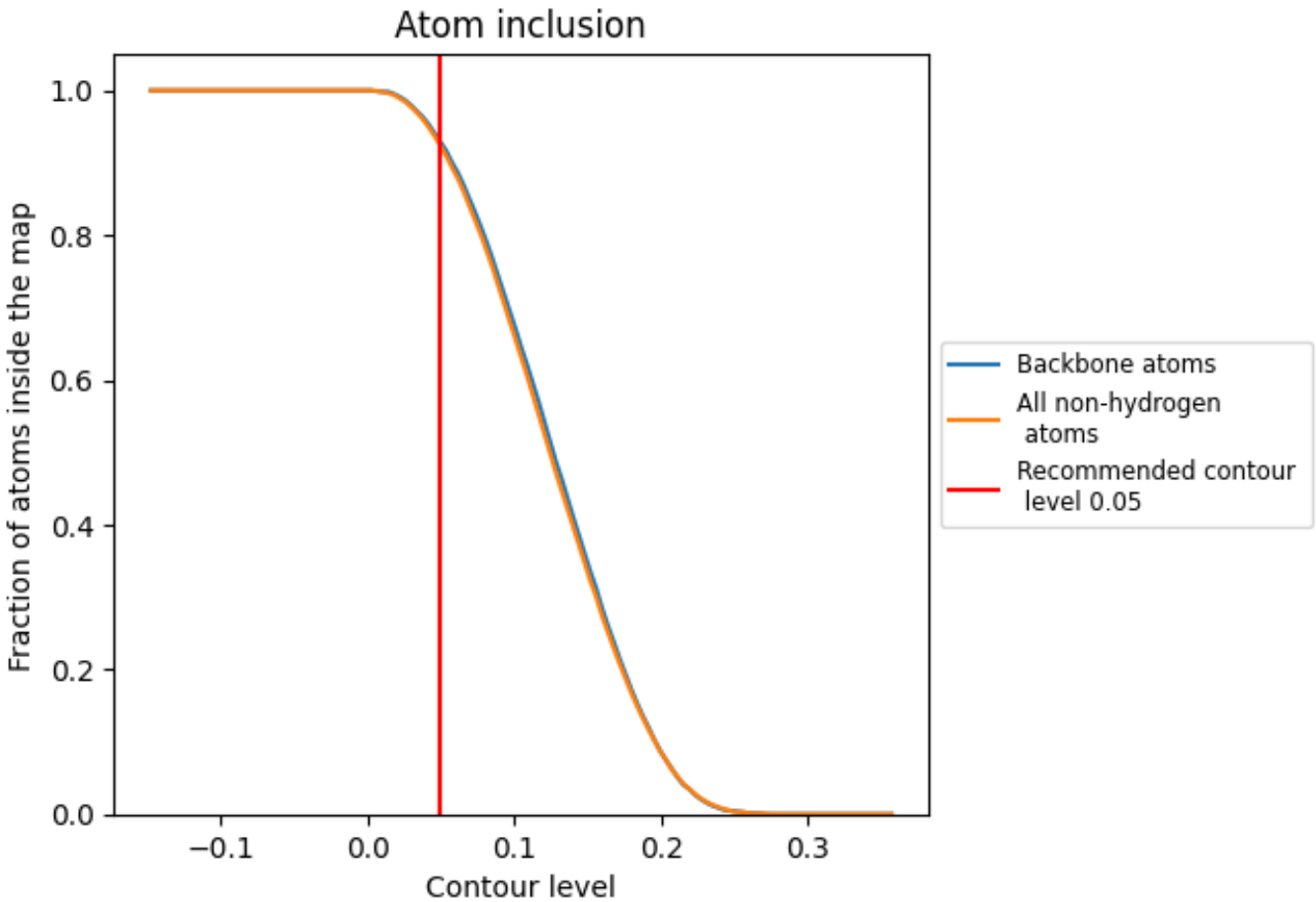
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9230	0.6620
A	0.9510	0.6780
B	0.9540	0.6830
C	0.9420	0.6640
D	0.9680	0.6890
E	0.8540	0.6220
F	0.8750	0.6310
G	0.9120	0.6480
H	0.9500	0.6670
I	0.9700	0.6710
J	0.8810	0.6410
K	0.9310	0.6360
L	0.8990	0.6540
M	0.9190	0.6550
O	0.8650	0.6300
P	0.6040	0.5400
R	0.6110	0.5510
T	0.9360	0.6690
U	0.8710	0.6360
V	0.8960	0.6400
X	0.8850	0.6350
Y	0.7770	0.5880
Z	0.8120	0.5820
a	0.9510	0.6780
b	0.9540	0.6830
c	0.9420	0.6640
d	0.9680	0.6900
e	0.8540	0.6250
f	0.8750	0.6290
g	0.9120	0.6520
h	0.9500	0.6640
i	0.9700	0.6730
j	0.8810	0.6390
k	0.9310	0.6410
l	0.8990	0.6550

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
m	0.9190	0.6530
o	0.8650	0.6310
p	0.6040	0.5440
r	0.6110	0.5530
t	0.9360	0.6710
u	0.8710	0.6370
v	0.8960	0.6400
x	0.8850	0.6360
y	0.7770	0.5910
z	0.8120	0.5810