



wwPDB EM Validation Summary Report ⓘ

Feb 19, 2025 – 12:24 PM JST

PDB ID : 9KQP
EMDB ID : EMD-62511
Title : PSI-LHCI supercomplex binding with 10 Lhcas from *C. subellipsoidea*
Authors : Tsai, P.-C.; Kato, K.; Shen, J.-R.; Akita, F.
Deposited on : 2024-11-26
Resolution : 1.92 Å(reported)
Based on initial model : 6zzx

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

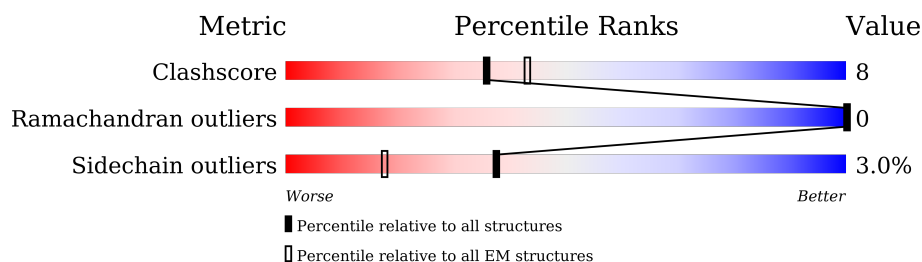
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.92 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	751	 89% 9% •
2	B	734	 92% 8%
3	C	81	 95% • •
4	D	192	 67% 7% 26%
5	E	71	 83% • 15%
6	F	245	 62% 5% 33%
7	G	138	 67% 7% • 25%
8	H	133	 7% 57% 11% 32%

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Mol	Chain	Length	Quality of chain
9	I	36	
10	J	41	
11	K	131	
12	M	31	
13	a	229	
13	b	229	
14	3	246	
15	7	259	
16	8	255	
17	9	230	
18	L	210	
19	O	142	
20	2	273	
21	4	246	
22	5	274	
23	6	272	

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
29	UNL	3	306	-	-	X	-
30	CL0	A	813	X	-	-	-
31	CLA	2	305	X	-	-	-
31	CLA	2	306	X	-	-	-
31	CLA	2	307	X	-	-	-
31	CLA	2	308	X	-	-	-
31	CLA	2	310	X	-	-	-
31	CLA	2	311	X	-	-	-
31	CLA	2	312	X	-	-	-
31	CLA	2	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	2	314	X	-	-	-
31	CLA	2	315	X	-	-	-
31	CLA	3	307	X	-	-	-
31	CLA	3	308	X	-	-	-
31	CLA	3	309	X	-	-	-
31	CLA	3	310	X	-	-	-
31	CLA	3	311	X	-	-	-
31	CLA	3	312	X	-	-	-
31	CLA	3	313	X	-	-	-
31	CLA	3	316	X	-	-	-
31	CLA	3	317	X	-	-	-
31	CLA	3	319	X	-	-	-
31	CLA	3	320	X	-	-	-
31	CLA	4	306	X	-	-	-
31	CLA	4	307	X	-	-	-
31	CLA	4	308	X	-	-	-
31	CLA	4	309	X	-	-	-
31	CLA	4	311	X	-	-	-
31	CLA	4	312	X	-	-	-
31	CLA	4	314	X	-	-	-
31	CLA	4	315	X	-	-	-
31	CLA	4	318	X	-	-	-
31	CLA	4	319	X	-	-	-
31	CLA	4	320	X	-	-	-
31	CLA	4	321	X	-	-	-
31	CLA	5	307	X	-	-	-
31	CLA	5	308	X	-	-	-
31	CLA	5	310	X	-	-	-
31	CLA	5	311	X	-	-	-
31	CLA	5	312	X	-	-	-
31	CLA	5	315	X	-	-	-
31	CLA	5	318	X	-	-	-
31	CLA	5	323	X	-	-	-
31	CLA	6	307	X	-	-	-
31	CLA	6	308	X	-	-	-
31	CLA	6	310	X	-	-	-
31	CLA	6	311	X	-	-	-
31	CLA	6	312	X	-	-	-
31	CLA	6	313	X	-	-	-
31	CLA	6	315	X	-	-	-
31	CLA	6	316	X	-	-	-
31	CLA	7	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	7	310	X	-	-	-
31	CLA	7	312	X	-	-	-
31	CLA	7	313	X	-	-	-
31	CLA	7	315	X	-	-	-
31	CLA	7	316	X	-	-	-
31	CLA	7	322	X	-	-	-
31	CLA	8	307	X	-	-	-
31	CLA	8	308	X	-	-	-
31	CLA	8	309	X	-	-	-
31	CLA	8	310	X	-	-	-
31	CLA	8	311	X	-	-	-
31	CLA	8	312	X	-	-	-
31	CLA	8	313	X	-	-	-
31	CLA	8	314	X	-	-	-
31	CLA	8	315	X	-	-	-
31	CLA	8	318	X	-	-	-
31	CLA	8	321	X	-	-	-
31	CLA	9	311	X	-	-	-
31	CLA	9	312	X	-	-	-
31	CLA	9	313	X	-	-	-
31	CLA	9	314	X	-	-	-
31	CLA	9	315	X	-	-	-
31	CLA	9	316	X	-	-	-
31	CLA	9	318	X	-	-	-
31	CLA	9	321	X	-	-	-
31	CLA	A	814	X	-	-	-
31	CLA	A	816	X	-	-	-
31	CLA	A	817	X	-	-	-
31	CLA	A	818	X	-	-	-
31	CLA	A	819	X	-	-	-
31	CLA	A	821	X	-	-	-
31	CLA	A	824	X	-	-	-
31	CLA	A	826	X	-	-	-
31	CLA	A	834	X	-	-	-
31	CLA	A	838	X	-	-	-
31	CLA	A	841	X	-	-	-
31	CLA	A	849	X	-	-	-
31	CLA	A	850	X	-	-	-
31	CLA	A	851	X	-	-	-
31	CLA	A	854	X	-	-	-
31	CLA	A	856	X	-	-	-
31	CLA	A	857	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	B	811	X	-	-	-
31	CLA	B	812	X	-	-	-
31	CLA	B	814	X	-	-	-
31	CLA	B	815	X	-	-	-
31	CLA	B	817	X	-	-	-
31	CLA	B	818	X	-	-	-
31	CLA	B	819	X	-	-	-
31	CLA	B	822	X	-	-	-
31	CLA	B	823	X	-	-	-
31	CLA	B	827	X	-	-	-
31	CLA	B	828	X	-	-	-
31	CLA	B	832	X	-	-	-
31	CLA	B	833	X	-	-	-
31	CLA	B	834	X	-	-	-
31	CLA	B	835	X	-	-	-
31	CLA	B	840	X	-	-	-
31	CLA	B	842	X	-	-	-
31	CLA	B	843	X	-	-	-
31	CLA	B	844	X	-	-	-
31	CLA	B	848	X	-	-	-
31	CLA	B	849	X	-	-	-
31	CLA	F	301	X	-	-	-
31	CLA	F	305	X	-	-	-
31	CLA	F	306	X	-	-	-
31	CLA	G	204	X	-	-	-
31	CLA	G	205	X	-	-	-
31	CLA	G	206	X	-	-	-
31	CLA	H	901	X	-	-	-
31	CLA	H	902	X	-	-	-
31	CLA	J	105	X	-	-	-
31	CLA	K	205	X	-	-	-
31	CLA	L	307	X	-	-	-
31	CLA	O	202	X	-	-	-
31	CLA	O	203	X	-	-	-
31	CLA	O	204	X	-	-	-
31	CLA	a	309	X	-	-	-
31	CLA	a	310	X	-	-	-
31	CLA	a	311	X	-	-	-
31	CLA	a	312	X	-	-	-
31	CLA	a	313	X	-	-	-
31	CLA	a	314	X	-	-	-
31	CLA	a	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	a	319	X	-	-	-
31	CLA	a	322	X	-	-	-
31	CLA	b	302	X	-	-	-
31	CLA	b	303	X	-	-	-
31	CLA	b	304	X	-	-	-
31	CLA	b	305	X	-	-	-
31	CLA	b	307	X	-	-	-
31	CLA	b	310	X	-	-	-
31	CLA	b	311	X	-	-	-
31	CLA	b	313	X	-	-	-
32	CHL	3	315	X	-	-	-
32	CHL	4	310	X	-	-	-
32	CHL	4	313	X	-	-	-
32	CHL	4	317	X	-	-	-
32	CHL	5	316	X	-	-	-
32	CHL	5	317	X	-	-	-
32	CHL	5	319	X	-	-	-
32	CHL	5	322	X	-	-	-
32	CHL	6	309	X	-	-	-
32	CHL	6	317	X	-	-	-
32	CHL	6	318	X	-	-	-
32	CHL	6	319	X	-	-	-
32	CHL	6	320	X	-	-	-
32	CHL	6	321	X	-	-	-
32	CHL	7	317	X	-	-	-
32	CHL	7	318	X	-	-	-
32	CHL	7	319	X	-	-	-
32	CHL	7	320	X	-	-	-
32	CHL	7	324	X	-	-	-
32	CHL	8	316	X	-	-	-
32	CHL	8	319	X	-	-	-
32	CHL	9	320	X	-	-	-
32	CHL	9	322	X	-	-	-
32	CHL	A	831	X	-	-	-
32	CHL	A	839	X	-	-	-
32	CHL	A	840	X	-	-	-
32	CHL	K	201	X	-	-	-
32	CHL	a	317	X	-	-	-
32	CHL	a	318	X	-	-	-
32	CHL	a	320	X	-	-	-
32	CHL	b	309	X	-	-	-
36	LUT	4	302	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	LUT	6	303	-	X	-	-
36	LUT	9	302	-	X	-	-
36	LUT	9	305	-	X	-	-
36	LUT	F	304	-	X	-	-
36	LUT	a	305	-	X	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 52991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5814	3800	992	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5808	3812	985	998	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			596	365	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1110	711	193	203	3		

- Molecule 5 is a protein called Photosystem I reaction centre subunit IV/PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	60	Total	C	N	O	S	0	0
			490	316	83	90	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1264	805	223	234	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	103	Total	C	N	O	S	0	0
			767	488	132	146	1		

- Molecule 8 is a protein called Photosystem I reaction centre subunit VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	S	0	0
			706	449	120	137			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			248	171	34	41	2		

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	39	Total	C	N	O	S	0	0
			319	220	46	52	1		

- Molecule 11 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			560	356	96	107	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			237	160	35	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	195	Total	C	N	O	S	0	0
			1458	944	245	267	2		
13	b	126	Total	C	N	O	S	0	0
			952	606	168	176	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	203	Total	C	N	O	S	0	0
			1580	1036	255	286	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	214	Total	C	N	O	S	0	0
			1633	1059	276	296	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	8	222	Total	C	N	O	S	0	0
			1701	1112	276	310	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	9	184	Total	C	N	O	S	0	0
			1414	915	238	258	3		

- Molecule 18 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	148	Total	C	N	O	S	0	0
			1102	723	183	194	2		

- Molecule 19 is a protein called Photosystem I PsaO.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	78	Total	C	N	O	0	0
			605	403	98	104		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic/Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	204	Total	C	N	O	S	0	0
			1606	1046	270	286	4		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4	193	Total	C	N	O	S	0	0
			1506	984	246	273	3		

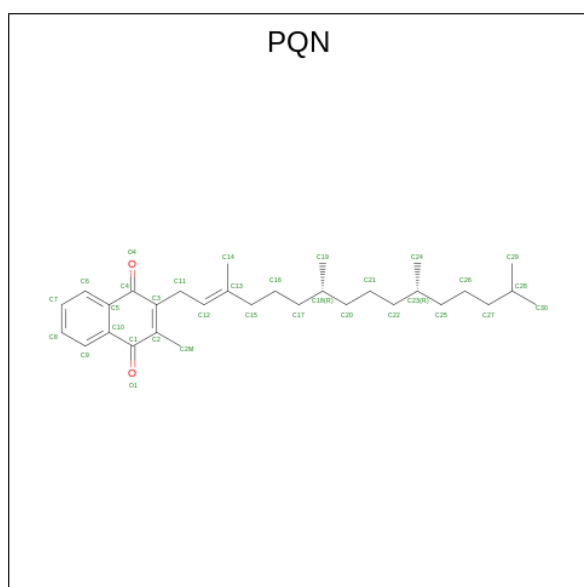
- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

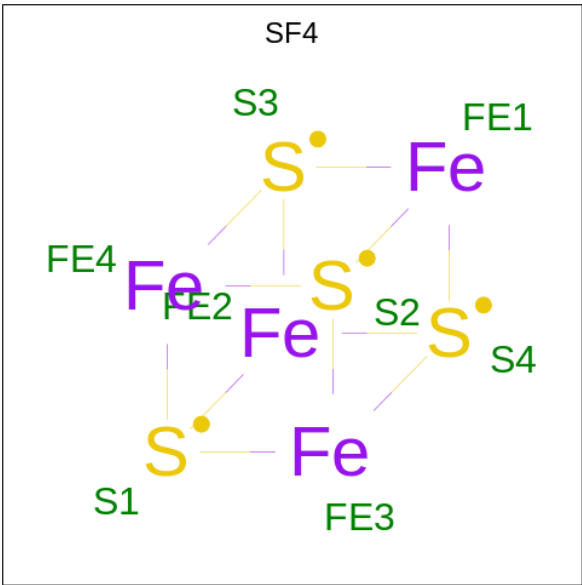
Mol	Chain	Residues	Atoms					AltConf	Trace
22	5	229	Total	C	N	O	S	0	0
			1766	1152	303	307	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	219	Total	C	N	O	S	0	0
			1658	1088	276	287	7		

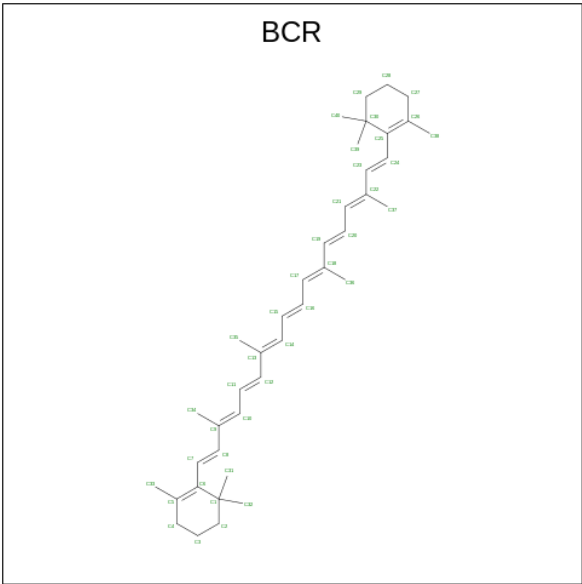
- Molecule 24 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



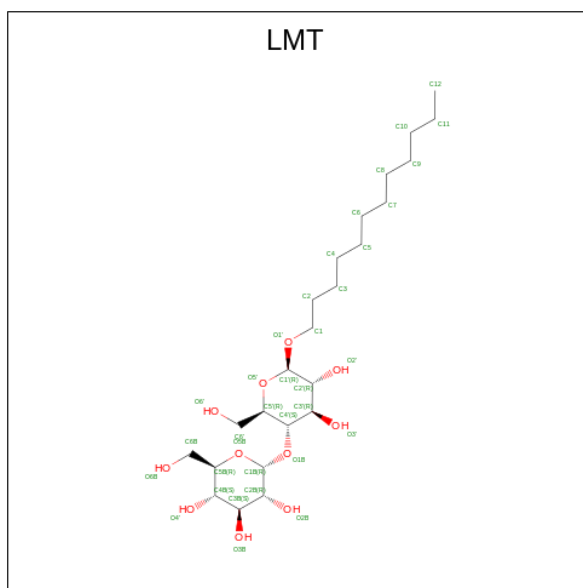
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	I	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	M	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	7	1	Total C 40 40	0
26	8	1	Total C 40 40	0

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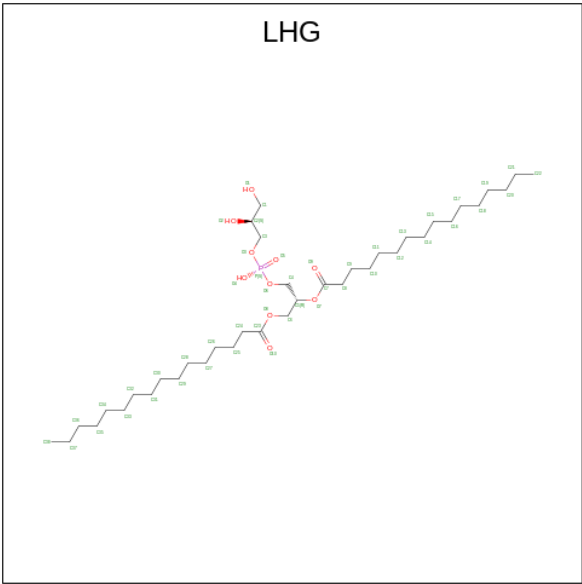
Mol	Chain	Residues	Atoms	AltConf
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	O	1	Total C 40 40	0
26	2	1	Total C 40 40	0
26	5	1	Total C 40 40	0
26	6	1	Total C 40 40	0

- Molecule 27 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C O 35 24 11	0
27	A	1	Total C O 35 24 11	0
27	9	1	Total C O 35 24 11	0
27	5	1	Total C O 35 24 11	0

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

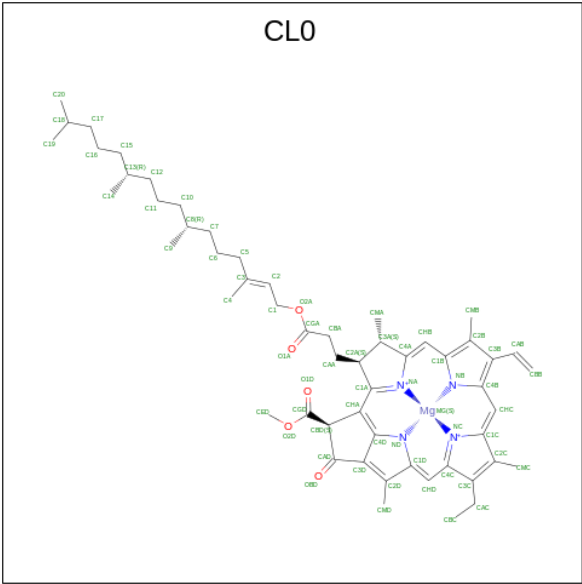


Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			42	31	10	1	
28	A	1	Total	C	O	P	0
			42	31	10	1	
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	B	1	Total	C	O	P	0
			32	21	10	1	
28	a	1	Total	C	O	P	0
			49	38	10	1	
28	7	1	Total	C	O	P	0
			49	38	10	1	
28	7	1	Total	C	O	P	0
			37	26	10	1	
28	8	1	Total	C	O	P	0
			49	38	10	1	
28	5	1	Total	C	O	P	0
			35	24	10	1	
28	6	1	Total	C	O	P	0
			27	16	10	1	
28	6	1	Total	C	O	P	0
			32	21	10	1	

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

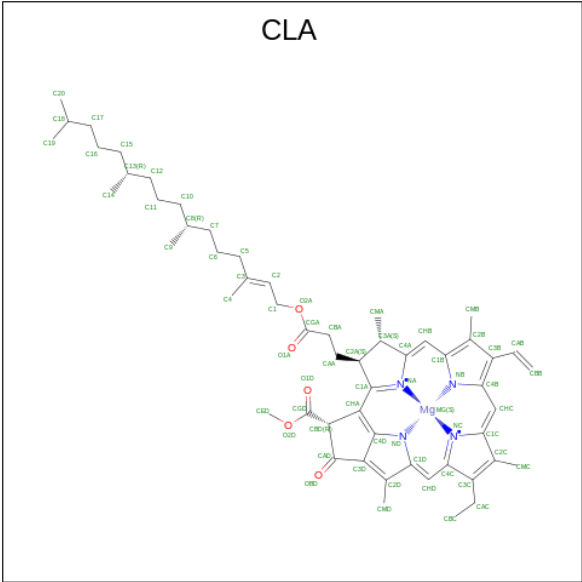
Mol	Chain	Residues	Atoms		AltConf
29	A	2	Total	C	0
			20	20	
29	B	2	Total	C	0
			24	24	
29	a	2	Total	C	0
			27	27	
29	3	1	Total	C	0
			11	11	
29	7	1	Total	C	0
			8	8	
29	8	1	Total	C	0
			18	18	
29	9	6	Total	C	0
			81	81	
29	2	1	Total	C	0
			11	11	
29	4	1	Total	C	0
			13	13	

- Molecule 30 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	7	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	9	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
31	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	2	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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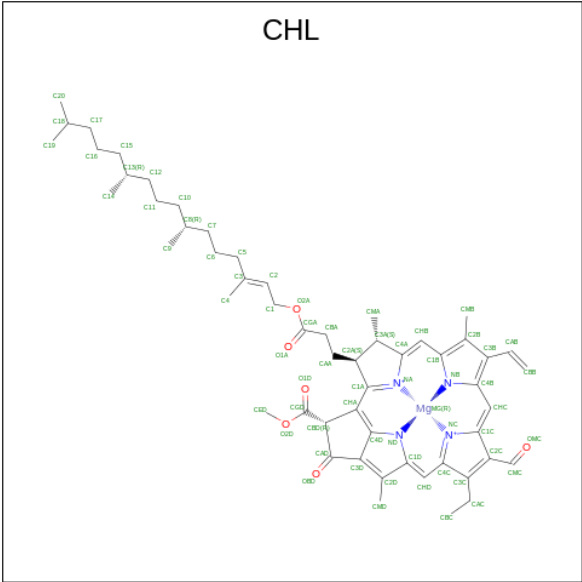
Mol	Chain	Residues	Atoms					AltConf
31	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 32 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



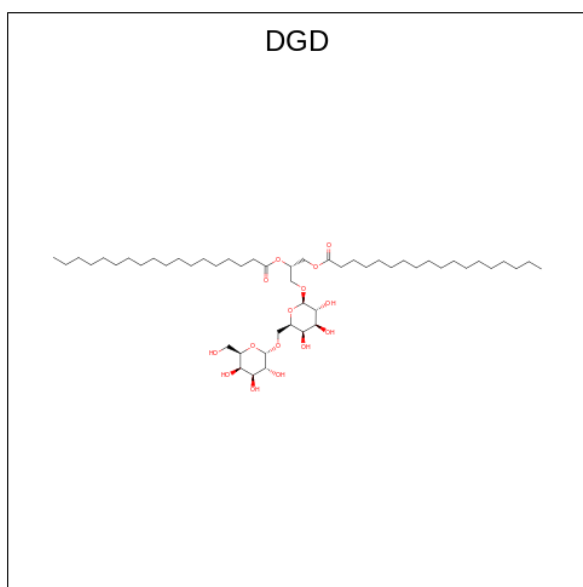
Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total 58	C 47	Mg 1	N 4	O 6	0
32	A	1	Total 56	C 45	Mg 1	N 4	O 6	0
32	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
32	K	1	Total 47	C 36	Mg 1	N 4	O 6	0
32	a	1	Total 61	C 50	Mg 1	N 4	O 6	0
32	a	1	Total 48	C 37	Mg 1	N 4	O 6	0
32	a	1	Total 48	C 37	Mg 1	N 4	O 6	0
32	3	1	Total 56	C 45	Mg 1	N 4	O 6	0
32	7	1	Total 57	C 46	Mg 1	N 4	O 6	0
32	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
32	7	1	Total 47	C 36	Mg 1	N 4	O 6	0
32	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
32	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
32	8	1	Total 66	C 55	Mg 1	N 4	O 6	0

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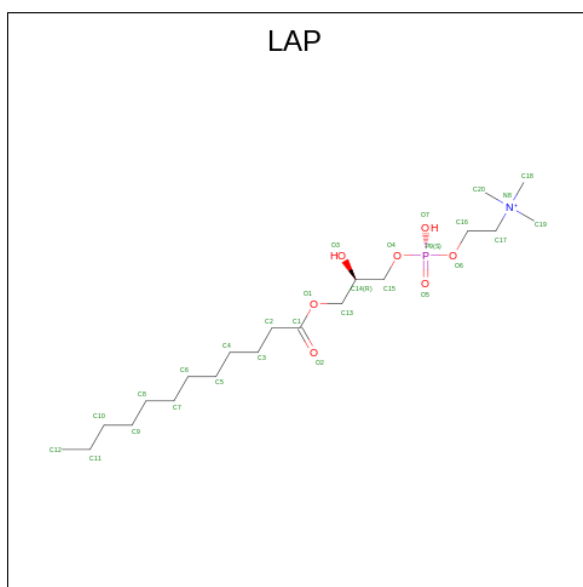
Mol	Chain	Residues	Atoms					AltConf
32	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



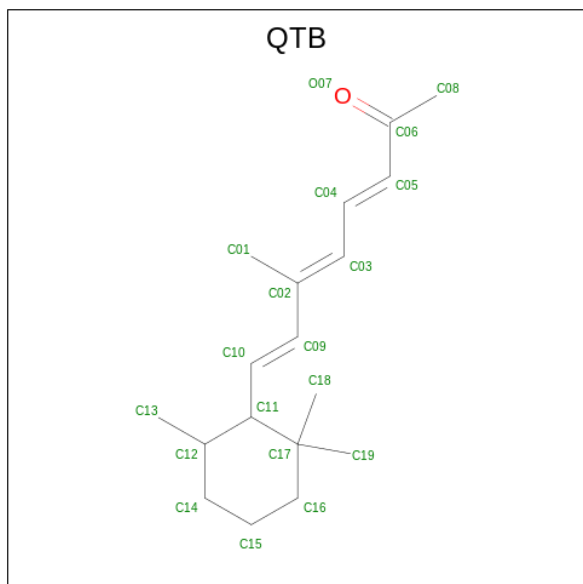
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			61	46	15	
33	7	1	Total	C	O	0
			52	37	15	

- Molecule 34 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (three-letter code: LAP) (formula: C₂₀H₄₃NO₇P) (labeled as "Ligand of Interest" by depositor).



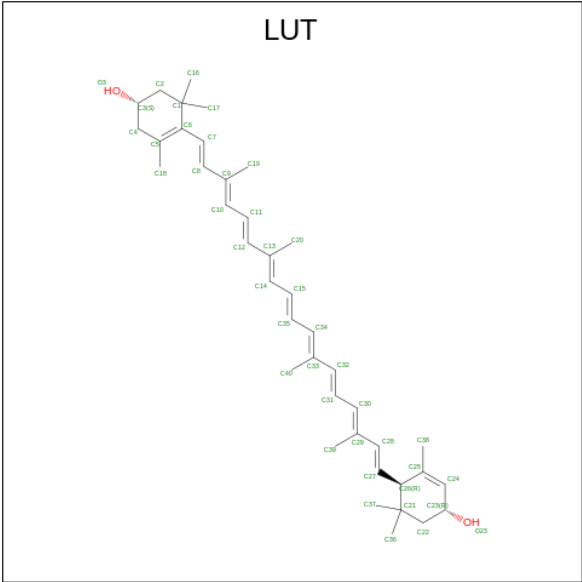
Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 35 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (three-letter code: QTB) (formula: C₁₈H₂₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	F	1	Total	C	O	0
			19	18	1	
35	a	1	Total	C	O	0
			19	18	1	
35	7	1	Total	C	O	0
			19	18	1	
35	9	1	Total	C	O	0
			19	18	1	

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



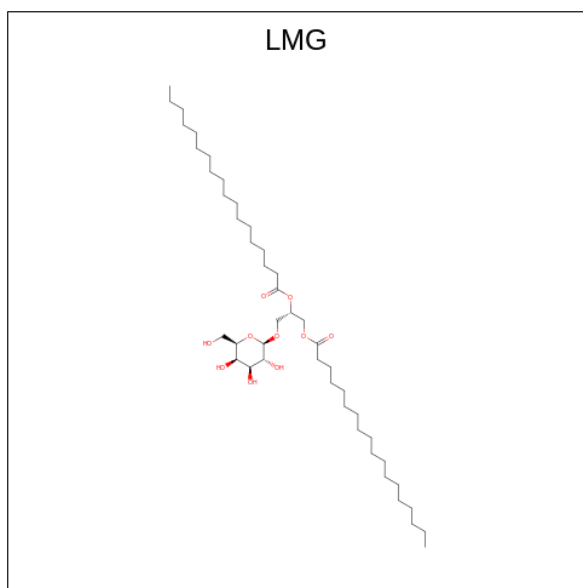
Mol	Chain	Residues	Atoms			AltConf
36	F	1	Total	C	O	0
			42	40	2	
36	J	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	7	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	L	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	

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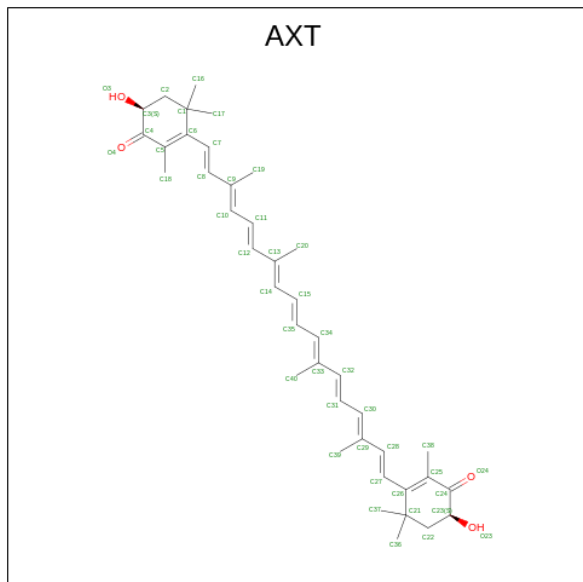
Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



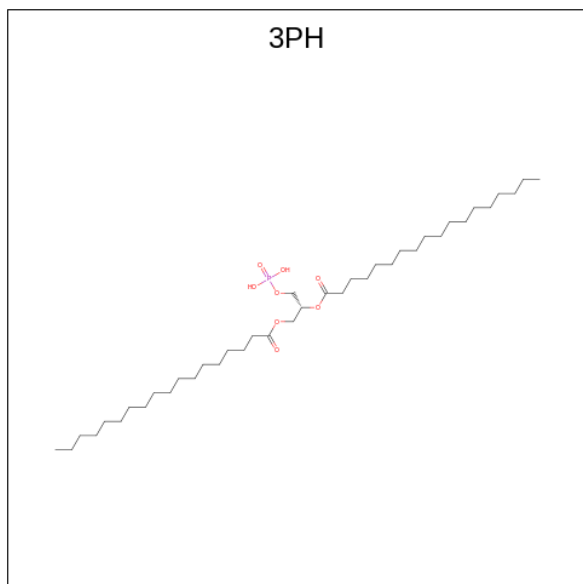
Mol	Chain	Residues	Atoms			AltConf
37	G	1	Total	C	O	0
			44	34	10	
37	J	1	Total	C	O	0
			49	39	10	
37	J	1	Total	C	O	0
			29	19	10	
37	a	1	Total	C	O	0
			42	32	10	

- Molecule 38 is ASTAXANTHIN (three-letter code: AXT) (formula: $C_{40}H_{52}O_4$) (labeled as "Ligand of Interest" by depositor).



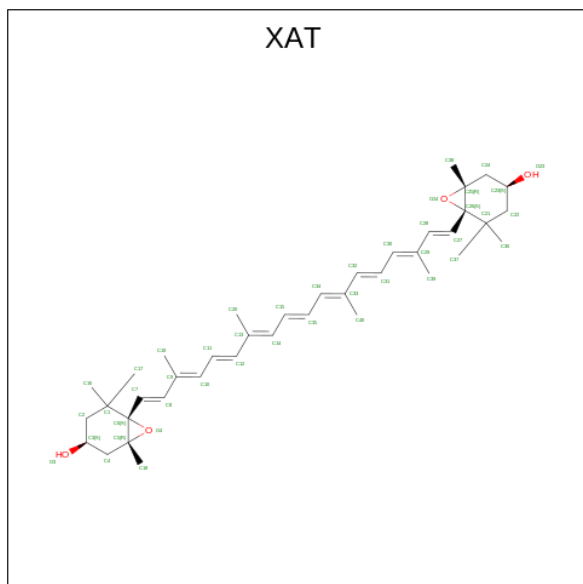
Mol	Chain	Residues	Atoms			AltConf
38	a	1	Total	C	O	0
			43	40	3	

- Molecule 39 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



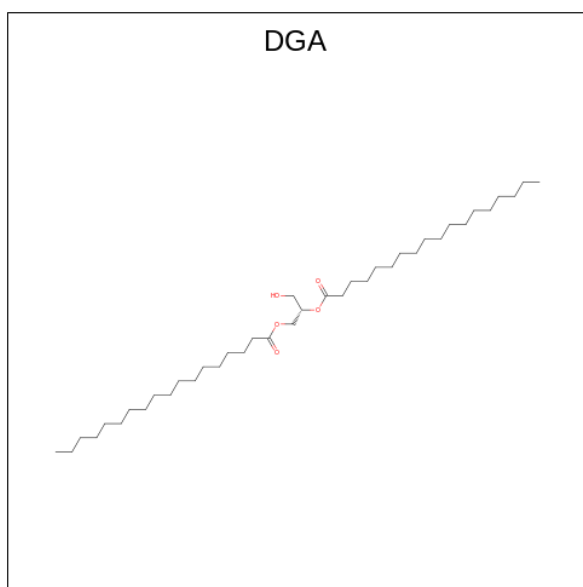
Mol	Chain	Residues	Atoms				AltConf
39	7	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 40 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



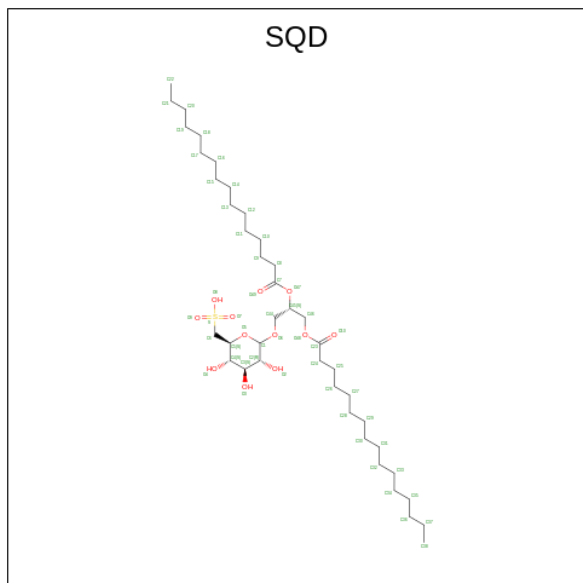
Mol	Chain	Residues	Atoms			AltConf
40	7	1	Total	C	O	0
			44	40	4	

- Molecule 41 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



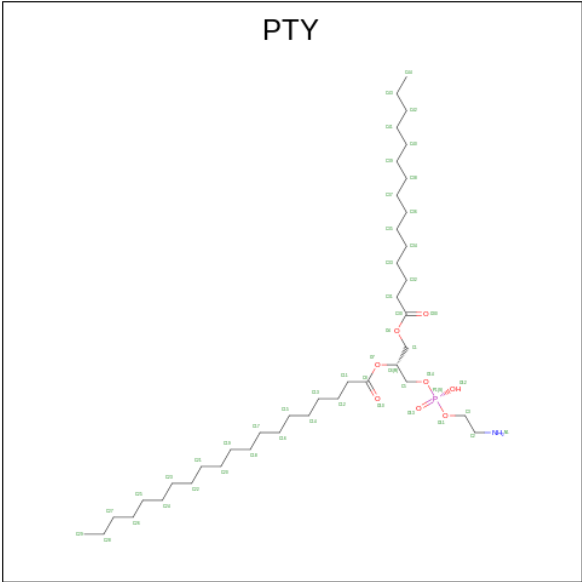
Mol	Chain	Residues	Atoms			AltConf
41	8	1	Total	C	O	0
			28	23	5	

- Molecule 42 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
42	4	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 43 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
43	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	A	297	Total	O	0
			297	297	
44	B	311	Total	O	0
			311	311	
44	C	60	Total	O	0
			60	60	
44	D	53	Total	O	0
			53	53	
44	E	28	Total	O	0
			28	28	
44	F	57	Total	O	0
			57	57	
44	G	18	Total	O	0
			18	18	
44	H	6	Total	O	0
			6	6	
44	I	6	Total	O	0
			6	6	
44	J	16	Total	O	0
			16	16	
44	K	2	Total	O	0
			2	2	

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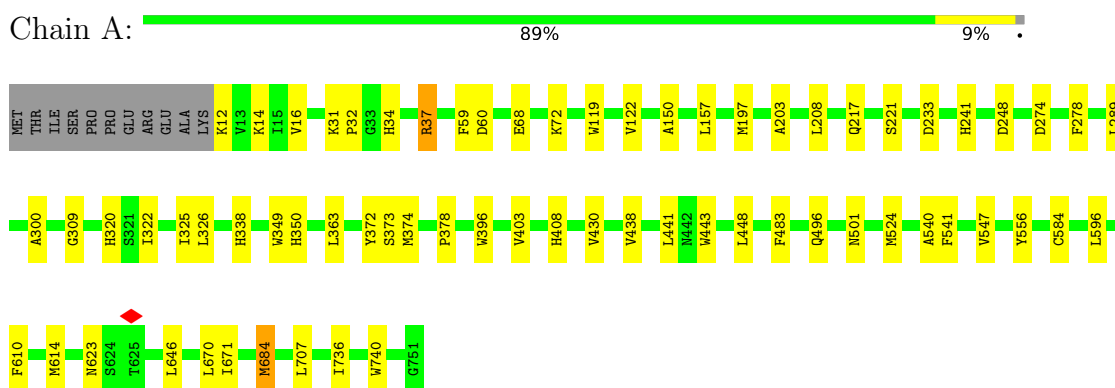
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Mol	Chain	Residues	Atoms		AltConf
44	M	5	Total 5	O 5	0
44	a	34	Total 34	O 34	0
44	3	32	Total 32	O 32	0
44	7	39	Total 39	O 39	0
44	8	37	Total 37	O 37	0
44	9	21	Total 21	O 21	0
44	L	17	Total 17	O 17	0
44	O	4	Total 4	O 4	0
44	2	3	Total 3	O 3	0
44	4	1	Total 1	O 1	0
44	5	11	Total 11	O 11	0
44	6	2	Total 2	O 2	0

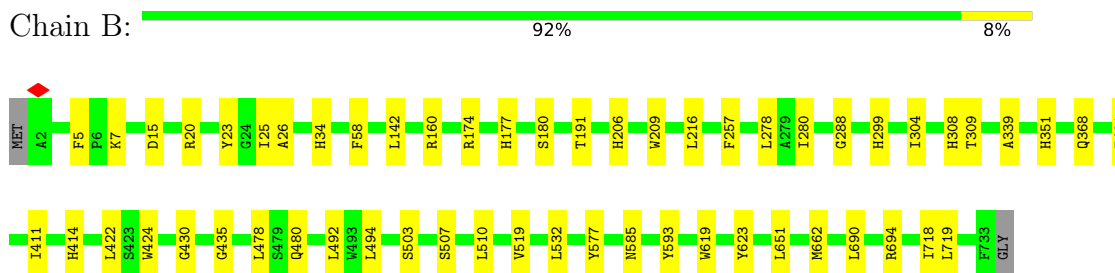
3 Residue-property plots [i](#)

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

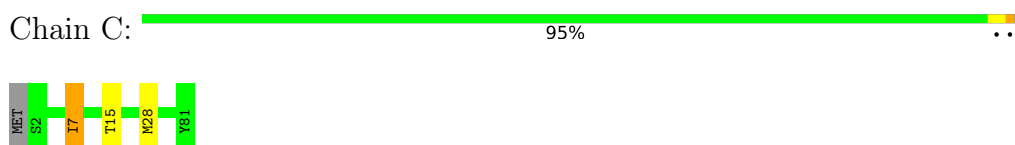
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



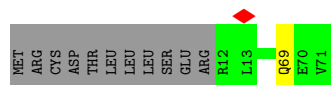
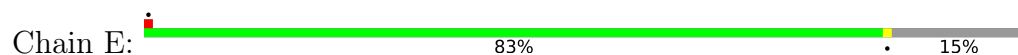
- Molecule 3: Photosystem I iron-sulfur center



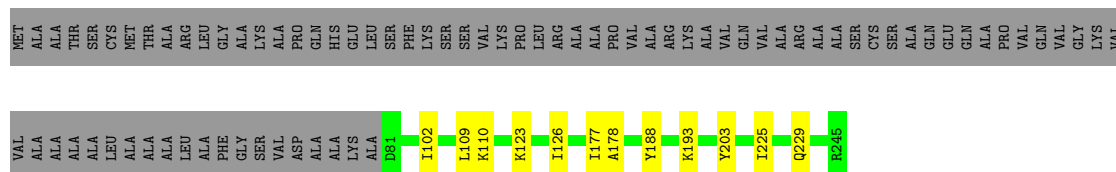
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



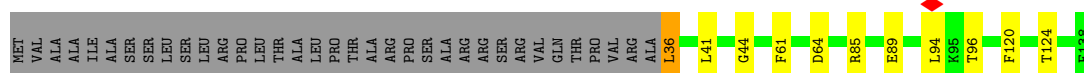
- Molecule 5: Photosystem I reaction centre subunit IV/PsaE



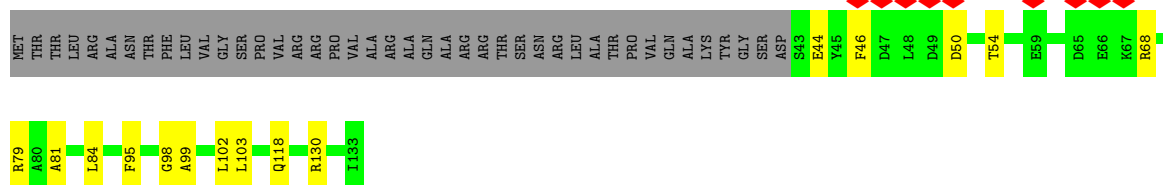
- Molecule 6: Photosystem I reaction center subunit III



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




- Molecule 8: Photosystem I reaction centre subunit VI



- Molecule 9: Photosystem I reaction center subunit VIII



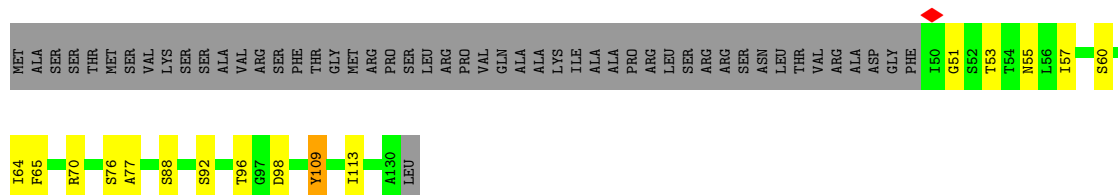
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  78% 17% 5%



- Molecule 11: PSI-K

Chain K:  50% 11% 38%




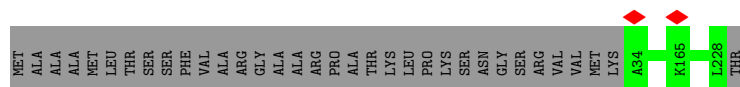
- Molecule 12: Photosystem I reaction center subunit XII

Chain M:  87% 13%



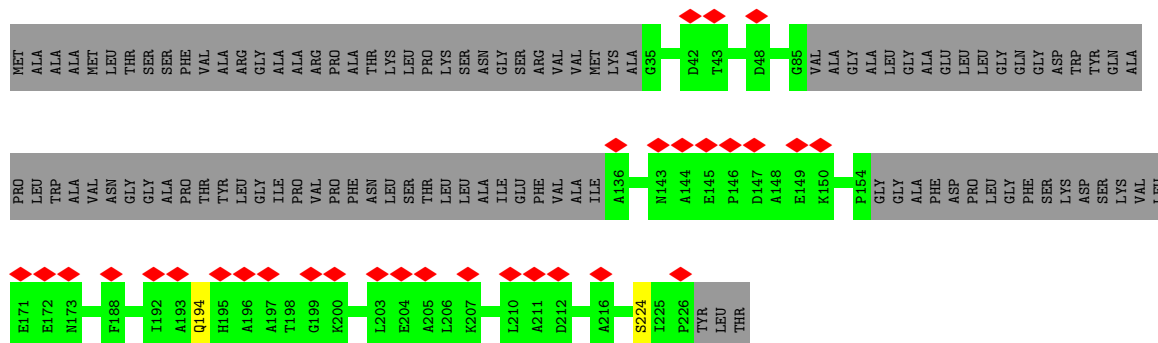
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain a:  85% 15%



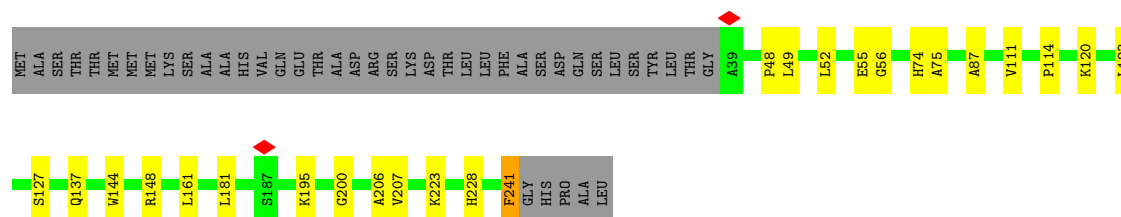
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain b:  14% 54% 45%

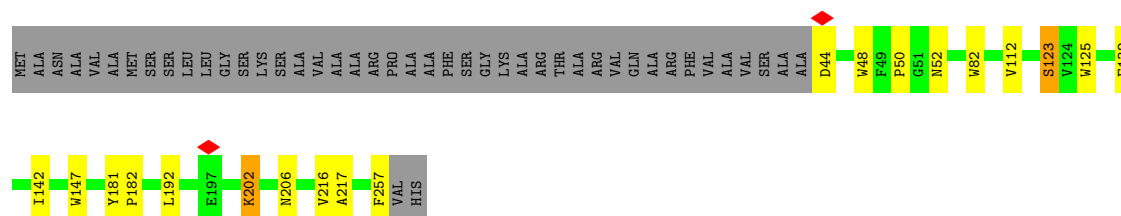
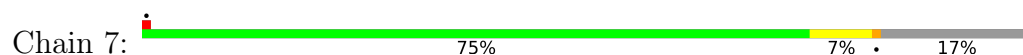


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

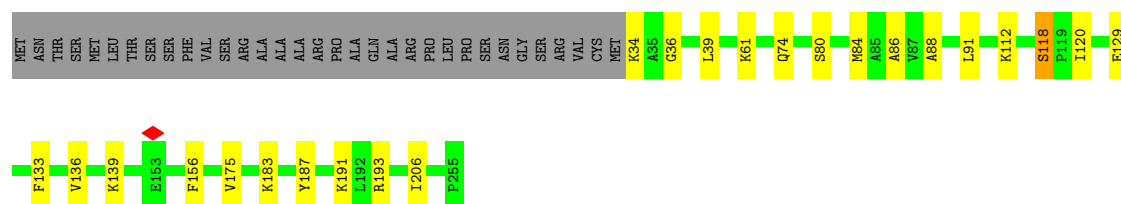
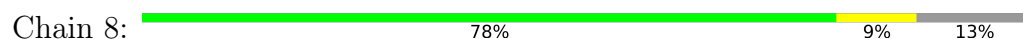
Chain 3:  72% 10% 17%



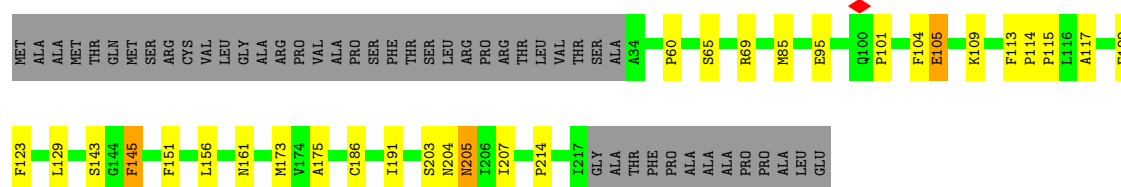
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



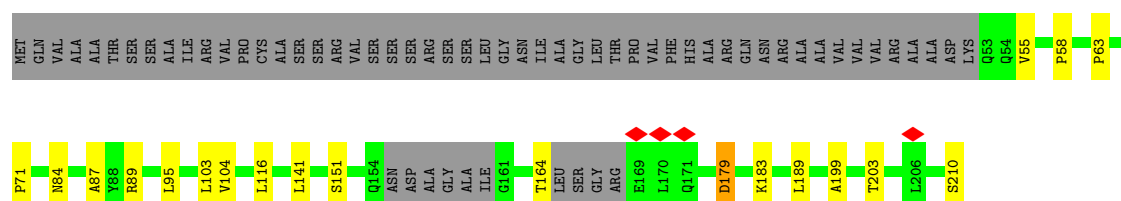
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



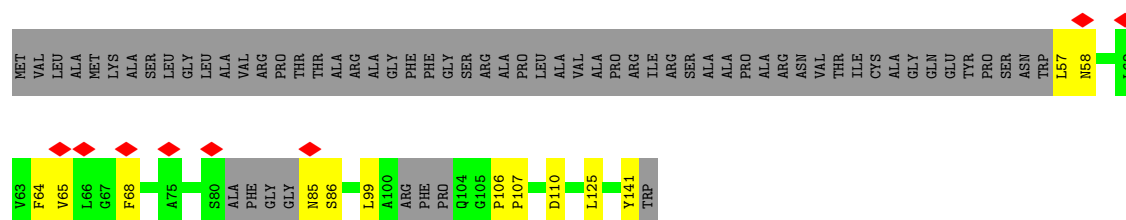
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



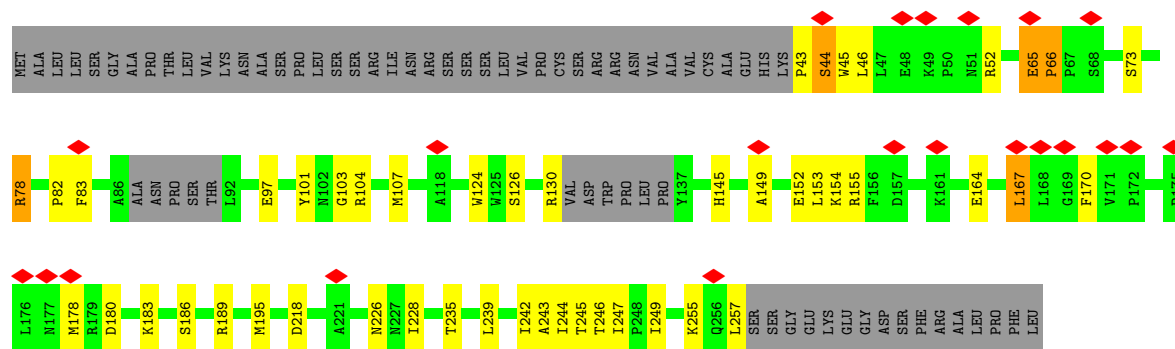
- Molecule 18: PSI subunit V



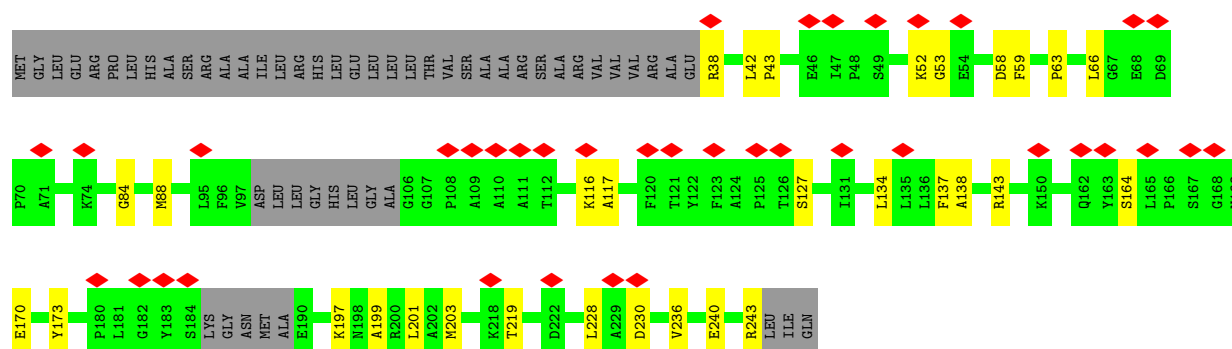
- Molecule 19: Photosystem I PsaO



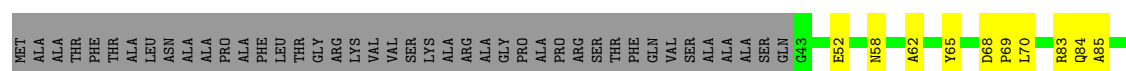
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic/Lhca2

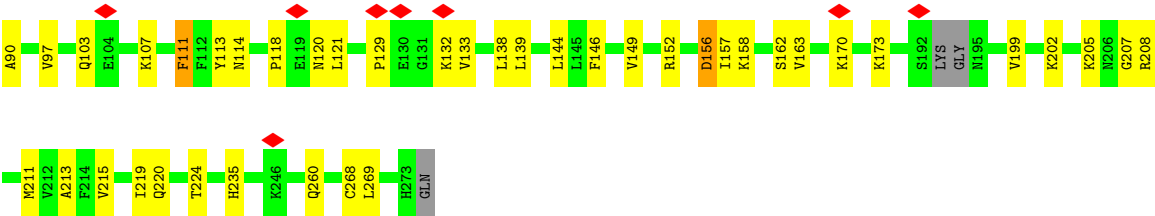


- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

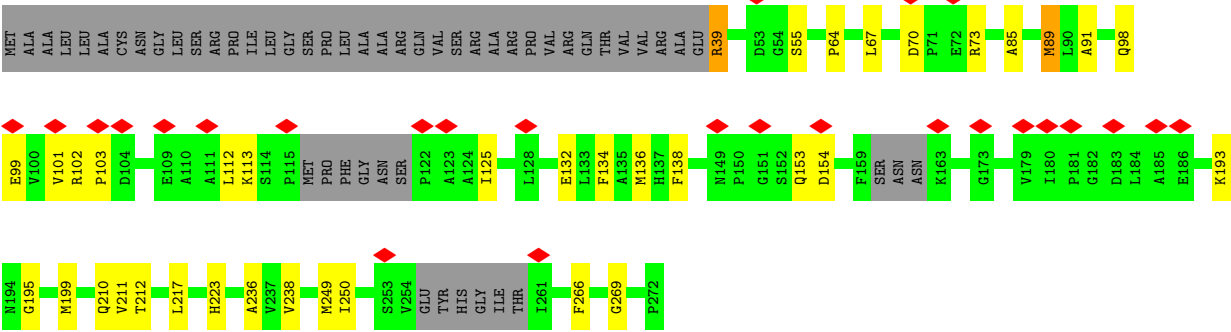


- Molecule 22: Chlorophyll a-b binding protein, chloroplastic





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224674	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.393	Depositor
Minimum map value	-0.655	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.085	Depositor
Map size (\AA)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, CLA, AXT, PQN, BCR, UNL, DGA, QTB, DGD, LUT, CHL, XAT, PTY, LAP, LHG, LMT, 3PH, SF4, SQD, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	0/6012	0.50	1/8202 (0.0%)
2	B	0.30	0/6017	0.51	0/8218
3	C	0.30	0/606	0.64	0/822
4	D	0.29	0/1136	0.53	0/1537
5	E	0.31	0/502	0.57	0/686
6	F	0.29	0/1288	0.51	0/1737
7	G	0.27	0/783	0.50	0/1063
8	H	0.29	0/722	0.56	0/972
9	I	0.34	0/254	0.54	0/347
10	J	0.29	0/330	0.47	0/452
11	K	0.28	0/568	0.49	0/773
12	M	0.29	0/240	0.41	0/325
13	a	0.30	0/1501	0.51	0/2045
13	b	0.25	0/977	0.46	0/1322
14	3	0.32	0/1629	0.50	0/2217
15	7	0.29	0/1684	0.47	0/2298
16	8	0.30	0/1752	0.46	0/2379
17	9	0.29	0/1451	0.50	0/1964
18	L	0.29	0/1129	0.50	0/1542
19	O	0.27	0/619	0.53	1/839 (0.1%)
20	2	0.29	0/1654	0.62	2/2254 (0.1%)
21	4	0.28	0/1553	0.47	0/2113
22	5	0.30	0/1820	0.54	2/2477 (0.1%)
23	6	0.28	0/1709	0.47	0/2328
All	All	0.29	0/35936	0.51	6/48912 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	6	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	66	PRO	CA-N-CD	-8.31	99.87	111.50
22	5	129	PRO	N-CD-CG	-7.27	92.30	103.20
20	2	65	GLU	C-N-CD	6.92	142.93	128.40
1	A	233	ASP	CB-CG-OD1	5.66	123.39	118.30
22	5	156	ASP	CB-CG-OD1	5.35	123.11	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	6	39	ARG	Sidechain

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	5814	0	5649	51	0
2	B	5808	0	5584	38	0
3	C	596	0	573	3	0
4	D	1110	0	1131	9	0
5	E	490	0	482	0	0
6	F	1264	0	1300	9	0
7	G	767	0	749	6	0
8	H	706	0	687	12	0
9	I	248	0	269	4	0
10	J	319	0	326	7	0
11	K	560	0	583	8	0
12	M	237	0	260	2	0
13	a	1458	0	1423	0	0
13	b	952	0	917	0	0
14	3	1580	0	1546	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	7	1633	0	1579	17	0
16	8	1701	0	1683	14	0
17	9	1414	0	1405	20	0
18	L	1102	0	1129	15	0
19	O	605	0	616	7	0
20	2	1606	0	1578	37	0
21	4	1506	0	1468	26	0
22	5	1766	0	1746	36	0
23	6	1658	0	1657	28	0
24	A	33	0	46	1	0
24	B	33	0	46	2	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	2	40	0	56	3	0
26	3	120	0	168	9	0
26	5	40	0	56	2	0
26	6	40	0	56	2	0
26	7	40	0	56	6	0
26	8	40	0	56	2	0
26	A	160	0	224	12	0
26	B	200	0	280	16	0
26	F	40	0	56	2	0
26	G	80	0	112	2	0
26	I	40	0	56	1	0
26	J	40	0	56	1	0
26	K	80	0	112	8	0
26	L	120	0	168	6	0
26	M	40	0	56	3	0
26	O	40	0	56	2	0
27	5	35	0	44	2	0
27	9	35	0	44	0	0
27	A	70	0	89	4	0
28	5	35	0	40	2	0
28	6	59	0	58	4	0
28	7	86	0	118	10	0
28	8	49	0	74	0	0
28	A	133	0	188	8	0
28	B	32	0	34	0	0
28	a	49	0	74	0	0
29	2	11	0	0	0	0
29	3	11	0	0	4	0
29	4	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	7	8	0	0	0	0
29	8	18	0	0	0	0
29	9	81	0	0	0	0
29	A	20	0	0	0	0
29	B	24	0	0	0	0
29	a	27	0	0	0	0
30	A	65	0	72	3	0
31	2	574	0	442	19	0
31	3	736	0	697	19	0
31	4	685	0	550	27	0
31	5	678	0	588	26	0
31	6	545	0	436	16	0
31	7	523	0	445	15	0
31	8	692	0	606	25	0
31	9	524	0	452	7	0
31	A	2450	0	2472	113	0
31	B	2382	0	2381	76	0
31	F	161	0	144	5	0
31	G	141	0	105	6	0
31	H	138	0	99	11	0
31	J	42	0	31	1	0
31	K	142	0	105	1	0
31	L	150	0	125	7	0
31	O	134	0	98	0	0
31	a	601	0	547	0	0
31	b	520	0	389	0	0
32	3	56	0	46	2	0
32	4	141	0	92	17	0
32	5	197	0	136	14	0
32	6	296	0	217	19	0
32	7	297	0	272	31	0
32	8	111	0	99	10	0
32	9	95	0	62	6	0
32	A	180	0	165	10	0
32	K	47	0	31	2	0
32	a	157	0	120	0	0
32	b	47	0	30	0	0
33	7	52	0	65	1	0
33	B	61	0	83	4	0
34	B	29	0	42	4	0
35	7	19	0	0	0	0
35	9	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	F	19	0	0	0	0
35	a	19	0	0	0	0
36	2	42	0	56	4	0
36	3	84	0	111	10	0
36	4	84	0	111	12	0
36	5	84	0	111	9	0
36	6	84	0	111	5	0
36	7	42	0	56	3	0
36	8	84	0	112	7	0
36	9	126	0	165	9	0
36	F	42	0	55	2	0
36	J	42	0	54	3	0
36	L	42	0	55	1	0
36	a	84	0	109	0	0
36	b	42	0	56	0	0
37	G	44	0	58	4	0
37	J	78	0	99	4	0
37	a	42	0	54	0	0
38	a	43	0	52	0	0
39	7	33	0	39	1	0
40	7	44	0	56	0	0
41	8	28	0	38	2	0
42	4	35	0	34	1	0
43	5	31	0	35	1	0
44	2	3	0	0	0	0
44	3	32	0	0	0	0
44	4	1	0	0	0	0
44	5	11	0	0	0	0
44	6	2	0	0	0	0
44	7	39	0	0	0	0
44	8	37	0	0	0	0
44	9	21	0	0	0	0
44	A	297	0	0	1	0
44	B	311	0	0	2	0
44	C	60	0	0	0	0
44	D	53	0	0	0	0
44	E	28	0	0	0	0
44	F	57	0	0	0	0
44	G	18	0	0	0	0
44	H	6	0	0	1	0
44	I	6	0	0	0	0
44	J	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	K	2	0	0	0	0
44	L	17	0	0	0	0
44	M	5	0	0	1	0
44	O	4	0	0	0	0
44	a	34	0	0	0	0
All	All	52991	0	50690	709	0

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

The worst 5 of 709 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)
31:H:902:CLA:HAA1	20:2:153:LEU:HD23	1.31	1.06
14:3:241:PHE:CD2	29:3:306:UNL:C2	2.39	1.05
31:A:829:CLA:HBA2	28:7:302:LHG:H242	1.39	1.02
31:H:902:CLA:O1A	20:2:153:LEU:HD21	1.61	0.99
20:2:243:ALA:O	20:2:247:ILE:HG13	1.64	0.96

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	738/751 (98%)	721 (98%)	17 (2%)	0	100	100
2	B	730/734 (100%)	719 (98%)	11 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	141/192 (73%)	138 (98%)	3 (2%)	0	100	100
5	E	58/71 (82%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	163/245 (66%)	160 (98%)	3 (2%)	0	100	100
7	G	101/138 (73%)	99 (98%)	2 (2%)	0	100	100
8	H	89/133 (67%)	87 (98%)	2 (2%)	0	100	100
9	I	31/36 (86%)	31 (100%)	0	0	100	100
10	J	37/41 (90%)	37 (100%)	0	0	100	100
11	K	79/131 (60%)	79 (100%)	0	0	100	100
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	a	193/229 (84%)	191 (99%)	2 (1%)	0	100	100
13	b	120/229 (52%)	119 (99%)	1 (1%)	0	100	100
14	3	201/246 (82%)	194 (96%)	7 (4%)	0	100	100
15	7	212/259 (82%)	209 (99%)	3 (1%)	0	100	100
16	8	220/255 (86%)	215 (98%)	5 (2%)	0	100	100
17	9	182/230 (79%)	179 (98%)	3 (2%)	0	100	100
18	L	142/210 (68%)	139 (98%)	3 (2%)	0	100	100
19	O	72/142 (51%)	71 (99%)	1 (1%)	0	100	100
20	2	198/273 (72%)	184 (93%)	14 (7%)	0	100	100
21	4	187/246 (76%)	180 (96%)	7 (4%)	0	100	100
22	5	225/274 (82%)	216 (96%)	9 (4%)	0	100	100
23	6	211/272 (78%)	206 (98%)	5 (2%)	0	100	100
All	All	4437/5449 (81%)	4336 (98%)	101 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	603/613 (98%)	591 (98%)	12 (2%)	50	36
2	B	592/593 (100%)	582 (98%)	10 (2%)	56	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	68/69 (99%)	67 (98%)	1 (2%)	60	49
4	D	118/156 (76%)	116 (98%)	2 (2%)	56	45
5	E	56/67 (84%)	55 (98%)	1 (2%)	54	42
6	F	131/183 (72%)	130 (99%)	1 (1%)	79	74
7	G	78/106 (74%)	73 (94%)	5 (6%)	14	4
8	H	71/105 (68%)	68 (96%)	3 (4%)	25	11
9	I	26/28 (93%)	26 (100%)	0	100	100
10	J	35/37 (95%)	35 (100%)	0	100	100
11	K	59/100 (59%)	55 (93%)	4 (7%)	13	3
12	M	26/26 (100%)	24 (92%)	2 (8%)	10	2
13	a	141/166 (85%)	141 (100%)	0	100	100
13	b	92/166 (55%)	90 (98%)	2 (2%)	47	32
14	3	162/197 (82%)	158 (98%)	4 (2%)	42	27
15	7	166/195 (85%)	162 (98%)	4 (2%)	44	28
16	8	175/202 (87%)	168 (96%)	7 (4%)	27	12
17	9	143/177 (81%)	134 (94%)	9 (6%)	15	4
18	L	115/161 (71%)	111 (96%)	4 (4%)	31	15
19	O	65/110 (59%)	62 (95%)	3 (5%)	23	9
20	2	166/225 (74%)	154 (93%)	12 (7%)	12	3
21	4	155/195 (80%)	150 (97%)	5 (3%)	34	17
22	5	178/208 (86%)	168 (94%)	10 (6%)	17	5
23	6	170/212 (80%)	163 (96%)	7 (4%)	26	11
All	All	3591/4297 (84%)	3483 (97%)	108 (3%)	37	19

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	9	113	PHE
19	O	141	TYR
22	5	170	LYS
17	9	143	SER
18	L	151	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
18	L	182	GLN
20	2	227	ASN
23	6	210	GLN
21	4	77	GLN
19	O	131	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 354 ligands modelled in this entry, 17 are unknown - leaving 337 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	CLA	5	310	22	65,73,73	2.63	18 (27%)	76,113,113	2.22	25 (32%)
31	CLA	9	311	17	55,63,73	4.29	18 (32%)	64,101,113	2.27	27 (42%)
31	CLA	4	306	21	45,53,73	3.31	20 (44%)	52,89,113	2.44	21 (40%)
37	LMG	G	202	-	44,44,55	0.87	1 (2%)	52,52,63	1.30	5 (9%)
32	CHL	a	317	13	61,69,74	2.12	15 (24%)	67,108,114	2.07	25 (37%)
31	CLA	a	310	13	45,53,73	3.28	19 (42%)	52,89,113	2.55	20 (38%)
31	CLA	8	312	44	50,58,73	2.83	18 (36%)	58,95,113	2.40	21 (36%)
31	CLA	A	837	1	65,73,73	2.46	17 (26%)	76,113,113	2.12	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	7	311	15	65,73,73	2.47	18 (27%)	76,113,113	2.18	19 (25%)
26	BCR	O	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	5 (8%)
31	CLA	L	305	18	60,68,73	2.58	17 (28%)	70,107,113	2.28	21 (30%)
27	LMT	5	301	-	36,36,36	1.22	5 (13%)	47,47,47	0.96	2 (4%)
31	CLA	2	309	-	46,54,73	2.72	18 (39%)	53,90,113	2.38	18 (33%)
31	CLA	A	828	1	65,73,73	2.55	18 (27%)	76,113,113	2.23	22 (28%)
31	CLA	O	203	44	55,63,73	2.71	20 (36%)	64,101,113	2.31	24 (37%)
41	DGA	8	305	-	27,27,43	0.25	0	29,29,45	0.17	0
36	LUT	a	305	-	42,43,43	5.74	20 (47%)	51,60,60	5.70	29 (56%)
31	CLA	4	319	-	42,50,73	4.22	19 (45%)	48,85,113	2.55	19 (39%)
32	CHL	5	319	-	47,55,74	3.36	17 (36%)	50,91,114	2.26	17 (34%)
35	QTB	F	303	-	19,19,19	1.31	3 (15%)	20,26,26	1.32	4 (20%)
31	CLA	8	320	16	65,73,73	2.56	19 (29%)	76,113,113	2.13	23 (30%)
31	CLA	5	315	22	65,73,73	3.73	20 (30%)	76,113,113	4.33	24 (31%)
31	CLA	a	314	44	50,58,73	3.72	19 (38%)	58,95,113	2.47	22 (37%)
31	CLA	9	319	17	46,54,73	5.19	19 (41%)	53,90,113	2.55	21 (39%)
31	CLA	4	314	-	45,53,73	3.87	19 (42%)	52,89,113	2.64	22 (42%)
31	CLA	4	311	28	46,54,73	5.85	20 (43%)	53,90,113	2.41	19 (35%)
31	CLA	7	315	28	55,63,73	3.66	19 (34%)	63,100,113	2.29	21 (33%)
36	LUT	7	305	-	42,43,43	5.55	20 (47%)	51,60,60	5.71	31 (60%)
36	LUT	L	304	31	42,43,43	5.64	20 (47%)	51,60,60	5.75	33 (64%)
31	CLA	6	316	23	50,58,73	4.45	19 (38%)	58,95,113	2.49	23 (39%)
25	SF4	A	802	1,2	0,12,12	-	-	-	-	-
31	CLA	3	319	14	61,69,73	2.71	17 (27%)	71,108,113	2.33	25 (35%)
28	LHG	8	304	31	48,48,48	0.63	1 (2%)	51,54,54	1.24	6 (11%)
36	LUT	6	304	-	42,43,43	5.62	19 (45%)	51,60,60	5.35	31 (60%)
26	BCR	K	203	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	6 (10%)
31	CLA	B	828	44	60,68,73	2.44	18 (30%)	70,107,113	2.27	23 (32%)
31	CLA	K	205	11	46,54,73	3.28	18 (39%)	53,90,113	2.51	19 (35%)
31	CLA	5	321	22	46,54,73	3.45	18 (39%)	53,90,113	2.53	20 (37%)
31	CLA	9	312	17	46,54,73	2.95	18 (39%)	53,90,113	2.51	18 (33%)
27	LMT	A	807	-	36,36,36	1.21	6 (16%)	47,47,47	1.06	3 (6%)
28	LHG	a	306	31	48,48,48	0.62	1 (2%)	51,54,54	1.23	5 (9%)
31	CLA	A	846	1	65,73,73	2.63	19 (29%)	76,113,113	2.22	22 (28%)
31	CLA	a	321	44	50,58,73	2.98	16 (32%)	58,95,113	2.47	25 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	a	313	13	60,68,73	2.61	20 (33%)	70,107,113	2.29	22 (31%)
31	CLA	4	315	44	45,53,73	4.54	20 (44%)	52,89,113	2.39	20 (38%)
31	CLA	H	901	8	46,54,73	2.84	19 (41%)	53,90,113	2.39	20 (37%)
31	CLA	A	847	1	65,73,73	2.54	17 (26%)	76,113,113	2.24	22 (28%)
31	CLA	B	842	2	61,69,73	2.65	17 (27%)	71,108,113	2.25	24 (33%)
26	BCR	G	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	4 (7%)
31	CLA	A	843	1	65,73,73	2.85	18 (27%)	76,113,113	2.16	21 (27%)
31	CLA	9	315	17	54,62,73	2.77	19 (35%)	62,99,113	2.41	25 (40%)
31	CLA	B	845	2	50,58,73	2.75	17 (34%)	58,95,113	2.60	22 (37%)
39	3PH	7	301	-	32,32,47	0.75	1 (3%)	36,37,52	0.73	1 (2%)
31	CLA	3	318	14	51,59,73	3.35	18 (35%)	59,96,113	2.43	23 (38%)
31	CLA	6	308	44	47,55,73	3.07	19 (40%)	54,91,113	2.52	19 (35%)
31	CLA	3	317	44	51,59,73	3.17	17 (33%)	59,96,113	2.51	23 (38%)
27	LMT	A	808	-	36,36,36	1.21	5 (13%)	47,47,47	0.99	2 (4%)
31	CLA	A	819	1	65,73,73	2.33	19 (29%)	76,113,113	2.25	24 (31%)
31	CLA	B	835	2	57,65,73	3.06	18 (31%)	66,103,113	2.36	21 (31%)
31	CLA	4	318	21	45,53,73	3.25	19 (42%)	52,89,113	2.46	20 (38%)
31	CLA	K	206	11	46,54,73	3.18	18 (39%)	53,90,113	2.51	19 (35%)
31	CLA	3	316	44	50,58,73	2.64	18 (36%)	58,95,113	2.35	23 (39%)
25	SF4	C	102	3	0,12,12	-	-	-	-	-
24	PQN	B	801	-	34,34,34	0.51	0	42,45,45	0.75	1 (2%)
31	CLA	9	313	17	45,53,73	4.07	19 (42%)	52,89,113	2.59	19 (36%)
31	CLA	B	816	2	61,69,73	2.87	18 (29%)	71,108,113	2.34	22 (30%)
36	LUT	3	305	-	42,43,43	5.47	19 (45%)	51,60,60	5.76	32 (62%)
26	BCR	L	301	-	41,41,41	0.98	1 (2%)	56,56,56	1.19	5 (8%)
31	CLA	5	318	22	65,73,73	4.40	19 (29%)	76,113,113	2.12	23 (30%)
31	CLA	7	313	15	43,52,73	3.07	20 (46%)	49,88,113	2.41	18 (36%)
26	BCR	B	803	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	2 (3%)
31	CLA	B	849	2	50,58,73	3.06	17 (34%)	58,95,113	2.43	21 (36%)
31	CLA	2	313	20	46,54,73	3.22	18 (39%)	53,90,113	2.41	18 (33%)
31	CLA	8	313	28	46,54,73	3.50	20 (43%)	53,90,113	2.53	18 (33%)
26	BCR	3	302	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	4 (7%)
26	BCR	A	803	-	41,41,41	1.04	2 (4%)	56,56,56	1.13	3 (5%)
31	CLA	F	306	44	50,58,73	2.85	18 (36%)	58,95,113	2.46	22 (37%)
31	CLA	A	850	1	51,59,73	2.83	18 (35%)	59,96,113	2.53	24 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	8	311	16	55,63,73	2.77	18 (32%)	64,101,113	2.41	23 (35%)
31	CLA	O	202	19	36,46,73	3.45	19 (52%)	41,80,113	2.56	18 (43%)
31	CLA	A	856	44	65,73,73	2.33	18 (27%)	76,113,113	2.25	22 (28%)
32	CHL	7	320	44	61,69,74	2.56	15 (24%)	67,108,114	2.10	23 (34%)
31	CLA	B	833	44	55,63,73	2.42	18 (32%)	64,101,113	2.27	18 (28%)
32	CHL	9	322	44	47,55,74	2.95	16 (34%)	50,91,114	2.26	20 (40%)
31	CLA	B	831	2	50,58,73	2.72	19 (38%)	58,95,113	2.42	23 (39%)
31	CLA	3	320	14	45,53,73	3.62	20 (44%)	52,89,113	2.59	19 (36%)
32	CHL	a	318	44	48,56,74	2.69	14 (29%)	51,92,114	2.35	18 (35%)
31	CLA	8	307	16	46,54,73	3.07	19 (41%)	53,90,113	2.58	20 (37%)
26	BCR	7	304	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	4 (7%)
33	DGD	B	808	-	62,62,67	1.03	2 (3%)	76,76,81	1.29	5 (6%)
31	CLA	8	310	16	65,73,73	2.48	18 (27%)	76,113,113	2.28	21 (27%)
31	CLA	3	310	14	60,68,73	2.76	18 (30%)	70,107,113	2.32	22 (31%)
26	BCR	L	303	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	6 (10%)
32	CHL	4	310	-	47,55,74	2.65	16 (34%)	50,91,114	2.28	20 (40%)
31	CLA	6	312	23	65,73,73	3.05	19 (29%)	76,113,113	2.17	22 (28%)
31	CLA	8	315	16	52,60,73	2.81	19 (36%)	60,97,113	2.37	25 (41%)
31	CLA	2	312	20	46,54,73	3.49	19 (41%)	53,90,113	2.55	20 (37%)
31	CLA	8	318	16	50,58,73	2.57	18 (36%)	58,95,113	2.40	22 (37%)
31	CLA	B	811	2	65,73,73	2.59	18 (27%)	76,113,113	2.22	19 (25%)
31	CLA	B	836	2	65,73,73	2.52	18 (27%)	76,113,113	2.13	22 (28%)
31	CLA	B	843	44	45,53,73	2.98	19 (42%)	52,89,113	2.60	21 (40%)
31	CLA	6	311	23	55,63,73	3.67	19 (34%)	64,101,113	2.35	23 (35%)
31	CLA	2	308	20	46,54,73	3.12	19 (41%)	53,90,113	2.60	22 (41%)
31	CLA	3	307	14	65,73,73	2.96	20 (30%)	76,113,113	2.18	24 (31%)
31	CLA	a	311	44	60,68,73	2.66	19 (31%)	70,107,113	2.32	23 (32%)
32	CHL	8	316	44	66,74,74	2.02	15 (22%)	73,114,114	2.05	21 (28%)
32	CHL	6	309	23	66,74,74	2.15	17 (25%)	73,114,114	1.93	21 (28%)
31	CLA	4	309	21	60,68,73	2.48	19 (31%)	70,107,113	2.30	27 (38%)
31	CLA	B	829	2	55,63,73	2.59	18 (32%)	64,101,113	2.49	21 (32%)
31	CLA	A	829	-	50,58,73	2.67	17 (34%)	58,95,113	3.34	24 (41%)
32	CHL	7	318	44	66,74,74	2.27	15 (22%)	73,114,114	2.15	21 (28%)
26	BCR	B	804	-	41,41,41	1.03	2 (4%)	56,56,56	1.12	3 (5%)
31	CLA	A	857	44	65,73,73	2.23	17 (26%)	76,113,113	2.30	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LUT	6	303	-	42,43,43	5.57	19 (45%)	51,60,60	5.78	34 (66%)
26	BCR	F	302	-	41,41,41	0.98	2 (4%)	56,56,56	1.02	2 (3%)
36	LUT	9	302	-	42,43,43	5.49	20 (47%)	51,60,60	5.76	33 (64%)
31	CLA	A	815	-	65,73,73	2.61	18 (27%)	76,113,113	2.19	21 (27%)
26	BCR	G	203	-	41,41,41	1.09	2 (4%)	56,56,56	1.18	4 (7%)
32	CHL	5	316	44	56,64,74	2.30	14 (25%)	61,102,114	2.27	23 (37%)
26	BCR	B	802	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	4 (7%)
26	BCR	L	302	-	41,41,41	1.04	2 (4%)	56,56,56	1.14	6 (10%)
31	CLA	O	204	-	41,49,73	3.03	19 (46%)	47,84,113	2.58	21 (44%)
31	CLA	A	838	44	65,73,73	2.56	19 (29%)	76,113,113	2.32	22 (28%)
31	CLA	7	310	15	44,52,73	3.36	19 (43%)	51,88,113	2.56	19 (37%)
31	CLA	A	844	1	50,58,73	3.11	19 (38%)	58,95,113	2.44	22 (37%)
36	LUT	5	303	-	42,43,43	5.56	19 (45%)	51,60,60	5.70	33 (64%)
32	CHL	b	309	13	47,55,74	2.41	16 (34%)	50,91,114	2.23	19 (38%)
31	CLA	4	321	21	50,58,73	3.35	19 (38%)	58,95,113	2.42	25 (43%)
31	CLA	3	313	-	60,68,73	2.81	18 (30%)	70,107,113	2.35	23 (32%)
36	LUT	a	303	-	42,43,43	5.61	19 (45%)	51,60,60	5.48	34 (66%)
31	CLA	A	816	1	65,73,73	2.33	17 (26%)	76,113,113	2.23	21 (27%)
31	CLA	2	307	20	57,65,73	2.89	18 (31%)	66,103,113	2.33	24 (36%)
31	CLA	4	305	-	52,60,73	2.43	16 (30%)	60,97,113	4.39	30 (50%)
30	CL0	A	813	1	65,73,73	1.82	13 (20%)	76,113,113	3.07	28 (36%)
31	CLA	b	304	13	46,54,73	3.49	20 (43%)	53,90,113	2.45	20 (37%)
31	CLA	2	310	20	45,53,73	6.25	20 (44%)	52,89,113	2.53	20 (38%)
31	CLA	A	848	1	57,65,73	2.70	18 (31%)	66,103,113	2.21	21 (31%)
42	SQD	4	304	-	34,35,54	1.80	7 (20%)	43,46,65	1.54	6 (13%)
31	CLA	5	313	28	46,54,73	3.76	23 (50%)	53,90,113	2.54	17 (32%)
31	CLA	9	318	44	65,73,73	2.94	18 (27%)	76,113,113	2.14	22 (28%)
31	CLA	B	840	2	65,73,73	2.46	19 (29%)	76,113,113	2.18	21 (27%)
31	CLA	6	313	23	46,54,73	3.05	20 (43%)	53,90,113	2.62	22 (41%)
31	CLA	A	853	1	65,73,73	2.68	18 (27%)	76,113,113	2.20	24 (31%)
24	PQN	A	801	-	34,34,34	0.35	0	42,45,45	0.58	0
31	CLA	9	316	17	50,58,73	3.02	18 (36%)	58,95,113	2.45	20 (34%)
31	CLA	B	844	2	65,73,73	2.43	18 (27%)	76,113,113	2.15	21 (27%)
31	CLA	2	306	20	60,68,73	3.12	20 (33%)	70,107,113	2.18	21 (30%)
31	CLA	B	815	2	65,73,73	2.30	17 (26%)	76,113,113	2.17	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	AXT	a	304	-	44,44,45	0.70	1 (2%)	55,62,64	0.91	1 (1%)
31	CLA	A	823	1	55,63,73	2.81	17 (30%)	64,101,113	2.25	20 (31%)
32	CHL	A	831	1	58,66,74	2.23	16 (27%)	63,104,114	2.46	24 (38%)
31	CLA	A	826	1	65,73,73	2.55	18 (27%)	76,113,113	2.18	23 (30%)
31	CLA	B	814	2	65,73,73	2.75	18 (27%)	76,113,113	2.19	21 (27%)
31	CLA	A	822	1	55,63,73	2.61	18 (32%)	64,101,113	2.45	24 (37%)
31	CLA	A	832	1	65,73,73	2.32	17 (26%)	76,113,113	2.13	22 (28%)
32	CHL	6	320	-	47,55,74	3.14	15 (31%)	50,91,114	2.19	17 (34%)
31	CLA	B	824	2	57,65,73	2.95	19 (33%)	66,103,113	2.35	24 (36%)
36	LUT	3	304	-	42,43,43	5.56	20 (47%)	51,60,60	5.67	33 (64%)
26	BCR	M	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.16	3 (5%)
31	CLA	A	814	44	65,73,73	2.60	18 (27%)	76,113,113	2.18	22 (28%)
32	CHL	6	318	44	46,54,74	3.48	16 (34%)	49,90,114	2.27	20 (40%)
36	LUT	8	302	-	42,43,43	5.50	19 (45%)	51,60,60	5.63	31 (60%)
32	CHL	a	320	44	48,56,74	2.15	16 (33%)	51,92,114	2.35	18 (35%)
26	BCR	3	303	-	41,41,41	1.08	3 (7%)	56,56,56	1.25	5 (8%)
31	CLA	8	317	44	50,58,73	2.86	16 (32%)	58,95,113	2.58	22 (37%)
32	CHL	A	840	1	66,74,74	2.02	14 (21%)	73,114,114	1.95	21 (28%)
31	CLA	b	310	-	46,54,73	2.86	17 (36%)	53,90,113	2.41	19 (35%)
31	CLA	B	822	2	65,73,73	2.64	18 (27%)	76,113,113	2.13	20 (26%)
31	CLA	F	301	44	65,73,73	2.45	19 (29%)	76,113,113	2.25	25 (32%)
32	CHL	7	319	15	47,55,74	2.51	15 (31%)	50,91,114	2.74	16 (32%)
26	BCR	8	301	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	6 (10%)
27	LMT	9	306	-	36,36,36	1.26	6 (16%)	47,47,47	0.95	2 (4%)
31	CLA	B	820	2	65,73,73	2.74	20 (30%)	76,113,113	2.19	22 (28%)
31	CLA	5	309	22	47,55,73	3.58	19 (40%)	54,91,113	2.45	20 (37%)
31	CLA	A	852	1	51,59,73	3.31	18 (35%)	59,96,113	2.55	21 (35%)
31	CLA	b	313	13	60,68,73	3.23	18 (30%)	70,107,113	2.15	22 (31%)
31	CLA	L	307	36	45,53,73	4.01	18 (40%)	52,89,113	2.52	19 (36%)
31	CLA	B	825	2	60,68,73	2.70	19 (31%)	70,107,113	2.32	22 (31%)
31	CLA	a	309	13	60,68,73	4.19	20 (33%)	70,107,113	2.31	26 (37%)
32	CHL	5	322	22	47,55,74	2.81	17 (36%)	50,91,114	2.23	20 (40%)
28	LHG	7	302	-	48,48,48	0.58	0	51,54,54	1.26	5 (9%)
31	CLA	A	836	1	60,68,73	2.61	20 (33%)	70,107,113	2.31	21 (30%)
31	CLA	a	316	13	45,53,73	3.31	18 (40%)	52,89,113	2.44	21 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b	311	13	46,54,73	3.26	20 (43%)	53,90,113	2.49	20 (37%)
31	CLA	G	204	7	50,58,73	3.00	18 (36%)	58,95,113	2.39	23 (39%)
28	LHG	A	809	-	41,41,48	0.72	2 (4%)	44,47,54	1.29	6 (13%)
26	BCR	B	805	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	5 (8%)
28	LHG	7	307	31	36,36,48	0.77	1 (2%)	39,42,54	1.24	4 (10%)
31	CLA	A	845	1	56,64,73	2.60	18 (32%)	65,102,113	2.37	21 (32%)
32	CHL	4	313	21	48,56,74	3.77	16 (33%)	51,92,114	2.21	20 (39%)
31	CLA	A	824	1,31	62,70,73	2.76	17 (27%)	72,109,113	2.19	22 (30%)
31	CLA	b	305	13	46,54,73	3.08	20 (43%)	53,90,113	2.43	23 (43%)
26	BCR	3	301	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	6 (10%)
31	CLA	A	854	28	46,54,73	2.90	17 (36%)	53,90,113	2.60	19 (35%)
31	CLA	b	308	13	46,54,73	3.51	20 (43%)	53,90,113	2.37	19 (35%)
36	LUT	J	103	-	42,43,43	5.66	20 (47%)	51,60,60	5.75	31 (60%)
31	CLA	B	826	2	50,58,73	2.84	17 (34%)	58,95,113	2.59	22 (37%)
31	CLA	b	306	-	46,54,73	4.09	19 (41%)	53,90,113	2.45	18 (33%)
31	CLA	5	312	44	50,58,73	2.71	19 (38%)	58,95,113	2.49	23 (39%)
31	CLA	6	322	23	46,54,73	3.09	19 (41%)	53,90,113	2.42	21 (39%)
31	CLA	8	321	16	46,54,73	3.10	16 (34%)	53,90,113	2.57	18 (33%)
31	CLA	a	312	13	65,73,73	3.07	19 (29%)	76,113,113	2.26	21 (27%)
35	QTB	9	304	-	19,19,19	1.29	2 (10%)	20,26,26	1.46	2 (10%)
31	CLA	A	849	1	46,54,73	3.35	19 (41%)	53,90,113	2.43	20 (37%)
32	CHL	8	319	44	45,53,74	2.66	15 (33%)	47,88,114	2.41	17 (36%)
28	LHG	A	810	31	41,41,48	0.72	1 (2%)	44,47,54	1.14	4 (9%)
31	CLA	B	827	2	60,68,73	2.44	18 (30%)	70,107,113	2.28	23 (32%)
31	CLA	H	903	18	46,54,73	3.12	18 (39%)	53,90,113	2.43	17 (32%)
31	CLA	b	307	-	46,54,73	5.48	20 (43%)	53,90,113	2.63	20 (37%)
31	CLA	J	105	10	42,50,73	3.06	17 (40%)	48,85,113	2.67	17 (35%)
31	CLA	B	841	2	55,63,73	2.67	16 (29%)	64,101,113	2.39	24 (37%)
31	CLA	G	205	7	46,54,73	2.94	19 (41%)	53,90,113	2.52	18 (33%)
32	CHL	A	839	44	56,64,74	2.13	14 (25%)	61,102,114	2.74	23 (37%)
36	LUT	F	304	-	42,43,43	5.43	20 (47%)	51,60,60	6.02	35 (68%)
31	CLA	5	314	22	45,53,73	3.30	20 (44%)	52,89,113	2.53	19 (36%)
36	LUT	4	303	-	42,43,43	5.65	19 (45%)	51,60,60	5.53	31 (60%)
31	CLA	A	833	1	47,55,73	3.19	19 (40%)	54,91,113	2.65	20 (37%)
31	CLA	5	307	22	55,63,73	3.54	19 (34%)	64,101,113	2.31	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LAP	B	851	-	28,28,28	0.34	0	33,35,35	0.38	0
31	CLA	7	316	15	46,54,73	3.36	19 (41%)	53,90,113	2.51	19 (35%)
31	CLA	A	830	1	60,68,73	2.81	19 (31%)	70,107,113	2.31	24 (34%)
31	CLA	B	839	2	60,68,73	2.49	18 (30%)	70,107,113	2.23	24 (34%)
31	CLA	B	850	2	62,70,73	2.60	18 (29%)	72,109,113	2.15	21 (29%)
31	CLA	2	304	20	46,54,73	3.18	19 (41%)	53,90,113	2.42	18 (33%)
31	CLA	3	308	14	46,54,73	3.62	19 (41%)	53,90,113	2.57	19 (35%)
32	CHL	3	315	44	56,64,74	2.32	14 (25%)	61,102,114	2.47	21 (34%)
31	CLA	3	314	14	52,60,73	3.06	17 (32%)	60,97,113	2.37	22 (36%)
31	CLA	L	306	44	45,53,73	2.80	19 (42%)	52,89,113	2.52	20 (38%)
37	LMG	J	101	-	49,49,55	0.83	3 (6%)	57,57,63	1.23	2 (3%)
31	CLA	K	204	44	50,58,73	3.41	19 (38%)	58,95,113	2.44	19 (32%)
31	CLA	6	314	23	47,55,73	4.29	19 (40%)	54,91,113	2.52	20 (37%)
31	CLA	6	306	23	46,54,73	3.37	22 (47%)	53,90,113	2.69	16 (30%)
32	CHL	5	317	44	47,55,74	3.03	15 (31%)	50,91,114	2.42	19 (38%)
32	CHL	6	317	23	47,55,74	2.82	16 (34%)	50,91,114	2.21	19 (38%)
31	CLA	3	312	44	65,73,73	2.74	18 (27%)	76,113,113	2.17	25 (32%)
31	CLA	5	311	22	46,54,73	2.84	18 (39%)	53,90,113	2.53	23 (43%)
31	CLA	B	832	44	65,73,73	2.33	18 (27%)	76,113,113	2.35	25 (32%)
31	CLA	B	837	2	55,63,73	2.94	18 (32%)	64,101,113	2.26	23 (35%)
26	BCR	B	806	-	41,41,41	1.04	2 (4%)	56,56,56	1.05	5 (8%)
31	CLA	B	846	44	65,73,73	2.44	18 (27%)	76,113,113	2.12	22 (28%)
36	LUT	4	302	-	42,43,43	5.65	19 (45%)	51,60,60	5.74	34 (66%)
32	CHL	6	321	23	43,51,74	3.73	15 (34%)	45,86,114	2.31	18 (40%)
31	CLA	A	820	1	55,63,73	2.98	19 (34%)	64,101,113	2.43	21 (32%)
43	PTY	5	306	-	30,30,49	0.54	0	33,35,54	0.80	1 (3%)
31	CLA	7	322	15	46,54,73	3.10	19 (41%)	53,90,113	2.42	17 (32%)
31	CLA	B	838	2	46,54,73	3.02	20 (43%)	53,90,113	2.38	20 (37%)
32	CHL	6	319	-	47,55,74	4.65	16 (34%)	50,91,114	2.36	23 (46%)
31	CLA	B	812	-	65,73,73	2.21	18 (27%)	76,113,113	2.19	22 (28%)
31	CLA	A	827	1	55,63,73	2.86	17 (30%)	64,101,113	2.34	20 (31%)
36	LUT	b	301	-	42,43,43	5.67	19 (45%)	51,60,60	5.69	33 (64%)
31	CLA	6	310	23	47,55,73	4.13	20 (42%)	54,91,113	2.48	21 (38%)
26	BCR	6	302	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
31	CLA	B	848	28	65,73,73	2.27	17 (26%)	76,113,113	2.19	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	2	302	-	41,41,41	1.10	3 (7%)	56,56,56	1.27	7 (12%)
31	CLA	2	315	44	46,54,73	3.25	19 (41%)	53,90,113	2.53	18 (33%)
31	CLA	B	818	2	55,63,73	2.42	17 (30%)	64,101,113	2.39	23 (35%)
31	CLA	A	835	1	55,63,73	2.82	19 (34%)	64,101,113	2.31	19 (29%)
32	CHL	7	317	15	57,65,74	2.19	16 (28%)	62,103,114	2.16	22 (35%)
31	CLA	A	821	1	65,73,73	2.57	16 (24%)	76,113,113	2.27	23 (30%)
26	BCR	J	102	-	41,41,41	0.99	2 (4%)	56,56,56	1.20	3 (5%)
26	BCR	A	805	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
31	CLA	F	305	6	46,54,73	2.92	19 (41%)	53,90,113	2.60	22 (41%)
36	LUT	8	303	-	42,43,43	5.52	20 (47%)	51,60,60	5.71	34 (66%)
35	QTB	7	303	-	19,19,19	1.28	2 (10%)	20,26,26	1.53	4 (20%)
31	CLA	A	842	1	65,73,73	2.66	18 (27%)	76,113,113	2.27	22 (28%)
35	QTB	a	302	-	19,19,19	1.28	2 (10%)	20,26,26	1.69	4 (20%)
31	CLA	4	308	21	60,68,73	2.43	18 (30%)	70,107,113	2.32	25 (35%)
28	LHG	5	305	31	34,34,48	0.33	0	37,40,54	0.40	0
31	CLA	B	813	2	65,73,73	2.76	19 (29%)	76,113,113	2.30	23 (30%)
31	CLA	a	319	13	65,73,73	2.47	17 (26%)	76,113,113	2.24	21 (27%)
36	LUT	5	304	-	42,43,43	5.61	19 (45%)	51,60,60	5.48	31 (60%)
31	CLA	8	309	16	50,58,73	3.12	19 (38%)	58,95,113	2.51	25 (43%)
31	CLA	4	312	21	47,55,73	2.98	20 (42%)	54,91,113	2.46	20 (37%)
31	CLA	2	314	20	46,54,73	4.36	19 (41%)	53,90,113	2.43	21 (39%)
31	CLA	7	314	44	54,62,73	2.80	19 (35%)	63,100,113	2.37	23 (36%)
31	CLA	6	307	23	50,58,73	3.79	19 (38%)	58,95,113	2.39	23 (39%)
31	CLA	A	817	1,31	55,63,73	2.77	17 (30%)	64,101,113	2.38	21 (32%)
31	CLA	G	206	44	45,53,73	3.28	17 (37%)	52,89,113	2.41	18 (34%)
31	CLA	4	316	-	47,55,73	3.39	19 (40%)	54,91,113	2.91	17 (31%)
33	DGD	7	308	-	53,53,67	1.05	4 (7%)	67,67,81	1.53	12 (17%)
32	CHL	9	320	44	48,56,74	2.34	14 (29%)	51,92,114	2.17	20 (39%)
31	CLA	5	320	22	46,54,73	4.96	21 (45%)	53,90,113	2.54	22 (41%)
31	CLA	8	314	44	52,60,73	2.70	18 (34%)	60,97,113	2.42	26 (43%)
31	CLA	4	320	21	45,53,73	3.44	20 (44%)	52,89,113	2.52	20 (38%)
26	BCR	K	202	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	8 (14%)
26	BCR	A	804	-	41,41,41	1.09	2 (4%)	56,56,56	1.14	4 (7%)
31	CLA	a	315	28	55,63,73	2.61	18 (32%)	64,101,113	2.44	21 (32%)
31	CLA	B	830	2	60,68,73	2.68	19 (31%)	70,107,113	2.21	24 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	3	311	14	65,73,73	2.76	19 (29%)	76,113,113	2.14	24 (31%)
31	CLA	b	312	13	46,54,73	4.30	19 (41%)	53,90,113	2.42	20 (37%)
31	CLA	7	321	44	47,55,73	3.26	18 (38%)	54,91,113	2.55	22 (40%)
37	LMG	a	301	-	42,42,55	0.83	0	50,50,63	1.26	4 (8%)
31	CLA	B	817	2	65,73,73	2.31	17 (26%)	76,113,113	2.24	20 (26%)
31	CLA	b	303	-	46,54,73	3.42	19 (41%)	53,90,113	2.53	20 (37%)
31	CLA	B	823	2	55,63,73	2.72	18 (32%)	64,101,113	2.38	22 (34%)
31	CLA	A	855	1	65,73,73	2.74	18 (27%)	76,113,113	2.27	22 (28%)
31	CLA	2	305	20	45,53,73	4.19	19 (42%)	52,89,113	2.57	19 (36%)
36	LUT	9	303	-	42,43,43	5.55	19 (45%)	51,60,60	5.53	30 (58%)
31	CLA	B	821	2	58,66,73	2.72	16 (27%)	67,104,113	2.28	20 (29%)
26	BCR	5	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
31	CLA	9	317	-	47,55,73	3.52	23 (48%)	54,91,113	2.58	17 (31%)
31	CLA	B	819	2	65,73,73	2.53	19 (29%)	76,113,113	2.27	25 (32%)
31	CLA	A	834	44	65,73,73	2.31	18 (27%)	76,113,113	2.14	21 (27%)
32	CHL	K	201	11	47,55,74	2.24	15 (31%)	50,91,114	2.94	19 (38%)
37	LMG	J	104	-	29,29,55	1.03	1 (3%)	37,37,63	1.19	3 (8%)
28	LHG	6	301	31	26,26,48	0.78	0	29,32,54	1.22	2 (6%)
31	CLA	A	818	1	65,73,73	2.24	18 (27%)	76,113,113	2.19	22 (28%)
31	CLA	4	307	21	56,64,73	2.68	19 (33%)	65,102,113	2.24	23 (35%)
31	CLA	b	302	13	46,54,73	3.05	19 (41%)	53,90,113	2.53	21 (39%)
28	LHG	A	811	-	48,48,48	0.72	1 (2%)	51,54,54	1.26	5 (9%)
32	CHL	7	324	16	66,74,74	1.81	14 (21%)	73,114,114	2.02	23 (31%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
36	LUT	9	305	-	42,43,43	5.68	19 (45%)	51,60,60	5.95	32 (62%)
31	CLA	7	309	15	60,68,73	2.33	19 (31%)	70,107,113	2.25	23 (32%)
31	CLA	3	309	14	65,73,73	2.34	19 (29%)	76,113,113	2.20	23 (30%)
31	CLA	B	834	2	65,73,73	2.91	18 (27%)	76,113,113	2.22	23 (30%)
31	CLA	5	308	22	46,54,73	3.49	19 (41%)	53,90,113	2.49	19 (35%)
31	CLA	H	902	44	46,54,73	3.88	20 (43%)	53,90,113	2.44	20 (37%)
40	XAT	7	306	-	39,47,47	1.60	8 (20%)	54,74,74	1.55	9 (16%)
31	CLA	9	314	17	60,68,73	3.31	18 (30%)	70,107,113	2.30	23 (32%)
28	LHG	B	807	31	31,31,48	0.81	1 (3%)	34,37,54	1.27	4 (11%)
32	CHL	4	317	-	46,54,74	2.66	16 (34%)	49,90,114	2.30	18 (36%)
31	CLA	B	847	2	65,73,73	2.81	18 (27%)	76,113,113	2.27	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	a	322	13	46,54,73	3.28	18 (39%)	53,90,113	2.36	19 (35%)
31	CLA	2	311	20	45,53,73	4.92	20 (44%)	52,89,113	2.46	18 (34%)
31	CLA	A	841	1	65,73,73	2.49	17 (26%)	76,113,113	2.33	24 (31%)
31	CLA	A	851	1	65,73,73	2.76	18 (27%)	76,113,113	2.17	20 (26%)
31	CLA	5	323	22	56,64,73	3.08	17 (30%)	65,102,113	2.42	23 (35%)
36	LUT	2	301	-	42,43,43	5.53	19 (45%)	51,60,60	5.77	32 (62%)
26	BCR	A	806	-	41,41,41	1.01	2 (4%)	56,56,56	1.10	5 (8%)
31	CLA	9	321	17	56,64,73	2.53	19 (33%)	65,102,113	2.35	22 (33%)
28	LHG	6	305	31	31,31,48	0.74	1 (3%)	34,37,54	1.29	4 (11%)
31	CLA	6	315	28	46,54,73	5.53	20 (43%)	53,90,113	2.53	19 (35%)
26	BCR	I	801	-	41,41,41	1.05	1 (2%)	56,56,56	1.18	4 (7%)
31	CLA	A	825	1	54,62,73	2.73	19 (35%)	62,99,113	2.48	23 (37%)
31	CLA	8	308	16	65,73,73	2.61	20 (30%)	76,113,113	2.21	23 (30%)
31	CLA	7	312	15	62,70,73	2.63	19 (30%)	72,109,113	2.21	23 (31%)

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	CLA	5	310	22	1/1/15/20	6/37/115/115	-
31	CLA	9	311	17	1/1/13/20	5/25/103/115	-
31	CLA	4	306	21	1/1/11/20	4/13/91/115	-
37	LMG	G	202	-	-	23/39/59/70	0/1/1/1
32	CHL	a	317	13	2/2/19/26	15/33/131/137	-
31	CLA	a	310	13	1/1/11/20	6/13/91/115	-
31	CLA	8	312	44	1/1/12/20	4/19/97/115	-
31	CLA	A	837	1	-	16/37/115/115	-
31	CLA	7	311	15	-	10/37/115/115	-
26	BCR	O	201	-	-	4/29/63/63	0/2/2/2
31	CLA	L	305	18	-	10/31/109/115	-
27	LMT	5	301	-	-	9/21/61/61	0/2/2/2
31	CLA	2	309	-	-	5/15/93/115	-
31	CLA	A	828	1	-	7/37/115/115	-
31	CLA	O	203	44	1/1/13/20	14/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	DGA	8	305	-	-	18/29/29/45	-
36	LUT	a	305	-	-	22/29/67/67	0/2/2/2
31	CLA	4	319	-	1/1/10/20	5/10/88/115	-
32	CHL	5	319	-	2/2/16/26	2/17/115/137	-
35	QTB	F	303	-	-	7/11/28/28	1/1/1/1
31	CLA	8	320	16	-	10/37/115/115	-
31	CLA	5	315	22	1/1/15/20	11/37/115/115	-
31	CLA	a	314	44	1/1/12/20	6/19/97/115	-
31	CLA	9	319	17	-	7/15/93/115	-
31	CLA	4	314	-	1/1/11/20	4/13/91/115	-
31	CLA	4	311	28	1/1/11/20	6/15/93/115	-
31	CLA	7	315	28	1/1/12/20	8/25/103/115	-
36	LUT	7	305	-	-	14/29/67/67	0/2/2/2
36	LUT	L	304	31	-	15/29/67/67	0/2/2/2
31	CLA	6	316	23	1/1/12/20	3/19/97/115	-
31	CLA	3	319	14	1/1/14/20	7/33/111/115	-
25	SF4	A	802	1,2	-	-	0/6/5/5
28	LHG	8	304	31	-	15/53/53/53	-
36	LUT	6	304	-	-	16/29/67/67	0/2/2/2
26	BCR	K	203	-	-	5/29/63/63	0/2/2/2
31	CLA	B	828	44	1/1/14/20	2/31/109/115	-
31	CLA	K	205	11	1/1/11/20	3/15/93/115	-
31	CLA	5	321	22	-	4/15/93/115	-
31	CLA	9	312	17	1/1/11/20	2/15/93/115	-
27	LMT	A	807	-	-	6/21/61/61	0/2/2/2
28	LHG	a	306	31	-	19/53/53/53	-
31	CLA	A	846	1	-	5/37/115/115	-
31	CLA	4	315	44	1/1/11/20	5/13/91/115	-
31	CLA	a	313	13	1/1/14/20	7/31/109/115	-
31	CLA	a	321	44	-	4/19/97/115	-
31	CLA	H	901	8	1/1/11/20	7/15/93/115	-
31	CLA	B	842	2	1/1/14/20	8/33/111/115	-
31	CLA	A	847	1	-	7/37/115/115	-
26	BCR	G	201	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	843	1	-	9/37/115/115	-
31	CLA	9	315	17	1/1/12/20	9/24/102/115	-
31	CLA	B	845	2	-	1/19/97/115	-
39	3PH	7	301	-	-	15/34/34/49	-
31	CLA	3	318	14	-	7/21/99/115	-
31	CLA	6	308	44	1/1/11/20	5/16/94/115	-
31	CLA	3	317	44	1/1/12/20	8/21/99/115	-
27	LMT	A	808	-	-	6/21/61/61	0/2/2/2
31	CLA	A	819	1	1/1/15/20	8/37/115/115	-
31	CLA	B	835	2	1/1/13/20	8/28/106/115	-
31	CLA	4	318	21	1/1/11/20	5/13/91/115	-
31	CLA	K	206	11	-	5/15/93/115	-
31	CLA	3	316	44	1/1/12/20	4/19/97/115	-
25	SF4	C	102	3	-	-	0/6/5/5
24	PQN	B	801	-	-	4/23/43/43	0/2/2/2
31	CLA	9	313	17	1/1/11/20	6/13/91/115	-
31	CLA	B	816	2	-	5/33/111/115	-
36	LUT	3	305	-	-	13/29/67/67	0/2/2/2
26	BCR	L	301	-	-	9/29/63/63	0/2/2/2
31	CLA	5	318	22	1/1/15/20	11/37/115/115	-
31	CLA	7	313	15	1/1/11/20	4/11/89/115	-
26	BCR	B	803	-	-	9/29/63/63	0/2/2/2
31	CLA	B	849	2	1/1/12/20	4/19/97/115	-
31	CLA	2	313	20	1/1/11/20	8/15/93/115	-
31	CLA	8	313	28	1/1/11/20	6/15/93/115	-
26	BCR	3	302	-	-	8/29/63/63	0/2/2/2
26	BCR	A	803	-	-	5/29/63/63	0/2/2/2
31	CLA	F	306	44	1/1/12/20	2/19/97/115	-
31	CLA	A	850	1	1/1/12/20	8/21/99/115	-
31	CLA	8	311	16	1/1/13/20	10/25/103/115	-
31	CLA	O	202	19	1/1/9/20	1/4/78/115	-
31	CLA	A	856	44	1/1/15/20	6/37/115/115	-
32	CHL	7	320	44	3/3/19/26	12/33/131/137	-
31	CLA	B	833	44	1/1/13/20	7/25/103/115	-
32	CHL	9	322	44	3/3/16/26	4/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	831	2	-	6/19/97/115	-
31	CLA	3	320	14	1/1/11/20	2/13/91/115	-
32	CHL	a	318	44	2/2/16/26	6/18/116/137	-
31	CLA	8	307	16	1/1/11/20	3/15/93/115	-
26	BCR	7	304	-	-	7/29/63/63	0/2/2/2
33	DGD	B	808	-	-	22/50/90/95	0/2/2/2
31	CLA	8	310	16	1/1/15/20	10/37/115/115	-
31	CLA	3	310	14	1/1/14/20	8/31/109/115	-
32	CHL	4	310	-	2/2/16/26	6/17/115/137	-
26	BCR	L	303	-	-	7/29/63/63	0/2/2/2
31	CLA	6	312	23	1/1/15/20	10/37/115/115	-
31	CLA	8	315	16	1/1/12/20	5/22/100/115	-
31	CLA	2	312	20	1/1/11/20	4/15/93/115	-
31	CLA	8	318	16	1/1/12/20	2/19/97/115	-
31	CLA	B	811	2	1/1/15/20	6/37/115/115	-
31	CLA	B	836	2	-	6/37/115/115	-
31	CLA	B	843	44	1/1/11/20	5/13/91/115	-
31	CLA	6	311	23	1/1/13/20	10/25/103/115	-
31	CLA	2	308	20	1/1/11/20	3/15/93/115	-
31	CLA	3	307	14	1/1/15/20	10/37/115/115	-
31	CLA	a	311	44	1/1/14/20	9/31/109/115	-
32	CHL	8	316	44	3/3/20/26	12/39/137/137	-
32	CHL	6	309	23	3/3/20/26	18/39/137/137	-
31	CLA	4	309	21	1/1/14/20	10/31/109/115	-
31	CLA	B	829	2	-	5/25/103/115	-
31	CLA	A	829	-	-	5/19/97/115	-
32	CHL	7	318	44	3/3/20/26	23/39/137/137	-
26	BCR	B	804	-	-	5/29/63/63	0/2/2/2
31	CLA	A	857	44	1/1/15/20	14/37/115/115	-
36	LUT	6	303	-	-	18/29/67/67	0/2/2/2
26	BCR	F	302	-	-	7/29/63/63	0/2/2/2
36	LUT	9	302	-	-	17/29/67/67	0/2/2/2
31	CLA	A	815	-	-	5/37/115/115	-
26	BCR	G	203	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CHL	5	316	44	3/3/18/26	12/27/125/137	-
26	BCR	B	802	-	-	5/29/63/63	0/2/2/2
31	CLA	O	204	-	1/1/10/20	2/8/86/115	-
26	BCR	L	302	-	-	6/29/63/63	0/2/2/2
31	CLA	A	838	44	1/1/15/20	11/37/115/115	-
31	CLA	7	310	15	1/1/11/20	4/11/89/115	-
31	CLA	A	844	1	-	3/19/97/115	-
36	LUT	5	303	-	-	13/29/67/67	0/2/2/2
32	CHL	b	309	13	2/2/16/26	10/17/115/137	-
31	CLA	4	321	21	1/1/12/20	6/19/97/115	-
31	CLA	3	313	-	1/1/14/20	10/31/109/115	-
36	LUT	a	303	-	-	14/29/67/67	0/2/2/2
31	CLA	A	816	1	1/1/15/20	6/37/115/115	-
31	CLA	2	307	20	1/1/13/20	9/28/106/115	-
31	CLA	4	305	-	-	5/22/100/115	-
30	CL0	A	813	1	1/1/20/25	7/37/135/135	-
31	CLA	b	304	13	1/1/11/20	5/15/93/115	-
31	CLA	2	310	20	1/1/11/20	4/13/91/115	-
31	CLA	A	848	1	-	11/28/106/115	-
42	SQD	4	304	-	-	12/30/50/69	0/1/1/1
31	CLA	5	313	28	-	4/15/93/115	-
31	CLA	9	318	44	1/1/15/20	8/37/115/115	-
31	CLA	B	840	2	1/1/15/20	12/37/115/115	-
31	CLA	6	313	23	1/1/11/20	5/15/93/115	-
31	CLA	A	853	1	-	10/37/115/115	-
31	CLA	9	316	17	1/1/12/20	5/19/97/115	-
24	PQN	A	801	-	-	2/23/43/43	0/2/2/2
31	CLA	B	844	2	1/1/15/20	10/37/115/115	-
31	CLA	2	306	20	1/1/14/20	9/31/109/115	-
31	CLA	B	815	2	1/1/15/20	15/37/115/115	-
38	AXT	a	304	-	-	2/29/71/75	0/2/2/2
31	CLA	A	823	1	-	7/25/103/115	-
32	CHL	A	831	1	2/2/18/26	11/30/128/137	-
31	CLA	A	826	1	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	814	2	1/1/15/20	16/37/115/115	-
31	CLA	A	822	1	-	9/25/103/115	-
31	CLA	A	832	1	-	6/37/115/115	-
32	CHL	6	320	-	3/3/16/26	10/17/115/137	-
31	CLA	B	824	2	-	10/28/106/115	-
36	LUT	3	304	-	-	13/29/67/67	0/2/2/2
26	BCR	M	101	-	-	7/29/63/63	0/2/2/2
31	CLA	A	814	44	1/1/15/20	10/37/115/115	-
32	CHL	6	318	44	3/3/16/26	9/15/113/137	-
36	LUT	8	302	-	-	16/29/67/67	0/2/2/2
32	CHL	a	320	44	3/3/16/26	7/18/116/137	-
26	BCR	3	303	-	-	9/29/63/63	0/2/2/2
31	CLA	8	317	44	-	2/19/97/115	-
32	CHL	A	840	1	2/2/20/26	13/39/137/137	-
31	CLA	b	310	-	1/1/11/20	6/15/93/115	-
31	CLA	B	822	2	1/1/15/20	17/37/115/115	-
31	CLA	F	301	44	1/1/15/20	7/37/115/115	-
32	CHL	7	319	15	3/3/16/26	1/17/115/137	-
26	BCR	8	301	-	-	6/29/63/63	0/2/2/2
27	LMT	9	306	-	-	10/21/61/61	0/2/2/2
31	CLA	B	820	2	-	11/37/115/115	-
31	CLA	5	309	22	-	5/16/94/115	-
31	CLA	A	852	1	-	2/21/99/115	-
31	CLA	b	313	13	1/1/14/20	12/31/109/115	-
31	CLA	L	307	36	1/1/11/20	7/13/91/115	-
31	CLA	B	825	2	-	8/31/109/115	-
31	CLA	a	309	13	1/1/14/20	6/31/109/115	-
32	CHL	5	322	22	3/3/16/26	5/17/115/137	-
28	LHG	7	302	-	-	32/53/53/53	-
31	CLA	A	836	1	-	6/31/109/115	-
31	CLA	a	316	13	-	9/13/91/115	-
31	CLA	b	311	13	1/1/11/20	5/15/93/115	-
31	CLA	G	204	7	1/1/12/20	5/19/97/115	-
28	LHG	A	809	-	-	20/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	805	-	-	7/29/63/63	0/2/2/2
28	LHG	7	307	31	-	21/41/41/53	-
31	CLA	A	845	1	-	7/27/105/115	-
32	CHL	4	313	21	2/2/16/26	8/18/116/137	-
31	CLA	A	824	1,31	1/1/14/20	8/34/112/115	-
31	CLA	b	305	13	1/1/11/20	6/15/93/115	-
26	BCR	3	301	-	-	9/29/63/63	0/2/2/2
31	CLA	A	854	28	1/1/11/20	6/15/93/115	-
31	CLA	b	308	13	-	5/15/93/115	-
36	LUT	J	103	-	-	16/29/67/67	0/2/2/2
31	CLA	B	826	2	-	9/19/97/115	-
31	CLA	b	306	-	-	5/15/93/115	-
31	CLA	5	312	44	1/1/12/20	8/19/97/115	-
31	CLA	6	322	23	-	5/15/93/115	-
31	CLA	8	321	16	1/1/11/20	3/15/93/115	-
31	CLA	a	312	13	1/1/15/20	13/37/115/115	-
35	QTB	9	304	-	-	6/11/28/28	0/1/1/1
31	CLA	A	849	1	1/1/11/20	7/15/93/115	-
32	CHL	8	319	44	3/3/15/26	3/14/112/137	-
28	LHG	A	810	31	-	18/46/46/53	-
31	CLA	B	827	2	1/1/14/20	9/31/109/115	-
31	CLA	H	903	18	-	5/15/93/115	-
31	CLA	b	307	-	1/1/11/20	5/15/93/115	-
31	CLA	J	105	10	1/1/10/20	4/10/88/115	-
31	CLA	B	841	2	-	10/25/103/115	-
31	CLA	G	205	7	1/1/11/20	6/15/93/115	-
32	CHL	A	839	44	2/2/18/26	6/27/125/137	-
36	LUT	F	304	-	-	17/29/67/67	0/2/2/2
31	CLA	5	314	22	-	5/13/91/115	-
36	LUT	4	303	-	-	16/29/67/67	0/2/2/2
31	CLA	A	833	1	-	7/16/94/115	-
31	CLA	5	307	22	1/1/13/20	5/25/103/115	-
34	LAP	B	851	-	-	16/30/30/30	-
31	CLA	7	316	15	1/1/11/20	3/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	830	1	-	11/31/109/115	-
31	CLA	B	839	2	-	10/31/109/115	-
31	CLA	B	850	2	-	6/34/112/115	-
31	CLA	2	304	20	-	11/15/93/115	-
31	CLA	3	308	14	1/1/11/20	5/15/93/115	-
32	CHL	3	315	44	2/2/18/26	7/27/125/137	-
31	CLA	3	314	14	-	7/22/100/115	-
31	CLA	L	306	44	-	4/13/91/115	-
37	LMG	J	101	-	-	20/44/64/70	0/1/1/1
31	CLA	K	204	44	-	3/19/97/115	-
31	CLA	6	314	23	-	4/16/94/115	-
31	CLA	6	306	23	-	5/15/93/115	-
32	CHL	5	317	44	2/2/16/26	6/17/115/137	-
32	CHL	6	317	23	2/2/16/26	8/17/115/137	-
31	CLA	3	312	44	1/1/15/20	9/37/115/115	-
31	CLA	5	311	22	1/1/11/20	5/15/93/115	-
31	CLA	B	832	44	1/1/15/20	9/37/115/115	-
31	CLA	B	837	2	-	6/25/103/115	-
26	BCR	B	806	-	-	6/29/63/63	0/2/2/2
31	CLA	B	846	44	-	8/37/115/115	-
36	LUT	4	302	-	-	16/29/67/67	0/2/2/2
32	CHL	6	321	23	3/3/15/26	7/12/110/137	-
31	CLA	A	820	1	-	4/25/103/115	-
43	PTY	5	306	-	-	17/34/34/53	-
31	CLA	7	322	15	1/1/11/20	4/15/93/115	-
31	CLA	B	838	2	-	3/15/93/115	-
32	CHL	6	319	-	1/1/16/26	6/17/115/137	-
31	CLA	B	812	-	1/1/15/20	9/37/115/115	-
31	CLA	A	827	1	-	9/25/103/115	-
36	LUT	b	301	-	-	14/29/67/67	0/2/2/2
31	CLA	6	310	23	1/1/11/20	4/16/94/115	-
26	BCR	6	302	-	-	15/29/63/63	0/2/2/2
31	CLA	B	848	28	1/1/15/20	9/37/115/115	-
26	BCR	2	302	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	2	315	44	1/1/11/20	6/15/93/115	-
31	CLA	B	818	2	1/1/13/20	5/25/103/115	-
31	CLA	A	835	1	-	5/25/103/115	-
32	CHL	7	317	15	3/3/18/26	10/29/127/137	-
31	CLA	A	821	1	1/1/15/20	12/37/115/115	-
26	BCR	J	102	-	-	6/29/63/63	0/2/2/2
26	BCR	A	805	-	-	8/29/63/63	0/2/2/2
31	CLA	F	305	6	1/1/11/20	4/15/93/115	-
36	LUT	8	303	-	-	14/29/67/67	0/2/2/2
35	QTB	7	303	-	-	10/11/28/28	1/1/1/1
31	CLA	A	842	1	-	5/37/115/115	-
35	QTB	a	302	-	-	5/11/28/28	0/1/1/1
31	CLA	4	308	21	1/1/14/20	8/31/109/115	-
28	LHG	5	305	31	-	24/39/39/53	-
31	CLA	B	813	2	-	8/37/115/115	-
31	CLA	a	319	13	1/1/15/20	11/37/115/115	-
36	LUT	5	304	-	-	16/29/67/67	0/2/2/2
31	CLA	8	309	16	1/1/12/20	6/19/97/115	-
31	CLA	4	312	21	1/1/11/20	7/16/94/115	-
31	CLA	2	314	20	1/1/11/20	2/15/93/115	-
31	CLA	7	314	44	-	7/23/101/115	-
31	CLA	6	307	23	1/1/12/20	5/19/97/115	-
31	CLA	A	817	1,31	1/1/13/20	6/25/103/115	-
31	CLA	G	206	44	1/1/11/20	2/13/91/115	-
31	CLA	4	316	-	-	6/16/94/115	-
33	DGD	7	308	-	-	14/41/81/95	0/2/2/2
32	CHL	9	320	44	3/3/16/26	7/18/116/137	-
31	CLA	5	320	22	-	3/15/93/115	-
31	CLA	8	314	44	1/1/12/20	4/22/100/115	-
31	CLA	4	320	21	1/1/11/20	7/13/91/115	-
26	BCR	K	202	-	-	9/29/63/63	0/2/2/2
26	BCR	A	804	-	-	9/29/63/63	0/2/2/2
31	CLA	a	315	28	1/1/13/20	7/25/103/115	-
31	CLA	B	830	2	-	7/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	3	311	14	1/1/15/20	11/37/115/115	-
31	CLA	b	312	13	-	3/15/93/115	-
31	CLA	7	321	44	-	7/16/94/115	-
37	LMG	a	301	-	-	21/37/57/70	0/1/1/1
31	CLA	B	817	2	1/1/15/20	11/37/115/115	-
31	CLA	b	303	-	1/1/11/20	5/15/93/115	-
31	CLA	B	823	2	1/1/13/20	9/25/103/115	-
31	CLA	A	855	1	-	13/37/115/115	-
31	CLA	2	305	20	1/1/11/20	5/13/91/115	-
36	LUT	9	303	-	-	16/29/67/67	0/2/2/2
31	CLA	B	821	2	-	4/29/107/115	-
26	BCR	5	302	-	-	13/29/63/63	0/2/2/2
31	CLA	9	317	-	-	6/16/94/115	-
31	CLA	B	819	2	1/1/15/20	6/37/115/115	-
31	CLA	A	834	44	1/1/15/20	10/37/115/115	-
32	CHL	K	201	11	3/3/16/26	7/17/115/137	-
37	LMG	J	104	-	-	11/24/44/70	0/1/1/1
31	CLA	A	818	1	1/1/15/20	10/37/115/115	-
28	LHG	6	301	31	-	16/31/31/53	-
31	CLA	4	307	21	1/1/13/20	8/27/105/115	-
31	CLA	b	302	13	1/1/11/20	6/15/93/115	-
28	LHG	A	811	-	-	19/53/53/53	-
32	CHL	7	324	16	2/2/20/26	14/39/137/137	-
25	SF4	C	101	3	-	-	0/6/5/5
36	LUT	9	305	-	-	18/29/67/67	0/2/2/2
31	CLA	7	309	15	1/1/14/20	4/31/109/115	-
31	CLA	3	309	14	1/1/15/20	14/37/115/115	-
31	CLA	B	834	2	1/1/15/20	5/37/115/115	-
31	CLA	5	308	22	1/1/11/20	2/15/93/115	-
31	CLA	H	902	44	1/1/11/20	3/15/93/115	-
40	XAT	7	306	-	-	4/31/93/93	0/4/4/4
31	CLA	9	314	17	1/1/14/20	10/31/109/115	-
28	LHG	B	807	31	-	7/36/36/53	-
32	CHL	4	317	-	3/3/16/26	10/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	847	2	-	9/37/115/115	-
31	CLA	a	322	13	1/1/11/20	6/15/93/115	-
31	CLA	2	311	20	1/1/11/20	6/13/91/115	-
31	CLA	A	841	1	1/1/15/20	13/37/115/115	-
31	CLA	A	851	1	1/1/15/20	9/37/115/115	-
31	CLA	5	323	22	1/1/13/20	9/27/105/115	-
36	LUT	2	301	-	-	13/29/67/67	0/2/2/2
26	BCR	A	806	-	-	7/29/63/63	0/2/2/2
31	CLA	9	321	17	1/1/13/20	12/27/105/115	-
28	LHG	6	305	31	-	8/36/36/53	-
31	CLA	6	315	28	1/1/11/20	3/15/93/115	-
26	BCR	I	801	-	-	6/29/63/63	0/2/2/2
31	CLA	A	825	1	-	2/24/102/115	-
31	CLA	8	308	16	1/1/15/20	13/37/115/115	-
31	CLA	7	312	15	1/1/14/20	11/34/112/115	-

The worst 5 of 5056 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	310	CLA	MG-NA	30.68	2.79	2.06
31	b	307	CLA	MG-NA	29.70	2.76	2.06
31	6	315	CLA	MG-NA	29.56	2.76	2.06
31	5	318	CLA	MG-ND	-28.84	1.48	2.05
31	9	319	CLA	MG-NA	28.29	2.73	2.06

The worst 5 of 6253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	315	CLA	C4-C3-C5	-19.91	81.78	115.27
31	5	315	CLA	C5-C3-C2	19.18	159.93	121.12
31	5	315	CLA	C4-C3-C2	-17.67	78.34	123.68
36	7	305	LUT	C15-C14-C13	-17.12	102.87	127.31
36	2	301	LUT	C15-C14-C13	-16.15	104.26	127.31

5 of 223 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	A	813	CL0	NC

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Mol	Chain	Res	Type	Atom
31	A	814	CLA	ND
31	A	816	CLA	ND
31	A	817	CLA	ND
31	A	818	CLA	ND

5 of 2779 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	804	BCR	C7-C8-C9-C10
26	A	804	BCR	C7-C8-C9-C34
26	A	804	BCR	C20-C21-C22-C23
26	A	805	BCR	C7-C8-C9-C34
26	A	805	BCR	C20-C21-C22-C37

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	F	303	QTB	C11-C12-C14-C15-C16-C17
35	7	303	QTB	C11-C12-C14-C15-C16-C17

256 monomers are involved in 557 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	5	310	CLA	5	0
31	9	311	CLA	1	0
37	G	202	LMG	4	0
31	A	837	CLA	4	0
31	7	311	CLA	3	0
26	O	201	BCR	2	0
31	L	305	CLA	7	0
27	5	301	LMT	2	0
31	A	828	CLA	2	0
41	8	305	DGA	2	0
31	4	319	CLA	1	0
32	5	319	CHL	4	0
31	8	320	CLA	1	0
31	5	315	CLA	2	0
31	4	314	CLA	5	0
31	4	311	CLA	1	0
31	7	315	CLA	6	0
36	7	305	LUT	3	0
36	L	304	LUT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	6	316	CLA	1	0
31	3	319	CLA	3	0
36	6	304	LUT	3	0
26	K	203	BCR	4	0
31	B	828	CLA	1	0
31	5	321	CLA	1	0
27	A	807	LMT	4	0
31	A	846	CLA	3	0
31	4	315	CLA	2	0
31	H	901	CLA	3	0
31	A	847	CLA	1	0
31	B	842	CLA	4	0
26	G	201	BCR	2	0
31	A	843	CLA	2	0
31	9	315	CLA	2	0
31	B	845	CLA	4	0
39	7	301	3PH	1	0
31	6	308	CLA	1	0
31	A	819	CLA	3	0
31	B	835	CLA	2	0
31	4	318	CLA	5	0
31	K	206	CLA	1	0
24	B	801	PQN	2	0
31	9	313	CLA	1	0
31	B	816	CLA	1	0
36	3	305	LUT	7	0
26	L	301	BCR	1	0
31	5	318	CLA	5	0
31	7	313	CLA	2	0
26	B	803	BCR	1	0
31	B	849	CLA	1	0
31	2	313	CLA	2	0
31	8	313	CLA	1	0
26	3	302	BCR	5	0
26	A	803	BCR	3	0
31	F	306	CLA	1	0
31	A	850	CLA	3	0
31	8	311	CLA	5	0
31	A	856	CLA	4	0
32	7	320	CHL	7	0
31	B	833	CLA	2	0
32	9	322	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	831	CLA	2	0
31	3	320	CLA	1	0
31	8	307	CLA	1	0
26	7	304	BCR	6	0
33	B	808	DGD	4	0
31	8	310	CLA	3	0
31	3	310	CLA	1	0
26	L	303	BCR	3	0
32	4	310	CHL	7	0
31	6	312	CLA	1	0
31	8	315	CLA	1	0
31	2	312	CLA	1	0
31	8	318	CLA	1	0
31	B	811	CLA	1	0
31	B	836	CLA	1	0
31	B	843	CLA	2	0
31	6	311	CLA	1	0
31	2	308	CLA	1	0
32	8	316	CHL	9	0
32	6	309	CHL	8	0
31	B	829	CLA	2	0
31	A	829	CLA	12	0
32	7	318	CHL	9	0
26	B	804	BCR	4	0
31	A	857	CLA	3	0
36	6	303	LUT	2	0
26	F	302	BCR	2	0
36	9	302	LUT	2	0
31	A	815	CLA	3	0
32	5	316	CHL	6	0
26	B	802	BCR	4	0
26	L	302	BCR	2	0
31	A	838	CLA	4	0
36	5	303	LUT	3	0
31	4	321	CLA	1	0
31	3	313	CLA	2	0
31	A	816	CLA	2	0
31	2	307	CLA	2	0
31	4	305	CLA	6	0
30	A	813	CL0	3	0
31	A	848	CLA	1	0
42	4	304	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	5	313	CLA	1	0
31	9	318	CLA	1	0
31	B	840	CLA	2	0
31	6	313	CLA	2	0
31	A	853	CLA	3	0
24	A	801	PQN	1	0
31	B	844	CLA	3	0
31	2	306	CLA	3	0
31	B	815	CLA	1	0
31	A	823	CLA	3	0
32	A	831	CHL	3	0
31	A	826	CLA	3	0
31	B	814	CLA	4	0
31	A	822	CLA	4	0
31	A	832	CLA	2	0
32	6	320	CHL	1	0
36	3	304	LUT	3	0
26	M	101	BCR	3	0
31	A	814	CLA	6	0
32	6	318	CHL	5	0
36	8	302	LUT	5	0
26	3	303	BCR	2	0
31	8	317	CLA	2	0
32	A	840	CHL	5	0
31	B	822	CLA	4	0
31	F	301	CLA	4	0
32	7	319	CHL	4	0
26	8	301	BCR	2	0
31	B	820	CLA	4	0
31	5	309	CLA	3	0
31	A	852	CLA	2	0
31	B	825	CLA	4	0
32	5	322	CHL	3	0
28	7	302	LHG	6	0
31	A	836	CLA	3	0
31	G	204	CLA	1	0
28	A	809	LHG	3	0
26	B	805	BCR	5	0
28	7	307	LHG	4	0
31	A	845	CLA	4	0
32	4	313	CHL	4	0
31	A	824	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	3	301	BCR	2	0
31	A	854	CLA	1	0
36	J	103	LUT	3	0
31	B	826	CLA	1	0
31	5	312	CLA	1	0
31	6	322	CLA	3	0
31	8	321	CLA	3	0
31	A	849	CLA	2	0
32	8	319	CHL	1	0
28	A	810	LHG	2	0
31	H	903	CLA	3	0
31	J	105	CLA	1	0
31	B	841	CLA	4	0
31	G	205	CLA	1	0
32	A	839	CHL	4	0
36	F	304	LUT	2	0
31	5	314	CLA	1	0
36	4	303	LUT	4	0
31	A	833	CLA	3	0
31	5	307	CLA	2	0
34	B	851	LAP	4	0
31	A	830	CLA	3	0
31	B	839	CLA	2	0
31	B	850	CLA	3	0
31	2	304	CLA	6	0
31	3	308	CLA	2	0
32	3	315	CHL	2	0
31	3	314	CLA	2	0
37	J	101	LMG	4	0
31	6	314	CLA	2	0
31	6	306	CLA	5	0
32	5	317	CHL	4	0
32	6	317	CHL	3	0
31	5	311	CLA	1	0
31	B	832	CLA	3	0
31	B	837	CLA	5	0
26	B	806	BCR	2	0
31	B	846	CLA	3	0
36	4	302	LUT	8	0
32	6	321	CHL	2	0
31	A	820	CLA	2	0
43	5	306	PTY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	7	322	CLA	1	0
31	B	838	CLA	1	0
32	6	319	CHL	2	0
31	B	812	CLA	2	0
31	A	827	CLA	3	0
26	6	302	BCR	2	0
31	B	848	CLA	4	0
26	2	302	BCR	3	0
31	2	315	CLA	1	0
31	B	818	CLA	2	0
31	A	835	CLA	3	0
32	7	317	CHL	8	0
31	A	821	CLA	2	0
26	J	102	BCR	1	0
26	A	805	BCR	3	0
36	8	303	LUT	2	0
31	A	842	CLA	1	0
31	4	308	CLA	1	0
28	5	305	LHG	2	0
31	B	813	CLA	6	0
36	5	304	LUT	6	0
31	8	309	CLA	1	0
31	4	312	CLA	1	0
31	2	314	CLA	3	0
31	6	307	CLA	2	0
31	G	206	CLA	4	0
31	4	316	CLA	4	0
33	7	308	DGD	1	0
32	9	320	CHL	3	0
31	5	320	CLA	1	0
31	8	314	CLA	1	0
26	K	202	BCR	4	0
26	A	804	BCR	2	0
31	B	830	CLA	1	0
31	3	311	CLA	2	0
31	7	321	CLA	2	0
31	B	817	CLA	1	0
31	B	823	CLA	1	0
31	A	855	CLA	3	0
36	9	303	LUT	6	0
26	5	302	BCR	2	0
31	B	819	CLA	2	0

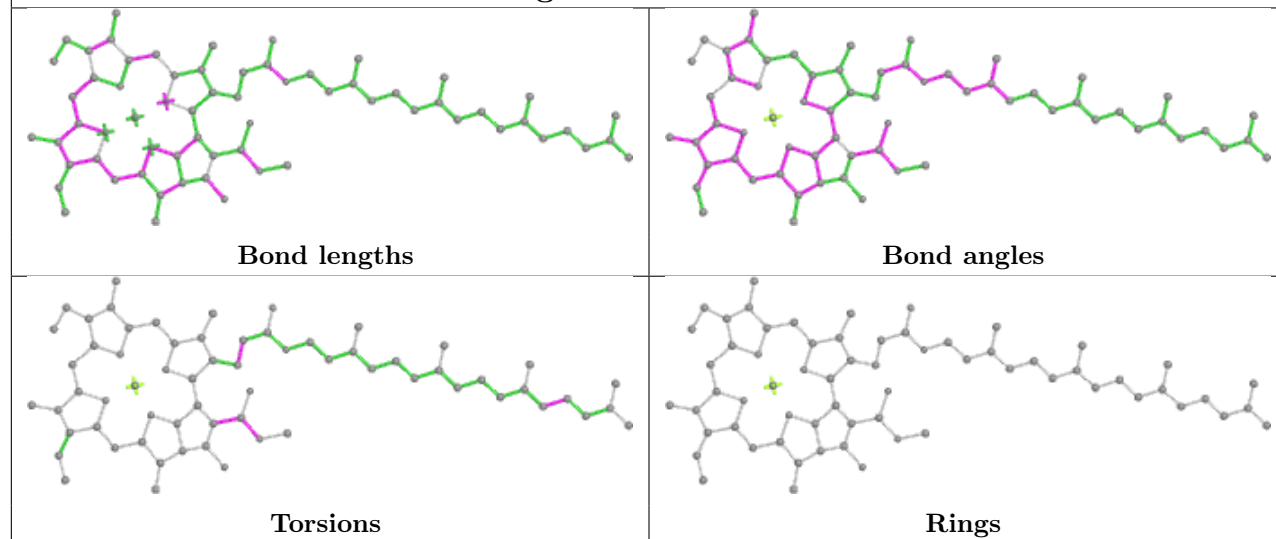
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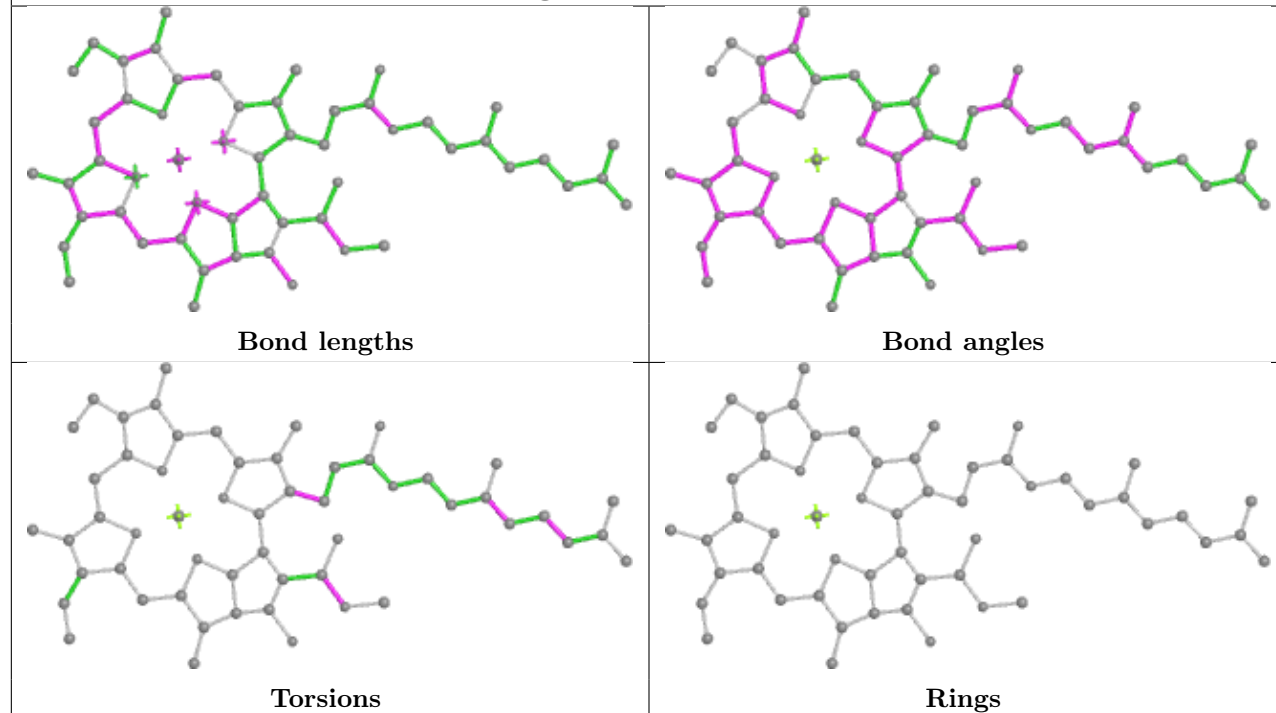
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	834	CLA	7	0
32	K	201	CHL	2	0
28	6	301	LHG	3	0
31	A	818	CLA	4	0
31	4	307	CLA	1	0
28	A	811	LHG	3	0
32	7	324	CHL	5	0
36	9	305	LUT	1	0
31	7	309	CLA	2	0
31	3	309	CLA	7	0
31	B	834	CLA	3	0
31	5	308	CLA	1	0
31	H	902	CLA	6	0
31	9	314	CLA	2	0
32	4	317	CHL	10	0
31	B	847	CLA	2	0
31	2	311	CLA	1	0
31	A	841	CLA	8	0
31	A	851	CLA	5	0
31	5	323	CLA	3	0
36	2	301	LUT	4	0
26	A	806	BCR	4	0
28	6	305	LHG	1	0
31	6	315	CLA	1	0
26	I	801	BCR	1	0
31	A	825	CLA	3	0
31	8	308	CLA	6	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

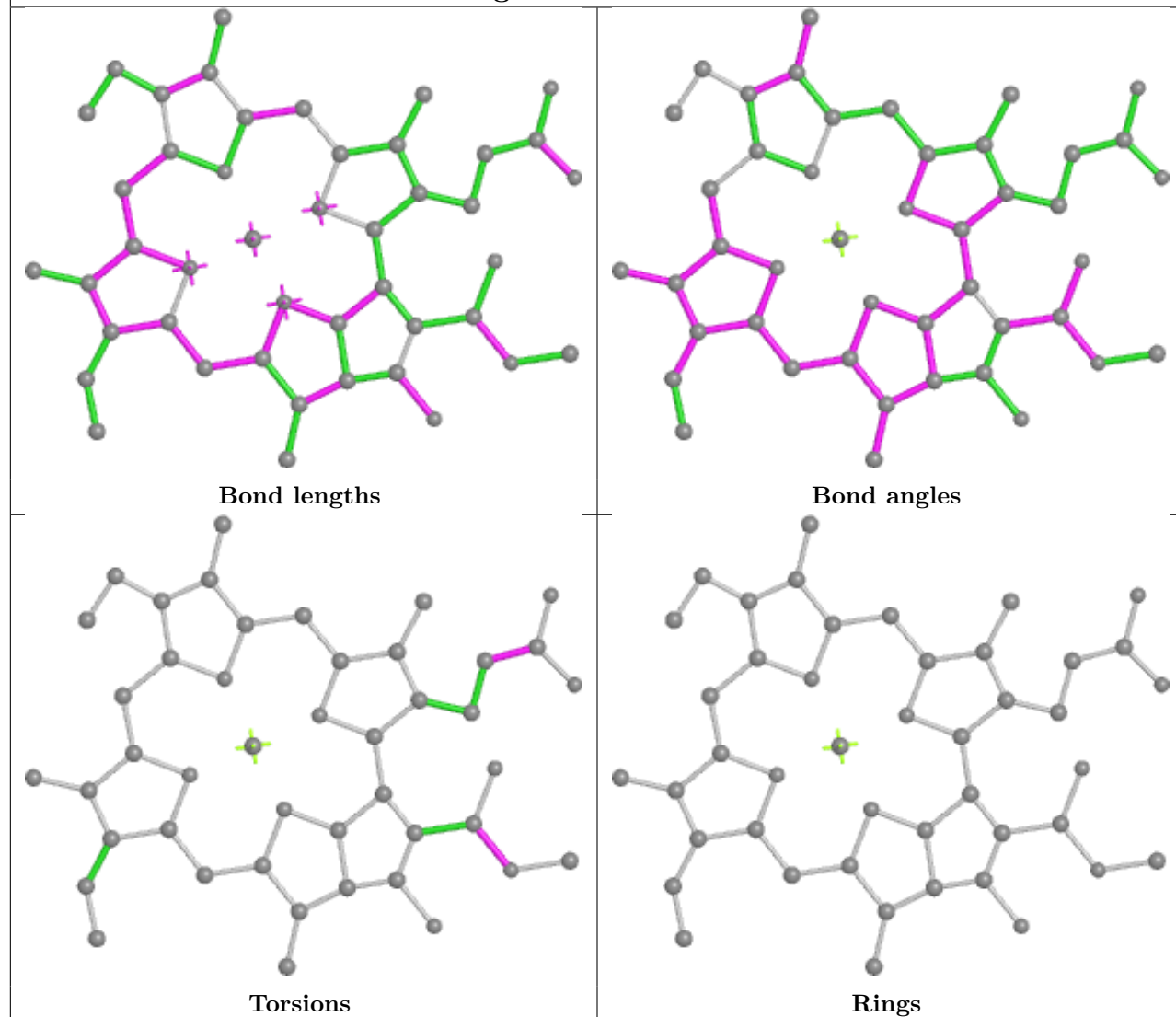
Ligand CLA 5 310



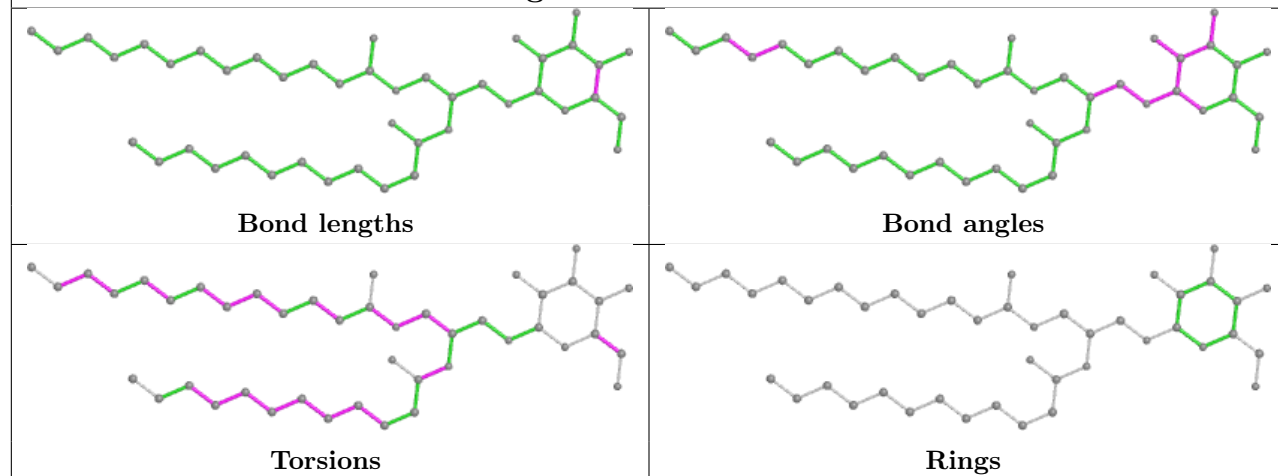
Ligand CLA 9 311

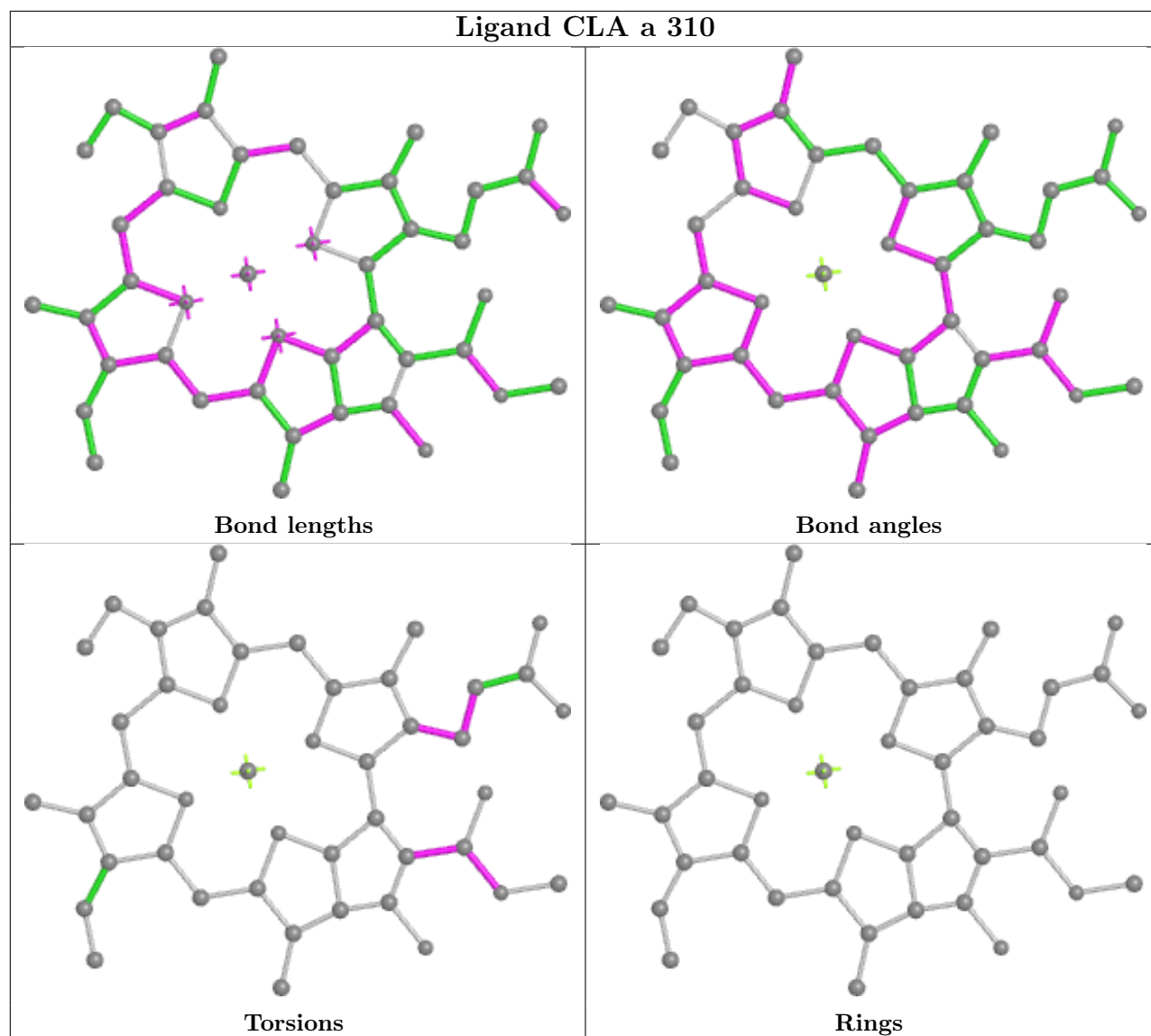
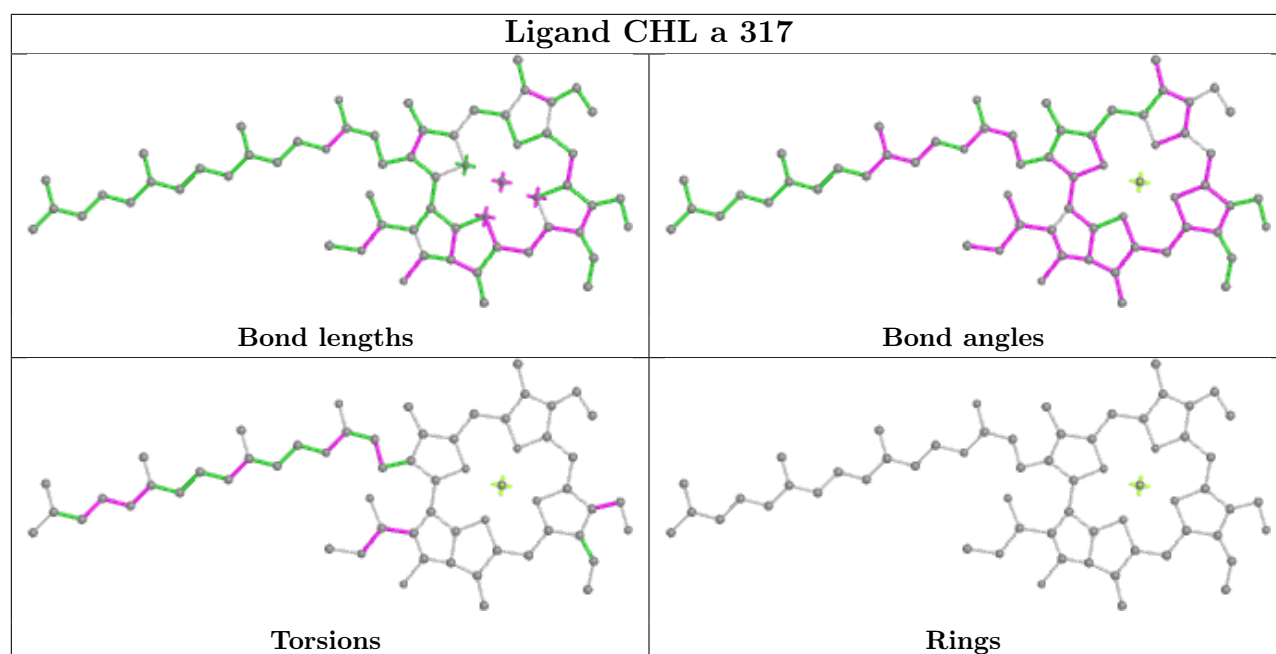


Ligand CLA 4 306

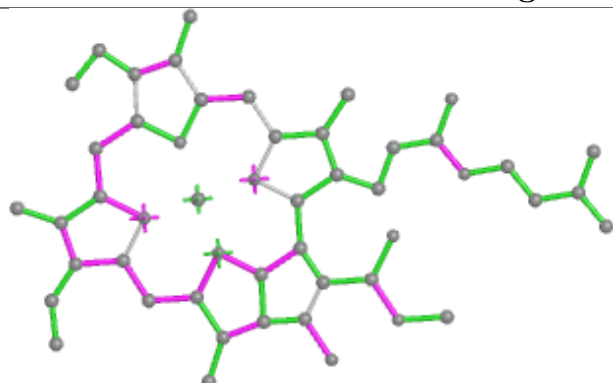


Ligand LMG G 202

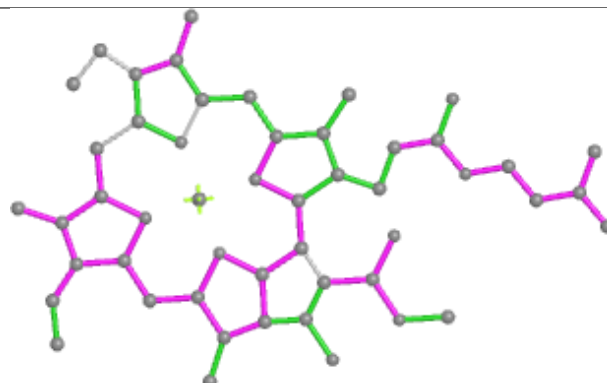




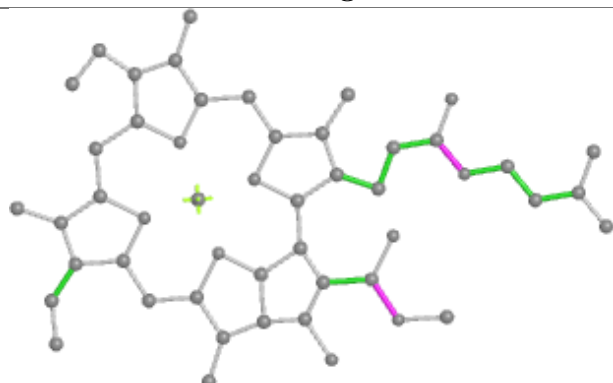
Ligand CLA 8 312



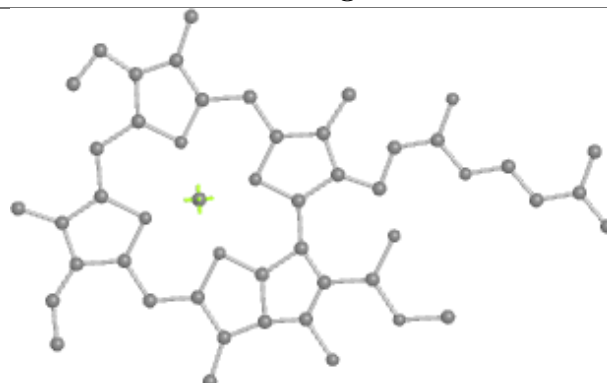
Bond lengths



Bond angles

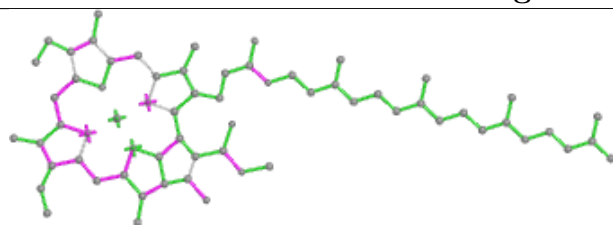


Torsions

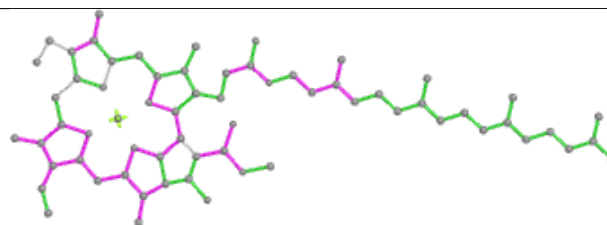


Rings

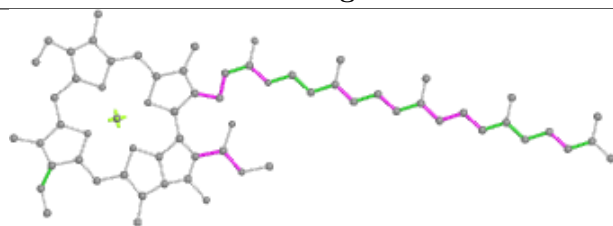
Ligand CLA A 837



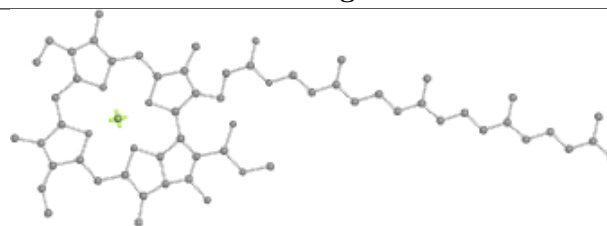
Bond lengths



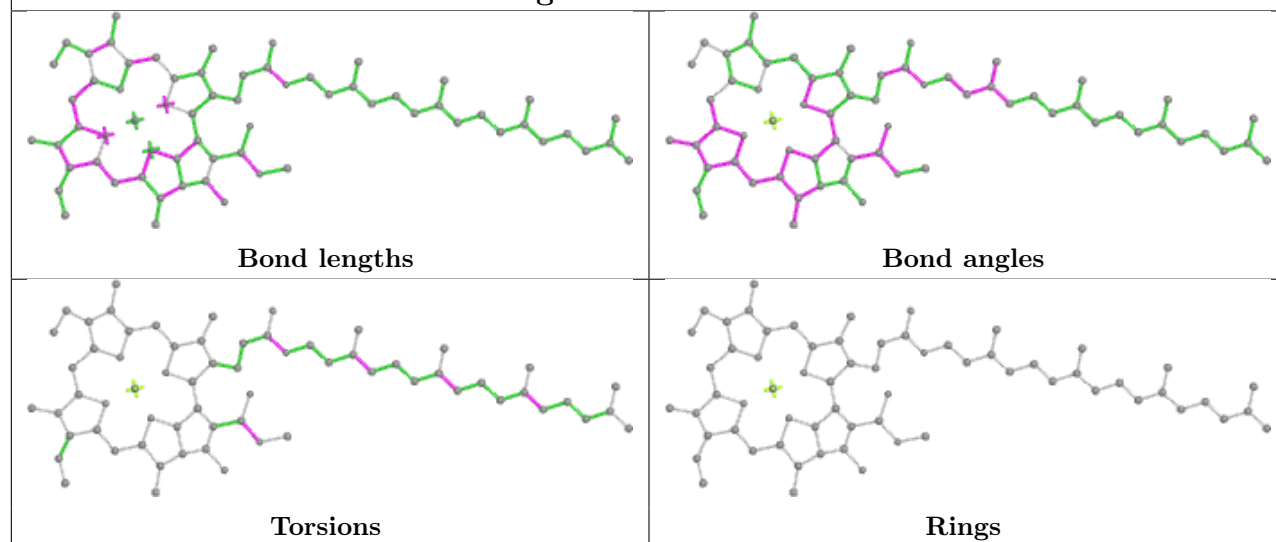
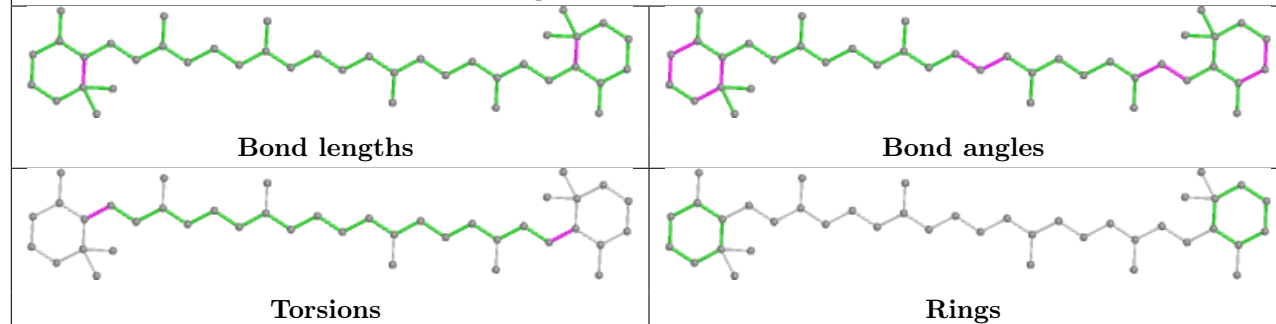
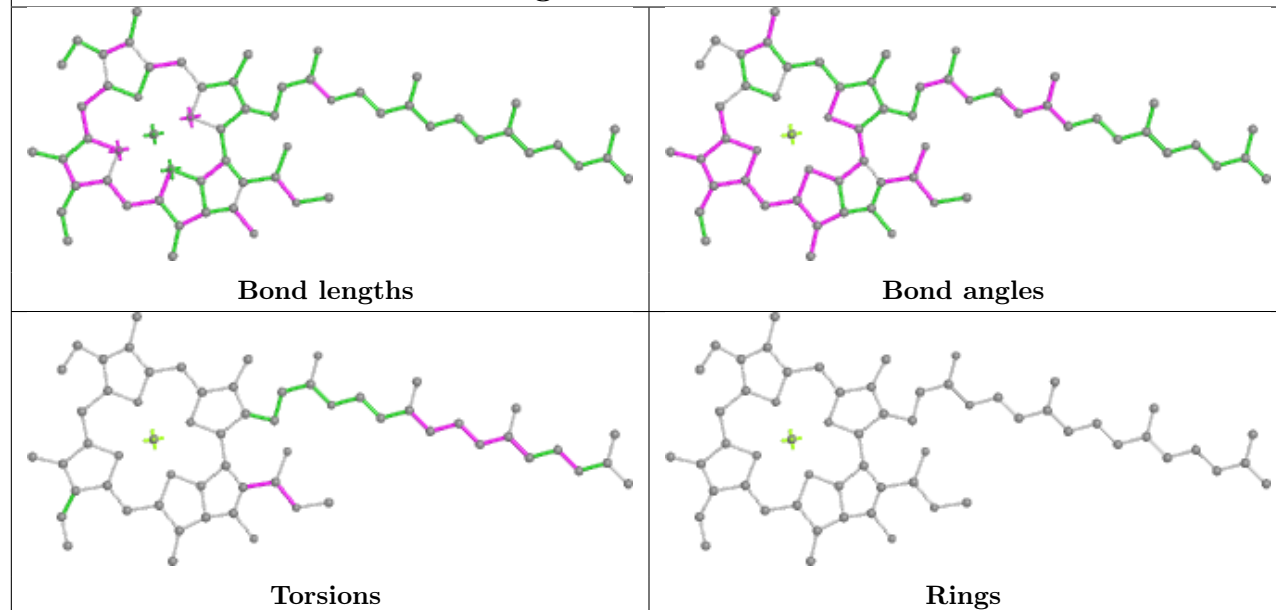
Bond angles

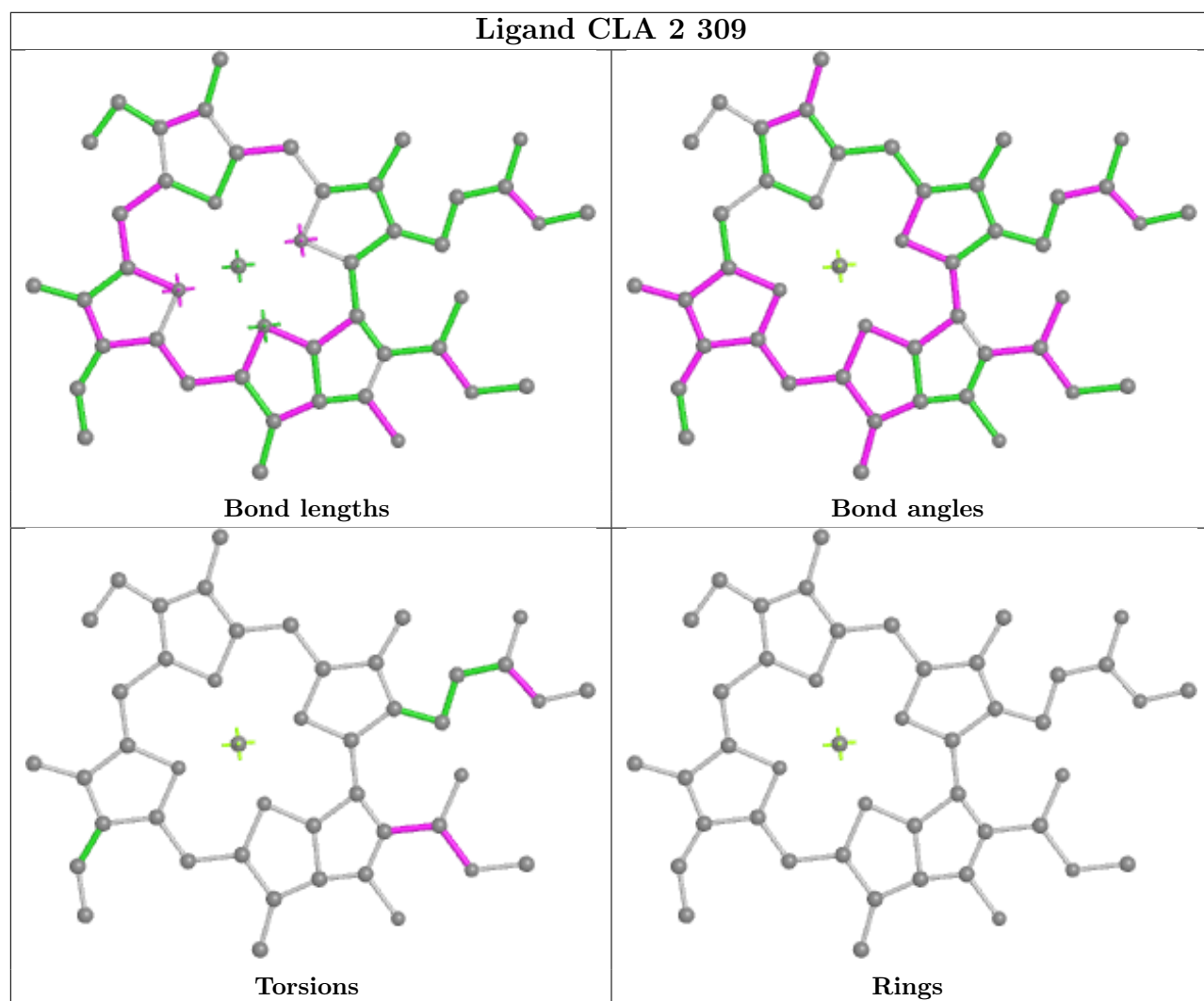
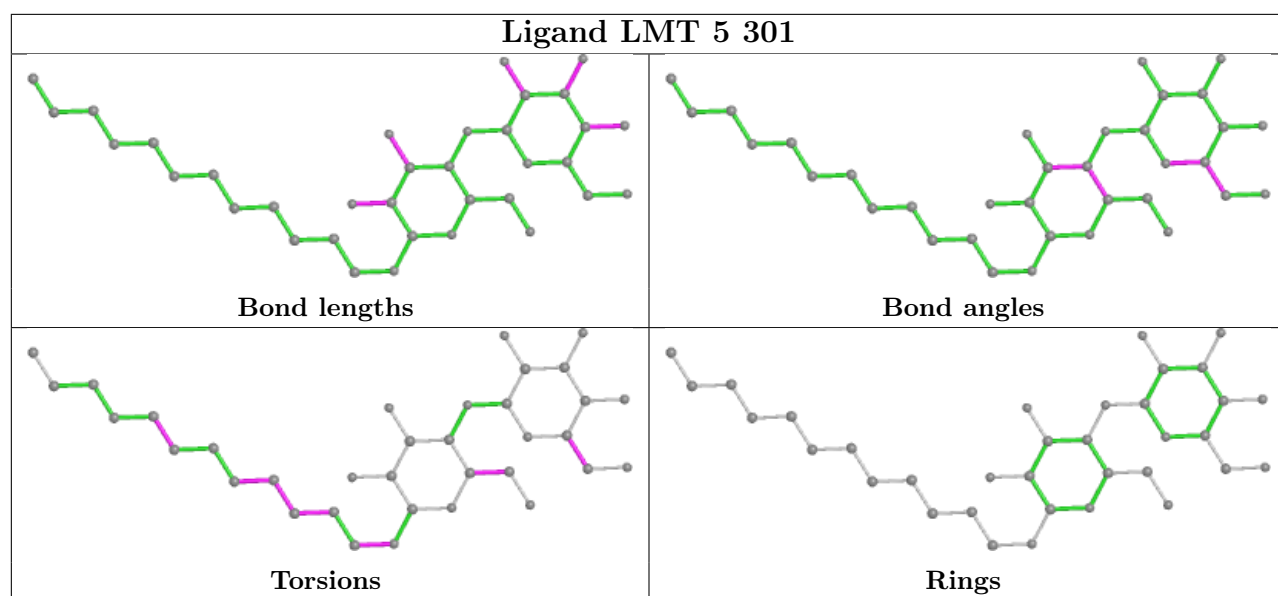


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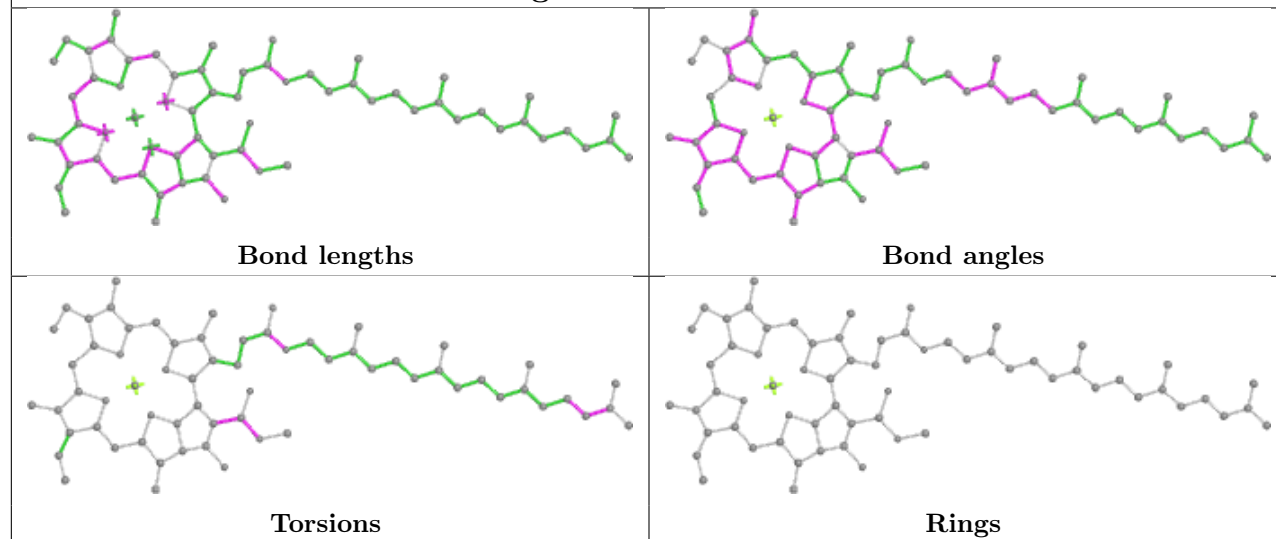


Rings

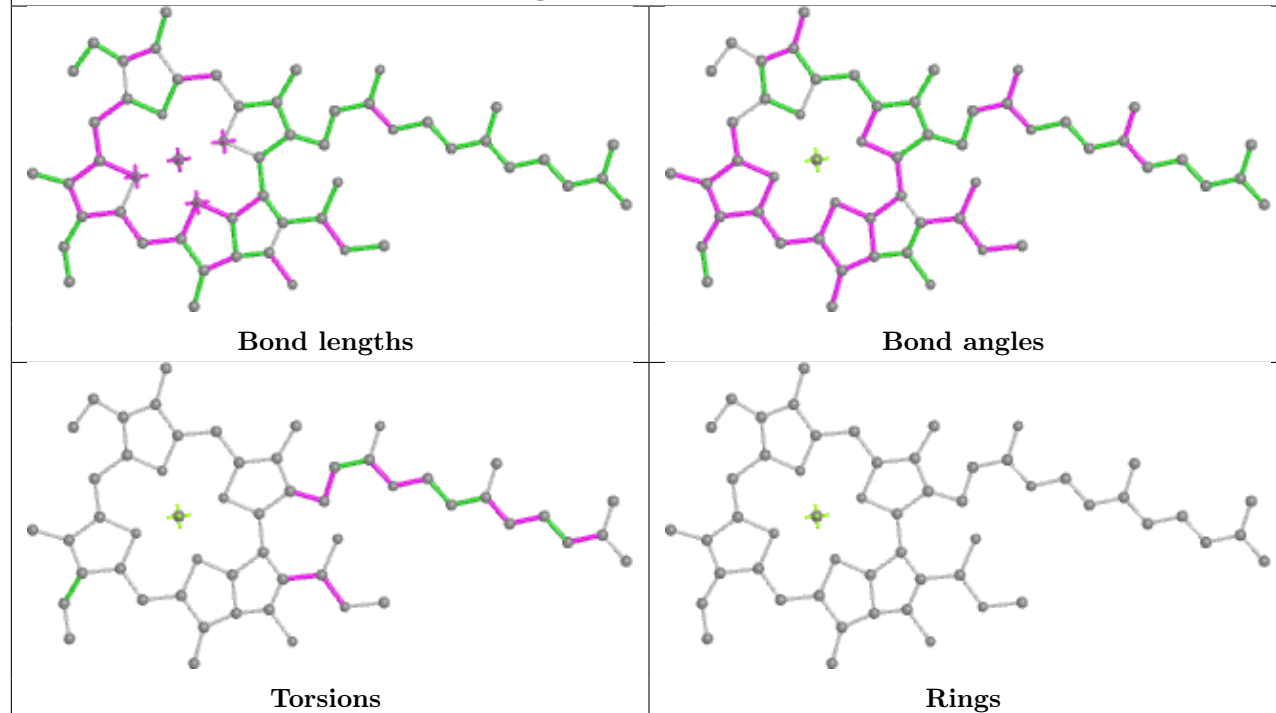
Ligand CLA 7 311**Ligand BCR O 201****Ligand CLA L 305**



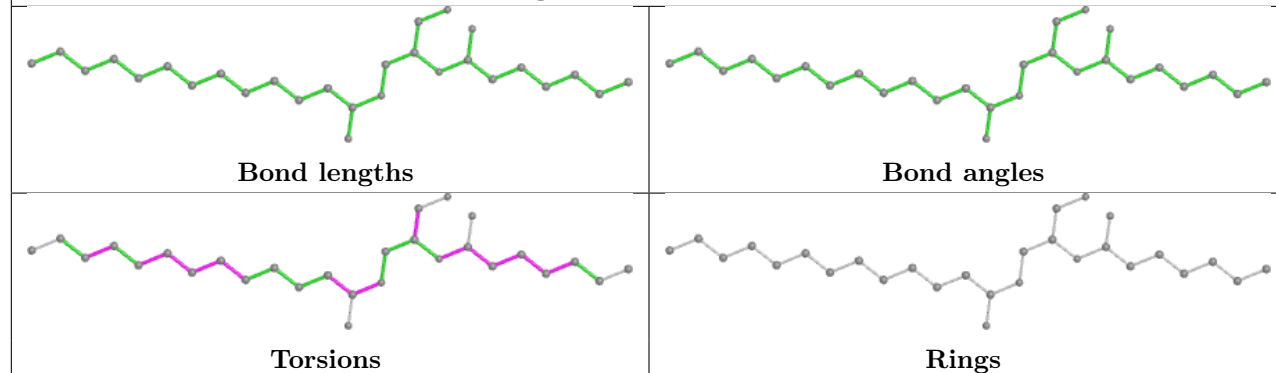
Ligand CLA A 828

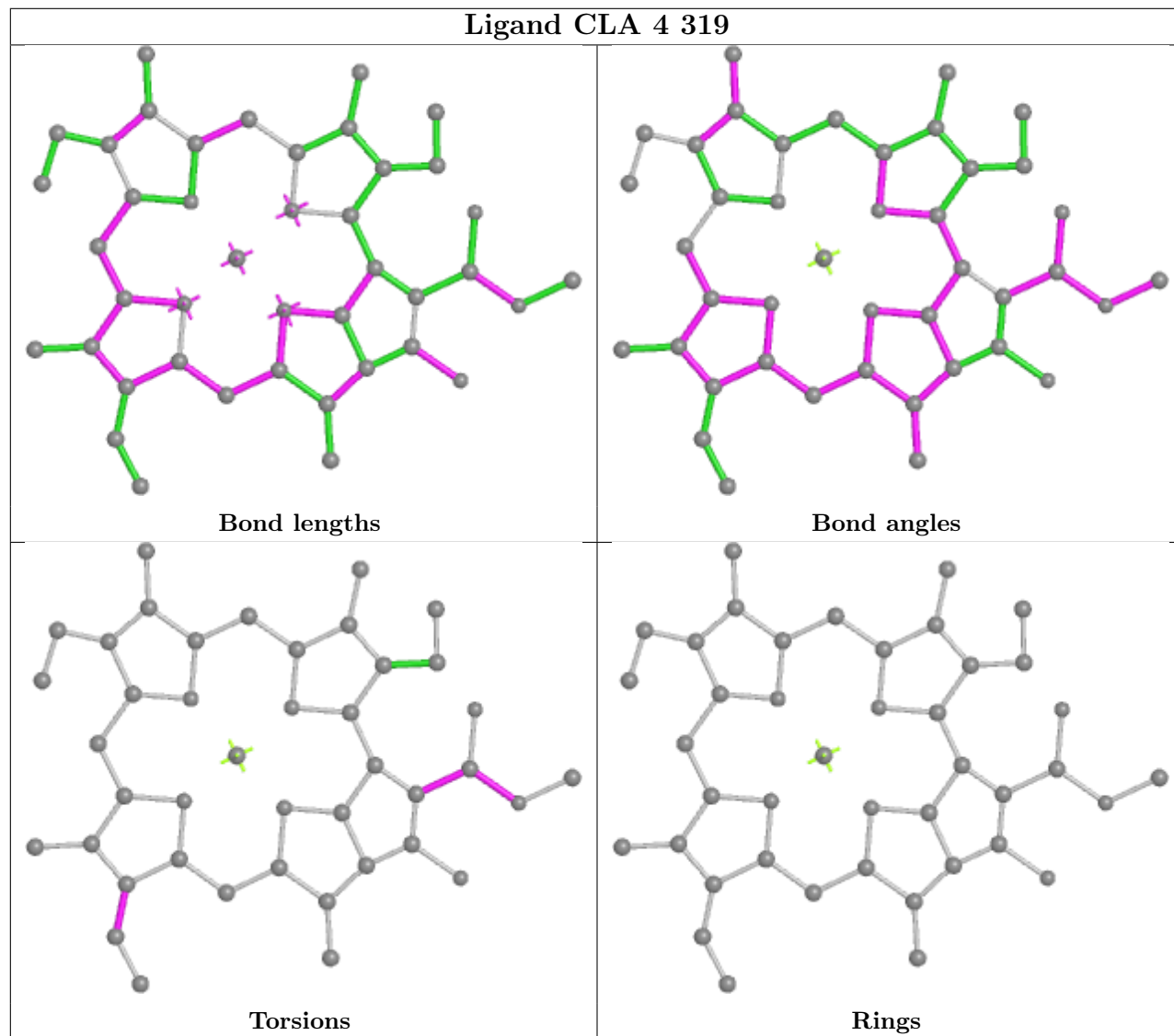
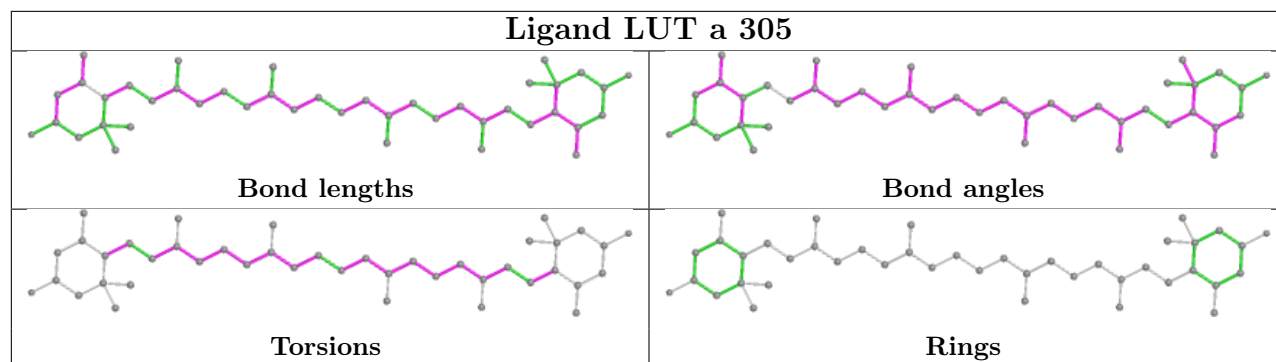


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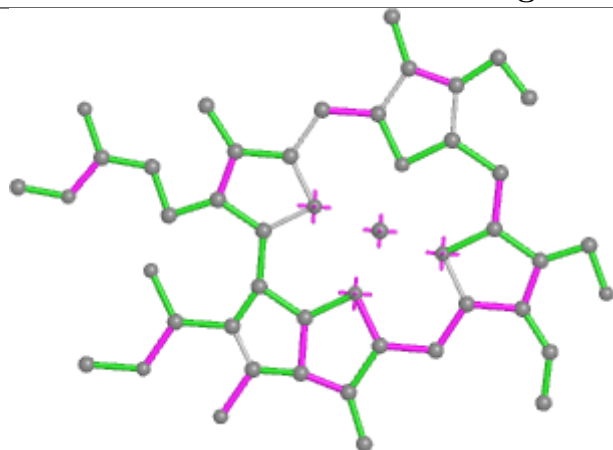


Ligand DGA 8 305

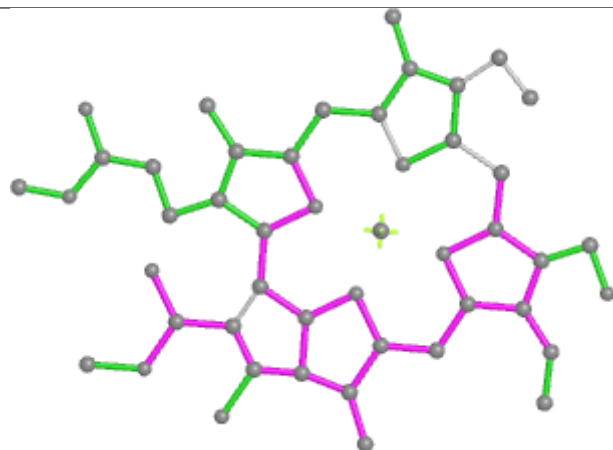




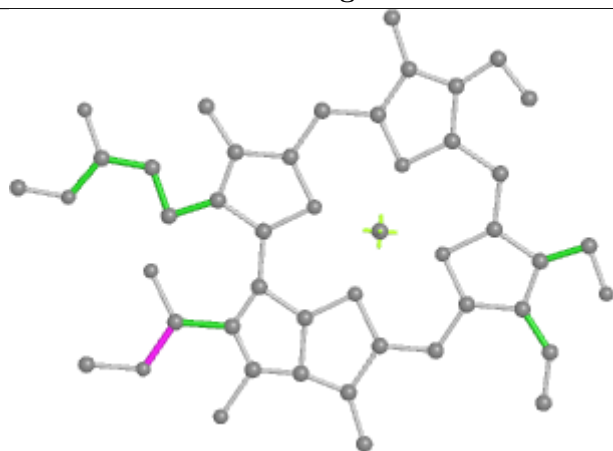
Ligand CHL 5 319



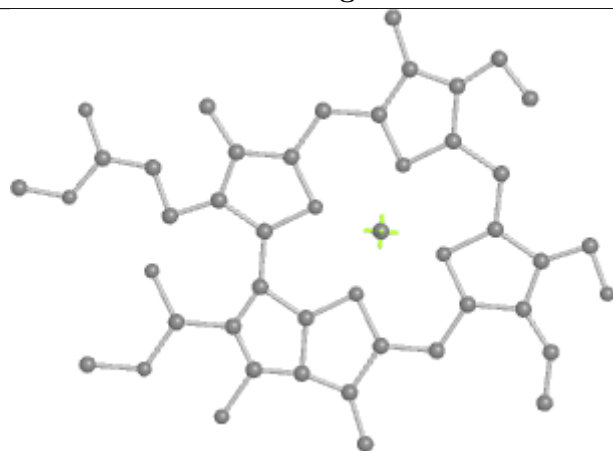
Bond lengths



Bond angles

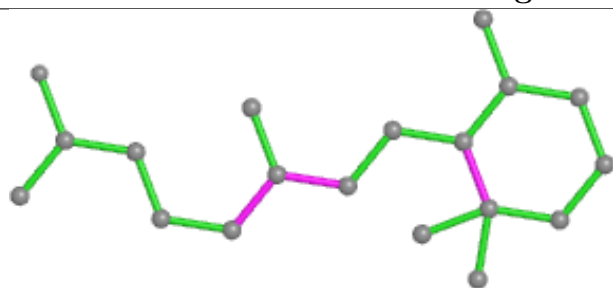


Torsions

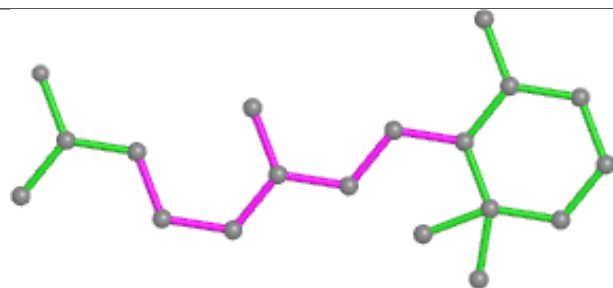


Rings

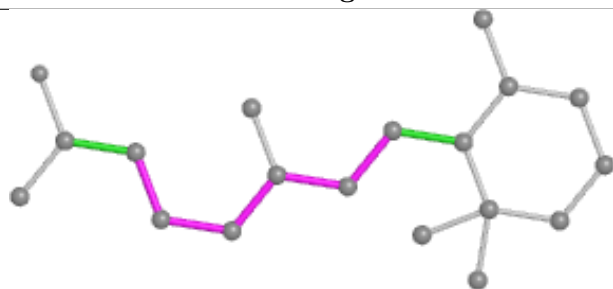
Ligand QTB F 303



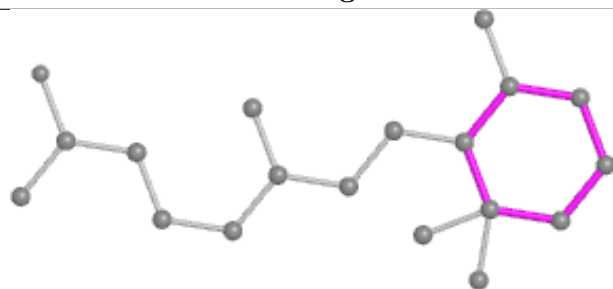
Bond lengths



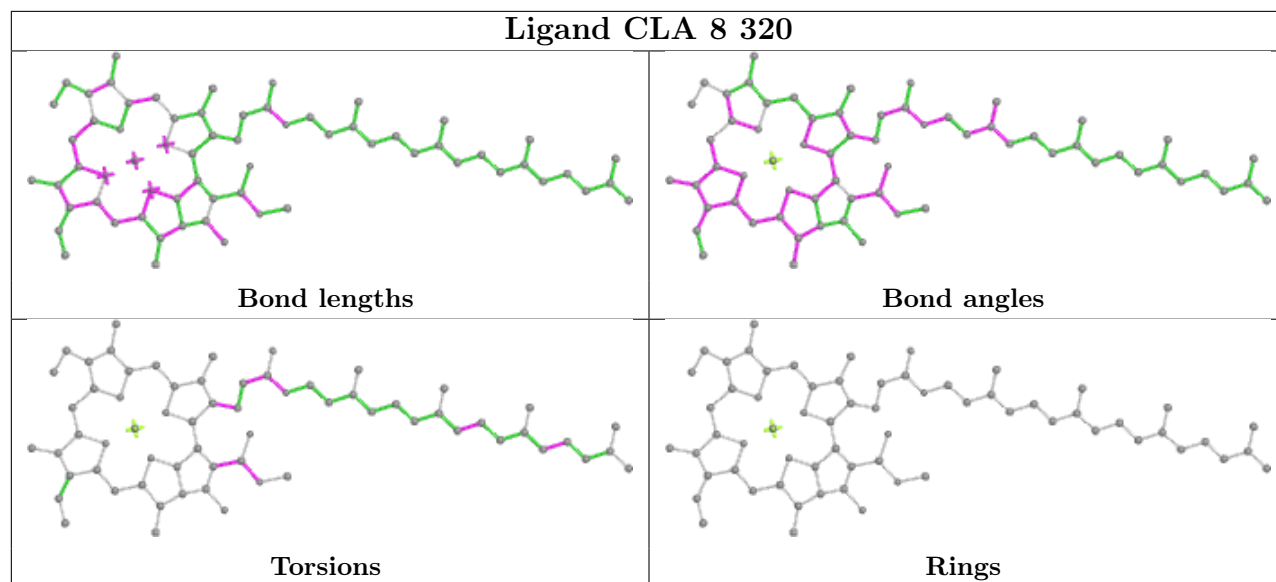
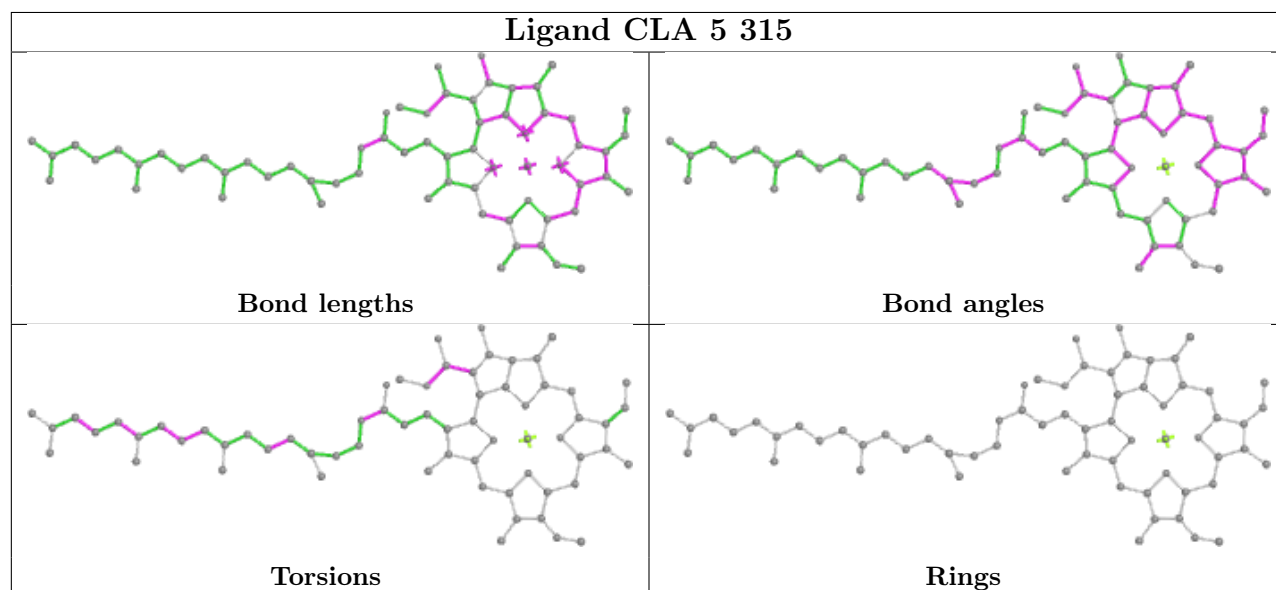
Bond angles



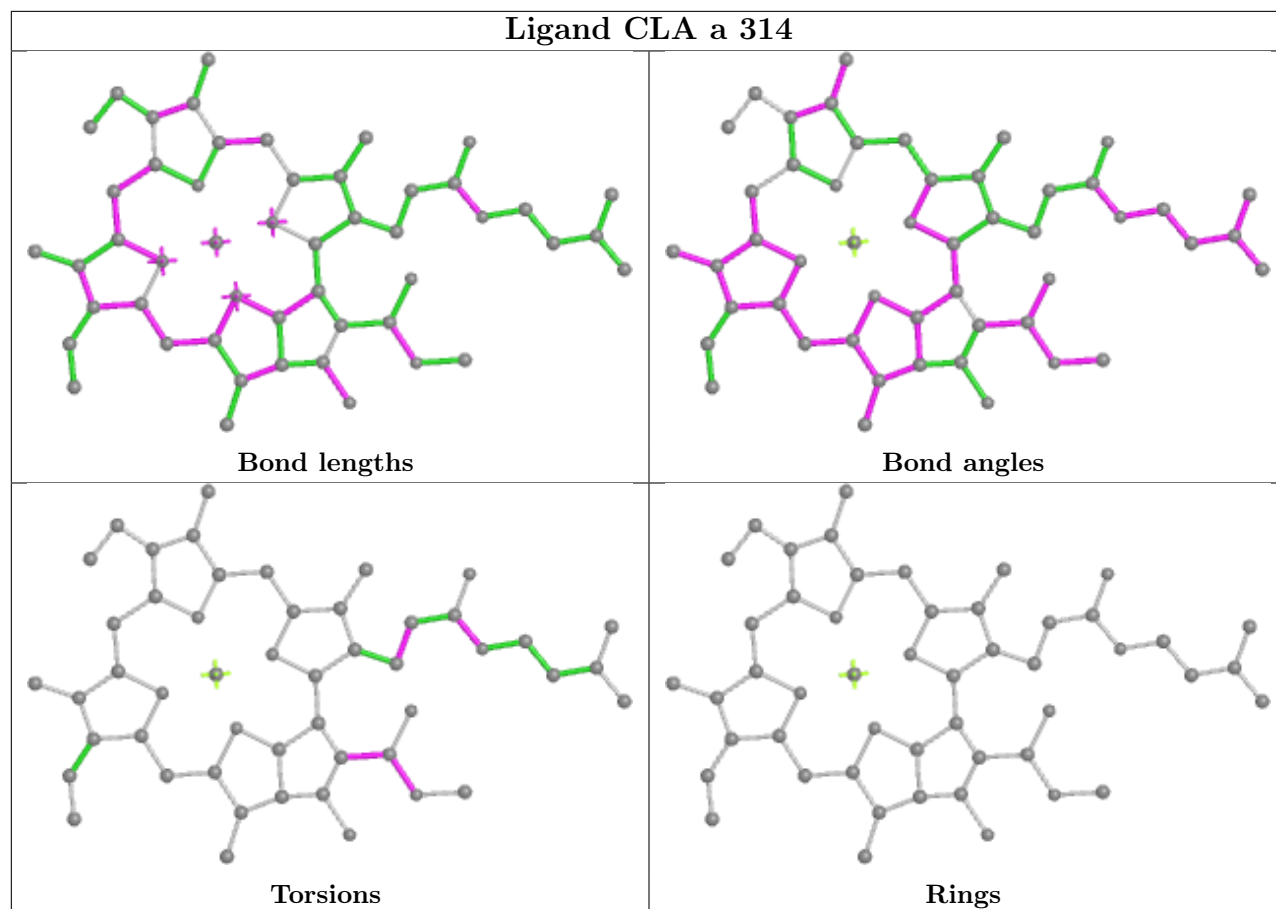
Torsions



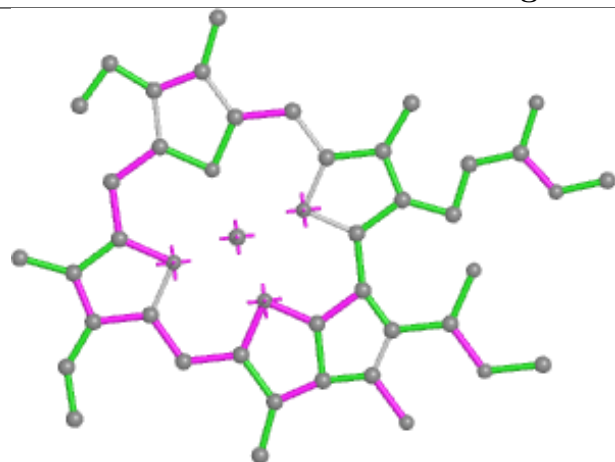
Rings

Ligand CLA 8 320**Ligand CLA 5 315**

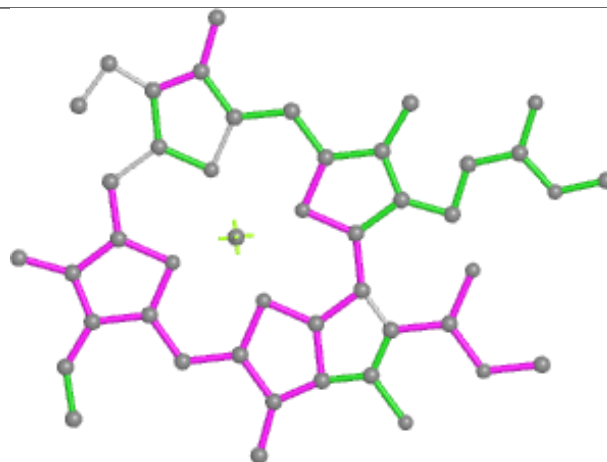
Ligand CLA a 314



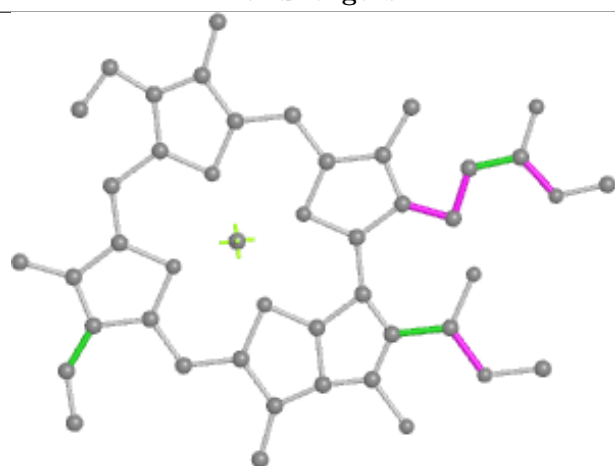
Ligand CLA 9 319



Bond lengths



Bond angles

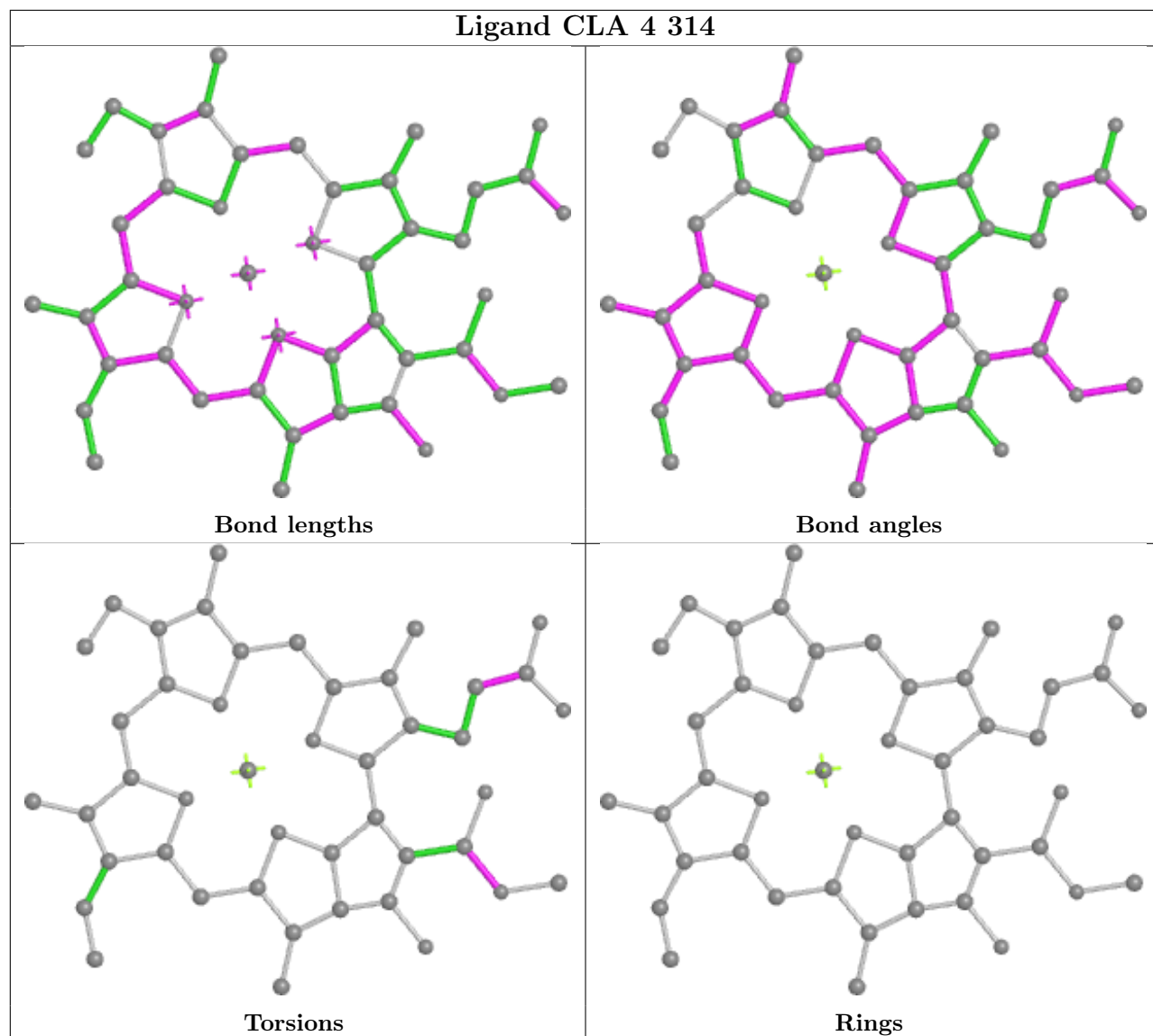


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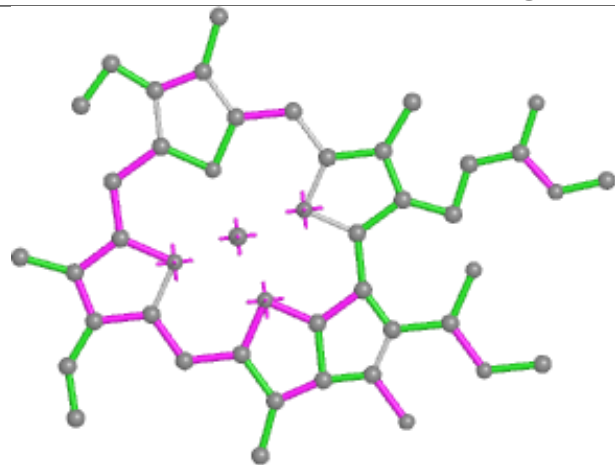


Rings

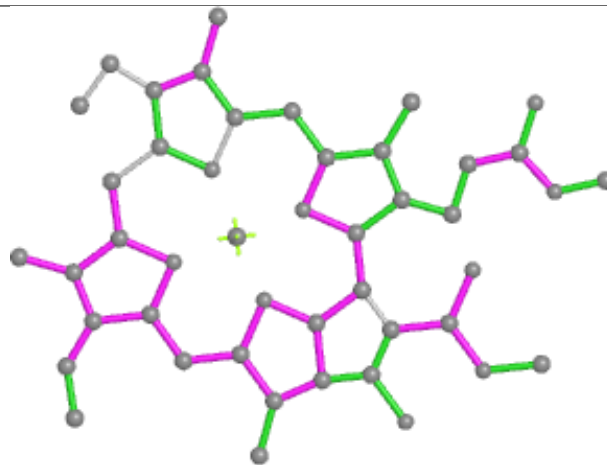
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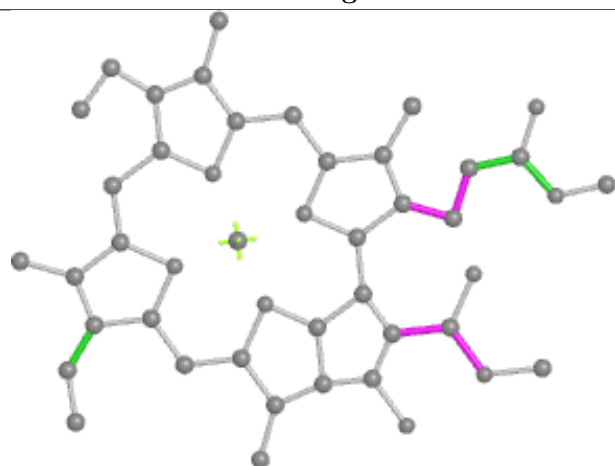
Ligand CLA 4 311



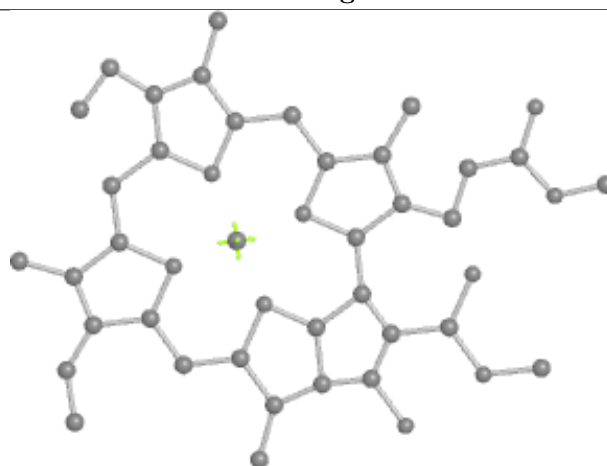
Bond lengths



Bond angles

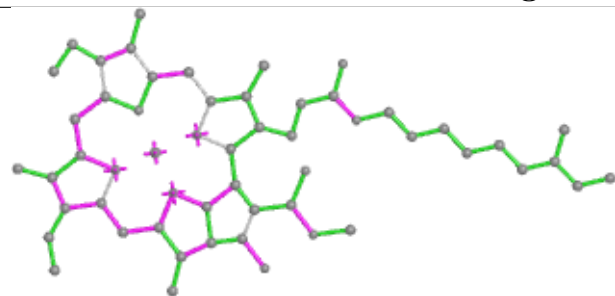


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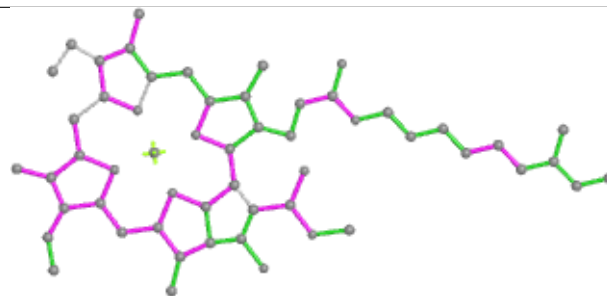


Rings

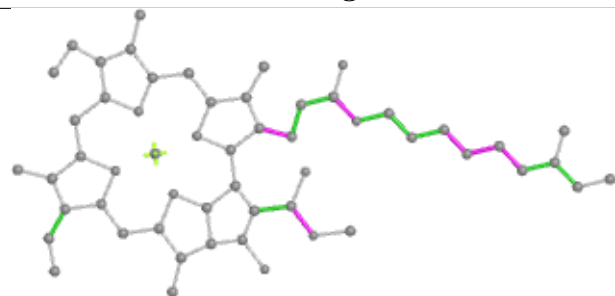
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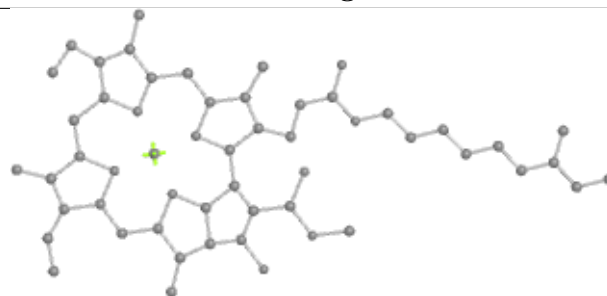
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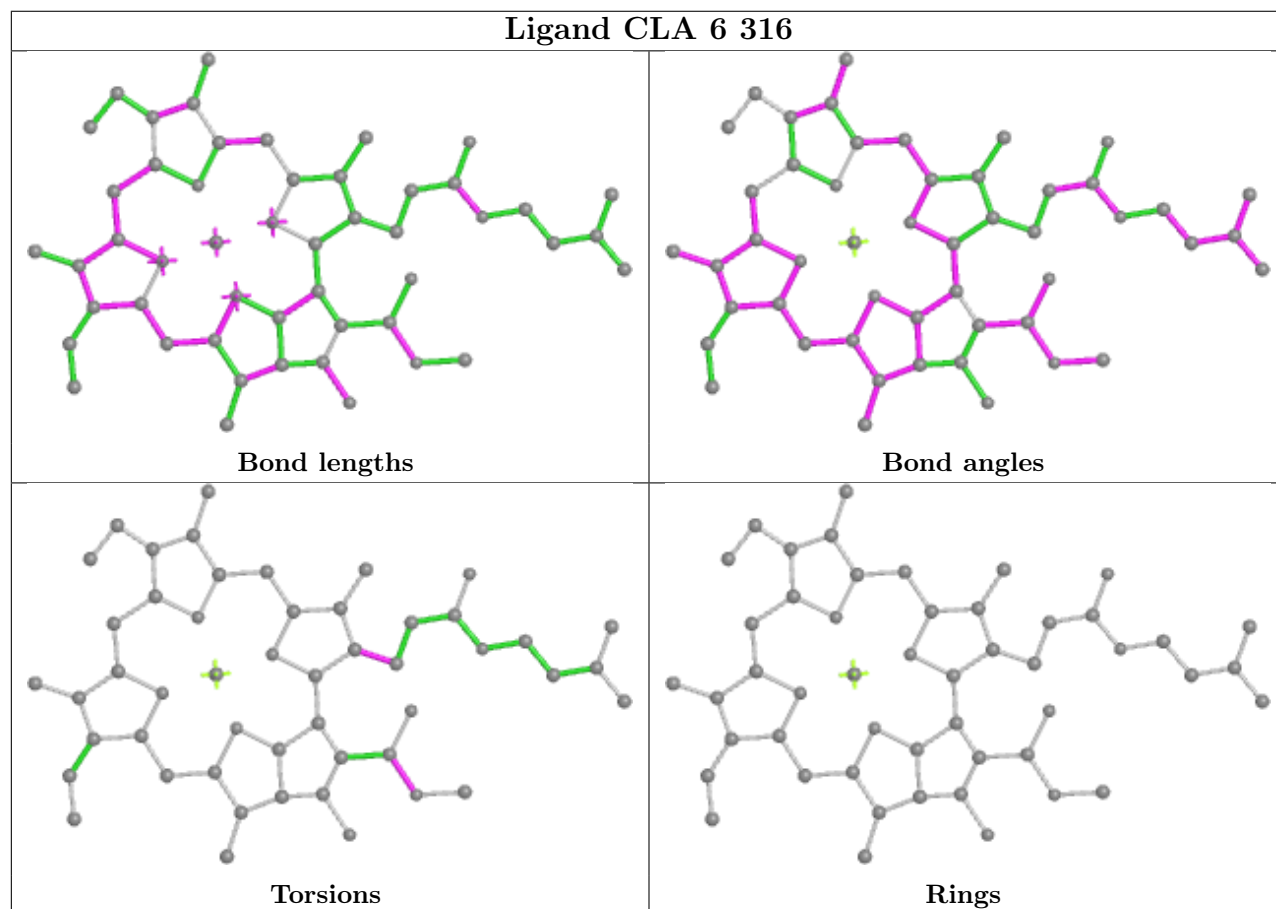
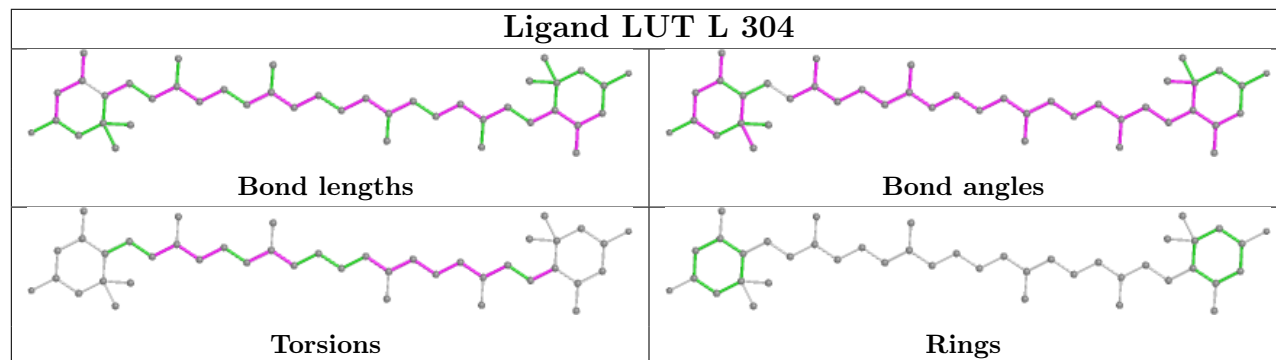
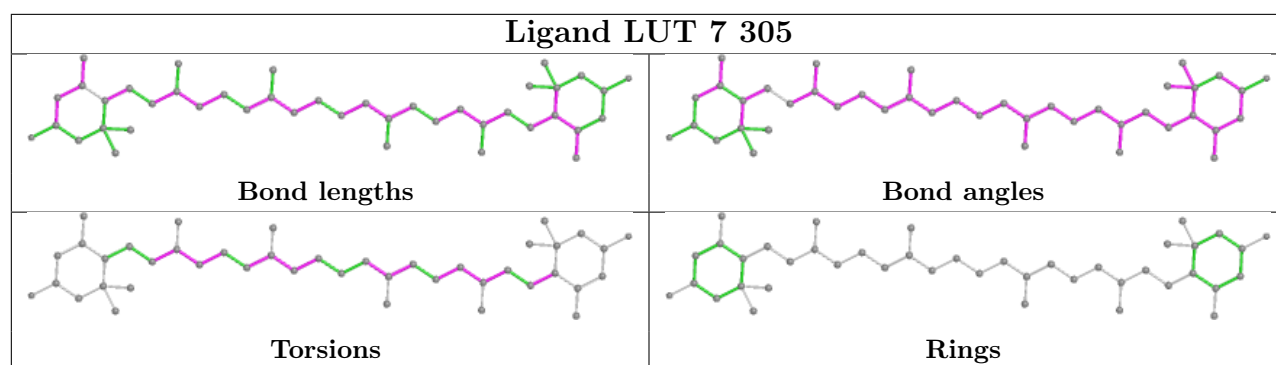
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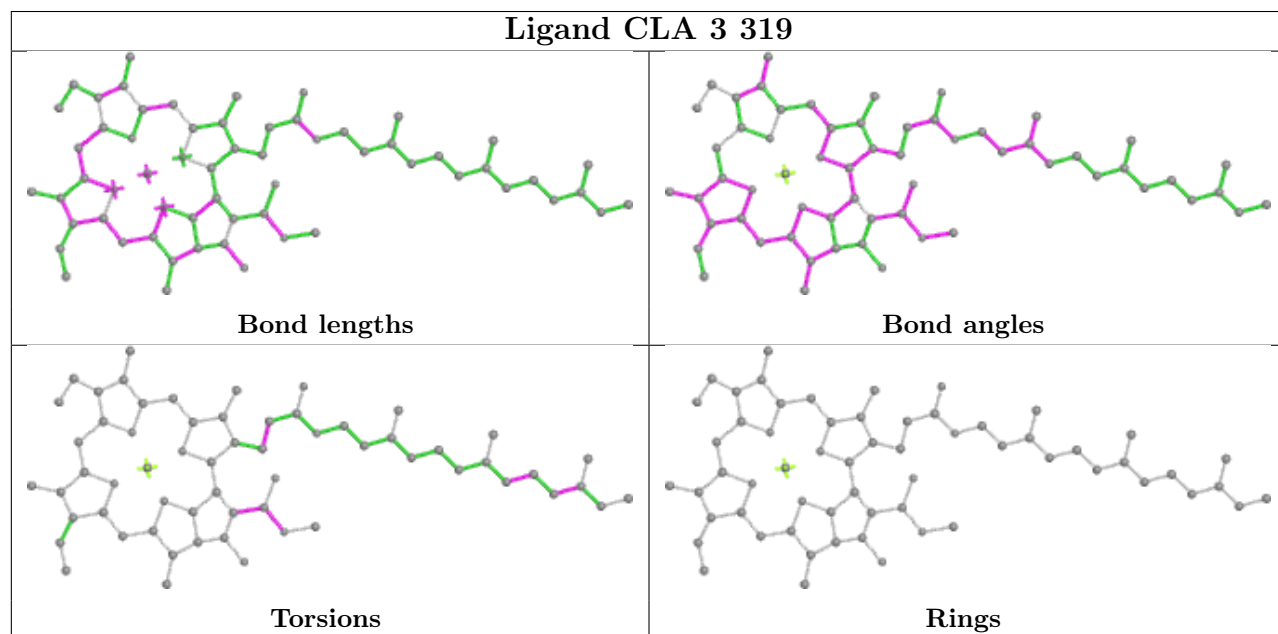
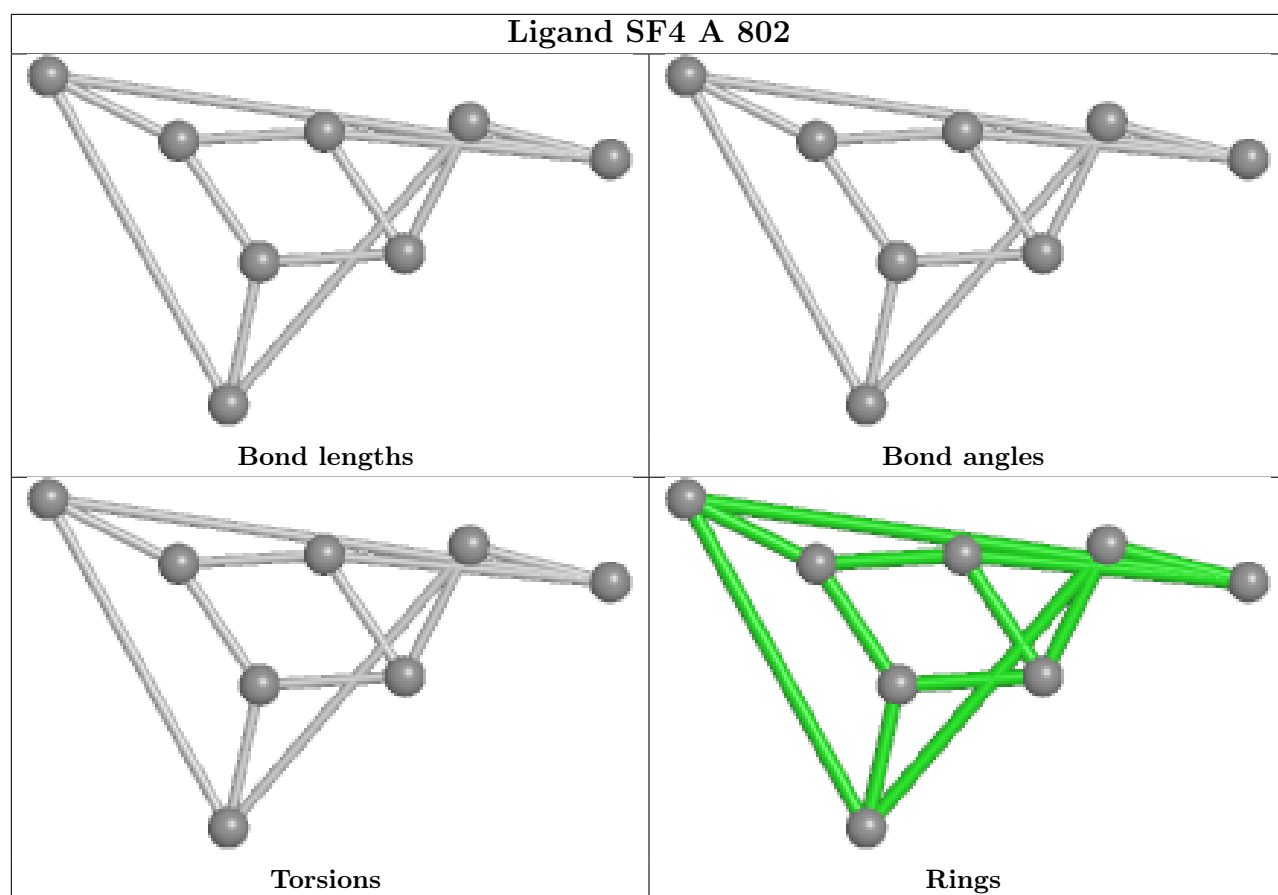


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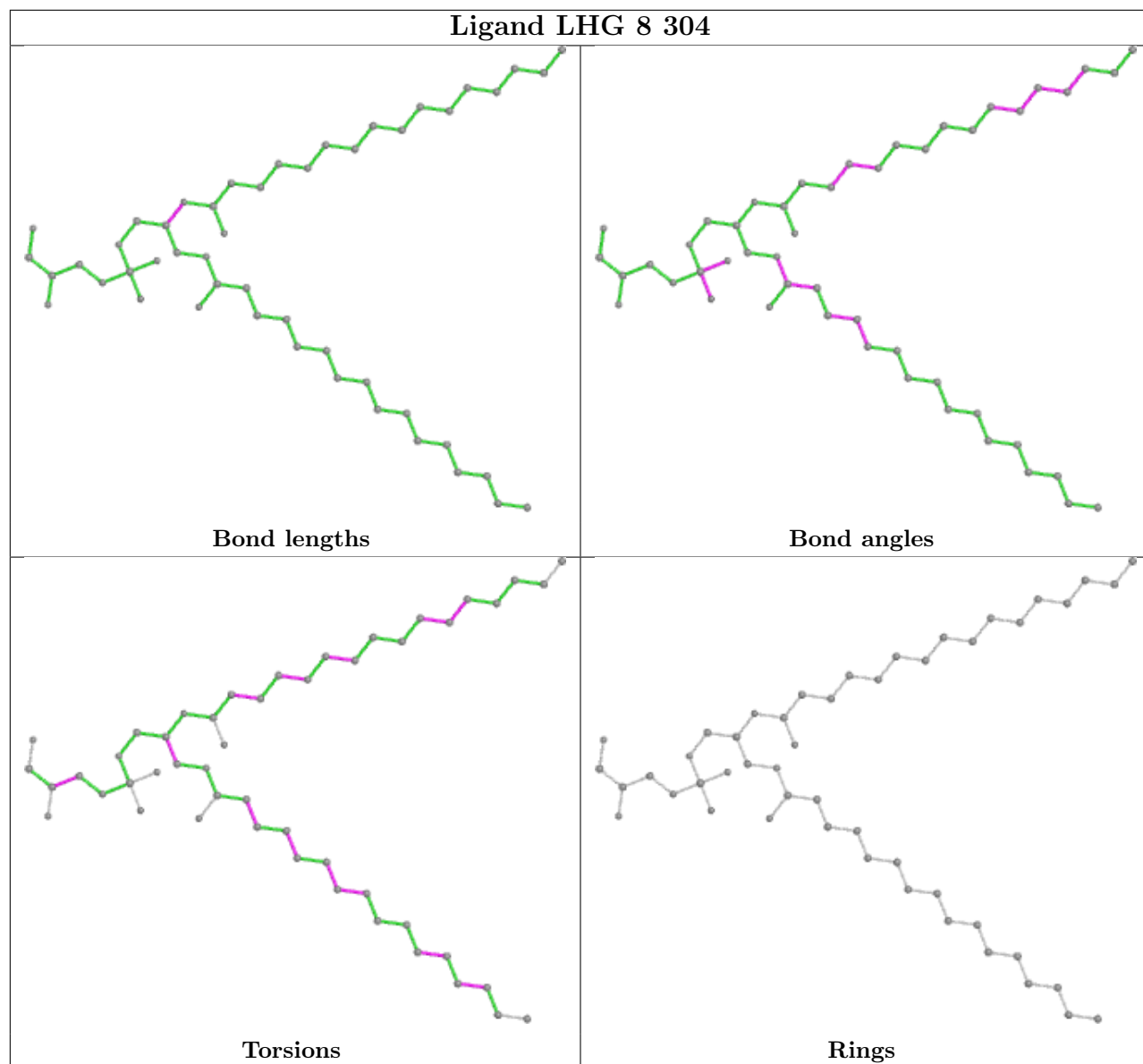


Rings

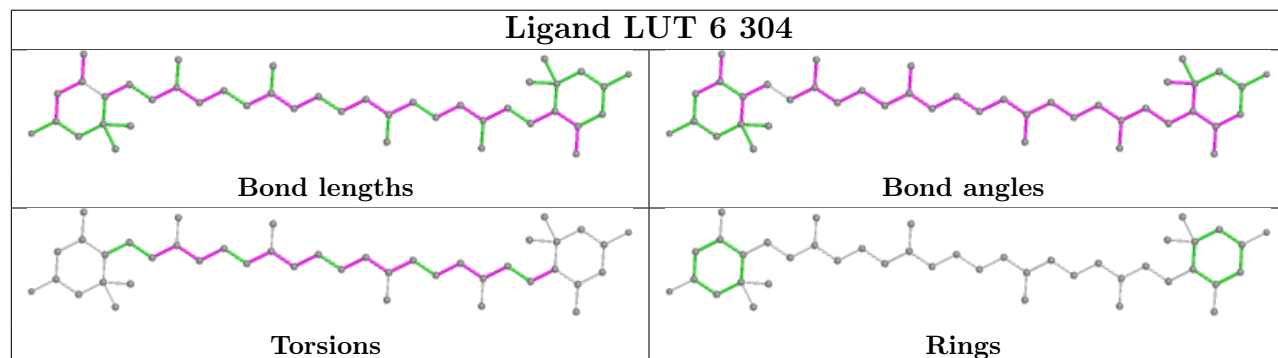


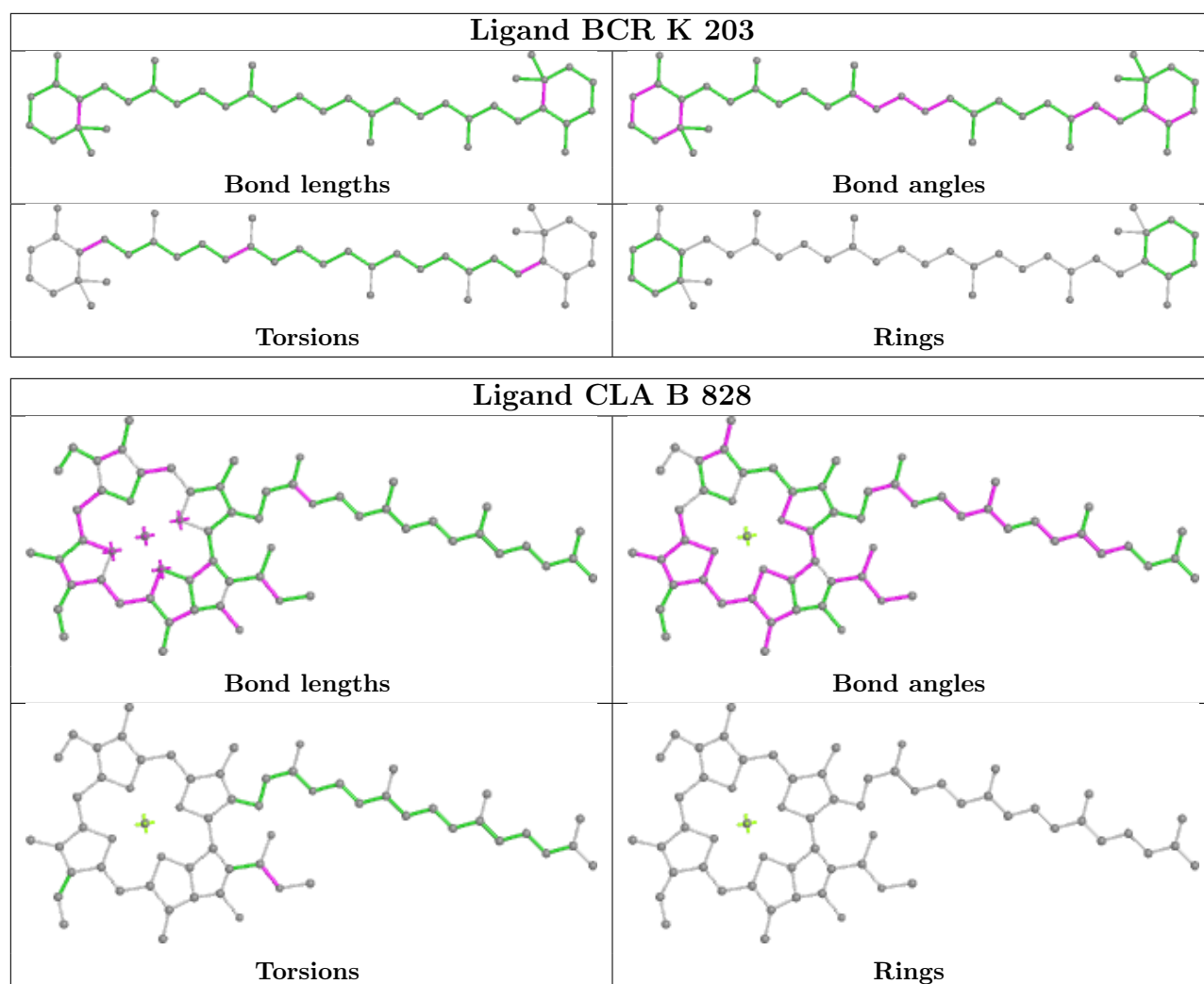


Ligand LHG 8 304

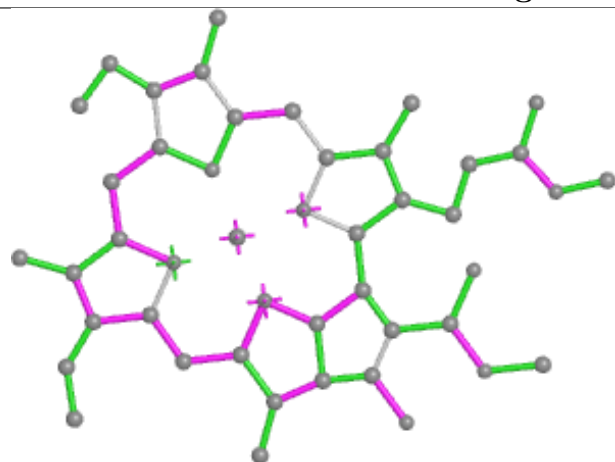


Ligand LUT 6 304

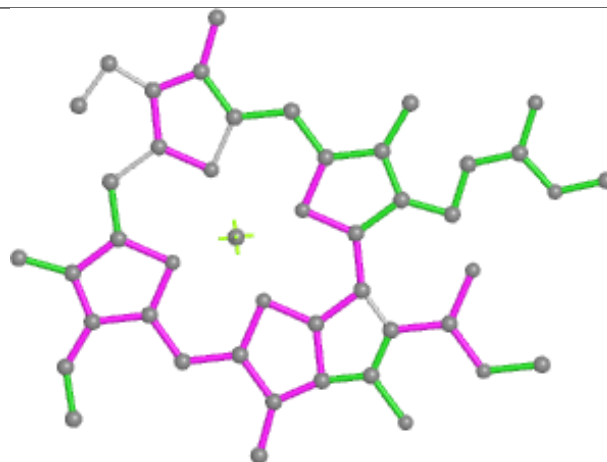




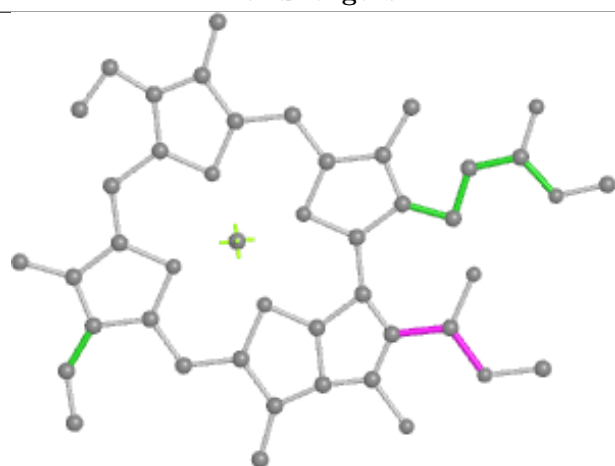
Ligand CLA K 205



Bond lengths



Bond angles

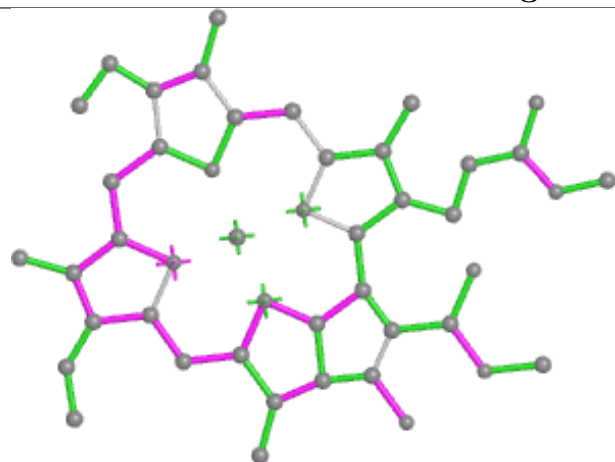


Torsions

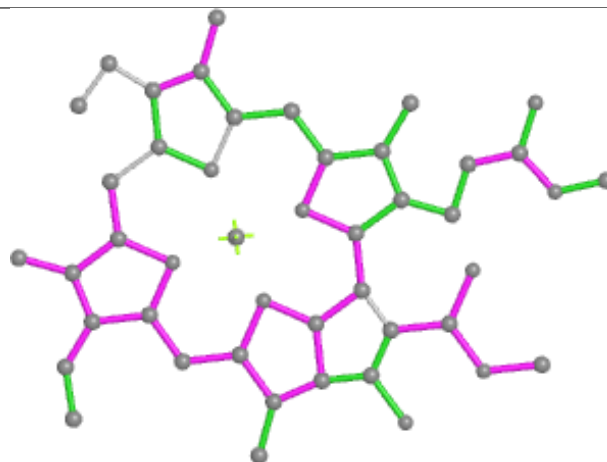


Rings

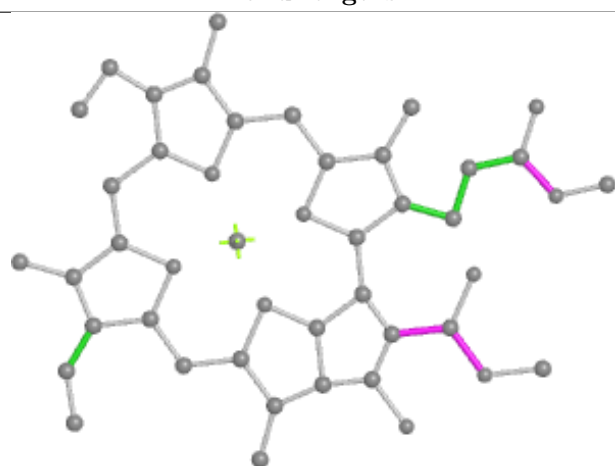
Ligand CLA 5 321



Bond lengths



Bond angles

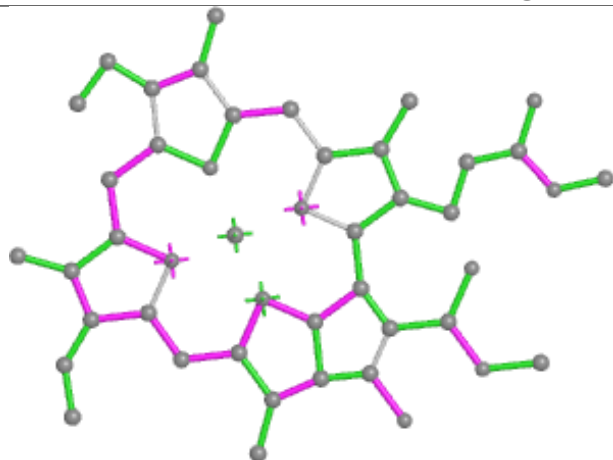


Torsions

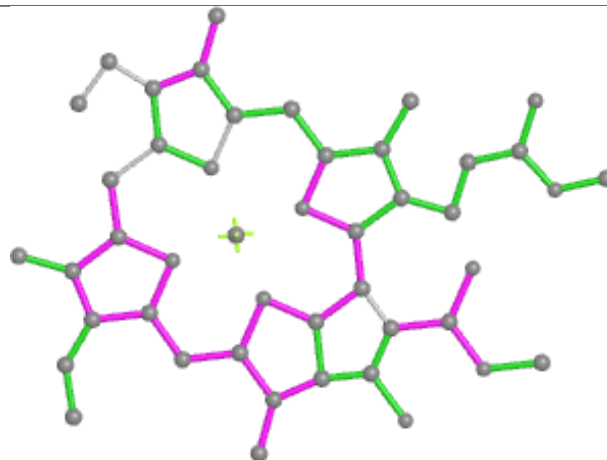


Rings

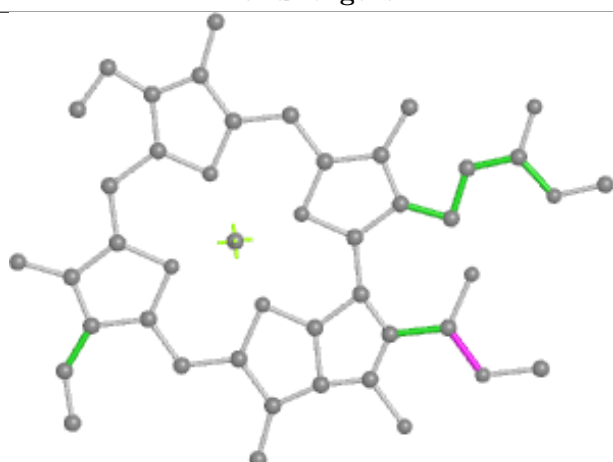
Ligand CLA 9 312



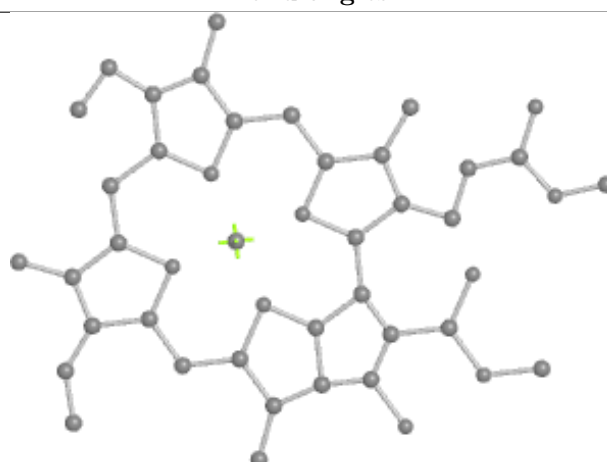
Bond lengths



Bond angles

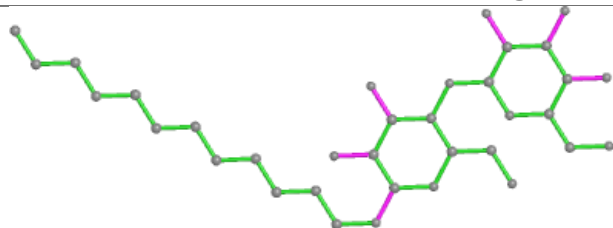


Torsions

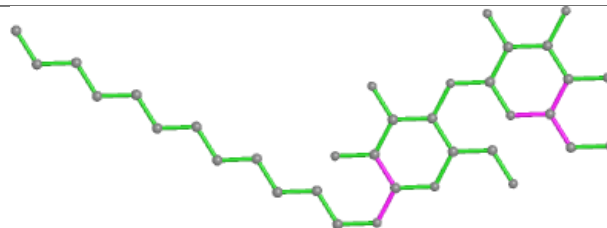


Rings

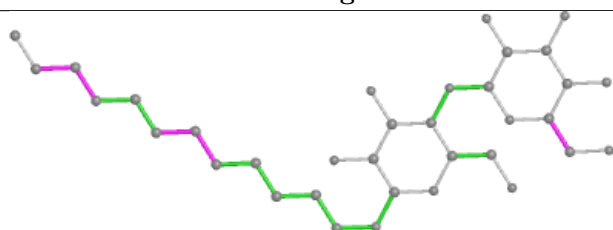
Ligand LMT A 807



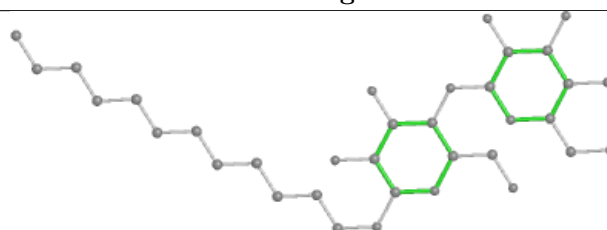
Bond lengths



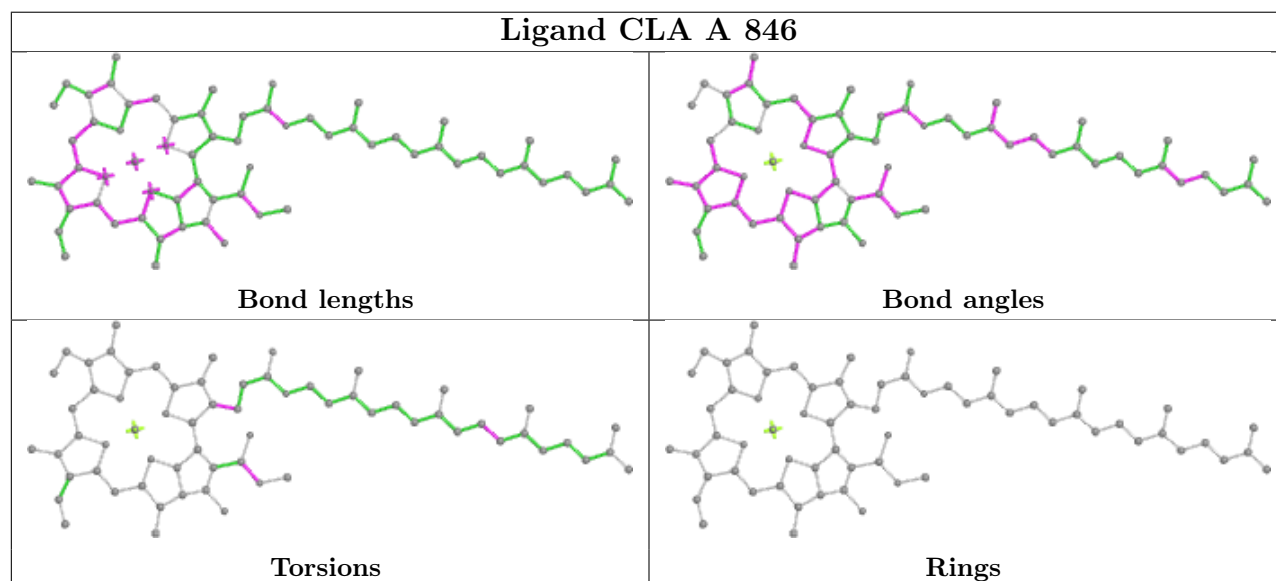
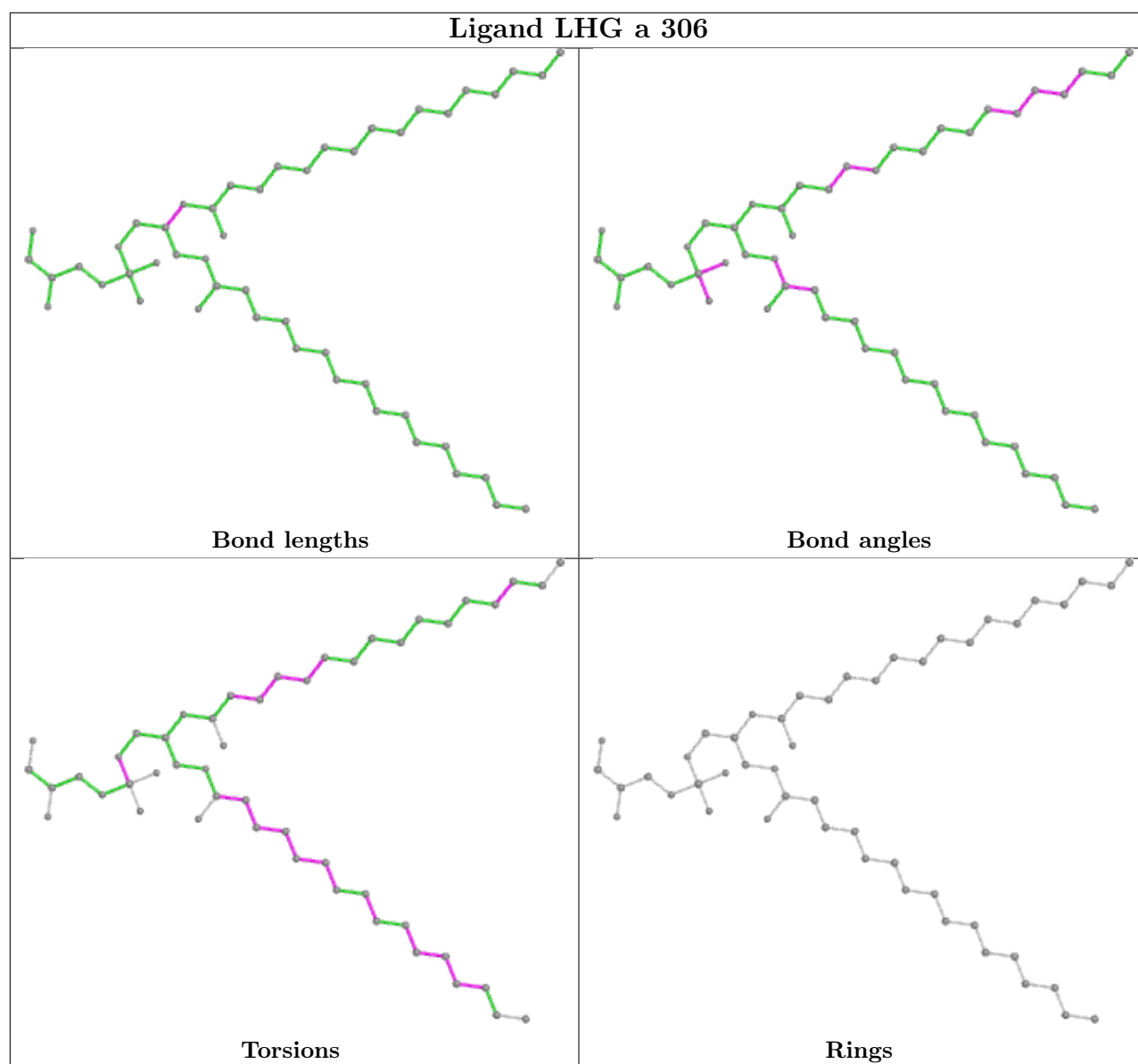
Bond angles



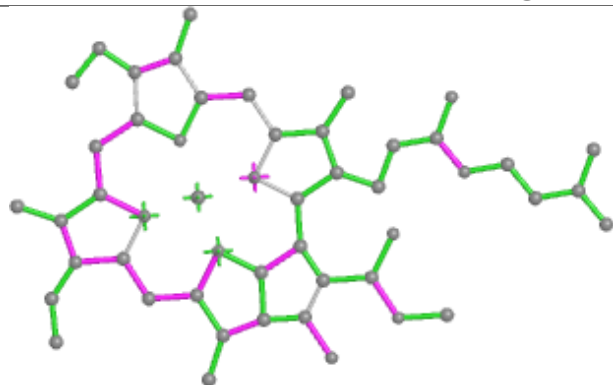
Torsions



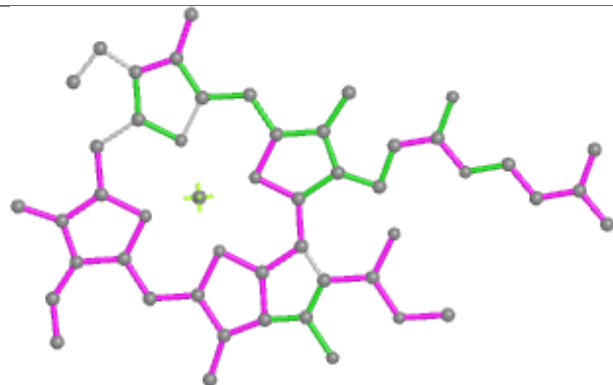
Rings



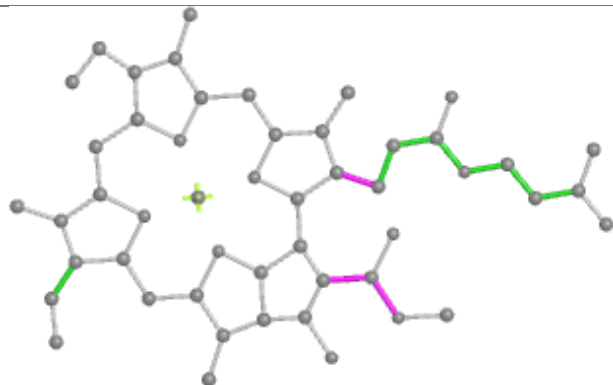
Ligand CLA a 321



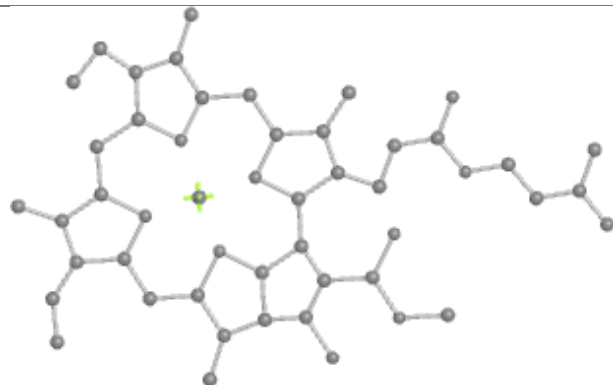
Bond lengths



Bond angles

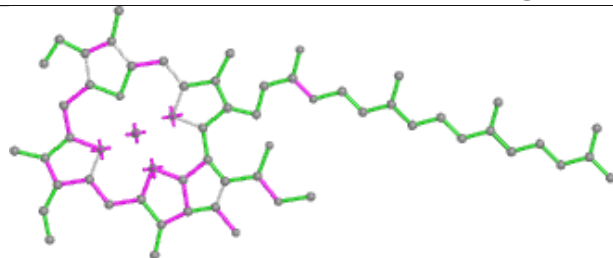


Torsions

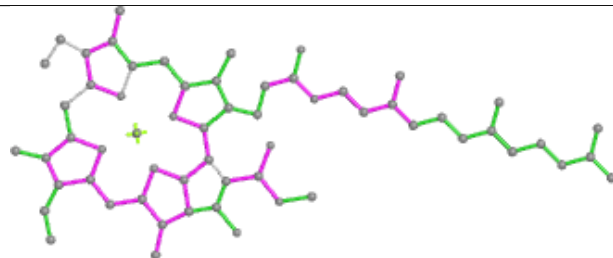


Rings

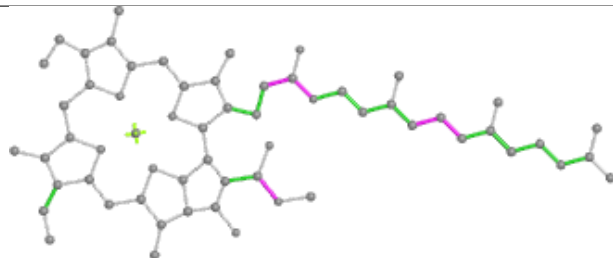
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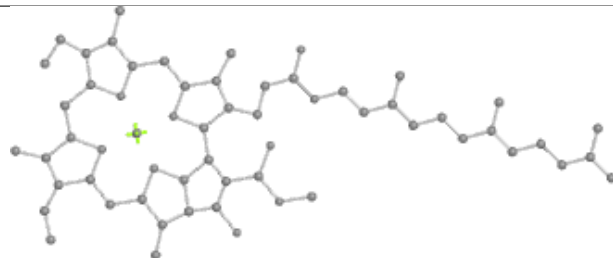
Bond lengths



Bond angles

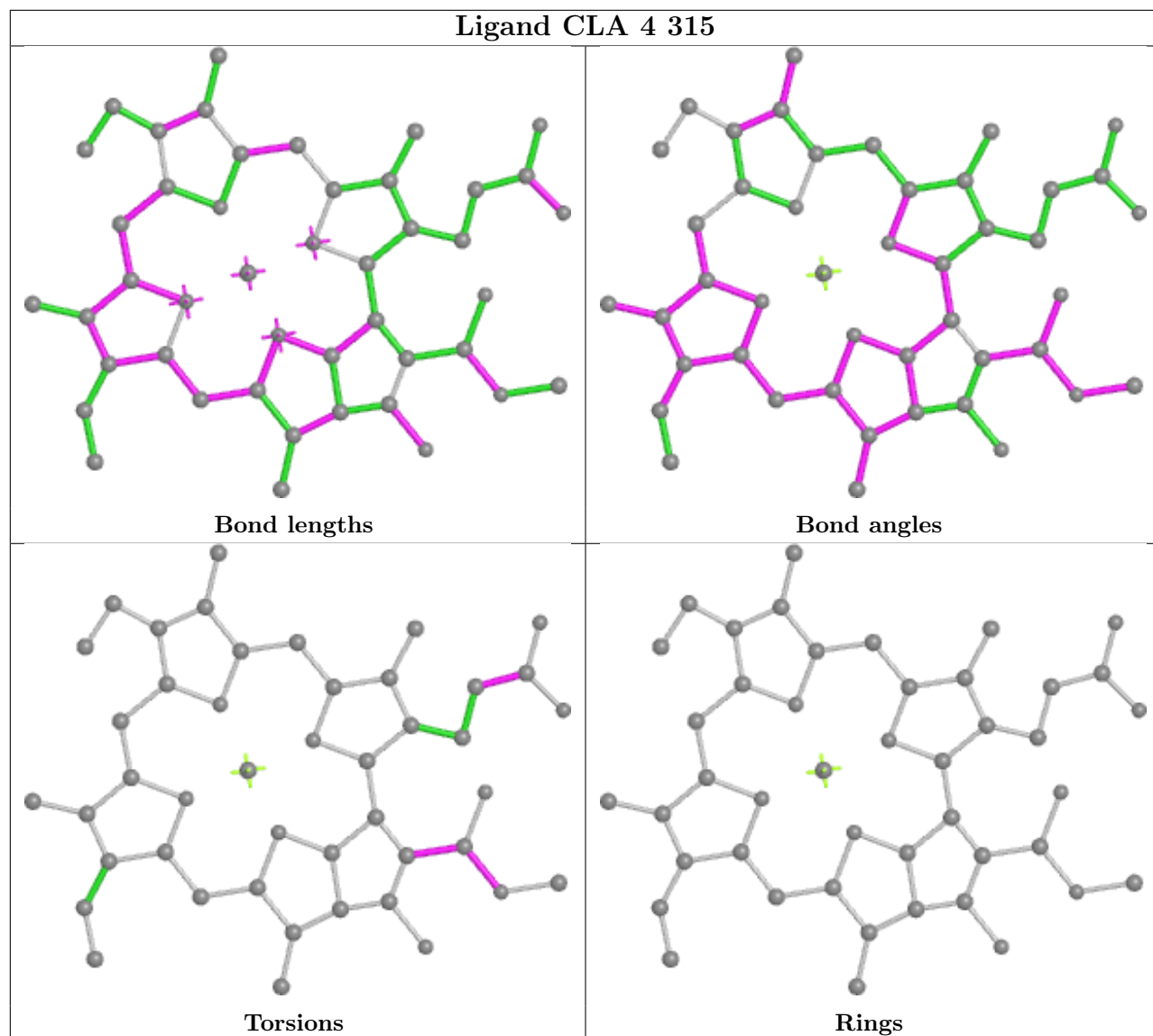


Torsions

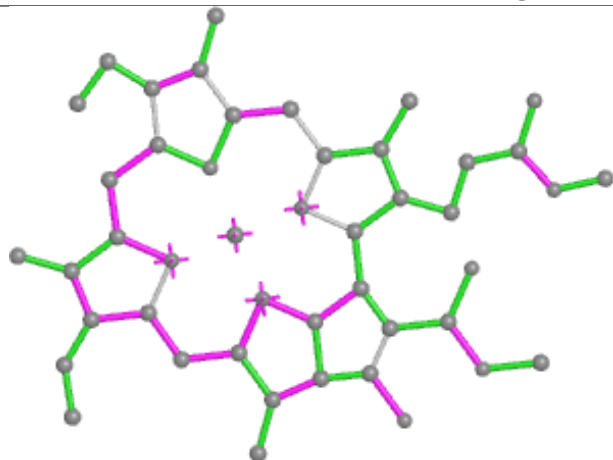


Rings

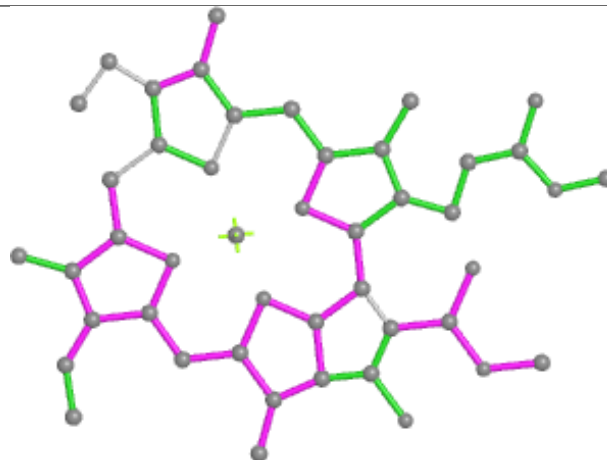
Ligand CLA 4 315



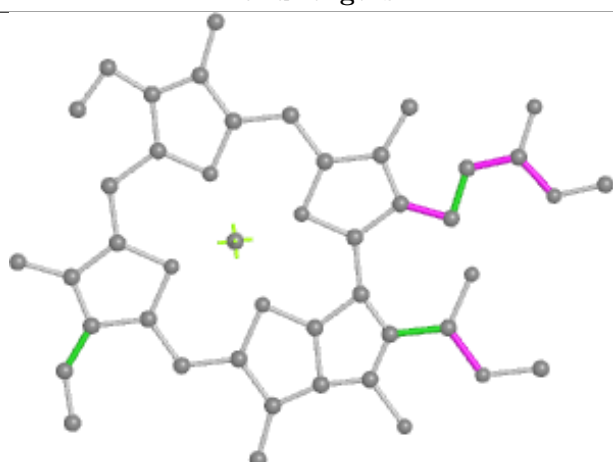
Ligand CLA H 901



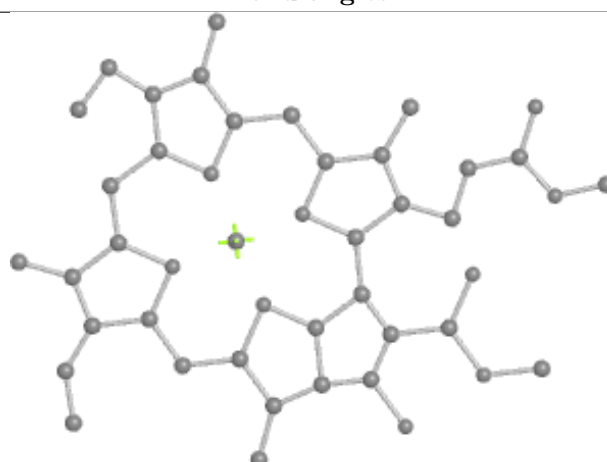
Bond lengths



Bond angles

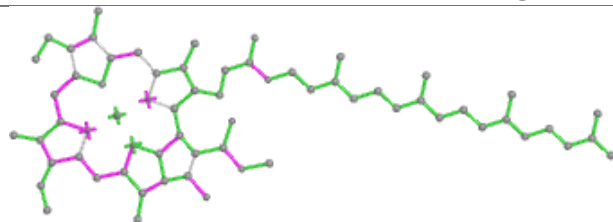


Torsions

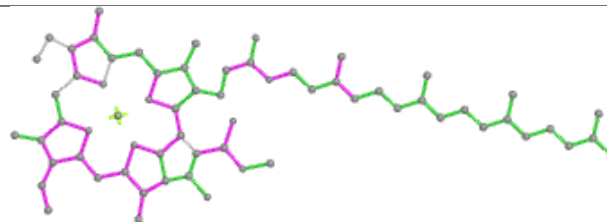


Rings

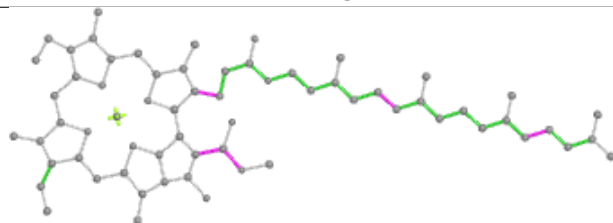
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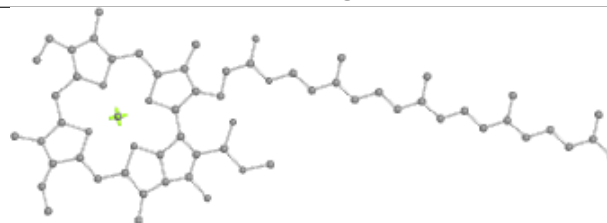
Bond lengths



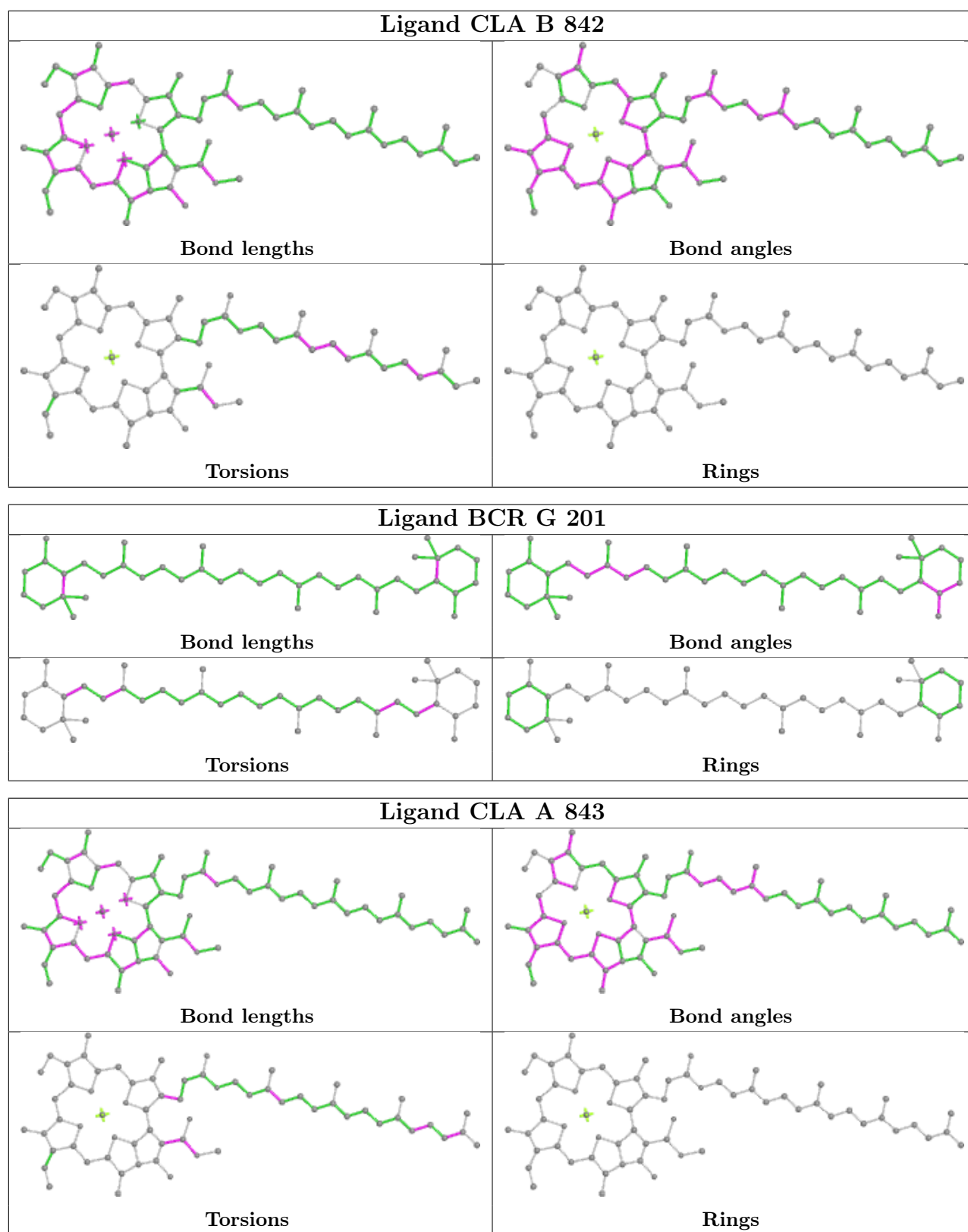
Bond angles



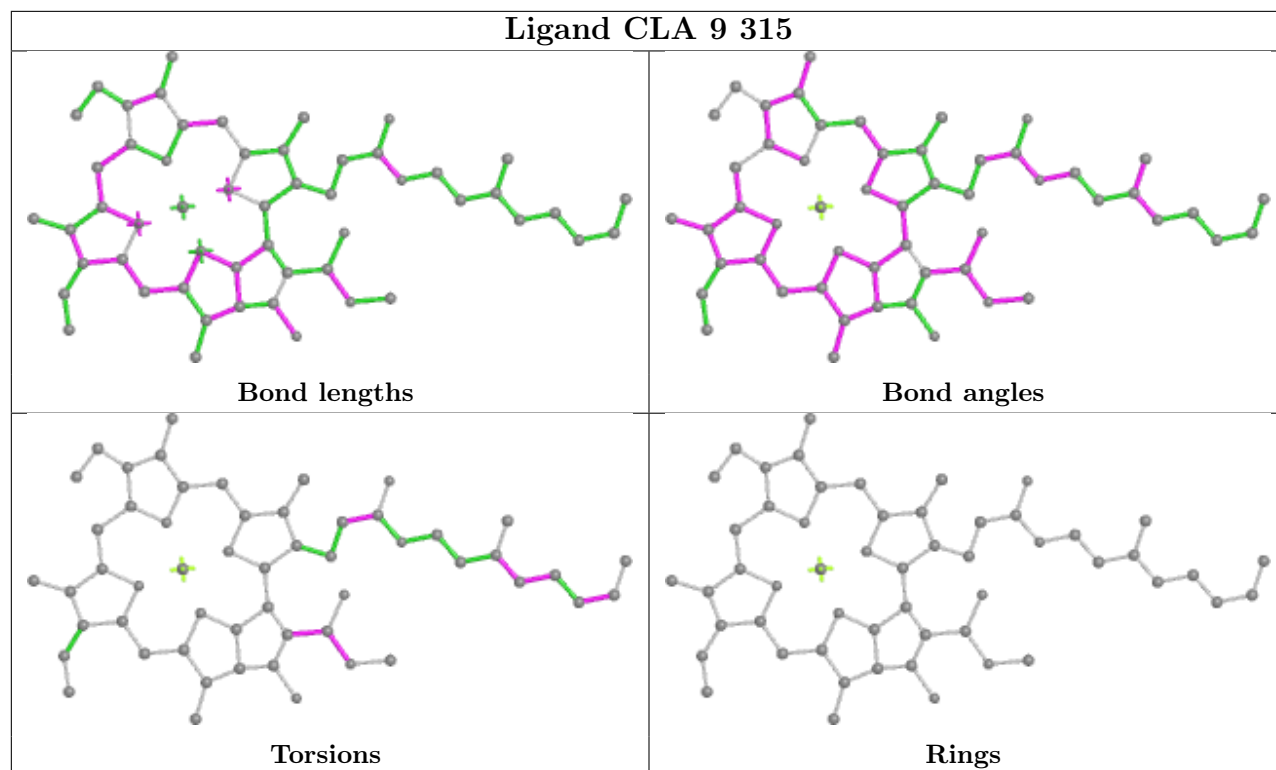
Torsions



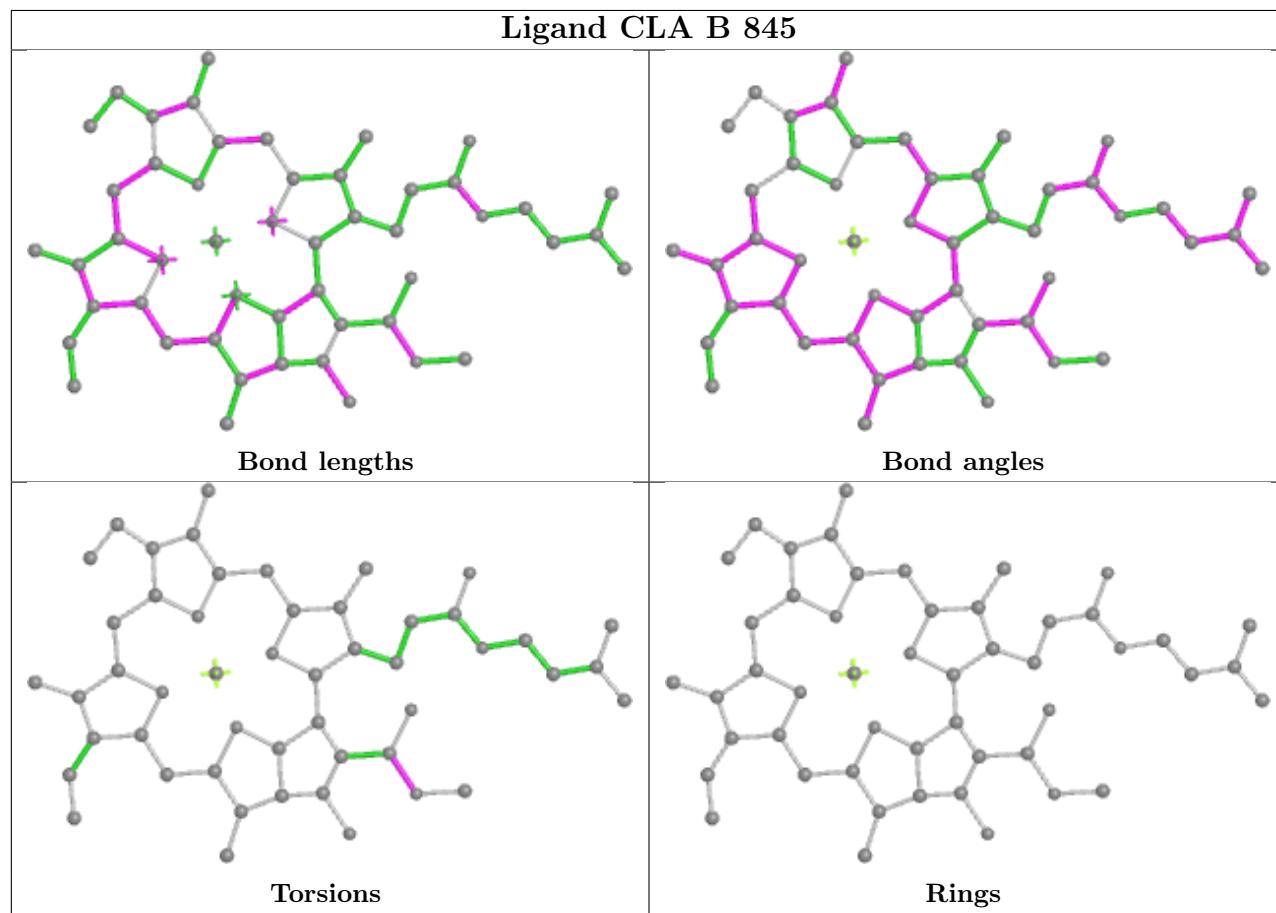
Rings

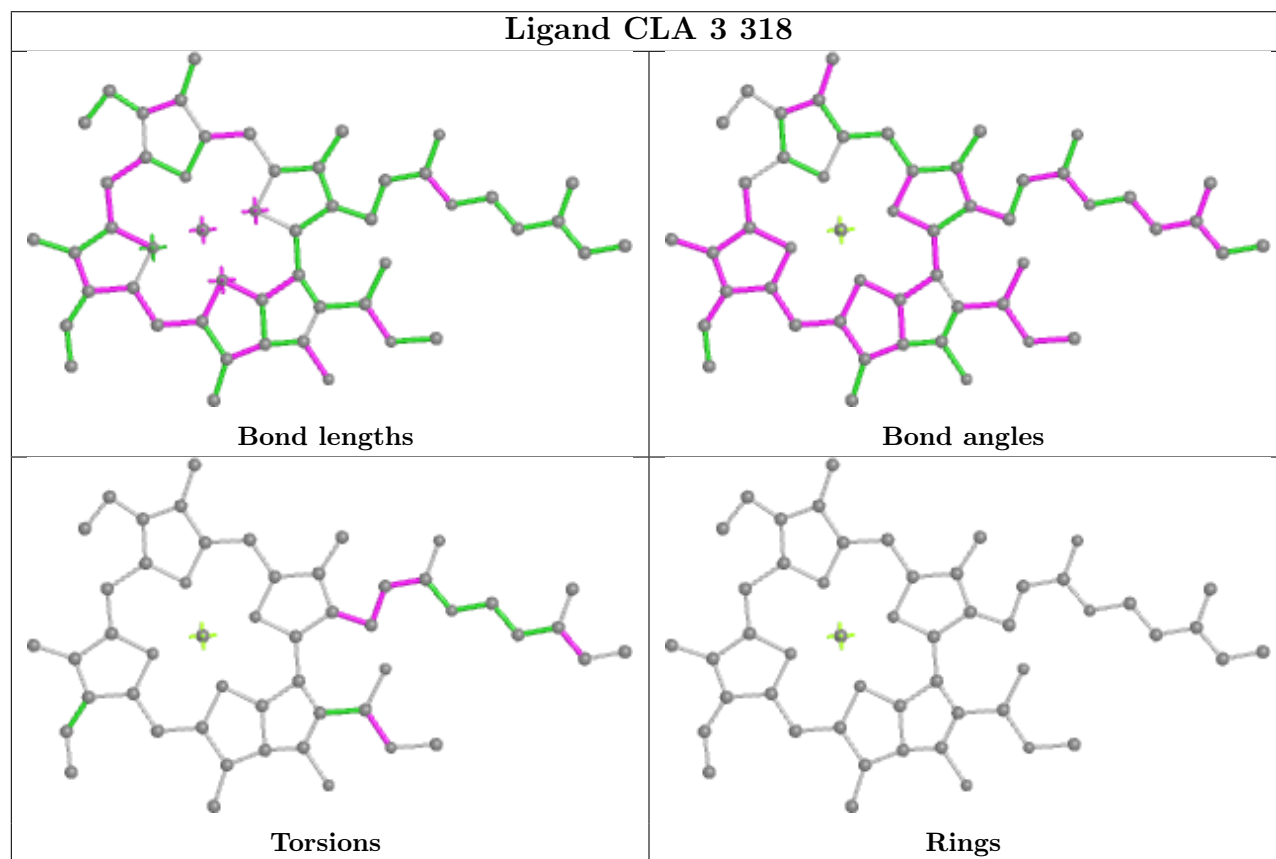
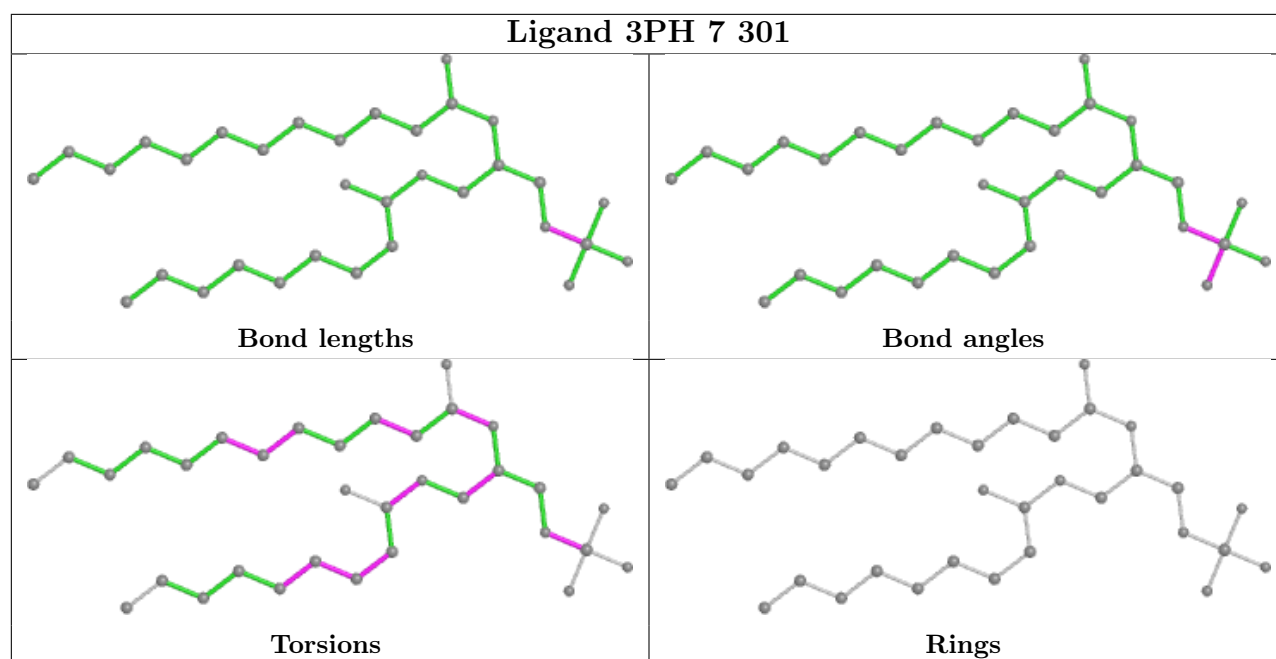


Ligand CLA 9 315

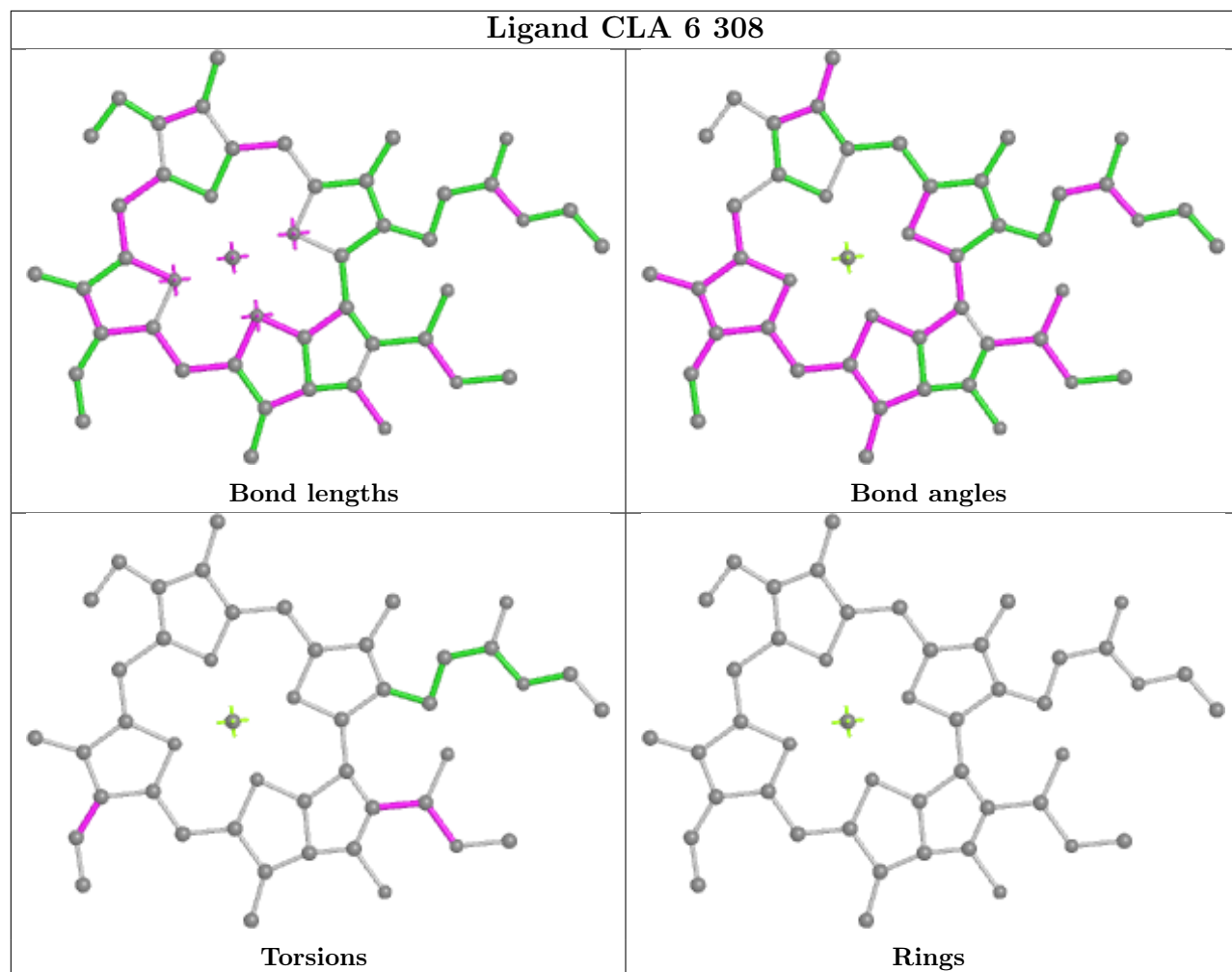


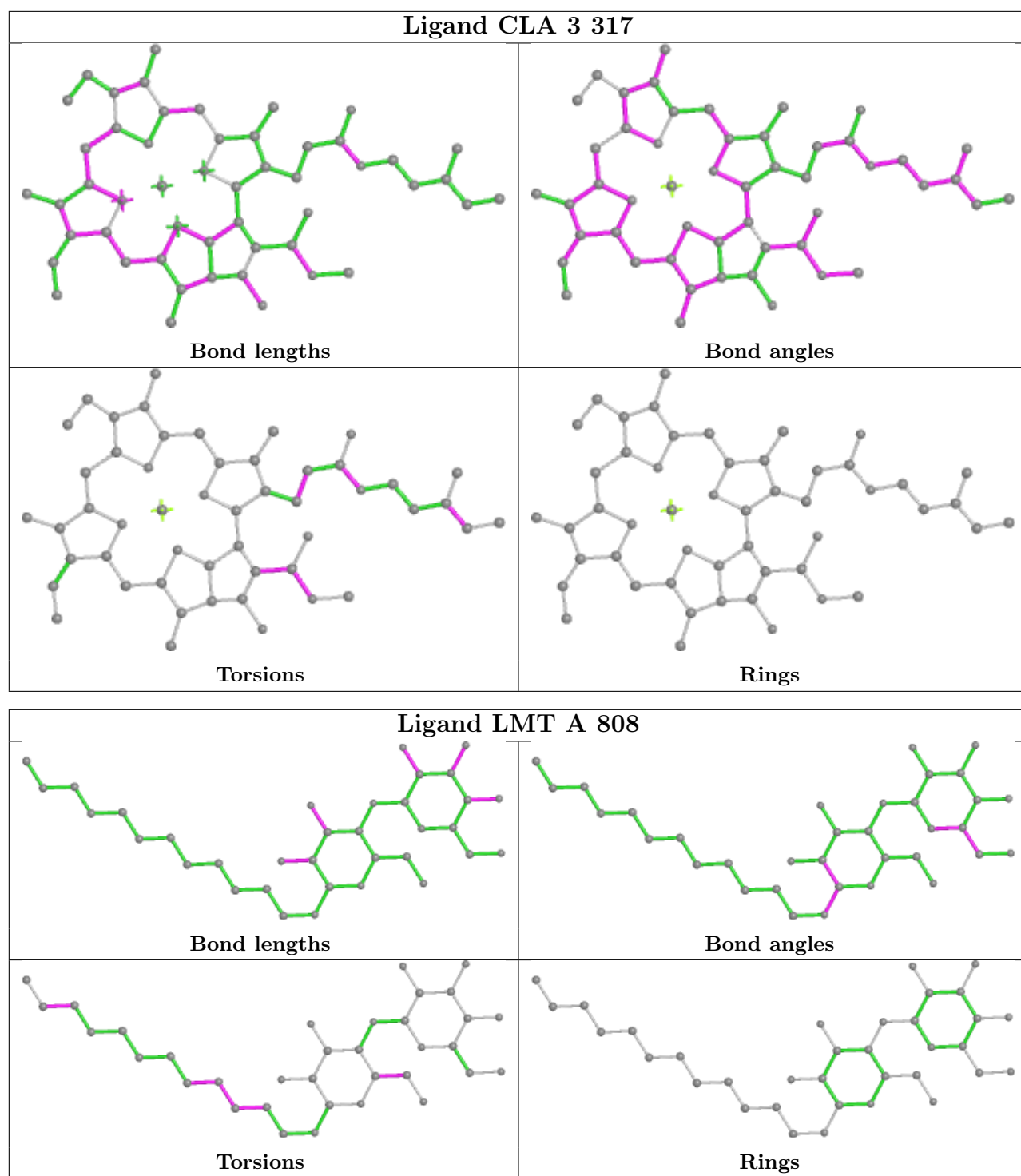
Ligand CLA B 845

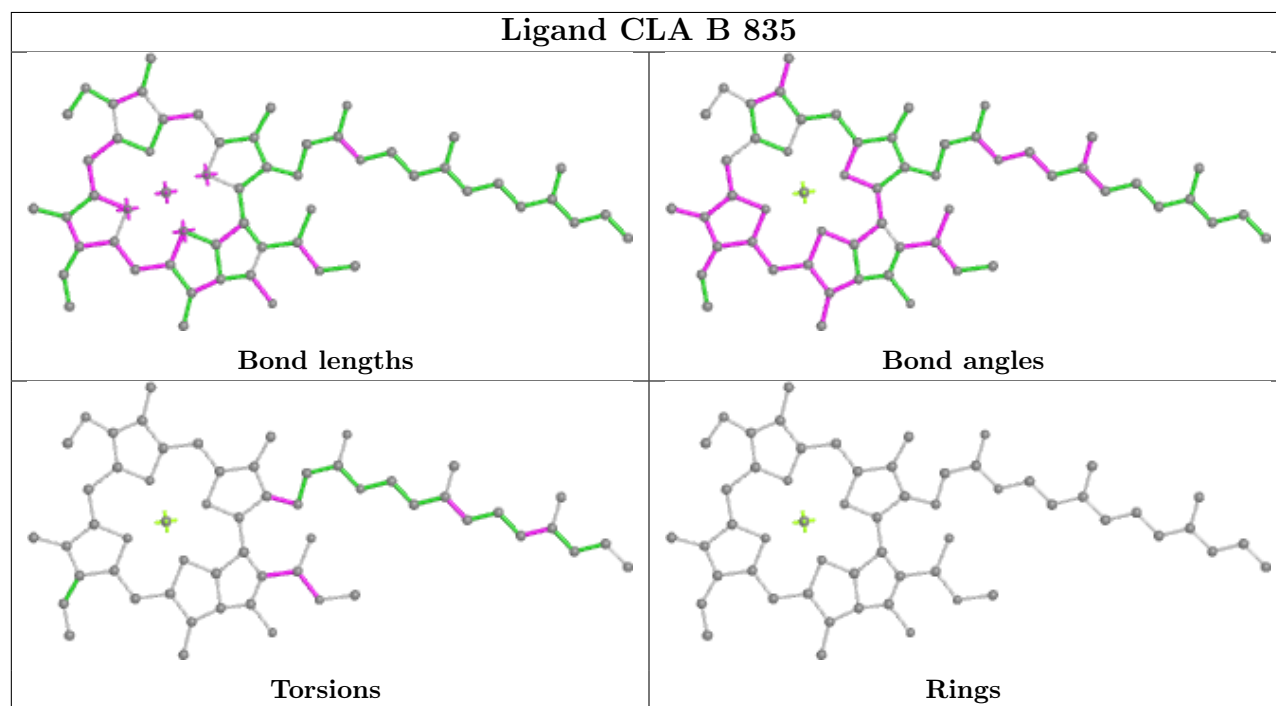
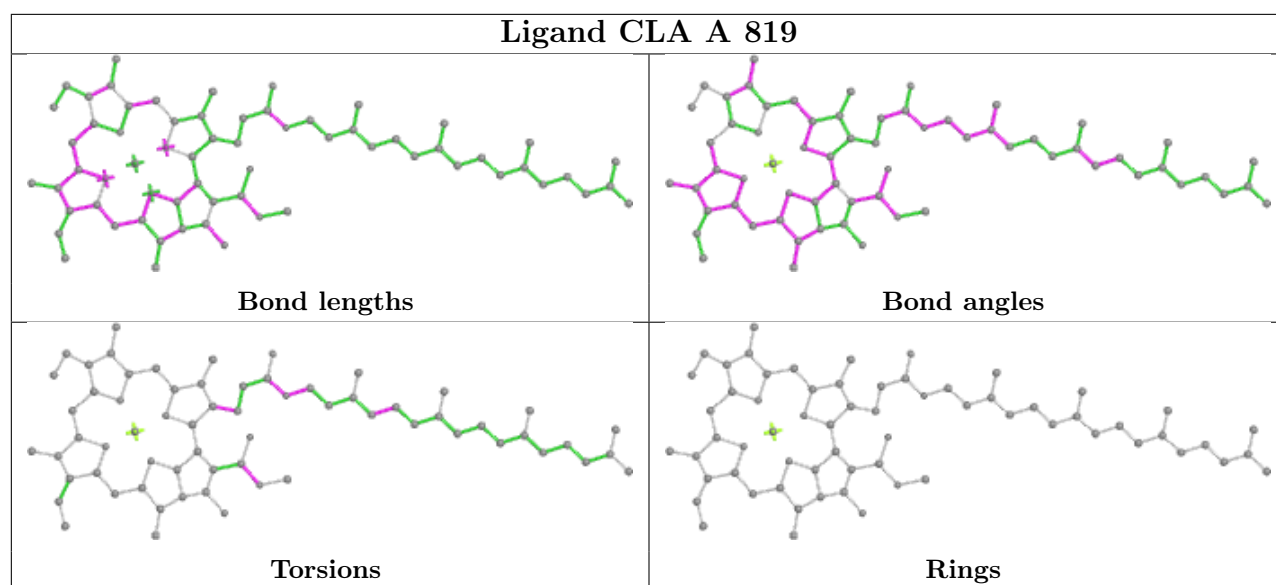




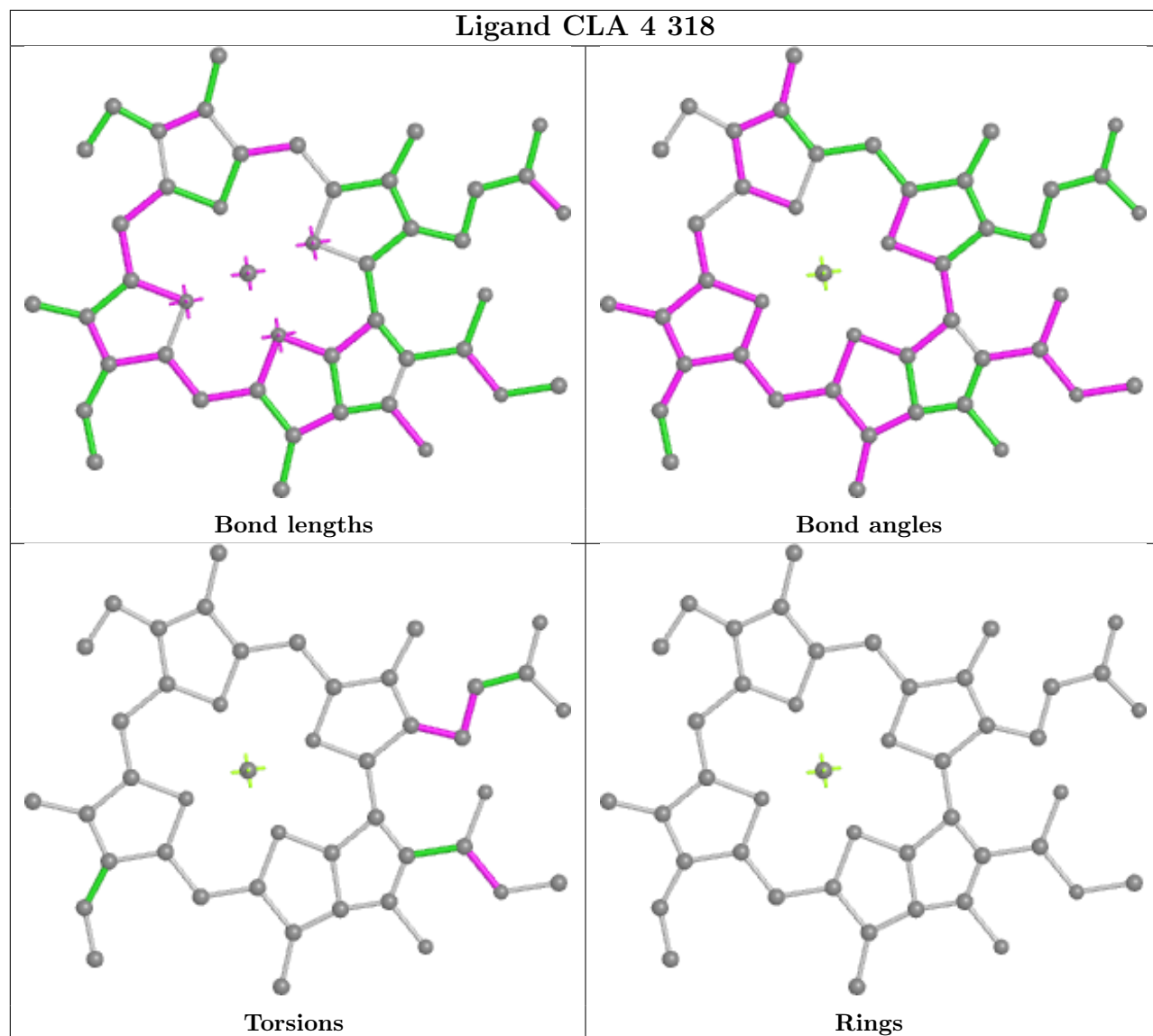
Ligand CLA 6 308



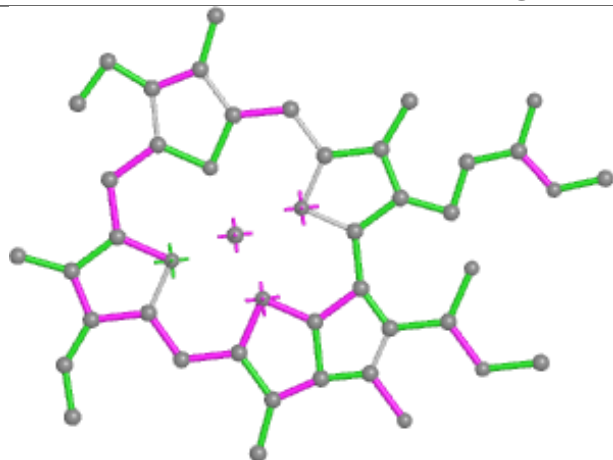




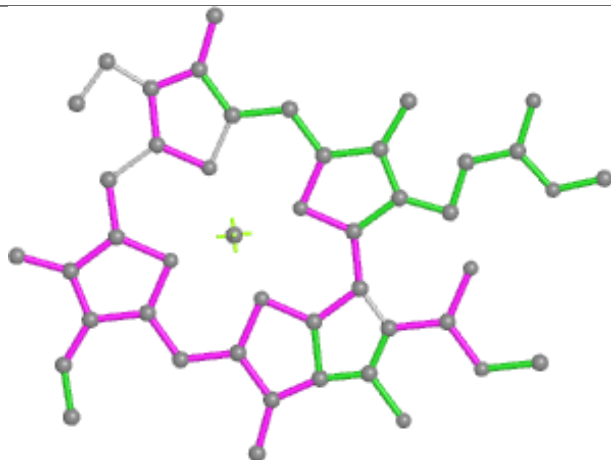
Ligand CLA 4 318



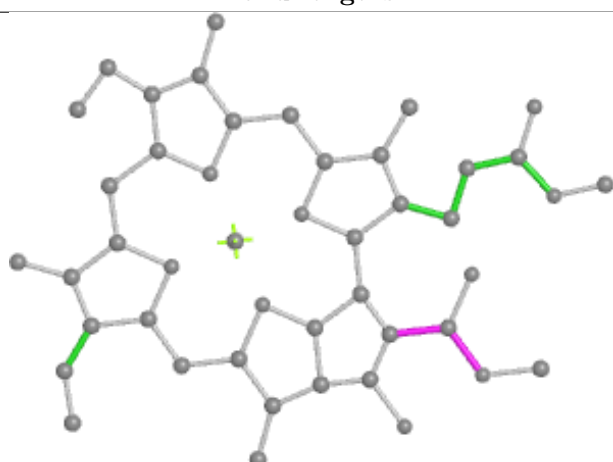
Ligand CLA K 206



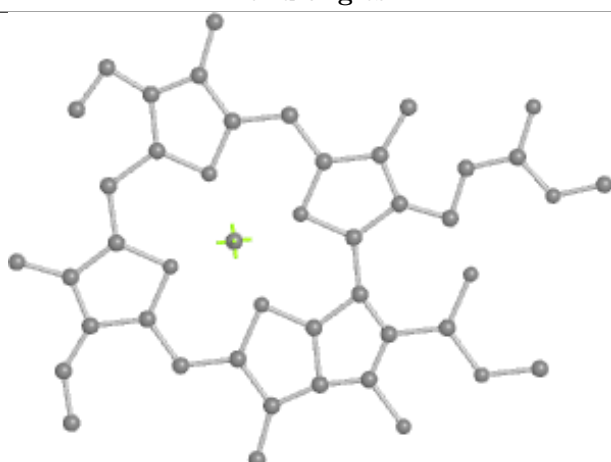
Bond lengths



Bond angles

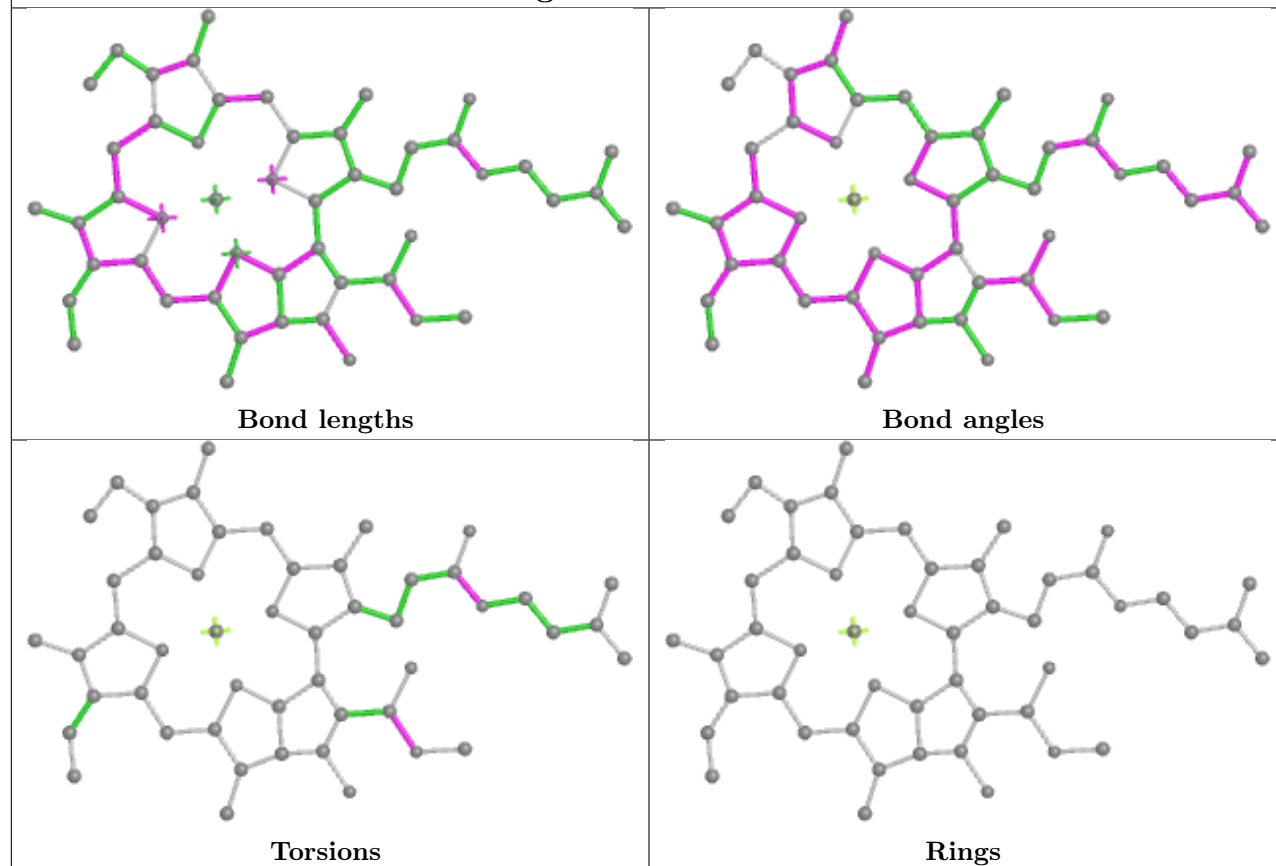


Torsions

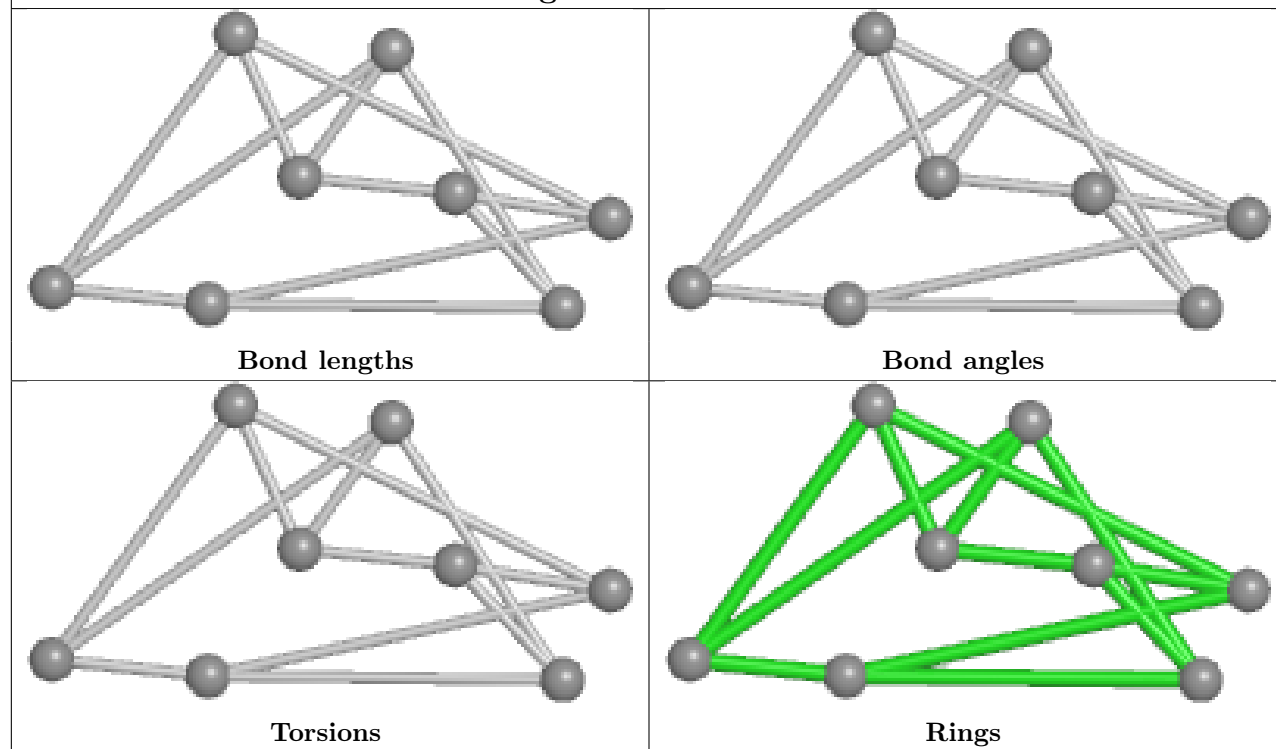


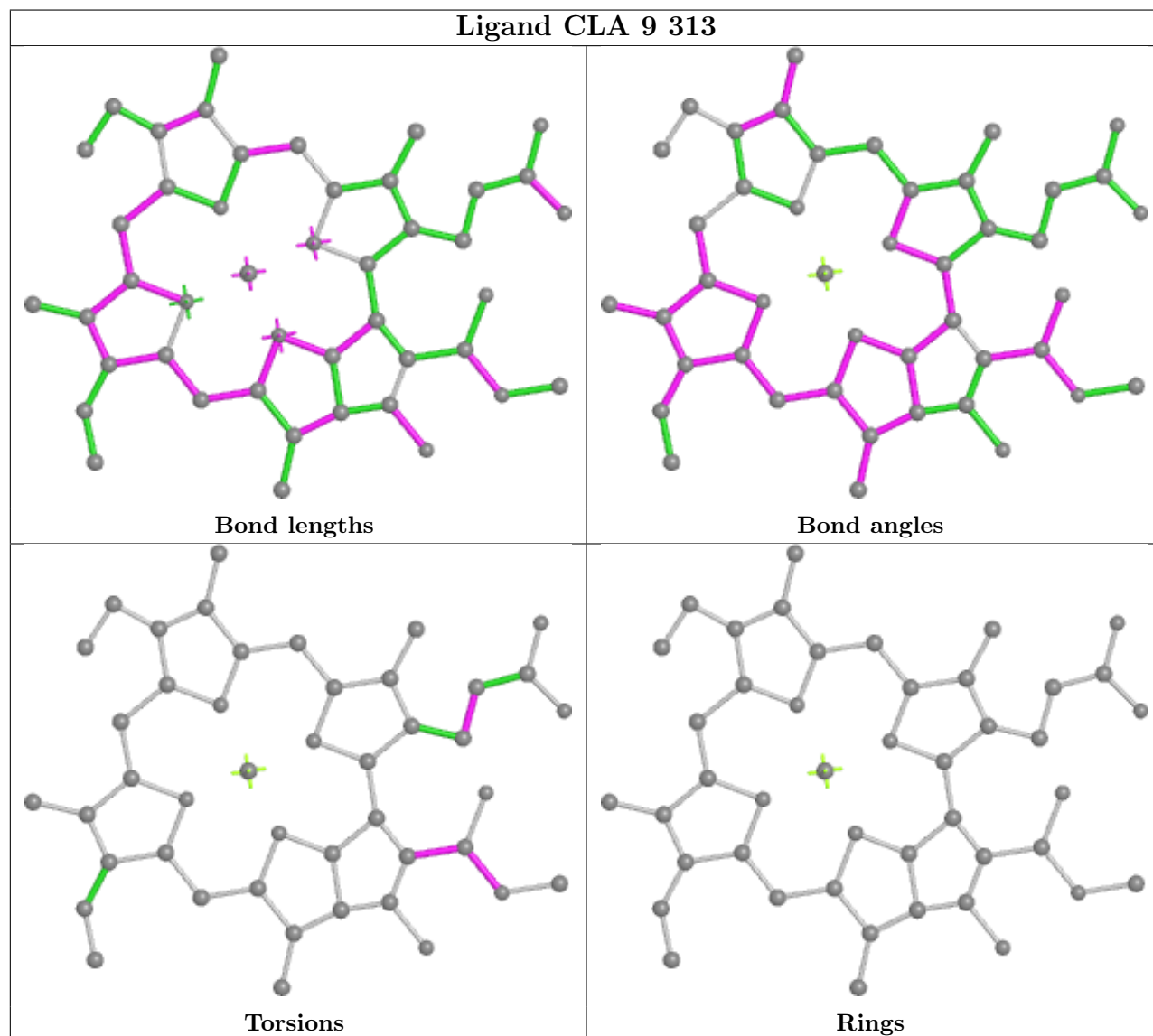
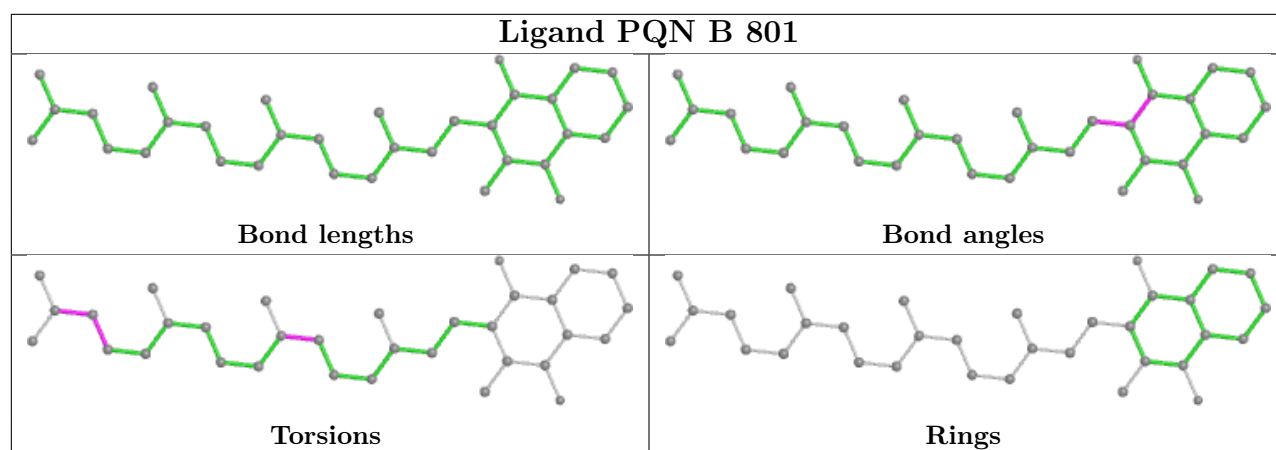
Rings

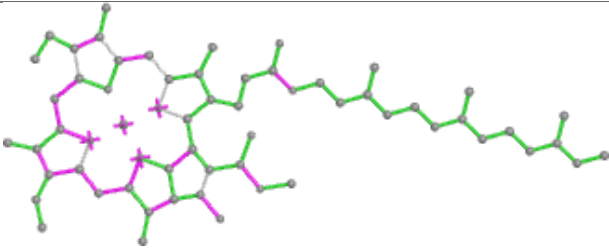
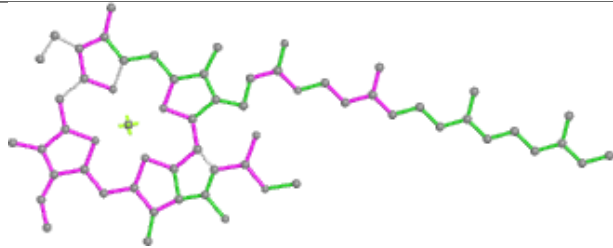
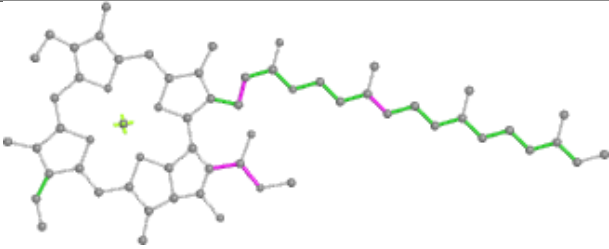
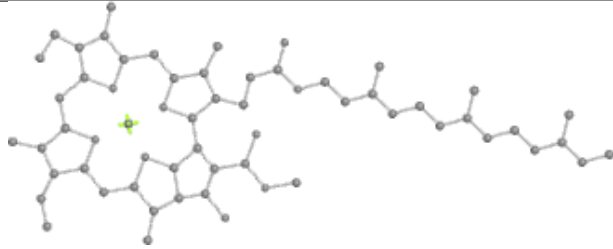
Ligand CLA 3 316

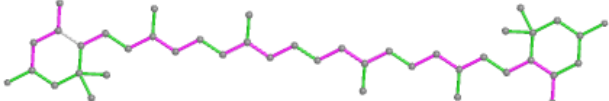
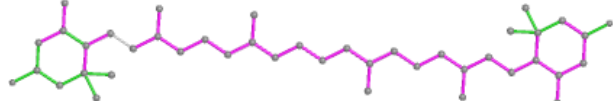
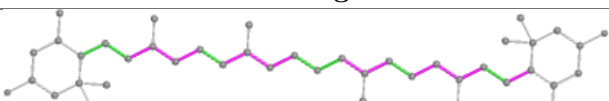



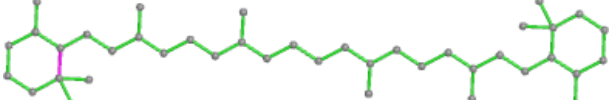
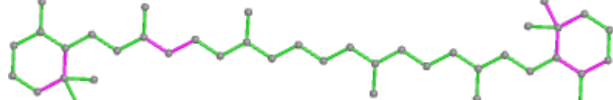
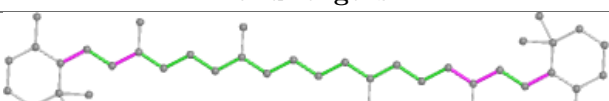
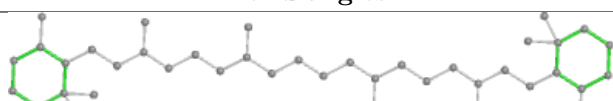
Ligand SF4 C 102

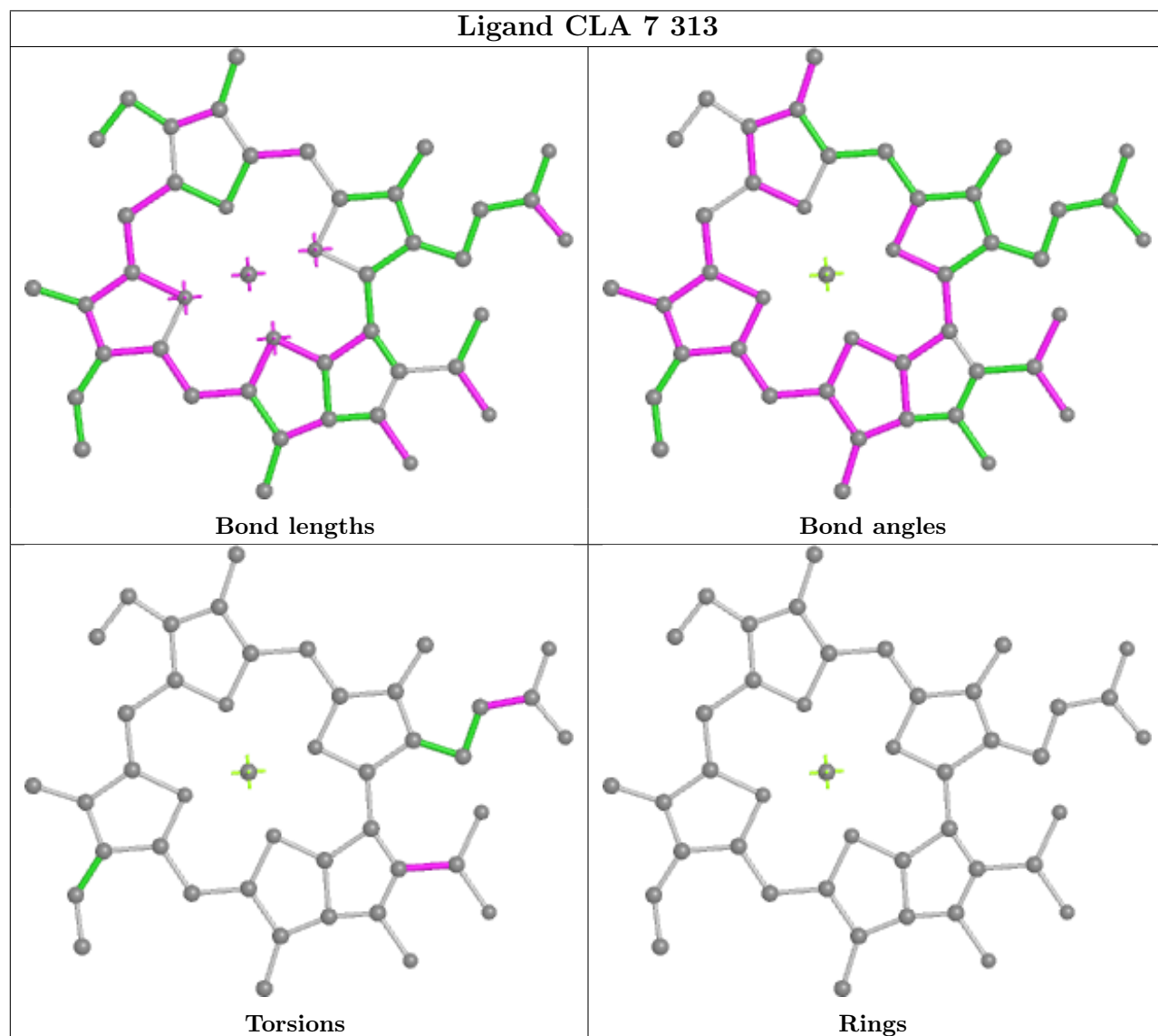
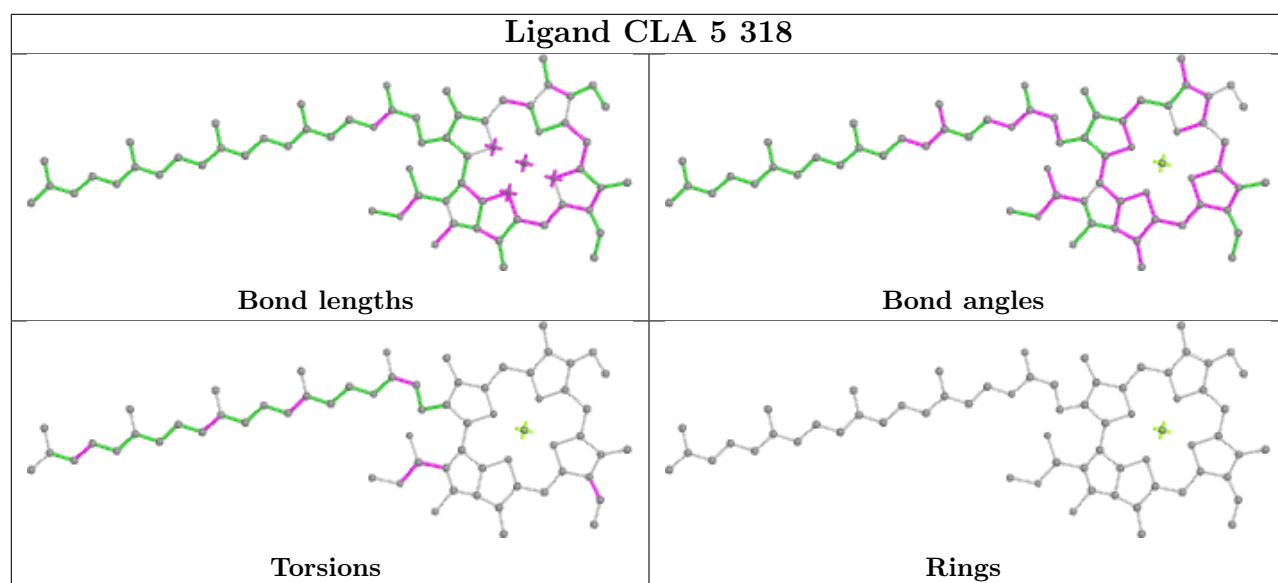


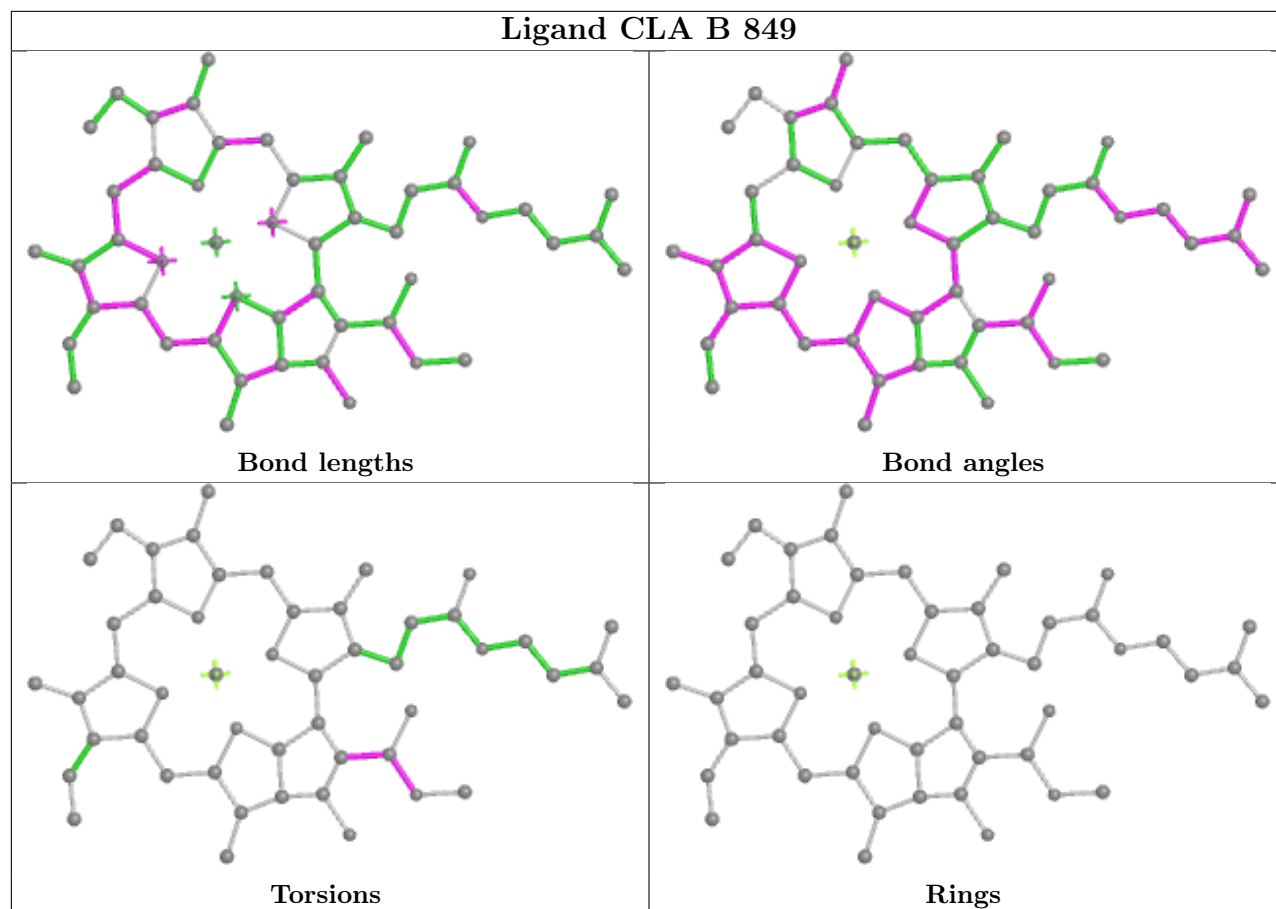
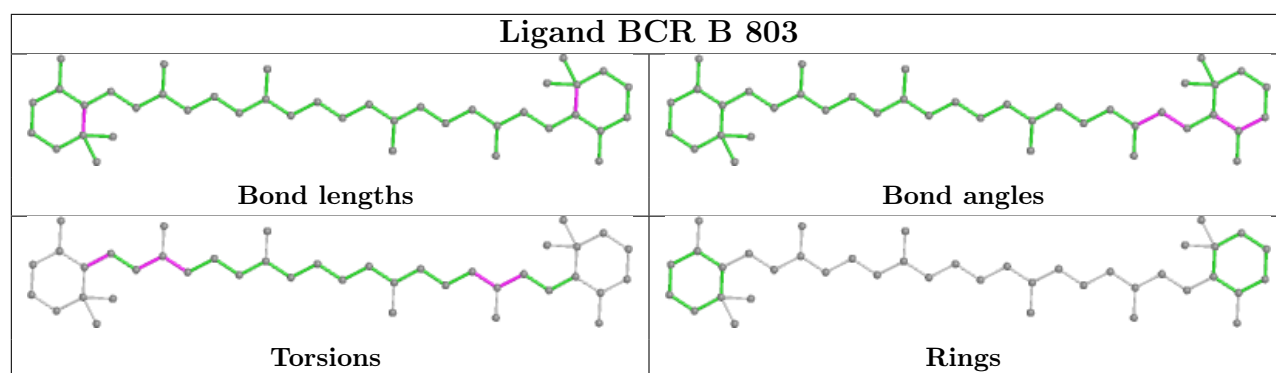


Ligand CLA B 816	
	Bond lengths
	Bond angles
	Torsions
	Rings

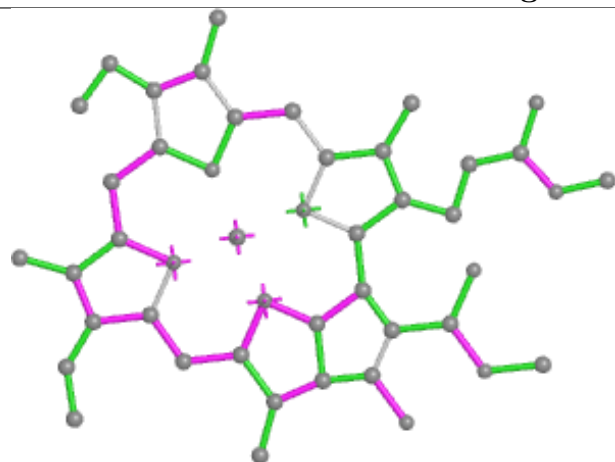
Ligand LUT 3 305	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR L 301	
	Bond lengths
	Bond angles
	Torsions
	Rings

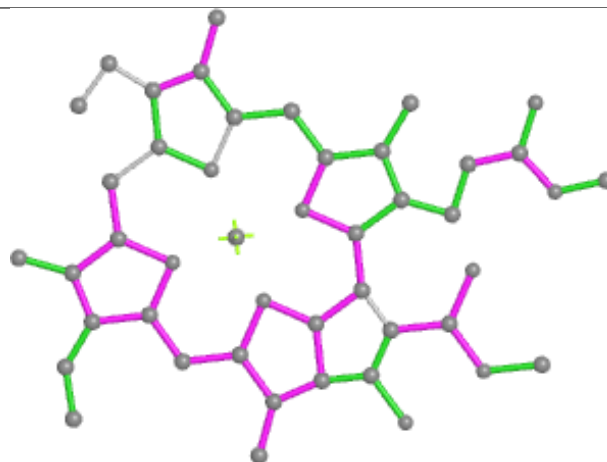




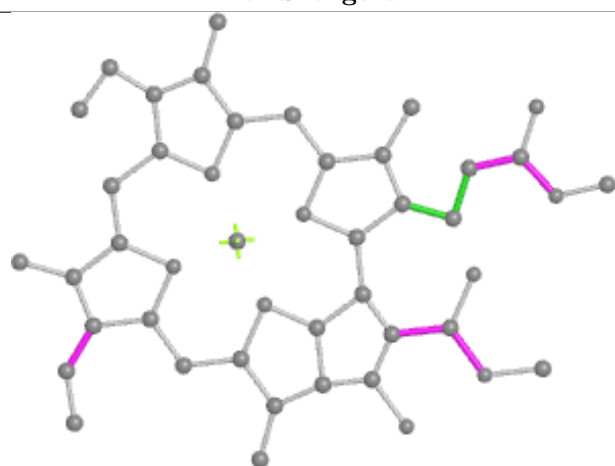
Ligand CLA 2 313



Bond lengths



Bond angles

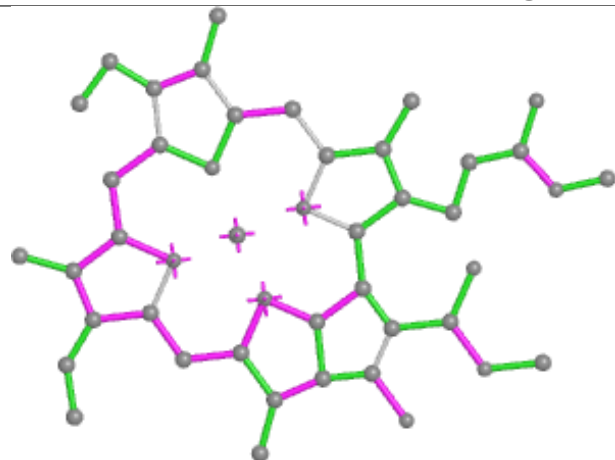


Torsions

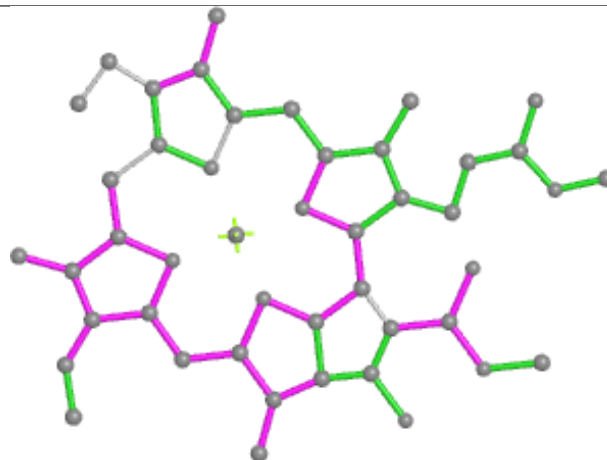


Rings

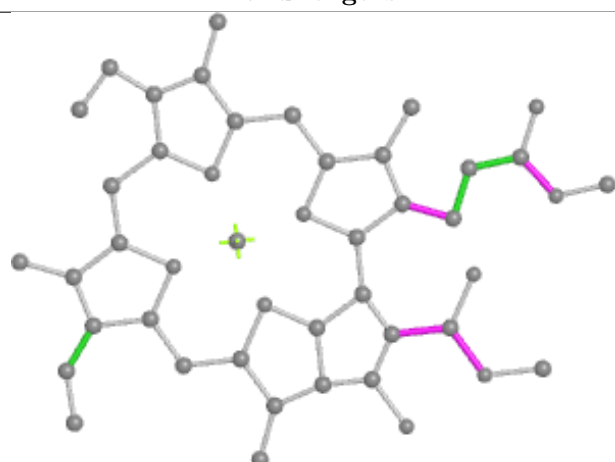
Ligand CLA 8 313



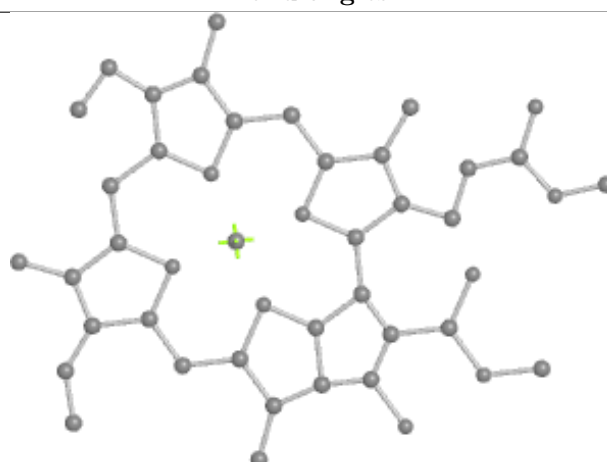
Bond lengths



Bond angles

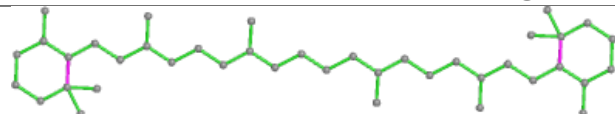


Torsions

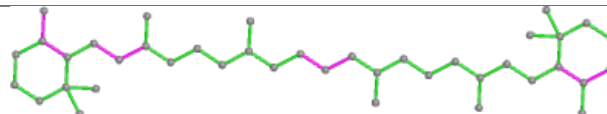


Rings

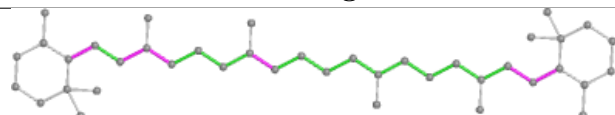
Ligand BCR 3 302



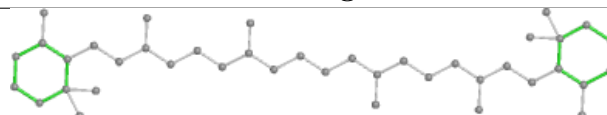
Bond lengths



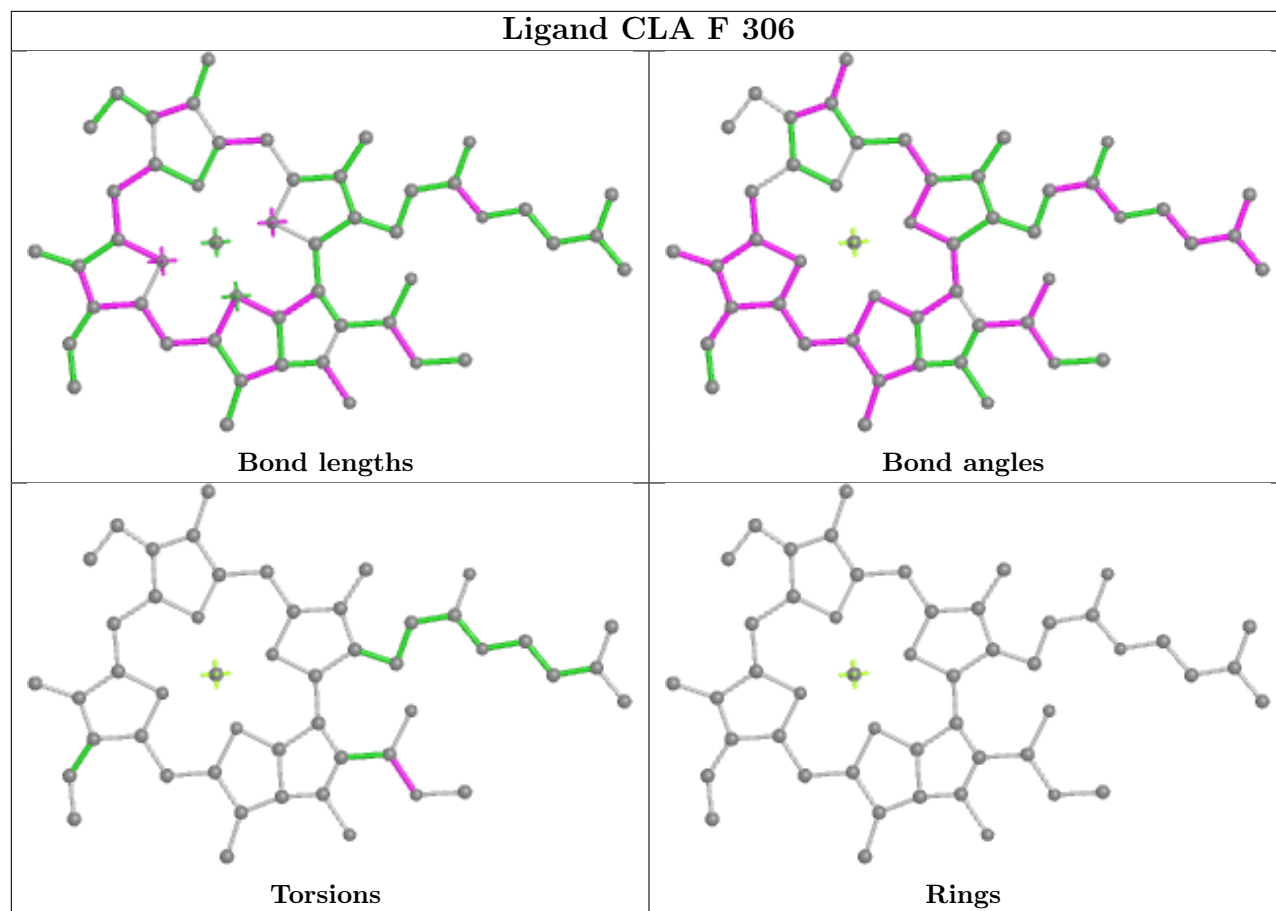
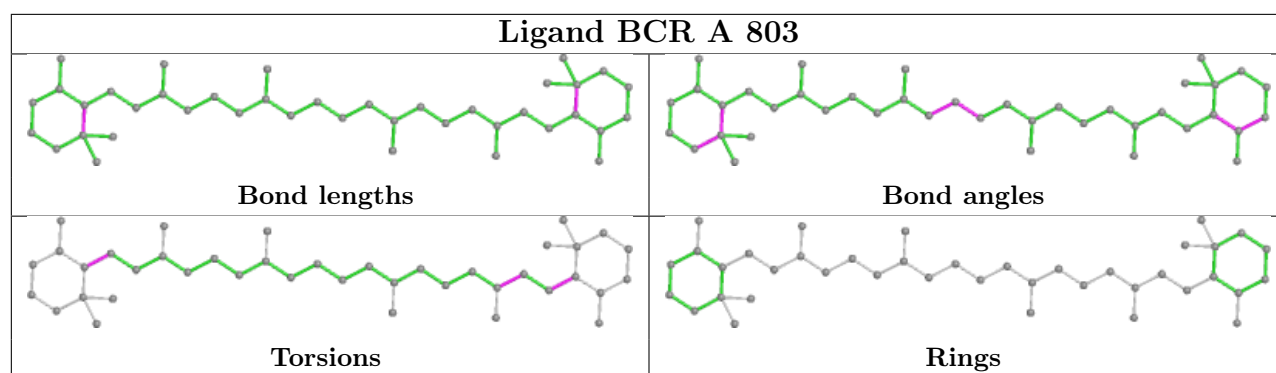
Bond angles

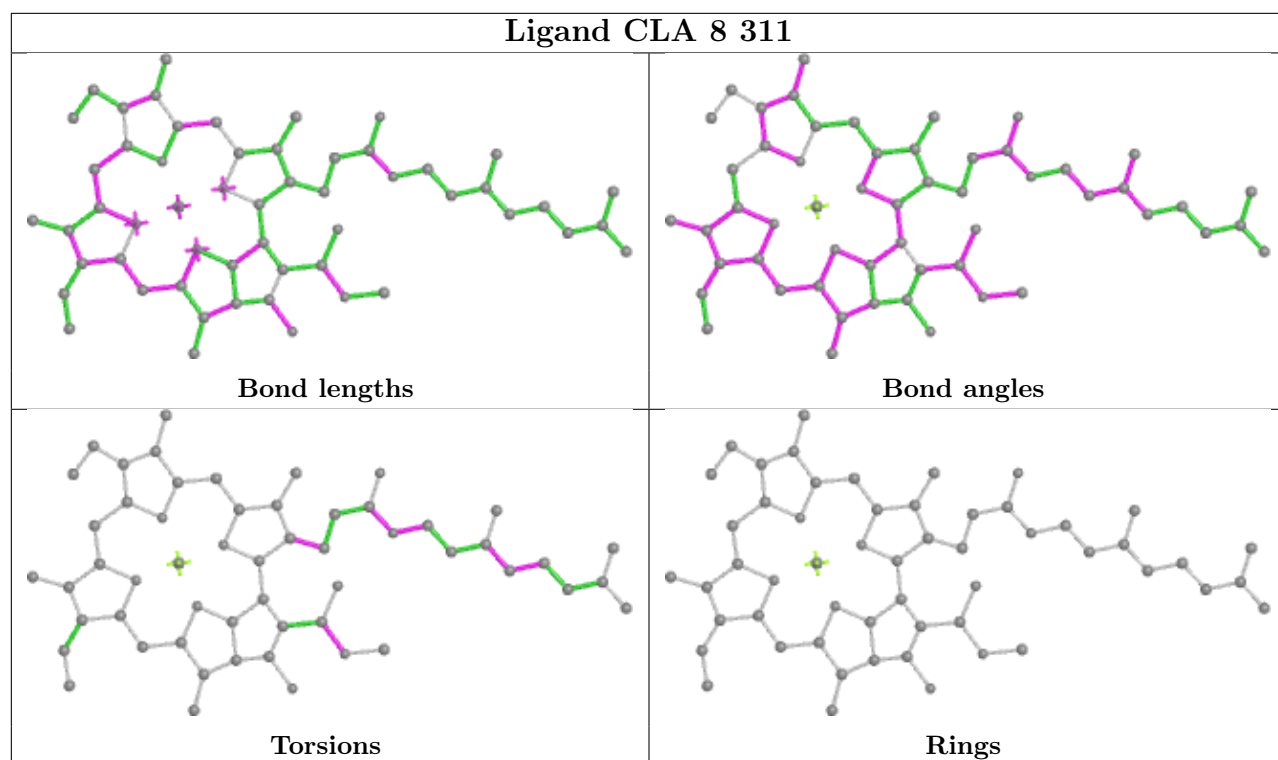
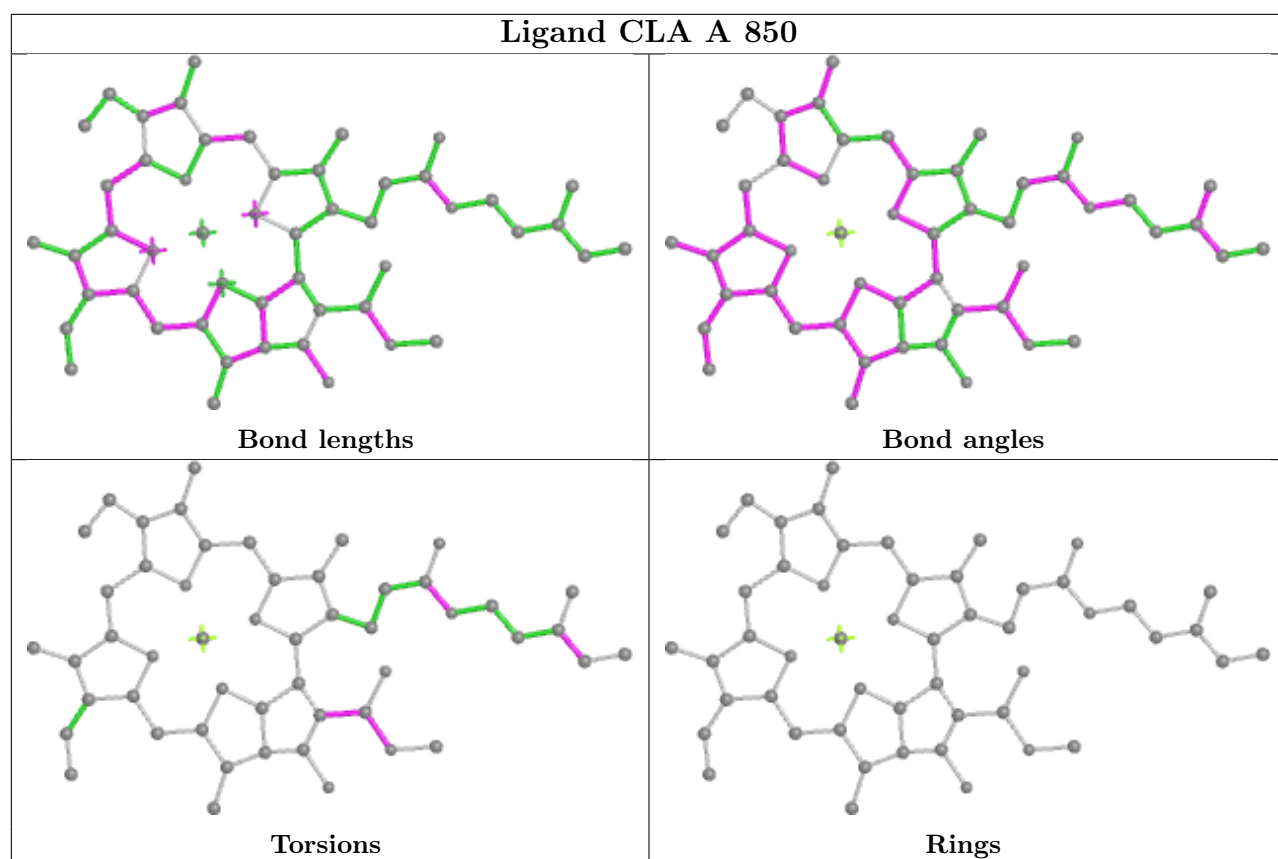


Torsions

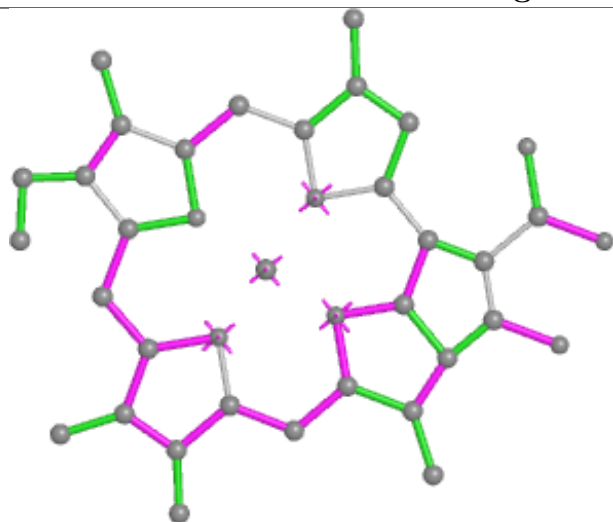


Rings

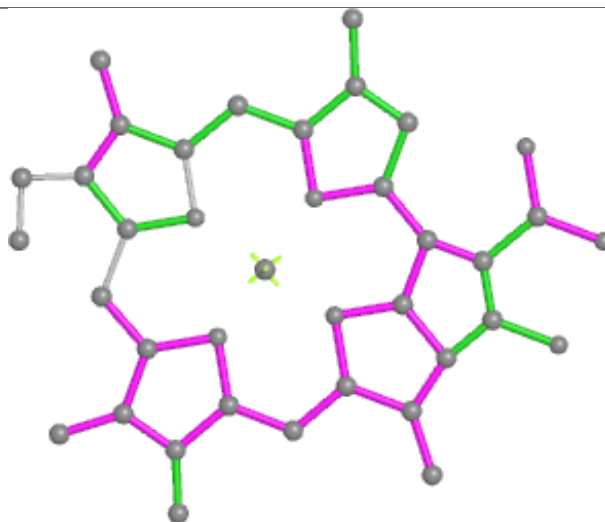




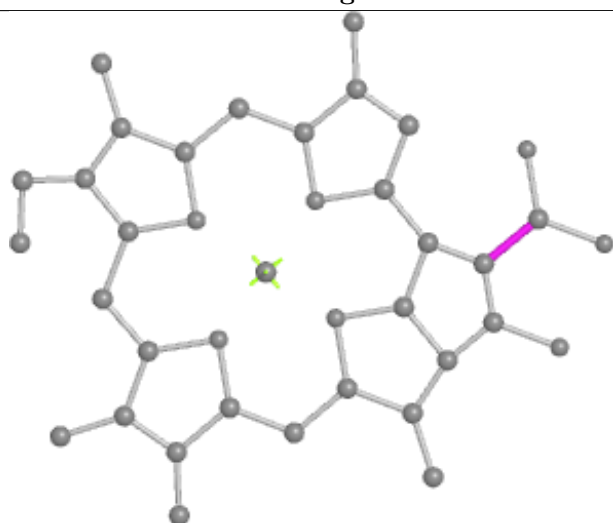
Ligand CLA O 202



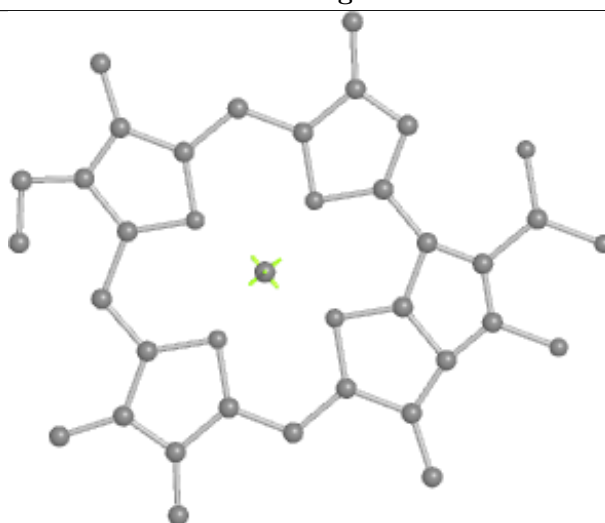
Bond lengths



Bond angles

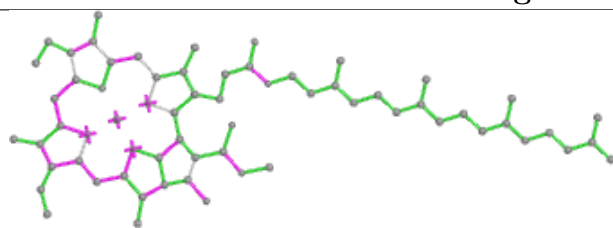


Torsions

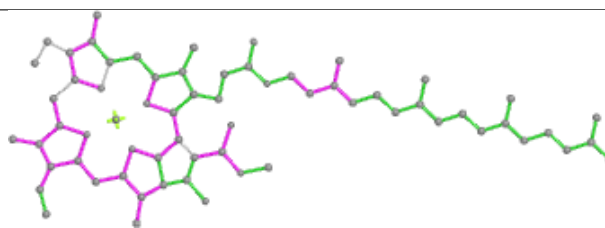


Rings

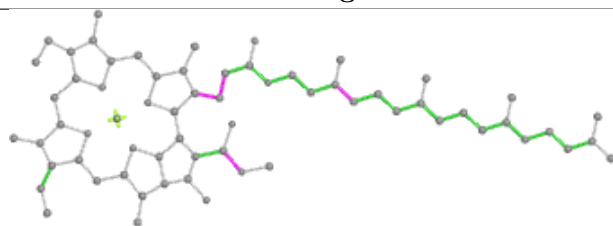
Ligand CLA A 856



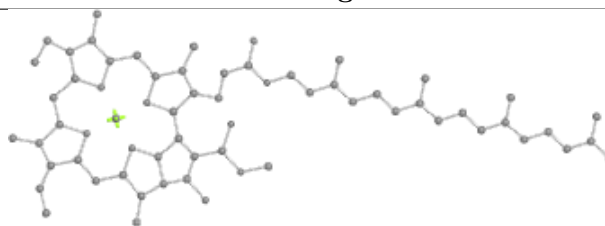
Bond lengths



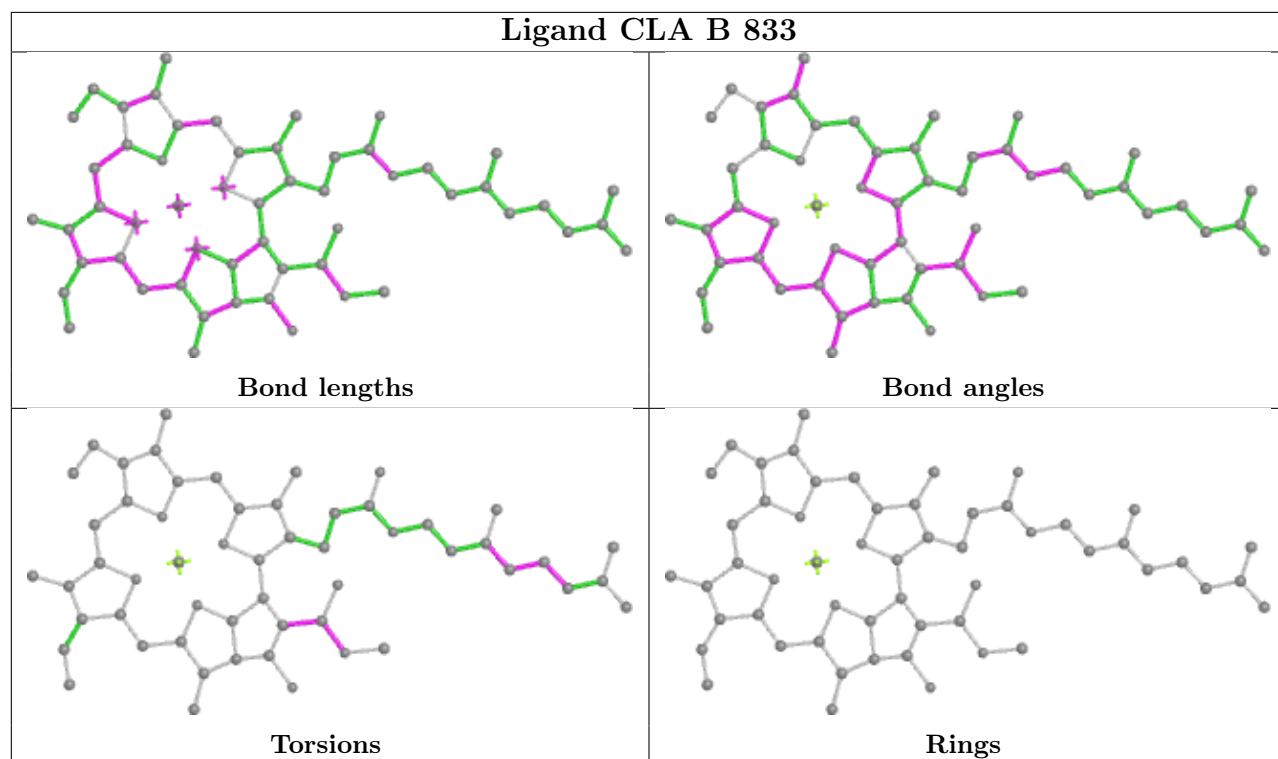
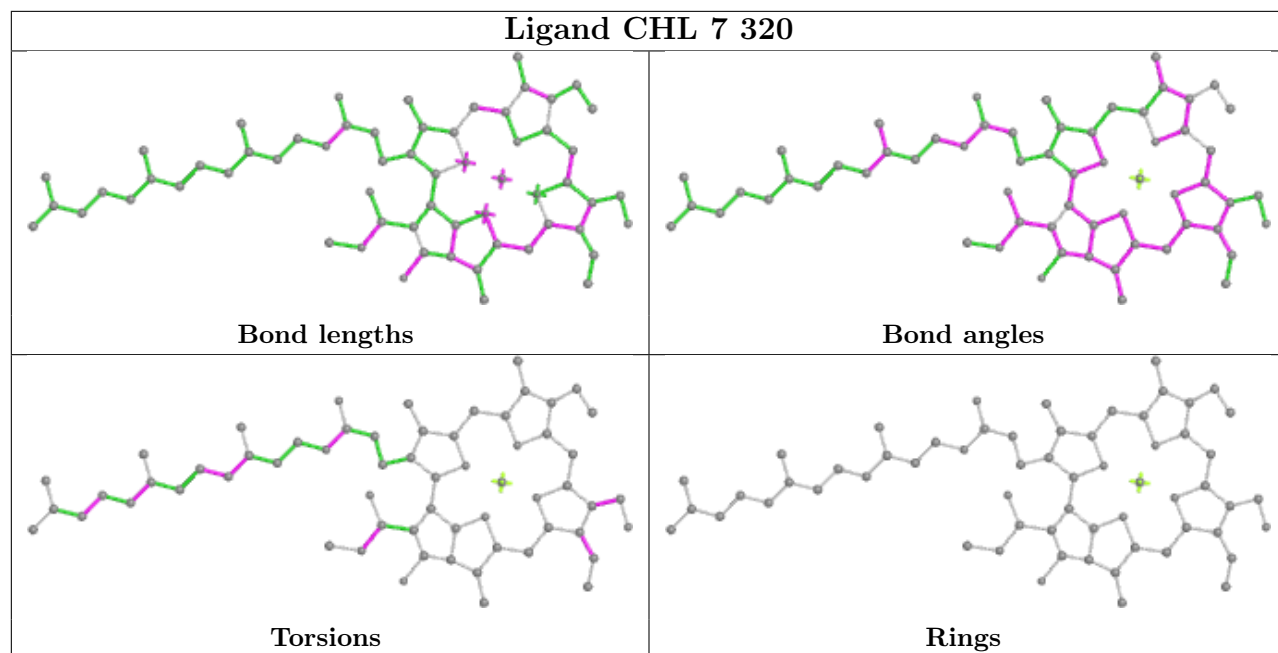
Bond angles



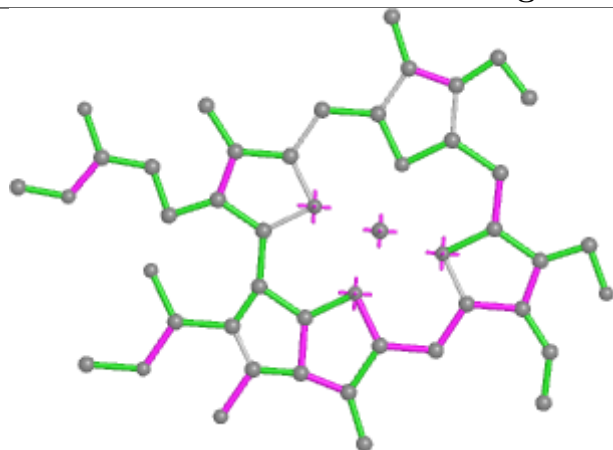
Torsions



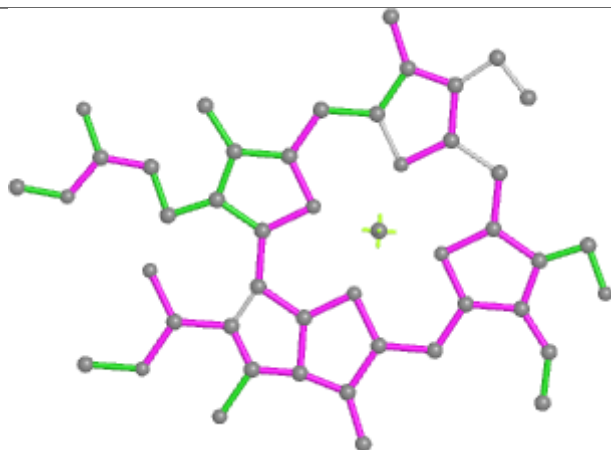
Rings



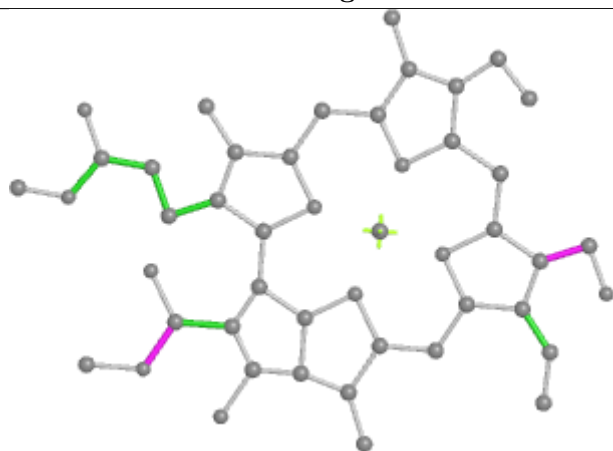
Ligand CHL 9 322



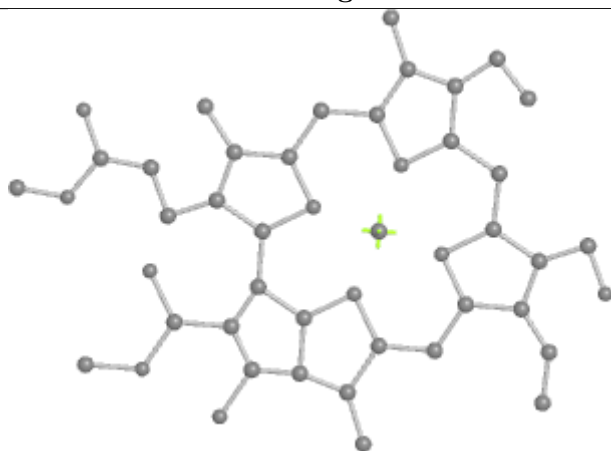
Bond lengths



Bond angles

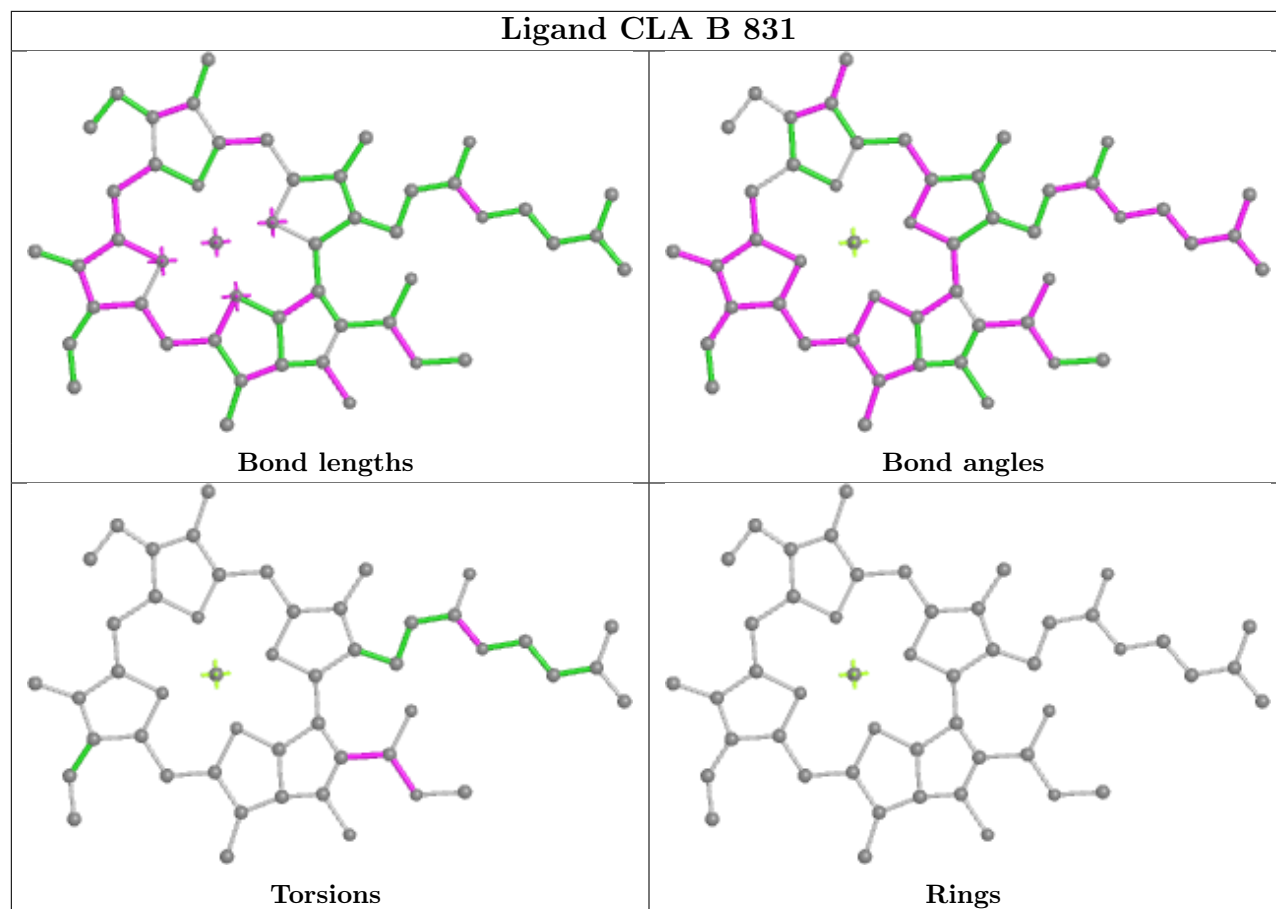


Torsions

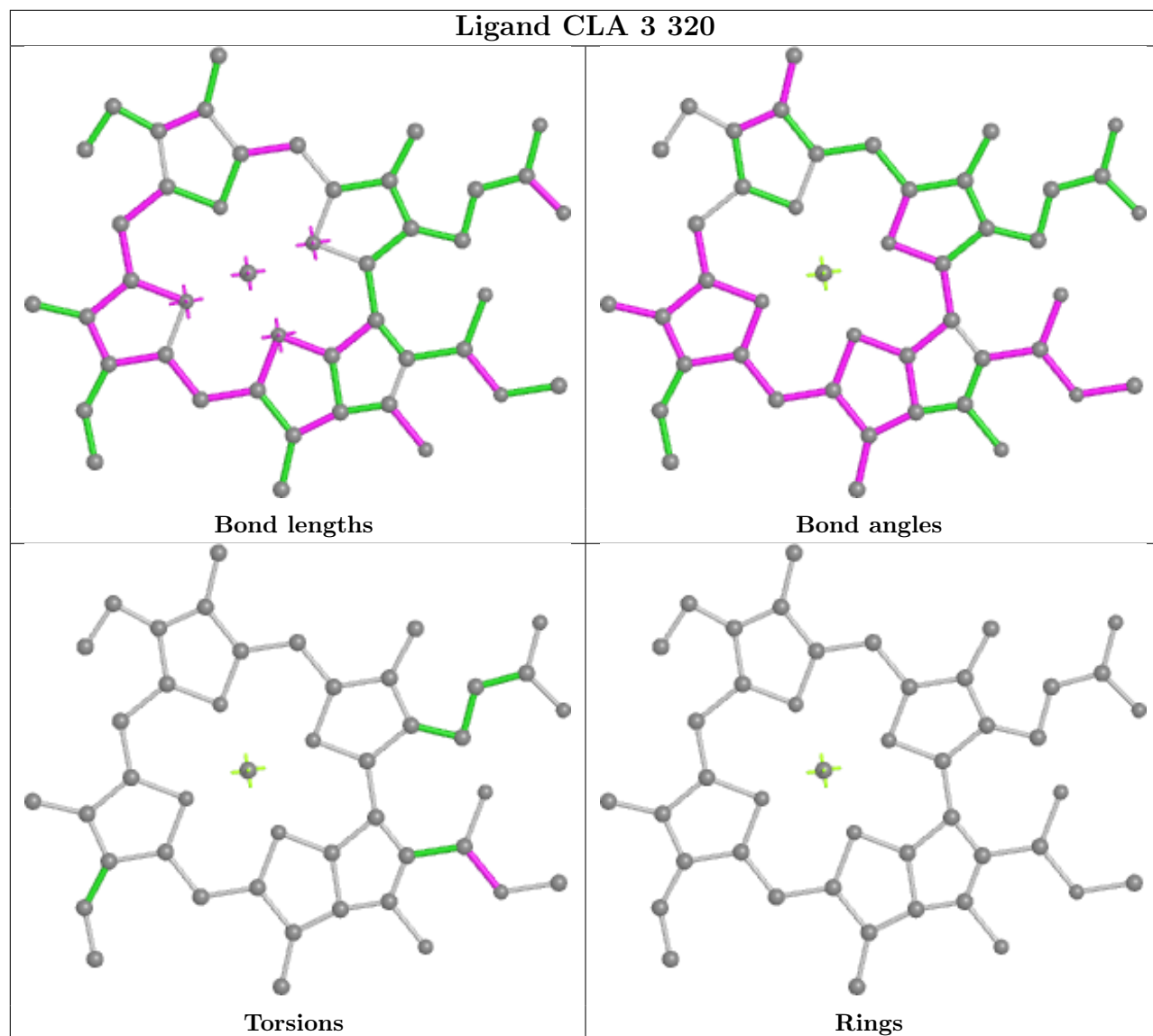


Rings

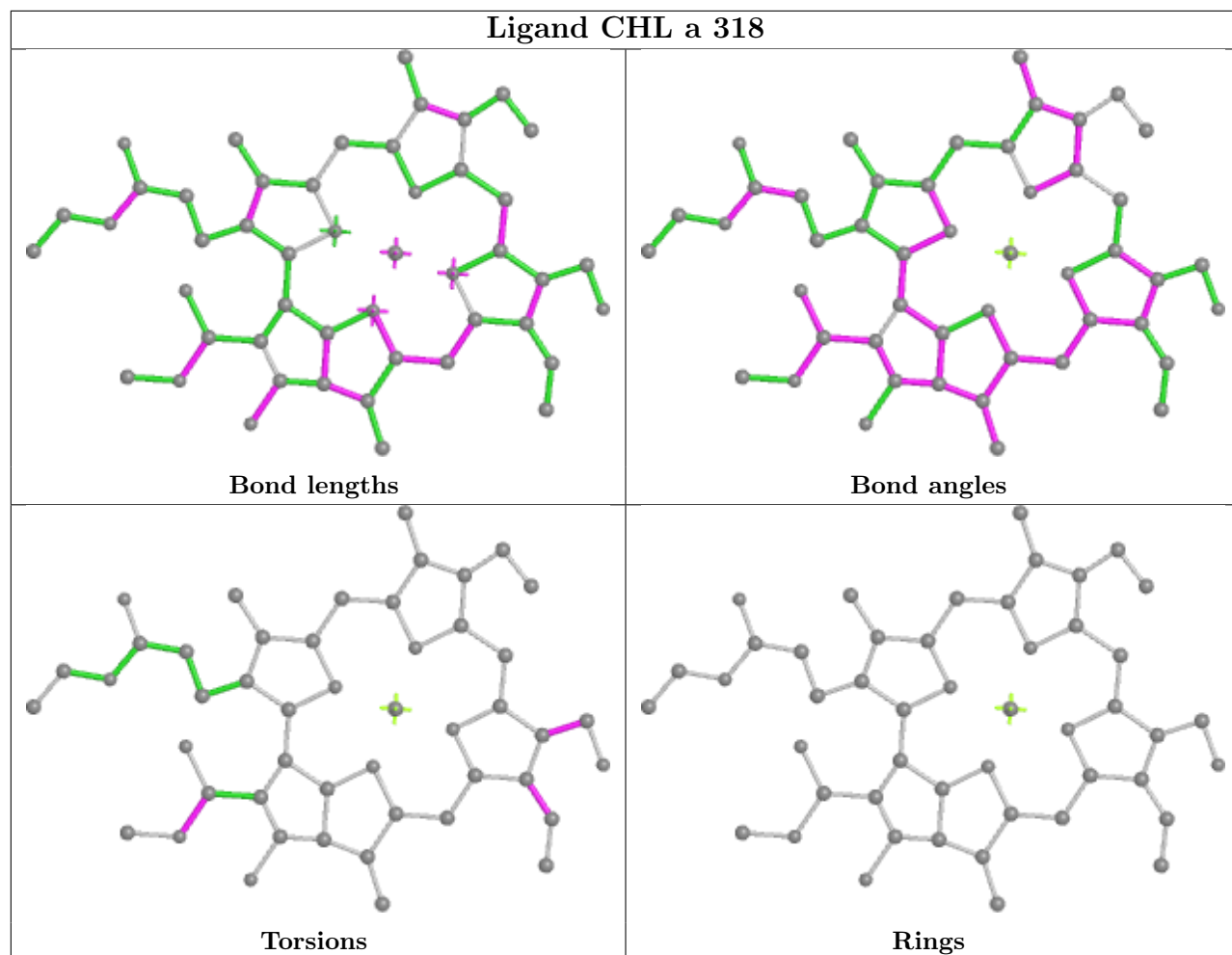
Ligand CLA B 831



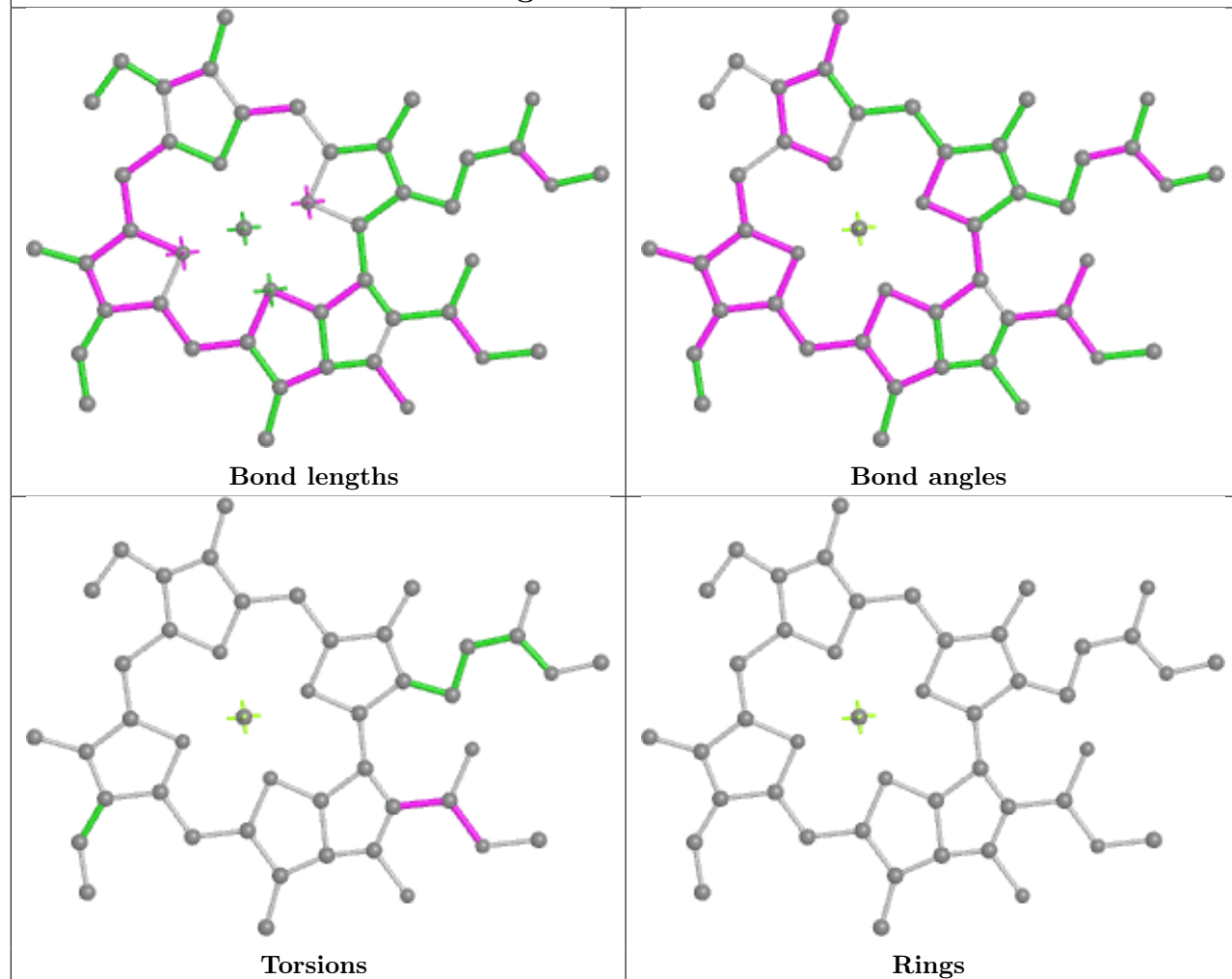
Ligand CLA 3 320



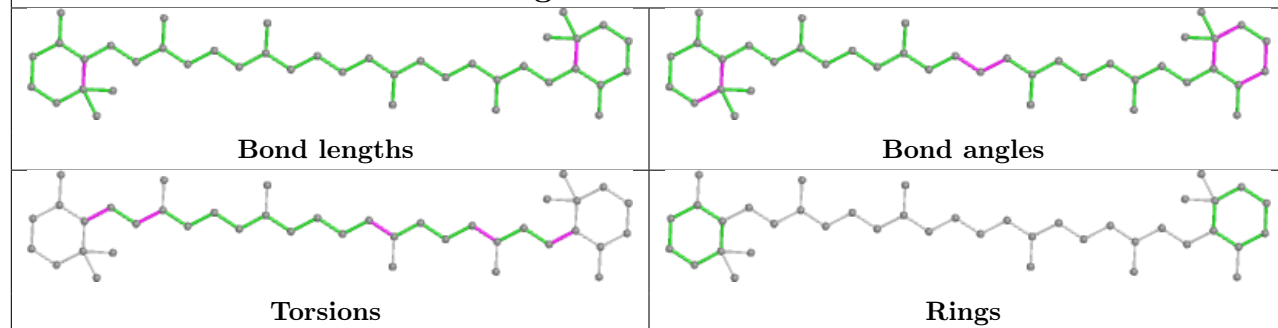
Ligand CHL a 318

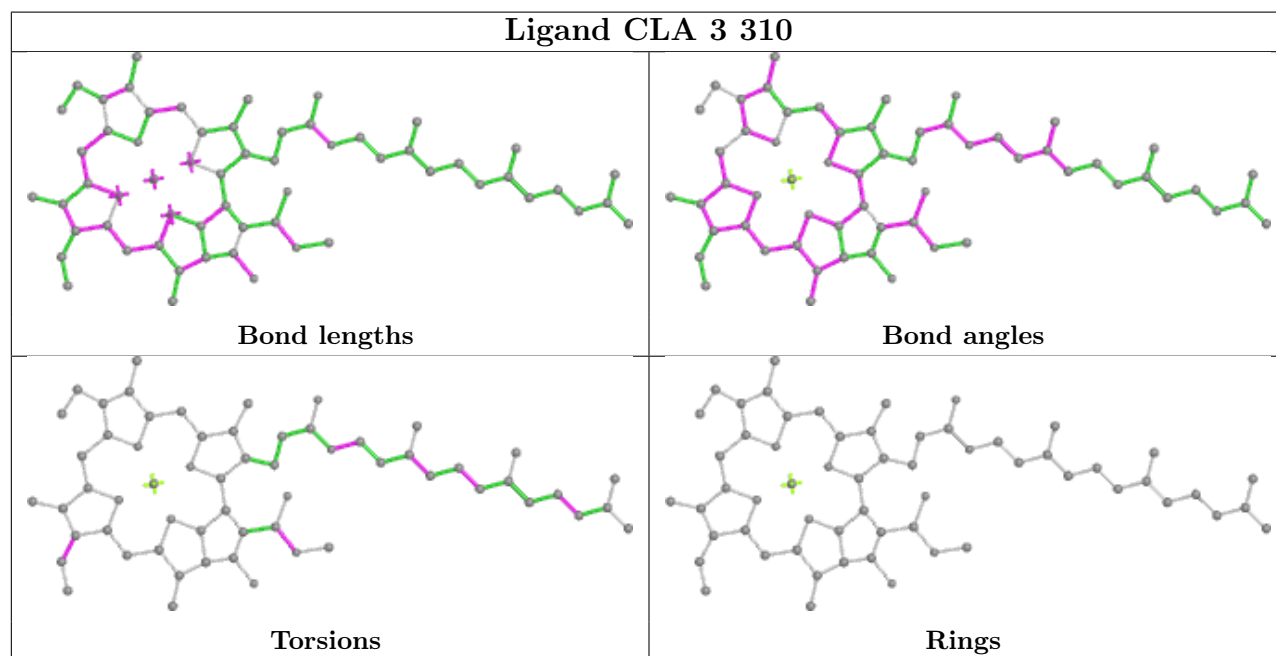
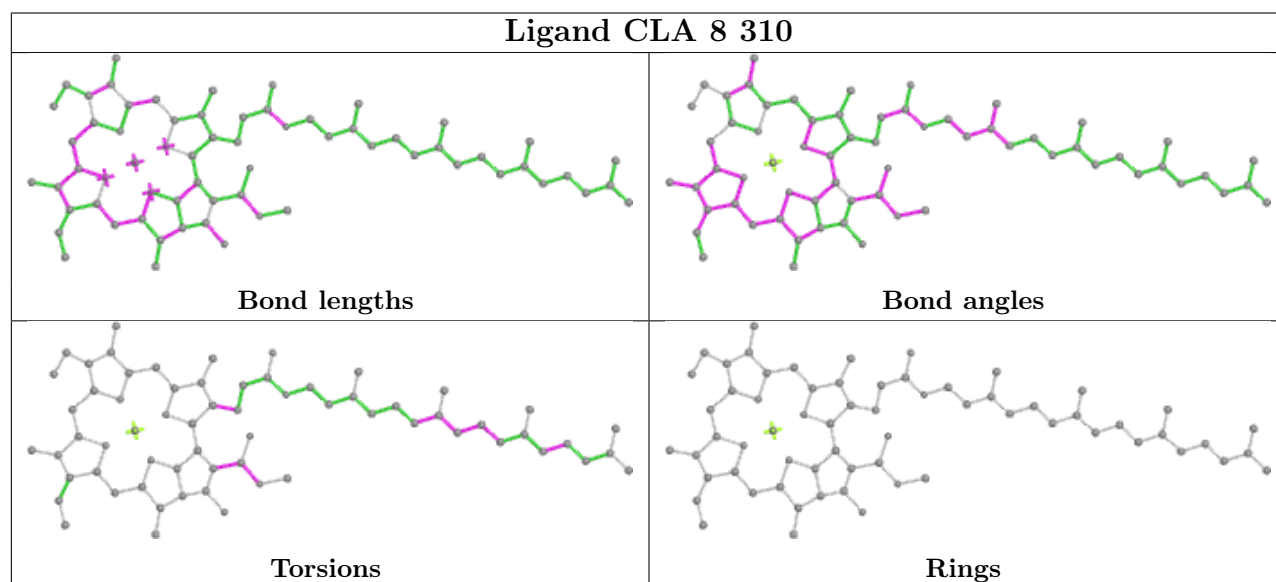
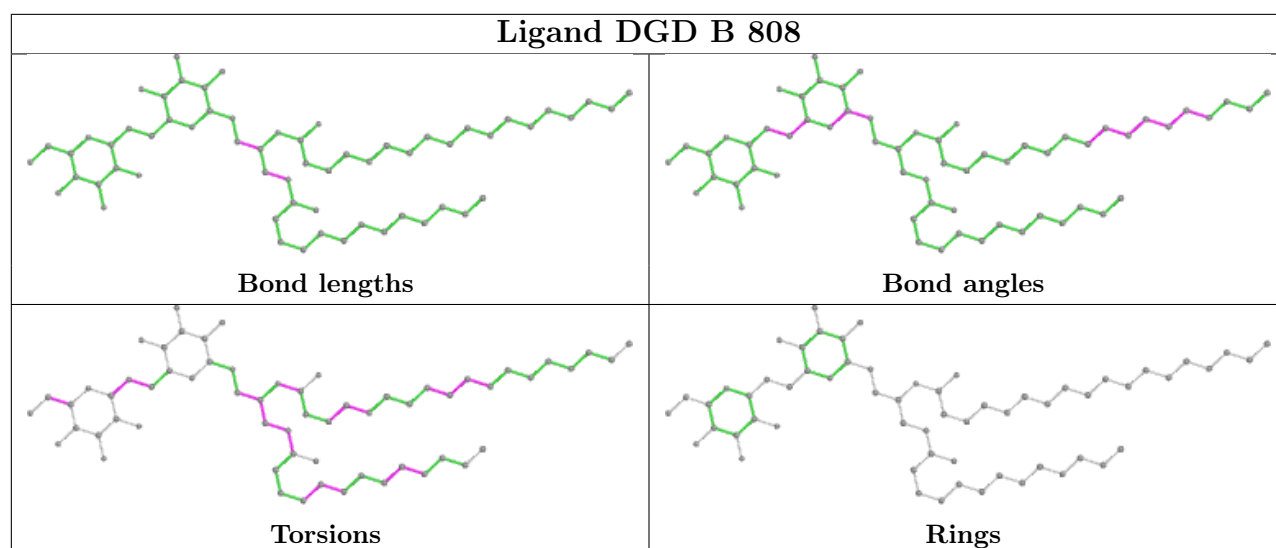


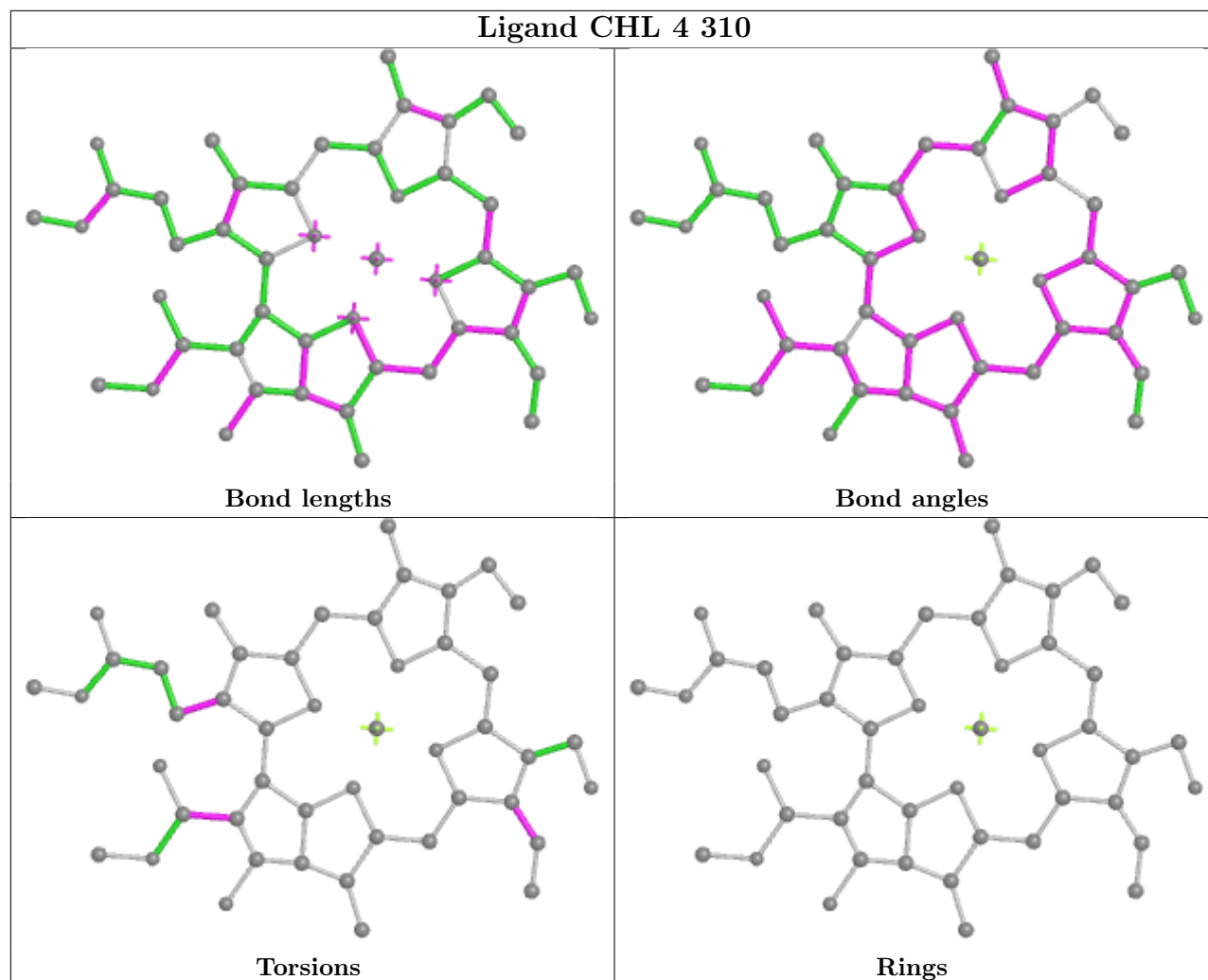
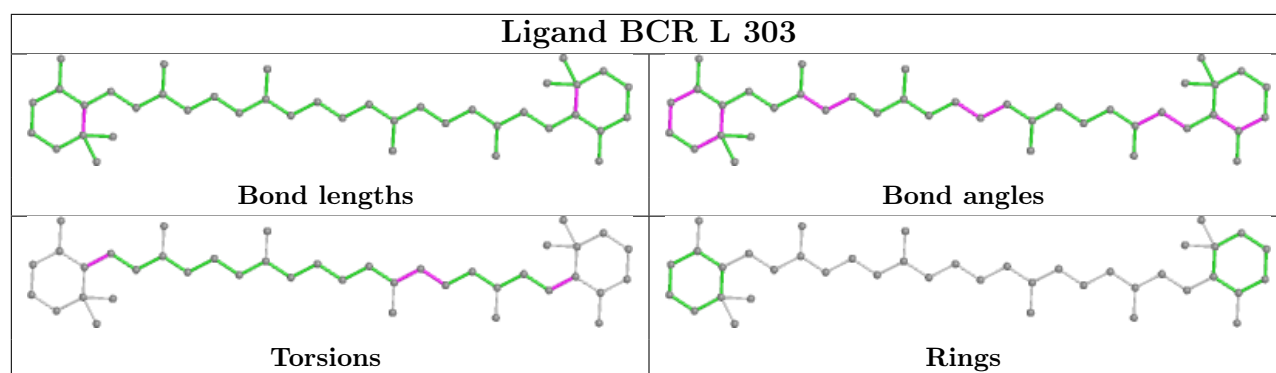
Ligand CLA 8 307



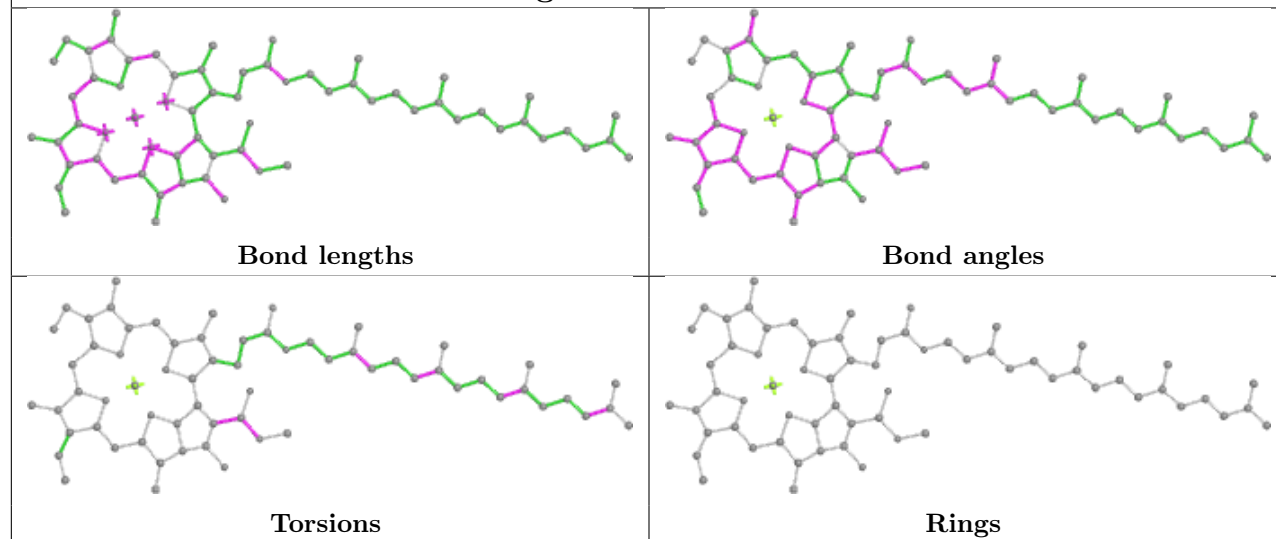
Ligand BCR 7 304



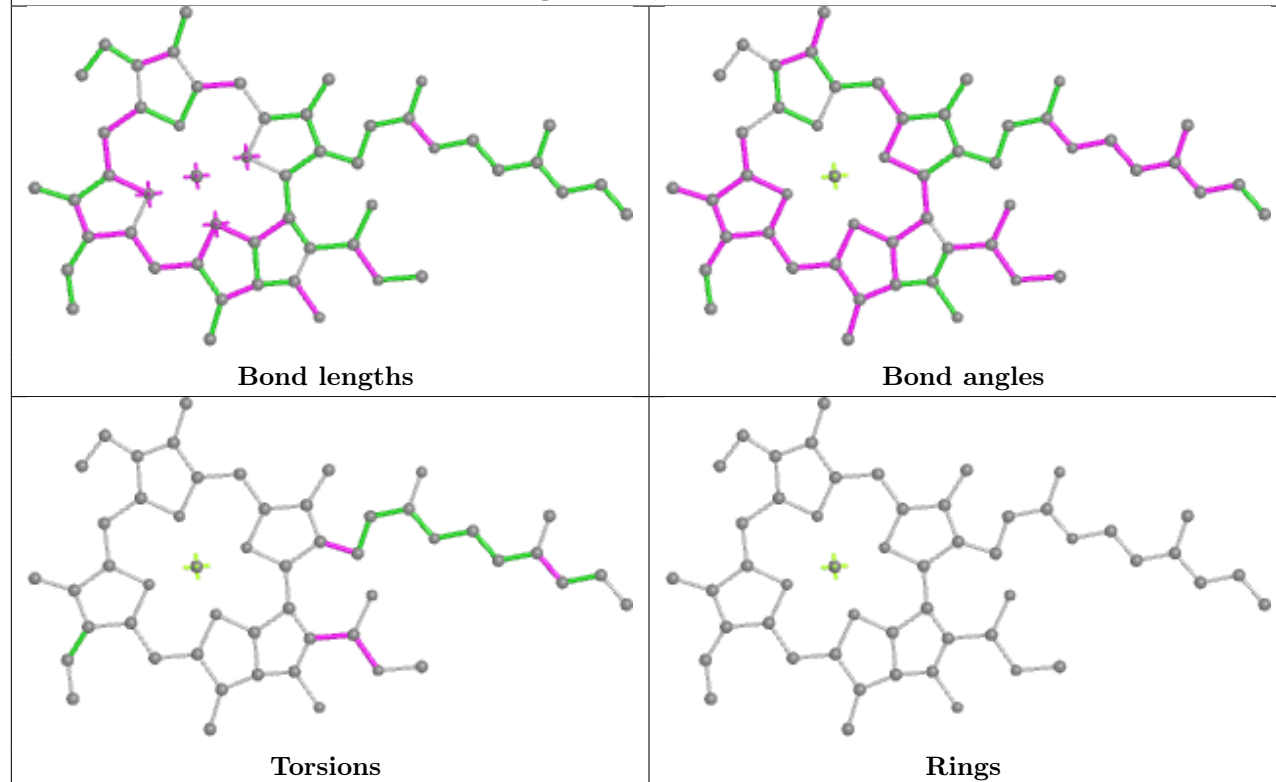




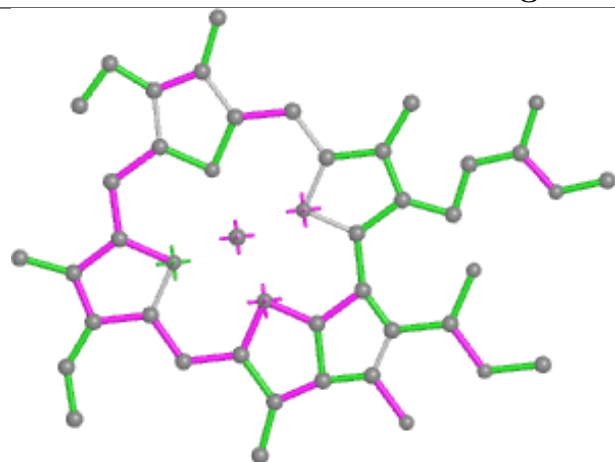
Ligand CLA 6 312



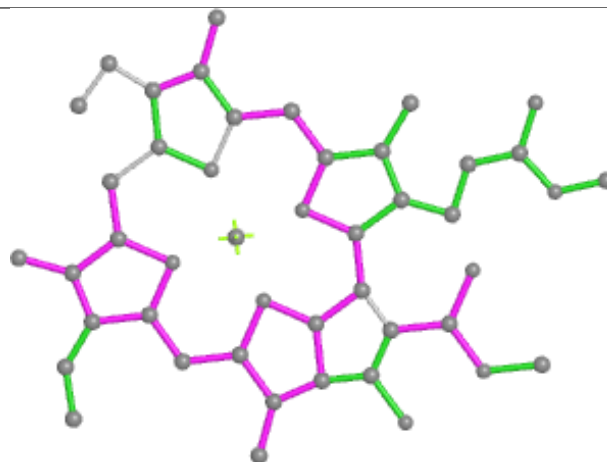
Ligand CLA 8 315



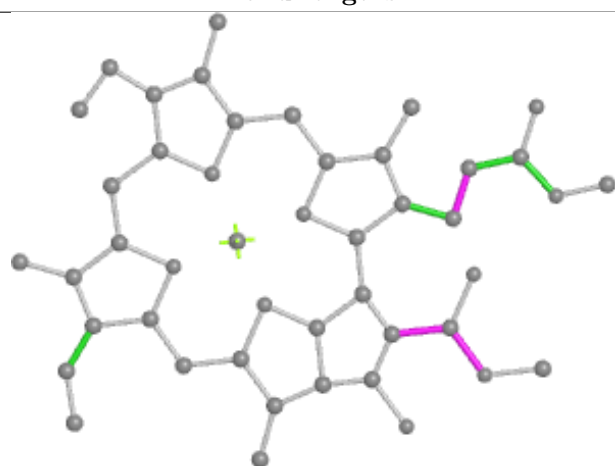
Ligand CLA 2 312



Bond lengths



Bond angles

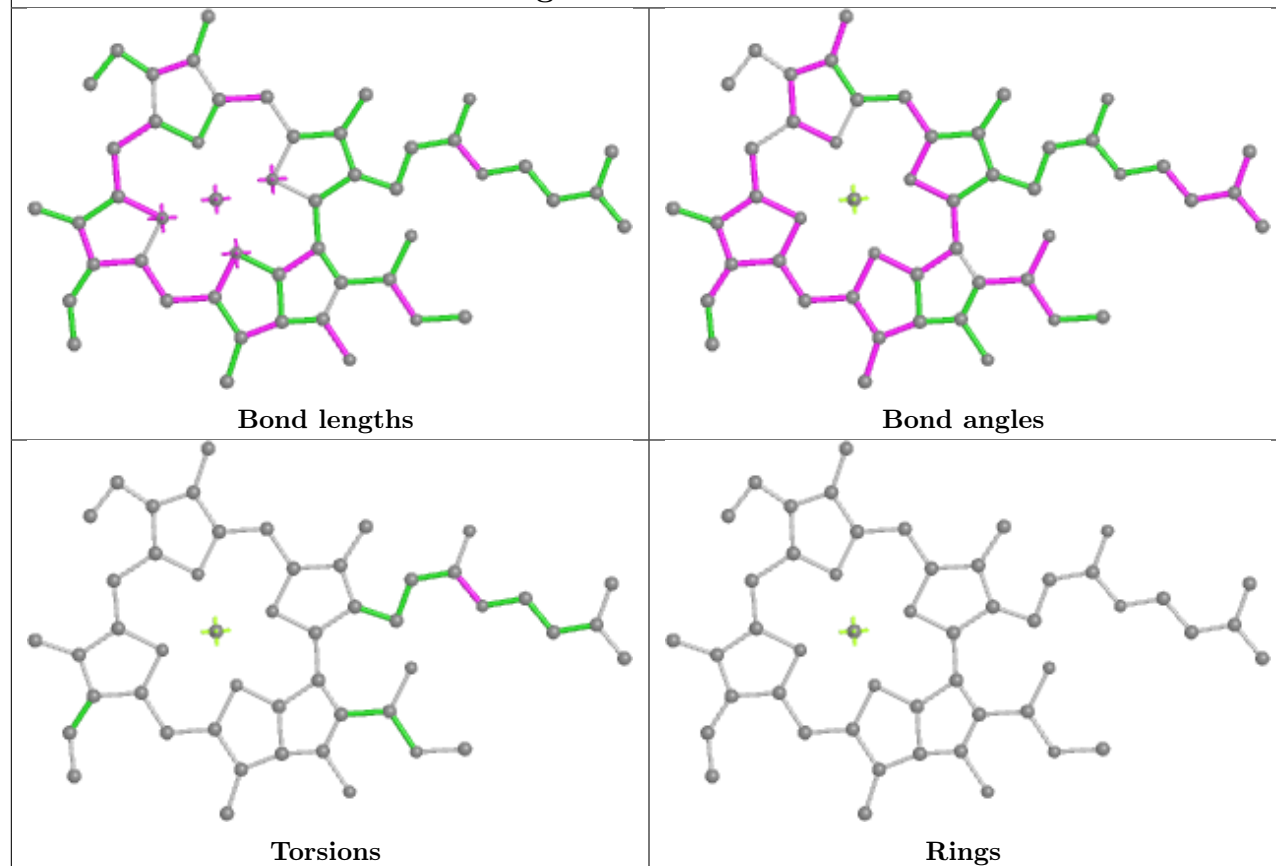


Torsions

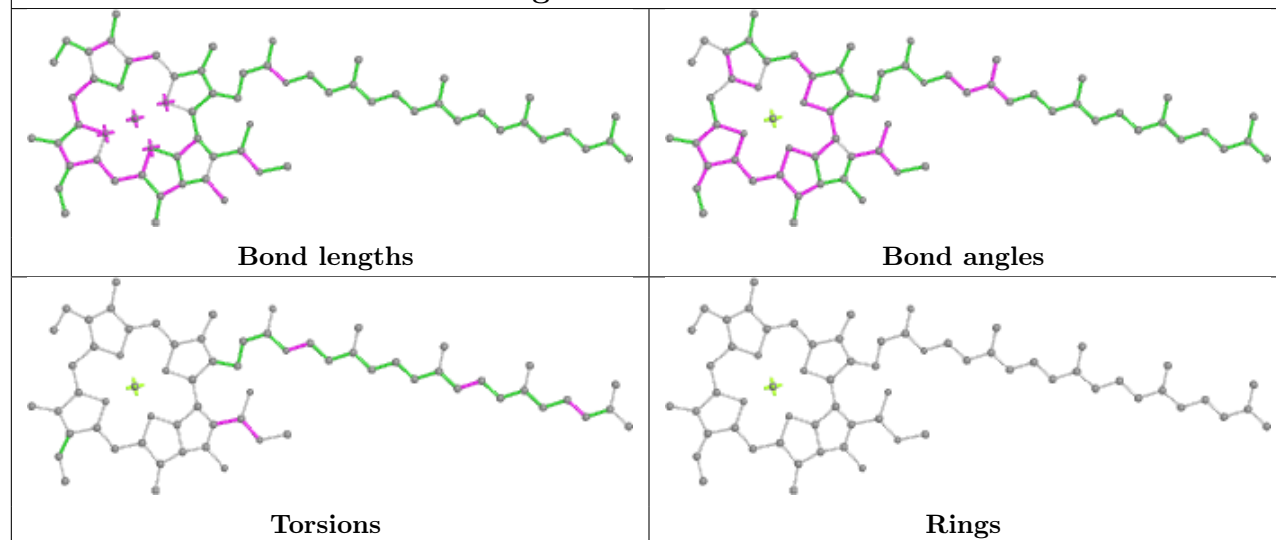


Rings

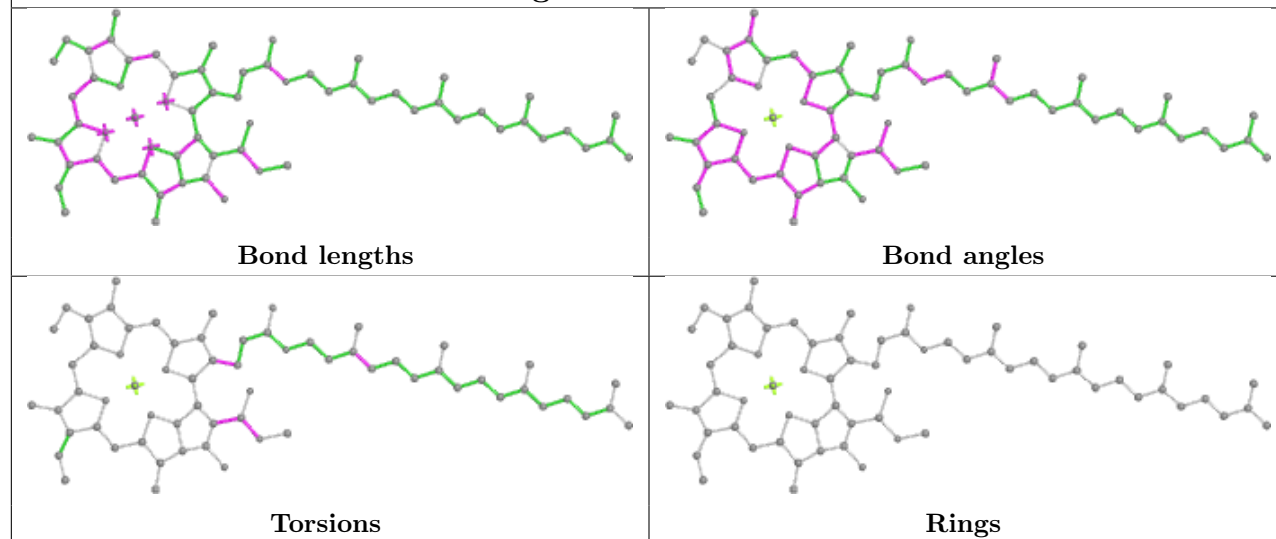
Ligand CLA 8 318



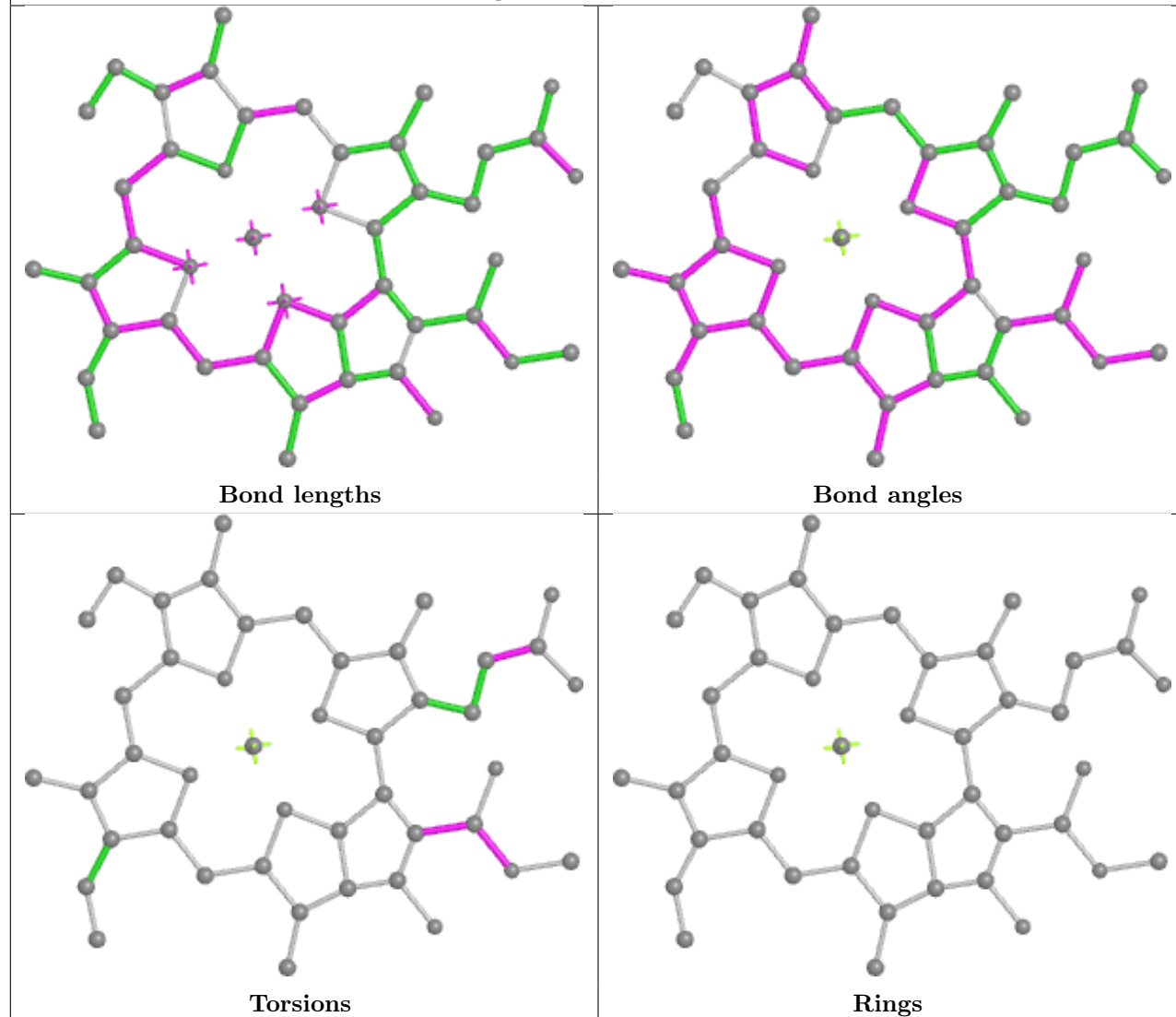
Ligand CLA B 811

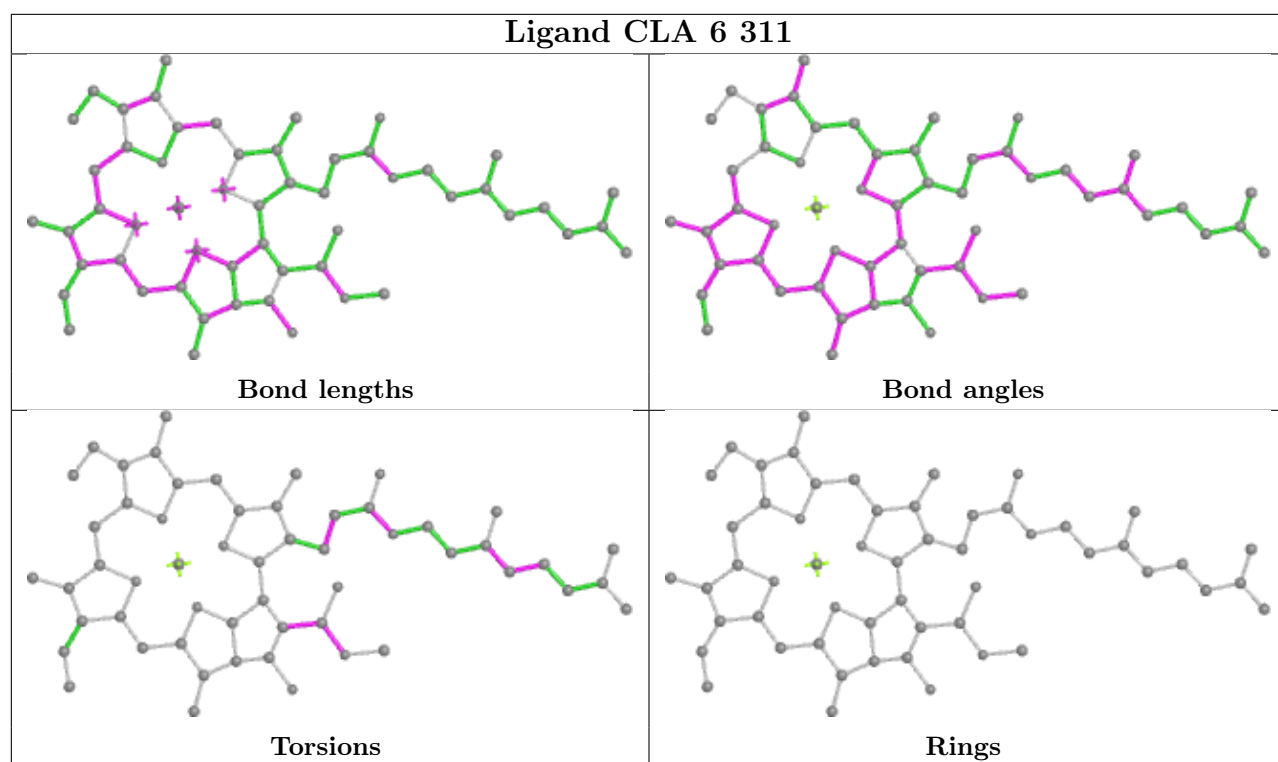


Ligand CLA B 836

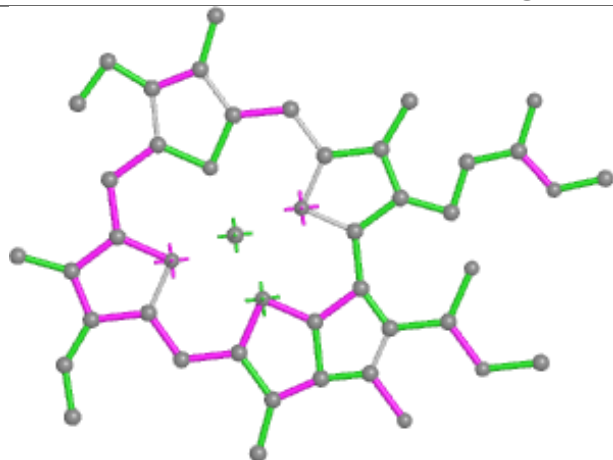


Ligand CLA B 843

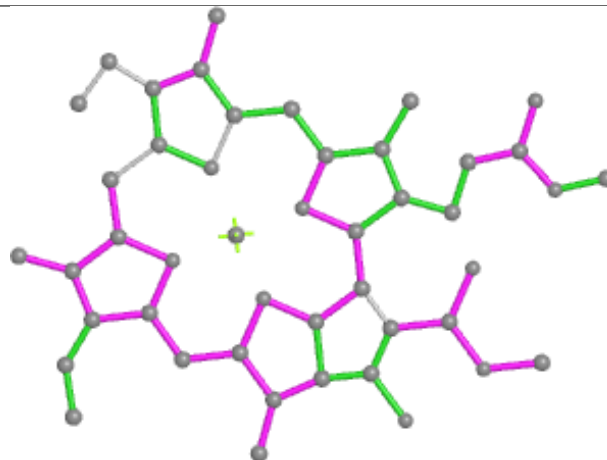




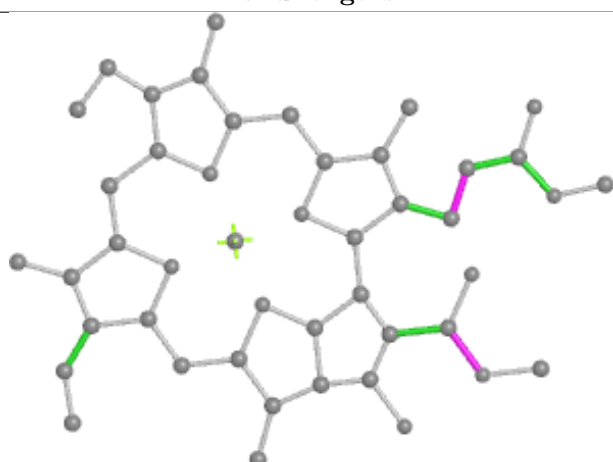
Ligand CLA 2 308



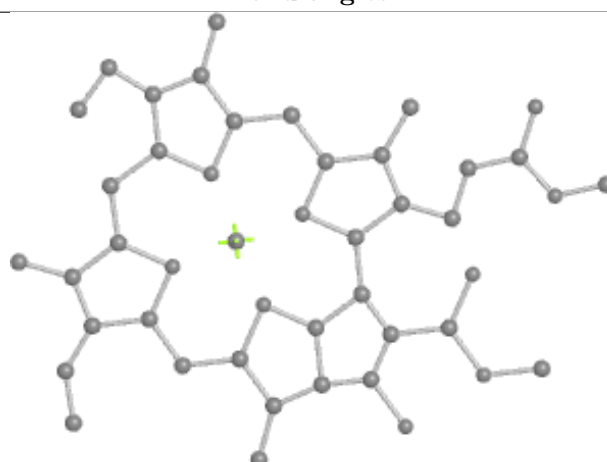
Bond lengths



Bond angles

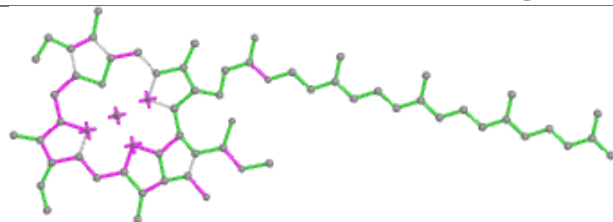


Torsions

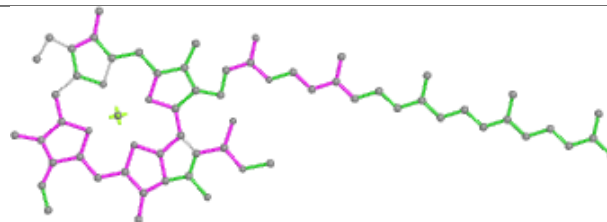


Rings

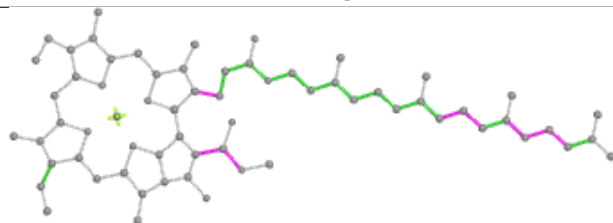
Ligand CLA 3 307



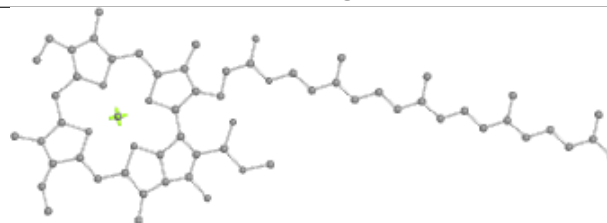
Bond lengths



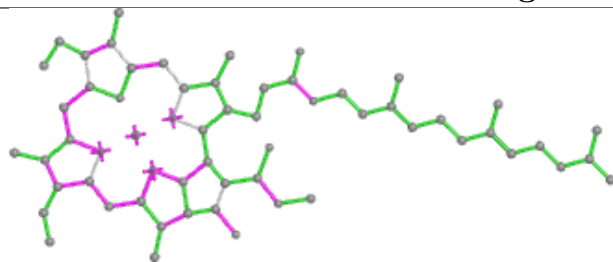
Bond angles



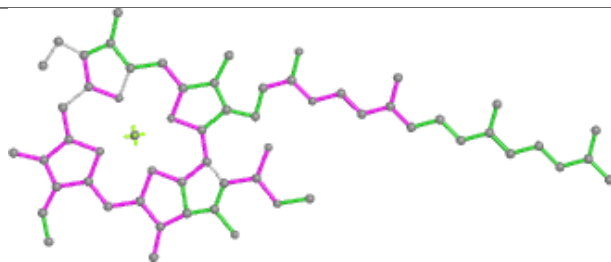
Torsions



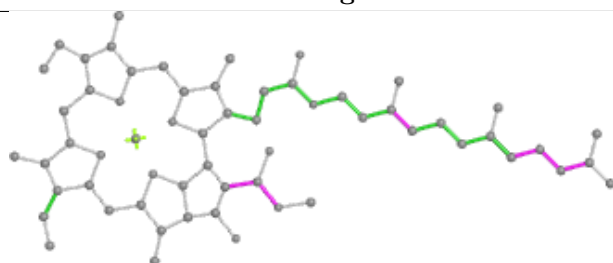
Rings

Ligand CLA a 311

Bond lengths



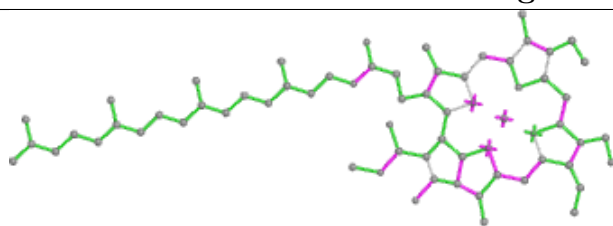
Bond angles



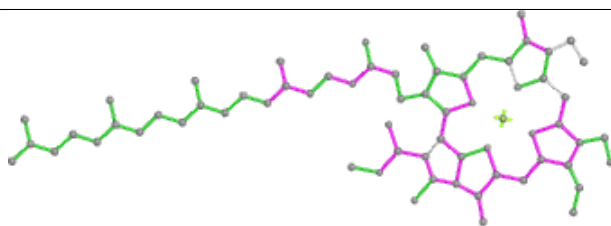
Torsions



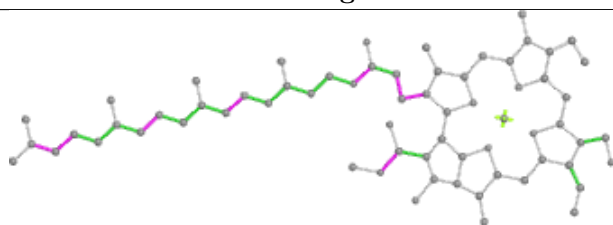
Rings

Ligand CHL 8 316

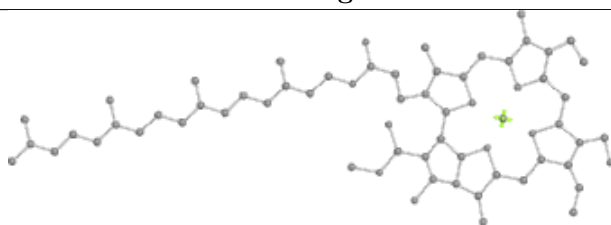
Bond lengths



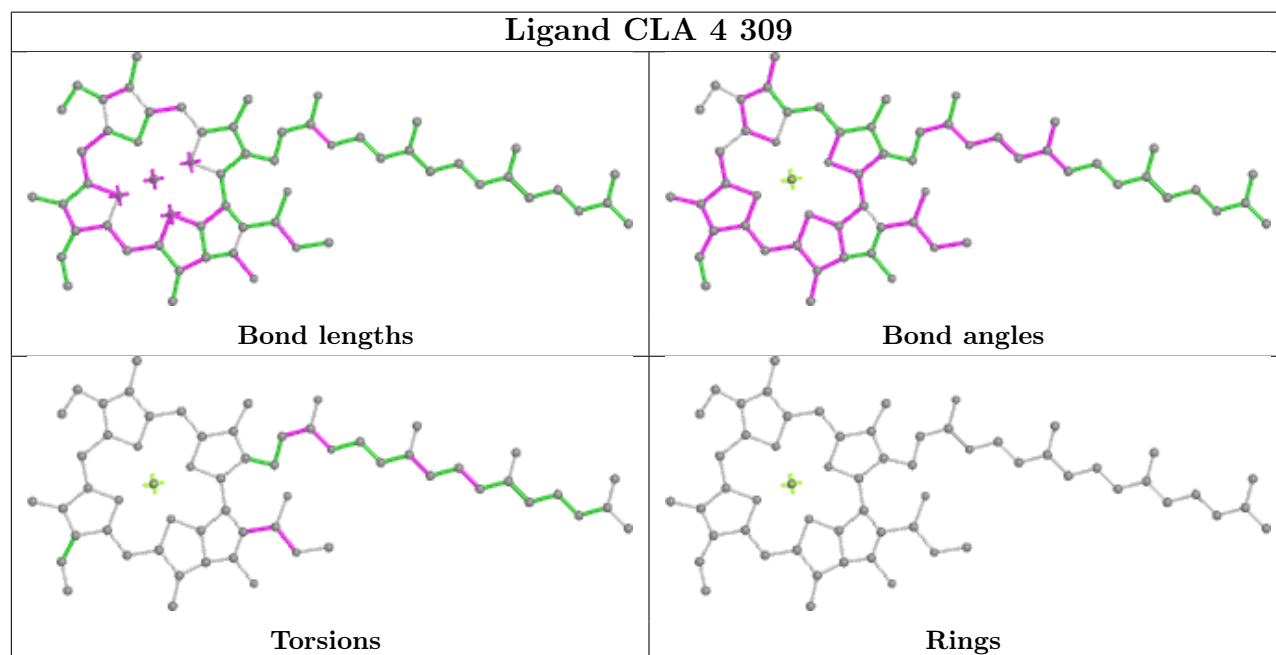
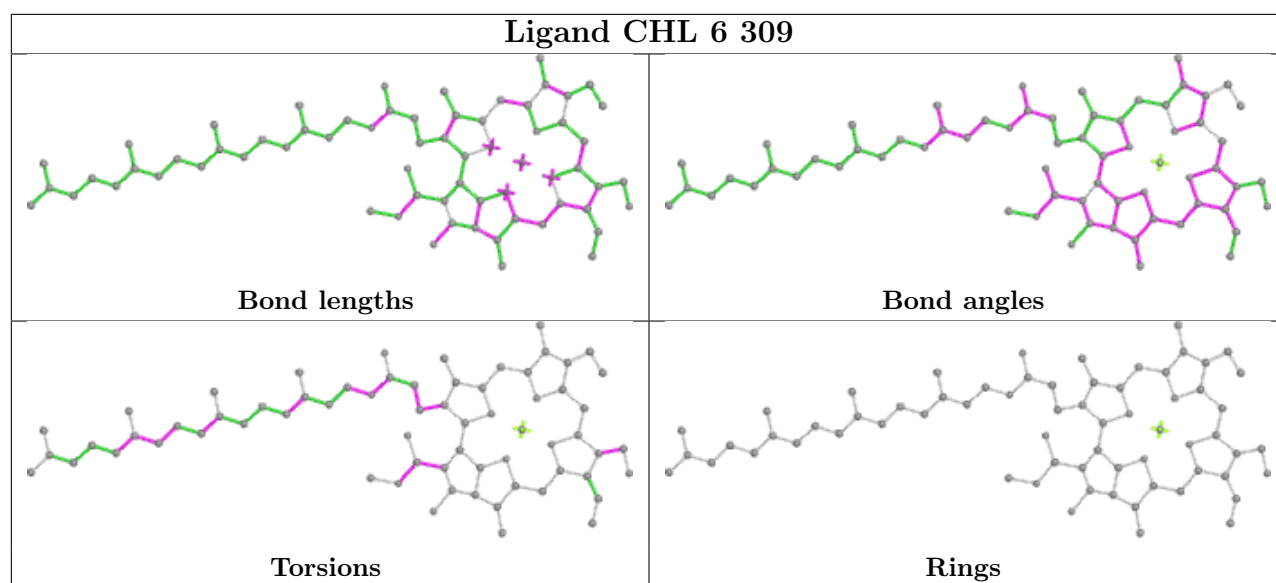
Bond angles



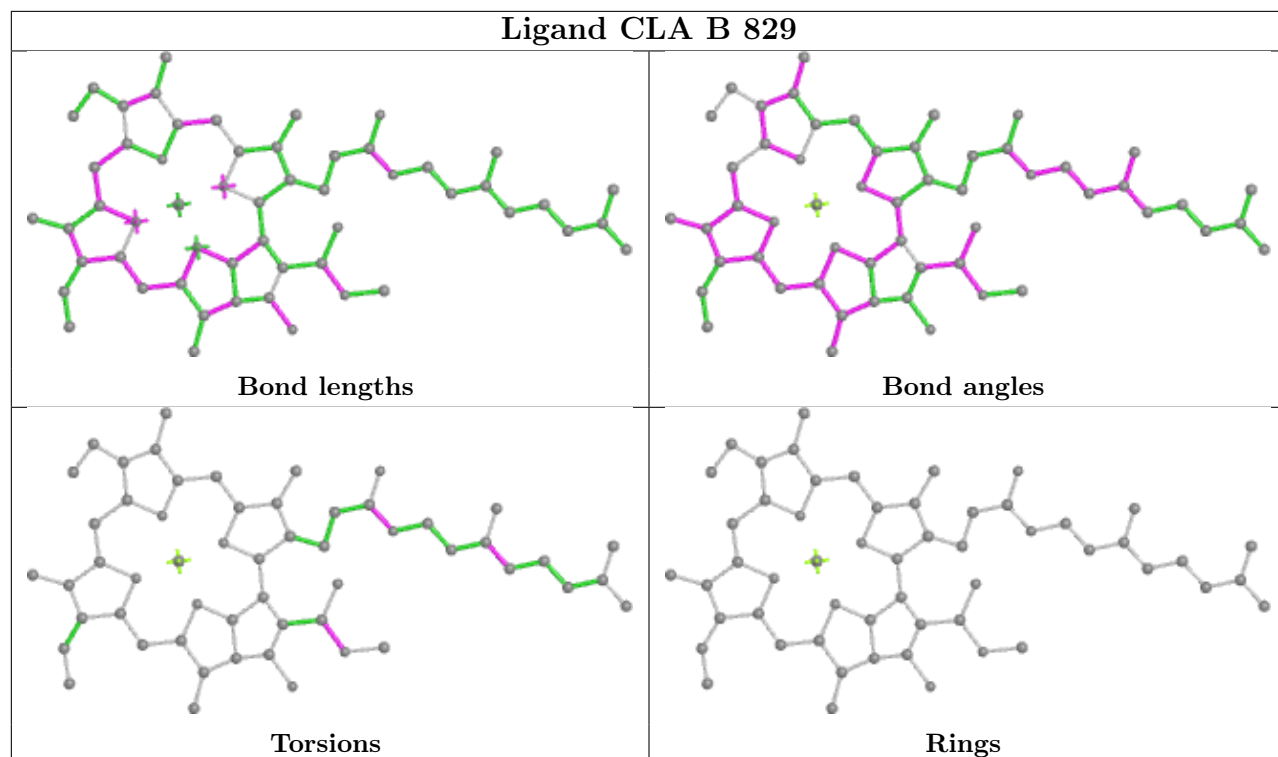
Torsions



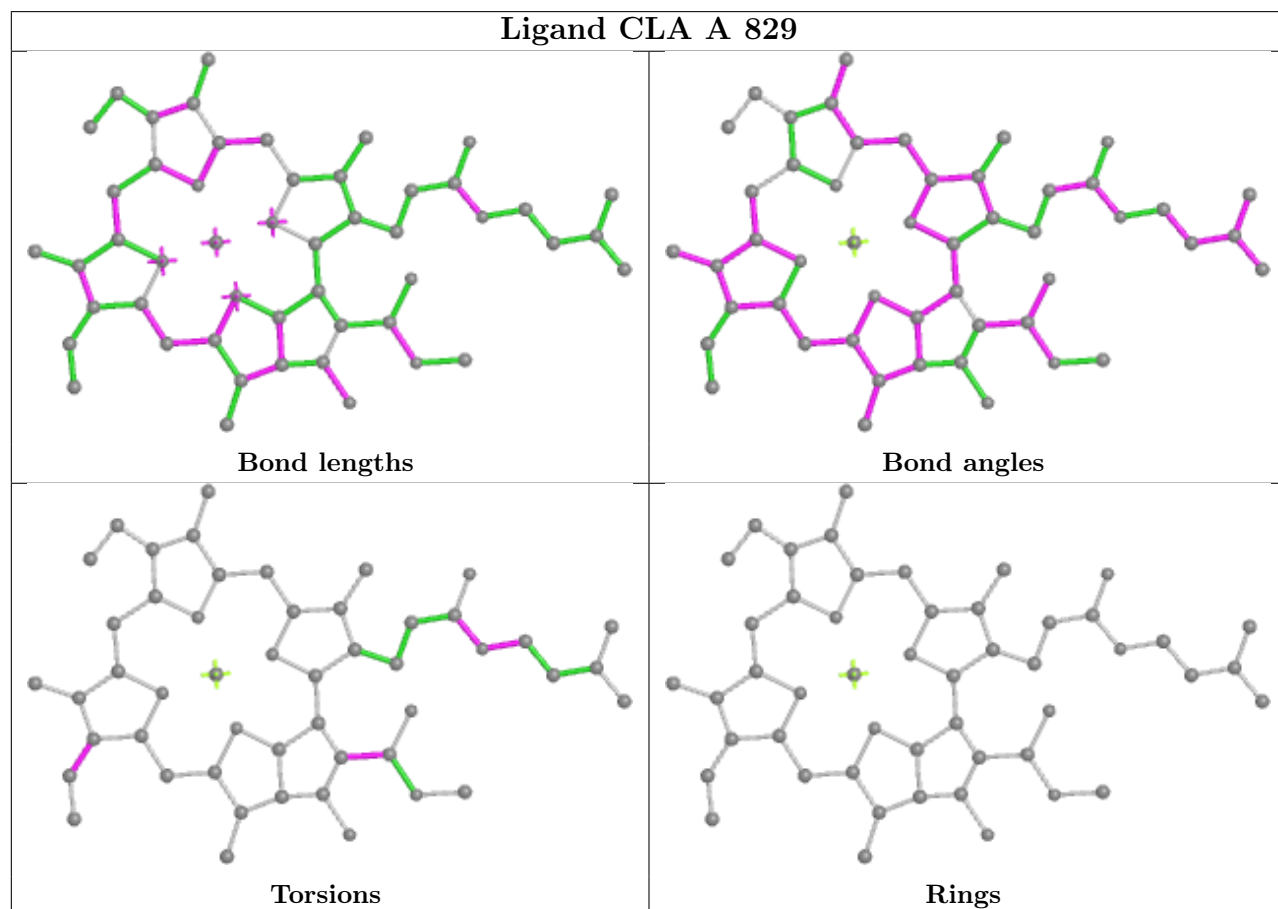
Rings

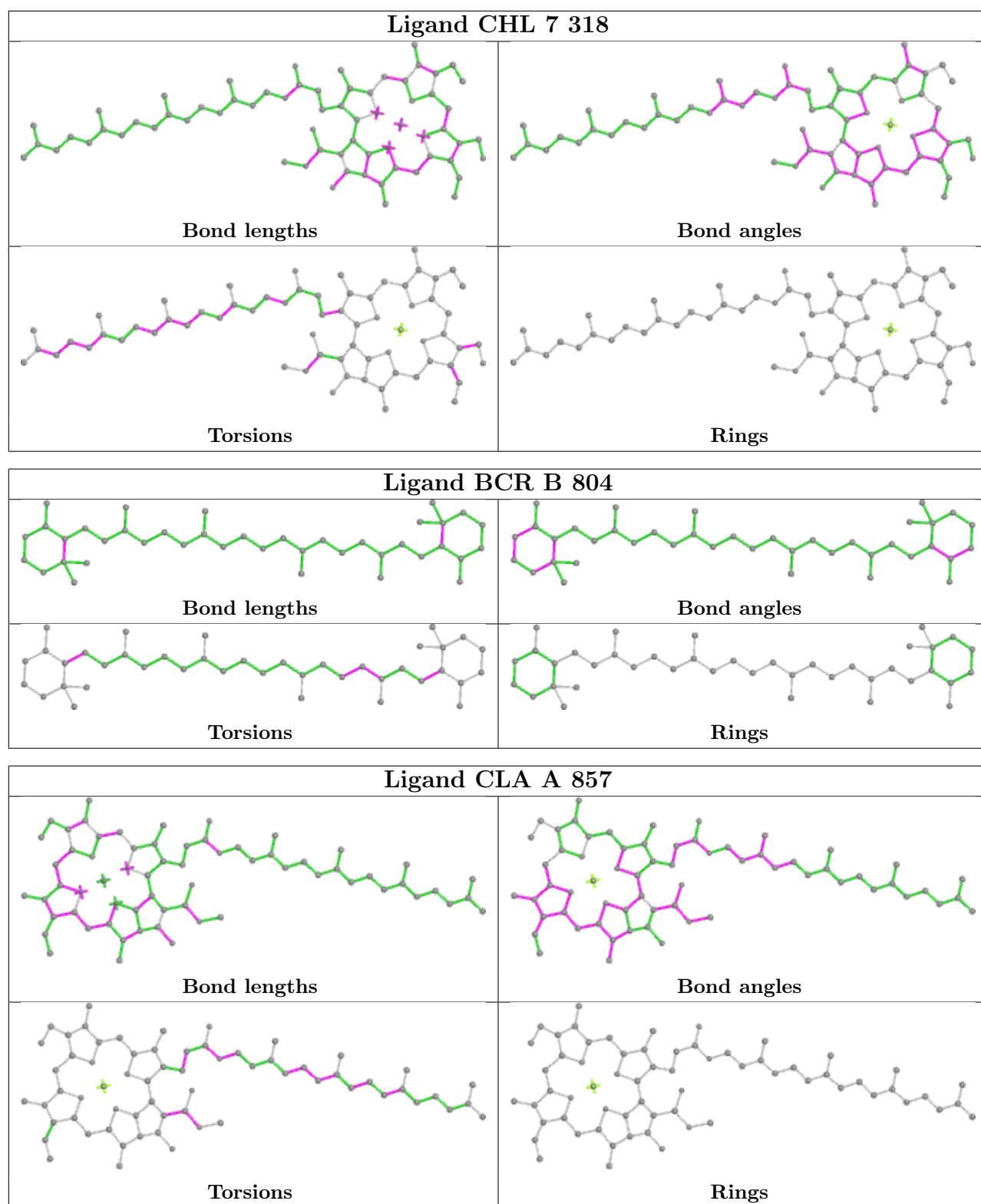


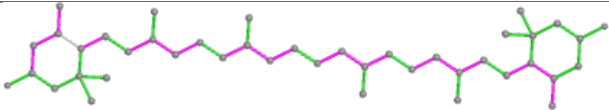
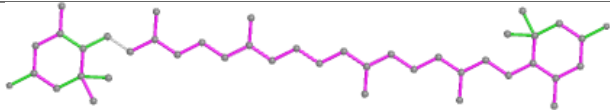
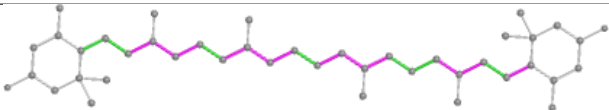
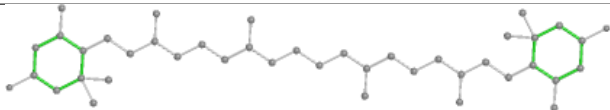
Ligand CLA B 829

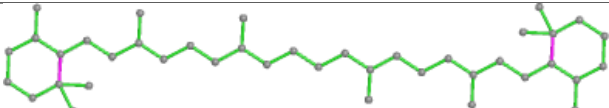
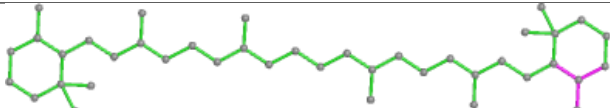
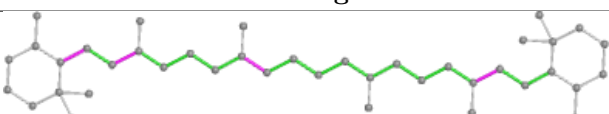
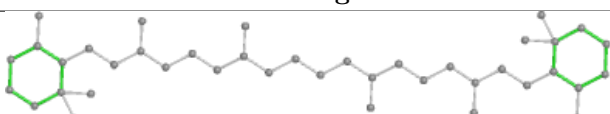


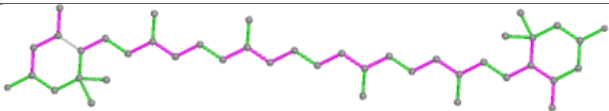
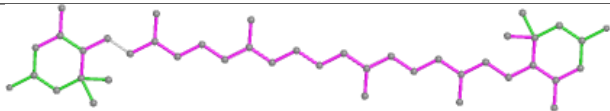
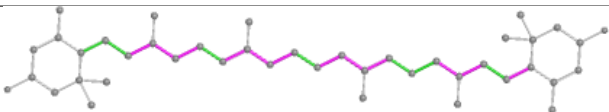
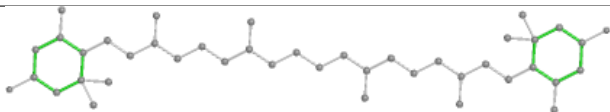
Ligand CLA A 829

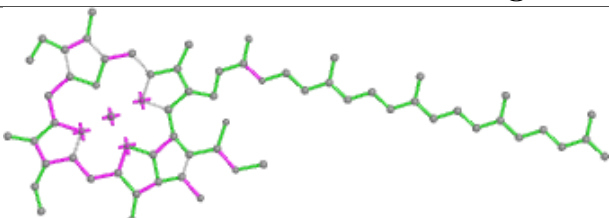
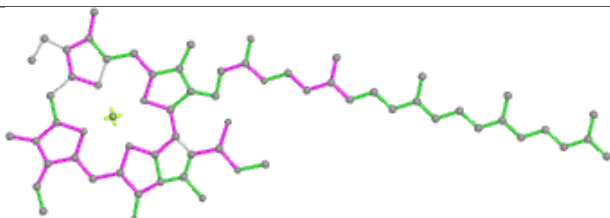
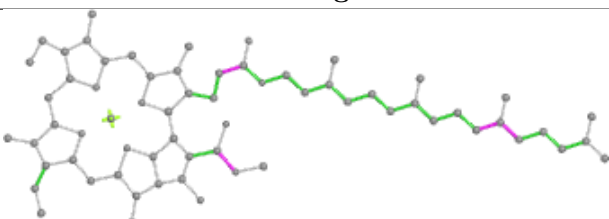
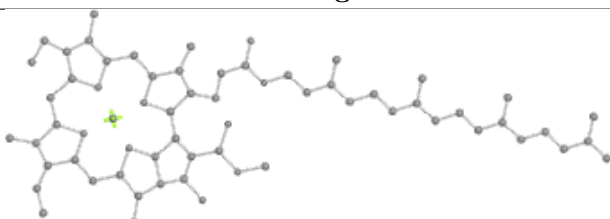


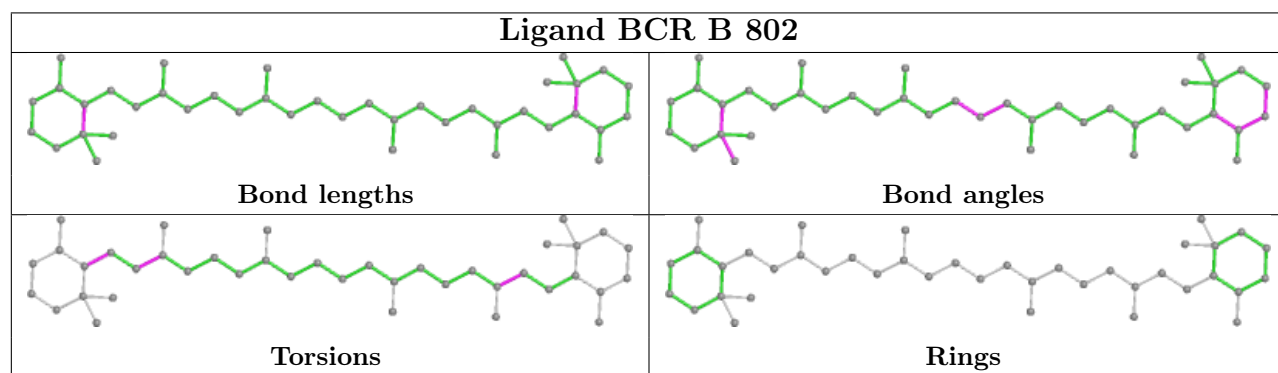
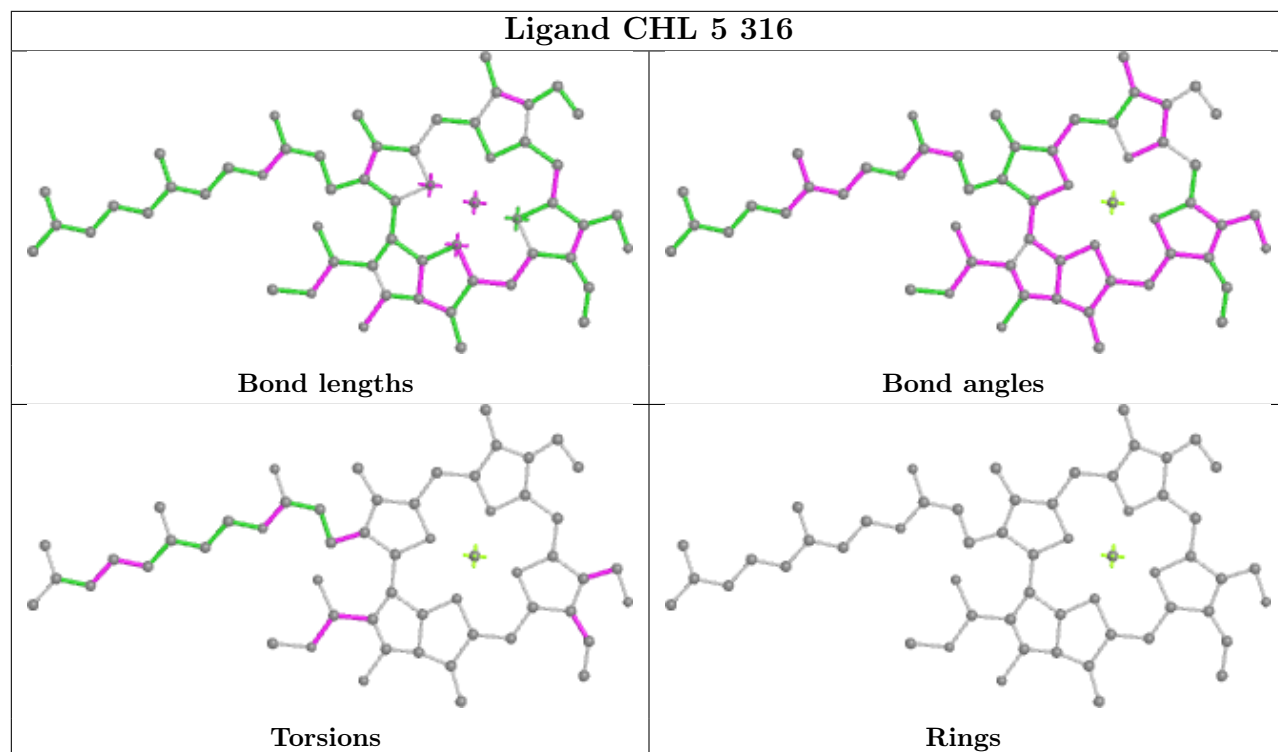
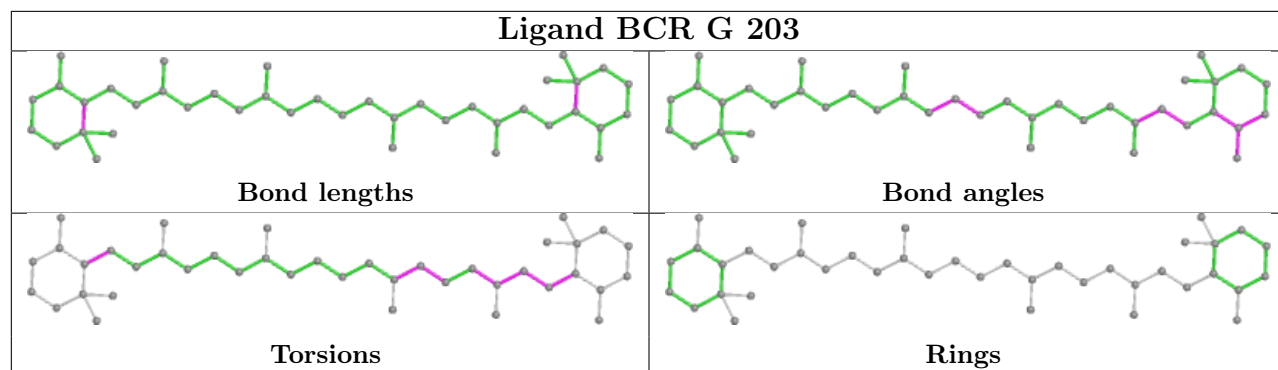


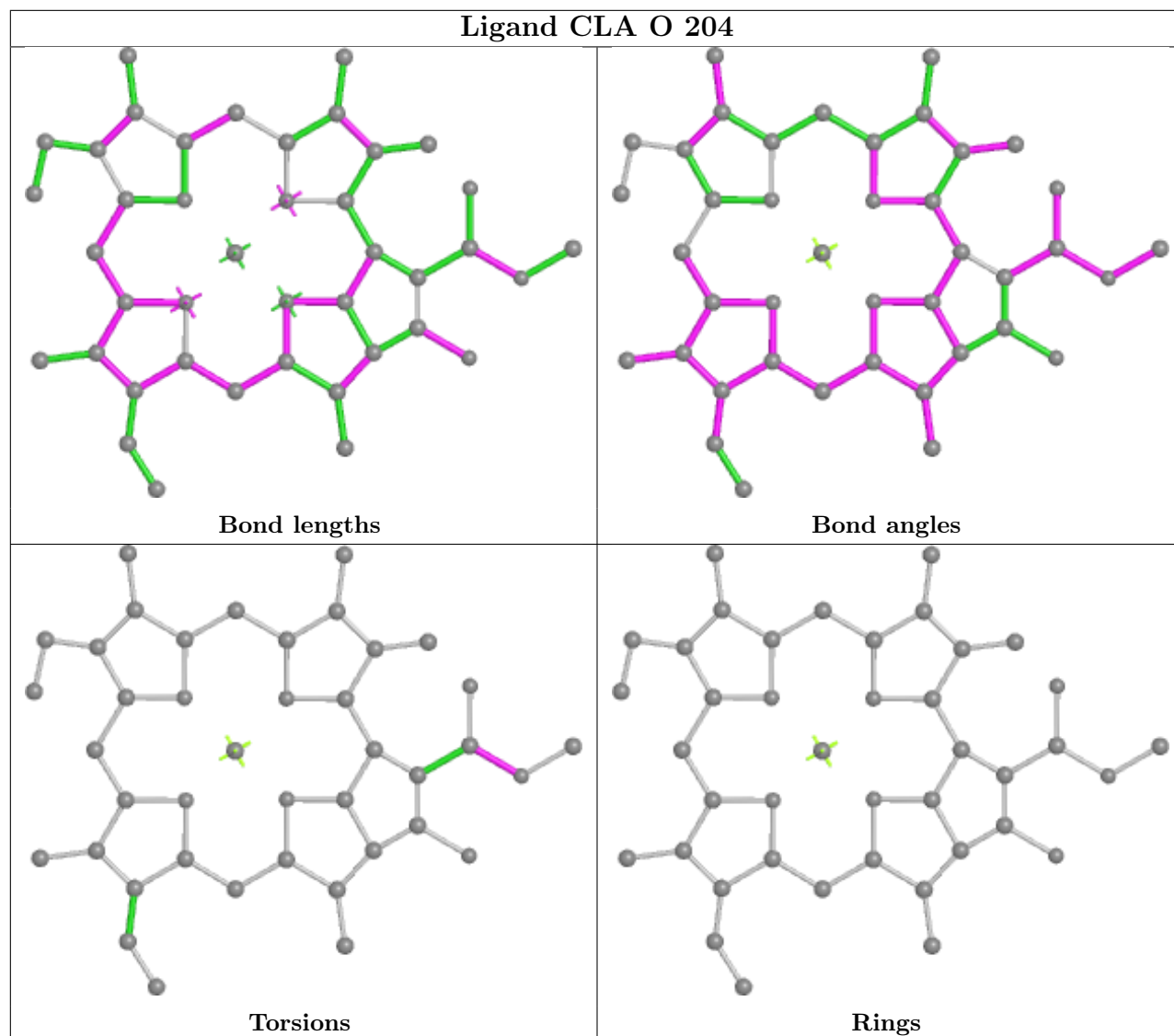
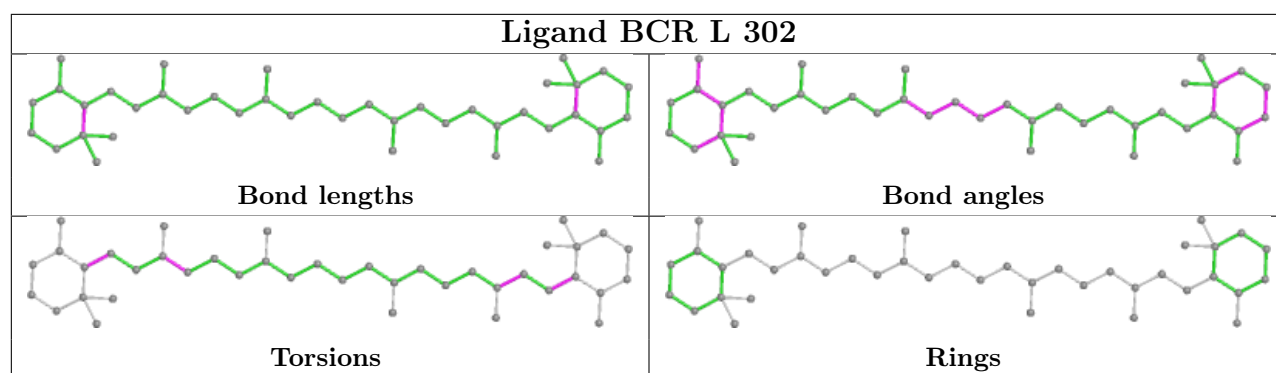
Ligand LUT 6 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

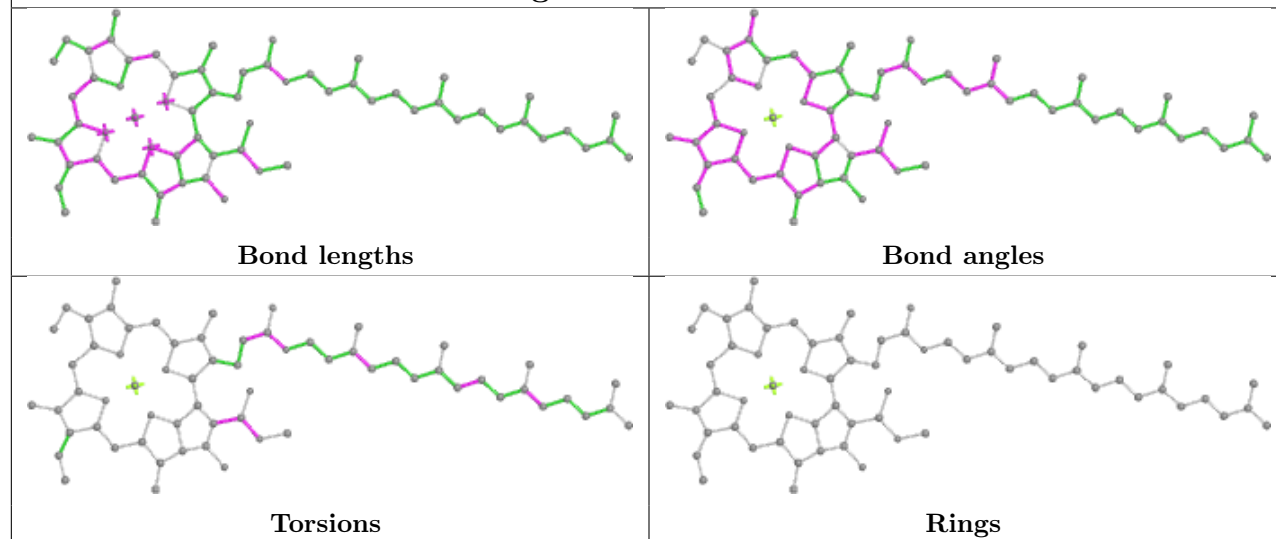
Ligand LUT 9 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

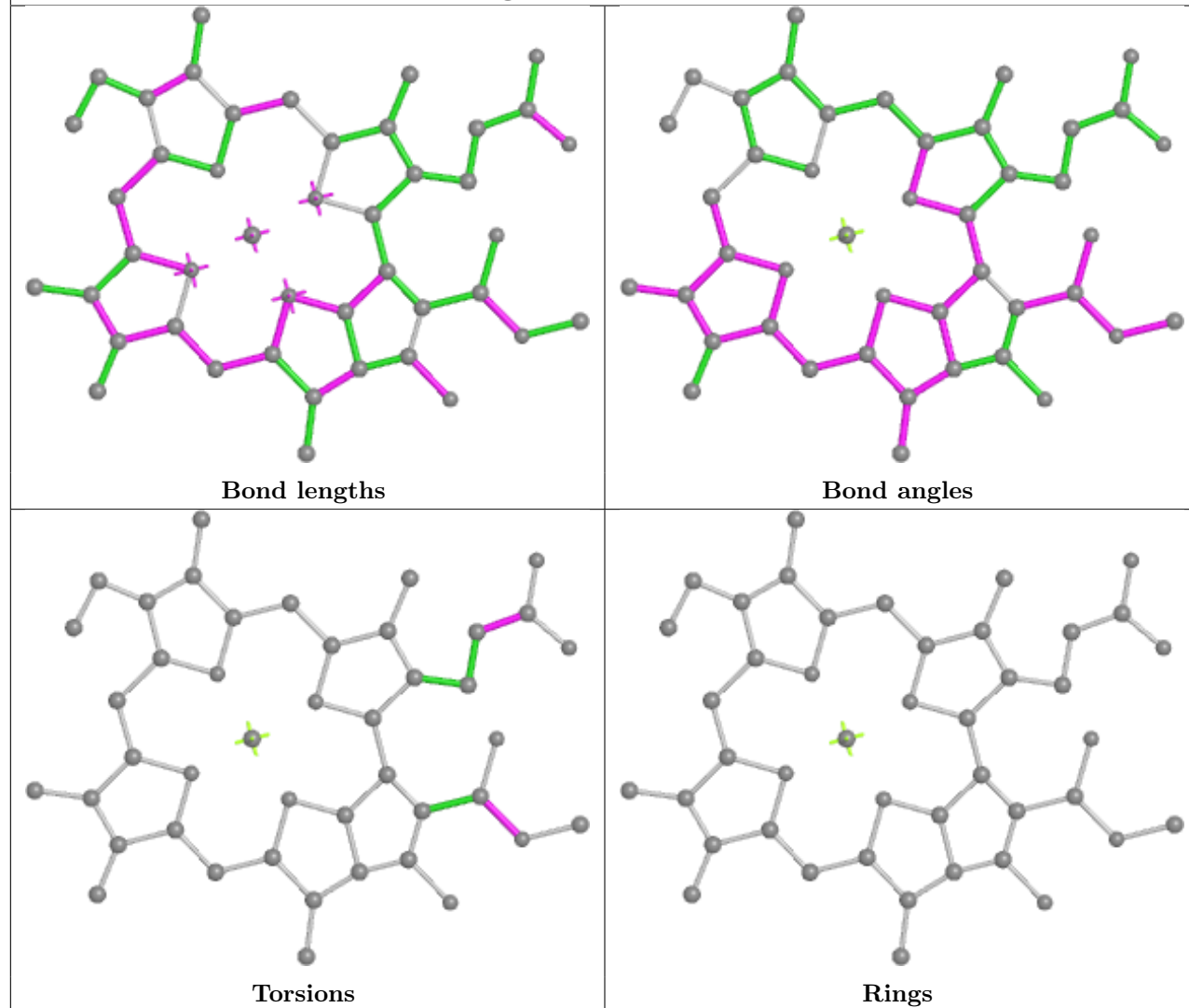




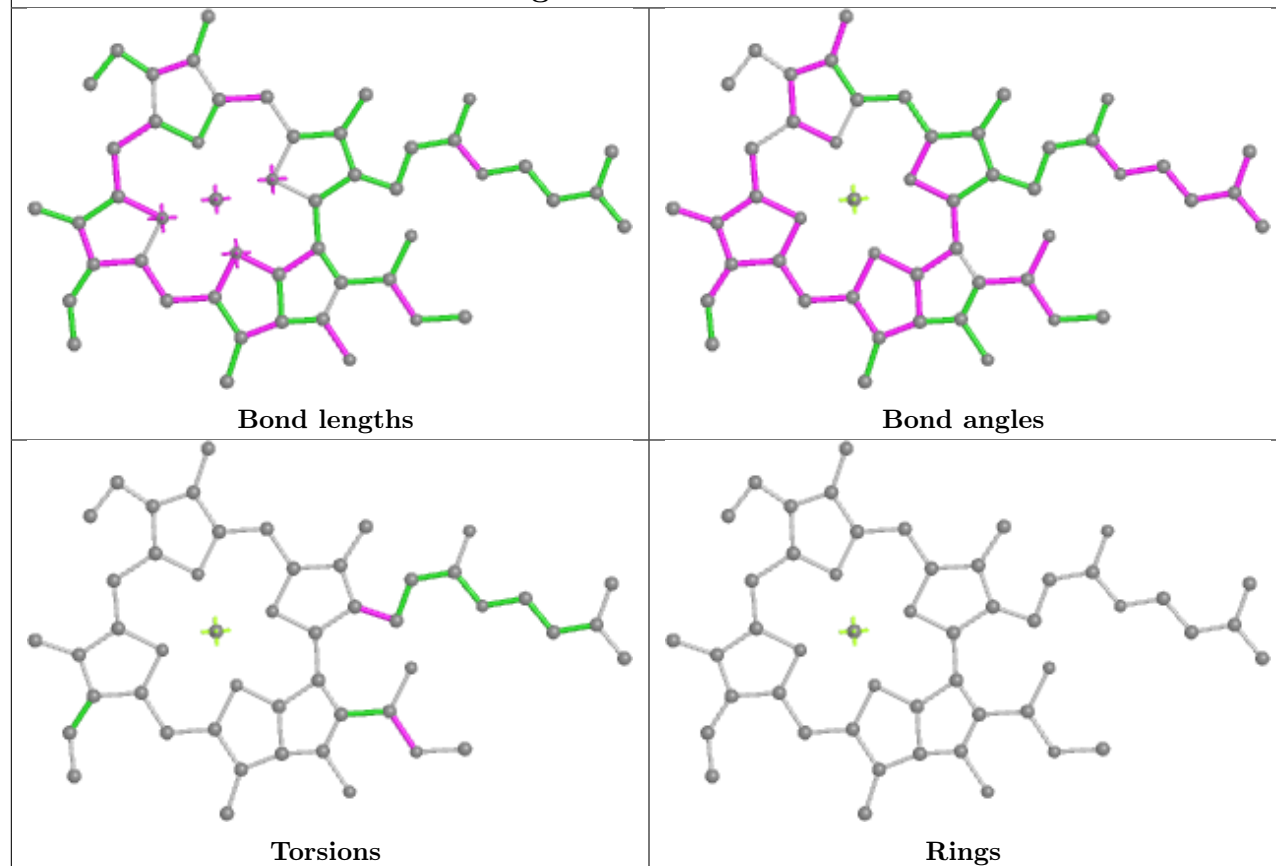
Ligand CLA A 838



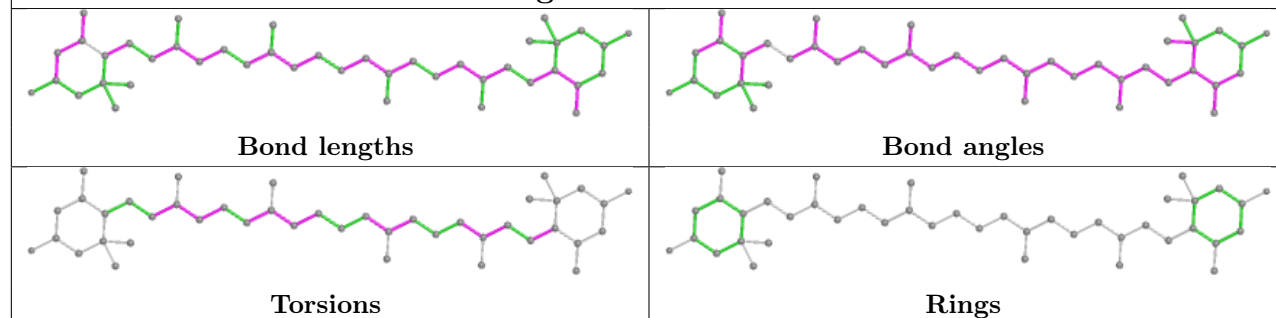
Ligand CLA 7 310



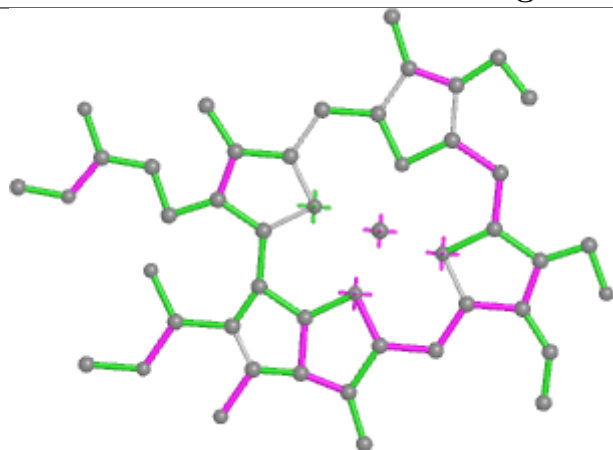
Ligand CLA A 844



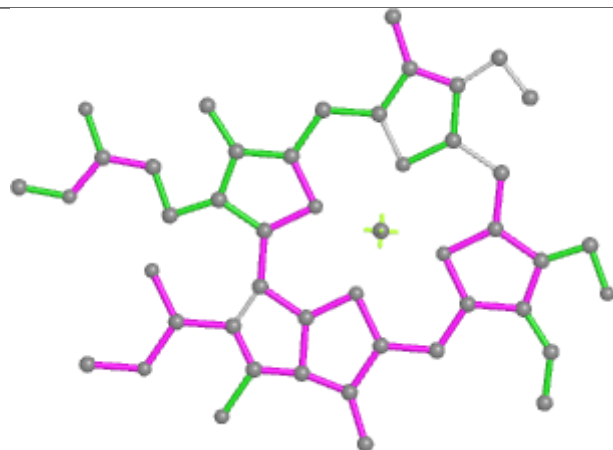
Ligand LUT 5 303



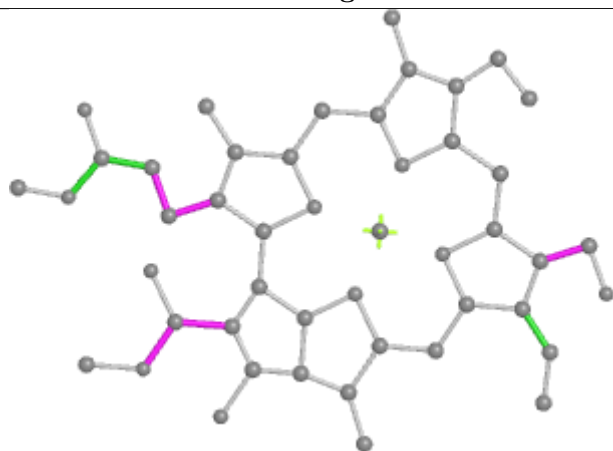
Ligand CHL b 309



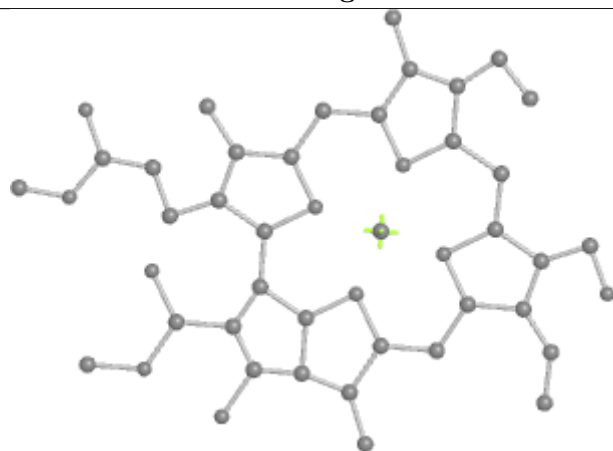
Bond lengths



Bond angles

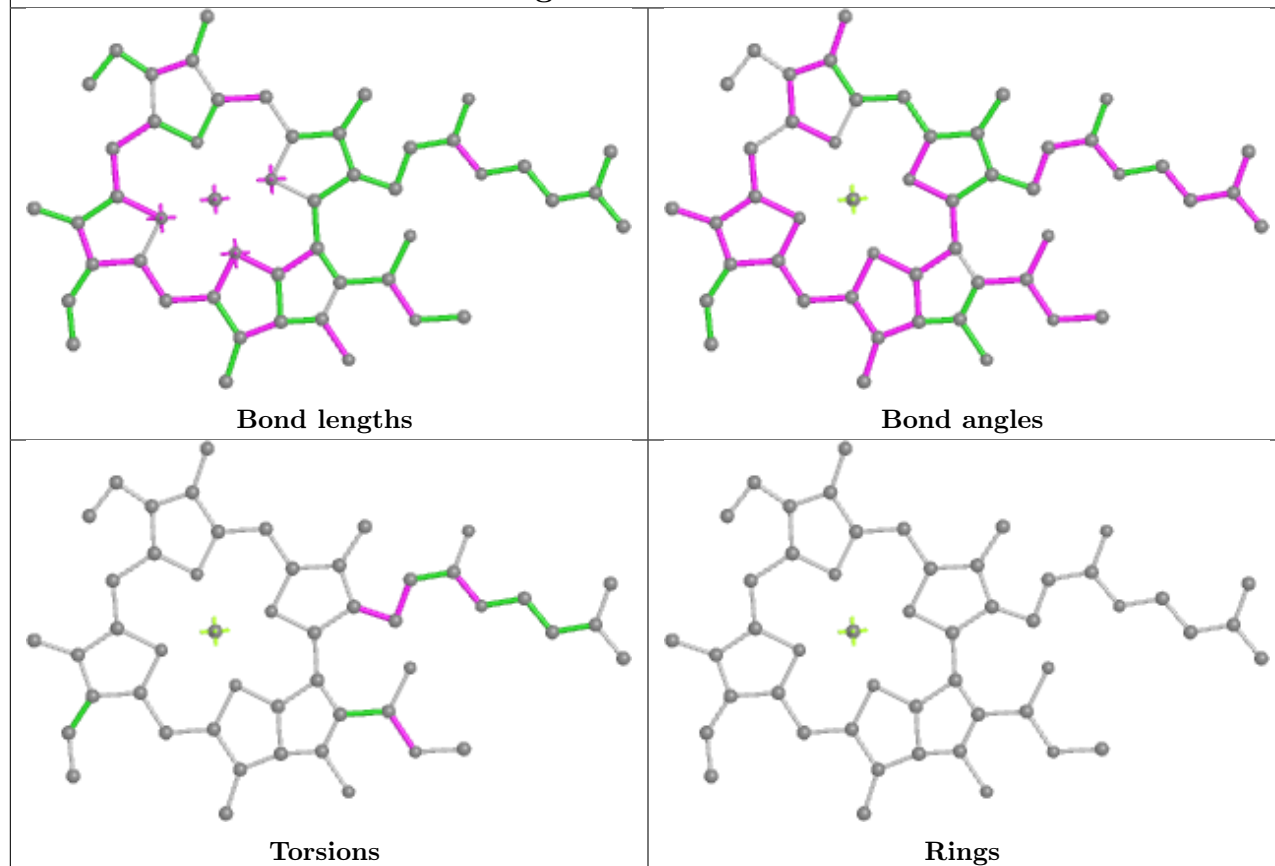


Torsions

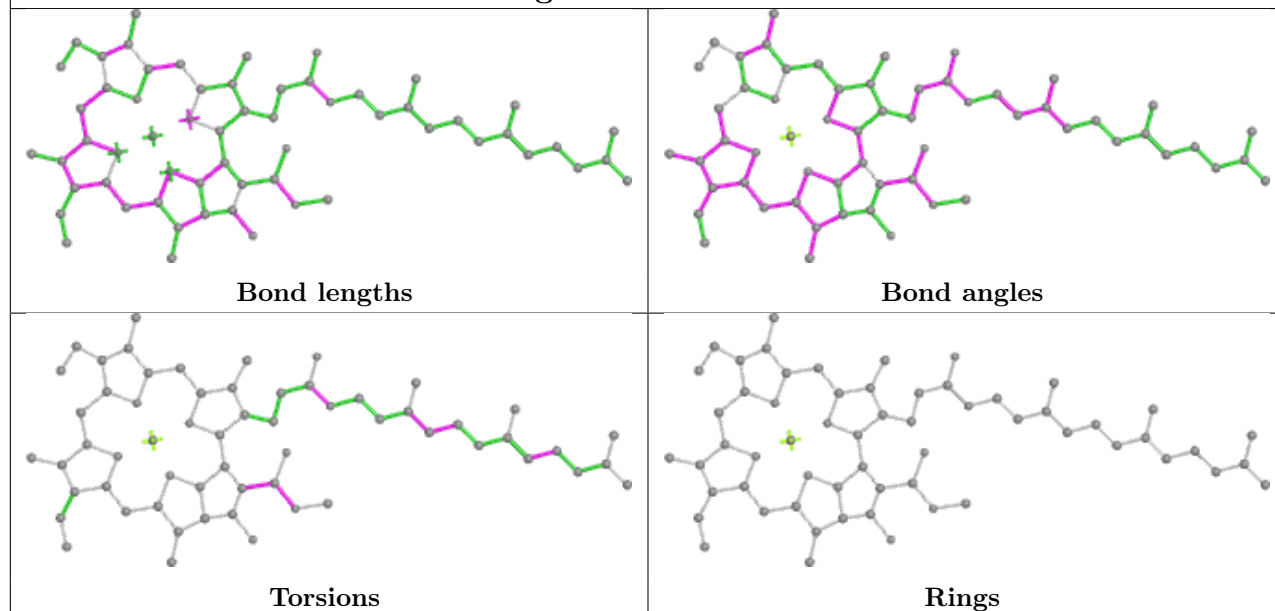


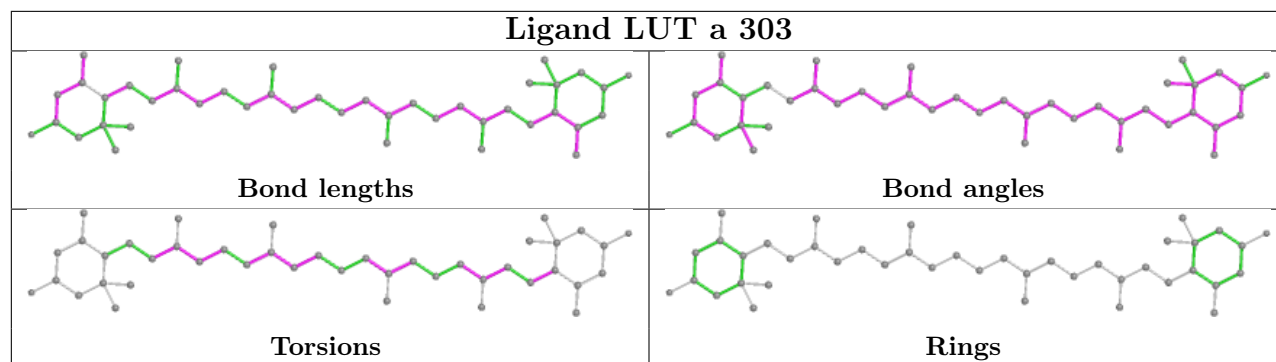
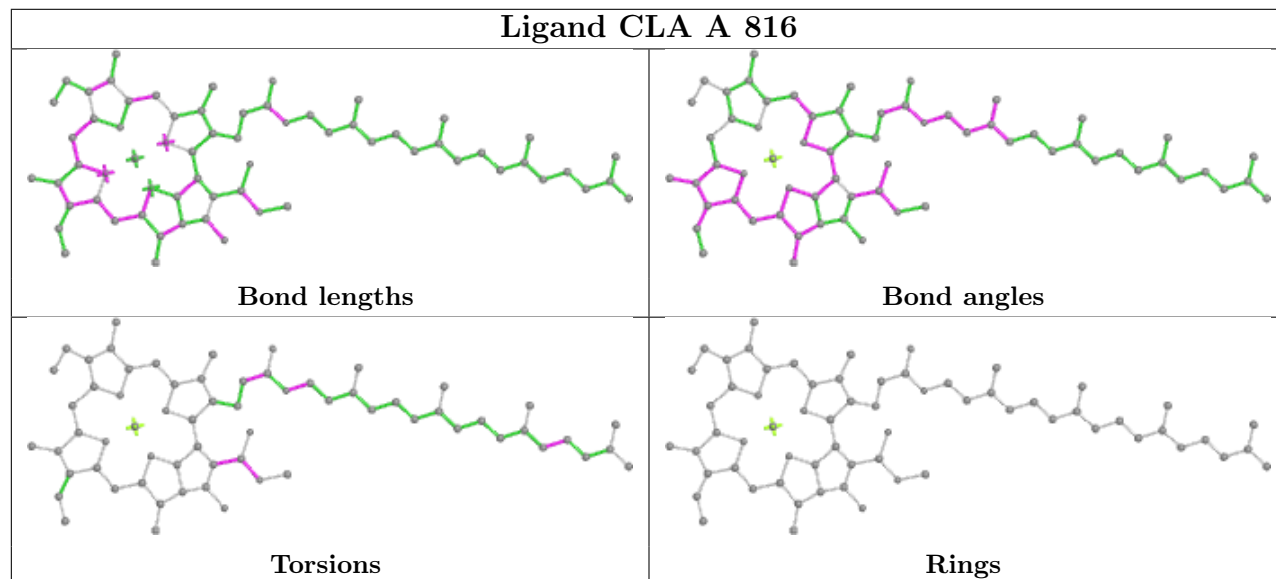
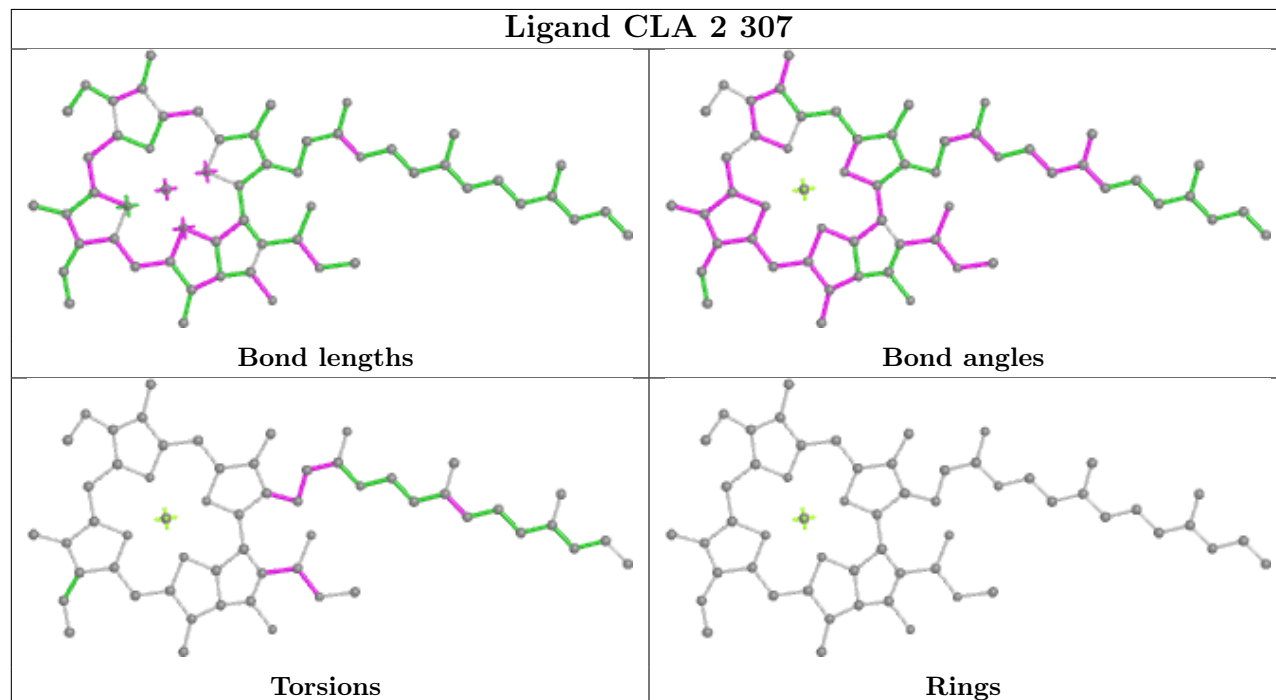
Rings

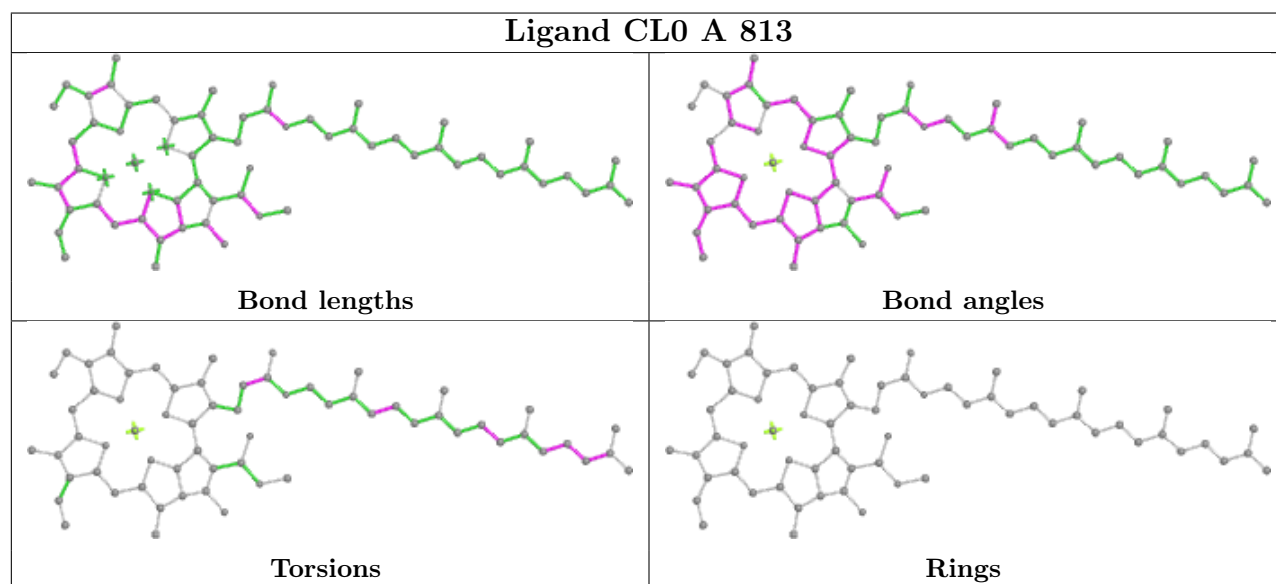
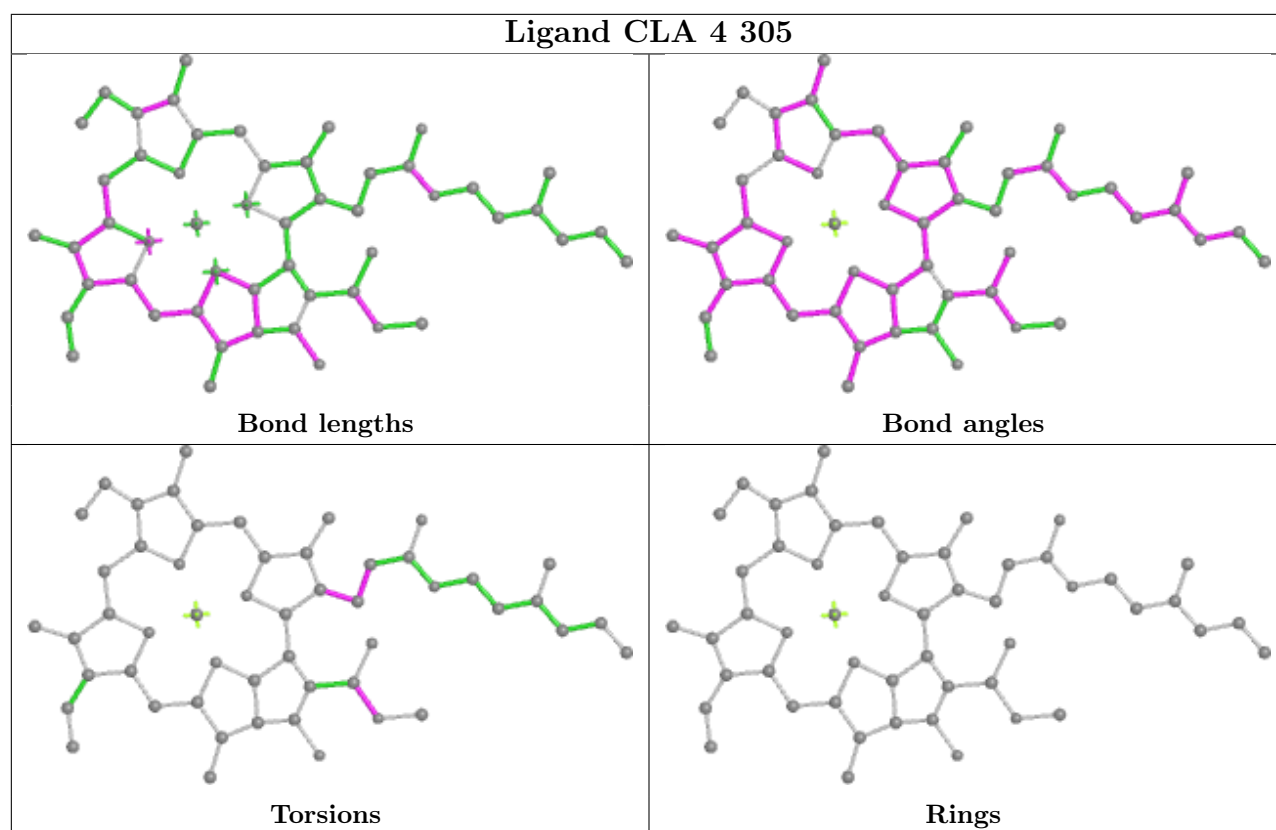
Ligand CLA 4 321



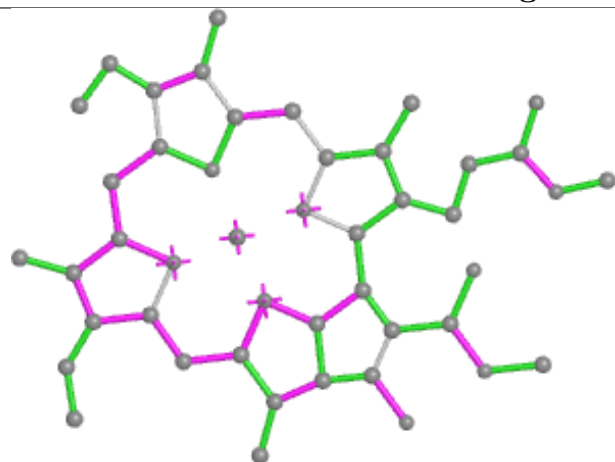
Ligand CLA 3 313



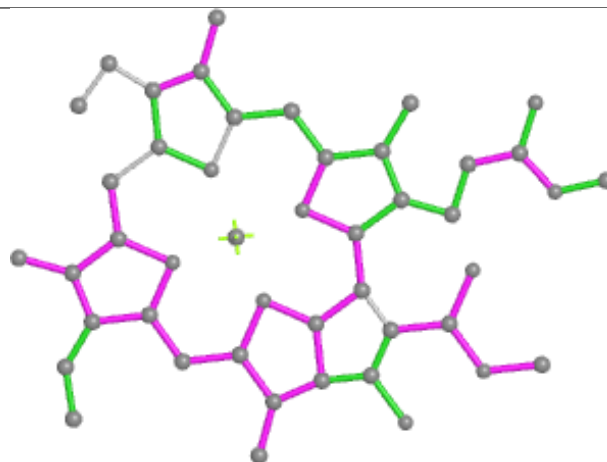
Ligand LUT a 303**Ligand CLA A 816****Ligand CLA 2 307**



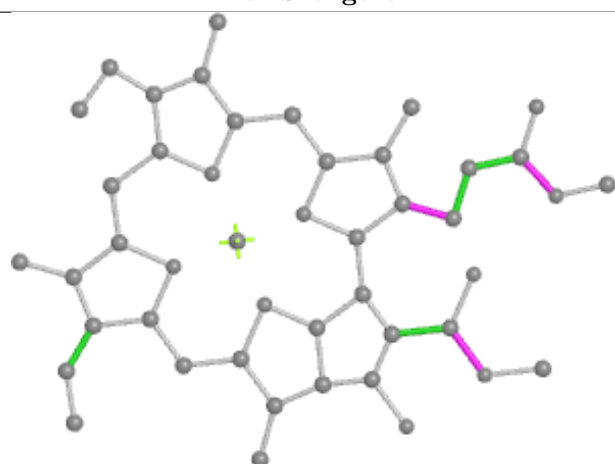
Ligand CLA b 304



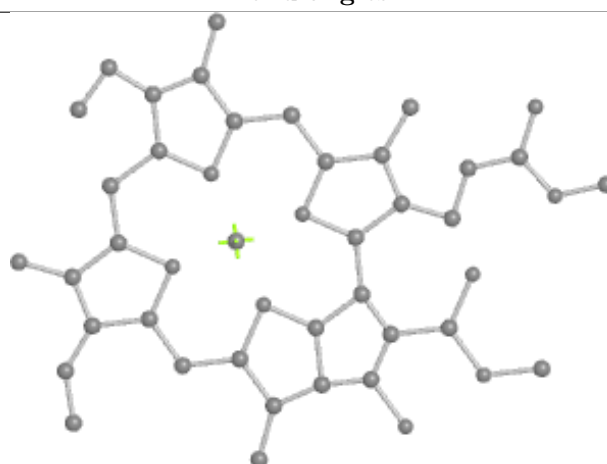
Bond lengths



Bond angles

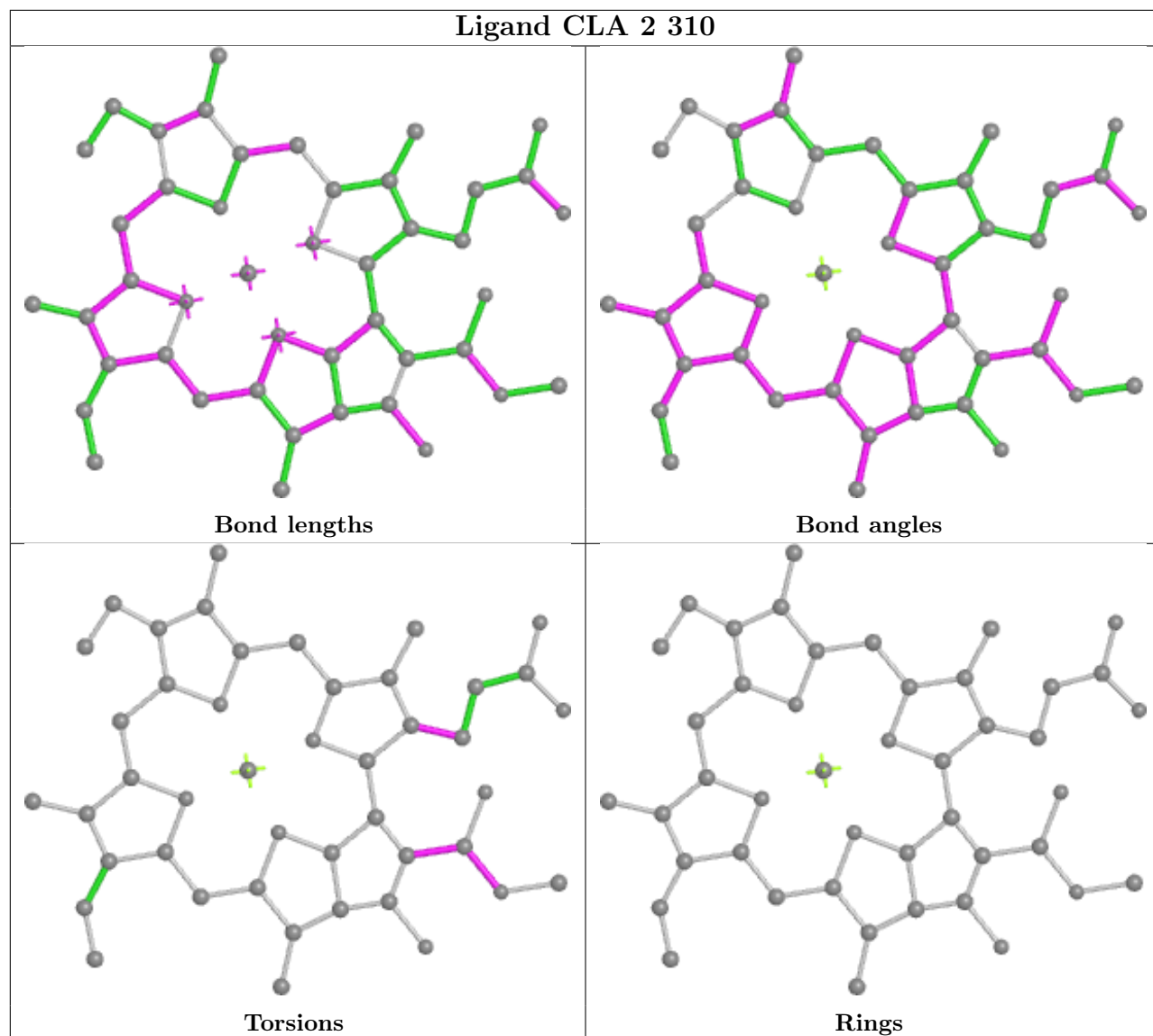


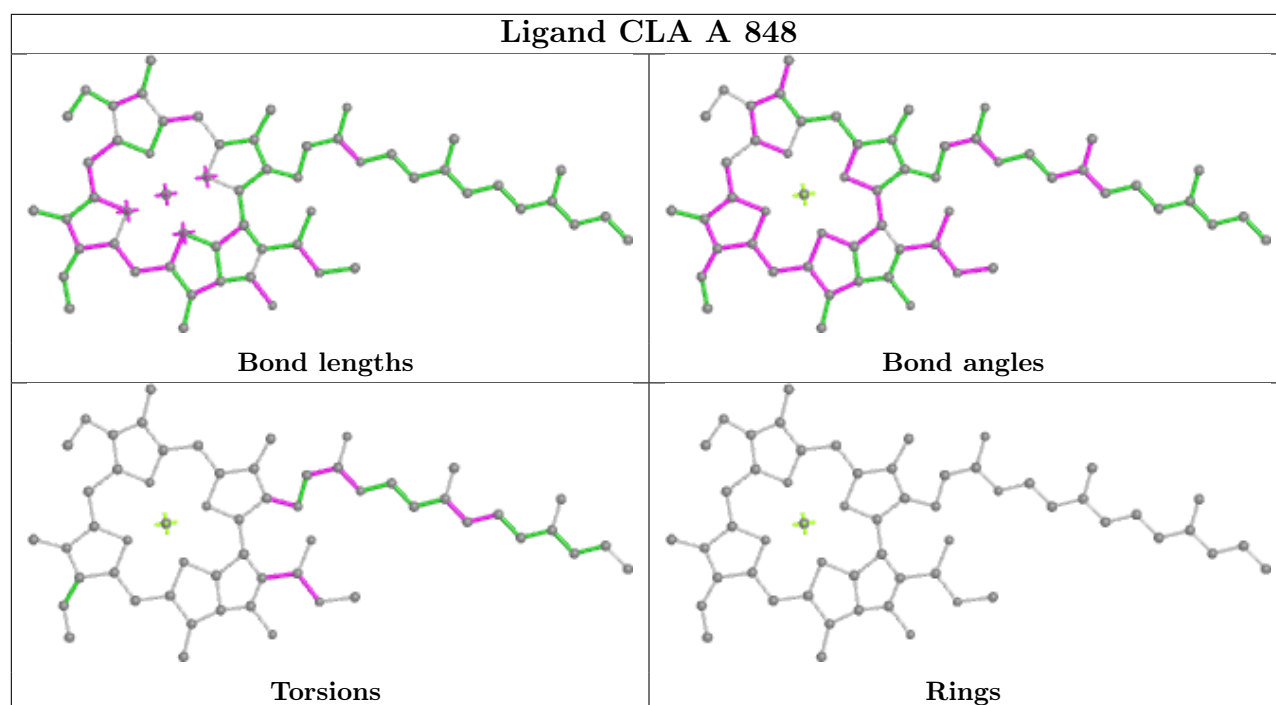
Torsions



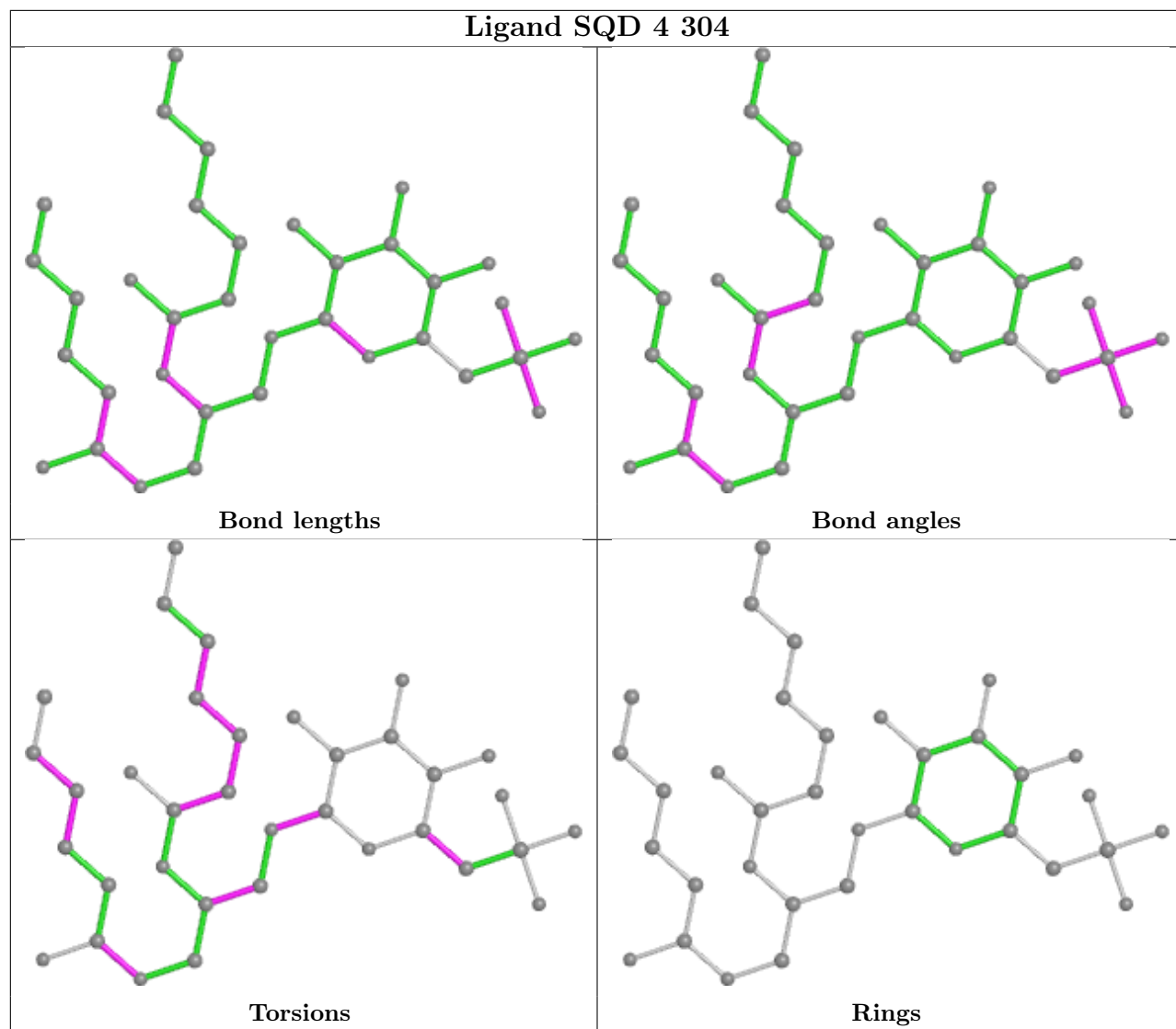
Rings

Ligand CLA 2 310

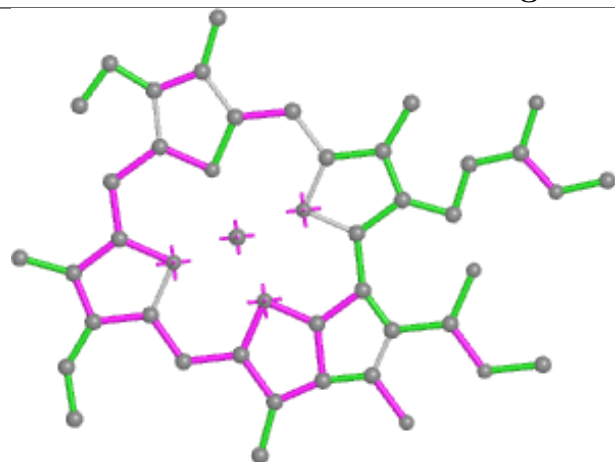




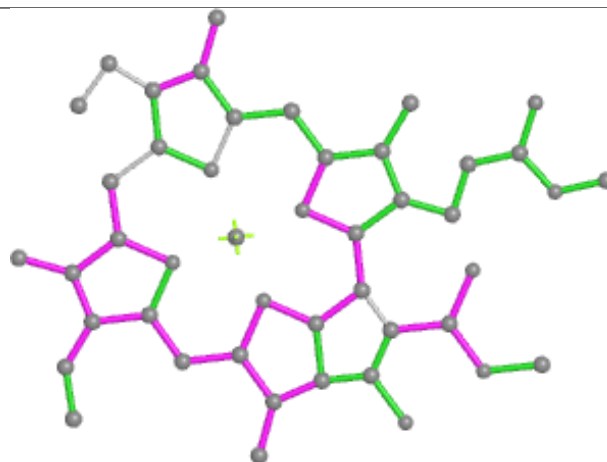
Ligand SQD 4 304



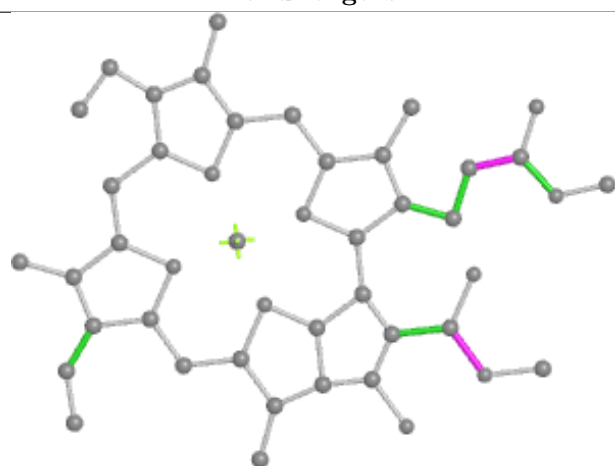
Ligand CLA 5 313



Bond lengths



Bond angles

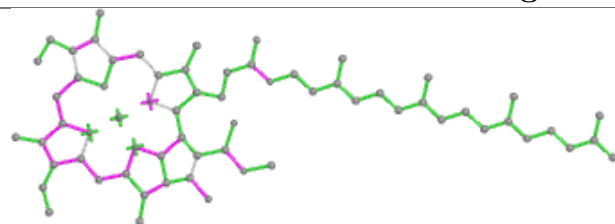


Torsions

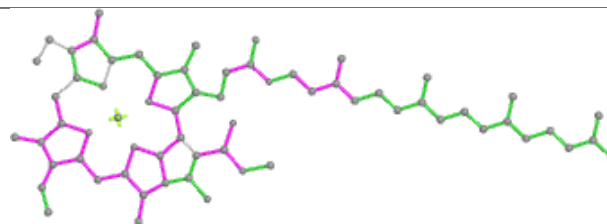


Rings

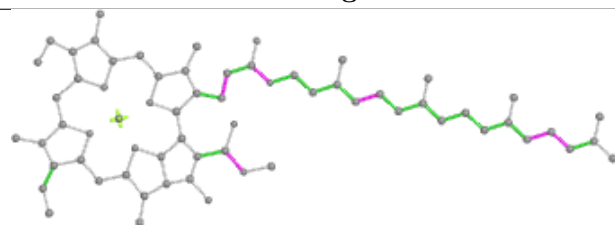
Ligand CLA 9 318



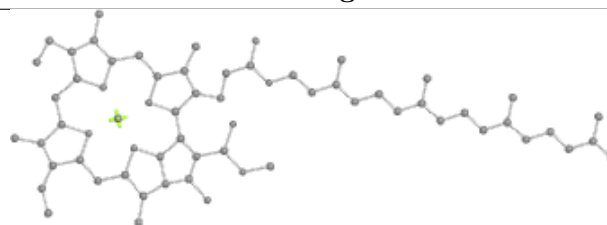
Bond lengths



Bond angles

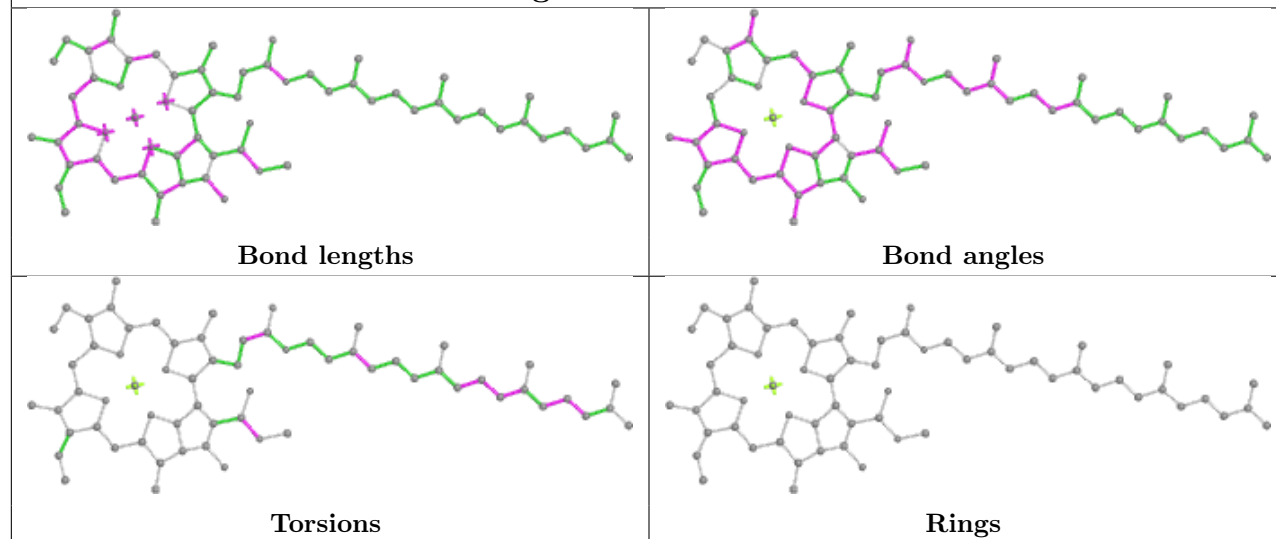


Torsions

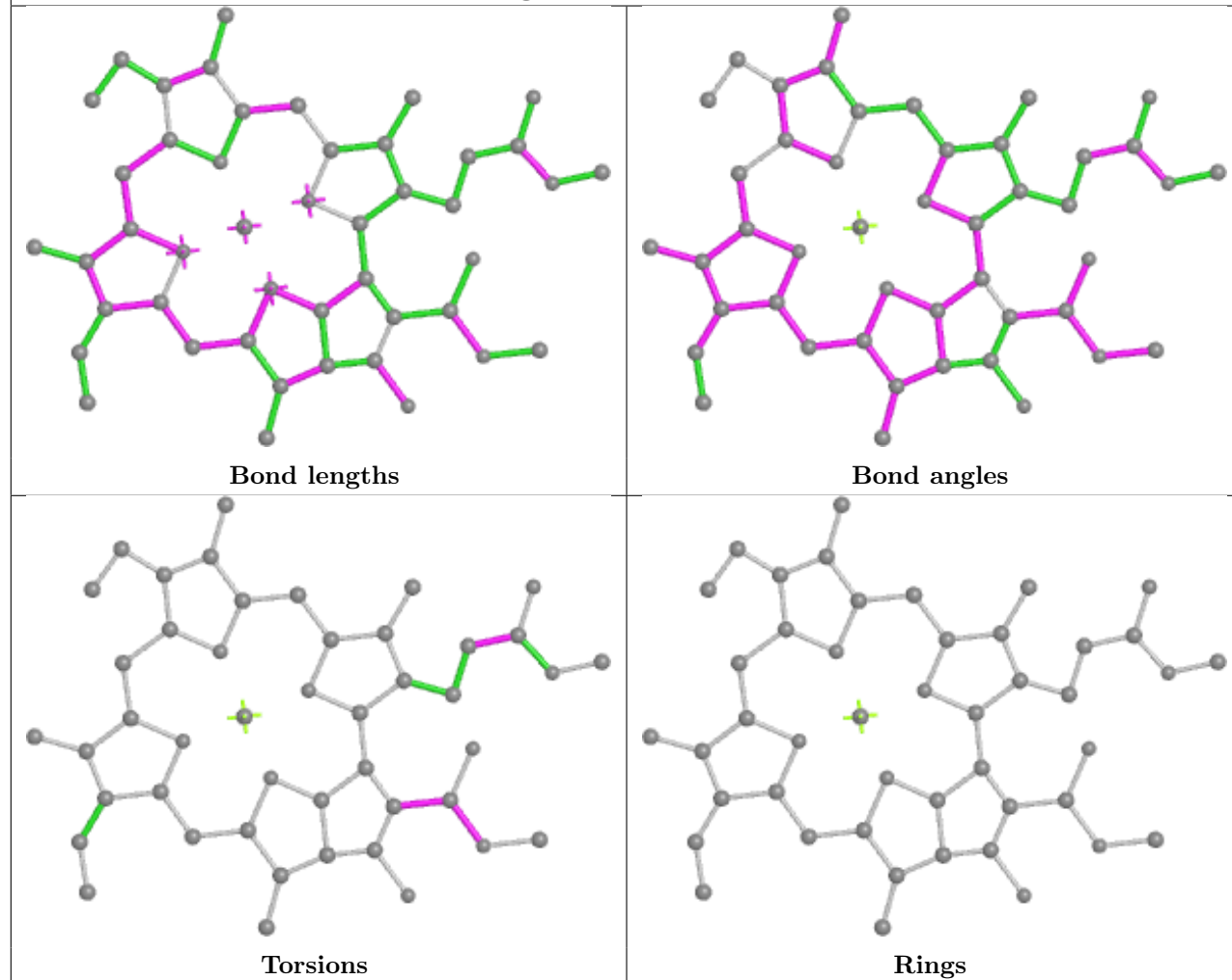


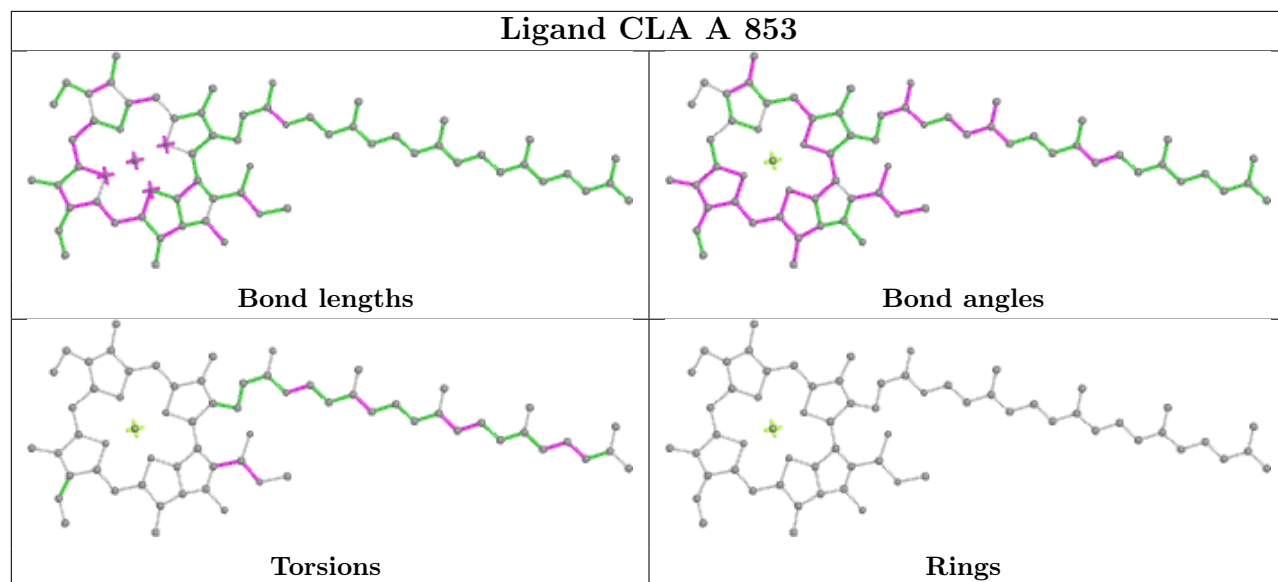
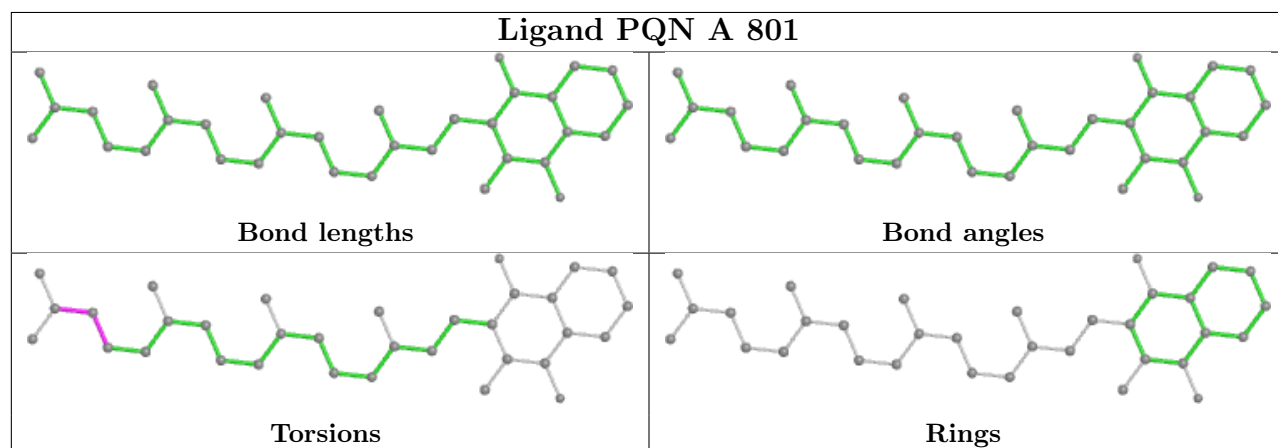
Rings

Ligand CLA B 840

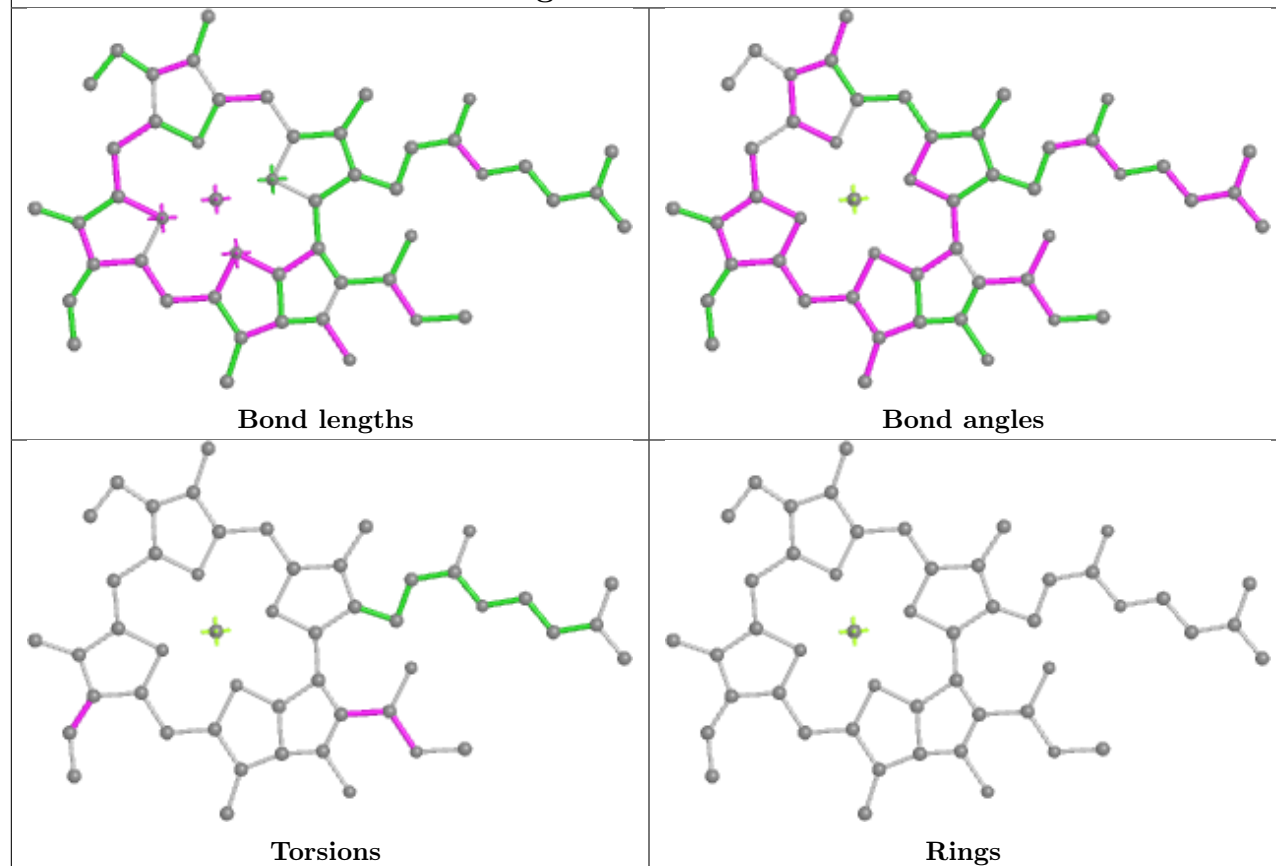


Ligand CLA 6 313

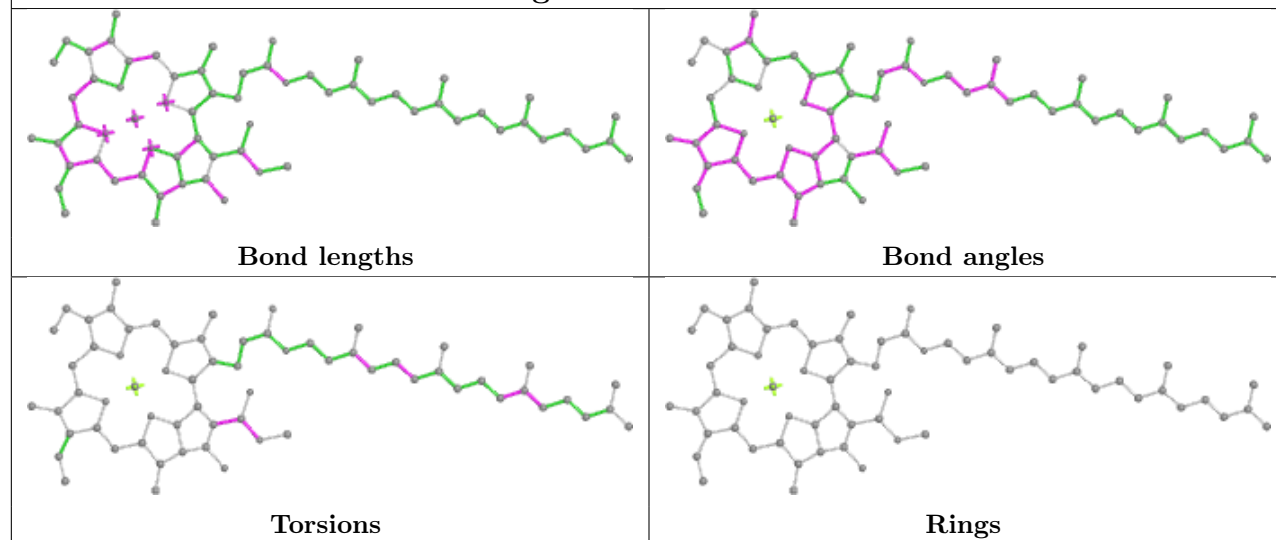


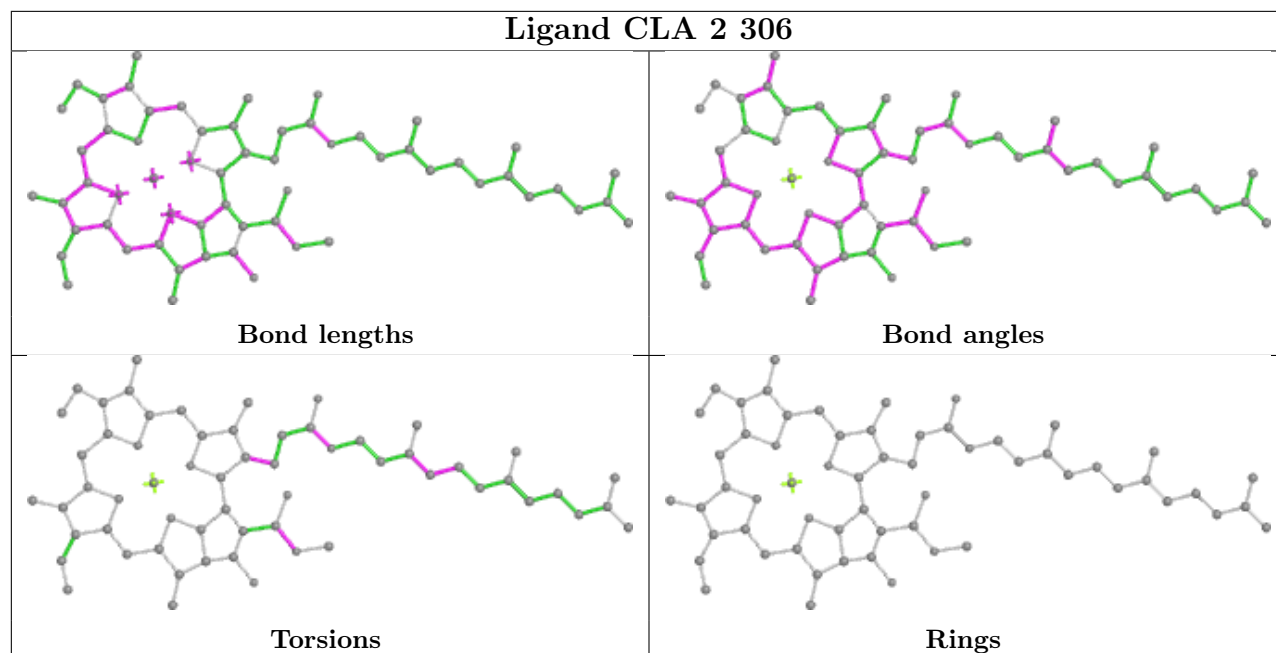
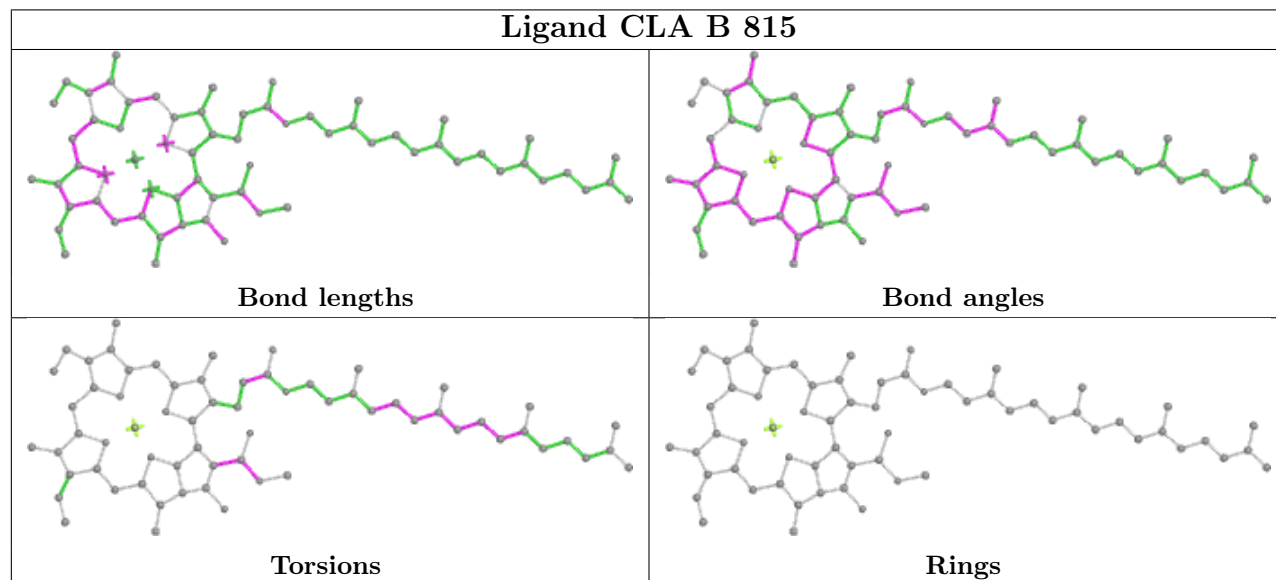
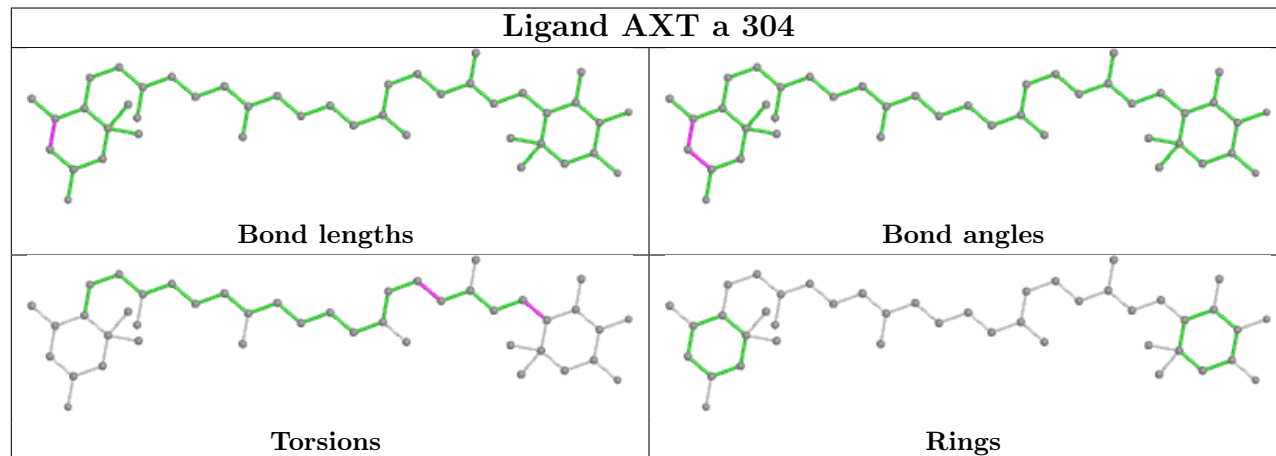
Ligand CLA A 853**Ligand PQN A 801**

Ligand CLA 9 316

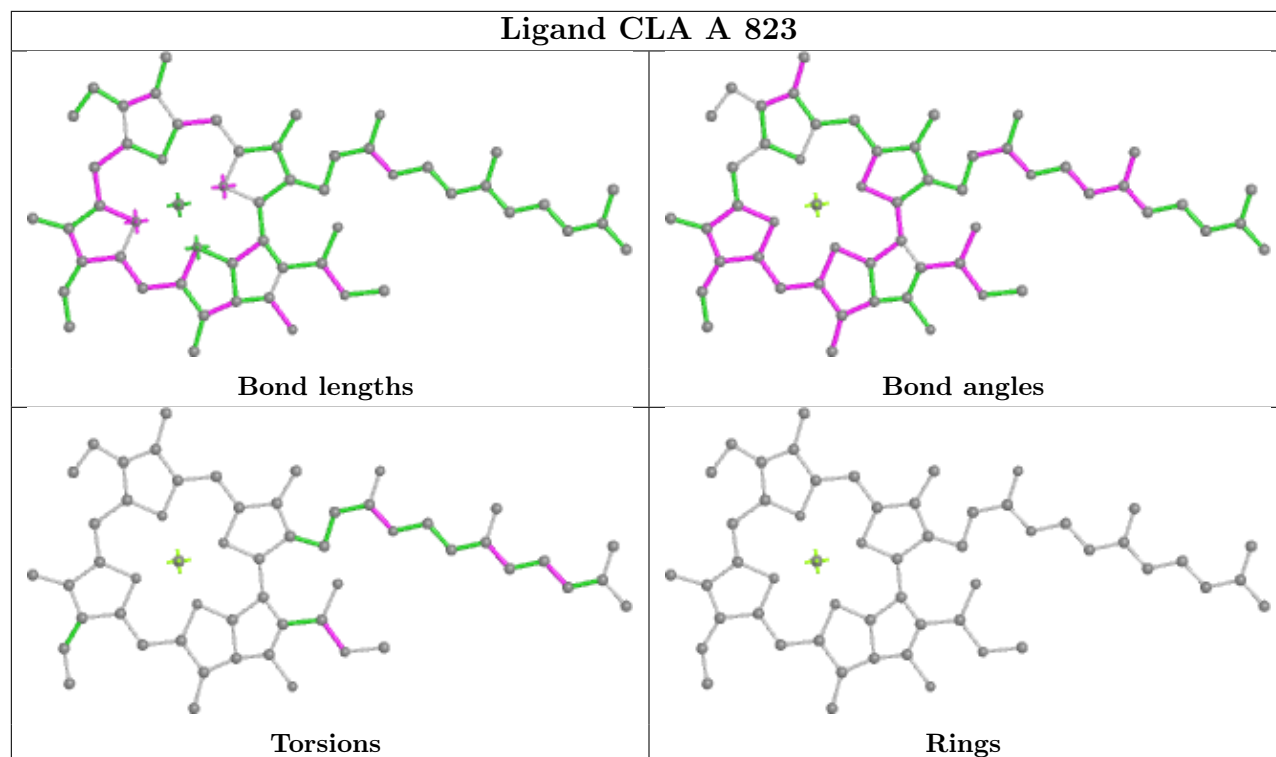


Ligand CLA B 844

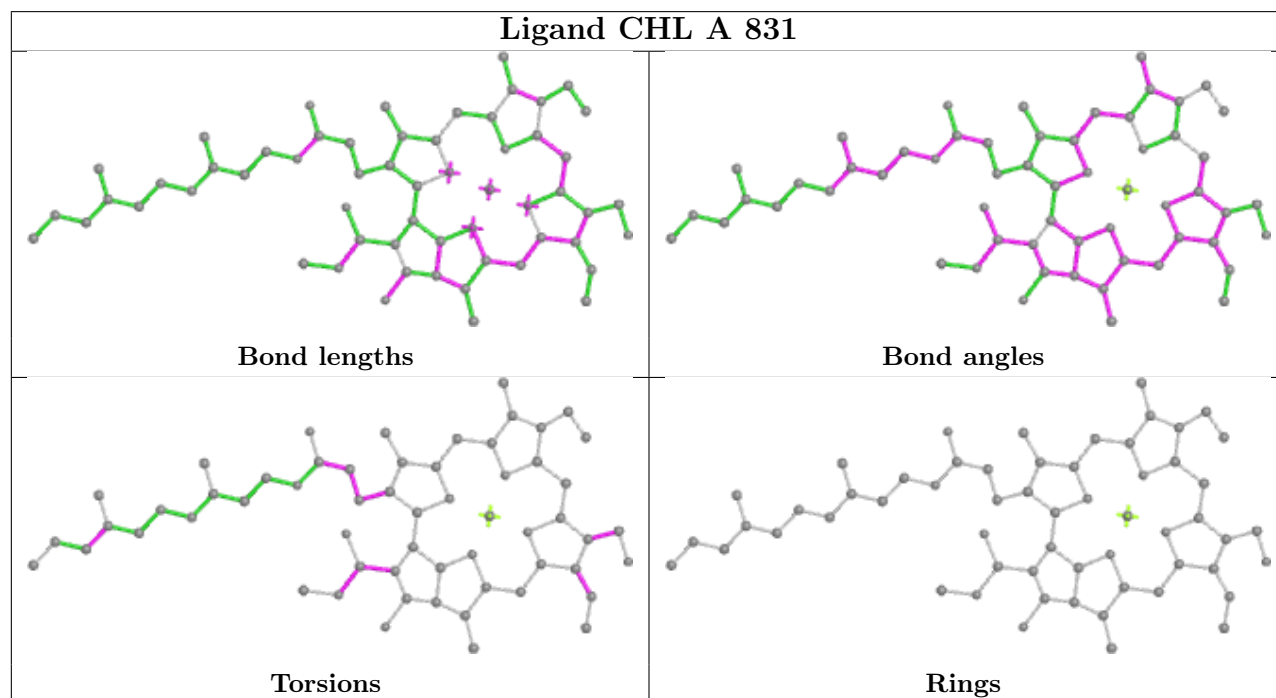


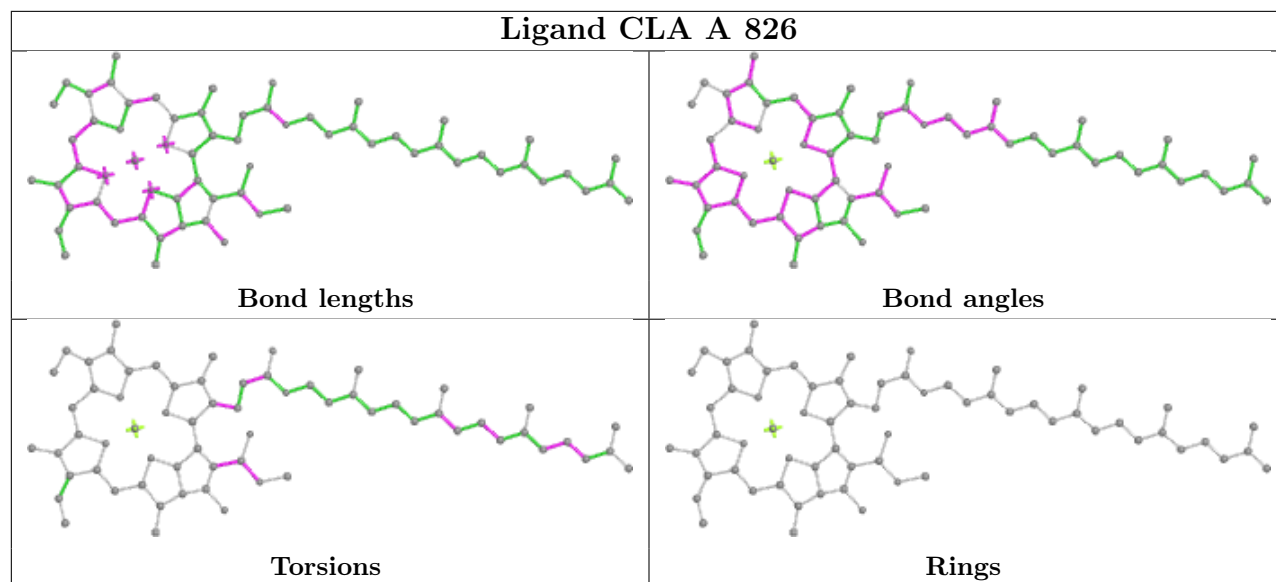
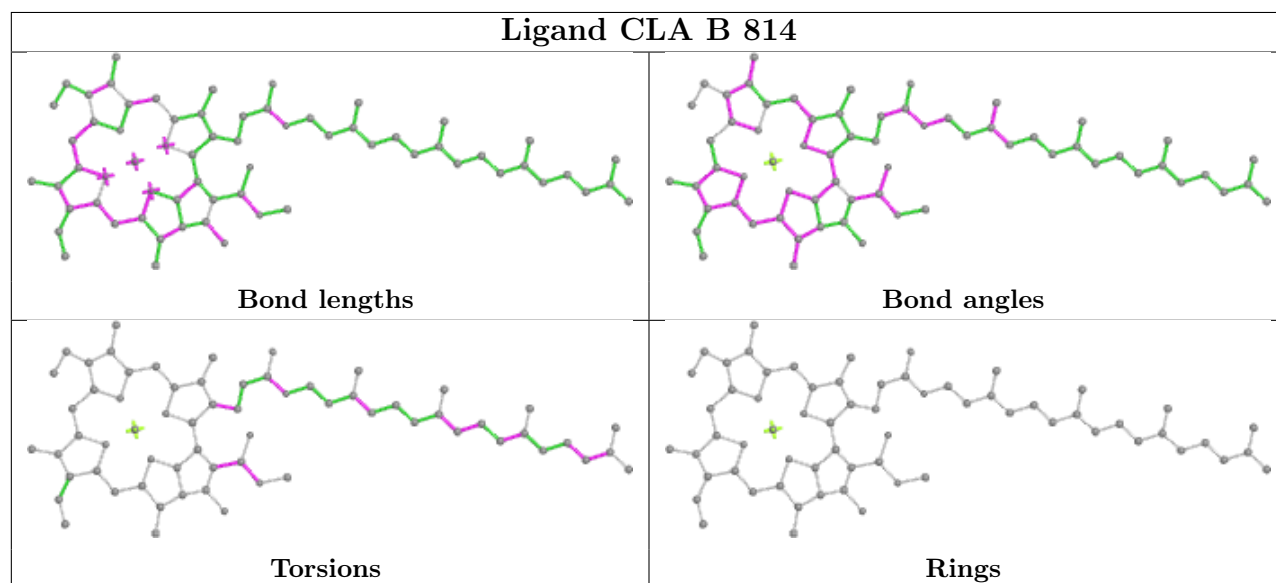
Ligand CLA 2 306**Ligand CLA B 815****Ligand AXT a 304**

Ligand CLA A 823

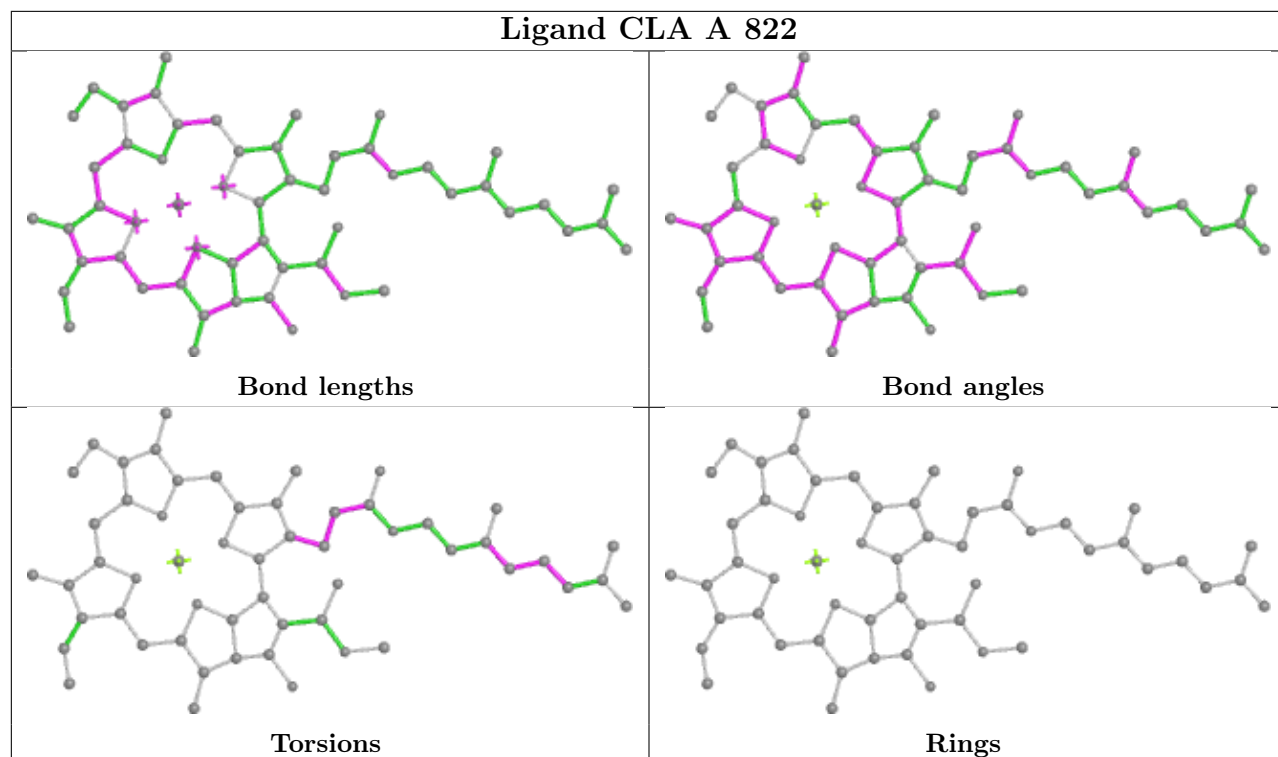


Ligand CHL A 831

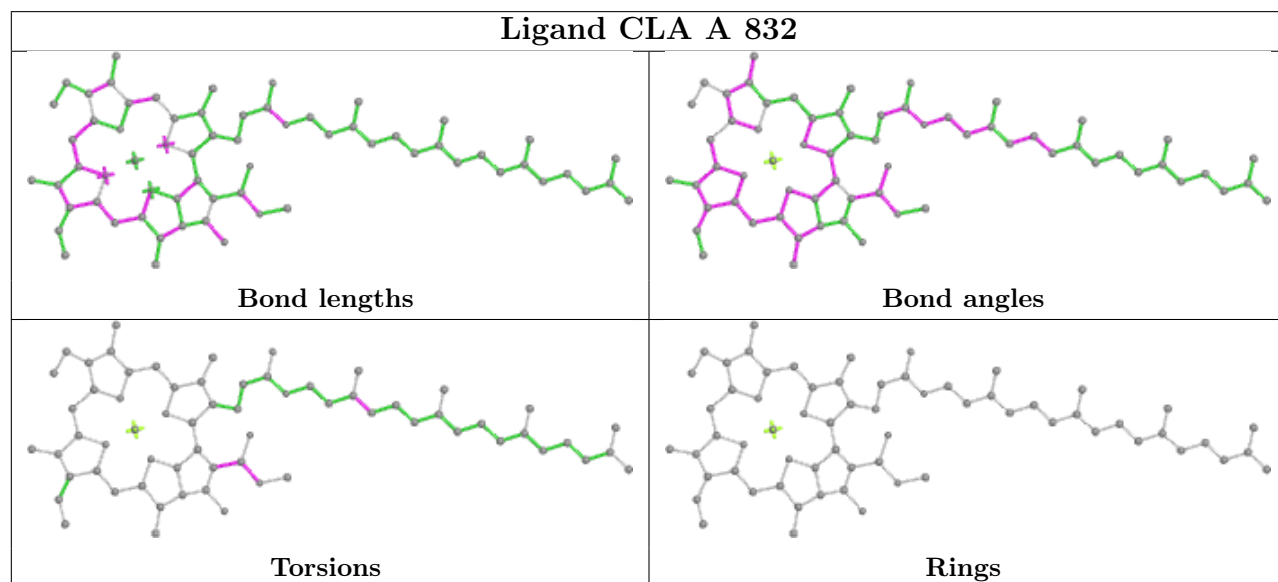


Ligand CLA A 826**Ligand CLA B 814**

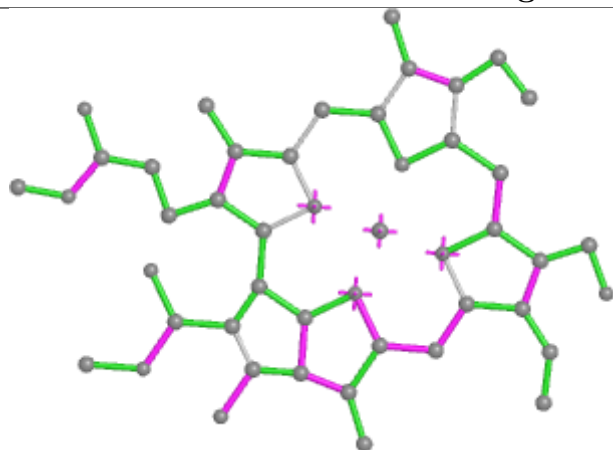
Ligand CLA A 822



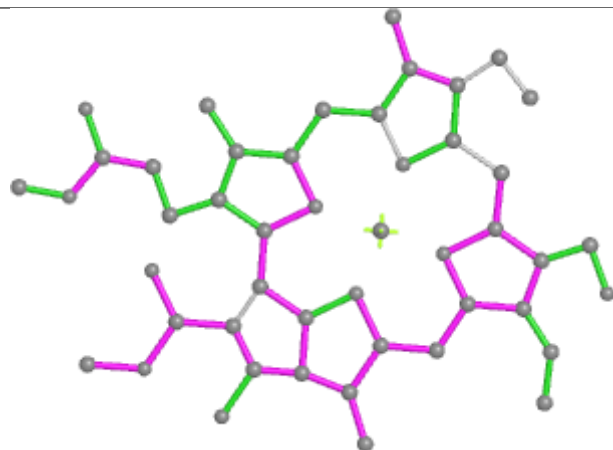
Ligand CLA A 832



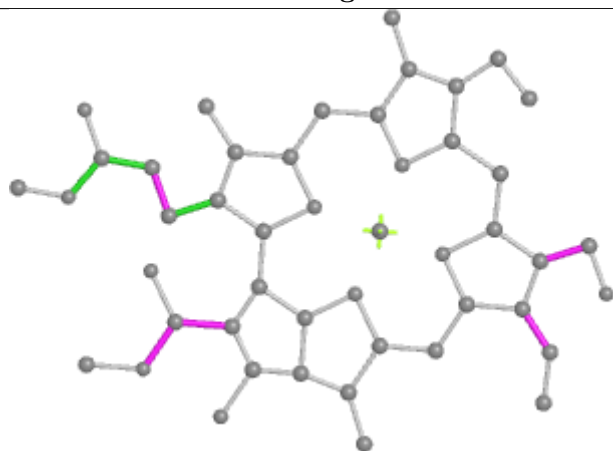
Ligand CHL 6 320



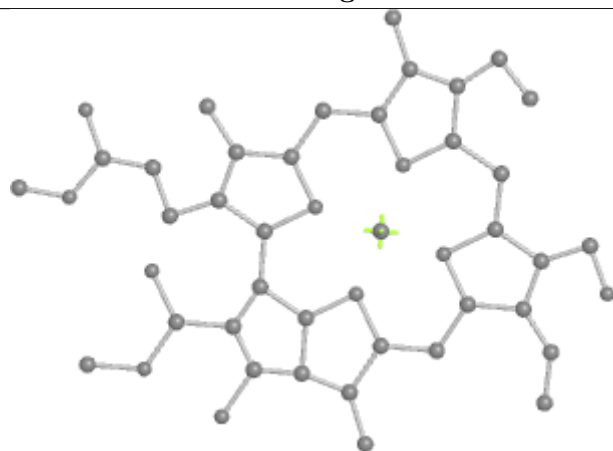
Bond lengths



Bond angles

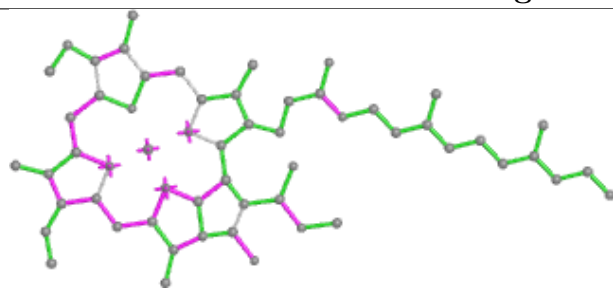


Torsions

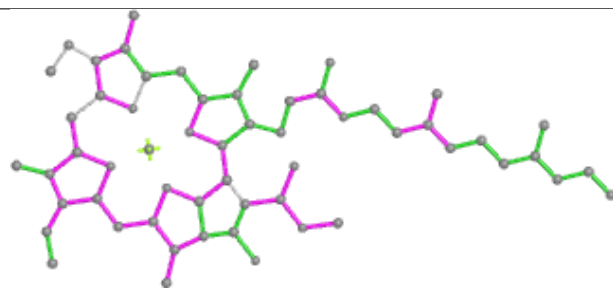


Rings

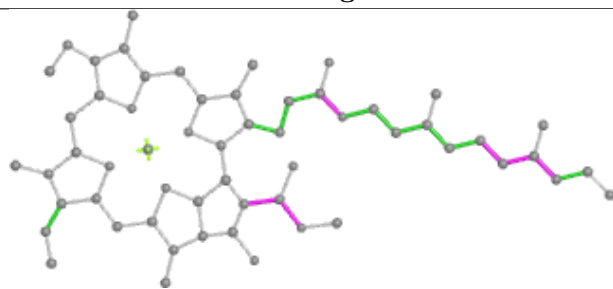
Ligand CLA B 824



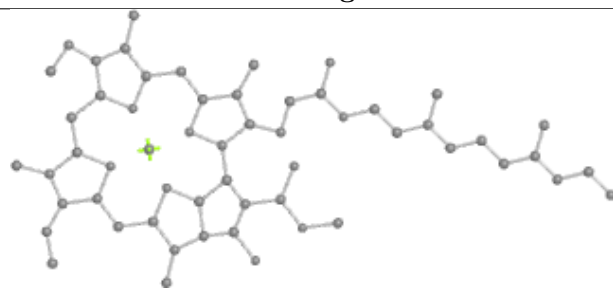
Bond lengths



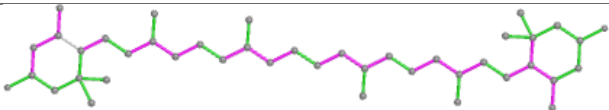
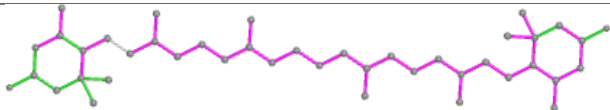
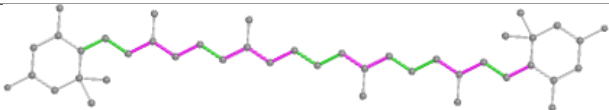
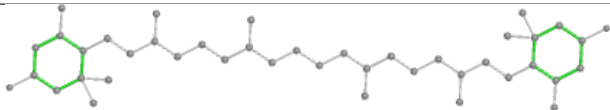
Bond angles

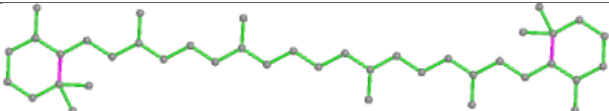
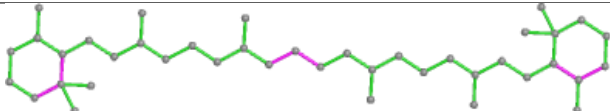
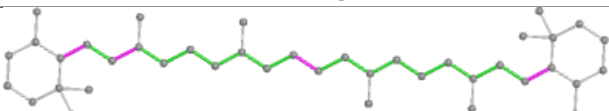
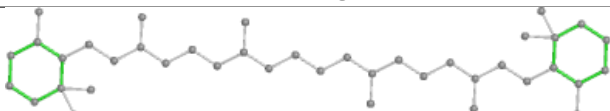


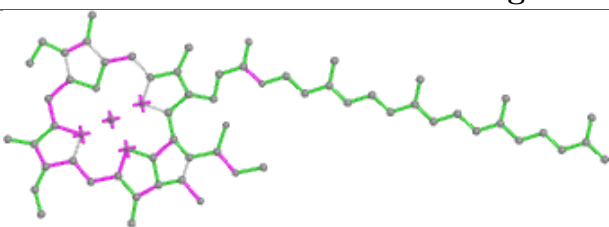
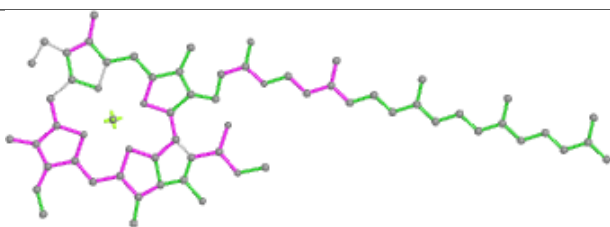
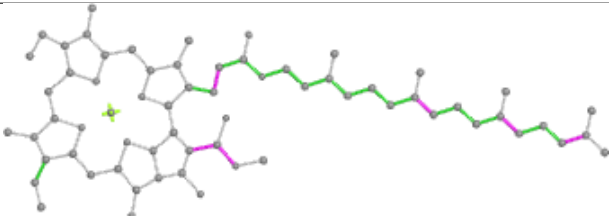
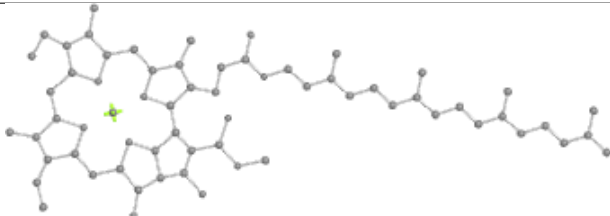
Torsions



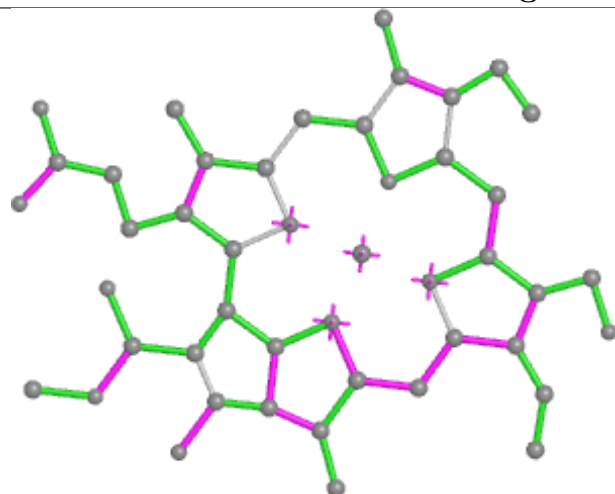
Rings

Ligand LUT 3 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

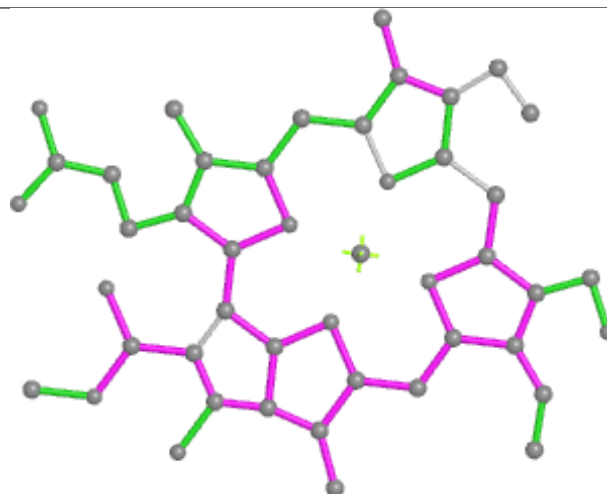
Ligand BCR M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

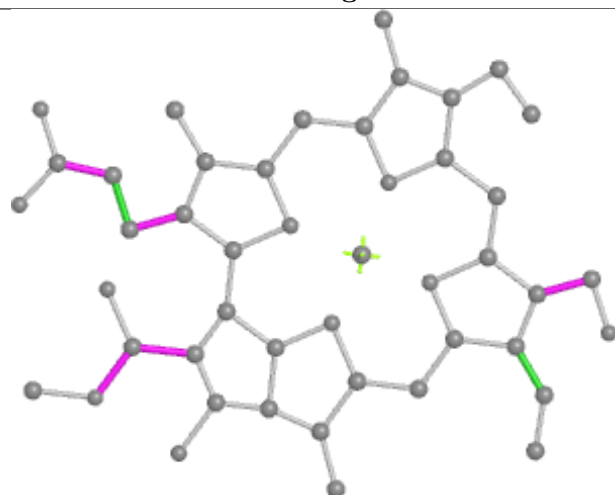
Ligand CHL 6 318



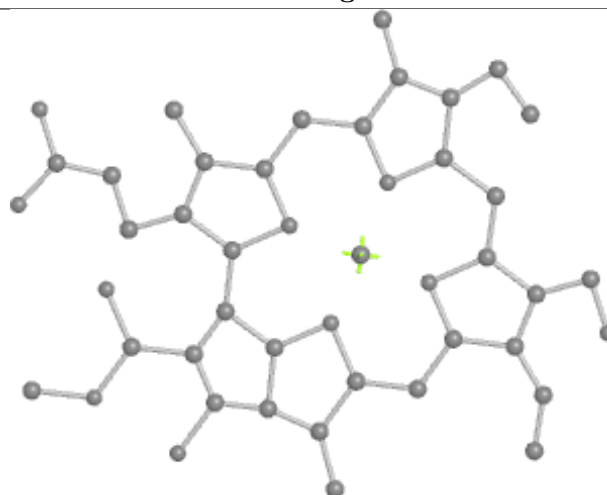
Bond lengths



Bond angles

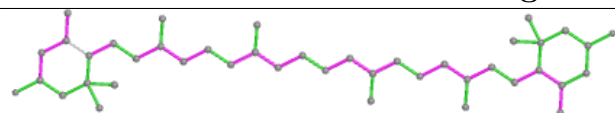


Torsions

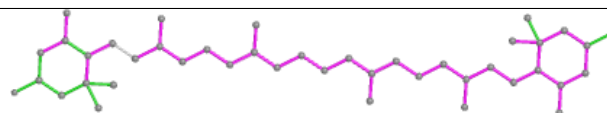


Rings

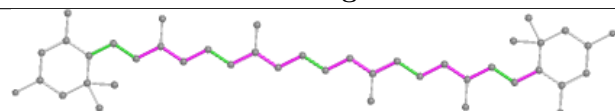
Ligand LUT 8 302



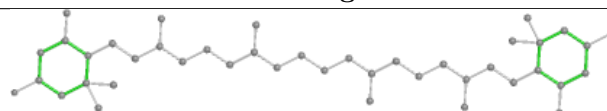
Bond lengths



Bond angles

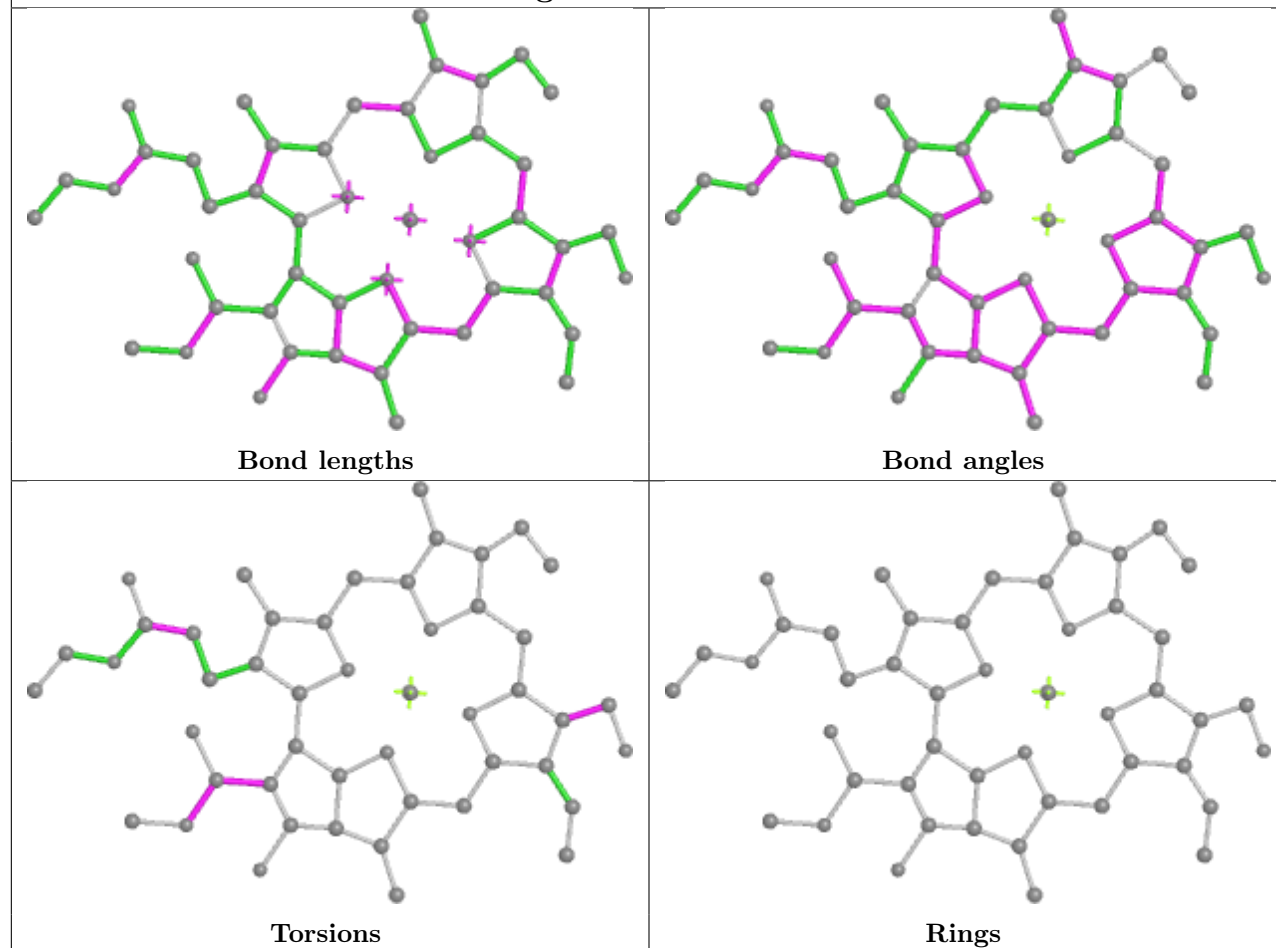


Torsions

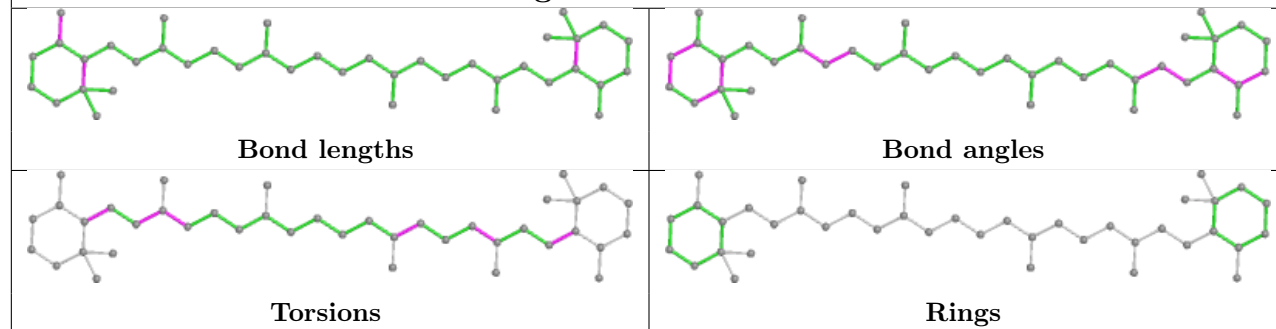


Rings

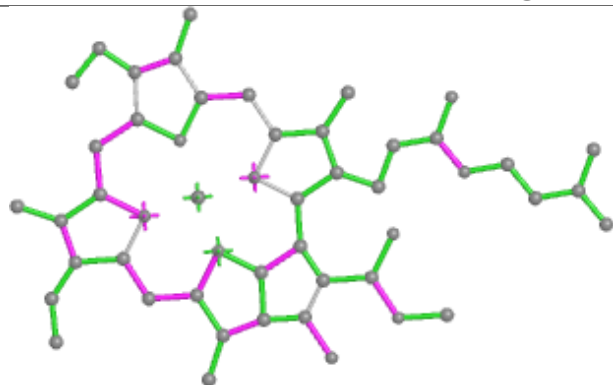
Ligand CHL a 320



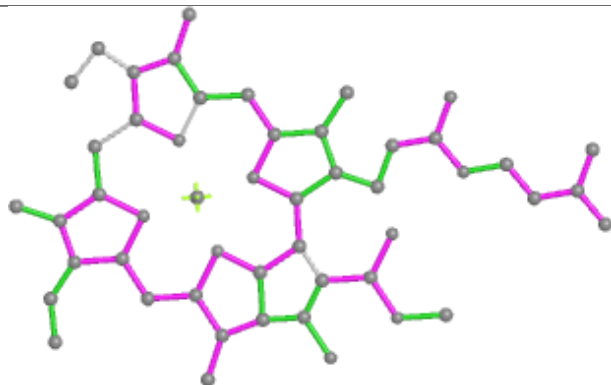
Ligand BCR 3 303



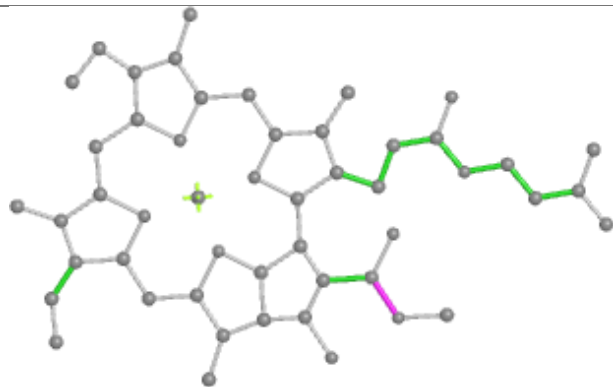
Ligand CLA 8 317



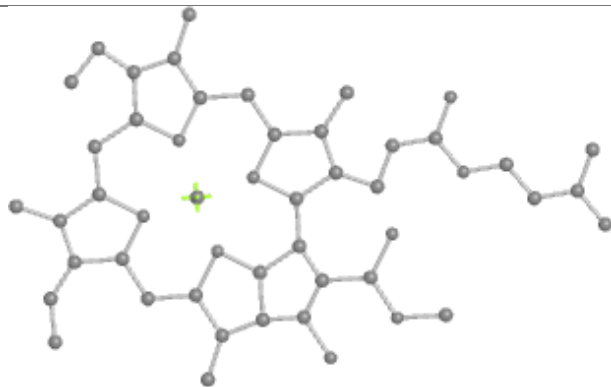
Bond lengths



Bond angles

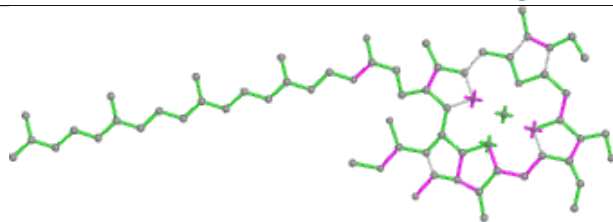


Torsions

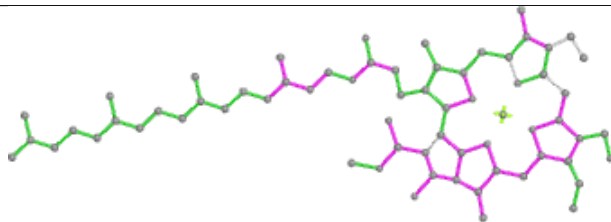


Rings

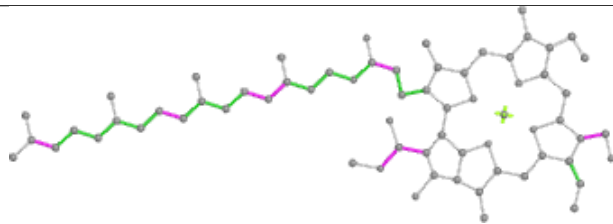
Ligand CHL A 840



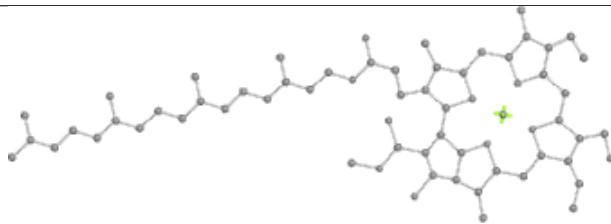
Bond lengths



Bond angles

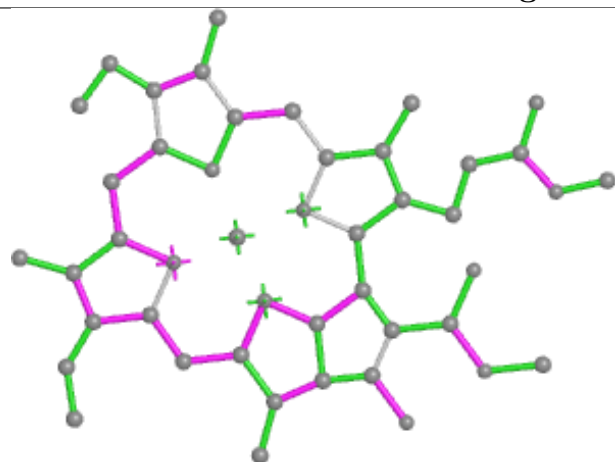


Torsions

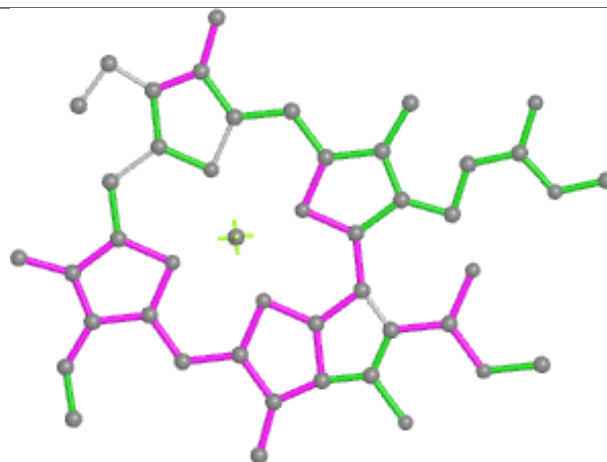


Rings

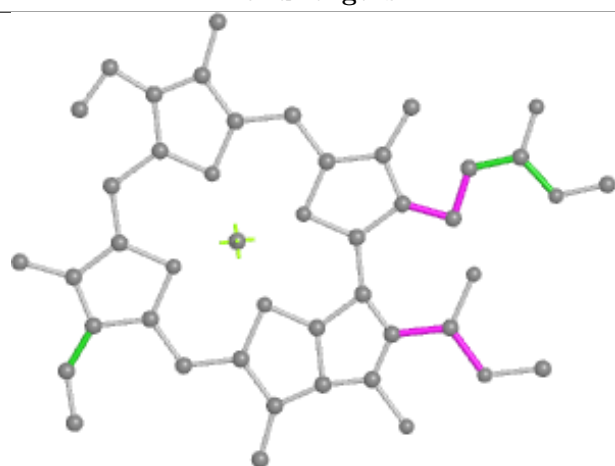
Ligand CLA b 310



Bond lengths



Bond angles

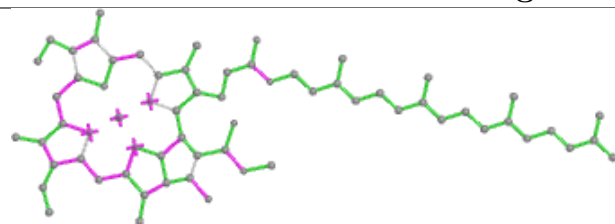


Torsions

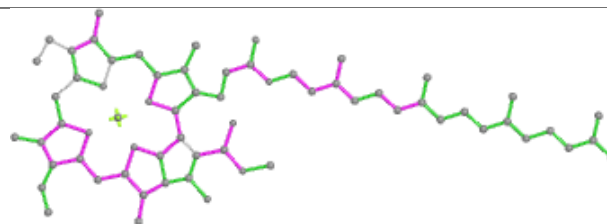


Rings

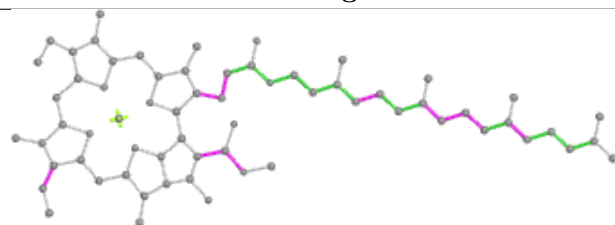
Ligand CLA B 822



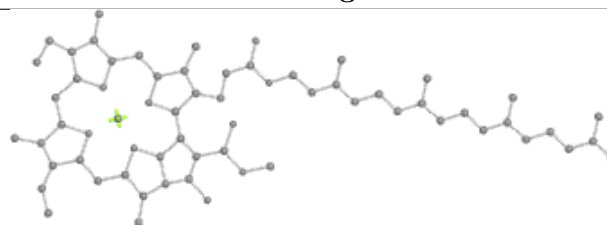
Bond lengths



Bond angles

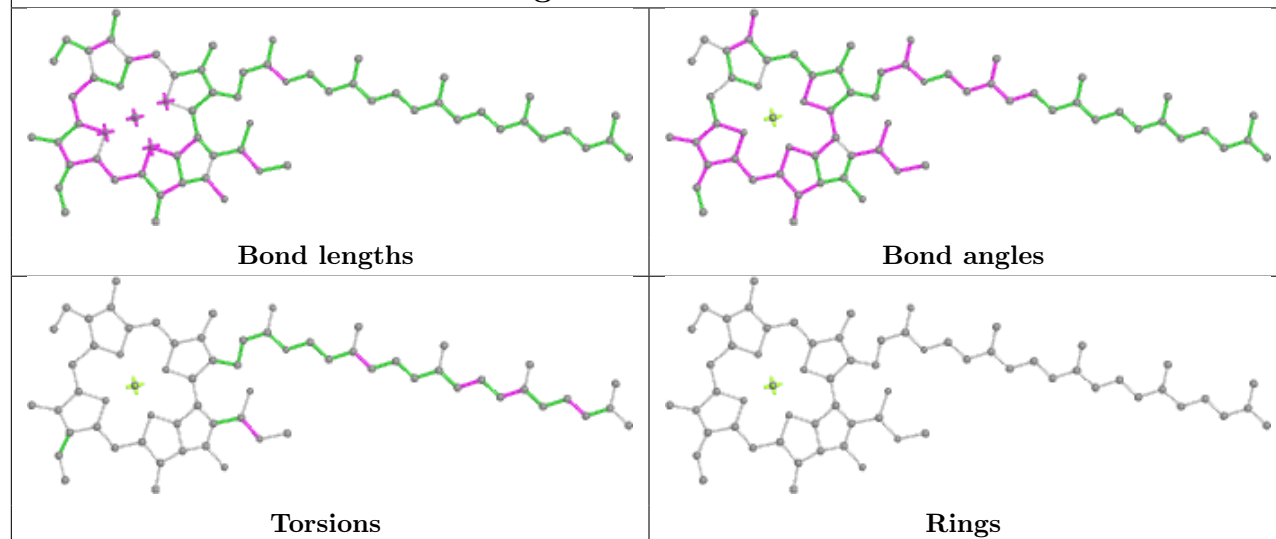


Torsions

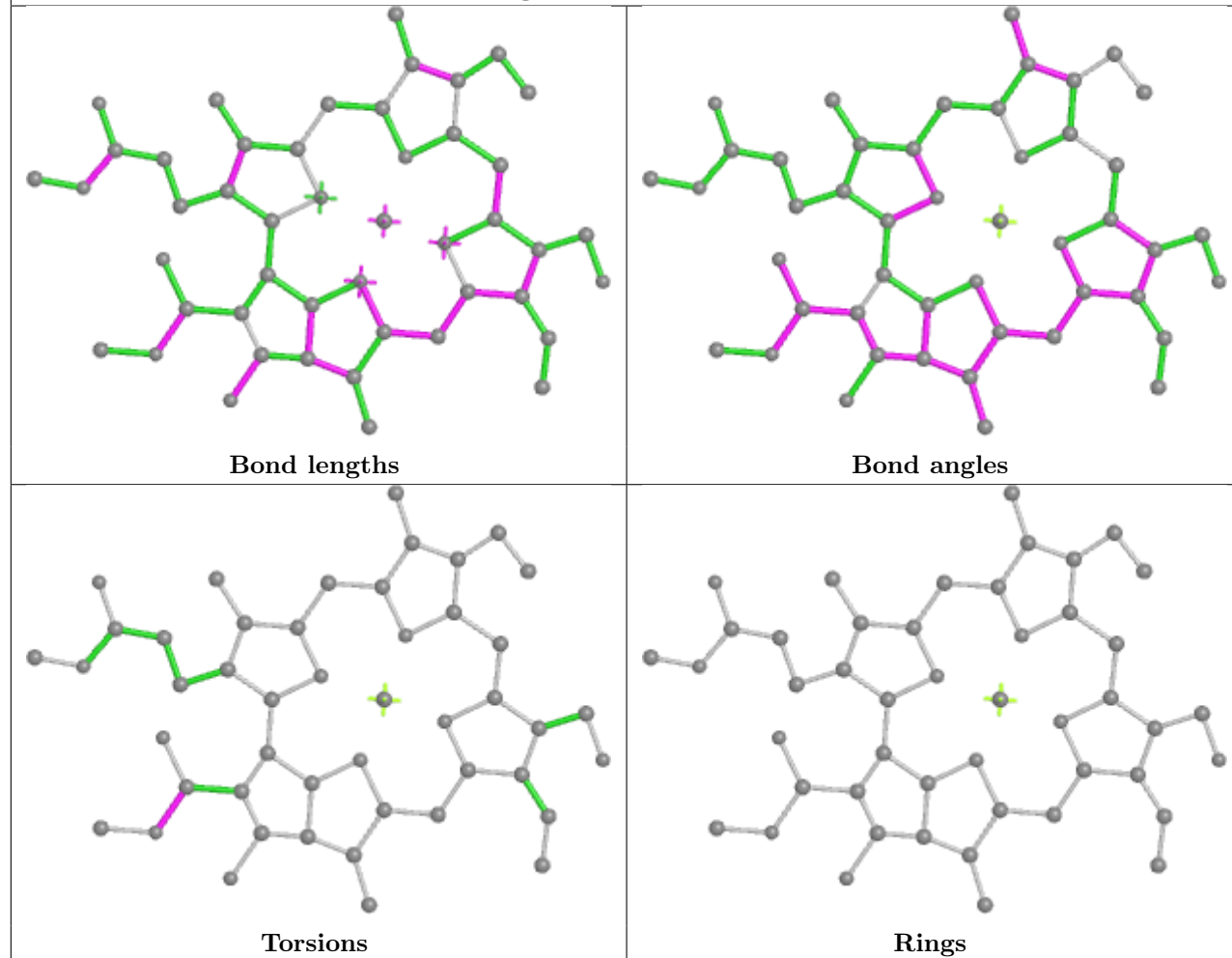


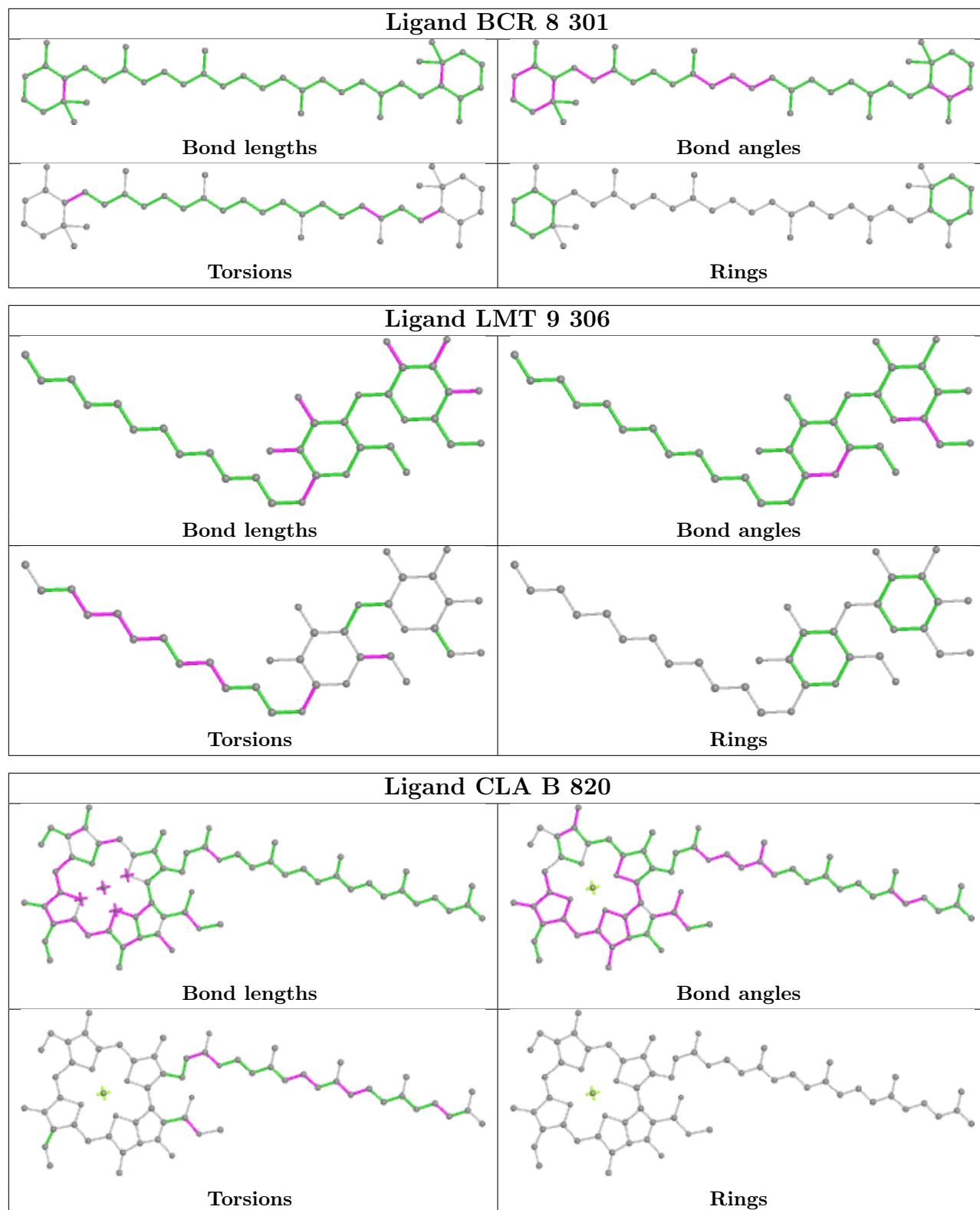
Rings

Ligand CLA F 301

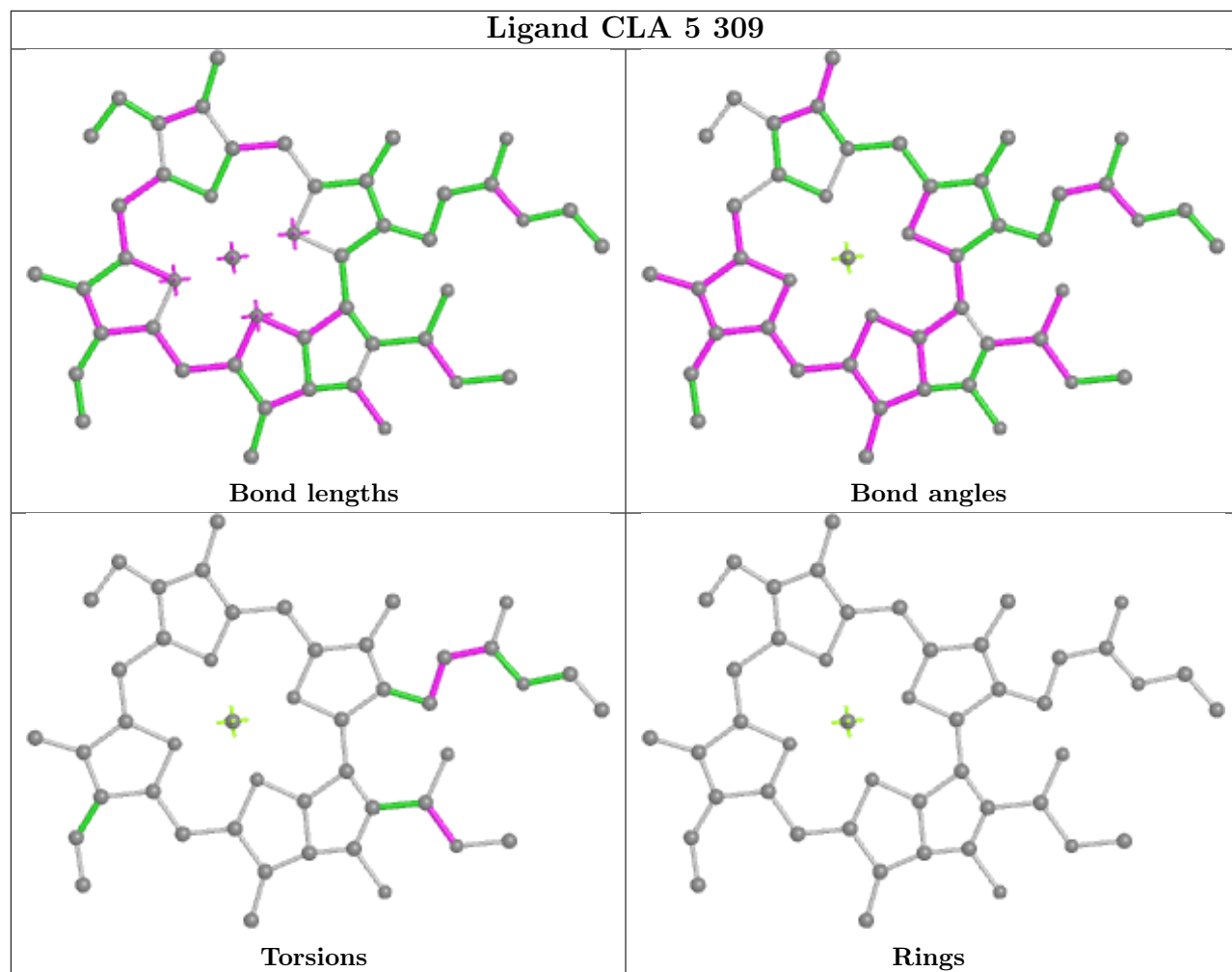


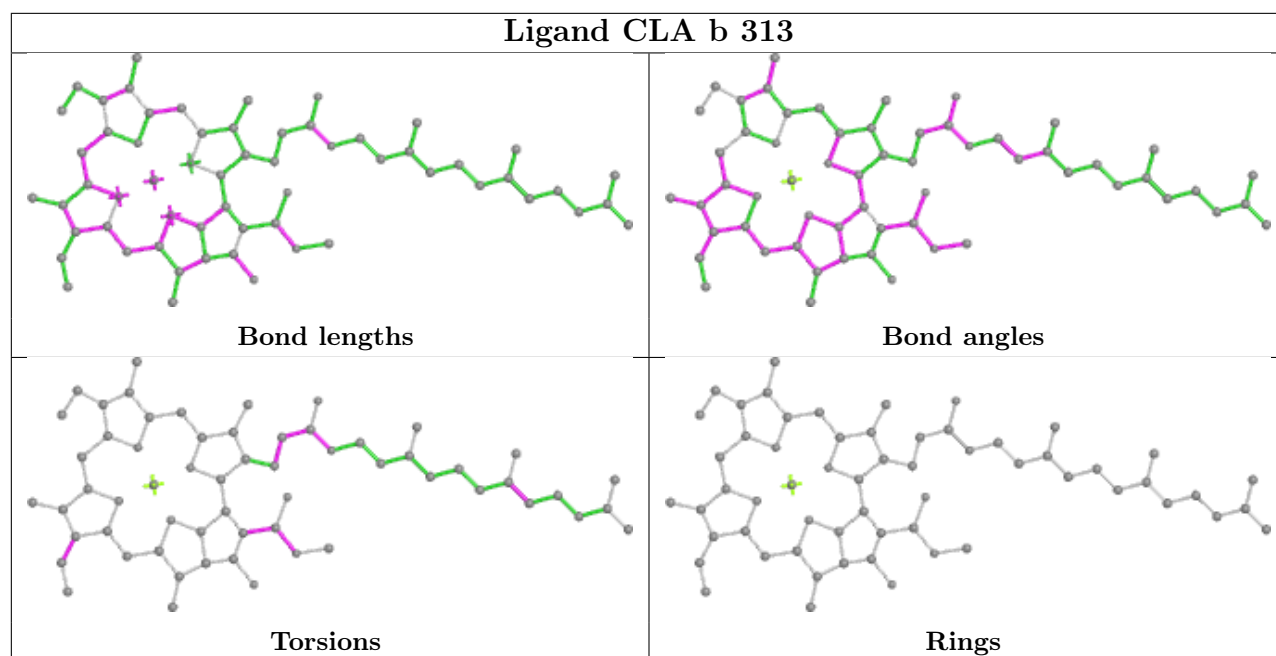
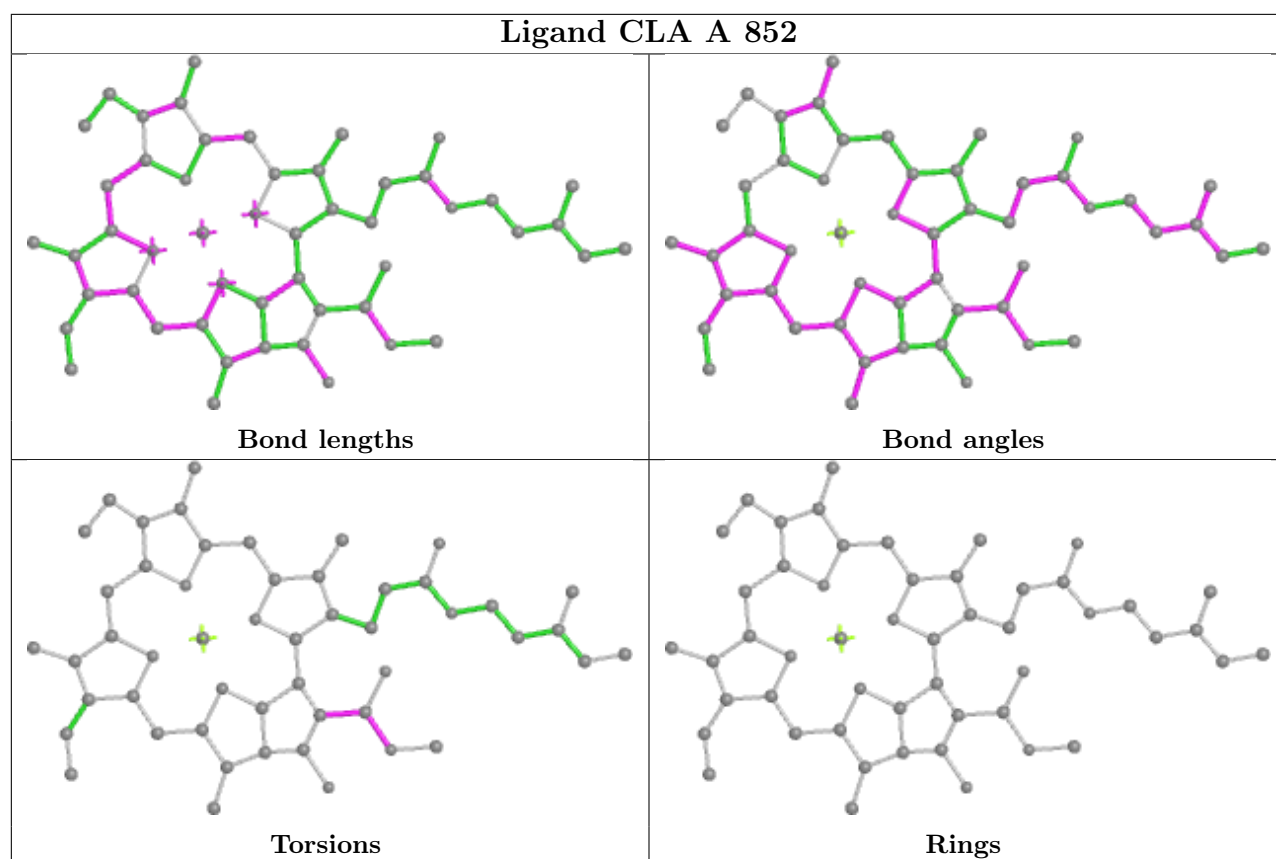
Ligand CHL 7 319



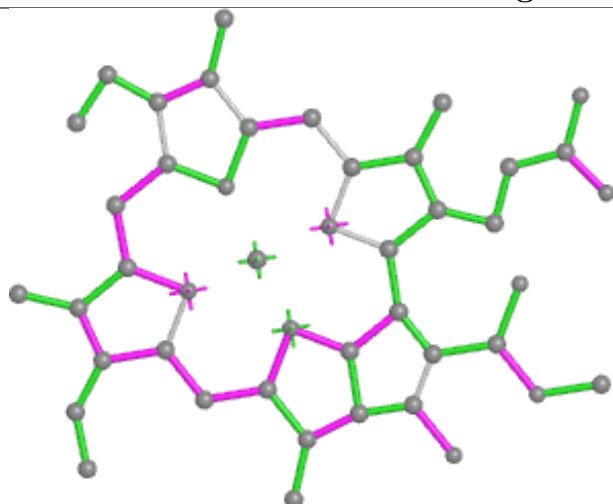


Ligand CLA 5 309

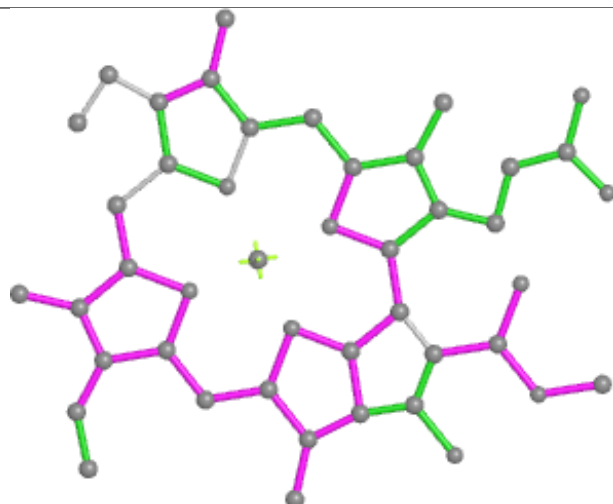




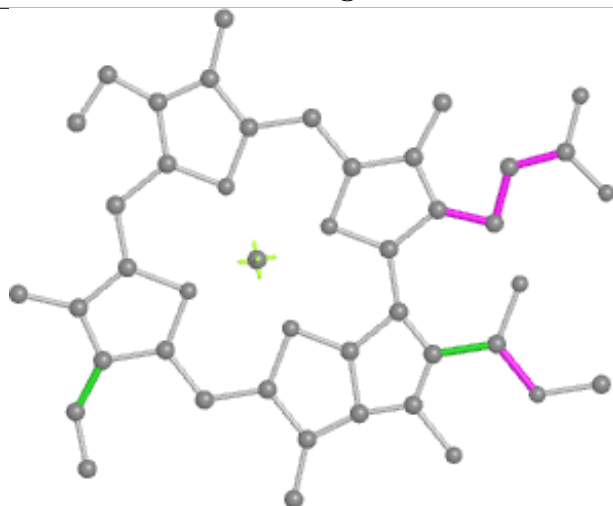
Ligand CLA L 307



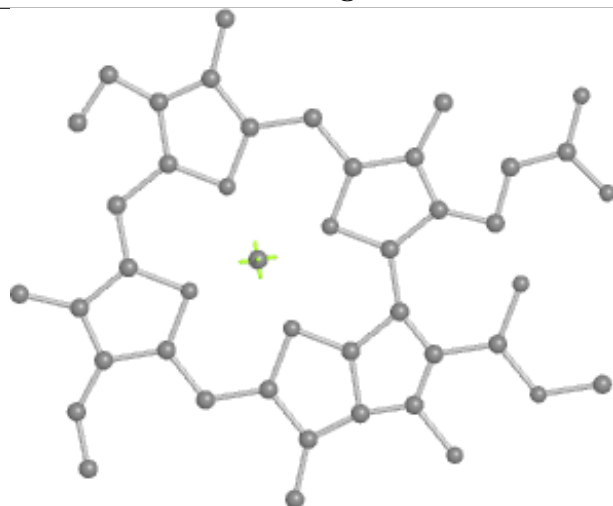
Bond lengths



Bond angles

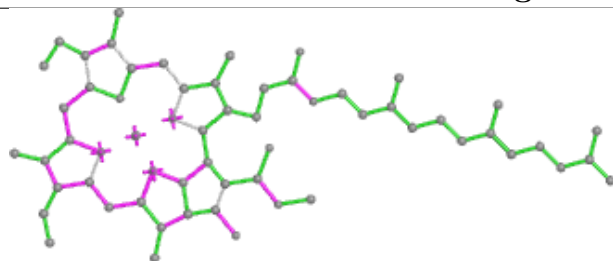


Torsions

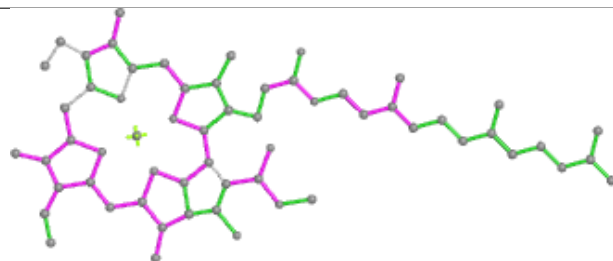


Rings

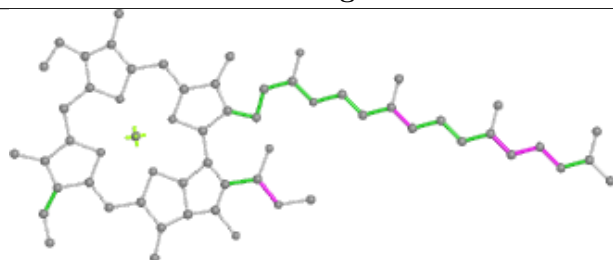
Ligand CLA B 825



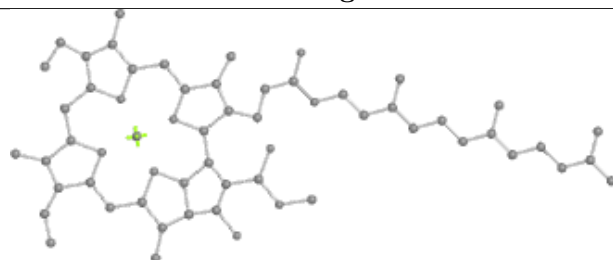
Bond lengths



Bond angles

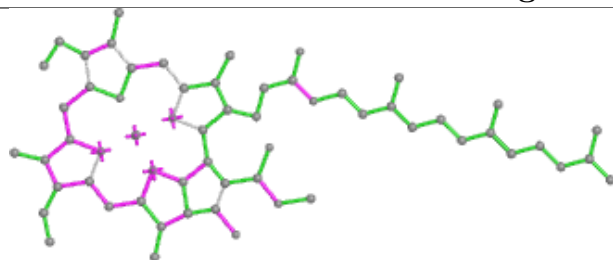


Torsions

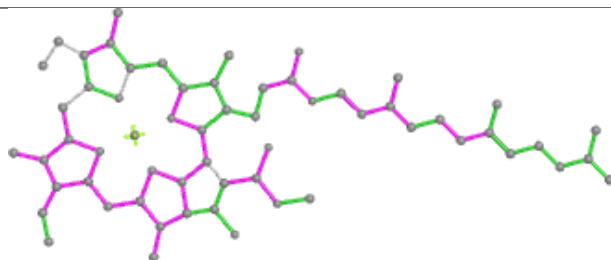


Rings

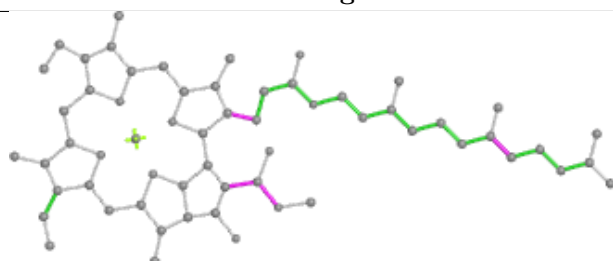
Ligand CLA a 309



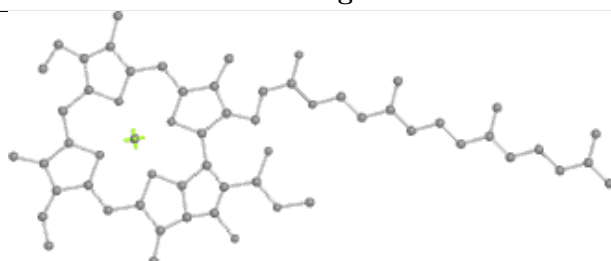
Bond lengths



Bond angles

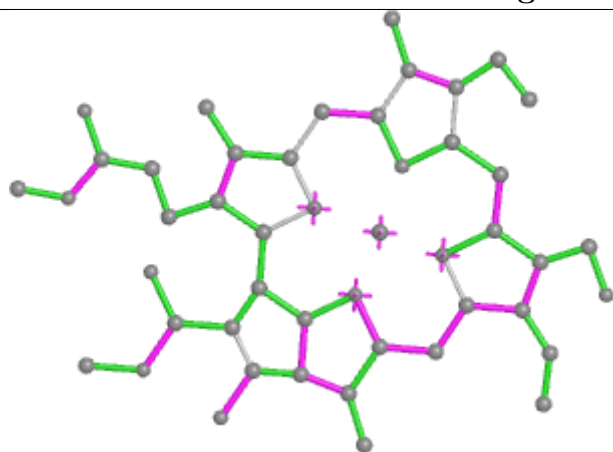


Torsions

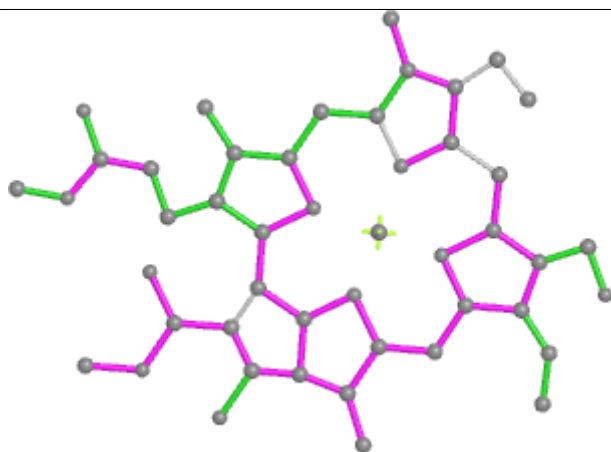


Rings

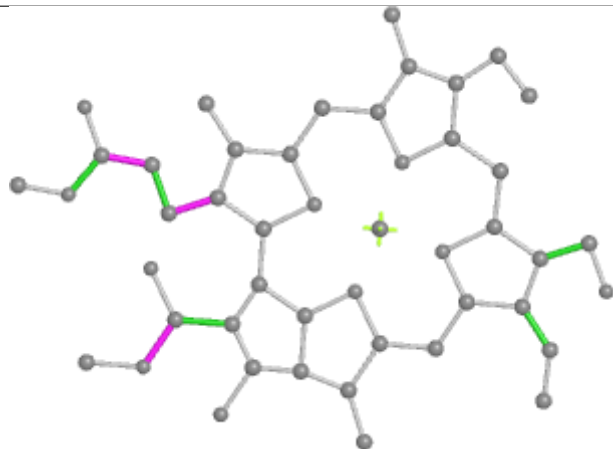
Ligand CHL 5 322



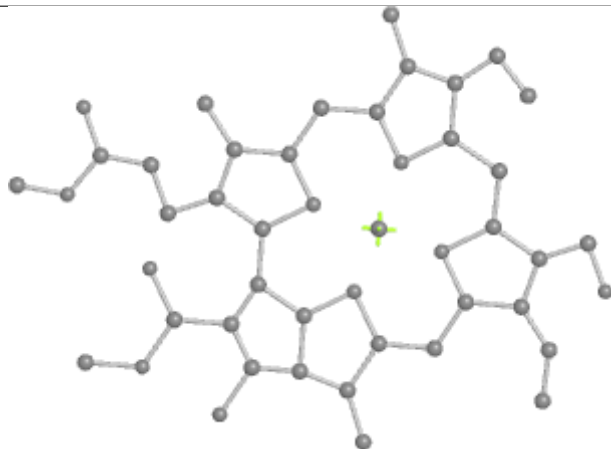
Bond lengths



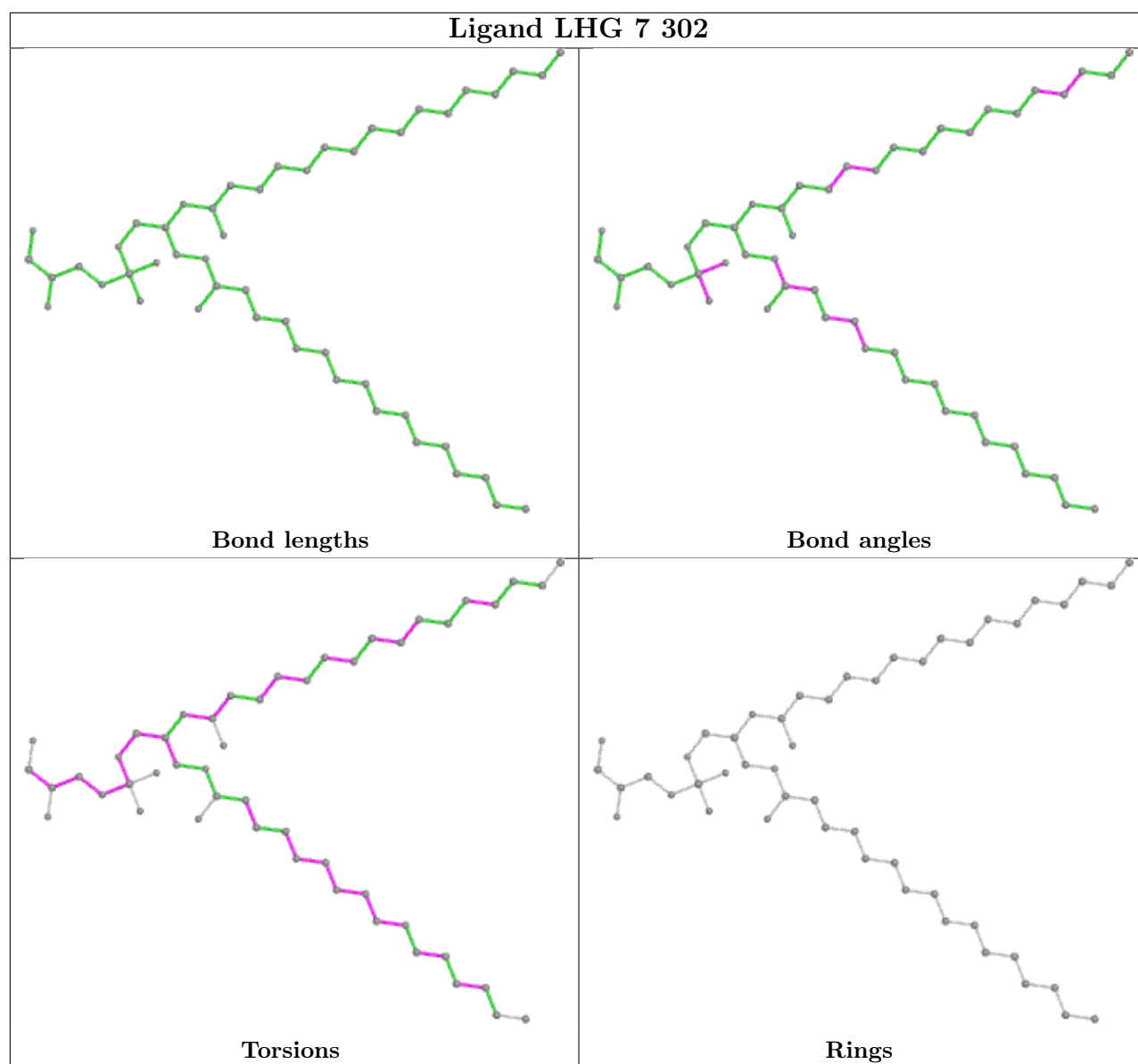
Bond angles



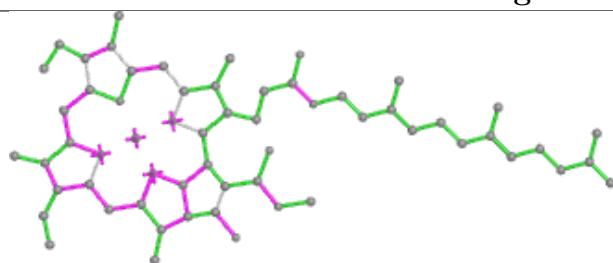
Torsions



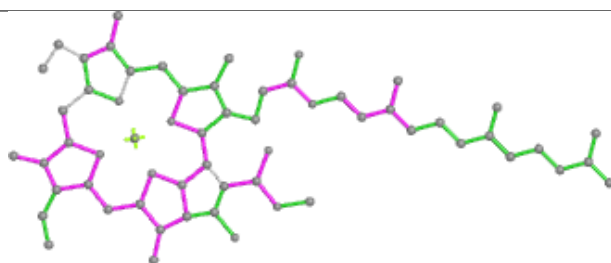
Rings



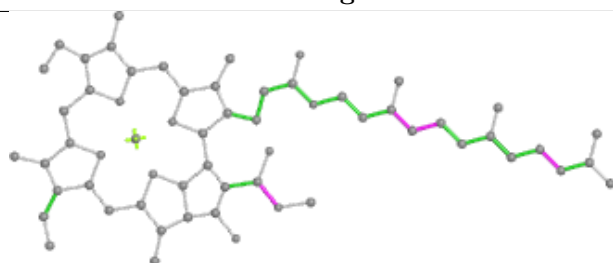
Ligand CLA A 836



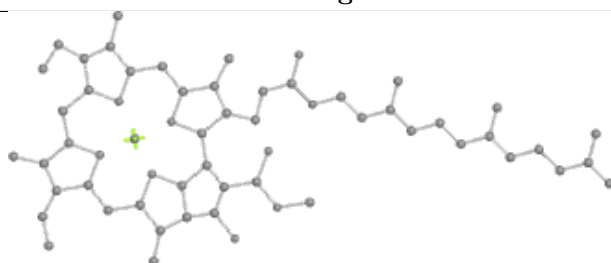
Bond lengths



Bond angles

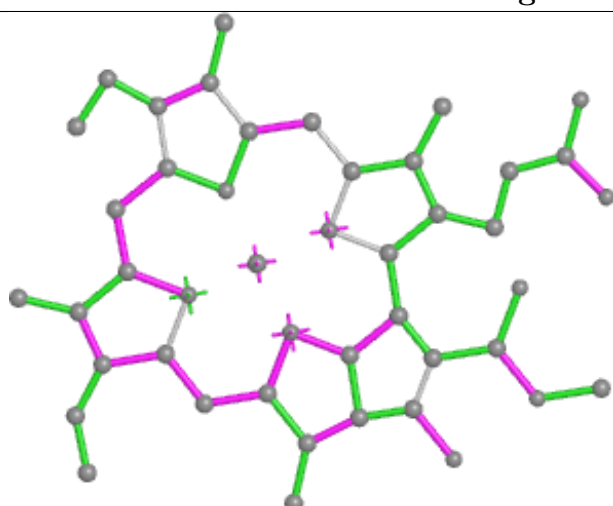


Torsions

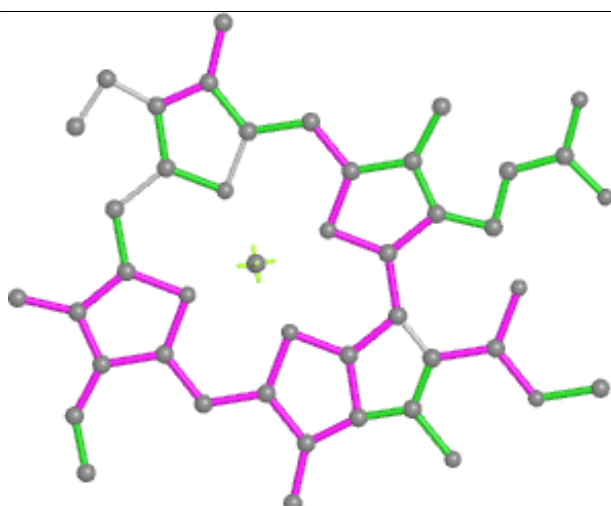


Rings

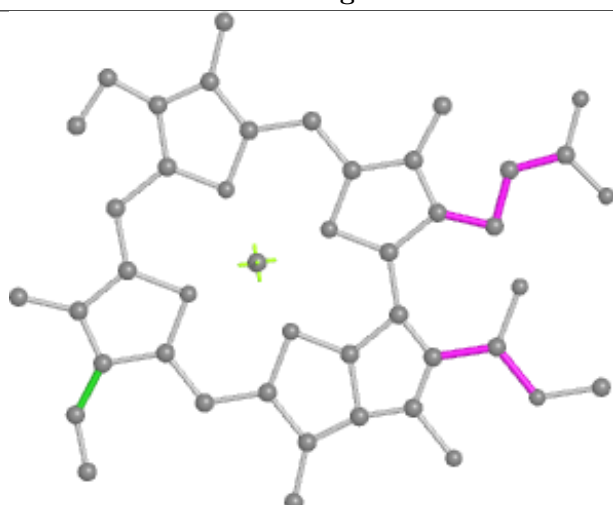
Ligand CLA a 316



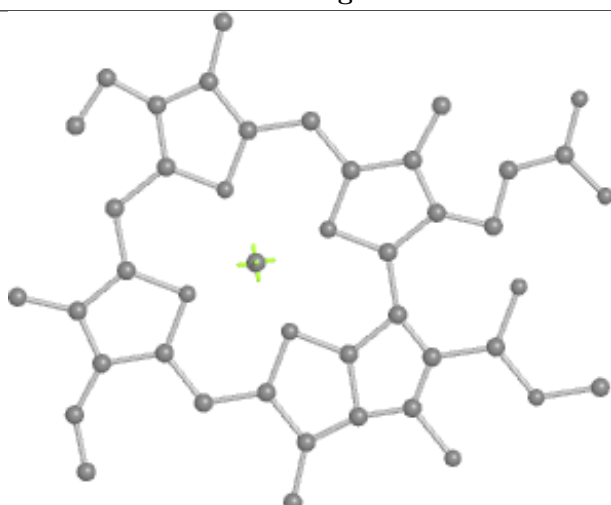
Bond lengths



Bond angles

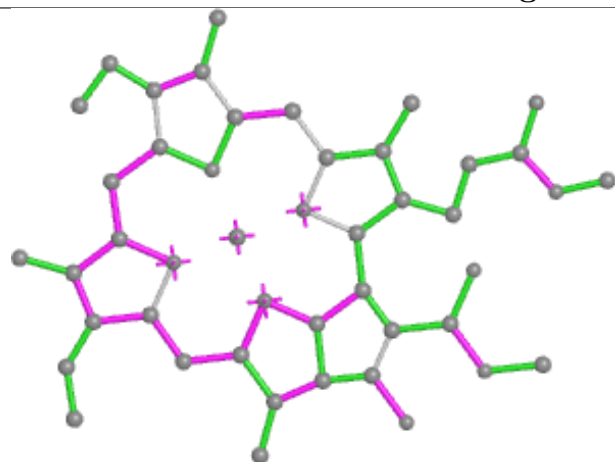


Torsions

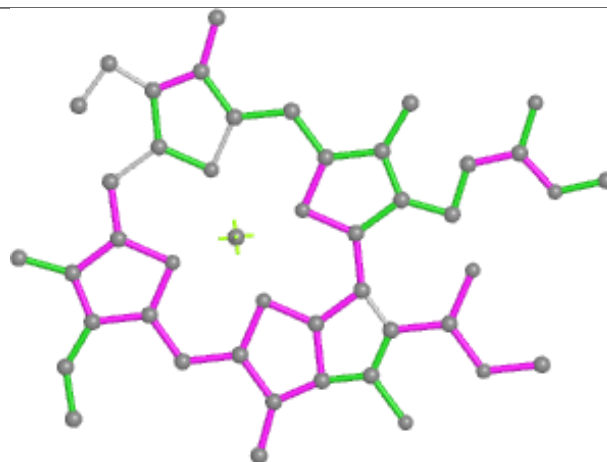


Rings

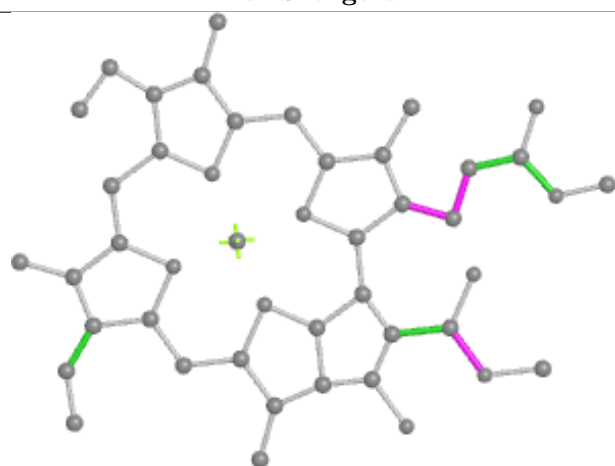
Ligand CLA b 311



Bond lengths



Bond angles

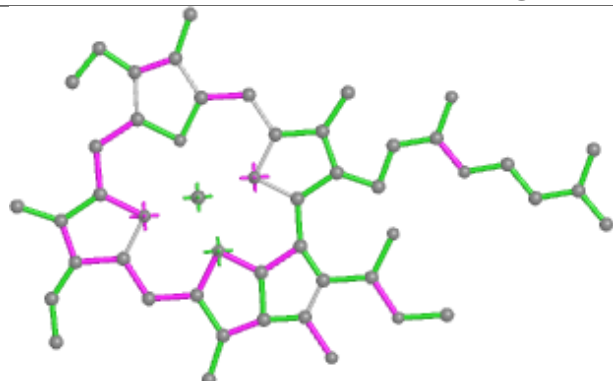


Torsions

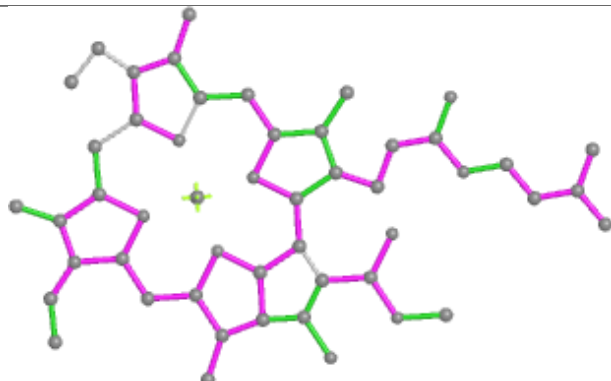


Rings

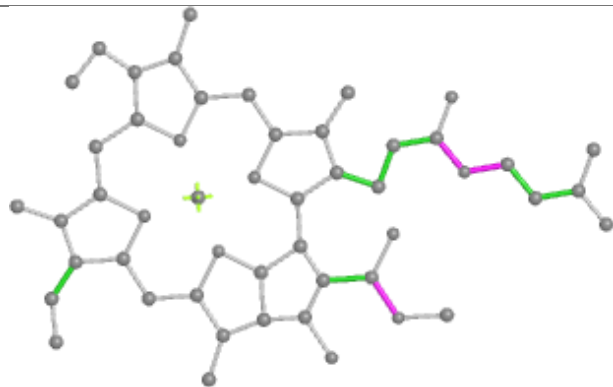
Ligand CLA G 204



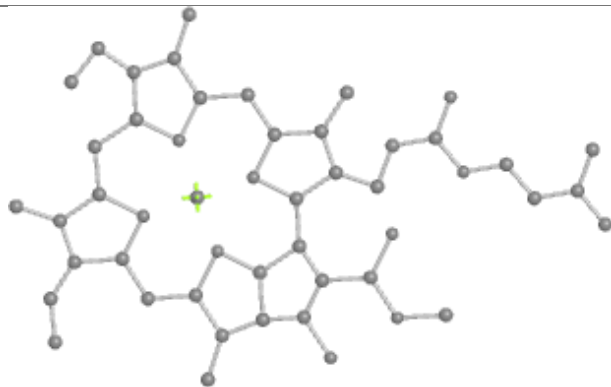
Bond lengths



Bond angles

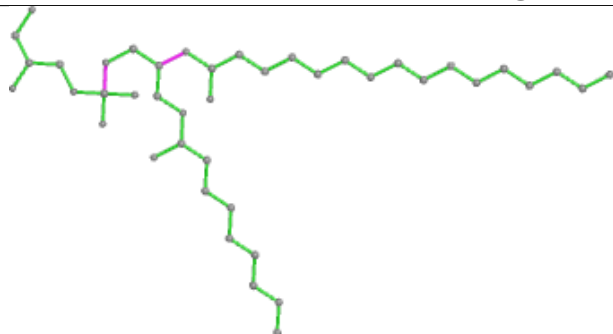


Torsions

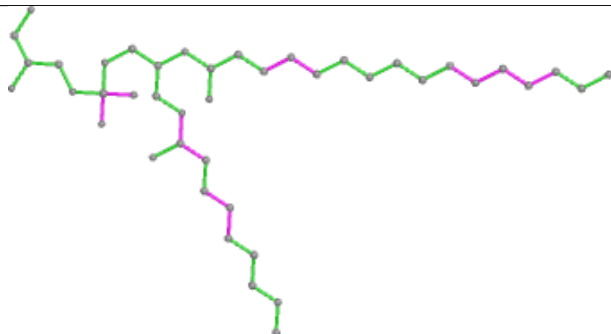


Rings

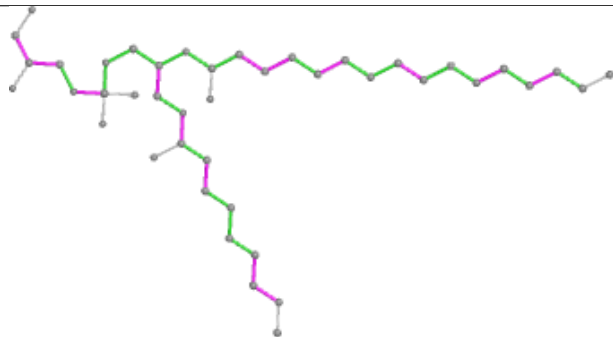
Ligand LHG A 809



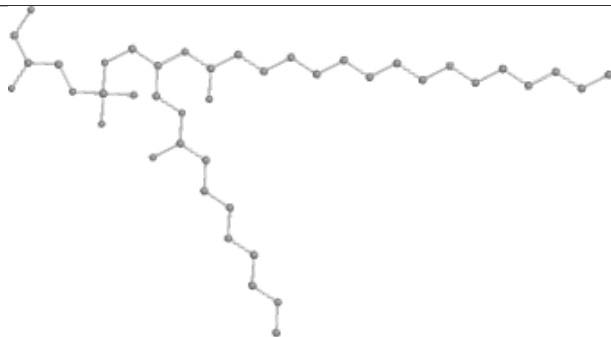
Bond lengths



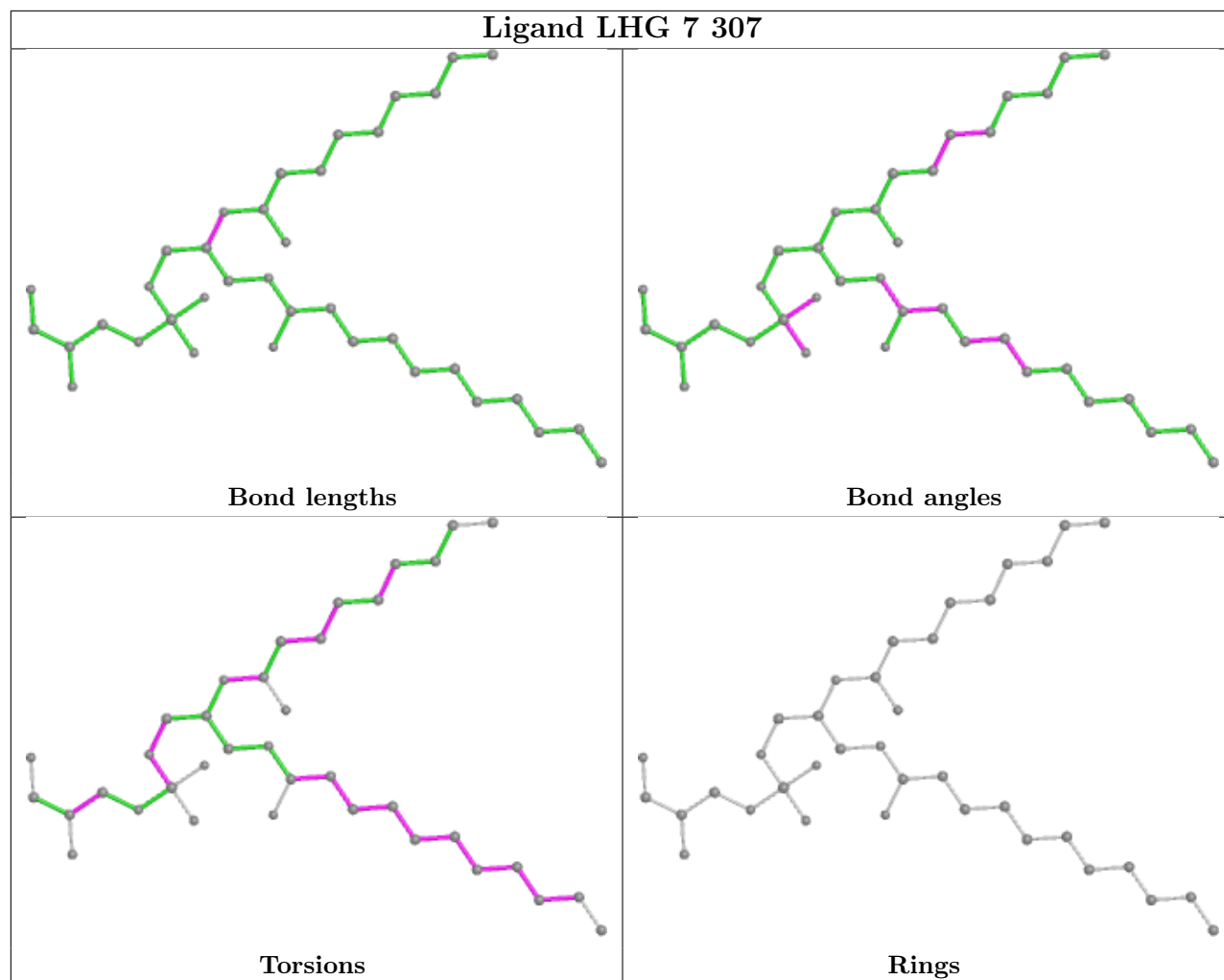
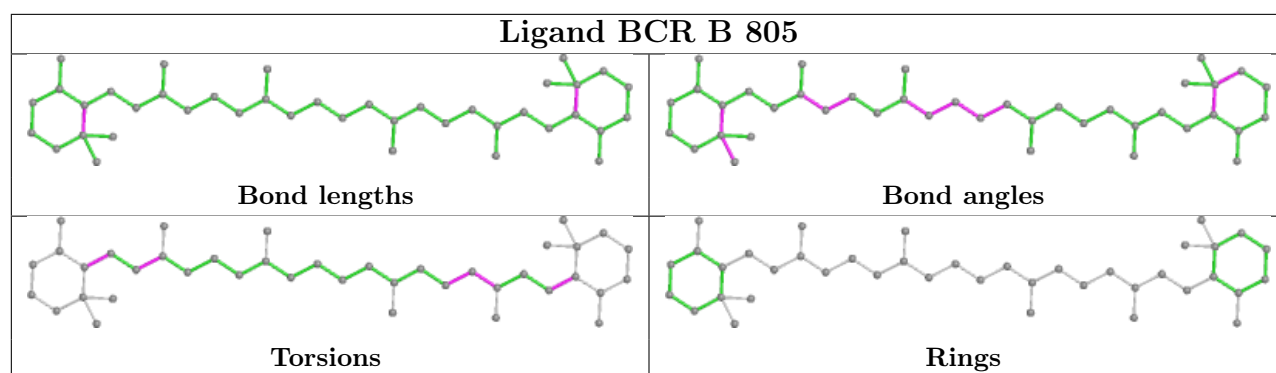
Bond angles



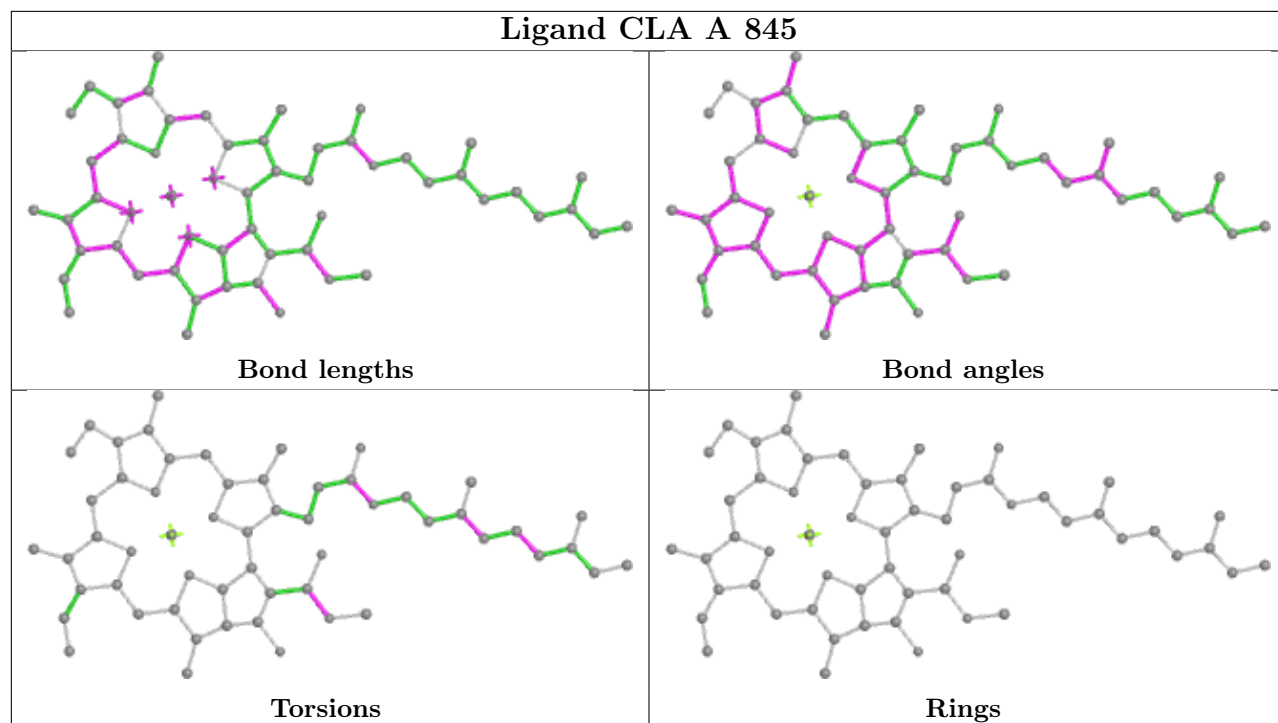
Torsions



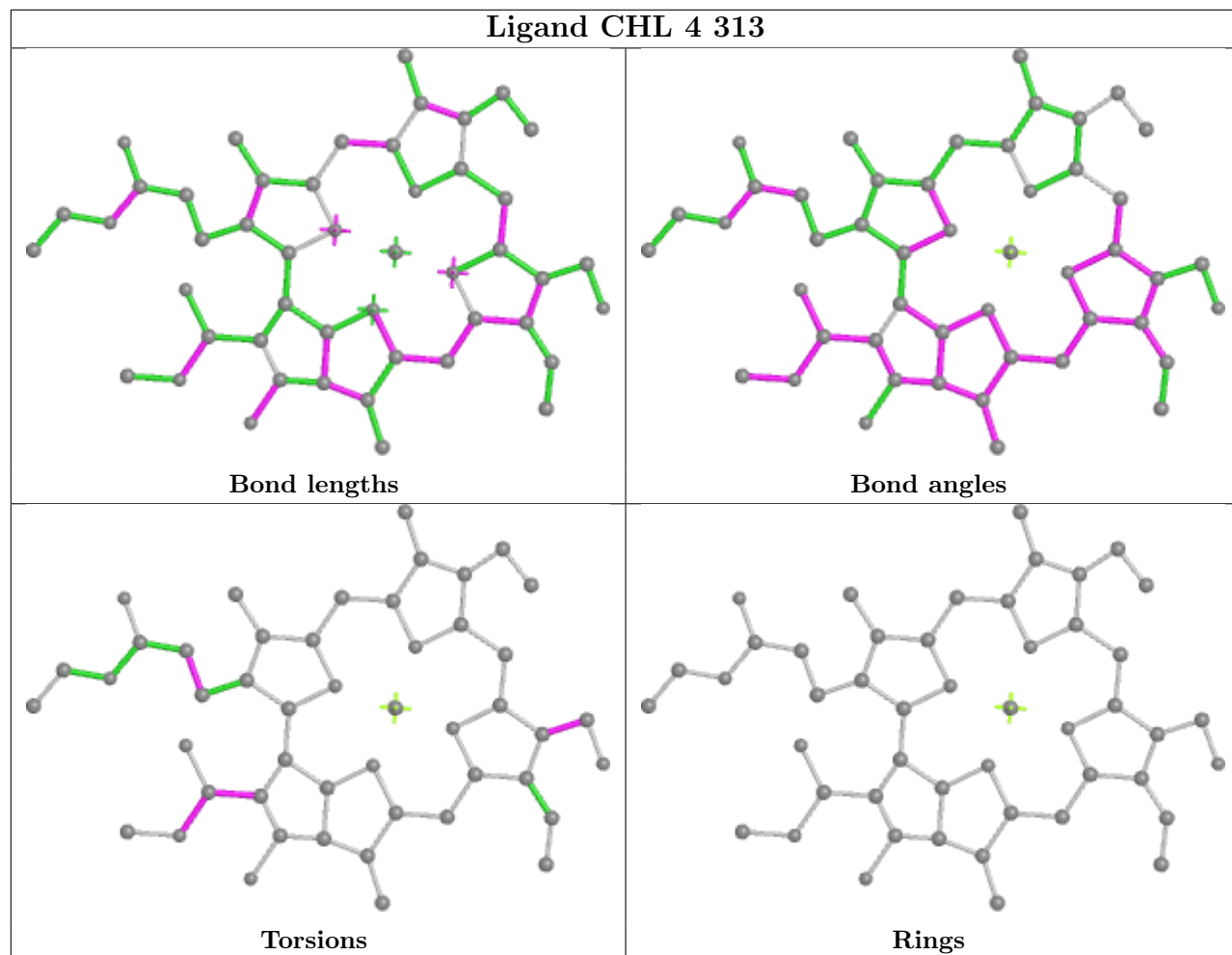
Rings

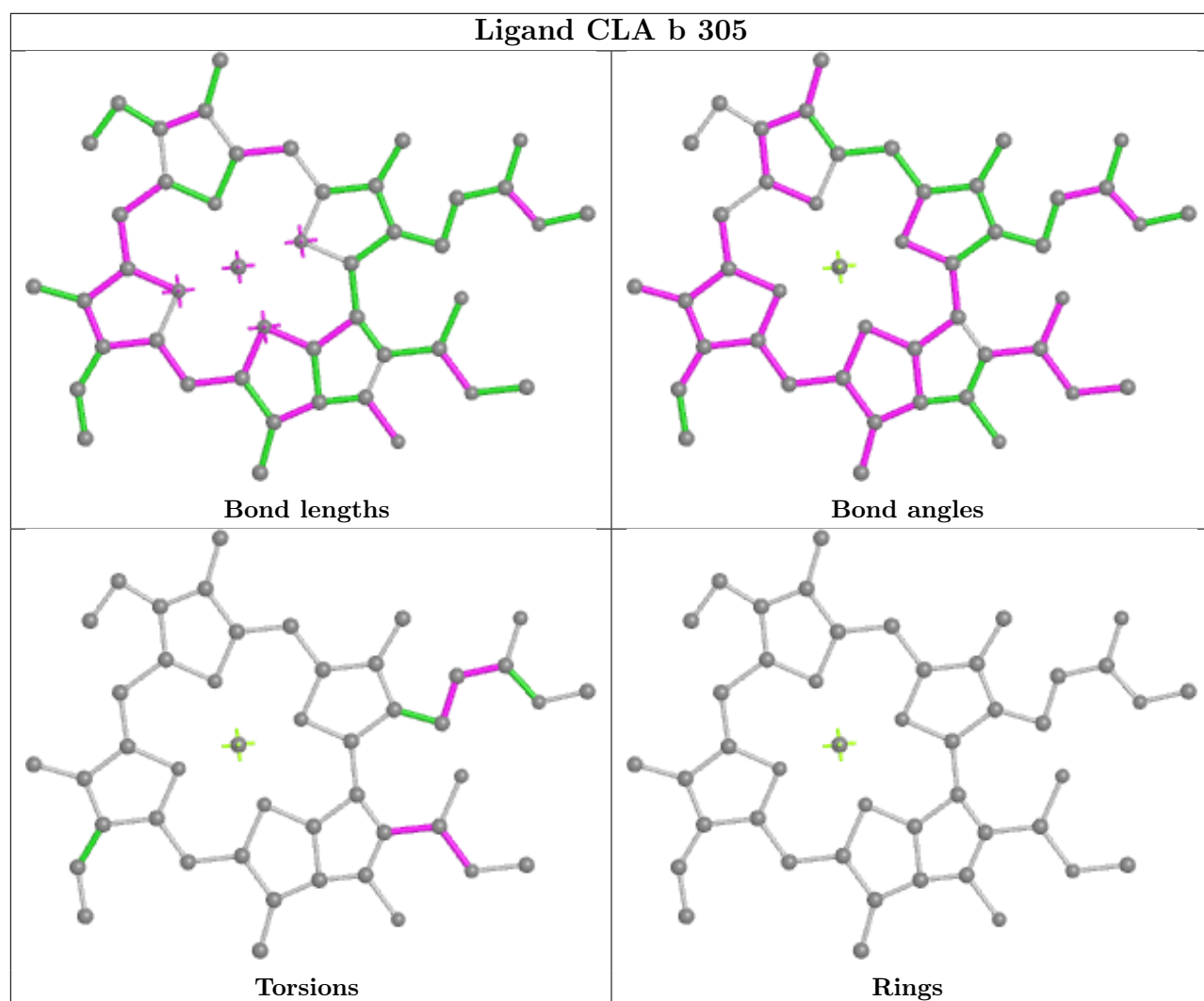
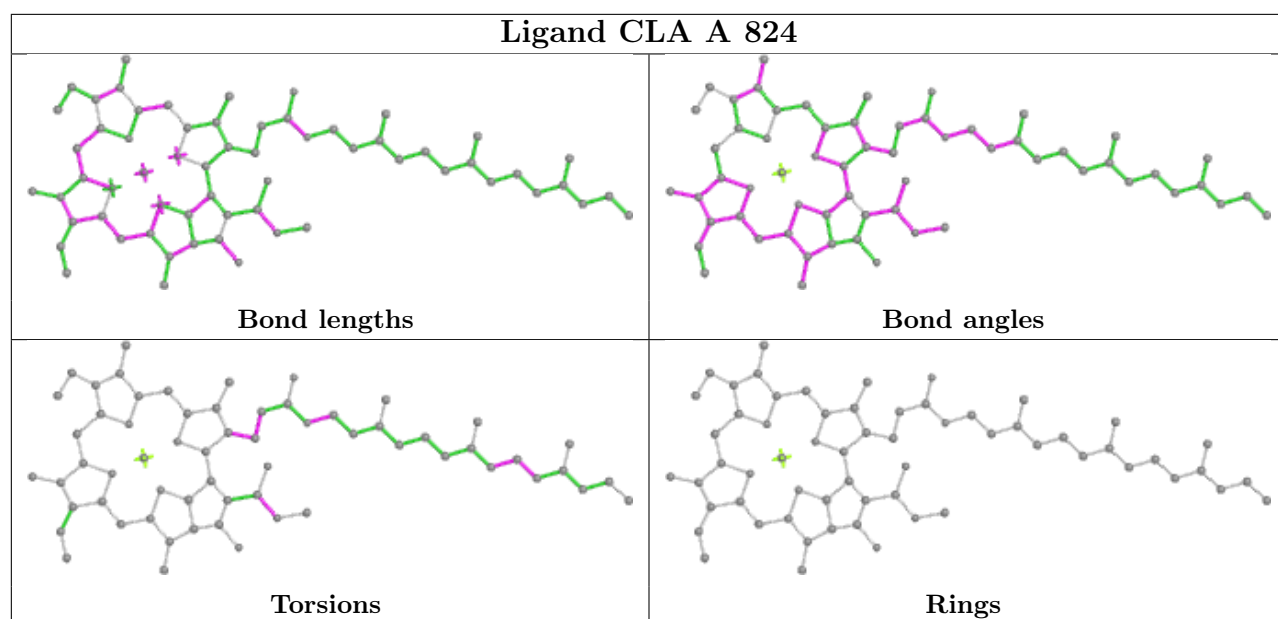


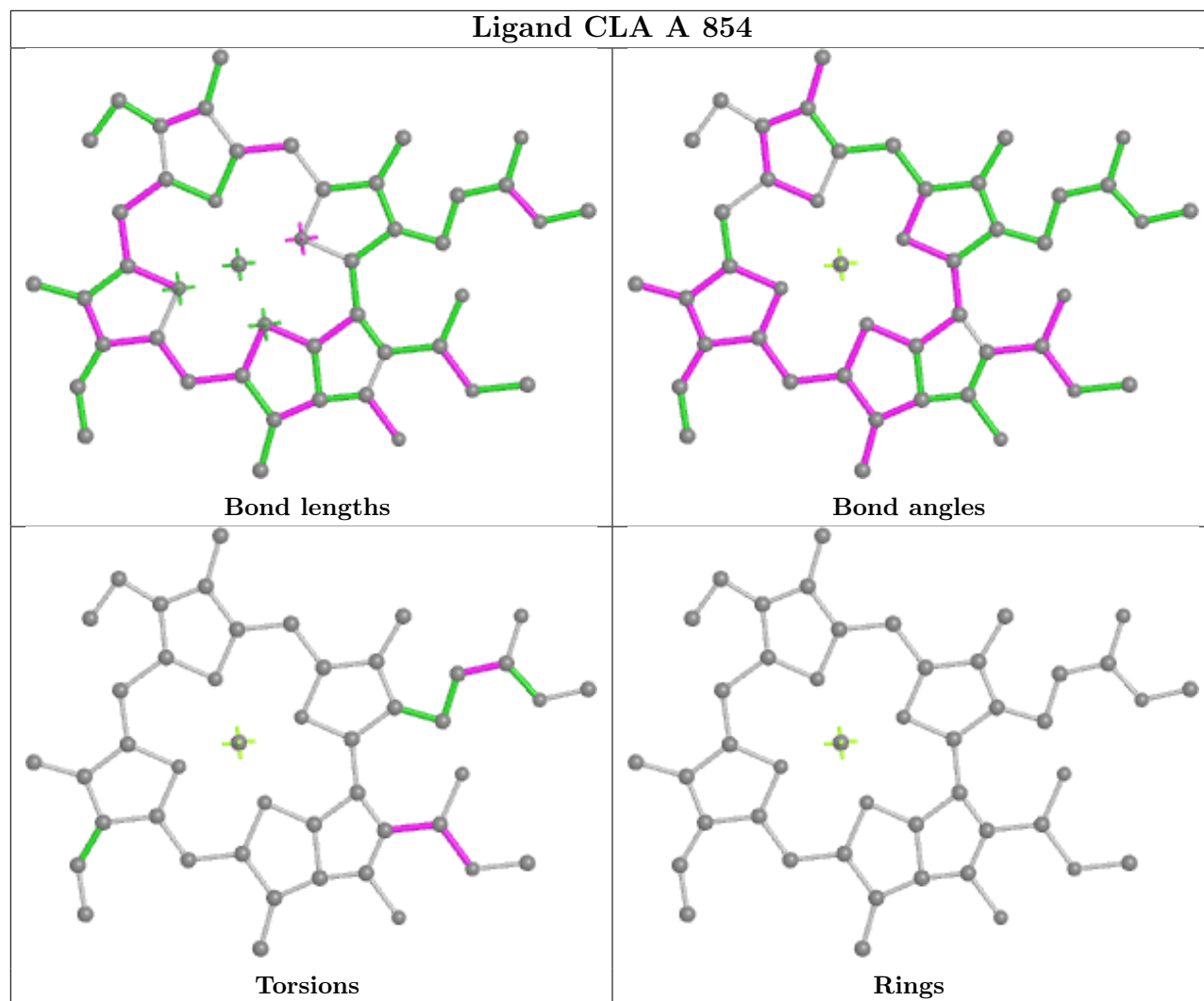
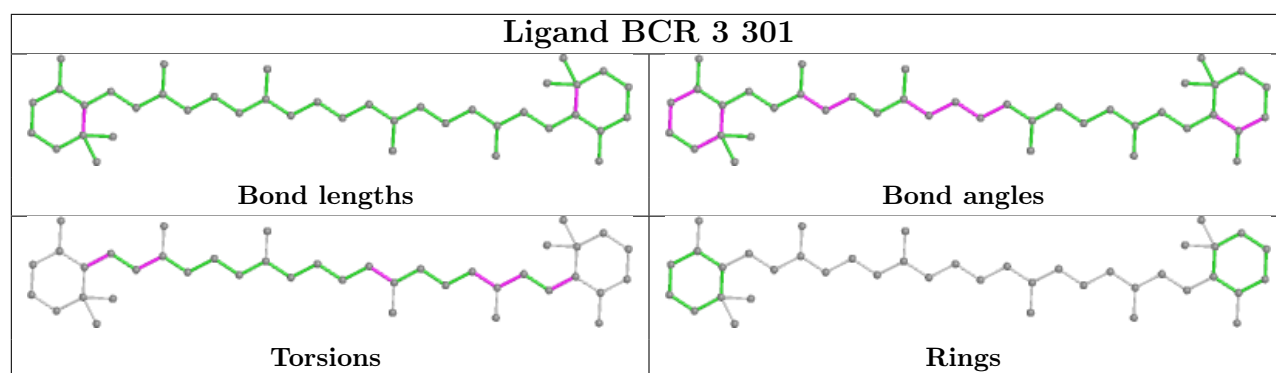
Ligand CLA A 845



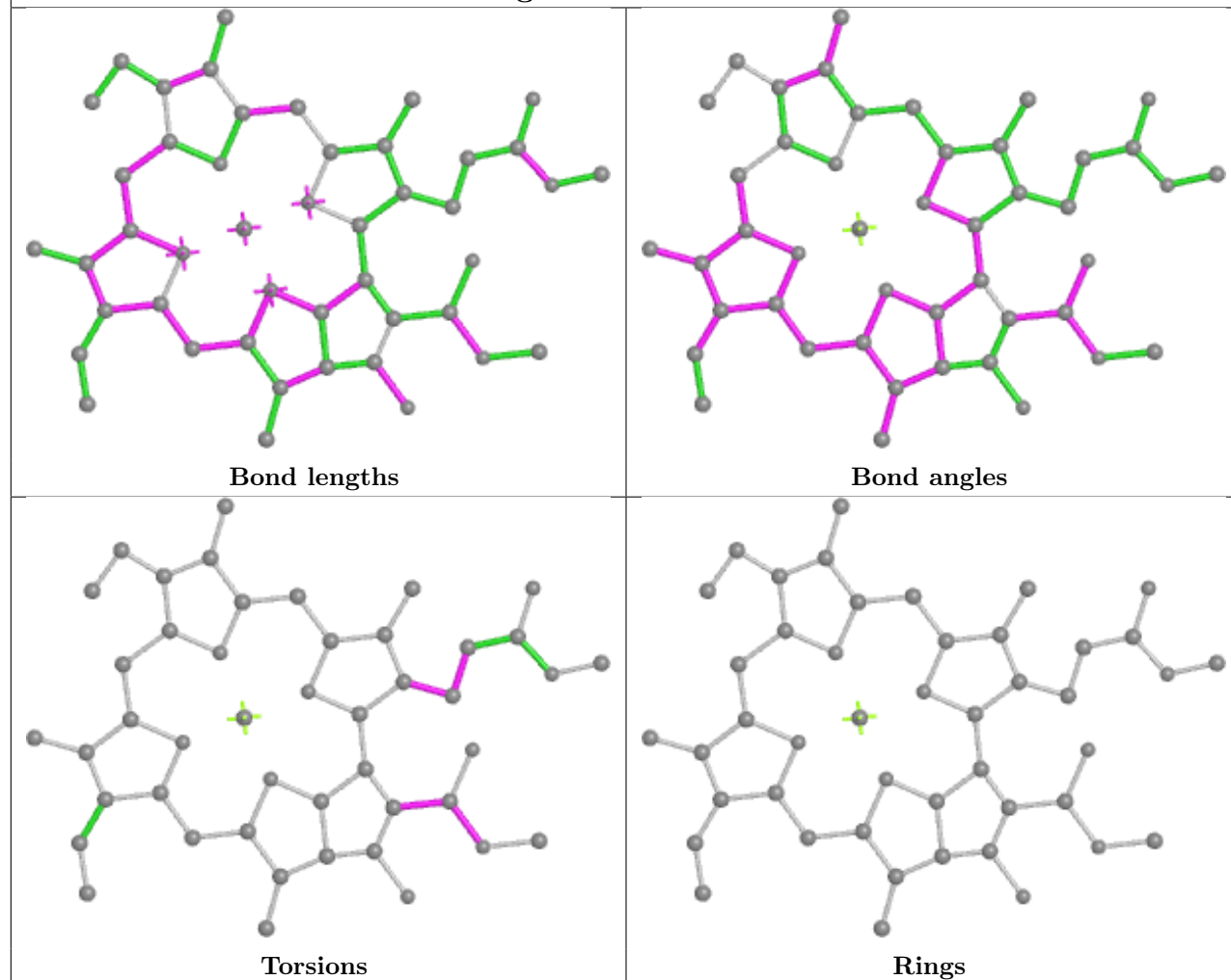
Ligand CHL 4 313



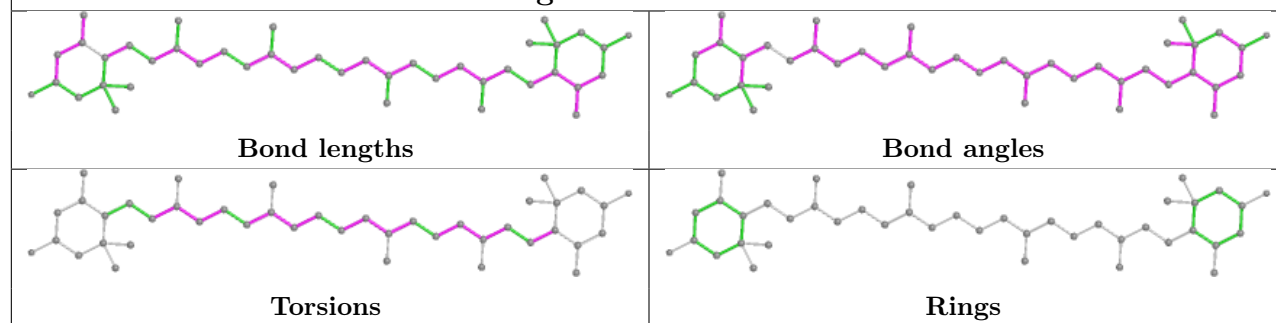




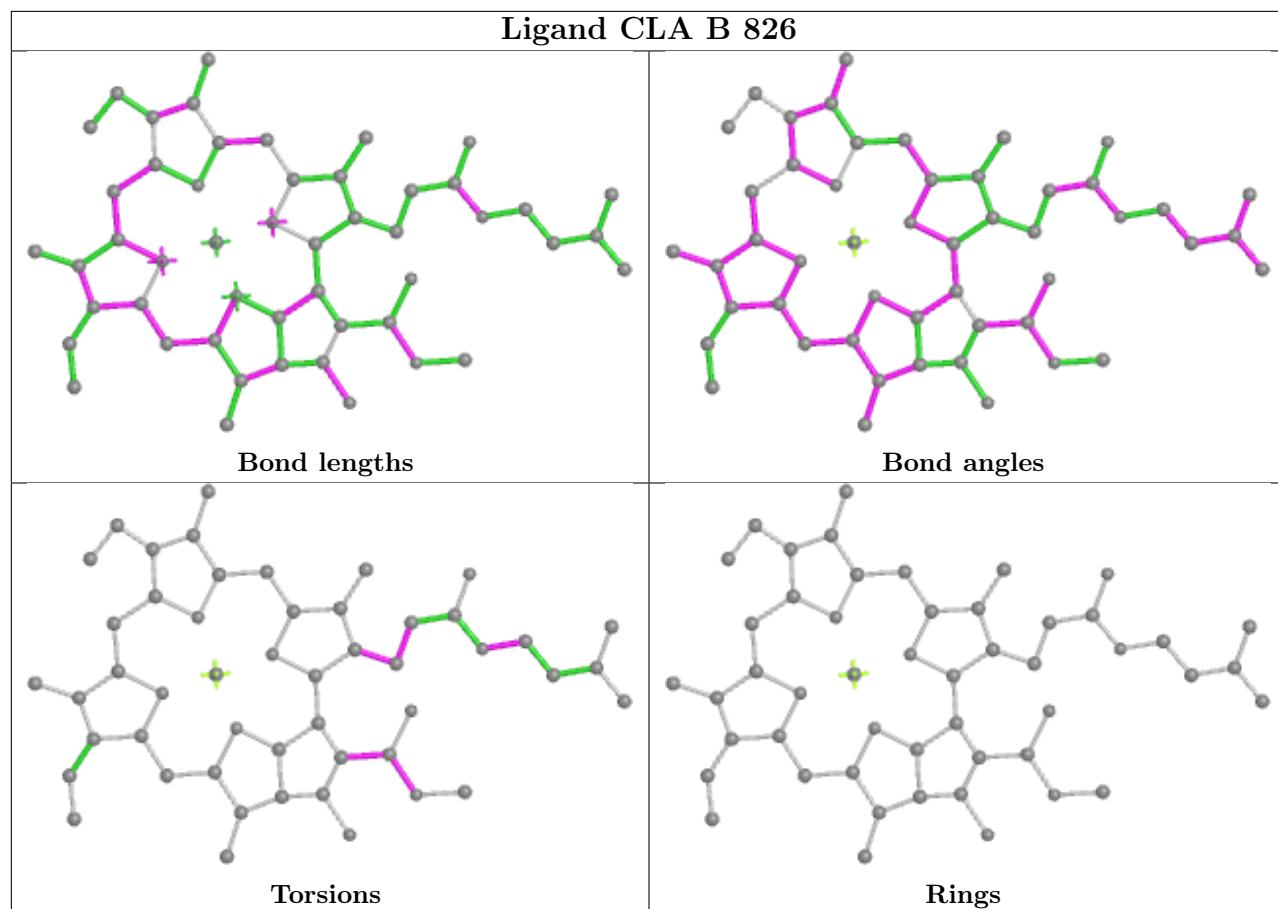
Ligand CLA b 308



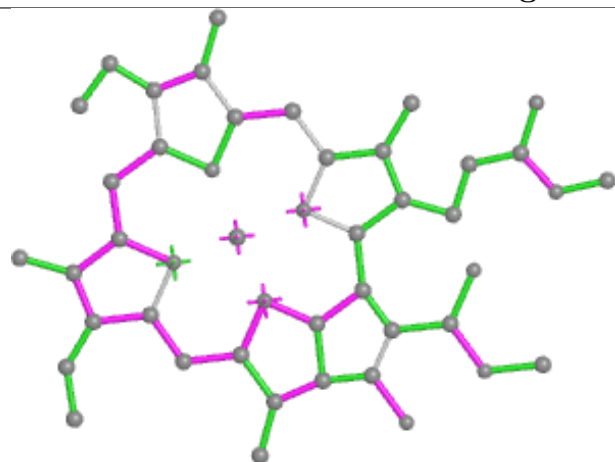
Ligand LUT J 103



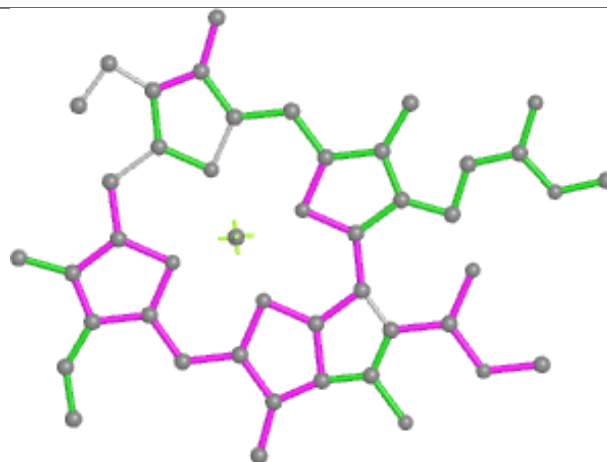
Ligand CLA B 826



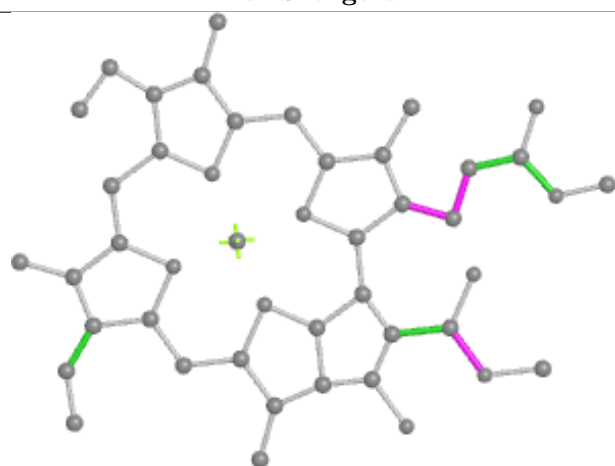
Ligand CLA b 306



Bond lengths



Bond angles

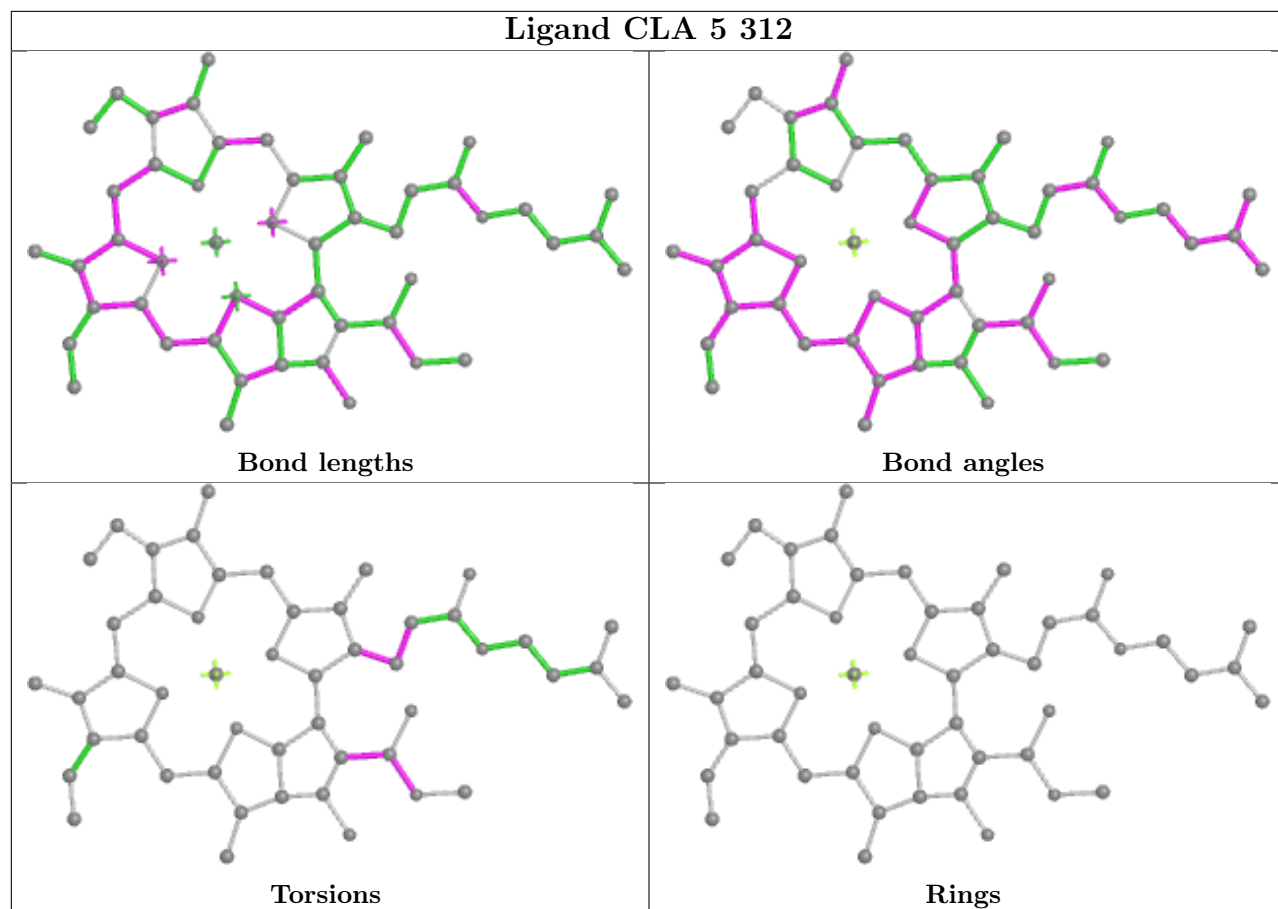


Torsions

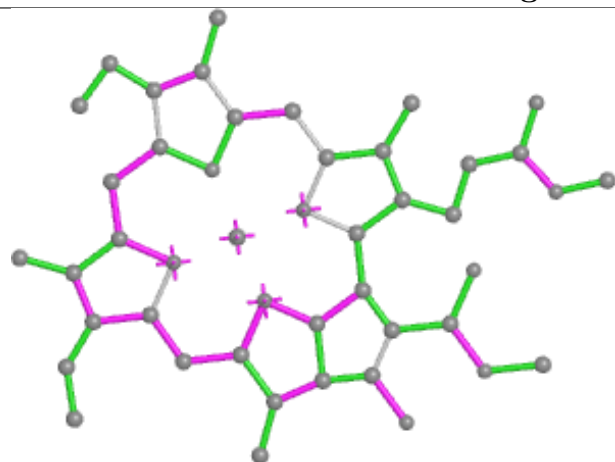


Rings

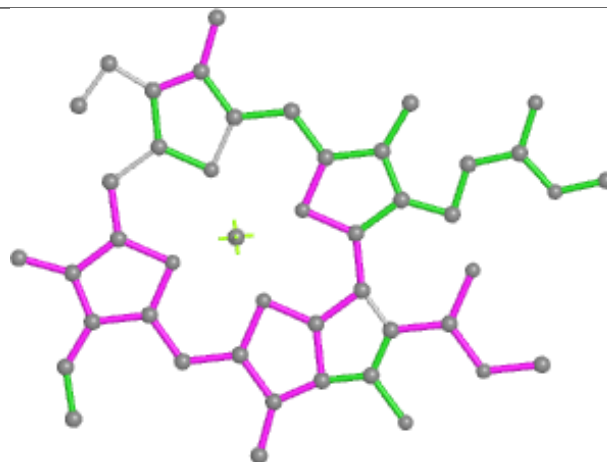
Ligand CLA 5 312



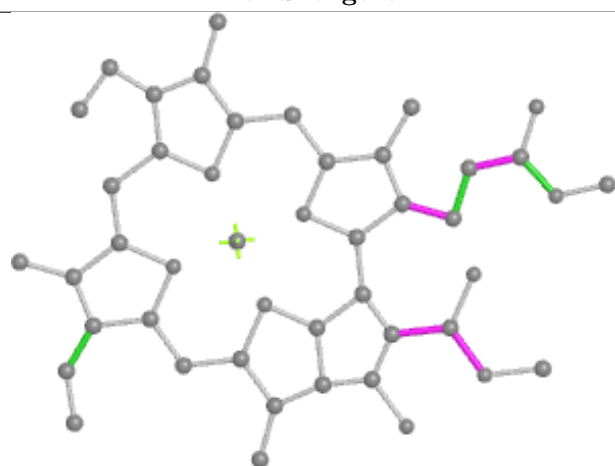
Ligand CLA 6 322



Bond lengths



Bond angles

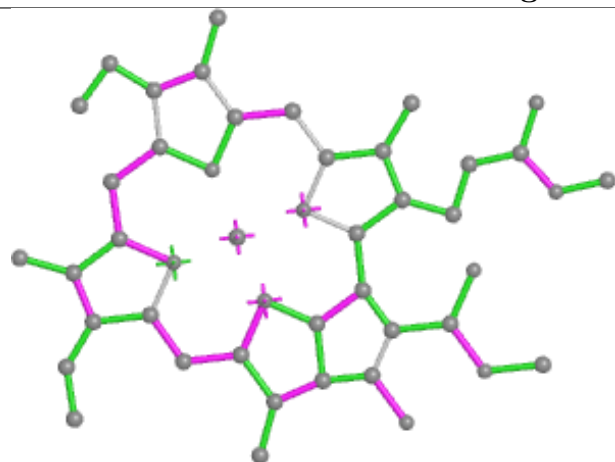


Torsions

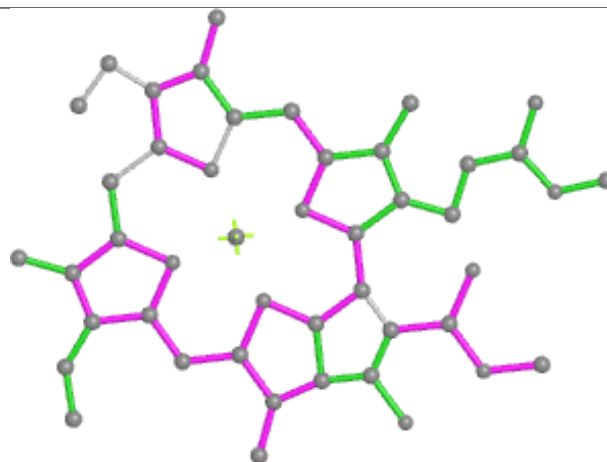


Rings

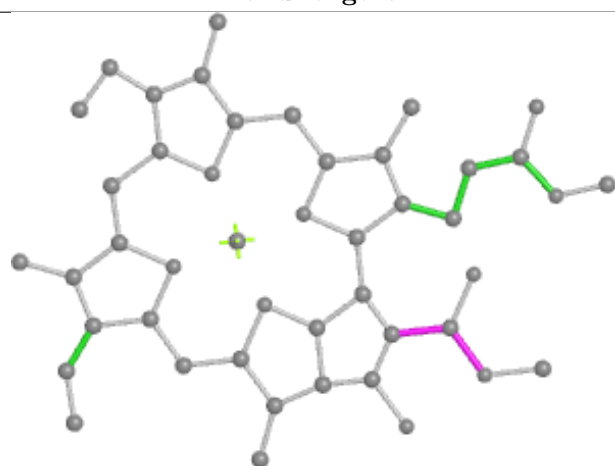
Ligand CLA 8 321



Bond lengths



Bond angles

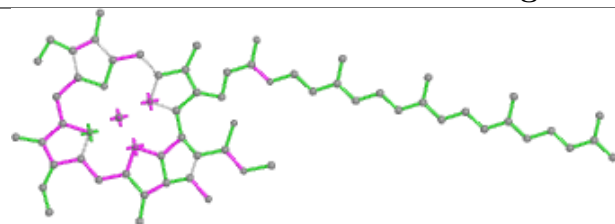


Torsions

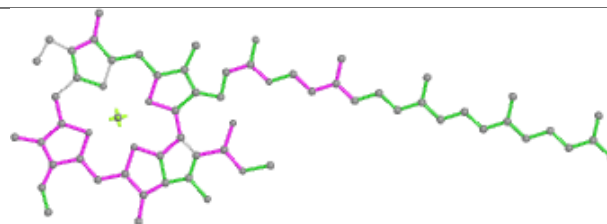


Rings

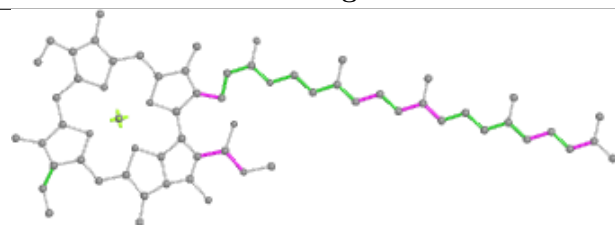
Ligand CLA a 312



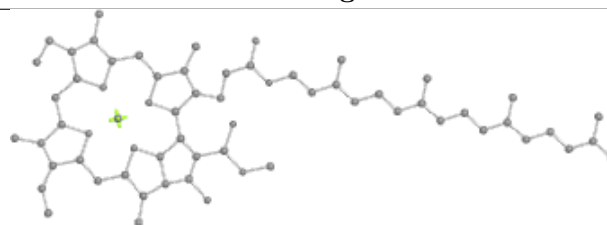
Bond lengths



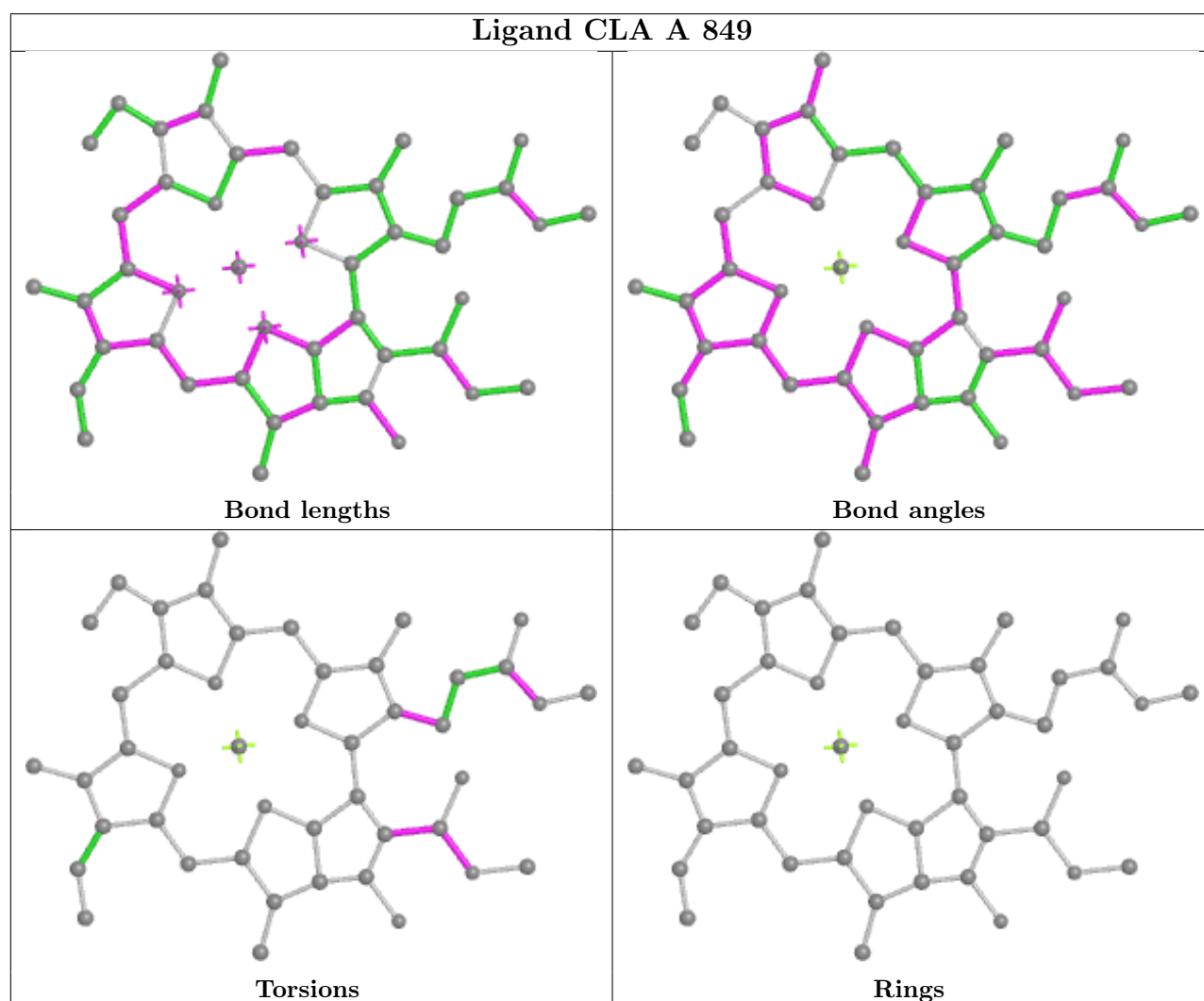
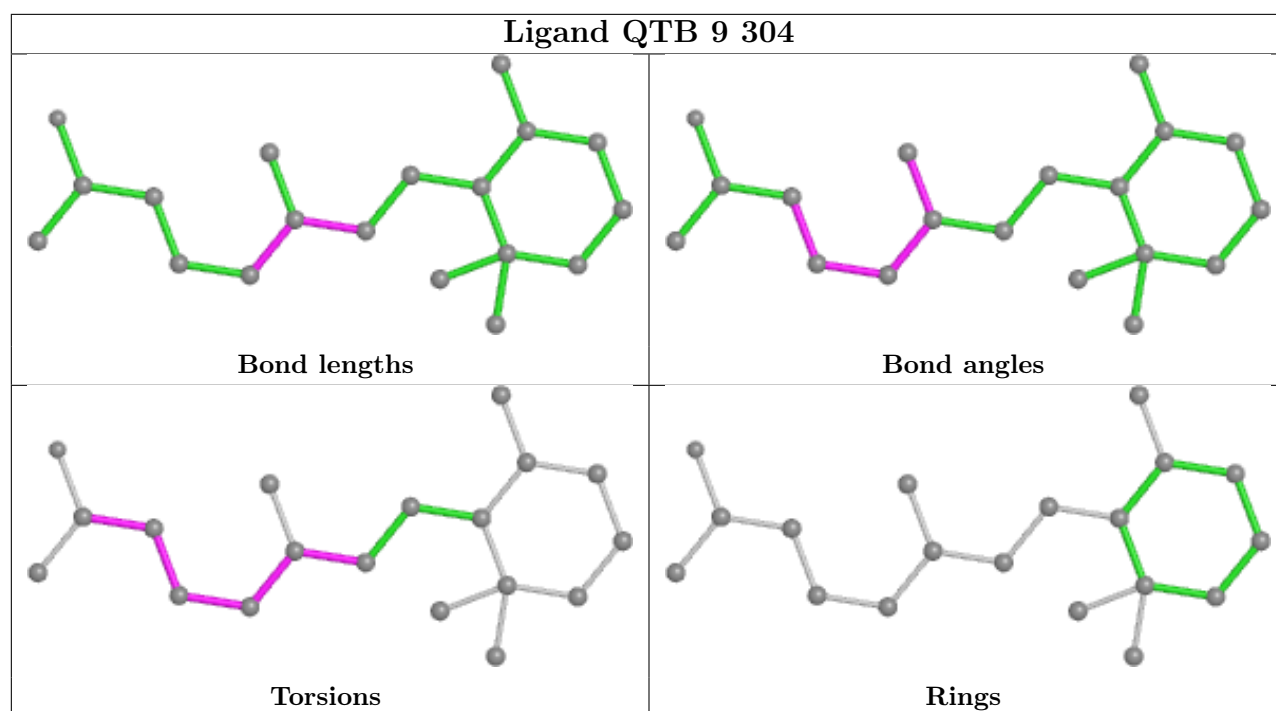
Bond angles



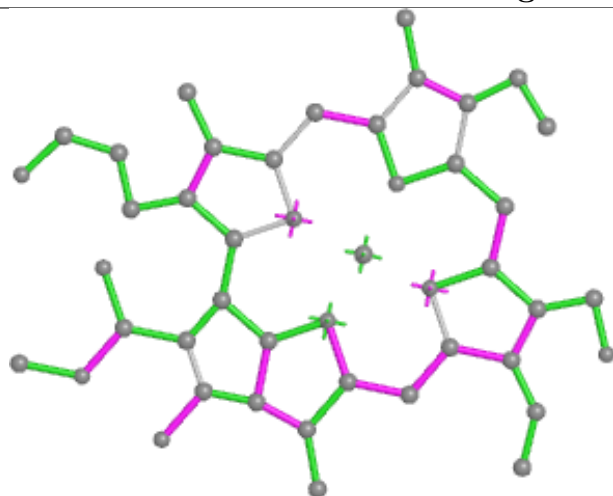
Torsions



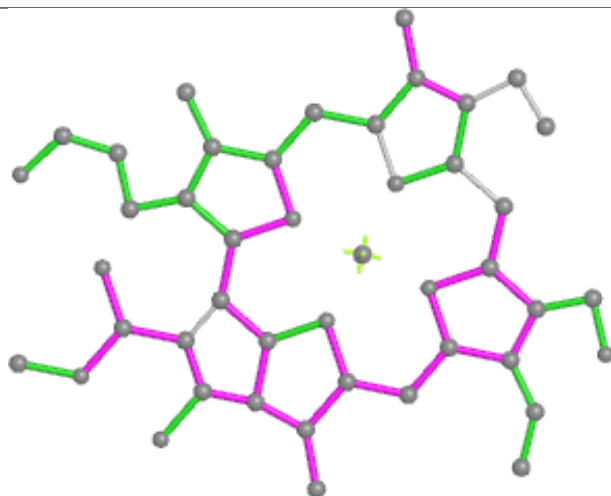
Rings



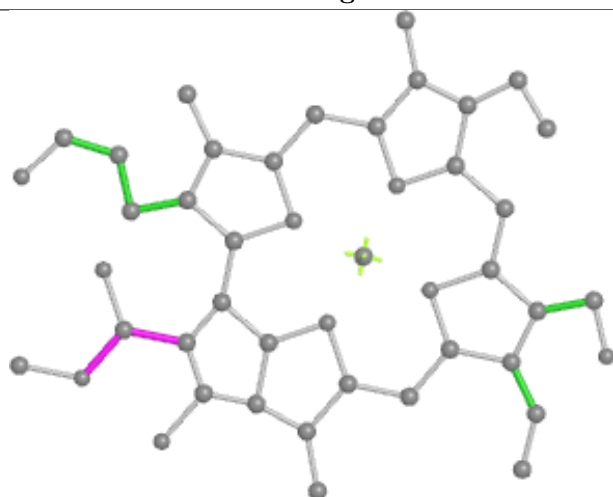
Ligand CHL 8 319



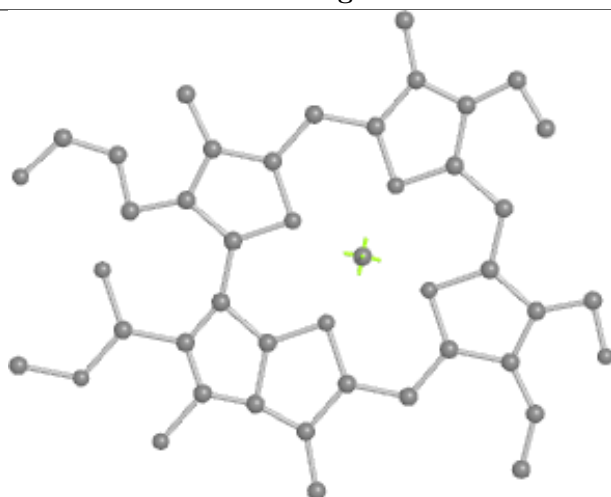
Bond lengths



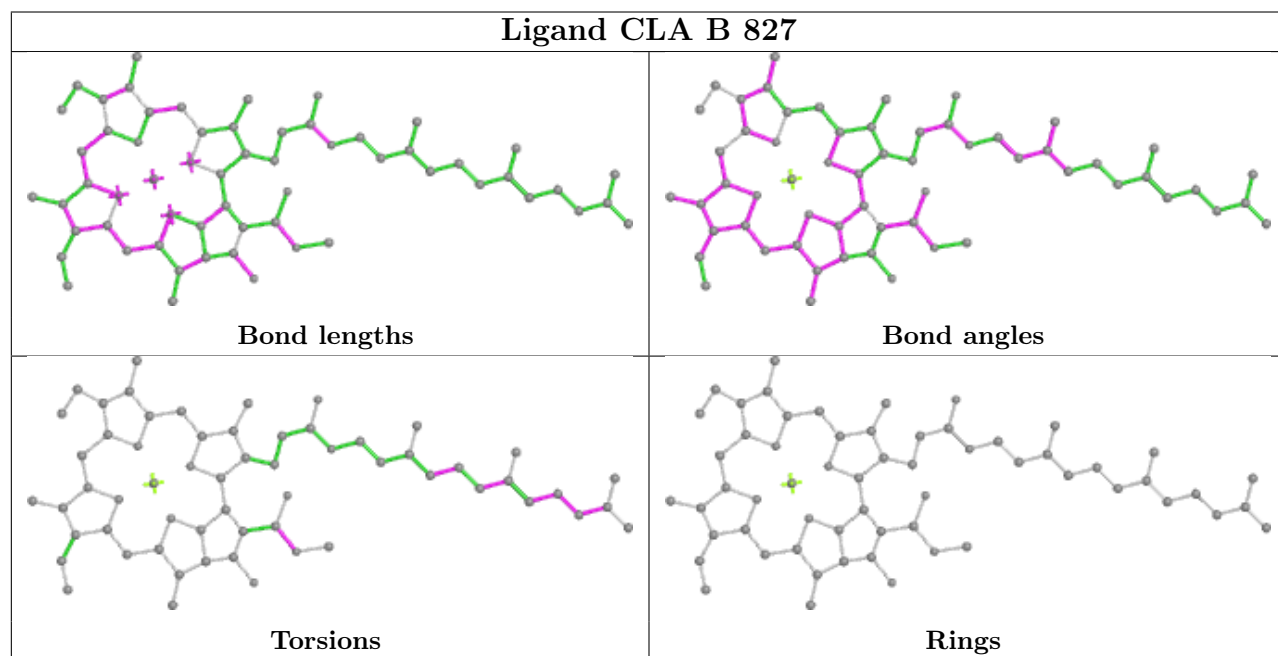
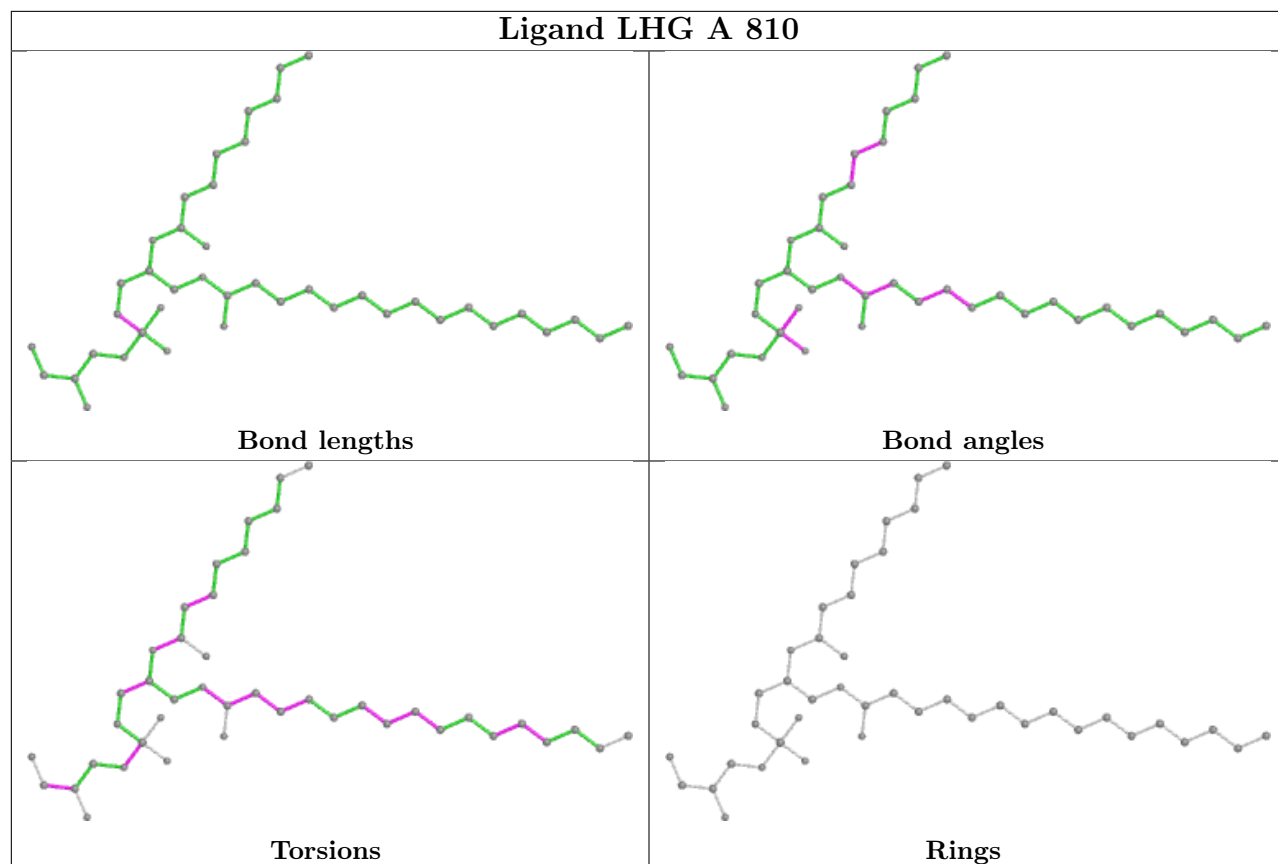
Bond angles



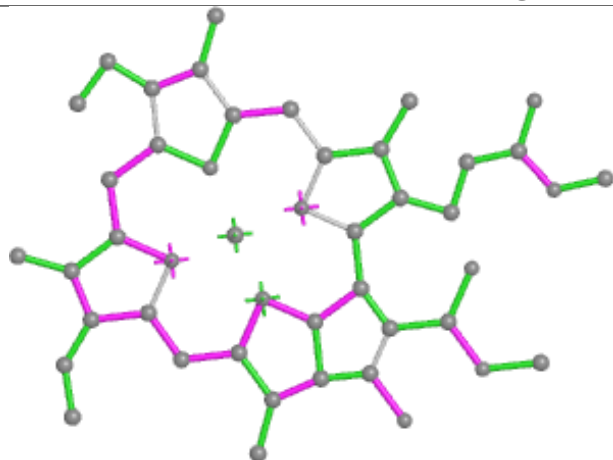
Torsions



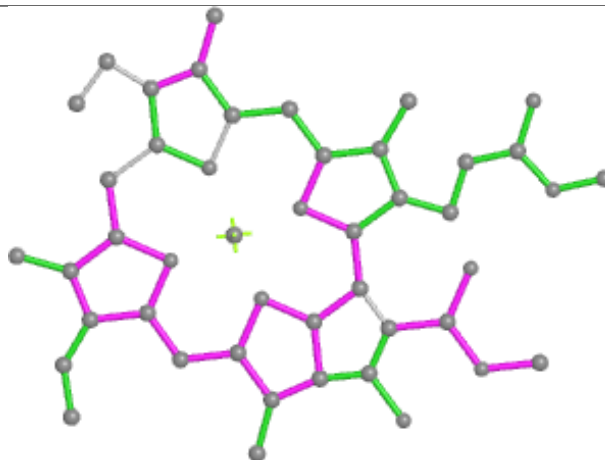
Rings



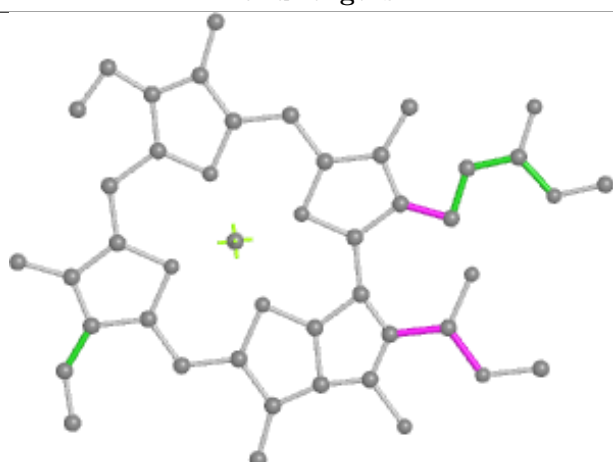
Ligand CLA H 903



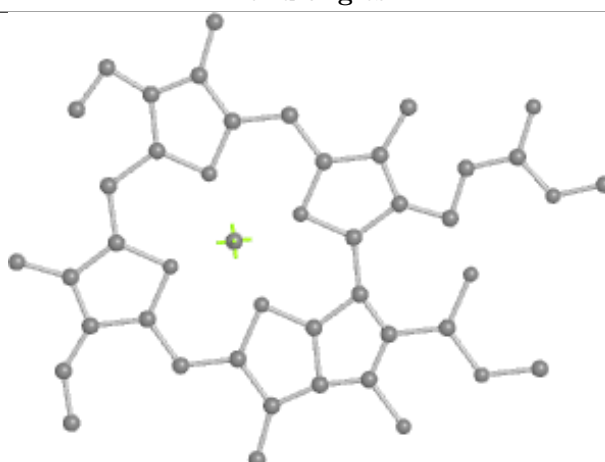
Bond lengths



Bond angles

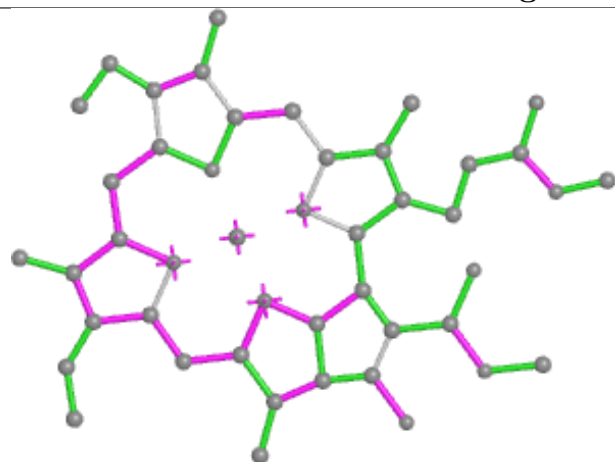


Torsions

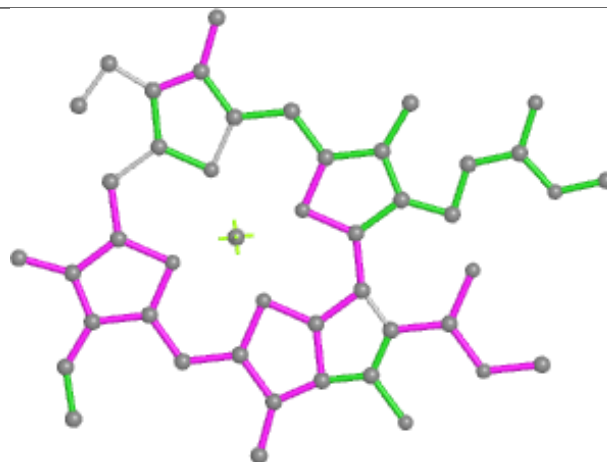


Rings

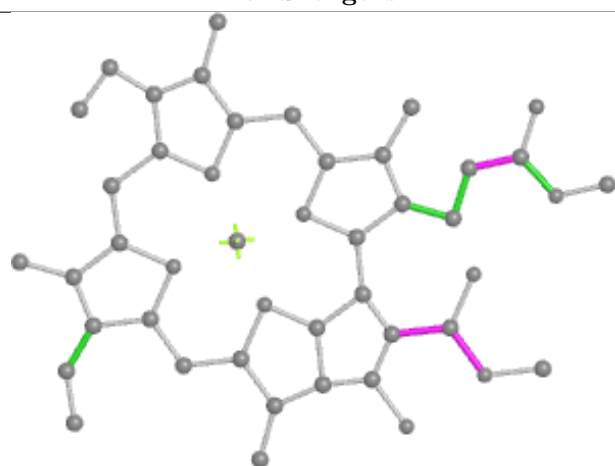
Ligand CLA b 307



Bond lengths



Bond angles

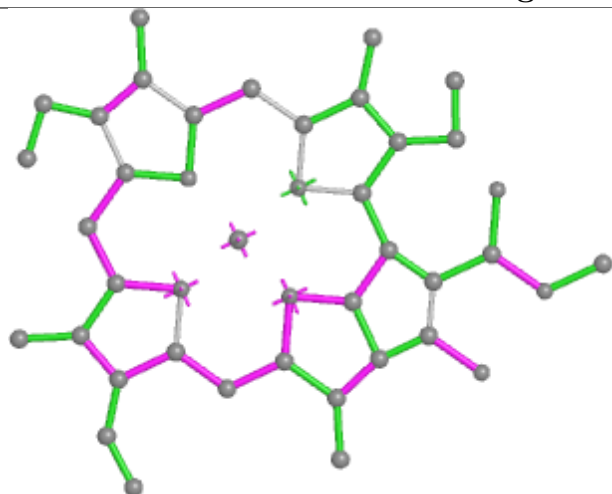


Torsions

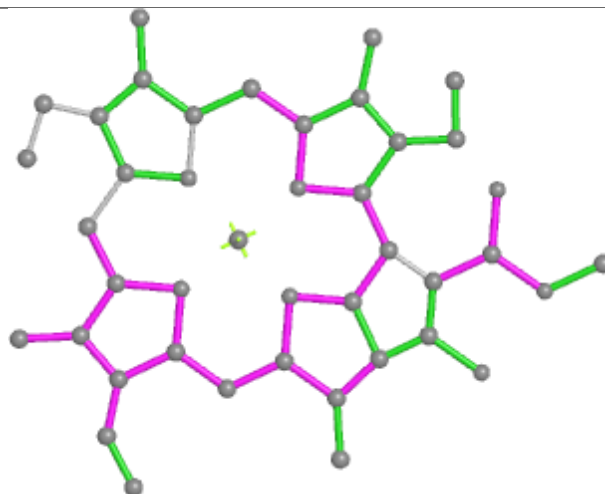


Rings

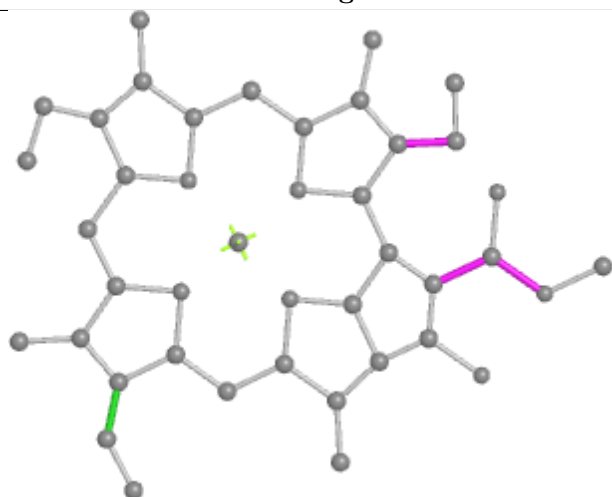
Ligand CLA J 105



Bond lengths



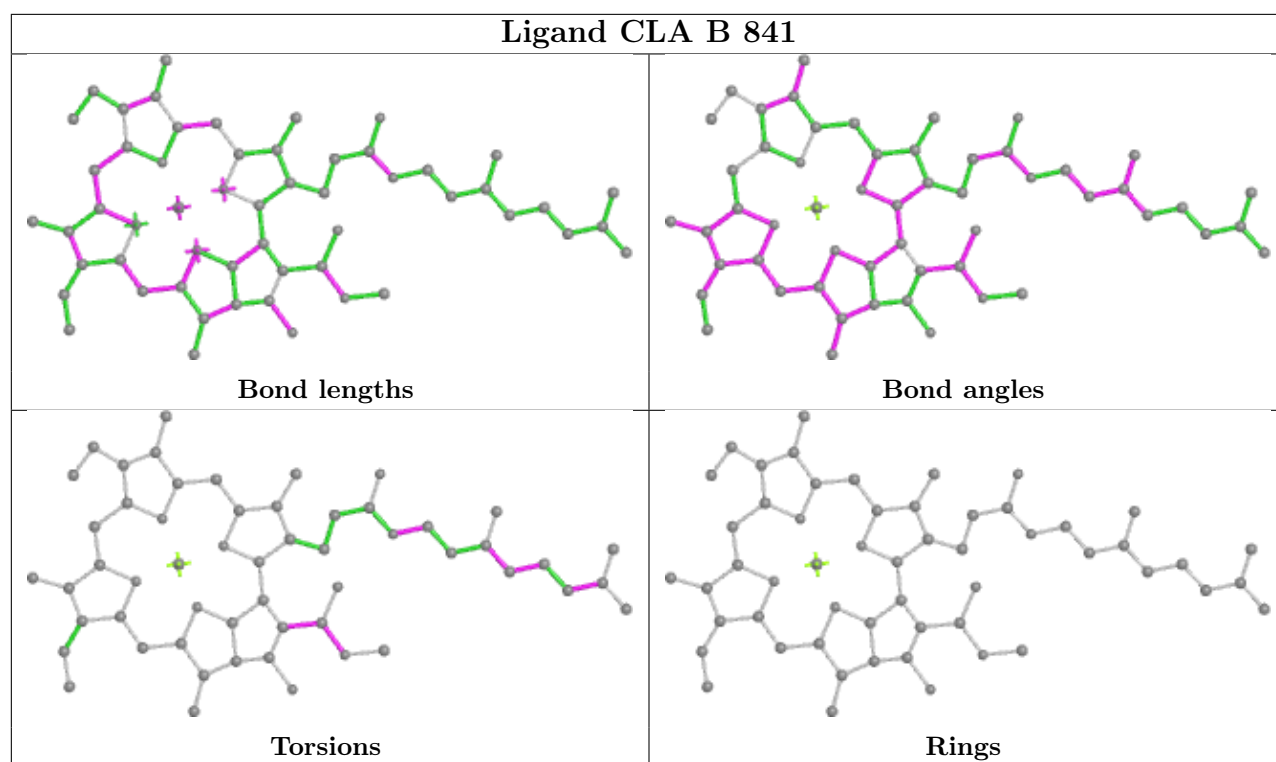
Bond angles

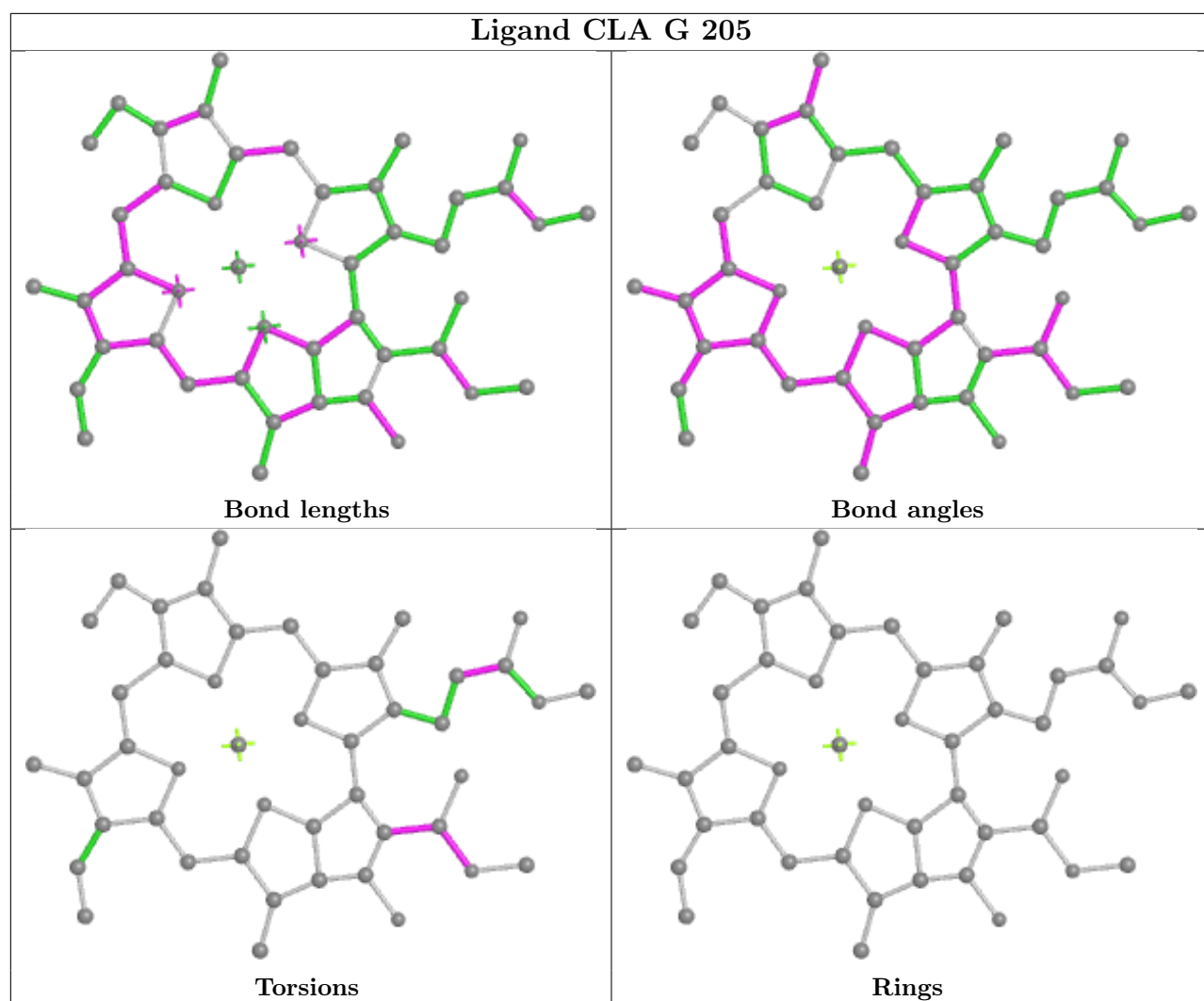


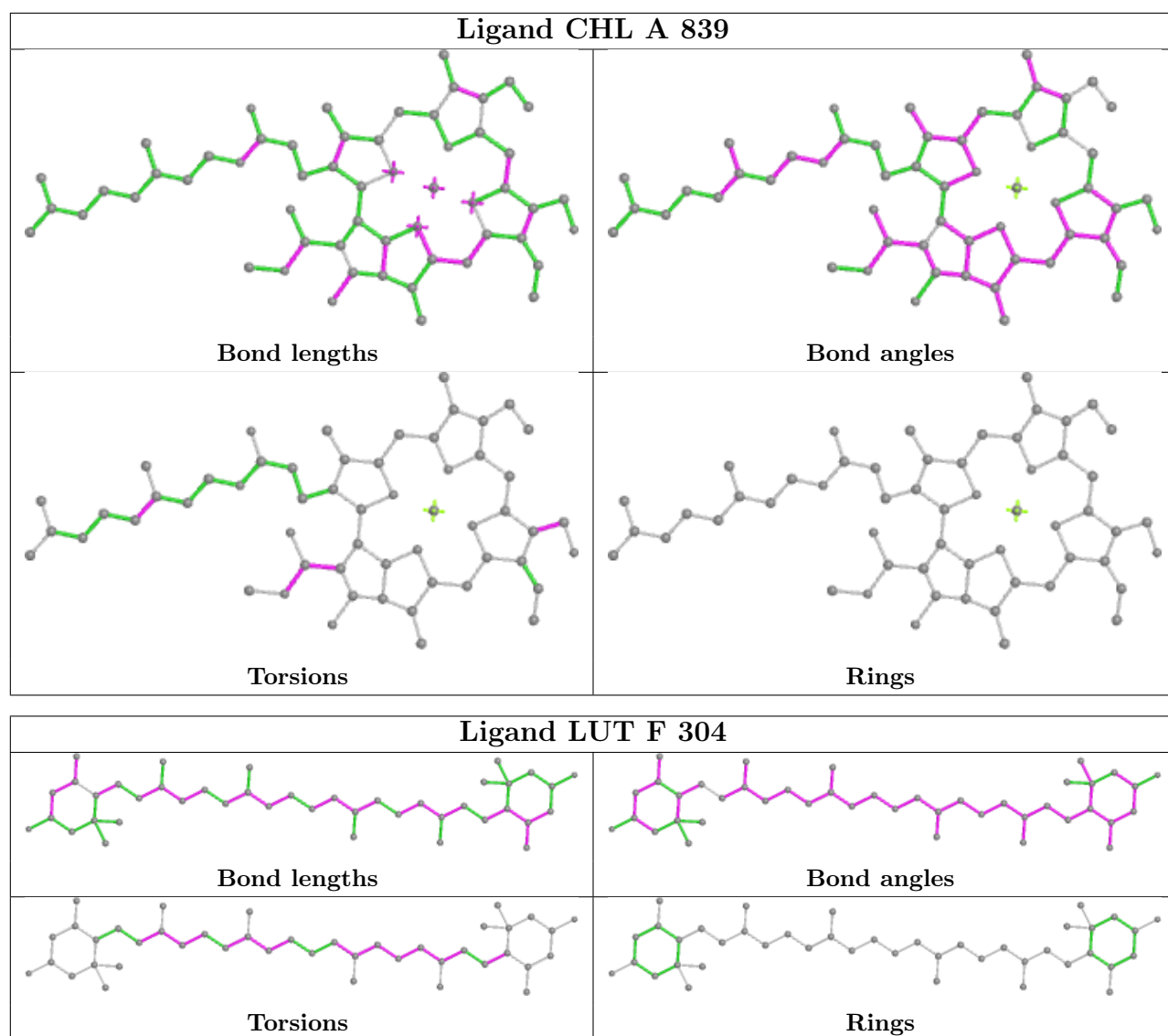
Torsions



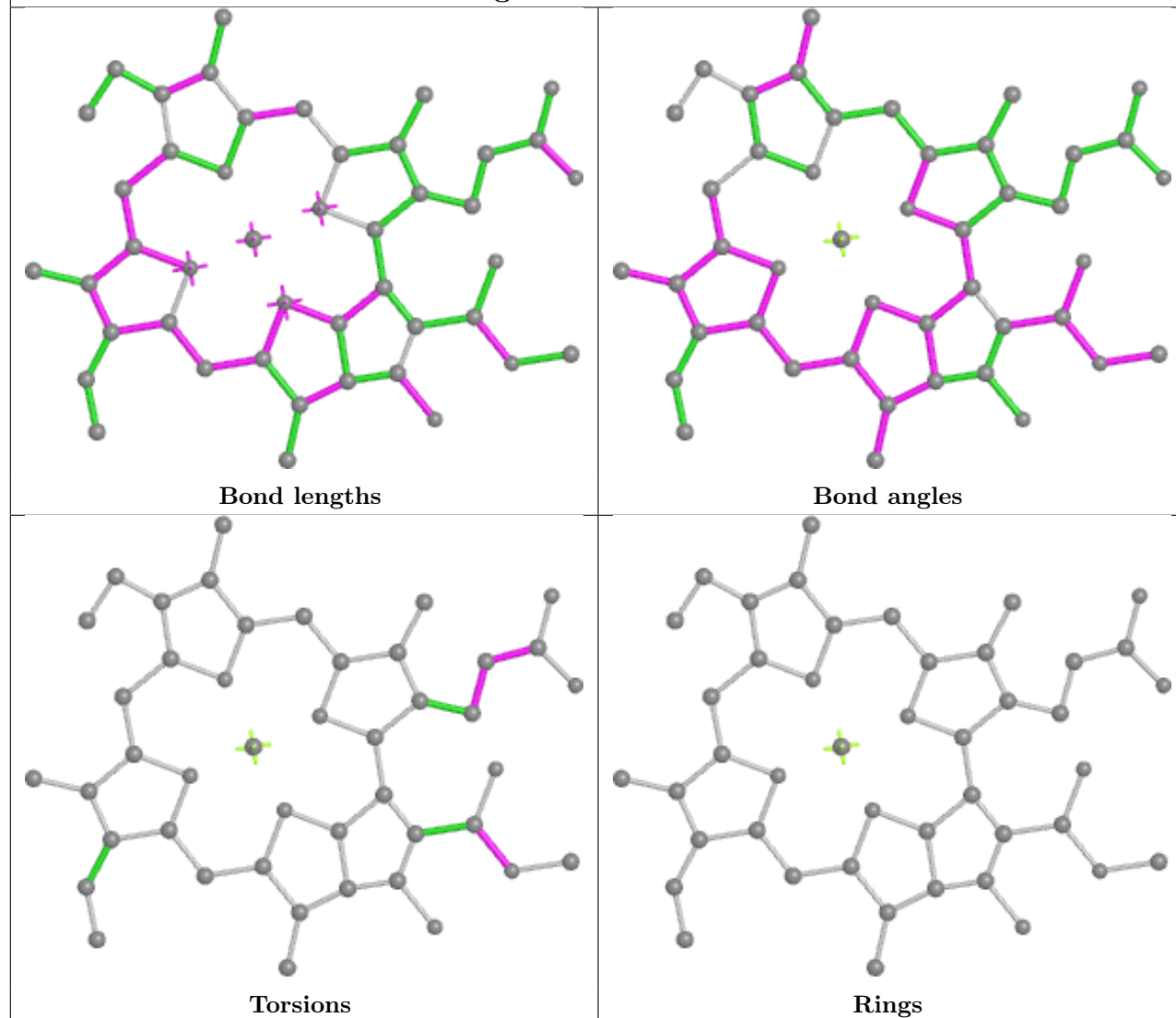
Rings



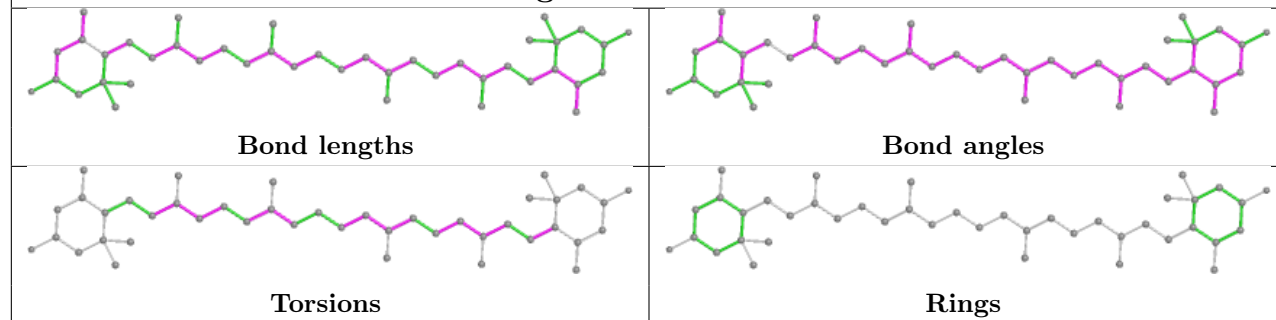




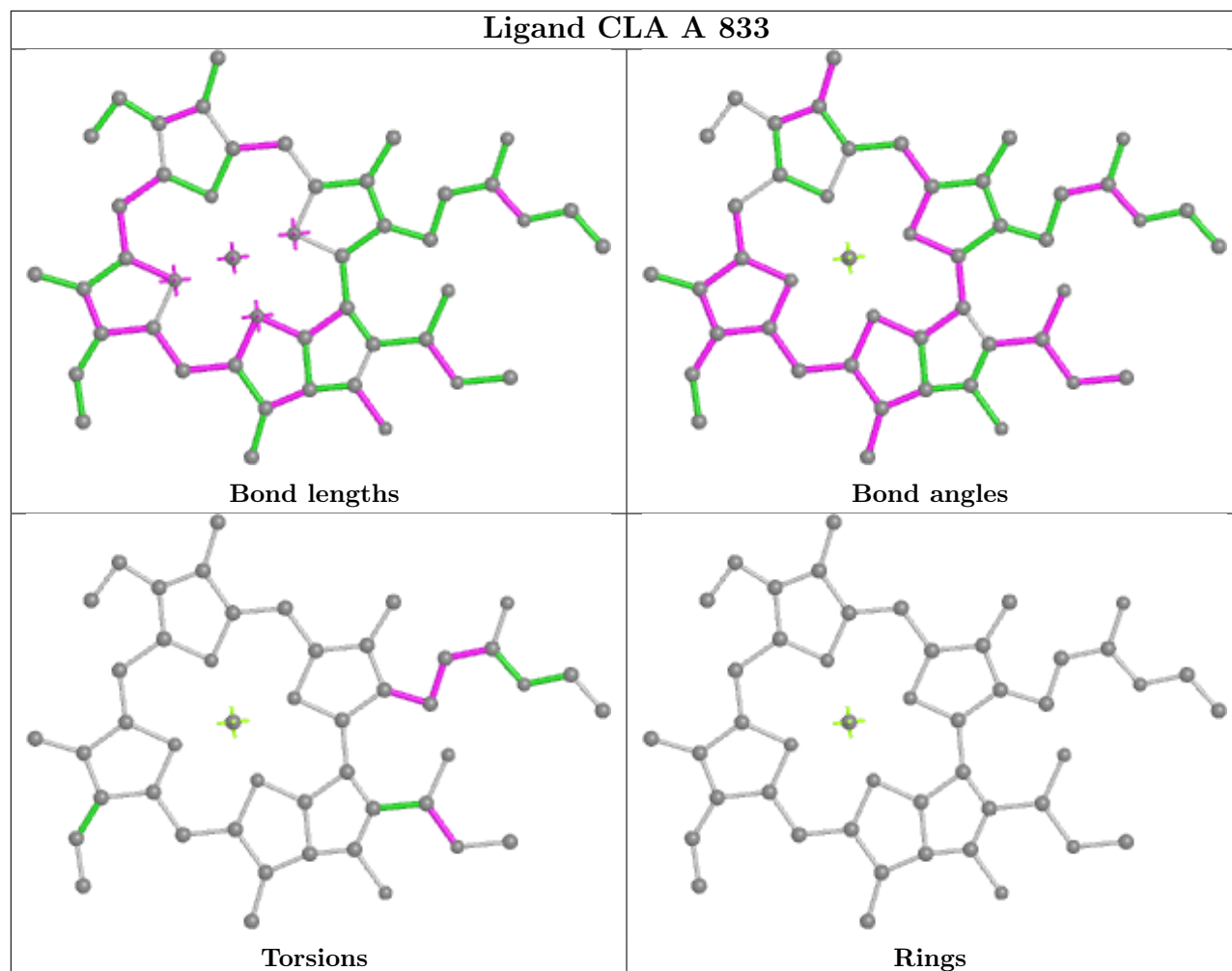
Ligand CLA 5 314



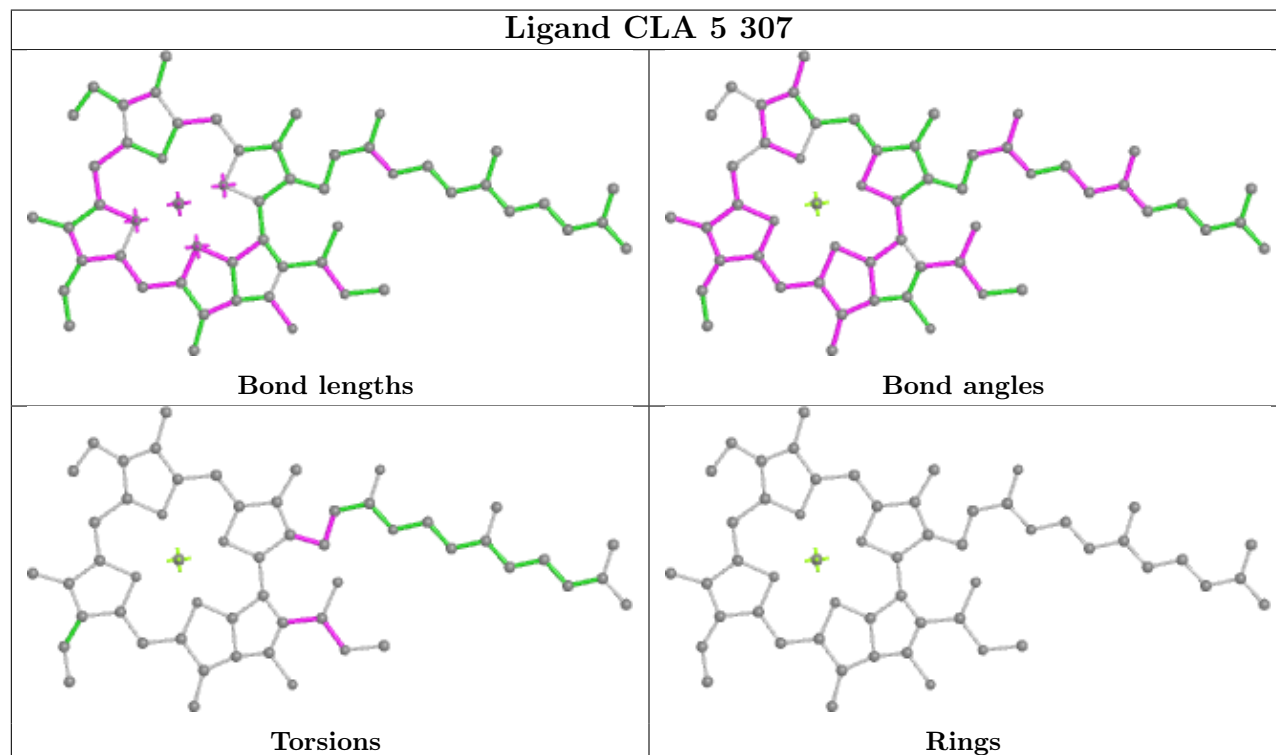
Ligand LUT 4 303



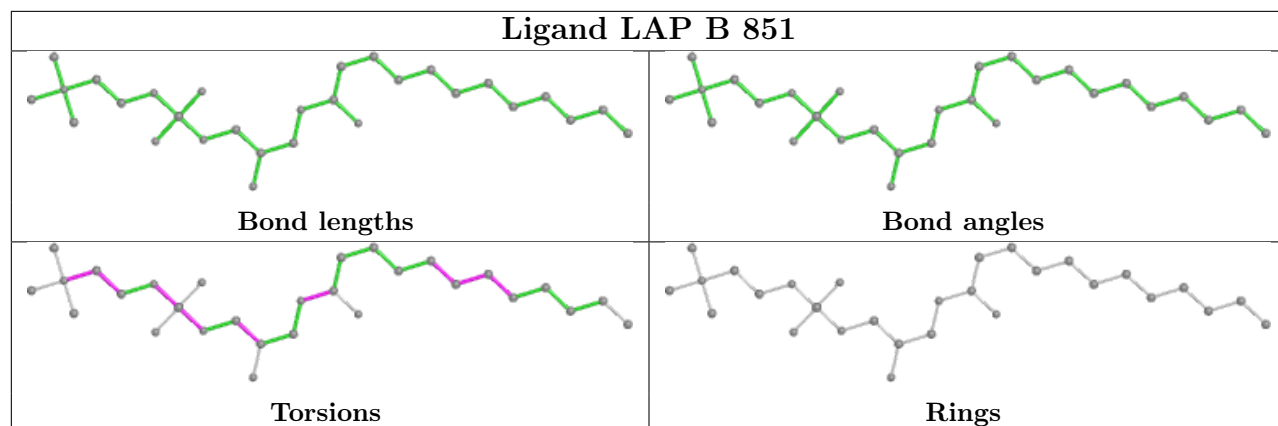
Ligand CLA A 833



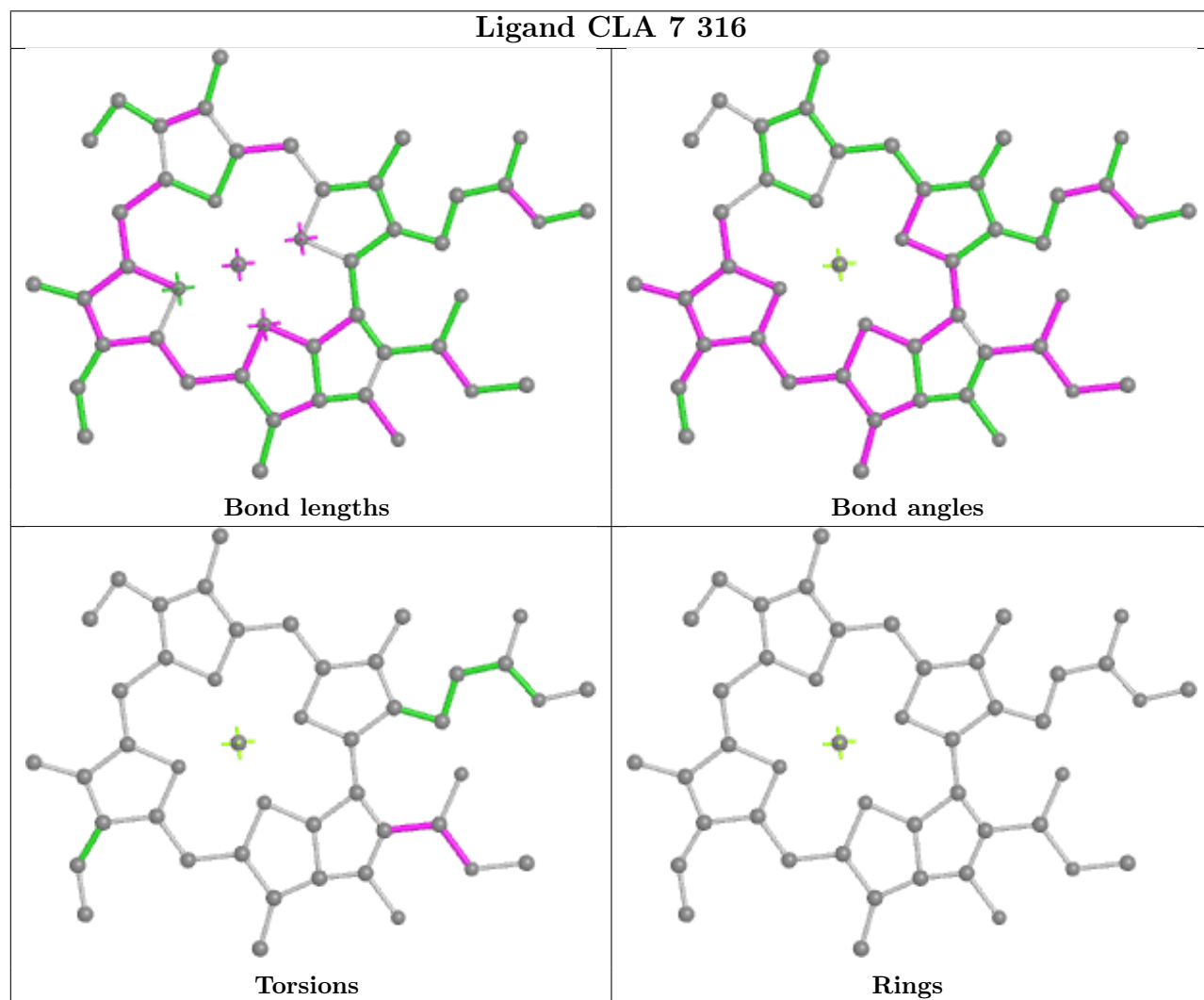
Ligand CLA 5 307

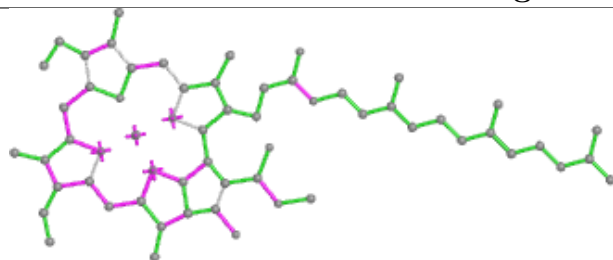


Ligand LAP B 851

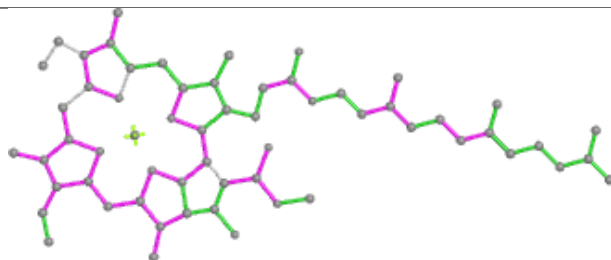


Ligand CLA 7 316

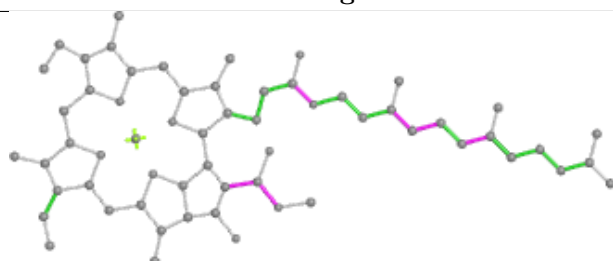


Ligand CLA A 830

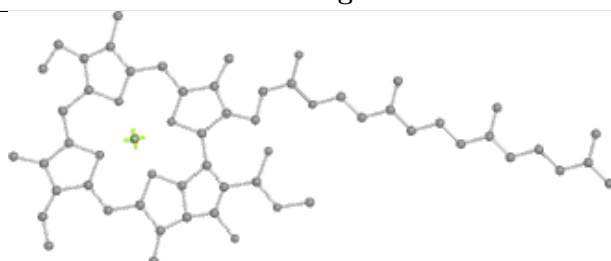
Bond lengths



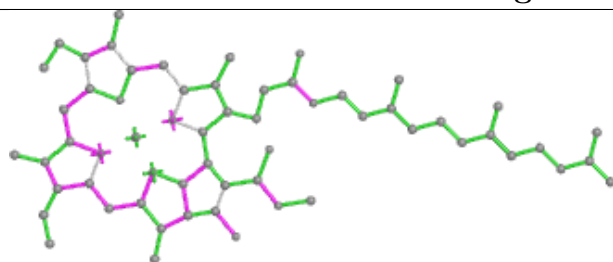
Bond angles



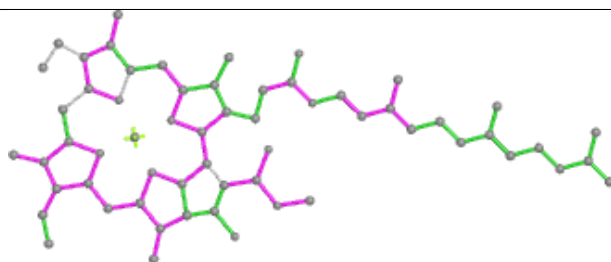
Torsions



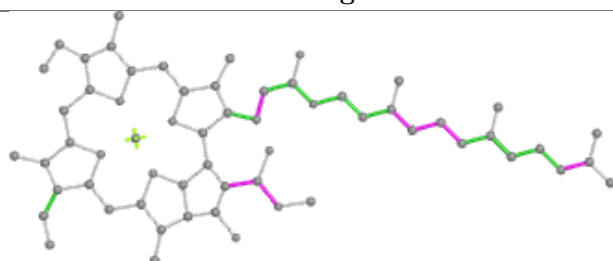
Rings

Ligand CLA B 839

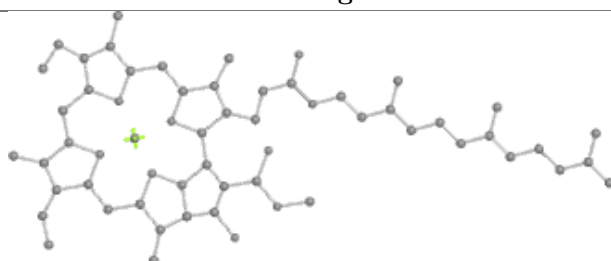
Bond lengths



Bond angles

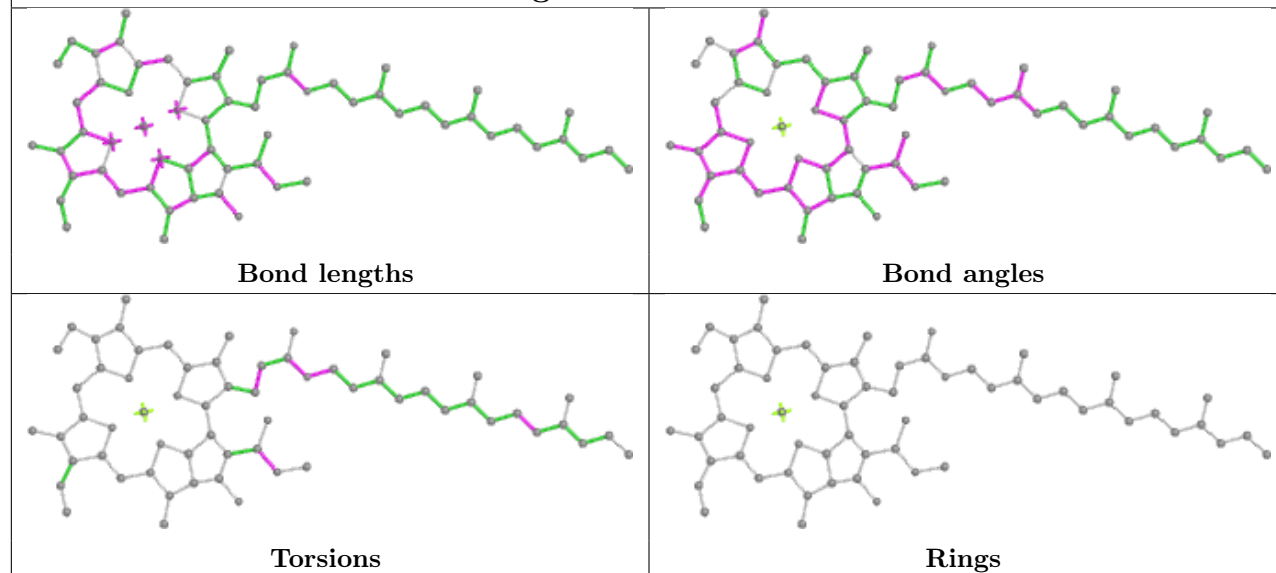


Torsions

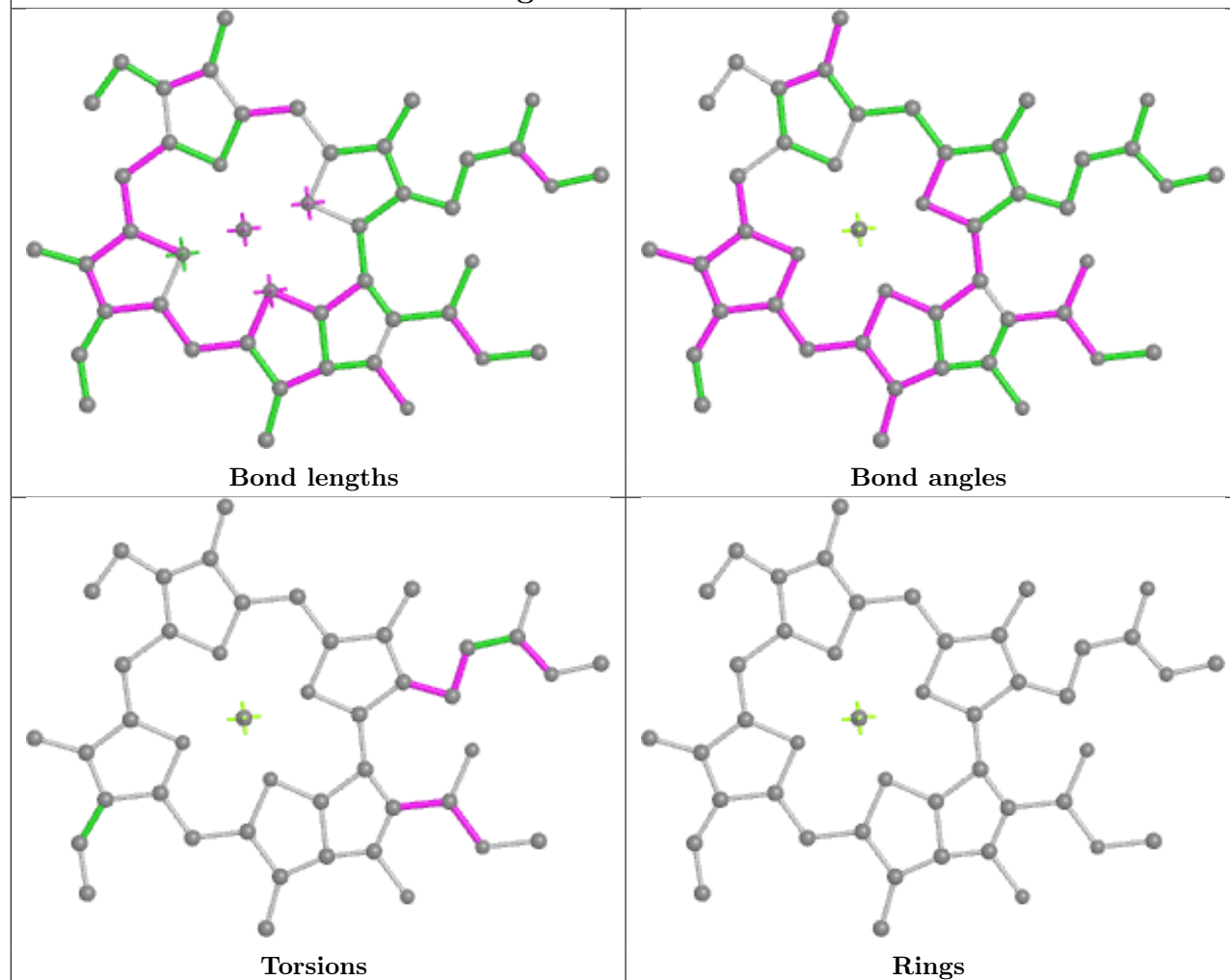


Rings

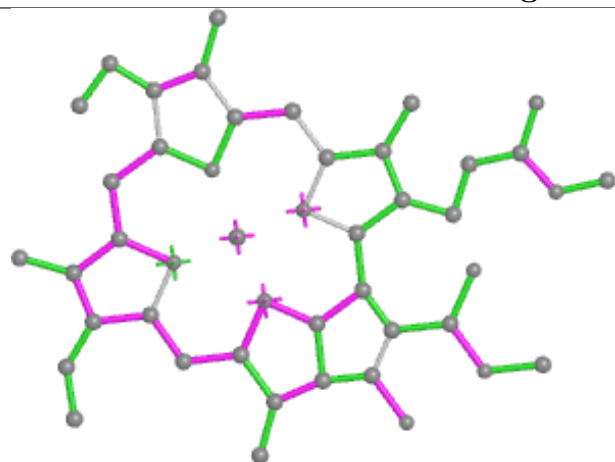
Ligand CLA B 850



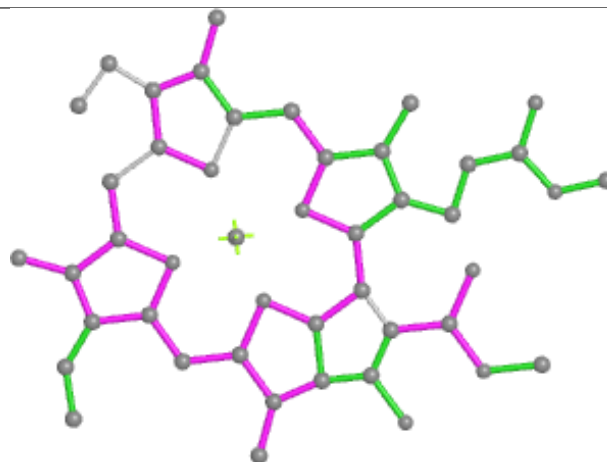
Ligand CLA 2 304



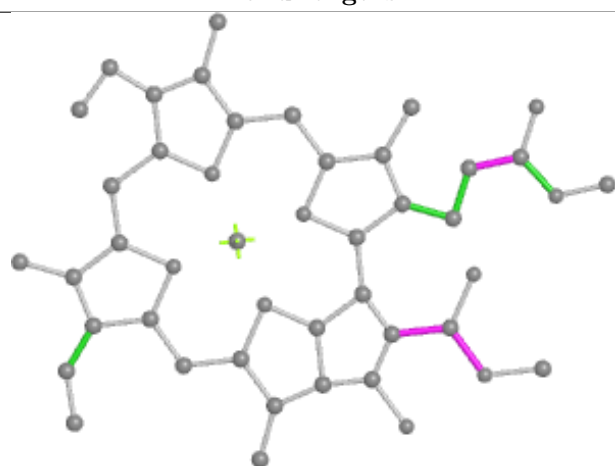
Ligand CLA 3 308



Bond lengths



Bond angles

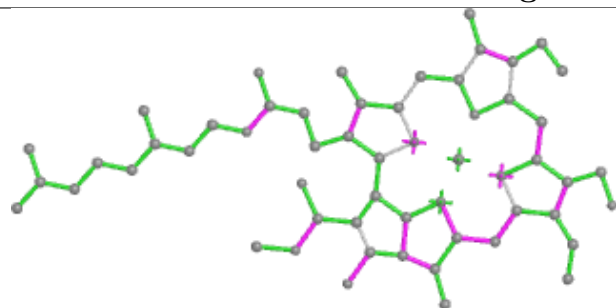


Torsions

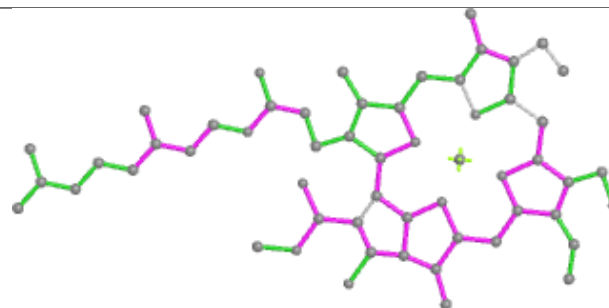


Rings

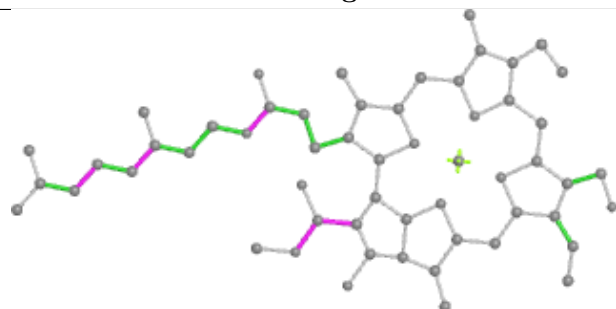
Ligand CHL 3 315



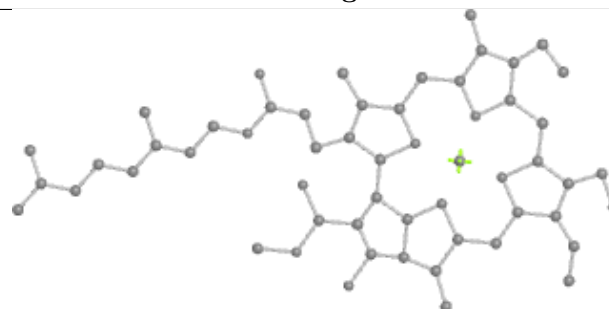
Bond lengths



Bond angles

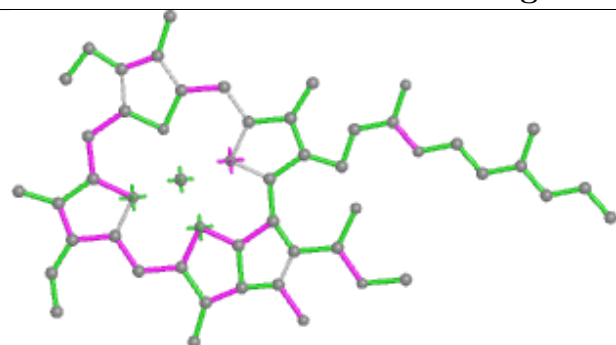


Torsions

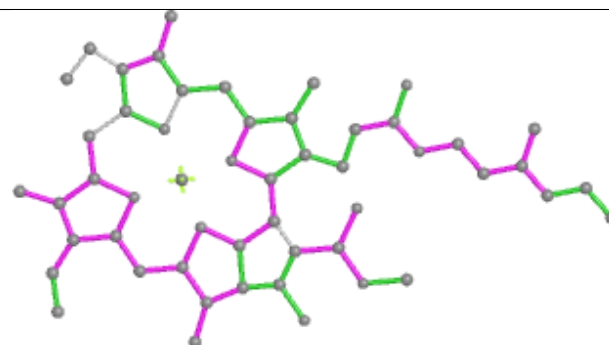


Rings

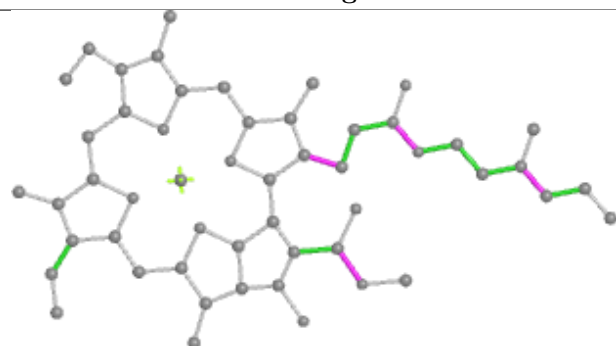
Ligand CLA 3 314



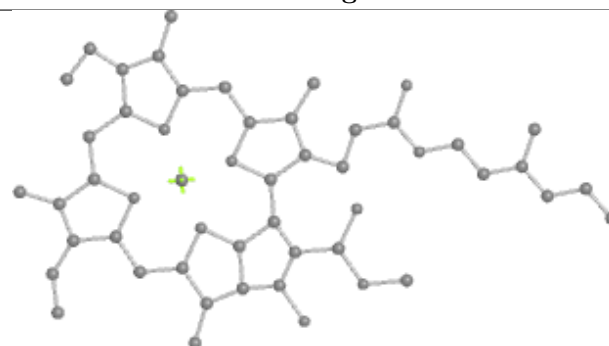
Bond lengths



Bond angles

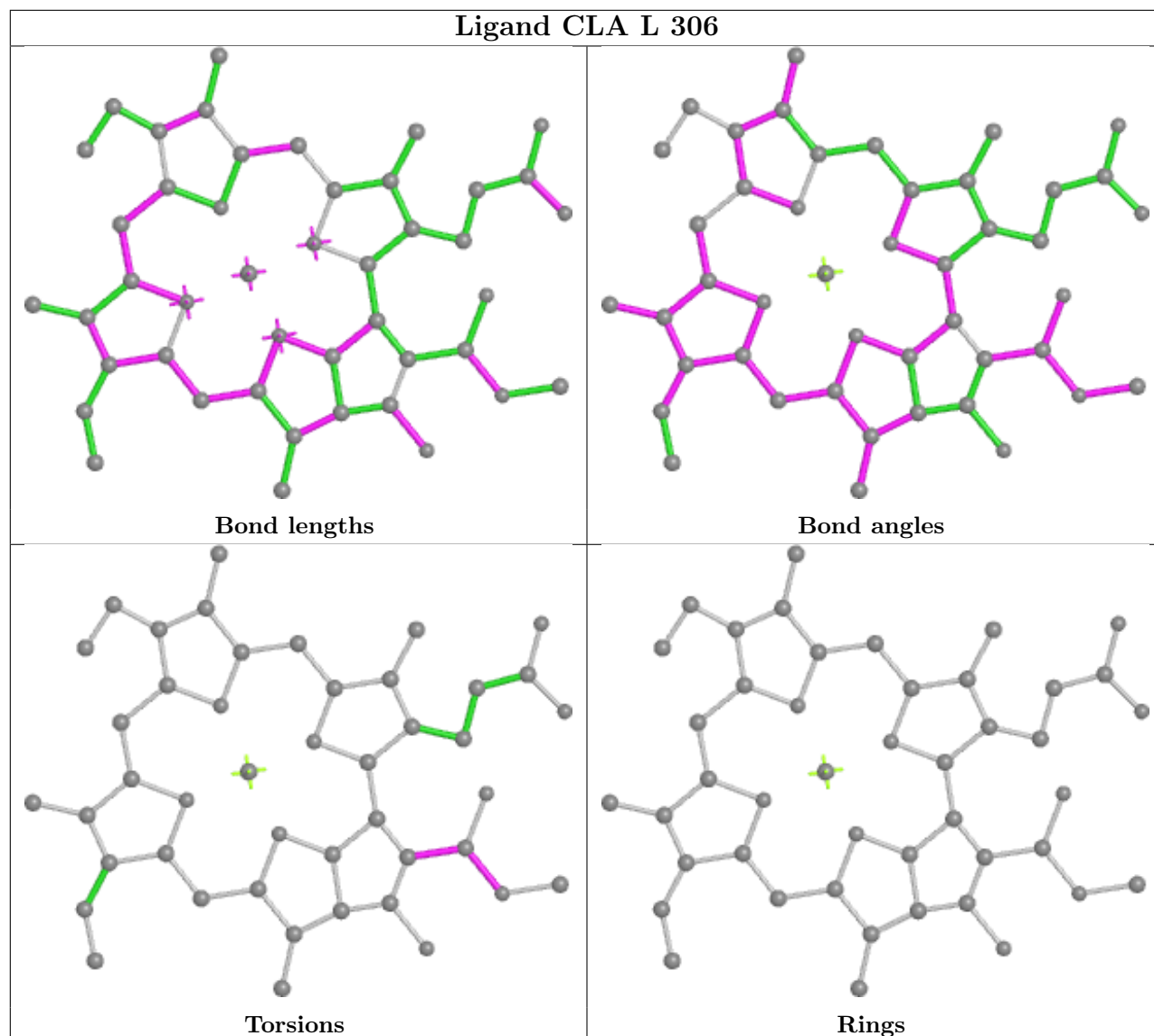


Torsions

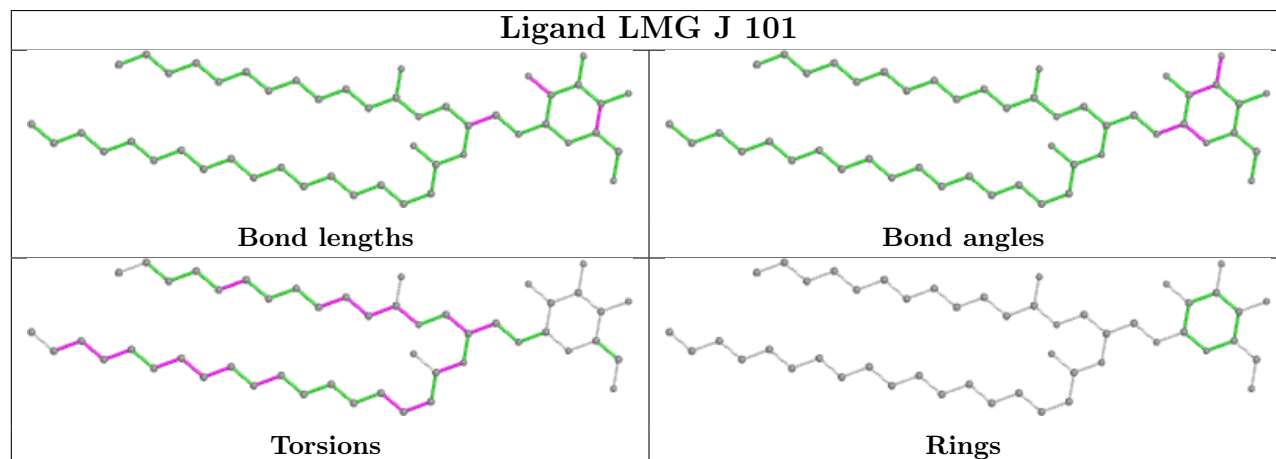


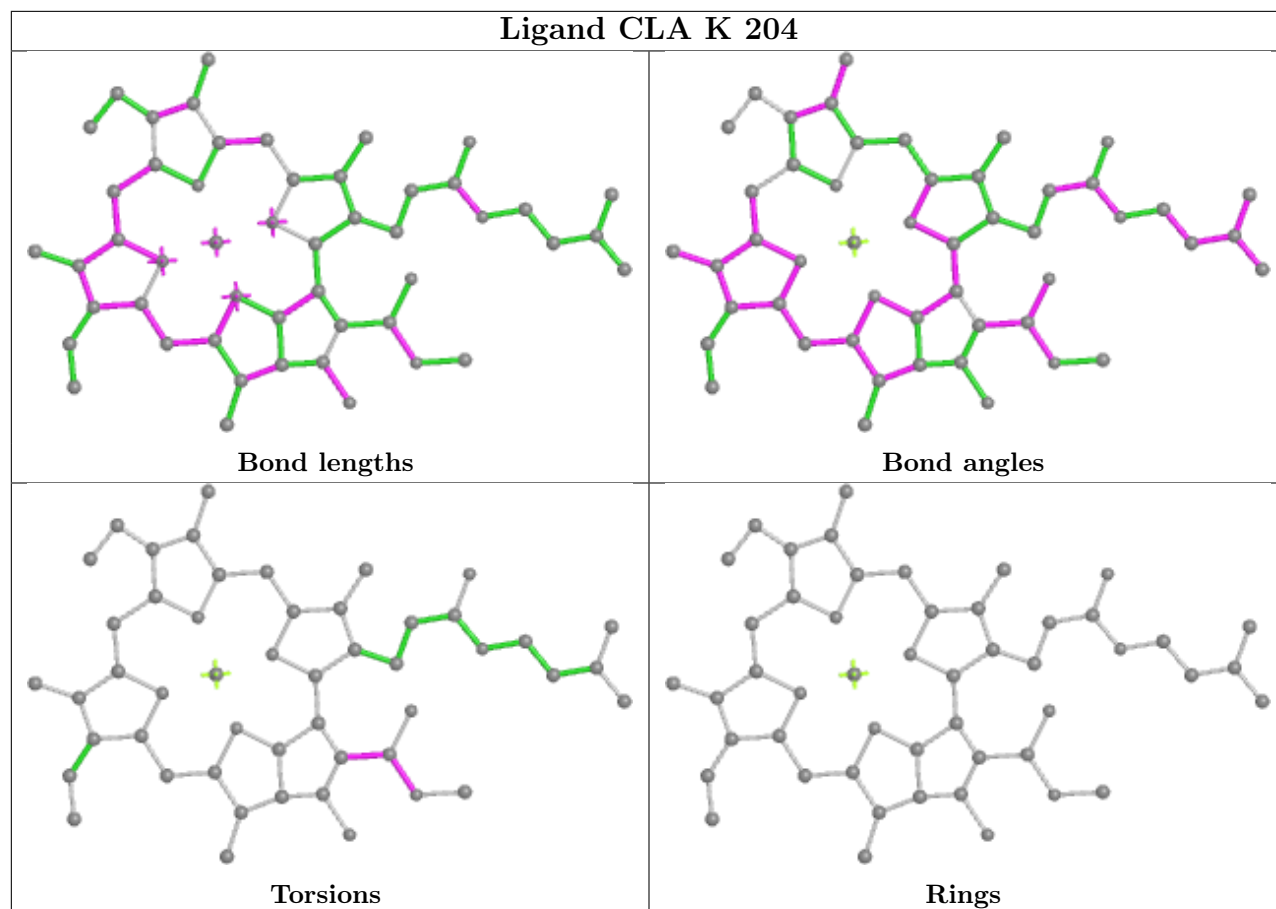
Rings

Ligand CLA L 306

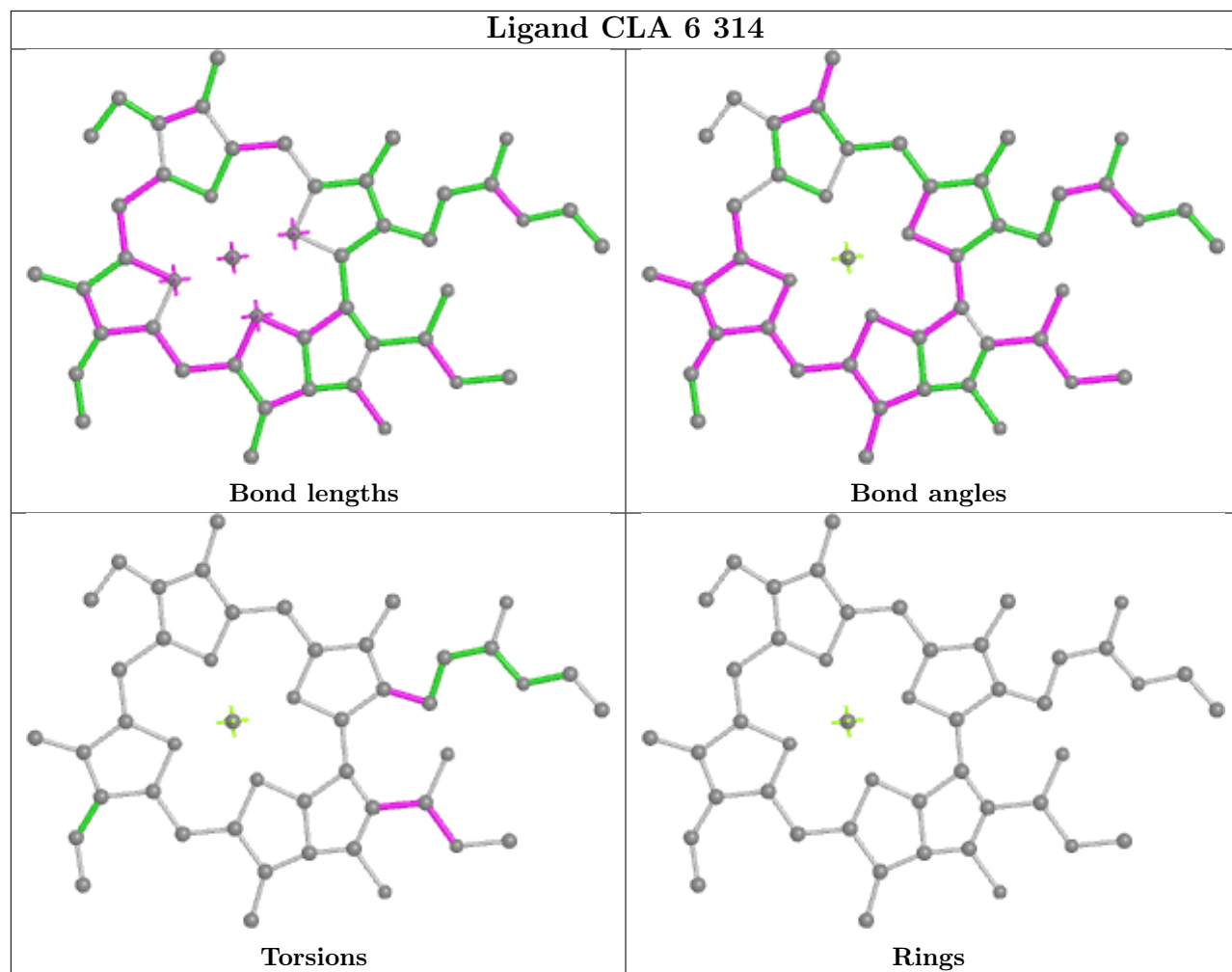


Ligand LMG J 101

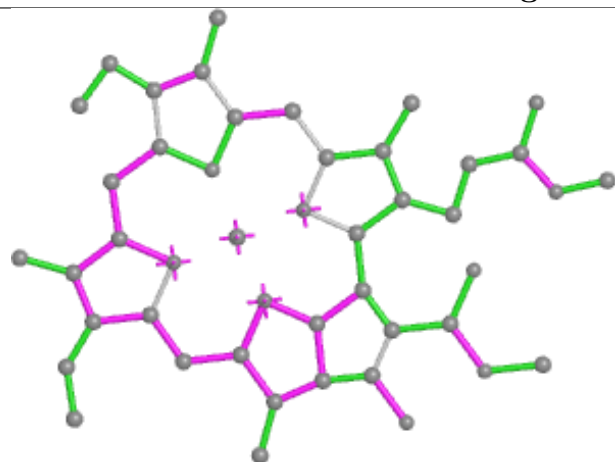




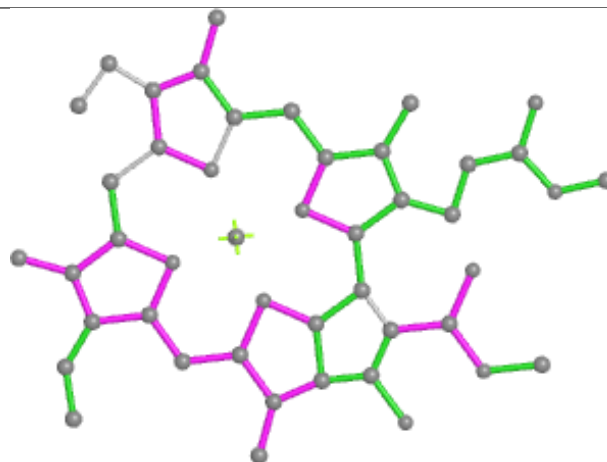
Ligand CLA 6 314



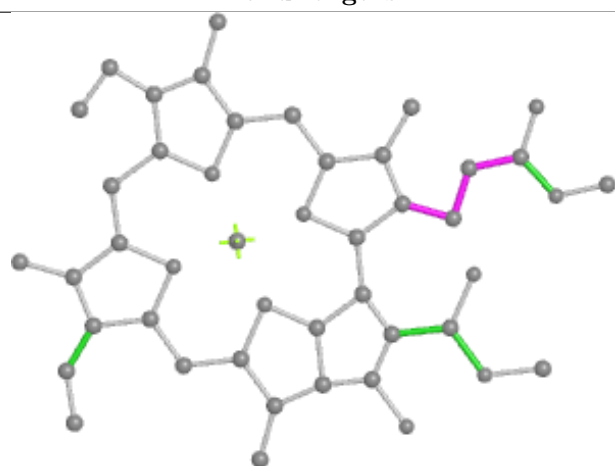
Ligand CLA 6 306



Bond lengths



Bond angles

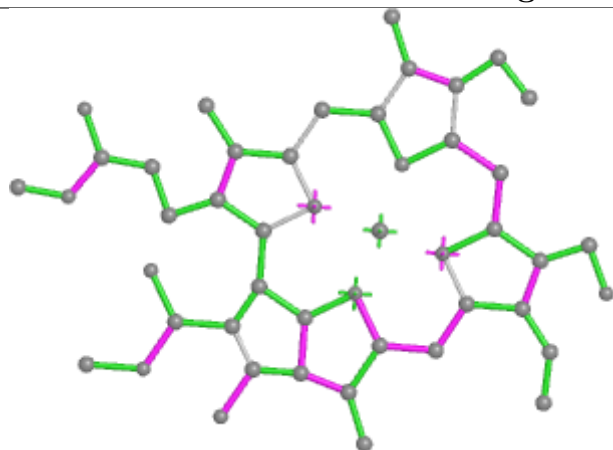


Torsions

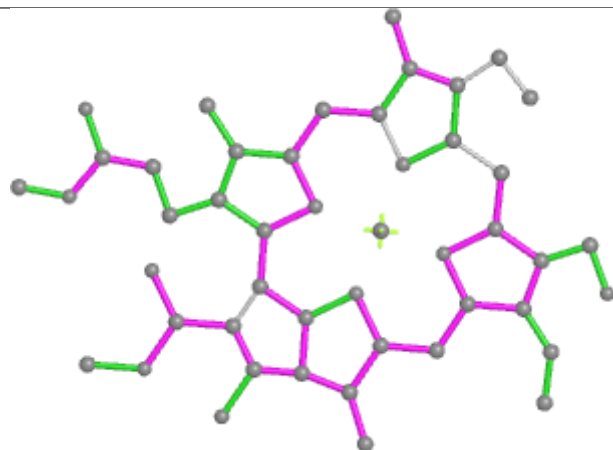


Rings

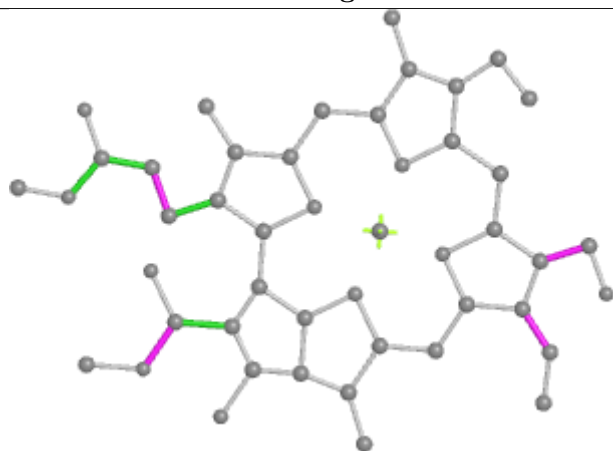
Ligand CHL 5 317



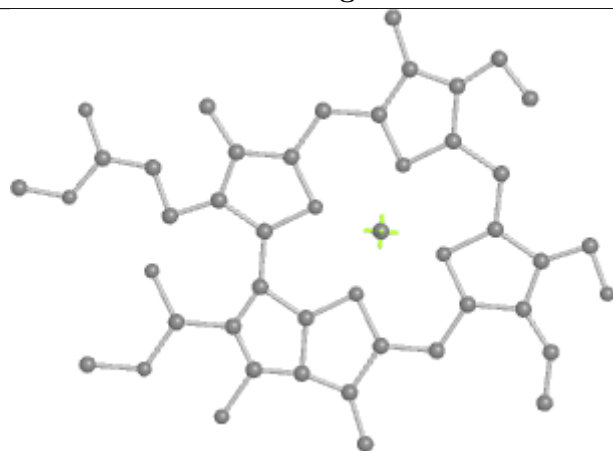
Bond lengths



Bond angles

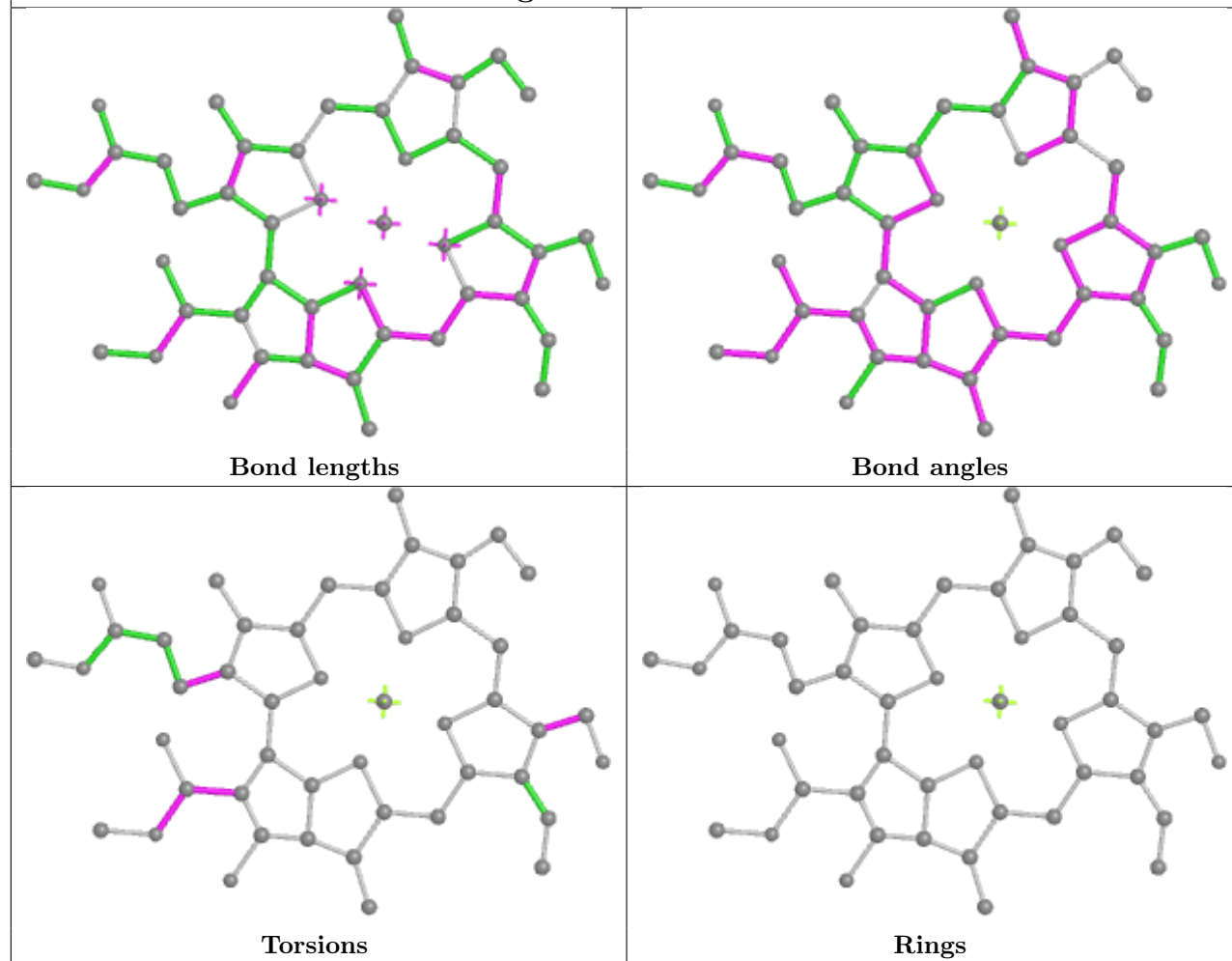


Torsions

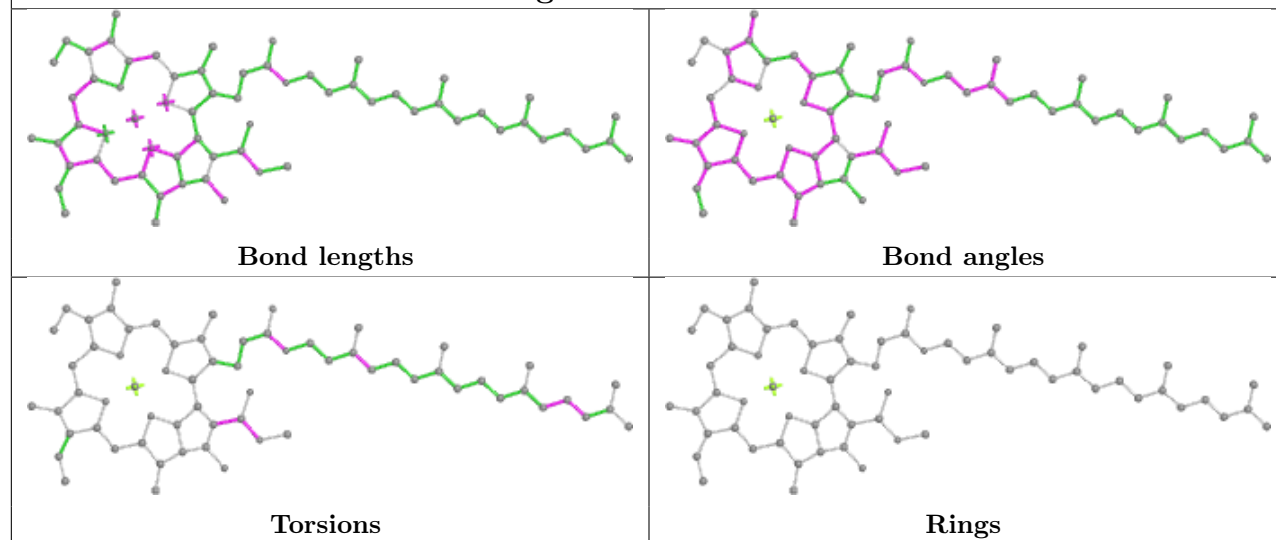


Rings

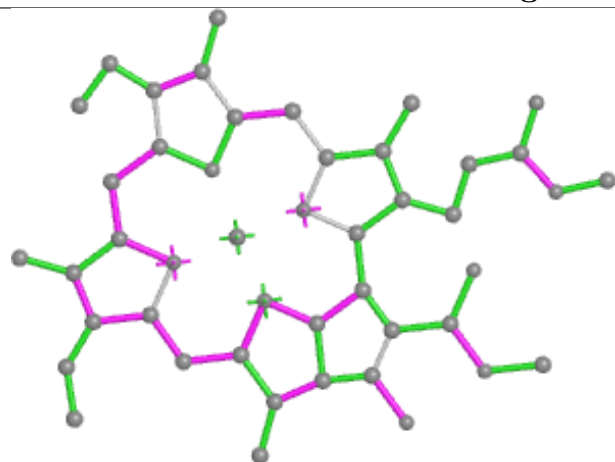
Ligand CHL 6 317



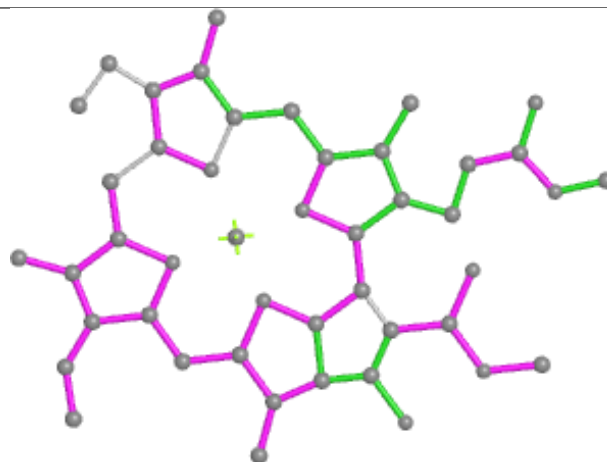
Ligand CLA 3 312



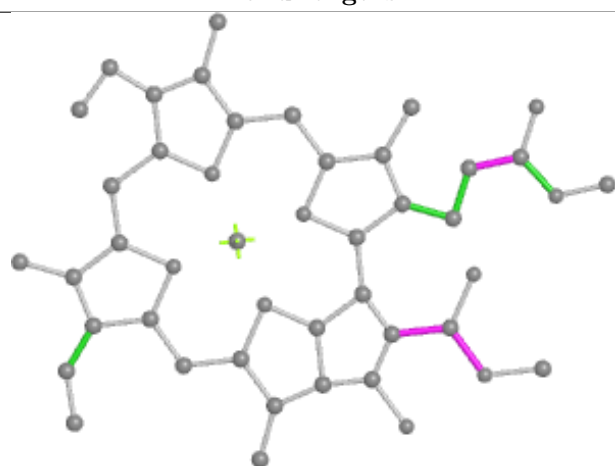
Ligand CLA 5 311



Bond lengths



Bond angles

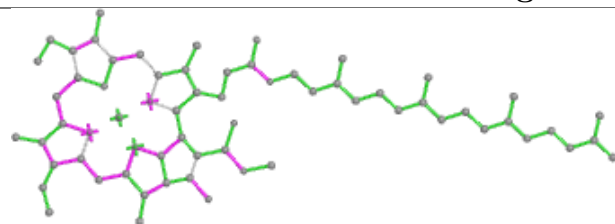


Torsions

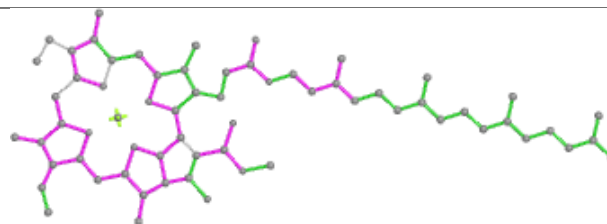


Rings

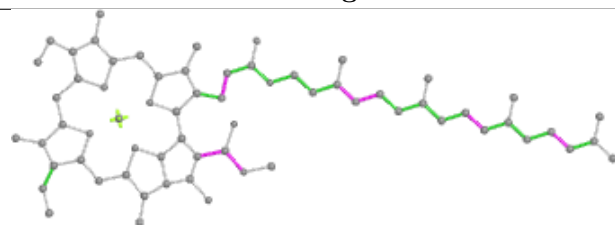
Ligand CLA B 832



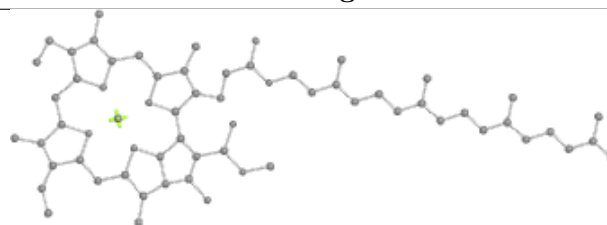
Bond lengths



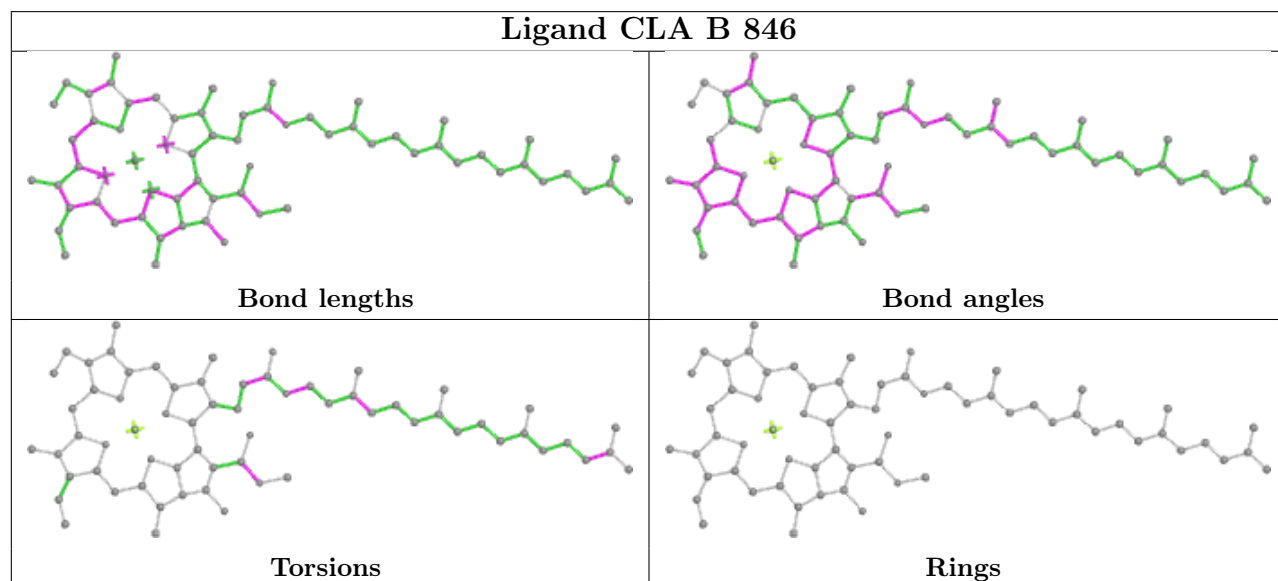
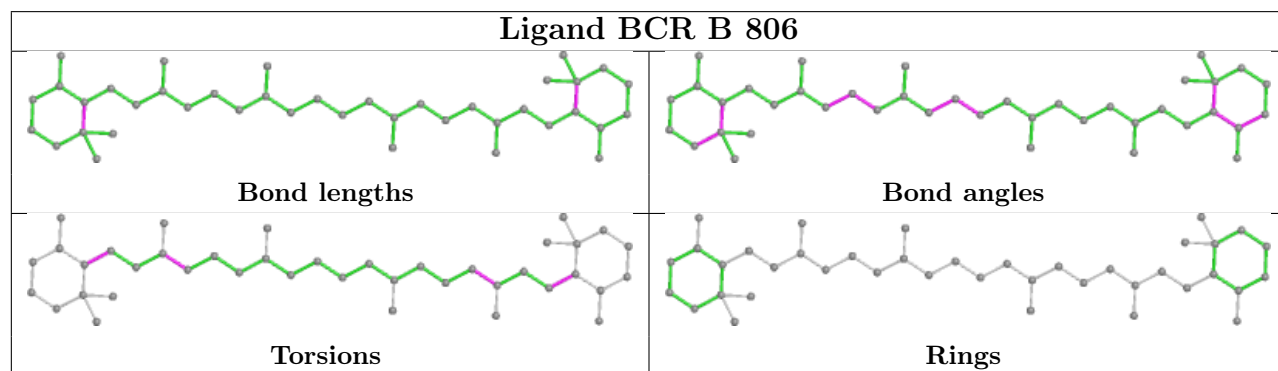
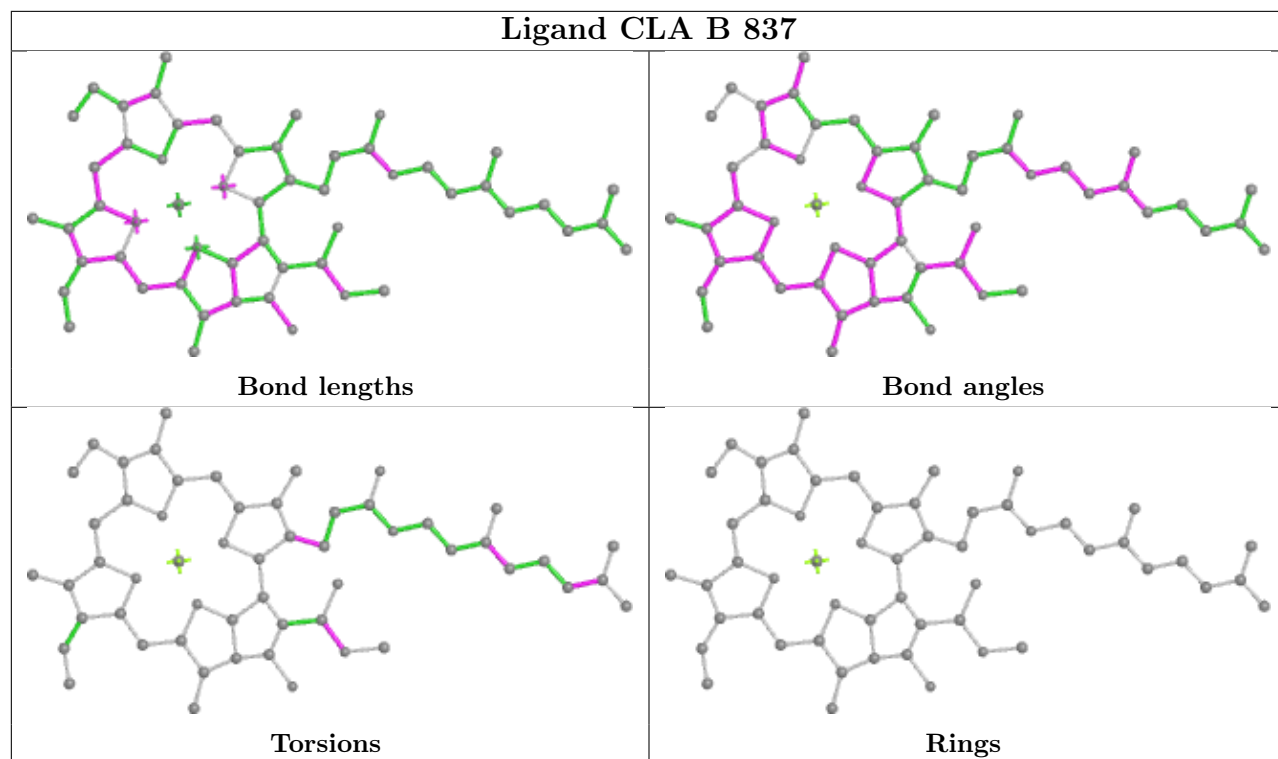
Bond angles

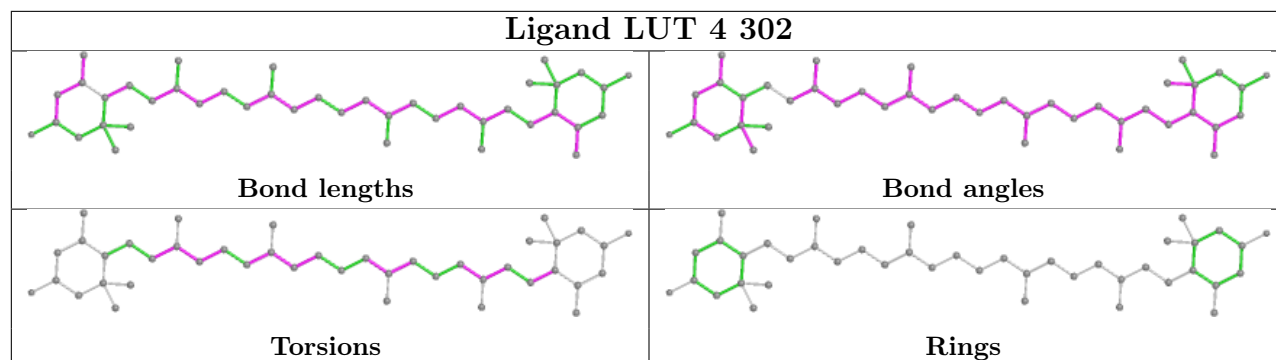
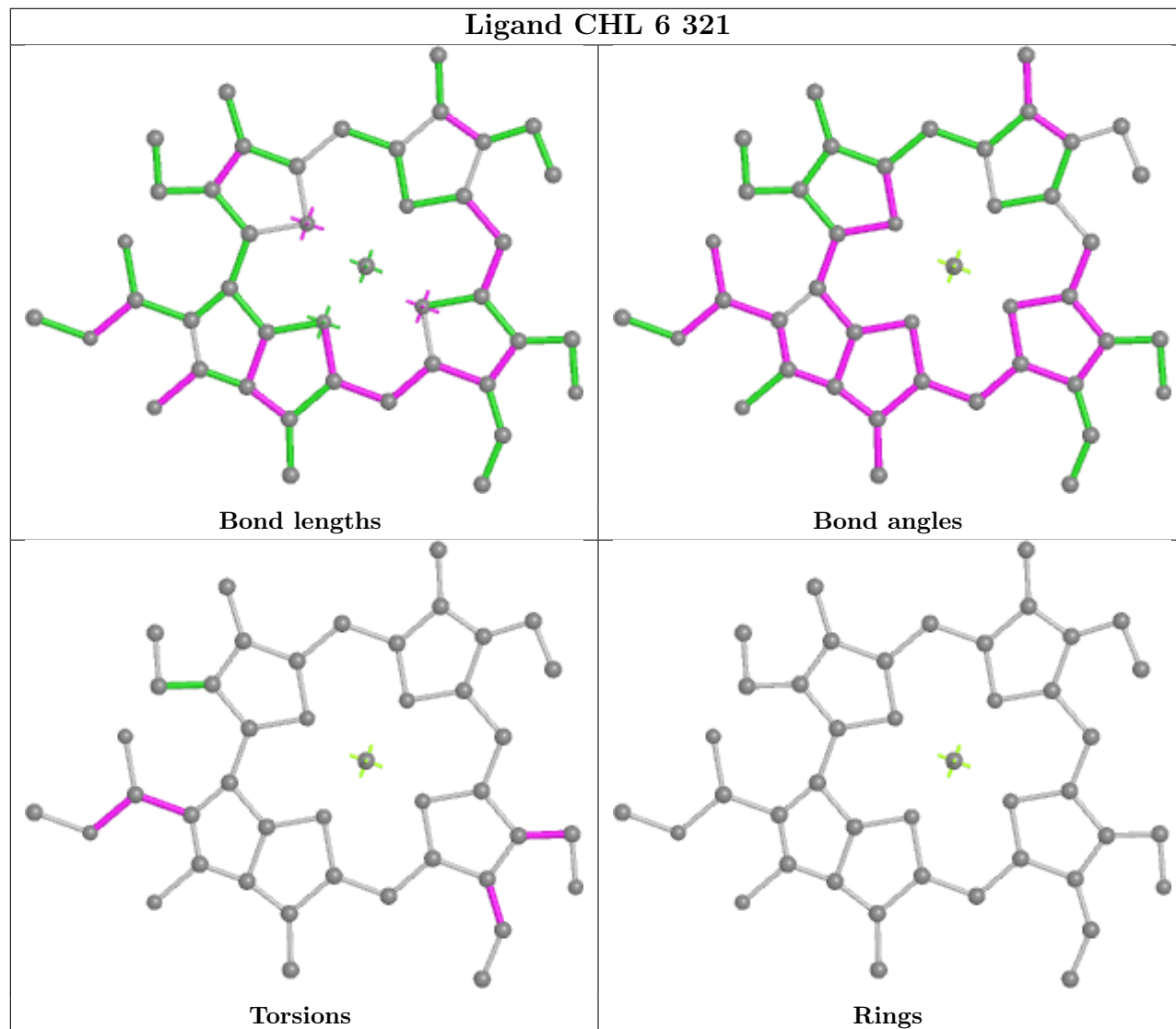


Torsions

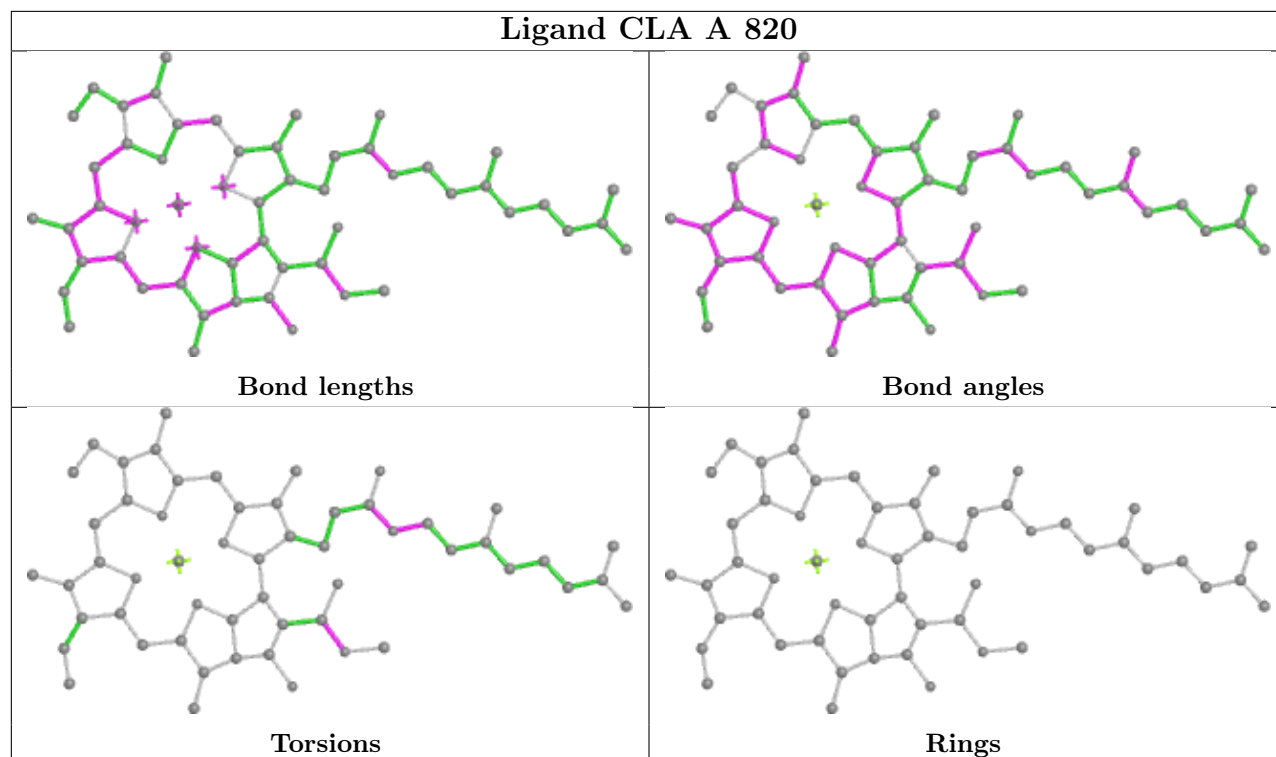


Rings

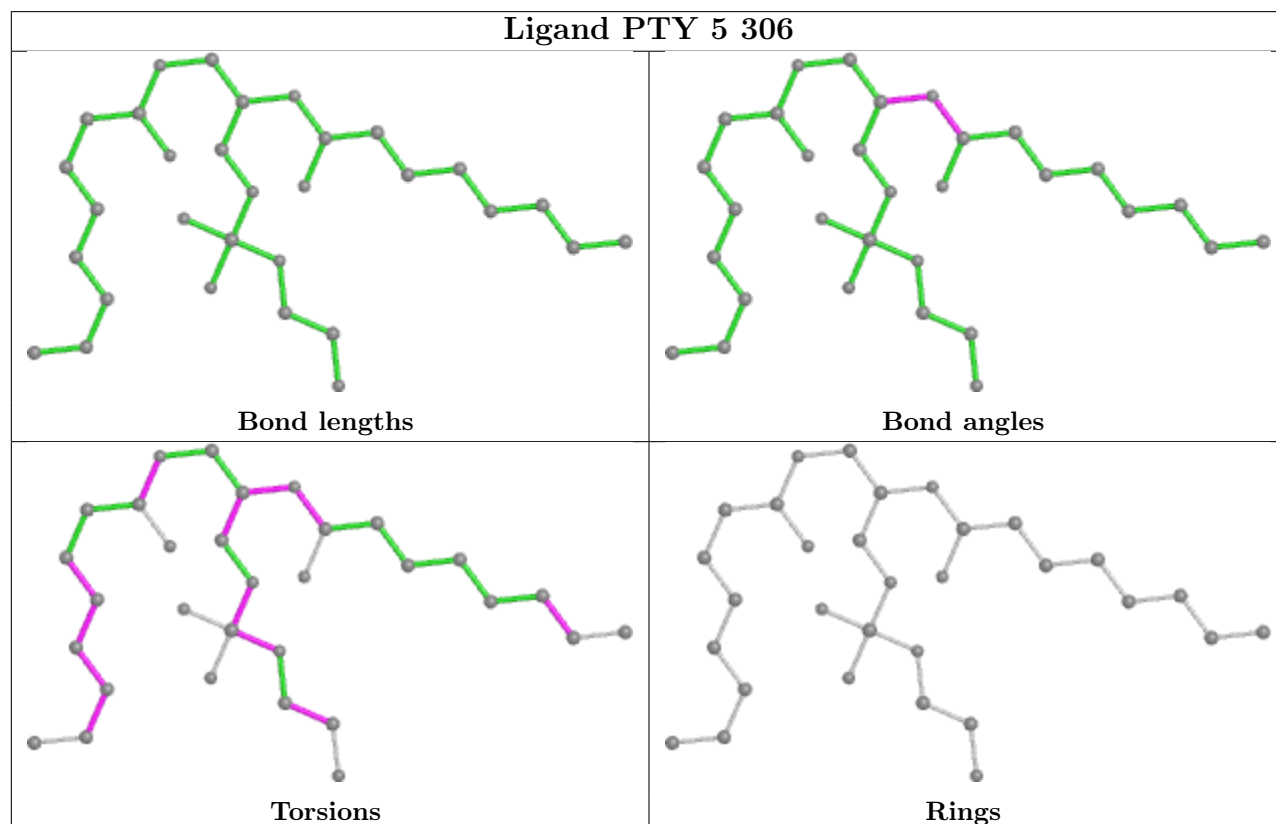


Ligand LUT 4 302**Ligand CHL 6 321**

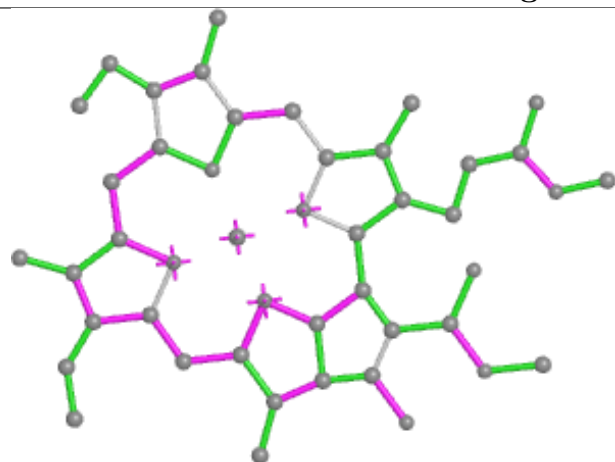
Ligand CLA A 820



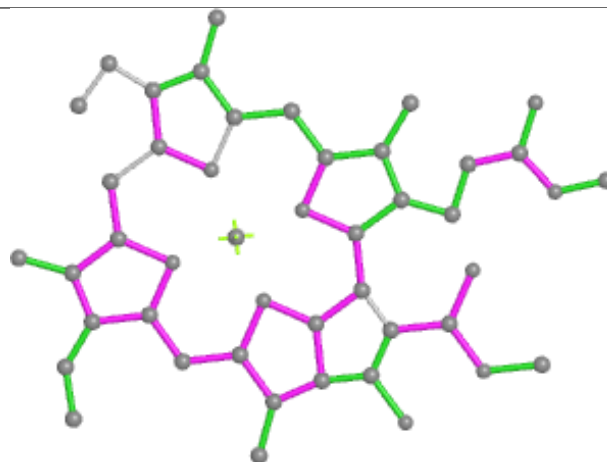
Ligand PTY 5 306



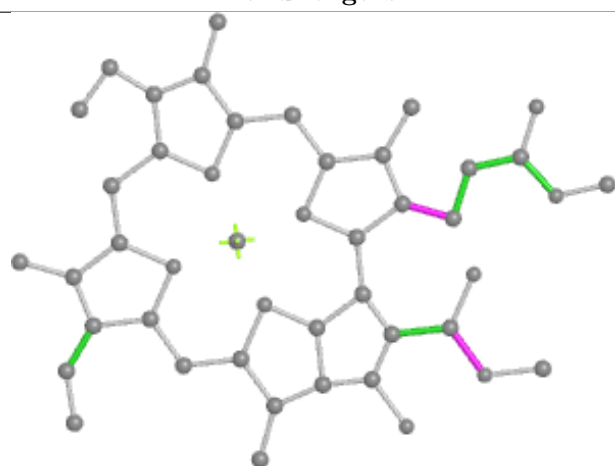
Ligand CLA 7 322



Bond lengths



Bond angles

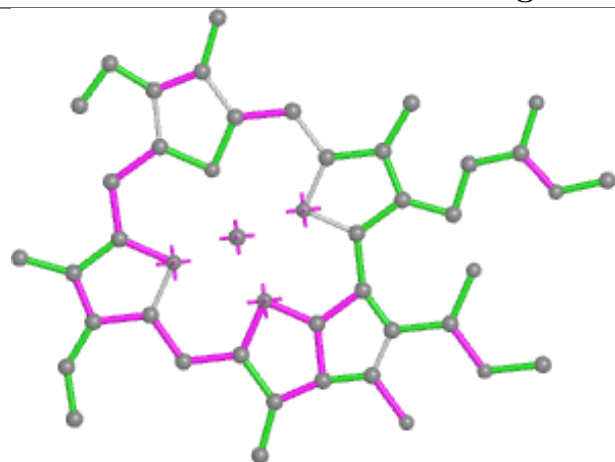


Torsions

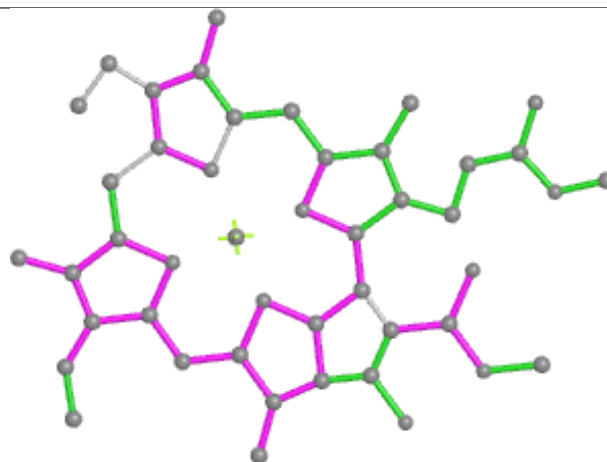


Rings

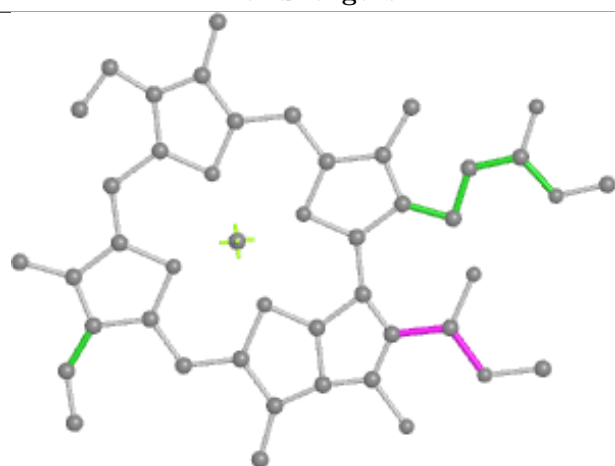
Ligand CLA B 838



Bond lengths



Bond angles

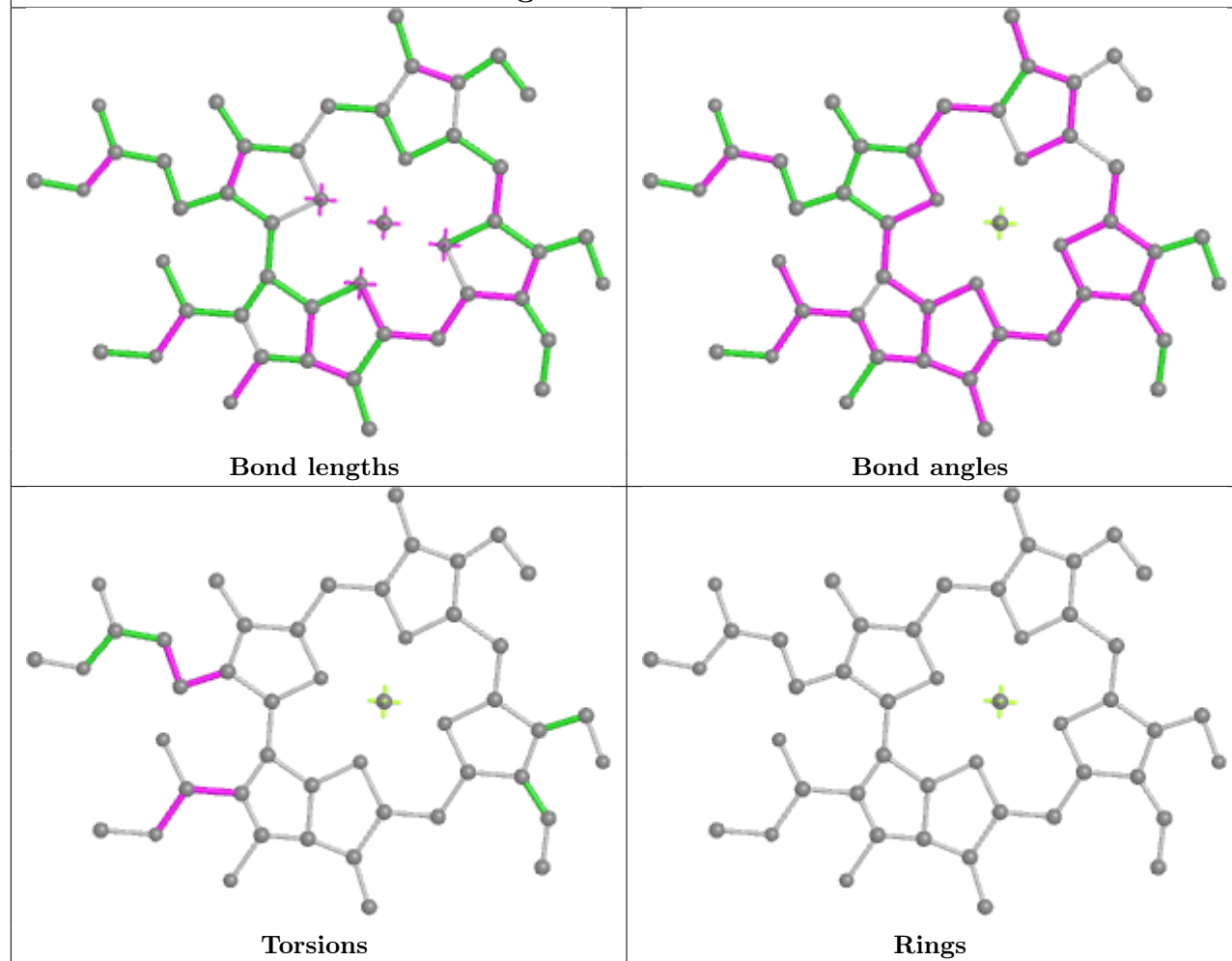


Torsions

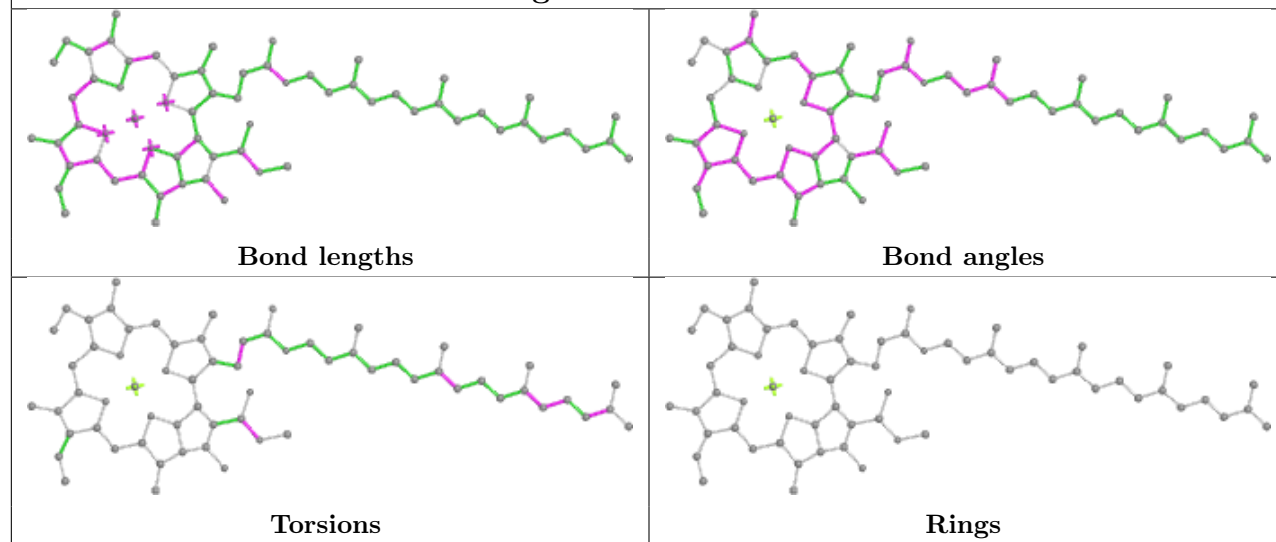


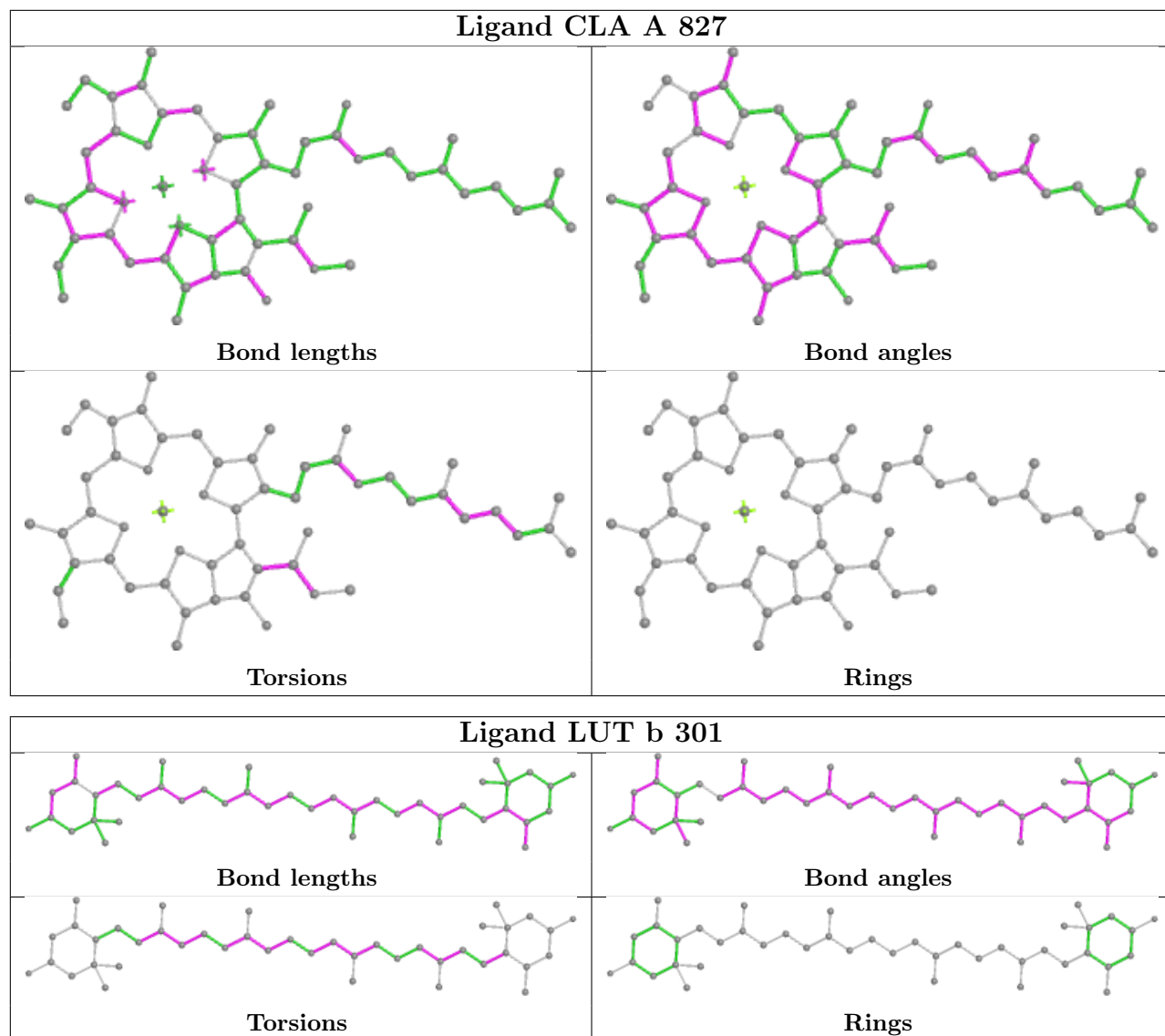
Rings

Ligand CHL 6 319

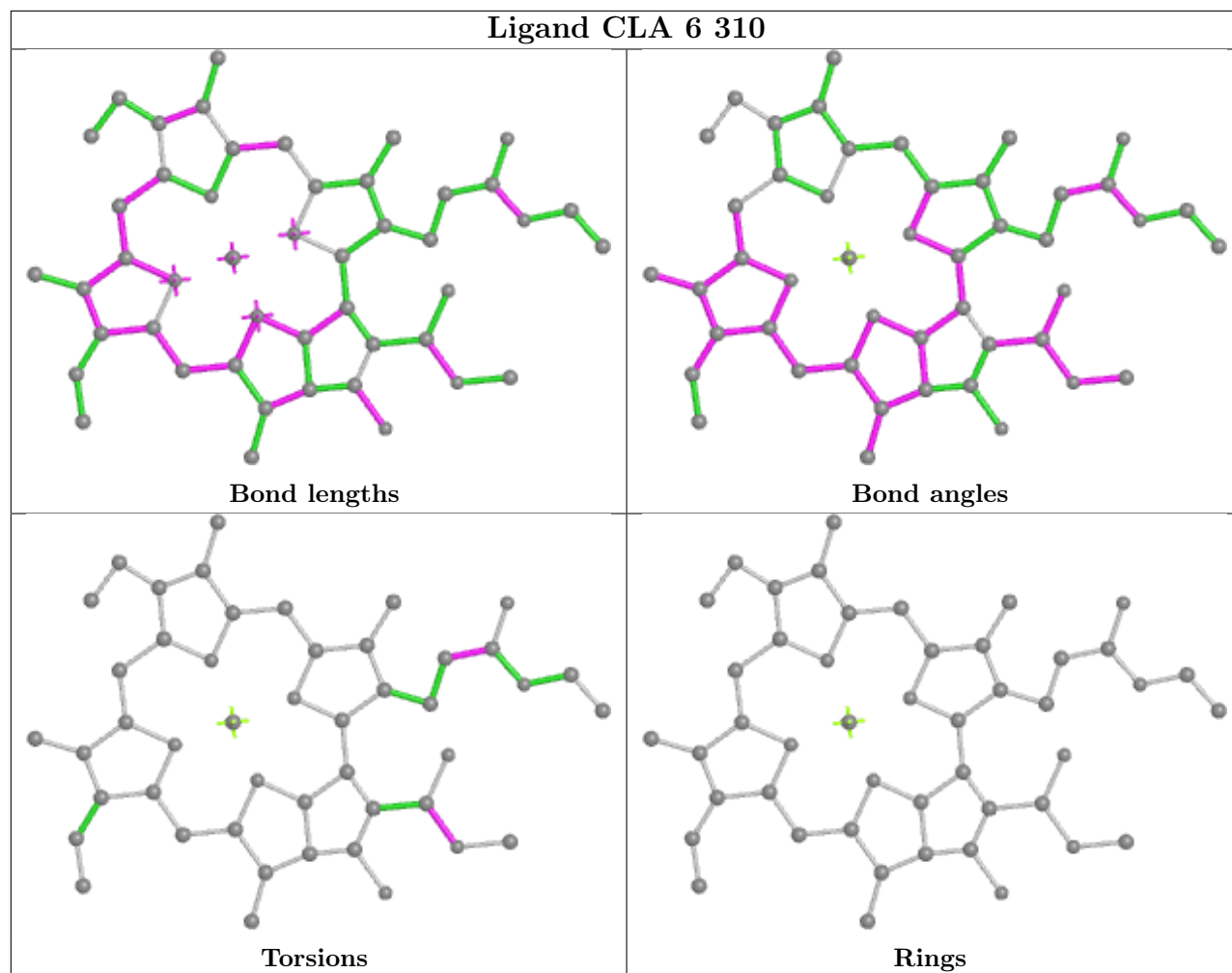


Ligand CLA B 812

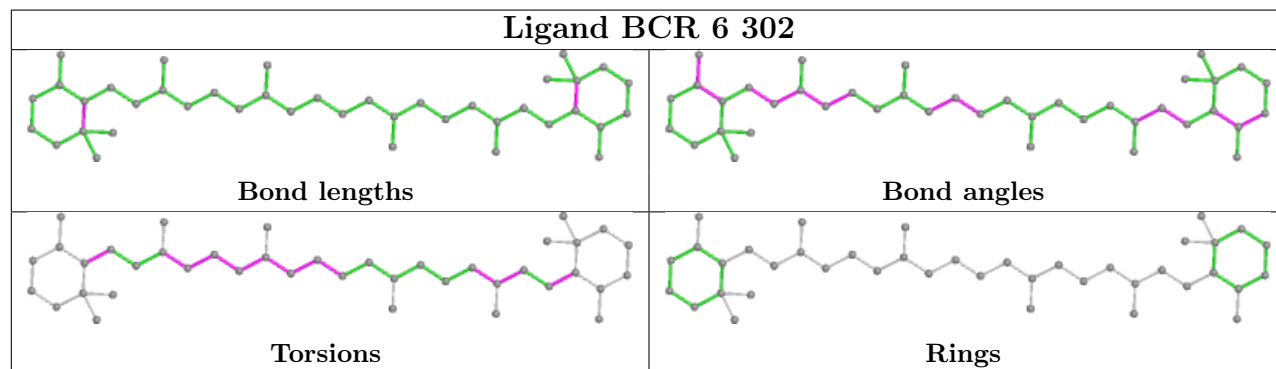


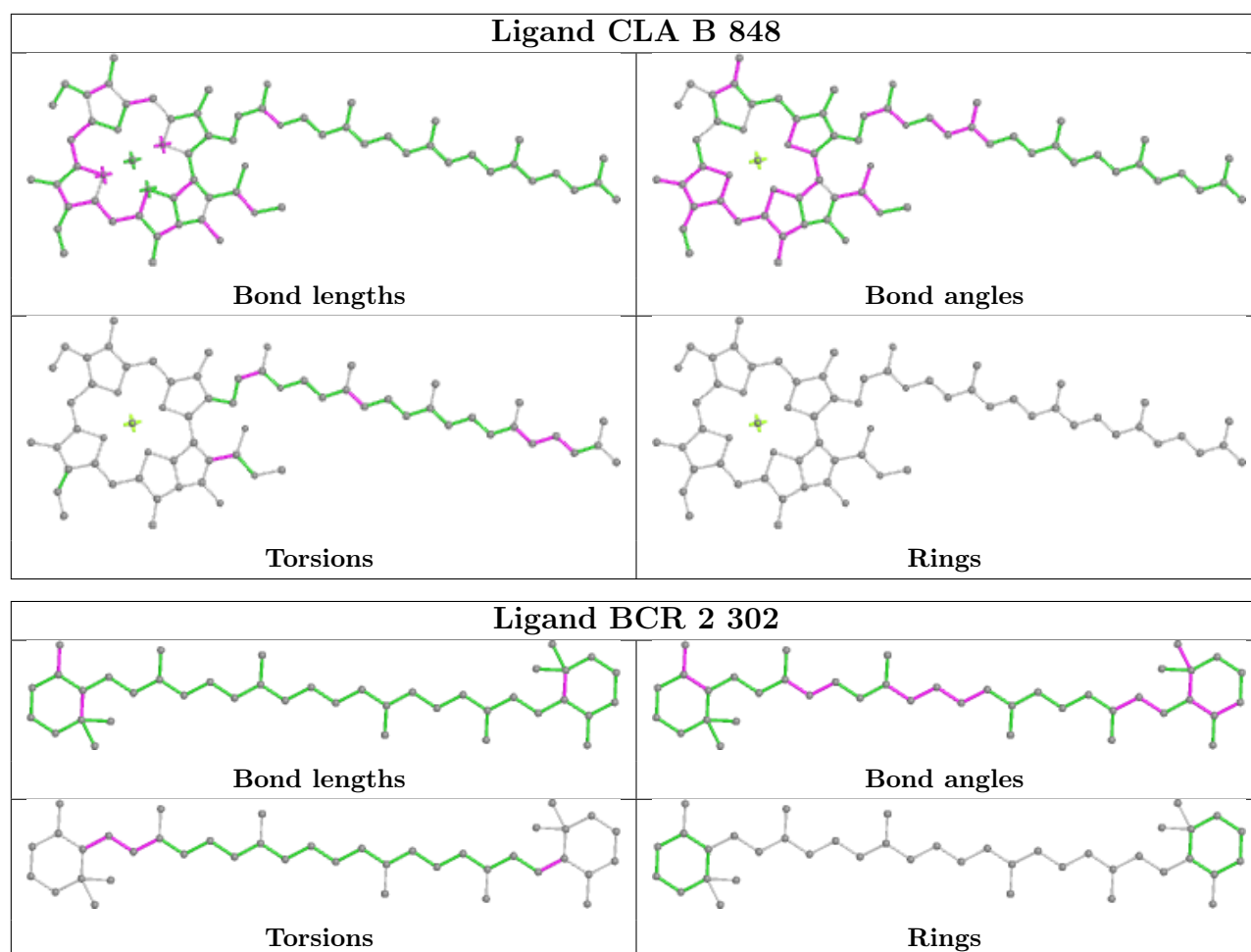


Ligand CLA 6 310

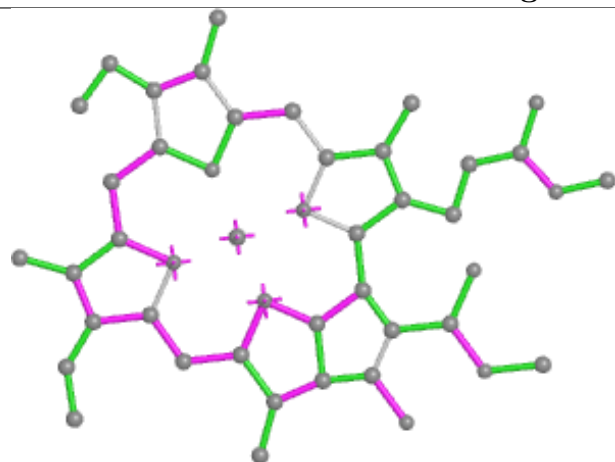


Ligand BCR 6 302

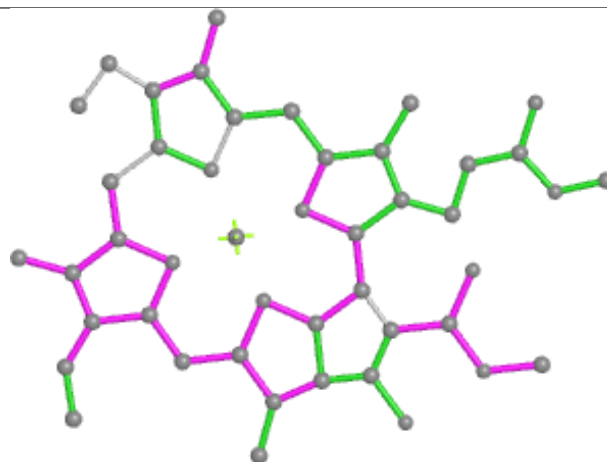




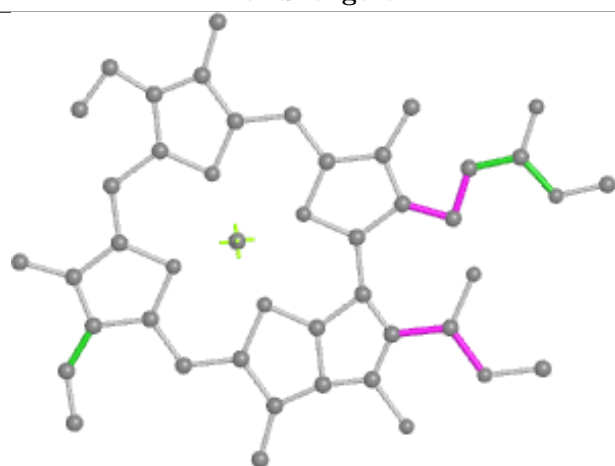
Ligand CLA 2 315



Bond lengths



Bond angles

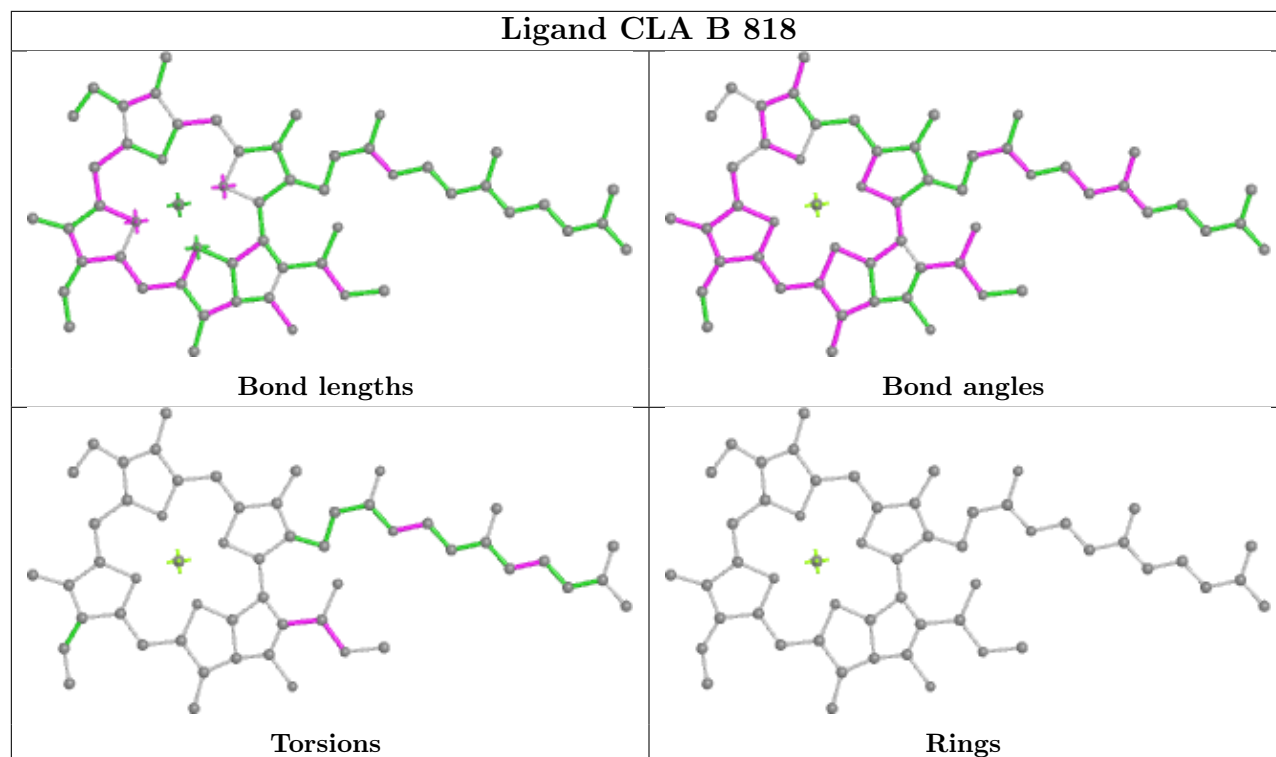


Torsions

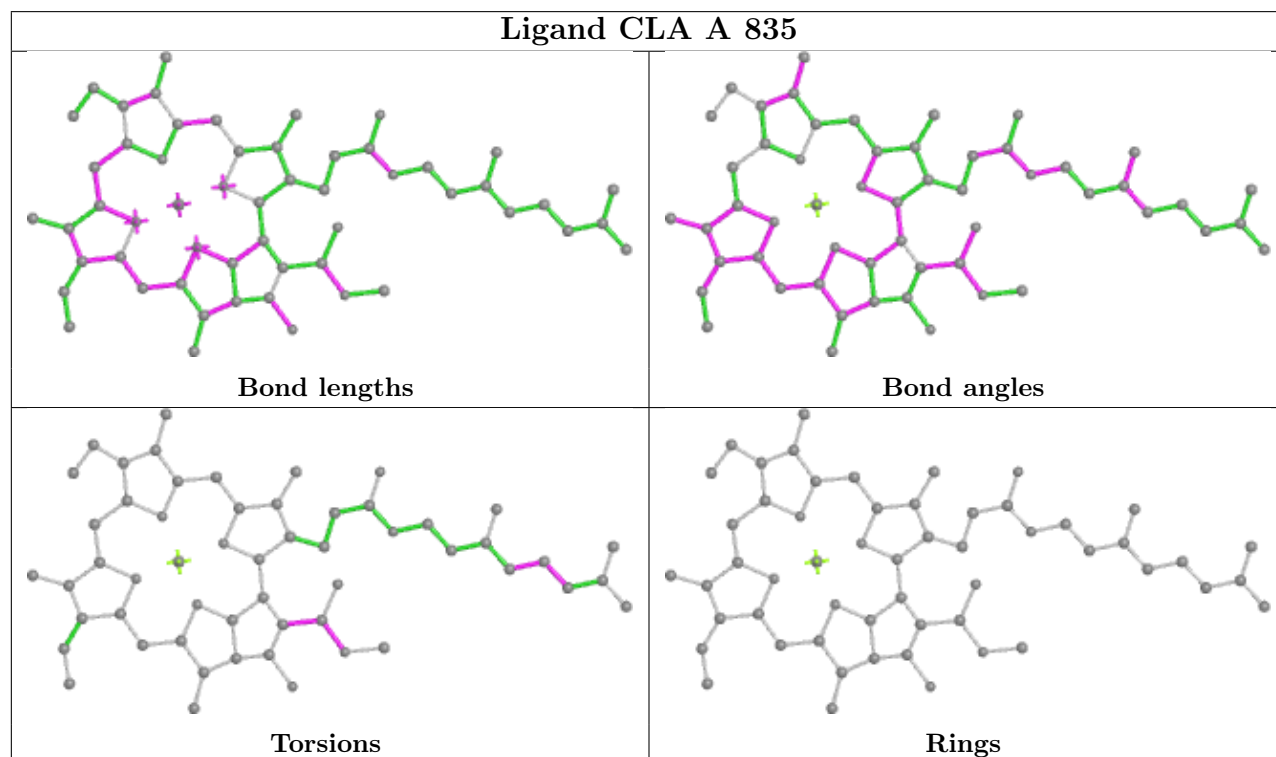


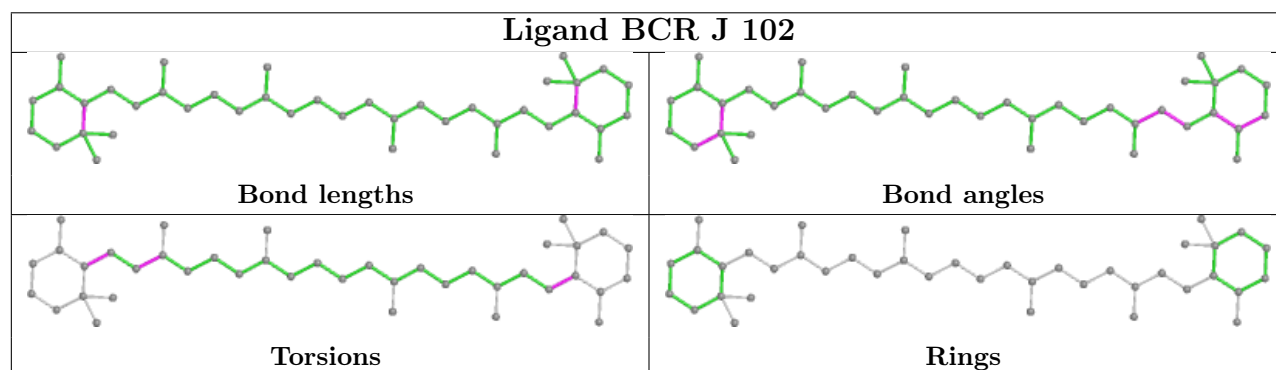
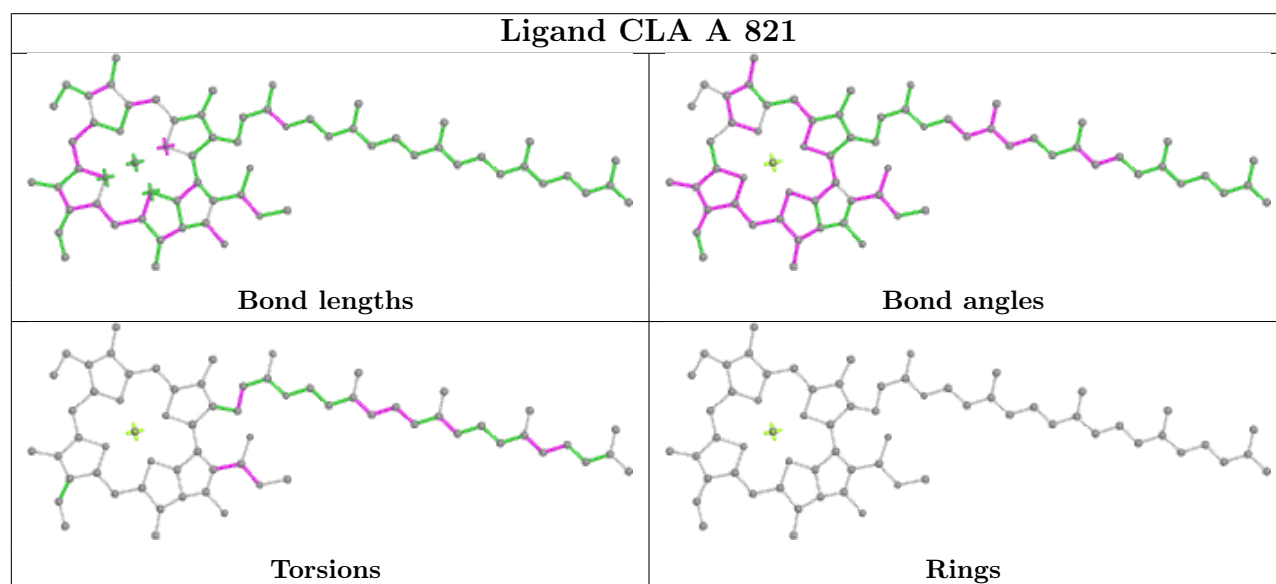
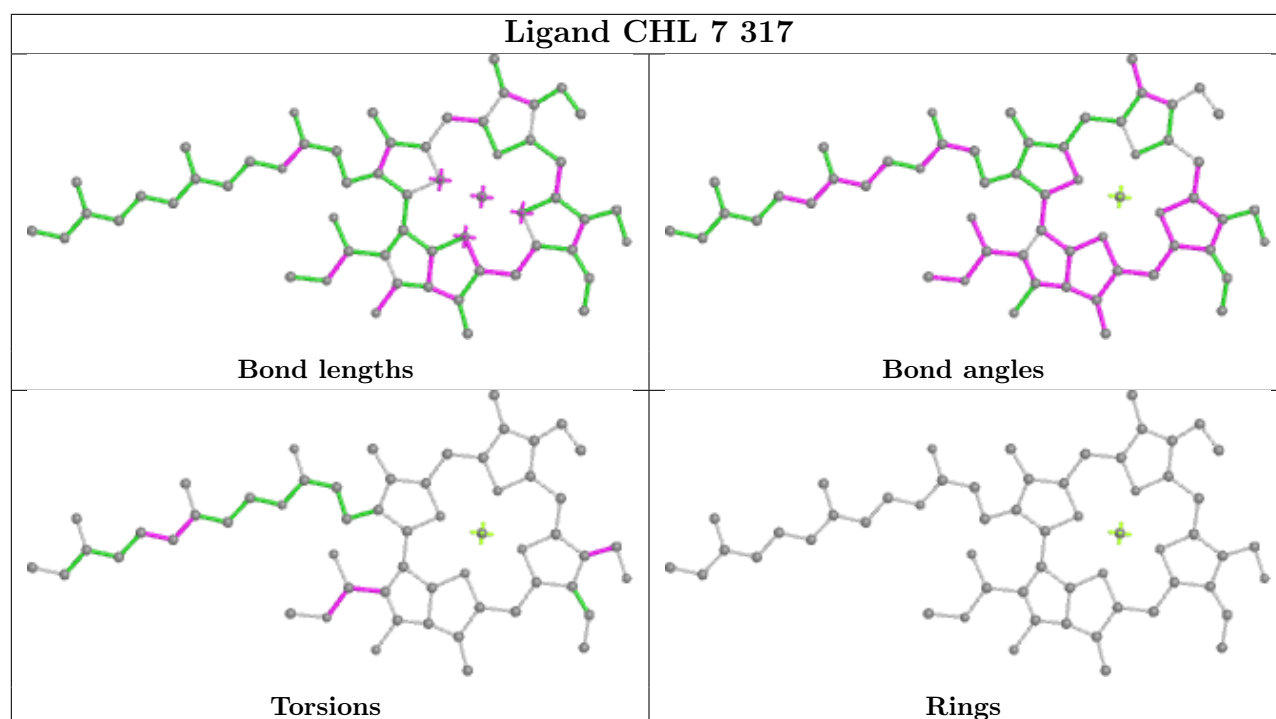
Rings

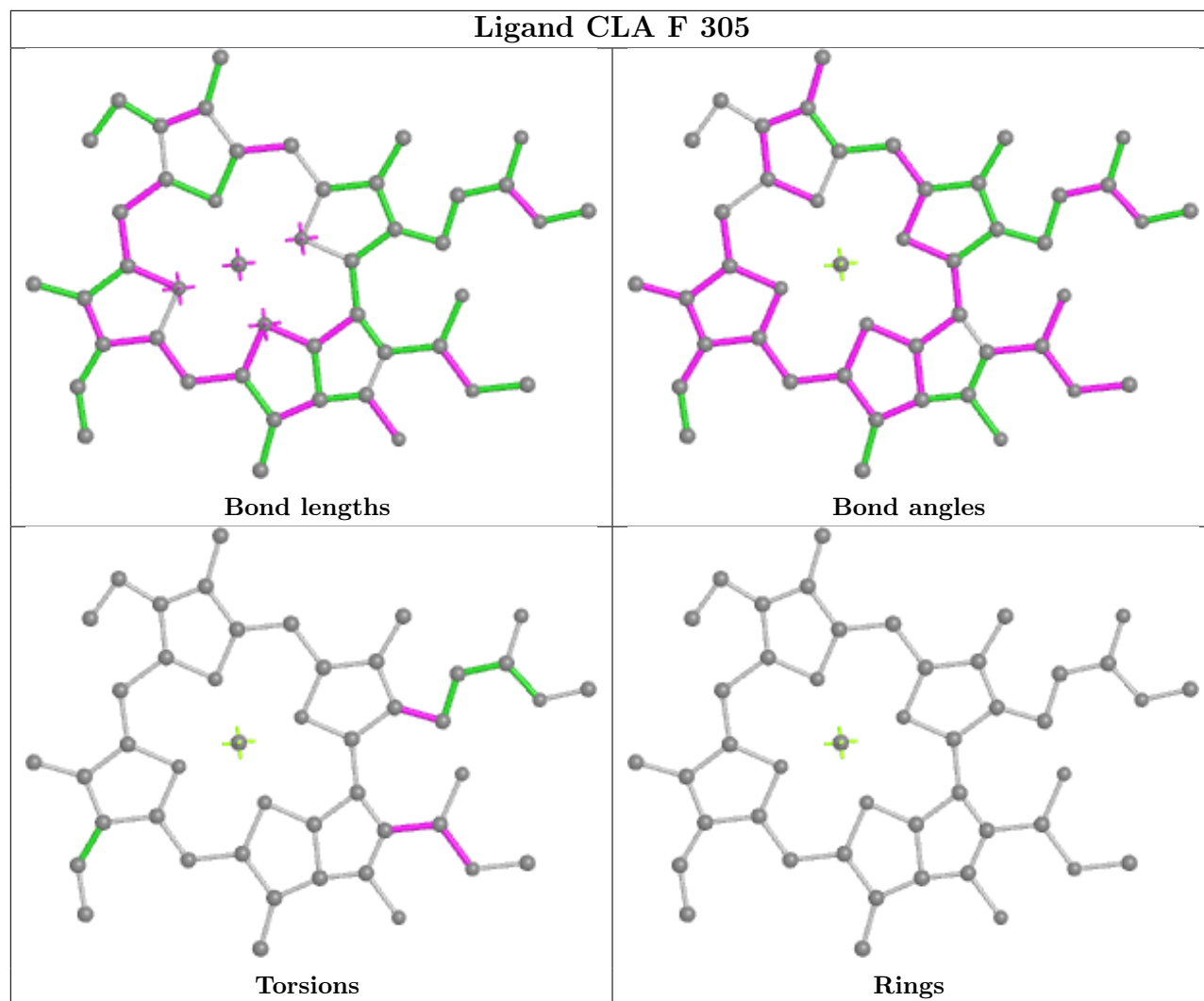
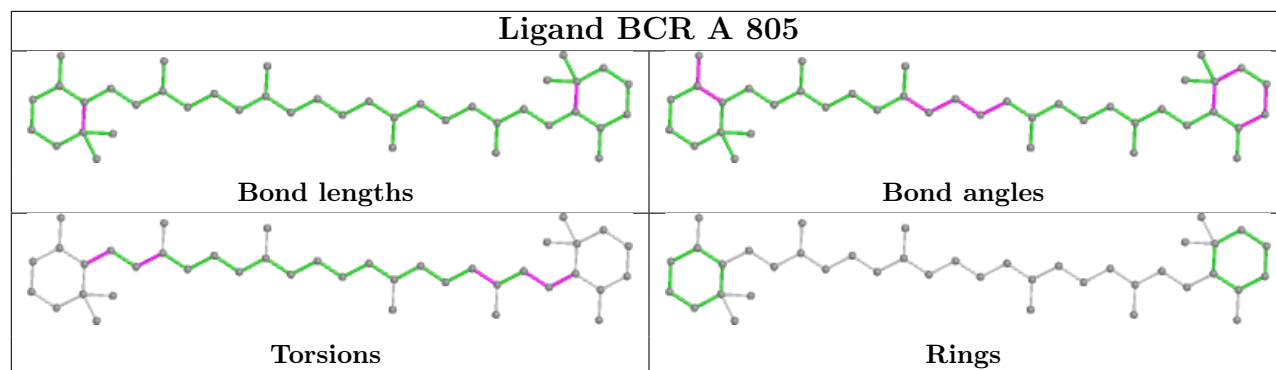
Ligand CLA B 818

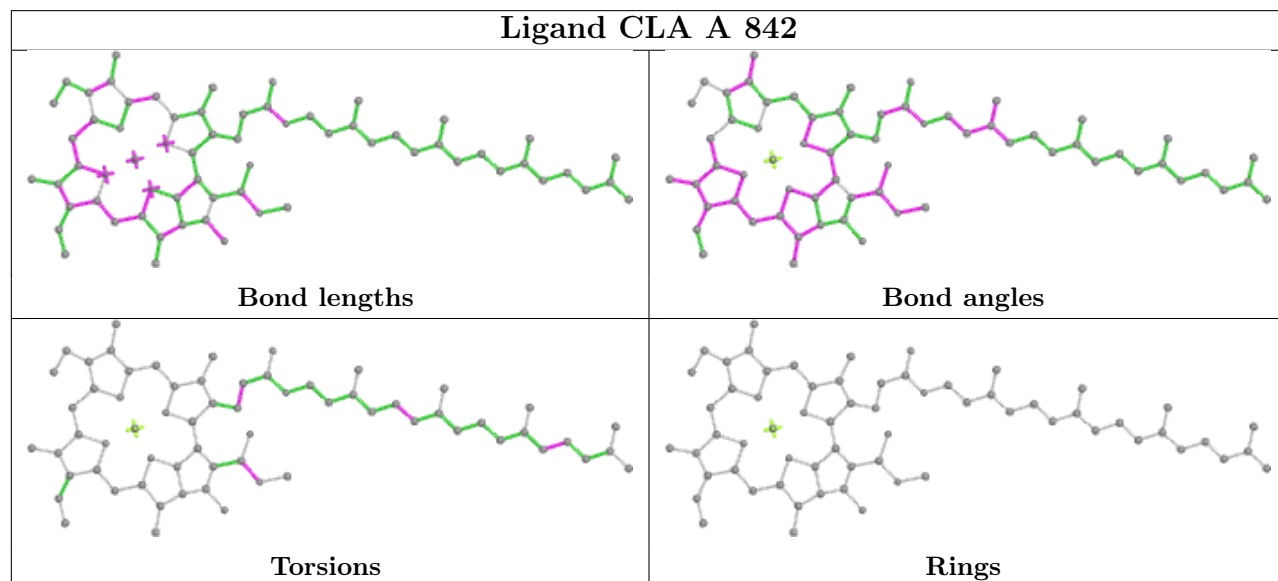
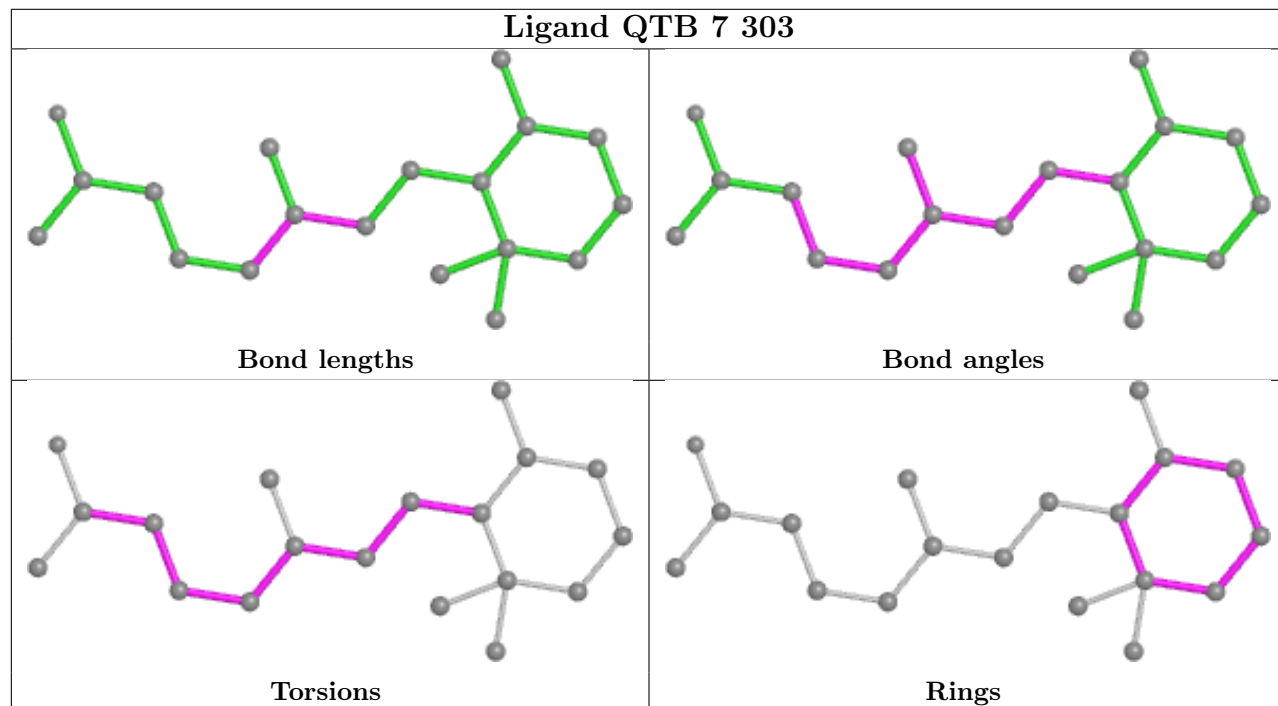
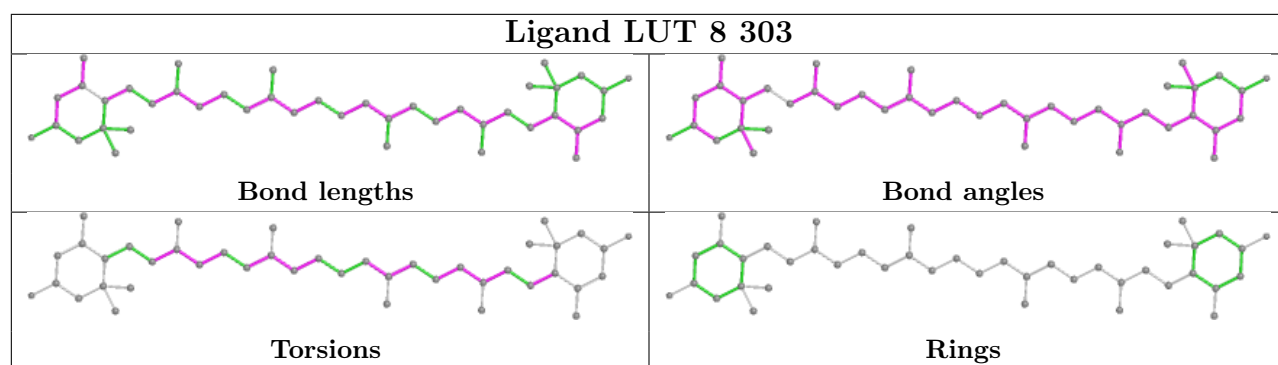


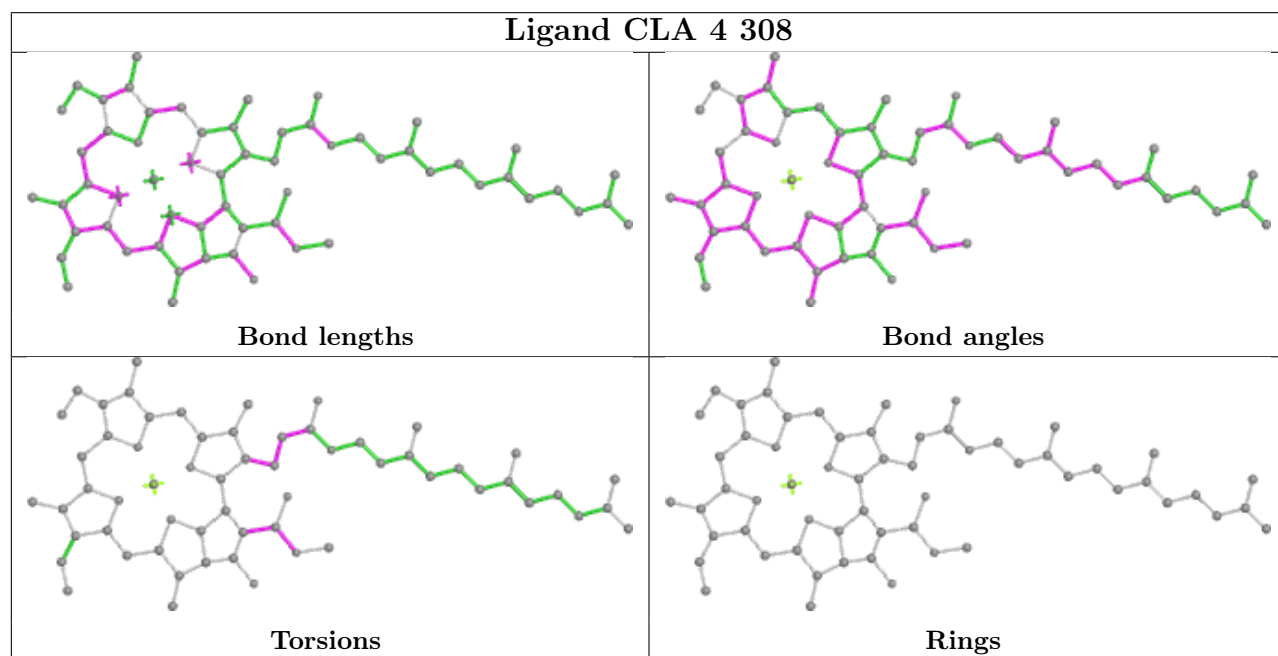
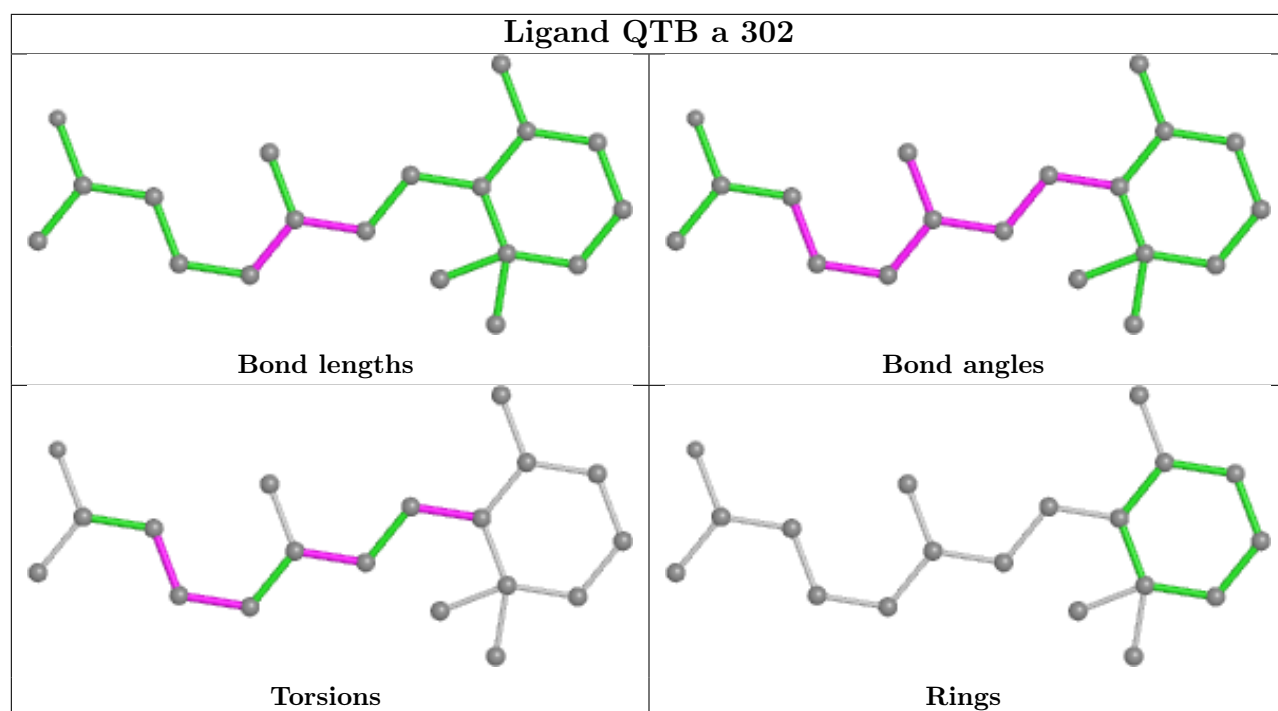
Ligand CLA A 835

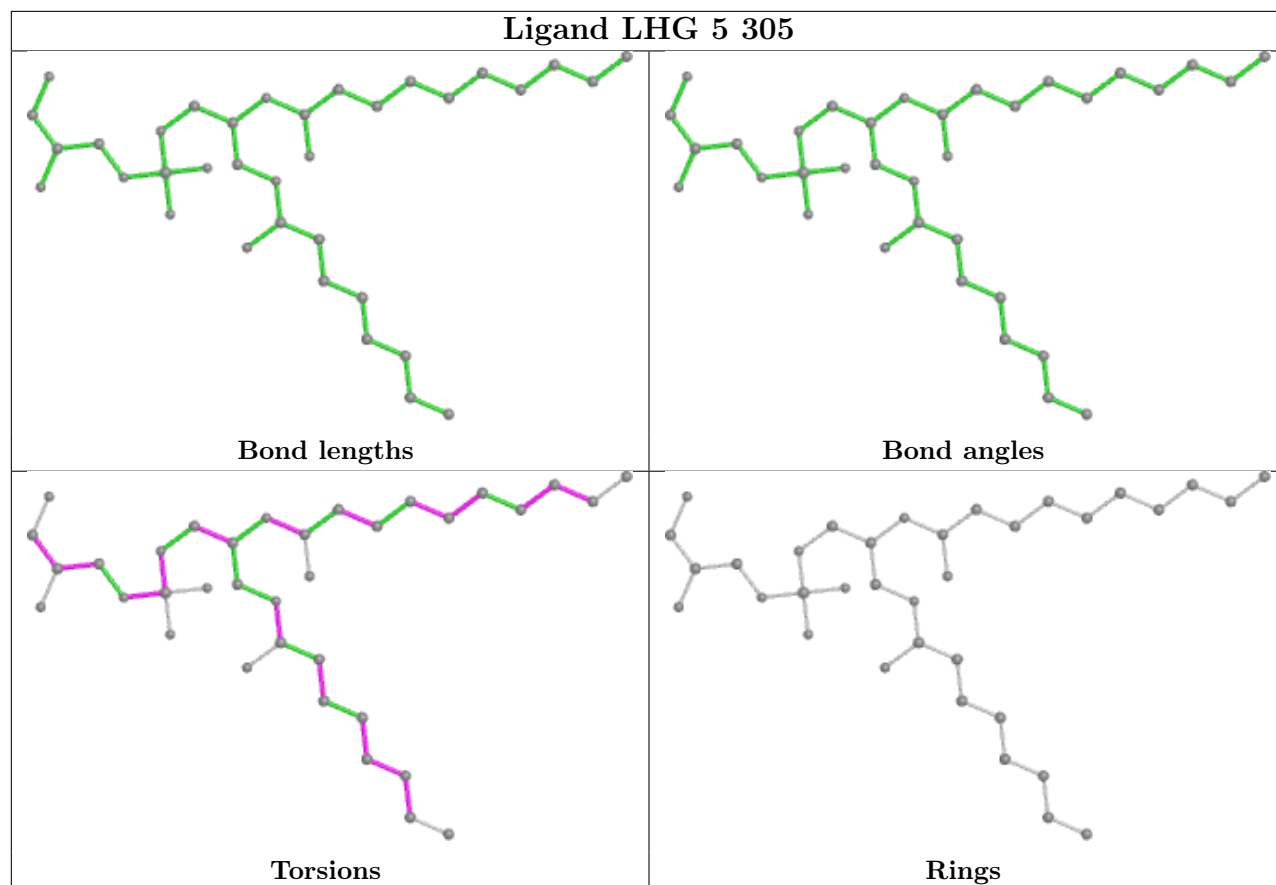
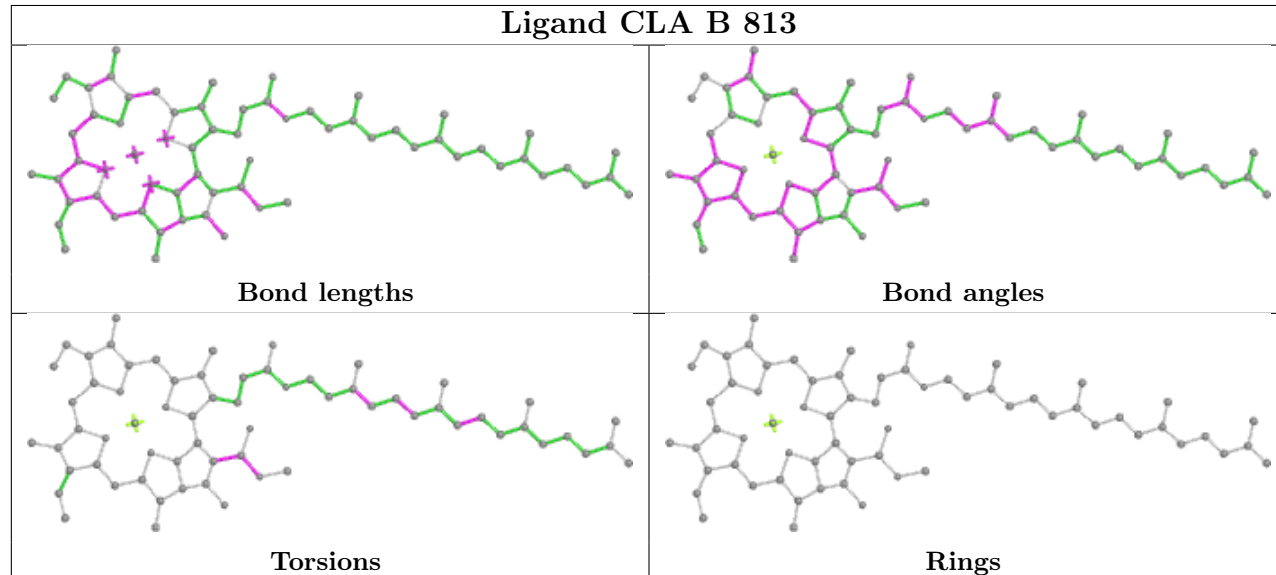


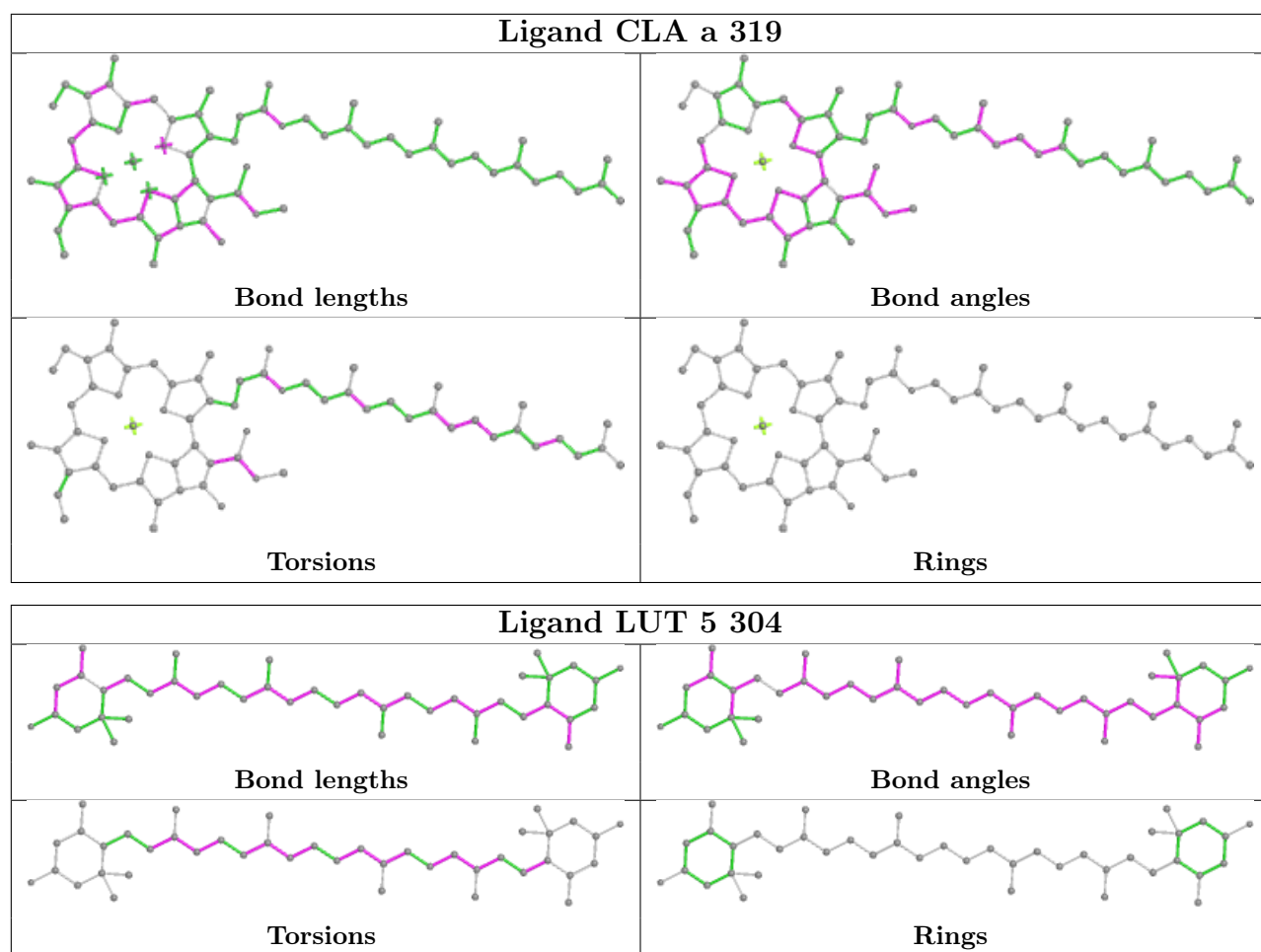




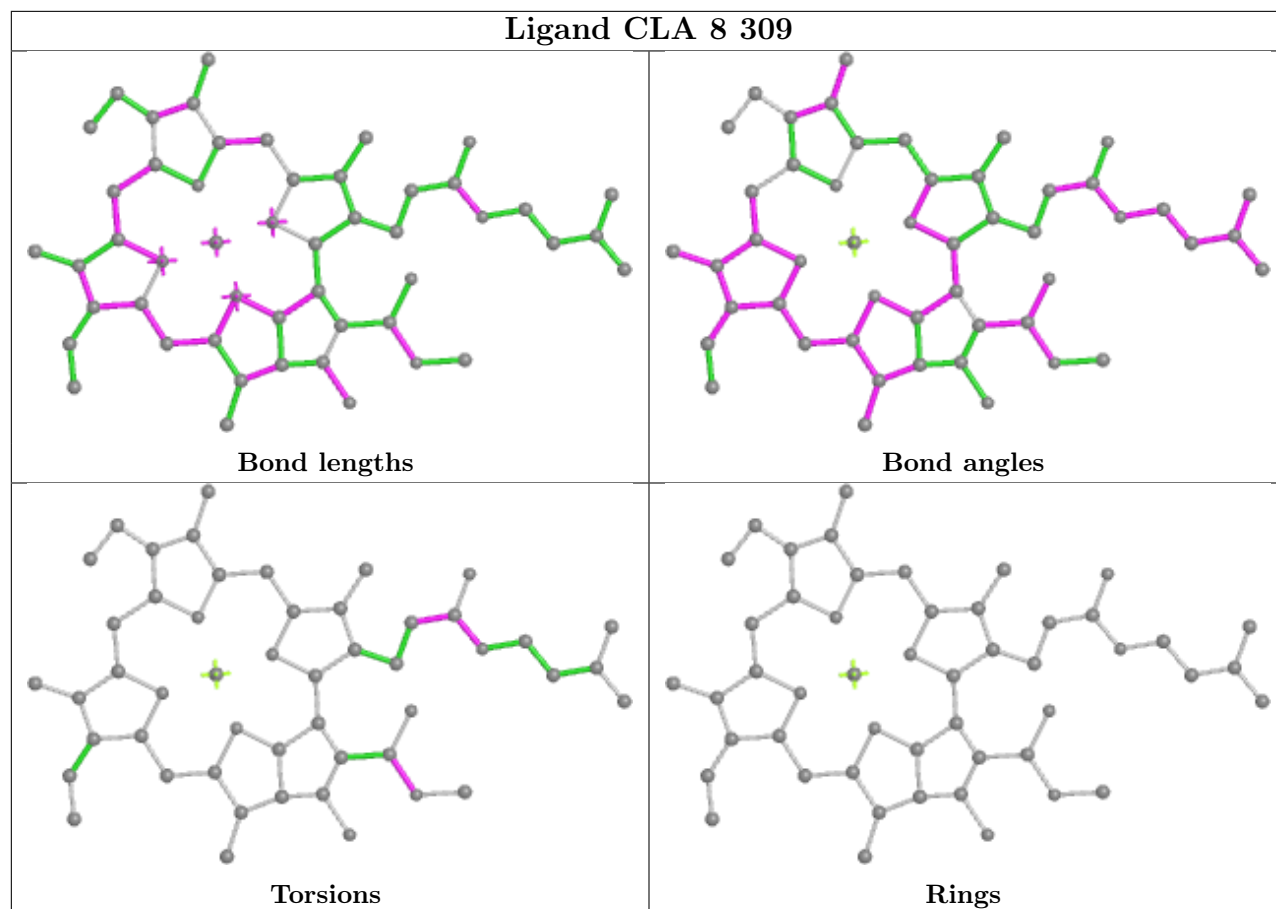




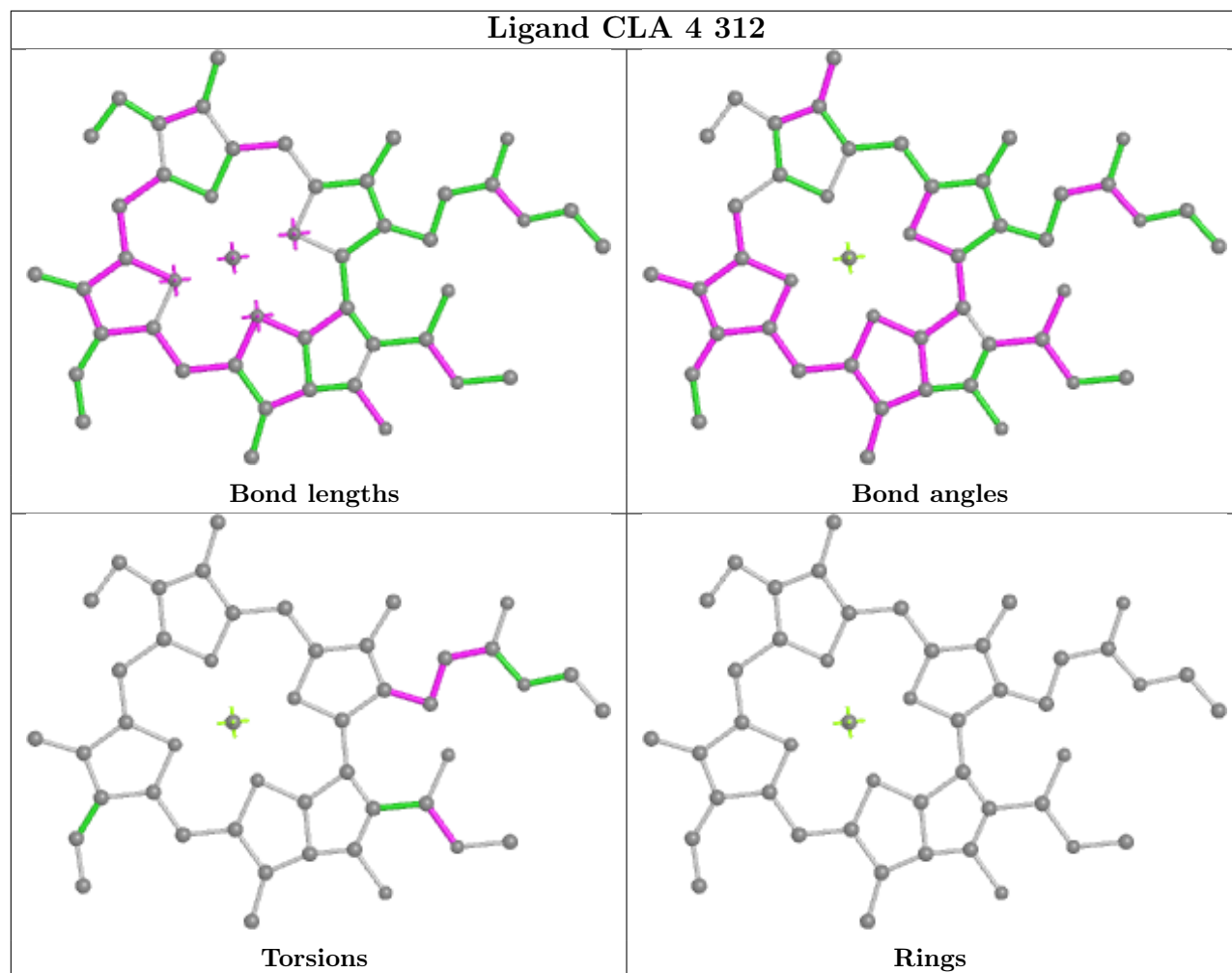
Ligand LHG 5 305**Ligand CLA B 813**



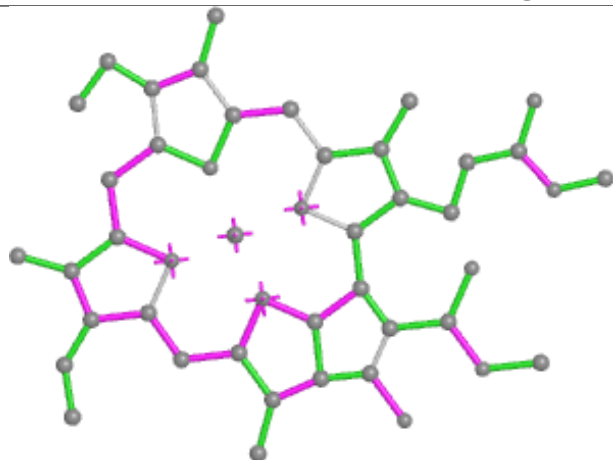
Ligand CLA 8 309



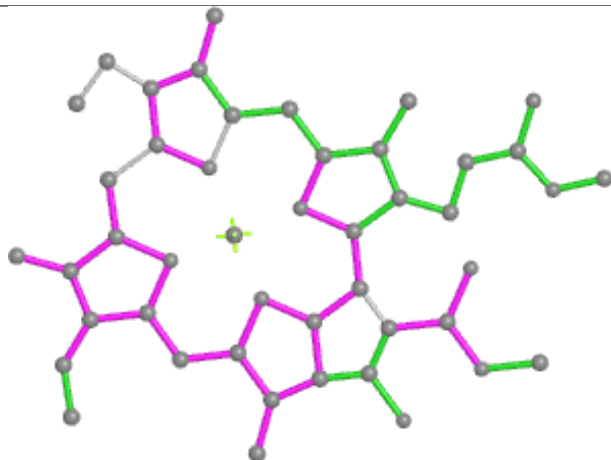
Ligand CLA 4 312



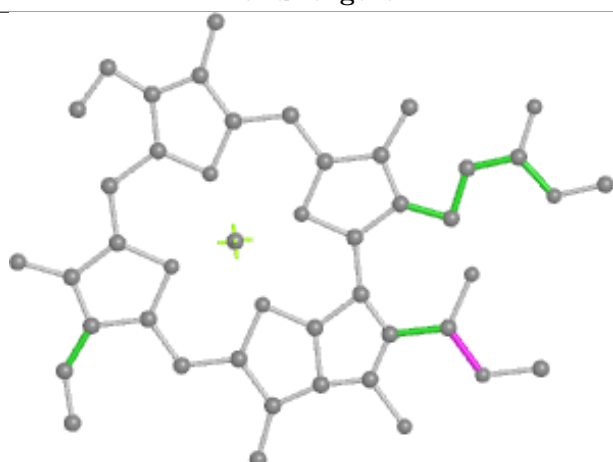
Ligand CLA 2 314



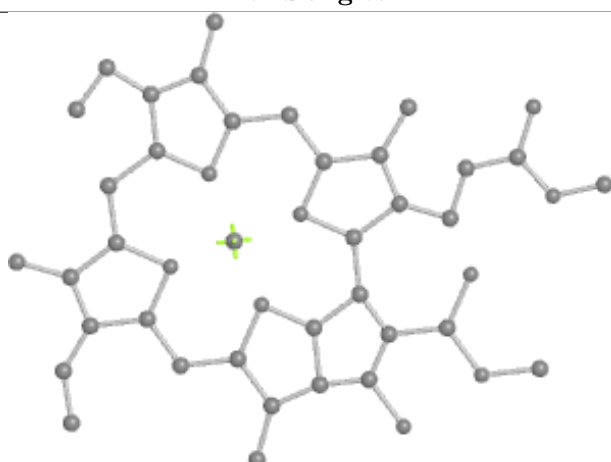
Bond lengths



Bond angles

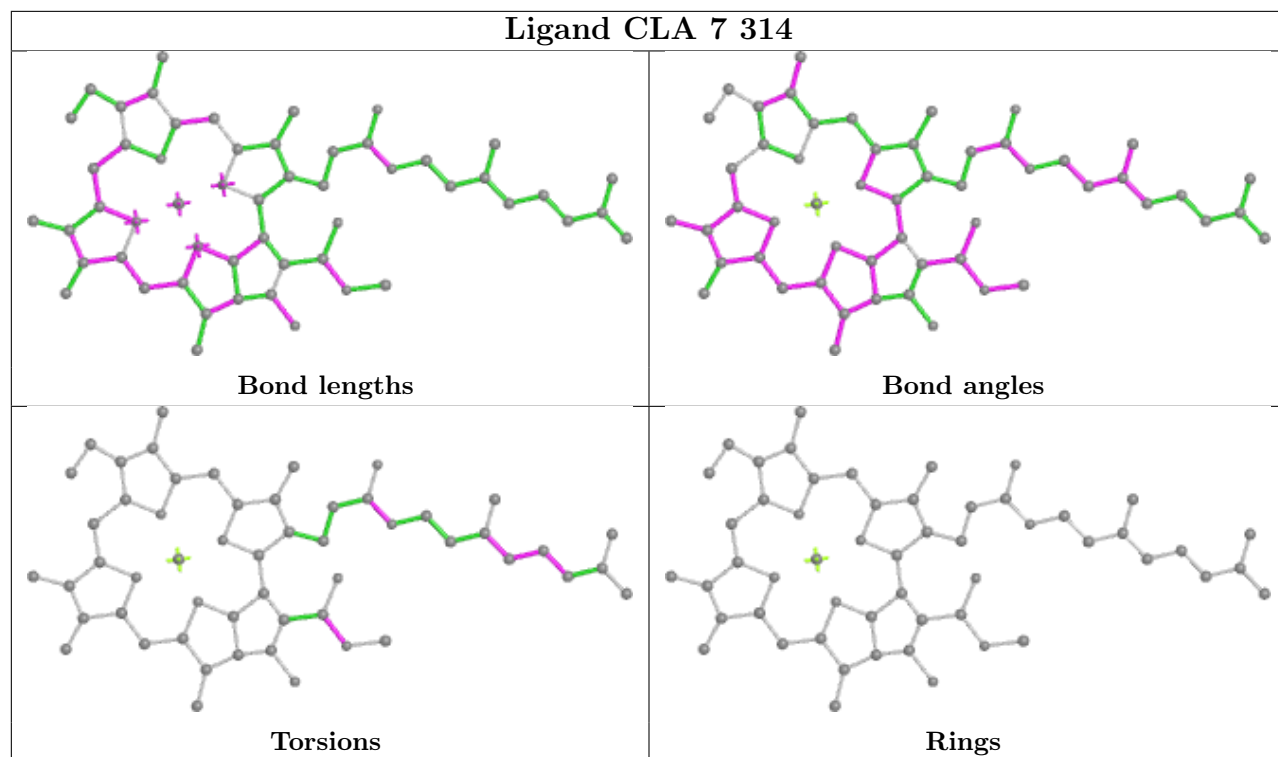


Torsions

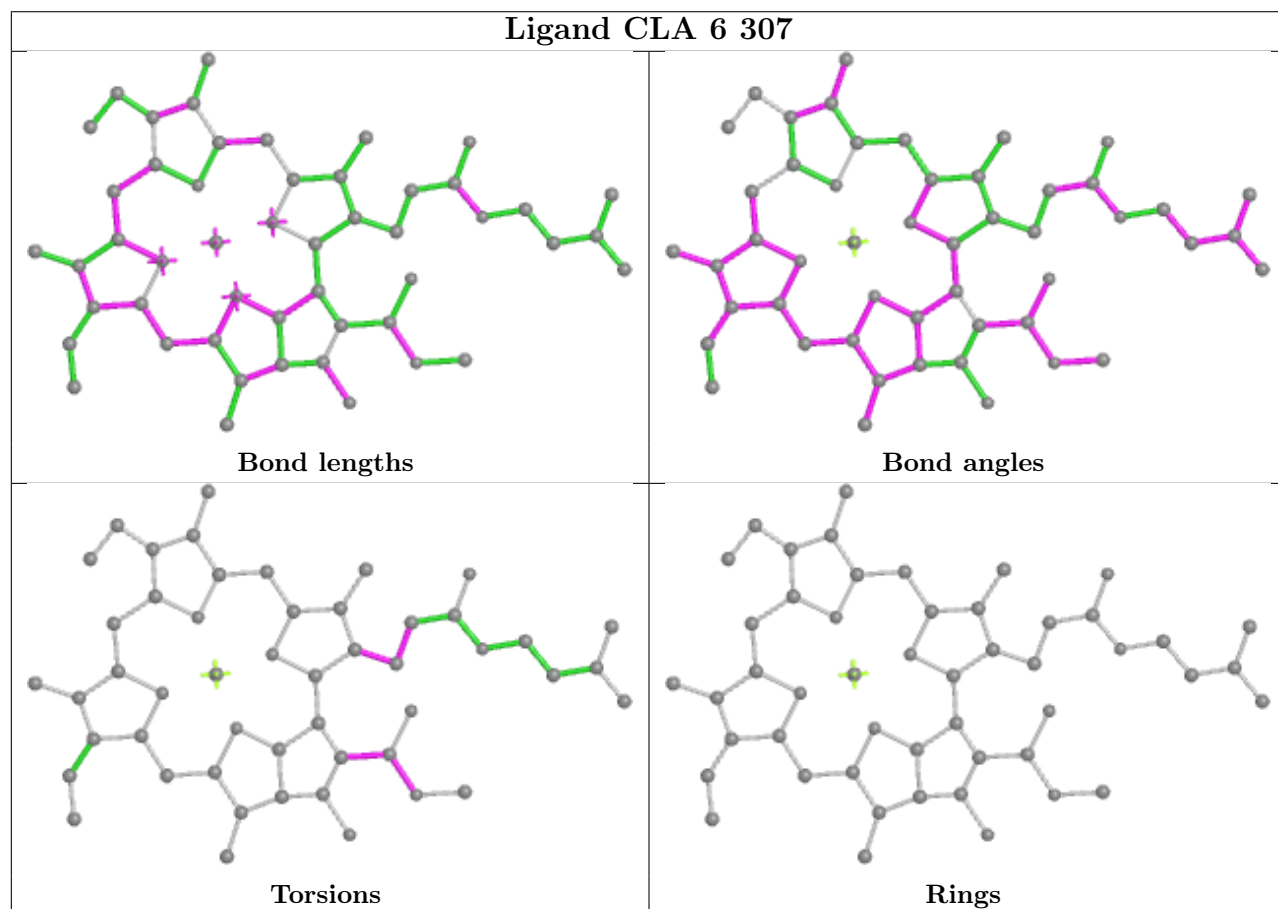


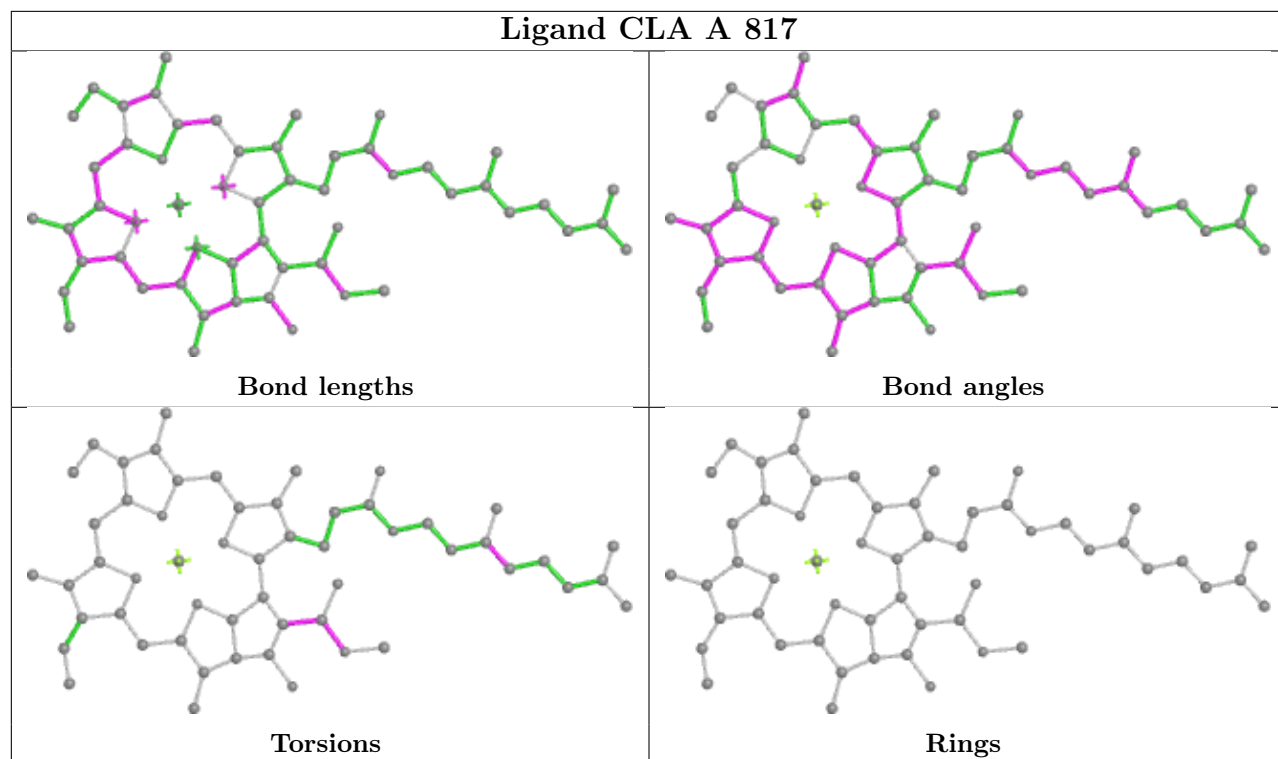
Rings

Ligand CLA 7 314

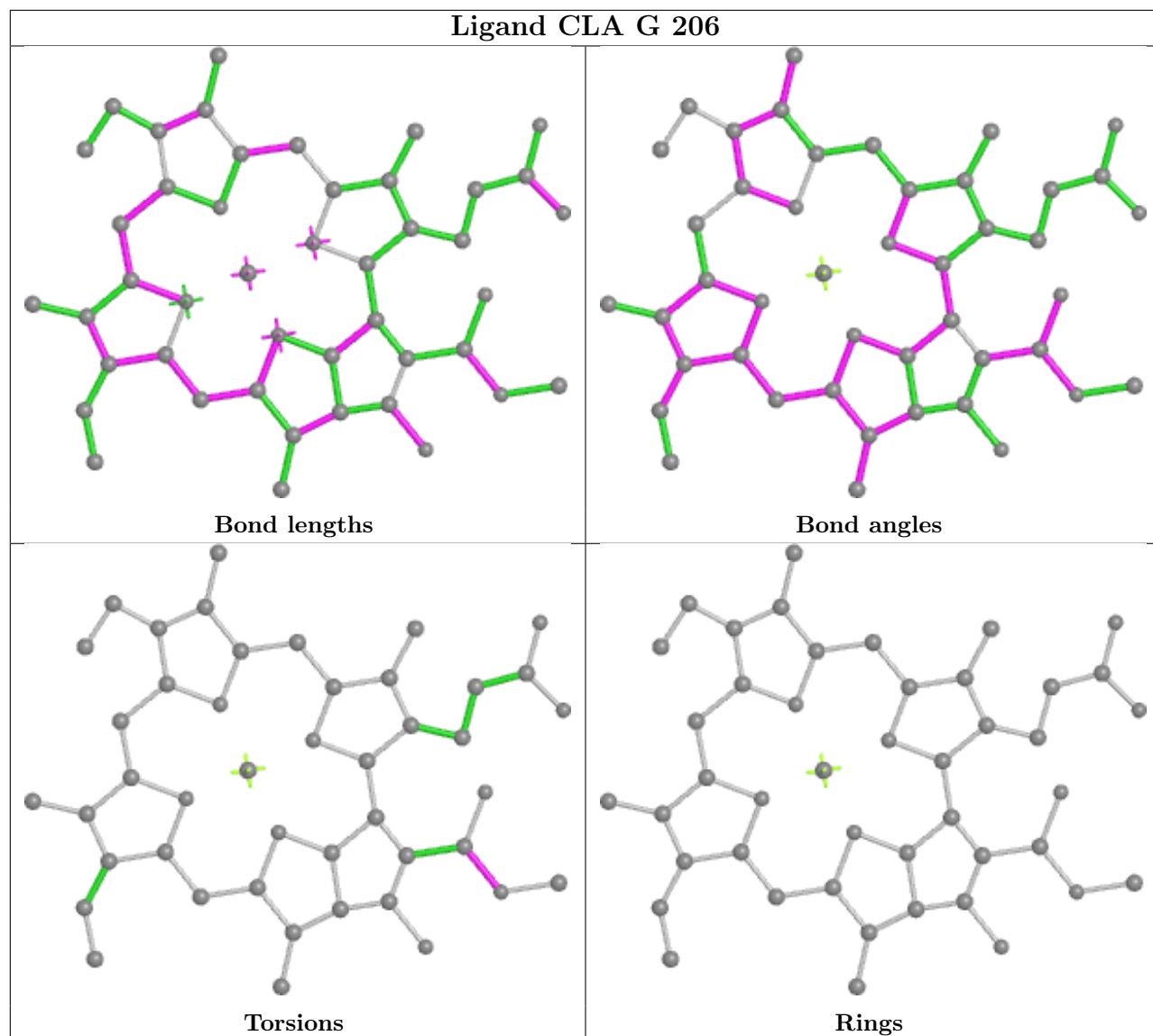


Ligand CLA 6 307

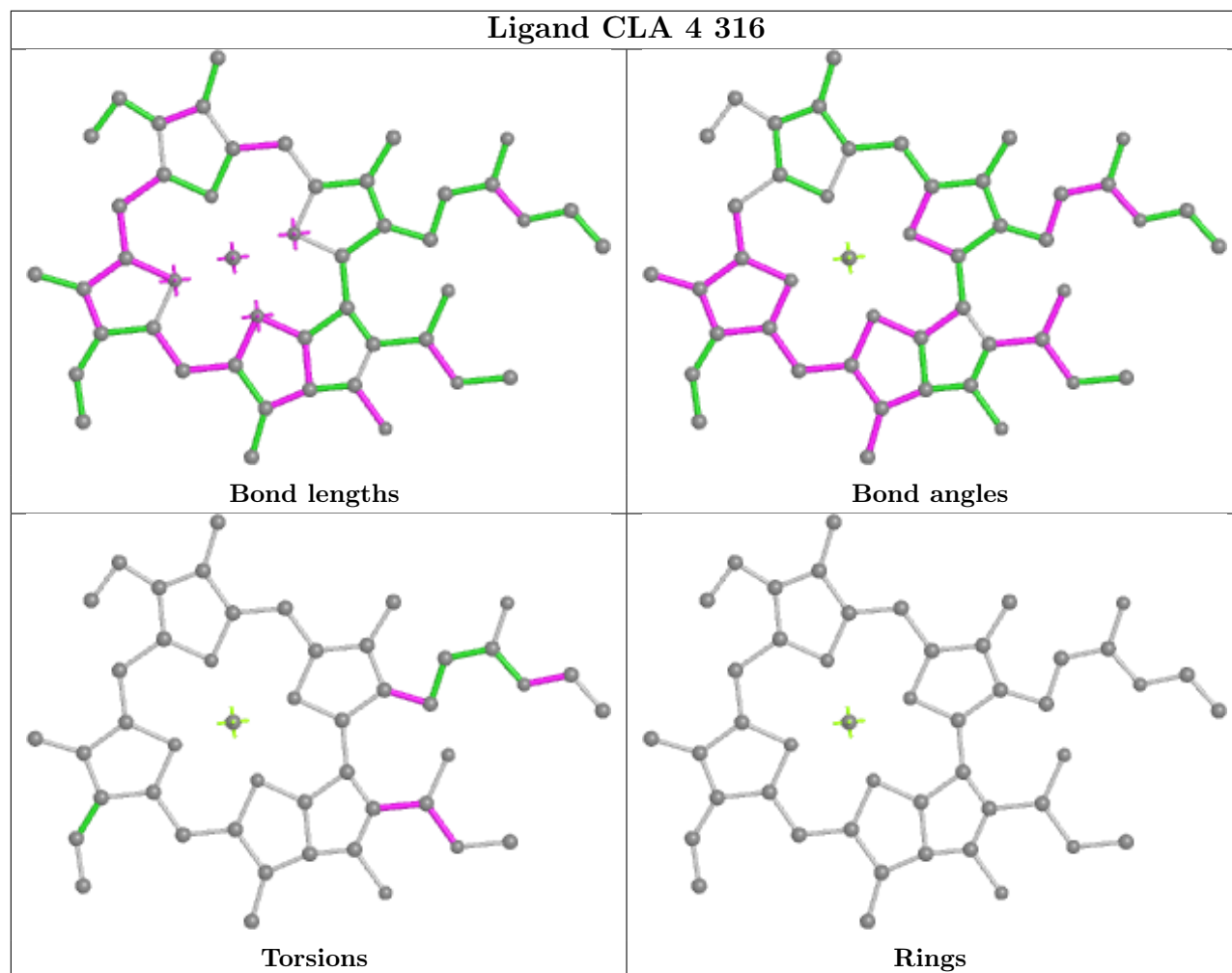




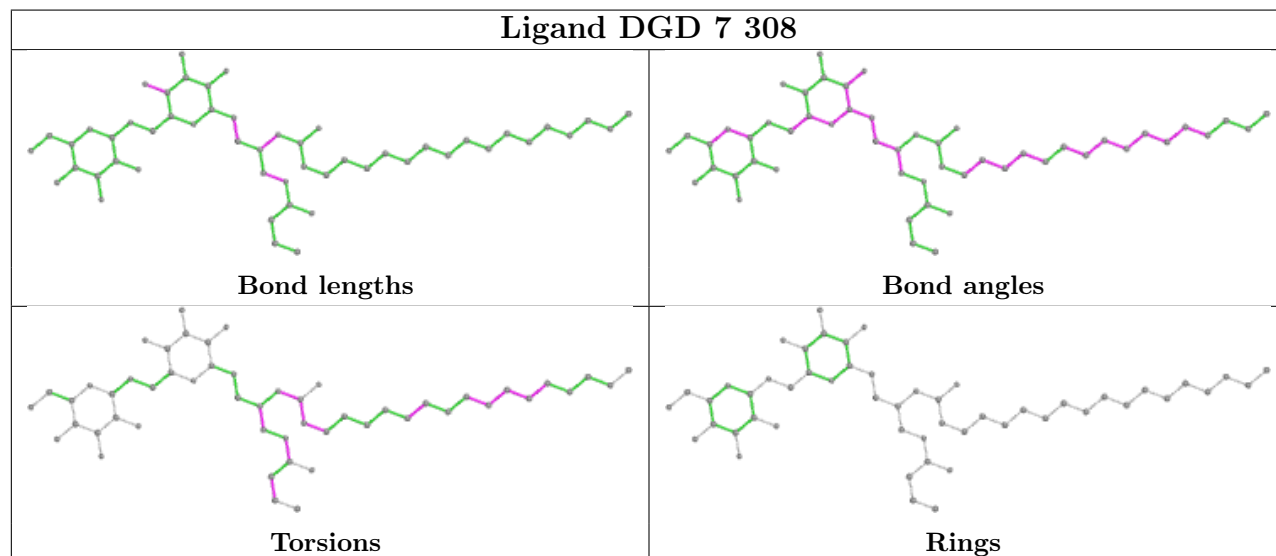
Ligand CLA G 206



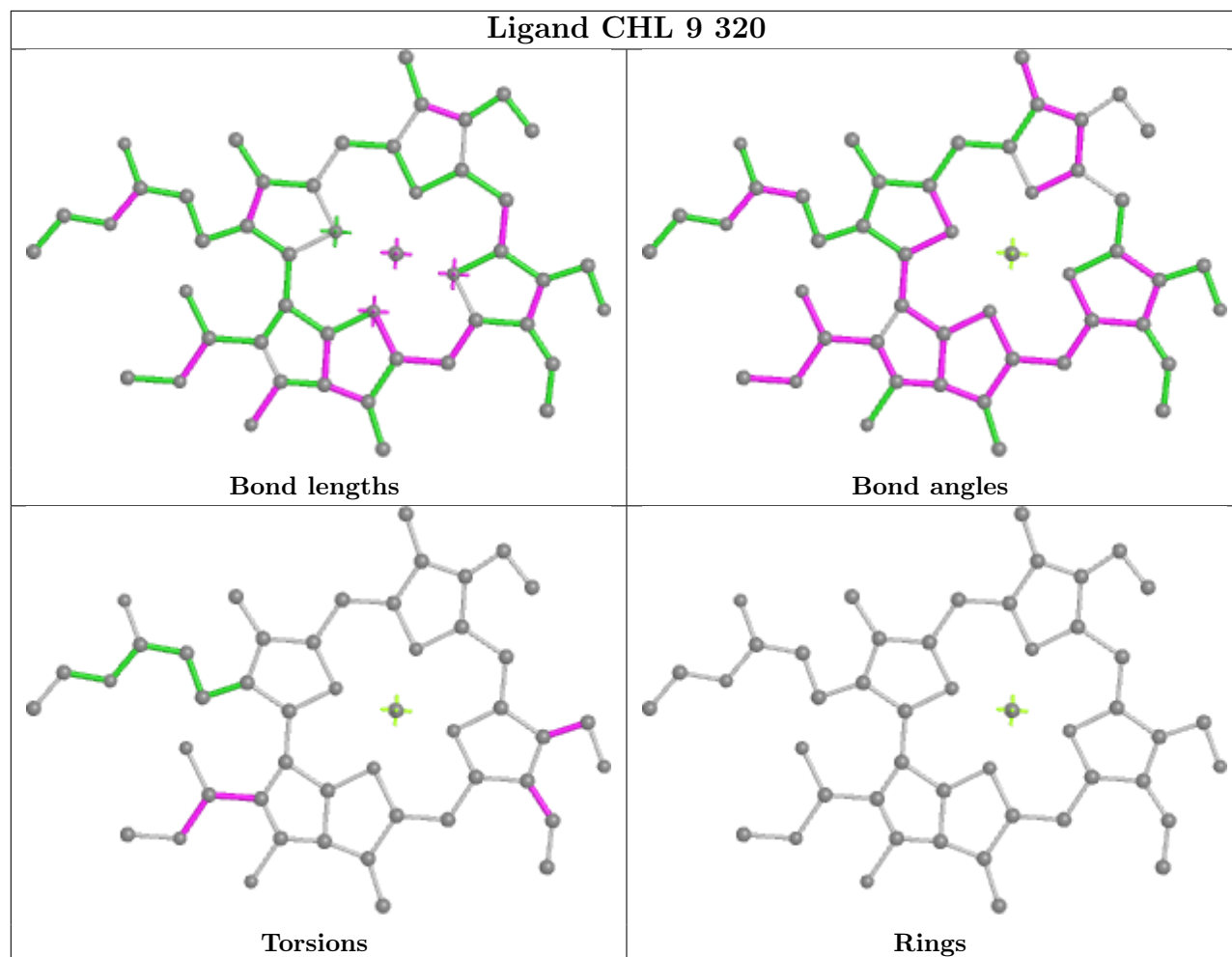
Ligand CLA 4 316



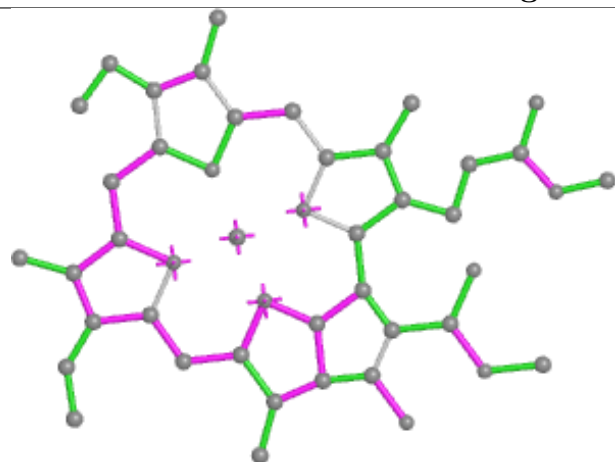
Ligand DGD 7 308



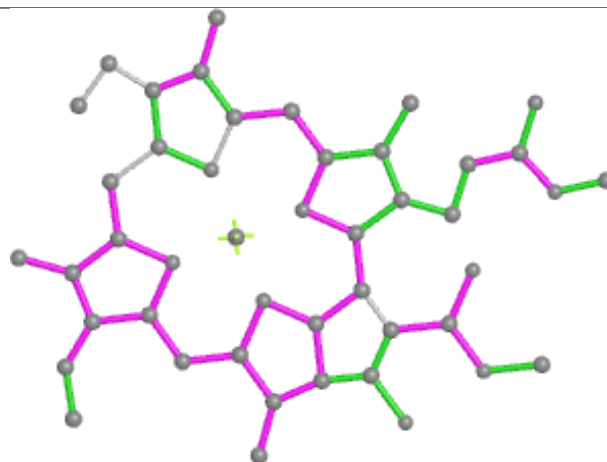
Ligand CHL 9 320



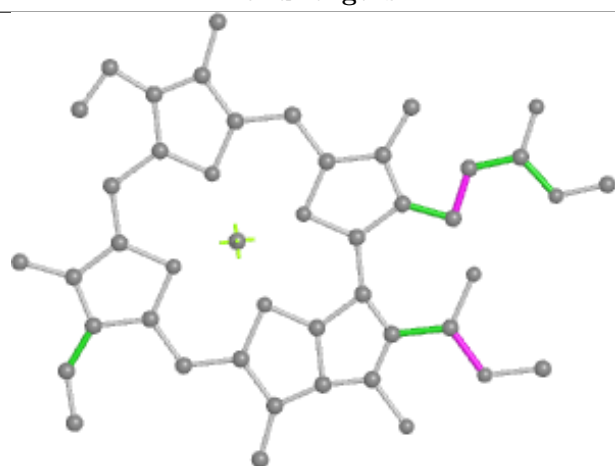
Ligand CLA 5 320



Bond lengths



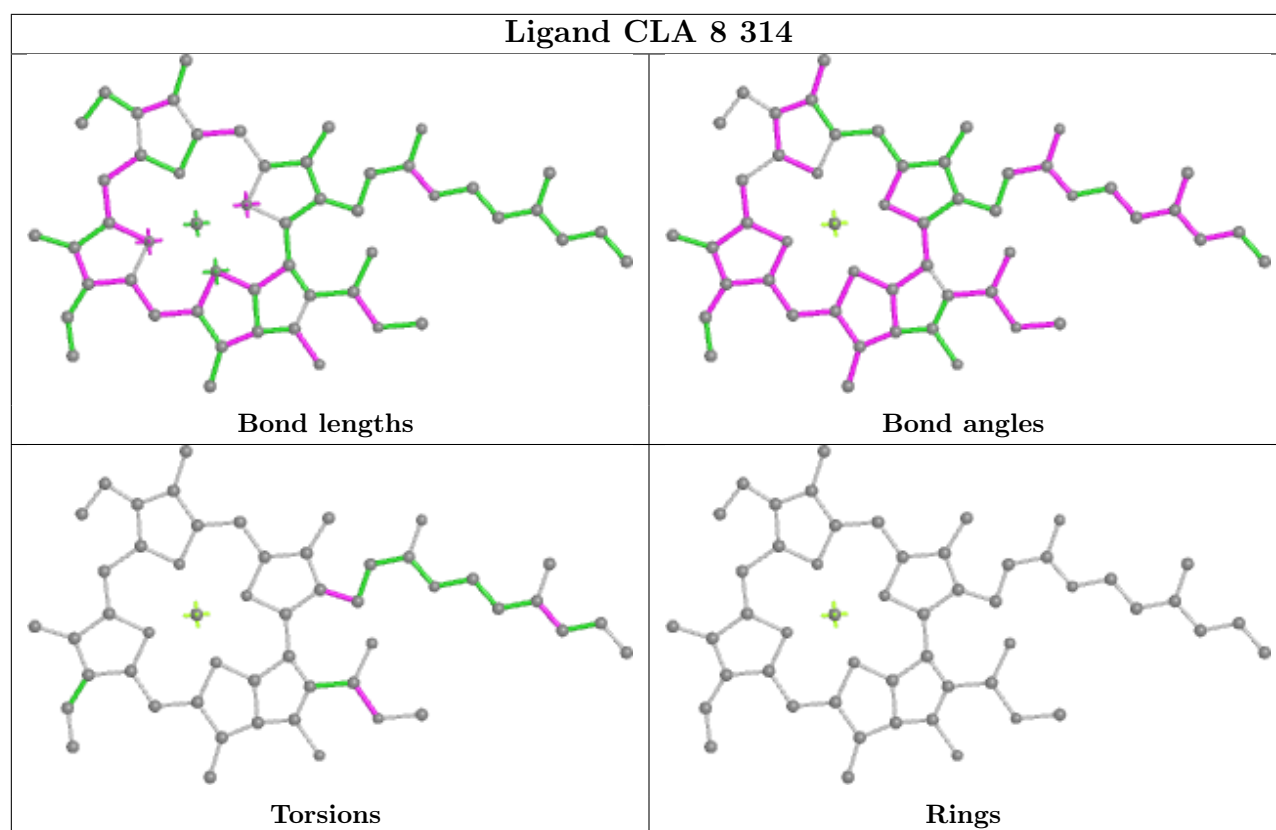
Bond angles



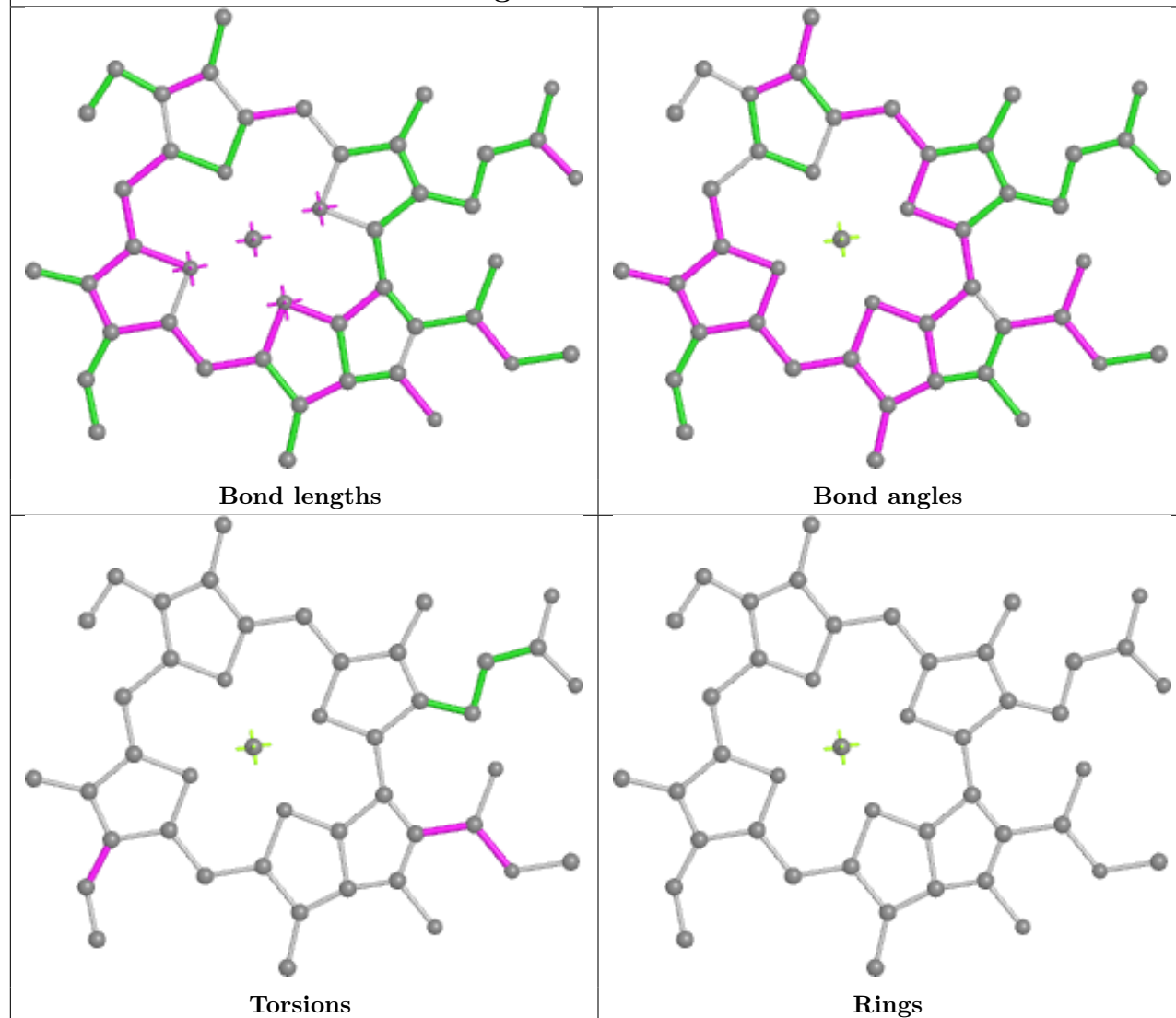
Torsions



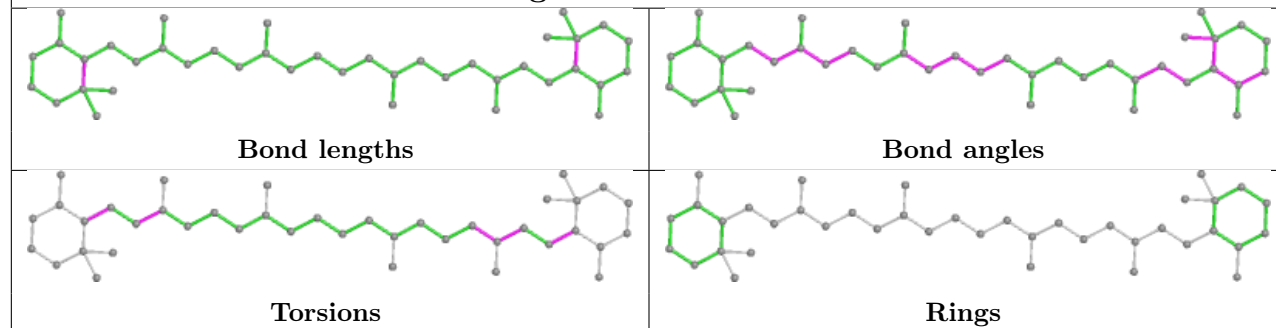
Rings

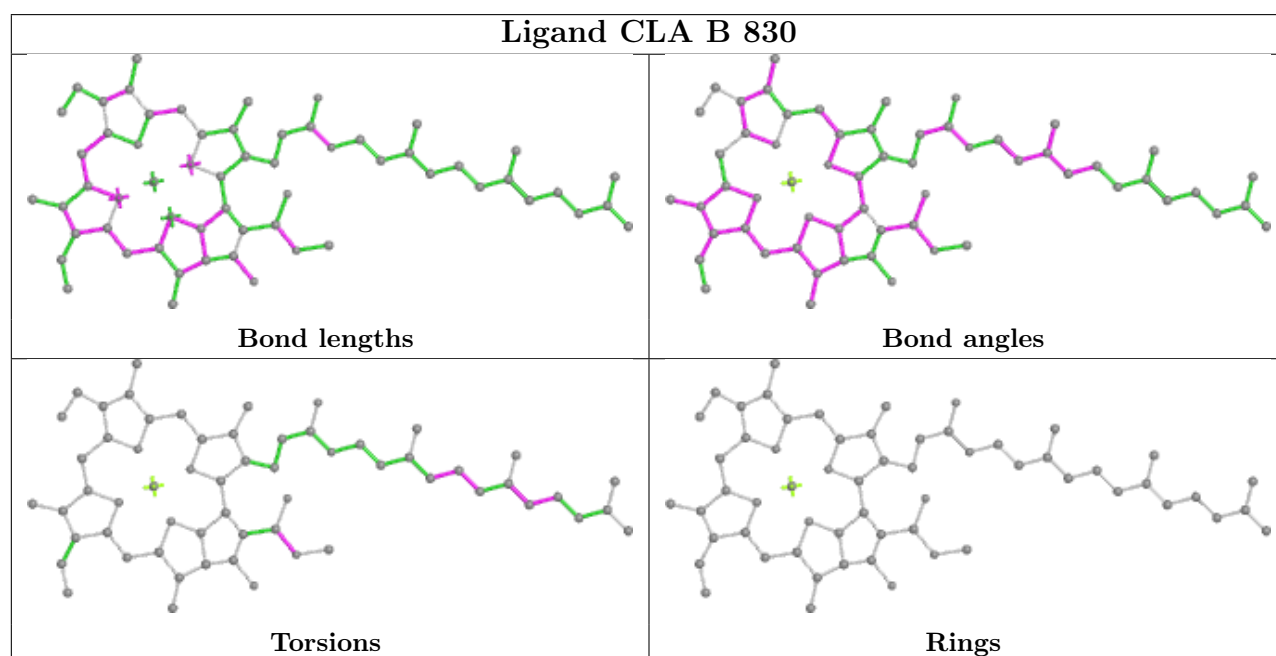
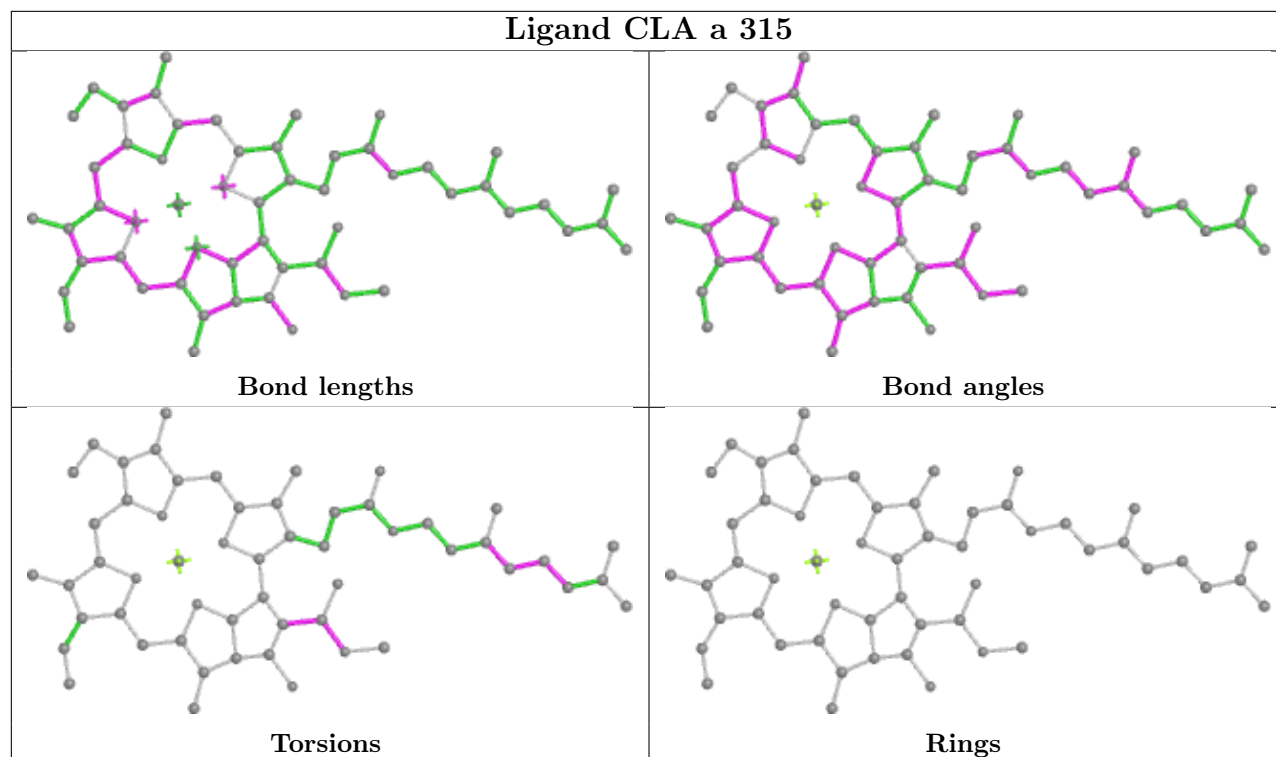
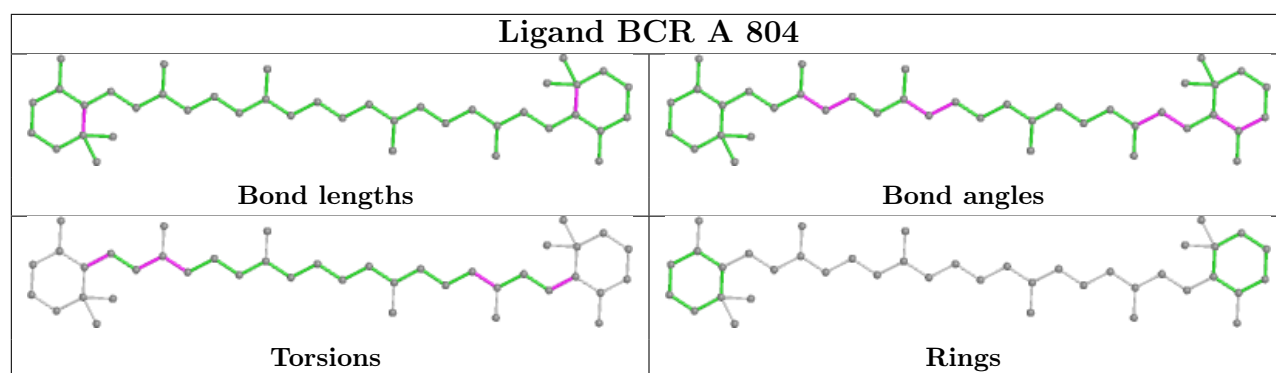


Ligand CLA 4 320

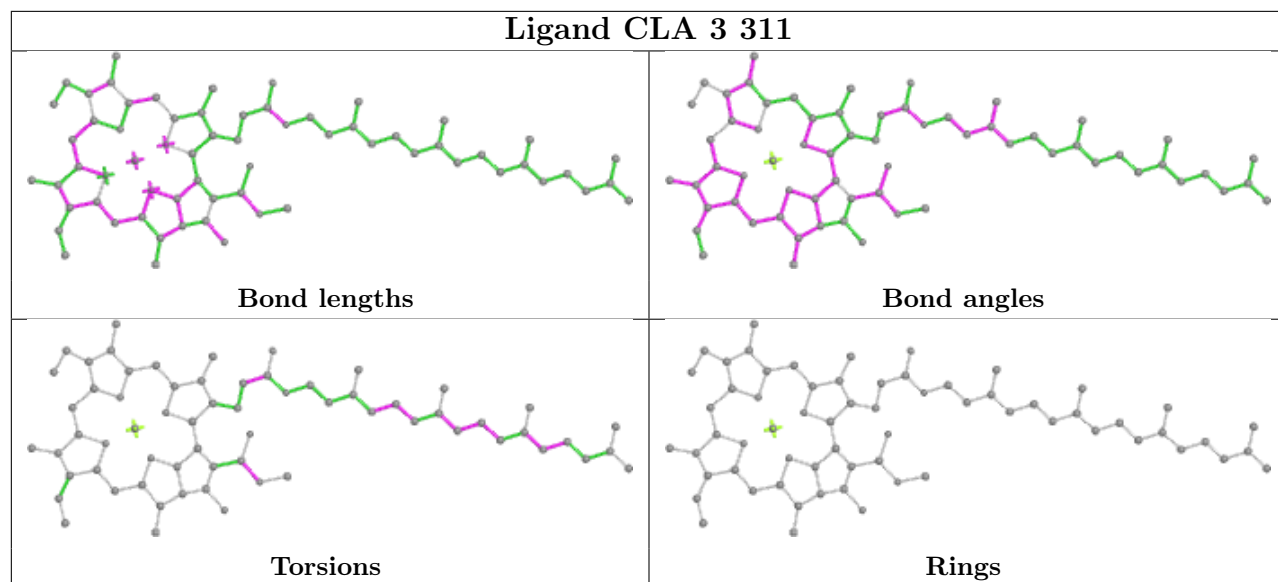


Ligand BCR K 202

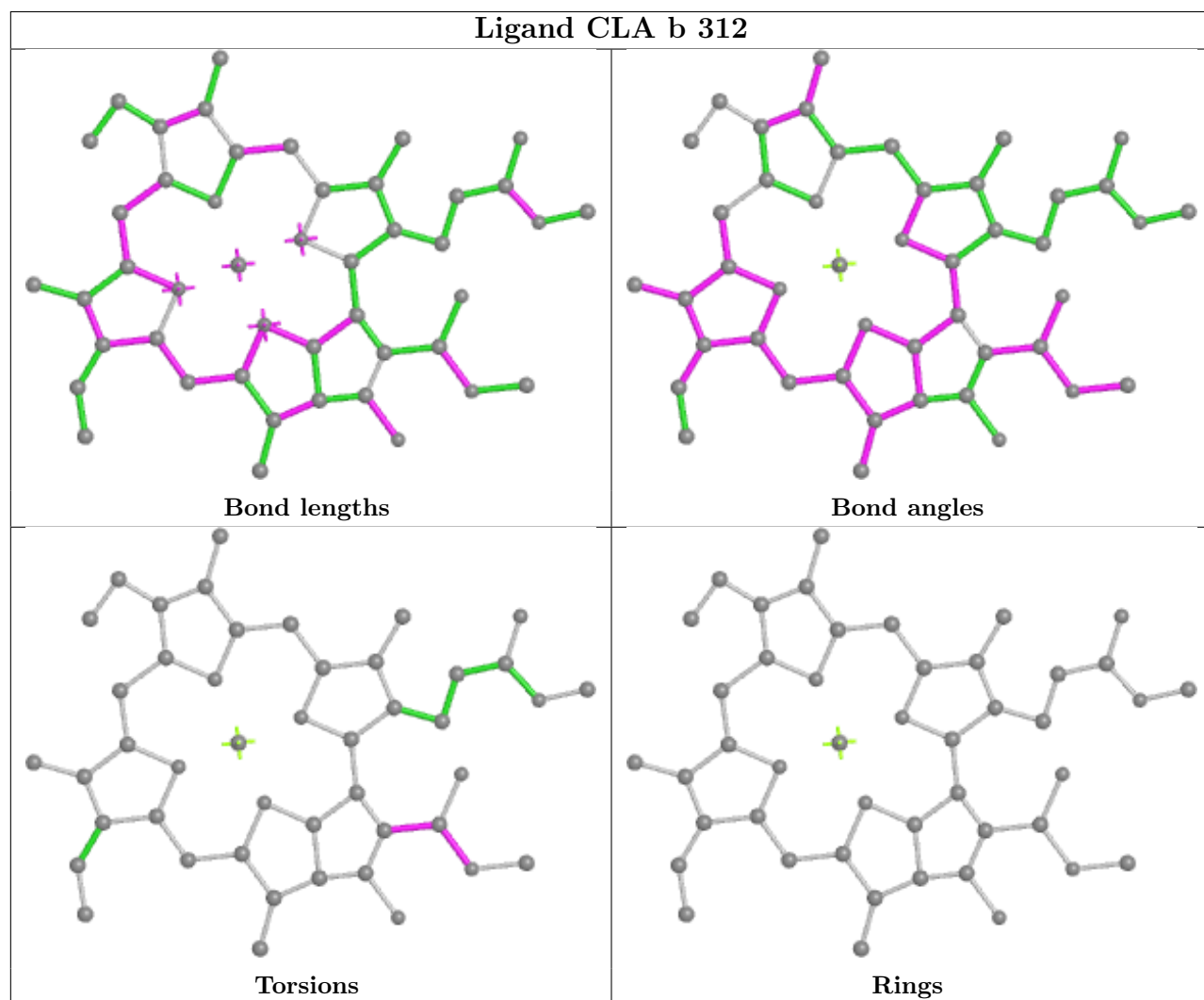




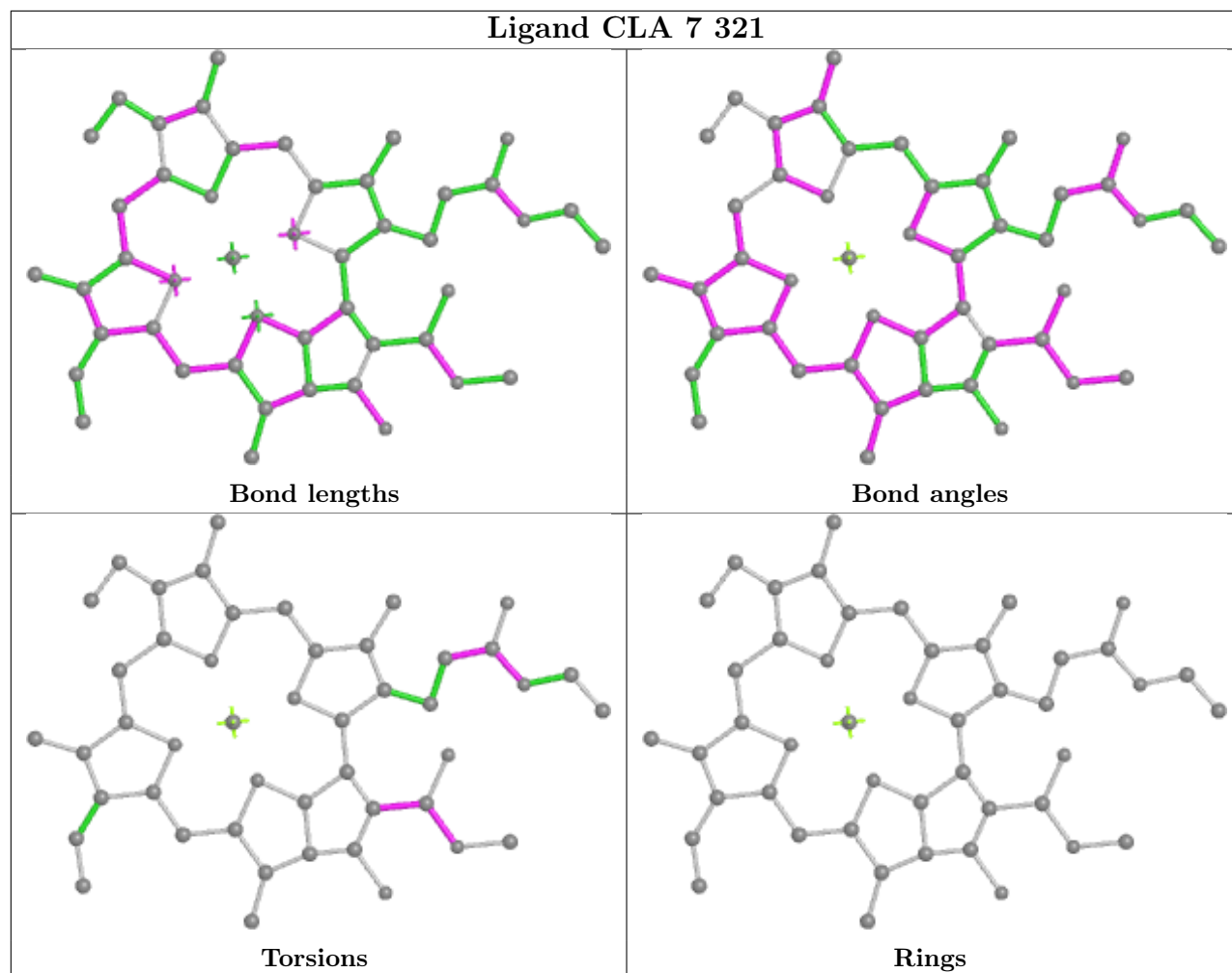
Ligand CLA 3 311



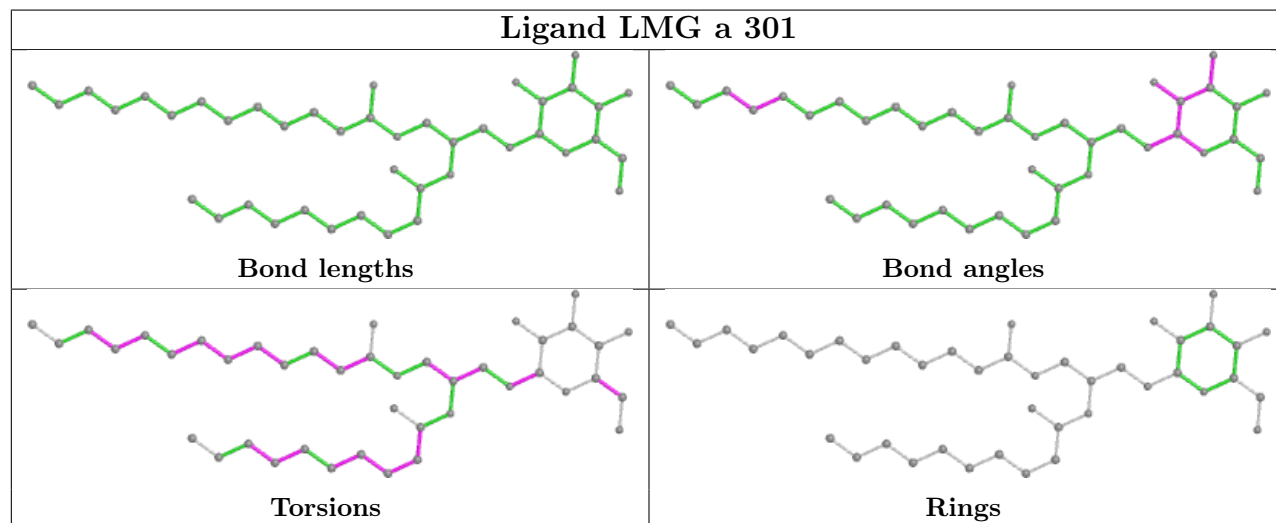
Ligand CLA b 312



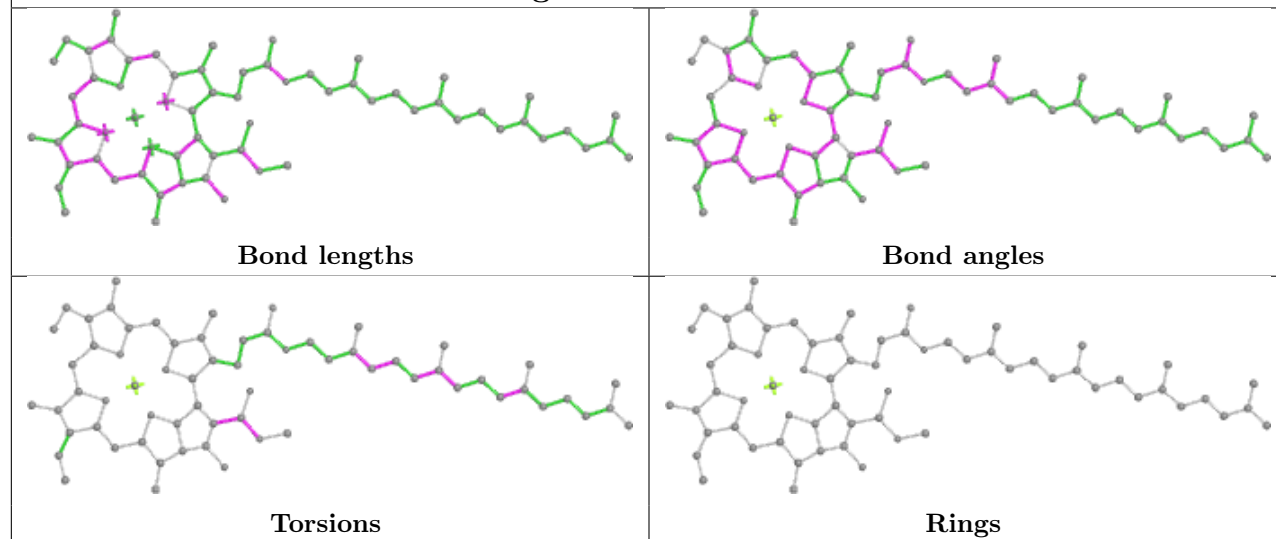
Ligand CLA 7 321



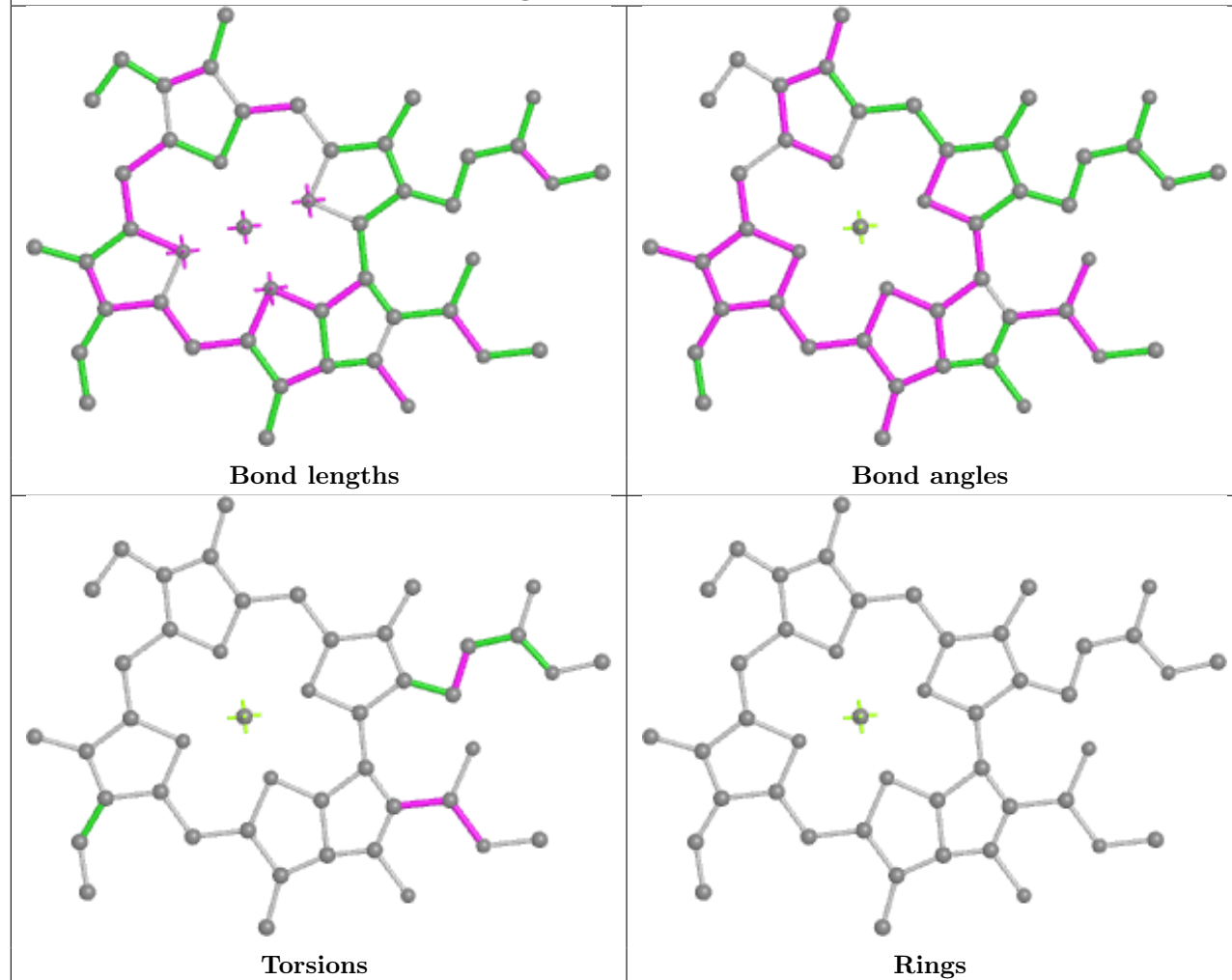
Ligand LMG a 301

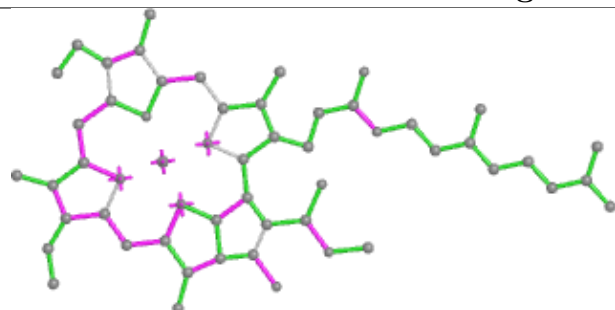


Ligand CLA B 817

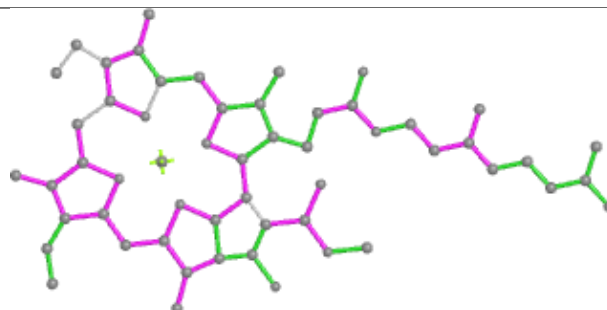


Ligand CLA b 303

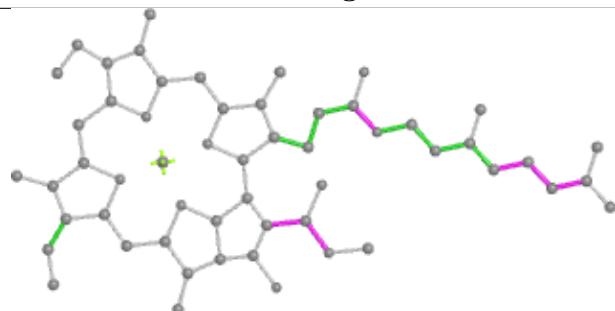


Ligand CLA B 823

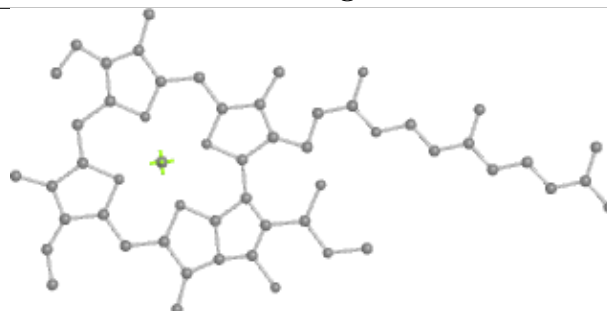
Bond lengths



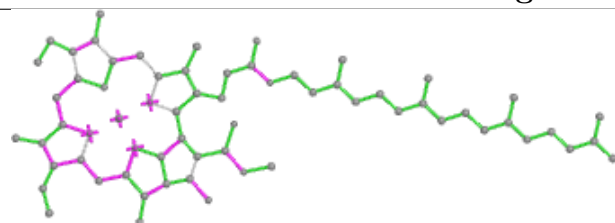
Bond angles



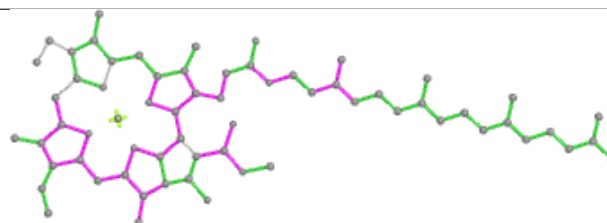
Torsions



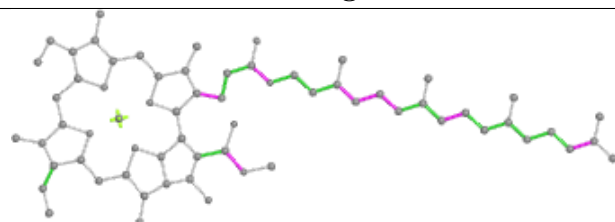
Rings

Ligand CLA A 855

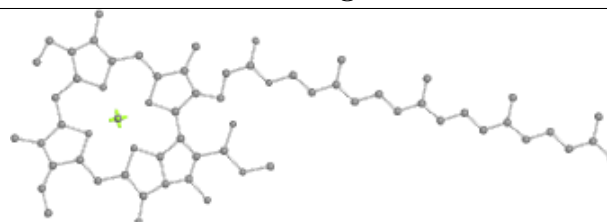
Bond lengths



Bond angles

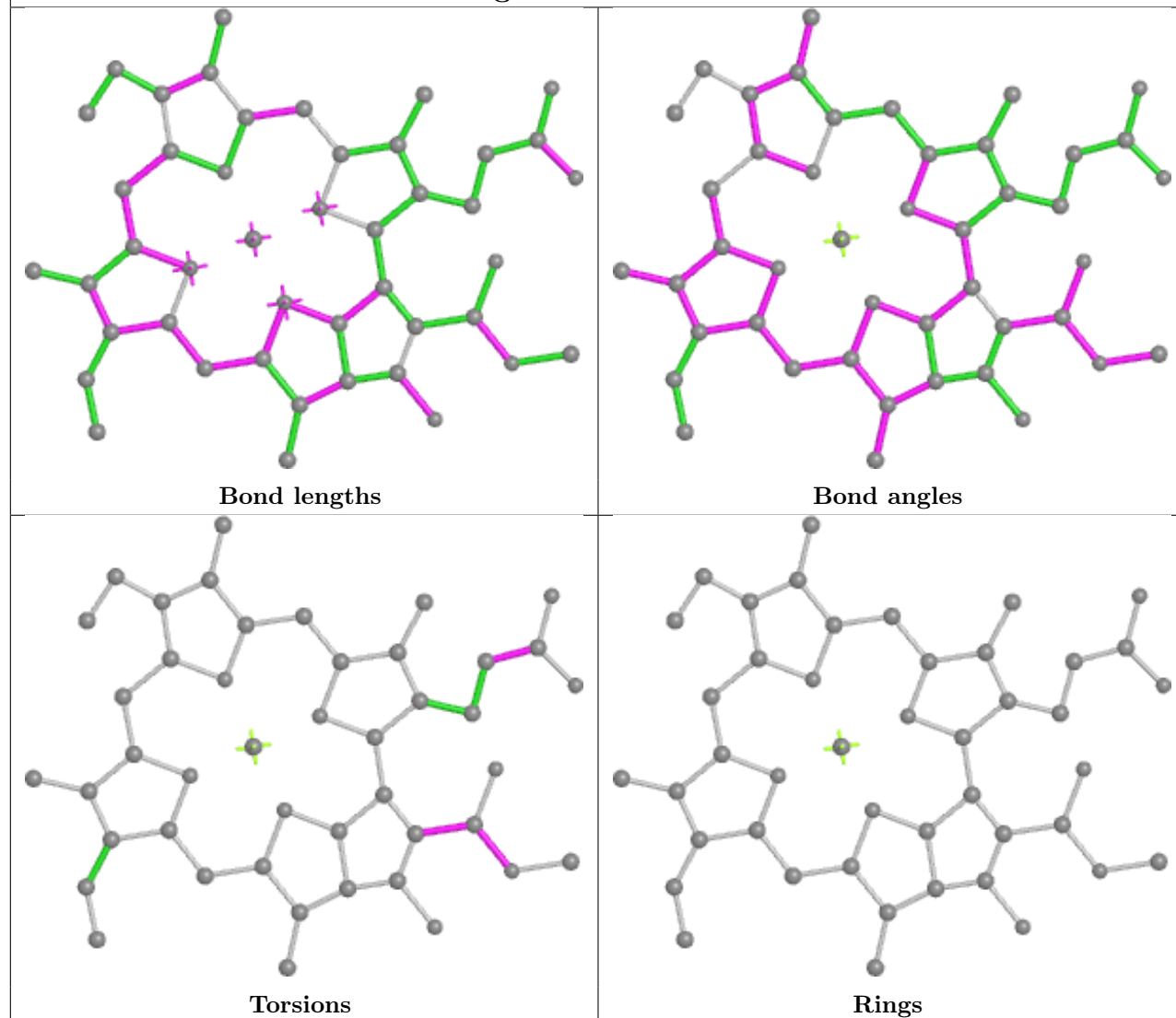


Torsions

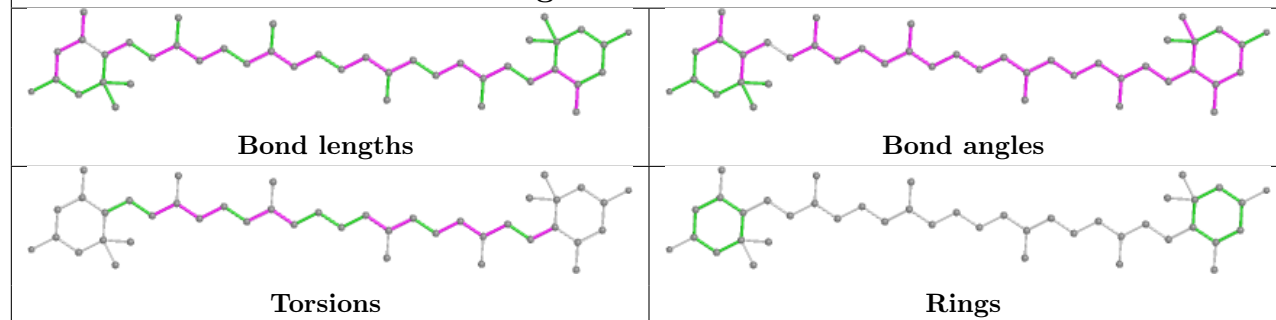


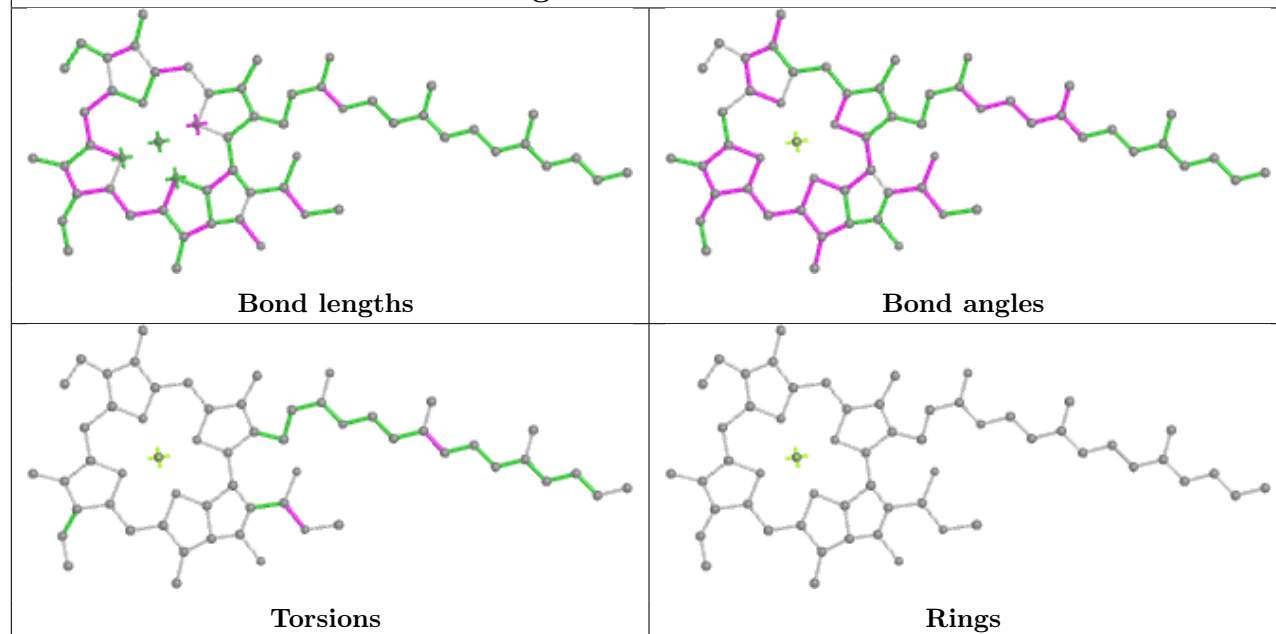
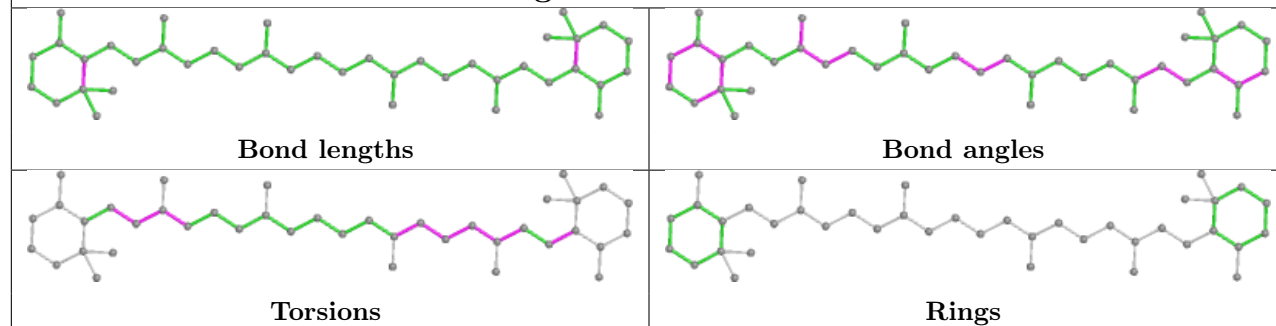
Rings

Ligand CLA 2 305

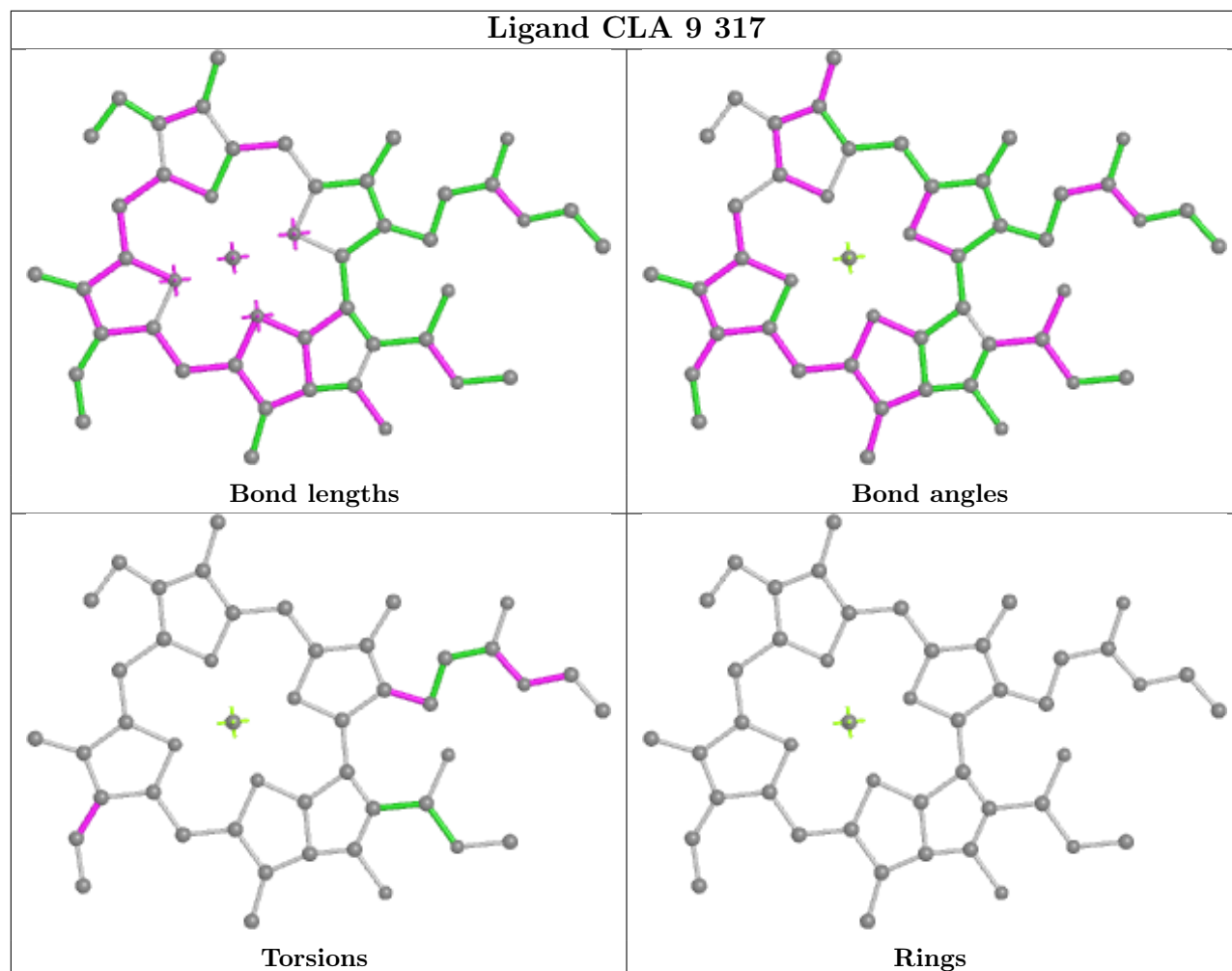


Ligand LUT 9 303

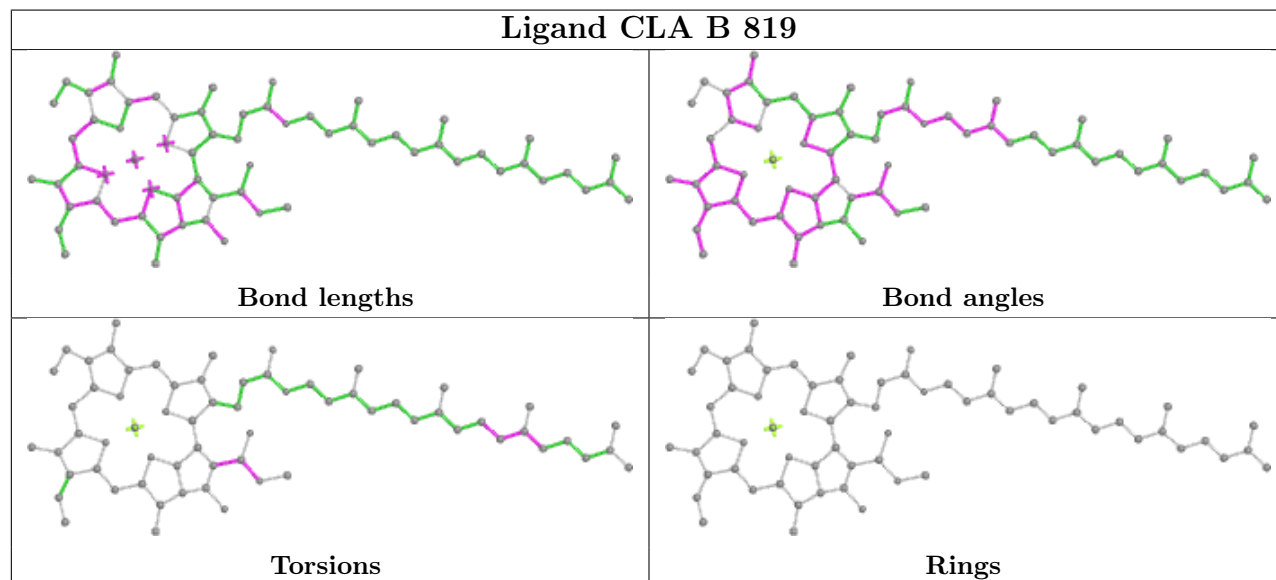


Ligand CLA B 821**Ligand BCR 5 302**

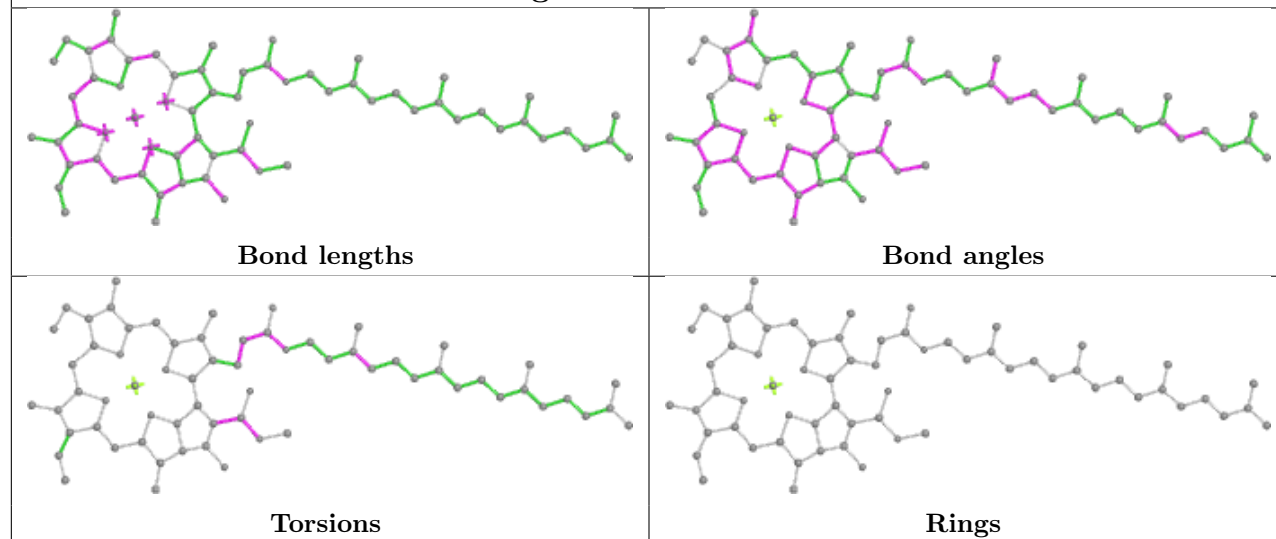
Ligand CLA 9 317



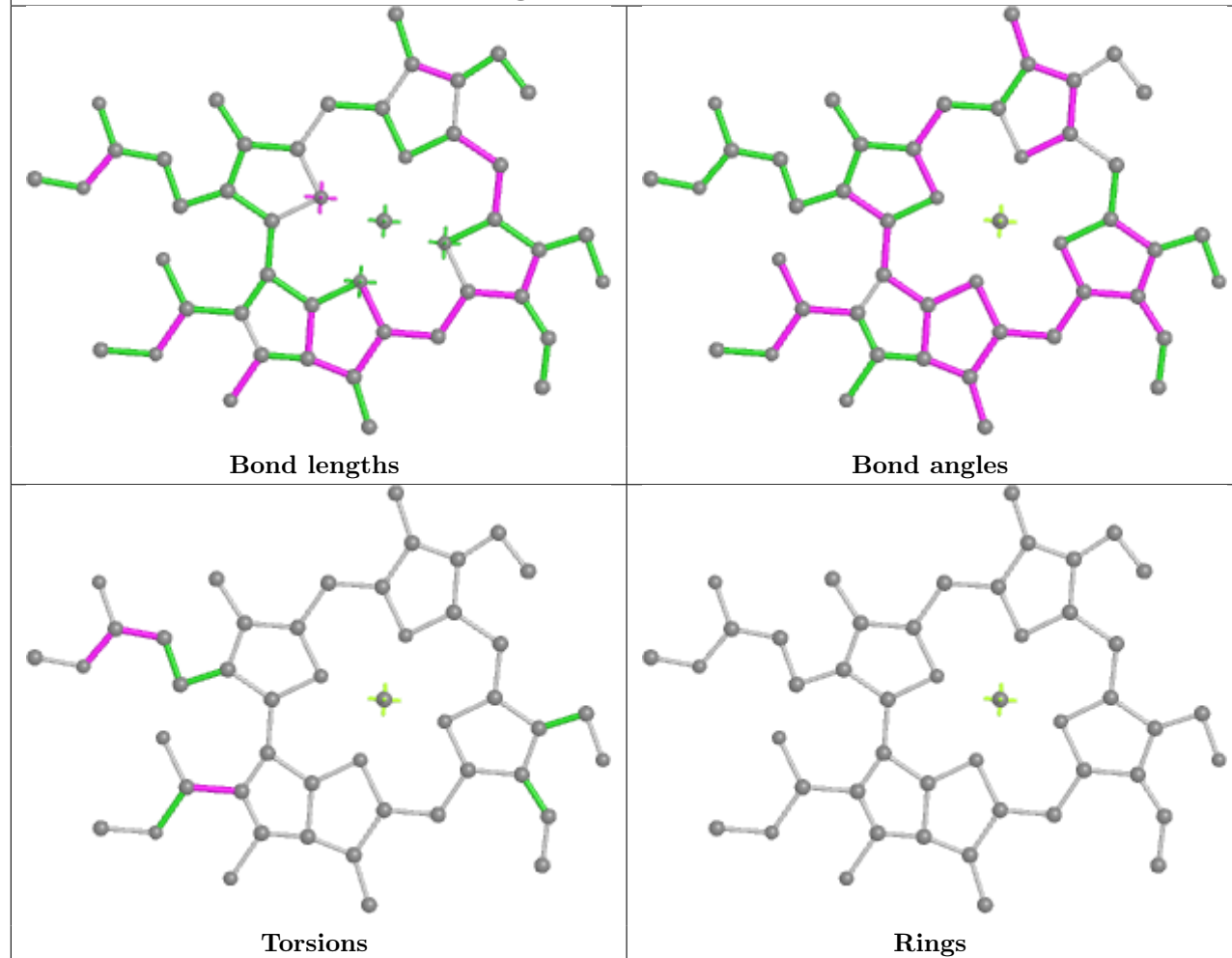
Ligand CLA B 819

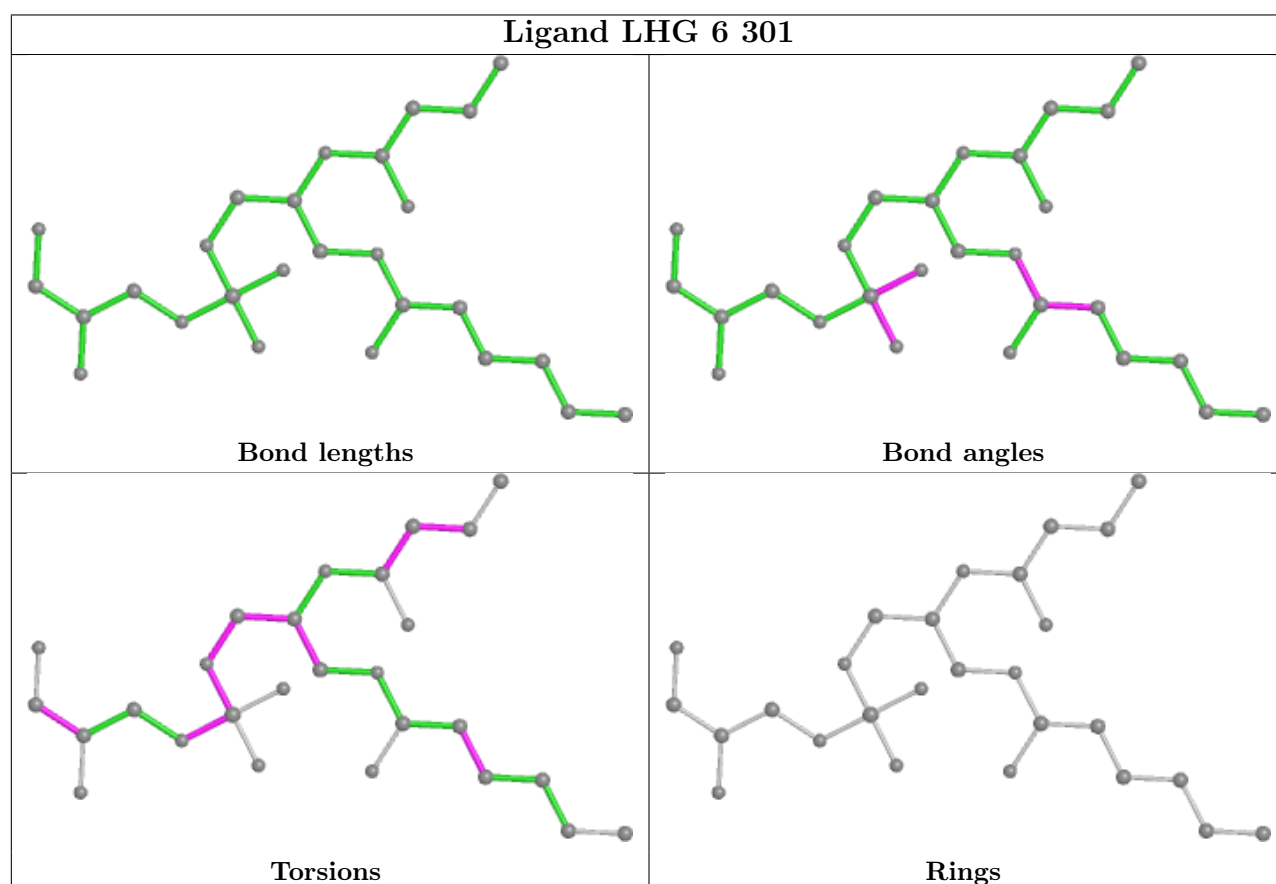
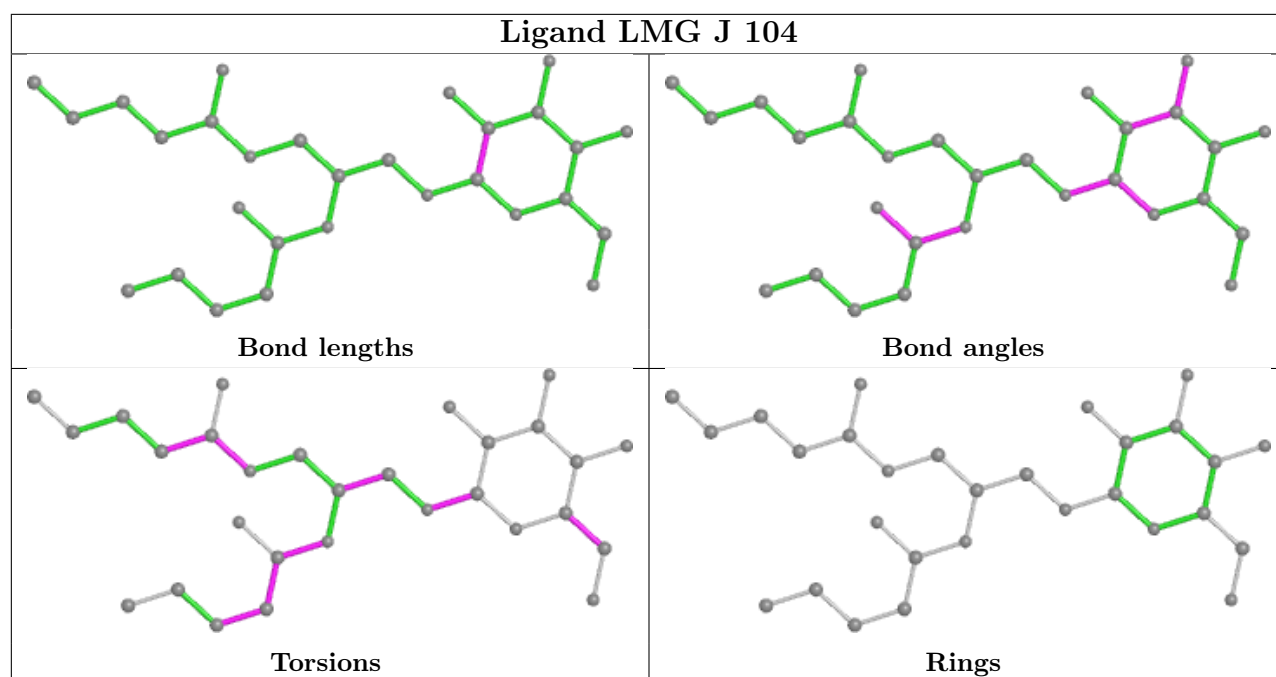


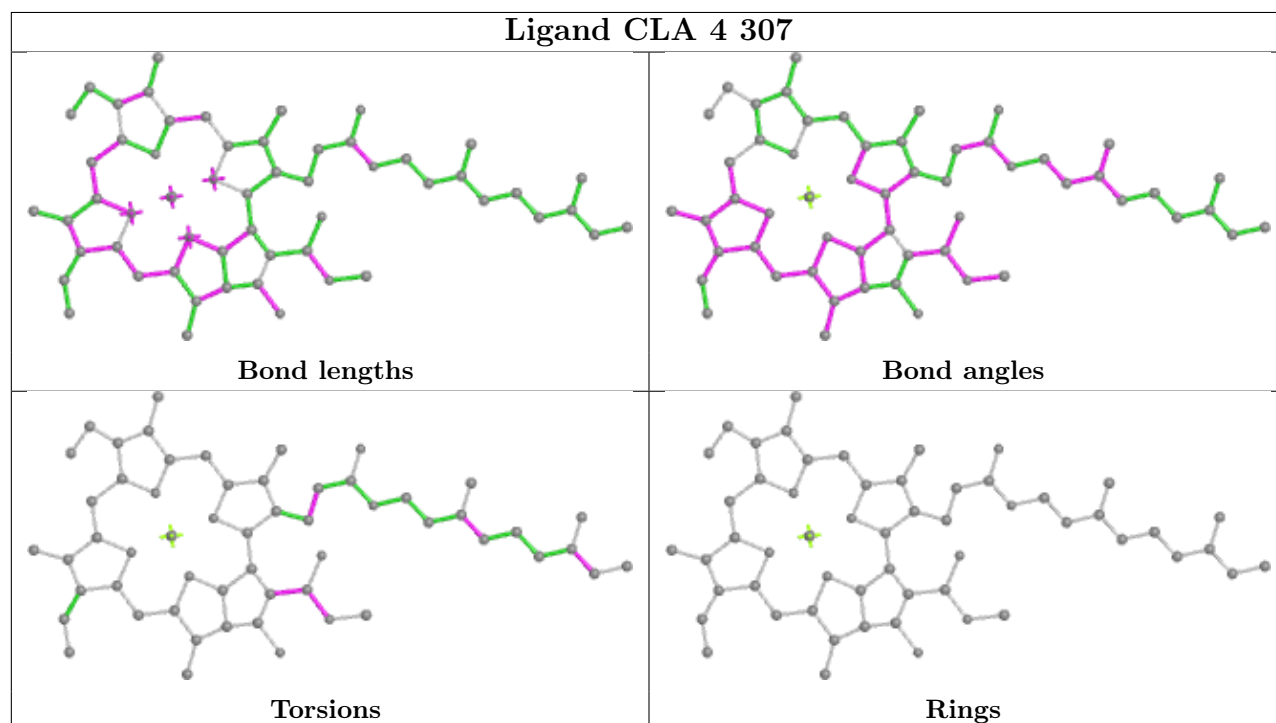
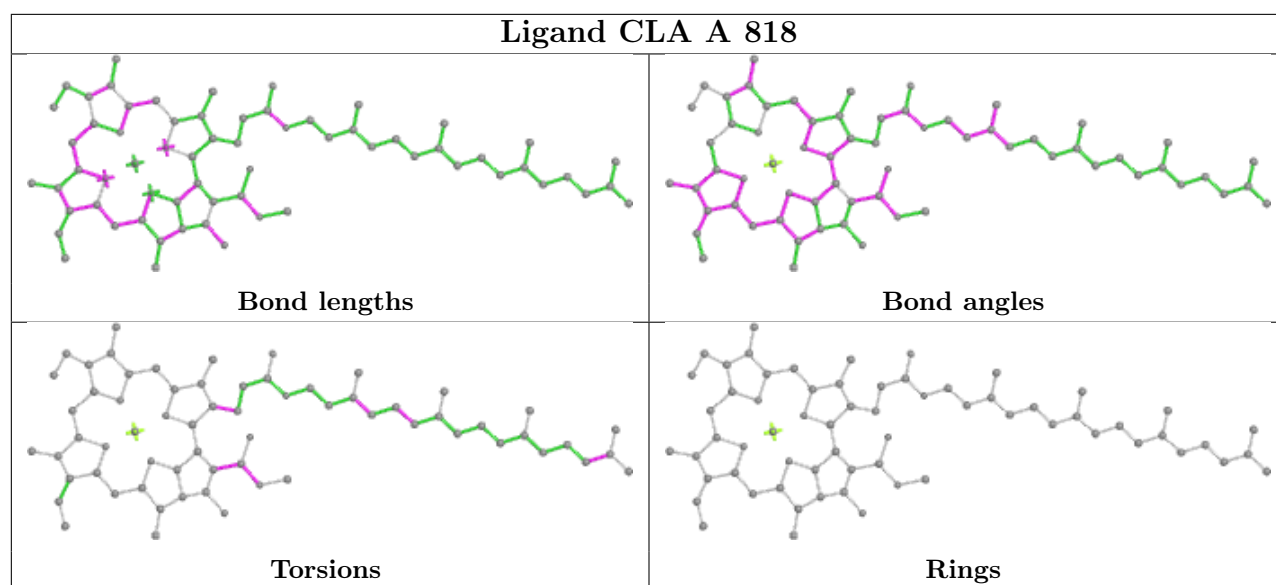
Ligand CLA A 834



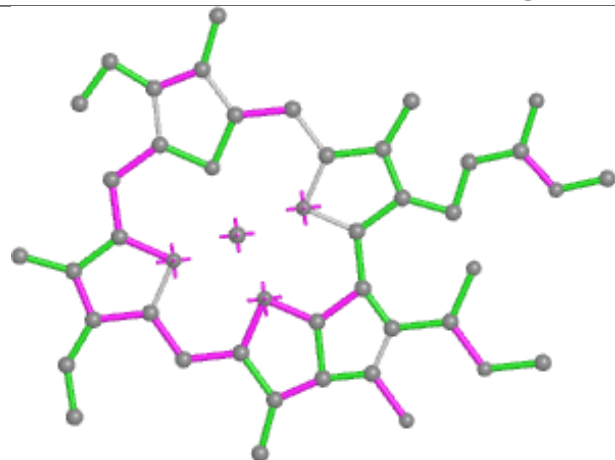
Ligand CHL K 201



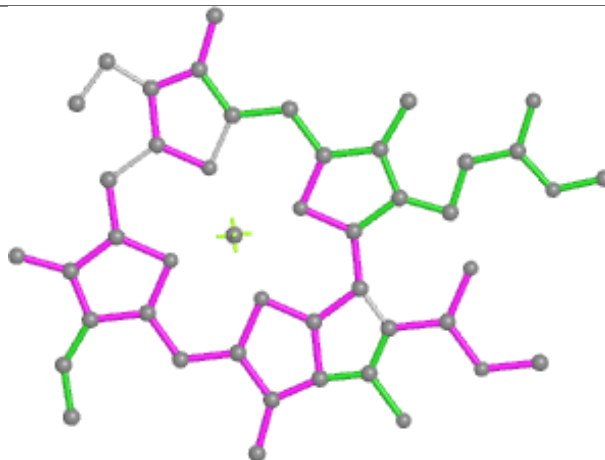




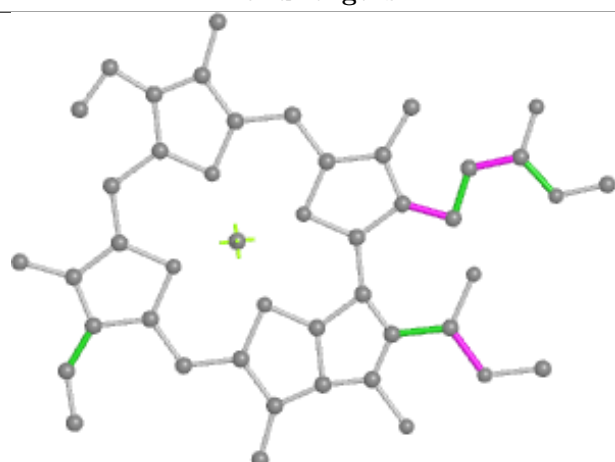
Ligand CLA b 302



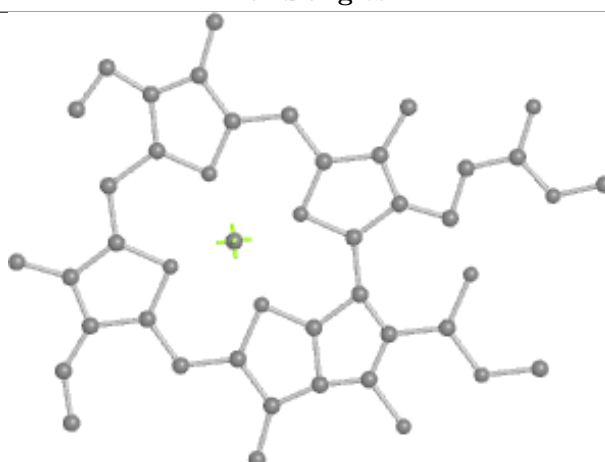
Bond lengths



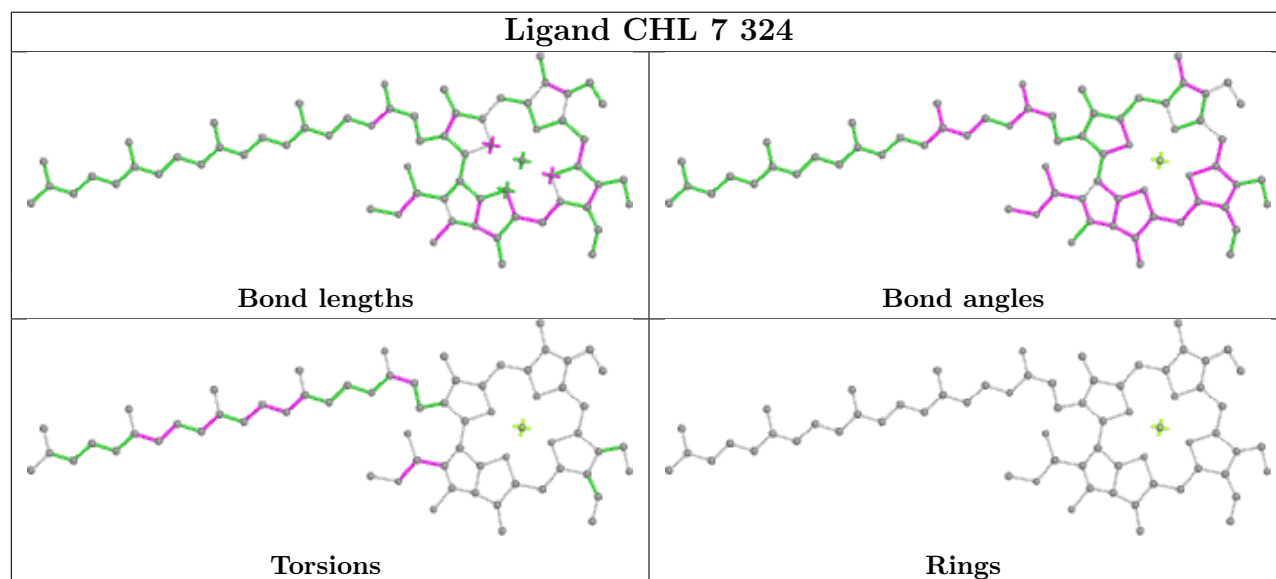
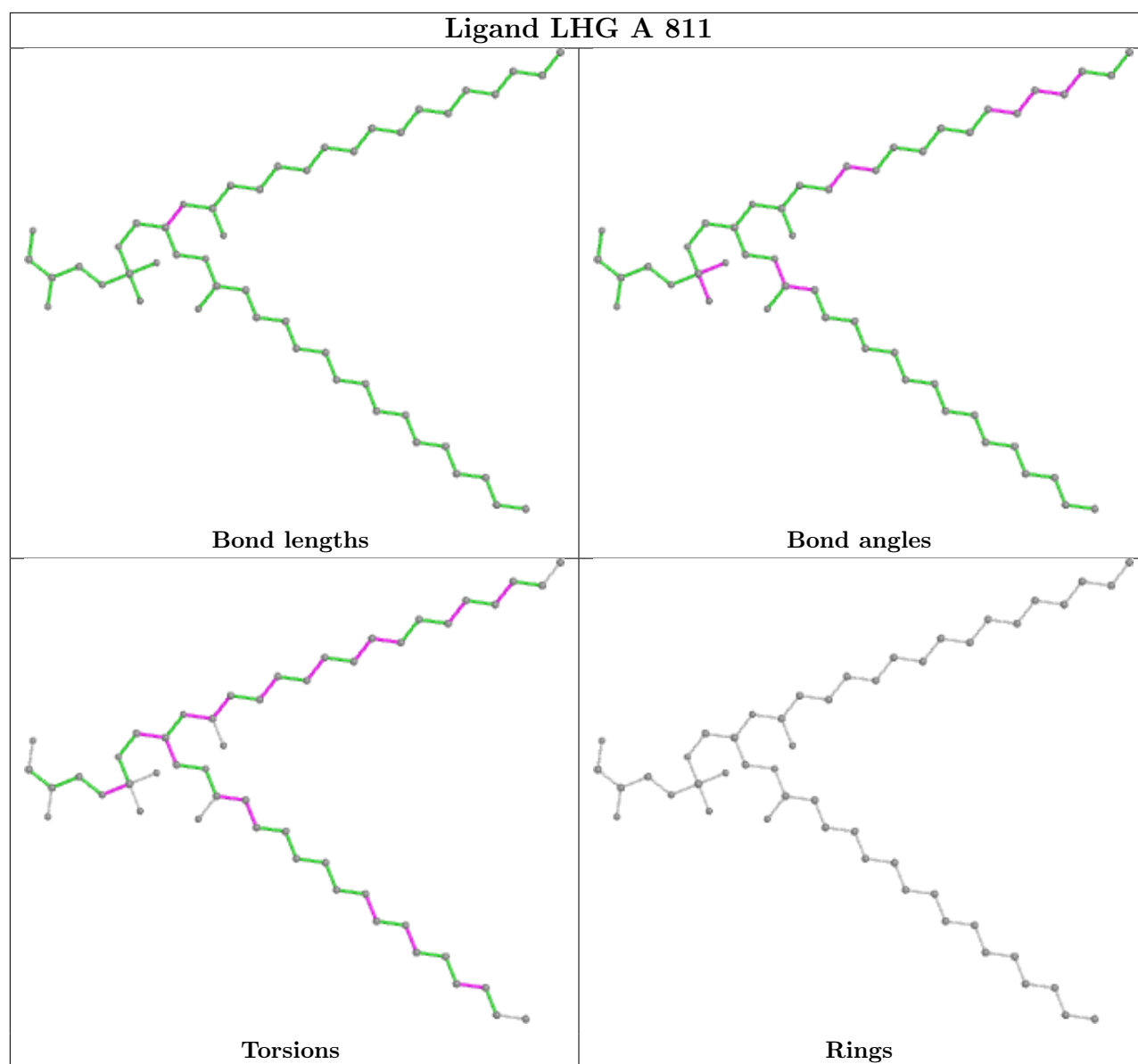
Bond angles

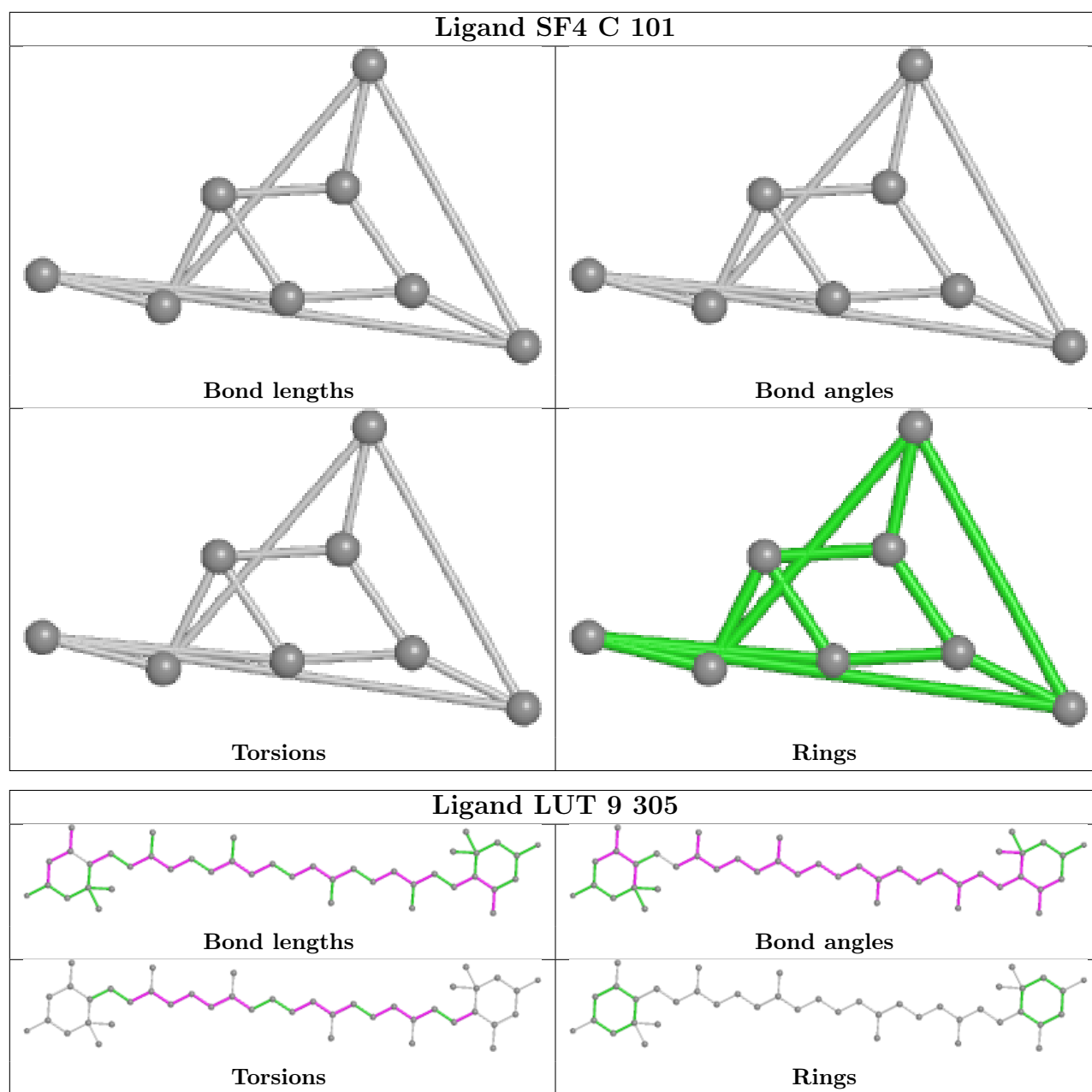


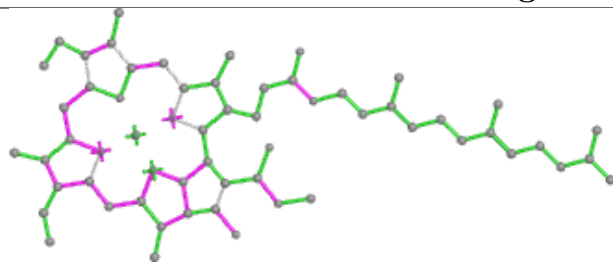
Torsions



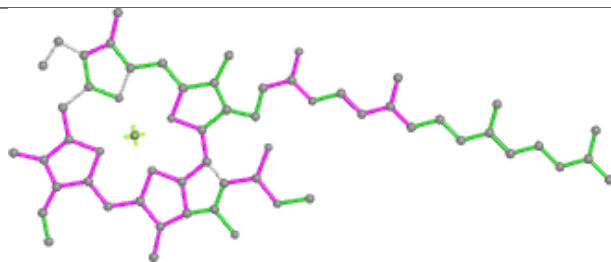
Rings



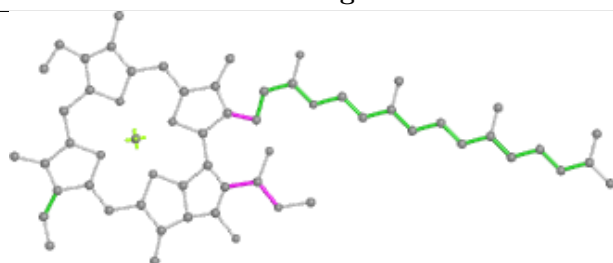


Ligand CLA 7 309

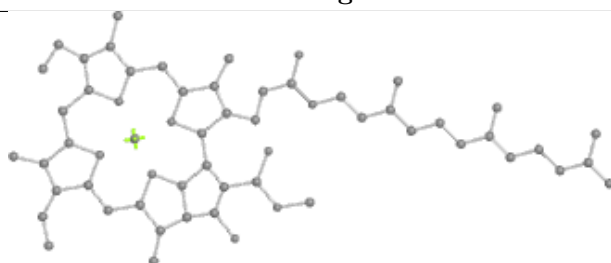
Bond lengths



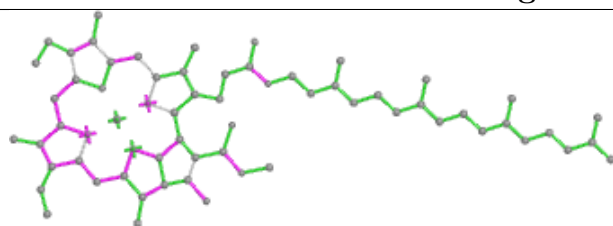
Bond angles



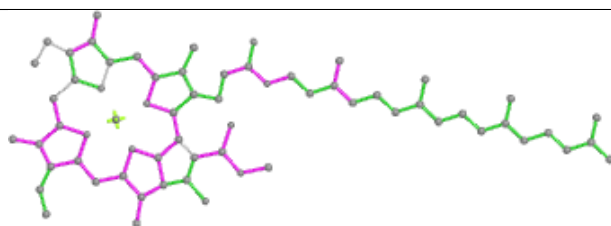
Torsions



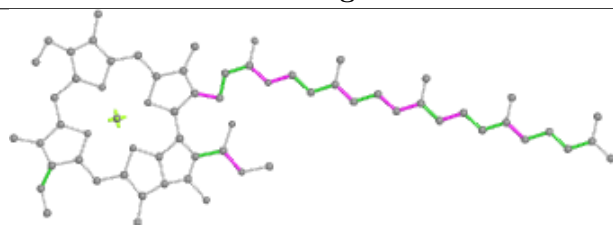
Rings

Ligand CLA 3 309

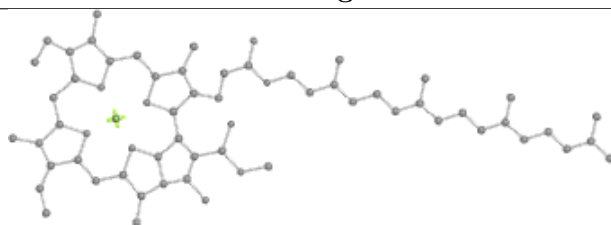
Bond lengths



Bond angles

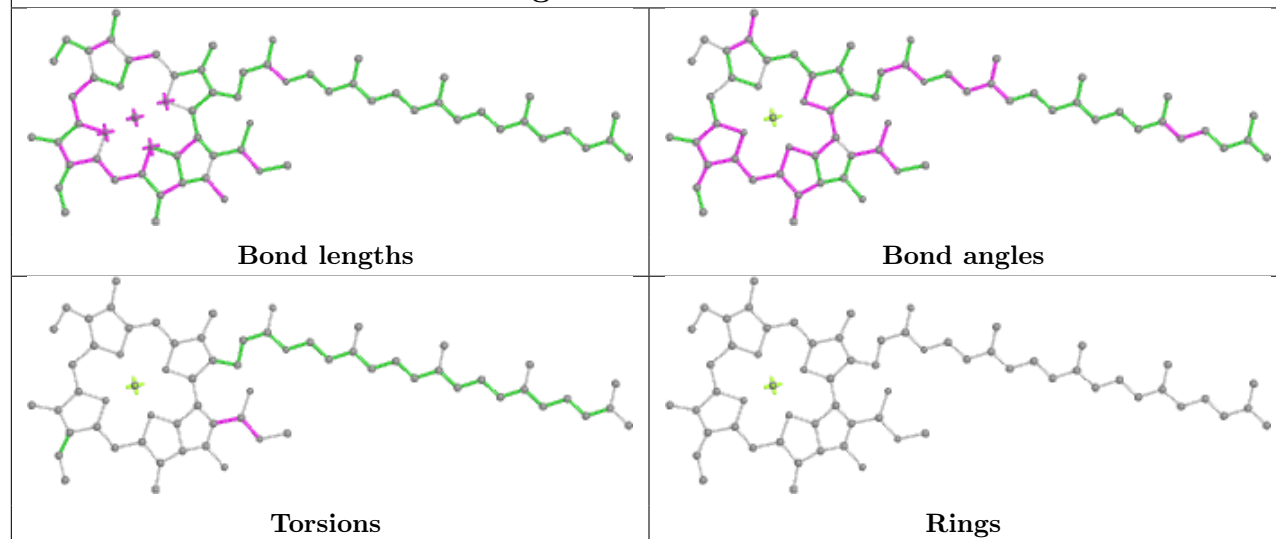


Torsions

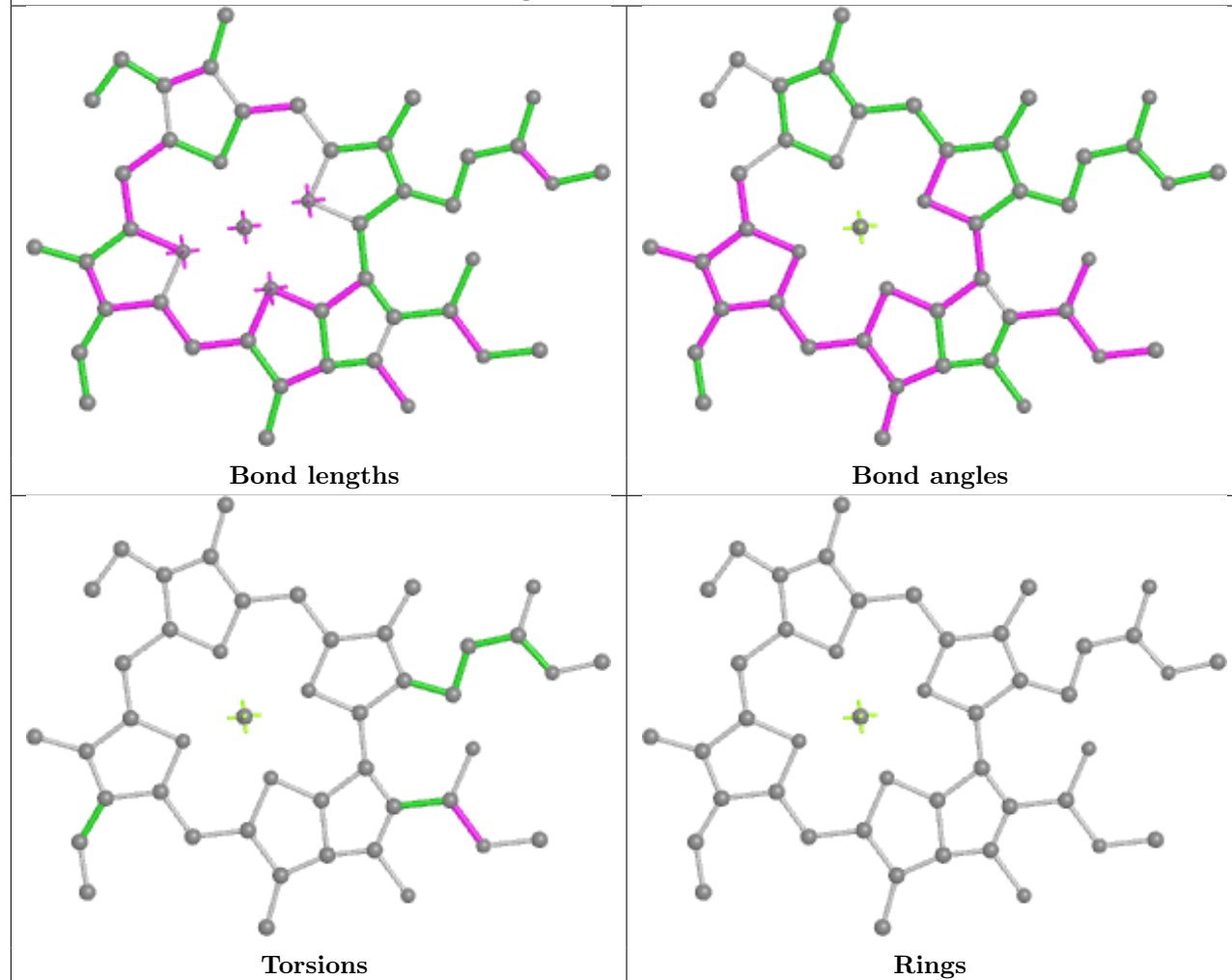


Rings

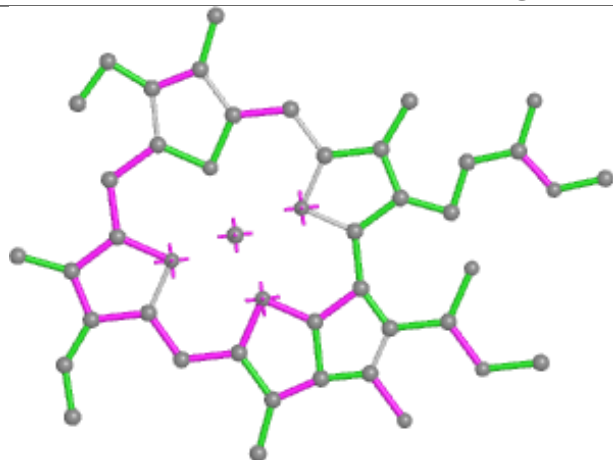
Ligand CLA B 834



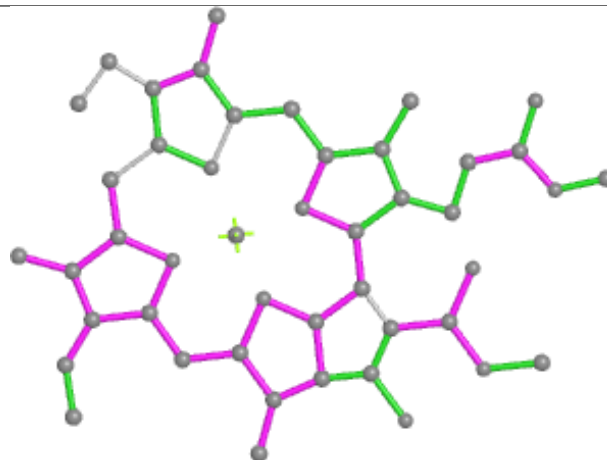
Ligand CLA 5 308



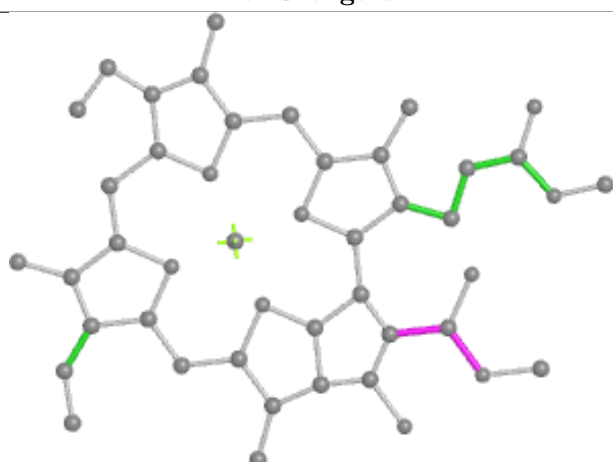
Ligand CLA H 902



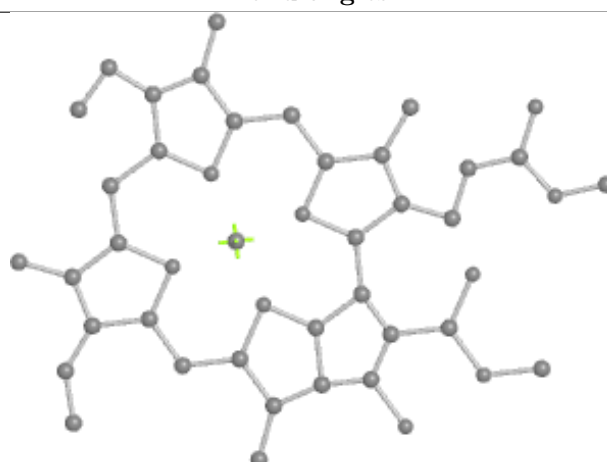
Bond lengths



Bond angles

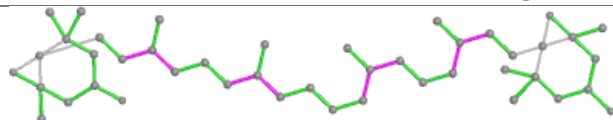


Torsions

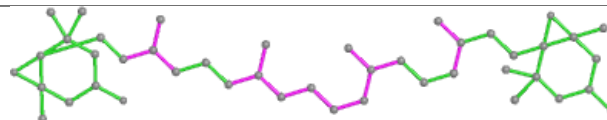


Rings

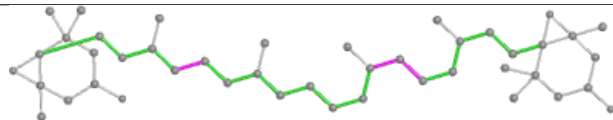
Ligand XAT 7 306



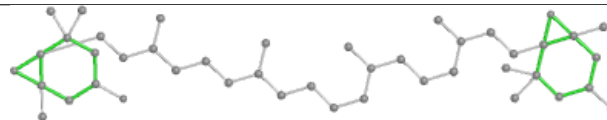
Bond lengths



Bond angles

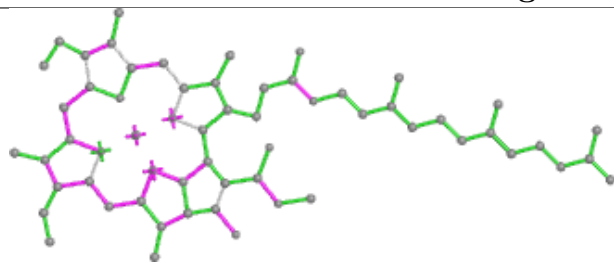


Torsions

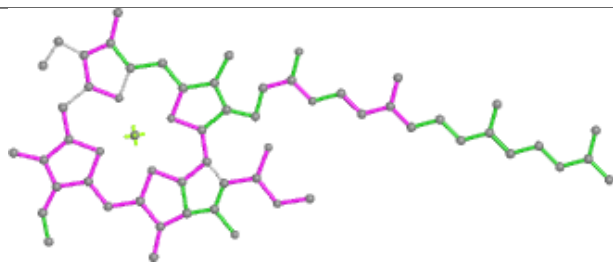


Rings

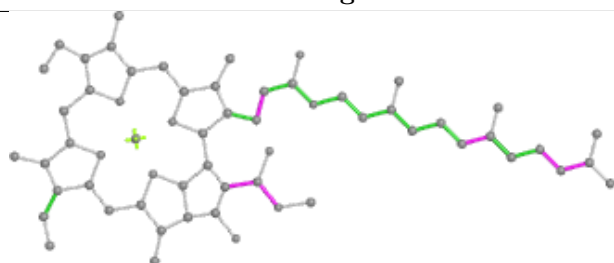
Ligand CLA 9 314



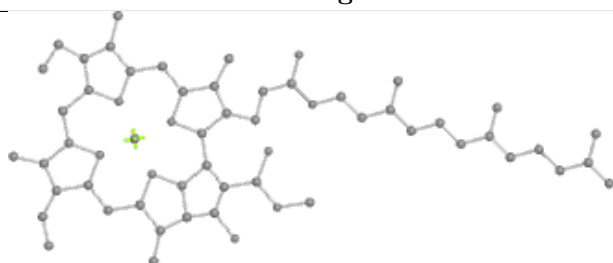
Bond lengths



Bond angles

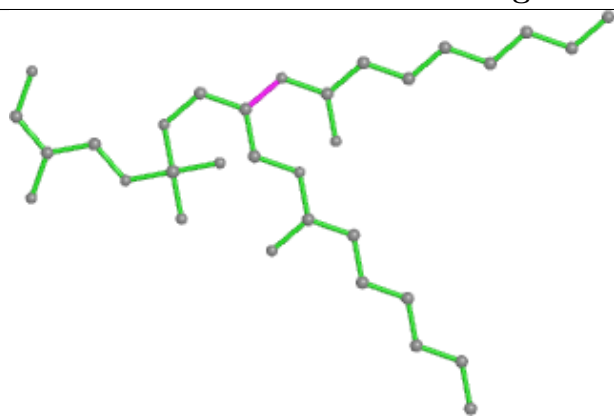


Torsions

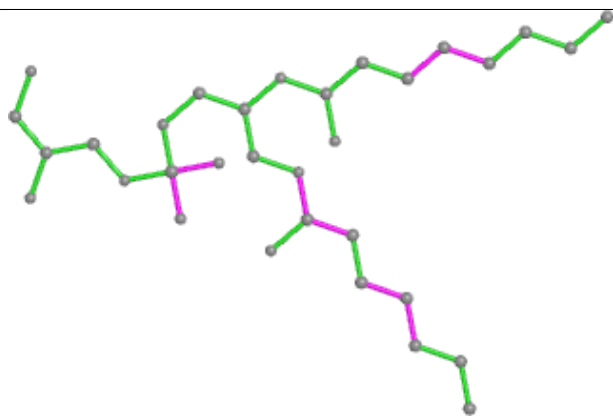


Rings

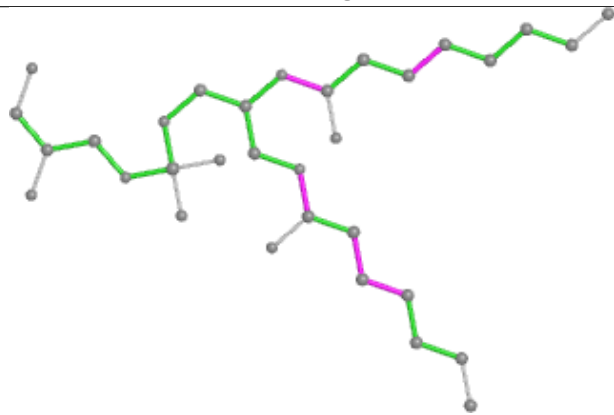
Ligand LHG B 807



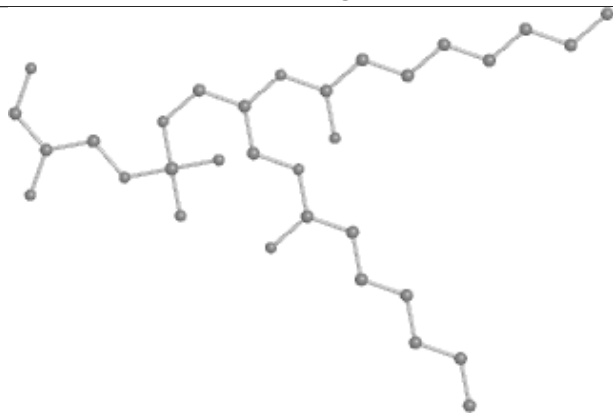
Bond lengths



Bond angles

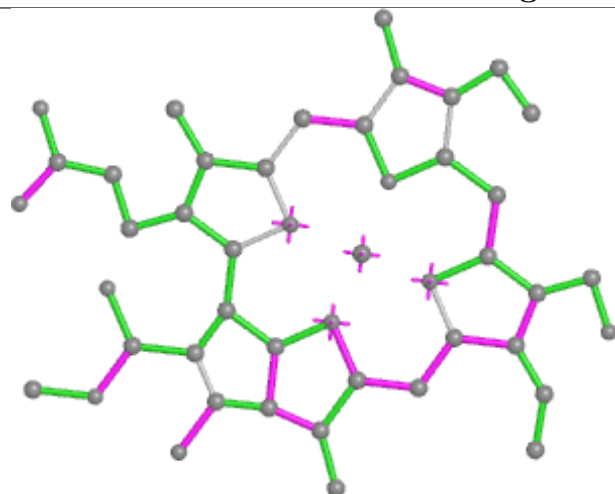


Torsions

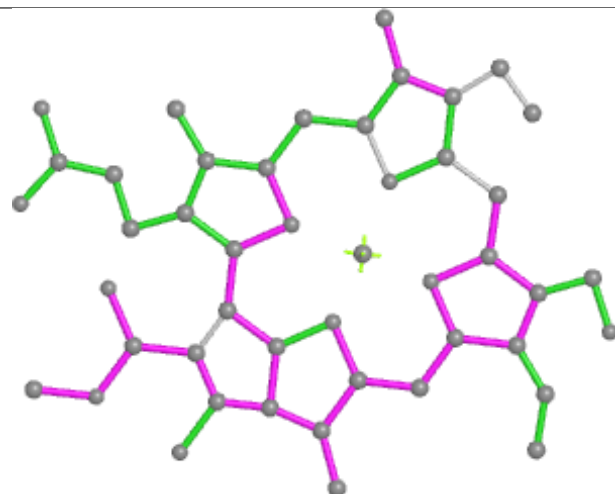


Rings

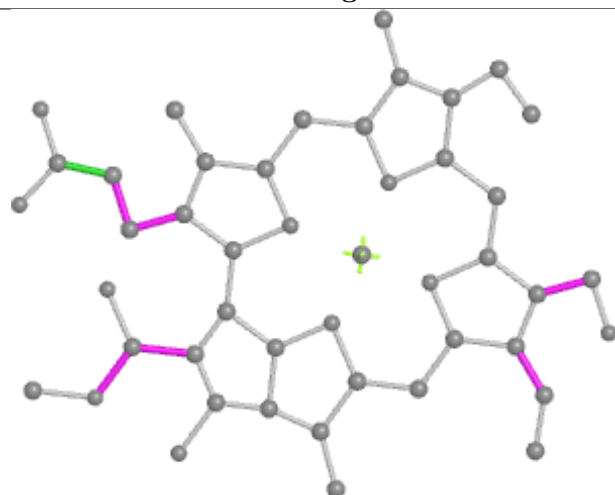
Ligand CHL 4 317



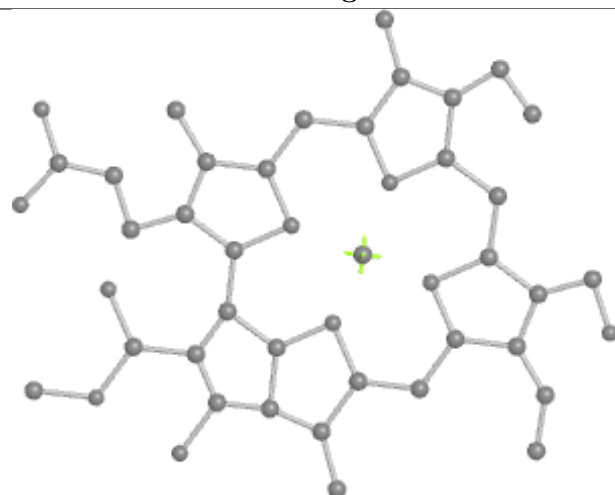
Bond lengths



Bond angles

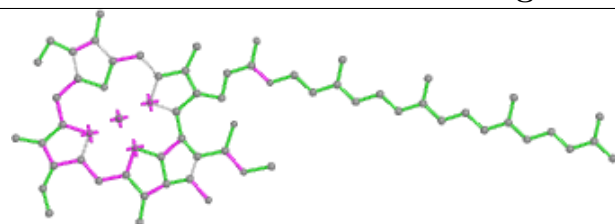


Torsions

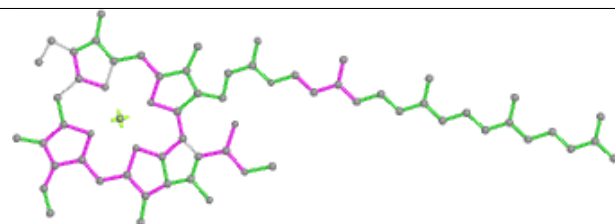


Rings

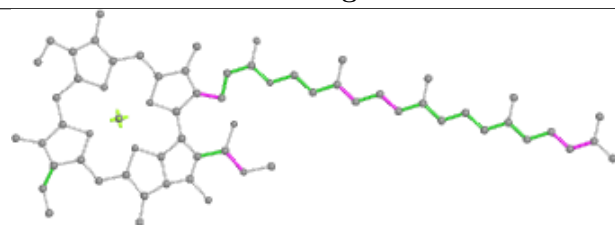
Ligand CLA B 847



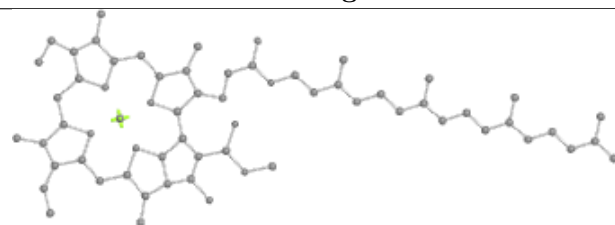
Bond lengths



Bond angles

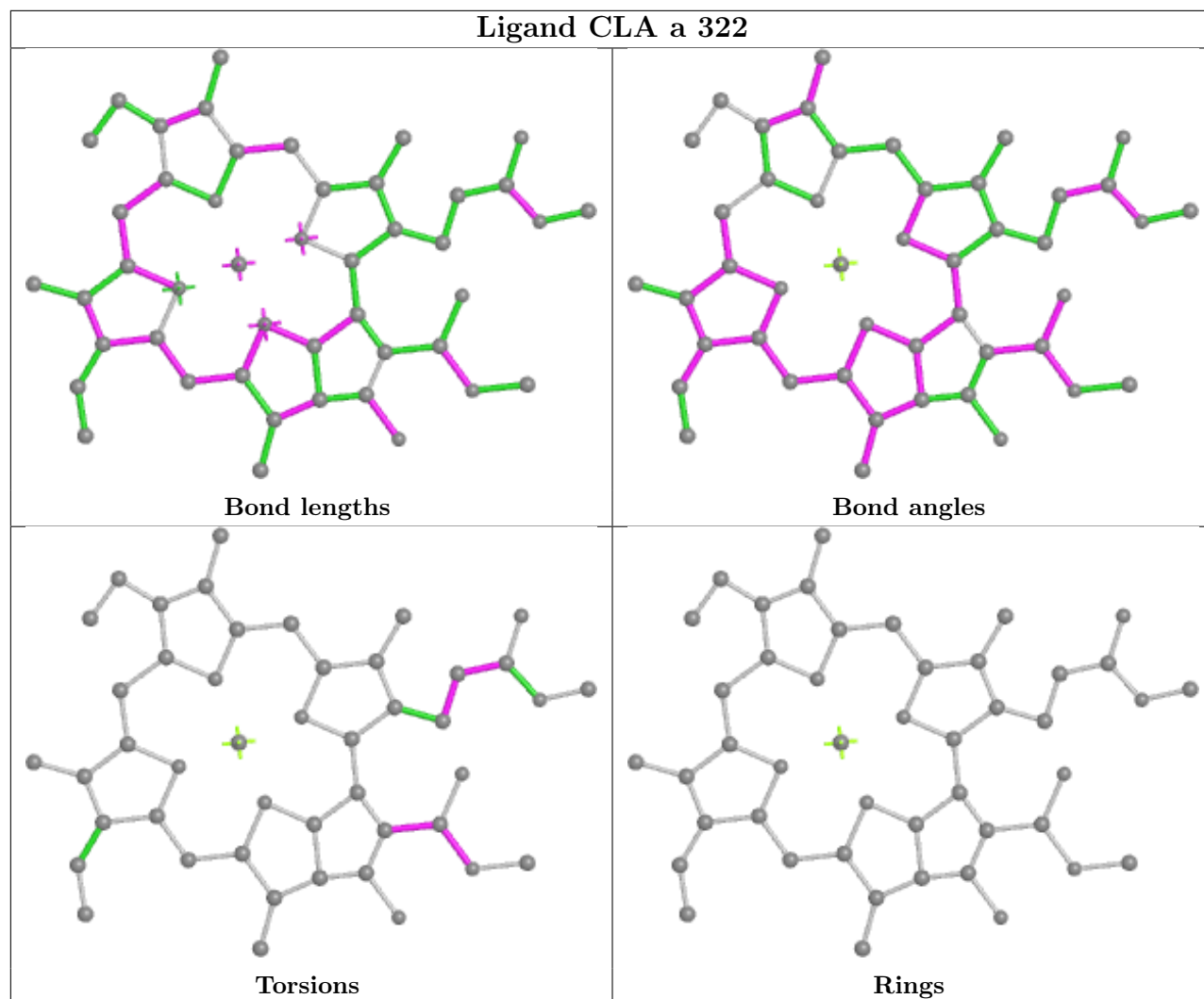


Torsions

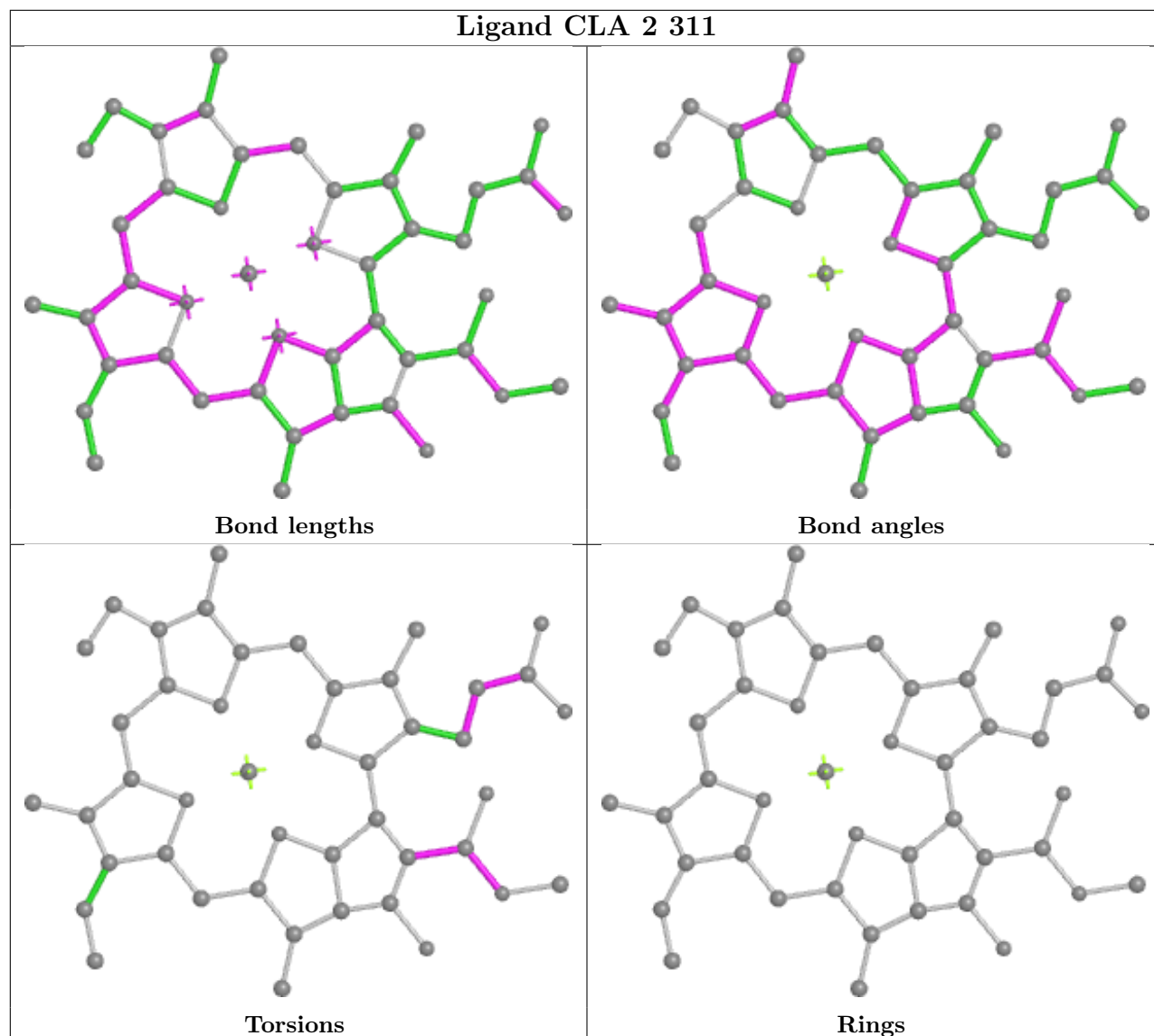


Rings

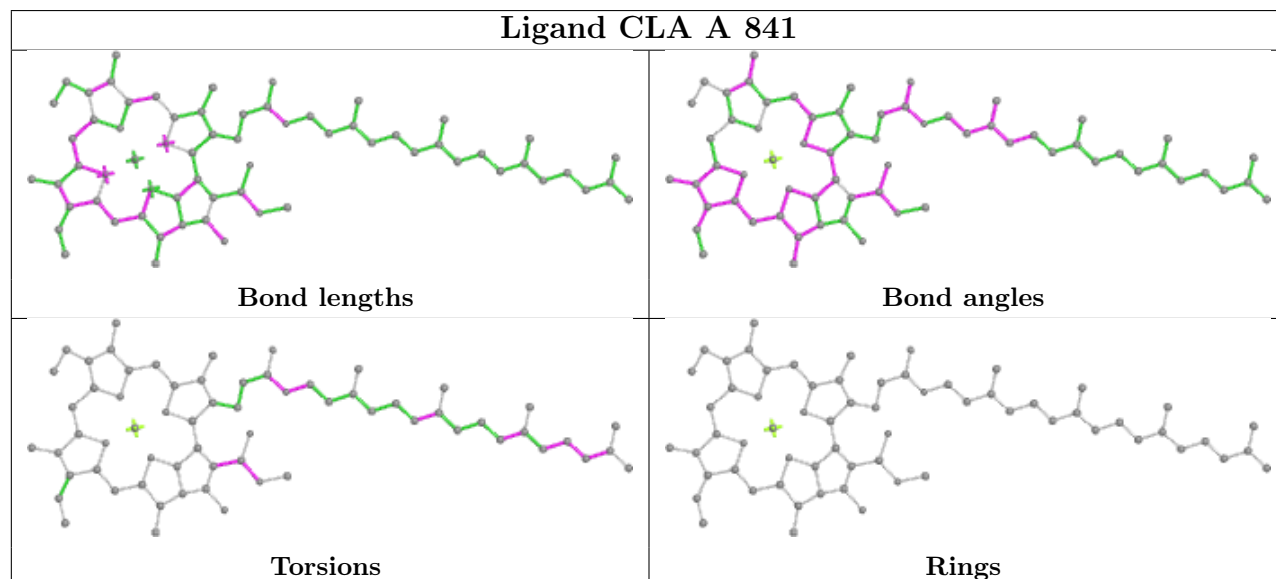
Ligand CLA a 322



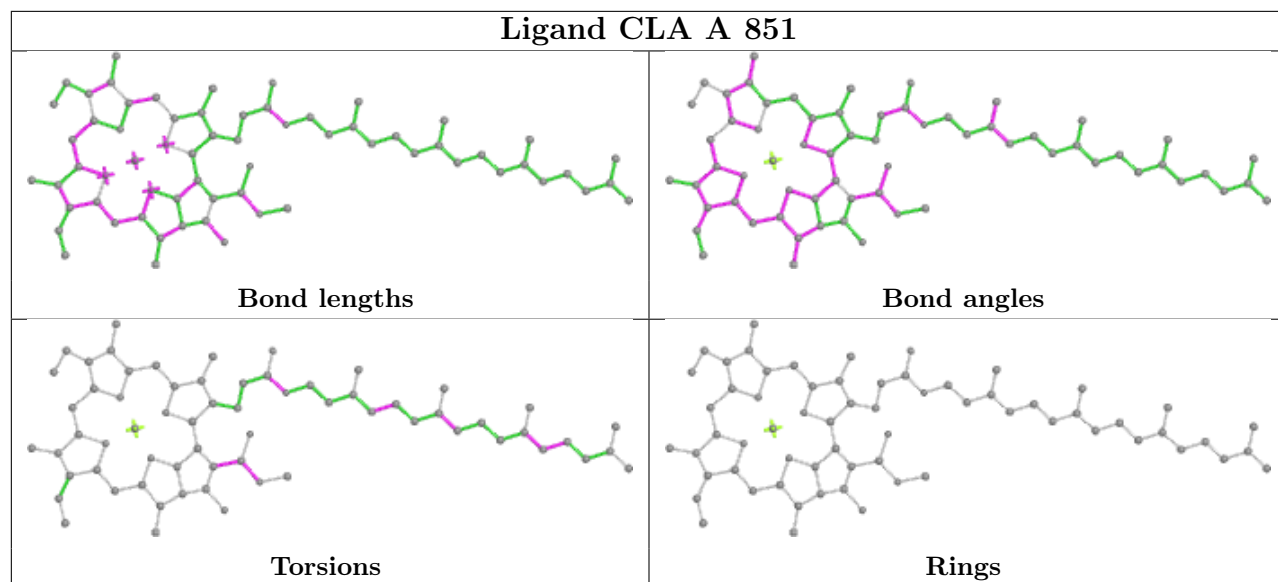
Ligand CLA 2 311



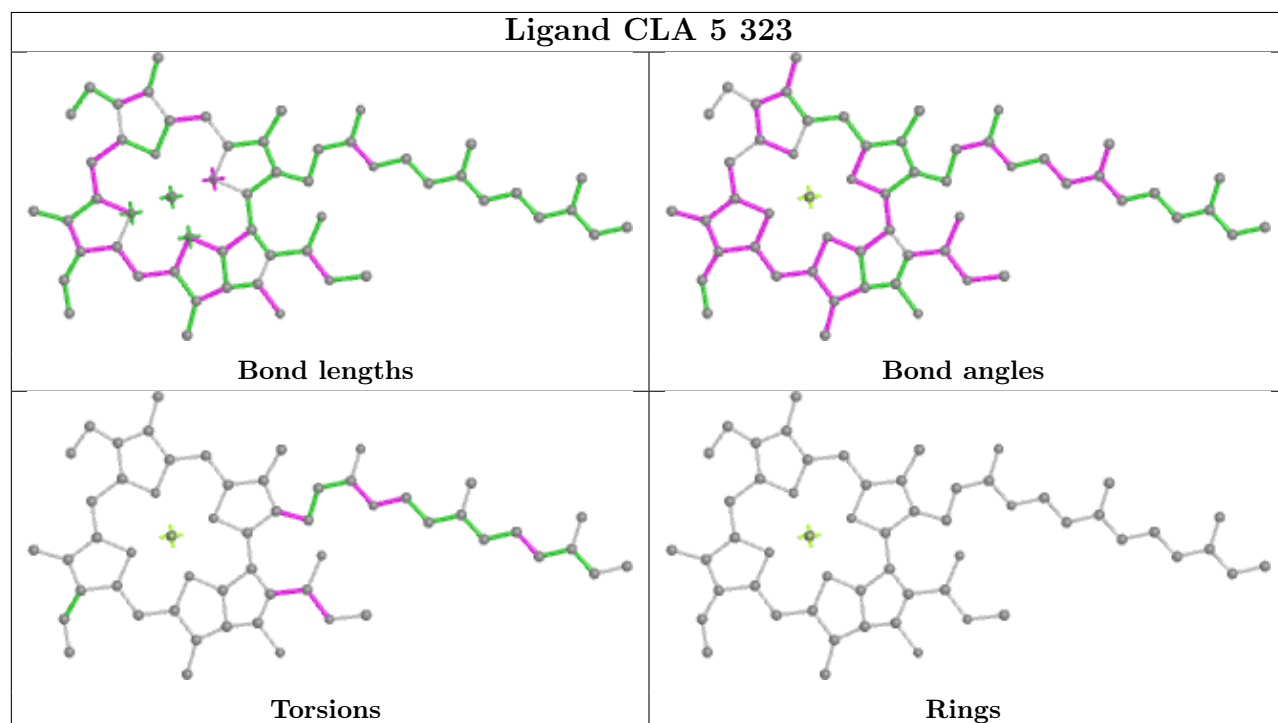
Ligand CLA A 841



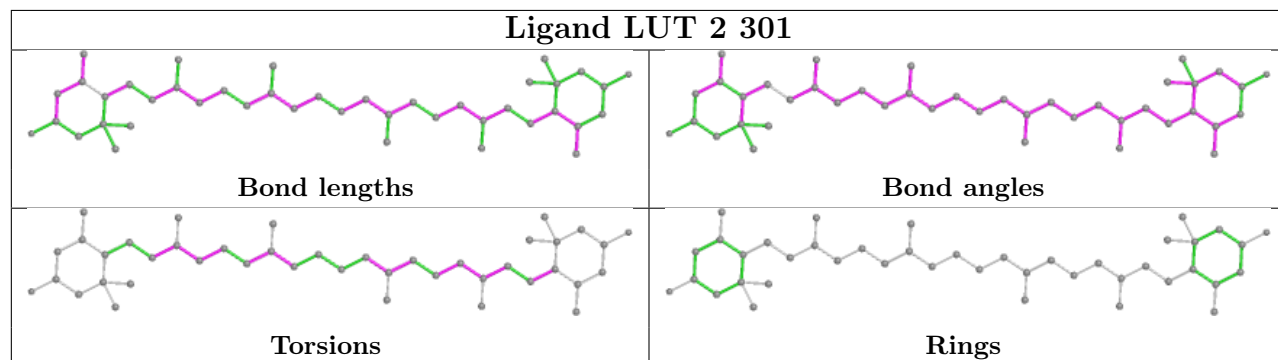
Ligand CLA A 851

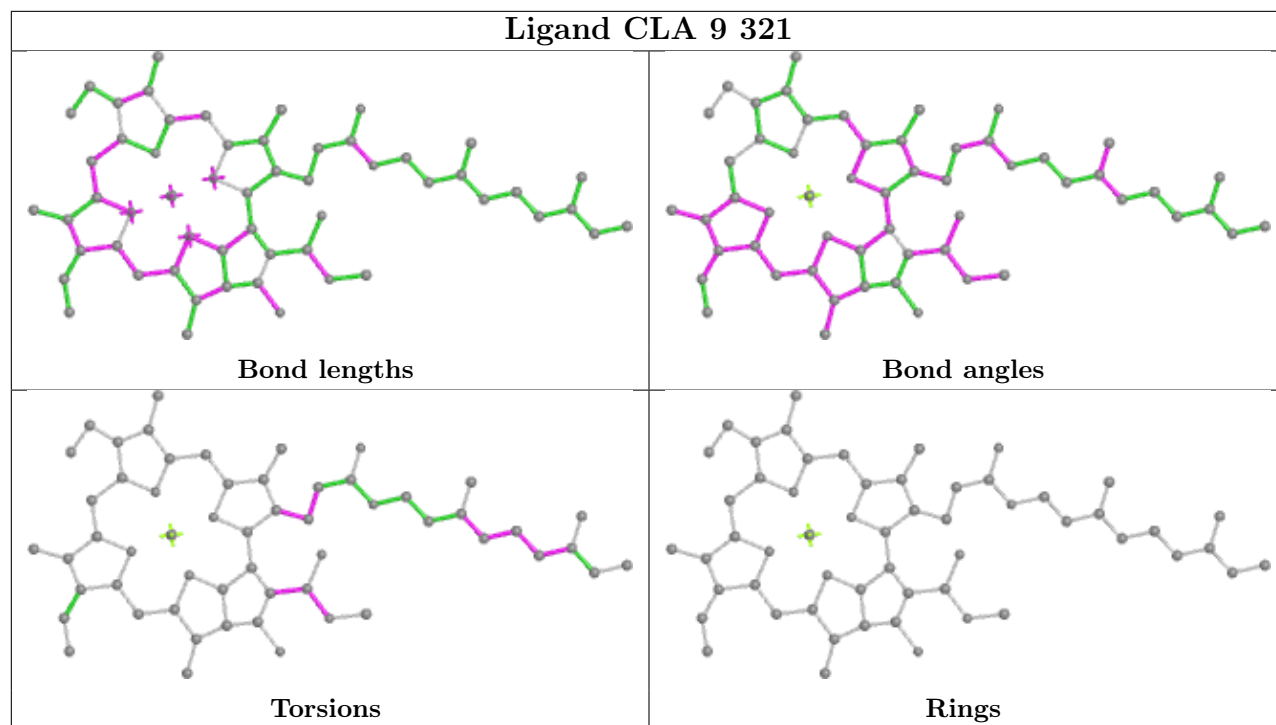
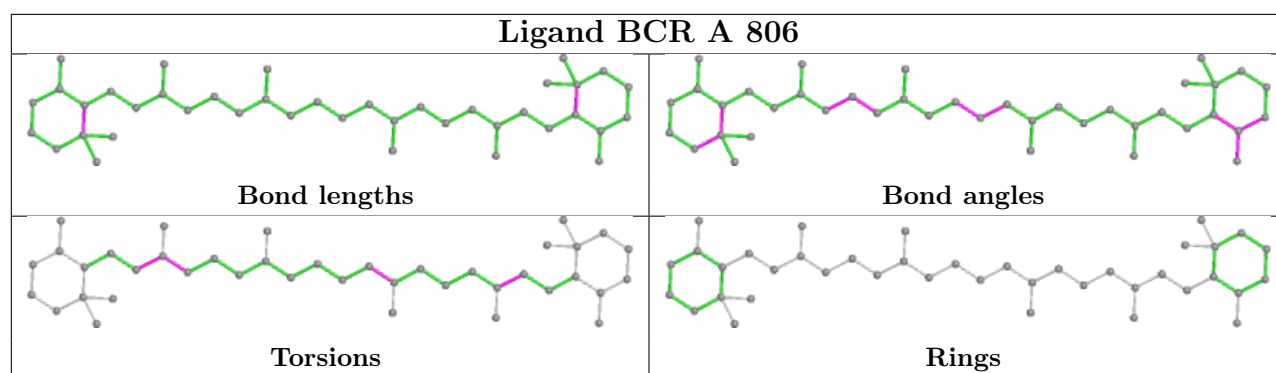


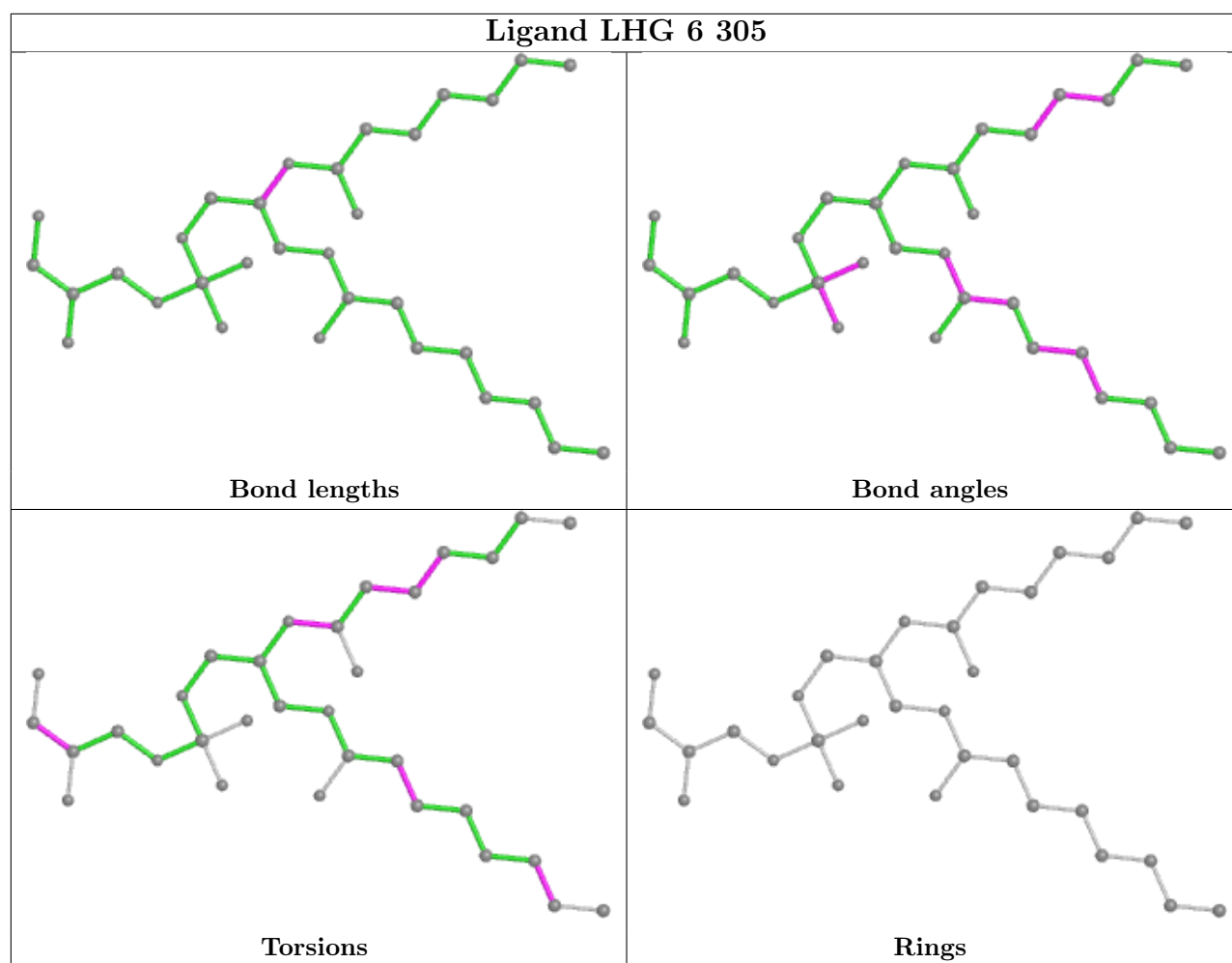
Ligand CLA 5 323



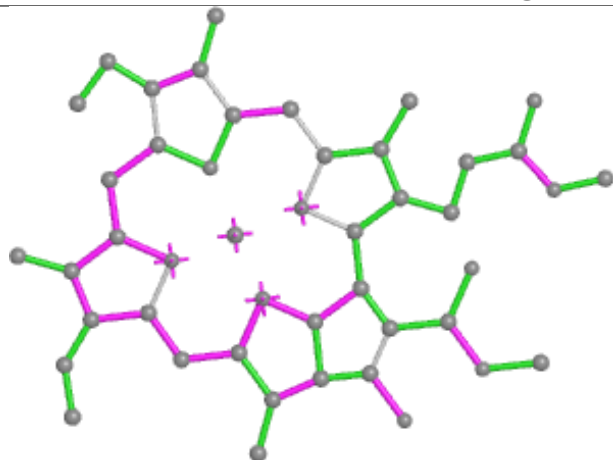
Ligand LUT 2 301



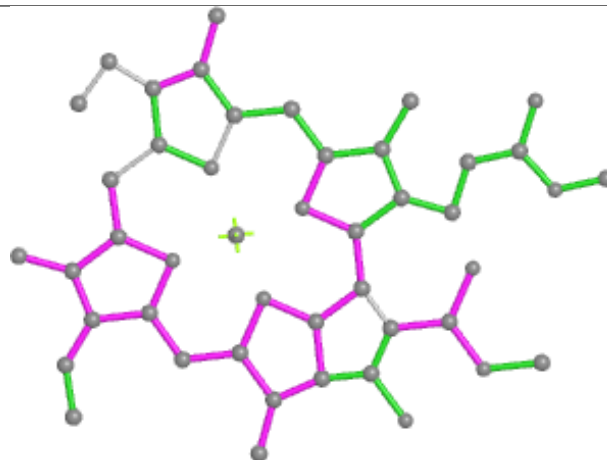




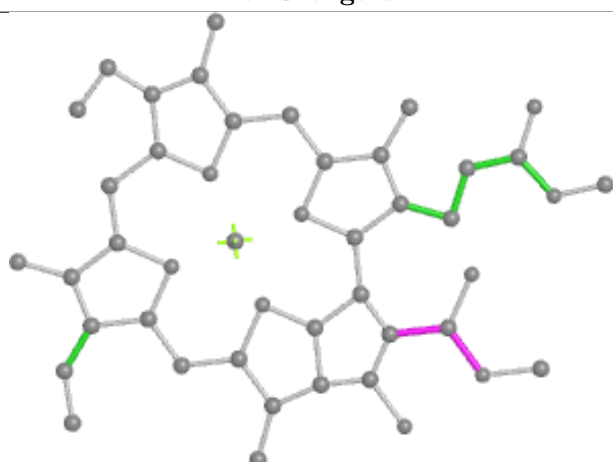
Ligand CLA 6 315



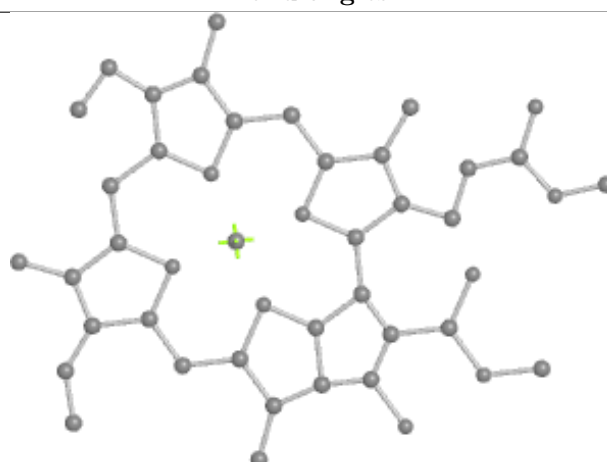
Bond lengths



Bond angles

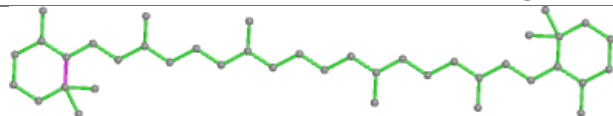


Torsions

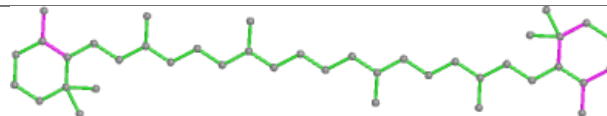


Rings

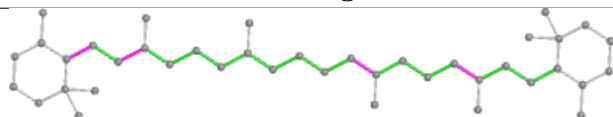
Ligand BCR I 801



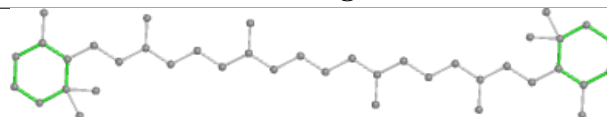
Bond lengths



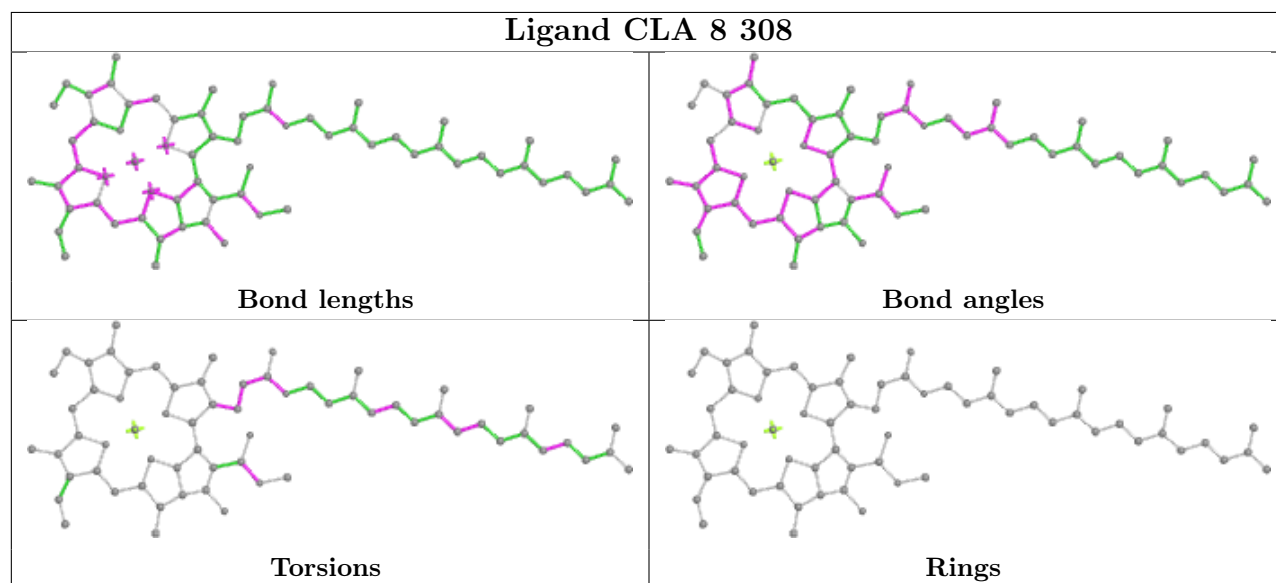
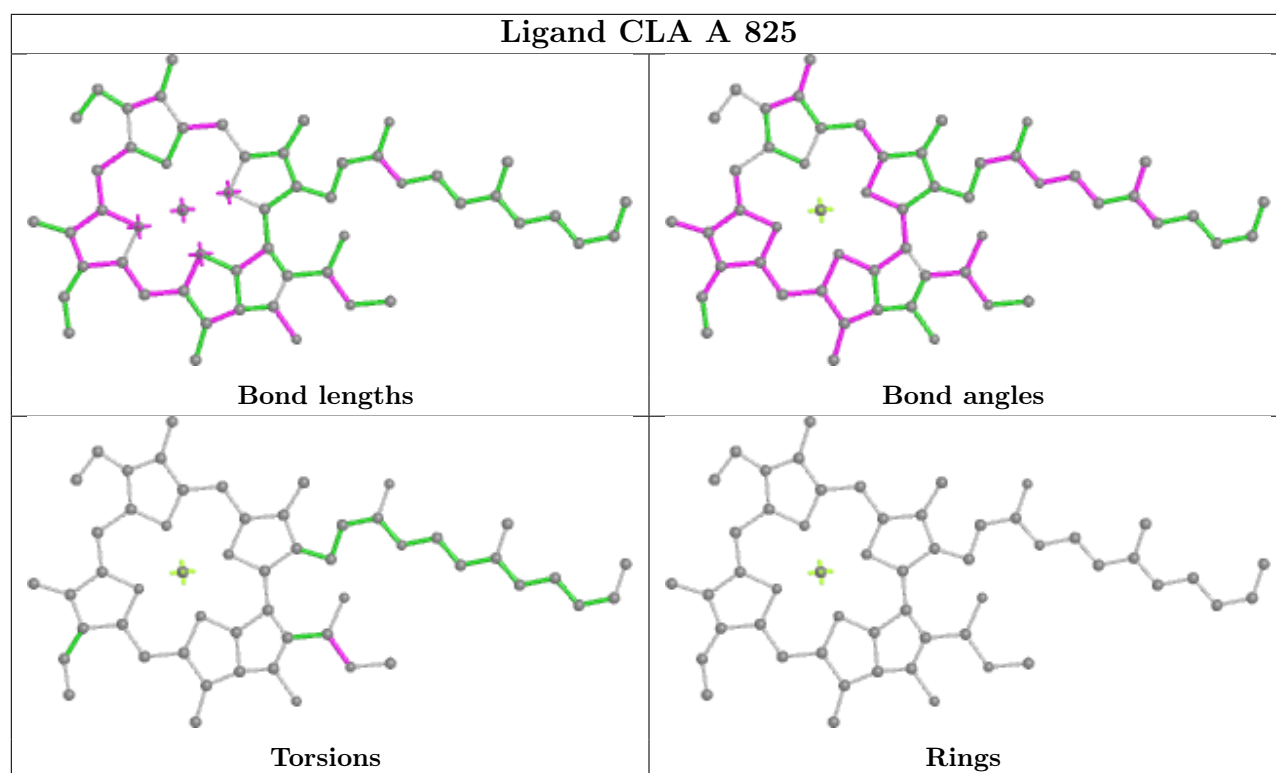
Bond angles

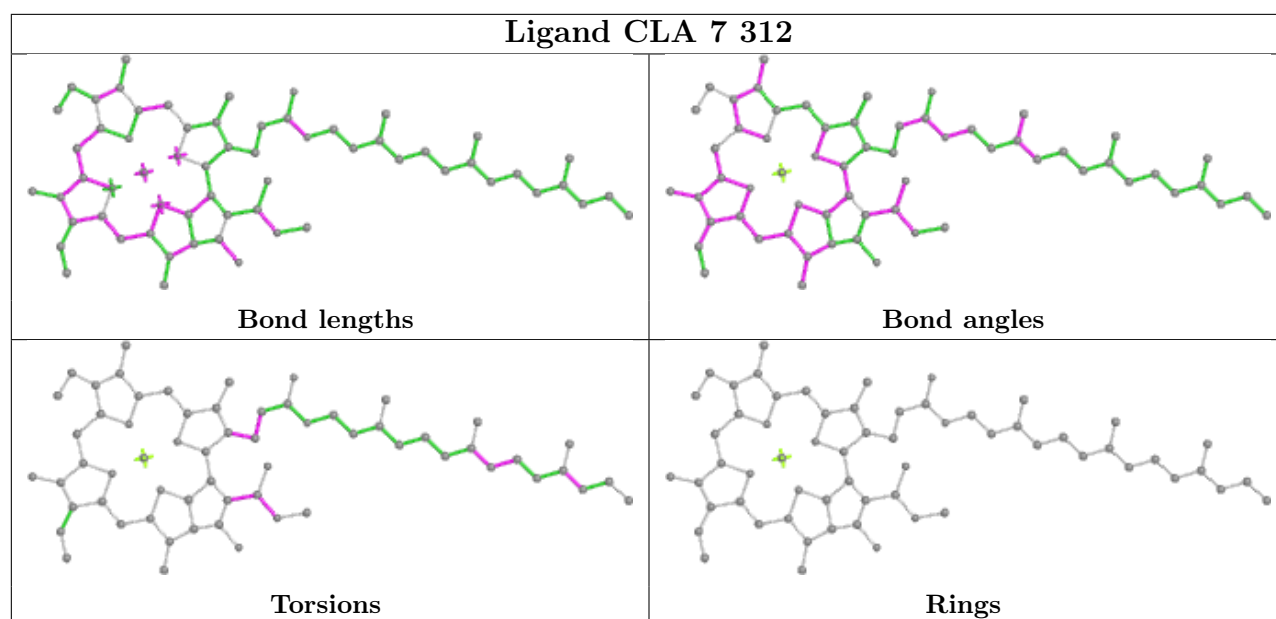


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

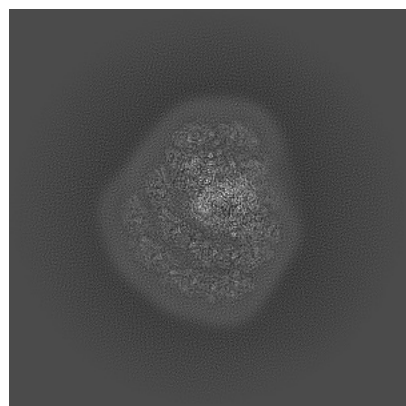
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62511. These allow visual inspection of the internal detail of the map and identification of artifacts.

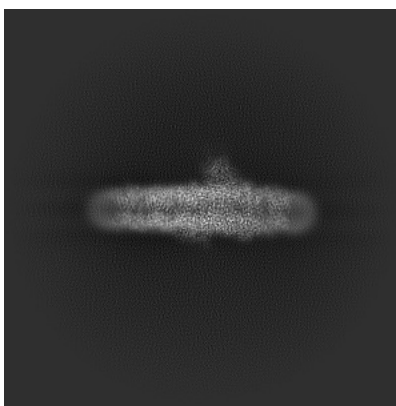
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

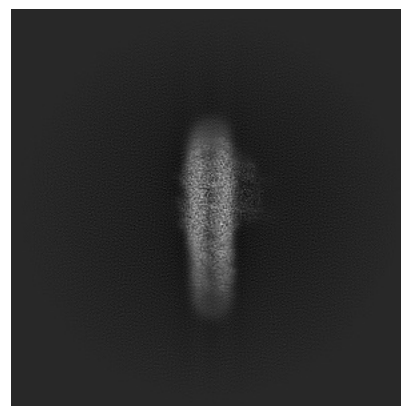
6.1.1 Primary map



X

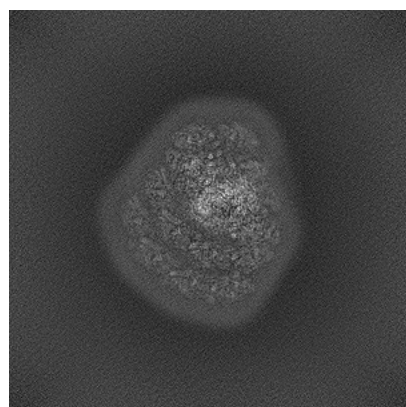


Y

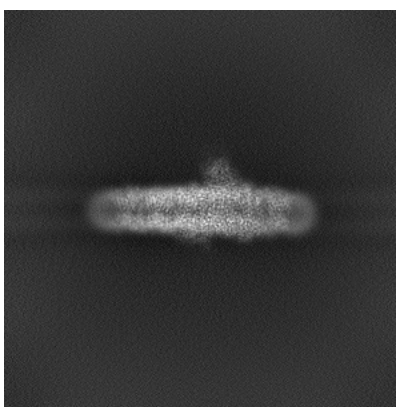


Z

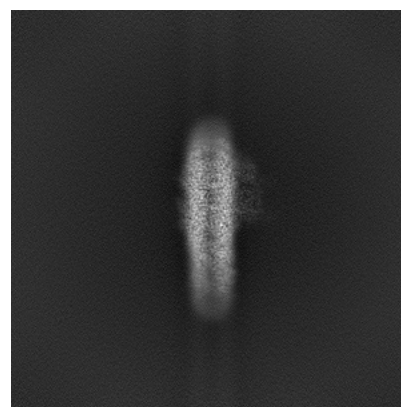
6.1.2 Raw map



X



Y

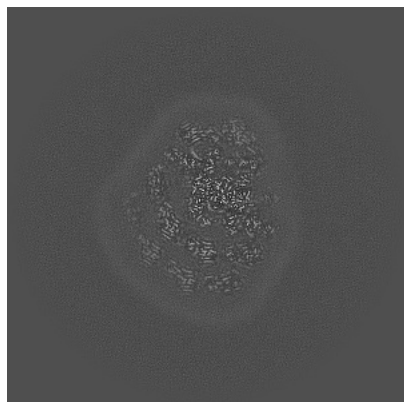


Z

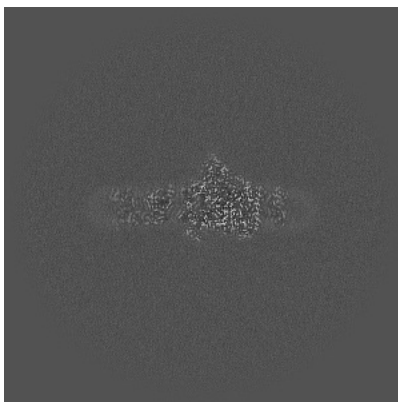
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

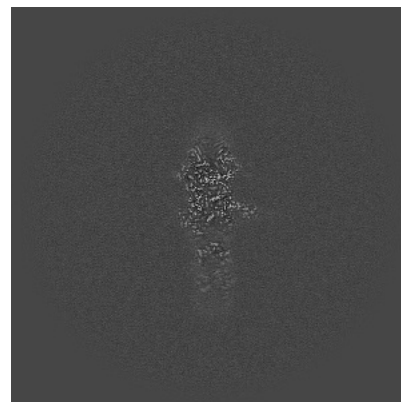
6.2.1 Primary map



X Index: 300

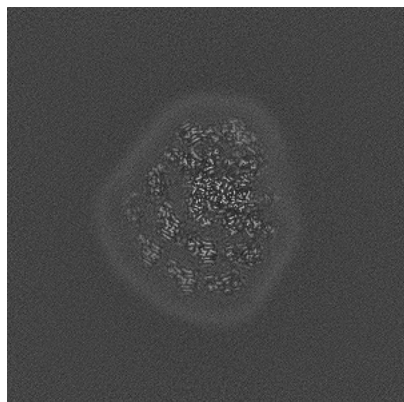


Y Index: 300

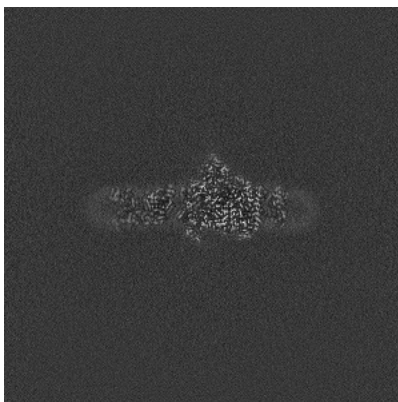


Z Index: 300

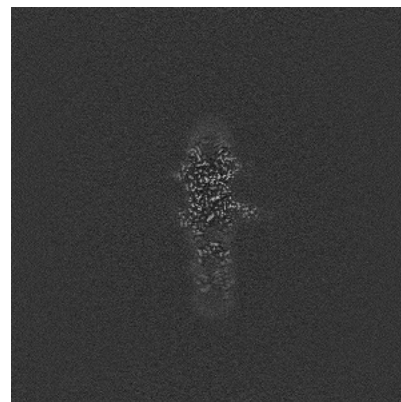
6.2.2 Raw map



X Index: 300



Y Index: 300

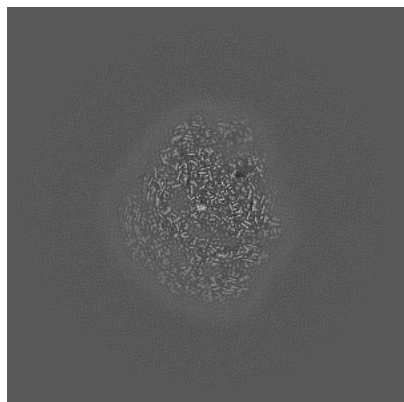


Z Index: 300

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

6.3 Largest variance slices [i](#)

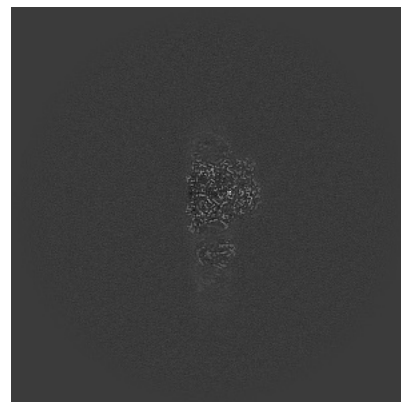
6.3.1 Primary map



X Index: 316

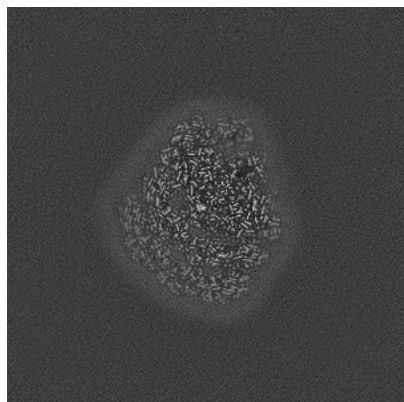


Y Index: 307

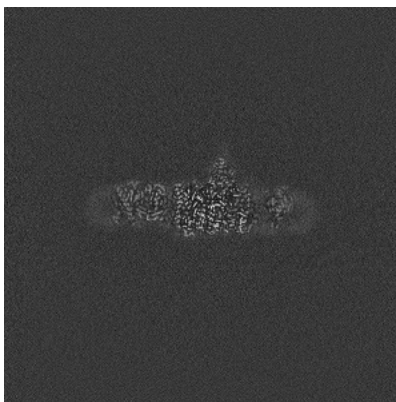


Z Index: 320

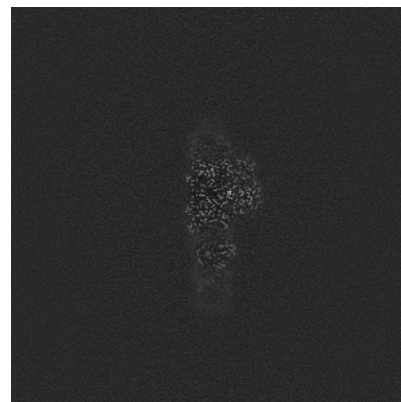
6.3.2 Raw map



X Index: 316



Y Index: 339

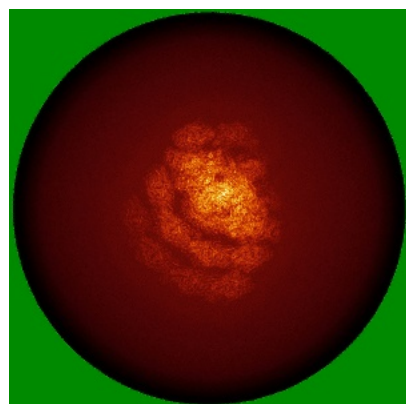


Z Index: 320

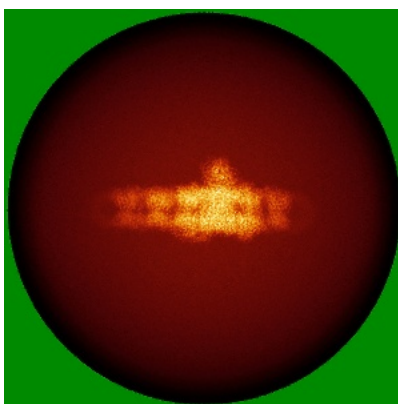
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

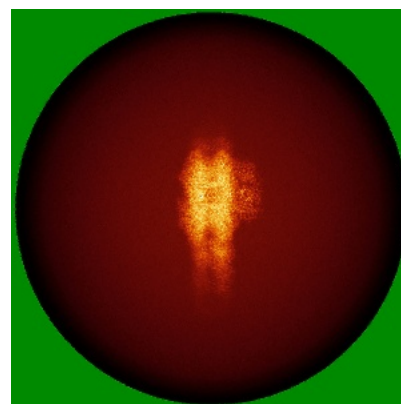
6.4.1 Primary map



X

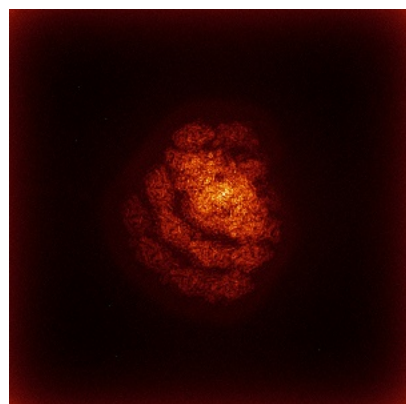


Y

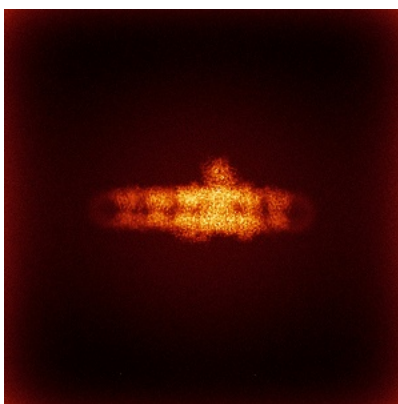


Z

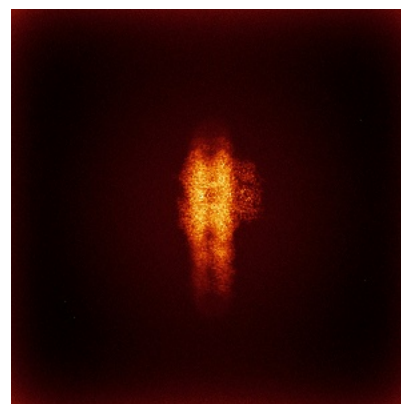
6.4.2 Raw map



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 0.085. 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.

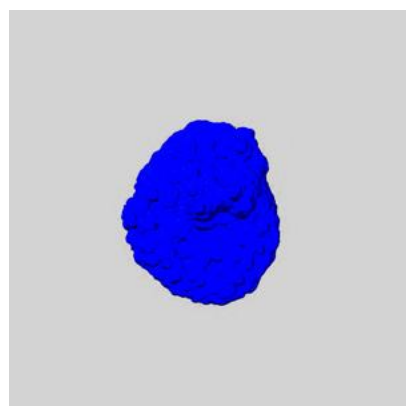
6.6 Mask visualisation [i](#)

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

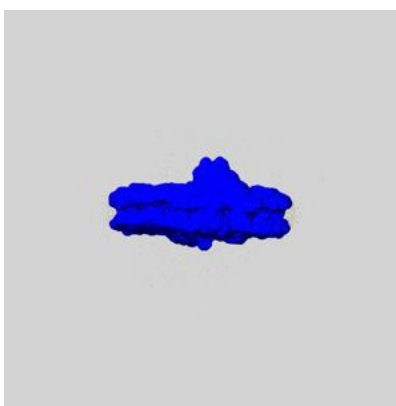
A mask typically either:

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

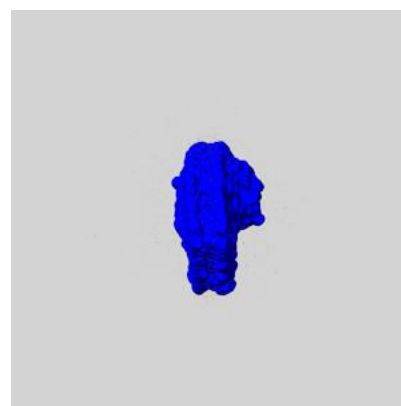
6.6.1 emd_62511_msk_1.map [i](#)



X



Y

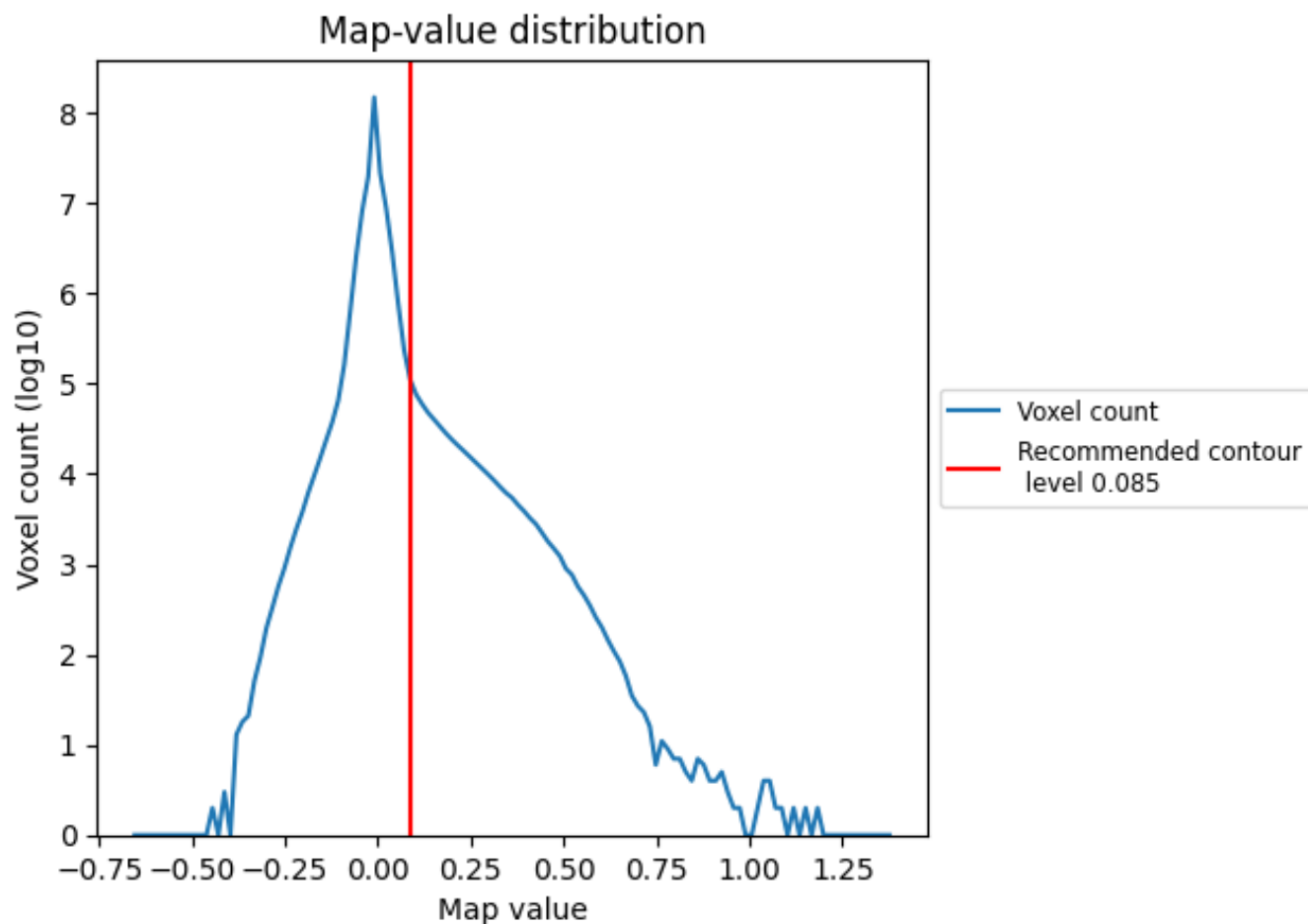


Z

7 Map analysis [i](#)

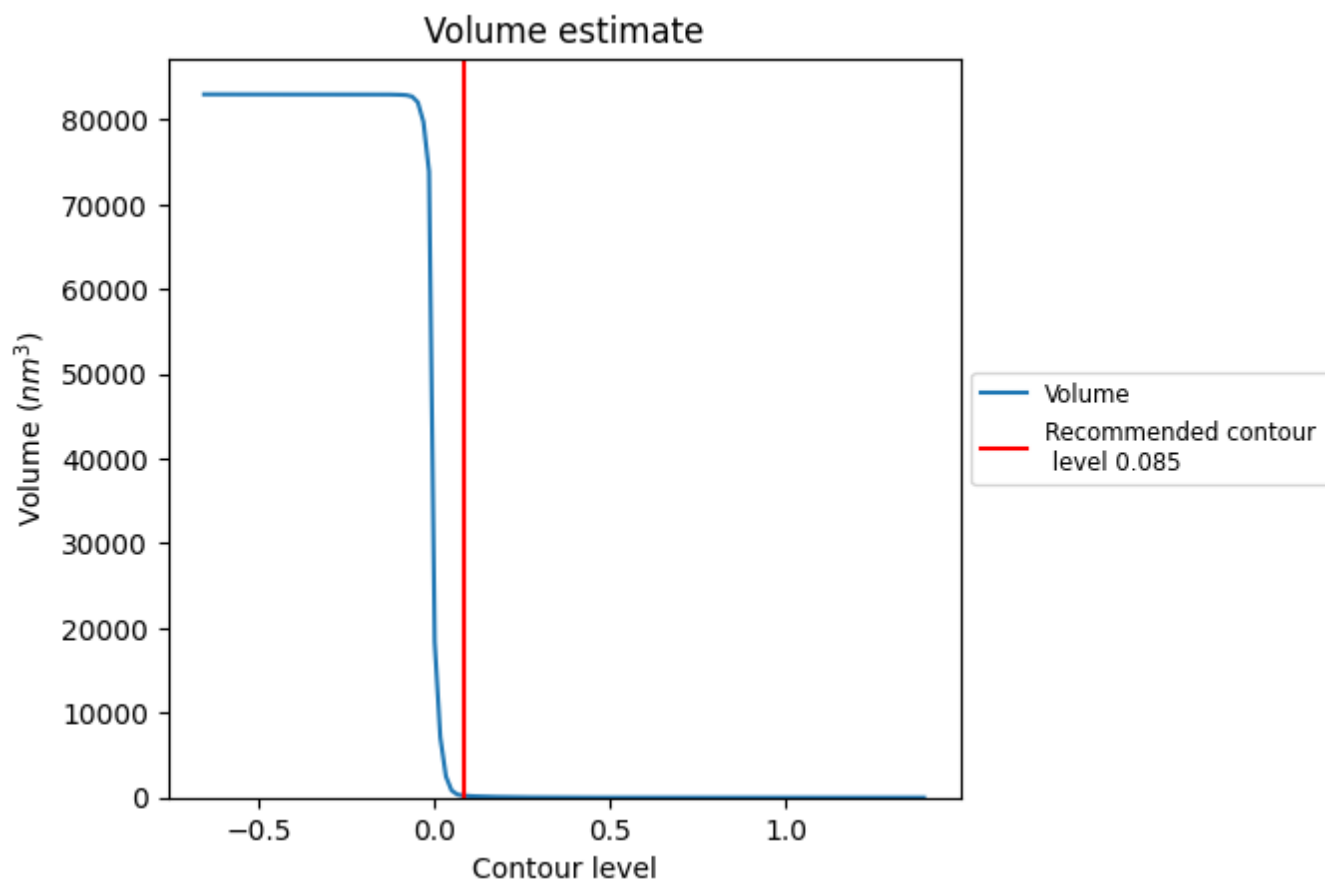
This section contains the results of statistical analysis of the map.

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.

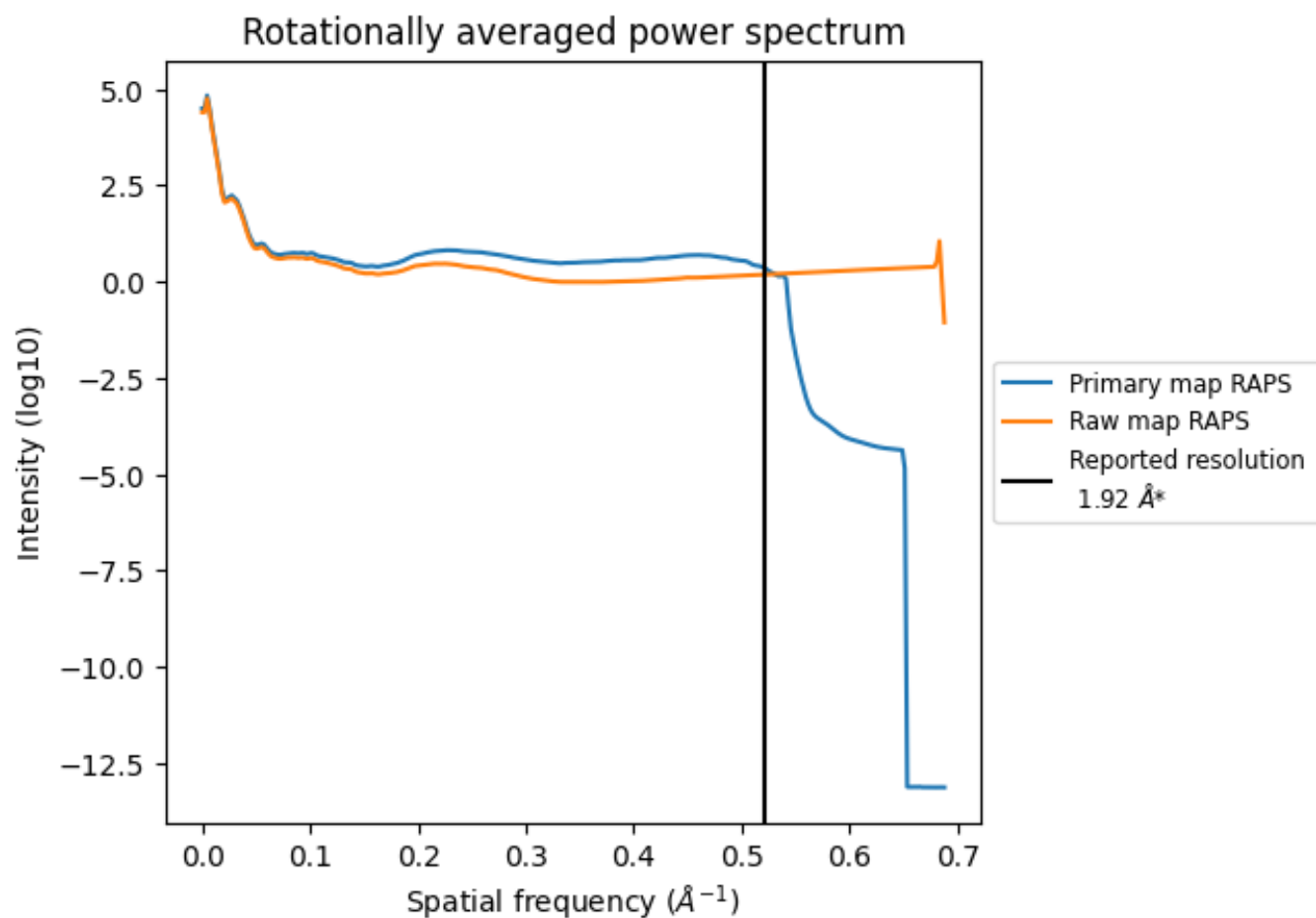
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm^3 ; this corresponds to an approximate mass of 205 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 ⓘ

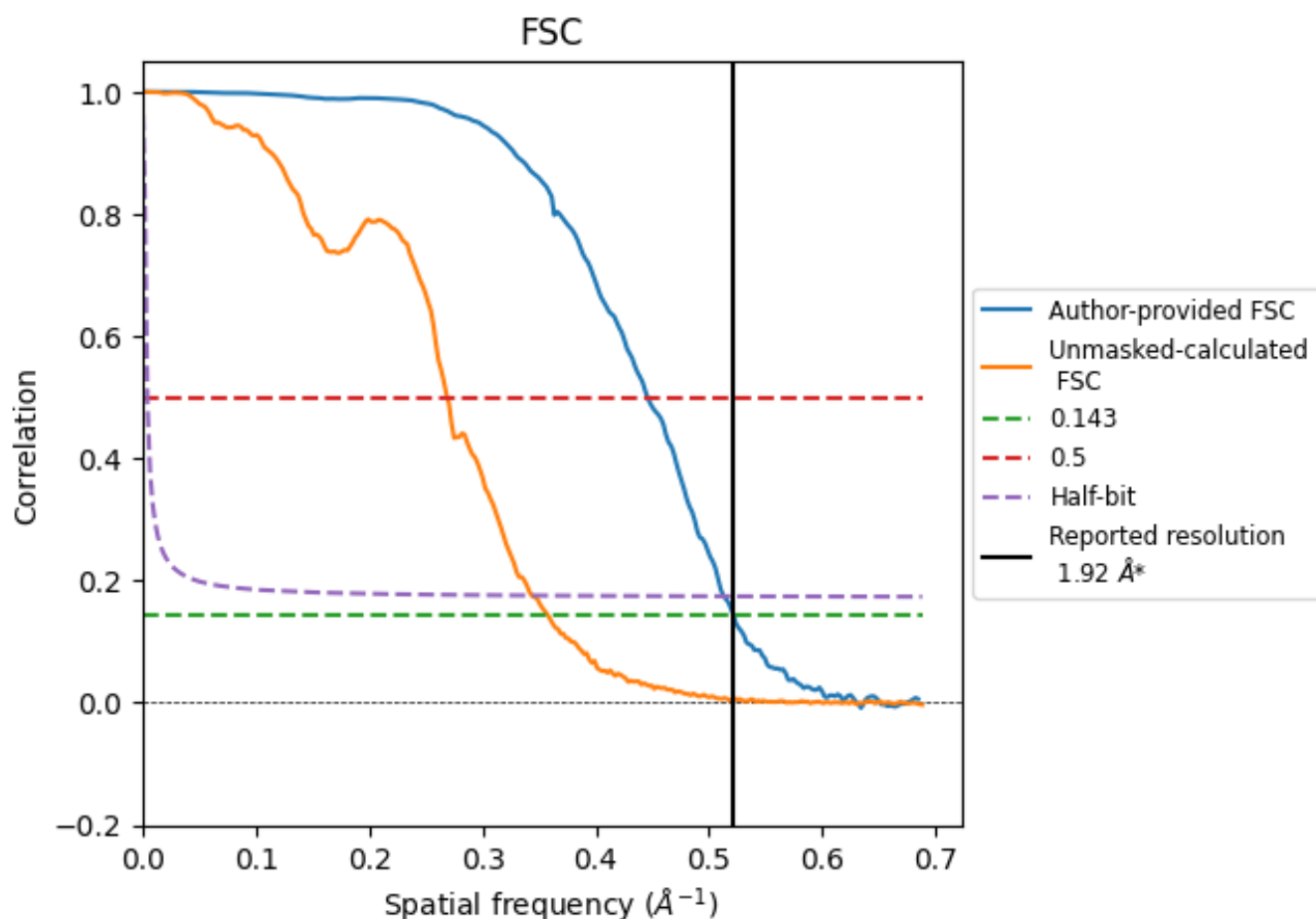


*Reported resolution corresponds to spatial frequency of 0.521 \AA^{-1}

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 0.521 \AA^{-1}

8.2 Resolution estimates [i](#)

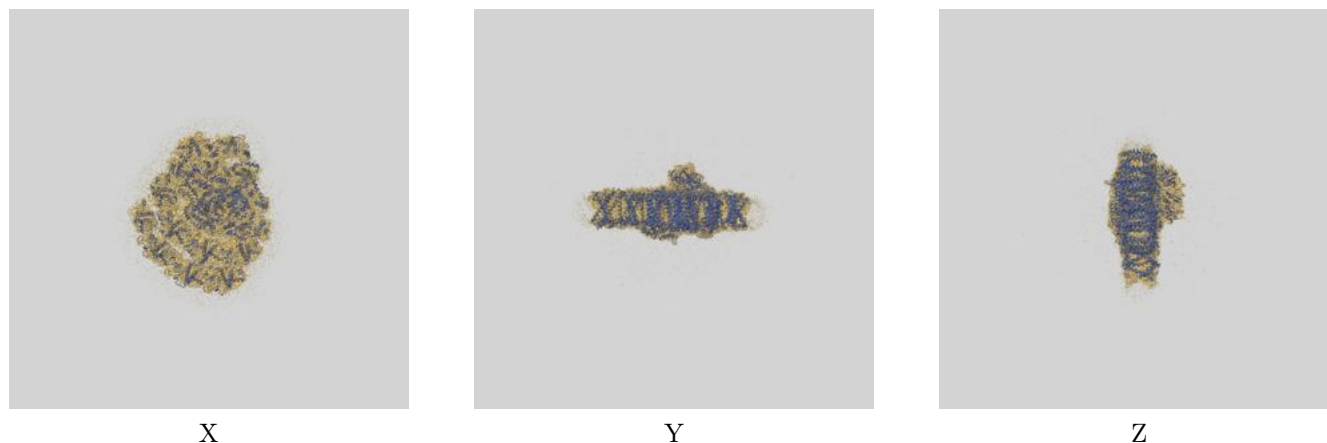
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.92	-	-
Author-provided FSC curve	1.92	2.24	1.95
Unmasked-calculated*	2.79	3.72	2.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.79 differs from the reported value 1.92 by more than 10 %

9 Map-model fit [i](#)

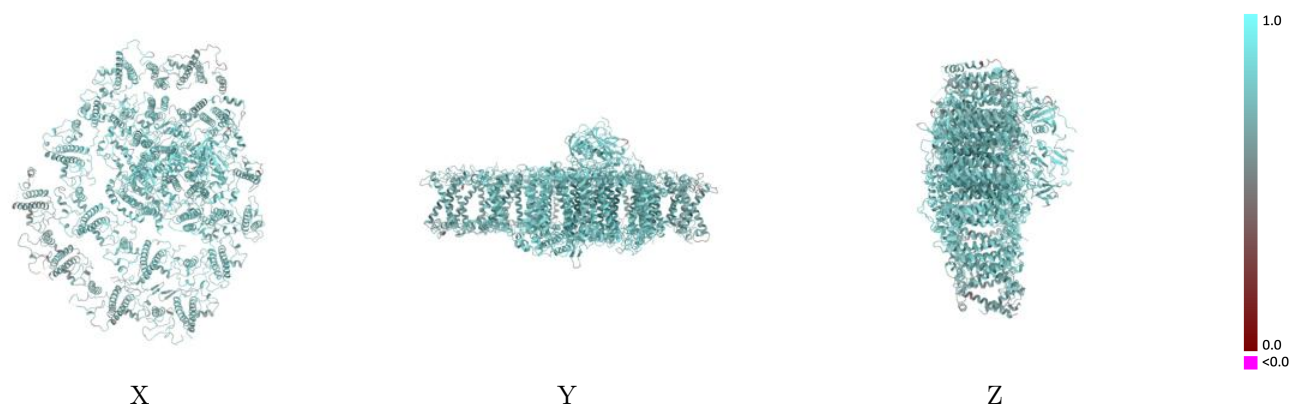
This section contains information regarding the fit between EMDB map EMD-62511 and PDB model 9KQP. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

9.1 Map-model overlay [i](#)



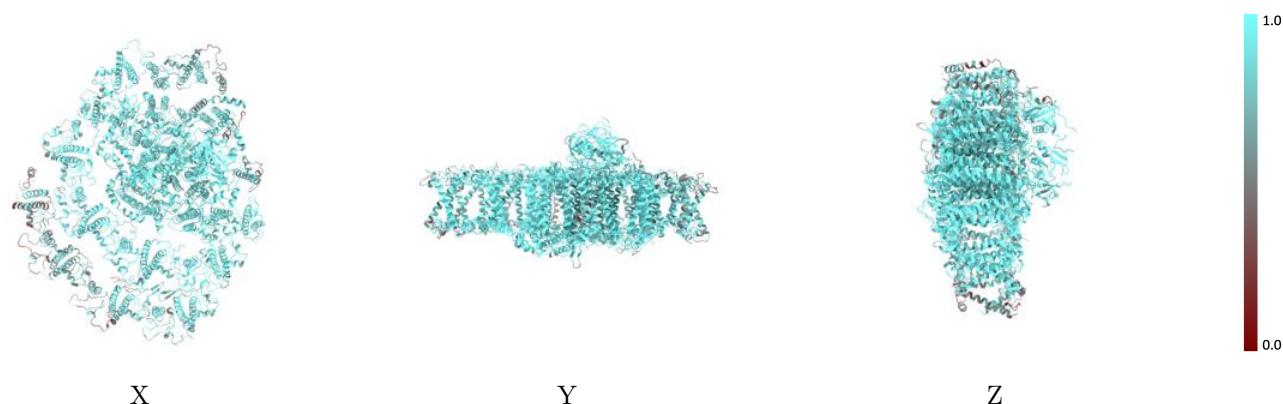
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



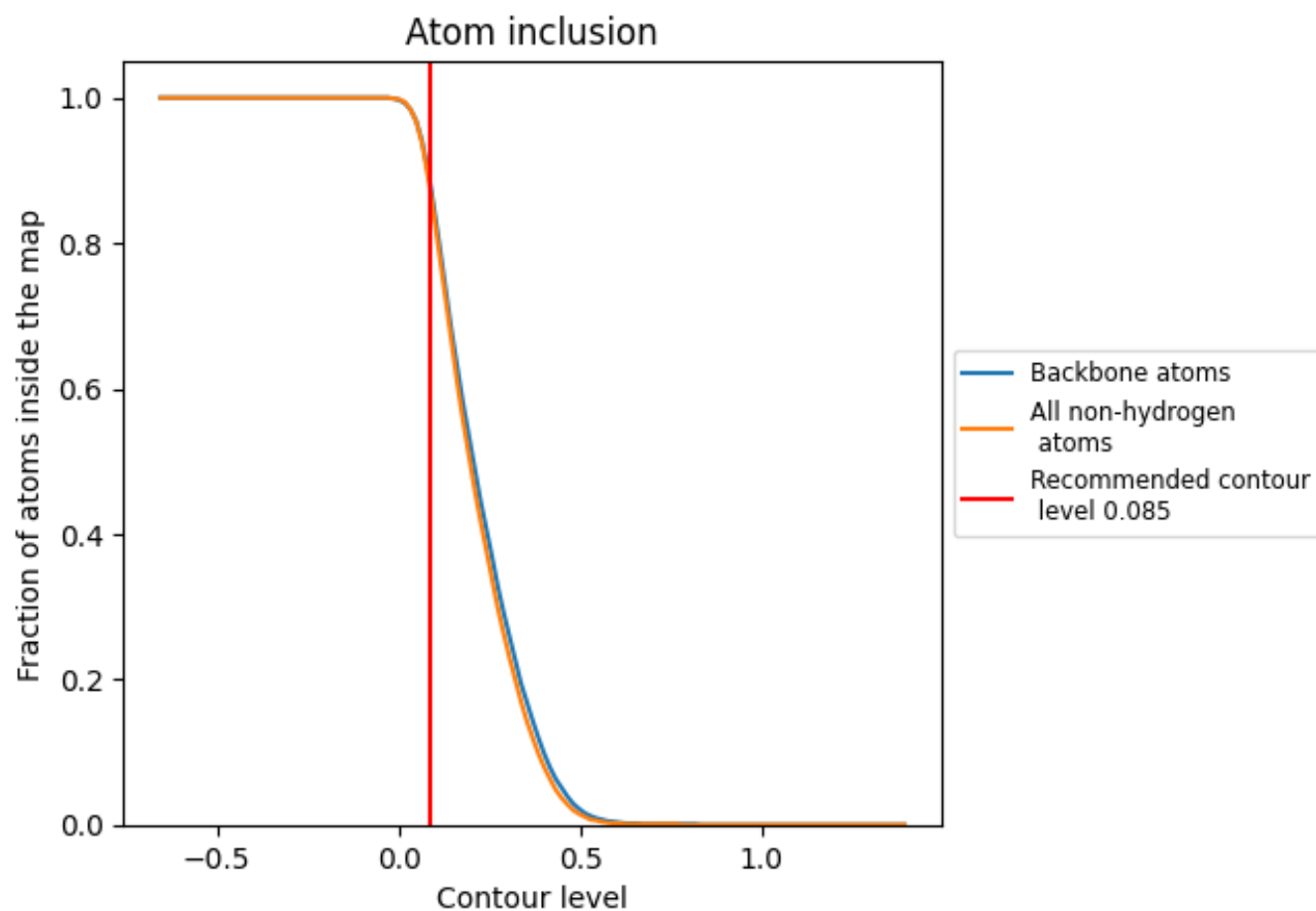
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.085).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.7230
2	 0.7470	 0.6320
3	 0.9070	 0.7070
4	 0.6450	 0.5770
5	 0.7930	 0.6420
6	 0.7360	 0.6210
7	 0.9190	 0.7280
8	 0.9100	 0.7290
9	 0.8830	 0.6910
A	 0.9650	 0.7910
B	 0.9690	 0.7950
C	 0.9920	 0.8120
D	 0.9590	 0.7800
E	 0.9200	 0.7700
F	 0.9490	 0.7810
G	 0.9090	 0.7300
H	 0.7620	 0.6860
I	 0.9760	 0.7770
J	 0.9690	 0.7790
K	 0.8840	 0.6980
L	 0.9000	 0.7320
M	 0.9530	 0.7720
O	 0.6770	 0.6560
a	 0.8890	 0.7080
b	 0.5990	 0.5800

