



wwPDB EM Validation Summary Report ⓘ

Feb 19, 2025 – 12:26 PM JST

PDB ID : 9KQQ
EMDB ID : EMD-62512
Title : PSI-LHCI supercomplex binding with 8 Lhcas from *C. subellipsoidea*
Authors : Tsai, P.-C.; Kato, K.; Shen, J.-R.; Akita, F.
Deposited on : 2024-11-26
Resolution : 2.06 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:

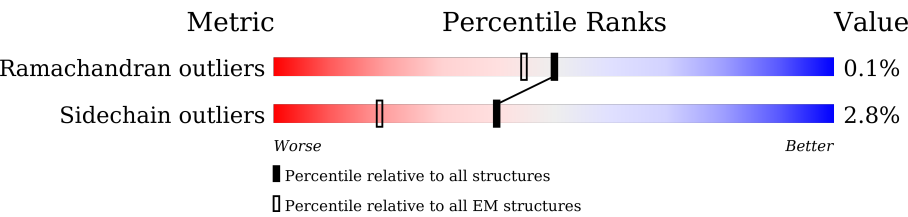
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

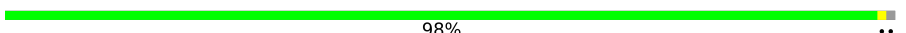
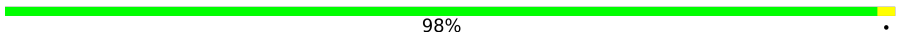
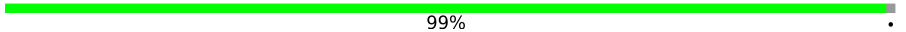





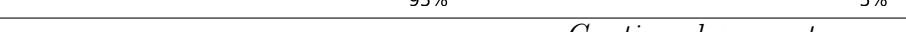
The reported resolution of this entry is 2.06 Å.

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.



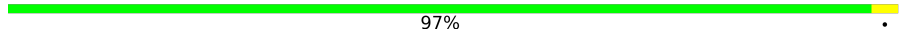







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	 98% ..
2	B	734	 98% .
3	C	81	 99% .
4	D	192	 73% . 26%
5	E	71	 85% 15%
6	F	245	 65% . 33%
7	G	138	 7% 14% . 86%
8	I	36	 89% . 8%
9	J	41	 95% 5%

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Mol	Chain	Length	Quality of chain
10	K	131	
11	M	31	
12	a	229	
12	b	229	
13	3	246	
14	4	246	
15	5	274	
16	6	272	
17	7	259	
18	8	255	
19	L	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CL0	A	815	X	-	-	-
27	CHL	3	308	X	-	-	-
27	CHL	3	309	X	-	-	-
27	CHL	3	310	X	-	-	-
27	CHL	3	311	X	-	-	-
27	CHL	3	312	X	-	-	-
27	CHL	3	313	X	-	-	-
27	CHL	3	314	X	-	-	-
27	CHL	3	315	X	-	-	-
27	CHL	3	316	X	-	-	-
27	CHL	3	317	X	-	-	-
27	CHL	3	318	X	-	-	-
27	CHL	3	319	X	-	-	-
27	CHL	3	320	X	-	-	-
27	CHL	3	321	X	-	-	-
27	CHL	4	304	X	-	-	-
27	CHL	4	305	X	-	-	-
27	CHL	4	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	4	307	X	-	-	-
27	CHL	4	308	X	-	-	-
27	CHL	4	309	X	-	-	-
27	CHL	4	310	X	-	-	-
27	CHL	4	311	X	-	-	-
27	CHL	4	312	X	-	-	-
27	CHL	4	313	X	-	-	-
27	CHL	4	314	X	-	-	-
27	CHL	4	315	X	-	-	-
27	CHL	4	316	X	-	-	-
27	CHL	4	317	X	-	-	-
27	CHL	4	318	X	-	-	-
27	CHL	4	319	X	-	-	-
27	CHL	4	320	X	-	-	-
27	CHL	5	307	X	-	-	-
27	CHL	5	308	X	-	-	-
27	CHL	5	309	X	-	-	-
27	CHL	5	310	X	-	-	-
27	CHL	5	311	X	-	-	-
27	CHL	5	312	X	-	-	-
27	CHL	5	313	X	-	-	-
27	CHL	5	314	X	-	-	-
27	CHL	5	315	X	-	-	-
27	CHL	5	316	X	-	-	-
27	CHL	5	317	X	-	-	-
27	CHL	5	318	X	-	-	-
27	CHL	5	319	X	-	-	-
27	CHL	5	320	X	-	-	-
27	CHL	5	321	X	-	-	-
27	CHL	5	322	X	-	-	-
27	CHL	5	323	X	-	-	-
27	CHL	5	325	X	-	-	-
27	CHL	6	305	X	-	-	-
27	CHL	6	306	X	-	-	-
27	CHL	6	307	X	-	-	-
27	CHL	6	308	X	-	-	-
27	CHL	6	309	X	-	-	-
27	CHL	6	310	X	-	-	-
27	CHL	6	311	X	-	-	-
27	CHL	6	312	X	-	-	-
27	CHL	6	313	X	-	-	-
27	CHL	6	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	6	315	X	-	-	-
27	CHL	6	316	X	-	-	-
27	CHL	6	317	X	-	-	-
27	CHL	6	318	X	-	-	-
27	CHL	6	319	X	-	-	-
27	CHL	6	320	X	-	-	-
27	CHL	7	311	X	-	-	-
27	CHL	7	312	X	-	-	-
27	CHL	7	313	X	-	-	-
27	CHL	7	314	X	-	-	-
27	CHL	7	315	X	-	-	-
27	CHL	7	316	X	-	-	-
27	CHL	7	317	X	-	-	-
27	CHL	7	318	X	-	-	-
27	CHL	7	319	X	-	-	-
27	CHL	7	320	X	-	-	-
27	CHL	7	321	X	-	-	-
27	CHL	7	322	X	-	-	-
27	CHL	7	323	X	-	-	-
27	CHL	7	324	X	-	-	-
27	CHL	8	311	X	-	-	-
27	CHL	8	312	X	-	-	-
27	CHL	8	313	X	-	-	-
27	CHL	8	314	X	-	-	-
27	CHL	8	315	X	-	-	-
27	CHL	8	316	X	-	-	-
27	CHL	8	317	X	-	-	-
27	CHL	8	318	X	-	-	-
27	CHL	8	319	X	-	-	-
27	CHL	8	320	X	-	-	-
27	CHL	8	321	X	-	-	-
27	CHL	8	322	X	-	-	-
27	CHL	8	323	X	-	-	-
27	CHL	8	324	X	-	-	-
27	CHL	8	325	X	-	-	-
27	CHL	8	326	X	-	-	-
27	CHL	A	816	X	-	-	-
27	CHL	A	817	X	-	-	-
27	CHL	A	818	X	-	-	-
27	CHL	A	819	X	-	-	-
27	CHL	A	820	X	-	-	-
27	CHL	A	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	A	822	X	-	-	-
27	CHL	A	823	X	-	-	-
27	CHL	A	824	X	-	-	-
27	CHL	A	825	X	-	-	-
27	CHL	A	826	X	-	-	-
27	CHL	A	827	X	-	-	-
27	CHL	A	828	X	-	-	-
27	CHL	A	829	X	-	-	-
27	CHL	A	830	X	-	-	-
27	CHL	A	831	X	-	-	-
27	CHL	A	832	X	-	-	-
27	CHL	A	833	X	-	-	-
27	CHL	A	834	X	-	-	-
27	CHL	A	835	X	-	-	-
27	CHL	A	836	X	-	-	-
27	CHL	A	837	X	-	-	-
27	CHL	A	838	X	-	-	-
27	CHL	A	839	X	-	-	-
27	CHL	A	840	X	-	-	-
27	CHL	A	841	X	-	-	-
27	CHL	A	842	X	-	-	-
27	CHL	A	843	X	-	-	-
27	CHL	A	844	X	-	-	-
27	CHL	A	845	X	-	-	-
27	CHL	A	846	X	-	-	-
27	CHL	A	847	X	-	-	-
27	CHL	A	848	X	-	-	-
27	CHL	A	849	X	-	-	-
27	CHL	A	850	X	-	-	-
27	CHL	A	851	X	-	-	-
27	CHL	A	852	X	-	-	-
27	CHL	A	853	X	-	-	-
27	CHL	A	854	X	-	-	-
27	CHL	A	855	X	-	-	-
27	CHL	A	856	X	-	-	-
27	CHL	A	857	X	-	-	-
27	CHL	A	858	X	-	-	-
27	CHL	A	859	X	-	-	-
27	CHL	B	811	X	-	-	-
27	CHL	B	812	X	-	-	-
27	CHL	B	813	X	-	-	-
27	CHL	B	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	B	815	X	-	-	-
27	CHL	B	816	X	-	-	-
27	CHL	B	817	X	-	-	-
27	CHL	B	818	X	-	-	-
27	CHL	B	819	X	-	-	-
27	CHL	B	820	X	-	-	-
27	CHL	B	821	X	-	-	-
27	CHL	B	822	X	-	-	-
27	CHL	B	823	X	-	-	-
27	CHL	B	824	X	-	-	-
27	CHL	B	825	X	-	-	-
27	CHL	B	826	X	-	-	-
27	CHL	B	827	X	-	-	-
27	CHL	B	828	X	-	-	-
27	CHL	B	829	X	-	-	-
27	CHL	B	830	X	-	-	-
27	CHL	B	831	X	-	-	-
27	CHL	B	832	X	-	-	-
27	CHL	B	833	X	-	-	-
27	CHL	B	834	X	-	-	-
27	CHL	B	835	X	-	-	-
27	CHL	B	836	X	-	-	-
27	CHL	B	837	X	-	-	-
27	CHL	B	838	X	-	-	-
27	CHL	B	839	X	-	-	-
27	CHL	B	840	X	-	-	-
27	CHL	B	841	X	-	-	-
27	CHL	B	842	X	-	-	-
27	CHL	B	843	X	-	-	-
27	CHL	B	844	X	-	-	-
27	CHL	B	845	X	-	-	-
27	CHL	B	846	X	-	-	-
27	CHL	B	847	X	-	-	-
27	CHL	B	848	X	-	-	-
27	CHL	B	849	X	-	-	-
27	CHL	B	850	X	-	-	-
27	CHL	B	851	X	-	-	-
27	CHL	F	308	X	-	-	-
27	CHL	F	309	X	-	-	-
27	CHL	J	106	X	-	-	-
27	CHL	K	204	X	-	-	-
27	CHL	K	205	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	K	206	X	-	-	-
27	CHL	K	207	X	-	-	-
27	CHL	L	303	X	-	-	-
27	CHL	L	304	X	-	-	-
27	CHL	a	307	X	-	-	-
27	CHL	a	308	X	-	-	-
27	CHL	a	309	X	-	-	-
27	CHL	a	310	X	-	-	-
27	CHL	a	311	X	-	-	-
27	CHL	a	312	X	-	-	-
27	CHL	a	313	X	-	-	-
27	CHL	a	314	X	-	-	-
27	CHL	a	315	X	-	-	-
27	CHL	a	316	X	-	-	-
27	CHL	a	317	X	-	-	-
27	CHL	a	318	X	-	-	-
27	CHL	a	319	X	-	-	-
27	CHL	a	320	X	-	-	-
27	CHL	b	304	X	-	-	-
27	CHL	b	305	X	-	-	-
27	CHL	b	306	X	-	-	-
27	CHL	b	307	X	-	-	-
27	CHL	b	308	X	-	-	-
27	CHL	b	309	X	-	-	-
27	CHL	b	310	X	-	-	-
27	CHL	b	311	X	-	-	-
27	CHL	b	312	X	-	-	-
27	CHL	b	313	X	-	-	-
27	CHL	b	314	X	-	-	-
27	CHL	b	315	X	-	-	-
27	CHL	b	316	X	-	-	-
27	CHL	b	317	X	-	-	-
29	LUT	4	301	-	X	-	-
29	LUT	4	302	-	X	-	-
29	LUT	5	303	-	X	-	-
29	LUT	6	303	-	X	-	-
29	LUT	F	303	-	X	-	-
29	LUT	J	103	-	X	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 46812 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	741	Total	C	N	O	S	0	0
			5823	3806	994	1005	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	3	0
			5832	3829	989	1001	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	20	Total	C	N	O	0	0
			159	107	23	29		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			336	232	48	55	1		

- Molecule 10 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	82	Total	C	N	O	S	0	0
			571	365	97	108	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	195	Total	C	N	O	S	0	0
			1458	944	245	267	2		
12	b	192	Total	C	N	O	S	0	0
			1441	933	242	264	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	220	Total	C	N	O	S	0	0
			1707	1117	275	312	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	207	Total	C	N	O	S	0	0
			1603	1045	264	290	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	231	Total	C	N	O	S	0	0
			1779	1160	306	309	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	234	Total	C	N	O	S	0	0
			1774	1159	296	311	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	7	216	Total	C	N	O	S	0	0
			1650	1070	280	298	2		

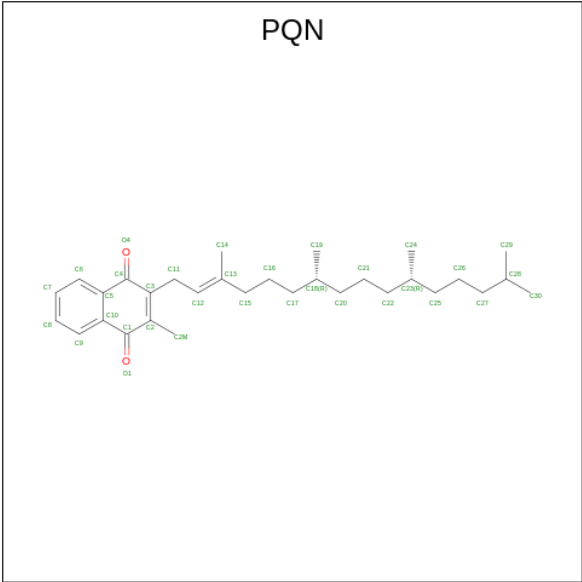
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	8	222	Total	C	N	O	S	0	0
			1701	1112	276	310	3		

- Molecule 19 is a protein called PSI subunit V.

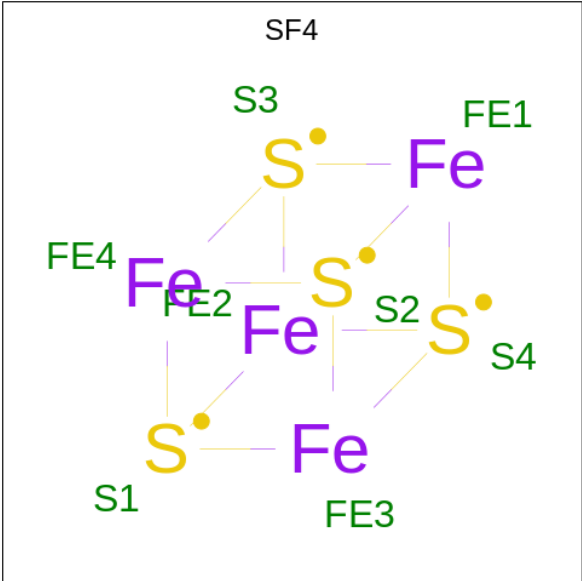
Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	122	Total	C	N	O	S	0	0
			890	585	148	155	2		

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



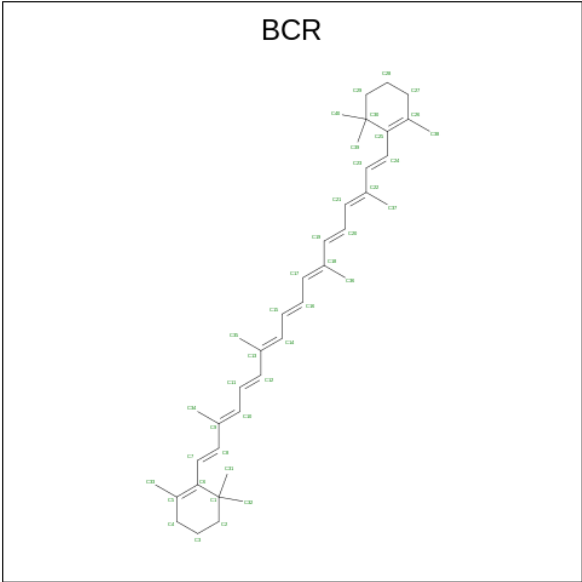
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

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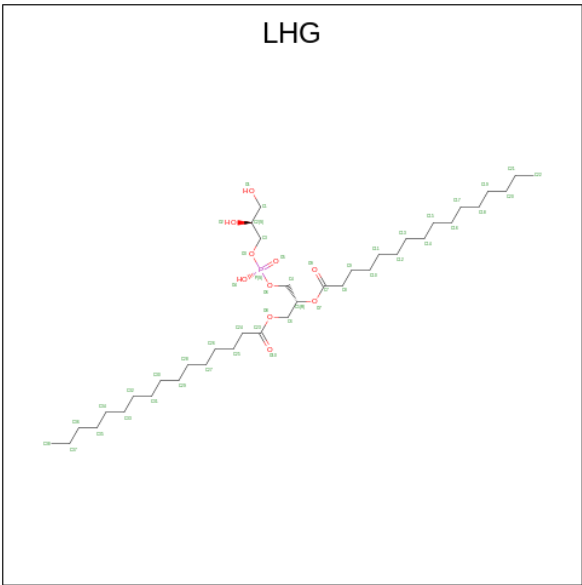
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	M	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	5	1	Total C 40 40	0
22	6	1	Total C 40 40	0
22	7	1	Total C 40 40	0
22	8	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total 35	C 24	O 11	0
23	A	1	Total 35	C 24	O 11	0
23	B	1	Total 35	C 24	O 11	0
23	F	1	Total 29	C 18	O 11	0
23	5	1	Total 30	C 19	O 11	0
23	5	1	Total 35	C 24	O 11	0
23	7	1	Total 35	C 24	O 11	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

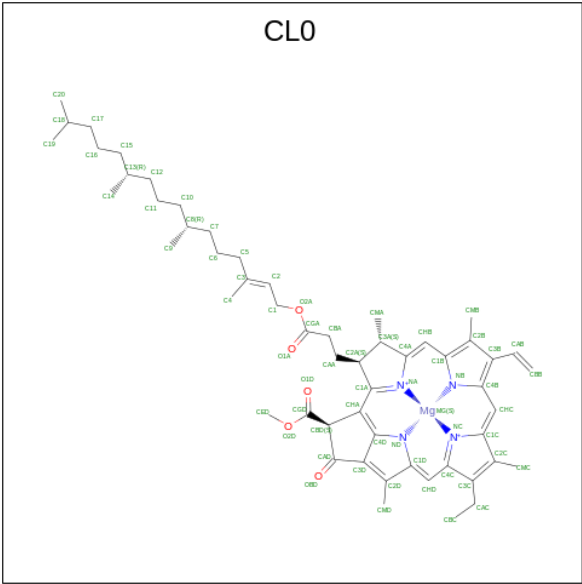


Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			42	31	10	1	
24	A	1	Total	C	O	P	0
			42	31	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	B	1	Total	C	O	P	0
			32	21	10	1	
24	a	1	Total	C	O	P	0
			49	38	10	1	
24	4	1	Total	C	O	P	0
			49	38	10	1	
24	5	1	Total	C	O	P	0
			35	24	10	1	
24	5	1	Total	C	O	P	0
			32	21	10	1	
24	7	1	Total	C	O	P	0
			49	38	10	1	
24	7	1	Total	C	O	P	0
			44	33	10	1	
24	8	1	Total	C	O	P	0
			49	38	10	1	
24	b	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 25 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

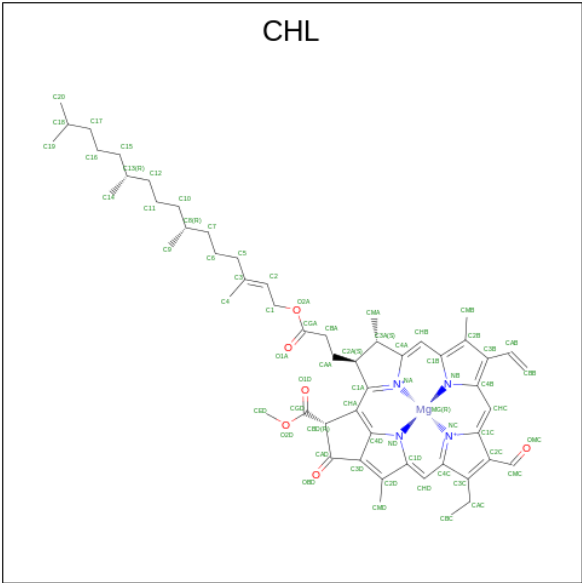
Mol	Chain	Residues	Atoms	AltConf
25	A	3	Total C 43 43	0
25	F	4	Total C 66 66	0
25	J	1	Total C 14 14	0
25	K	1	Total C 18 18	0
25	M	1	Total C 18 18	0
25	a	1	Total C 18 18	0
25	3	2	Total C 32 32	0
25	4	1	Total C 18 18	0
25	6	1	Total C 18 18	0
25	7	3	Total C 43 43	0
25	8	3	Total C 46 46	0

- Molecule 26 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	K	1	Total 47	C 36	Mg 1	N 4	O 6	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	a	1	Total 61	C 50	Mg 1	N 4	O 6	0
27	a	1	Total 48	C 37	Mg 1	N 4	O 6	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 37	Mg 1	N 4	O 6	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	3	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
27	3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
27	6	1	Total 47	C 36	Mg 1	N 4	O 6	0
27	6	1	Total 47	C 36	Mg 1	N 4	O 6	0
27	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
27	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	7	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	7	1	Total 65	C 55	Mg 1	N 4	O 5	0

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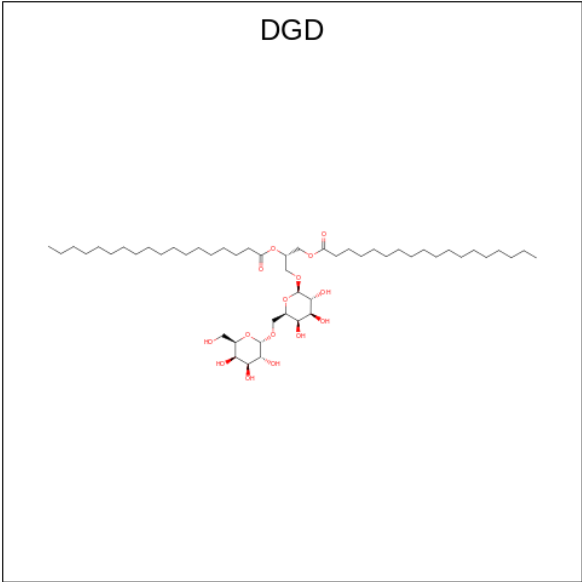
Mol	Chain	Residues	Atoms					AltConf
27	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	7	1	Total 47	C 36	Mg 1	N 4	O 6	0
27	7	1	Total 47	C 36	Mg 1	N 4	O 6	0
27	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
27	7	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	8	1	Total 45	C 35	Mg 1	N 4	O 5	0

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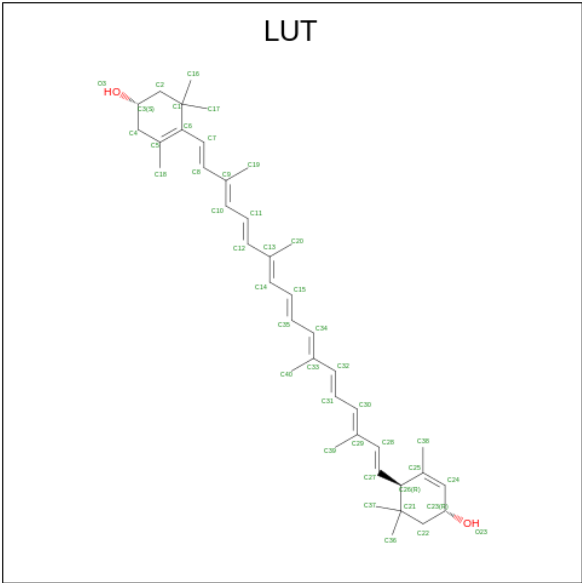
Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	b	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			61	46	15	
28	7	1	Total	C	O	0
			66	51	15	

- Molecule 29 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).



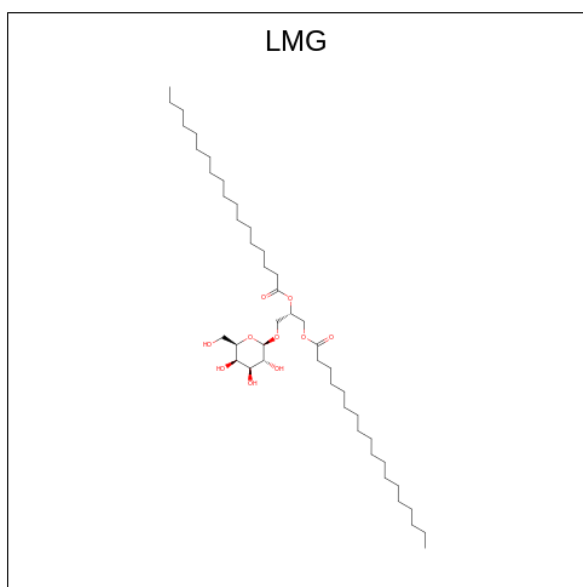
Mol	Chain	Residues	Atoms			AltConf
29	F	1	Total	C	O	0
			42	40	2	

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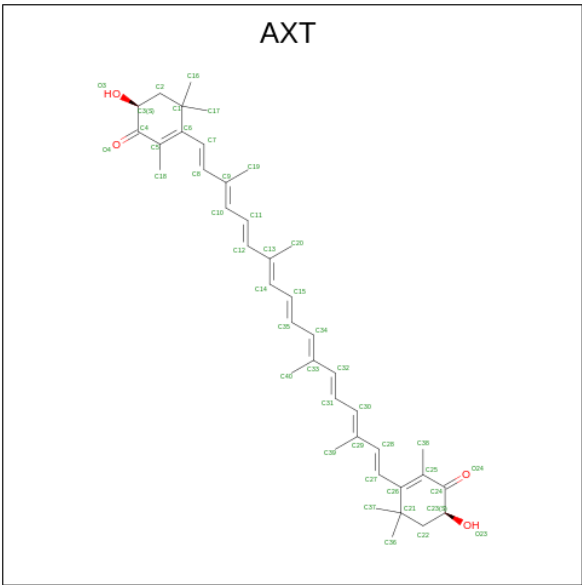
Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



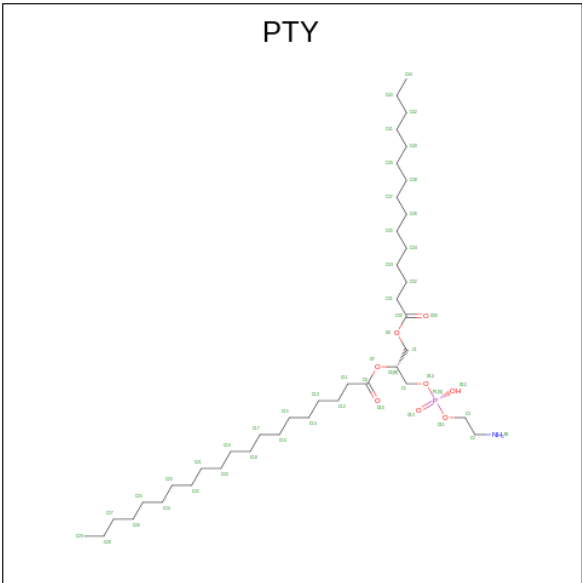
Mol	Chain	Residues	Atoms			AltConf
30	J	1	Total	C	O	0
			49	39	10	
30	J	1	Total	C	O	0
			29	19	10	
30	a	1	Total	C	O	0
			44	34	10	
30	7	1	Total	C	O	0
			41	31	10	
30	8	1	Total	C	O	0
			32	22	10	

- Molecule 31 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
31	a	1	Total	C	O	0
			43	40	3	

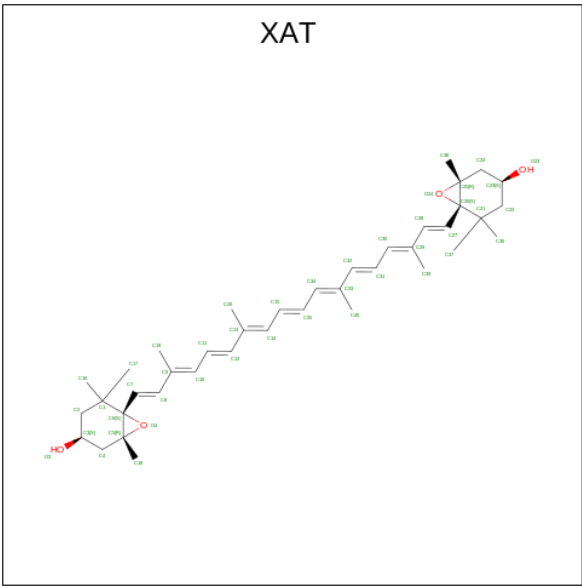
- Molecule 32 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

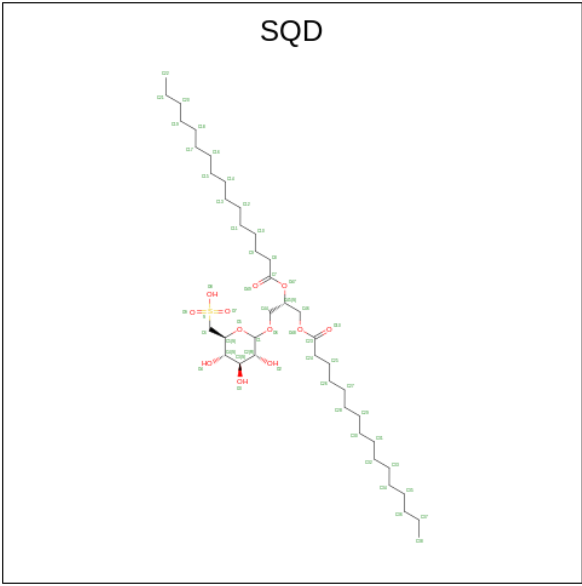
- Molecule 33 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as

"Ligand of Interest" by depositor).



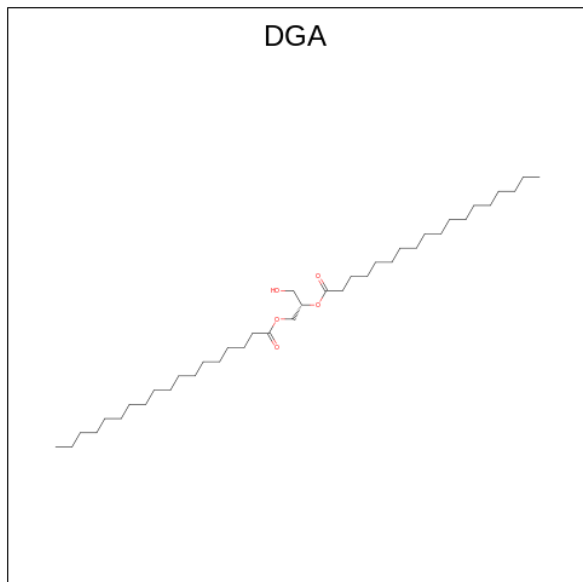
Mol	Chain	Residues	Atoms			AltConf
33	7	1	Total	C	O	0
			44	40	4	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
34	8	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 35 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
35	8	1	Total	C	O	0
			28	23	5	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	189	Total	O	0
			189	189	
36	B	174	Total	O	0
			174	174	
36	C	37	Total	O	0
			37	37	
36	D	26	Total	O	0
			26	26	
36	E	9	Total	O	0
			9	9	
36	F	30	Total	O	0
			30	30	
36	I	1	Total	O	0
			1	1	
36	J	5	Total	O	0
			5	5	
36	K	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
36	a	13	Total 13	O 13	0
36	3	25	Total 25	O 25	0
36	5	7	Total 7	O 7	0
36	6	2	Total 2	O 2	0
36	7	25	Total 25	O 25	0
36	8	24	Total 24	O 24	0
36	L	1	Total 1	O 1	0

3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:  98% ..



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  98% .



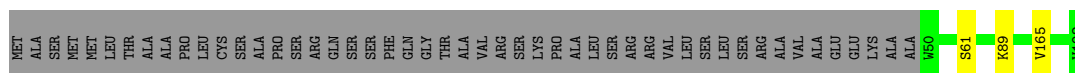
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  99% .




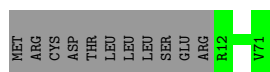
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:  73% . 26%



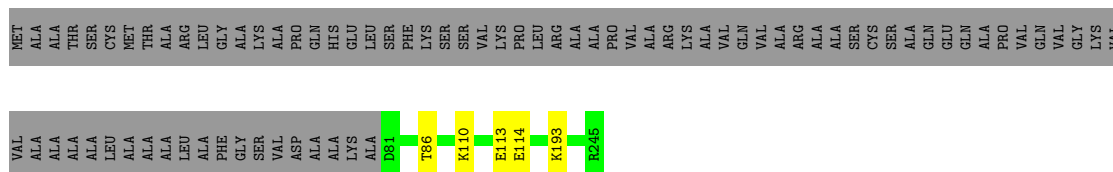
- Molecule 5: Photosystem I reaction centre subunit IV/PsaE

Chain E:  85% 15%



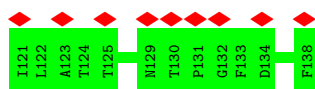
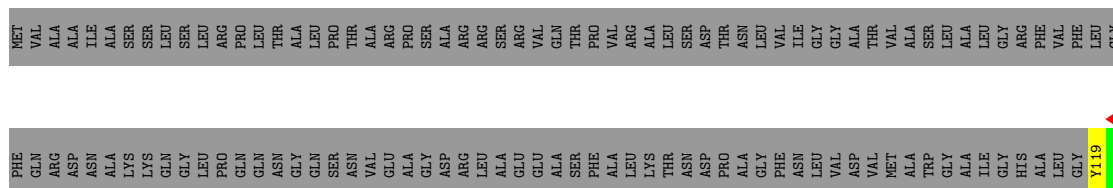
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  65% 33%




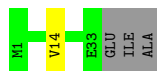
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:  7% 14% 86%



- Molecule 8: Photosystem I reaction center subunit VIII

Chain I:  89% 8%



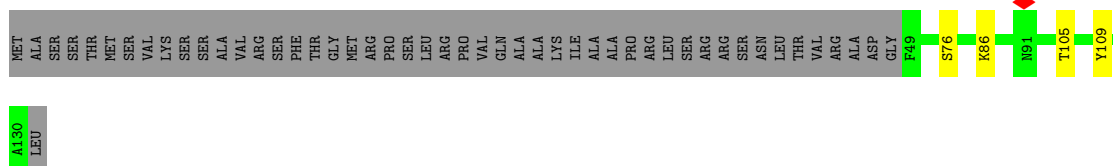
- Molecule 9: Photosystem I reaction center subunit IX

Chain J:  95% 5%



- Molecule 10: PSI-K

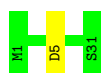
Chain K:  60% 37%



- Molecule 11: Photosystem I reaction center subunit XII

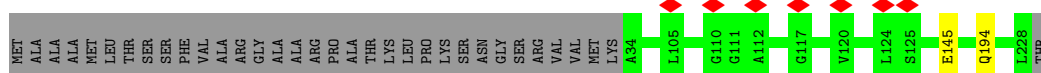
Chain M:  97%





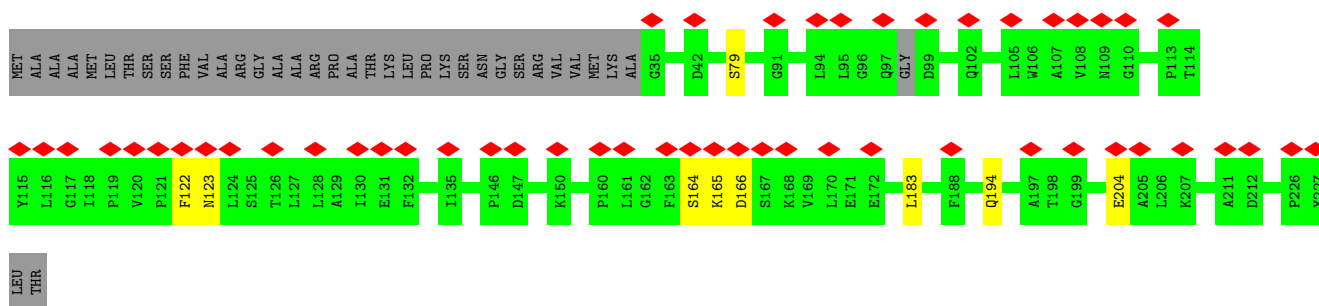
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain a: 84% 15%



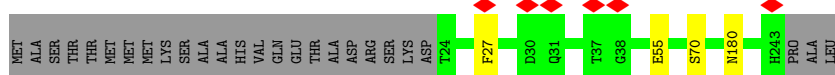
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain b: 23% 80% 16%



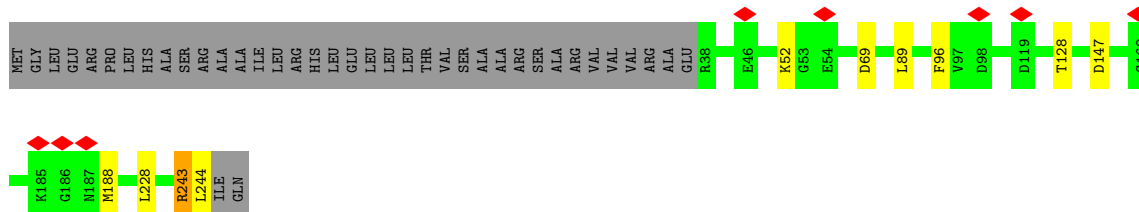
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 88% 11%



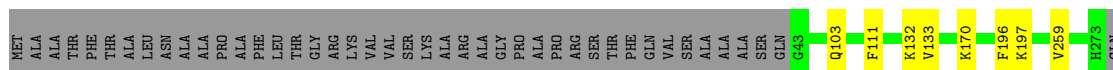
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 80% 16%




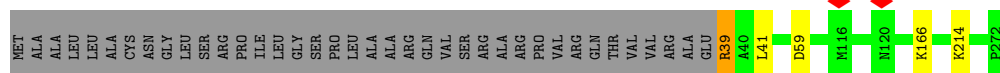
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 81% 16%




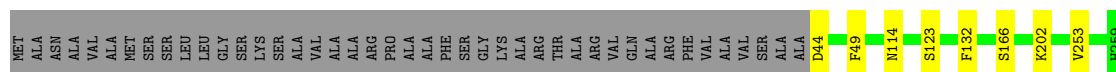
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 6:  84% 14%




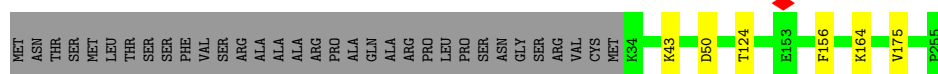
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  80% 17%



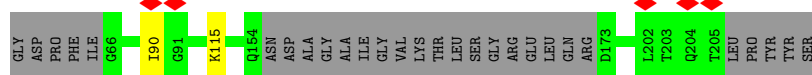
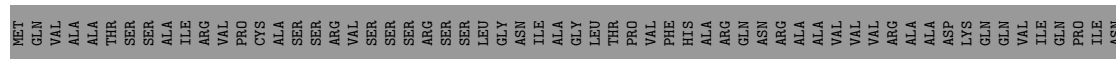
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  85% 13%



- Molecule 19: PSI subunit V

Chain L:  57% 42%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63984	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	0.519	Depositor
Minimum map value	-0.166	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: LHG, DGD, BCR, CL0, LMG, LUT, AXT, PQN, SQD, DGA, SF4, XAT, LMT, UNL, PTY, CHL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/6021	0.49	1/8213 (0.0%)
2	B	0.30	0/6041	0.48	0/8247
3	C	0.32	0/606	0.57	0/822
4	D	0.29	0/1136	0.53	0/1537
5	E	0.32	0/502	0.51	0/686
6	F	0.28	0/1288	0.50	0/1737
7	G	0.25	0/165	0.35	0/226
8	I	0.35	0/254	0.58	0/347
9	J	0.29	0/348	0.45	0/476
10	K	0.27	0/580	0.47	0/789
11	M	0.30	0/240	0.54	0/325
12	a	0.28	0/1501	0.47	0/2045
12	b	0.30	0/1483	0.51	1/2019 (0.0%)
13	3	0.31	0/1759	0.47	0/2394
14	4	0.30	0/1653	0.50	1/2250 (0.0%)
15	5	0.29	0/1834	0.49	0/2496
16	6	0.29	0/1832	0.48	1/2501 (0.0%)
17	7	0.29	0/1702	0.45	0/2323
18	8	0.30	0/1752	0.45	0/2379
19	L	0.27	0/912	0.45	0/1247
All	All	0.30	0/31609	0.48	4/43059 (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
14	4	0	1
16	6	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	147	ASP	CB-CG-OD1	6.54	124.19	118.30
16	6	59	ASP	CB-CG-OD1	6.31	123.97	118.30
1	A	157	LEU	CA-CB-CG	5.87	128.79	115.30
12	b	183	LEU	CA-CB-CG	5.33	127.57	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	4	243	ARG	Sidechain
16	6	39	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	720 (97%)	19 (3%)	0	100	100
2	B	732/734 (100%)	719 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/192 (73%)	138 (98%)	3 (2%)	0	100	100
5	E	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
6	F	163/245 (66%)	161 (99%)	2 (1%)	0	100	100
7	G	18/138 (13%)	17 (94%)	1 (6%)	0	100	100
8	I	31/36 (86%)	31 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
10	K	80/131 (61%)	80 (100%)	0	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
12	a	193/229 (84%)	188 (97%)	5 (3%)	0	100	100
12	b	188/229 (82%)	177 (94%)	9 (5%)	2 (1%)	12	4
13	3	218/246 (89%)	214 (98%)	4 (2%)	0	100	100
14	4	205/246 (83%)	198 (97%)	7 (3%)	0	100	100
15	5	229/274 (84%)	219 (96%)	10 (4%)	0	100	100
16	6	232/272 (85%)	227 (98%)	5 (2%)	0	100	100
17	7	214/259 (83%)	209 (98%)	5 (2%)	0	100	100
18	8	220/255 (86%)	217 (99%)	3 (1%)	0	100	100
19	L	118/210 (56%)	116 (98%)	2 (2%)	0	100	100
All	All	3925/4671 (84%)	3831 (98%)	92 (2%)	2 (0%)	50	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	b	165	LYS
12	b	164	SER

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	604/613 (98%)	597 (99%)	7 (1%)	67	68
2	B	594/593 (100%)	578 (97%)	16 (3%)	40	35
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	118/156 (76%)	115 (98%)	3 (2%)	42	38
5	E	56/67 (84%)	56 (100%)	0	100	100
6	F	131/183 (72%)	126 (96%)	5 (4%)	28	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	18/106 (17%)	17 (94%)	1 (6%)	17	10
8	I	26/28 (93%)	25 (96%)	1 (4%)	28	22
9	J	37/37 (100%)	35 (95%)	2 (5%)	18	11
10	K	60/100 (60%)	56 (93%)	4 (7%)	13	7
11	M	26/26 (100%)	25 (96%)	1 (4%)	28	22
12	a	141/166 (85%)	139 (99%)	2 (1%)	62	62
12	b	140/166 (84%)	134 (96%)	6 (4%)	25	18
13	3	176/197 (89%)	172 (98%)	4 (2%)	45	41
14	4	164/195 (84%)	155 (94%)	9 (6%)	18	11
15	5	179/208 (86%)	171 (96%)	8 (4%)	23	17
16	6	183/212 (86%)	179 (98%)	4 (2%)	47	43
17	7	168/195 (86%)	160 (95%)	8 (5%)	21	15
18	8	175/202 (87%)	169 (97%)	6 (3%)	32	26
19	L	91/161 (56%)	89 (98%)	2 (2%)	47	43
All	All	3155/3680 (86%)	3066 (97%)	89 (3%)	40	34

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	5	132	LYS
17	7	132	PHE
15	5	170	LYS
16	6	166	LYS
18	8	43	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
15	5	260	GLN
12	b	72	GLN
17	7	114	ASN
12	b	194	GLN
19	L	176	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 318 ligands modelled in this entry, 21 are unknown - leaving 297 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	$\# Z > 2$
27	CHL	5	315	15	65,73,74	2.59	19 (29%)	76,113,114	4.35	24 (31%)
29	LUT	3	304	-	42,43,43	5.53	19 (45%)	51,60,60	5.58	32 (62%)
27	CHL	4	309	-	47,55,74	2.54	15 (31%)	50,91,114	2.09	17 (34%)
27	CHL	6	310	16	55,63,74	2.85	21 (38%)	64,101,114	2.34	23 (35%)
27	CHL	7	316	36	54,62,74	2.62	18 (33%)	63,100,114	2.30	23 (36%)
27	CHL	A	851	1	46,54,74	2.78	19 (41%)	53,90,114	2.55	20 (37%)
29	LUT	7	304	-	42,43,43	5.54	21 (50%)	51,60,60	5.78	29 (56%)
29	LUT	4	302	-	42,43,43	5.62	19 (45%)	51,60,60	5.60	31 (60%)
27	CHL	B	822	2	65,73,74	2.59	18 (27%)	76,113,114	2.14	21 (27%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
22	BCR	3	301	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
27	CHL	8	321	36	66,74,74	2.11	15 (22%)	73,114,114	2.03	21 (28%)
27	CHL	a	318	36	48,56,74	2.69	17 (35%)	51,92,114	2.24	19 (37%)
22	BCR	K	203	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	A	841	36	56,64,74	2.07	15 (26%)	61,102,114	2.42	23 (37%)
21	SF4	A	802	1,2	0,12,12	-	-	-		
27	CHL	a	307	12	60,68,74	2.76	19 (31%)	70,107,114	2.21	23 (32%)
27	CHL	6	318	-	47,55,74	2.77	14 (29%)	50,91,114	2.21	17 (34%)
27	CHL	A	834	1	65,73,74	2.35	19 (29%)	76,113,114	2.07	23 (30%)
27	CHL	B	836	2	65,73,74	2.56	18 (27%)	76,113,114	2.04	20 (26%)
27	CHL	B	850	2	50,58,74	3.05	20 (40%)	58,95,114	2.54	25 (43%)
22	BCR	A	807	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
27	CHL	5	318	15	65,73,74	2.65	18 (27%)	76,113,114	2.17	24 (31%)
27	CHL	A	838	1	60,68,74	2.74	18 (30%)	70,107,114	2.22	23 (32%)
27	CHL	5	320	15	46,54,74	2.86	20 (43%)	53,90,114	2.44	21 (39%)
27	CHL	A	846	-	50,58,74	2.22	12 (24%)	58,95,114	4.33	29 (50%)
29	LUT	8	304	-	42,43,43	5.52	19 (45%)	51,60,60	5.83	33 (64%)
27	CHL	4	307	14	60,68,74	2.50	19 (31%)	70,107,114	2.24	23 (32%)
27	CHL	A	825	1	65,73,74	2.73	19 (29%)	76,113,114	2.21	24 (31%)
27	CHL	A	823	1	65,73,74	2.27	17 (26%)	76,113,114	2.21	24 (31%)
27	CHL	A	837	1	55,63,74	2.73	19 (34%)	64,101,114	2.41	22 (34%)
24	LHG	b	302	27	34,34,48	0.74	1 (2%)	37,40,54	1.28	4 (10%)
27	CHL	A	839	1	65,73,74	2.46	18 (27%)	76,113,114	2.15	23 (30%)
23	LMT	7	308	-	36,36,36	1.19	6 (16%)	47,47,47	0.89	0
27	CHL	B	831	2	46,54,74	2.79	19 (41%)	53,90,114	2.43	22 (41%)
22	BCR	I	801	-	41,41,41	1.11	2 (4%)	56,56,56	1.15	4 (7%)
27	CHL	A	816	36	65,73,74	2.38	18 (27%)	76,113,114	2.21	22 (28%)
23	LMT	5	326	-	36,36,36	1.23	6 (16%)	47,47,47	0.94	2 (4%)
27	CHL	B	851	2	62,70,74	2.64	20 (32%)	72,109,114	2.17	24 (33%)
27	CHL	3	315	13	52,60,74	2.54	18 (34%)	60,97,114	2.39	22 (36%)
20	PQN	B	801	-	34,34,34	0.47	0	42,45,45	0.73	1 (2%)
27	CHL	8	323	-	50,58,74	3.27	21 (42%)	58,95,114	2.79	23 (39%)
27	CHL	B	819	2	65,73,74	2.53	19 (29%)	76,113,114	2.21	22 (28%)
22	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	5 (8%)
27	CHL	3	320	13	61,69,74	2.28	18 (29%)	71,108,114	2.25	26 (36%)
22	BCR	3	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	5 (8%)
27	CHL	B	846	36	65,73,74	2.30	18 (27%)	76,113,114	2.17	23 (30%)
32	PTY	5	305	-	30,30,49	0.56	0	33,35,54	0.55	1 (3%)
27	CHL	B	834	2	65,73,74	3.02	18 (27%)	76,113,114	2.27	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	4	316	-	46,54,74	2.85	15 (32%)	49,90,114	2.16	18 (36%)
27	CHL	B	820	2	65,73,74	2.61	19 (29%)	76,113,114	2.14	23 (30%)
27	CHL	8	326	18	46,54,74	3.06	17 (36%)	53,90,114	2.60	22 (41%)
27	CHL	A	843	1	65,73,74	1.95	12 (18%)	76,113,114	4.66	36 (47%)
27	CHL	A	828	1	65,73,74	2.52	19 (29%)	76,113,114	2.14	22 (28%)
27	CHL	A	819	1	55,63,74	2.68	19 (34%)	64,101,114	2.35	20 (31%)
27	CHL	4	317	14	45,53,74	2.77	18 (40%)	52,89,114	3.00	18 (34%)
22	BCR	L	302	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	4 (7%)
24	LHG	a	305	27	48,48,48	0.28	0	51,54,54	0.30	0
24	LHG	4	303	27	48,48,48	0.27	0	51,54,54	0.37	0
27	CHL	B	848	2	65,73,74	2.69	19 (29%)	76,113,114	2.16	21 (27%)
27	CHL	8	320	18	52,60,74	2.86	19 (36%)	60,97,114	2.43	23 (38%)
24	LHG	A	811	27	41,41,48	0.69	2 (4%)	44,47,54	1.18	4 (9%)
27	CHL	B	847	36	65,73,74	2.90	19 (29%)	76,113,114	2.19	23 (30%)
27	CHL	b	307	12	55,63,74	2.57	18 (32%)	64,101,114	2.25	24 (37%)
24	LHG	7	306	27	43,43,48	0.70	1 (2%)	46,49,54	1.22	4 (8%)
30	LMG	J	104	-	29,29,55	0.99	1 (3%)	37,37,63	1.21	3 (8%)
27	CHL	B	813	2	55,63,74	2.76	20 (36%)	64,101,114	2.43	21 (32%)
35	DGA	8	306	-	27,27,43	0.22	0	29,29,45	0.17	0
27	CHL	3	308	13	65,73,74	2.88	18 (27%)	76,113,114	2.26	25 (32%)
27	CHL	L	304	-	45,53,74	2.88	19 (42%)	52,89,114	2.47	19 (36%)
27	CHL	b	306	12	46,54,74	4.26	18 (39%)	53,90,114	2.38	22 (41%)
27	CHL	5	313	-	57,65,74	2.10	12 (21%)	66,103,114	4.36	34 (51%)
27	CHL	5	325	16	47,55,74	2.21	16 (34%)	50,91,114	2.21	20 (40%)
27	CHL	a	312	36	50,58,74	3.31	18 (36%)	58,95,114	2.43	22 (37%)
27	CHL	7	320	36,28	47,55,74	2.10	14 (29%)	50,91,114	2.41	19 (38%)
27	CHL	5	323	15	56,64,74	3.20	17 (30%)	65,102,114	2.43	23 (35%)
27	CHL	B	817	2	65,73,74	2.39	18 (27%)	76,113,114	2.29	22 (28%)
27	CHL	A	835	1	47,55,74	3.12	19 (40%)	54,91,114	2.51	21 (38%)
27	CHL	B	842	2	65,73,74	2.78	18 (27%)	76,113,114	2.24	23 (30%)
27	CHL	4	314	-	45,53,74	2.96	20 (44%)	52,89,114	2.47	21 (40%)
27	CHL	B	840	2	65,73,74	2.63	17 (26%)	76,113,114	2.18	23 (30%)
27	CHL	B	833	36	55,63,74	2.62	19 (34%)	64,101,114	2.26	22 (34%)
23	LMT	A	808	-	36,36,36	1.24	6 (16%)	47,47,47	1.05	2 (4%)
30	LMG	J	101	-	49,49,55	0.81	1 (2%)	57,57,63	1.26	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	A	858	1	65,73,74	2.60	19 (29%)	76,113,114	2.23	25 (32%)
27	CHL	b	313	12	46,54,74	3.66	19 (41%)	53,90,114	2.48	20 (37%)
27	CHL	B	843	36	45,53,74	3.13	17 (37%)	52,89,114	2.52	18 (34%)
27	CHL	b	314	12	46,54,74	3.00	19 (41%)	53,90,114	2.40	21 (39%)
27	CHL	A	856	36	65,73,74	2.35	18 (27%)	76,113,114	2.22	25 (32%)
27	CHL	7	321	17	47,55,74	2.53	15 (31%)	50,91,114	2.53	18 (36%)
27	CHL	A	855	1	65,73,74	2.48	19 (29%)	76,113,114	2.18	24 (31%)
27	CHL	3	321	13	45,53,74	3.25	19 (42%)	52,89,114	2.50	18 (34%)
27	CHL	5	311	15	46,54,74	3.04	19 (41%)	53,90,114	2.59	24 (45%)
27	CHL	b	305	-	46,54,74	3.39	19 (41%)	53,90,114	2.52	20 (37%)
23	LMT	5	306	-	31,31,36	1.28	5 (16%)	42,42,47	0.96	3 (7%)
27	CHL	7	319	17	66,74,74	1.77	15 (22%)	73,114,114	2.08	23 (31%)
27	CHL	B	811	2	65,73,74	2.50	18 (27%)	76,113,114	2.26	23 (30%)
27	CHL	6	305	16	46,54,74	2.74	19 (41%)	53,90,114	2.40	19 (35%)
27	CHL	8	324	36	45,53,74	2.40	16 (35%)	46,88,114	2.36	19 (41%)
27	CHL	b	316	-	48,56,74	2.60	16 (33%)	51,92,114	2.17	19 (37%)
27	CHL	7	317	24	65,73,74	2.44	19 (29%)	76,113,114	2.18	23 (30%)
27	CHL	8	313	18	50,58,74	3.08	19 (38%)	58,95,114	2.46	22 (37%)
27	CHL	A	857	24	46,54,74	2.89	17 (36%)	53,90,114	2.56	22 (41%)
27	CHL	A	852	1	51,59,74	3.23	17 (33%)	59,96,114	2.64	25 (42%)
27	CHL	4	320	14	50,58,74	2.89	20 (40%)	58,95,114	2.43	25 (43%)
27	CHL	A	832	1	60,68,74	2.83	19 (31%)	70,107,114	2.38	24 (34%)
22	BCR	B	805	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	4 (7%)
27	CHL	A	826	1	62,70,74	2.81	18 (29%)	72,109,114	2.21	22 (30%)
27	CHL	a	313	24	55,63,74	2.57	19 (34%)	64,101,114	2.33	24 (37%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
27	CHL	B	814	2	65,73,74	2.46	19 (29%)	76,113,114	2.18	23 (30%)
22	BCR	B	802	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	7 (12%)
27	CHL	6	313	16	47,55,74	3.65	19 (40%)	54,91,114	2.50	21 (38%)
27	CHL	b	312	-	46,54,74	3.10	18 (39%)	53,90,114	2.43	22 (41%)
27	CHL	3	313	36	65,73,74	2.50	19 (29%)	76,113,114	2.13	23 (30%)
27	CHL	5	321	15	46,54,74	3.09	18 (39%)	53,90,114	2.47	21 (39%)
27	CHL	5	314	15	45,53,74	3.29	18 (40%)	52,89,114	2.43	18 (34%)
27	CHL	3	309	13	46,54,74	3.22	19 (41%)	53,90,114	2.52	19 (35%)
22	BCR	B	804	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	7	303	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	5 (8%)
27	CHL	A	859	36	65,73,74	2.72	17 (26%)	76,113,114	2.20	25 (32%)
27	CHL	B	832	36	65,73,74	2.36	18 (27%)	76,113,114	2.23	26 (34%)
27	CHL	a	316	36	48,56,74	2.47	15 (31%)	51,92,114	2.20	20 (39%)
27	CHL	5	319	-	47,55,74	2.83	16 (34%)	50,91,114	2.16	19 (38%)
27	CHL	8	314	18	66,74,74	1.91	14 (21%)	73,114,114	1.97	24 (32%)
33	XAT	7	305	-	39,47,47	1.64	8 (20%)	54,74,74	1.61	10 (18%)
27	CHL	4	319	14	45,53,74	3.07	19 (42%)	52,89,114	2.60	17 (32%)
27	CHL	6	316	36	46,54,74	2.91	16 (34%)	49,90,114	2.31	18 (36%)
27	CHL	B	844	2	65,73,74	2.40	18 (27%)	76,113,114	2.12	23 (30%)
29	LUT	6	303	-	42,43,43	5.58	20 (47%)	51,60,60	5.63	32 (62%)
28	DGD	7	307	27	67,67,67	0.91	2 (2%)	81,81,81	1.38	10 (12%)
29	LUT	3	305	-	42,43,43	5.47	19 (45%)	51,60,60	5.84	33 (64%)
27	CHL	A	847	1	56,64,74	2.85	18 (32%)	65,102,114	2.30	23 (35%)
23	LMT	A	809	-	36,36,36	1.21	5 (13%)	47,47,47	0.93	1 (2%)
27	CHL	4	308	14	60,68,74	2.80	19 (31%)	70,107,114	2.23	23 (32%)
27	CHL	6	307	-	65,73,74	1.99	14 (21%)	76,113,114	4.03	33 (43%)
31	AXT	a	303	-	44,44,45	0.70	1 (2%)	55,62,64	0.99	1 (1%)
27	CHL	8	316	18	65,73,74	2.53	19 (29%)	76,113,114	2.13	24 (31%)
27	CHL	B	849	24	65,73,74	2.42	19 (29%)	76,113,114	2.10	21 (27%)
22	BCR	5	301	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	4 (7%)
27	CHL	3	319	13	55,63,74	2.98	18 (32%)	64,101,114	2.30	21 (32%)
27	CHL	6	314	24	46,54,74	3.24	19 (41%)	53,90,114	2.50	19 (35%)
27	CHL	3	311	13	60,68,74	2.50	17 (28%)	70,107,114	2.28	23 (32%)
27	CHL	F	309	36	50,58,74	2.78	19 (38%)	58,95,114	2.45	22 (37%)
27	CHL	7	314	17	62,70,74	3.03	18 (29%)	72,109,114	2.21	23 (31%)
27	CHL	4	315	14	47,55,74	2.79	19 (40%)	54,91,114	2.48	21 (38%)
27	CHL	A	827	1	54,62,74	2.77	19 (35%)	62,99,114	2.35	22 (35%)
27	CHL	K	204	36	50,58,74	3.77	20 (40%)	58,95,114	2.45	22 (37%)
27	CHL	8	311	18	46,54,74	2.93	19 (41%)	53,90,114	2.48	19 (35%)
27	CHL	8	322	36	50,58,74	2.63	16 (32%)	58,95,114	2.53	21 (36%)
29	LUT	b	303	-	42,43,43	1.65	8 (19%)	51,60,60	1.74	10 (19%)
22	BCR	K	202	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	6 (10%)
27	CHL	B	845	2	50,58,74	2.67	18 (36%)	58,95,114	2.55	24 (41%)
30	LMG	8	307	-	32,32,55	0.27	0	40,40,63	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMT	F	302	-	30,30,36	1.33	6 (20%)	41,41,47	1.01	3 (7%)
27	CHL	A	836	36	65,73,74	2.73	19 (29%)	76,113,114	2.14	23 (30%)
27	CHL	A	844	1	65,73,74	2.60	20 (30%)	76,113,114	2.12	21 (27%)
27	CHL	A	842	1	66,74,74	2.10	15 (22%)	73,114,114	1.89	21 (28%)
27	CHL	b	310	12	46,54,74	3.59	20 (43%)	53,90,114	2.48	22 (41%)
27	CHL	B	841	2	55,63,74	2.51	17 (30%)	64,101,114	2.35	21 (32%)
27	CHL	7	322	36	61,69,74	2.10	17 (27%)	67,108,114	2.10	23 (34%)
22	BCR	B	806	-	41,41,41	1.10	2 (4%)	56,56,56	1.36	5 (8%)
27	CHL	8	312	18	65,73,74	2.82	18 (27%)	76,113,114	2.11	23 (30%)
27	CHL	B	827	2	60,68,74	2.36	17 (28%)	70,107,114	2.22	24 (34%)
27	CHL	4	305	14	45,53,74	3.14	18 (40%)	52,89,114	2.42	21 (40%)
27	CHL	4	304	14	55,63,74	2.83	18 (32%)	64,101,114	2.32	24 (37%)
27	CHL	7	312	17	44,52,74	3.08	18 (40%)	51,88,114	2.52	21 (41%)
22	BCR	B	807	-	41,41,41	1.11	2 (4%)	56,56,56	1.09	3 (5%)
27	CHL	B	821	2	58,66,74	2.54	19 (32%)	67,104,114	2.31	23 (34%)
27	CHL	B	829	2	55,63,74	2.61	19 (34%)	64,101,114	2.36	23 (35%)
27	CHL	3	310	13	65,73,74	2.37	19 (29%)	76,113,114	2.12	22 (28%)
27	CHL	7	311	17	60,68,74	2.43	19 (31%)	70,107,114	2.24	26 (37%)
27	CHL	a	319	36	50,58,74	2.83	19 (38%)	58,95,114	2.46	24 (41%)
27	CHL	b	309	24	46,54,74	3.72	19 (41%)	53,90,114	2.50	21 (39%)
27	CHL	8	315	18	65,73,74	2.30	19 (29%)	76,113,114	2.20	21 (27%)
27	CHL	6	309	16	47,55,74	3.14	19 (40%)	54,91,114	2.38	20 (37%)
29	LUT	6	302	-	42,43,43	5.56	19 (45%)	51,60,60	5.91	31 (60%)
27	CHL	B	839	2	60,68,74	2.59	19 (31%)	70,107,114	2.22	24 (34%)
22	BCR	8	302	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	8 (14%)
27	CHL	B	816	2	61,69,74	2.62	18 (29%)	71,108,114	2.26	25 (35%)
27	CHL	5	316	36	66,74,74	1.78	13 (19%)	73,114,114	2.57	22 (30%)
27	CHL	6	308	16	66,74,74	1.85	15 (22%)	73,114,114	2.50	22 (30%)
27	CHL	b	311	12	47,55,74	2.67	16 (34%)	50,91,114	2.20	21 (42%)
28	DGD	B	809	-	62,62,67	0.98	2 (3%)	76,76,81	1.35	10 (13%)
29	LUT	8	303	-	42,43,43	5.48	19 (45%)	51,60,60	5.73	33 (64%)
27	CHL	J	106	9	42,50,74	3.34	18 (42%)	48,85,114	2.54	18 (37%)
27	CHL	6	315	16	50,58,74	3.42	20 (40%)	58,95,114	2.46	23 (39%)
27	CHL	A	853	1	65,73,74	2.53	19 (29%)	76,113,114	2.18	23 (30%)
27	CHL	4	313	-	45,53,74	3.32	17 (37%)	52,89,114	3.09	20 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	7	315	17	43,52,74	3.04	20 (46%)	49,88,114	2.40	19 (38%)
27	CHL	8	325	18	65,73,74	2.41	18 (27%)	76,113,114	2.10	21 (27%)
27	CHL	b	308	-	46,54,74	5.19	22 (47%)	53,90,114	5.00	23 (43%)
27	CHL	A	849	1	65,73,74	2.58	19 (29%)	76,113,114	2.19	21 (27%)
27	CHL	B	838	2	65,73,74	2.61	18 (27%)	76,113,114	2.15	23 (30%)
27	CHL	3	316	36	66,74,74	1.87	13 (19%)	73,114,114	2.09	24 (32%)
29	LUT	a	302	-	42,43,43	5.58	19 (45%)	51,60,60	5.75	34 (66%)
24	LHG	A	812	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	6 (11%)
27	CHL	K	206	10	46,54,74	3.16	19 (41%)	53,90,114	2.48	21 (39%)
27	CHL	5	308	15	46,54,74	3.03	18 (39%)	53,90,114	2.52	19 (35%)
27	CHL	B	828	36	60,68,74	2.38	18 (30%)	70,107,114	2.21	24 (34%)
27	CHL	7	323	-	52,60,74	2.95	17 (32%)	60,97,114	2.74	23 (38%)
27	CHL	8	319	36	55,63,74	2.71	19 (34%)	64,101,114	2.36	23 (35%)
27	CHL	b	315	12	65,73,74	2.94	20 (30%)	76,113,114	2.16	22 (28%)
34	SQD	8	301	-	34,35,54	1.79	7 (20%)	43,46,65	1.51	6 (13%)
22	BCR	A	805	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	5 (8%)
24	LHG	5	324	27	31,31,48	0.79	1 (3%)	34,37,54	1.27	4 (11%)
29	LUT	a	304	-	42,43,43	5.54	19 (45%)	51,60,60	6.07	32 (62%)
27	CHL	a	309	36	60,68,74	3.25	19 (31%)	70,107,114	2.31	24 (34%)
27	CHL	4	312	14	48,56,74	2.16	16 (33%)	51,92,114	2.21	20 (39%)
27	CHL	B	824	2	57,65,74	2.69	18 (31%)	66,103,114	2.33	24 (36%)
22	BCR	A	803	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	3 (5%)
27	CHL	4	311	14	47,55,74	3.73	19 (40%)	54,91,114	2.47	21 (38%)
29	LUT	F	303	-	42,43,43	5.51	19 (45%)	51,60,60	5.90	33 (64%)
27	CHL	8	318	24	46,54,74	3.48	18 (39%)	53,90,114	2.44	18 (33%)
27	CHL	a	317	12	65,73,74	2.36	19 (29%)	76,113,114	2.14	22 (28%)
27	CHL	6	306	16	57,65,74	4.24	19 (33%)	66,103,114	2.31	25 (37%)
27	CHL	A	829	1	55,63,74	2.62	18 (32%)	64,101,114	2.39	20 (31%)
27	CHL	L	303	-	60,68,74	2.03	14 (23%)	70,107,114	4.14	30 (42%)
27	CHL	a	314	12	45,53,74	2.96	19 (42%)	52,89,114	2.46	21 (40%)
27	CHL	5	309	15	60,68,74	2.49	19 (31%)	70,107,114	2.23	23 (32%)
27	CHL	6	317	-	47,55,74	2.98	16 (34%)	50,91,114	2.36	20 (40%)
29	LUT	5	303	-	42,43,43	5.51	20 (47%)	51,60,60	5.89	32 (62%)
27	CHL	B	830	2	60,68,74	2.64	20 (33%)	70,107,114	2.27	23 (32%)
27	CHL	K	207	10	47,55,74	3.21	16 (34%)	50,91,114	2.11	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	6	319	16	43,51,74	2.42	16 (37%)	45,86,114	2.89	17 (37%)
27	CHL	8	317	36	65,73,74	2.37	19 (29%)	76,113,114	2.14	22 (28%)
22	BCR	B	803	-	41,41,41	1.15	2 (4%)	56,56,56	1.13	4 (7%)
27	CHL	A	817	-	65,73,74	2.58	17 (26%)	76,113,114	2.19	22 (28%)
27	CHL	7	313	17	65,73,74	2.61	19 (29%)	76,113,114	2.15	22 (28%)
27	CHL	a	315	12	61,69,74	2.36	16 (26%)	67,108,114	2.09	25 (37%)
27	CHL	A	840	36	65,73,74	2.69	19 (29%)	76,113,114	2.25	22 (28%)
27	CHL	5	310	15	65,73,74	3.39	20 (30%)	76,113,114	2.26	22 (28%)
27	CHL	A	833	1	61,69,74	2.05	15 (24%)	67,108,114	2.22	24 (35%)
27	CHL	7	318	17	55,63,74	2.78	19 (34%)	64,101,114	2.42	23 (35%)
29	LUT	J	103	-	42,43,43	5.59	20 (47%)	51,60,60	5.87	31 (60%)
27	CHL	4	310	24	46,54,74	3.83	20 (43%)	53,90,114	2.50	22 (41%)
27	CHL	A	850	1	65,73,74	2.37	18 (27%)	76,113,114	2.12	23 (30%)
30	LMG	a	301	-	44,44,55	0.87	2 (4%)	52,52,63	1.27	6 (11%)
20	PQN	A	801	-	34,34,34	0.37	0	42,45,45	0.56	0
22	BCR	F	301	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	4 (7%)
27	CHL	a	308	12	45,53,74	3.09	19 (42%)	52,89,114	2.58	20 (38%)
29	LUT	b	301	-	42,43,43	5.62	19 (45%)	51,60,60	5.71	34 (66%)
30	LMG	7	301	-	41,41,55	0.87	1 (2%)	49,49,63	1.21	3 (6%)
27	CHL	a	310	12	65,73,74	2.93	18 (27%)	76,113,114	2.17	22 (28%)
27	CHL	5	307	15	55,63,74	3.45	18 (32%)	64,101,114	2.30	25 (39%)
27	CHL	a	311	12	60,68,74	2.71	18 (30%)	70,107,114	2.33	24 (34%)
27	CHL	5	322	15	47,55,74	2.80	16 (34%)	50,91,114	2.23	19 (38%)
27	CHL	B	823	2	55,63,74	2.64	19 (34%)	64,101,114	2.37	23 (35%)
27	CHL	B	835	2	57,65,74	2.66	19 (33%)	66,103,114	2.36	22 (33%)
27	CHL	A	854	1	56,64,74	2.91	20 (35%)	65,102,114	2.41	23 (35%)
27	CHL	3	314	36	60,68,74	2.68	17 (28%)	70,107,114	2.29	22 (31%)
22	BCR	A	804	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	5 (8%)
24	LHG	8	305	27	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
27	CHL	B	826	2	50,58,74	3.33	19 (38%)	58,95,114	2.48	21 (36%)
27	CHL	A	821	1	65,73,74	2.51	20 (30%)	76,113,114	2.17	23 (30%)
27	CHL	A	824	1	60,68,74	2.46	17 (28%)	70,107,114	2.20	22 (31%)
27	CHL	F	308	6	46,54,74	3.17	19 (41%)	53,90,114	2.48	19 (35%)
26	CL0	A	815	1	65,73,73	1.79	11 (16%)	76,113,113	3.37	29 (38%)
24	LHG	5	304	-	34,34,48	0.36	0	37,40,54	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	B	818	2	55,63,74	2.59	19 (34%)	64,101,114	2.38	21 (32%)
27	CHL	A	830	1	65,73,74	2.39	18 (27%)	76,113,114	2.27	22 (28%)
22	BCR	L	301	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	4 (7%)
27	CHL	A	831	-	55,63,74	2.15	11 (20%)	64,101,114	4.15	31 (48%)
27	CHL	5	312	36	50,58,74	3.81	19 (38%)	58,95,114	2.42	22 (37%)
27	CHL	b	317	-	48,56,74	2.83	16 (33%)	51,92,114	2.20	19 (37%)
22	BCR	6	301	-	41,41,41	1.68	8 (19%)	56,56,56	1.61	11 (19%)
27	CHL	5	317	36	47,55,74	2.26	14 (29%)	50,91,114	2.29	19 (38%)
22	BCR	M	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	5 (8%)
22	BCR	3	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	7 (12%)
27	CHL	a	320	12	46,54,74	3.19	19 (41%)	53,90,114	2.40	21 (39%)
27	CHL	K	205	10	46,54,74	3.04	19 (41%)	53,90,114	2.40	20 (37%)
27	CHL	4	318	-	42,50,74	3.94	19 (45%)	48,85,114	2.52	20 (41%)
27	CHL	B	825	2	60,68,74	2.71	20 (33%)	70,107,114	2.30	26 (37%)
27	CHL	6	320	16	46,54,74	3.33	17 (36%)	53,90,114	2.44	21 (39%)
27	CHL	B	837	2	65,73,74	2.73	19 (29%)	76,113,114	2.12	23 (30%)
24	LHG	7	302	-	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
27	CHL	A	845	1	65,73,74	2.79	19 (29%)	76,113,114	2.14	23 (30%)
27	CHL	A	818	1	65,73,74	2.32	20 (30%)	76,113,114	2.20	25 (32%)
27	CHL	7	324	17	46,54,74	2.83	19 (41%)	53,90,114	2.35	18 (33%)
27	CHL	3	318	36	51,59,74	2.76	20 (39%)	59,96,114	2.46	23 (38%)
27	CHL	3	317	36	62,70,74	2.53	19 (30%)	72,109,114	2.26	21 (29%)
27	CHL	A	820	1	65,73,74	2.40	18 (27%)	76,113,114	2.24	24 (31%)
24	LHG	A	810	-	41,41,48	0.68	1 (2%)	44,47,54	1.32	6 (13%)
24	LHG	B	808	27	31,31,48	0.78	1 (3%)	34,37,54	1.31	4 (11%)
27	CHL	A	822	1	55,63,74	2.92	20 (36%)	64,101,114	2.37	24 (37%)
27	CHL	B	812	-	65,73,74	2.47	17 (26%)	76,113,114	2.24	22 (28%)
23	LMT	B	810	-	36,36,36	1.20	5 (13%)	47,47,47	0.94	1 (2%)
27	CHL	B	815	2	65,73,74	2.45	20 (30%)	76,113,114	2.17	26 (34%)
22	BCR	A	806	-	41,41,41	1.15	2 (4%)	56,56,56	1.28	6 (10%)
27	CHL	3	312	13	65,73,74	2.80	20 (30%)	76,113,114	2.16	24 (31%)
27	CHL	4	306	14	56,64,74	2.63	18 (32%)	65,102,114	2.31	23 (35%)
27	CHL	6	312	16	46,54,74	3.25	19 (41%)	53,90,114	2.55	22 (41%)
27	CHL	6	311	16	65,73,74	2.67	19 (29%)	76,113,114	2.20	24 (31%)
27	CHL	b	304	12	46,54,74	3.62	19 (41%)	53,90,114	2.50	22 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	A	848	1	65,73,74	2.43	18 (27%)	76,113,114	2.18	22 (28%)
29	LUT	5	302	-	42,43,43	5.57	19 (45%)	51,60,60	5.71	33 (64%)
29	LUT	4	301	-	42,43,43	5.61	20 (47%)	51,60,60	5.69	34 (66%)

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
27	CHL	5	315	15	3/3/20/26	8/37/135/137	-
29	LUT	3	304	-	-	15/29/67/67	0/2/2/2
27	CHL	4	309	-	3/3/16/26	9/17/115/137	-
27	CHL	6	310	16	3/3/18/26	10/25/123/137	-
27	CHL	7	316	36	3/3/18/26	9/23/121/137	-
27	CHL	A	851	1	3/3/16/26	4/15/113/137	-
29	LUT	7	304	-	-	17/29/67/67	0/2/2/2
29	LUT	4	302	-	-	19/29/67/67	0/2/2/2
27	CHL	B	822	2	2/2/20/26	14/37/135/137	-
22	BCR	3	301	-	-	8/29/63/63	0/2/2/2
21	SF4	C	102	3	-	-	0/6/5/5
27	CHL	8	321	36	3/3/20/26	17/39/137/137	-
27	CHL	a	318	36	3/3/16/26	6/18/116/137	-
22	BCR	K	203	-	-	5/29/63/63	0/2/2/2
27	CHL	A	841	36	3/3/18/26	10/27/125/137	-
27	CHL	a	307	12	3/3/19/26	4/31/129/137	-
21	SF4	A	802	1,2	-	-	0/6/5/5
27	CHL	6	318	-	3/3/16/26	9/17/115/137	-
27	CHL	A	834	1	2/2/20/26	6/37/135/137	-
27	CHL	B	836	2	2/2/20/26	5/37/135/137	-
27	CHL	B	850	2	2/2/17/26	3/19/117/137	-
22	BCR	A	807	-	-	11/29/63/63	0/2/2/2
27	CHL	5	318	15	3/3/20/26	9/37/135/137	-
27	CHL	A	838	1	1/1/19/26	8/31/129/137	-
27	CHL	5	320	15	3/3/16/26	2/15/113/137	-
27	CHL	A	846	-	2/2/17/26	3/19/117/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LUT	8	304	-	-	14/29/67/67	0/2/2/2
27	CHL	4	307	14	2/2/19/26	7/31/129/137	-
27	CHL	A	825	1	1/1/20/26	11/37/135/137	-
27	CHL	A	823	1	3/3/20/26	13/37/135/137	-
27	CHL	A	837	1	2/2/18/26	5/25/123/137	-
27	CHL	A	839	1	2/2/20/26	13/37/135/137	-
27	CHL	B	831	2	2/2/16/26	4/15/113/137	-
27	CHL	B	851	2	2/2/19/26	7/34/132/137	-
27	CHL	5	323	15	2/2/18/26	8/27/125/137	-
27	CHL	A	816	36	3/3/20/26	6/37/135/137	-
27	CHL	b	305	-	3/3/16/26	6/15/113/137	-
27	CHL	3	315	13	2/2/17/26	8/22/120/137	-
22	BCR	I	801	-	-	11/29/63/63	0/2/2/2
23	LMT	5	326	-	-	9/21/61/61	0/2/2/2
27	CHL	8	323	-	2/2/17/26	4/19/117/137	-
20	PQN	B	801	-	-	3/23/43/43	0/2/2/2
27	CHL	B	819	2	3/3/20/26	11/37/135/137	-
27	CHL	3	320	13	3/3/19/26	6/33/131/137	-
22	BCR	J	102	-	-	8/29/63/63	0/2/2/2
22	BCR	3	302	-	-	11/29/63/63	0/2/2/2
27	CHL	B	846	36	3/3/20/26	13/37/135/137	-
32	PTY	5	305	-	-	17/34/34/53	-
27	CHL	B	834	2	3/3/20/26	6/37/135/137	-
27	CHL	4	316	-	3/3/16/26	8/15/113/137	-
27	CHL	B	820	2	1/1/20/26	10/37/135/137	-
27	CHL	8	326	18	3/3/16/26	3/15/113/137	-
27	CHL	A	843	1	2/2/20/26	13/37/135/137	-
27	CHL	A	828	1	2/2/20/26	12/37/135/137	-
27	CHL	A	819	1	2/2/18/26	8/25/123/137	-
27	CHL	4	317	14	2/2/16/26	6/13/111/137	-
22	BCR	L	302	-	-	8/29/63/63	0/2/2/2
27	CHL	B	848	2	1/1/20/26	7/37/135/137	-
24	LHG	a	305	27	-	24/53/53/53	-
24	LHG	4	303	27	-	30/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	8	320	18	2/2/17/26	6/22/120/137	-
24	LHG	A	811	27	-	26/46/46/53	-
27	CHL	B	847	36	2/2/20/26	8/37/135/137	-
27	CHL	b	307	12	2/2/18/26	6/25/123/137	-
24	LHG	7	306	27	-	20/48/48/53	-
30	LMG	J	104	-	-	7/24/44/70	0/1/1/1
27	CHL	B	813	2	3/3/18/26	9/25/123/137	-
35	DGA	8	306	-	-	5/29/29/45	-
27	CHL	3	308	13	3/3/20/26	6/37/135/137	-
27	CHL	L	304	-	2/2/16/26	2/13/111/137	-
27	CHL	b	306	12	2/2/16/26	5/15/113/137	-
27	CHL	5	313	-	2/2/18/26	10/28/126/137	-
27	CHL	5	325	16	2/2/16/26	8/17/115/137	-
27	CHL	a	312	36	3/3/17/26	4/19/117/137	-
27	CHL	7	320	36,28	2/2/16/26	8/17/115/137	-
27	CHL	B	817	2	3/3/20/26	9/37/135/137	-
27	CHL	A	835	1	3/3/16/26	6/16/114/137	-
27	CHL	B	842	2	2/2/20/26	5/37/135/137	-
27	CHL	4	314	-	3/3/16/26	5/13/111/137	-
27	CHL	B	840	2	3/3/20/26	10/37/135/137	-
27	CHL	B	833	36	3/3/18/26	7/25/123/137	-
23	LMT	A	808	-	-	8/21/61/61	0/2/2/2
30	LMG	J	101	-	-	26/44/64/70	0/1/1/1
27	CHL	A	858	1	2/2/20/26	14/37/135/137	-
27	CHL	b	313	12	3/3/16/26	7/15/113/137	-
27	CHL	B	843	36	3/3/16/26	2/13/111/137	-
27	CHL	b	314	12	3/3/16/26	4/15/113/137	-
27	CHL	A	856	36	2/2/20/26	4/37/135/137	-
27	CHL	7	321	17	3/3/16/26	1/17/115/137	-
27	CHL	A	855	1	1/1/20/26	10/37/135/137	-
27	CHL	3	321	13	2/2/16/26	5/13/111/137	-
27	CHL	5	311	15	3/3/16/26	5/15/113/137	-
23	LMT	5	306	-	-	6/16/56/61	0/2/2/2
27	CHL	7	319	17	3/3/20/26	19/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	B	811	2	2/2/20/26	7/37/135/137	-
27	CHL	6	305	16	3/3/16/26	7/15/113/137	-
27	CHL	8	324	36	3/3/15/26	2/13/112/137	-
27	CHL	b	316	-	3/3/16/26	6/18/116/137	-
27	CHL	7	317	24	3/3/20/26	13/37/135/137	-
27	CHL	8	313	18	3/3/17/26	4/19/117/137	-
27	CHL	A	857	24	3/3/16/26	5/15/113/137	-
27	CHL	A	852	1	3/3/17/26	4/21/119/137	-
27	CHL	4	320	14	3/3/17/26	7/19/117/137	-
27	CHL	A	832	1	2/2/19/26	13/31/129/137	-
22	BCR	B	805	-	-	8/29/63/63	0/2/2/2
27	CHL	A	826	1	1/1/19/26	11/34/132/137	-
27	CHL	a	313	24	3/3/18/26	10/25/123/137	-
27	CHL	B	814	2	3/3/20/26	15/37/135/137	-
21	SF4	C	101	3	-	-	0/6/5/5
27	CHL	b	312	-	1/1/16/26	4/15/113/137	-
27	CHL	6	313	16	2/2/16/26	6/16/114/137	-
22	BCR	B	802	-	-	9/29/63/63	0/2/2/2
27	CHL	3	313	36	3/3/20/26	7/37/135/137	-
27	CHL	5	321	15	2/2/16/26	3/15/113/137	-
27	CHL	5	314	15	2/2/16/26	4/13/111/137	-
27	CHL	3	309	13	3/3/16/26	2/15/113/137	-
22	BCR	B	804	-	-	10/29/63/63	0/2/2/2
27	CHL	5	319	-	2/2/16/26	10/17/115/137	-
27	CHL	A	859	36	3/3/20/26	7/37/135/137	-
27	CHL	B	832	36	3/3/20/26	7/37/135/137	-
27	CHL	a	316	36	3/3/16/26	8/18/116/137	-
27	CHL	8	314	18	3/3/20/26	10/39/137/137	-
22	BCR	7	303	-	-	8/29/63/63	0/2/2/2
33	XAT	7	305	-	-	7/31/93/93	0/4/4/4
27	CHL	4	319	14	2/2/16/26	5/13/111/137	-
27	CHL	6	316	36	3/3/16/26	9/15/113/137	-
27	CHL	B	844	2	3/3/20/26	11/37/135/137	-
29	LUT	6	303	-	-	18/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	7	307	27	-	22/55/95/95	0/2/2/2
29	LUT	3	305	-	-	12/29/67/67	0/2/2/2
27	CHL	A	847	1	2/2/18/26	6/27/125/137	-
27	CHL	4	308	14	3/3/19/26	9/31/129/137	-
27	CHL	6	307	-	2/2/20/26	14/37/135/137	-
23	LMT	A	809	-	-	6/21/61/61	0/2/2/2
31	AXT	a	303	-	-	1/29/71/75	0/2/2/2
27	CHL	8	316	18	2/2/20/26	11/37/135/137	-
27	CHL	B	849	24	3/3/20/26	6/37/135/137	-
22	BCR	5	301	-	-	13/29/63/63	0/2/2/2
27	CHL	3	319	13	2/2/18/26	9/25/123/137	-
27	CHL	6	314	24	3/3/16/26	3/15/113/137	-
27	CHL	3	311	13	3/3/19/26	15/31/129/137	-
27	CHL	F	309	36	3/3/17/26	5/19/117/137	-
27	CHL	7	314	17	3/3/19/26	9/34/132/137	-
27	CHL	4	315	14	3/3/16/26	2/16/114/137	-
27	CHL	A	827	1	2/2/17/26	7/24/122/137	-
27	CHL	K	204	36	3/3/17/26	4/19/117/137	-
27	CHL	8	311	18	3/3/16/26	2/15/113/137	-
27	CHL	8	322	36	2/2/17/26	2/19/117/137	-
29	LUT	b	303	-	-	23/29/67/67	0/2/2/2
22	BCR	K	202	-	-	9/29/63/63	0/2/2/2
27	CHL	B	845	2	2/2/17/26	2/19/117/137	-
30	LMG	8	307	-	-	13/27/47/70	0/1/1/1
23	LMT	F	302	-	-	5/15/55/61	0/2/2/2
27	CHL	A	836	36	3/3/20/26	11/37/135/137	-
27	CHL	A	844	1	1/1/20/26	6/37/135/137	-
24	LHG	b	302	27	-	17/39/39/53	-
27	CHL	A	842	1	2/2/20/26	8/39/137/137	-
27	CHL	b	310	12	2/2/16/26	4/15/113/137	-
27	CHL	B	841	2	2/2/18/26	7/25/123/137	-
27	CHL	7	322	36	2/2/19/26	10/33/131/137	-
27	CHL	8	312	18	3/3/20/26	14/37/135/137	-
22	BCR	B	806	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	B	827	2	3/3/19/26	10/31/129/137	-
27	CHL	4	305	14	3/3/16/26	4/13/111/137	-
27	CHL	4	304	14	3/3/18/26	4/25/123/137	-
27	CHL	7	312	17	3/3/16/26	4/11/109/137	-
27	CHL	B	821	2	2/2/18/26	9/29/127/137	-
27	CHL	B	829	2	2/2/18/26	7/25/123/137	-
27	CHL	3	310	13	3/3/20/26	13/37/135/137	-
22	BCR	B	807	-	-	6/29/63/63	0/2/2/2
27	CHL	7	311	17	3/3/19/26	4/31/129/137	-
27	CHL	a	319	36	2/2/17/26	6/19/117/137	-
27	CHL	b	309	24	3/3/16/26	3/15/113/137	-
27	CHL	8	315	18	2/2/20/26	14/37/135/137	-
27	CHL	6	309	16	3/3/16/26	5/16/114/137	-
29	LUT	6	302	-	-	16/29/67/67	0/2/2/2
27	CHL	B	839	2	2/2/19/26	6/31/129/137	-
22	BCR	8	302	-	-	7/29/63/63	0/2/2/2
27	CHL	B	816	2	3/3/19/26	6/33/131/137	-
27	CHL	5	316	36	3/3/20/26	25/39/137/137	-
27	CHL	6	308	16	3/3/20/26	19/39/137/137	-
27	CHL	b	311	12	3/3/16/26	8/17/115/137	-
28	DGD	B	809	-	-	22/50/90/95	0/2/2/2
29	LUT	8	303	-	-	13/29/67/67	0/2/2/2
27	CHL	J	106	9	3/3/15/26	4/10/108/137	-
27	CHL	6	315	16	2/2/17/26	2/19/117/137	-
27	CHL	A	853	1	3/3/20/26	10/37/135/137	-
27	CHL	4	313	-	1/1/16/26	6/13/111/137	-
27	CHL	7	315	17	2/2/16/26	3/11/109/137	-
27	CHL	8	325	18	2/2/20/26	10/37/135/137	-
27	CHL	b	308	-	2/2/16/26	5/15/113/137	-
27	CHL	A	849	1	2/2/20/26	7/37/135/137	-
27	CHL	B	838	2	1/1/20/26	11/37/135/137	-
27	CHL	3	316	36	2/2/20/26	8/39/137/137	-
29	LUT	a	302	-	-	15/29/67/67	0/2/2/2
24	LHG	A	812	-	-	21/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	K	206	10	2/2/16/26	2/15/113/137	-
27	CHL	5	308	15	3/3/16/26	3/15/113/137	-
27	CHL	B	828	36	3/3/19/26	2/31/129/137	-
27	CHL	7	323	-	2/2/17/26	8/22/120/137	-
27	CHL	8	319	36	3/3/18/26	6/25/123/137	-
27	CHL	b	315	12	3/3/20/26	14/37/135/137	-
34	SQD	8	301	-	-	15/30/50/69	0/1/1/1
22	BCR	A	805	-	-	4/29/63/63	0/2/2/2
24	LHG	5	324	27	-	14/36/36/53	-
29	LUT	a	304	-	-	14/29/67/67	0/2/2/2
27	CHL	a	309	36	3/3/19/26	7/31/129/137	-
27	CHL	4	312	14	2/2/16/26	9/18/116/137	-
27	CHL	B	824	2	2/2/18/26	6/28/126/137	-
22	BCR	A	803	-	-	7/29/63/63	0/2/2/2
27	CHL	4	311	14	3/3/16/26	5/16/114/137	-
29	LUT	F	303	-	-	18/29/67/67	0/2/2/2
27	CHL	8	318	24	3/3/16/26	6/15/113/137	-
27	CHL	a	317	12	3/3/20/26	9/37/135/137	-
27	CHL	6	306	16	3/3/18/26	10/28/126/137	-
27	CHL	A	829	1	2/2/18/26	9/25/123/137	-
27	CHL	L	303	-	2/2/19/26	10/31/129/137	-
27	CHL	a	314	12	2/2/16/26	8/13/111/137	-
27	CHL	5	309	15	2/2/19/26	15/31/129/137	-
27	CHL	6	317	-	2/2/16/26	7/17/115/137	-
29	LUT	5	303	-	-	19/29/67/67	0/2/2/2
27	CHL	B	830	2	2/2/19/26	3/31/129/137	-
27	CHL	K	207	10	3/3/16/26	6/17/115/137	-
27	CHL	6	319	16	3/3/15/26	6/12/110/137	-
27	CHL	8	317	36	3/3/20/26	12/37/135/137	-
22	BCR	B	803	-	-	9/29/63/63	0/2/2/2
27	CHL	A	817	-	1/1/20/26	3/37/135/137	-
27	CHL	7	313	17	2/2/20/26	10/37/135/137	-
27	CHL	a	315	12	2/2/19/26	12/33/131/137	-
27	CHL	A	840	36	3/3/20/26	8/37/135/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	5	310	15	3/3/20/26	5/37/135/137	-
27	CHL	A	833	1	2/2/19/26	11/33/131/137	-
27	CHL	7	318	17	2/2/18/26	7/25/123/137	-
29	LUT	J	103	-	-	18/29/67/67	0/2/2/2
27	CHL	4	310	24	3/3/16/26	6/15/113/137	-
27	CHL	A	850	1	1/1/20/26	10/37/135/137	-
30	LMG	a	301	-	-	16/39/59/70	0/1/1/1
27	CHL	a	308	12	3/3/16/26	5/13/111/137	-
20	PQN	A	801	-	-	3/23/43/43	0/2/2/2
22	BCR	F	301	-	-	10/29/63/63	0/2/2/2
29	LUT	b	301	-	-	15/29/67/67	0/2/2/2
30	LMG	7	301	-	-	18/36/56/70	0/1/1/1
27	CHL	a	310	12	2/2/20/26	12/37/135/137	-
27	CHL	5	307	15	3/3/18/26	6/25/123/137	-
27	CHL	a	311	12	2/2/19/26	7/31/129/137	-
27	CHL	5	322	15	3/3/16/26	3/17/115/137	-
27	CHL	B	823	2	3/3/18/26	8/25/123/137	-
27	CHL	B	835	2	2/2/18/26	11/28/126/137	-
24	LHG	B	808	27	-	6/36/36/53	-
27	CHL	A	854	1	1/1/18/26	3/27/125/137	-
27	CHL	3	314	36	3/3/19/26	10/31/129/137	-
27	CHL	B	826	2	1/1/17/26	7/19/117/137	-
22	BCR	A	804	-	-	6/29/63/63	0/2/2/2
24	LHG	8	305	27	-	16/53/53/53	-
27	CHL	A	821	1	3/3/20/26	11/37/135/137	-
27	CHL	A	824	1	2/2/19/26	8/31/129/137	-
27	CHL	F	308	6	3/3/16/26	6/15/113/137	-
26	CL0	A	815	1	1/1/20/25	6/37/135/135	-
27	CHL	B	818	2	2/2/18/26	6/25/123/137	-
24	LHG	5	304	-	-	21/39/39/53	-
27	CHL	A	830	1	2/2/20/26	7/37/135/137	-
27	CHL	A	831	-	2/2/18/26	12/25/123/137	-
27	CHL	5	312	36	3/3/17/26	4/19/117/137	-
27	CHL	b	317	-	2/2/16/26	5/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	L	301	-	-	10/29/63/63	0/2/2/2
22	BCR	6	301	-	-	23/29/63/63	0/2/2/2
27	CHL	5	317	36	2/2/16/26	5/17/115/137	-
22	BCR	M	102	-	-	9/29/63/63	0/2/2/2
27	CHL	4	318	-	3/3/15/26	3/10/108/137	-
27	CHL	a	320	12	3/3/16/26	5/15/113/137	-
27	CHL	K	205	10	3/3/16/26	3/15/113/137	-
22	BCR	3	303	-	-	10/29/63/63	0/2/2/2
27	CHL	B	825	2	2/2/19/26	8/31/129/137	-
27	CHL	6	320	16	3/3/16/26	4/15/113/137	-
27	CHL	B	837	2	1/1/20/26	9/37/135/137	-
24	LHG	7	302	-	-	32/53/53/53	-
27	CHL	A	845	1	1/1/20/26	10/37/135/137	-
27	CHL	A	818	1	3/3/20/26	7/37/135/137	-
27	CHL	7	324	17	2/2/16/26	6/15/113/137	-
27	CHL	3	318	36	3/3/17/26	7/21/119/137	-
27	CHL	3	317	36	2/2/19/26	9/34/132/137	-
27	CHL	A	820	1	3/3/20/26	7/37/135/137	-
24	LHG	A	810	-	-	21/46/46/53	-
27	CHL	A	822	1	1/1/18/26	5/25/123/137	-
27	CHL	B	812	-	2/2/20/26	6/37/135/137	-
27	CHL	4	306	14	3/3/18/26	7/27/125/137	-
27	CHL	B	815	2	3/3/20/26	12/37/135/137	-
27	CHL	6	312	16	3/3/16/26	7/15/113/137	-
22	BCR	A	806	-	-	9/29/63/63	0/2/2/2
27	CHL	3	312	13	2/2/20/26	7/37/135/137	-
23	LMT	B	810	-	-	7/21/61/61	0/2/2/2
23	LMT	7	308	-	-	9/21/61/61	0/2/2/2
27	CHL	6	311	16	3/3/20/26	9/37/135/137	-
27	CHL	b	304	12	2/2/16/26	4/15/113/137	-
27	CHL	A	848	1	2/2/20/26	4/37/135/137	-
29	LUT	5	302	-	-	14/29/67/67	0/2/2/2
29	LUT	4	301	-	-	15/29/67/67	0/2/2/2

The worst 5 of 4370 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	306	CHL	MG-NA	23.77	2.62	2.06
27	6	306	CHL	MG-NA	23.39	2.61	2.06
27	5	310	CHL	MG-NA	20.63	2.55	2.06
27	b	308	CHL	C1B-NB	20.41	1.53	1.35
27	5	312	CHL	MG-NA	19.85	2.53	2.06

The worst 5 of 5620 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	308	CHL	CMB-C2B-C1B	-25.31	89.57	128.46
27	5	315	CHL	C4-C3-C5	-19.98	81.67	115.27
27	5	315	CHL	C5-C3-C2	19.36	160.28	121.12
27	5	313	CHL	C1D-ND-C4D	-17.88	93.63	106.33
27	A	843	CHL	O2A-CGA-O1A	-17.87	78.49	123.59

5 of 530 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	815	CL0	NC
27	A	816	CHL	ND
27	A	816	CHL	NA
27	A	816	CHL	NC
27	A	817	CHL	NC

5 of 2594 torsion outliers are listed below:

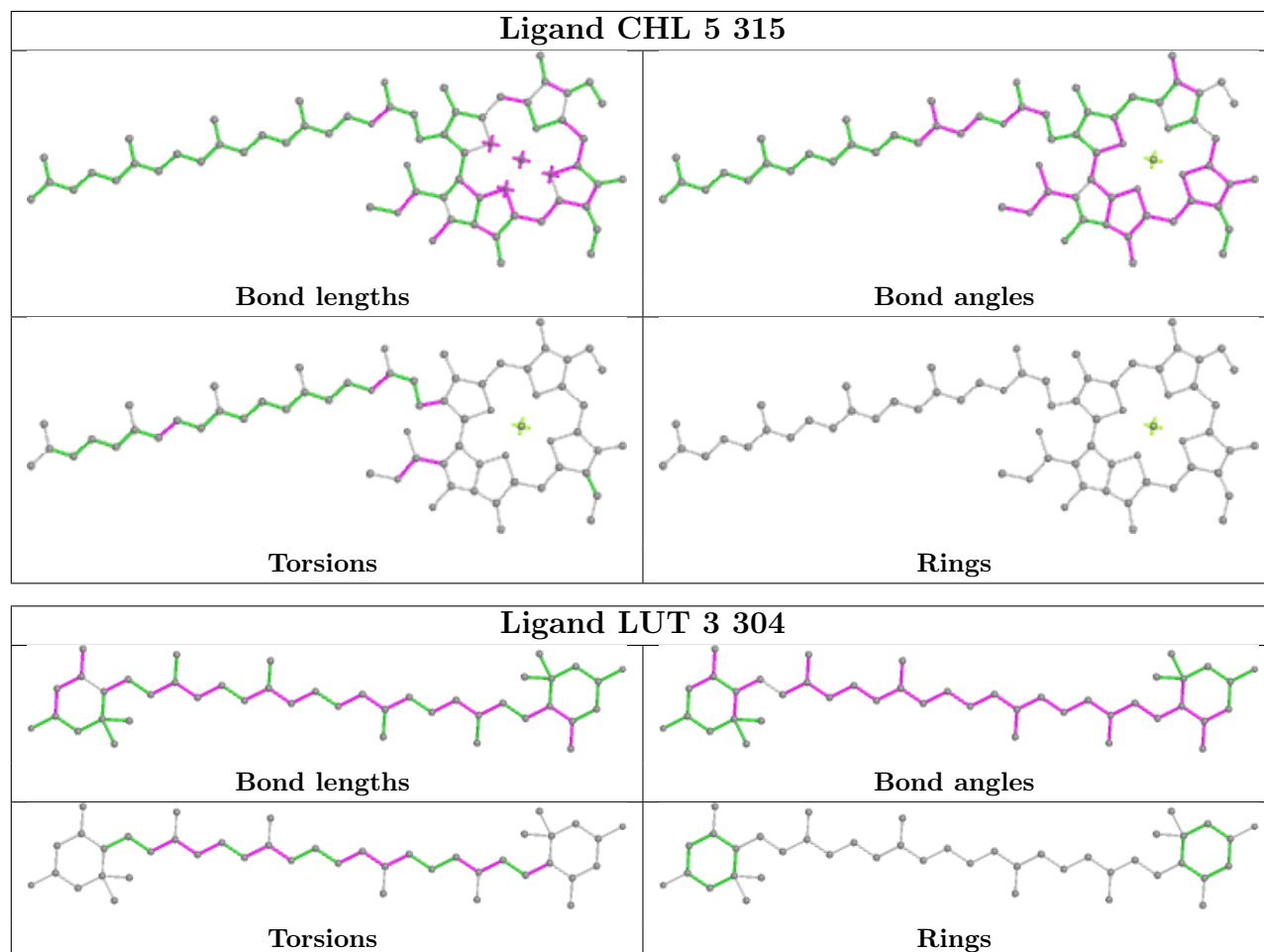
Mol	Chain	Res	Type	Atoms
22	A	804	BCR	C7-C8-C9-C10
22	A	804	BCR	C7-C8-C9-C34
22	A	805	BCR	C1-C6-C7-C8
22	A	806	BCR	C1-C6-C7-C8
22	A	806	BCR	C7-C8-C9-C34

There are no ring outliers.

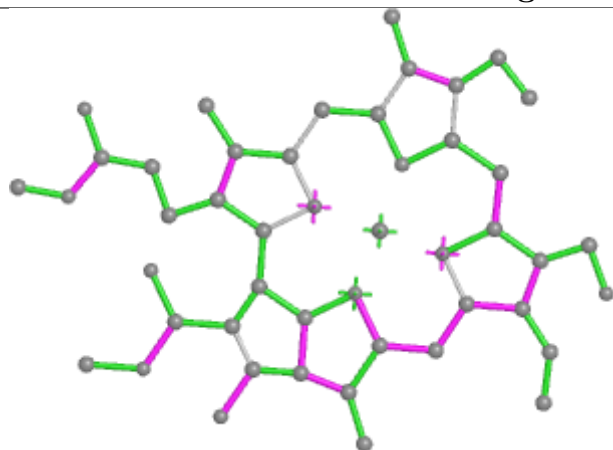
No monomer is involved in short contacts.

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

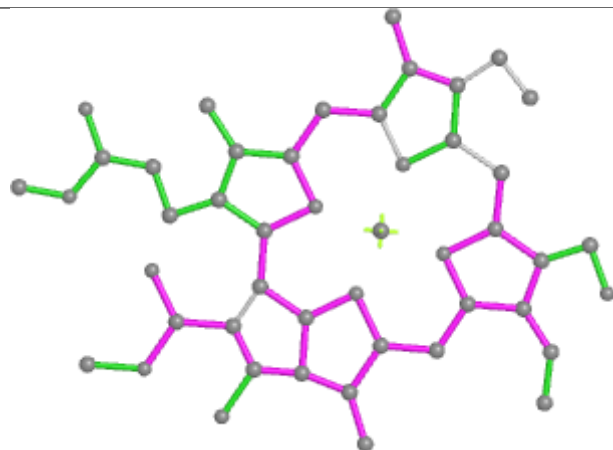
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



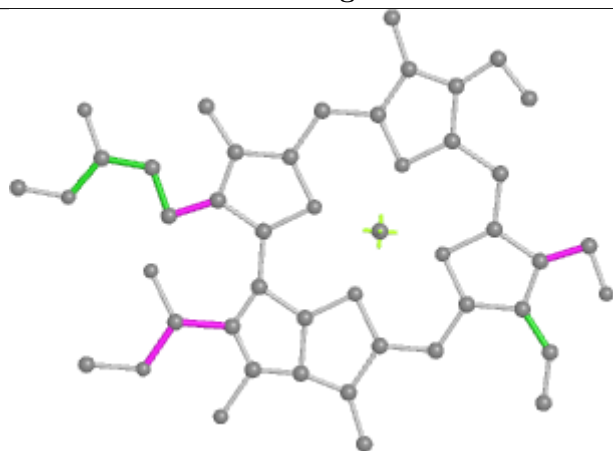
Ligand CHL 4 309



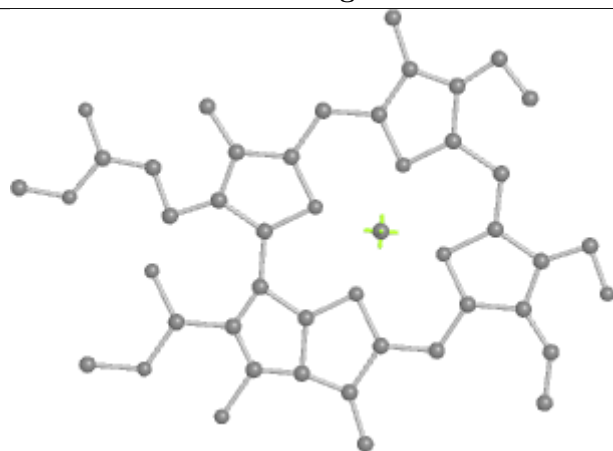
Bond lengths



Bond angles

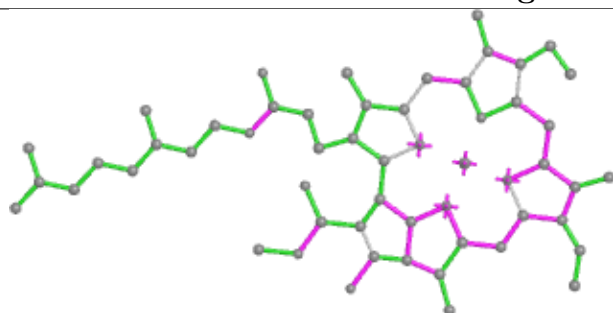


Torsions

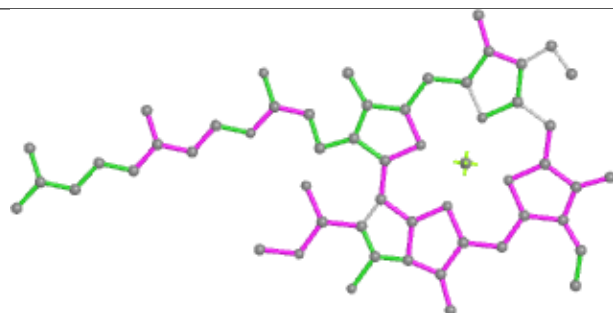


Rings

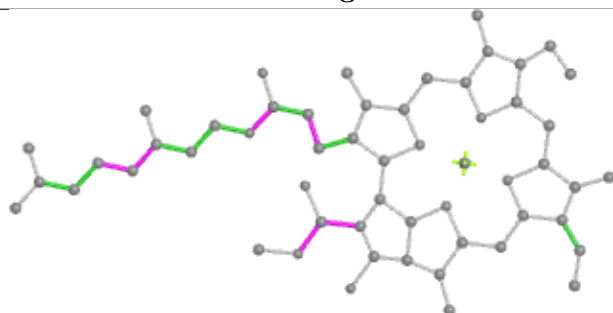
Ligand CHL 6 310



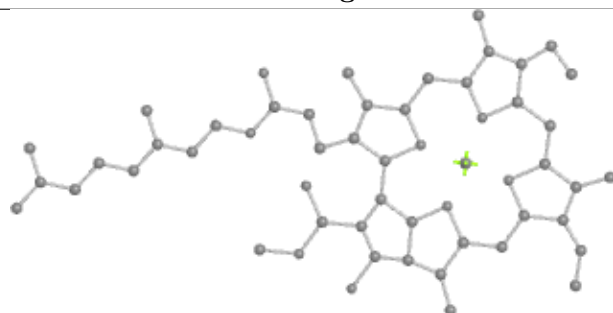
Bond lengths



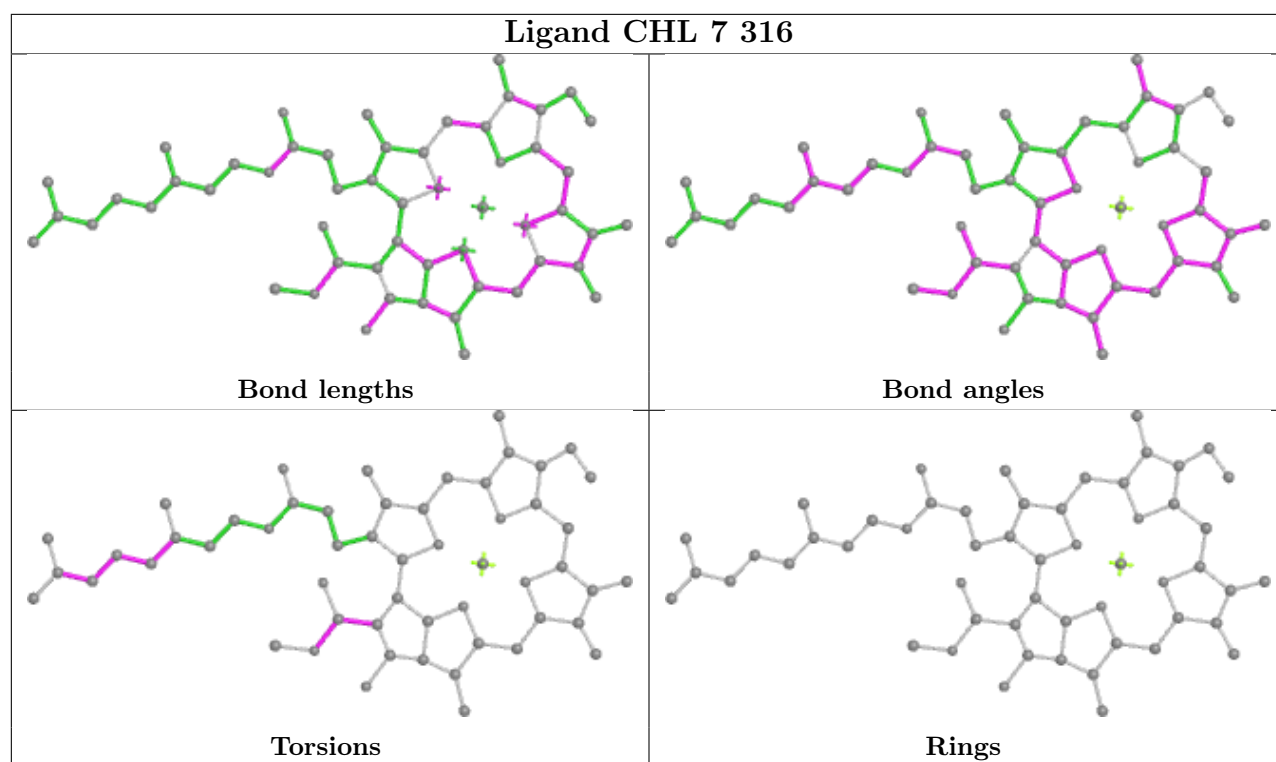
Bond angles



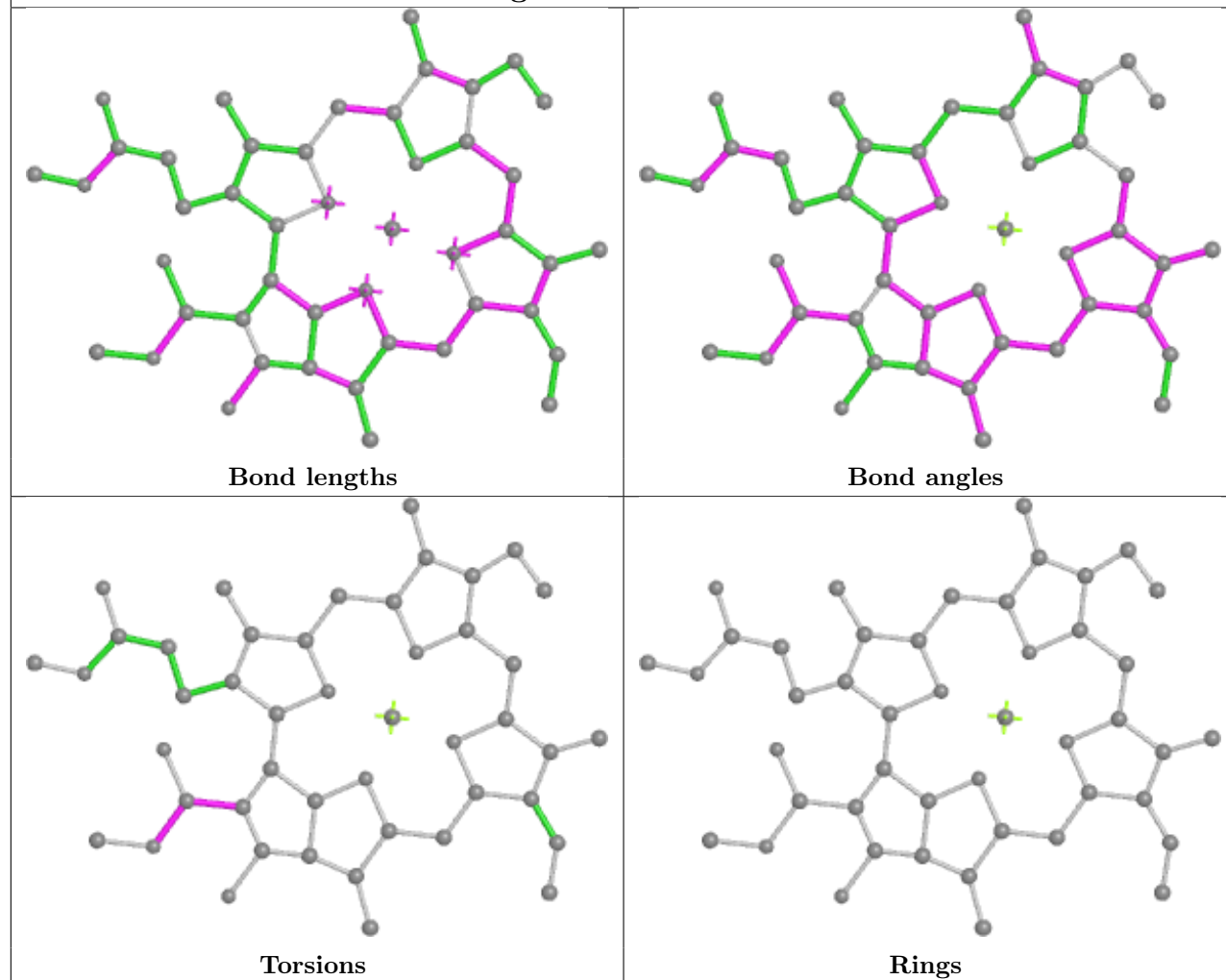
Torsions



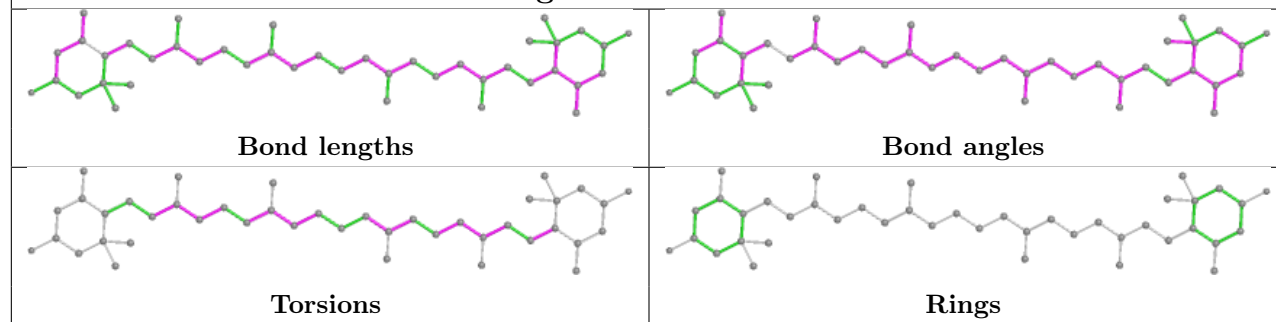
Rings

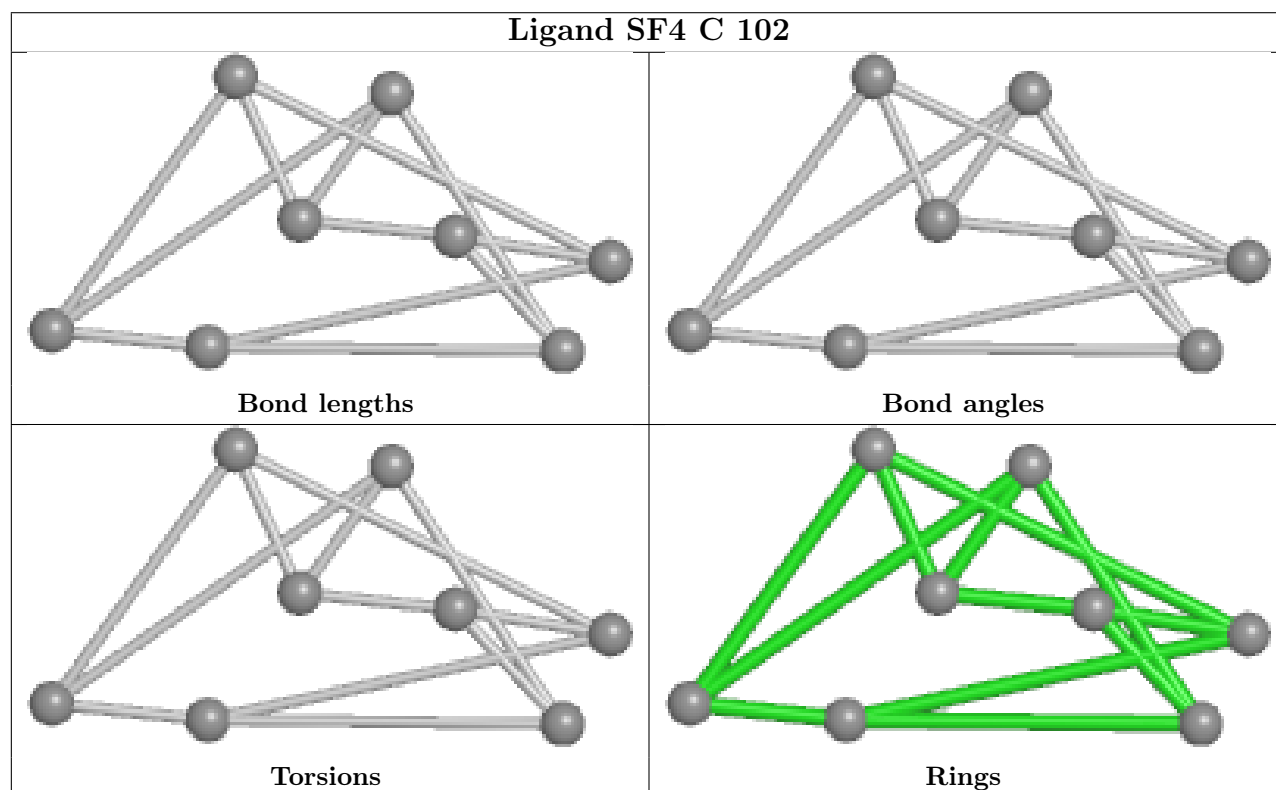
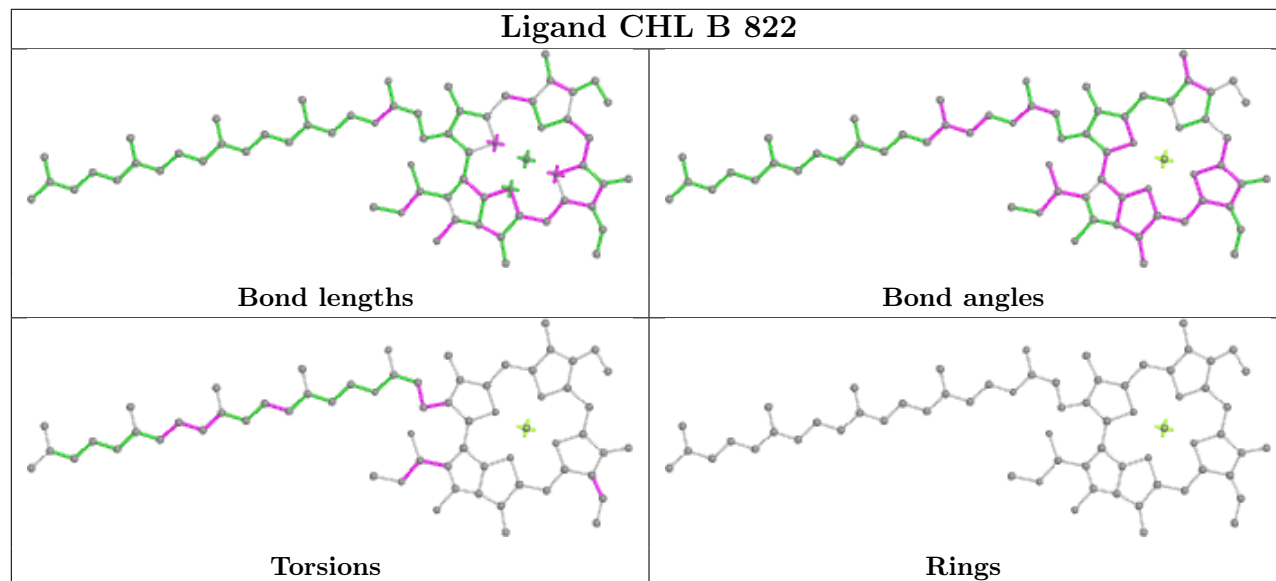
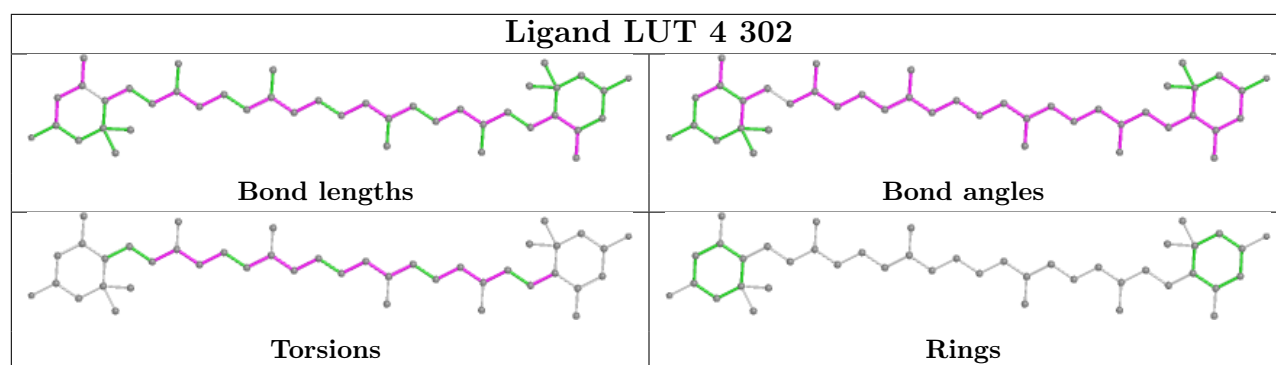


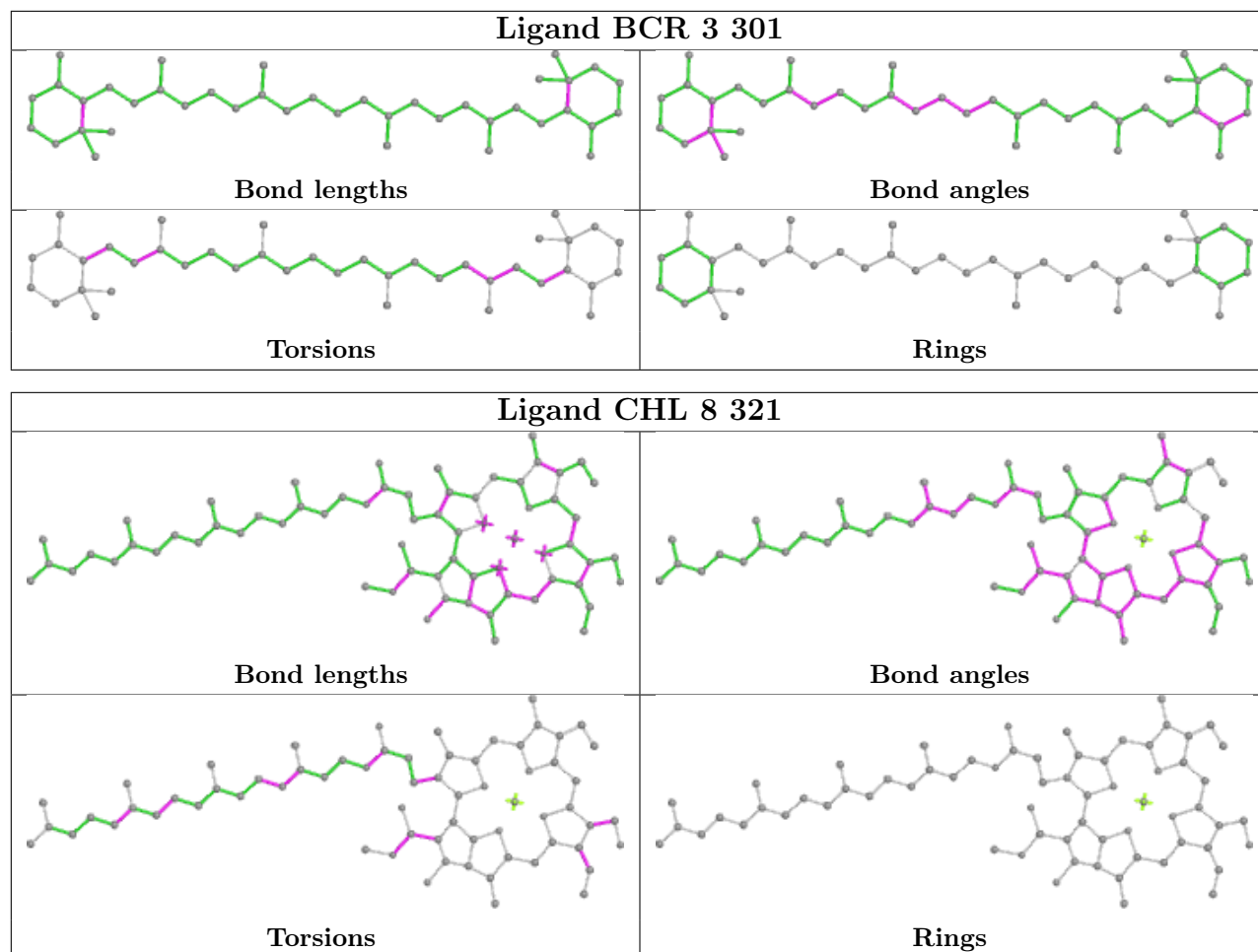
Ligand CHL A 851



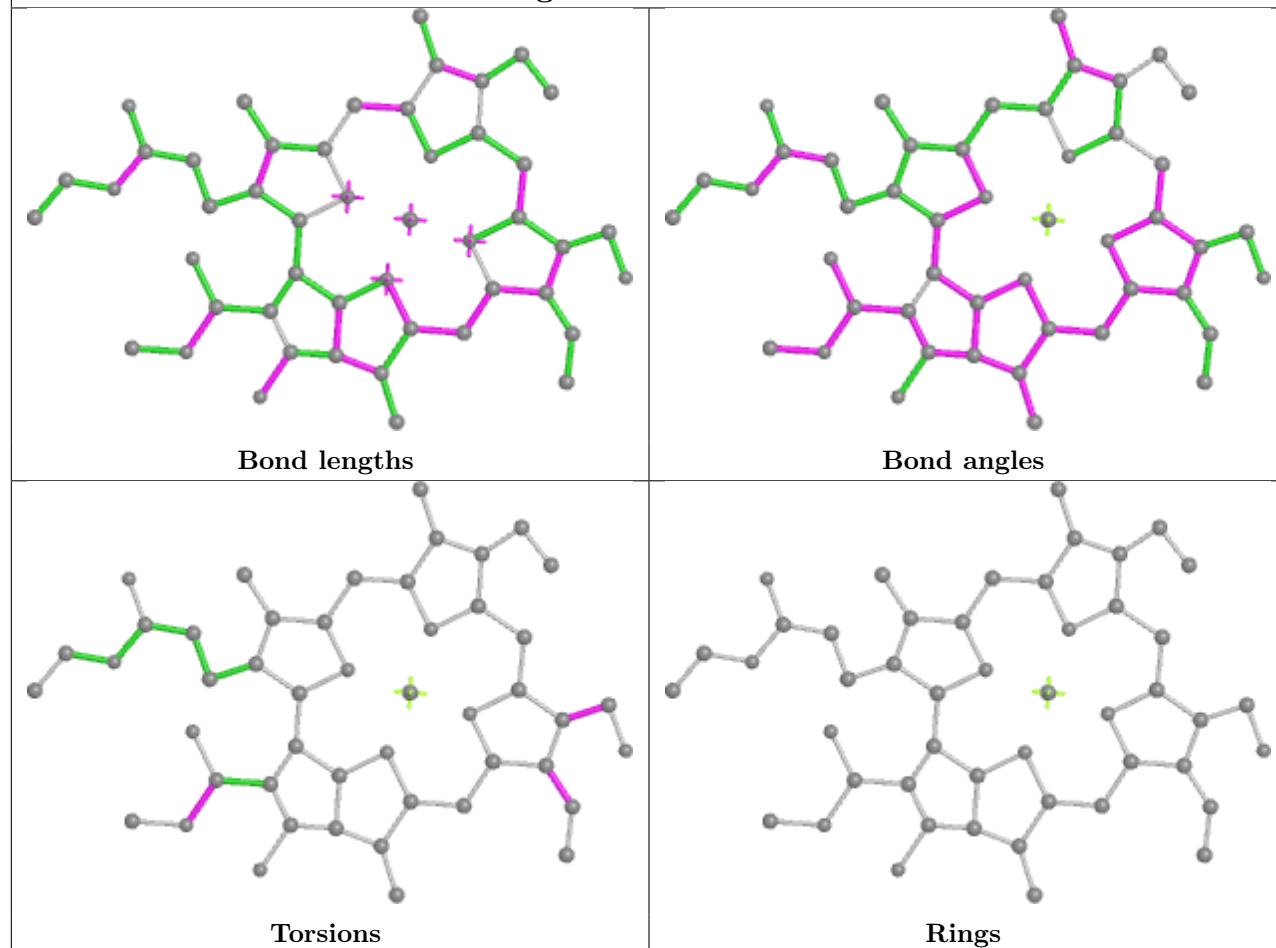
Ligand LUT 7 304



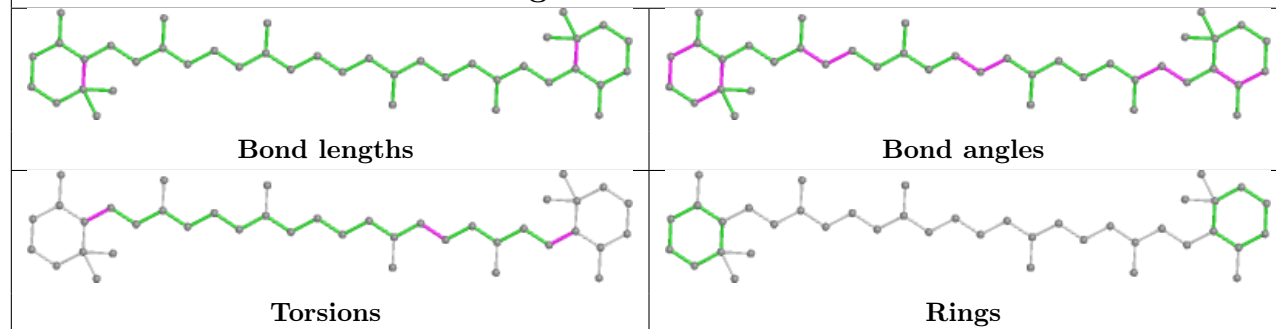


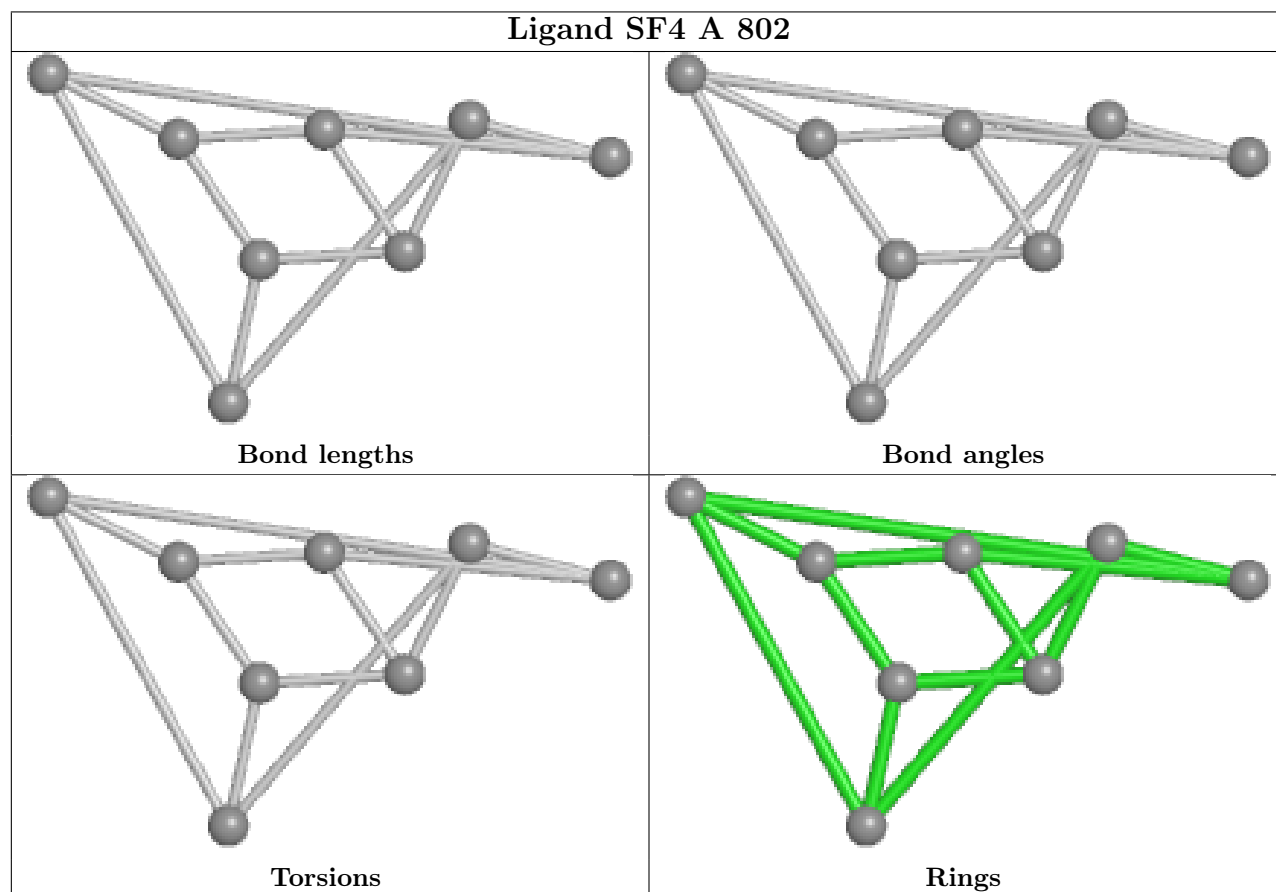
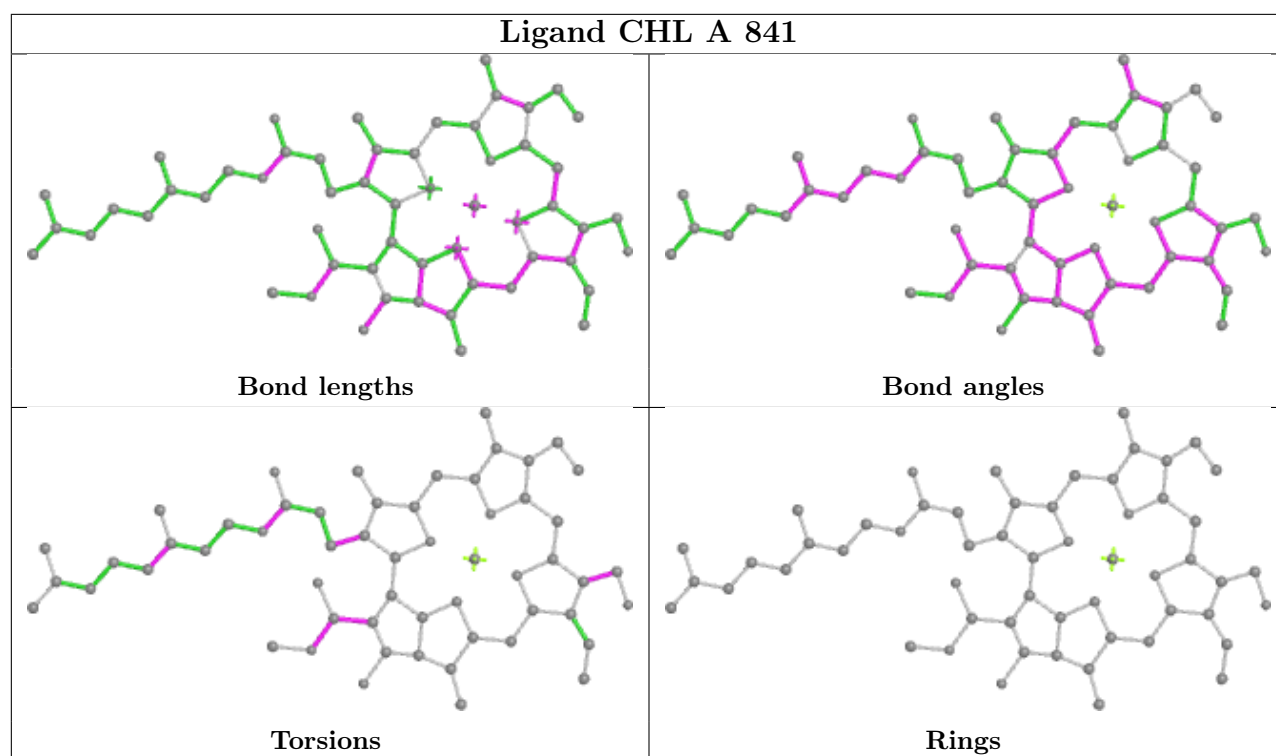


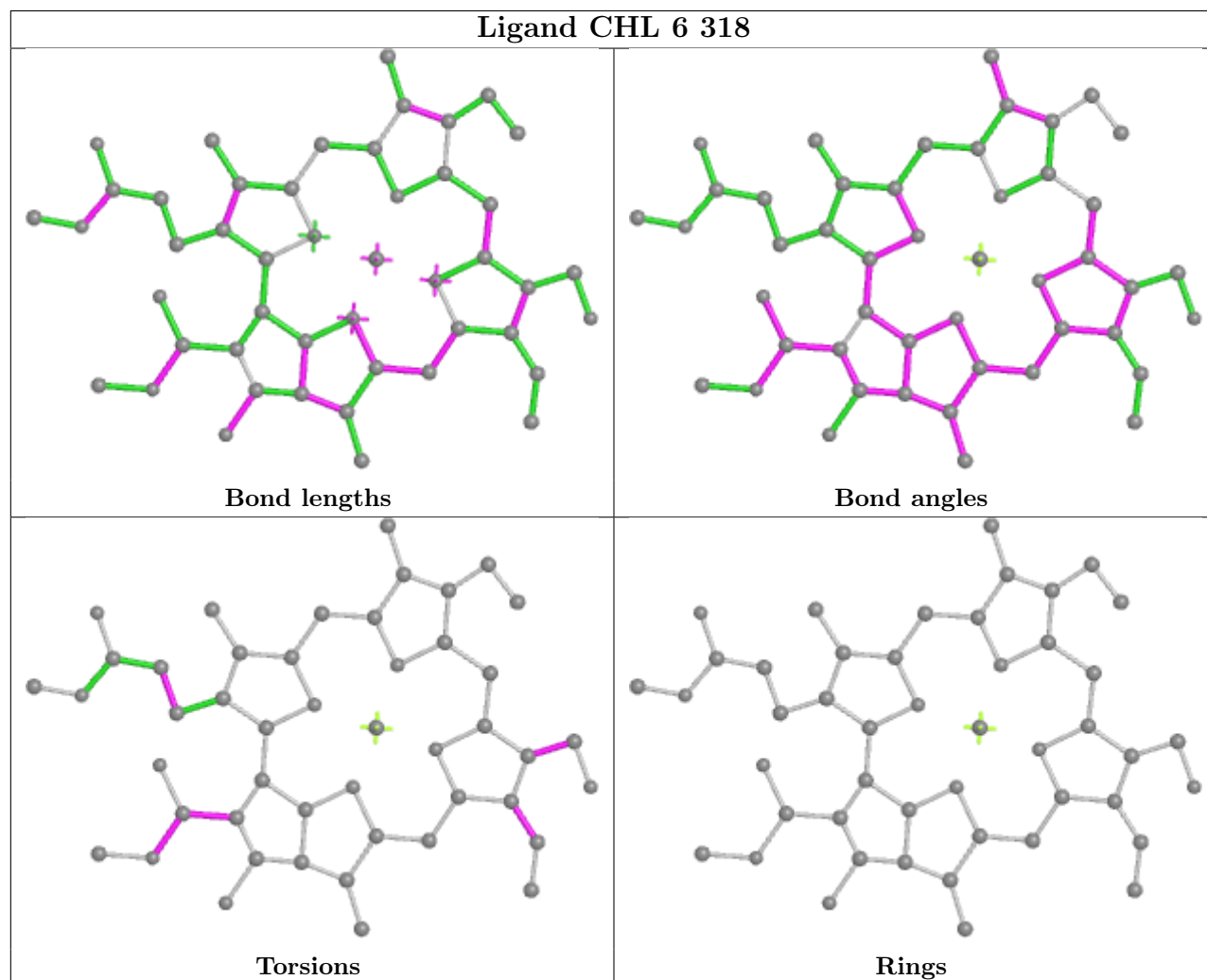
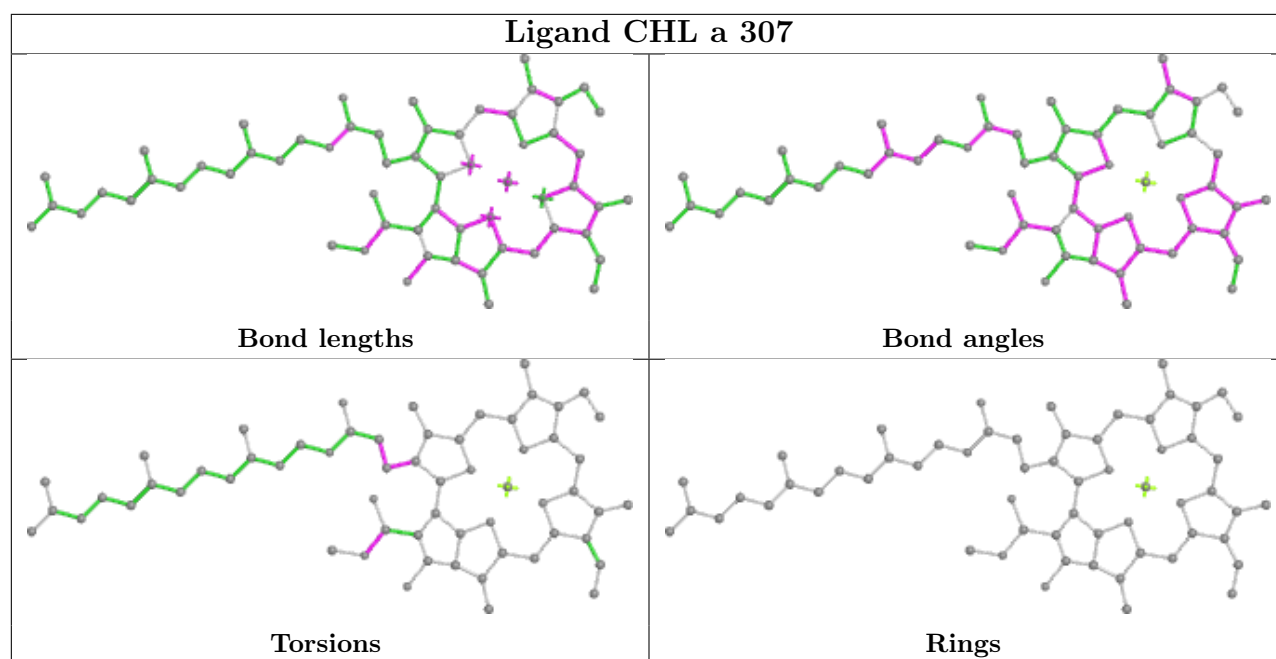
Ligand CHL a 318

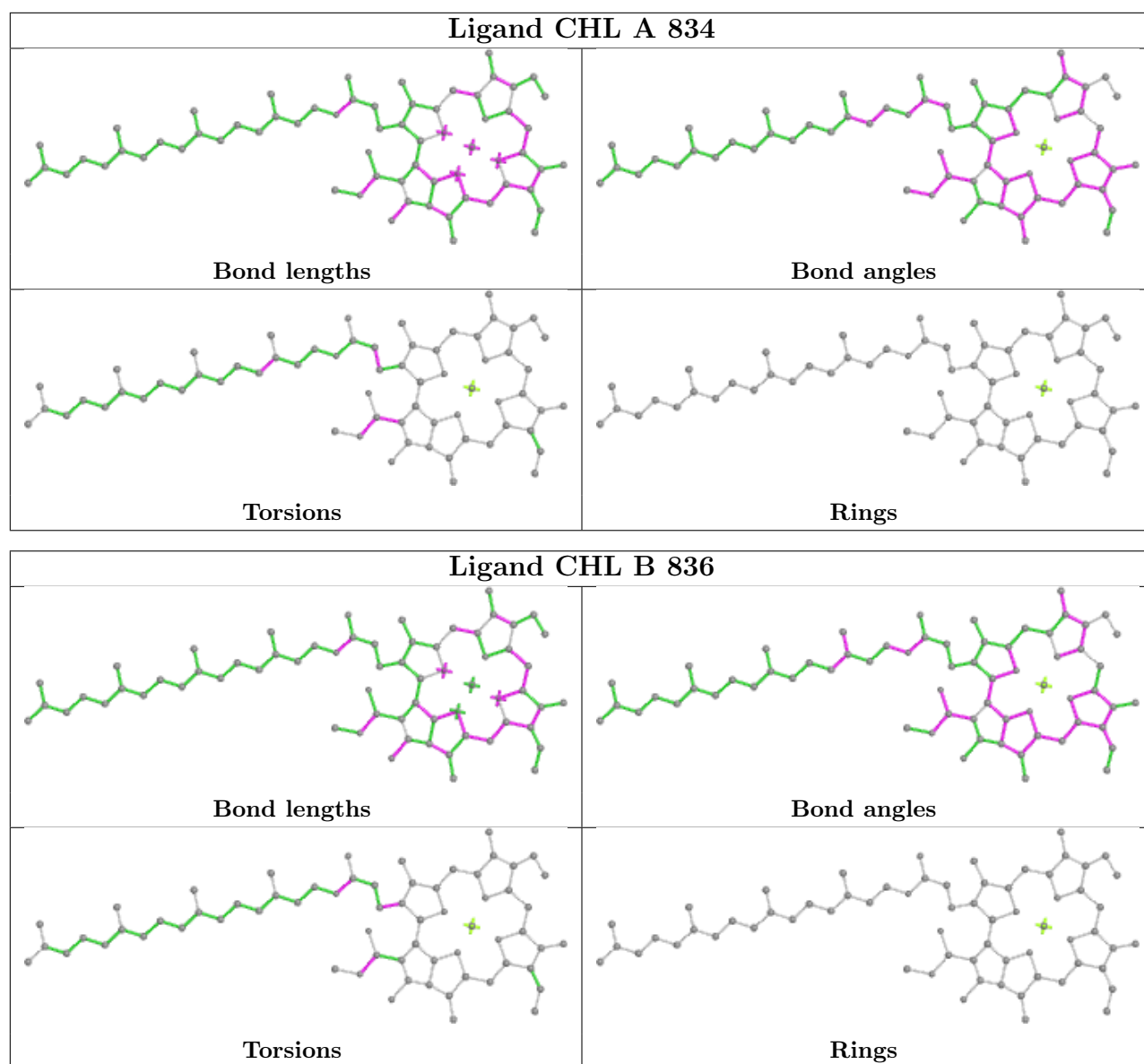


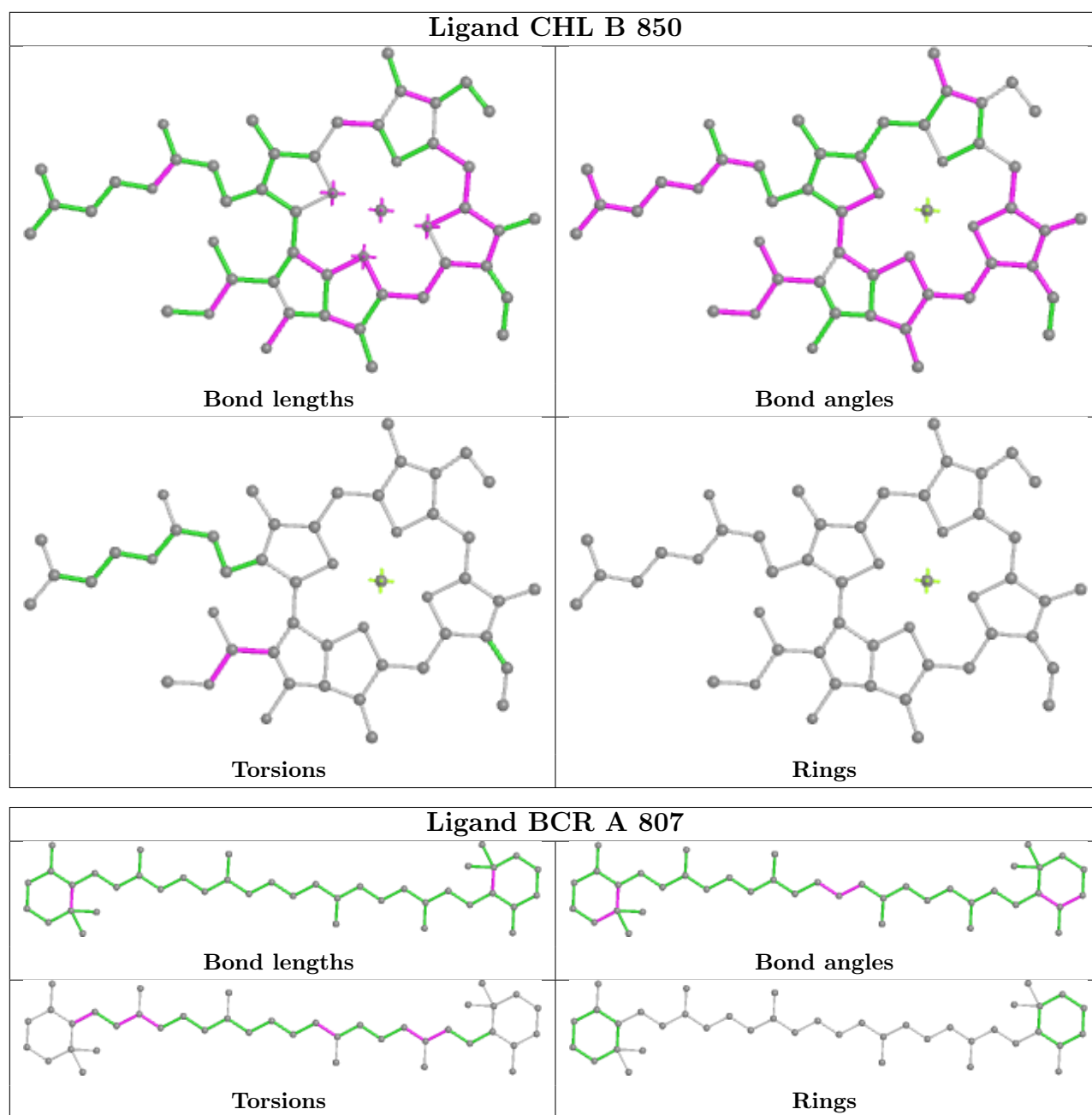
Ligand BCR K 203

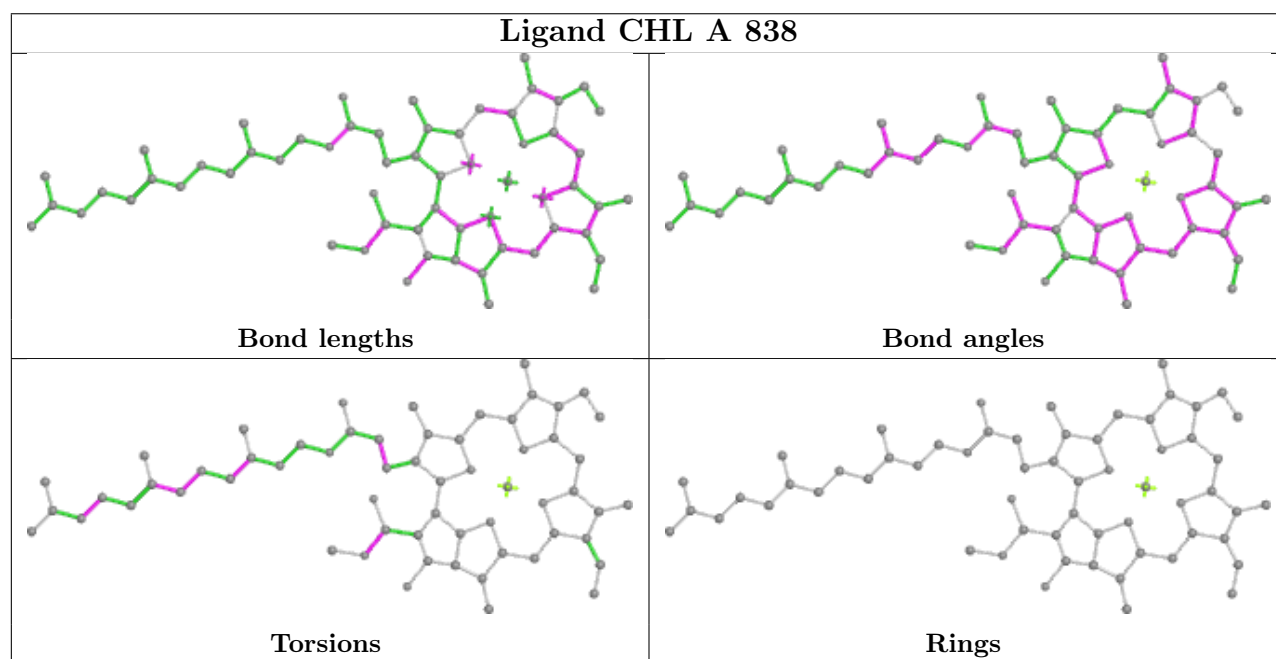
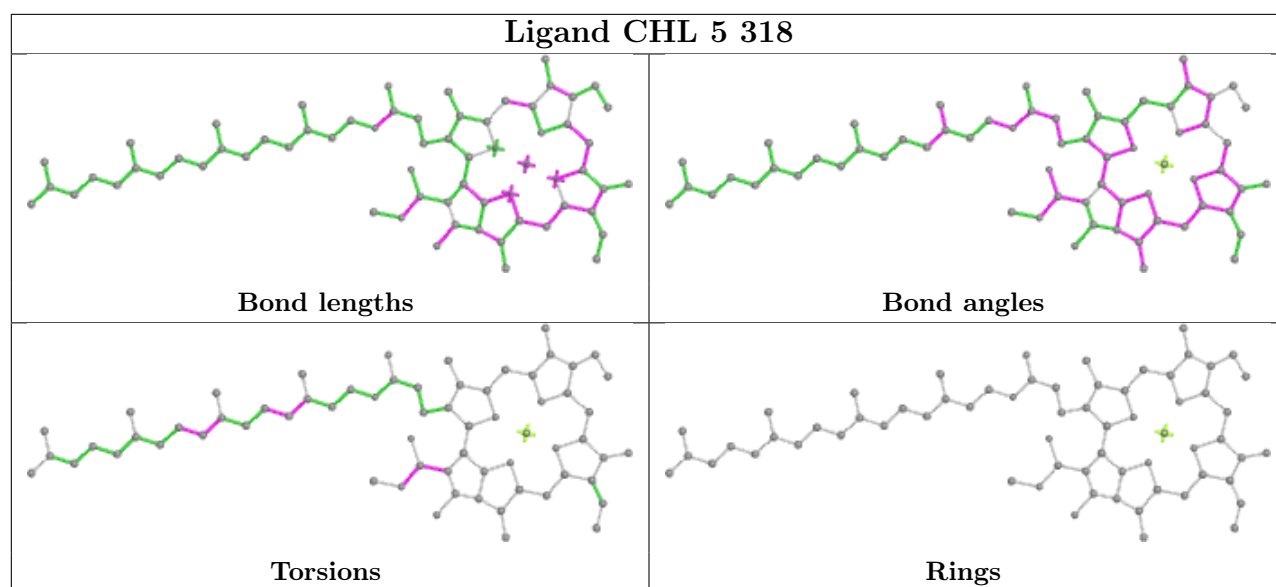




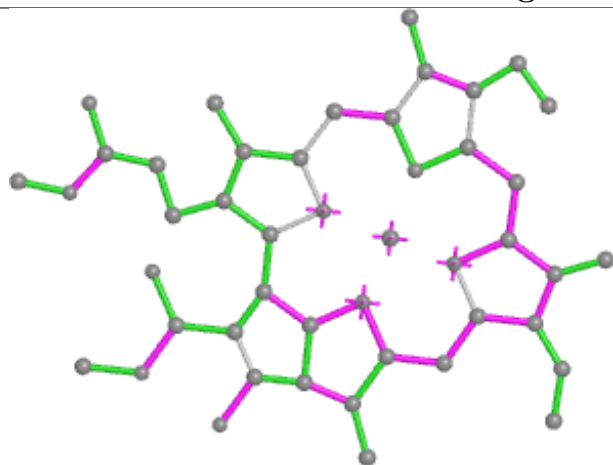




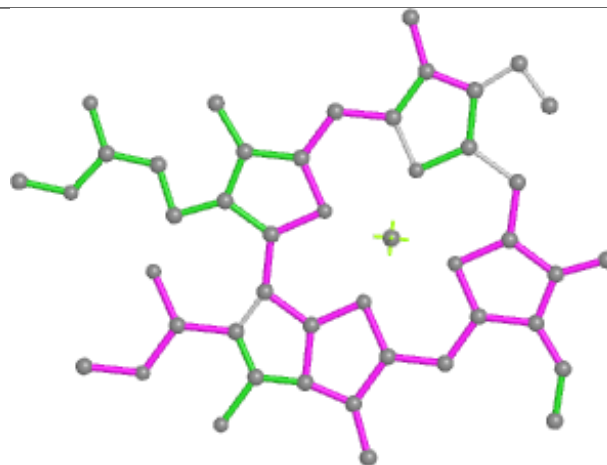




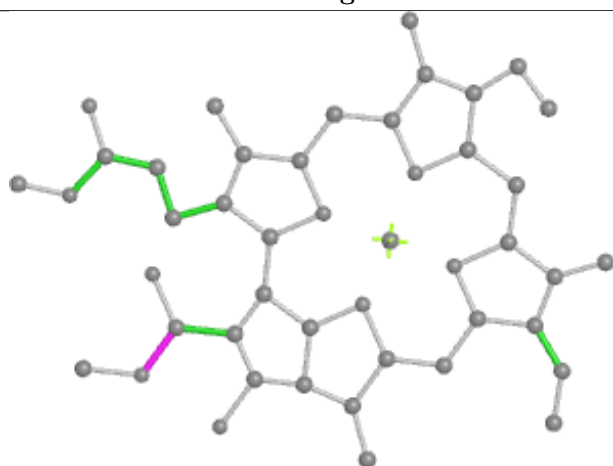
Ligand CHL 5 320



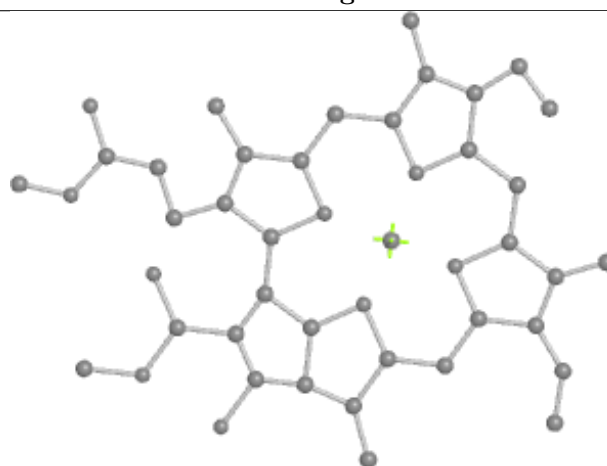
Bond lengths



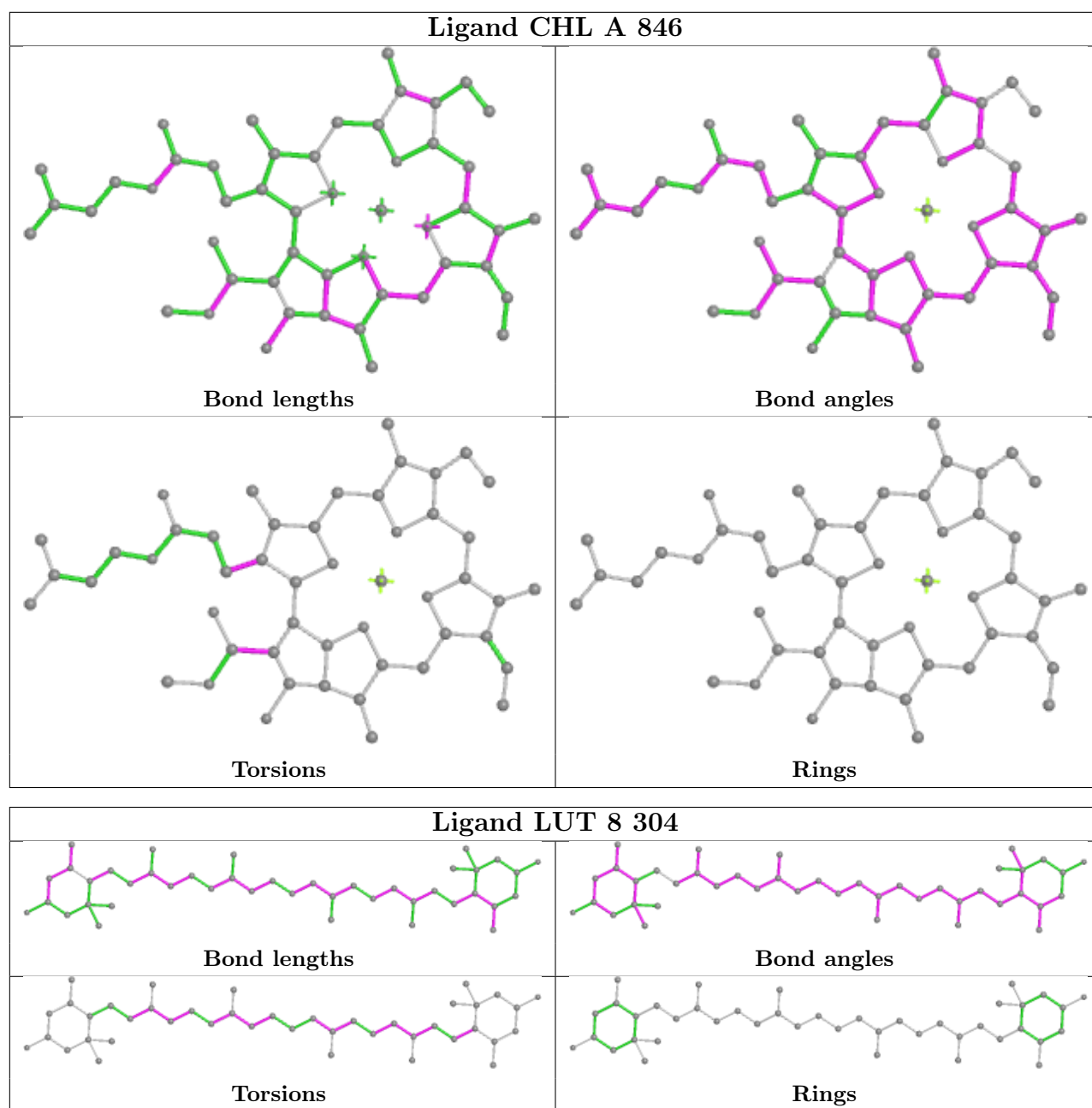
Bond angles

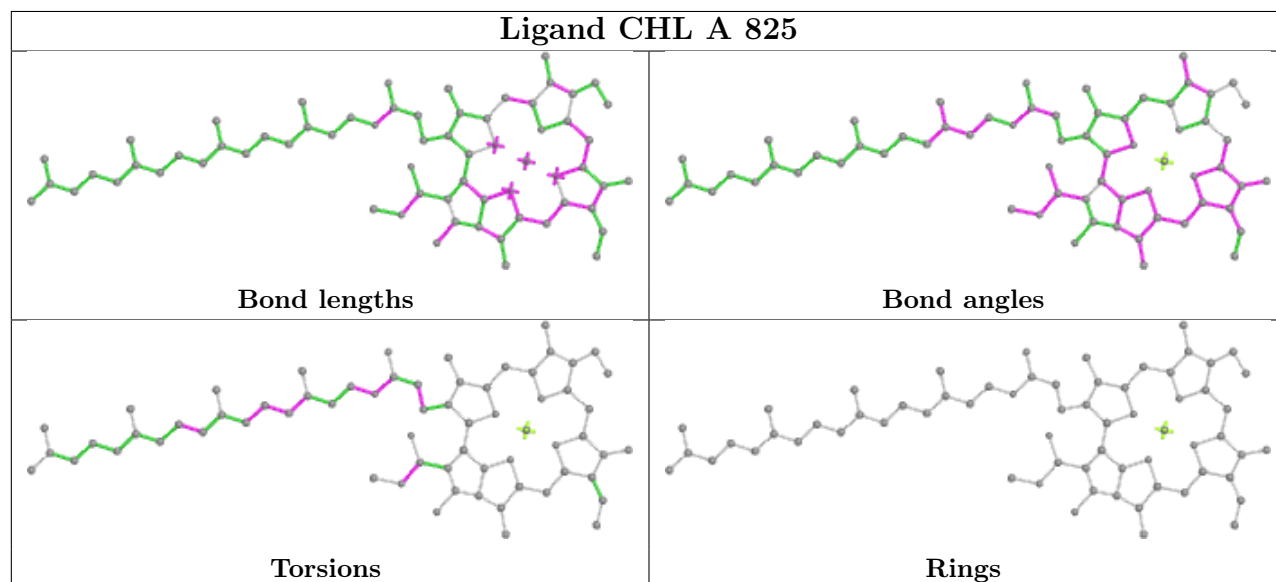
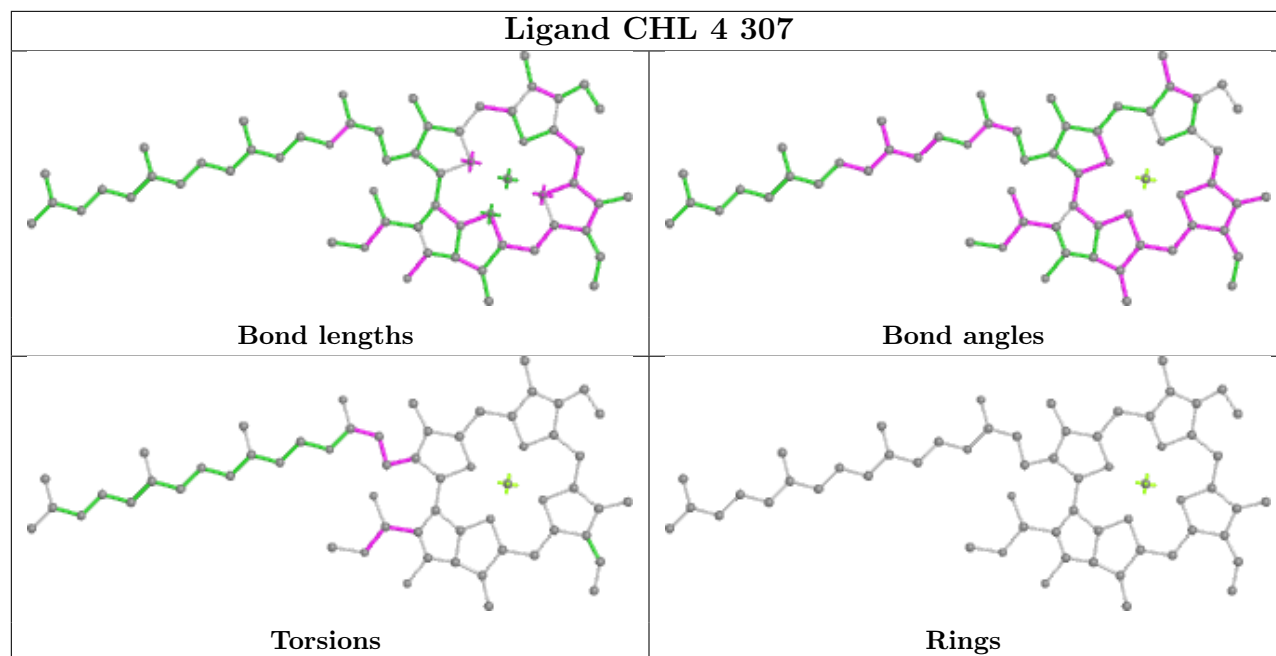


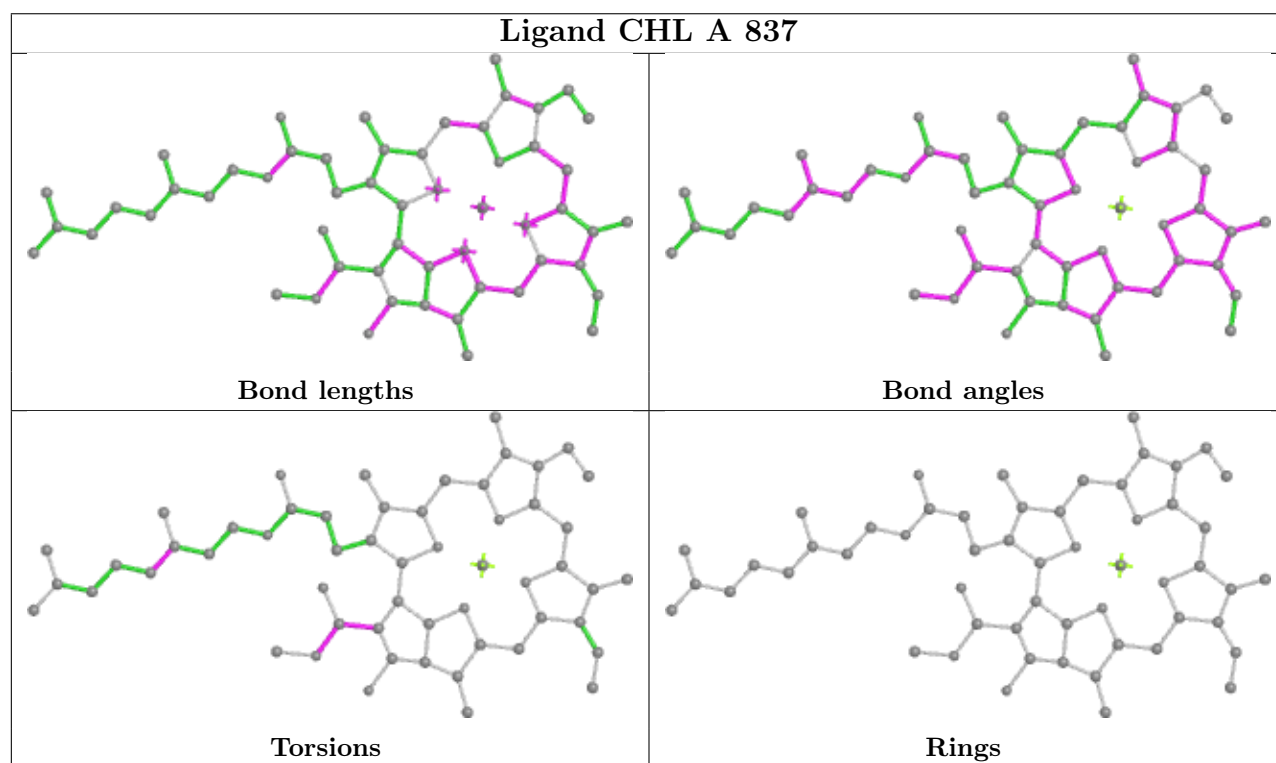
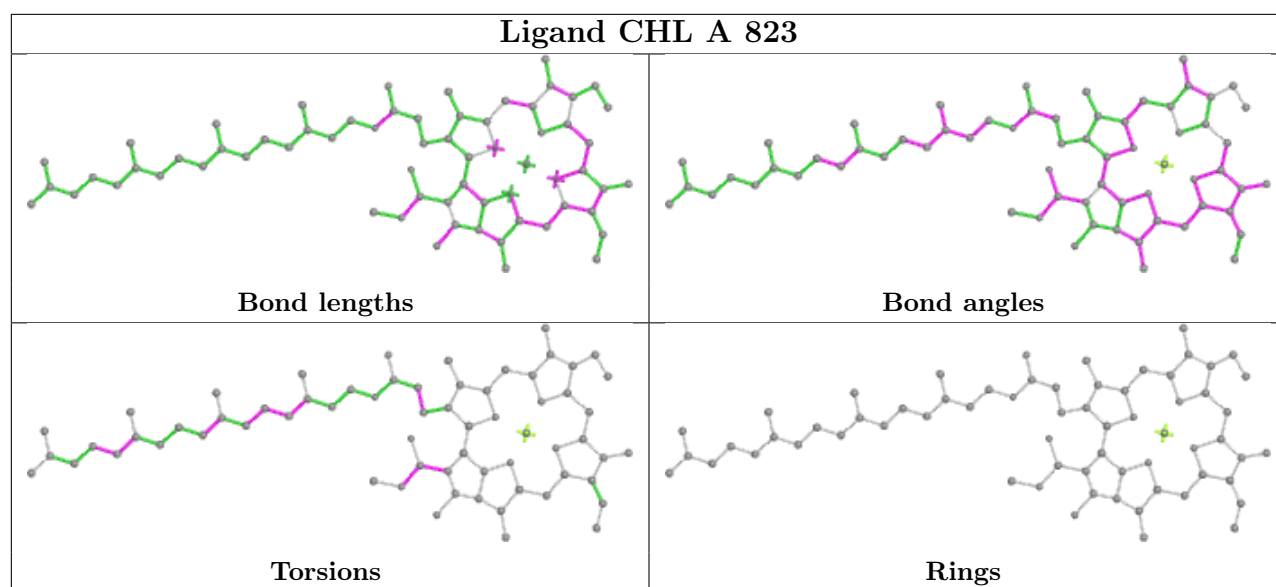
Torsions



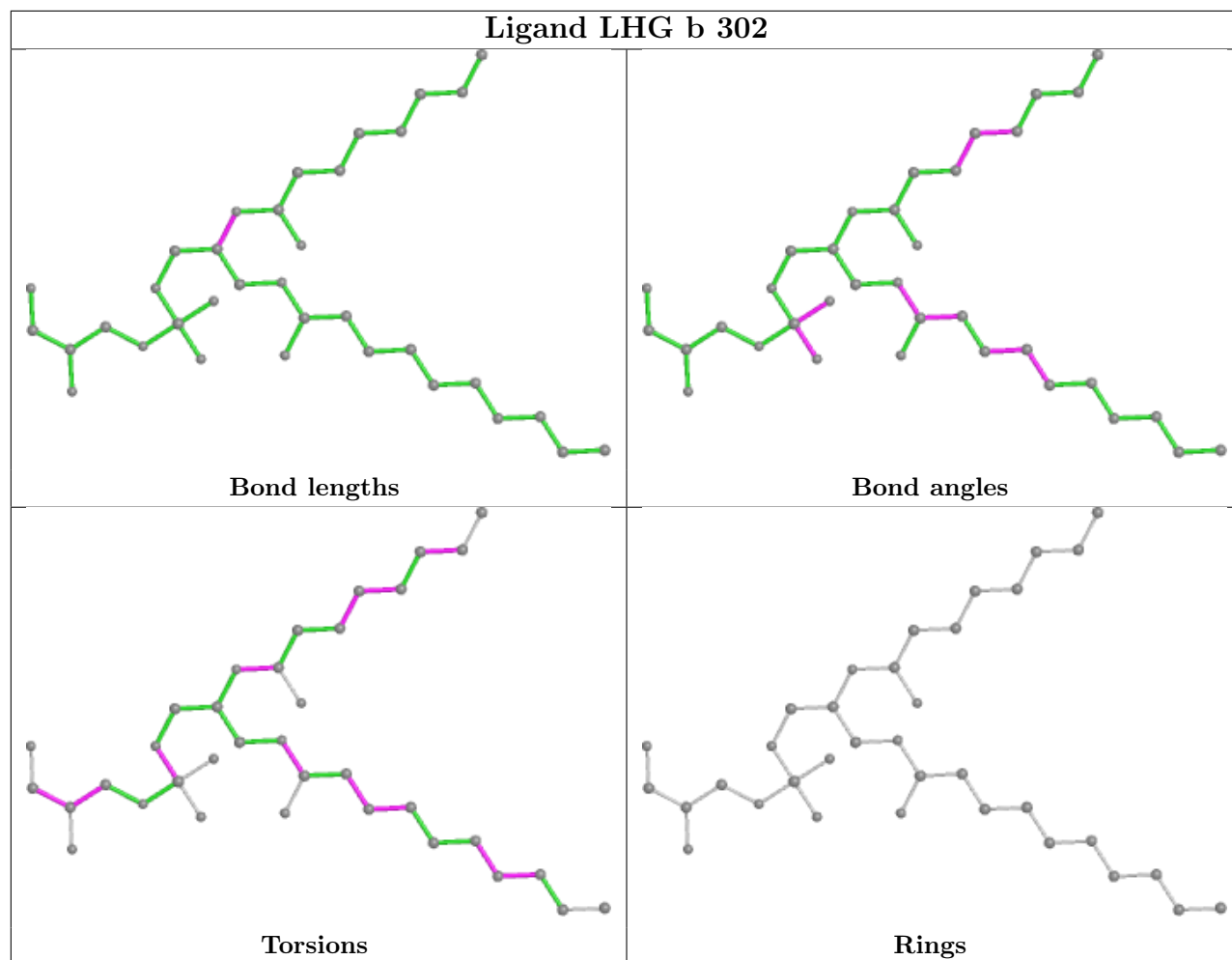
Rings



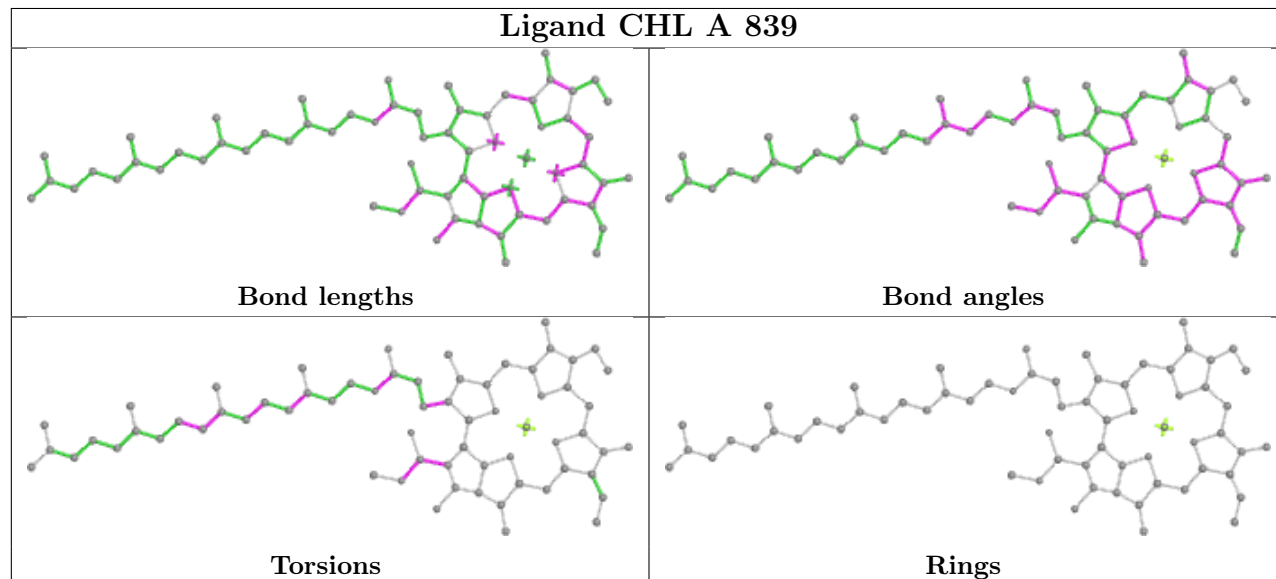


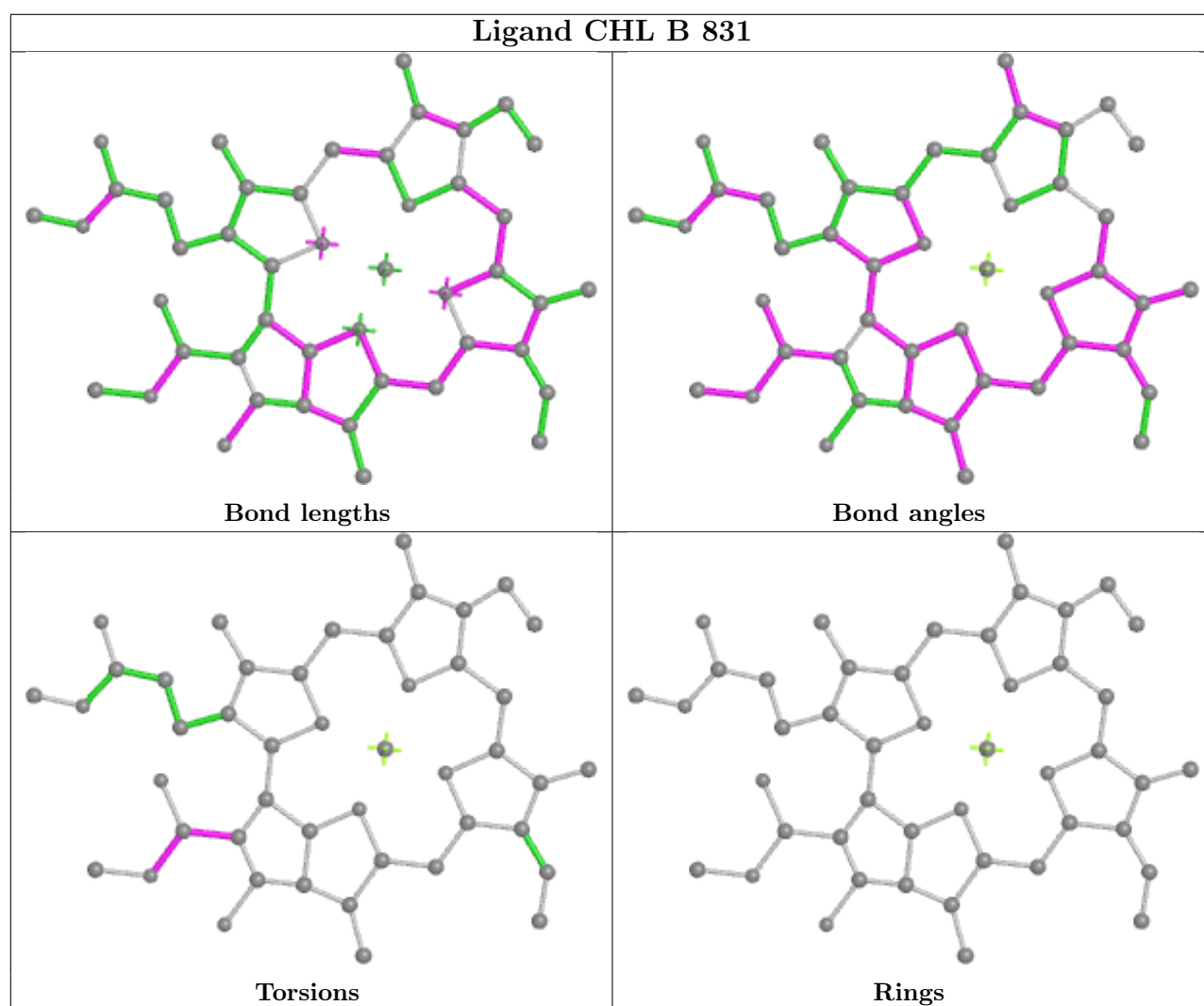
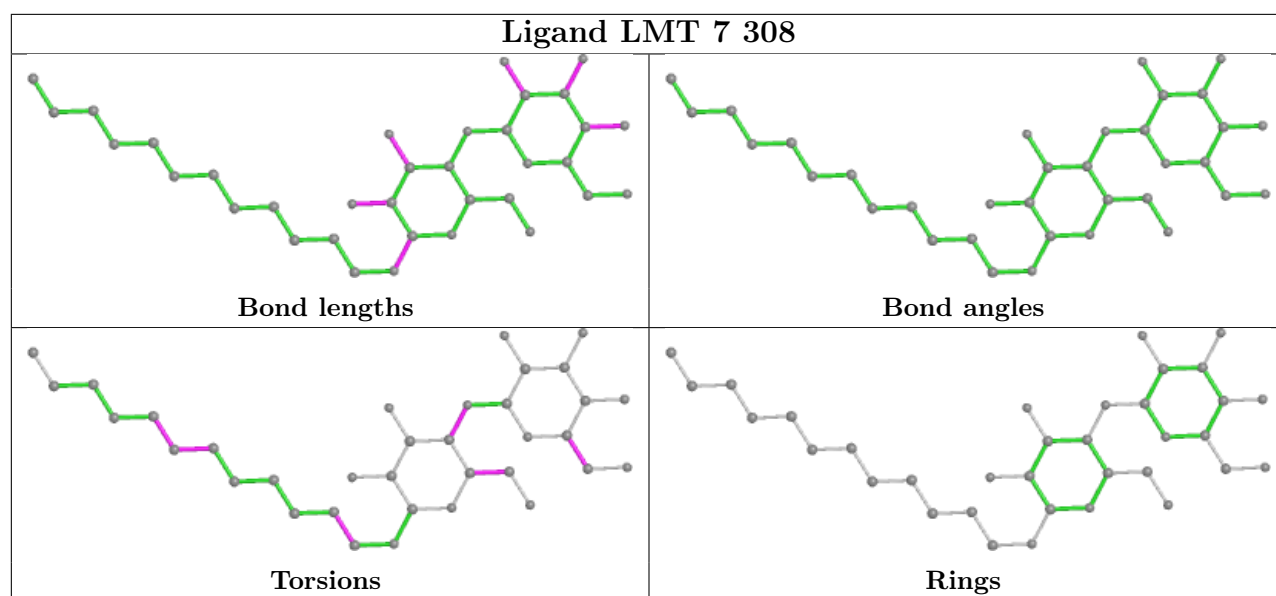


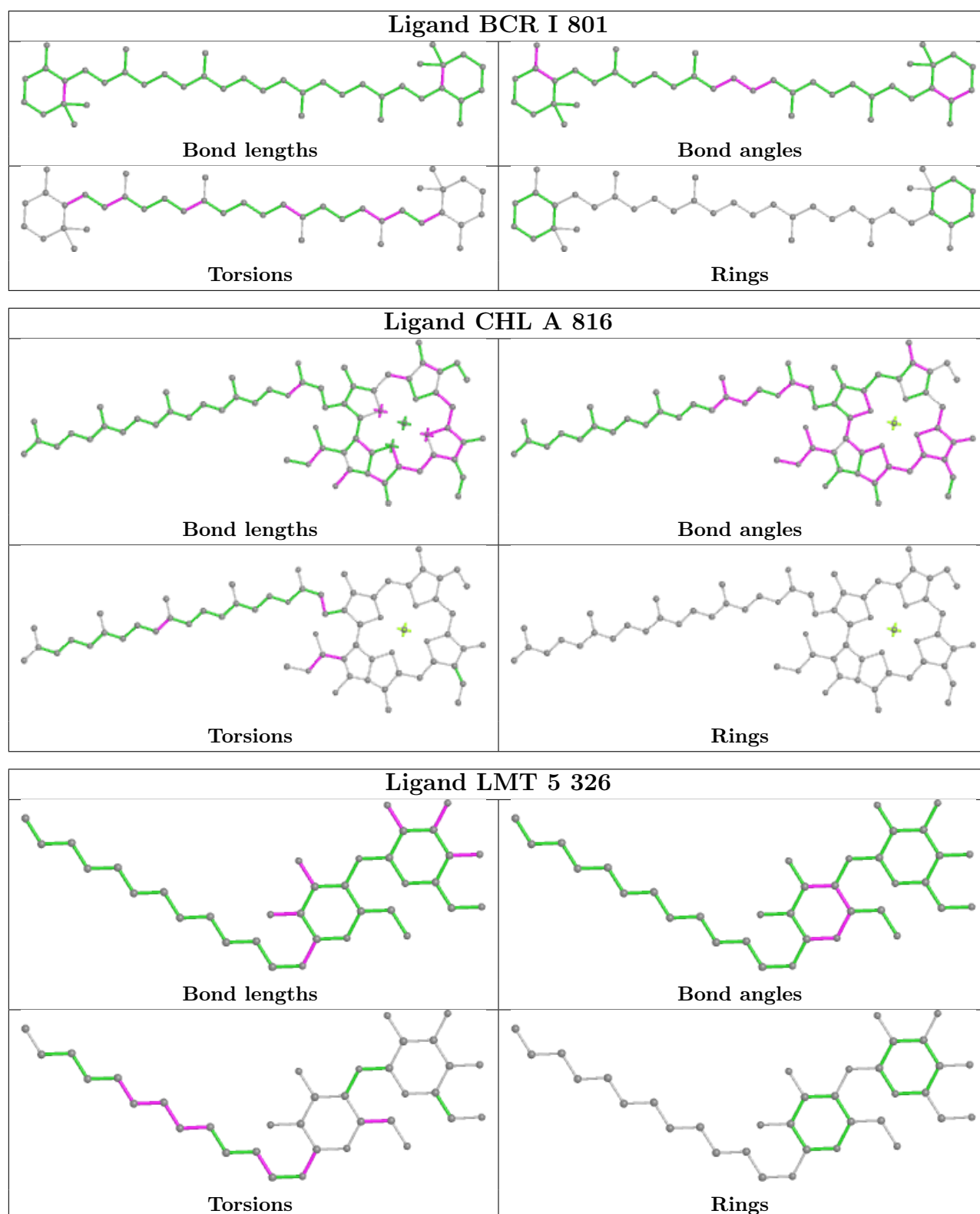
Ligand LHG b 302

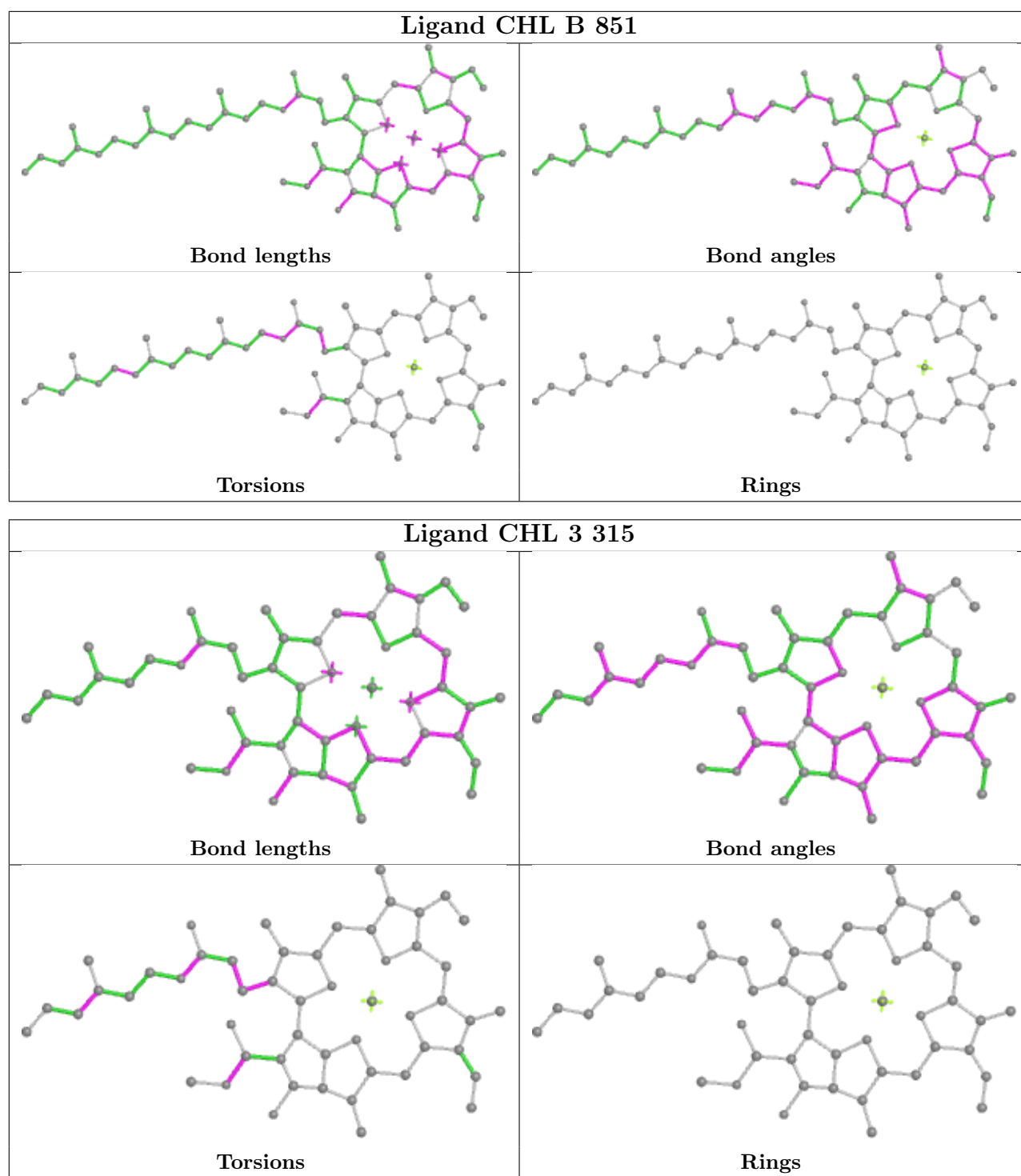


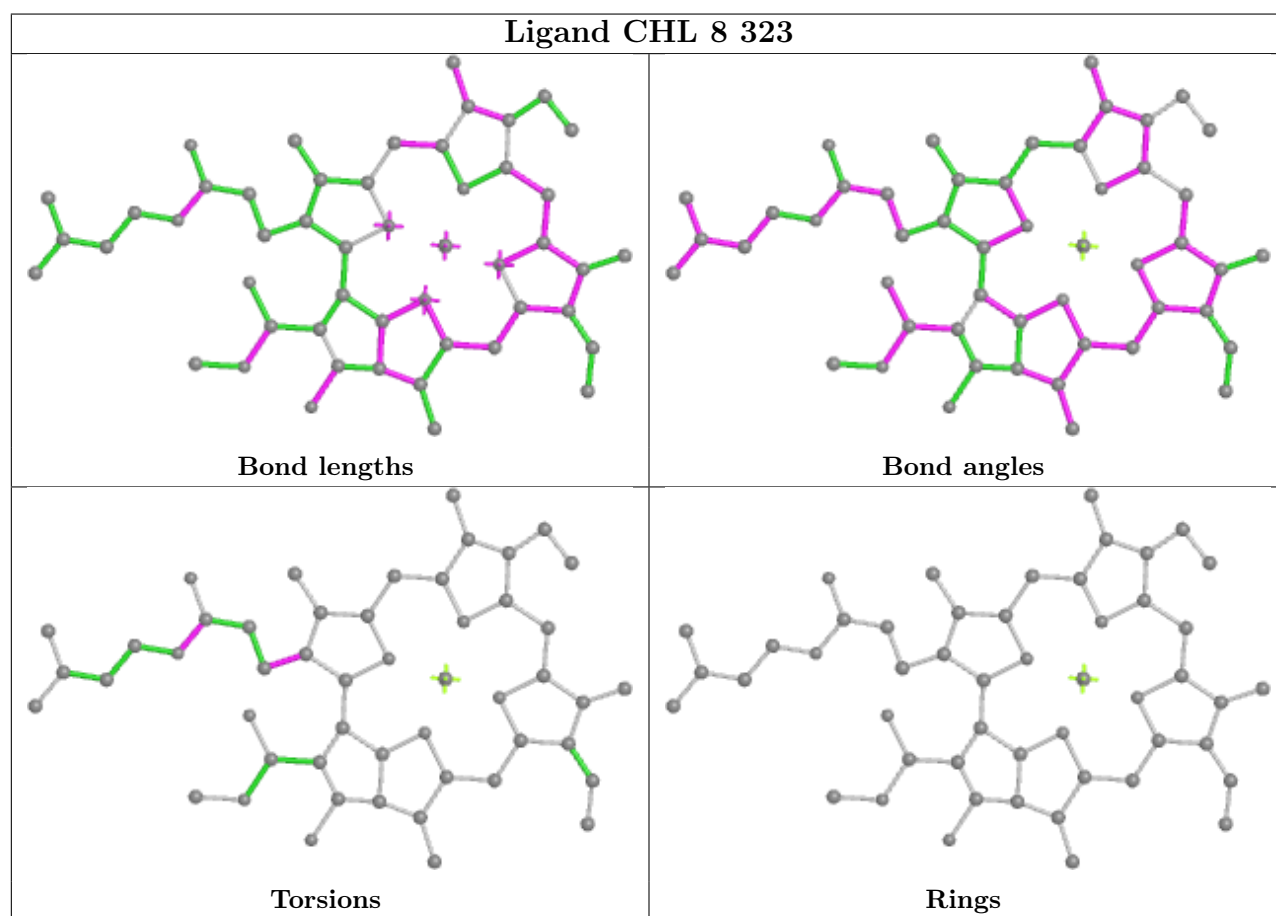
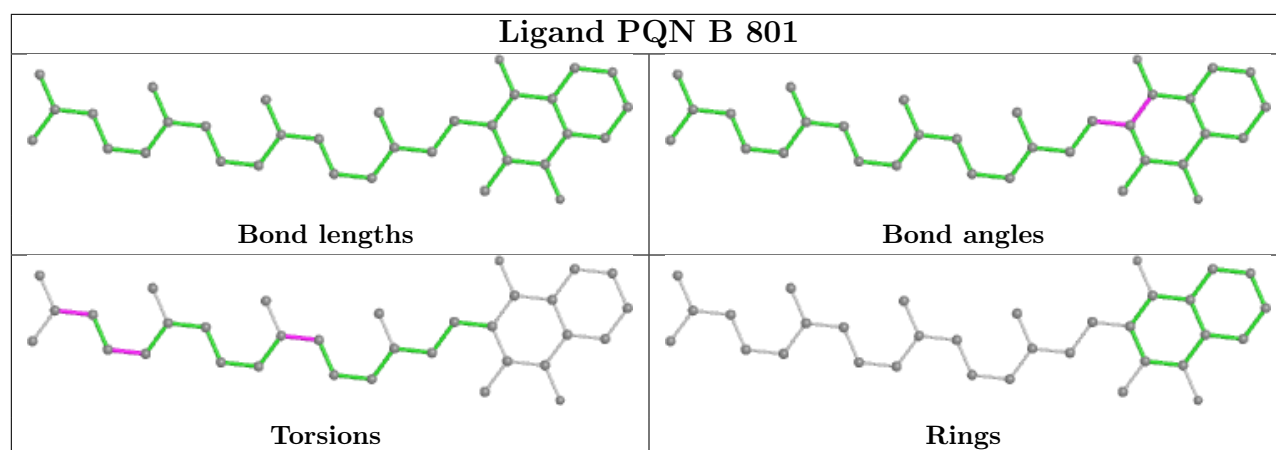
Ligand CHL A 839

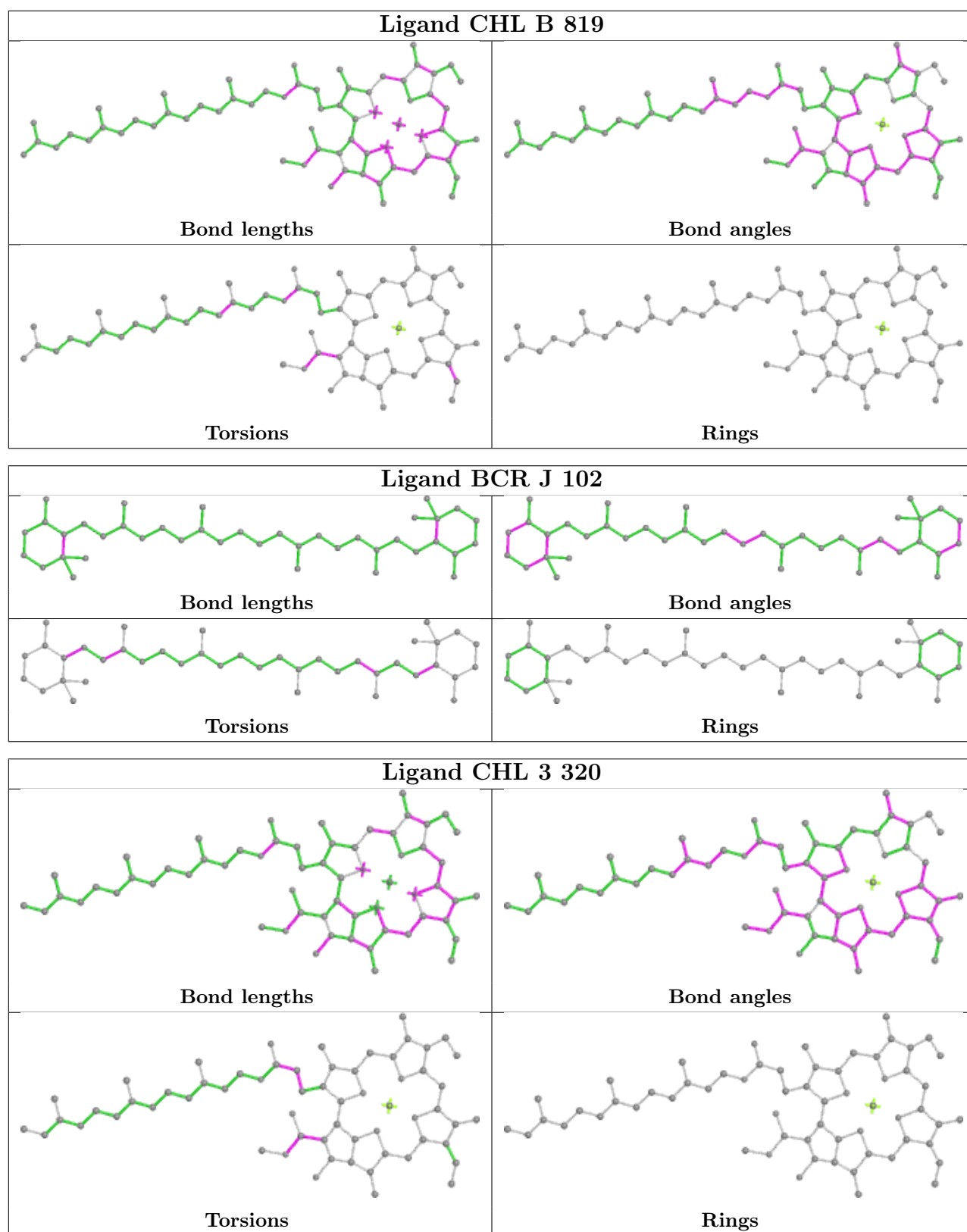


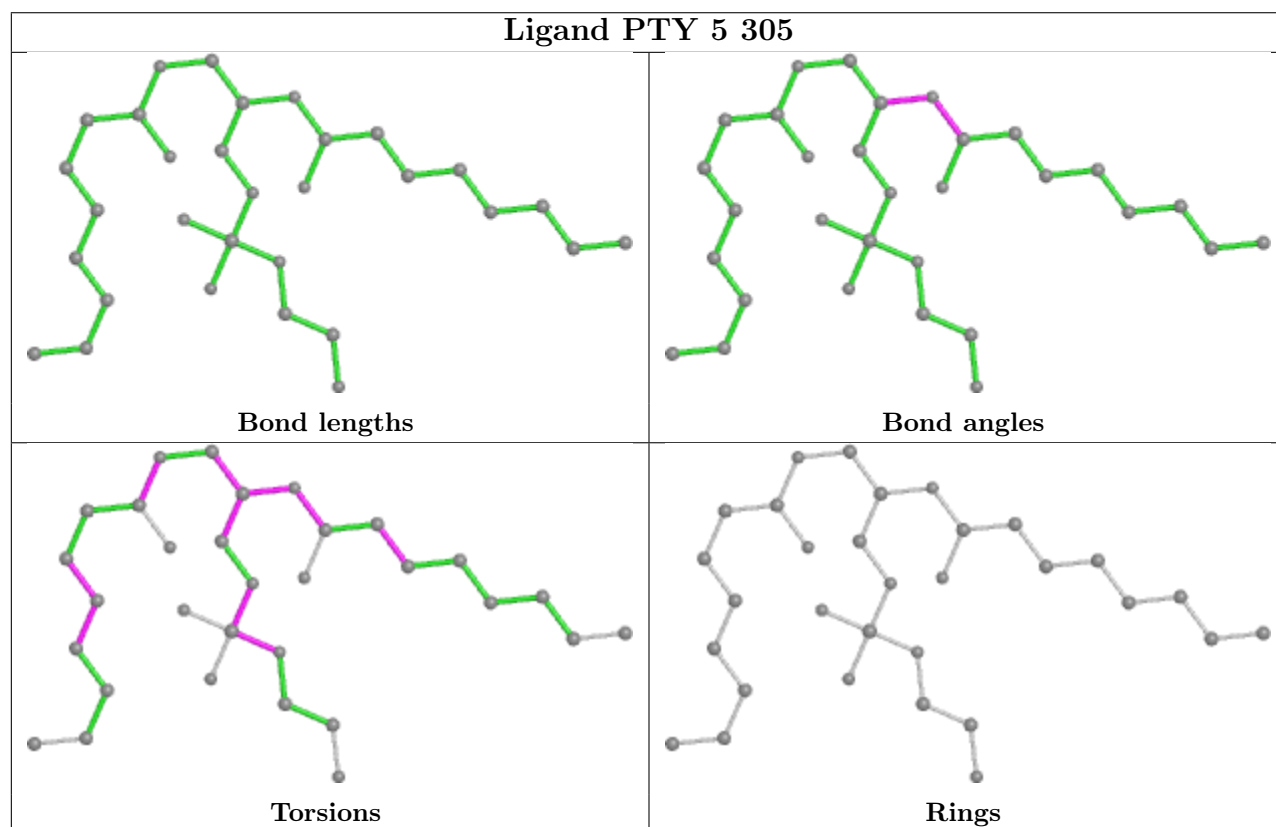
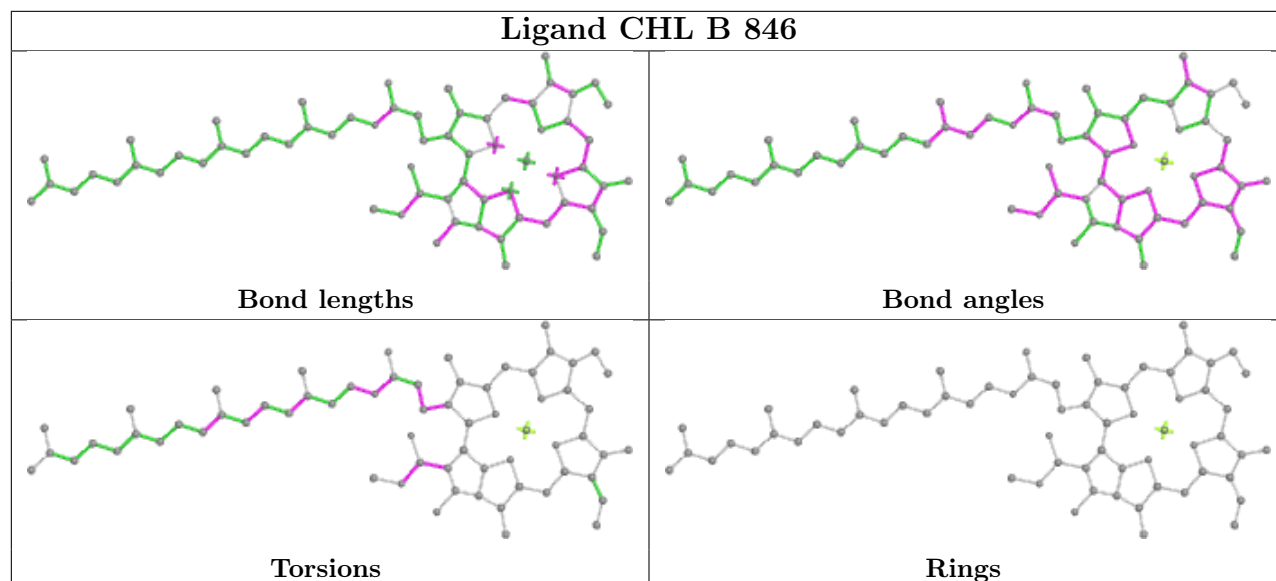
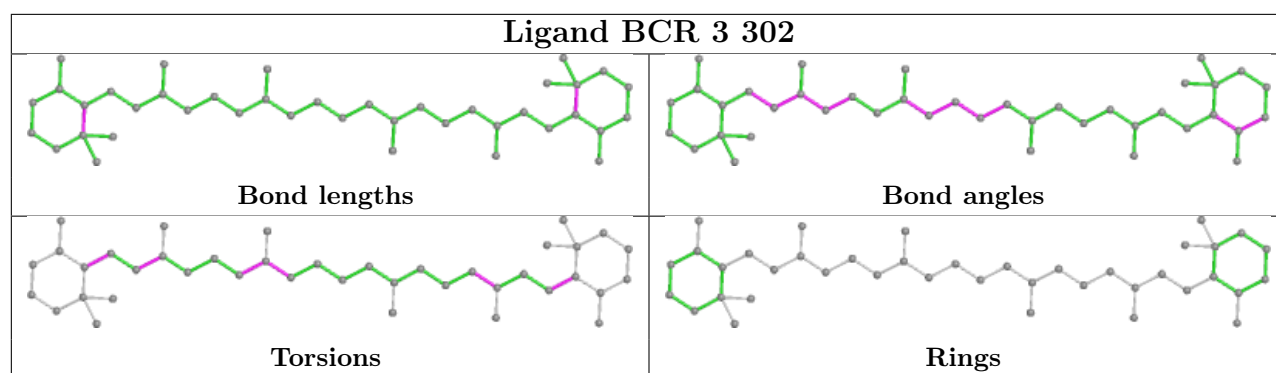


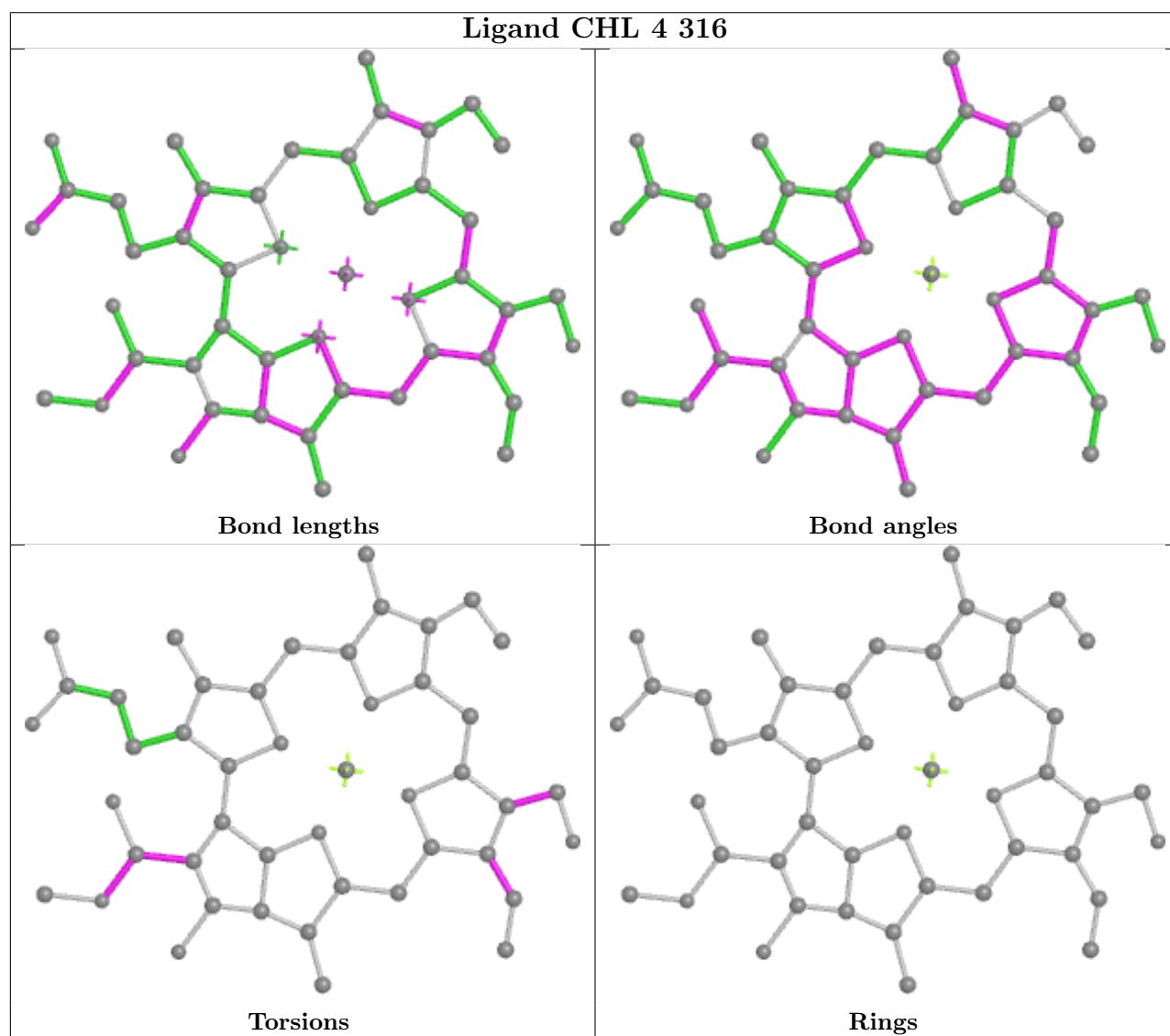
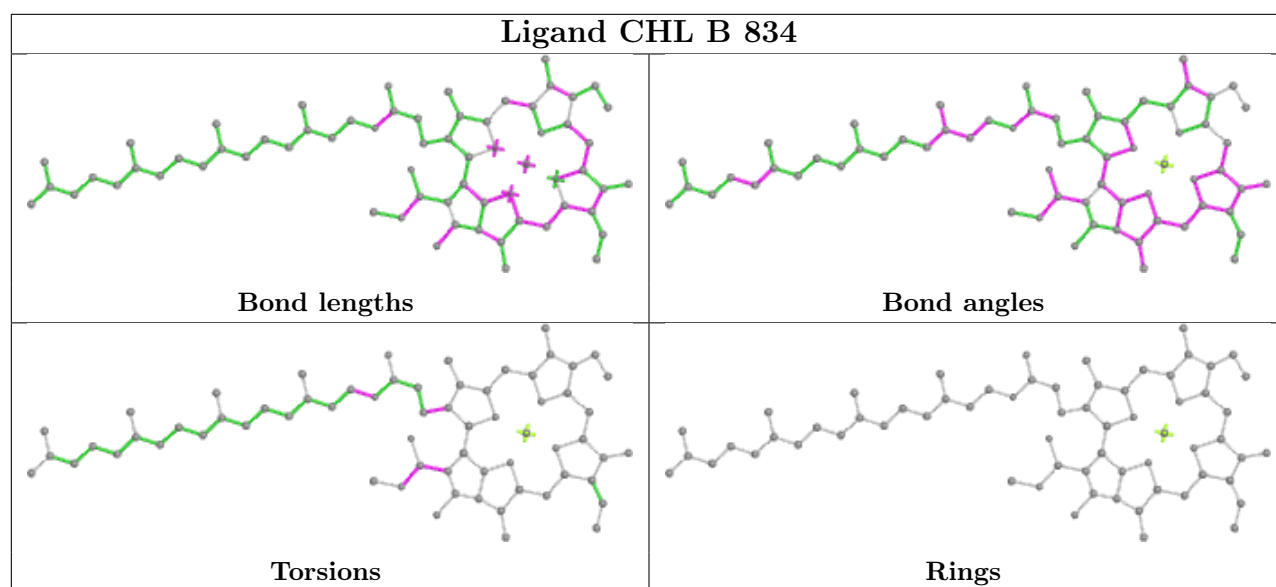


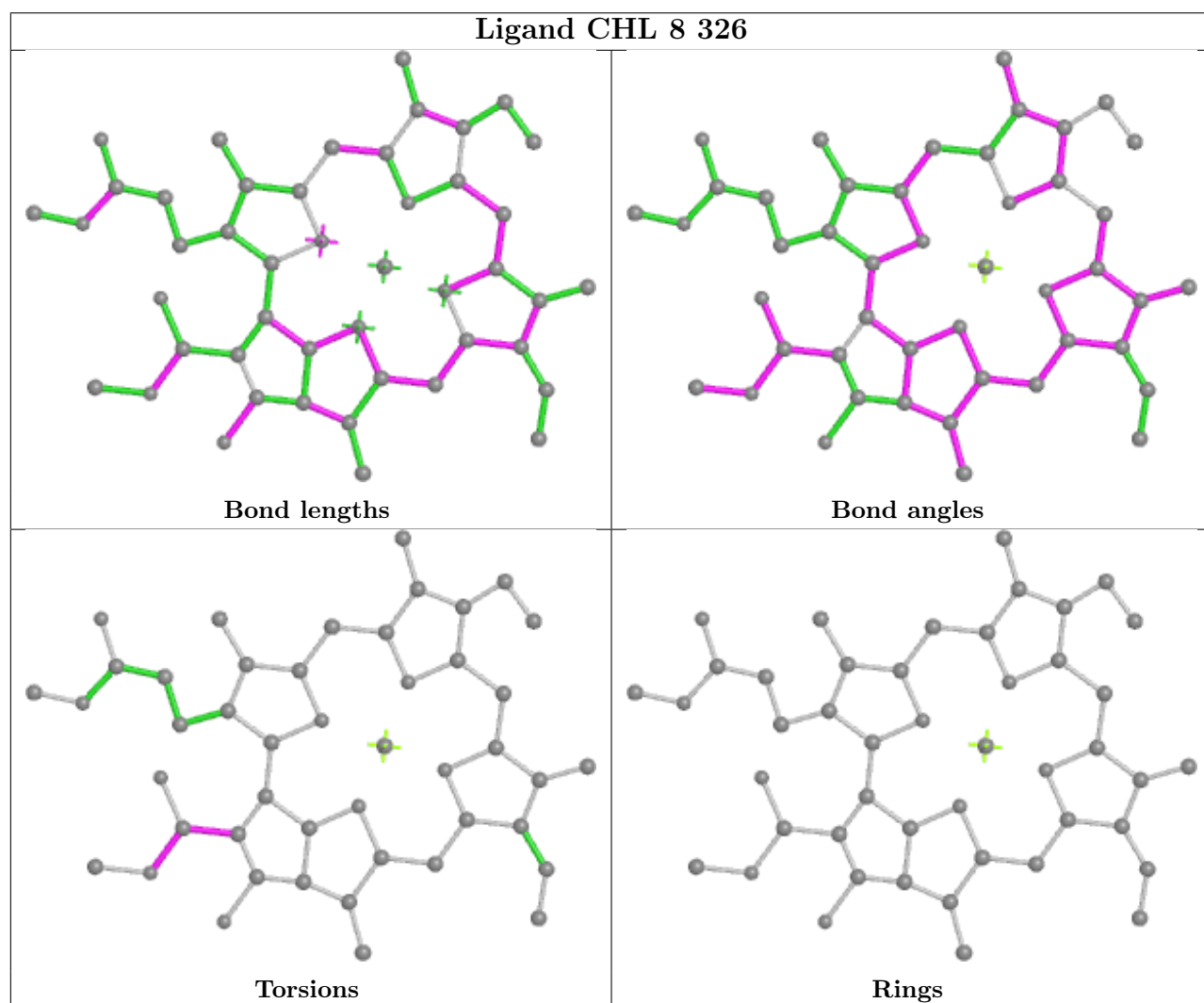
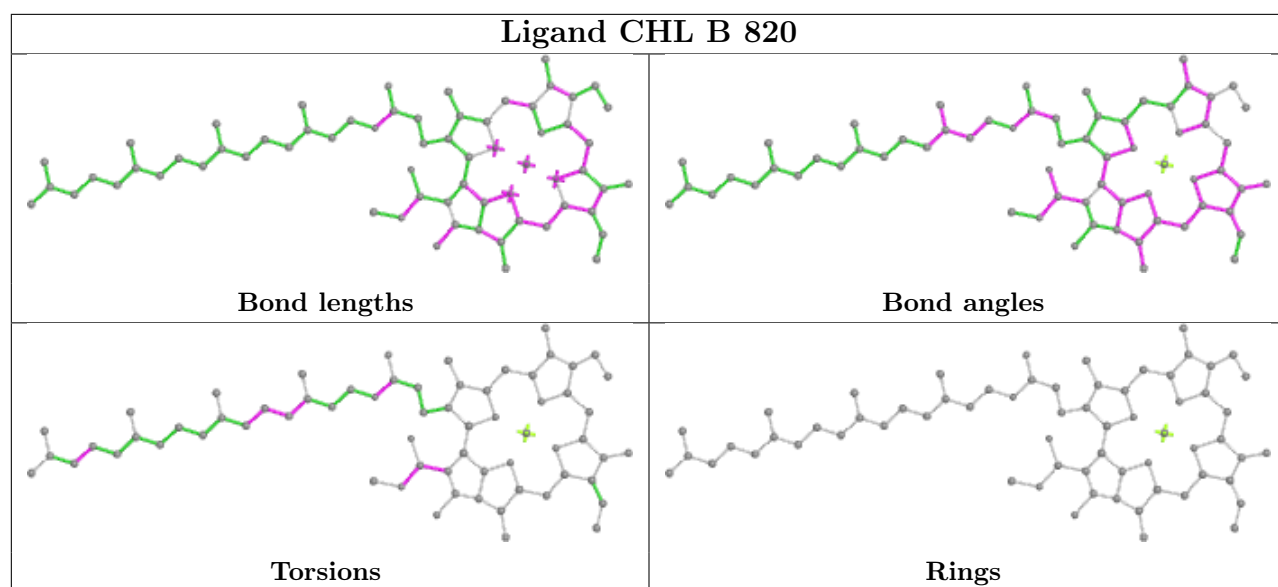


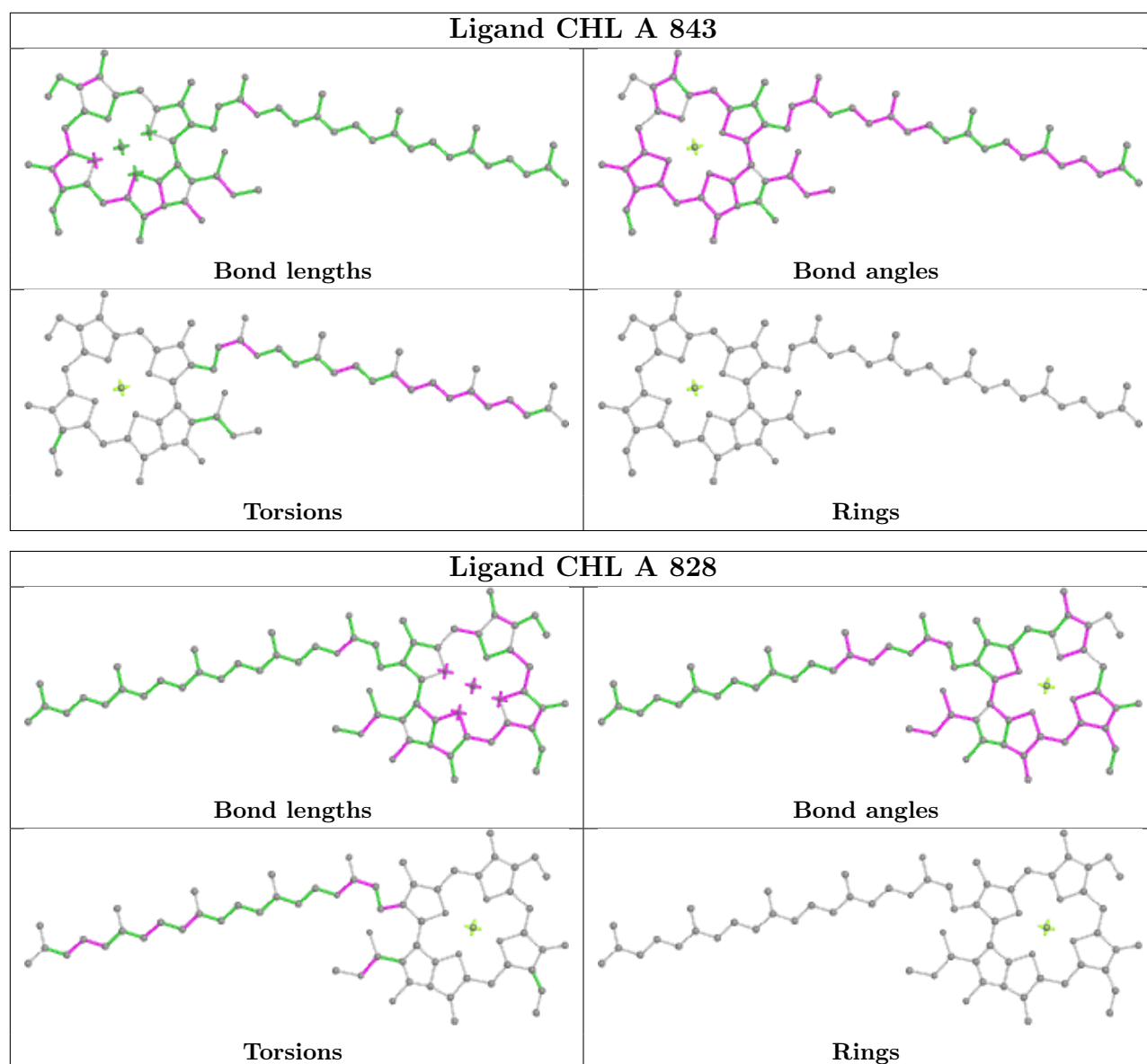


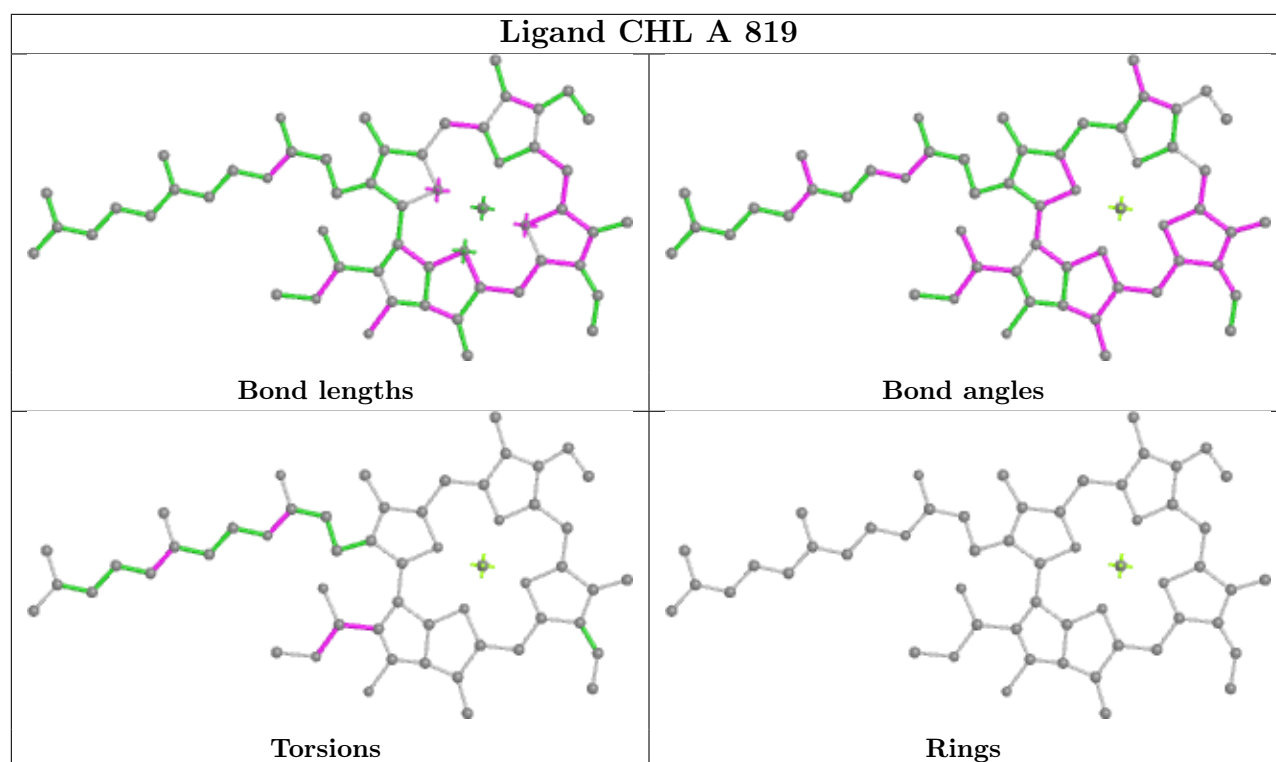




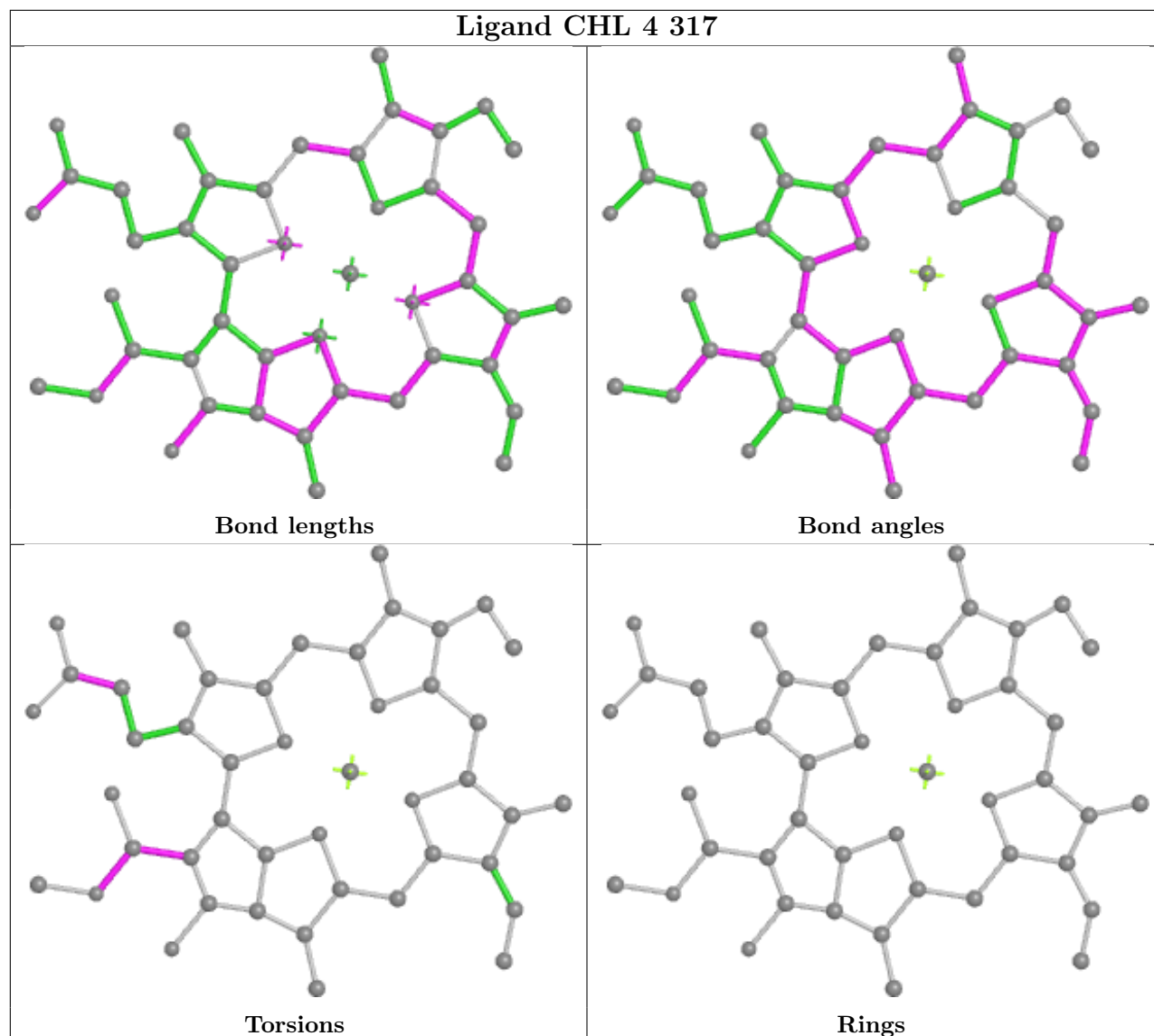




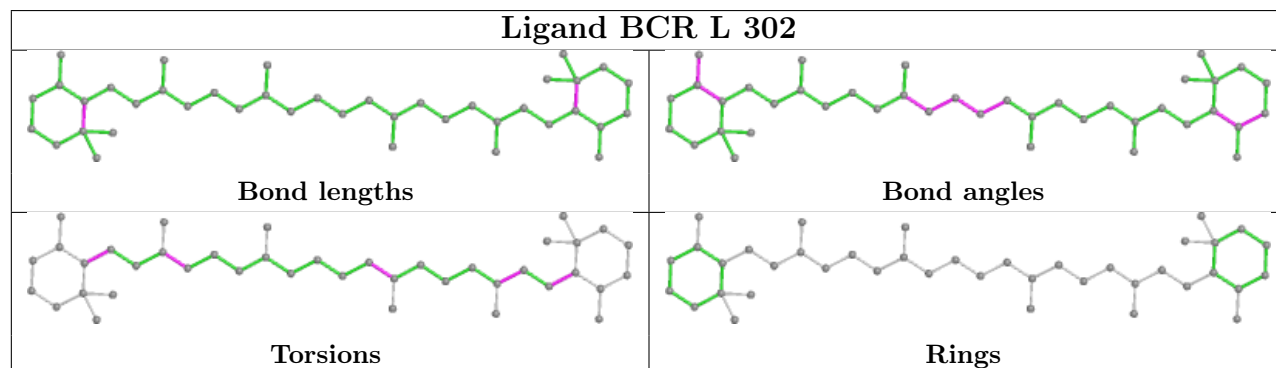


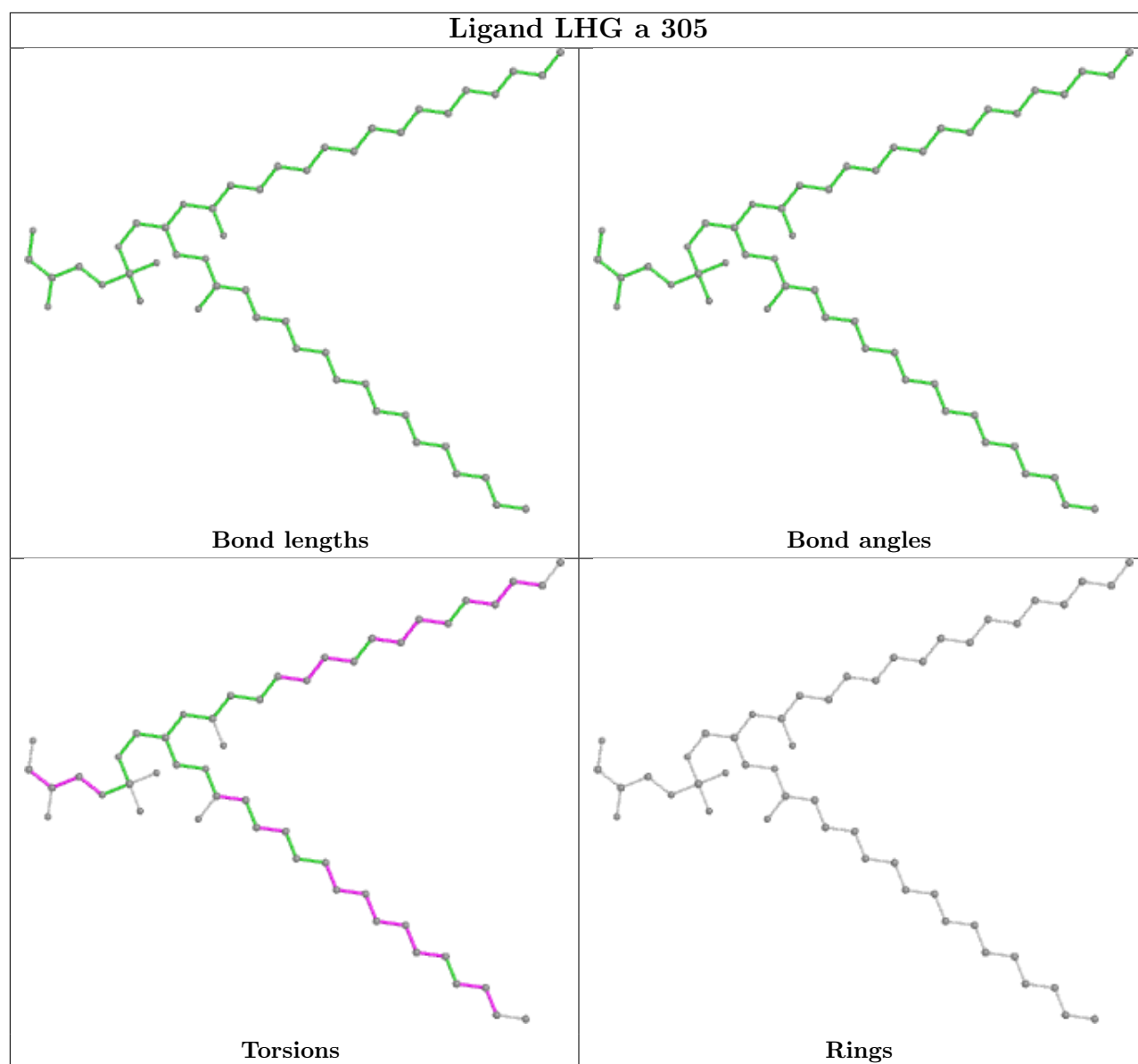


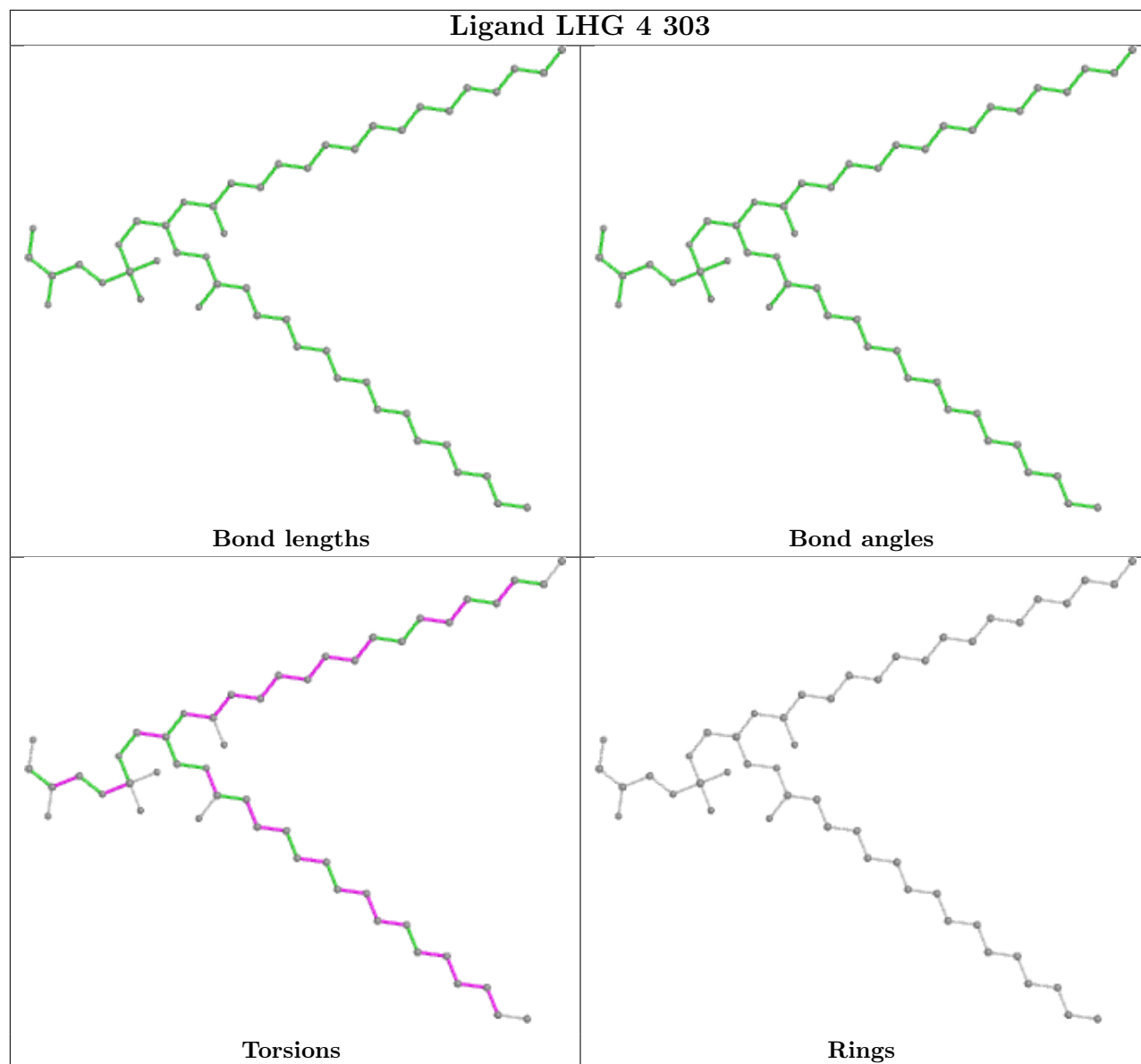
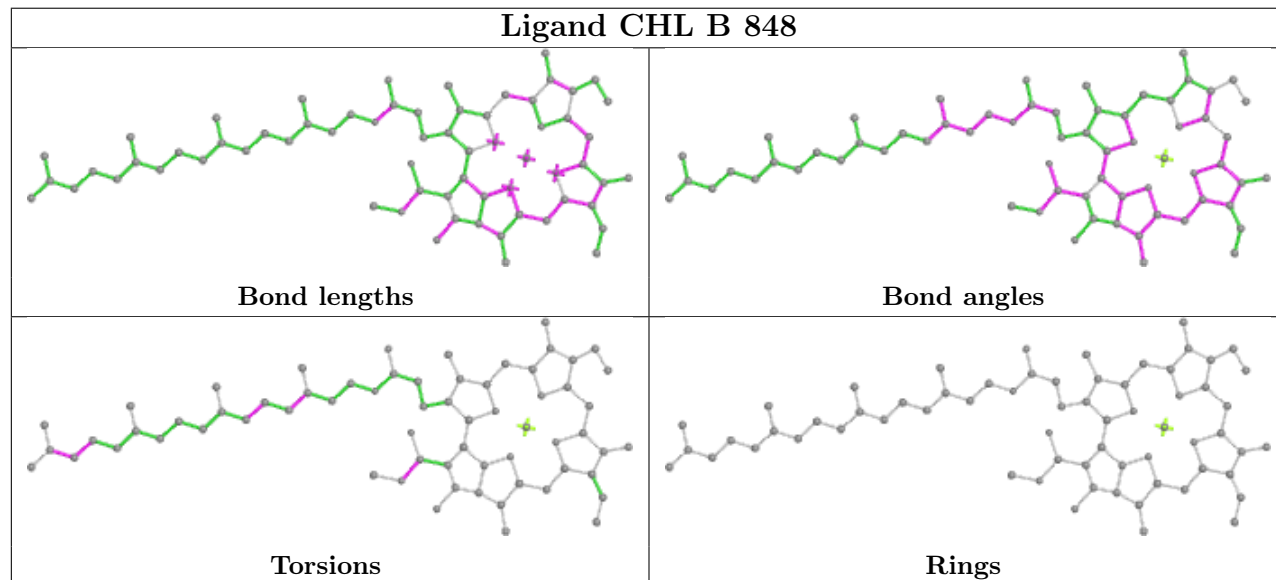
Ligand CHL 4 317

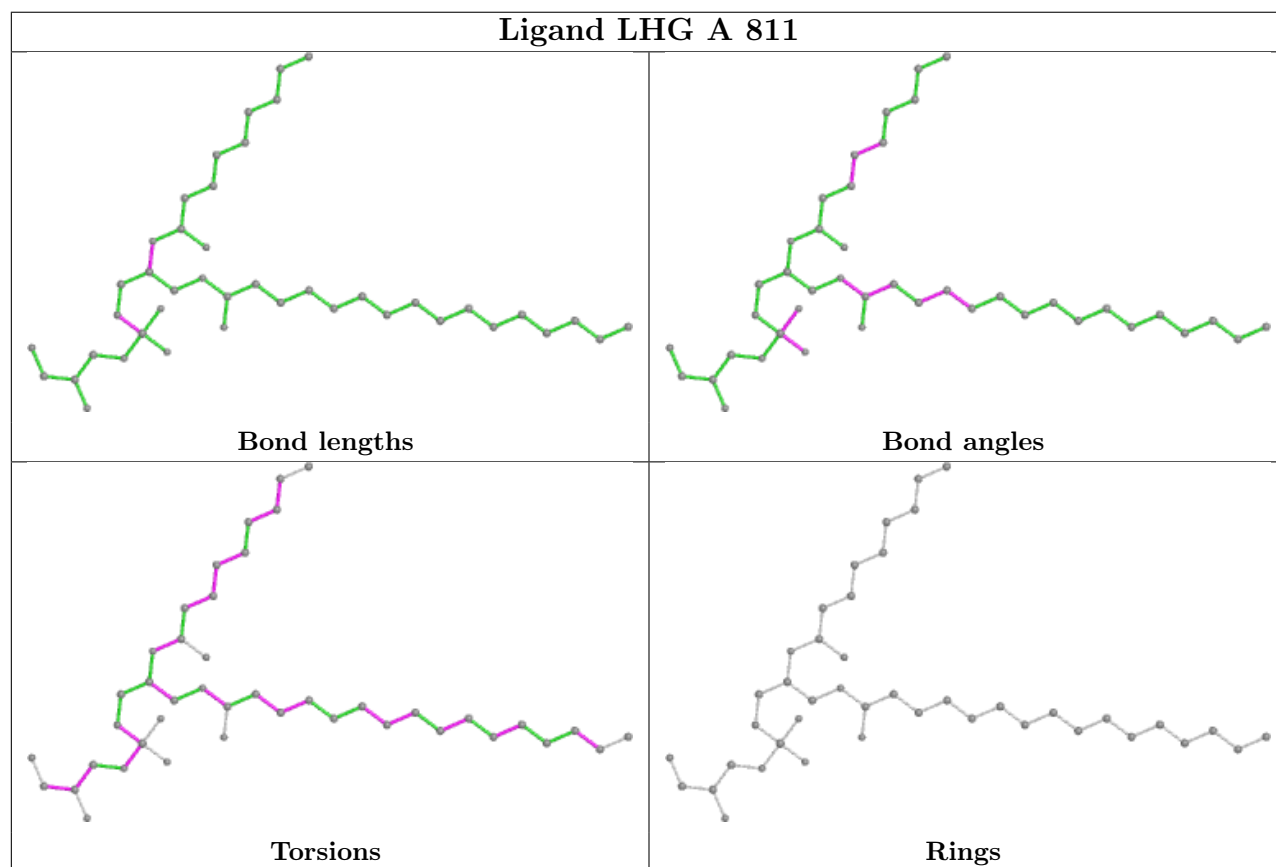
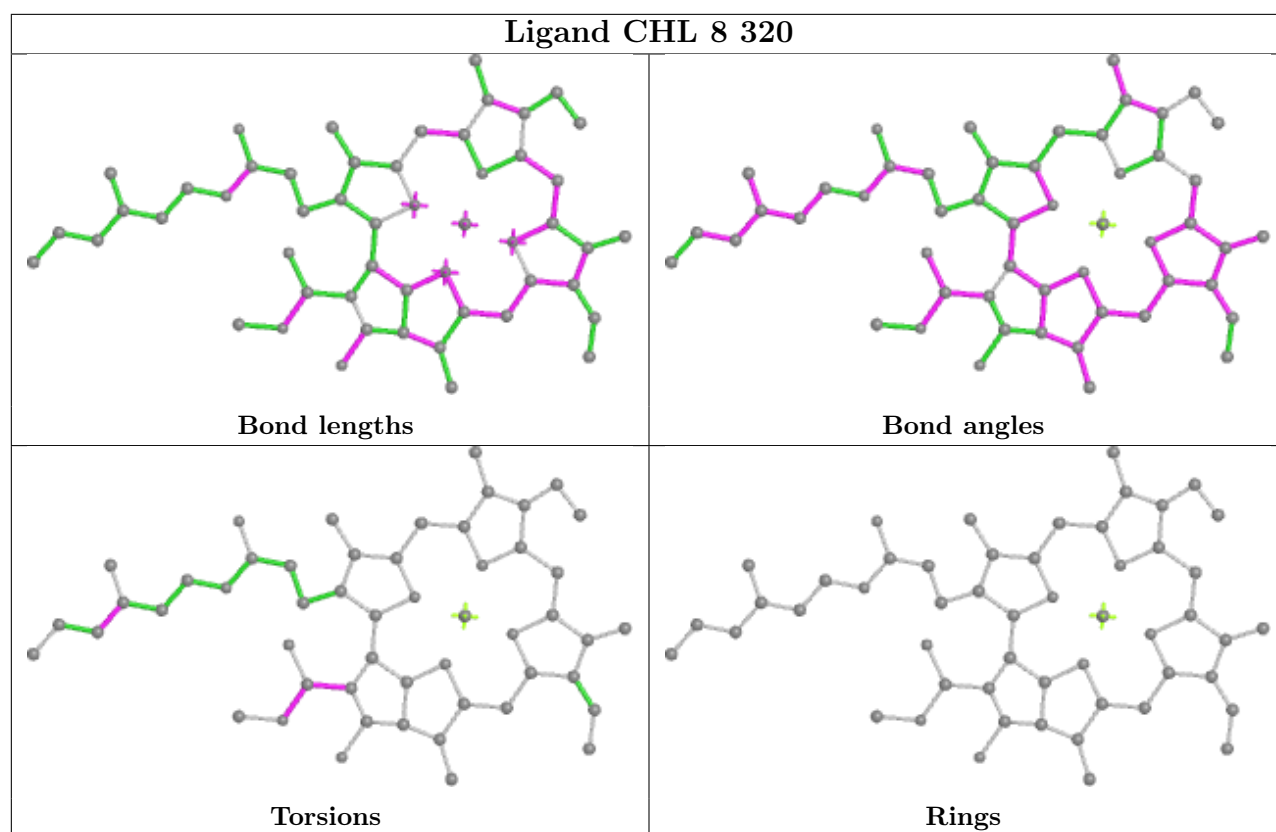


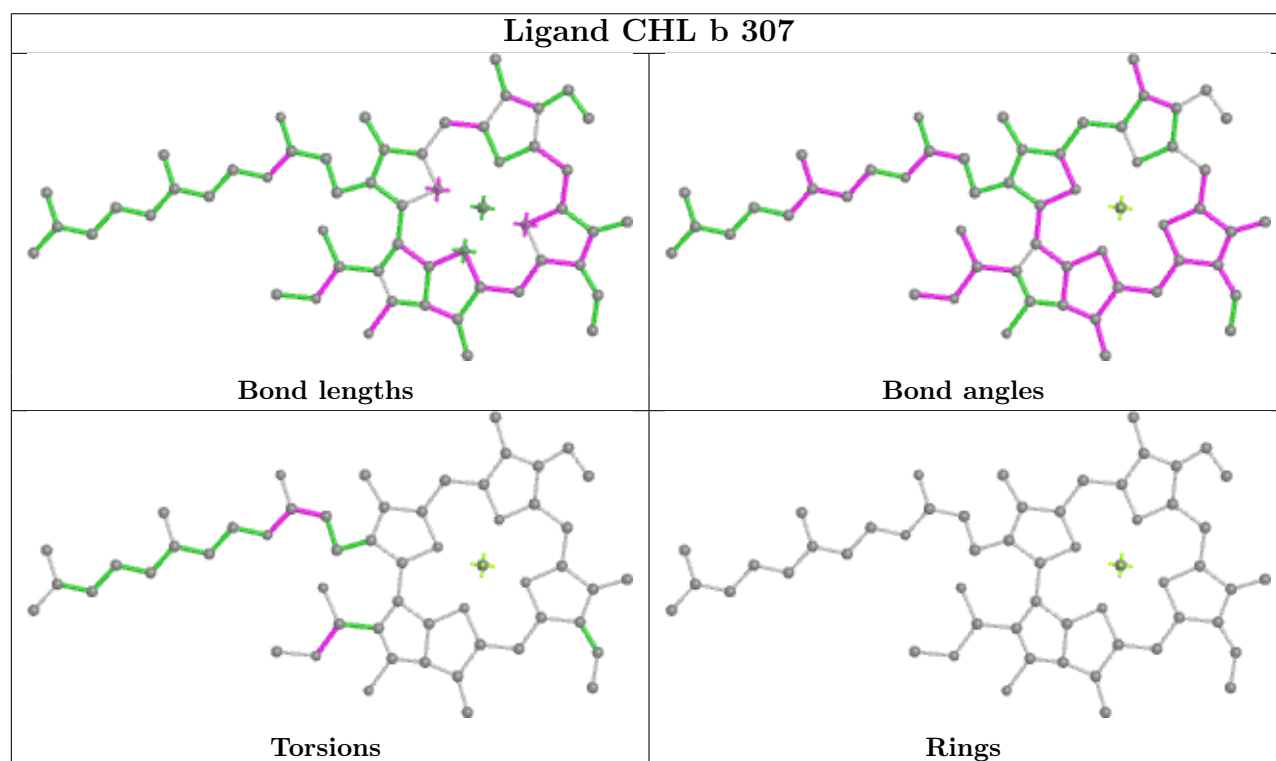
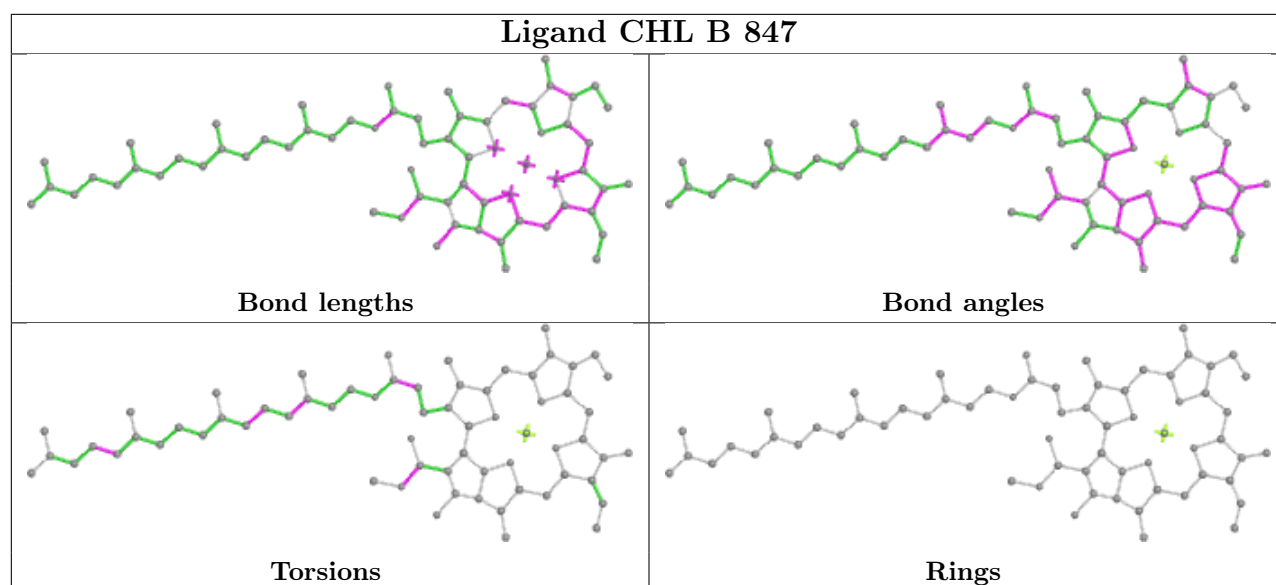
Ligand BCR L 302



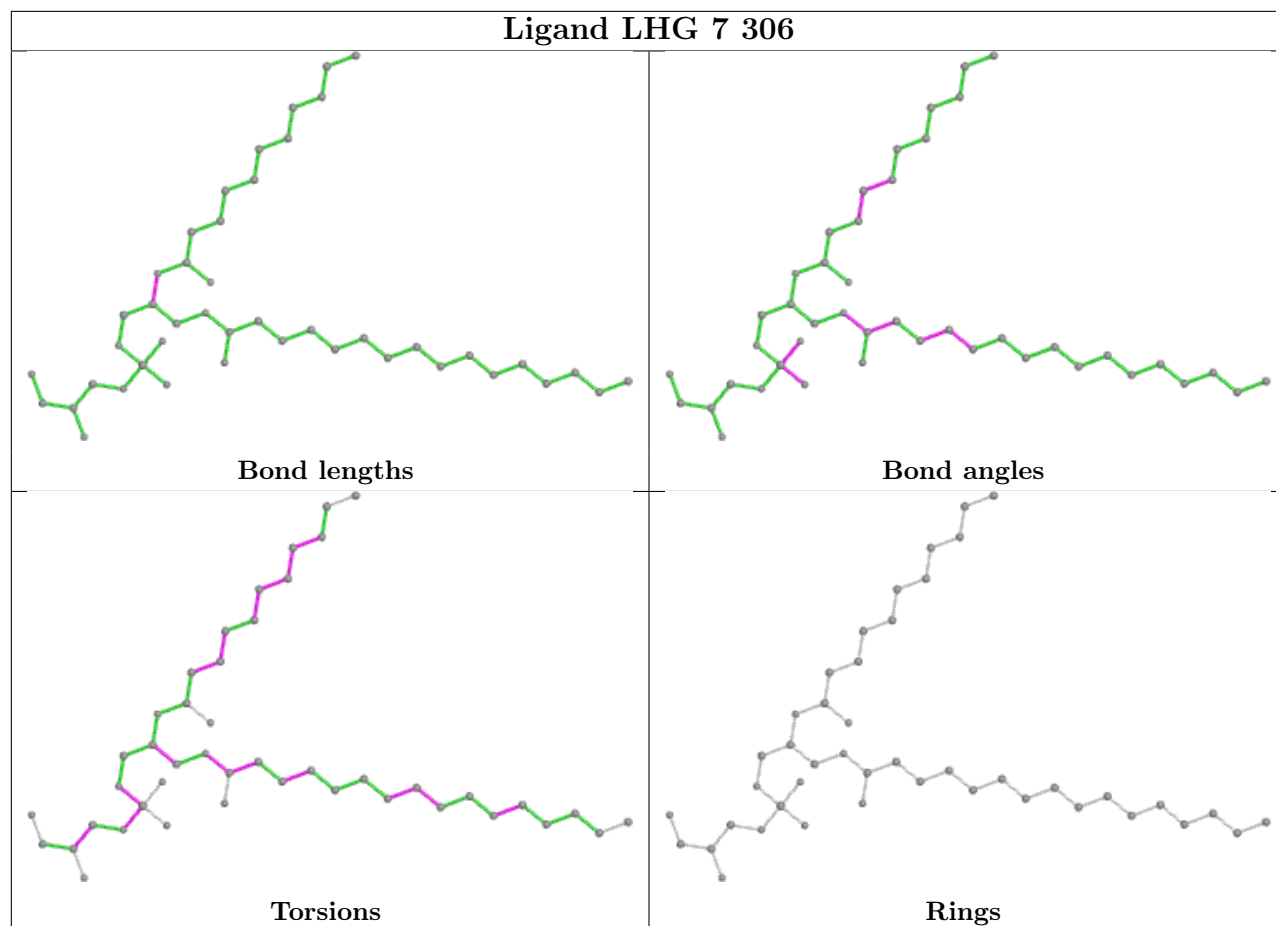


Ligand LHG 4 303**Ligand CHL B 848**

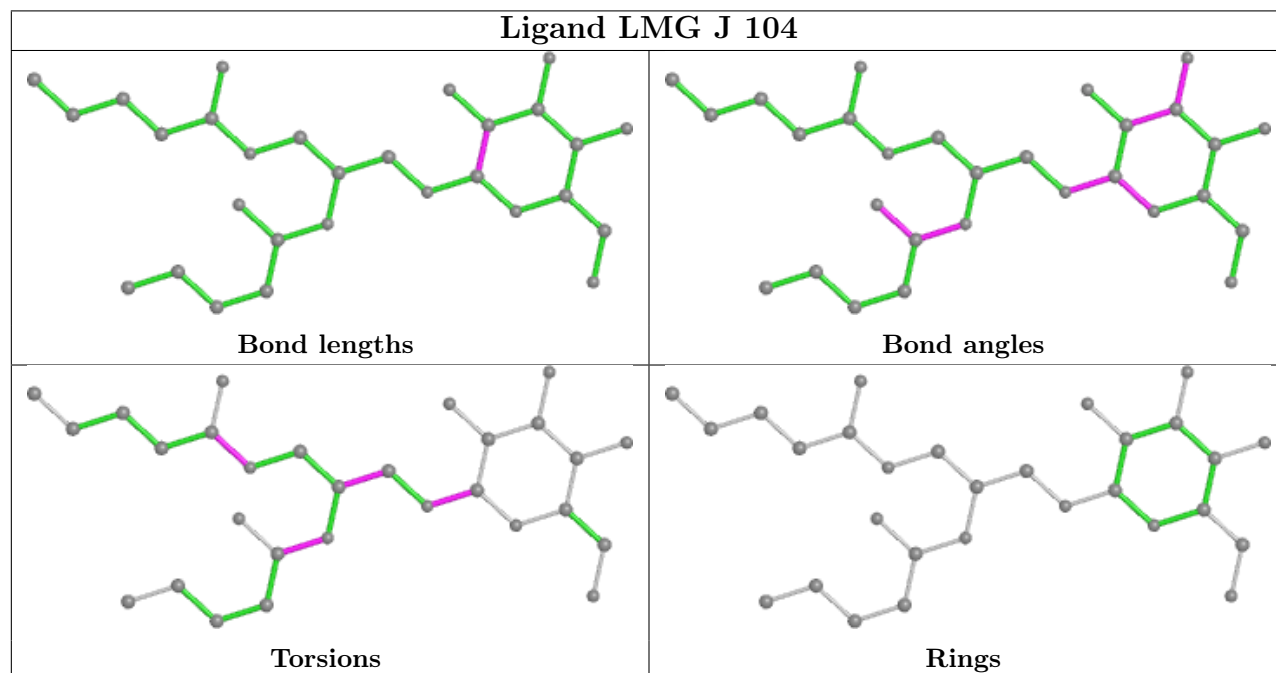


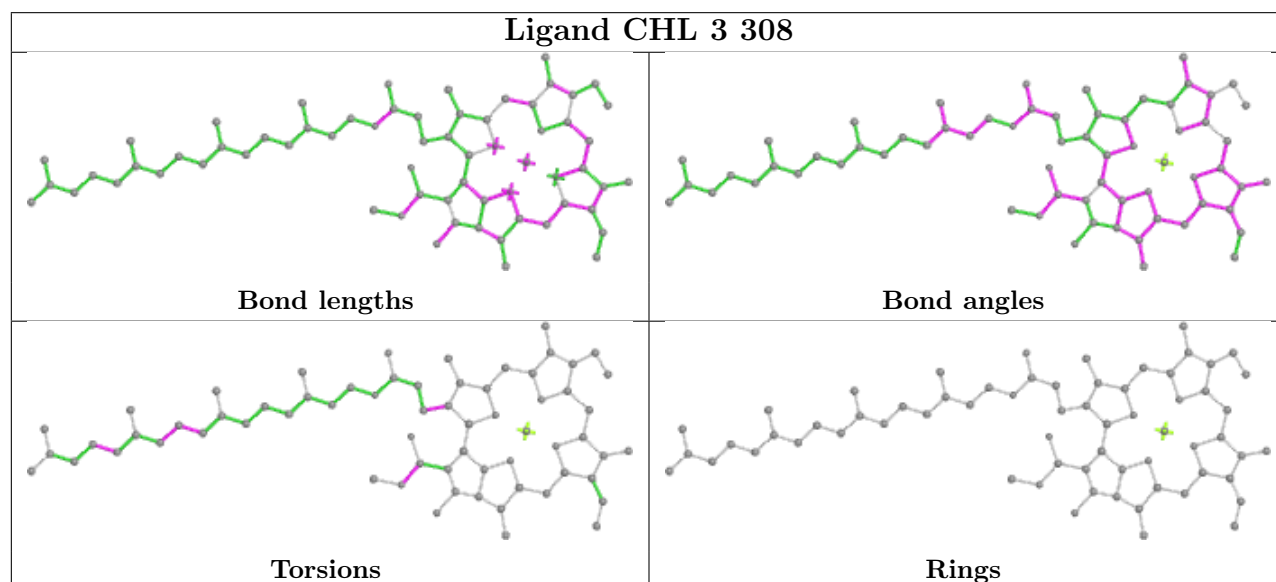
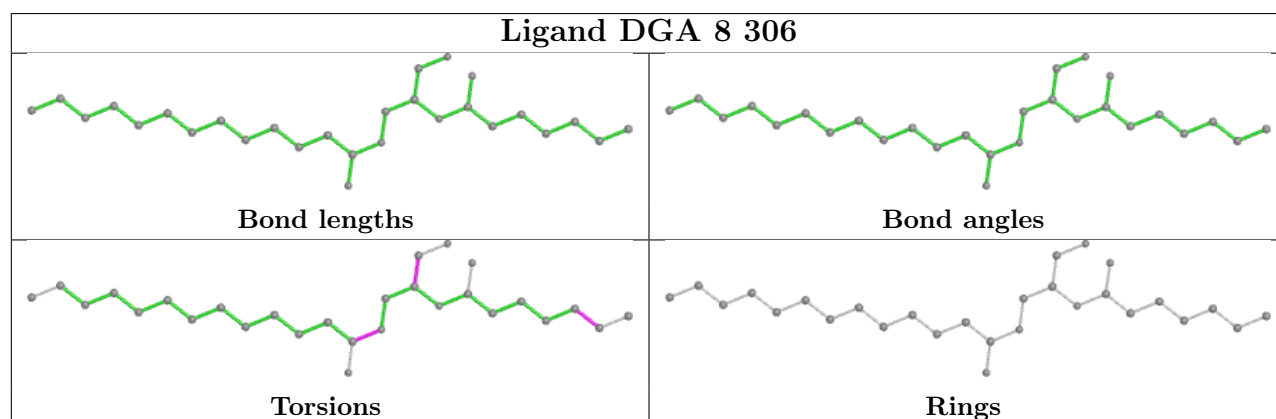
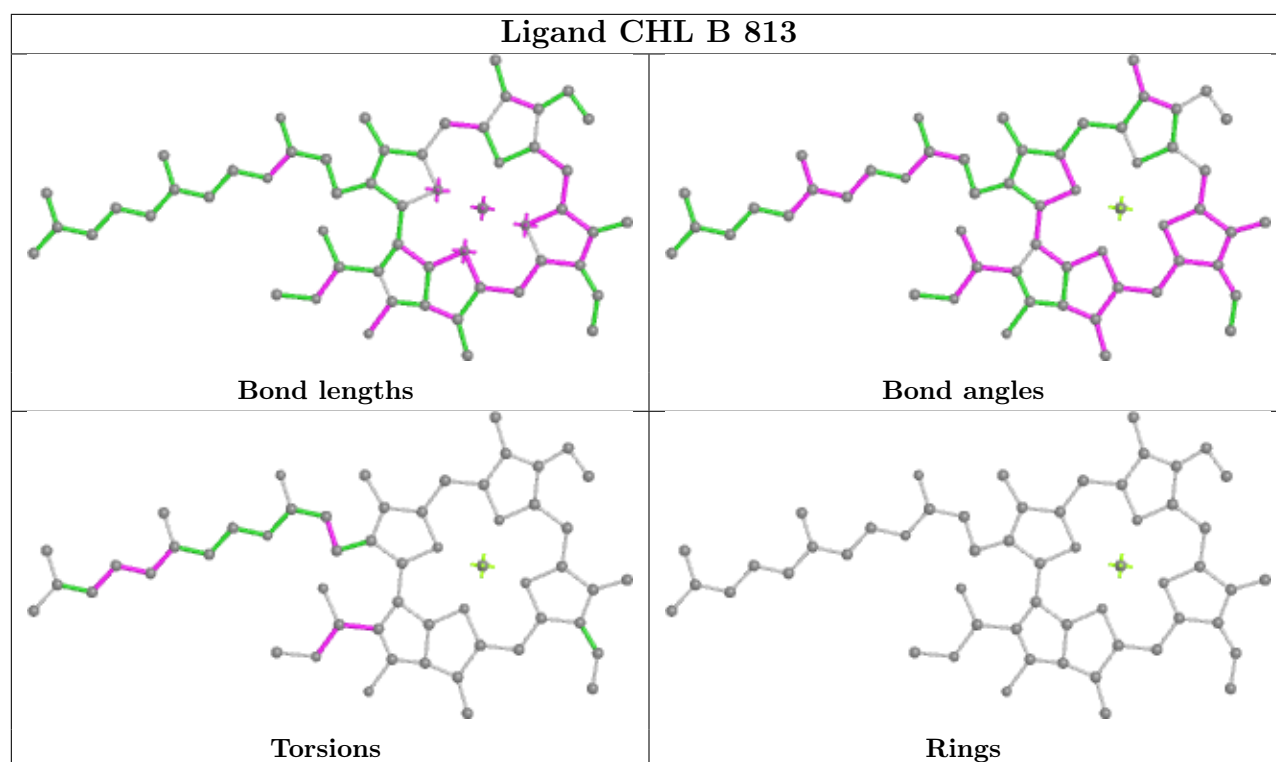


Ligand LHG 7 306

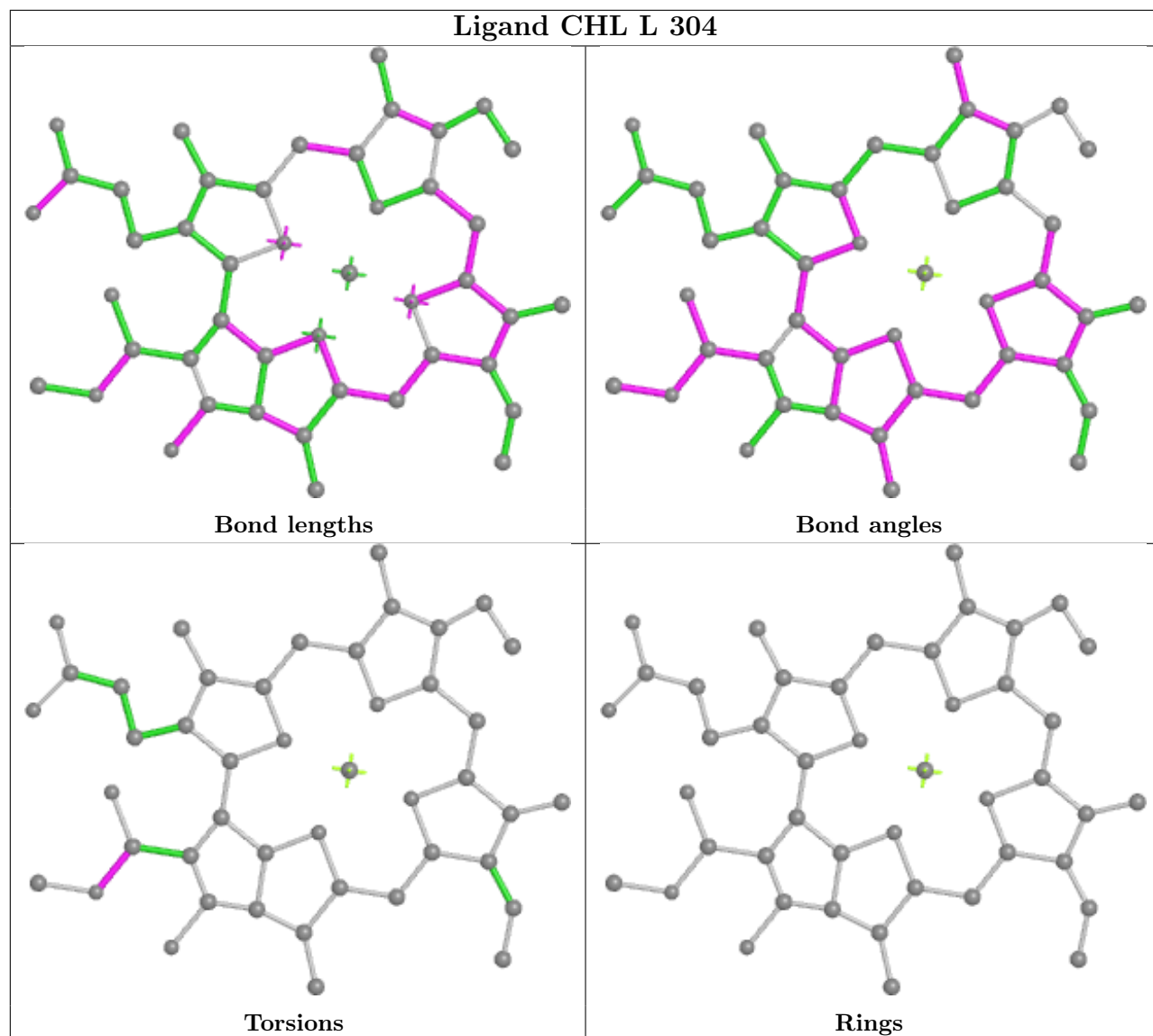


Ligand LMG J 104

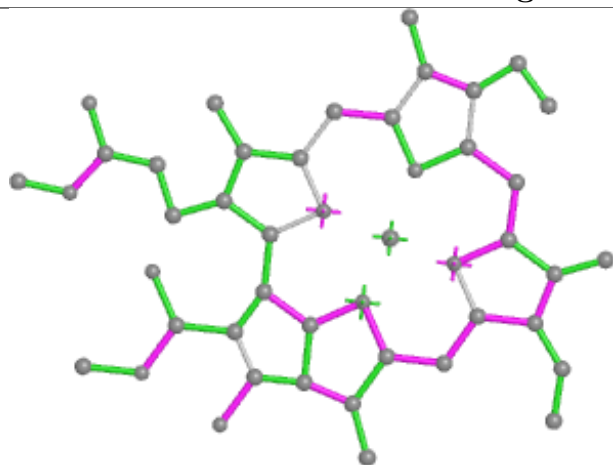




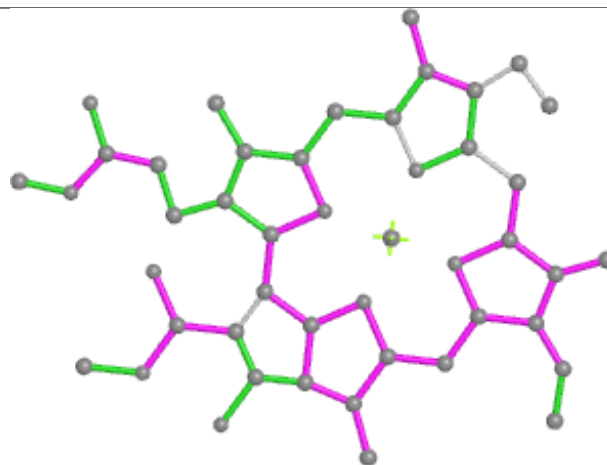
Ligand CHL L 304



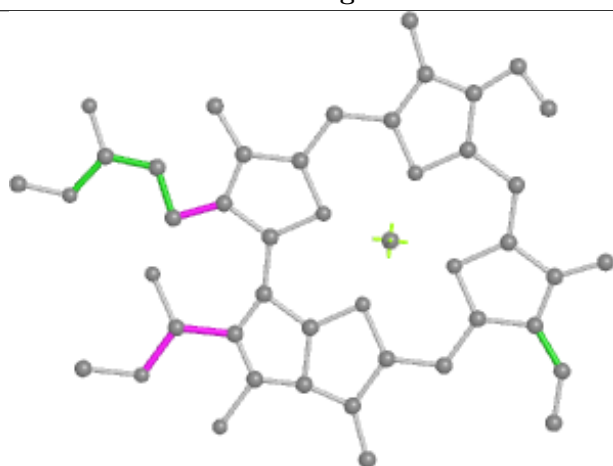
Ligand CHL b 306



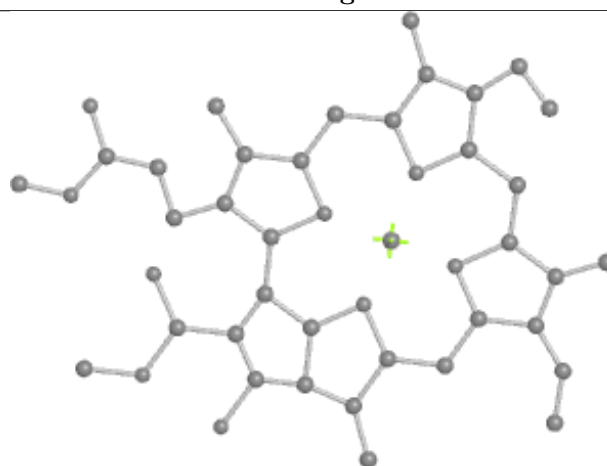
Bond lengths



Bond angles

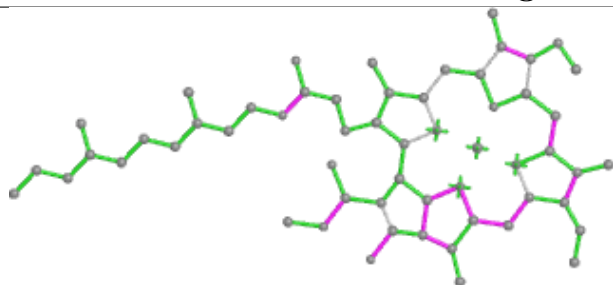


Torsions

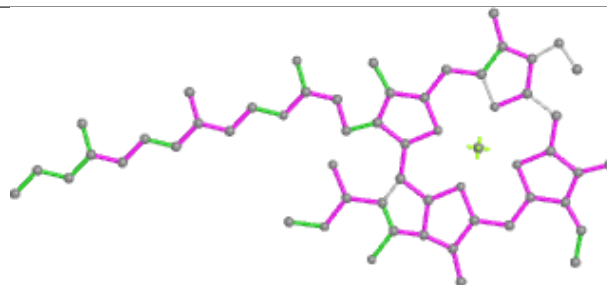


Rings

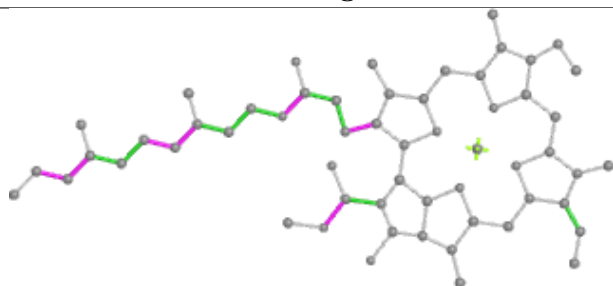
Ligand CHL 5 313



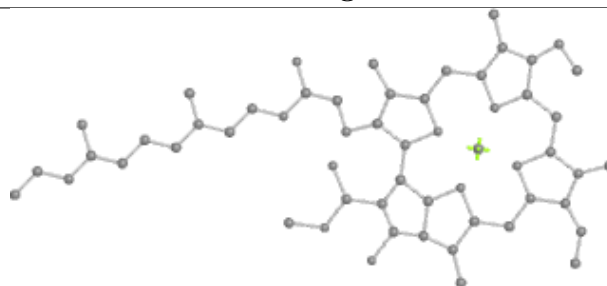
Bond lengths



Bond angles

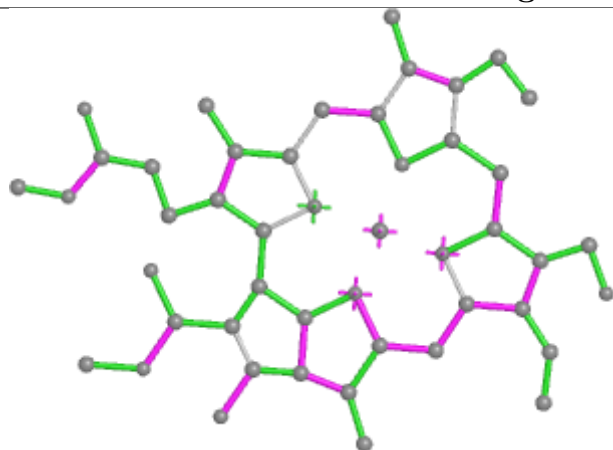


Torsions

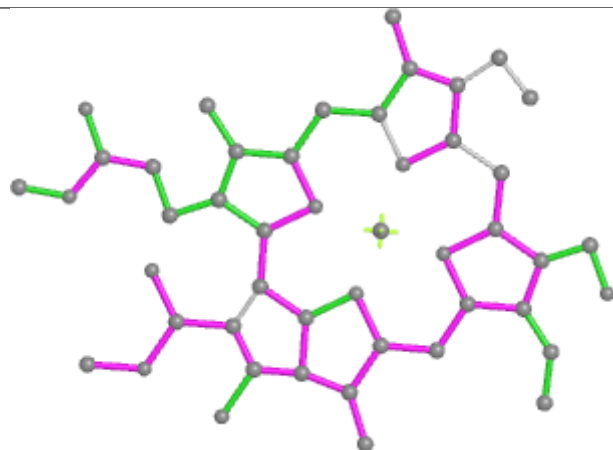


Rings

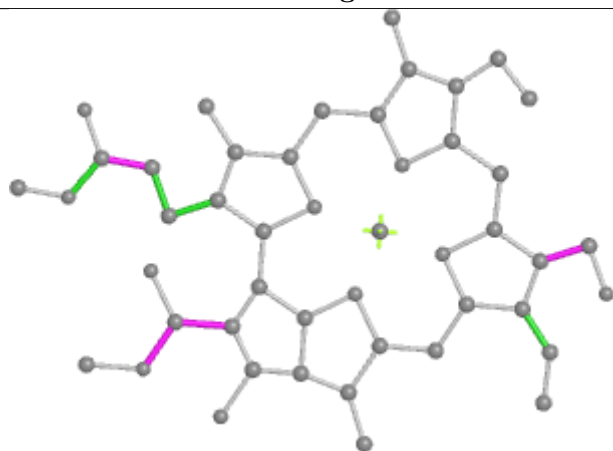
Ligand CHL 5 325



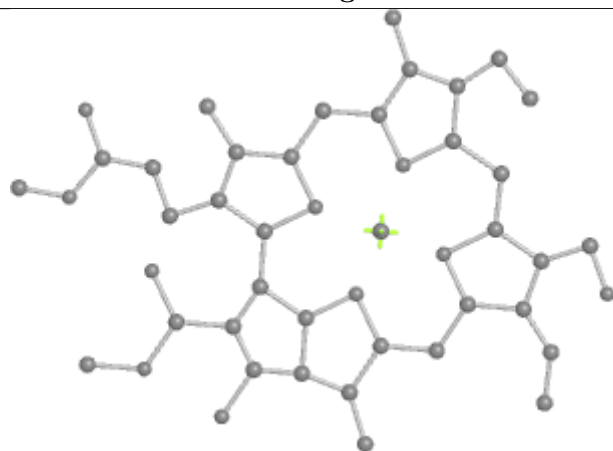
Bond lengths



Bond angles

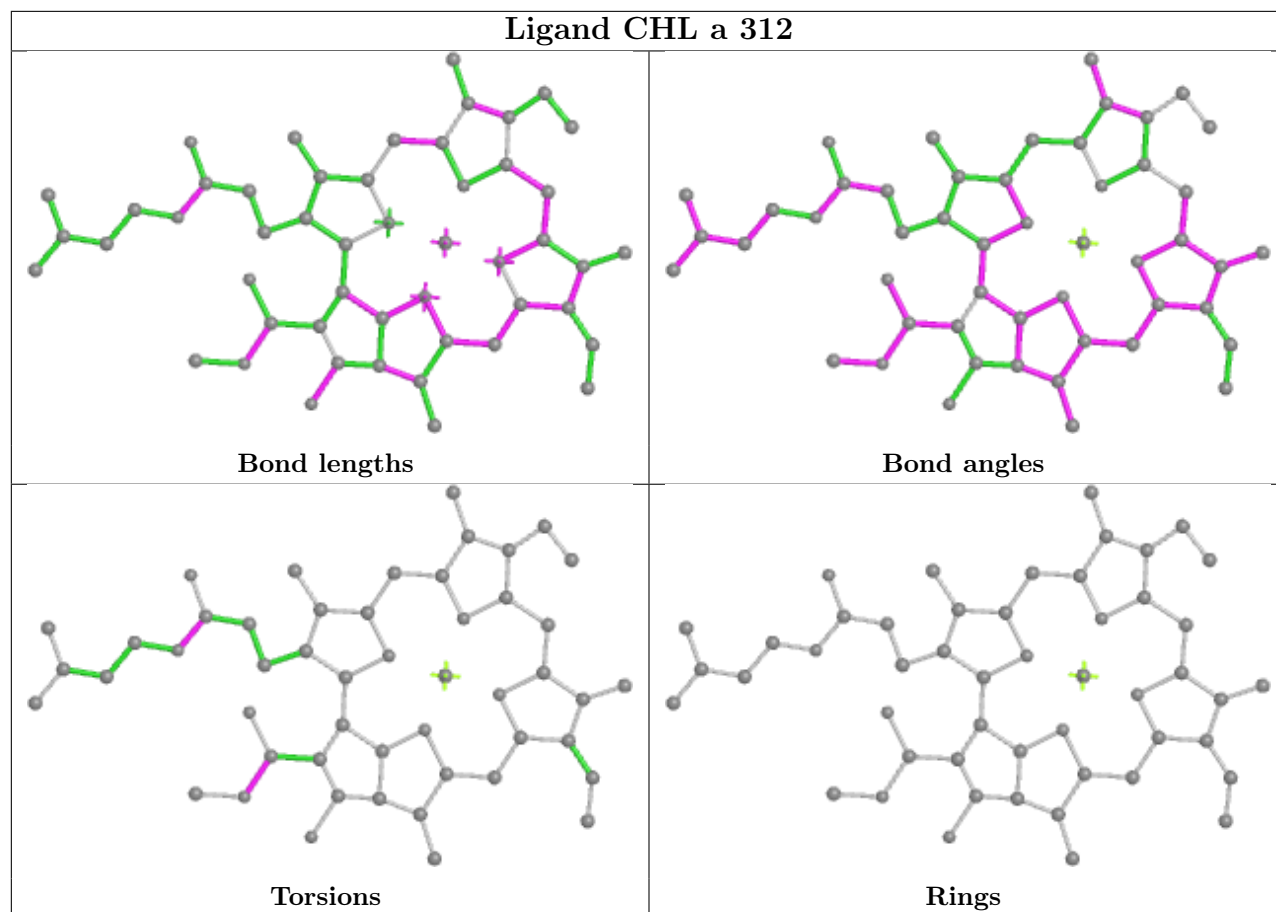


Torsions

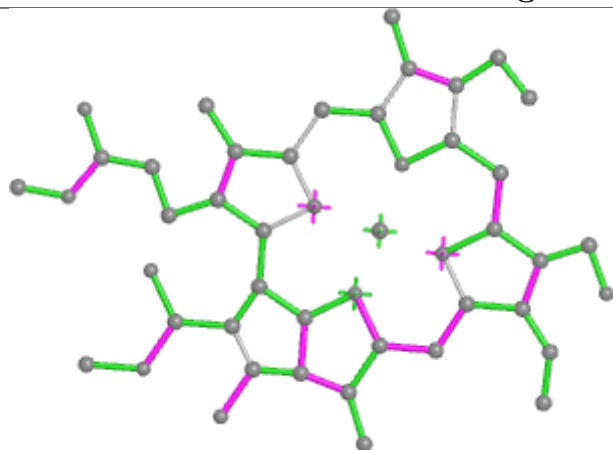


Rings

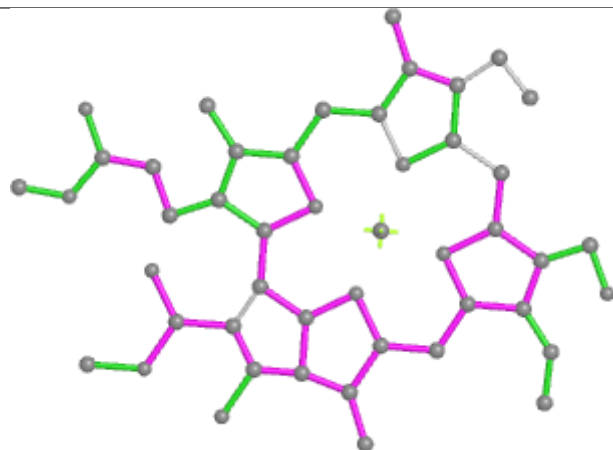
Ligand CHL a 312



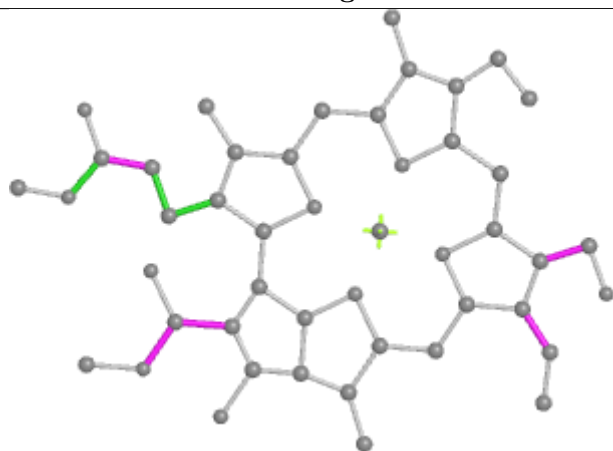
Ligand CHL 7 320



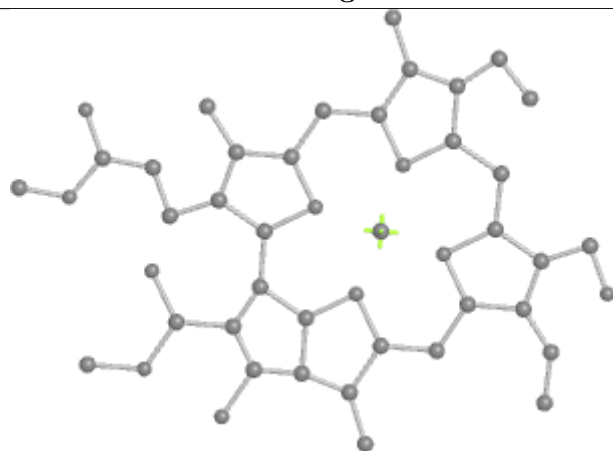
Bond lengths



Bond angles

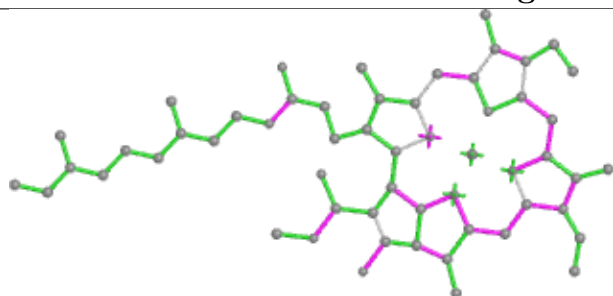


Torsions

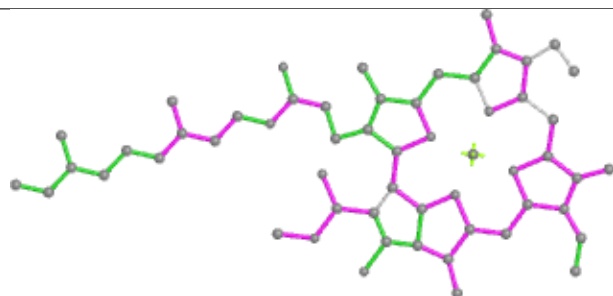


Rings

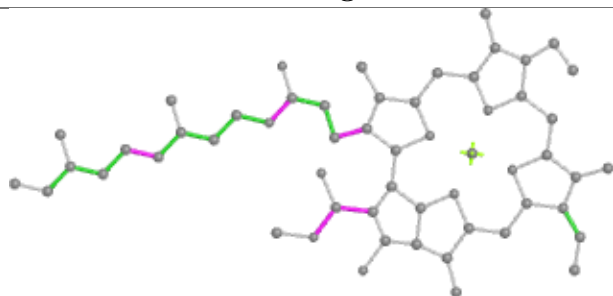
Ligand CHL 5 323



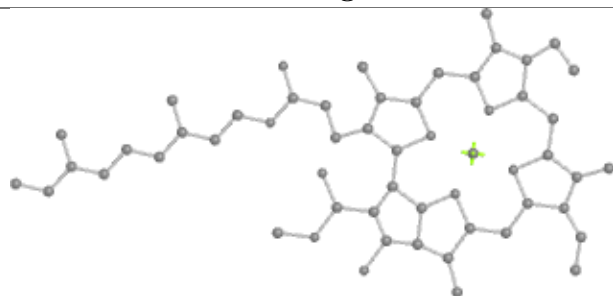
Bond lengths



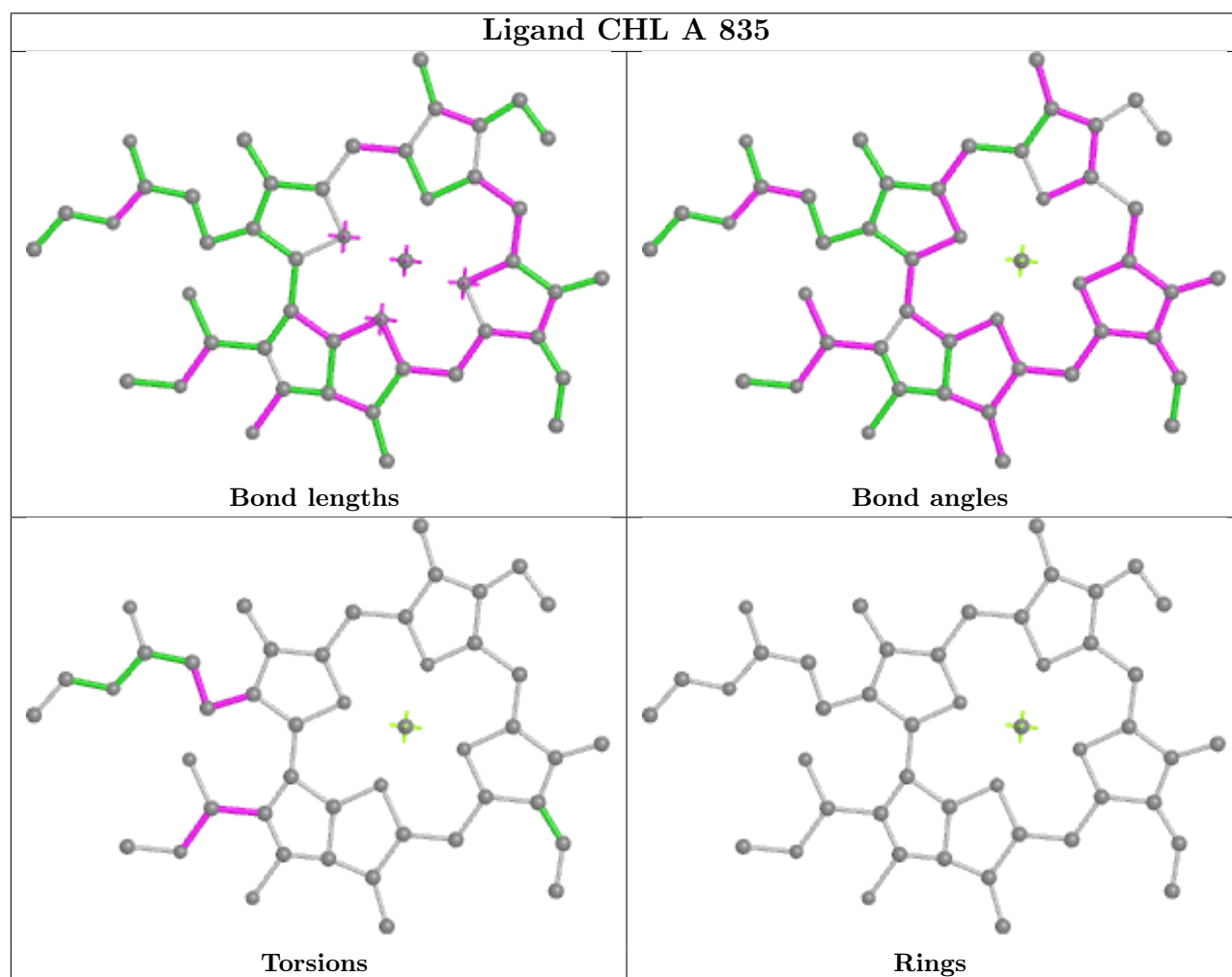
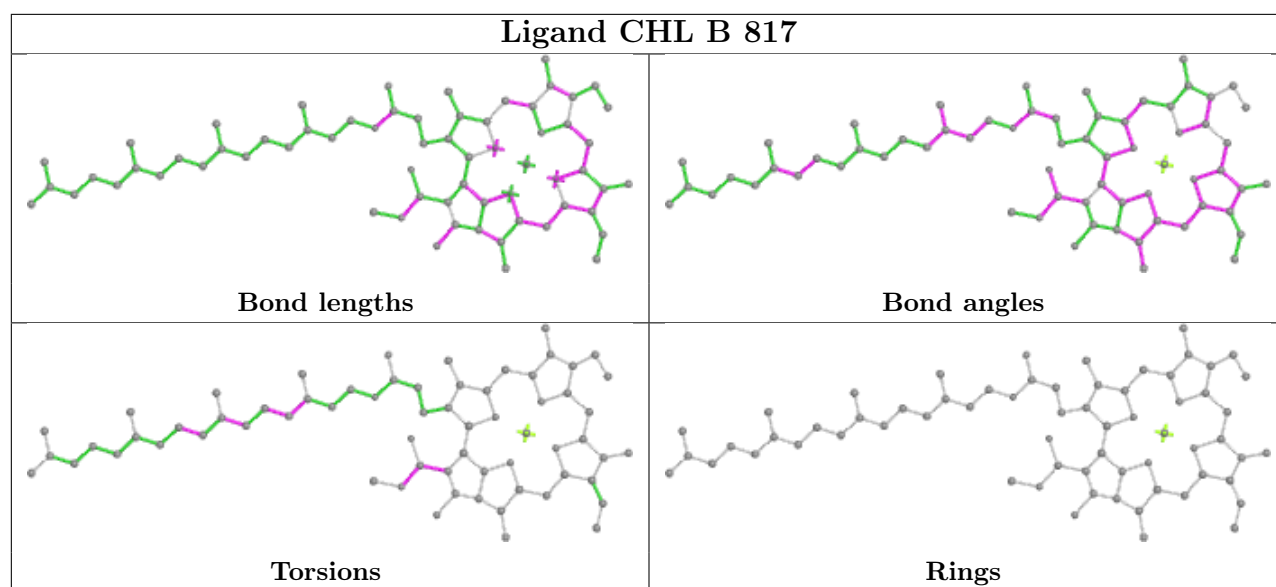
Bond angles

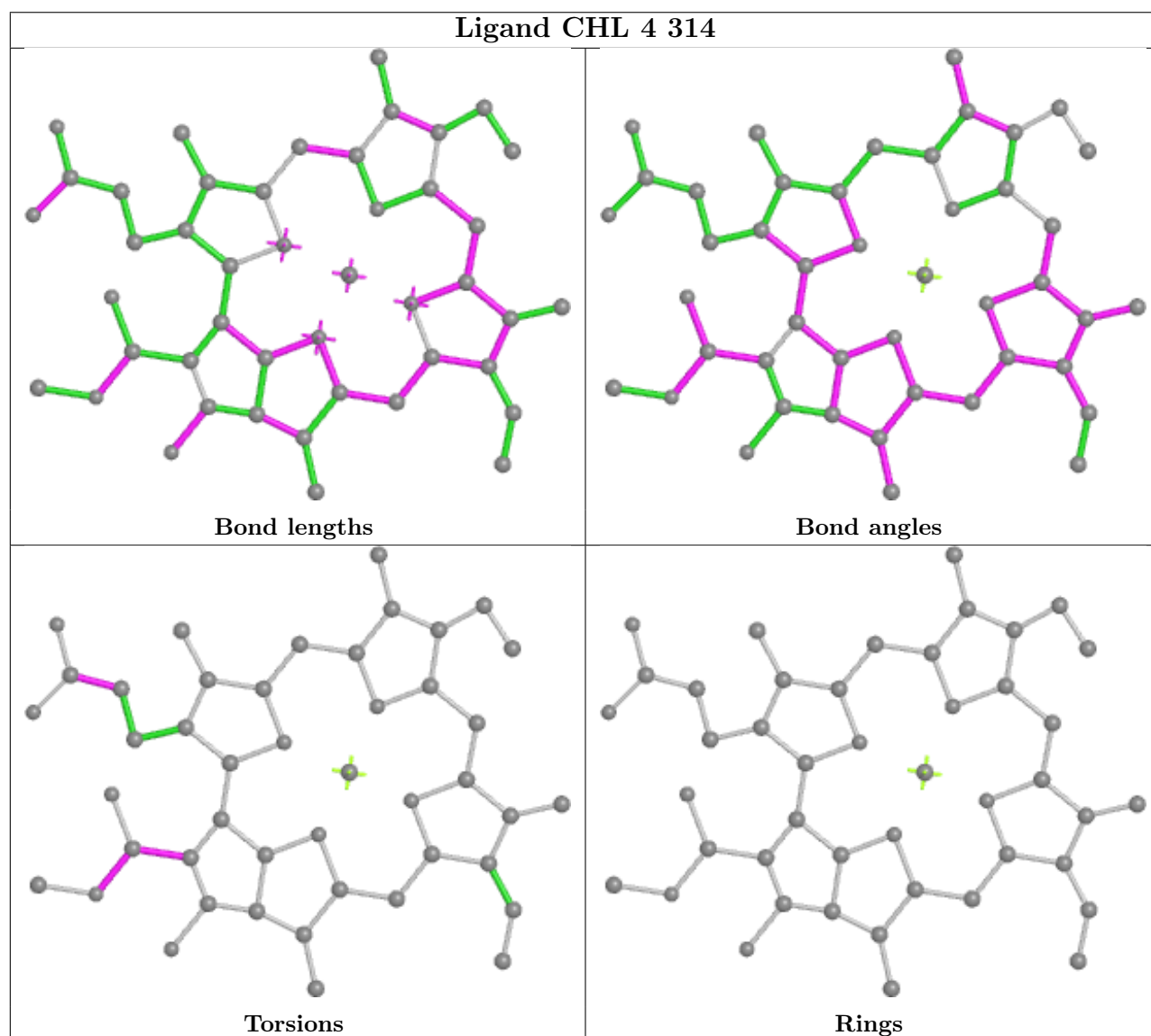
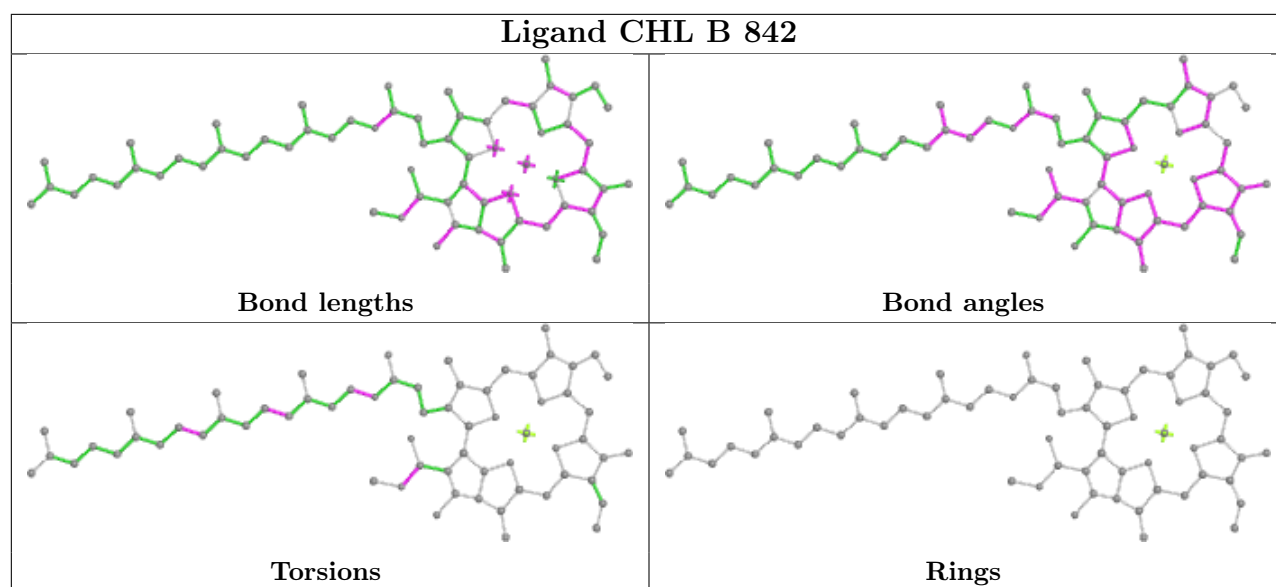


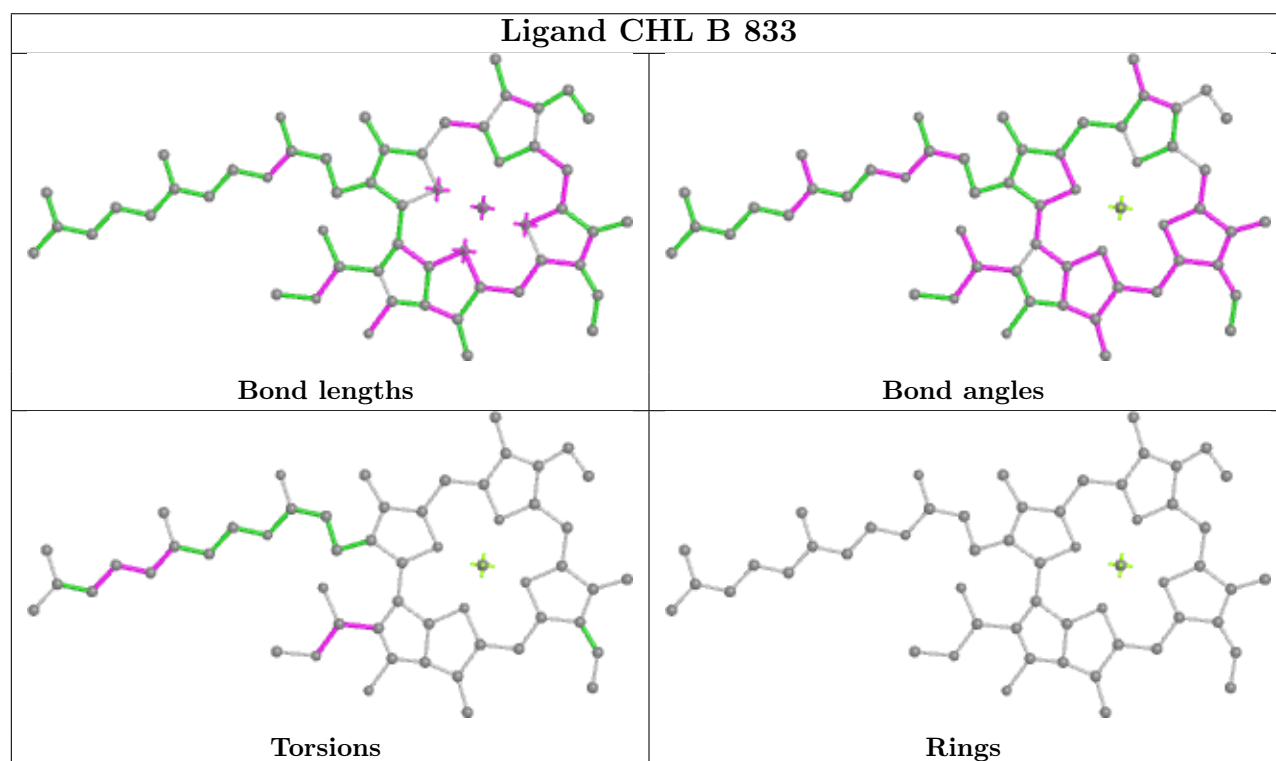
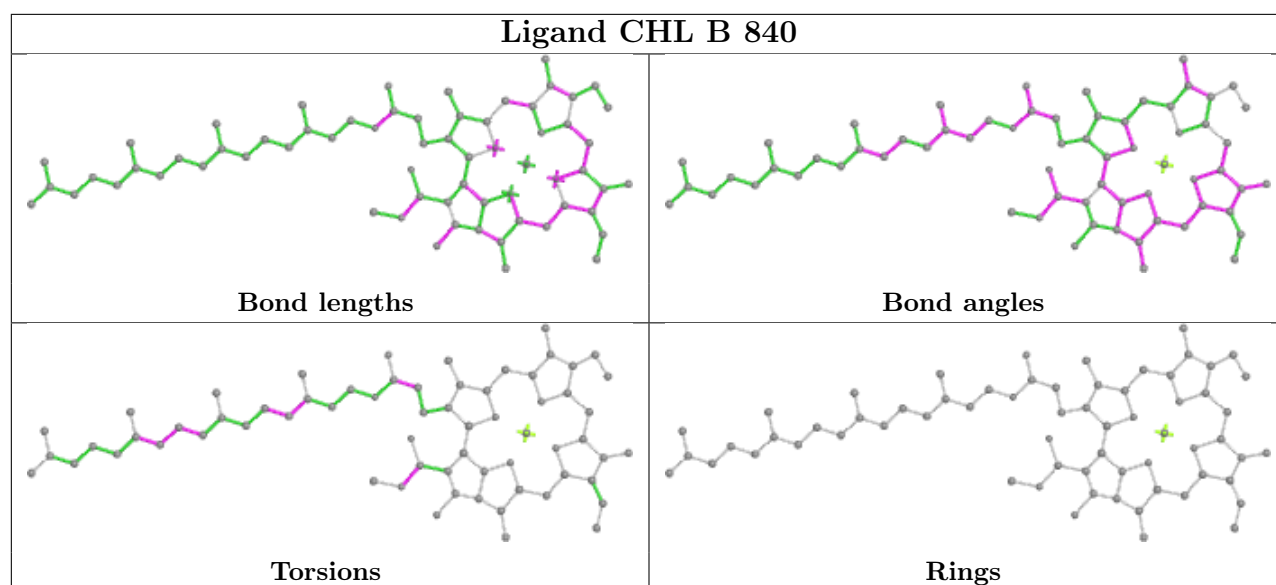
Torsions

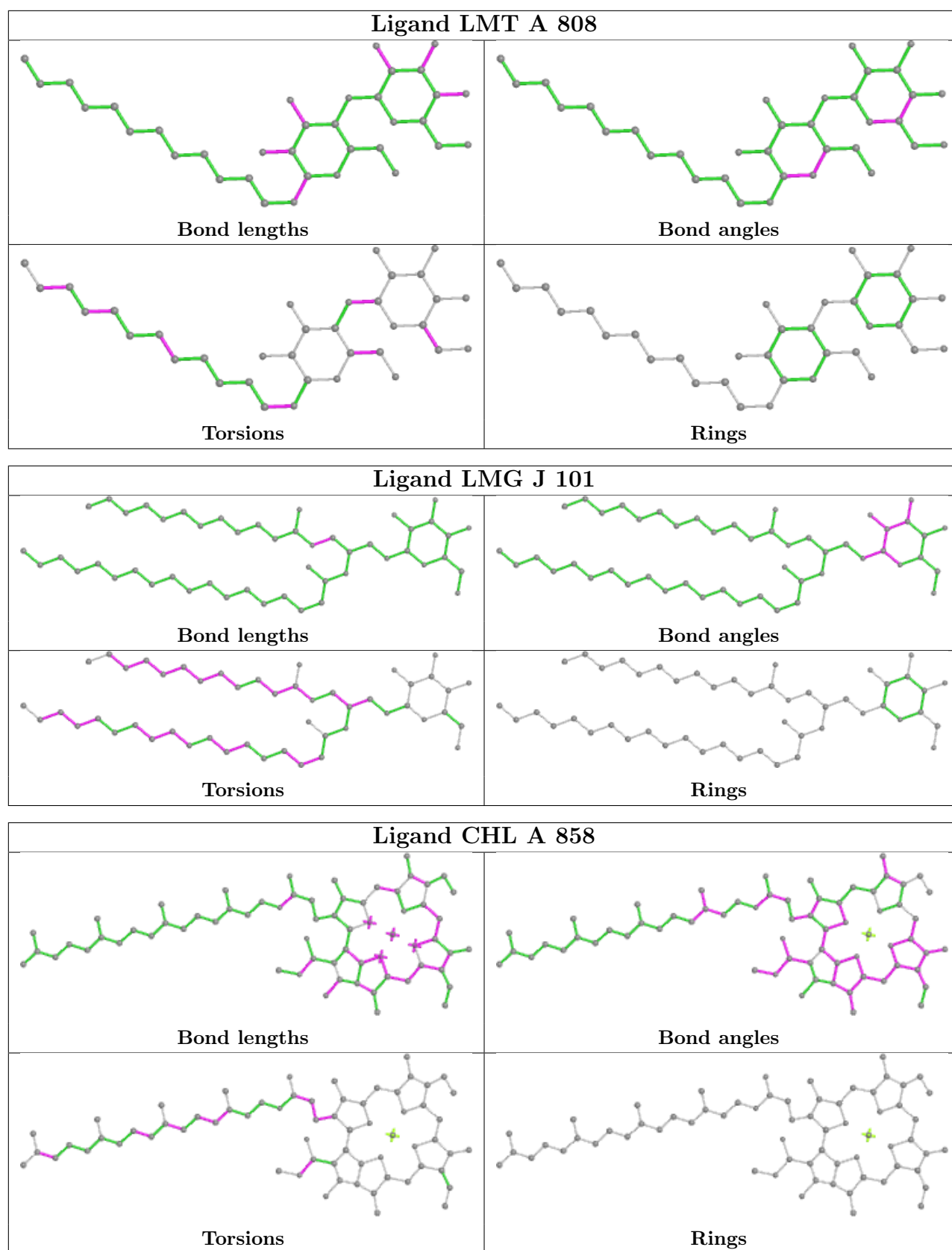


Rings

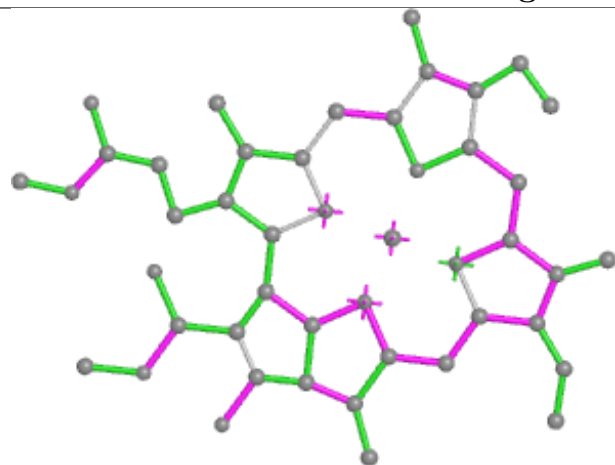




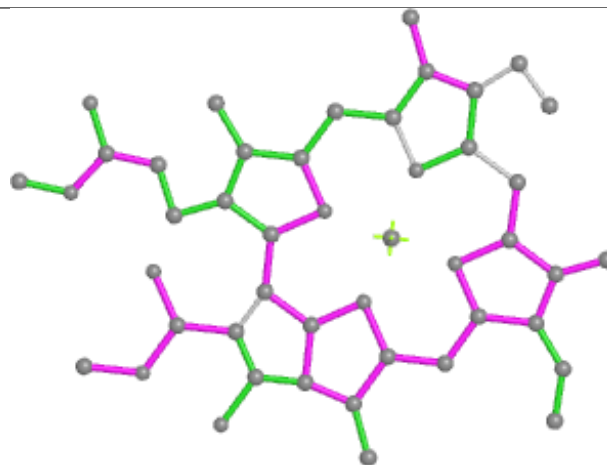




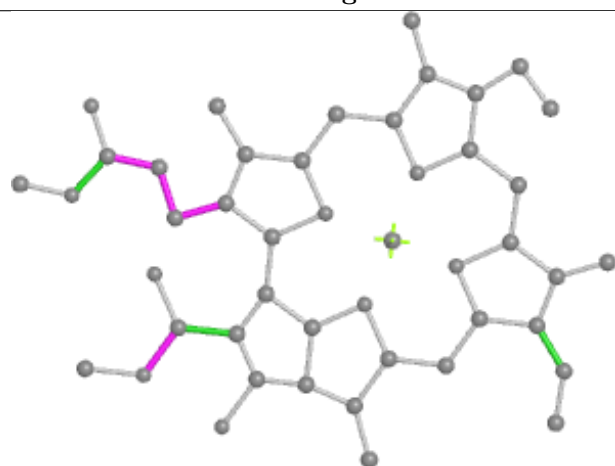
Ligand CHL b 313



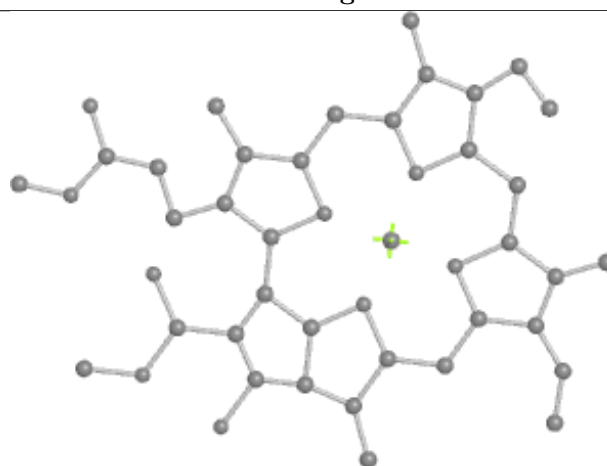
Bond lengths



Bond angles

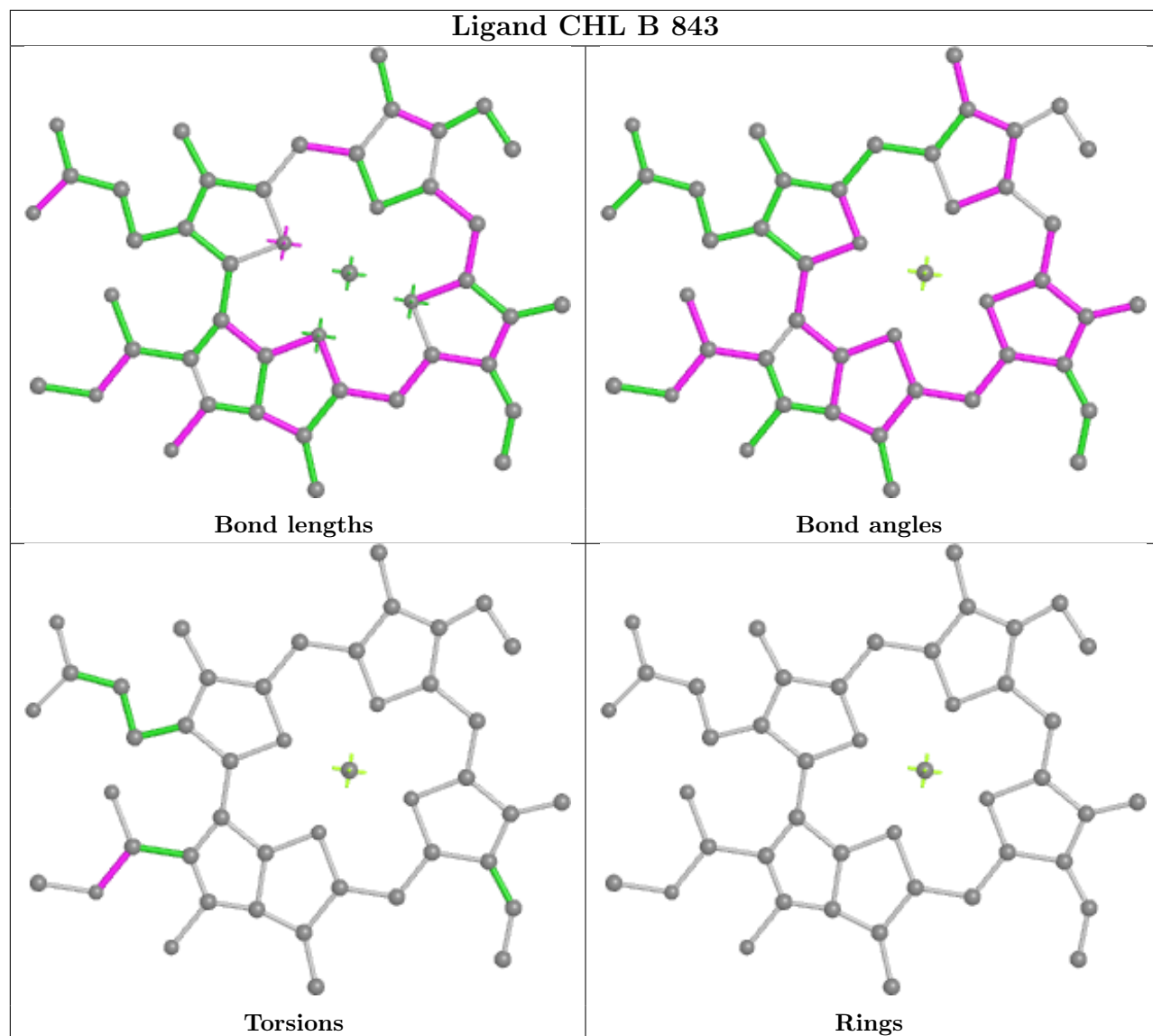


Torsions

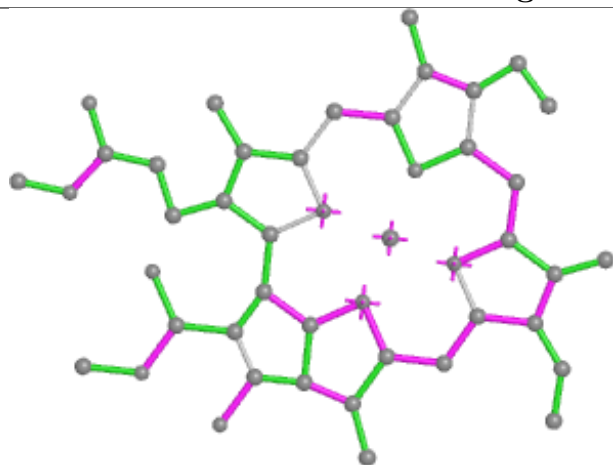


Rings

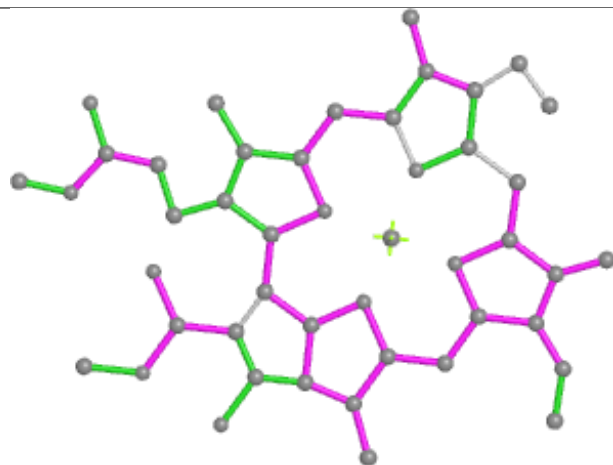
Ligand CHL B 843



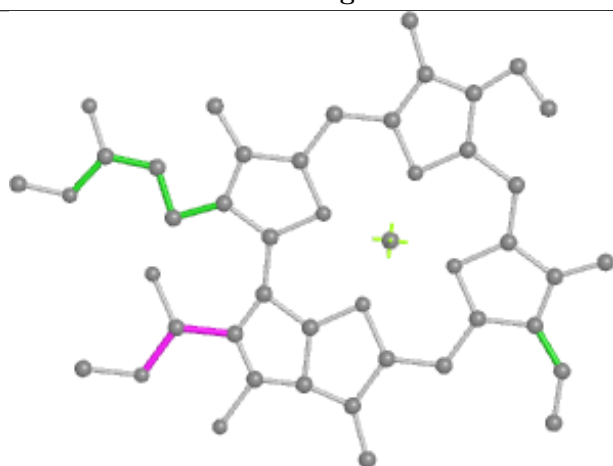
Ligand CHL b 314



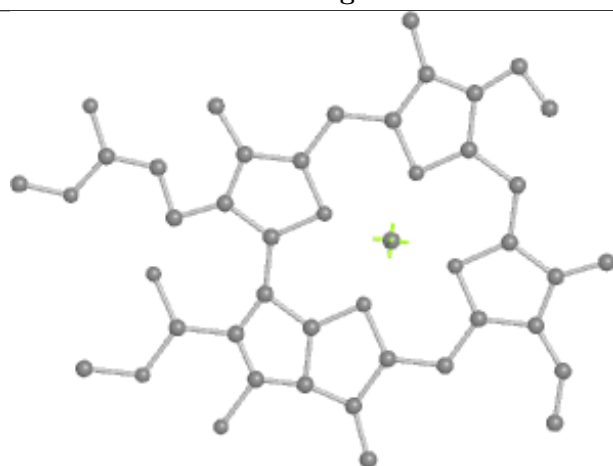
Bond lengths



Bond angles

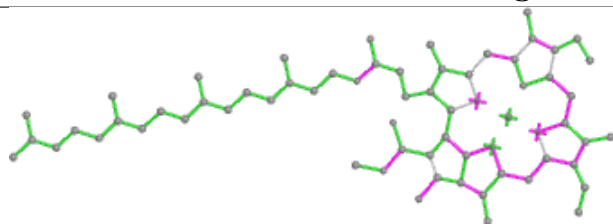


Torsions

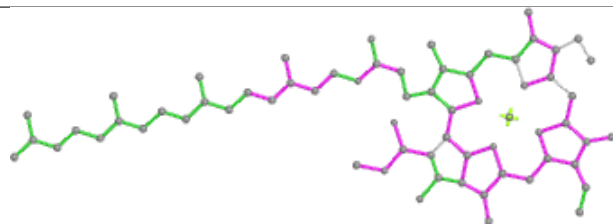


Rings

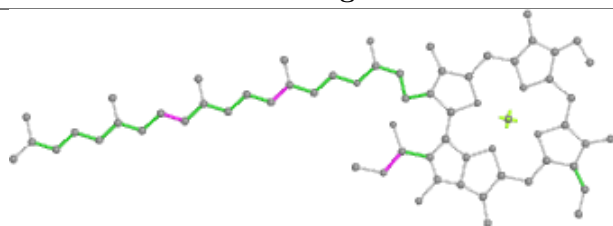
Ligand CHL A 856



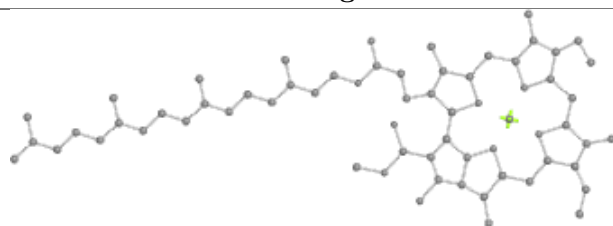
Bond lengths



Bond angles

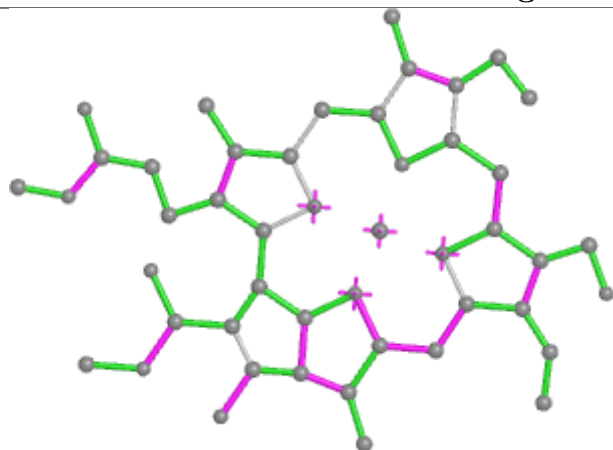


Torsions

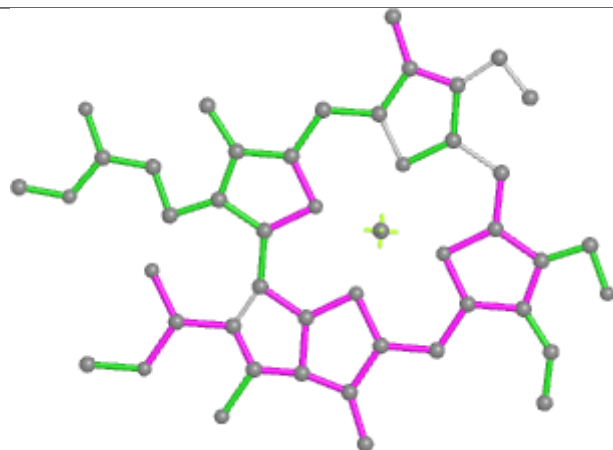


Rings

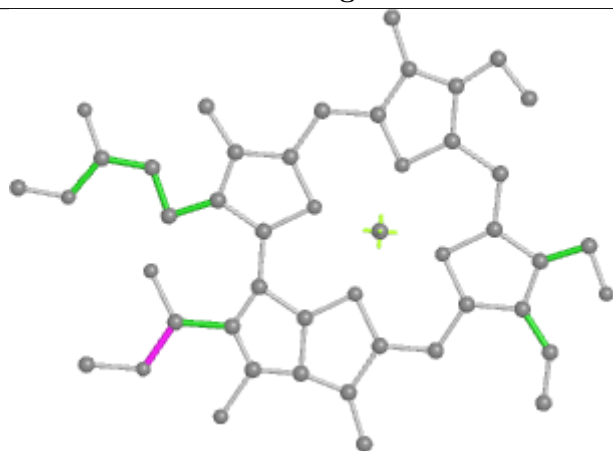
Ligand CHL 7 321



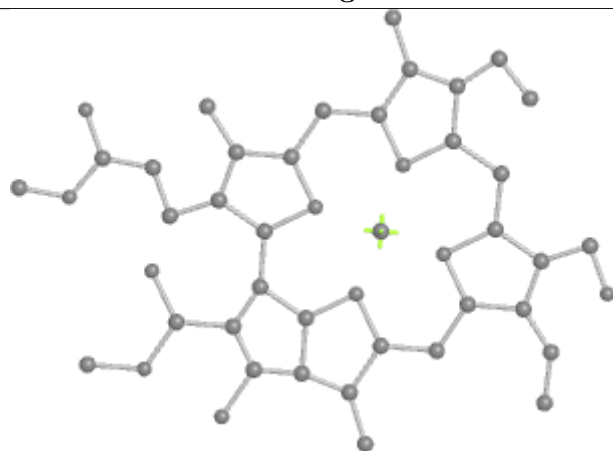
Bond lengths



Bond angles

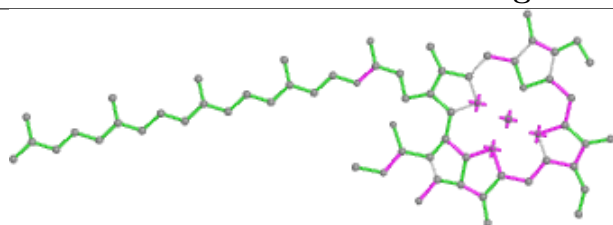


Torsions

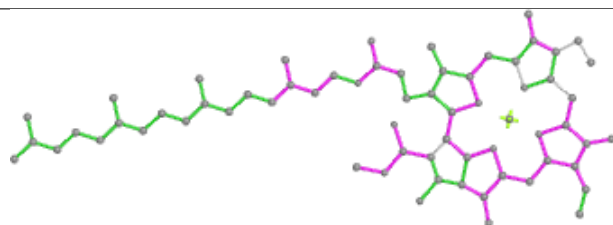


Rings

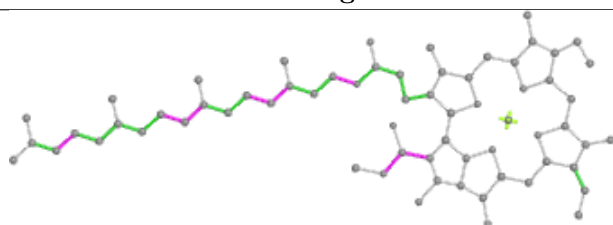
Ligand CHL A 855



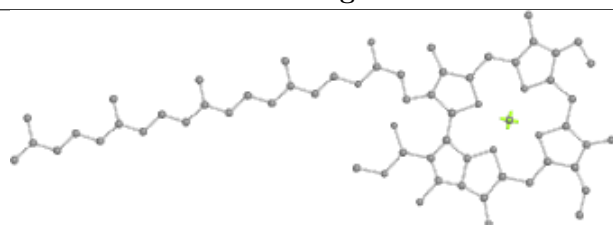
Bond lengths



Bond angles

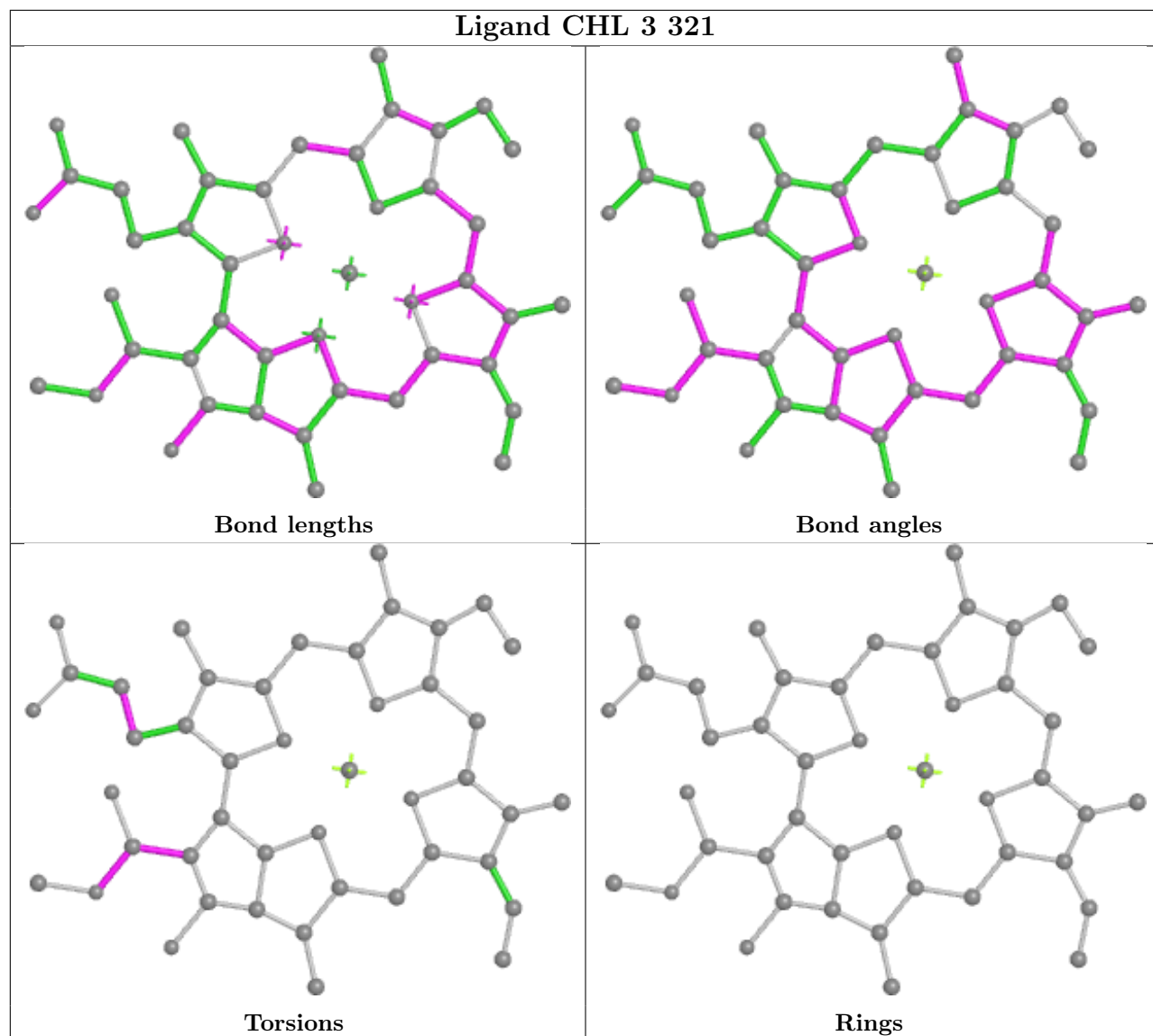


Torsions

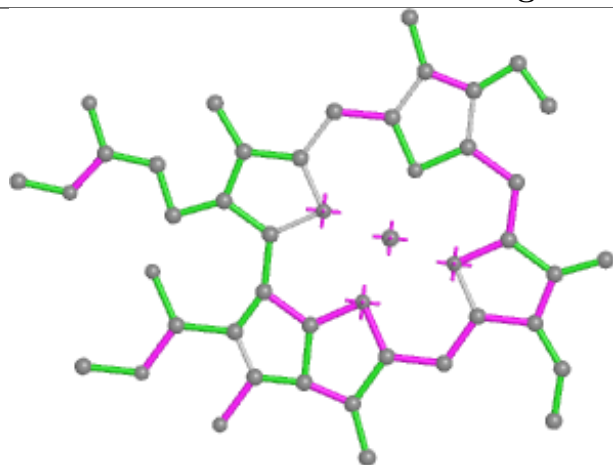


Rings

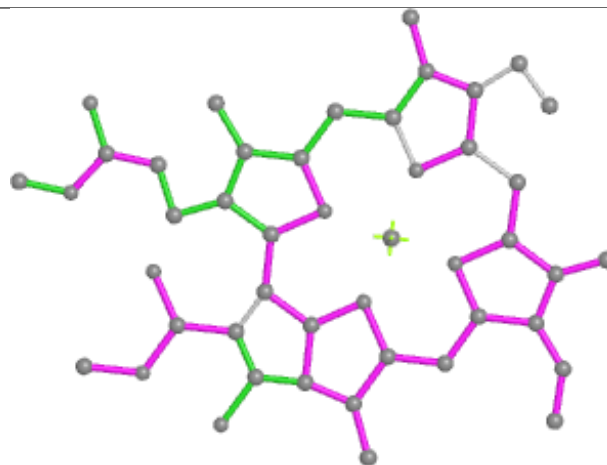
Ligand CHL 3 321



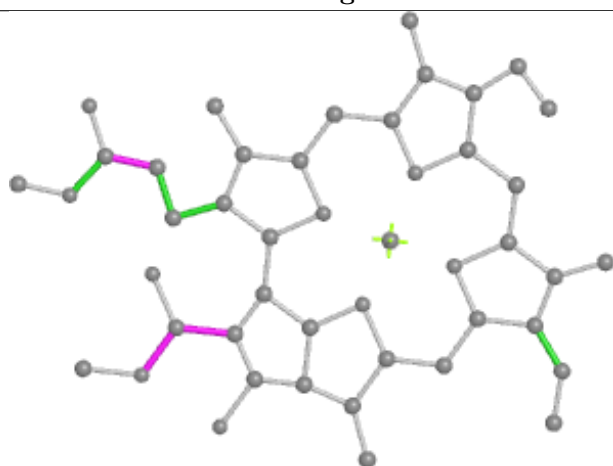
Ligand CHL 5 311



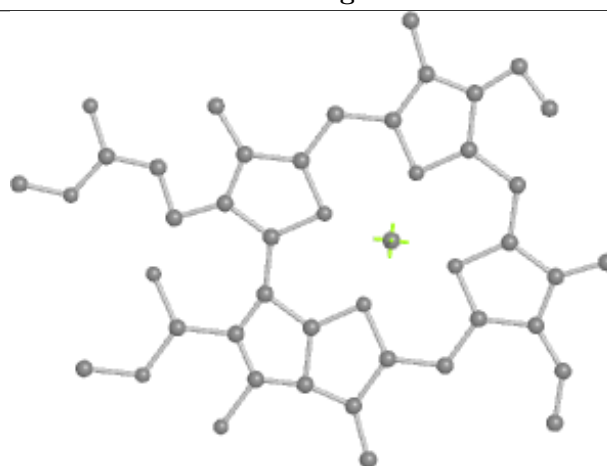
Bond lengths



Bond angles

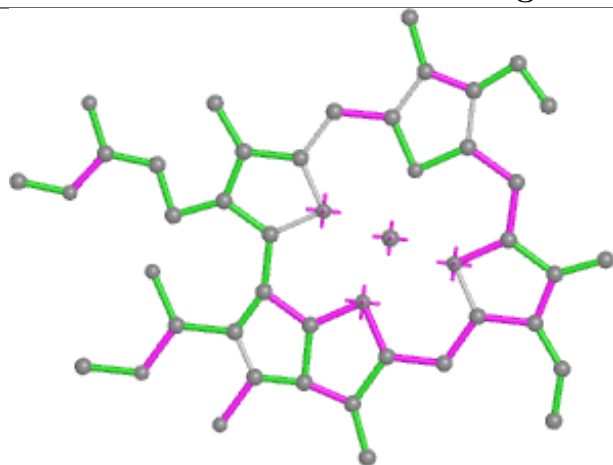


Torsions

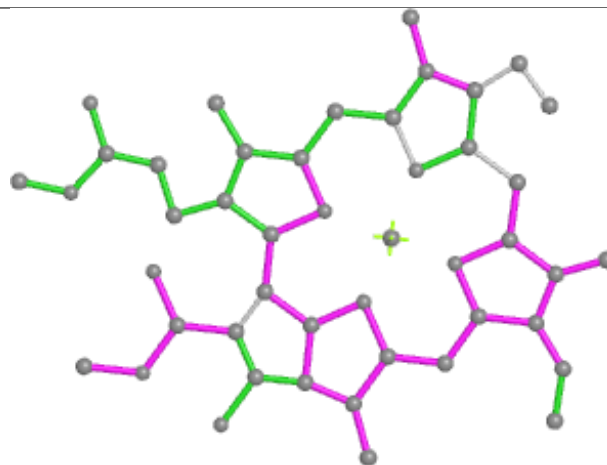


Rings

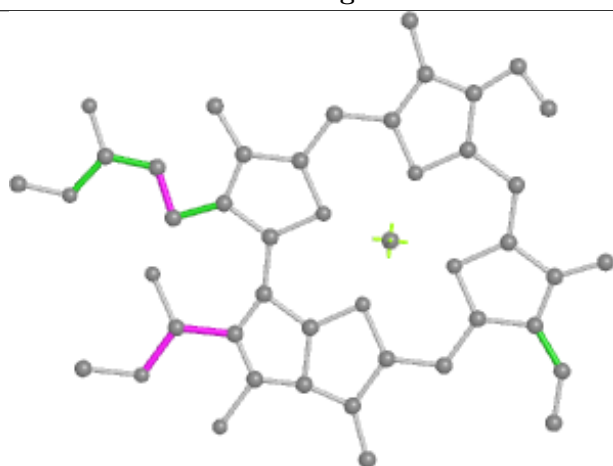
Ligand CHL b 305



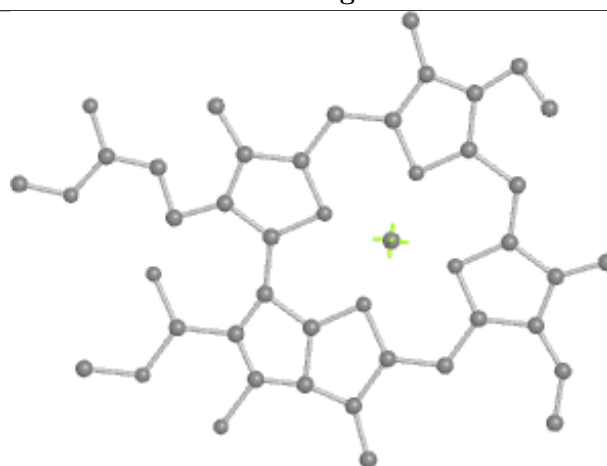
Bond lengths



Bond angles

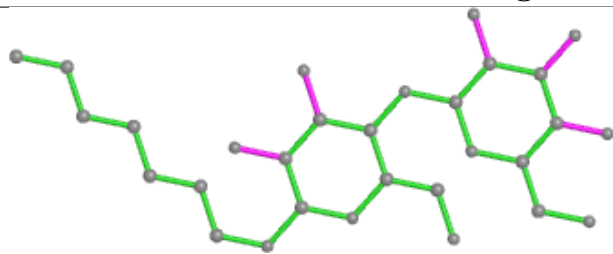


Torsions

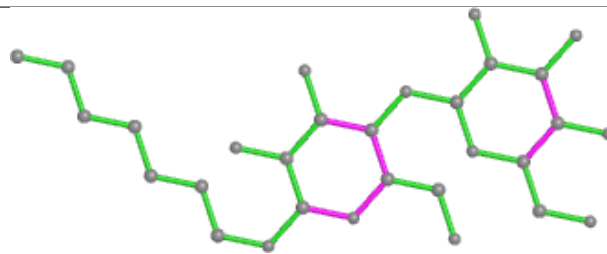


Rings

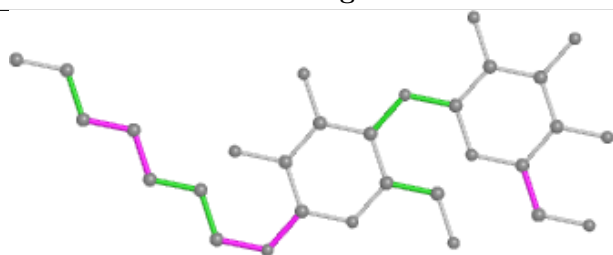
Ligand LMT 5 306



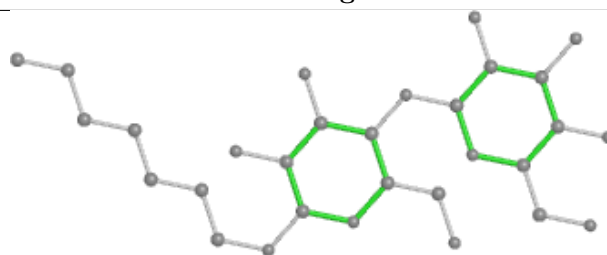
Bond lengths



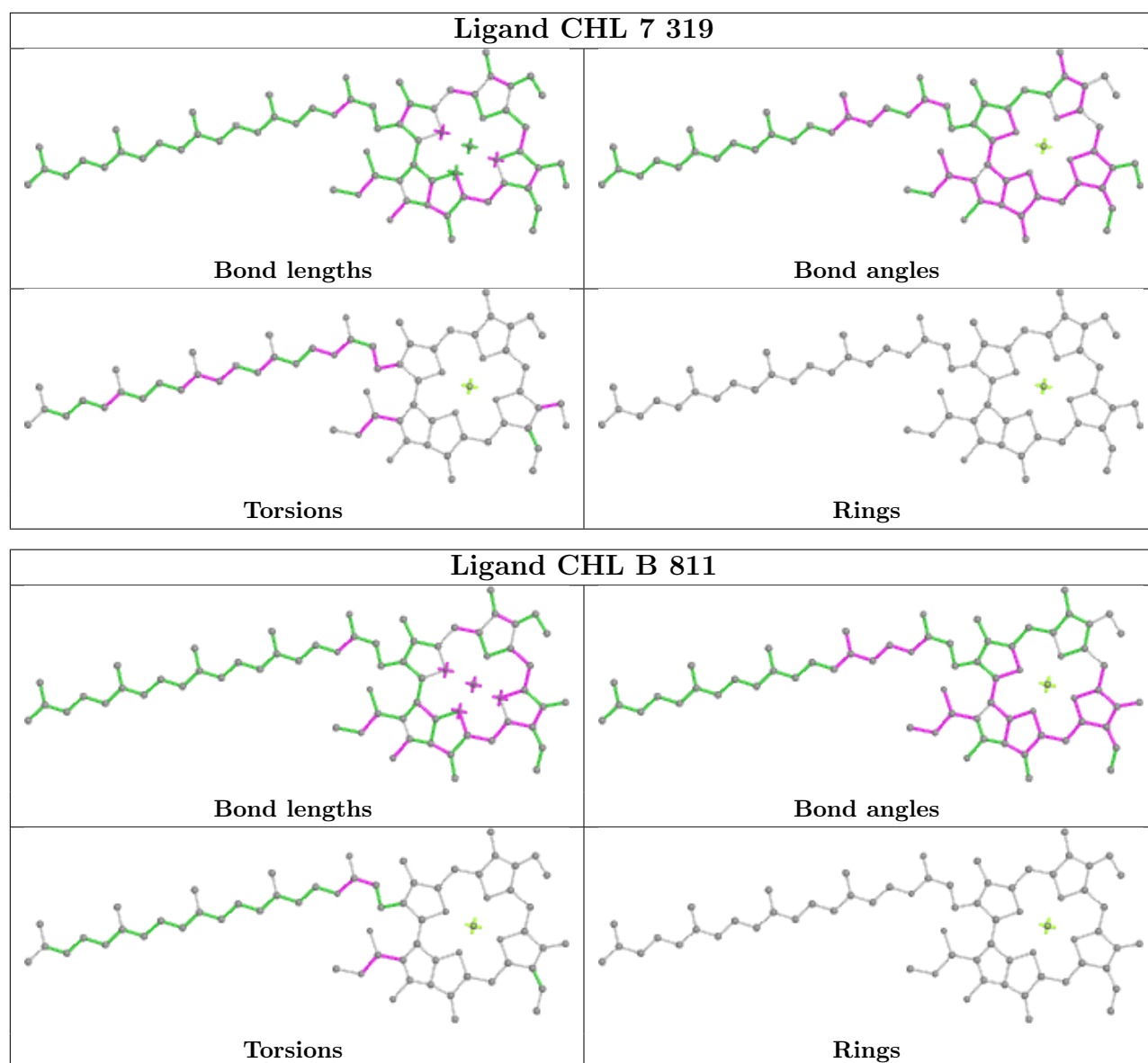
Bond angles



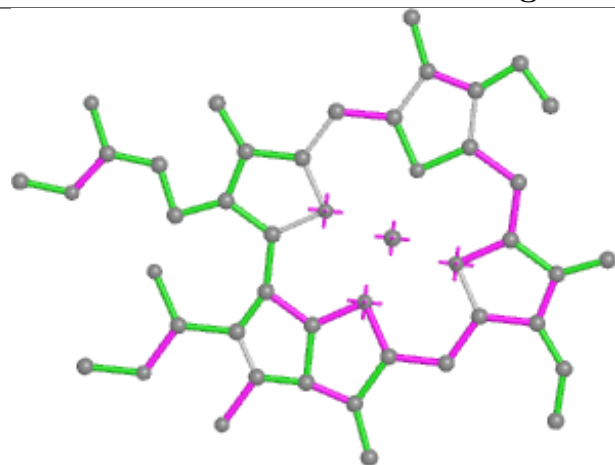
Torsions



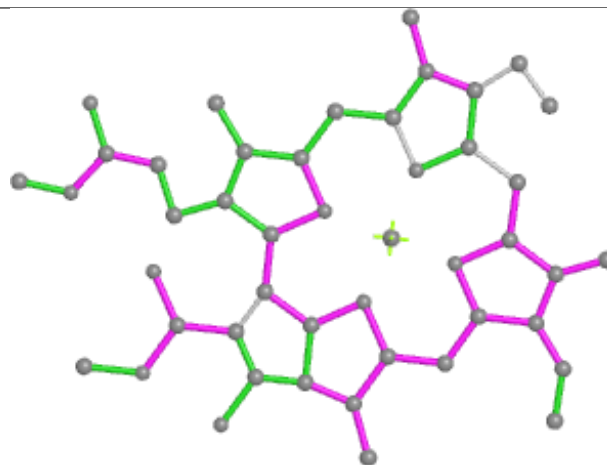
Rings



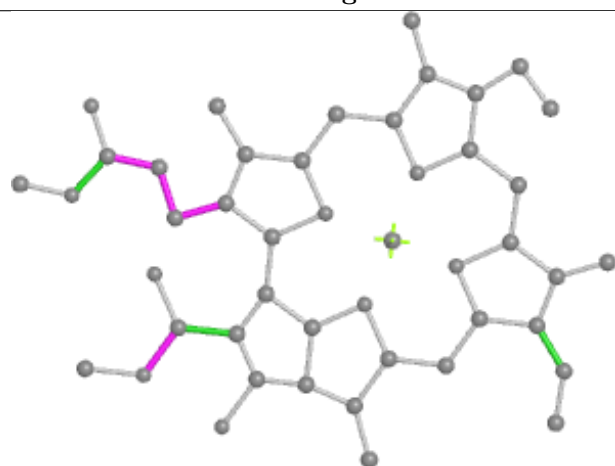
Ligand CHL 6 305



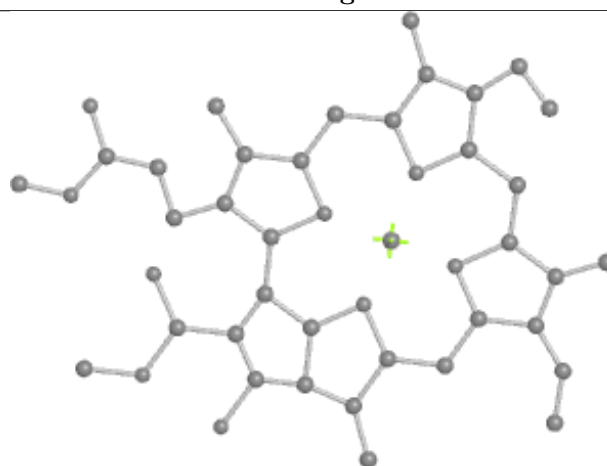
Bond lengths



Bond angles

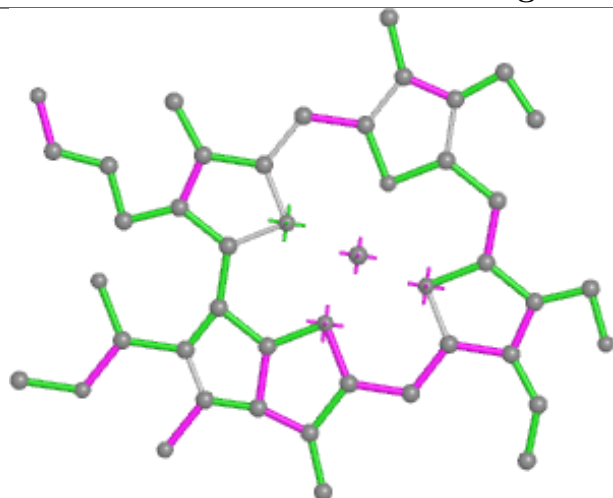


Torsions

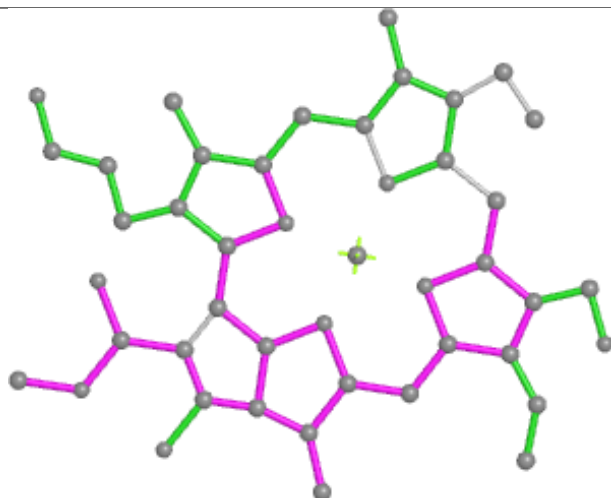


Rings

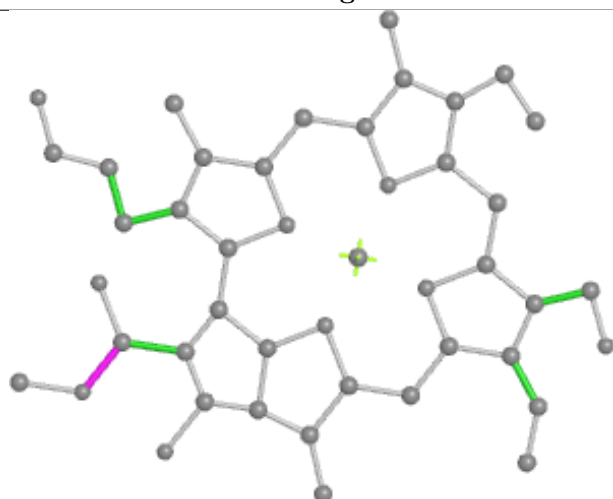
Ligand CHL 8 324



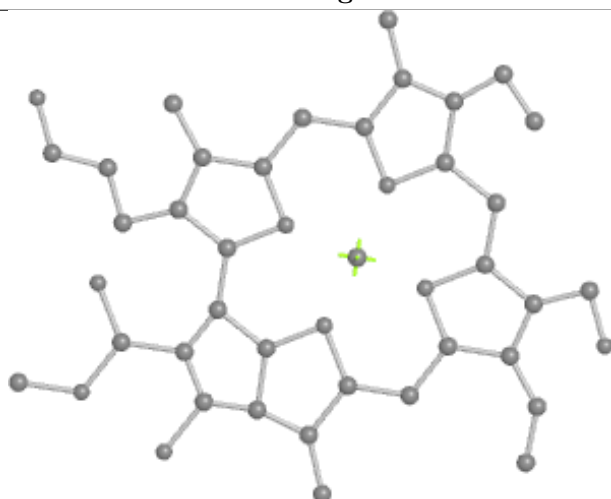
Bond lengths



Bond angles

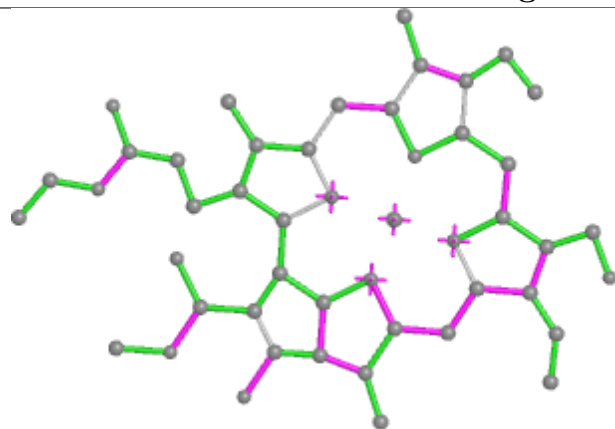


Torsions

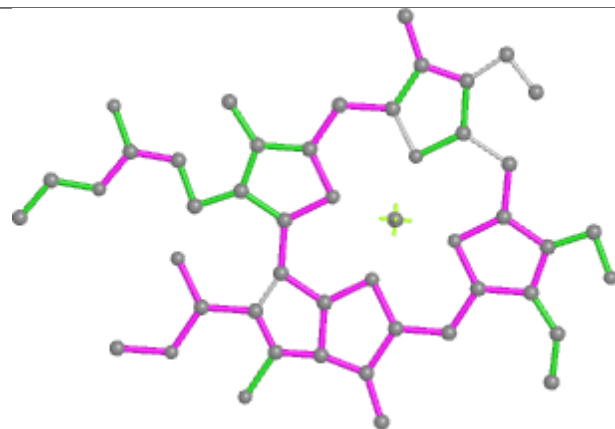


Rings

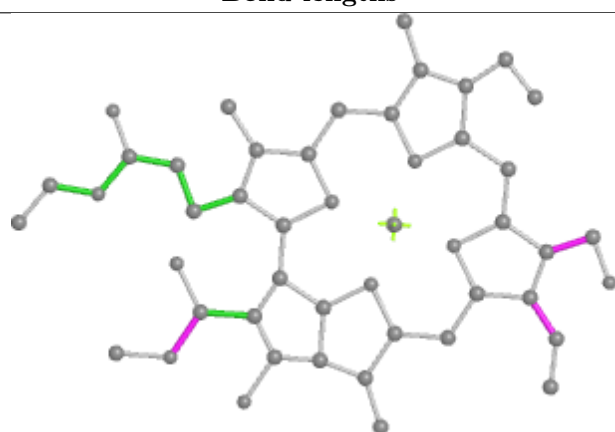
Ligand CHL b 316



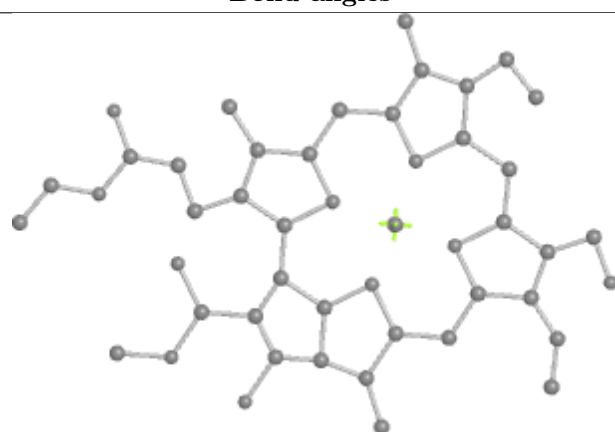
Bond lengths



Bond angles

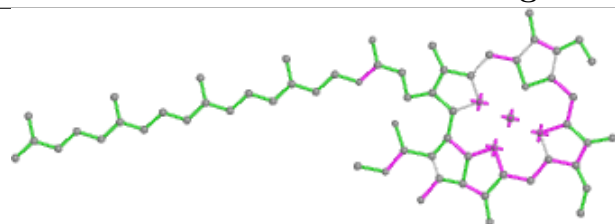


Torsions

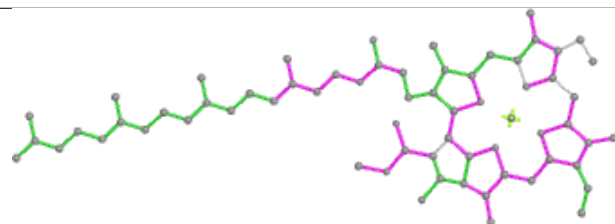


Rings

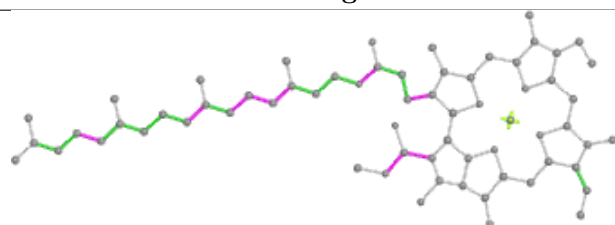
Ligand CHL 7 317



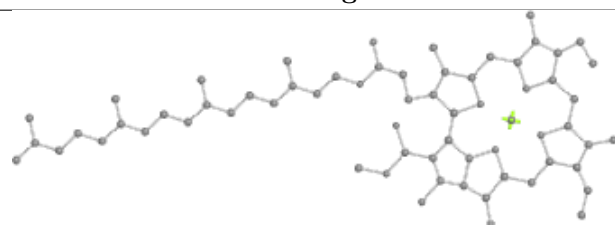
Bond lengths



Bond angles

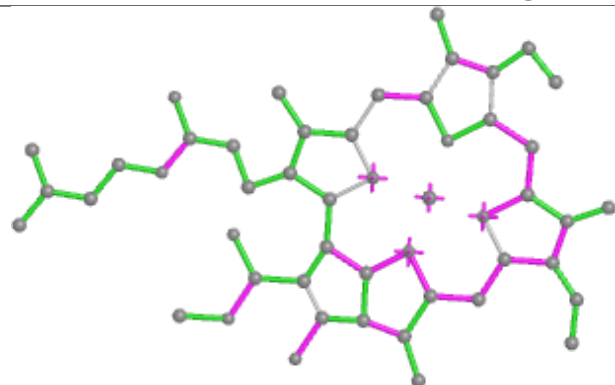


Torsions

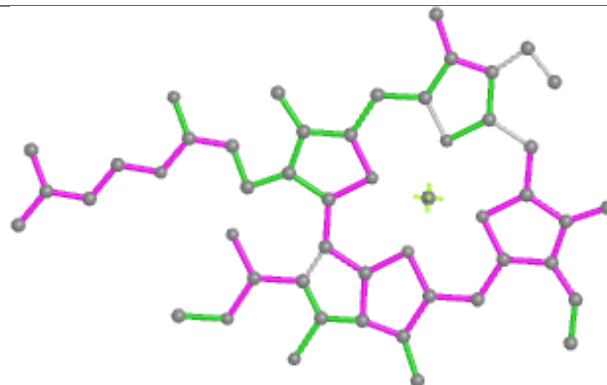


Rings

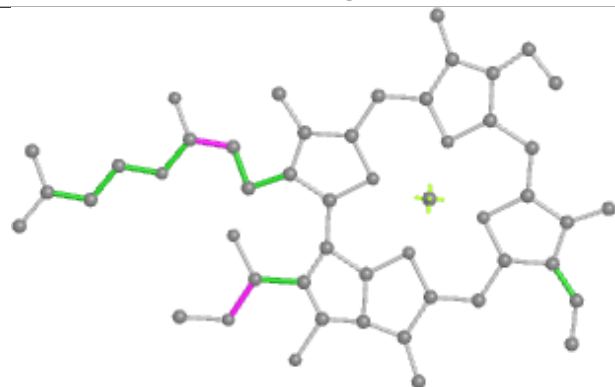
Ligand CHL 8 313



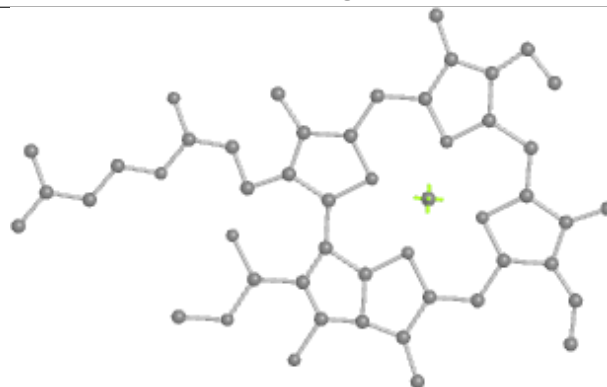
Bond lengths



Bond angles

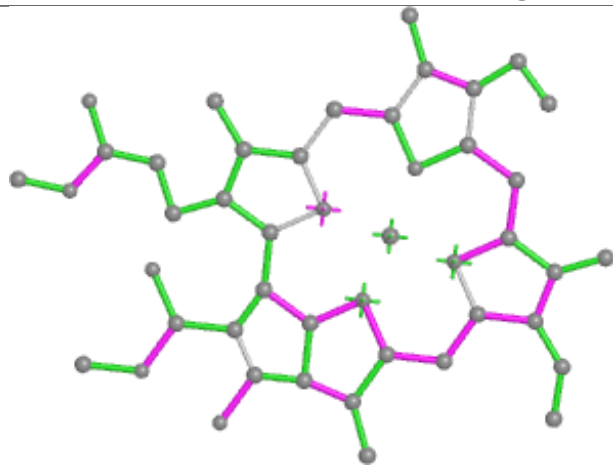


Torsions

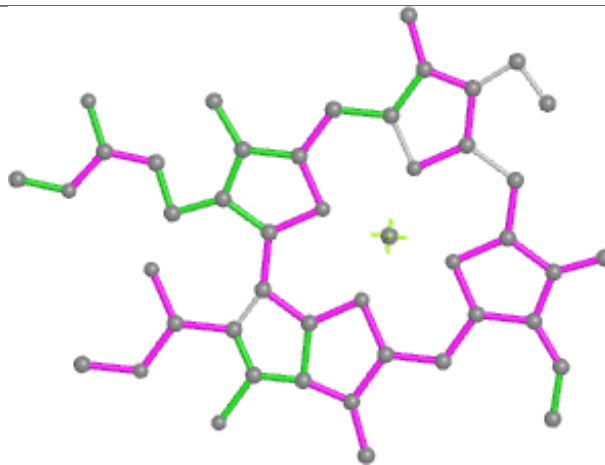


Rings

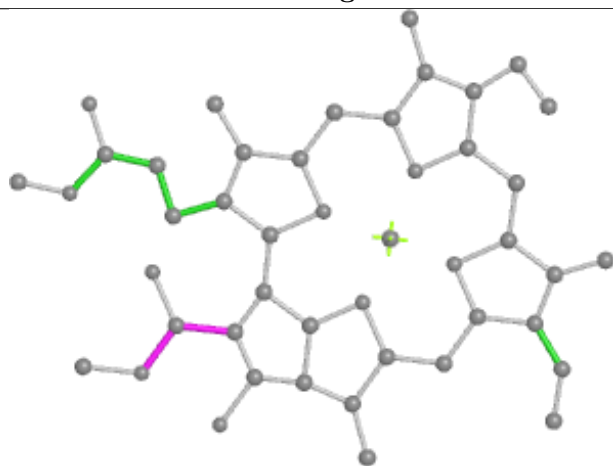
Ligand CHL A 857



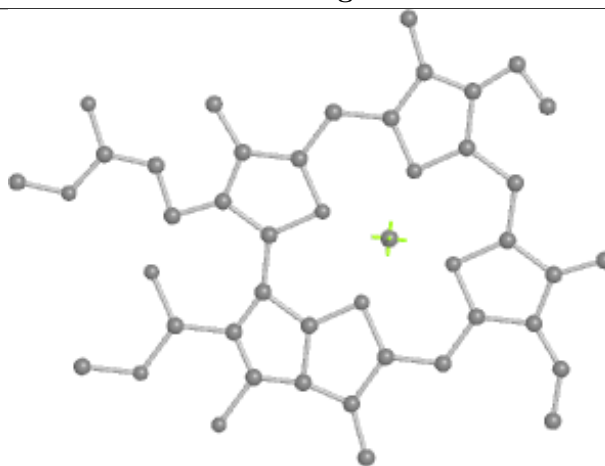
Bond lengths



Bond angles

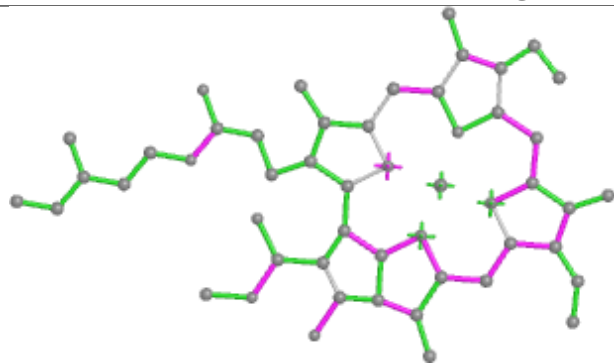


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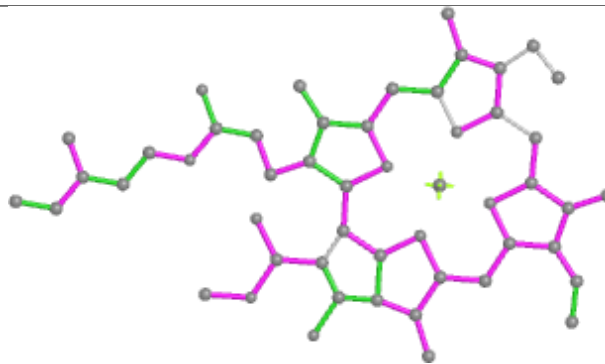


Rings

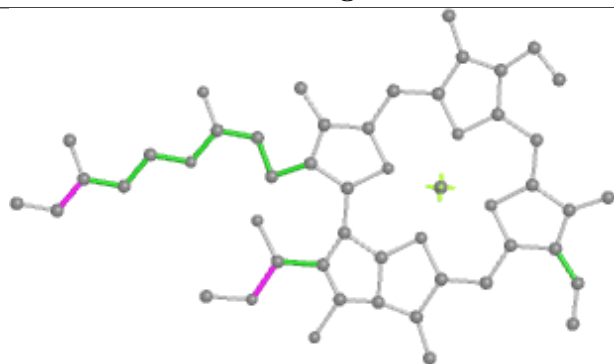
Ligand CHL A 852



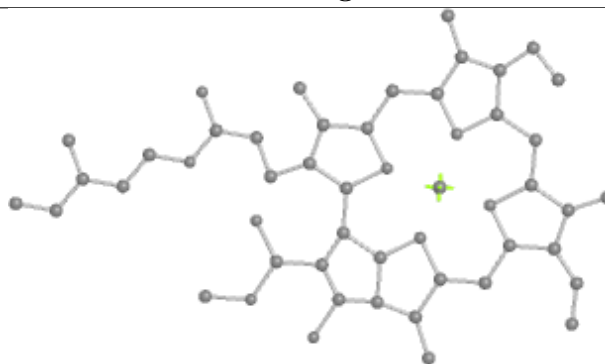
Bond lengths



Bond angles

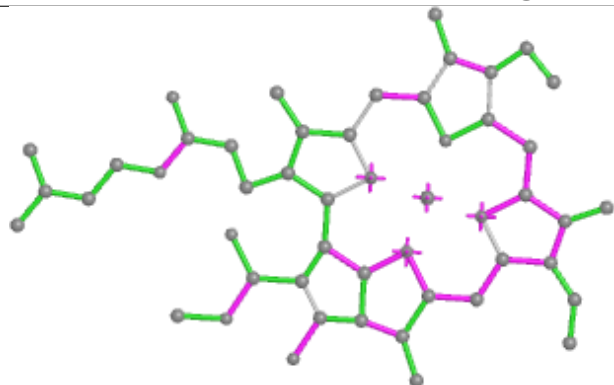


Torsions

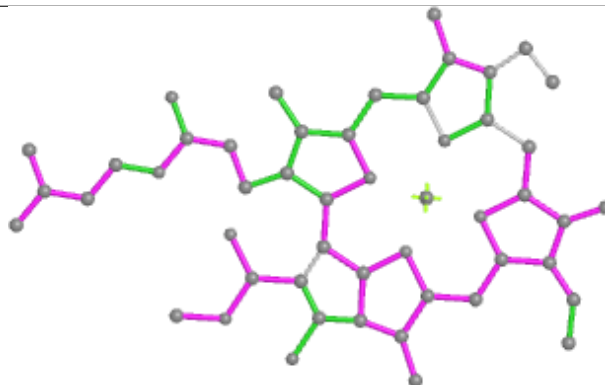


Rings

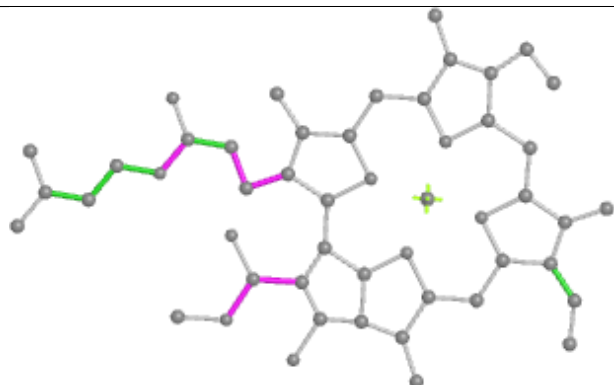
Ligand CHL 4 320



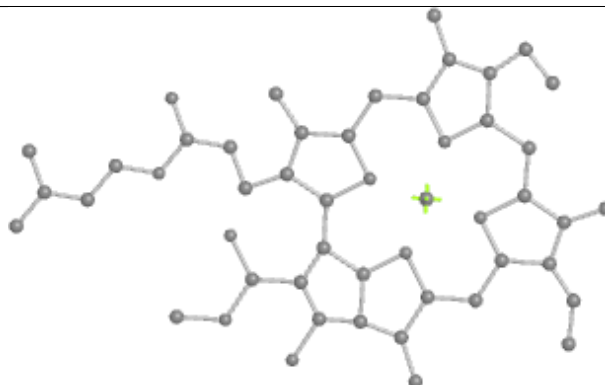
Bond lengths



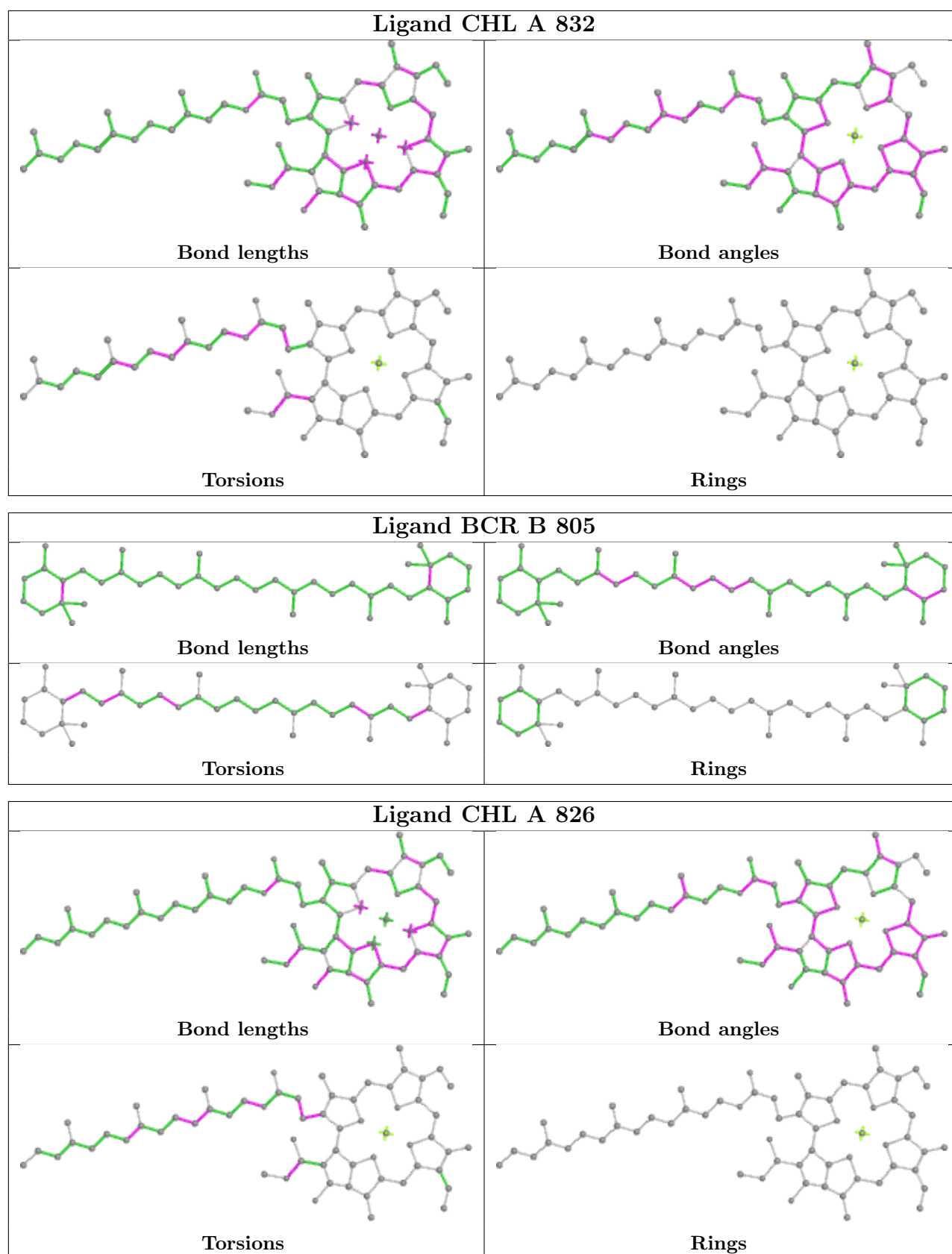
Bond angles

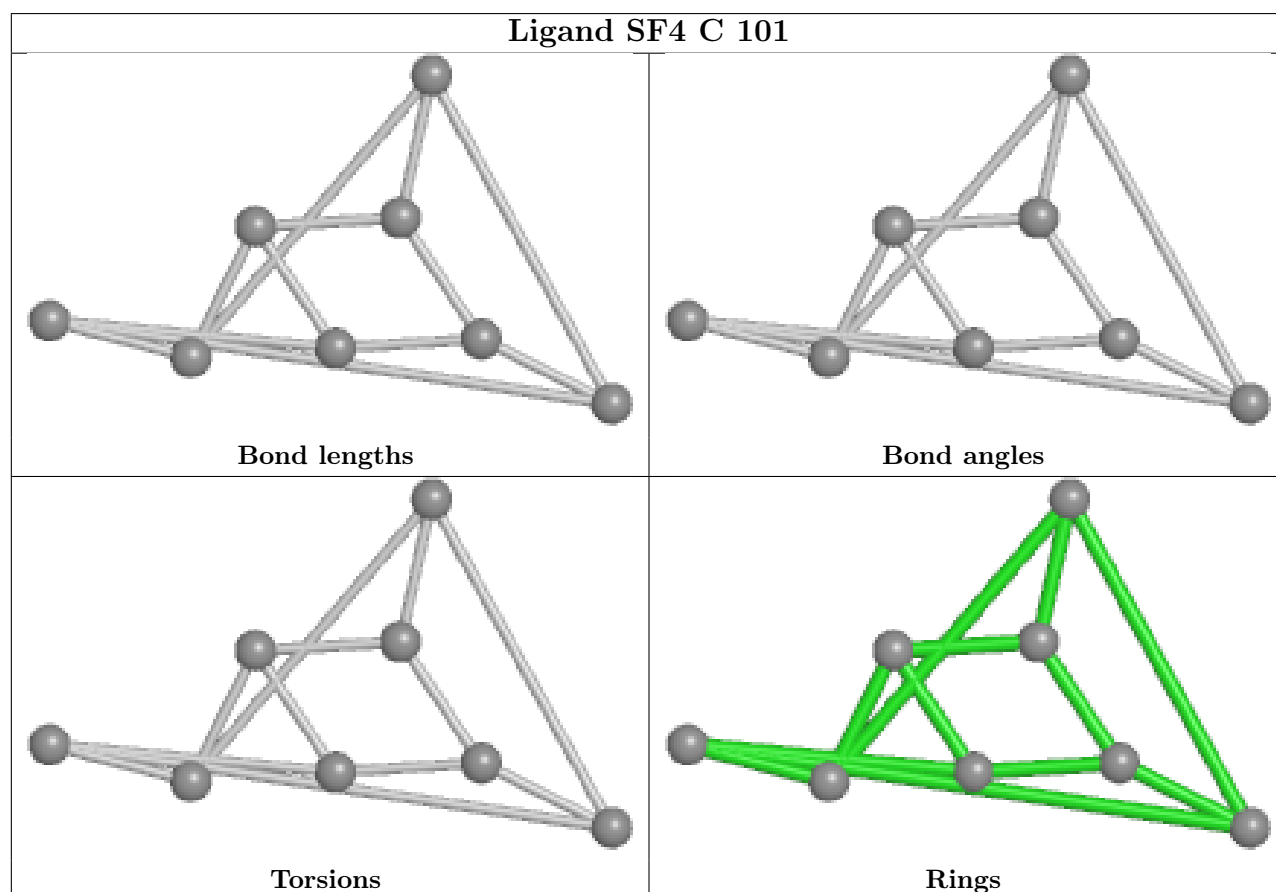
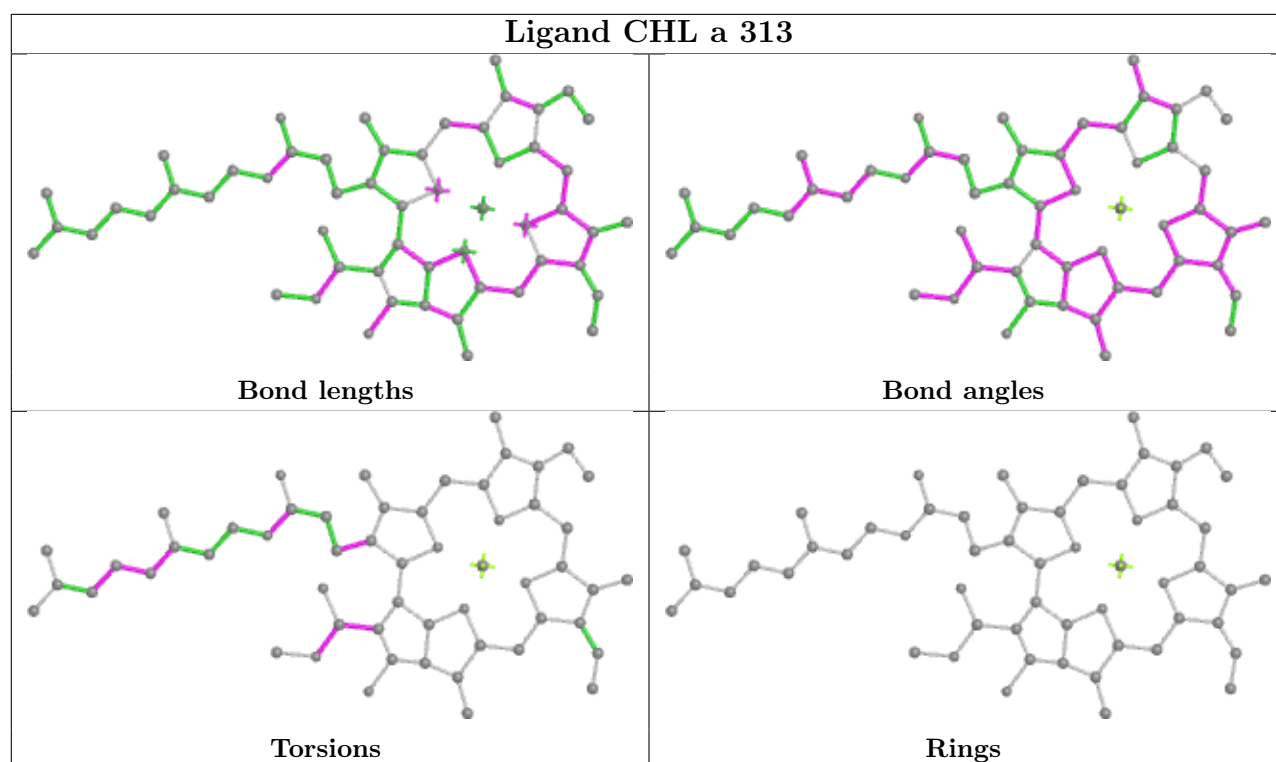


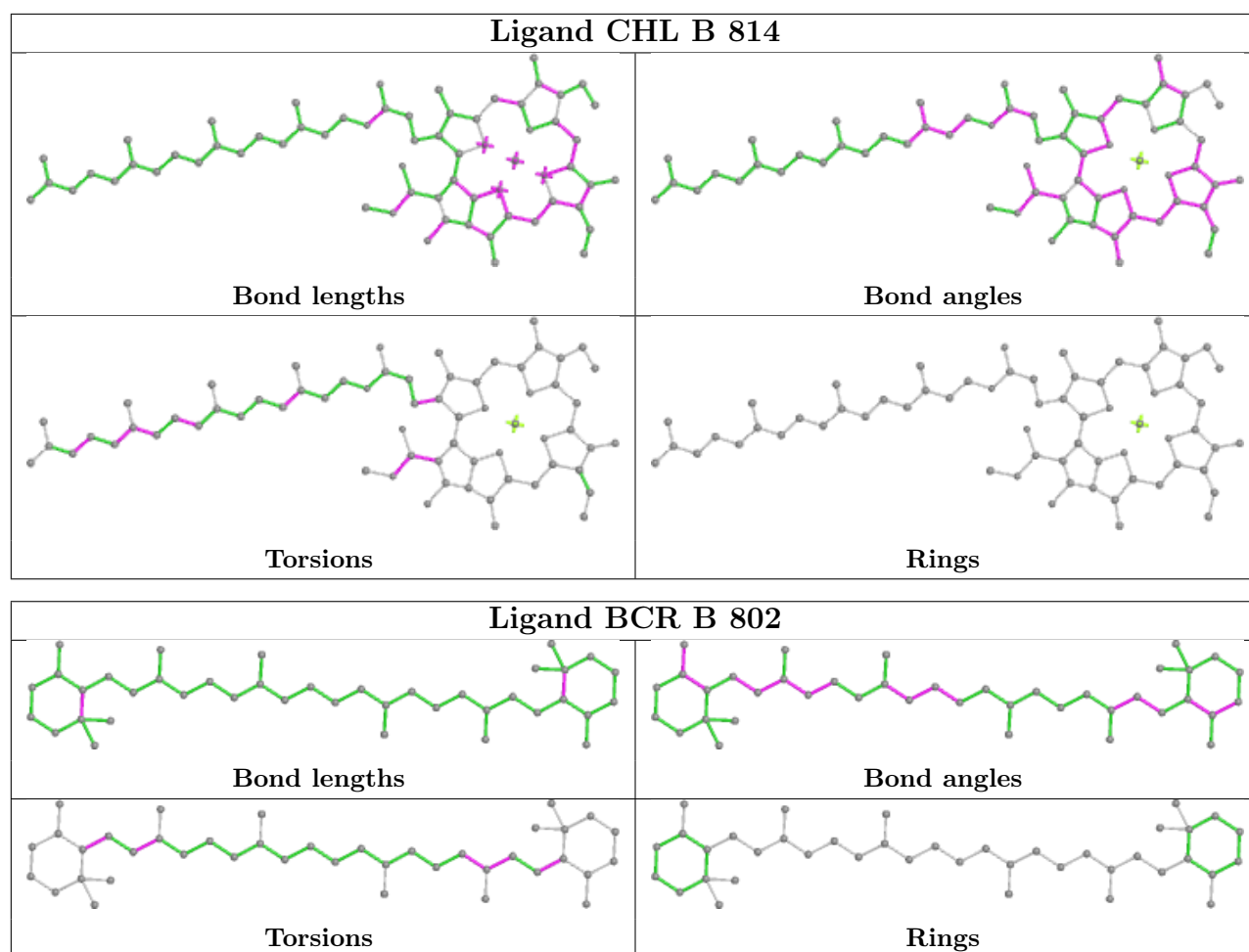
Torsions



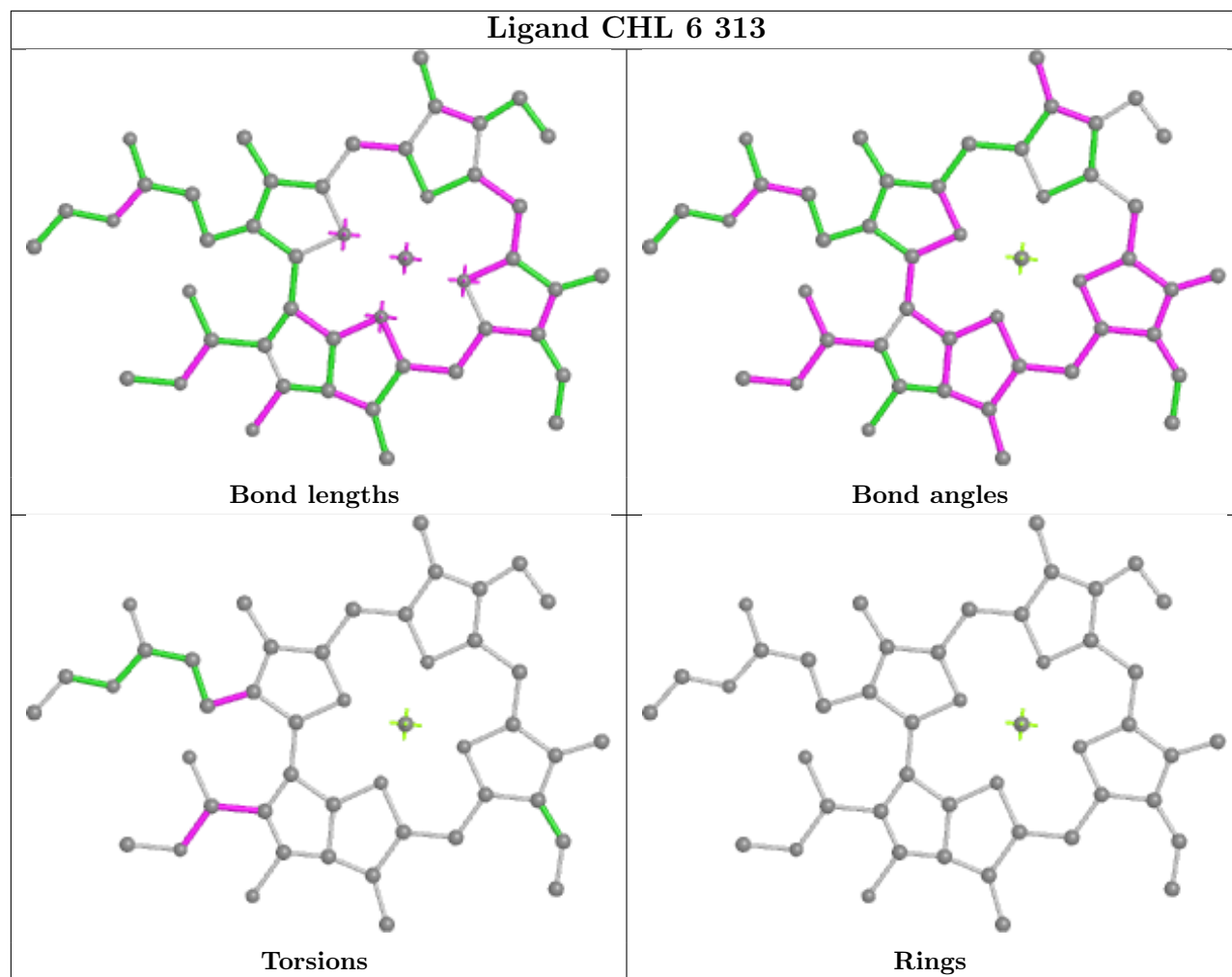
Rings



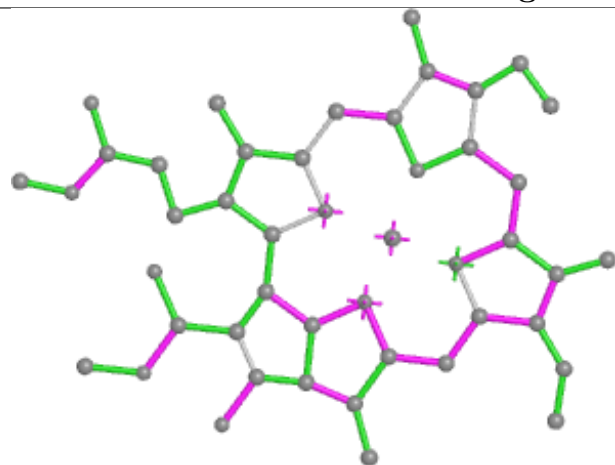




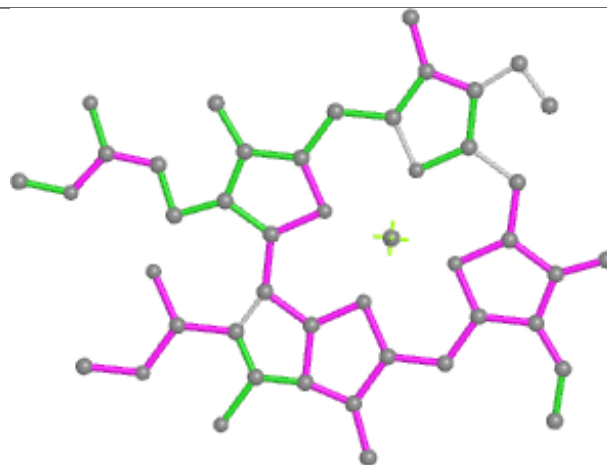
Ligand CHL 6 313



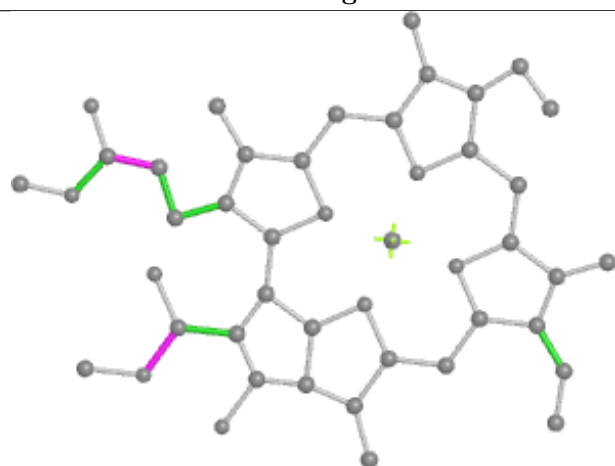
Ligand CHL b 312



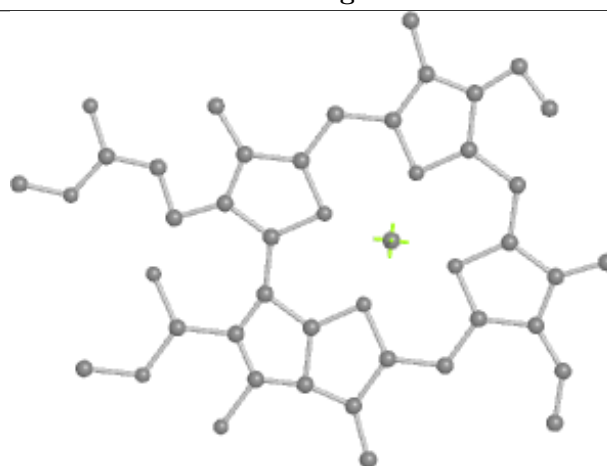
Bond lengths



Bond angles

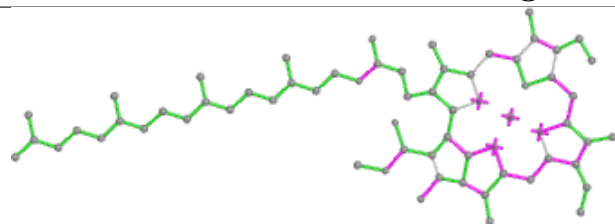


Torsions

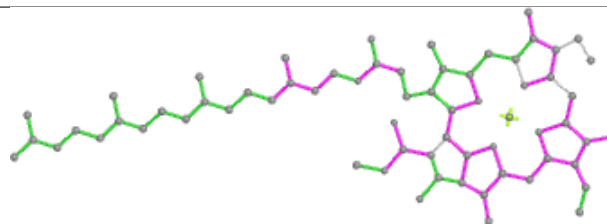


Rings

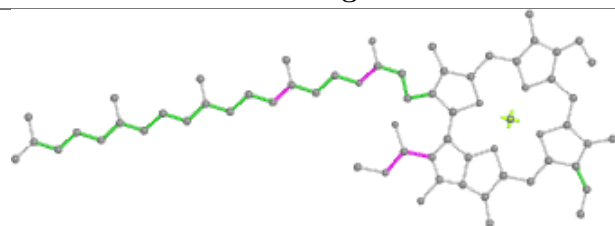
Ligand CHL 3 313



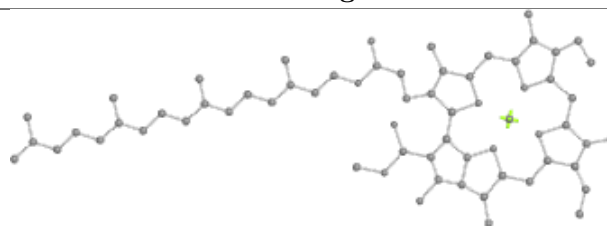
Bond lengths



Bond angles

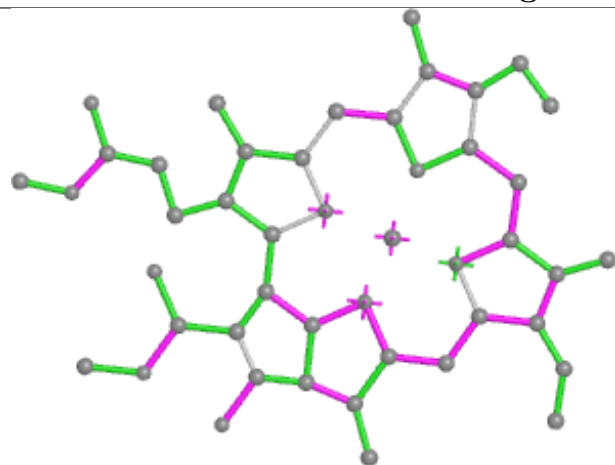


Torsions

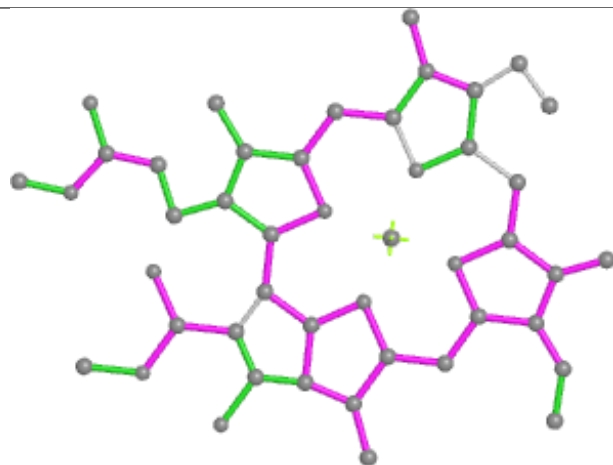


Rings

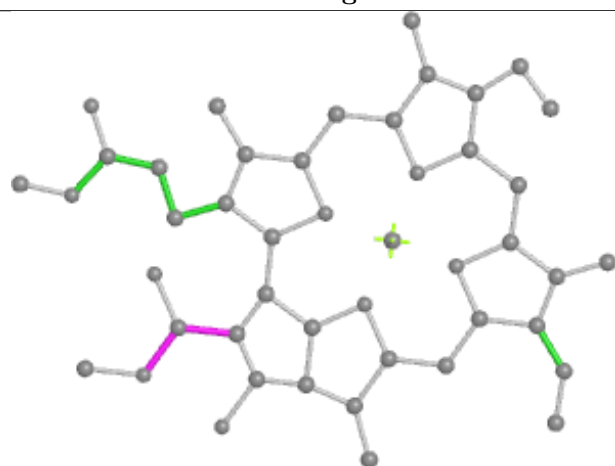
Ligand CHL 5 321



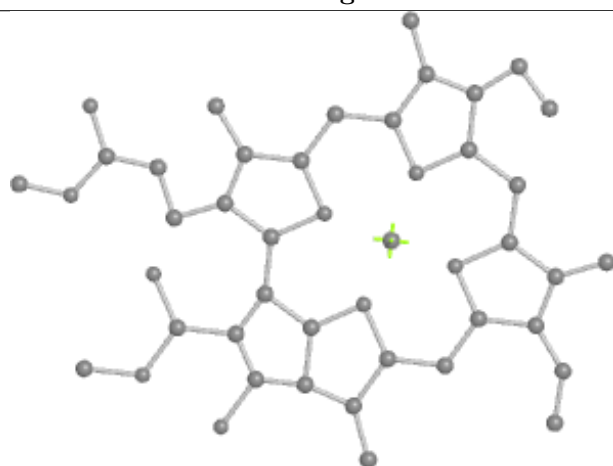
Bond lengths



Bond angles

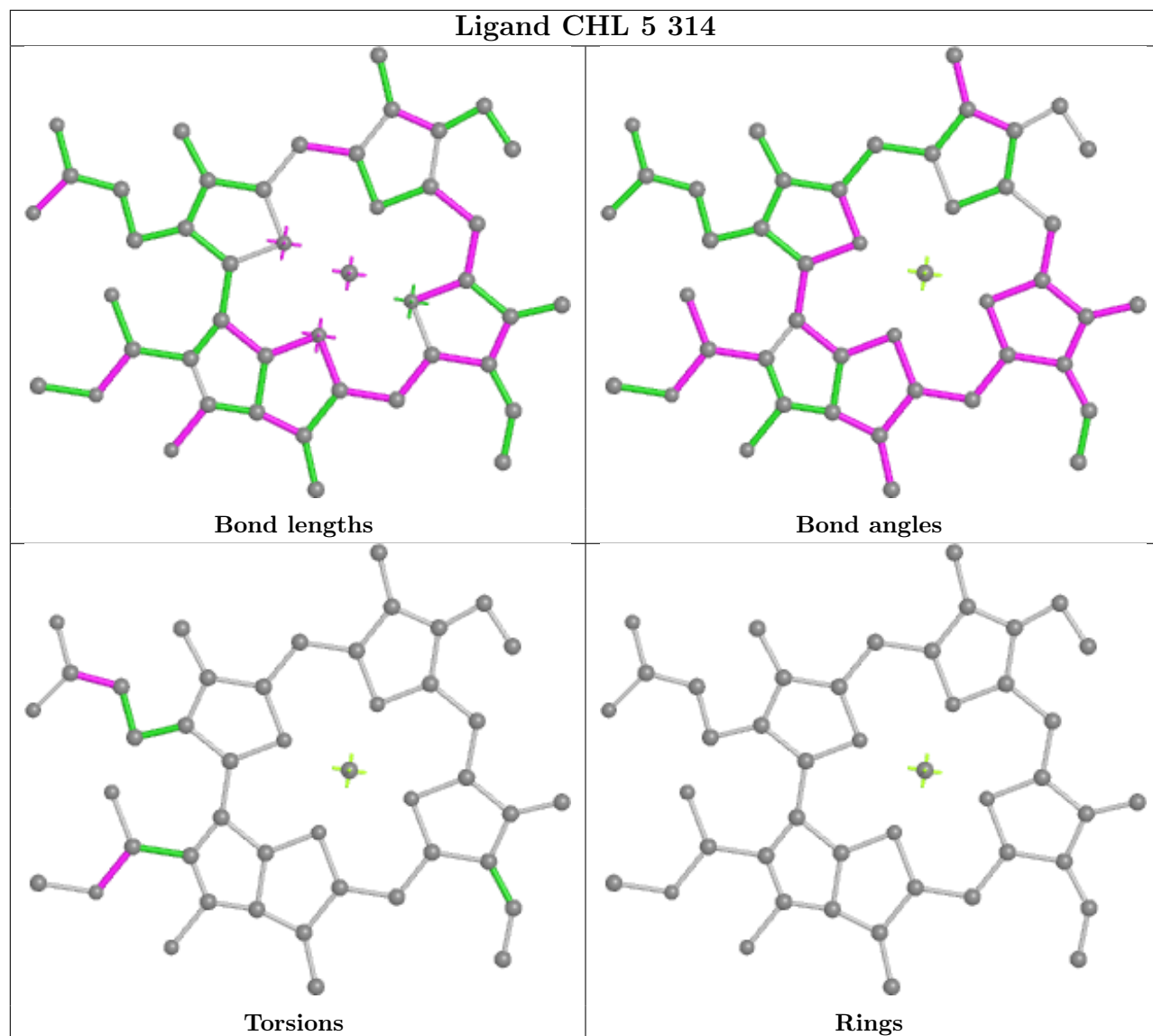


Torsions

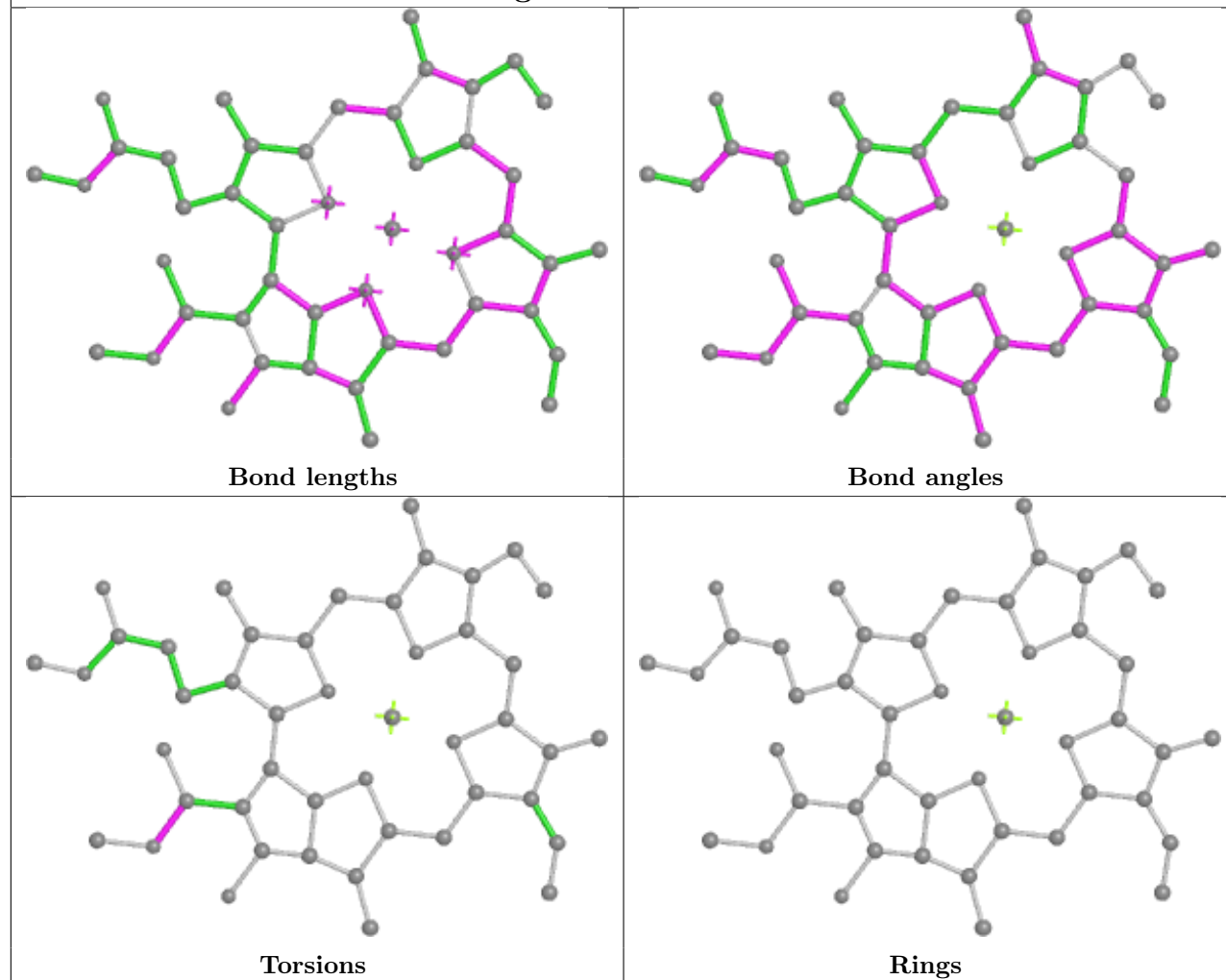


Rings

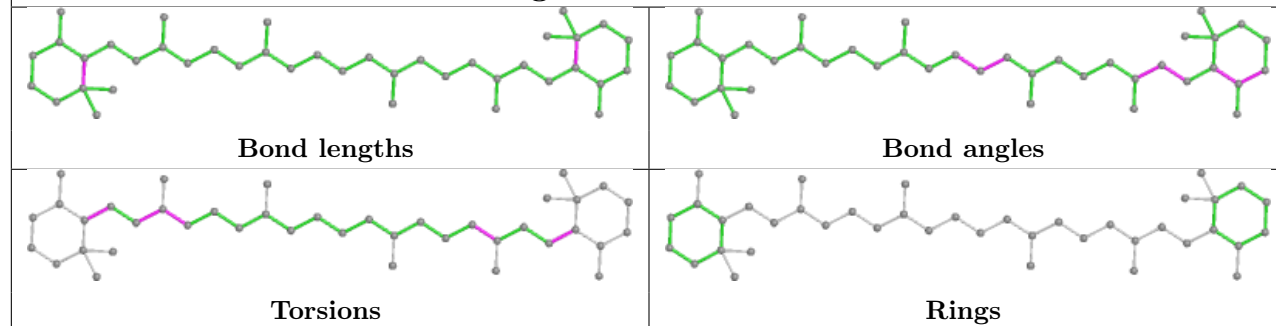
Ligand CHL 5 314

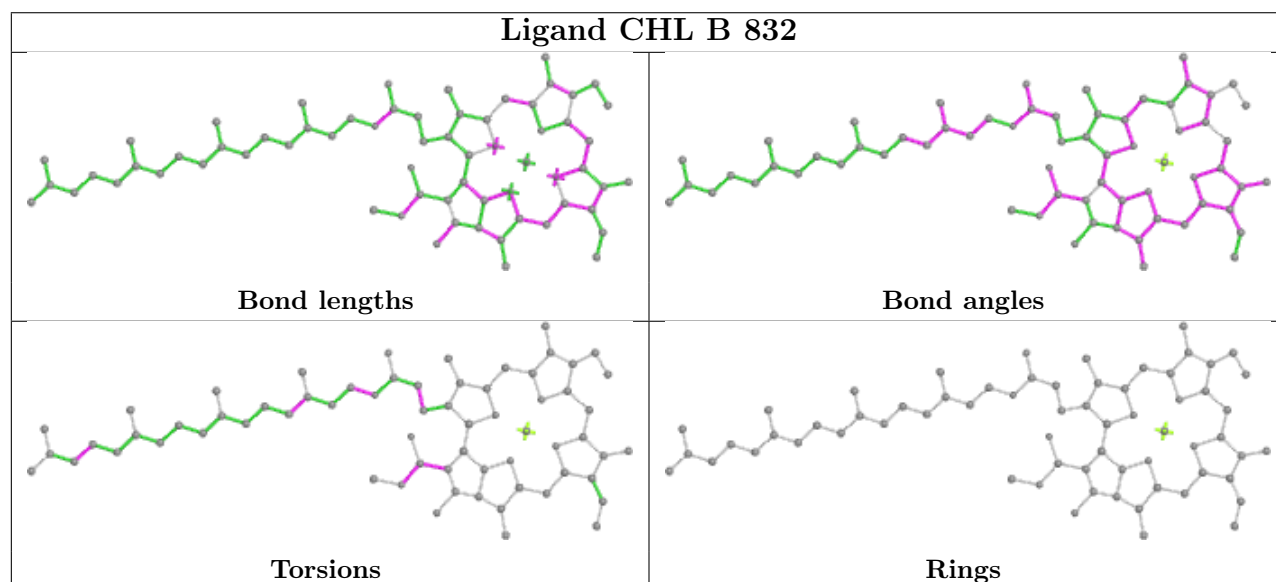
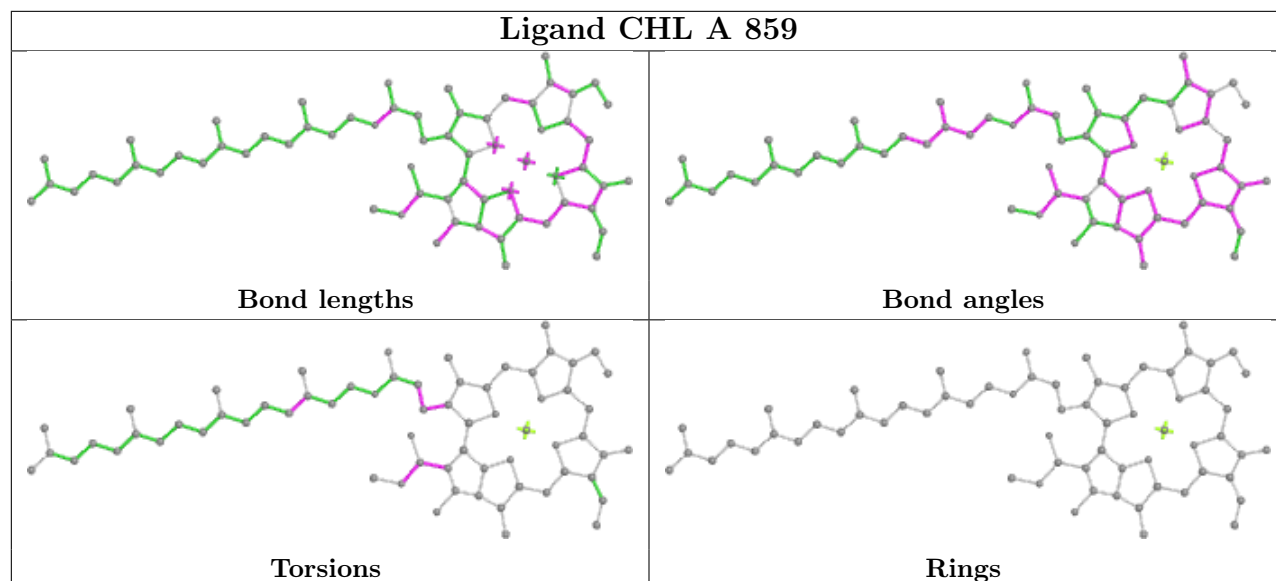
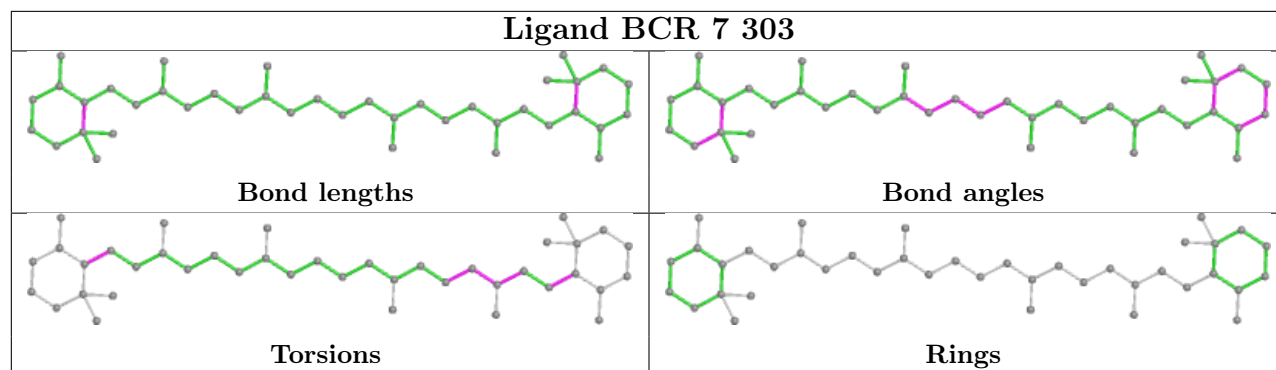


Ligand CHL 3 309

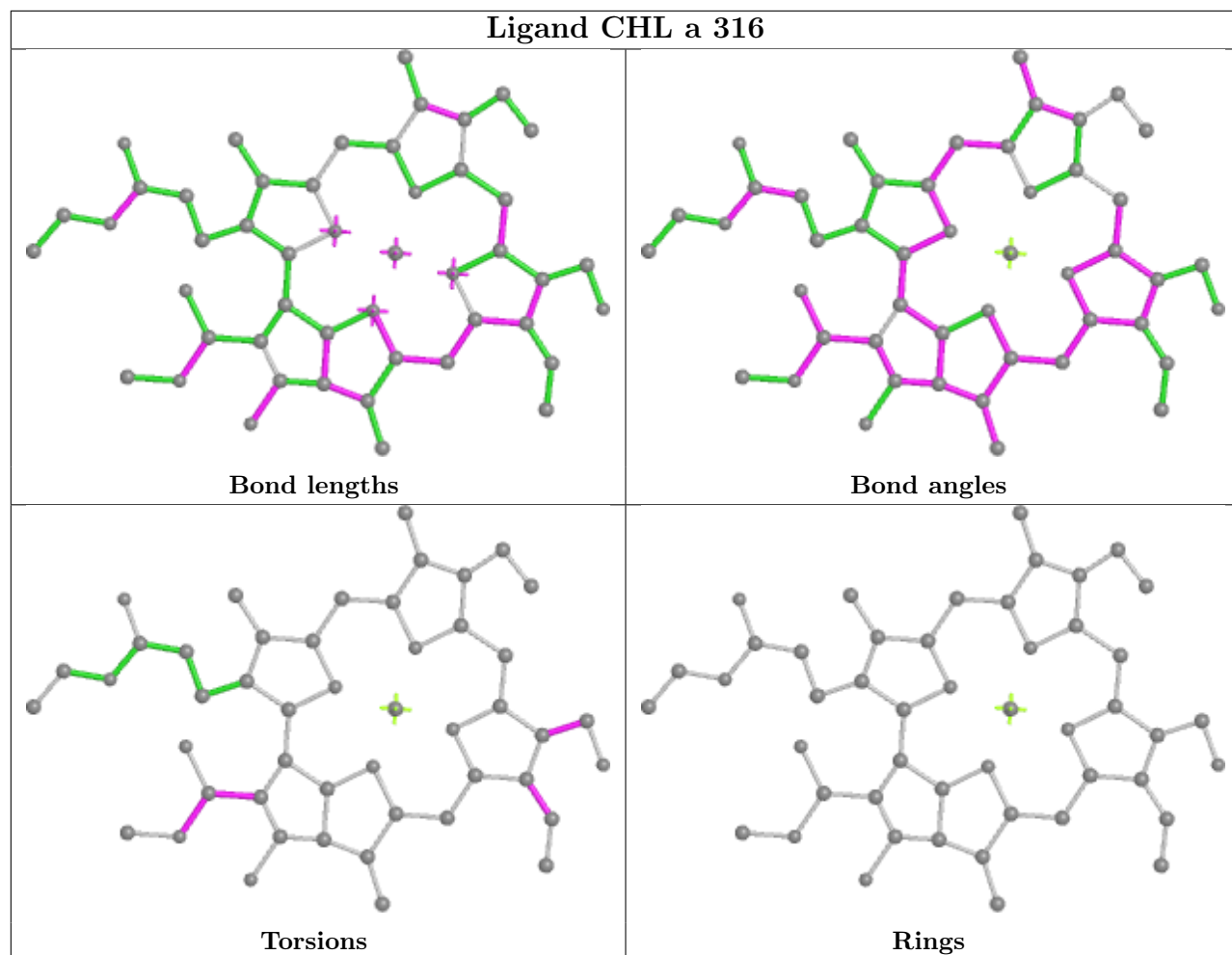


Ligand BCR B 804

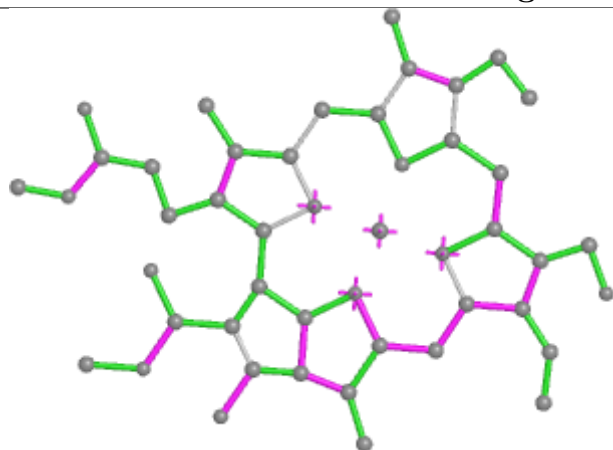




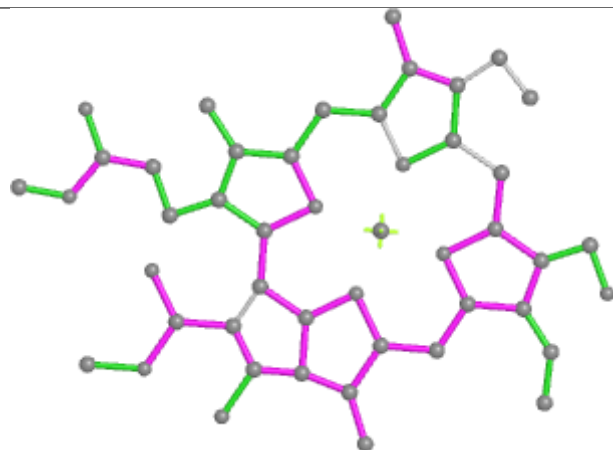
Ligand CHL a 316



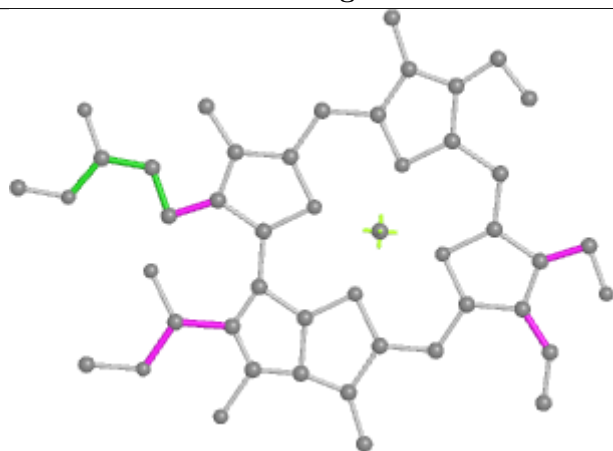
Ligand CHL 5 319



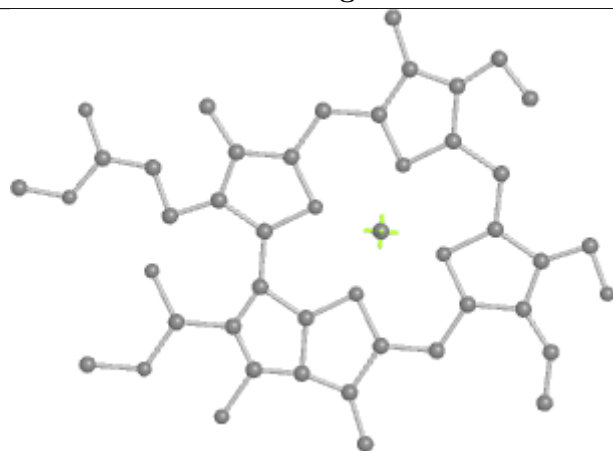
Bond lengths



Bond angles

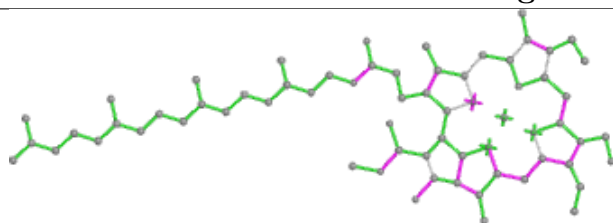


Torsions

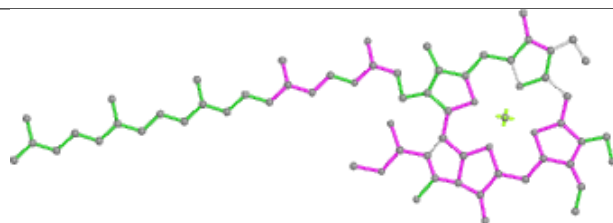


Rings

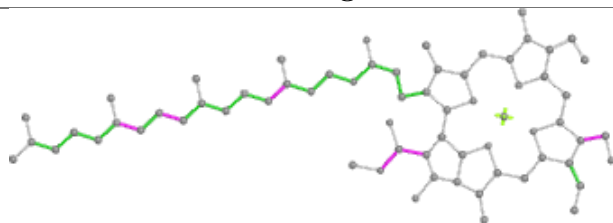
Ligand CHL 8 314



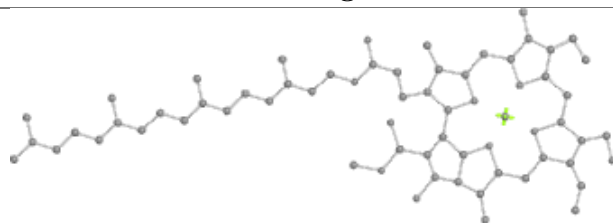
Bond lengths



Bond angles

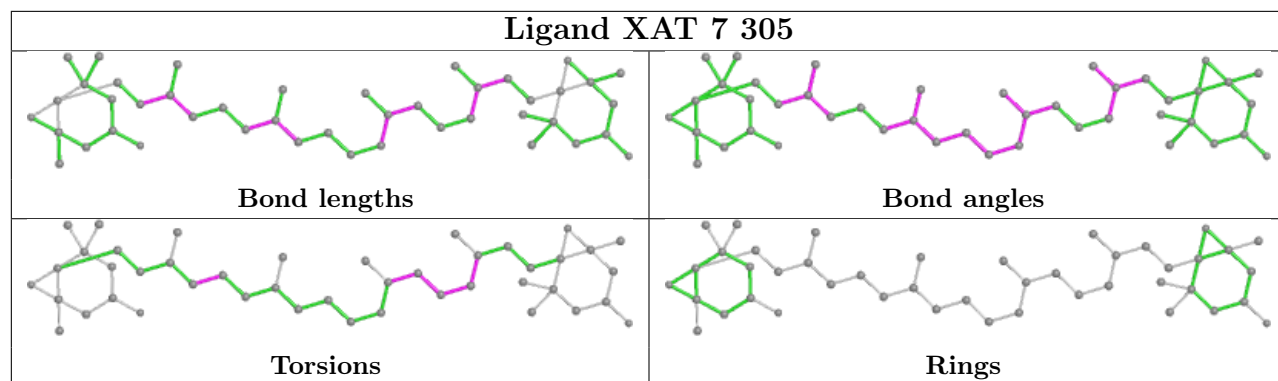


Torsions

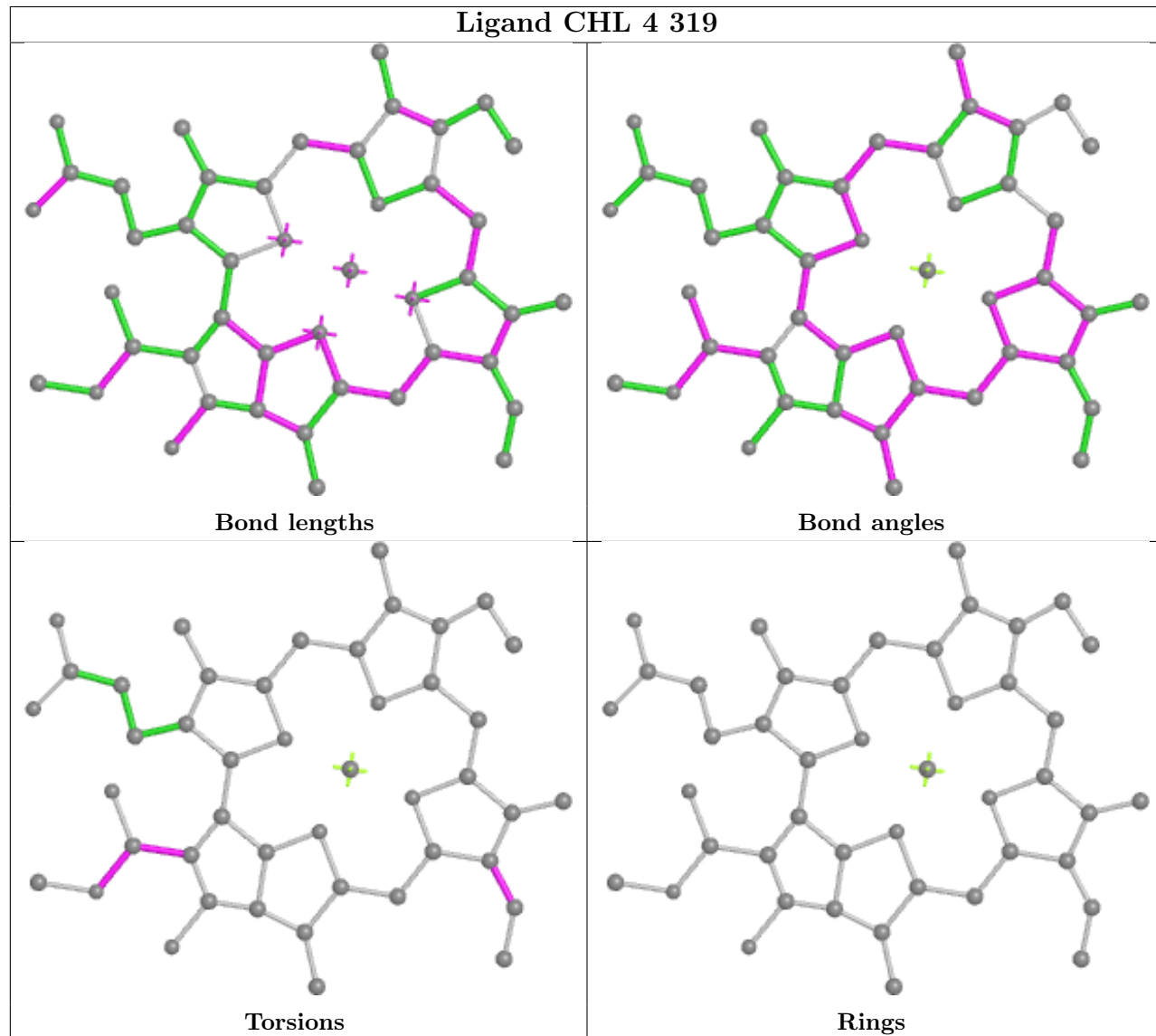


Rings

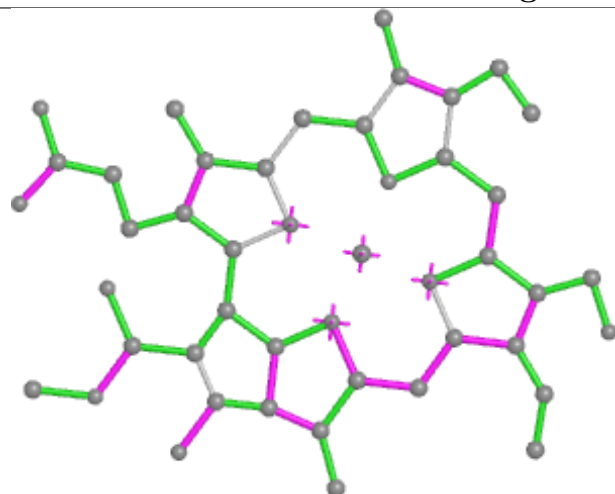
Ligand XAT 7 305



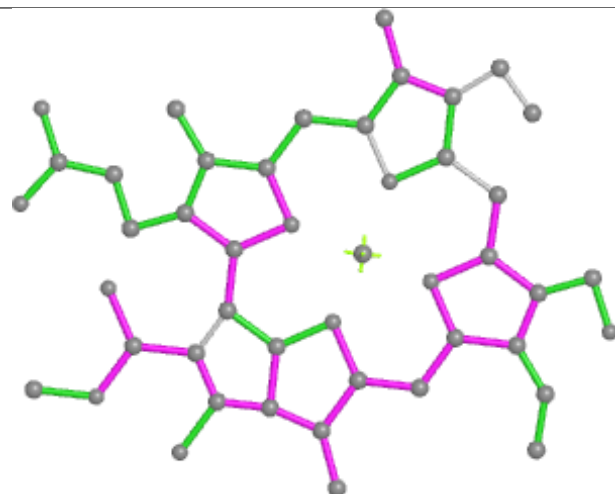
Ligand CHL 4 319



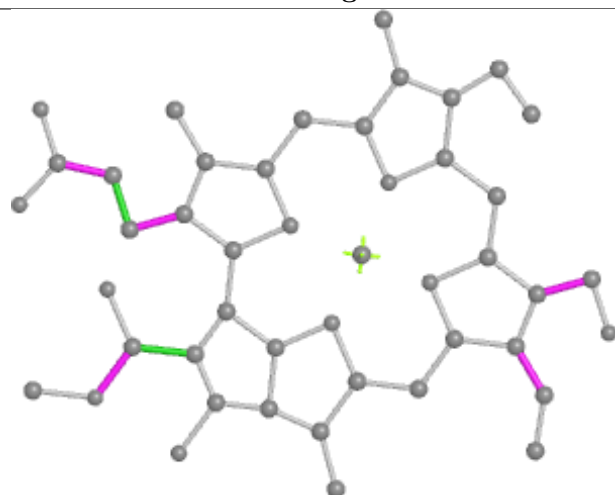
Ligand CHL 6 316



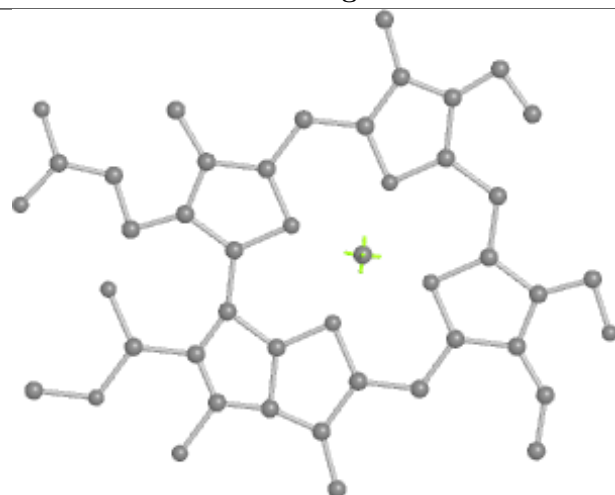
Bond lengths



Bond angles

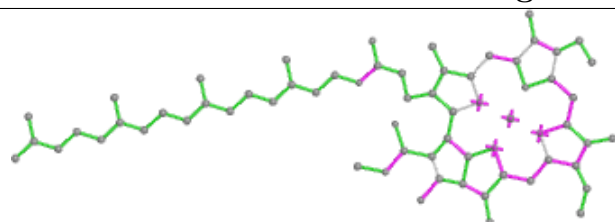


Torsions

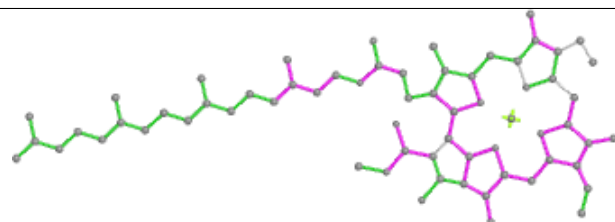


Rings

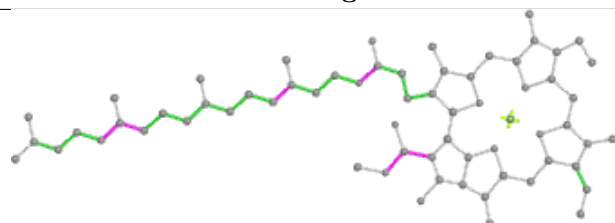
Ligand CHL B 844



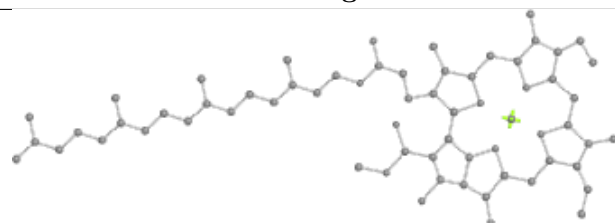
Bond lengths



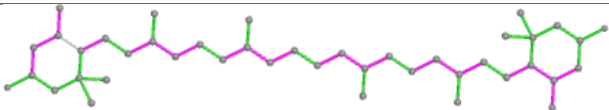
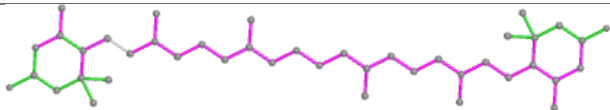
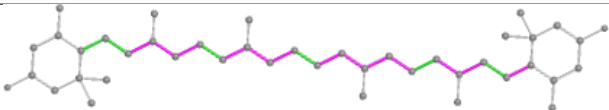
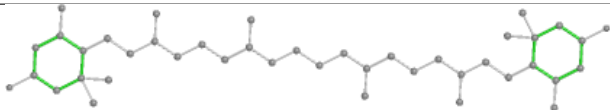
Bond angles

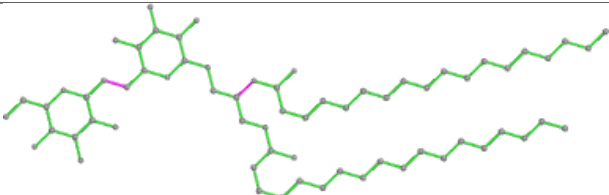
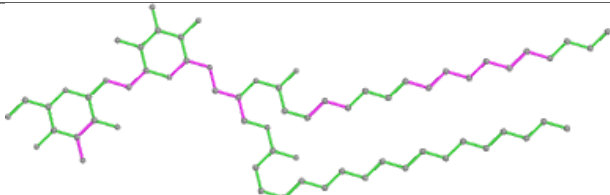
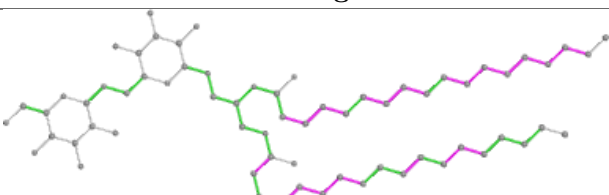
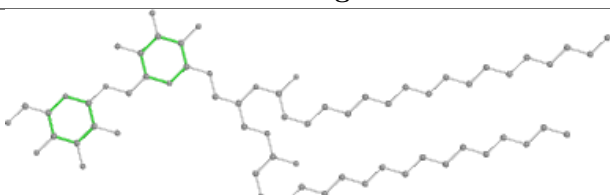


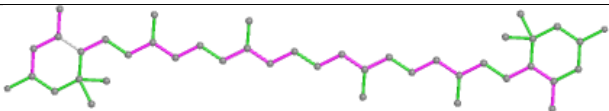
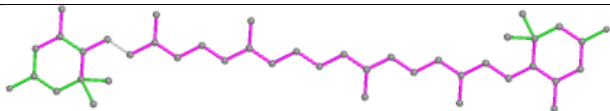
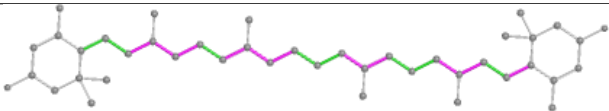
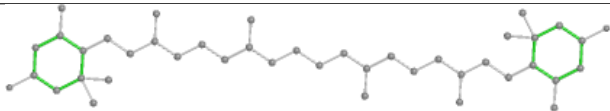
Torsions

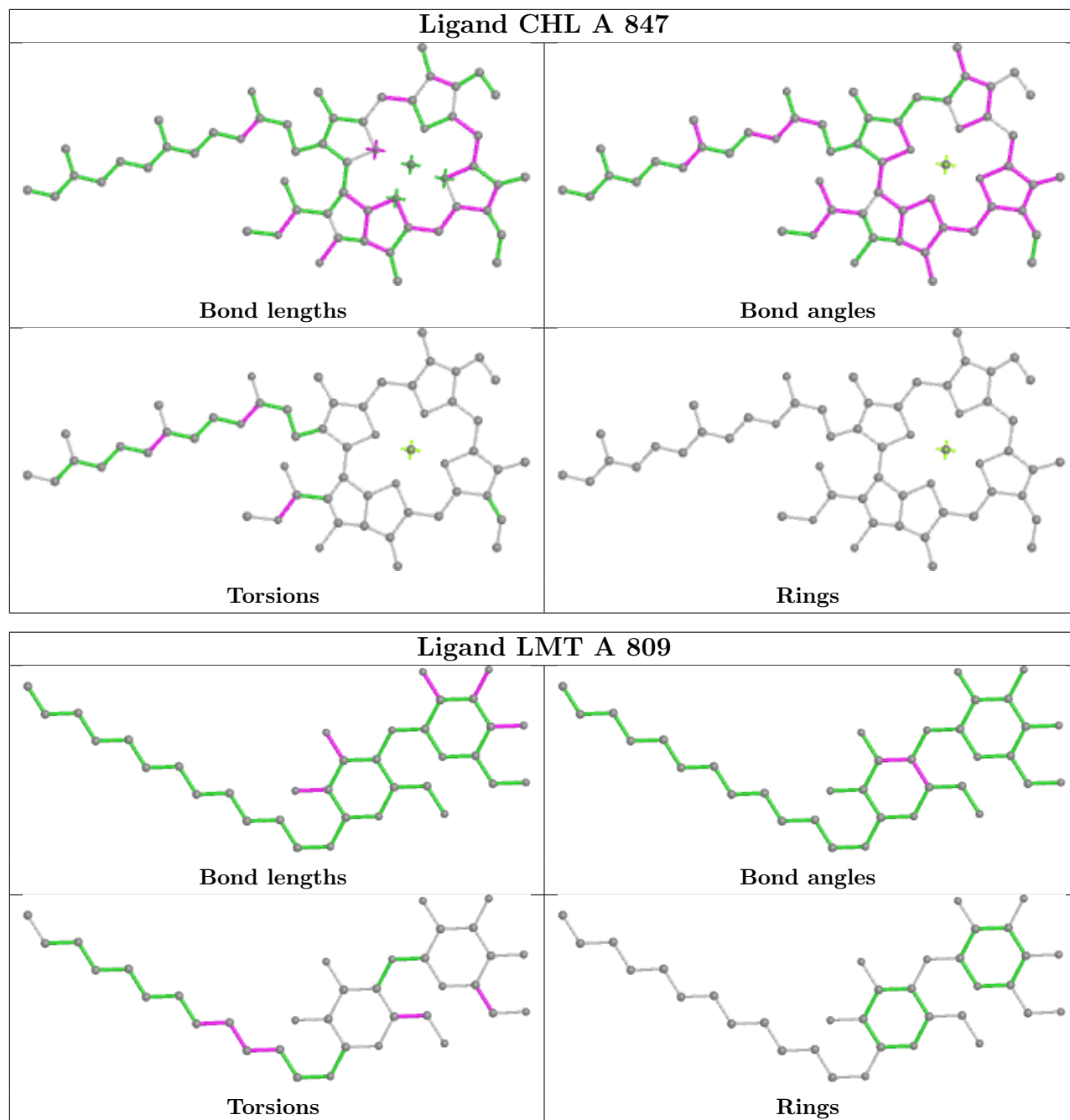


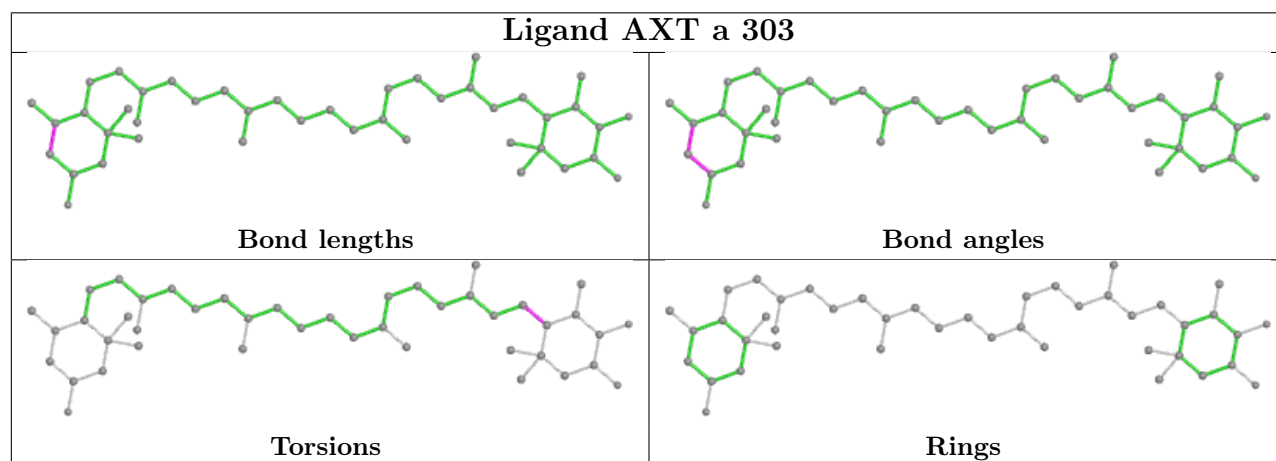
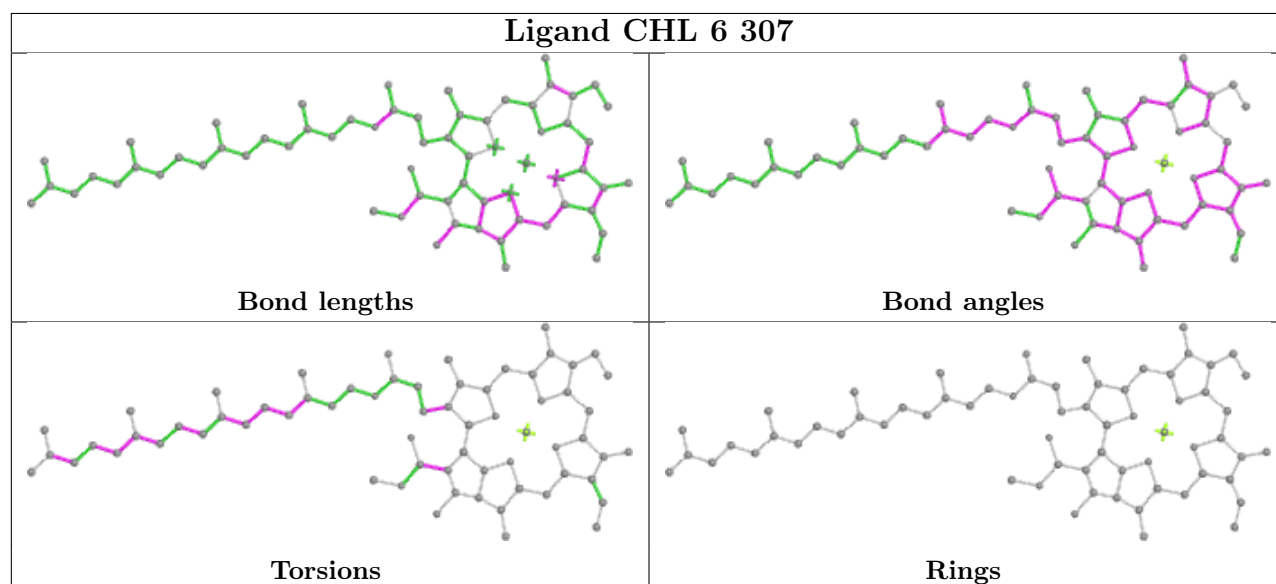
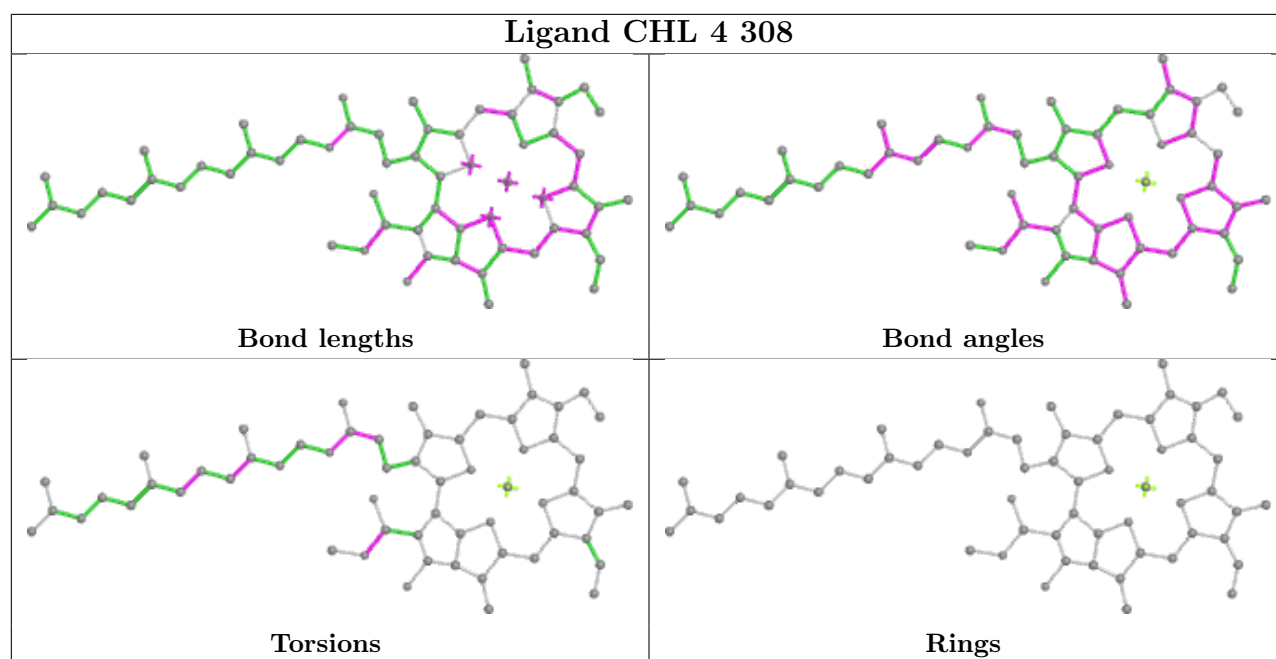
Rings

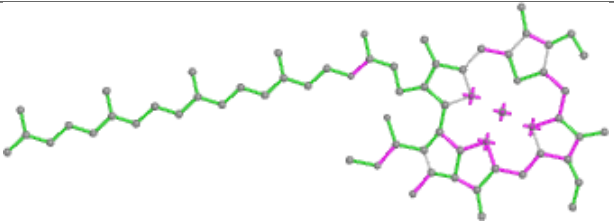
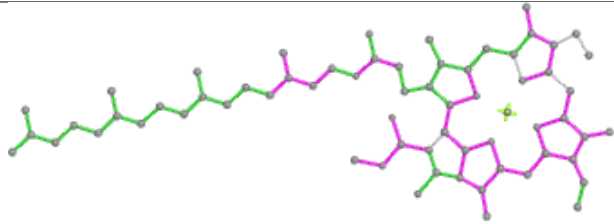
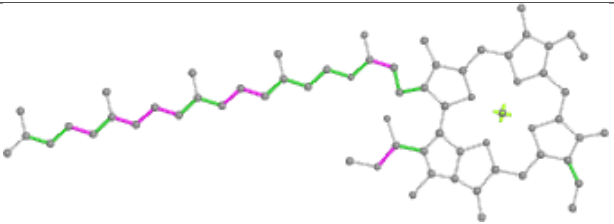
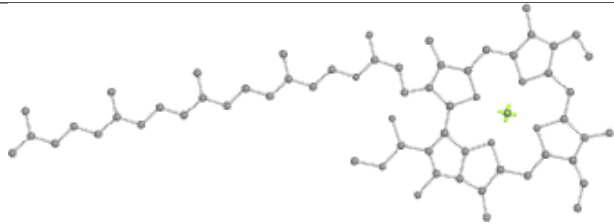
Ligand LUT 6 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

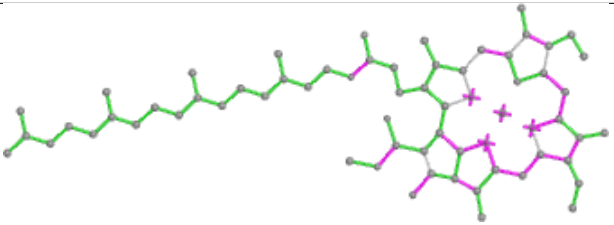
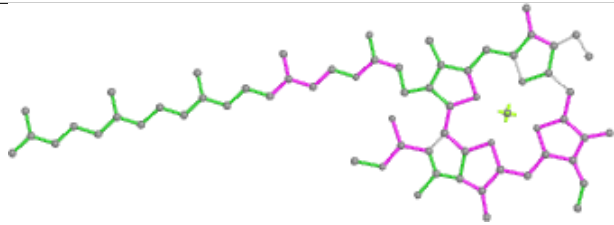
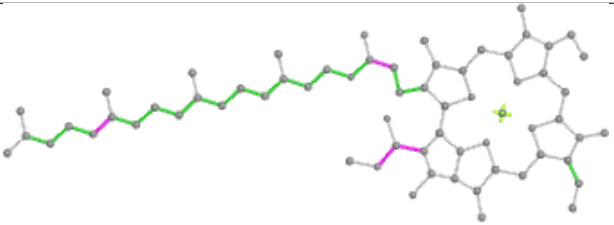
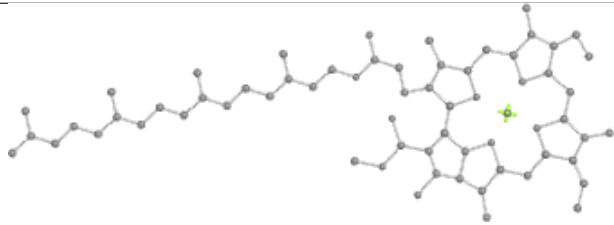
Ligand DGD 7 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

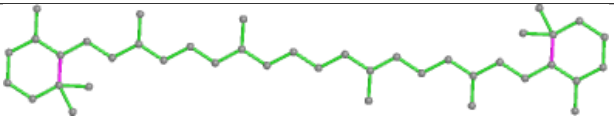
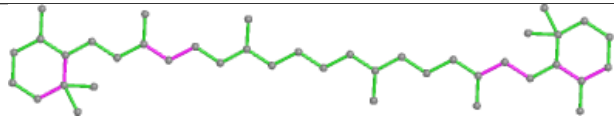
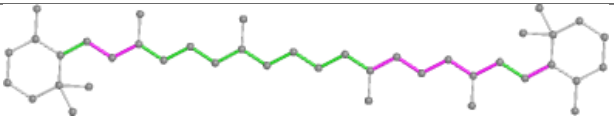
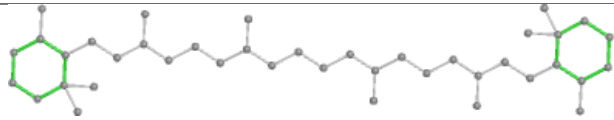
Ligand LUT 3 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

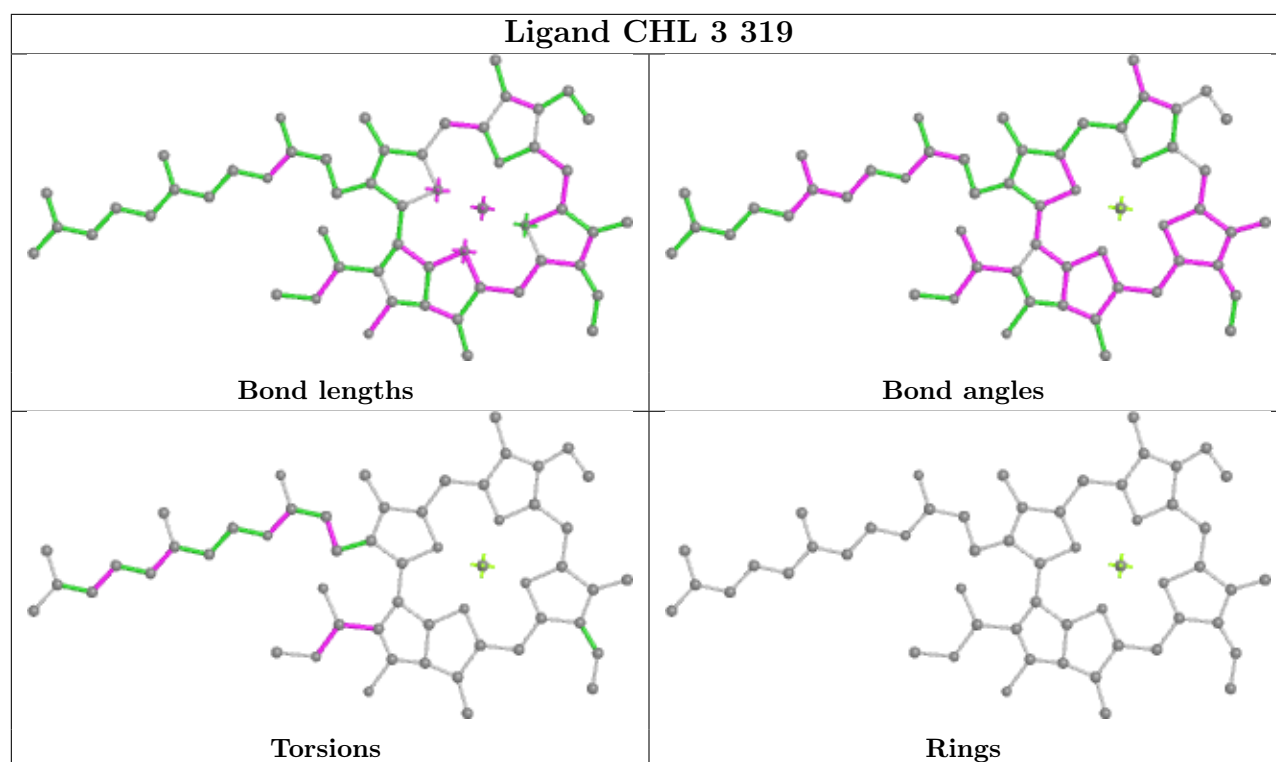




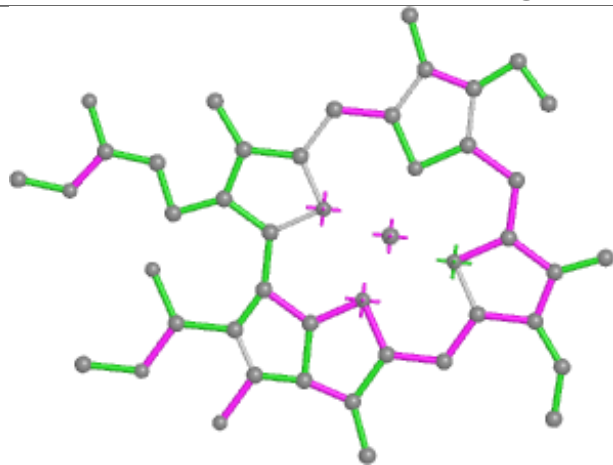
Ligand CHL 8 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL B 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

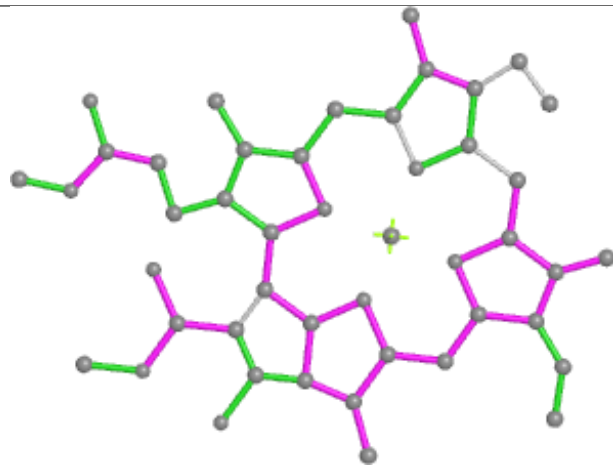
Ligand BCR 5 301	
	
Bond lengths	Bond angles
	
Torsions	Rings



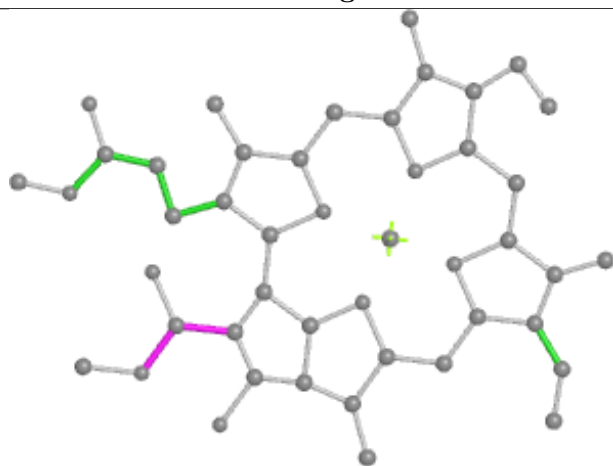
Ligand CHL 6 314



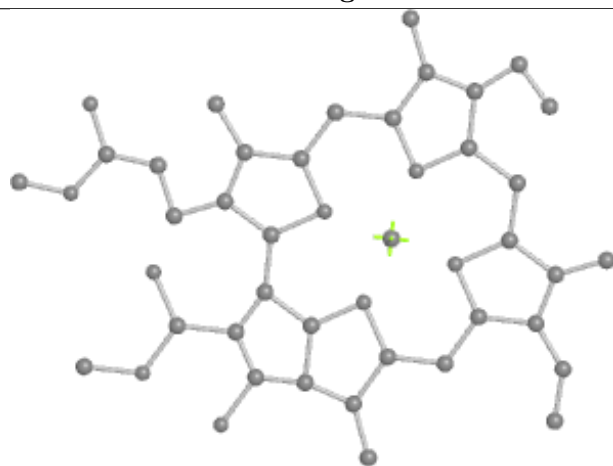
Bond lengths



Bond angles

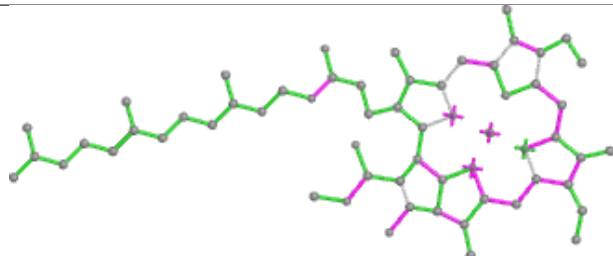


Torsions

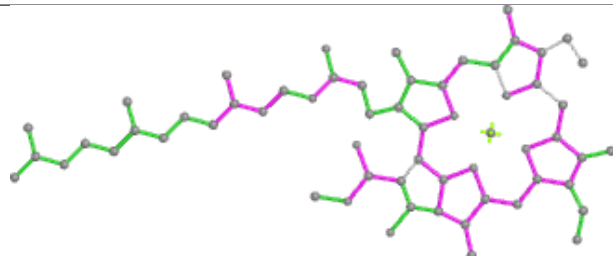


Rings

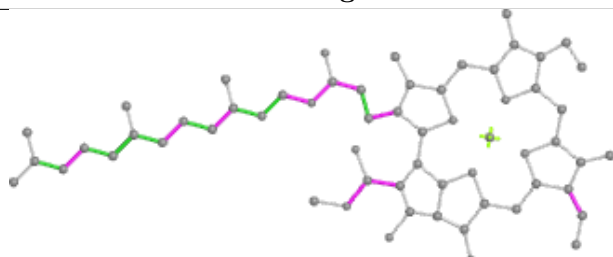
Ligand CHL 3 311



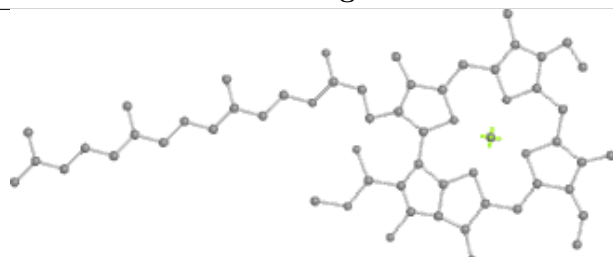
Bond lengths



Bond angles

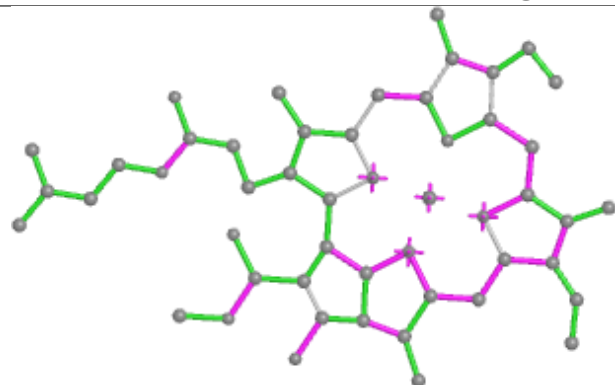


Torsions

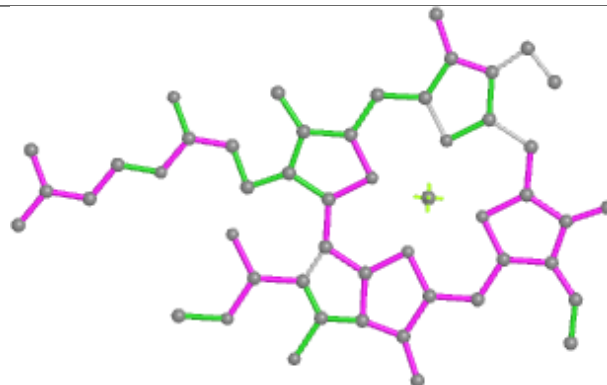


Rings

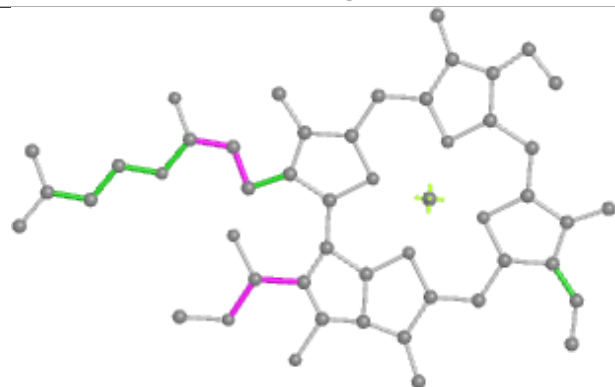
Ligand CHL F 309



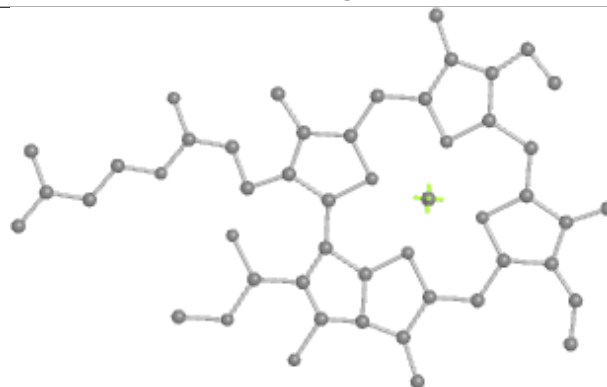
Bond lengths



Bond angles

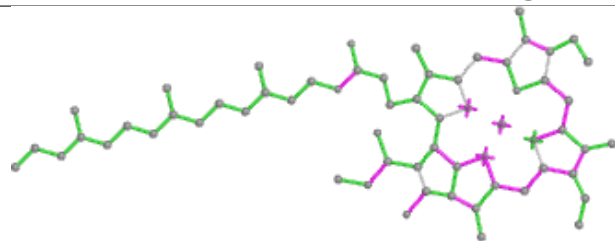


Torsions

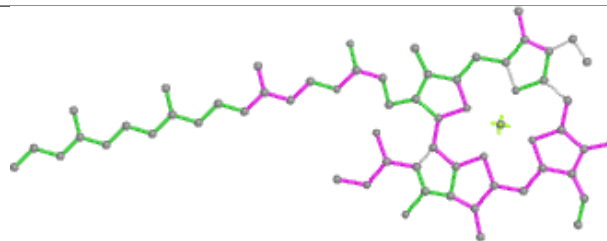


Rings

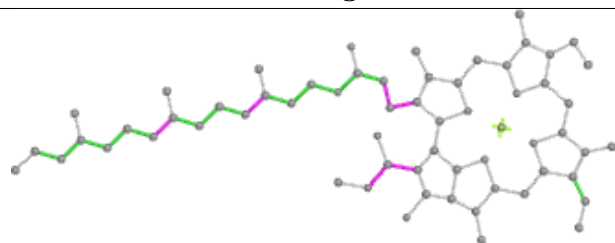
Ligand CHL 7 314



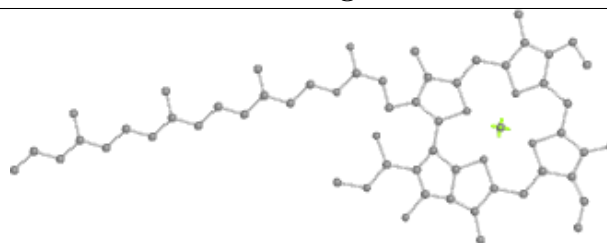
Bond lengths



Bond angles

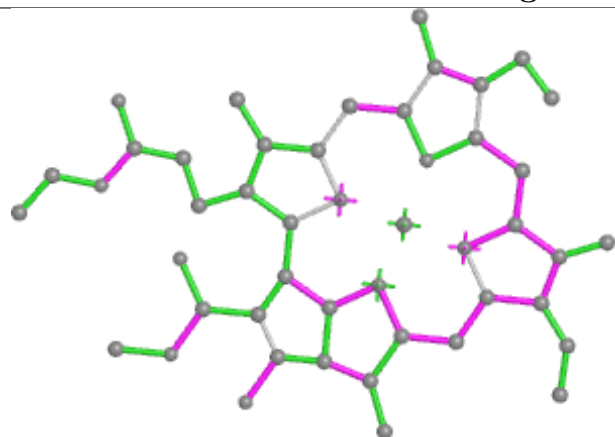


Torsions

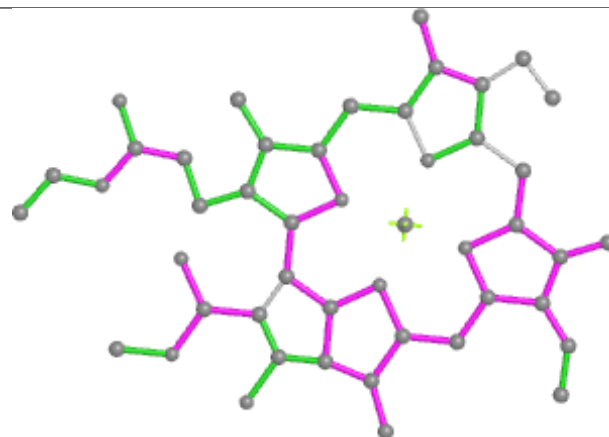


Rings

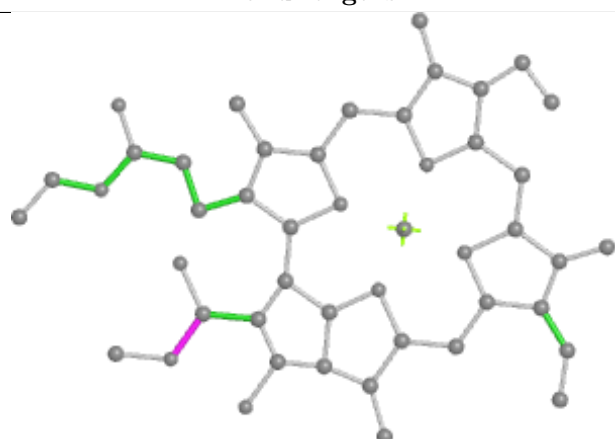
Ligand CHL 4 315



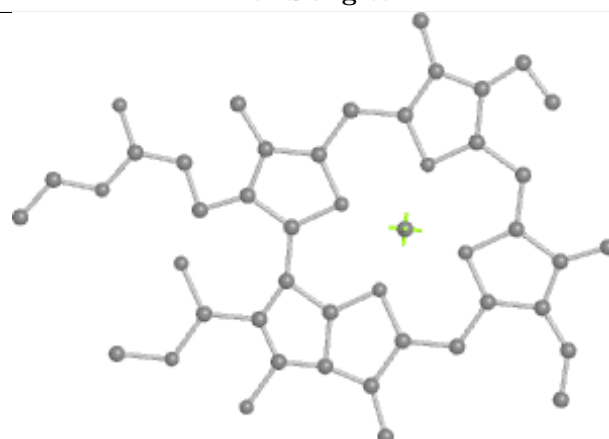
Bond lengths



Bond angles

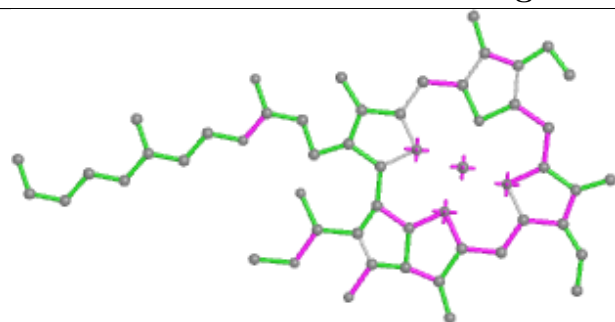


Torsions

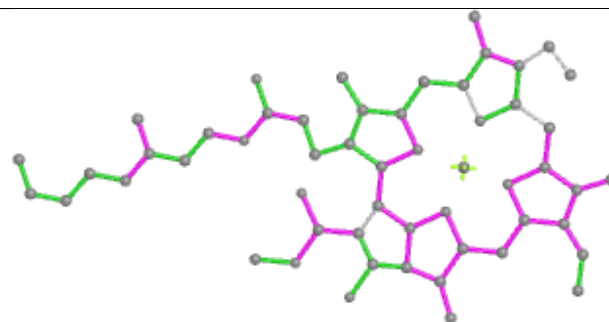


Rings

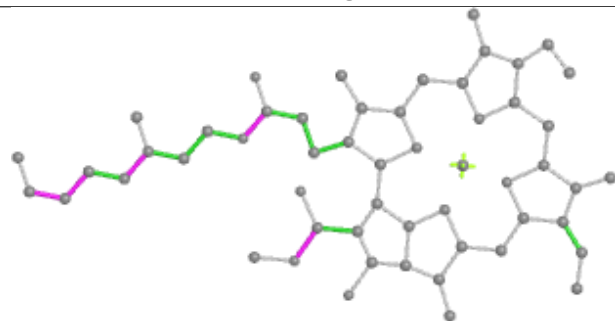
Ligand CHL A 827



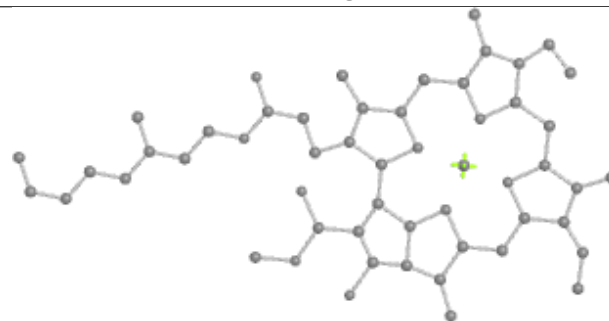
Bond lengths



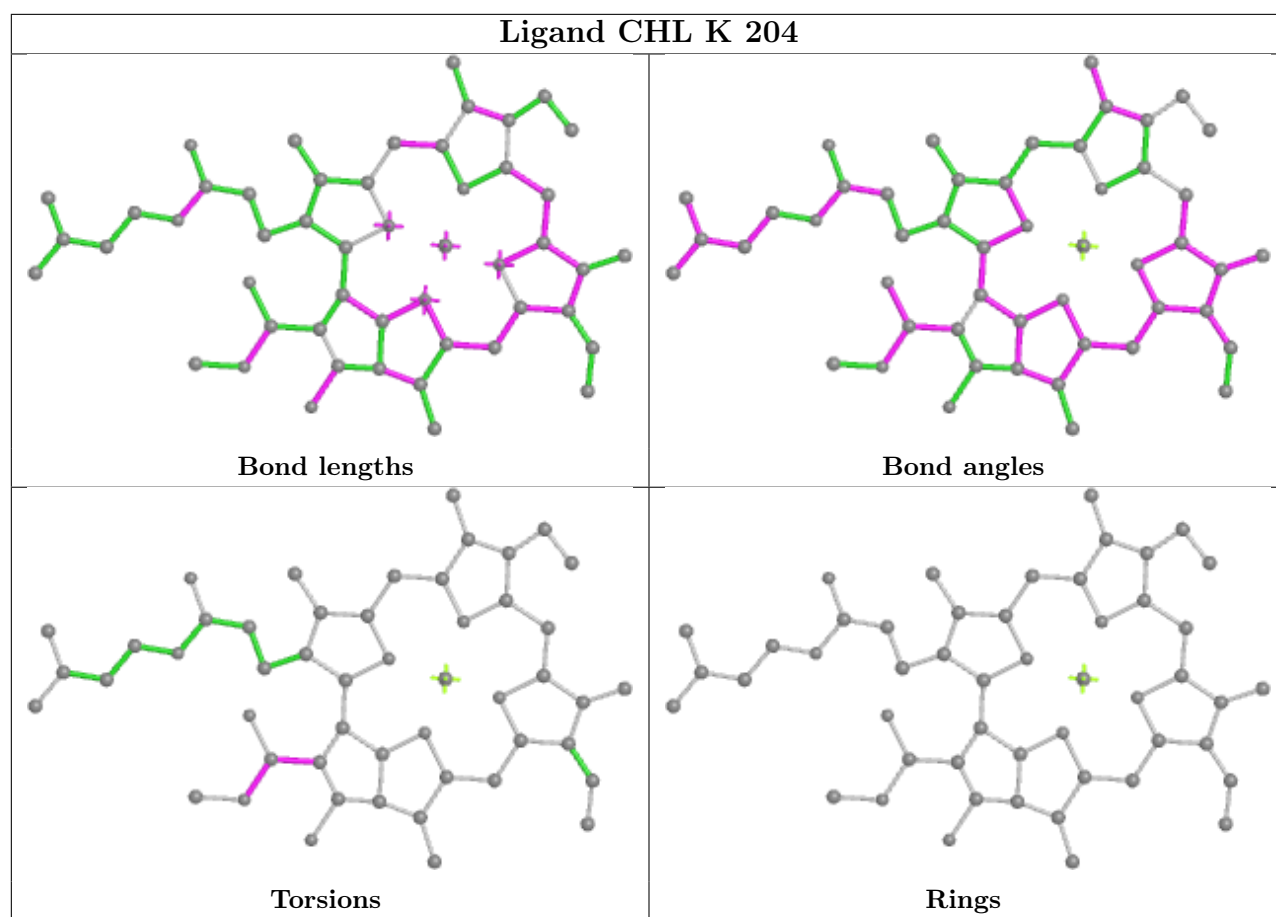
Bond angles



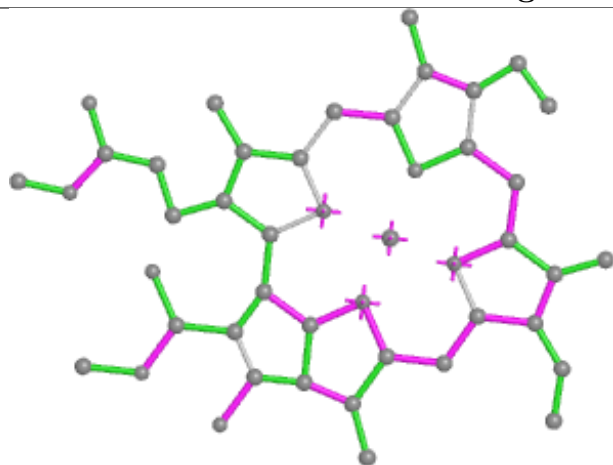
Torsions



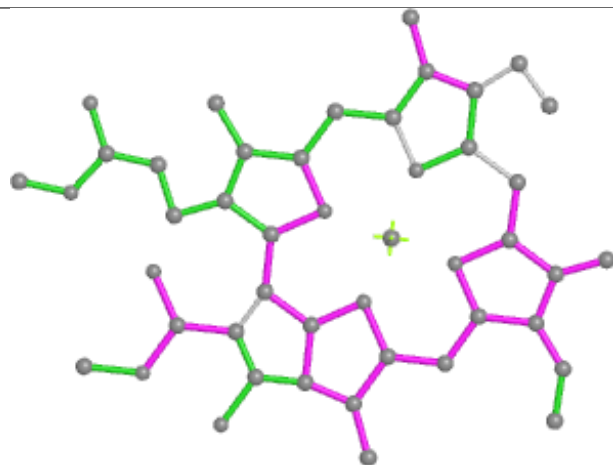
Rings



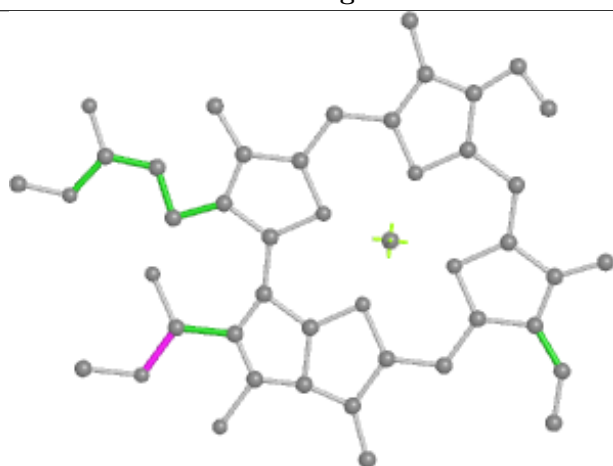
Ligand CHL 8 311



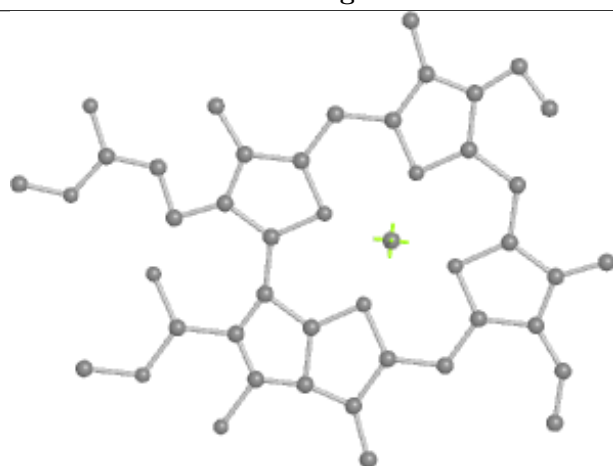
Bond lengths



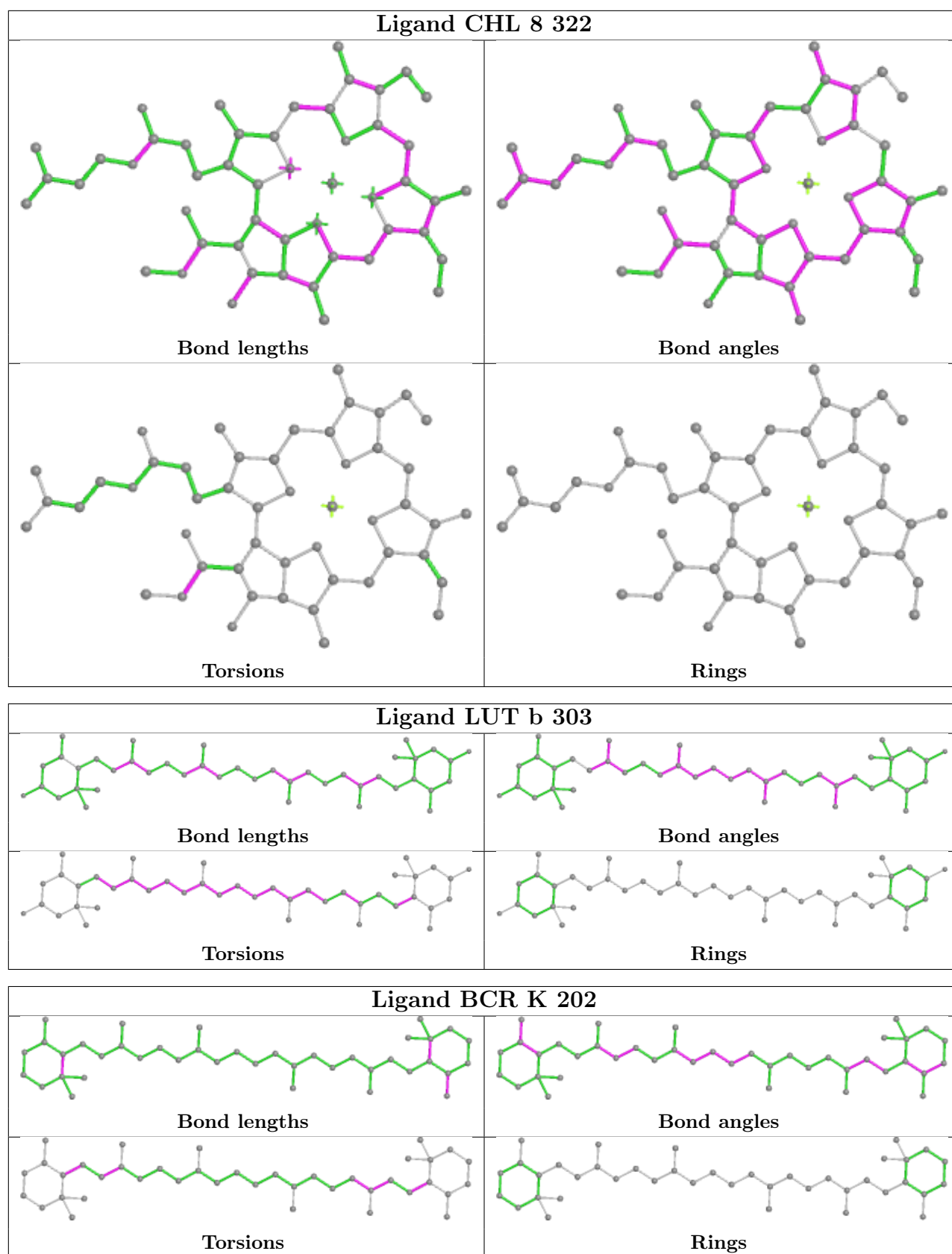
Bond angles

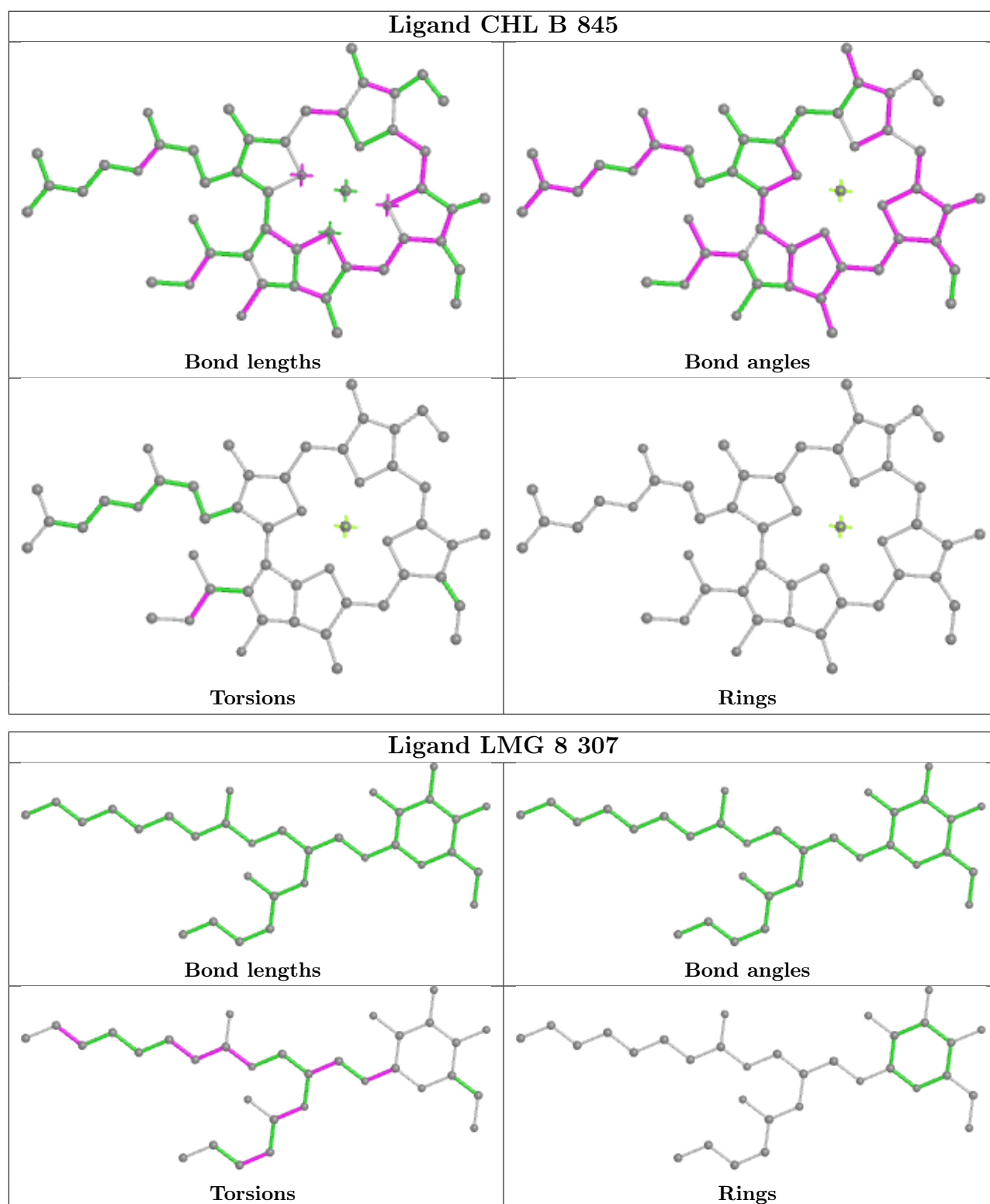


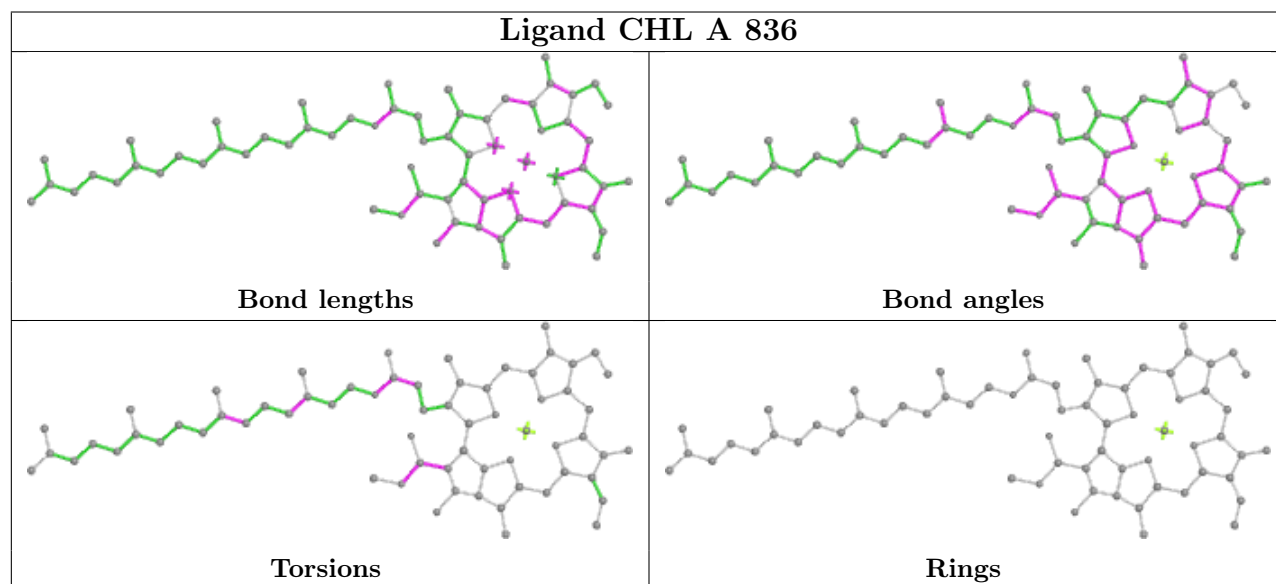
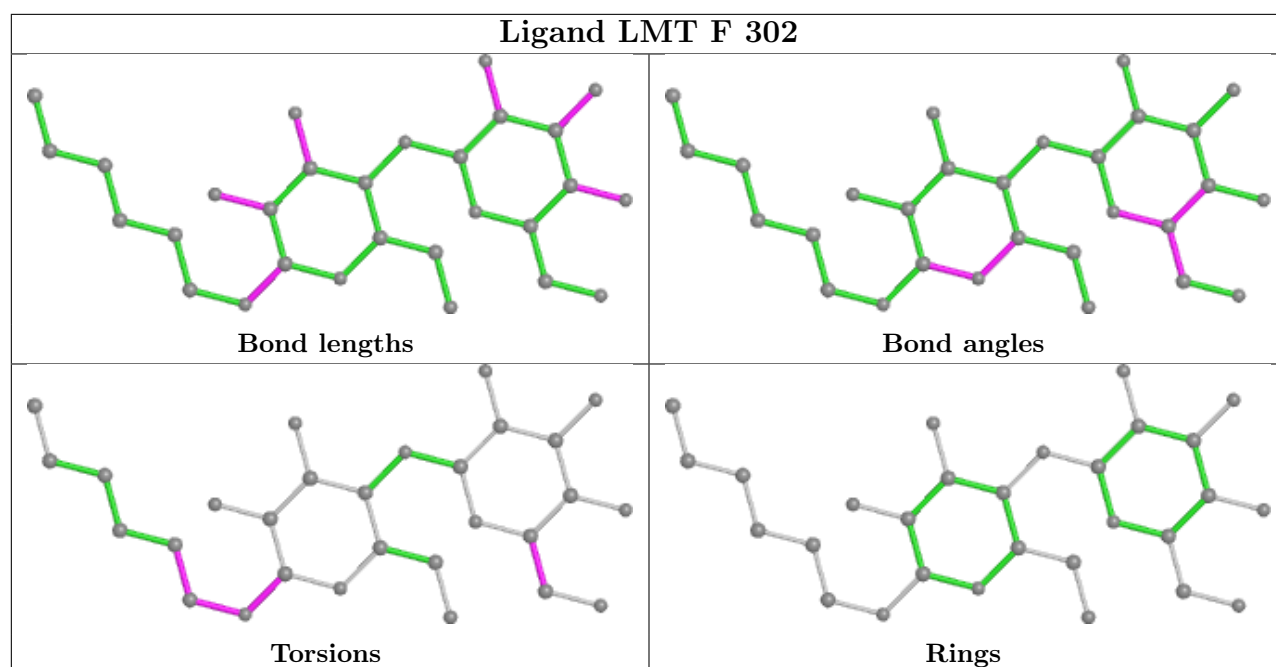
Torsions

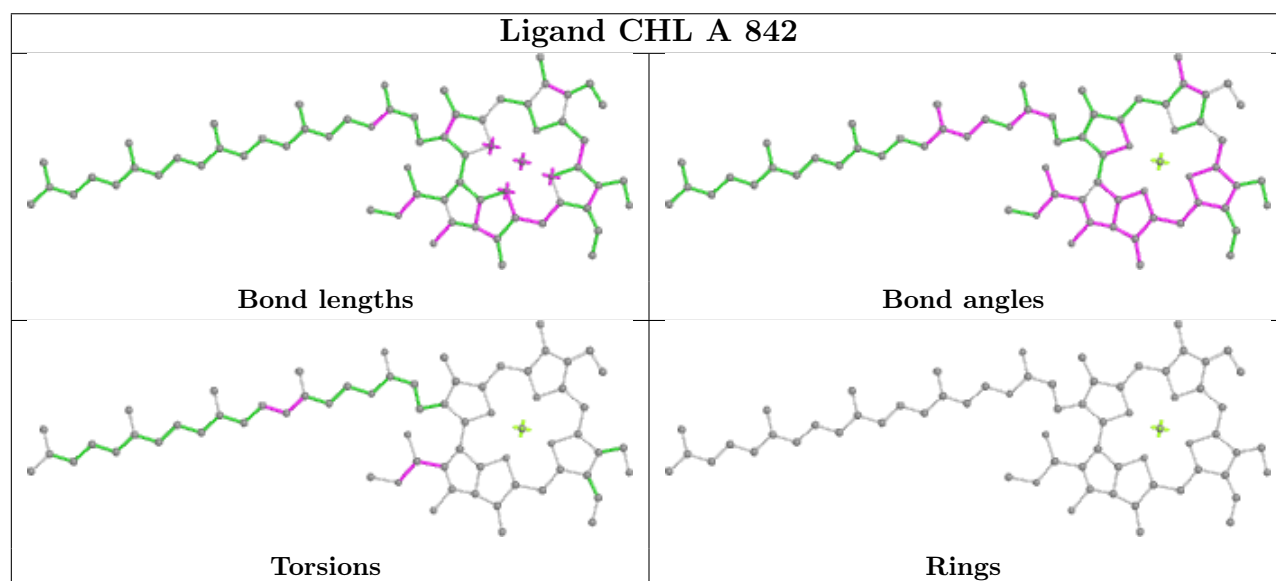
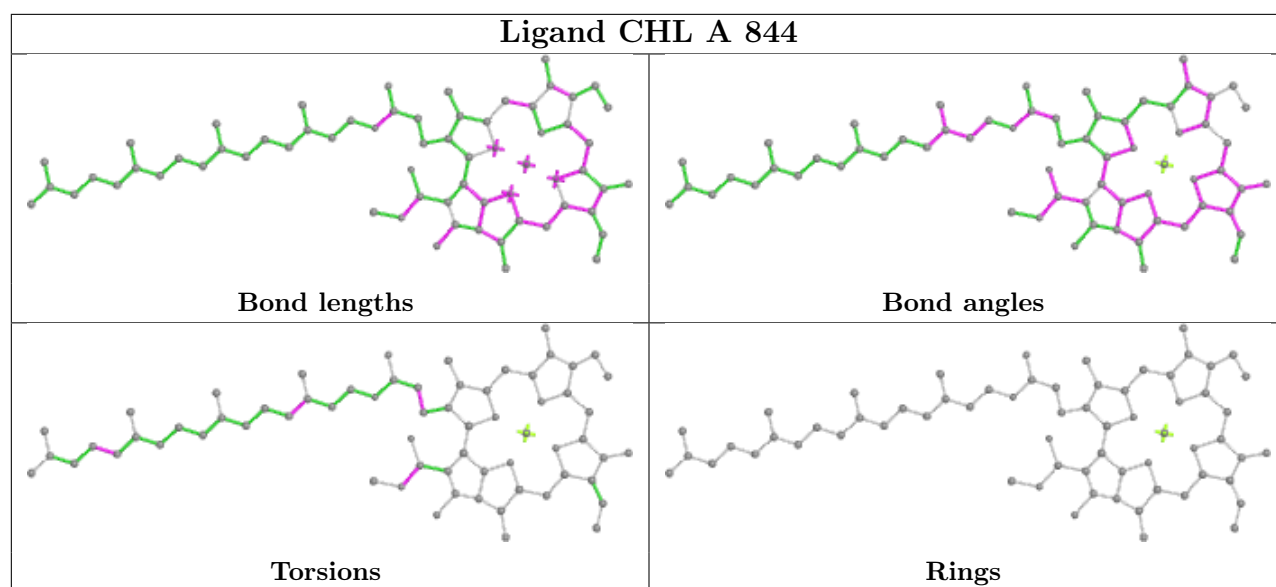


Rings

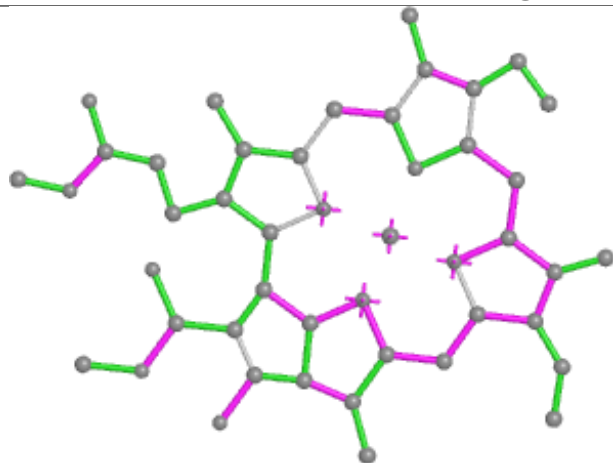




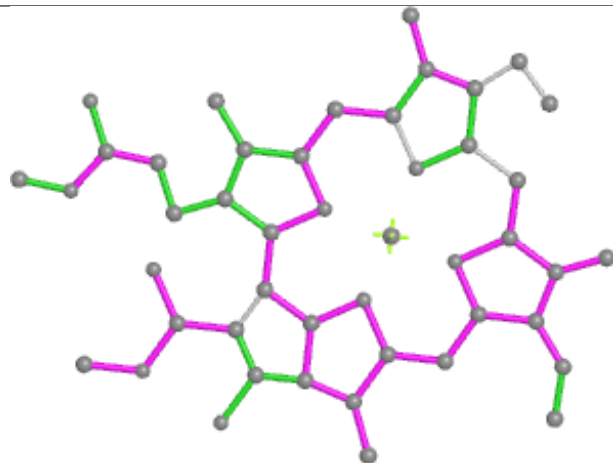




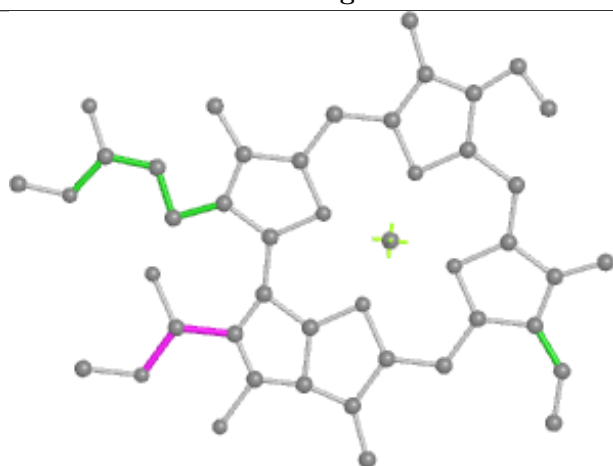
Ligand CHL b 310



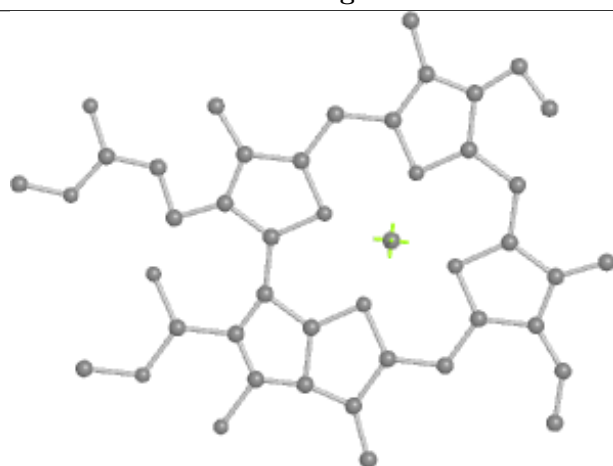
Bond lengths



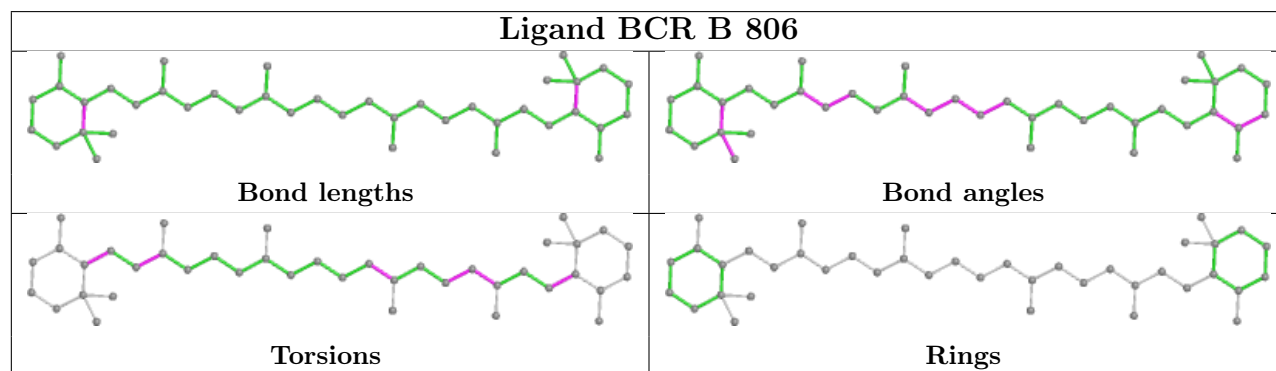
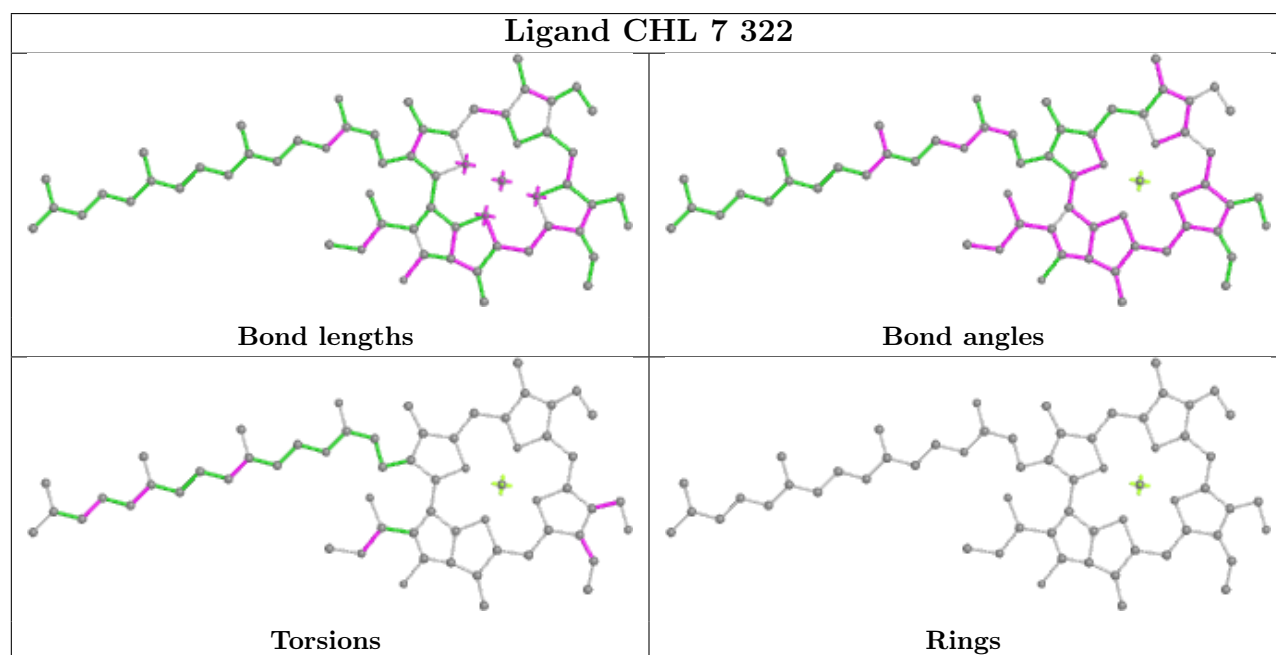
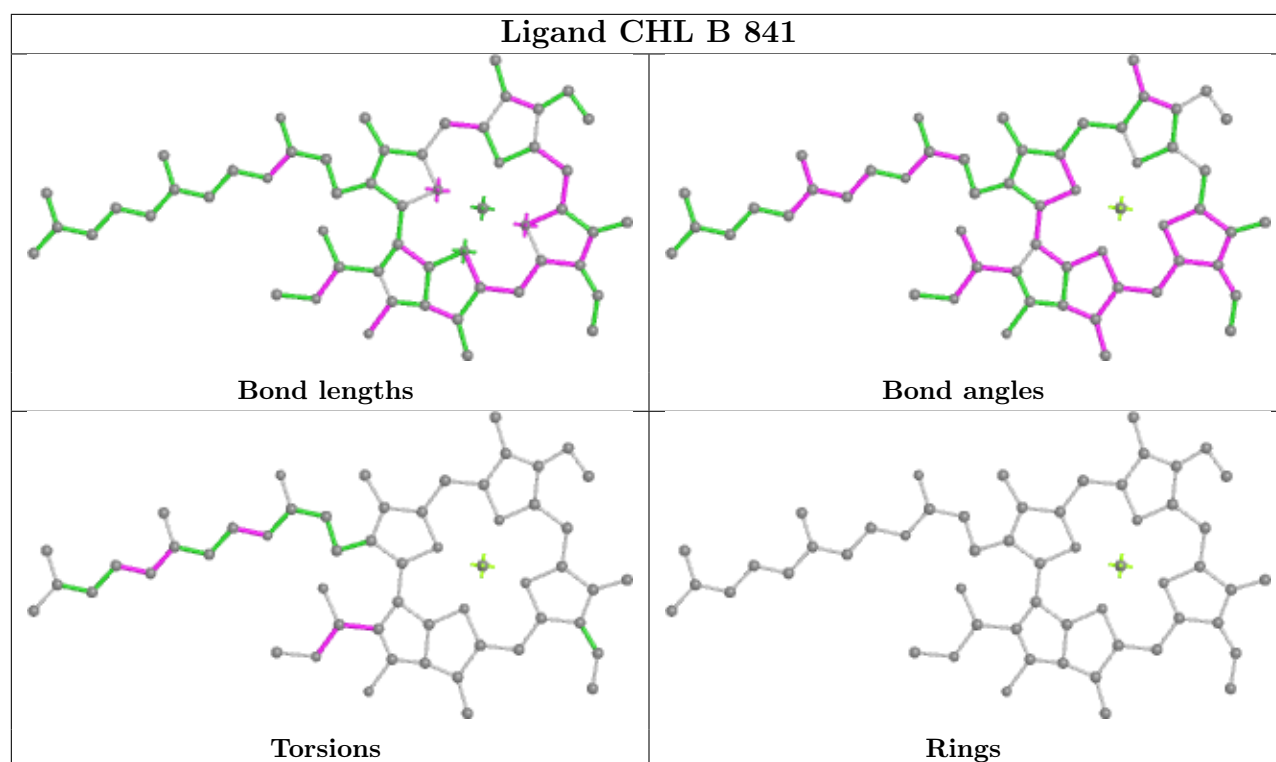
Bond angles

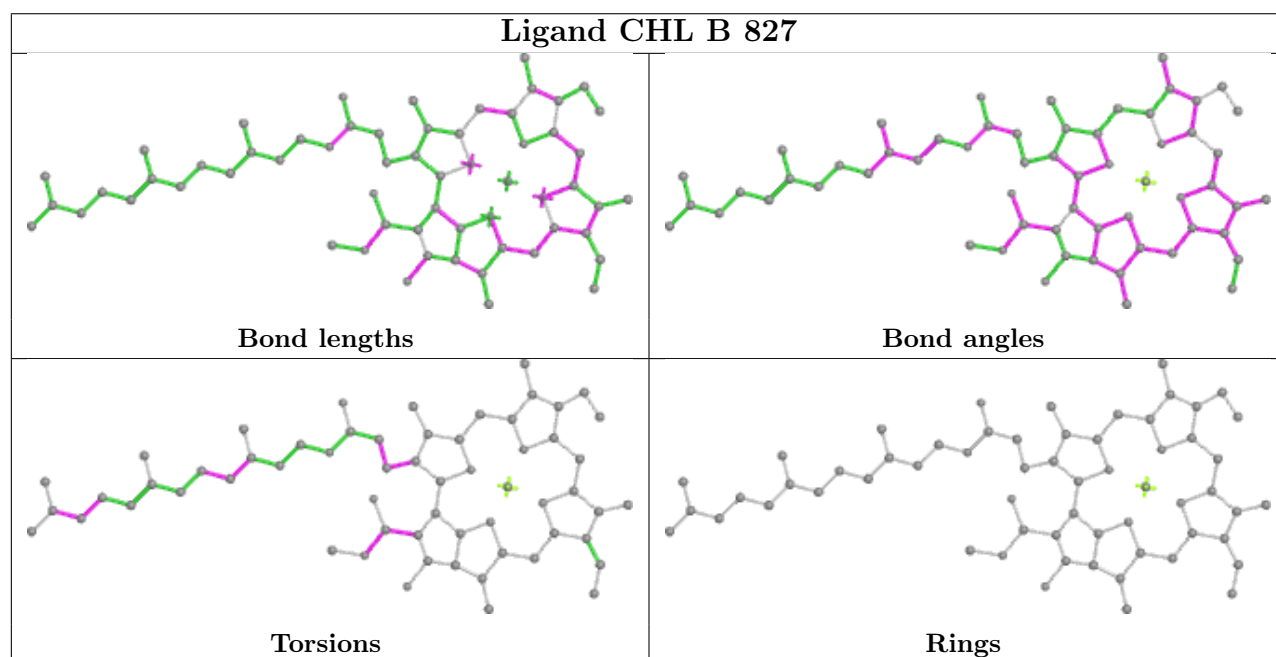
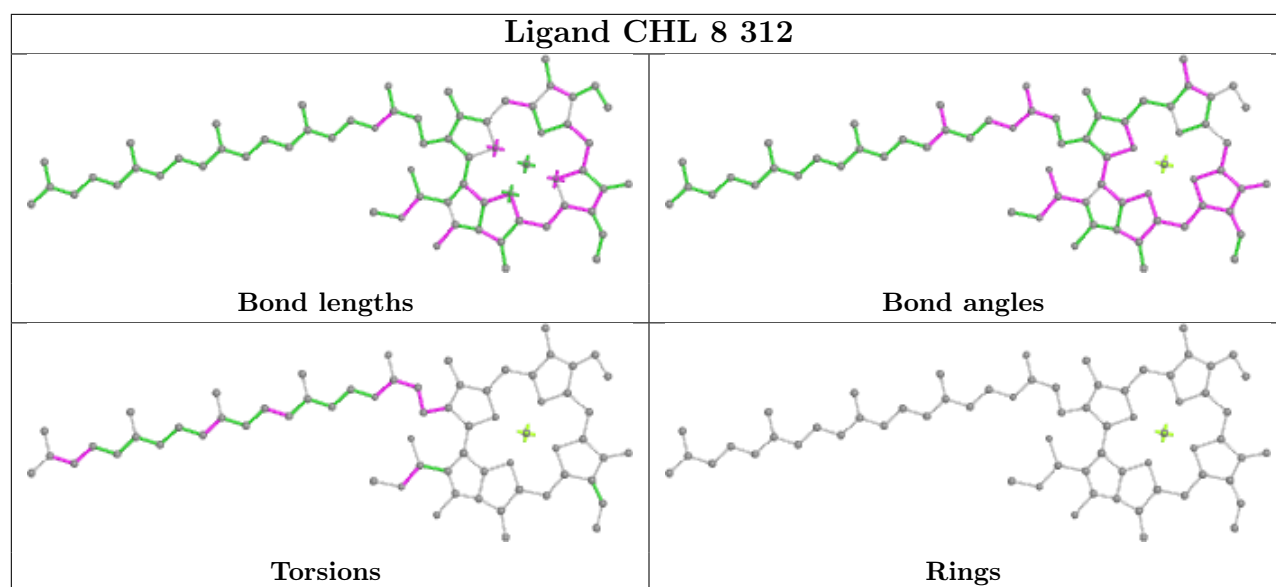


Torsions

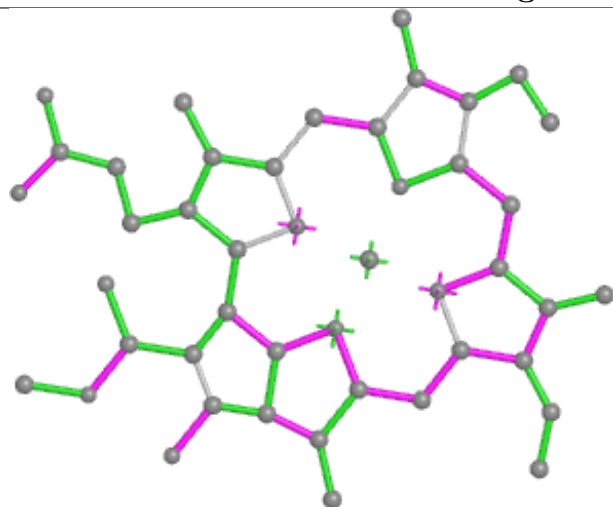


Rings

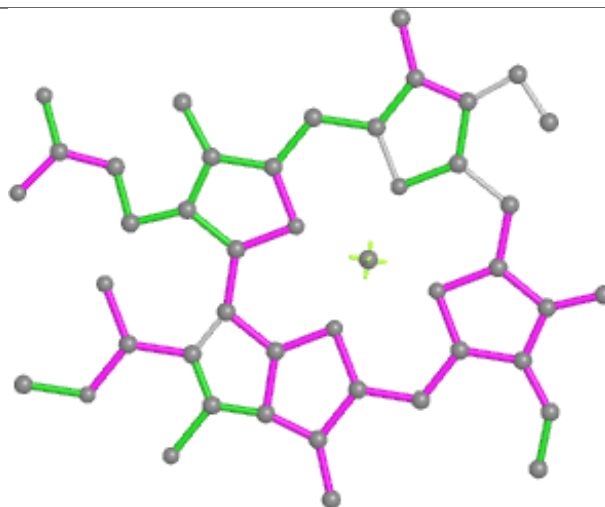




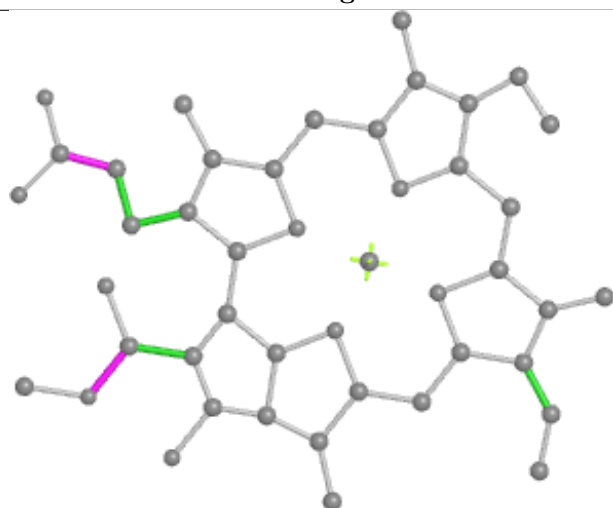
Ligand CHL 4 305



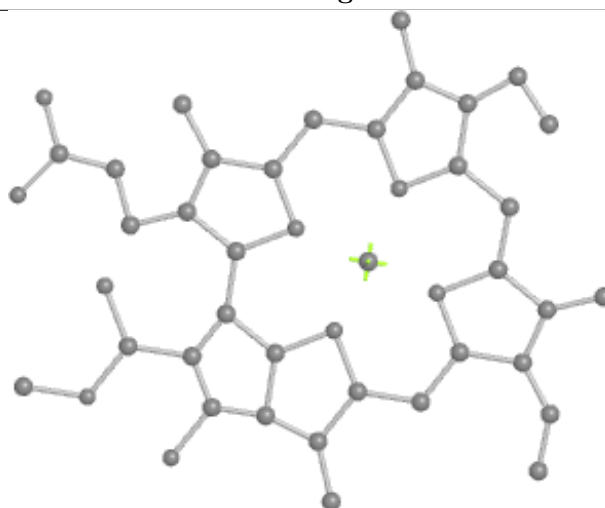
Bond lengths



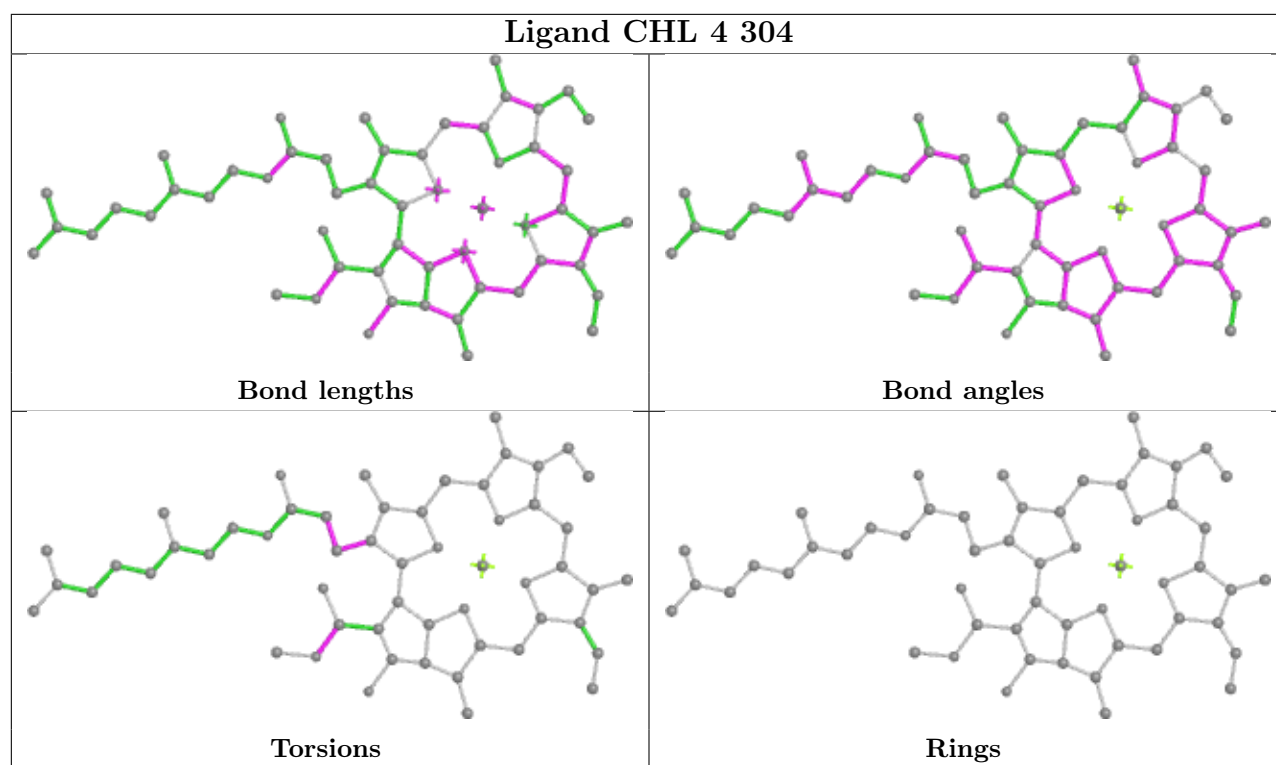
Bond angles



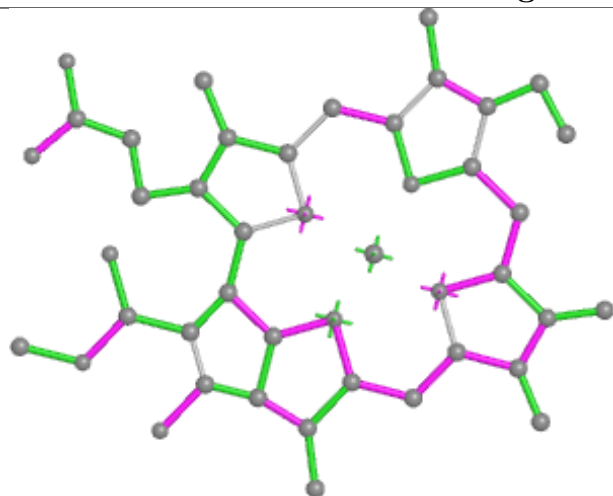
Torsions



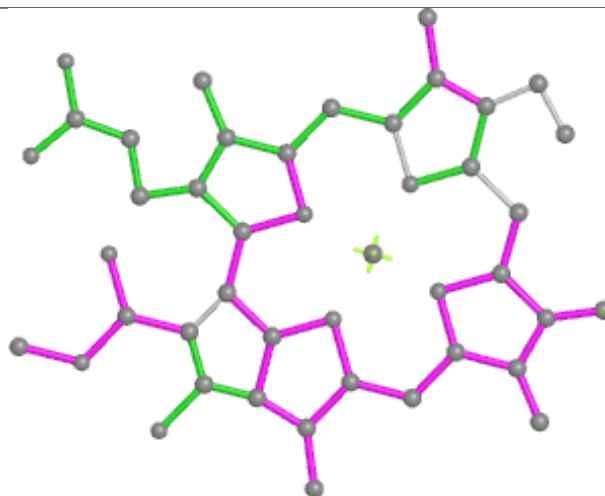
Rings



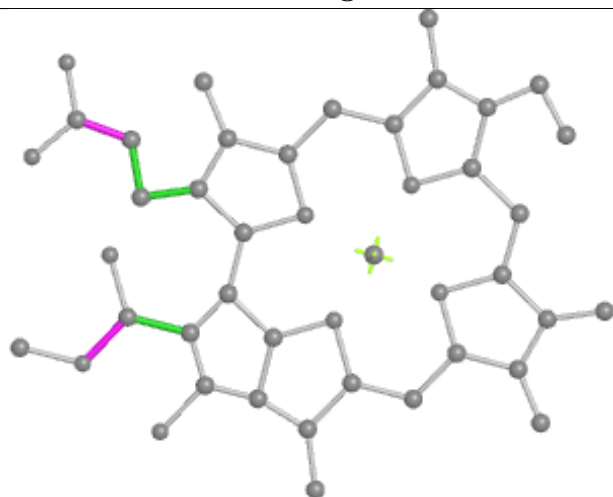
Ligand CHL 7 312



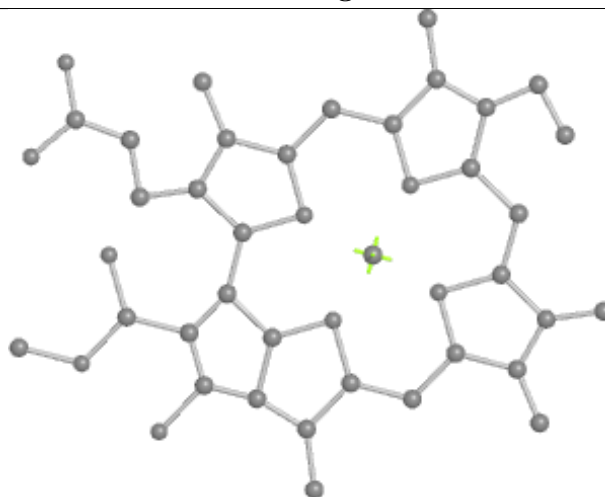
Bond lengths



Bond angles

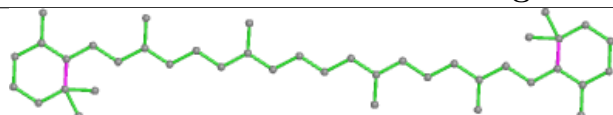


Torsions

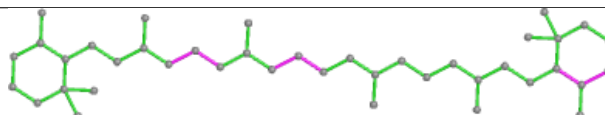


Rings

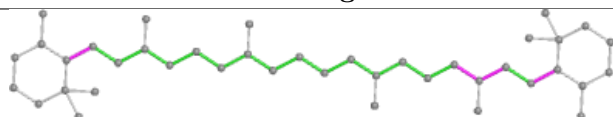
Ligand BCR B 807



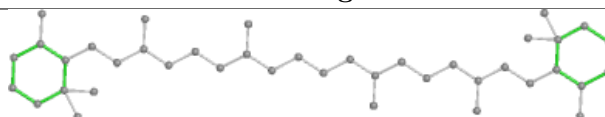
Bond lengths



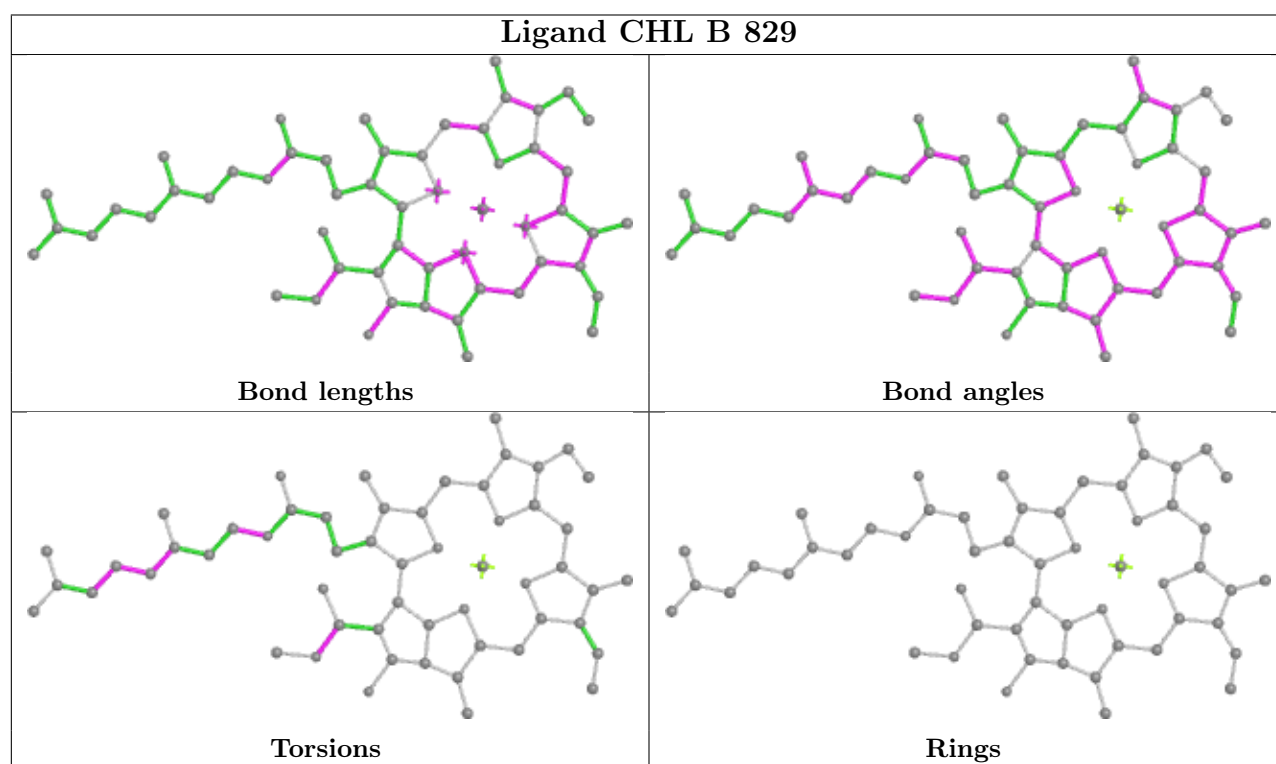
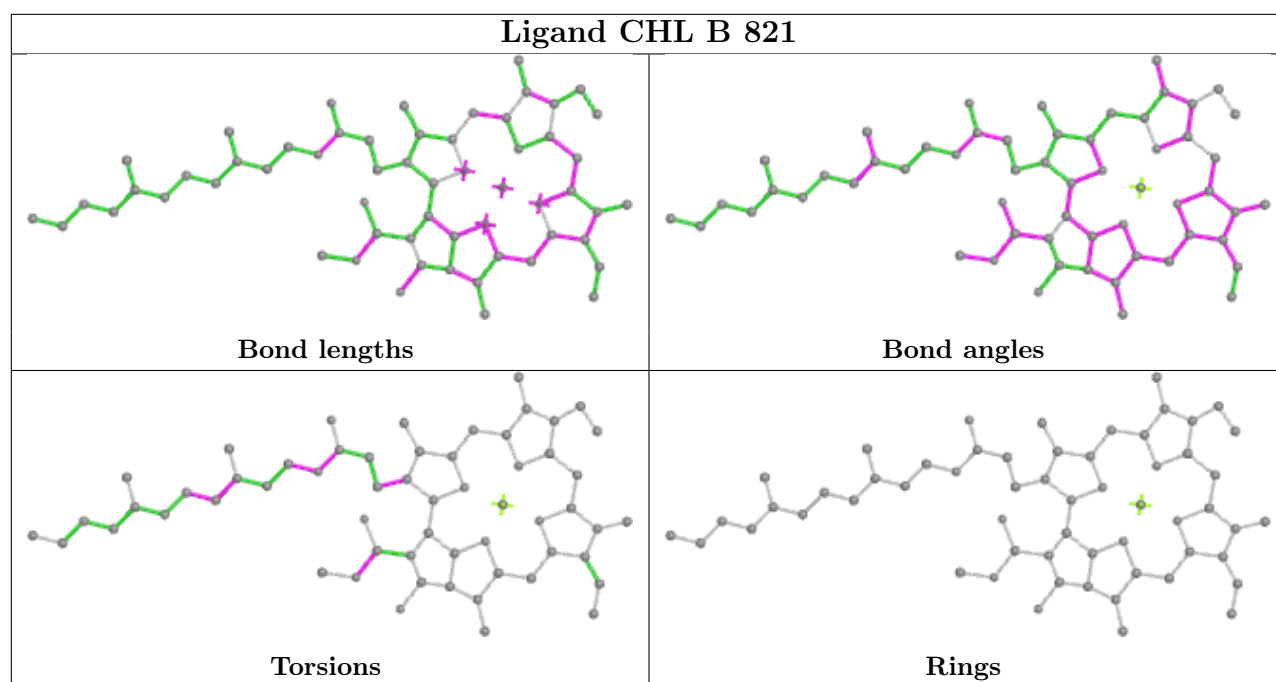
Bond angles

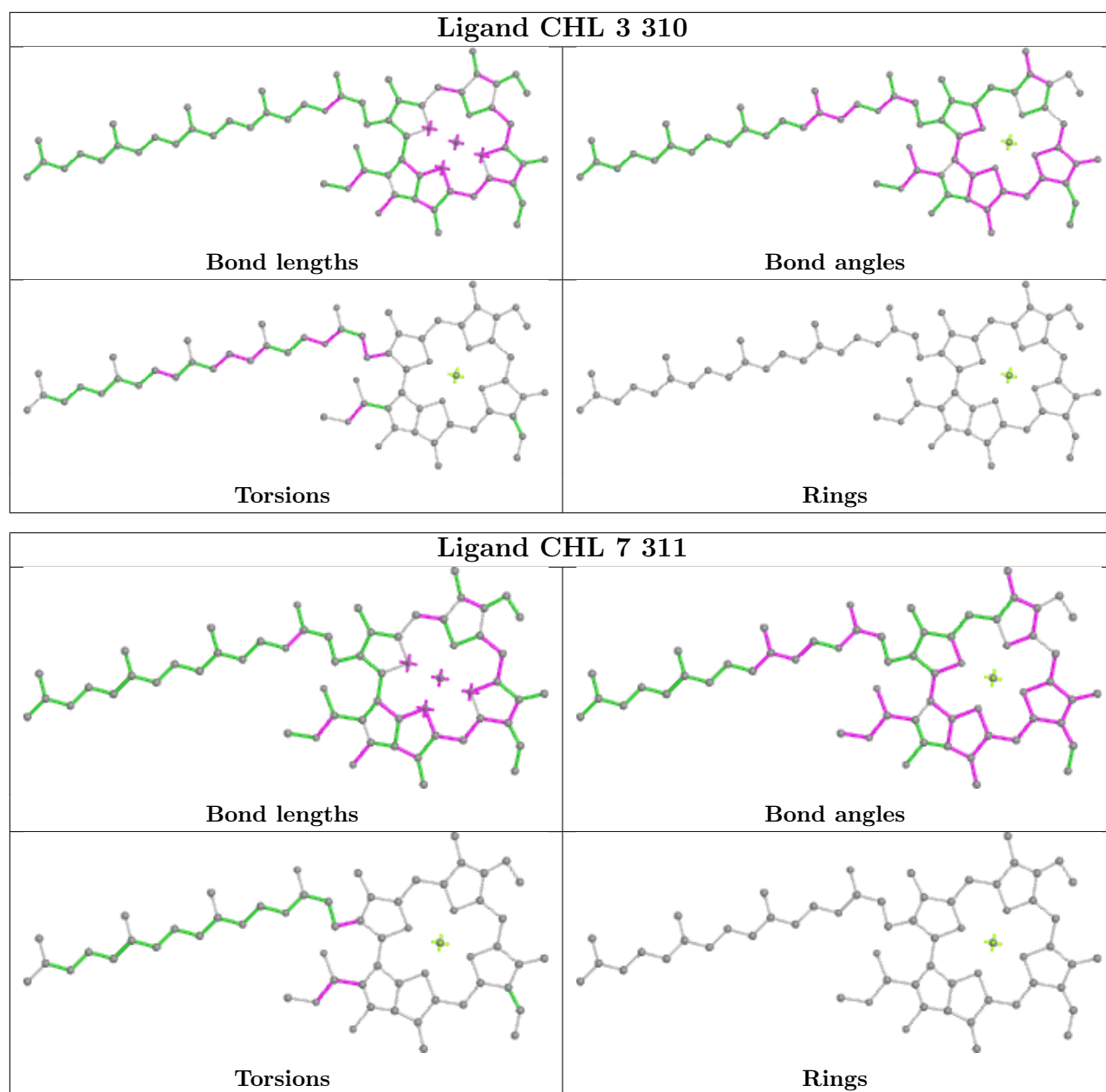


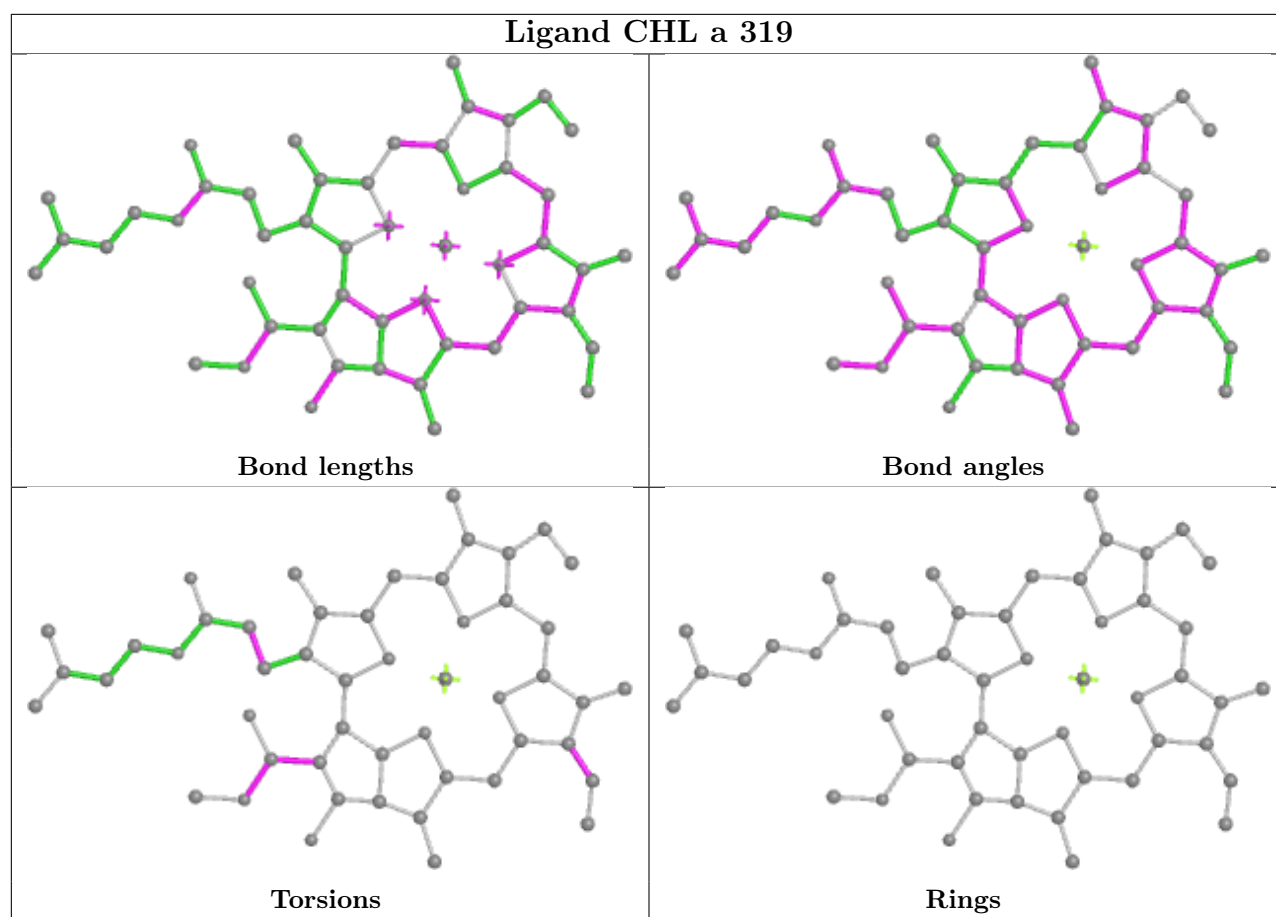
Torsions



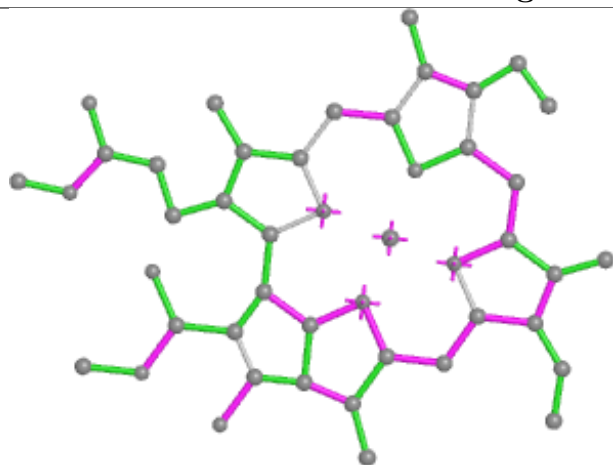
Rings



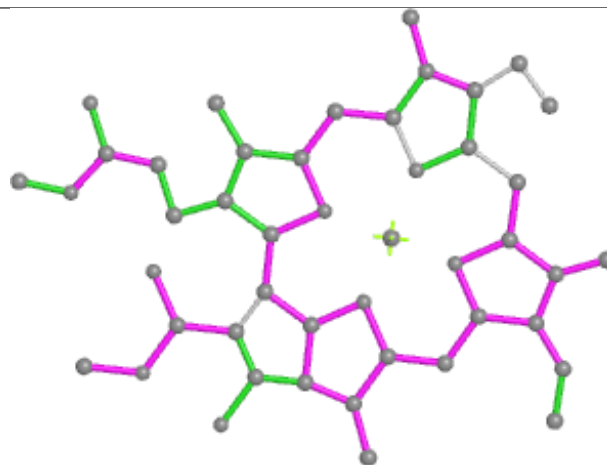




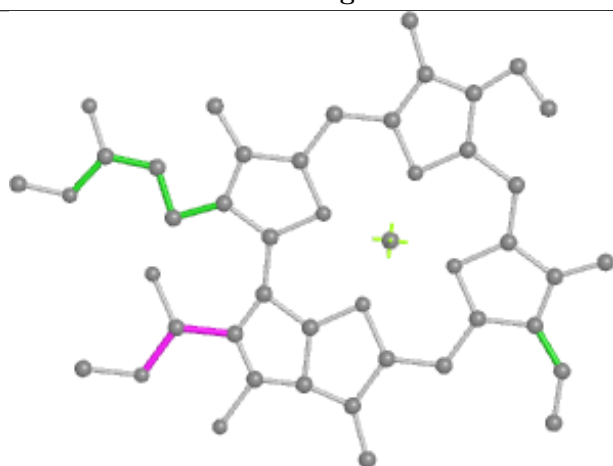
Ligand CHL b 309



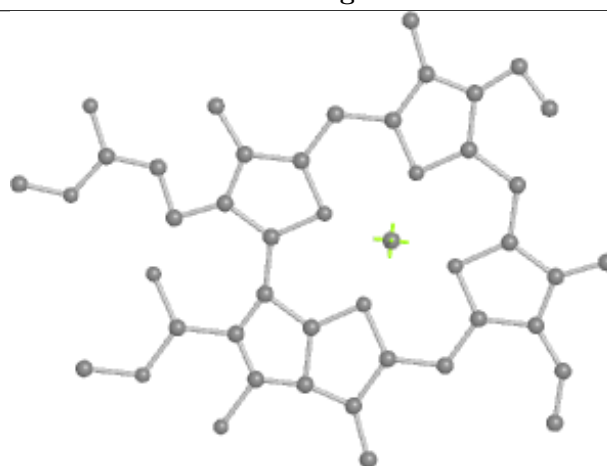
Bond lengths



Bond angles

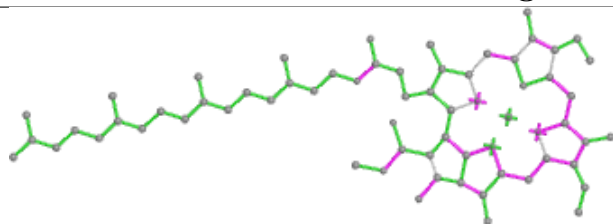


Torsions

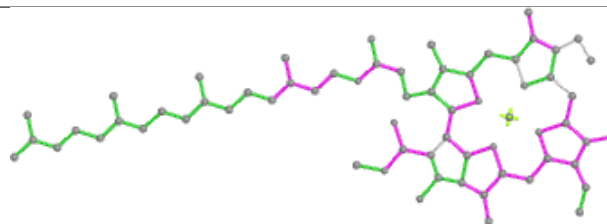


Rings

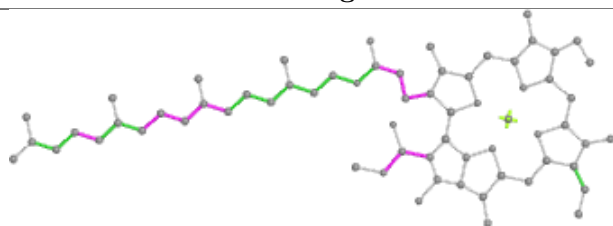
Ligand CHL 8 315



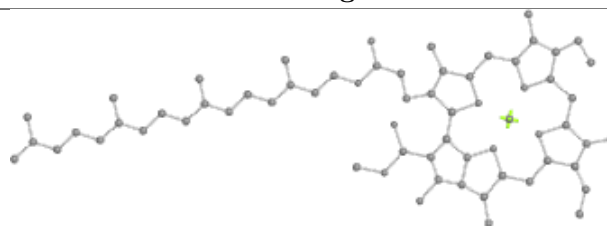
Bond lengths



Bond angles

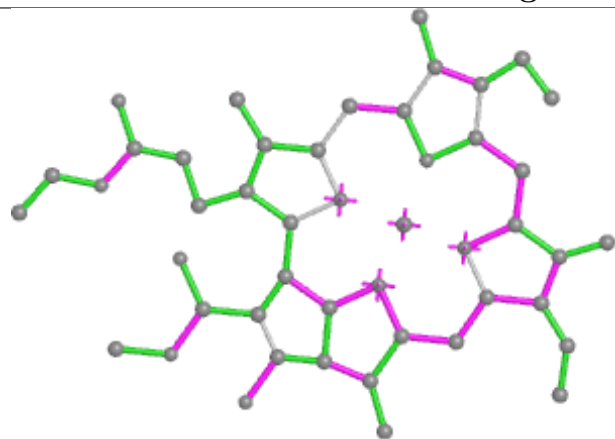


Torsions

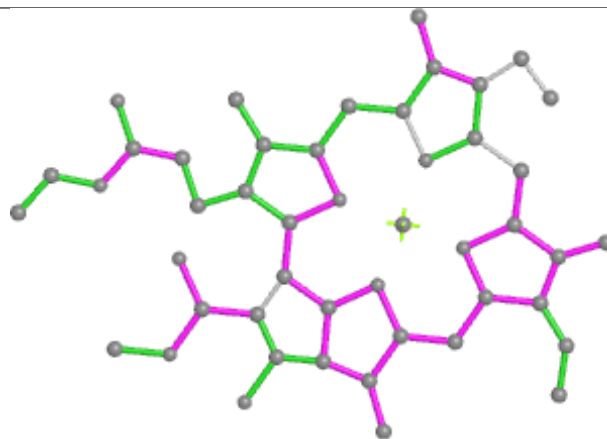


Rings

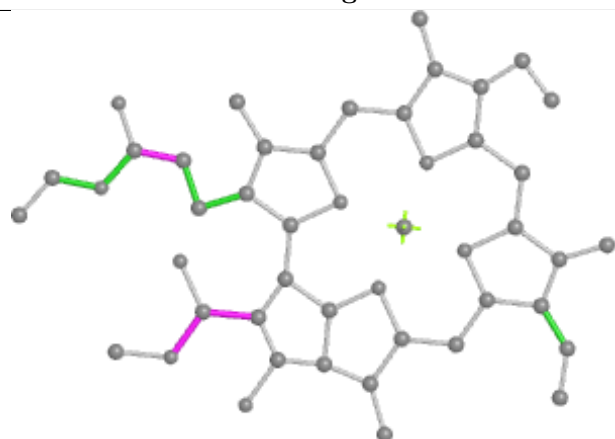
Ligand CHL 6 309



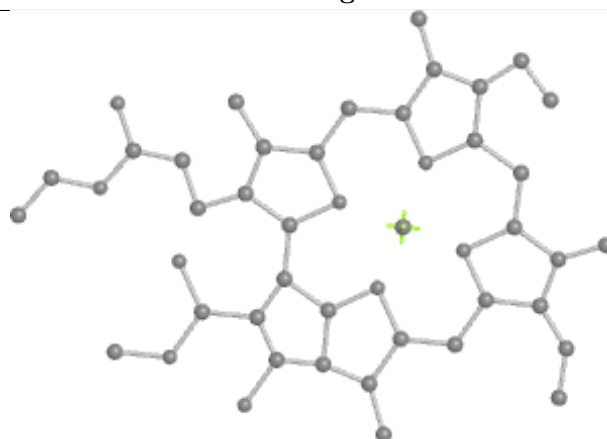
Bond lengths



Bond angles

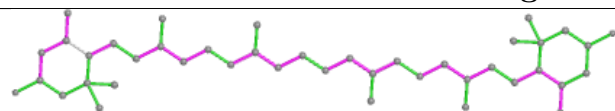


Torsions

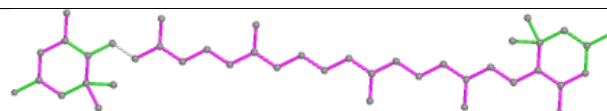


Rings

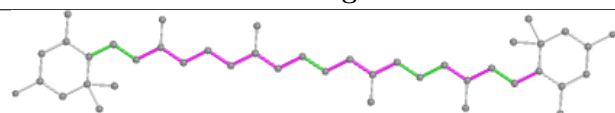
Ligand LUT 6 302



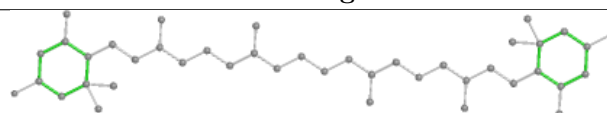
Bond lengths



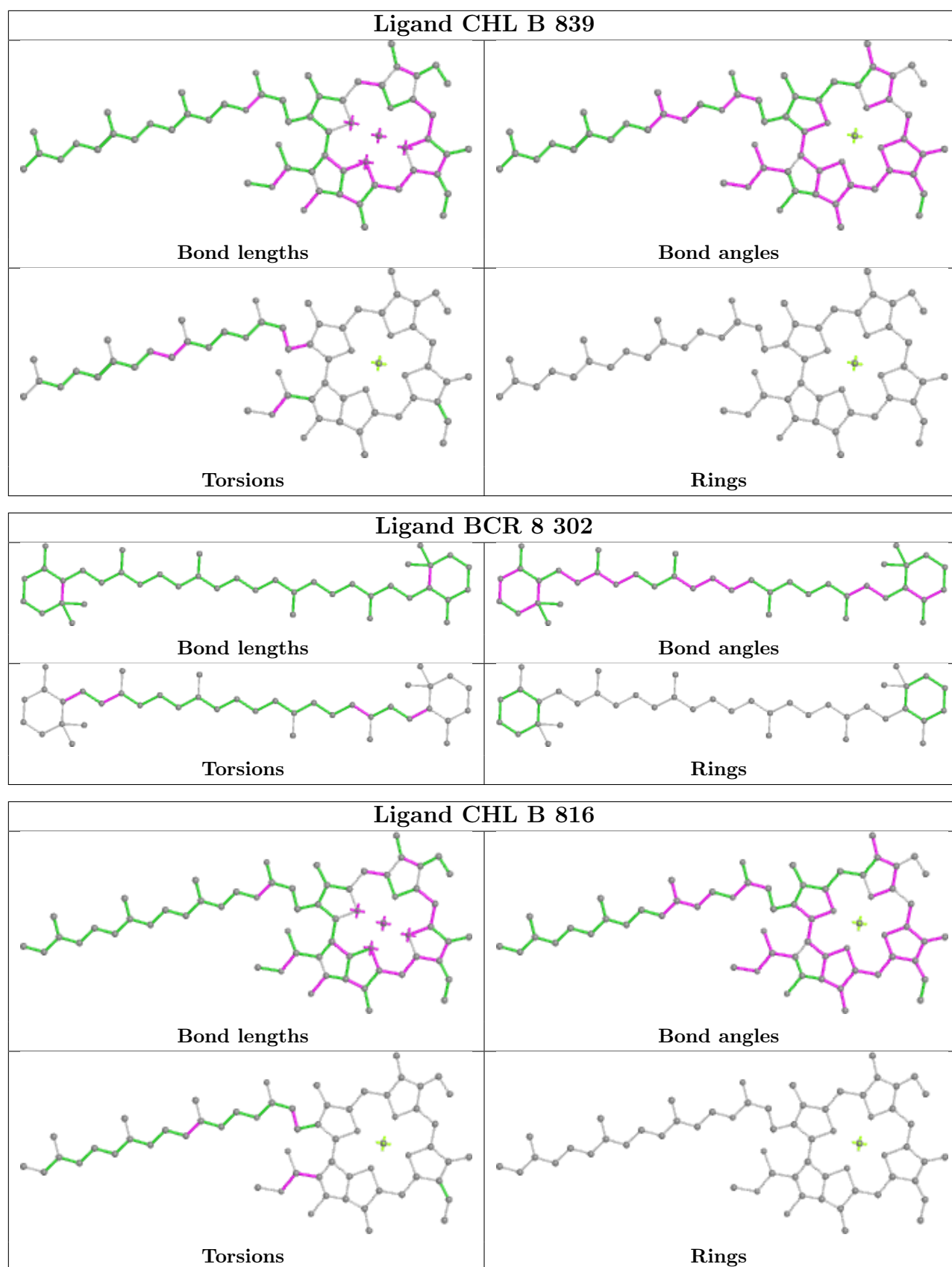
Bond angles

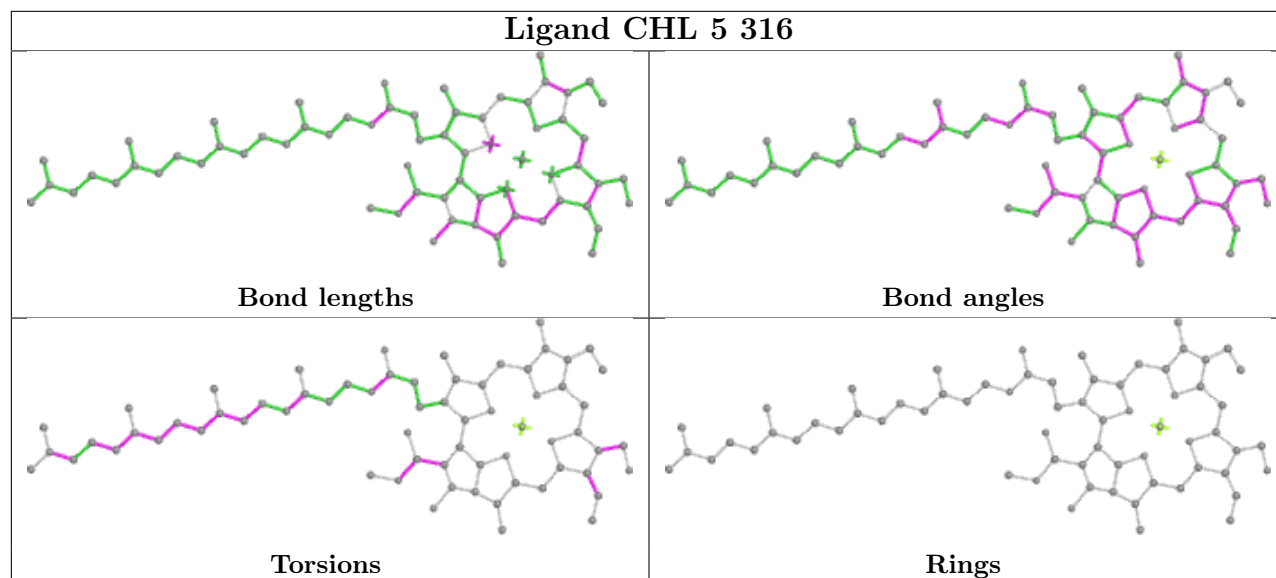
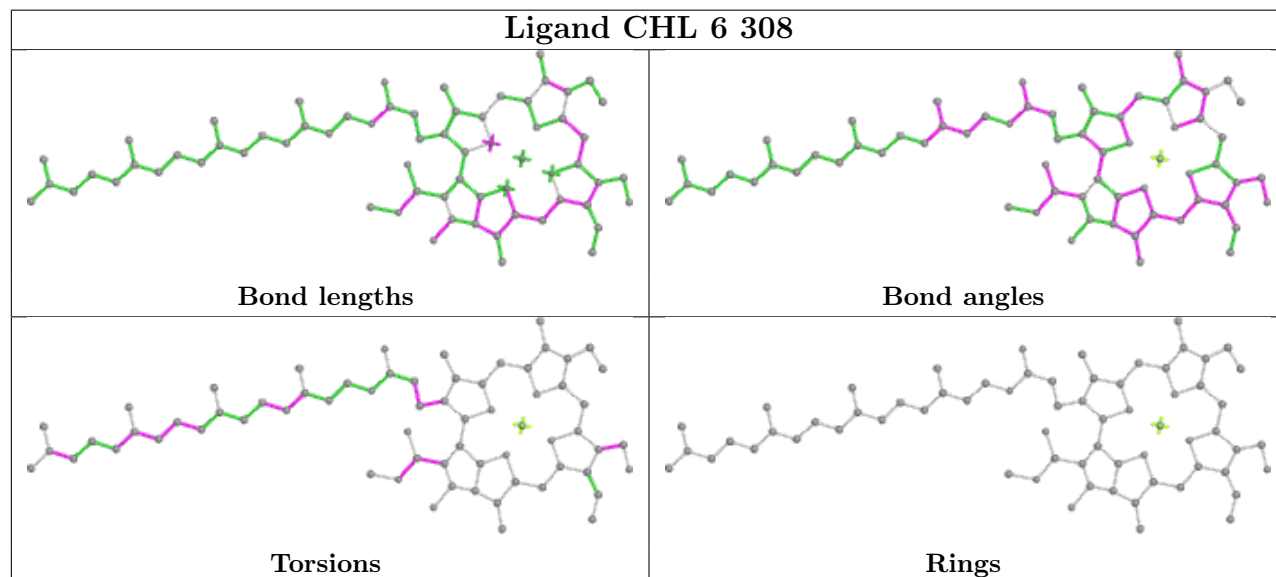


Torsions

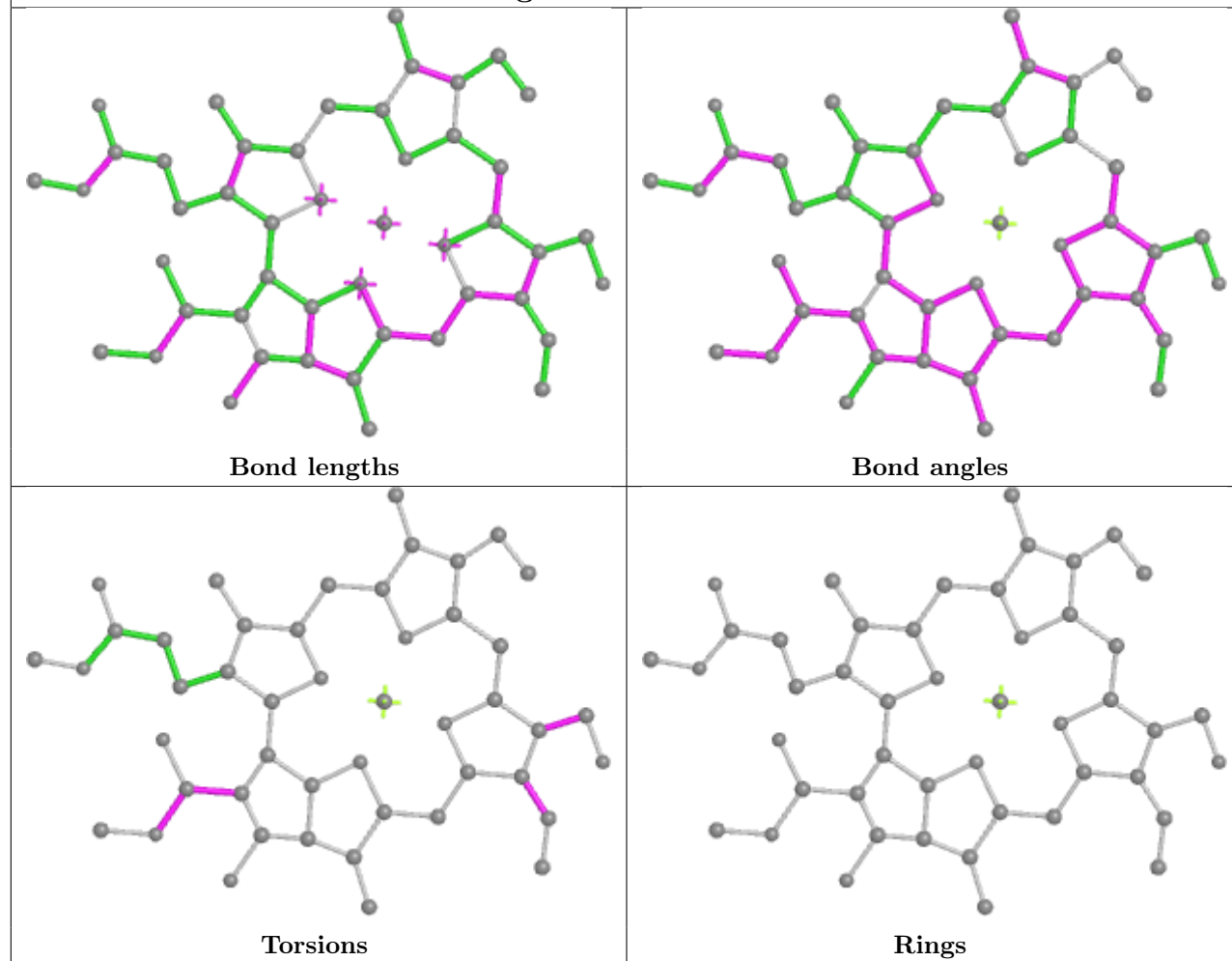


Rings

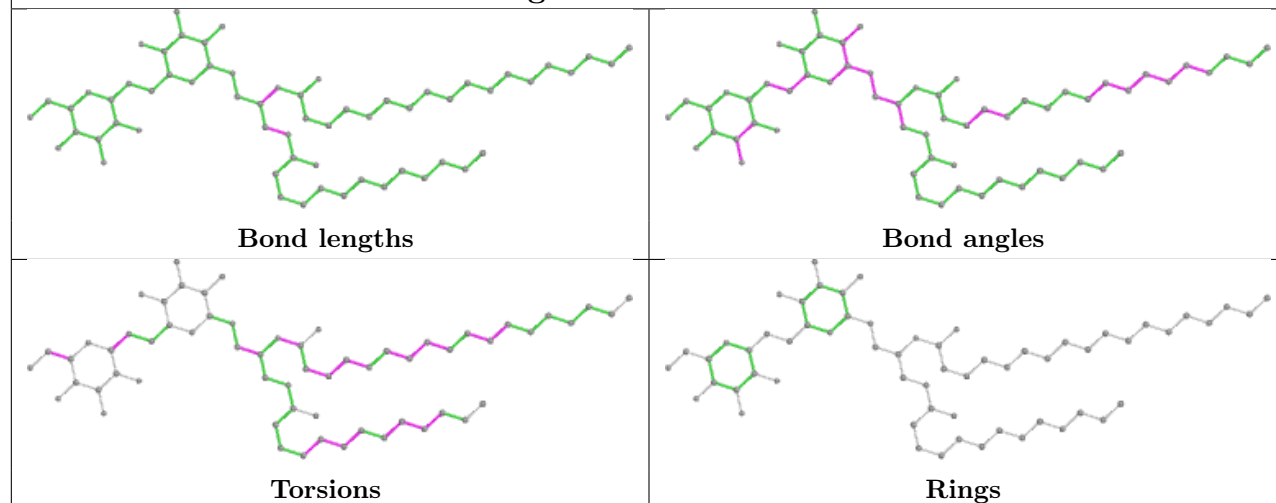


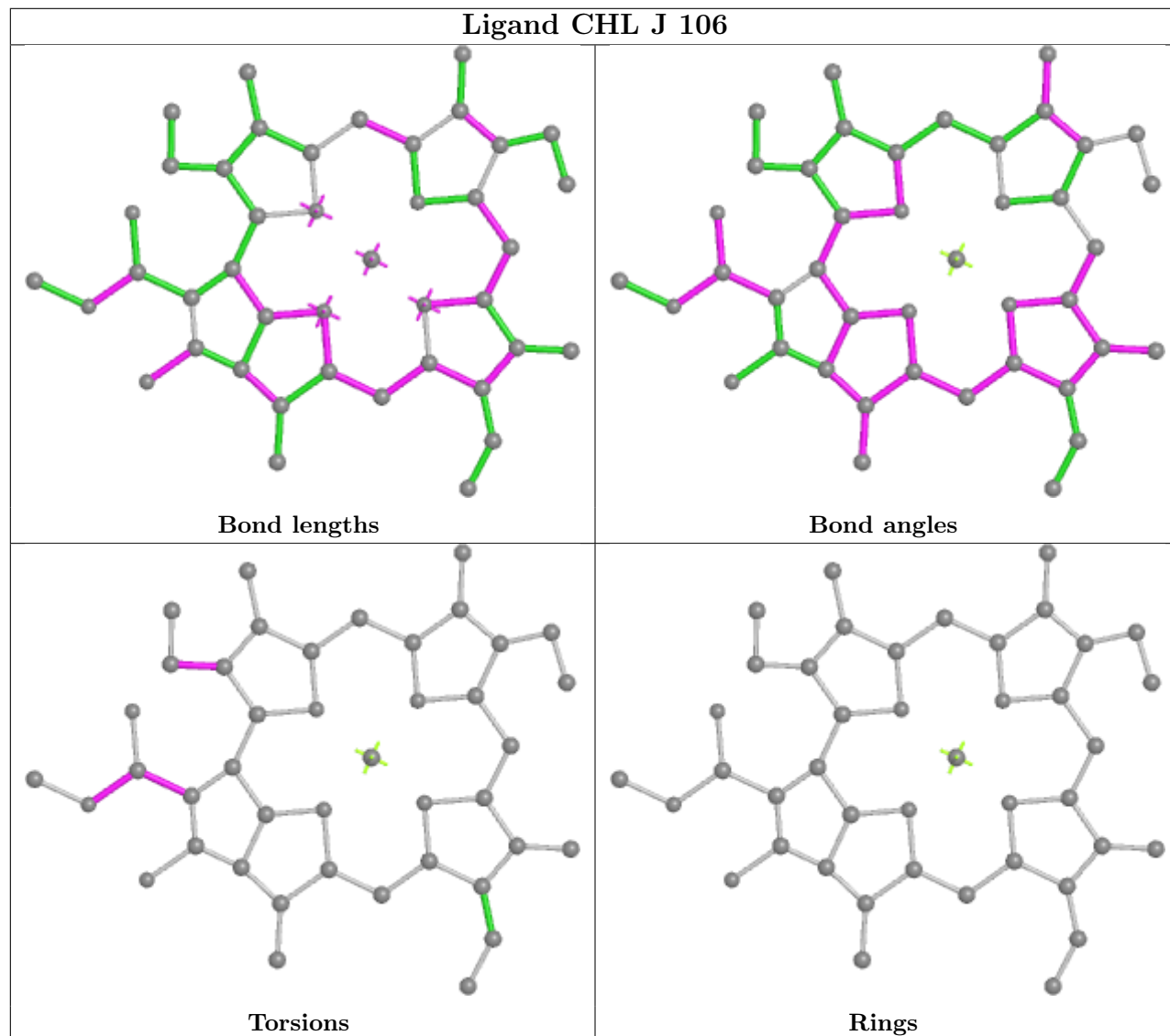
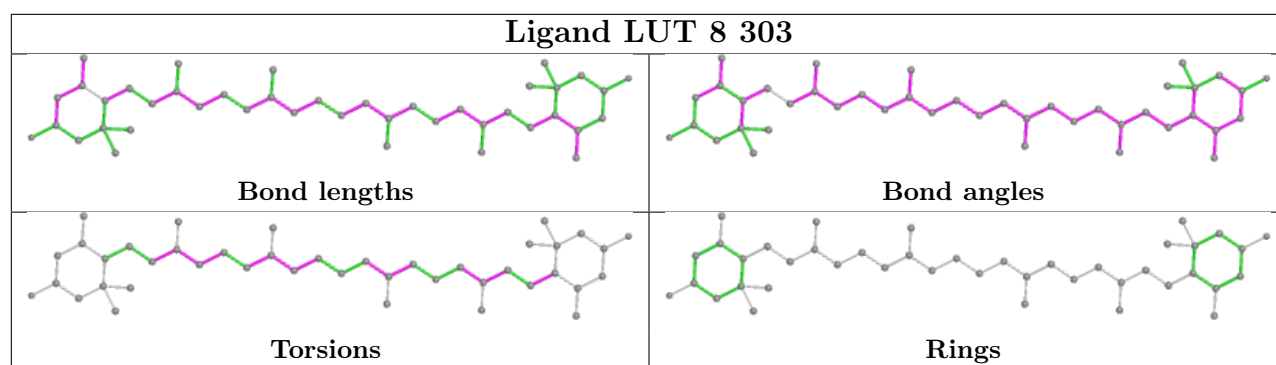
Ligand CHL 5 316**Ligand CHL 6 308**

Ligand CHL b 311

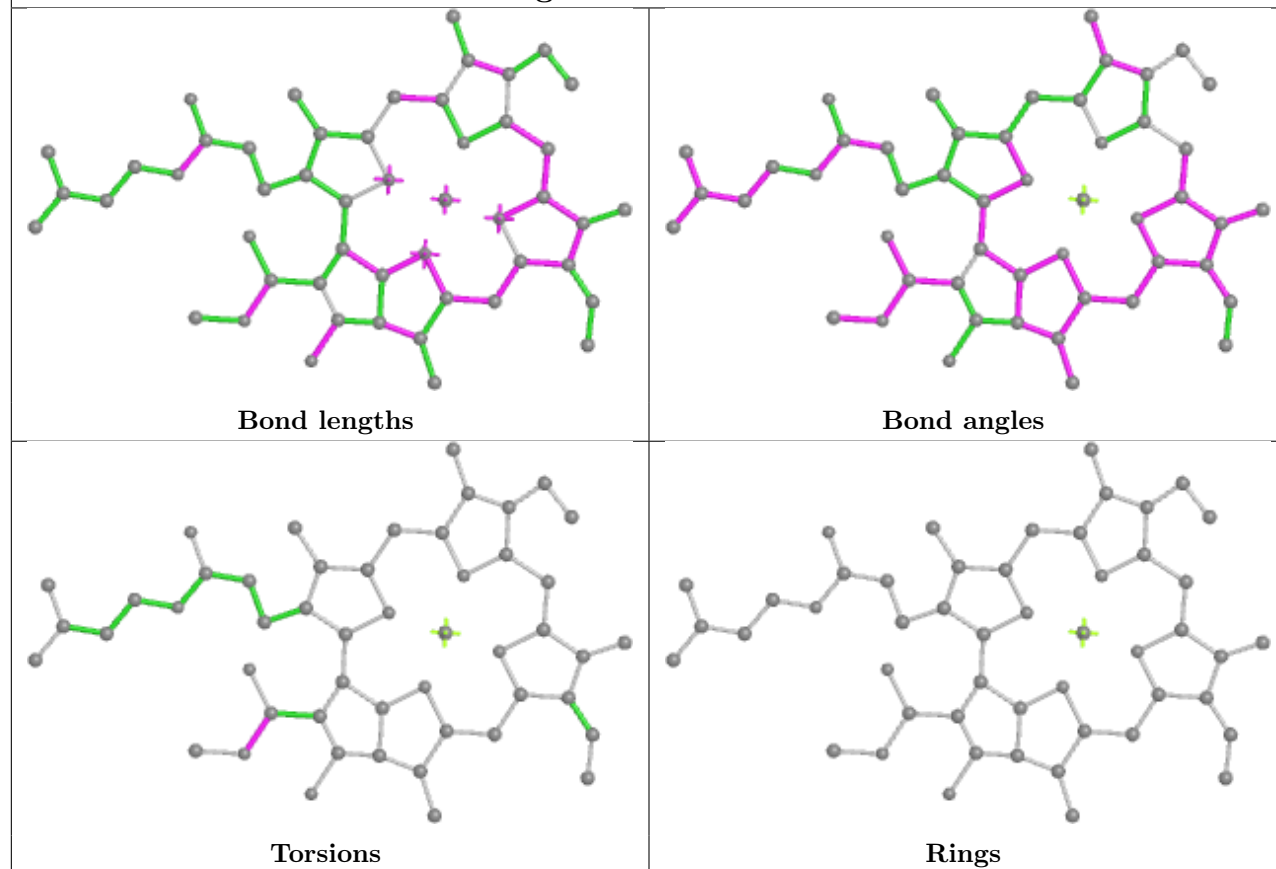


Ligand DGD B 809

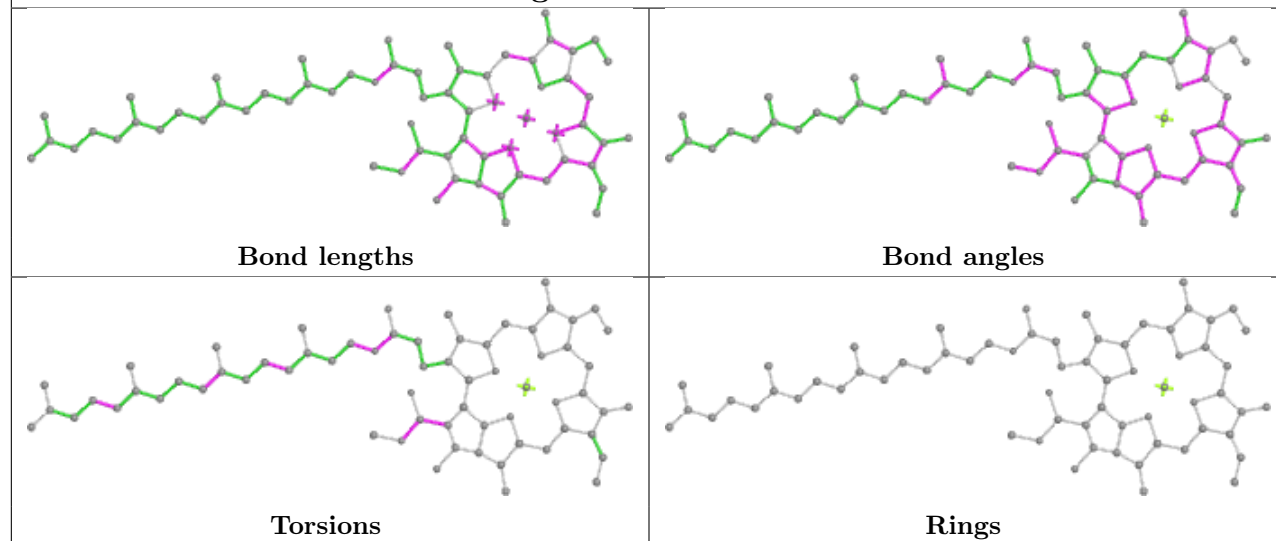




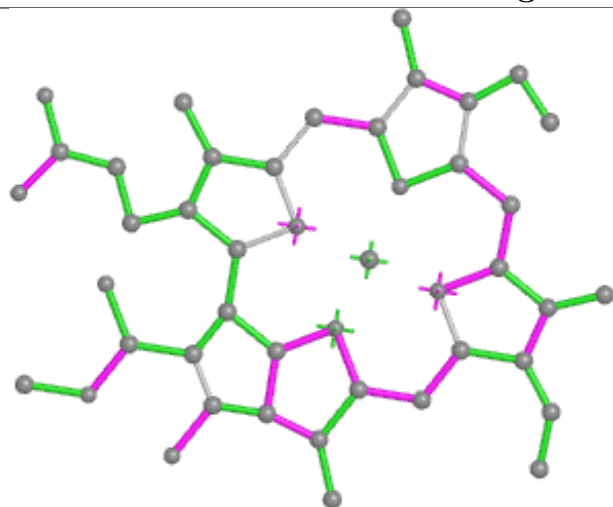
Ligand CHL 6 315



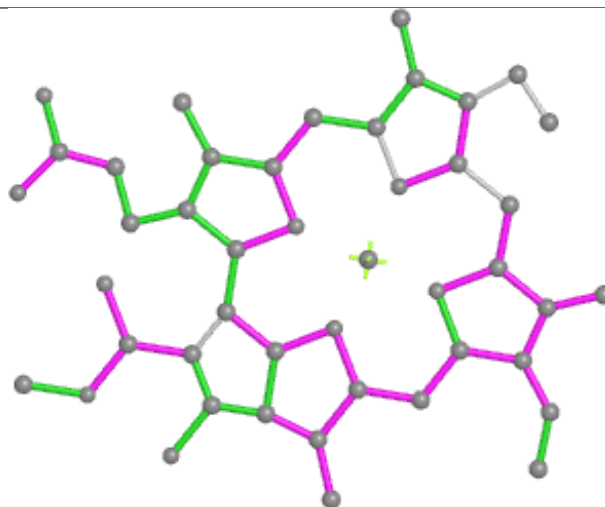
Ligand CHL A 853



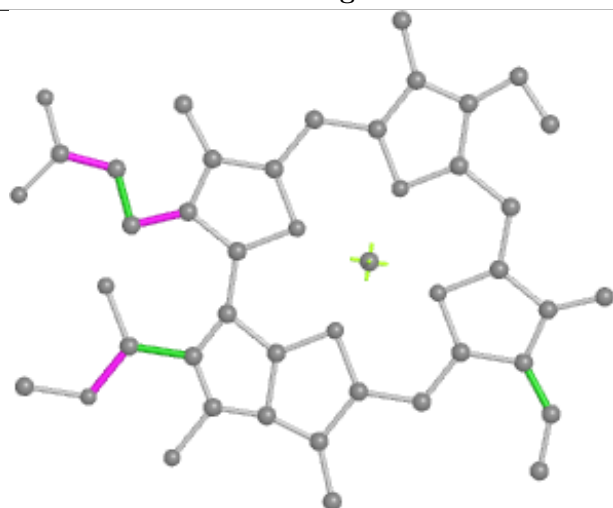
Ligand CHL 4 313



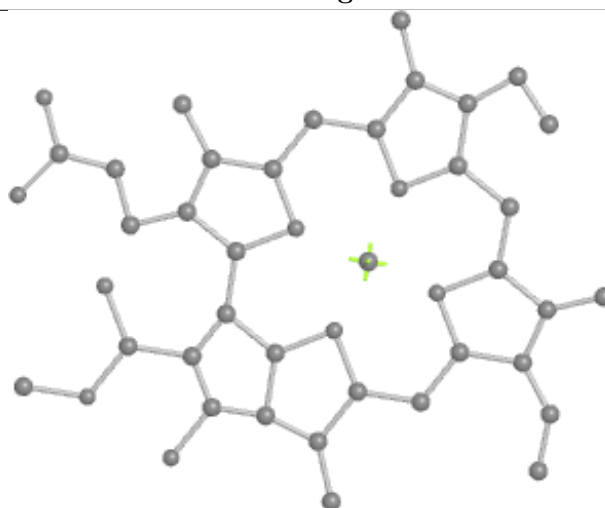
Bond lengths



Bond angles

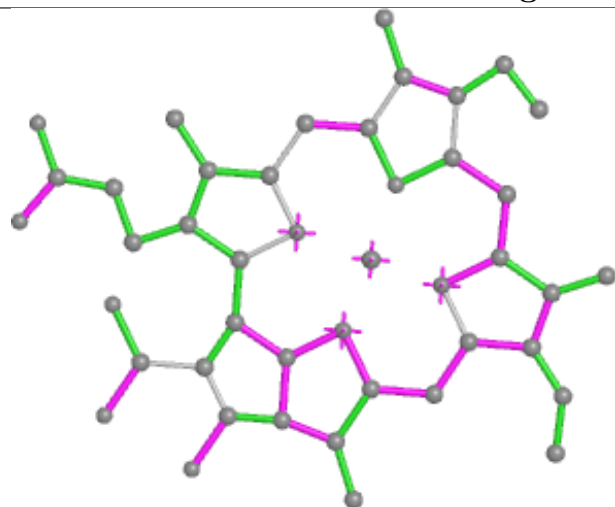


Torsions

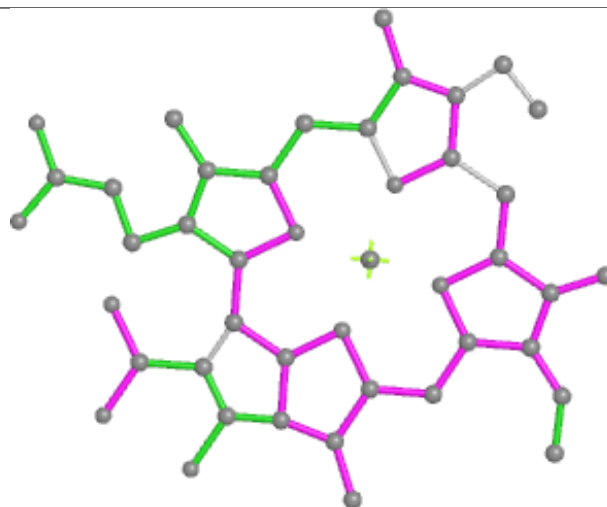


Rings

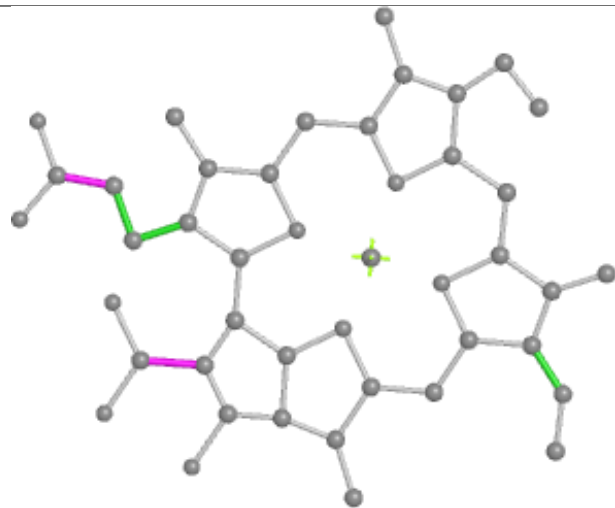
Ligand CHL 7 315



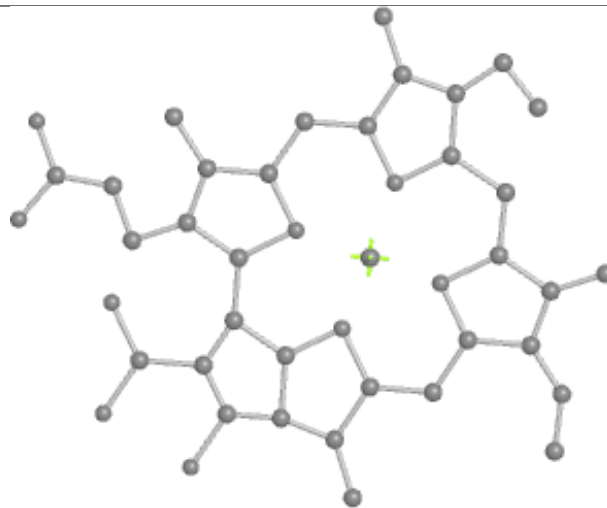
Bond lengths



Bond angles

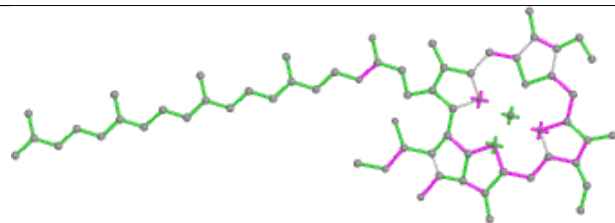


Torsions

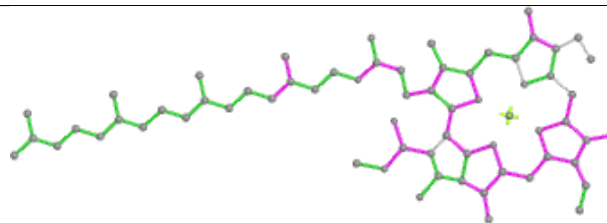


Rings

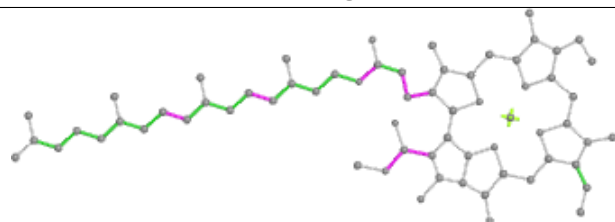
Ligand CHL 8 325



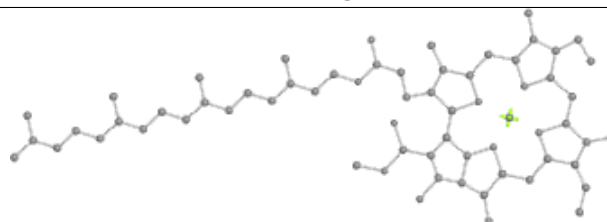
Bond lengths



Bond angles

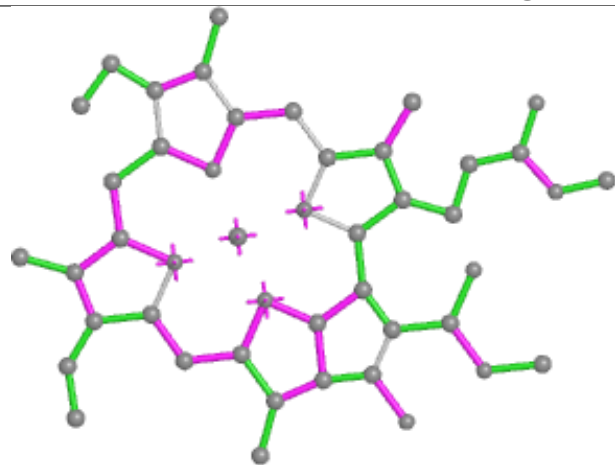


Torsions

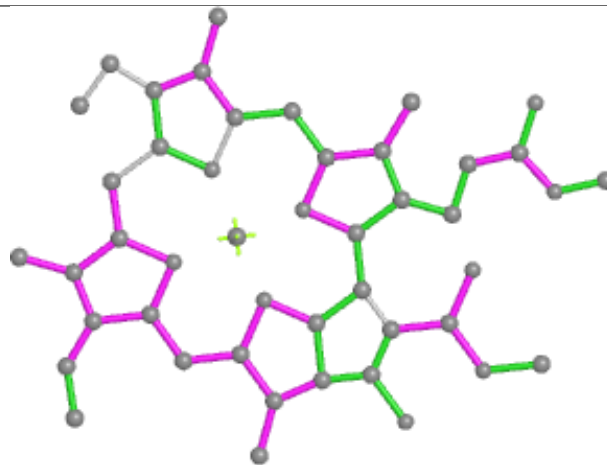


Rings

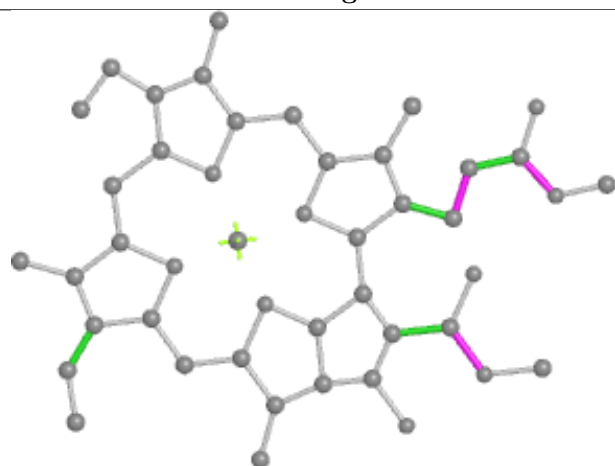
Ligand CHL b 308



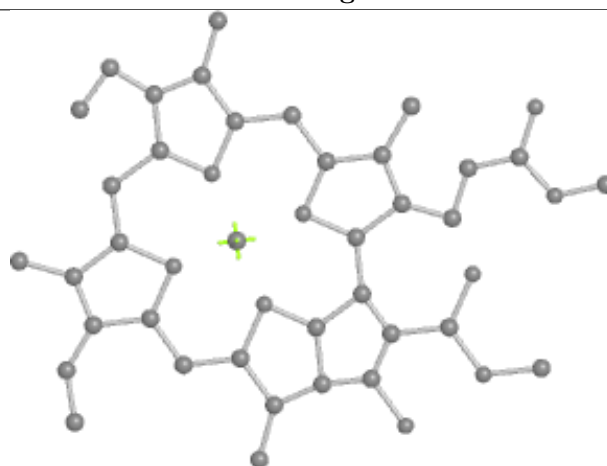
Bond lengths



Bond angles

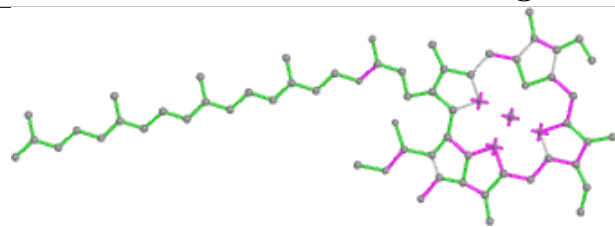


Torsions

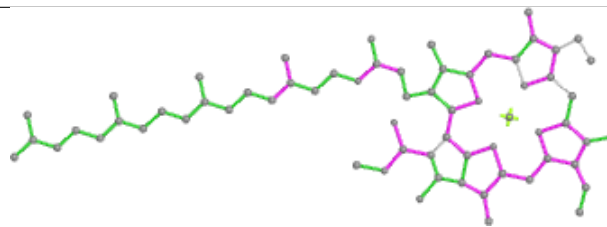


Rings

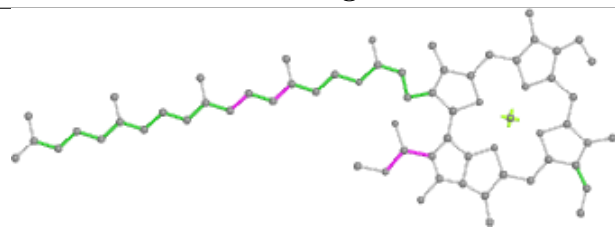
Ligand CHL A 849



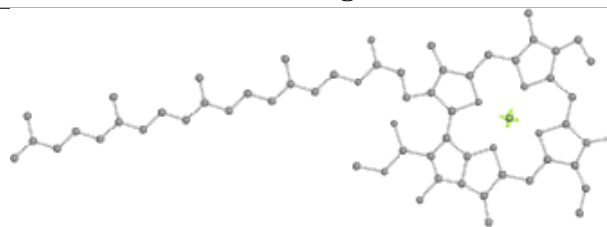
Bond lengths



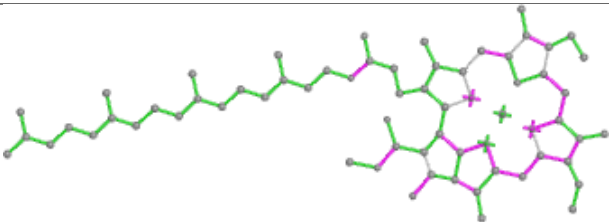
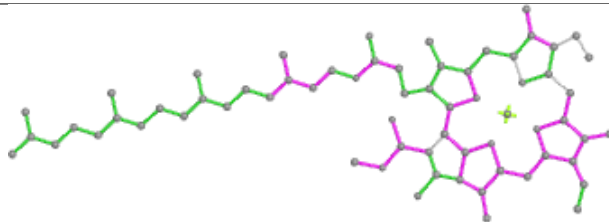
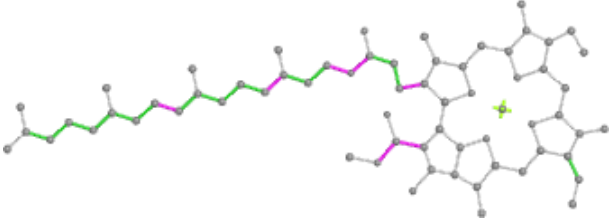
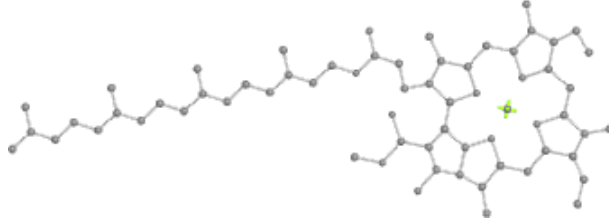
Bond angles

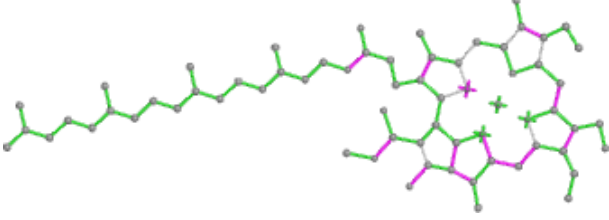
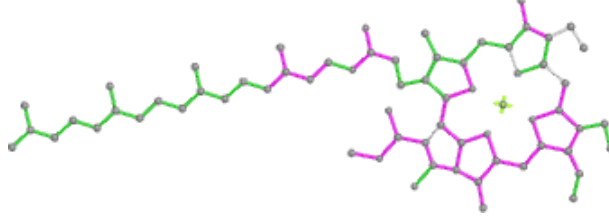
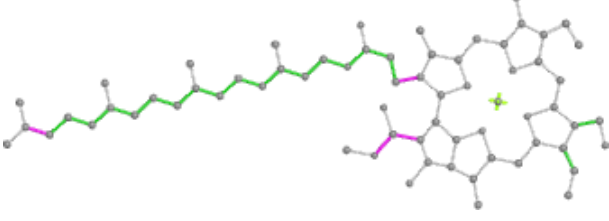
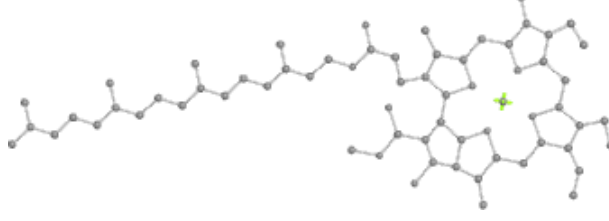


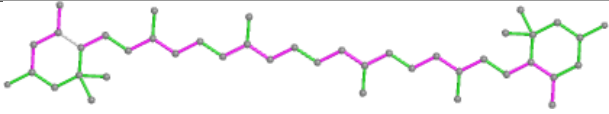
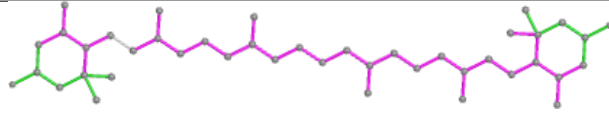
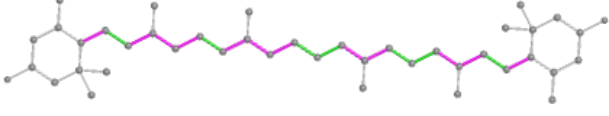
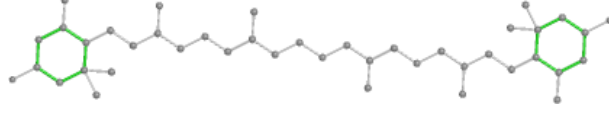
Torsions

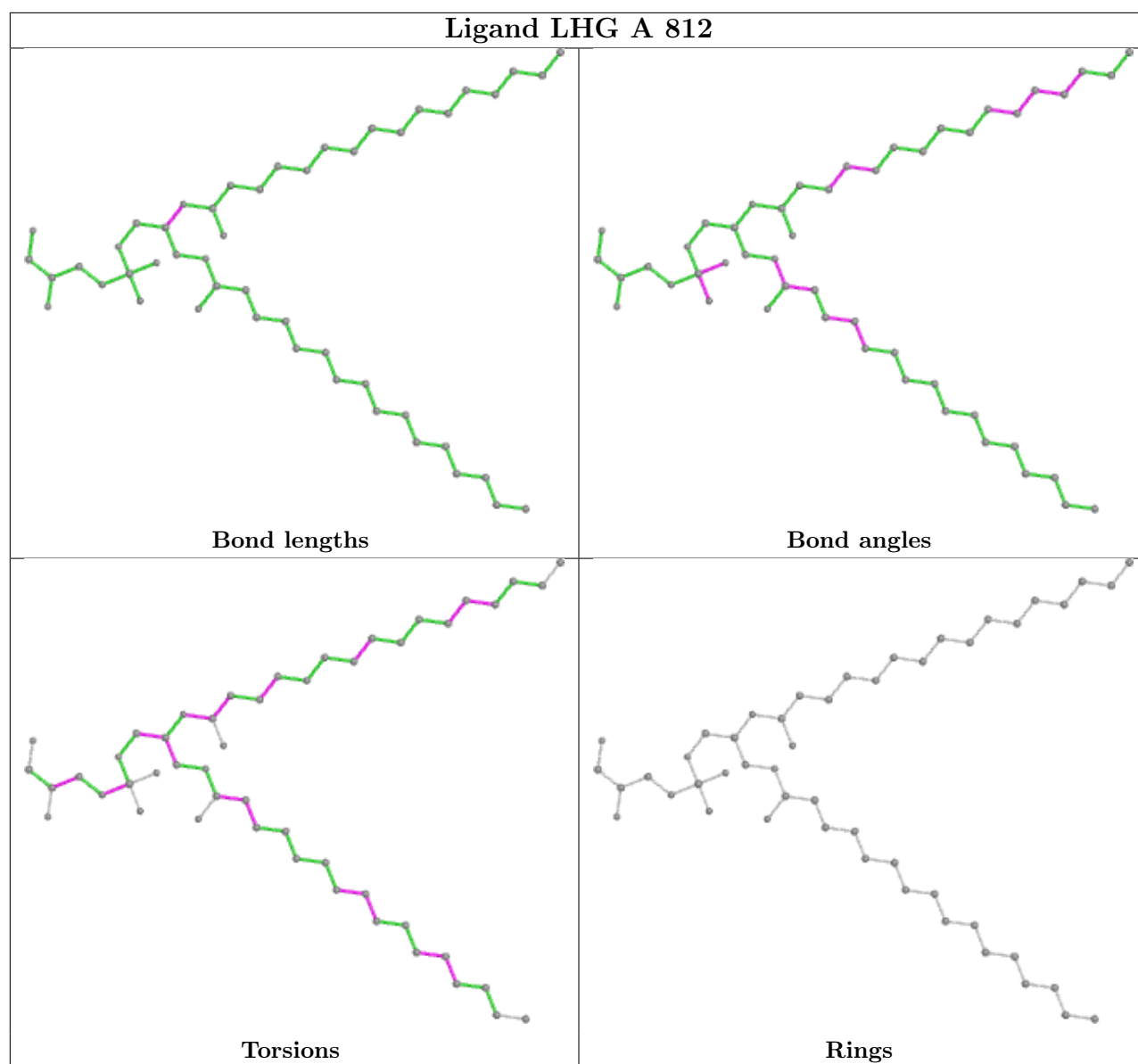


Rings

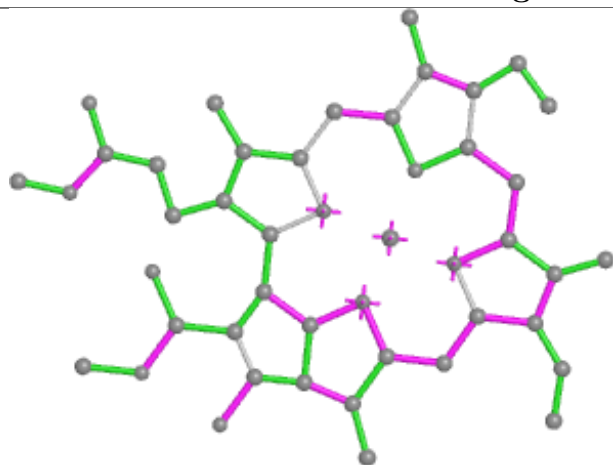
Ligand CHL B 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 3 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

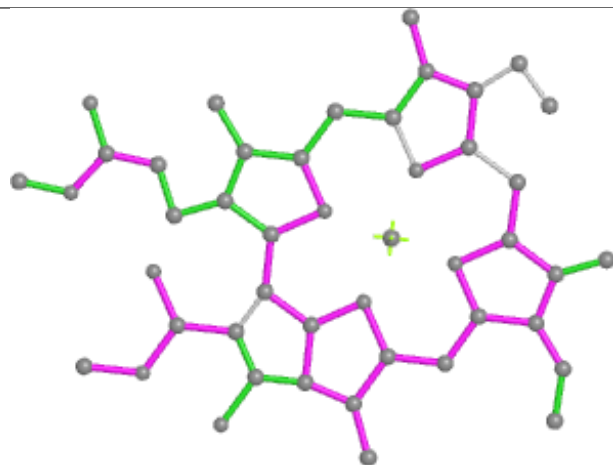
Ligand LUT a 302	
	
Bond lengths	Bond angles
	
Torsions	Rings



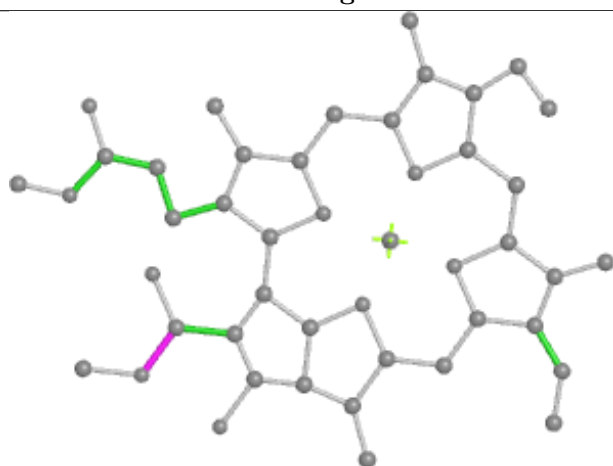
Ligand CHL K 206



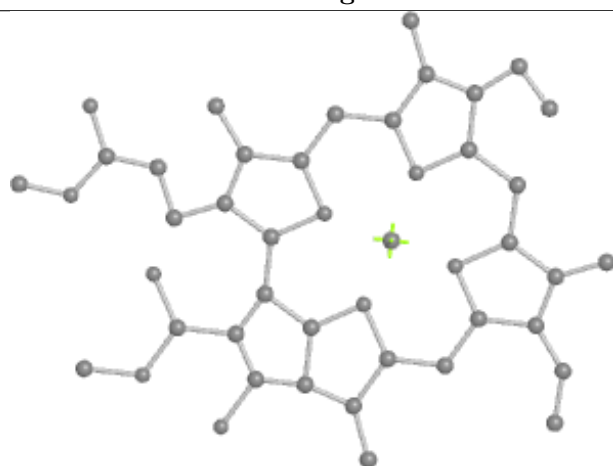
Bond lengths



Bond angles

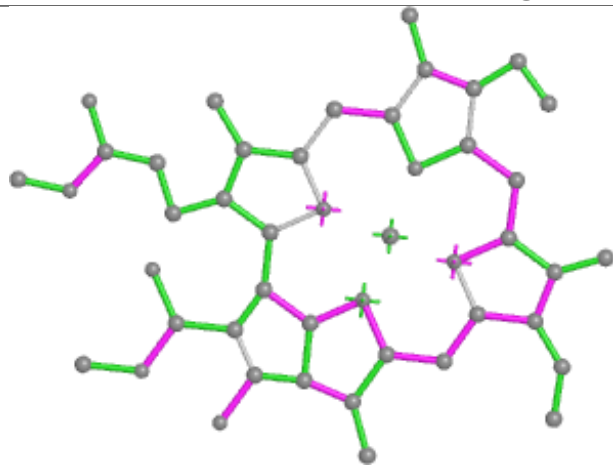


Torsions

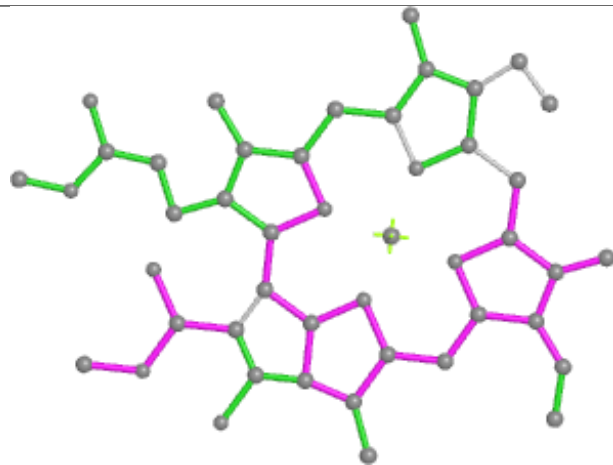


Rings

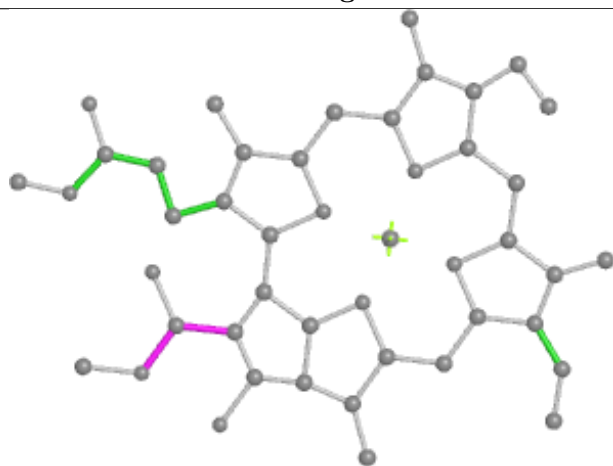
Ligand CHL 5 308



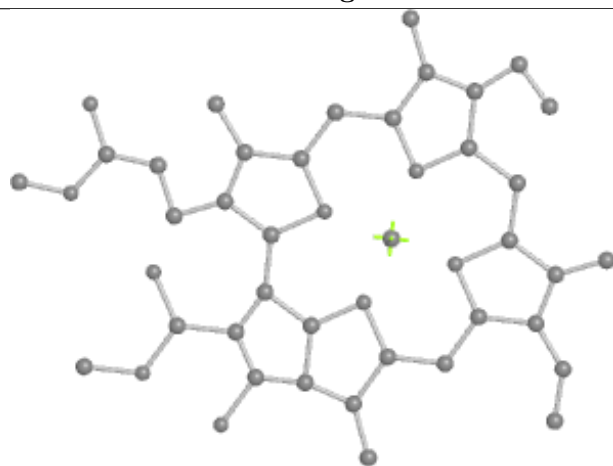
Bond lengths



Bond angles

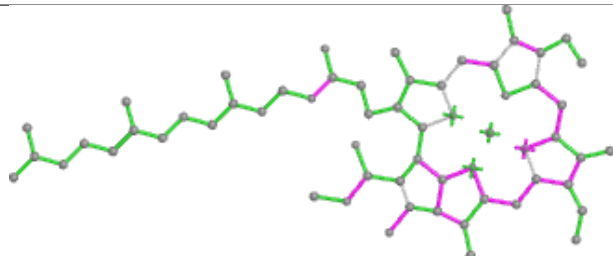


Torsions

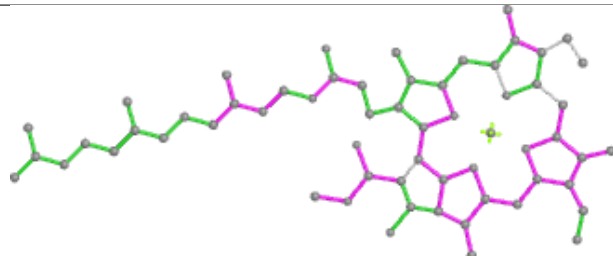


Rings

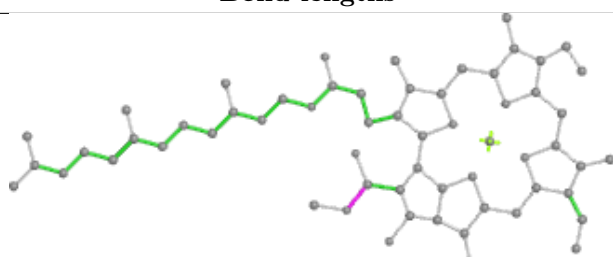
Ligand CHL B 828



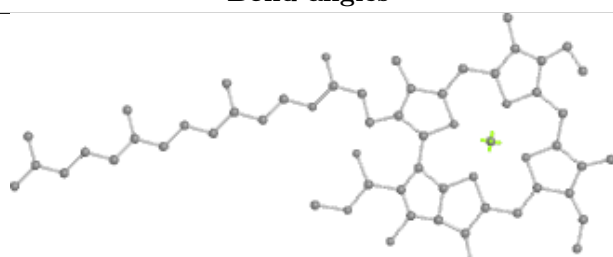
Bond lengths



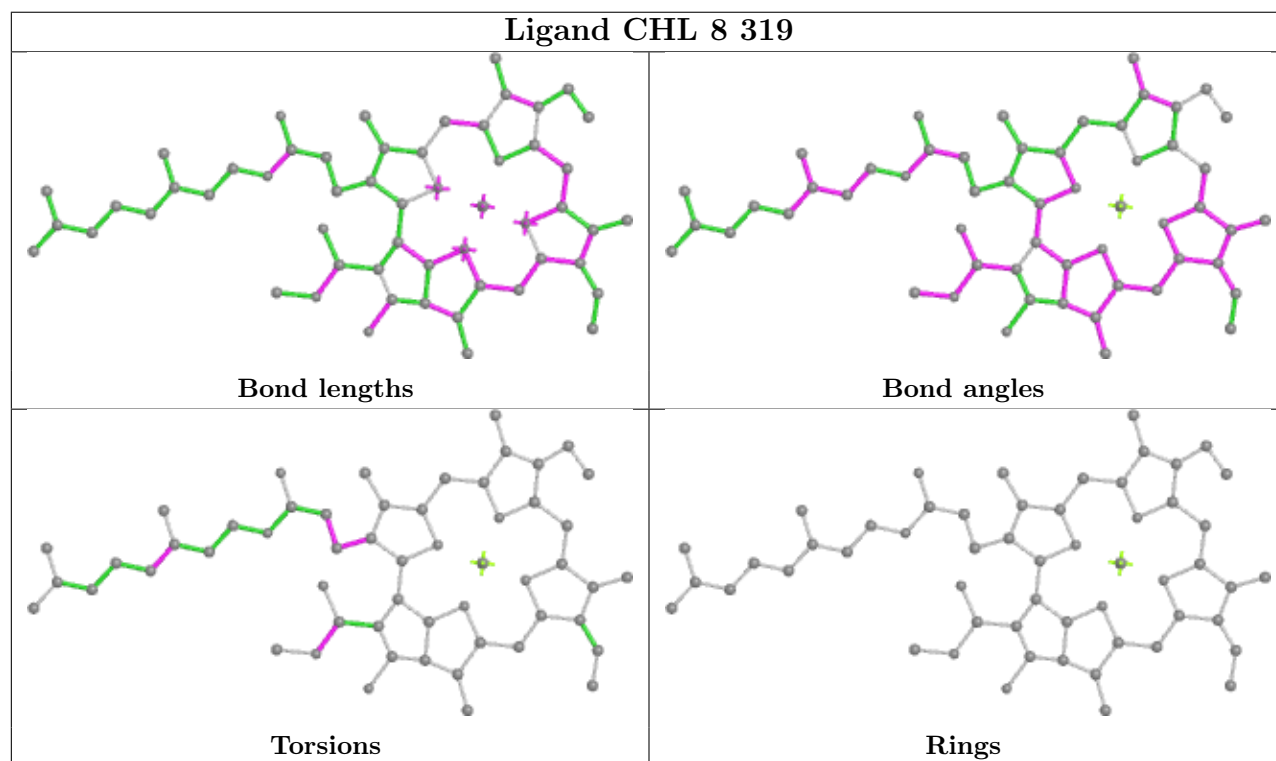
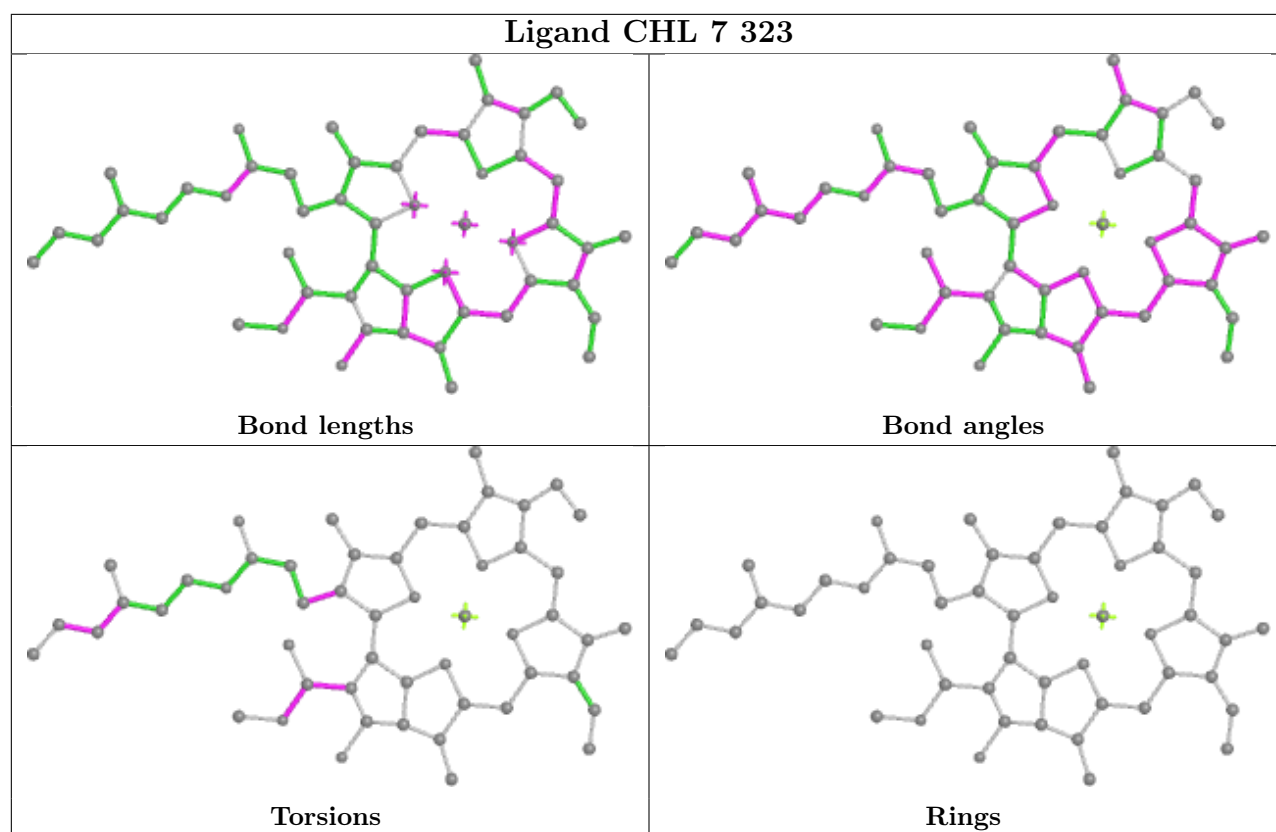
Bond angles

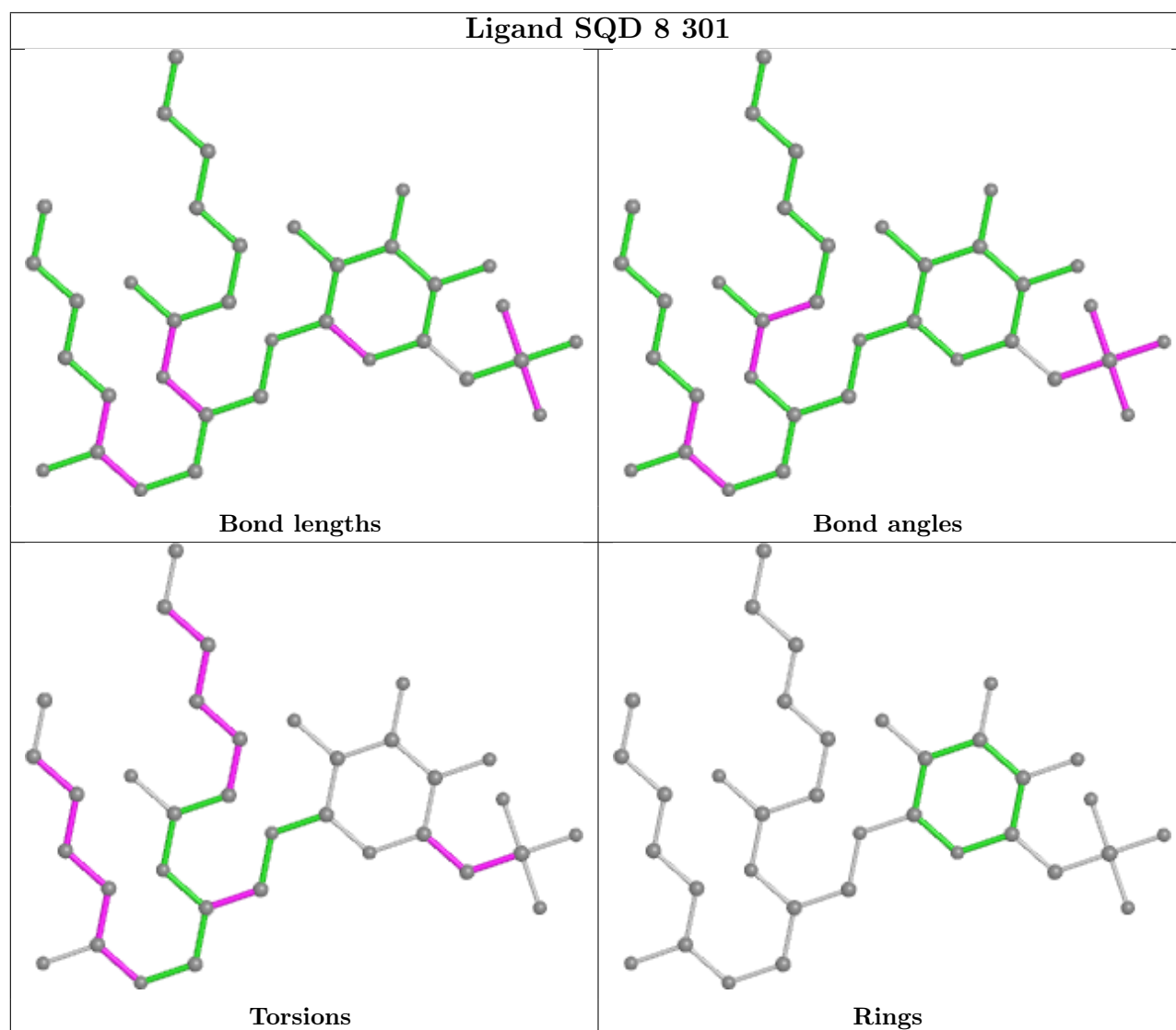
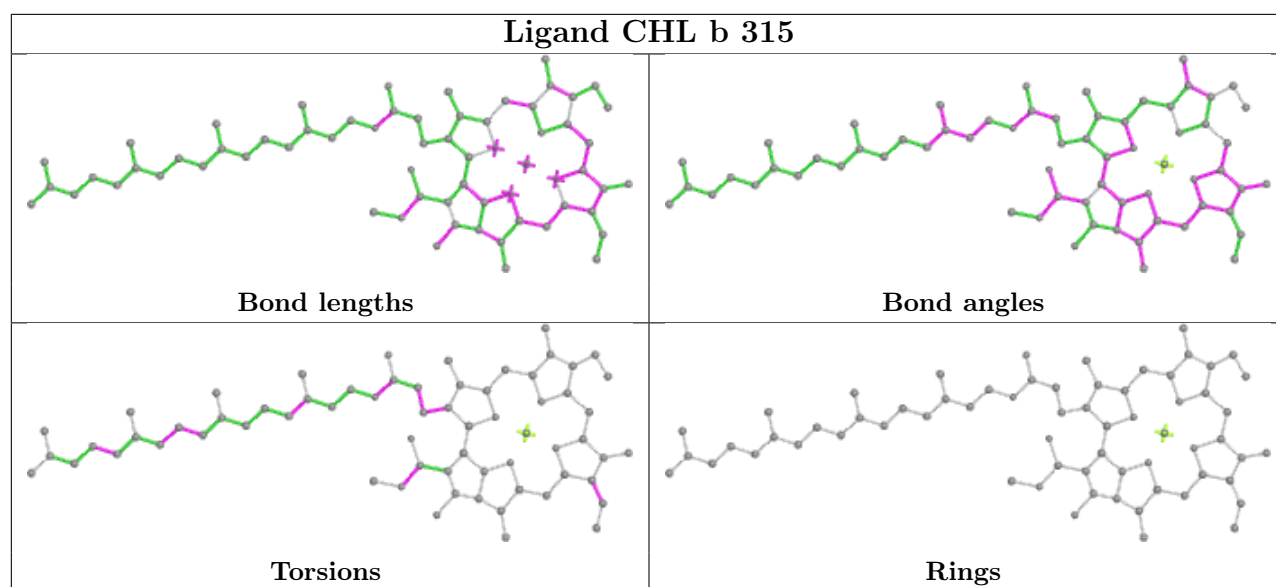


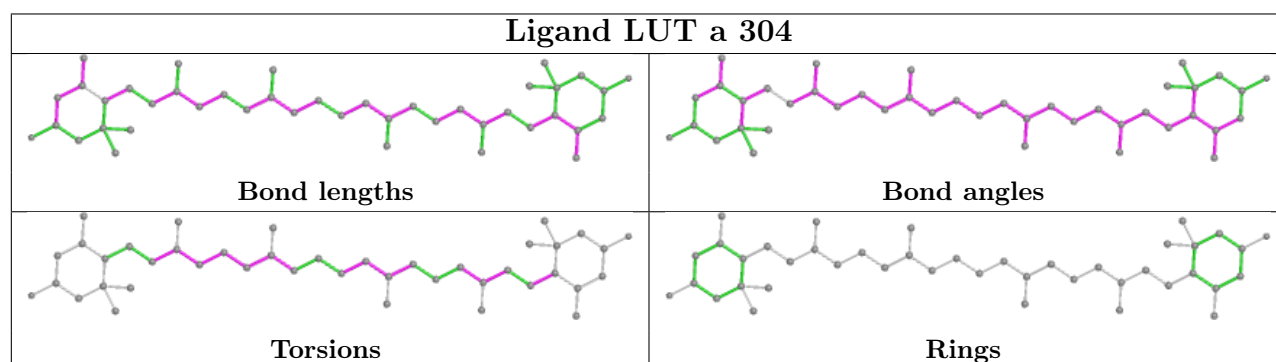
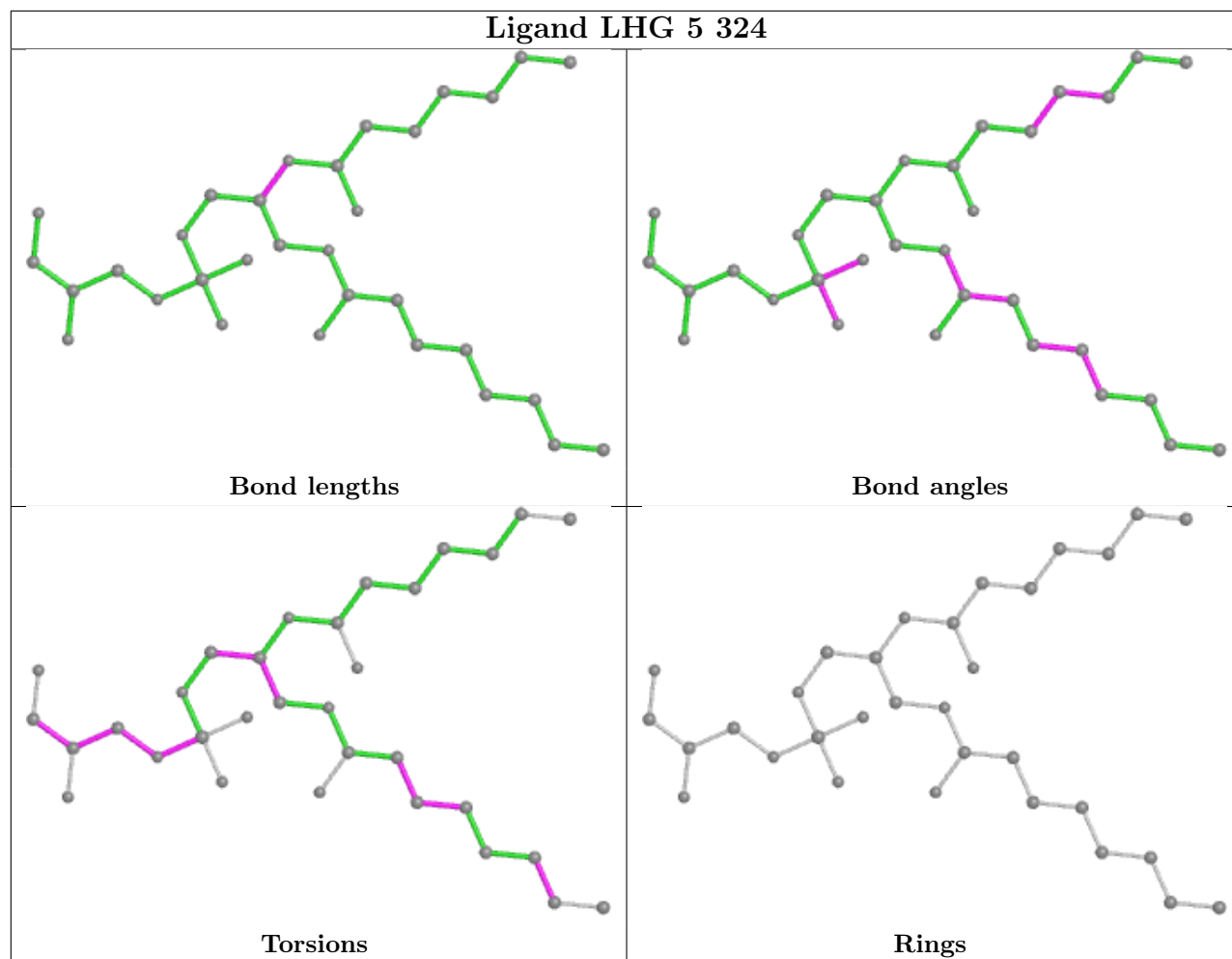
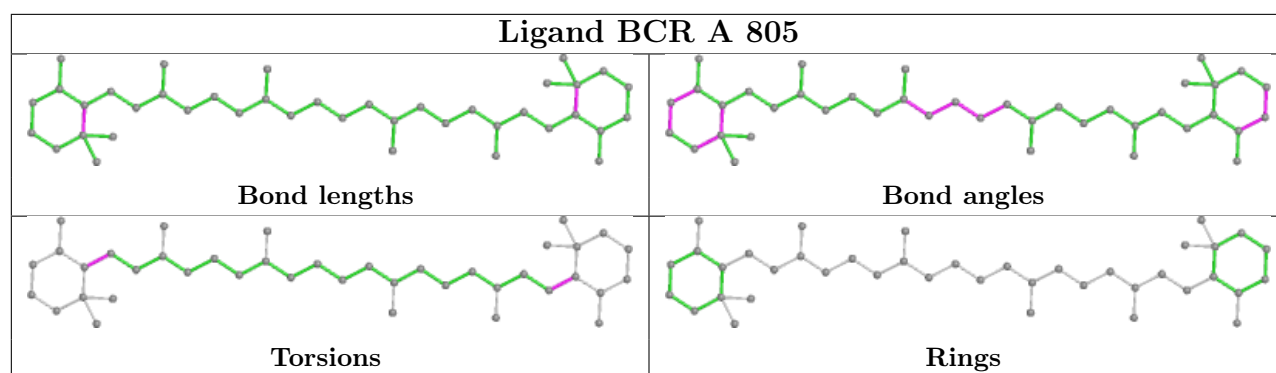
Torsions

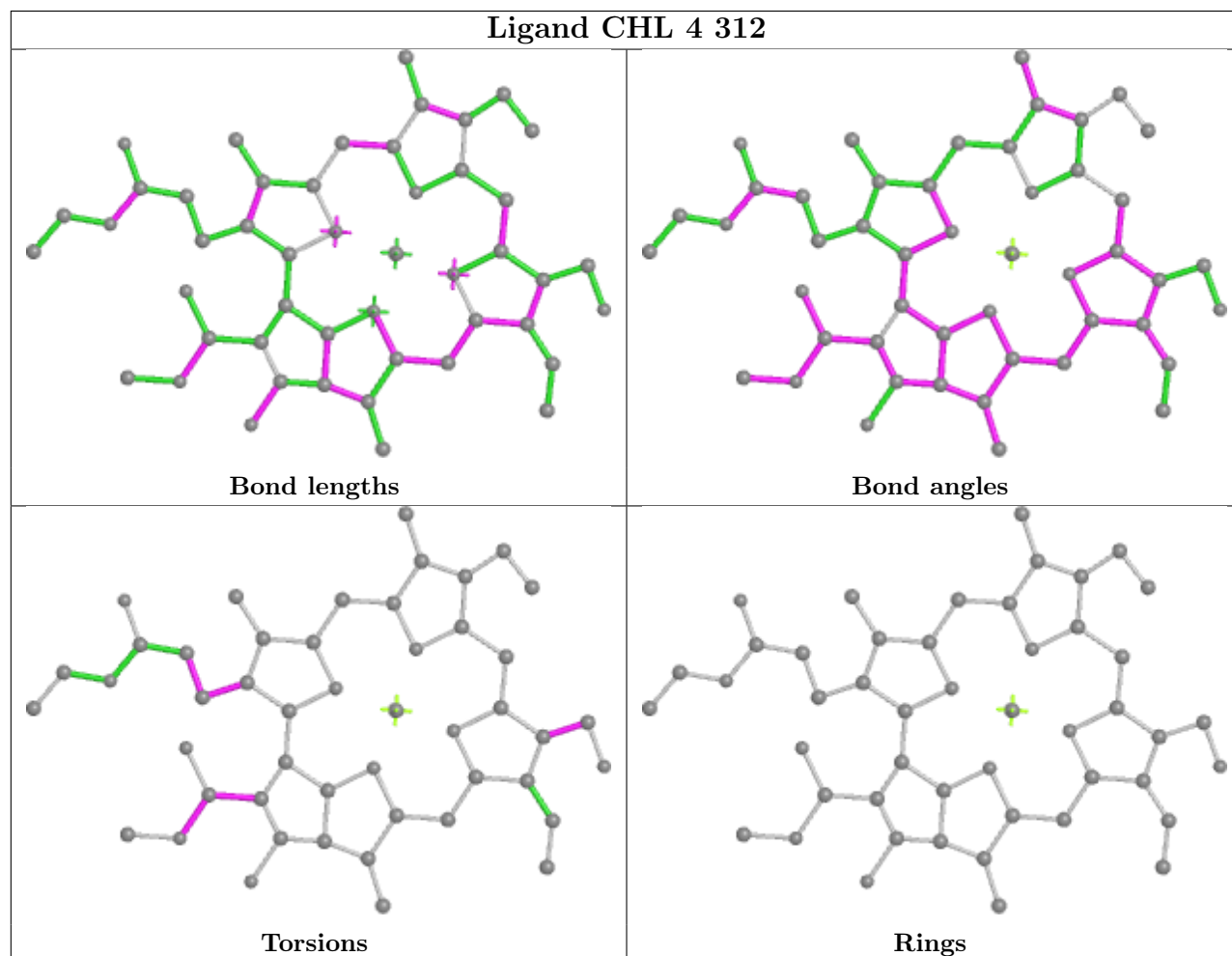
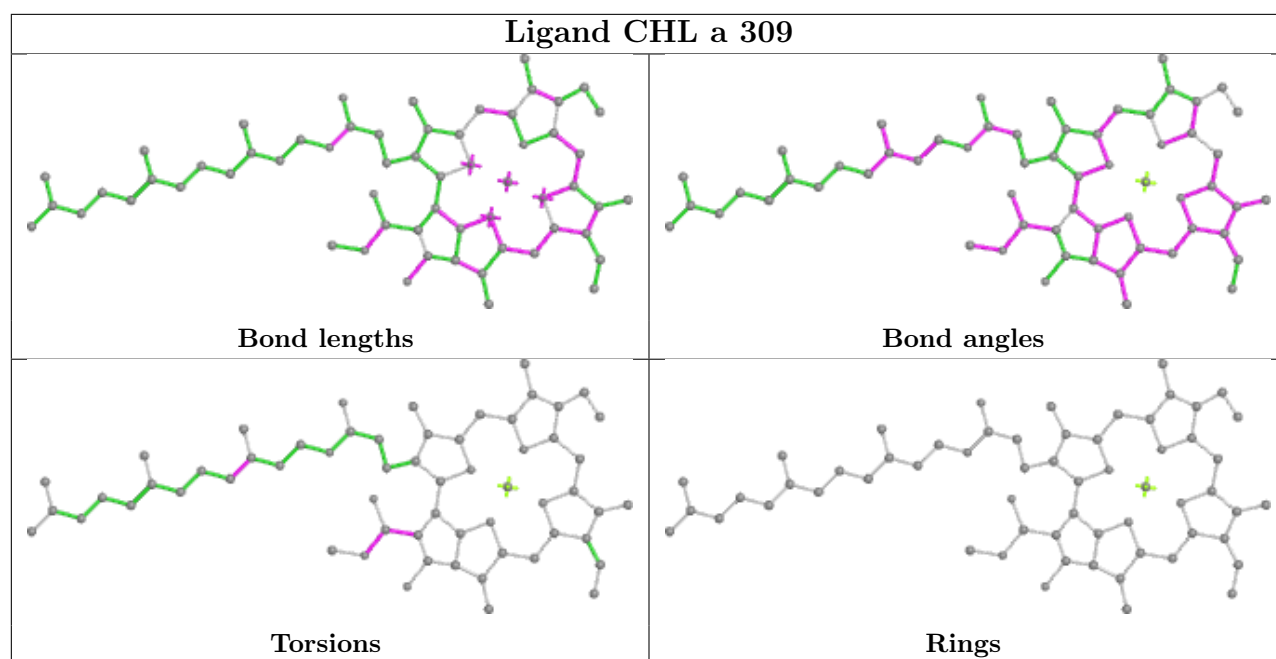


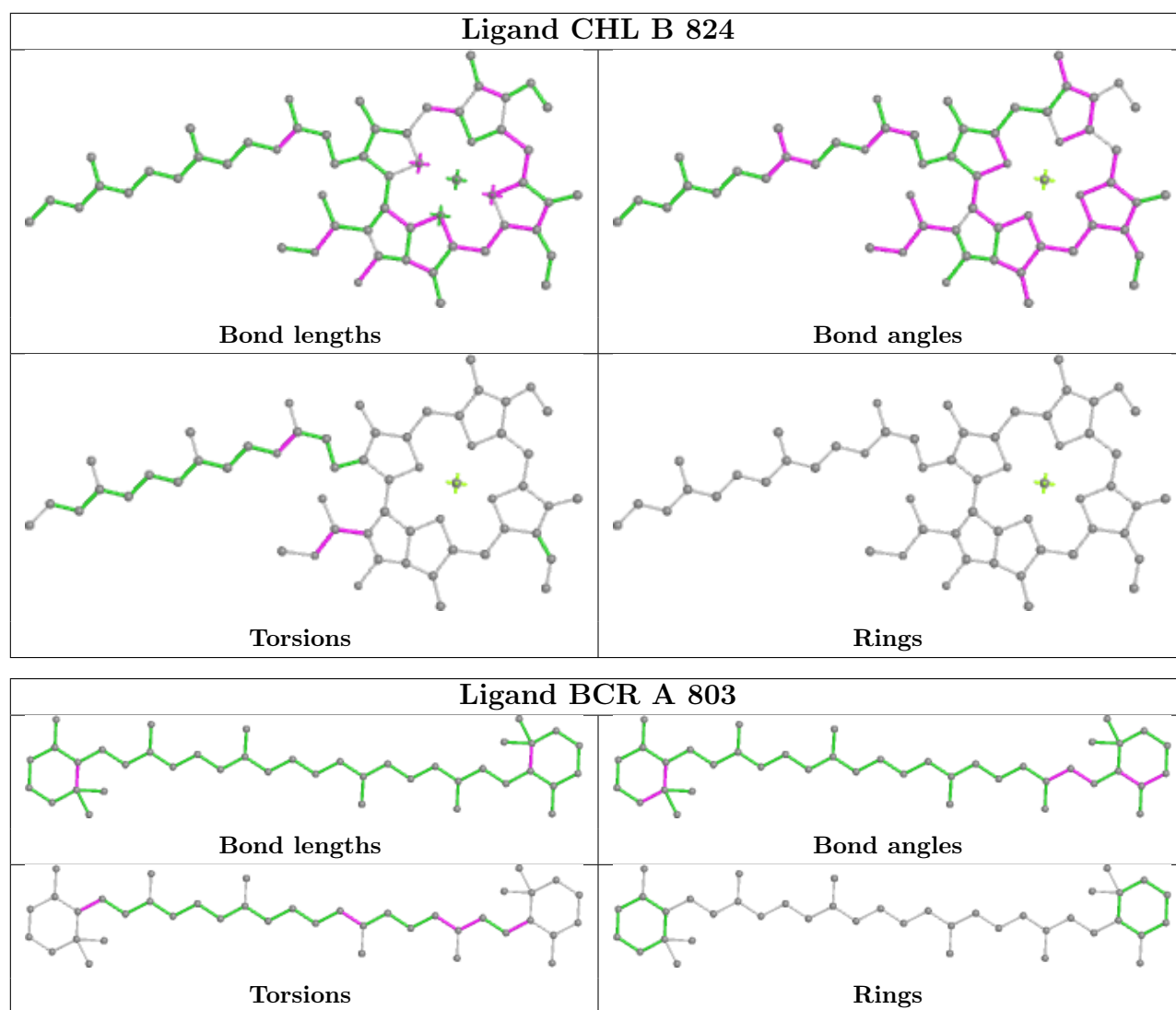
Rings



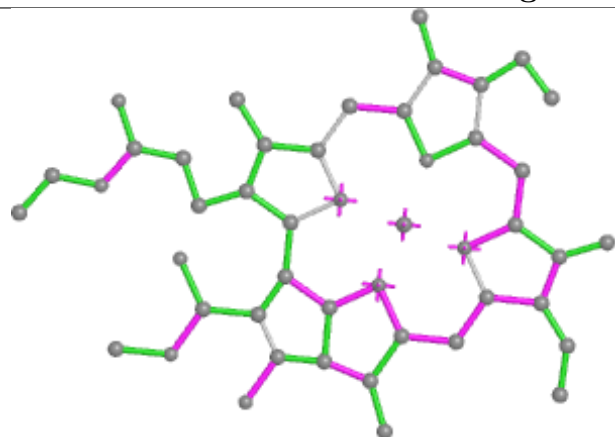




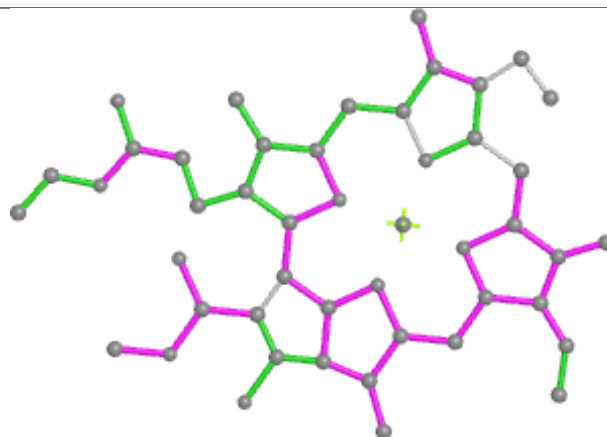




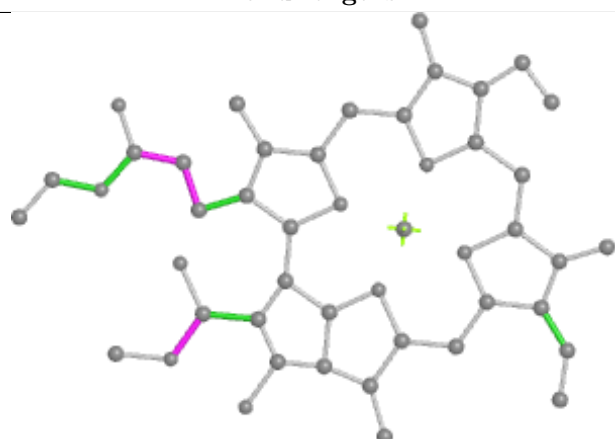
Ligand CHL 4 311



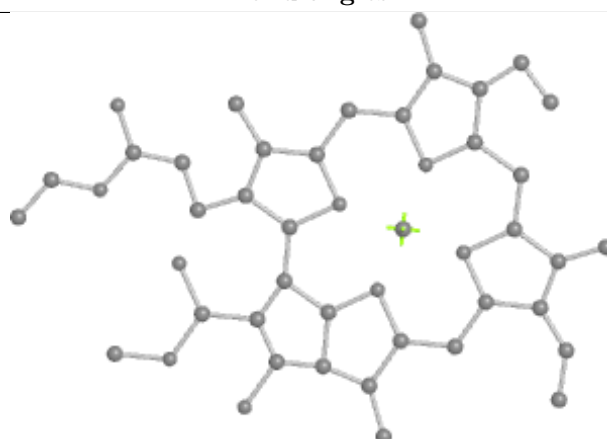
Bond lengths



Bond angles

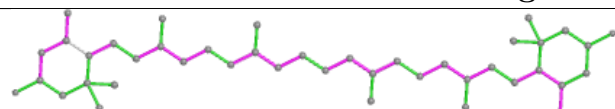


Torsions

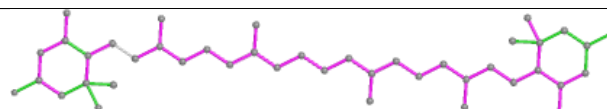


Rings

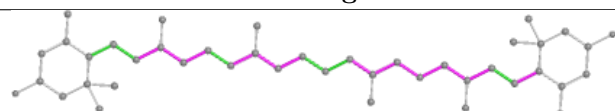
Ligand LUT F 303



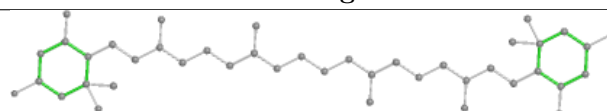
Bond lengths



Bond angles

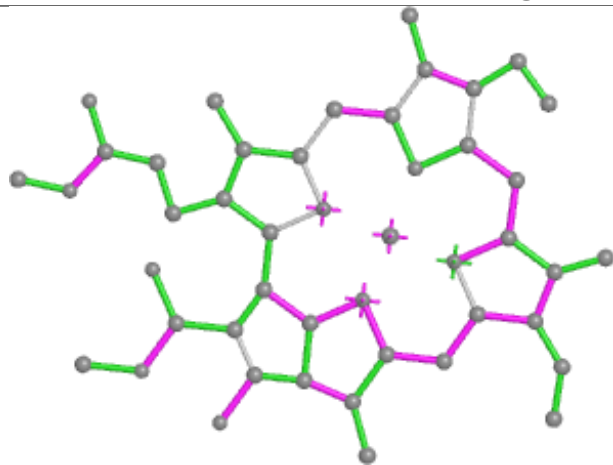


Torsions

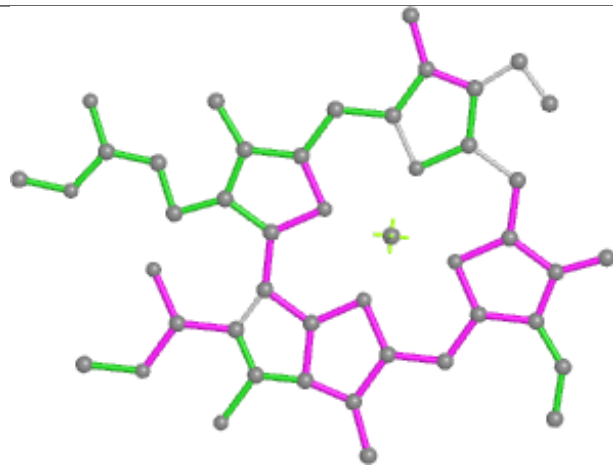


Rings

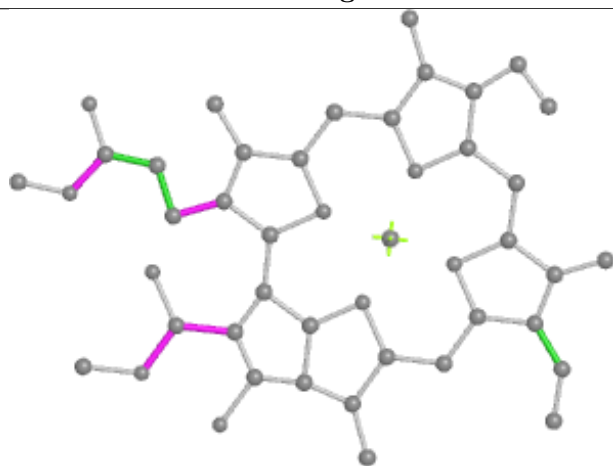
Ligand CHL 8 318



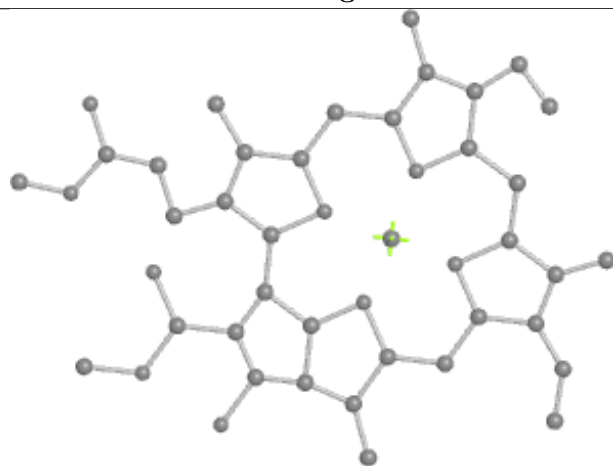
Bond lengths



Bond angles

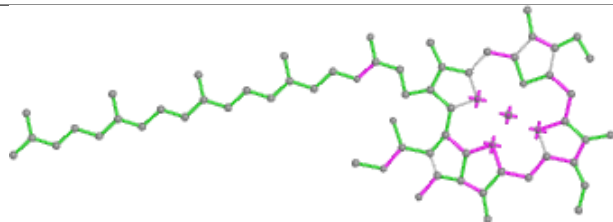


Torsions

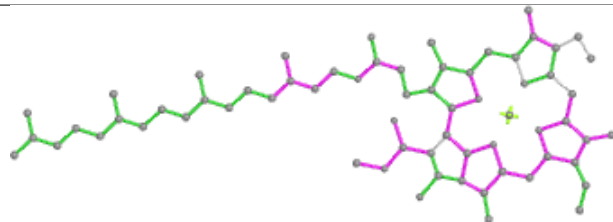


Rings

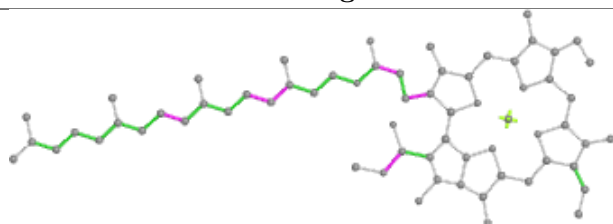
Ligand CHL a 317



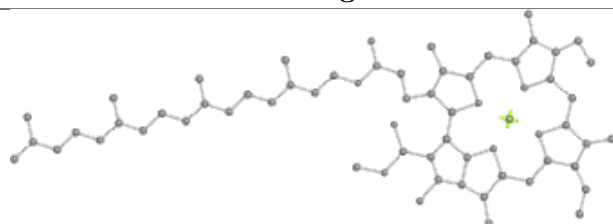
Bond lengths



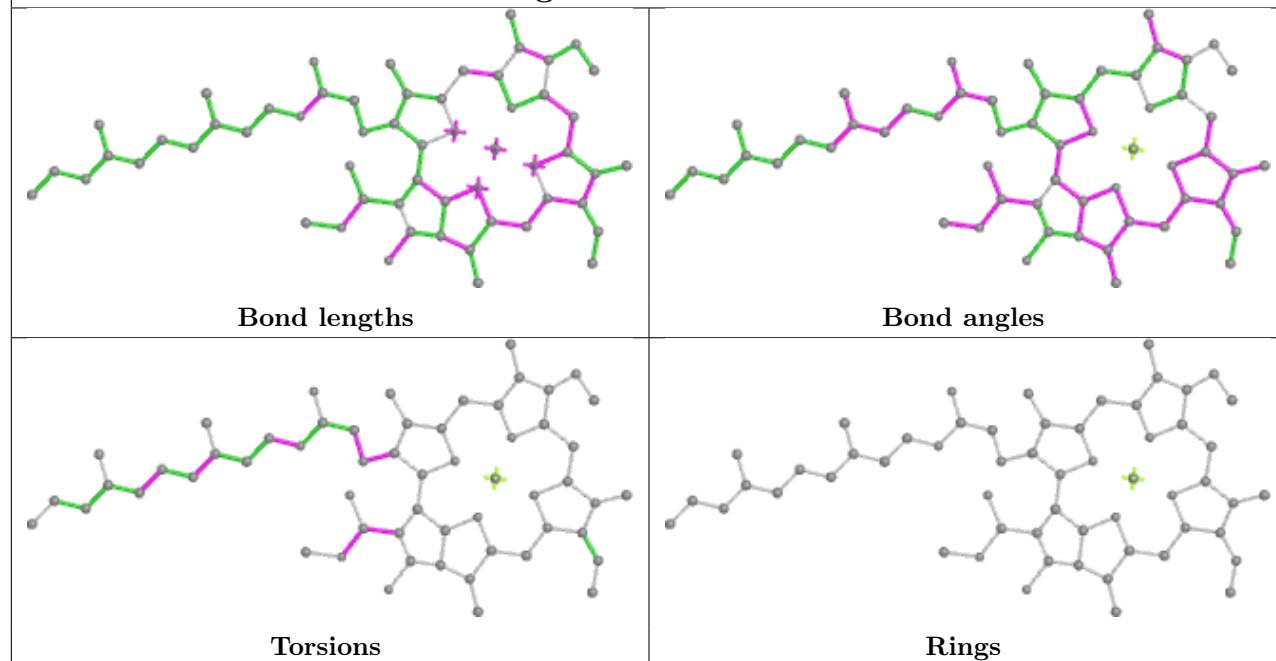
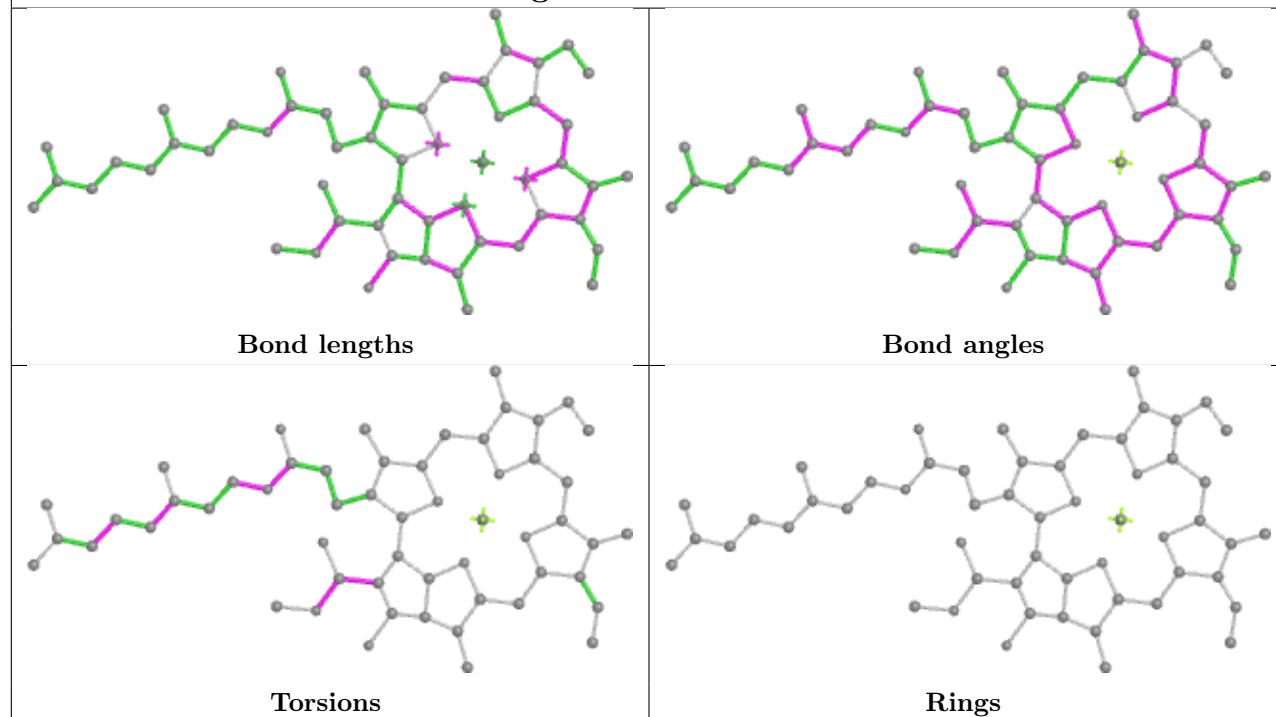
Bond angles

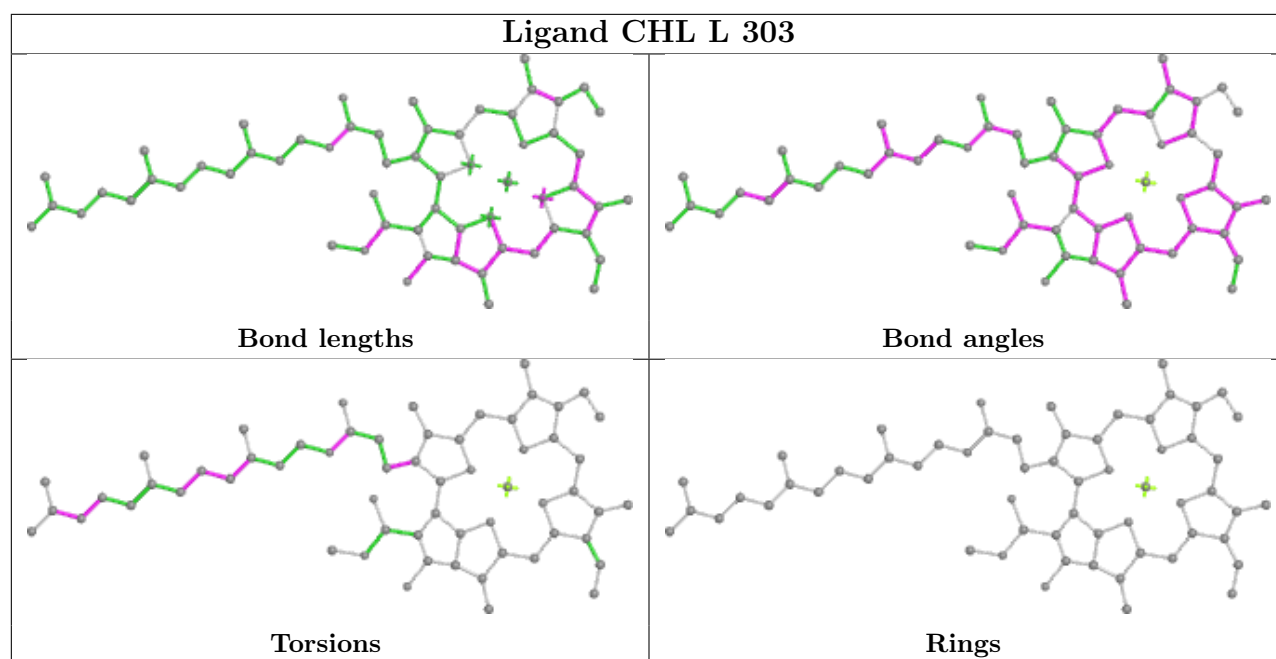


Torsions

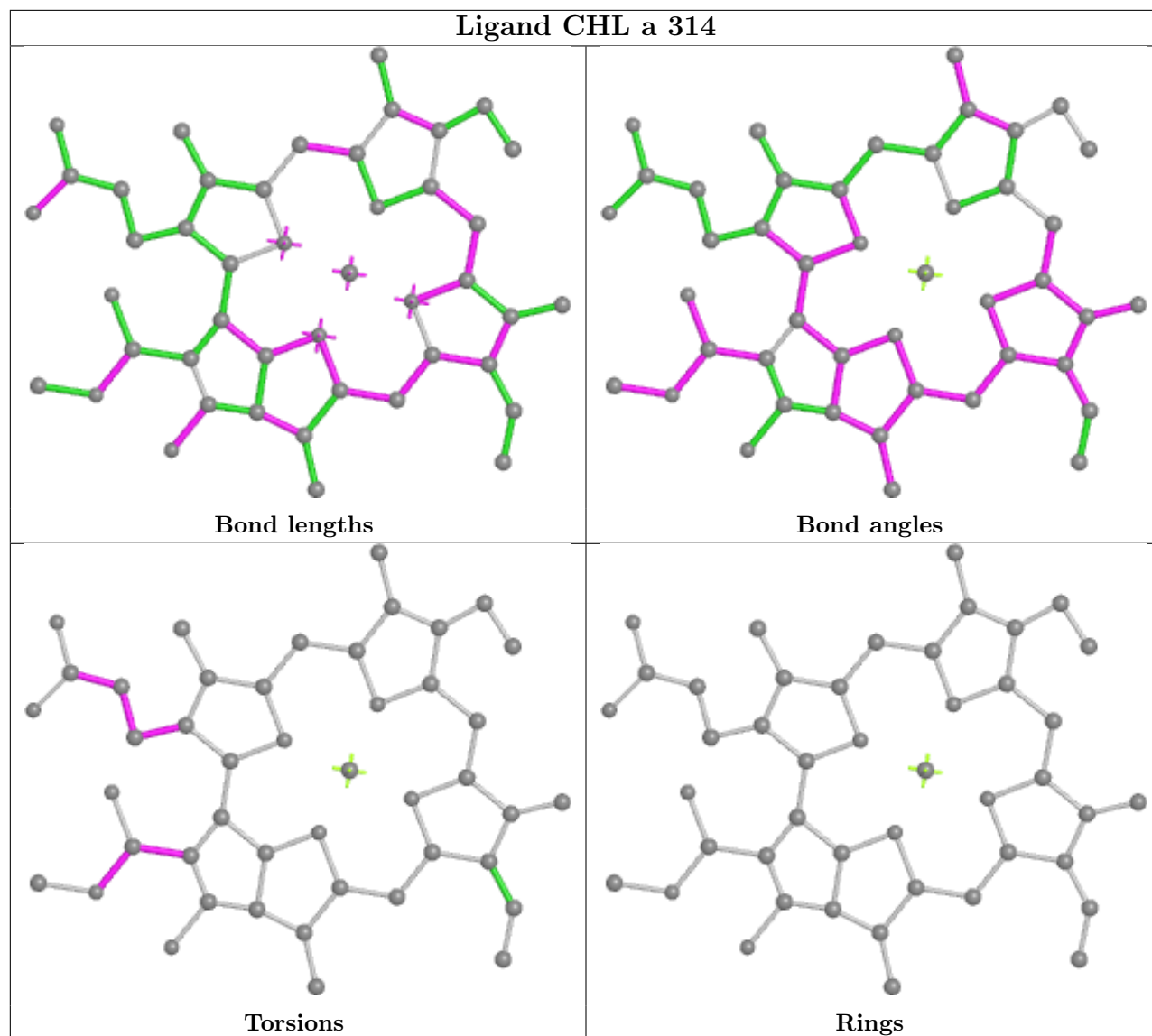


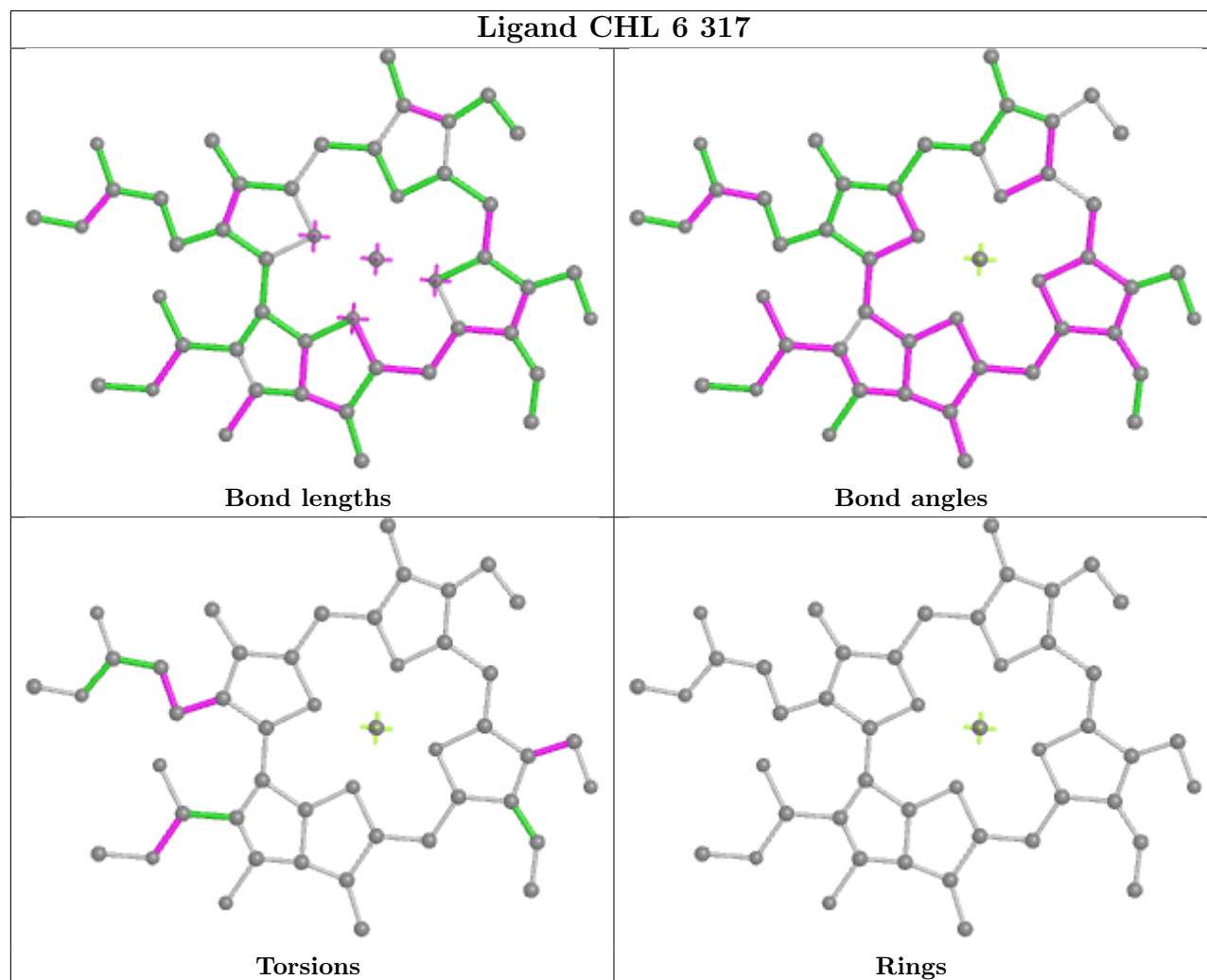
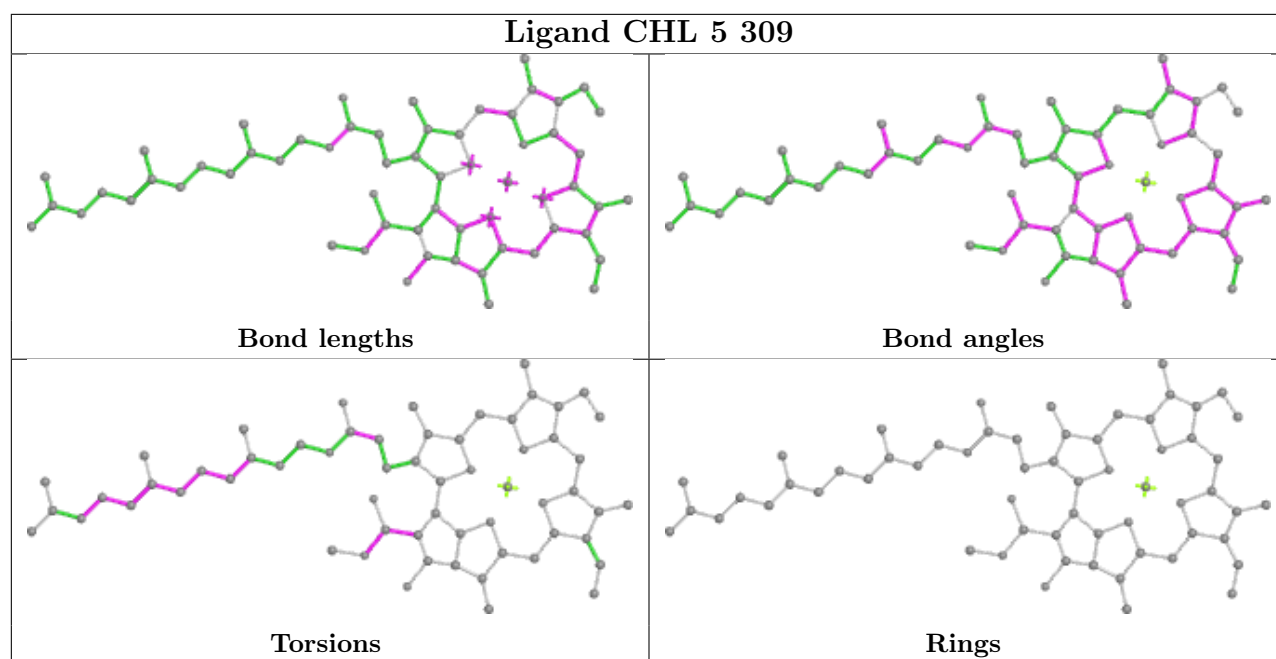
Rings

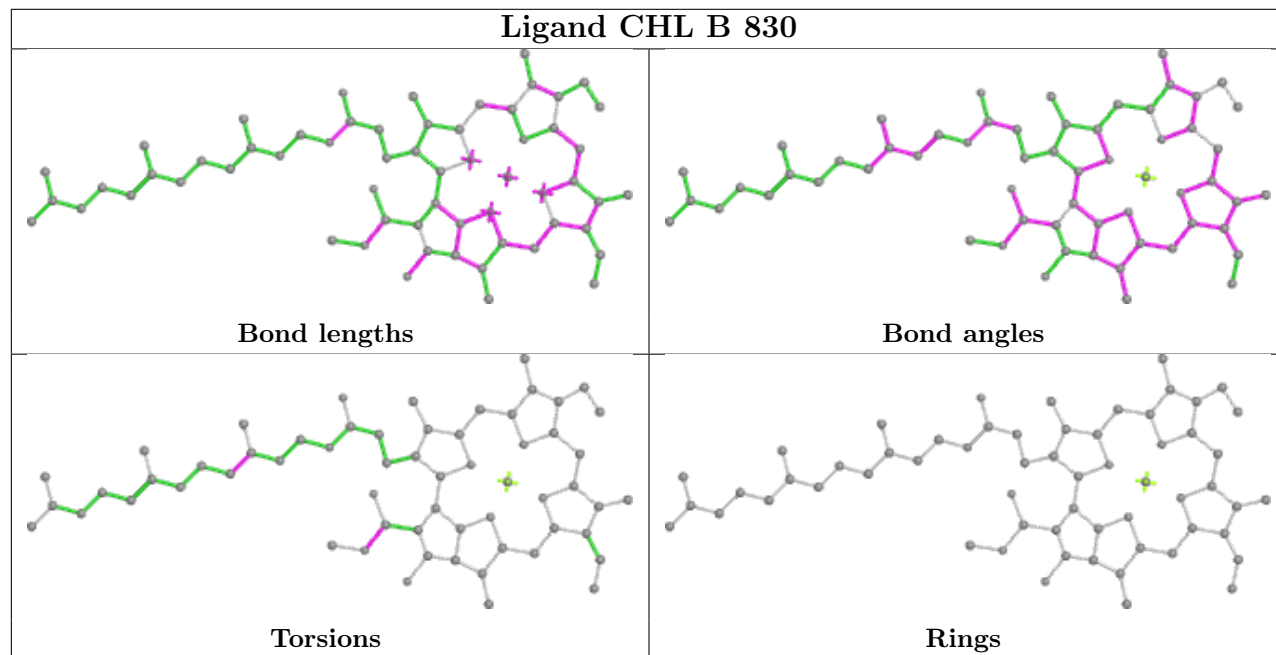
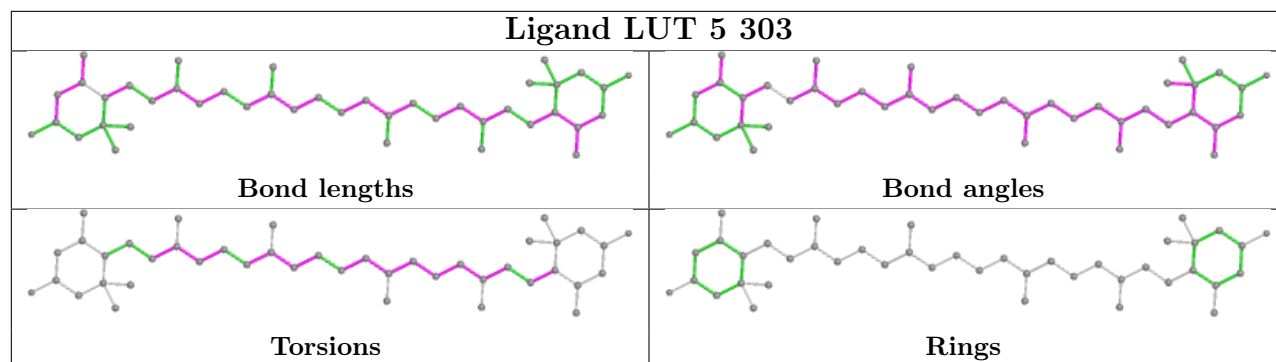
Ligand CHL 6 306**Ligand CHL A 829**



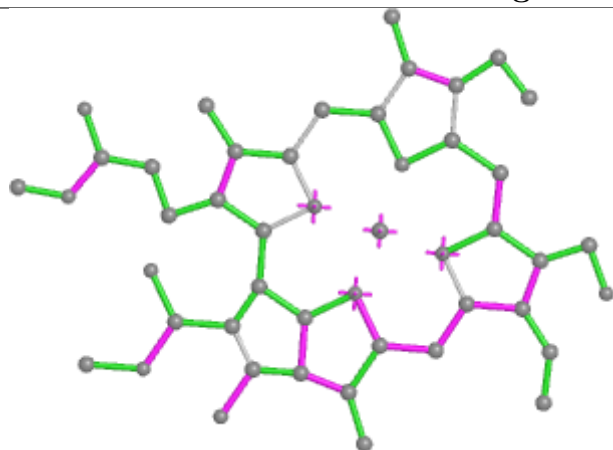
Ligand CHL a 314



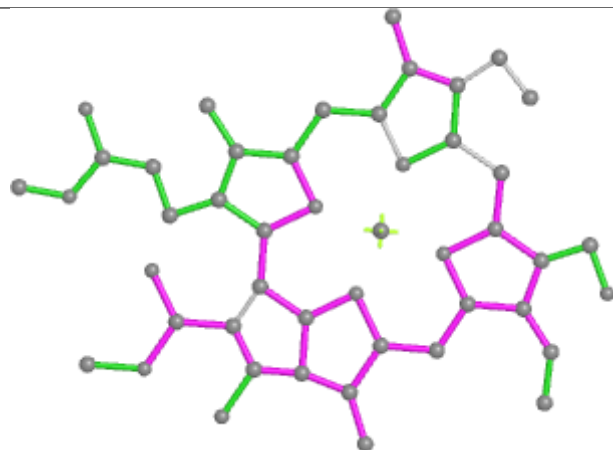




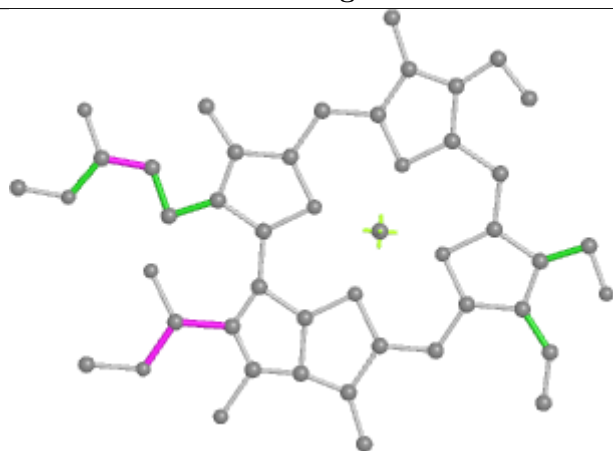
Ligand CHL K 207



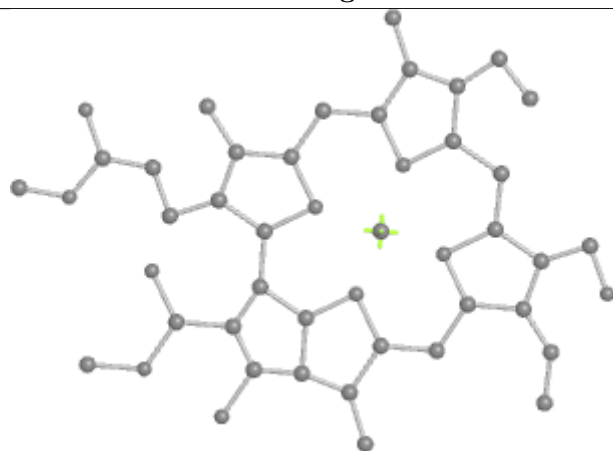
Bond lengths



Bond angles

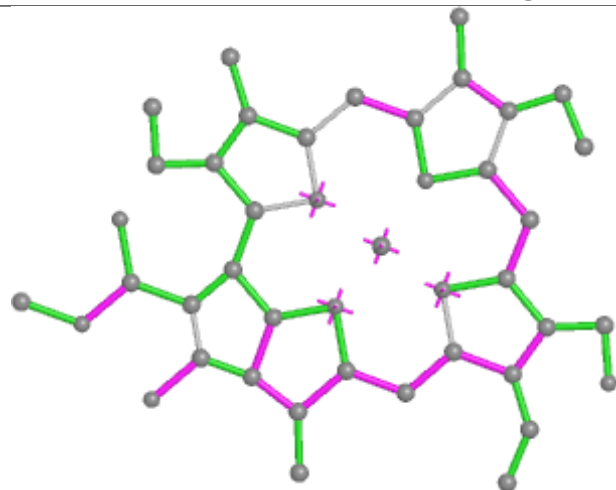


Torsions

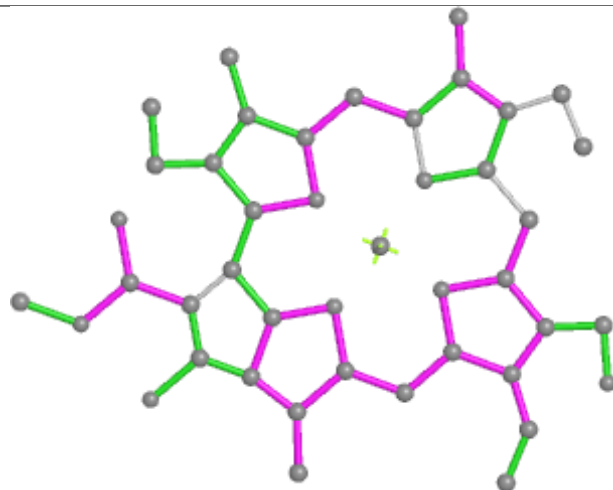


Rings

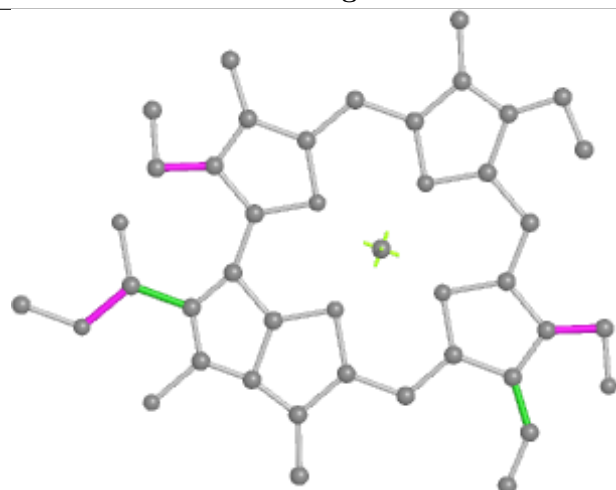
Ligand CHL 6 319



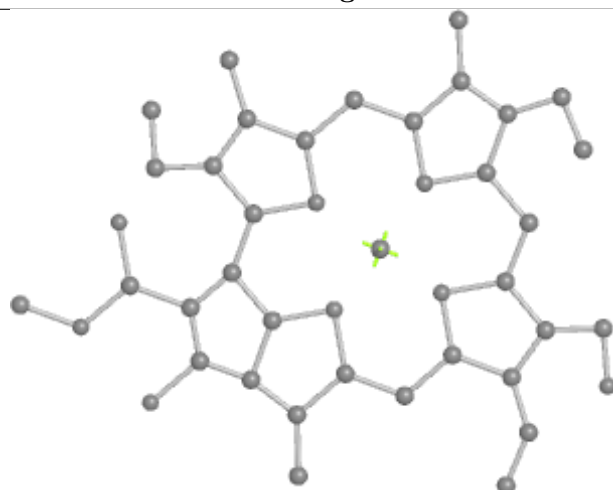
Bond lengths



Bond angles

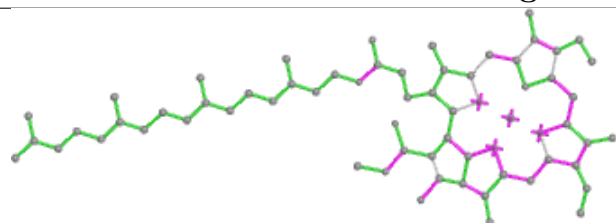


Torsions

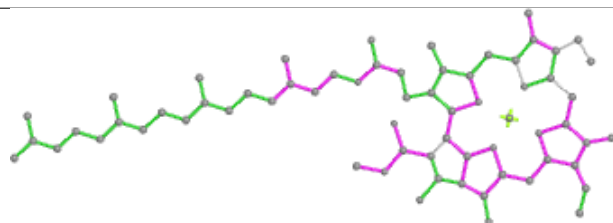


Rings

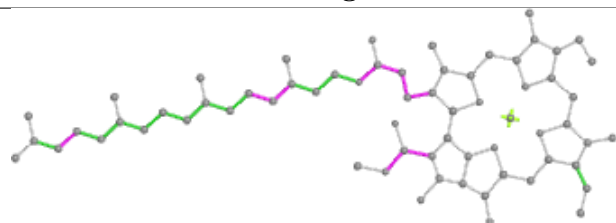
Ligand CHL 8 317



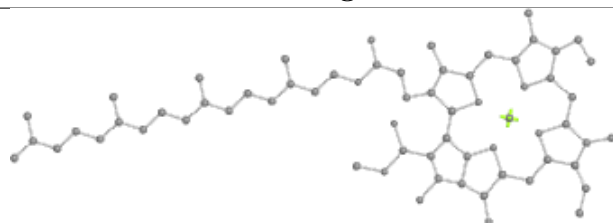
Bond lengths



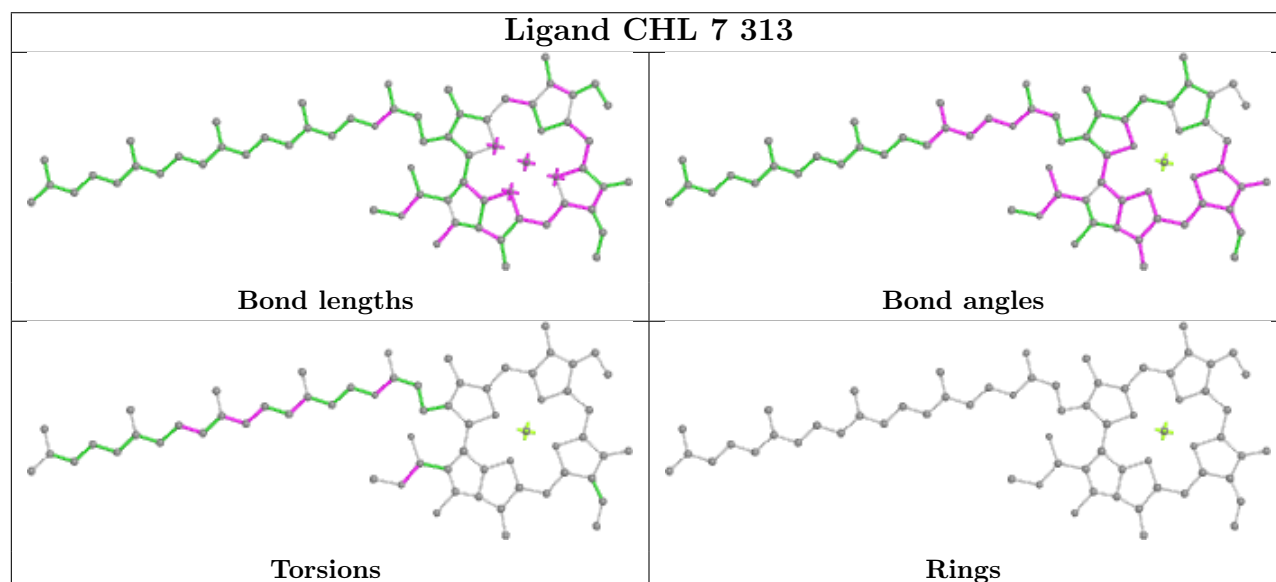
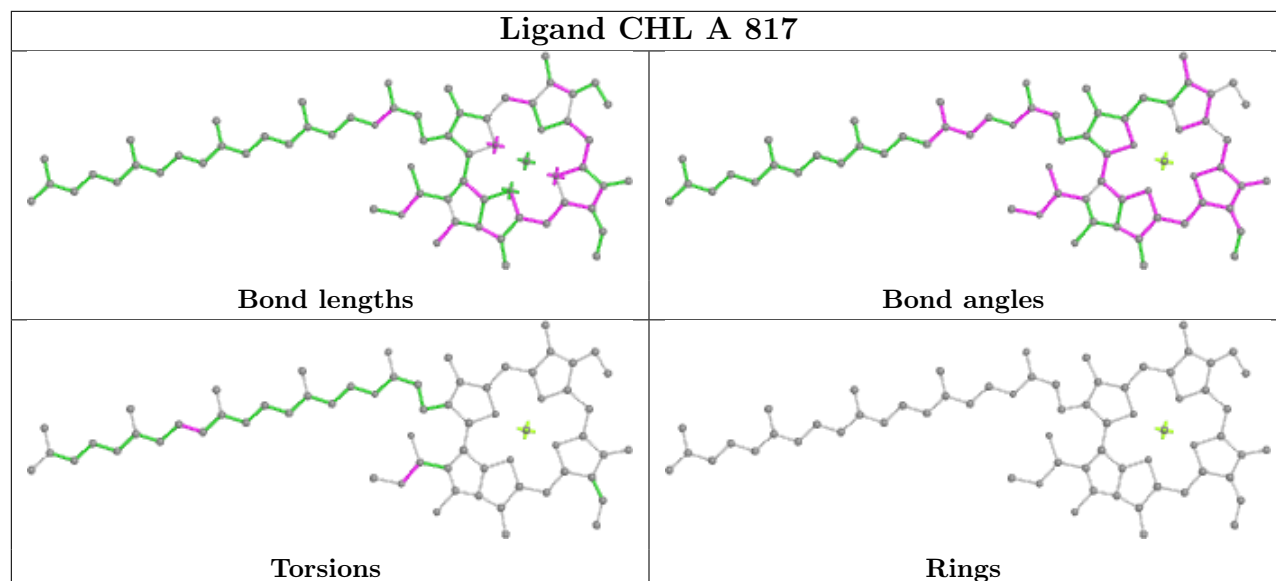
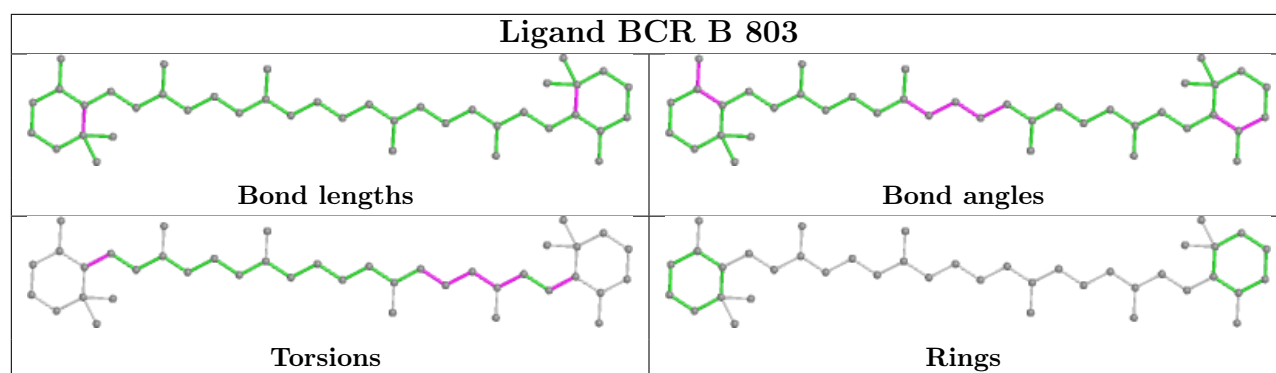
Bond angles

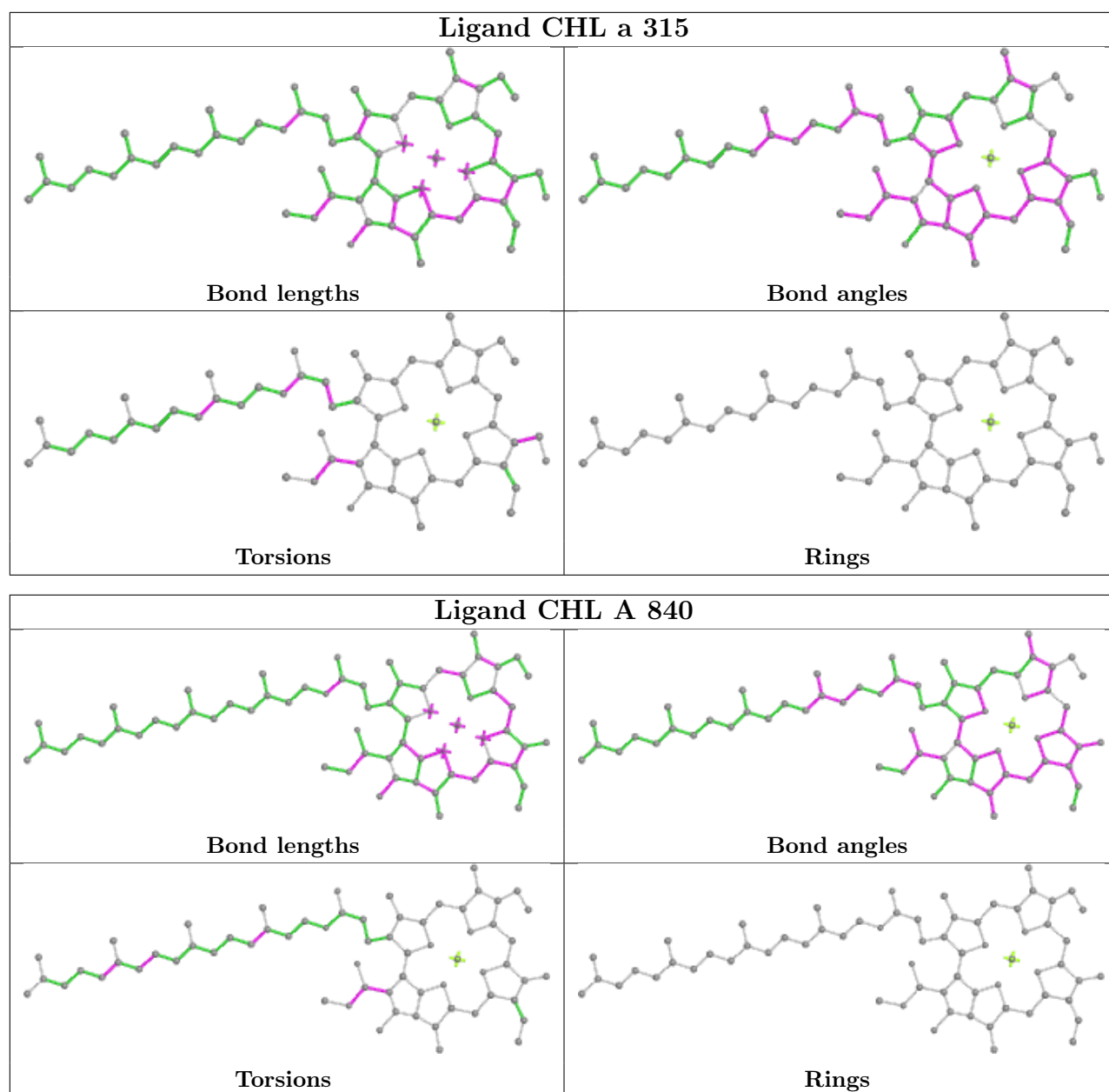


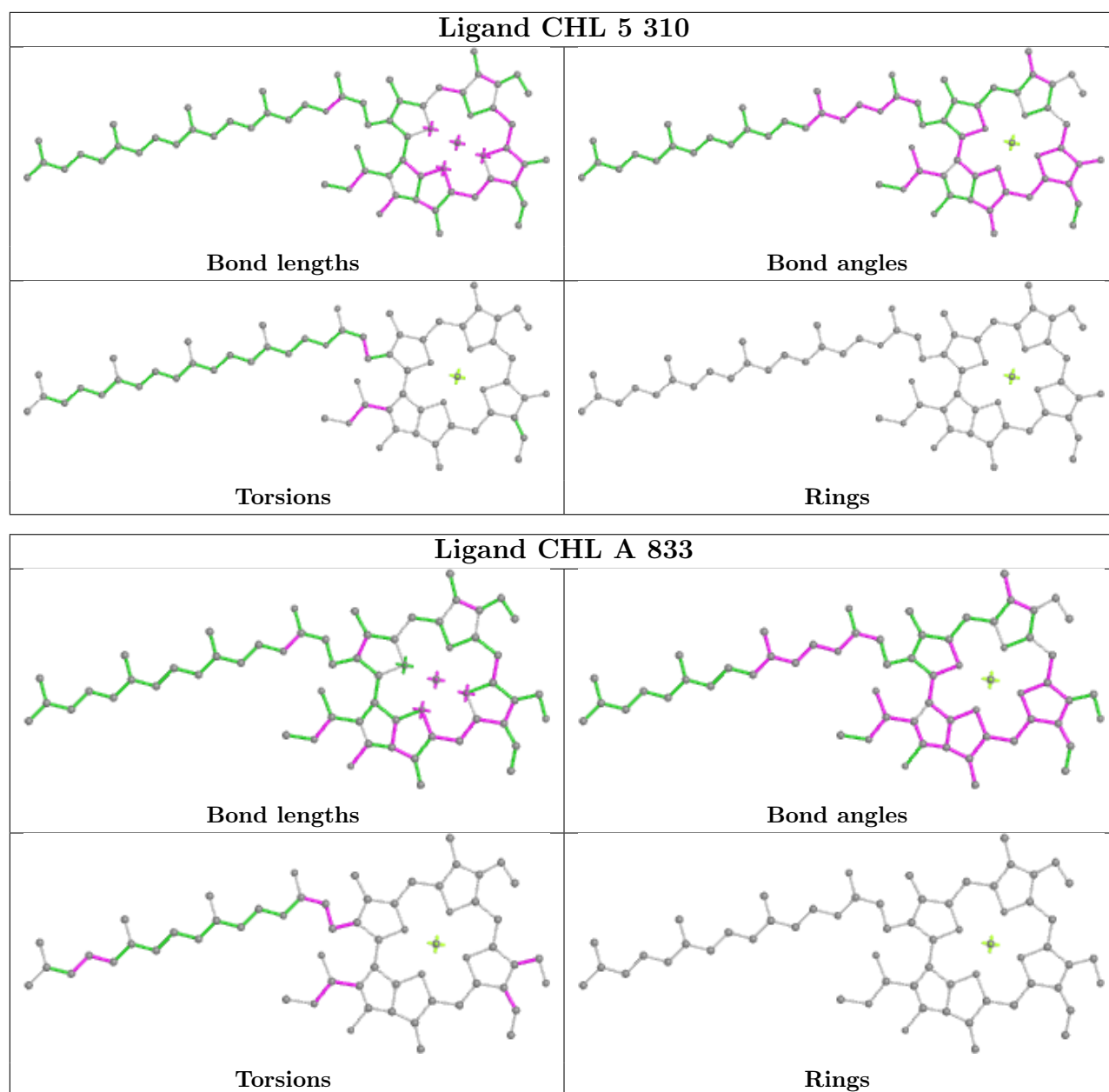
Torsions

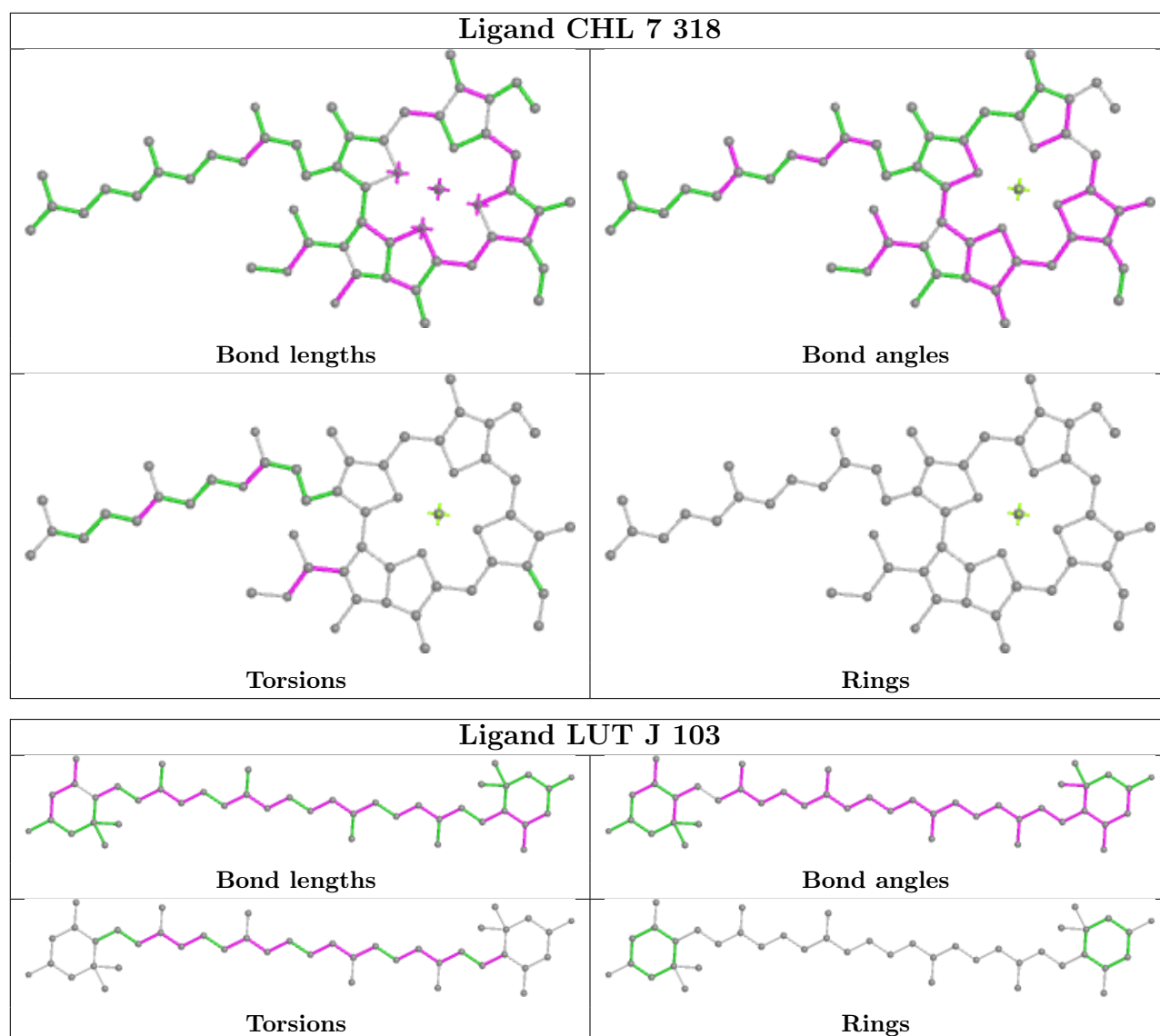


Rings

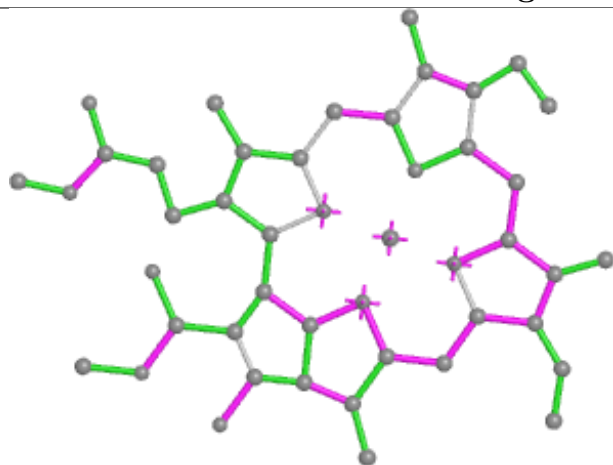




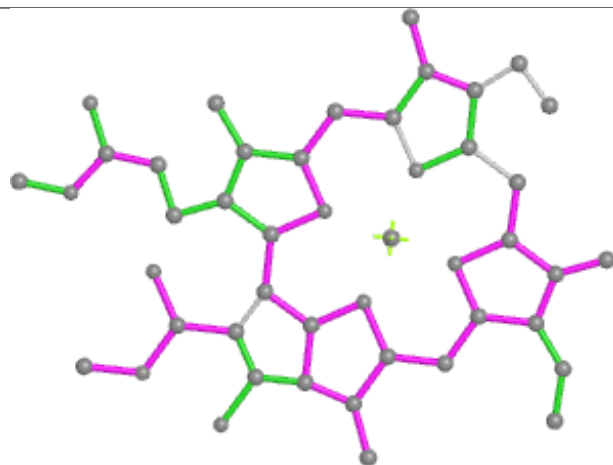




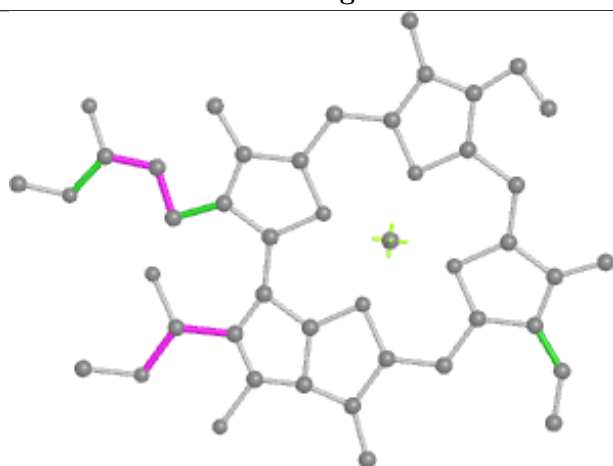
Ligand CHL 4 310



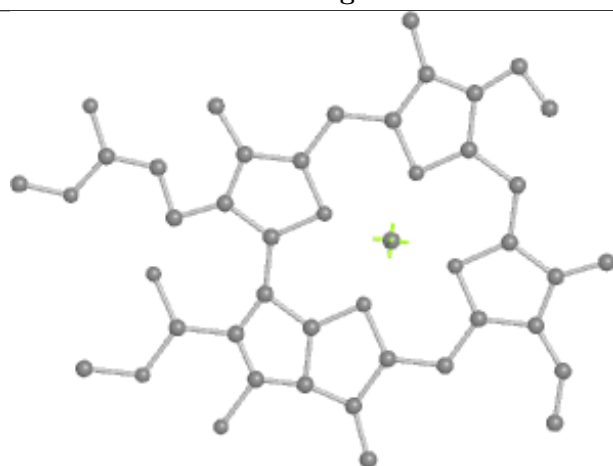
Bond lengths



Bond angles

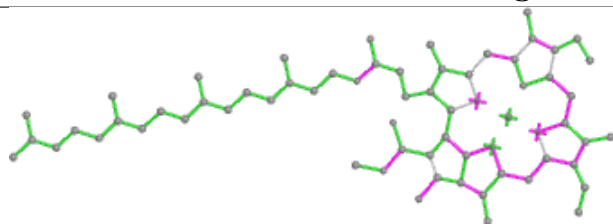


Torsions

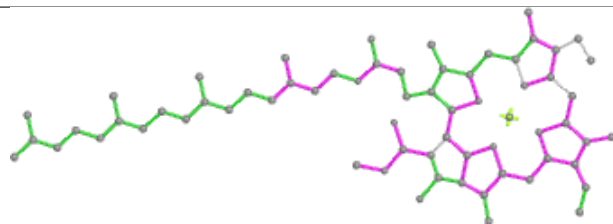


Rings

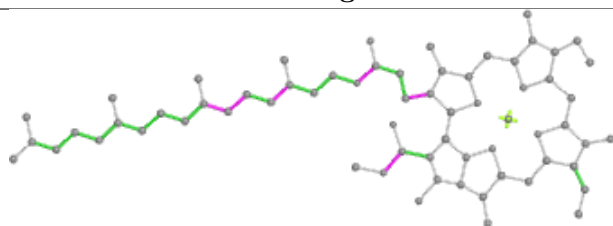
Ligand CHL A 850



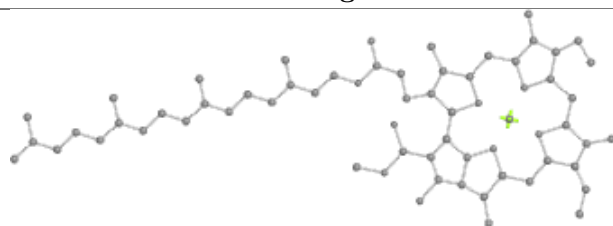
Bond lengths



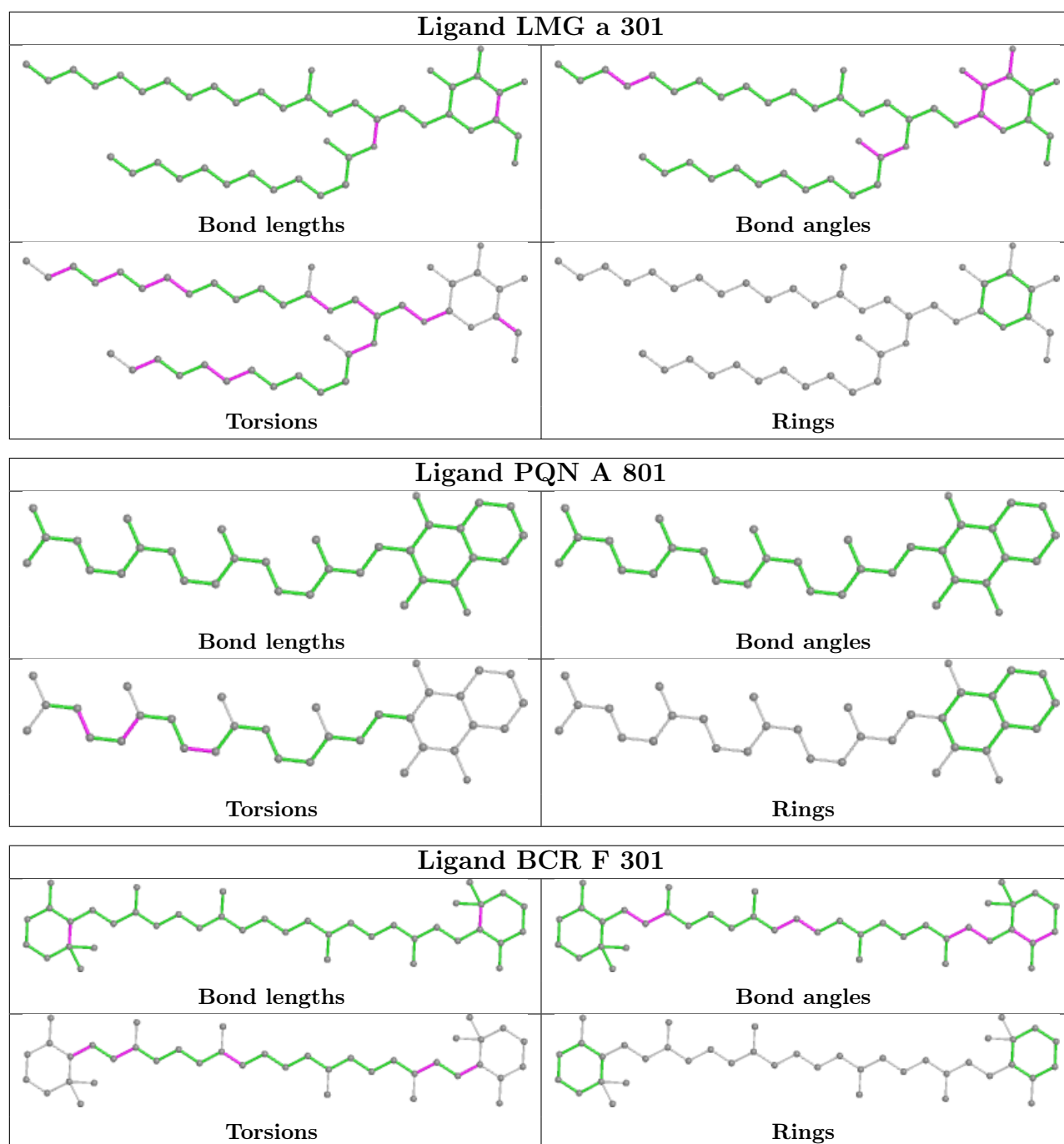
Bond angles



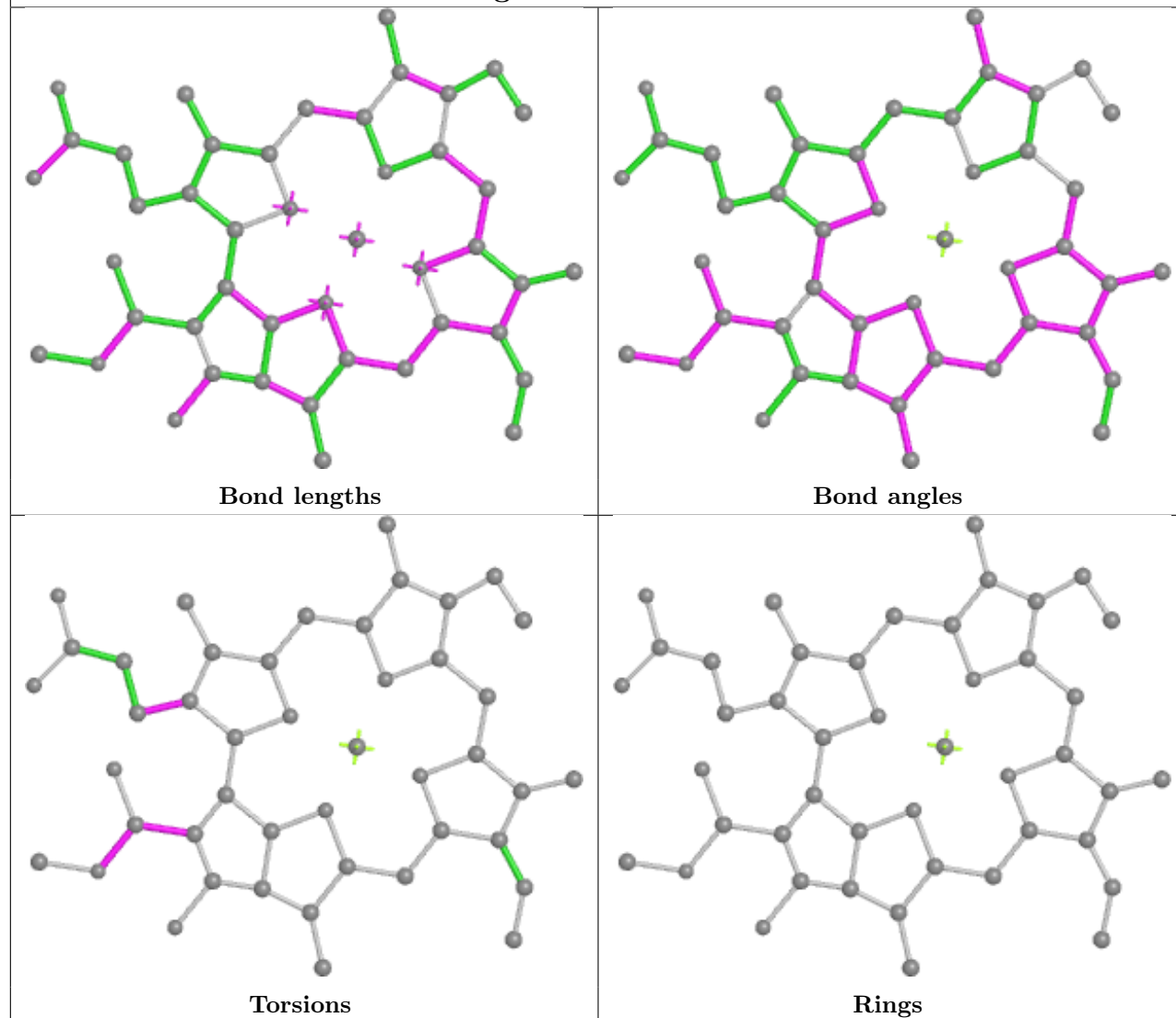
Torsions



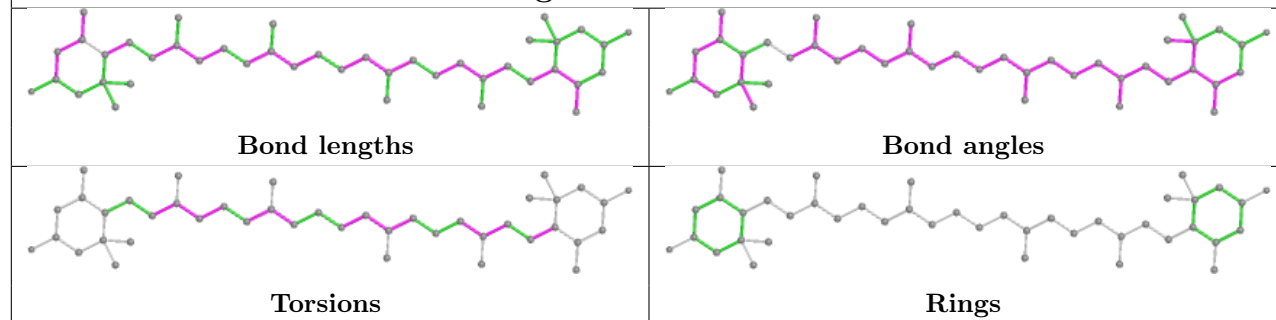
Rings

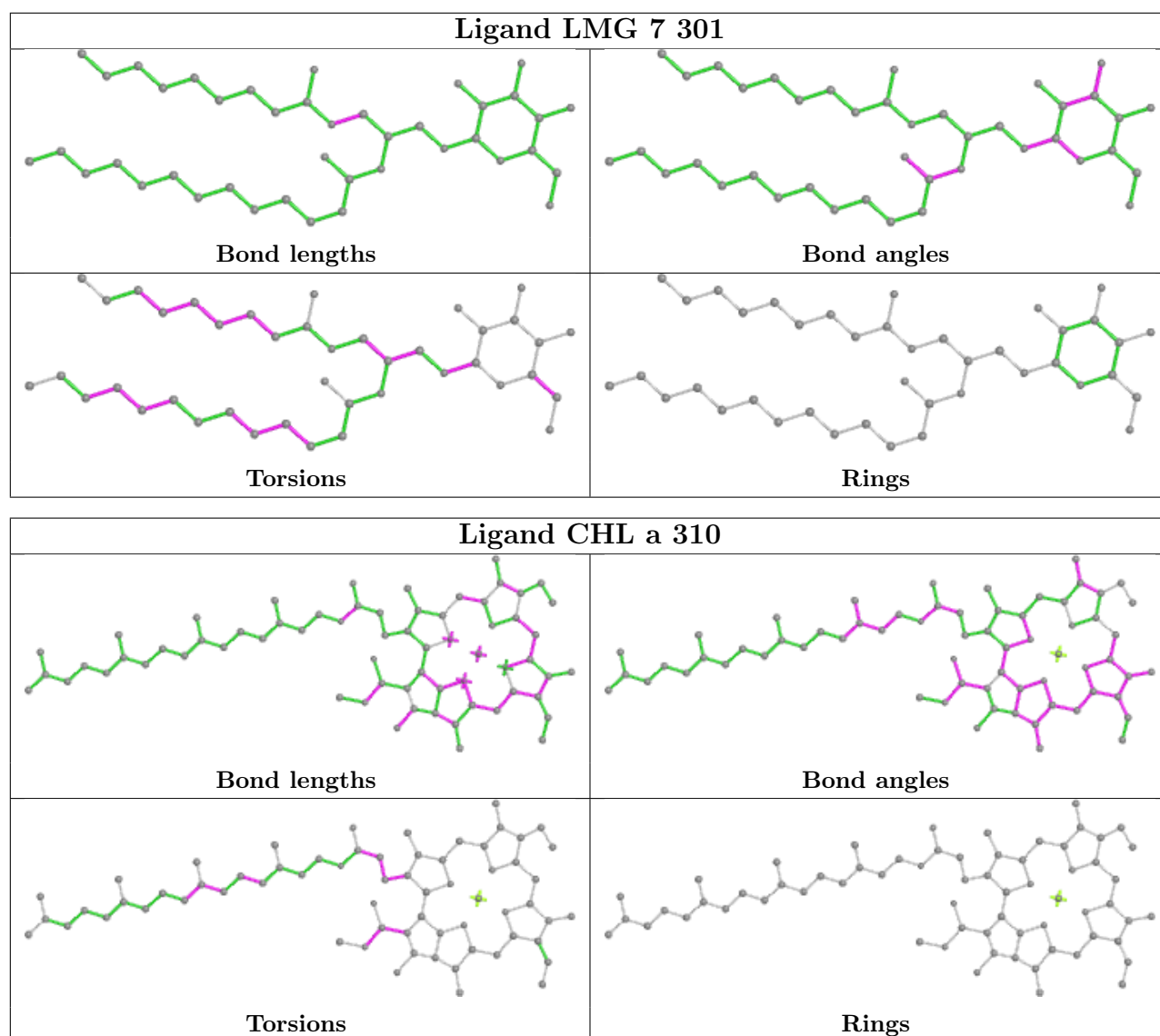


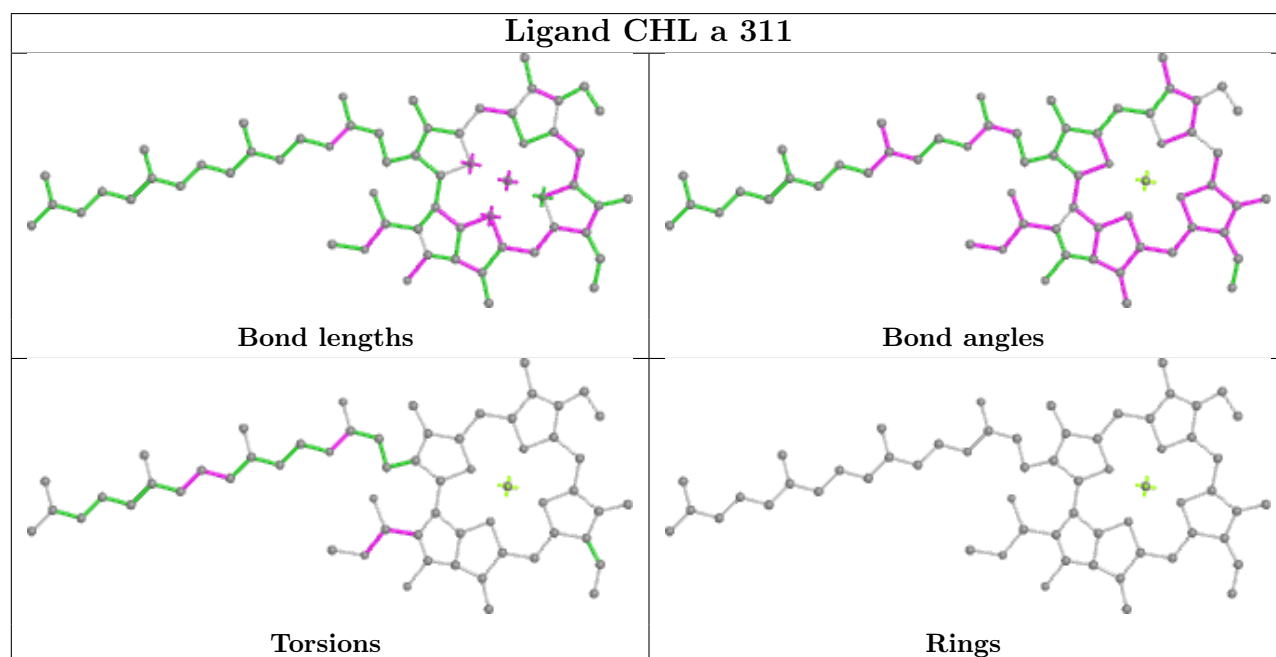
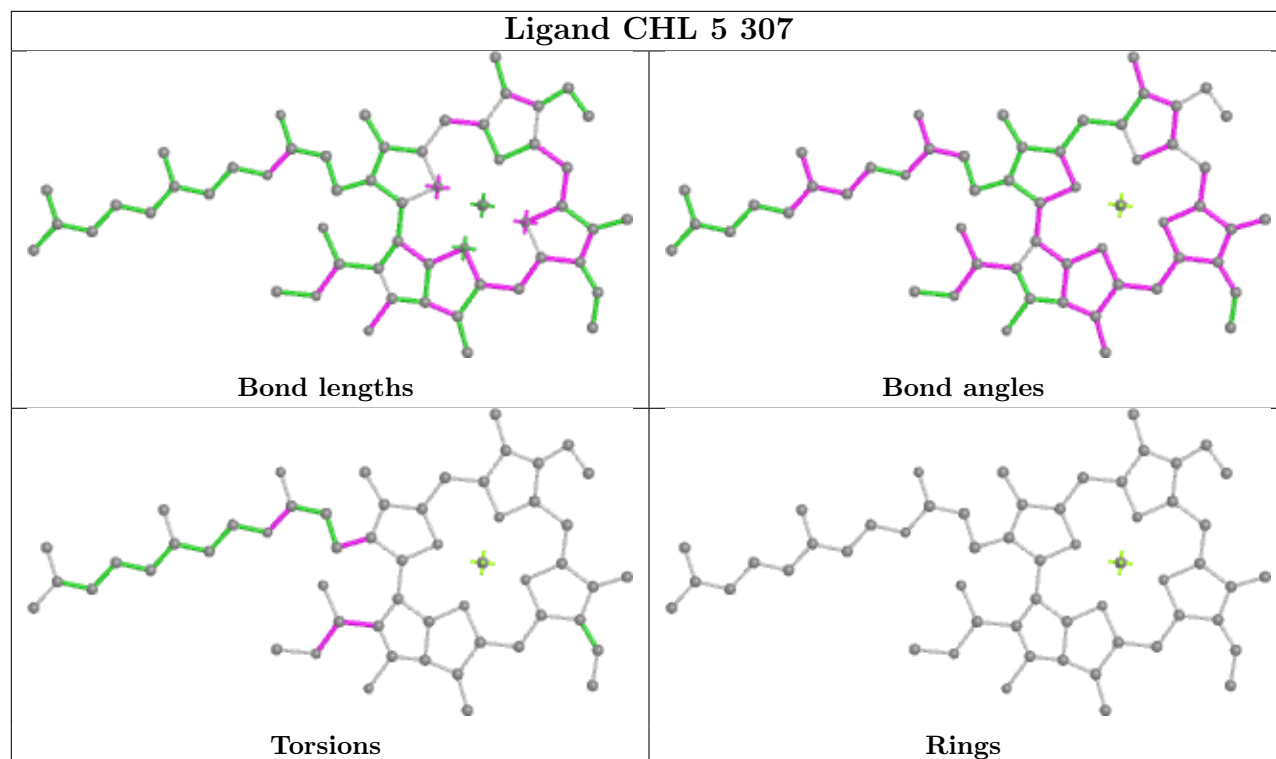
Ligand CHL a 308



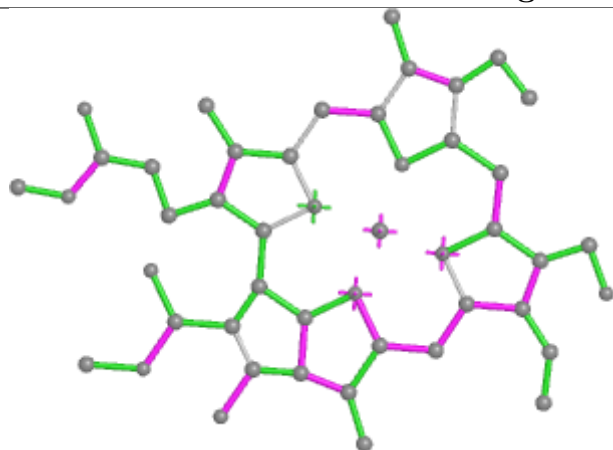
Ligand LUT b 301



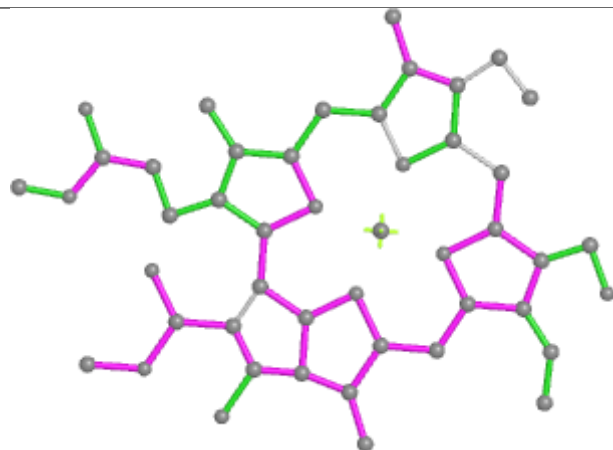




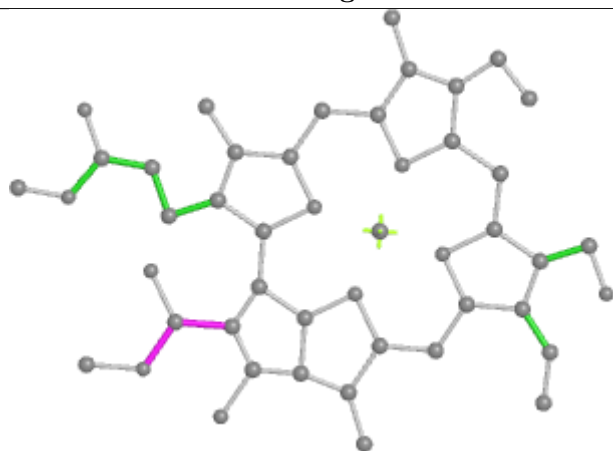
Ligand CHL 5 322



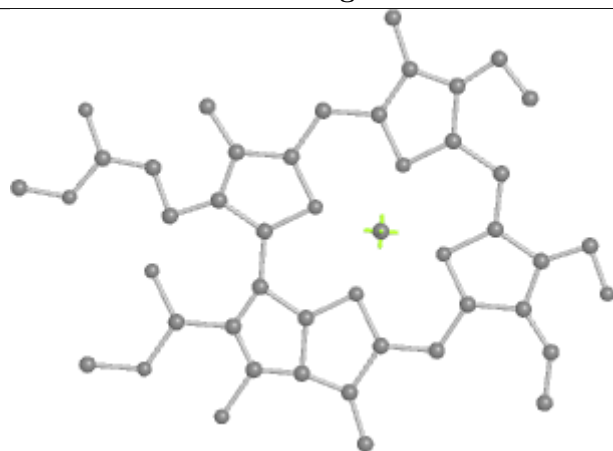
Bond lengths



Bond angles

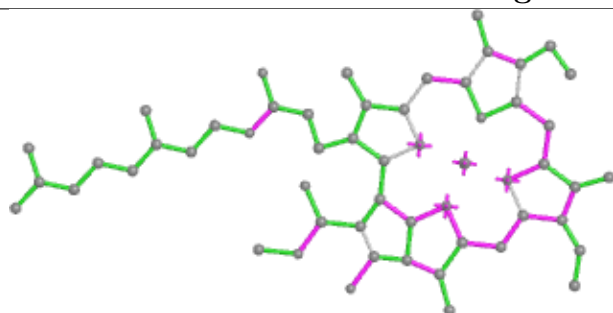


Torsions

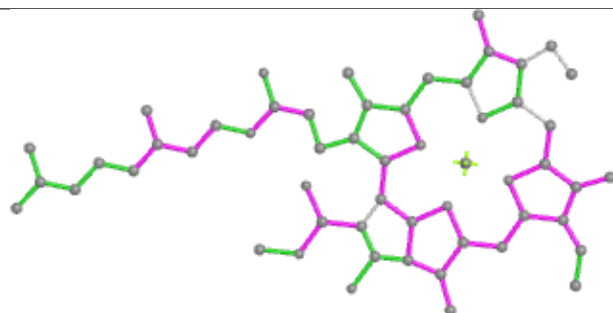


Rings

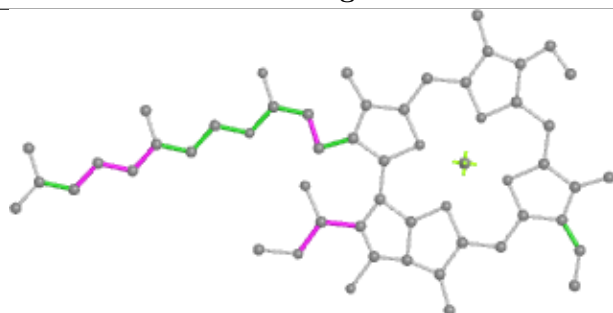
Ligand CHL B 823



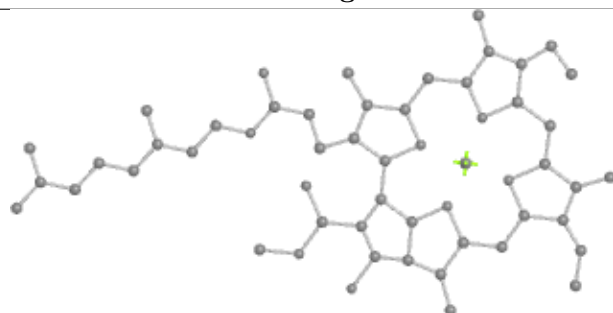
Bond lengths



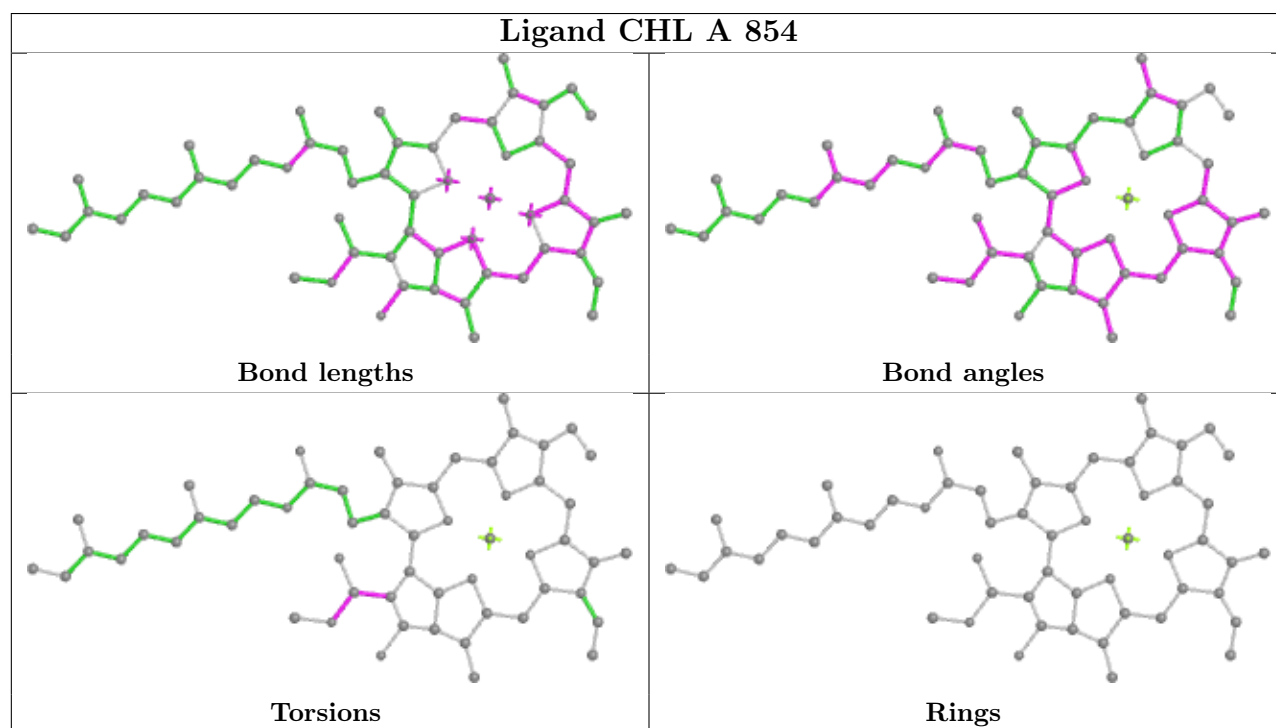
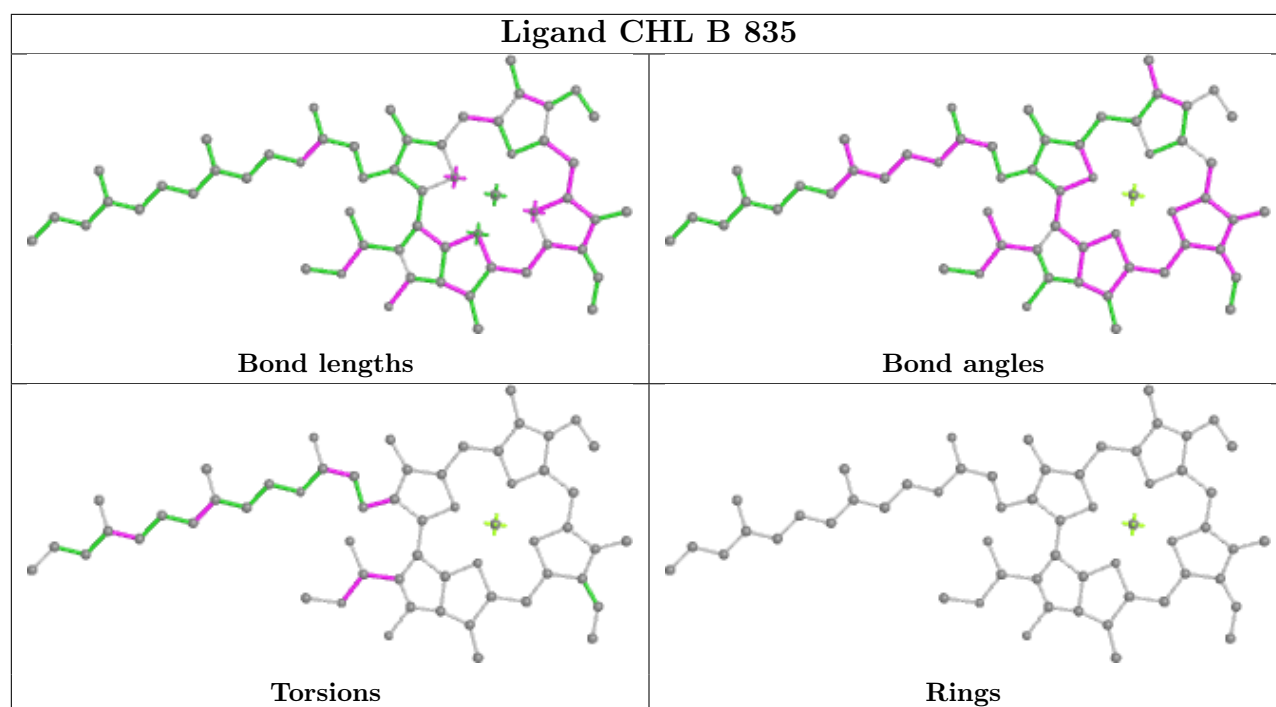
Bond angles

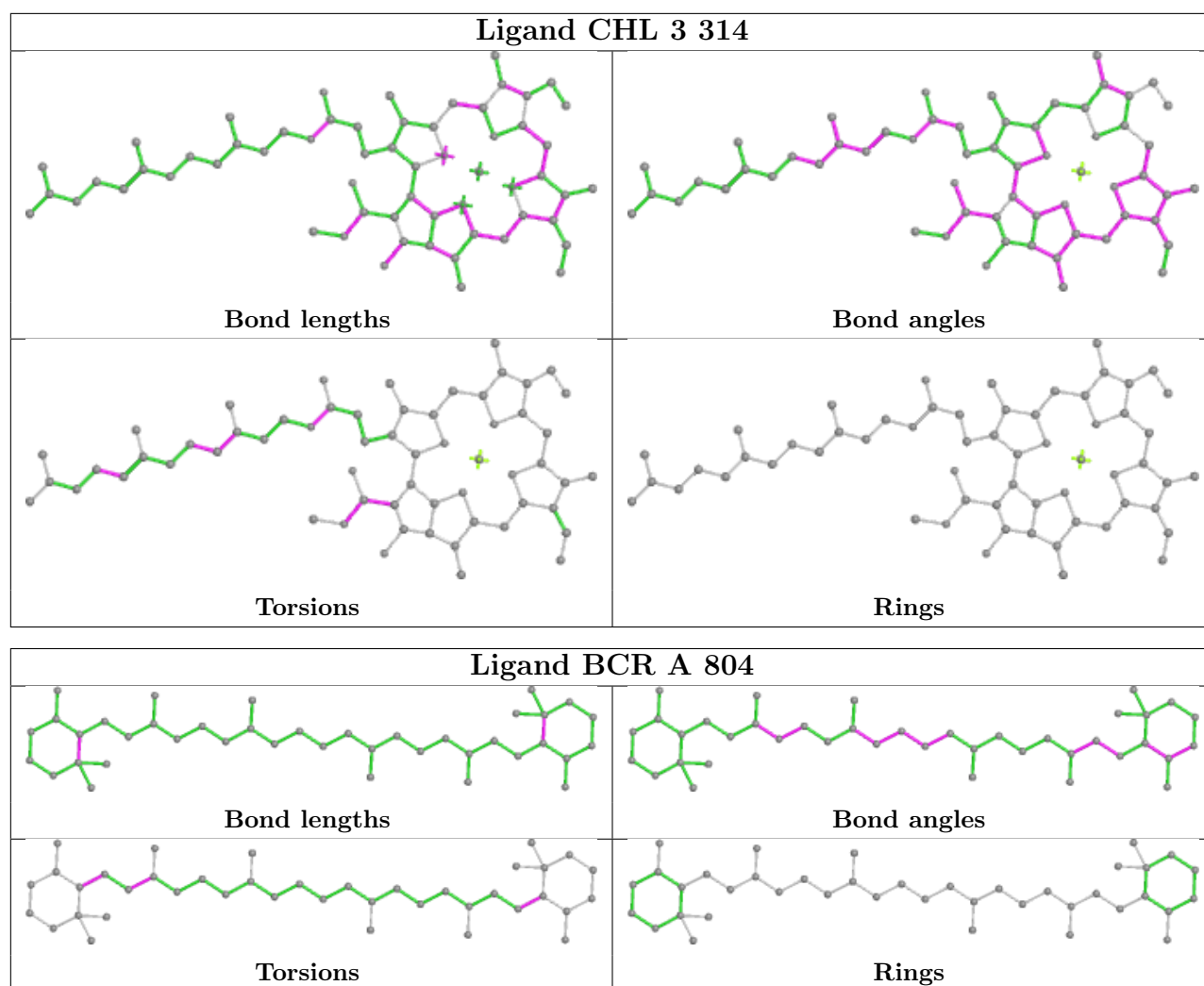


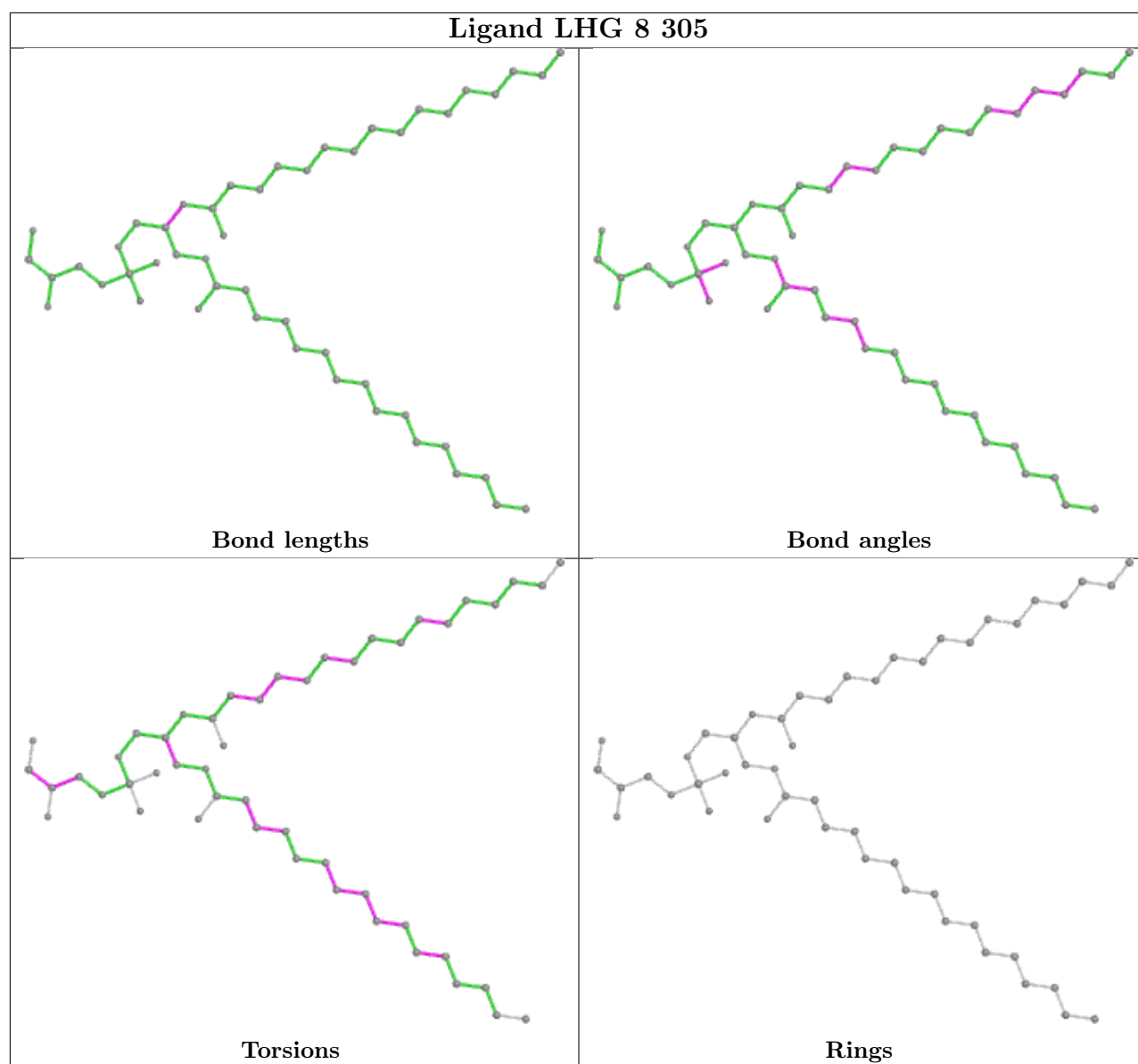
Torsions

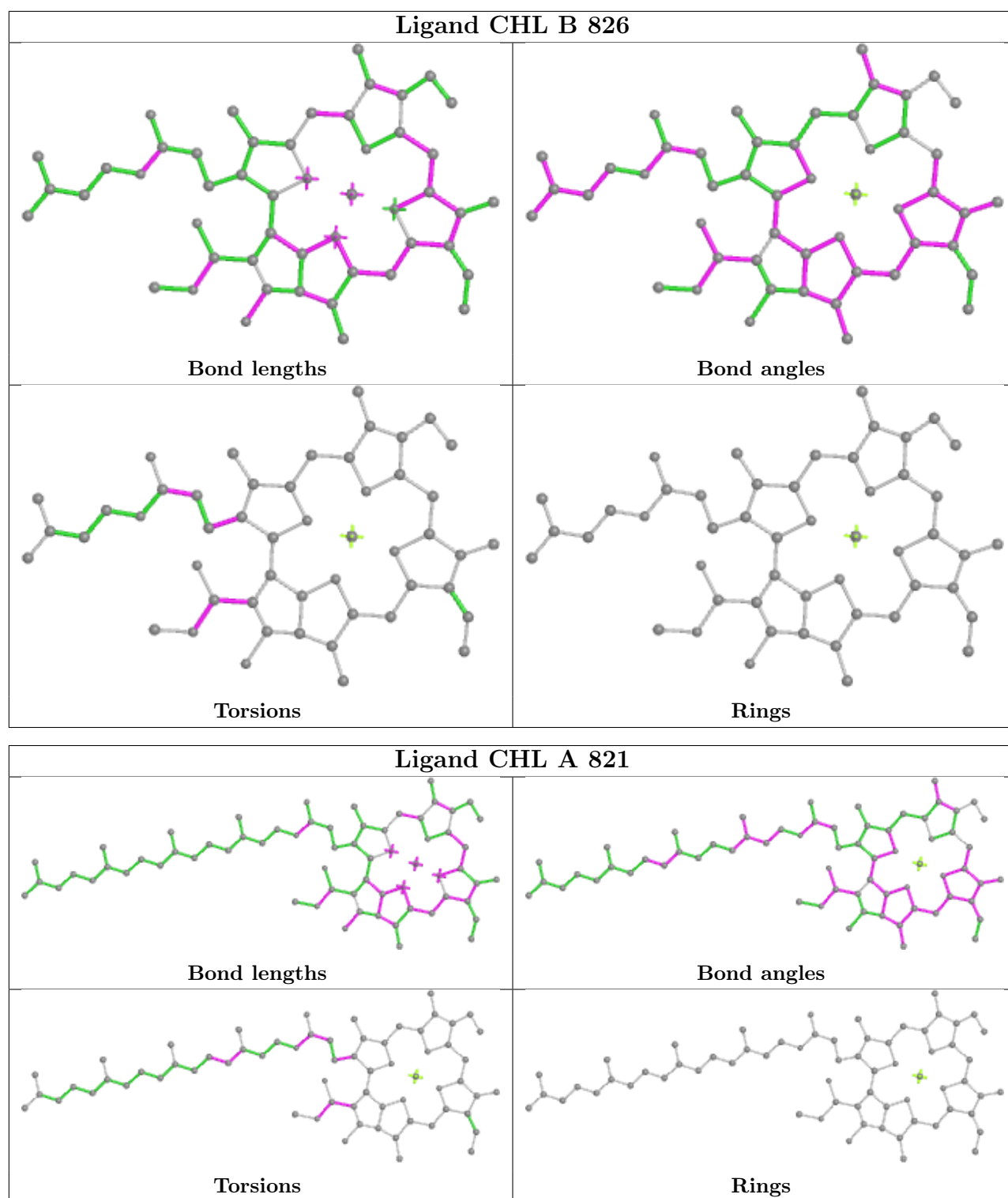


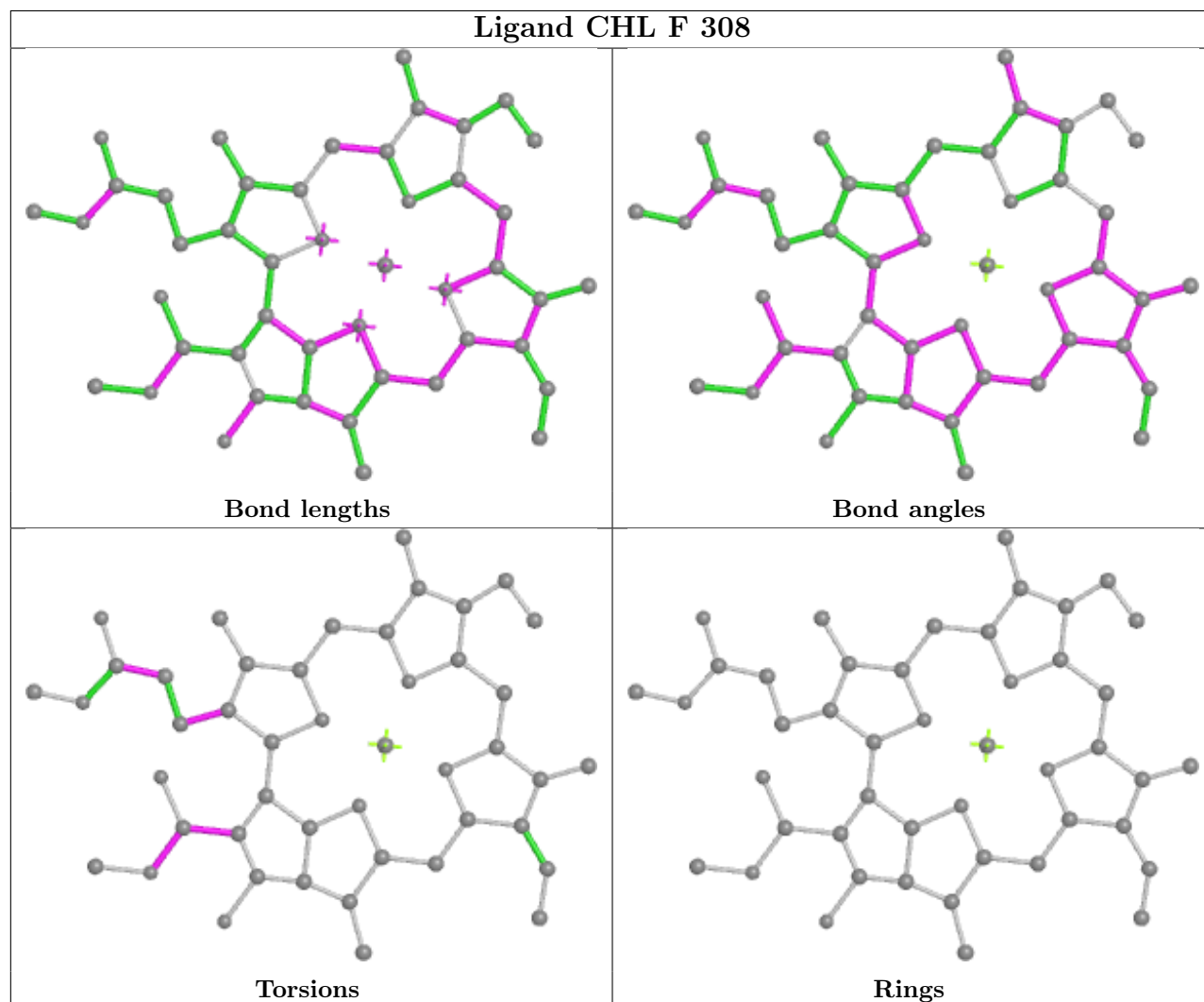
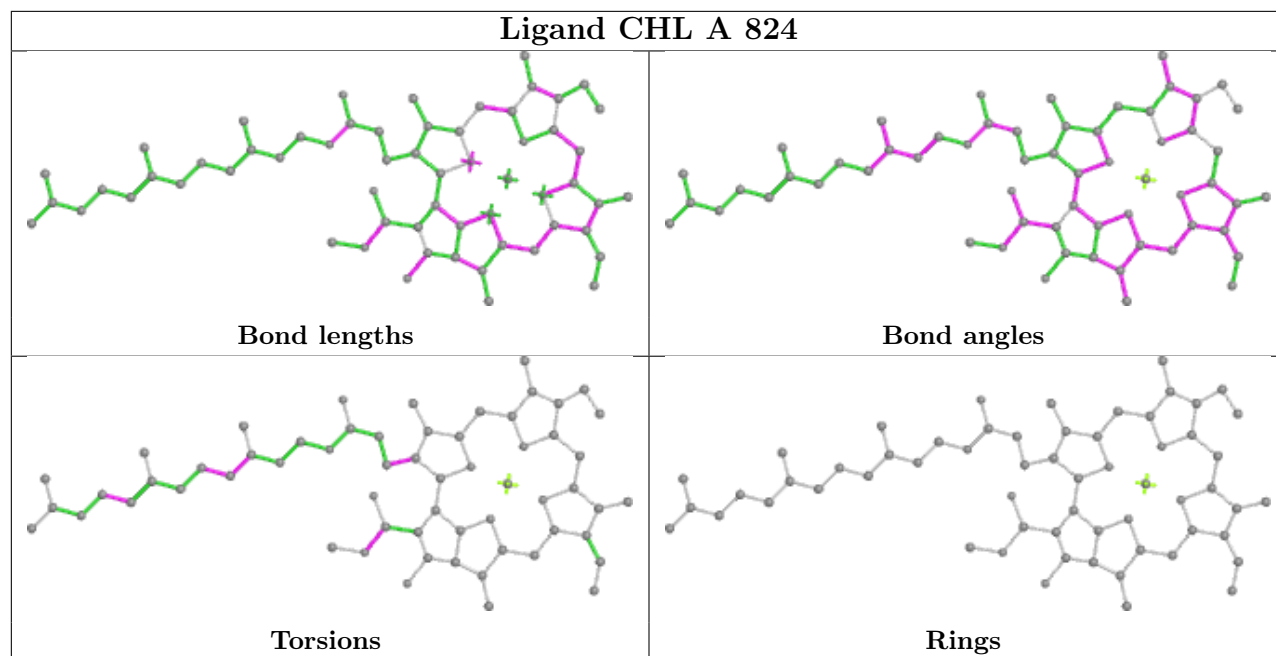
Rings

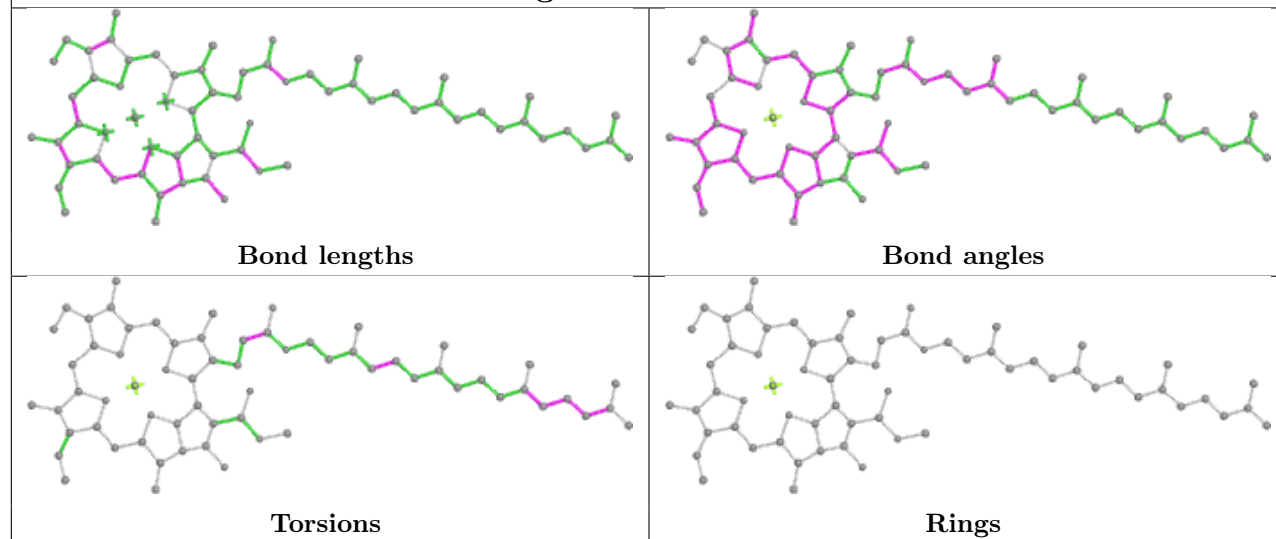
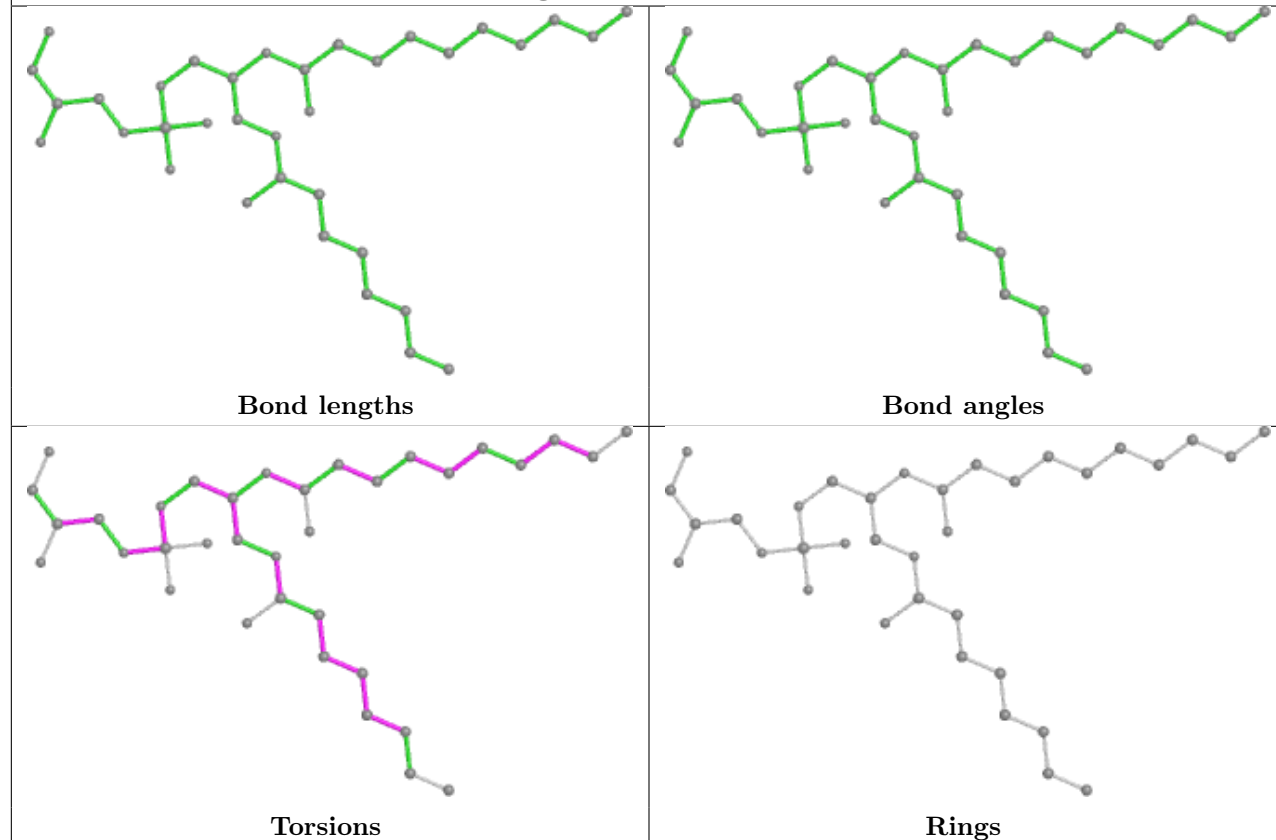


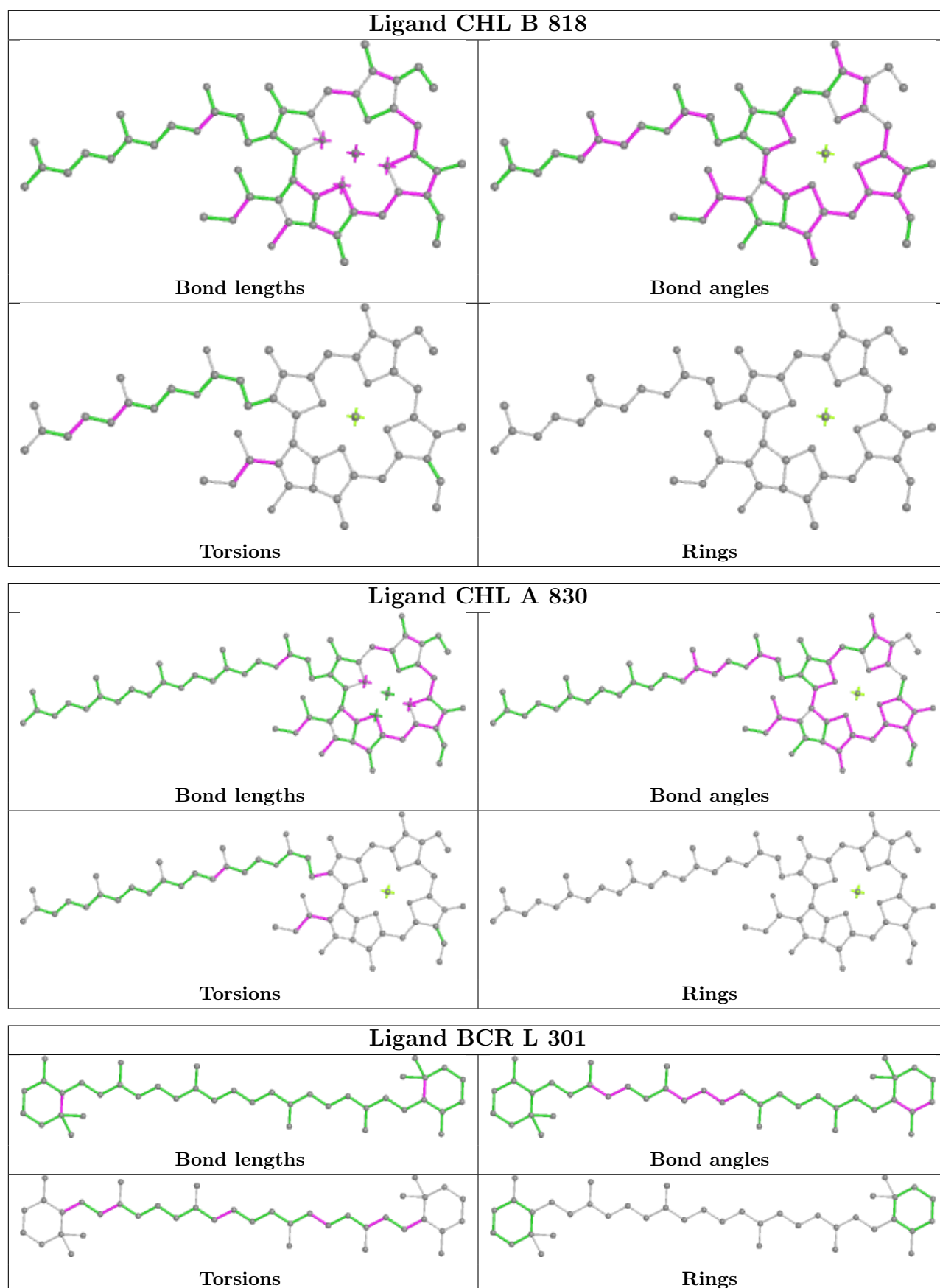


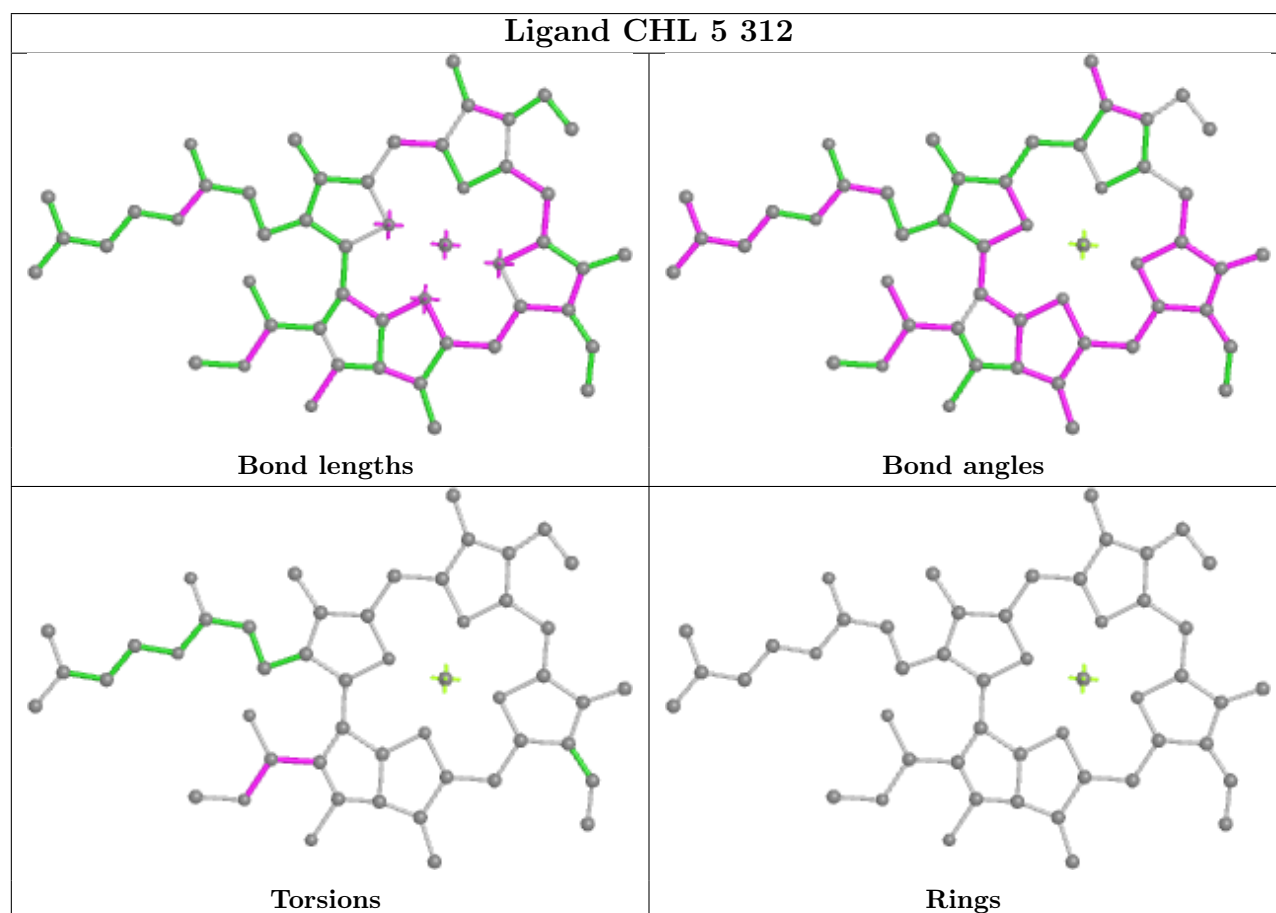
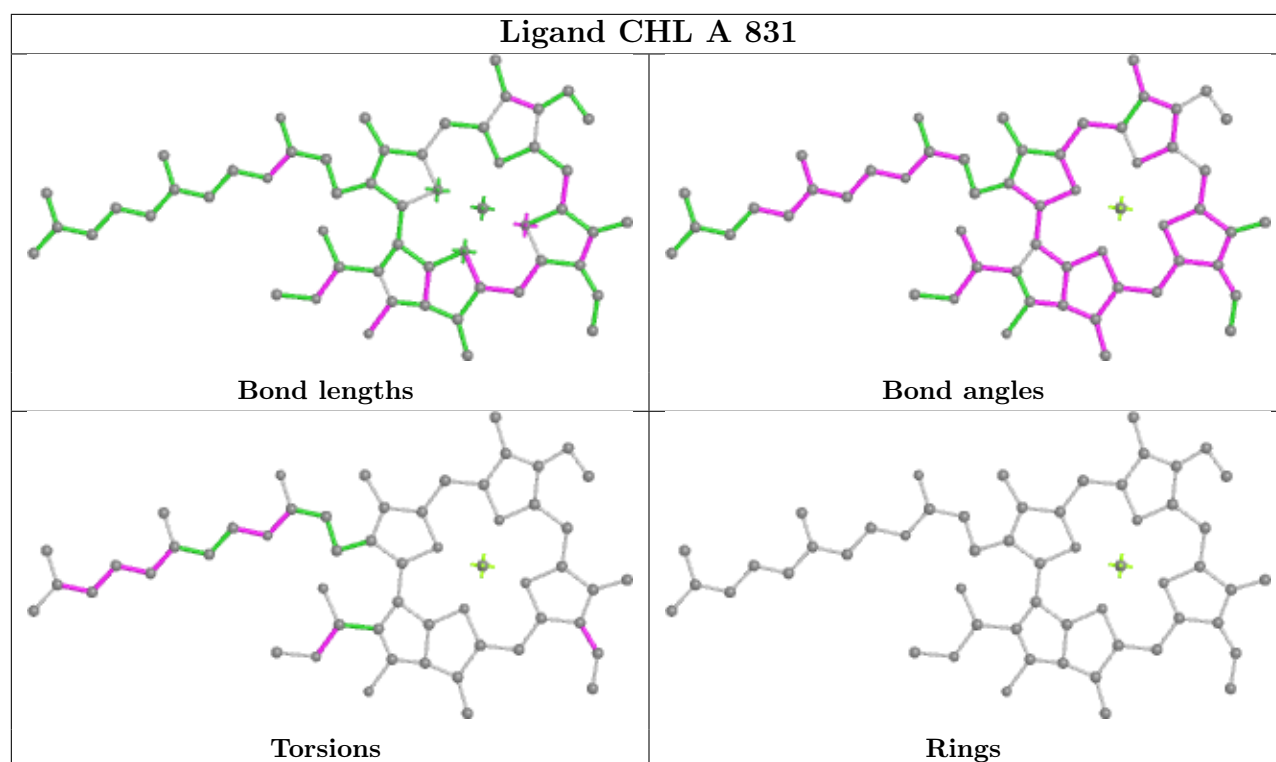




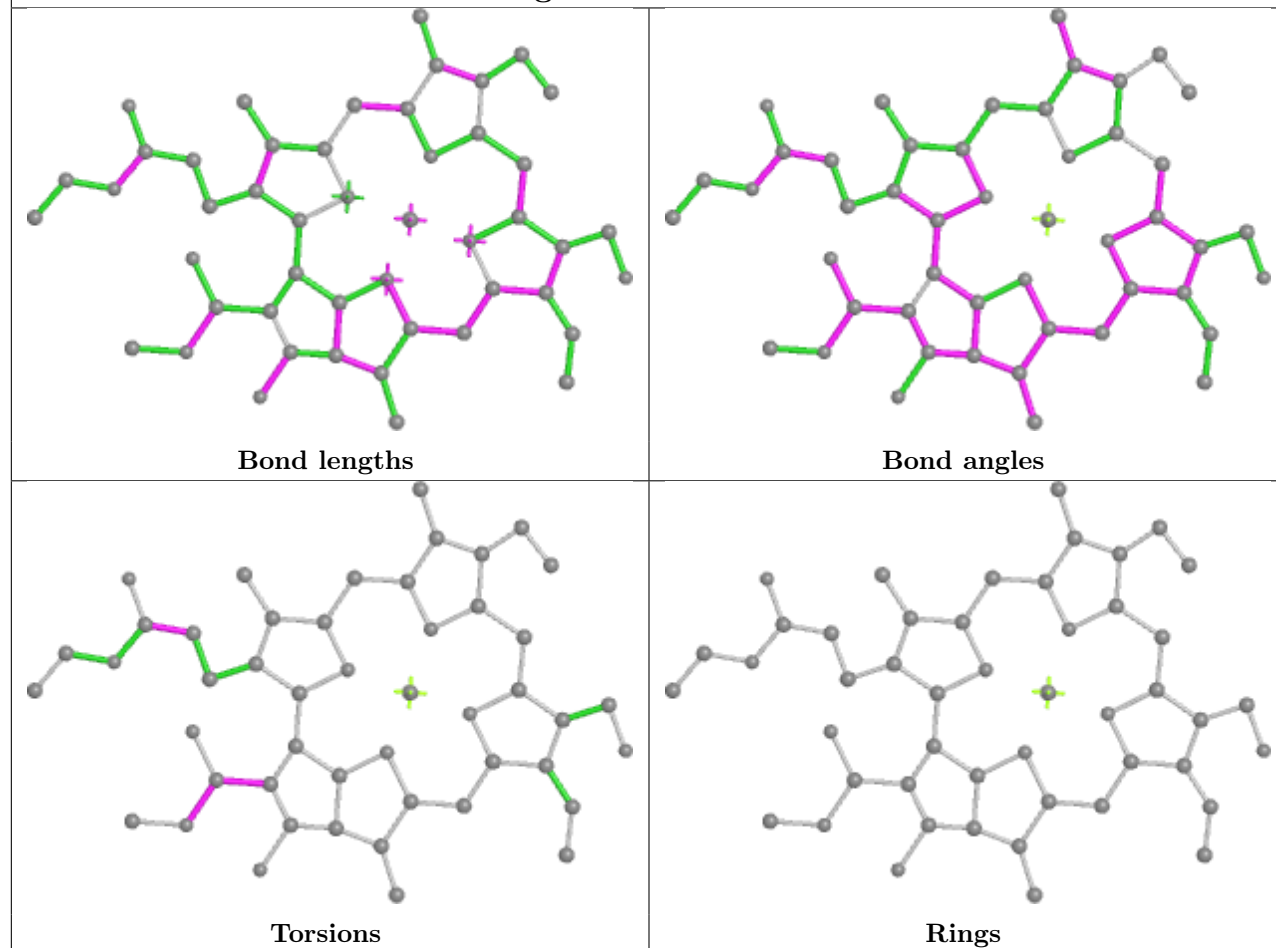


Ligand CL0 A 815**Ligand LHG 5 304**

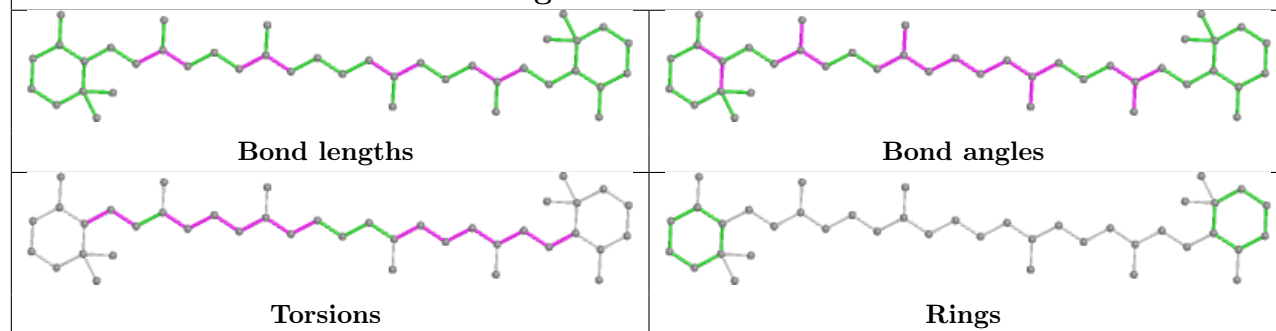




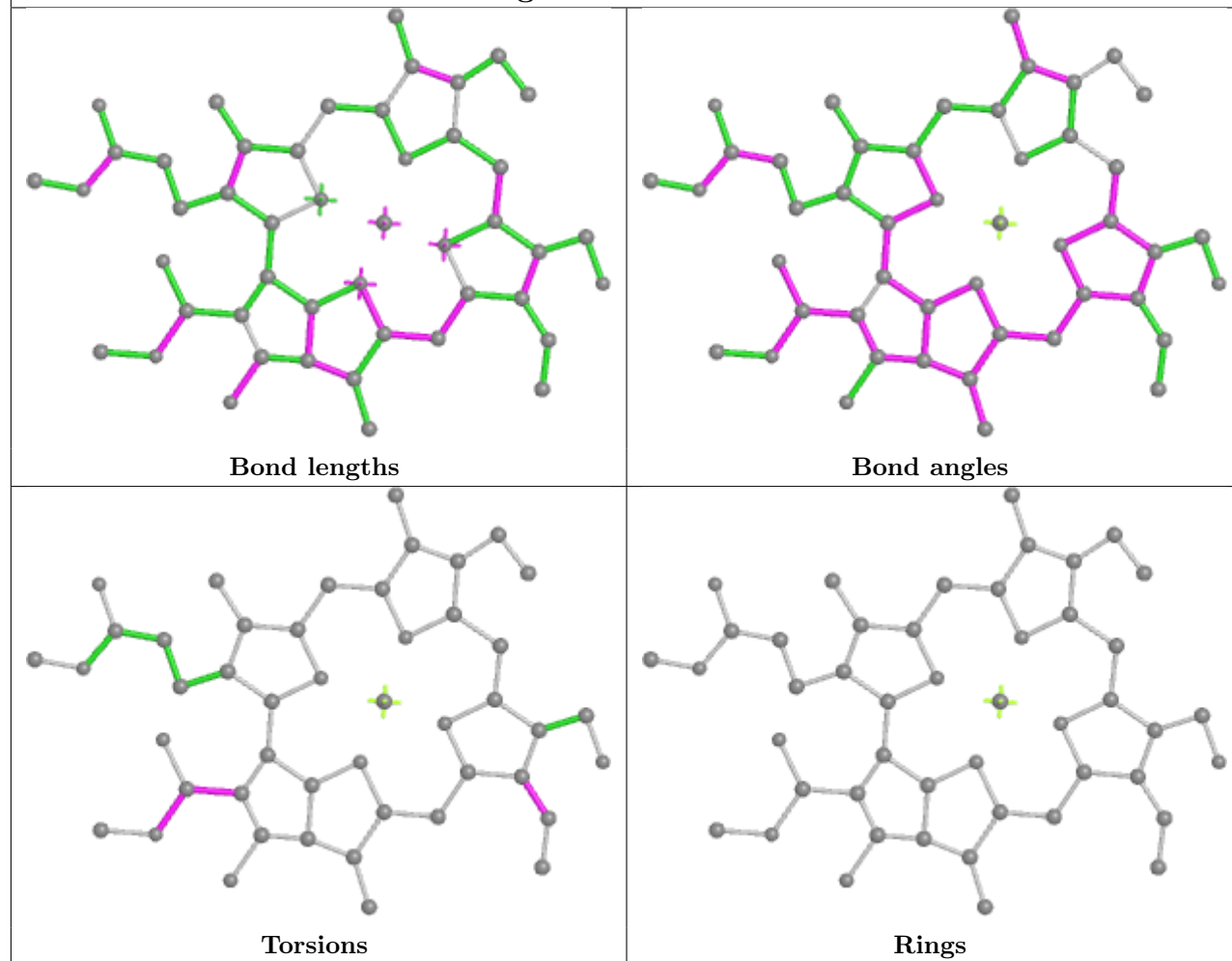
Ligand CHL b 317



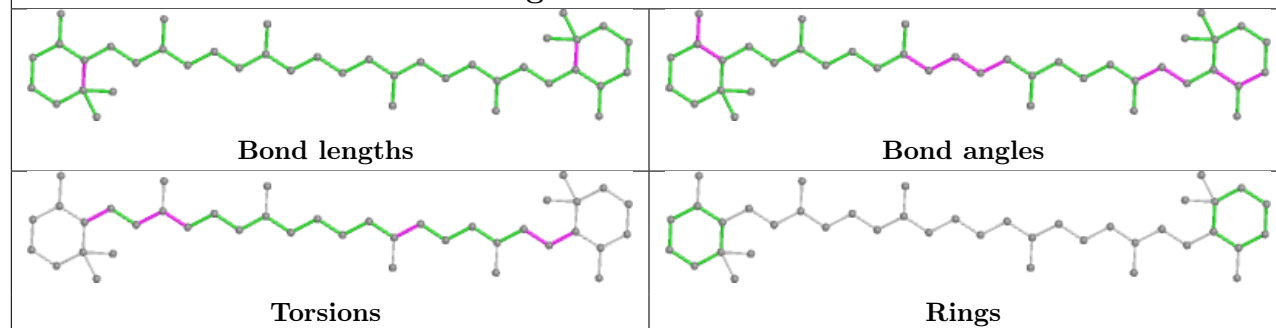
Ligand BCR 6 301



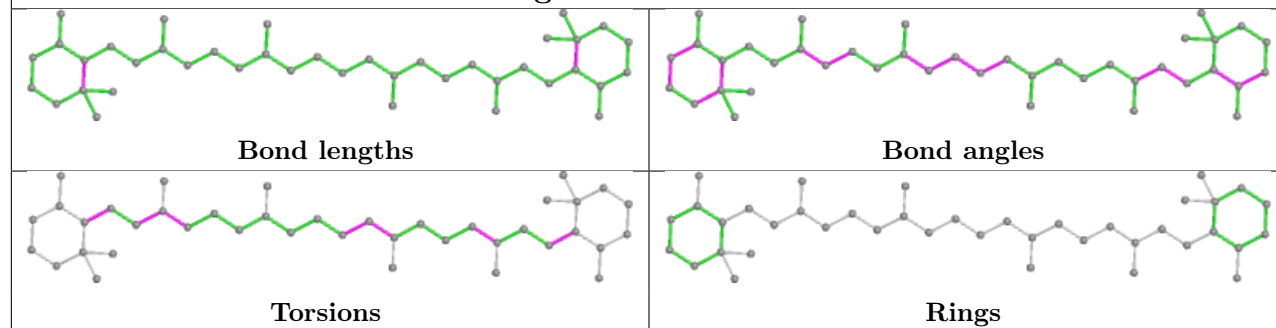
Ligand CHL 5 317



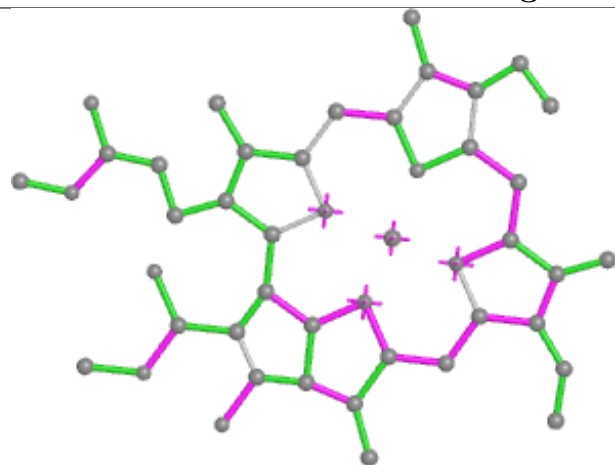
Ligand BCR M 102



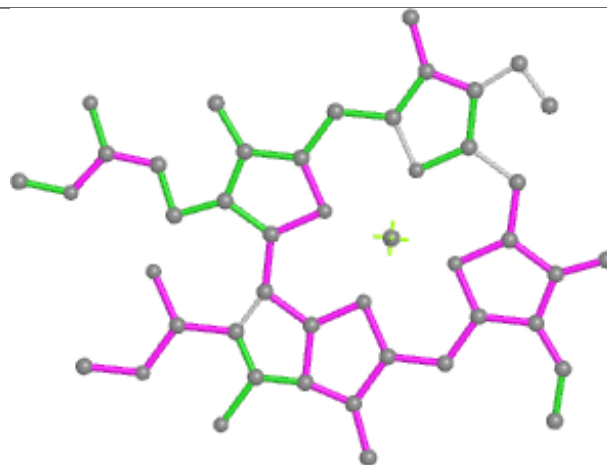
Ligand BCR 3 303



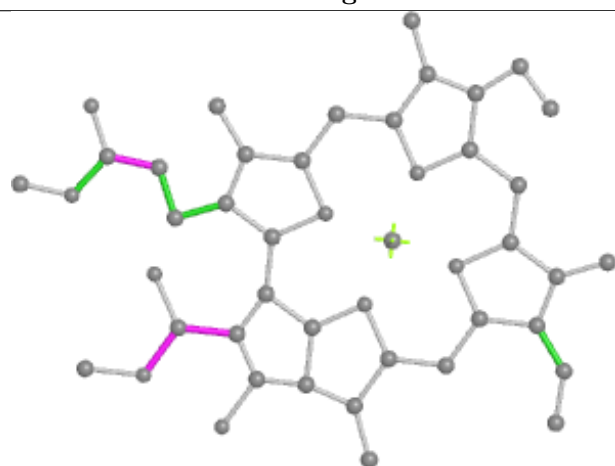
Ligand CHL a 320



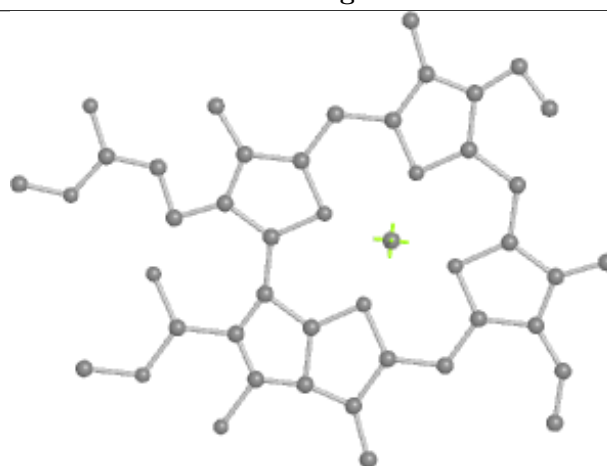
Bond lengths



Bond angles

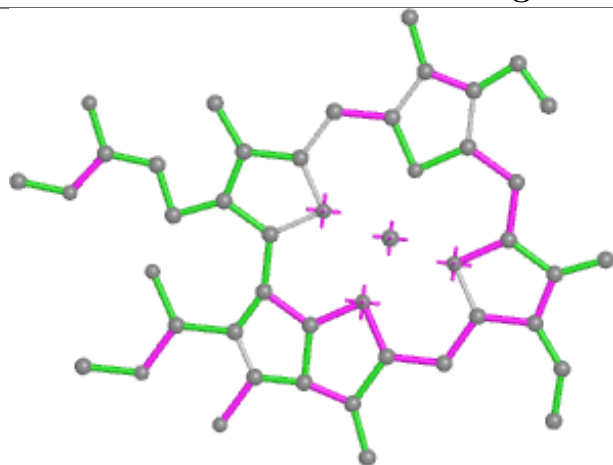


Torsions

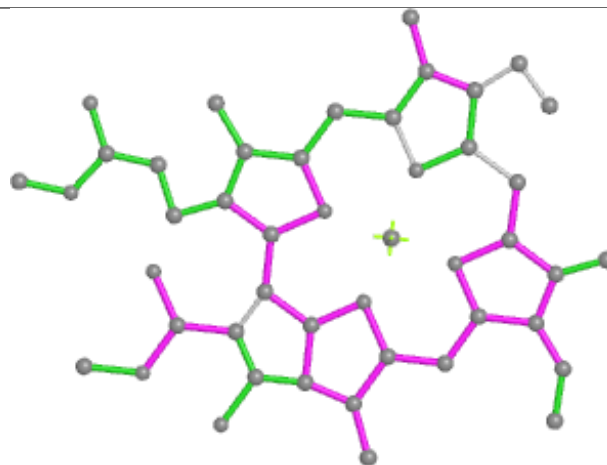


Rings

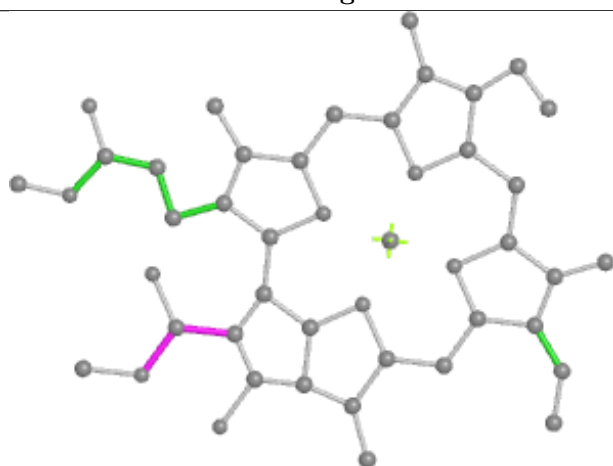
Ligand CHL K 205



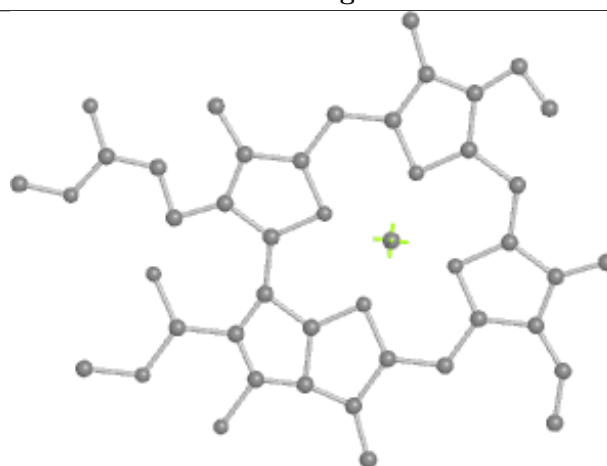
Bond lengths



Bond angles

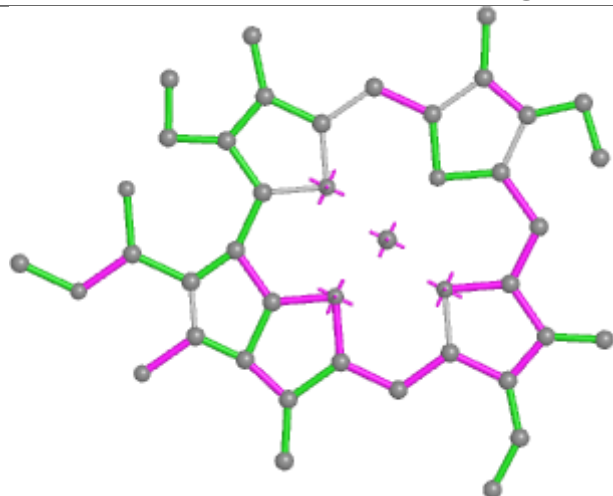


Torsions

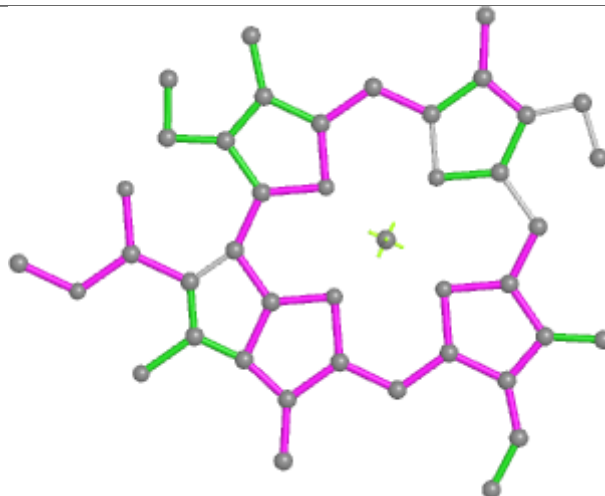


Rings

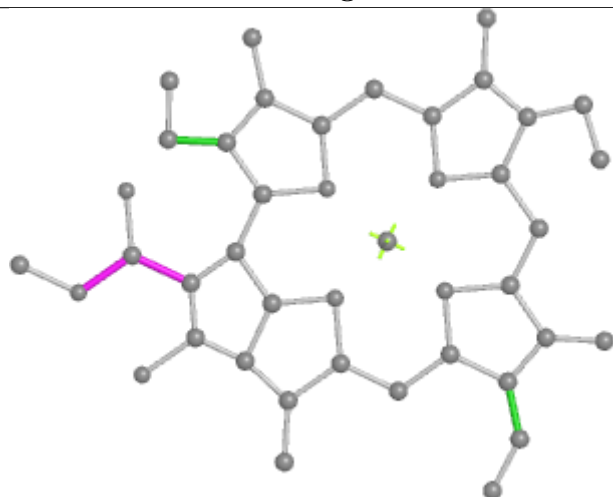
Ligand CHL 4 318



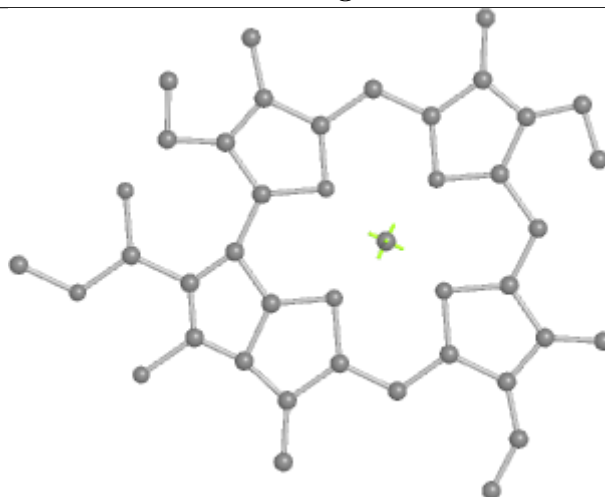
Bond lengths



Bond angles

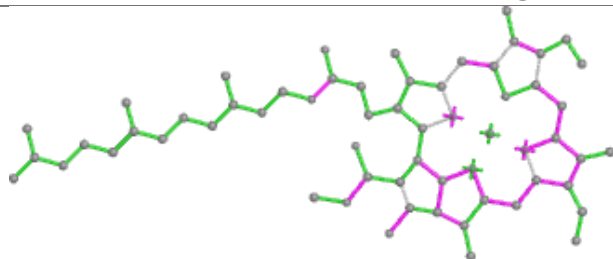


Torsions

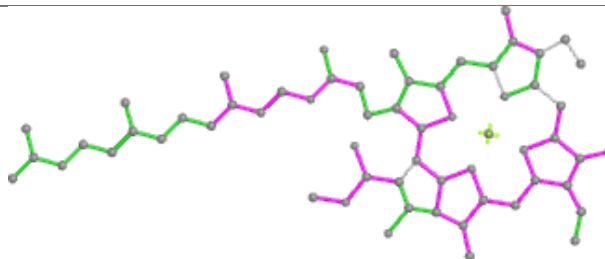


Rings

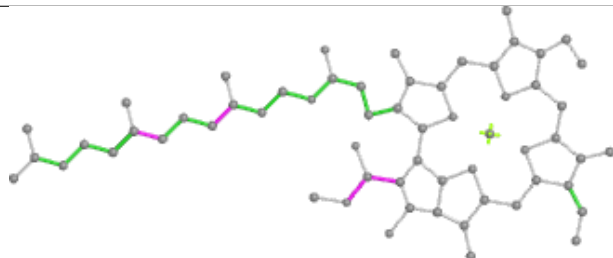
Ligand CHL B 825



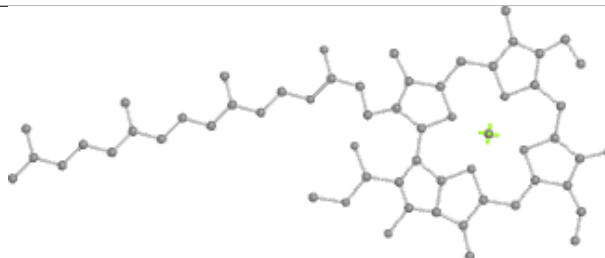
Bond lengths



Bond angles

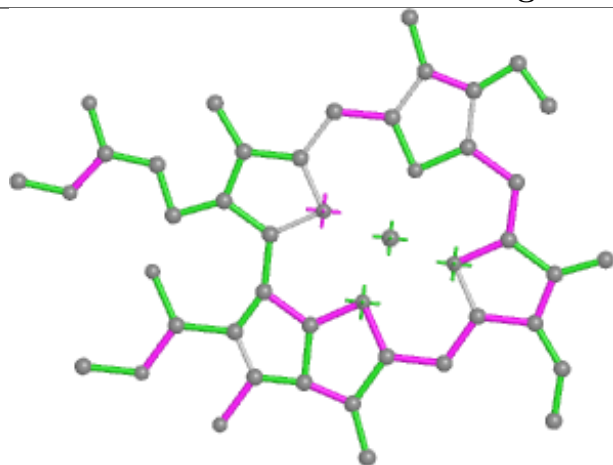


Torsions

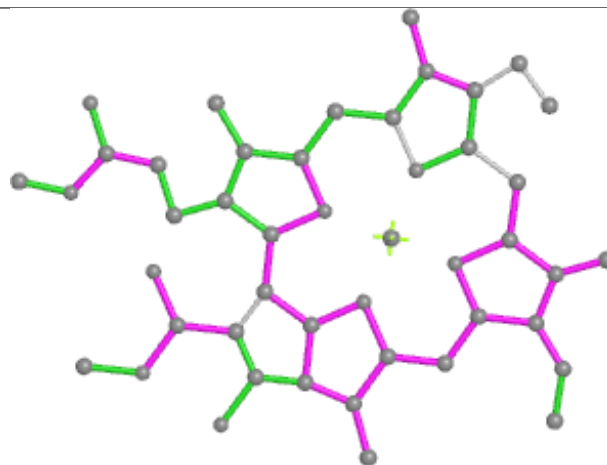


Rings

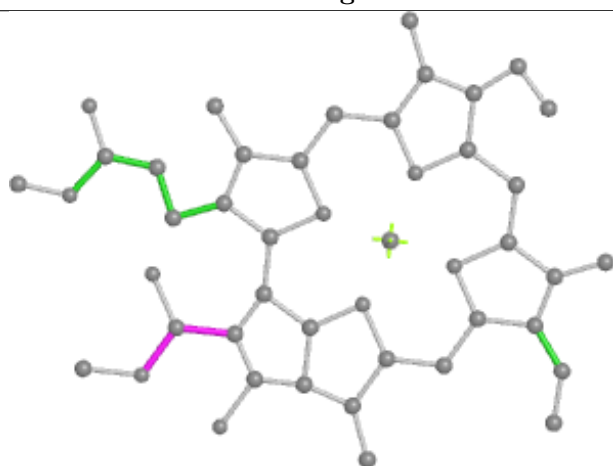
Ligand CHL 6 320



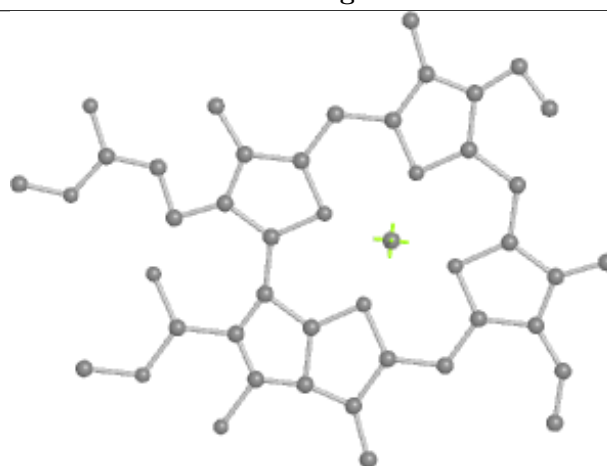
Bond lengths



Bond angles

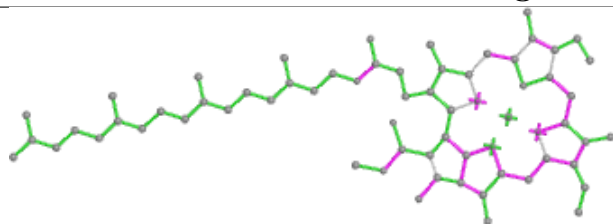


Torsions

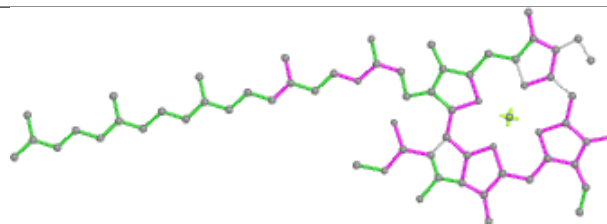


Rings

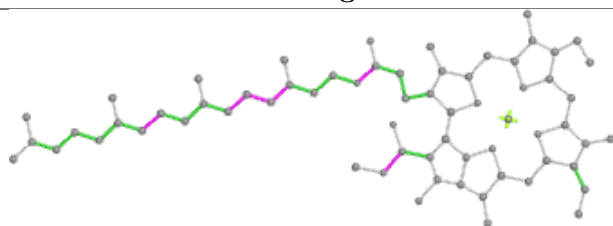
Ligand CHL B 837



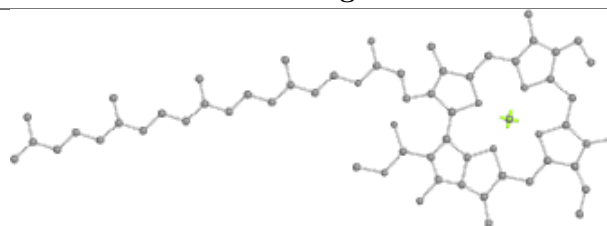
Bond lengths



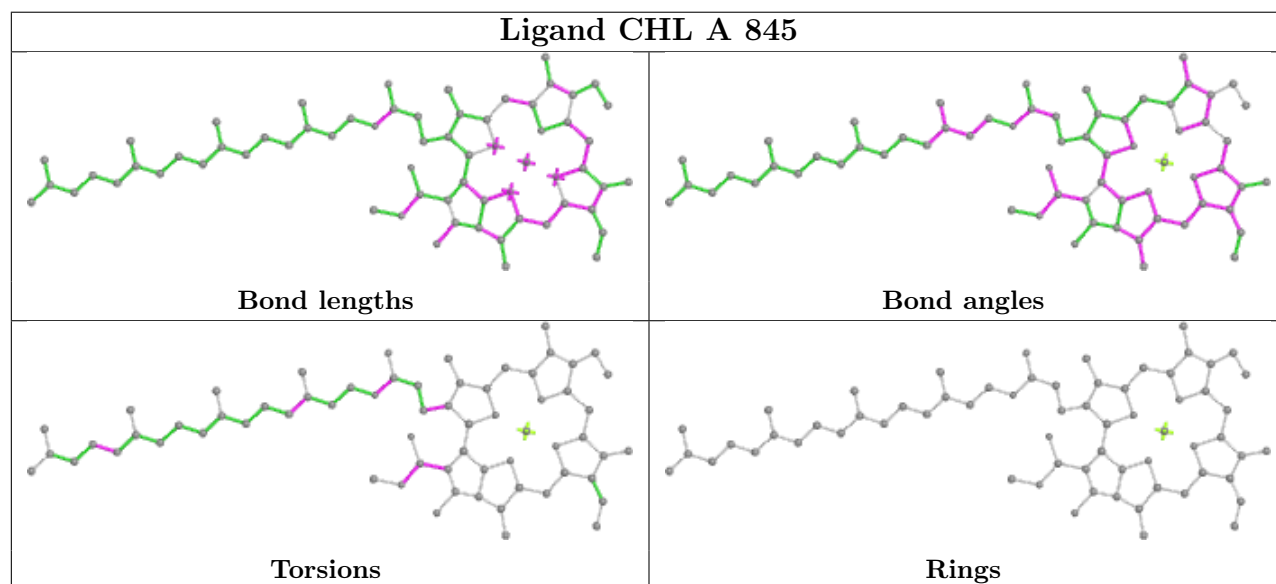
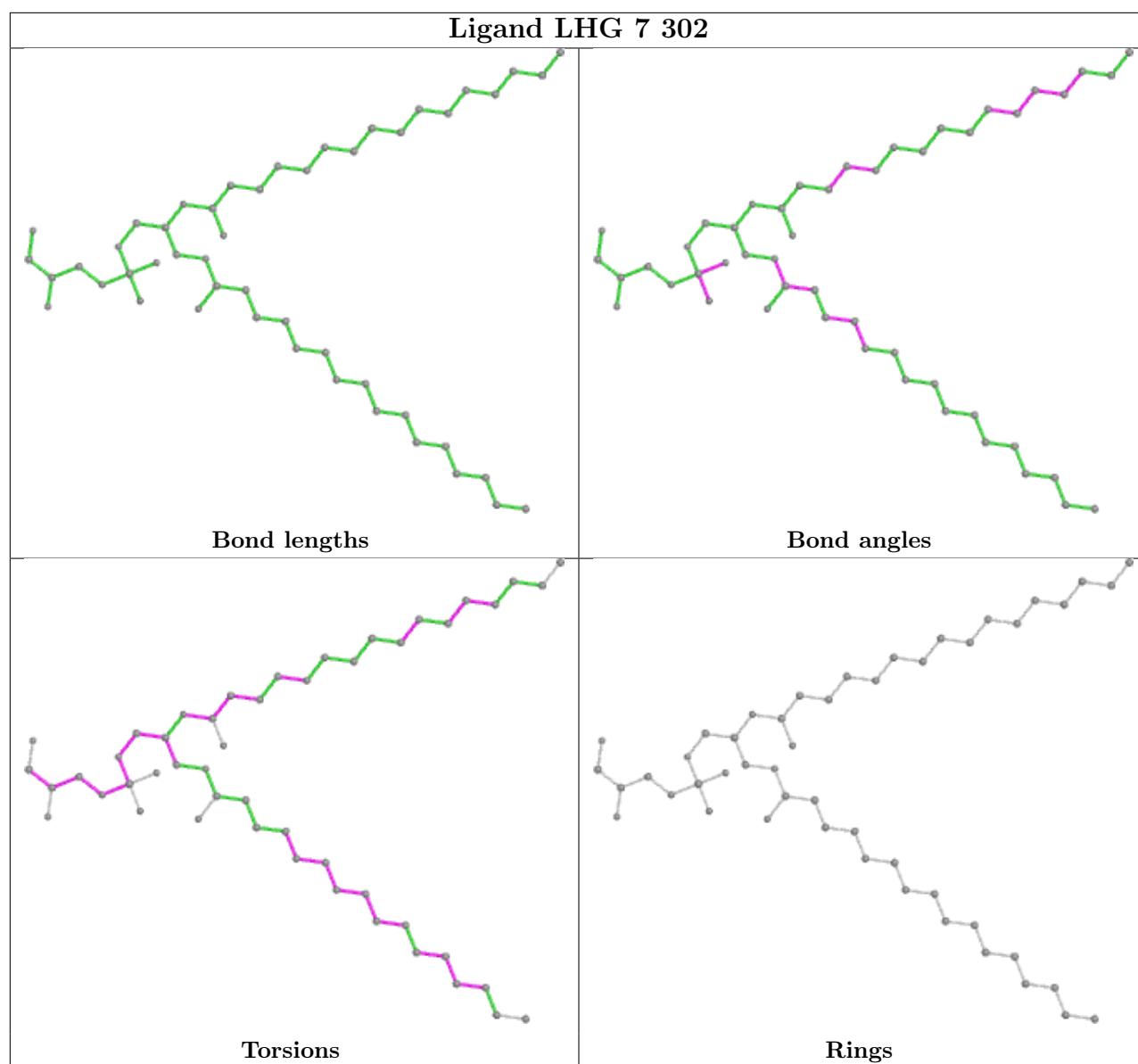
Bond angles

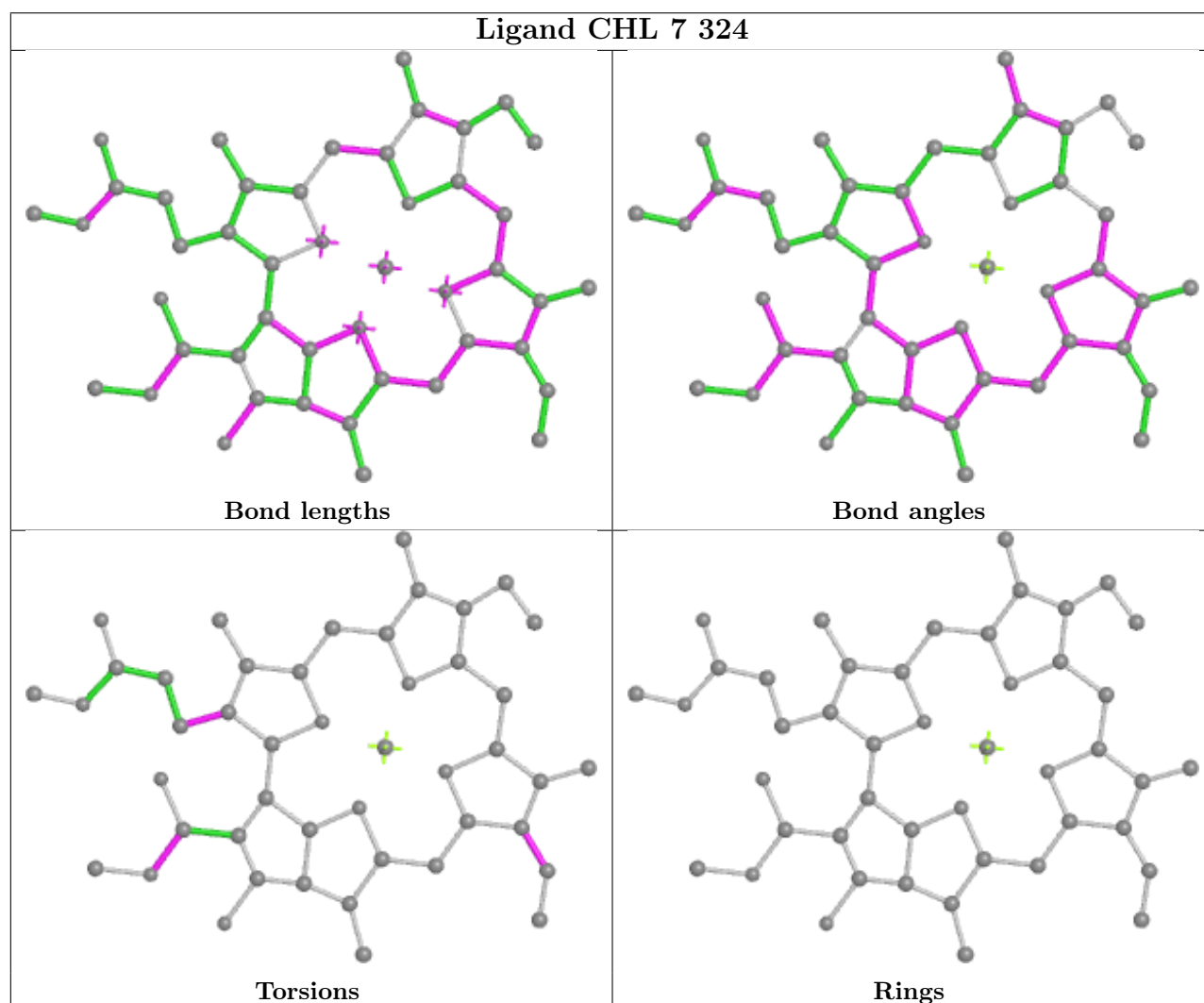
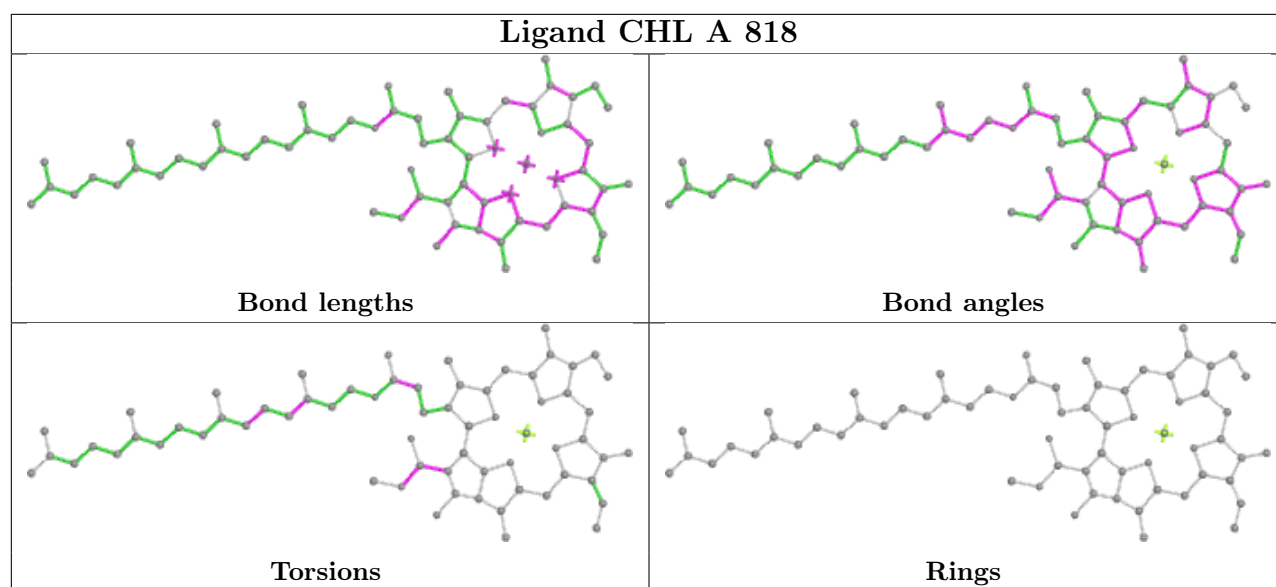


Torsions

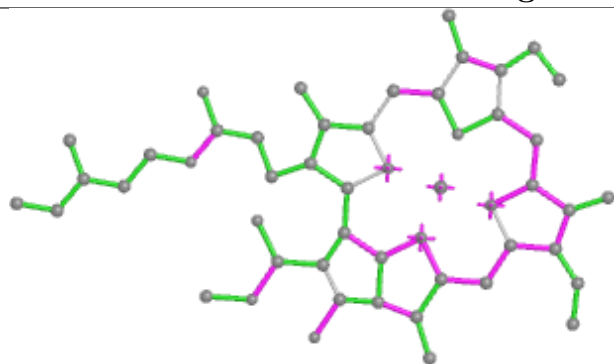


Rings

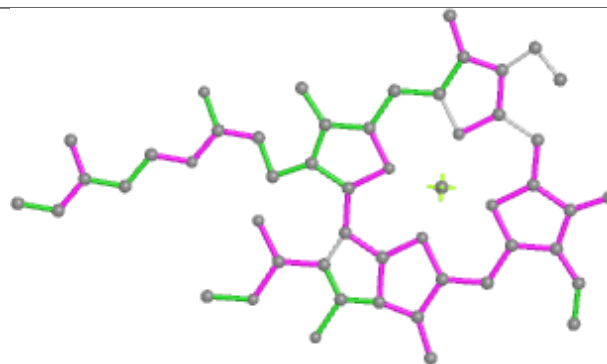




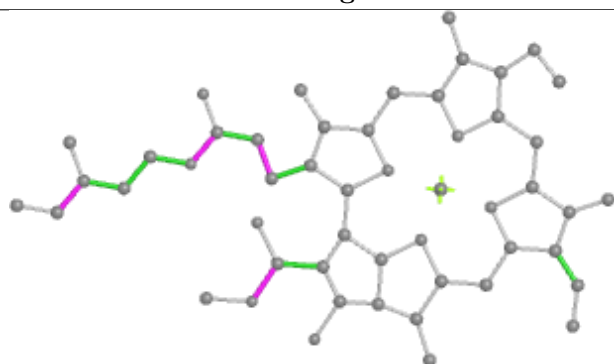
Ligand CHL 3 318



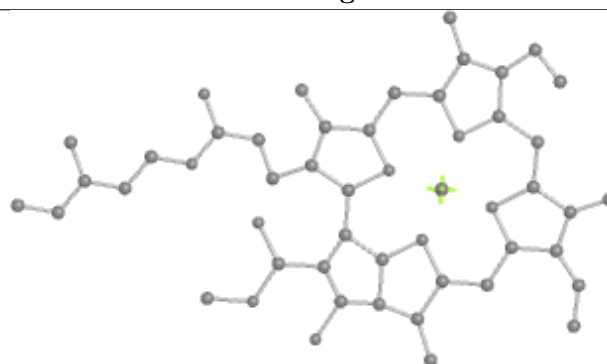
Bond lengths



Bond angles

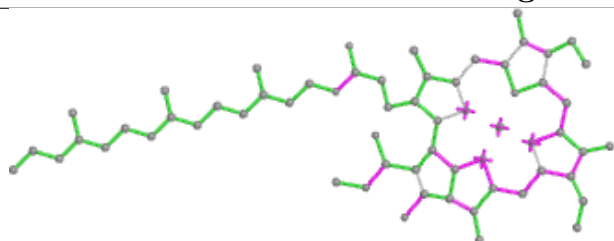


Torsions

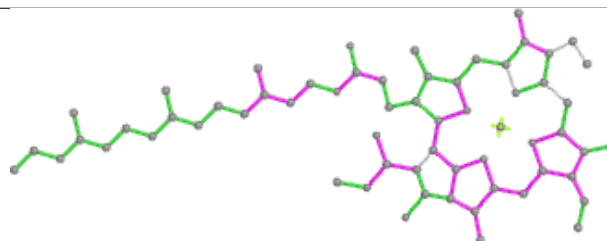


Rings

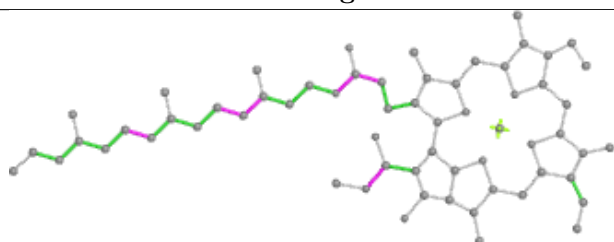
Ligand CHL 3 317



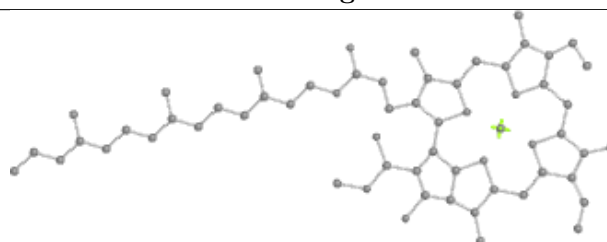
Bond lengths



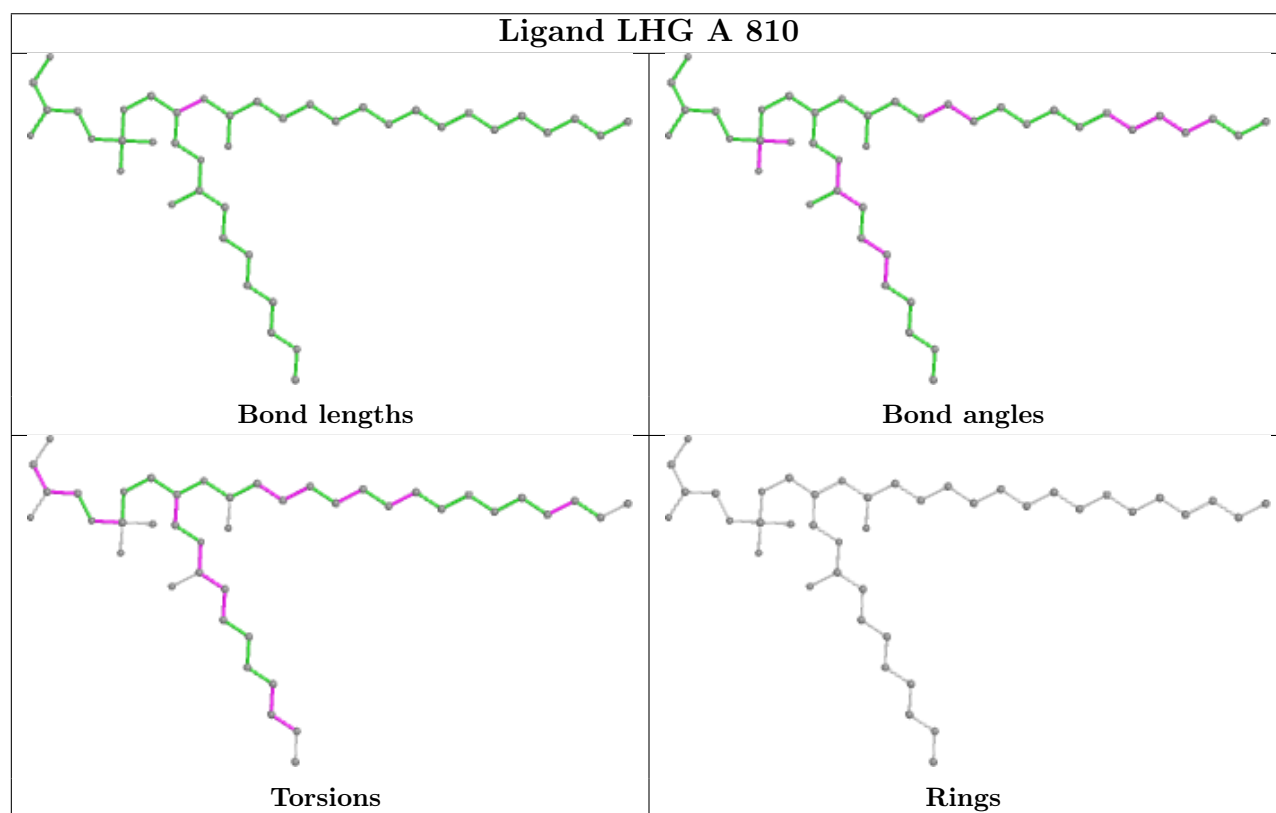
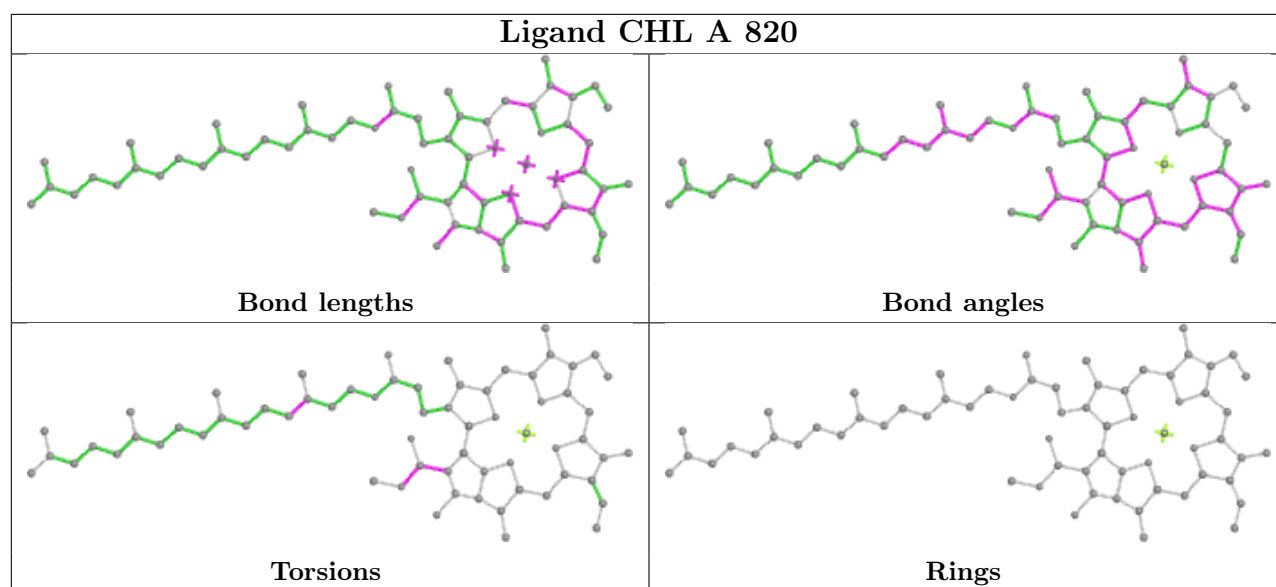
Bond angles

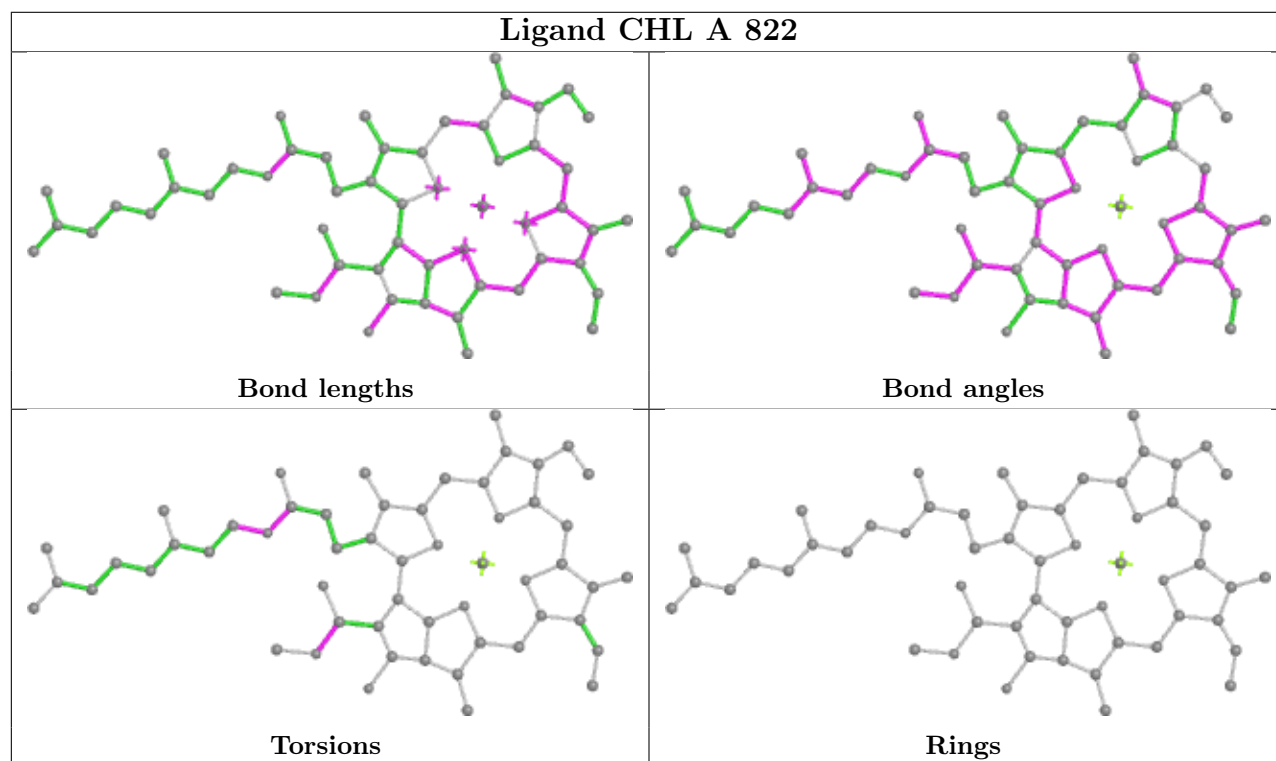
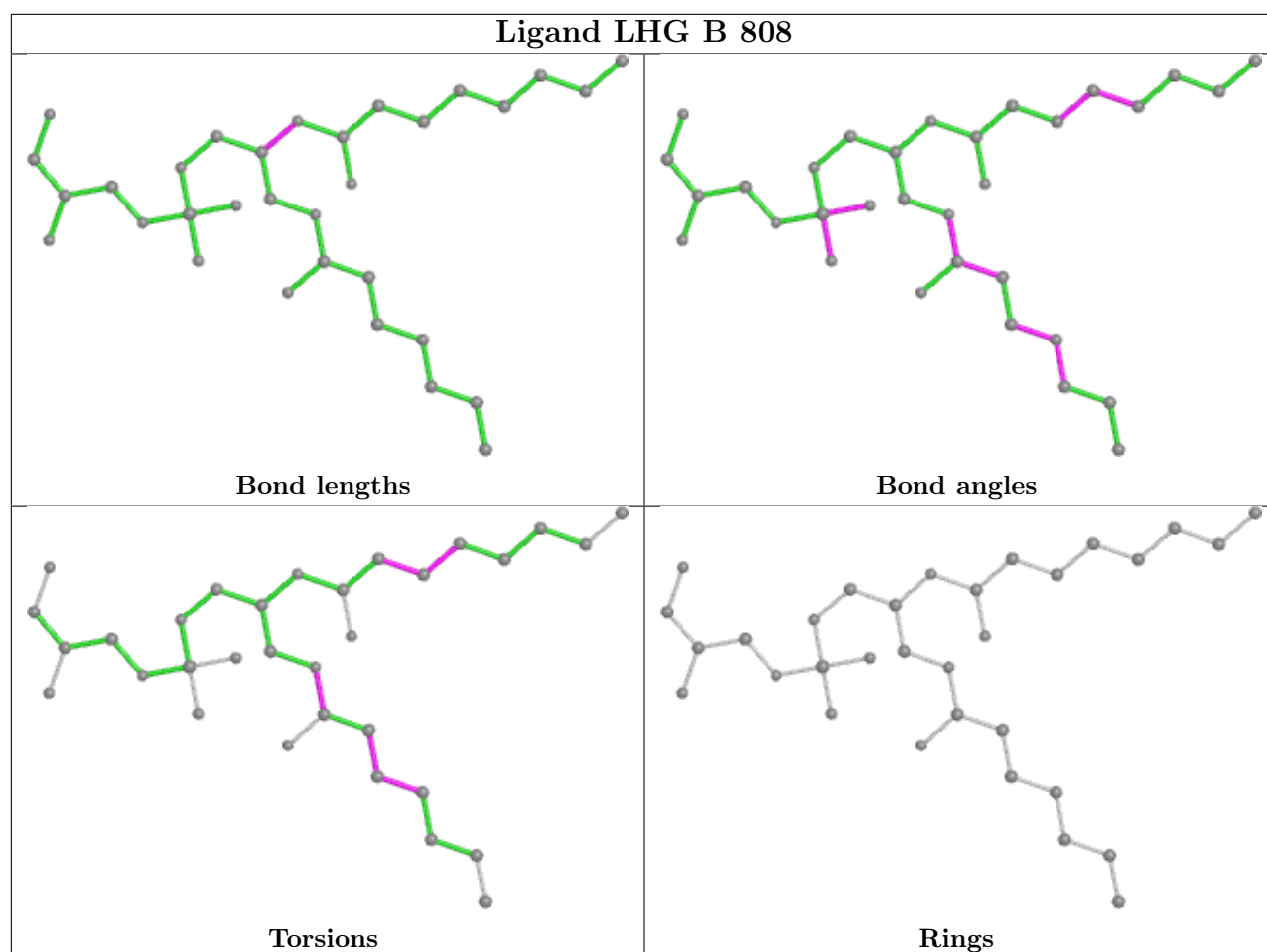


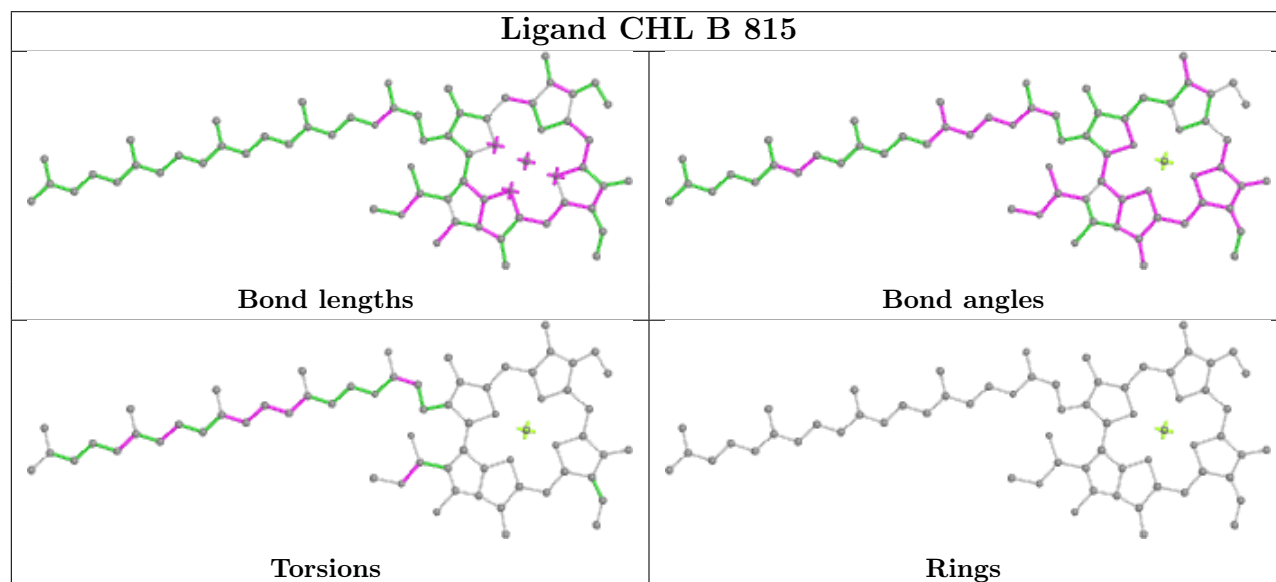
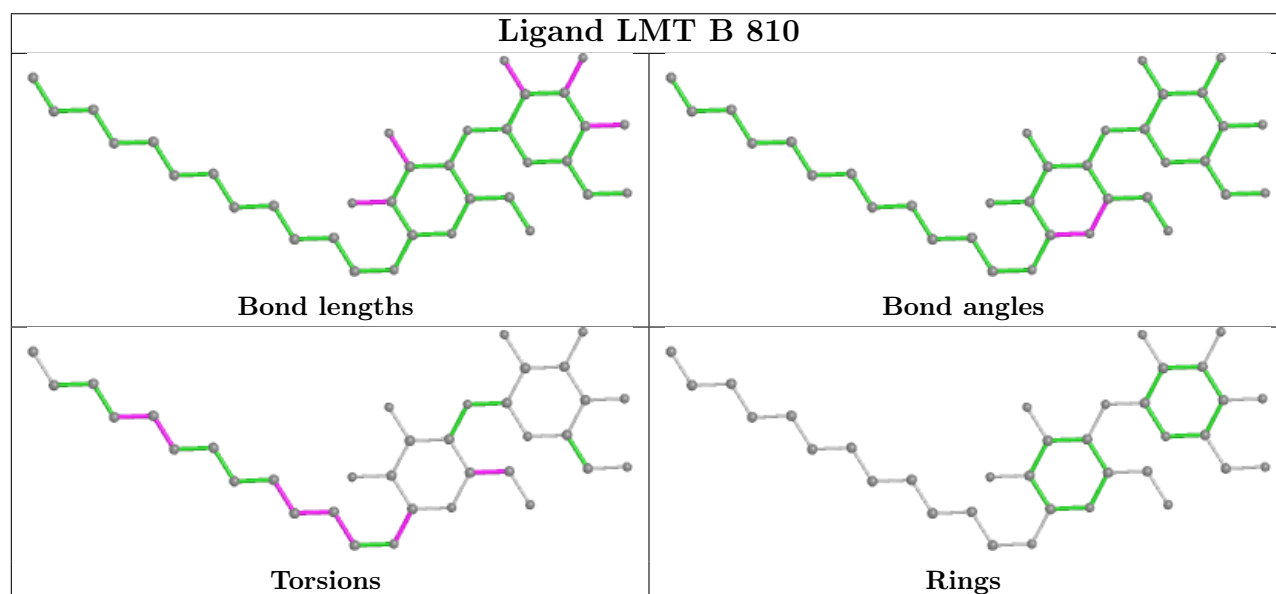
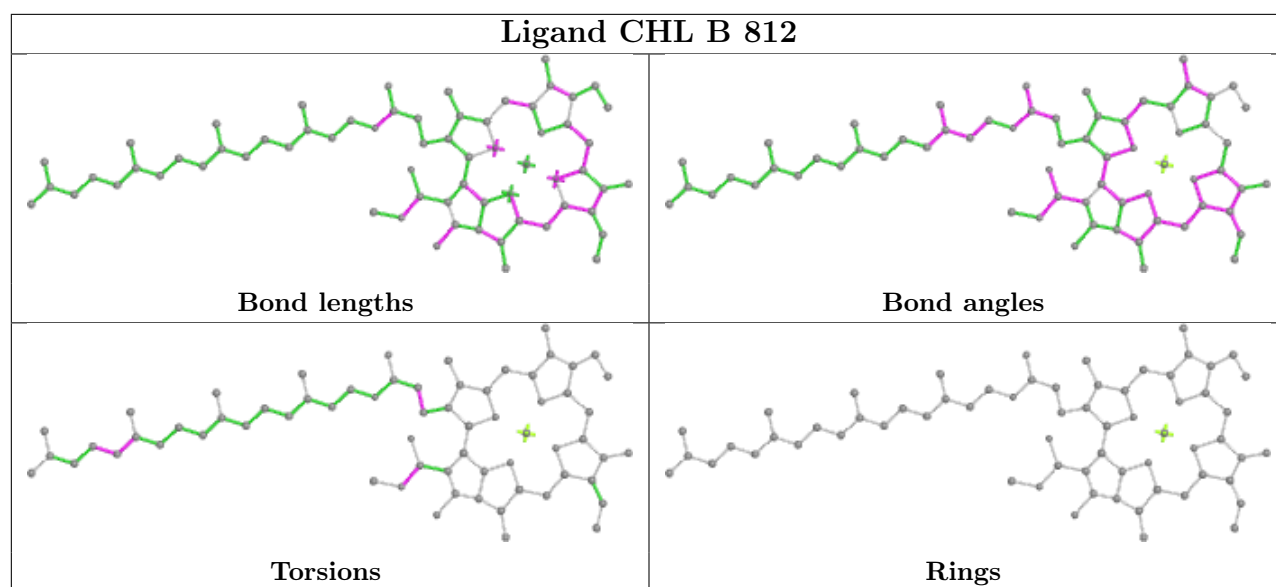
Torsions

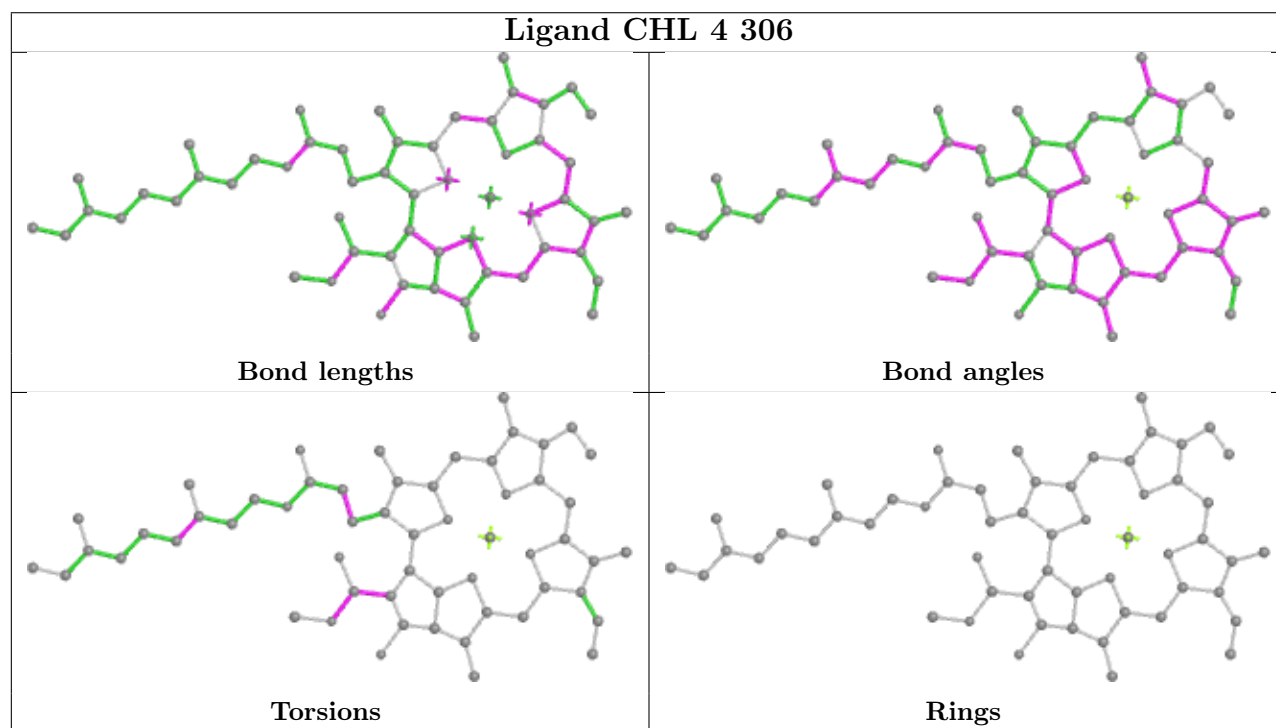
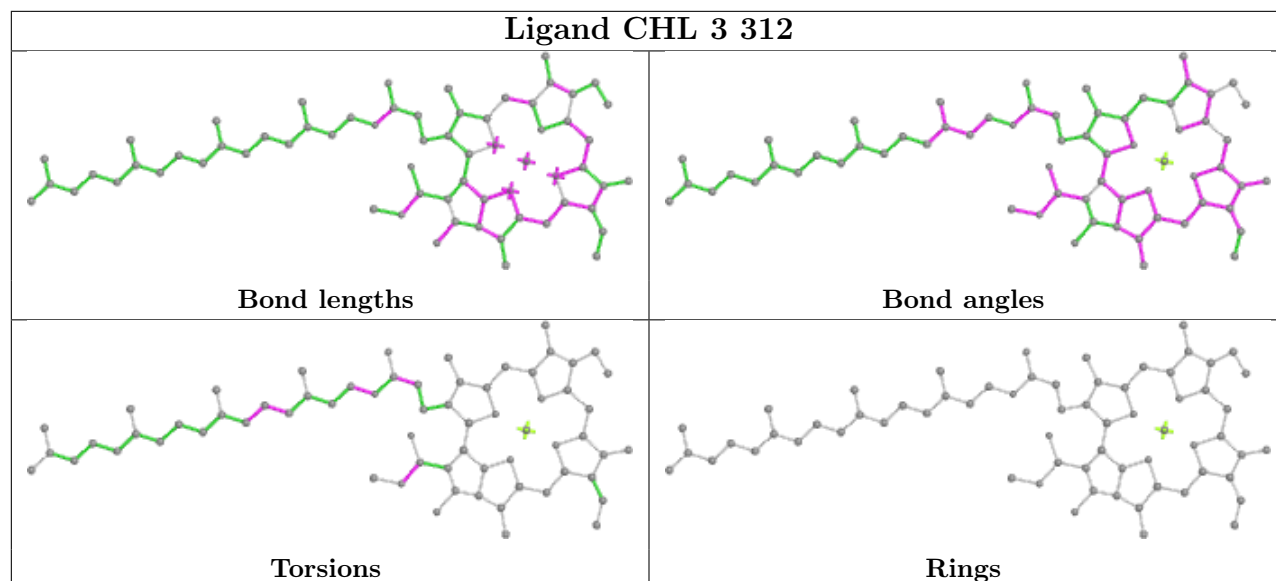
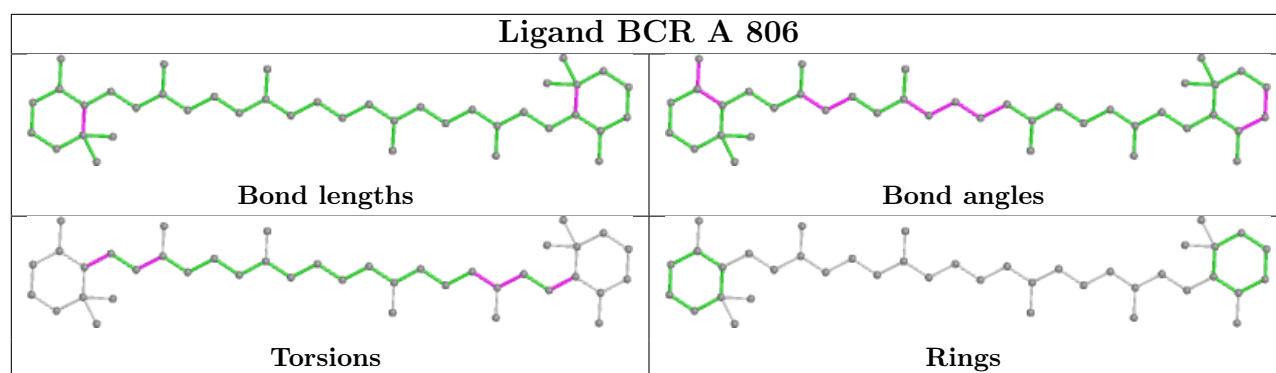


Rings

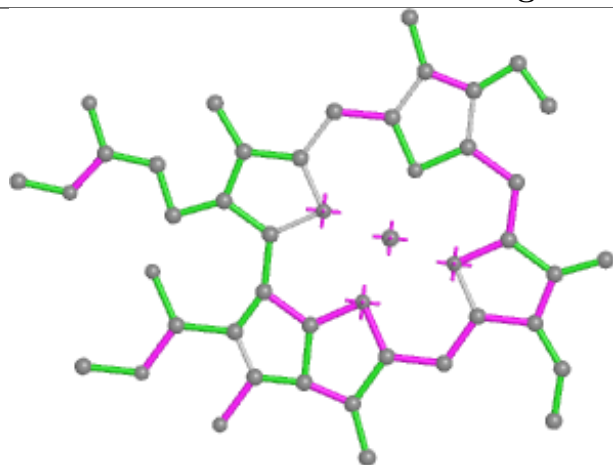




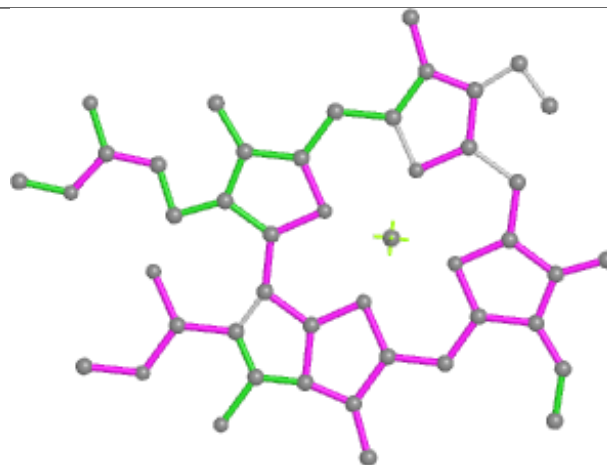




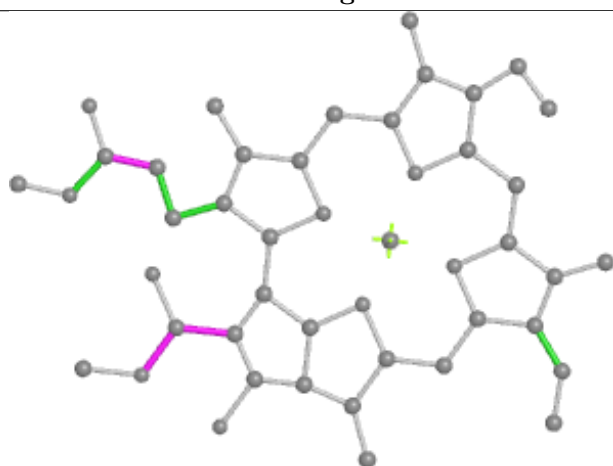
Ligand CHL 6 312



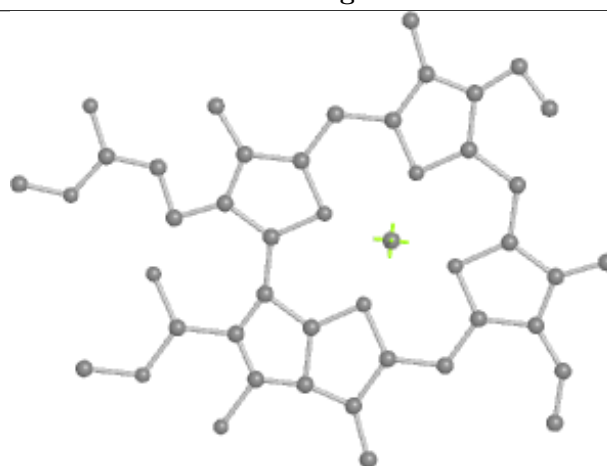
Bond lengths



Bond angles

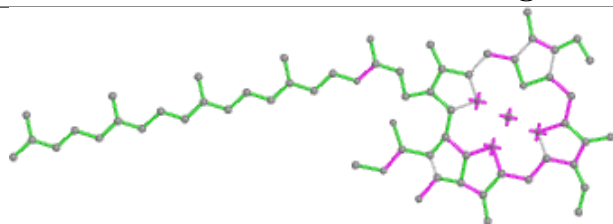


Torsions

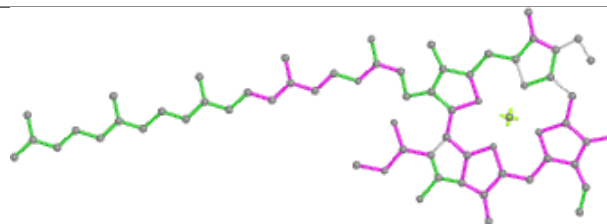


Rings

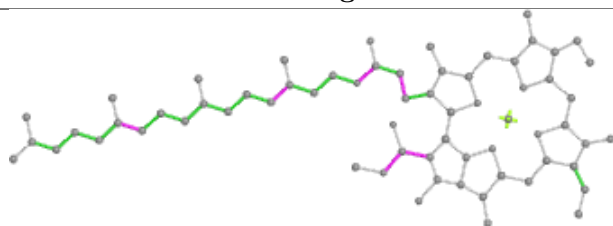
Ligand CHL 6 311



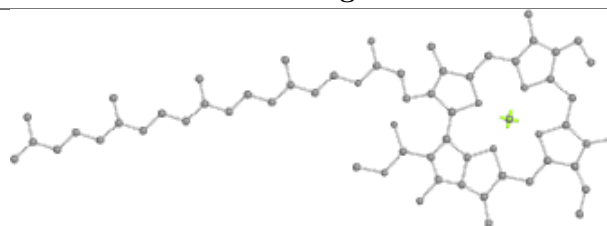
Bond lengths



Bond angles

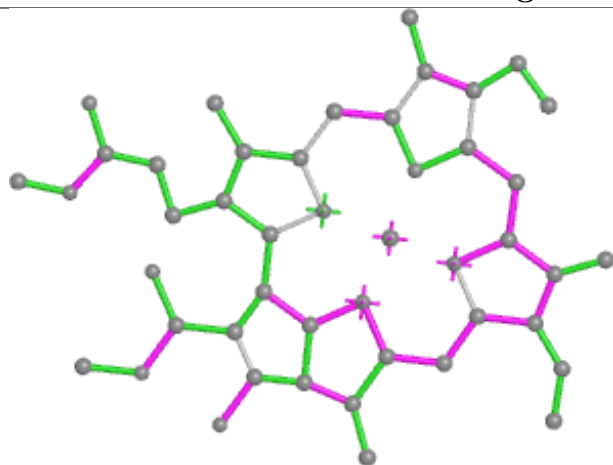


Torsions

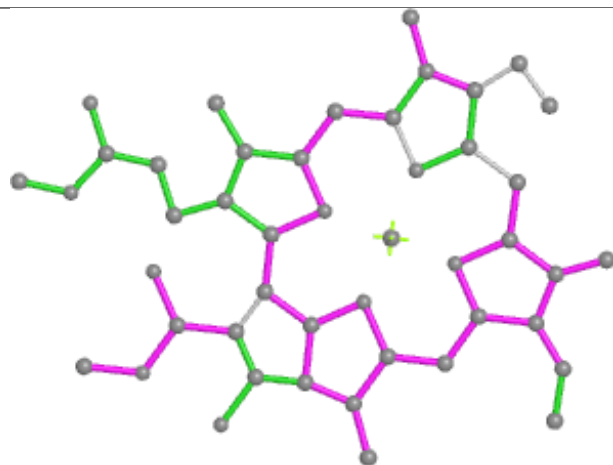


Rings

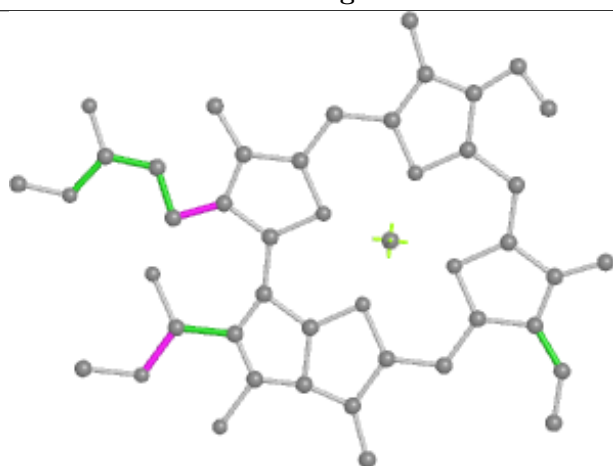
Ligand CHL b 304



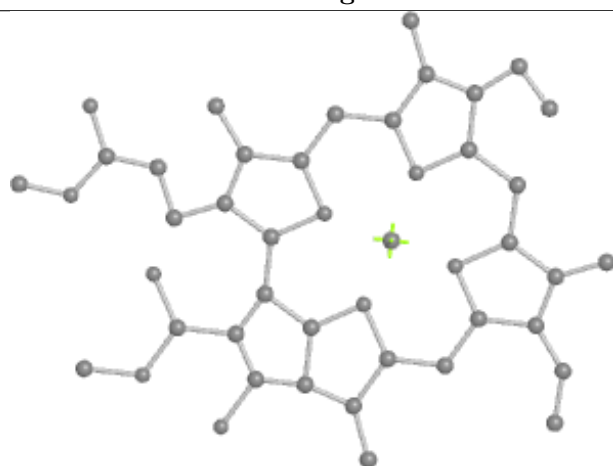
Bond lengths



Bond angles

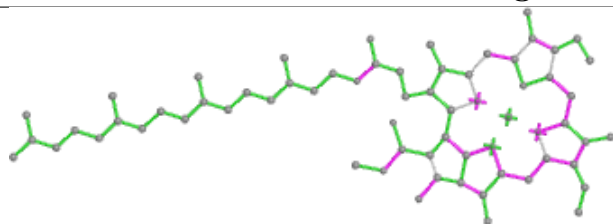


Torsions

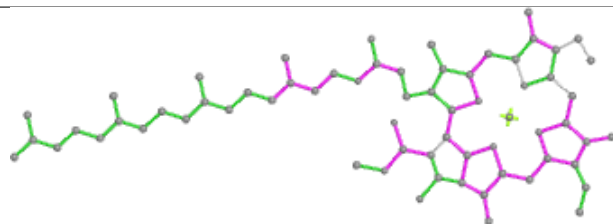


Rings

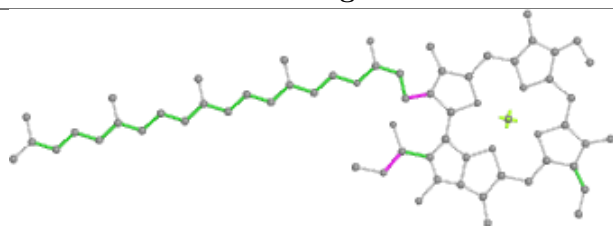
Ligand CHL A 848



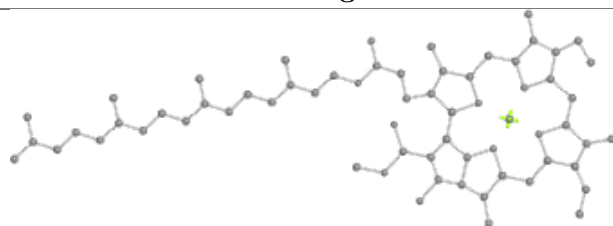
Bond lengths



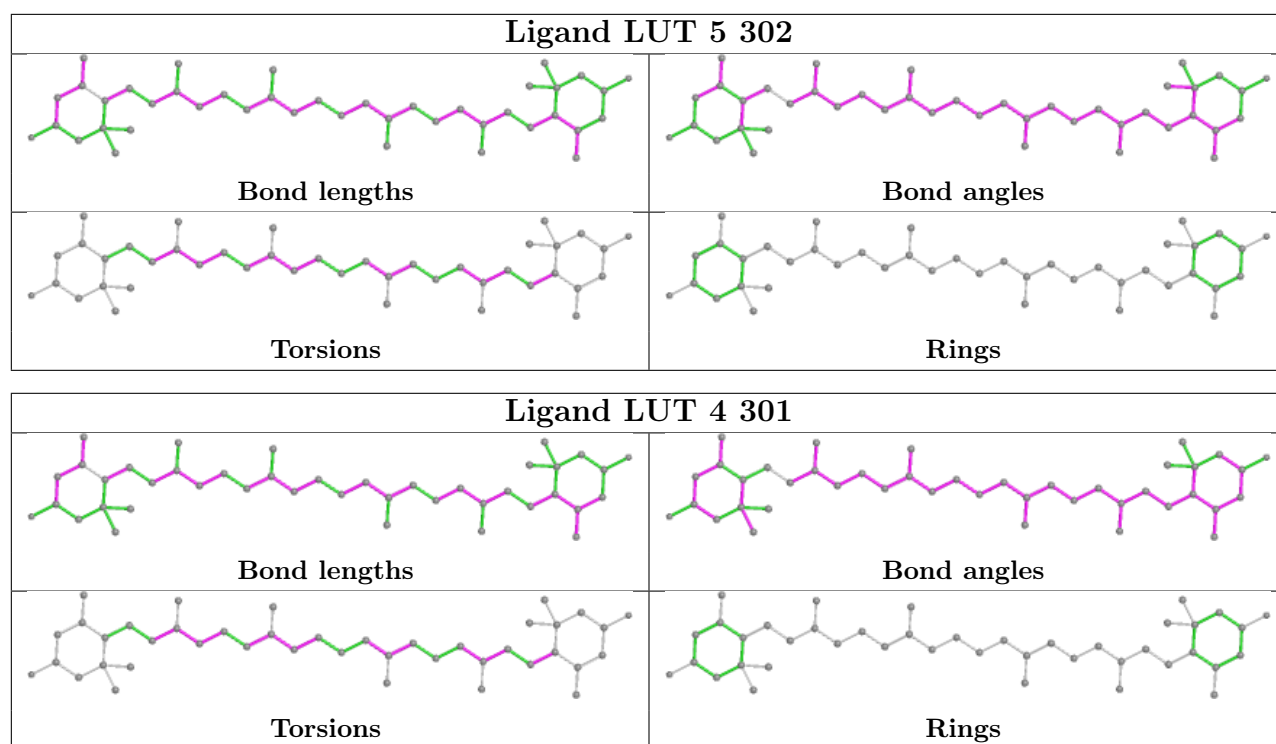
Bond angles



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.

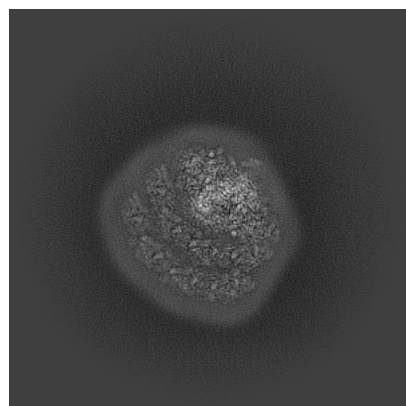
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62512. These allow visual inspection of the internal detail of the map and identification of artifacts.

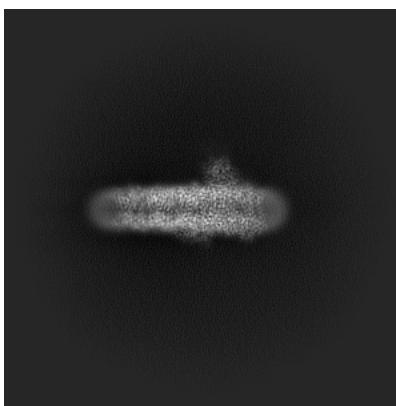
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

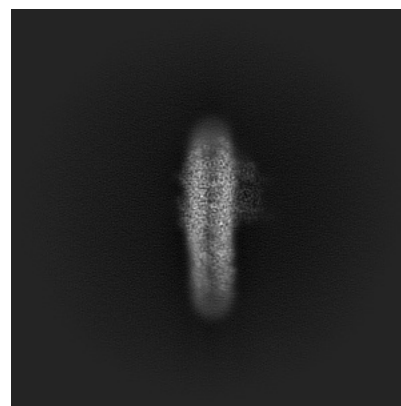
6.1.1 Primary map



X

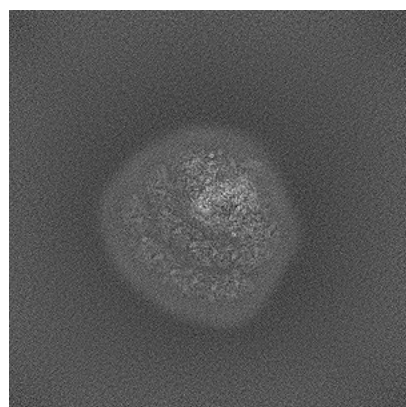


Y

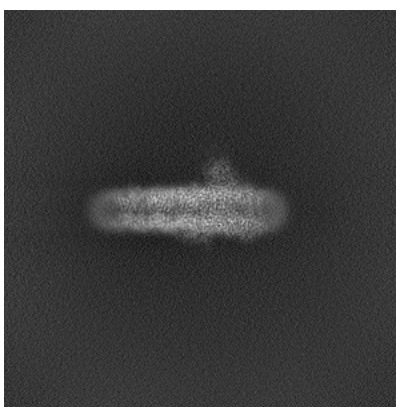


Z

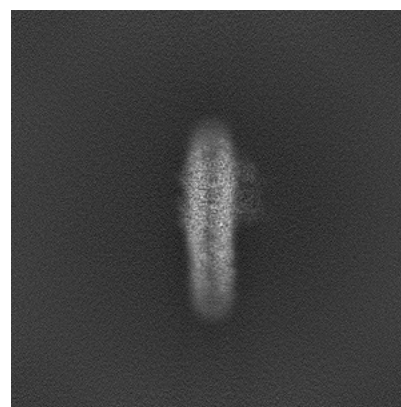
6.1.2 Raw map



X



Y

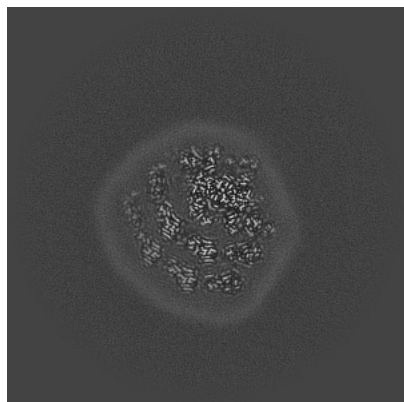


Z

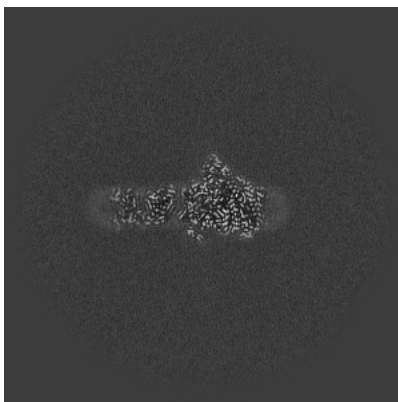
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

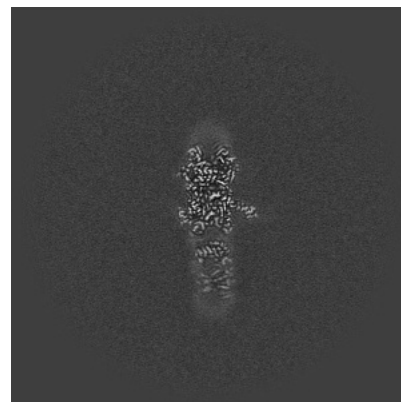
6.2.1 Primary map



X Index: 300

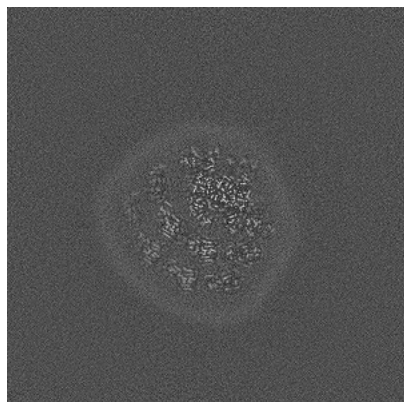


Y Index: 300

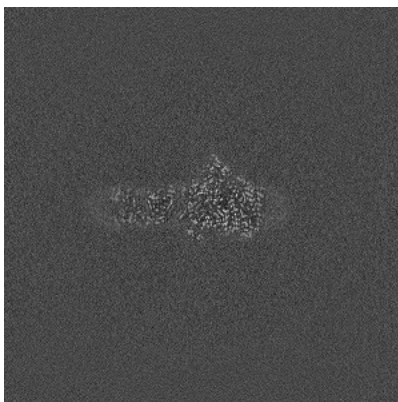


Z Index: 300

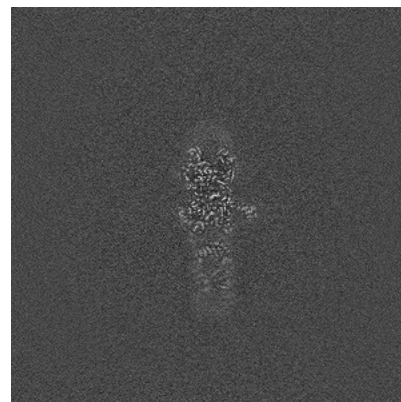
6.2.2 Raw map



X Index: 300



Y Index: 300

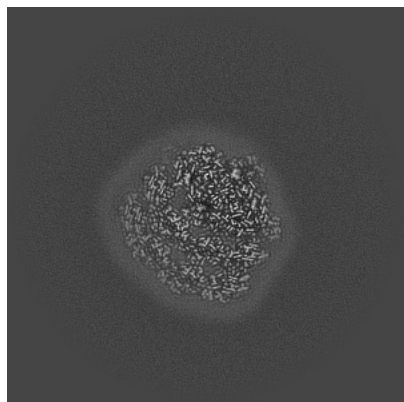


Z Index: 300

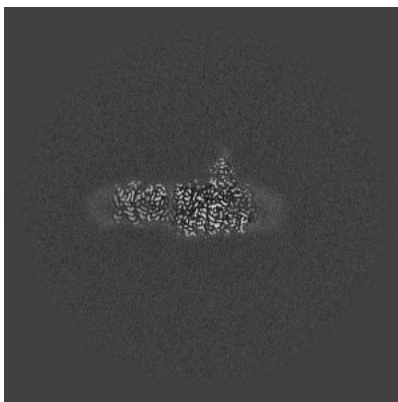
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

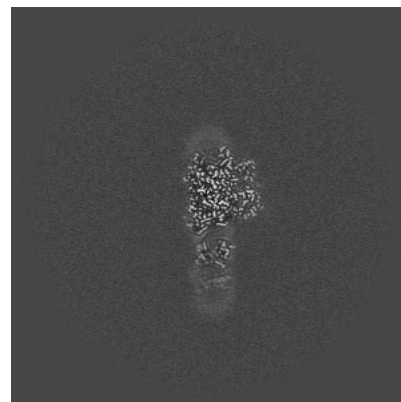
6.3.1 Primary map



X Index: 317

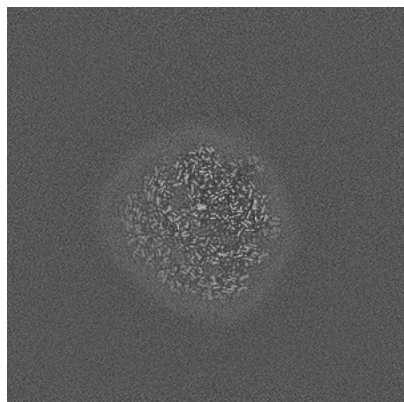


Y Index: 340

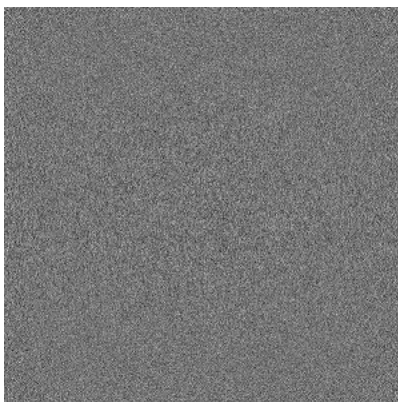


Z Index: 316

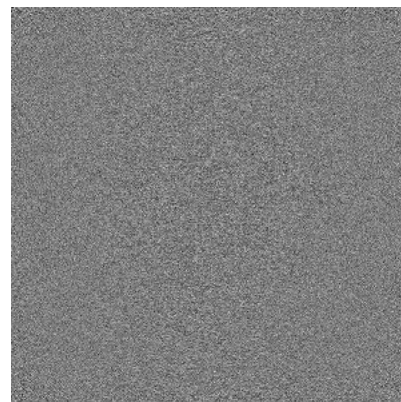
6.3.2 Raw map



X Index: 316



Y Index: 0

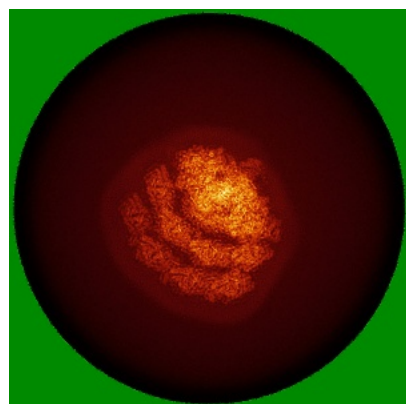


Z Index: 0

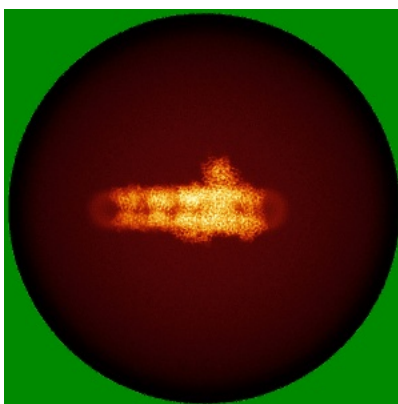
The images above show the largest variance slices of the map in three orthogonal directions.

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

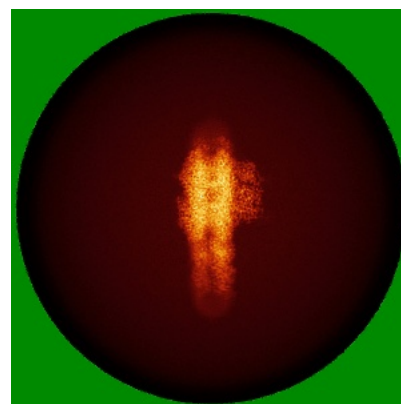
6.4.1 Primary map



X

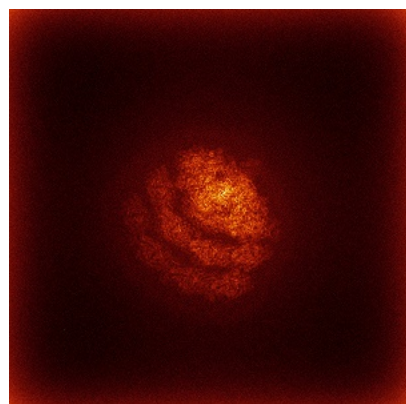


Y

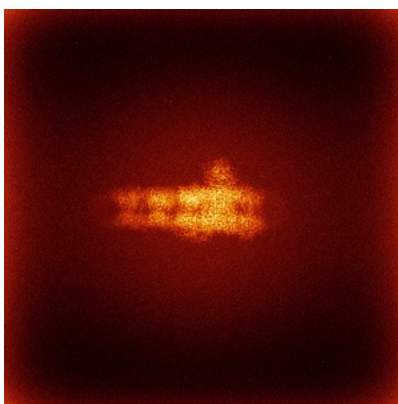


Z

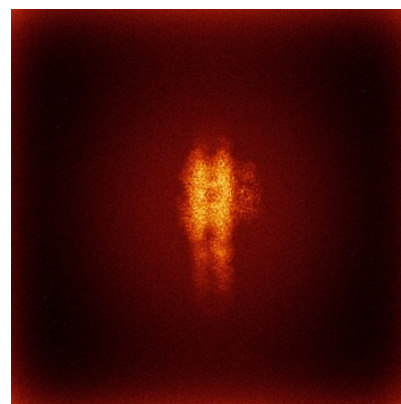
6.4.2 Raw map



X



Y

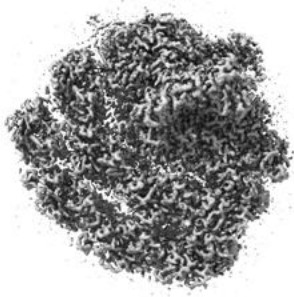


Z

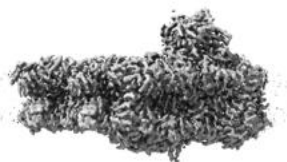
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



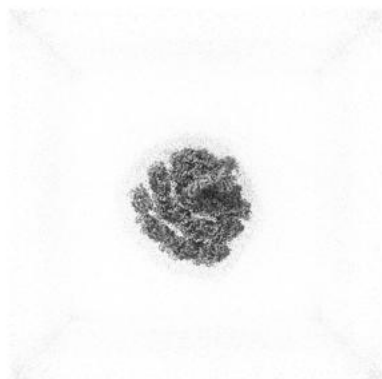
Y



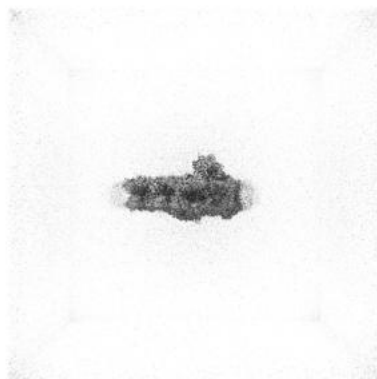
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

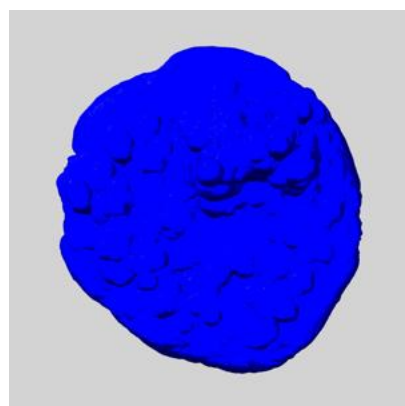
6.6 Mask visualisation [i](#)

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

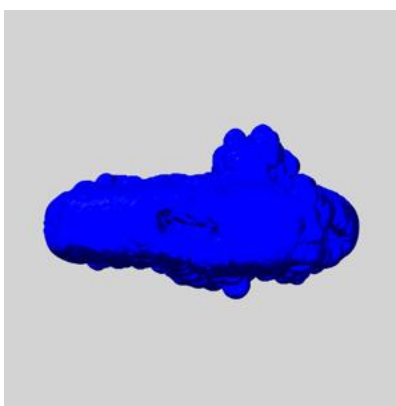
A mask typically either:

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

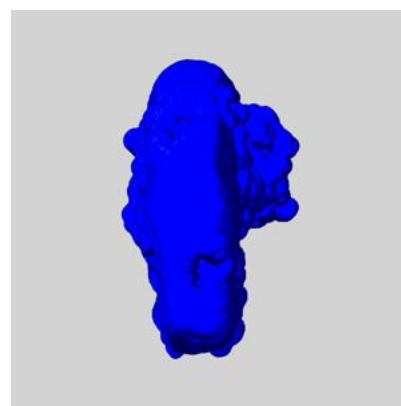
6.6.1 emd_62512_msk_1.map [i](#)



X



Y

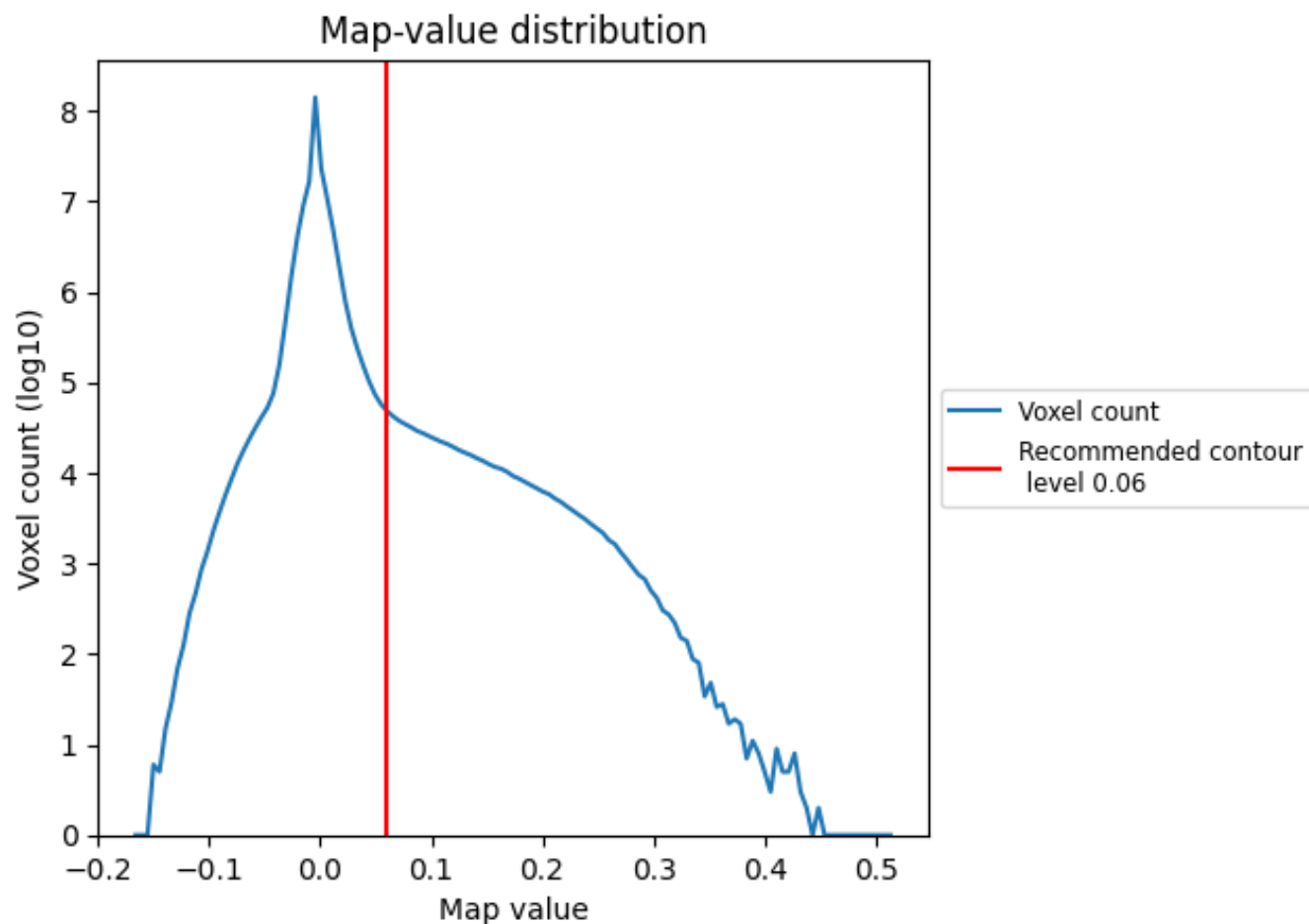


Z

7 Map analysis [i](#)

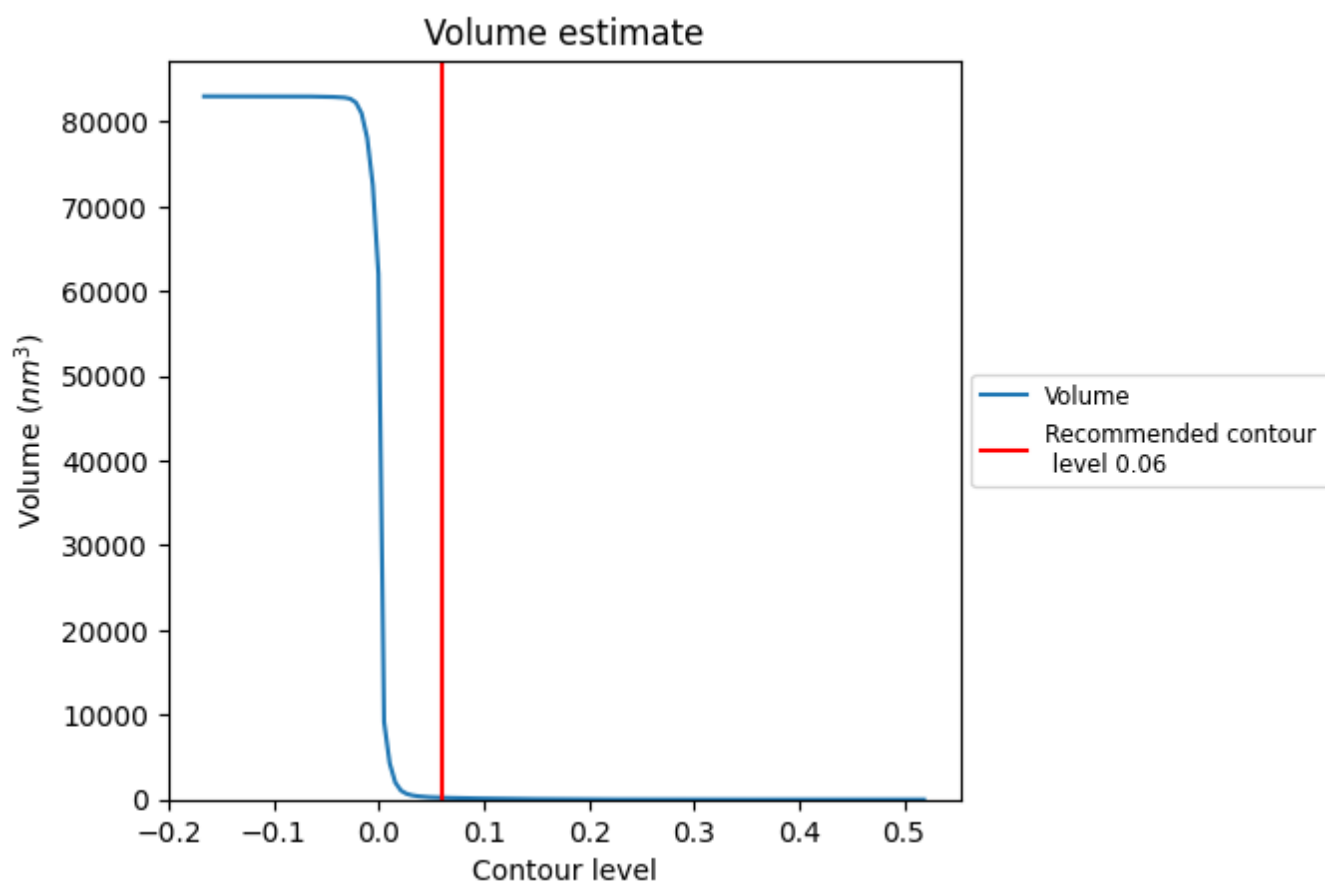
This section contains the results of statistical analysis of the map.

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.

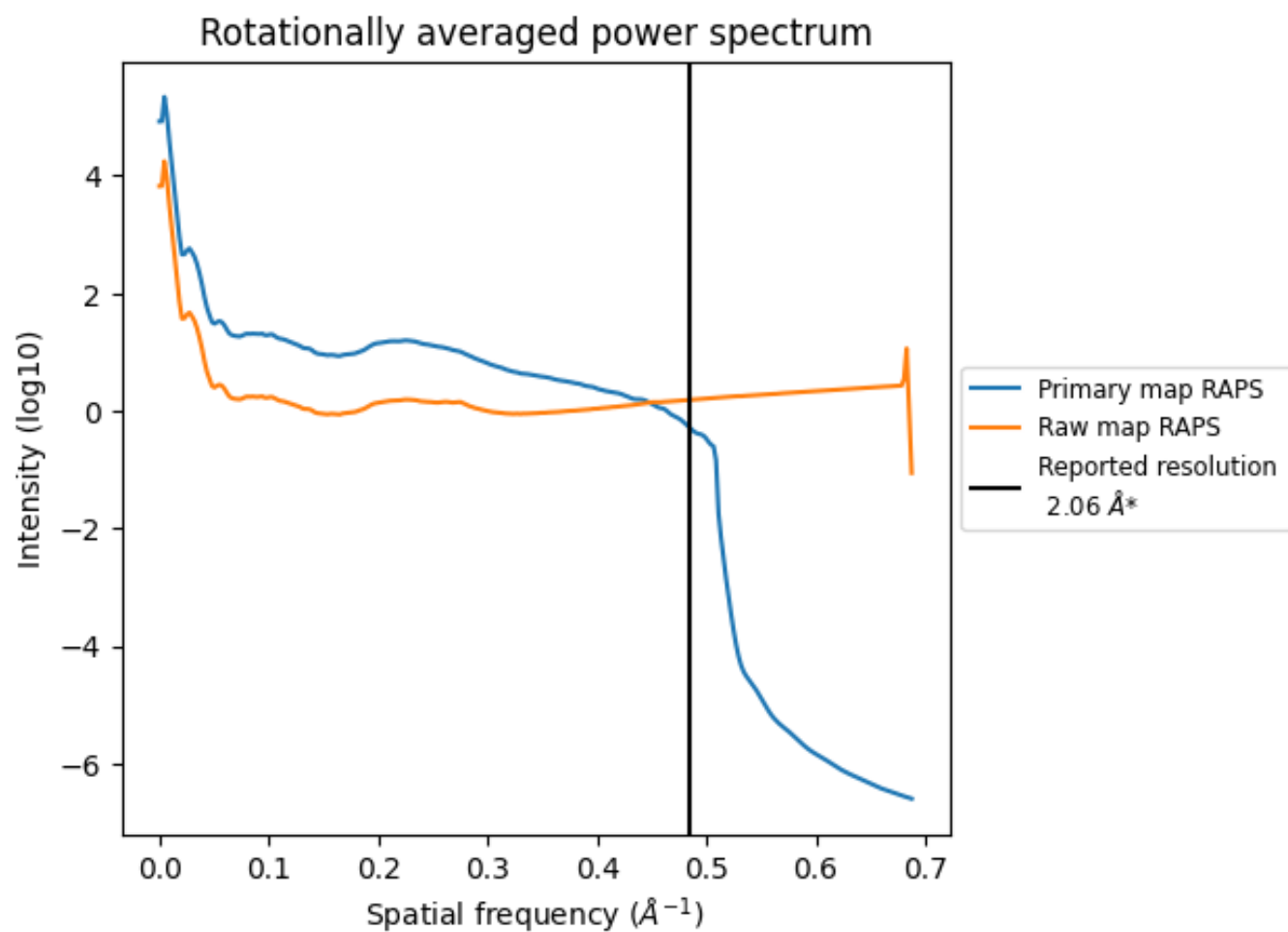
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm³; this corresponds to an approximate mass of 203 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 ⓘ

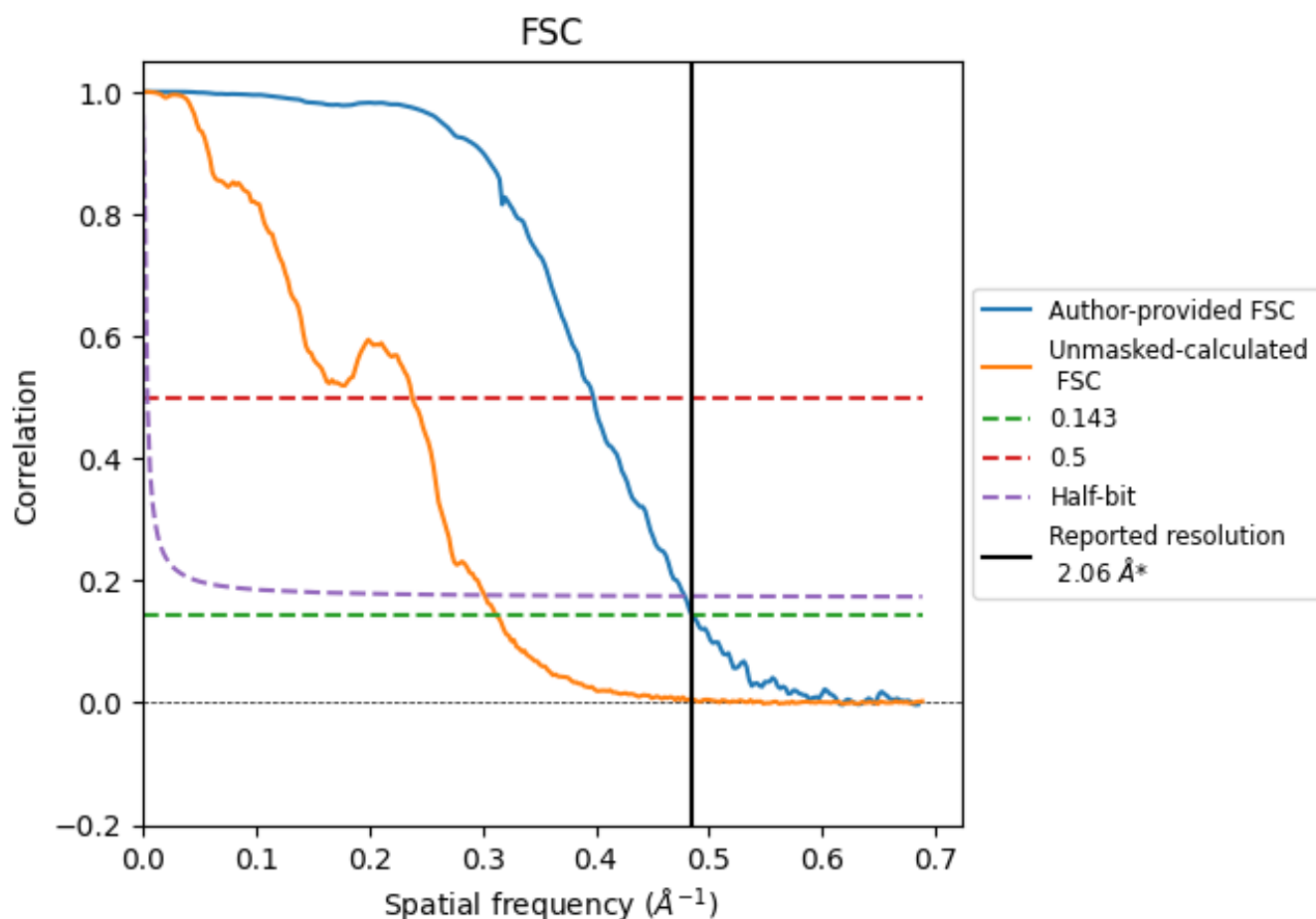


*Reported resolution corresponds to spatial frequency of 0.485 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.485 \AA^{-1}

8.2 Resolution estimates [i](#)

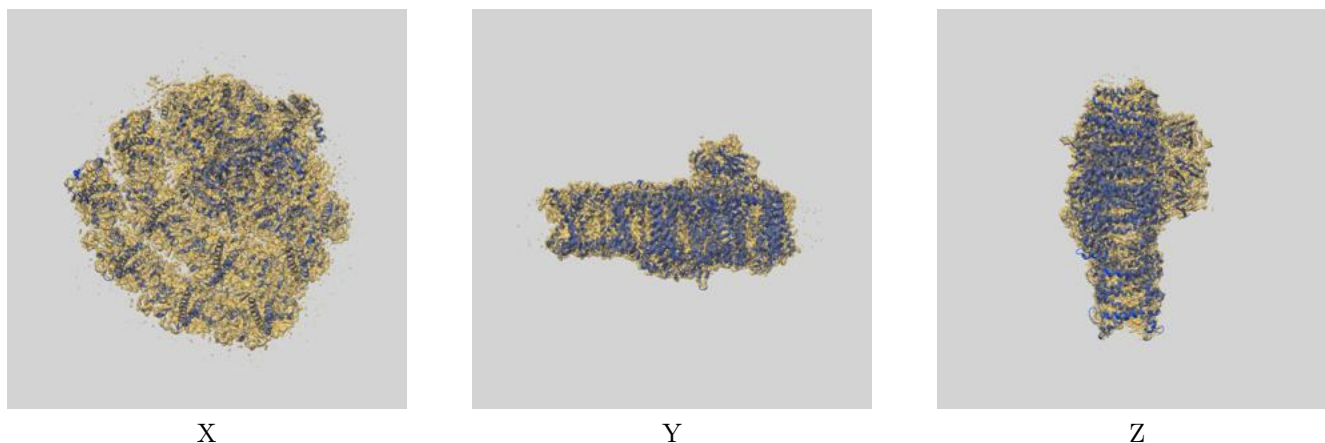
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.51	2.09
Unmasked-calculated*	3.20	4.20	3.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.06 by more than 10 %

9 Map-model fit [i](#)

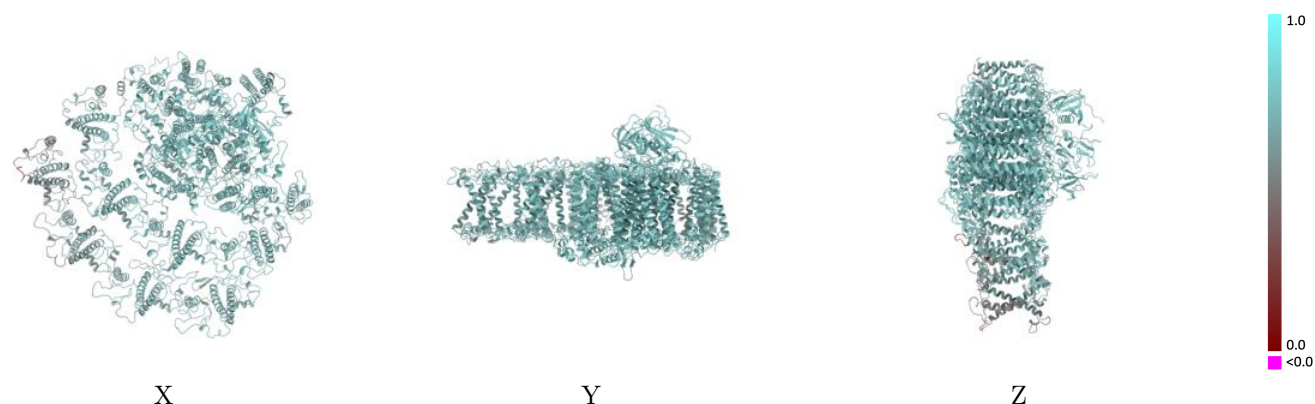
This section contains information regarding the fit between EMDB map EMD-62512 and PDB model 9KQQ. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



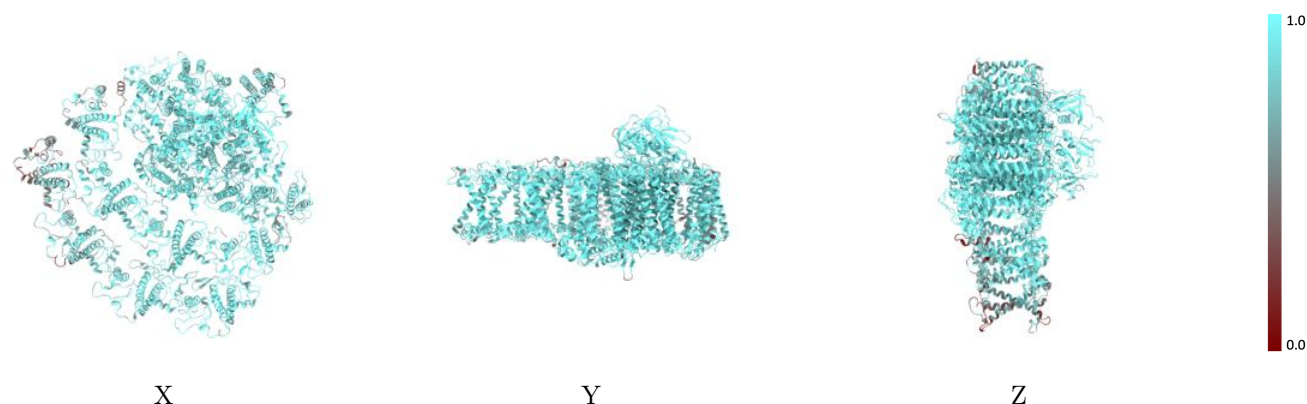
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



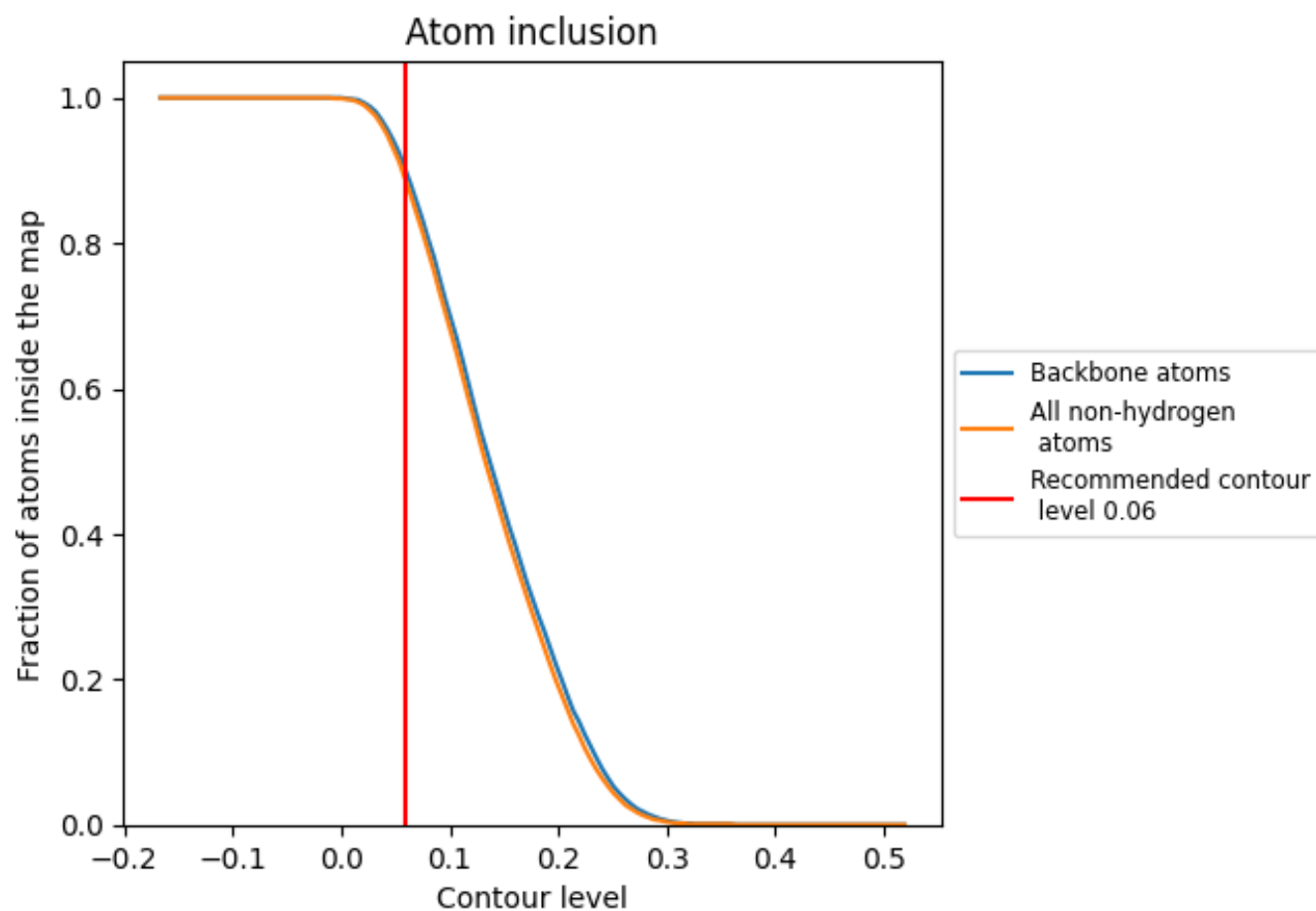
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8840	<div></div> 0.6680
3	<div></div> 0.8930	<div></div> 0.6640
4	<div></div> 0.7630	<div></div> 0.5820
5	<div></div> 0.8680	<div></div> 0.6390
6	<div></div> 0.8360	<div></div> 0.6240
7	<div></div> 0.9100	<div></div> 0.6740
8	<div></div> 0.8850	<div></div> 0.6680
A	<div></div> 0.9530	<div></div> 0.7160
B	<div></div> 0.9420	<div></div> 0.7060
C	<div></div> 0.9880	<div></div> 0.7270
D	<div></div> 0.9490	<div></div> 0.7040
E	<div></div> 0.9240	<div></div> 0.6890
F	<div></div> 0.9120	<div></div> 0.6940
G	<div></div> 0.4050	<div></div> 0.5050
I	<div></div> 0.9020	<div></div> 0.6870
J	<div></div> 0.9300	<div></div> 0.6950
K	<div></div> 0.8180	<div></div> 0.6410
L	<div></div> 0.8030	<div></div> 0.6480
M	<div></div> 0.8490	<div></div> 0.6630
a	<div></div> 0.8080	<div></div> 0.6200
b	<div></div> 0.6100	<div></div> 0.5250

