



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:36 AM UTC

PDB ID : 7YCA / pdb_00007yca
EMDB ID : EMD-33737
Title : Cryo-EM structure of the PSI-LHCI-Lhcp supercomplex from *Ostreococcus tauri*
Authors : Shan, J.; Sheng, X.; Ishii, A.; Watanabe, A.; Song, C.; Murata, K.; Minagawa, J.; Liu, Z.
Deposited on : 2022-07-01
Resolution : 2.94 Å (reported)
Based on initial models : 5ZJI, 7D0J

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:

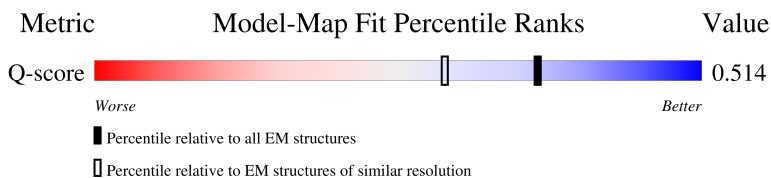
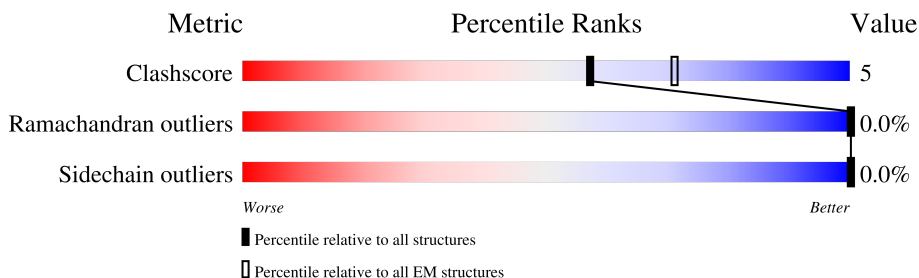
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	1	225	
2	2	242	
3	3	272	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	4	236	
5	5	217	
6	6	249	
7	A	751	
8	B	733	
9	C	81	
10	D	188	
11	E	101	
12	F	231	
13	G	132	
14	H	166	
15	I	35	
16	J	42	
17	K	131	
18	L	204	
19	M	31	
20	N	139	
21	O	136	
22	P	233	
22	R	233	
22	S	233	
22	T	233	
22	U	233	
22	V	233	
22	W	233	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
22	X	233	84% 72% 12% 16%
23	Q	226	28% 83% 16%

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
24	CHL	1	601	X	-	-	-
24	CHL	1	604	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	605	X	-	-	-
24	CHL	2	607	X	-	-	-
24	CHL	2	615	X	-	-	-
24	CHL	3	306	X	-	-	-
24	CHL	4	302	X	-	-	-
24	CHL	4	306	X	-	-	-
24	CHL	4	307	X	-	-	-
24	CHL	4	308	X	-	-	-
24	CHL	5	605	X	-	-	-
24	CHL	6	601	X	-	-	-
24	CHL	6	605	X	-	-	-
24	CHL	6	606	X	-	-	-
24	CHL	P	304	X	-	-	-
24	CHL	P	305	X	-	-	-
24	CHL	P	306	X	-	-	-
24	CHL	P	307	X	-	-	-
24	CHL	P	314	X	-	-	-
24	CHL	Q	307	X	-	-	-
24	CHL	Q	308	X	-	-	-
24	CHL	Q	309	X	-	-	-
24	CHL	Q	316	X	-	-	-
24	CHL	R	302	X	-	-	-
24	CHL	R	308	X	-	-	-
24	CHL	R	309	X	-	-	-
24	CHL	R	310	X	-	-	-
24	CHL	R	311	X	-	-	-
24	CHL	R	318	X	-	-	-
24	CHL	S	304	X	-	-	-
24	CHL	S	305	X	-	-	-
24	CHL	S	306	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	S	307	X	-	-	-
24	CHL	S	314	X	-	-	-
24	CHL	T	304	X	-	-	-
24	CHL	T	305	X	-	-	-
24	CHL	T	306	X	-	-	-
24	CHL	T	307	X	-	-	-
24	CHL	T	314	X	-	-	-
24	CHL	T	320	X	-	-	-
24	CHL	U	304	X	-	-	-
24	CHL	U	305	X	-	-	-
24	CHL	U	306	X	-	-	-
24	CHL	U	313	X	-	-	-
24	CHL	V	304	X	-	-	-
24	CHL	V	305	X	-	-	-
24	CHL	V	306	X	-	-	-
24	CHL	V	307	X	-	-	-
24	CHL	V	314	X	-	-	-
24	CHL	W	304	X	-	-	-
24	CHL	W	305	X	-	-	-
24	CHL	W	306	X	-	-	-
24	CHL	W	307	X	-	-	-
24	CHL	W	314	X	-	-	-
24	CHL	X	305	X	-	-	-
24	CHL	X	306	X	-	-	-
24	CHL	X	307	X	-	-	-
24	CHL	X	308	X	-	-	-
24	CHL	X	315	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	605	X	-	-	-
25	CLA	1	606	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	608	X	-	-	-
25	CLA	1	609	X	-	-	-
25	CLA	1	613	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	606	X	-	-	-
25	CLA	2	608	X	-	-	-
25	CLA	2	609	X	-	-	-
25	CLA	2	610	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	613	X	-	-	-
25	CLA	2	614	X	-	-	-
25	CLA	3	301	X	-	-	-
25	CLA	3	302	X	-	-	-
25	CLA	3	303	X	-	-	-
25	CLA	3	304	X	-	-	-
25	CLA	3	305	X	-	-	-
25	CLA	3	307	X	-	-	-
25	CLA	3	308	X	-	-	-
25	CLA	3	309	X	-	-	-
25	CLA	3	310	X	-	-	-
25	CLA	3	311	X	-	-	-
25	CLA	3	312	X	-	-	-
25	CLA	3	313	X	-	-	-
25	CLA	4	303	X	-	-	-
25	CLA	4	304	X	-	-	-
25	CLA	4	305	X	-	-	-
25	CLA	4	309	X	-	-	-
25	CLA	4	310	X	-	-	-
25	CLA	4	311	X	-	-	-
25	CLA	4	312	X	-	-	-
25	CLA	4	314	X	-	-	-
25	CLA	4	315	X	-	-	-
25	CLA	4	316	X	-	-	-
25	CLA	5	601	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	606	X	-	-	-
25	CLA	5	607	X	-	-	-
25	CLA	5	608	X	-	-	-
25	CLA	5	609	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	607	X	-	-	-
25	CLA	6	608	X	-	-	-
25	CLA	6	609	X	-	-	-
25	CLA	6	610	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	6	611	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	A	803	X	-	-	-
25	CLA	A	804	X	-	-	-
25	CLA	A	805	X	-	-	-
25	CLA	A	806	X	-	-	-
25	CLA	A	807	X	-	-	-
25	CLA	A	808	X	-	-	-
25	CLA	A	809	X	-	-	-
25	CLA	A	810	X	-	-	-
25	CLA	A	811	X	-	-	-
25	CLA	A	812	X	-	-	-
25	CLA	A	813	X	-	-	-
25	CLA	A	814	X	-	-	-
25	CLA	A	815	X	-	-	-
25	CLA	A	816	X	-	-	-
25	CLA	A	818	X	-	-	-
25	CLA	A	819	X	-	-	-
25	CLA	A	820	X	-	-	-
25	CLA	A	821	X	-	-	-
25	CLA	A	822	X	-	-	-
25	CLA	A	823	X	-	-	-
25	CLA	A	824	X	-	-	-
25	CLA	A	825	X	-	-	-
25	CLA	A	826	X	-	-	-
25	CLA	A	827	X	-	-	-
25	CLA	A	829	X	-	-	-
25	CLA	A	830	X	-	-	-
25	CLA	A	831	X	-	-	-
25	CLA	A	832	X	-	-	-
25	CLA	A	834	X	-	-	-
25	CLA	A	835	X	-	-	-
25	CLA	A	836	X	-	-	-
25	CLA	A	837	X	-	-	-
25	CLA	A	839	X	-	-	-
25	CLA	A	841	X	-	-	-
25	CLA	A	842	X	-	-	-
25	CLA	A	843	X	-	-	-
25	CLA	A	845	X	-	-	-
25	CLA	A	856	X	-	-	-
25	CLA	B	802	X	-	-	-
25	CLA	B	803	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	804	X	-	-	-
25	CLA	B	805	X	-	-	-
25	CLA	B	806	X	-	-	-
25	CLA	B	807	X	-	-	-
25	CLA	B	808	X	-	-	-
25	CLA	B	809	X	-	-	-
25	CLA	B	810	X	-	-	-
25	CLA	B	811	X	-	-	-
25	CLA	B	812	X	-	-	-
25	CLA	B	813	X	-	-	-
25	CLA	B	814	X	-	-	-
25	CLA	B	815	X	-	-	-
25	CLA	B	816	X	-	-	-
25	CLA	B	817	X	-	-	-
25	CLA	B	818	X	-	-	-
25	CLA	B	819	X	-	-	-
25	CLA	B	820	X	-	-	-
25	CLA	B	821	X	-	-	-
25	CLA	B	822	X	-	-	-
25	CLA	B	823	X	-	-	-
25	CLA	B	824	X	-	-	-
25	CLA	B	825	X	-	-	-
25	CLA	B	826	X	-	-	-
25	CLA	B	827	X	-	-	-
25	CLA	B	828	X	-	-	-
25	CLA	B	829	X	-	-	-
25	CLA	B	830	X	-	-	-
25	CLA	B	831	X	-	-	-
25	CLA	B	832	X	-	-	-
25	CLA	B	833	X	-	-	-
25	CLA	B	834	X	-	-	-
25	CLA	B	835	X	-	-	-
25	CLA	B	837	X	-	-	-
25	CLA	B	838	X	-	-	-
25	CLA	B	839	X	-	-	-
25	CLA	B	841	X	-	-	-
25	CLA	B	842	X	-	-	-
25	CLA	B	843	X	-	-	-
25	CLA	F	802	X	-	-	-
25	CLA	F	803	X	-	-	-
25	CLA	G	202	X	-	-	-
25	CLA	G	203	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	G	204	X	-	-	-
25	CLA	H	301	X	-	-	-
25	CLA	H	302	X	-	-	-
25	CLA	H	304	X	-	-	-
25	CLA	J	102	X	-	-	-
25	CLA	K	201	X	-	-	-
25	CLA	K	203	X	-	-	-
25	CLA	K	204	X	-	-	-
25	CLA	K	206	X	-	-	-
25	CLA	L	301	X	-	-	-
25	CLA	L	303	X	-	-	-
25	CLA	L	304	X	-	-	-
25	CLA	N	202	X	-	-	-
25	CLA	N	203	X	-	-	-
25	CLA	O	2001	X	-	-	-
25	CLA	O	2002	X	-	-	-
25	CLA	O	2003	X	-	-	-
25	CLA	O	2004	X	-	-	-
25	CLA	O	2005	X	-	-	-
25	CLA	P	301	X	-	-	-
25	CLA	P	302	X	-	-	-
25	CLA	P	303	X	-	-	-
25	CLA	P	309	X	-	-	-
25	CLA	P	310	X	-	-	-
25	CLA	P	311	X	-	-	-
25	CLA	P	312	X	-	-	-
25	CLA	Q	301	X	-	-	-
25	CLA	Q	304	X	-	-	-
25	CLA	Q	305	X	-	-	-
25	CLA	Q	306	X	-	-	-
25	CLA	Q	311	X	-	-	-
25	CLA	Q	312	X	-	-	-
25	CLA	Q	313	X	-	-	-
25	CLA	Q	314	X	-	-	-
25	CLA	Q	315	X	-	-	-
25	CLA	R	305	X	-	-	-
25	CLA	R	306	X	-	-	-
25	CLA	R	307	X	-	-	-
25	CLA	R	313	X	-	-	-
25	CLA	R	314	X	-	-	-
25	CLA	R	315	X	-	-	-
25	CLA	R	316	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	301	X	-	-	-
25	CLA	S	302	X	-	-	-
25	CLA	S	303	X	-	-	-
25	CLA	S	309	X	-	-	-
25	CLA	S	310	X	-	-	-
25	CLA	S	311	X	-	-	-
25	CLA	S	312	X	-	-	-
25	CLA	S	313	X	-	-	-
25	CLA	T	301	X	-	-	-
25	CLA	T	302	X	-	-	-
25	CLA	T	303	X	-	-	-
25	CLA	T	309	X	-	-	-
25	CLA	T	310	X	-	-	-
25	CLA	T	311	X	-	-	-
25	CLA	T	312	X	-	-	-
25	CLA	T	313	X	-	-	-
25	CLA	U	301	X	-	-	-
25	CLA	U	302	X	-	-	-
25	CLA	U	303	X	-	-	-
25	CLA	U	308	X	-	-	-
25	CLA	U	309	X	-	-	-
25	CLA	U	310	X	-	-	-
25	CLA	U	311	X	-	-	-
25	CLA	U	312	X	-	-	-
25	CLA	V	301	X	-	-	-
25	CLA	V	302	X	-	-	-
25	CLA	V	303	X	-	-	-
25	CLA	V	309	X	-	-	-
25	CLA	V	310	X	-	-	-
25	CLA	V	311	X	-	-	-
25	CLA	V	313	X	-	-	-
25	CLA	W	301	X	-	-	-
25	CLA	W	302	X	-	-	-
25	CLA	W	303	X	-	-	-
25	CLA	W	309	X	-	-	-
25	CLA	W	310	X	-	-	-
25	CLA	W	311	X	-	-	-
25	CLA	W	312	X	-	-	-
25	CLA	W	313	X	-	-	-
25	CLA	X	302	X	-	-	-
25	CLA	X	303	X	-	-	-
25	CLA	X	304	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	X	310	X	-	-	-
25	CLA	X	311	X	-	-	-
25	CLA	X	312	X	-	-	-
25	CLA	X	313	X	-	-	-
25	CLA	X	314	X	-	-	-
33	CL0	A	802	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 64832 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 Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	159	Total	C	N	O	S	0	0
			1209	768	219	213	9		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	205	Total	C	N	O	S	0	0
			1583	1023	265	286	9		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	227	Total	C	N	O	S	0	0
			1717	1111	279	311	16		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	203	Total	C	N	O	S	0	0
			1579	1021	267	280	11		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	166	Total	C	N	O	S	0	0
			1278	826	215	226	11		

- Molecule 6 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	194	Total	C	N	O	S	0	0
			1484	963	243	269	9		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	742	Total	C	N	O	S	0	0
			5819	3802	990	1000	27		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	732	Total	C	N	O	S	0	0
			5773	3793	966	996	18		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	80	Total	C	N	O	S	0	0
			593	364	103	115	11		

- Molecule 10 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	143	Total	C	N	O	S	0	0
			1116	717	197	196	6		

- Molecule 11 is a protein called Photosystem I reaction centre subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	62	Total	C	N	O	S	0	0
			503	324	84	94	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	165	Total	C	N	O	S	0	0
			1259	808	212	235	4		

- Molecule 13 is a protein called PsuG.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	95	Total	C	N	O	S	0	0
			717	453	124	137	3		

- Molecule 14 is a protein called Photosystem I PsuH, reaction centre subunit VI.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	H	96	Total	C	N	O	0	0
			721	456	122	143		

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total	C	N	O	S	0	0
			264	181	37	44	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	41	Total	C	N	O	S	0	0
			328	225	49	53	1		

- Molecule 17 is a protein called Photosystem I PsaG/PsaK protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	87	Total	C	N	O	S	0	0
			625	393	106	121	5		

- Molecule 18 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	158	Total	C	N	O	S	0	0
			1169	759	190	217	3		

- Molecule 19 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	31	Total	C	N	O	S	0	0
			239	159	37	42	1		

- Molecule 20 is a protein called Photosystem I PsaN, reaction centre subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	91	Total	C	N	O	S	0	0
			676	415	118	138	5		

- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	96	Total	C	N	O	S	0	0
			759	498	123	132	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	R	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	S	202	Total	C	N	O	S	0	0
			1512	971	247	288	6		
22	T	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	U	201	Total	C	N	O	S	0	0
			1507	968	246	287	6		
22	V	197	Total	C	N	O	S	0	0
			1484	956	242	280	6		
22	W	200	Total	C	N	O	S	0	0
			1499	964	245	284	6		
22	X	196	Total	C	N	O	S	0	0
			1474	949	241	278	6		

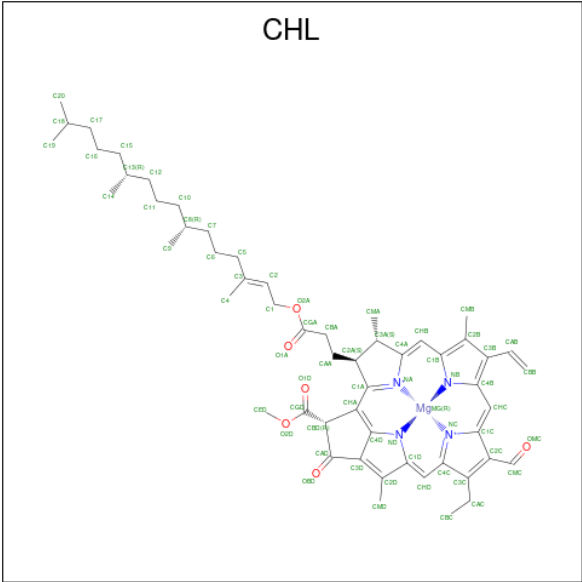
- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Q	226	Total	C	N	O	P	S	0	0
			1706	1100	285	313	1	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	28	ACE	-	acetylation	UNP A0A090LYE8

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	P	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	P	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	P	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	P	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	Q	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	Q	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	Q	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	R	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	R	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

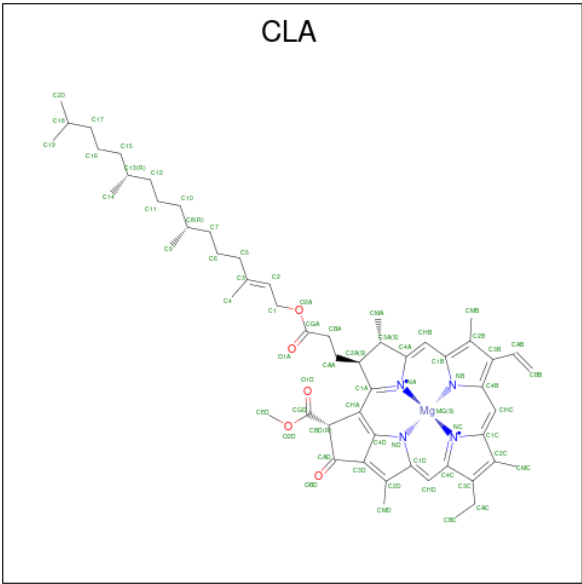
Mol	Chain	Residues	Atoms					AltConf
24	T	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	T	1	Total 49	C 38	Mg 1	N 4	O 6	0
24	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	T	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	T	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	U	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	U	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	U	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	V	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	V	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	W	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	W	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	W	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	W	1	Total 41	C 32	Mg 1	N 4	O 4	0
24	X	1	Total 42	C 33	Mg 1	N 4	O 4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
24	X	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	X	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
24	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			37	30	1	4	2	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	2	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	2	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	3	1	Total 43	C 33	Mg 1	N 4	O 5	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 42	C 34	Mg 1	N 4	O 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	4	1	Total 43	C 33	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 38	C 30	Mg 1	N 4	O 3	0
25	5	1	Total 40	C 32	Mg 1	N 4	O 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	5	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	6	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	6	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	H	1	Total 44	C 35	Mg 1	N 4	O 4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	K	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	N	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	O	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 50	C 40	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	P	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	P	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	P	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	Q	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	Q	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	Q	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	R	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 55	C 45	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	T	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	T	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	T	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	T	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	U	1	Total 41	C 33	Mg 1	N 4	O 3	0

Continued on next page...

Continued from previous page...

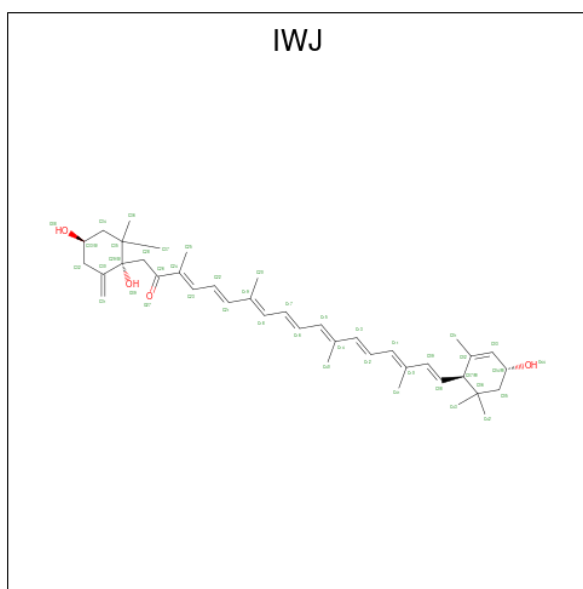
Mol	Chain	Residues	Atoms					AltConf
25	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	U	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	V	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	V	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	V	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	V	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	W	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	W	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	X	1	Total 55	C 45	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
25	X	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	X	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 26 is (3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-1-[(1 {S},4 {S})-2,2-dimethyl-6-methylidene-1,4-bis(oxidanyl)cyclohexyl]-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-2-one (CCD ID: IWJ) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



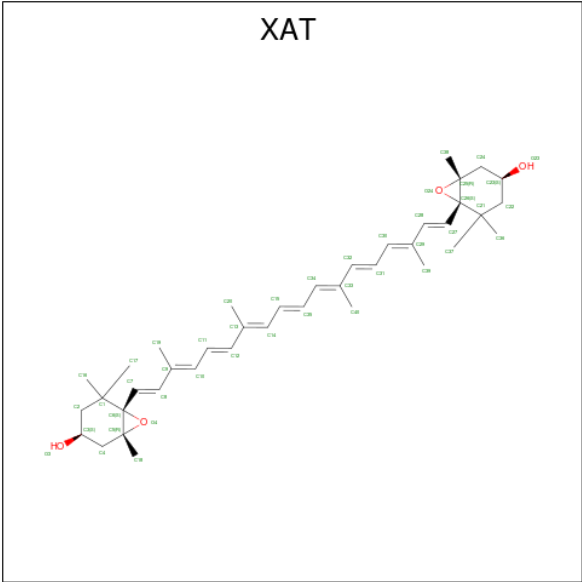
Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			44	40	4	
26	3	1	Total	C	O	0
			44	40	4	
26	4	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

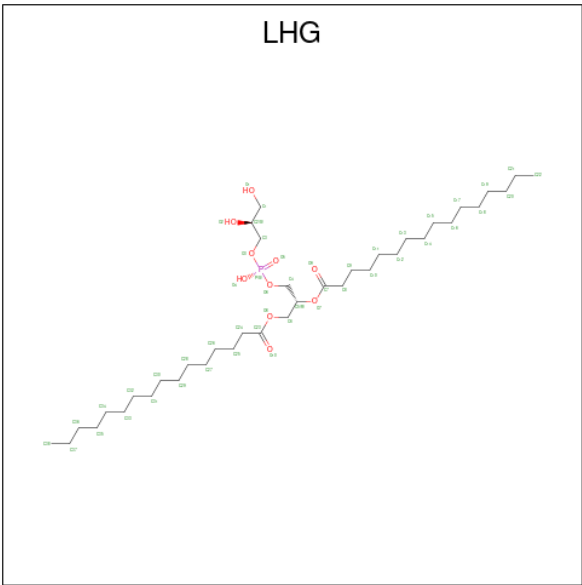
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	
26	6	1	Total	C	O	0
			44	40	4	
26	P	1	Total	C	O	0
			44	40	4	
26	P	1	Total	C	O	0
			44	40	4	
26	Q	1	Total	C	O	0
			44	40	4	
26	Q	1	Total	C	O	0
			44	40	4	
26	R	1	Total	C	O	0
			44	40	4	
26	R	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	S	1	Total	C	O	0
			44	40	4	
26	T	1	Total	C	O	0
			44	40	4	
26	T	1	Total	C	O	0
			44	40	4	
26	U	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	V	1	Total	C	O	0
			44	40	4	
26	W	1	Total	C	O	0
			44	40	4	
26	X	1	Total	C	O	0
			44	40	4	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



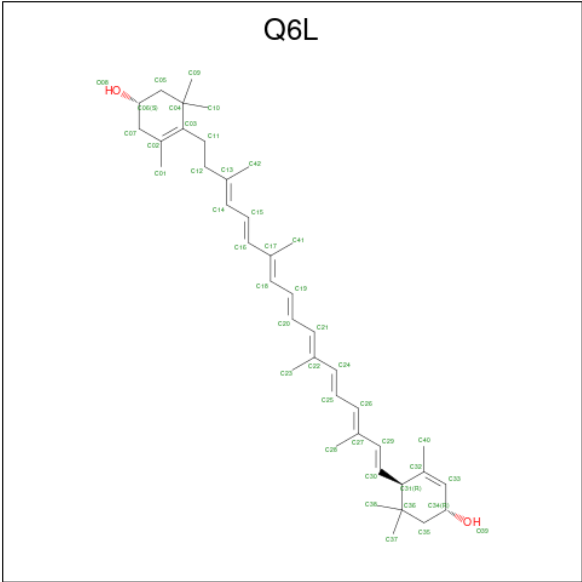
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
28	1	1	Total	C	O	P	0
			35	24	10	1	
28	2	1	Total	C	O	P	0
			33	22	10	1	
28	3	1	Total	C	O	P	0
			23	13	9	1	
28	3	1	Total	C	O	P	0
			43	32	10	1	
28	3	1	Total	C	O	P	0
			36	25	10	1	
28	3	1	Total	C	O	P	0
			43	32	10	1	
28	6	1	Total	C	O	P	0
			46	35	10	1	
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	A	1	Total	C	O	P	0
			30	19	10	1	
28	Q	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 29 is (1 {S})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaenyl]cyclohex-3-en-1-ol (CCD ID: Q6L) (formula: C₄₀H₅₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	P	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	Q	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

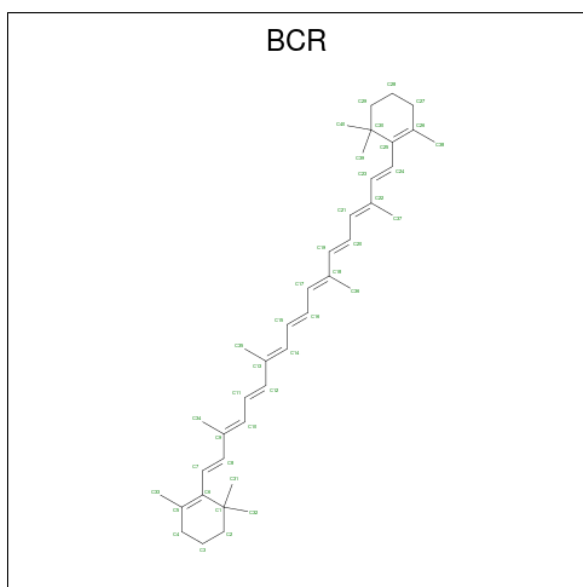
Mol	Chain	Residues	Atoms			AltConf
29	R	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	U	1	Total 42	C 40	O 2	0
29	U	1	Total 42	C 40	O 2	0
29	U	1	Total 42	C 40	O 2	0
29	V	1	Total 42	C 40	O 2	0
29	V	1	Total 42	C 40	O 2	0
29	V	1	Total 42	C 40	O 2	0
29	V	1	Total 42	C 40	O 2	0
29	W	1	Total 42	C 40	O 2	0
29	W	1	Total 42	C 40	O 2	0
29	W	1	Total 42	C 40	O 2	0
29	W	1	Total 42	C 40	O 2	0

Continued on next page...

Continued from previous page...

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

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



Mol	Chain	Residues	Atoms	AltConf
30	2	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	4	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

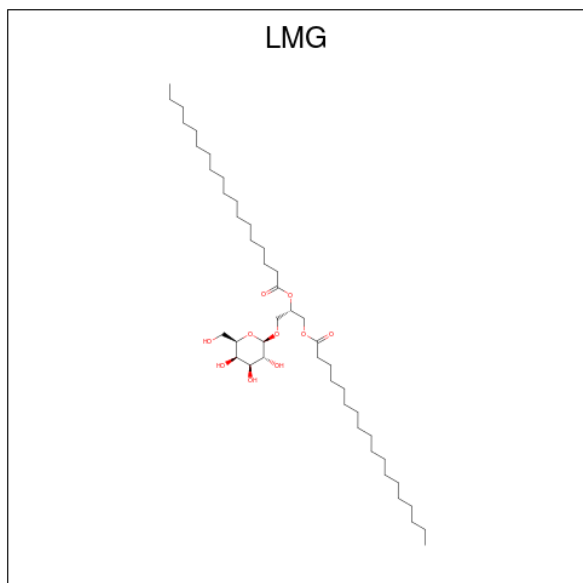
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	I	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
30	L	1	Total	C	0
			40	40	
30	M	1	Total	C	0
			40	40	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



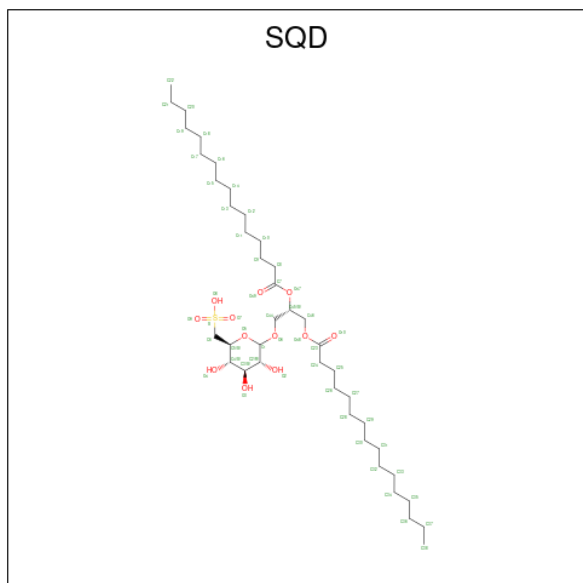
Mol	Chain	Residues	Atoms			AltConf
31	2	1	Total	C	O	0
			31	21	10	
31	5	1	Total	C	O	0
			54	44	10	
31	A	1	Total	C	O	0
			31	21	10	
31	A	1	Total	C	O	0
			27	17	10	
31	A	1	Total	C	O	0
			46	36	10	
31	B	1	Total	C	O	0
			38	28	10	
31	F	1	Total	C	O	0
			31	21	10	
31	J	1	Total	C	O	0
			46	36	10	
31	L	1	Total	C	O	0
			31	21	10	

Continued on next page...

Continued from previous page...

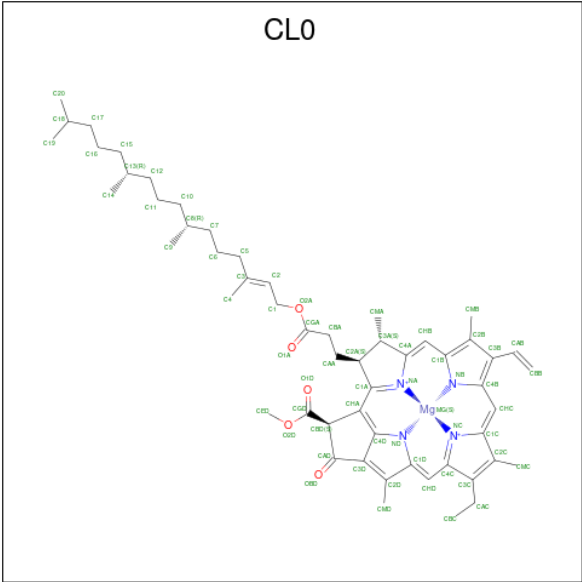
Mol	Chain	Residues	Atoms			AltConf
31	N	1	Total	C	O	0
			55	45	10	
31	O	1	Total	C	O	0
			39	29	10	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



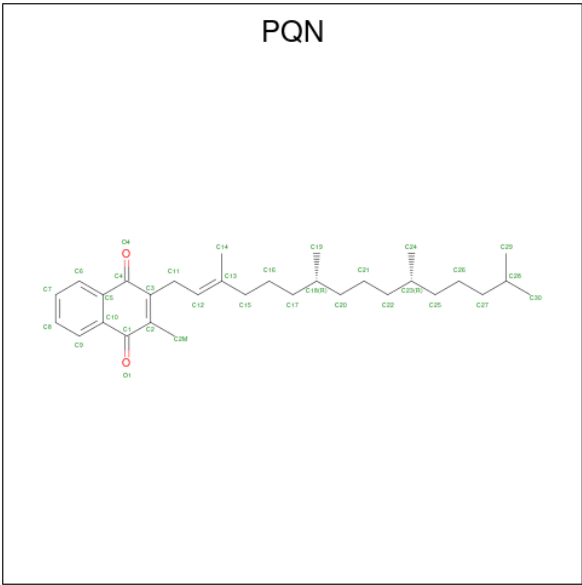
Mol	Chain	Residues	Atoms				AltConf
32	6	1	Total	C	O	S	0
			54	41	12	1	
32	H	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 33 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



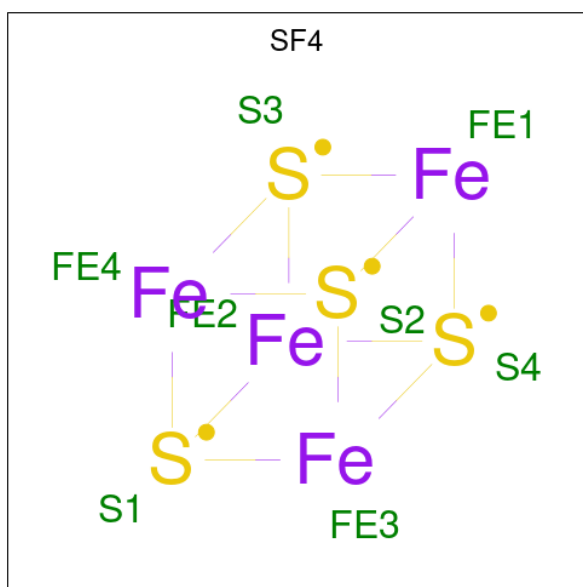
Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 34 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



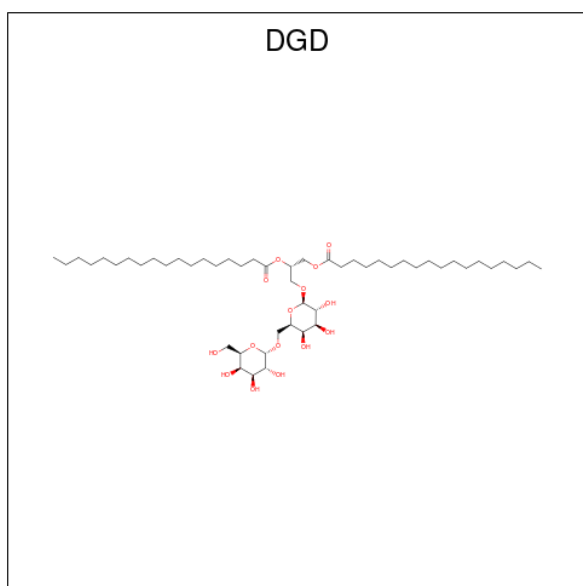
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			33	31	2	
34	B	1	Total	C	O	0
			33	31	2	

- Molecule 35 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



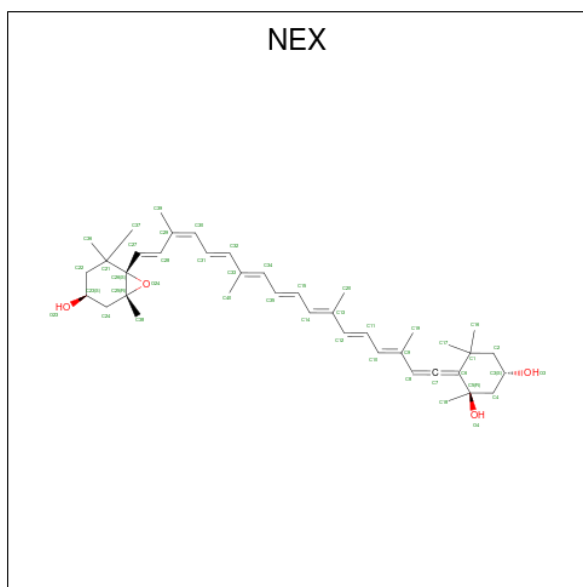
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	Fe	S	0
			8	4	4	
35	C	1	Total	Fe	S	0
			8	4	4	
35	C	1	Total	Fe	S	0
			8	4	4	

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



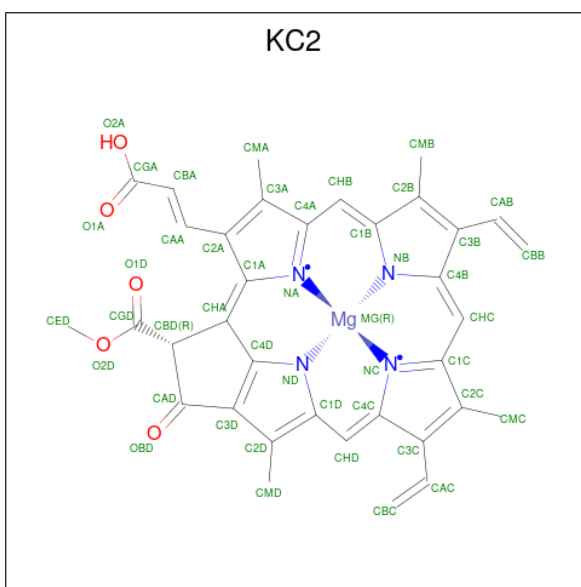
Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			51	36	15	
36	B	1	Total	C	O	0
			59	44	15	

- Molecule 37 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
37	H	1	Total	C	O	0
			44	40	4	
37	P	1	Total	C	O	0
			44	40	4	
37	R	1	Total	C	O	0
			44	40	4	
37	S	1	Total	C	O	0
			44	40	4	
37	T	1	Total	C	O	0
			44	40	4	
37	W	1	Total	C	O	0
			44	40	4	

- Molecule 38 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
38	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	X	1	Total 45	C 35	Mg 1	N 4	O 5	0

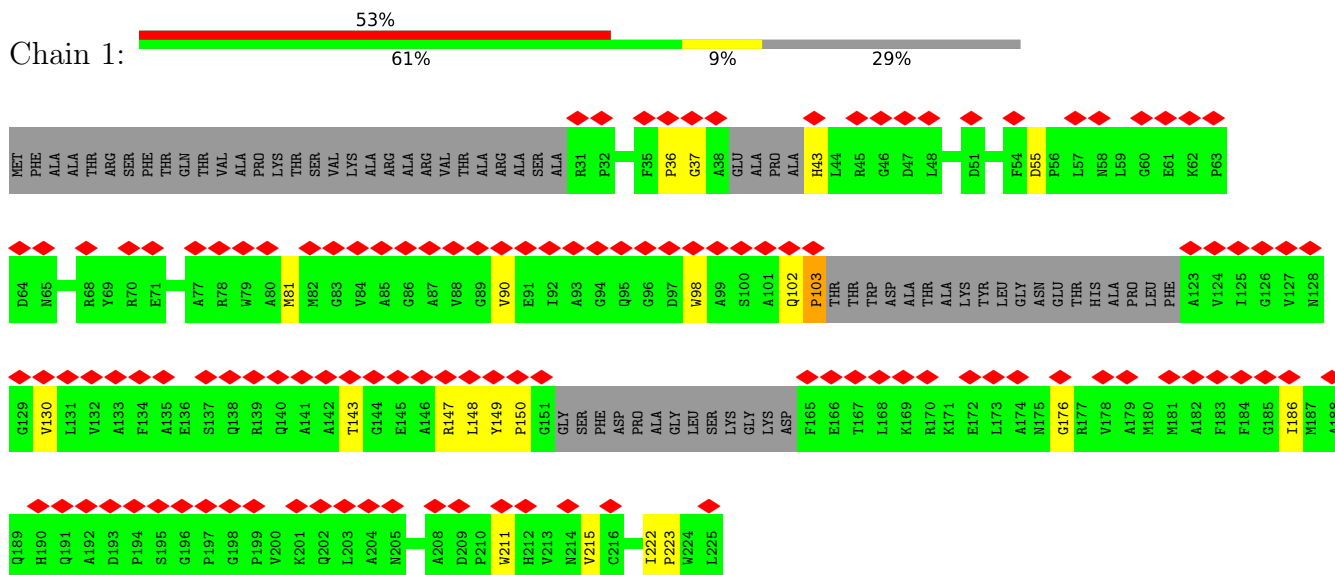
- Molecule 39 is water.

Mol	Chain	Residues	Atoms	AltConf
39	A	3	Total O 3 3	0
39	Q	1	Total O 1 1	0

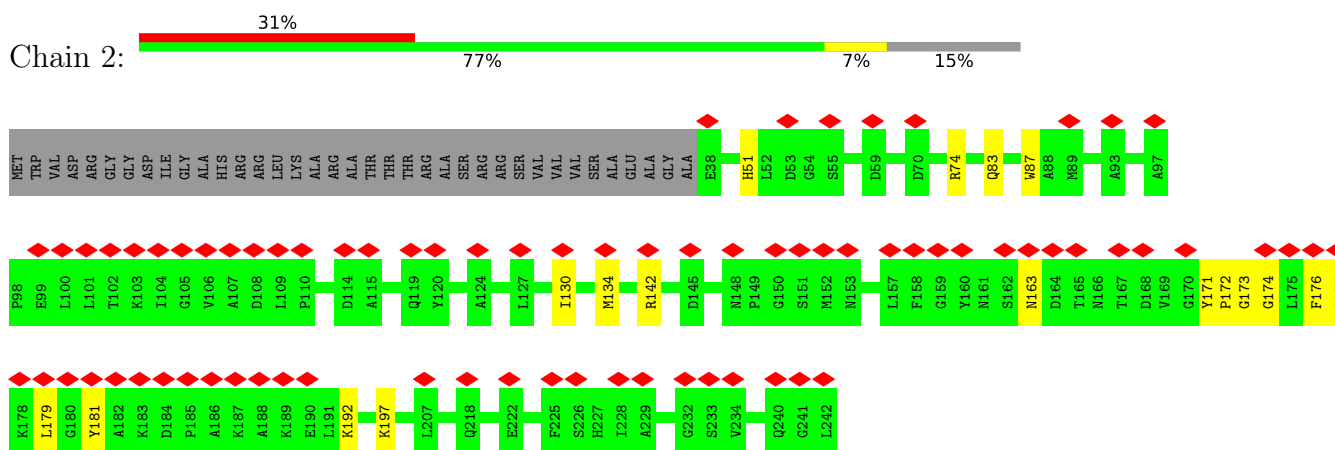
3 Residue-property plots

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: Lhca1

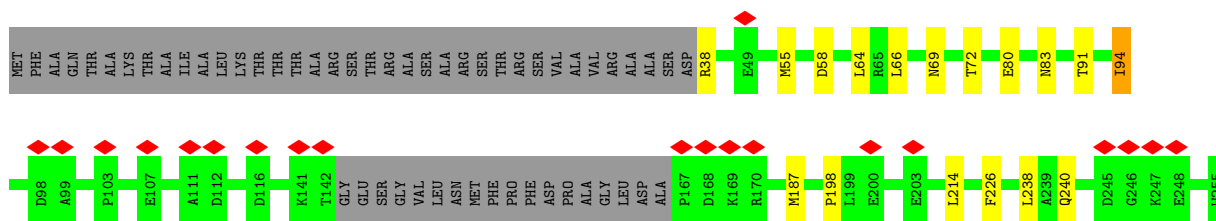


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



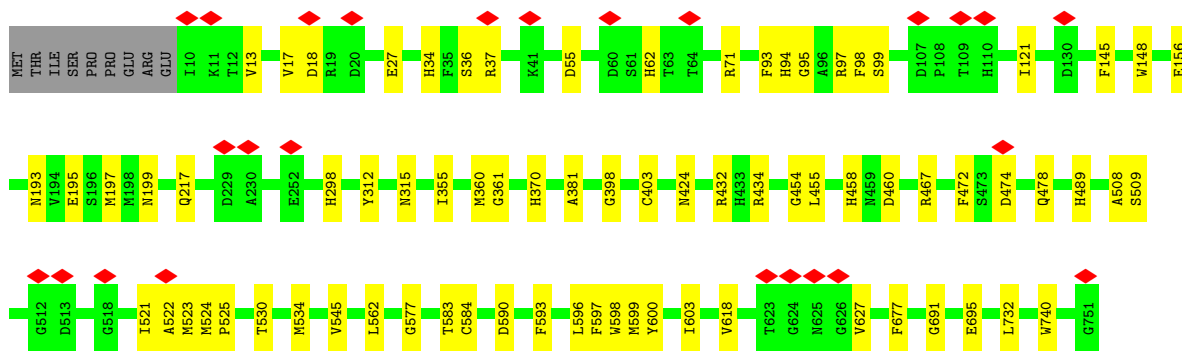
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic





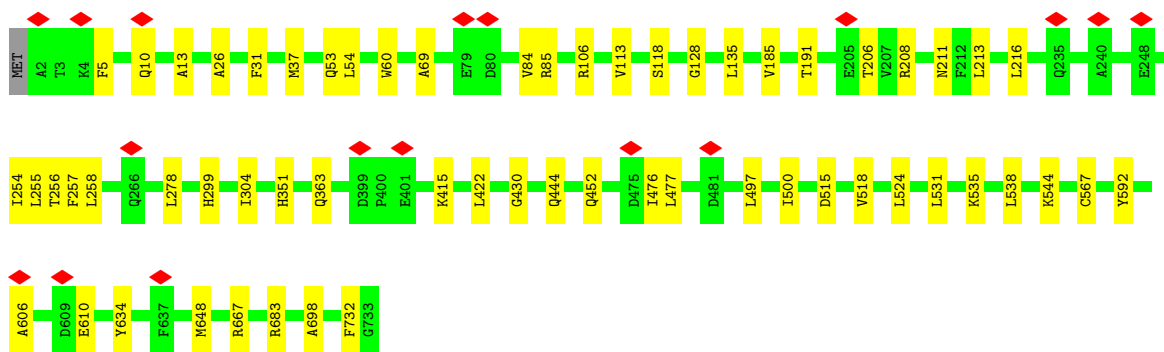
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 89% 10%



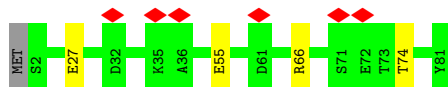
• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 92% 8%



• Molecule 9: Photosystem I iron-sulfur center

Chain C: 94% 7% 5%

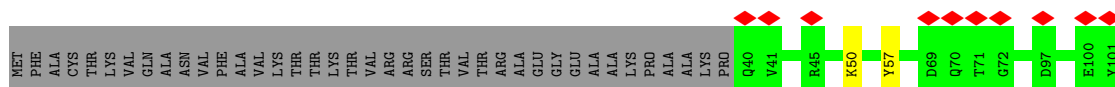


• Molecule 10: Photosystem I reaction center subunit II, chloroplastic

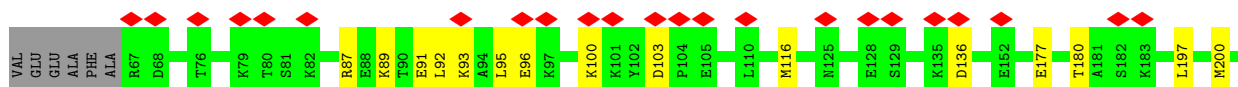
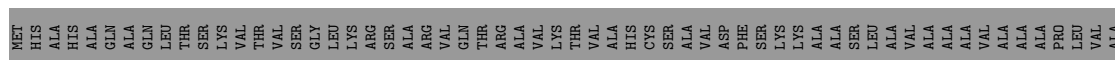
Chain D: 69% 14% 7% 24%



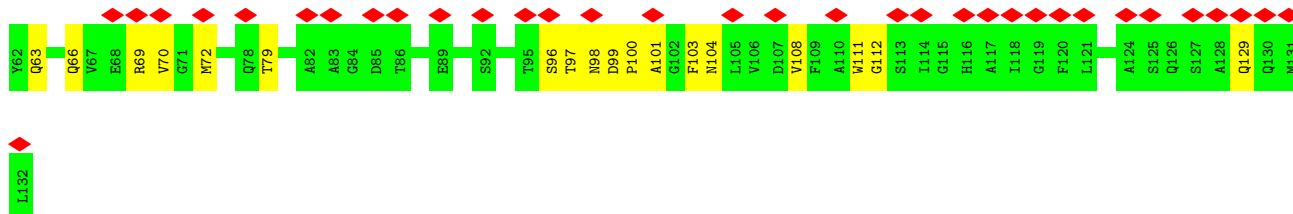
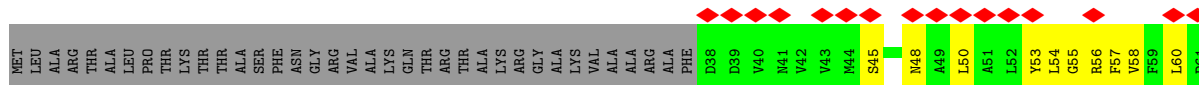
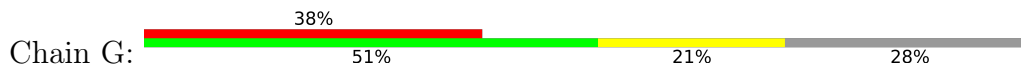
- Molecule 11: Photosystem I reaction centre subunit IV



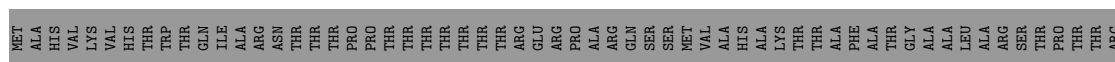
- Molecule 12: Photosystem I reaction center subunit III

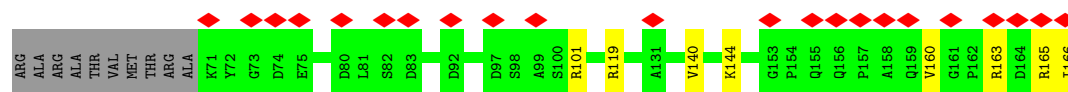


- Molecule 13: PsaG



- Molecule 14: Photosystem I PsaH, reaction centre subunit VI

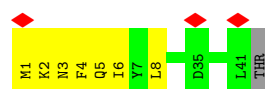
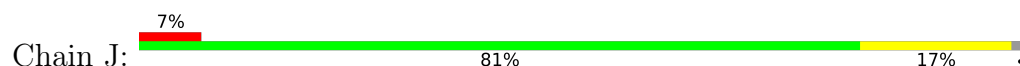




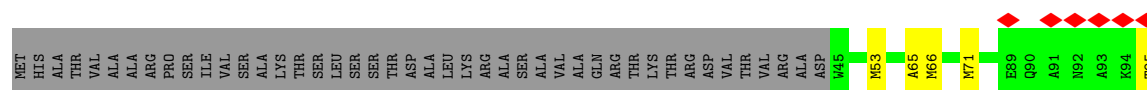
- Molecule 15: Photosystem I reaction center subunit VIII



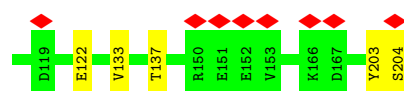
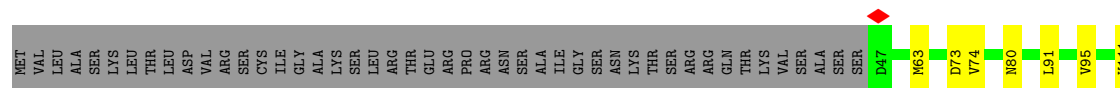
- Molecule 16: Photosystem I reaction center subunit IX



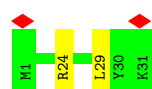
- Molecule 17: Photosystem I PsaG/PsaK protein



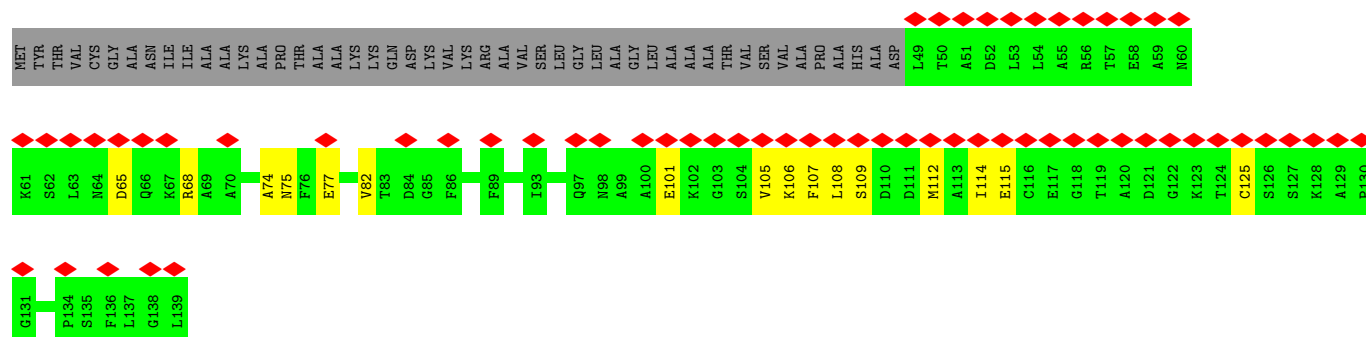
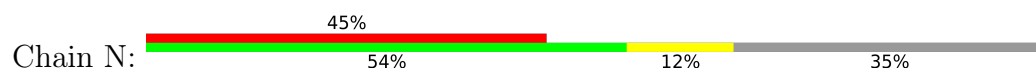
- Molecule 18: PSI subunit V



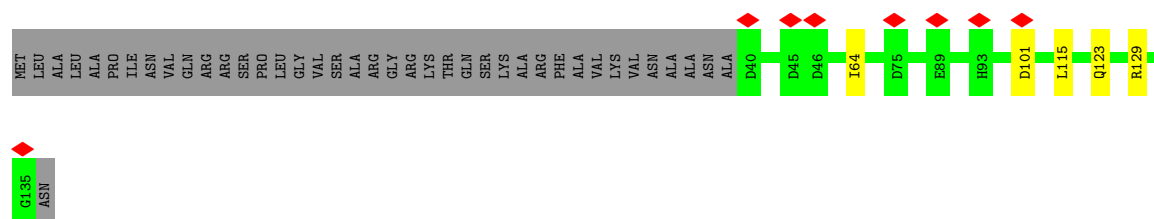
- Molecule 19: Photosystem I reaction center subunit XII



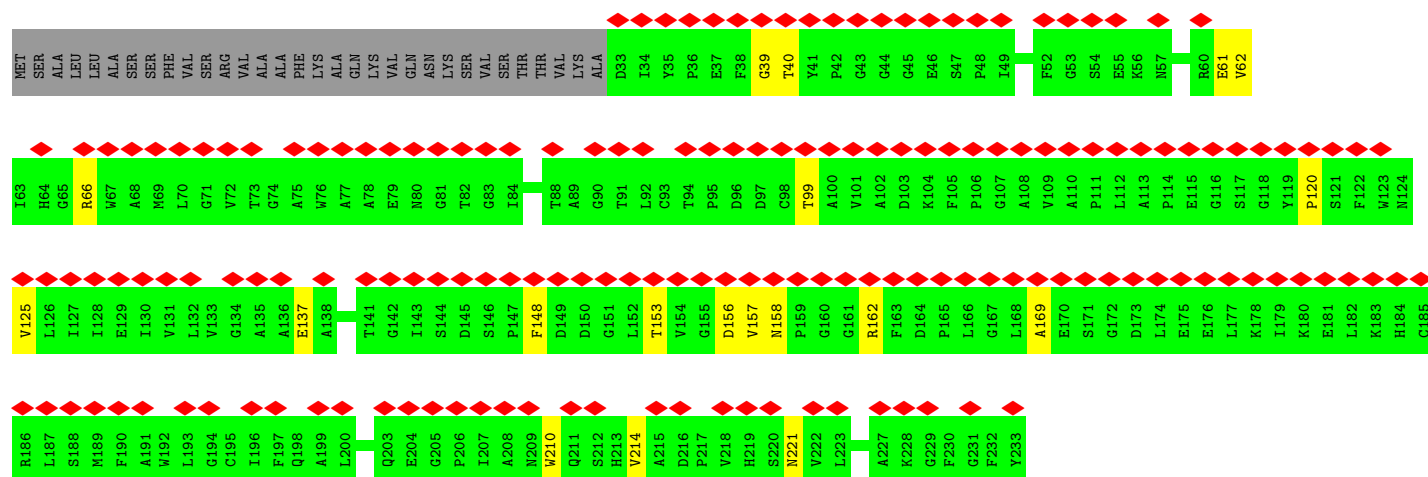
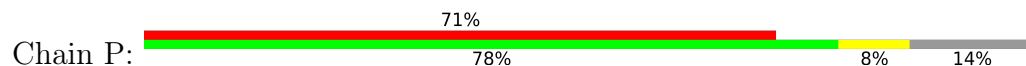
- Molecule 20: Photosystem I PsaN, reaction centre subunit N



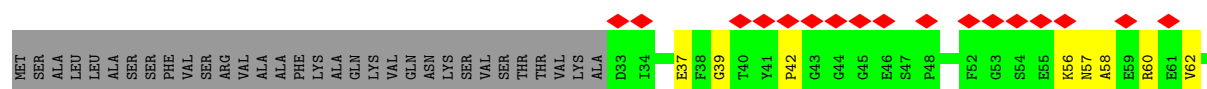
• Molecule 21: PsaO

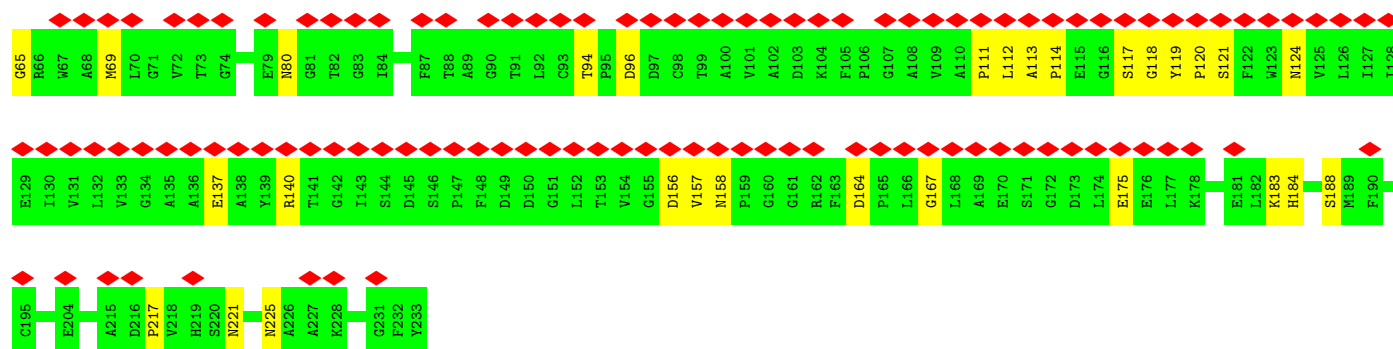


• Molecule 22: Chlorophyll a-b binding protein, chloroplastic



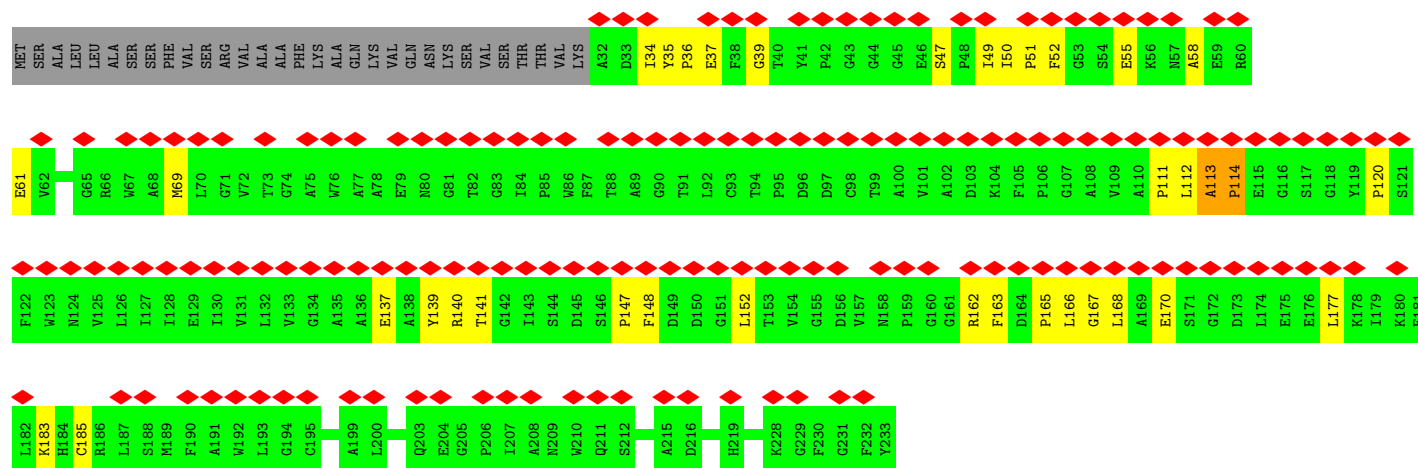
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic





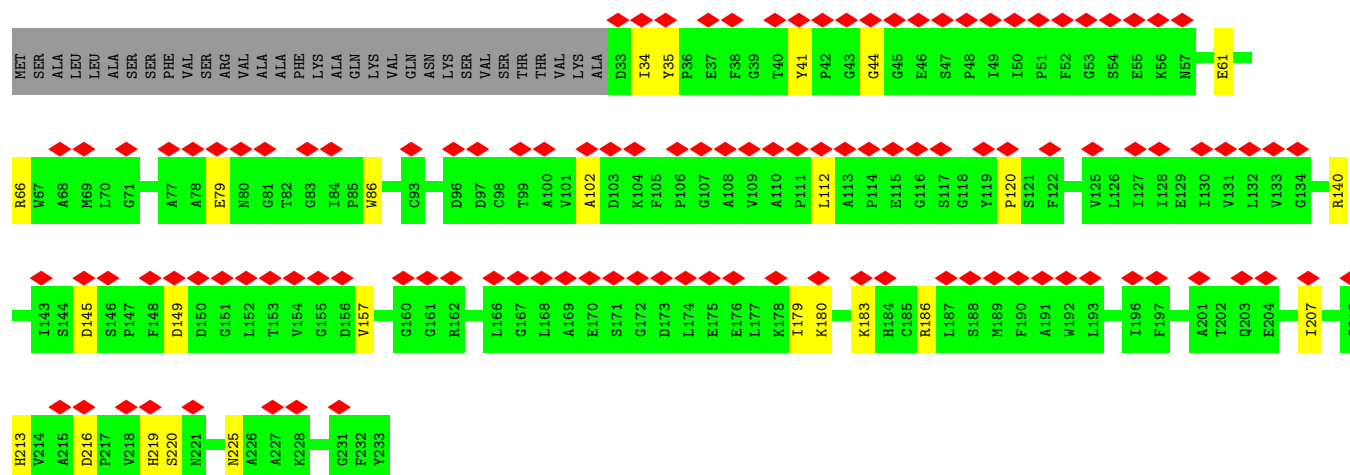
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain S: 68% 71% 15% 13%

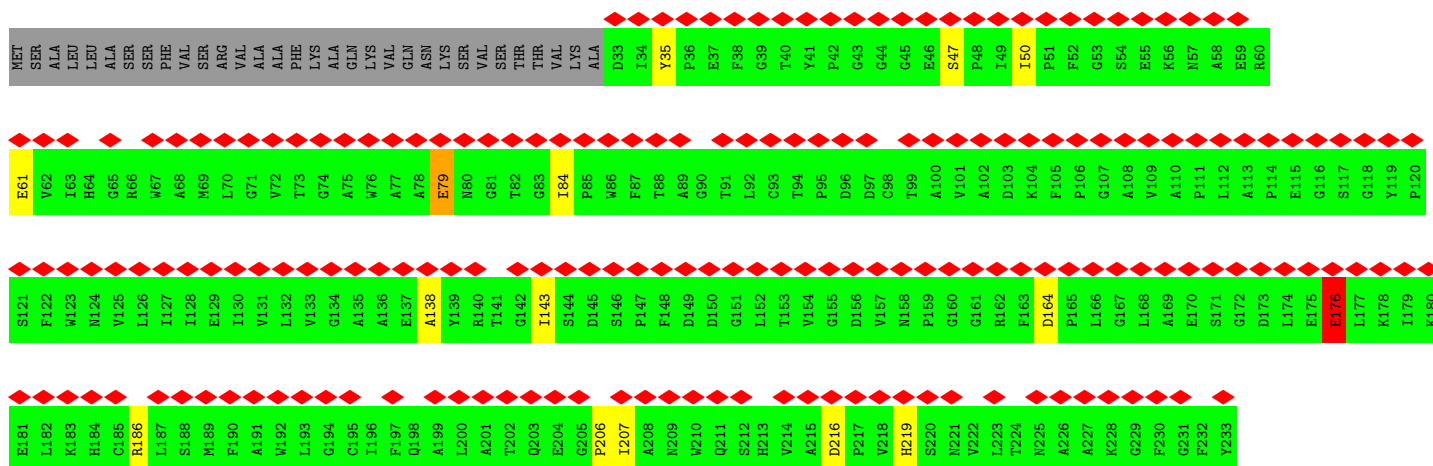
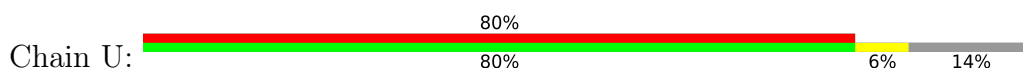


- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

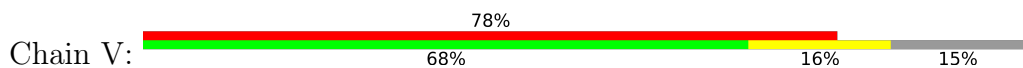
Chain T: 50% 76% 11% 14%



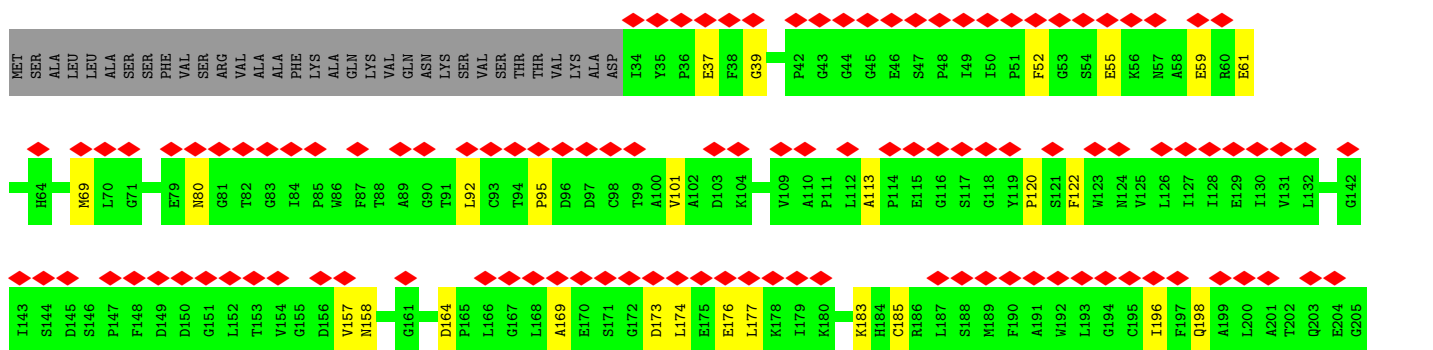
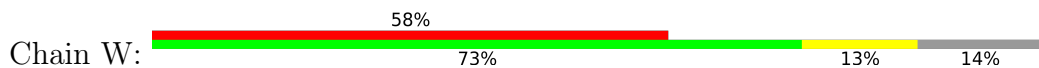
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



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

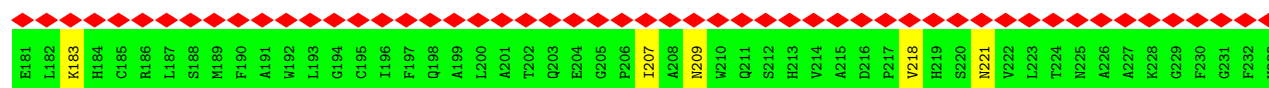
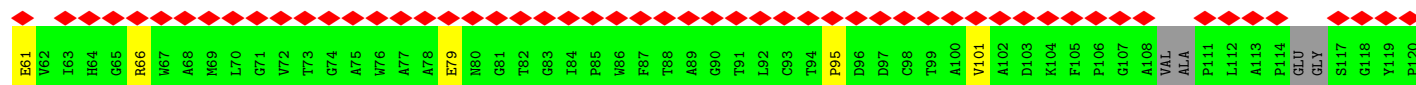
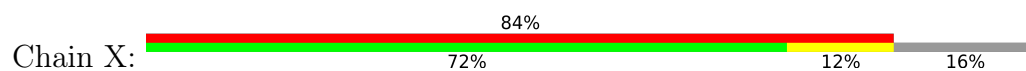


• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

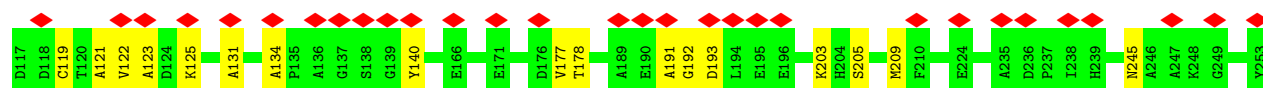
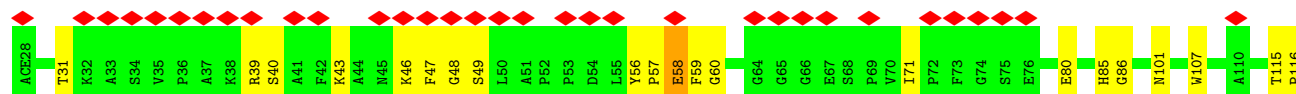
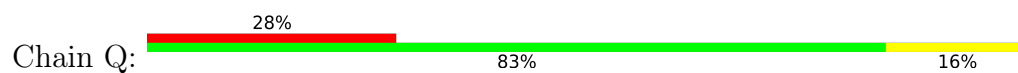




- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80366	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IWJ, KC2, TPO, BCR, PQN, SF4, CLA, CHL, SQD, XAT, LMG, DGD, ACE, LHG, NEX, Q6L, CL0

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	1	0.59	1/1242 (0.1%)	0.71	2/1686 (0.1%)
2	2	0.48	0/1634	0.63	0/2224
3	3	0.51	0/1768	0.70	0/2394
4	4	0.47	0/1630	0.65	1/2215 (0.0%)
5	5	0.50	1/1312 (0.1%)	0.64	0/1783
6	6	0.41	1/1522 (0.1%)	0.56	0/2068
7	A	0.41	0/6017	0.55	0/8202
8	B	0.41	0/5981	0.54	0/8166
9	C	0.43	0/603	0.64	0/818
10	D	0.46	0/1142	0.66	1/1537 (0.1%)
11	E	0.35	0/516	0.57	0/703
12	F	0.40	0/1286	0.57	0/1739
13	G	0.49	0/732	0.70	0/995
14	H	0.35	0/736	0.52	0/1001
15	I	0.57	0/270	0.69	0/368
16	J	0.43	0/338	0.58	0/462
17	K	0.40	0/635	0.55	0/860
18	L	0.41	0/1197	0.52	0/1635
19	M	0.43	0/242	0.46	0/328
20	N	0.47	0/685	0.75	1/921 (0.1%)
21	O	0.45	1/787 (0.1%)	0.52	0/1070
22	P	0.46	0/1553	0.69	0/2122
22	R	0.47	0/1553	0.77	2/2122 (0.1%)
22	S	0.46	0/1558	0.72	2/2129 (0.1%)
22	T	0.43	1/1553 (0.1%)	0.62	0/2122
22	U	0.46	1/1553 (0.1%)	0.67	1/2122 (0.0%)
22	V	0.54	2/1529 (0.1%)	0.70	1/2089 (0.0%)
22	W	0.45	0/1545	0.66	1/2111 (0.0%)
22	X	0.44	0/1518	0.69	2/2070 (0.1%)
23	Q	0.50	1/1746 (0.1%)	0.72	1/2379 (0.0%)
All	All	0.45	9/44383 (0.0%)	0.63	15/60441 (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
22	U	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	103	PRO	CB-CG	9.42	1.96	1.49
22	T	35	TYR	C-O	7.19	1.27	1.23
21	O	64	ILE	CA-CB	-7.08	1.50	1.54
22	V	164	ASP	N-CA	6.34	1.50	1.46
5	5	212	ILE	CA-CB	-6.25	1.50	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	111	PRO	CA-N-CD	-8.52	100.07	112.00
1	1	103	PRO	CB-CG-CD	-7.69	81.50	106.10
22	S	114	PRO	CA-N-CD	-7.23	101.88	112.00
22	X	149	ASP	CA-C-N	6.53	133.24	122.73
22	X	149	ASP	C-N-CA	6.53	133.24	122.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	U	176	GLU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1209	0	1167	16	0
2	2	1583	0	1529	17	0
3	3	1717	0	1657	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4	1579	0	1521	27	0
5	5	1278	0	1267	16	0
6	6	1484	0	1465	13	0
7	A	5819	0	5655	60	0
8	B	5773	0	5540	45	0
9	C	593	0	573	4	0
10	D	1116	0	1151	9	0
11	E	503	0	489	2	0
12	F	1259	0	1285	16	0
13	G	717	0	685	35	0
14	H	721	0	698	8	0
15	I	264	0	286	8	0
16	J	328	0	341	6	0
17	K	625	0	625	10	0
18	L	1169	0	1186	7	0
19	M	239	0	262	2	0
20	N	676	0	650	13	0
21	O	759	0	722	7	0
22	P	1507	0	1429	20	0
22	R	1507	0	1429	40	0
22	S	1512	0	1434	35	0
22	T	1507	0	1429	20	0
22	U	1507	0	1429	11	0
22	V	1484	0	1411	33	0
22	W	1499	0	1425	25	0
22	X	1474	0	1401	26	0
23	Q	1706	0	1649	33	0
24	1	96	0	68	1	0
24	2	177	0	115	0	0
24	3	45	0	30	2	0
24	4	181	0	117	4	0
24	5	41	0	24	0	0
24	6	127	0	77	0	0
24	P	233	0	163	1	0
24	Q	185	0	130	1	0
24	R	284	0	200	9	0
24	S	223	0	151	7	0
24	T	282	0	199	2	0
24	U	175	0	118	1	0
24	V	221	0	153	3	0
24	W	243	0	189	1	0
24	X	225	0	155	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	1	424	0	334	5	0
25	2	530	0	430	6	0
25	3	602	0	470	5	0
25	4	510	0	396	4	0
25	5	430	0	345	2	0
25	6	494	0	412	5	0
25	A	2557	0	2585	16	0
25	B	2465	0	2485	25	0
25	F	83	0	60	1	0
25	G	132	0	97	3	0
25	H	154	0	138	0	0
25	J	42	0	31	1	0
25	K	218	0	201	3	0
25	L	188	0	152	0	0
25	N	87	0	61	0	0
25	O	247	0	217	2	0
25	P	467	0	454	5	0
25	Q	458	0	387	8	0
25	R	467	0	454	5	0
25	S	443	0	414	13	0
25	T	438	0	411	3	0
25	U	378	0	296	1	0
25	V	412	0	347	13	0
25	W	427	0	379	11	0
25	X	373	0	290	9	0
26	1	44	0	0	0	0
26	3	44	0	0	1	0
26	4	88	0	0	2	0
26	5	44	0	0	0	0
26	6	44	0	0	2	0
26	P	88	0	0	2	0
26	Q	88	0	0	1	0
26	R	88	0	0	1	0
26	S	132	0	0	2	0
26	T	88	0	0	2	0
26	U	44	0	0	0	0
26	V	132	0	0	2	0
26	W	44	0	0	2	0
26	X	44	0	0	0	0
27	1	44	0	56	0	0
27	2	44	0	56	0	0
27	3	44	0	56	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	4	44	0	56	1	0
27	5	44	0	56	0	0
27	6	44	0	56	1	0
28	1	35	0	40	1	0
28	2	33	0	36	1	0
28	3	145	0	180	0	0
28	6	46	0	65	1	0
28	A	79	0	104	0	0
28	Q	35	0	40	0	0
29	2	42	0	0	1	0
29	O	84	0	0	1	0
29	P	168	0	0	1	0
29	Q	126	0	0	1	0
29	R	210	0	0	0	0
29	S	210	0	0	1	0
29	T	168	0	0	1	0
29	U	126	0	0	2	0
29	V	168	0	0	1	0
29	W	168	0	0	2	0
29	X	166	0	0	1	0
30	2	40	0	56	0	0
30	3	120	0	168	1	0
30	4	40	0	56	2	0
30	A	200	0	280	3	0
30	B	200	0	280	2	0
30	F	80	0	112	1	0
30	G	80	0	112	4	0
30	H	40	0	56	0	0
30	I	40	0	56	0	0
30	J	80	0	112	2	0
30	K	120	0	168	2	0
30	L	120	0	168	2	0
30	M	40	0	56	1	0
31	2	31	0	32	0	0
31	5	54	0	81	0	0
31	A	104	0	121	0	0
31	B	38	0	46	0	0
31	F	31	0	32	1	0
31	J	46	0	65	0	0
31	L	31	0	32	0	0
31	N	55	0	86	0	0
31	O	39	0	48	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	6	54	0	78	0	0
32	H	48	0	60	1	0
33	A	65	0	72	0	0
34	A	33	0	46	1	0
34	B	33	0	46	0	0
35	A	8	0	0	0	0
35	C	16	0	0	0	0
36	A	51	0	60	1	0
36	B	59	0	79	1	0
37	H	44	0	56	0	0
37	P	44	0	56	1	0
37	R	44	0	56	0	0
37	S	44	0	56	0	0
37	T	44	0	56	0	0
37	W	44	0	56	0	0
38	P	45	0	0	1	0
38	Q	45	0	0	0	0
38	R	45	0	0	2	0
38	S	45	0	0	1	0
38	T	45	0	0	1	0
38	U	45	0	0	0	0
38	V	45	0	0	1	0
38	W	45	0	0	0	0
38	X	45	0	0	0	0
39	A	3	0	0	0	0
39	Q	1	0	0	0	0
All	All	64832	0	59326	584	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 584 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:103:PRO:CG	1:1:103:PRO:CB	1.96	1.39
7:A:489:HIS:NE2	21:O:101:ASP:OD1	1.65	1.30
5:5:97:GLU:OE2	5:5:103:ALA:HB2	1.12	1.28
5:5:97:GLU:OE2	5:5:103:ALA:CB	1.84	1.25
15:I:23:MET:HE2	30:L:305:BCR:H352	1.23	1.15

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1	151/225 (67%)	144 (95%)	6 (4%)	1 (1%)	18	40
2	2	203/242 (84%)	197 (97%)	6 (3%)	0	100	100
3	3	225/272 (83%)	215 (96%)	10 (4%)	0	100	100
4	4	199/236 (84%)	190 (96%)	9 (4%)	0	100	100
5	5	162/217 (75%)	158 (98%)	4 (2%)	0	100	100
6	6	190/249 (76%)	187 (98%)	3 (2%)	0	100	100
7	A	740/751 (98%)	724 (98%)	16 (2%)	0	100	100
8	B	730/733 (100%)	706 (97%)	24 (3%)	0	100	100
9	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
10	D	141/188 (75%)	135 (96%)	6 (4%)	0	100	100
11	E	60/101 (59%)	59 (98%)	1 (2%)	0	100	100
12	F	163/231 (71%)	159 (98%)	4 (2%)	0	100	100
13	G	93/132 (70%)	89 (96%)	4 (4%)	0	100	100
14	H	94/166 (57%)	93 (99%)	1 (1%)	0	100	100
15	I	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
16	J	39/42 (93%)	37 (95%)	2 (5%)	0	100	100
17	K	85/131 (65%)	84 (99%)	1 (1%)	0	100	100
18	L	156/204 (76%)	153 (98%)	3 (2%)	0	100	100
19	M	29/31 (94%)	29 (100%)	0	0	100	100
20	N	89/139 (64%)	83 (93%)	6 (7%)	0	100	100
21	O	94/136 (69%)	93 (99%)	1 (1%)	0	100	100
22	P	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
22	R	199/233 (85%)	185 (93%)	14 (7%)	0	100	100
22	S	200/233 (86%)	190 (95%)	9 (4%)	1 (0%)	24	49
22	T	199/233 (85%)	189 (95%)	10 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	U	199/233 (85%)	191 (96%)	8 (4%)	0	100	100
22	V	193/233 (83%)	188 (97%)	5 (3%)	0	100	100
22	W	198/233 (85%)	188 (95%)	10 (5%)	0	100	100
22	X	190/233 (82%)	184 (97%)	6 (3%)	0	100	100
23	Q	223/226 (99%)	212 (95%)	11 (5%)	0	100	100
All	All	5554/6632 (84%)	5362 (96%)	190 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	S	120	PRO
1	1	150	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	118/166 (71%)	118 (100%)	0	100	100
2	2	160/186 (86%)	160 (100%)	0	100	100
3	3	173/208 (83%)	173 (100%)	0	100	100
4	4	159/186 (86%)	159 (100%)	0	100	100
5	5	127/163 (78%)	127 (100%)	0	100	100
6	6	148/188 (79%)	148 (100%)	0	100	100
7	A	600/609 (98%)	600 (100%)	0	100	100
8	B	584/585 (100%)	584 (100%)	0	100	100
9	C	66/67 (98%)	66 (100%)	0	100	100
10	D	118/150 (79%)	118 (100%)	0	100	100
11	E	55/85 (65%)	55 (100%)	0	100	100
12	F	130/176 (74%)	130 (100%)	0	100	100
13	G	73/99 (74%)	73 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	H	72/128 (56%)	72 (100%)	0	100	100
15	I	29/29 (100%)	29 (100%)	0	100	100
16	J	35/36 (97%)	35 (100%)	0	100	100
17	K	66/101 (65%)	66 (100%)	0	100	100
18	L	125/165 (76%)	125 (100%)	0	100	100
19	M	27/27 (100%)	27 (100%)	0	100	100
20	N	72/103 (70%)	72 (100%)	0	100	100
21	O	80/110 (73%)	80 (100%)	0	100	100
22	P	153/179 (86%)	153 (100%)	0	100	100
22	R	153/179 (86%)	153 (100%)	0	100	100
22	S	153/179 (86%)	153 (100%)	0	100	100
22	T	153/179 (86%)	153 (100%)	0	100	100
22	U	153/179 (86%)	153 (100%)	0	100	100
22	V	151/179 (84%)	151 (100%)	0	100	100
22	W	152/179 (85%)	152 (100%)	0	100	100
22	X	150/179 (84%)	150 (100%)	0	100	100
23	Q	167/167 (100%)	166 (99%)	1 (1%)	78	89
All	All	4402/5166 (85%)	4401 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	Q	58	GLU

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

Mol	Chain	Res	Type
16	J	30	ASN
23	Q	229	ASN
22	V	209	ASN
22	U	219	HIS
8	B	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	TPO	Q	31	23	8,10,11	1.75	1 (12%)	10,14,16	1.21	1 (10%)

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
23	TPO	Q	31	23	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Q	31	TPO	P-O1P	3.60	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	31	TPO	P-OG1-CB	-2.57	116.33	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Q	31	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

449 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	6	601	6	36,50,74	2.84	9 (25%)	31,85,114	1.93	11 (35%)
25	CLA	A	828	-	63,67,73	1.25	8 (12%)	74,105,113	1.27	9 (12%)
25	CLA	A	829	-	69,73,73	1.16	6 (8%)	82,113,113	1.42	15 (18%)
25	CLA	B	803	-	69,73,73	1.22	9 (13%)	82,113,113	1.46	14 (17%)
25	CLA	A	833	-	54,58,73	1.38	8 (14%)	64,95,113	1.32	9 (14%)
25	CLA	A	810	7	69,73,73	1.17	10 (14%)	82,113,113	1.31	9 (10%)
25	CLA	Q	301	14	59,63,73	1.30	8 (13%)	70,101,113	1.56	11 (15%)
24	CHL	1	601	1	49,63,74	2.67	12 (24%)	45,101,114	1.76	11 (24%)
24	CHL	S	314	22	38,53,74	2.96	9 (23%)	31,88,114	1.87	10 (32%)
25	CLA	L	301	18	45,49,73	1.40	7 (15%)	54,84,113	1.35	5 (9%)
25	CLA	B	843	28	69,73,73	1.14	8 (11%)	82,113,113	1.44	10 (12%)
31	LMG	N	201	-	55,55,55	0.91	2 (3%)	63,63,63	1.16	4 (6%)
31	LMG	L	308	-	31,31,55	1.21	2 (6%)	39,39,63	1.04	2 (5%)
25	CLA	U	310	-	47,52,73	1.38	7 (14%)	55,87,113	1.32	8 (14%)
26	IWJ	5	611	-	43,45,45	1.56	4 (9%)	47,65,65	1.41	6 (12%)
37	NEX	T	317	-	40,46,46	1.35	6 (15%)	50,70,70	2.40	16 (32%)
24	CHL	U	306	-	38,52,74	3.04	11 (28%)	31,87,114	1.73	9 (29%)
30	BCR	H	305	-	41,41,41	1.18	3 (7%)	56,56,56	1.80	18 (32%)
25	CLA	X	314	-	45,49,73	1.41	6 (13%)	54,84,113	1.32	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	J	102	16	46,50,73	1.35	8 (17%)	53,85,113	1.46	5 (9%)
25	CLA	A	831	-	69,73,73	1.21	10 (14%)	82,113,113	1.40	8 (9%)
29	Q6L	R	323	-	42,43,43	1.93	7 (16%)	51,60,60	1.94	10 (19%)
26	IWJ	Q	303	-	43,45,45	1.58	6 (13%)	47,65,65	1.50	9 (19%)
29	Q6L	T	315	-	42,43,43	1.89	8 (19%)	51,60,60	1.63	7 (13%)
25	CLA	5	608	5	45,49,73	1.43	7 (15%)	54,84,113	1.44	5 (9%)
38	KC2	X	309	22	49,53,53	2.21	16 (32%)	60,89,89	2.28	21 (35%)
38	KC2	R	312	22	49,53,53	2.16	14 (28%)	60,89,89	2.18	19 (31%)
28	LHG	A	846	-	48,48,48	0.93	2 (4%)	51,54,54	0.98	2 (3%)
25	CLA	A	832	-	69,73,73	1.19	5 (7%)	82,113,113	1.15	5 (6%)
35	SF4	C	102	9	0,12,12	-	-	-	-	-
25	CLA	P	310	22	64,68,73	1.22	6 (9%)	76,107,113	1.28	8 (10%)
30	BCR	2	618	-	41,41,41	1.14	3 (7%)	56,56,56	2.18	14 (25%)
38	KC2	S	308	22	49,53,53	2.17	14 (28%)	60,89,89	2.22	15 (25%)
24	CHL	2	615	2	37,51,74	3.07	11 (29%)	30,86,114	2.08	12 (40%)
25	CLA	A	805	-	69,73,73	1.20	5 (7%)	82,113,113	1.49	10 (12%)
25	CLA	A	822	-	49,53,73	1.36	8 (16%)	58,89,113	1.26	7 (12%)
25	CLA	N	202	20	48,53,73	1.37	6 (12%)	56,89,113	1.33	5 (8%)
29	Q6L	U	317	-	42,43,43	1.90	8 (19%)	51,60,60	1.82	8 (15%)
25	CLA	P	311	-	64,68,73	1.18	4 (6%)	76,107,113	1.39	12 (15%)
24	CHL	P	305	-	40,54,74	3.09	12 (30%)	34,90,114	1.97	11 (32%)
25	CLA	3	312	-	43,48,73	1.45	8 (18%)	51,83,113	1.33	8 (15%)
25	CLA	X	311	22	54,58,73	1.31	6 (11%)	64,95,113	1.21	5 (7%)
25	CLA	T	312	22	59,63,73	1.25	8 (13%)	70,101,113	1.32	7 (10%)
29	Q6L	S	316	-	42,43,43	1.90	7 (16%)	51,60,60	1.96	9 (17%)
24	CHL	R	308	22	40,54,74	2.89	11 (27%)	34,90,114	1.83	13 (38%)
24	CHL	S	307	-	36,50,74	3.15	11 (30%)	29,85,114	2.07	12 (41%)
25	CLA	4	313	4	61,65,73	1.25	7 (11%)	72,103,113	1.45	8 (11%)
25	CLA	B	838	-	54,58,73	1.28	8 (14%)	64,95,113	1.40	5 (7%)
25	CLA	B	840	-	51,55,73	1.35	7 (13%)	60,91,113	1.41	6 (10%)
29	Q6L	W	320	-	42,43,43	1.91	7 (16%)	51,60,60	1.77	7 (13%)
25	CLA	T	301	22	69,73,73	1.19	9 (13%)	82,113,113	1.50	14 (17%)
25	CLA	W	310	22	64,68,73	1.21	6 (9%)	76,107,113	1.11	4 (5%)
24	CHL	R	310	-	46,60,74	2.73	13 (28%)	40,97,114	1.93	14 (35%)
24	CHL	X	307	-	46,60,74	2.76	11 (23%)	40,97,114	2.63	16 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	6	609	-	48,52,73	1.43	4 (8%)	57,88,113	1.62	10 (17%)
24	CHL	P	306	-	46,60,74	2.68	14 (30%)	40,97,114	1.77	15 (37%)
27	XAT	4	318	-	41,47,47	1.17	5 (12%)	54,74,74	3.04	24 (44%)
25	CLA	2	606	-	49,53,73	1.36	7 (14%)	58,89,113	1.39	7 (12%)
25	CLA	V	309	22	46,50,73	1.57	8 (17%)	53,85,113	1.79	13 (24%)
25	CLA	B	839	-	69,73,73	1.20	8 (11%)	82,113,113	1.24	5 (6%)
25	CLA	B	804	-	69,73,73	1.19	9 (13%)	82,113,113	1.29	7 (8%)
26	IWJ	P	320	-	43,45,45	1.61	6 (13%)	47,65,65	1.70	7 (14%)
25	CLA	P	313	-	52,56,73	1.33	6 (11%)	61,92,113	1.24	6 (9%)
25	CLA	X	303	-	55,59,73	1.27	5 (9%)	64,96,113	1.18	4 (6%)
26	IWJ	S	318	-	43,45,45	1.51	5 (11%)	47,65,65	1.63	6 (12%)
25	CLA	6	607	6	49,53,73	1.45	11 (22%)	58,89,113	1.46	8 (13%)
25	CLA	S	301	22	69,73,73	1.23	9 (13%)	82,113,113	1.30	13 (15%)
25	CLA	6	612	6	49,53,73	1.37	7 (14%)	58,89,113	1.23	5 (8%)
25	CLA	A	827	39	69,73,73	1.26	10 (14%)	82,113,113	1.57	16 (19%)
25	CLA	1	602	1	60,64,73	1.32	7 (11%)	71,102,113	1.26	9 (12%)
27	XAT	3	316	-	41,47,47	1.22	6 (14%)	54,74,74	3.02	23 (42%)
25	CLA	U	301	22	49,53,73	1.40	7 (14%)	58,89,113	1.44	10 (17%)
25	CLA	B	841	-	69,73,73	1.23	10 (14%)	82,113,113	1.36	11 (13%)
29	Q6L	W	319	-	42,43,43	1.91	7 (16%)	51,60,60	1.75	7 (13%)
38	KC2	U	307	22	49,53,53	2.15	13 (26%)	60,89,89	2.12	14 (23%)
30	BCR	L	306	-	41,41,41	1.15	4 (9%)	56,56,56	2.07	20 (35%)
24	CHL	V	305	22	37,51,74	2.85	12 (32%)	30,86,114	2.07	13 (43%)
25	CLA	A	803	-	69,73,73	1.15	6 (8%)	82,113,113	1.39	11 (13%)
25	CLA	B	828	-	69,73,73	1.19	8 (11%)	82,113,113	1.28	9 (10%)
24	CHL	X	305	22	36,50,74	3.03	13 (36%)	29,85,114	1.81	11 (37%)
25	CLA	B	829	-	69,73,73	1.20	8 (11%)	82,113,113	1.44	10 (12%)
25	CLA	F	802	-	46,50,73	1.42	10 (21%)	53,85,113	1.38	7 (13%)
35	SF4	A	853	8,7	0,12,12	-	-	-	-	-
25	CLA	B	830	-	69,73,73	1.18	7 (10%)	82,113,113	1.22	8 (9%)
30	BCR	A	849	-	41,41,41	1.10	3 (7%)	56,56,56	2.24	19 (33%)
27	XAT	1	612	-	41,47,47	1.31	7 (17%)	54,74,74	3.02	28 (51%)
24	CHL	T	305	-	43,57,74	2.88	12 (27%)	37,93,114	2.15	13 (35%)
27	XAT	2	617	-	41,47,47	1.16	4 (9%)	54,74,74	2.80	27 (50%)
25	CLA	O	2003	-	45,49,73	1.39	6 (13%)	54,84,113	1.19	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	U	312	-	45,49,73	1.41	6 (13%)	54,84,113	1.23	5 (9%)
25	CLA	O	2004	-	45,49,73	1.40	7 (15%)	54,84,113	1.43	6 (11%)
25	CLA	T	313	-	46,50,73	1.39	8 (17%)	53,85,113	1.20	3 (5%)
25	CLA	T	310	22	46,50,73	1.42	7 (15%)	53,85,113	1.18	3 (5%)
25	CLA	B	815	-	69,73,73	1.20	9 (13%)	82,113,113	1.68	11 (13%)
25	CLA	P	301	22	69,73,73	1.16	8 (11%)	82,113,113	1.36	10 (12%)
32	SQD	H	303	-	46,48,54	1.23	3 (6%)	56,59,65	1.11	3 (5%)
25	CLA	W	311	-	49,53,73	1.34	7 (14%)	58,89,113	1.39	7 (12%)
25	CLA	P	309	22	68,72,73	1.12	7 (10%)	80,111,113	1.47	11 (13%)
31	LMG	O	2008	-	39,39,55	1.06	2 (5%)	47,47,63	1.15	3 (6%)
30	BCR	K	207	-	41,41,41	1.26	5 (12%)	56,56,56	2.10	14 (25%)
25	CLA	Q	304	23	69,73,73	1.21	8 (11%)	82,113,113	1.54	6 (7%)
25	CLA	V	311	-	64,68,73	1.21	6 (9%)	76,107,113	1.27	7 (9%)
25	CLA	6	603	6	47,52,73	1.51	9 (19%)	55,88,113	1.43	11 (20%)
24	CHL	R	311	-	38,52,74	3.12	14 (36%)	31,87,114	1.86	7 (22%)
30	BCR	L	307	-	41,41,41	1.12	2 (4%)	56,56,56	2.59	19 (33%)
24	CHL	2	605	-	36,50,74	3.00	12 (33%)	31,85,114	1.86	8 (25%)
25	CLA	B	818	-	59,63,73	1.28	7 (11%)	70,101,113	1.47	12 (17%)
29	Q6L	T	319	-	42,43,43	1.89	7 (16%)	51,60,60	1.96	7 (13%)
24	CHL	R	302	-	41,55,74	2.87	12 (29%)	35,91,114	1.95	12 (34%)
24	CHL	4	308	-	40,54,74	3.04	11 (27%)	34,90,114	2.15	12 (35%)
25	CLA	T	311	-	64,68,73	1.20	6 (9%)	76,107,113	1.34	8 (10%)
29	Q6L	O	2007	-	42,43,43	1.97	9 (21%)	51,60,60	1.71	8 (15%)
25	CLA	F	803	12	45,49,73	1.42	7 (15%)	54,84,113	1.54	9 (16%)
25	CLA	Q	305	-	47,52,73	1.39	6 (12%)	55,87,113	1.22	4 (7%)
25	CLA	2	604	-	46,51,73	1.39	4 (8%)	54,86,113	1.28	8 (14%)
24	CHL	V	307	-	38,52,74	3.05	10 (26%)	31,87,114	1.83	9 (29%)
26	IWJ	Q	320	-	43,45,45	1.44	4 (9%)	47,65,65	1.67	9 (19%)
25	CLA	L	304	-	46,50,73	1.37	8 (17%)	53,85,113	1.42	5 (9%)
25	CLA	B	813	-	69,73,73	1.21	8 (11%)	82,113,113	1.57	17 (20%)
25	CLA	1	608	1	69,73,73	1.23	8 (11%)	82,113,113	1.24	8 (9%)
24	CHL	4	302	4	46,60,74	2.77	15 (32%)	40,97,114	2.07	15 (37%)
26	IWJ	4	301	-	43,45,45	1.56	4 (9%)	47,65,65	1.26	4 (8%)
29	Q6L	X	301	-	42,43,43	1.94	8 (19%)	51,60,60	1.74	8 (15%)
24	CHL	3	306	-	38,53,74	2.90	15 (39%)	36,89,114	1.72	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	T	306	-	46,60,74	2.57	12 (26%)	40,97,114	1.73	15 (37%)
25	CLA	4	314	-	45,49,73	1.38	6 (13%)	54,84,113	1.39	6 (11%)
24	CHL	R	309	-	44,58,74	2.82	13 (29%)	37,94,114	2.16	15 (40%)
25	CLA	A	823	39	69,73,73	1.23	8 (11%)	82,113,113	1.36	12 (14%)
25	CLA	W	303	-	54,58,73	1.30	9 (16%)	64,95,113	1.38	10 (15%)
24	CHL	6	605	-	36,50,74	2.98	9 (25%)	31,85,114	1.79	8 (25%)
25	CLA	B	814	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	8 (9%)
25	CLA	2	614	2	47,52,73	1.31	6 (12%)	55,87,113	1.45	7 (12%)
25	CLA	B	812	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	9 (10%)
25	CLA	A	821	-	69,73,73	1.23	8 (11%)	82,113,113	1.35	12 (14%)
31	LMG	B	801	-	38,38,55	1.15	3 (7%)	46,46,63	1.13	3 (6%)
30	BCR	I	101	-	41,41,41	1.00	4 (9%)	56,56,56	2.46	21 (37%)
24	CHL	4	307	-	37,50,74	2.97	14 (37%)	31,85,114	2.47	12 (38%)
25	CLA	B	825	-	49,53,73	1.36	7 (14%)	58,89,113	1.30	9 (15%)
25	CLA	3	302	-	59,63,73	1.39	10 (16%)	70,101,113	1.73	17 (24%)
25	CLA	R	306	-	69,73,73	1.15	7 (10%)	82,113,113	1.14	3 (3%)
25	CLA	T	302	-	69,73,73	1.21	7 (10%)	82,113,113	1.19	5 (6%)
37	NEX	W	317	-	40,46,46	1.22	5 (12%)	50,70,70	2.44	14 (28%)
25	CLA	U	303	-	54,58,73	1.34	6 (11%)	64,95,113	1.28	6 (9%)
25	CLA	A	830	-	69,73,73	1.22	7 (10%)	82,113,113	1.60	13 (15%)
25	CLA	G	204	13	49,53,73	1.50	8 (16%)	58,89,113	1.49	10 (17%)
30	BCR	M	101	-	41,41,41	1.33	8 (19%)	56,56,56	2.33	23 (41%)
25	CLA	6	604	-	46,51,73	1.38	6 (13%)	54,86,113	1.28	6 (11%)
29	Q6L	R	319	-	42,43,43	1.93	8 (19%)	51,60,60	1.68	6 (11%)
26	IWJ	R	322	-	43,45,45	1.52	4 (9%)	47,65,65	1.19	4 (8%)
25	CLA	4	305	-	47,51,73	1.54	10 (21%)	58,87,113	1.26	5 (8%)
24	CHL	Q	308	23	44,58,74	3.00	16 (36%)	37,94,114	1.79	5 (13%)
25	CLA	A	843	-	69,73,73	1.17	6 (8%)	82,113,113	1.48	8 (9%)
25	CLA	T	303	-	54,58,73	1.33	7 (12%)	64,95,113	1.27	6 (9%)
24	CHL	2	601	2	41,55,74	3.00	14 (34%)	35,91,114	1.66	9 (25%)
24	CHL	P	314	22	38,53,74	3.02	10 (26%)	31,88,114	1.81	10 (32%)
25	CLA	A	825	-	69,73,73	1.23	6 (8%)	82,113,113	1.61	16 (19%)
25	CLA	N	203	-	46,50,73	1.52	8 (17%)	53,85,113	1.33	10 (18%)
24	CHL	W	306	-	46,60,74	2.72	15 (32%)	40,97,114	1.96	15 (37%)
26	IWJ	U	316	-	43,45,45	1.50	7 (16%)	47,65,65	2.05	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	5	613	-	54,54,55	0.92	2 (3%)	62,62,63	0.84	1 (1%)
25	CLA	6	610	-	65,69,73	1.18	6 (9%)	77,108,113	1.17	5 (6%)
25	CLA	A	809	-	54,58,73	1.27	8 (14%)	64,95,113	1.40	9 (14%)
26	IWJ	T	321	-	43,45,45	1.58	6 (13%)	47,65,65	1.36	5 (10%)
25	CLA	1	607	1	40,44,73	1.61	8 (20%)	48,74,113	2.24	10 (20%)
24	CHL	2	607	-	38,53,74	3.08	15 (39%)	31,88,114	1.87	9 (29%)
25	CLA	P	312	22	59,63,73	1.26	5 (8%)	70,101,113	1.34	8 (11%)
30	BCR	F	801	-	41,41,41	1.14	4 (9%)	56,56,56	1.98	17 (30%)
25	CLA	A	815	-	69,73,73	1.21	6 (8%)	82,113,113	1.56	10 (12%)
25	CLA	H	302	-	69,73,73	1.14	7 (10%)	82,113,113	1.42	9 (10%)
24	CHL	X	315	22	38,53,74	2.93	8 (21%)	31,88,114	1.81	11 (35%)
29	Q6L	X	319	-	42,43,43	1.96	8 (19%)	51,60,60	2.05	9 (17%)
31	LMG	J	104	-	46,46,55	0.98	2 (4%)	54,54,63	0.89	2 (3%)
24	CHL	S	304	22	36,50,74	3.01	14 (38%)	29,85,114	2.06	14 (48%)
24	CHL	Q	309	-	38,52,74	3.01	10 (26%)	31,87,114	1.96	12 (38%)
36	DGD	B	850	-	60,60,67	0.95	3 (5%)	74,74,81	0.96	4 (5%)
24	CHL	W	307	-	60,74,74	2.41	8 (13%)	58,114,114	1.72	15 (25%)
25	CLA	A	806	-	56,60,73	1.31	6 (10%)	65,97,113	1.47	10 (15%)
29	Q6L	R	301	-	42,43,43	1.91	7 (16%)	51,60,60	2.04	8 (15%)
29	Q6L	S	321	-	42,43,43	2.00	10 (23%)	51,60,60	1.78	10 (19%)
25	CLA	U	311	22	59,63,73	1.27	8 (13%)	70,101,113	1.47	10 (14%)
28	LHG	2	619	25	32,32,48	1.13	2 (6%)	35,38,54	1.08	4 (11%)
25	CLA	5	602	5	64,68,73	1.21	5 (7%)	76,107,113	1.35	10 (13%)
25	CLA	B	822	-	54,58,73	1.31	7 (12%)	64,95,113	1.36	6 (9%)
25	CLA	A	834	-	60,64,73	1.25	6 (10%)	71,102,113	1.25	8 (11%)
25	CLA	2	602	2	65,69,73	1.27	6 (9%)	77,108,113	1.61	15 (19%)
30	BCR	J	101	-	41,41,41	1.19	4 (9%)	56,56,56	2.57	22 (39%)
25	CLA	B	805	-	69,73,73	1.21	8 (11%)	82,113,113	1.30	10 (12%)
28	LHG	1	614	25	34,34,48	1.12	2 (5%)	37,40,54	1.19	3 (8%)
25	CLA	P	303	-	54,58,73	1.31	5 (9%)	64,95,113	1.31	9 (14%)
29	Q6L	V	321	-	42,43,43	1.90	8 (19%)	51,60,60	1.71	7 (13%)
25	CLA	A	840	-	59,63,73	1.26	6 (10%)	70,101,113	1.45	6 (8%)
29	Q6L	P	321	-	42,43,43	1.92	8 (19%)	51,60,60	1.58	7 (13%)
33	CL0	A	802	-	58,73,73	2.15	13 (22%)	60,113,113	1.55	11 (18%)
25	CLA	2	608	2	49,53,73	1.36	4 (8%)	58,89,113	1.36	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	2	611	2	47,52,73	1.38	4 (8%)	55,88,113	1.40	4 (7%)
29	Q6L	U	314	-	42,43,43	1.89	7 (16%)	51,60,60	1.87	8 (15%)
24	CHL	T	320	-	46,60,74	2.64	10 (21%)	40,97,114	2.10	15 (37%)
26	IWJ	X	318	-	43,45,45	1.63	7 (16%)	47,65,65	1.72	10 (21%)
25	CLA	O	2001	-	63,67,73	1.20	5 (7%)	74,105,113	1.44	7 (9%)
25	CLA	B	835	-	49,53,73	1.40	6 (12%)	58,89,113	1.20	4 (6%)
25	CLA	S	309	22	64,68,73	1.22	9 (14%)	76,107,113	1.16	6 (7%)
29	Q6L	Q	318	-	42,43,43	1.81	6 (14%)	51,60,60	1.63	7 (13%)
25	CLA	A	820	-	63,67,73	1.28	9 (14%)	74,105,113	1.41	11 (14%)
32	SQD	6	617	-	52,54,54	1.12	3 (5%)	62,65,65	1.09	4 (6%)
25	CLA	5	607	5	69,73,73	1.16	6 (8%)	82,113,113	1.27	6 (7%)
25	CLA	3	305	3	45,49,73	1.51	10 (22%)	54,84,113	1.32	7 (12%)
37	NEX	S	317	-	40,46,46	1.42	5 (12%)	50,70,70	2.44	17 (34%)
38	KC2	P	308	22	49,53,53	2.13	15 (30%)	60,89,89	2.40	17 (28%)
28	LHG	A	847	25	29,29,48	1.18	2 (6%)	32,35,54	1.06	2 (6%)
25	CLA	B	809	-	69,73,73	1.23	9 (13%)	82,113,113	1.37	10 (12%)
25	CLA	O	2005	-	45,49,73	1.39	6 (13%)	54,84,113	1.39	5 (9%)
24	CHL	T	314	22	36,50,74	2.97	9 (25%)	29,85,114	2.01	9 (31%)
25	CLA	B	802	-	69,73,73	1.18	7 (10%)	82,113,113	1.44	11 (13%)
30	BCR	4	319	-	41,41,41	1.30	5 (12%)	56,56,56	2.34	23 (41%)
25	CLA	2	609	2	59,63,73	1.22	6 (10%)	70,101,113	1.32	8 (11%)
30	BCR	G	205	-	41,41,41	1.21	5 (12%)	56,56,56	2.00	14 (25%)
25	CLA	B	831	-	69,73,73	1.23	8 (11%)	82,113,113	1.47	10 (12%)
25	CLA	1	613	-	56,60,73	1.30	5 (8%)	65,97,113	1.25	8 (12%)
25	CLA	B	816	-	55,59,73	1.28	7 (12%)	64,96,113	1.27	7 (10%)
24	CHL	V	304	22	40,54,74	2.84	11 (27%)	34,90,114	1.79	10 (29%)
25	CLA	B	817	-	47,51,73	1.39	9 (19%)	55,86,113	1.30	4 (7%)
25	CLA	L	302	-	64,68,73	1.24	7 (10%)	76,107,113	1.41	7 (9%)
24	CHL	W	305	-	36,50,74	3.07	14 (38%)	29,85,114	2.09	11 (37%)
28	LHG	3	323	-	42,42,48	1.00	2 (4%)	45,48,54	0.93	3 (6%)
25	CLA	A	811	7	54,58,73	1.29	4 (7%)	64,95,113	1.48	7 (10%)
24	CHL	U	313	22	37,51,74	2.96	10 (27%)	30,86,114	1.88	10 (33%)
30	BCR	K	205	-	41,41,41	1.21	4 (9%)	56,56,56	2.09	16 (28%)
37	NEX	P	317	-	40,46,46	1.33	8 (20%)	50,70,70	2.45	16 (32%)
25	CLA	6	608	6	46,50,73	1.37	5 (10%)	53,85,113	1.47	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	5	609	-	57,62,73	1.27	7 (12%)	67,100,113	1.31	5 (7%)
25	CLA	2	610	28	46,50,73	1.38	6 (13%)	53,85,113	1.36	6 (11%)
25	CLA	S	302	-	69,73,73	1.20	7 (10%)	82,113,113	1.24	6 (7%)
38	KC2	V	308	22	49,53,53	2.29	13 (26%)	60,89,89	2.09	19 (31%)
25	CLA	A	856	-	61,65,73	1.21	5 (8%)	72,103,113	1.65	13 (18%)
25	CLA	4	309	4	49,53,73	1.40	7 (14%)	58,89,113	1.66	11 (18%)
25	CLA	A	842	-	69,73,73	1.20	9 (13%)	82,113,113	1.42	12 (14%)
29	Q6L	S	315	-	42,43,43	1.78	5 (11%)	51,60,60	1.72	10 (19%)
25	CLA	5	604	-	41,46,73	1.61	10 (24%)	51,81,113	1.29	6 (11%)
25	CLA	A	818	-	49,53,73	1.37	5 (10%)	58,89,113	1.39	7 (12%)
26	IWJ	T	318	-	43,45,45	1.58	4 (9%)	47,65,65	1.37	6 (12%)
25	CLA	W	309	22	68,72,73	1.16	7 (10%)	80,111,113	1.44	9 (11%)
30	BCR	B	848	-	41,41,41	1.29	4 (9%)	56,56,56	2.23	19 (33%)
25	CLA	B	832	-	47,51,73	1.50	10 (21%)	55,86,113	1.54	12 (21%)
24	CHL	Q	316	23	38,53,74	3.04	10 (26%)	31,88,114	2.12	13 (41%)
25	CLA	3	311	3	57,62,73	1.33	8 (14%)	67,100,113	1.66	12 (17%)
25	CLA	B	806	-	69,73,73	1.19	8 (11%)	82,113,113	1.53	12 (14%)
25	CLA	S	310	22	64,68,73	1.19	8 (12%)	76,107,113	1.25	7 (9%)
24	CHL	5	605	-	35,49,74	2.98	9 (25%)	28,84,114	1.88	9 (32%)
28	LHG	3	322	-	35,35,48	1.04	2 (5%)	38,41,54	1.08	3 (7%)
30	BCR	A	850	-	41,41,41	1.26	5 (12%)	56,56,56	2.40	22 (39%)
29	Q6L	R	304	-	42,43,43	1.94	8 (19%)	51,60,60	1.68	7 (13%)
30	BCR	L	305	-	41,41,41	1.04	1 (2%)	56,56,56	2.31	20 (35%)
30	BCR	A	852	-	41,41,41	1.16	4 (9%)	56,56,56	2.17	13 (23%)
25	CLA	X	310	22	46,50,73	1.39	7 (15%)	53,85,113	1.34	7 (13%)
24	CHL	W	304	22	36,50,74	3.02	10 (27%)	29,85,114	1.80	9 (31%)
25	CLA	R	314	22	64,68,73	1.24	6 (9%)	76,107,113	1.43	9 (11%)
25	CLA	A	816	-	49,53,73	1.36	7 (14%)	58,89,113	1.52	8 (13%)
29	Q6L	P	316	-	42,43,43	1.96	9 (21%)	51,60,60	1.77	9 (17%)
25	CLA	A	807	-	68,72,73	1.23	8 (11%)	80,111,113	1.33	8 (10%)
31	LMG	A	801	-	31,31,55	1.15	2 (6%)	39,39,63	0.93	1 (2%)
30	BCR	K	202	-	41,41,41	1.20	6 (14%)	56,56,56	2.61	26 (46%)
38	KC2	Q	310	23	49,53,53	2.20	13 (26%)	60,89,89	2.26	13 (21%)
29	Q6L	V	315	-	42,43,43	1.93	7 (16%)	51,60,60	1.91	7 (13%)
25	CLA	Q	315	-	52,56,73	1.32	7 (13%)	61,92,113	1.41	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	P	307	-	38,52,74	3.26	11 (28%)	31,87,114	1.99	10 (32%)
25	CLA	3	309	28	46,50,73	1.40	6 (13%)	53,85,113	1.33	6 (11%)
24	CHL	6	606	-	37,51,74	3.08	8 (21%)	30,86,114	2.11	11 (36%)
30	BCR	B	849	-	41,41,41	1.07	2 (4%)	56,56,56	2.31	17 (30%)
30	BCR	A	851	-	41,41,41	0.95	2 (4%)	56,56,56	2.45	22 (39%)
25	CLA	K	203	-	66,70,73	1.19	7 (10%)	78,109,113	1.42	7 (8%)
25	CLA	2	613	-	45,50,73	1.39	6 (13%)	52,85,113	1.31	8 (15%)
25	CLA	B	823	-	51,55,73	1.37	5 (9%)	60,91,113	1.20	4 (6%)
25	CLA	H	301	14	47,52,73	1.34	5 (10%)	55,87,113	1.36	7 (12%)
26	IWJ	V	317	-	43,45,45	1.58	4 (9%)	47,65,65	1.38	4 (8%)
30	BCR	F	804	-	41,41,41	1.17	3 (7%)	56,56,56	2.37	22 (39%)
24	CHL	V	314	22	38,52,74	2.90	11 (28%)	31,87,114	1.80	10 (32%)
25	CLA	A	813	-	69,73,73	1.19	7 (10%)	82,113,113	1.13	5 (6%)
24	CHL	S	305	22	36,50,74	2.91	12 (33%)	29,85,114	2.18	15 (51%)
25	CLA	R	305	22	69,73,73	1.20	5 (7%)	82,113,113	1.37	8 (9%)
25	CLA	B	807	-	69,73,73	1.20	8 (11%)	82,113,113	1.44	9 (10%)
25	CLA	S	313	-	45,49,73	1.43	6 (13%)	54,84,113	1.29	5 (9%)
24	CHL	X	306	-	36,50,74	2.95	12 (33%)	29,85,114	2.46	12 (41%)
29	Q6L	P	319	-	42,43,43	1.91	7 (16%)	51,60,60	1.76	9 (17%)
25	CLA	K	201	17	49,53,73	1.40	4 (8%)	58,89,113	1.70	12 (20%)
25	CLA	X	313	22	45,49,73	1.40	8 (17%)	54,84,113	1.33	7 (12%)
25	CLA	A	838	7	69,73,73	1.19	7 (10%)	82,113,113	1.42	11 (13%)
26	IWJ	S	322	-	43,45,45	1.60	5 (11%)	47,65,65	1.49	5 (10%)
25	CLA	A	812	-	68,72,73	1.17	7 (10%)	80,111,113	1.30	6 (7%)
25	CLA	B	821	-	59,63,73	1.31	7 (11%)	70,101,113	1.33	10 (14%)
25	CLA	3	307	3	65,69,73	1.26	9 (13%)	77,108,113	1.53	10 (12%)
25	CLA	6	611	-	47,51,73	1.36	5 (10%)	55,86,113	1.37	8 (14%)
31	LMG	A	857	-	46,46,55	0.97	2 (4%)	54,54,63	0.89	2 (3%)
25	CLA	5	606	-	44,48,73	1.50	7 (15%)	55,83,113	1.51	8 (14%)
25	CLA	A	808	7	69,73,73	1.18	7 (10%)	82,113,113	1.44	9 (10%)
25	CLA	A	839	-	69,73,73	1.13	6 (8%)	82,113,113	1.38	11 (13%)
26	IWJ	S	319	-	43,45,45	1.57	6 (13%)	47,65,65	1.54	8 (17%)
25	CLA	Q	314	23	57,61,73	1.24	5 (8%)	67,98,113	1.37	7 (10%)
25	CLA	X	302	22	59,63,73	1.25	10 (16%)	70,101,113	1.36	11 (15%)
28	LHG	3	320	25	22,22,48	1.10	1 (4%)	24,27,54	1.08	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	KC2	W	308	22	49,53,53	2.18	15 (30%)	60,89,89	2.07	18 (30%)
25	CLA	2	603	-	47,52,73	1.42	7 (14%)	55,88,113	1.42	7 (12%)
29	Q6L	O	2006	-	42,43,43	1.94	8 (19%)	51,60,60	1.79	7 (13%)
24	CHL	U	305	-	40,54,74	2.97	10 (25%)	34,90,114	2.25	11 (32%)
25	CLA	B	826	-	69,73,73	1.26	11 (15%)	82,113,113	1.49	14 (17%)
25	CLA	5	601	5	50,54,73	1.35	7 (14%)	59,90,113	1.64	12 (20%)
25	CLA	4	312	4	44,49,73	1.43	6 (13%)	50,84,113	1.41	7 (14%)
29	Q6L	T	322	-	42,43,43	1.94	8 (19%)	51,60,60	1.99	8 (15%)
25	CLA	R	316	22	59,63,73	1.27	6 (10%)	70,101,113	1.54	9 (12%)
30	BCR	A	848	-	41,41,41	1.34	5 (12%)	56,56,56	2.14	19 (33%)
24	CHL	R	318	22	38,53,74	3.02	9 (23%)	31,88,114	1.85	10 (32%)
28	LHG	6	616	-	45,45,48	0.96	2 (4%)	48,51,54	1.09	3 (6%)
24	CHL	V	306	-	38,52,74	2.96	13 (34%)	31,87,114	1.93	10 (32%)
28	LHG	3	321	-	42,42,48	1.00	2 (4%)	45,48,54	0.90	1 (2%)
29	Q6L	X	317	-	42,43,43	1.90	8 (19%)	51,60,60	2.02	8 (15%)
25	CLA	B	837	-	46,50,73	1.42	6 (13%)	53,85,113	1.43	7 (13%)
29	Q6L	T	316	-	42,43,43	1.89	7 (16%)	51,60,60	2.02	12 (23%)
25	CLA	S	311	-	51,55,73	1.31	5 (9%)	60,91,113	1.47	8 (13%)
29	Q6L	2	616	-	42,43,43	1.85	7 (16%)	51,60,60	2.24	14 (27%)
25	CLA	3	314	3	43,48,73	1.44	5 (11%)	51,83,113	1.34	7 (13%)
29	Q6L	Q	317	-	42,43,43	1.85	6 (14%)	51,60,60	1.76	9 (17%)
25	CLA	K	204	-	50,54,73	1.34	8 (16%)	59,90,113	1.56	8 (13%)
26	IWJ	R	303	-	43,45,45	1.55	5 (11%)	47,65,65	1.40	7 (14%)
29	Q6L	X	316	-	40,41,43	1.90	6 (15%)	50,56,60	1.93	10 (20%)
30	BCR	B	845	-	41,41,41	1.30	4 (9%)	56,56,56	2.74	25 (44%)
25	CLA	A	826	-	59,63,73	1.23	5 (8%)	70,101,113	1.35	7 (10%)
24	CHL	X	308	-	38,52,74	2.94	10 (26%)	31,87,114	1.97	11 (35%)
29	Q6L	Q	319	-	42,43,43	1.91	7 (16%)	51,60,60	1.86	12 (23%)
29	Q6L	W	315	-	42,43,43	1.86	8 (19%)	51,60,60	1.74	8 (15%)
25	CLA	Q	311	23	59,63,73	1.22	5 (8%)	70,101,113	1.25	8 (11%)
27	XAT	6	615	-	41,47,47	1.11	3 (7%)	54,74,74	2.77	25 (46%)
25	CLA	U	302	-	60,64,73	1.28	8 (13%)	71,102,113	1.36	8 (11%)
25	CLA	V	310	22	51,55,73	1.35	6 (11%)	60,91,113	1.25	8 (13%)
25	CLA	B	810	-	69,73,73	1.21	7 (10%)	82,113,113	1.26	8 (9%)
25	CLA	B	836	8	64,68,73	1.22	8 (12%)	76,107,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	4	304	-	48,52,73	1.48	8 (16%)	59,88,113	1.64	9 (15%)
25	CLA	B	827	-	54,58,73	1.30	4 (7%)	64,95,113	1.42	9 (14%)
24	CHL	Q	307	23	40,54,74	3.01	8 (20%)	34,90,114	2.07	12 (35%)
38	KC2	T	308	22	49,53,53	2.14	13 (26%)	60,89,89	2.20	16 (26%)
26	IWJ	V	318	-	43,45,45	1.60	4 (9%)	47,65,65	1.70	9 (19%)
25	CLA	U	308	22	45,49,73	1.35	7 (15%)	54,84,113	1.67	10 (18%)
25	CLA	A	837	-	69,73,73	1.21	7 (10%)	82,113,113	1.32	9 (10%)
25	CLA	6	602	6	66,70,73	1.16	4 (6%)	78,109,113	1.39	10 (12%)
30	BCR	3	319	-	41,41,41	1.25	5 (12%)	56,56,56	2.04	15 (26%)
25	CLA	R	313	22	68,72,73	1.20	7 (10%)	80,111,113	1.31	10 (12%)
25	CLA	V	302	-	54,58,73	1.29	7 (12%)	64,95,113	1.29	8 (12%)
26	IWJ	1	611	-	43,45,45	1.73	5 (11%)	47,65,65	1.27	5 (10%)
29	Q6L	V	319	-	42,43,43	1.83	8 (19%)	51,60,60	2.12	16 (31%)
25	CLA	K	206	17	69,73,73	1.18	6 (8%)	82,113,113	1.35	10 (12%)
25	CLA	O	2002	-	69,73,73	1.23	8 (11%)	82,113,113	1.60	17 (20%)
25	CLA	Q	312	23	46,50,73	1.41	7 (15%)	53,85,113	1.18	4 (7%)
25	CLA	P	302	-	69,73,73	1.14	7 (10%)	82,113,113	1.34	10 (12%)
29	Q6L	R	320	-	42,43,43	1.92	7 (16%)	51,60,60	1.74	10 (19%)
29	Q6L	S	323	-	42,43,43	1.89	6 (14%)	51,60,60	1.78	12 (23%)
25	CLA	H	304	18	49,53,73	1.33	8 (16%)	58,89,113	1.41	8 (13%)
25	CLA	A	814	-	58,62,73	1.34	9 (15%)	68,99,113	1.32	11 (16%)
25	CLA	5	603	5	49,53,73	1.42	7 (14%)	58,89,113	1.39	6 (10%)
25	CLA	4	310	4	58,62,73	1.23	5 (8%)	68,99,113	1.34	11 (16%)
37	NEX	H	306	-	40,46,46	1.42	9 (22%)	50,70,70	2.32	18 (36%)
24	CHL	T	307	-	38,52,74	3.04	11 (28%)	31,87,114	1.94	10 (32%)
25	CLA	G	203	-	46,50,73	1.42	6 (13%)	53,85,113	1.49	5 (9%)
25	CLA	A	836	-	69,73,73	1.18	9 (13%)	82,113,113	1.38	5 (6%)
25	CLA	A	817	-	69,73,73	1.21	6 (8%)	82,113,113	1.27	8 (9%)
25	CLA	V	303	-	54,58,73	1.34	7 (12%)	64,95,113	1.50	8 (12%)
25	CLA	A	804	39	69,73,73	1.28	8 (11%)	82,113,113	1.46	15 (18%)
30	BCR	J	103	-	41,41,41	1.09	4 (9%)	56,56,56	2.22	19 (33%)
25	CLA	A	835	-	69,73,73	1.21	7 (10%)	82,113,113	1.27	6 (7%)
25	CLA	4	315	-	45,49,73	1.41	5 (11%)	54,84,113	1.28	7 (12%)
24	CHL	U	304	22	36,50,74	2.94	13 (36%)	29,85,114	1.93	10 (34%)
25	CLA	R	315	-	64,68,73	1.26	7 (10%)	76,107,113	1.37	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	U	309	22	50,54,73	1.31	6 (12%)	59,90,113	1.24	4 (6%)
26	IWJ	V	320	-	43,45,45	1.57	5 (11%)	47,65,65	1.40	4 (8%)
25	CLA	4	311	-	46,50,73	1.57	6 (13%)	53,85,113	1.68	11 (20%)
25	CLA	V	313	-	52,56,73	1.31	6 (11%)	61,92,113	1.20	5 (8%)
37	NEX	R	321	-	40,46,46	1.43	8 (20%)	50,70,70	2.42	17 (34%)
25	CLA	R	307	-	54,58,73	1.32	7 (12%)	64,95,113	1.26	6 (9%)
25	CLA	Q	306	39	54,58,73	1.35	9 (16%)	64,95,113	1.52	12 (18%)
24	CHL	T	304	22	37,51,74	3.09	11 (29%)	30,86,114	2.06	11 (36%)
25	CLA	2	612	2	69,73,73	1.20	6 (8%)	82,113,113	1.34	12 (14%)
29	Q6L	V	316	-	42,43,43	1.98	7 (16%)	51,60,60	1.99	9 (17%)
30	BCR	G	201	-	41,41,41	1.08	3 (7%)	56,56,56	2.22	19 (33%)
25	CLA	1	605	-	44,49,73	1.44	7 (15%)	50,84,113	1.22	3 (6%)
25	CLA	B	811	8	69,73,73	1.21	9 (13%)	82,113,113	1.30	6 (7%)
25	CLA	3	304	3	44,49,73	1.45	9 (20%)	50,84,113	1.46	7 (14%)
25	CLA	1	609	-	41,46,73	1.52	6 (14%)	51,81,113	1.47	8 (15%)
24	CHL	P	304	22	40,54,74	3.03	10 (25%)	34,90,114	2.19	16 (47%)
25	CLA	A	845	28	54,58,73	1.25	6 (11%)	64,95,113	1.35	7 (10%)
24	CHL	4	306	-	35,49,74	3.11	10 (28%)	30,84,114	1.68	8 (26%)
25	CLA	W	302	-	59,63,73	1.26	7 (11%)	70,101,113	1.17	5 (7%)
25	CLA	3	310	-	47,51,73	1.38	5 (10%)	55,86,113	1.30	7 (12%)
25	CLA	1	606	1	44,48,73	1.49	6 (13%)	55,83,113	1.39	9 (16%)
26	IWJ	4	317	-	43,45,45	1.64	6 (13%)	47,65,65	1.51	9 (19%)
36	DGD	A	854	-	52,52,67	1.05	3 (5%)	66,66,81	1.21	6 (9%)
25	CLA	B	842	-	69,73,73	1.22	8 (11%)	82,113,113	1.56	11 (13%)
25	CLA	X	312	-	55,59,73	1.29	7 (12%)	64,96,113	1.40	7 (10%)
31	LMG	2	620	-	31,31,55	1.18	2 (6%)	39,39,63	1.29	4 (10%)
25	CLA	3	303	-	47,51,73	1.53	9 (19%)	58,87,113	1.38	6 (10%)
25	CLA	B	833	-	47,51,73	1.36	5 (10%)	55,86,113	1.50	5 (9%)
25	CLA	V	301	22	64,68,73	1.16	5 (7%)	76,107,113	1.47	10 (13%)
25	CLA	X	304	-	46,50,73	1.44	8 (17%)	53,85,113	1.45	8 (15%)
25	CLA	A	841	-	54,58,73	1.34	6 (11%)	64,95,113	1.36	5 (7%)
24	CHL	W	314	22	35,49,74	3.11	11 (31%)	30,83,114	2.11	12 (40%)
26	IWJ	W	318	-	43,45,45	1.59	4 (9%)	47,65,65	1.51	8 (17%)
25	CLA	W	313	-	47,51,73	1.37	7 (14%)	55,86,113	1.17	4 (7%)
31	LMG	A	855	-	27,27,55	1.27	2 (7%)	35,35,63	1.32	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.32	8 (9%)
25	CLA	4	303	4	64,68,73	1.26	9 (14%)	76,107,113	1.25	11 (14%)
25	CLA	L	303	-	49,53,73	1.40	6 (12%)	58,89,113	1.56	13 (22%)
28	LHG	Q	302	-	34,34,48	1.10	2 (5%)	37,40,54	1.07	2 (5%)
25	CLA	Q	313	-	50,54,73	1.33	7 (14%)	59,90,113	1.45	6 (10%)
29	Q6L	U	315	-	42,43,43	1.93	8 (19%)	51,60,60	2.04	12 (23%)
25	CLA	1	610	1	44,48,73	1.51	7 (15%)	53,83,113	1.48	12 (22%)
25	CLA	5	610	-	45,49,73	1.42	7 (15%)	54,84,113	1.23	5 (9%)
25	CLA	W	312	22	59,63,73	1.21	7 (11%)	70,101,113	1.56	12 (17%)
25	CLA	A	819	-	64,68,73	1.17	5 (7%)	76,107,113	1.47	8 (10%)
25	CLA	V	312	22	59,63,73	1.26	7 (11%)	70,101,113	1.30	8 (11%)
26	IWJ	6	614	-	43,45,45	1.53	4 (9%)	47,65,65	1.43	5 (10%)
30	BCR	3	318	-	41,41,41	1.28	6 (14%)	56,56,56	2.19	19 (33%)
25	CLA	6	613	6	69,73,73	1.22	6 (8%)	82,113,113	1.30	9 (10%)
30	BCR	B	846	-	41,41,41	1.09	5 (12%)	56,56,56	2.35	19 (33%)
25	CLA	B	820	-	64,68,73	1.24	10 (15%)	76,107,113	1.43	13 (17%)
26	IWJ	3	315	-	43,45,45	1.46	7 (16%)	47,65,65	1.93	5 (10%)
26	IWJ	P	318	-	43,45,45	1.49	5 (11%)	47,65,65	1.27	4 (8%)
29	Q6L	S	320	-	42,43,43	1.96	7 (16%)	51,60,60	1.83	12 (23%)
25	CLA	3	313	-	45,49,73	1.40	6 (13%)	54,84,113	1.30	5 (9%)
34	PQN	B	844	-	34,34,34	2.99	11 (32%)	43,45,45	2.01	9 (20%)
25	CLA	S	303	-	54,58,73	1.35	8 (14%)	64,95,113	1.37	8 (12%)
27	XAT	5	612	-	41,47,47	1.07	2 (4%)	54,74,74	2.84	24 (44%)
29	Q6L	W	316	-	42,43,43	1.95	9 (21%)	51,60,60	2.04	13 (25%)
25	CLA	B	808	8	69,73,73	1.20	10 (14%)	82,113,113	1.31	11 (13%)
25	CLA	1	603	-	59,63,73	1.28	7 (11%)	70,101,113	1.63	13 (18%)
25	CLA	T	309	22	63,67,73	1.22	8 (12%)	74,105,113	1.32	8 (10%)
25	CLA	B	819	-	63,67,73	1.25	6 (9%)	74,105,113	1.27	9 (12%)
35	SF4	C	101	9	0,12,12	-	-	-	-	-
30	BCR	B	847	-	41,41,41	1.33	6 (14%)	56,56,56	2.52	22 (39%)
25	CLA	3	308	3	45,49,73	1.40	7 (15%)	54,84,113	1.37	8 (14%)
34	PQN	A	844	-	34,34,34	3.02	10 (29%)	43,45,45	1.93	8 (18%)
24	CHL	S	306	-	46,60,74	2.78	12 (26%)	40,97,114	2.19	14 (35%)
25	CLA	R	317	-	52,56,73	1.32	6 (11%)	61,92,113	1.36	8 (13%)
30	BCR	3	317	-	41,41,41	1.10	3 (7%)	56,56,56	1.90	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	824	-	64,68,73	1.29	10 (15%)	76,107,113	1.29	9 (11%)
24	CHL	1	604	1	35,49,74	3.05	10 (28%)	28,84,114	1.72	10 (35%)
25	CLA	S	312	22	59,63,73	1.25	8 (13%)	70,101,113	1.26	7 (10%)
25	CLA	G	202	-	49,53,73	1.40	7 (14%)	58,89,113	1.25	6 (10%)
29	Q6L	P	315	-	42,43,43	1.96	8 (19%)	51,60,60	1.63	7 (13%)
25	CLA	3	301	3	64,68,73	1.28	8 (12%)	76,107,113	1.41	5 (6%)
25	CLA	W	301	22	59,63,73	1.24	7 (11%)	70,101,113	1.33	4 (5%)
31	LMG	F	805	-	31,31,55	1.15	2 (6%)	39,39,63	1.13	3 (7%)
25	CLA	A	824	-	46,50,73	1.45	6 (13%)	53,85,113	1.38	6 (11%)
25	CLA	4	316	4	46,50,73	1.36	5 (10%)	53,85,113	1.33	7 (13%)

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
24	CHL	6	601	6	3/3/15/26	1/10/108/137	-
25	CLA	A	828	-	-	5/32/108/115	-
25	CLA	A	829	-	1/1/15/20	14/39/115/115	-
25	CLA	B	803	-	1/1/15/20	10/39/115/115	-
25	CLA	A	833	-	-	5/21/97/115	-
25	CLA	A	810	7	1/1/15/20	7/39/115/115	-
25	CLA	Q	301	14	1/1/13/20	11/27/103/115	-
24	CHL	1	601	1	3/3/18/26	5/25/123/137	-
24	CHL	S	314	22	3/3/15/26	3/14/112/137	-
25	CLA	L	301	18	1/1/10/20	2/10/86/115	-
25	CLA	B	843	28	1/1/15/20	12/39/115/115	-
31	LMG	N	201	-	-	3/50/70/70	0/1/1/1
31	LMG	L	308	-	-	7/26/46/70	0/1/1/1
25	CLA	U	310	-	1/1/10/20	9/14/90/115	-
26	IWJ	5	611	-	-	5/33/76/76	1/2/2/2
37	NEX	T	317	-	-	3/27/83/83	0/3/3/3
24	CHL	U	306	-	3/3/15/26	5/13/111/137	-
30	BCR	H	305	-	-	6/29/63/63	0/2/2/2
25	CLA	X	314	-	1/1/10/20	6/10/86/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	J	102	16	1/1/10/20	7/12/88/115	-
25	CLA	A	831	-	1/1/15/20	15/39/115/115	-
29	Q6L	R	323	-	-	9/29/67/67	0/2/2/2
26	IWJ	Q	303	-	-	4/33/76/76	0/2/2/2
29	Q6L	T	315	-	-	6/29/67/67	0/2/2/2
25	CLA	5	608	5	1/1/10/20	4/10/86/115	-
38	KC2	X	309	22	-	9/15/71/71	-
38	KC2	R	312	22	-	7/15/71/71	-
28	LHG	A	846	-	-	10/53/53/53	-
25	CLA	A	832	-	1/1/15/20	12/39/115/115	-
35	SF4	C	102	9	-	-	0/6/5/5
25	CLA	P	310	22	1/1/14/20	8/33/109/115	-
30	BCR	2	618	-	-	4/29/63/63	0/2/2/2
38	KC2	S	308	22	-	7/15/71/71	-
24	CHL	2	615	2	3/3/15/26	4/12/110/137	-
25	CLA	A	805	-	1/1/15/20	13/39/115/115	-
25	CLA	A	822	-	1/1/11/20	3/15/91/115	-
25	CLA	N	202	20	1/1/11/20	2/15/91/115	-
29	Q6L	U	317	-	-	5/29/67/67	0/2/2/2
25	CLA	P	311	-	1/1/14/20	9/33/109/115	-
24	CHL	P	305	-	3/3/16/26	4/15/113/137	-
25	CLA	3	312	-	1/1/10/20	2/8/84/115	-
25	CLA	X	311	22	1/1/12/20	10/21/97/115	-
25	CLA	T	312	22	1/1/13/20	12/27/103/115	-
29	Q6L	S	316	-	-	2/29/67/67	0/2/2/2
24	CHL	R	308	22	3/3/16/26	3/15/113/137	-
24	CHL	S	307	-	3/3/15/26	5/10/108/137	-
25	CLA	4	313	4	-	7/30/106/115	-
25	CLA	B	838	-	1/1/12/20	2/21/97/115	-
25	CLA	B	840	-	-	9/18/94/115	-
29	Q6L	W	320	-	-	7/29/67/67	0/2/2/2
25	CLA	T	301	22	1/1/15/20	12/39/115/115	-
25	CLA	W	310	22	1/1/14/20	9/33/109/115	-
24	CHL	R	310	-	3/3/17/26	8/23/121/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	X	307	-	3/3/17/26	10/23/121/137	-
25	CLA	6	609	-	1/1/11/20	4/13/89/115	-
24	CHL	P	306	-	3/3/17/26	8/23/121/137	-
27	XAT	4	318	-	-	5/31/93/93	0/4/4/4
25	CLA	2	606	-	1/1/11/20	7/15/91/115	-
25	CLA	V	309	22	1/1/10/20	3/12/88/115	-
25	CLA	B	839	-	1/1/15/20	16/39/115/115	-
25	CLA	B	804	-	1/1/15/20	14/39/115/115	-
26	IWJ	P	320	-	-	3/33/76/76	0/2/2/2
25	CLA	P	313	-	-	6/19/95/115	-
25	CLA	X	303	-	1/1/12/20	8/23/99/115	-
26	IWJ	S	318	-	-	5/33/76/76	0/2/2/2
25	CLA	6	607	6	1/1/11/20	2/15/91/115	-
25	CLA	S	301	22	1/1/15/20	7/39/115/115	-
25	CLA	6	612	6	1/1/11/20	6/15/91/115	-
25	CLA	A	827	39	1/1/15/20	9/39/115/115	-
25	CLA	1	602	1	1/1/13/20	4/29/105/115	-
27	XAT	3	316	-	-	3/31/93/93	0/4/4/4
25	CLA	U	301	22	1/1/11/20	7/15/91/115	-
25	CLA	B	841	-	1/1/15/20	6/39/115/115	-
29	Q6L	W	319	-	-	9/29/67/67	0/2/2/2
38	KC2	U	307	22	-	10/15/71/71	-
30	BCR	L	306	-	-	2/29/63/63	0/2/2/2
24	CHL	V	305	22	3/3/15/26	4/12/110/137	-
25	CLA	A	803	-	1/1/15/20	6/39/115/115	-
25	CLA	B	828	-	1/1/15/20	4/39/115/115	-
24	CHL	X	305	22	3/3/15/26	0/10/108/137	-
25	CLA	B	829	-	1/1/15/20	16/39/115/115	-
25	CLA	F	802	-	1/1/10/20	3/12/88/115	-
35	SF4	A	853	8,7	-	-	0/6/5/5
25	CLA	B	830	-	1/1/15/20	12/39/115/115	-
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2
27	XAT	1	612	-	-	6/31/93/93	0/4/4/4
24	CHL	T	305	-	3/3/16/26	5/19/117/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	2	617	-	-	0/31/93/93	0/4/4/4
25	CLA	O	2003	-	1/1/10/20	2/10/86/115	-
25	CLA	U	312	-	1/1/10/20	2/10/86/115	-
25	CLA	O	2004	-	1/1/10/20	6/10/86/115	-
25	CLA	T	313	-	1/1/10/20	5/12/88/115	-
25	CLA	T	310	22	1/1/10/20	3/12/88/115	-
25	CLA	B	815	-	1/1/15/20	12/39/115/115	-
25	CLA	P	301	22	1/1/15/20	10/39/115/115	-
32	SQD	H	303	-	-	10/43/63/69	0/1/1/1
25	CLA	W	311	-	1/1/11/20	5/15/91/115	-
25	CLA	P	309	22	1/1/14/20	15/38/114/115	-
31	LMG	O	2008	-	-	2/34/54/70	0/1/1/1
30	BCR	K	207	-	-	3/29/63/63	0/2/2/2
25	CLA	Q	304	23	1/1/15/20	11/39/115/115	-
25	CLA	V	311	-	1/1/14/20	12/33/109/115	-
25	CLA	6	603	6	1/1/11/20	3/13/89/115	-
24	CHL	R	311	-	3/3/15/26	2/13/111/137	-
30	BCR	L	307	-	-	4/29/63/63	0/2/2/2
24	CHL	2	605	-	3/3/15/26	6/10/108/137	-
25	CLA	B	818	-	1/1/13/20	10/27/103/115	-
29	Q6L	T	319	-	-	8/29/67/67	0/2/2/2
24	CHL	R	302	-	3/3/16/26	7/17/115/137	-
24	CHL	4	308	-	3/3/16/26	3/15/113/137	-
25	CLA	T	311	-	1/1/14/20	12/33/109/115	-
29	Q6L	O	2007	-	-	6/29/67/67	0/2/2/2
25	CLA	F	803	12	1/1/10/20	4/10/86/115	-
25	CLA	Q	305	-	1/1/10/20	0/14/90/115	-
25	CLA	2	604	-	1/1/10/20	4/12/88/115	-
24	CHL	V	307	-	3/3/15/26	4/13/111/137	-
26	IWJ	Q	320	-	-	11/33/76/76	0/2/2/2
25	CLA	L	304	-	1/1/10/20	5/12/88/115	-
25	CLA	B	813	-	1/1/15/20	14/39/115/115	-
25	CLA	1	608	1	1/1/15/20	12/39/115/115	-
24	CHL	4	302	4	3/3/17/26	4/23/121/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	IWJ	4	301	-	-	6/33/76/76	0/2/2/2
29	Q6L	X	301	-	-	9/29/67/67	0/2/2/2
24	CHL	3	306	-	3/3/16/26	7/13/111/137	-
24	CHL	T	306	-	3/3/17/26	9/23/121/137	-
25	CLA	4	314	-	1/1/10/20	4/10/86/115	-
24	CHL	R	309	-	3/3/16/26	6/20/118/137	-
25	CLA	A	823	39	1/1/15/20	11/39/115/115	-
25	CLA	W	303	-	1/1/12/20	4/21/97/115	-
24	CHL	6	605	-	3/3/15/26	3/10/108/137	-
25	CLA	B	814	-	1/1/15/20	11/39/115/115	-
25	CLA	2	614	2	1/1/10/20	8/14/90/115	-
25	CLA	B	812	-	1/1/15/20	12/39/115/115	-
25	CLA	A	821	-	1/1/15/20	15/39/115/115	-
31	LMG	B	801	-	-	4/33/53/70	0/1/1/1
30	BCR	I	101	-	-	9/29/63/63	0/2/2/2
24	CHL	4	307	-	3/3/15/26	6/12/108/137	-
25	CLA	B	825	-	1/1/11/20	4/15/91/115	-
25	CLA	3	302	-	1/1/13/20	7/27/103/115	-
25	CLA	R	306	-	1/1/15/20	13/39/115/115	-
25	CLA	T	302	-	1/1/15/20	10/39/115/115	-
37	NEX	W	317	-	-	2/27/83/83	0/3/3/3
25	CLA	U	303	-	1/1/12/20	5/21/97/115	-
25	CLA	A	830	-	1/1/15/20	19/39/115/115	-
25	CLA	G	204	13	1/1/11/20	8/15/91/115	-
30	BCR	M	101	-	-	6/29/63/63	0/2/2/2
25	CLA	6	604	-	1/1/10/20	3/12/88/115	-
29	Q6L	R	319	-	-	10/29/67/67	0/2/2/2
26	IWJ	R	322	-	-	7/33/76/76	1/2/2/2
25	CLA	4	305	-	1/1/11/20	0/11/87/115	-
24	CHL	Q	308	23	3/3/16/26	6/20/118/137	-
25	CLA	A	843	-	1/1/15/20	7/39/115/115	-
25	CLA	T	303	-	1/1/12/20	4/21/97/115	-
24	CHL	2	601	2	3/3/16/26	2/17/115/137	-
24	CHL	P	314	22	3/3/15/26	4/14/112/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	825	-	1/1/15/20	17/39/115/115	-
25	CLA	N	203	-	1/1/10/20	4/12/88/115	-
24	CHL	W	306	-	3/3/17/26	3/23/121/137	-
26	IWJ	U	316	-	-	2/33/76/76	0/2/2/2
31	LMG	5	613	-	-	6/49/69/70	0/1/1/1
25	CLA	6	610	-	1/1/14/20	12/35/111/115	-
25	CLA	A	809	-	1/1/12/20	5/21/97/115	-
26	IWJ	T	321	-	-	4/33/76/76	1/2/2/2
25	CLA	1	607	1	1/1/7/20	2/8/68/115	-
24	CHL	2	607	-	3/3/15/26	5/14/112/137	-
25	CLA	P	312	22	1/1/13/20	10/27/103/115	-
30	BCR	F	801	-	-	4/29/63/63	0/2/2/2
25	CLA	A	815	-	1/1/15/20	11/39/115/115	-
25	CLA	H	302	-	1/1/15/20	11/39/115/115	-
24	CHL	X	315	22	3/3/15/26	6/14/112/137	-
29	Q6L	X	319	-	-	10/29/67/67	0/2/2/2
31	LMG	J	104	-	-	6/41/61/70	0/1/1/1
24	CHL	S	304	22	3/3/15/26	2/10/108/137	-
24	CHL	Q	309	-	3/3/15/26	2/13/111/137	-
36	DGD	B	850	-	-	12/48/88/95	0/2/2/2
24	CHL	W	307	-	3/3/20/26	13/39/137/137	-
25	CLA	A	806	-	1/1/12/20	5/24/100/115	-
29	Q6L	R	301	-	-	10/29/67/67	0/2/2/2
29	Q6L	S	321	-	-	11/29/67/67	0/2/2/2
25	CLA	U	311	22	1/1/13/20	5/27/103/115	-
28	LHG	2	619	25	-	7/37/37/53	-
25	CLA	5	602	5	1/1/14/20	10/33/109/115	-
25	CLA	B	822	-	1/1/12/20	2/21/97/115	-
25	CLA	A	834	-	1/1/13/20	4/29/105/115	-
25	CLA	2	602	2	1/1/14/20	15/35/111/115	-
30	BCR	J	101	-	-	4/29/63/63	0/2/2/2
25	CLA	B	805	-	1/1/15/20	15/39/115/115	-
28	LHG	1	614	25	-	11/39/39/53	-
25	CLA	P	303	-	1/1/12/20	9/21/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	Q6L	V	321	-	-	6/29/67/67	0/2/2/2
25	CLA	A	840	-	-	6/27/103/115	-
29	Q6L	P	321	-	-	7/29/67/67	0/2/2/2
33	CL0	A	802	-	3/3/20/25	10/37/135/135	-
25	CLA	2	608	2	1/1/11/20	6/15/91/115	-
25	CLA	2	611	2	1/1/11/20	5/13/89/115	-
29	Q6L	U	314	-	-	7/29/67/67	0/2/2/2
24	CHL	T	320	-	3/3/17/26	6/23/121/137	-
26	IWJ	X	318	-	-	7/33/76/76	1/2/2/2
25	CLA	O	2001	-	1/1/13/20	8/32/108/115	-
25	CLA	B	835	-	1/1/11/20	4/15/91/115	-
25	CLA	S	309	22	1/1/14/20	12/33/109/115	-
29	Q6L	Q	318	-	-	6/29/67/67	0/2/2/2
25	CLA	A	820	-	1/1/13/20	11/32/108/115	-
32	SQD	6	617	-	-	13/49/69/69	0/1/1/1
25	CLA	5	607	5	1/1/15/20	14/39/115/115	-
25	CLA	3	305	3	1/1/10/20	1/10/86/115	-
37	NEX	S	317	-	-	3/27/83/83	0/3/3/3
38	KC2	P	308	22	-	8/15/71/71	-
28	LHG	A	847	25	-	7/34/34/53	-
25	CLA	B	809	-	1/1/15/20	10/39/115/115	-
25	CLA	O	2005	-	1/1/10/20	2/10/86/115	-
24	CHL	T	314	22	3/3/15/26	2/10/108/137	-
25	CLA	B	802	-	1/1/15/20	9/39/115/115	-
30	BCR	4	319	-	-	2/29/63/63	0/2/2/2
25	CLA	2	609	2	1/1/13/20	7/27/103/115	-
30	BCR	G	205	-	-	2/29/63/63	0/2/2/2
25	CLA	B	831	-	1/1/15/20	13/39/115/115	-
25	CLA	1	613	-	1/1/12/20	7/24/100/115	-
25	CLA	B	816	-	1/1/12/20	4/23/99/115	-
24	CHL	V	304	22	3/3/16/26	6/15/113/137	-
25	CLA	B	817	-	1/1/10/20	3/13/89/115	-
25	CLA	L	302	-	-	12/33/109/115	-
24	CHL	W	305	-	3/3/15/26	2/10/108/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	3	323	-	-	13/47/47/53	-
25	CLA	A	811	7	1/1/12/20	2/21/97/115	-
24	CHL	U	313	22	3/3/15/26	2/12/110/137	-
30	BCR	K	205	-	-	2/29/63/63	0/2/2/2
37	NEX	P	317	-	-	2/27/83/83	0/3/3/3
25	CLA	6	608	6	1/1/10/20	4/12/88/115	-
25	CLA	5	609	-	1/1/13/20	9/25/101/115	-
25	CLA	2	610	28	1/1/10/20	4/12/88/115	-
25	CLA	S	302	-	1/1/15/20	12/39/115/115	-
38	KC2	V	308	22	-	11/15/71/71	-
25	CLA	A	856	-	1/1/13/20	12/30/106/115	-
25	CLA	4	309	4	1/1/11/20	6/15/91/115	-
25	CLA	A	842	-	1/1/15/20	14/39/115/115	-
29	Q6L	S	315	-	-	5/29/67/67	0/2/2/2
25	CLA	5	604	-	1/1/10/20	0/4/80/115	-
25	CLA	A	818	-	1/1/11/20	4/15/91/115	-
26	IWJ	T	318	-	-	6/33/76/76	0/2/2/2
25	CLA	W	309	22	1/1/14/20	9/38/114/115	-
30	BCR	B	848	-	-	2/29/63/63	0/2/2/2
25	CLA	B	832	-	1/1/10/20	5/13/89/115	-
24	CHL	Q	316	23	3/3/15/26	5/14/112/137	-
25	CLA	3	311	3	1/1/13/20	10/25/101/115	-
25	CLA	B	806	-	1/1/15/20	12/39/115/115	-
25	CLA	S	310	22	1/1/14/20	11/33/109/115	-
24	CHL	5	605	-	3/3/15/26	1/8/106/137	-
28	LHG	3	322	-	-	8/40/40/53	-
30	BCR	A	850	-	-	1/29/63/63	0/2/2/2
29	Q6L	R	304	-	-	5/29/67/67	0/2/2/2
30	BCR	L	305	-	-	3/29/63/63	0/2/2/2
30	BCR	A	852	-	-	4/29/63/63	0/2/2/2
25	CLA	X	310	22	1/1/10/20	2/12/88/115	-
24	CHL	W	304	22	3/3/15/26	1/10/108/137	-
25	CLA	R	314	22	1/1/14/20	12/33/109/115	-
25	CLA	A	816	-	1/1/11/20	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	Q6L	P	316	-	-	2/29/67/67	0/2/2/2
25	CLA	A	807	-	1/1/14/20	17/38/114/115	-
31	LMG	A	801	-	-	1/26/46/70	0/1/1/1
30	BCR	K	202	-	-	0/29/63/63	0/2/2/2
38	KC2	Q	310	23	-	6/15/71/71	-
29	Q6L	V	315	-	-	11/29/67/67	0/2/2/2
25	CLA	Q	315	-	1/1/11/20	4/19/95/115	-
24	CHL	P	307	-	3/3/15/26	2/13/111/137	-
25	CLA	3	309	28	1/1/10/20	5/12/88/115	-
24	CHL	6	606	-	3/3/15/26	6/12/110/137	-
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
30	BCR	A	851	-	-	5/29/63/63	0/2/2/2
25	CLA	K	203	-	1/1/14/20	6/36/112/115	-
25	CLA	2	613	-	1/1/10/20	5/11/87/115	-
25	CLA	B	823	-	1/1/11/20	6/18/94/115	-
25	CLA	H	301	14	1/1/10/20	8/14/90/115	-
26	IWJ	V	317	-	-	5/33/76/76	0/2/2/2
30	BCR	F	804	-	-	6/29/63/63	0/2/2/2
24	CHL	V	314	22	3/3/15/26	4/13/111/137	-
25	CLA	A	813	-	1/1/15/20	15/39/115/115	-
24	CHL	S	305	22	3/3/15/26	3/10/108/137	-
25	CLA	R	305	22	1/1/15/20	11/39/115/115	-
25	CLA	B	807	-	1/1/15/20	11/39/115/115	-
25	CLA	S	313	-	1/1/10/20	2/10/86/115	-
24	CHL	X	306	-	3/3/15/26	2/10/108/137	-
29	Q6L	P	319	-	-	6/29/67/67	0/2/2/2
25	CLA	K	201	17	1/1/11/20	4/15/91/115	-
25	CLA	X	313	22	1/1/10/20	2/10/86/115	-
25	CLA	A	838	7	-	18/39/115/115	-
26	IWJ	S	322	-	-	5/33/76/76	0/2/2/2
25	CLA	A	812	-	1/1/14/20	9/38/114/115	-
25	CLA	B	821	-	1/1/13/20	9/27/103/115	-
25	CLA	3	307	3	1/1/14/20	11/35/111/115	-
25	CLA	6	611	-	1/1/10/20	6/13/89/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	A	857	-	-	9/41/61/70	0/1/1/1
25	CLA	5	606	-	1/1/10/20	0/8/84/115	-
25	CLA	A	808	7	1/1/15/20	9/39/115/115	-
25	CLA	A	839	-	1/1/15/20	16/39/115/115	-
26	IWJ	S	319	-	-	7/33/76/76	1/2/2/2
25	CLA	Q	314	23	1/1/12/20	10/25/101/115	-
25	CLA	X	302	22	1/1/13/20	9/27/103/115	-
28	LHG	3	320	25	-	3/26/26/53	-
38	KC2	W	308	22	-	9/15/71/71	-
25	CLA	2	603	-	1/1/11/20	4/13/89/115	-
29	Q6L	O	2006	-	-	9/29/67/67	0/2/2/2
24	CHL	U	305	-	3/3/16/26	8/15/113/137	-
25	CLA	B	826	-	1/1/15/20	8/39/115/115	-
25	CLA	5	601	5	1/1/11/20	11/17/93/115	-
25	CLA	4	312	4	1/1/10/20	2/10/86/115	-
29	Q6L	T	322	-	-	7/29/67/67	0/2/2/2
25	CLA	R	316	22	1/1/13/20	9/27/103/115	-
30	BCR	A	848	-	-	2/29/63/63	0/2/2/2
24	CHL	R	318	22	3/3/15/26	3/14/112/137	-
28	LHG	6	616	-	-	10/50/50/53	-
24	CHL	V	306	-	3/3/15/26	0/13/111/137	-
28	LHG	3	321	-	-	9/47/47/53	-
29	Q6L	X	317	-	-	2/29/67/67	0/2/2/2
25	CLA	B	837	-	1/1/10/20	2/12/88/115	-
29	Q6L	T	316	-	-	1/29/67/67	0/2/2/2
25	CLA	S	311	-	1/1/11/20	6/18/94/115	-
29	Q6L	2	616	-	-	11/29/67/67	0/2/2/2
25	CLA	3	314	3	-	0/8/84/115	-
29	Q6L	Q	317	-	-	7/29/67/67	0/2/2/2
25	CLA	K	204	-	1/1/11/20	7/17/93/115	-
26	IWJ	R	303	-	-	4/33/76/76	0/2/2/2
29	Q6L	X	316	-	-	7/29/63/67	0/2/2/2
30	BCR	B	845	-	-	2/29/63/63	0/2/2/2
25	CLA	A	826	-	1/1/13/20	9/27/103/115	-
24	CHL	X	308	-	3/3/15/26	6/13/111/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	Q6L	Q	319	-	-	5/29/67/67	0/2/2/2
29	Q6L	W	315	-	-	4/29/67/67	0/2/2/2
25	CLA	Q	311	23	1/1/13/20	7/27/103/115	-
27	XAT	6	615	-	-	0/31/93/93	0/4/4/4
25	CLA	U	302	-	1/1/13/20	9/29/105/115	-
25	CLA	V	310	22	1/1/11/20	8/18/94/115	-
25	CLA	B	810	-	1/1/15/20	18/39/115/115	-
25	CLA	B	836	8	-	7/33/109/115	-
25	CLA	4	304	-	1/1/11/20	4/13/89/115	-
25	CLA	B	827	-	1/1/12/20	4/21/97/115	-
24	CHL	Q	307	23	3/3/16/26	8/15/113/137	-
38	KC2	T	308	22	-	7/15/71/71	-
26	IWJ	V	318	-	-	4/33/76/76	0/2/2/2
25	CLA	U	308	22	1/1/10/20	0/10/86/115	-
25	CLA	A	837	-	1/1/15/20	11/39/115/115	-
25	CLA	6	602	6	1/1/14/20	11/36/112/115	-
30	BCR	3	319	-	-	1/29/63/63	0/2/2/2
25	CLA	R	313	22	1/1/14/20	16/38/114/115	-
25	CLA	V	302	-	1/1/12/20	9/21/97/115	-
26	IWJ	1	611	-	-	4/33/76/76	0/2/2/2
29	Q6L	V	319	-	-	9/29/67/67	0/2/2/2
25	CLA	K	206	17	1/1/15/20	13/39/115/115	-
25	CLA	O	2002	-	1/1/15/20	8/39/115/115	-
25	CLA	Q	312	23	1/1/10/20	3/12/88/115	-
25	CLA	P	302	-	1/1/15/20	15/39/115/115	-
29	Q6L	R	320	-	-	0/29/67/67	0/2/2/2
29	Q6L	S	323	-	-	9/29/67/67	0/2/2/2
25	CLA	H	304	18	1/1/11/20	5/15/91/115	-
25	CLA	A	814	-	1/1/12/20	6/26/102/115	-
25	CLA	5	603	5	1/1/11/20	5/15/91/115	-
25	CLA	4	310	4	1/1/12/20	4/26/102/115	-
37	NEX	H	306	-	-	3/27/83/83	0/3/3/3
24	CHL	T	307	-	3/3/15/26	3/13/111/137	-
25	CLA	G	203	-	1/1/10/20	4/12/88/115	-
25	CLA	A	836	-	1/1/15/20	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	817	-	-	11/39/115/115	-
25	CLA	V	303	-	1/1/12/20	4/21/97/115	-
25	CLA	A	804	39	1/1/15/20	14/39/115/115	-
30	BCR	J	103	-	-	1/29/63/63	0/2/2/2
25	CLA	A	835	-	1/1/15/20	13/39/115/115	-
25	CLA	4	315	-	1/1/10/20	4/10/86/115	-
24	CHL	U	304	22	3/3/15/26	3/10/108/137	-
25	CLA	R	315	-	1/1/14/20	10/33/109/115	-
25	CLA	U	309	22	1/1/11/20	8/17/93/115	-
26	IWJ	V	320	-	-	5/33/76/76	1/2/2/2
25	CLA	4	311	-	1/1/10/20	6/12/88/115	-
25	CLA	V	313	-	1/1/11/20	6/19/95/115	-
37	NEX	R	321	-	-	3/27/83/83	0/3/3/3
25	CLA	R	307	-	1/1/12/20	4/21/97/115	-
25	CLA	Q	306	39	1/1/12/20	7/21/97/115	-
24	CHL	T	304	22	3/3/15/26	4/12/110/137	-
25	CLA	2	612	2	1/1/15/20	15/39/115/115	-
29	Q6L	V	316	-	-	7/29/67/67	0/2/2/2
30	BCR	G	201	-	-	2/29/63/63	0/2/2/2
25	CLA	1	605	-	1/1/10/20	4/10/86/115	-
25	CLA	B	811	8	1/1/15/20	12/39/115/115	-
25	CLA	3	304	3	1/1/10/20	2/10/86/115	-
25	CLA	1	609	-	1/1/10/20	1/4/80/115	-
24	CHL	P	304	22	3/3/16/26	5/15/113/137	-
25	CLA	A	845	28	1/1/12/20	5/21/97/115	-
24	CHL	4	306	-	3/3/15/26	0/8/106/137	-
25	CLA	W	302	-	1/1/13/20	5/27/103/115	-
25	CLA	3	310	-	1/1/10/20	5/13/89/115	-
25	CLA	1	606	1	1/1/10/20	2/8/84/115	-
26	IWJ	4	317	-	-	8/33/76/76	0/2/2/2
36	DGD	A	854	-	-	4/40/80/95	0/2/2/2
25	CLA	B	842	-	1/1/15/20	17/39/115/115	-
25	CLA	X	312	-	1/1/12/20	6/23/99/115	-
31	LMG	2	620	-	-	3/26/46/70	0/1/1/1
25	CLA	3	303	-	1/1/11/20	0/11/87/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	833	-	1/1/10/20	0/13/89/115	-
25	CLA	V	301	22	1/1/14/20	10/33/109/115	-
25	CLA	X	304	-	1/1/10/20	3/12/88/115	-
25	CLA	A	841	-	1/1/12/20	4/21/97/115	-
24	CHL	W	314	22	3/3/14/26	3/10/104/137	-
26	IWJ	W	318	-	-	9/33/76/76	0/2/2/2
25	CLA	W	313	-	1/1/10/20	3/13/89/115	-
31	LMG	A	855	-	-	3/22/42/70	0/1/1/1
25	CLA	B	834	-	1/1/15/20	11/39/115/115	-
25	CLA	4	303	4	1/1/14/20	17/33/109/115	-
25	CLA	L	303	-	1/1/11/20	5/15/91/115	-
28	LHG	Q	302	-	-	5/39/39/53	-
25	CLA	Q	313	-	1/1/11/20	11/17/93/115	-
29	Q6L	U	315	-	-	2/29/67/67	0/2/2/2
25	CLA	1	610	1	-	6/8/84/115	-
25	CLA	5	610	-	1/1/10/20	4/10/86/115	-
25	CLA	W	312	22	1/1/13/20	7/27/103/115	-
25	CLA	A	819	-	1/1/14/20	13/33/109/115	-
25	CLA	V	312	22	-	7/27/103/115	-
26	IWJ	6	614	-	-	3/33/76/76	0/2/2/2
30	BCR	3	318	-	-	2/29/63/63	0/2/2/2
25	CLA	6	613	6	-	8/39/115/115	-
30	BCR	B	846	-	-	4/29/63/63	0/2/2/2
25	CLA	B	820	-	1/1/14/20	10/33/109/115	-
26	IWJ	3	315	-	-	3/33/76/76	1/2/2/2
26	IWJ	P	318	-	-	2/33/76/76	0/2/2/2
29	Q6L	S	320	-	-	7/29/67/67	0/2/2/2
25	CLA	3	313	-	1/1/10/20	2/10/86/115	-
34	PQN	B	844	-	-	6/23/43/43	0/2/2/2
25	CLA	S	303	-	1/1/12/20	2/21/97/115	-
27	XAT	5	612	-	-	0/31/93/93	0/4/4/4
29	Q6L	W	316	-	-	6/29/67/67	0/2/2/2
25	CLA	B	808	8	1/1/15/20	23/39/115/115	-
25	CLA	1	603	-	1/1/13/20	6/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	T	309	22	1/1/13/20	10/32/108/115	-
25	CLA	B	819	-	1/1/13/20	11/32/108/115	-
35	SF4	C	101	9	-	-	0/6/5/5
30	BCR	B	847	-	-	0/29/63/63	0/2/2/2
25	CLA	3	308	3	1/1/10/20	3/10/86/115	-
34	PQN	A	844	-	-	13/23/43/43	0/2/2/2
24	CHL	S	306	-	3/3/17/26	9/23/121/137	-
25	CLA	R	317	-	-	5/19/95/115	-
30	BCR	3	317	-	-	2/29/63/63	0/2/2/2
25	CLA	B	824	-	1/1/14/20	4/33/109/115	-
24	CHL	1	604	1	3/3/15/26	0/8/106/137	-
25	CLA	S	312	22	1/1/13/20	7/27/103/115	-
25	CLA	G	202	-	1/1/11/20	8/15/91/115	-
29	Q6L	P	315	-	-	6/29/67/67	0/2/2/2
25	CLA	3	301	3	1/1/14/20	7/33/109/115	-
25	CLA	W	301	22	1/1/13/20	9/27/103/115	-
31	LMG	F	805	-	-	2/26/46/70	0/1/1/1
25	CLA	A	824	-	1/1/10/20	5/12/88/115	-
25	CLA	4	316	4	1/1/10/20	3/12/88/115	-

The worst 5 of 3209 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	307	CHL	C3B-C4B	11.68	1.52	1.41
24	T	304	CHL	C3B-C4B	11.25	1.52	1.41
24	P	304	CHL	C3B-C4B	11.21	1.52	1.41
24	Q	308	CHL	C3B-C4B	11.02	1.52	1.41
24	T	305	CHL	C3B-C4B	10.96	1.52	1.41

The worst 5 of 4280 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	318	XAT	O4-C5-C4	12.50	125.20	113.49
37	S	317	NEX	O24-C25-C24	10.98	123.78	113.49
25	1	607	CLA	CHA-C4D-ND	10.67	134.35	125.22
37	R	321	NEX	O24-C25-C24	10.63	123.46	113.49
27	6	615	XAT	O4-C5-C4	10.55	123.38	113.49

5 of 413 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	601	CHL	ND
24	1	601	CHL	NC
24	1	601	CHL	NA
24	1	604	CHL	ND
24	1	604	CHL	NC

5 of 2891 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	2	601	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C3A-C2A-CAA-CBA
24	2	605	CHL	CAD-CBD-CGD-O1D
24	2	605	CHL	CAD-CBD-CGD-O2D

5 of 7 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	3	315	IWJ	C29-C30-C32-C33-C34-C35
26	X	318	IWJ	C29-C30-C32-C33-C34-C35
26	T	321	IWJ	C29-C30-C32-C33-C34-C35
26	S	319	IWJ	C29-C30-C32-C33-C34-C35
26	V	320	IWJ	C29-C30-C32-C33-C34-C35

159 monomers are involved in 236 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	803	CLA	1	0
24	1	601	CHL	1	0
25	B	843	CLA	1	0
25	J	102	CLA	1	0
38	R	312	KC2	2	0
25	A	832	CLA	1	0
38	S	308	KC2	1	0
25	A	822	CLA	1	0
24	P	305	CHL	1	0
25	X	311	CLA	3	0
25	T	312	CLA	1	0
24	R	308	CHL	7	0
24	S	307	CHL	5	0
27	4	318	XAT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	V	309	CLA	4	0
26	P	320	IWJ	1	0
25	6	607	CLA	1	0
25	S	301	CLA	7	0
25	6	612	CLA	1	0
25	A	827	CLA	1	0
27	3	316	XAT	1	0
25	U	301	CLA	1	0
24	V	305	CHL	1	0
25	A	803	CLA	1	0
25	B	829	CLA	2	0
25	F	802	CLA	1	0
25	T	310	CLA	1	0
25	B	815	CLA	3	0
25	P	301	CLA	3	0
32	H	303	SQD	1	0
25	P	309	CLA	2	0
30	K	207	BCR	2	0
25	Q	304	CLA	6	0
25	V	311	CLA	3	0
24	R	311	CHL	2	0
25	B	818	CLA	2	0
24	4	308	CHL	1	0
25	T	311	CLA	1	0
24	V	307	CHL	1	0
26	Q	320	IWJ	1	0
25	B	813	CLA	1	0
26	4	301	IWJ	1	0
24	3	306	CHL	2	0
25	W	303	CLA	1	0
25	B	825	CLA	1	0
25	R	306	CLA	1	0
25	A	830	CLA	1	0
25	G	204	CLA	1	0
30	M	101	BCR	1	0
26	R	322	IWJ	1	0
25	A	825	CLA	1	0
25	6	610	CLA	1	0
26	T	321	IWJ	1	0
25	1	607	CLA	3	0
30	F	801	BCR	1	0
25	A	815	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	319	Q6L	1	0
24	S	304	CHL	2	0
36	B	850	DGD	1	0
28	2	619	LHG	1	0
25	5	602	CLA	1	0
30	J	101	BCR	2	0
28	1	614	LHG	1	0
29	V	321	Q6L	1	0
25	2	608	CLA	1	0
29	U	314	Q6L	2	0
25	O	2001	CLA	1	0
25	B	835	CLA	1	0
25	S	309	CLA	4	0
25	A	820	CLA	1	0
25	5	607	CLA	1	0
38	P	308	KC2	1	0
30	4	319	BCR	2	0
25	2	609	CLA	4	0
37	P	317	NEX	1	0
38	V	308	KC2	1	0
25	A	856	CLA	1	0
25	4	309	CLA	1	0
29	S	315	Q6L	1	0
26	T	318	IWJ	1	0
25	W	309	CLA	5	0
30	B	848	BCR	1	0
25	B	832	CLA	1	0
25	B	806	CLA	1	0
25	S	310	CLA	2	0
30	A	850	BCR	1	0
30	L	305	BCR	2	0
30	A	852	BCR	2	0
25	X	310	CLA	1	0
25	A	816	CLA	1	0
29	P	316	Q6L	1	0
25	2	613	CLA	1	0
26	V	317	IWJ	1	0
24	V	314	CHL	1	0
25	A	813	CLA	1	0
25	R	305	CLA	3	0
24	X	306	CHL	1	0
25	X	313	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	S	322	IWJ	1	0
25	A	812	CLA	1	0
25	3	307	CLA	3	0
25	A	808	CLA	1	0
26	S	319	IWJ	1	0
25	Q	314	CLA	1	0
25	X	302	CLA	3	0
29	O	2006	Q6L	1	0
25	R	316	CLA	1	0
28	6	616	LHG	1	0
29	T	316	Q6L	1	0
29	2	616	Q6L	1	0
30	B	845	BCR	1	0
24	X	308	CHL	1	0
29	Q	319	Q6L	1	0
29	W	315	Q6L	2	0
27	6	615	XAT	1	0
25	B	810	CLA	1	0
24	Q	307	CHL	1	0
38	T	308	KC2	1	0
25	6	602	CLA	2	0
30	3	319	BCR	1	0
25	V	302	CLA	1	0
25	K	206	CLA	3	0
25	O	2002	CLA	1	0
25	Q	312	CLA	1	0
24	T	307	CHL	1	0
25	G	203	CLA	1	0
25	A	836	CLA	1	0
25	A	817	CLA	1	0
24	U	304	CHL	1	0
26	V	320	IWJ	1	0
25	4	311	CLA	1	0
24	T	304	CHL	1	0
30	G	201	BCR	4	0
25	1	605	CLA	1	0
24	4	306	CHL	3	0
26	4	317	IWJ	1	0
36	A	854	DGD	1	0
25	B	842	CLA	4	0
25	V	301	CLA	4	0
25	X	304	CLA	1	0

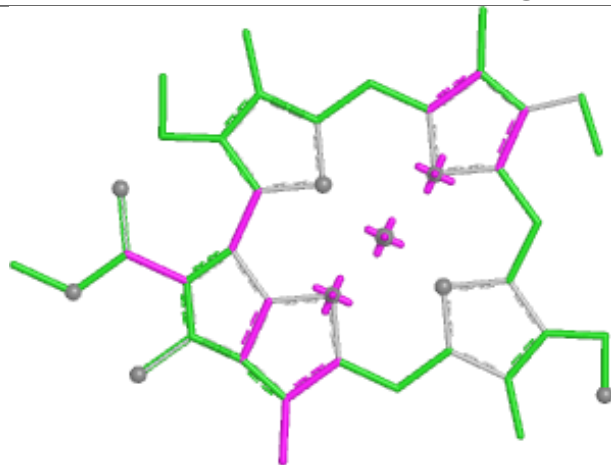
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	W	314	CHL	1	0
26	W	318	IWJ	2	0
25	4	303	CLA	2	0
25	1	610	CLA	1	0
25	W	312	CLA	2	0
25	V	312	CLA	2	0
26	6	614	IWJ	2	0
26	3	315	IWJ	1	0
26	P	318	IWJ	1	0
25	B	808	CLA	2	0
25	B	819	CLA	2	0
30	B	847	BCR	1	0
34	A	844	PQN	1	0
25	B	824	CLA	3	0
25	G	202	CLA	1	0
25	3	301	CLA	2	0
25	W	301	CLA	3	0
31	F	805	LMG	1	0
25	A	824	CLA	1	0

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

Ligand CHL 6 601



Bond lengths



Bond angles

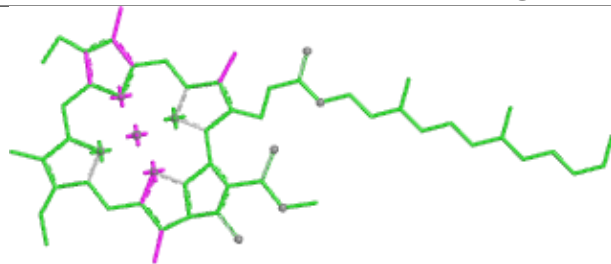


Torsions

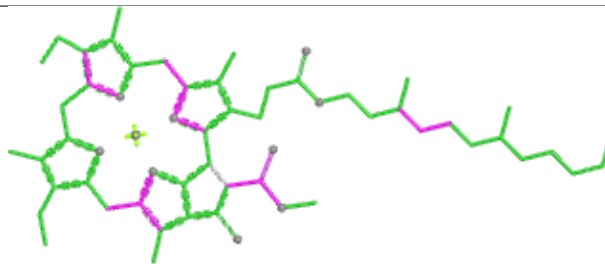


Rings

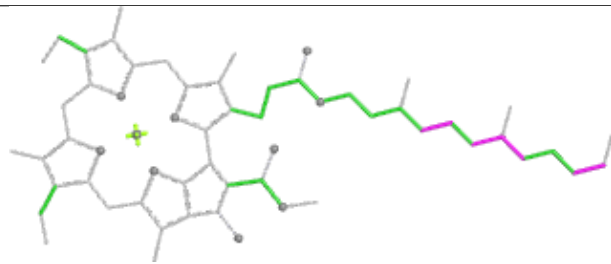
Ligand CLA A 828



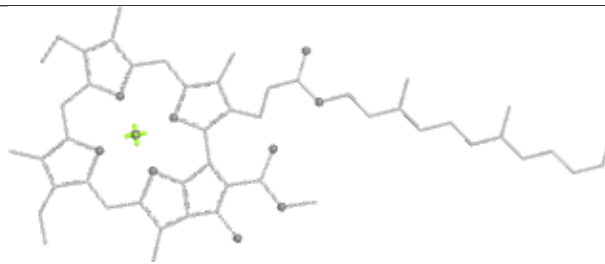
Bond lengths



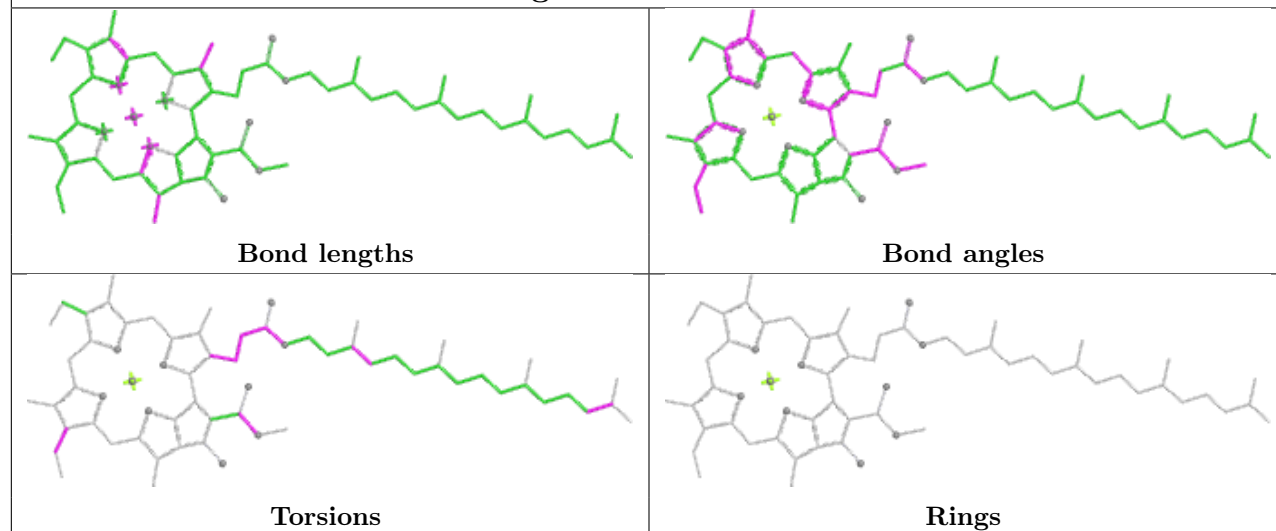
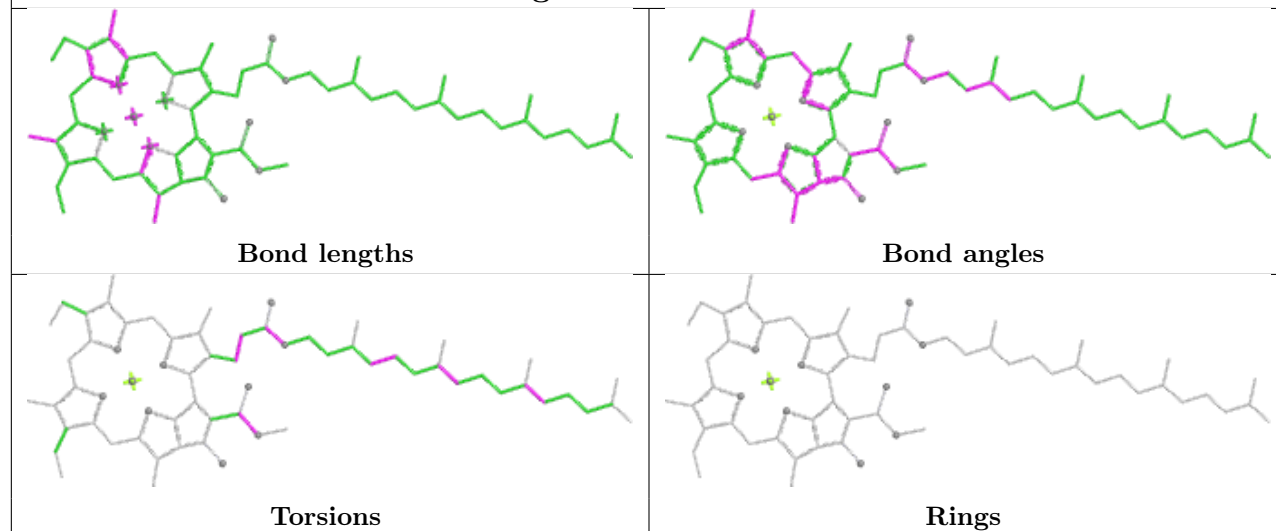
Bond angles



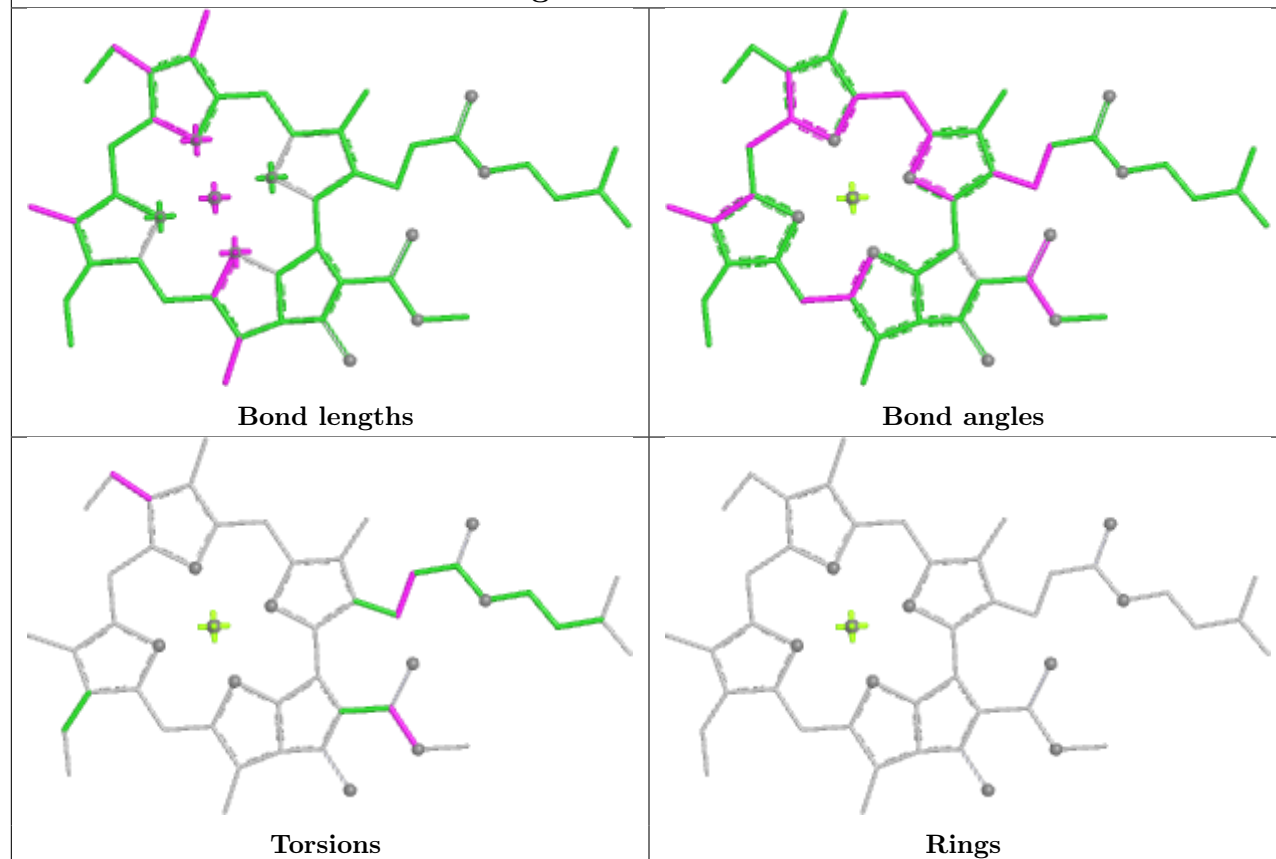
Torsions



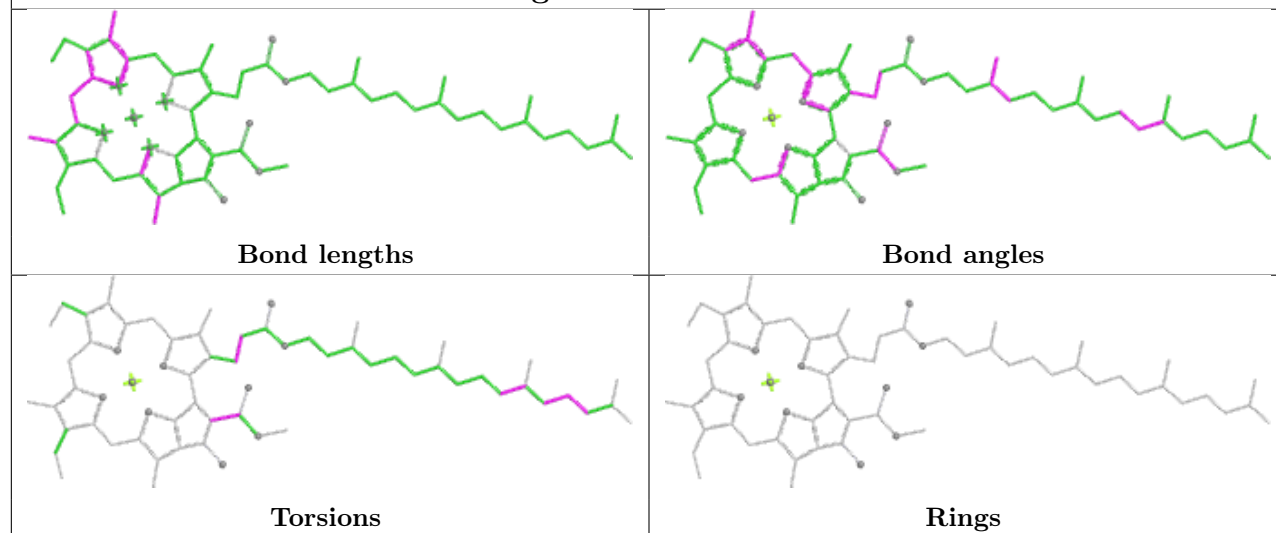
Rings

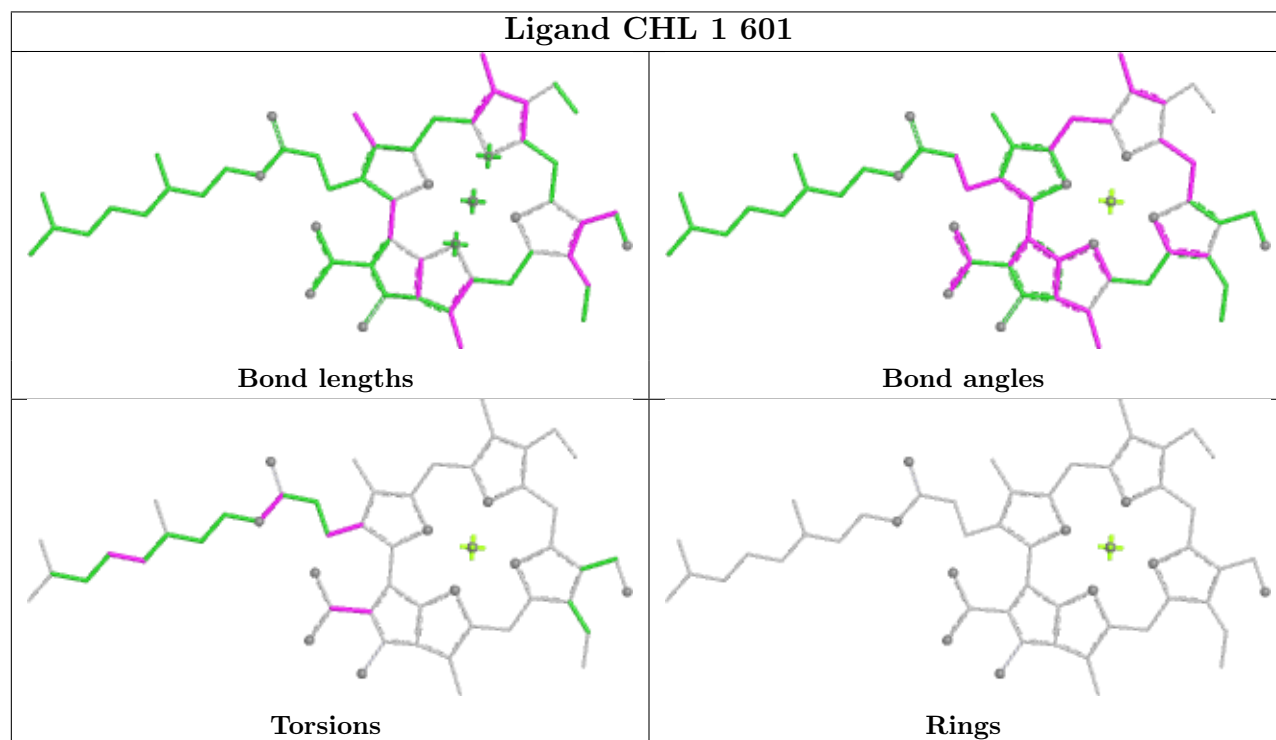
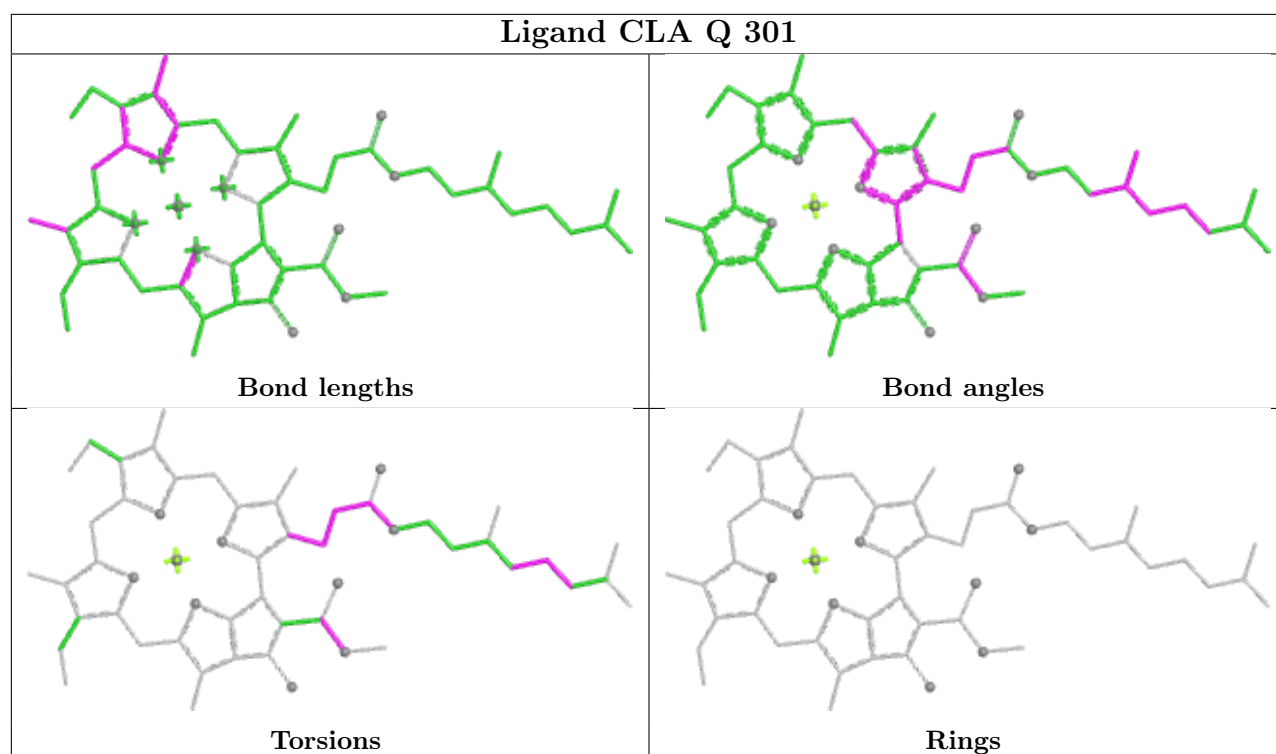
Ligand CLA A 829**Ligand CLA B 803**

Ligand CLA A 833

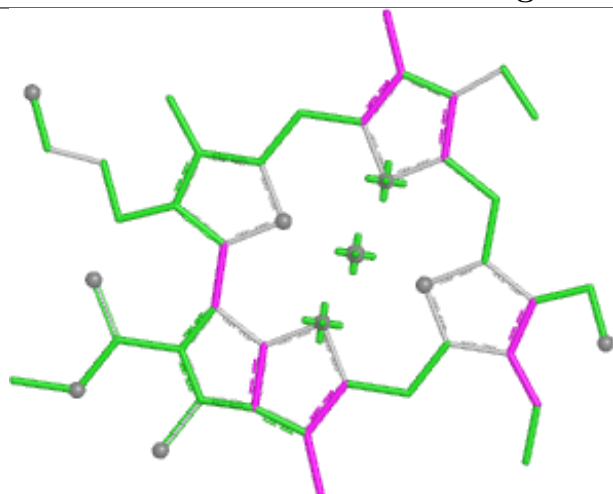


Ligand CLA A 810

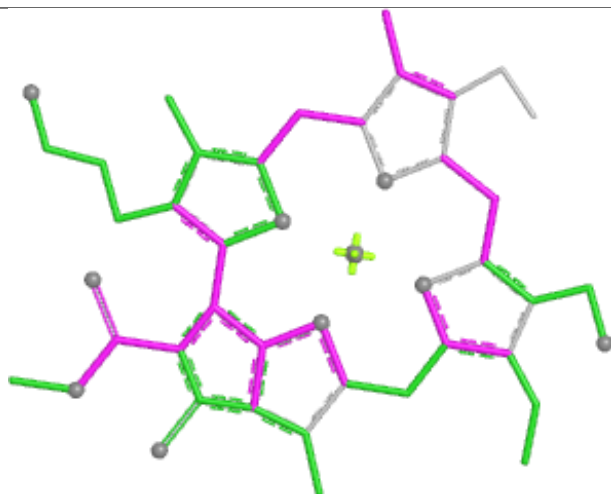




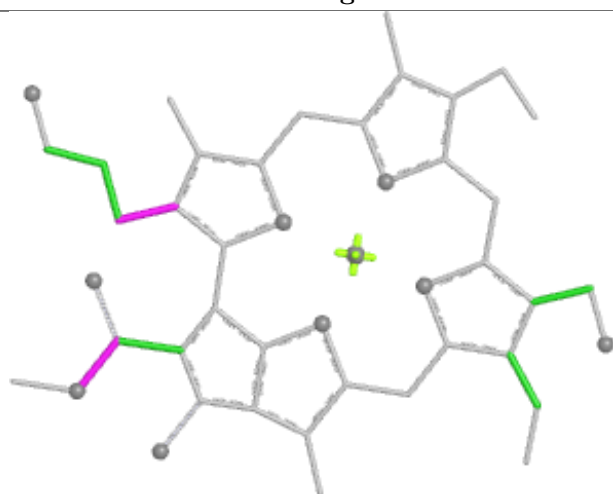
Ligand CHL S 314



Bond lengths



Bond angles

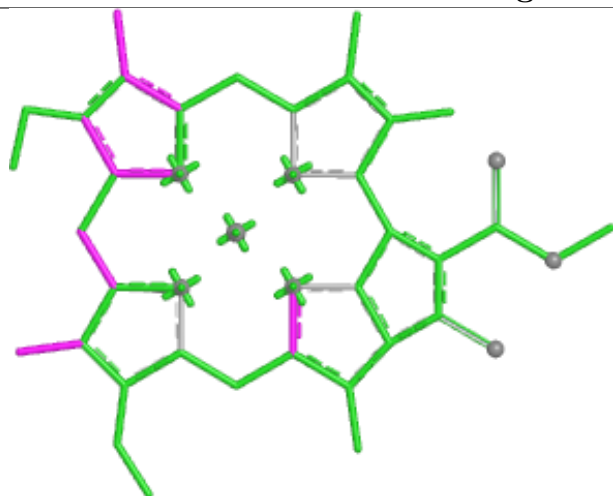


Torsions

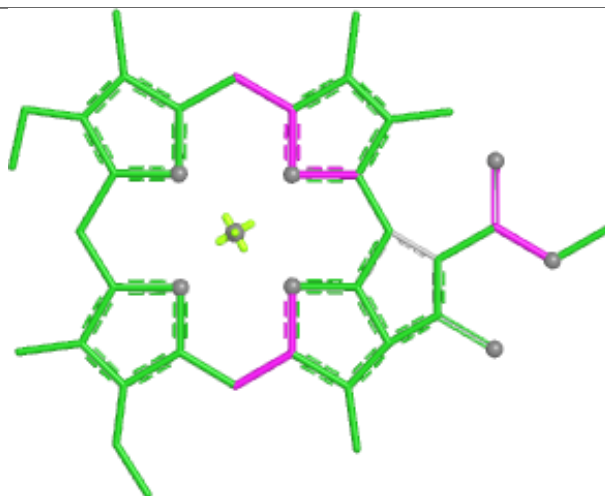


Rings

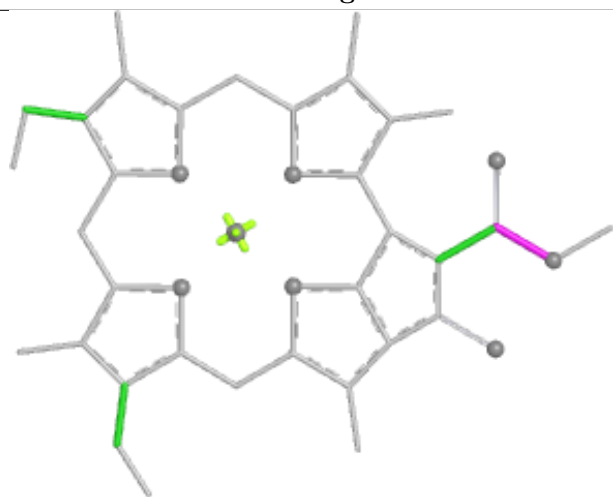
Ligand CLA L 301



Bond lengths



Bond angles

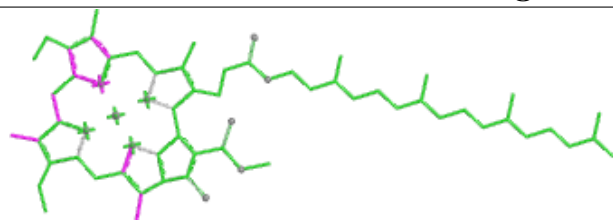


Torsions

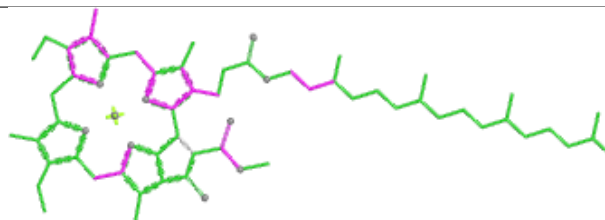


Rings

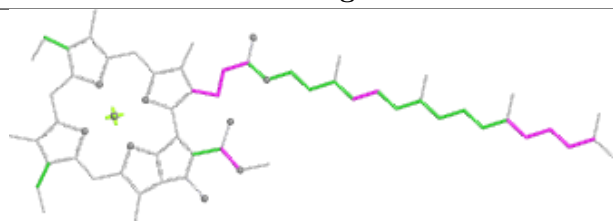
Ligand CLA B 843



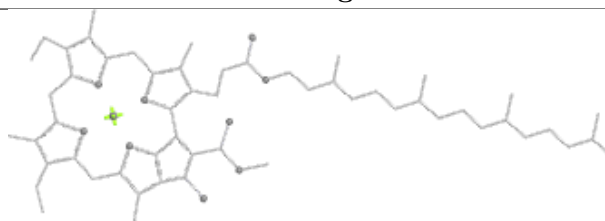
Bond lengths



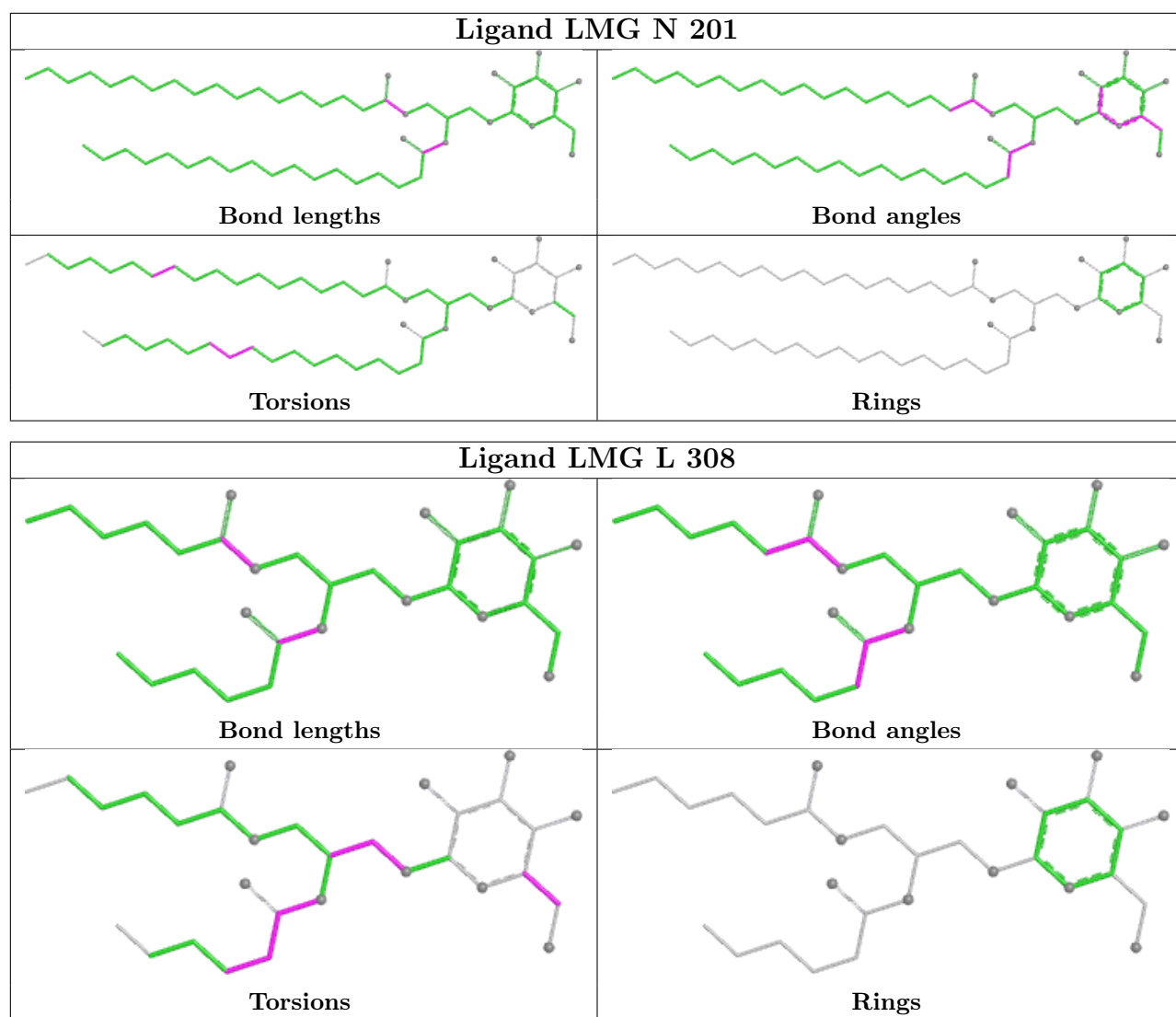
Bond angles



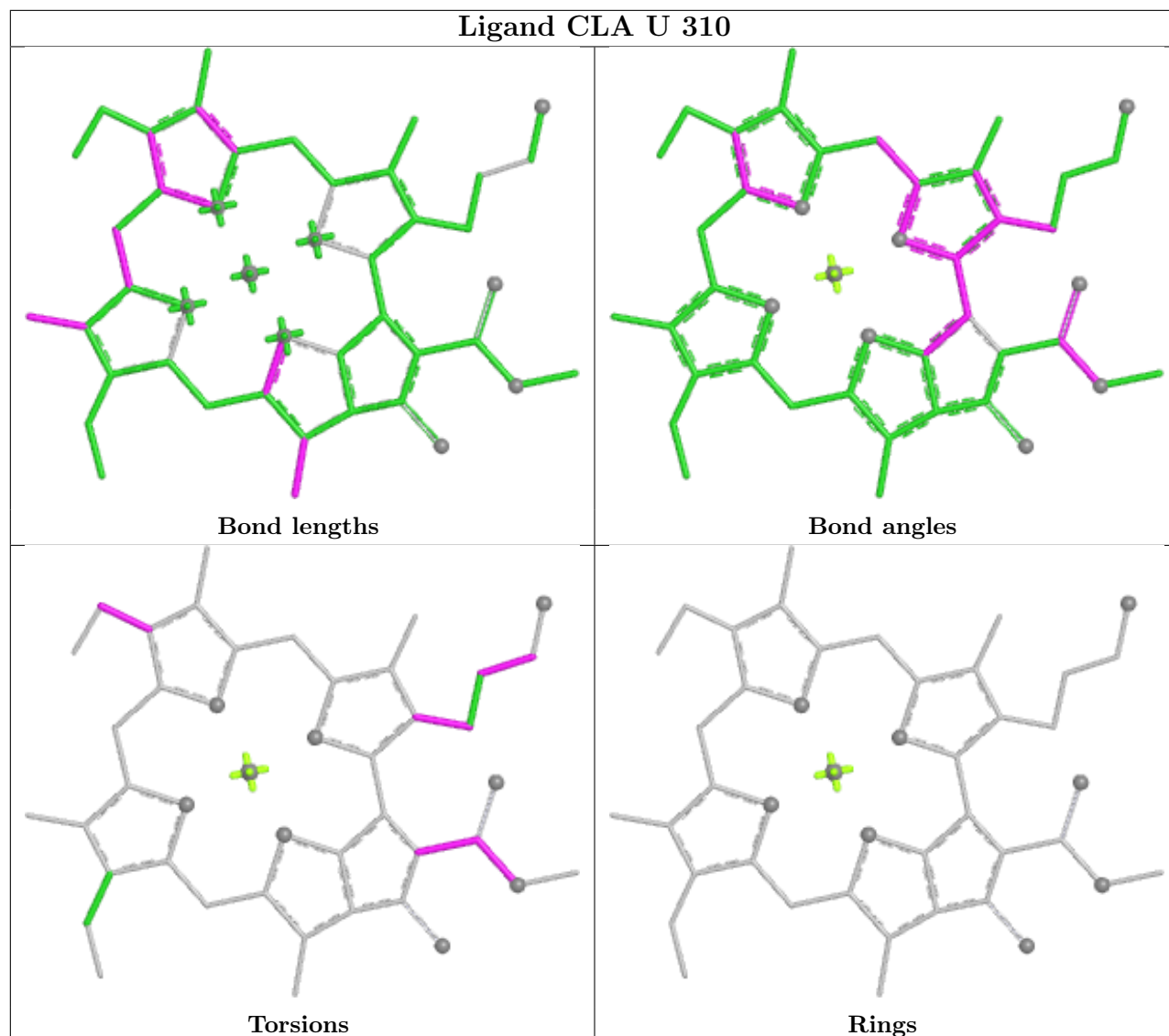
Torsions



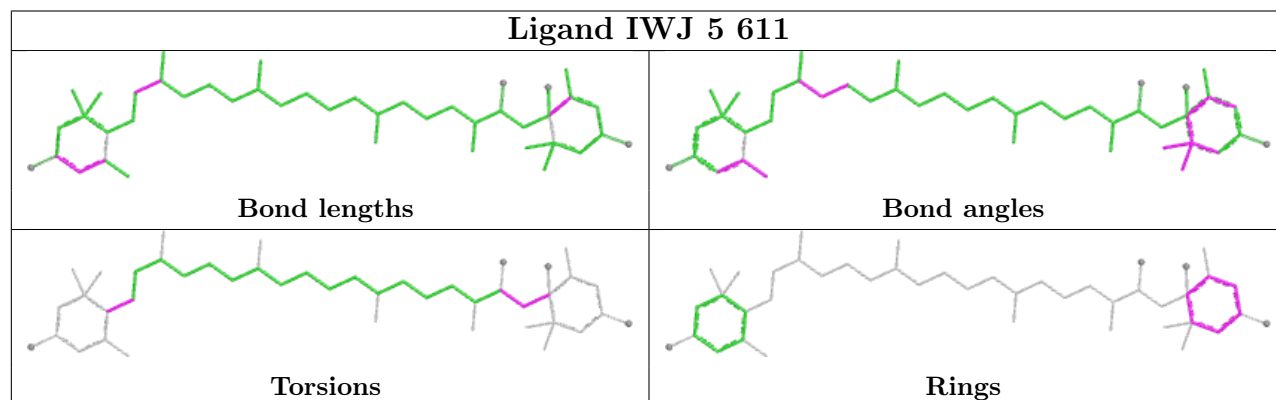
Rings

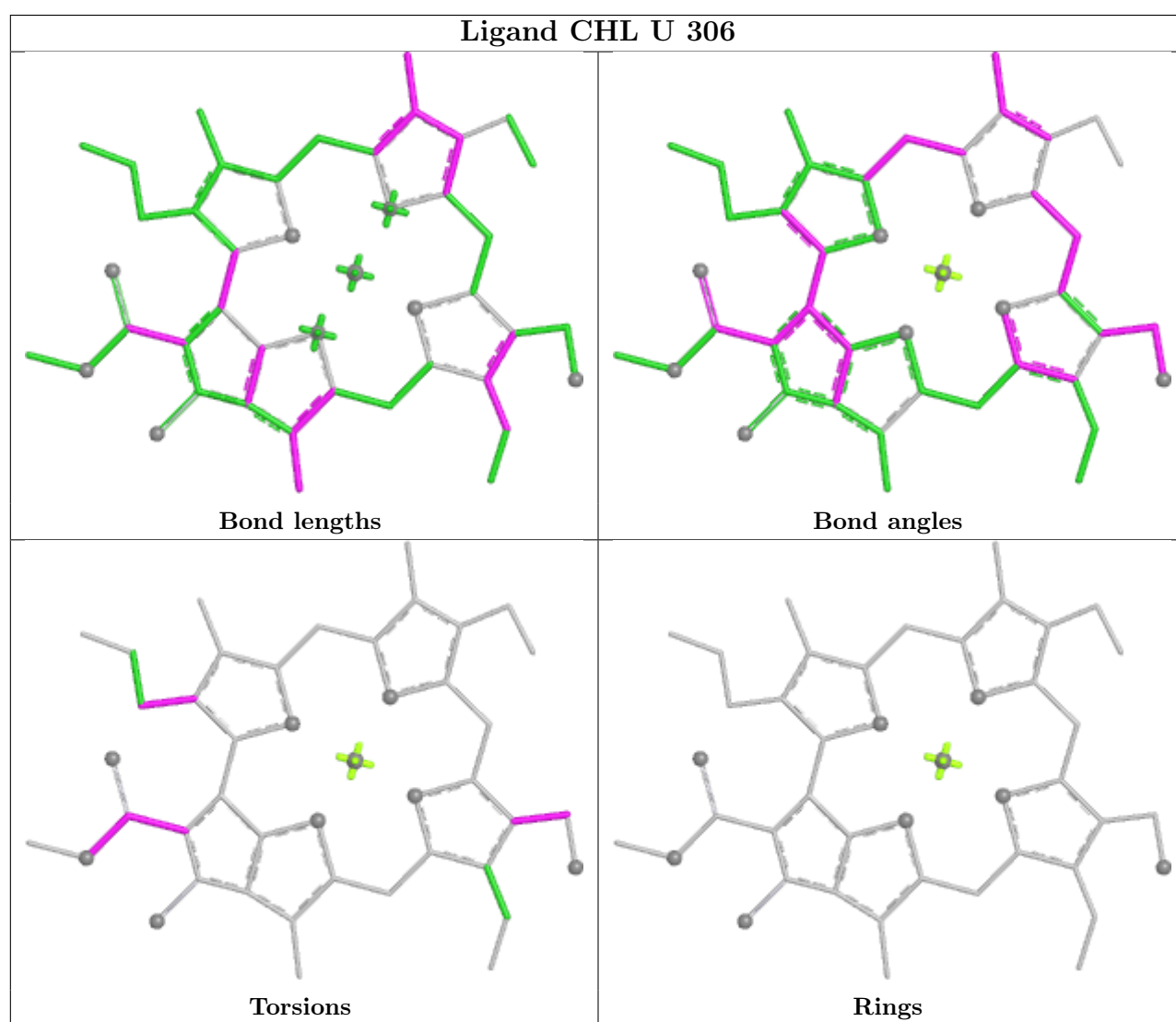
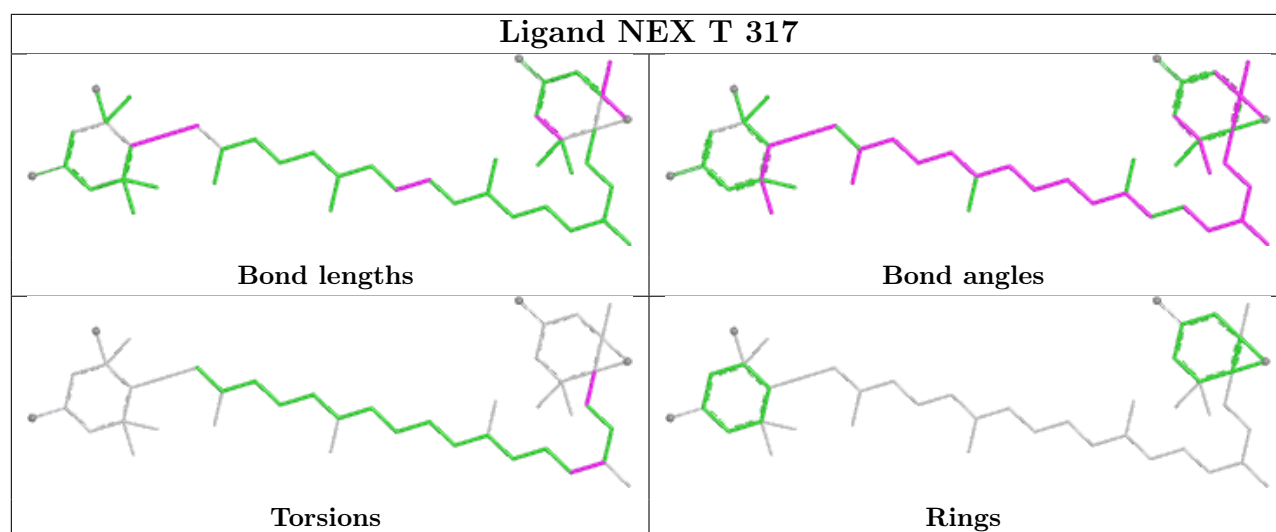


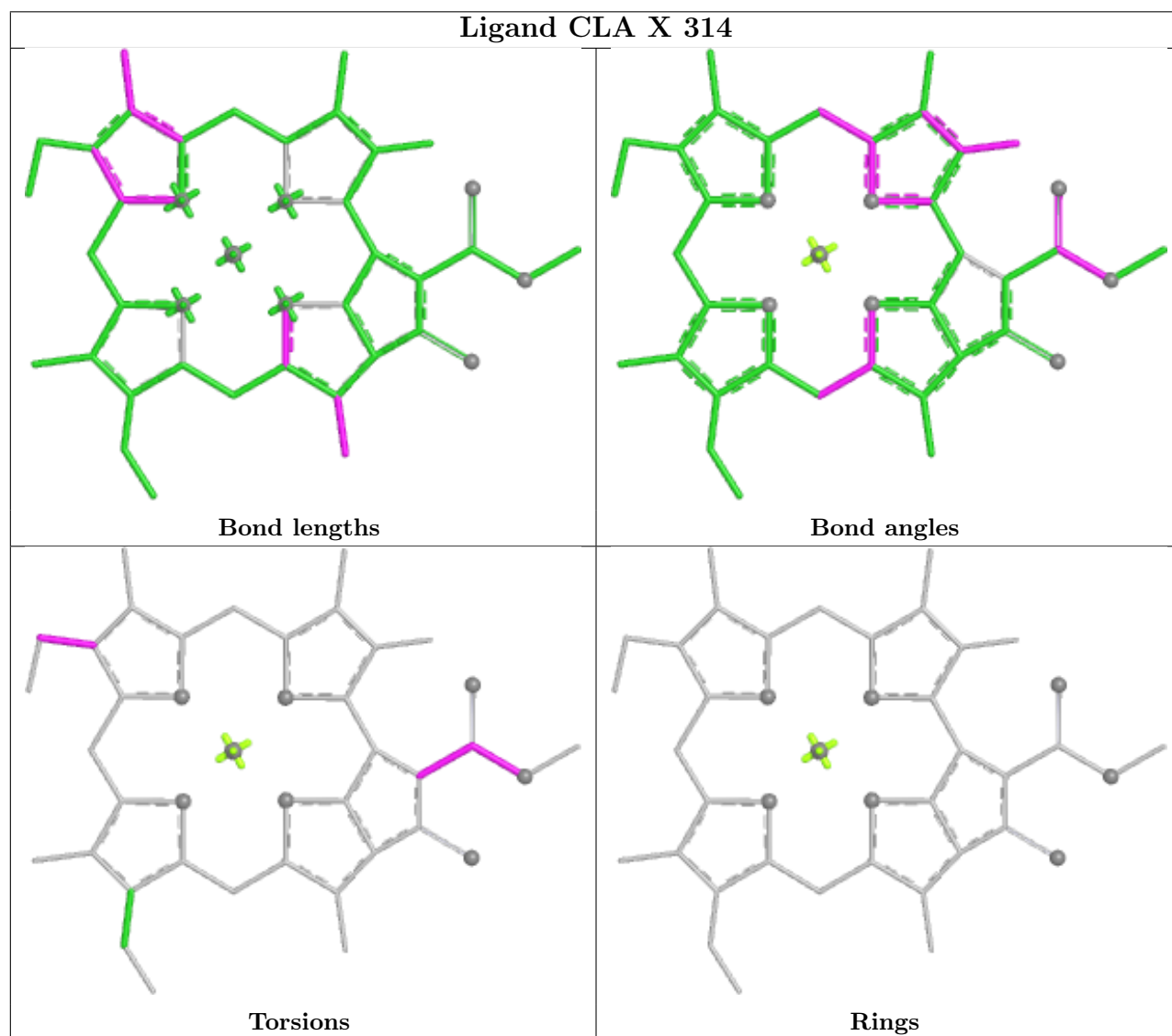
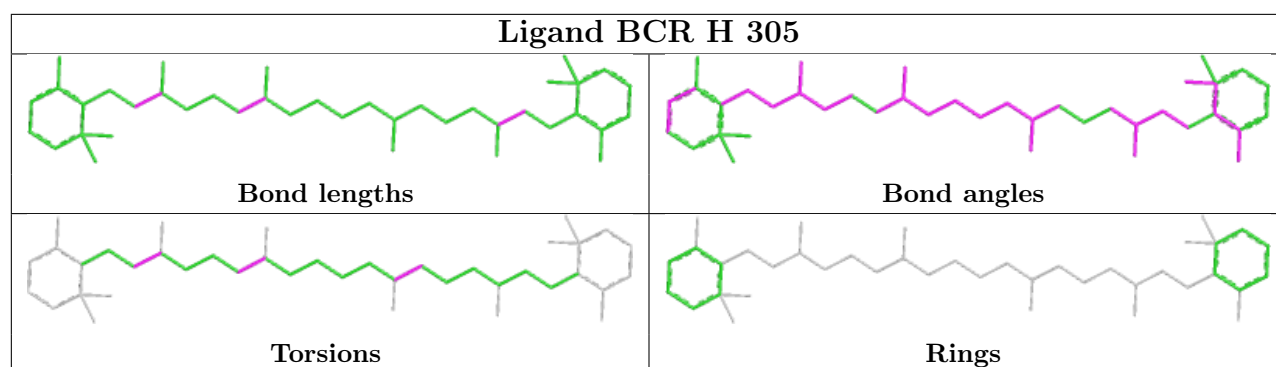
Ligand CLA U 310



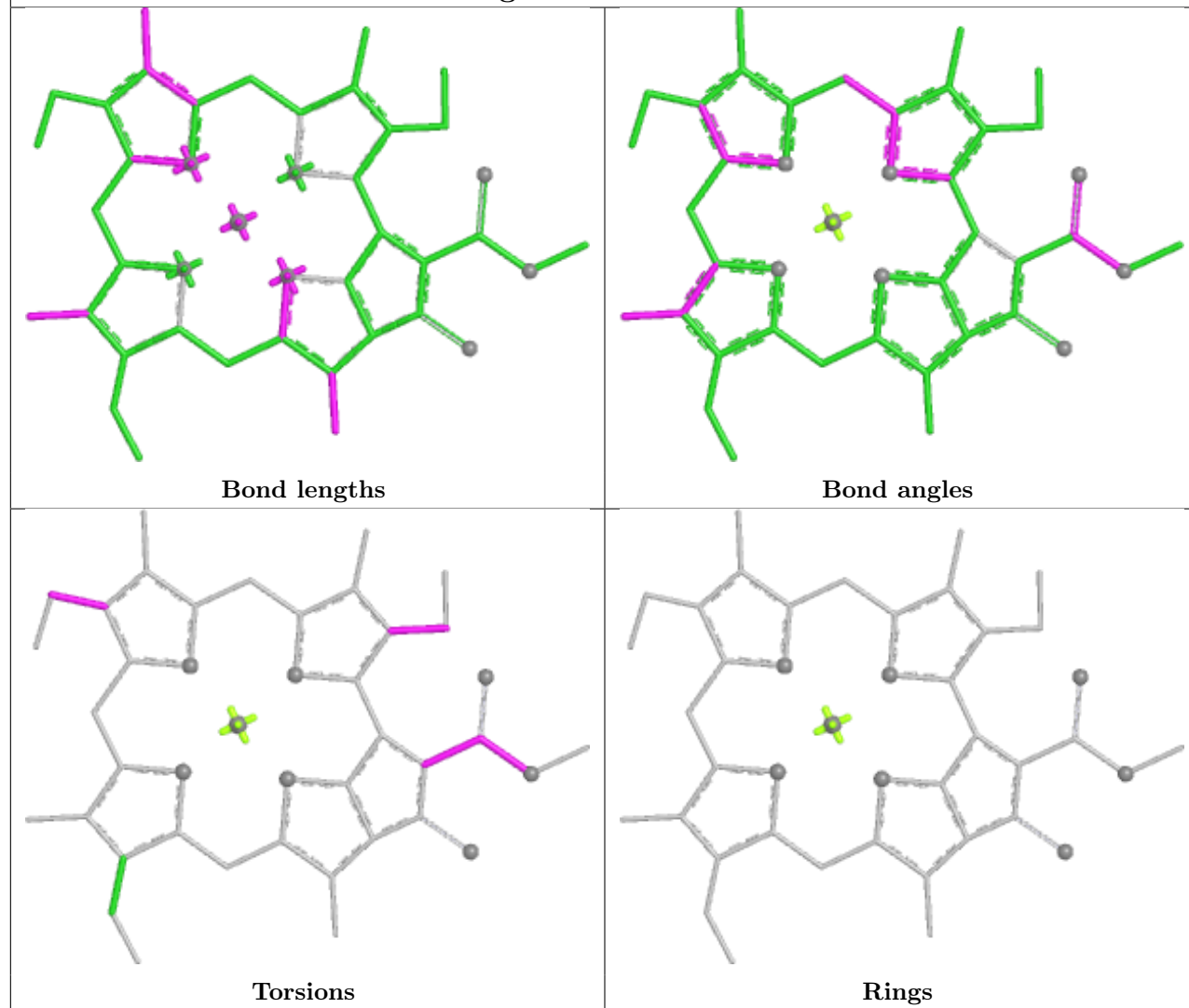
Ligand IWJ 5 611



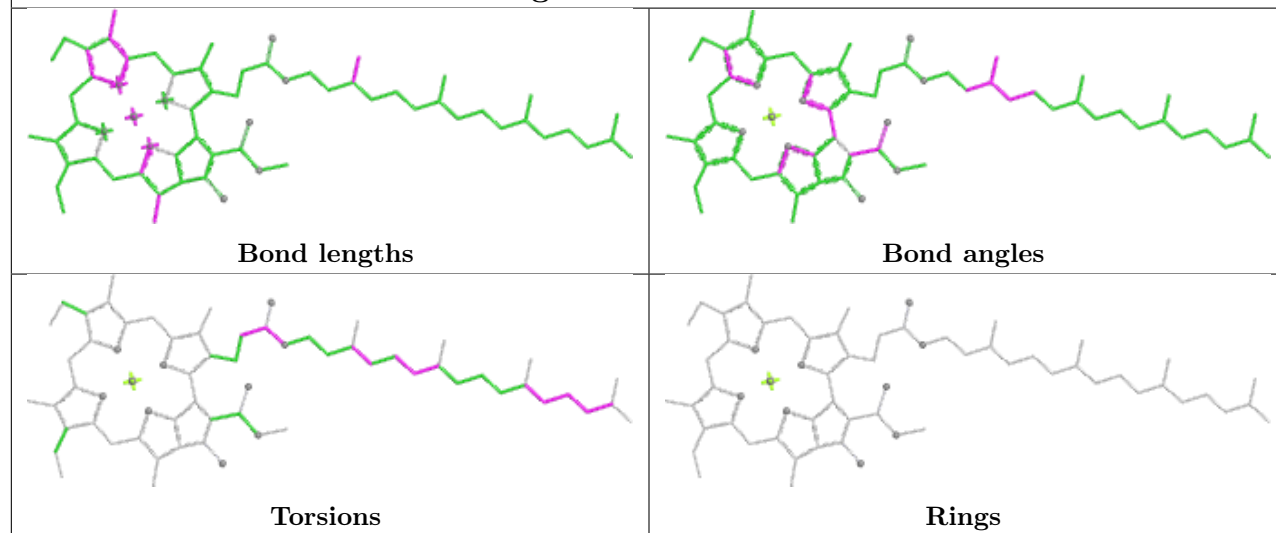




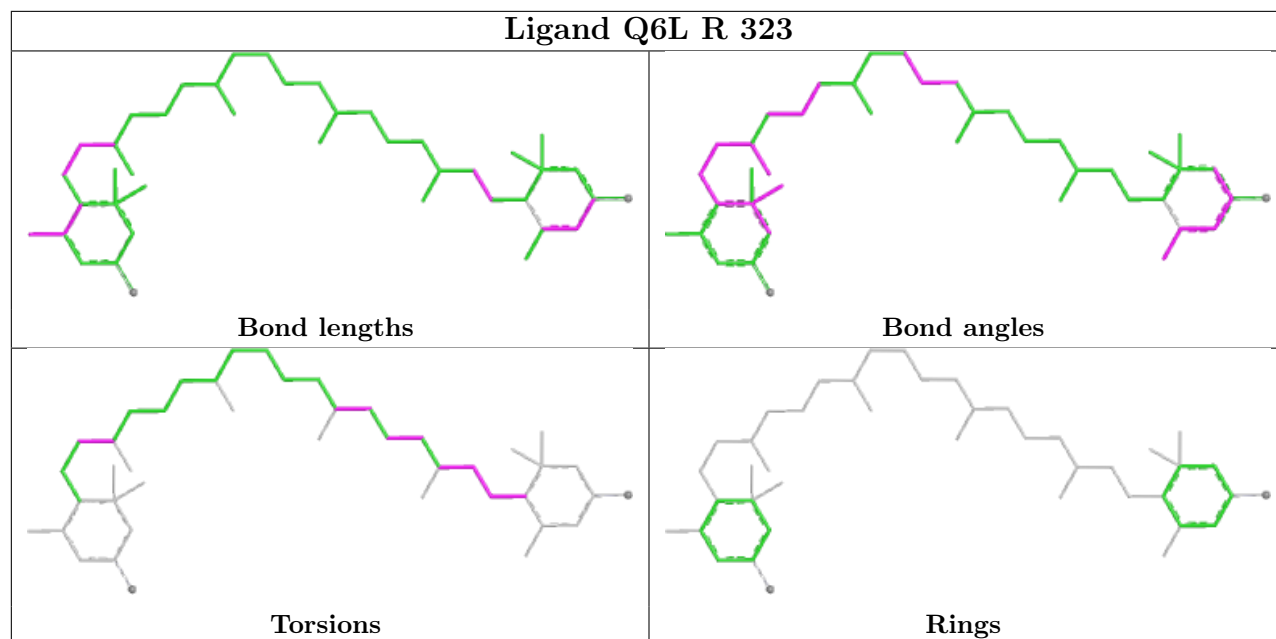
Ligand CLA J 102



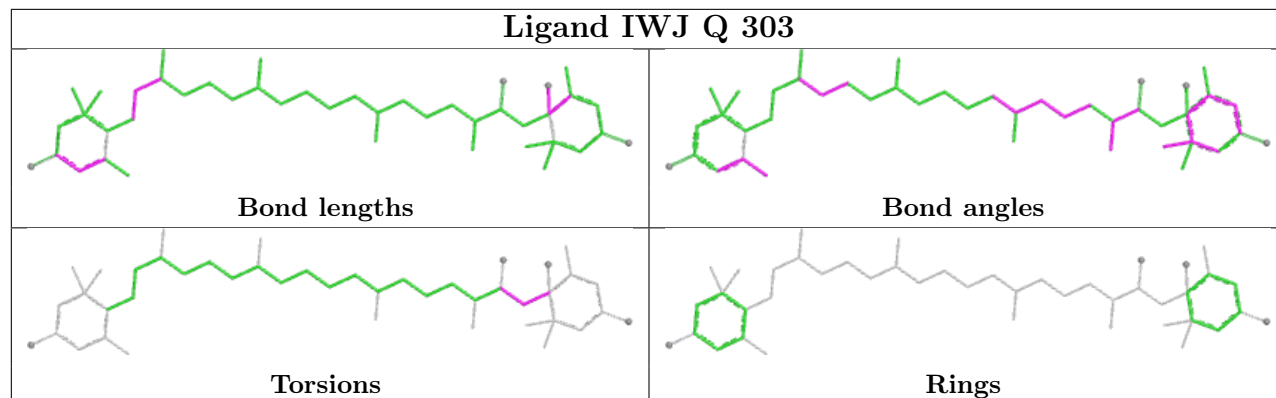
Ligand CLA A 831



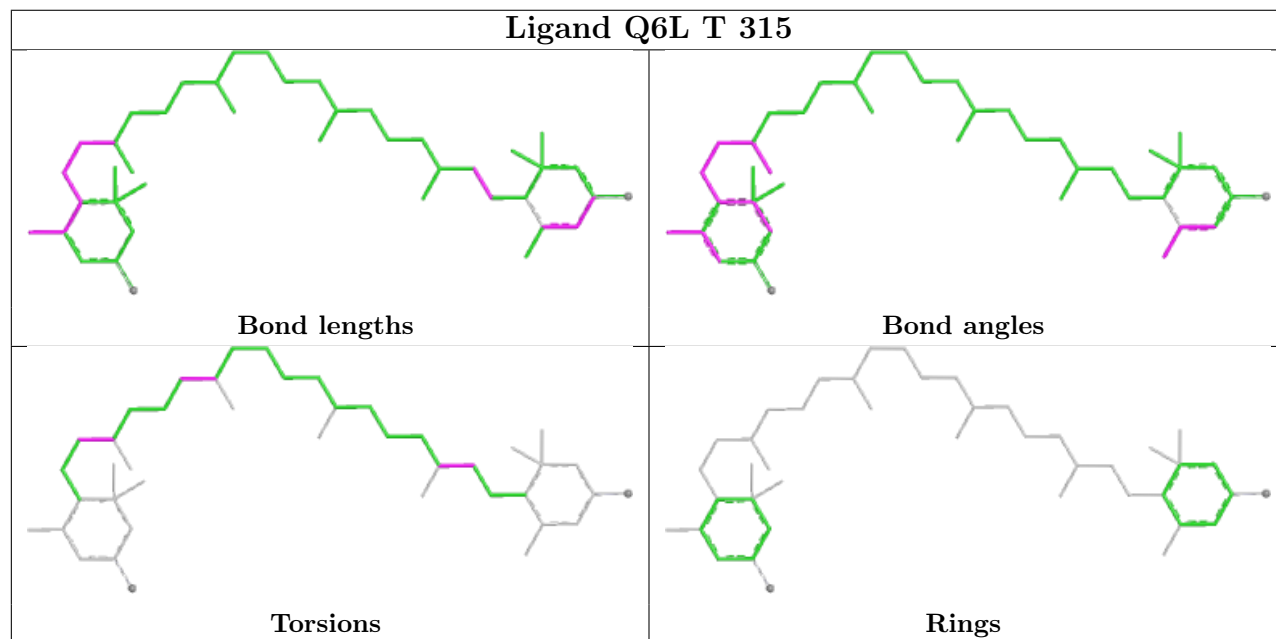
Ligand Q6L R 323



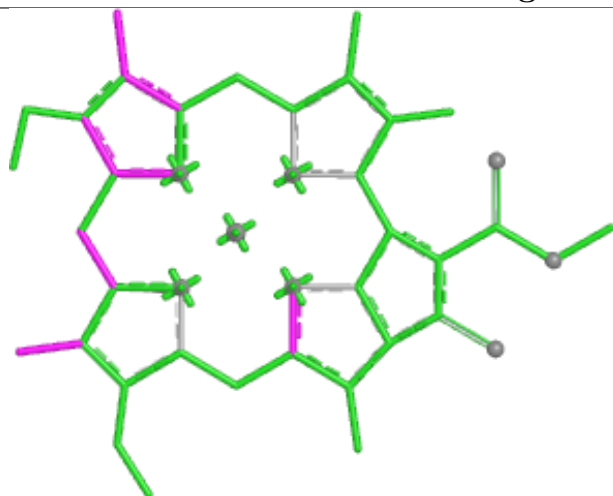
Ligand IWJ Q 303



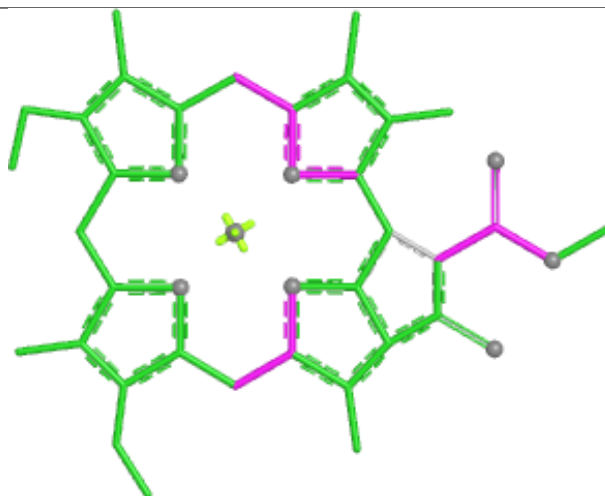
Ligand Q6L T 315



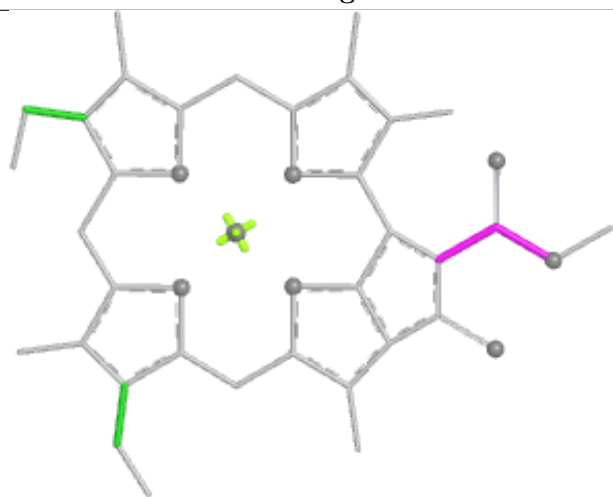
Ligand CLA 5 608



Bond lengths



Bond angles

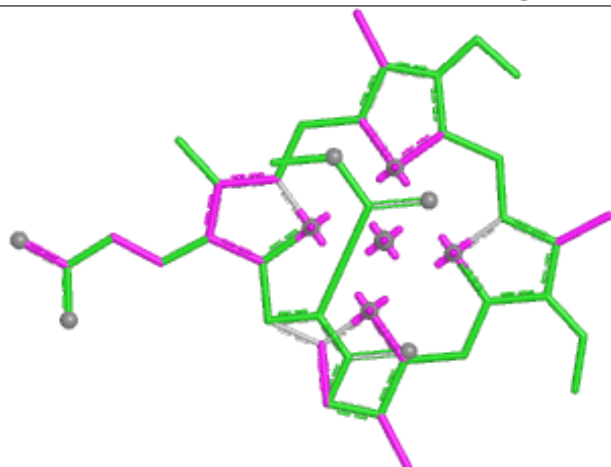


Torsions

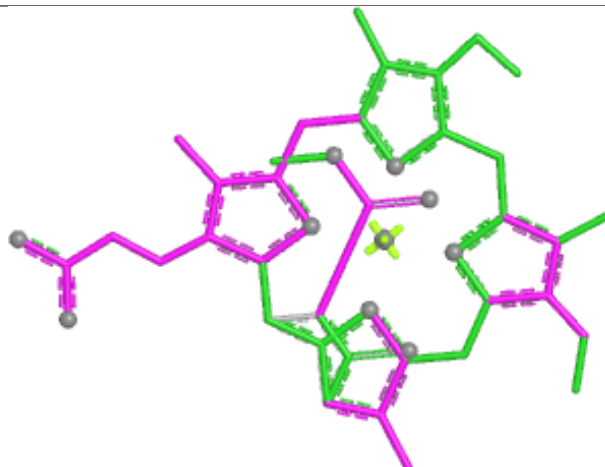


Rings

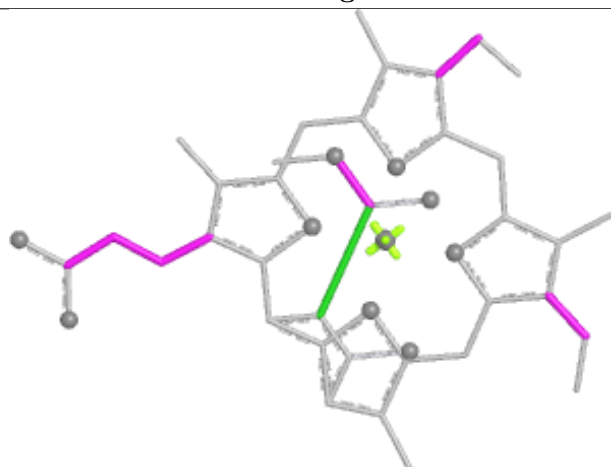
Ligand KC2 X 309



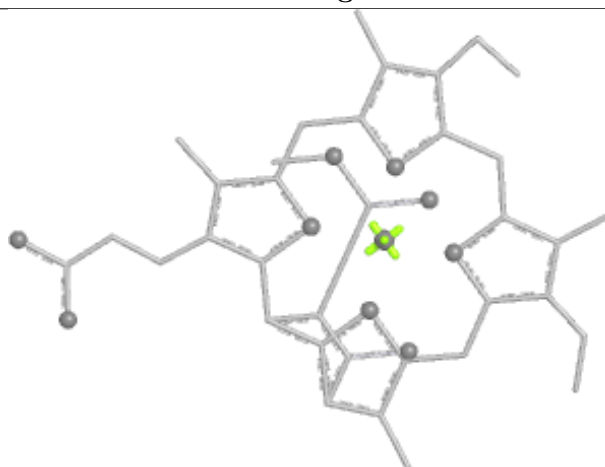
Bond lengths



Bond angles

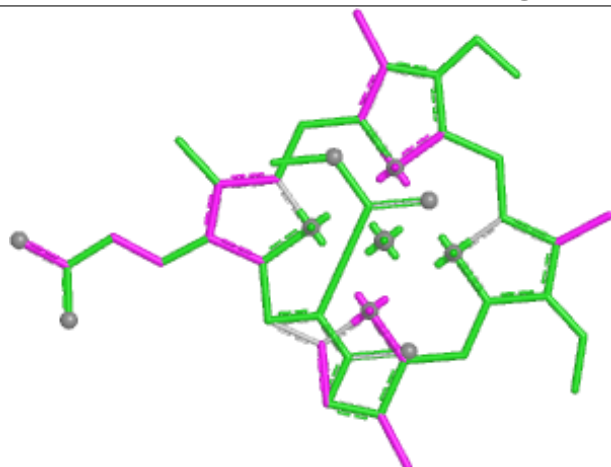


Torsions

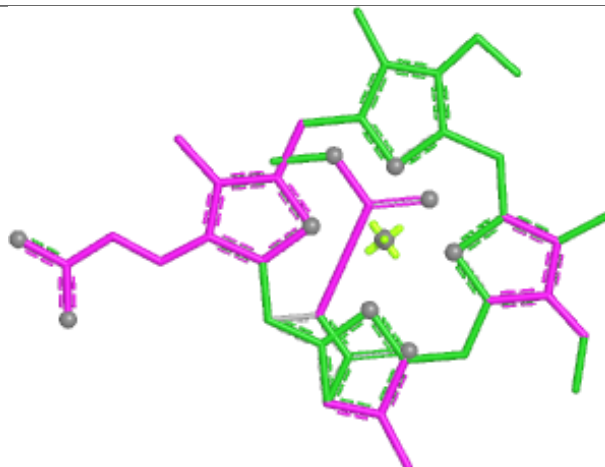


Rings

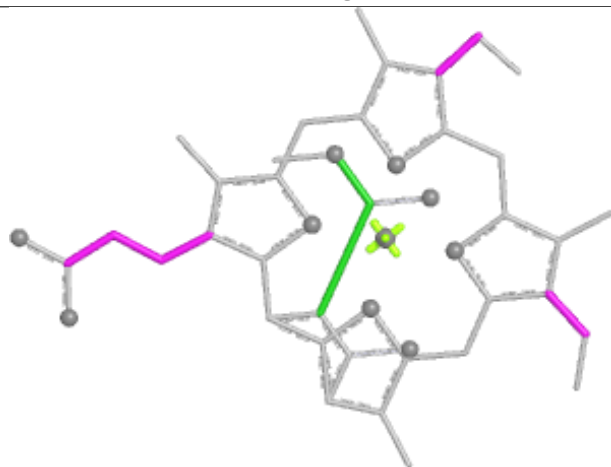
Ligand KC2 R 312



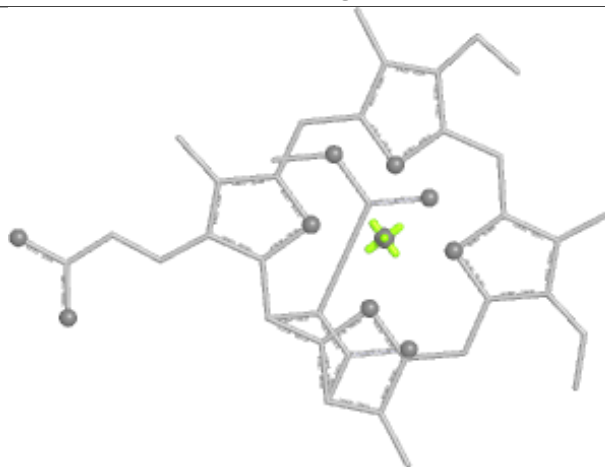
Bond lengths



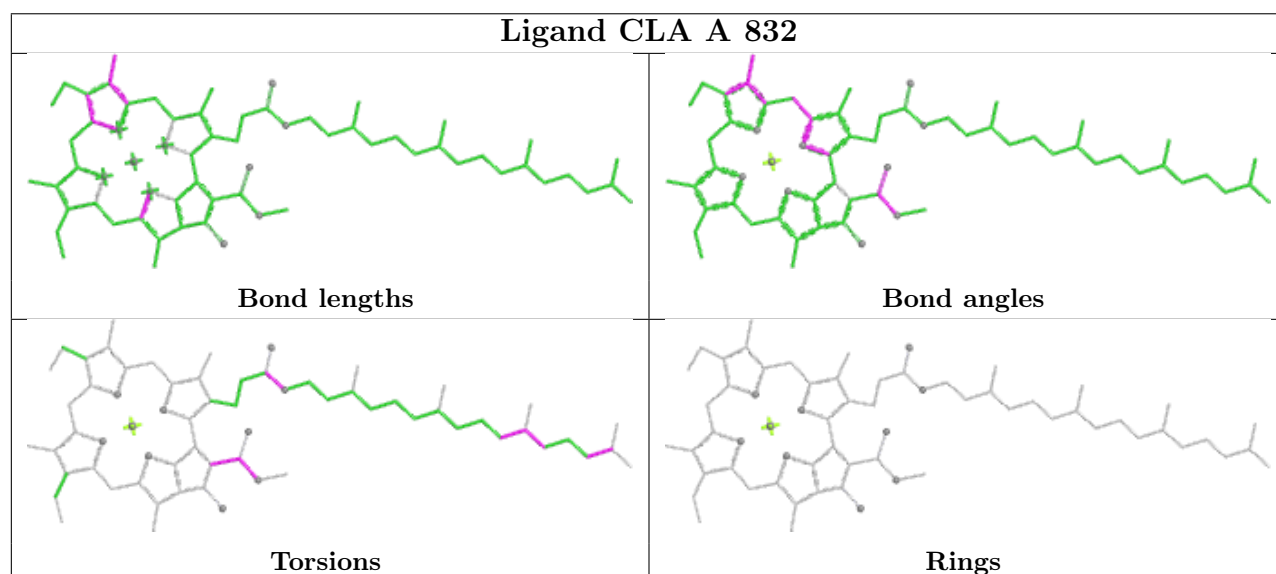
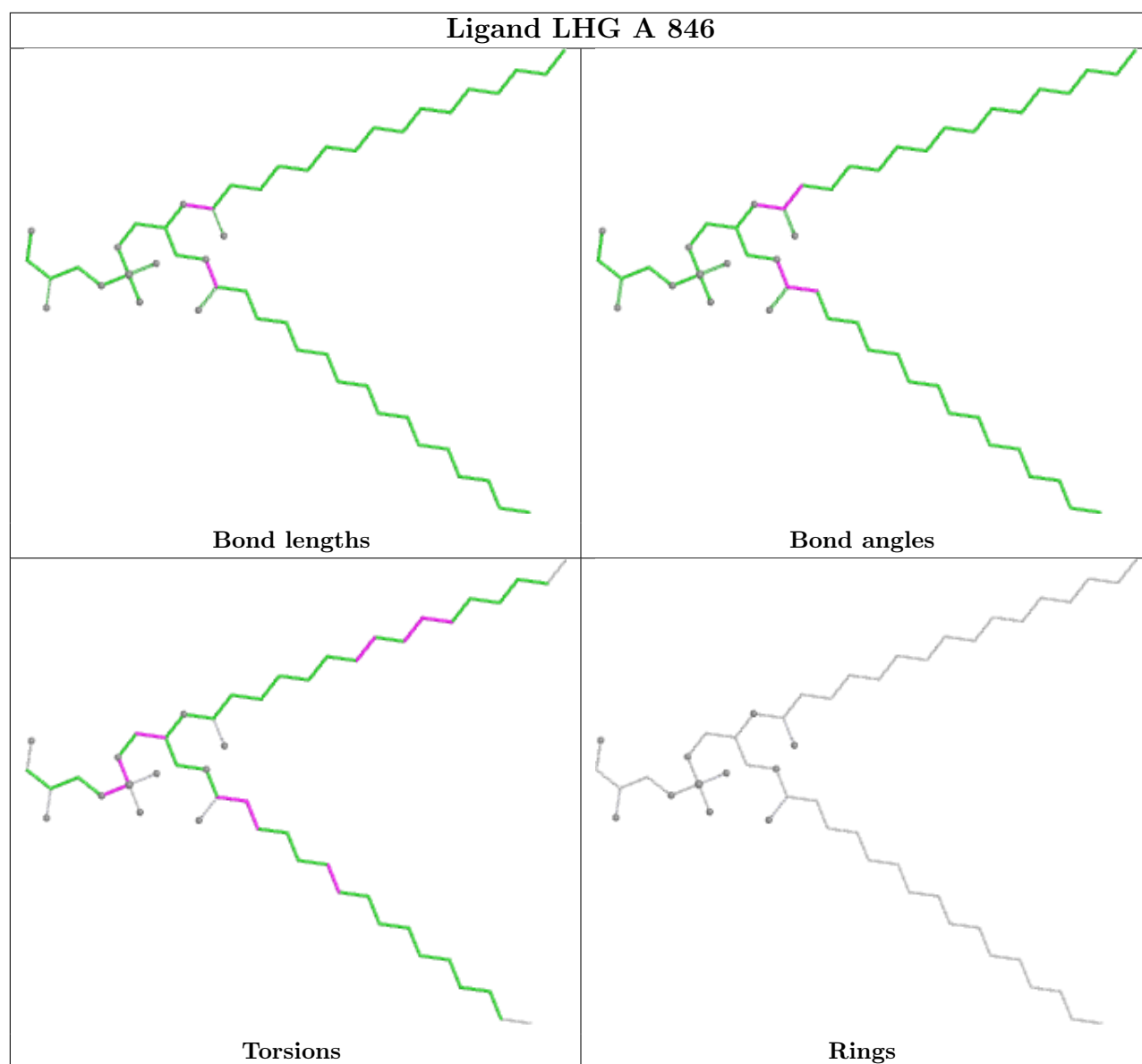
Bond angles

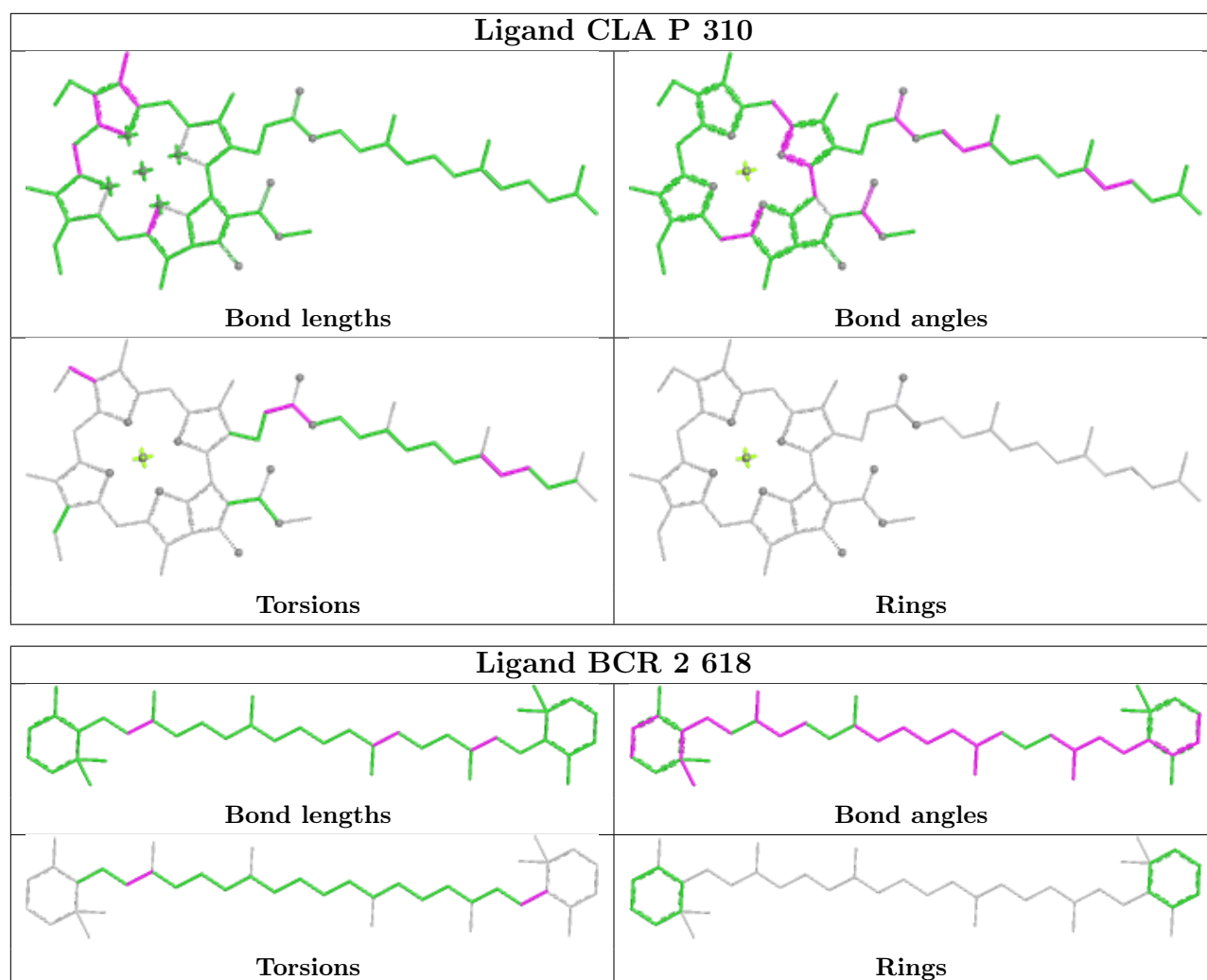


Torsions

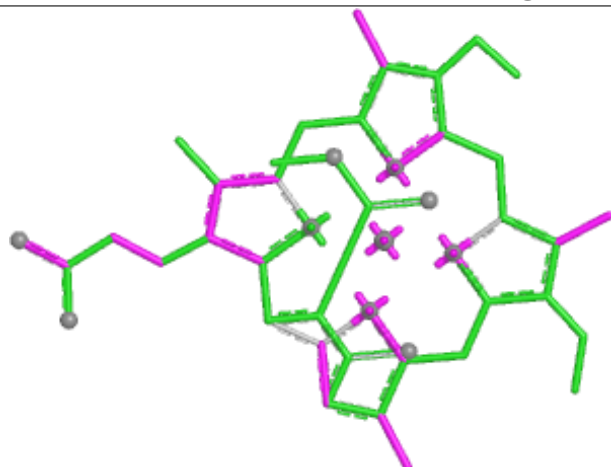


Rings

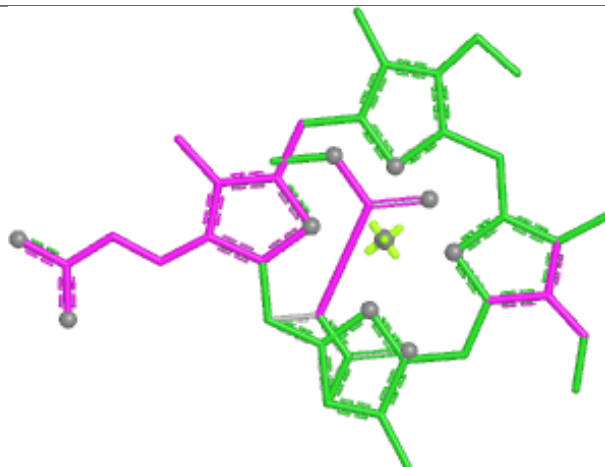




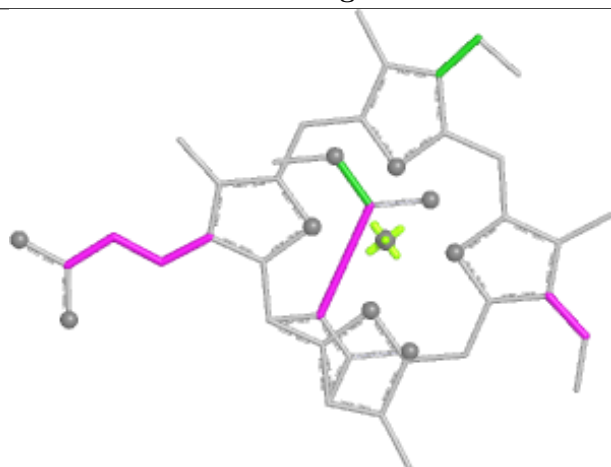
Ligand KC2 S 308



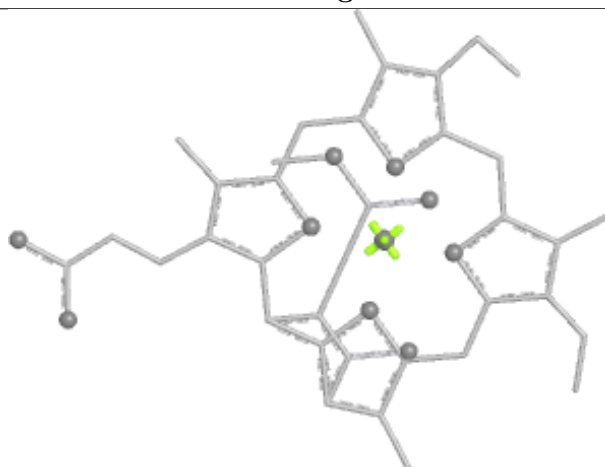
Bond lengths



Bond angles

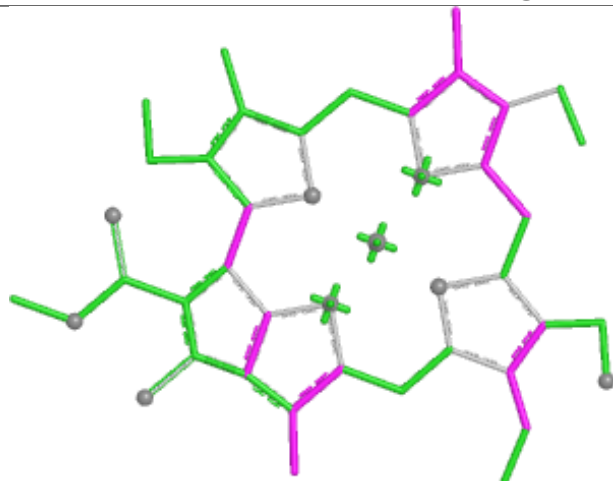


Torsions

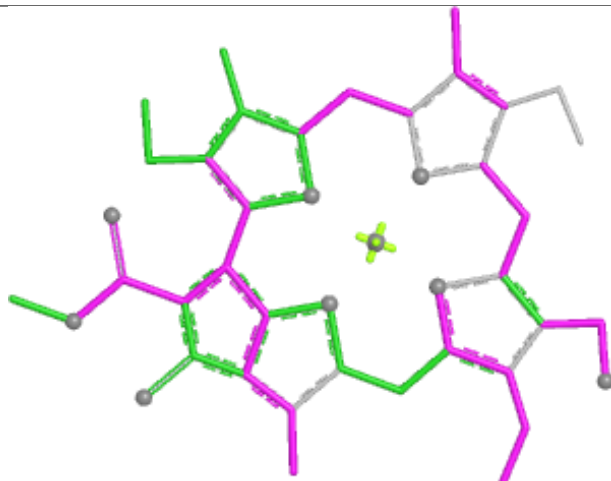


Rings

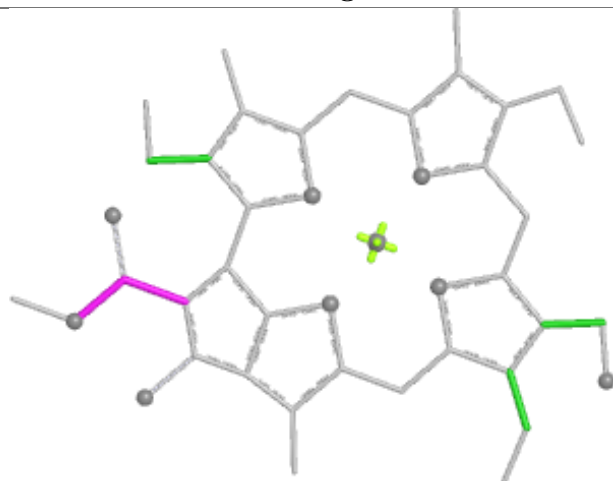
Ligand CHL 2 615



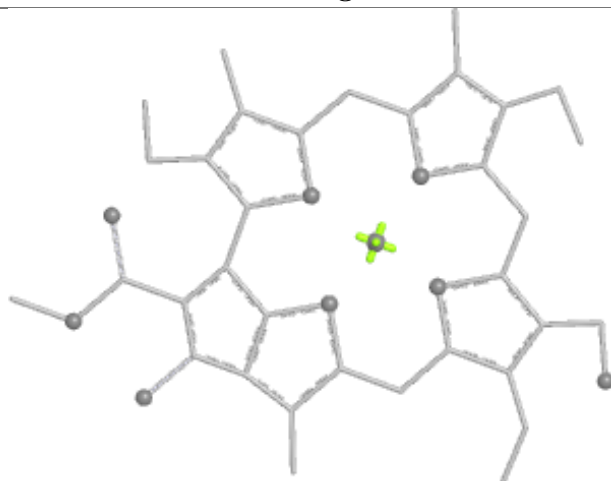
Bond lengths



Bond angles

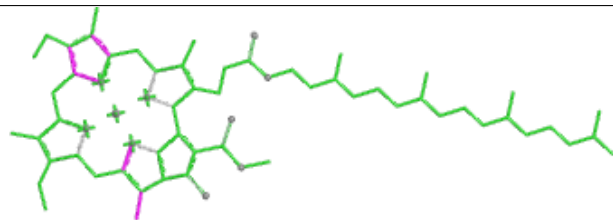


Torsions

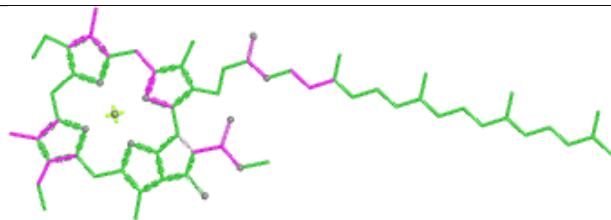


Rings

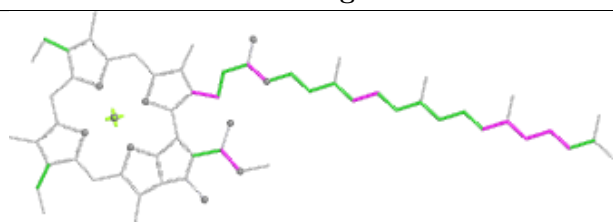
Ligand CLA A 805



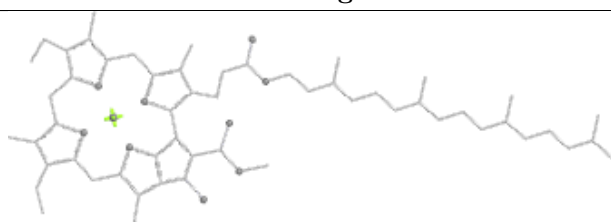
Bond lengths



Bond angles

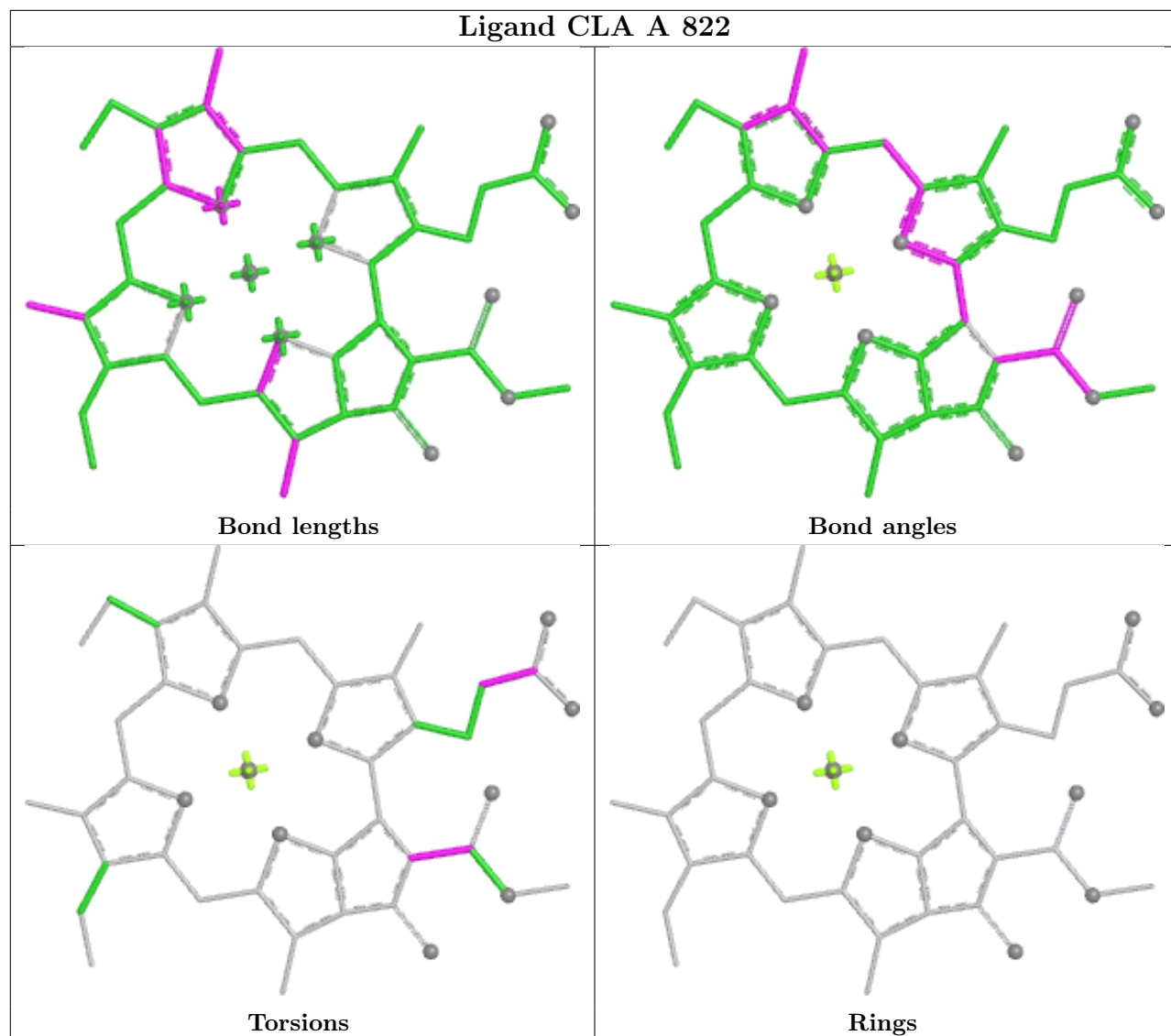


Torsions

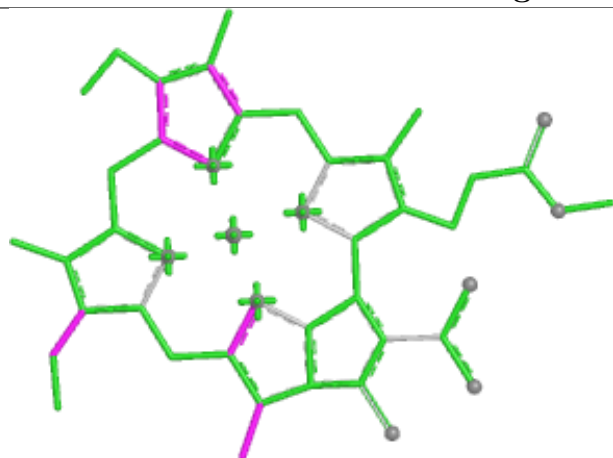


Rings

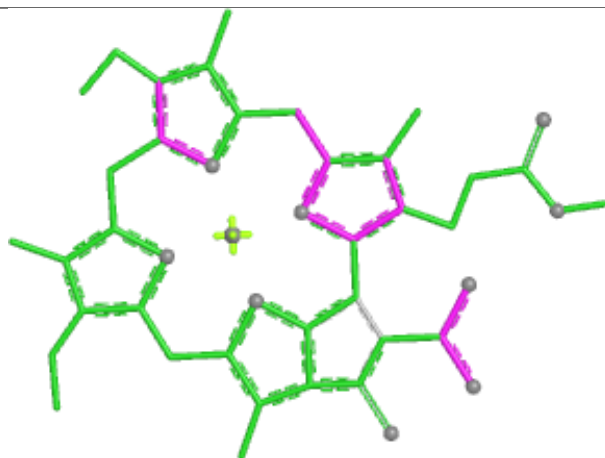
Ligand CLA A 822



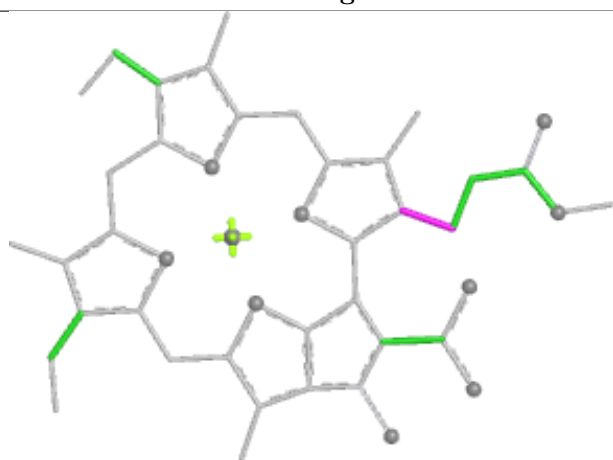
Ligand CLA N 202



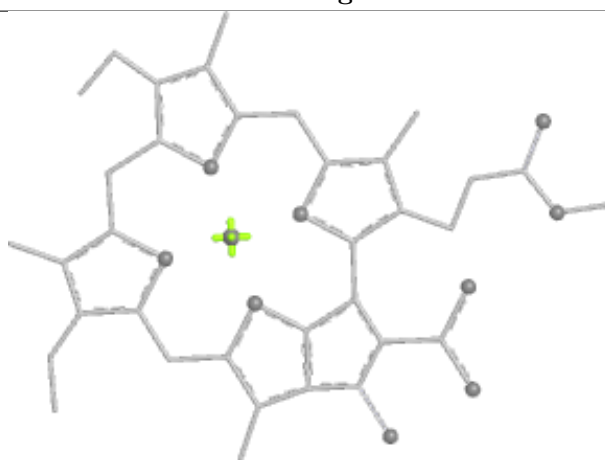
Bond lengths



Bond angles

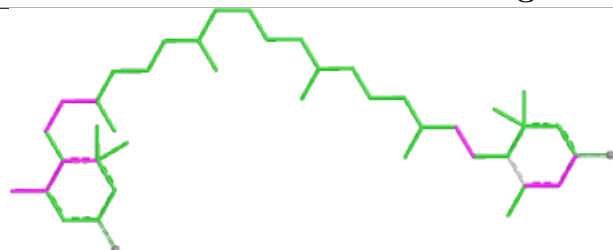


Torsions

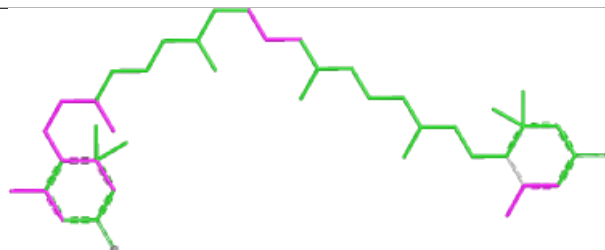


Rings

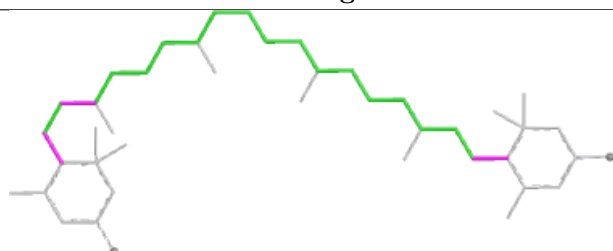
Ligand Q6L U 317



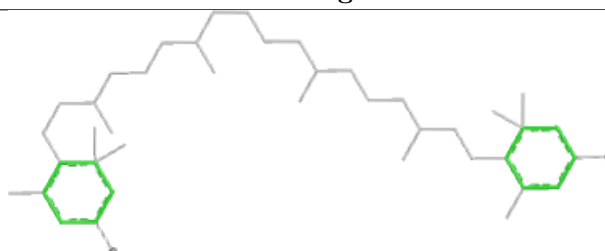
Bond lengths



Bond angles

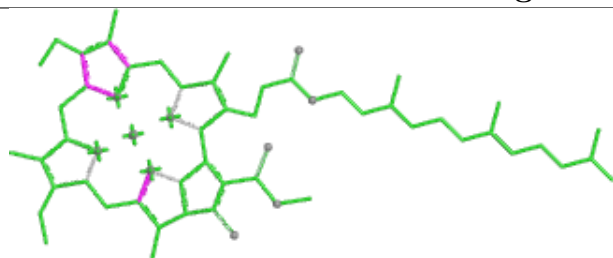


Torsions

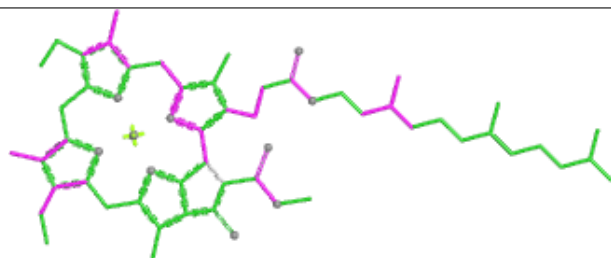


Rings

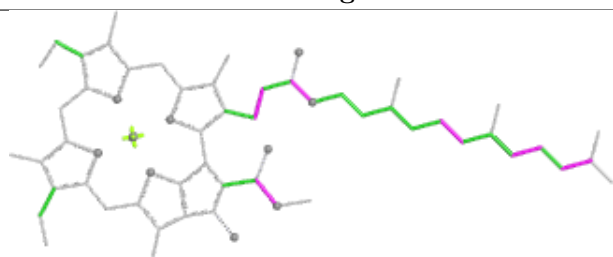
Ligand CLA P 311



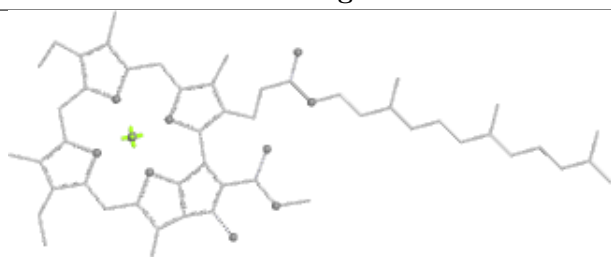
Bond lengths



Bond angles

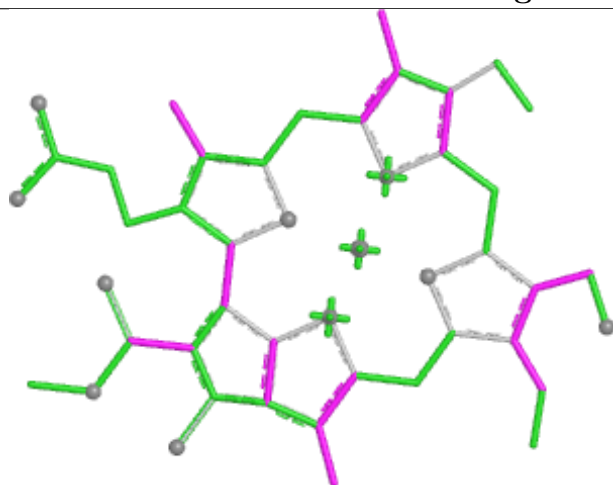


Torsions

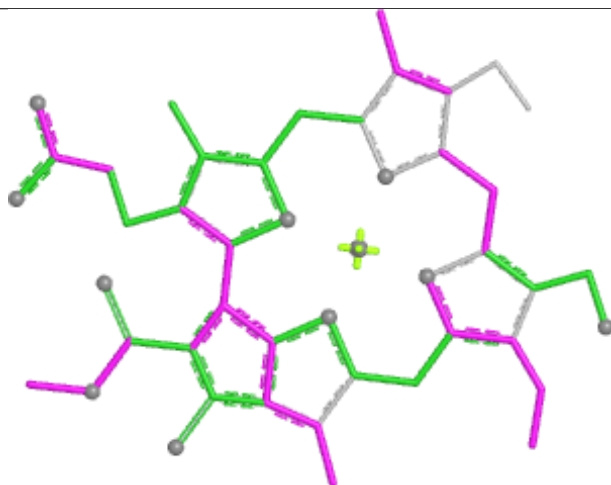


Rings

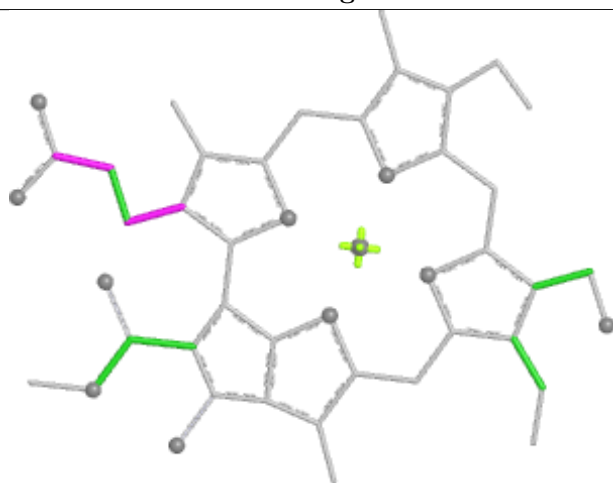
Ligand CHL P 305



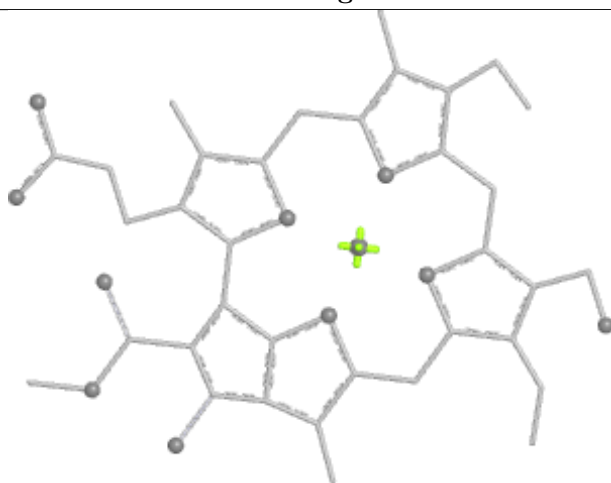
Bond lengths



Bond angles

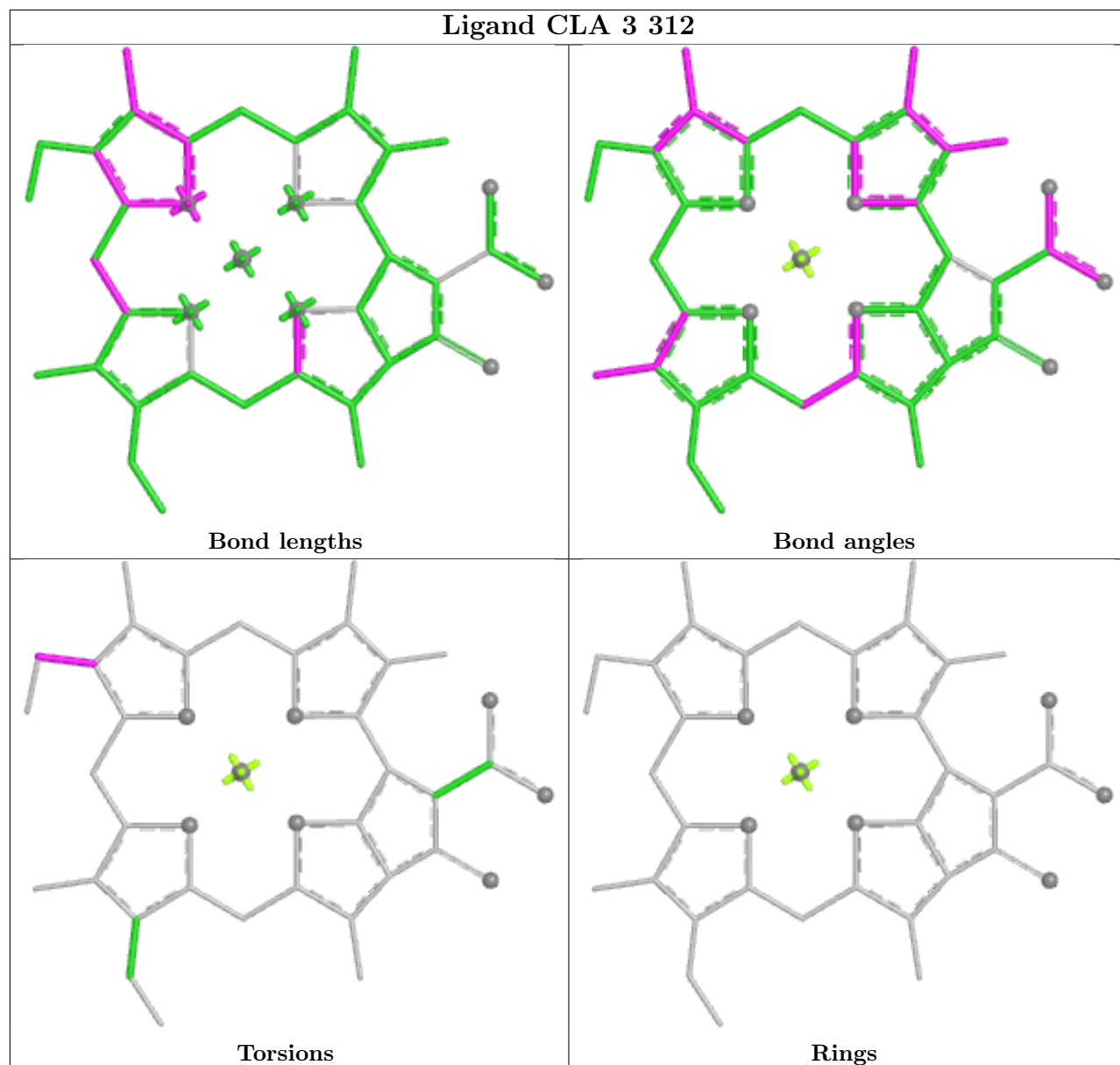


Torsions

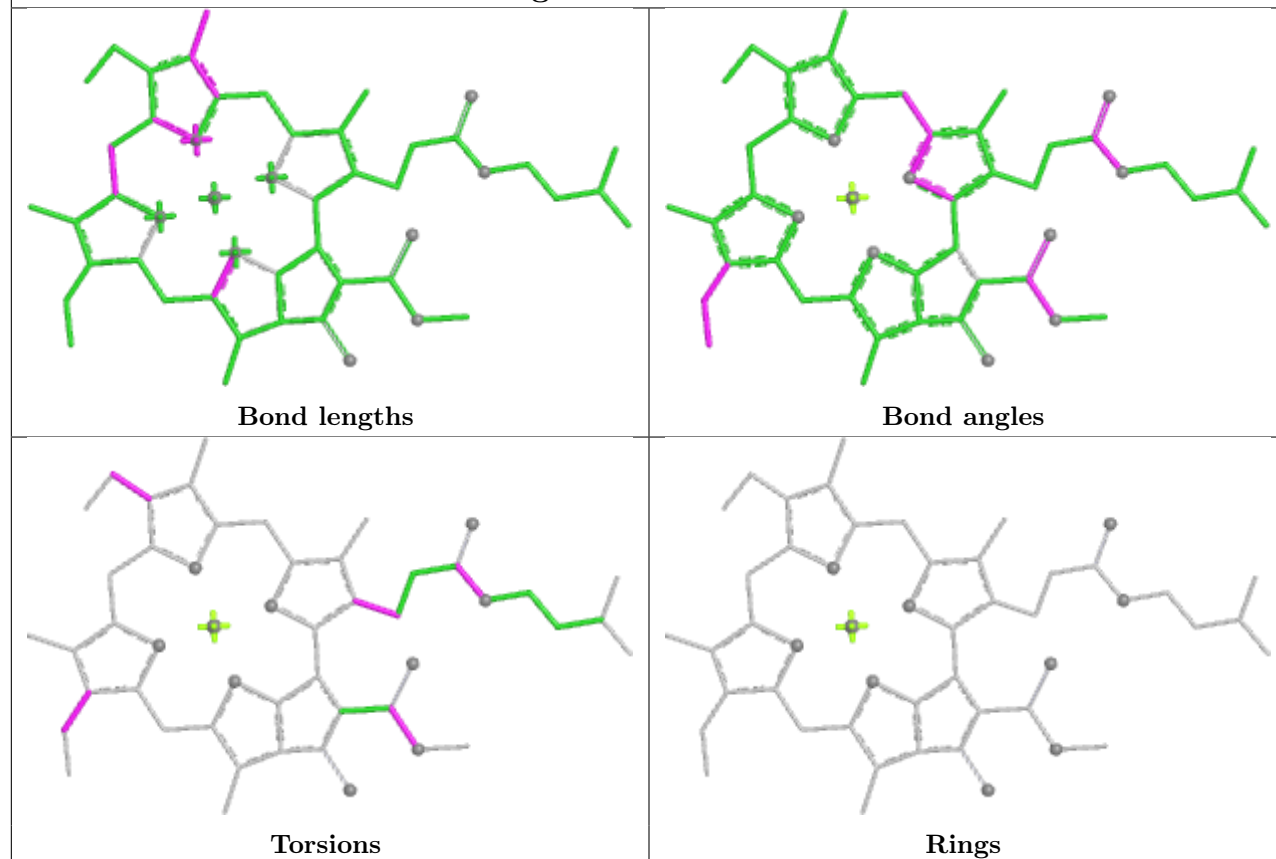


Rings

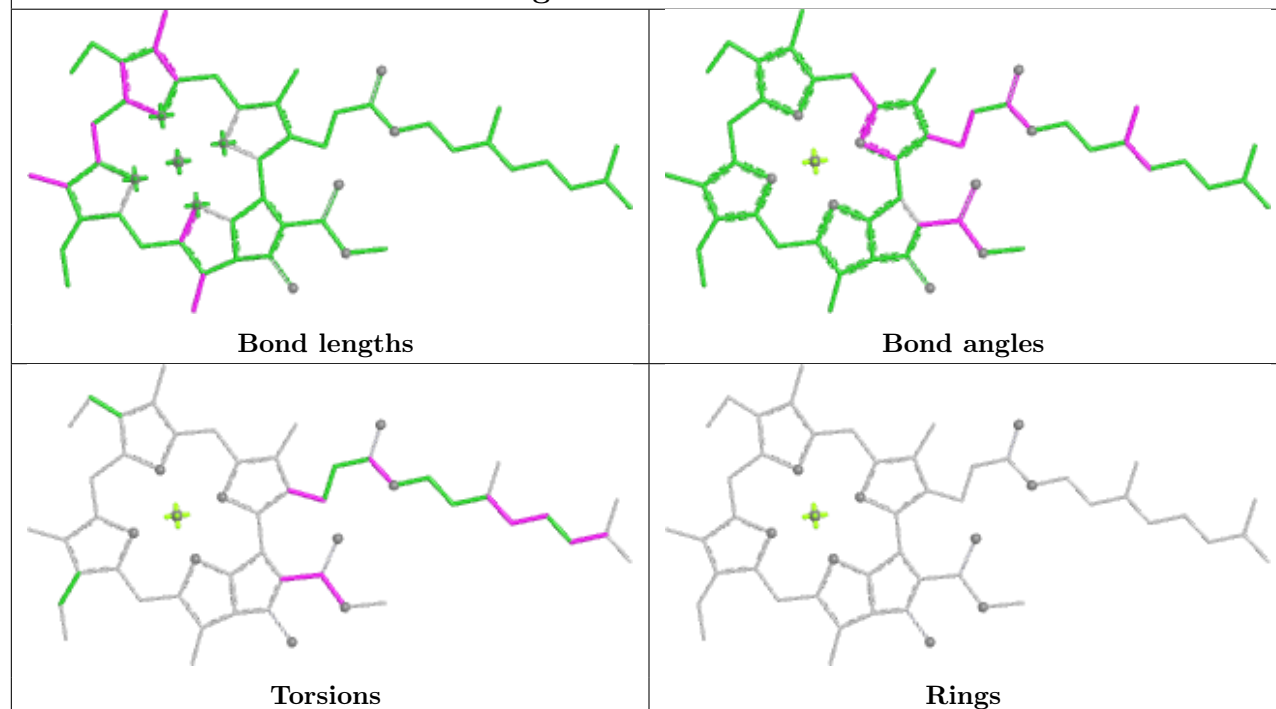
Ligand CLA 3 312

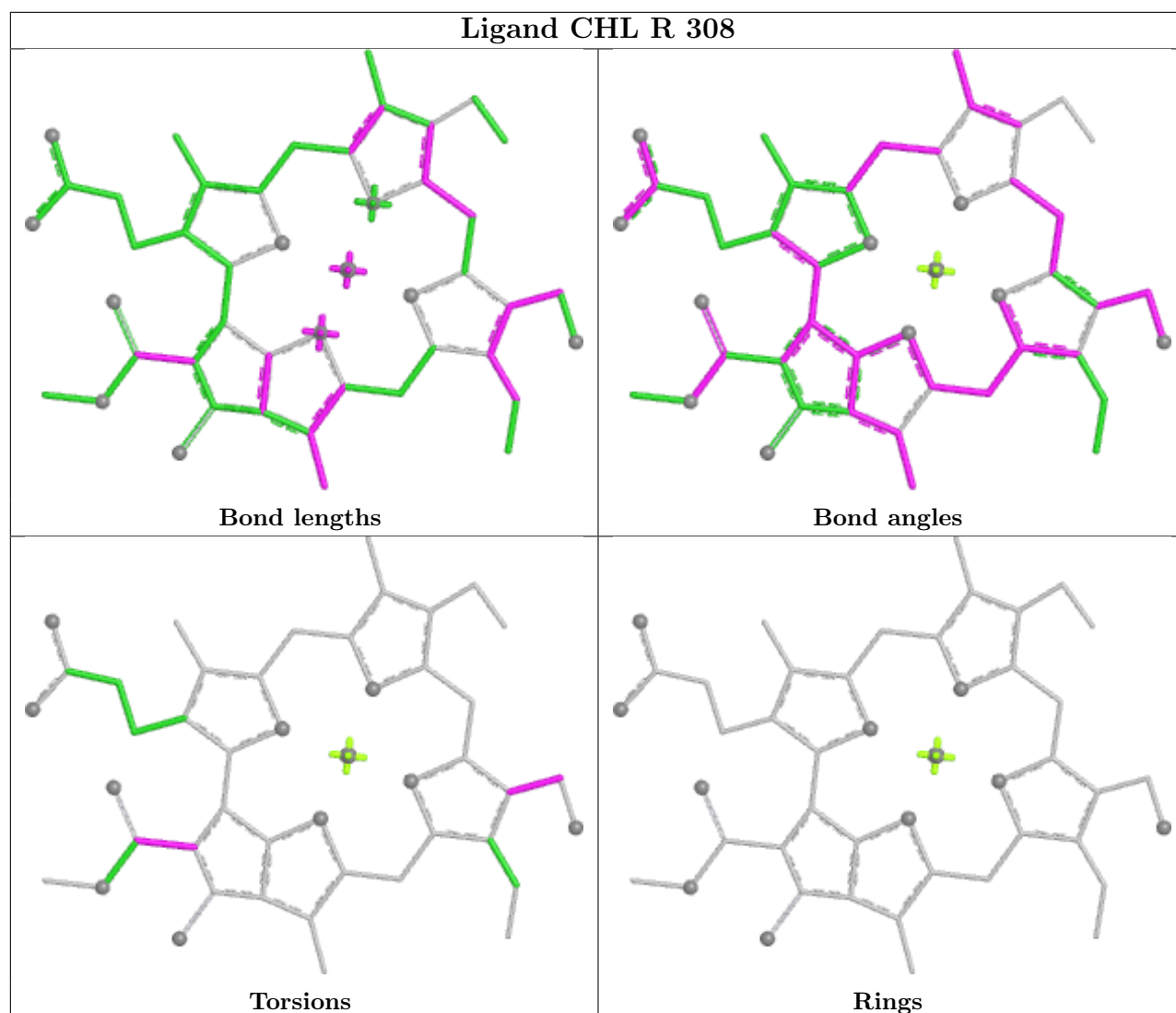
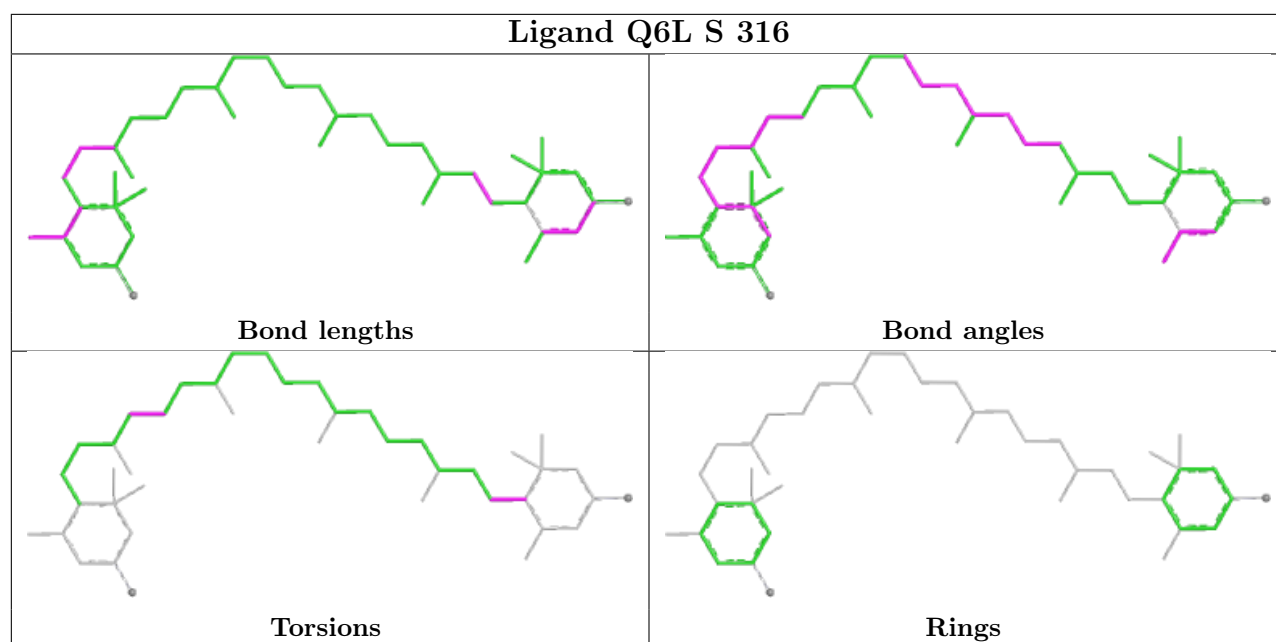


Ligand CLA X 311

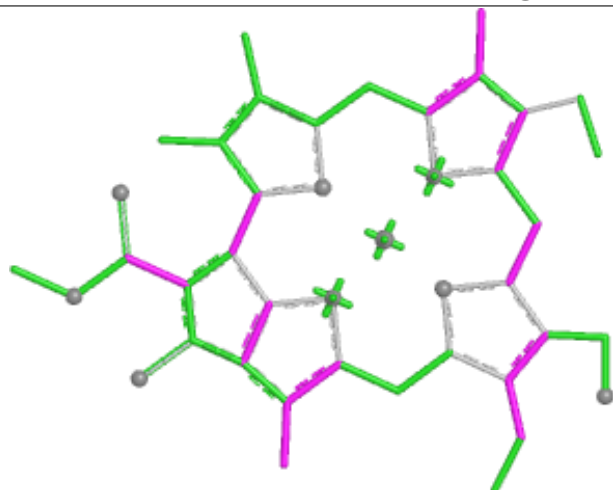


Ligand CLA T 312

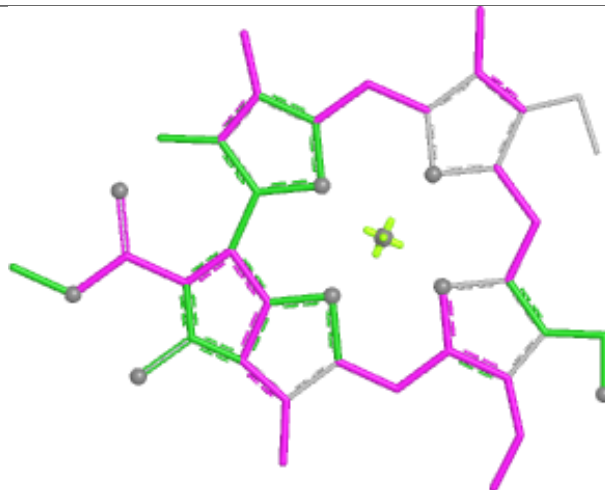




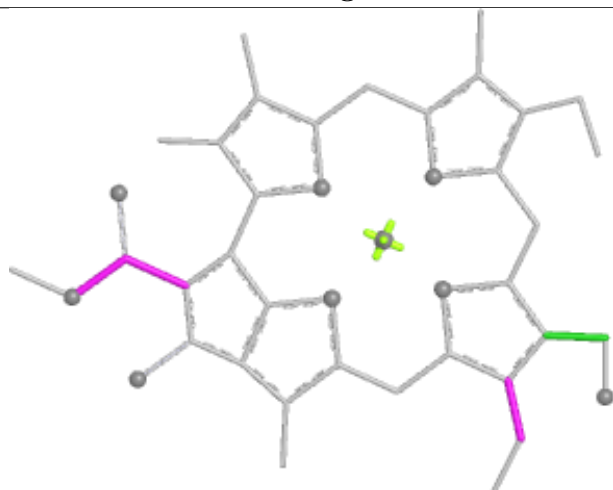
Ligand CHL S 307



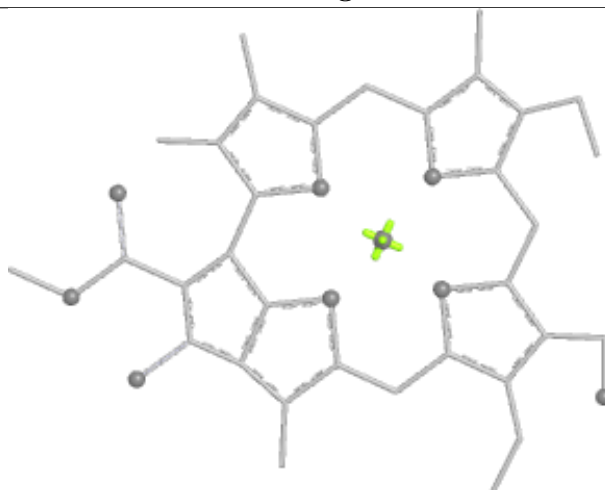
Bond lengths



Bond angles

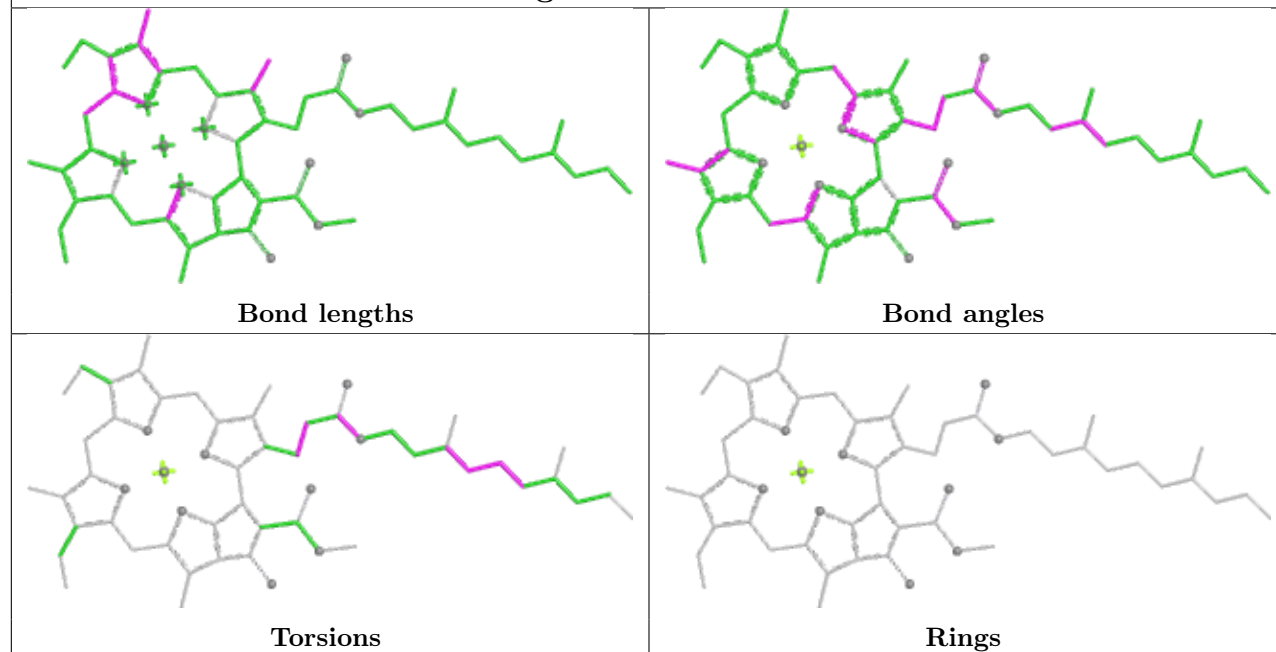


Torsions

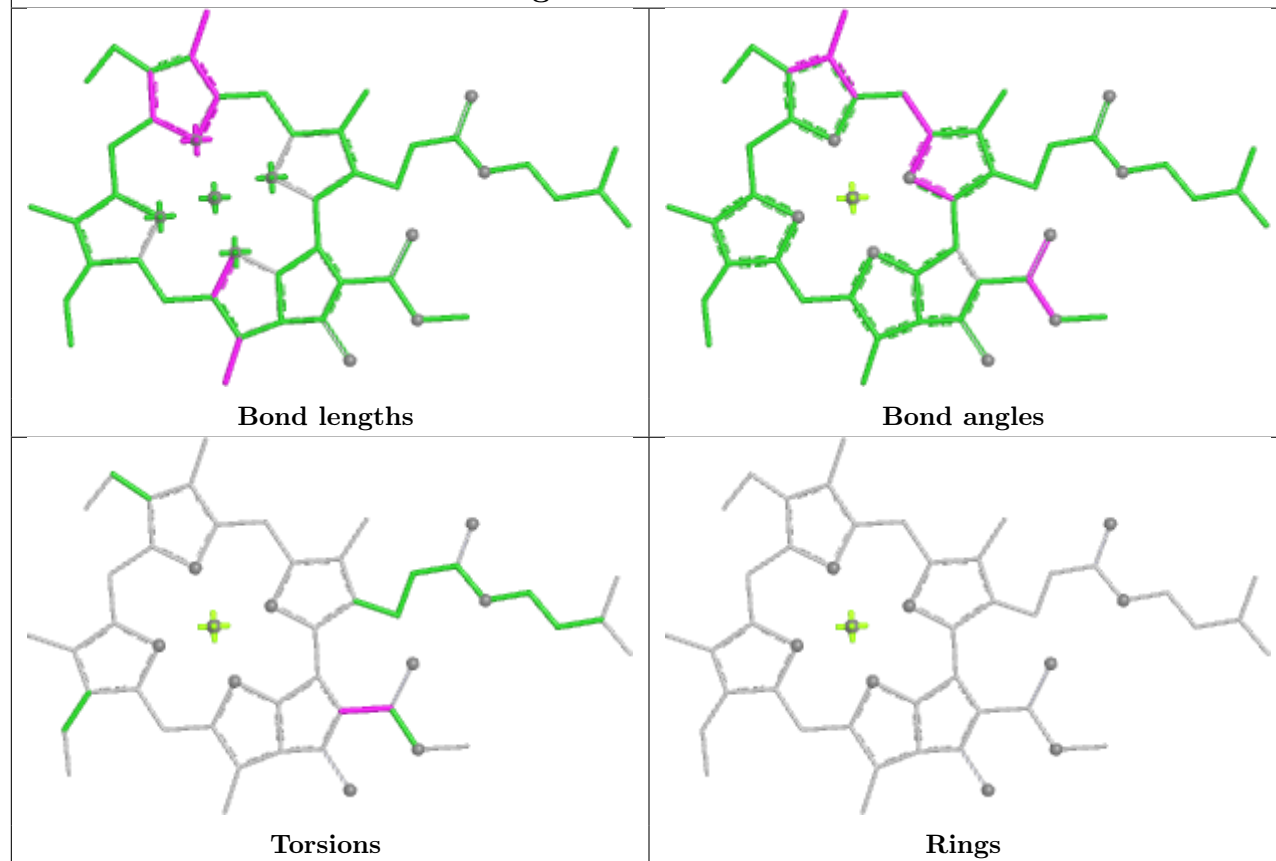


Rings

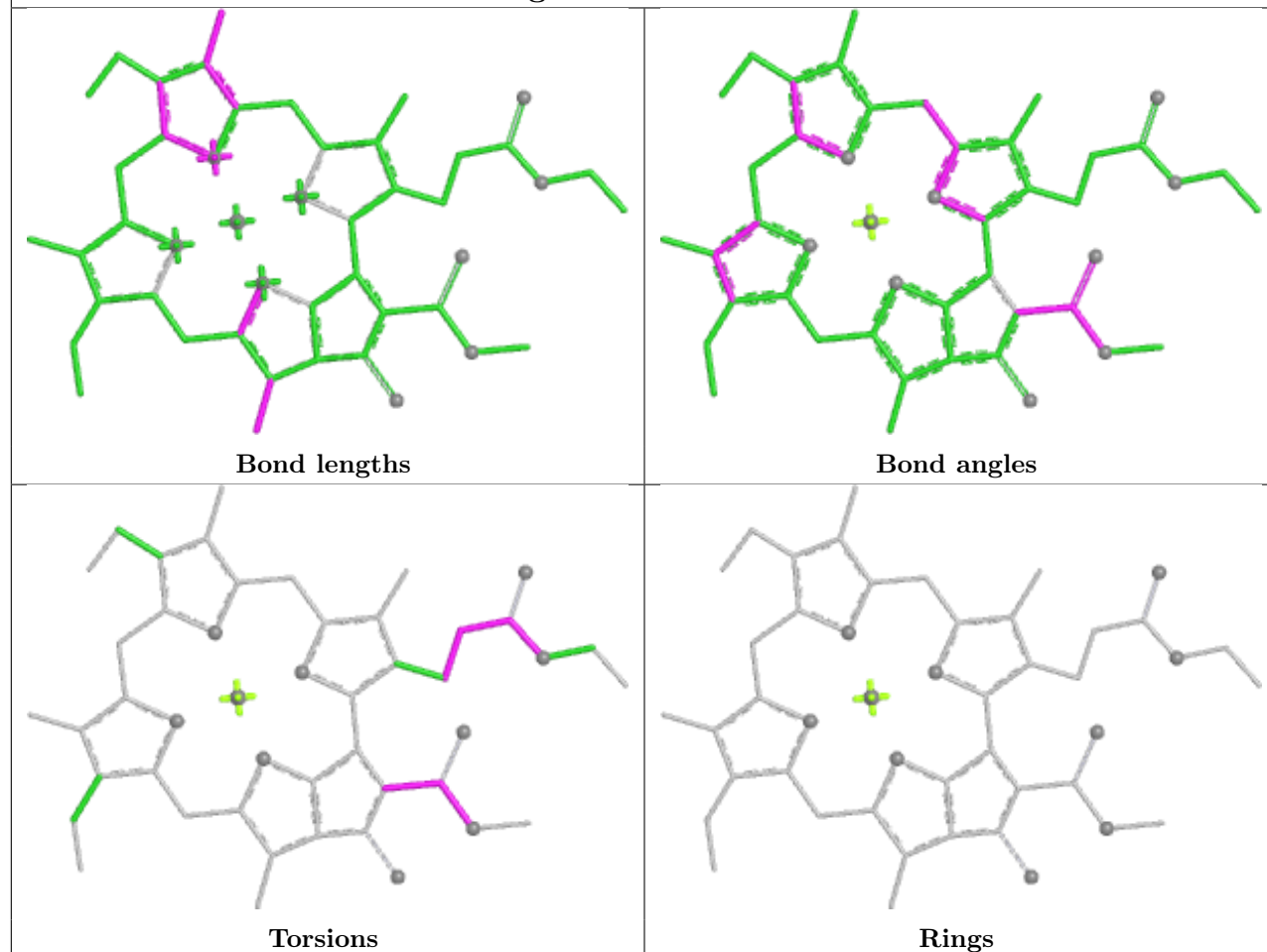
Ligand CLA 4 313



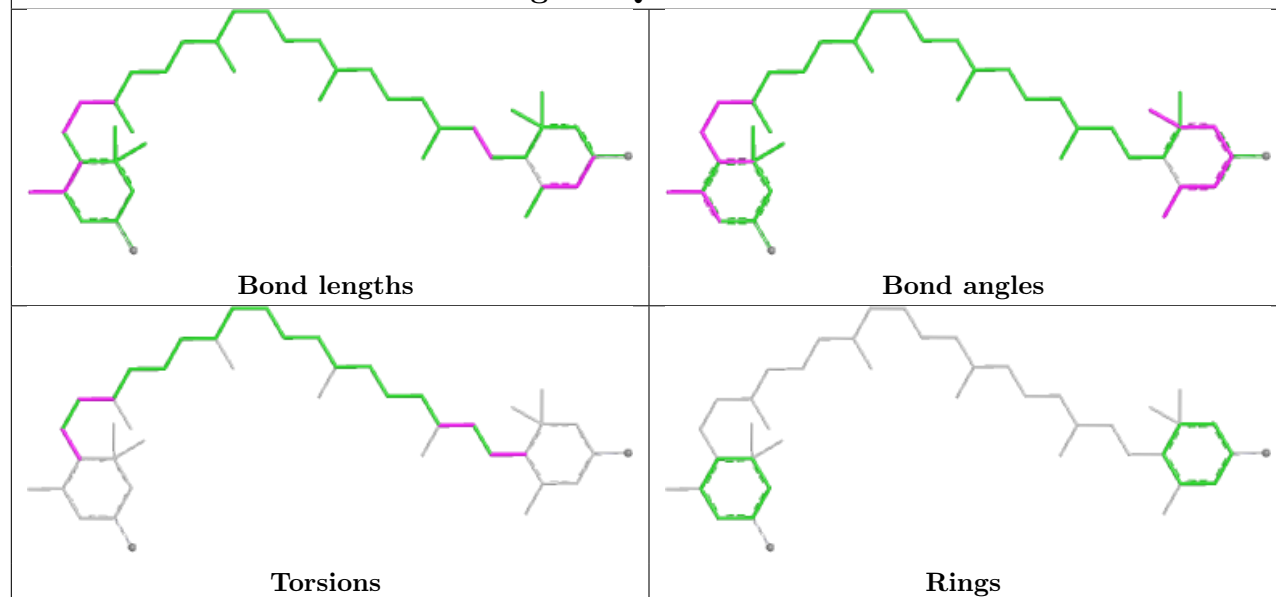
Ligand CLA B 838

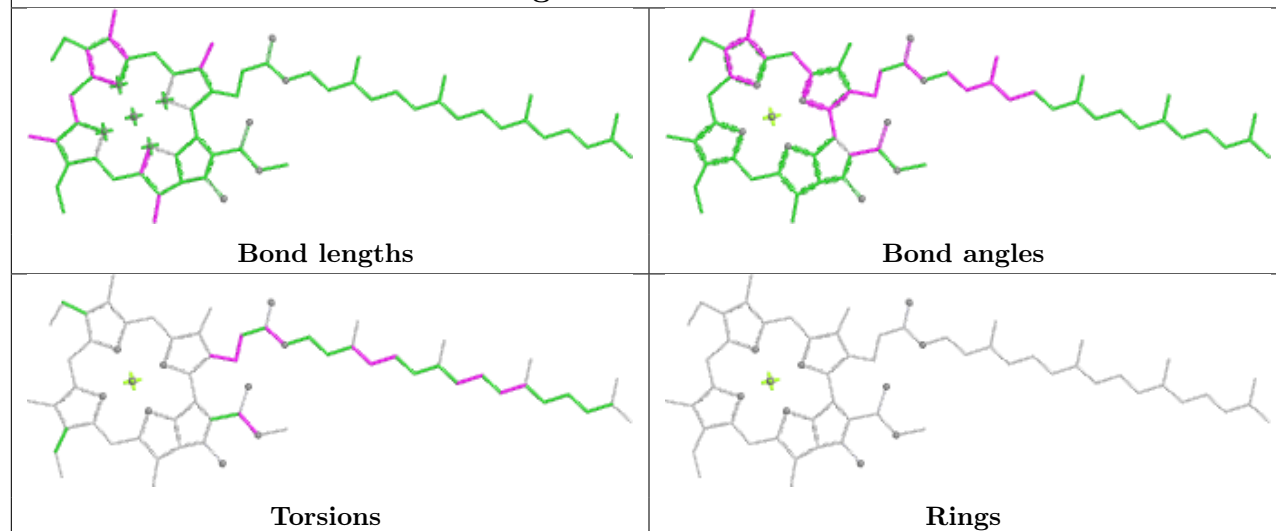
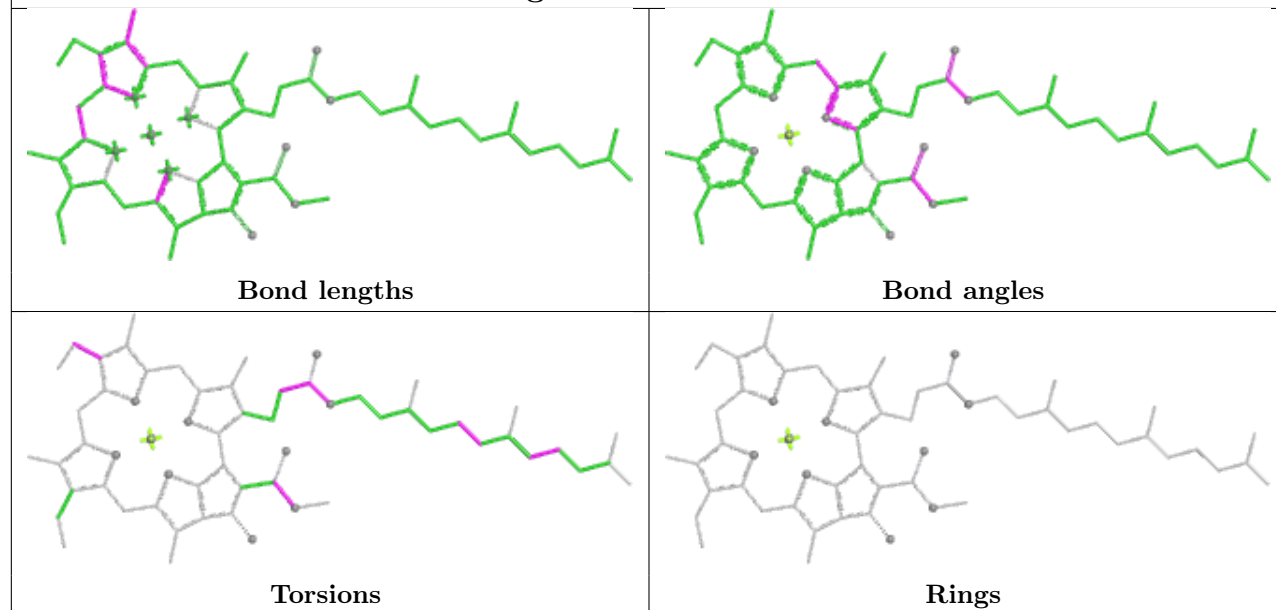


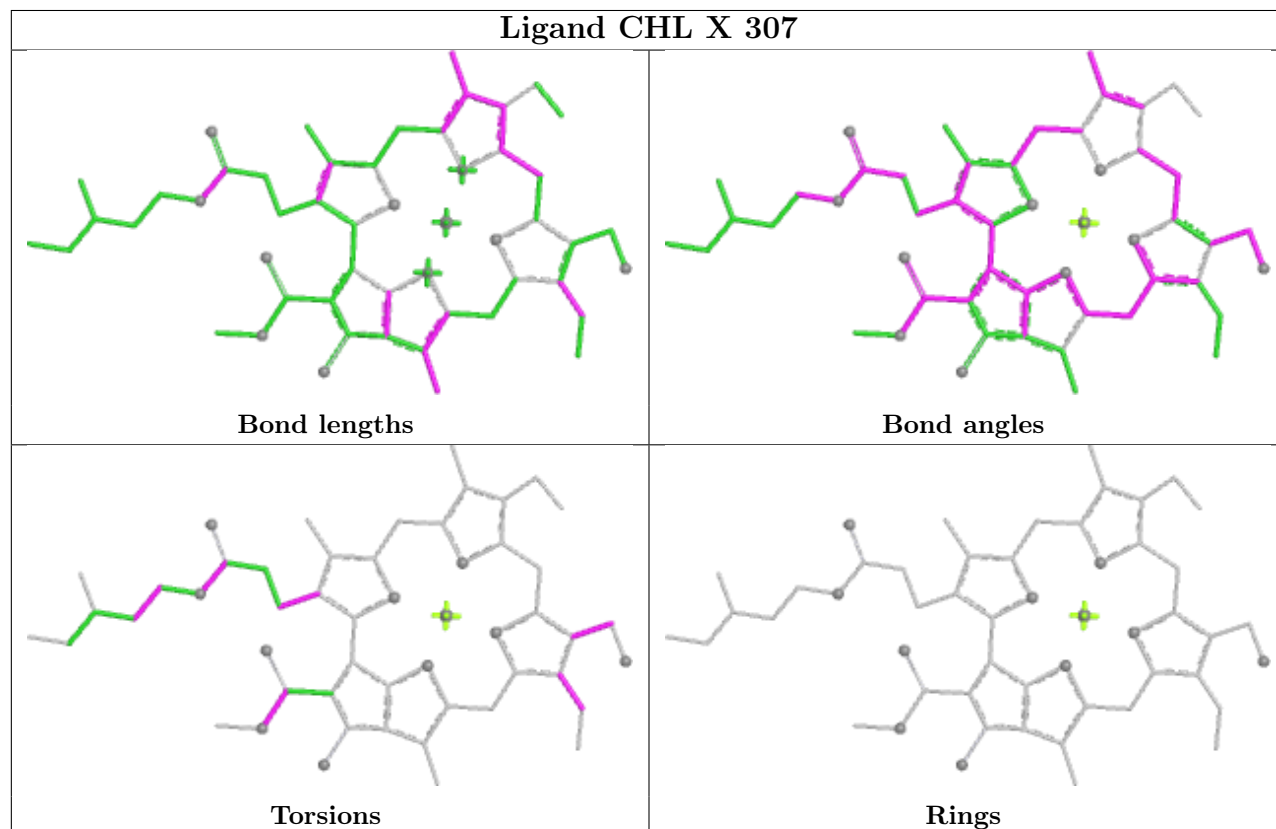
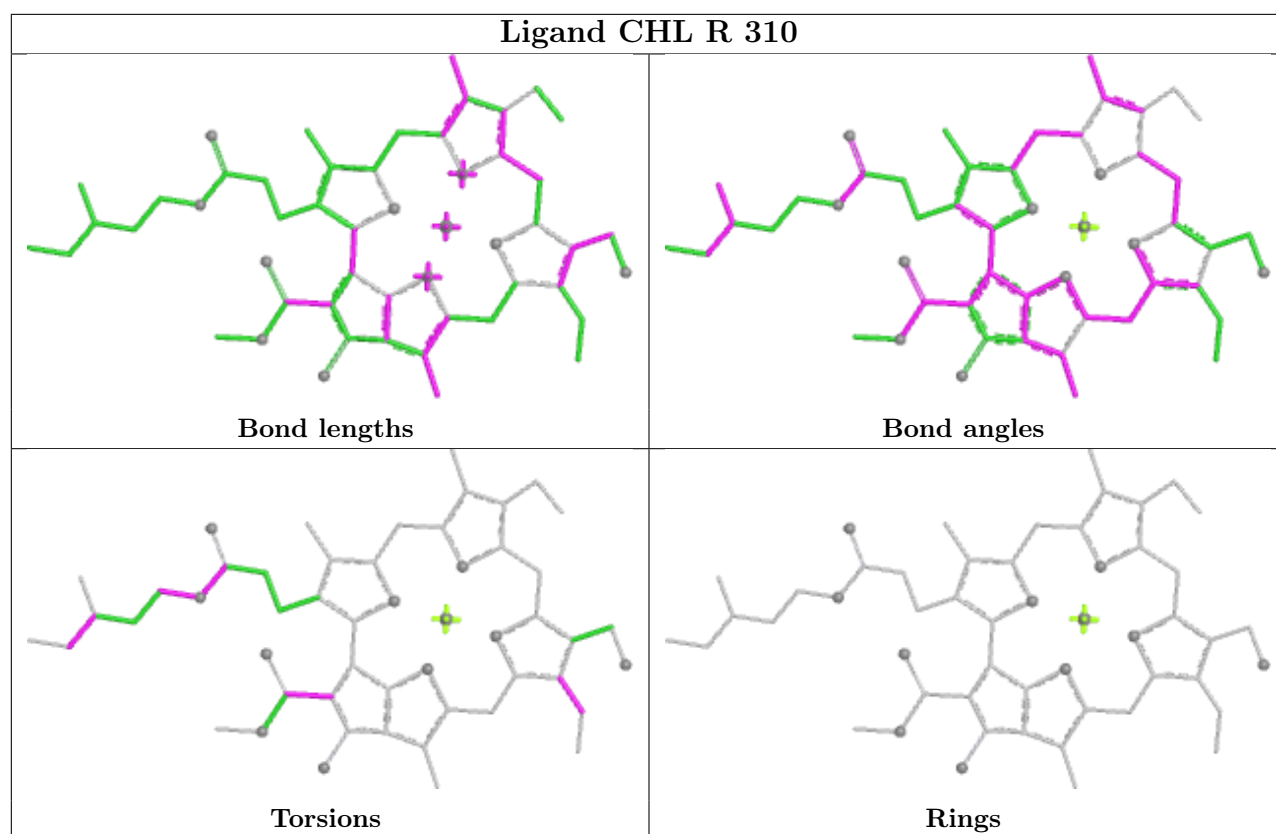
Ligand CLA B 840



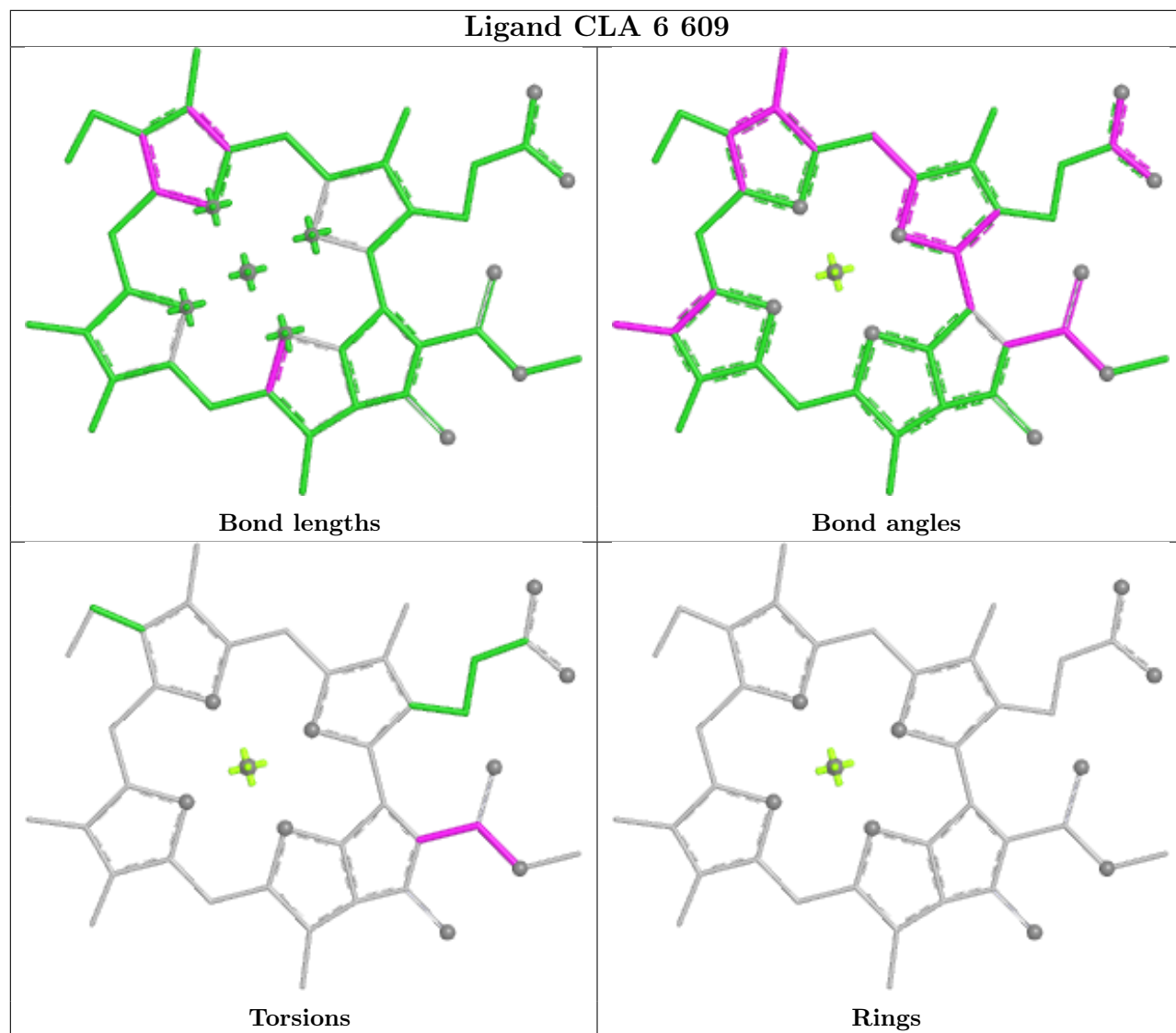
Ligand Q6L W 320

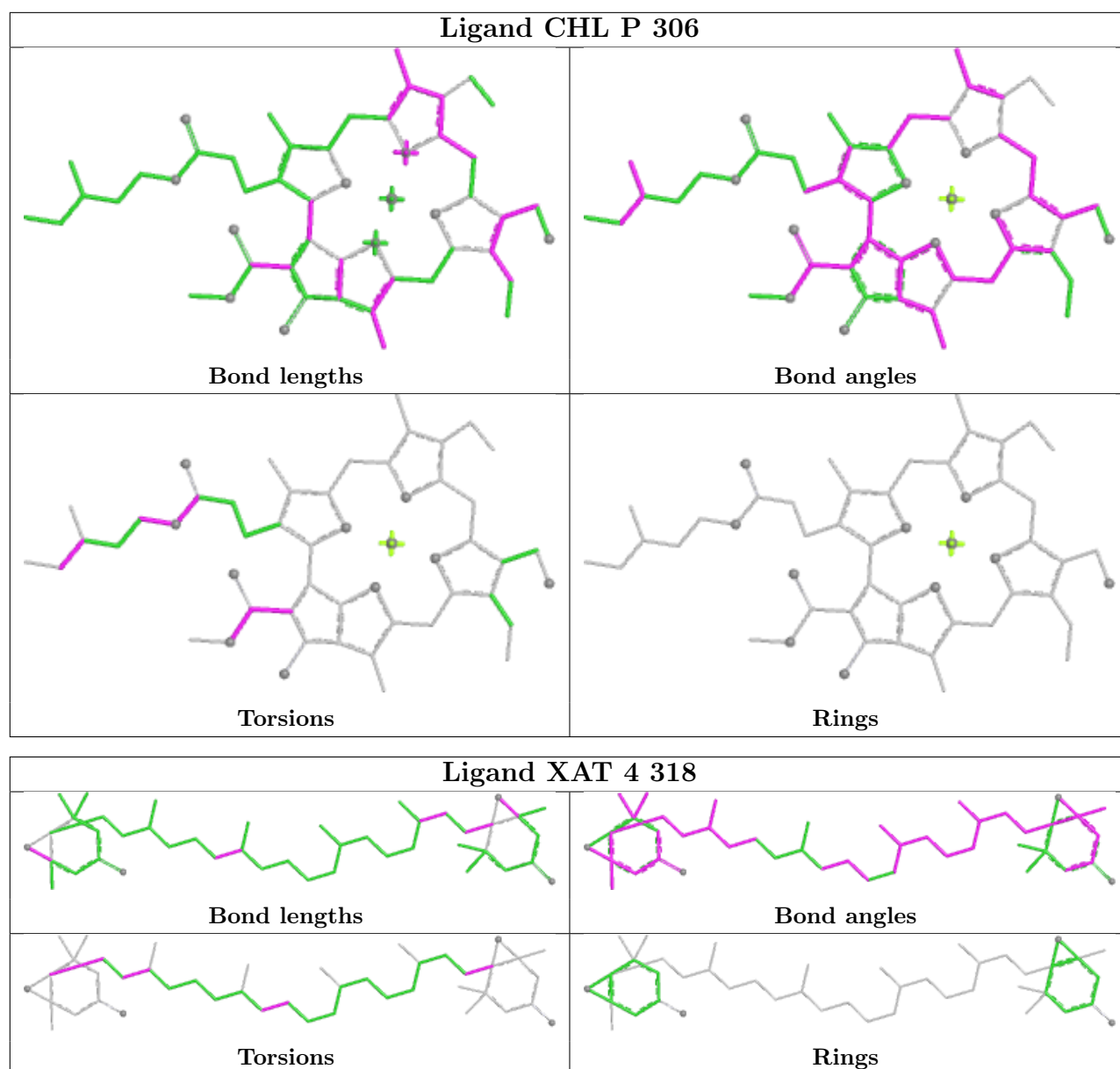


Ligand CLA T 301**Ligand CLA W 310**

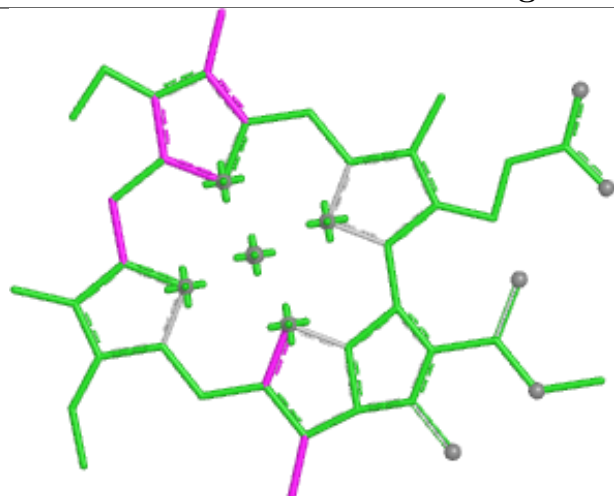


Ligand CLA 6 609

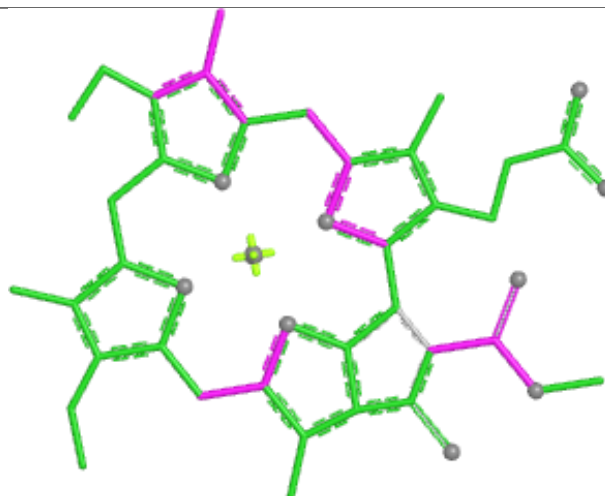




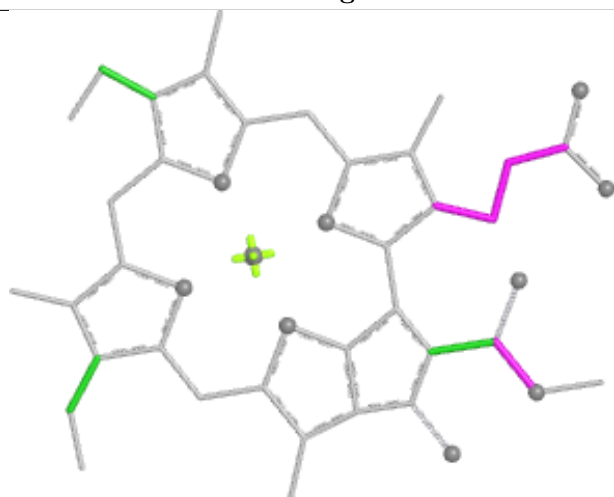
Ligand CLA 2 606



Bond lengths



Bond angles

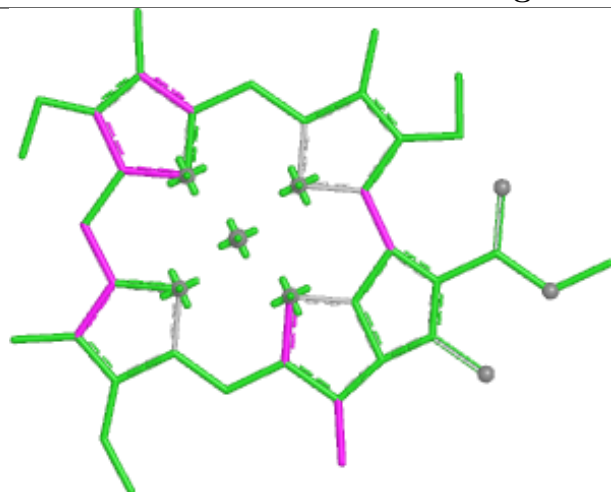


Torsions



Rings

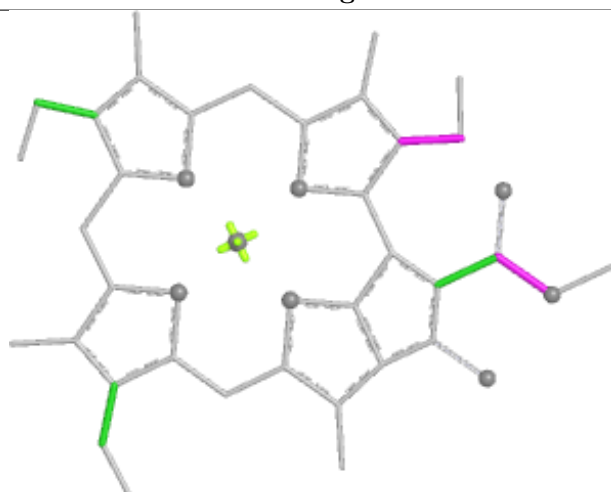
Ligand CLA V 309



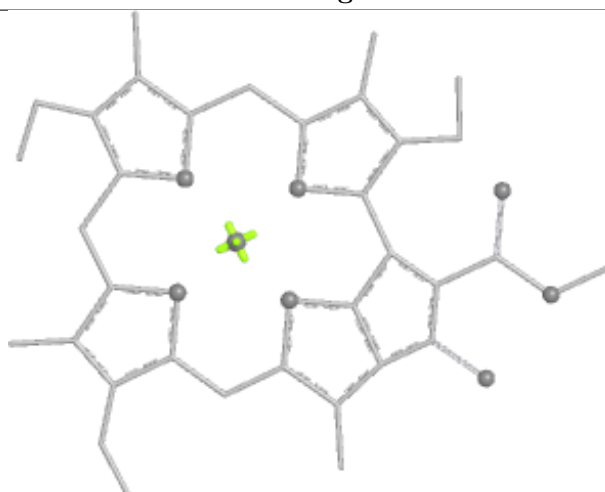
Bond lengths



Bond angles

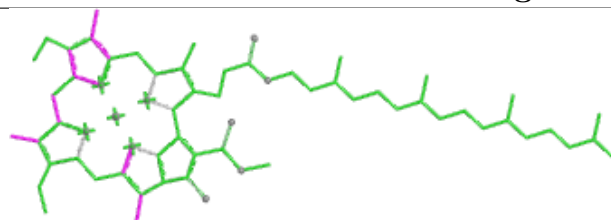


Torsions

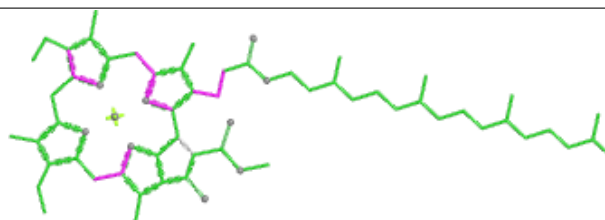


Rings

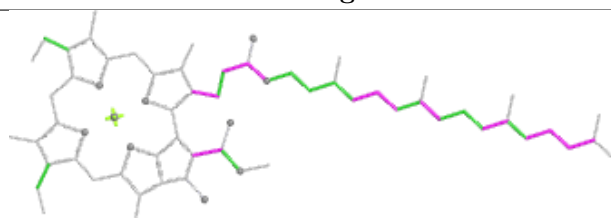
Ligand CLA B 839



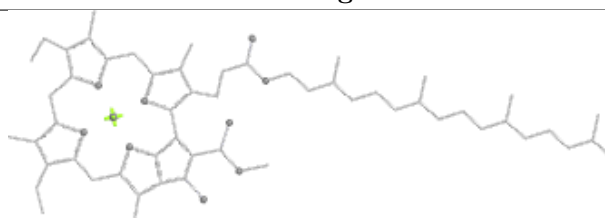
Bond lengths



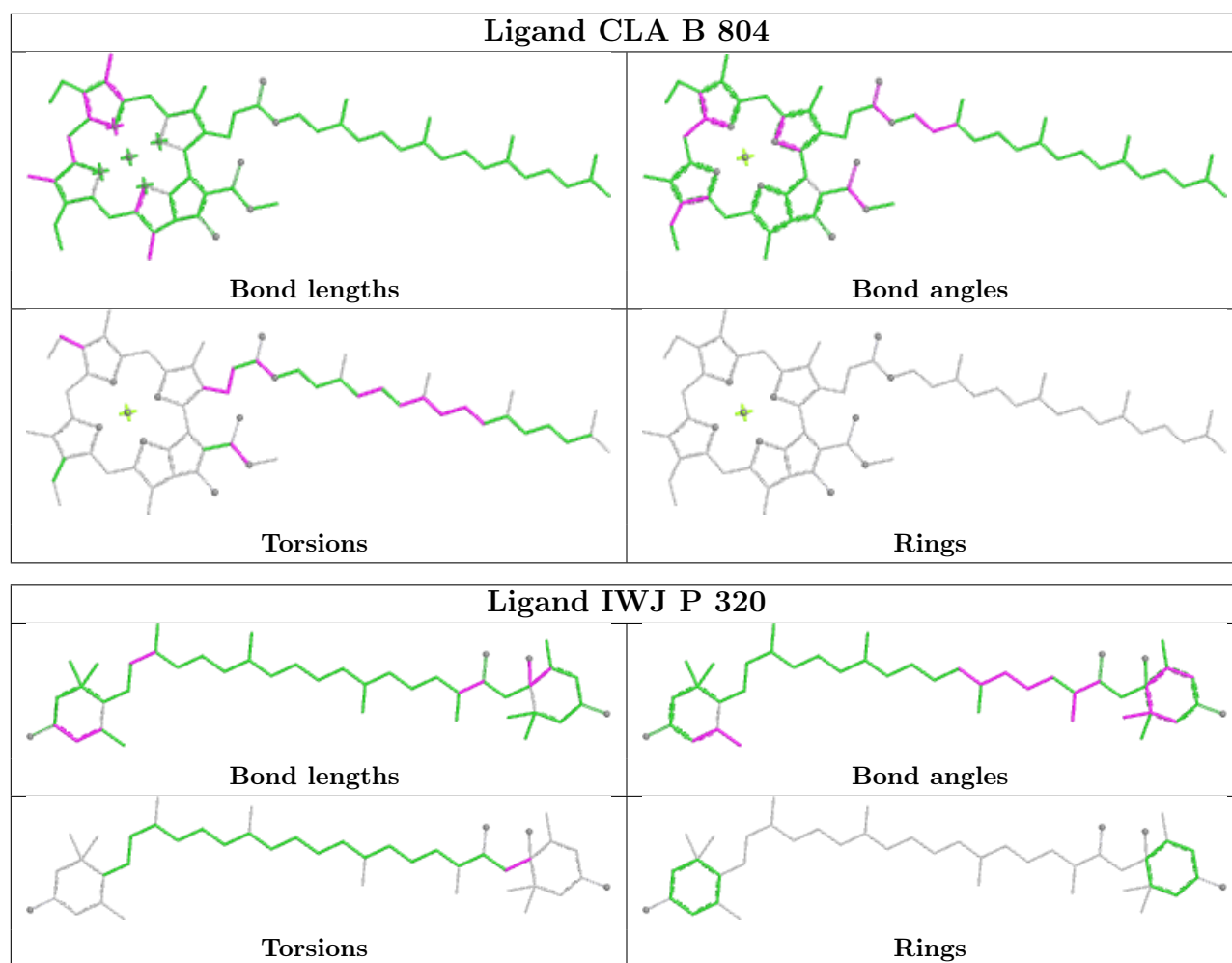
Bond angles



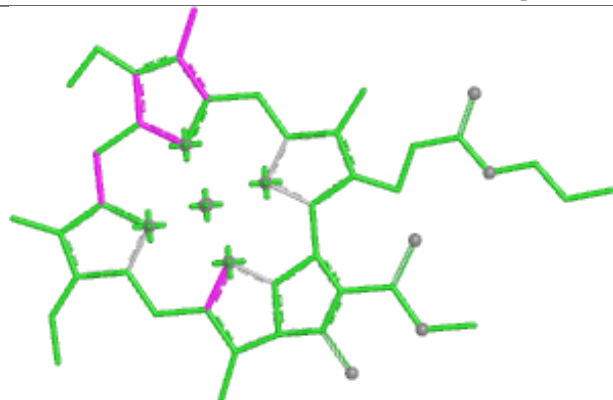
Torsions



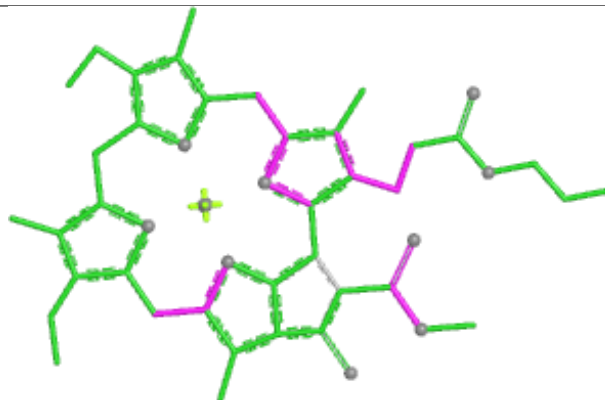
Rings



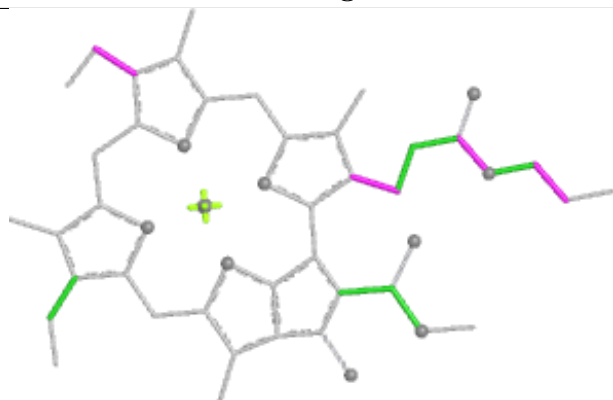
Ligand CLA P 313



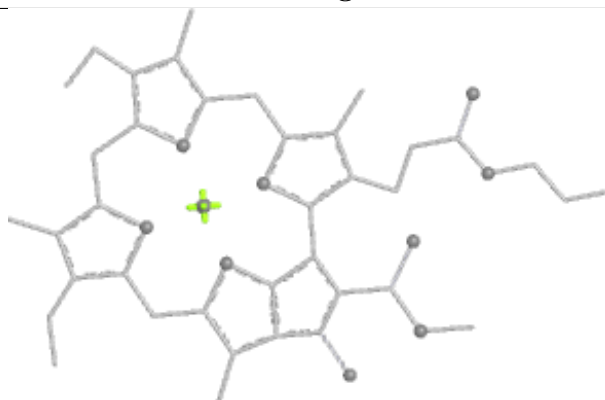
Bond lengths



Bond angles

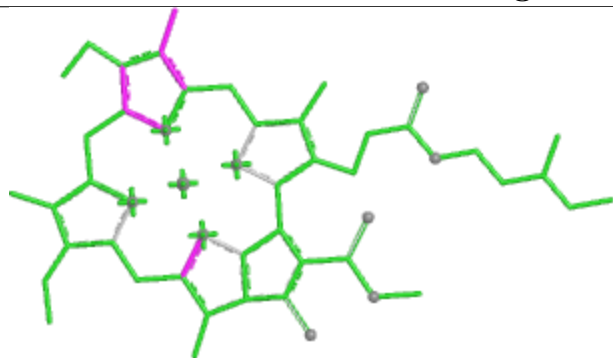


Torsions

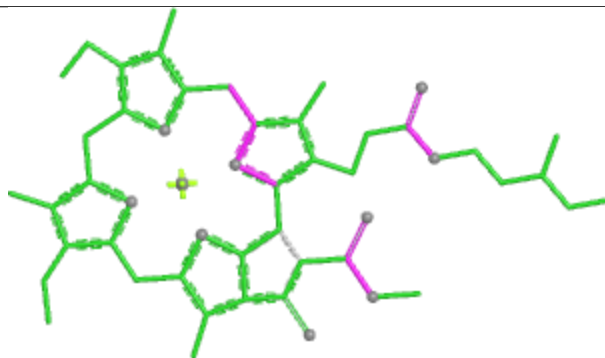


Rings

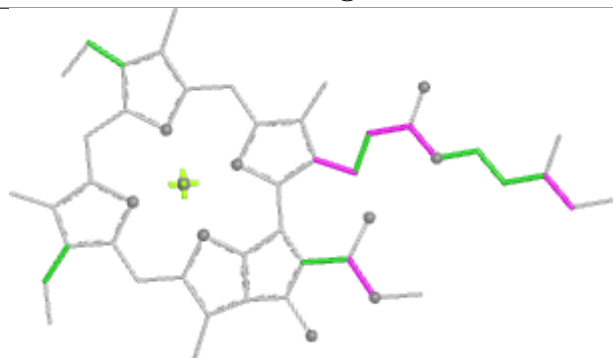
Ligand CLA X 303



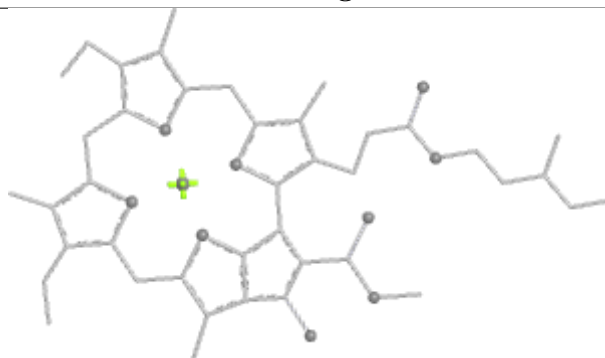
Bond lengths



Bond angles

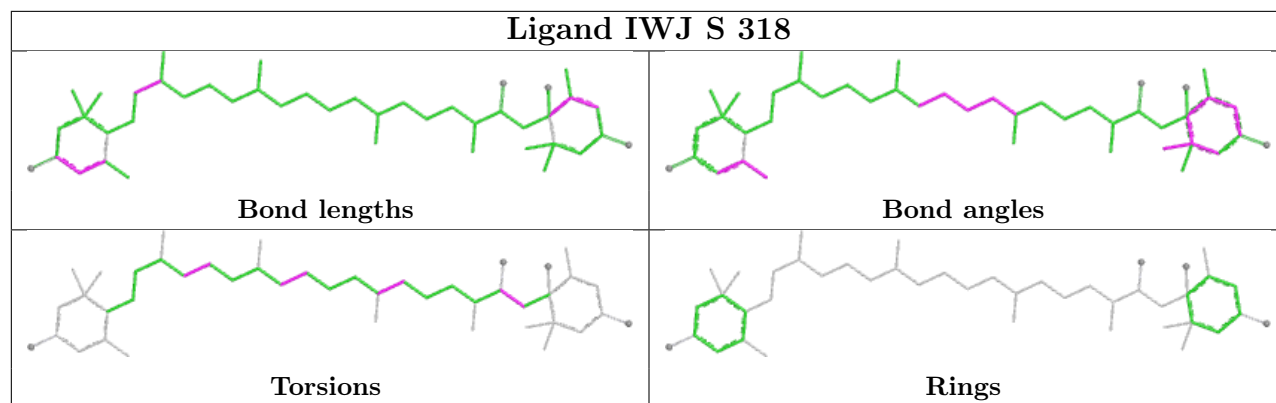


Torsions

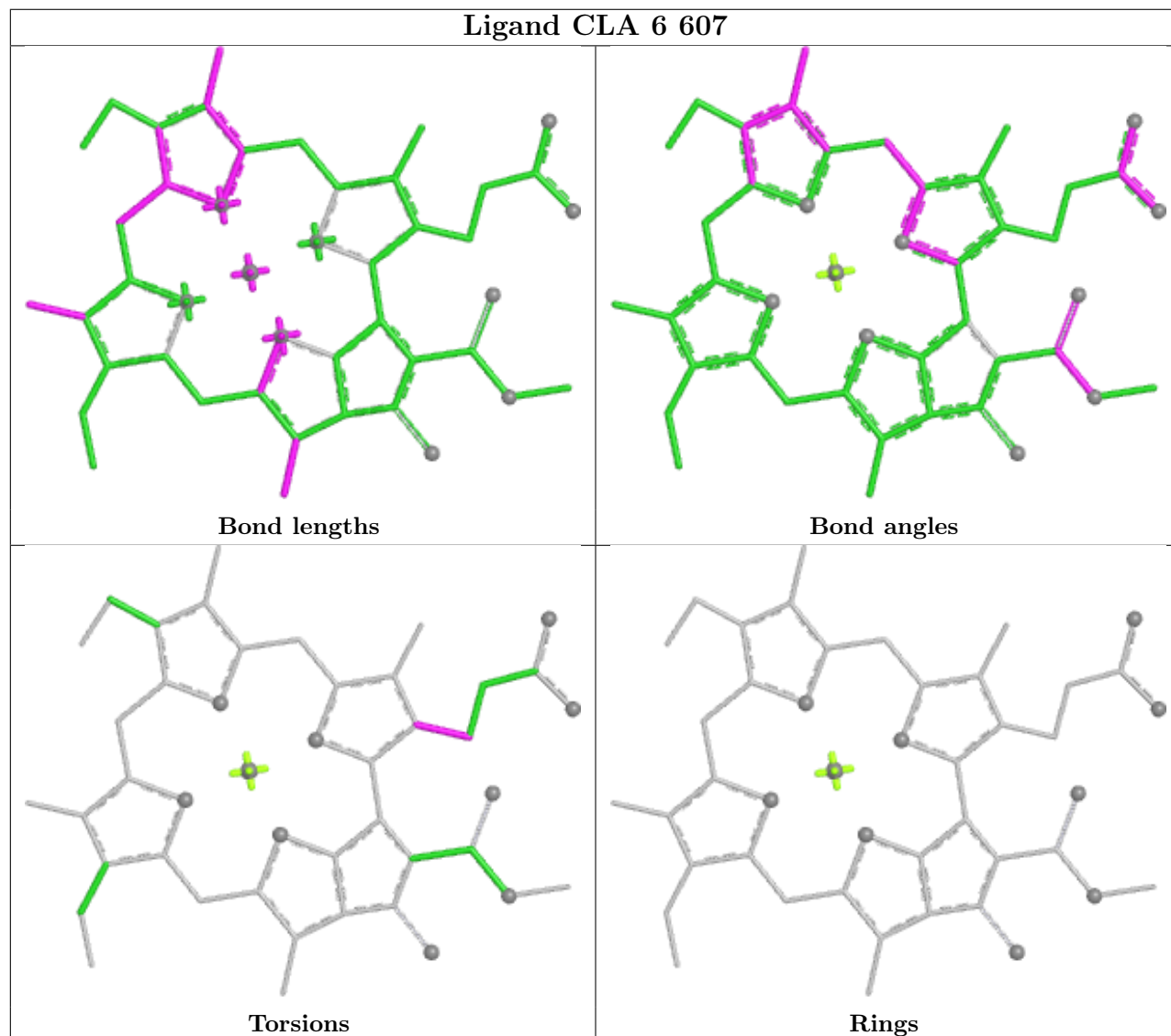


Rings

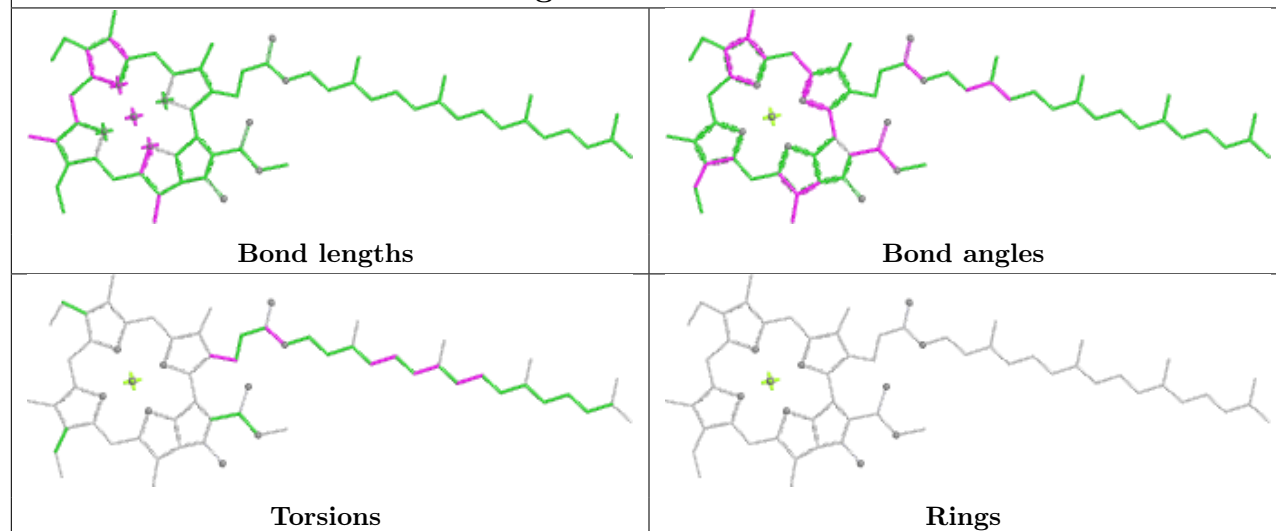
Ligand IWJ S 318



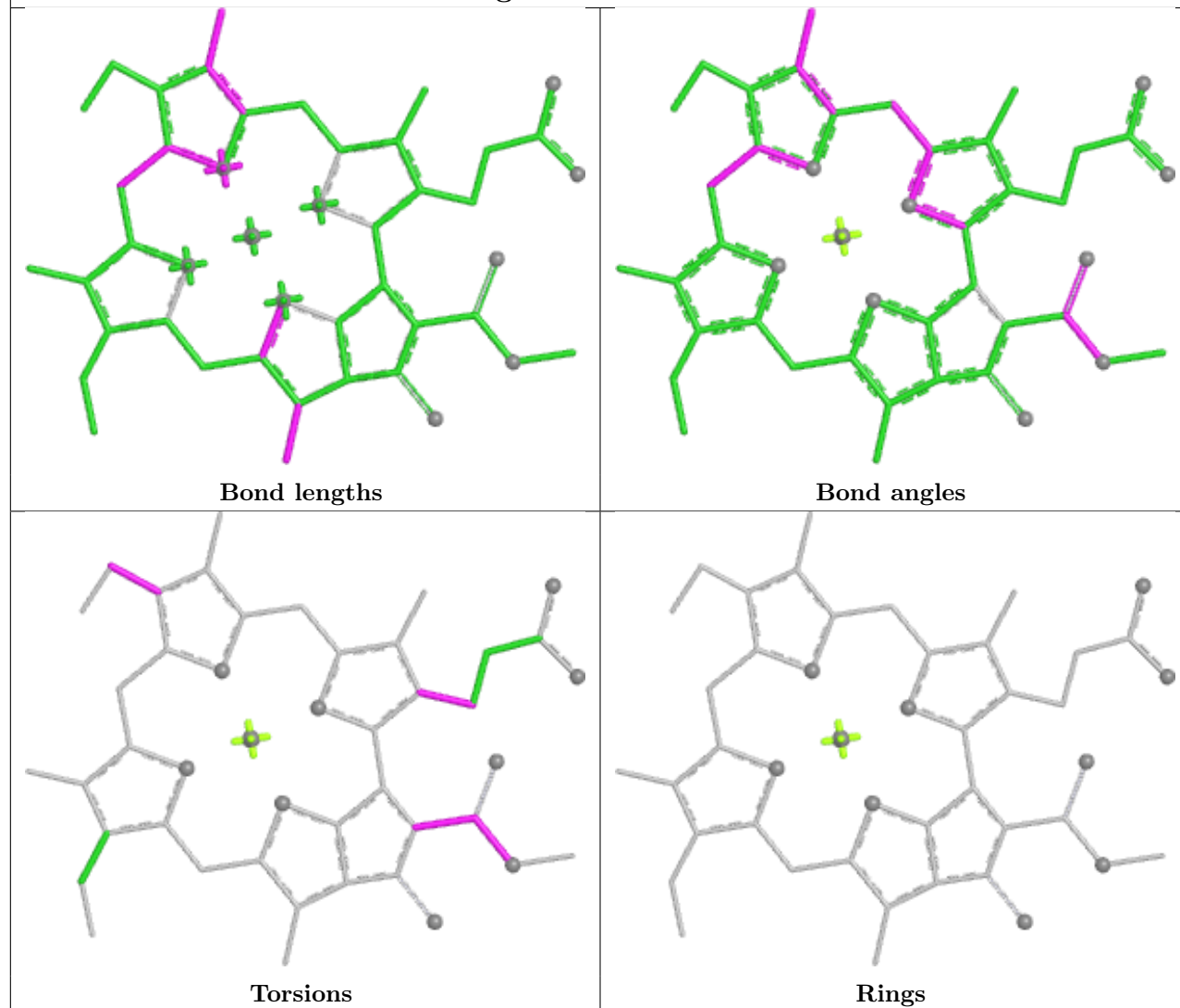
Ligand CLA 6 607

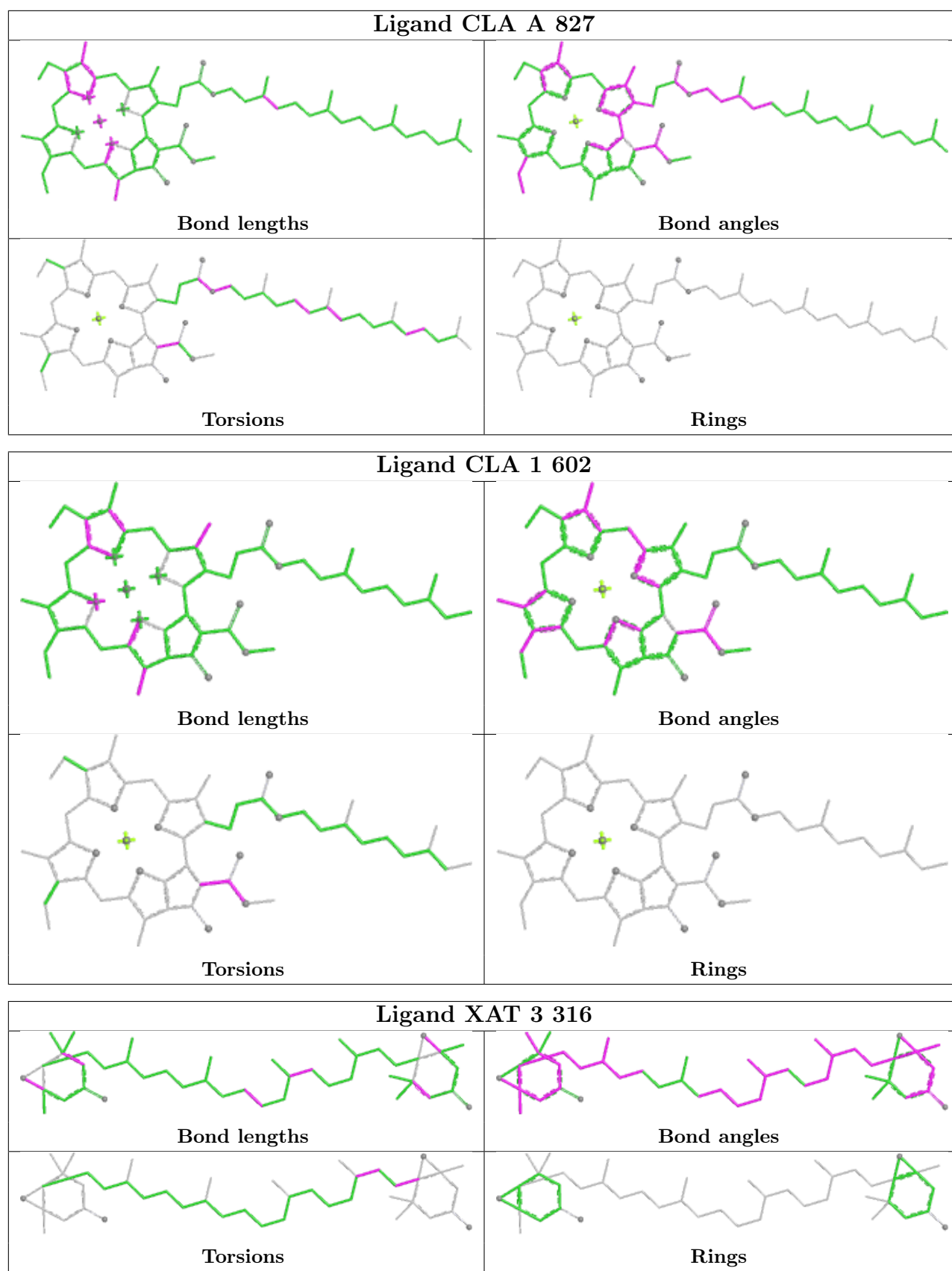


Ligand CLA S 301

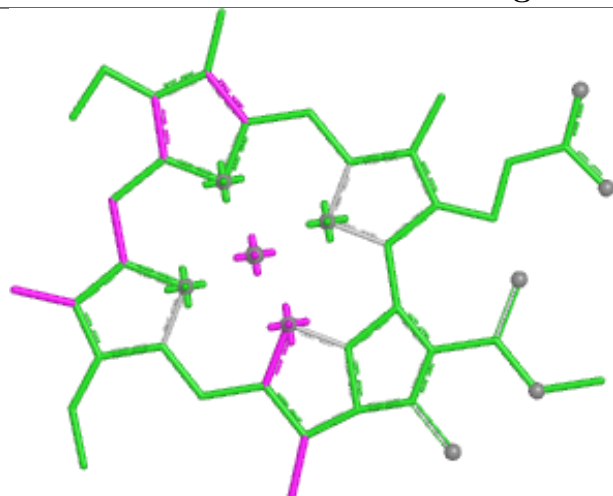


Ligand CLA 6 612

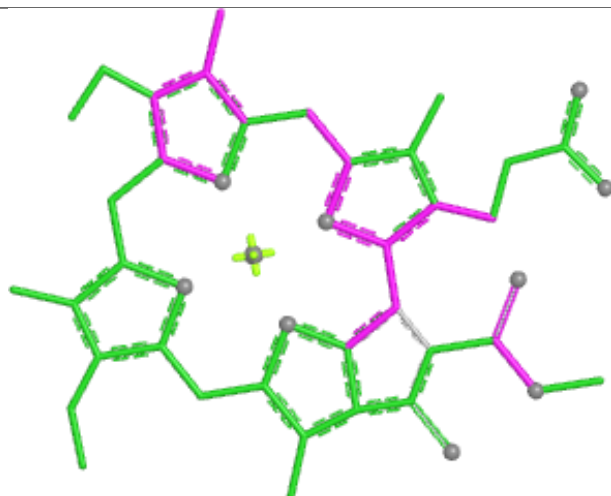




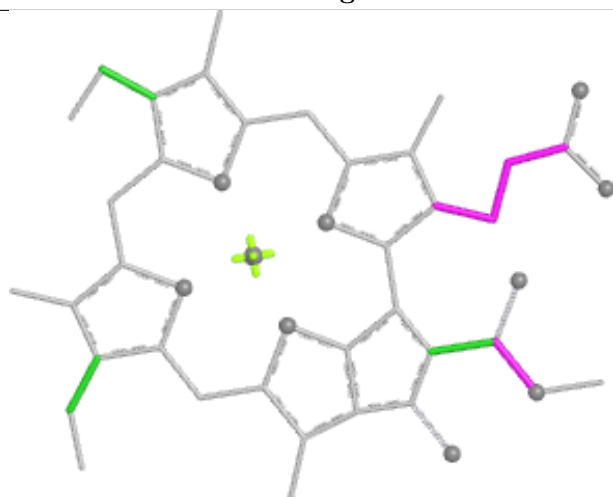
Ligand CLA U 301



Bond lengths



Bond angles

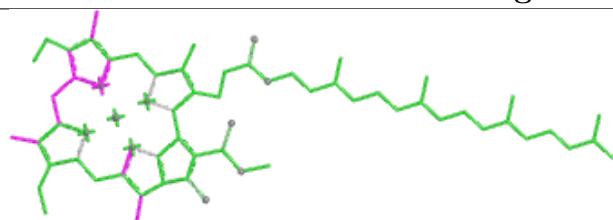


Torsions

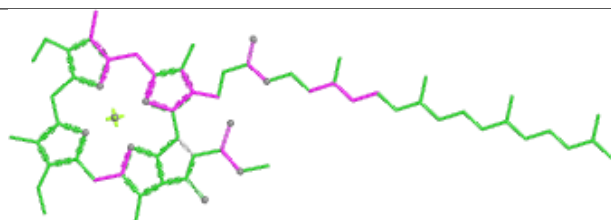


Rings

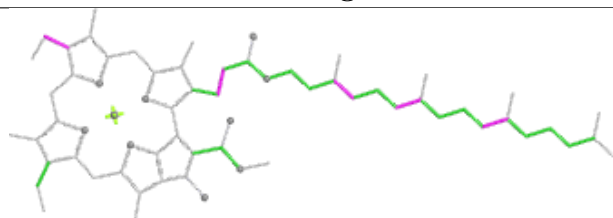
Ligand CLA B 841



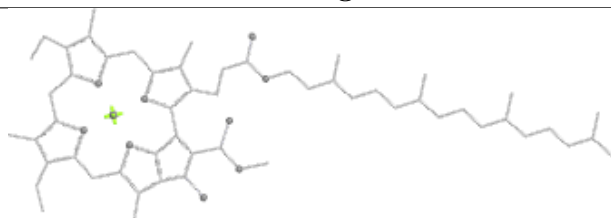
Bond lengths



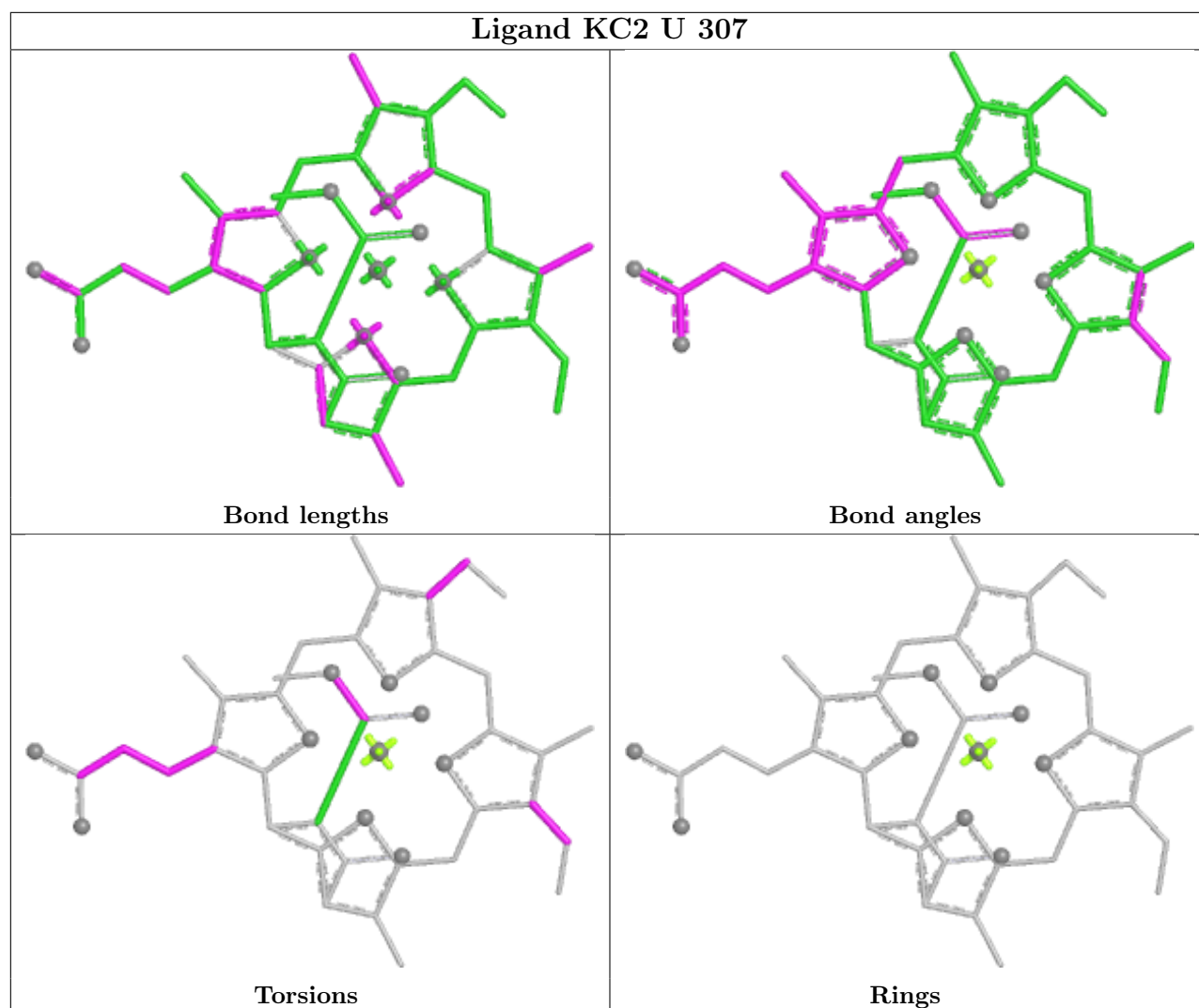
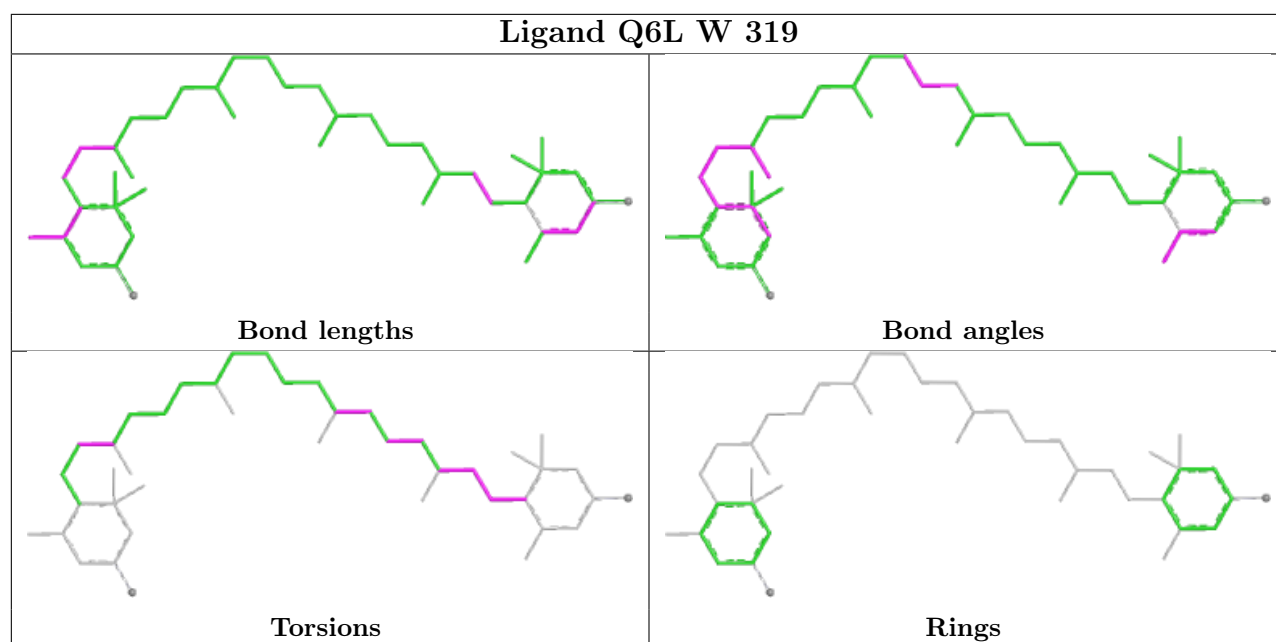
Bond angles

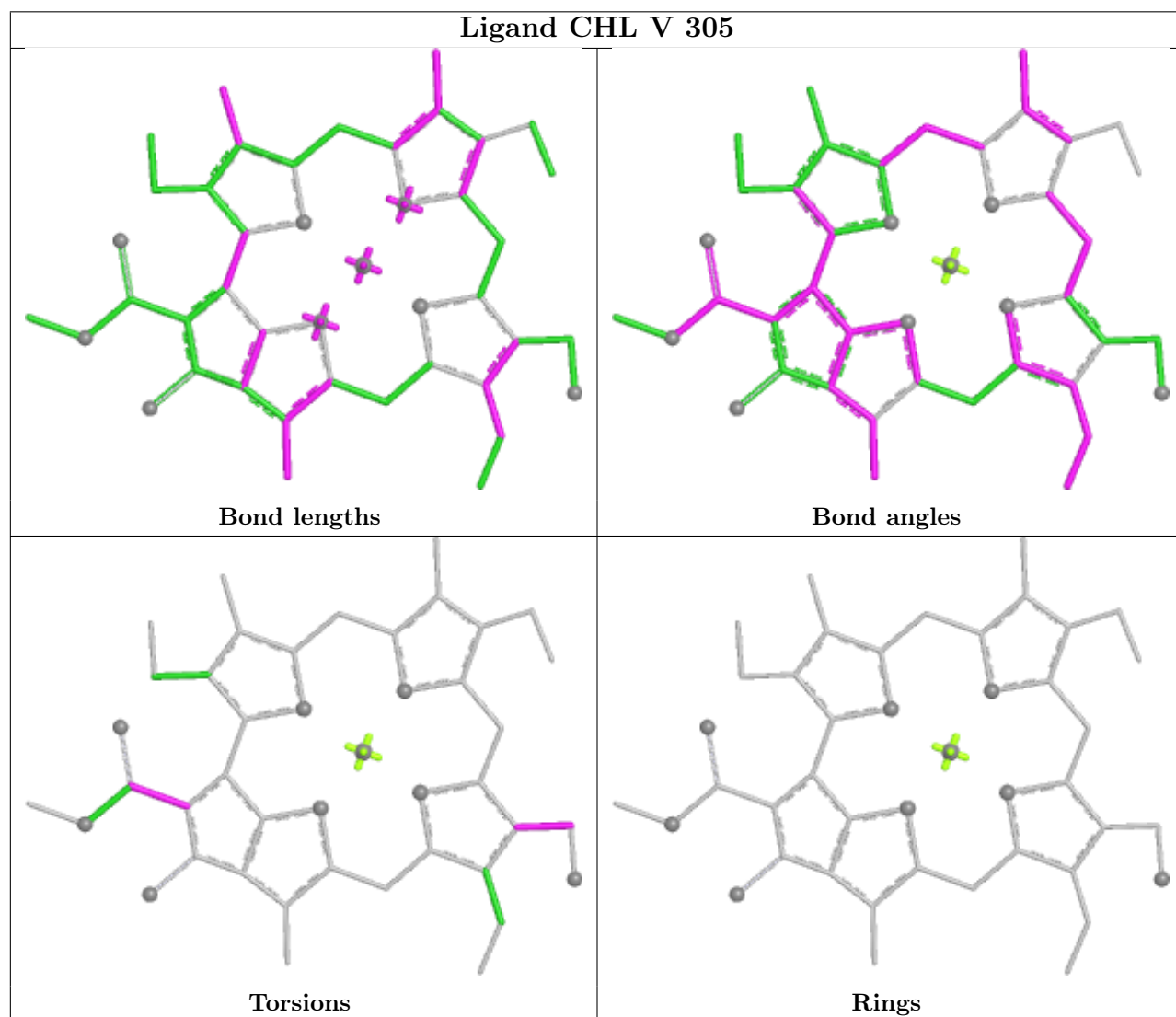
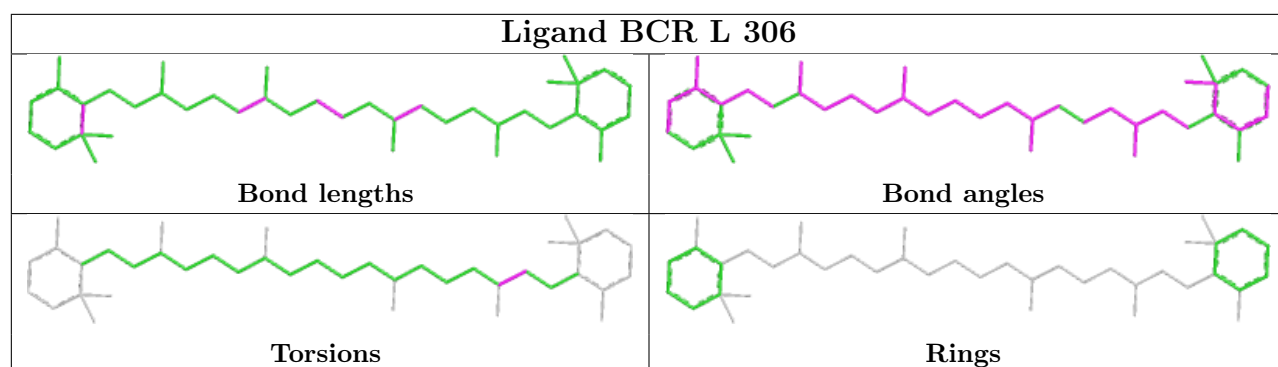


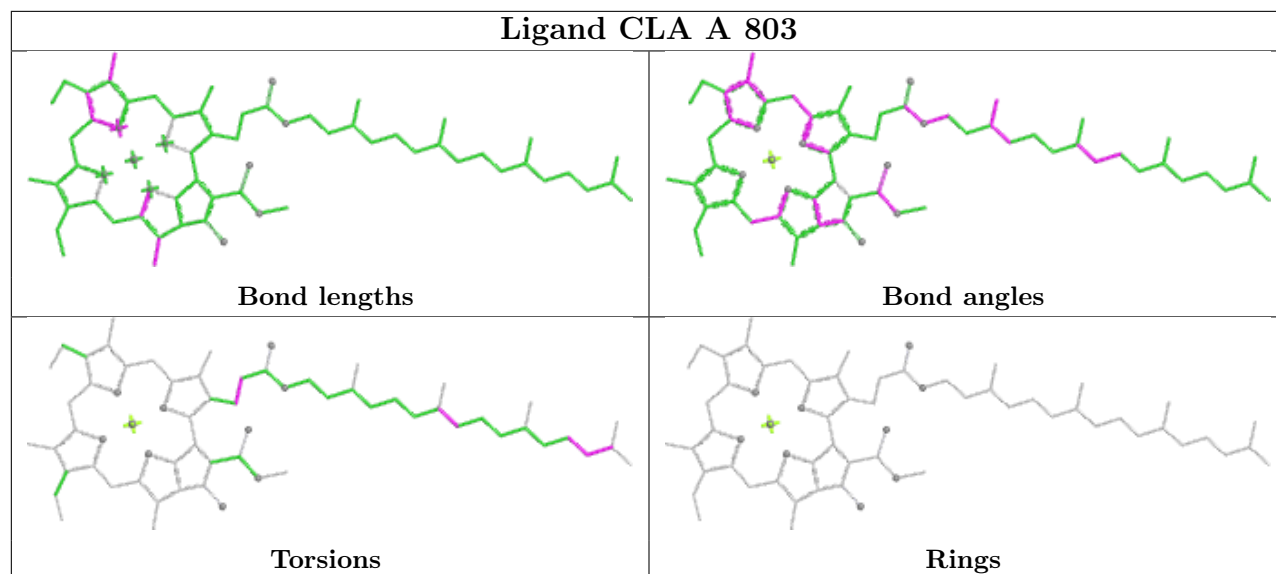
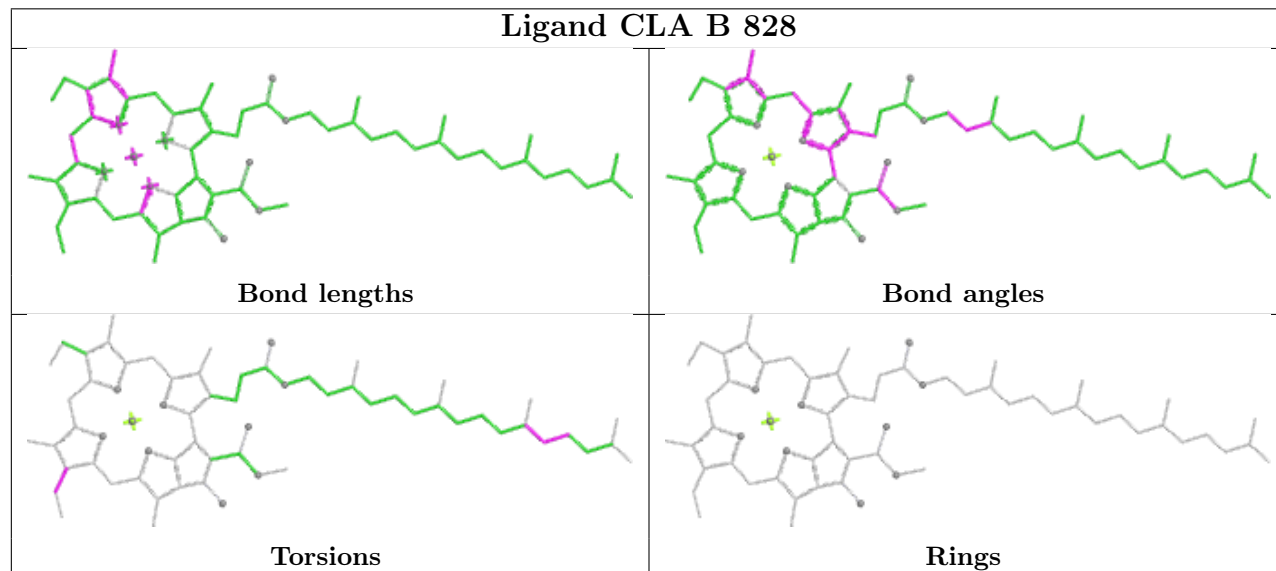
Torsions

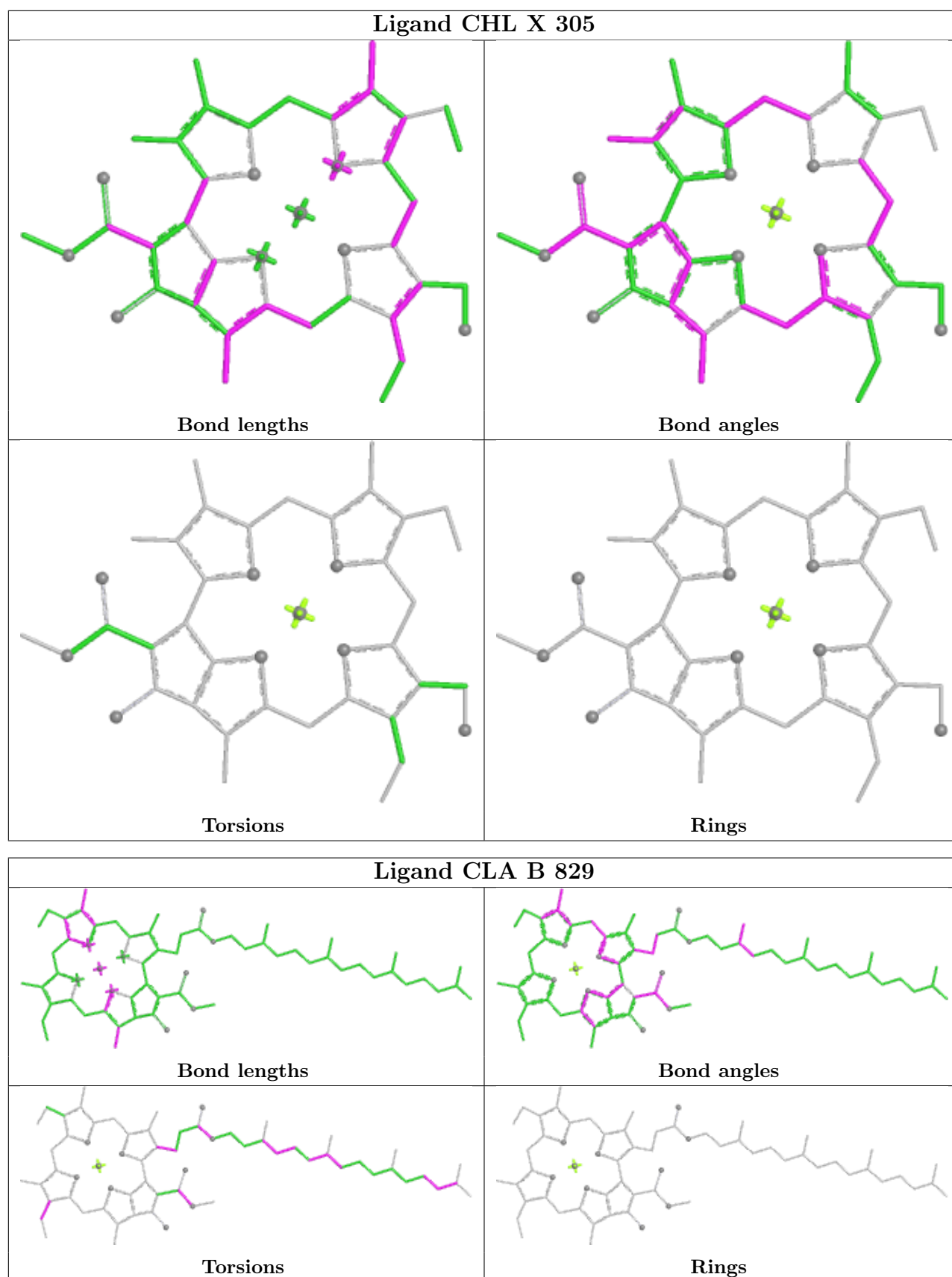


Rings

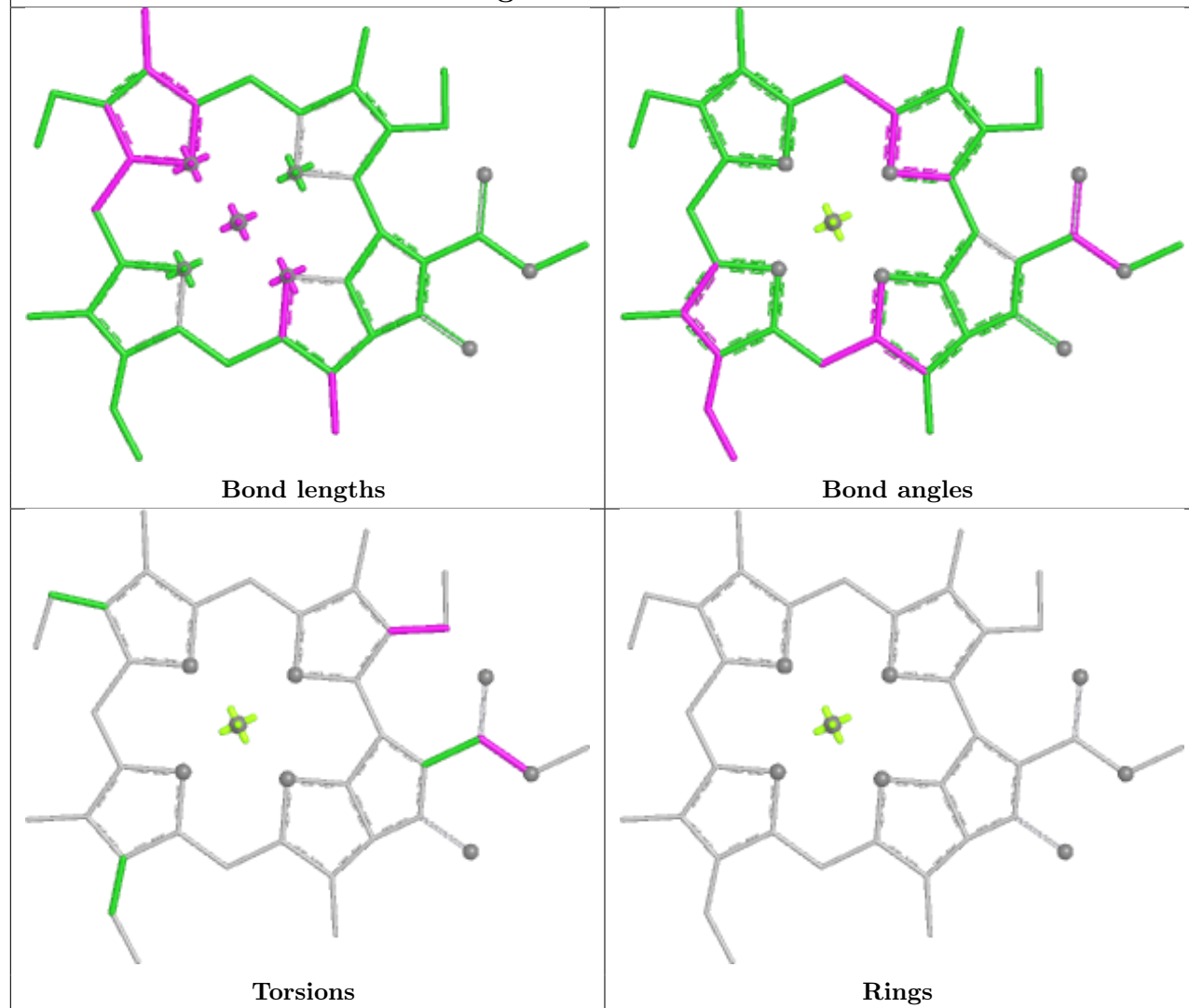




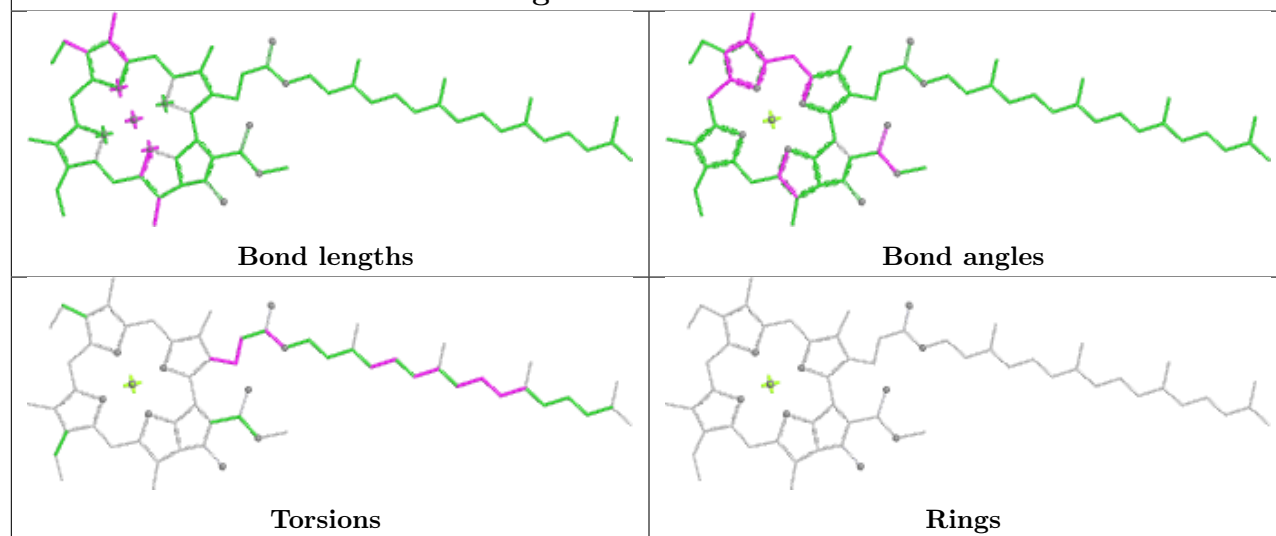
Ligand CLA A 803**Ligand CLA B 828**

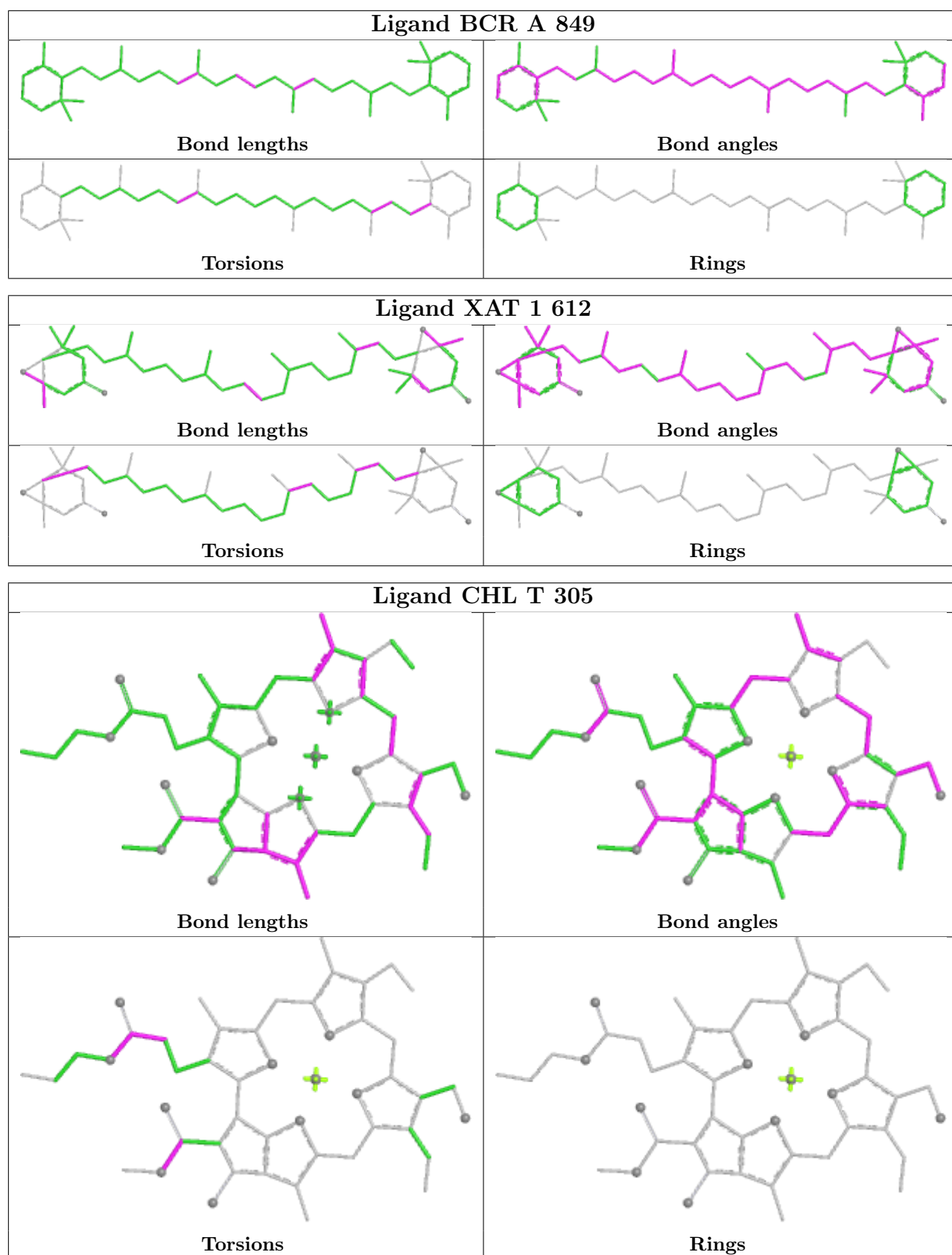


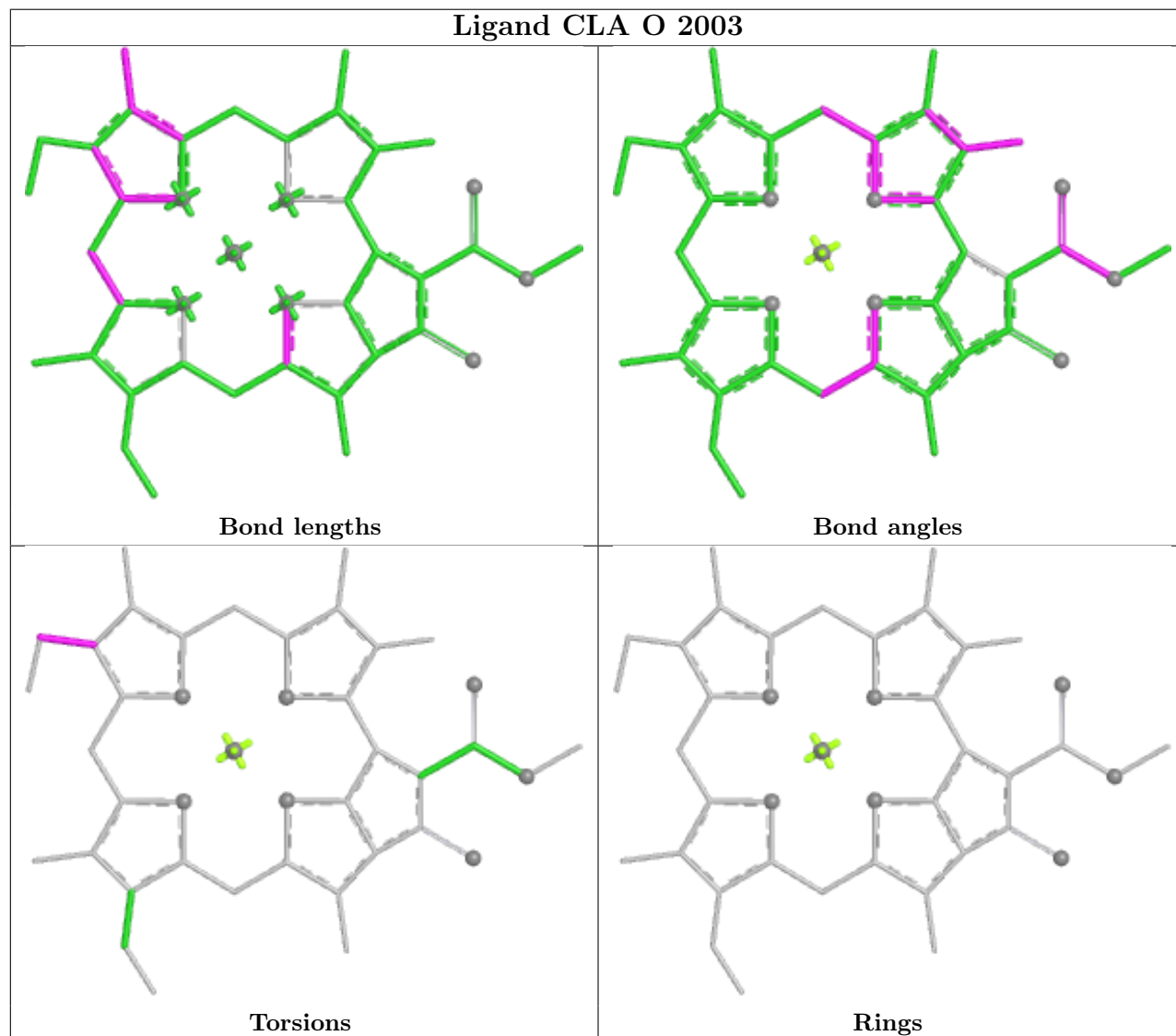
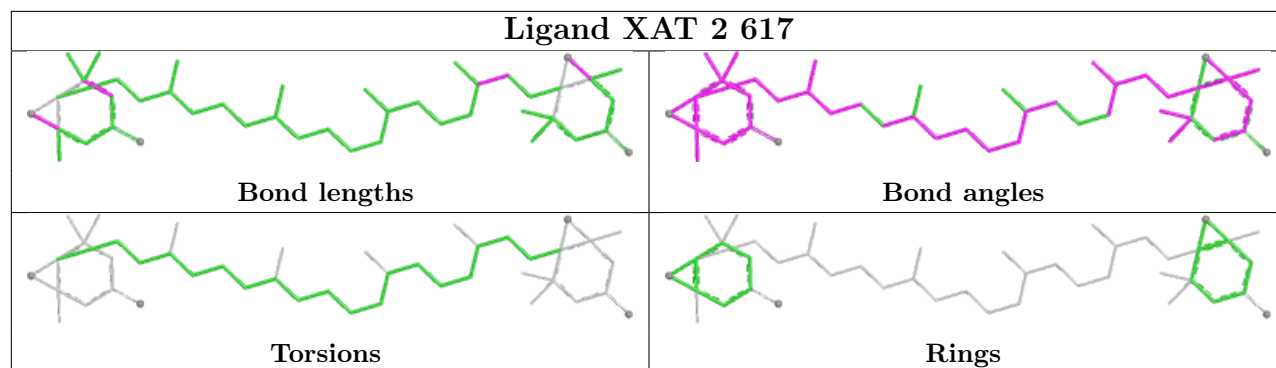
Ligand CLA F 802



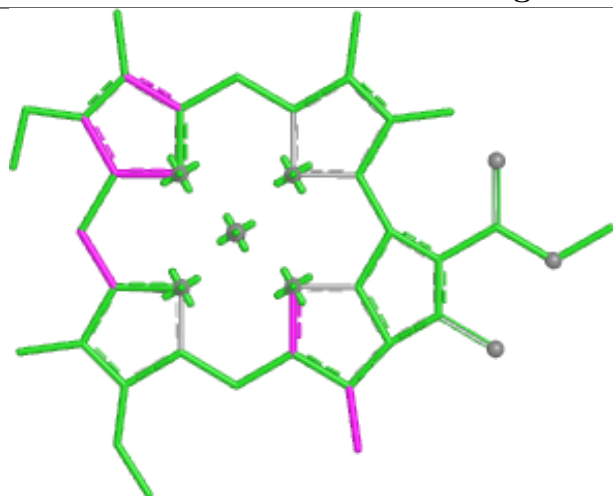
Ligand CLA B 830



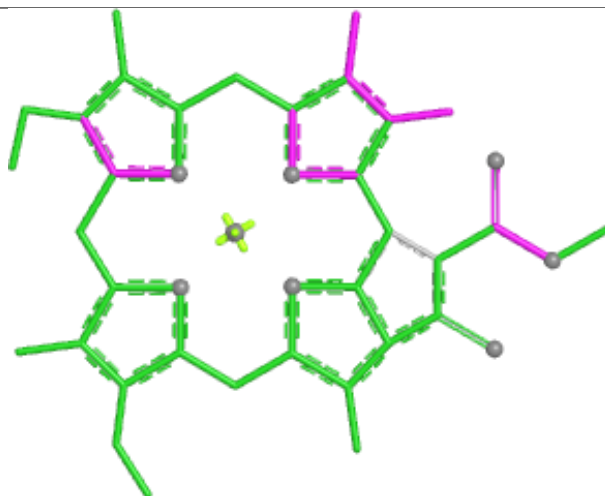




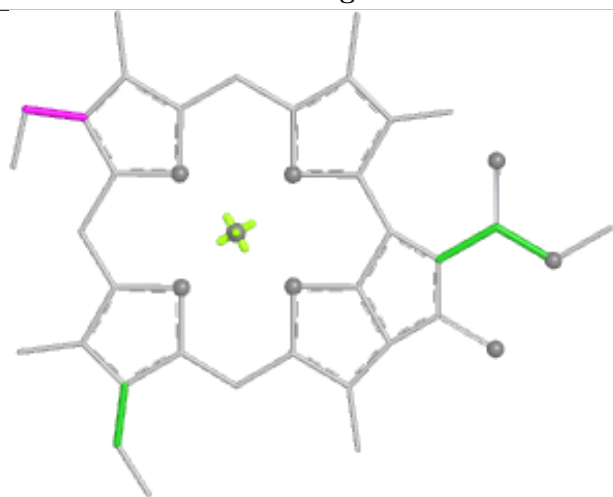
Ligand CLA U 312



Bond lengths



Bond angles

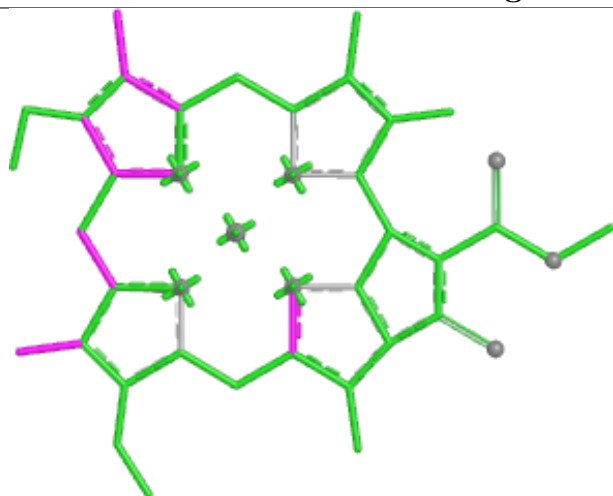


Torsions

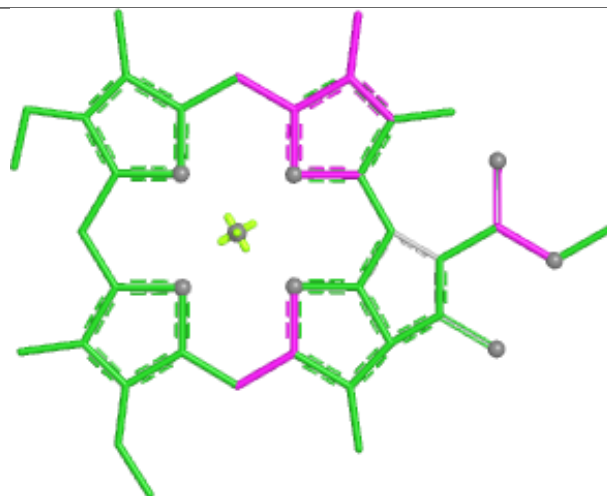


Rings

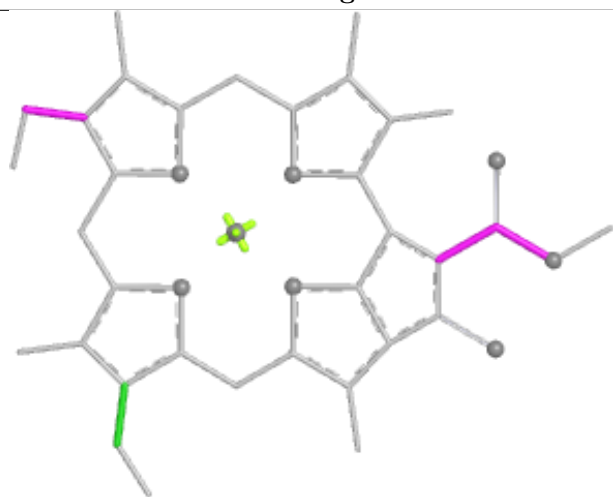
Ligand CLA O 2004



Bond lengths



Bond angles

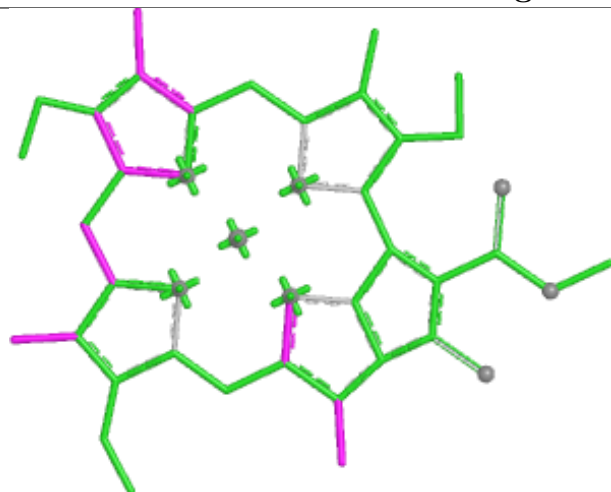


Torsions

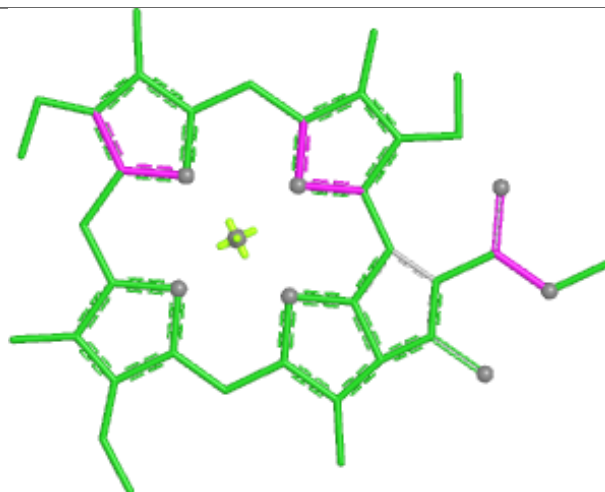


Rings

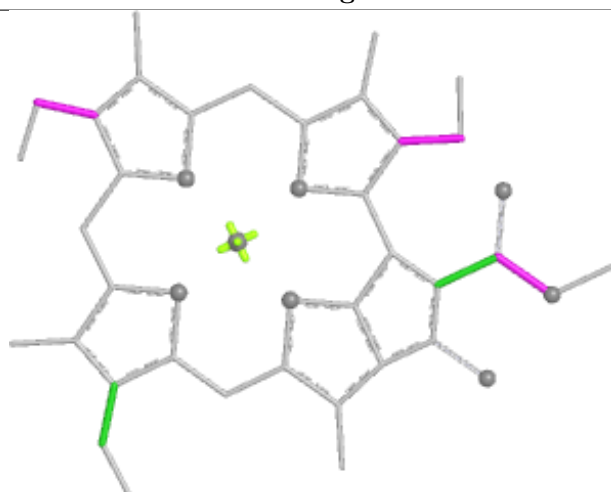
Ligand CLA T 313



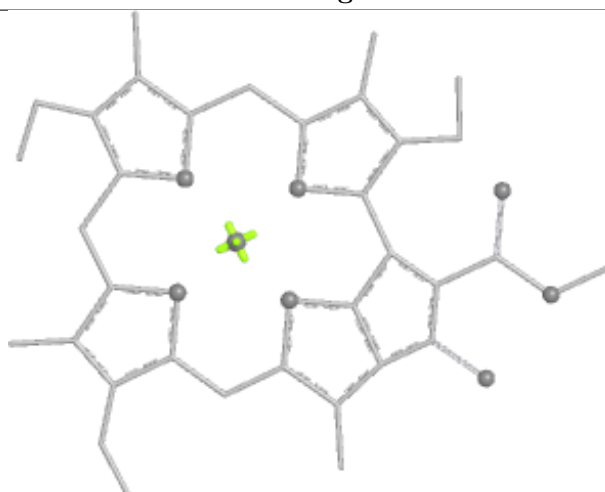
Bond lengths



Bond angles

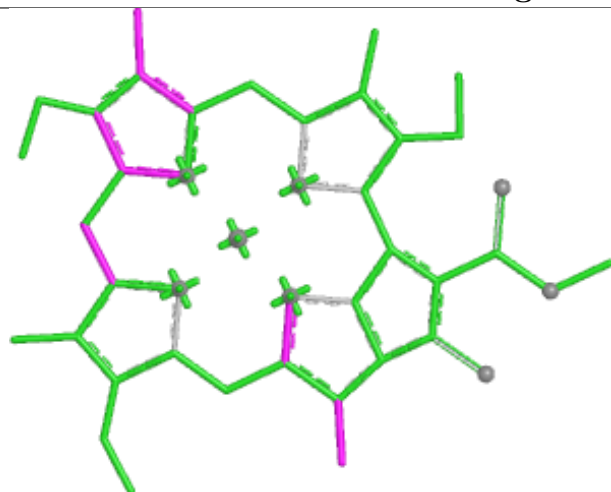


Torsions

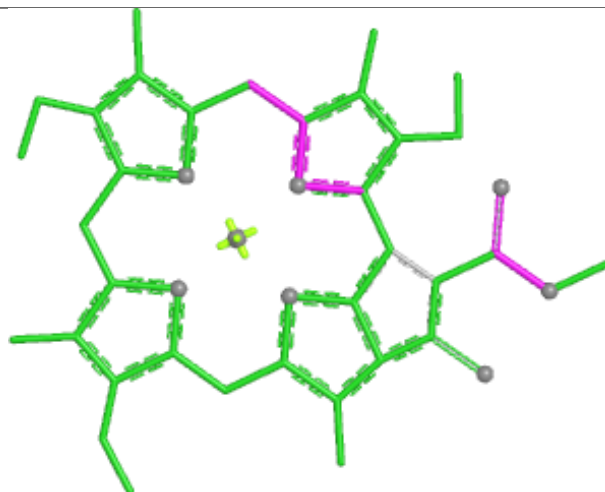


Rings

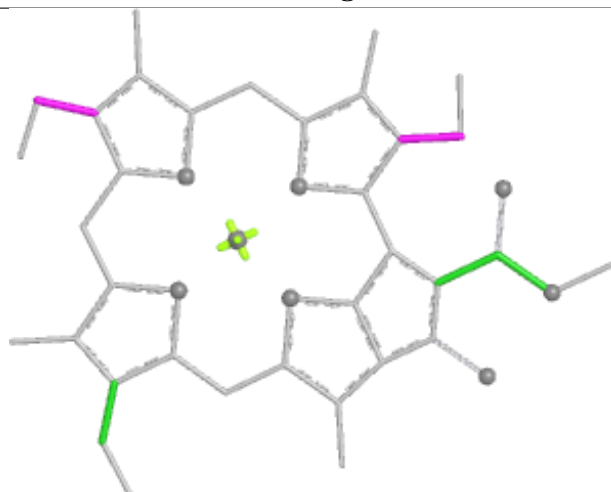
Ligand CLA T 310



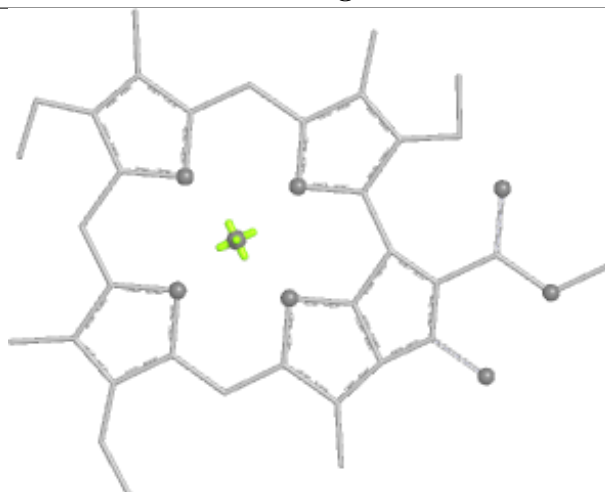
Bond lengths



Bond angles

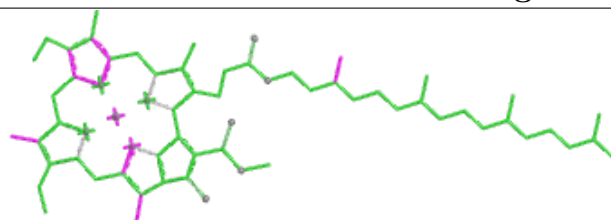


Torsions

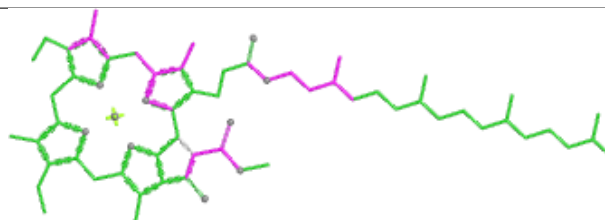


Rings

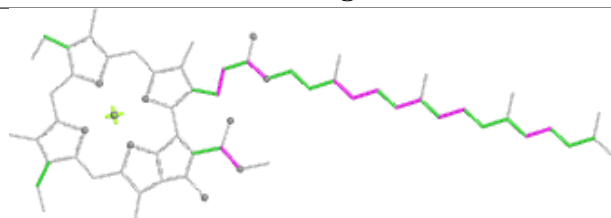
Ligand CLA B 815



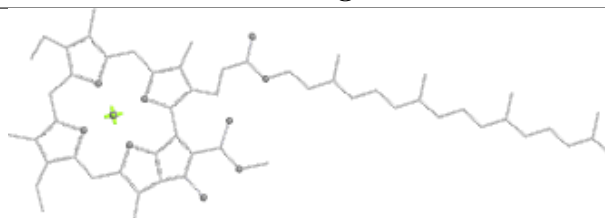
Bond lengths



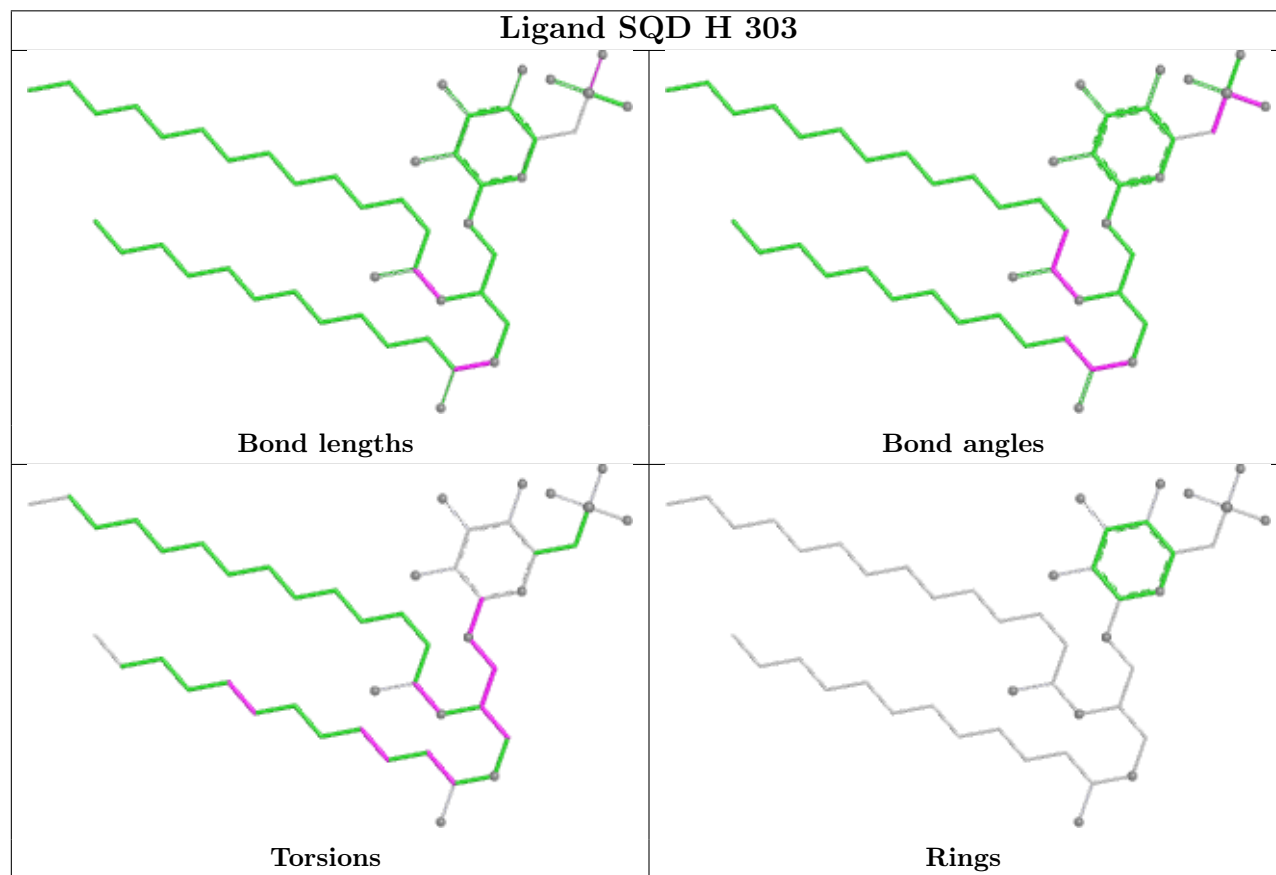
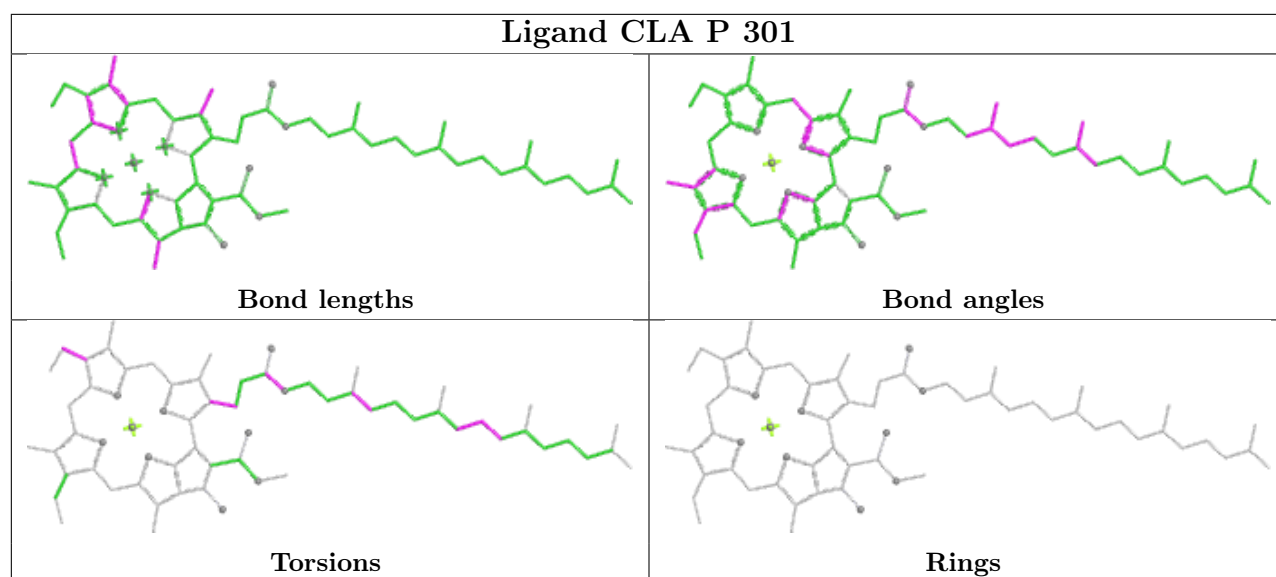
Bond angles

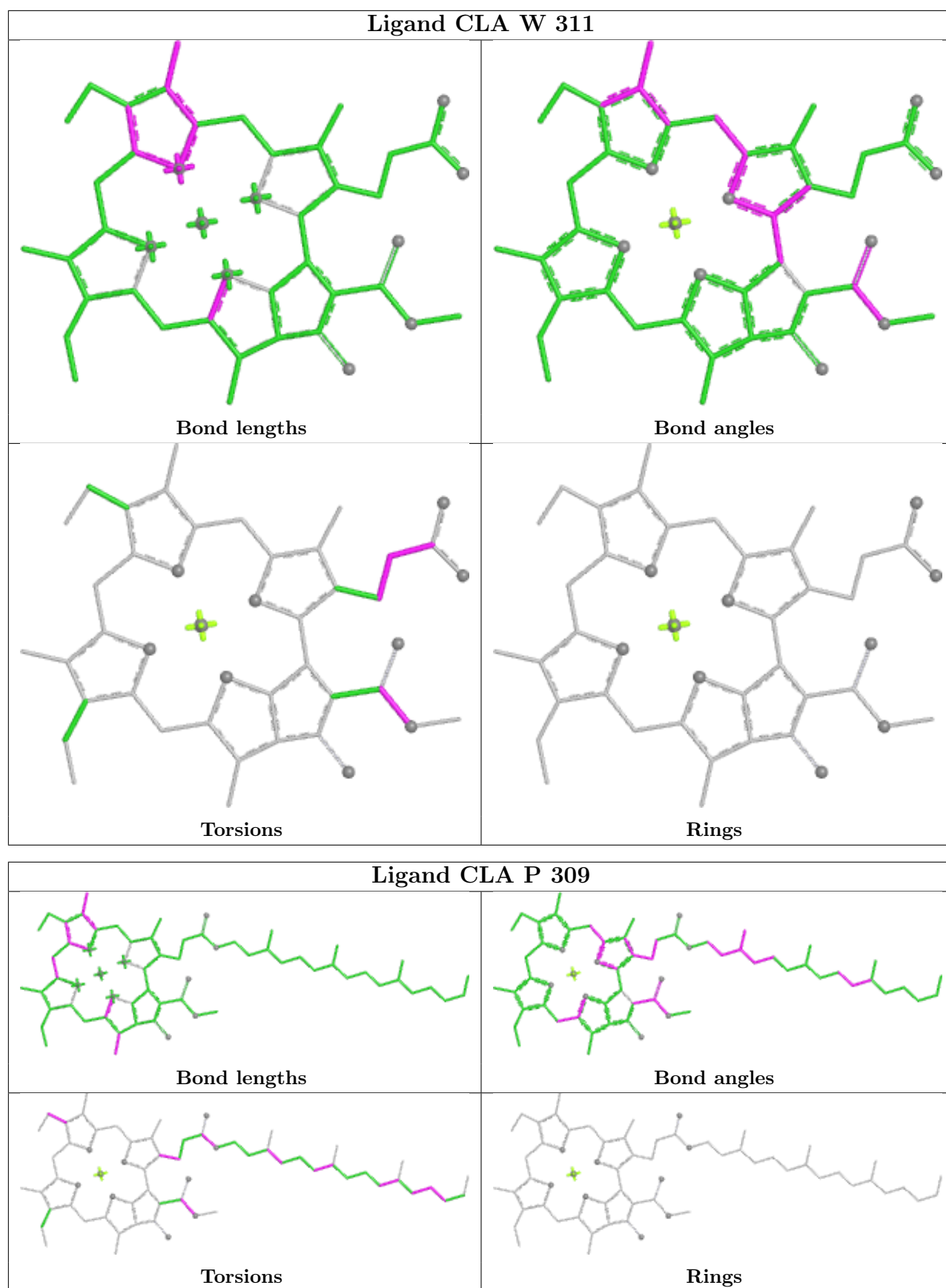


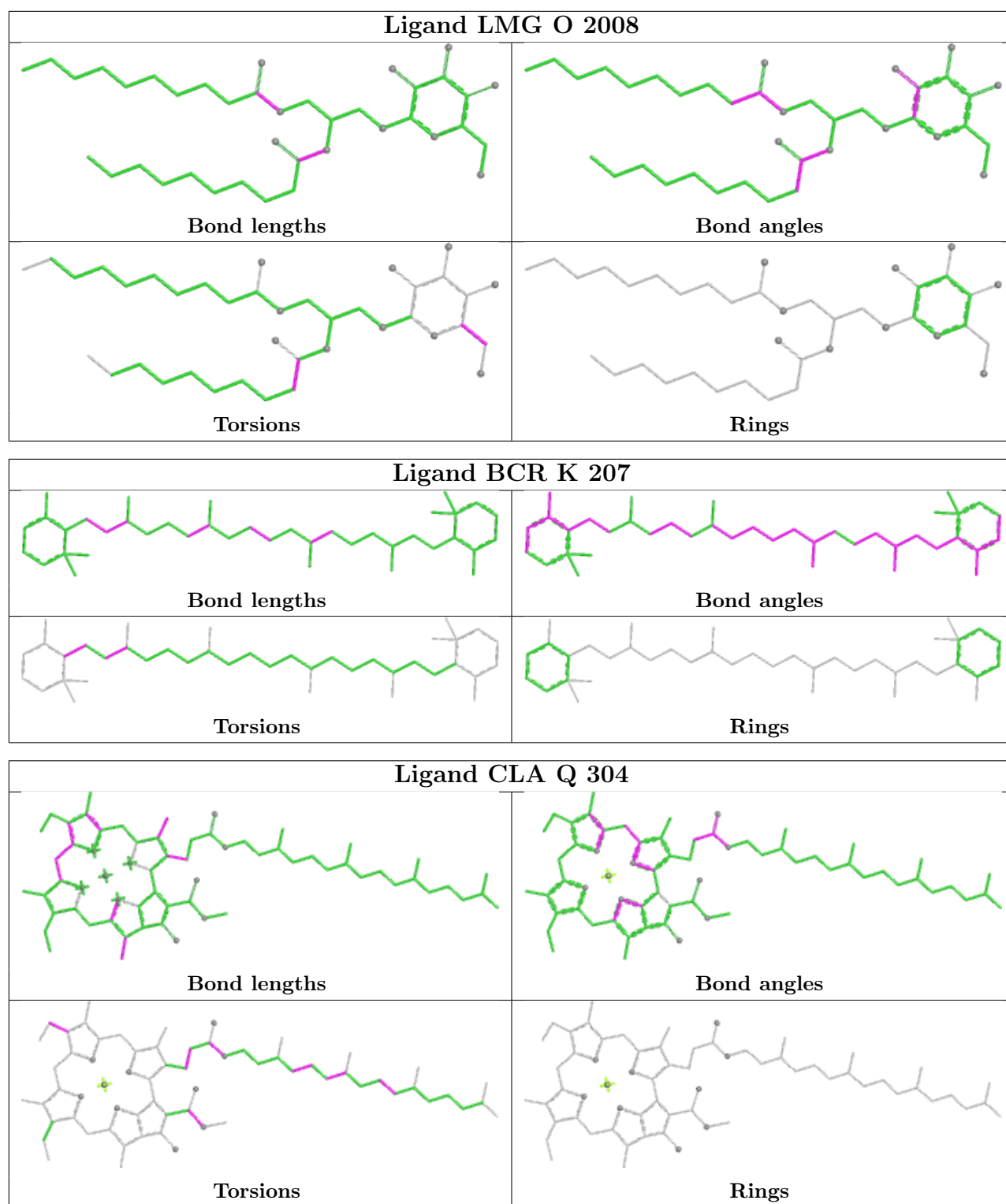
Torsions



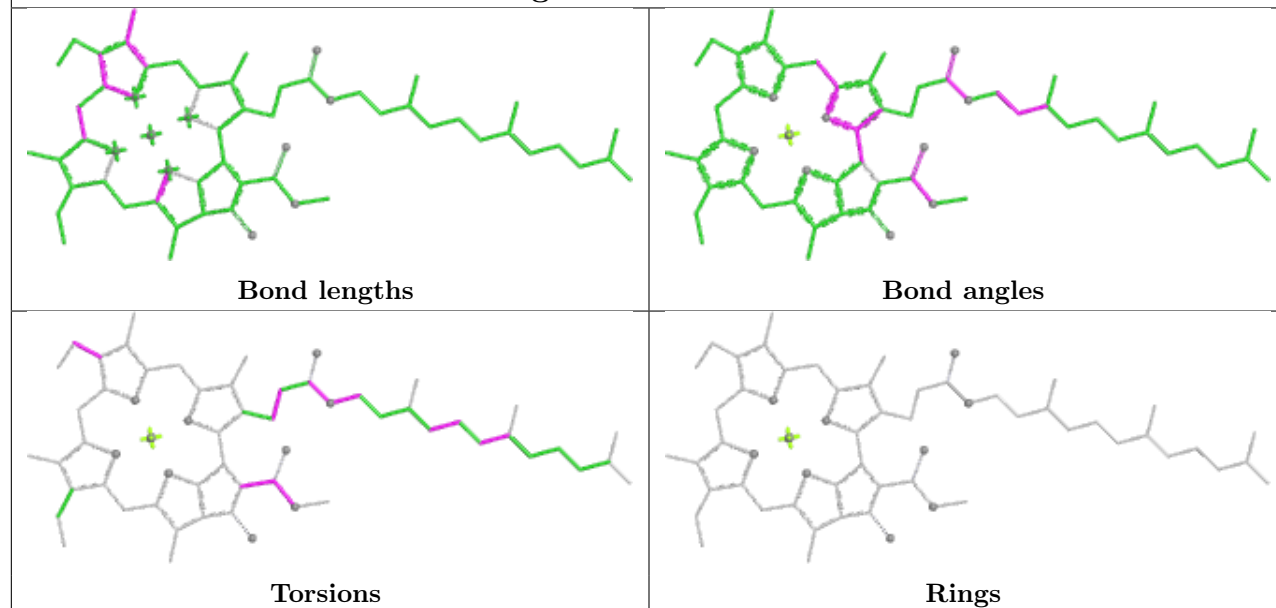
Rings



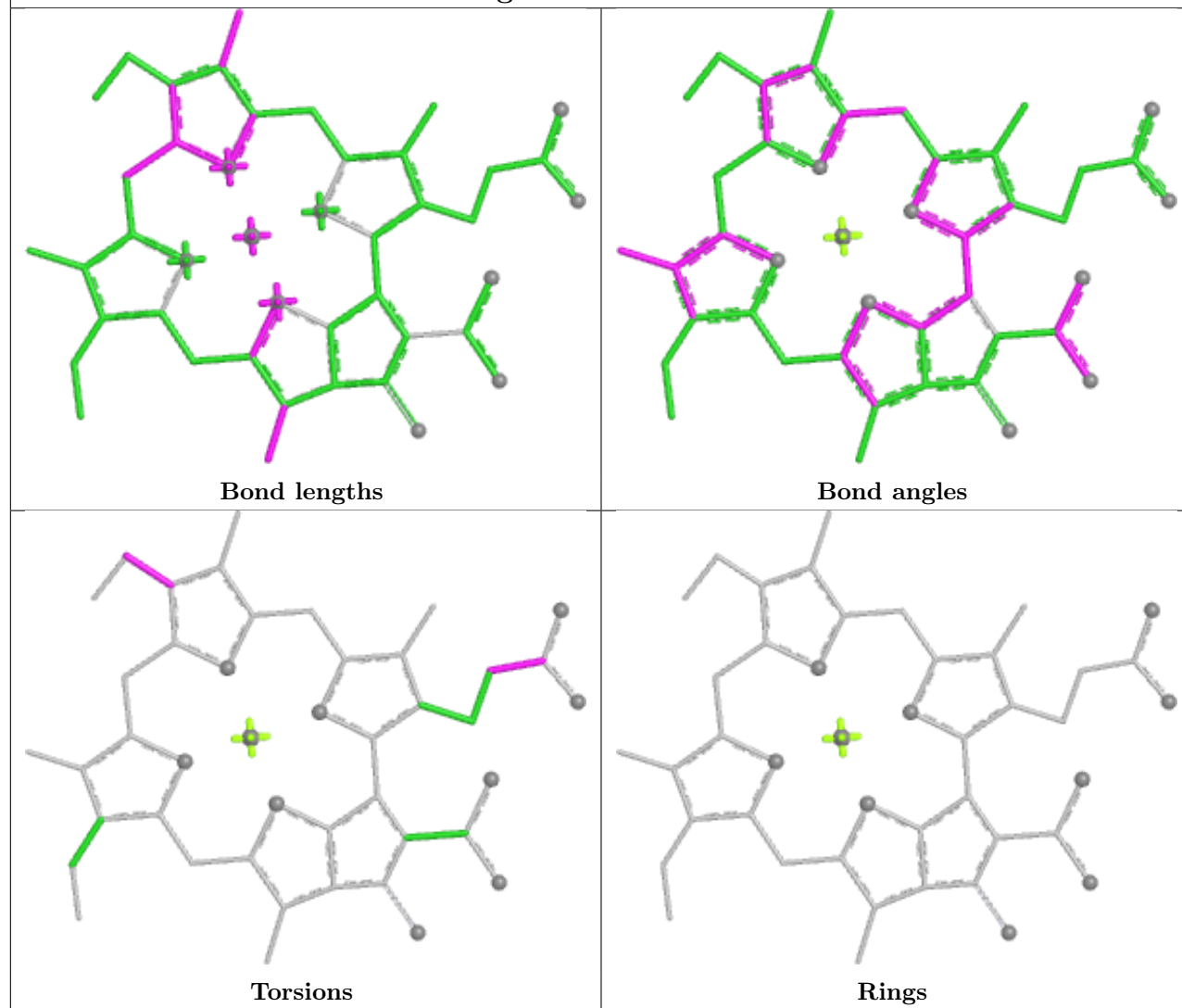




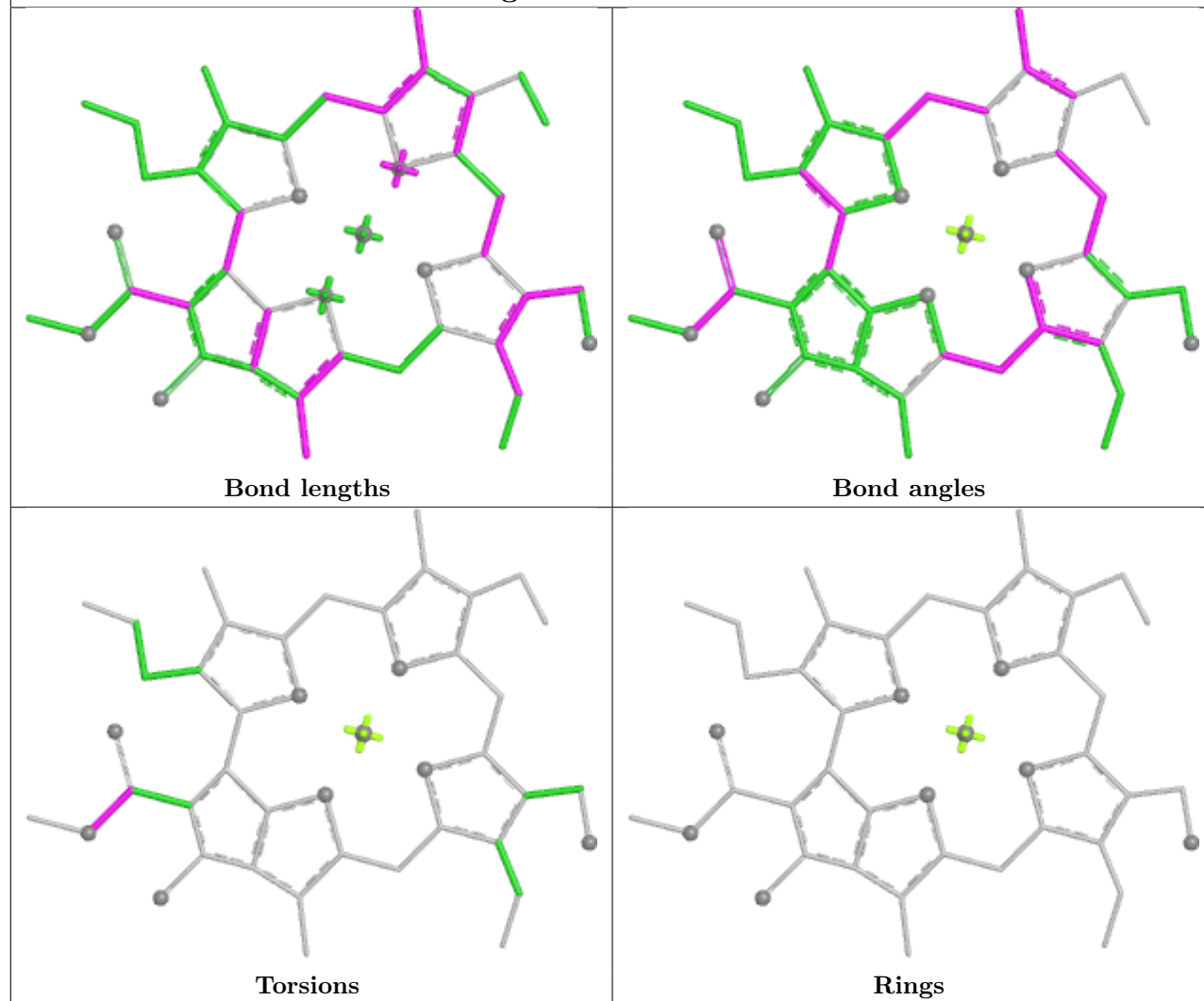
Ligand CLA V 311



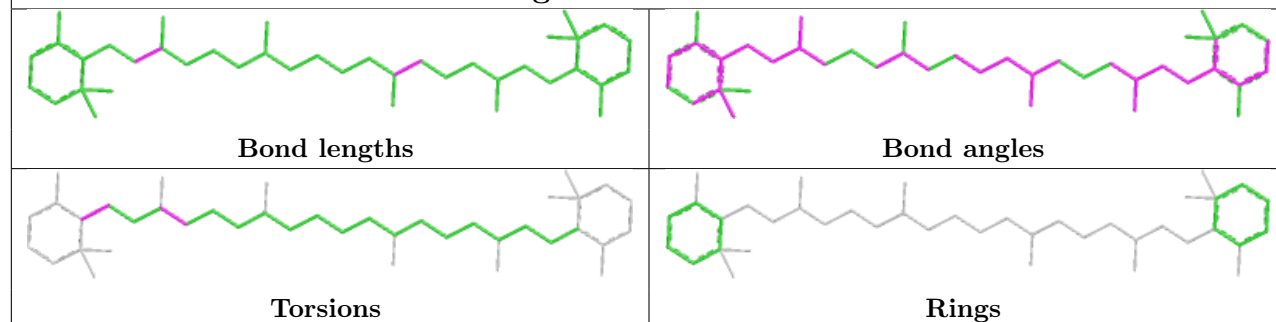
Ligand CLA 6 603



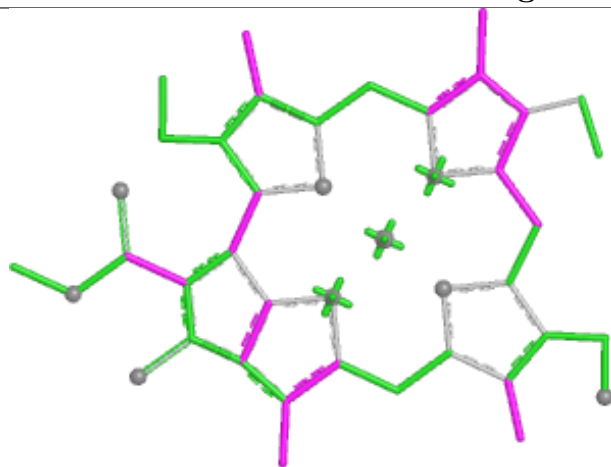
Ligand CHL R 311



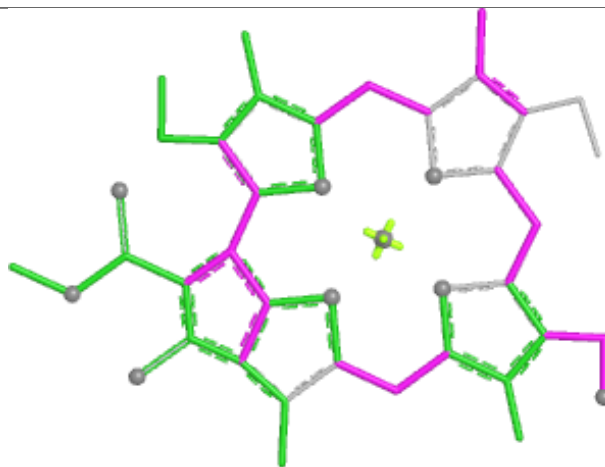
Ligand BCR L 307



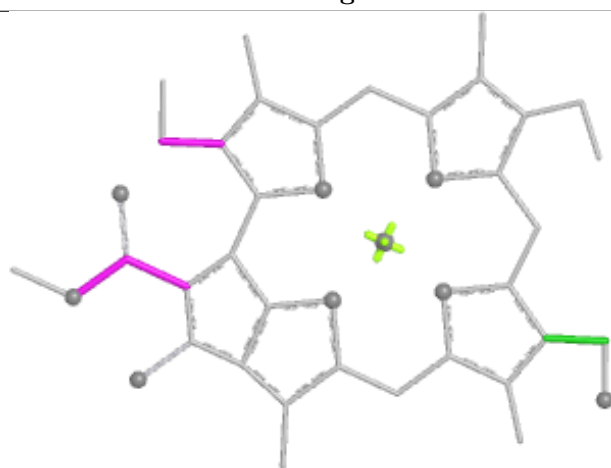
Ligand CHL 2 605



Bond lengths



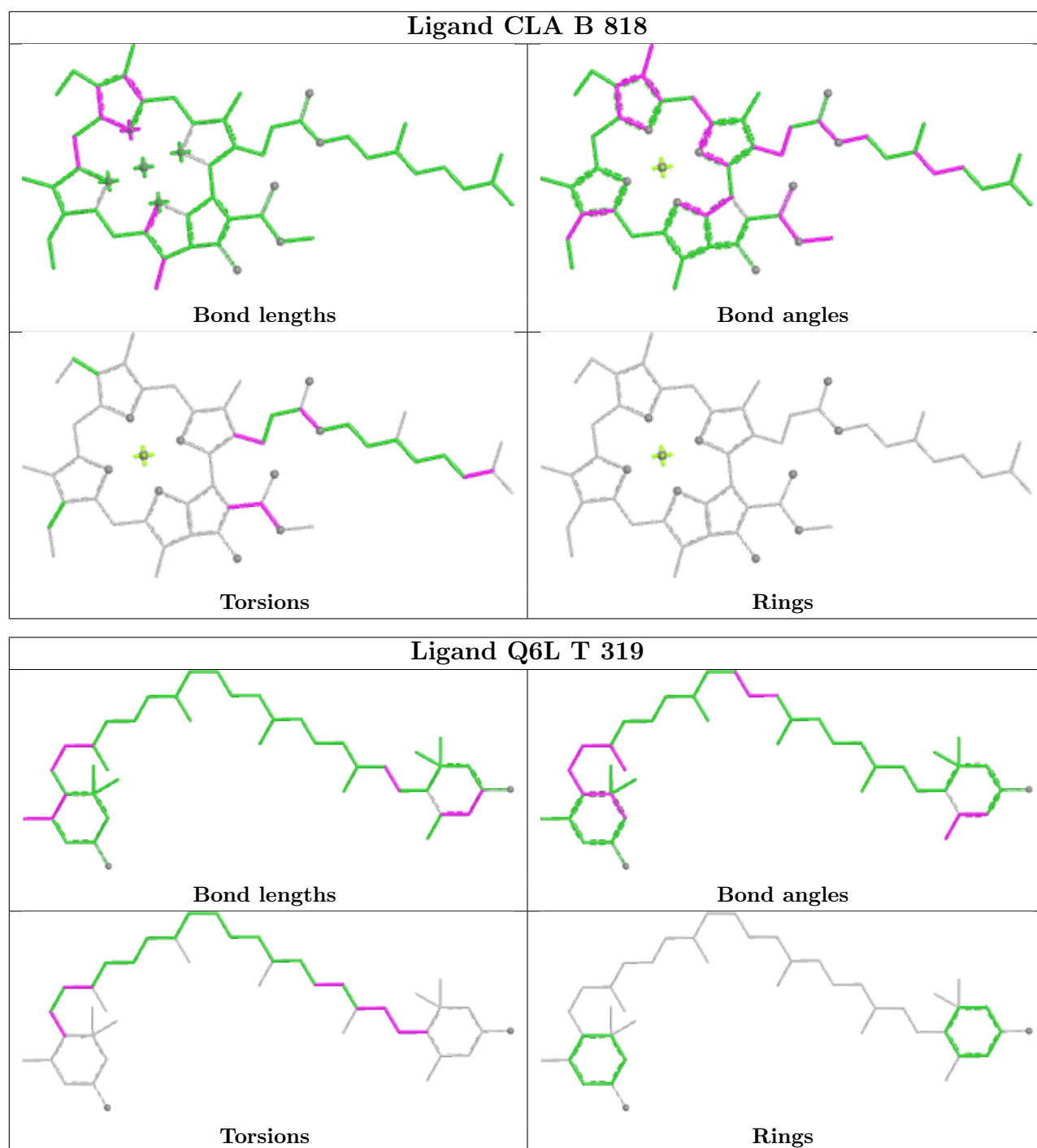
Bond angles



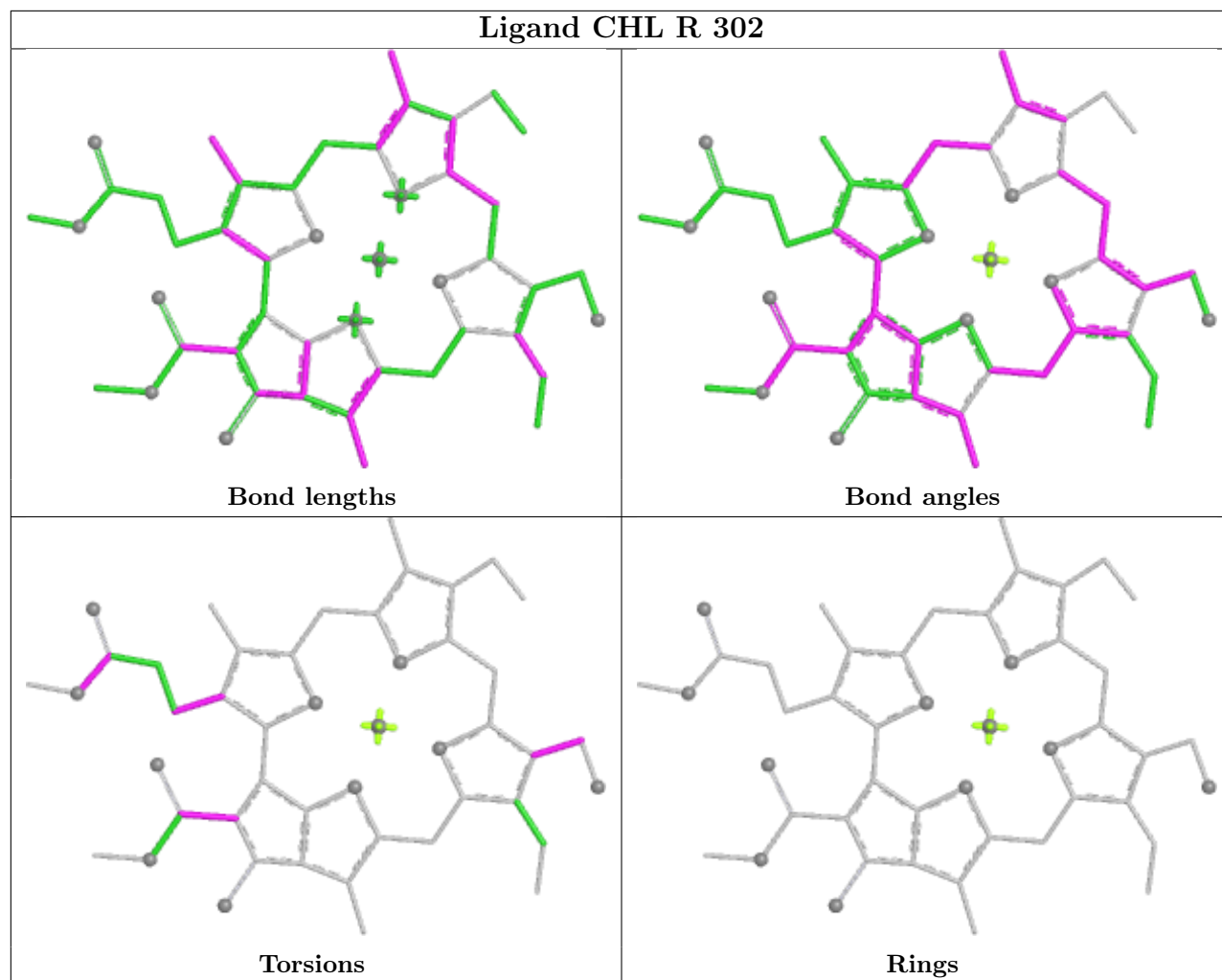
Torsions



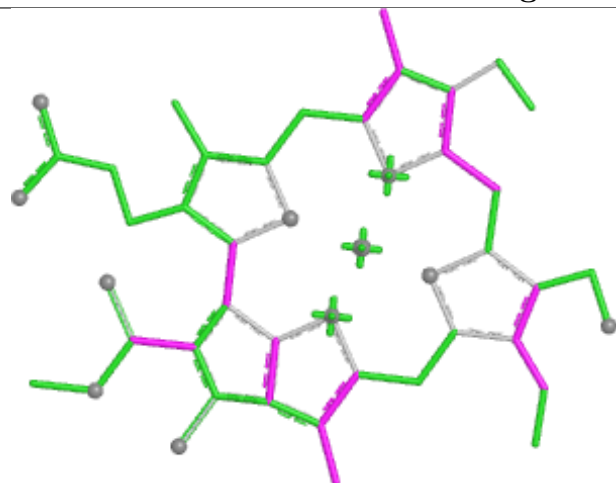
Rings



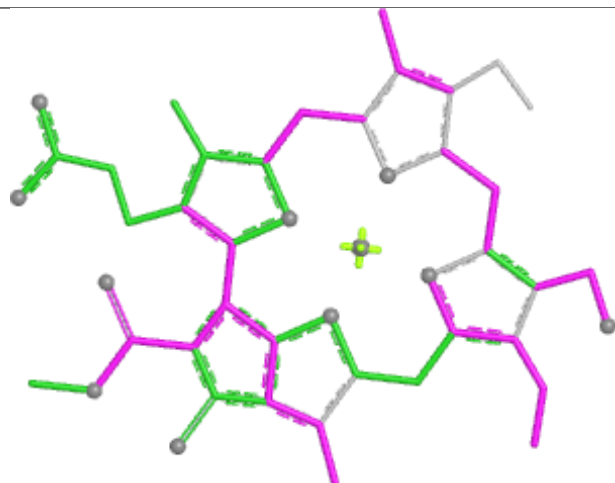
Ligand CHL R 302



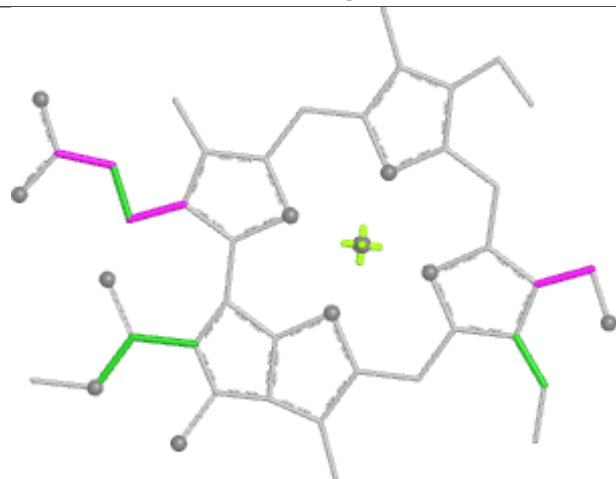
Ligand CHL 4 308



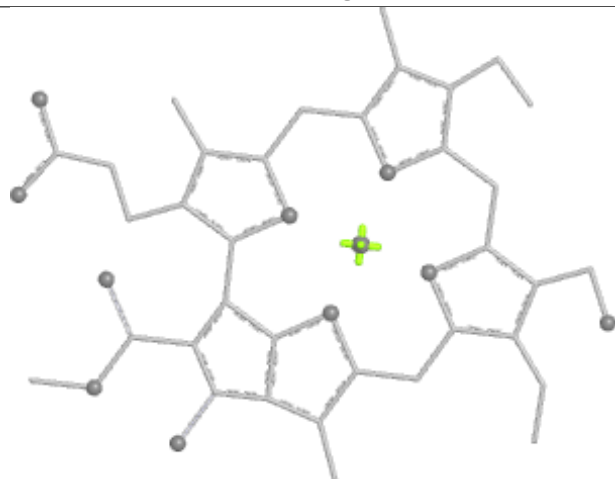
Bond lengths



Bond angles

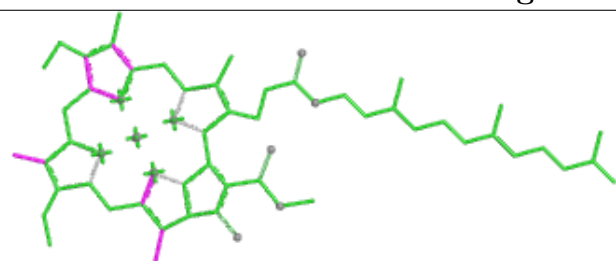


Torsions

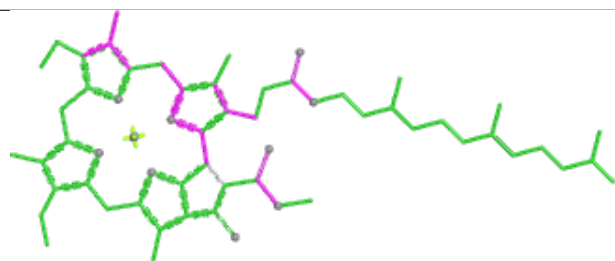


Rings

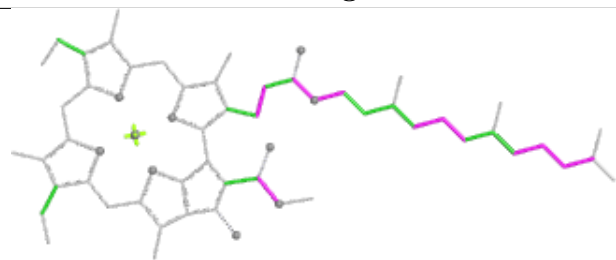
Ligand CLA T 311



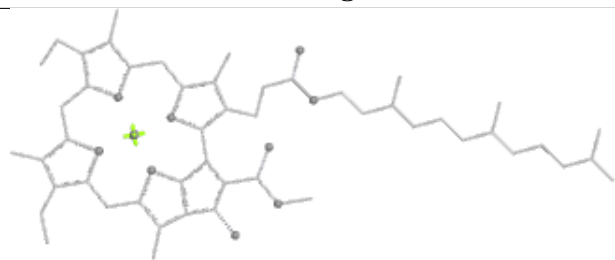
Bond lengths



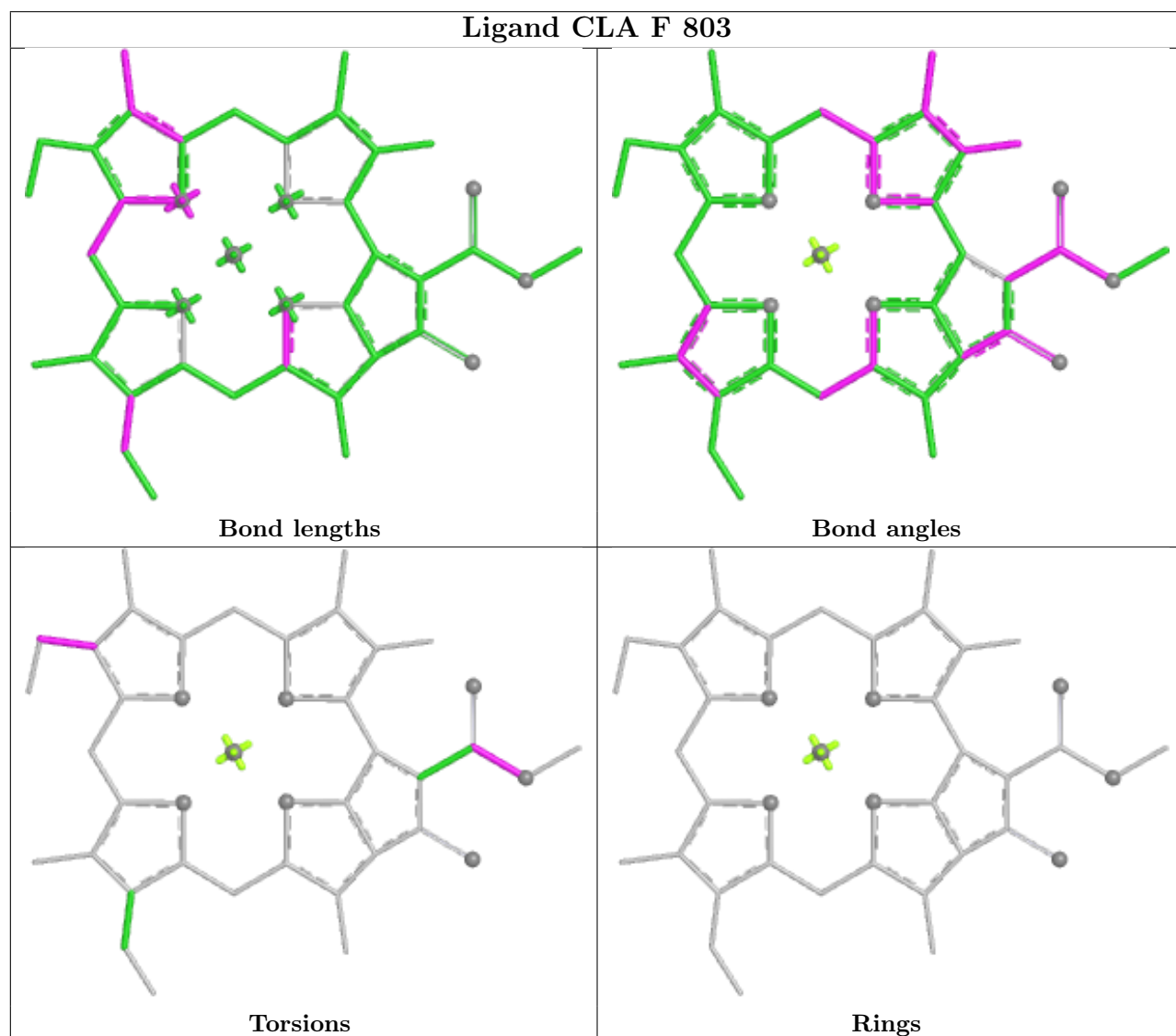
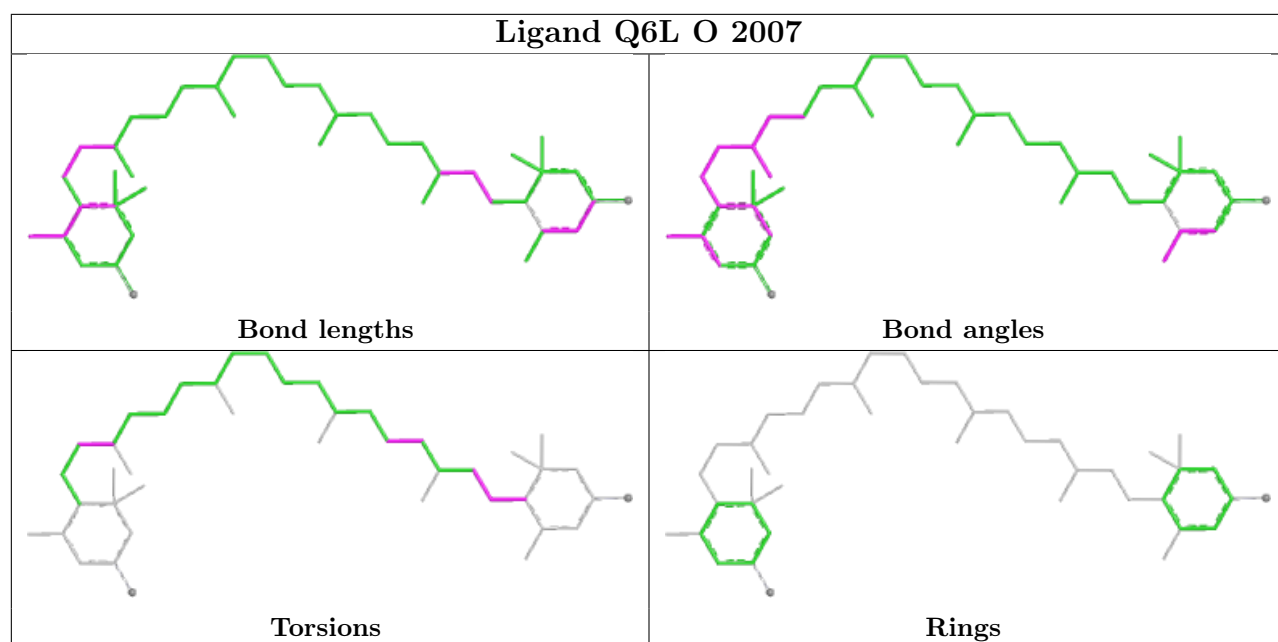
Bond angles

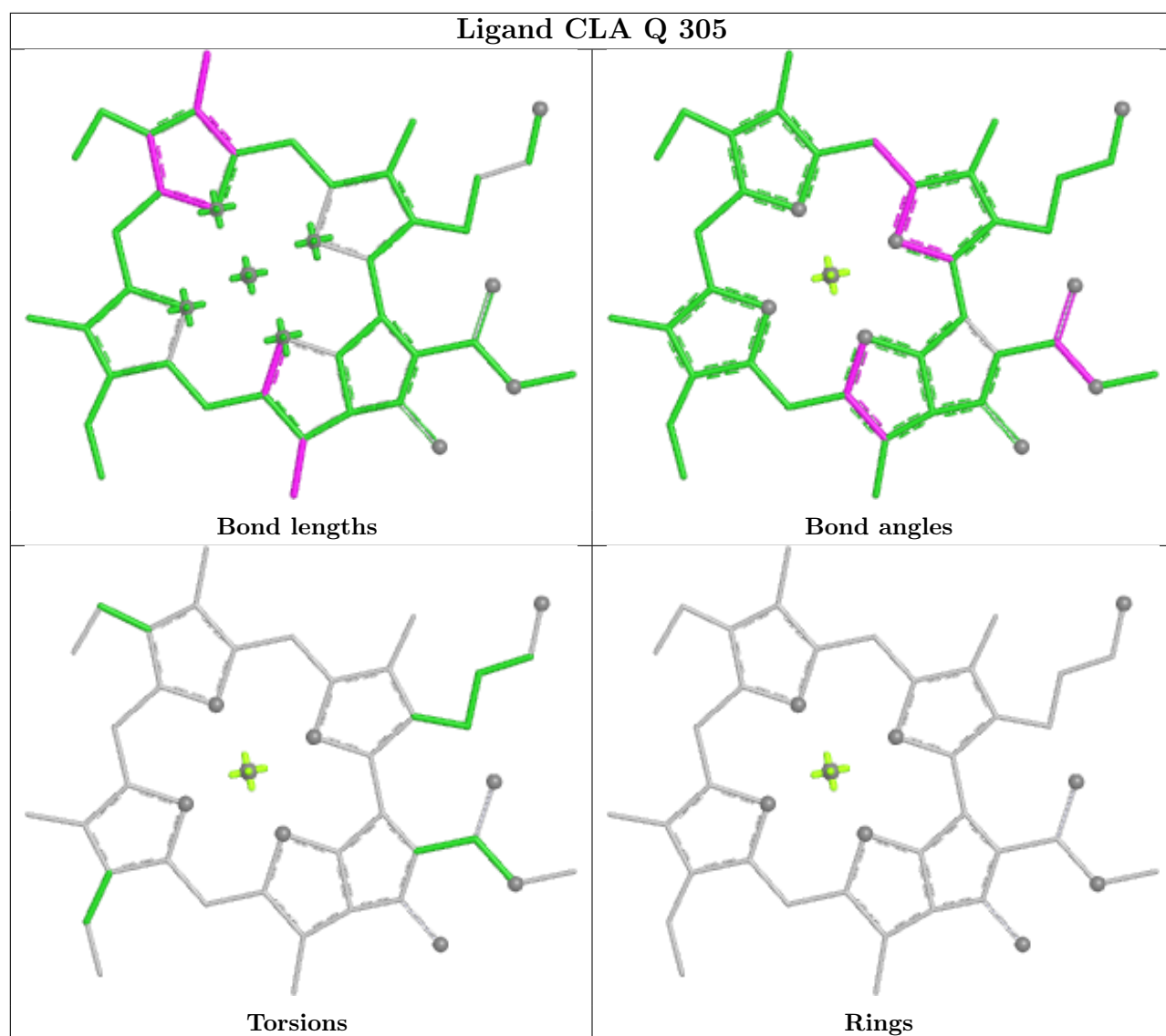


Torsions

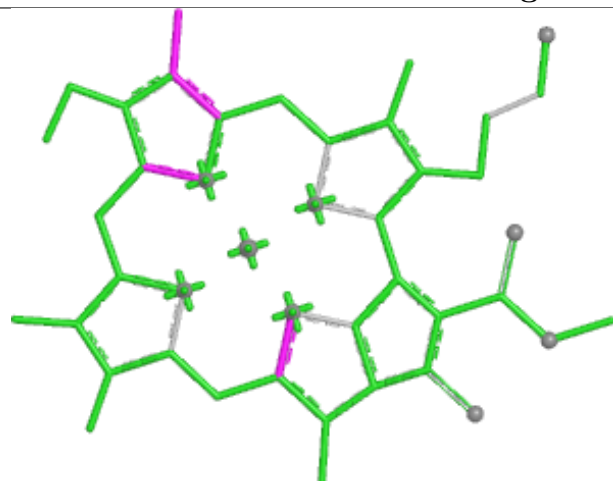


Rings

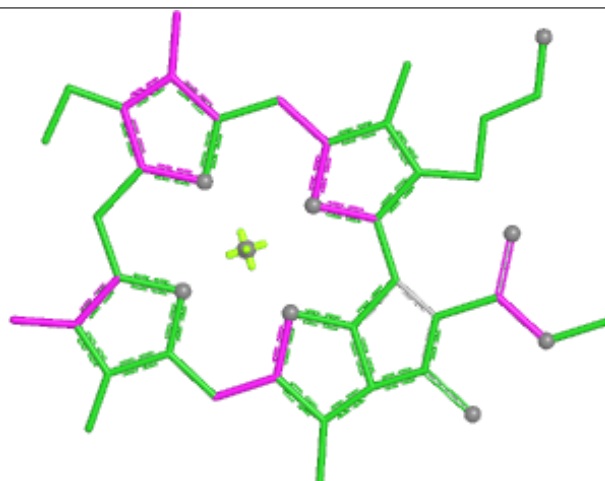




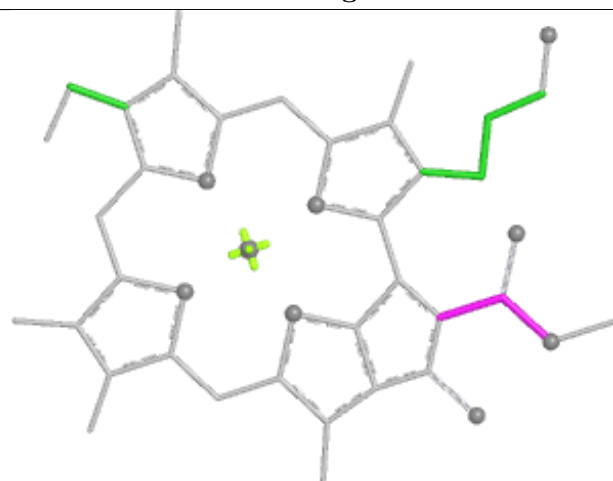
Ligand CLA 2 604



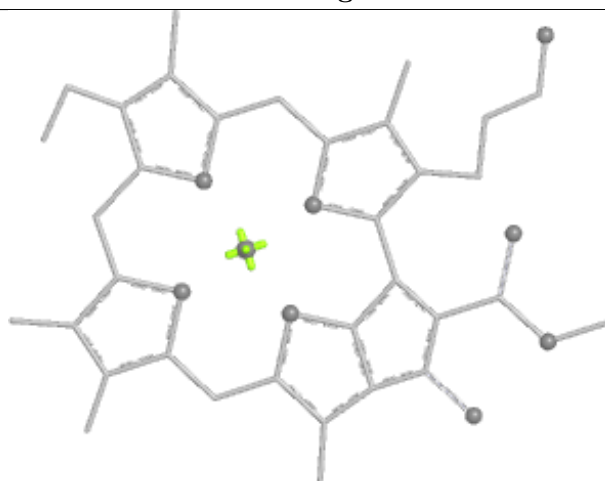
Bond lengths



Bond angles

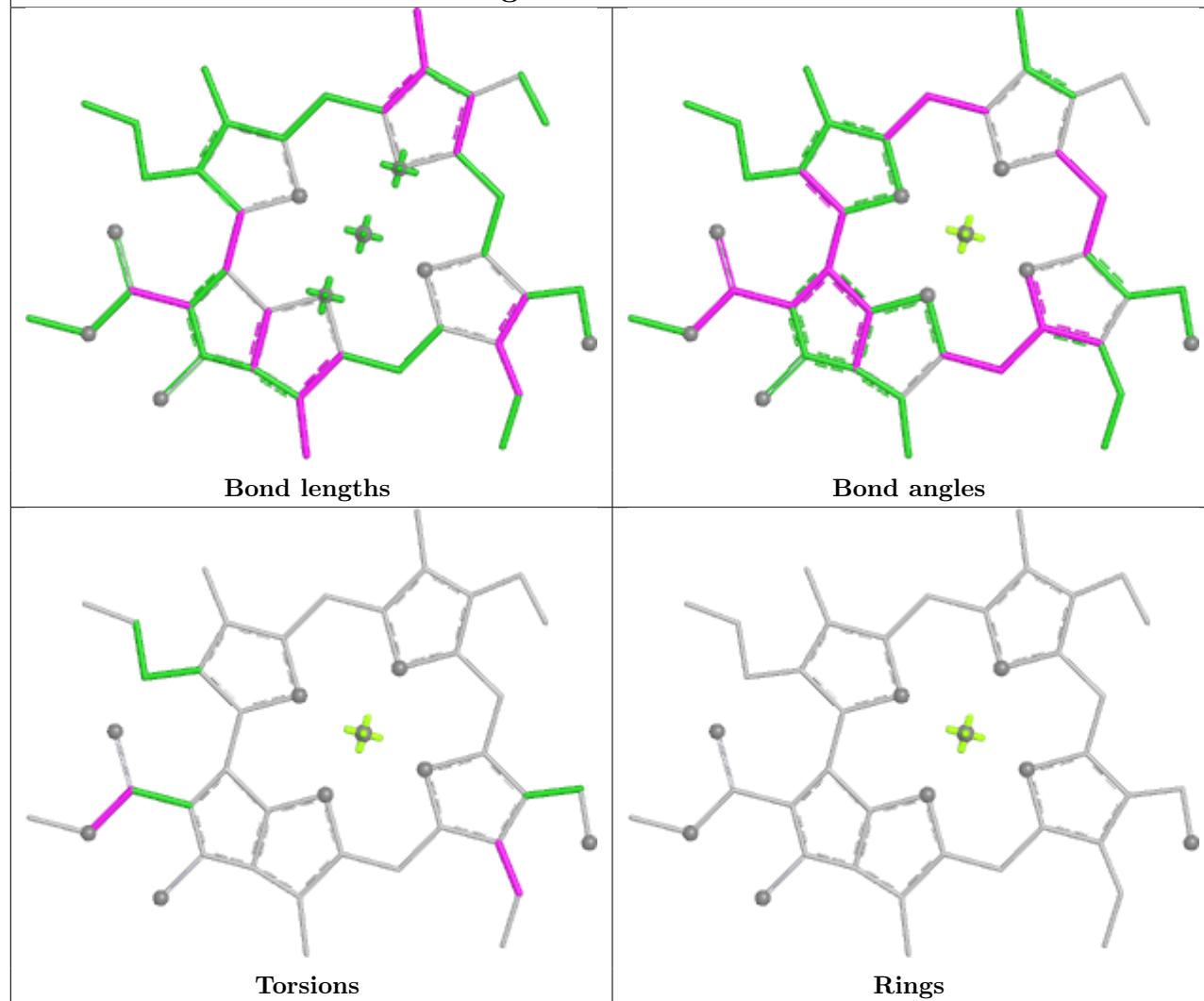


Torsions

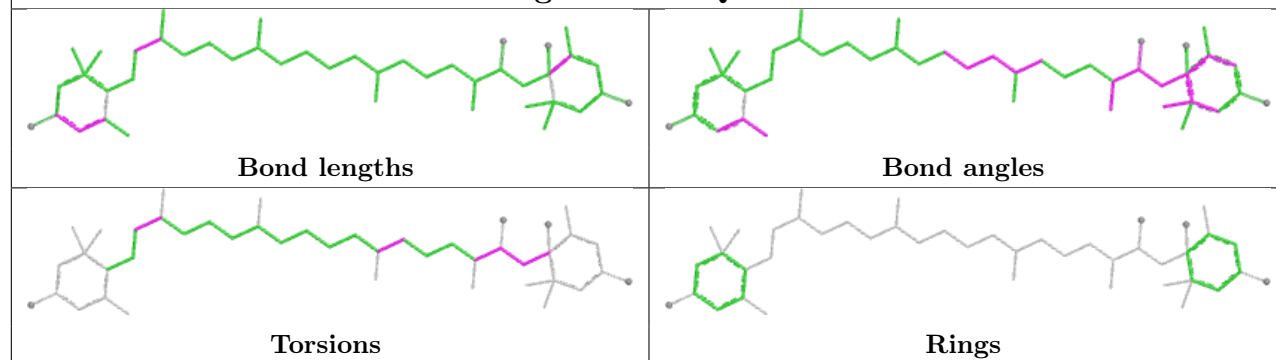


Rings

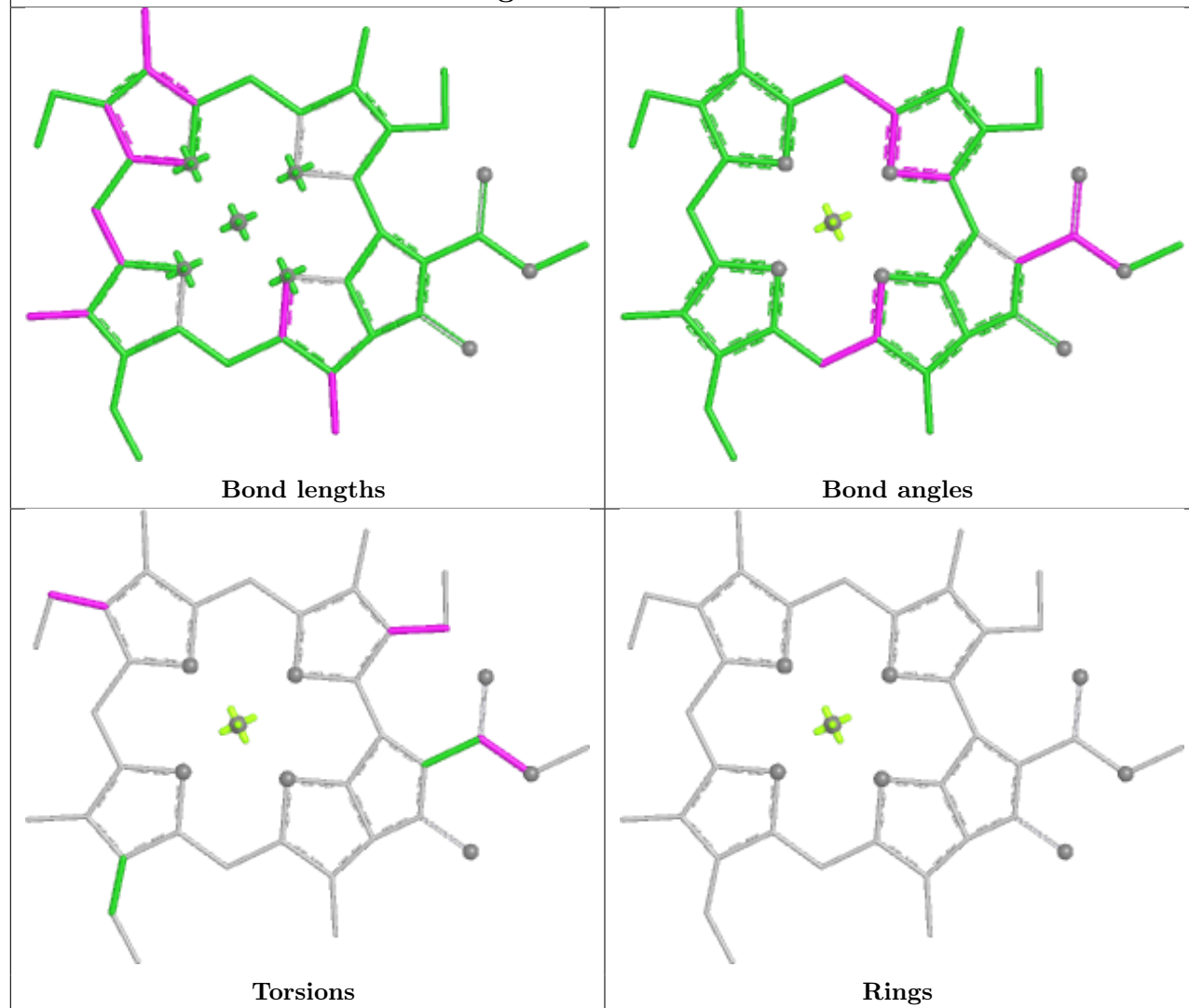
Ligand CHL V 307



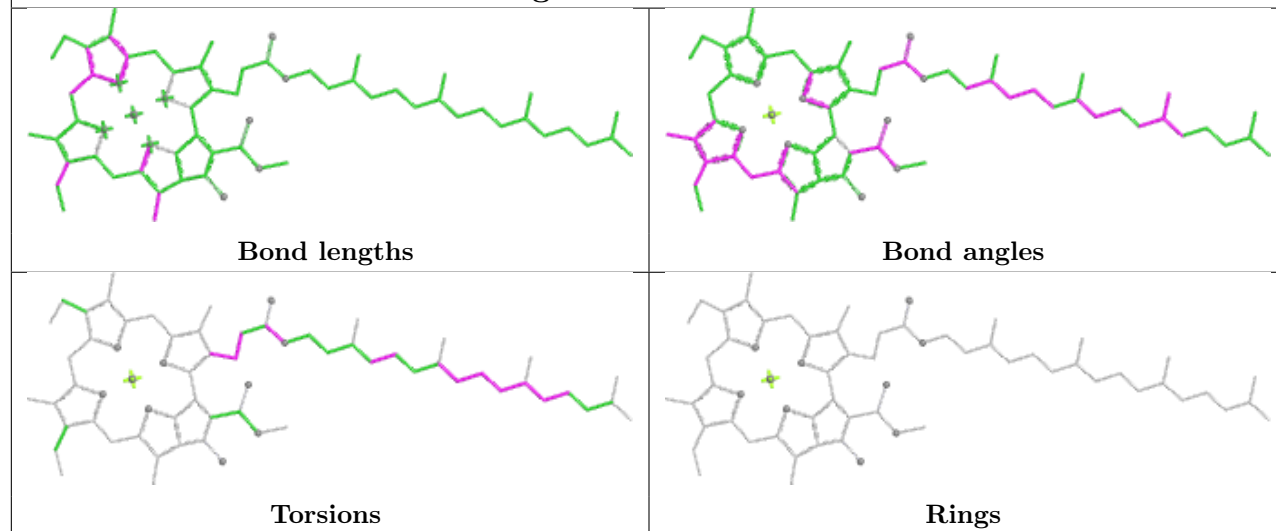
Ligand IWJ Q 320



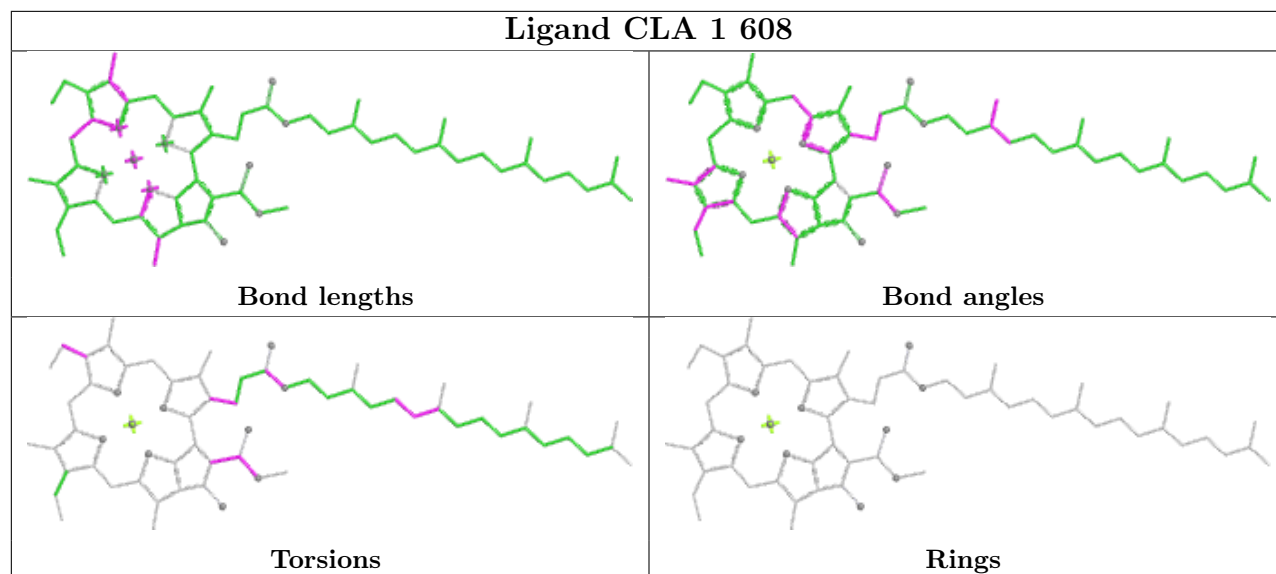
Ligand CLA L 304



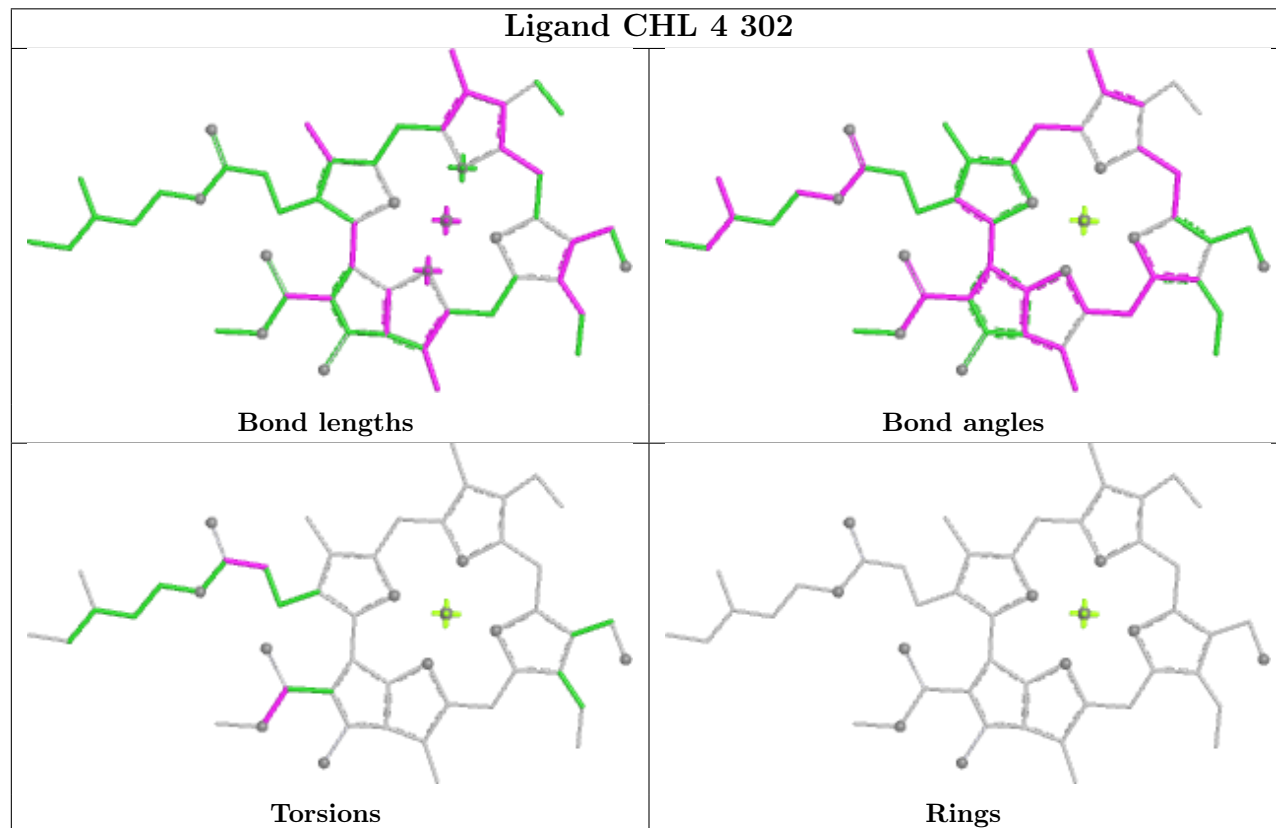
Ligand CLA B 813

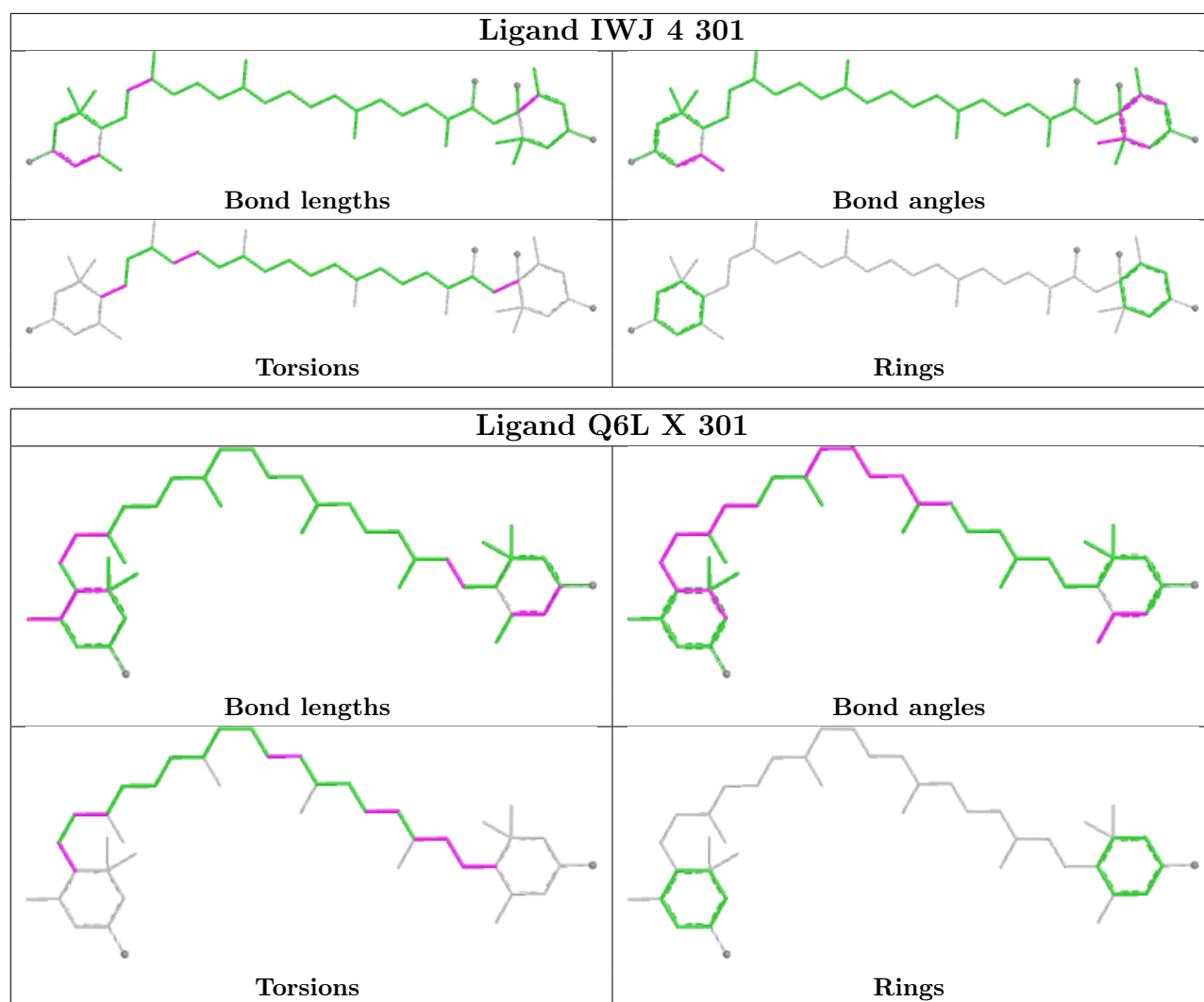


Ligand CLA 1 608

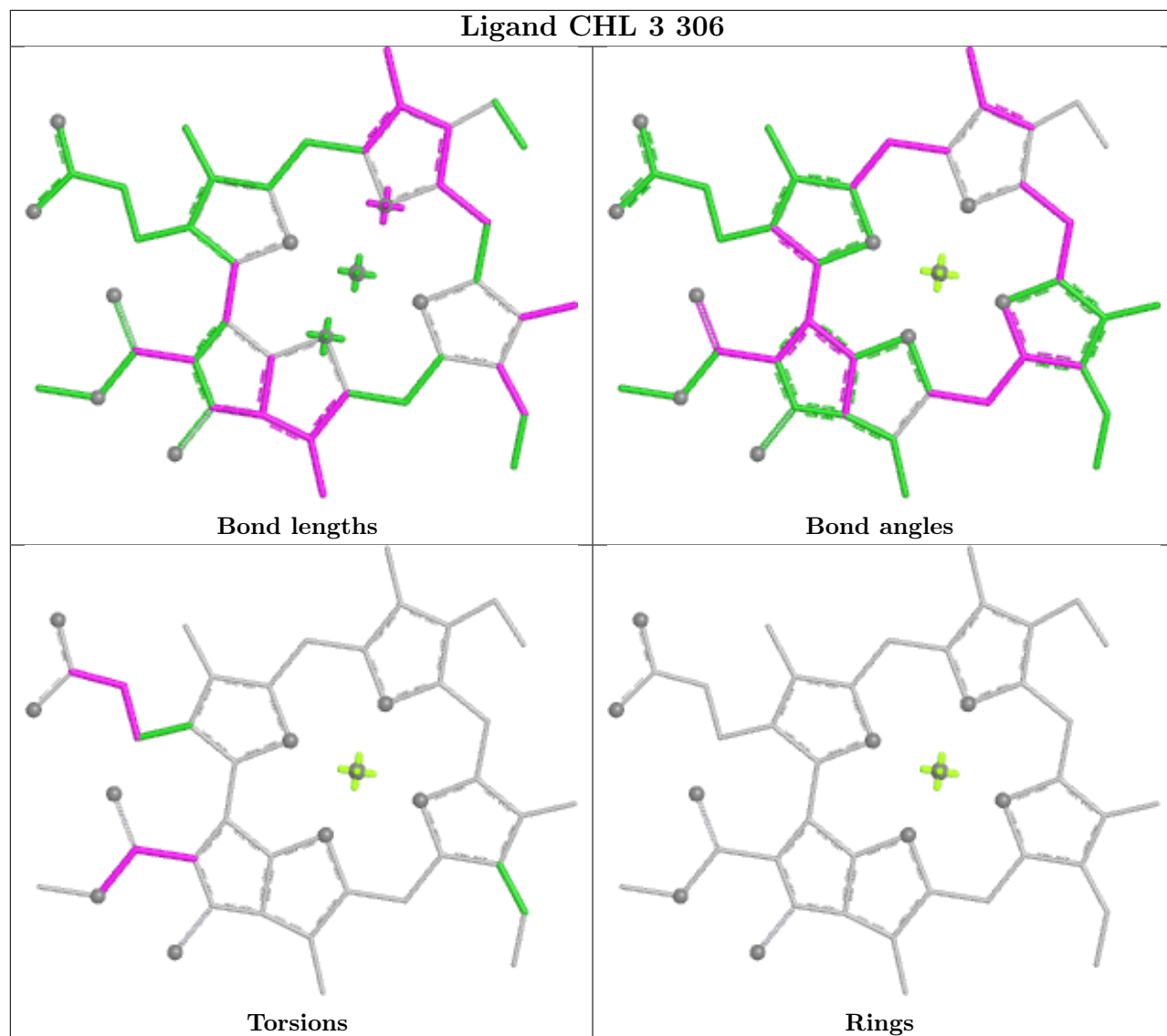


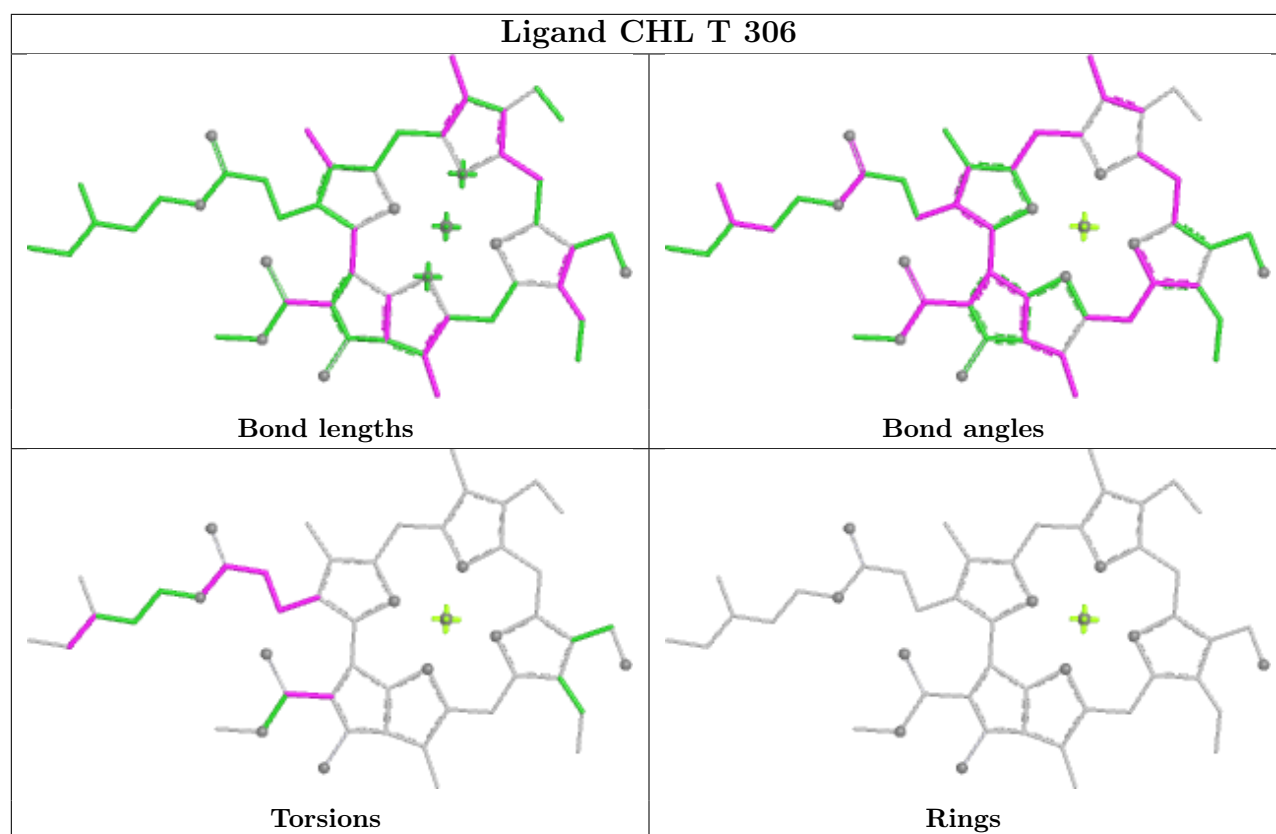
Ligand CHL 4 302



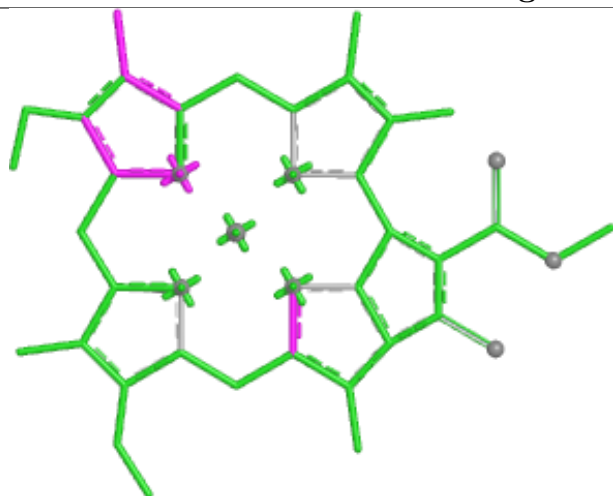


Ligand CHL 3 306

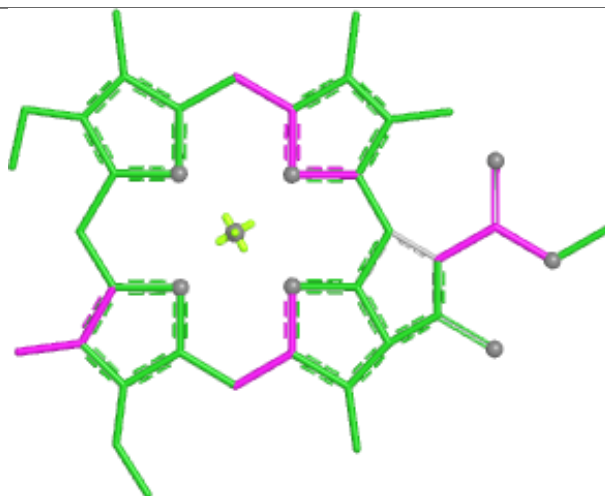




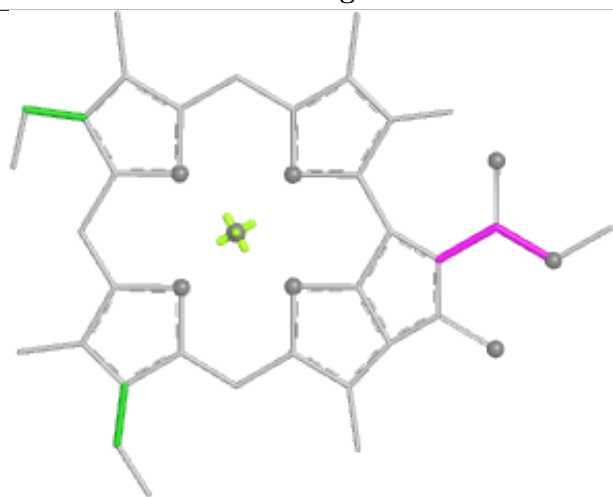
Ligand CLA 4 314



Bond lengths



Bond angles

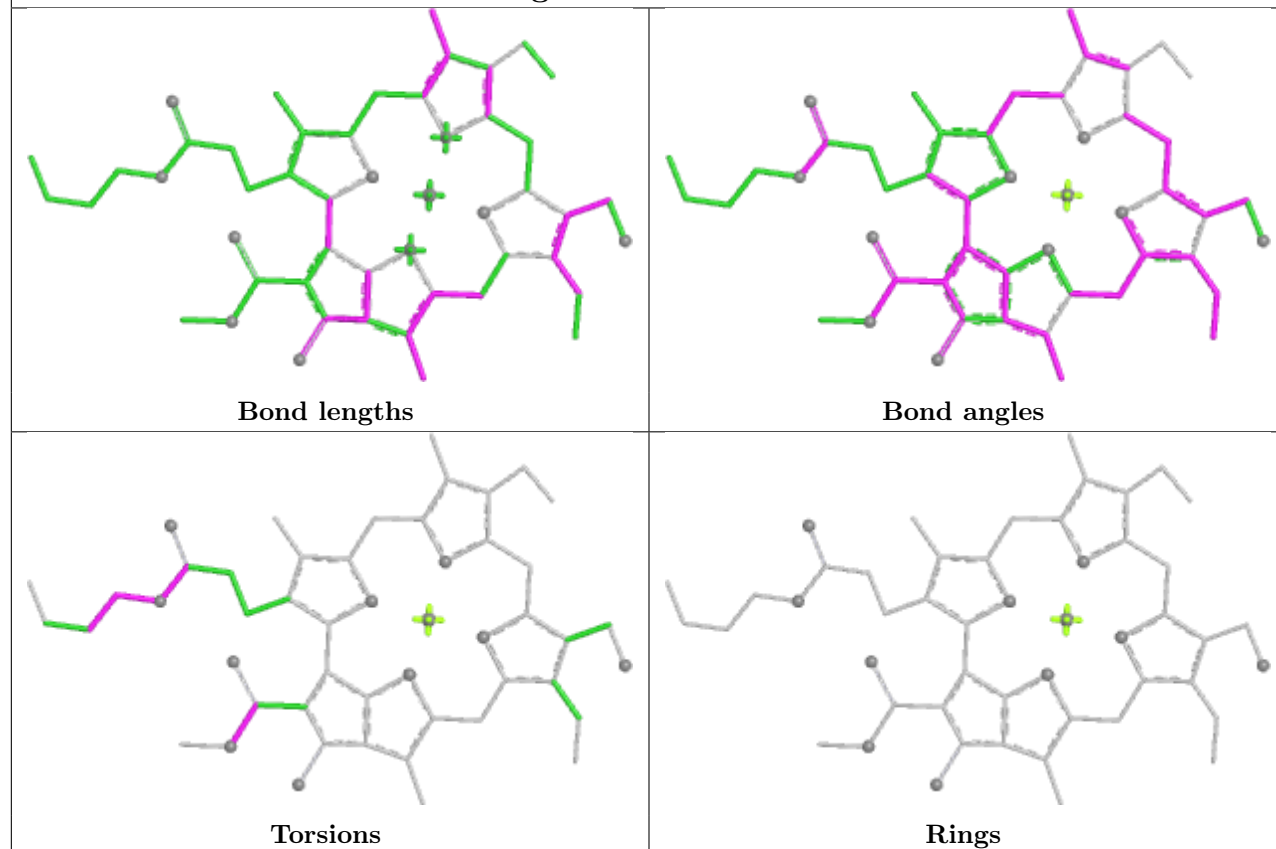


Torsions

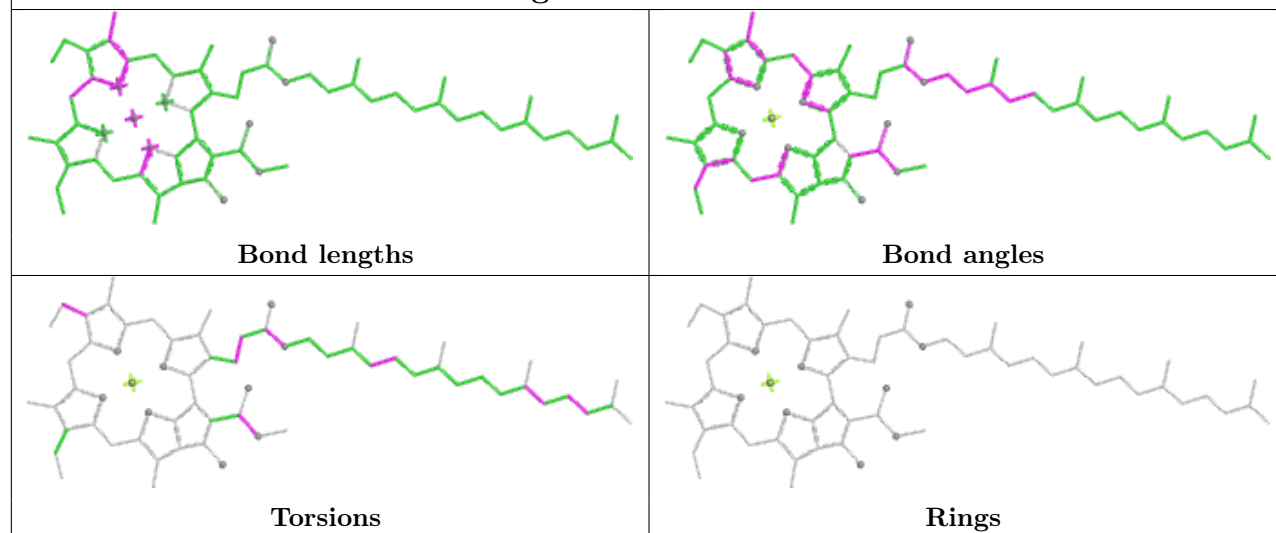


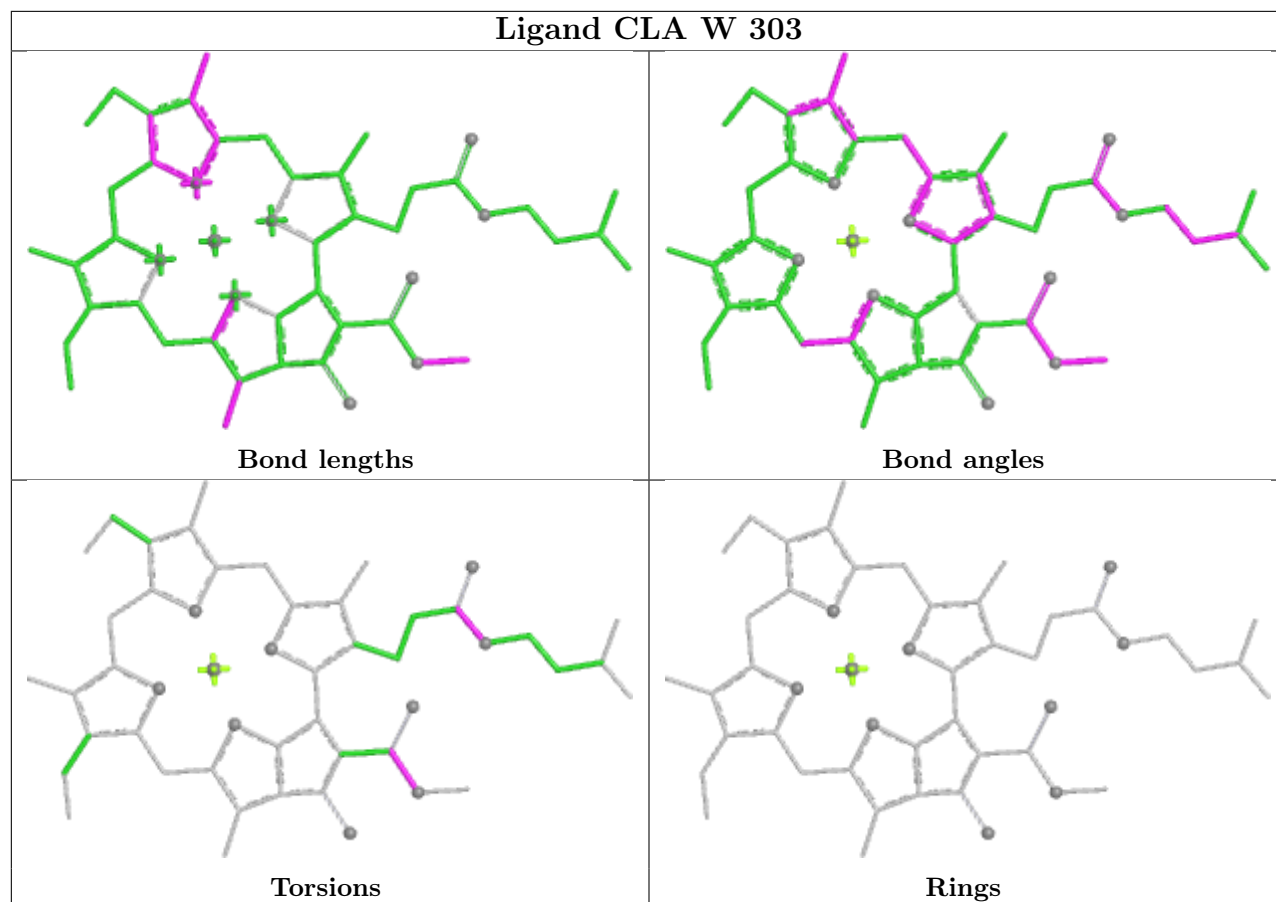
Rings

Ligand CHL R 309

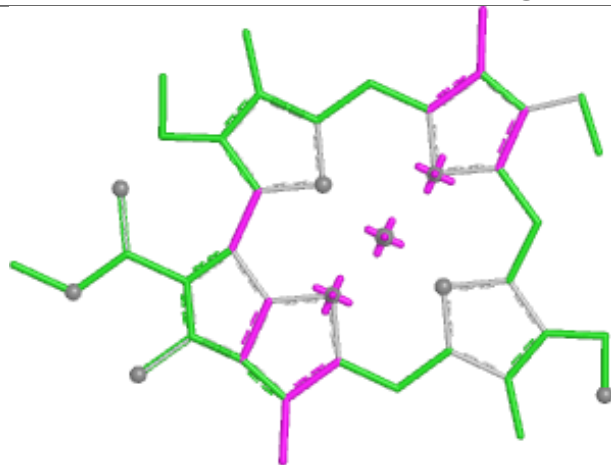


Ligand CLA A 823

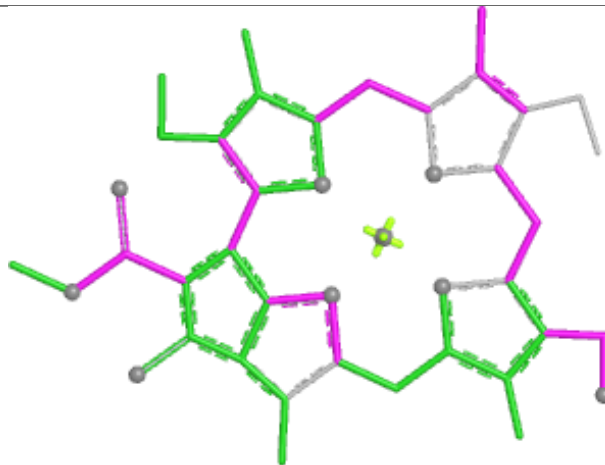




Ligand CHL 6 605



Bond lengths



Bond angles

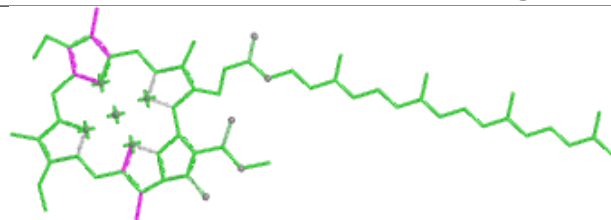


Torsions

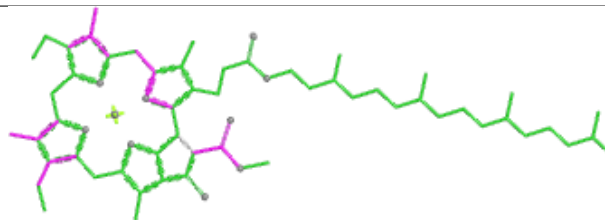


Rings

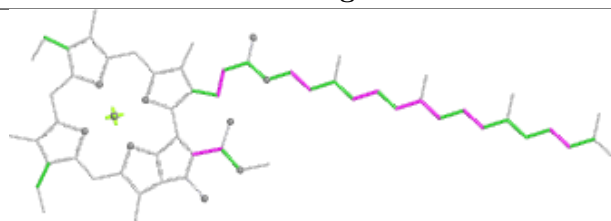
Ligand CLA B 814



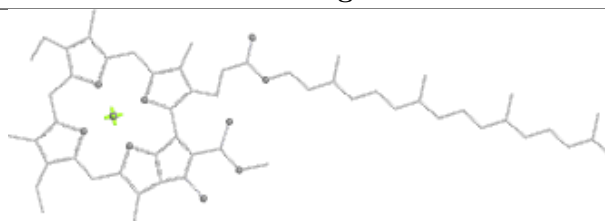
Bond lengths



Bond angles

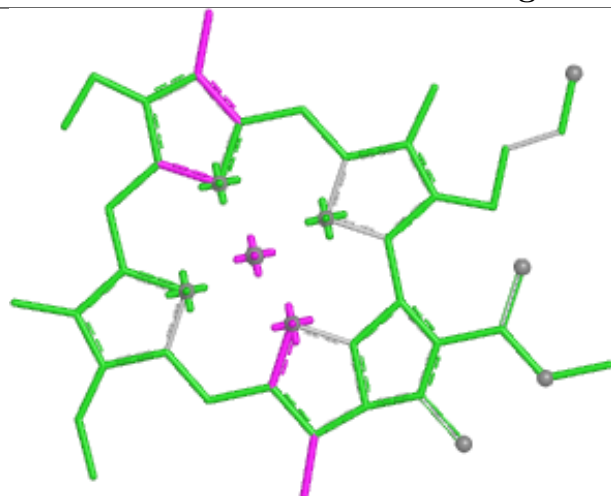


Torsions

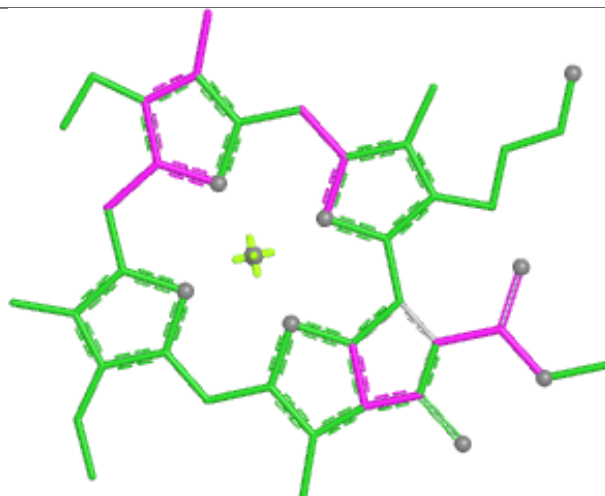


Rings

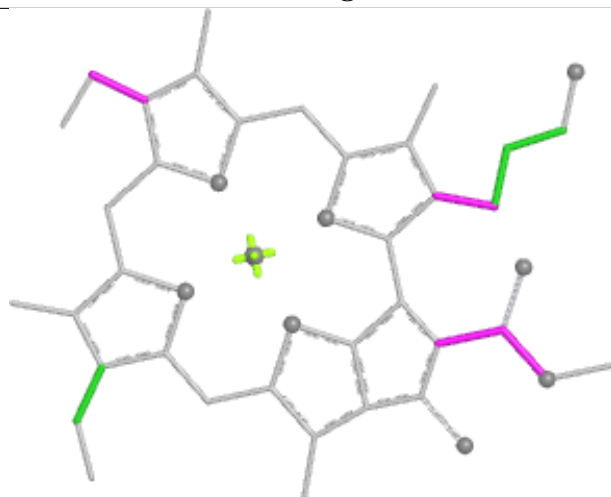
Ligand CLA 2 614



Bond lengths



Bond angles

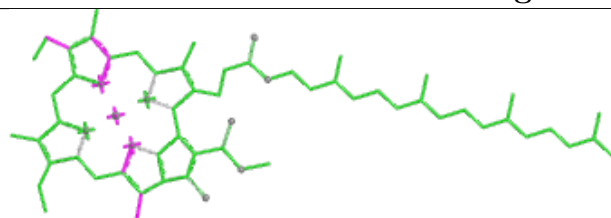


Torsions

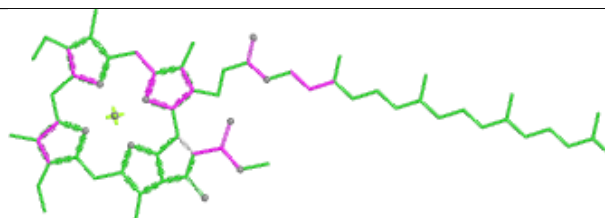


Rings

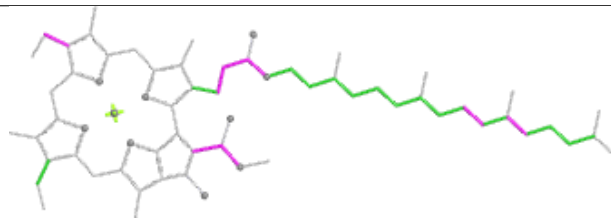
Ligand CLA B 812



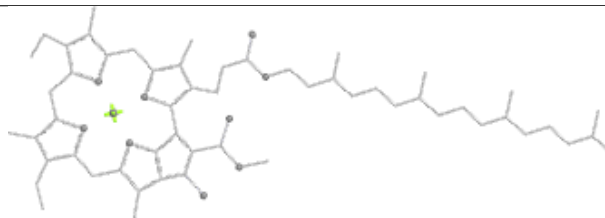
Bond lengths



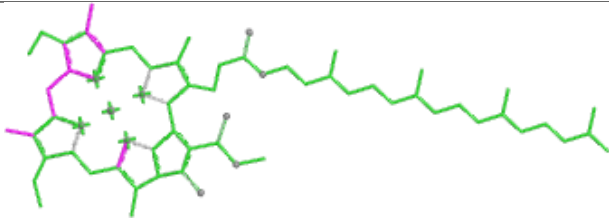
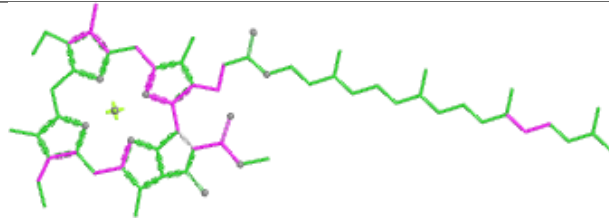
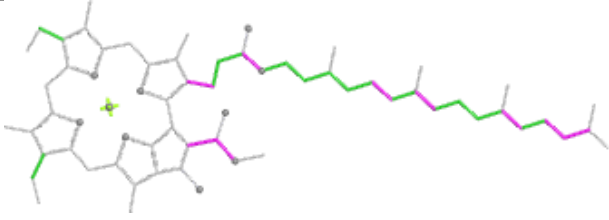
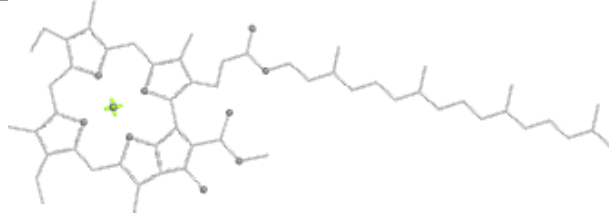
Bond angles

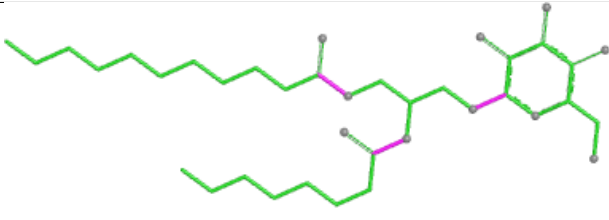
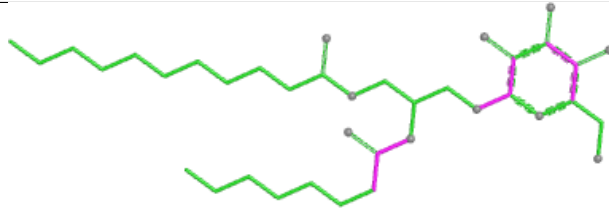
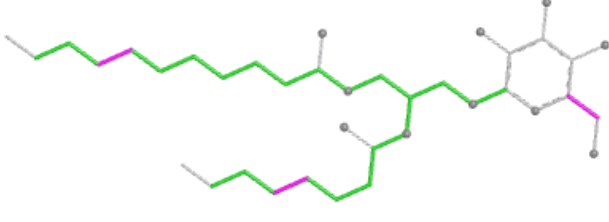
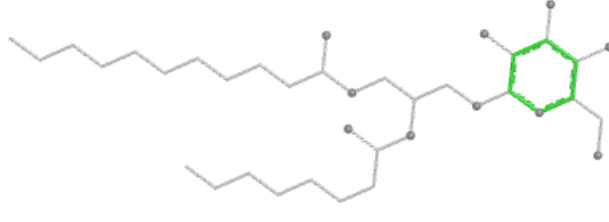


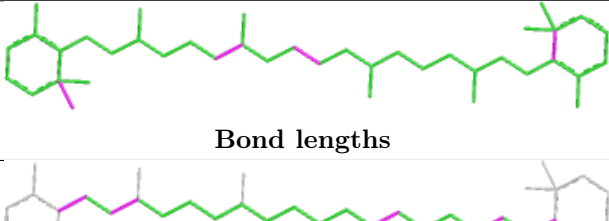
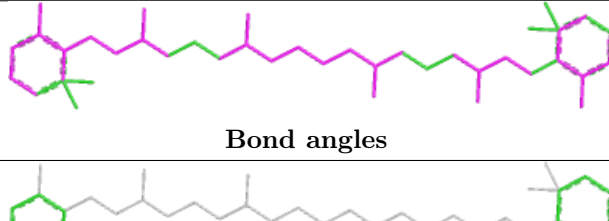
Torsions



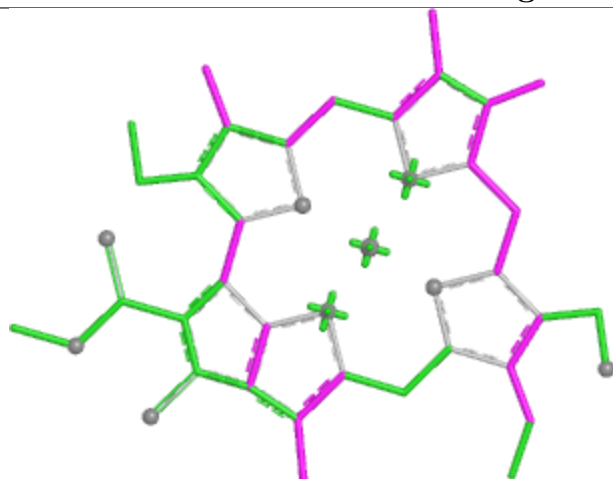
Rings

Ligand CLA A 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

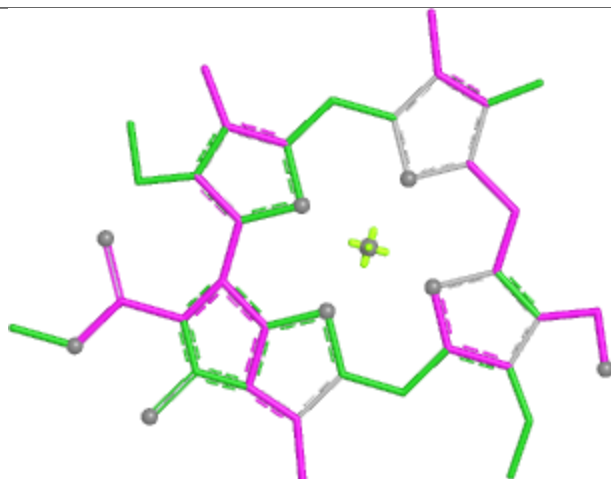
Ligand LMG B 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

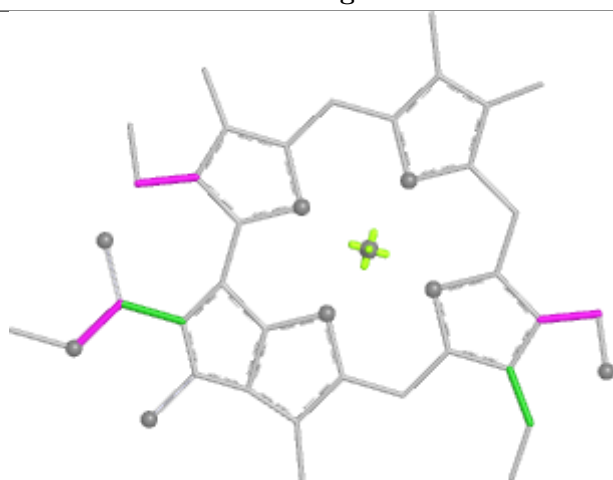
Ligand CHL 4 307



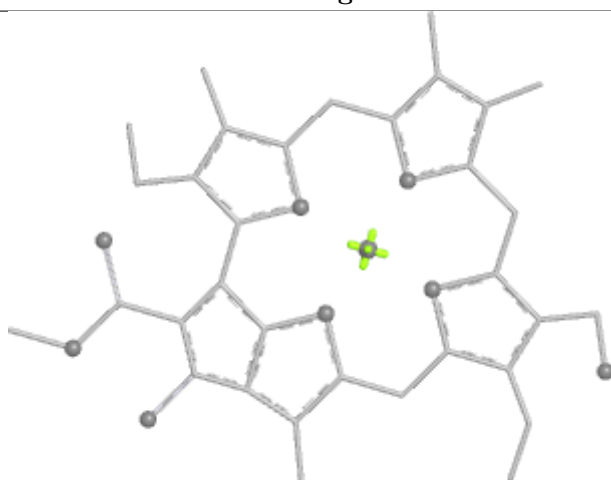
Bond lengths



Bond angles

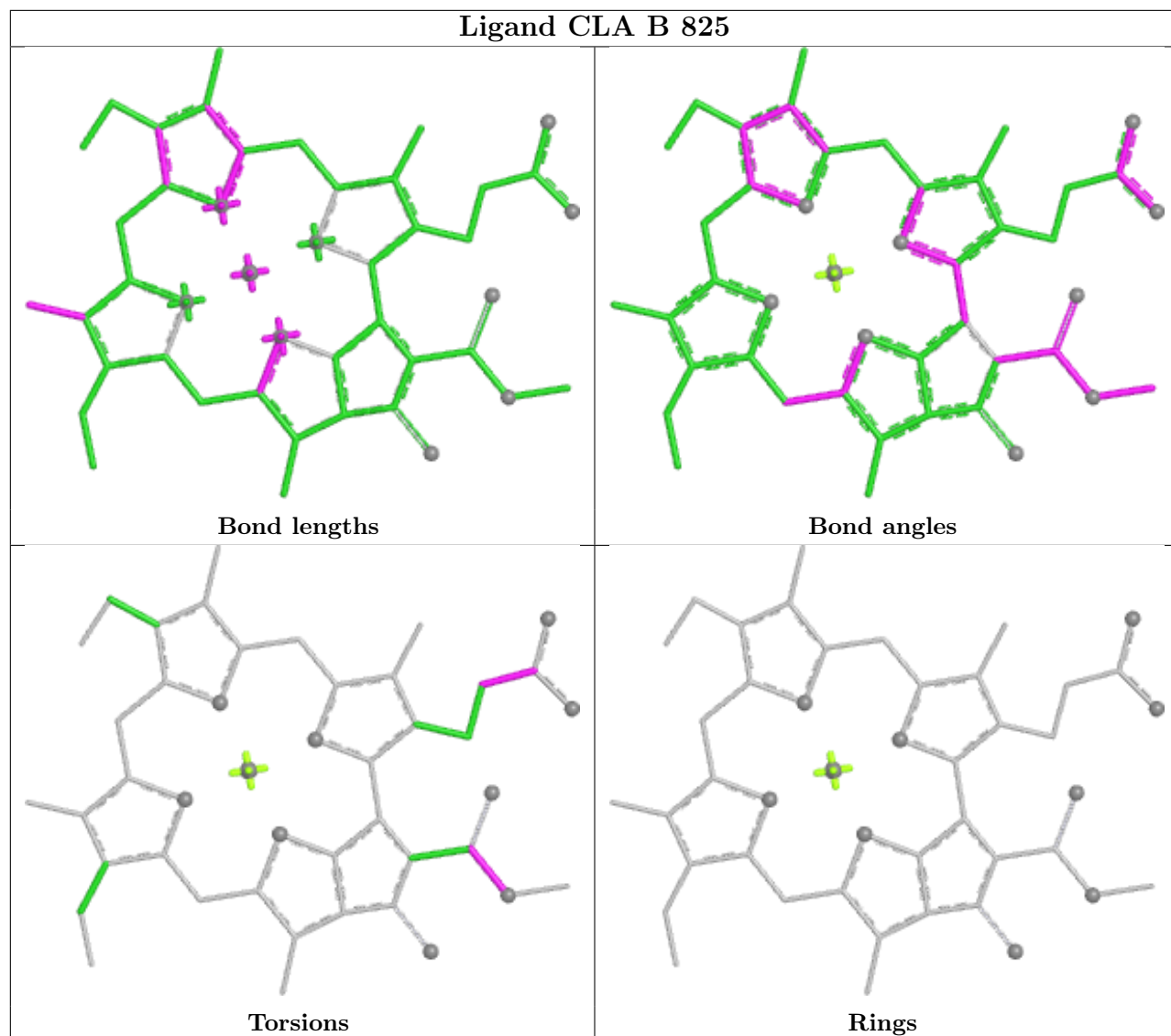


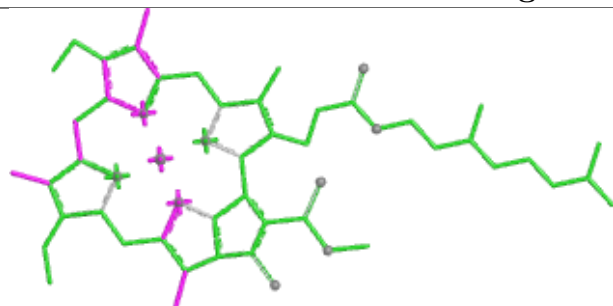
Torsions



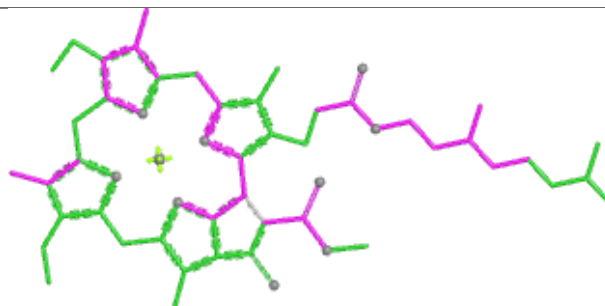
Rings

Ligand CLA B 825

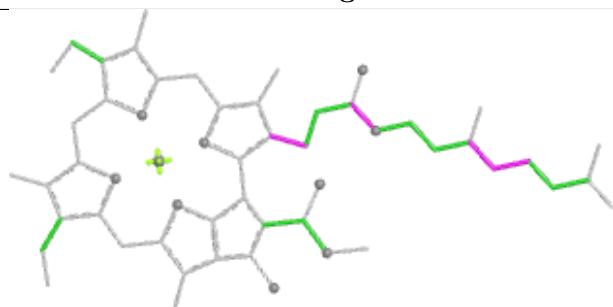


Ligand CLA 3 302

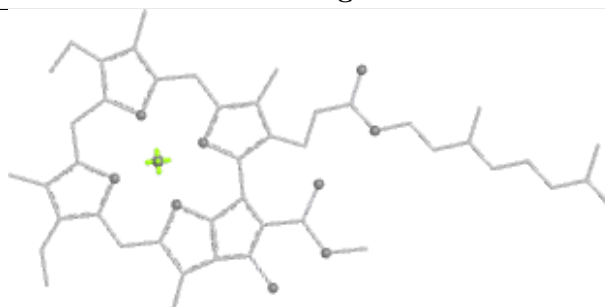
Bond lengths



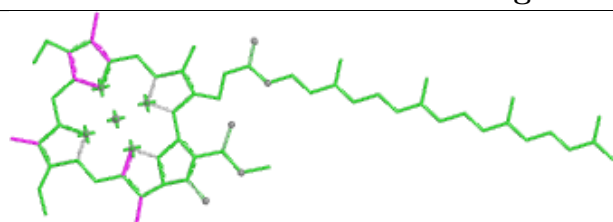
Bond angles



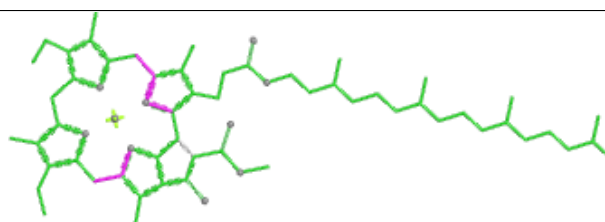
Torsions



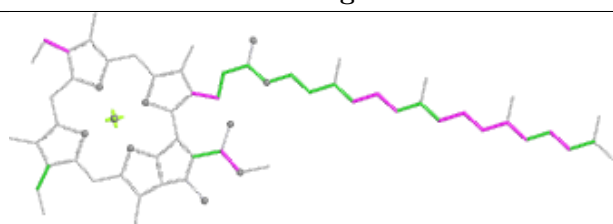
Rings

Ligand CLA R 306

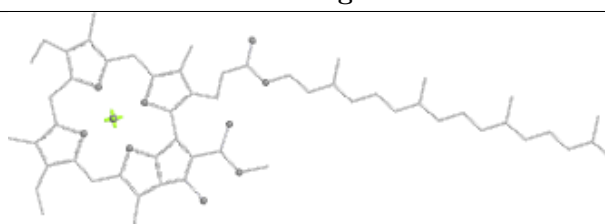
Bond lengths



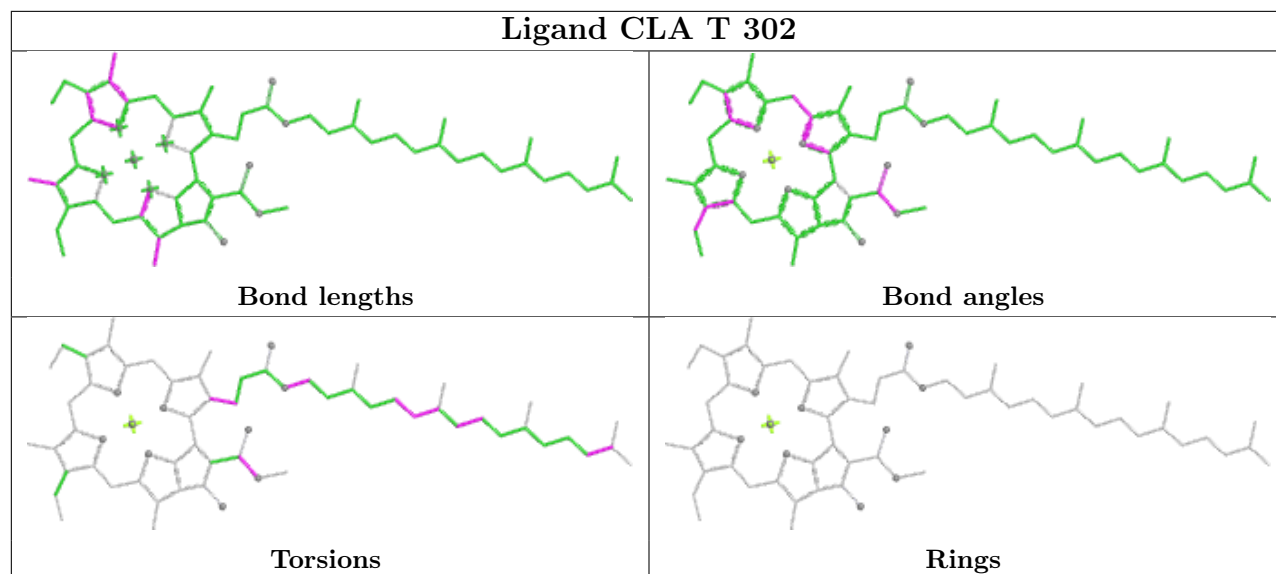
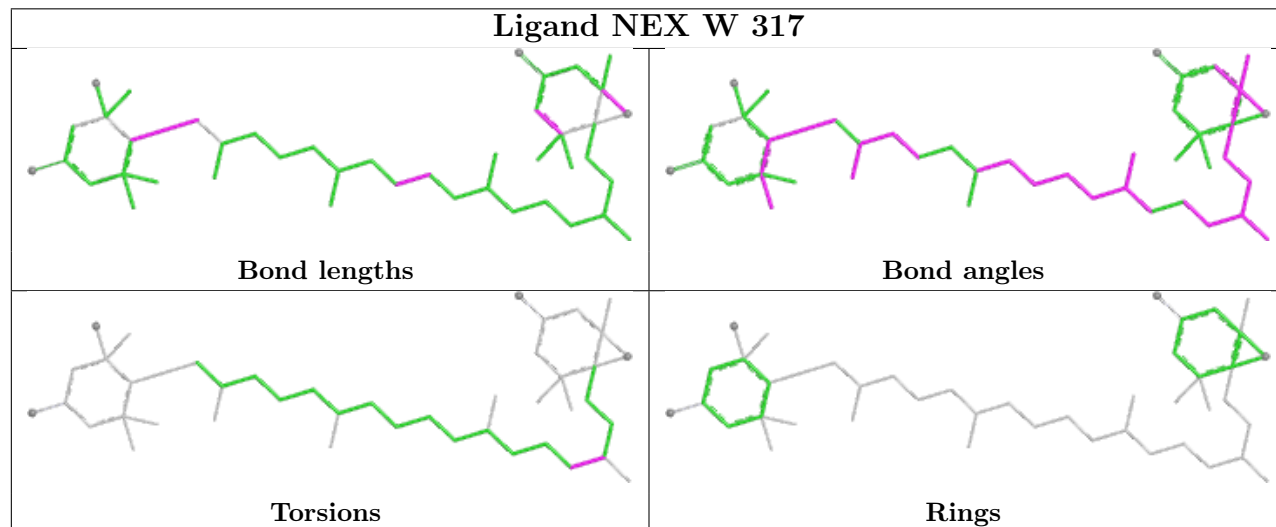
Bond angles



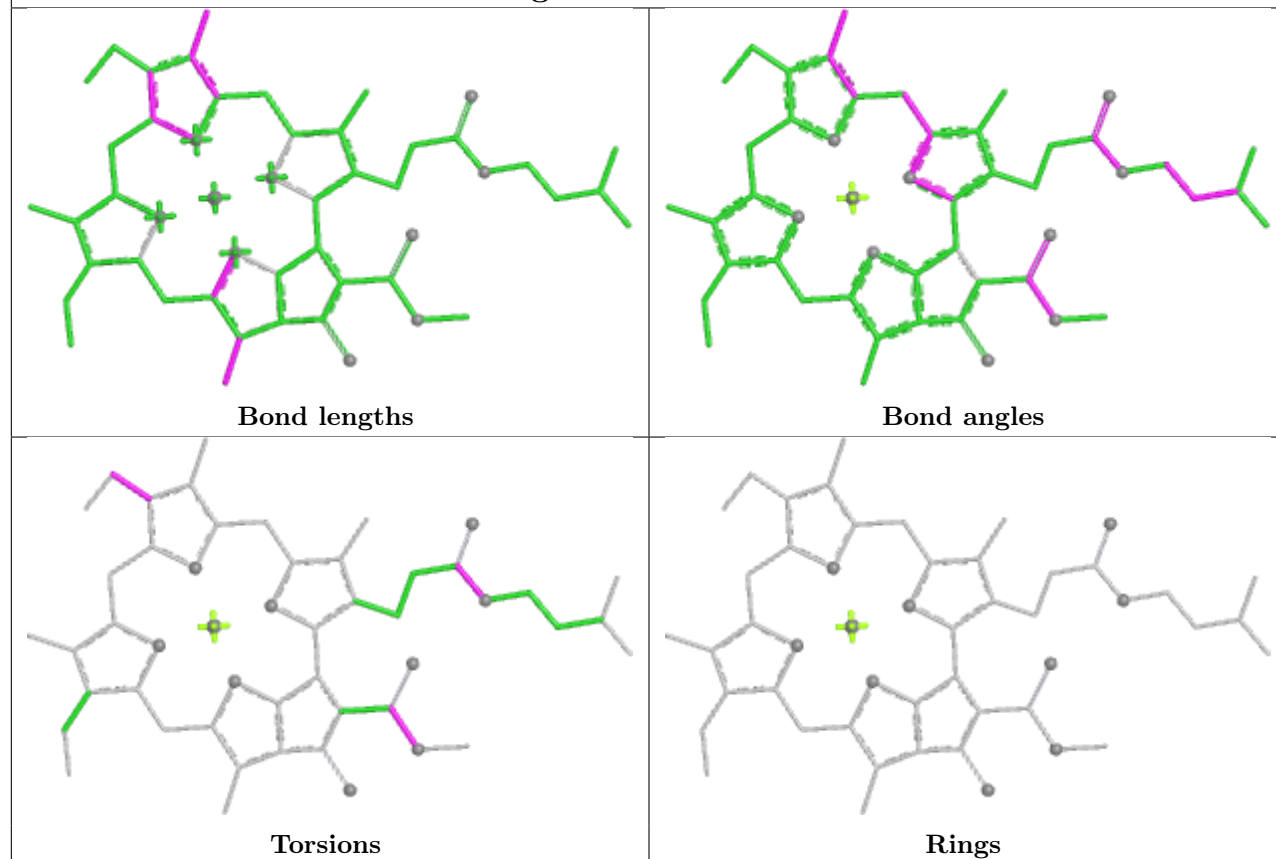
Torsions



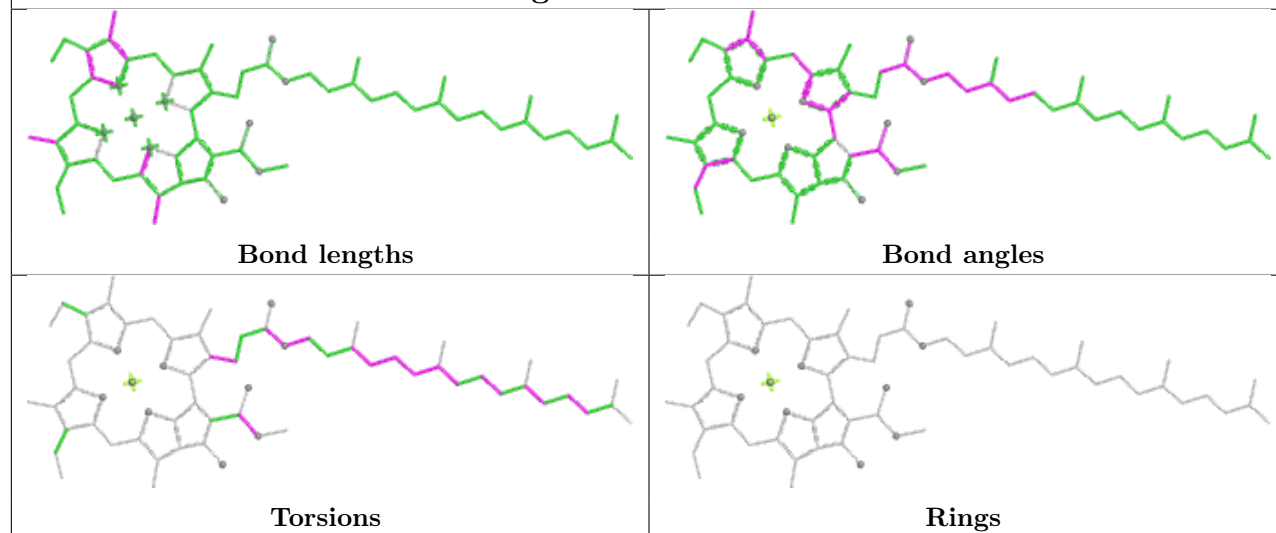
Rings

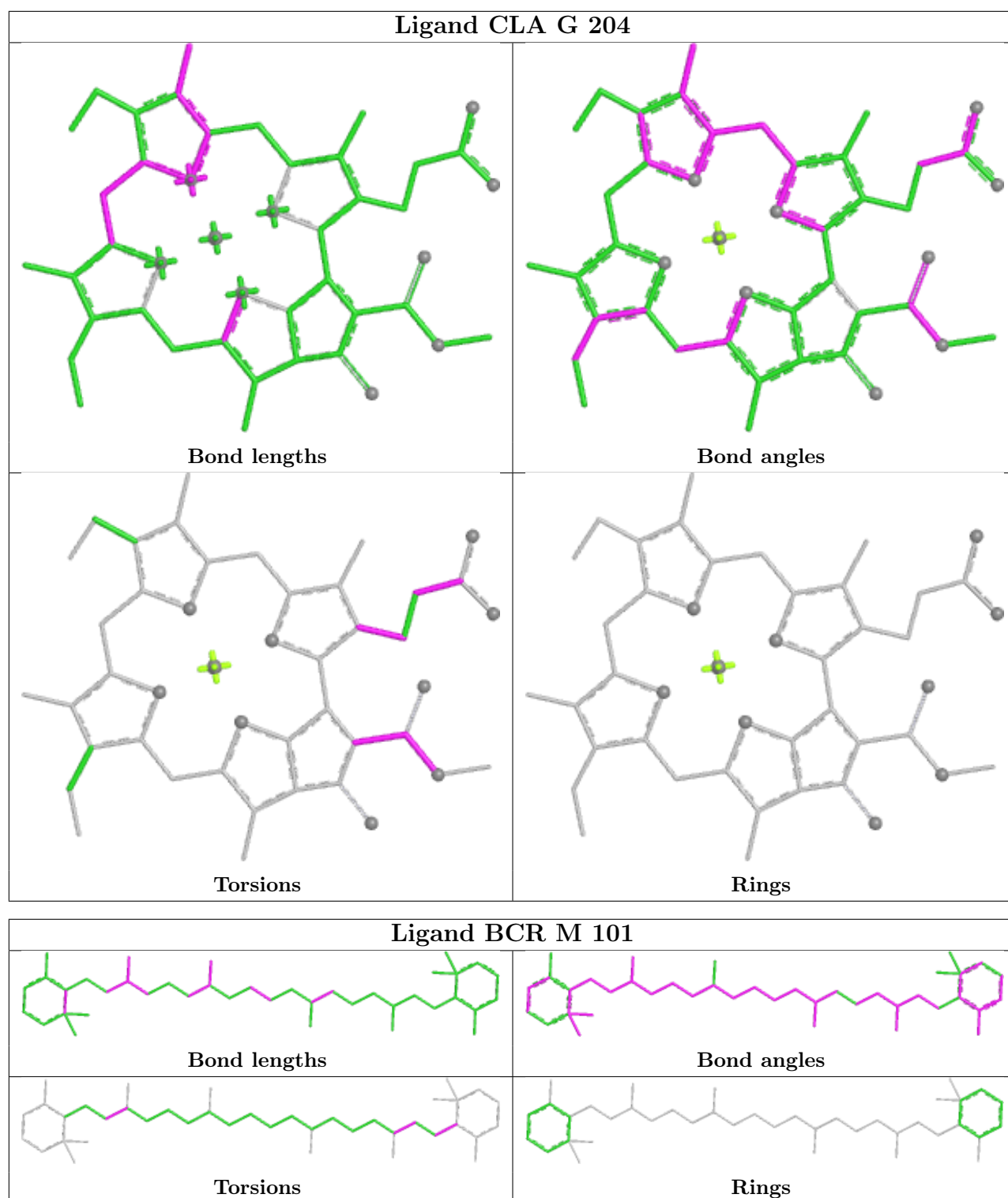
Ligand CLA T 302**Ligand NEX W 317**

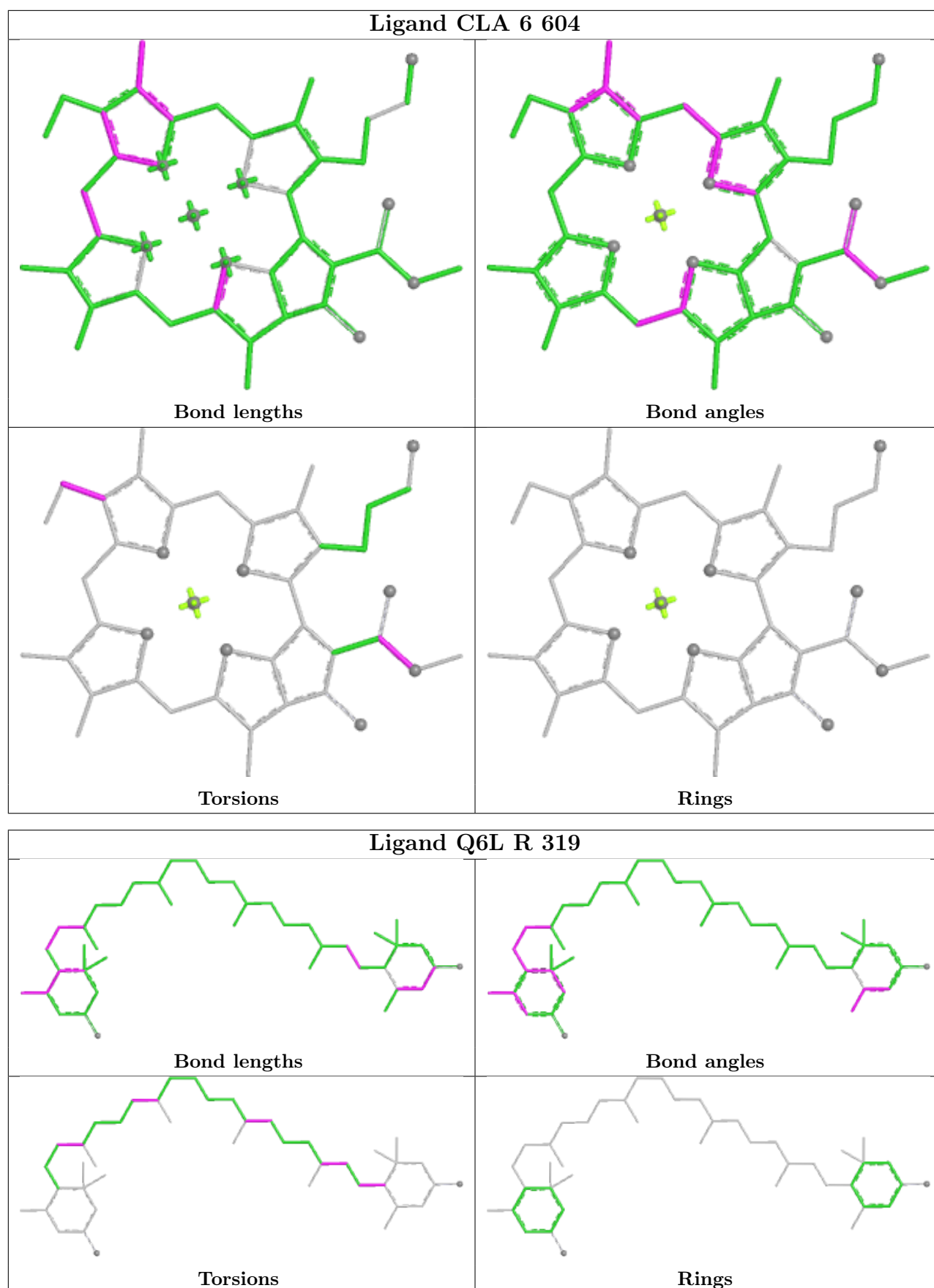
Ligand CLA U 303



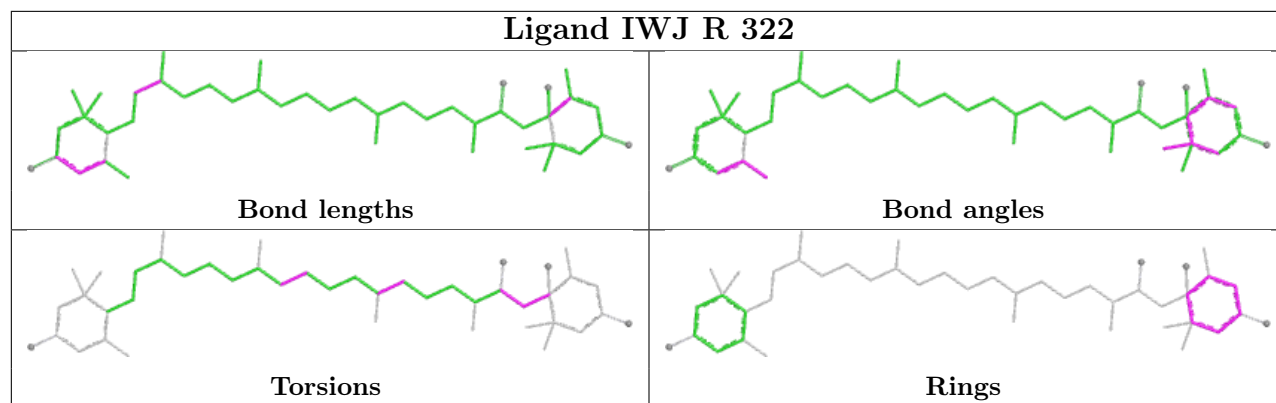
Ligand CLA A 830



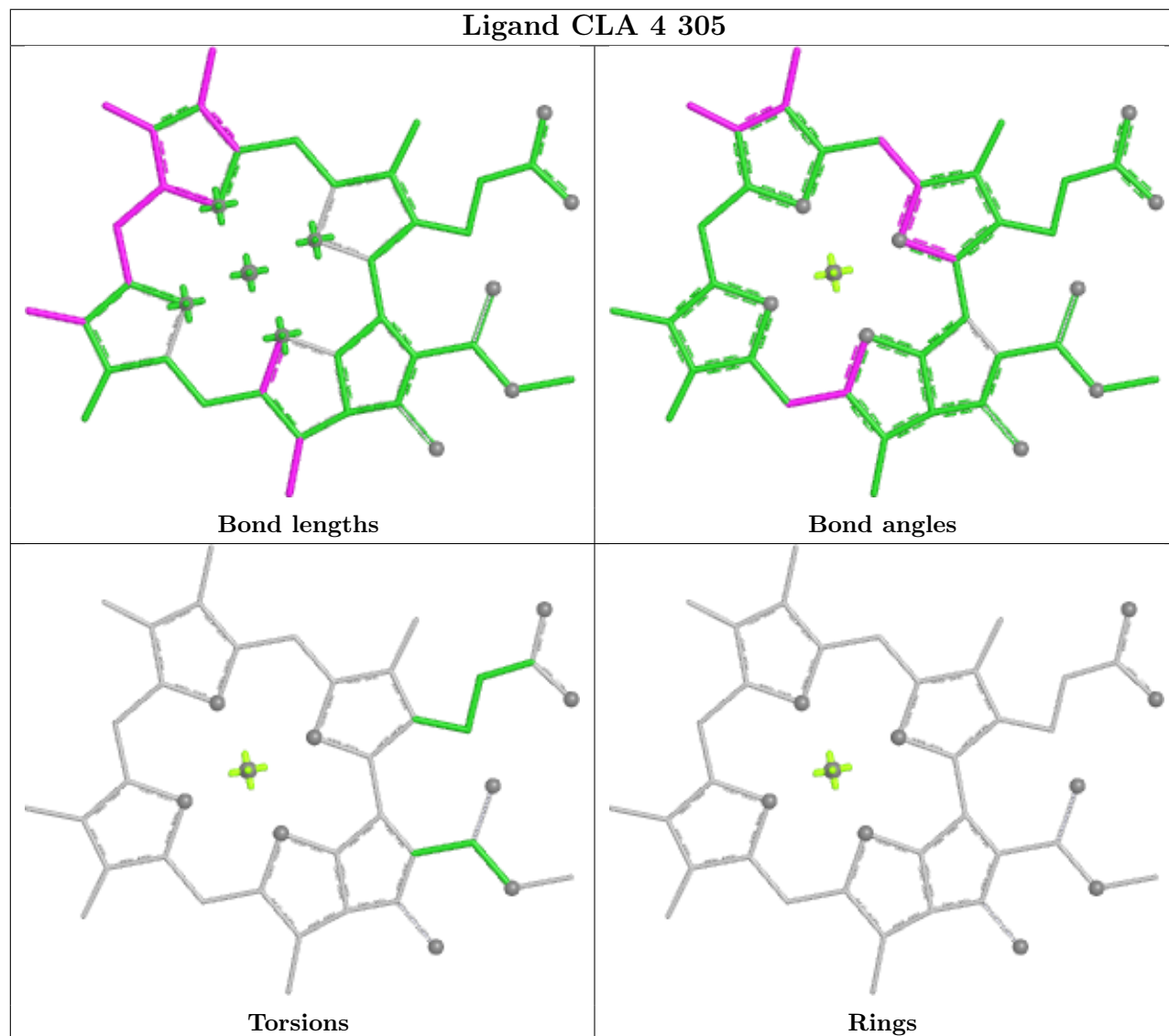


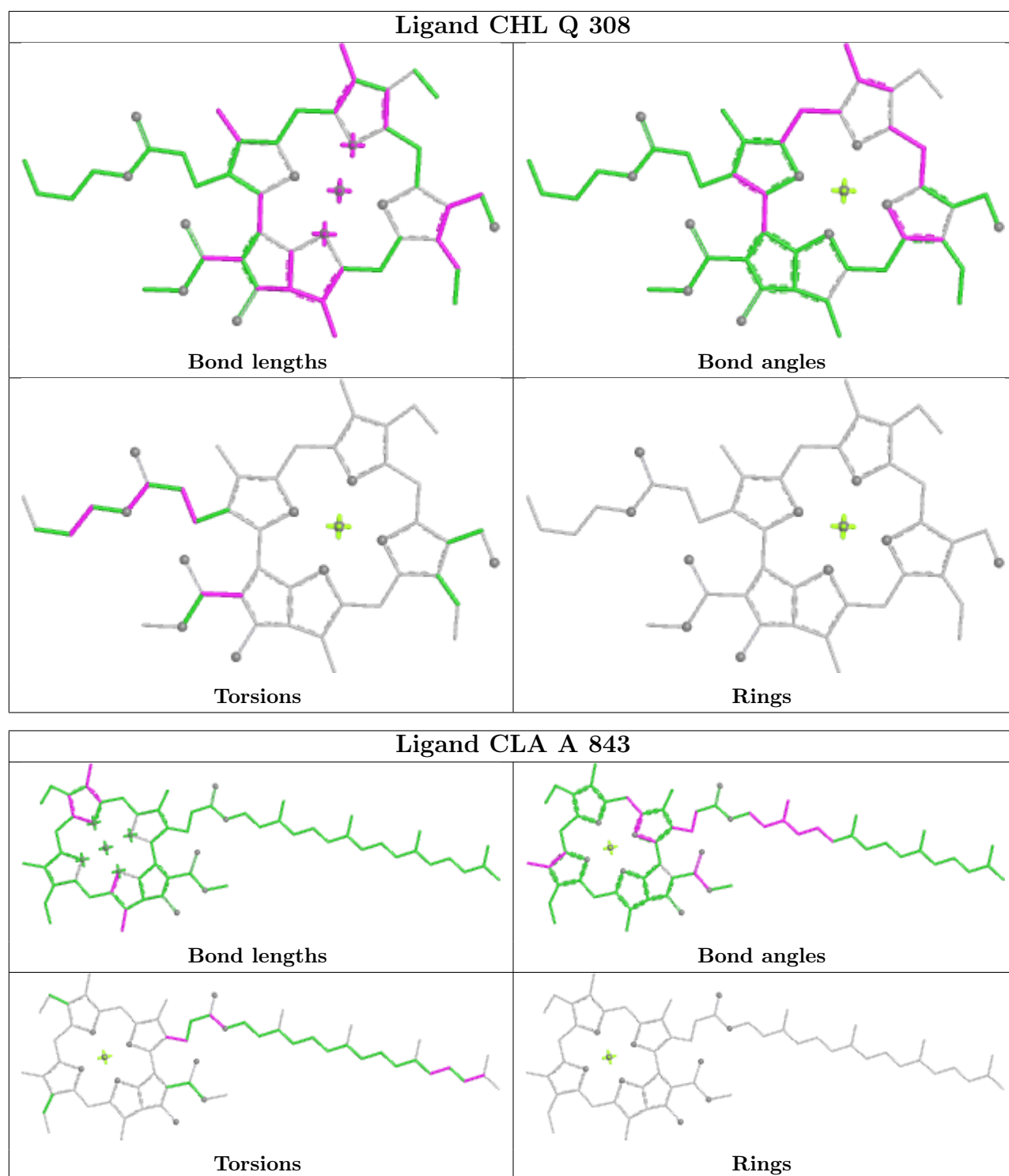


Ligand IWJ R 322

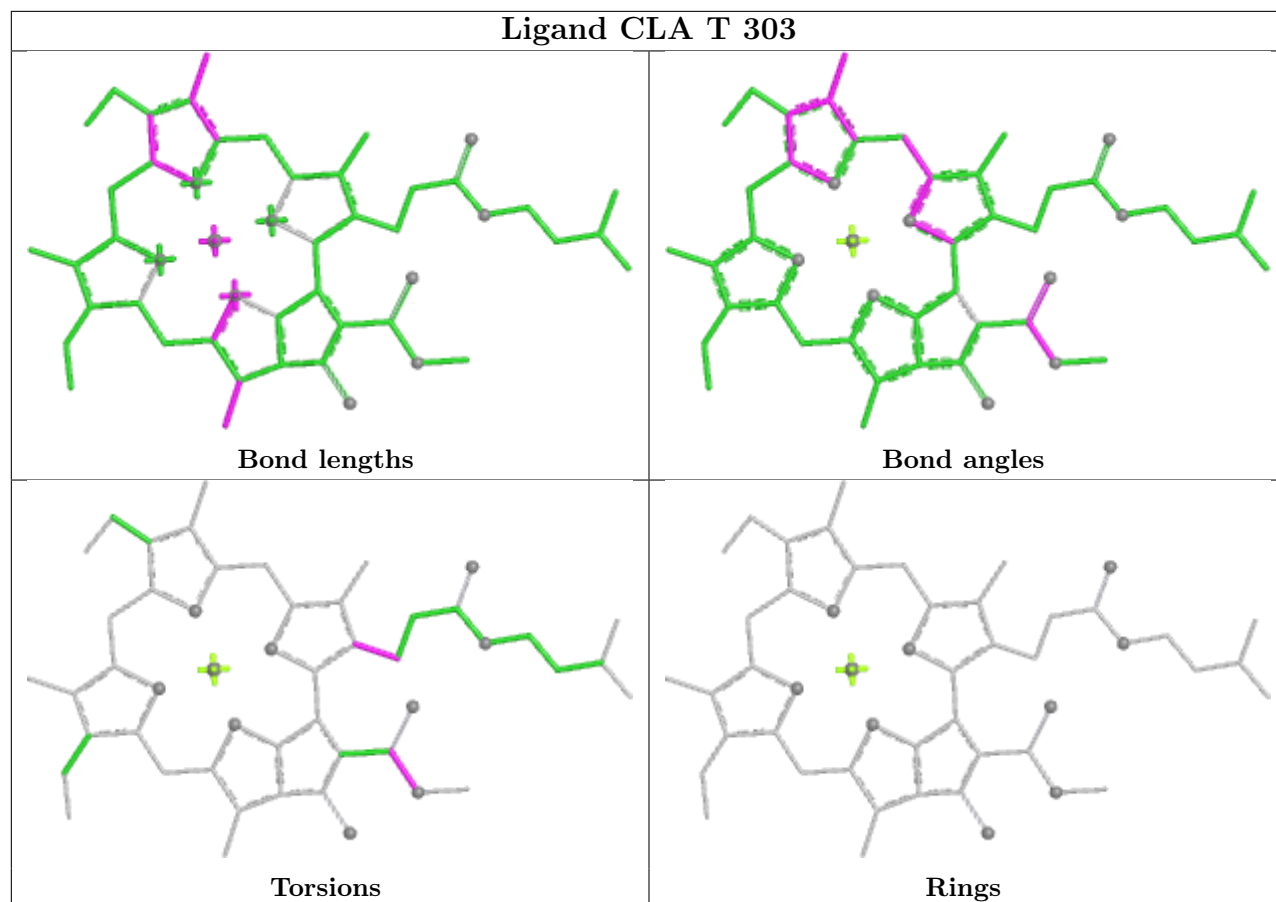


Ligand CLA 4 305

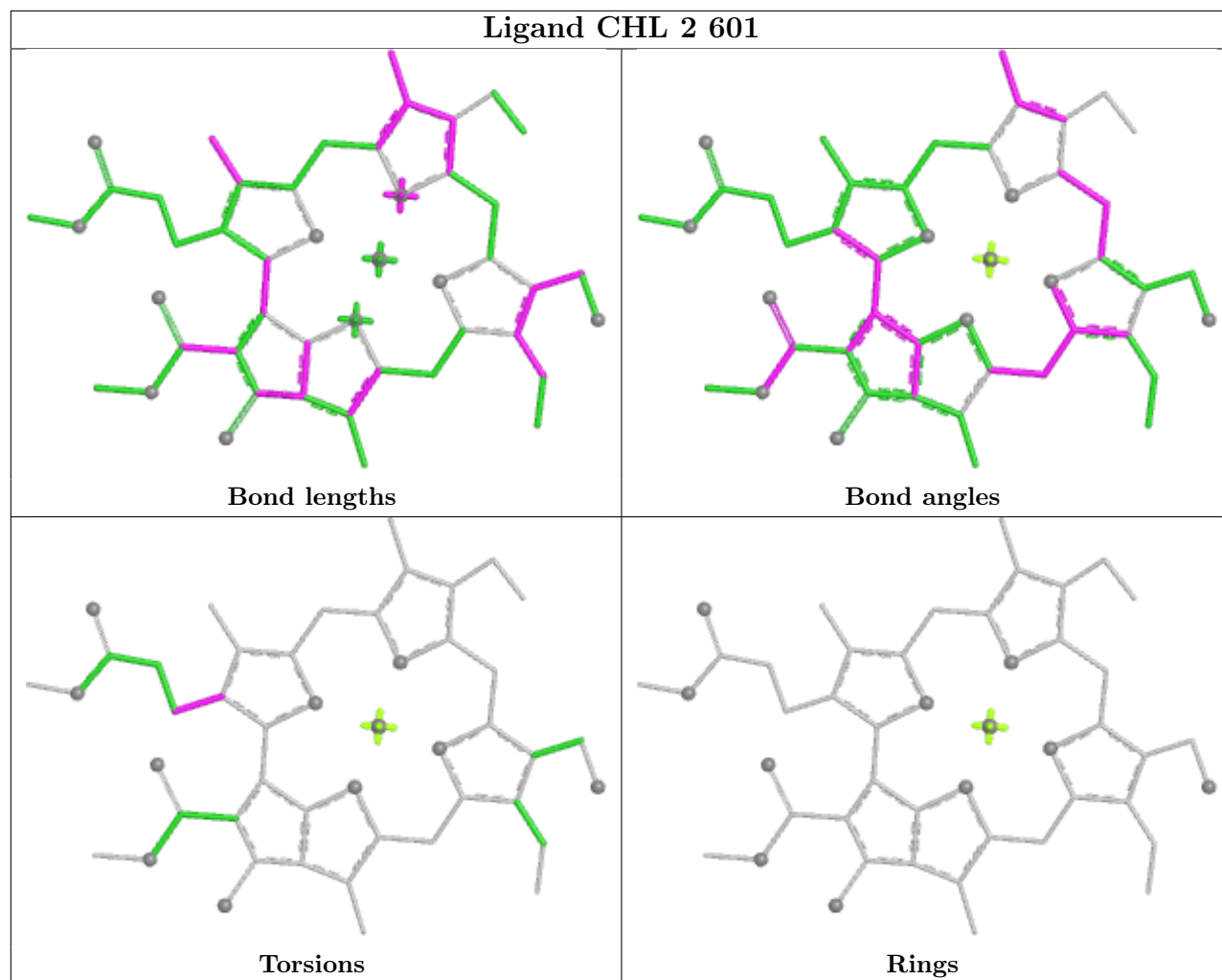




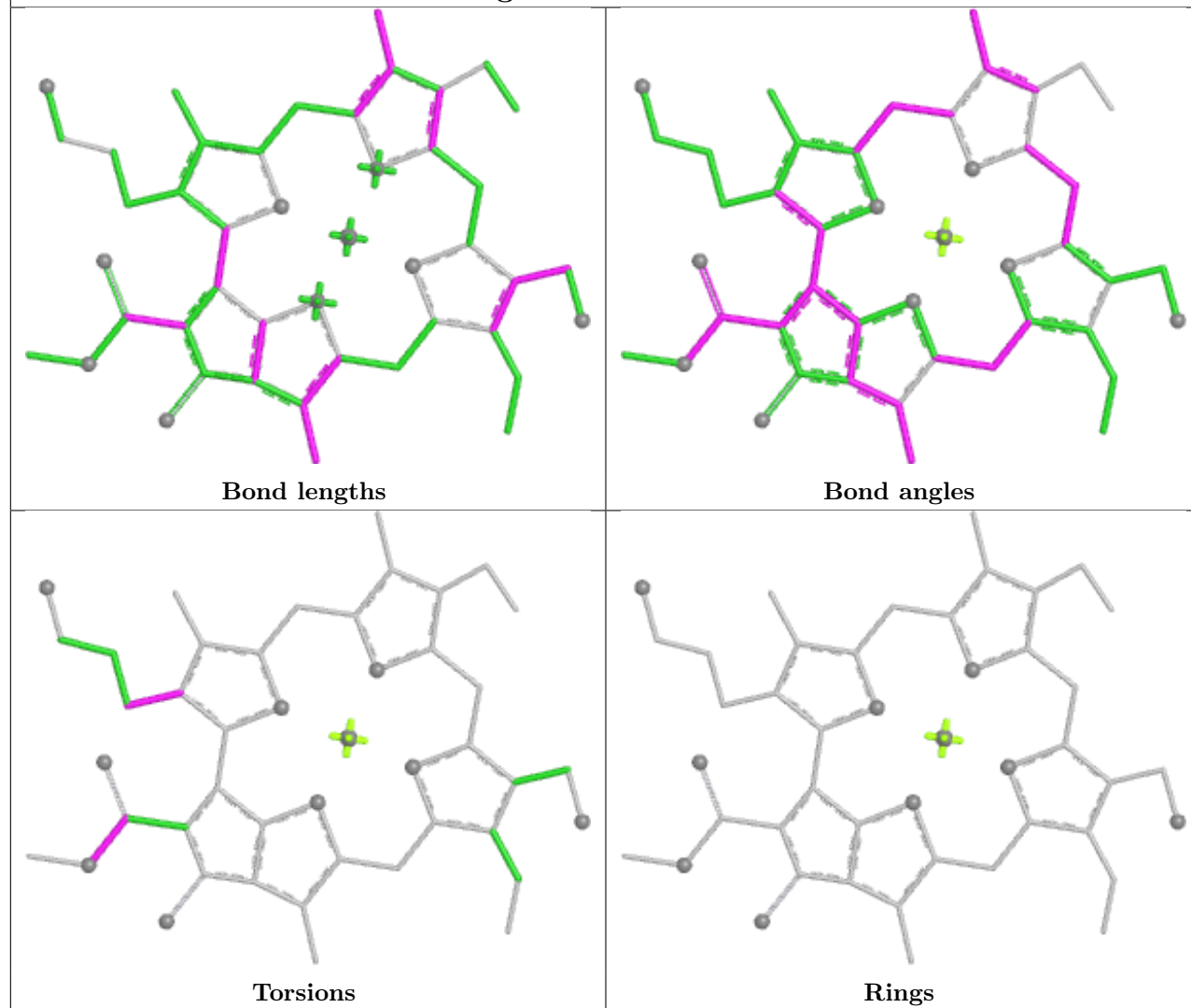
Ligand CLA T 303



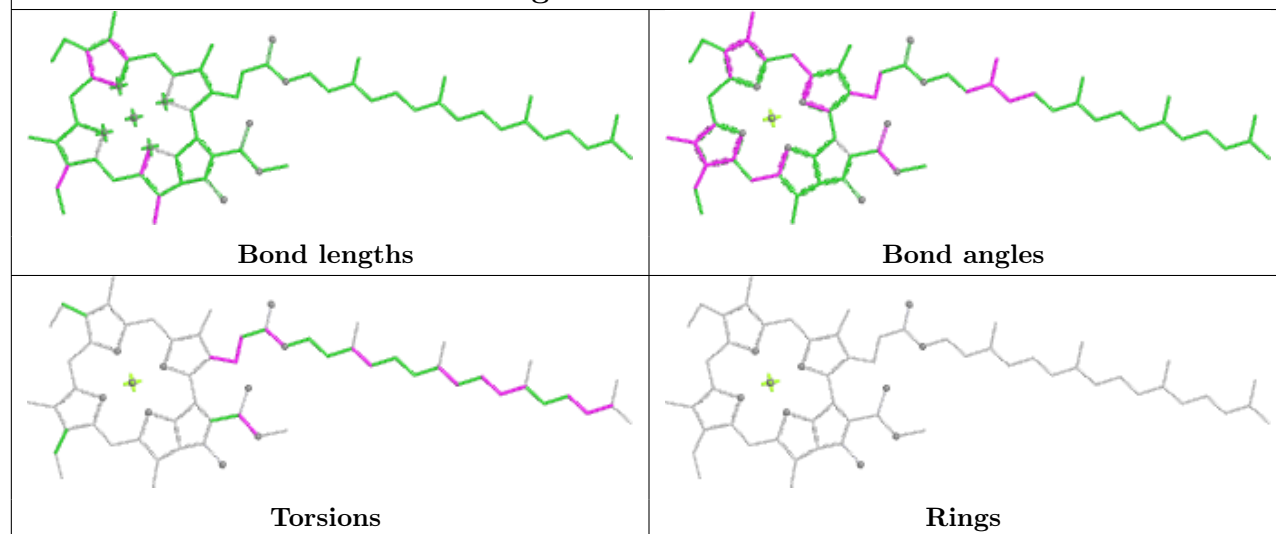
Ligand CHL 2 601



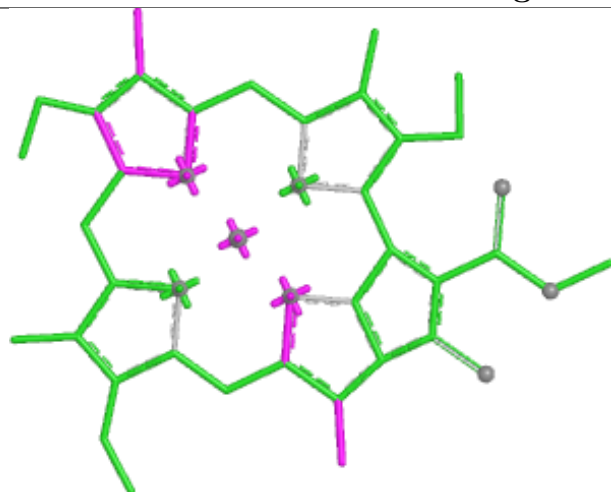
Ligand CHL P 314



Ligand CLA A 825



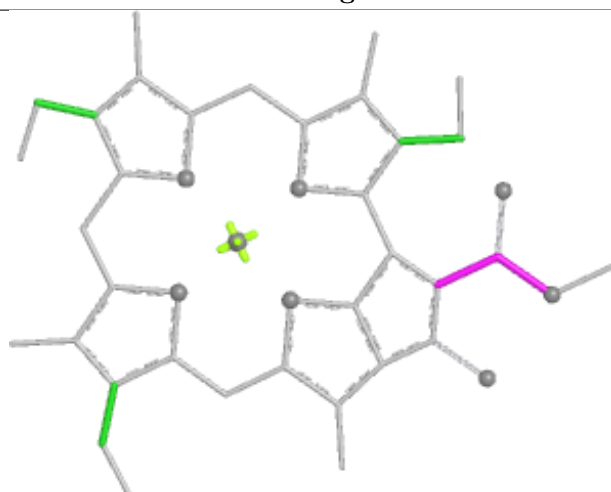
Ligand CLA N 203



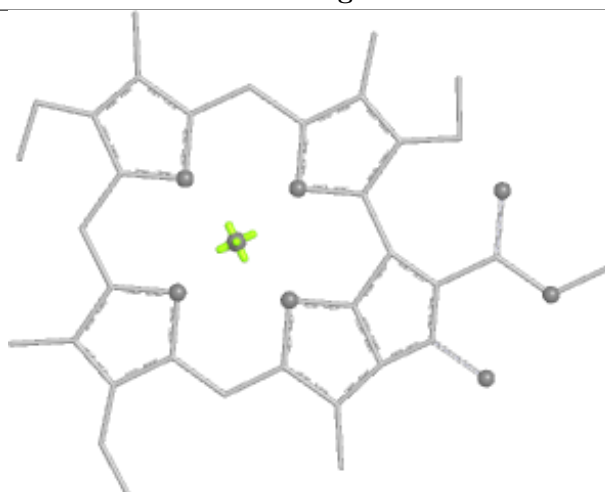
Bond lengths



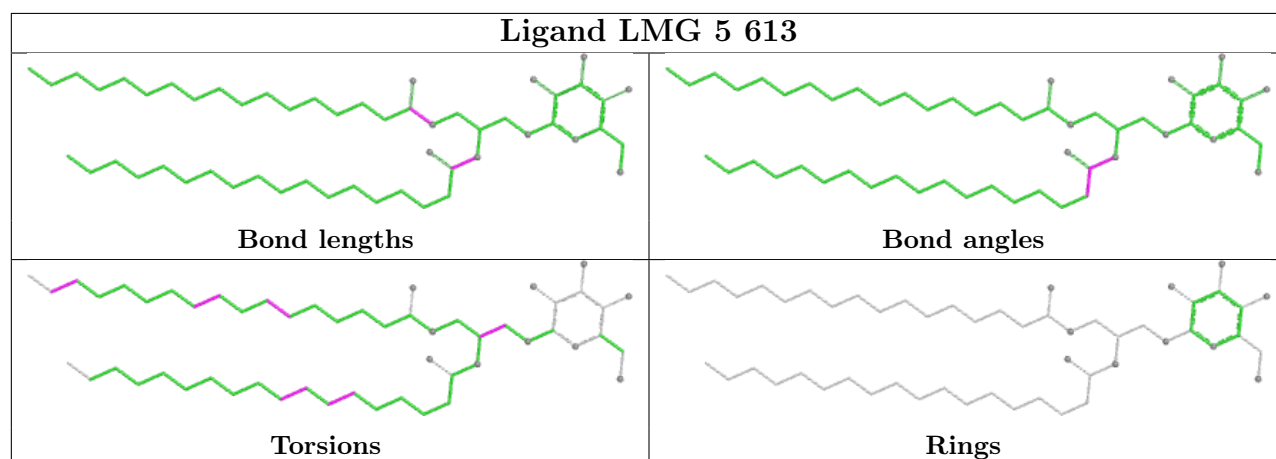
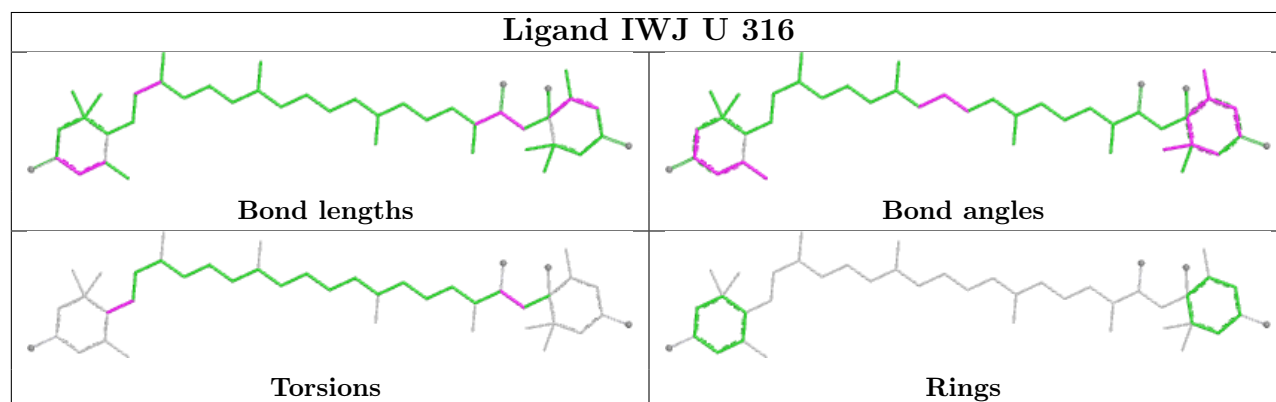
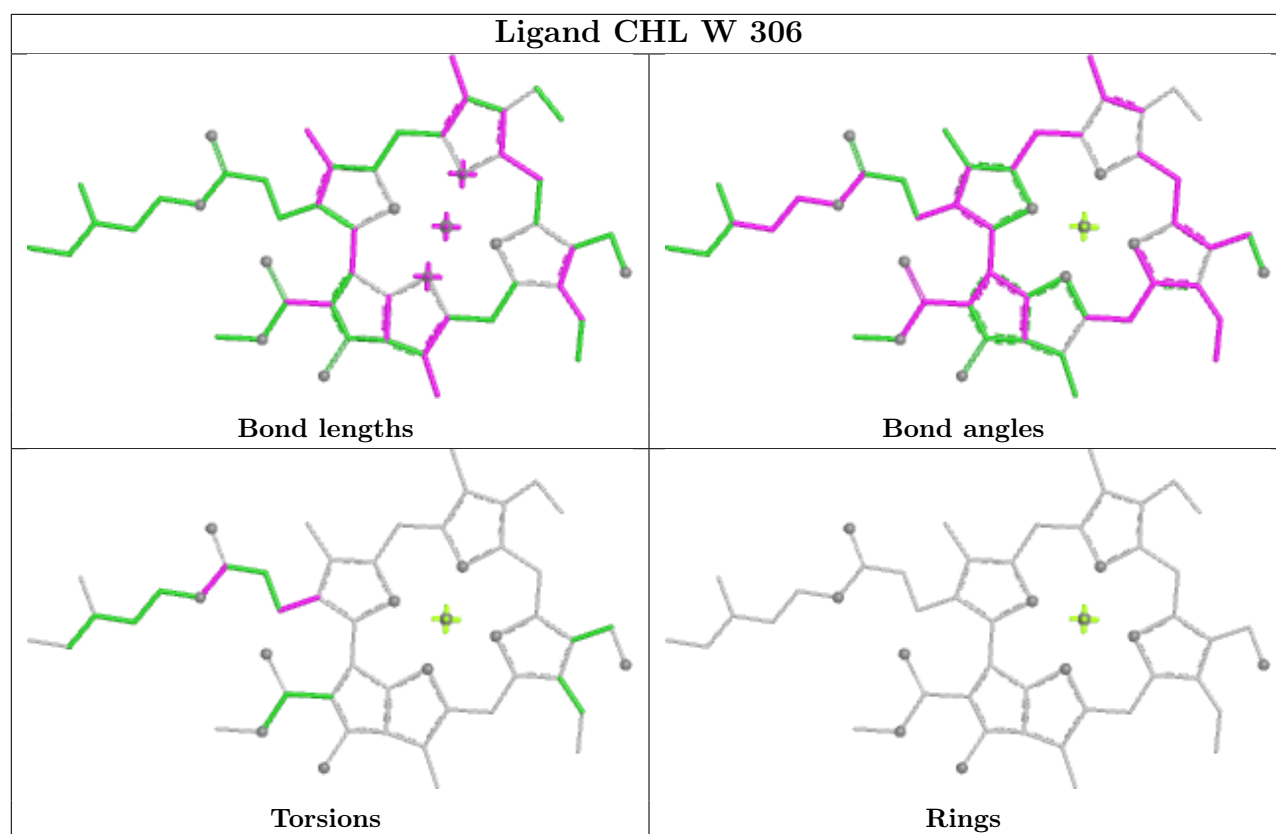
Bond angles



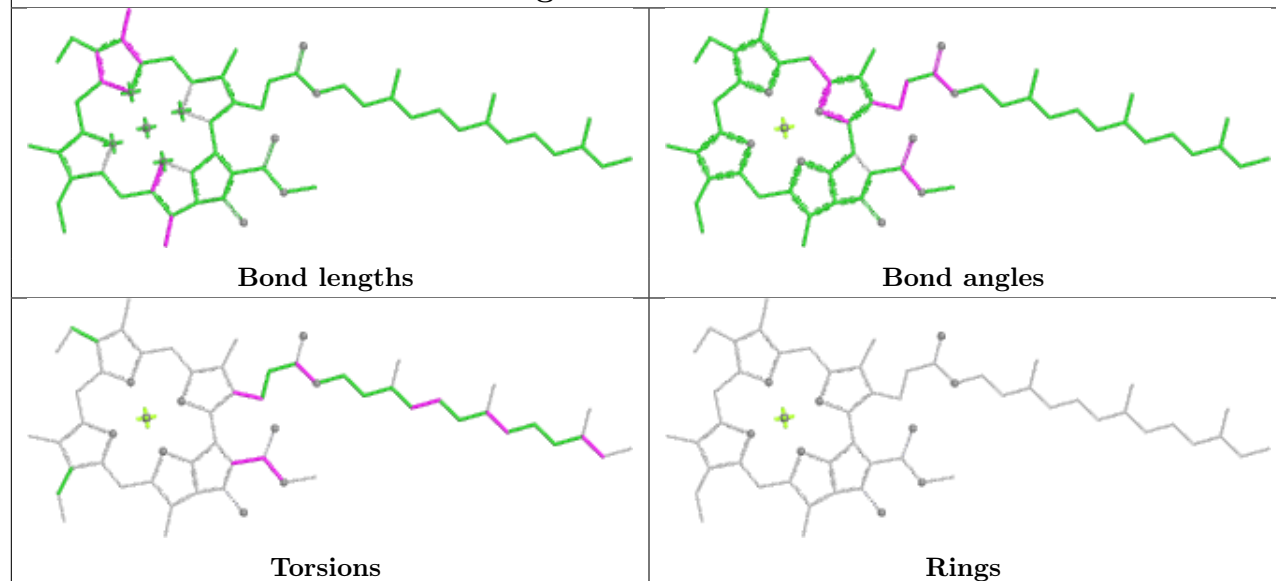
Torsions



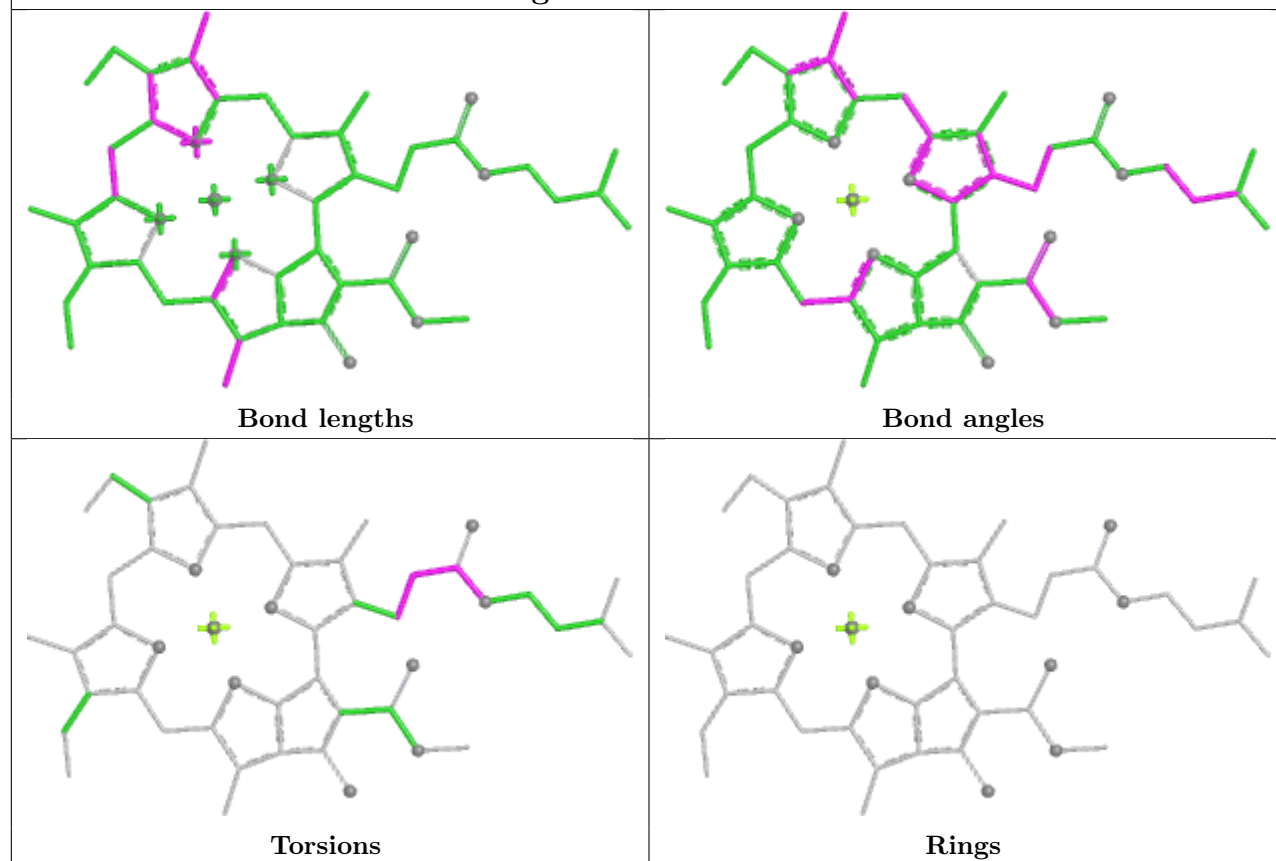
Rings



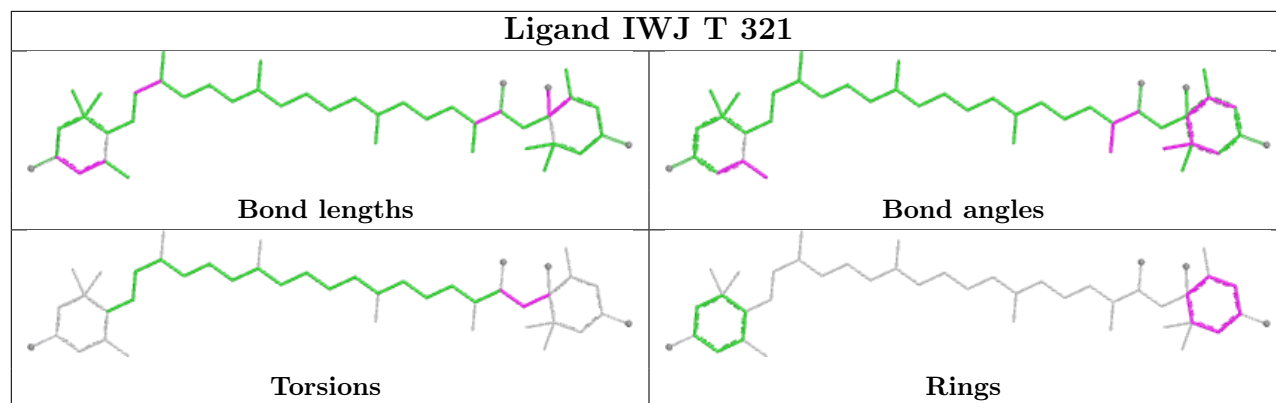
Ligand CLA 6 610



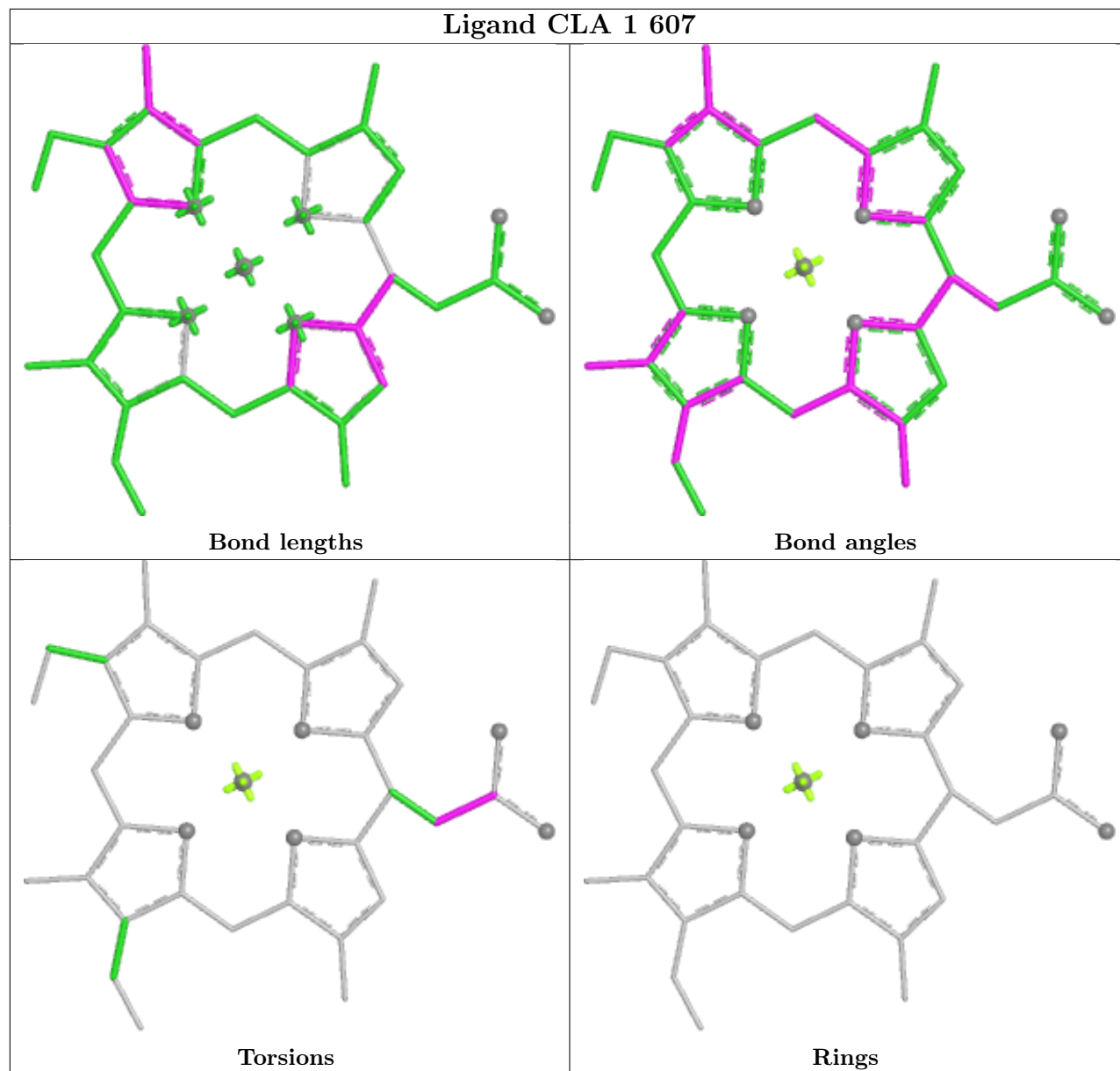
Ligand CLA A 809



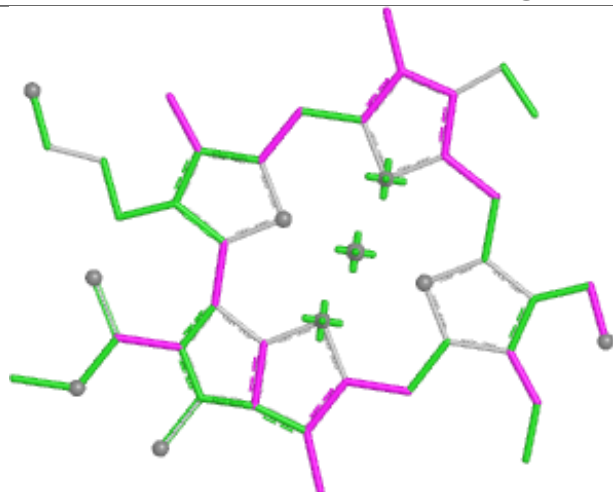
Ligand IWJ T 321



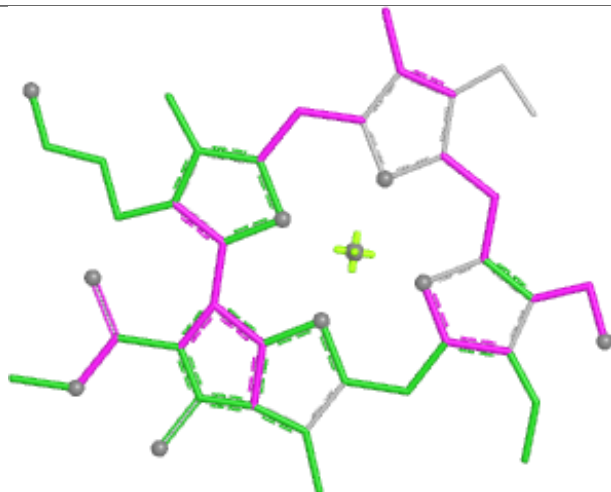
Ligand CLA 1 607



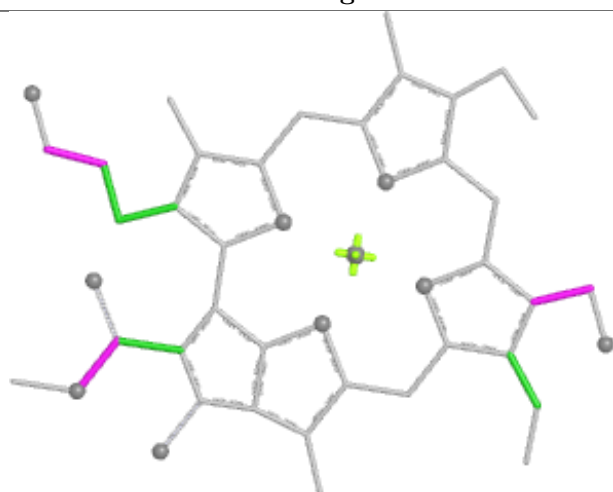
Ligand CHL 2 607



Bond lengths



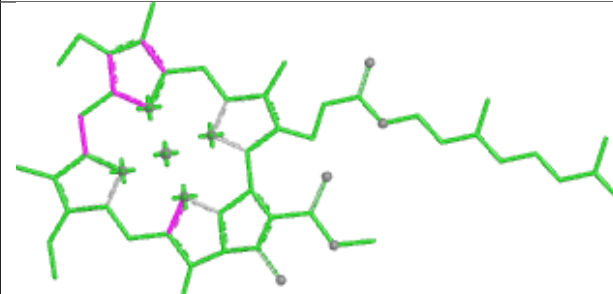
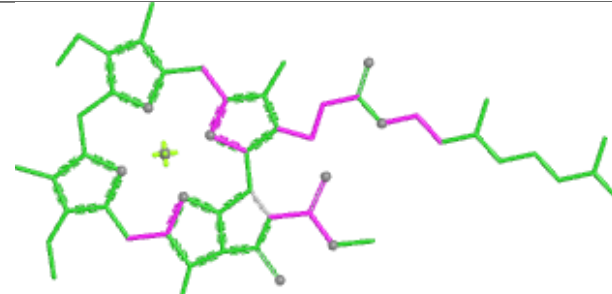
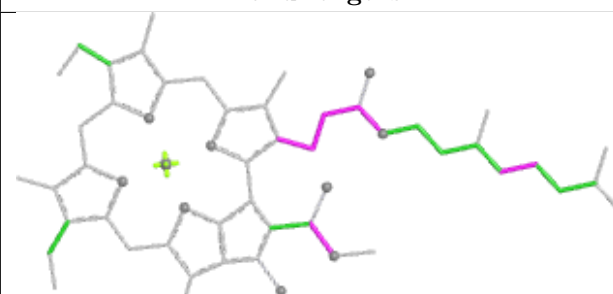
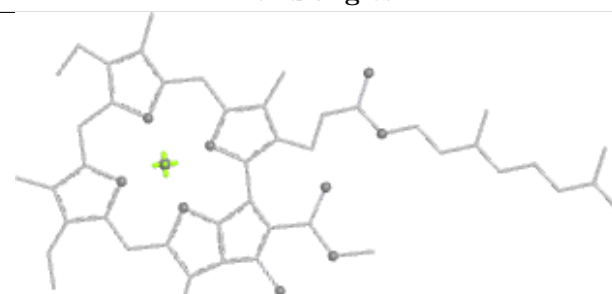
Bond angles

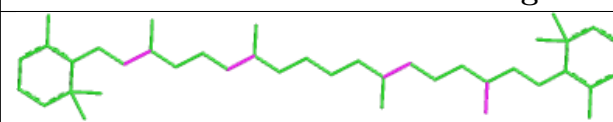
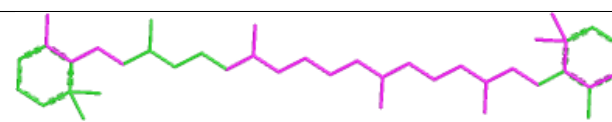
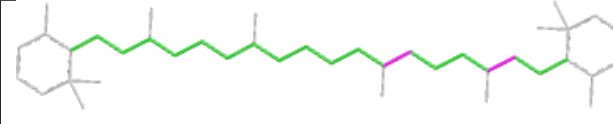
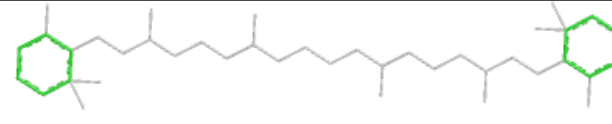


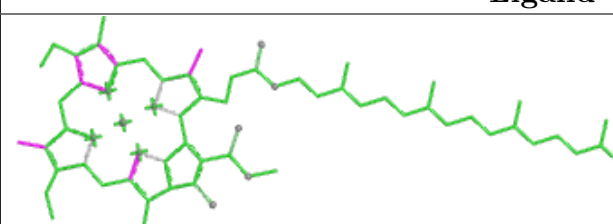
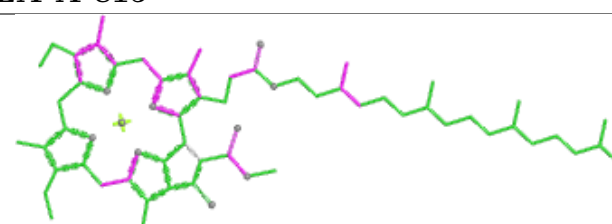
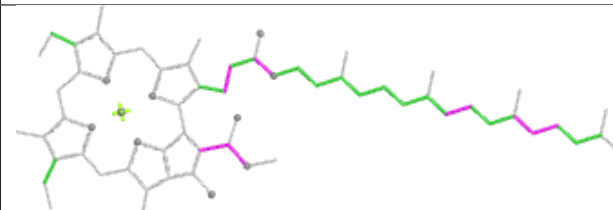
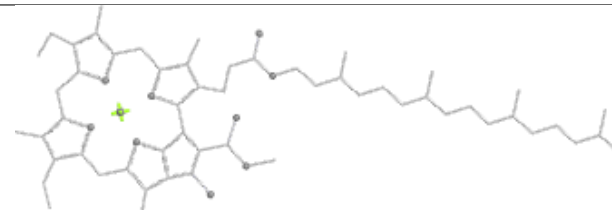
Torsions



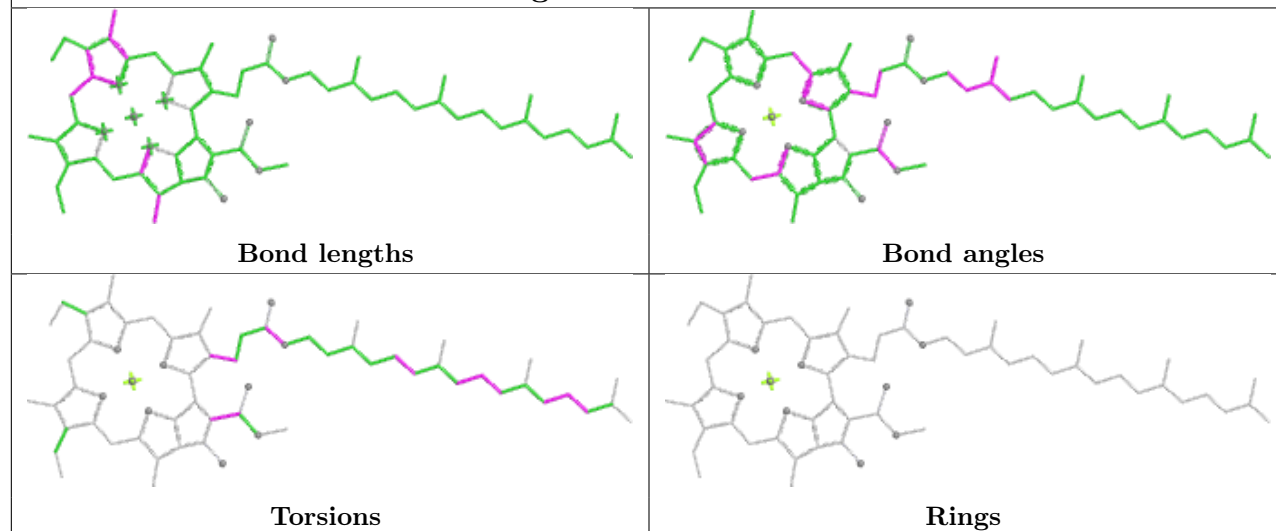
Rings

Ligand CLA P 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

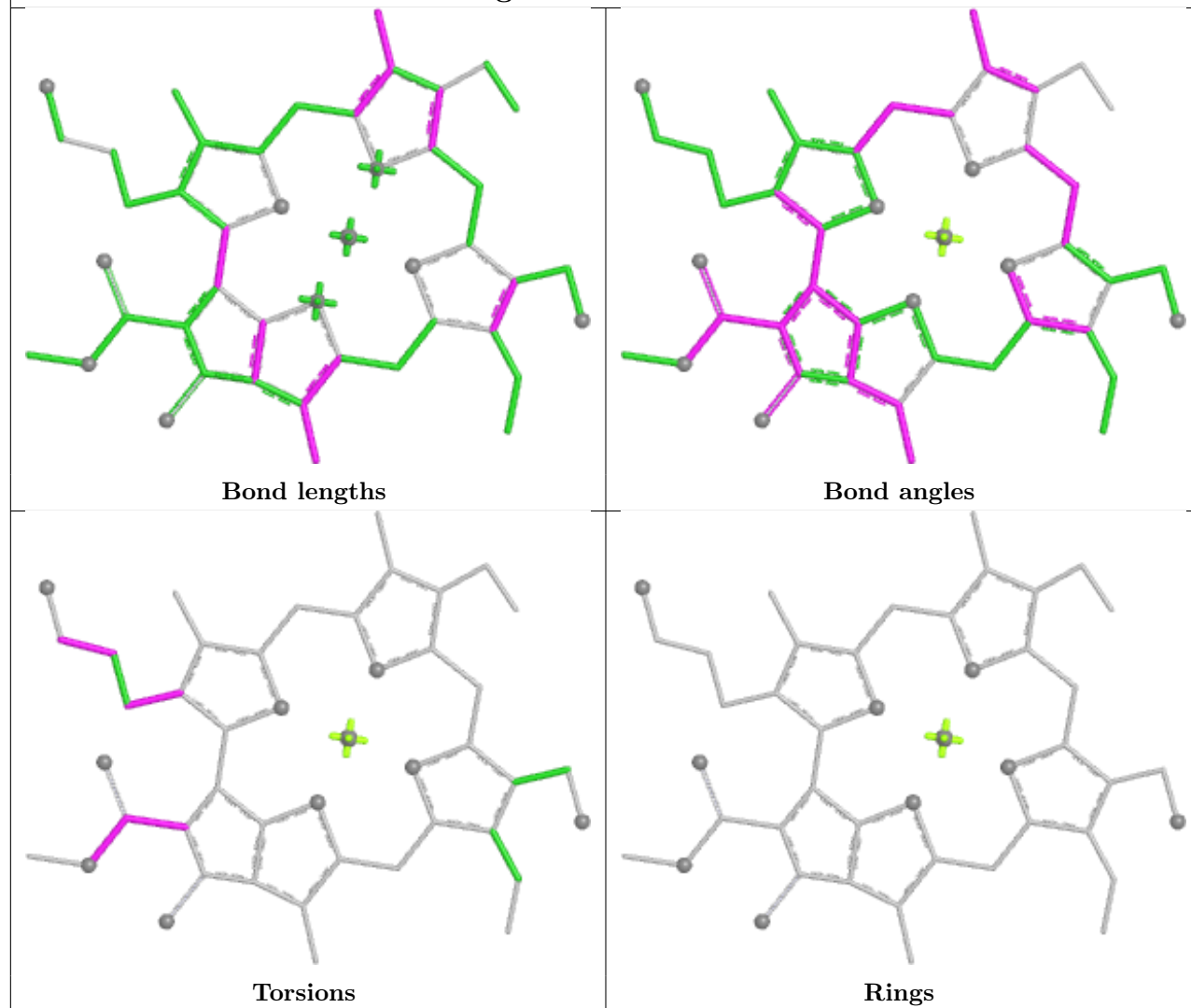
Ligand BCR F 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

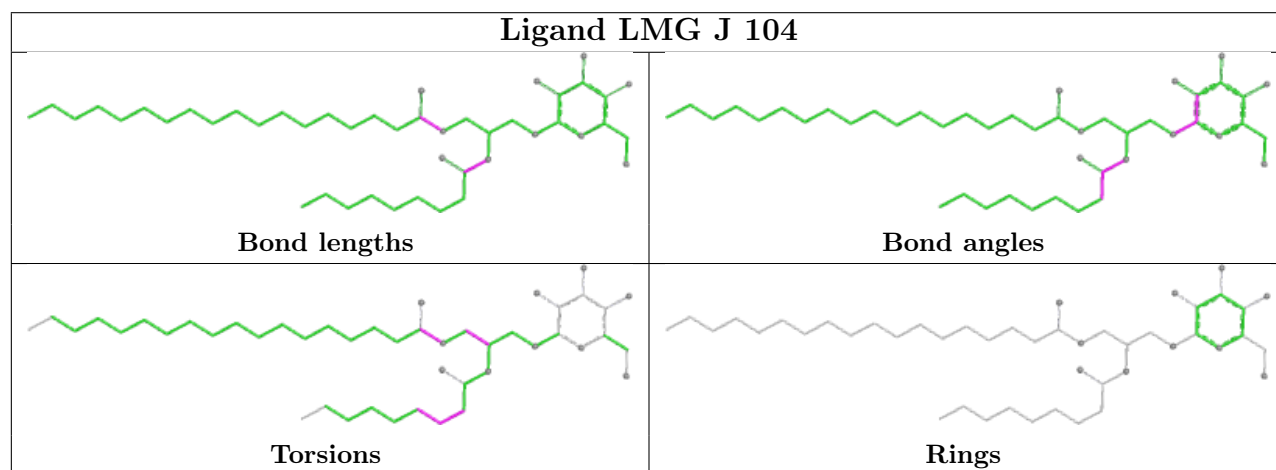
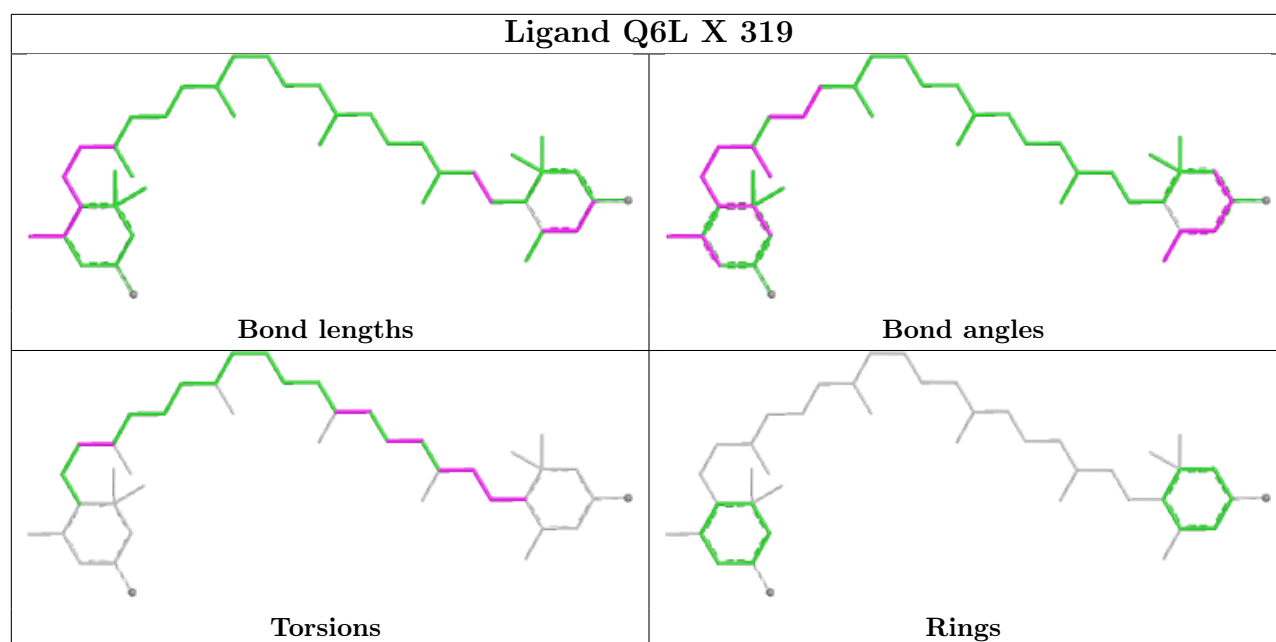
Ligand CLA A 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 302

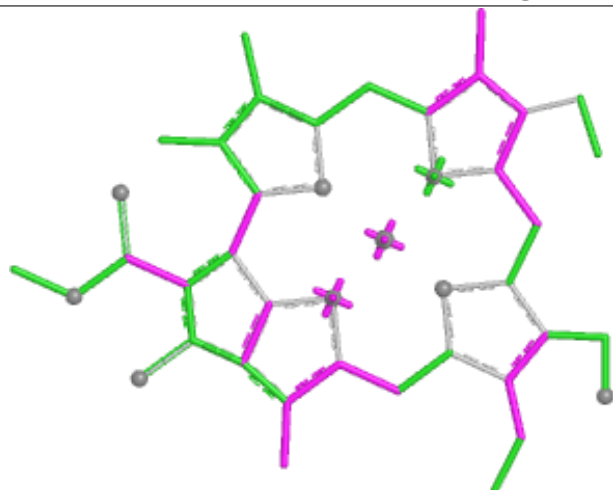


Ligand CHL X 315

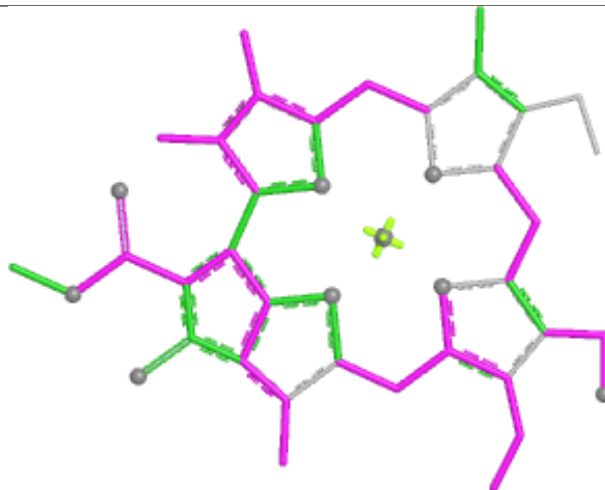




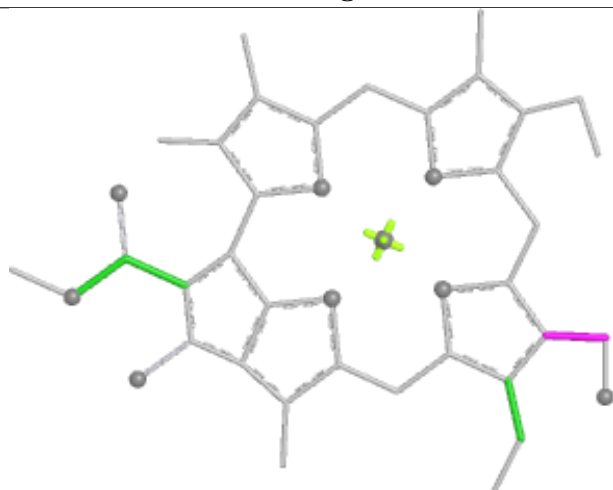
Ligand CHL S 304



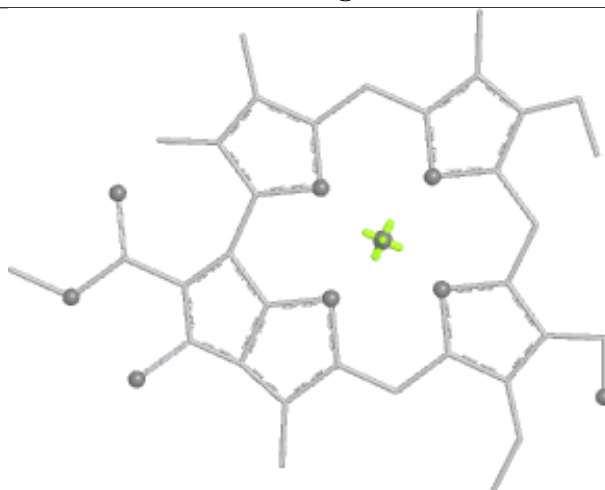
Bond lengths



Bond angles

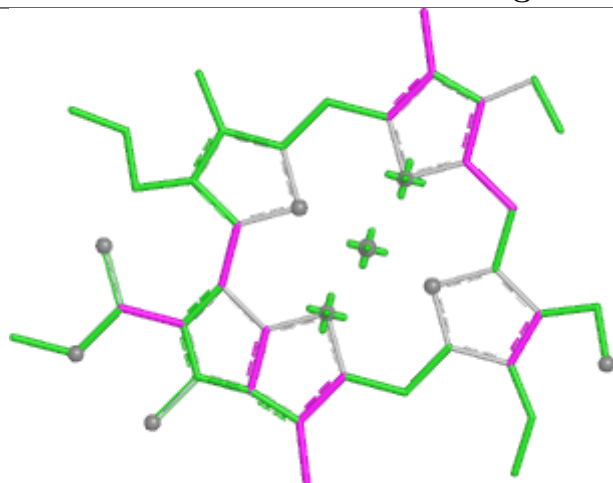


Torsions

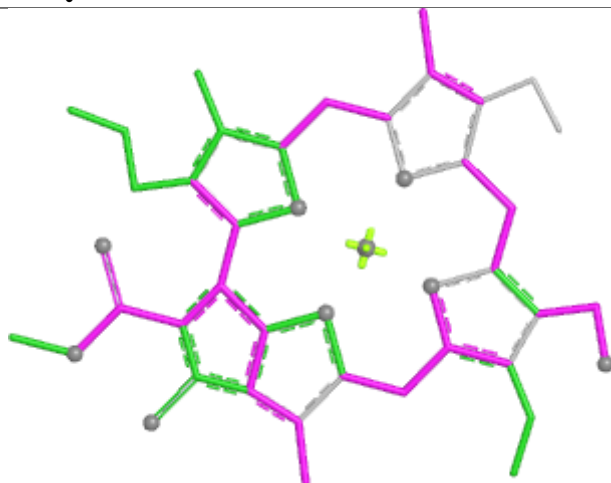


Rings

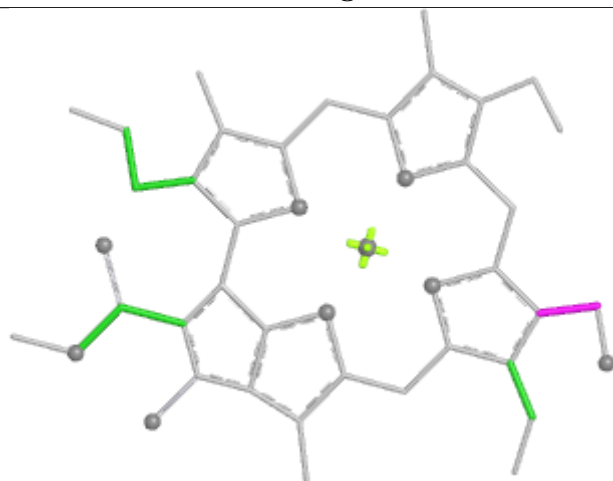
Ligand CHL Q 309



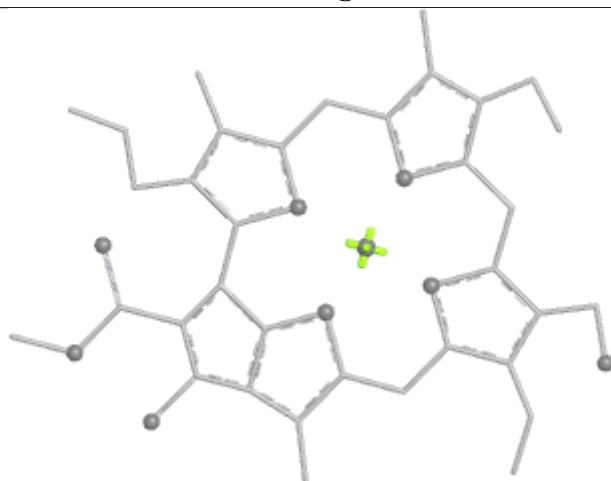
Bond lengths



Bond angles

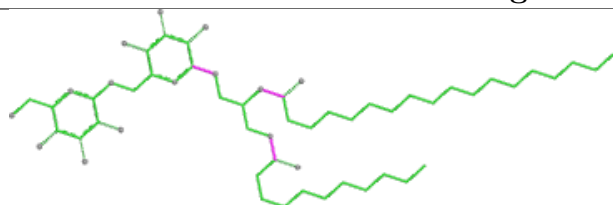


Torsions

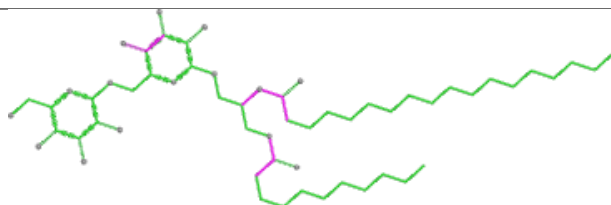


Rings

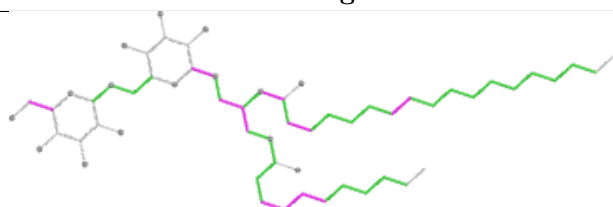
Ligand DGD B 850



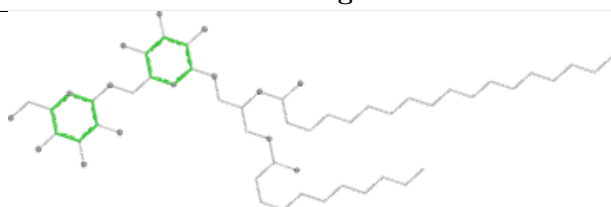
Bond lengths



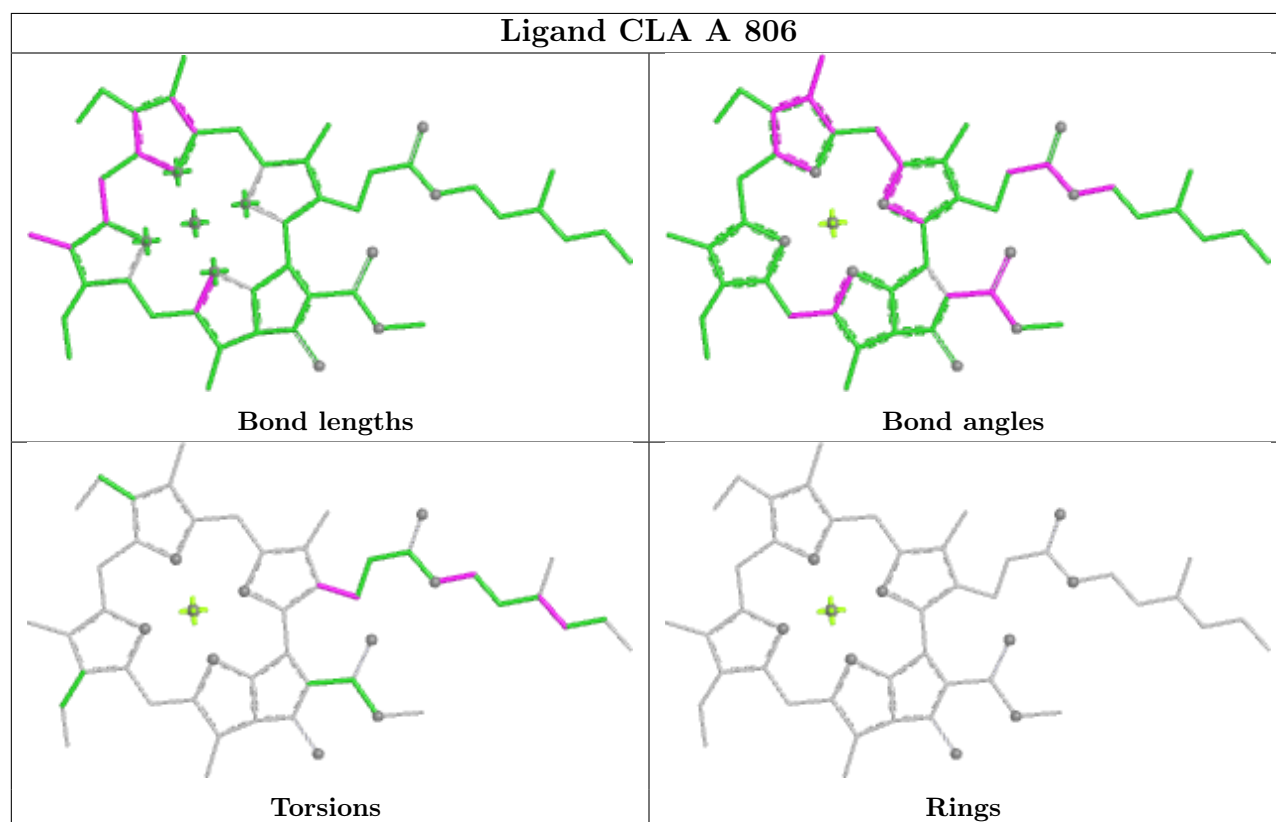
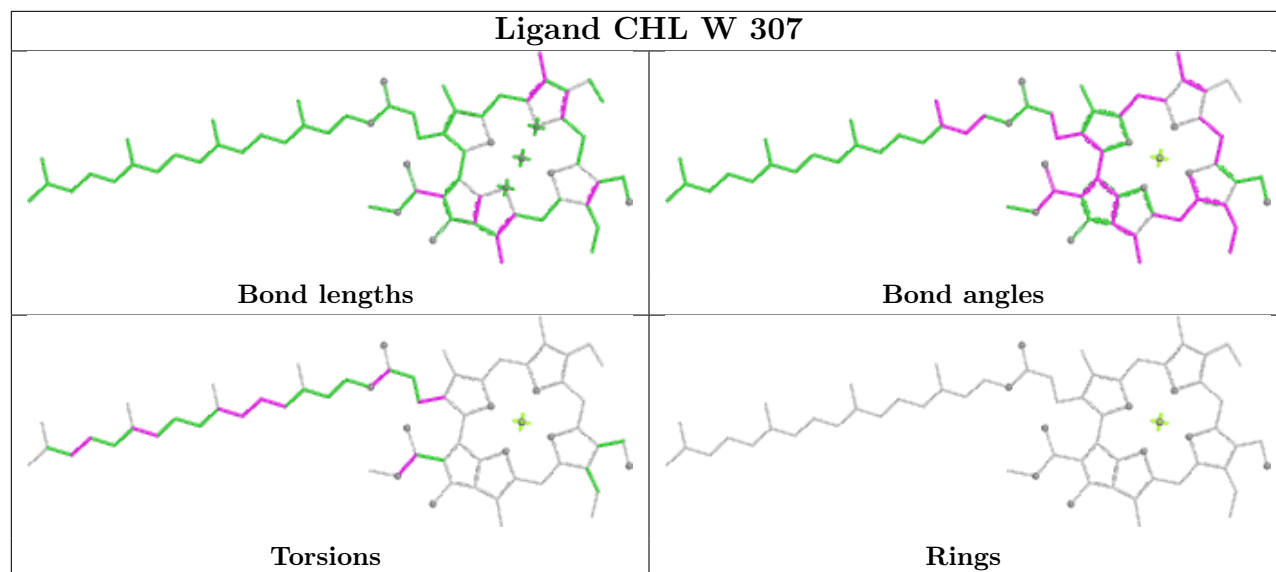
Bond angles

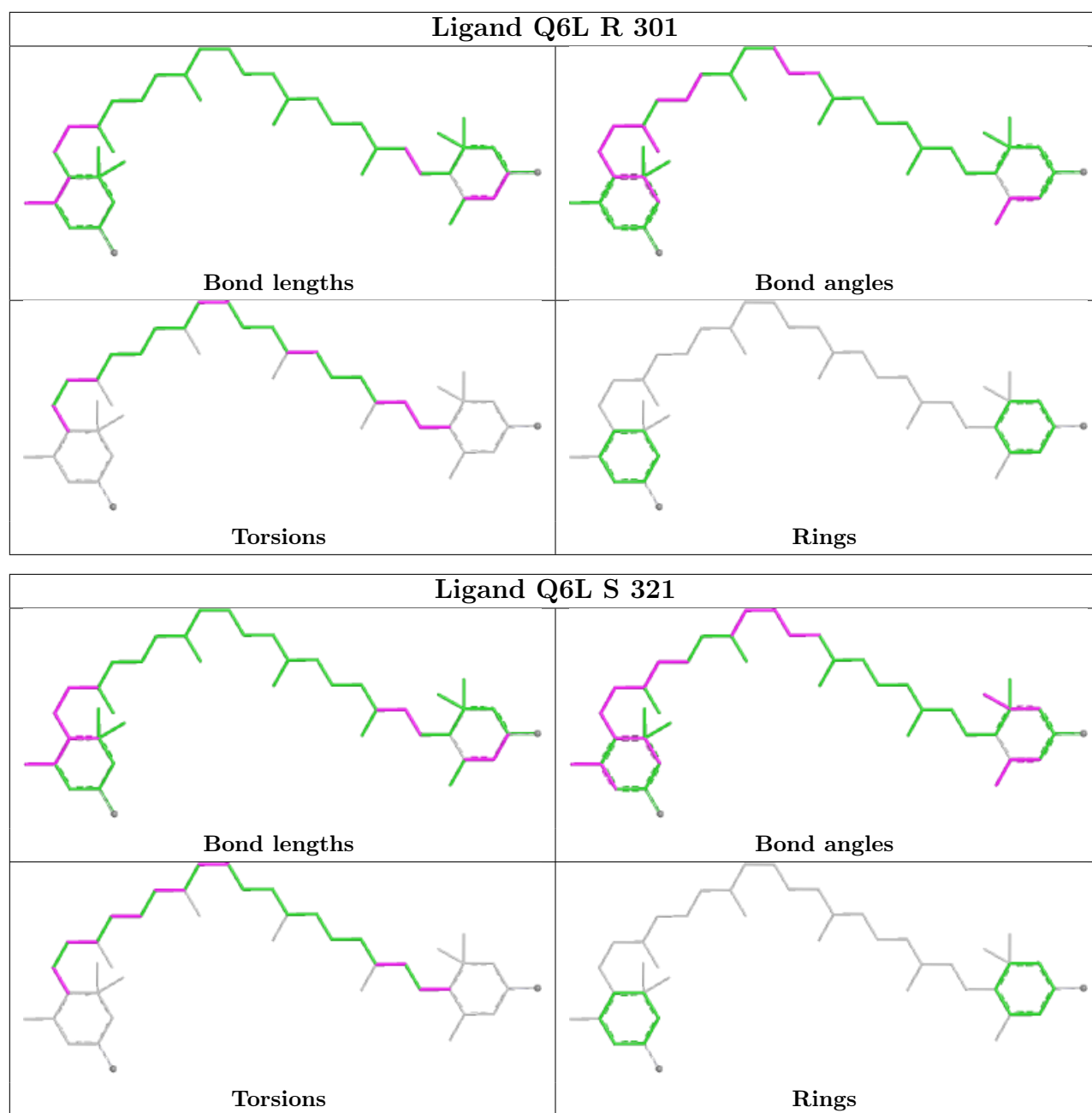


Torsions

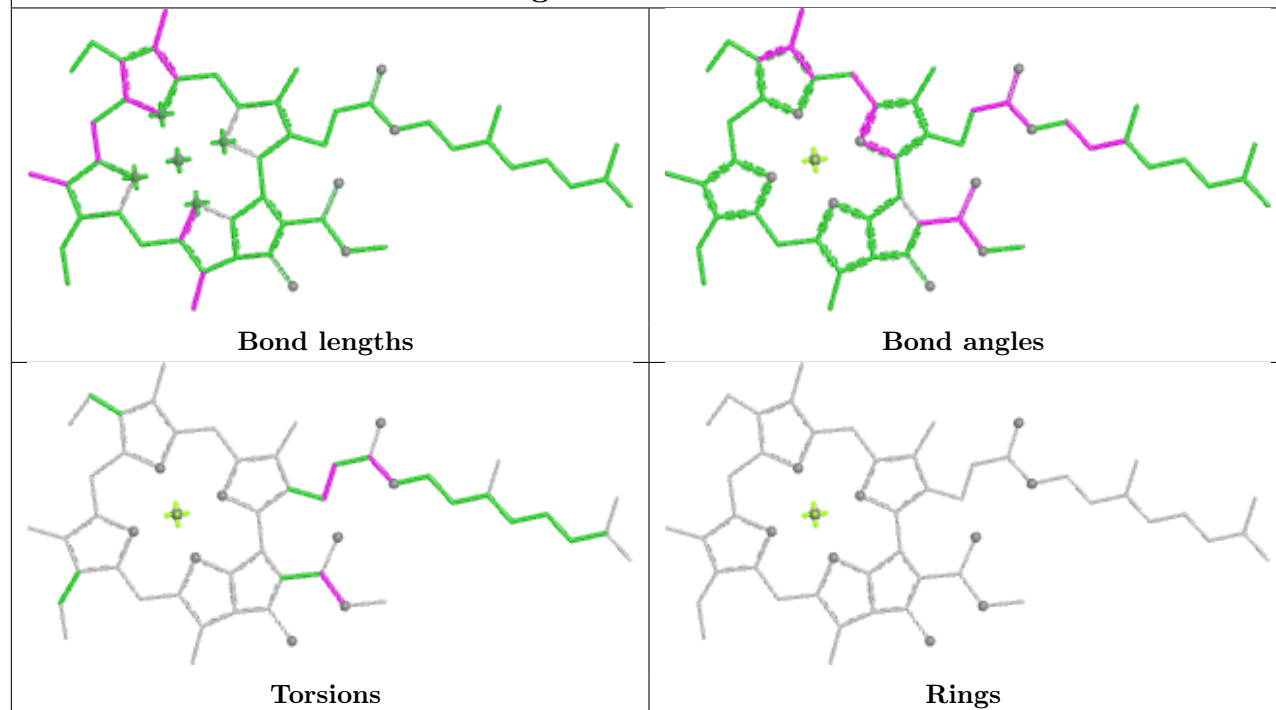


Rings

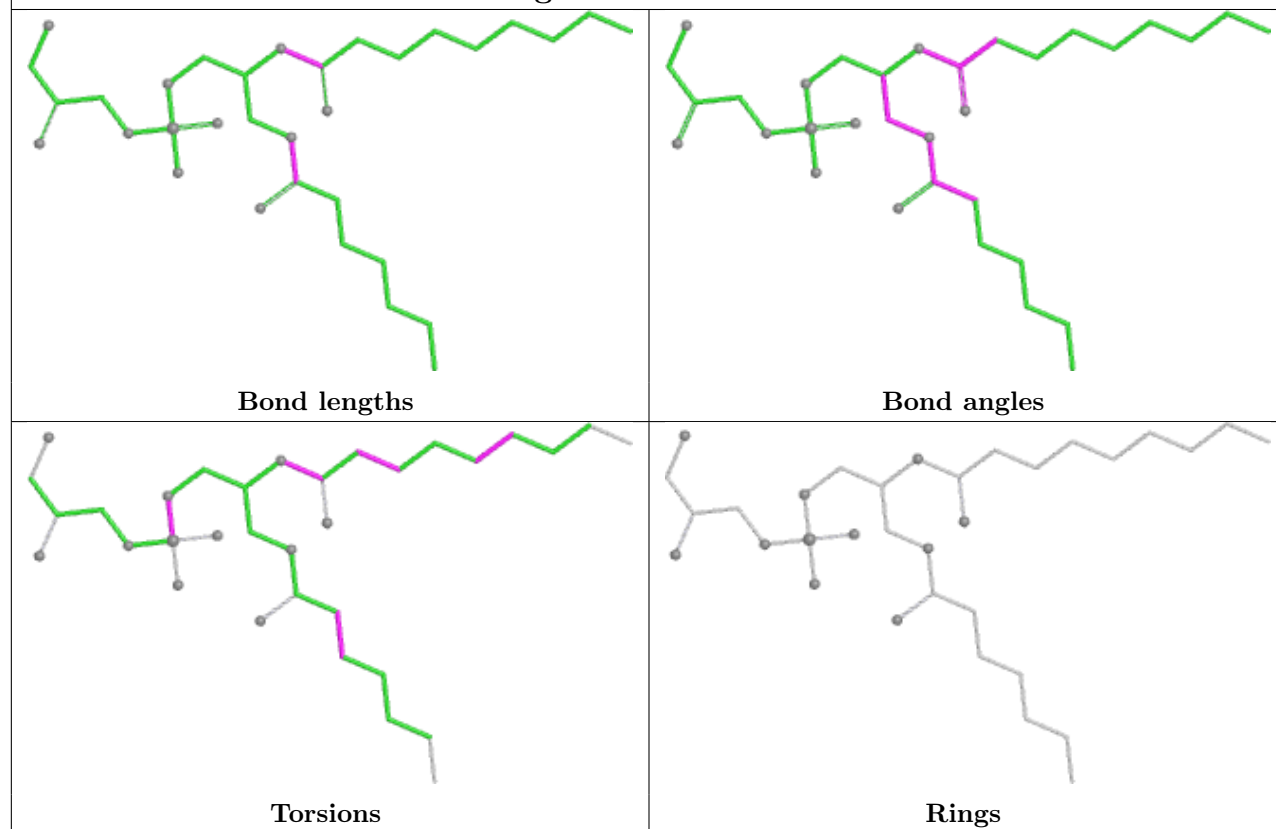




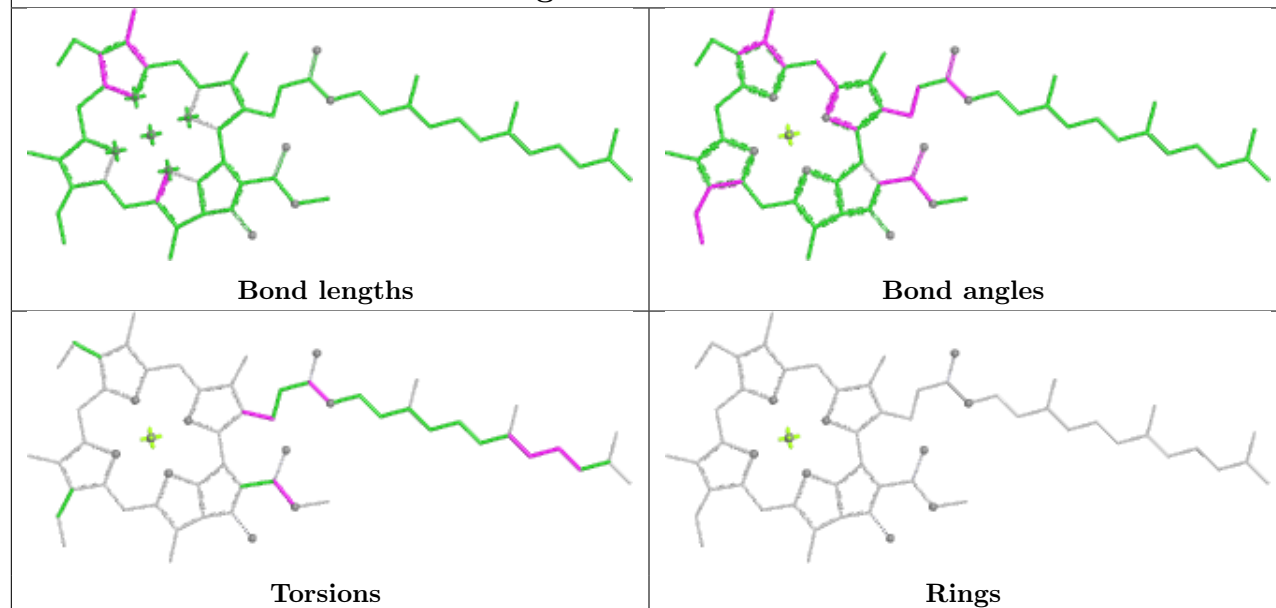
Ligand CLA U 311



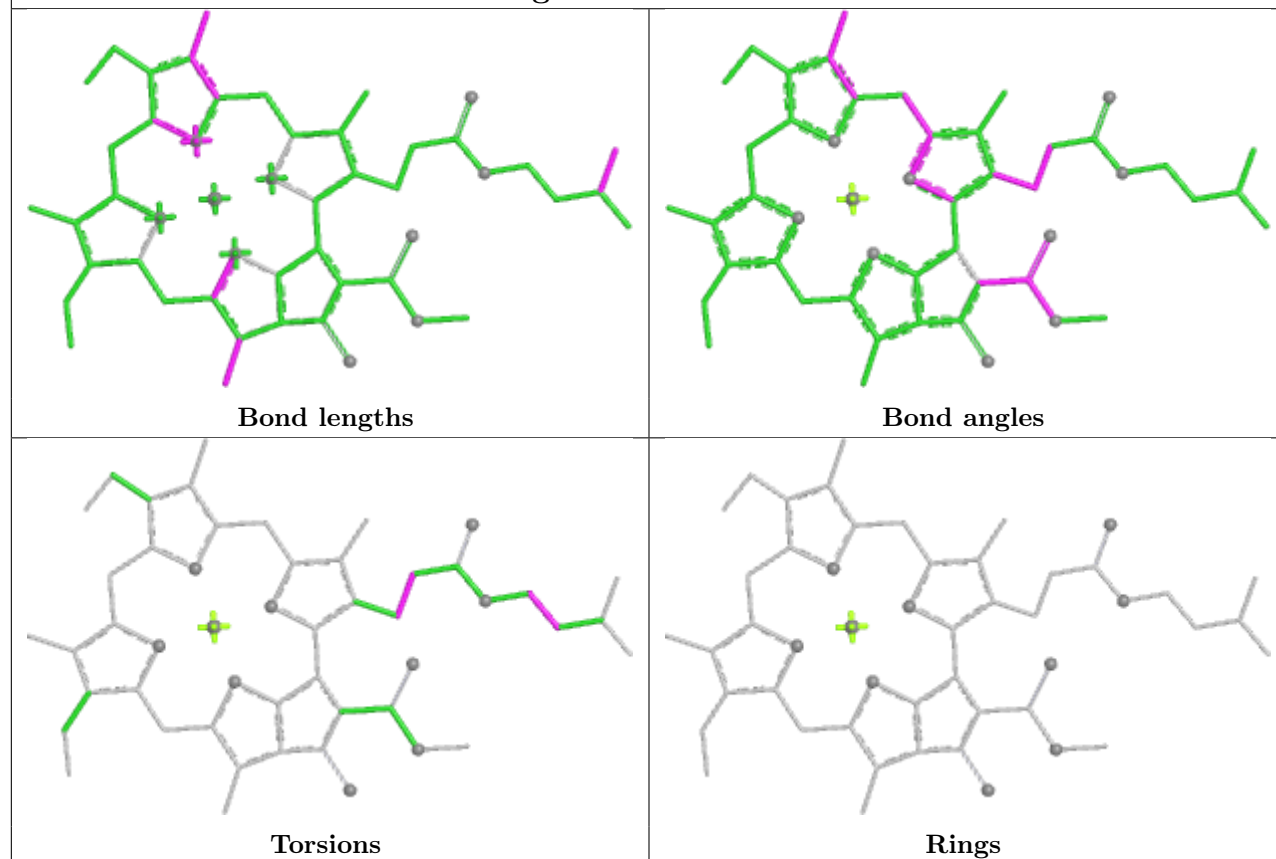
Ligand LHG 2 619



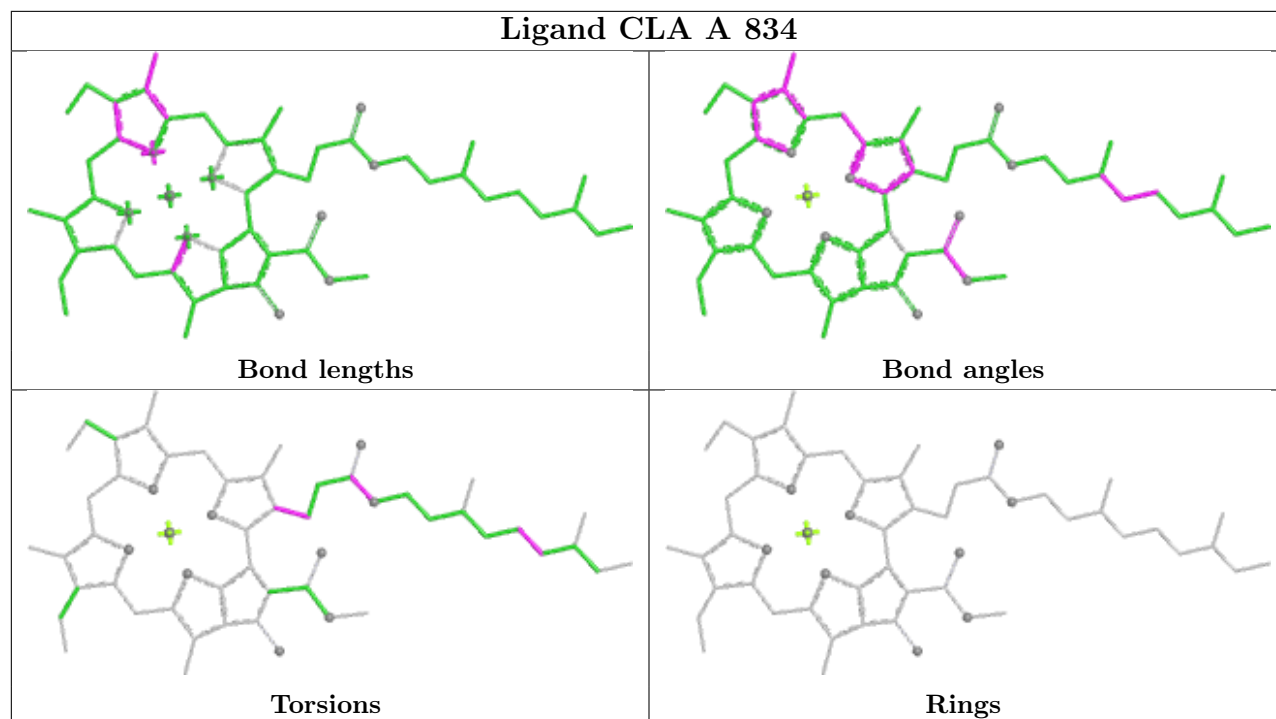
Ligand CLA 5 602



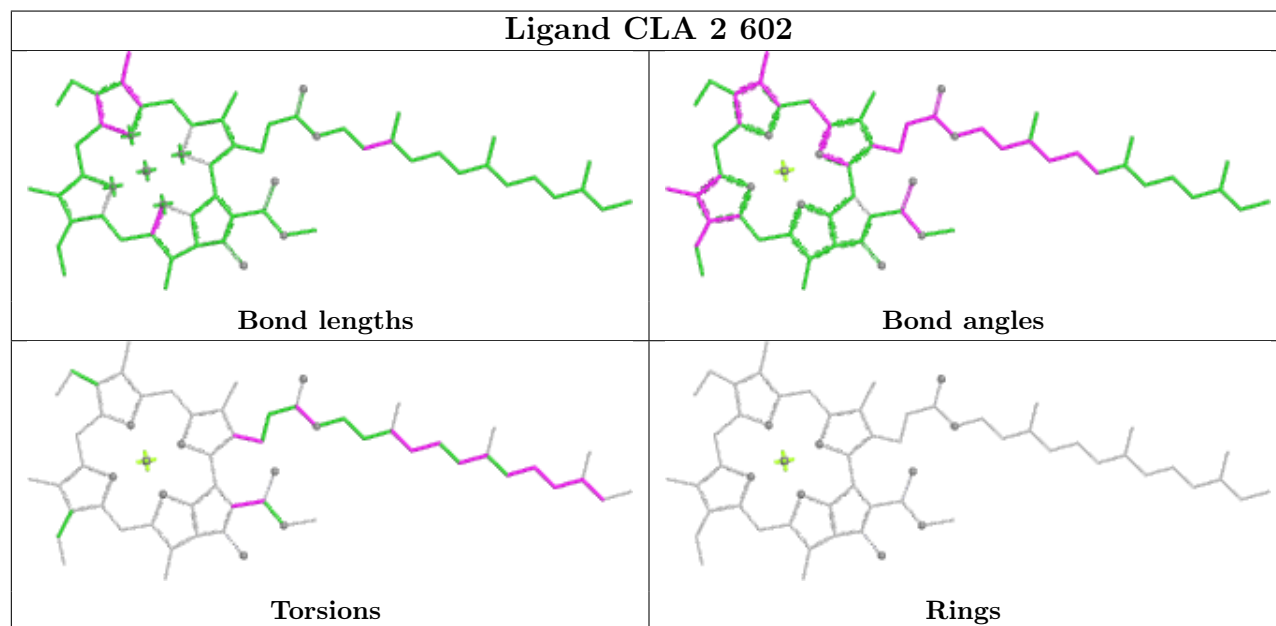
Ligand CLA B 822



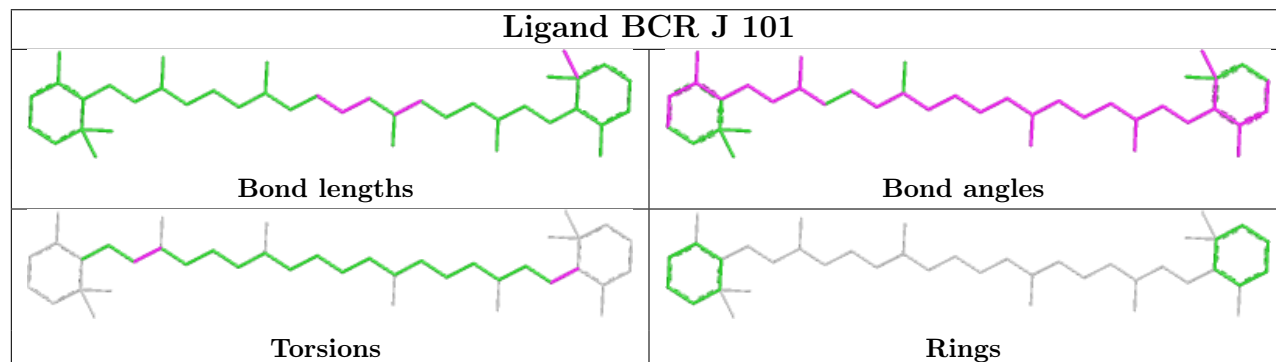
Ligand CLA A 834

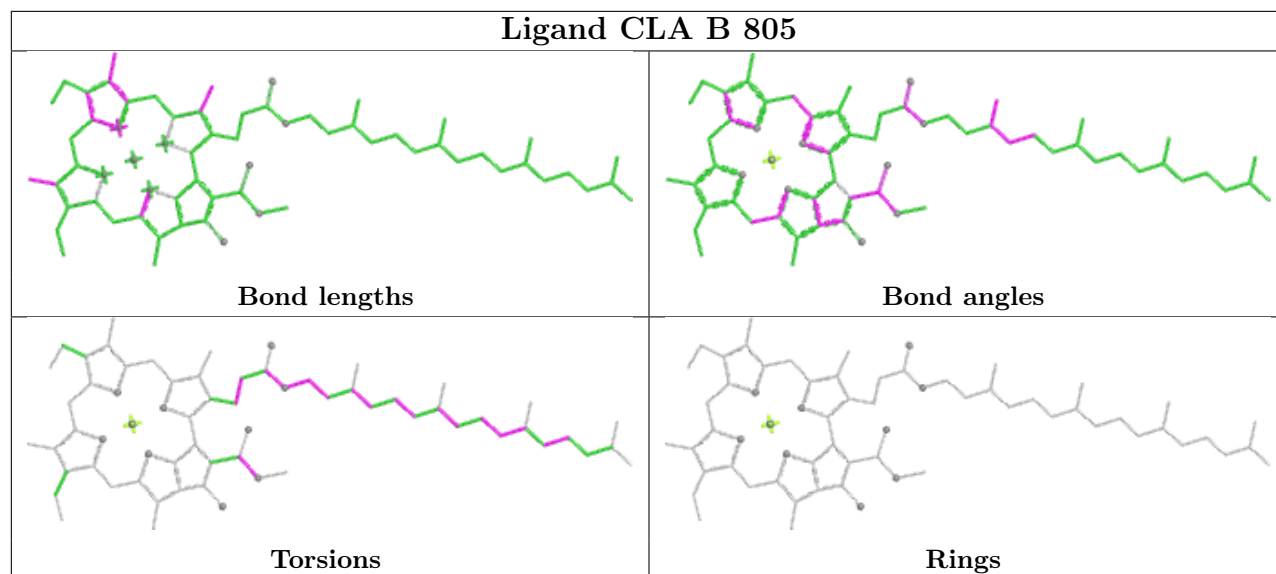
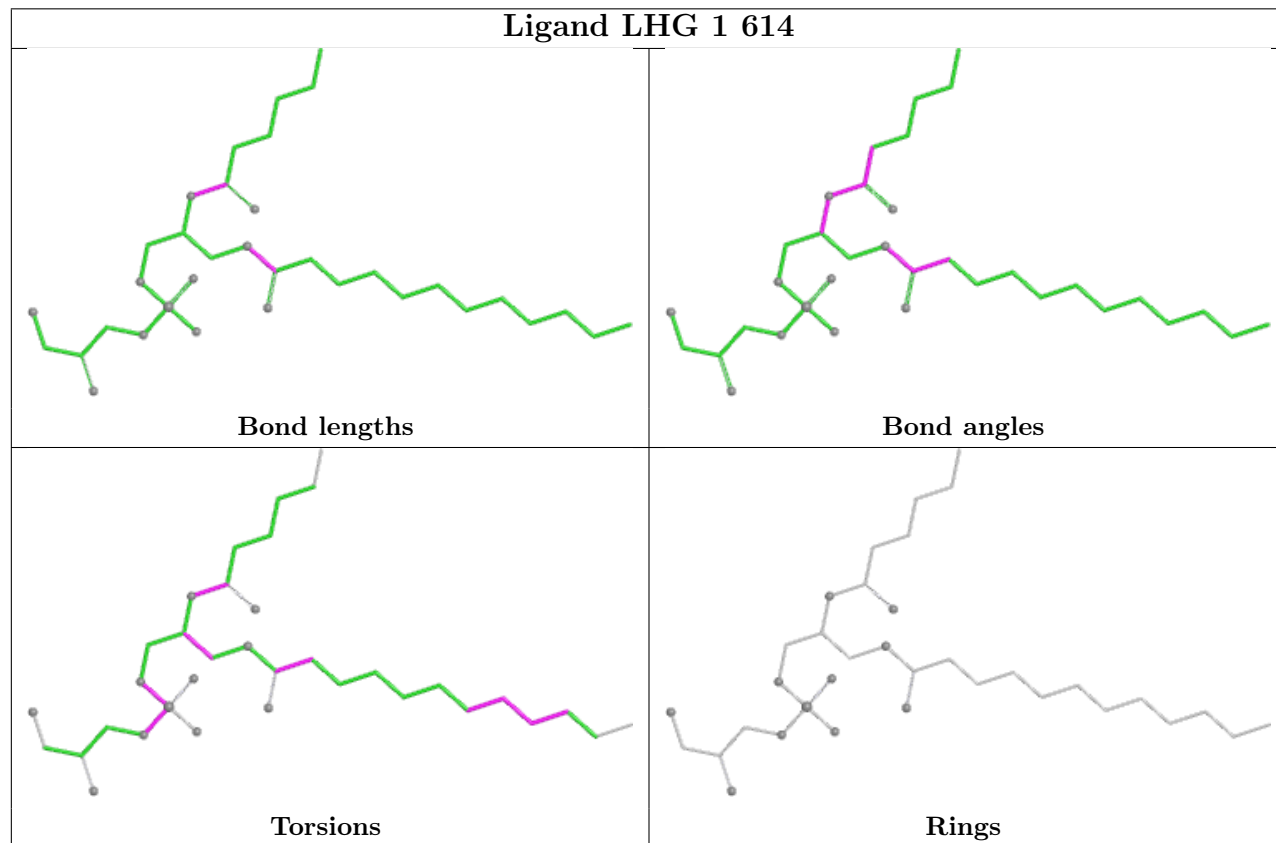


Ligand CLA 2 602

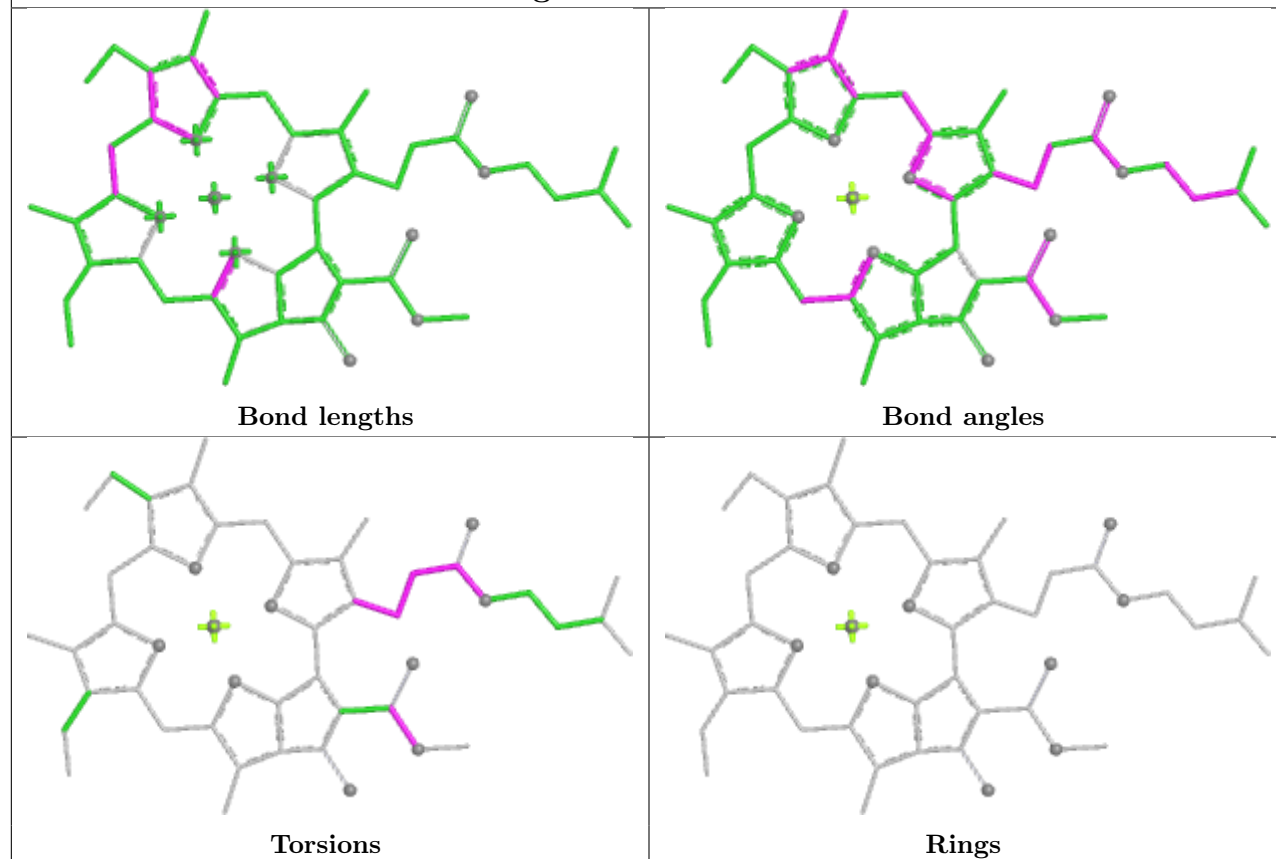


Ligand BCR J 101

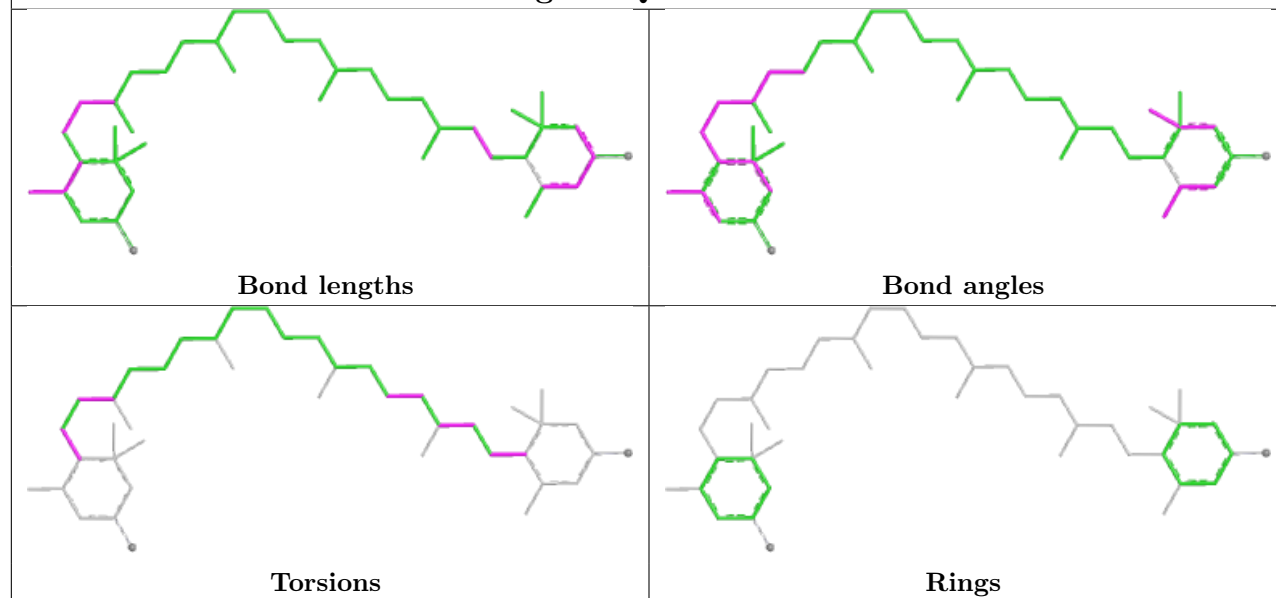


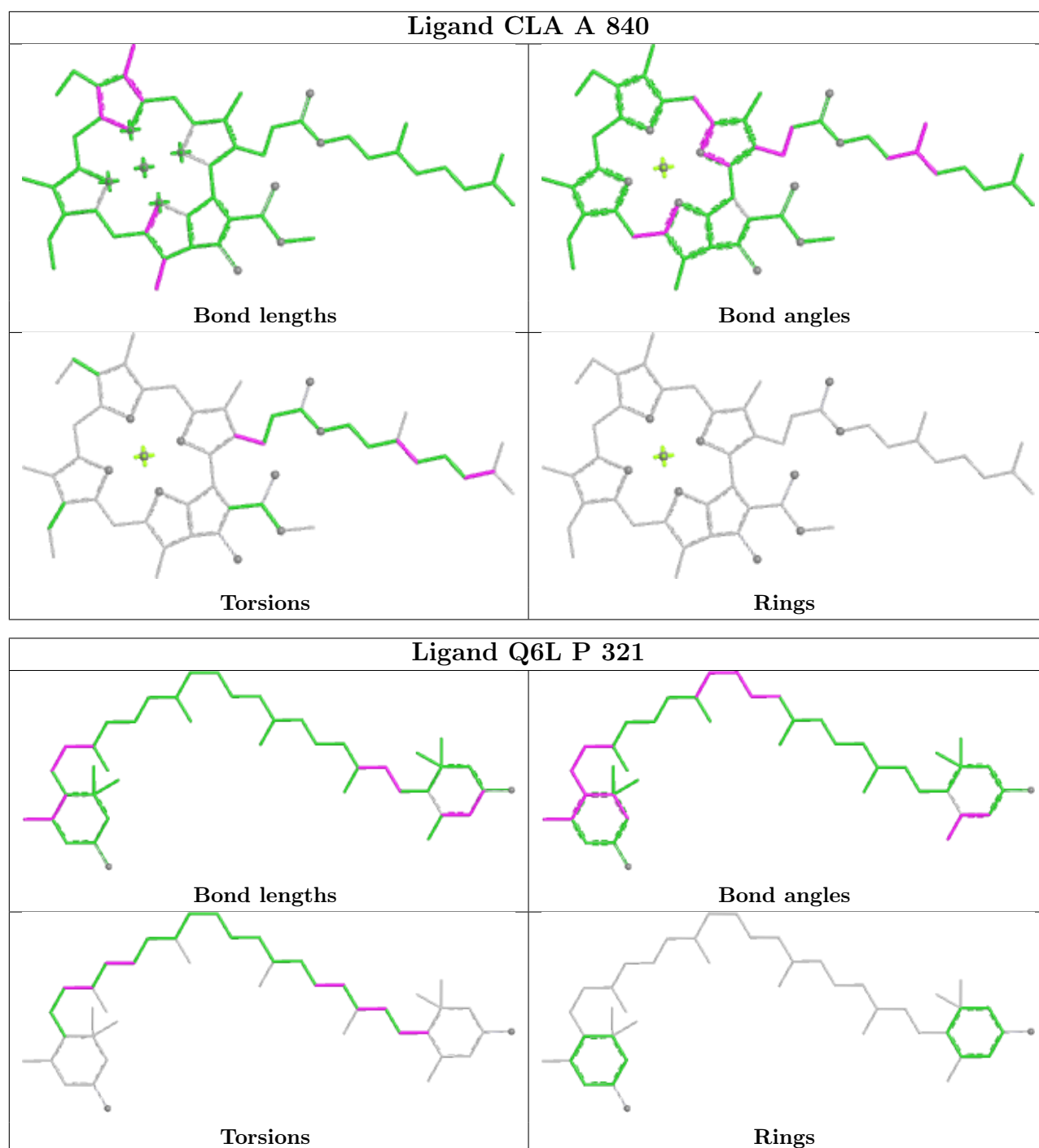
Ligand CLA B 805**Ligand LHG 1 614**

Ligand CLA P 303

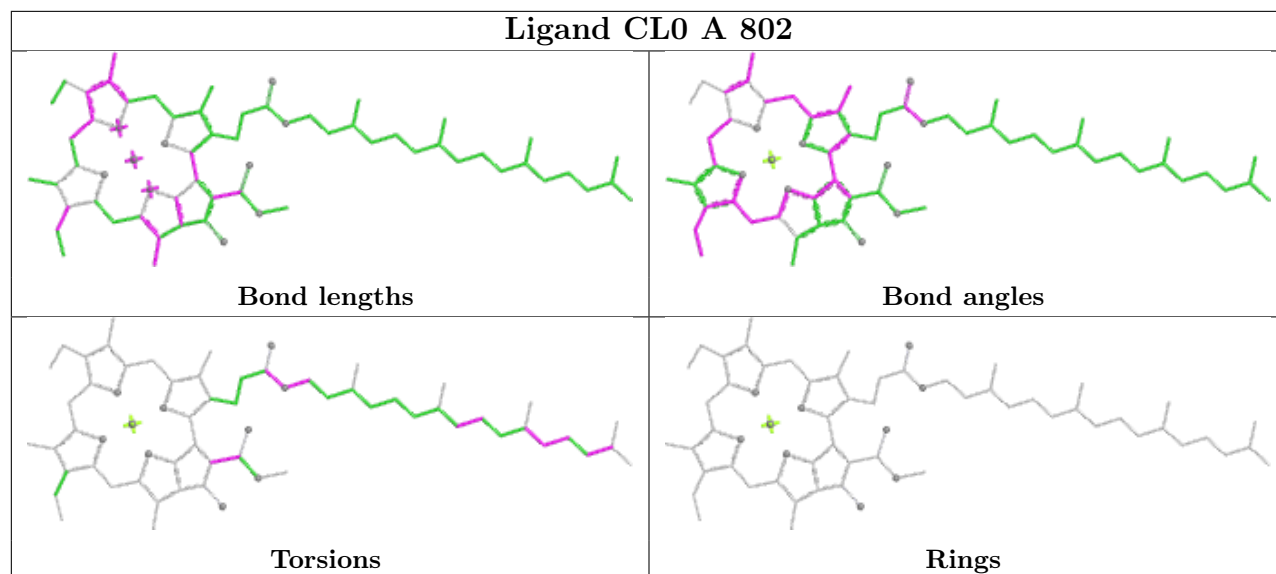


Ligand Q6L V 321

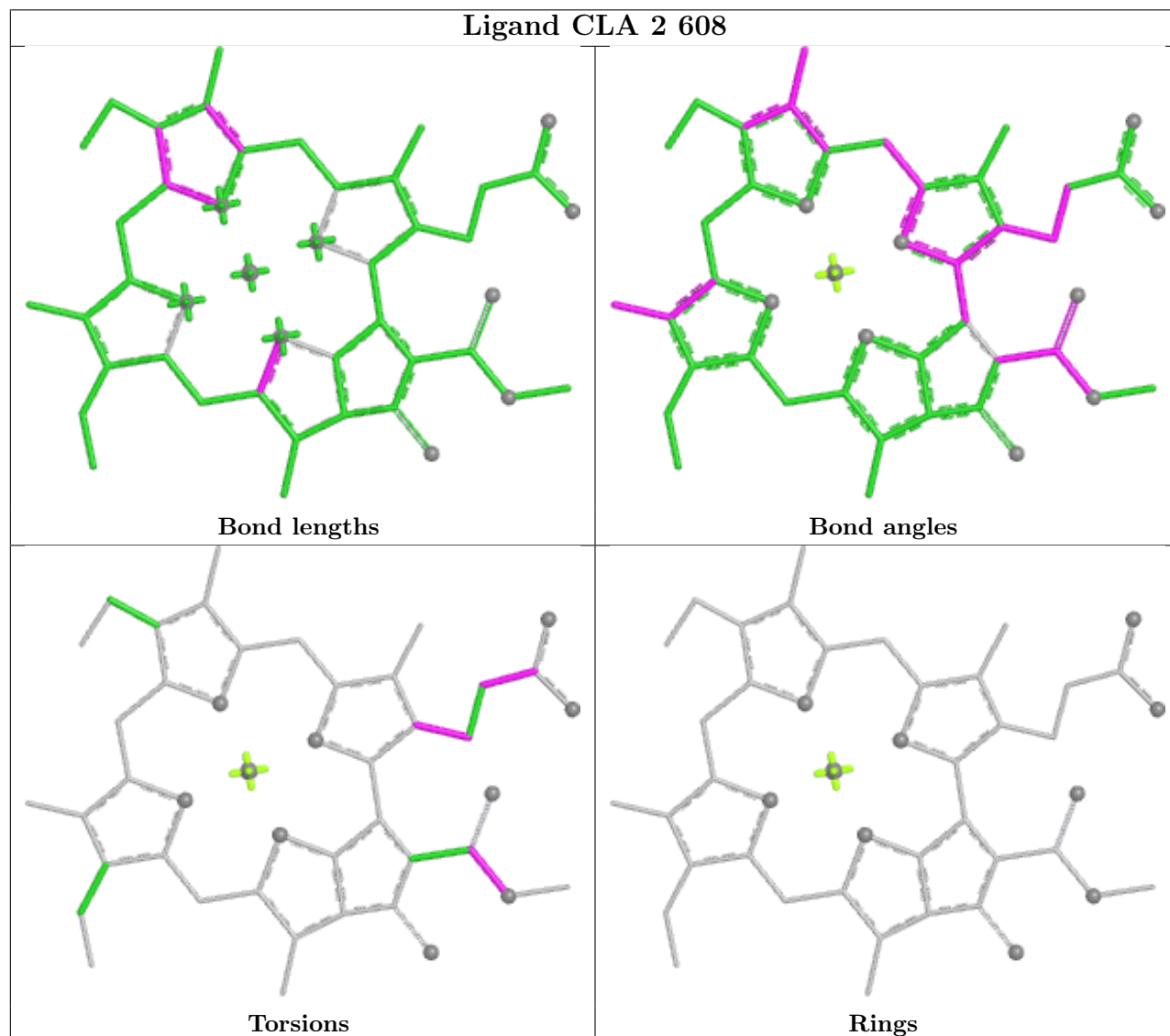




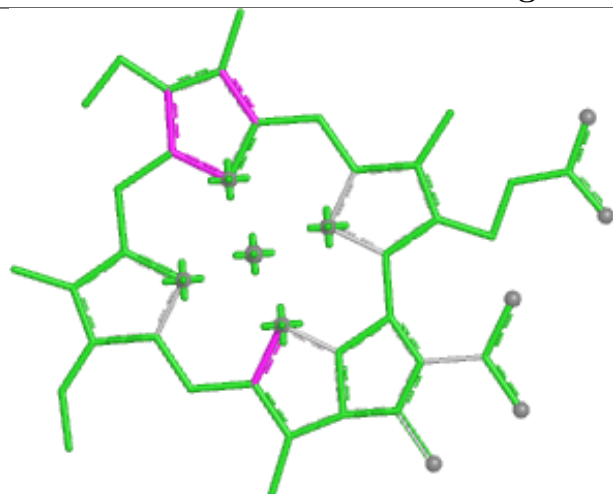
Ligand CL0 A 802



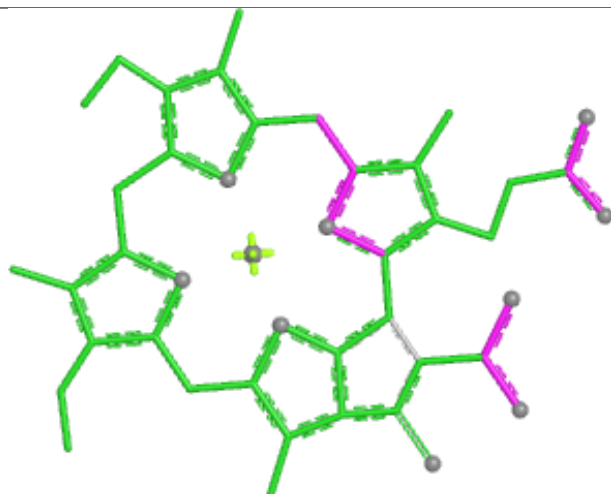
Ligand CLA 2 608



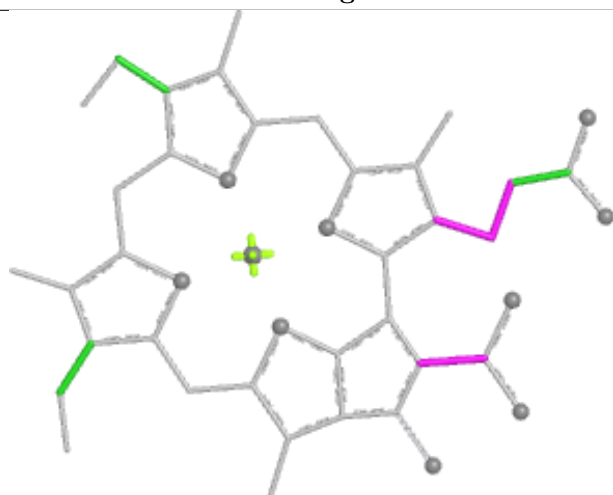
Ligand CLA 2 611



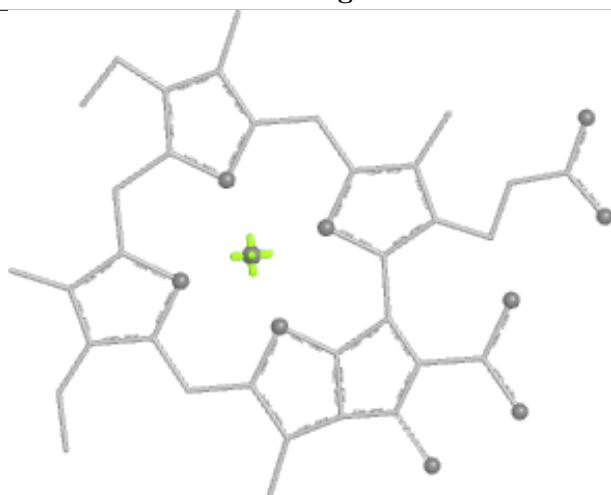
Bond lengths



Bond angles

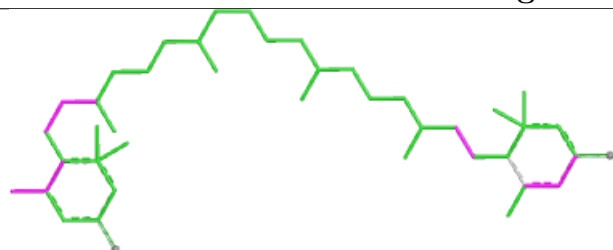


Torsions

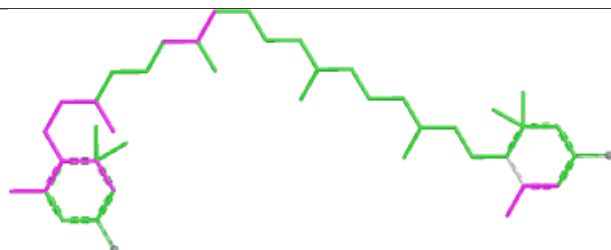


Rings

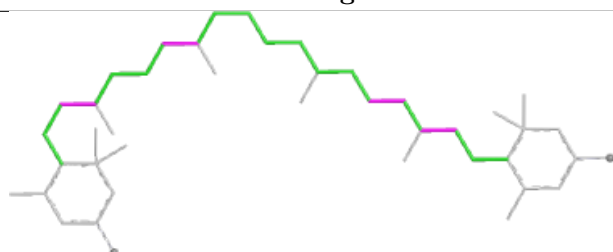
Ligand Q6L U 314



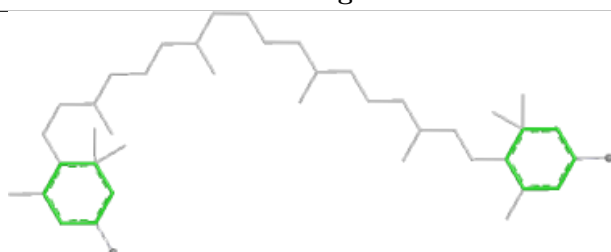
Bond lengths



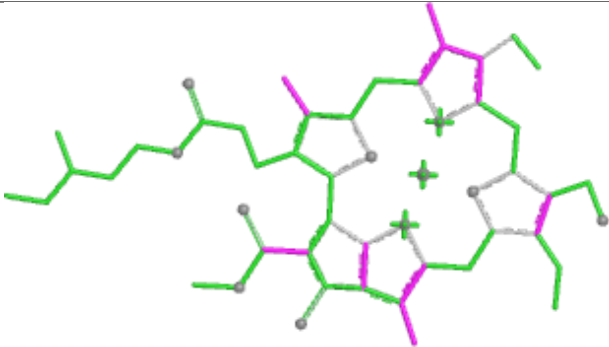
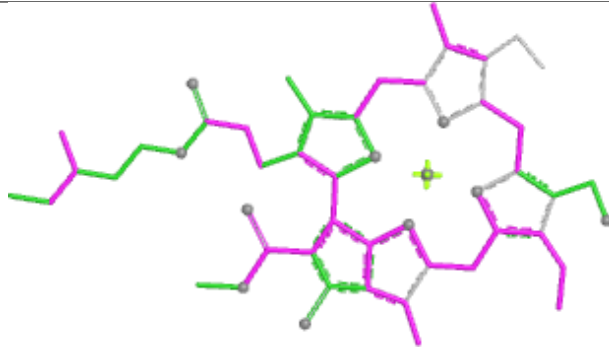
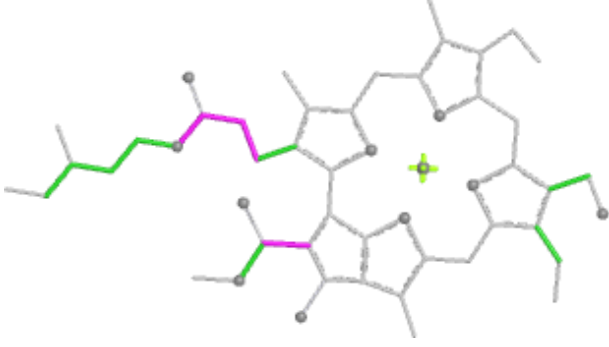
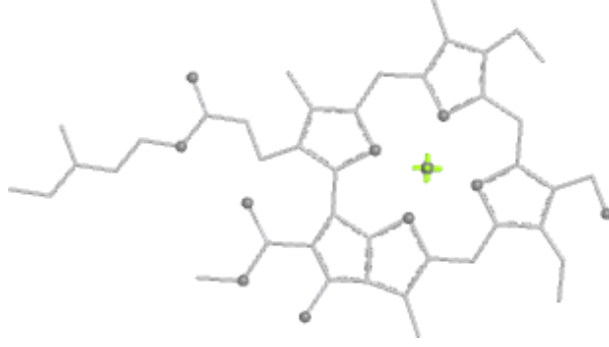
Bond angles

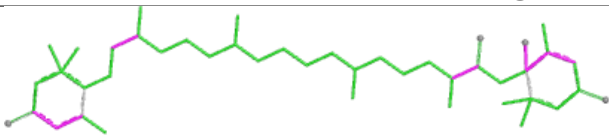
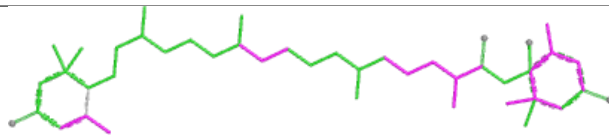
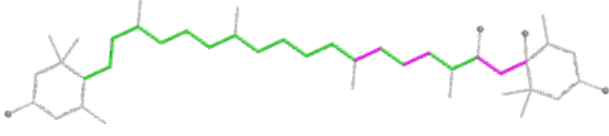
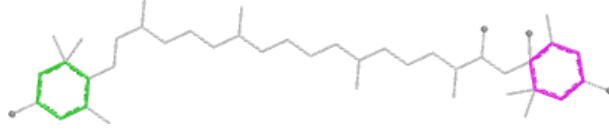


Torsions

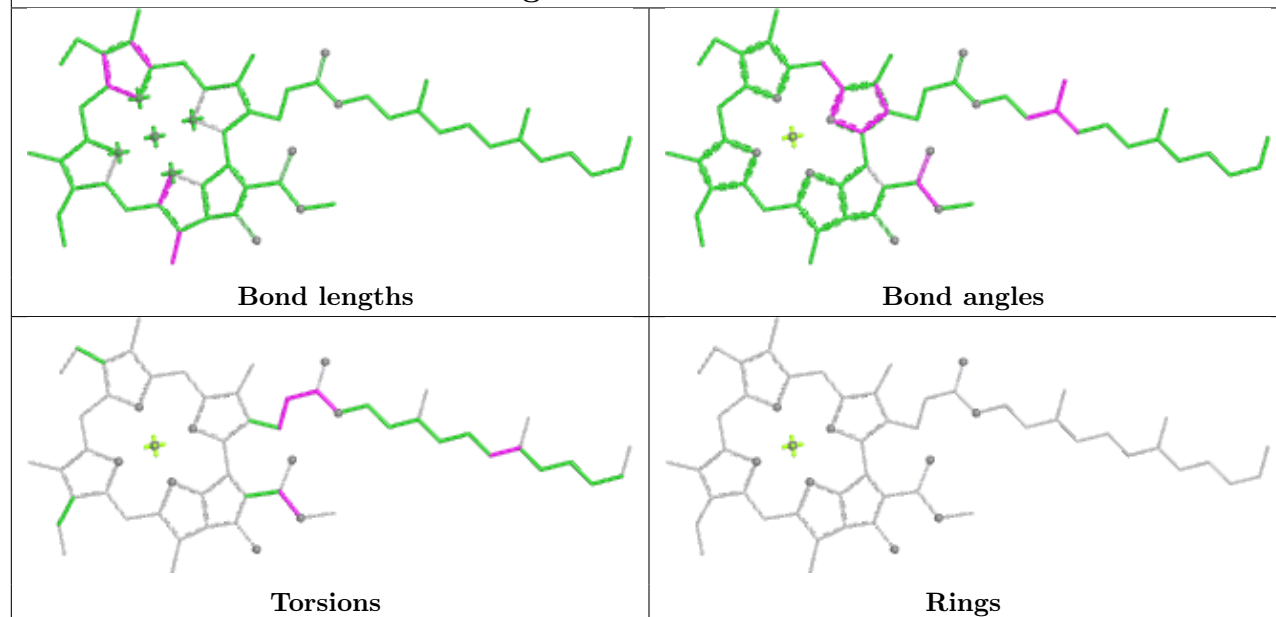


Rings

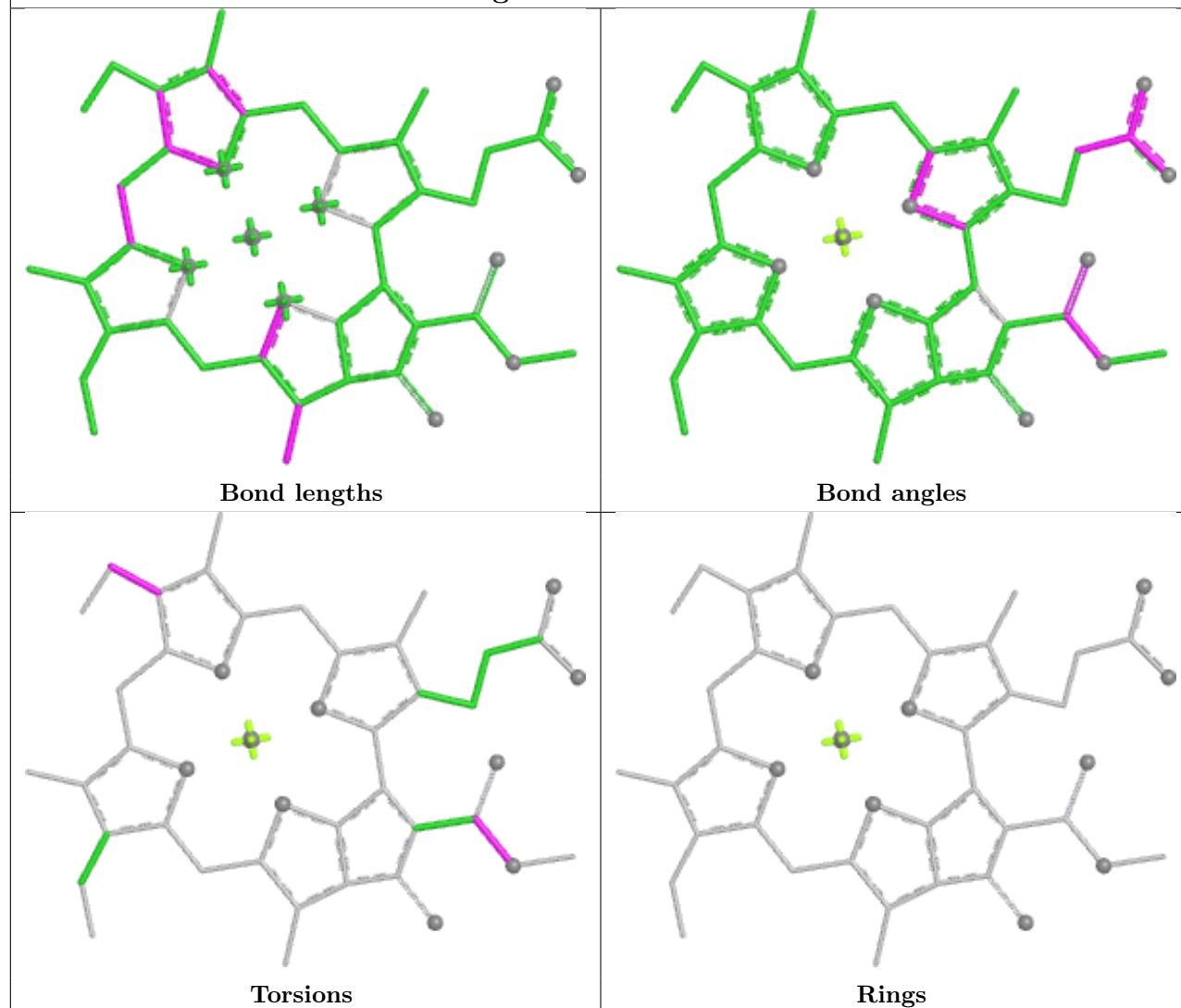
Ligand CHL T 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

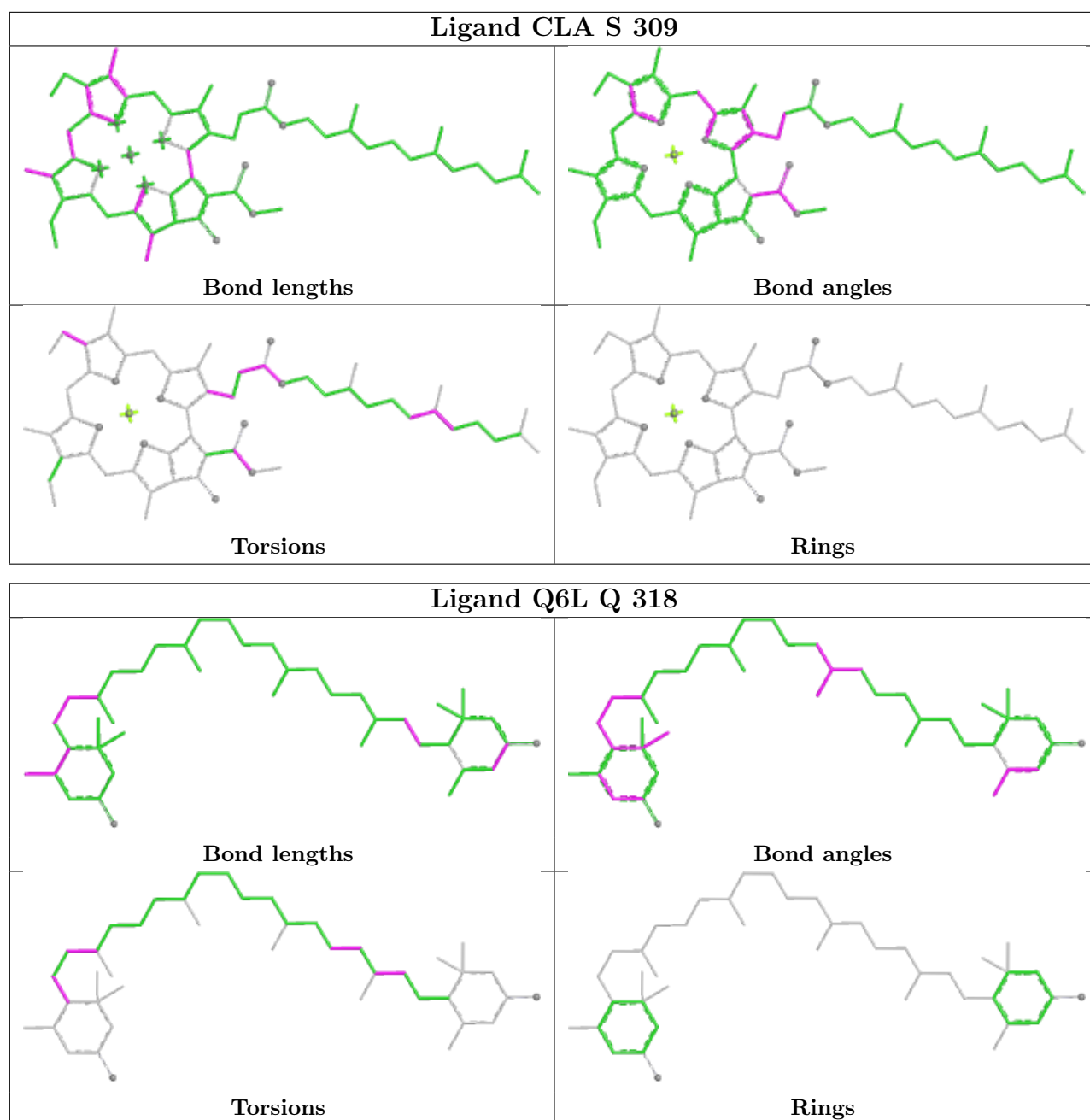
Ligand IWJ X 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA O 2001

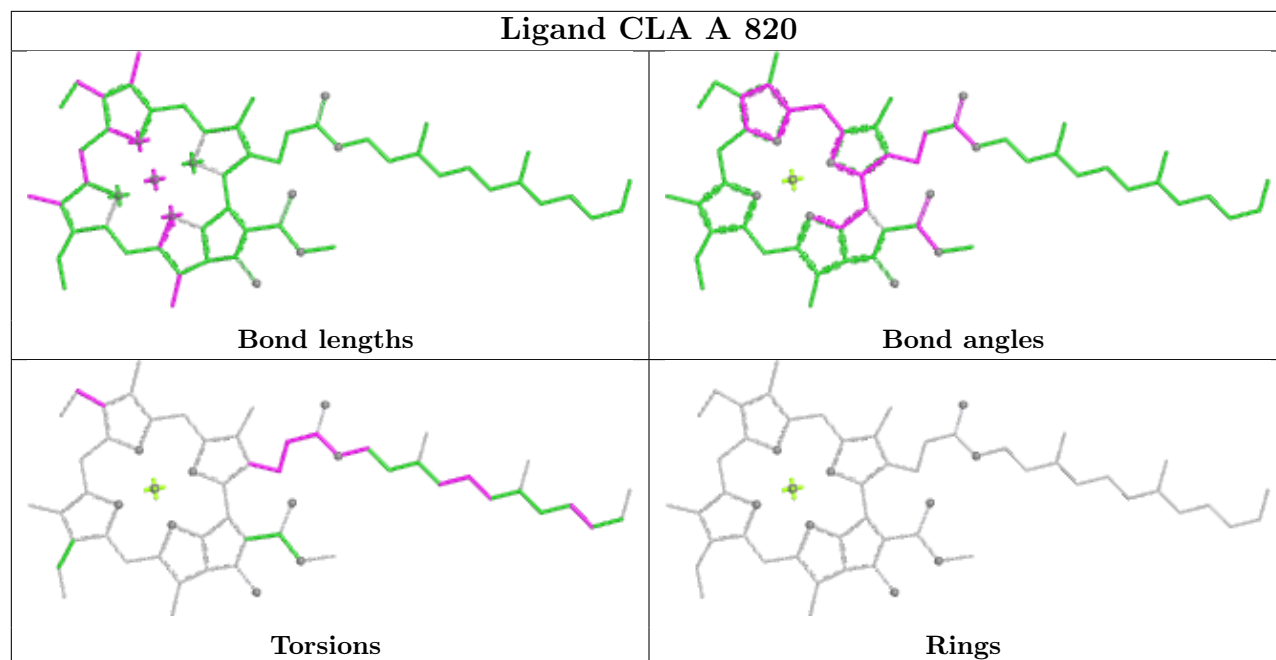


Ligand CLA B 835

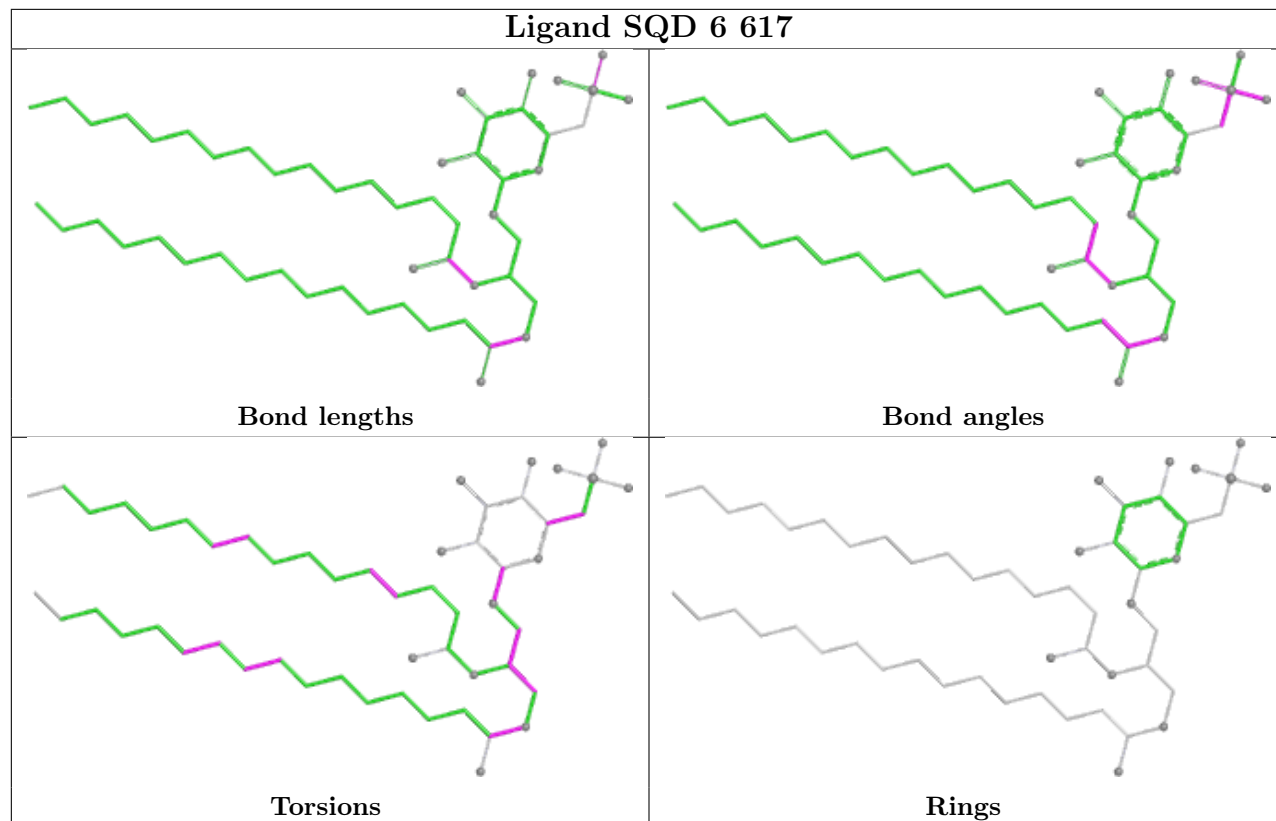




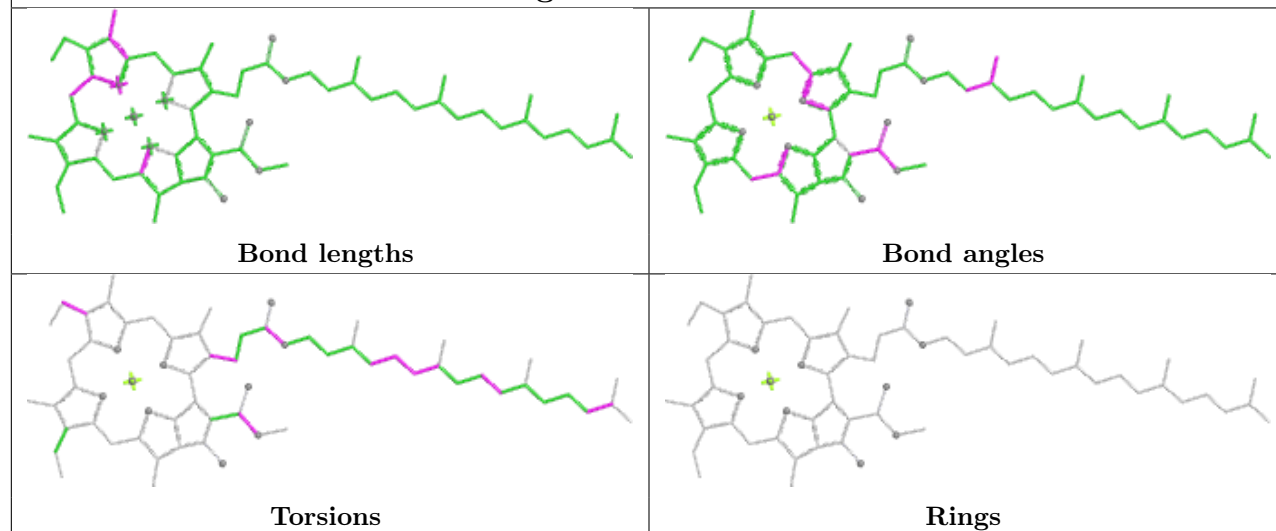
Ligand CLA A 820



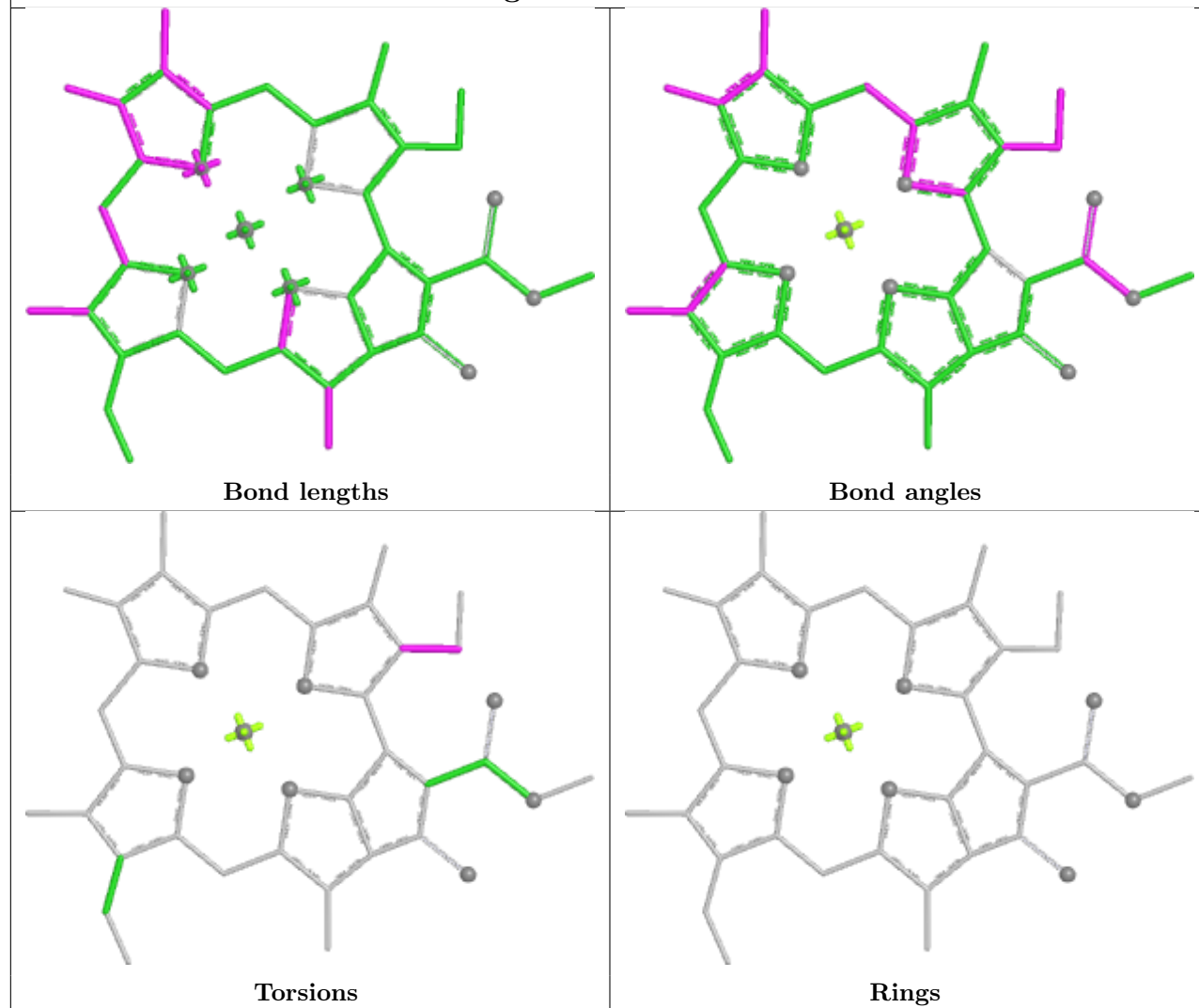
Ligand SQD 6 617



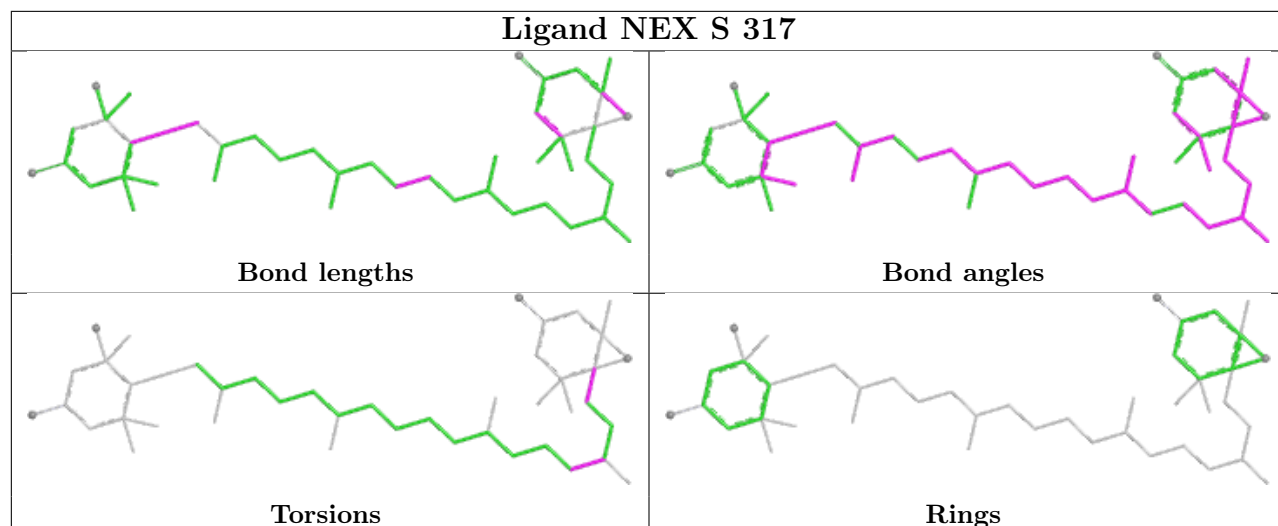
Ligand CLA 5 607



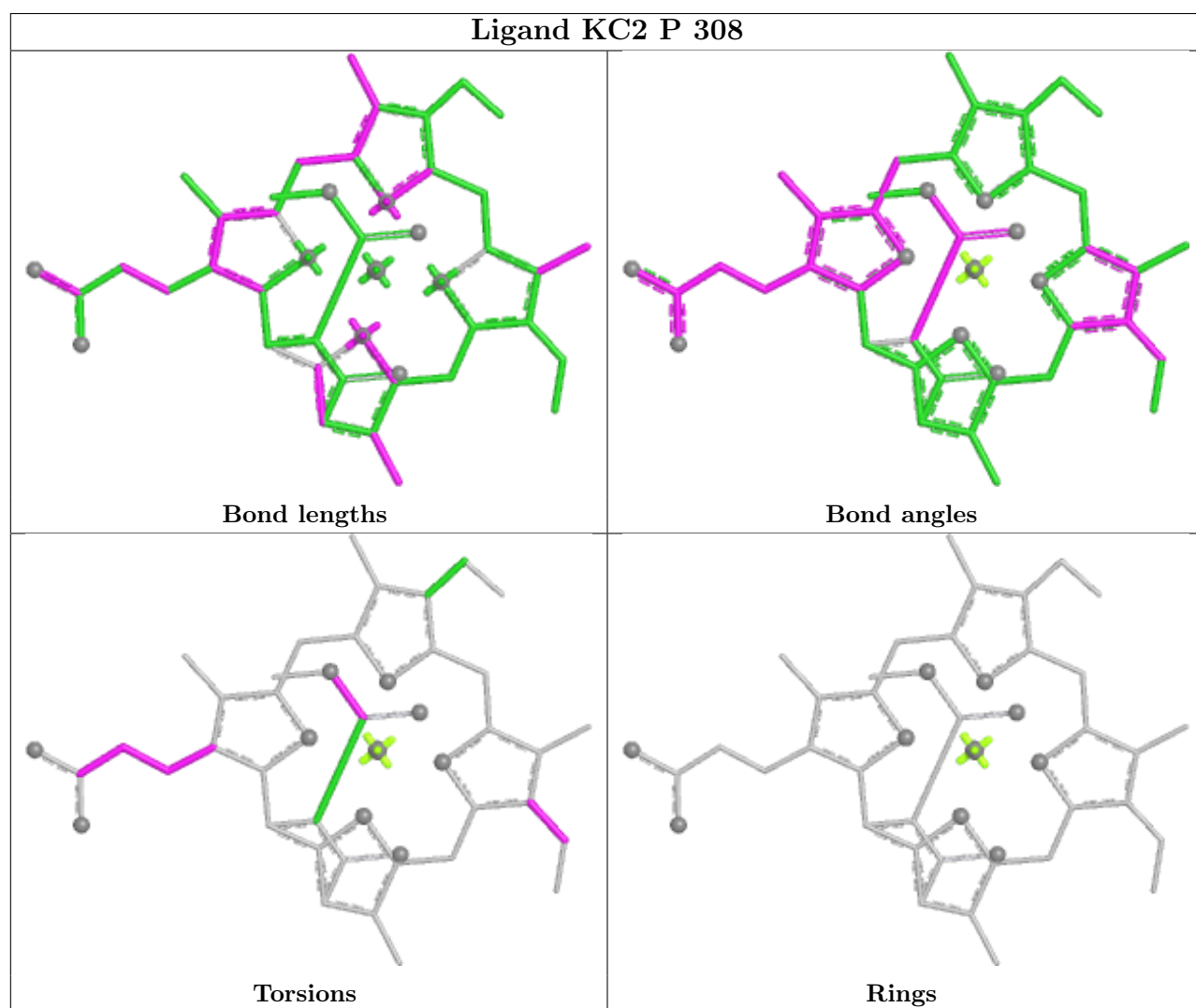
Ligand CLA 3 305

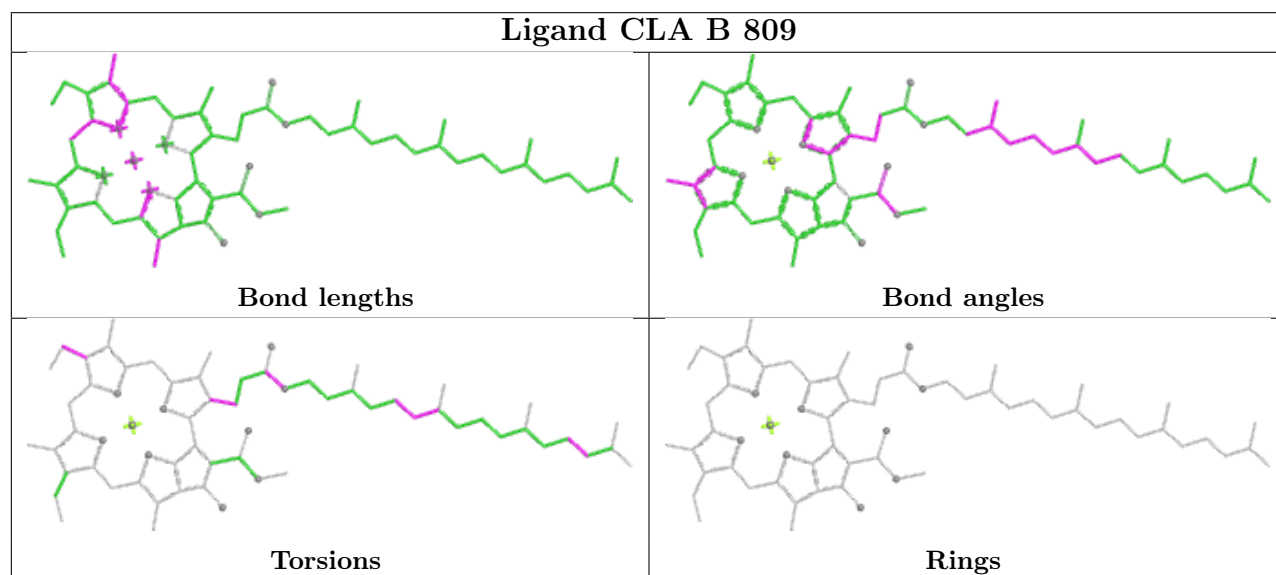
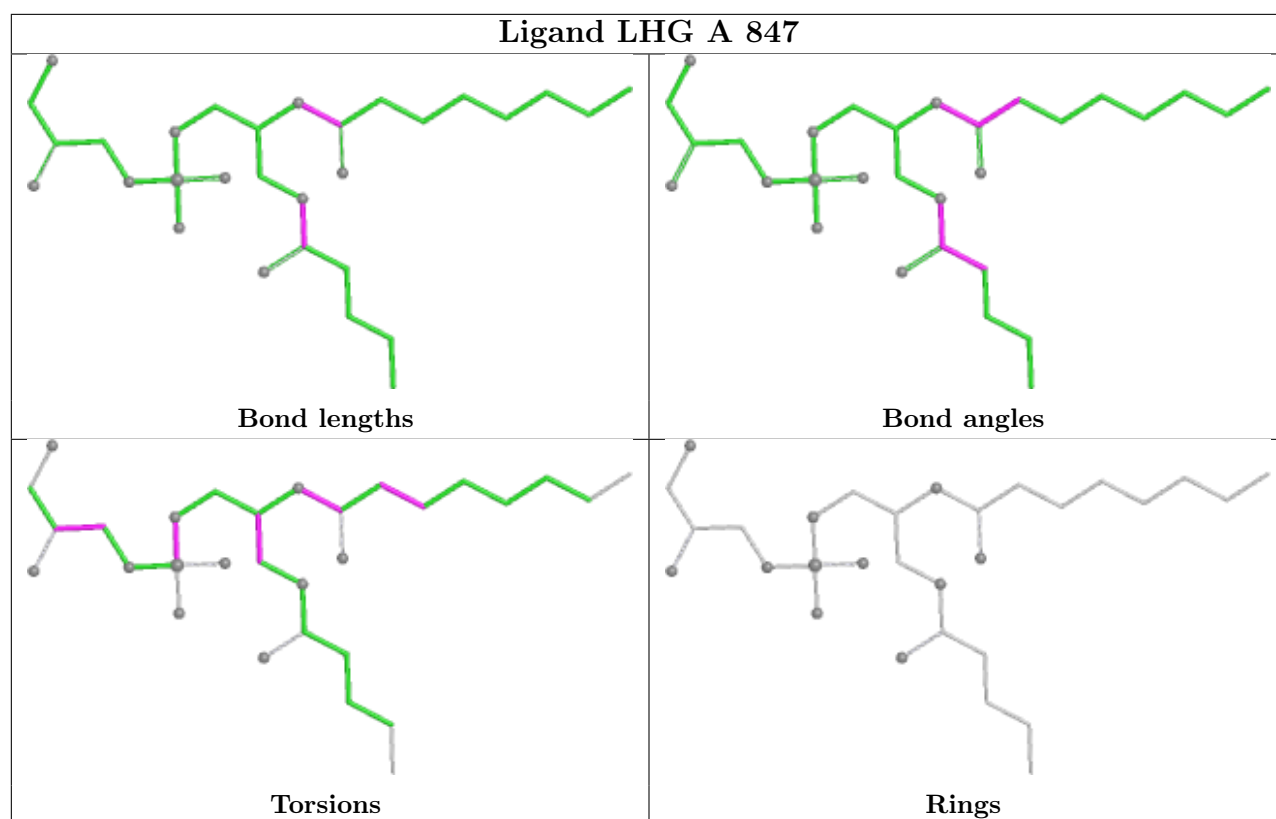


Ligand NEX S 317

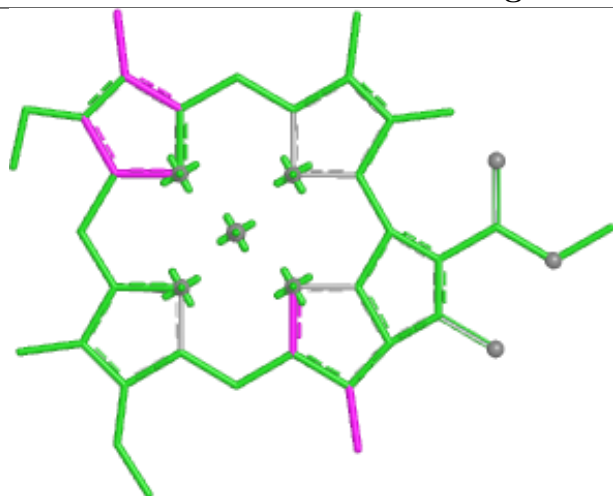


Ligand KC2 P 308

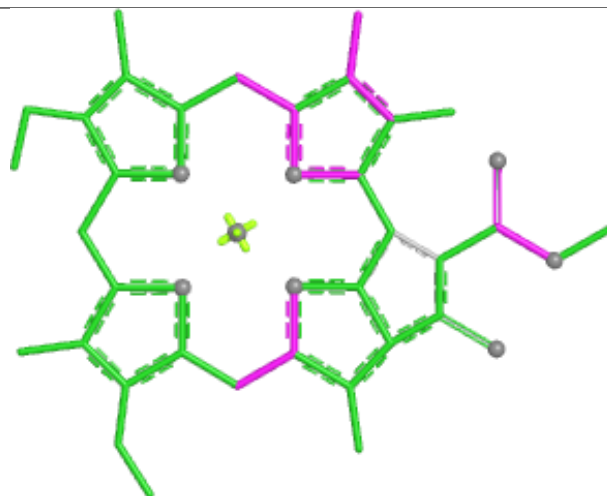




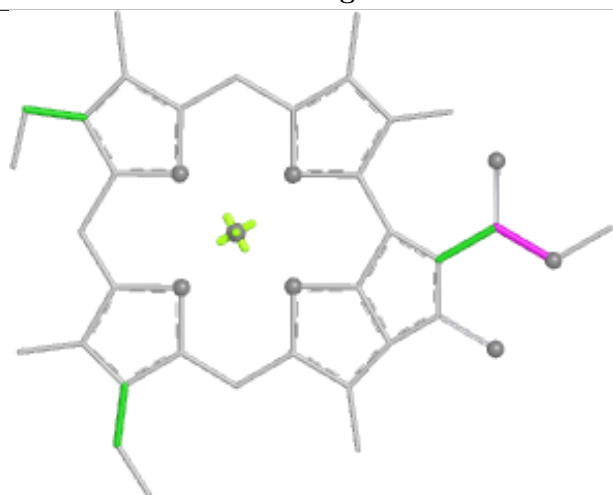
Ligand CLA O 2005



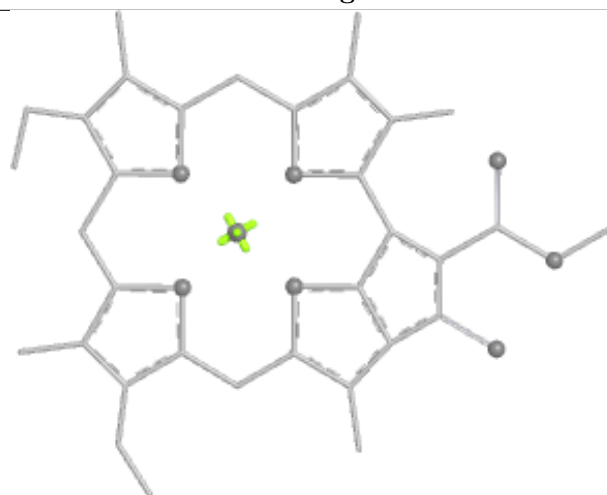
Bond lengths



Bond angles

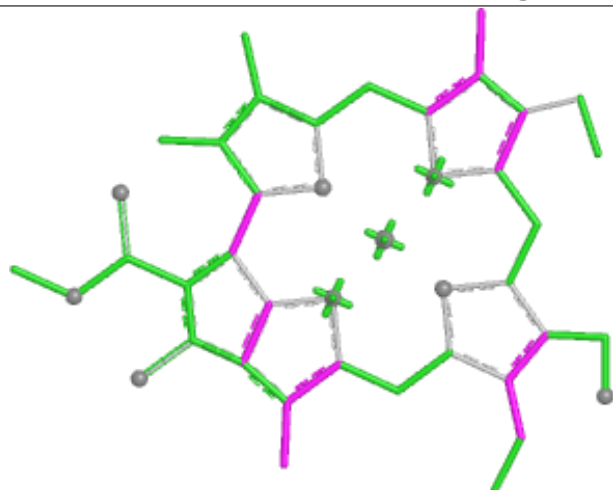


Torsions

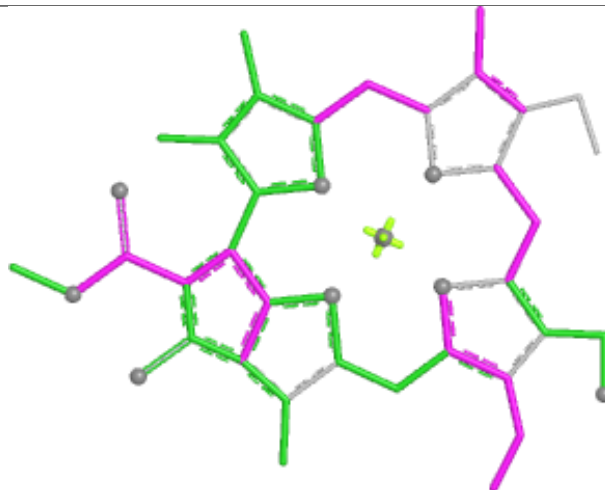


Rings

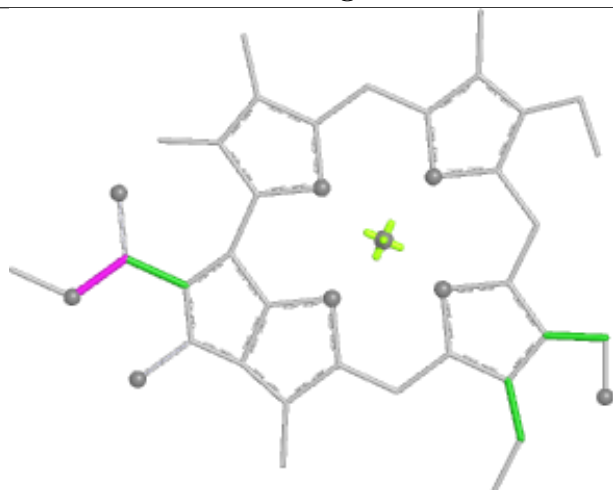
Ligand CHL T 314



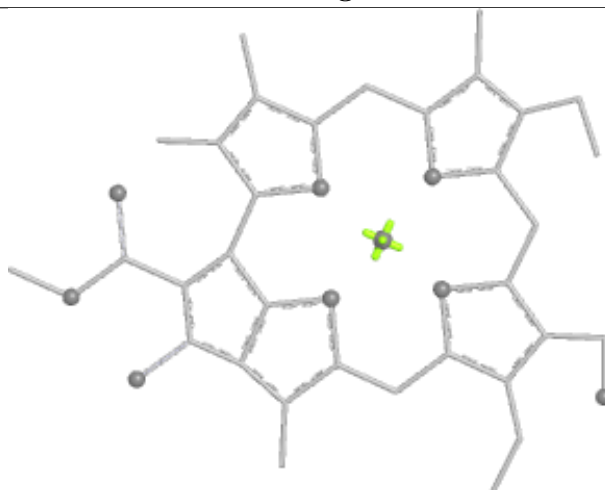
Bond lengths



Bond angles

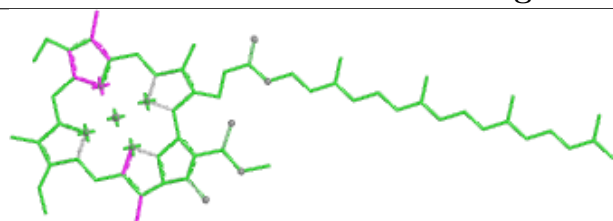


Torsions



Rings

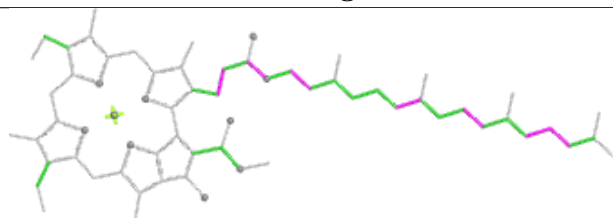
Ligand CLA B 802



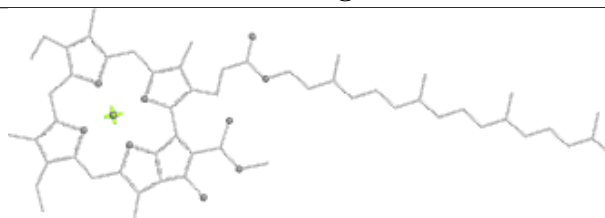
Bond lengths



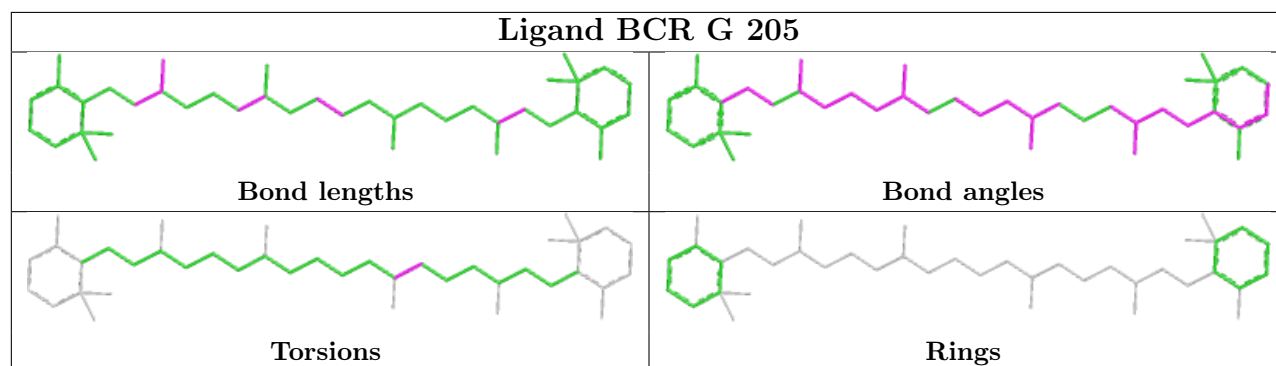
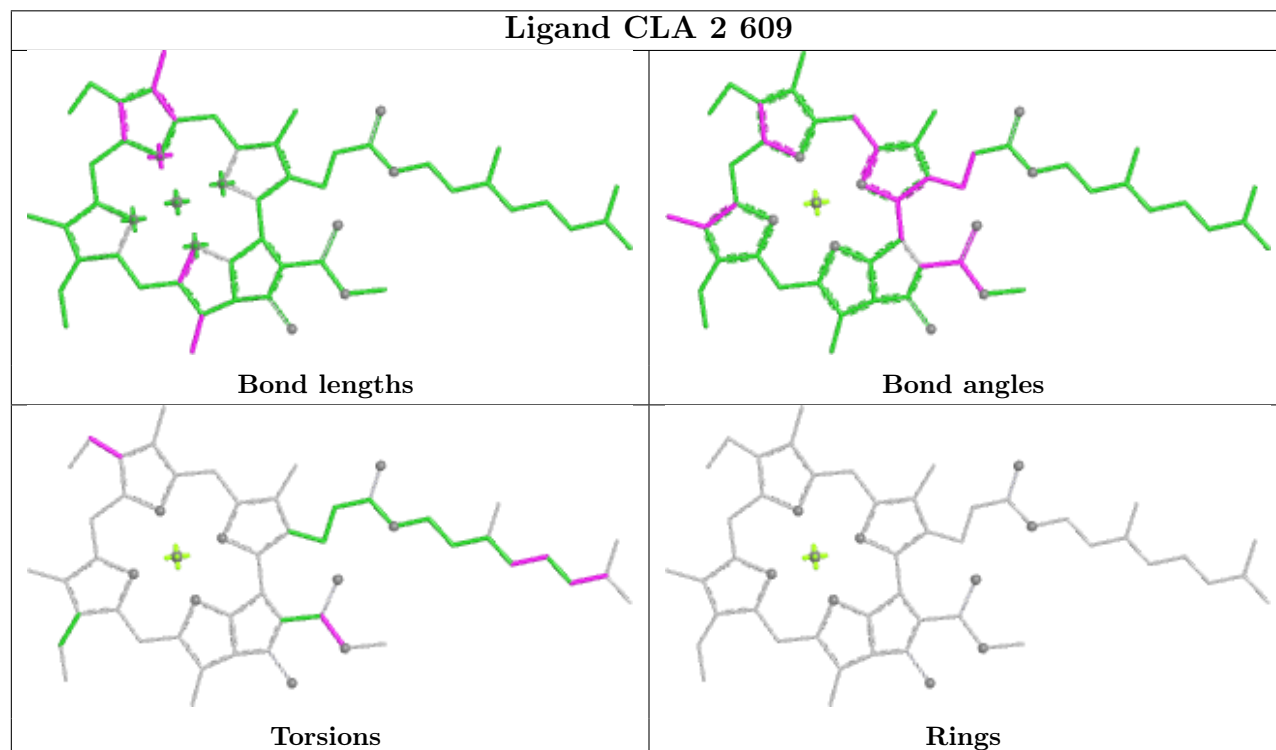
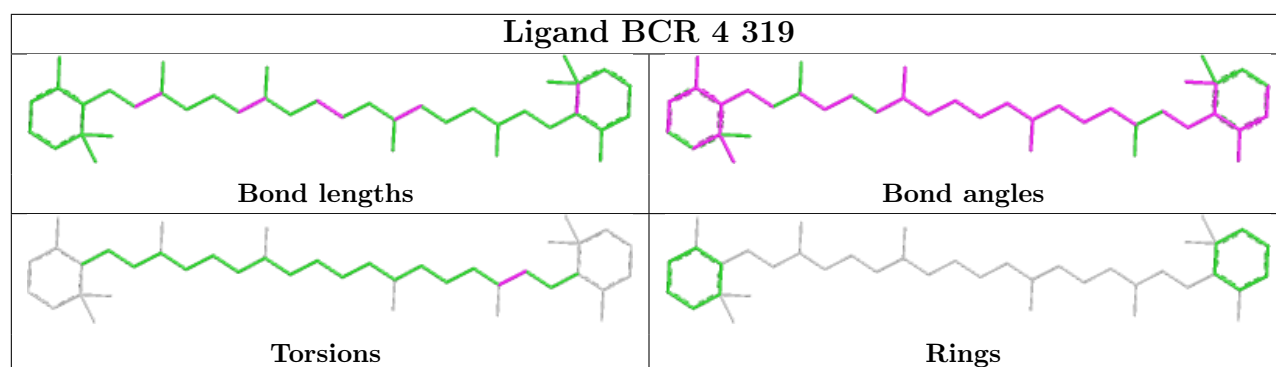
Bond angles

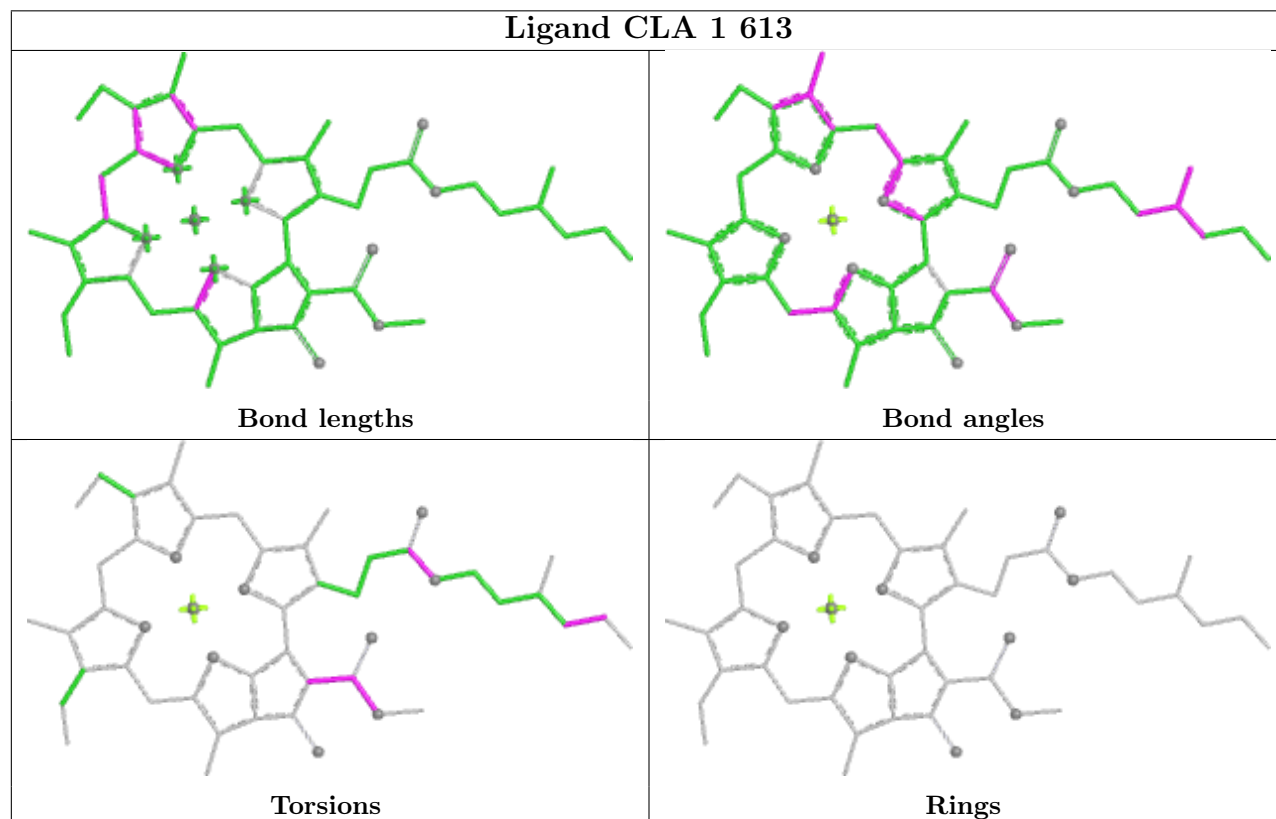
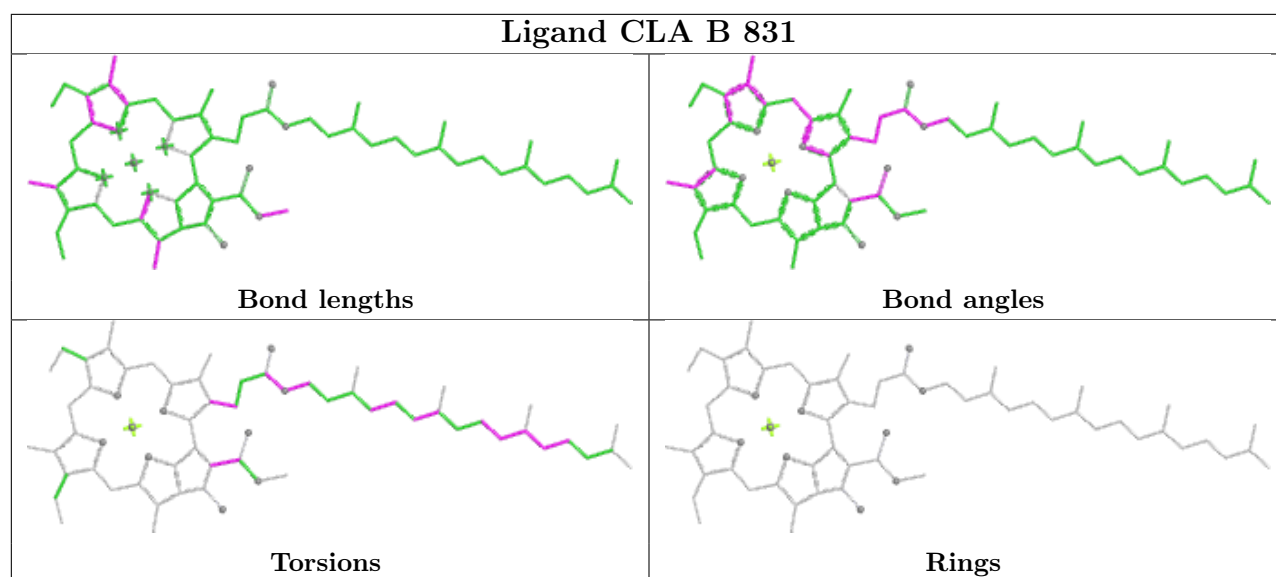


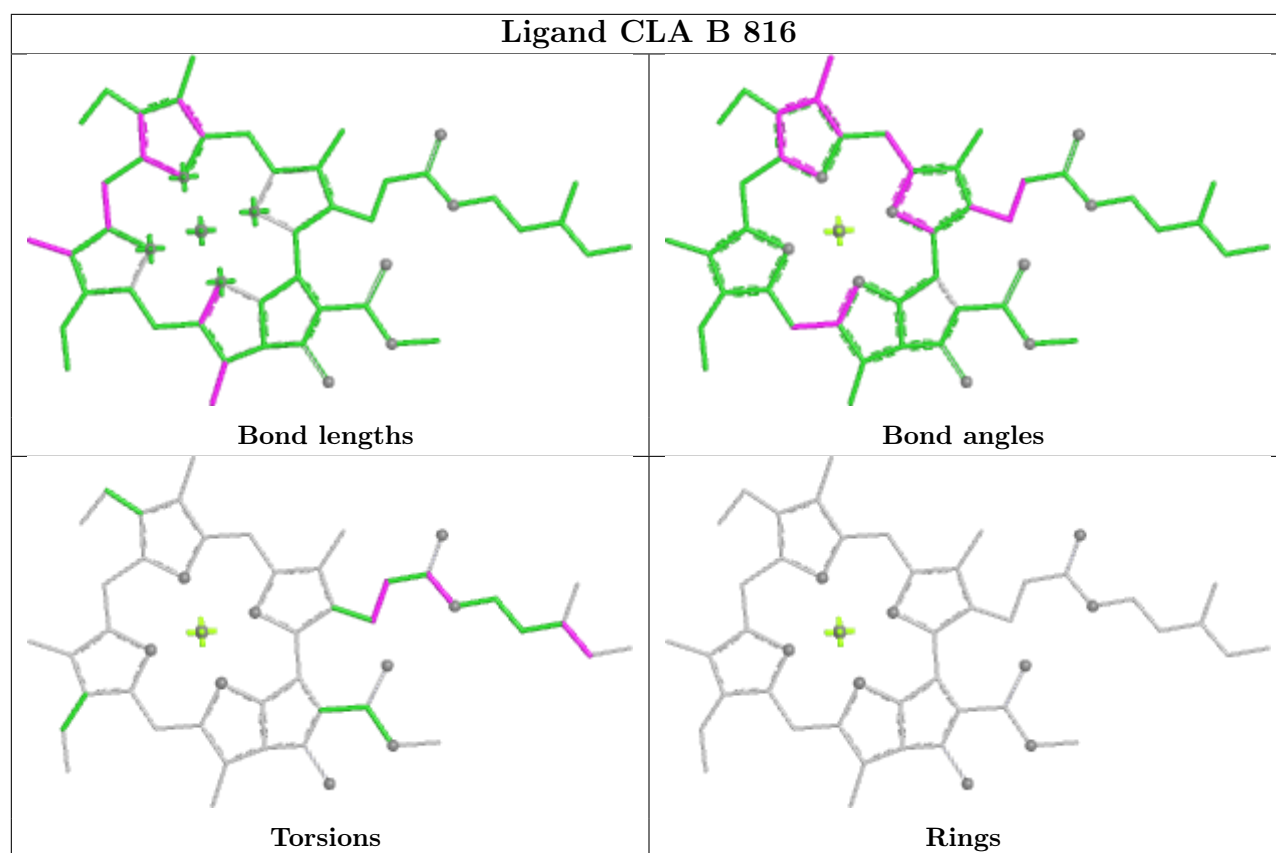
Torsions



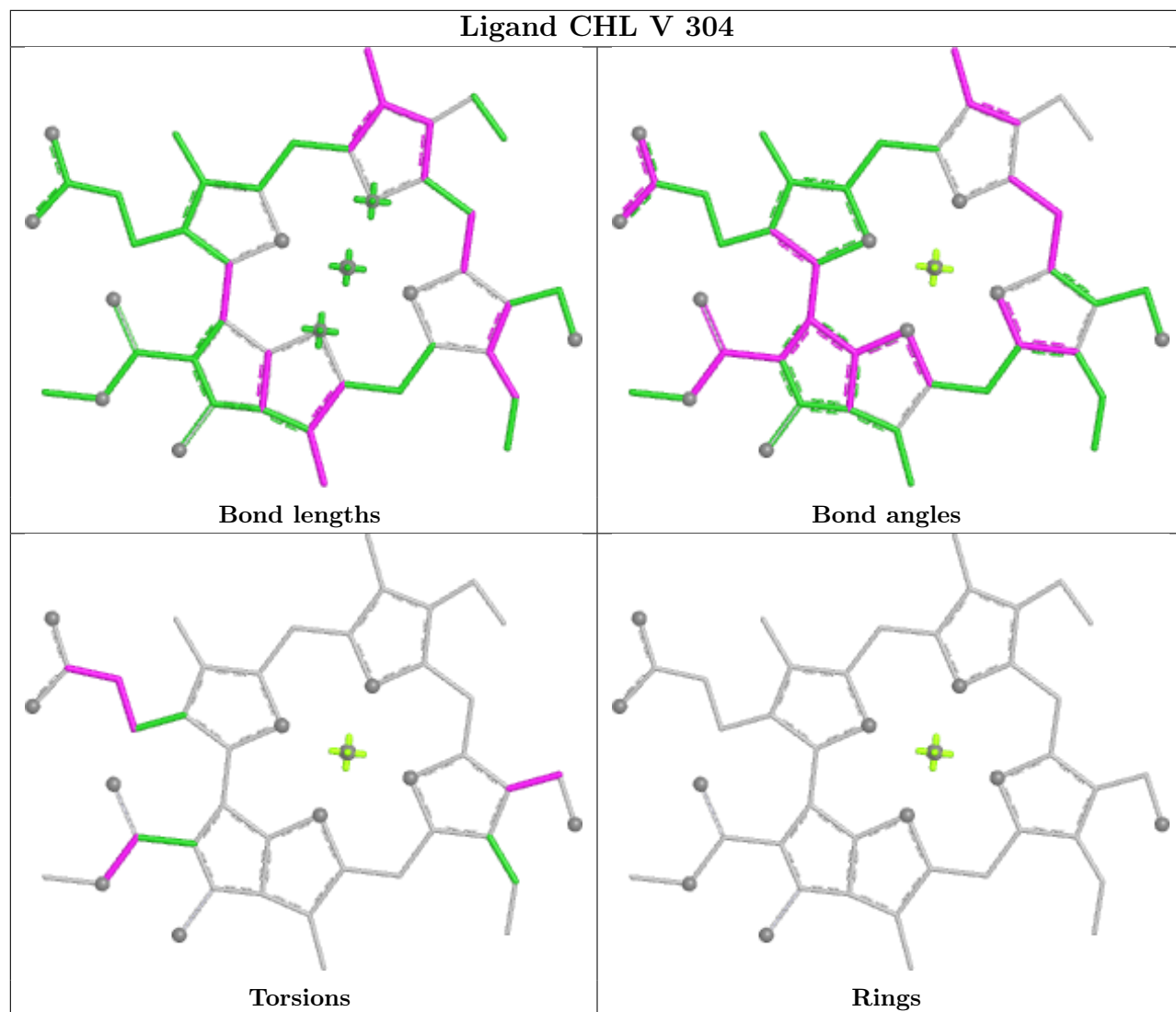
Rings



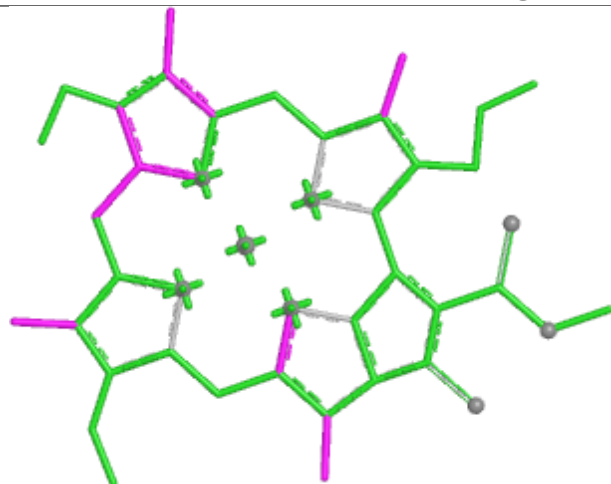




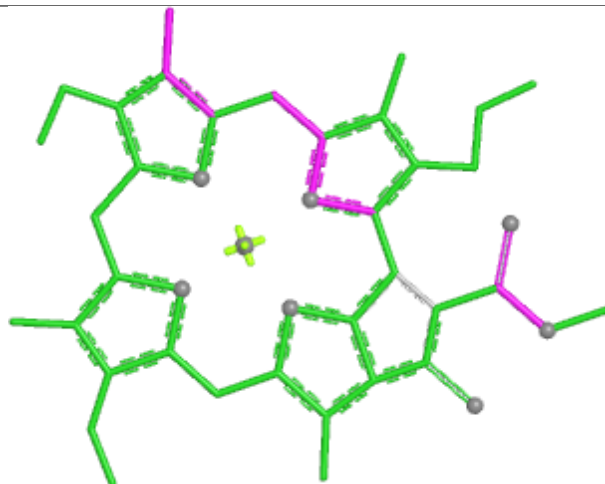
Ligand CHL V 304



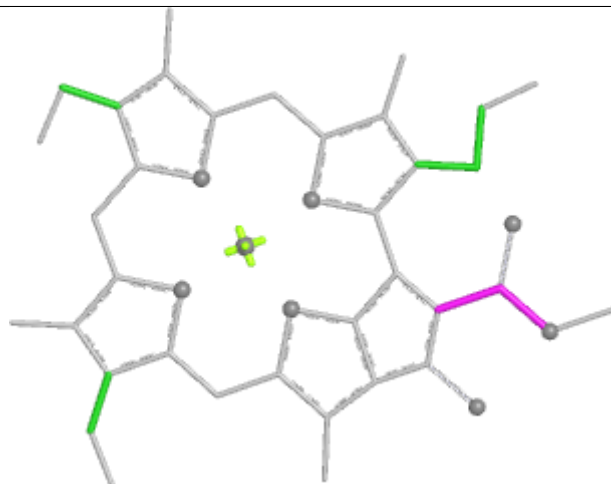
Ligand CLA B 817



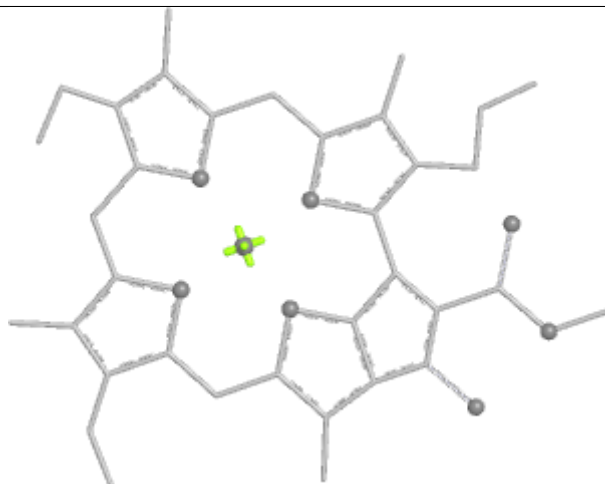
Bond lengths



Bond angles

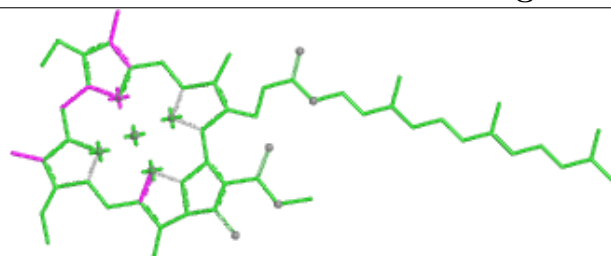


Torsions

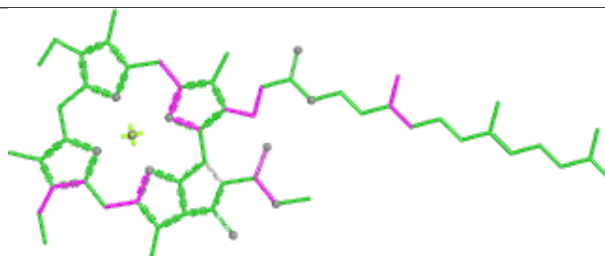


Rings

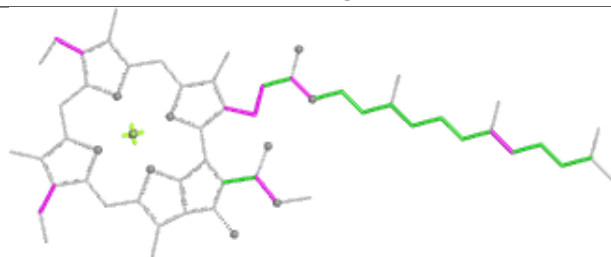
Ligand CLA L 302



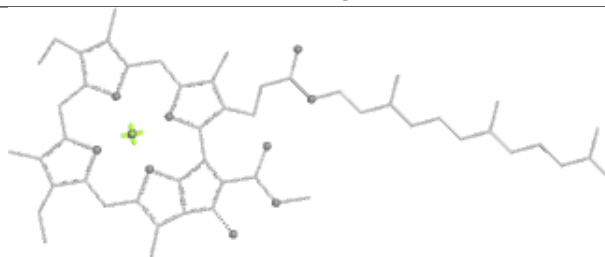
Bond lengths



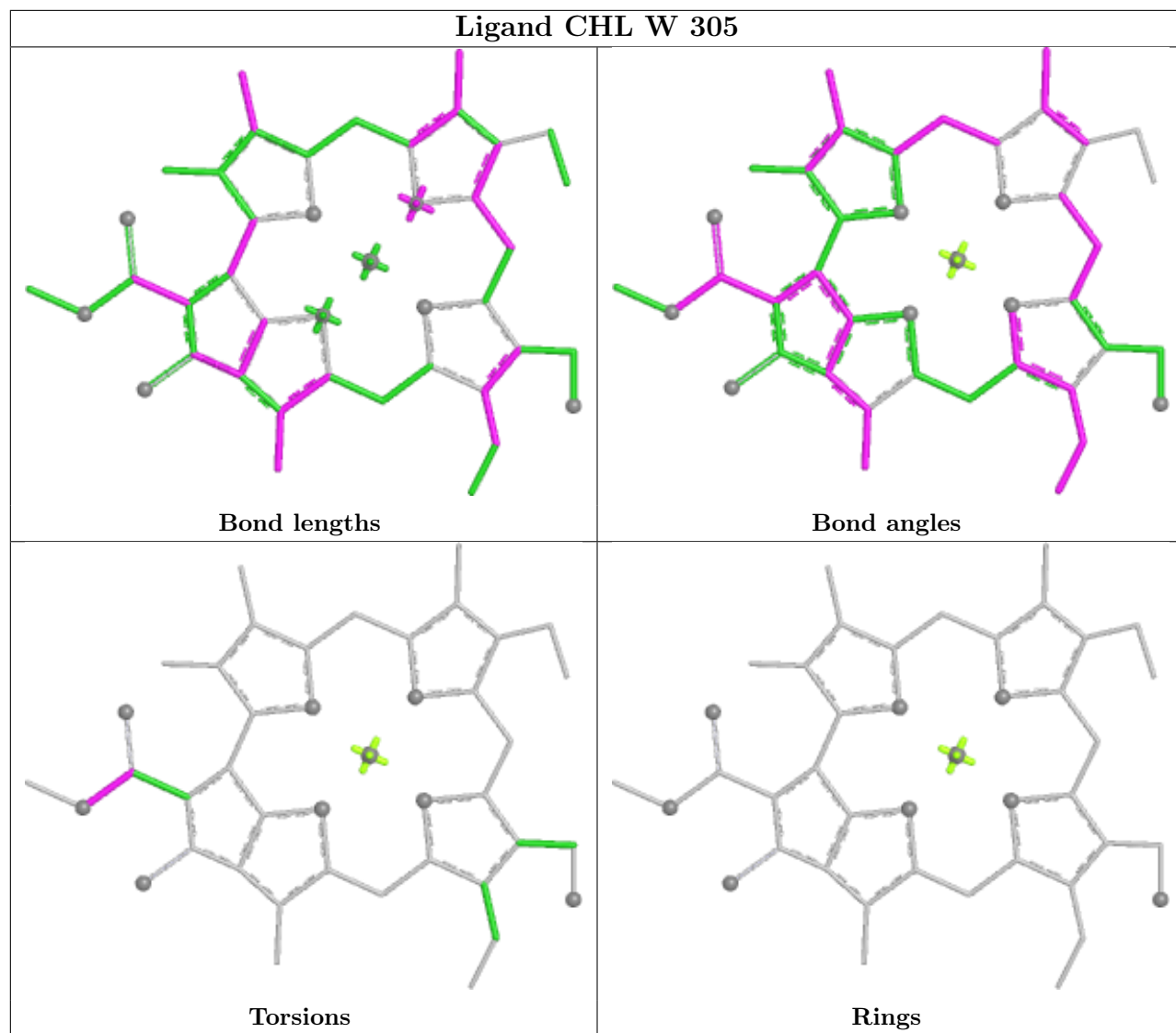
Bond angles



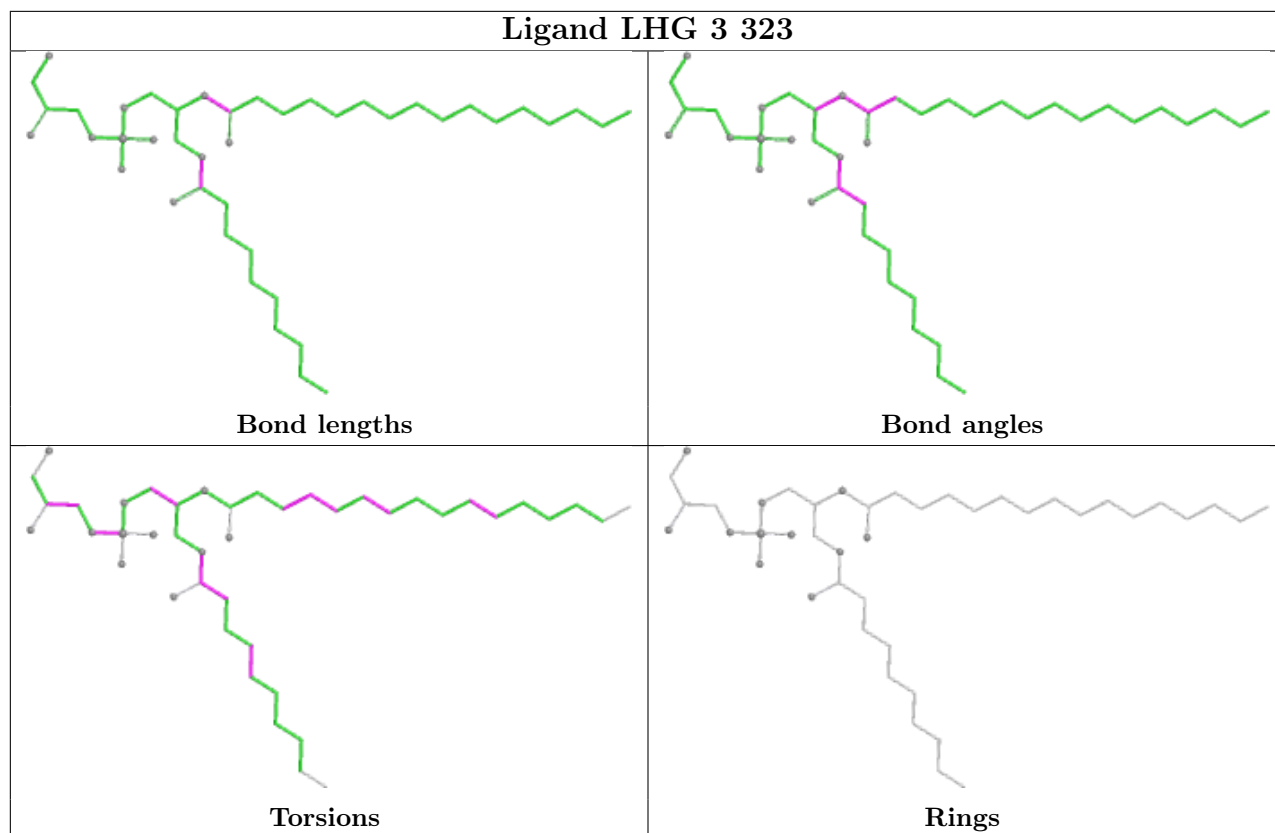
Torsions



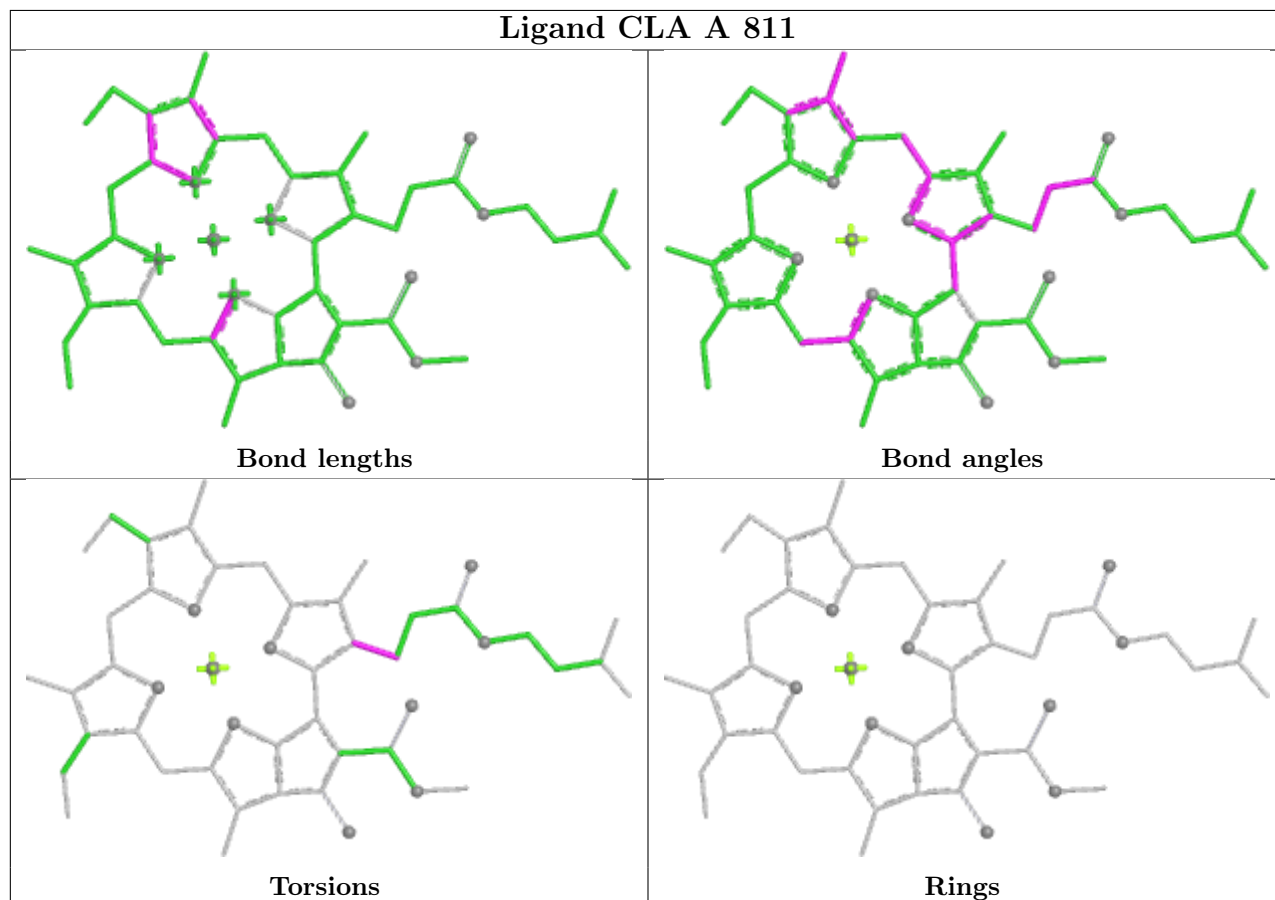
Rings

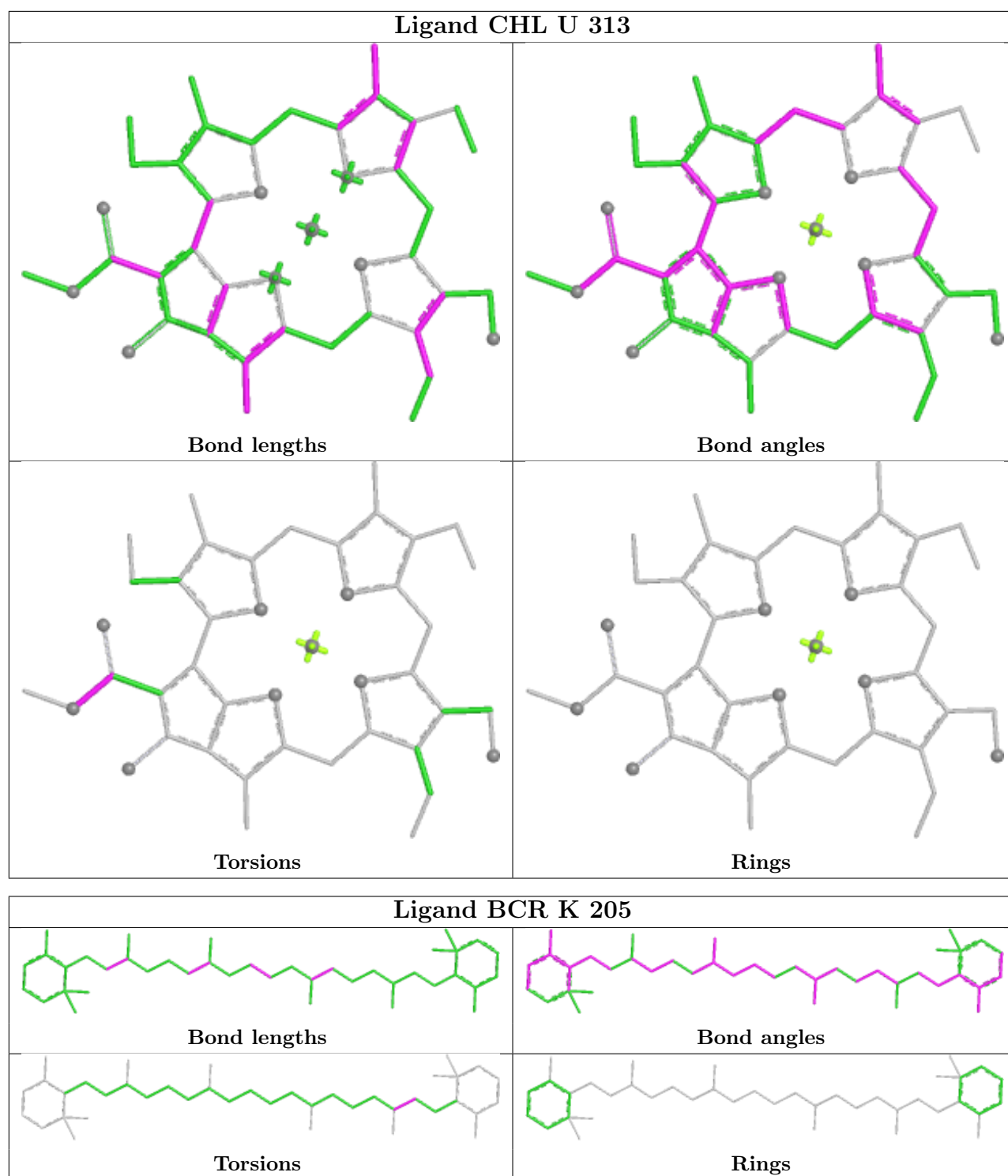


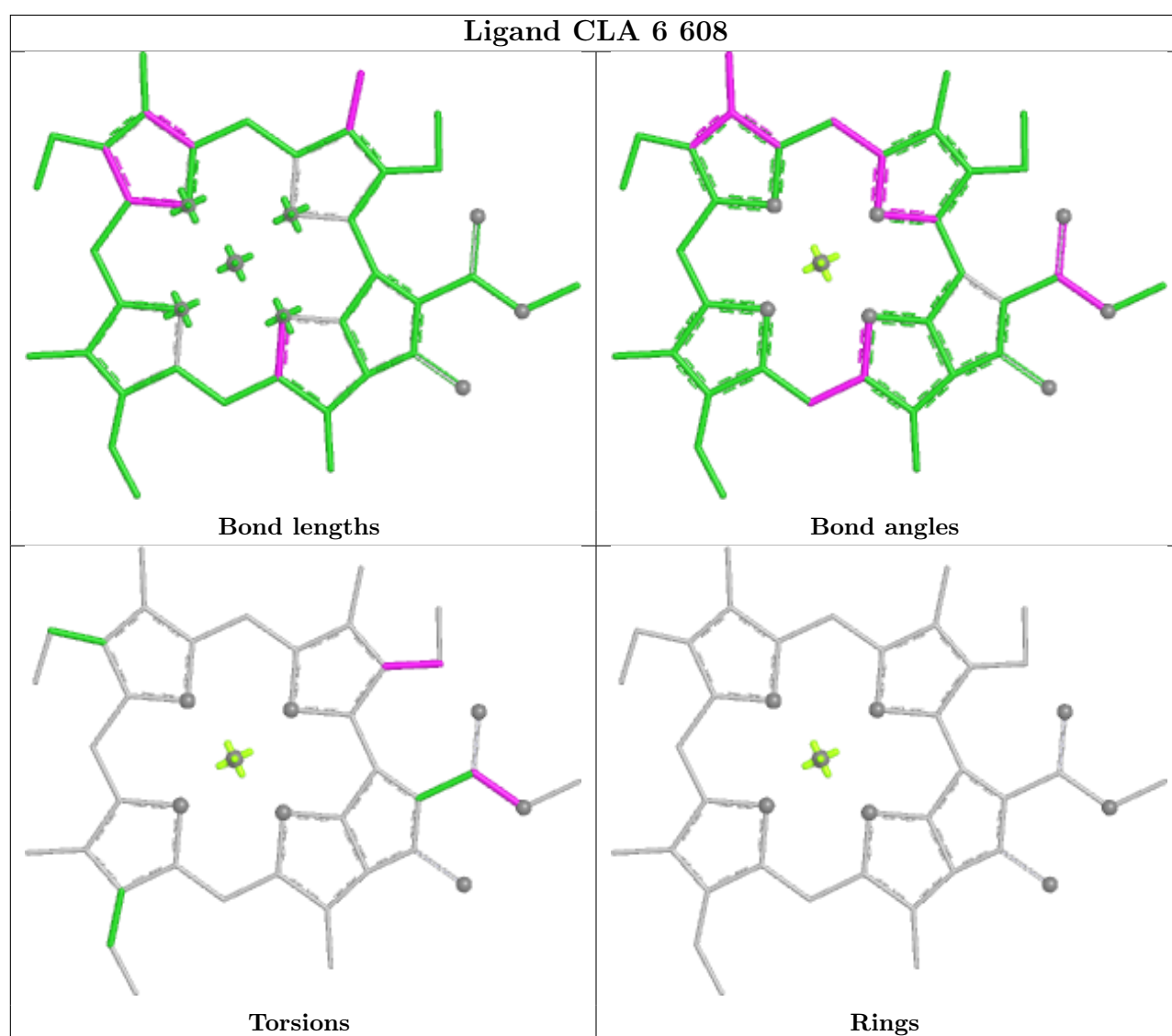
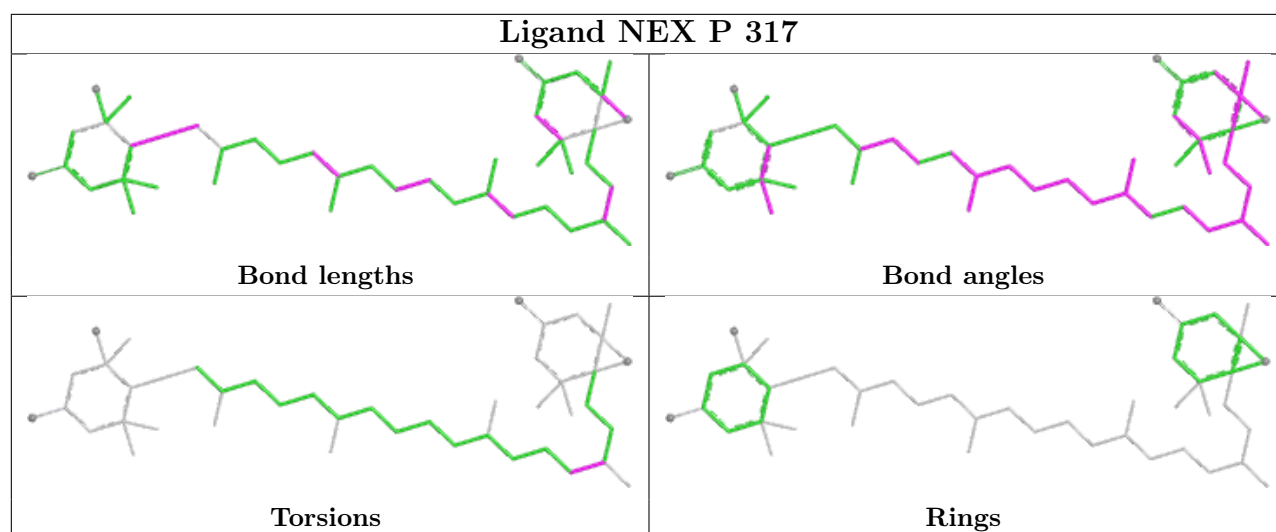
Ligand LHG 3 323

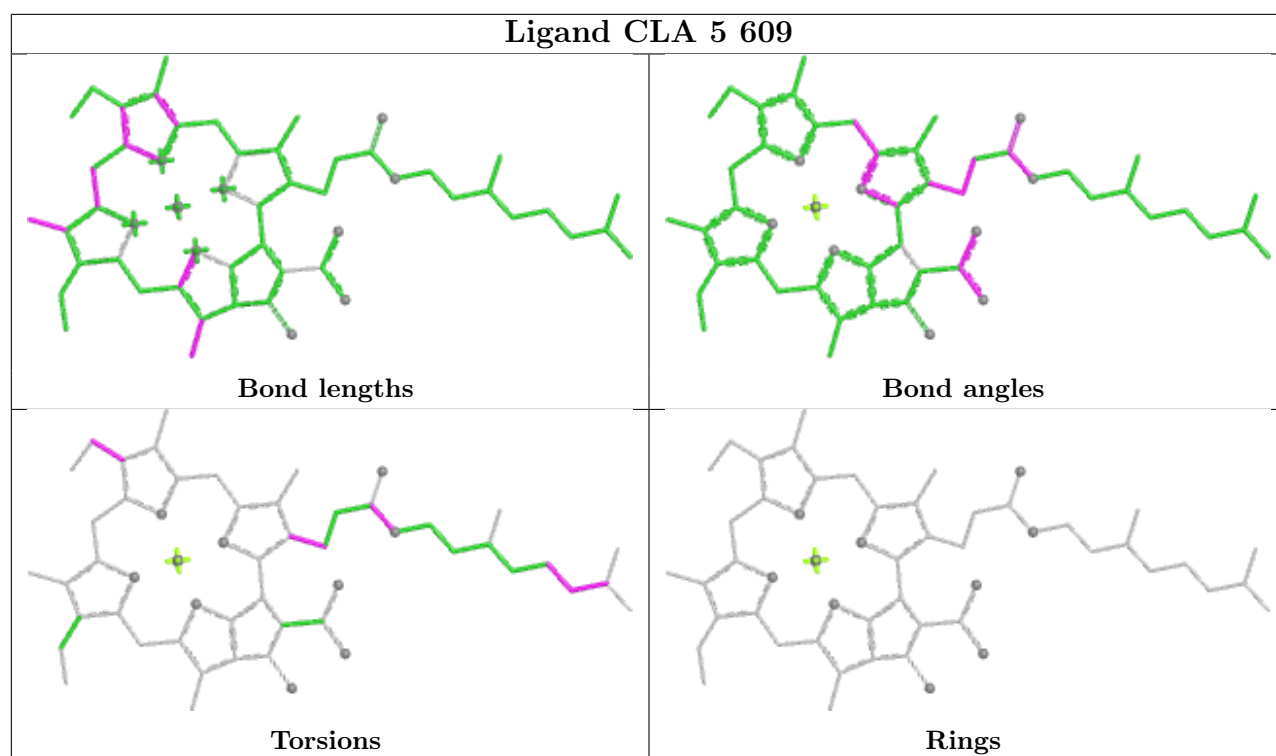


Ligand CLA A 811

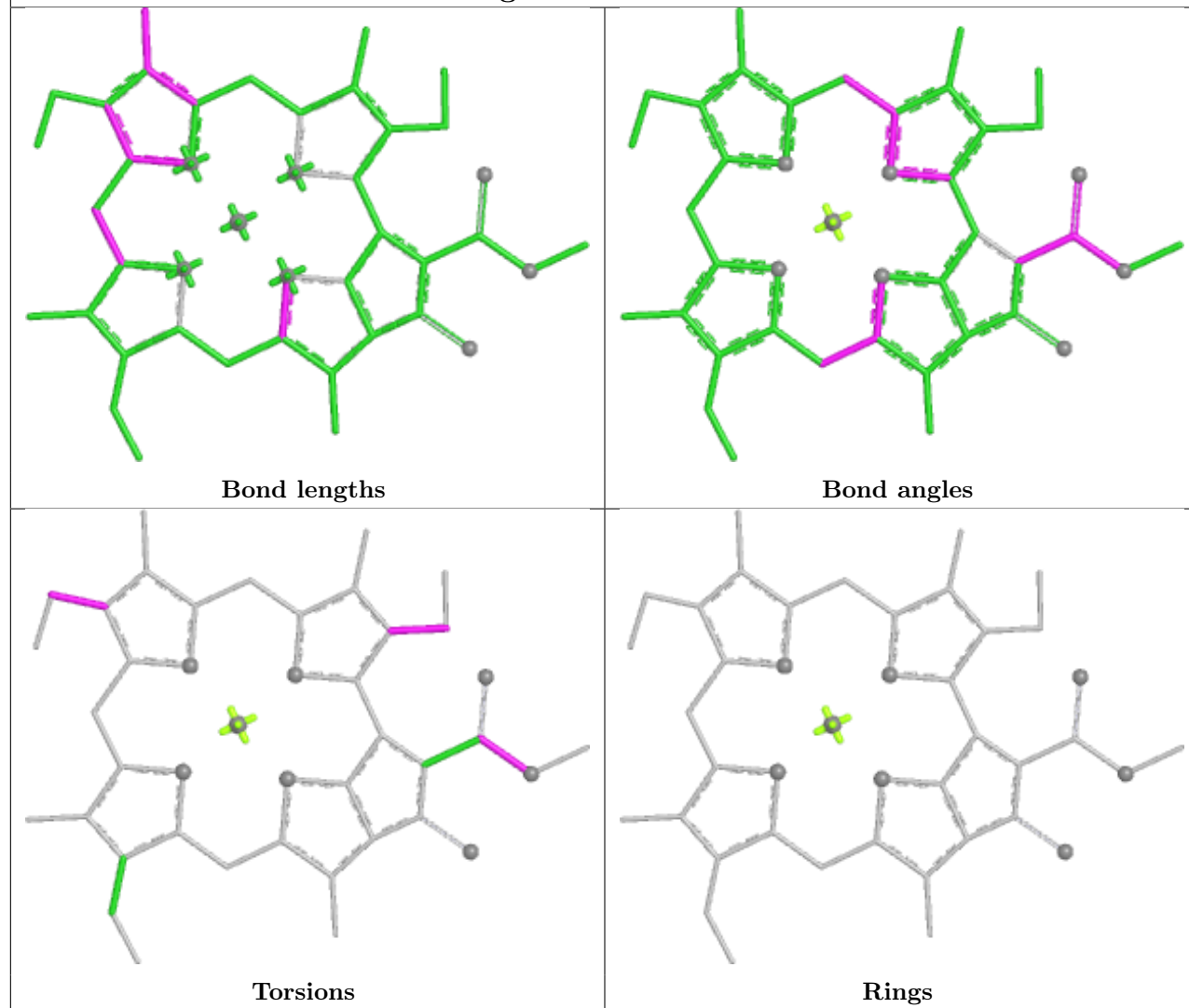




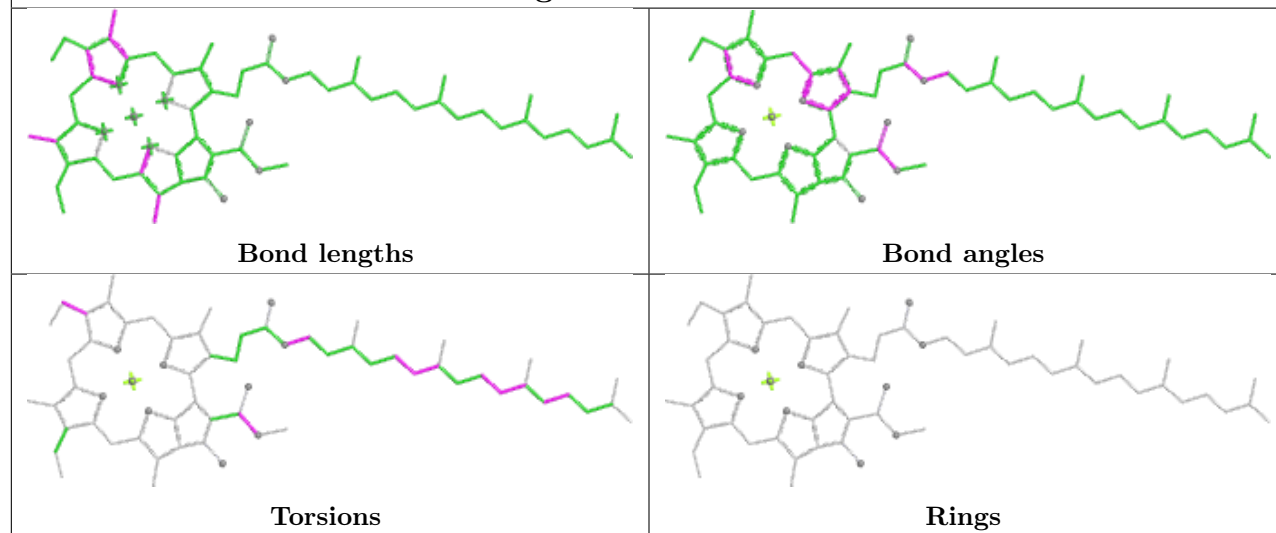




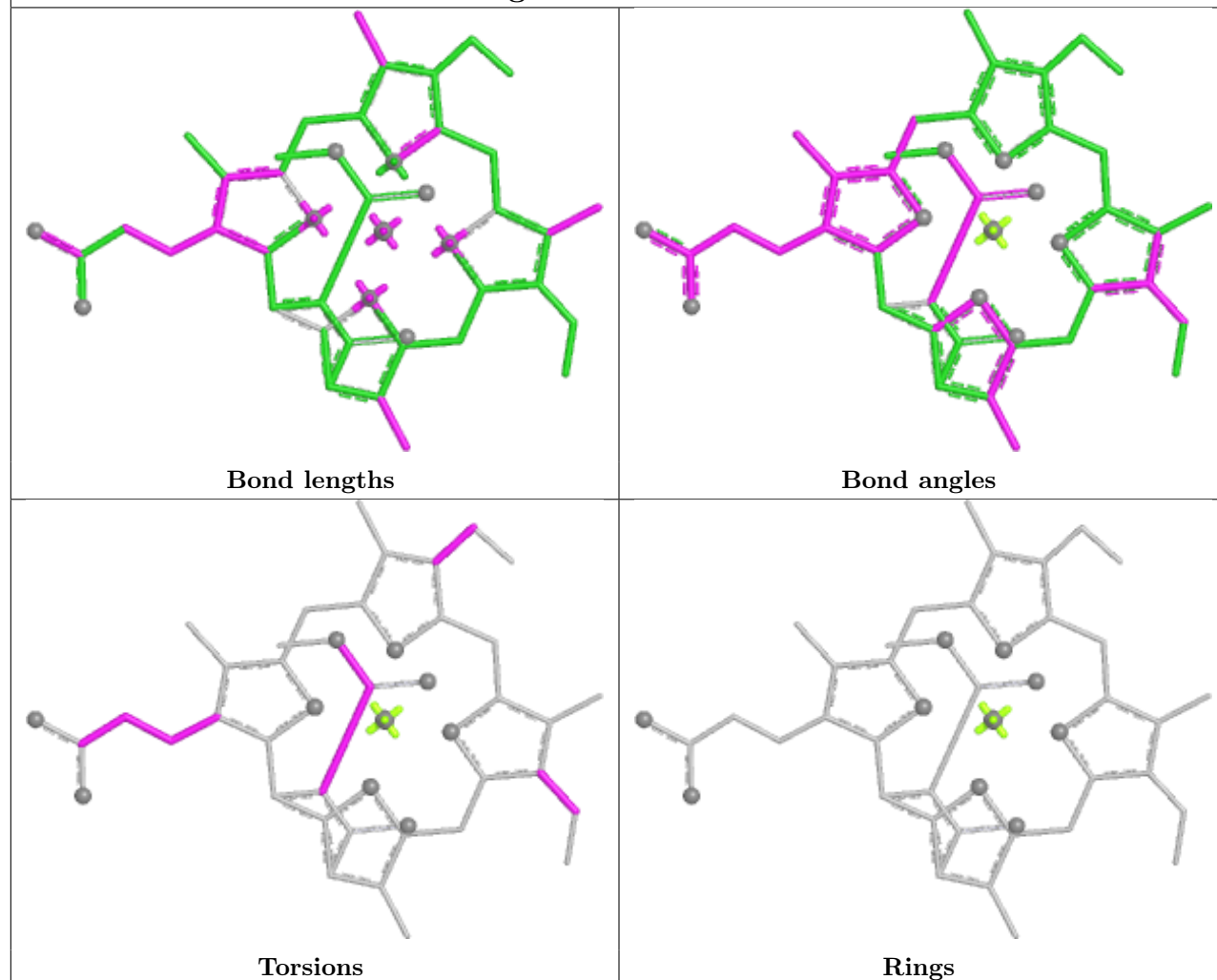
Ligand CLA 2 610



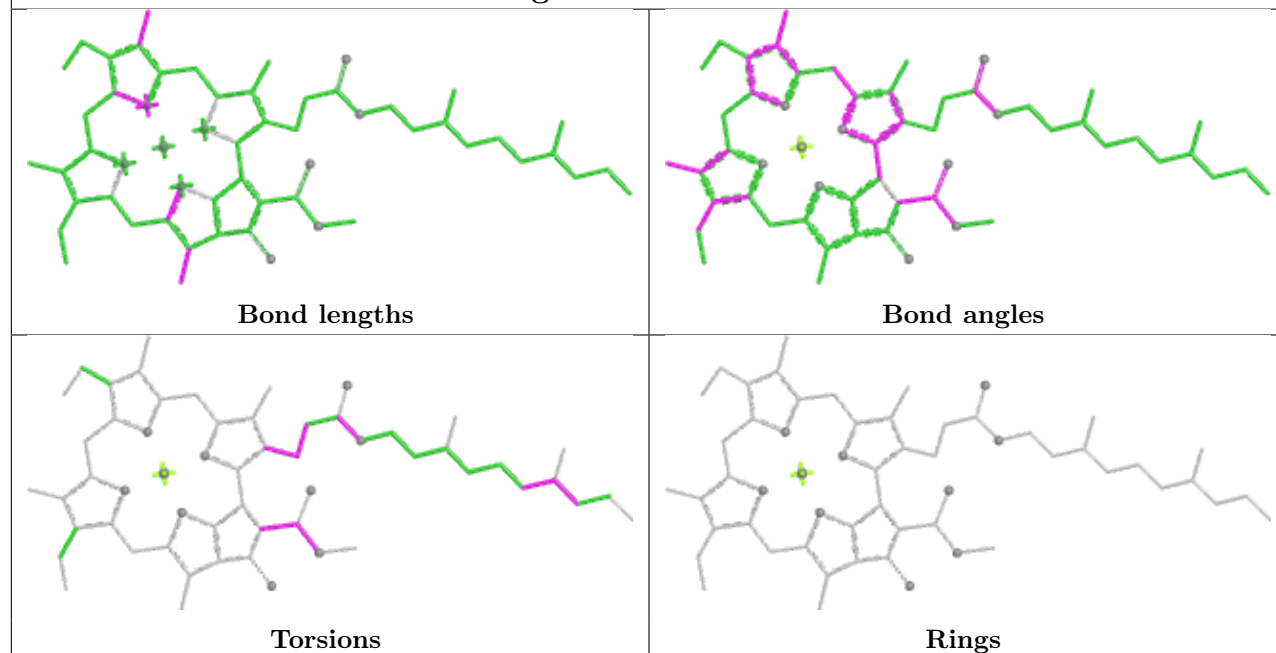
Ligand CLA S 302



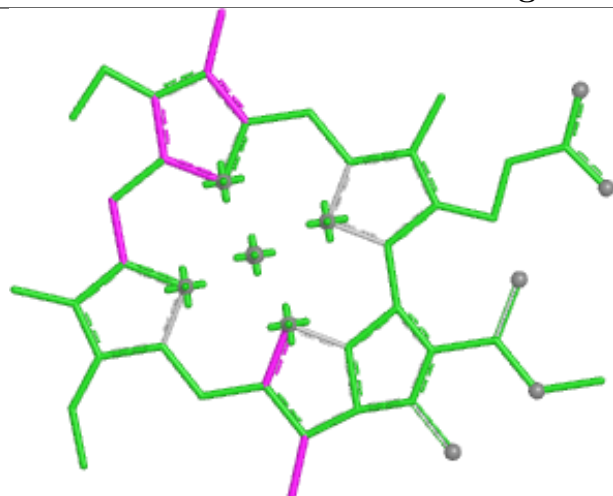
Ligand KC2 V 308



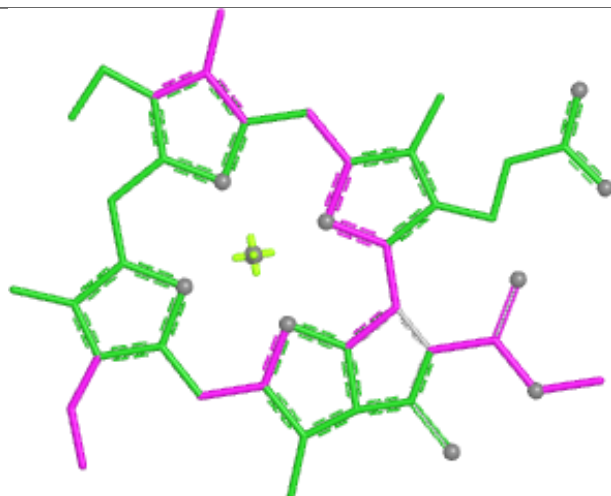
Ligand CLA A 856



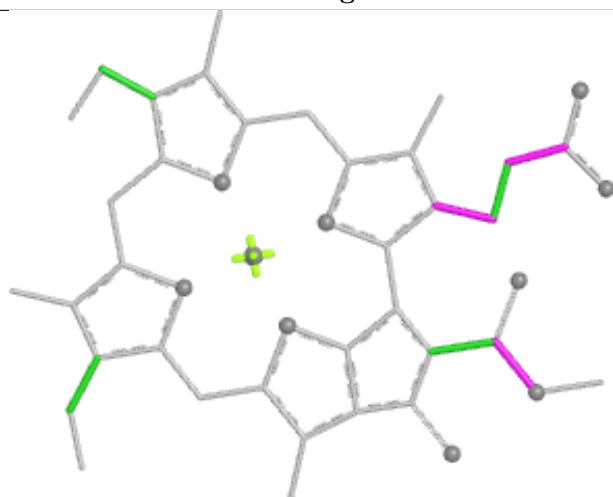
Ligand CLA 4 309



Bond lengths



Bond angles

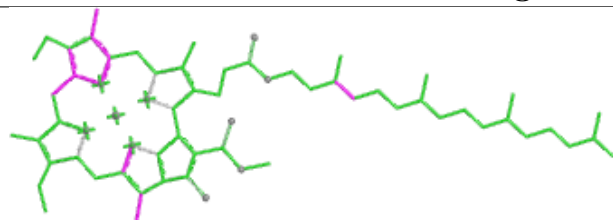


Torsions

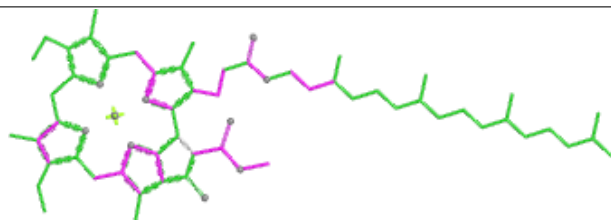


Rings

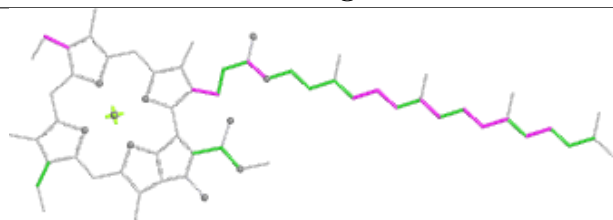
Ligand CLA A 842



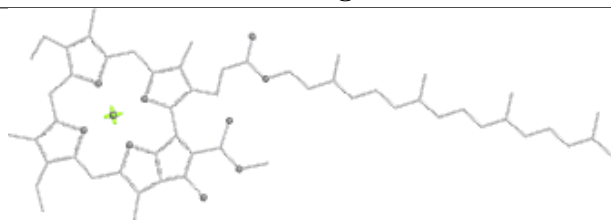
Bond lengths



Bond angles

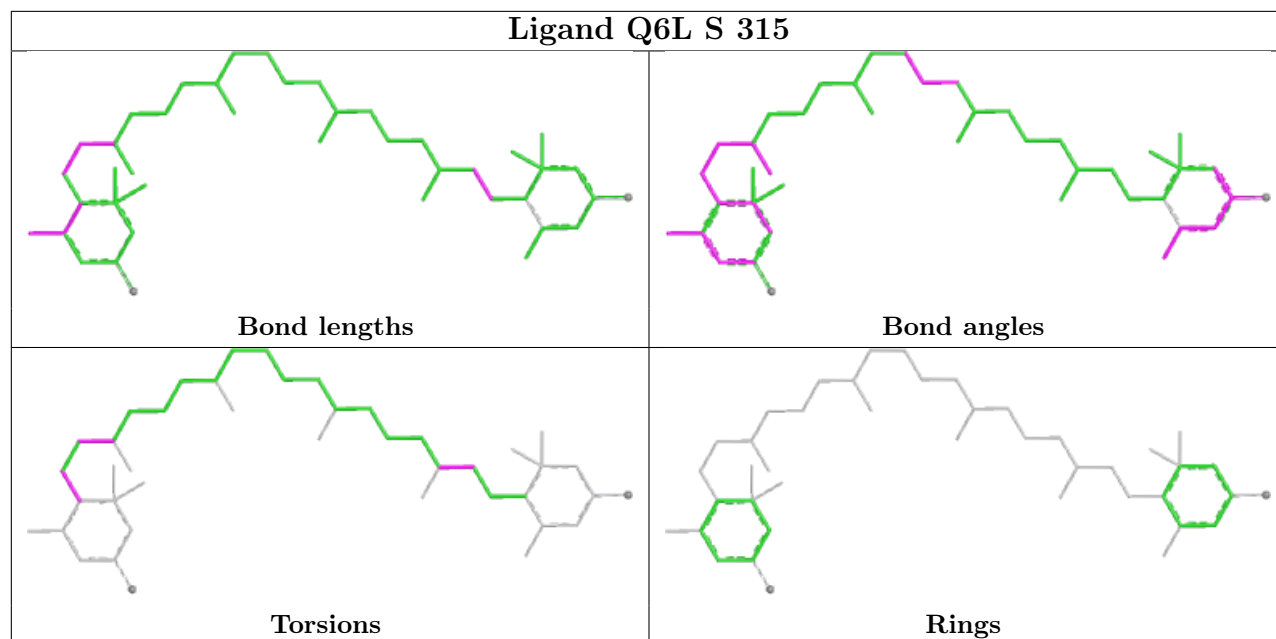


Torsions

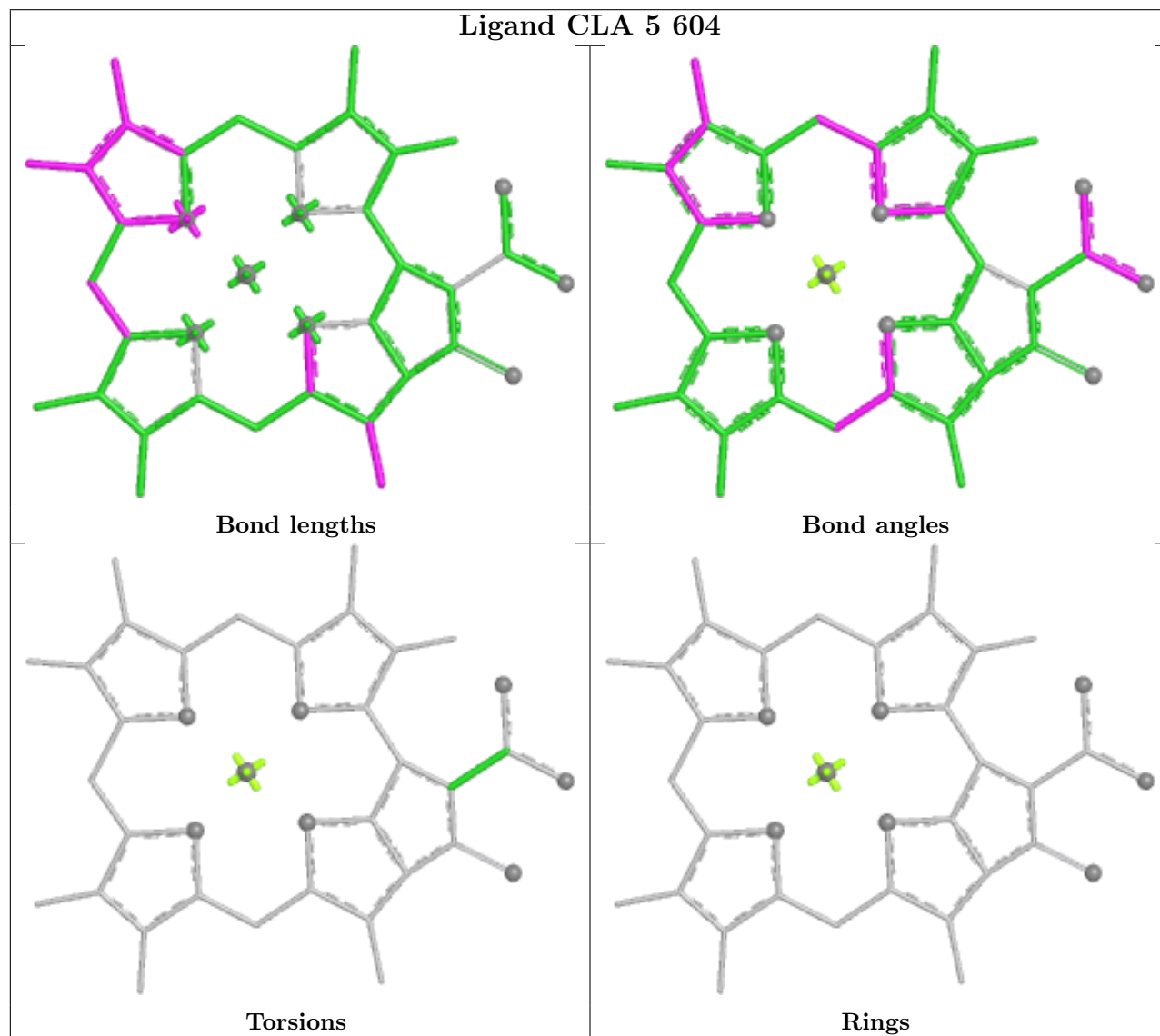


Rings

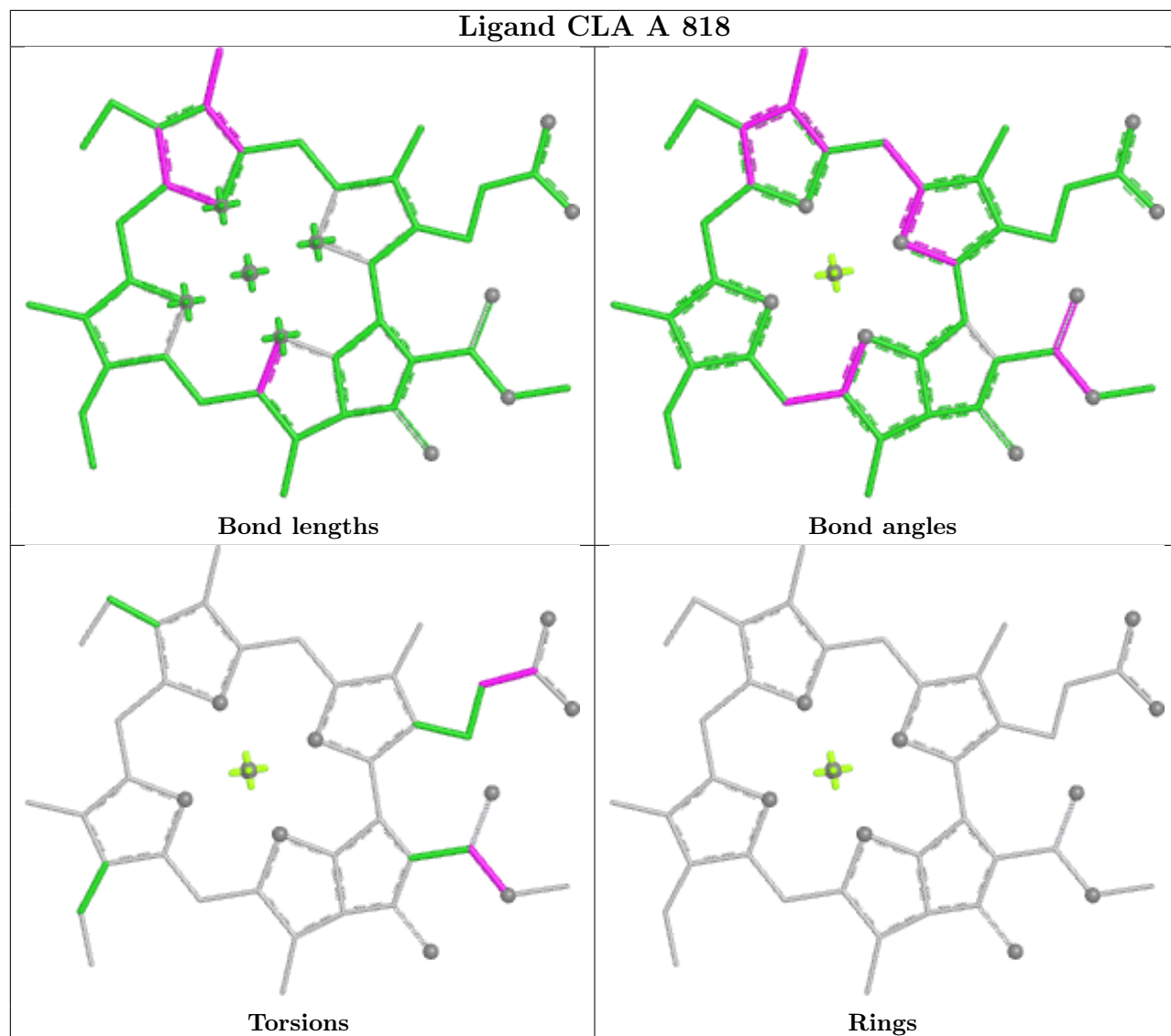
Ligand Q6L S 315



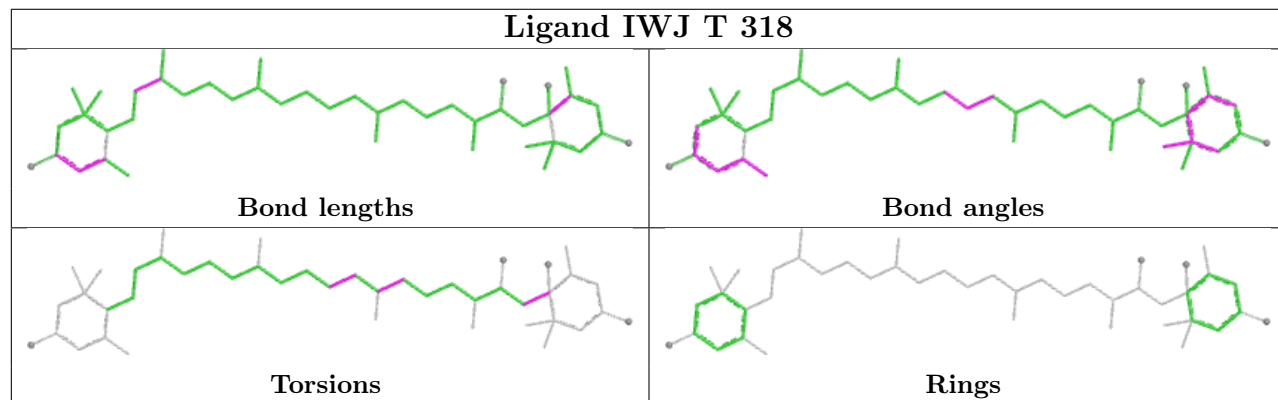
Ligand CLA 5 604

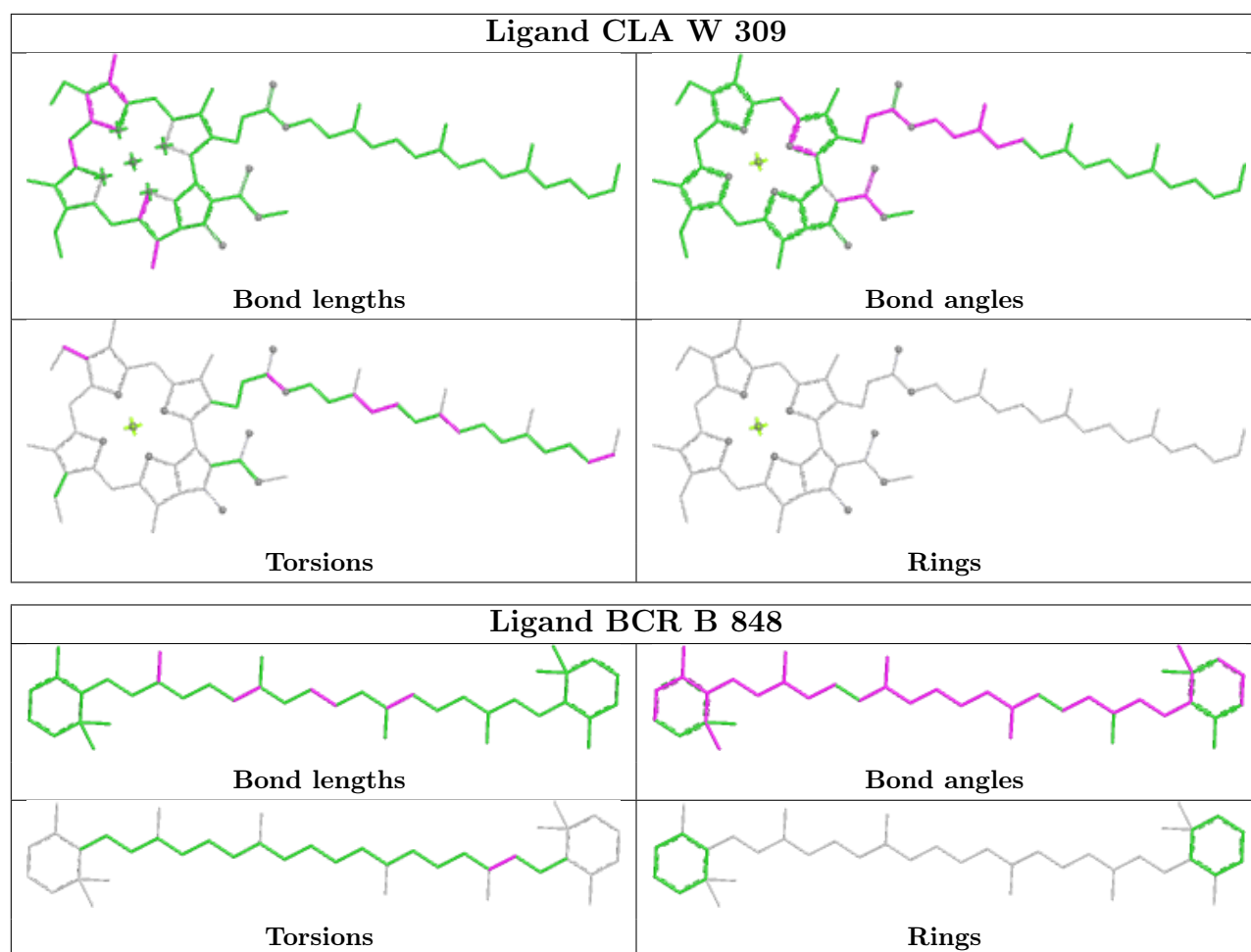


Ligand CLA A 818

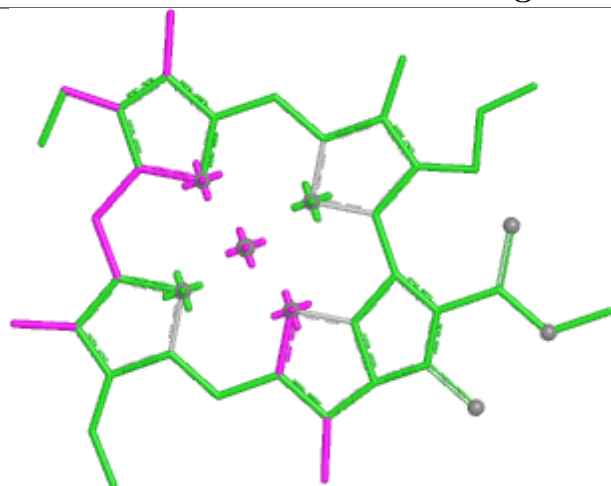


Ligand IWJ T 318

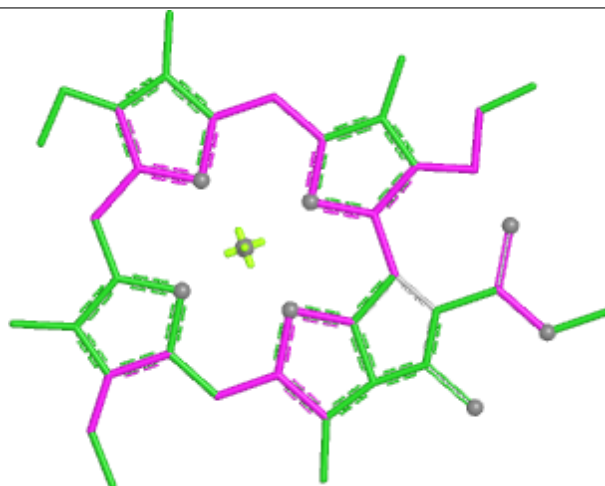




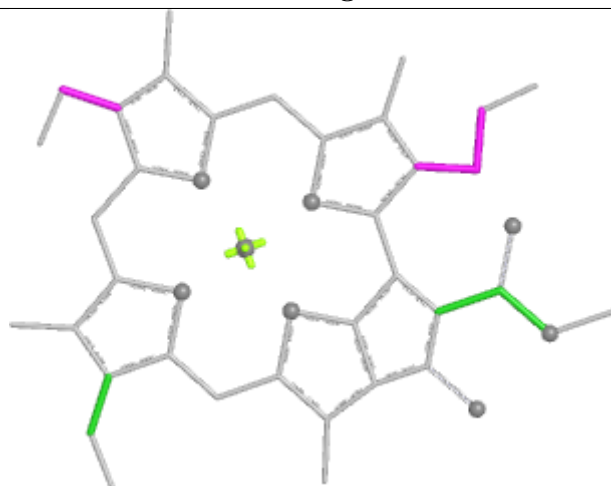
Ligand CLA B 832



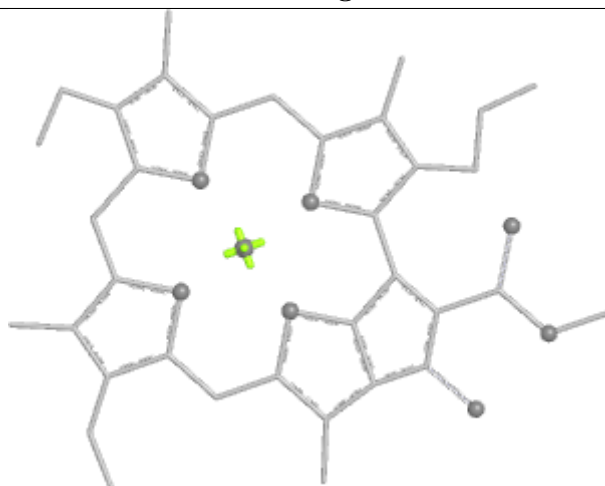
Bond lengths



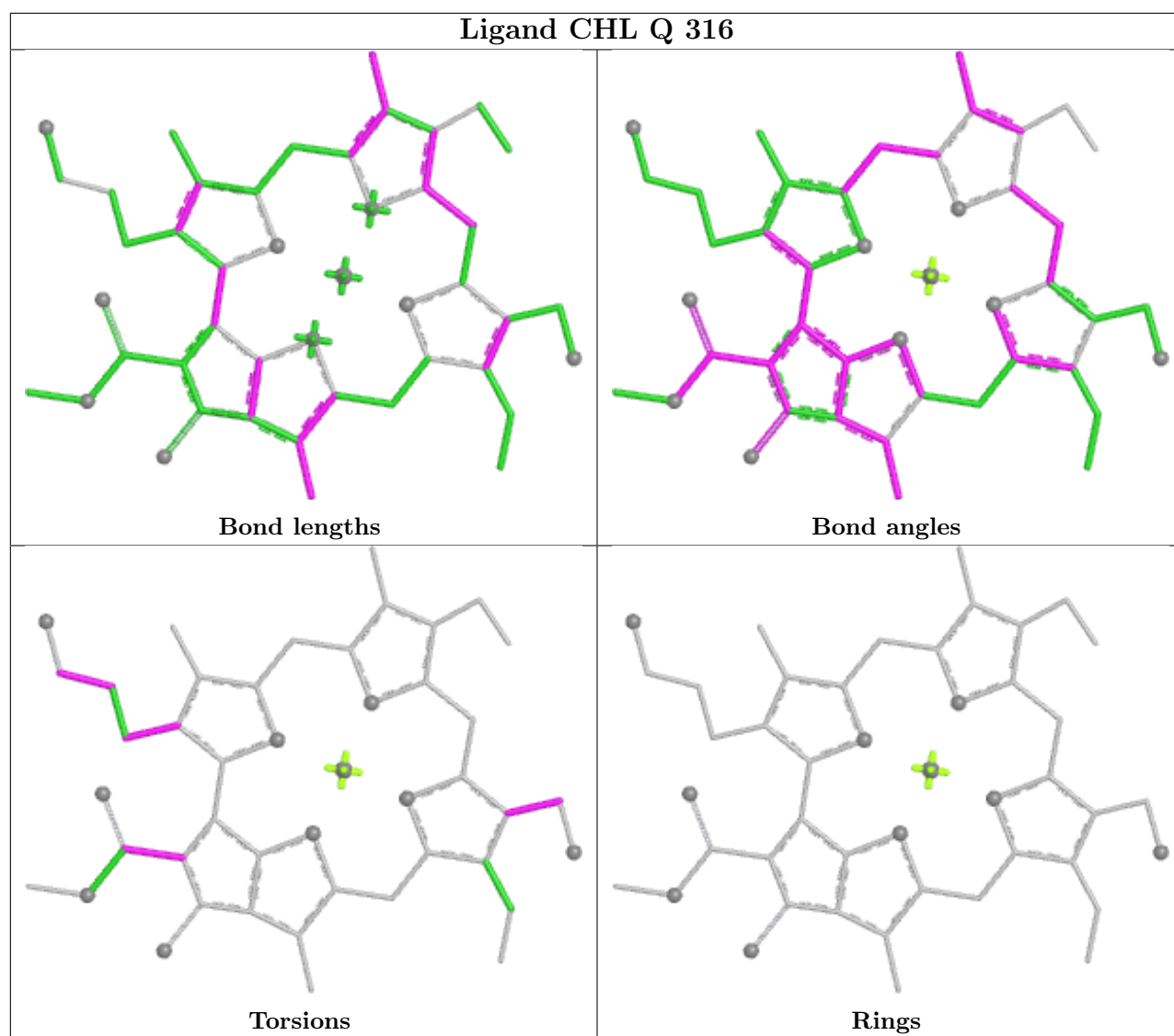
Bond angles

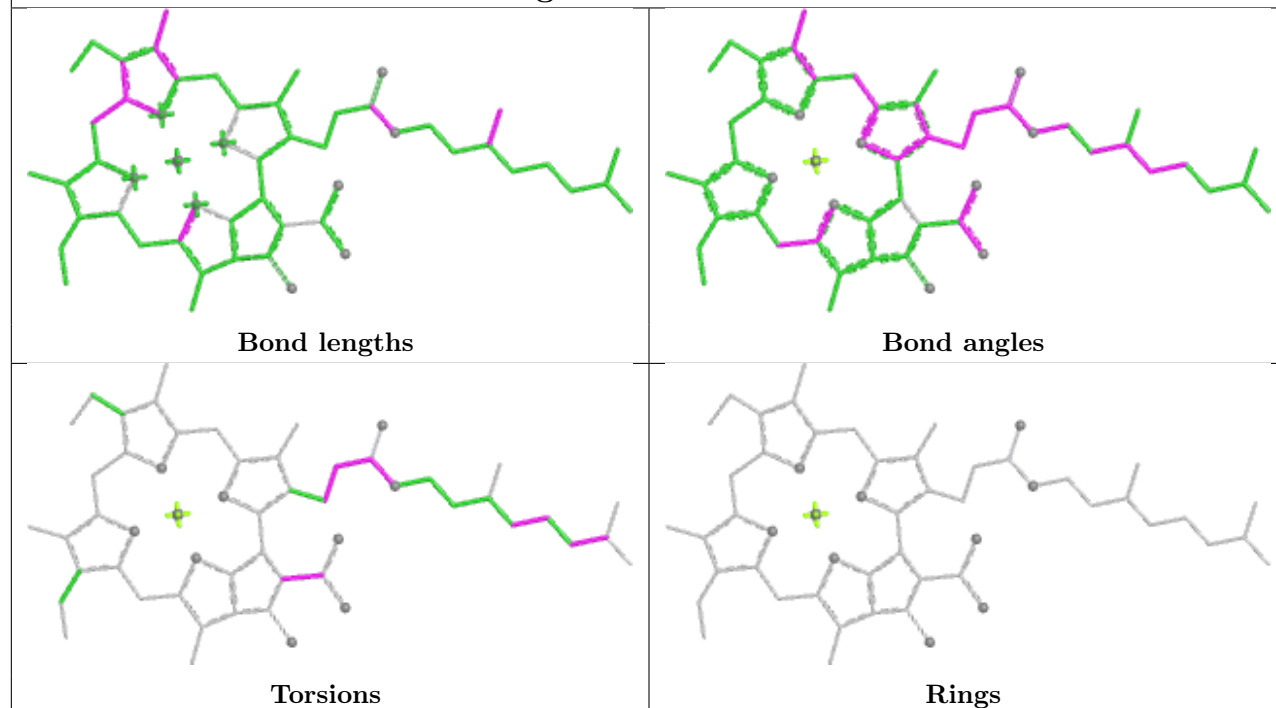
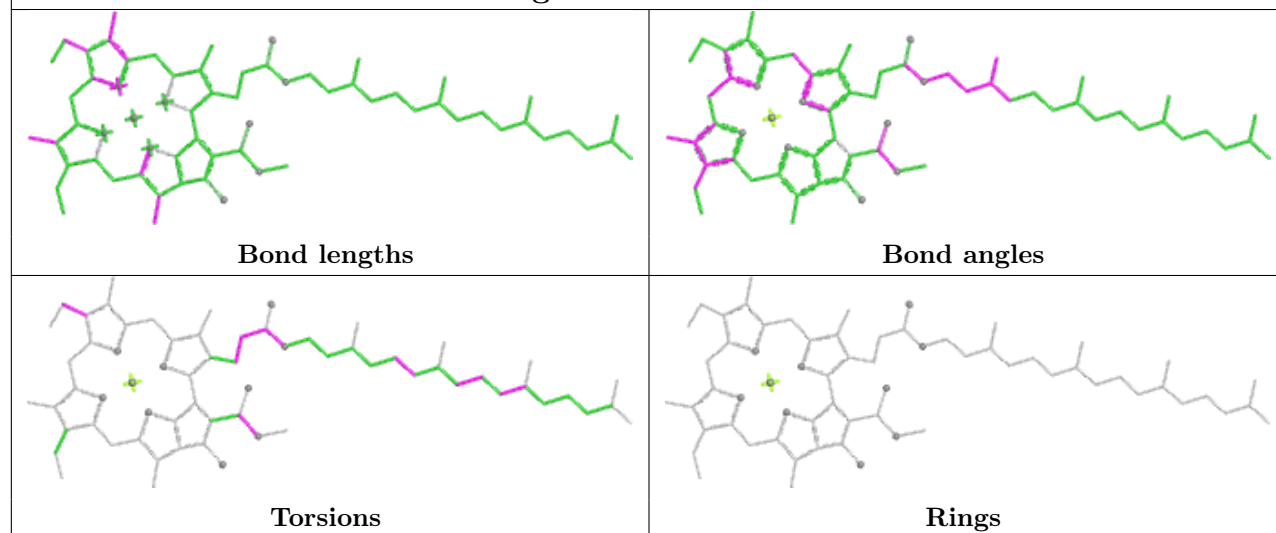


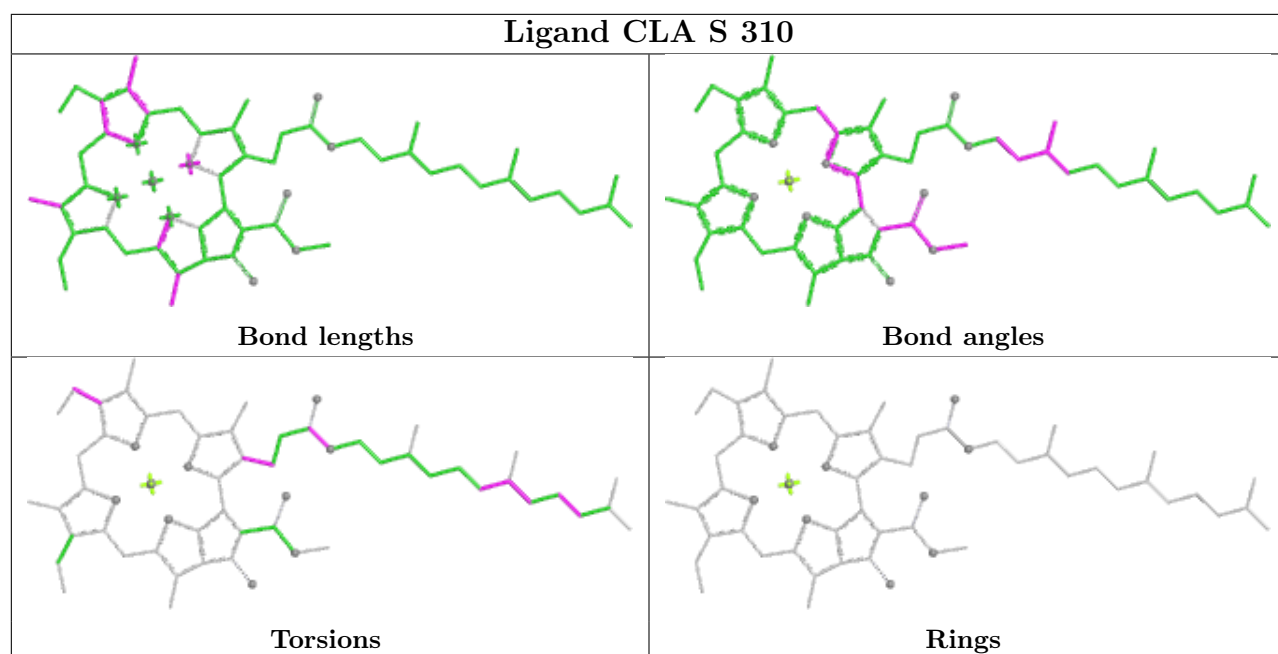
Torsions



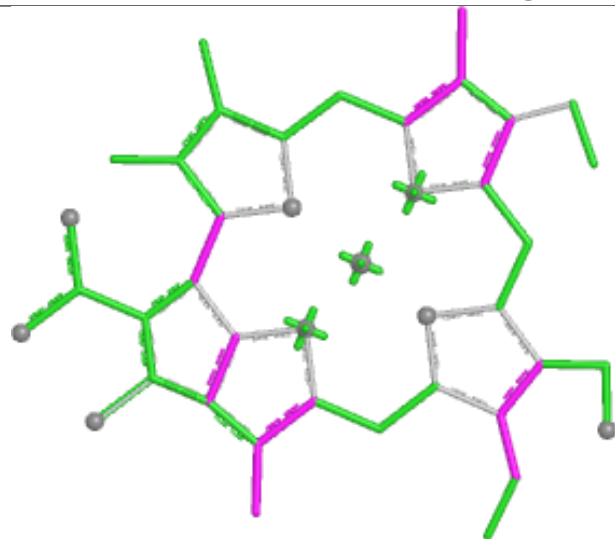
Rings



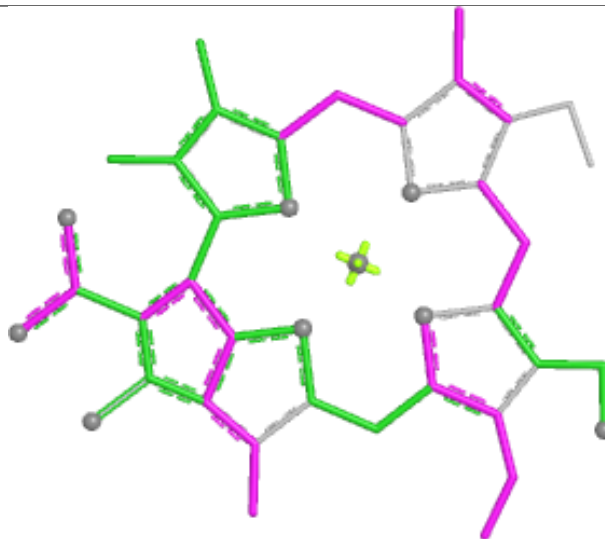
Ligand CLA 3 311**Ligand CLA B 806**



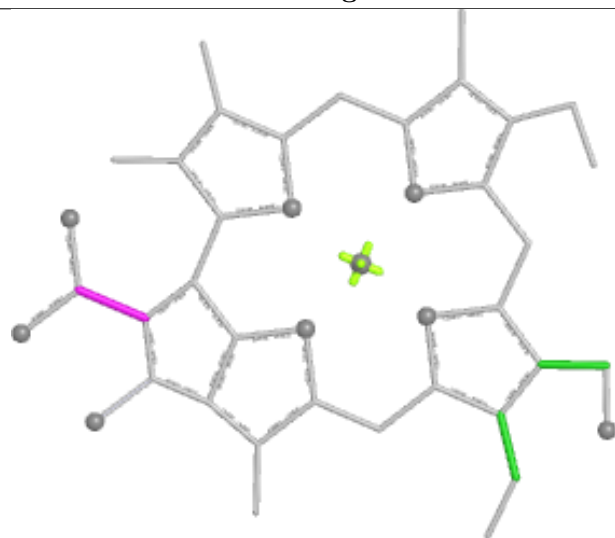
Ligand CHL 5 605



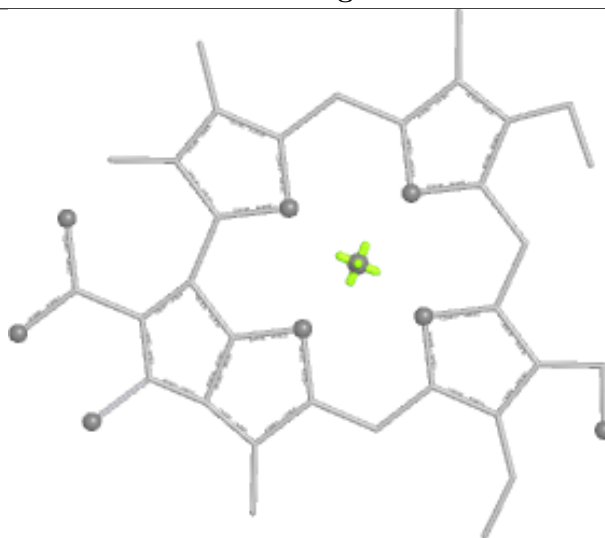
Bond lengths



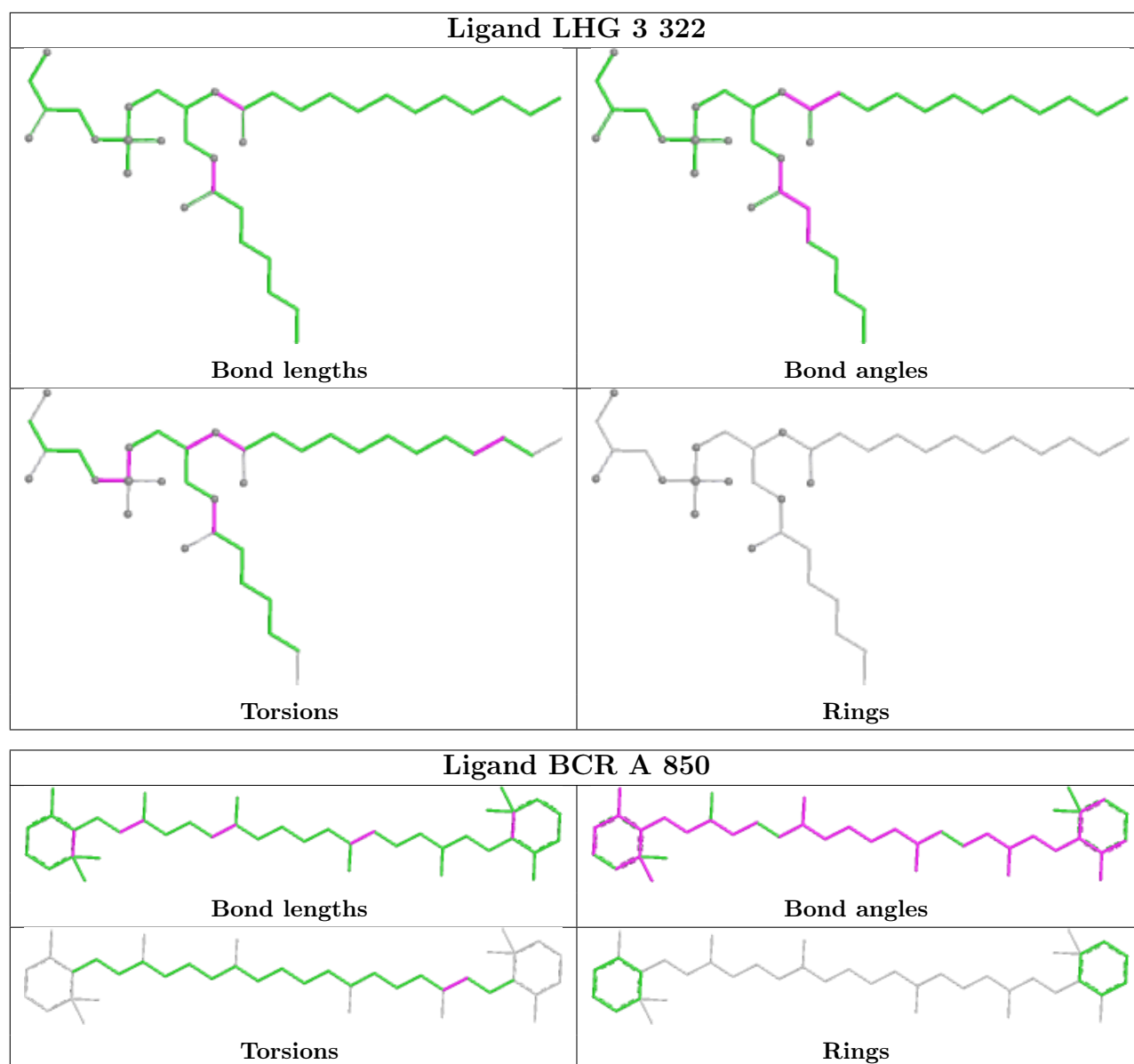
Bond angles

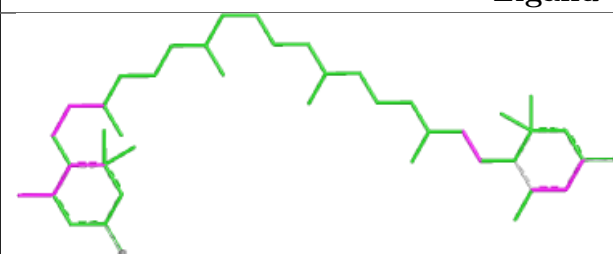
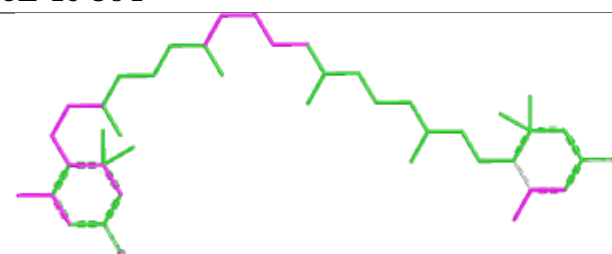
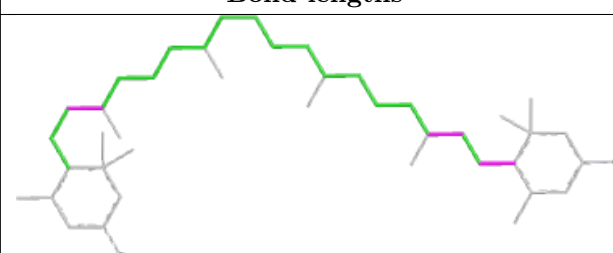
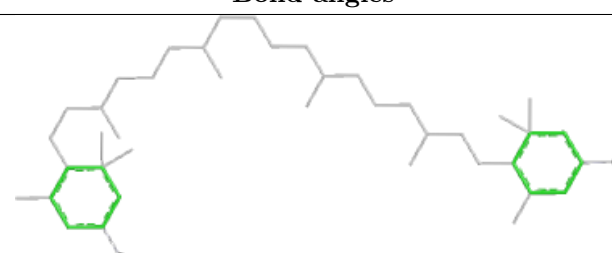


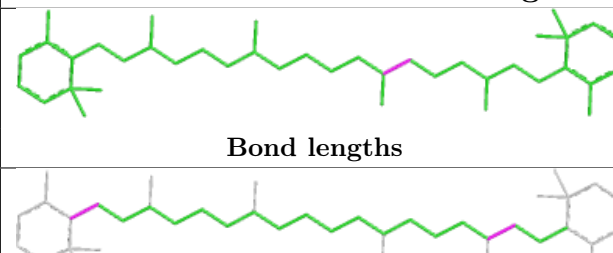
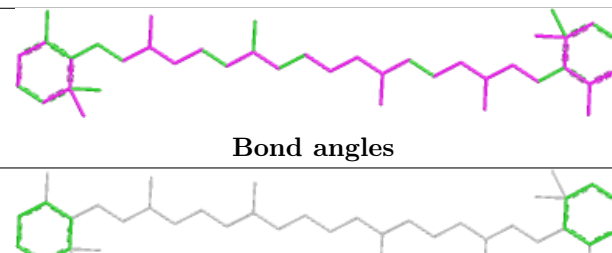
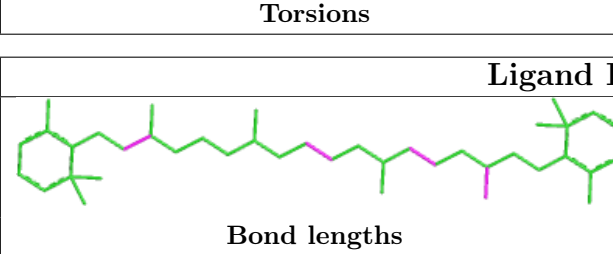
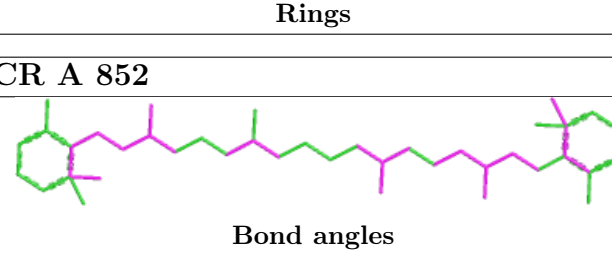
Torsions

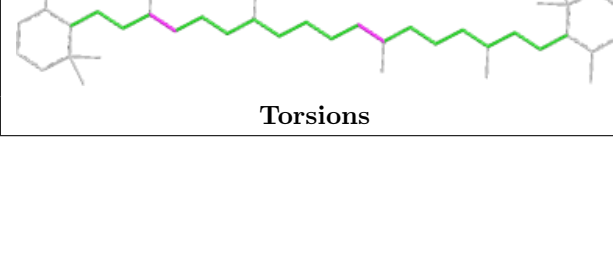
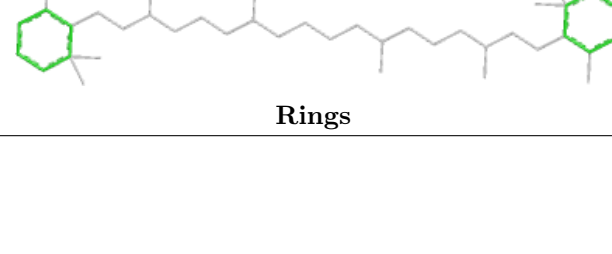


Rings

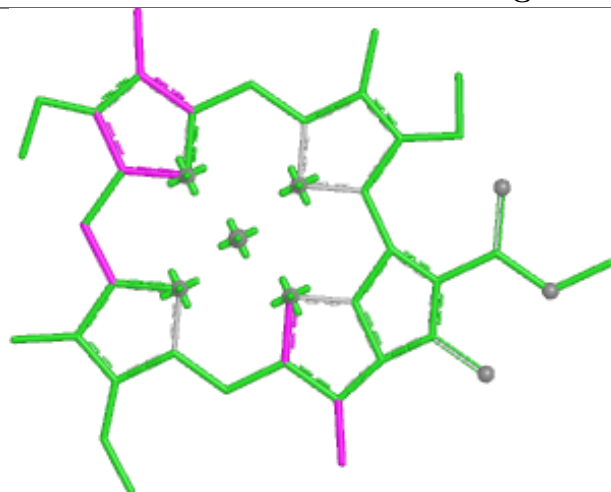


Ligand Q6L R 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

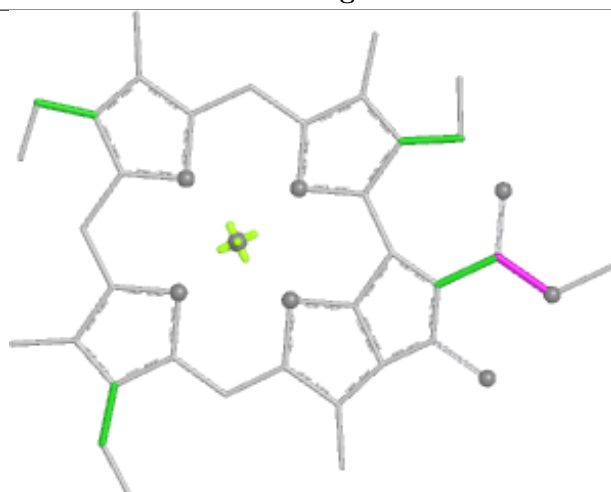
Ligand CLA X 310



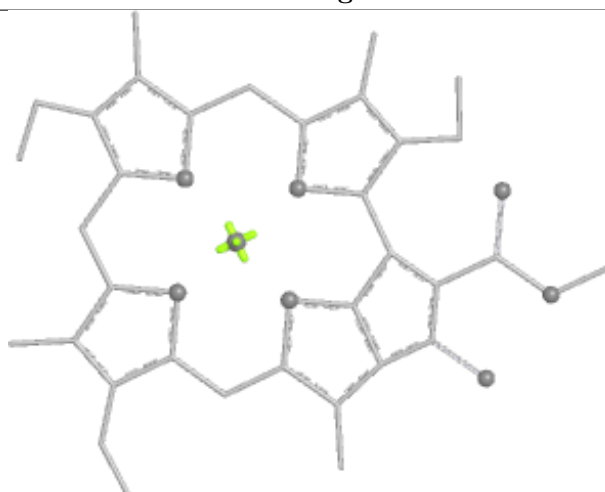
Bond lengths



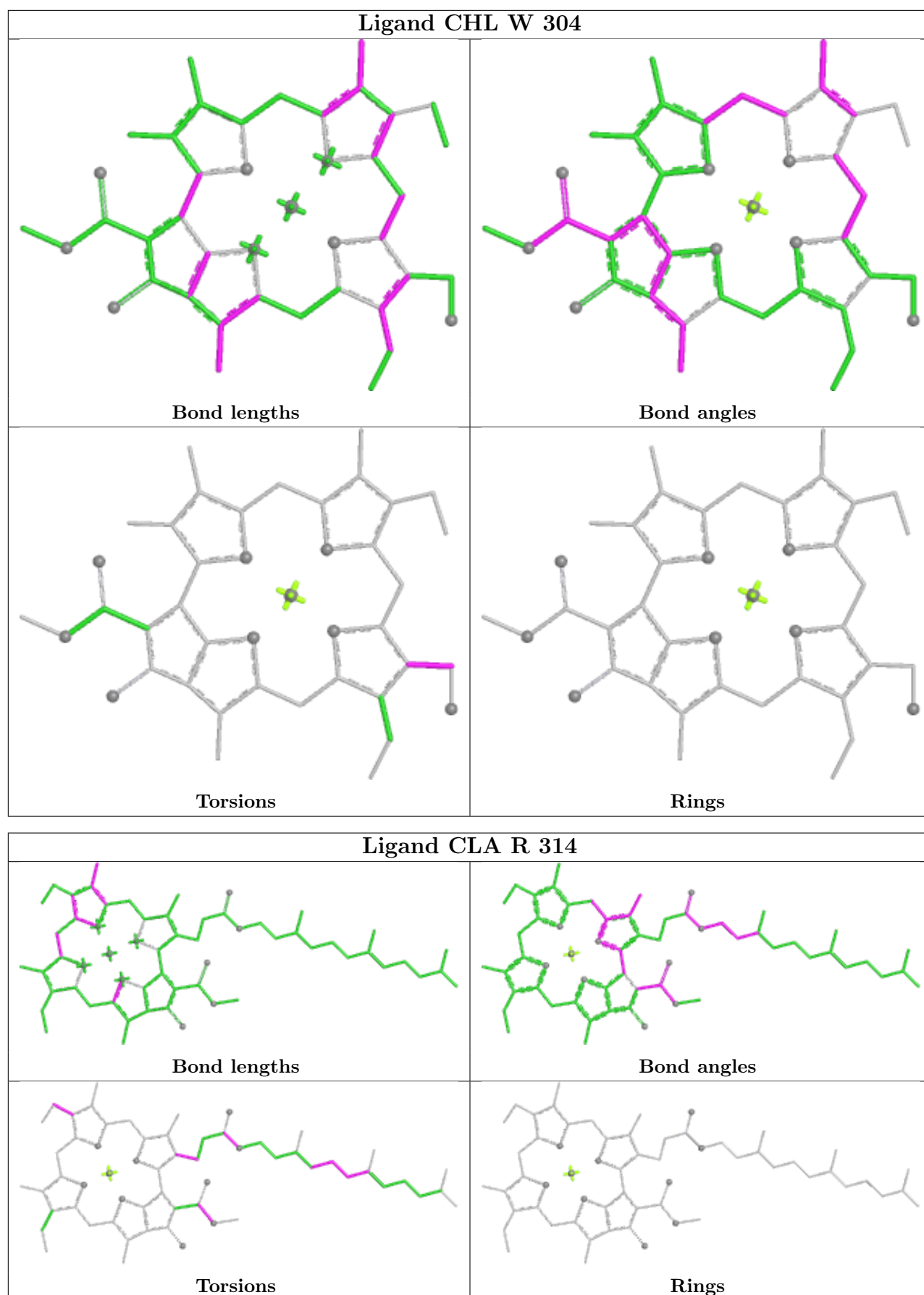
Bond angles



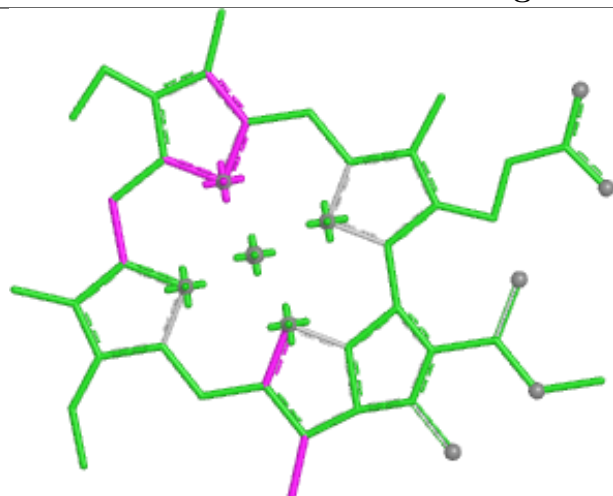
Torsions



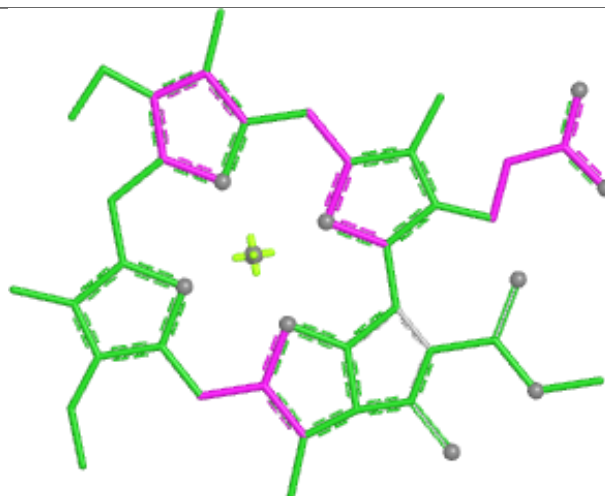
Rings



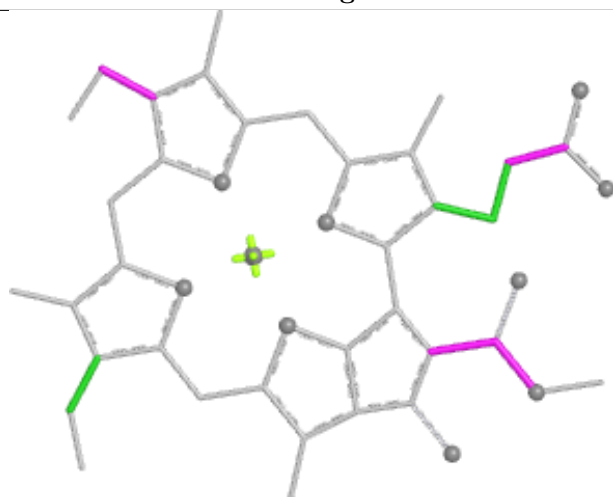
Ligand CLA A 816



Bond lengths



Bond angles

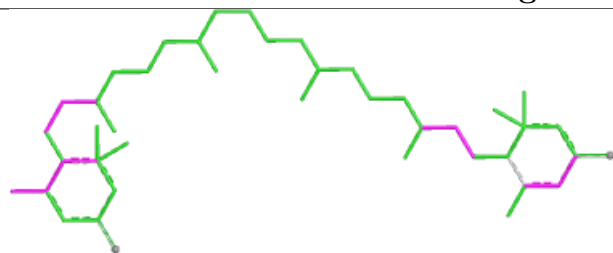


Torsions

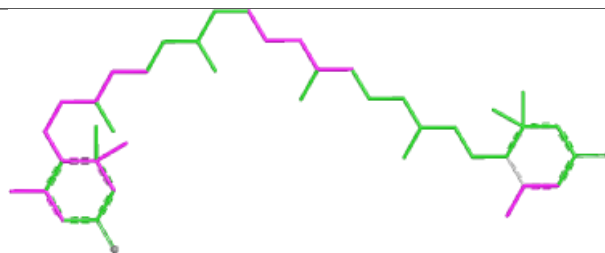


Rings

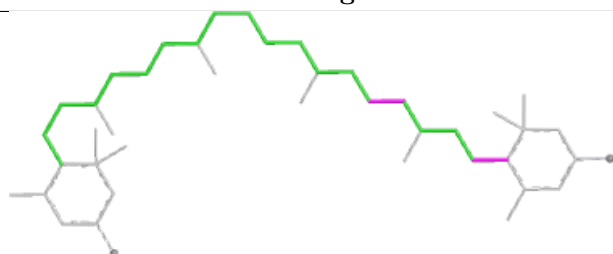
Ligand Q6L P 316



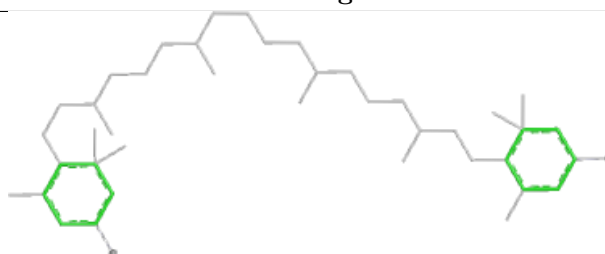
Bond lengths



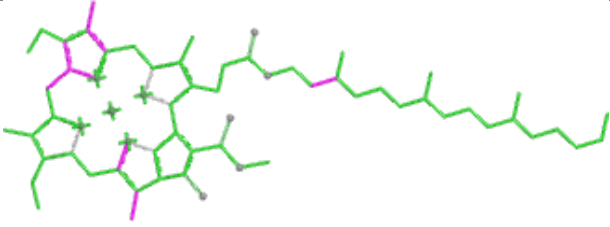
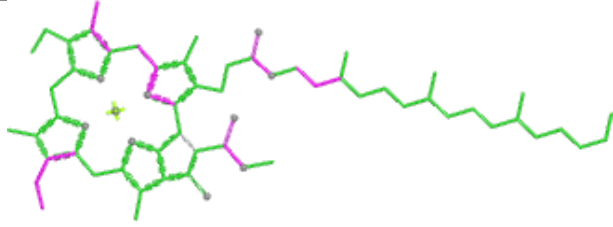
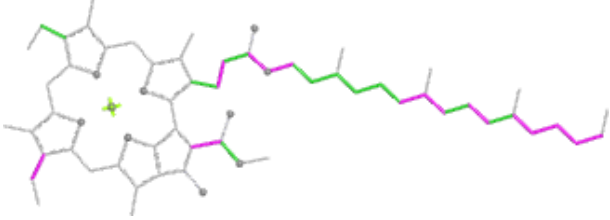
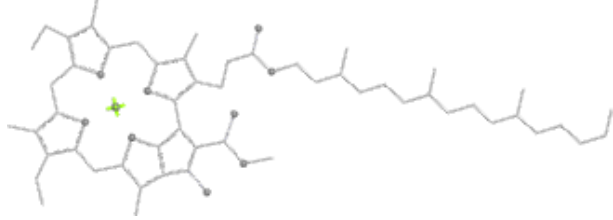
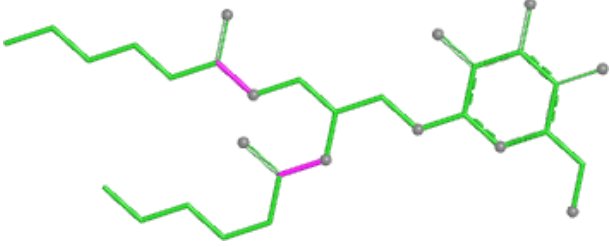
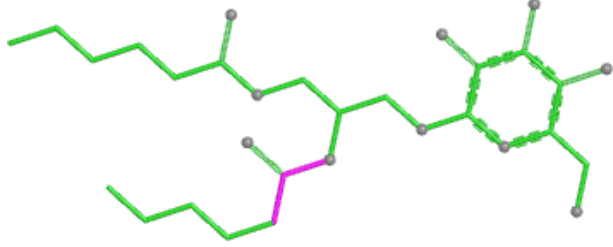
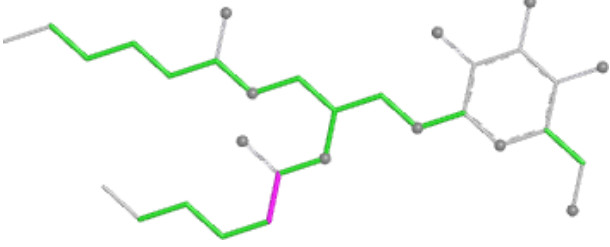
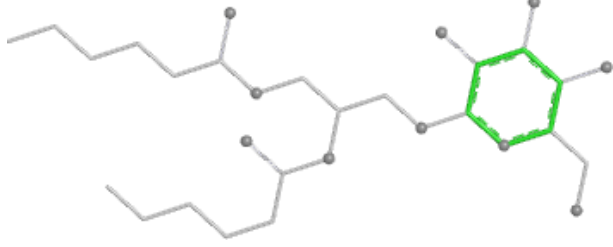
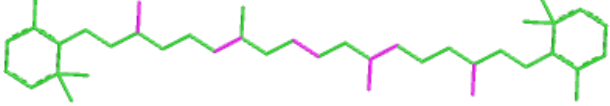
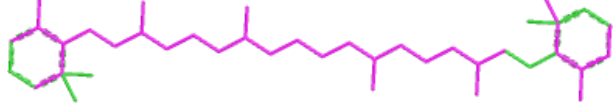
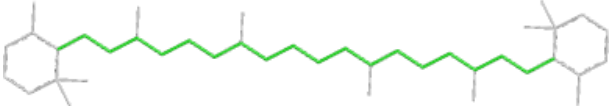
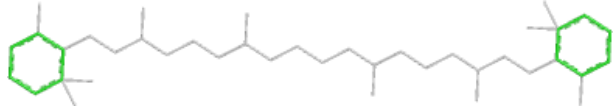
Bond angles



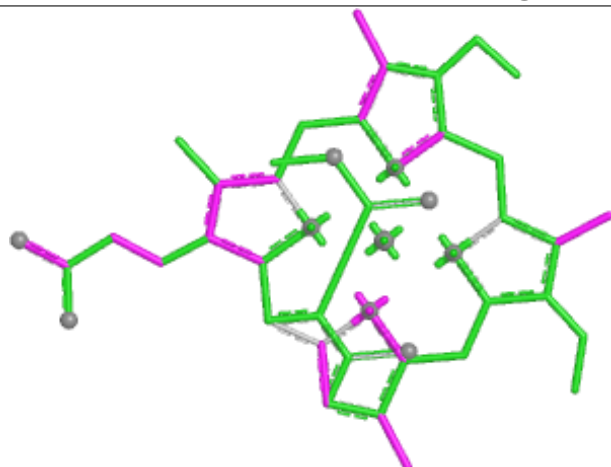
Torsions



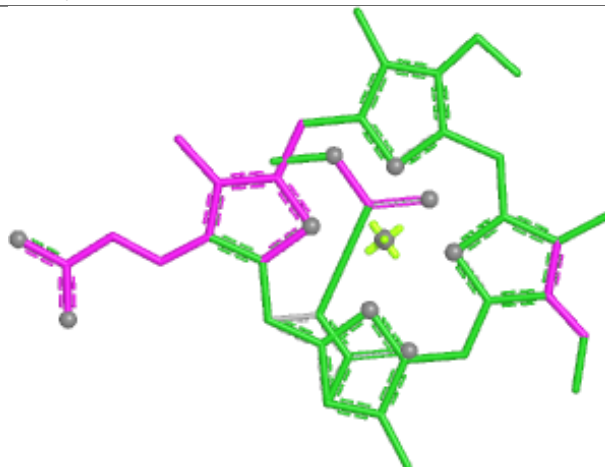
Rings

Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

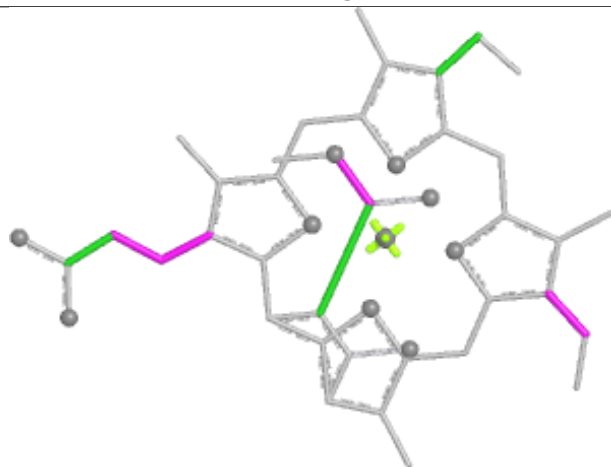
Ligand KC2 Q 310



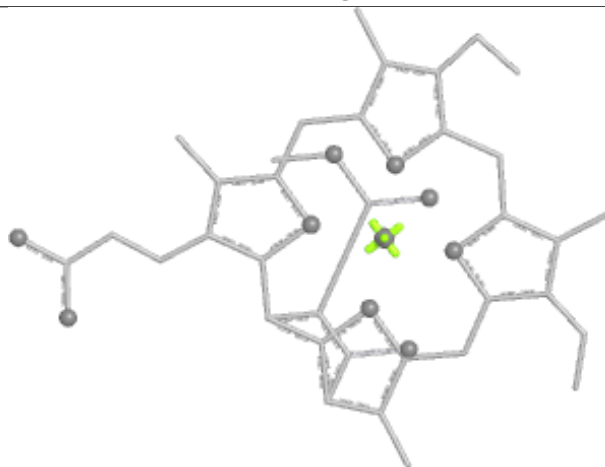
Bond lengths



Bond angles

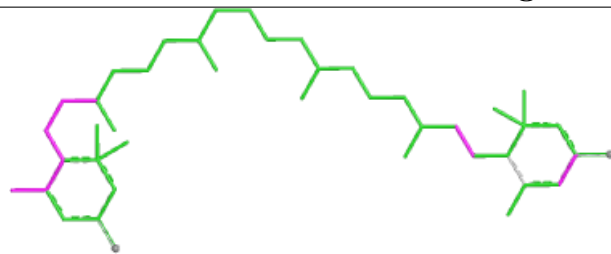


Torsions

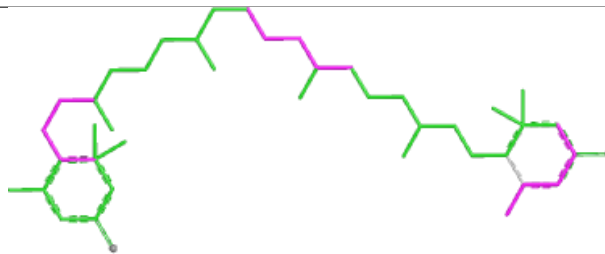


Rings

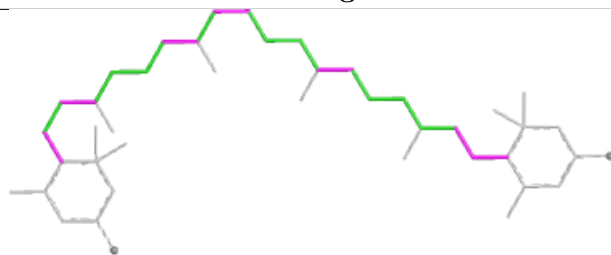
Ligand Q6L V 315



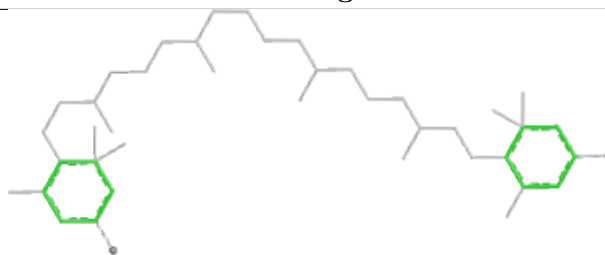
Bond lengths



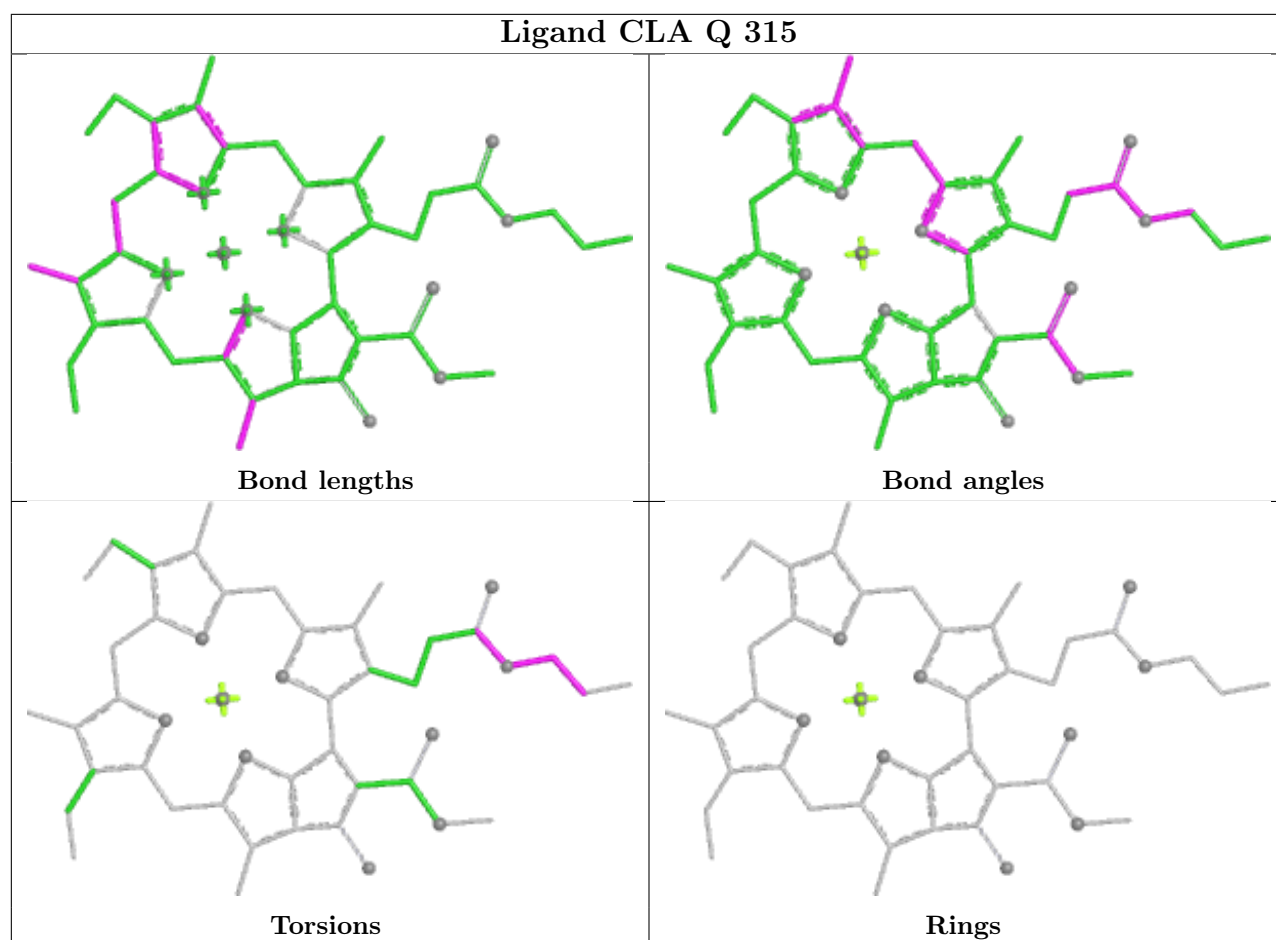
Bond angles



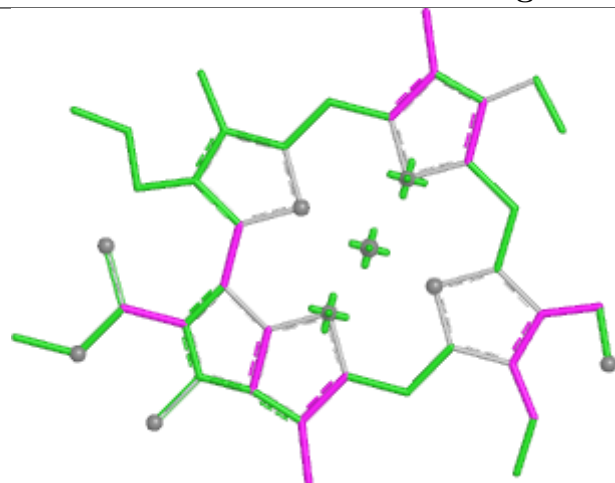
Torsions



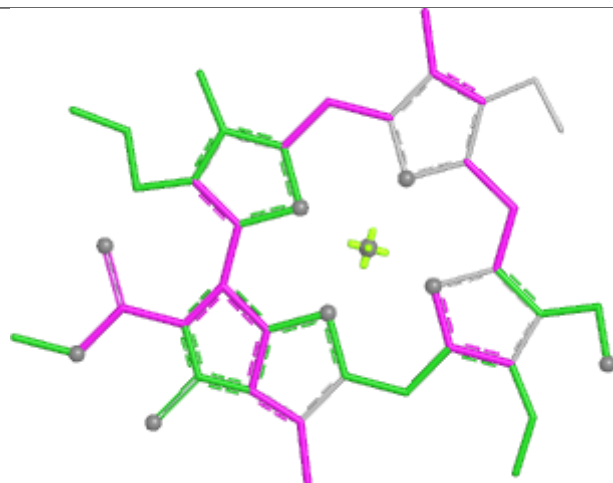
Rings



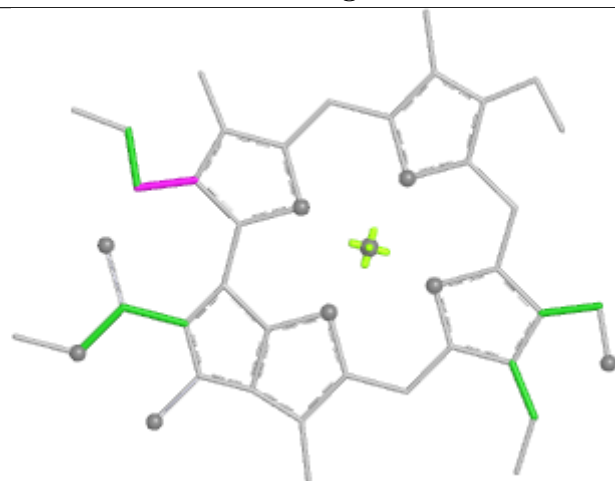
Ligand CHL P 307



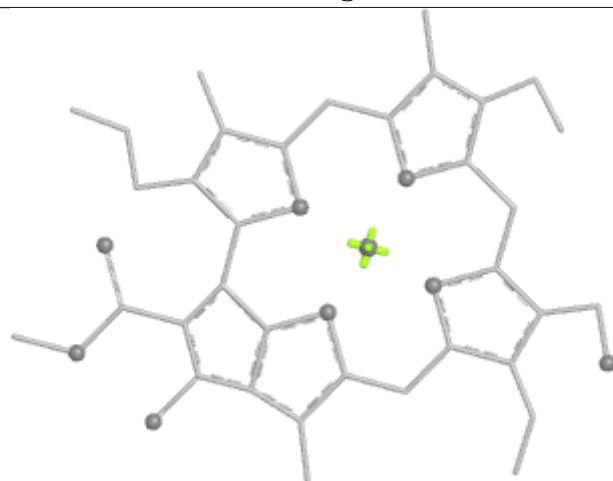
Bond lengths



Bond angles

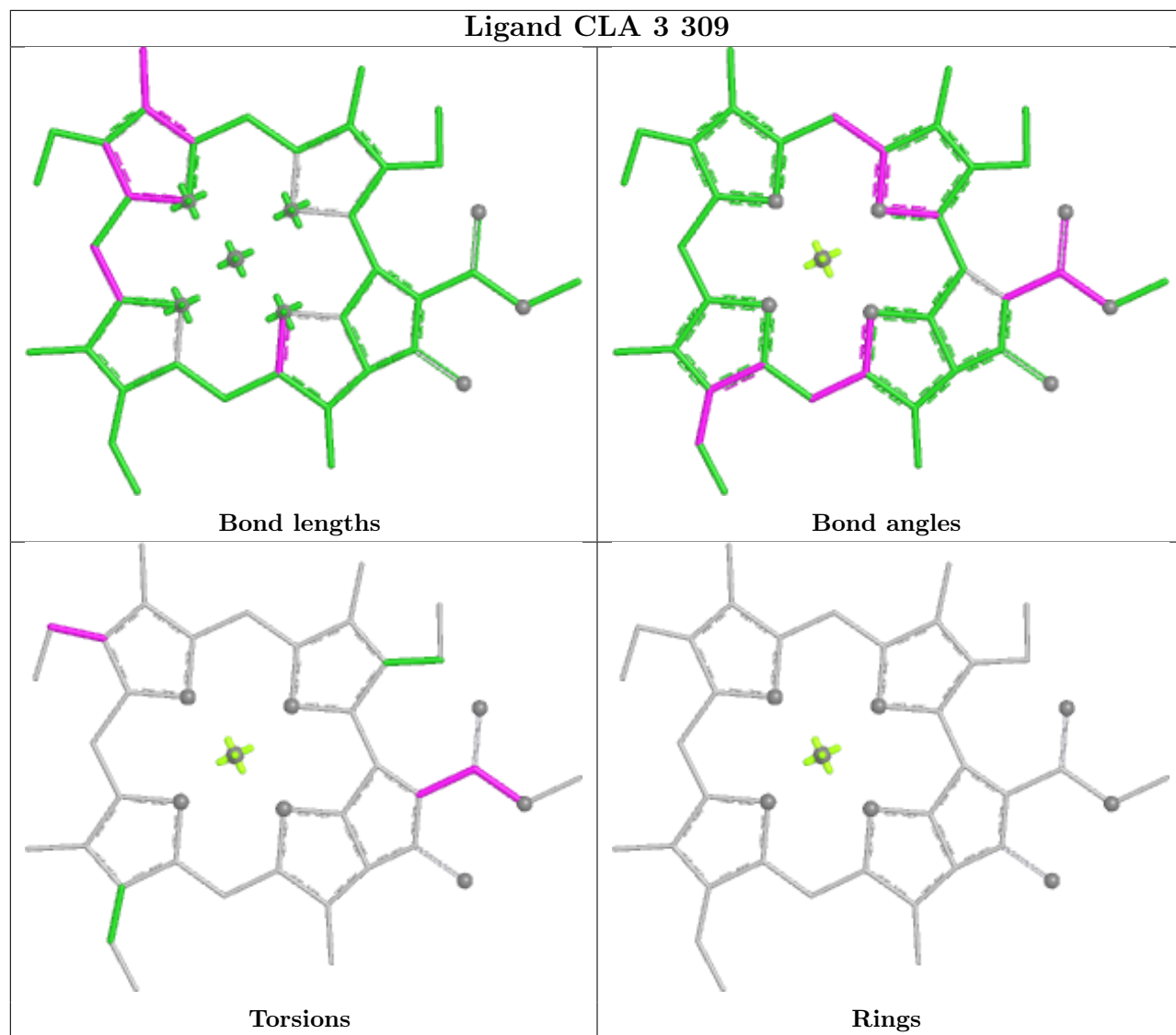


Torsions

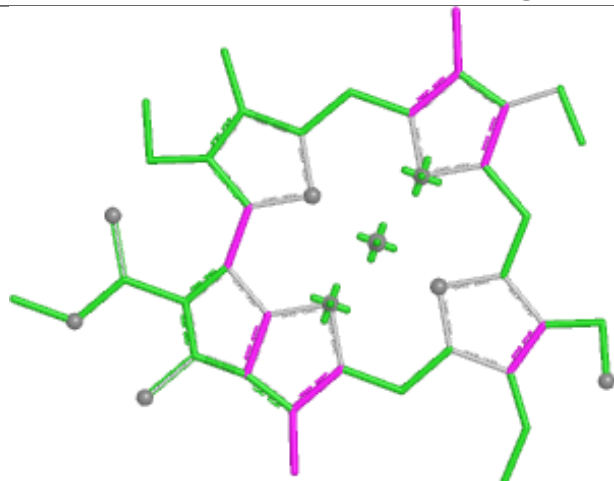


Rings

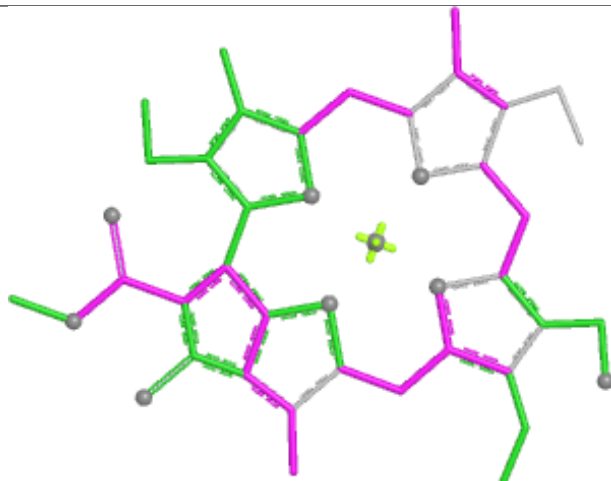
Ligand CLA 3 309



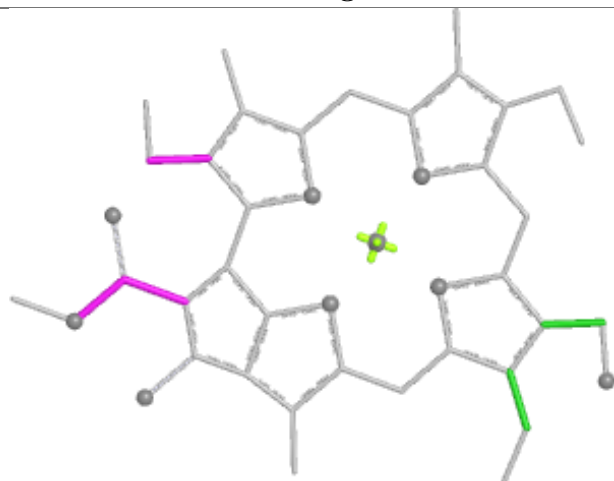
Ligand CHL 6 606



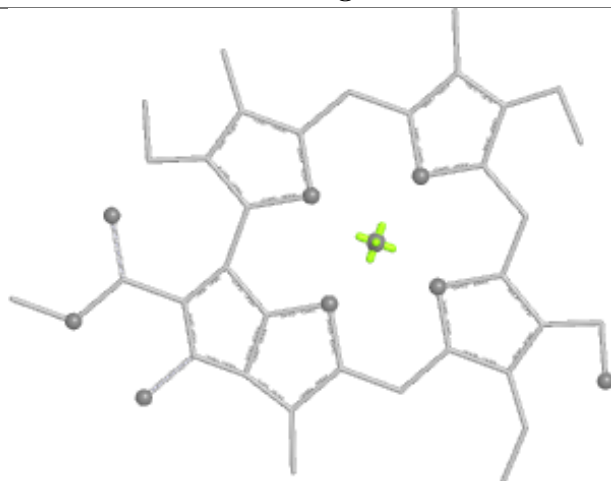
Bond lengths



Bond angles

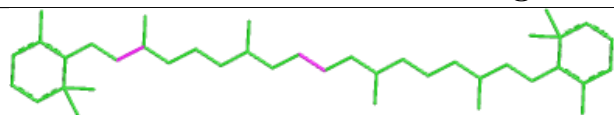


Torsions

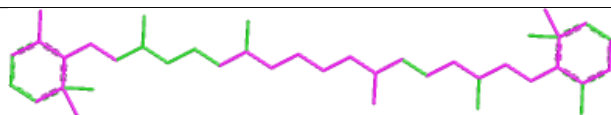


Rings

Ligand BCR B 849



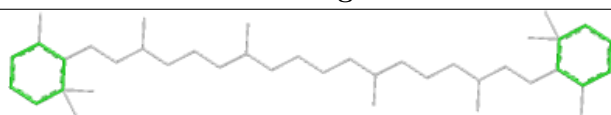
Bond lengths



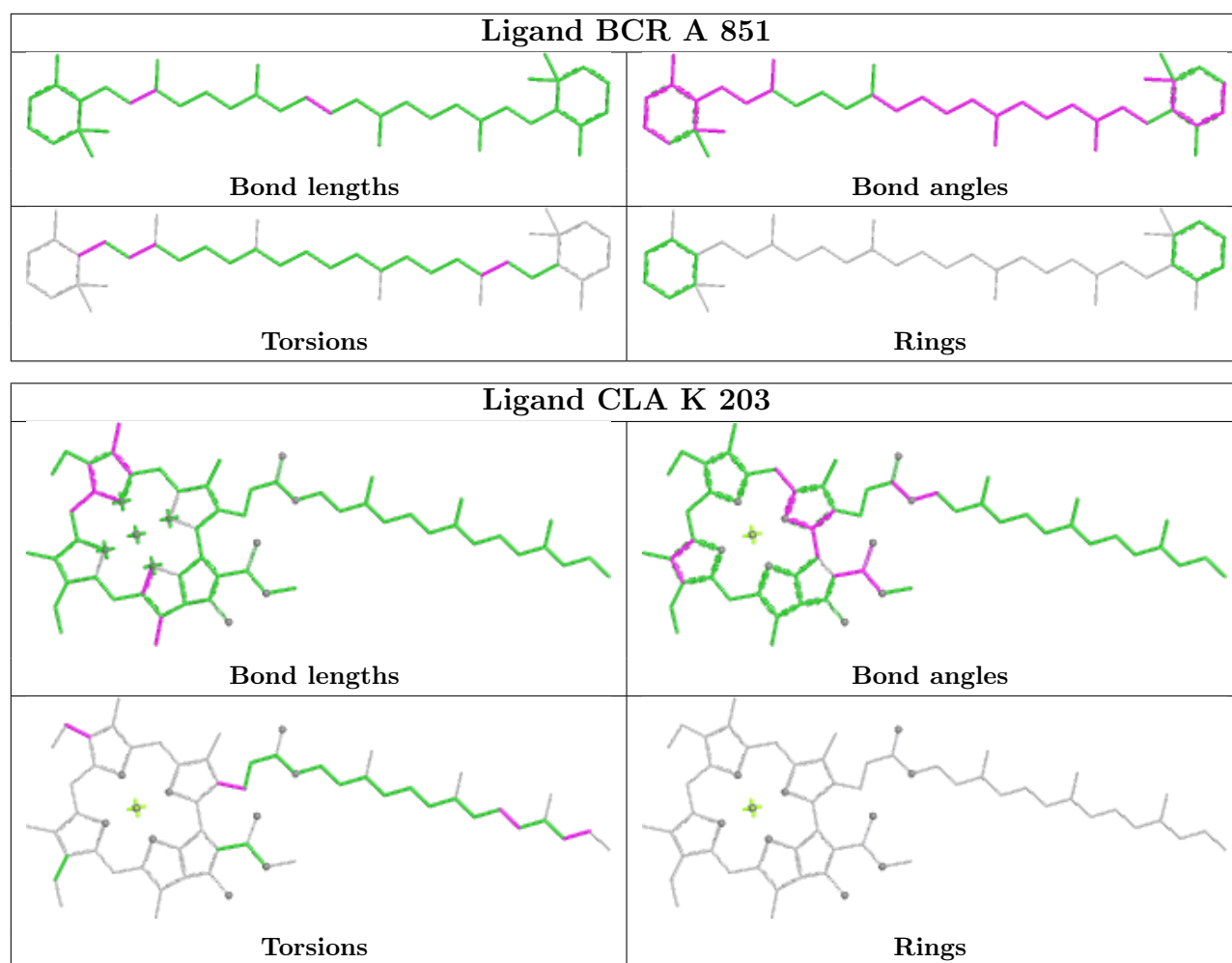
Bond angles



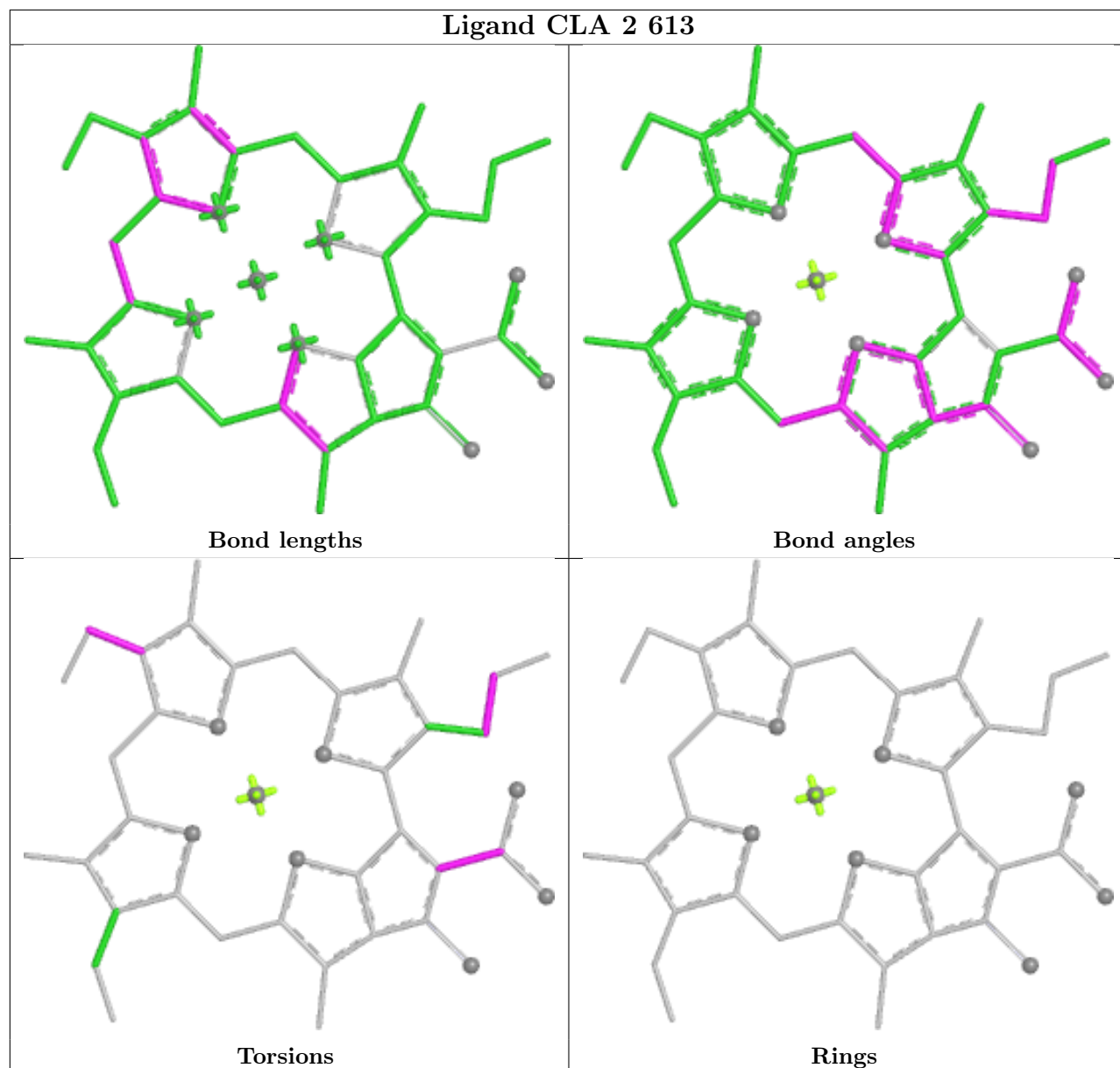
Torsions



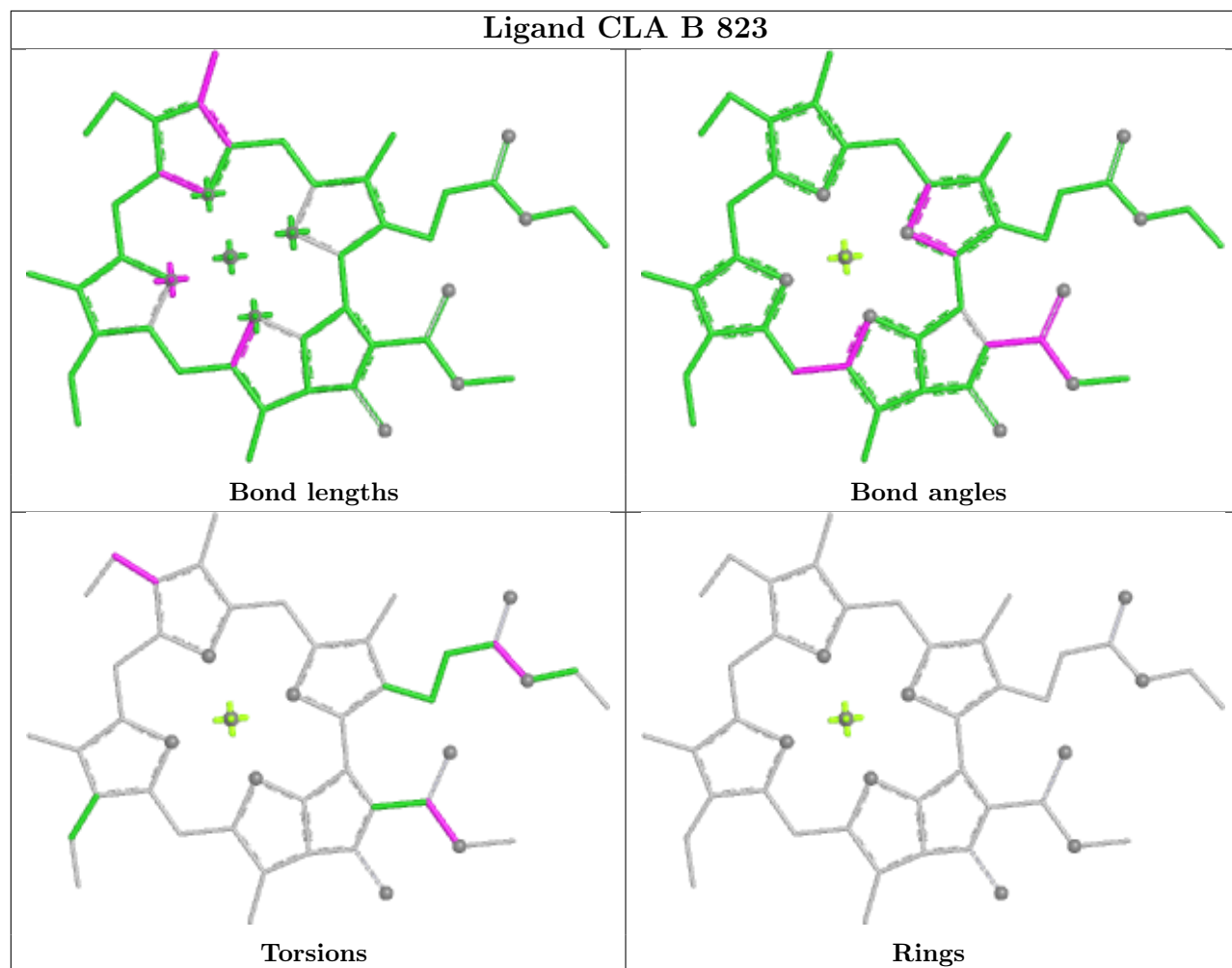
Rings



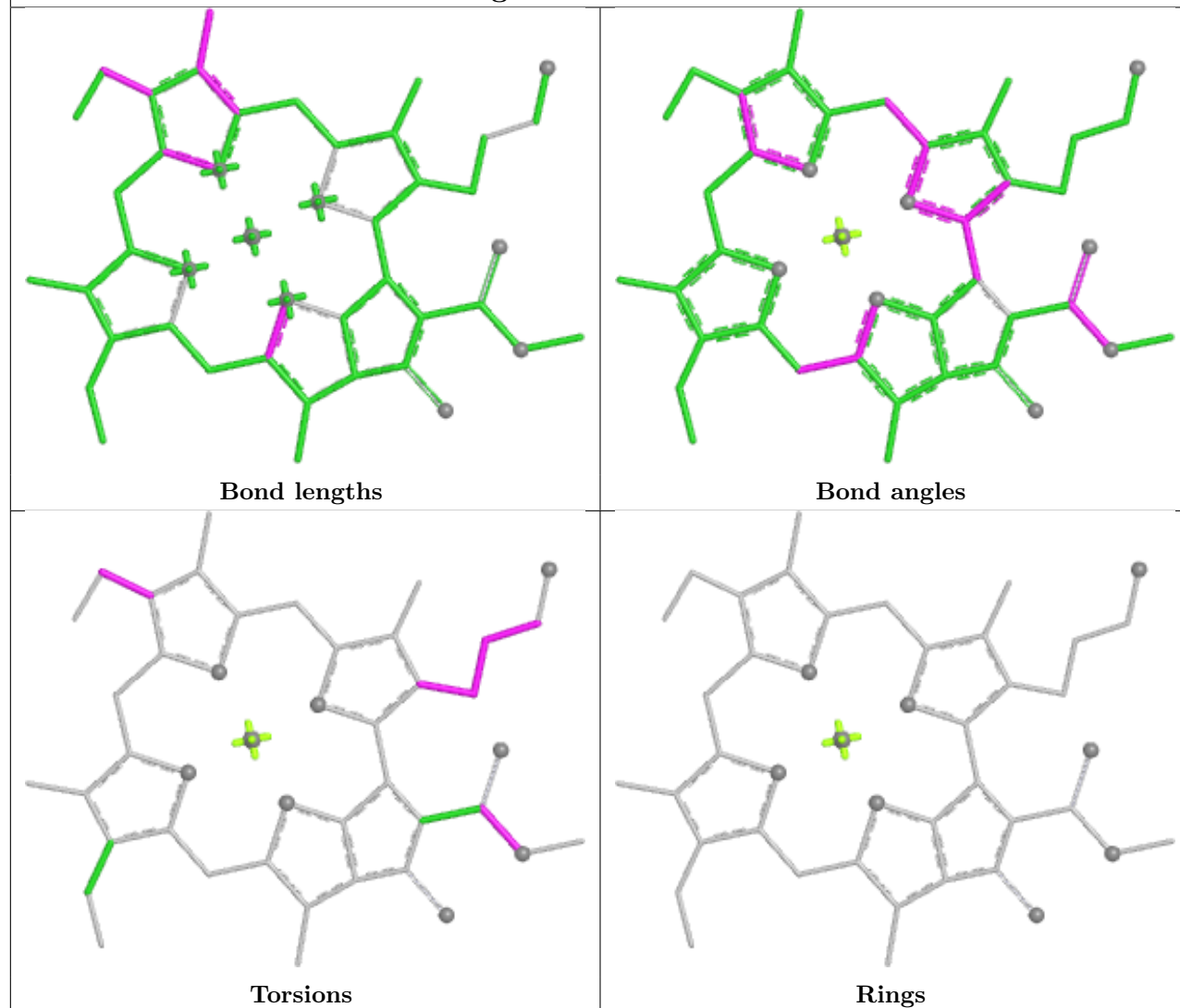
Ligand CLA 2 613



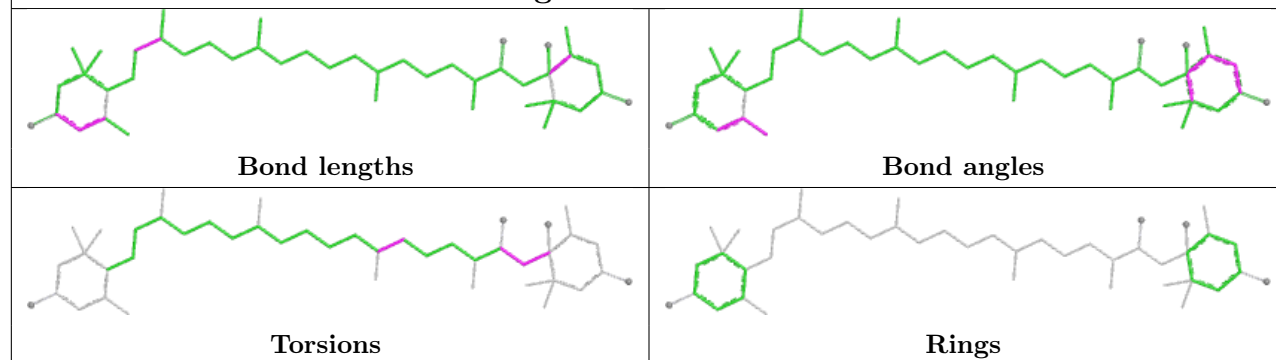
Ligand CLA B 823

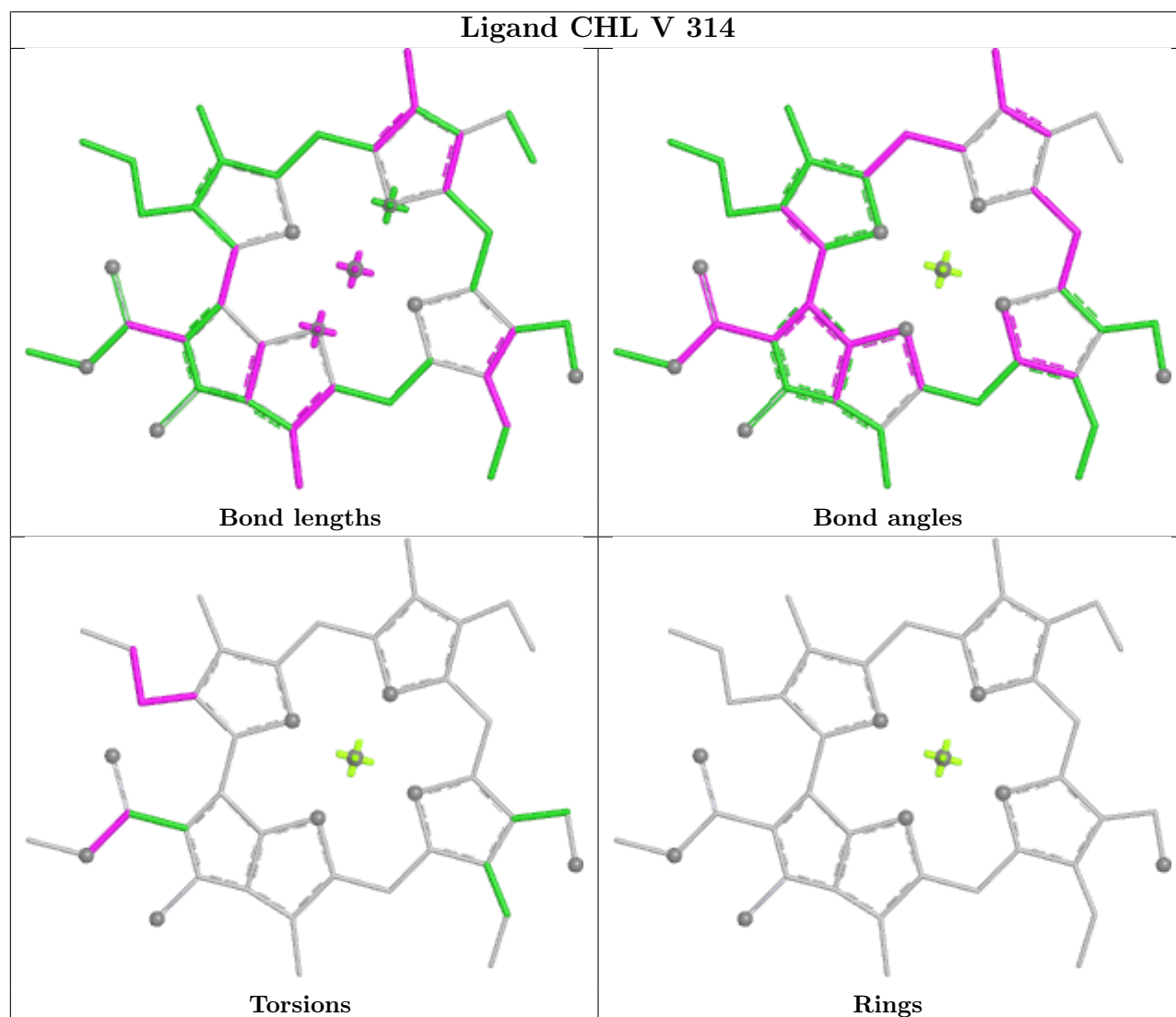
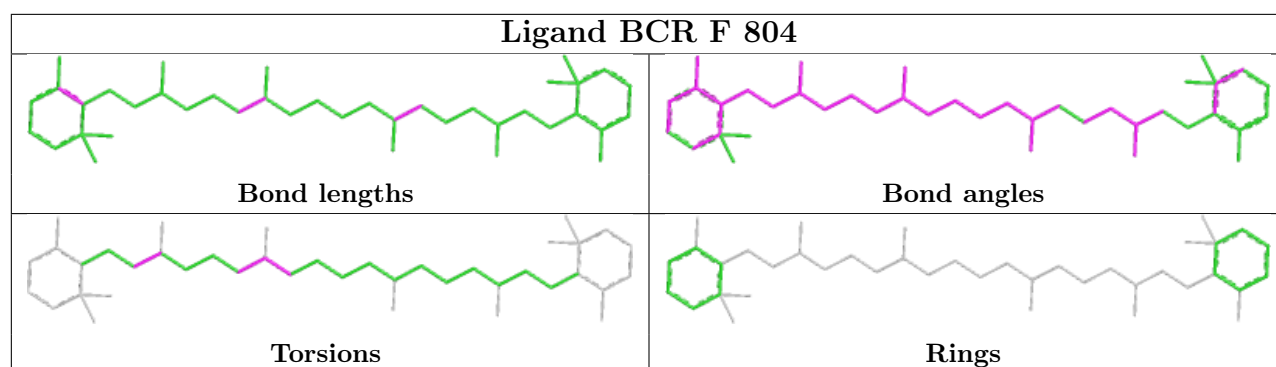


Ligand CLA H 301

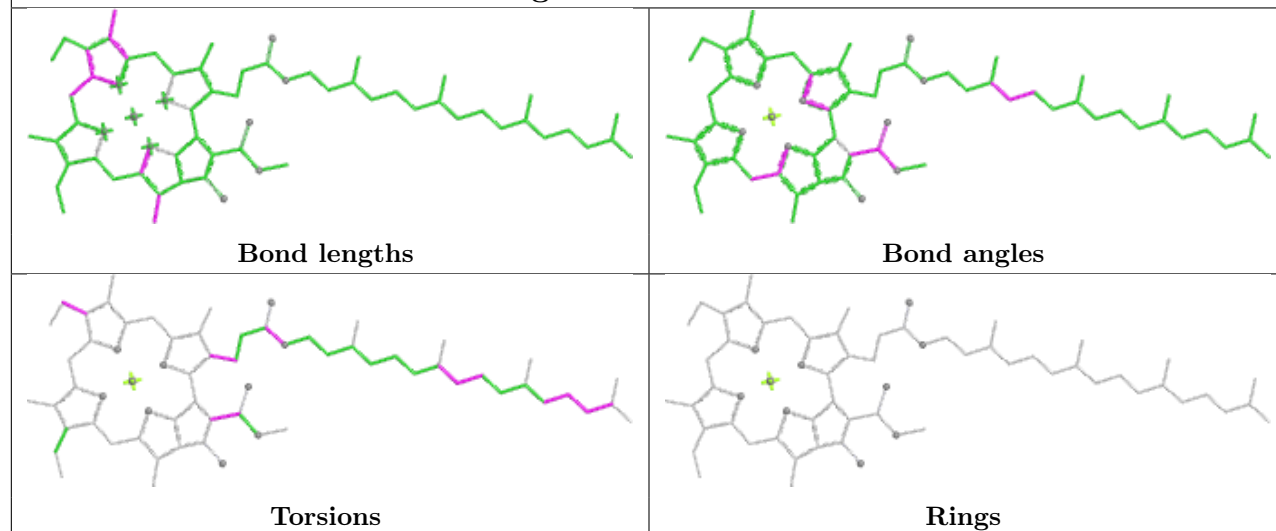


Ligand IWJ V 317

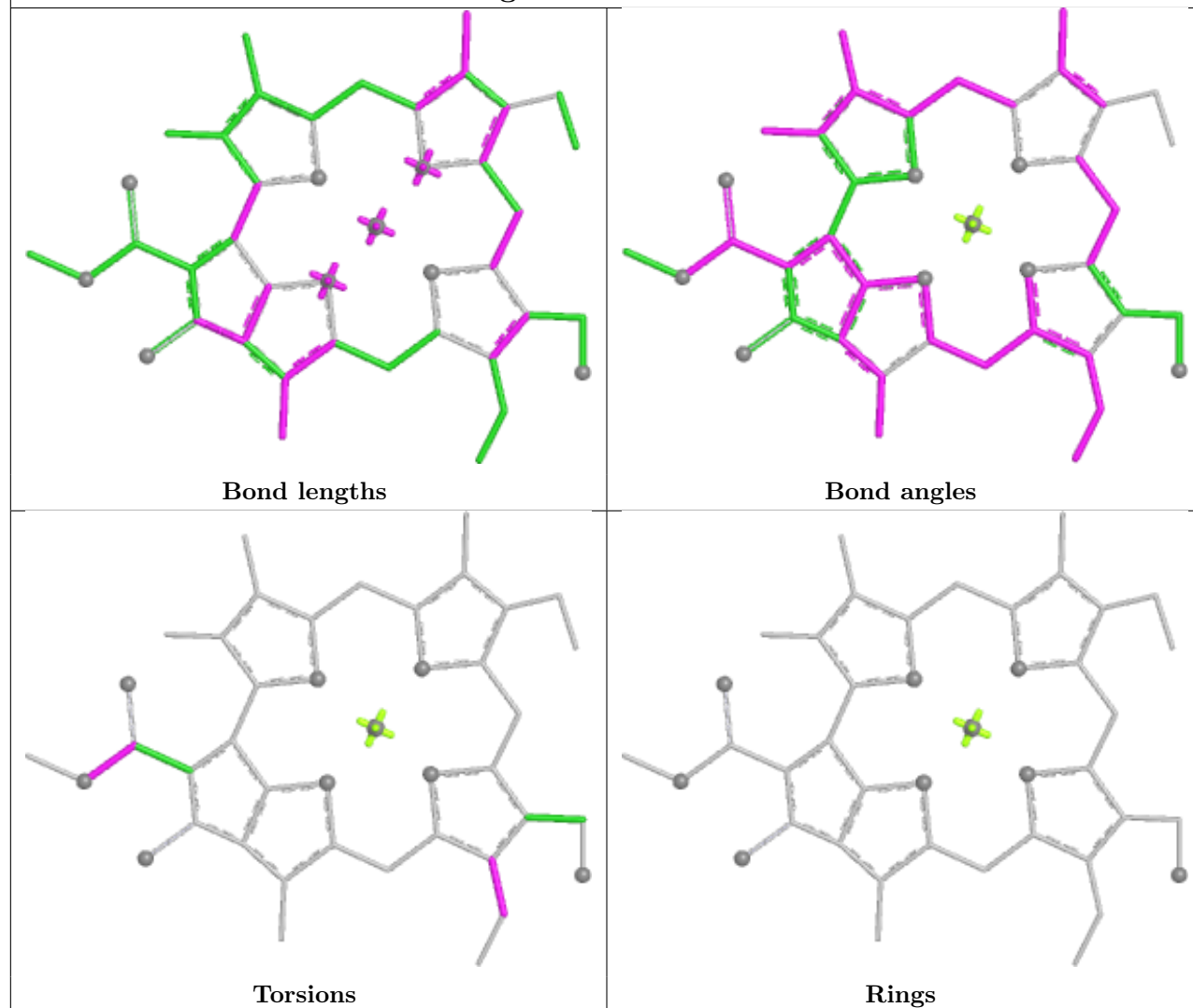


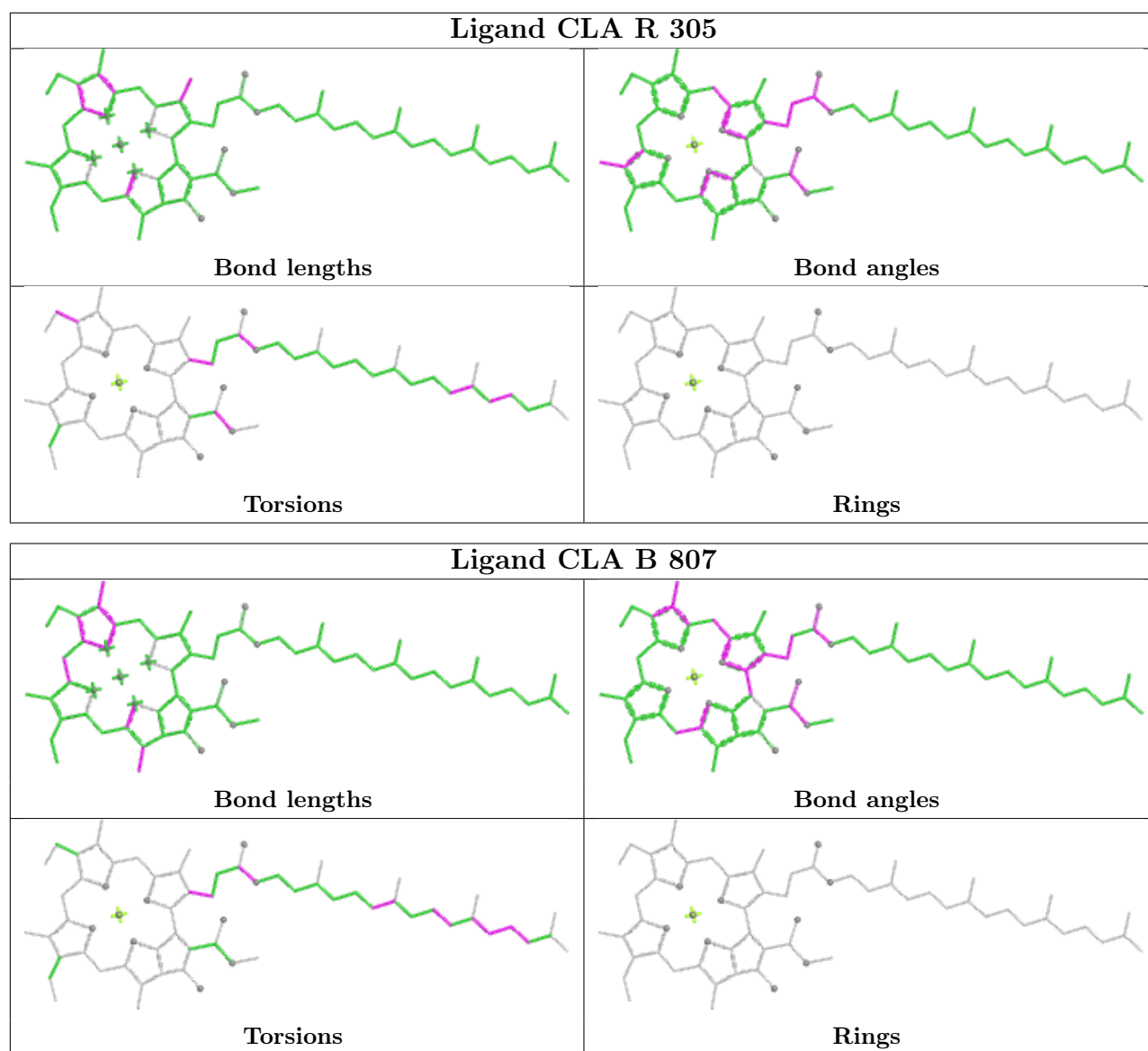


Ligand CLA A 813

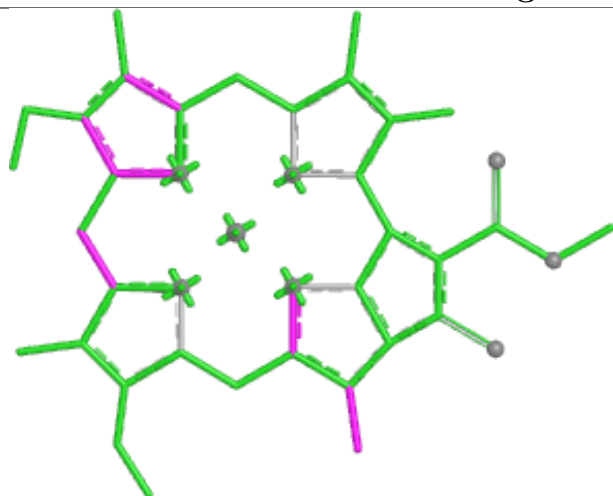


Ligand CHL S 305

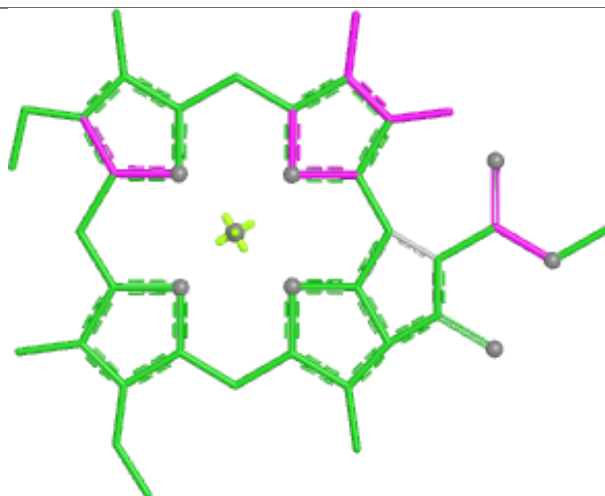




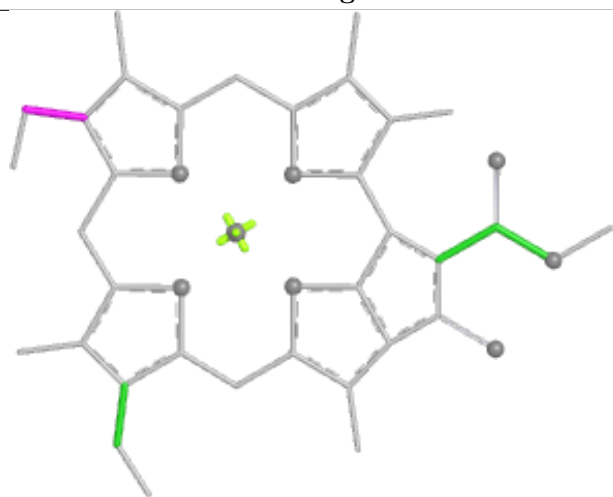
Ligand CLA S 313



Bond lengths



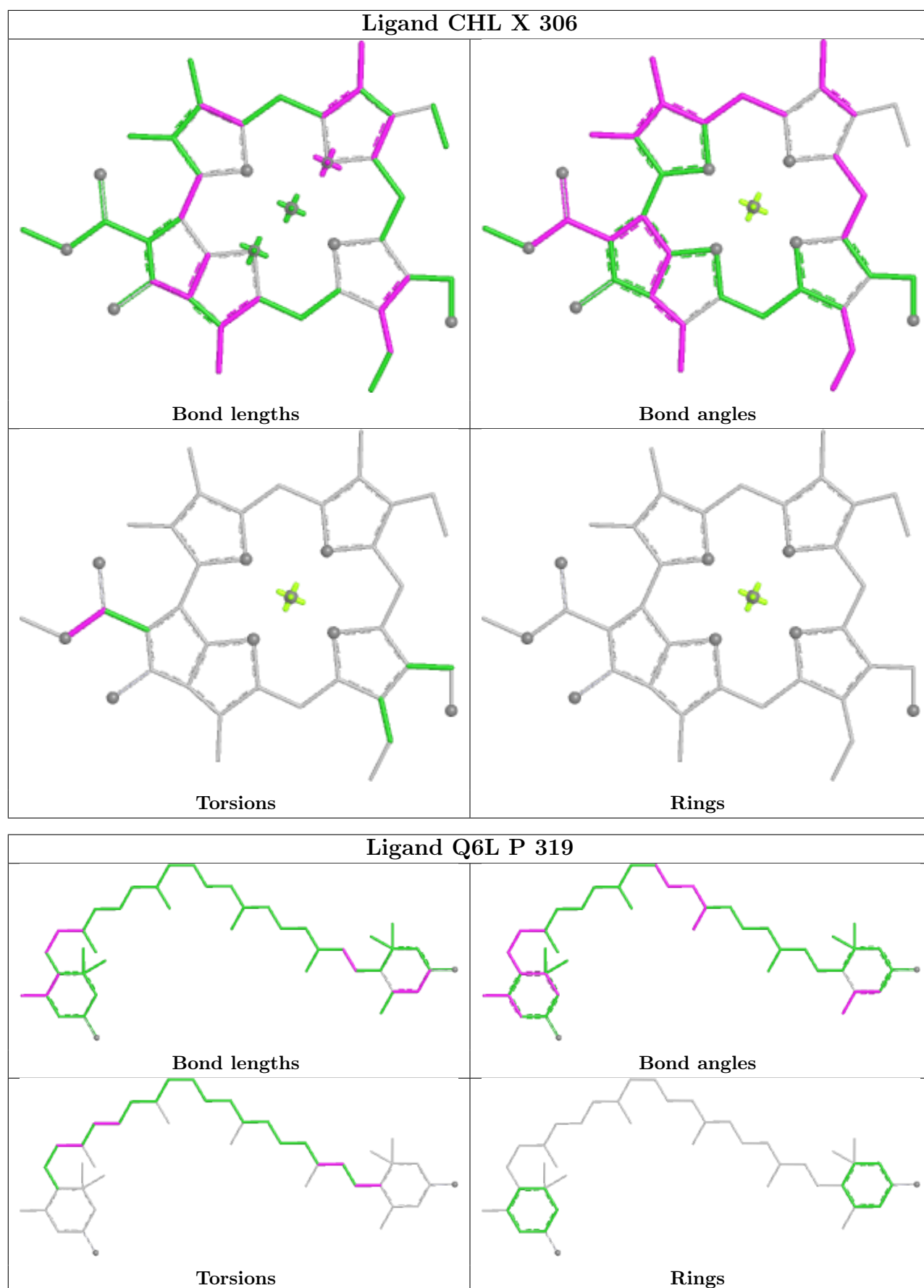
Bond angles

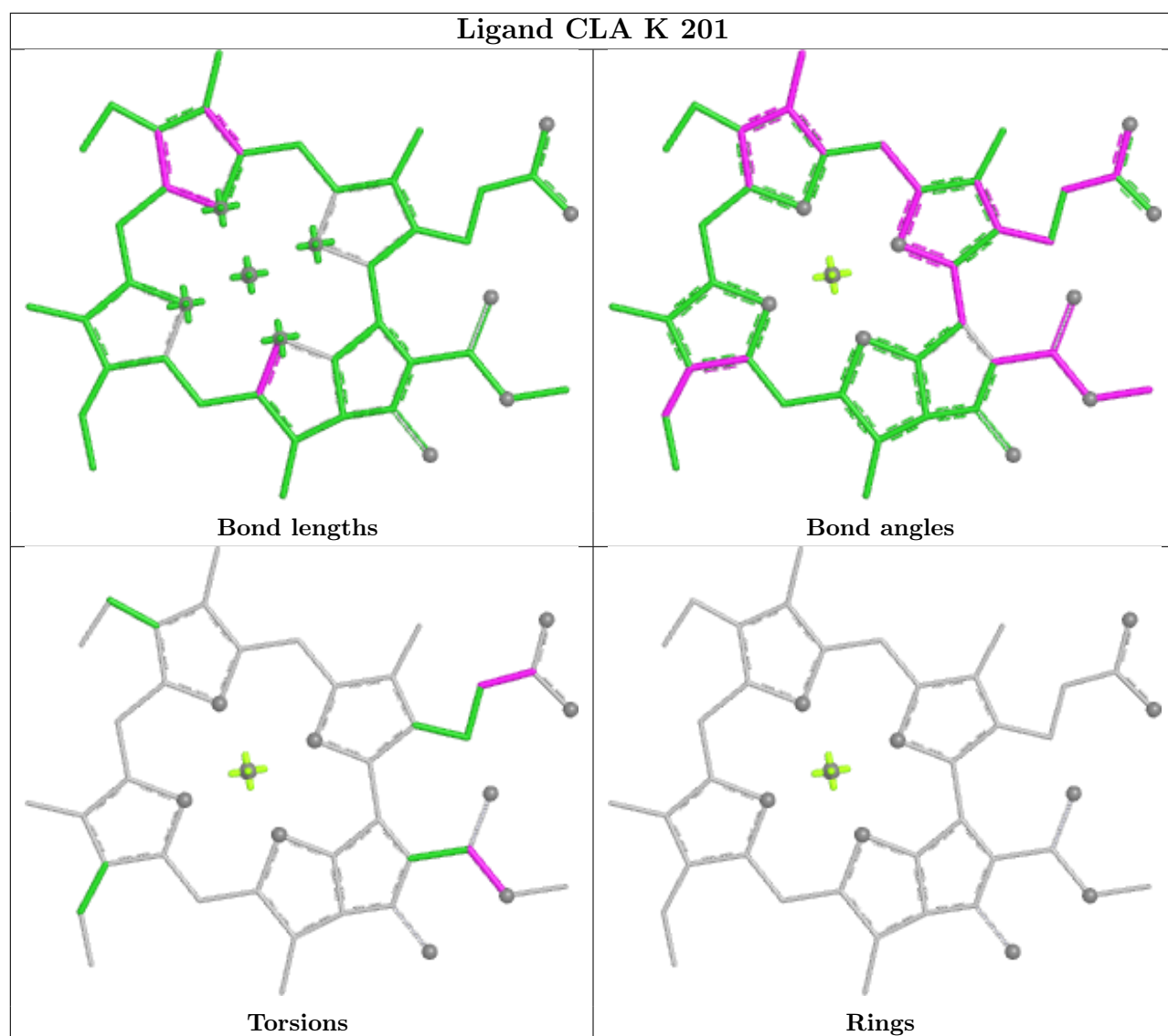


Torsions

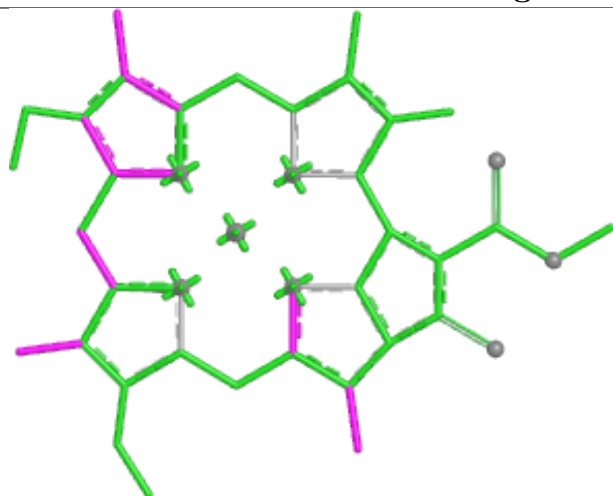


Rings

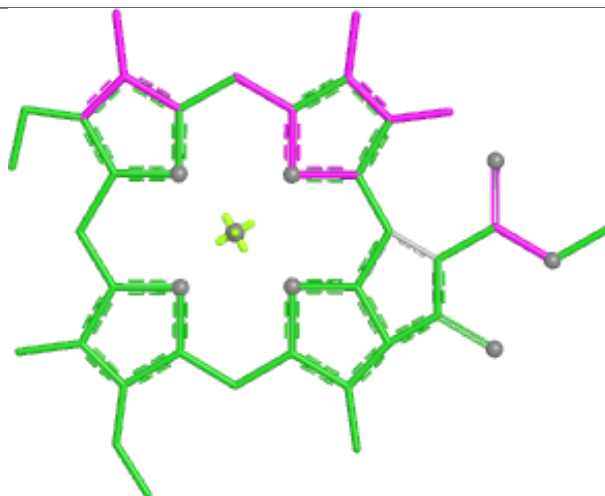




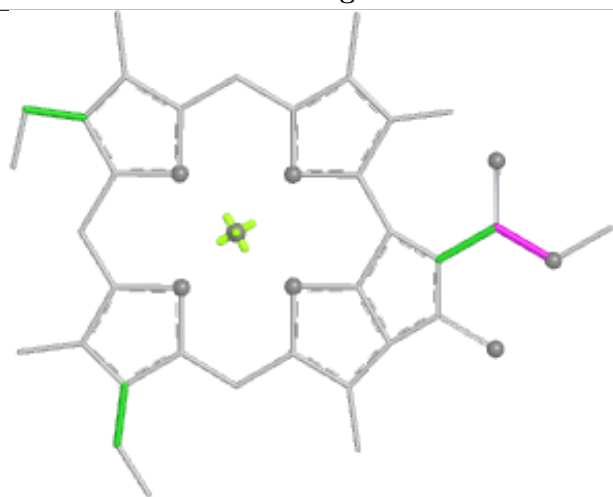
Ligand CLA X 313



Bond lengths



Bond angles

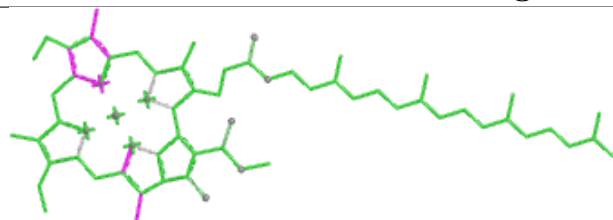


Torsions

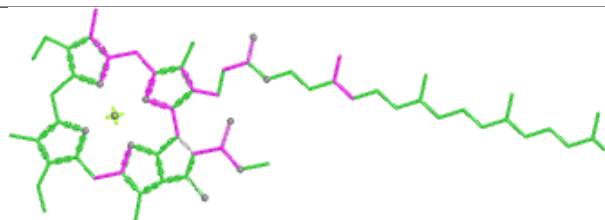


Rings

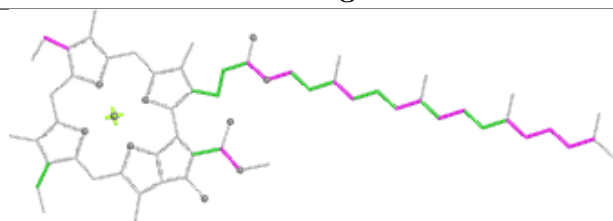
Ligand CLA A 838



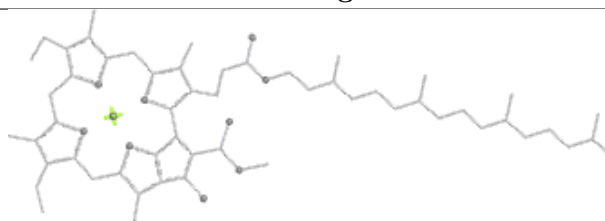
Bond lengths



Bond angles

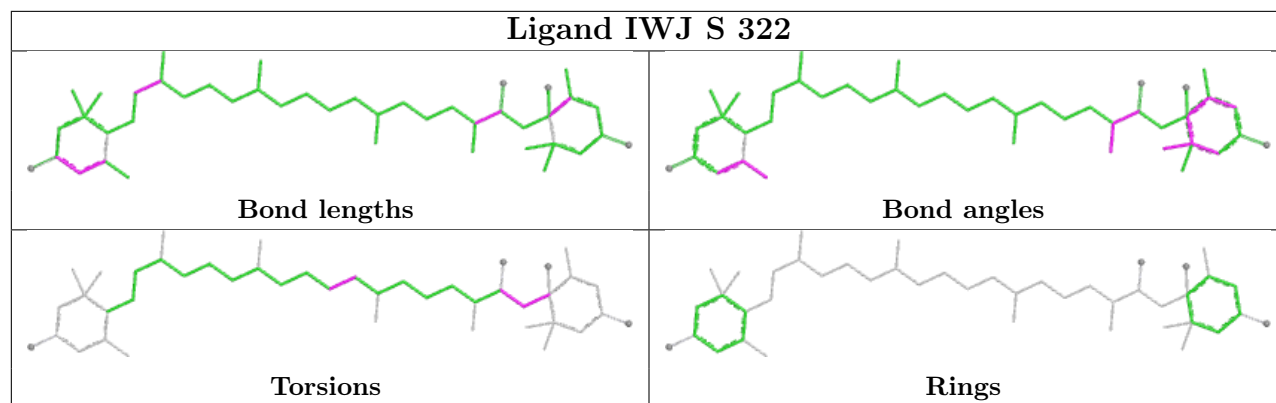


Torsions

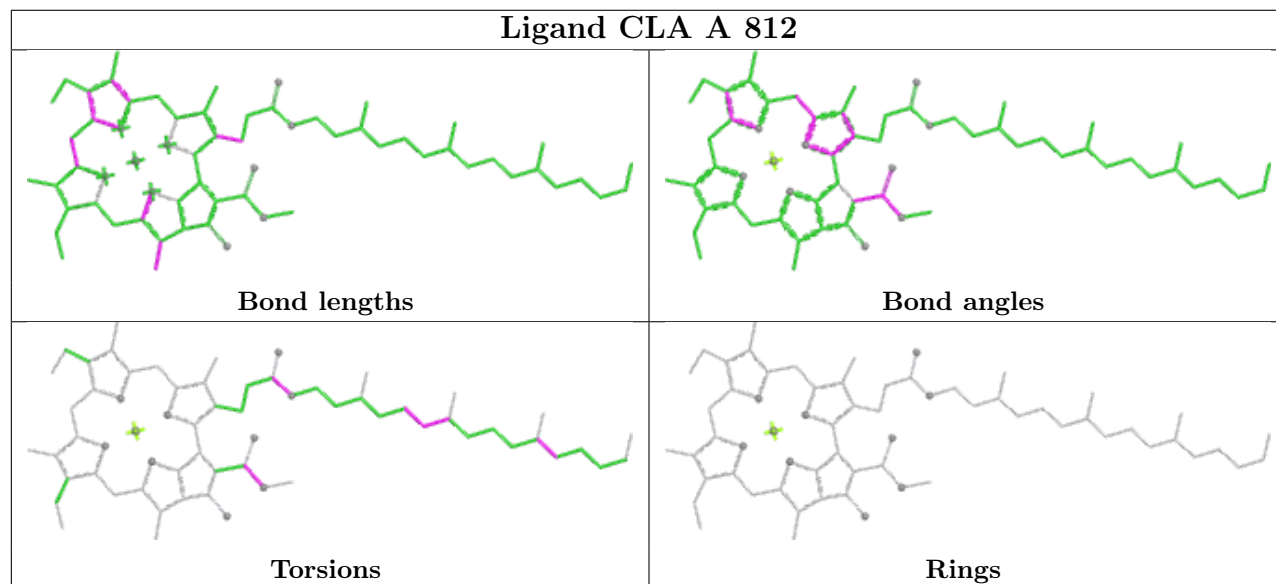


Rings

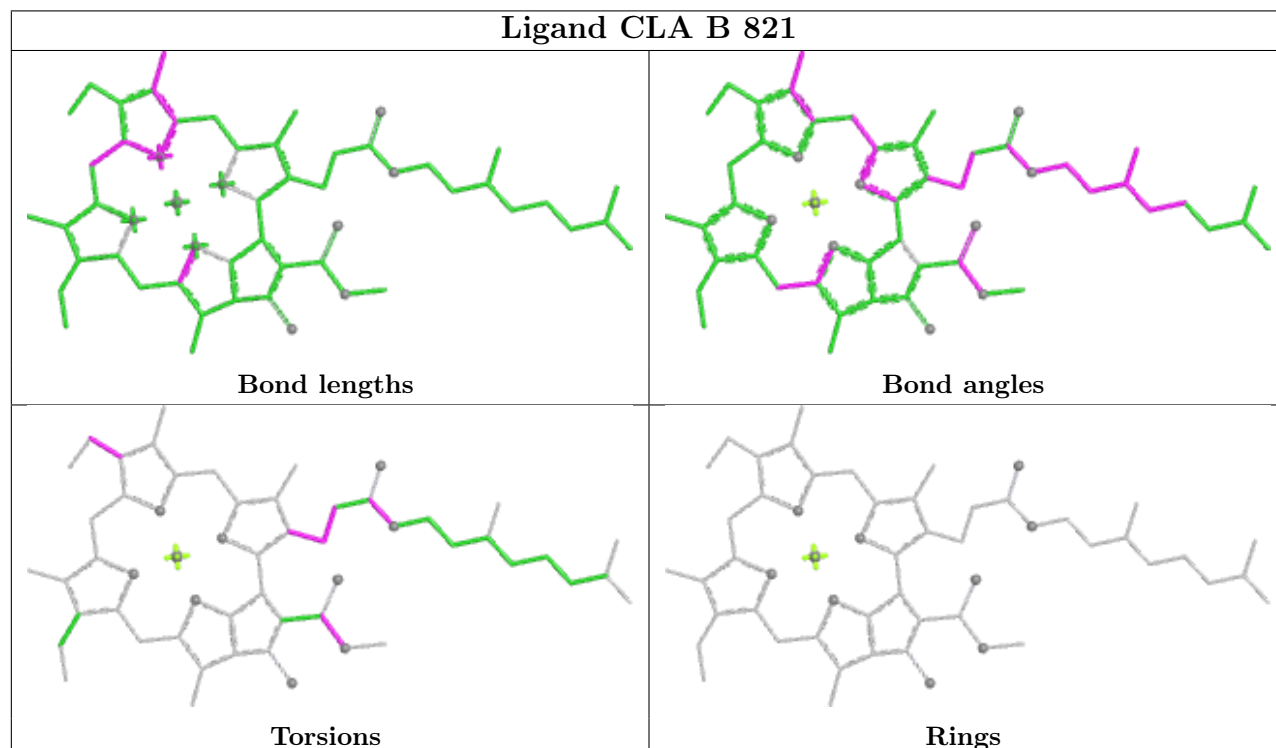
Ligand IWJ S 322



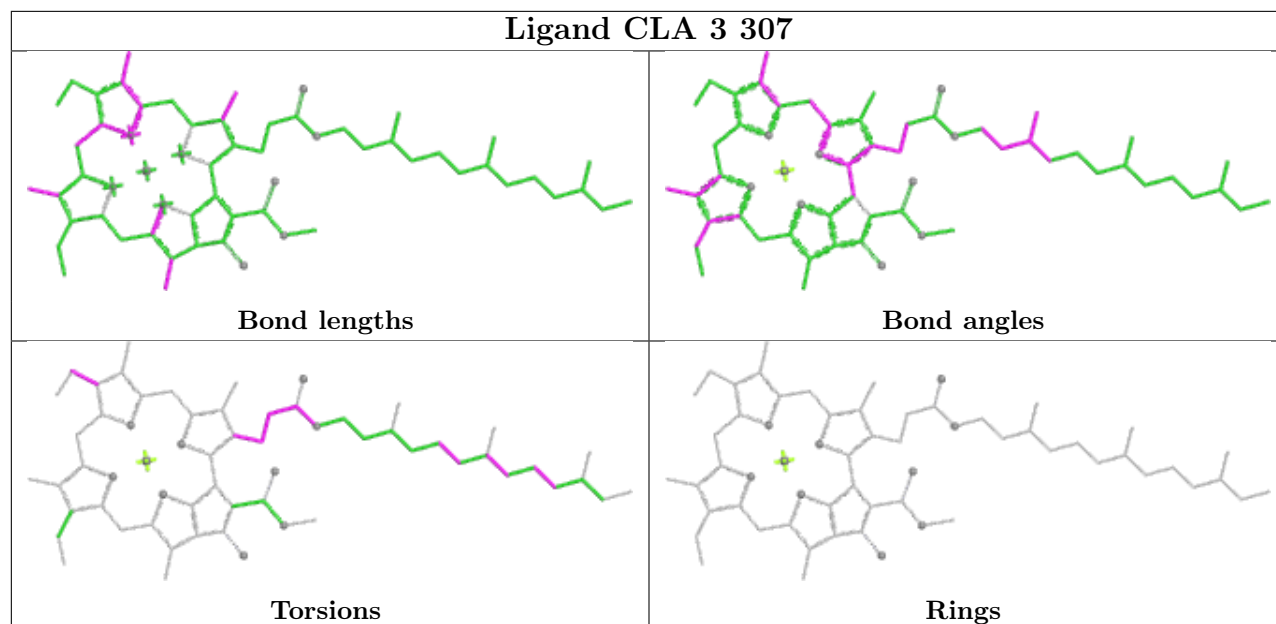
Ligand CLA A 812



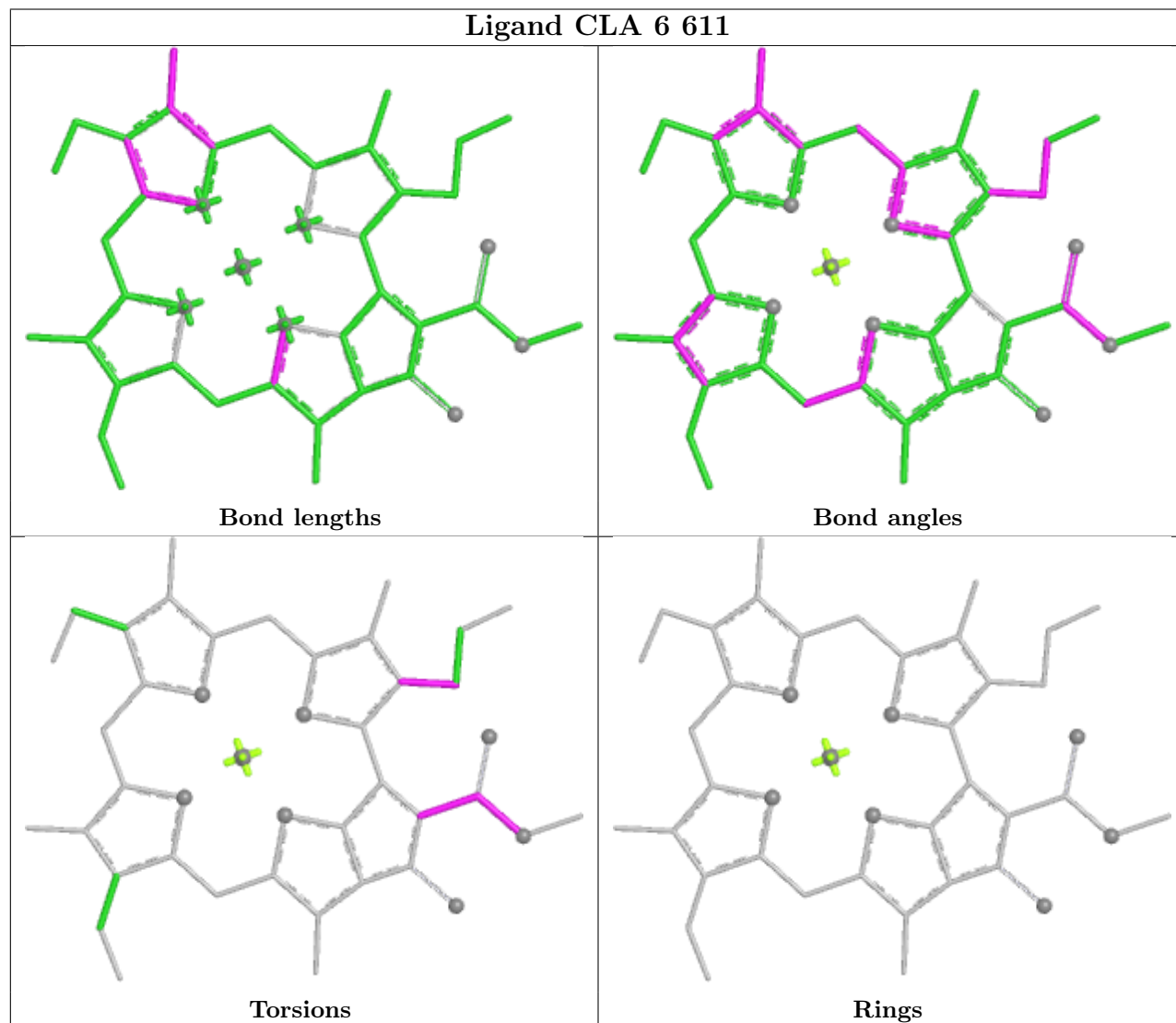
Ligand CLA B 821

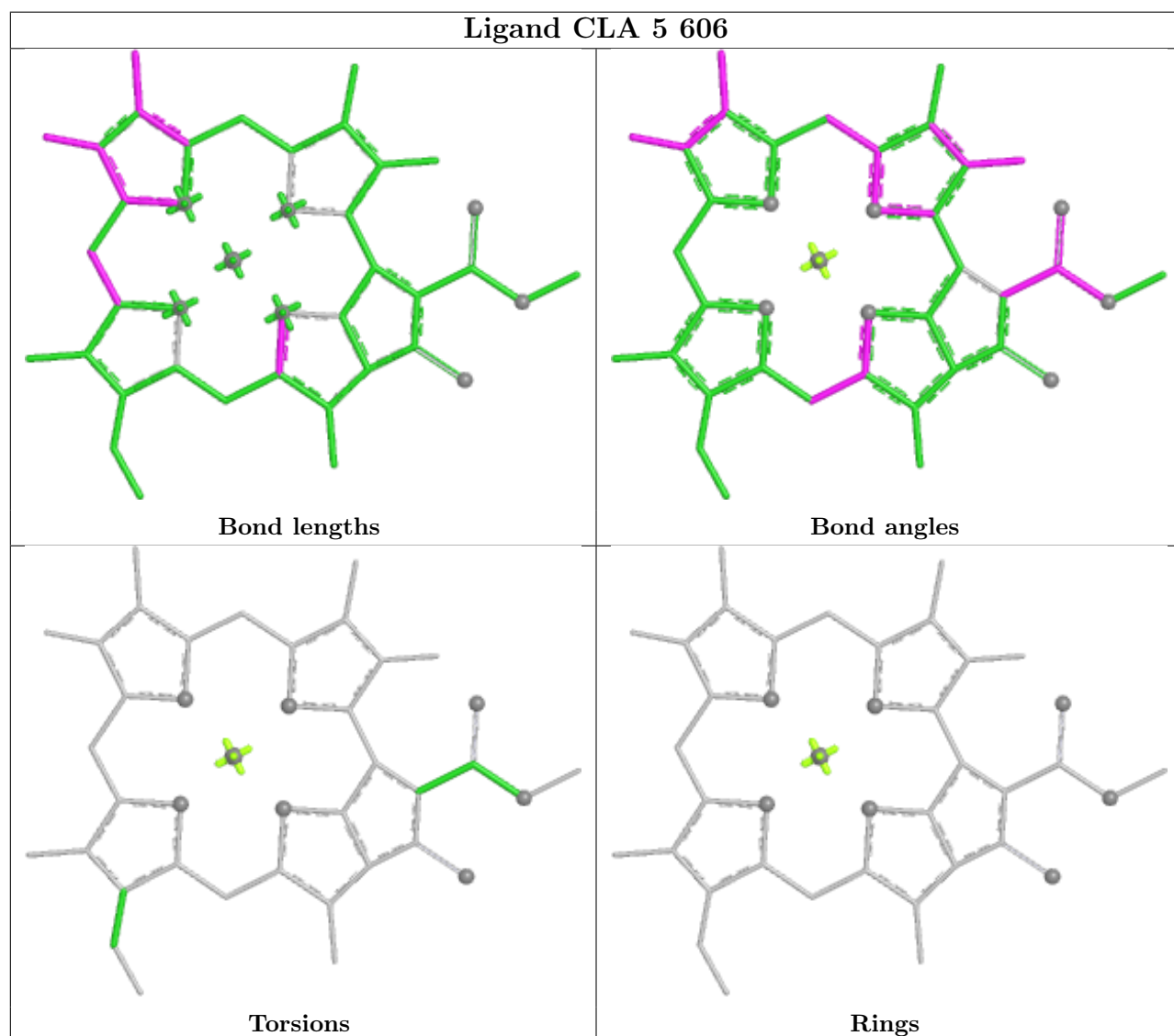
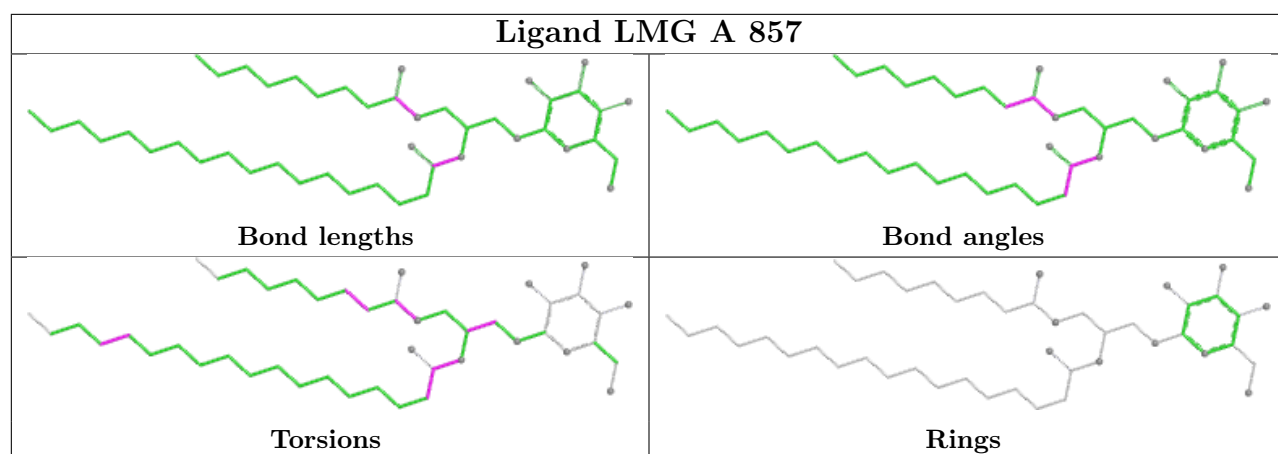


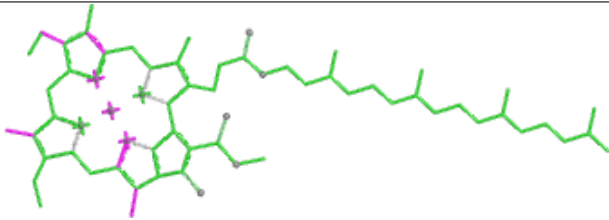
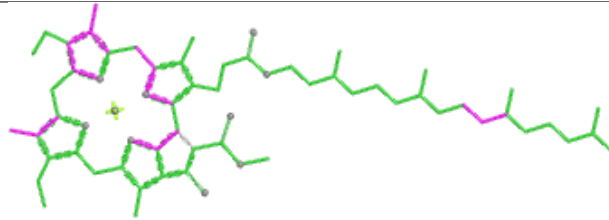
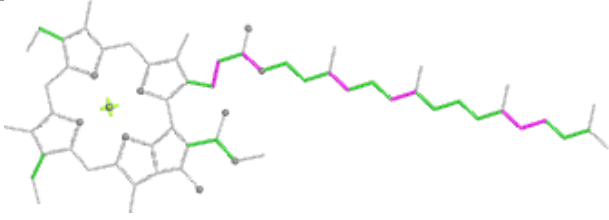
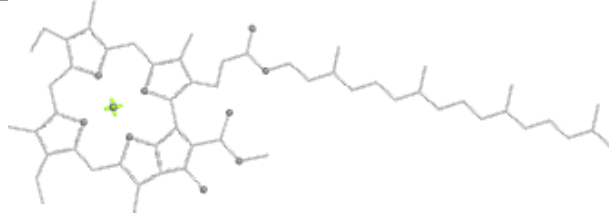
Ligand CLA 3 307

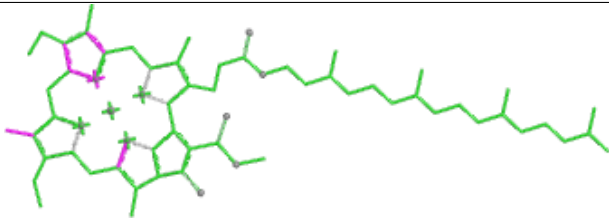
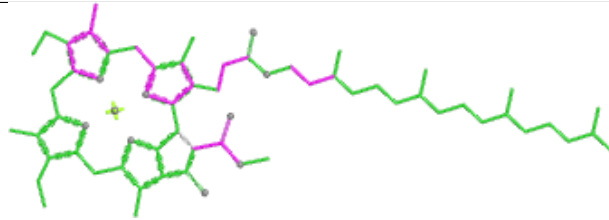
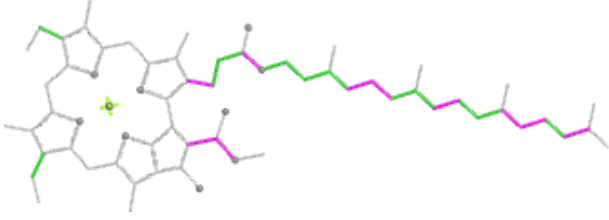
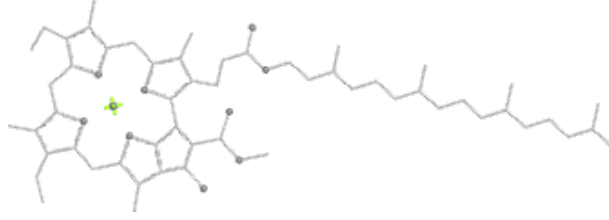


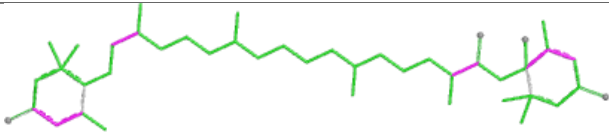
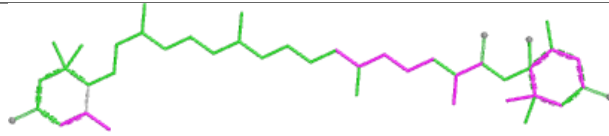
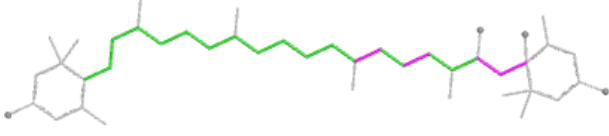
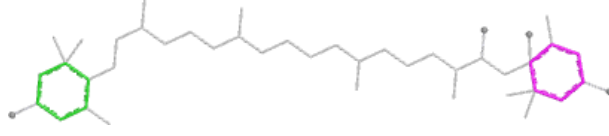
Ligand CLA 6 611



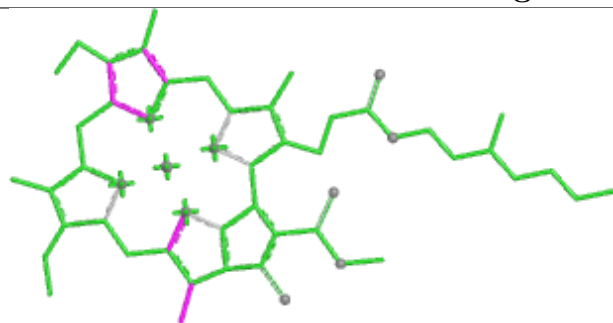


Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

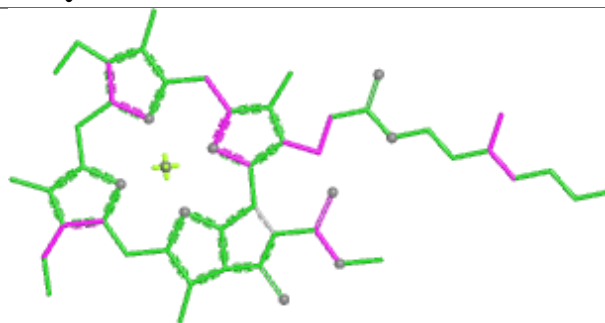
Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand IWJ S 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

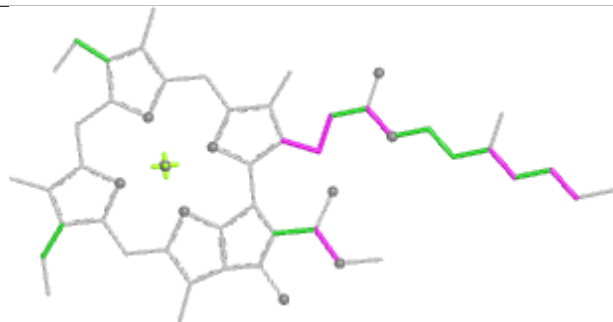
Ligand CLA Q 314



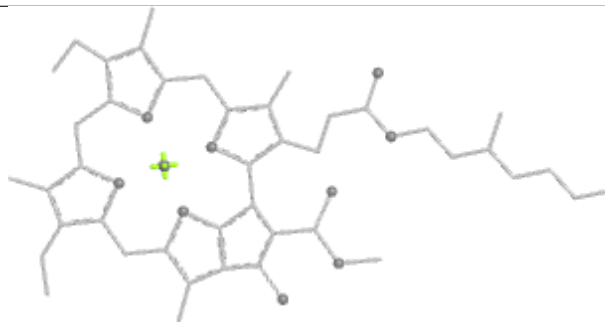
Bond lengths



Bond angles

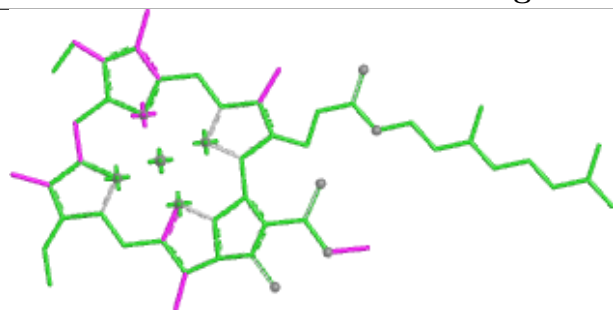


Torsions

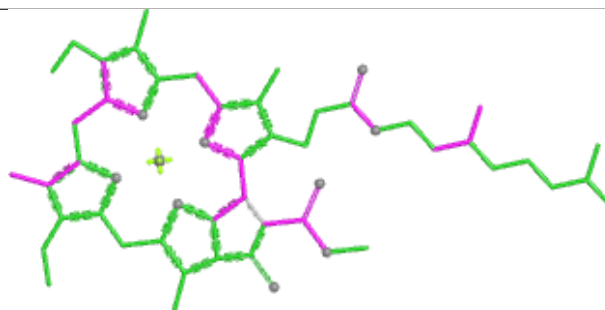


Rings

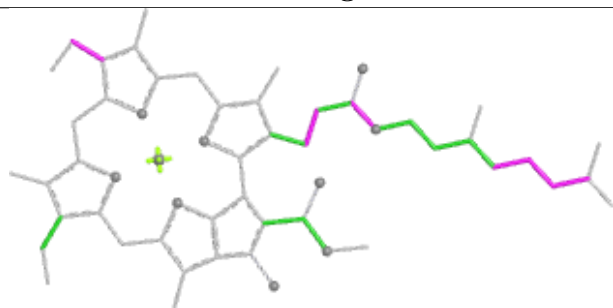
Ligand CLA X 302



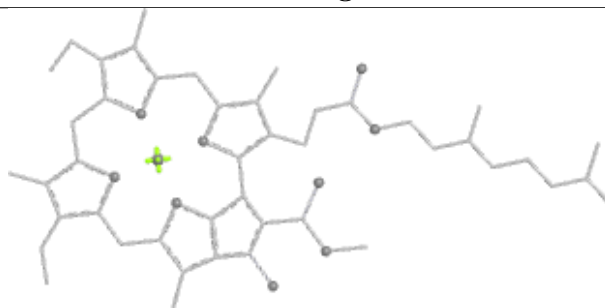
Bond lengths



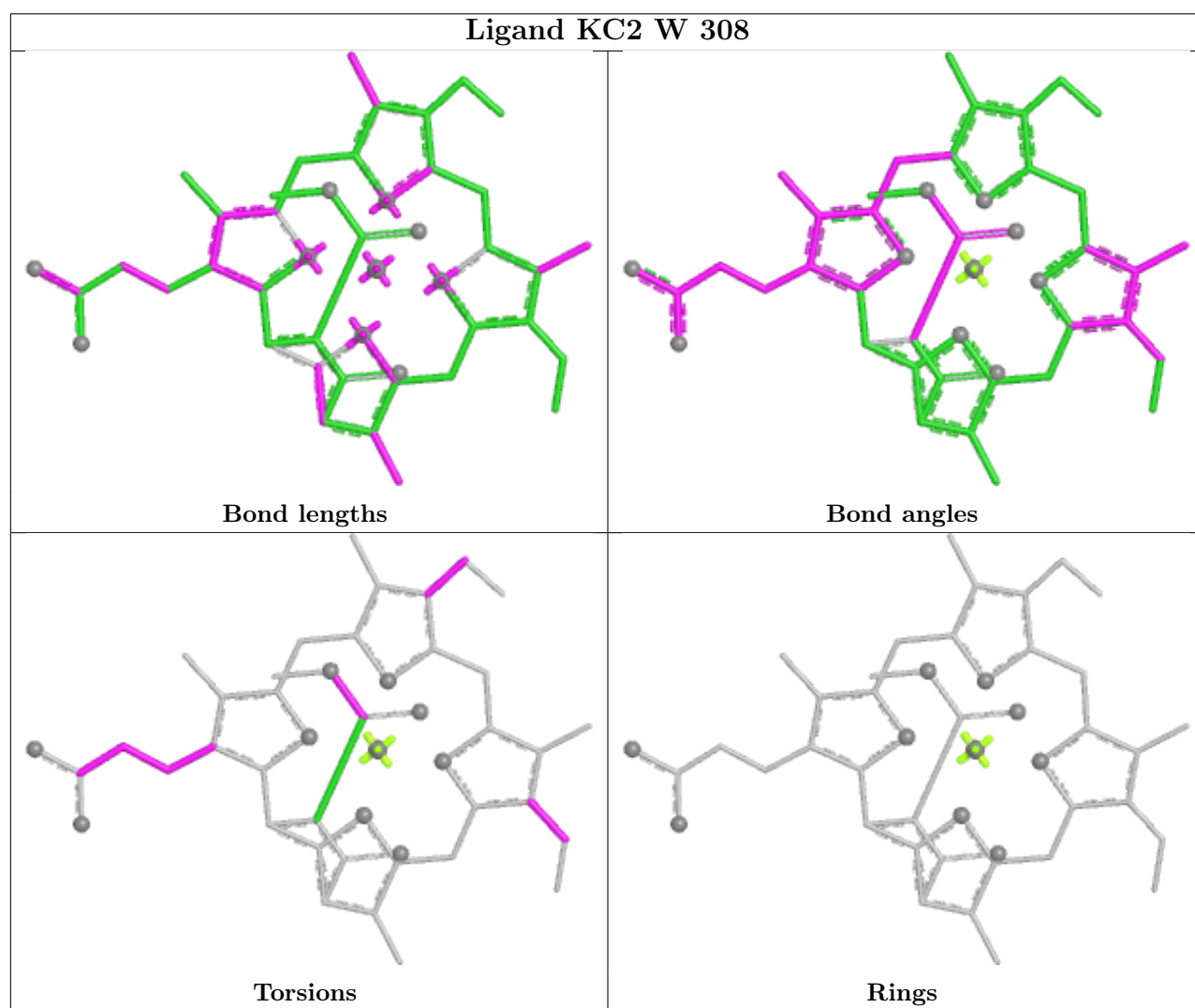
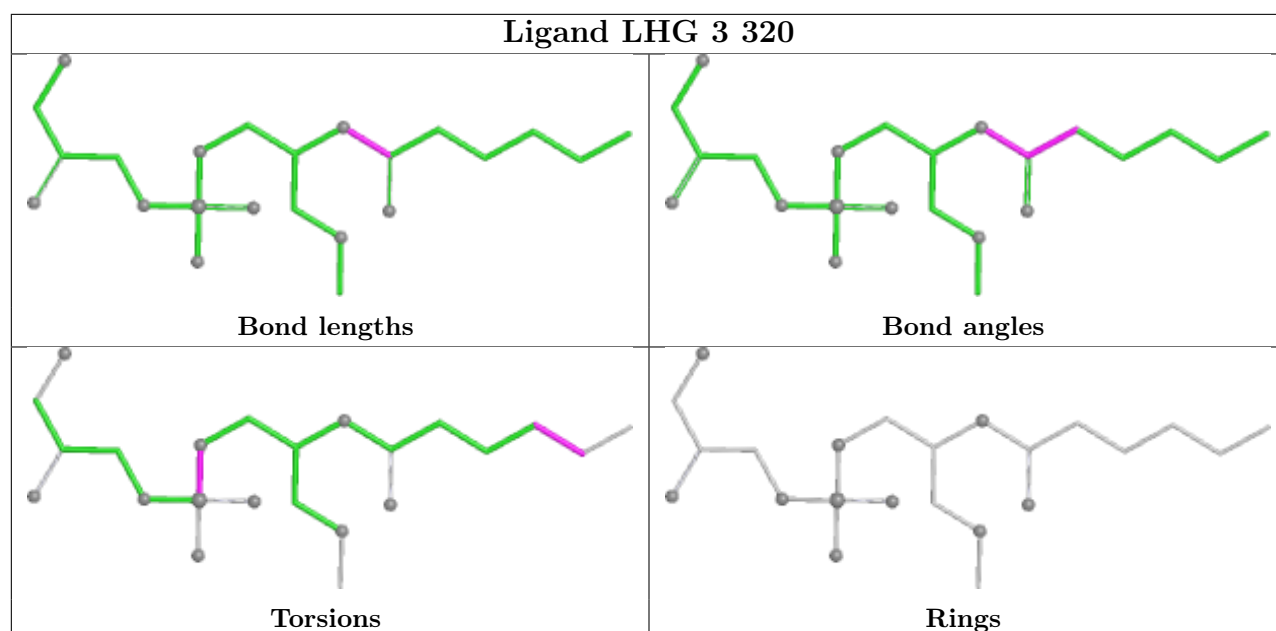
Bond angles



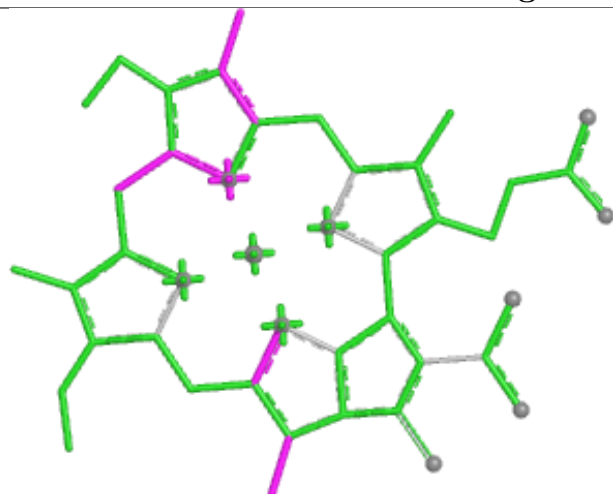
Torsions



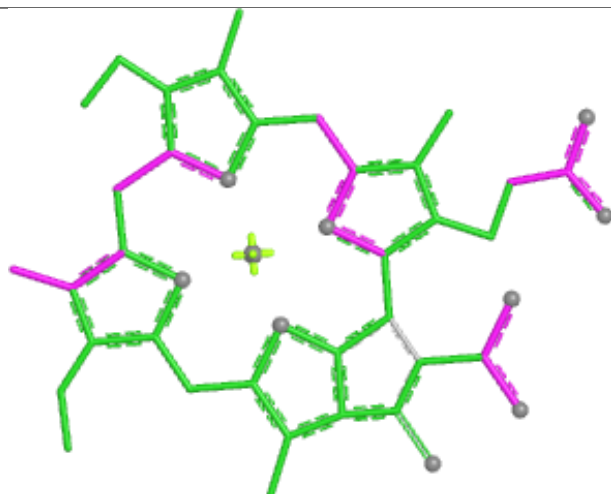
Rings



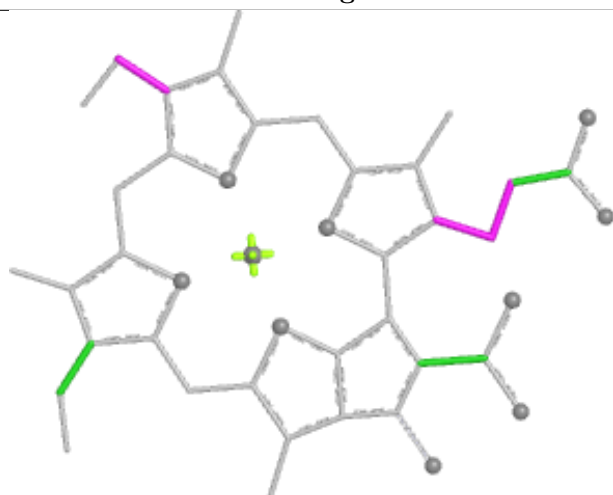
Ligand CLA 2 603



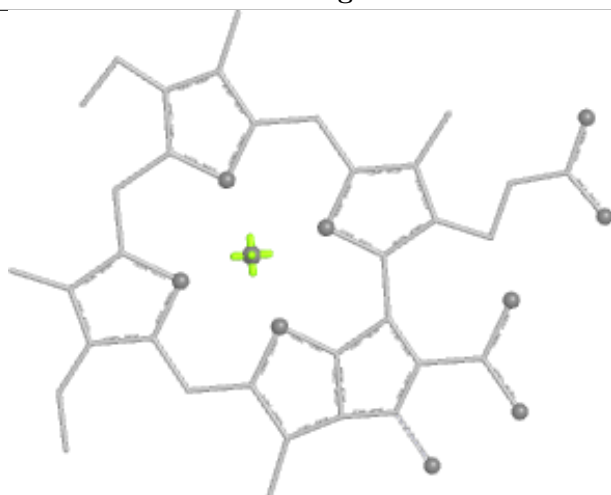
Bond lengths



Bond angles

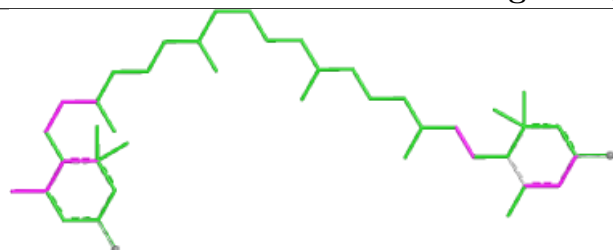


Torsions

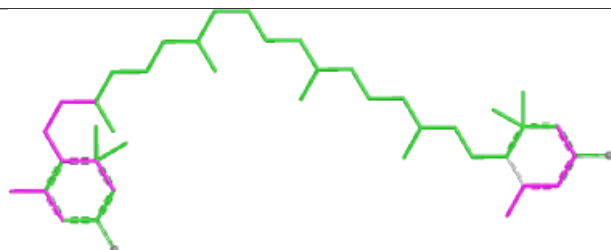


Rings

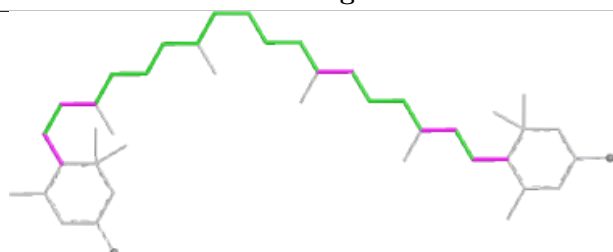
Ligand Q6L O 2006



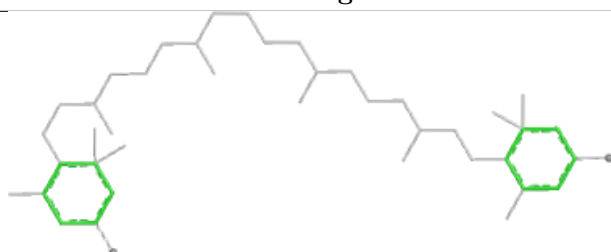
Bond lengths



Bond angles

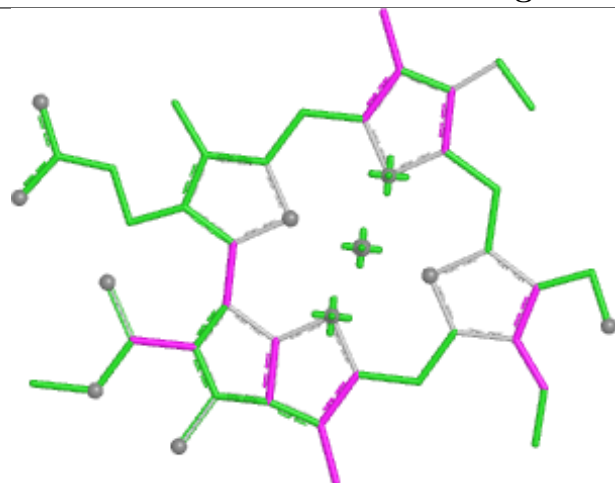


Torsions

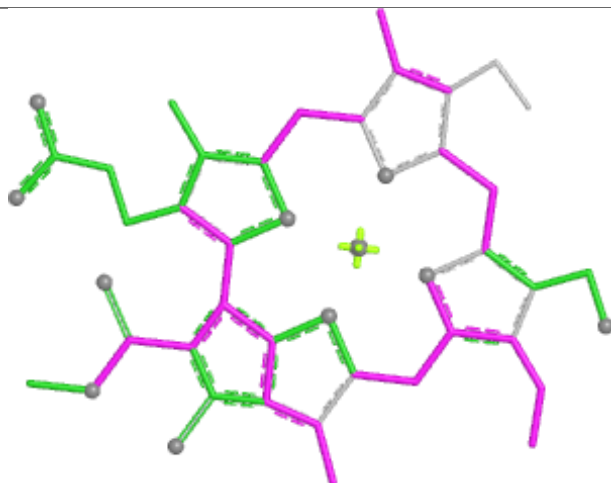


Rings

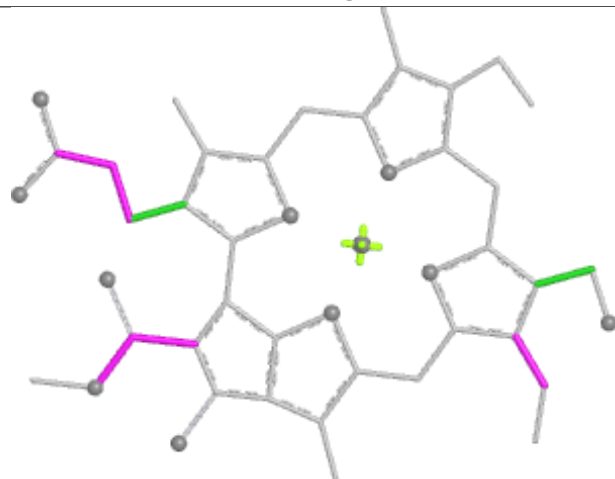
Ligand CHL U 305



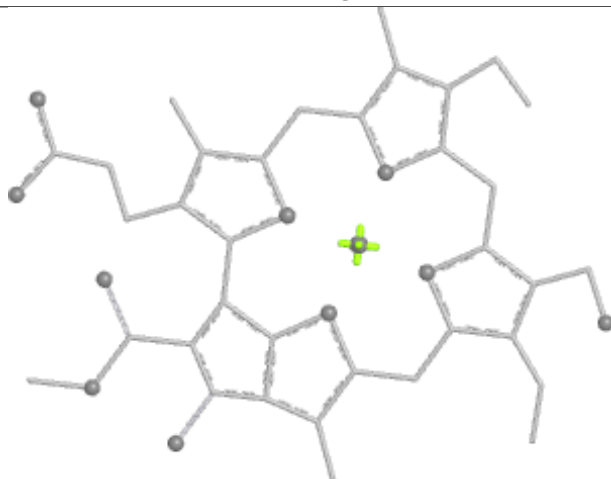
Bond lengths



Bond angles

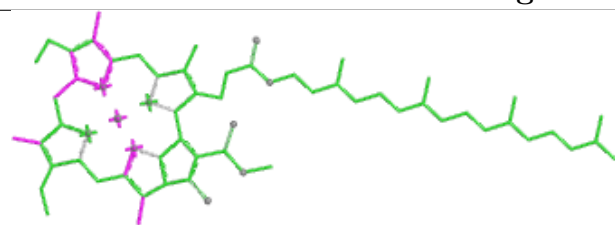


Torsions

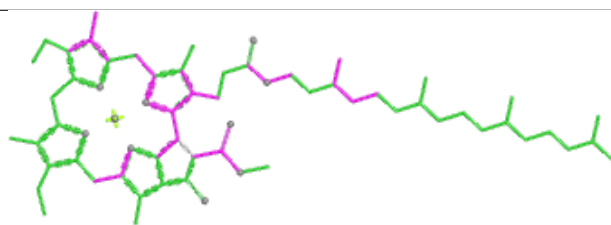


Rings

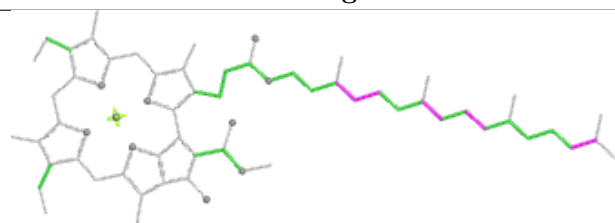
Ligand CLA B 826



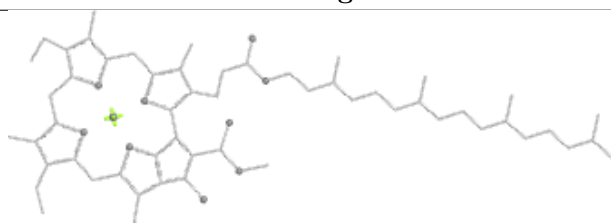
Bond lengths



Bond angles

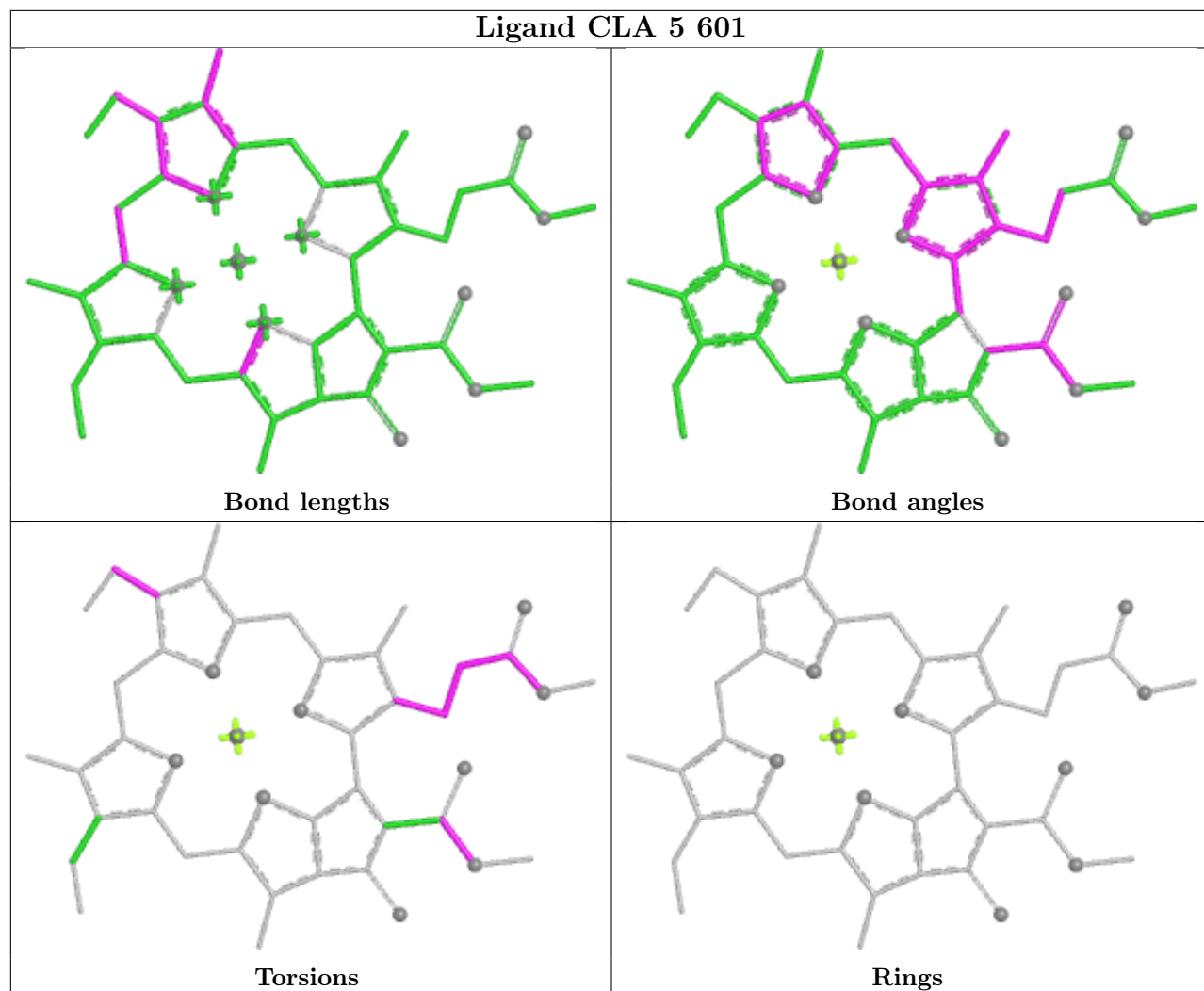


Torsions

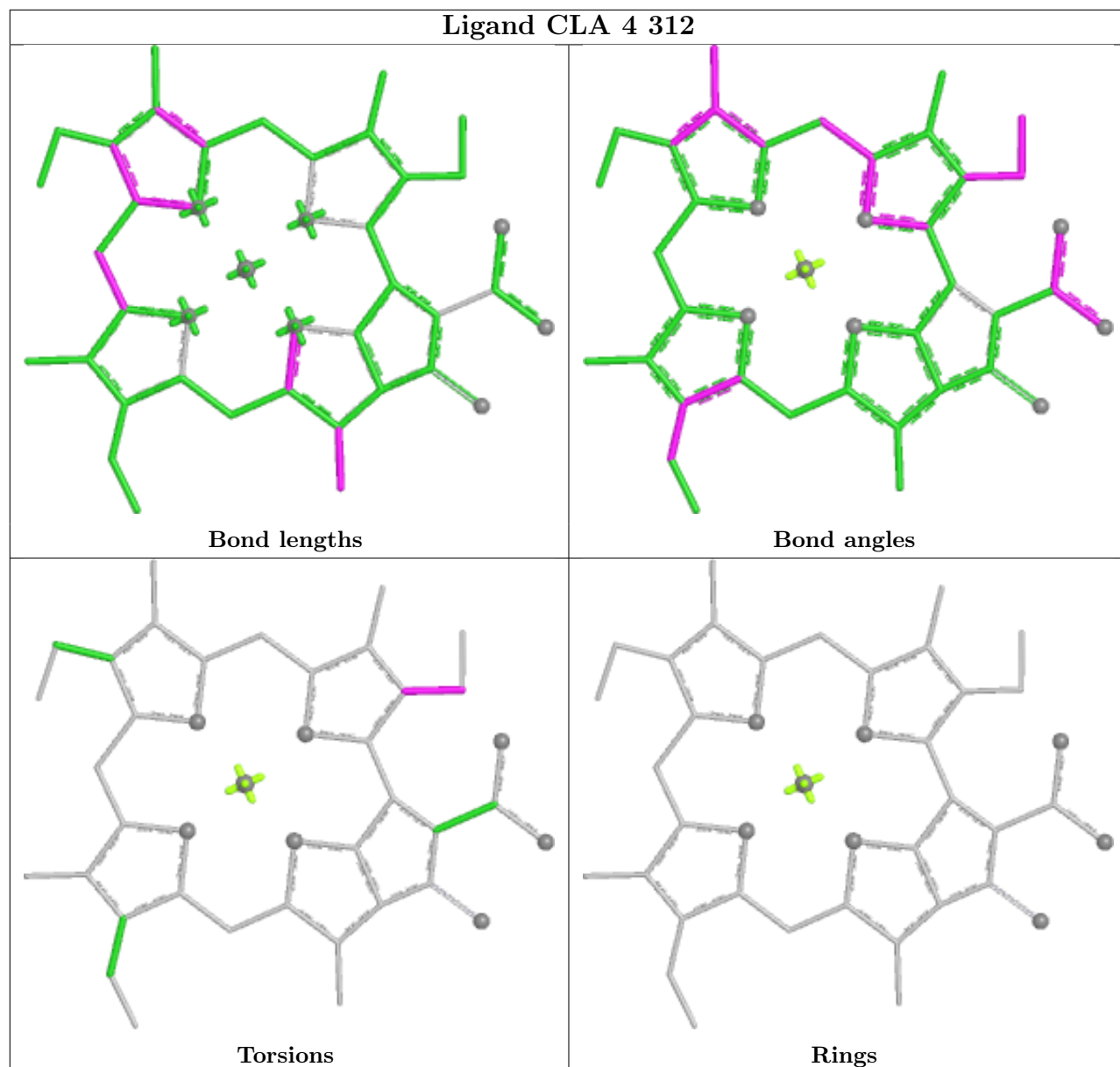


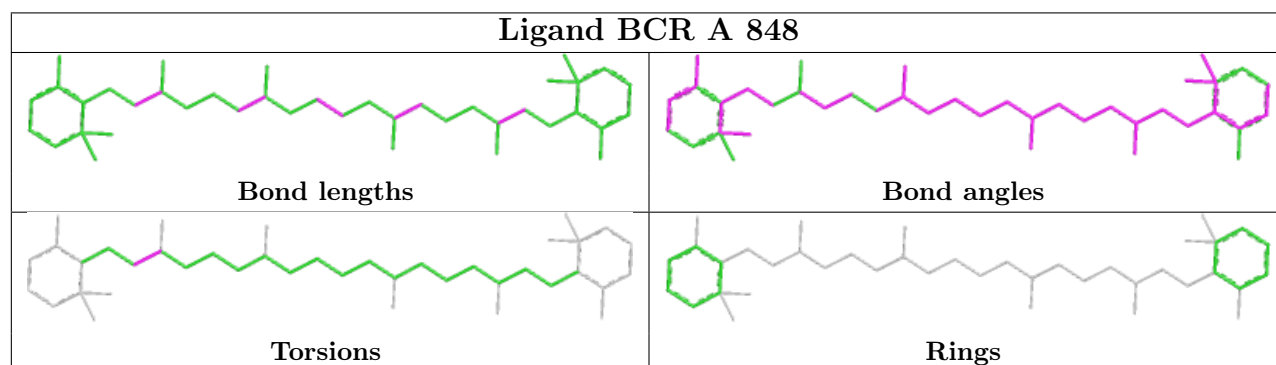
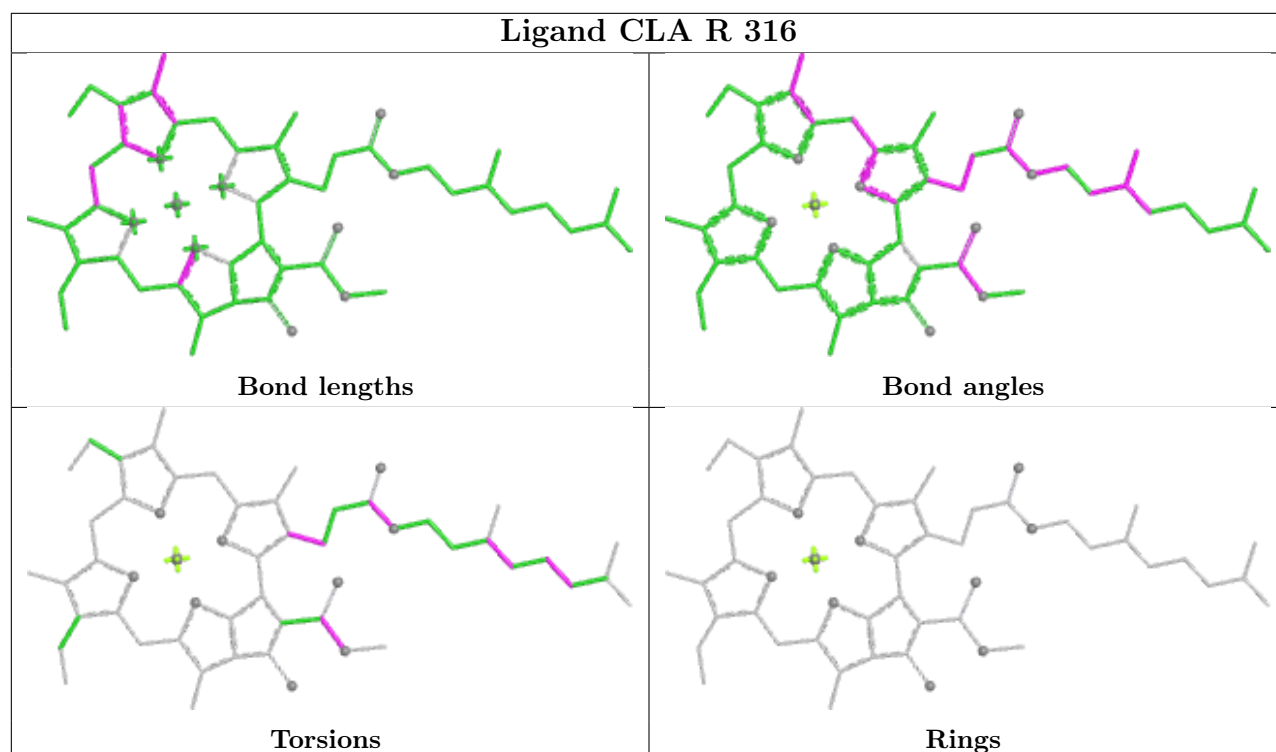
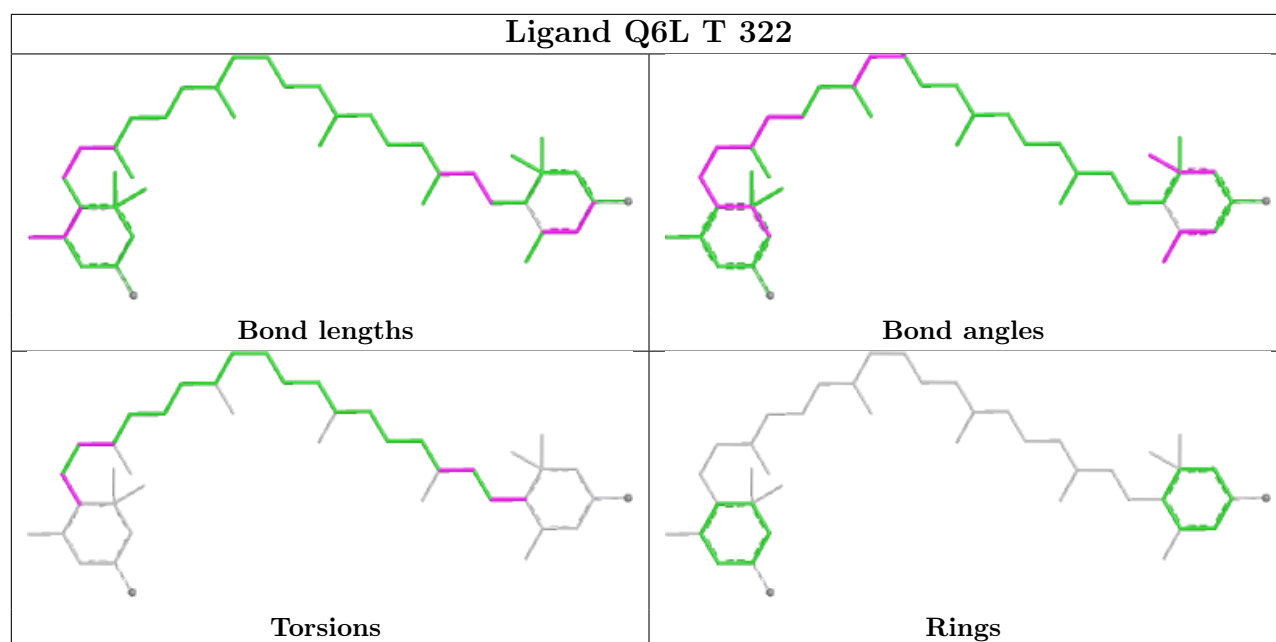
Rings

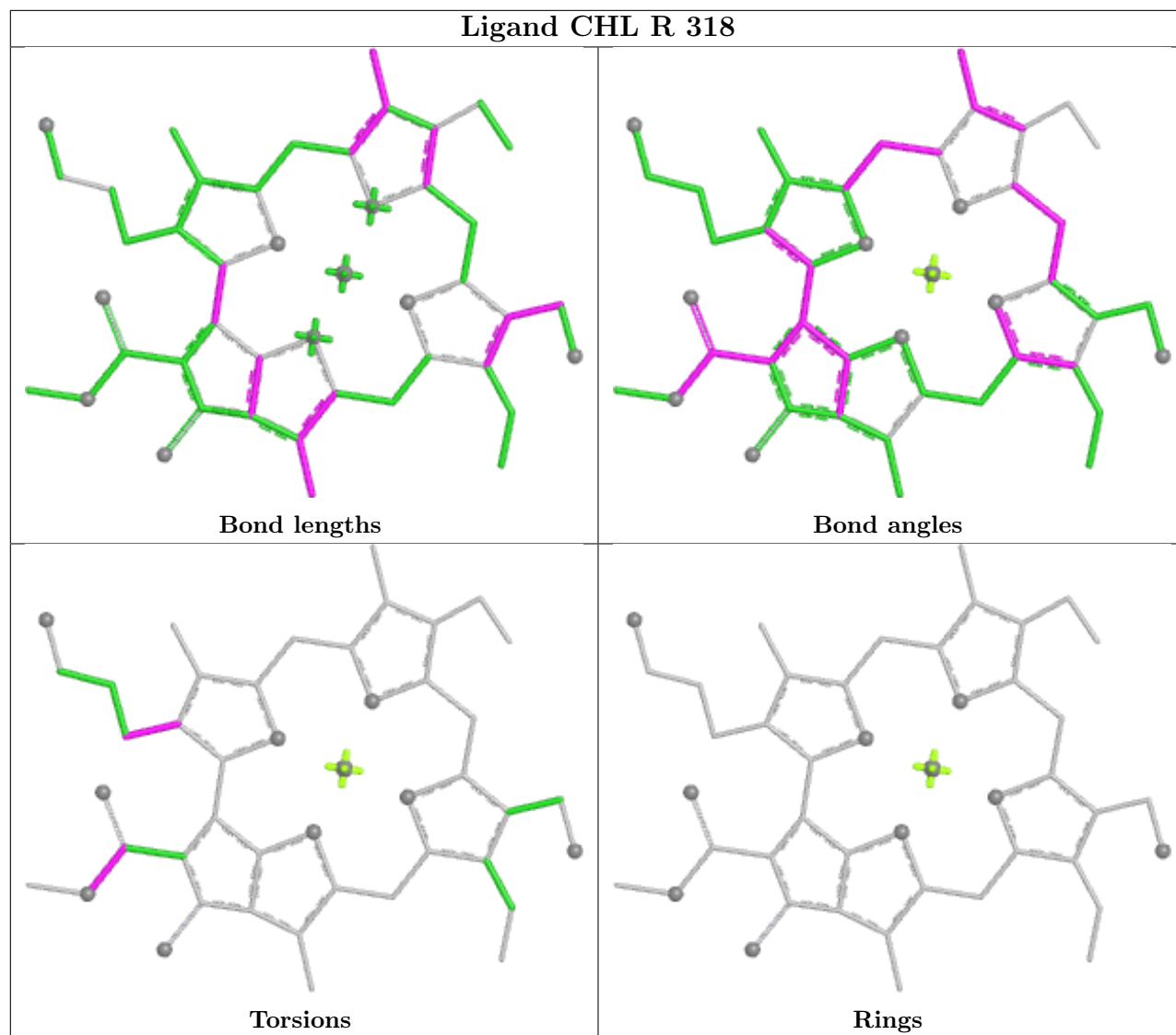
Ligand CLA 5 601

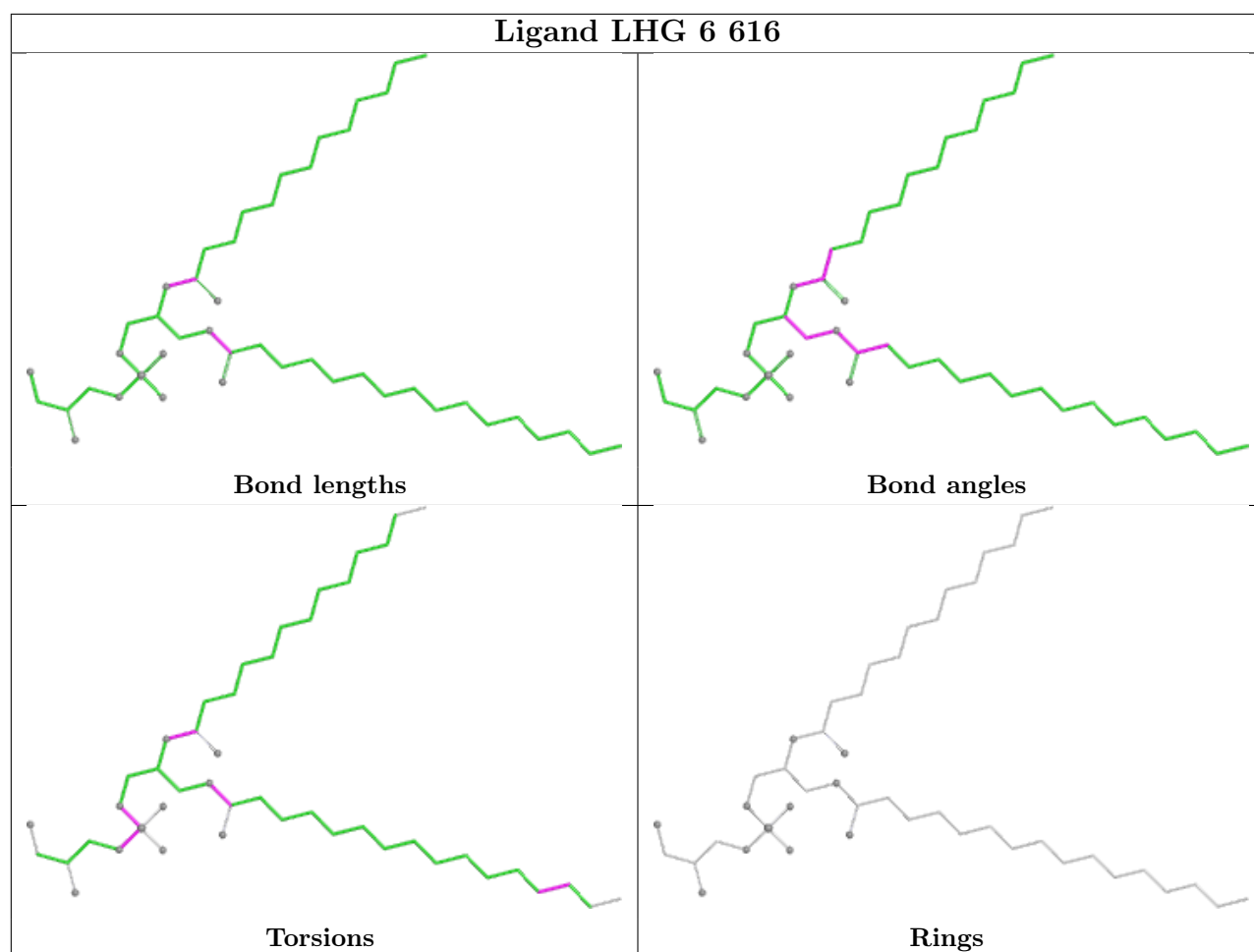


Ligand CLA 4 312

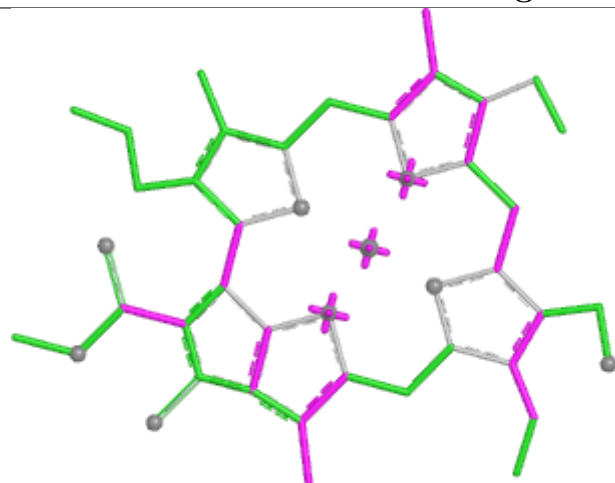




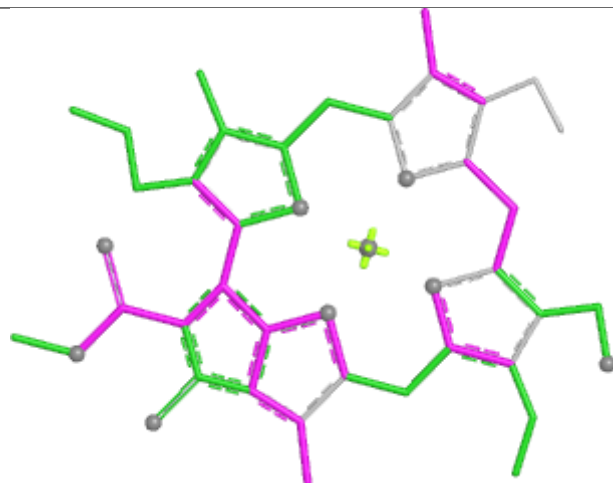




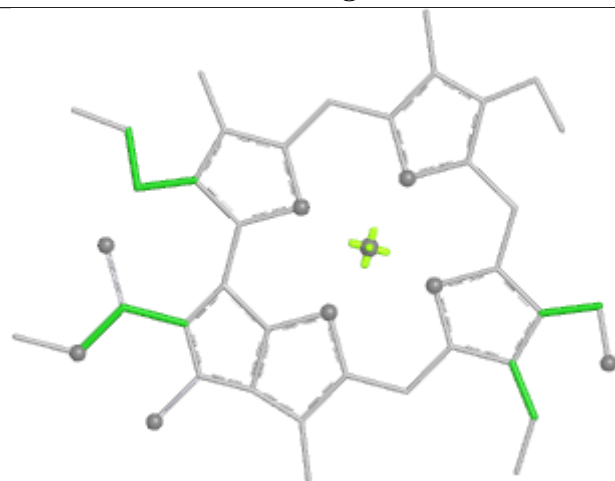
Ligand CHL V 306



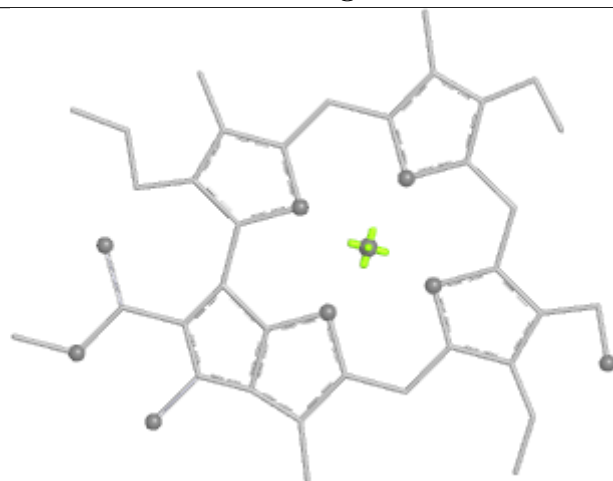
Bond lengths



Bond angles

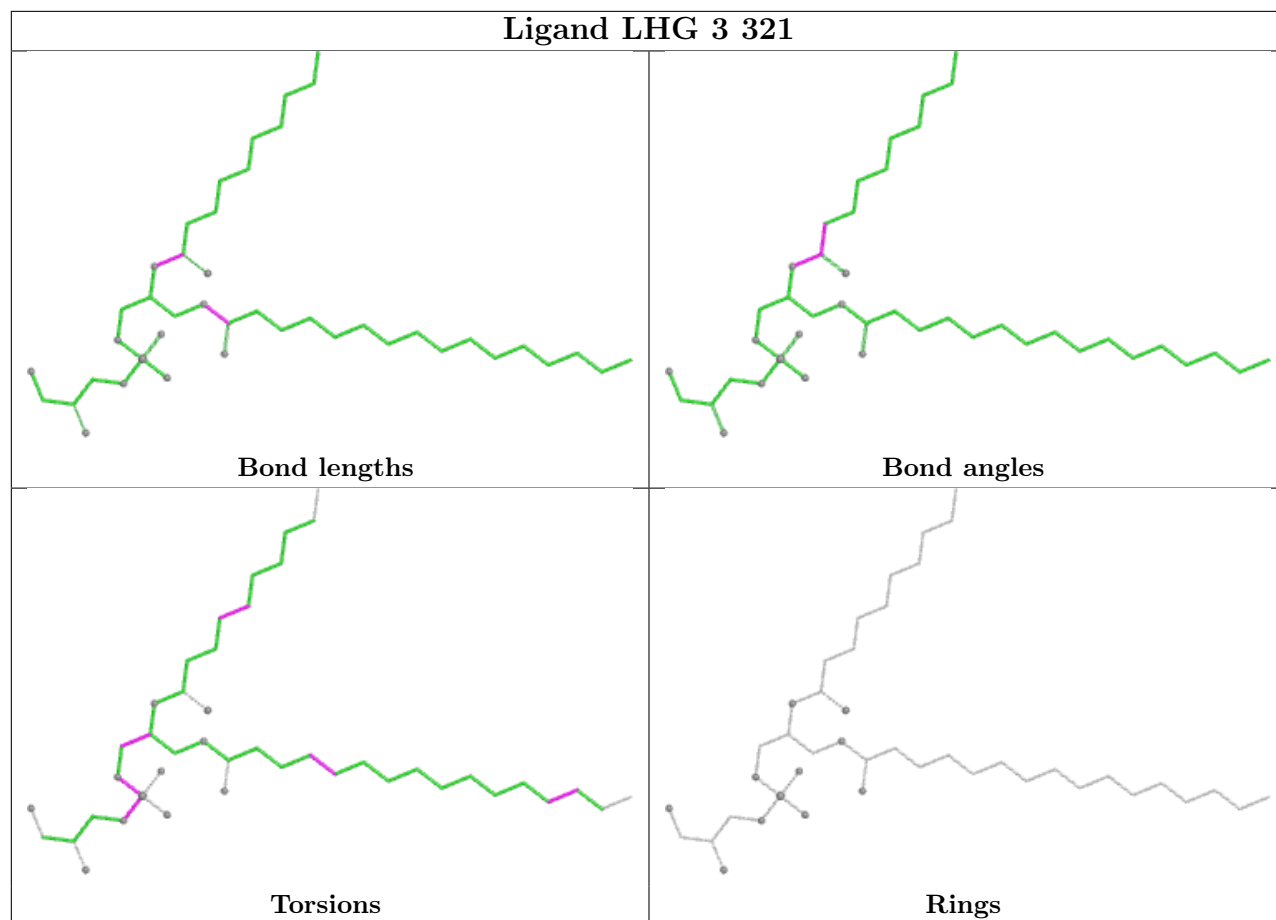


Torsions

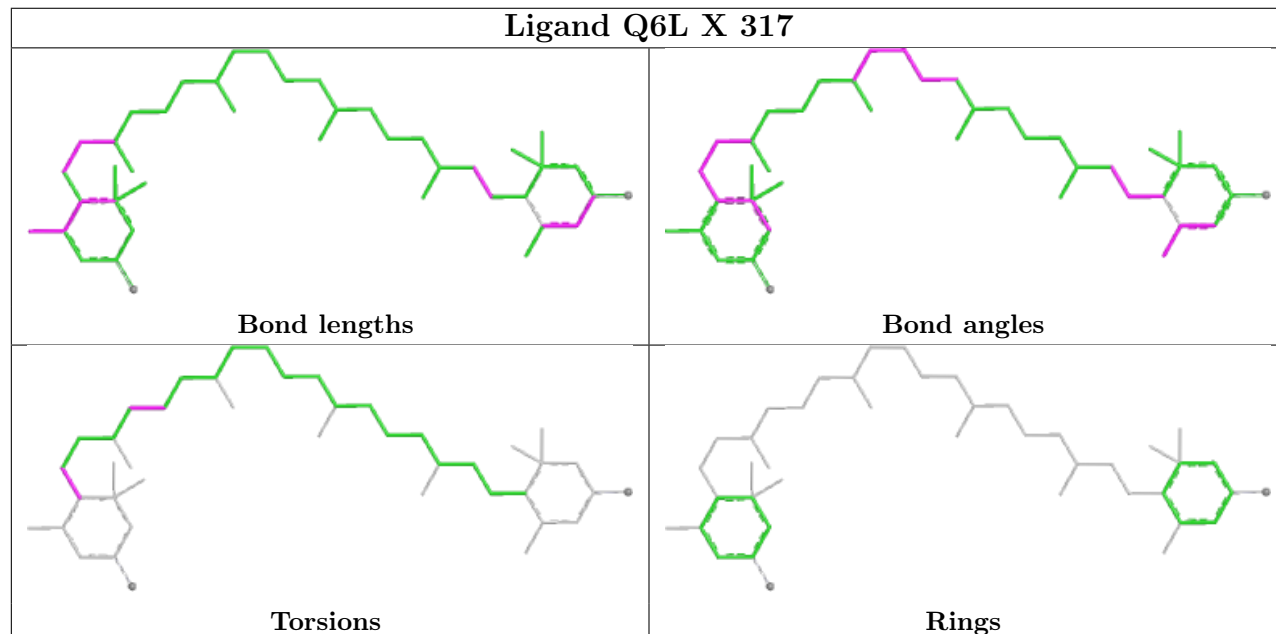


Rings

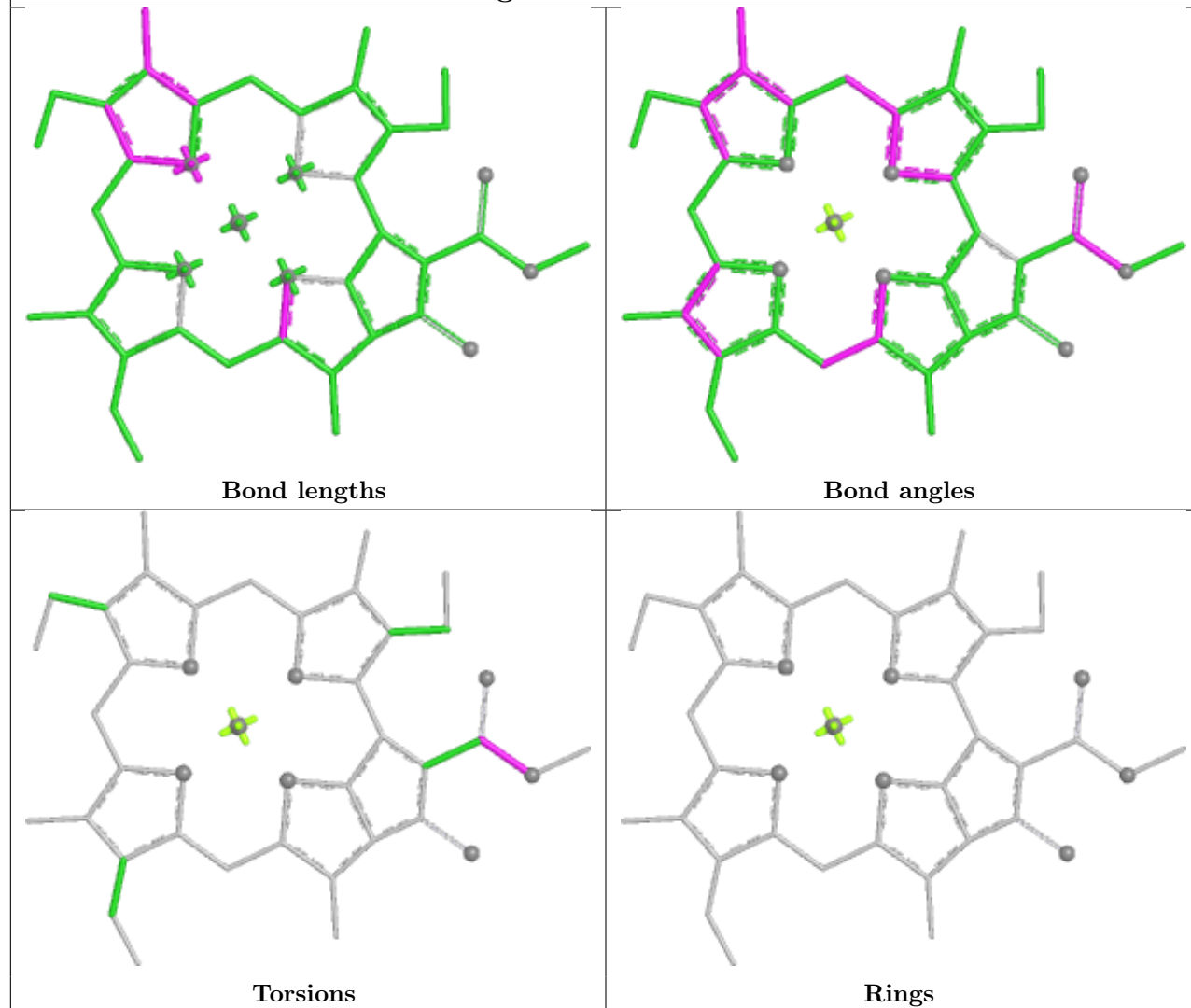
Ligand LHG 3 321



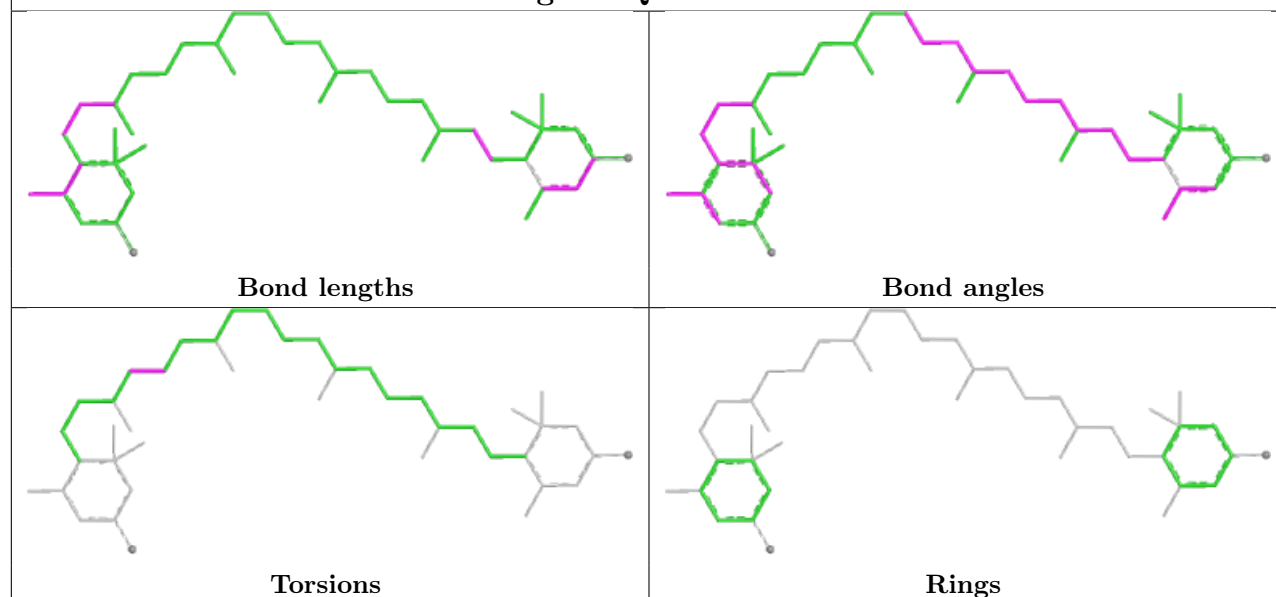
Ligand Q6L X 317



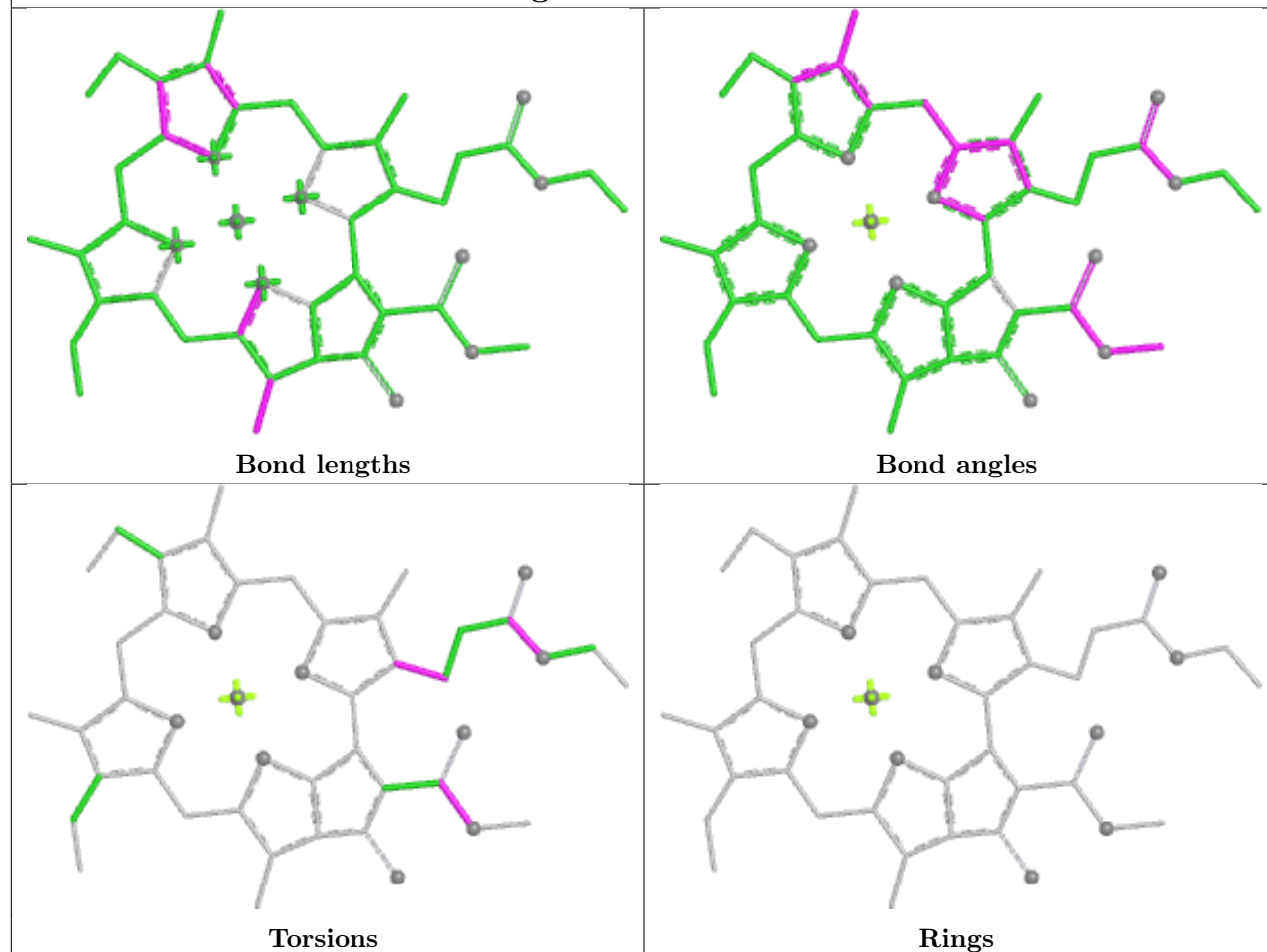
Ligand CLA B 837



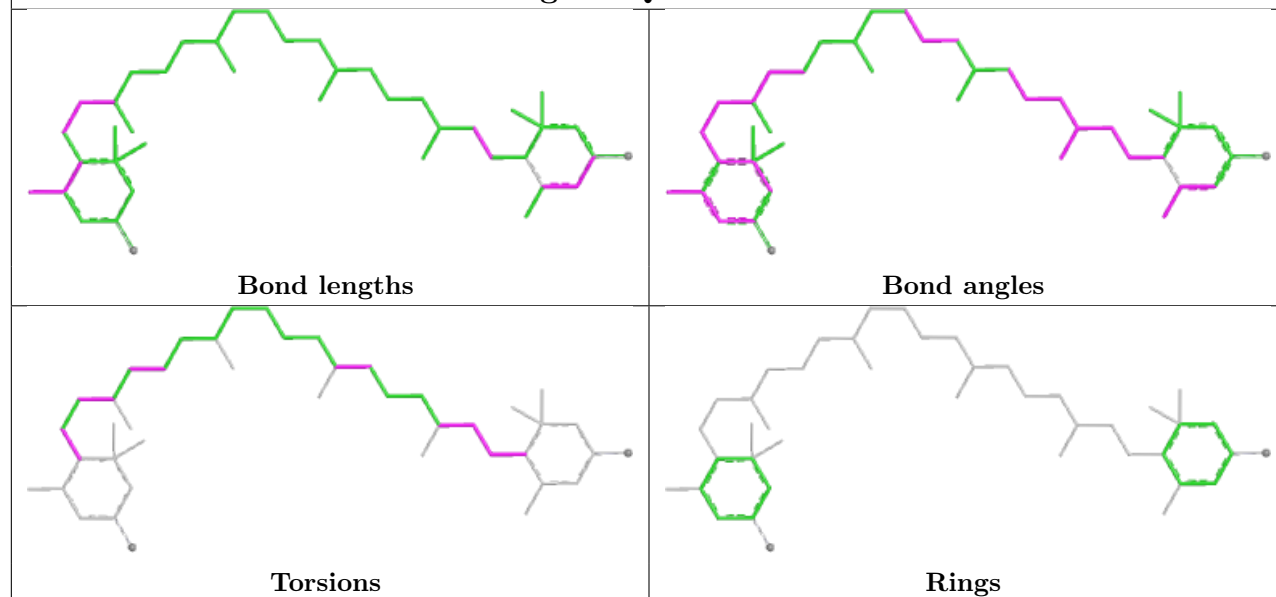
Ligand Q6L T 316



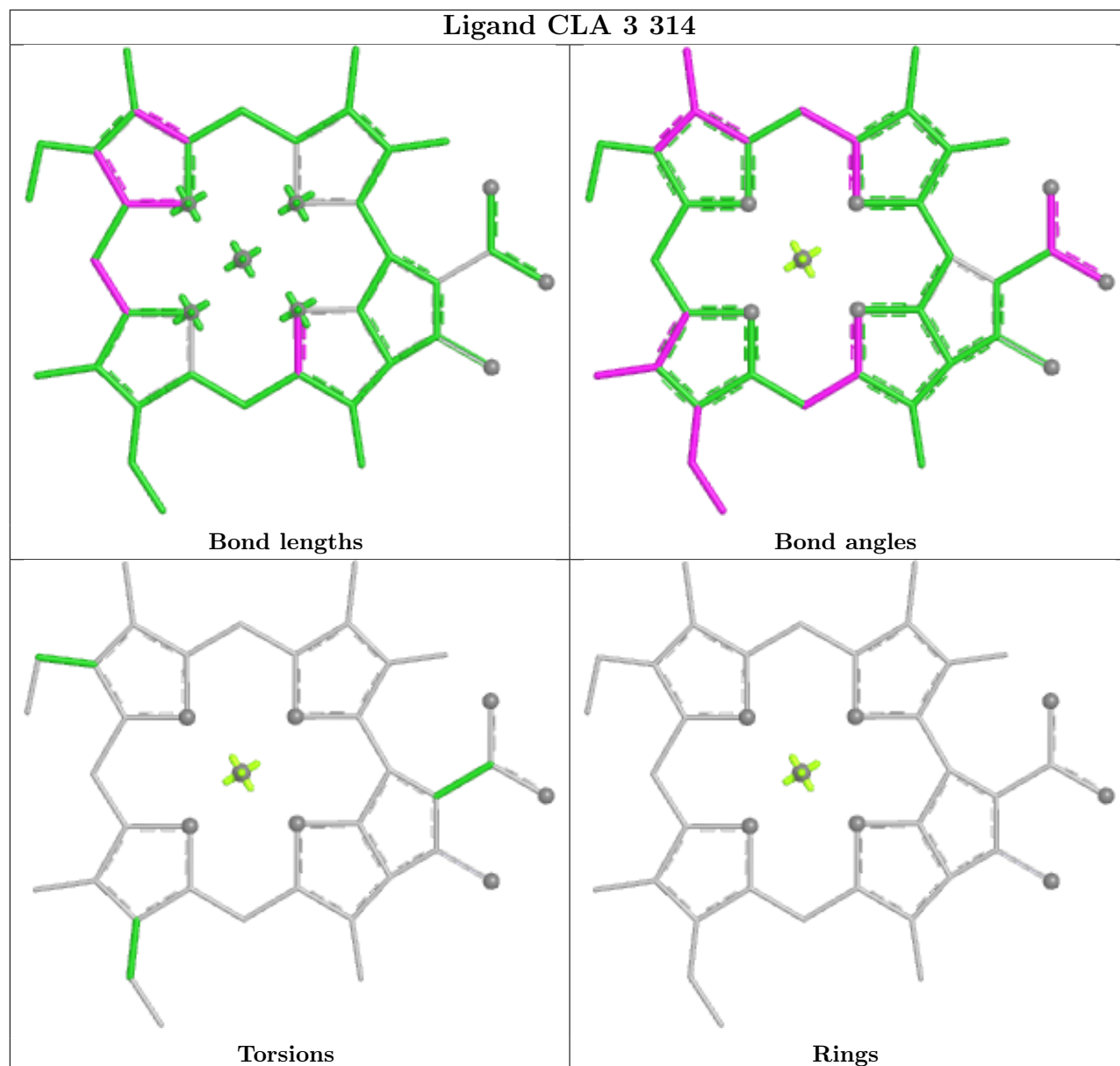
Ligand CLA S 311

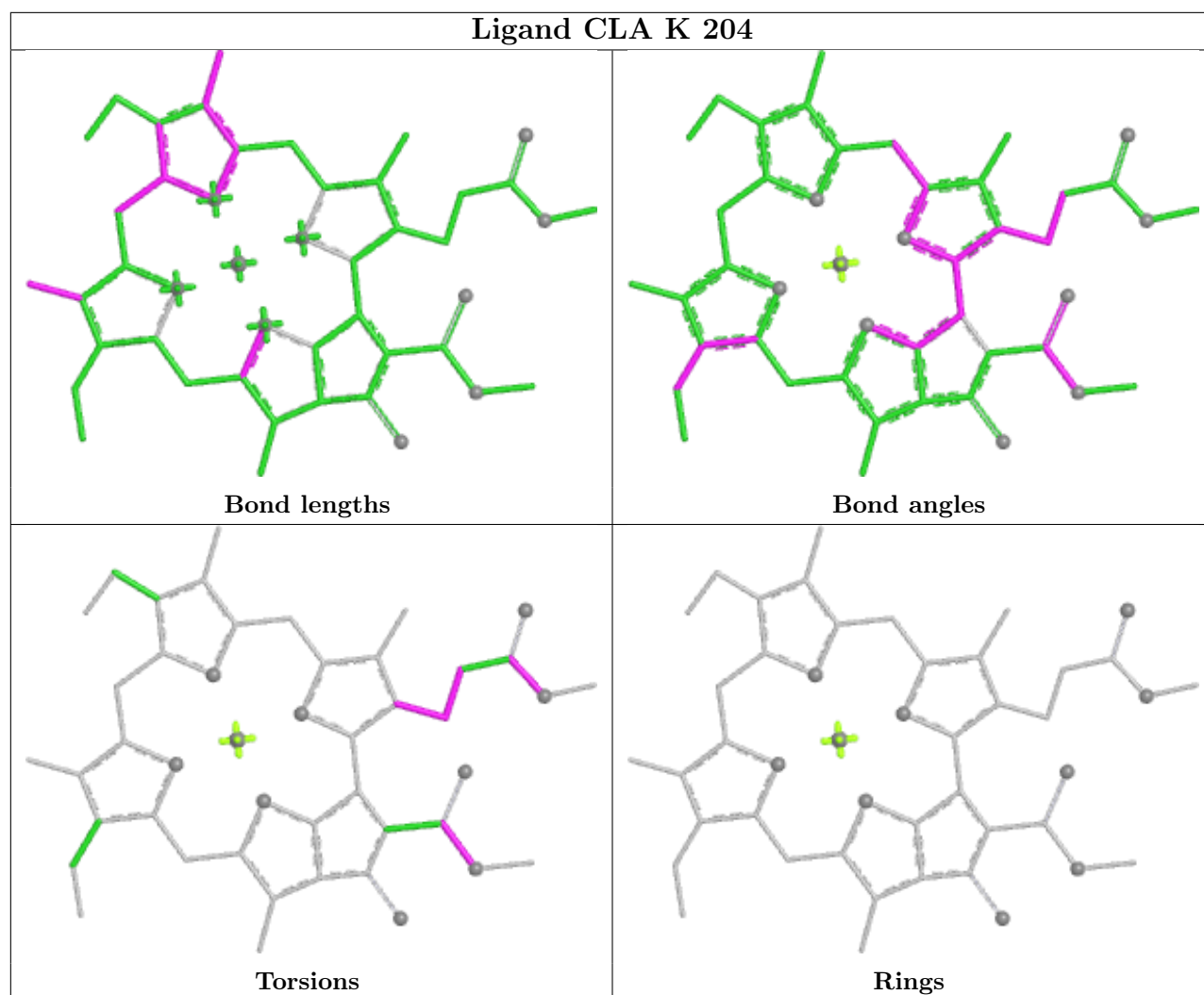
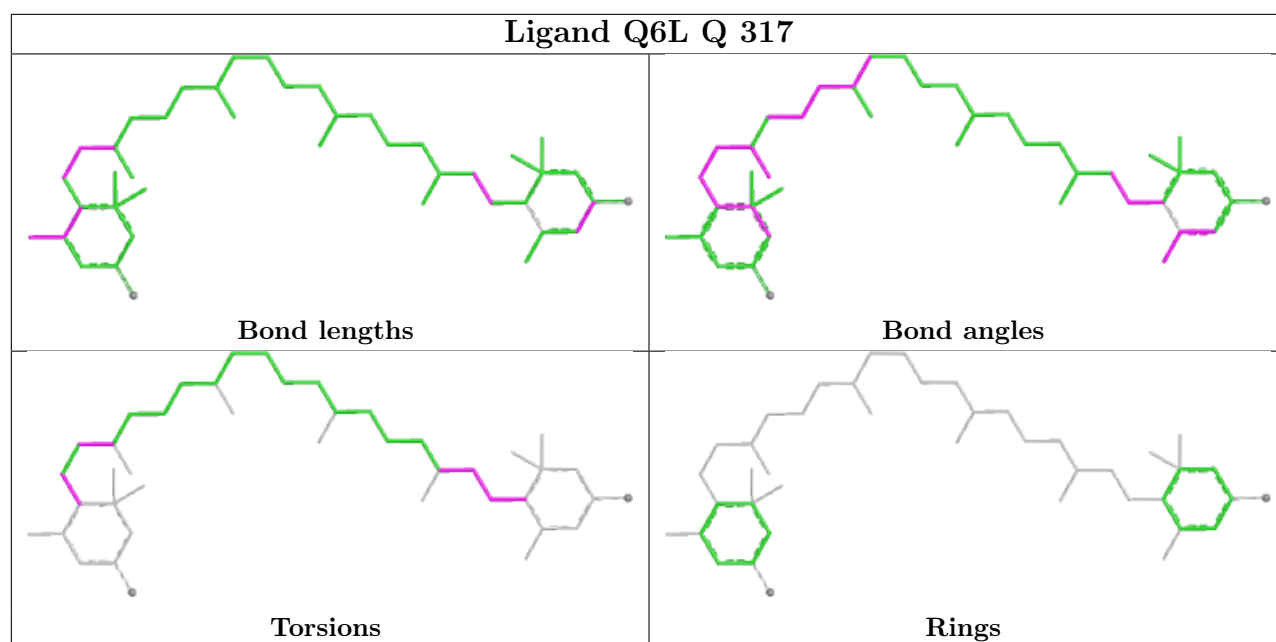


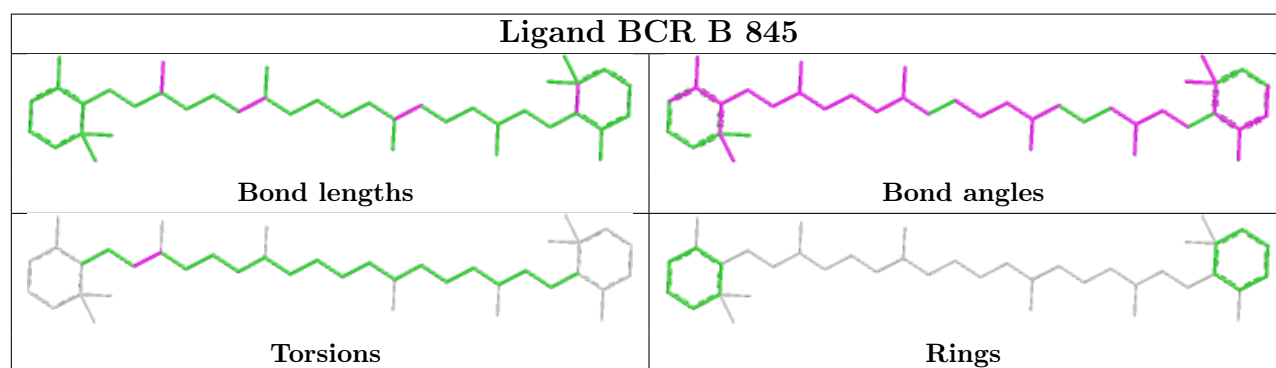
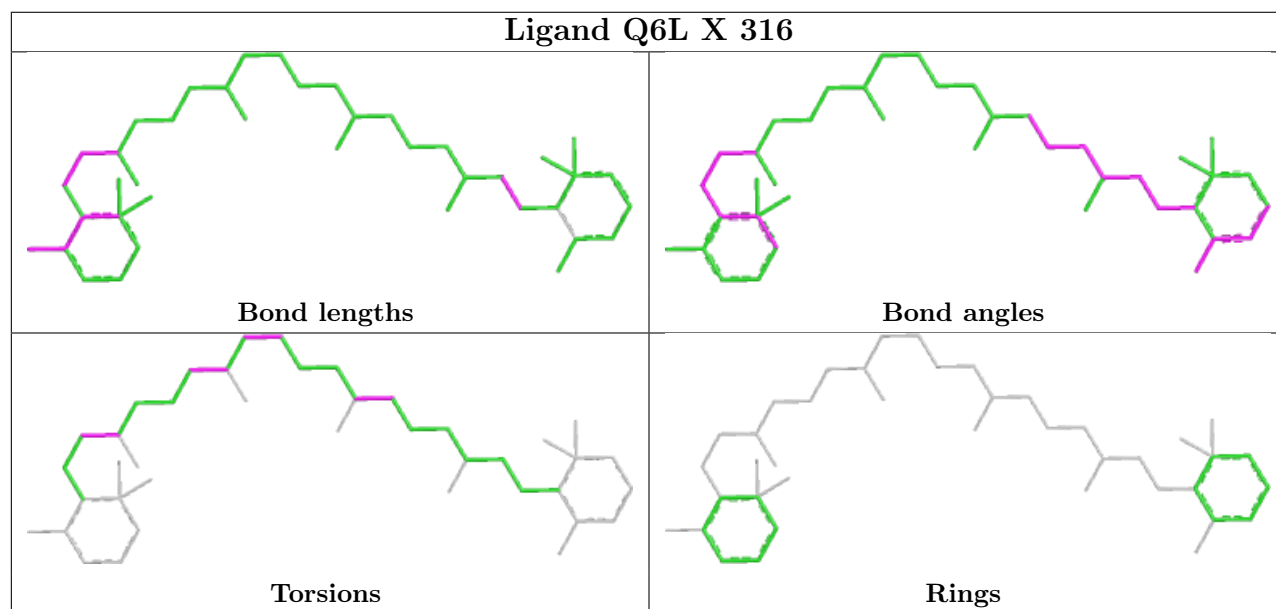
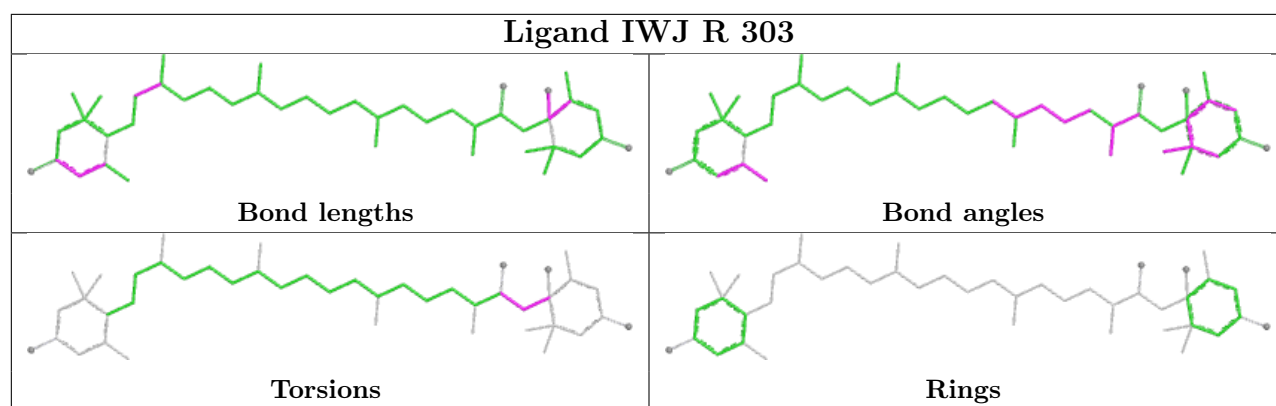
Ligand Q6L 2 616

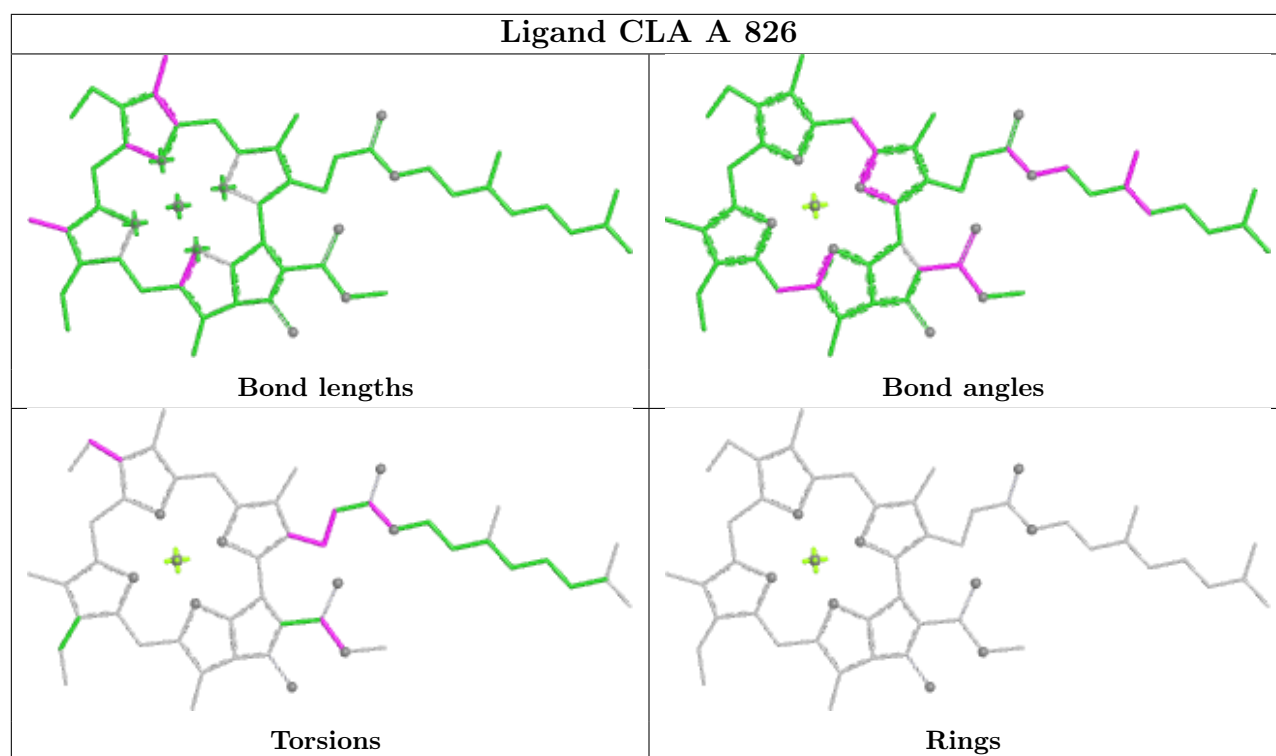


Ligand CLA 3 314

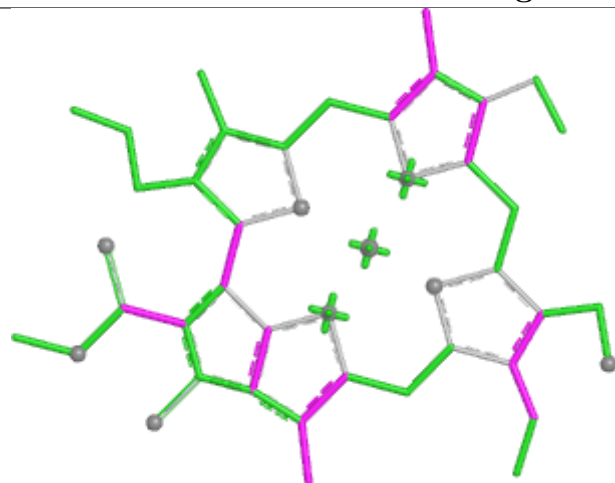




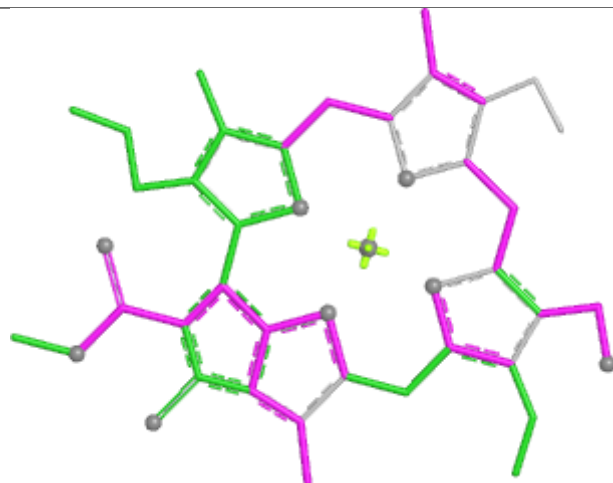




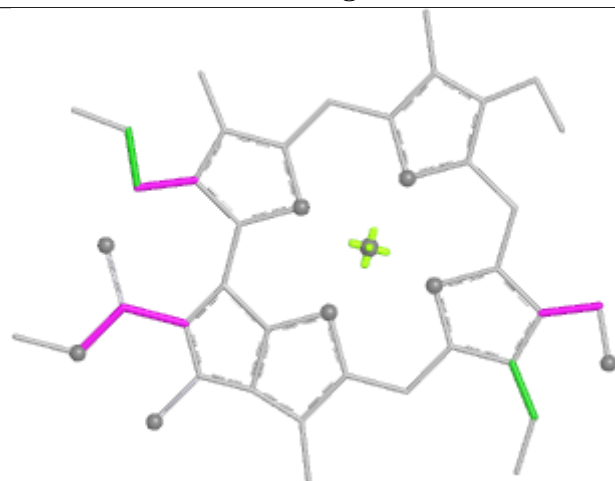
Ligand CHL X 308



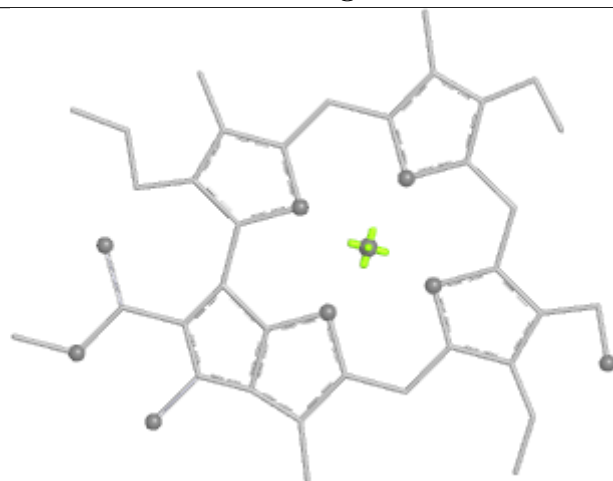
Bond lengths



Bond angles

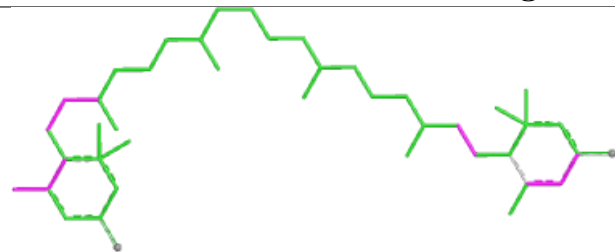


Torsions

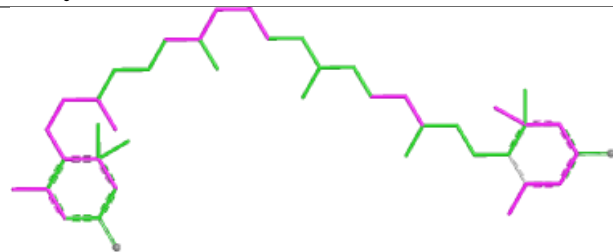


Rings

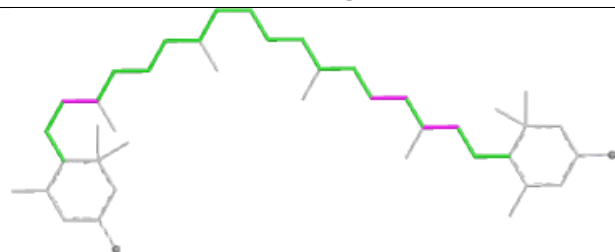
Ligand Q6L Q 319



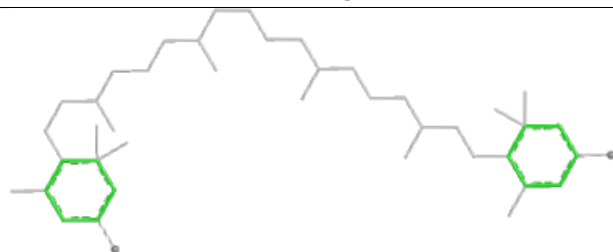
Bond lengths



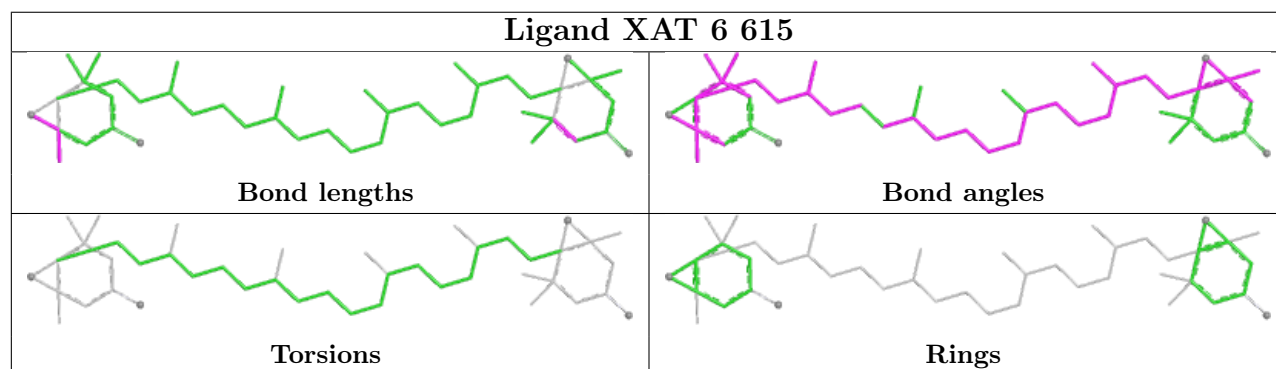
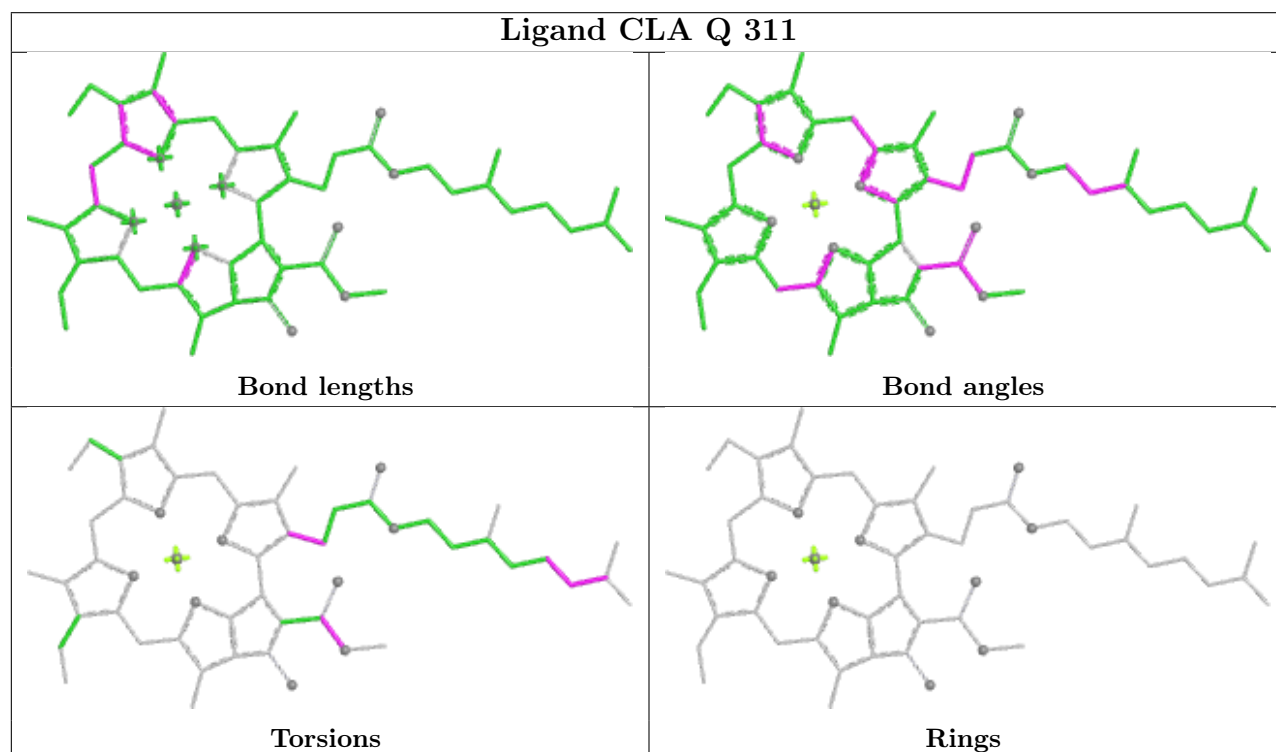
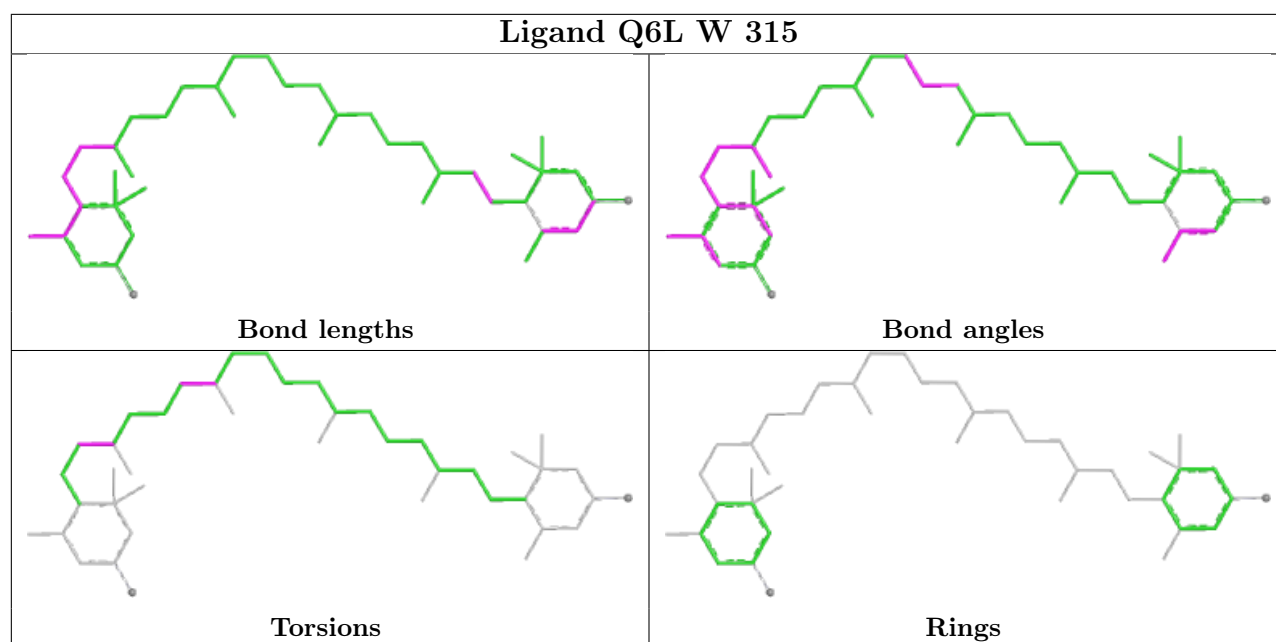
Bond angles



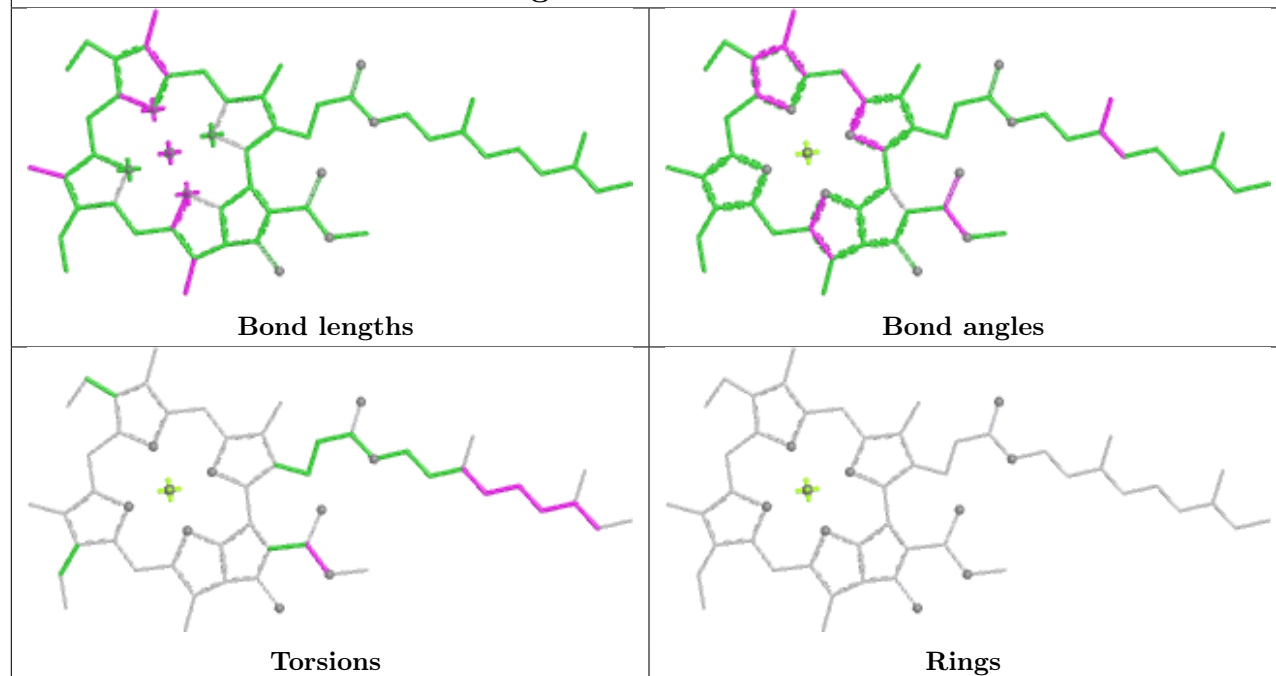
Torsions



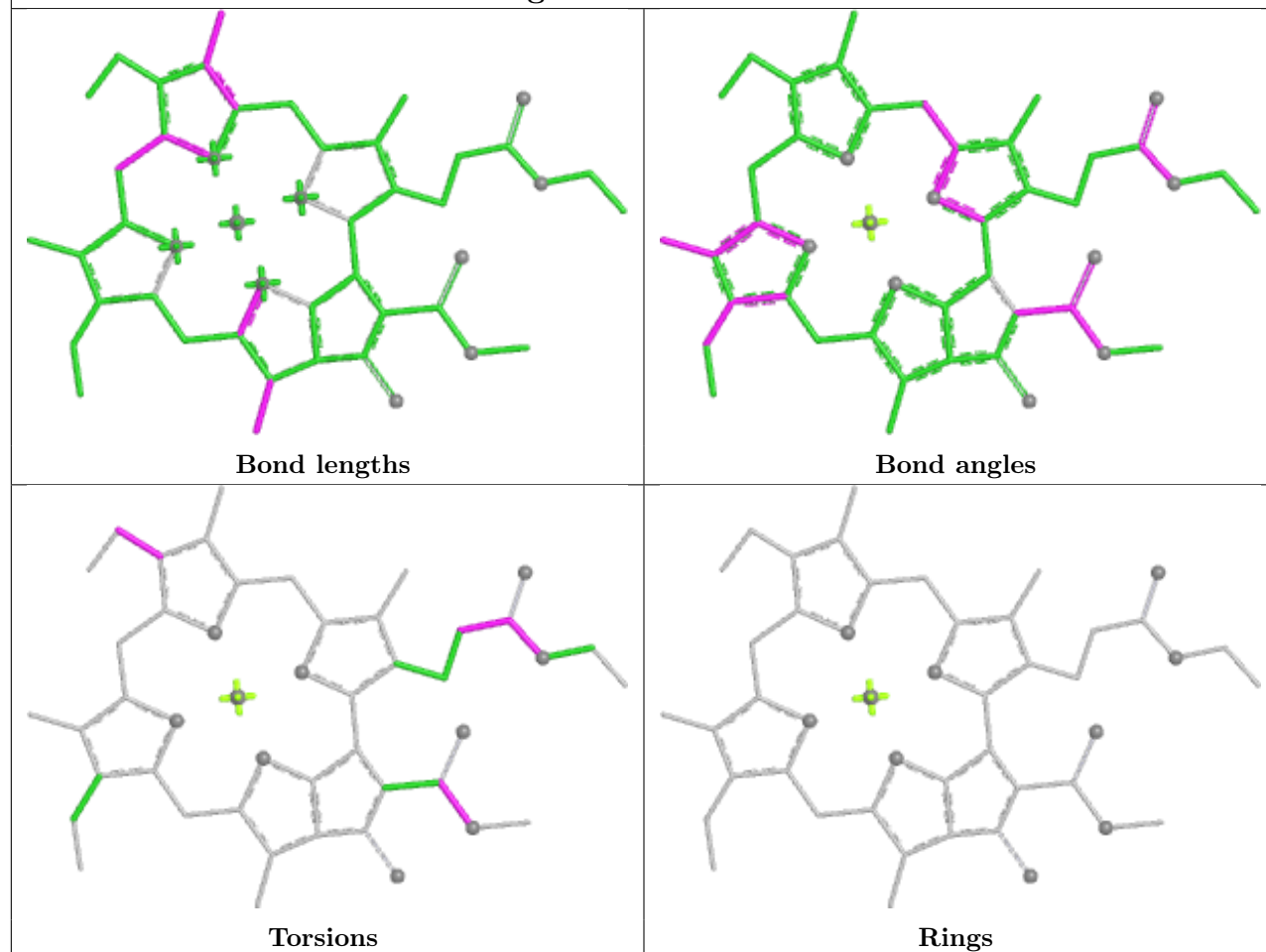
Rings

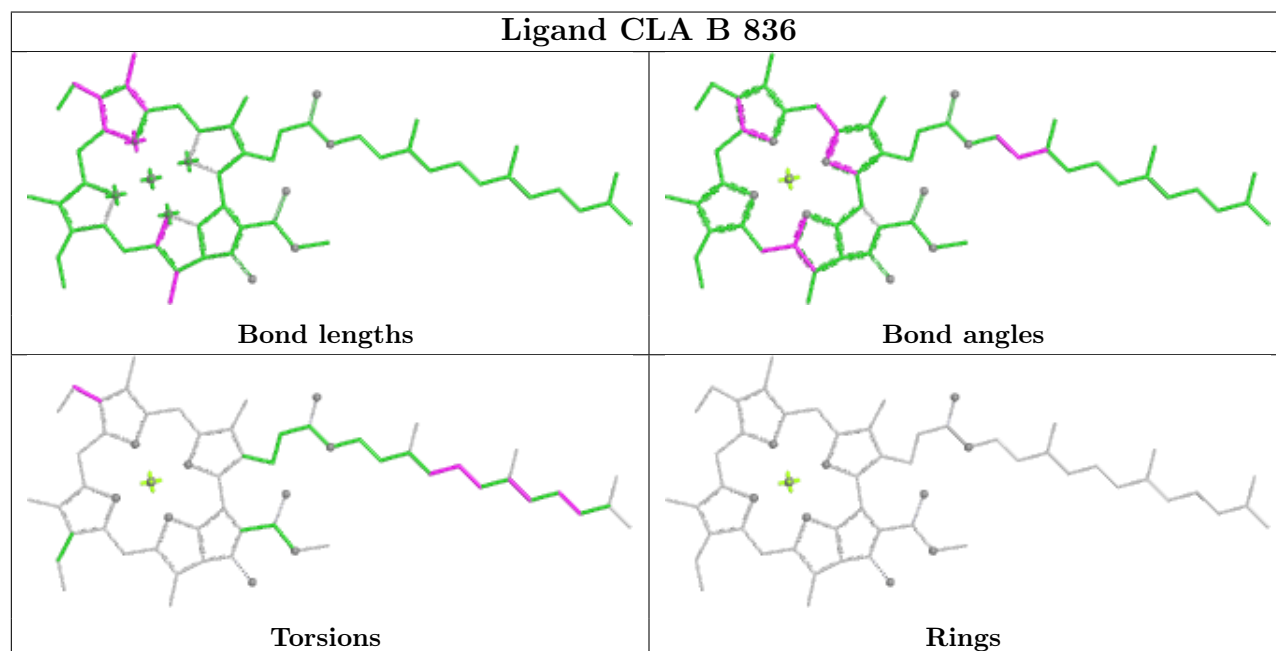
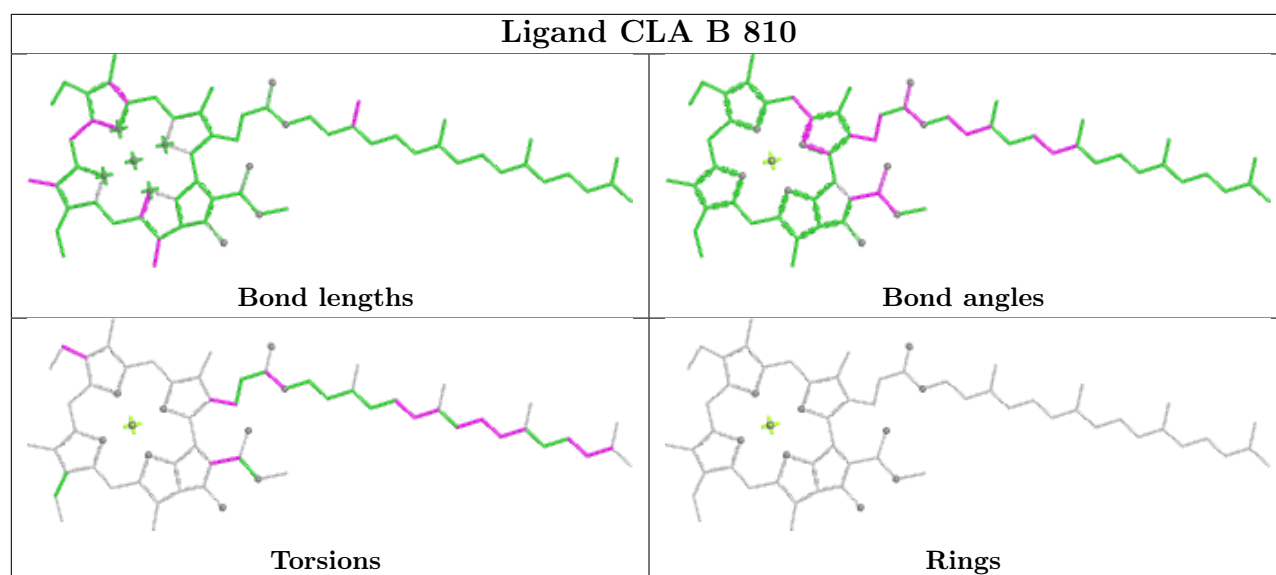


Ligand CLA U 302

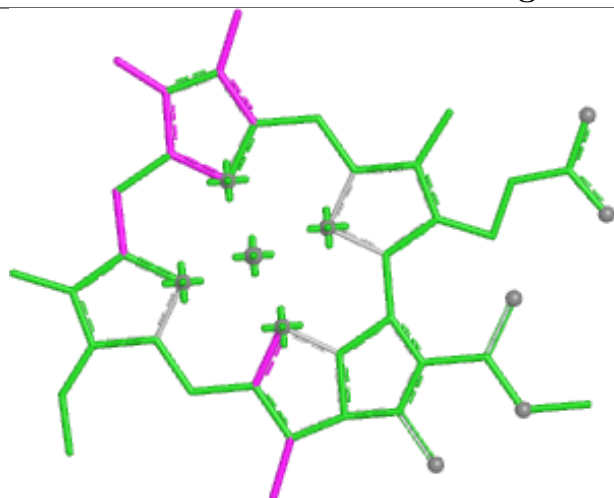


Ligand CLA V 310

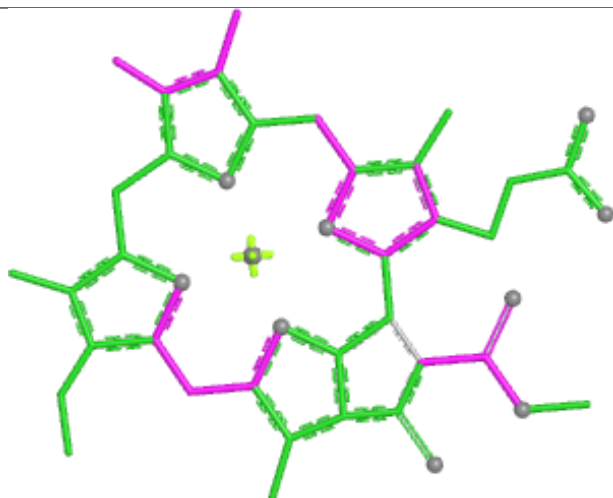




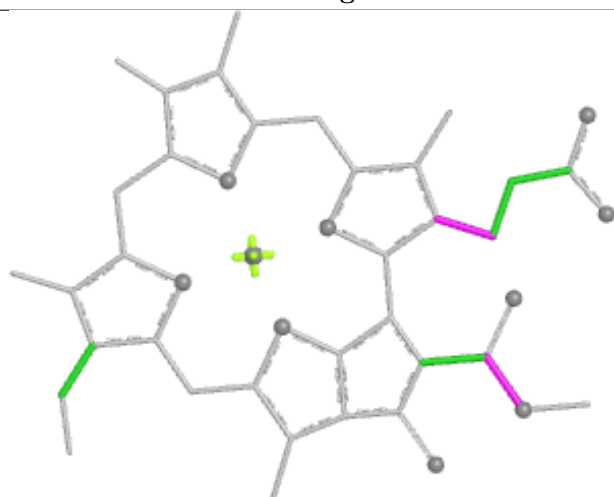
Ligand CLA 4 304



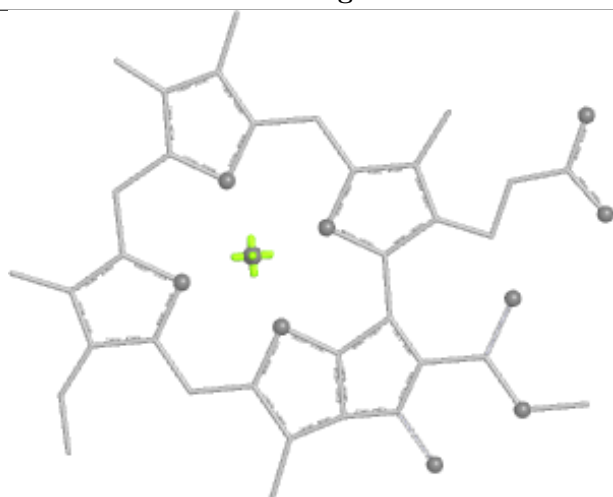
Bond lengths



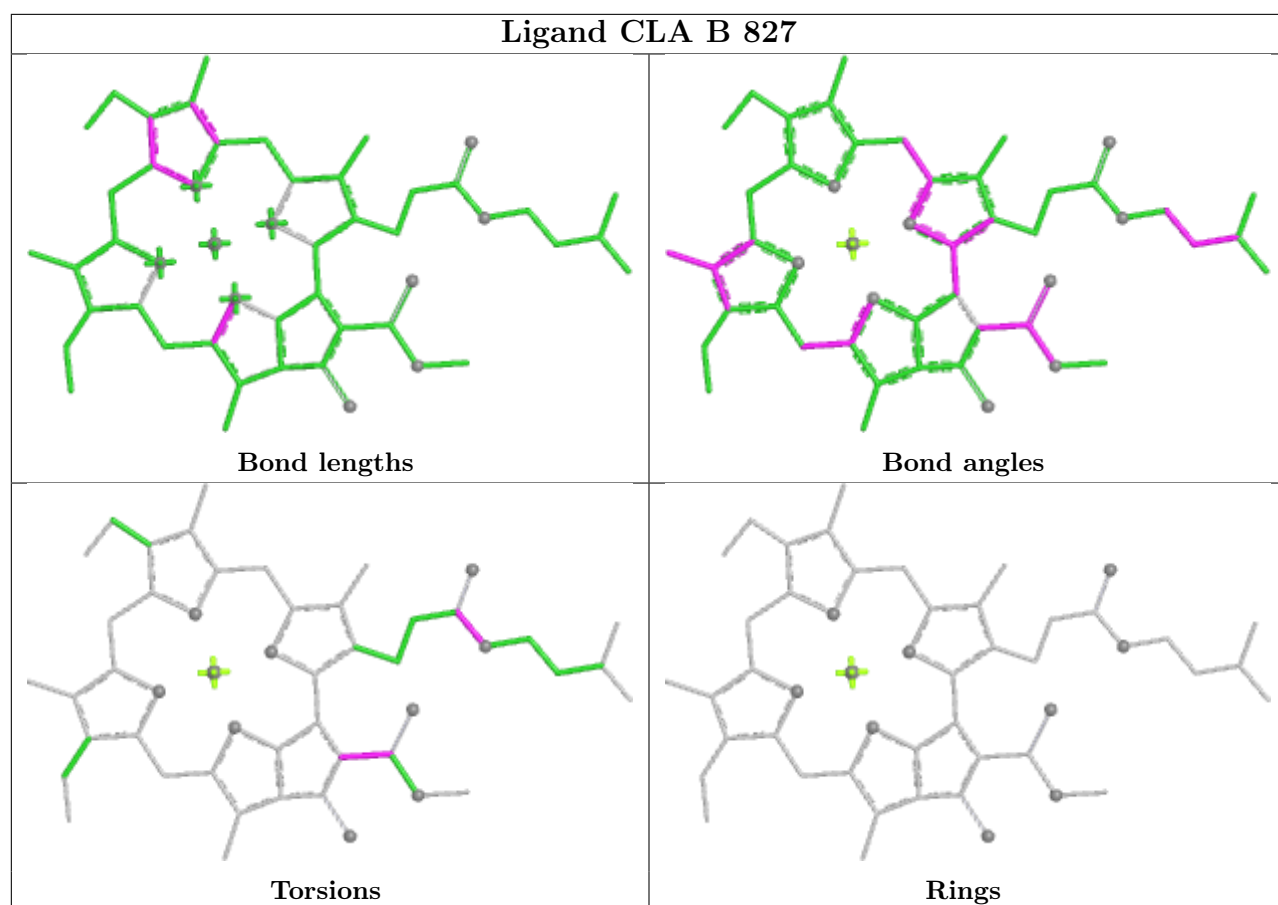
Bond angles

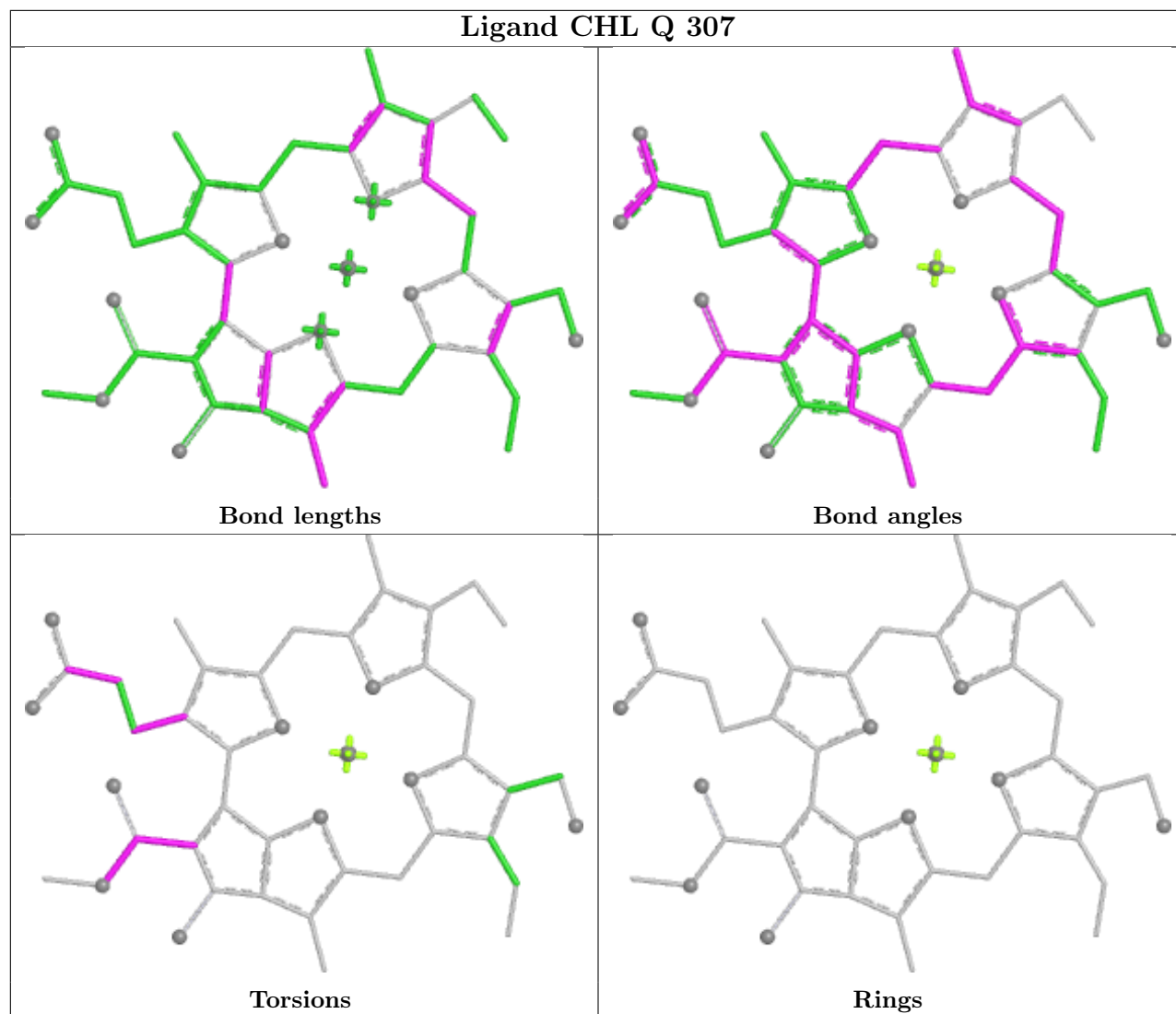


Torsions

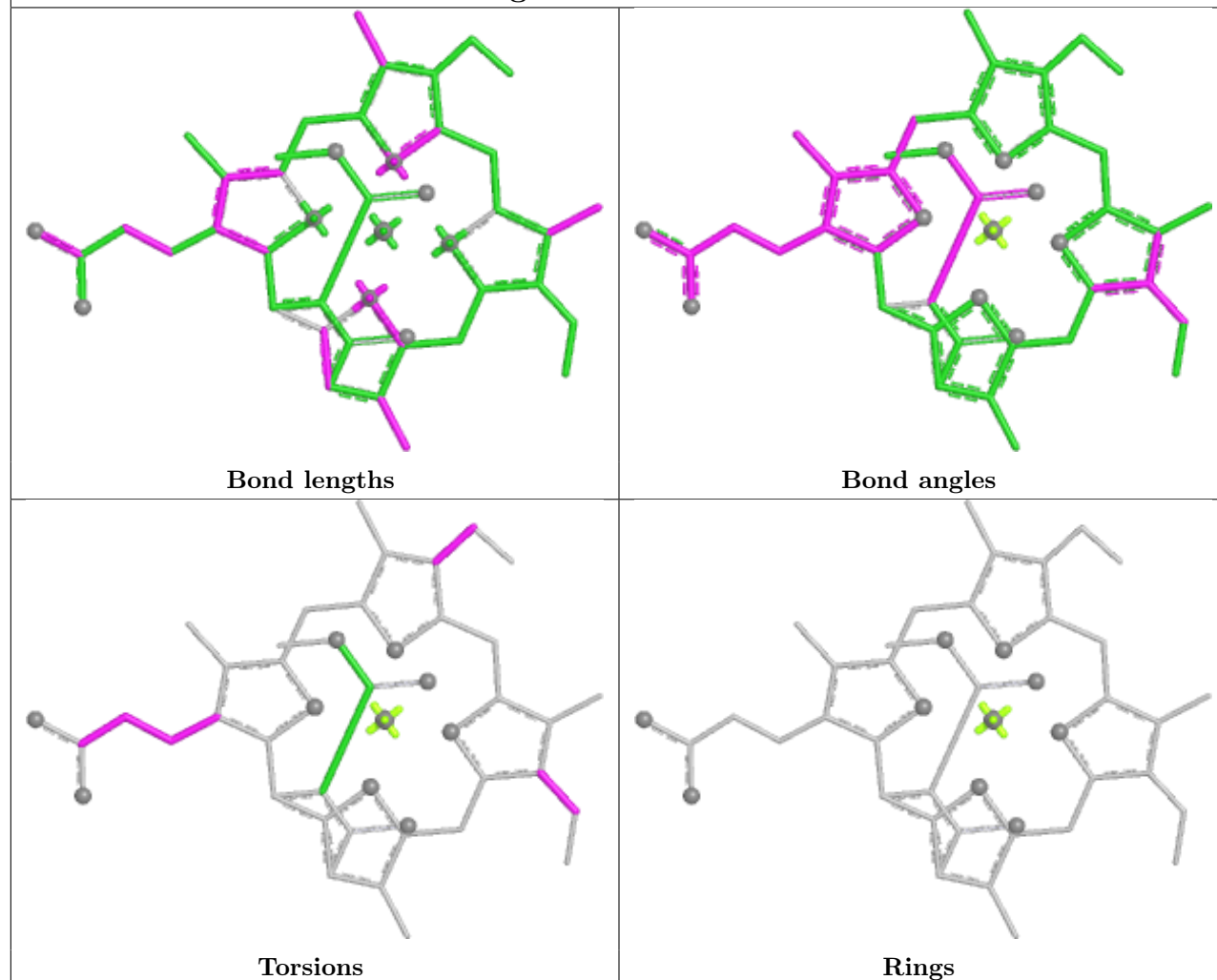


Rings

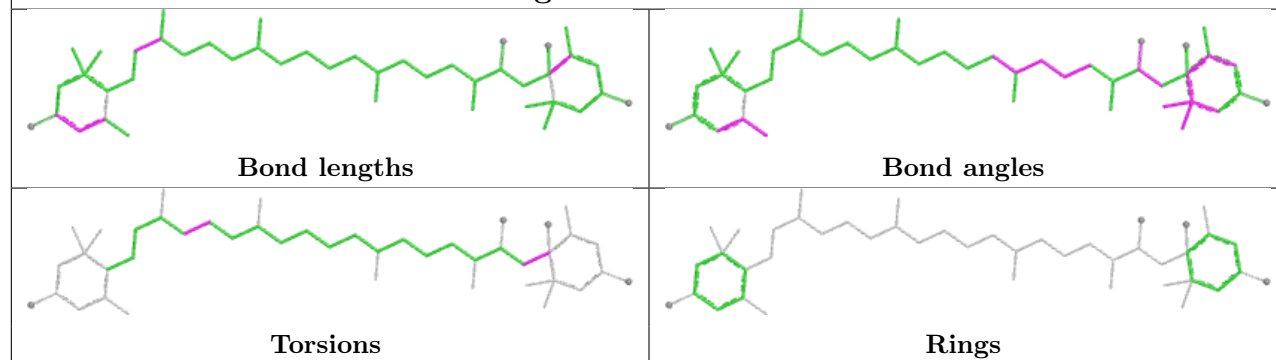




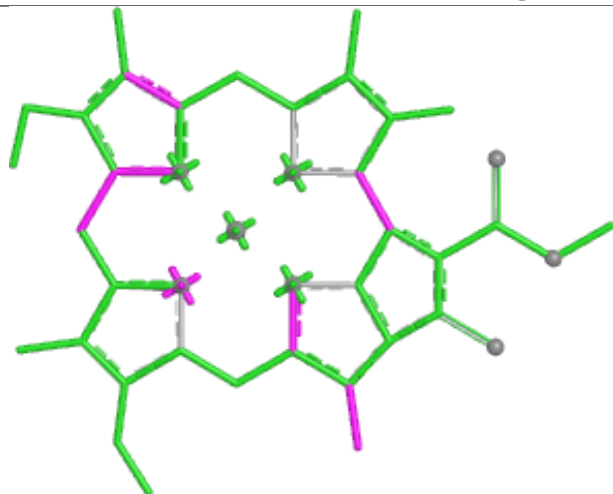
Ligand KC2 T 308



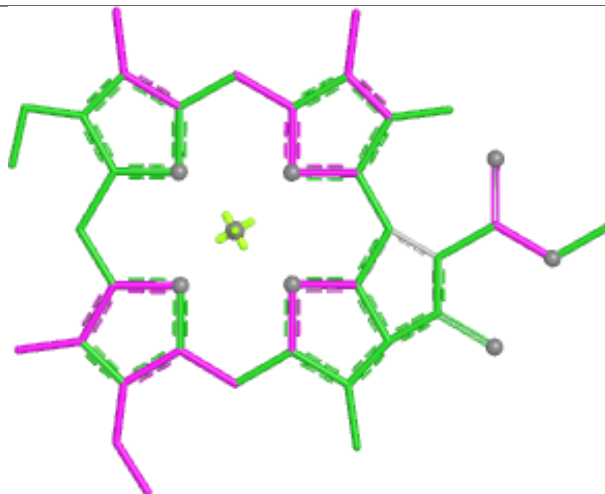
Ligand IWJ V 318



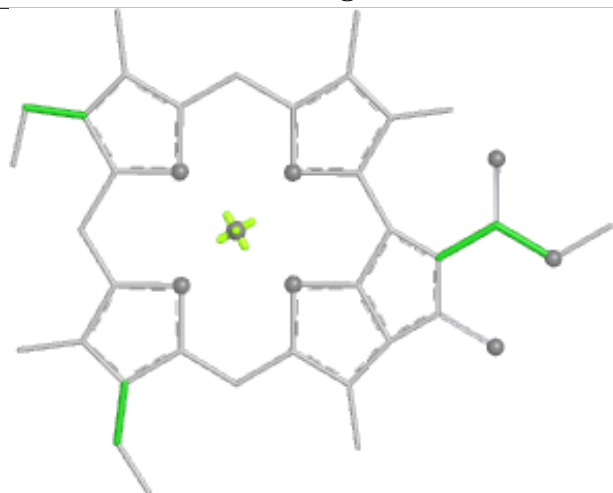
Ligand CLA U 308



Bond lengths



Bond angles

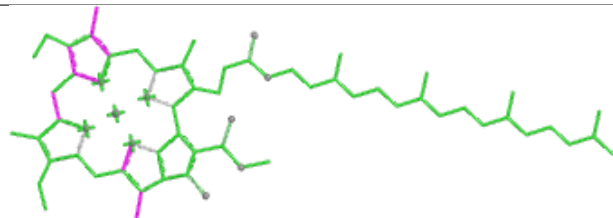


Torsions

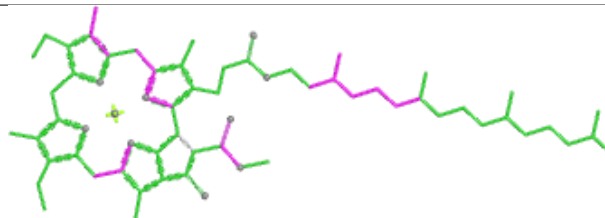


Rings

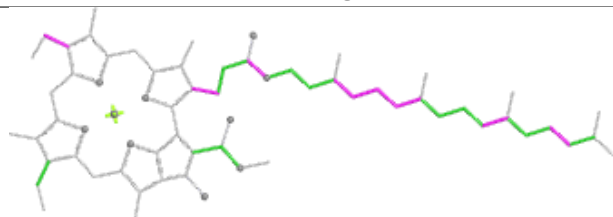
Ligand CLA A 837



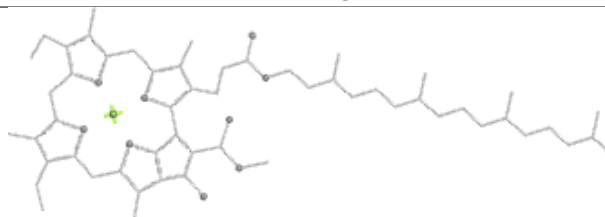
Bond lengths



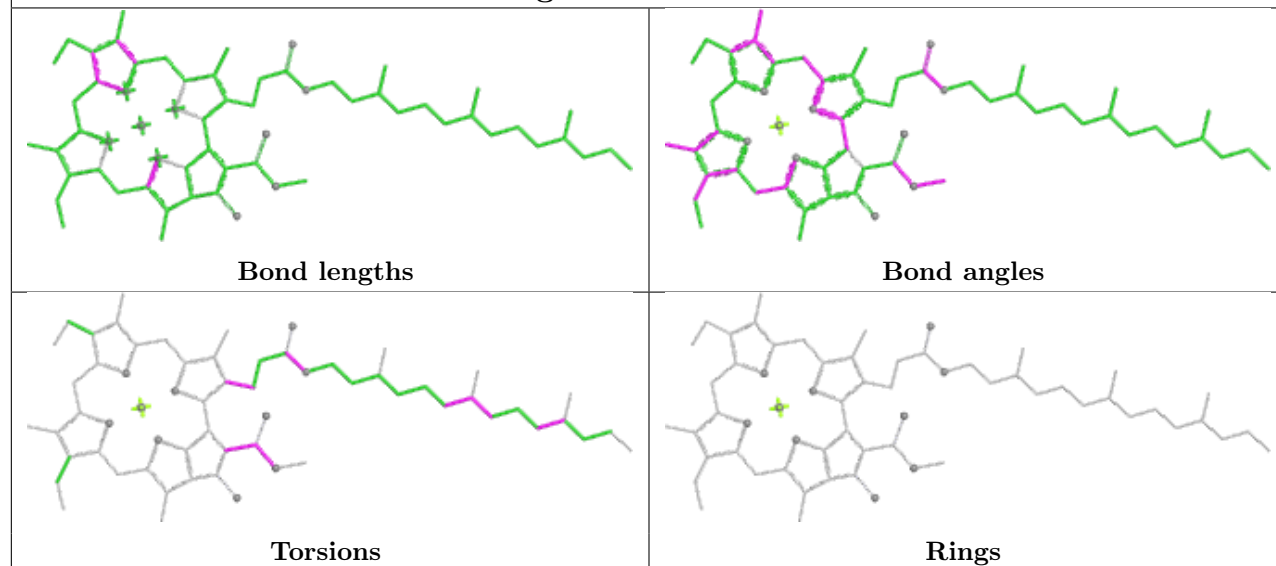
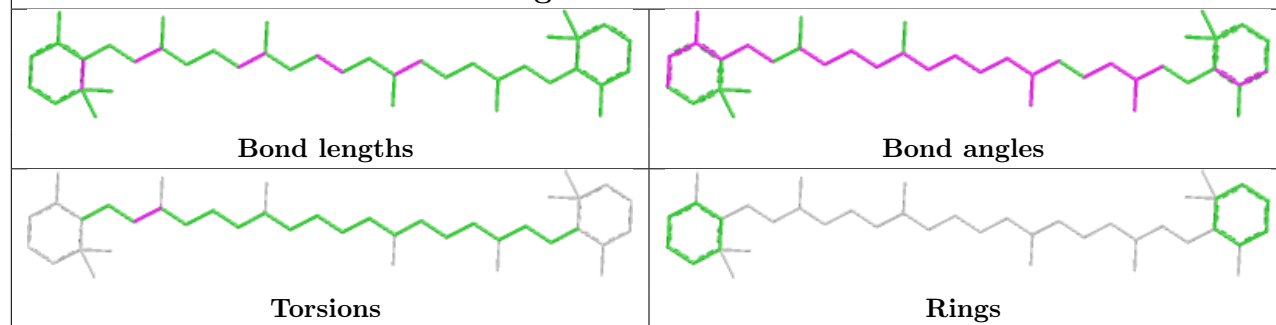
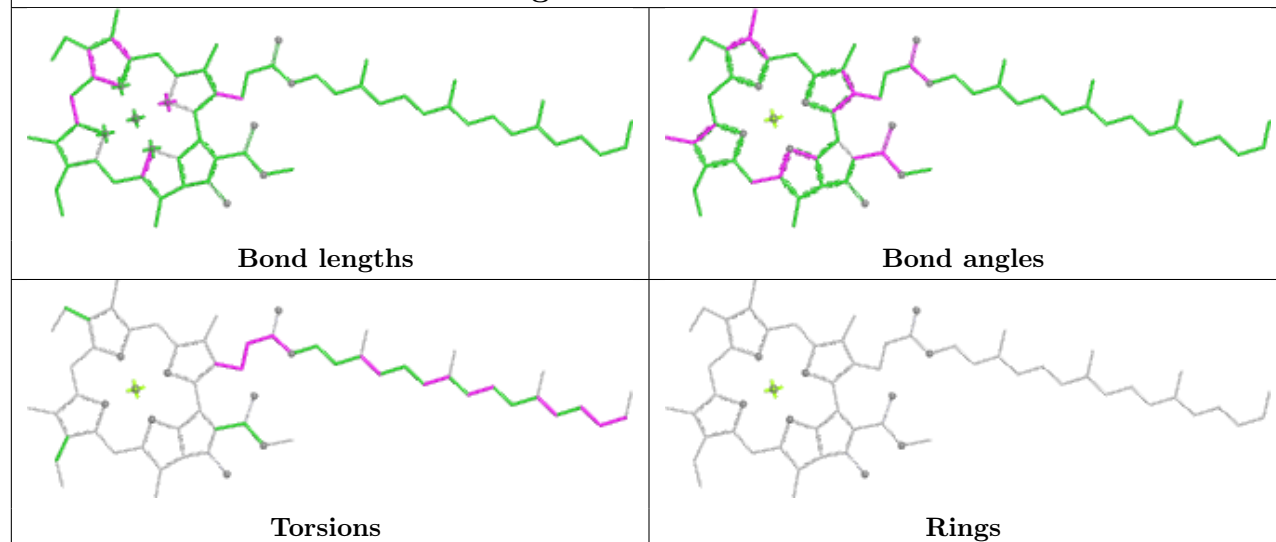
Bond angles



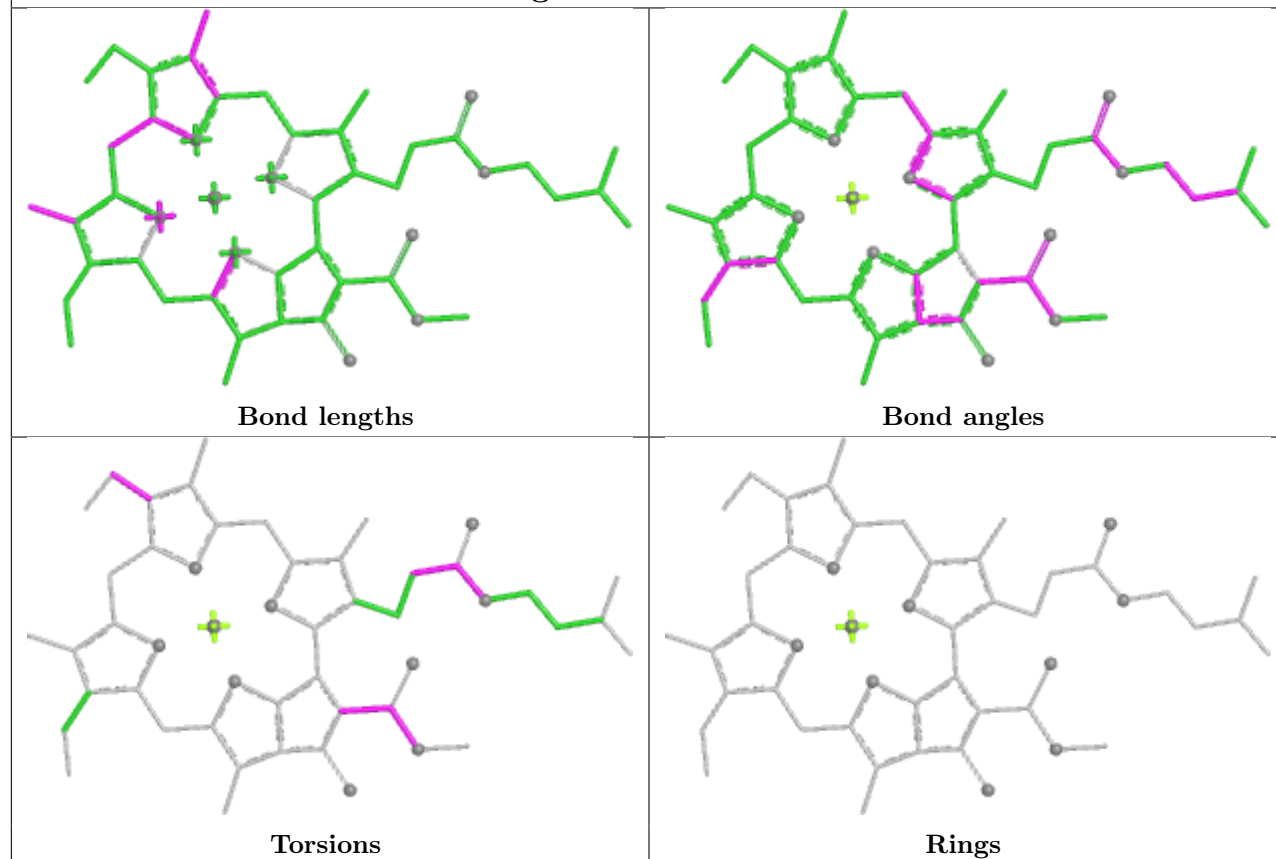
Torsions



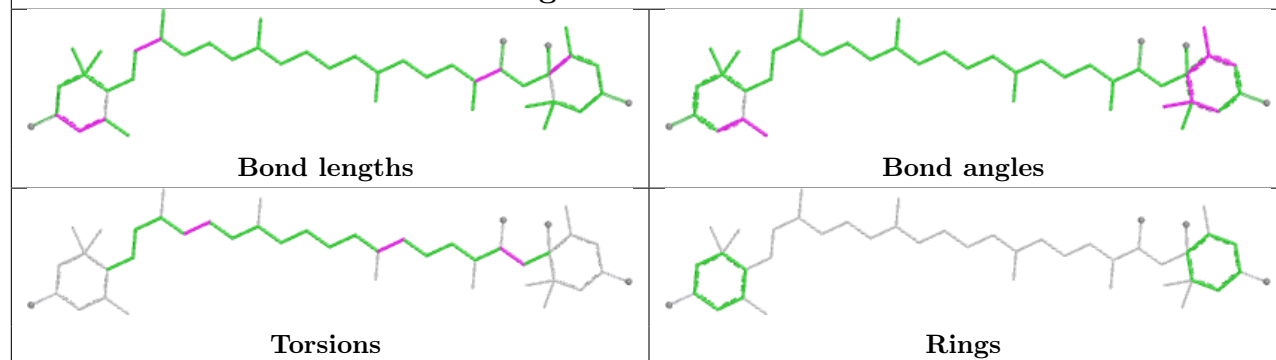
Rings

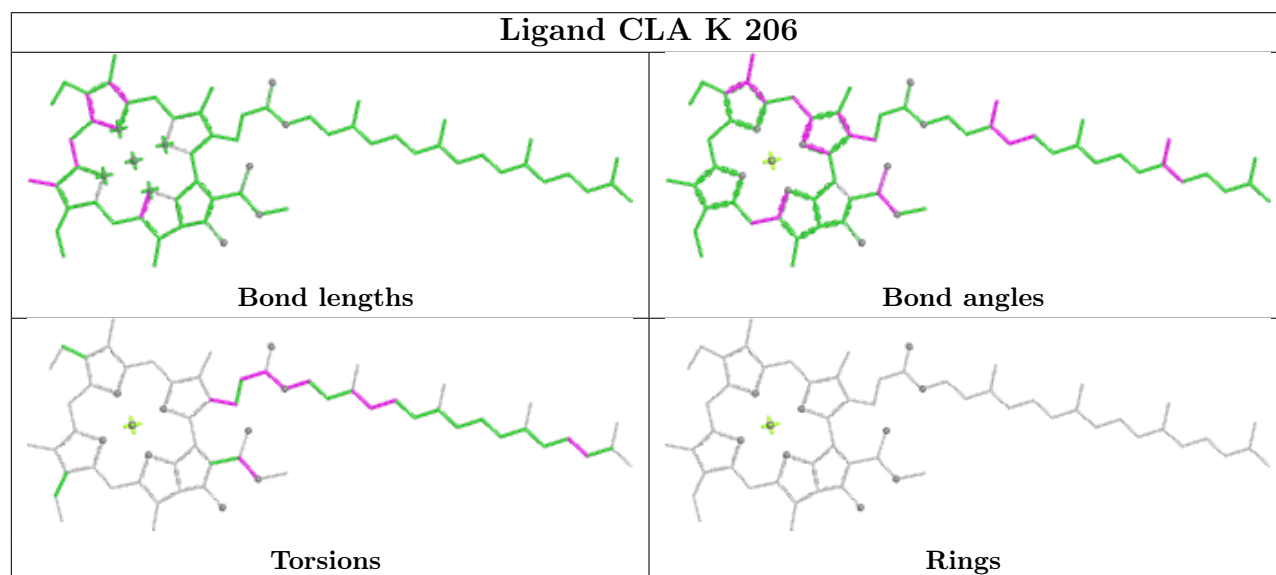
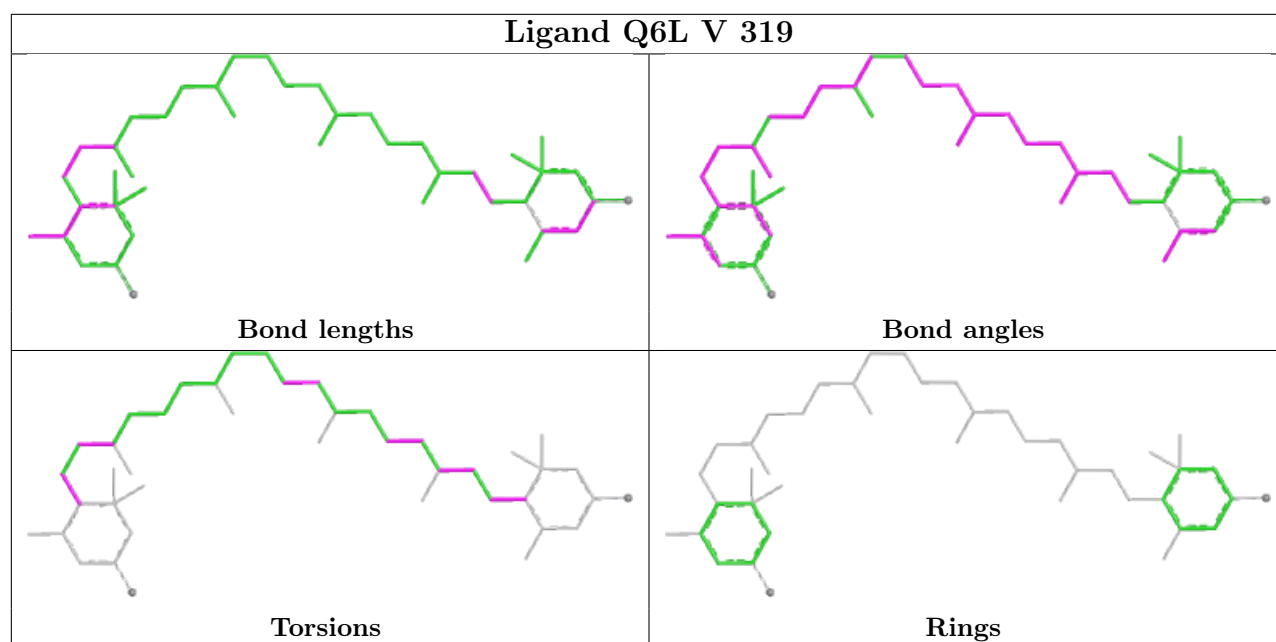
Ligand CLA 6 602**Ligand BCR 3 319****Ligand CLA R 313**

Ligand CLA V 302

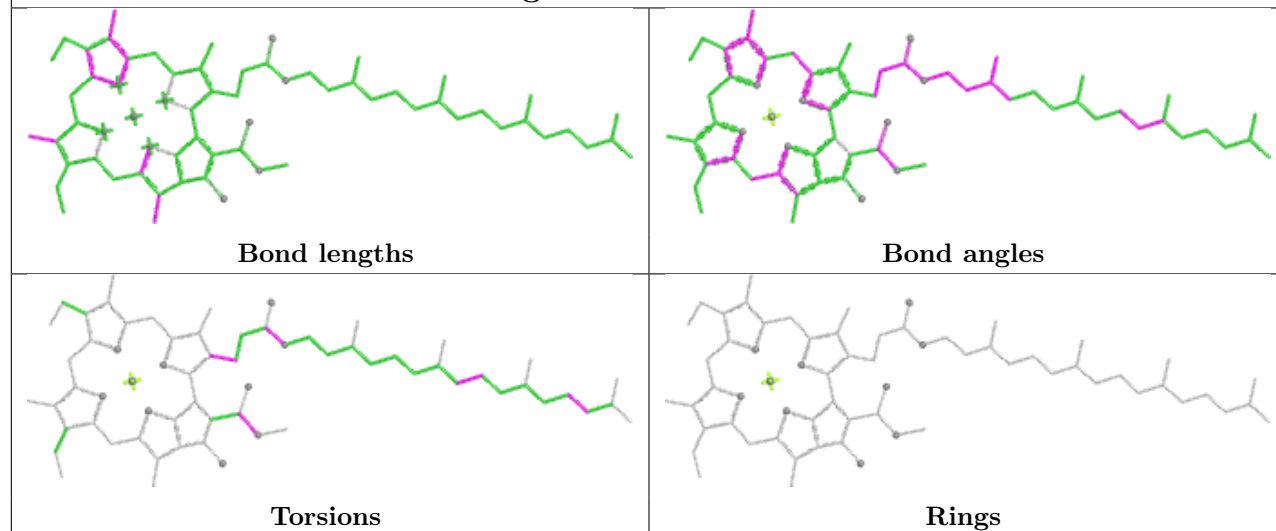


Ligand IWJ 1 611

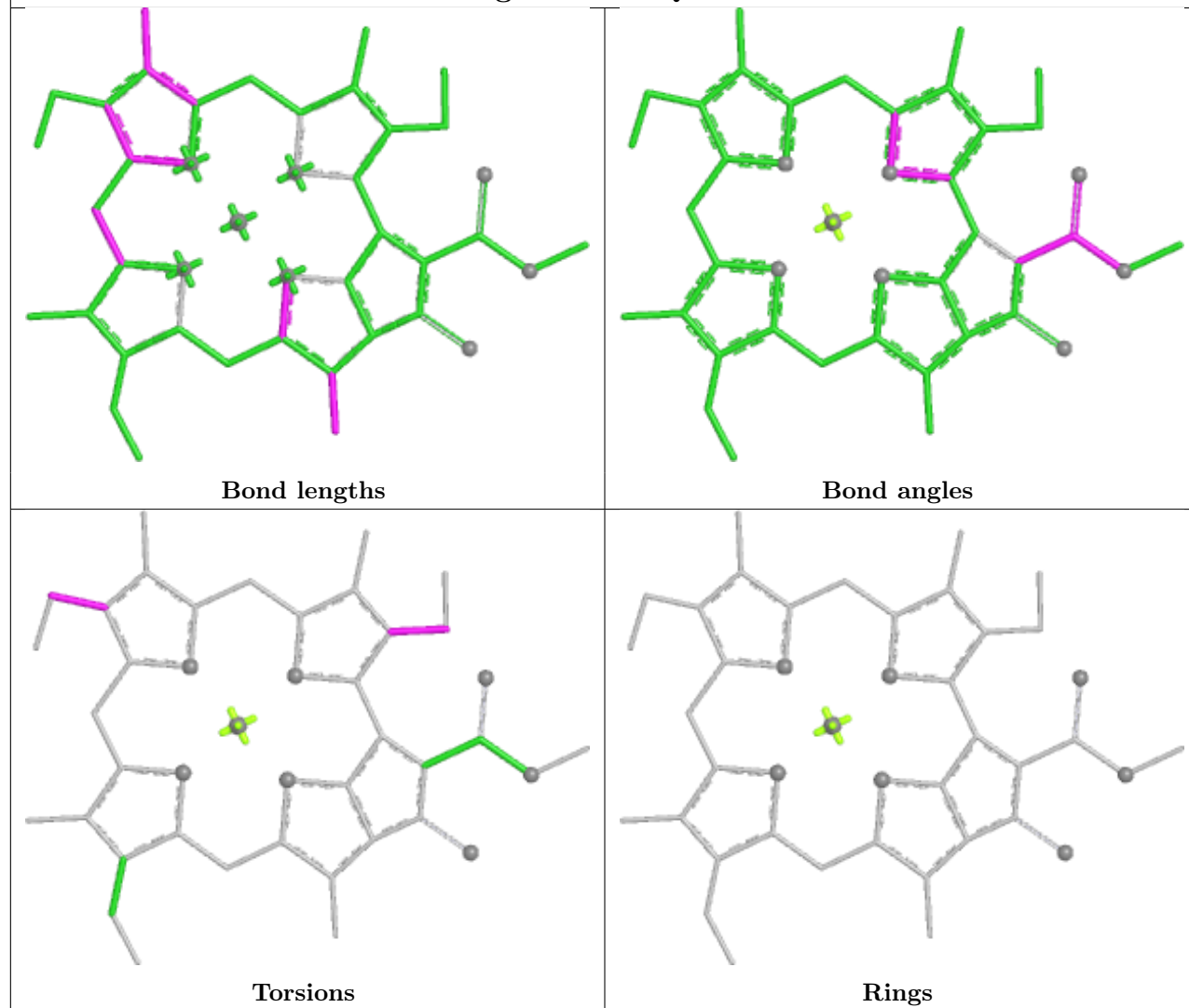


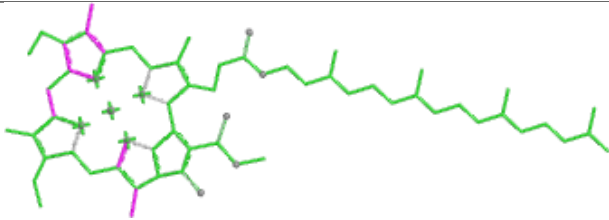
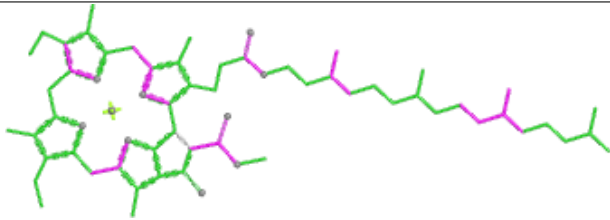
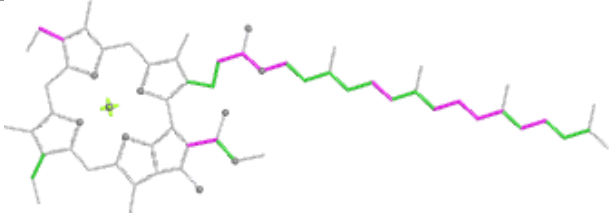
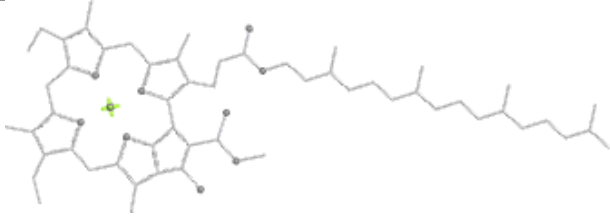


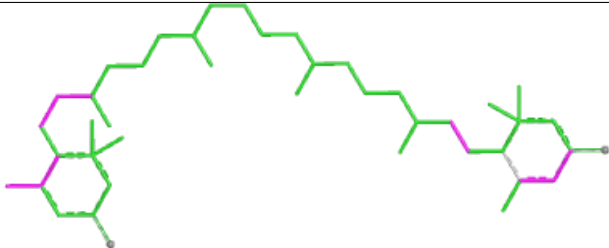
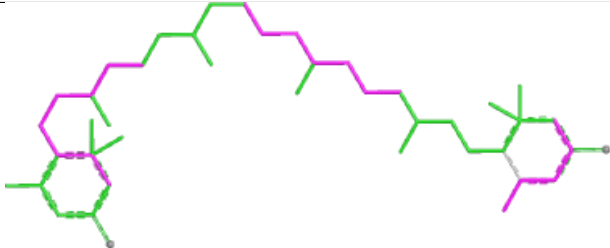
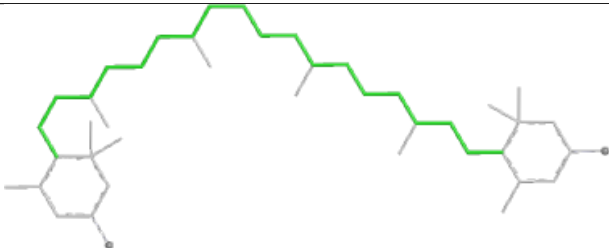
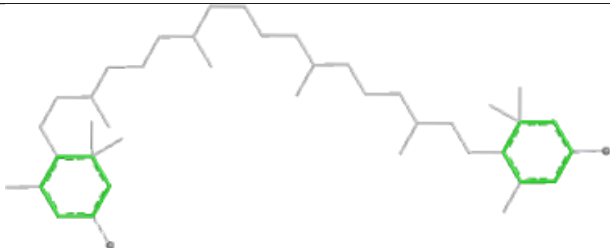
Ligand CLA O 2002



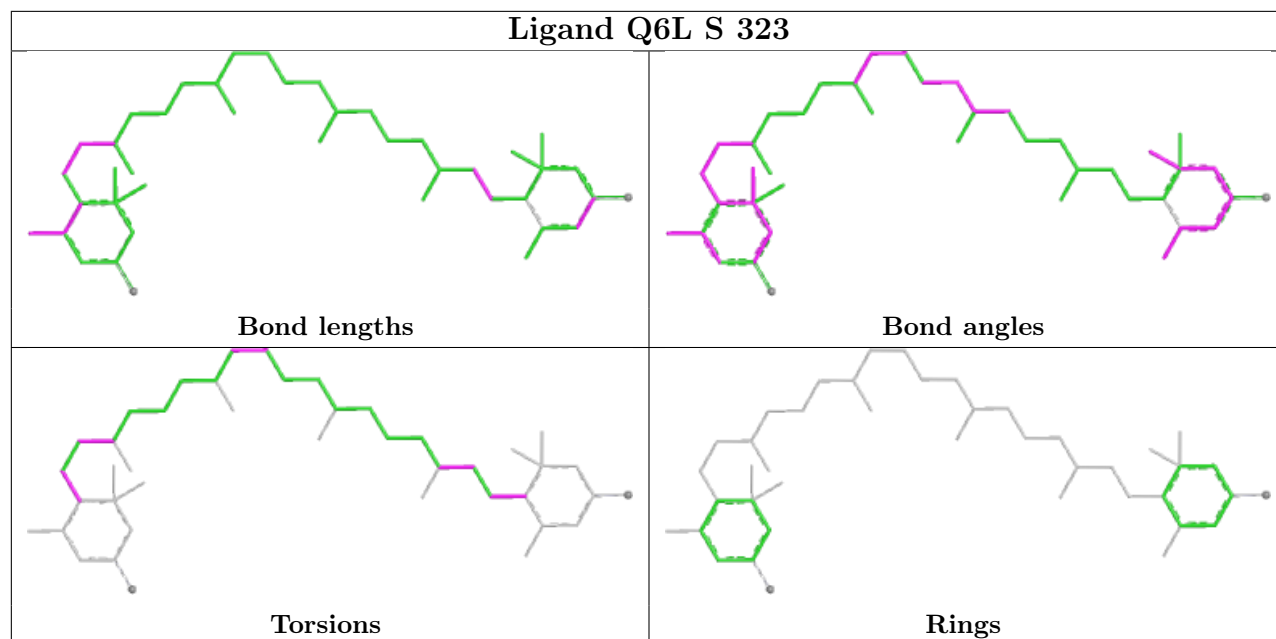
Ligand CLA Q 312



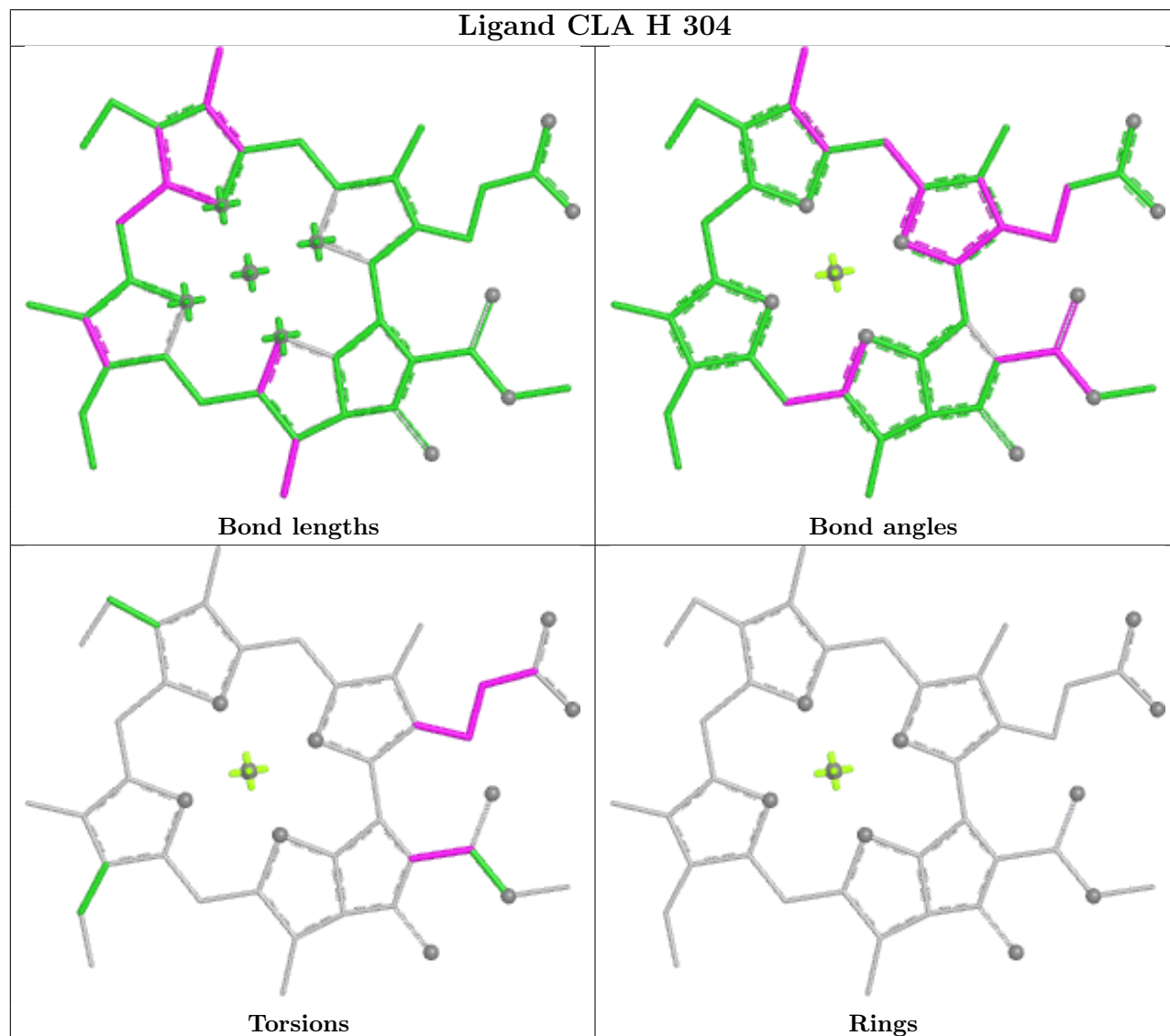
Ligand CLA P 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

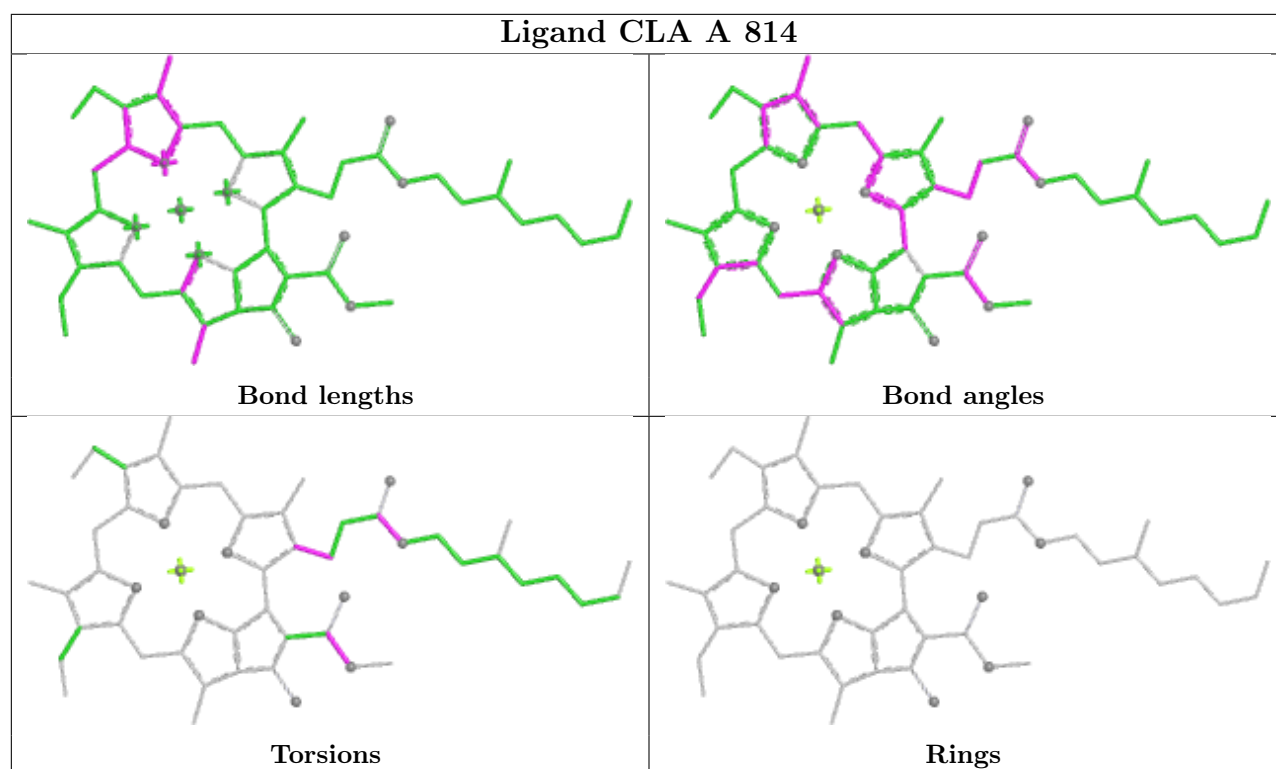
Ligand Q6L R 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand Q6L S 323

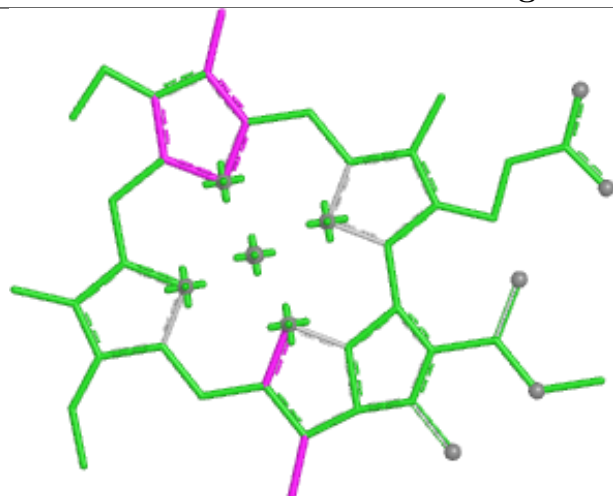


Ligand CLA H 304

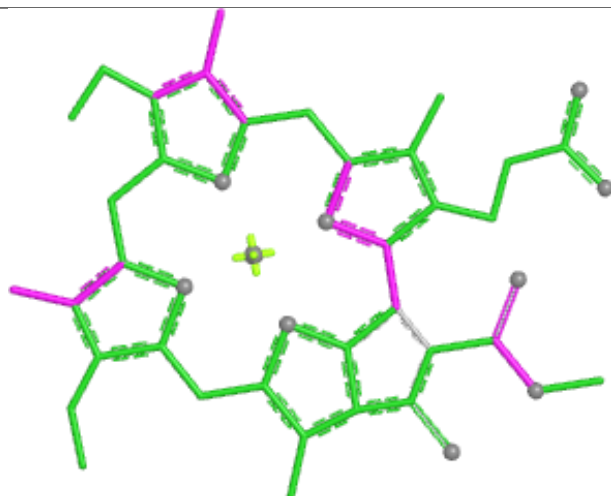




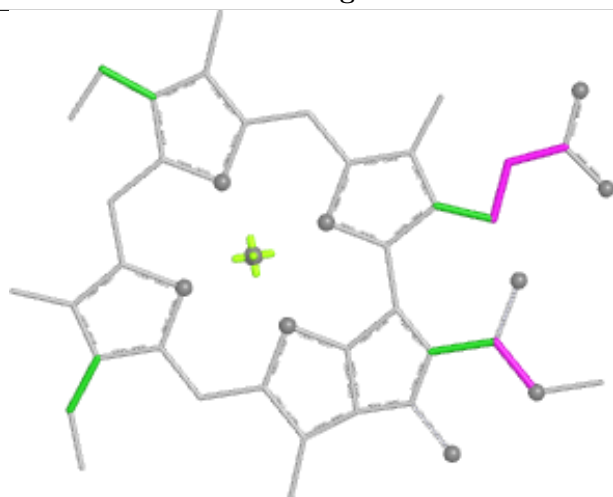
Ligand CLA 5 603



Bond lengths



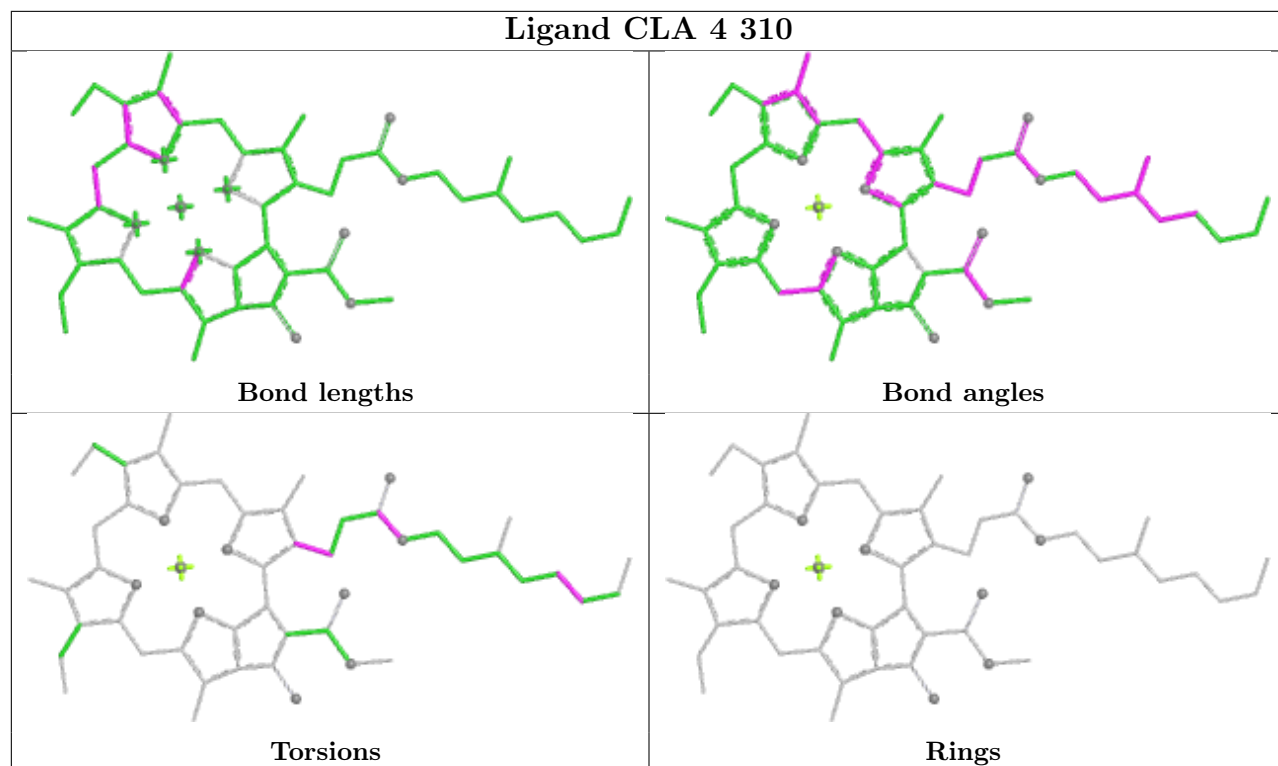
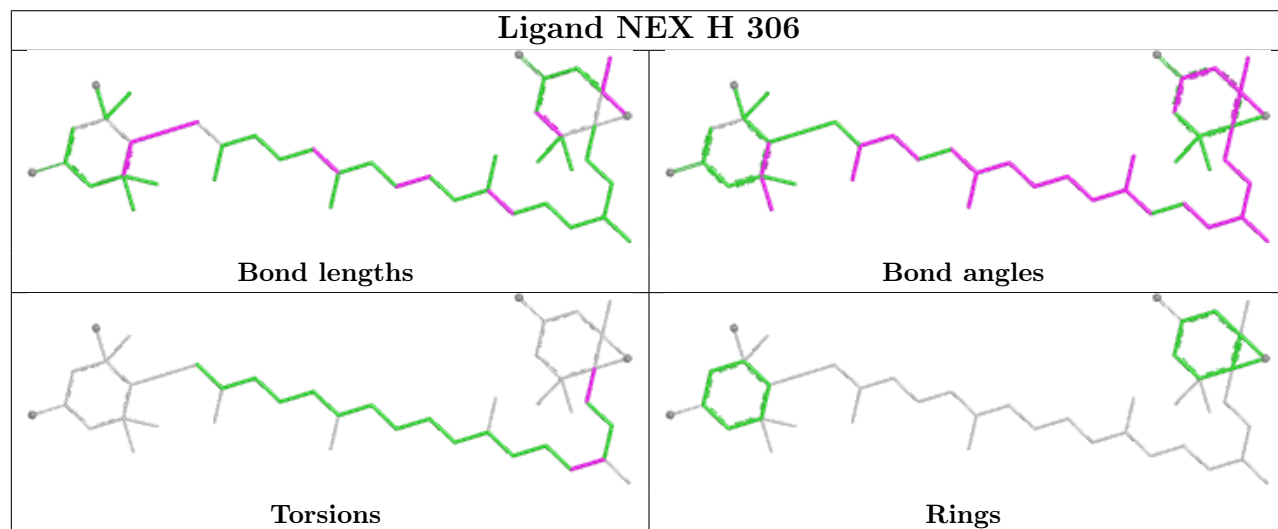
Bond angles



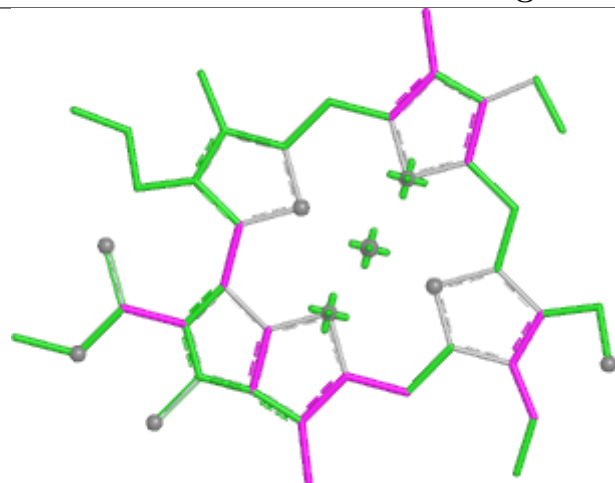
Torsions



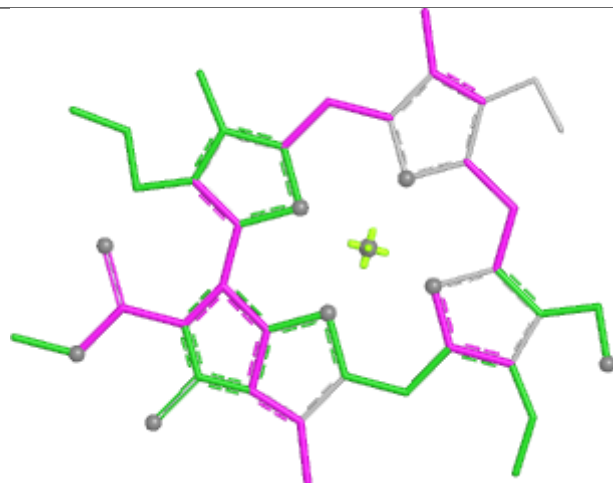
Rings

Ligand CLA 4 310**Ligand NEX H 306**

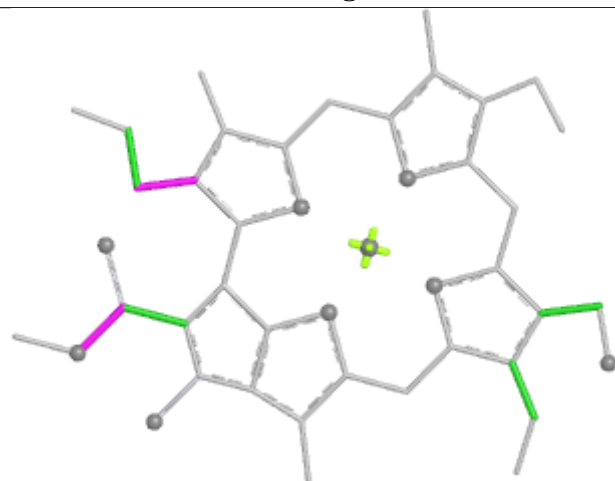
Ligand CHL T 307



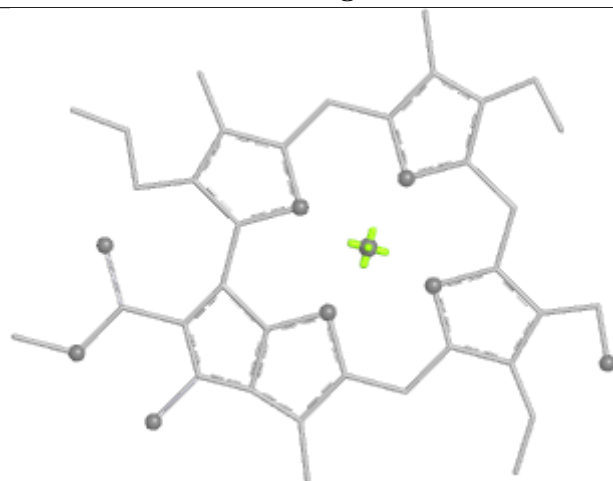
Bond lengths



Bond angles

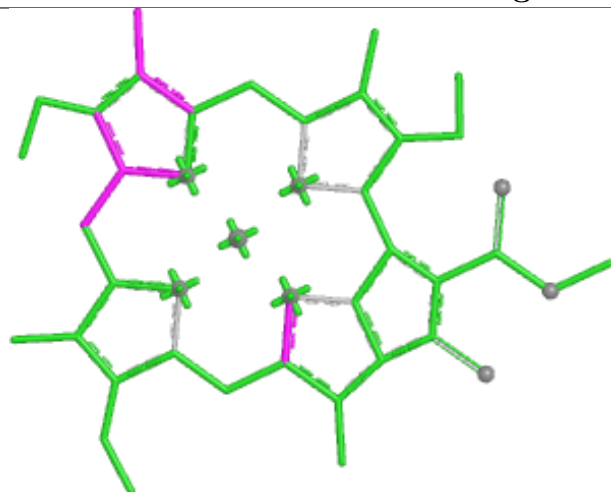


Torsions



Rings

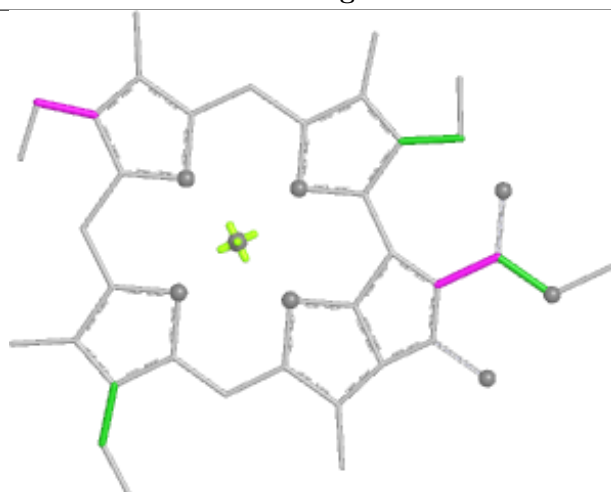
Ligand CLA G 203



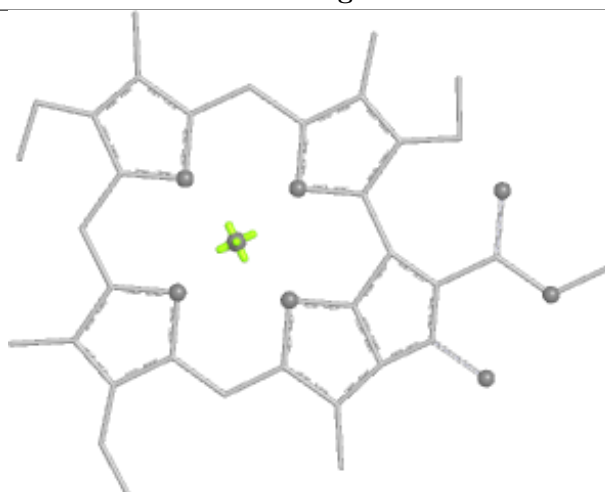
Bond lengths



Bond angles

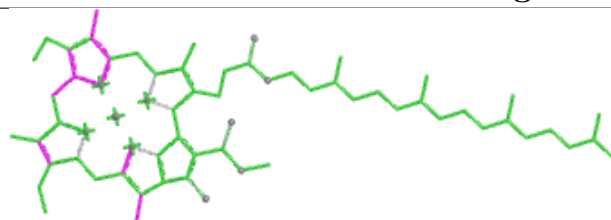


Torsions

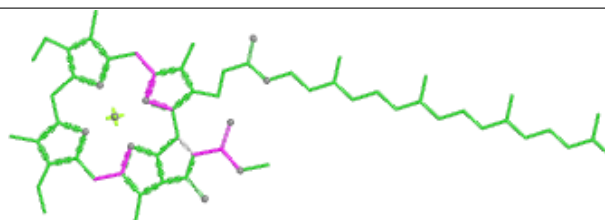


Rings

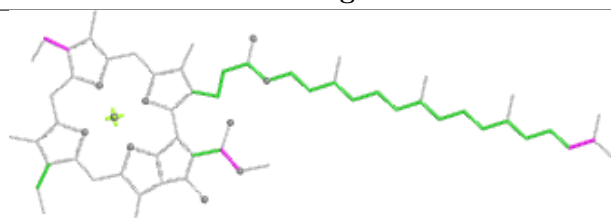
Ligand CLA A 836



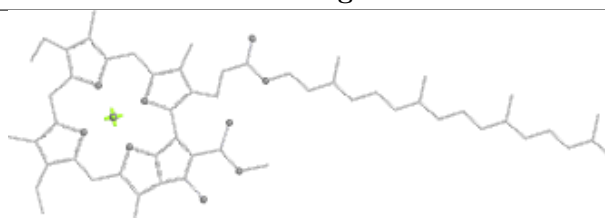
Bond lengths



Bond angles

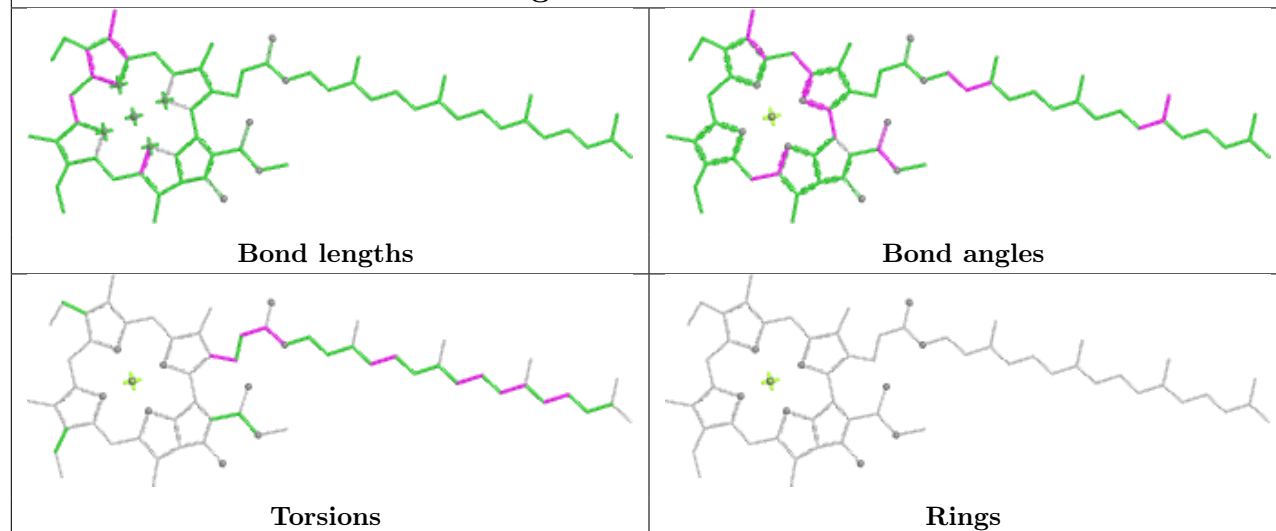


Torsions

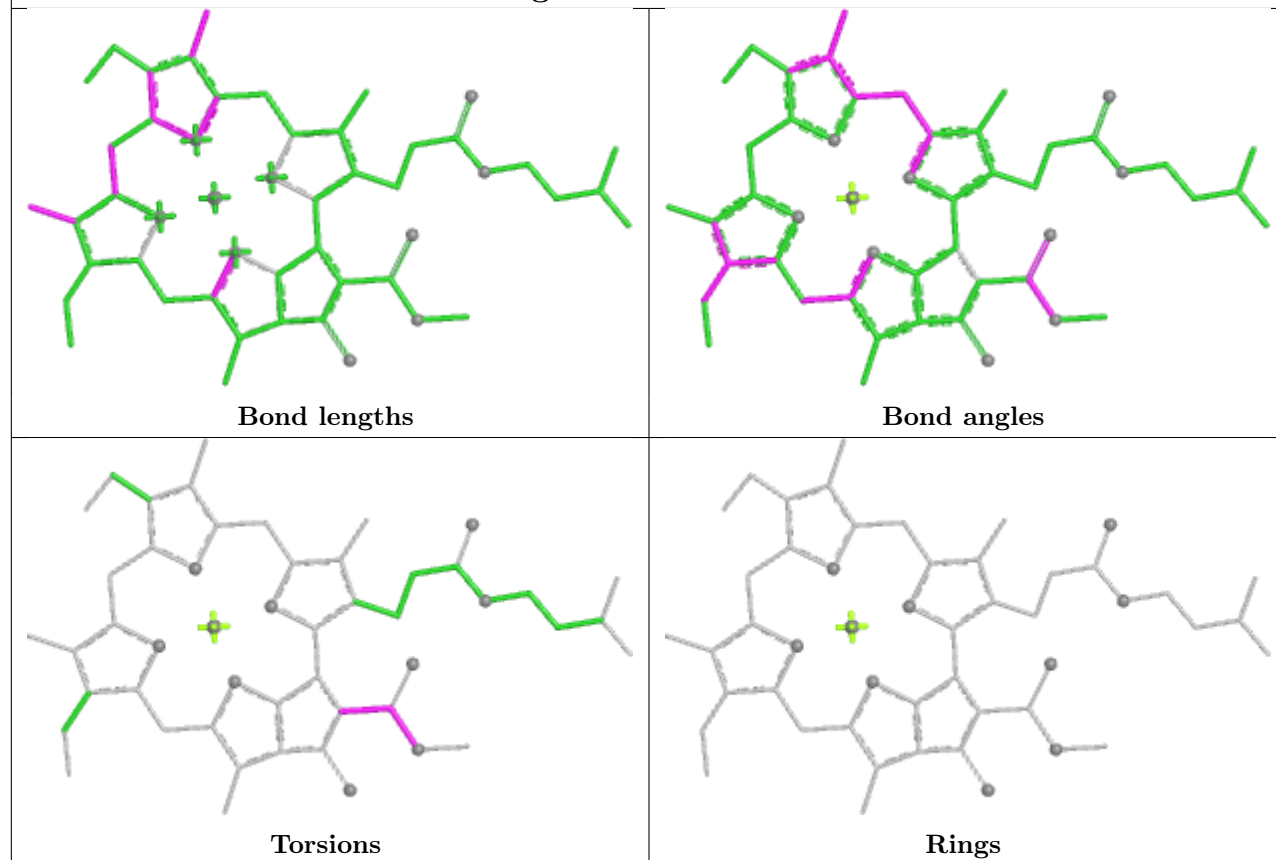


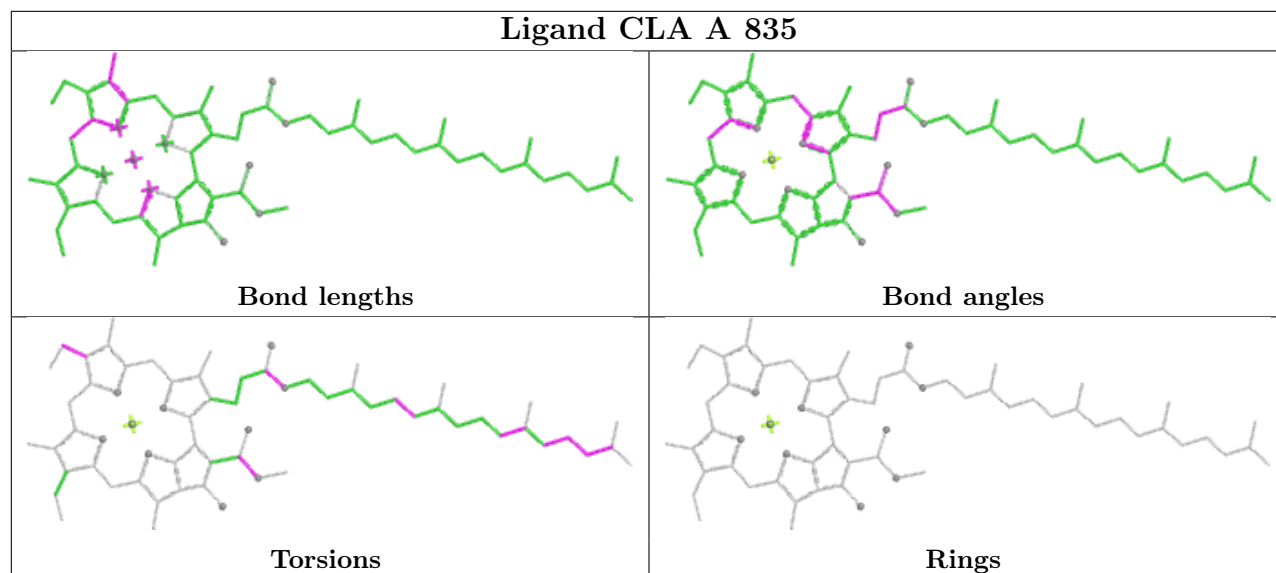
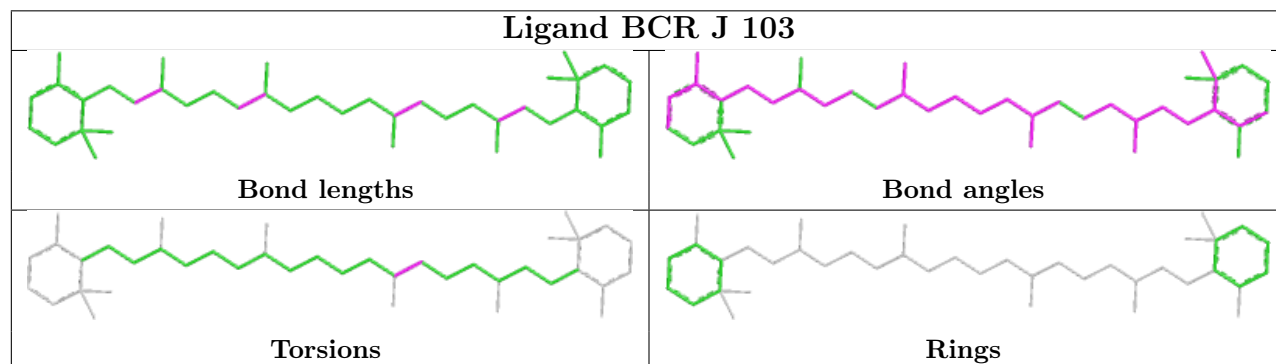
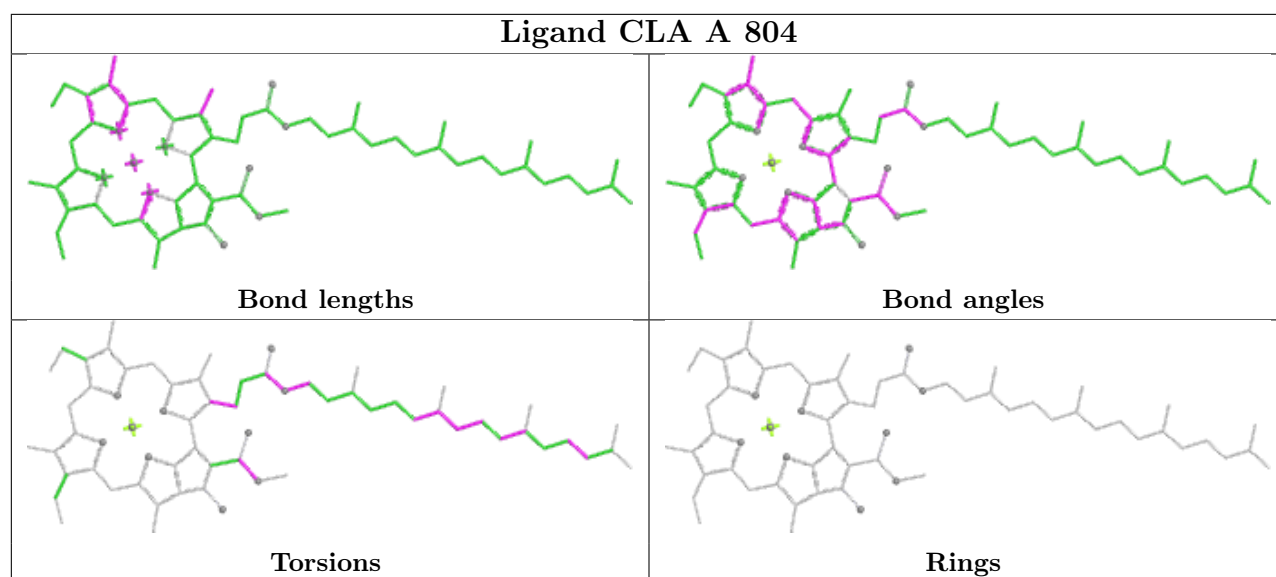
Rings

Ligand CLA A 817

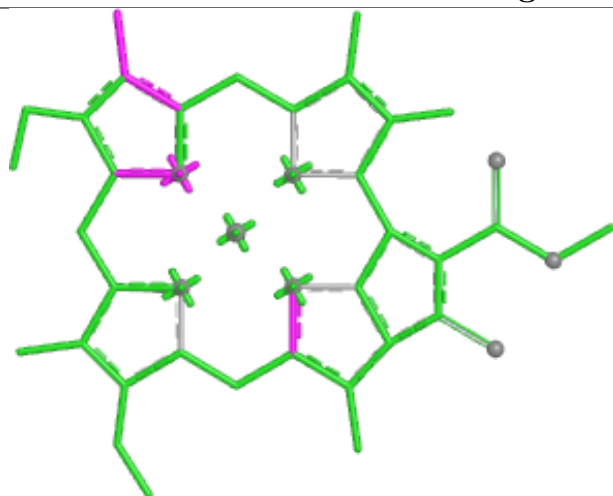


Ligand CLA V 303

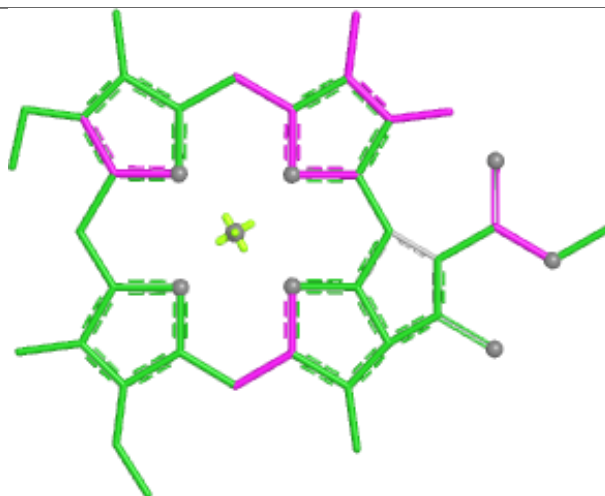




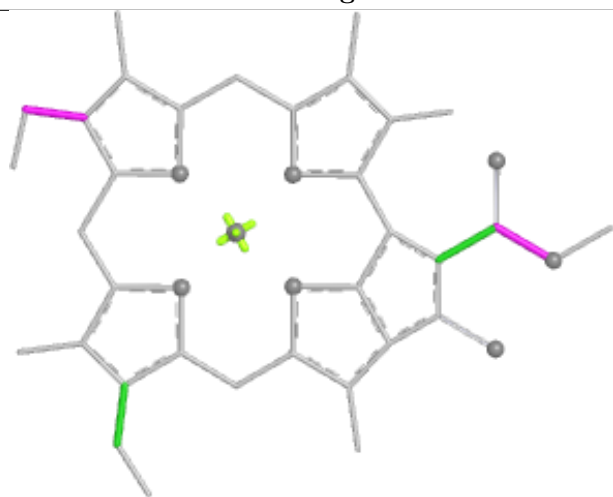
Ligand CLA 4 315



Bond lengths



Bond angles

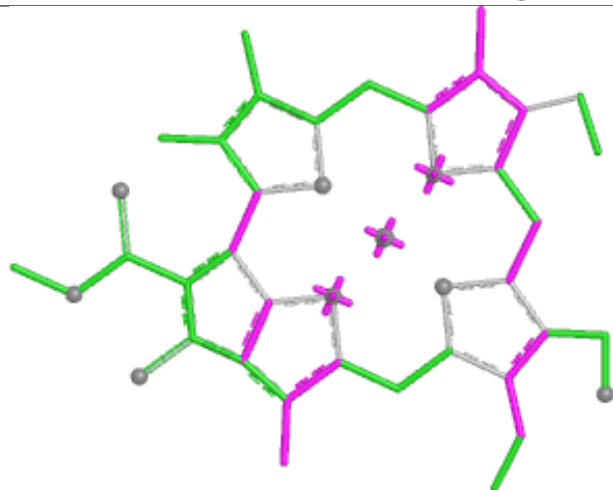


Torsions

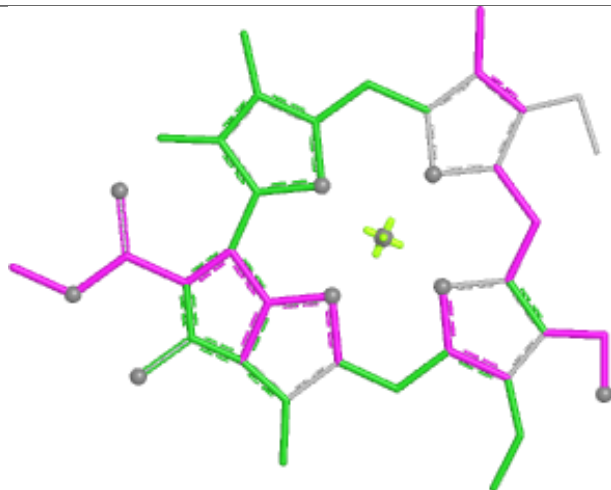


Rings

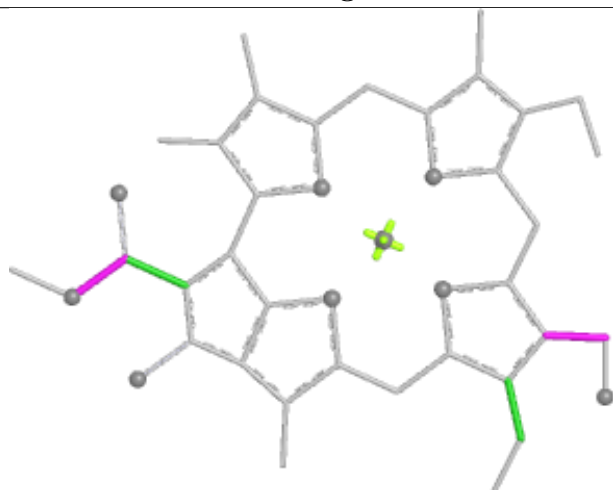
Ligand CHL U 304



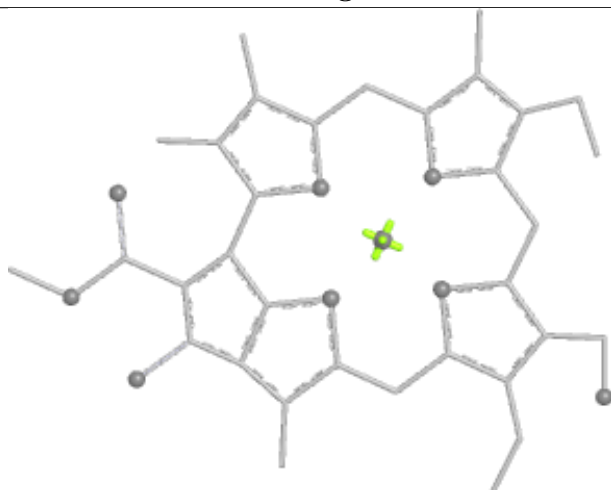
Bond lengths



Bond angles

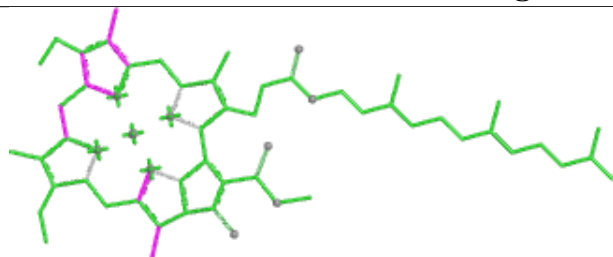


Torsions

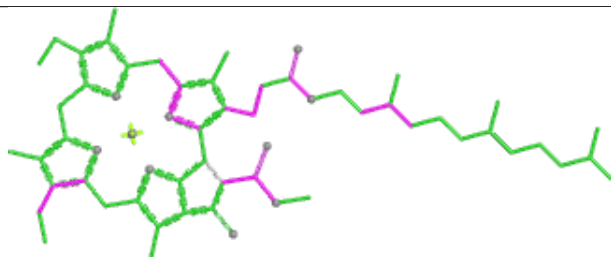


Rings

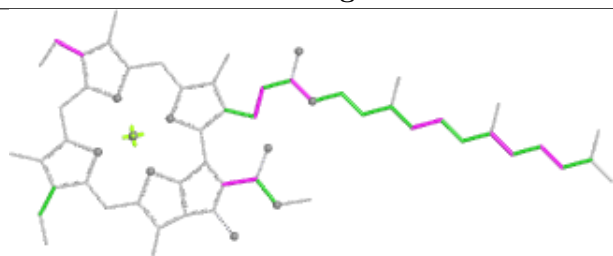
Ligand CLA R 315



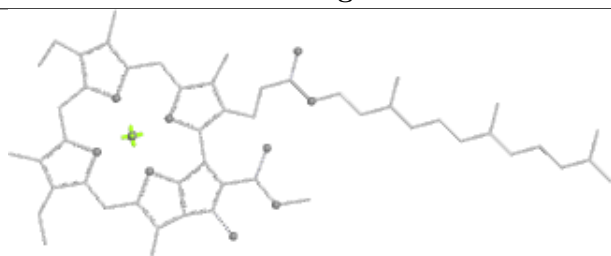
Bond lengths



Bond angles

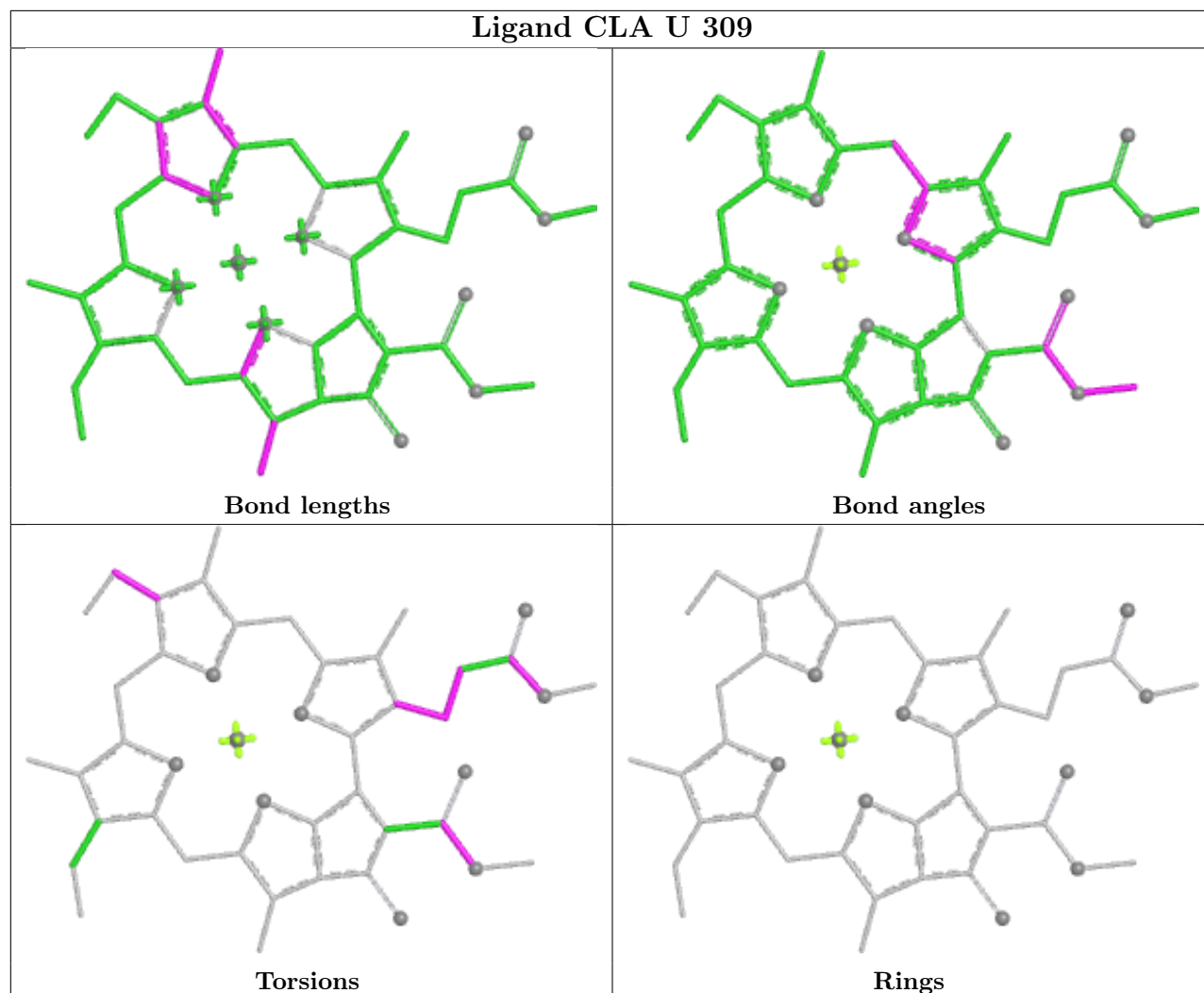


Torsions

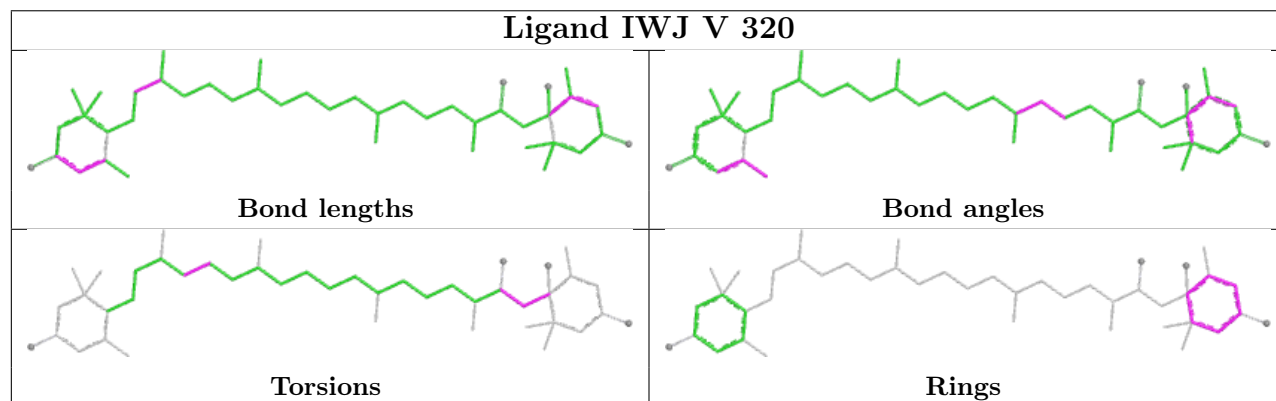


Rings

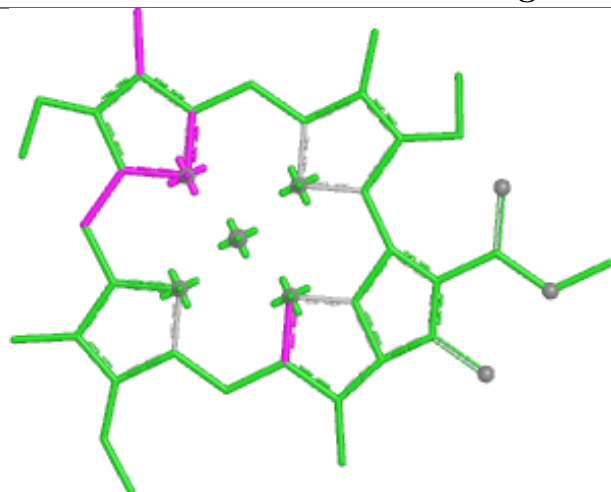
Ligand CLA U 309



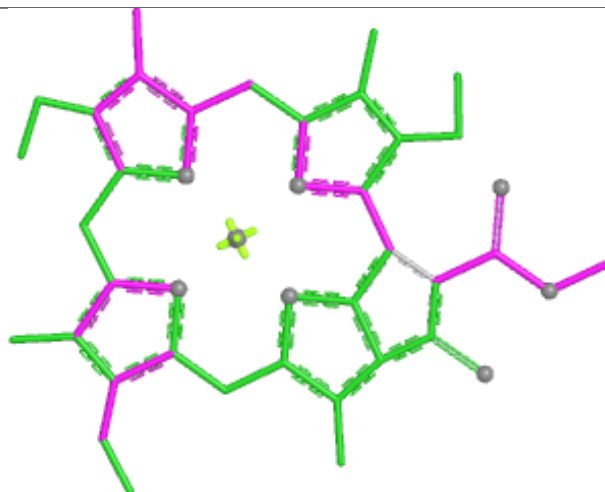
Ligand IWJ V 320



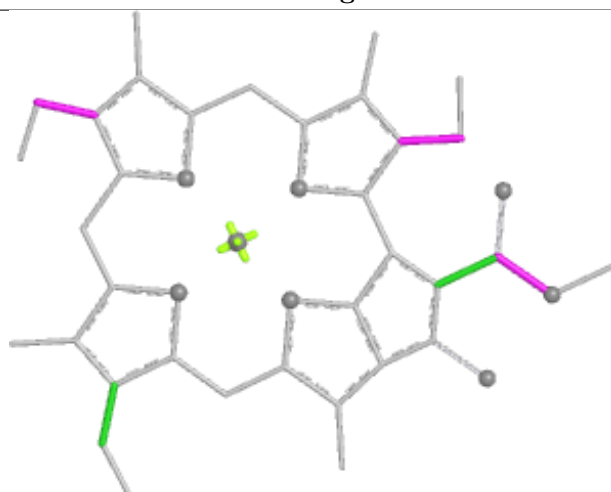
Ligand CLA 4 311



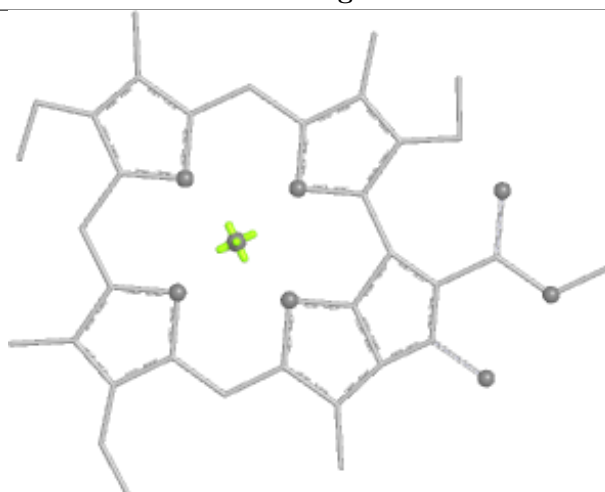
Bond lengths



Bond angles

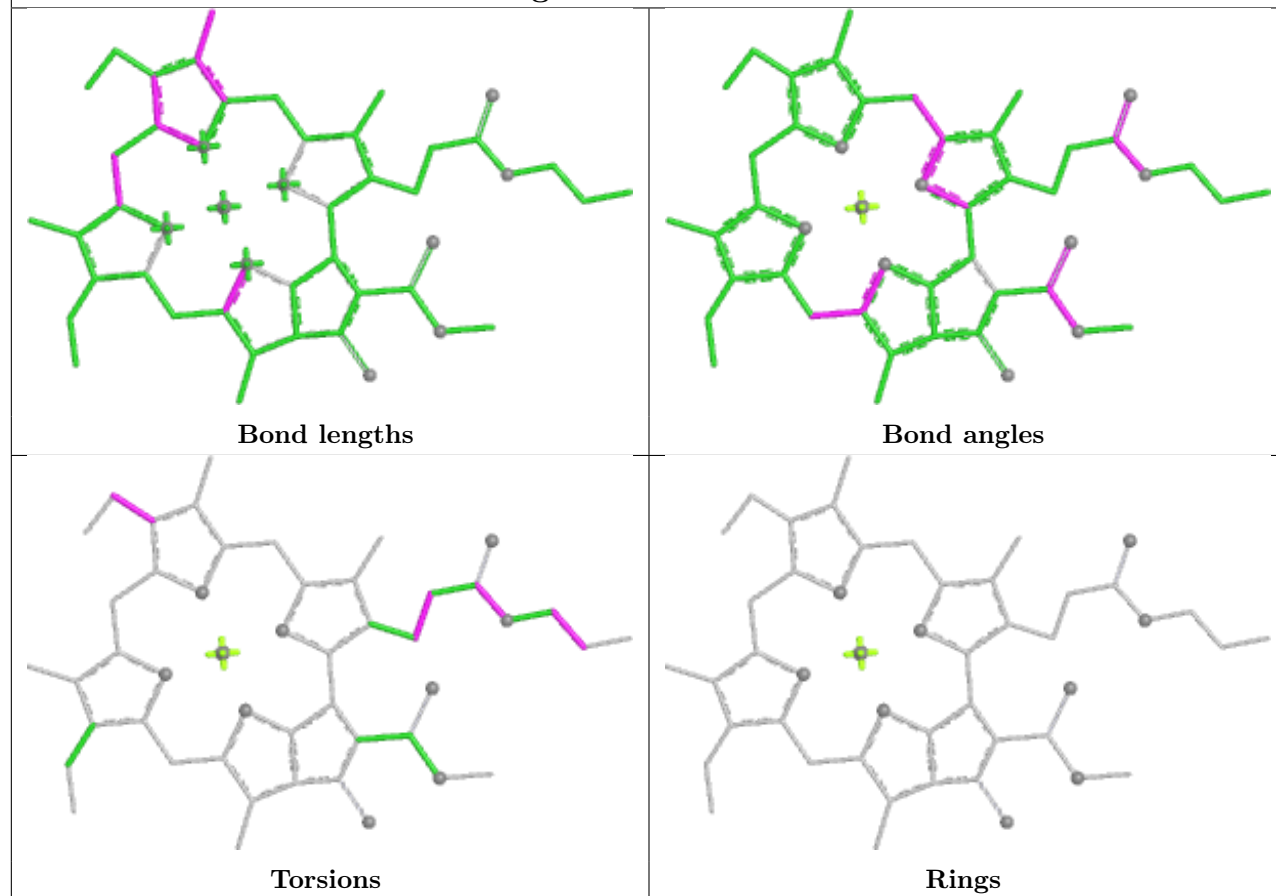


Torsions

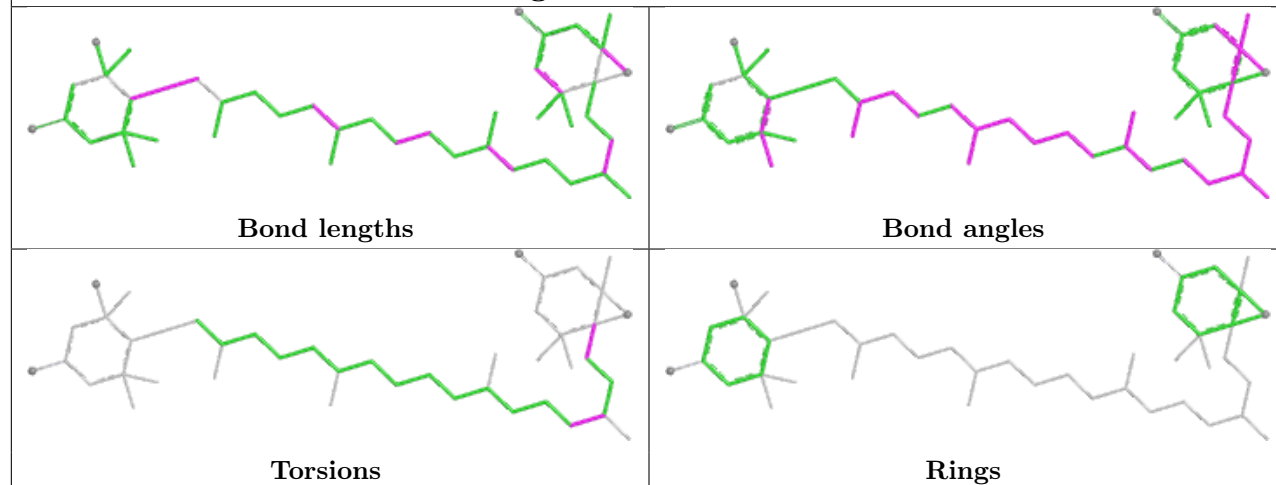


Rings

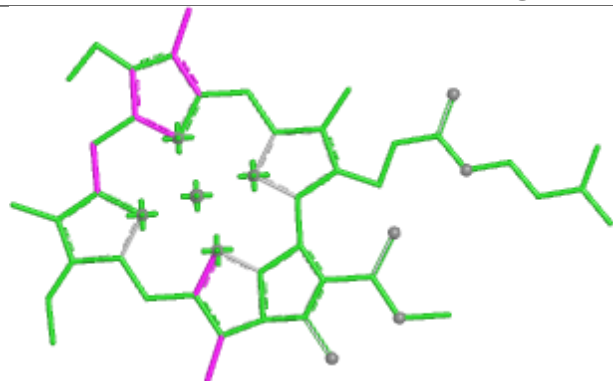
Ligand CLA V 313



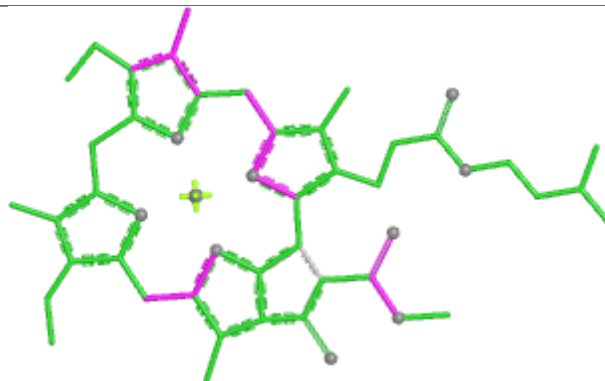
Ligand NEX R 321



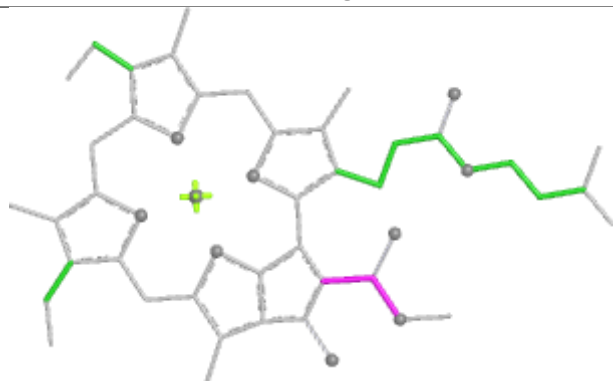
Ligand CLA R 307



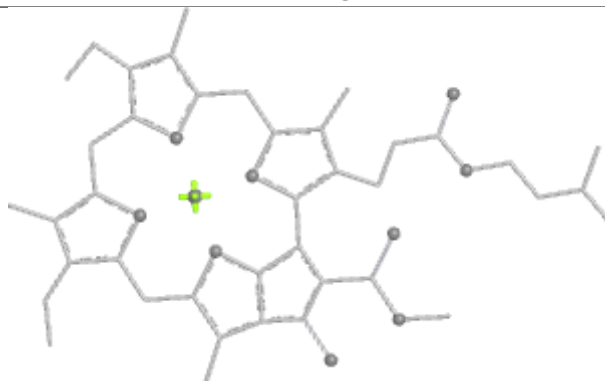
Bond lengths



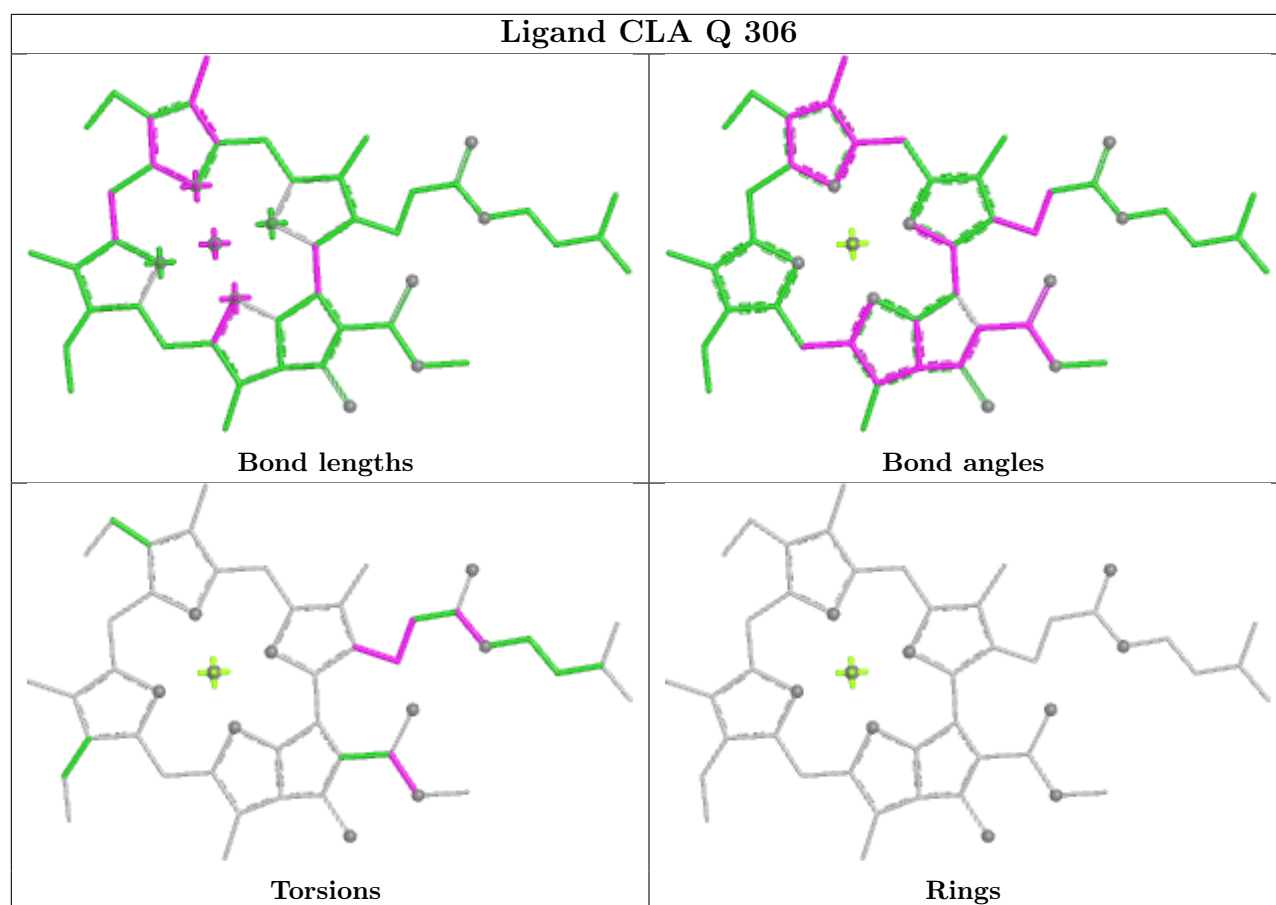
Bond angles



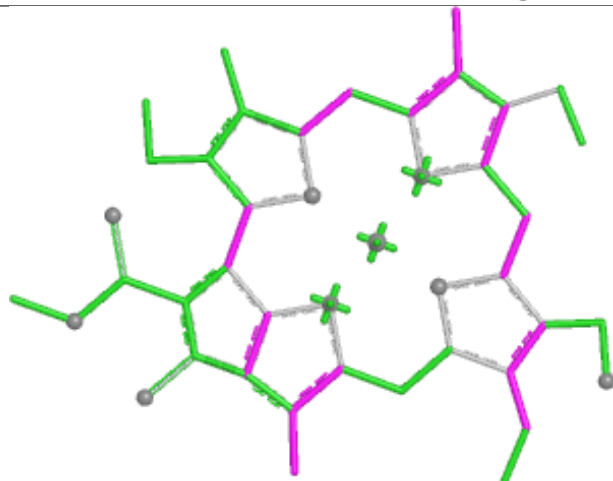
Torsions



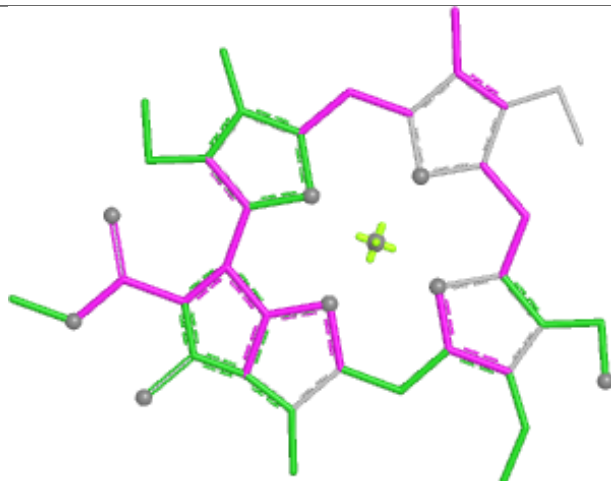
Rings



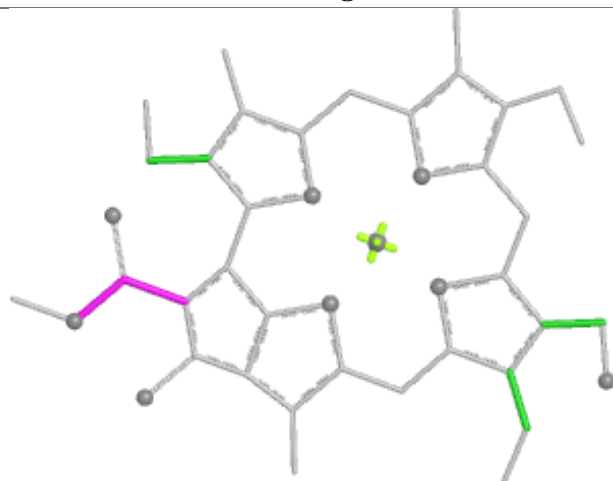
Ligand CHL T 304



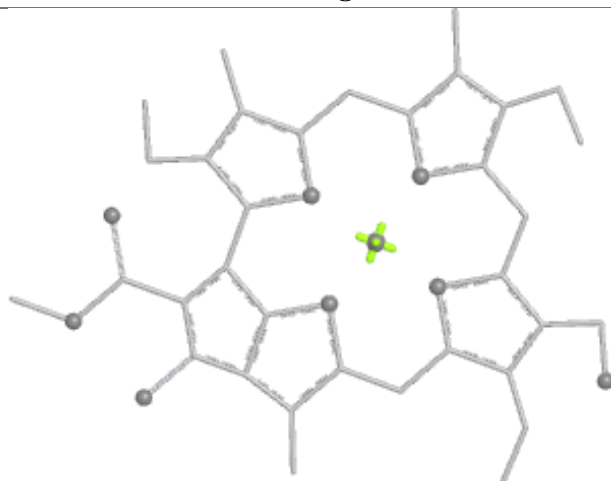
Bond lengths



Bond angles

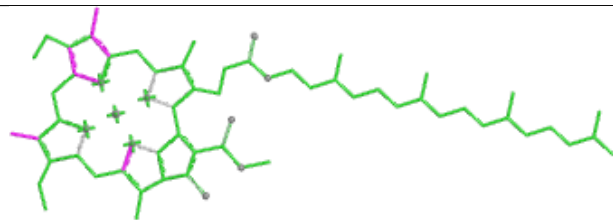


Torsions

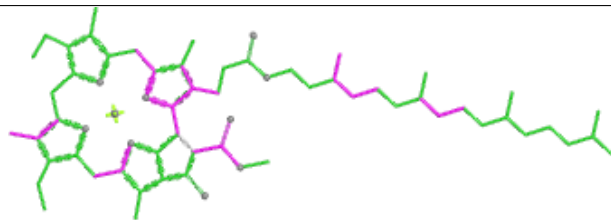


Rings

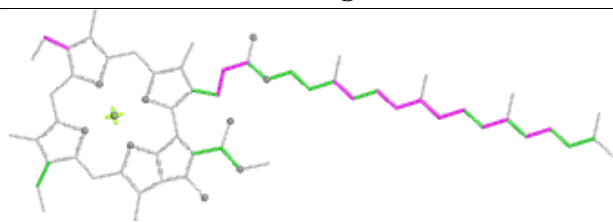
Ligand CLA 2 612



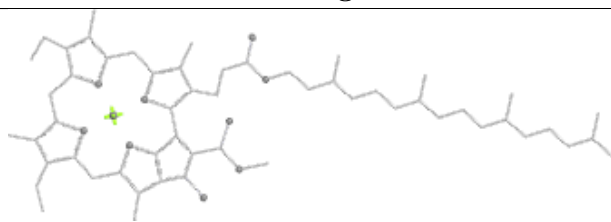
Bond lengths



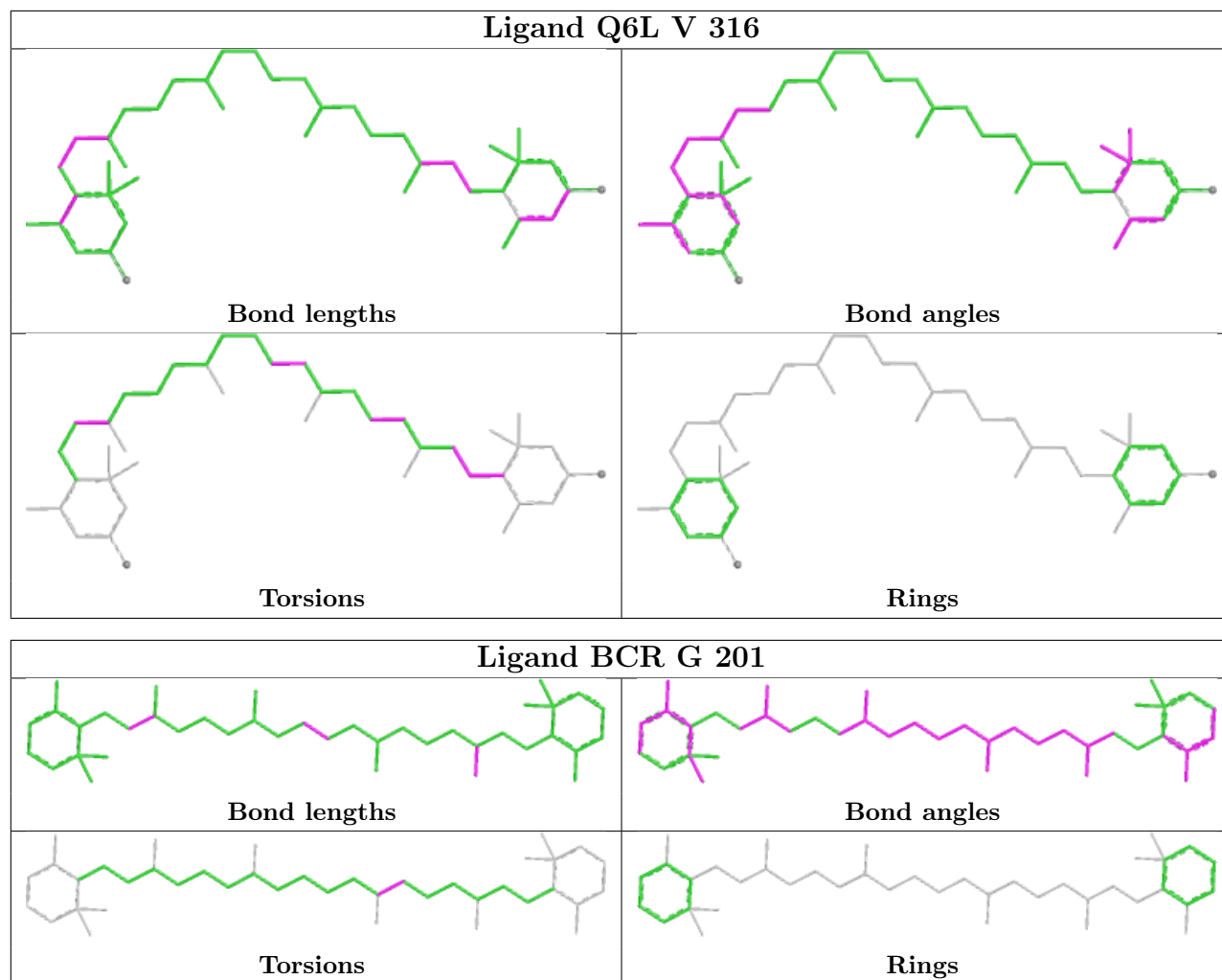
Bond angles



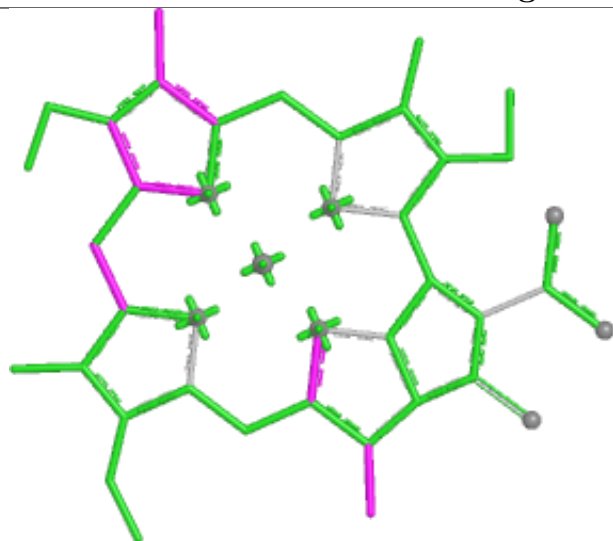
Torsions



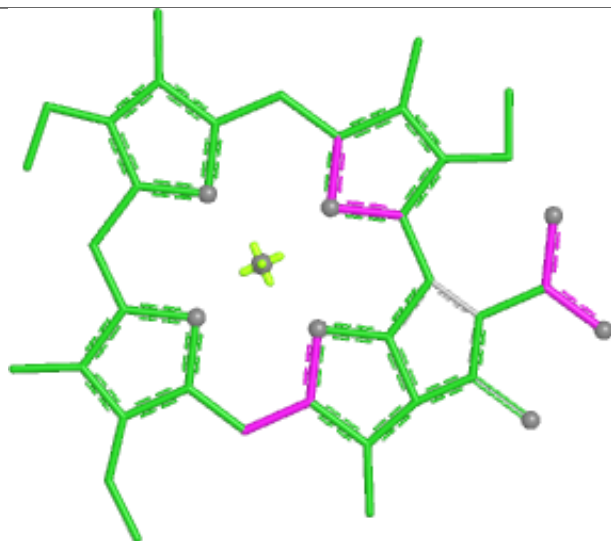
Rings



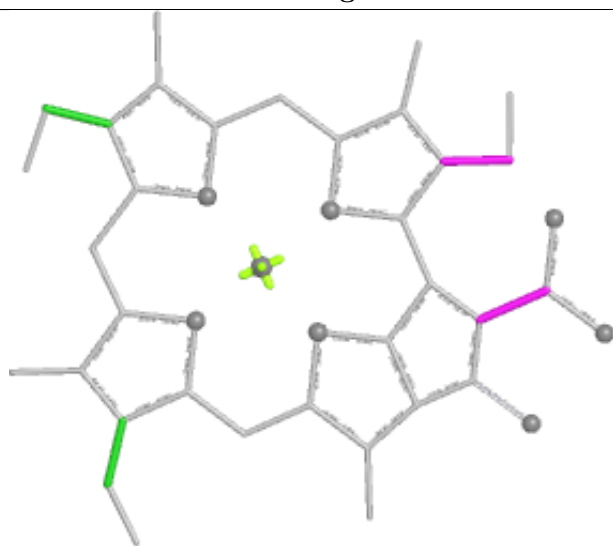
Ligand CLA 1 605



Bond lengths



Bond angles

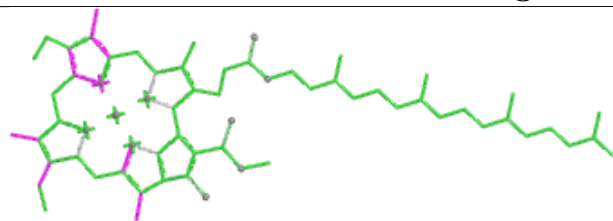


Torsions

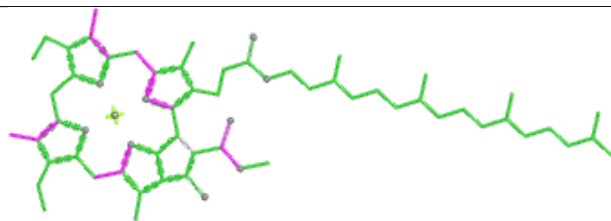


Rings

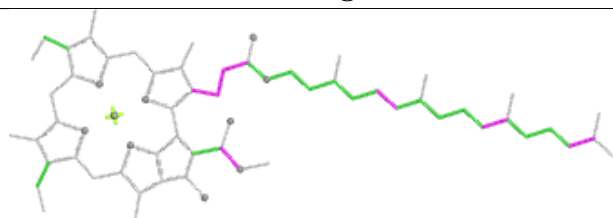
Ligand CLA B 811



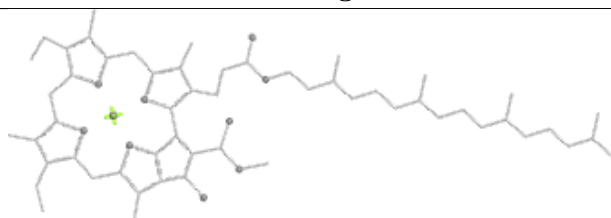
Bond lengths



Bond angles

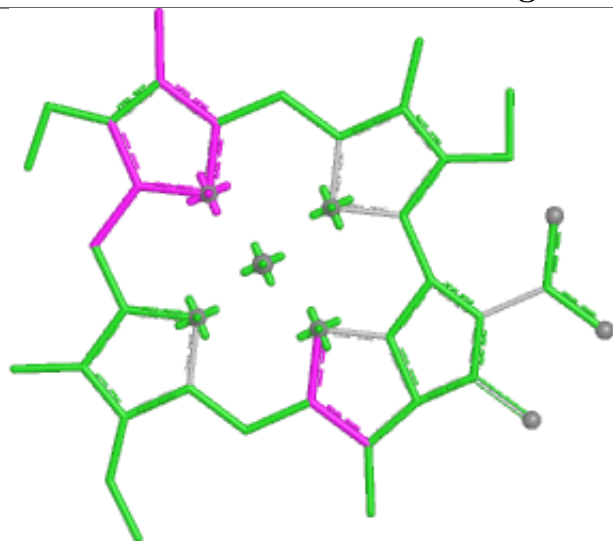


Torsions

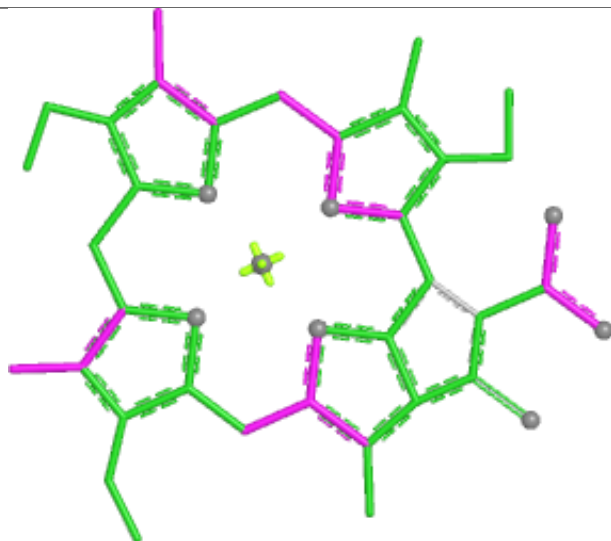


Rings

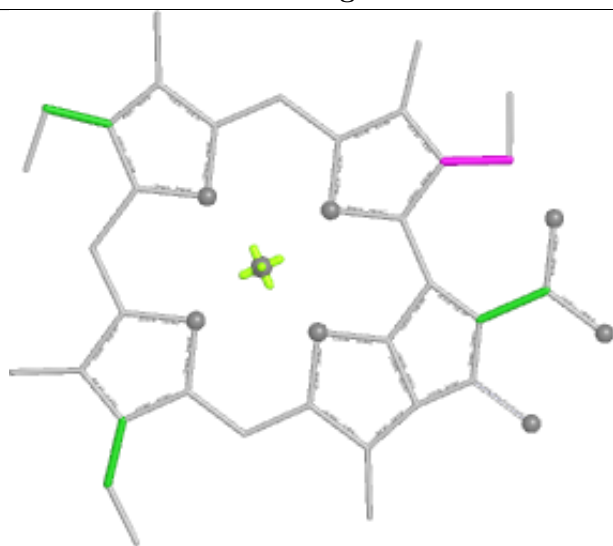
Ligand CLA 3 304



Bond lengths



Bond angles

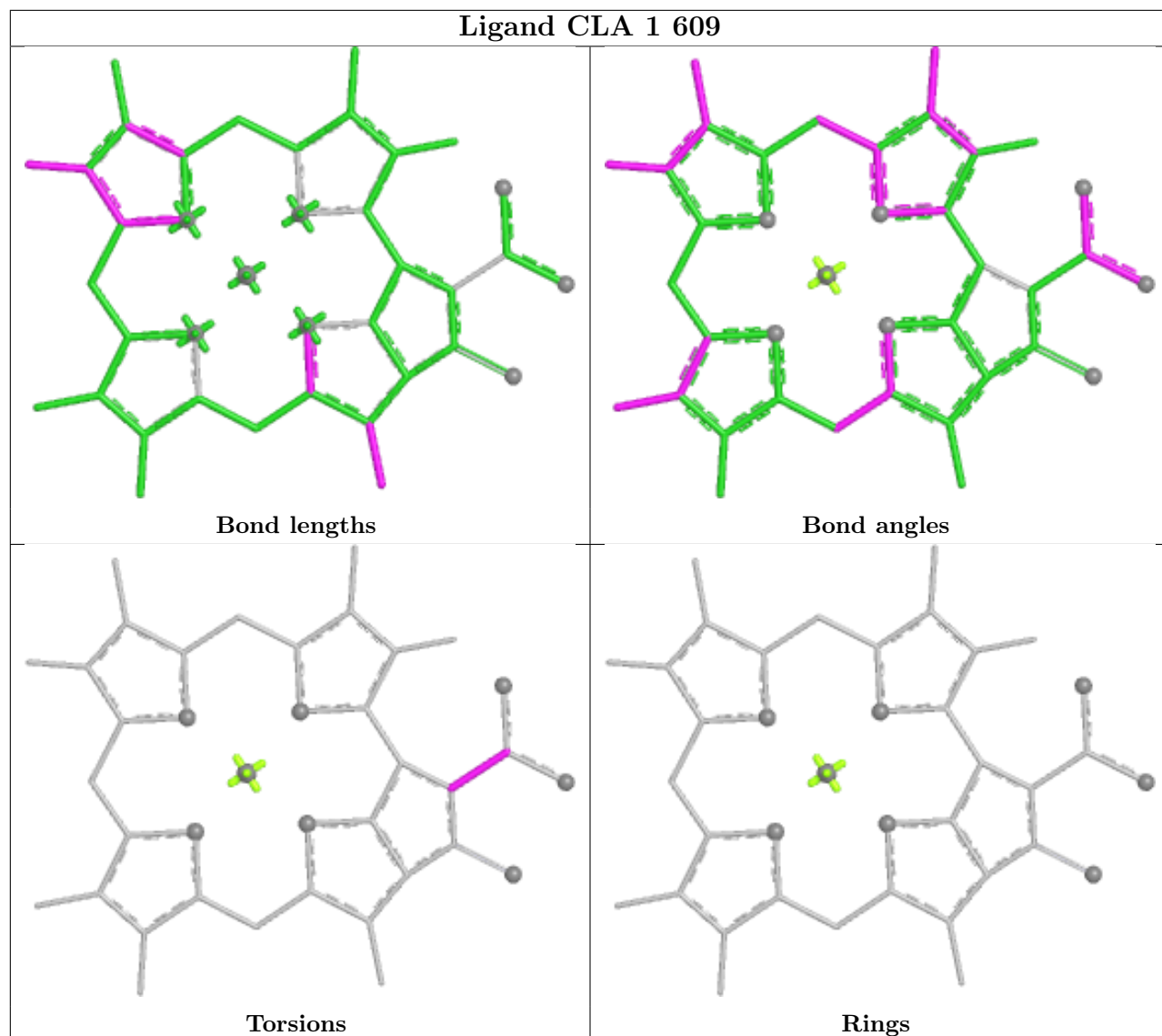


Torsions

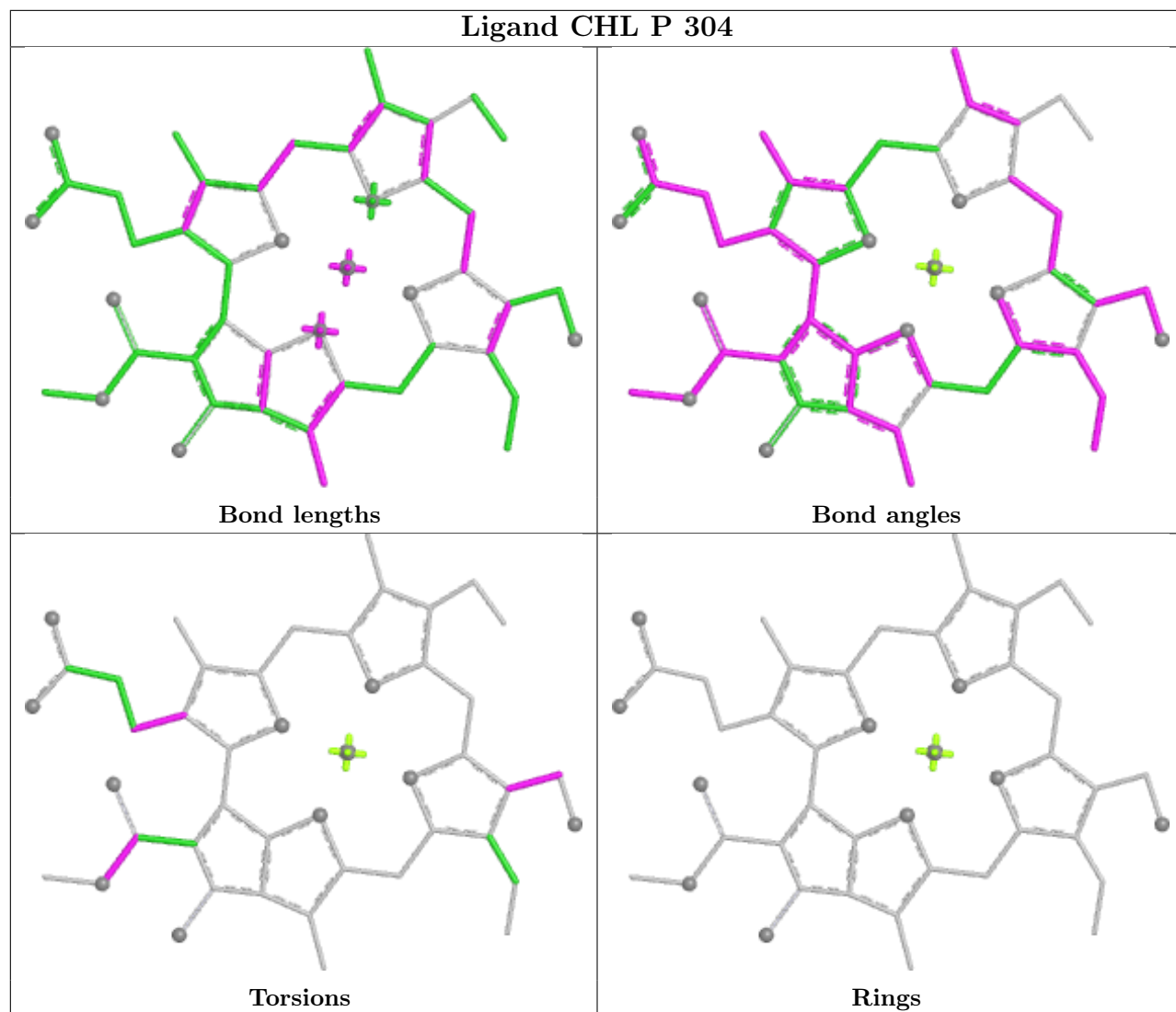


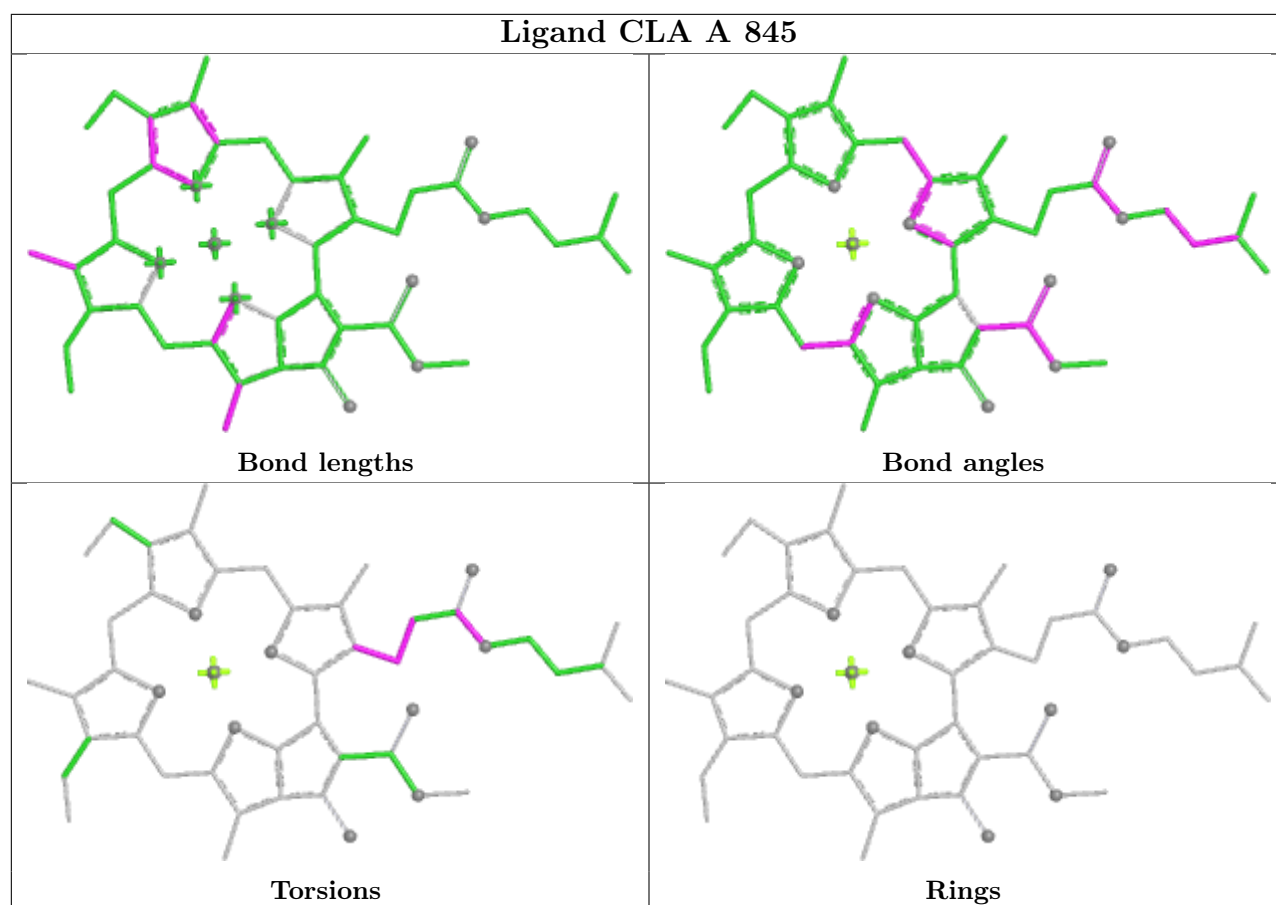
Rings

Ligand CLA 1 609

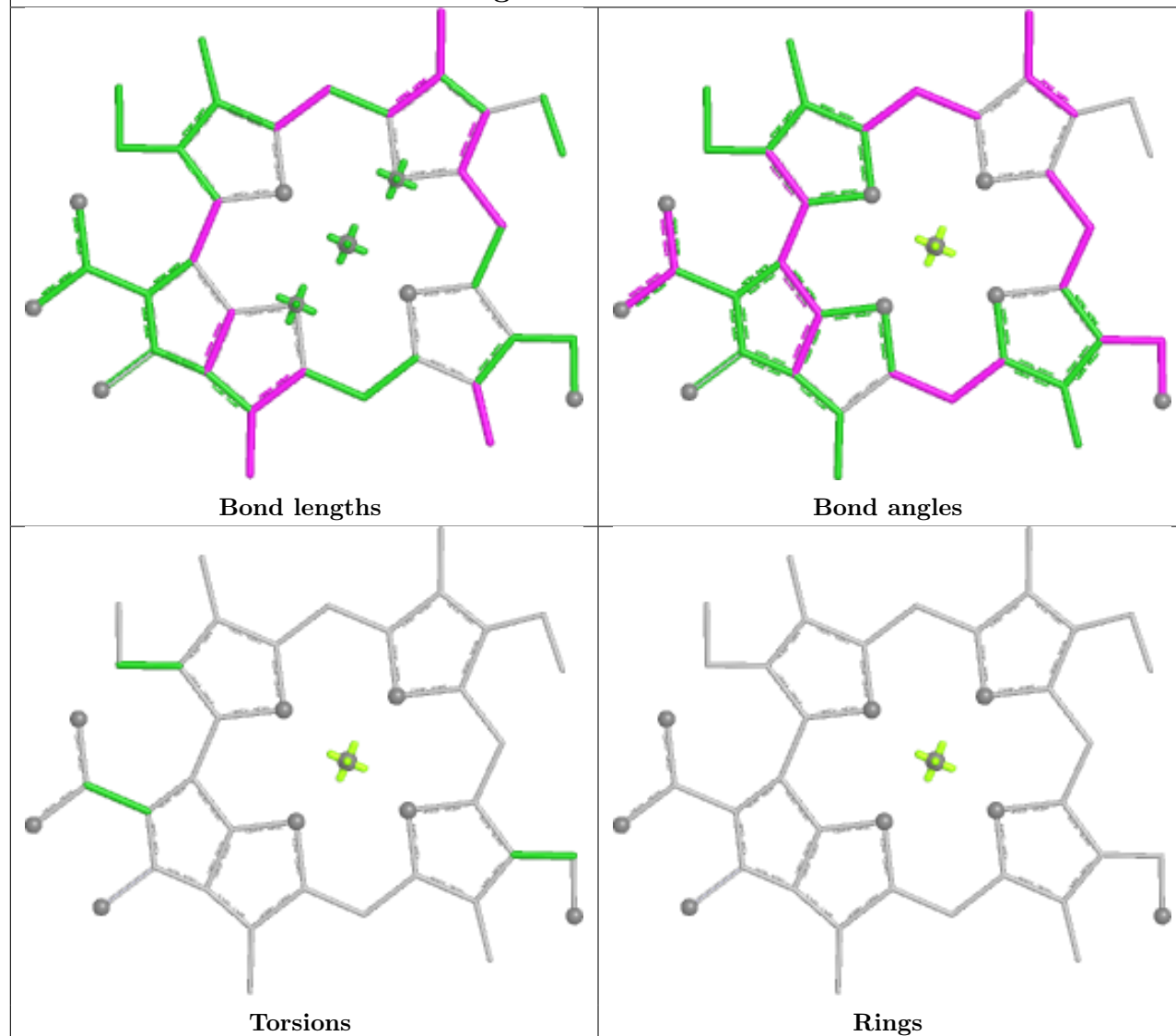


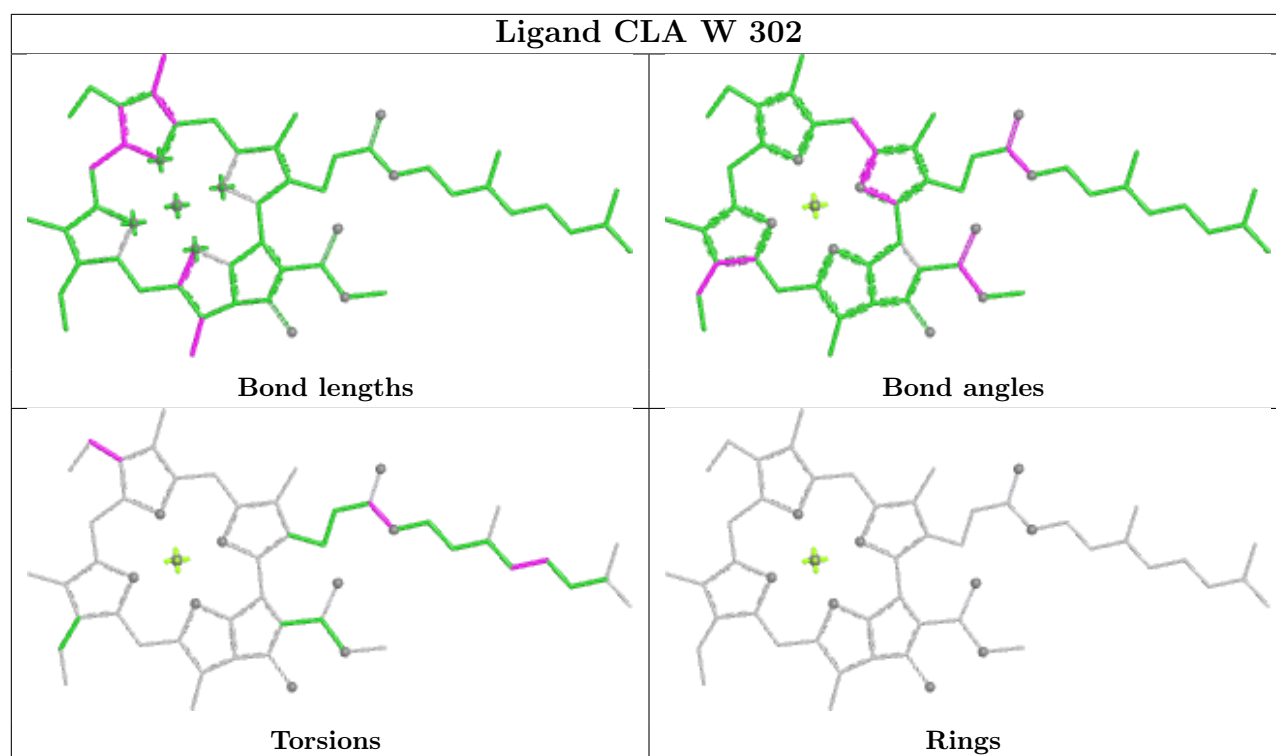
Ligand CHL P 304



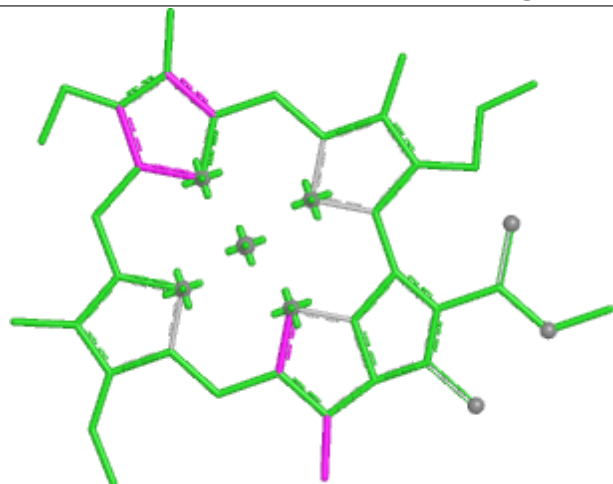


Ligand CHL 4 306

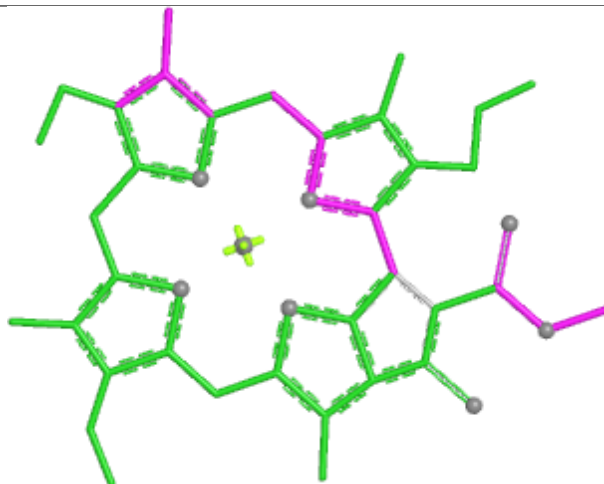




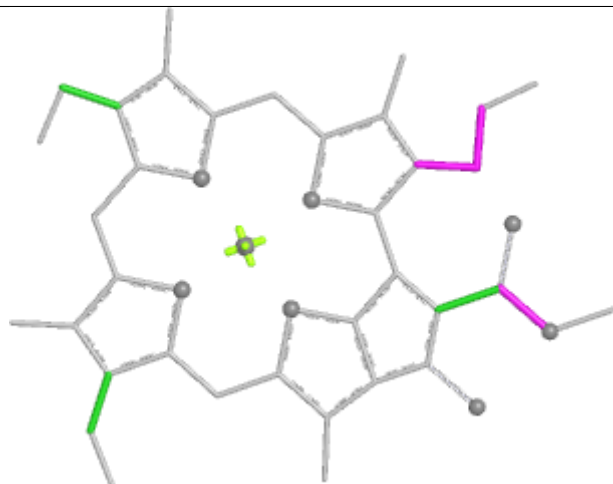
Ligand CLA 3 310



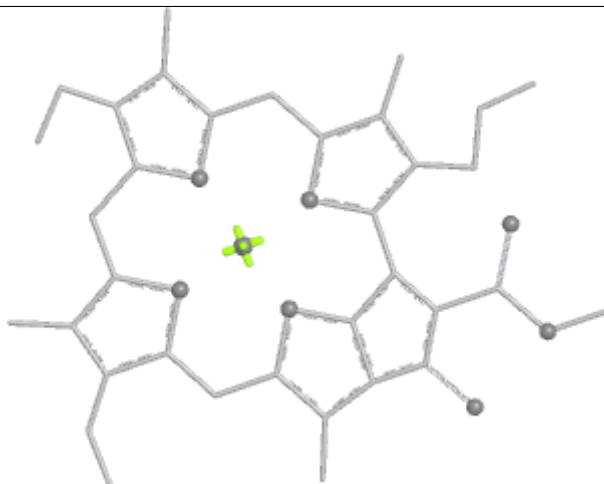
Bond lengths



Bond angles

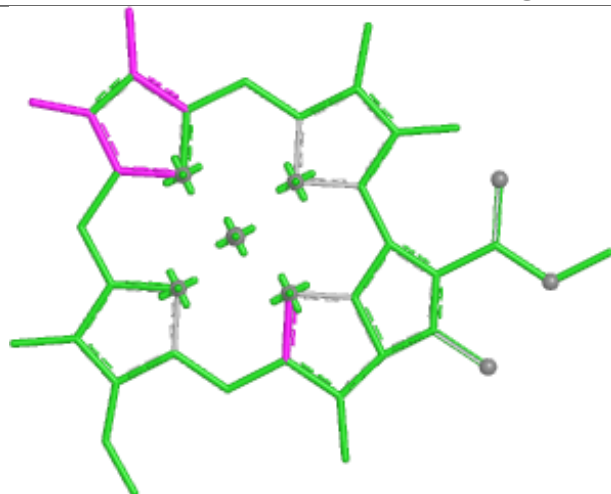


Torsions

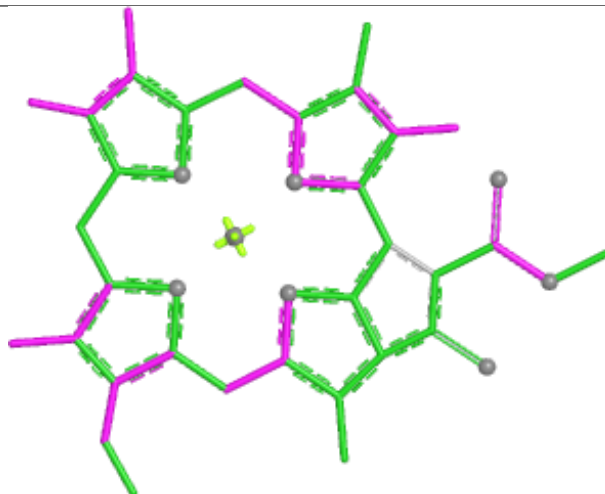


Rings

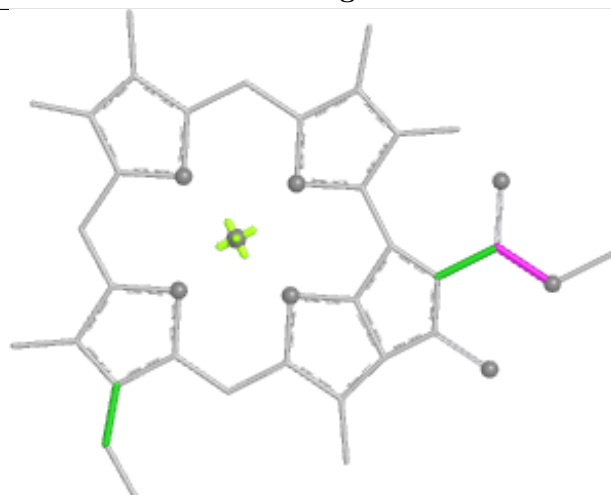
Ligand CLA 1 606



Bond lengths



Bond angles

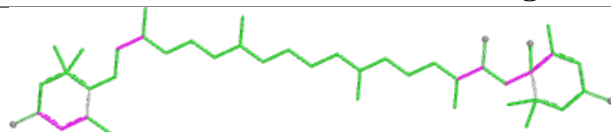


Torsions

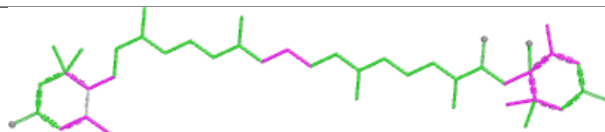


Rings

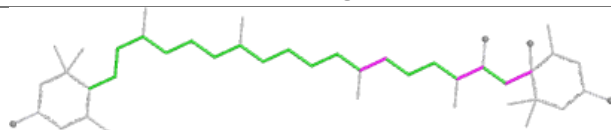
Ligand IWJ 4 317



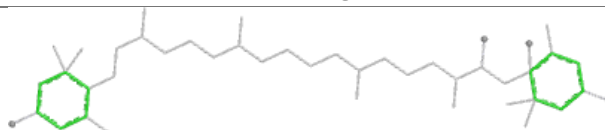
Bond lengths



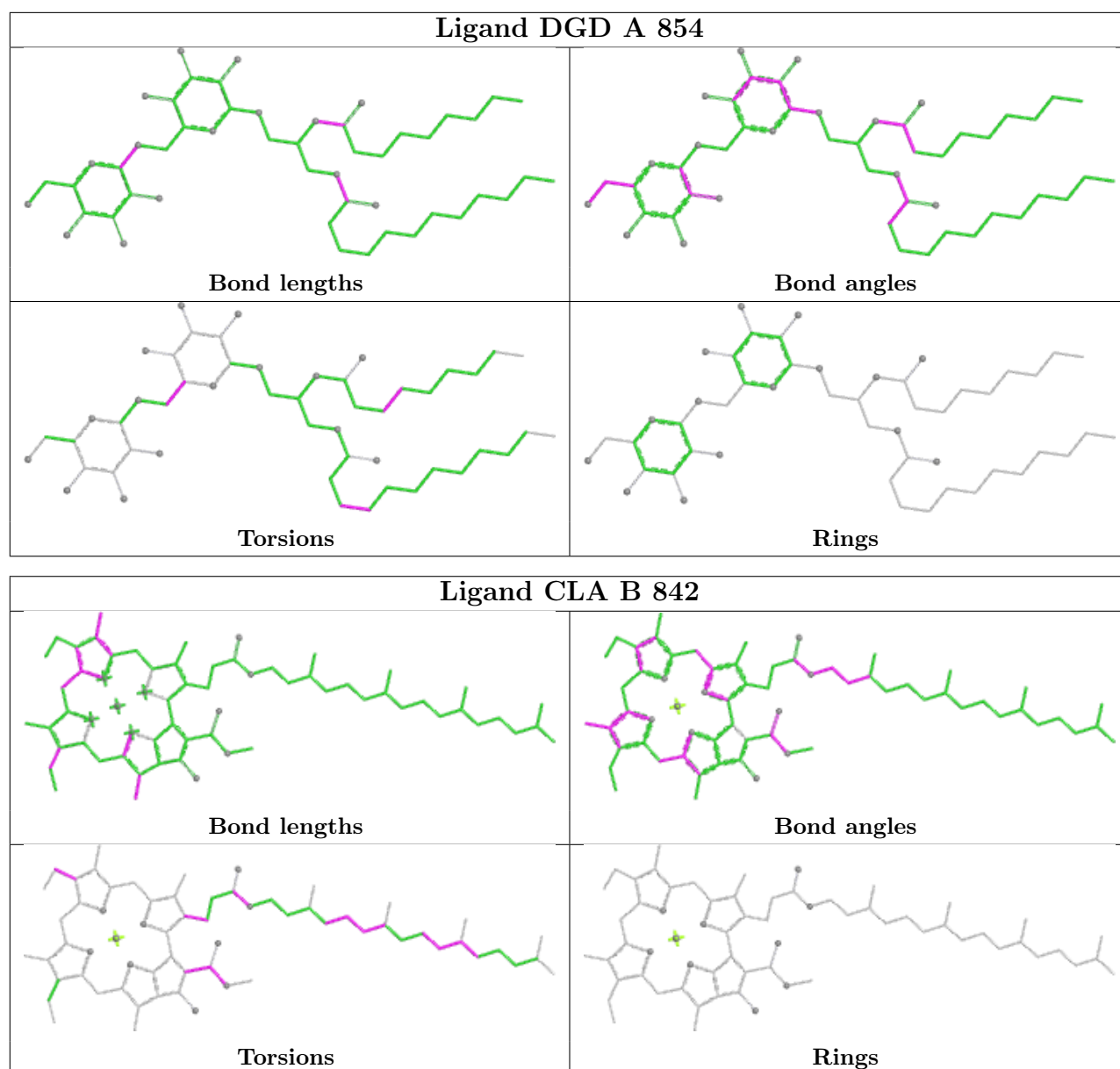
Bond angles



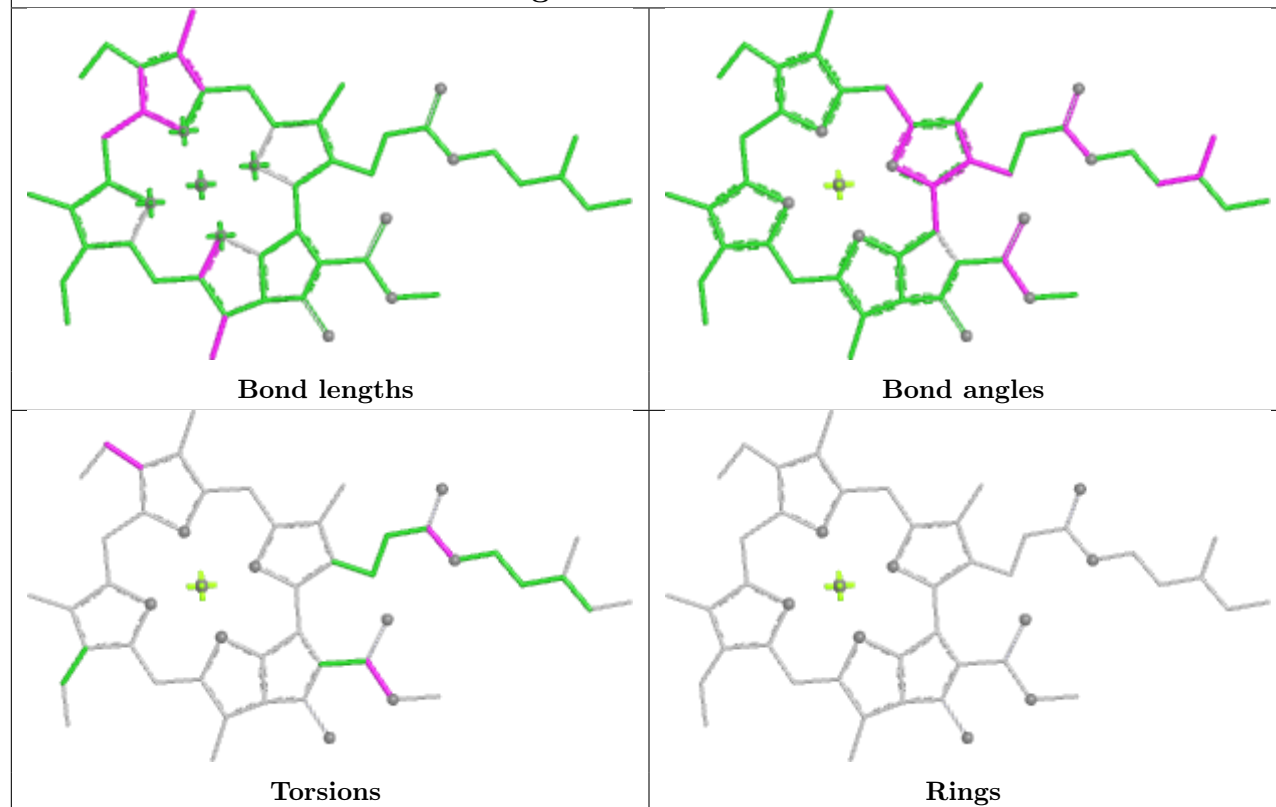
Torsions



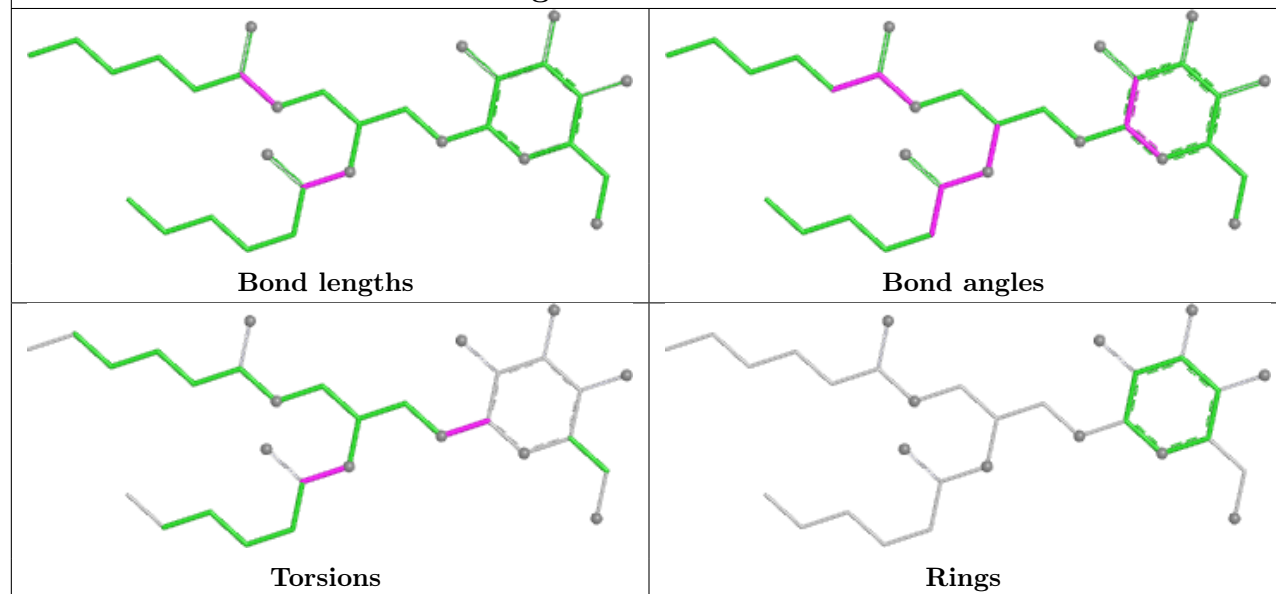
Rings



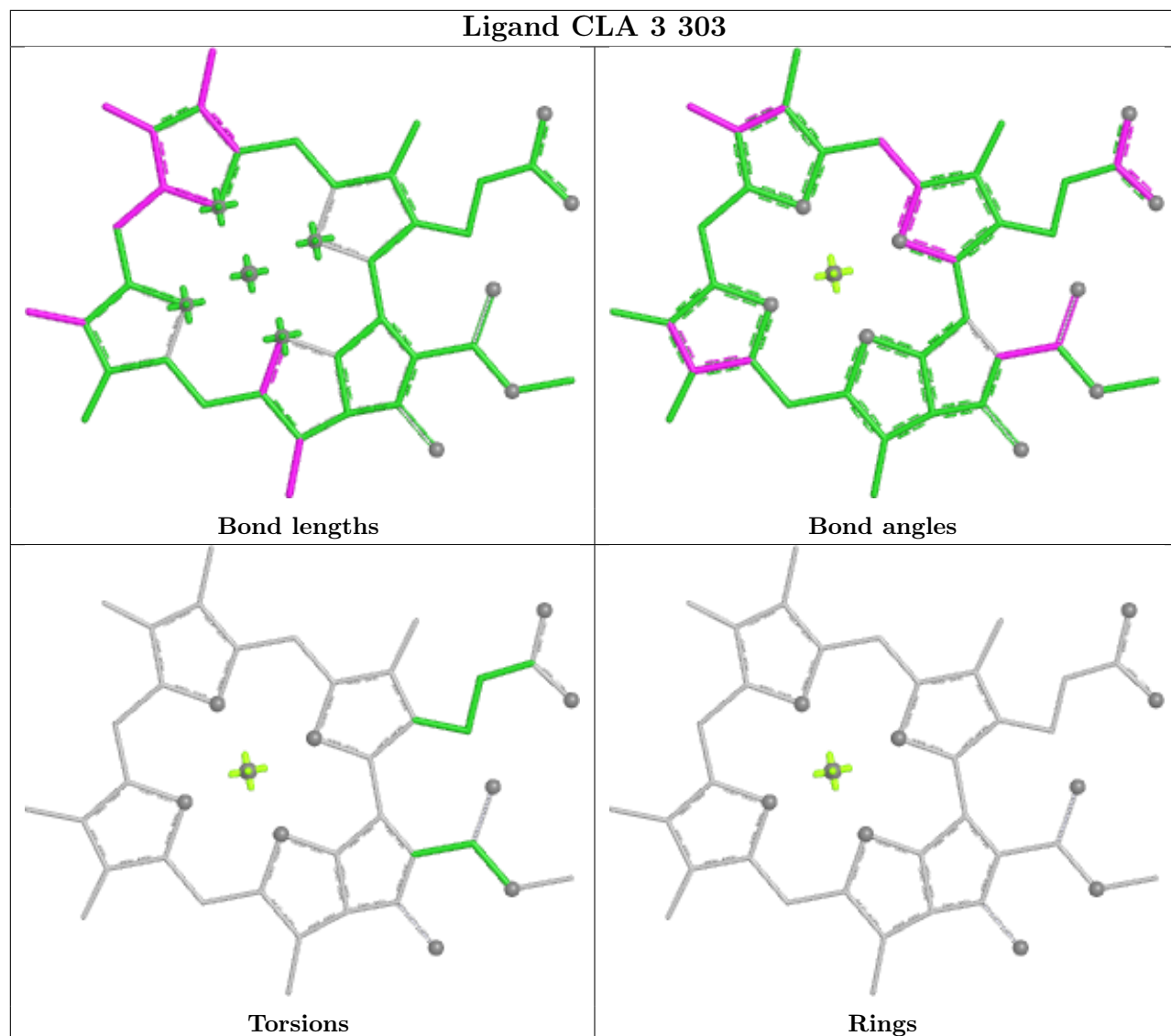
Ligand CLA X 312



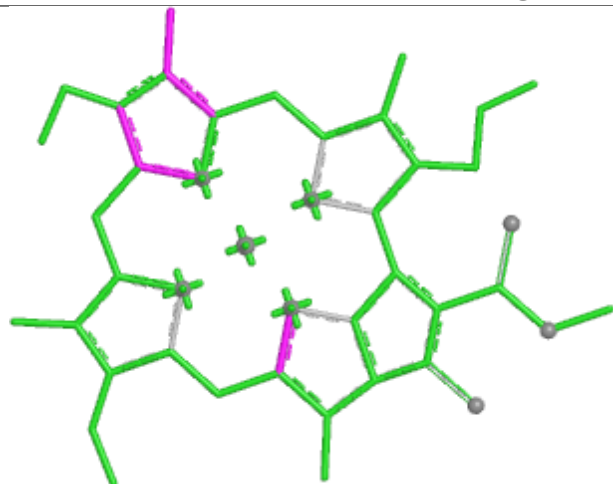
Ligand LMG 2 620



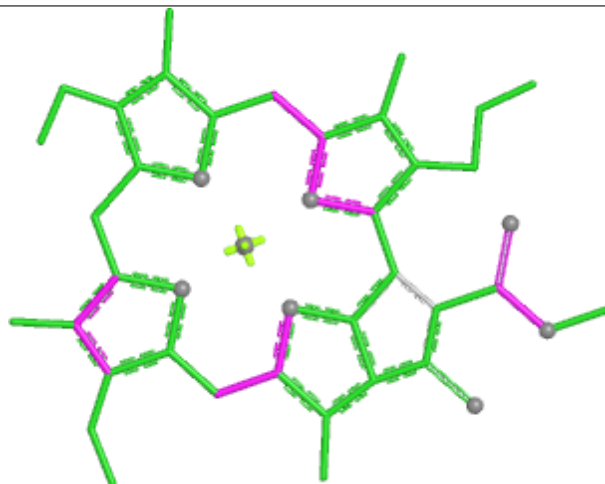
Ligand CLA 3 303



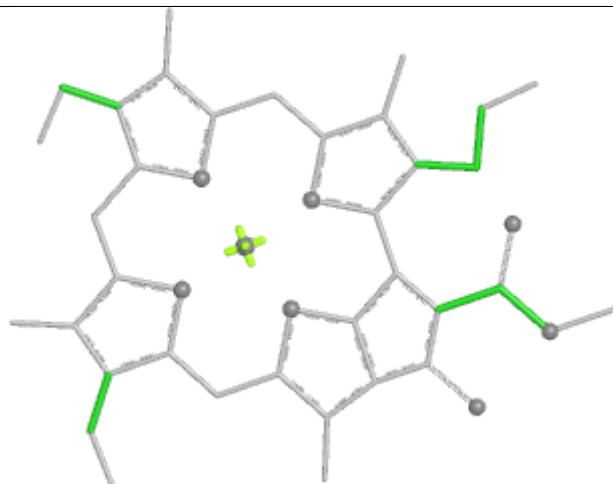
Ligand CLA B 833



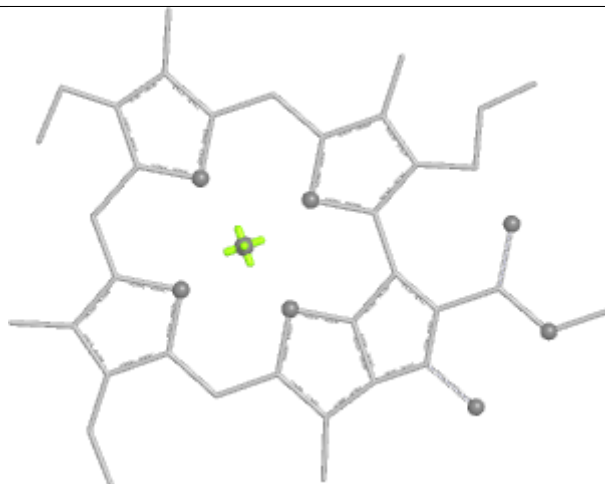
Bond lengths



Bond angles

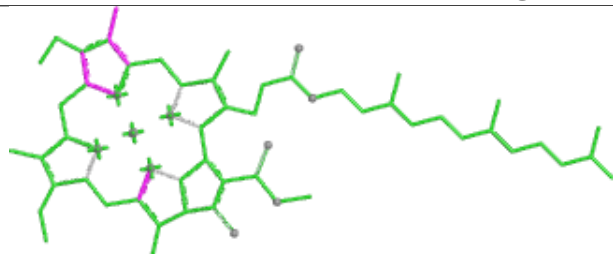


Torsions

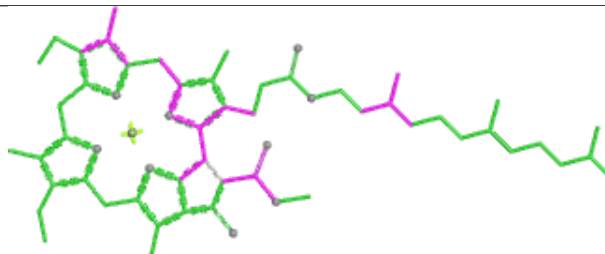


Rings

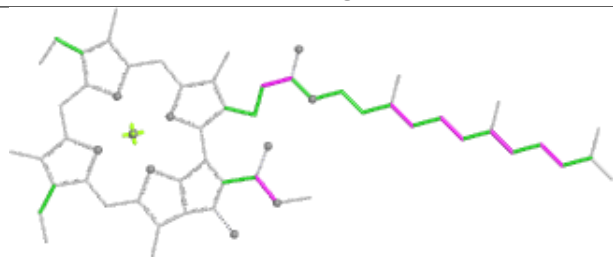
Ligand CLA V 301



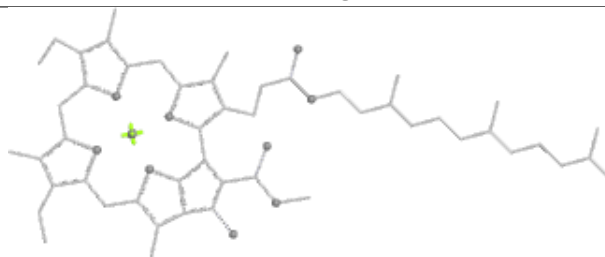
Bond lengths



Bond angles

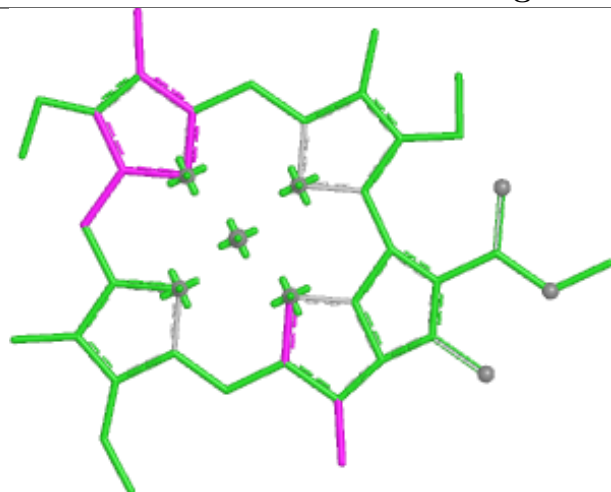


Torsions

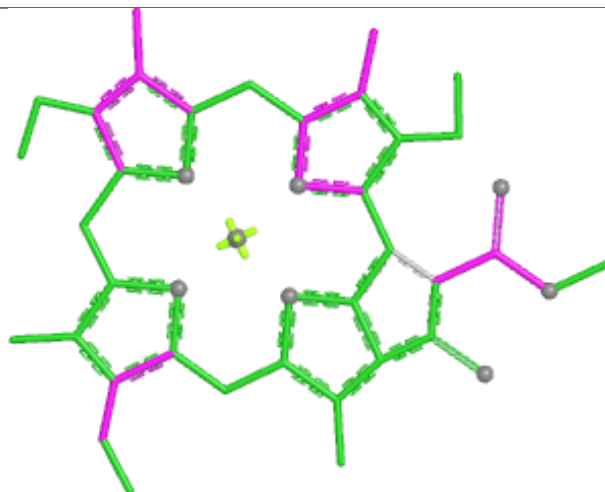


Rings

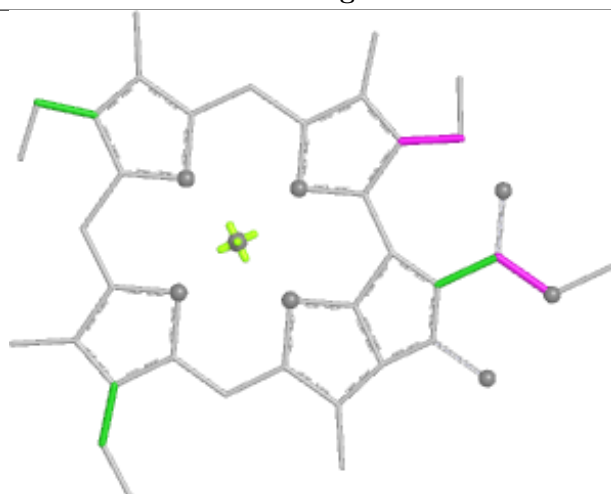
Ligand CLA X 304



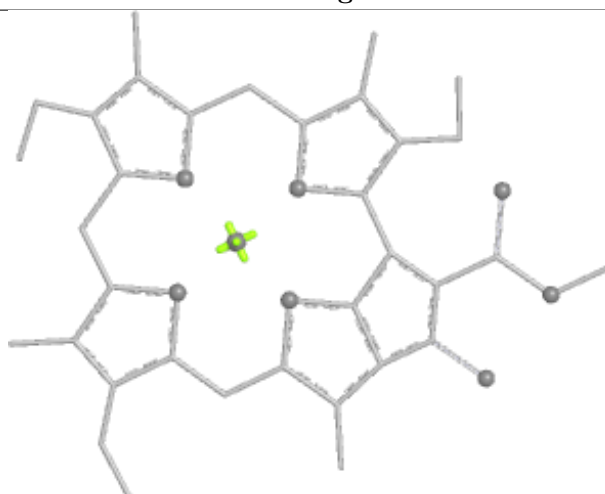
Bond lengths



Bond angles

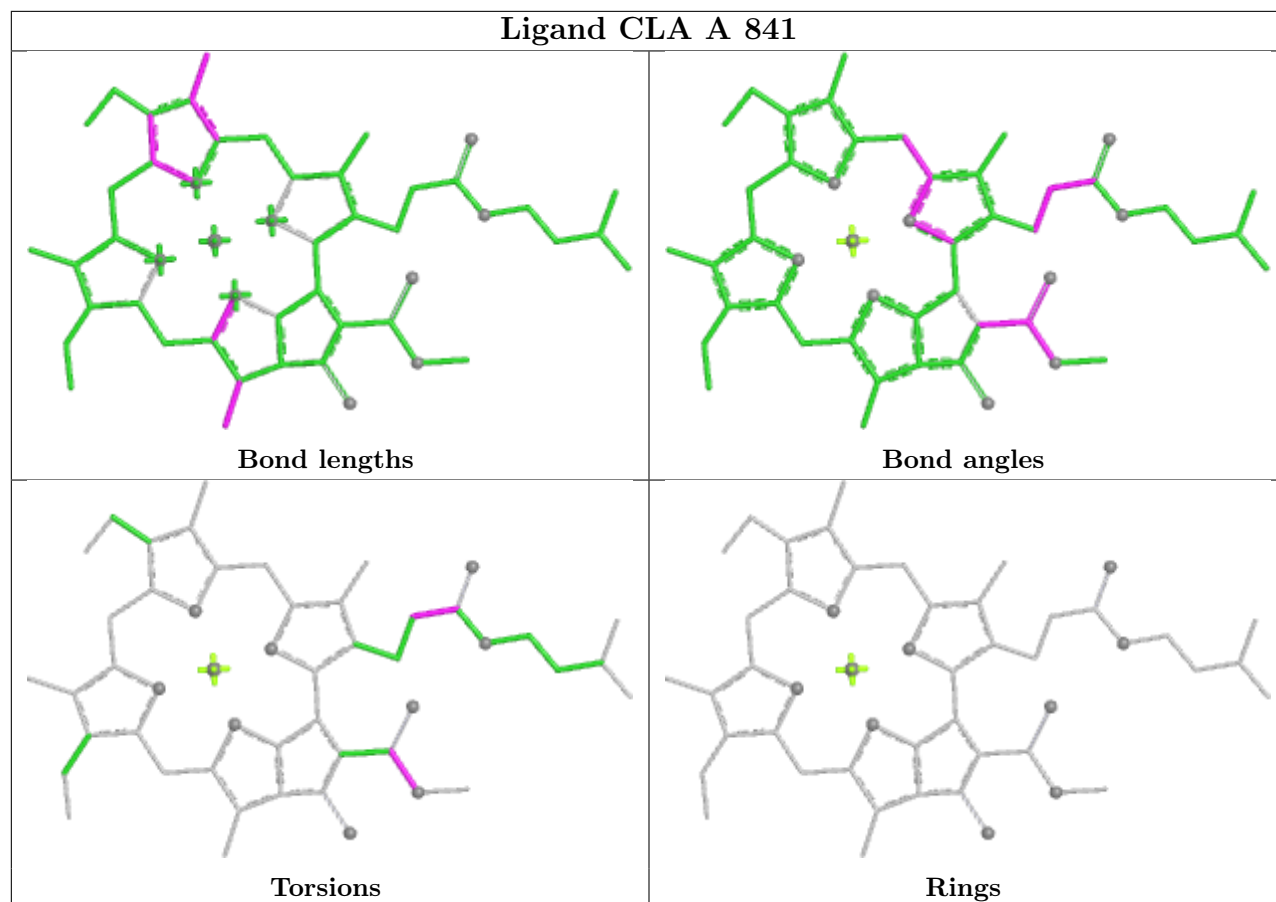


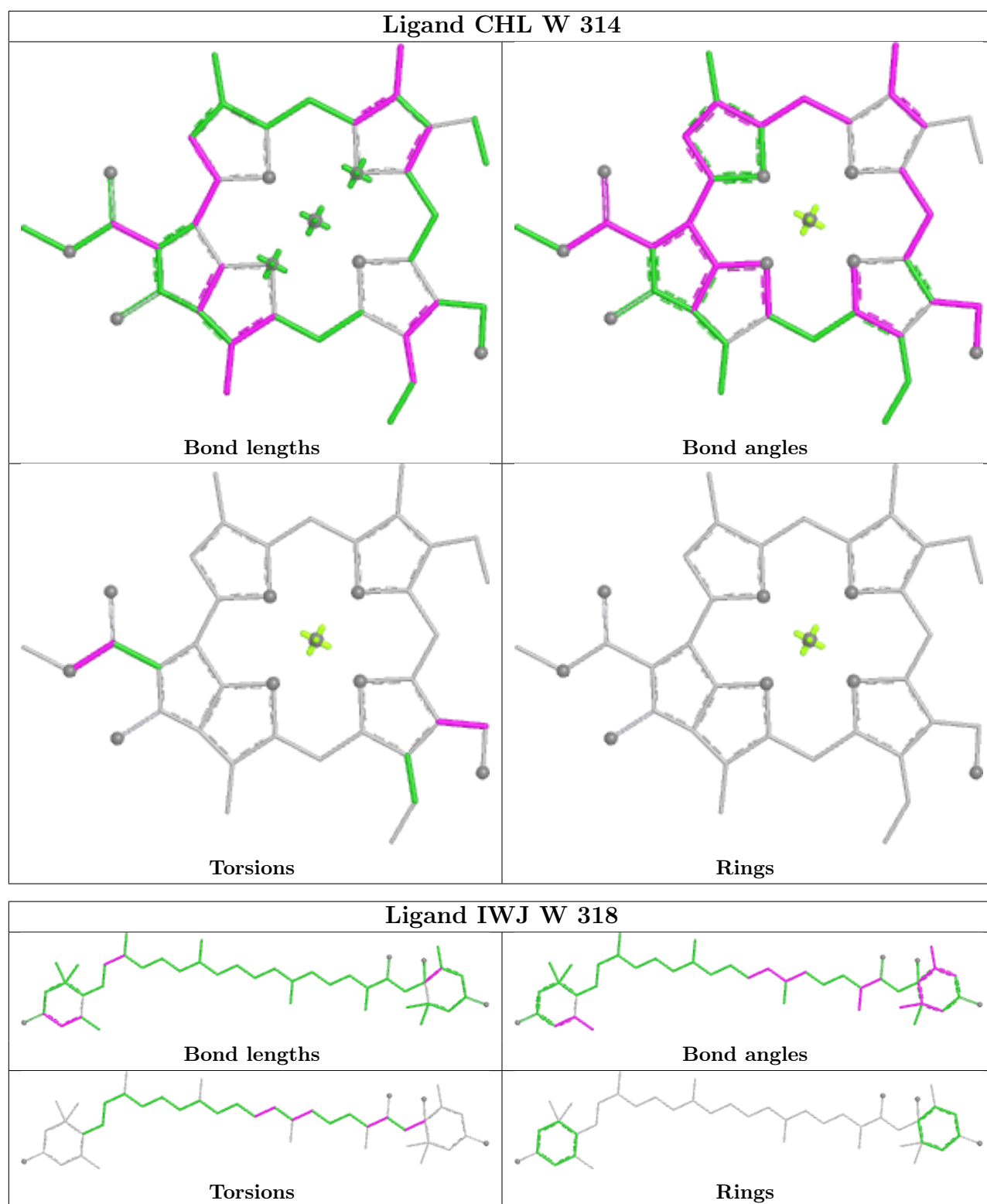
Torsions

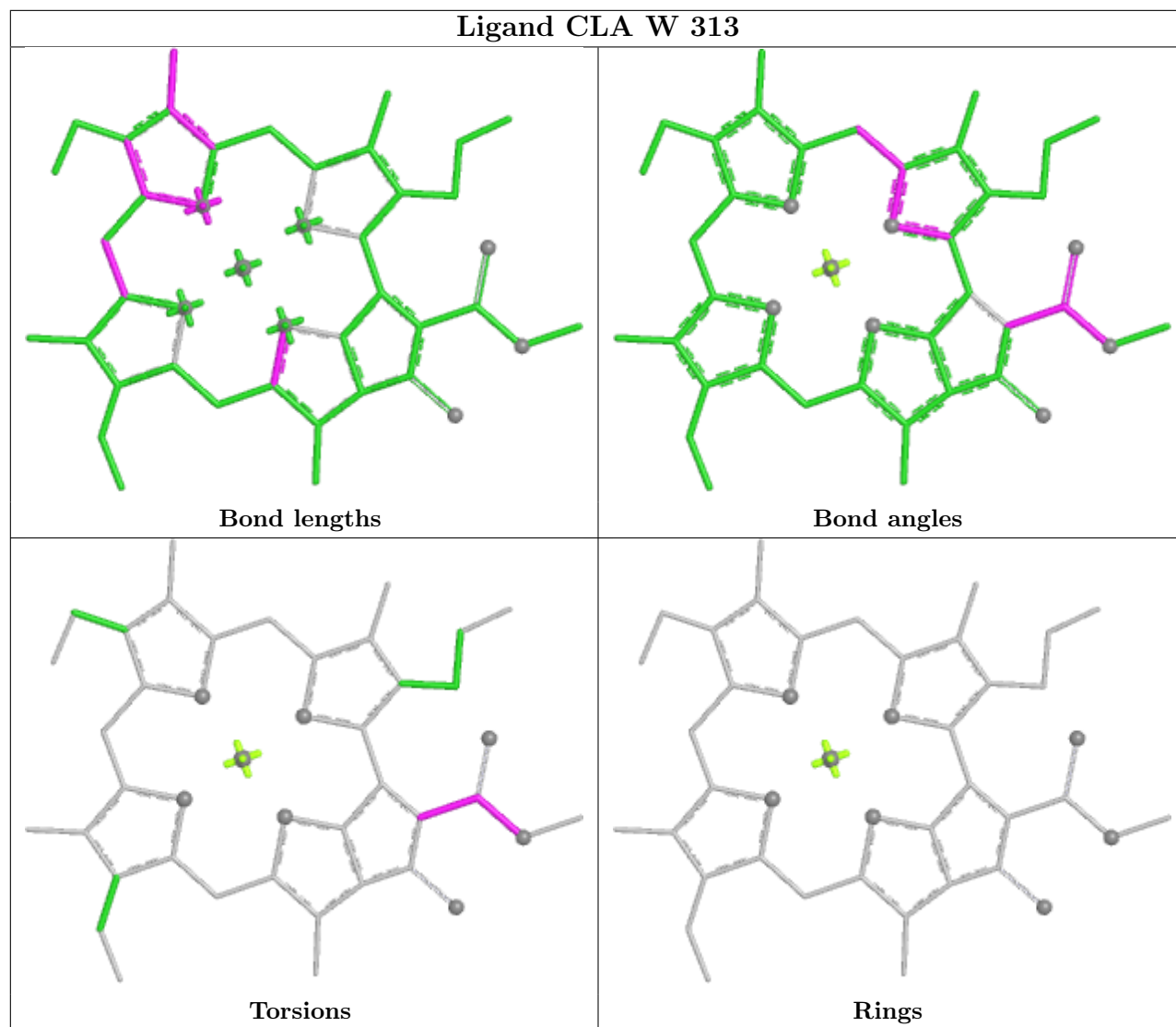


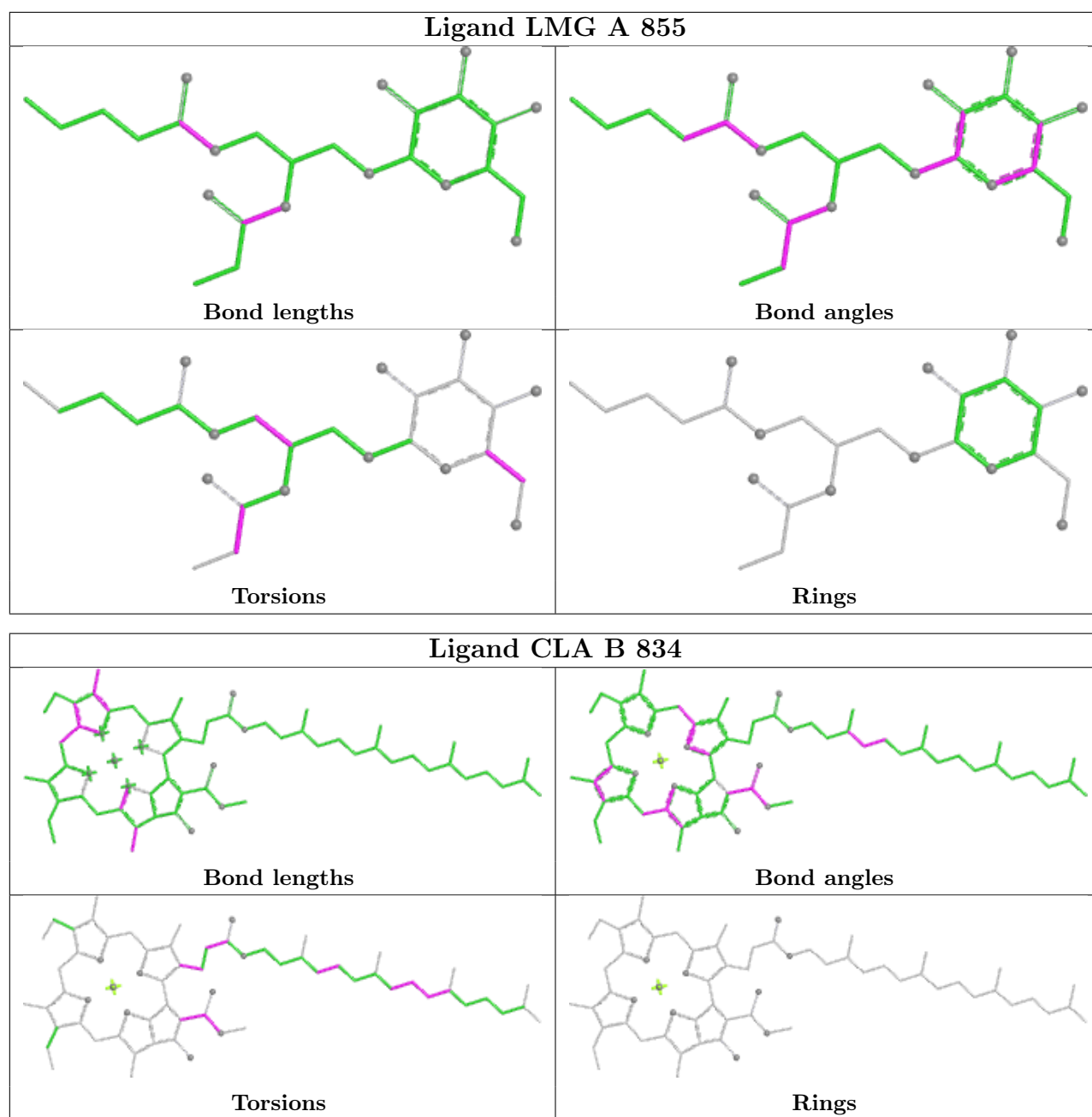
Rings

Ligand CLA A 841

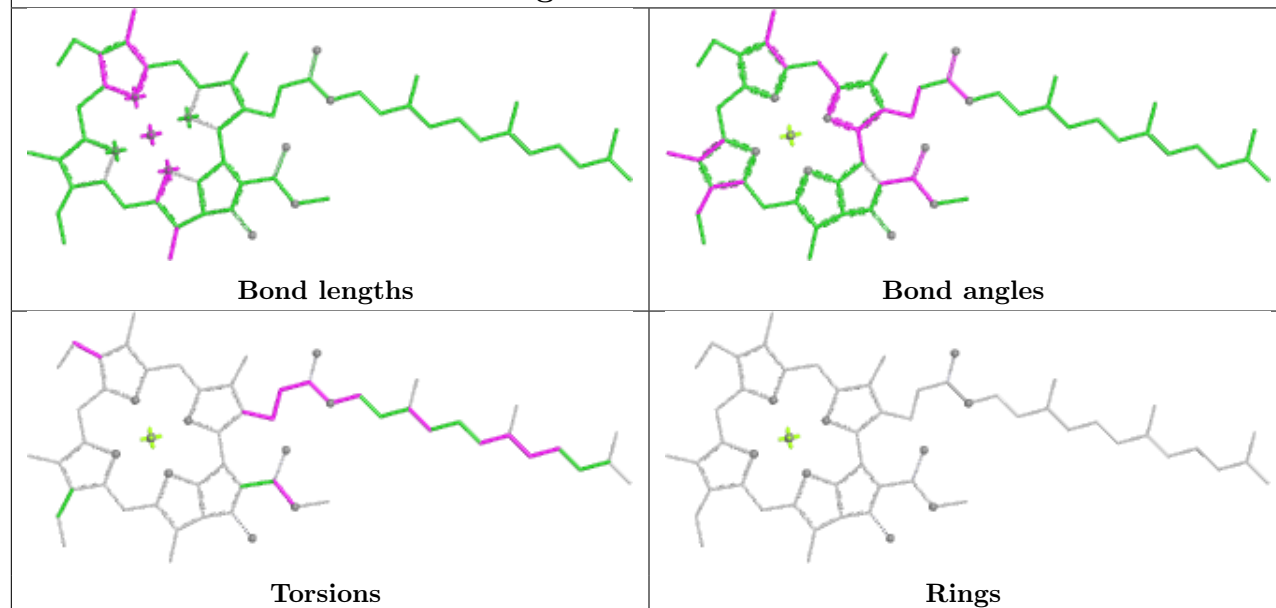




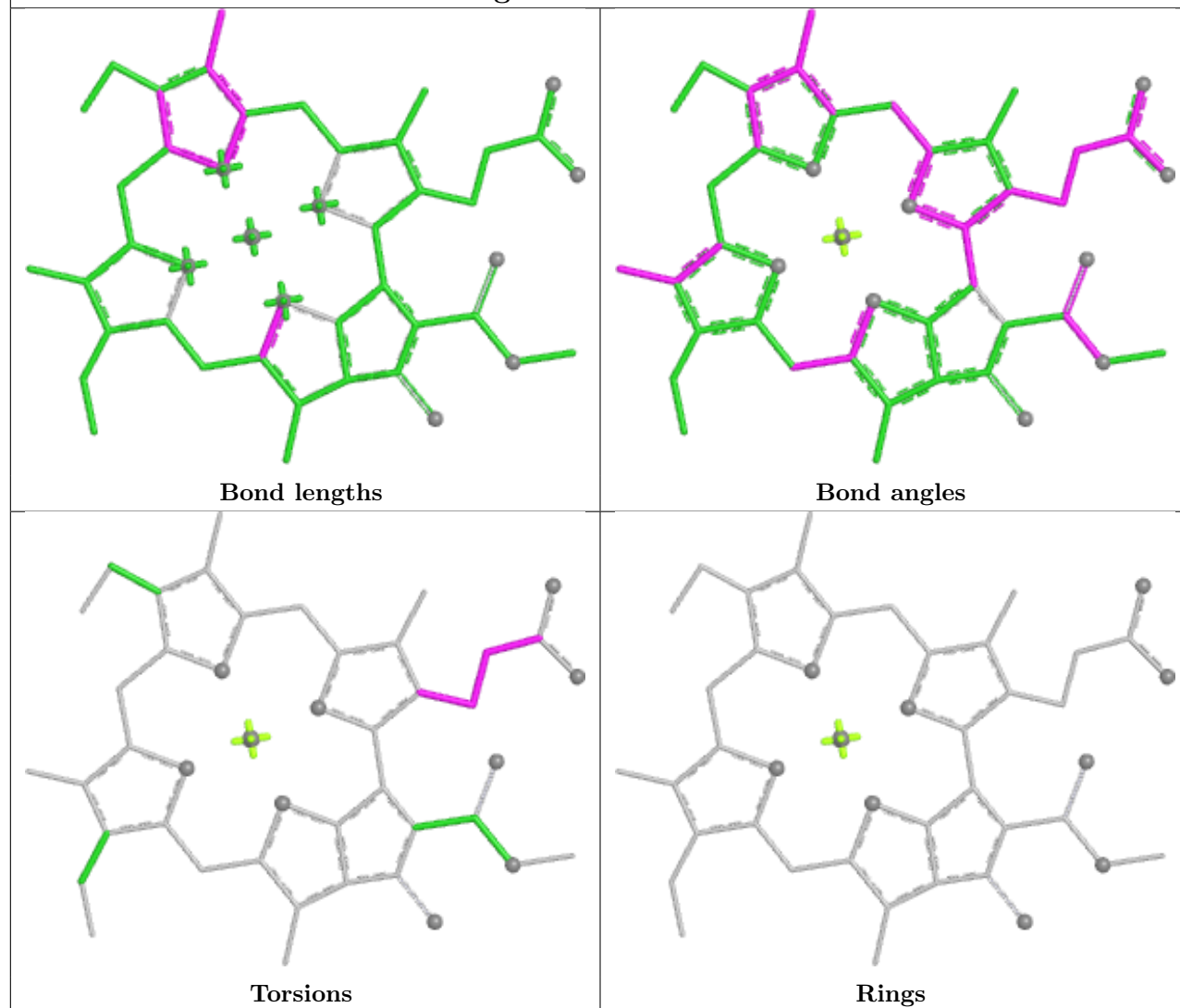


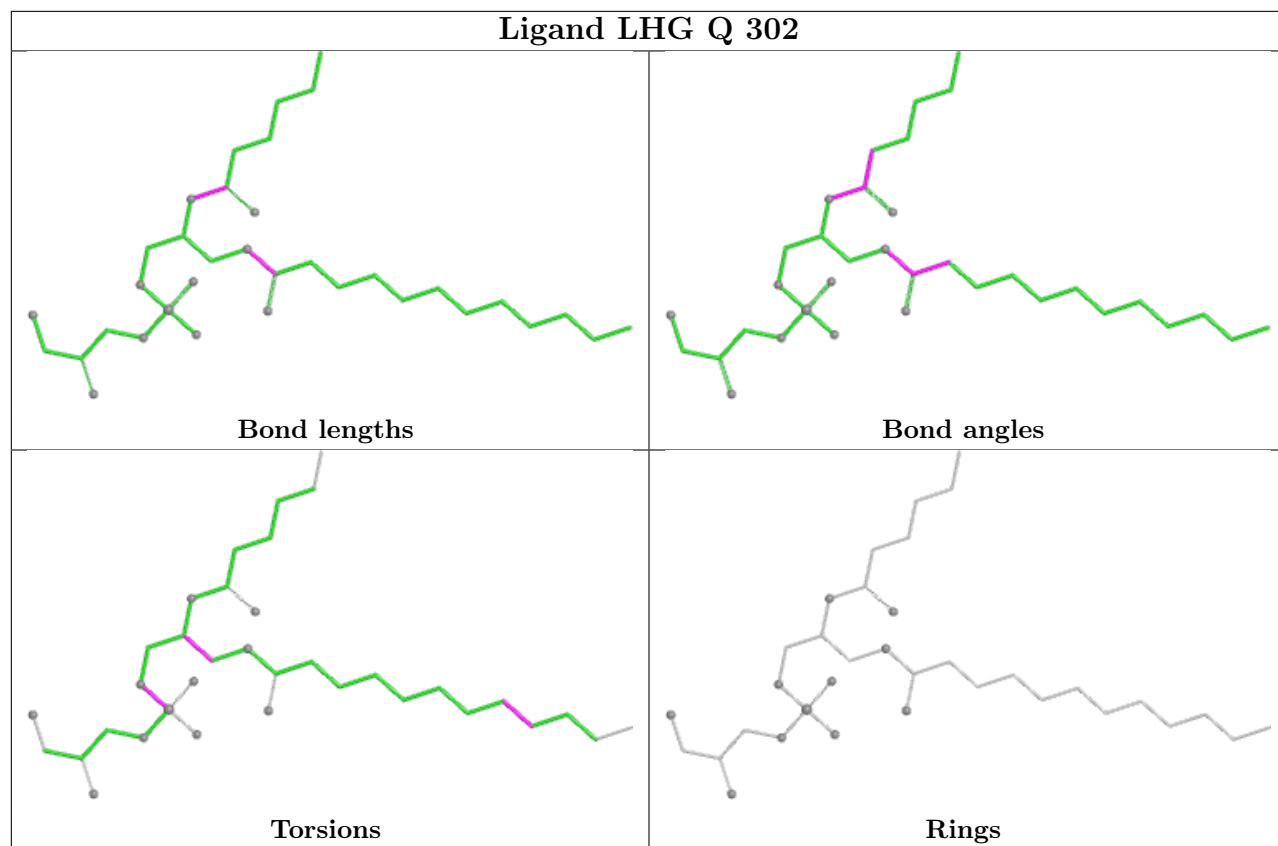


Ligand CLA 4 303

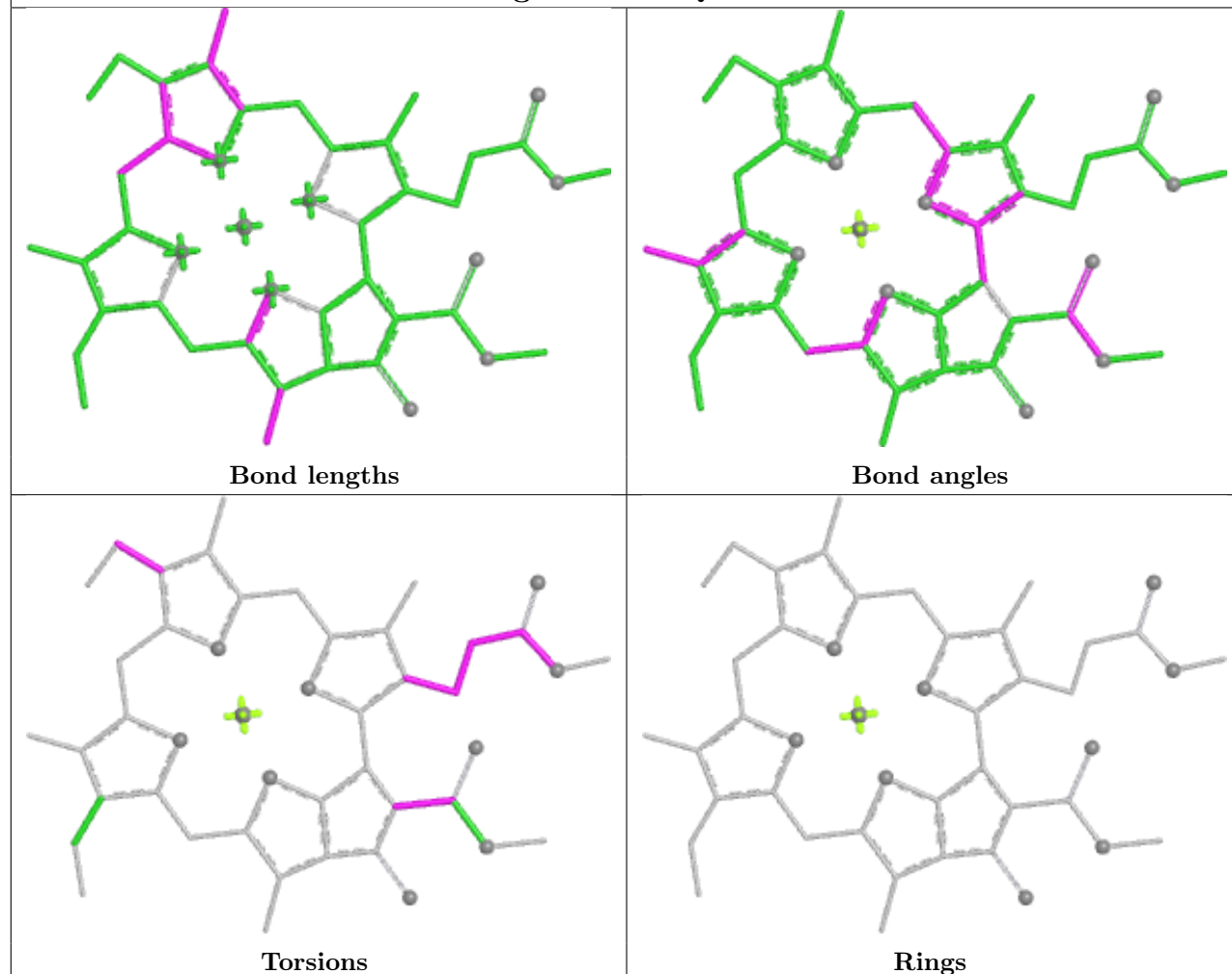


Ligand CLA L 303

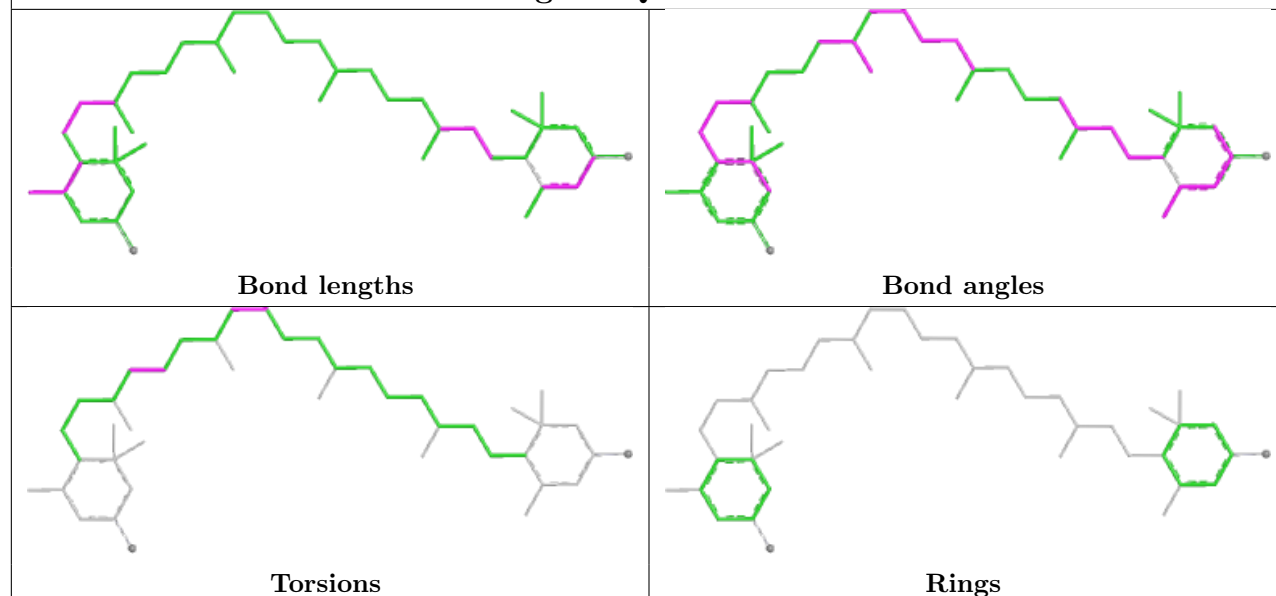




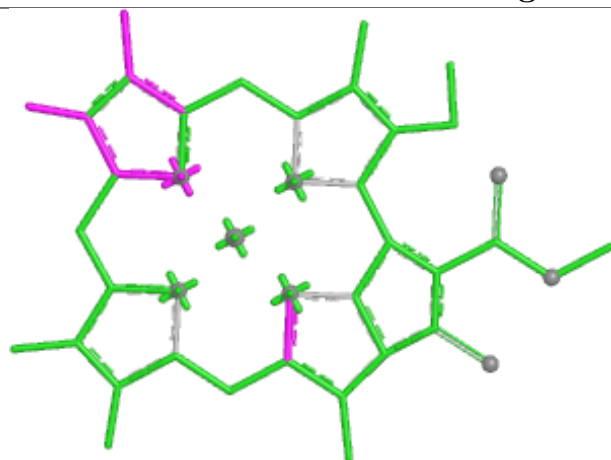
Ligand CLA Q 313



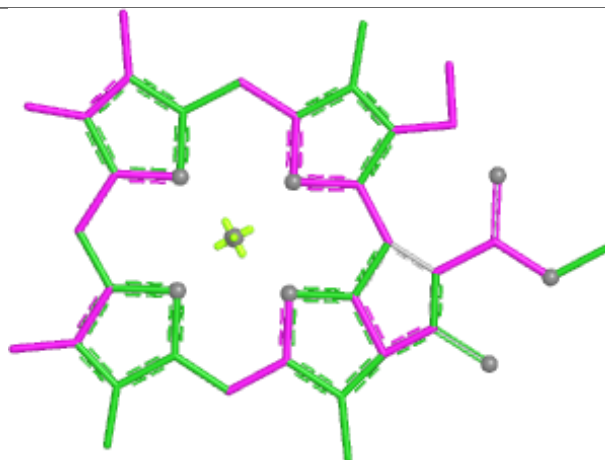
Ligand Q6L U 315



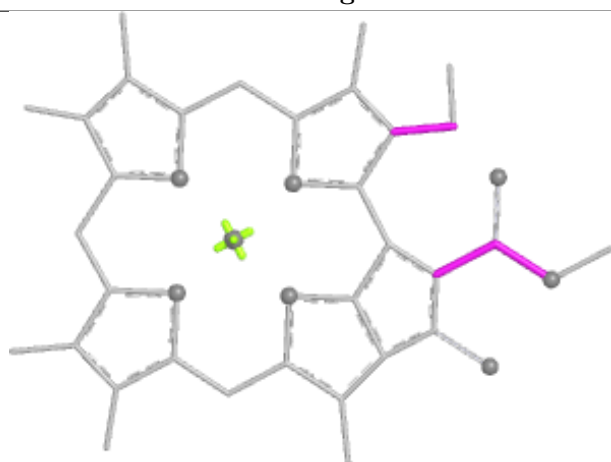
Ligand CLA 1 610



Bond lengths



Bond angles

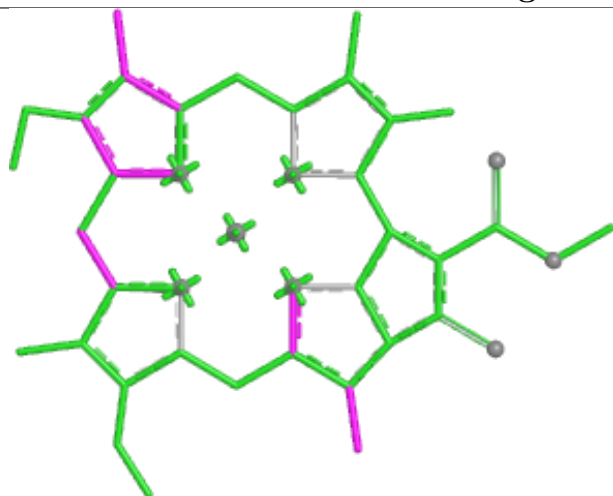


Torsions

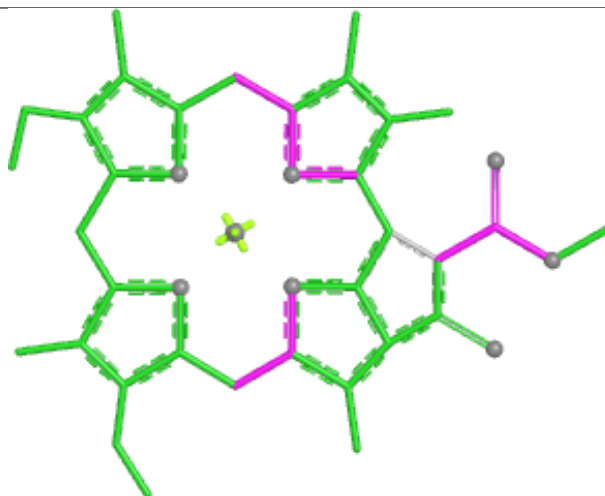


Rings

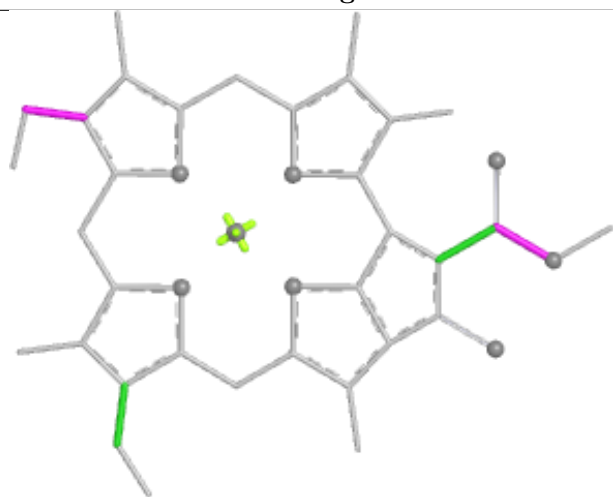
Ligand CLA 5 610



Bond lengths



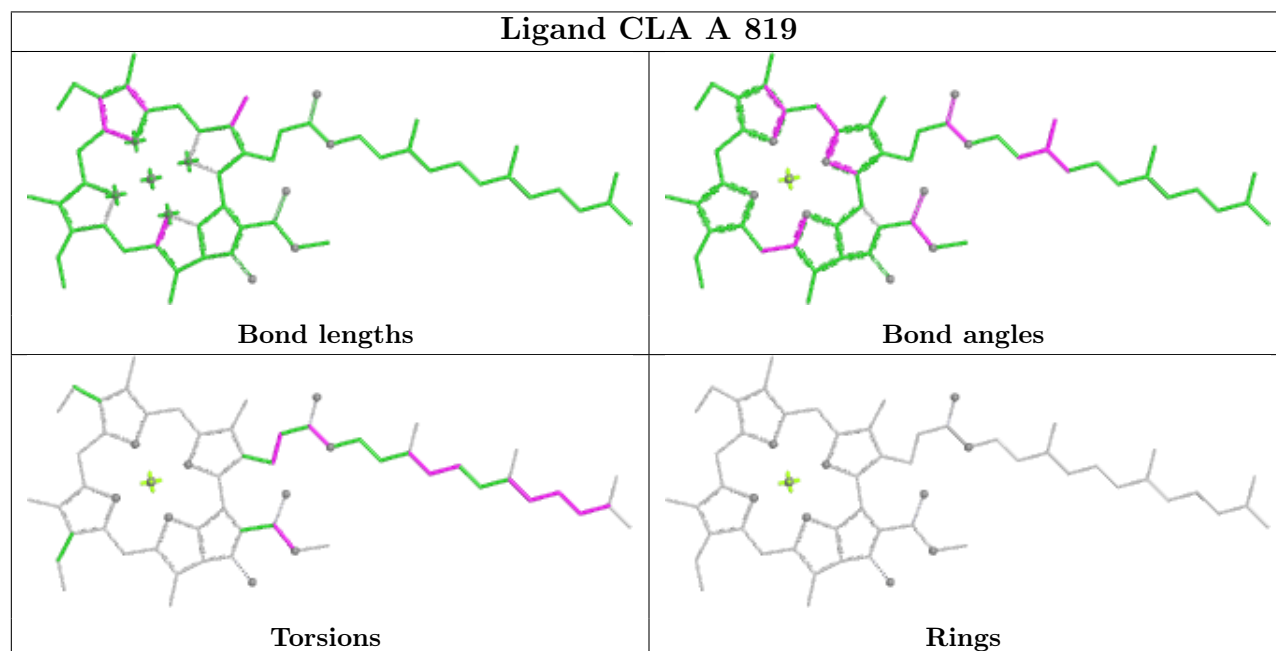
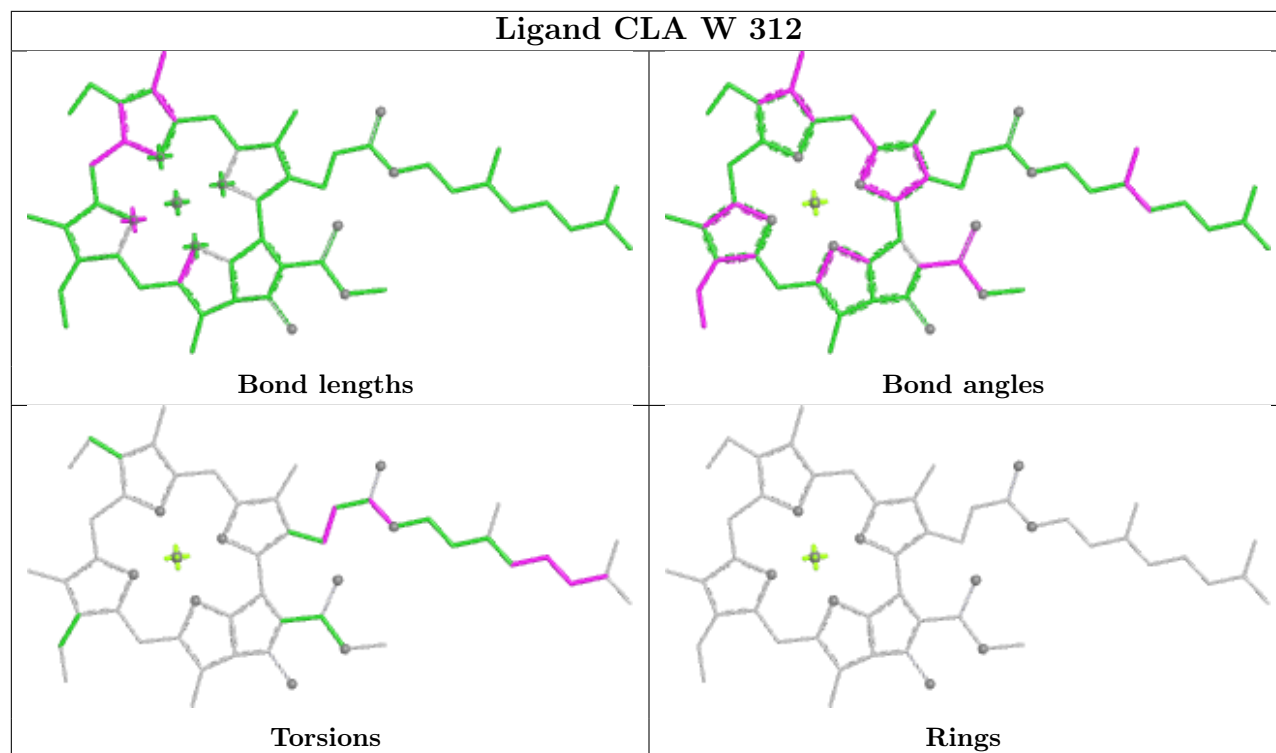
Bond angles

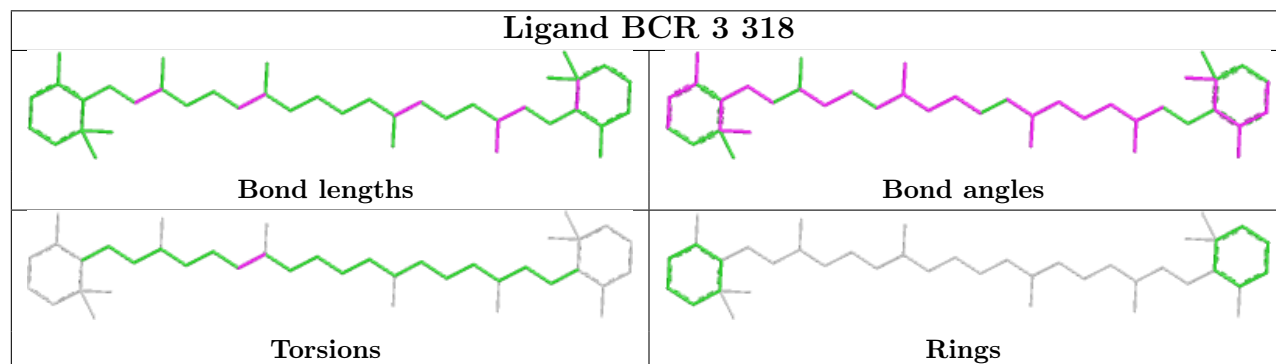
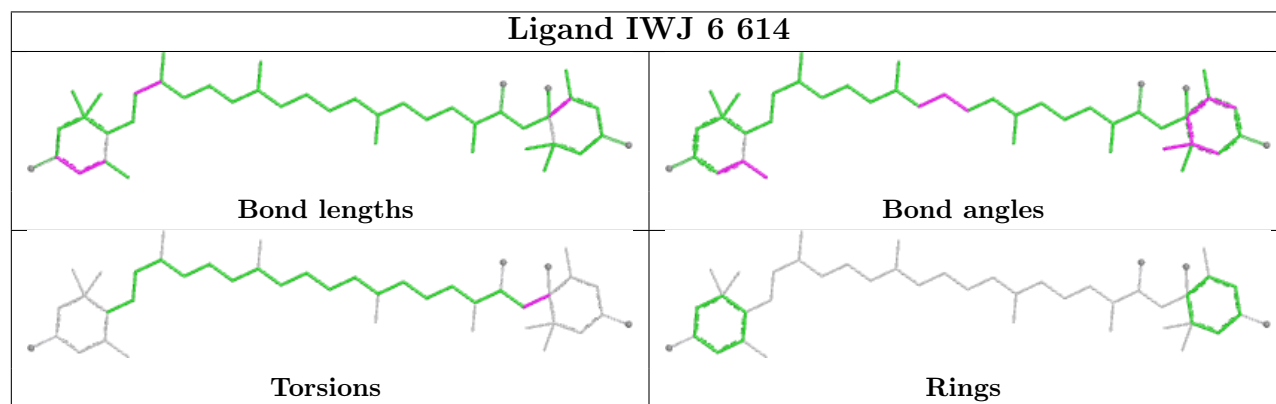
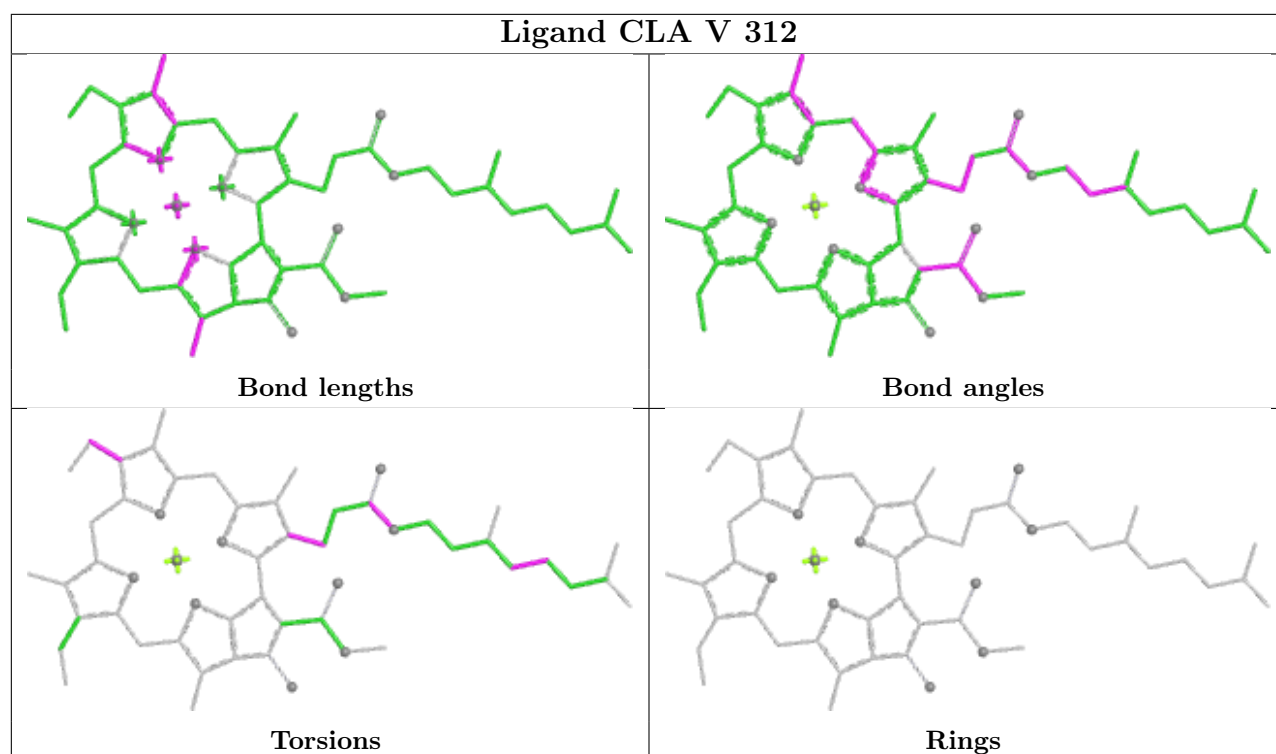


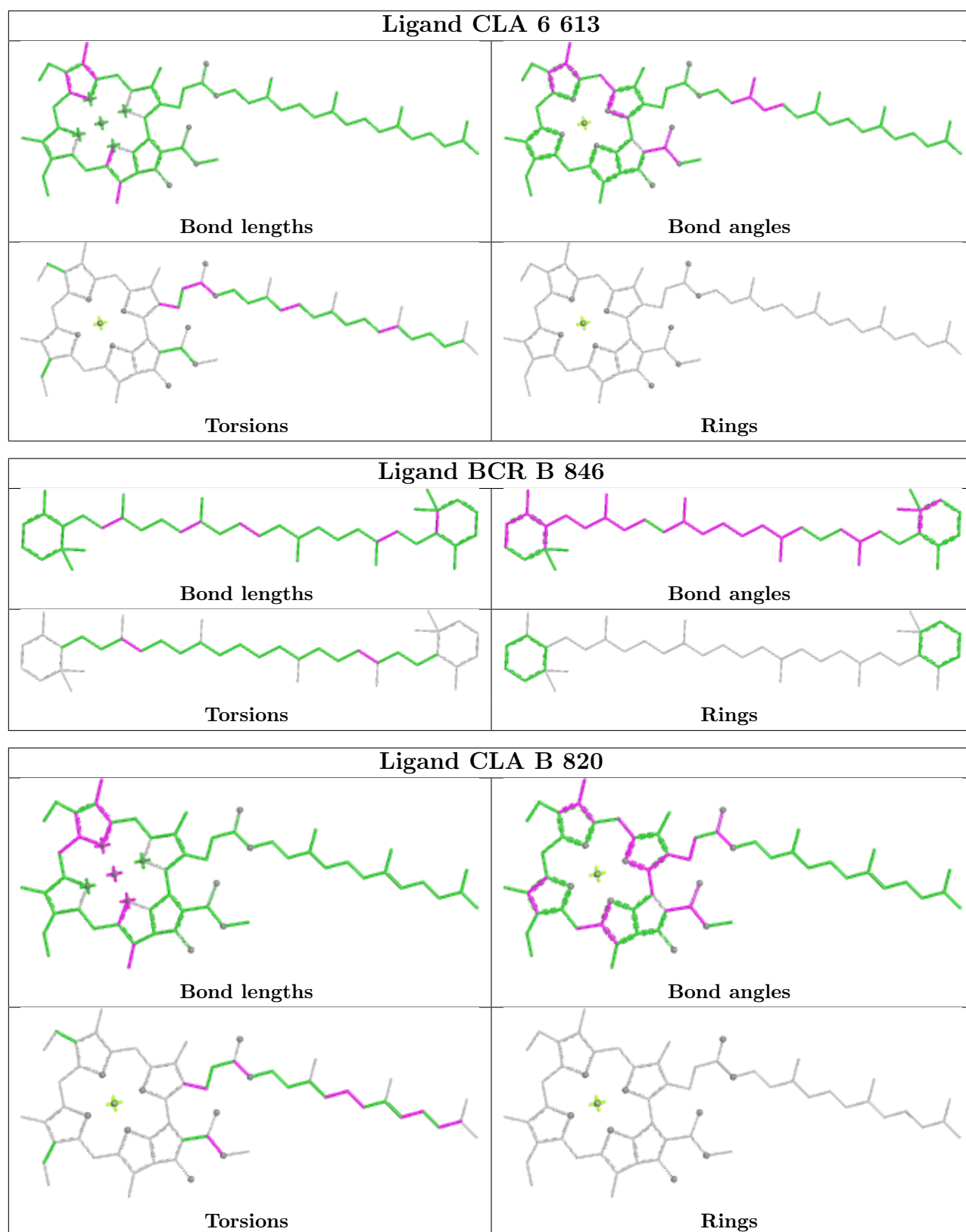
Torsions

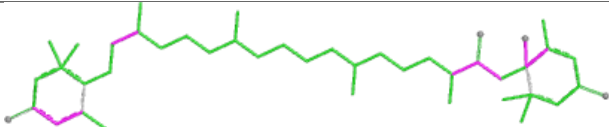
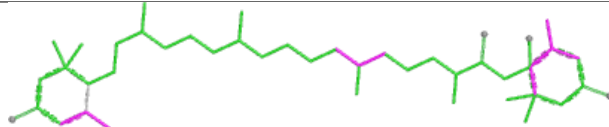
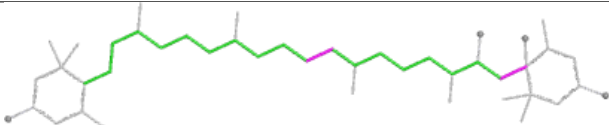
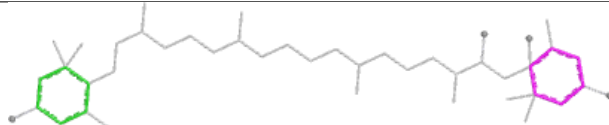


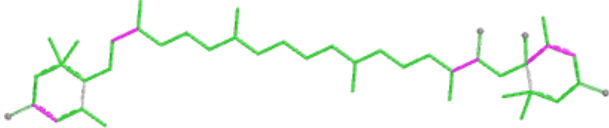
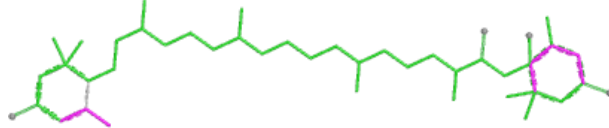
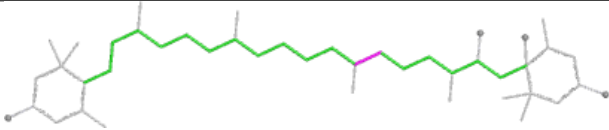
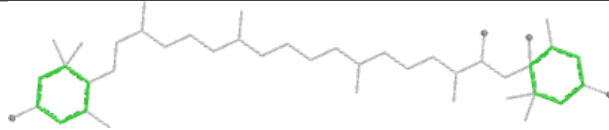
Rings

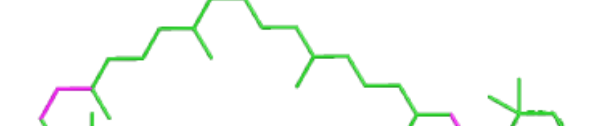
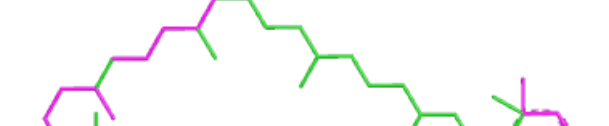
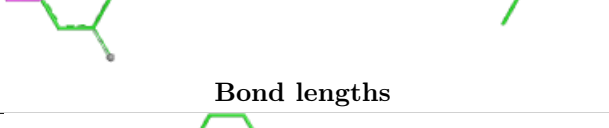




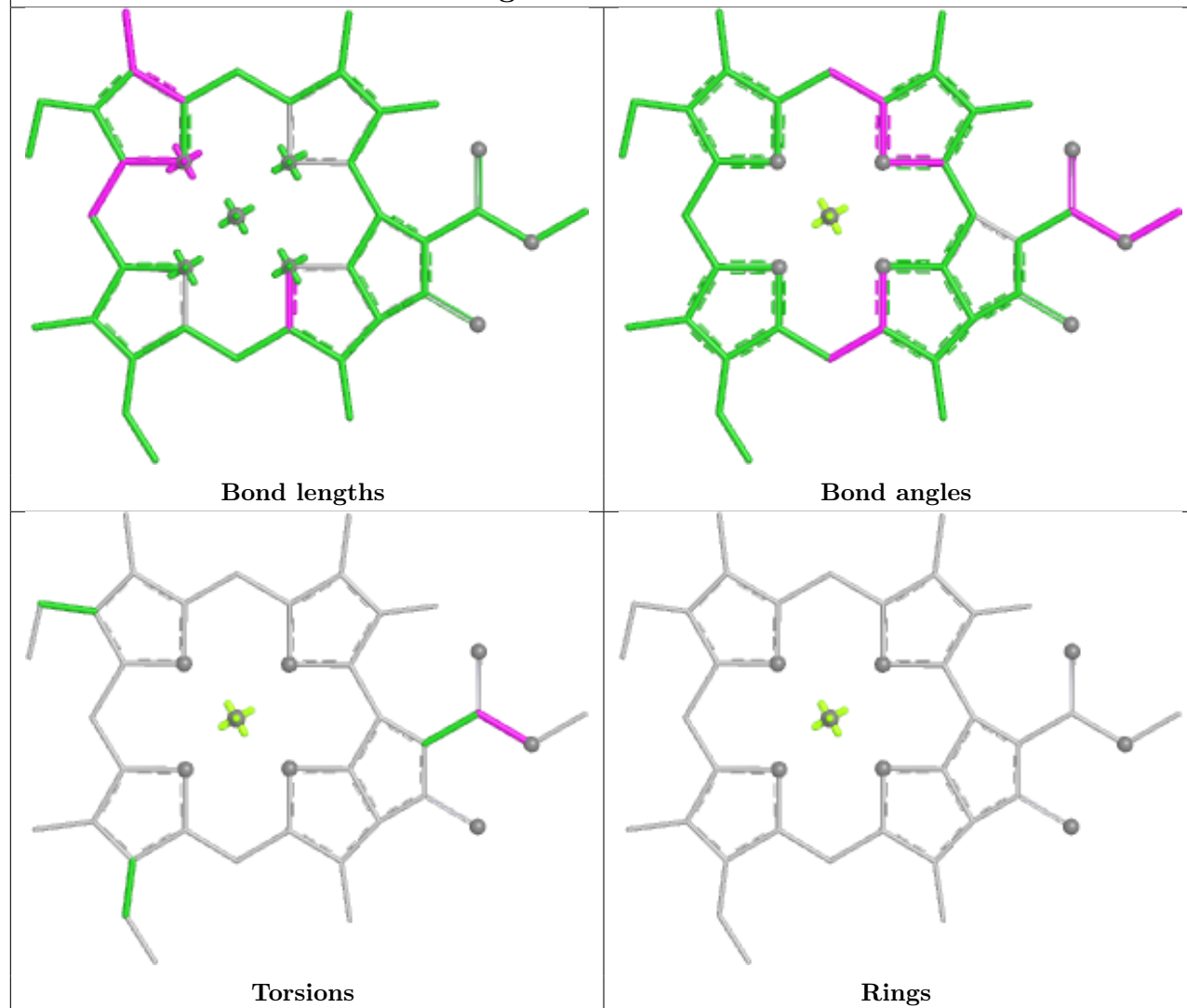


Ligand IWJ 3 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

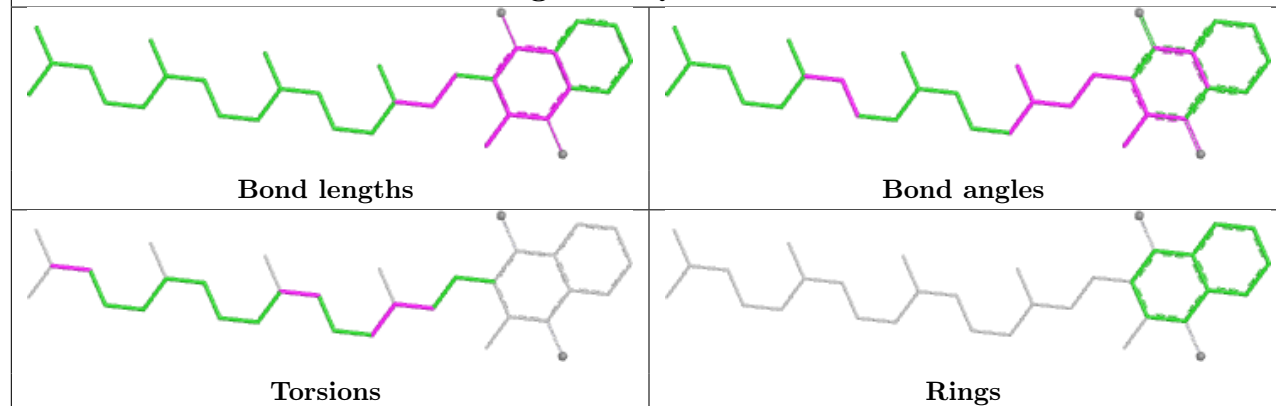
Ligand IWJ P 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand Q6L S 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

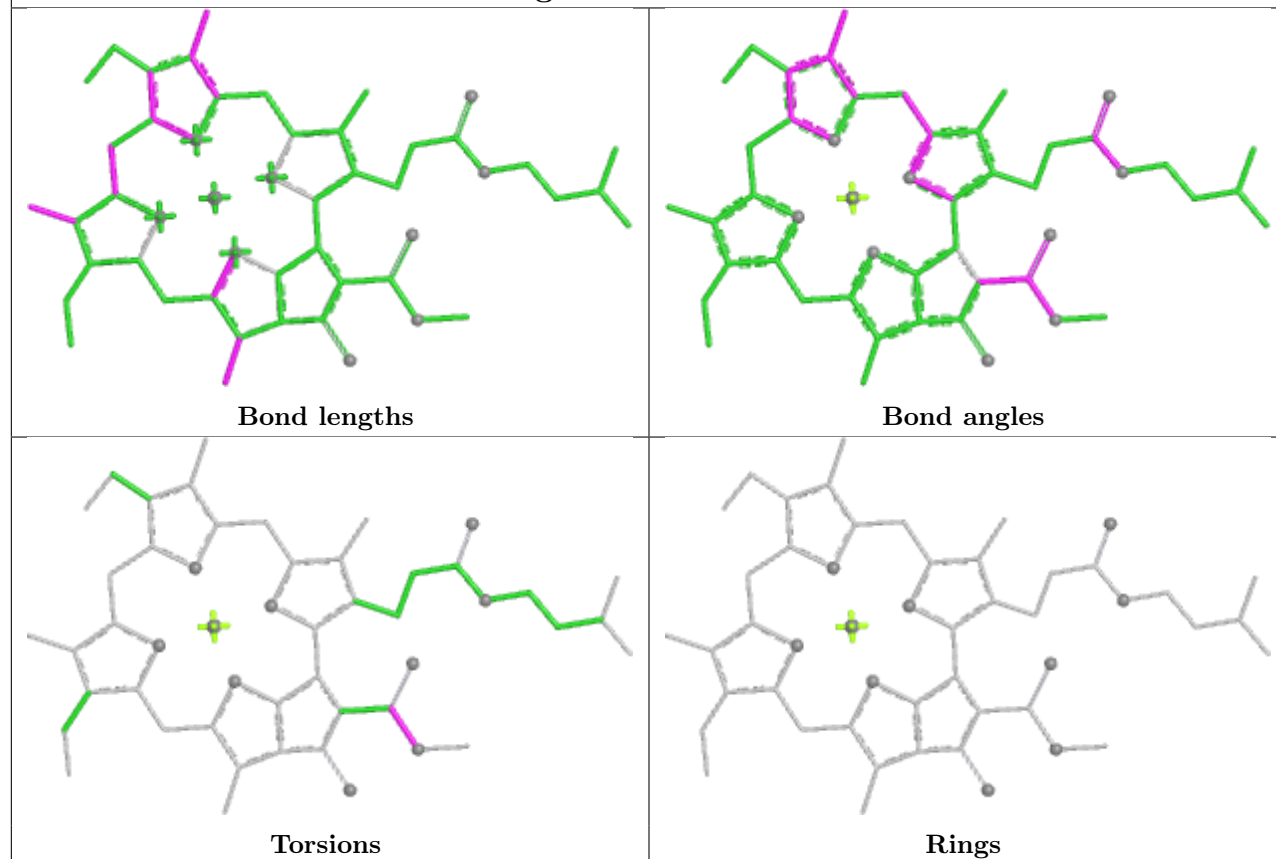
Ligand CLA 3 313



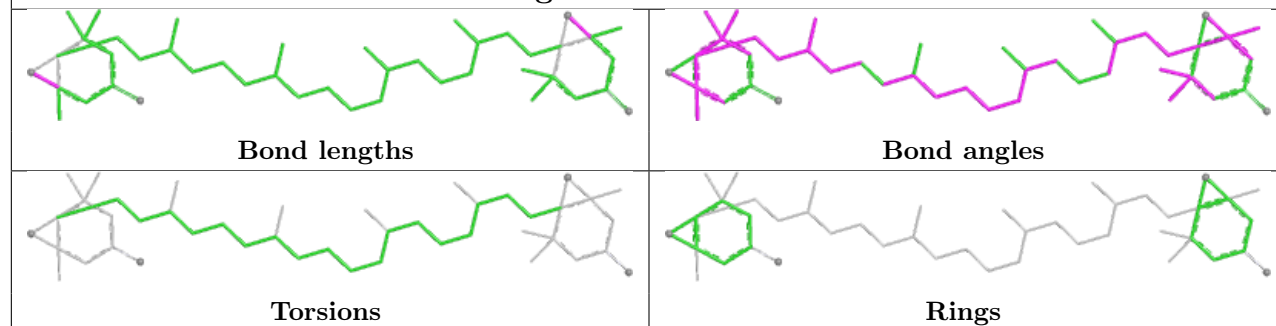
Ligand PQN B 844

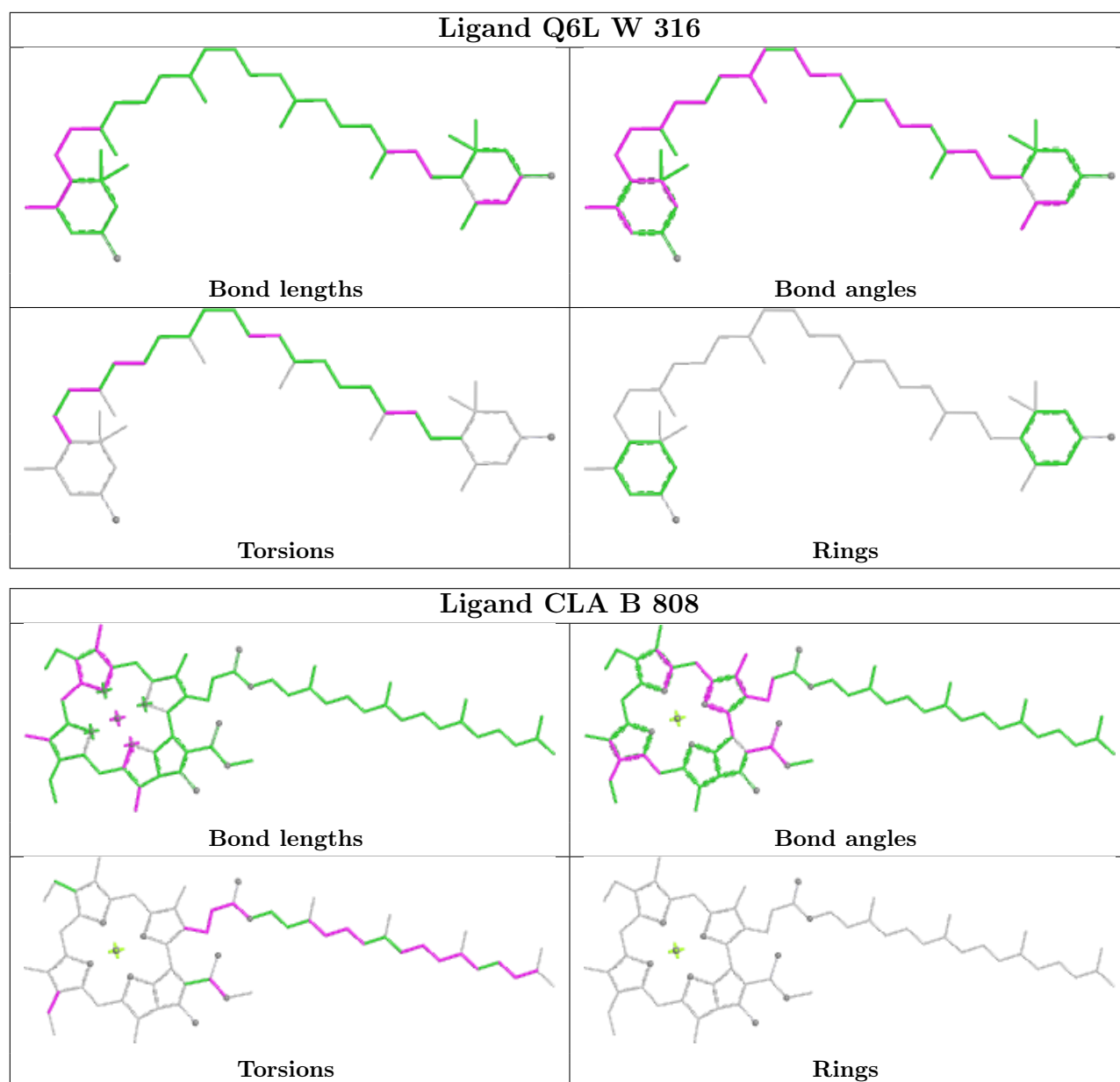


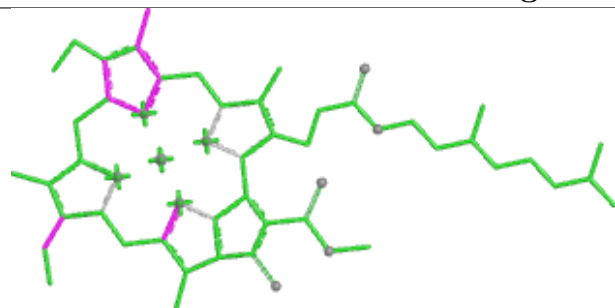
Ligand CLA S 303



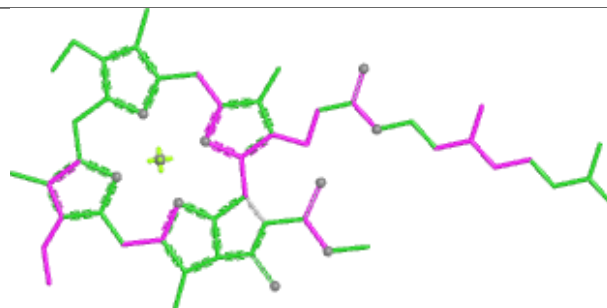
Ligand XAT 5 612



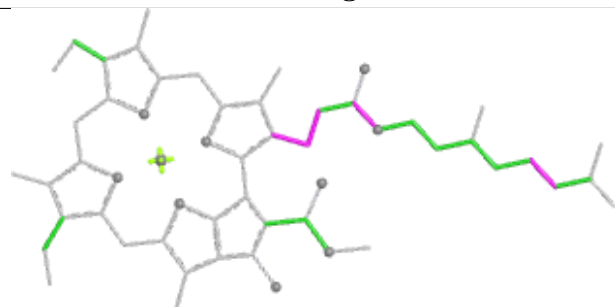


Ligand CLA 1 603

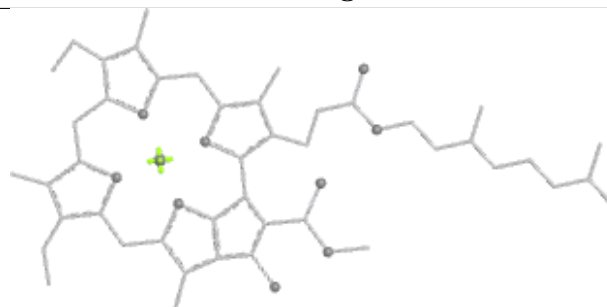
Bond lengths



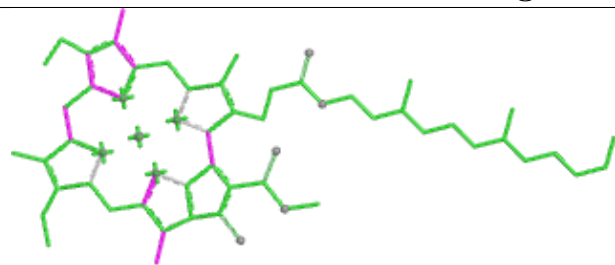
Bond angles



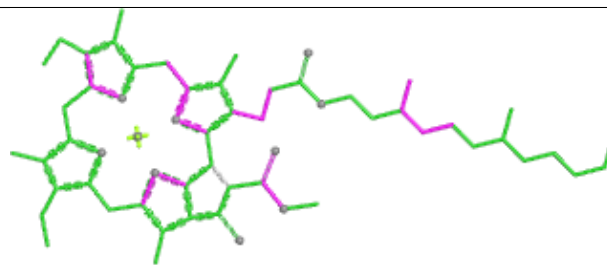
Torsions



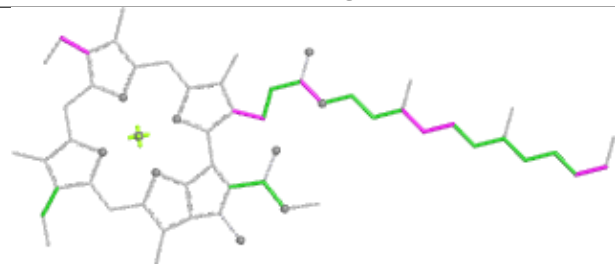
Rings

Ligand CLA T 309

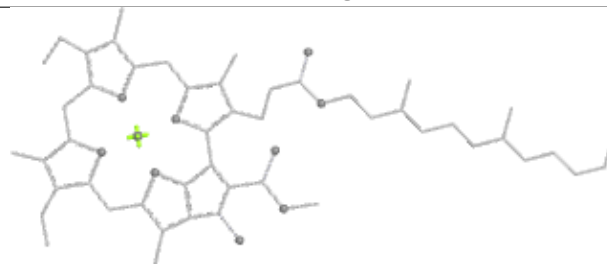
Bond lengths



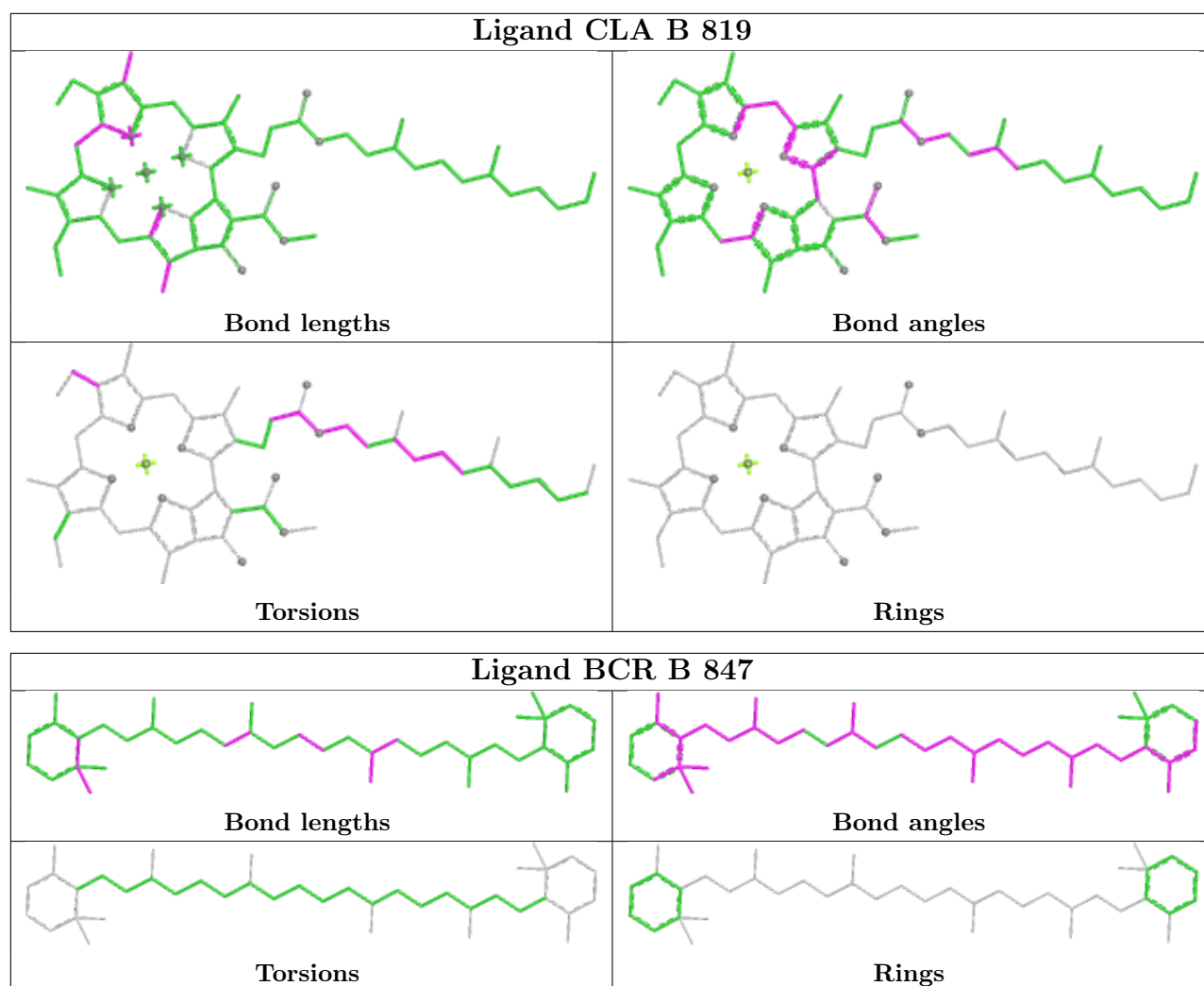
Bond angles



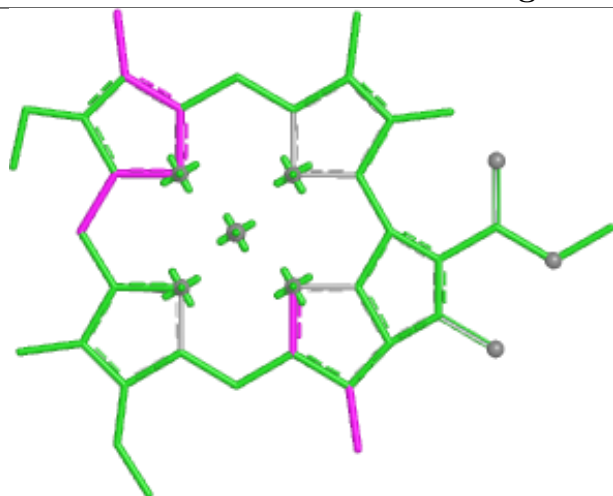
Torsions



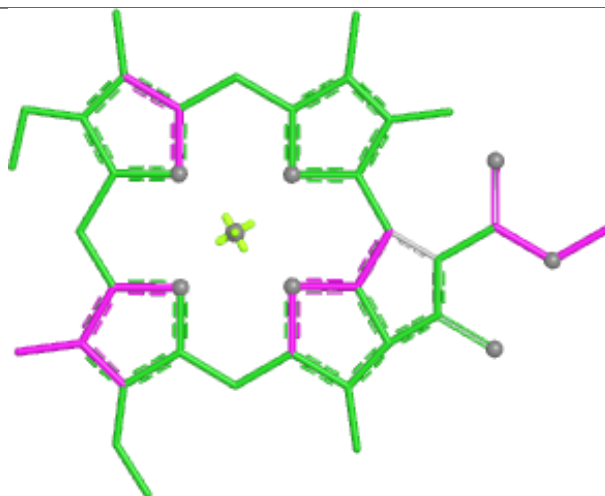
Rings



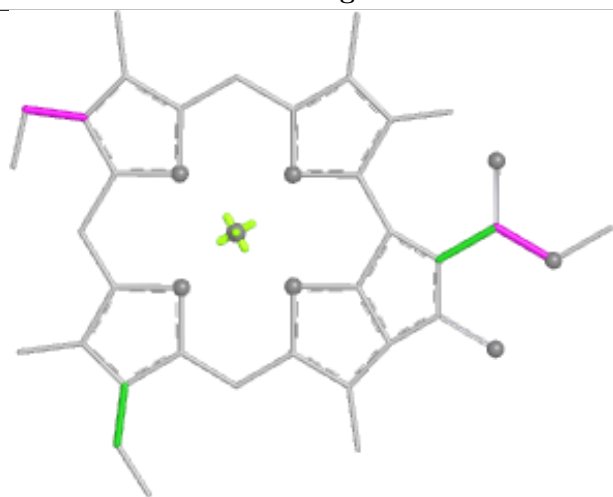
Ligand CLA 3 308



Bond lengths



Bond angles

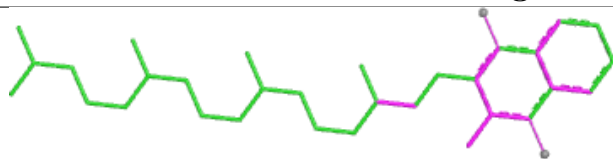


Torsions

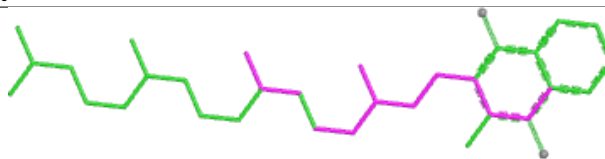


Rings

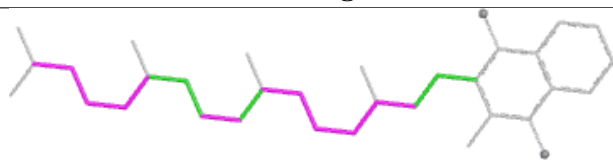
Ligand PQN A 844



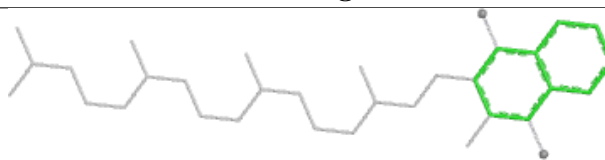
Bond lengths



Bond angles

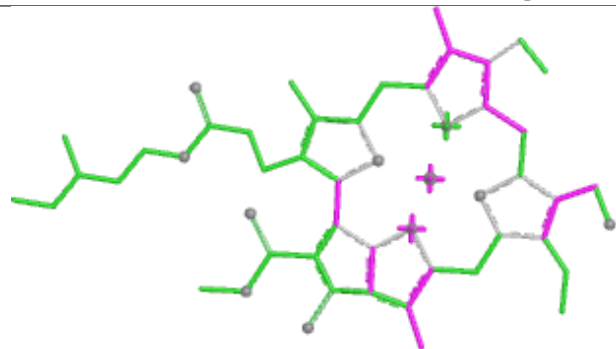


Torsions

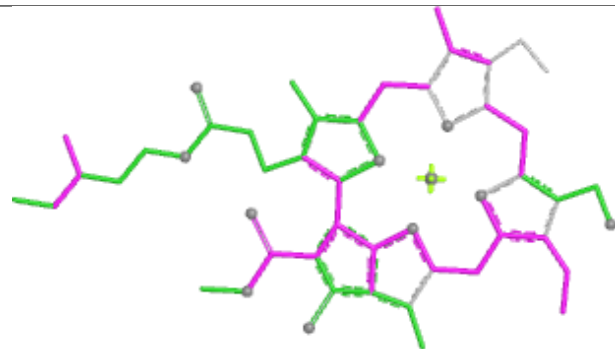


Rings

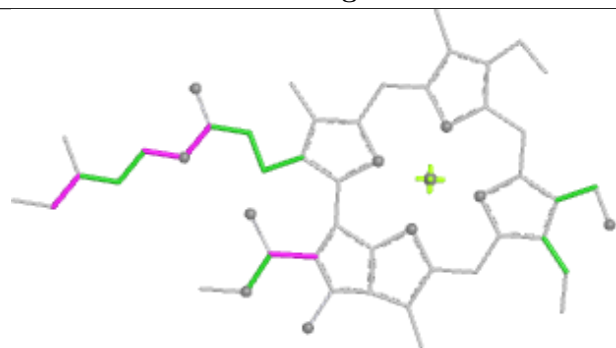
Ligand CHL S 306



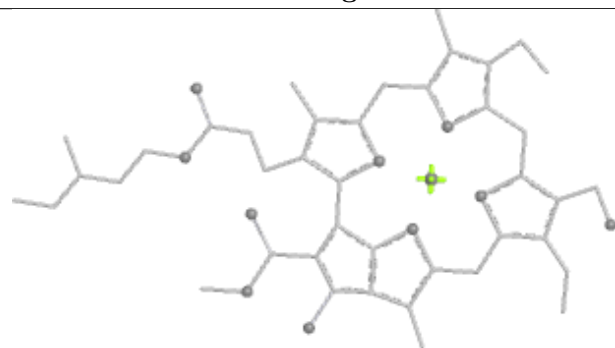
Bond lengths



Bond angles

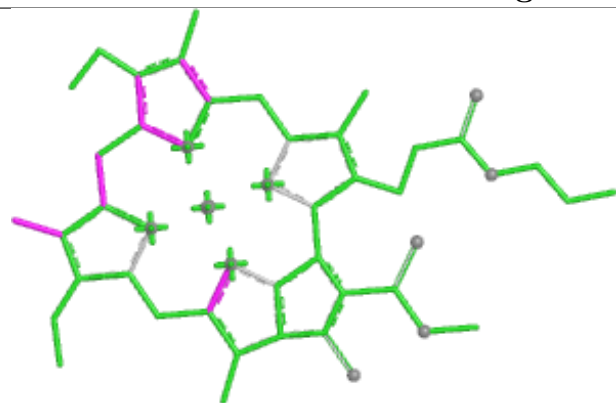


Torsions

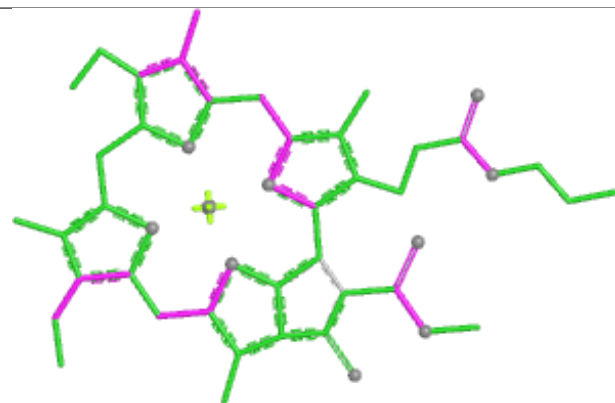


Rings

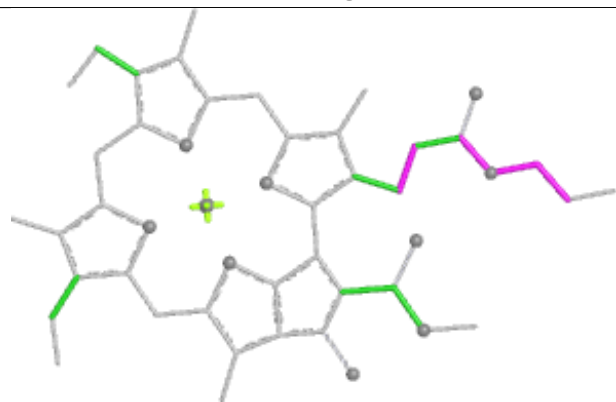
Ligand CLA R 317



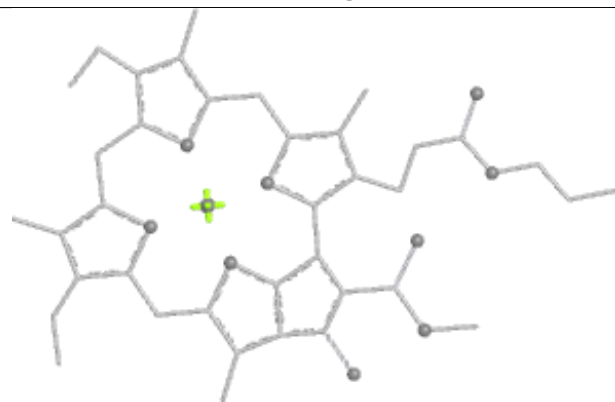
Bond lengths



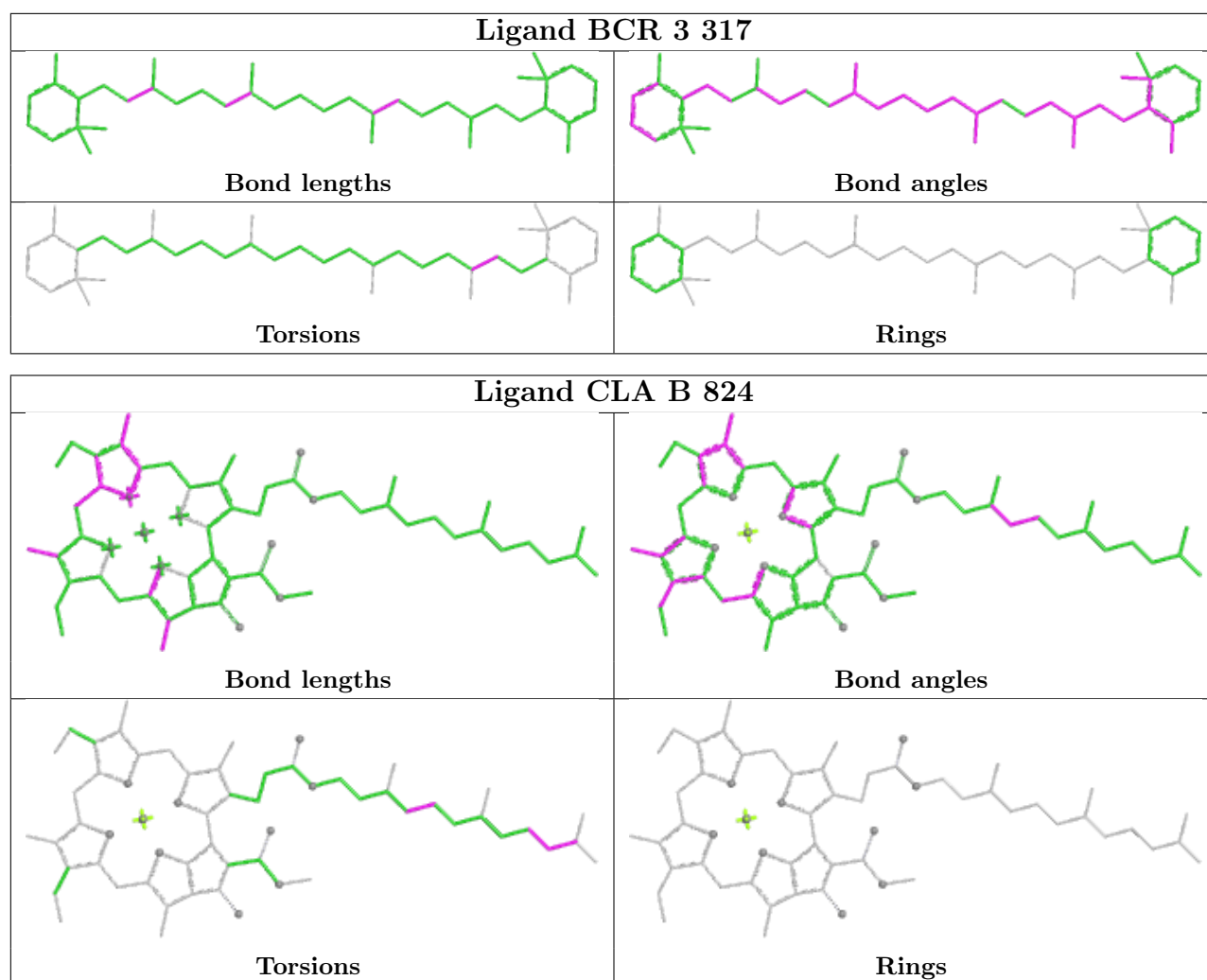
Bond angles



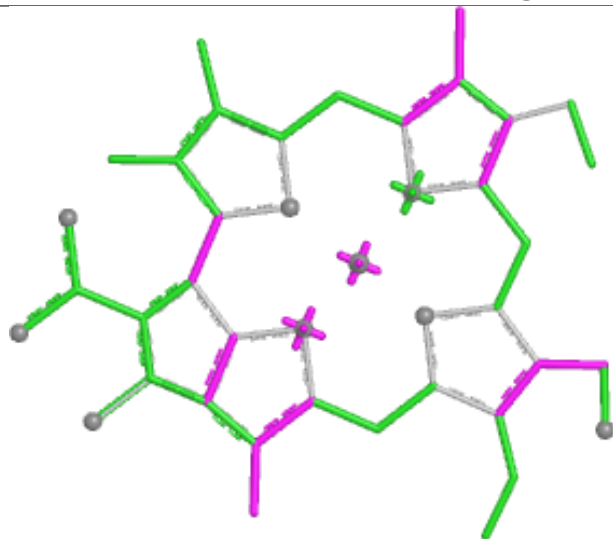
Torsions



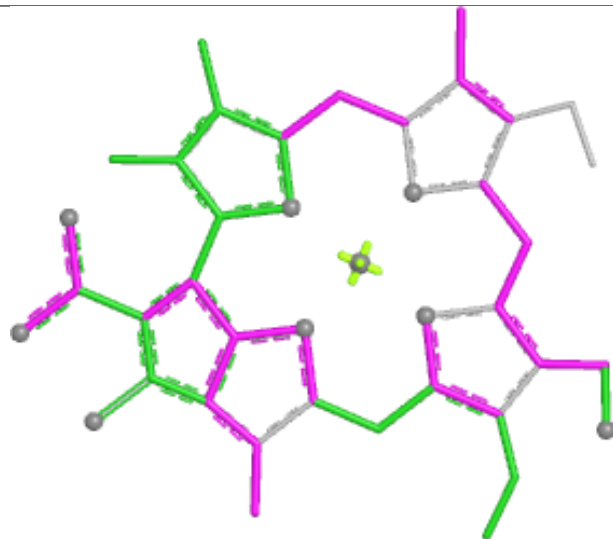
Rings



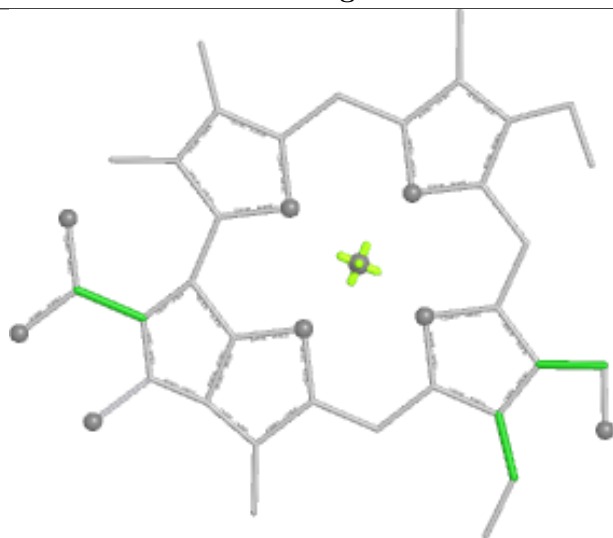
Ligand CHL 1 604



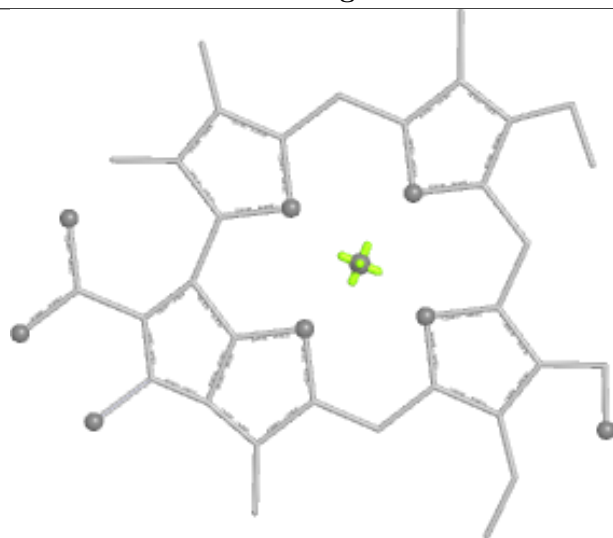
Bond lengths



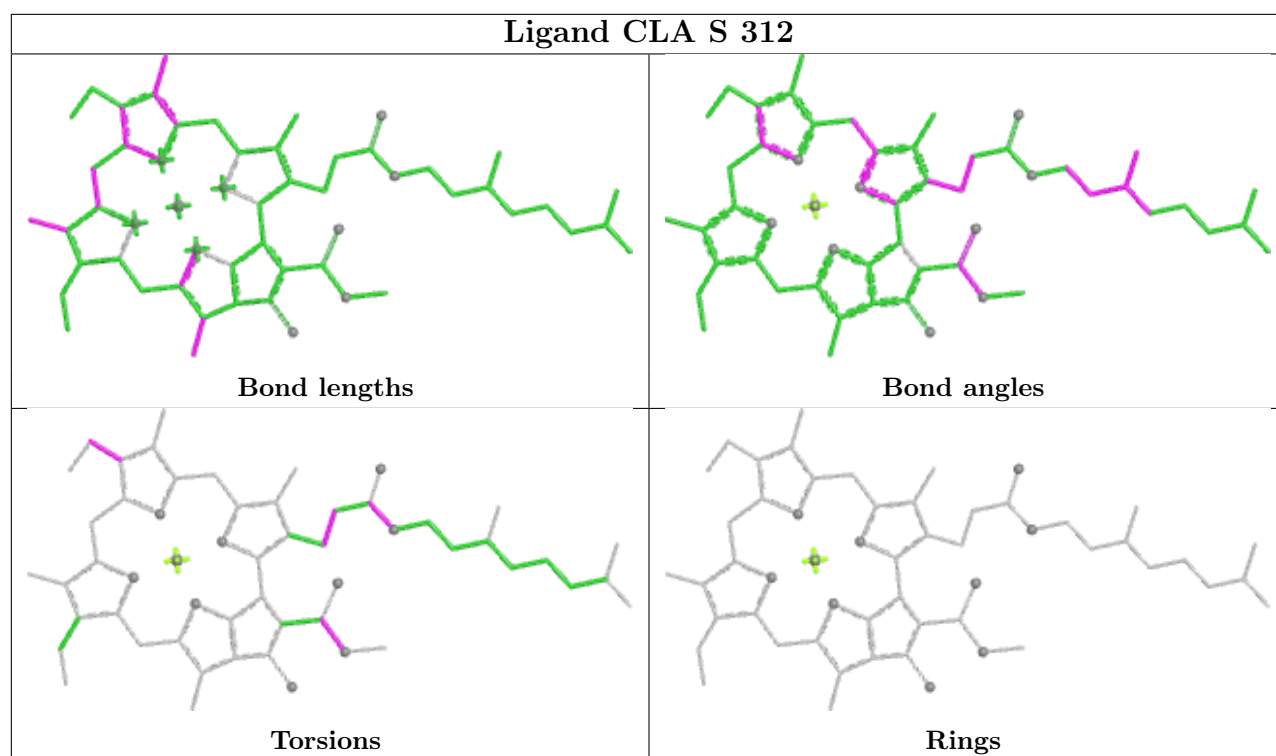
Bond angles

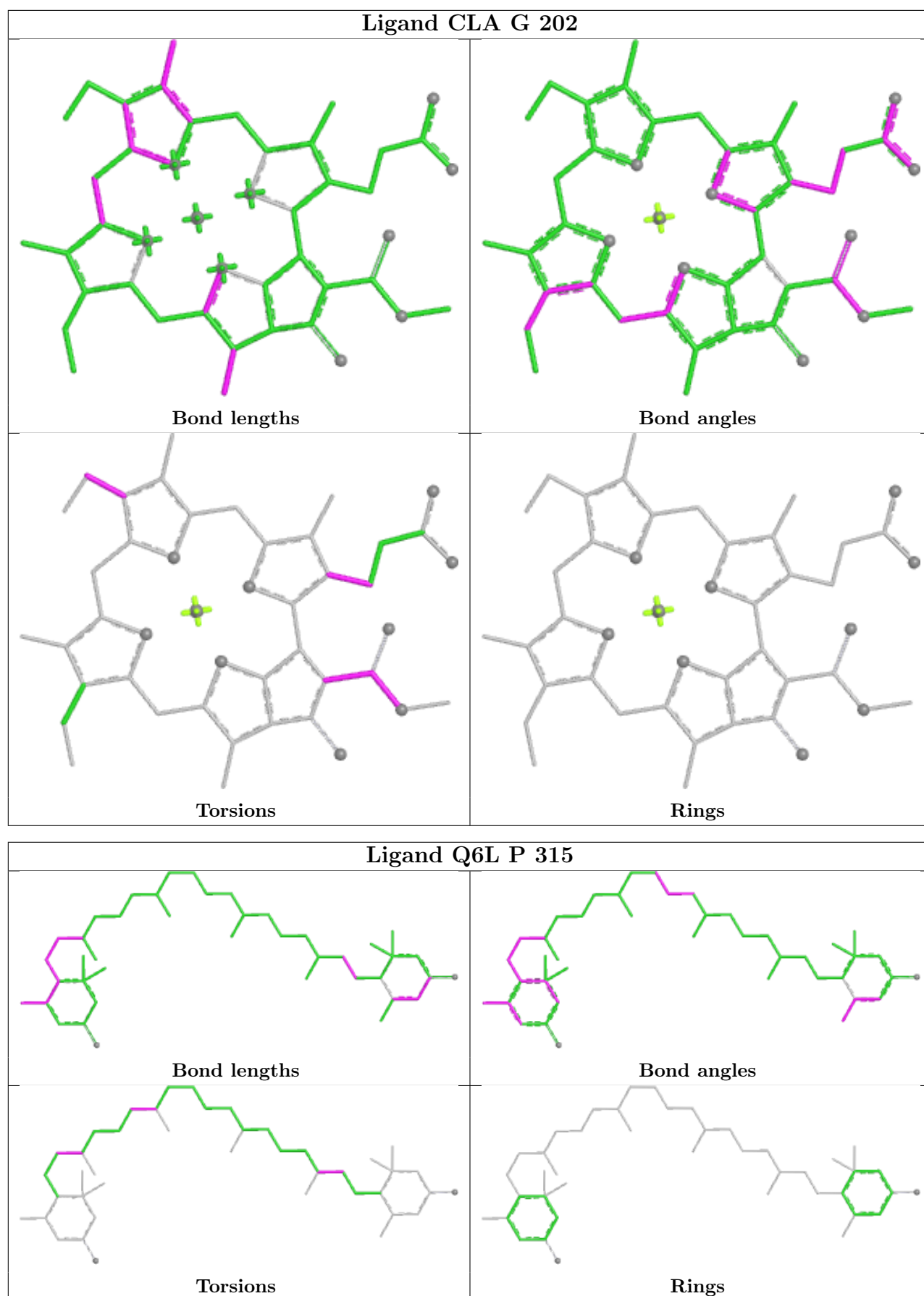


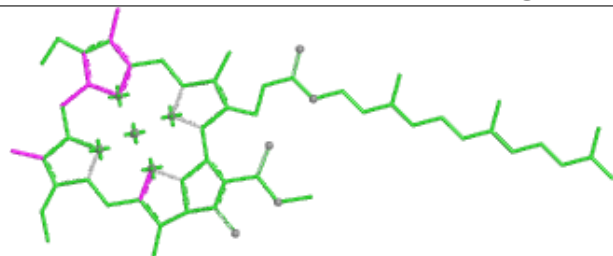
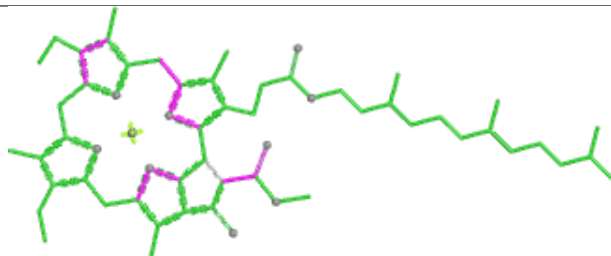
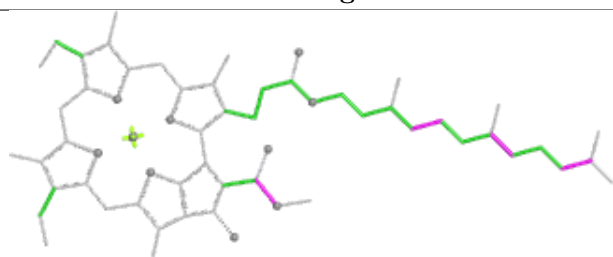
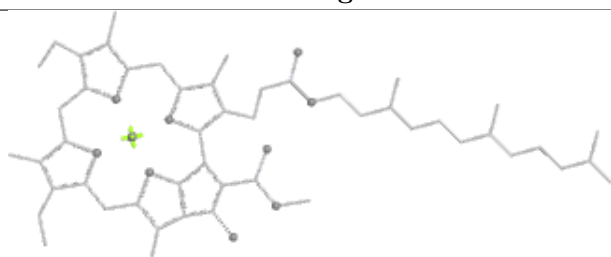
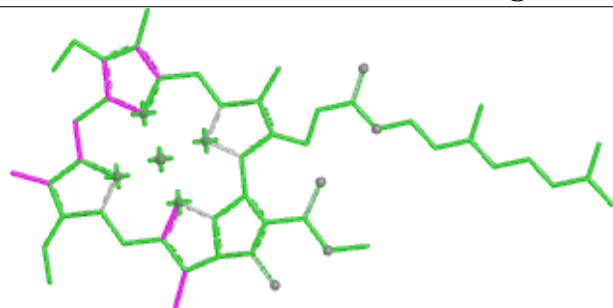
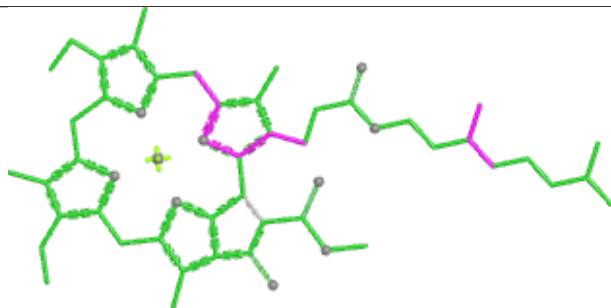
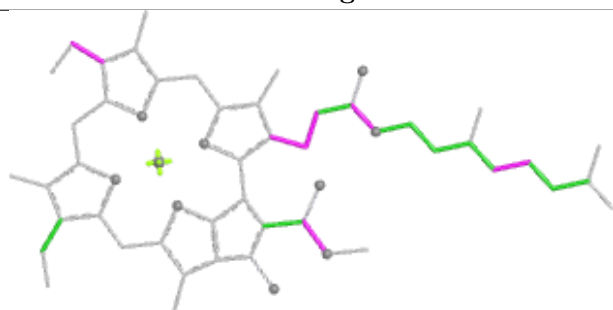
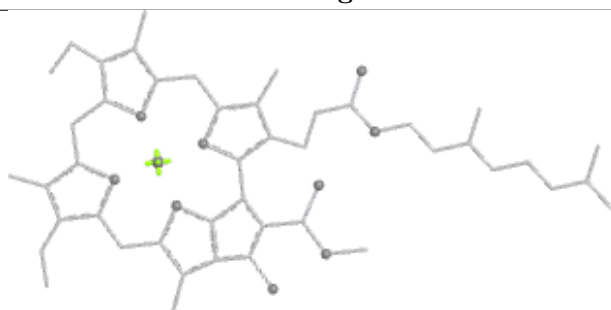
Torsions

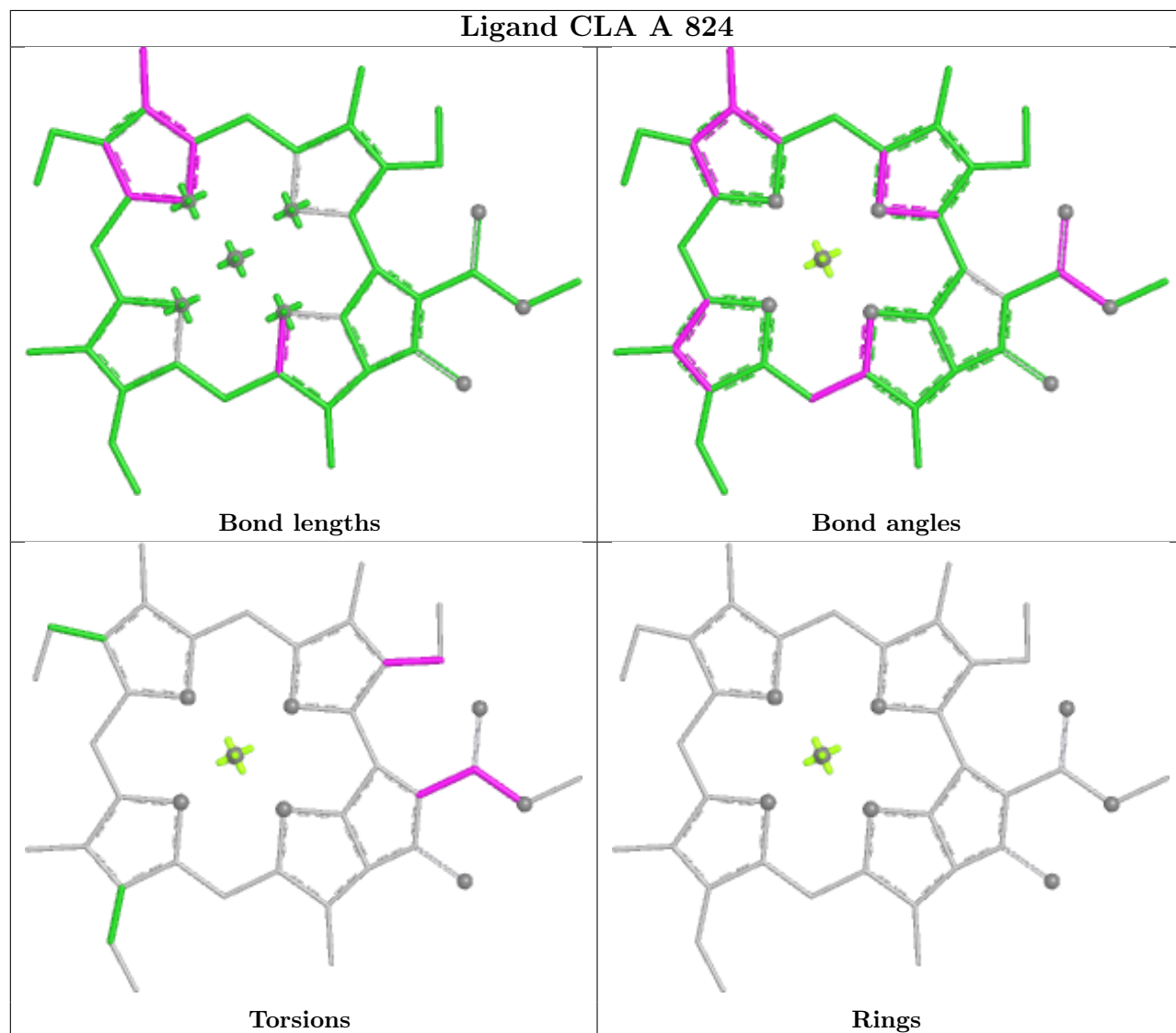
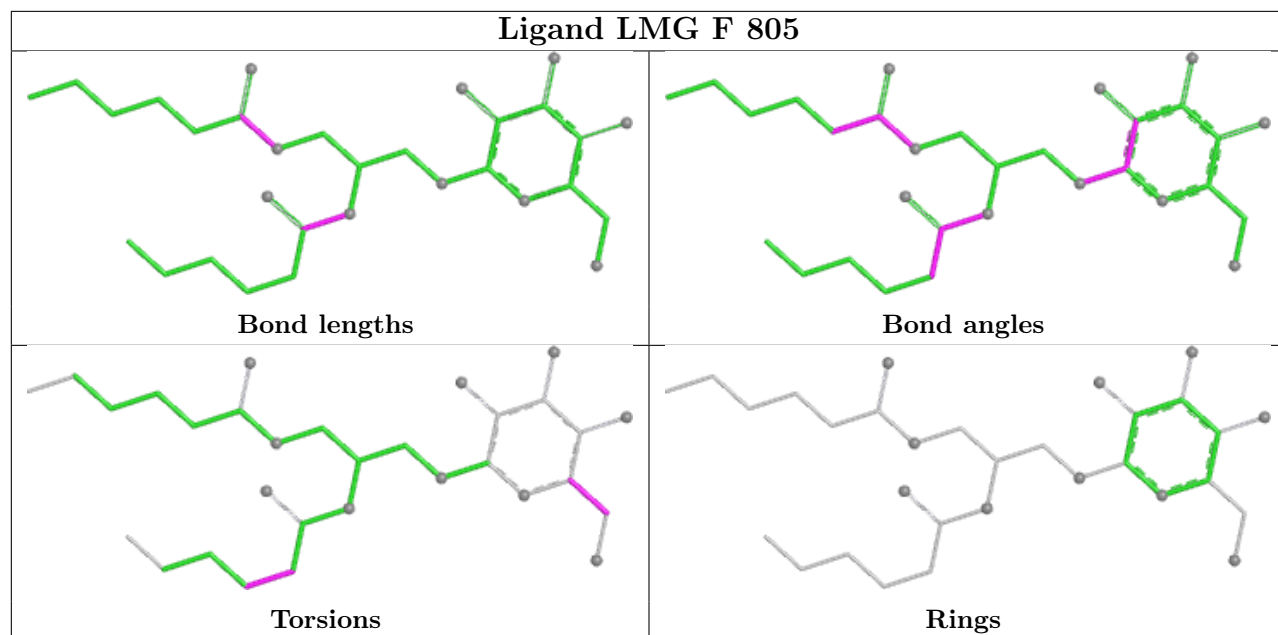


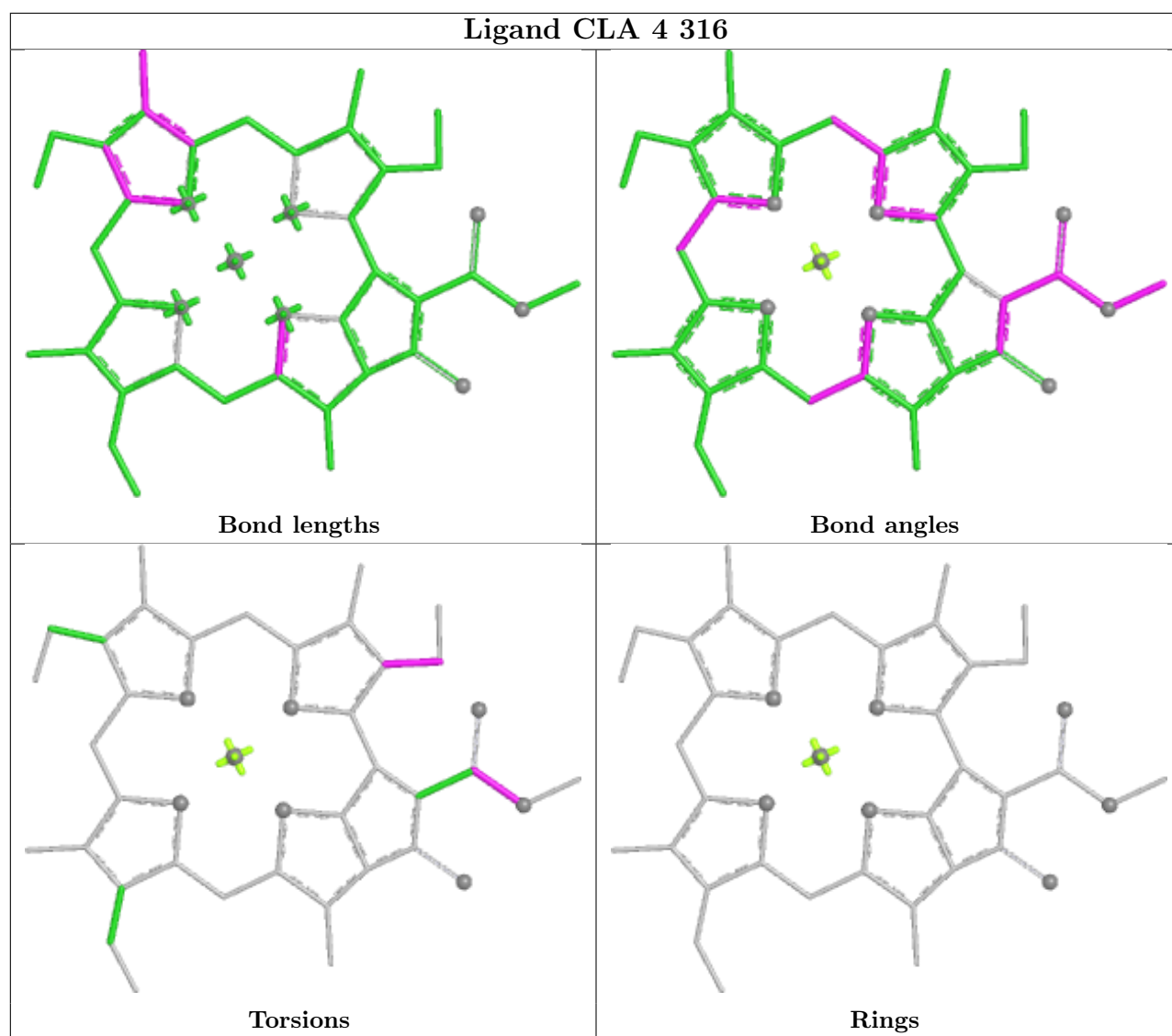
Rings





Ligand CLA 3 301**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA W 301****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.

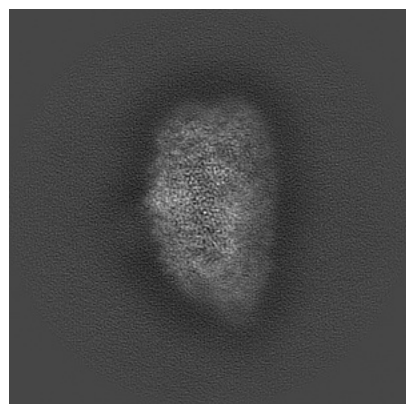
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33737. These allow visual inspection of the internal detail of the map and identification of artifacts.

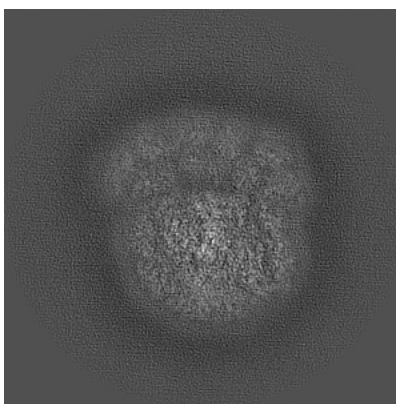
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

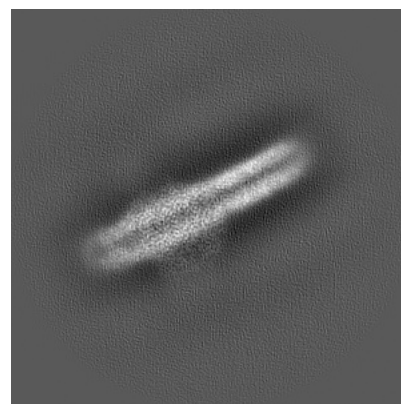
6.1.1 Primary map



X

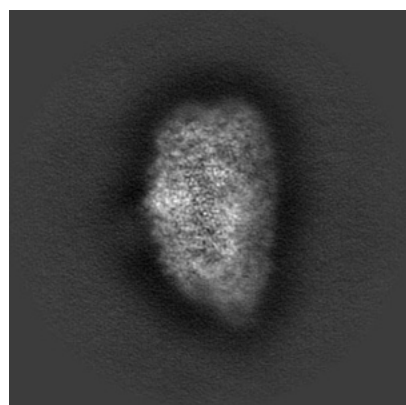


Y

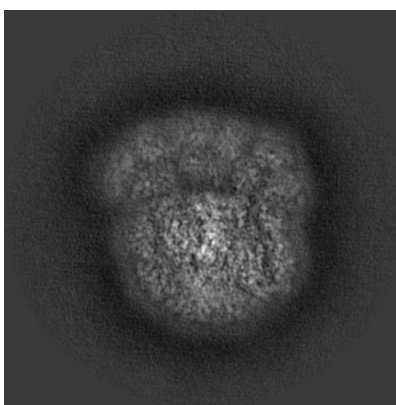


Z

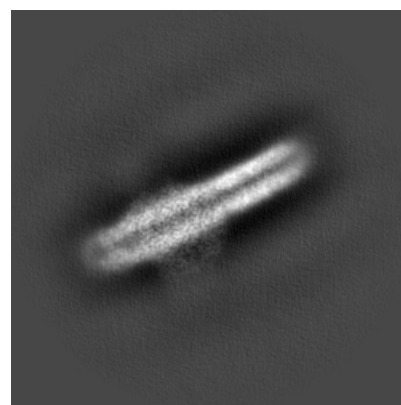
6.1.2 Raw map



X



Y

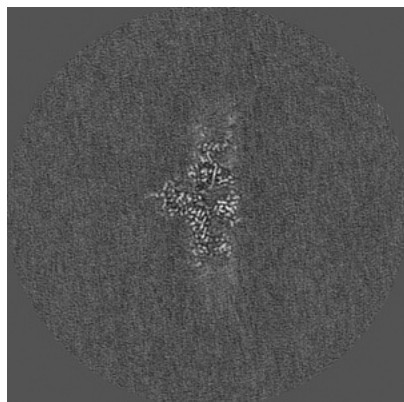


Z

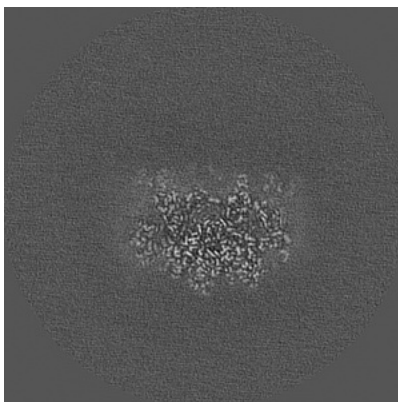
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

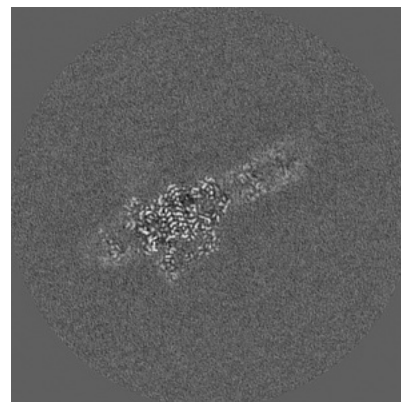
6.2.1 Primary map



X Index: 192

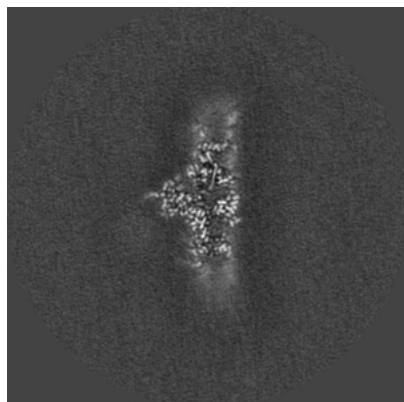


Y Index: 192

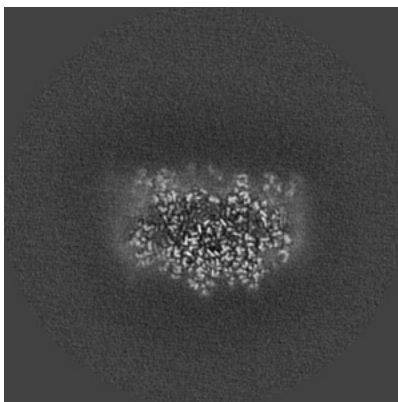


Z Index: 192

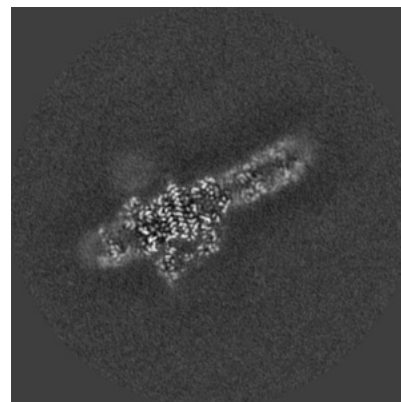
6.2.2 Raw map



X Index: 192



Y Index: 192

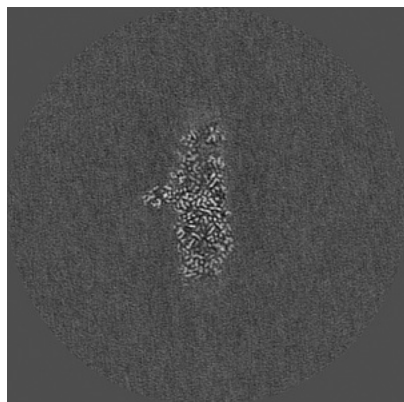


Z Index: 192

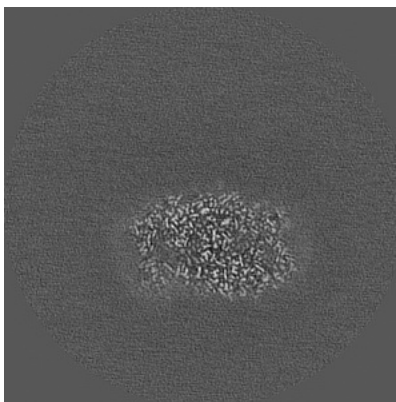
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

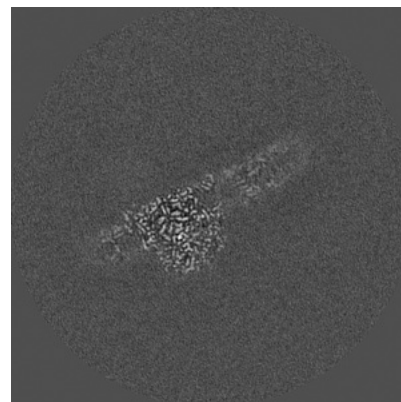
6.3.1 Primary map



X Index: 169

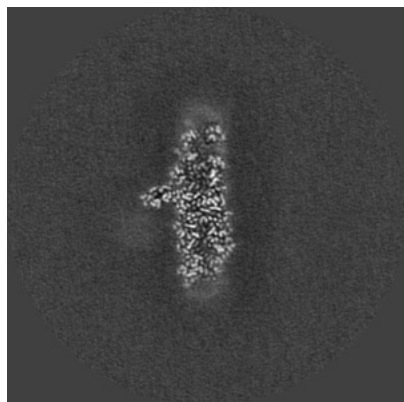


Y Index: 180

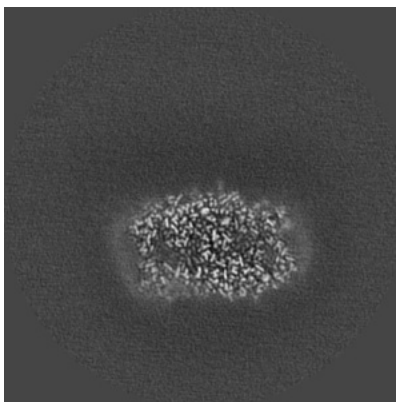


Z Index: 201

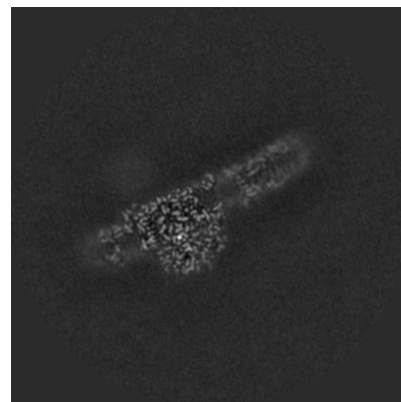
6.3.2 Raw map



X Index: 168



Y Index: 180

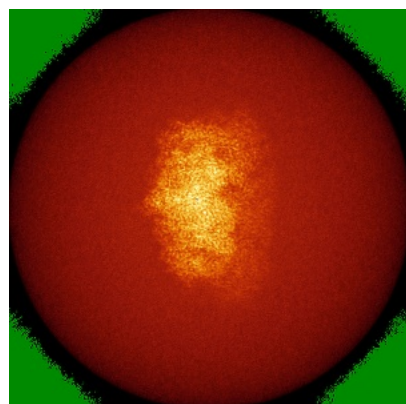


Z Index: 201

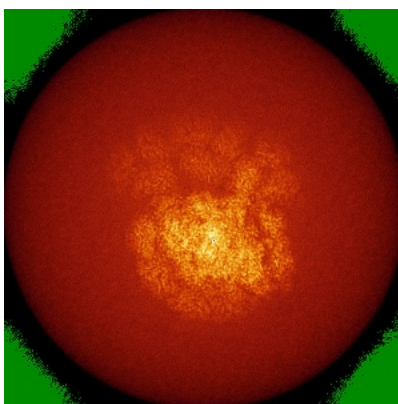
The images above show the largest variance slices of the map in three orthogonal directions.

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

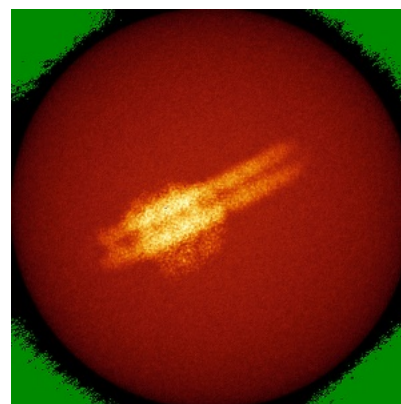
6.4.1 Primary map



X

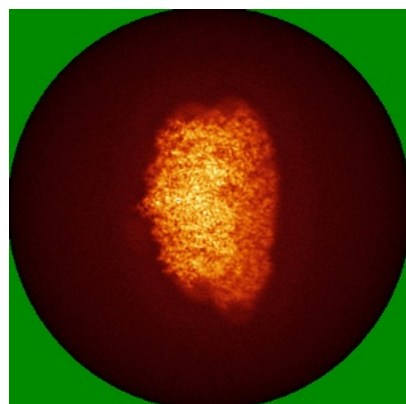


Y

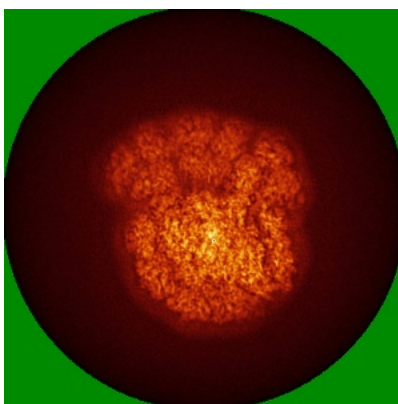


Z

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

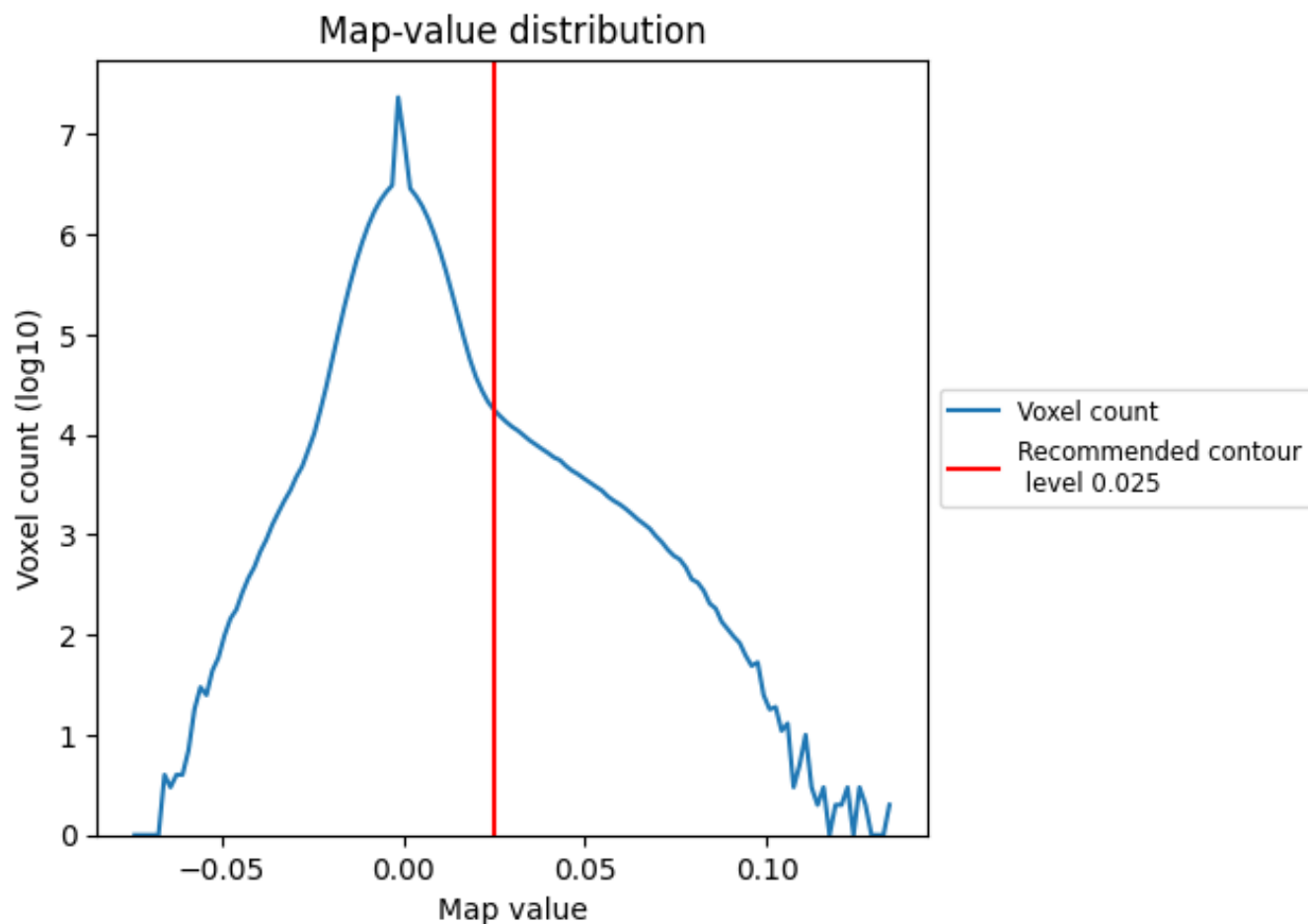
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

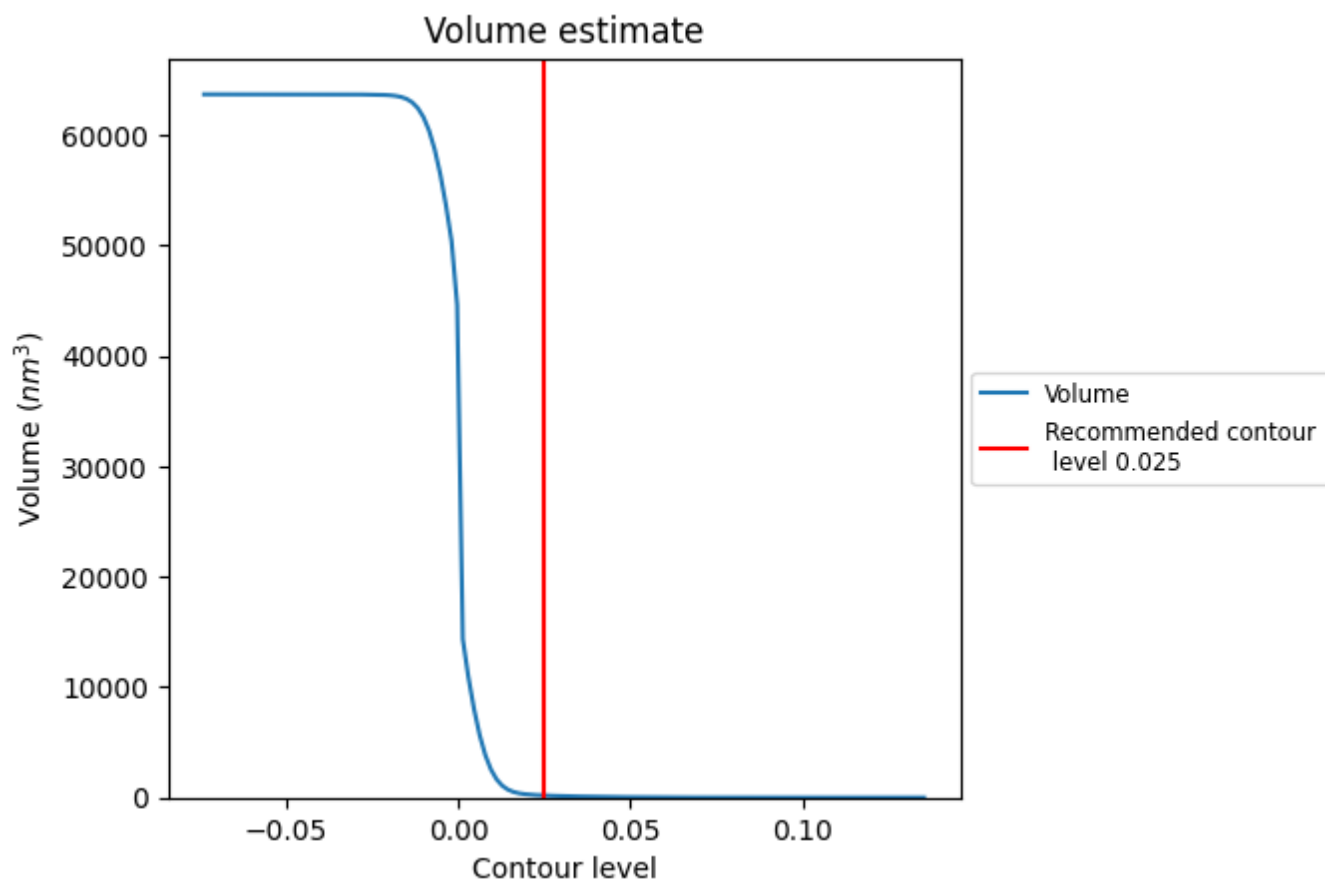
This section contains the results of statistical analysis of the map.

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.

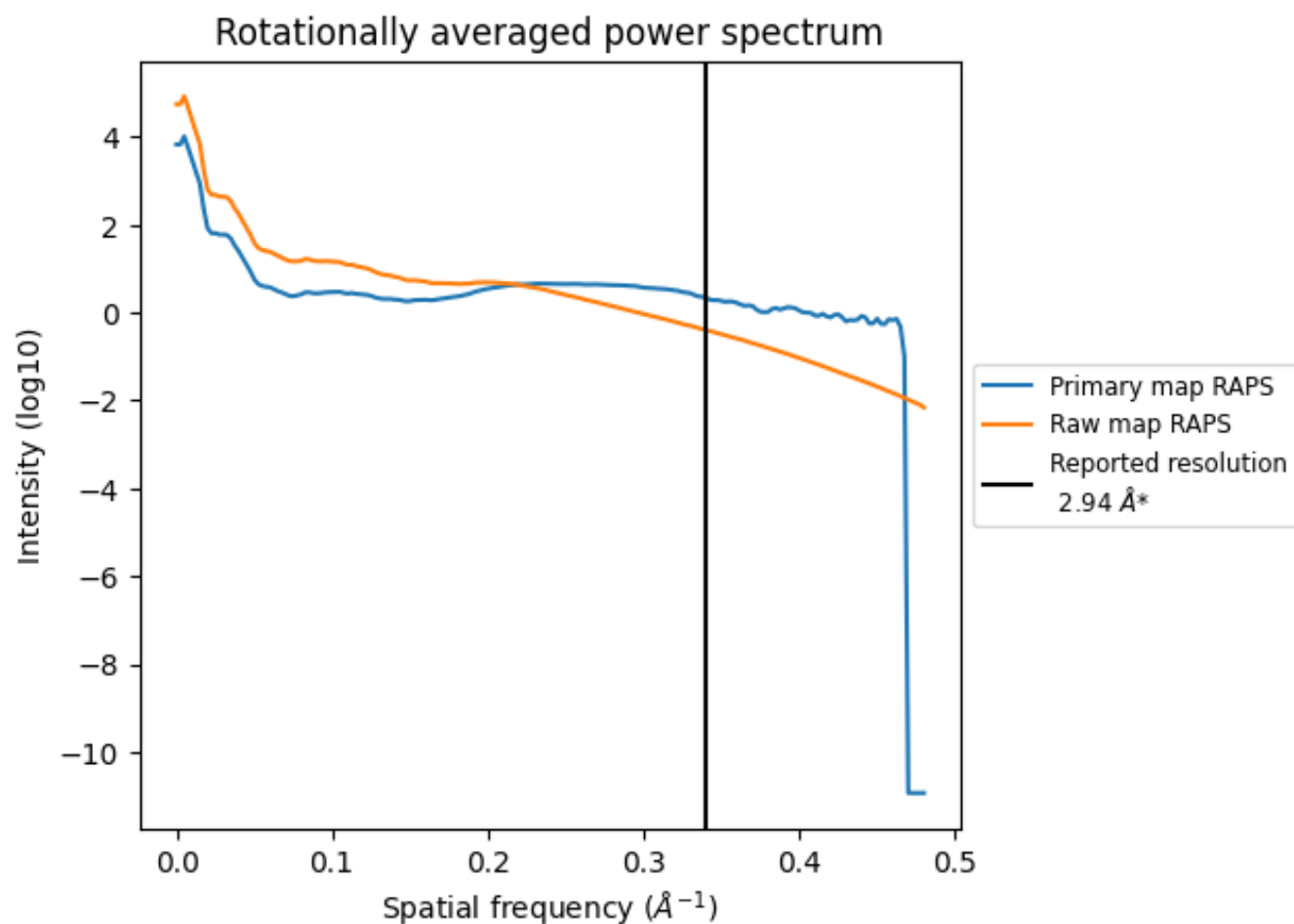
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm³; this corresponds to an approximate mass of 169 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 ⓘ

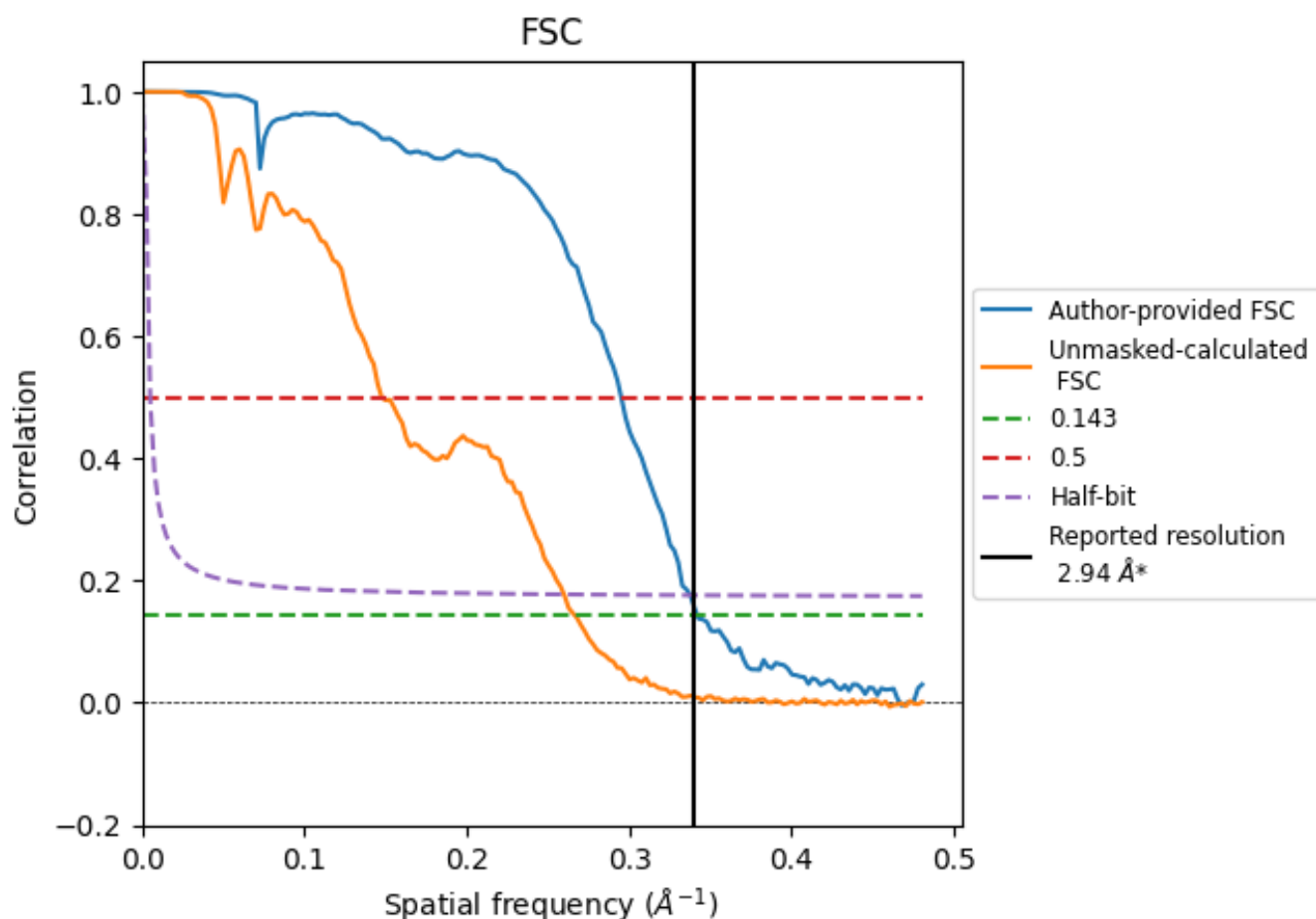


*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

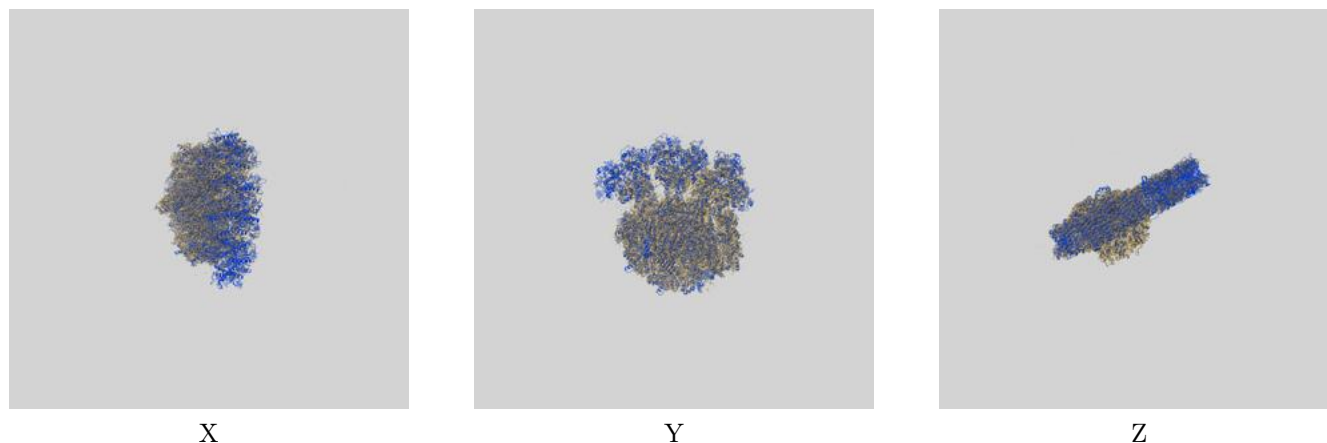
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.39	2.96
Unmasked-calculated*	3.75	6.77	3.85

*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 3.75 differs from the reported value 2.94 by more than 10 %

9 Map-model fit [i](#)

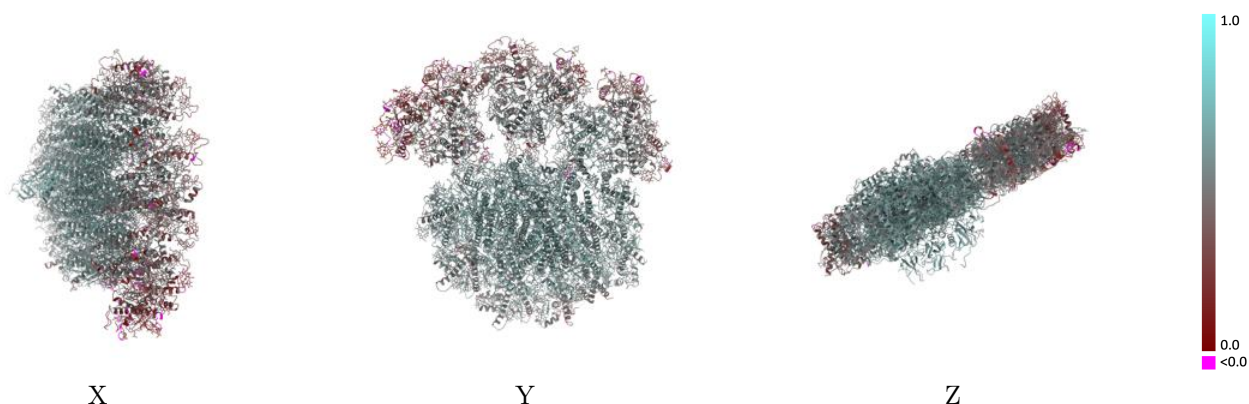
This section contains information regarding the fit between EMDB map EMD-33737 and PDB model 7YCA. Per-residue inclusion information can be found in [section 3](#) on [page 45](#).

9.1 Map-model overlay [i](#)



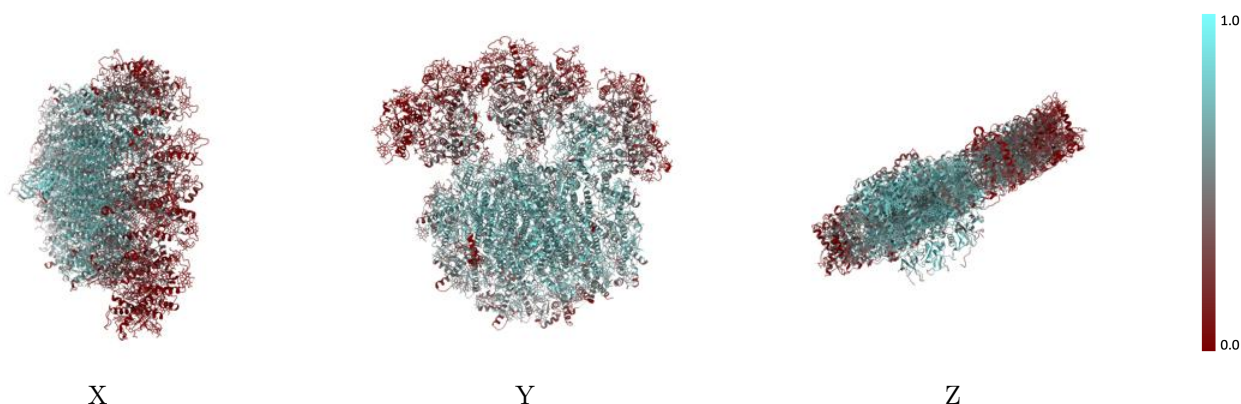
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



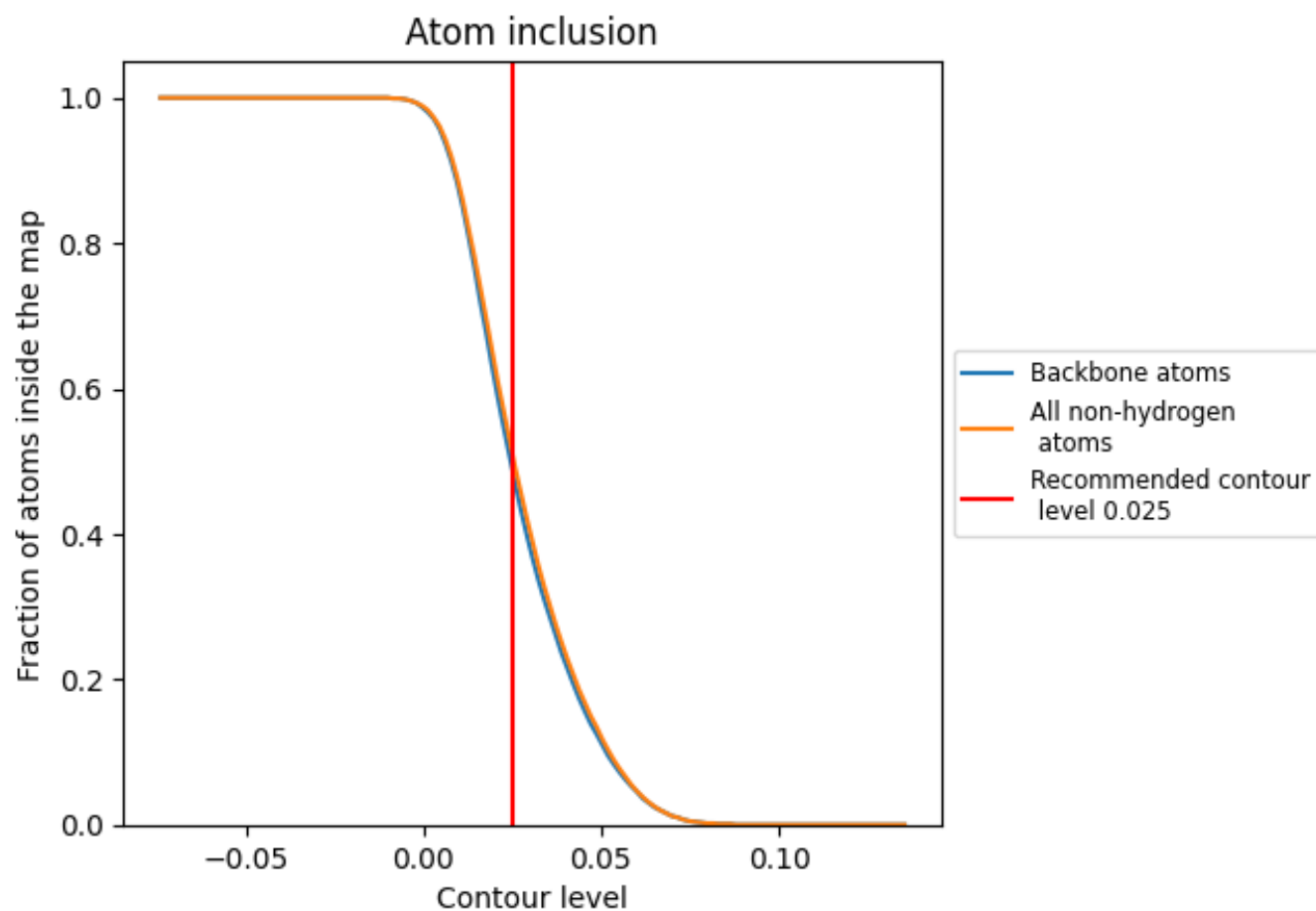
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 51% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5110	 0.5140
1	 0.3170	 0.4450
2	 0.5160	 0.5240
3	 0.5610	 0.5590
4	 0.4200	 0.4810
5	 0.5730	 0.5480
6	 0.6330	 0.5670
A	 0.7720	 0.6190
B	 0.7600	 0.6090
C	 0.7780	 0.6160
D	 0.6260	 0.5840
E	 0.6110	 0.5870
F	 0.5970	 0.5620
G	 0.3990	 0.4970
H	 0.6320	 0.5770
I	 0.6670	 0.5760
J	 0.6620	 0.5760
K	 0.6500	 0.5780
L	 0.7290	 0.6100
M	 0.6490	 0.5930
N	 0.3080	 0.4830
O	 0.6920	 0.5910
P	 0.2520	 0.3960
Q	 0.5640	 0.5220
R	 0.3340	 0.4370
S	 0.2460	 0.4000
T	 0.3560	 0.4660
U	 0.1480	 0.3670
V	 0.1590	 0.3420
W	 0.3080	 0.4200
X	 0.0560	 0.2600

