



# wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 11:27 PM JST

PDB ID : 7YCA  
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 : 7D0J, 5ZJI

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

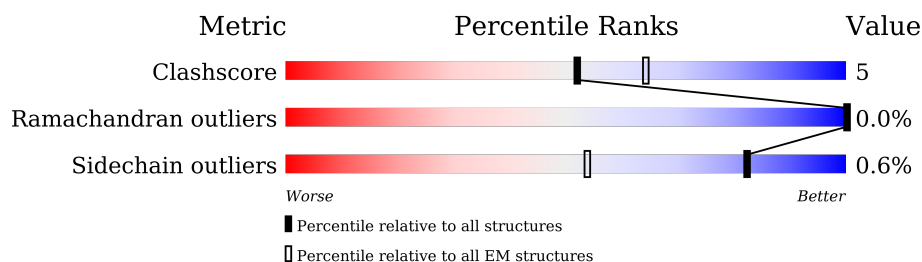
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
4	4	236	
5	5	217	
6	6	249	
7	A	751	
8	B	733	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
22	X	233	
23	Q	226	

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	-	-	-
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	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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 PsaG.

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 PsaH, 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		

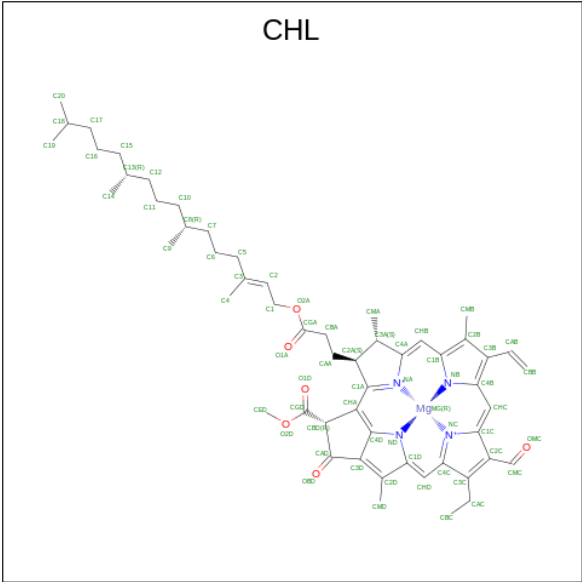
- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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 (three-letter code: 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...*

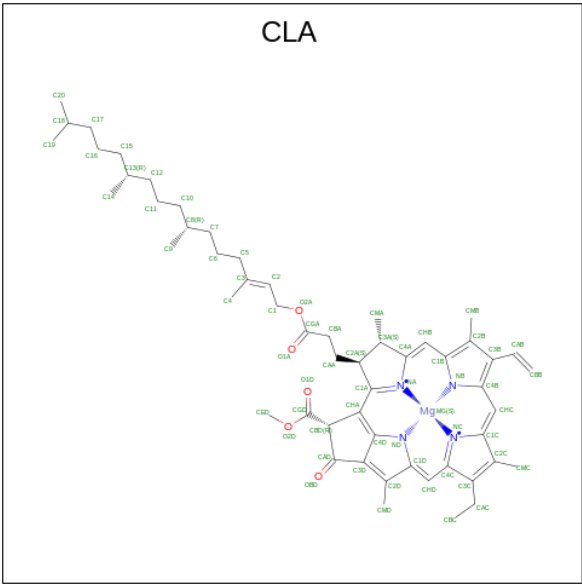
Mol	Chain	Residues	Atoms					AltConf
24	T	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	T	1	Total 49	C 38	Mg 1	N 4	O 6	0
24	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	T	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	T	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
24	U	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	U	1	Total 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 (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

*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...*

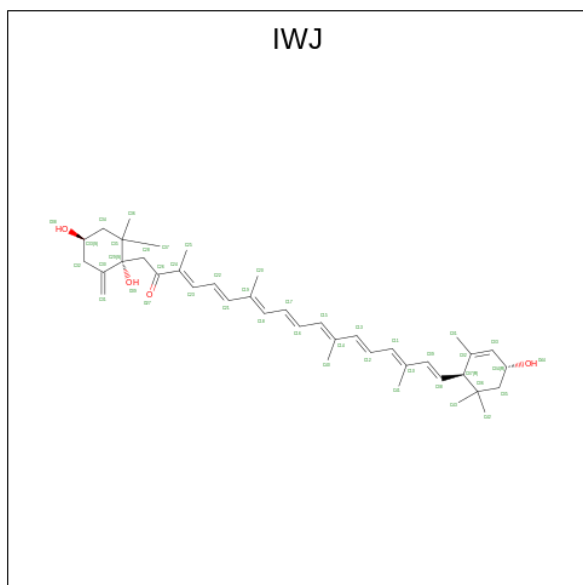
Mol	Chain	Residues	Atoms					AltConf
25	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	U	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	V	1	Total 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 (three-letter code: IWJ) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



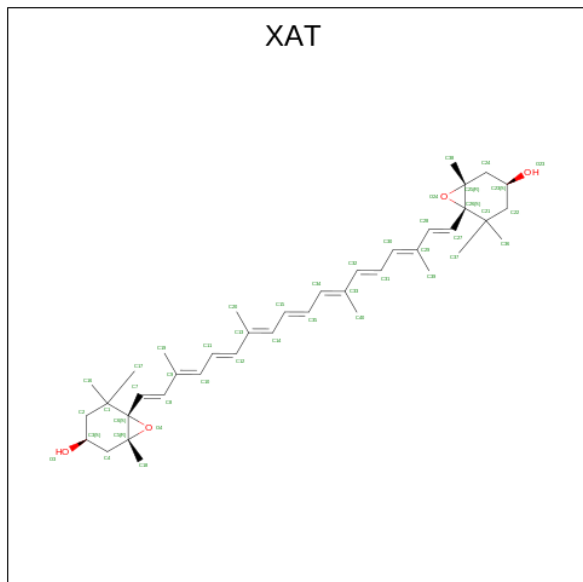
Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			44	40	4	
26	3	1	Total	C	O	0
			44	40	4	

Continued on next page...

*Continued from previous page...*

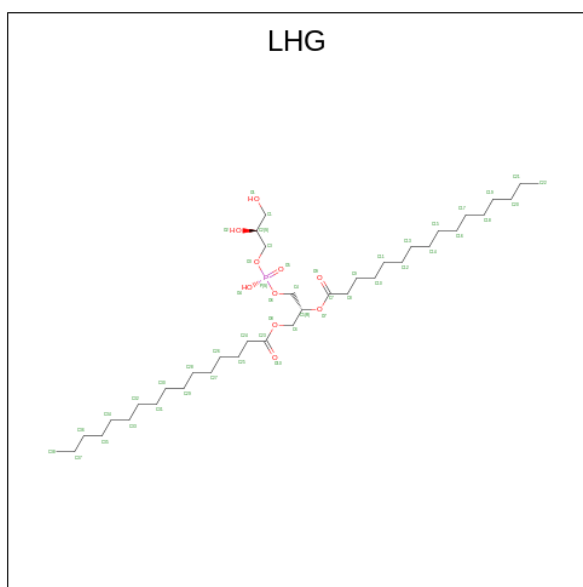
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total 44	C 40	O 4	0
26	4	1	Total 44	C 40	O 4	0
26	5	1	Total 44	C 40	O 4	0
26	6	1	Total 44	C 40	O 4	0
26	P	1	Total 44	C 40	O 4	0
26	P	1	Total 44	C 40	O 4	0
26	Q	1	Total 44	C 40	O 4	0
26	Q	1	Total 44	C 40	O 4	0
26	R	1	Total 44	C 40	O 4	0
26	R	1	Total 44	C 40	O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

- 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 (three-letter code: XAT) (formula:  $C_{40}H_{56}O_4$ ).



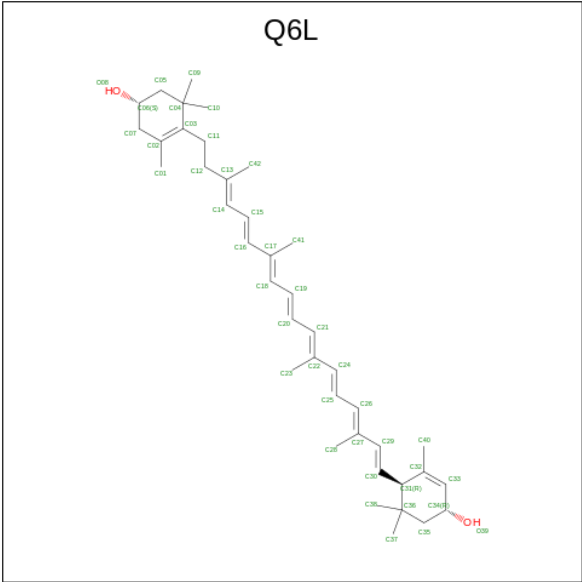
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



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 (three-letter code: Q6L) (formula: C<sub>40</sub>H<sub>58</sub>O<sub>2</sub>) (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...*

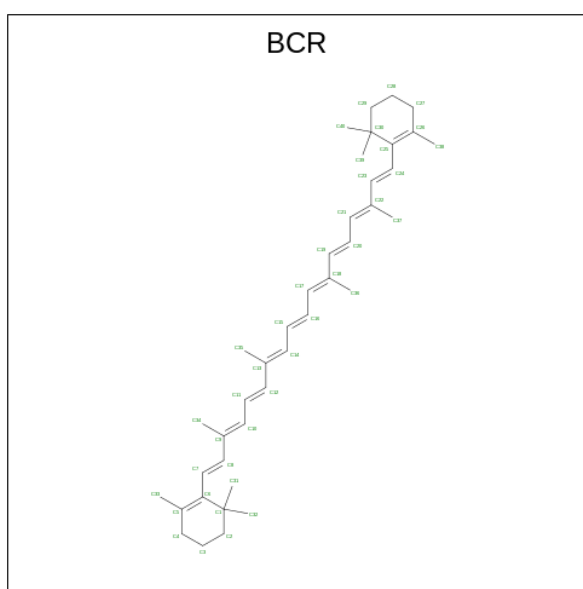
Mol	Chain	Residues	Atoms			AltConf
29	R	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	S	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O 2	0
29	T	1	Total 42	C 40	O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

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



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

*Continued on next page...*



*Continued from previous page...*

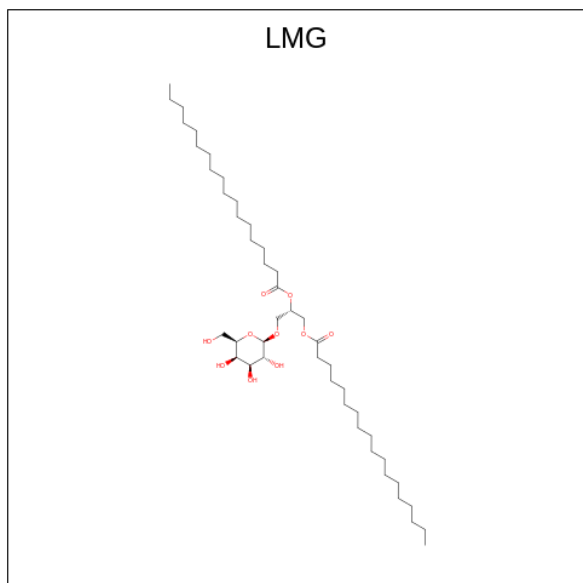
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	G	1	Total C 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 (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



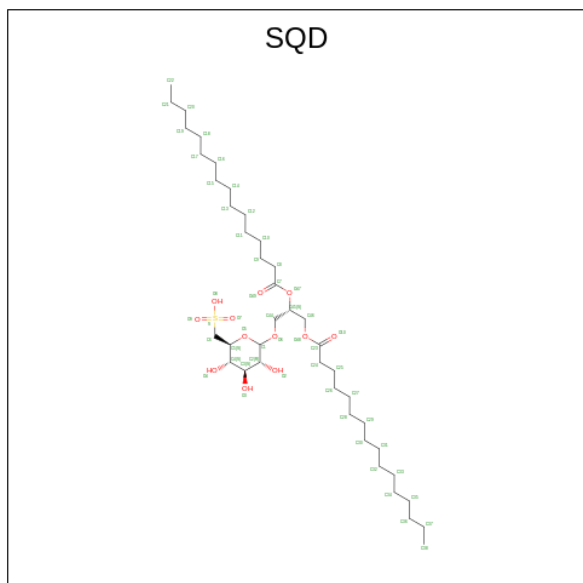
Mol	Chain	Residues	Atoms			AltConf
31	2	1	Total	C	O	0
			31	21	10	
31	5	1	Total	C	O	0
			54	44	10	
31	A	1	Total	C	O	0
			31	21	10	
31	A	1	Total	C	O	0
			27	17	10	
31	A	1	Total	C	O	0
			46	36	10	
31	B	1	Total	C	O	0
			38	28	10	
31	F	1	Total	C	O	0
			31	21	10	
31	J	1	Total	C	O	0
			46	36	10	
31	L	1	Total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

*Continued on next page...*

*Continued from previous page...*

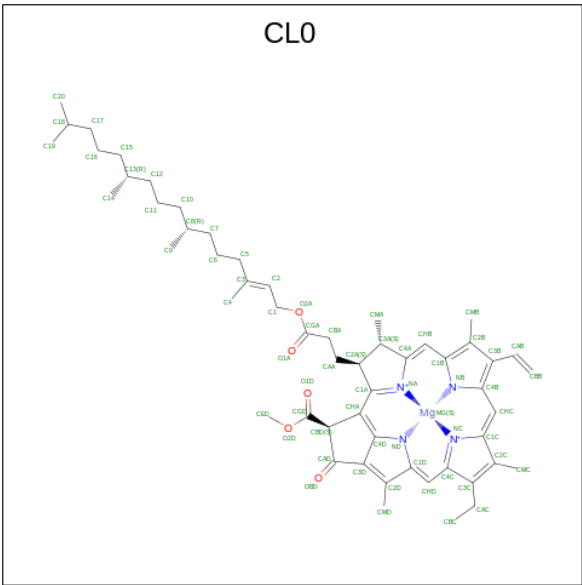
Mol	Chain	Residues	Atoms			AltConf
31	N	1	Total	C	O	0
			55	45	10	
31	O	1	Total	C	O	0
			39	29	10	

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



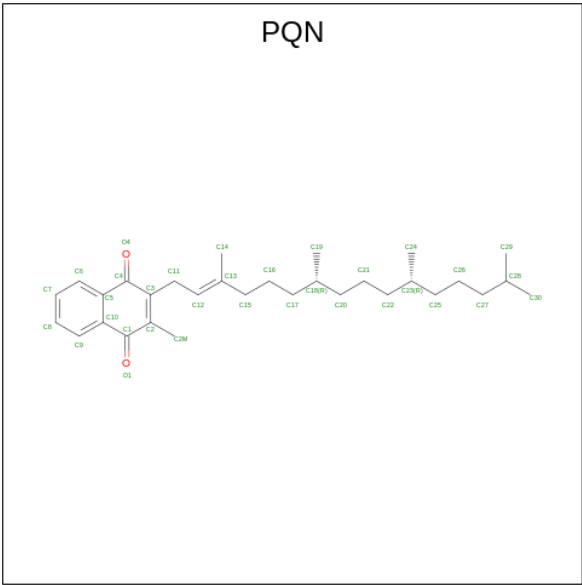
Mol	Chain	Residues	Atoms				AltConf
32	6	1	Total	C	O	S	0
			54	41	12	1	
32	H	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 33 is CHLOROPHYLL A ISOMER (three-letter code: 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 (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



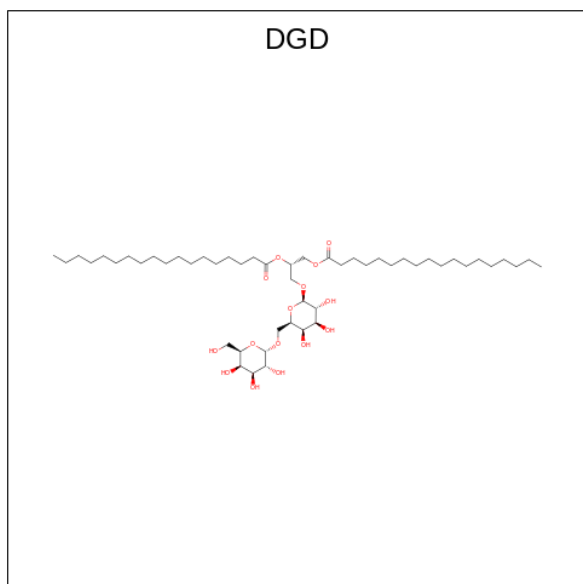
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			33	31	2	
34	B	1	Total	C	O	0
			33	31	2	

- Molecule 35 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



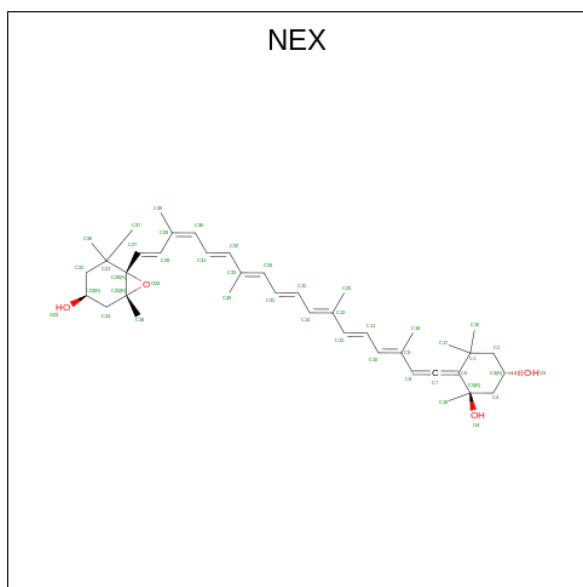
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	Fe	S	0
			8	4	4	
35	C	1	Total	Fe	S	0
			8	4	4	
35	C	1	Total	Fe	S	0
			8	4	4	

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



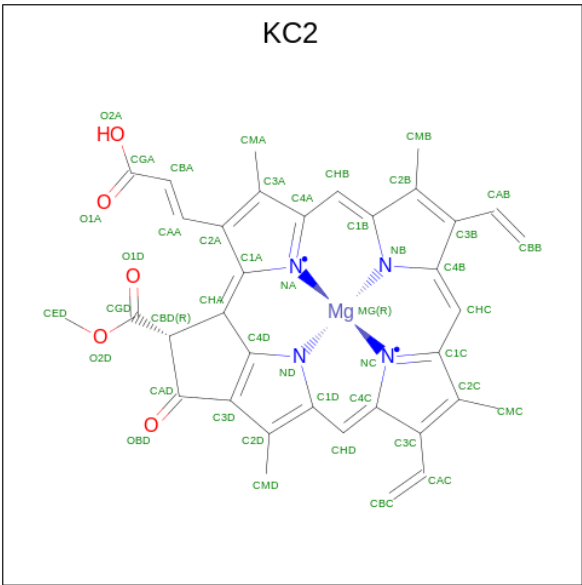
Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			51	36	15	
36	B	1	Total	C	O	0
			59	44	15	

- 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 (three-letter code: NEX) (formula:  $C_{40}H_{56}O_4$ ).



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 (three-letter code: KC2) (formula:  $C_{35}H_{28}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



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

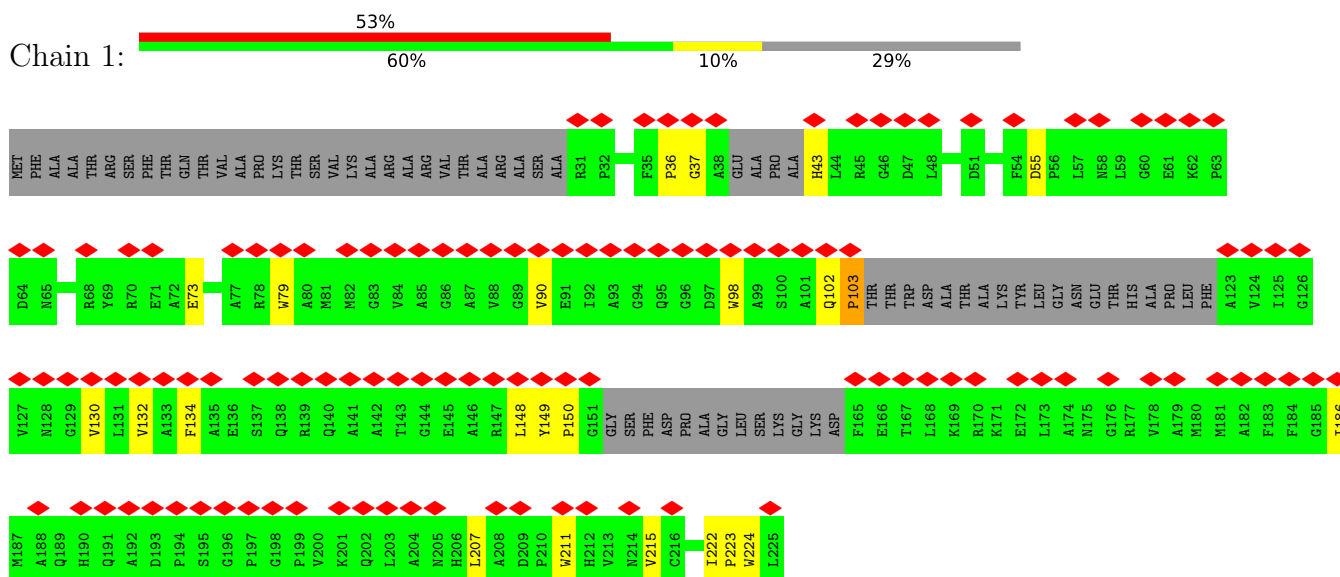
- Molecule 39 is water.

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

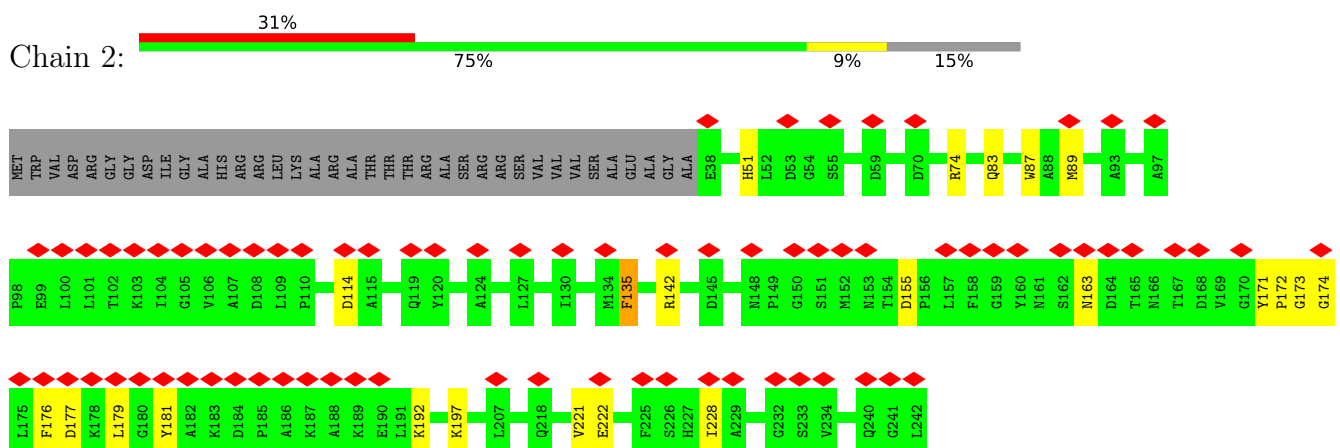
### 3 Residue-property plots

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



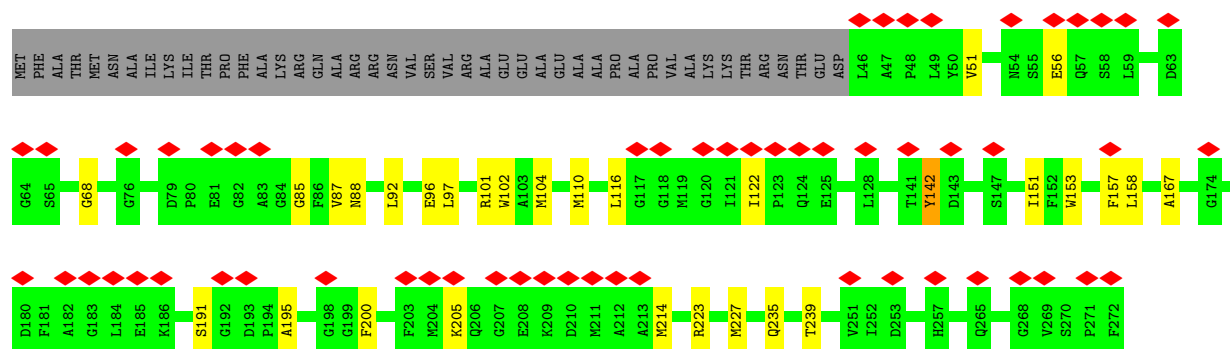
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



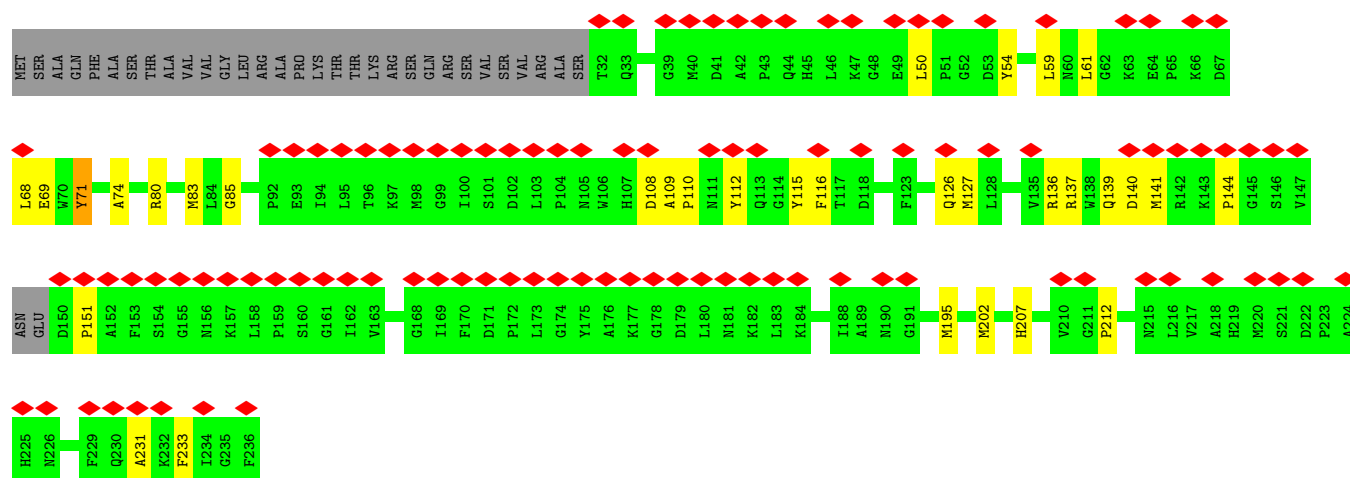
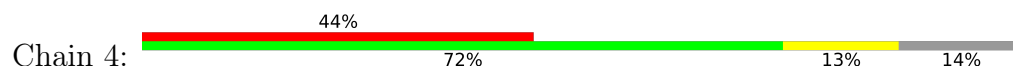
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



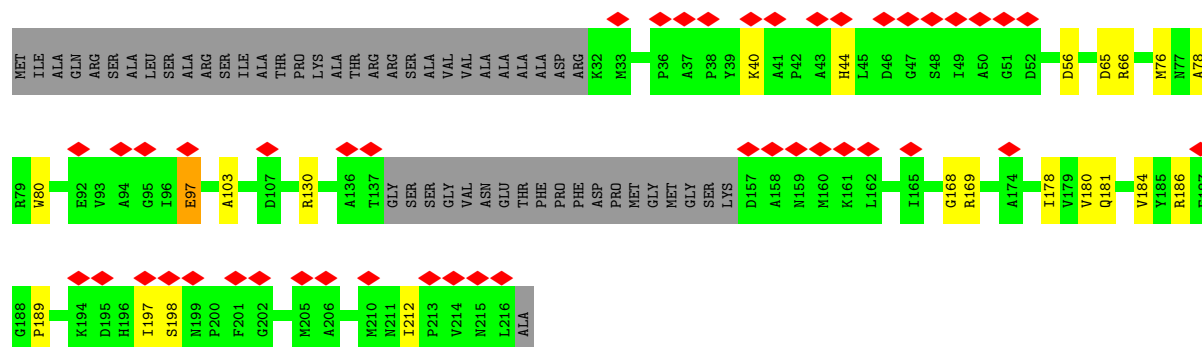




• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

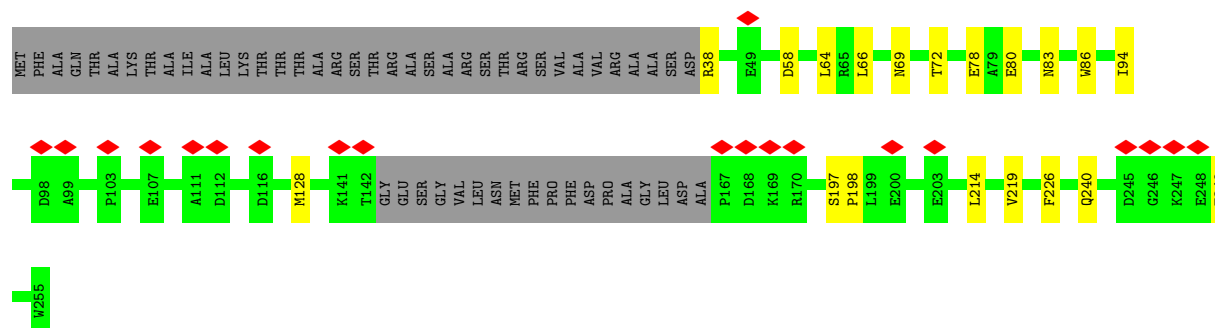


• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

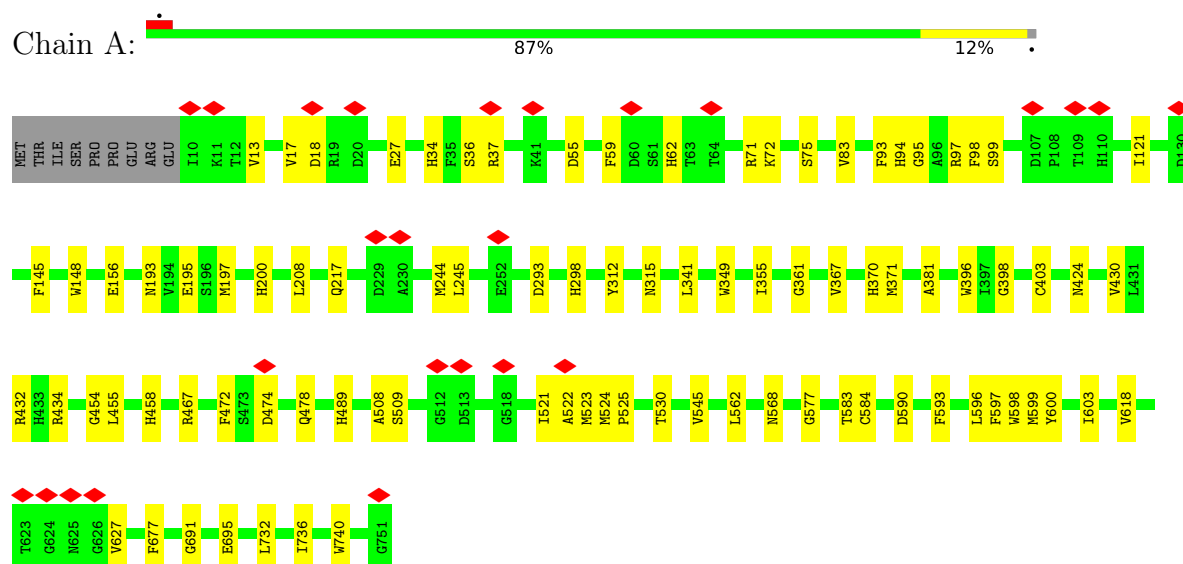


• Molecule 6: Lhca6

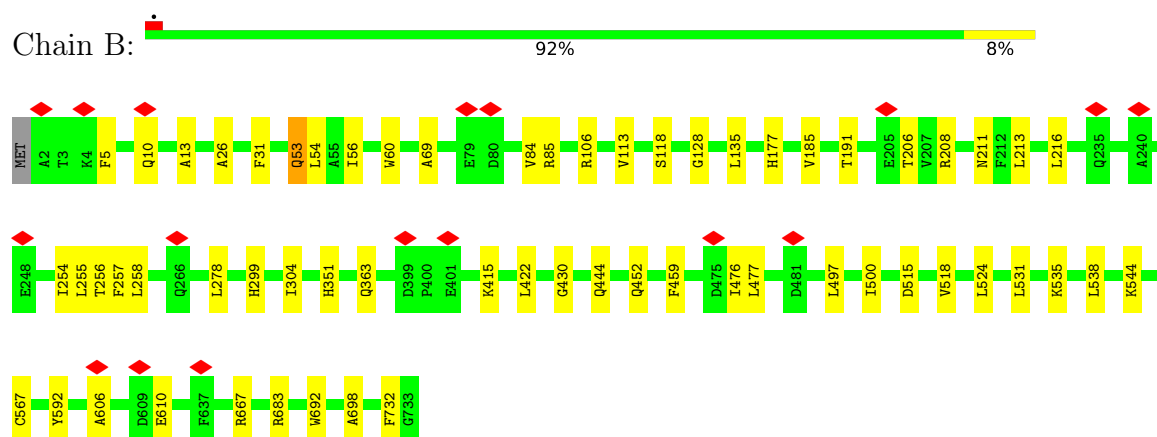




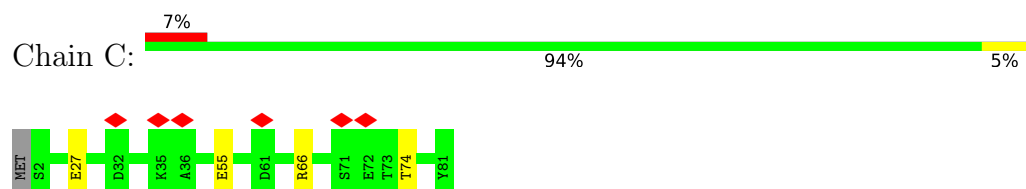
- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1



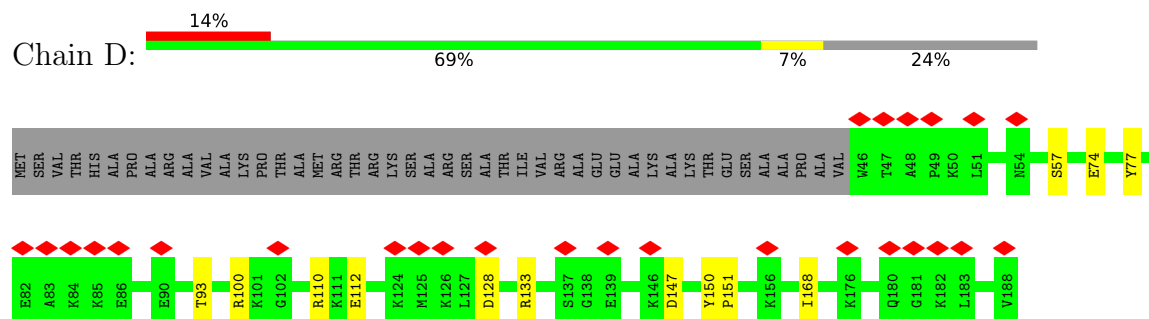
- Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2



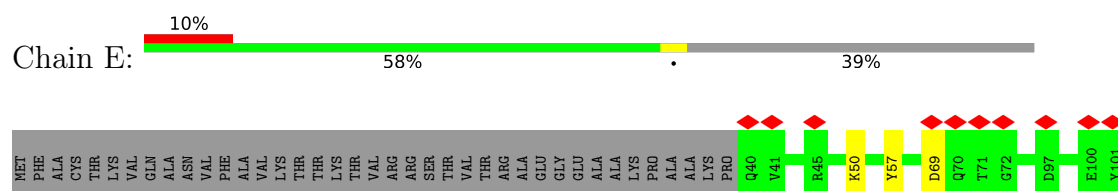
- Molecule 9: Photosystem I iron-sulfur center



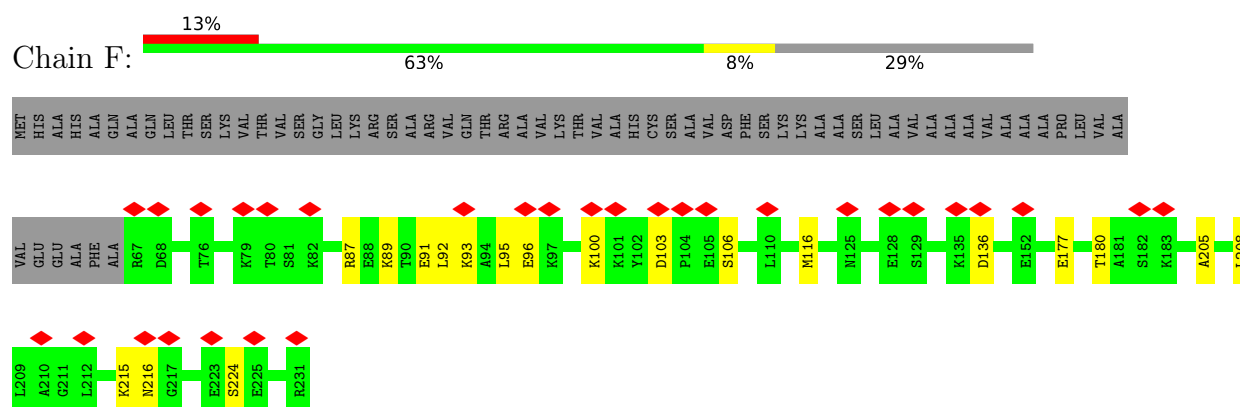
- Molecule 10: Photosystem I reaction center subunit II, chloroplastic



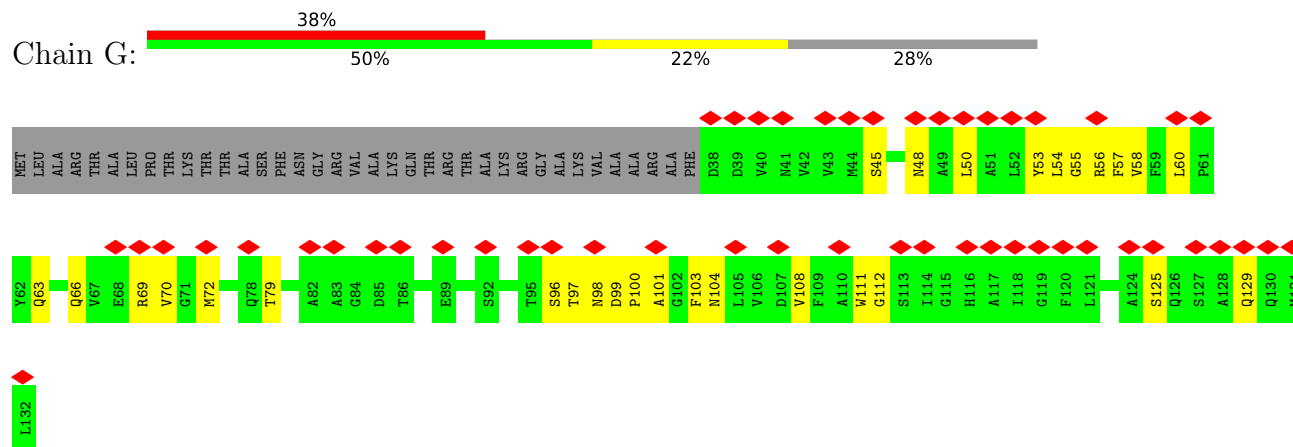
- Molecule 11: Photosystem I reaction centre subunit IV



- Molecule 12: Photosystem I reaction center subunit III



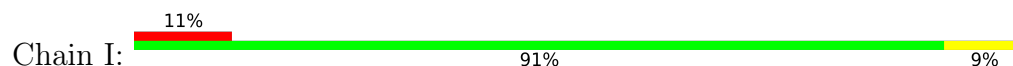
- Molecule 13: PsaG



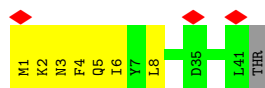
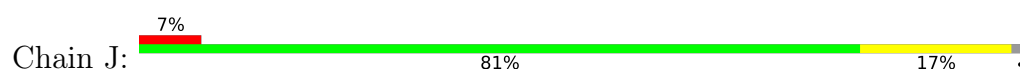
- Molecule 14: Photosystem I PsuH, reaction centre subunit VI



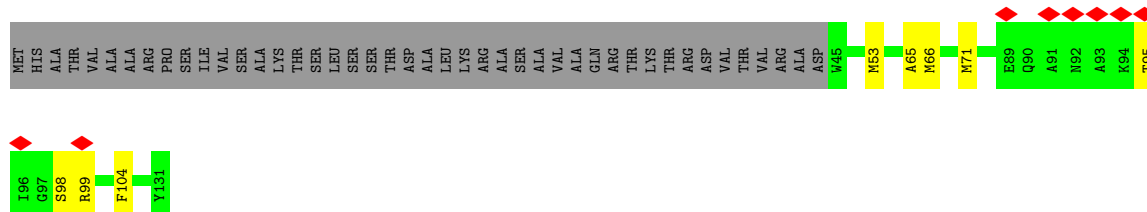
- Molecule 15: Photosystem I reaction center subunit VIII



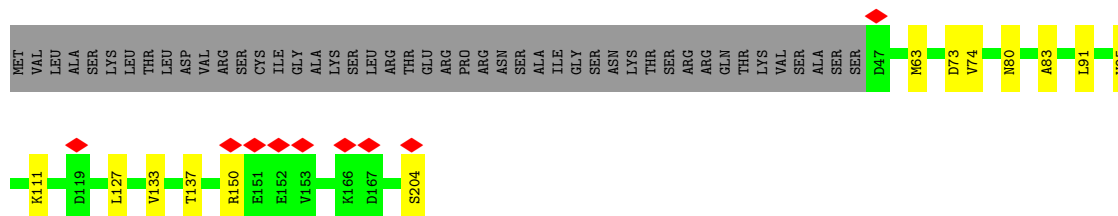
- Molecule 16: Photosystem I reaction center subunit IX



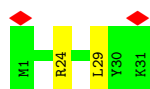
- Molecule 17: Photosystem I PsaG/PsaK protein



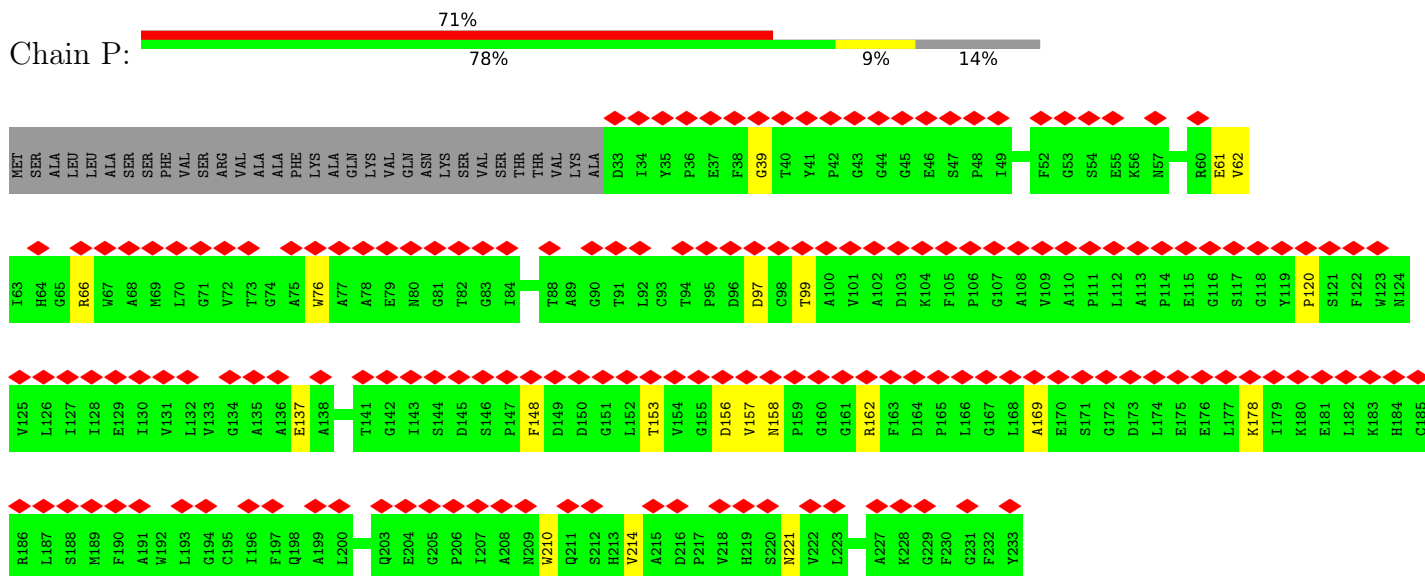
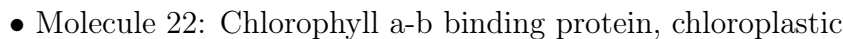
- Molecule 18: PSI subunit V



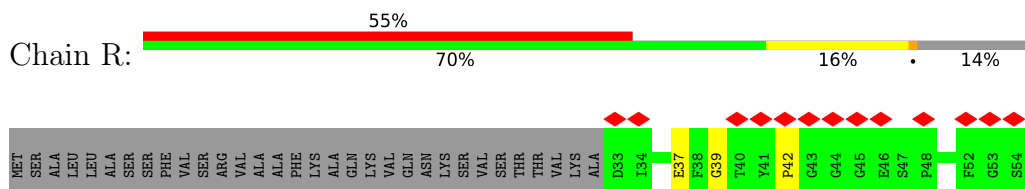
- Molecule 19: Photosystem I reaction center subunit XII

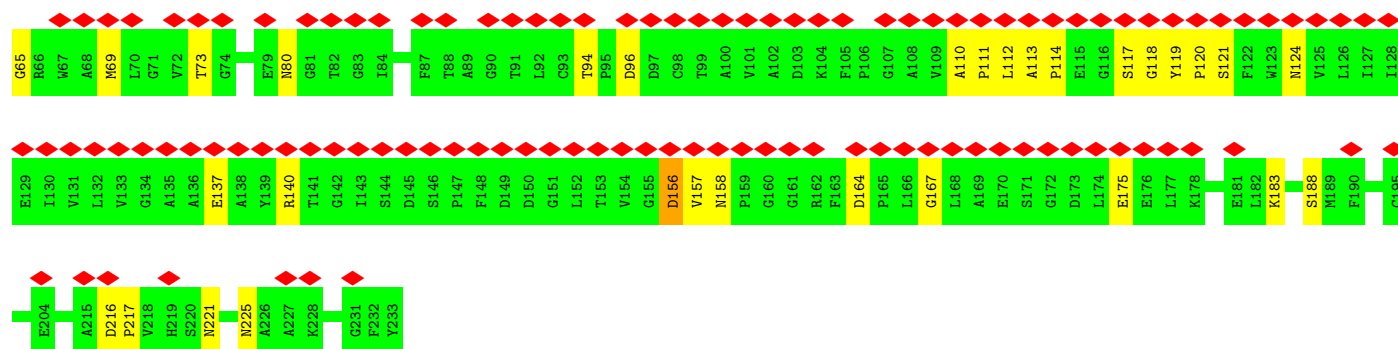


- Chain N:

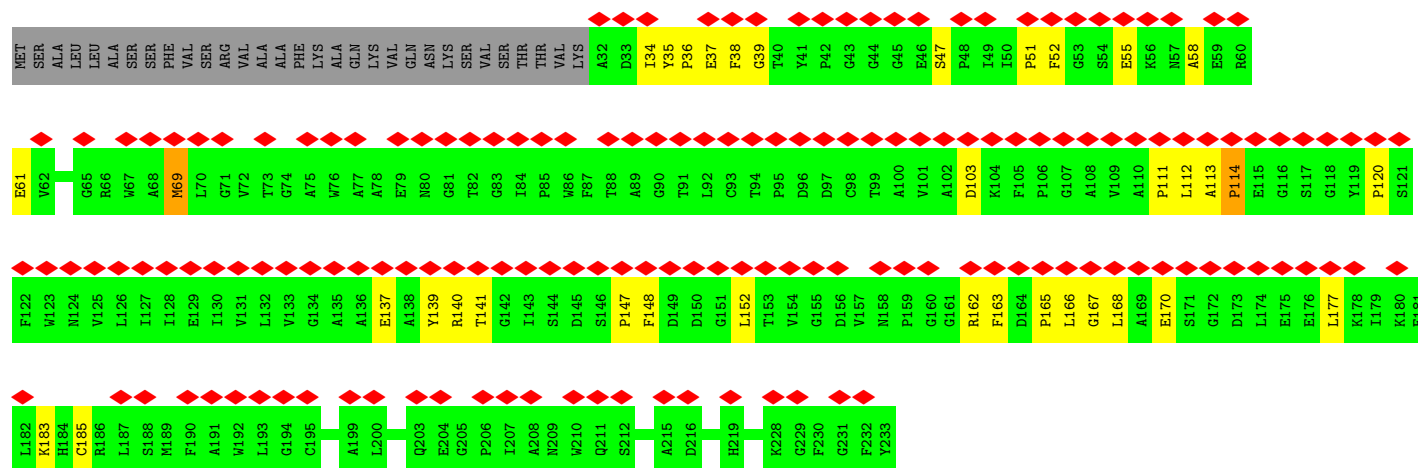


- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

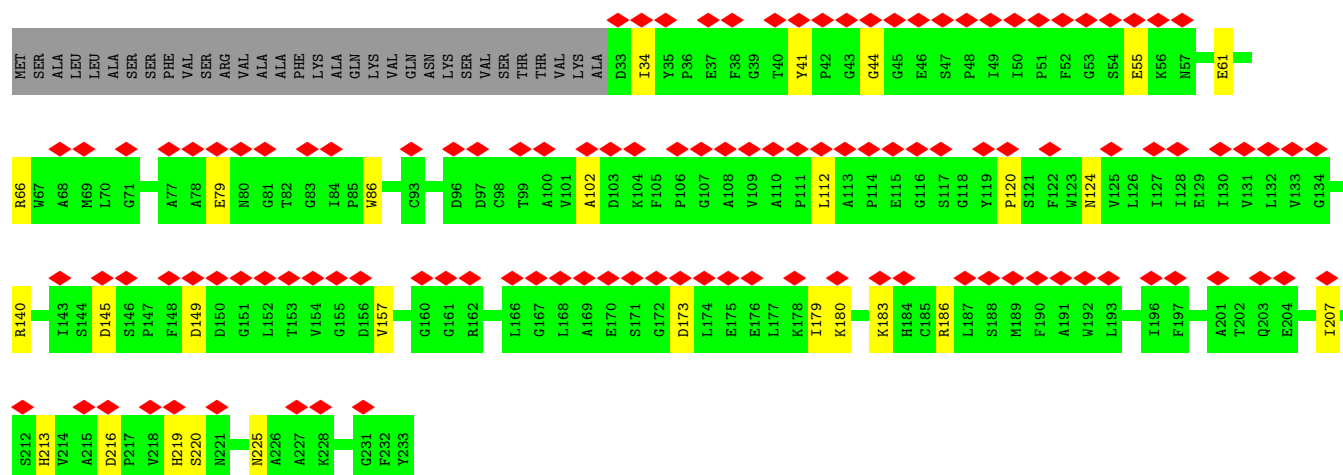
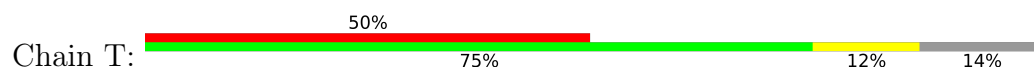




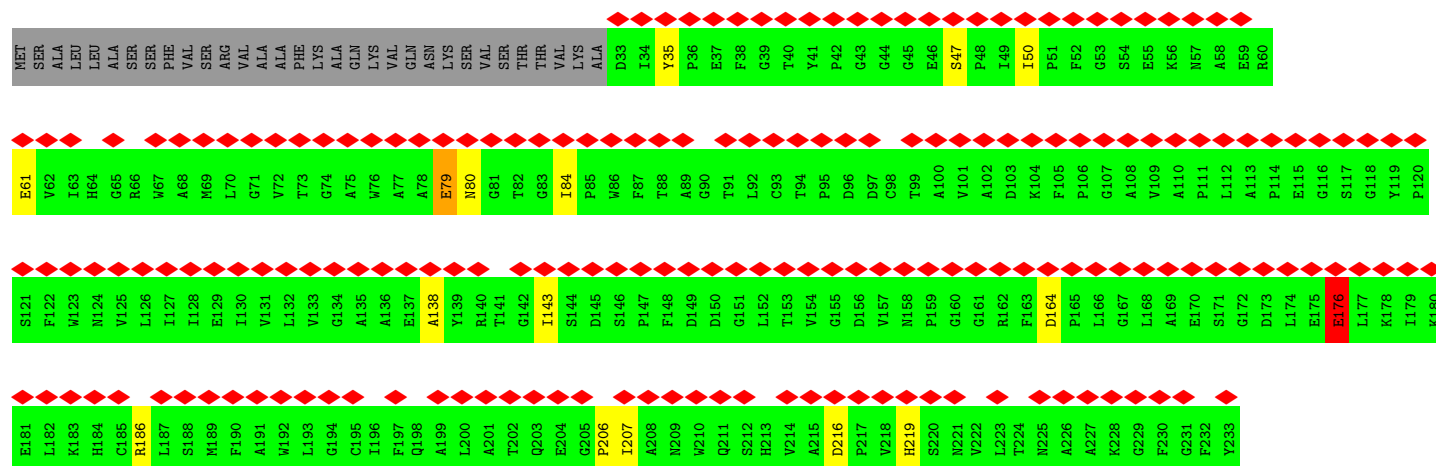
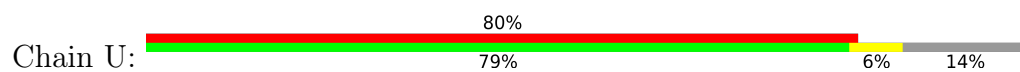
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



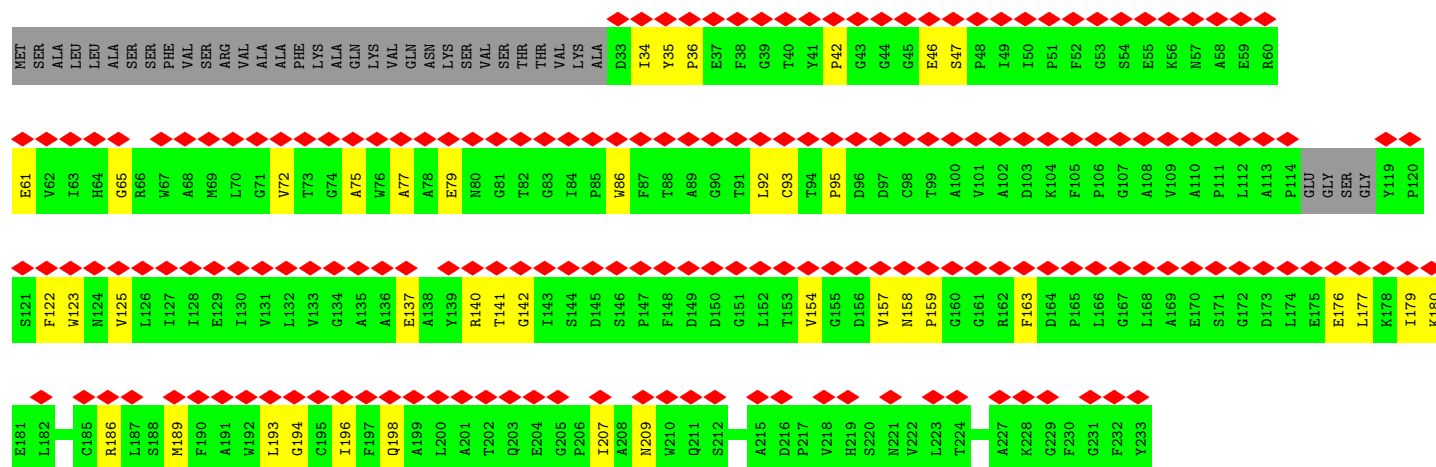
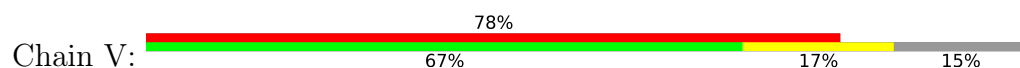
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



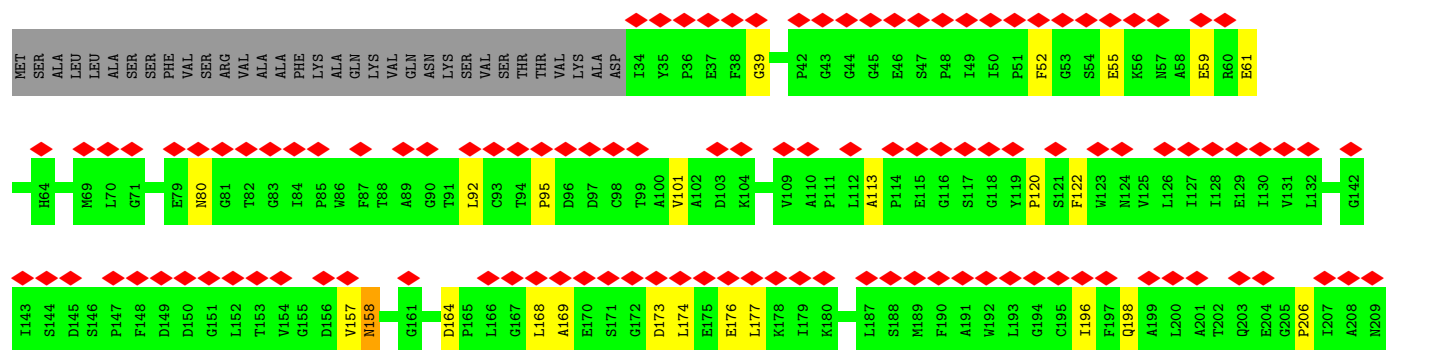
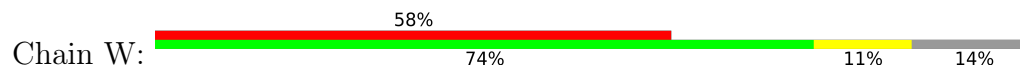
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

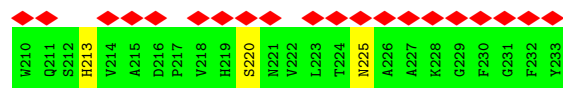


• Molecule 22: Chlorophyll a-b binding protein, chloroplastic



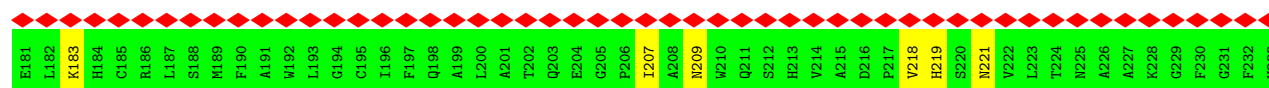
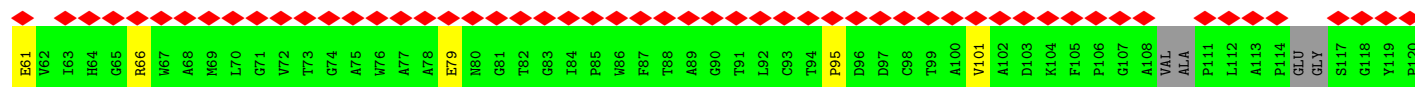
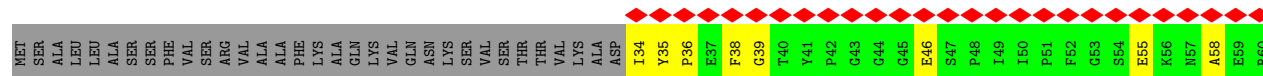
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic





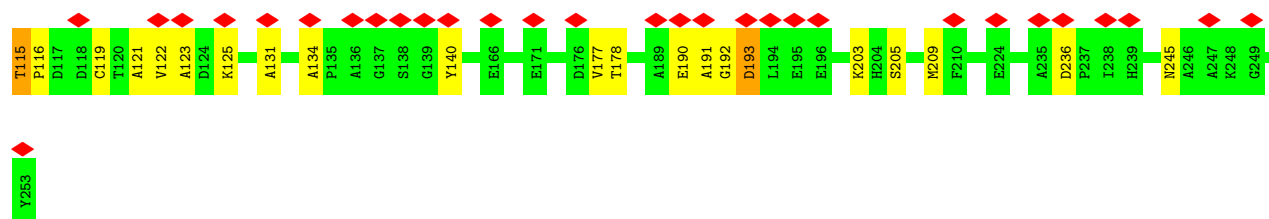
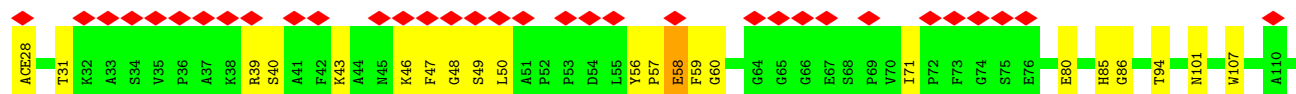
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain X: 84%  
72% 12% 16%



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

Chain Q: 28%  
81% 18%





## 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.61	2/1242 (0.2%)	0.79	3/1686 (0.2%)
2	2	0.57	3/1634 (0.2%)	0.70	1/2224 (0.0%)
3	3	0.56	1/1768 (0.1%)	0.78	1/2394 (0.0%)
4	4	0.54	2/1630 (0.1%)	0.71	1/2215 (0.0%)
5	5	0.54	1/1312 (0.1%)	0.73	1/1783 (0.1%)
6	6	0.46	0/1522	0.65	1/2068 (0.0%)
7	A	0.46	1/6017 (0.0%)	0.64	2/8202 (0.0%)
8	B	0.47	0/5981	0.64	0/8166
9	C	0.48	0/603	0.74	0/818
10	D	0.53	0/1142	0.82	2/1537 (0.1%)
11	E	0.46	0/516	0.77	1/703 (0.1%)
12	F	0.46	0/1286	0.67	0/1739
13	G	0.51	0/732	0.73	0/995
14	H	0.43	0/736	0.68	0/1001
15	I	0.59	0/270	0.72	0/368
16	J	0.46	0/338	0.61	0/462
17	K	0.45	0/635	0.66	0/860
18	L	0.46	0/1197	0.62	0/1635
19	M	0.46	0/242	0.62	0/328
20	N	0.49	0/685	0.75	1/921 (0.1%)
21	O	0.42	0/787	0.63	0/1070
22	P	0.50	1/1553 (0.1%)	0.73	1/2122 (0.0%)
22	R	0.49	0/1553	0.78	6/2122 (0.3%)
22	S	0.52	0/1558	0.72	3/2129 (0.1%)
22	T	0.48	0/1553	0.68	1/2122 (0.0%)
22	U	0.57	2/1553 (0.1%)	0.69	1/2122 (0.0%)
22	V	0.55	1/1529 (0.1%)	0.70	2/2089 (0.1%)
22	W	0.56	1/1545 (0.1%)	0.67	1/2111 (0.0%)
22	X	0.50	0/1518	0.68	1/2070 (0.0%)
23	Q	0.58	2/1746 (0.1%)	0.76	3/2379 (0.1%)
All	All	0.51	17/44383 (0.0%)	0.69	33/60441 (0.1%)

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 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	79	GLU	CG-CD	-9.89	1.37	1.51
1	1	103	PRO	CB-CG	9.36	1.96	1.50
23	Q	80	GLU	CD-OE1	-9.19	1.15	1.25
4	4	69	GLU	CD-OE1	-7.71	1.17	1.25
4	4	71	TYR	CD1-CE1	-6.08	1.30	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	69	GLU	OE1-CD-OE2	-11.52	109.47	123.30
10	D	147	ASP	CB-CG-OD1	10.91	128.12	118.30
1	1	102	GLN	C-N-CD	8.90	147.10	128.40
22	R	216	ASP	CB-CG-OD1	8.57	126.02	118.30
11	E	69	ASP	CB-CG-OD2	-8.19	110.93	118.30

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	18	0
2	2	1583	0	1529	19	0
3	3	1717	0	1657	23	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	17	0
6	6	1484	0	1465	13	0
7	A	5819	0	5655	69	0
8	B	5773	0	5540	48	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	15	0
13	G	717	0	685	34	0
14	H	721	0	698	8	0
15	I	264	0	286	10	0
16	J	328	0	341	6	0
17	K	625	0	625	10	0
18	L	1169	0	1186	8	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	19	0
22	R	1507	0	1429	40	0
22	S	1512	0	1434	33	0
22	T	1507	0	1429	19	0
22	U	1507	0	1429	11	0
22	V	1484	0	1411	35	0
22	W	1499	0	1425	23	0
22	X	1474	0	1401	26	0
23	Q	1706	0	1649	36	0
24	1	96	0	68	1	0
24	2	177	0	115	2	0
24	3	45	0	30	1	0
24	4	181	0	117	3	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	1	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	9	0
25	2	530	0	430	11	0
25	3	602	0	470	13	0
25	4	510	0	396	6	0
25	5	430	0	345	8	0
25	6	494	0	412	9	0
25	A	2557	0	2585	28	0
25	B	2465	0	2485	38	0
25	F	83	0	60	2	0
25	G	132	0	97	3	0
25	H	154	0	138	1	0
25	J	42	0	31	1	0
25	K	218	0	201	3	0
25	L	188	0	152	2	0
25	N	87	0	61	1	0
25	O	247	0	217	2	0
25	P	467	0	454	5	0
25	Q	458	0	387	10	0
25	R	467	0	454	8	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	15	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	2	0
26	4	88	0	0	3	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	1	0
27	3	44	0	56	2	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	1	0
27	6	44	0	56	2	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	2	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	2	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	5	0
30	B	200	0	280	2	0
30	F	80	0	112	1	0
30	G	80	0	112	5	0
30	H	40	0	56	0	0
30	I	40	0	56	0	0
30	J	80	0	112	4	0
30	K	120	0	168	2	0
30	L	120	0	168	3	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	1	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	634	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 634 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
13:G:53:TYR:CE1	13:G:57:PHE:CE2	2.38	1.12

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%)	19	41
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%)	25	50
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%)	117 (99%)	1 (1%)	79	87
2	2	160/186 (86%)	159 (99%)	1 (1%)	84	90
3	3	173/208 (83%)	171 (99%)	2 (1%)	67	81
4	4	159/186 (86%)	158 (99%)	1 (1%)	84	90
5	5	127/163 (78%)	124 (98%)	3 (2%)	44	68
6	6	148/188 (79%)	146 (99%)	2 (1%)	62	79
7	A	600/609 (98%)	598 (100%)	2 (0%)	91	95
8	B	584/585 (100%)	583 (100%)	1 (0%)	92	96
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%)	129 (99%)	1 (1%)	79	87
13	G	73/99 (74%)	72 (99%)	1 (1%)	62	79

*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%)	124 (99%)	1 (1%)	79	87
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%)	152 (99%)	1 (1%)	81	89
22	R	153/179 (86%)	152 (99%)	1 (1%)	81	89
22	S	153/179 (86%)	152 (99%)	1 (1%)	81	89
22	T	153/179 (86%)	151 (99%)	2 (1%)	65	80
22	U	153/179 (86%)	152 (99%)	1 (1%)	81	89
22	V	151/179 (84%)	151 (100%)	0	100	100
22	W	152/179 (85%)	151 (99%)	1 (1%)	81	89
22	X	150/179 (84%)	148 (99%)	2 (1%)	65	80
23	Q	167/167 (100%)	165 (99%)	2 (1%)	67	81
All	All	4402/5166 (85%)	4375 (99%)	27 (1%)	82	90

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	G	125	SER
23	Q	58	GLU
22	W	158	ASN
22	P	178	LYS
23	Q	190	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	209	ASN
22	W	209	ASN
16	J	3	ASN
16	J	5	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	P	158	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	1.69	1 (12%)	10,14,16	1.11	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	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Q	31	TPO	P-O1P	3.45	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	-2.28	116.33	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Q	31	TPO	O-C-CA-CB
23	Q	31	TPO	CB-OG1-P-O1P

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$
31	LMG	F	805	-	31,31,55	1.15	2 (6%)	39,39,63	1.12	3 (7%)
31	LMG	O	2008	-	39,39,55	1.06	2 (5%)	47,47,63	1.14	3 (6%)
25	CLA	V	301	22	60,68,73	1.48	5 (8%)	70,107,113	1.74	11 (15%)
24	CHL	5	605	-	40,49,74	1.81	6 (15%)	41,84,114	1.72	7 (17%)
29	Q6L	T	319	-	42,43,43	1.85	7 (16%)	47,60,60	1.46	5 (10%)
25	CLA	W	312	22	55,63,73	1.60	7 (12%)	64,101,113	1.79	13 (20%)
25	CLA	A	813	-	65,73,73	1.46	8 (12%)	76,113,113	1.28	7 (9%)
25	CLA	B	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.69	15 (19%)
25	CLA	H	302	-	65,73,73	1.47	7 (10%)	76,113,113	1.59	12 (15%)
25	CLA	B	821	-	55,63,73	1.71	8 (14%)	64,101,113	1.49	11 (17%)
35	SF4	C	101	9	0,12,12	-	-	-	-	-
24	CHL	T	307	-	44,52,74	1.76	6 (13%)	46,87,114	1.75	6 (13%)
25	CLA	R	316	22	55,63,73	1.62	5 (9%)	64,101,113	1.74	11 (17%)
25	CLA	A	823	39	65,73,73	1.57	9 (13%)	76,113,113	1.55	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CHL	2	605	-	42,50,74	1.92	8 (19%)	45,85,114	1.47	5 (11%)
25	CLA	R	313	22	64,72,73	1.54	7 (10%)	74,111,113	1.51	11 (14%)
24	CHL	R	318	22	45,53,74	1.80	6 (13%)	46,88,114	1.54	8 (17%)
25	CLA	B	836	8	60,68,73	1.58	8 (13%)	70,107,113	1.46	9 (12%)
25	CLA	Q	315	-	48,56,73	1.70	7 (14%)	55,92,113	1.62	10 (18%)
24	CHL	2	607	-	45,53,74	1.77	8 (17%)	46,88,114	1.58	8 (17%)
30	BCR	4	319	-	41,41,41	1.33	5 (12%)	56,56,56	2.31	23 (41%)
25	CLA	V	309	22	42,50,73	2.12	9 (21%)	48,85,113	2.06	14 (29%)
25	CLA	N	202	20	44,53,73	1.81	7 (15%)	50,89,113	1.45	5 (10%)
25	CLA	A	826	-	55,63,73	1.59	8 (14%)	64,101,113	1.47	7 (10%)
24	CHL	W	306	-	52,60,74	1.60	8 (15%)	56,97,114	2.11	14 (25%)
25	CLA	A	828	-	59,67,73	1.53	10 (16%)	68,105,113	1.42	11 (16%)
34	PQN	B	844	-	34,34,34	2.96	11 (32%)	42,45,45	2.05	7 (16%)
24	CHL	T	314	22	42,50,74	1.79	6 (14%)	44,85,114	1.69	8 (18%)
25	CLA	K	201	17	45,53,73	1.77	5 (11%)	52,89,113	1.96	12 (23%)
30	BCR	J	101	-	41,41,41	1.25	4 (9%)	56,56,56	2.59	24 (42%)
31	LMG	2	620	-	31,31,55	1.18	2 (6%)	39,39,63	1.28	4 (10%)
24	CHL	V	304	22	46,54,74	1.78	8 (17%)	49,90,114	1.49	8 (16%)
35	SF4	A	853	7,8	0,12,12	-	-	-	-	-
30	BCR	L	305	-	41,41,41	1.05	1 (2%)	56,56,56	2.31	20 (35%)
30	BCR	I	101	-	41,41,41	1.02	3 (7%)	56,56,56	2.42	22 (39%)
25	CLA	S	309	22	60,68,73	1.58	8 (13%)	70,107,113	1.36	10 (14%)
25	CLA	6	604	-	43,51,73	1.82	7 (16%)	48,86,113	1.53	7 (14%)
28	LHG	3	323	-	42,42,48	1.00	2 (4%)	45,48,54	0.92	3 (6%)
25	CLA	B	817	-	43,51,73	1.78	8 (18%)	49,86,113	1.57	7 (14%)
24	CHL	X	305	22	42,50,74	1.85	5 (11%)	44,85,114	1.43	8 (18%)
30	BCR	B	848	-	41,41,41	1.30	4 (9%)	56,56,56	2.23	18 (32%)
25	CLA	R	307	-	50,58,73	1.71	7 (14%)	58,95,113	1.50	7 (12%)
25	CLA	S	311	-	47,55,73	1.69	6 (12%)	54,91,113	1.71	9 (16%)
25	CLA	A	816	-	45,53,73	1.73	8 (17%)	52,89,113	1.64	8 (15%)
25	CLA	5	601	5	46,54,73	1.76	8 (17%)	53,90,113	1.76	13 (24%)
25	CLA	W	302	-	55,63,73	1.61	8 (14%)	64,101,113	1.34	8 (12%)
25	CLA	B	826	-	65,73,73	1.52	10 (15%)	76,113,113	1.67	15 (19%)
25	CLA	5	604	-	37,46,73	2.03	7 (18%)	46,81,113	1.50	8 (17%)
25	CLA	2	609	2	55,63,73	1.54	9 (16%)	64,101,113	1.44	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	X	314	-	41,49,73	1.85	7 (17%)	47,84,113	1.55	8 (17%)
25	CLA	Q	313	-	46,54,73	1.72	8 (17%)	53,90,113	1.66	9 (16%)
30	BCR	A	848	-	41,41,41	1.36	5 (12%)	56,56,56	2.12	19 (33%)
25	CLA	5	609	-	53,62,73	1.64	5 (9%)	61,100,113	1.43	8 (13%)
32	SQD	6	617	-	53,54,54	1.19	4 (7%)	62,65,65	1.13	5 (8%)
25	CLA	1	608	1	65,73,73	1.54	10 (15%)	76,113,113	1.36	10 (13%)
25	CLA	B	824	-	60,68,73	1.59	9 (15%)	70,107,113	1.46	7 (10%)
25	CLA	B	835	-	45,53,73	1.82	8 (17%)	52,89,113	1.36	8 (15%)
25	CLA	L	303	-	45,53,73	1.76	5 (11%)	52,89,113	1.86	13 (25%)
30	BCR	G	201	-	41,41,41	1.13	3 (7%)	56,56,56	2.21	19 (33%)
26	IWJ	V	320	-	43,45,45	1.16	5 (11%)	43,65,65	1.13	2 (4%)
25	CLA	B	839	-	65,73,73	1.55	9 (13%)	76,113,113	1.38	7 (9%)
25	CLA	B	811	8	65,73,73	1.48	11 (16%)	76,113,113	1.48	8 (10%)
29	Q6L	R	320	-	42,43,43	1.88	7 (16%)	47,60,60	1.40	5 (10%)
30	BCR	B	845	-	41,41,41	1.32	5 (12%)	56,56,56	2.71	25 (44%)
25	CLA	V	302	-	50,58,73	1.70	9 (18%)	58,95,113	1.47	11 (18%)
25	CLA	A	819	-	60,68,73	1.51	7 (11%)	70,107,113	1.59	10 (14%)
25	CLA	6	610	-	61,69,73	1.52	8 (13%)	71,108,113	1.32	10 (14%)
25	CLA	B	808	8	65,73,73	1.47	10 (15%)	76,113,113	1.44	14 (18%)
25	CLA	K	203	-	62,70,73	1.50	8 (12%)	72,109,113	1.56	11 (15%)
25	CLA	X	310	22	42,50,73	1.82	7 (16%)	48,85,113	1.58	9 (18%)
24	CHL	Q	307	23	46,54,74	1.63	4 (8%)	49,90,114	1.65	10 (20%)
36	DGD	A	854	-	52,52,67	1.05	3 (5%)	66,66,81	1.21	7 (10%)
25	CLA	5	606	-	40,48,73	1.89	6 (15%)	50,83,113	1.75	10 (20%)
25	CLA	W	303	-	50,58,73	1.65	8 (16%)	58,95,113	1.68	11 (18%)
25	CLA	R	305	22	65,73,73	1.52	7 (10%)	76,113,113	1.50	12 (15%)
24	CHL	4	302	4	52,60,74	1.63	9 (17%)	56,97,114	1.90	16 (28%)
25	CLA	A	824	-	42,50,73	1.86	7 (16%)	48,85,113	1.62	7 (14%)
25	CLA	S	312	22	55,63,73	1.63	8 (14%)	64,101,113	1.37	9 (14%)
25	CLA	4	315	-	41,49,73	1.85	5 (12%)	47,84,113	1.49	9 (19%)
24	CHL	V	314	22	44,52,74	1.79	7 (15%)	46,87,114	1.66	10 (21%)
37	NEX	T	317	-	38,46,46	1.26	4 (10%)	50,70,70	2.54	15 (30%)
30	BCR	K	202	-	41,41,41	1.26	7 (17%)	56,56,56	2.59	24 (42%)
32	SQD	H	303	-	47,48,54	1.30	4 (8%)	56,59,65	1.14	3 (5%)
26	IWJ	4	301	-	43,45,45	1.17	4 (9%)	43,65,65	1.09	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	Q	305	-	44,52,73	1.76	8 (18%)	49,87,113	1.47	7 (14%)
28	LHG	A	846	-	48,48,48	0.93	2 (4%)	51,54,54	0.98	2 (3%)
25	CLA	B	809	-	65,73,73	1.47	10 (15%)	76,113,113	1.46	14 (18%)
25	CLA	L	302	-	60,68,73	1.64	9 (15%)	70,107,113	1.58	9 (12%)
24	CHL	S	304	22	42,50,74	1.94	8 (19%)	44,85,114	1.77	9 (20%)
25	CLA	U	310	-	44,52,73	1.83	7 (15%)	49,87,113	1.46	10 (20%)
25	CLA	F	802	-	42,50,73	1.80	9 (21%)	48,85,113	1.59	11 (22%)
25	CLA	2	606	-	45,53,73	1.79	9 (20%)	52,89,113	1.66	8 (15%)
24	CHL	V	307	-	44,52,74	1.74	5 (11%)	46,87,114	1.53	9 (19%)
29	Q6L	R	319	-	42,43,43	1.90	7 (16%)	47,60,60	1.47	4 (8%)
30	BCR	3	318	-	41,41,41	1.30	6 (14%)	56,56,56	2.17	19 (33%)
25	CLA	P	309	22	64,72,73	1.45	5 (7%)	74,111,113	1.64	14 (18%)
25	CLA	3	310	-	43,51,73	1.76	6 (13%)	49,86,113	1.53	8 (16%)
25	CLA	B	829	-	65,73,73	1.44	8 (12%)	76,113,113	1.66	11 (14%)
29	Q6L	P	315	-	42,43,43	1.92	8 (19%)	47,60,60	1.38	5 (10%)
30	BCR	A	851	-	41,41,41	0.98	2 (4%)	56,56,56	2.42	22 (39%)
24	CHL	V	306	-	44,52,74	1.75	7 (15%)	46,87,114	1.96	12 (26%)
26	IWJ	Q	320	-	43,45,45	1.12	4 (9%)	43,65,65	1.29	7 (16%)
29	Q6L	T	322	-	42,43,43	1.91	8 (19%)	47,60,60	1.45	4 (8%)
24	CHL	W	314	22	40,49,74	1.84	6 (15%)	42,83,114	1.99	10 (23%)
25	CLA	2	611	2	43,52,73	1.75	6 (13%)	49,88,113	1.60	8 (16%)
29	Q6L	2	616	-	42,43,43	1.82	7 (16%)	47,60,60	1.54	8 (17%)
38	KC2	W	308	22	48,53,53	2.57	16 (33%)	54,89,89	2.32	20 (37%)
38	KC2	V	308	22	48,53,53	2.53	16 (33%)	54,89,89	2.21	19 (35%)
25	CLA	6	602	6	62,70,73	1.43	5 (8%)	72,109,113	1.63	11 (15%)
25	CLA	5	610	-	41,49,73	1.87	6 (14%)	47,84,113	1.46	8 (17%)
25	CLA	1	609	-	37,46,73	1.97	6 (16%)	46,81,113	1.74	11 (23%)
25	CLA	T	303	-	50,58,73	1.72	8 (16%)	58,95,113	1.51	6 (10%)
38	KC2	X	309	22	48,53,53	2.57	16 (33%)	54,89,89	2.54	21 (38%)
25	CLA	W	311	-	45,53,73	1.68	6 (13%)	52,89,113	1.62	8 (15%)
25	CLA	V	311	-	60,68,73	1.51	7 (11%)	70,107,113	1.40	11 (15%)
25	CLA	2	604	-	43,51,73	1.81	6 (13%)	48,86,113	1.53	8 (16%)
25	CLA	B	843	28	65,73,73	1.47	8 (12%)	76,113,113	1.59	10 (13%)
28	LHG	3	321	-	42,42,48	1.00	2 (4%)	45,48,54	0.89	1 (2%)
27	XAT	6	615	-	39,47,47	1.09	2 (5%)	54,74,74	2.99	25 (46%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	3	302	-	55,63,73	1.68	8 (14%)	64,101,113	1.93	17 (26%)
29	Q6L	S	323	-	42,43,43	1.86	6 (14%)	47,60,60	1.81	11 (23%)
25	CLA	6	612	6	45,53,73	1.76	9 (20%)	52,89,113	1.43	6 (11%)
25	CLA	A	831	-	65,73,73	1.48	9 (13%)	76,113,113	1.49	12 (15%)
26	IWJ	R	322	-	43,45,45	1.16	4 (9%)	43,65,65	1.00	2 (4%)
24	CHL	R	308	22	46,54,74	1.72	5 (10%)	49,90,114	1.50	8 (16%)
25	CLA	Q	311	23	55,63,73	1.55	7 (12%)	64,101,113	1.41	10 (15%)
24	CHL	P	307	-	44,52,74	1.76	7 (15%)	46,87,114	1.88	10 (21%)
25	CLA	H	301	14	44,52,73	1.80	7 (15%)	49,87,113	1.50	9 (18%)
29	Q6L	O	2007	-	42,43,43	1.92	8 (19%)	47,60,60	1.34	4 (8%)
25	CLA	A	818	-	45,53,73	1.77	5 (11%)	52,89,113	1.70	7 (13%)
24	CHL	Q	309	-	44,52,74	1.73	6 (13%)	46,87,114	1.61	8 (17%)
29	Q6L	T	315	-	42,43,43	1.86	7 (16%)	47,60,60	1.39	6 (12%)
25	CLA	A	830	-	65,73,73	1.51	8 (12%)	76,113,113	1.77	15 (19%)
25	CLA	B	831	-	65,73,73	1.52	7 (10%)	76,113,113	1.68	13 (17%)
25	CLA	4	314	-	41,49,73	1.85	6 (14%)	47,84,113	1.63	9 (19%)
25	CLA	P	302	-	65,73,73	1.50	8 (12%)	76,113,113	1.45	12 (15%)
29	Q6L	W	319	-	42,43,43	1.88	7 (16%)	47,60,60	1.45	7 (14%)
29	Q6L	Q	317	-	42,43,43	1.82	6 (14%)	47,60,60	1.61	6 (12%)
37	NEX	W	317	-	38,46,46	1.13	4 (10%)	50,70,70	2.59	13 (26%)
25	CLA	3	314	3	39,48,73	1.90	4 (10%)	44,83,113	1.69	8 (18%)
29	Q6L	V	319	-	42,43,43	1.81	7 (16%)	47,60,60	1.79	12 (25%)
29	Q6L	Q	318	-	42,43,43	1.81	6 (14%)	47,60,60	1.58	6 (12%)
29	Q6L	S	316	-	42,43,43	1.87	7 (16%)	47,60,60	1.56	5 (10%)
30	BCR	B	847	-	41,41,41	1.33	6 (14%)	56,56,56	2.49	22 (39%)
25	CLA	A	820	-	59,67,73	1.64	10 (16%)	68,105,113	1.46	11 (16%)
28	LHG	2	619	25	32,32,48	1.12	2 (6%)	35,38,54	1.07	3 (8%)
24	CHL	R	309	-	50,58,74	1.73	6 (12%)	52,94,114	1.57	10 (19%)
25	CLA	B	810	-	65,73,73	1.51	10 (15%)	76,113,113	1.30	9 (11%)
38	KC2	R	312	22	48,53,53	2.61	14 (29%)	54,89,89	2.49	21 (38%)
29	Q6L	R	304	-	42,43,43	1.90	7 (16%)	47,60,60	1.45	3 (6%)
25	CLA	4	309	4	45,53,73	1.86	9 (20%)	52,89,113	1.90	12 (23%)
25	CLA	O	2001	-	59,67,73	1.52	8 (13%)	68,105,113	1.58	11 (16%)
25	CLA	G	203	-	42,50,73	1.83	7 (16%)	48,85,113	1.69	9 (18%)
25	CLA	S	310	22	60,68,73	1.59	9 (15%)	70,107,113	1.41	11 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	BCR	B	849	-	41,41,41	1.08	3 (7%)	56,56,56	2.28	16 (28%)
29	Q6L	Q	319	-	42,43,43	1.87	7 (16%)	47,60,60	1.71	10 (21%)
25	CLA	U	303	-	50,58,73	1.76	8 (16%)	58,95,113	1.49	9 (15%)
26	IWJ	6	614	-	43,45,45	1.16	4 (9%)	43,65,65	1.30	3 (6%)
26	IWJ	W	318	-	43,45,45	1.15	4 (9%)	43,65,65	1.36	6 (13%)
24	CHL	X	315	22	45,53,74	1.83	6 (13%)	46,88,114	1.36	5 (10%)
26	IWJ	V	318	-	43,45,45	1.14	4 (9%)	43,65,65	1.43	8 (18%)
25	CLA	B	841	-	65,73,73	1.56	9 (13%)	76,113,113	1.55	12 (15%)
25	CLA	B	830	-	65,73,73	1.47	9 (13%)	76,113,113	1.31	6 (7%)
30	BCR	B	846	-	41,41,41	1.11	4 (9%)	56,56,56	2.46	18 (32%)
24	CHL	4	306	-	40,49,74	1.78	6 (15%)	42,84,114	2.07	11 (26%)
25	CLA	L	304	-	42,50,73	1.79	8 (19%)	48,85,113	1.65	8 (16%)
25	CLA	N	203	-	42,50,73	1.89	9 (21%)	48,85,113	1.58	11 (22%)
25	CLA	A	835	-	65,73,73	1.54	9 (13%)	76,113,113	1.36	9 (11%)
28	LHG	3	320	25	22,22,48	1.10	1 (4%)	24,27,54	1.07	1 (4%)
25	CLA	3	309	28	42,50,73	1.86	6 (14%)	48,85,113	1.56	9 (18%)
25	CLA	R	306	-	65,73,73	1.45	8 (12%)	76,113,113	1.30	6 (7%)
25	CLA	X	302	22	55,63,73	1.64	10 (18%)	64,101,113	1.48	13 (20%)
25	CLA	F	803	12	41,49,73	1.83	9 (21%)	47,84,113	1.72	12 (25%)
25	CLA	S	301	22	65,73,73	1.55	9 (13%)	76,113,113	1.41	13 (17%)
24	CHL	6	601	6	42,50,74	1.75	6 (14%)	45,85,114	1.87	13 (28%)
24	CHL	P	306	-	52,60,74	1.61	8 (15%)	56,97,114	1.70	12 (21%)
25	CLA	1	610	1	40,48,73	1.93	6 (15%)	50,83,113	1.68	14 (28%)
25	CLA	6	611	-	43,51,73	1.76	6 (13%)	49,86,113	1.63	8 (16%)
25	CLA	A	822	-	45,53,73	1.72	7 (15%)	52,89,113	1.52	9 (17%)
25	CLA	1	605	-	40,49,73	1.87	6 (15%)	45,84,113	1.51	6 (13%)
29	Q6L	X	301	-	42,43,43	1.90	7 (16%)	47,60,60	1.52	5 (10%)
25	CLA	U	311	22	55,63,73	1.64	8 (14%)	64,101,113	1.67	10 (15%)
38	KC2	T	308	22	48,53,53	2.57	14 (29%)	54,89,89	2.41	19 (35%)
25	CLA	3	311	3	53,62,73	1.68	9 (16%)	61,100,113	1.89	14 (22%)
25	CLA	R	315	-	60,68,73	1.59	7 (11%)	70,107,113	1.49	12 (17%)
38	KC2	P	308	22	48,53,53	2.62	16 (33%)	54,89,89	2.65	21 (38%)
26	IWJ	T	321	-	43,45,45	1.20	5 (11%)	43,65,65	1.10	3 (6%)
25	CLA	B	832	-	43,51,73	1.97	11 (25%)	49,86,113	1.69	13 (26%)
25	CLA	A	840	-	55,63,73	1.60	7 (12%)	64,101,113	1.62	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMG	A	801	-	31,31,55	1.14	2 (6%)	39,39,63	0.93	1 (2%)
30	BCR	H	305	-	41,41,41	1.19	3 (7%)	56,56,56	1.80	17 (30%)
25	CLA	B	815	-	65,73,73	1.41	8 (12%)	76,113,113	1.87	10 (13%)
25	CLA	T	309	22	59,67,73	1.63	10 (16%)	68,105,113	1.46	12 (17%)
29	Q6L	V	321	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	4 (8%)
24	CHL	W	305	-	42,50,74	1.81	6 (14%)	44,85,114	1.83	10 (22%)
24	CHL	Q	316	23	45,53,74	1.81	5 (11%)	46,88,114	1.57	11 (23%)
31	LMG	J	104	-	46,46,55	0.97	2 (4%)	54,54,63	0.88	2 (3%)
31	LMG	5	613	-	54,54,55	0.92	2 (3%)	62,62,63	0.84	1 (1%)
25	CLA	A	832	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
26	IWJ	U	316	-	43,45,45	1.15	4 (9%)	43,65,65	1.35	5 (11%)
24	CHL	X	307	-	52,60,74	1.58	10 (19%)	56,97,114	2.51	18 (32%)
26	IWJ	S	318	-	43,45,45	1.16	5 (11%)	43,65,65	1.38	6 (13%)
29	Q6L	V	316	-	42,43,43	1.94	7 (16%)	47,60,60	1.60	5 (10%)
24	CHL	T	304	22	43,51,74	1.76	5 (11%)	45,86,114	1.94	7 (15%)
30	BCR	J	103	-	41,41,41	1.12	4 (9%)	56,56,56	2.21	20 (35%)
30	BCR	L	306	-	41,41,41	1.18	4 (9%)	56,56,56	2.08	19 (33%)
24	CHL	P	304	22	46,54,74	1.78	6 (13%)	49,90,114	1.95	16 (32%)
26	IWJ	S	319	-	43,45,45	1.19	7 (16%)	43,65,65	1.26	6 (13%)
25	CLA	5	602	5	60,68,73	1.53	6 (10%)	70,107,113	1.51	12 (17%)
25	CLA	1	607	1	36,44,73	2.03	7 (19%)	39,74,113	2.98	11 (28%)
25	CLA	B	816	-	51,59,73	1.65	7 (13%)	59,96,113	1.52	7 (11%)
25	CLA	B	819	-	59,67,73	1.60	9 (15%)	68,105,113	1.42	11 (16%)
26	IWJ	R	303	-	43,45,45	1.18	5 (11%)	43,65,65	1.25	3 (6%)
29	Q6L	P	319	-	42,43,43	1.87	7 (16%)	47,60,60	1.60	7 (14%)
29	Q6L	W	320	-	42,43,43	1.88	7 (16%)	47,60,60	1.72	5 (10%)
26	IWJ	V	317	-	43,45,45	1.17	4 (9%)	43,65,65	1.20	2 (4%)
25	CLA	3	301	3	60,68,73	1.55	8 (13%)	70,107,113	1.57	9 (12%)
25	CLA	B	818	-	55,63,73	1.58	8 (14%)	64,101,113	1.61	13 (20%)
25	CLA	A	825	-	65,73,73	1.51	6 (9%)	76,113,113	1.80	17 (22%)
25	CLA	T	311	-	60,68,73	1.52	6 (10%)	70,107,113	1.55	9 (12%)
24	CHL	1	601	1	54,63,74	1.63	8 (14%)	58,101,114	1.43	11 (18%)
25	CLA	V	313	-	48,56,73	1.70	7 (14%)	55,92,113	1.37	8 (14%)
24	CHL	T	305	-	49,57,74	1.68	6 (12%)	52,93,114	1.88	11 (21%)
26	IWJ	T	318	-	43,45,45	1.17	5 (11%)	43,65,65	1.18	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	5	603	5	45,53,73	1.78	5 (11%)	52,89,113	1.66	7 (13%)
25	CLA	6	613	6	65,73,73	1.51	6 (9%)	76,113,113	1.45	11 (14%)
24	CHL	6	606	-	43,51,74	1.74	5 (11%)	45,86,114	1.76	10 (22%)
25	CLA	A	856	-	57,65,73	1.54	8 (14%)	66,103,113	1.81	14 (21%)
25	CLA	2	602	2	61,69,73	1.56	7 (11%)	71,108,113	1.83	17 (23%)
25	CLA	B	840	-	47,55,73	1.79	8 (17%)	54,91,113	1.56	9 (16%)
26	IWJ	P	318	-	43,45,45	1.16	4 (9%)	43,65,65	1.11	1 (2%)
25	CLA	B	842	-	65,73,73	1.49	8 (12%)	76,113,113	1.71	15 (19%)
37	NEX	H	306	-	38,46,46	1.33	7 (18%)	50,70,70	2.53	18 (36%)
25	CLA	6	603	6	43,52,73	1.87	8 (18%)	49,88,113	1.57	12 (24%)
24	CHL	2	601	2	47,55,74	1.73	9 (19%)	50,91,114	1.72	10 (20%)
25	CLA	A	805	-	65,73,73	1.44	7 (10%)	76,113,113	1.69	12 (15%)
24	CHL	S	306	-	52,60,74	1.67	11 (21%)	56,97,114	2.21	17 (30%)
31	LMG	N	201	-	55,55,55	0.90	2 (3%)	63,63,63	1.16	6 (9%)
24	CHL	X	306	-	42,50,74	1.79	6 (14%)	44,85,114	1.84	8 (18%)
25	CLA	R	314	22	60,68,73	1.59	6 (10%)	70,107,113	1.58	13 (18%)
25	CLA	G	204	13	45,53,73	1.78	6 (13%)	52,89,113	1.63	9 (17%)
25	CLA	P	312	22	55,63,73	1.65	5 (9%)	64,101,113	1.57	10 (15%)
28	LHG	6	616	-	45,45,48	0.95	2 (4%)	48,51,54	1.08	3 (6%)
25	CLA	W	313	-	43,51,73	1.77	6 (13%)	49,86,113	1.41	7 (14%)
29	Q6L	U	317	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	5 (10%)
25	CLA	O	2003	-	41,49,73	1.84	5 (12%)	47,84,113	1.41	7 (14%)
30	BCR	A	850	-	41,41,41	1.25	7 (17%)	56,56,56	2.38	22 (39%)
25	CLA	A	814	-	54,62,73	1.67	7 (12%)	62,99,113	1.50	12 (19%)
25	CLA	2	610	28	42,50,73	1.82	5 (11%)	48,85,113	1.58	8 (16%)
25	CLA	W	310	22	60,68,73	1.55	6 (10%)	70,107,113	1.30	8 (11%)
25	CLA	X	311	22	50,58,73	1.65	7 (14%)	58,95,113	1.41	8 (13%)
25	CLA	V	310	22	47,55,73	1.74	8 (17%)	54,91,113	1.48	10 (18%)
25	CLA	A	842	-	65,73,73	1.50	9 (13%)	76,113,113	1.58	14 (18%)
30	BCR	A	849	-	41,41,41	1.15	4 (9%)	56,56,56	2.23	18 (32%)
24	CHL	W	304	22	42,50,74	1.88	5 (11%)	44,85,114	1.58	7 (15%)
26	IWJ	X	318	-	43,45,45	1.18	7 (16%)	43,65,65	1.39	7 (16%)
29	Q6L	P	321	-	42,43,43	1.89	8 (19%)	47,60,60	1.54	6 (12%)
30	BCR	L	307	-	41,41,41	1.16	3 (7%)	56,56,56	2.65	18 (32%)
24	CHL	S	307	-	42,50,74	1.85	6 (14%)	44,85,114	1.80	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	U	309	22	46,54,73	1.75	7 (15%)	53,90,113	1.46	8 (15%)
25	CLA	A	807	-	64,72,73	1.49	9 (14%)	74,111,113	1.50	10 (13%)
25	CLA	W	309	22	64,72,73	1.51	6 (9%)	74,111,113	1.59	14 (18%)
24	CHL	R	311	-	44,52,74	1.86	8 (18%)	46,87,114	1.59	10 (21%)
25	CLA	6	607	6	45,53,73	1.81	9 (20%)	52,89,113	1.65	7 (13%)
25	CLA	A	845	28	50,58,73	1.60	6 (12%)	58,95,113	1.50	10 (17%)
26	IWJ	4	317	-	43,45,45	1.20	6 (13%)	43,65,65	1.25	4 (9%)
25	CLA	A	803	-	65,73,73	1.44	5 (7%)	76,113,113	1.55	10 (13%)
26	IWJ	Q	303	-	43,45,45	1.21	4 (9%)	43,65,65	1.27	6 (13%)
25	CLA	X	312	-	51,59,73	1.66	8 (15%)	59,96,113	1.56	11 (18%)
24	CHL	U	306	-	44,52,74	1.76	7 (15%)	46,87,114	1.34	5 (10%)
24	CHL	6	605	-	42,50,74	1.82	7 (16%)	45,85,114	1.73	7 (15%)
25	CLA	B	814	-	65,73,73	1.49	6 (9%)	76,113,113	1.45	10 (13%)
24	CHL	T	320	-	52,60,74	1.66	7 (13%)	56,97,114	1.65	12 (21%)
25	CLA	B	805	-	65,73,73	1.51	9 (13%)	76,113,113	1.47	12 (15%)
25	CLA	4	313	4	57,65,73	1.56	8 (14%)	66,103,113	1.66	11 (16%)
29	Q6L	X	319	-	42,43,43	1.92	6 (14%)	47,60,60	1.77	7 (14%)
25	CLA	3	308	3	41,49,73	1.77	9 (21%)	47,84,113	1.53	10 (21%)
26	IWJ	5	611	-	43,45,45	1.17	3 (6%)	43,65,65	1.28	4 (9%)
25	CLA	3	303	-	43,51,73	1.88	9 (20%)	54,87,113	1.58	9 (16%)
25	CLA	T	313	-	42,50,73	1.87	8 (19%)	48,85,113	1.35	6 (12%)
29	Q6L	U	314	-	42,43,43	1.85	7 (16%)	47,60,60	1.65	6 (12%)
25	CLA	S	313	-	41,49,73	1.88	6 (14%)	47,84,113	1.43	8 (17%)
36	DGD	B	850	-	60,60,67	0.95	2 (3%)	74,74,81	0.96	4 (5%)
25	CLA	B	813	-	65,73,73	1.44	9 (13%)	76,113,113	1.69	21 (27%)
25	CLA	A	834	-	56,64,73	1.56	7 (12%)	65,102,113	1.45	9 (13%)
29	Q6L	X	317	-	42,43,43	1.86	7 (16%)	47,60,60	1.57	5 (10%)
30	BCR	A	852	-	41,41,41	1.14	4 (9%)	56,56,56	2.20	12 (21%)
25	CLA	B	806	-	65,73,73	1.52	9 (13%)	76,113,113	1.62	15 (19%)
34	PQN	A	844	-	34,34,34	2.98	12 (35%)	42,45,45	1.95	6 (14%)
25	CLA	Q	314	23	53,61,73	1.59	6 (11%)	61,98,113	1.50	9 (14%)
29	Q6L	T	316	-	42,43,43	1.86	7 (16%)	47,60,60	1.62	10 (21%)
30	BCR	2	618	-	41,41,41	1.17	3 (7%)	56,56,56	2.18	15 (26%)
24	CHL	3	306	-	45,53,74	1.94	8 (17%)	52,89,114	1.58	7 (13%)
29	Q6L	P	316	-	42,43,43	1.91	8 (19%)	47,60,60	1.44	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	A	817	-	65,73,73	1.50	6 (9%)	76,113,113	1.45	10 (13%)
25	CLA	K	206	17	65,73,73	1.48	4 (6%)	76,113,113	1.53	11 (14%)
25	CLA	Q	306	39	50,58,73	1.78	7 (14%)	58,95,113	1.78	11 (18%)
25	CLA	4	304	-	44,52,73	1.85	6 (13%)	55,88,113	1.84	11 (20%)
28	LHG	Q	302	-	34,34,48	1.09	2 (5%)	37,40,54	1.06	2 (5%)
26	IWJ	1	611	-	43,45,45	1.22	5 (11%)	43,65,65	1.12	3 (6%)
25	CLA	1	602	1	56,64,73	1.70	10 (17%)	65,102,113	1.45	10 (15%)
30	BCR	3	319	-	41,41,41	1.27	5 (12%)	56,56,56	2.04	15 (26%)
24	CHL	Q	308	23	50,58,74	1.71	7 (14%)	52,94,114	1.96	12 (23%)
25	CLA	3	312	-	39,48,73	1.88	6 (15%)	44,83,113	1.62	9 (20%)
25	CLA	B	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.66	13 (17%)
25	CLA	5	607	5	65,73,73	1.52	8 (12%)	76,113,113	1.41	9 (11%)
25	CLA	2	603	-	43,52,73	1.82	8 (18%)	49,88,113	1.58	10 (20%)
24	CHL	S	305	22	42,50,74	1.77	8 (19%)	44,85,114	1.79	8 (18%)
25	CLA	P	313	-	48,56,73	1.74	6 (12%)	55,92,113	1.42	9 (16%)
25	CLA	T	301	22	65,73,73	1.54	8 (12%)	76,113,113	1.67	14 (18%)
25	CLA	A	806	-	52,60,73	1.68	6 (11%)	60,97,113	1.69	10 (16%)
25	CLA	A	833	-	50,58,73	1.80	10 (20%)	58,95,113	1.44	9 (15%)
27	XAT	2	617	-	39,47,47	1.12	3 (7%)	54,74,74	3.07	27 (50%)
30	BCR	G	205	-	41,41,41	1.25	5 (12%)	56,56,56	2.02	14 (25%)
28	LHG	1	614	25	34,34,48	1.11	2 (5%)	37,40,54	1.17	3 (8%)
25	CLA	P	310	22	60,68,73	1.58	6 (10%)	70,107,113	1.46	11 (15%)
24	CHL	U	305	-	46,54,74	1.75	6 (13%)	49,90,114	1.73	8 (16%)
25	CLA	K	204	-	46,54,73	1.68	8 (17%)	53,90,113	1.75	11 (20%)
25	CLA	O	2005	-	41,49,73	1.80	6 (14%)	47,84,113	1.66	8 (17%)
37	NEX	R	321	-	38,46,46	1.30	7 (18%)	50,70,70	2.71	17 (34%)
29	Q6L	X	316	-	40,41,43	1.86	5 (12%)	46,56,60	1.61	6 (13%)
30	BCR	K	207	-	41,41,41	1.26	5 (12%)	56,56,56	2.10	16 (28%)
26	IWJ	P	320	-	43,45,45	1.20	6 (13%)	43,65,65	1.36	5 (11%)
25	CLA	2	612	2	65,73,73	1.52	8 (12%)	76,113,113	1.48	15 (19%)
25	CLA	B	833	-	43,51,73	1.75	7 (16%)	49,86,113	1.74	8 (16%)
25	CLA	S	303	-	50,58,73	1.73	7 (14%)	58,95,113	1.66	10 (17%)
25	CLA	U	312	-	41,49,73	1.86	6 (14%)	47,84,113	1.41	6 (12%)
25	CLA	2	613	-	41,50,73	1.83	7 (17%)	46,85,113	1.54	10 (21%)
24	CHL	P	314	22	45,53,74	1.78	6 (13%)	46,88,114	1.50	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	A	836	-	65,73,73	1.44	8 (12%)	76,113,113	1.50	8 (10%)
25	CLA	J	102	16	42,50,73	1.77	9 (21%)	48,85,113	1.63	7 (14%)
30	BCR	F	804	-	41,41,41	1.18	3 (7%)	56,56,56	2.40	21 (37%)
25	CLA	B	837	-	42,50,73	1.84	6 (14%)	48,85,113	1.66	8 (16%)
29	Q6L	W	315	-	42,43,43	1.84	7 (16%)	47,60,60	1.54	7 (14%)
29	Q6L	V	315	-	42,43,43	1.91	7 (16%)	47,60,60	1.45	6 (12%)
25	CLA	H	304	18	45,53,73	1.71	9 (20%)	52,89,113	1.68	10 (19%)
25	CLA	X	313	22	41,49,73	1.86	8 (19%)	47,84,113	1.60	9 (19%)
24	CHL	W	307	-	66,74,74	1.46	6 (9%)	73,114,114	1.53	10 (13%)
25	CLA	1	606	1	40,48,73	1.91	7 (17%)	50,83,113	1.66	12 (24%)
25	CLA	B	820	-	60,68,73	1.50	9 (15%)	70,107,113	1.65	16 (22%)
25	CLA	X	304	-	42,50,73	1.86	8 (19%)	48,85,113	1.74	9 (18%)
25	CLA	B	804	-	65,73,73	1.51	7 (10%)	76,113,113	1.39	9 (11%)
25	CLA	U	301	22	45,53,73	1.76	10 (22%)	52,89,113	1.67	9 (17%)
25	CLA	B	827	-	50,58,73	1.60	4 (8%)	58,95,113	1.61	12 (20%)
30	BCR	M	101	-	41,41,41	1.40	8 (19%)	56,56,56	2.32	22 (39%)
24	CHL	2	615	2	43,51,74	1.67	7 (16%)	45,86,114	1.56	9 (20%)
25	CLA	B	823	-	47,55,73	1.83	8 (17%)	54,91,113	1.38	7 (12%)
25	CLA	A	839	-	65,73,73	1.41	6 (9%)	76,113,113	1.51	10 (13%)
35	SF4	C	102	9	0,12,12	-	-	-	-	-
29	Q6L	R	301	-	42,43,43	1.89	7 (16%)	47,60,60	1.73	6 (12%)
25	CLA	A	804	39	65,73,73	1.51	10 (15%)	76,113,113	1.65	16 (21%)
24	CHL	V	305	22	43,51,74	1.74	7 (16%)	45,86,114	1.76	7 (15%)
29	Q6L	W	316	-	42,43,43	1.91	9 (21%)	47,60,60	1.54	6 (12%)
25	CLA	P	303	-	50,58,73	1.70	5 (10%)	58,95,113	1.55	9 (15%)
38	KC2	S	308	22	48,53,53	2.58	15 (31%)	54,89,89	2.42	18 (33%)
25	CLA	B	822	-	50,58,73	1.68	7 (14%)	58,95,113	1.55	9 (15%)
29	Q6L	U	315	-	42,43,43	1.90	8 (19%)	47,60,60	1.73	9 (19%)
25	CLA	B	828	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	10 (13%)
25	CLA	Q	301	14	55,63,73	1.59	8 (14%)	64,101,113	1.72	13 (20%)
26	IWJ	3	315	-	43,45,45	1.13	6 (13%)	43,65,65	1.24	2 (4%)
24	CHL	R	310	-	52,60,74	1.63	8 (15%)	56,97,114	1.73	11 (19%)
25	CLA	P	311	-	60,68,73	1.51	6 (10%)	70,107,113	1.56	14 (20%)
25	CLA	4	310	4	54,62,73	1.58	5 (9%)	62,99,113	1.59	14 (22%)
24	CHL	X	308	-	44,52,74	1.72	6 (13%)	46,87,114	1.77	10 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	A	809	-	50,58,73	1.64	9 (18%)	58,95,113	1.64	10 (17%)
25	CLA	B	812	-	65,73,73	1.41	10 (15%)	76,113,113	1.36	11 (14%)
25	CLA	3	307	3	61,69,73	1.56	11 (18%)	71,108,113	1.72	14 (19%)
25	CLA	4	312	4	40,49,73	1.85	6 (15%)	45,84,113	1.67	8 (17%)
25	CLA	R	317	-	48,56,73	1.68	7 (14%)	55,92,113	1.60	9 (16%)
31	LMG	B	801	-	38,38,55	1.14	3 (7%)	46,46,63	1.14	3 (6%)
25	CLA	3	305	3	41,49,73	1.93	8 (19%)	51,84,113	1.51	11 (21%)
37	NEX	S	317	-	38,46,46	1.32	4 (10%)	50,70,70	2.71	16 (32%)
24	CHL	1	604	1	40,49,74	1.81	8 (20%)	41,84,114	1.61	10 (24%)
37	NEX	P	317	-	38,46,46	1.26	6 (15%)	50,70,70	2.62	17 (34%)
38	KC2	U	307	22	48,53,53	2.57	14 (29%)	54,89,89	2.35	18 (33%)
25	CLA	T	312	22	55,63,73	1.63	7 (12%)	64,101,113	1.48	10 (15%)
25	CLA	A	829	-	65,73,73	1.40	10 (15%)	76,113,113	1.55	14 (18%)
25	CLA	U	302	-	56,64,73	1.63	11 (19%)	65,102,113	1.53	8 (12%)
25	CLA	A	815	-	65,73,73	1.47	7 (10%)	76,113,113	1.78	9 (11%)
25	CLA	4	305	-	43,51,73	1.92	8 (18%)	54,87,113	1.48	8 (14%)
31	LMG	A	857	-	46,46,55	0.97	2 (4%)	54,54,63	0.89	2 (3%)
25	CLA	6	608	6	42,50,73	1.76	6 (14%)	48,85,113	1.77	7 (14%)
26	IWJ	S	322	-	43,45,45	1.18	5 (11%)	43,65,65	1.18	3 (6%)
24	CHL	S	314	22	45,53,74	1.76	5 (11%)	46,88,114	1.62	6 (13%)
25	CLA	6	609	-	44,52,73	1.79	4 (9%)	51,88,113	1.90	10 (19%)
25	CLA	A	808	7	65,73,73	1.43	11 (16%)	76,113,113	1.56	9 (11%)
29	Q6L	S	320	-	42,43,43	1.92	7 (16%)	47,60,60	1.65	9 (19%)
25	CLA	B	825	-	45,53,73	1.67	8 (17%)	52,89,113	1.41	8 (15%)
29	Q6L	O	2006	-	42,43,43	1.90	7 (16%)	47,60,60	1.42	5 (10%)
25	CLA	X	303	-	51,59,73	1.72	8 (15%)	59,96,113	1.32	7 (11%)
25	CLA	W	301	22	55,63,73	1.59	9 (16%)	64,101,113	1.53	9 (14%)
28	LHG	3	322	-	35,35,48	1.04	2 (5%)	38,41,54	1.06	3 (7%)
30	BCR	3	317	-	41,41,41	1.08	3 (7%)	56,56,56	1.89	18 (32%)
25	CLA	5	608	5	41,49,73	1.87	8 (19%)	47,84,113	1.65	8 (17%)
25	CLA	O	2004	-	41,49,73	1.84	7 (17%)	47,84,113	1.68	8 (17%)
28	LHG	A	847	25	29,29,48	1.17	2 (6%)	32,35,54	1.05	2 (6%)
25	CLA	A	827	39	65,73,73	1.49	8 (12%)	76,113,113	1.69	15 (19%)
25	CLA	G	202	-	45,53,73	1.80	8 (17%)	52,89,113	1.39	7 (13%)
25	CLA	B	807	-	65,73,73	1.47	7 (10%)	76,113,113	1.65	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CHL	R	302	-	47,55,74	1.73	6 (12%)	50,91,114	1.71	13 (26%)
25	CLA	B	838	-	50,58,73	1.57	5 (10%)	58,95,113	1.67	7 (12%)
25	CLA	U	308	22	41,49,73	1.90	10 (24%)	47,84,113	1.92	13 (27%)
27	XAT	1	612	-	39,47,47	1.34	6 (15%)	54,74,74	3.21	28 (51%)
25	CLA	L	301	18	41,49,73	1.82	8 (19%)	47,84,113	1.61	7 (14%)
25	CLA	P	301	22	65,73,73	1.43	7 (10%)	76,113,113	1.52	13 (17%)
33	CL0	A	802	-	65,73,73	1.54	10 (15%)	76,113,113	1.41	11 (14%)
31	LMG	A	855	-	27,27,55	1.27	2 (7%)	35,35,63	1.35	4 (11%)
38	KC2	Q	310	23	48,53,53	2.58	14 (29%)	54,89,89	2.51	18 (33%)
30	BCR	K	205	-	41,41,41	1.23	4 (9%)	56,56,56	2.07	16 (28%)
25	CLA	V	303	-	50,58,73	1.72	8 (16%)	58,95,113	1.73	8 (13%)
24	CHL	T	306	-	52,60,74	1.60	7 (13%)	56,97,114	1.63	11 (19%)
25	CLA	4	303	4	60,68,73	1.56	9 (15%)	70,107,113	1.39	12 (17%)
29	Q6L	S	315	-	42,43,43	1.76	5 (11%)	47,60,60	1.65	9 (19%)
25	CLA	A	843	-	65,73,73	1.47	7 (10%)	76,113,113	1.64	13 (17%)
25	CLA	2	614	2	44,52,73	1.73	8 (18%)	49,87,113	1.65	6 (12%)
25	CLA	T	310	22	42,50,73	1.89	7 (16%)	48,85,113	1.36	6 (12%)
30	BCR	F	801	-	41,41,41	1.14	4 (9%)	56,56,56	1.96	16 (28%)
25	CLA	A	841	-	50,58,73	1.72	7 (14%)	58,95,113	1.52	9 (15%)
25	CLA	1	603	-	55,63,73	1.62	8 (14%)	64,101,113	1.79	15 (23%)
25	CLA	1	613	-	52,60,73	1.68	5 (9%)	60,97,113	1.50	9 (15%)
25	CLA	A	810	7	65,73,73	1.46	9 (13%)	76,113,113	1.50	10 (13%)
25	CLA	3	304	3	40,49,73	1.87	7 (17%)	45,84,113	1.71	9 (20%)
25	CLA	4	316	4	42,50,73	1.83	6 (14%)	48,85,113	1.57	9 (18%)
24	CHL	U	313	22	43,51,74	1.81	6 (13%)	45,86,114	1.55	8 (17%)
25	CLA	A	838	7	65,73,73	1.52	7 (10%)	76,113,113	1.57	14 (18%)
29	Q6L	S	321	-	42,43,43	1.96	8 (19%)	47,60,60	1.41	6 (12%)
25	CLA	A	812	-	64,72,73	1.48	8 (12%)	74,111,113	1.43	9 (12%)
24	CHL	4	307	-	42,50,74	1.86	9 (21%)	48,85,114	2.11	13 (27%)
25	CLA	4	311	-	42,50,73	2.07	7 (16%)	48,85,113	1.75	12 (25%)
25	CLA	Q	304	23	65,73,73	1.45	10 (15%)	76,113,113	1.67	9 (11%)
24	CHL	P	305	-	46,54,74	1.77	6 (13%)	49,90,114	1.93	11 (22%)
27	XAT	5	612	-	39,47,47	1.03	2 (5%)	54,74,74	3.01	25 (46%)
31	LMG	L	308	-	31,31,55	1.20	2 (6%)	39,39,63	1.03	2 (5%)
25	CLA	V	312	22	55,63,73	1.60	9 (16%)	64,101,113	1.47	9 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	Q6L	R	323	-	42,43,43	1.89	6 (14%)	47,60,60	1.73	7 (14%)
27	XAT	3	316	-	39,47,47	1.23	5 (12%)	54,74,74	3.25	24 (44%)
25	CLA	Q	312	23	42,50,73	1.92	7 (16%)	48,85,113	1.41	7 (14%)
25	CLA	3	313	-	41,49,73	1.84	7 (17%)	47,84,113	1.55	8 (17%)
25	CLA	T	302	-	65,73,73	1.54	8 (12%)	76,113,113	1.34	9 (11%)
25	CLA	O	2002	-	65,73,73	1.46	9 (13%)	76,113,113	1.73	15 (19%)
25	CLA	A	821	-	65,73,73	1.50	7 (10%)	76,113,113	1.57	13 (17%)
25	CLA	S	302	-	65,73,73	1.53	10 (15%)	76,113,113	1.38	10 (13%)
25	CLA	A	811	7	50,58,73	1.60	4 (8%)	58,95,113	1.80	8 (13%)
24	CHL	4	308	-	46,54,74	1.75	6 (13%)	49,90,114	1.42	6 (12%)
25	CLA	B	834	-	65,73,73	1.44	8 (12%)	76,113,113	1.48	11 (14%)
25	CLA	2	608	2	45,53,73	1.79	6 (13%)	52,89,113	1.61	11 (21%)
27	XAT	4	318	-	39,47,47	1.10	5 (12%)	54,74,74	3.38	23 (42%)
25	CLA	A	837	-	65,73,73	1.57	7 (10%)	76,113,113	1.48	11 (14%)
24	CHL	U	304	22	42,50,74	1.82	9 (21%)	44,85,114	1.74	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	F	805	-	-	2/26/46/70	0/1/1/1
31	LMG	O	2008	-	-	2/34/54/70	0/1/1/1
25	CLA	V	301	22	1/1/14/20	10/31/109/115	-
24	CHL	5	605	-	3/3/15/26	2/8/106/137	-
29	Q6L	T	319	-	-	8/29/67/67	0/2/2/2
25	CLA	W	312	22	1/1/13/20	9/25/103/115	-
25	CLA	A	813	-	1/1/15/20	13/37/115/115	-
25	CLA	B	803	-	1/1/15/20	10/37/115/115	-
25	CLA	H	302	-	1/1/15/20	12/37/115/115	-
25	CLA	B	821	-	1/1/13/20	7/25/103/115	-
35	SF4	C	101	9	-	-	0/6/5/5
24	CHL	T	307	-	3/3/15/26	3/13/111/137	-
25	CLA	R	316	22	1/1/13/20	9/25/103/115	-
25	CLA	A	823	39	1/1/15/20	10/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	2	605	-	3/3/15/26	7/10/108/137	-
25	CLA	R	313	22	1/1/14/20	17/36/114/115	-
24	CHL	R	318	22	3/3/15/26	4/13/112/137	-
25	CLA	B	836	8	-	6/31/109/115	-
25	CLA	Q	315	-	1/1/11/20	5/17/95/115	-
24	CHL	2	607	-	3/3/15/26	4/13/112/137	-
30	BCR	4	319	-	-	3/29/63/63	0/2/2/2
25	CLA	V	309	22	1/1/10/20	4/10/88/115	-
25	CLA	N	202	20	1/1/11/20	3/13/91/115	-
25	CLA	A	826	-	1/1/13/20	8/25/103/115	-
24	CHL	W	306	-	3/3/17/26	5/23/121/137	-
25	CLA	A	828	-	-	8/30/108/115	-
34	PQN	B	844	-	-	6/23/43/43	0/2/2/2
24	CHL	T	314	22	3/3/15/26	3/10/108/137	-
25	CLA	K	201	17	1/1/11/20	6/13/91/115	-
30	BCR	J	101	-	-	4/29/63/63	0/2/2/2
31	LMG	2	620	-	-	3/26/46/70	0/1/1/1
24	CHL	V	304	22	3/3/16/26	8/15/113/137	-
35	SF4	A	853	7,8	-	-	0/6/5/5
30	BCR	L	305	-	-	4/29/63/63	0/2/2/2
30	BCR	I	101	-	-	9/29/63/63	0/2/2/2
25	CLA	S	309	22	1/1/14/20	12/31/109/115	-
25	CLA	6	604	-	1/1/10/20	2/9/88/115	-
28	LHG	3	323	-	-	15/47/47/53	-
25	CLA	B	817	-	1/1/10/20	4/11/89/115	-
24	CHL	X	305	22	3/3/15/26	1/10/108/137	-
30	BCR	B	848	-	-	2/29/63/63	0/2/2/2
25	CLA	R	307	-	1/1/12/20	2/19/97/115	-
25	CLA	S	311	-	1/1/11/20	6/16/94/115	-
25	CLA	A	816	-	1/1/11/20	6/13/91/115	-
25	CLA	5	601	5	1/1/11/20	9/15/93/115	-
25	CLA	W	302	-	1/1/13/20	5/25/103/115	-
25	CLA	B	826	-	1/1/15/20	8/37/115/115	-
25	CLA	5	604	-	1/1/10/20	0/4/80/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	609	2	1/1/13/20	7/25/103/115	-
25	CLA	X	314	-	1/1/10/20	5/8/86/115	-
25	CLA	Q	313	-	1/1/11/20	7/15/93/115	-
30	BCR	A	848	-	-	3/29/63/63	0/2/2/2
25	CLA	5	609	-	1/1/13/20	7/23/101/115	-
32	SQD	6	617	-	-	13/49/69/69	0/1/1/1
25	CLA	1	608	1	1/1/15/20	10/37/115/115	-
25	CLA	B	824	-	1/1/14/20	6/31/109/115	-
25	CLA	B	835	-	1/1/11/20	3/13/91/115	-
25	CLA	L	303	-	1/1/11/20	5/13/91/115	-
30	BCR	G	201	-	-	2/29/63/63	0/2/2/2
26	IWJ	V	320	-	-	5/33/76/76	1/2/2/2
25	CLA	B	839	-	1/1/15/20	20/37/115/115	-
25	CLA	B	811	8	1/1/15/20	13/37/115/115	-
29	Q6L	R	320	-	-	0/29/67/67	0/2/2/2
30	BCR	B	845	-	-	3/29/63/63	0/2/2/2
25	CLA	V	302	-	1/1/12/20	9/19/97/115	-
25	CLA	A	819	-	1/1/14/20	13/31/109/115	-
25	CLA	6	610	-	1/1/14/20	13/33/111/115	-
25	CLA	B	808	8	1/1/15/20	23/37/115/115	-
25	CLA	K	203	-	1/1/14/20	4/34/112/115	-
25	CLA	X	310	22	1/1/10/20	3/10/88/115	-
24	CHL	Q	307	23	3/3/16/26	6/15/113/137	-
36	DGD	A	854	-	-	4/40/80/95	0/2/2/2
25	CLA	5	606	-	1/1/10/20	0/8/84/115	-
25	CLA	W	303	-	1/1/12/20	4/19/97/115	-
25	CLA	R	305	22	1/1/15/20	9/37/115/115	-
24	CHL	4	302	4	3/3/17/26	4/23/121/137	-
25	CLA	A	824	-	1/1/10/20	6/10/88/115	-
25	CLA	S	312	22	1/1/13/20	7/25/103/115	-
25	CLA	4	315	-	1/1/10/20	3/8/86/115	-
24	CHL	V	314	22	3/3/15/26	5/13/111/137	-
37	NEX	T	317	-	-	3/27/83/83	0/3/3/3
30	BCR	K	202	-	-	0/29/63/63	0/2/2/2
32	SQD	H	303	-	-	10/43/63/69	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	IWJ	4	301	-	-	7/33/76/76	0/2/2/2
25	CLA	Q	305	-	1/1/10/20	0/11/90/115	-
28	LHG	A	846	-	-	12/53/53/53	-
25	CLA	B	809	-	1/1/15/20	9/37/115/115	-
25	CLA	L	302	-	-	10/31/109/115	-
24	CHL	S	304	22	3/3/15/26	3/10/108/137	-
25	CLA	U	310	-	1/1/10/20	5/11/90/115	-
25	CLA	F	802	-	1/1/10/20	4/10/88/115	-
25	CLA	2	606	-	1/1/11/20	10/13/91/115	-
24	CHL	V	307	-	3/3/15/26	5/13/111/137	-
29	Q6L	R	319	-	-	10/29/67/67	0/2/2/2
30	BCR	3	318	-	-	2/29/63/63	0/2/2/2
25	CLA	P	309	22	1/1/14/20	15/36/114/115	-
25	CLA	3	310	-	1/1/10/20	6/11/89/115	-
25	CLA	B	829	-	1/1/15/20	16/37/115/115	-
29	Q6L	P	315	-	-	6/29/67/67	0/2/2/2
30	BCR	A	851	-	-	6/29/63/63	0/2/2/2
24	CHL	V	306	-	3/3/15/26	0/13/111/137	-
26	IWJ	Q	320	-	-	12/33/76/76	0/2/2/2
29	Q6L	T	322	-	-	8/29/67/67	0/2/2/2
24	CHL	W	314	22	3/3/14/26	5/10/104/137	-
25	CLA	2	611	2	1/1/11/20	5/11/89/115	-
29	Q6L	2	616	-	-	11/29/67/67	0/2/2/2
38	KC2	W	308	22	-	10/15/71/71	-
38	KC2	V	308	22	-	10/15/71/71	-
25	CLA	6	602	6	1/1/14/20	13/34/112/115	-
25	CLA	5	610	-	1/1/10/20	4/8/86/115	-
25	CLA	1	609	-	1/1/10/20	2/4/80/115	-
25	CLA	T	303	-	1/1/12/20	6/19/97/115	-
38	KC2	X	309	22	-	10/15/71/71	-
25	CLA	W	311	-	1/1/11/20	5/13/91/115	-
25	CLA	V	311	-	1/1/14/20	10/31/109/115	-
25	CLA	2	604	-	1/1/10/20	3/9/88/115	-
25	CLA	B	843	28	1/1/15/20	14/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	3	321	-	-	9/47/47/53	-
27	XAT	6	615	-	-	0/31/93/93	0/4/4/4
25	CLA	3	302	-	1/1/13/20	7/25/103/115	-
29	Q6L	S	323	-	-	9/29/67/67	0/2/2/2
25	CLA	6	612	6	1/1/11/20	5/13/91/115	-
25	CLA	A	831	-	1/1/15/20	15/37/115/115	-
26	IWJ	R	322	-	-	7/33/76/76	1/2/2/2
24	CHL	R	308	22	3/3/16/26	3/15/113/137	-
25	CLA	Q	311	23	1/1/13/20	8/25/103/115	-
24	CHL	P	307	-	3/3/15/26	3/13/111/137	-
25	CLA	H	301	14	1/1/10/20	6/11/90/115	-
29	Q6L	O	2007	-	-	6/29/67/67	0/2/2/2
25	CLA	A	818	-	1/1/11/20	5/13/91/115	-
24	CHL	Q	309	-	3/3/15/26	3/13/111/137	-
29	Q6L	T	315	-	-	6/29/67/67	0/2/2/2
25	CLA	A	830	-	1/1/15/20	21/37/115/115	-
25	CLA	B	831	-	1/1/15/20	12/37/115/115	-
25	CLA	4	314	-	1/1/10/20	5/8/86/115	-
25	CLA	P	302	-	1/1/15/20	15/37/115/115	-
29	Q6L	W	319	-	-	9/29/67/67	0/2/2/2
29	Q6L	Q	317	-	-	6/29/67/67	0/2/2/2
37	NEX	W	317	-	-	2/27/83/83	0/3/3/3
25	CLA	3	314	3	-	0/6/84/115	-
29	Q6L	V	319	-	-	9/29/67/67	0/2/2/2
29	Q6L	Q	318	-	-	6/29/67/67	0/2/2/2
29	Q6L	S	316	-	-	3/29/67/67	0/2/2/2
30	BCR	B	847	-	-	0/29/63/63	0/2/2/2
25	CLA	A	820	-	1/1/13/20	11/30/108/115	-
28	LHG	2	619	25	-	8/37/37/53	-
24	CHL	R	309	-	3/3/16/26	7/20/118/137	-
25	CLA	B	810	-	1/1/15/20	16/37/115/115	-
38	KC2	R	312	22	-	8/15/71/71	-
29	Q6L	R	304	-	-	5/29/67/67	0/2/2/2
25	CLA	4	309	4	1/1/11/20	8/13/91/115	-
25	CLA	O	2001	-	1/1/13/20	13/30/108/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	203	-	1/1/10/20	3/10/88/115	-
25	CLA	S	310	22	1/1/14/20	11/31/109/115	-
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
29	Q6L	Q	319	-	-	5/29/67/67	0/2/2/2
25	CLA	U	303	-	1/1/12/20	6/19/97/115	-
26	IWJ	6	614	-	-	3/33/76/76	0/2/2/2
26	IWJ	W	318	-	-	10/33/76/76	0/2/2/2
24	CHL	X	315	22	3/3/15/26	4/13/112/137	-
26	IWJ	V	318	-	-	4/33/76/76	0/2/2/2
25	CLA	B	841	-	1/1/15/20	6/37/115/115	-
25	CLA	B	830	-	1/1/15/20	13/37/115/115	-
30	BCR	B	846	-	-	4/29/63/63	0/2/2/2
24	CHL	4	306	-	3/3/15/26	3/8/106/137	-
25	CLA	L	304	-	1/1/10/20	4/10/88/115	-
25	CLA	N	203	-	1/1/10/20	4/10/88/115	-
25	CLA	A	835	-	1/1/15/20	12/37/115/115	-
28	LHG	3	320	25	-	4/26/26/53	-
25	CLA	3	309	28	1/1/10/20	3/10/88/115	-
25	CLA	R	306	-	1/1/15/20	11/37/115/115	-
25	CLA	X	302	22	1/1/13/20	8/25/103/115	-
25	CLA	F	803	12	1/1/10/20	4/8/86/115	-
25	CLA	S	301	22	1/1/15/20	9/37/115/115	-
24	CHL	6	601	6	3/3/15/26	3/10/108/137	-
24	CHL	P	306	-	3/3/17/26	7/23/121/137	-
25	CLA	6	611	-	1/1/10/20	6/11/89/115	-
25	CLA	A	822	-	1/1/11/20	3/13/91/115	-
25	CLA	1	610	1	-	5/8/84/115	-
25	CLA	1	605	-	1/1/10/20	3/8/86/115	-
29	Q6L	X	301	-	-	8/29/67/67	0/2/2/2
25	CLA	U	311	22	1/1/13/20	6/25/103/115	-
38	KC2	T	308	22	-	8/15/71/71	-
25	CLA	3	311	3	1/1/13/20	10/23/101/115	-
25	CLA	R	315	-	1/1/14/20	10/31/109/115	-
38	KC2	P	308	22	-	9/15/71/71	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	IWJ	T	321	-	-	4/33/76/76	1/2/2/2
25	CLA	B	832	-	1/1/10/20	3/11/89/115	-
25	CLA	A	840	-	-	7/25/103/115	-
31	LMG	A	801	-	-	1/26/46/70	0/1/1/1
30	BCR	H	305	-	-	6/29/63/63	0/2/2/2
25	CLA	B	815	-	1/1/15/20	14/37/115/115	-
25	CLA	T	309	22	1/1/13/20	10/30/108/115	-
29	Q6L	V	321	-	-	6/29/67/67	0/2/2/2
24	CHL	W	305	-	3/3/15/26	2/10/108/137	-
24	CHL	Q	316	23	3/3/15/26	3/13/112/137	-
31	LMG	J	104	-	-	6/41/61/70	0/1/1/1
31	LMG	5	613	-	-	5/49/69/70	0/1/1/1
25	CLA	A	832	-	1/1/15/20	12/37/115/115	-
26	IWJ	U	316	-	-	2/33/76/76	0/2/2/2
24	CHL	X	307	-	3/3/17/26	10/23/121/137	-
26	IWJ	S	318	-	-	4/33/76/76	0/2/2/2
29	Q6L	V	316	-	-	8/29/67/67	0/2/2/2
24	CHL	T	304	22	3/3/15/26	5/12/110/137	-
30	BCR	J	103	-	-	2/29/63/63	0/2/2/2
30	BCR	L	306	-	-	3/29/63/63	0/2/2/2
24	CHL	P	304	22	3/3/16/26	6/15/113/137	-
26	IWJ	S	319	-	-	7/33/76/76	1/2/2/2
25	CLA	5	602	5	1/1/14/20	12/31/109/115	-
25	CLA	1	607	1	1/1/7/20	2/6/68/115	-
25	CLA	B	816	-	1/1/12/20	5/21/99/115	-
25	CLA	B	819	-	1/1/13/20	10/30/108/115	-
26	IWJ	R	303	-	-	4/33/76/76	0/2/2/2
29	Q6L	P	319	-	-	6/29/67/67	0/2/2/2
29	Q6L	W	320	-	-	7/29/67/67	0/2/2/2
26	IWJ	V	317	-	-	6/33/76/76	0/2/2/2
25	CLA	3	301	3	1/1/14/20	7/31/109/115	-
25	CLA	B	818	-	1/1/13/20	9/25/103/115	-
25	CLA	A	825	-	1/1/15/20	18/37/115/115	-
25	CLA	T	311	-	1/1/14/20	15/31/109/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	1	601	1	3/3/18/26	8/25/123/137	-
25	CLA	V	313	-	1/1/11/20	4/17/95/115	-
24	CHL	T	305	-	3/3/16/26	5/19/117/137	-
26	IWJ	T	318	-	-	6/33/76/76	0/2/2/2
25	CLA	5	603	5	1/1/11/20	6/13/91/115	-
25	CLA	6	613	6	-	8/37/115/115	-
24	CHL	6	606	-	3/3/15/26	8/12/110/137	-
25	CLA	A	856	-	1/1/13/20	12/28/106/115	-
25	CLA	2	602	2	1/1/14/20	15/33/111/115	-
25	CLA	B	840	-	-	8/16/94/115	-
26	IWJ	P	318	-	-	2/33/76/76	0/2/2/2
25	CLA	B	842	-	1/1/15/20	18/37/115/115	-
37	NEX	H	306	-	-	3/27/83/83	0/3/3/3
25	CLA	6	603	6	1/1/11/20	2/11/89/115	-
24	CHL	2	601	2	3/3/16/26	2/17/115/137	-
25	CLA	A	805	-	1/1/15/20	13/37/115/115	-
24	CHL	S	306	-	3/3/17/26	7/23/121/137	-
31	LMG	N	201	-	-	3/50/70/70	0/1/1/1
24	CHL	X	306	-	3/3/15/26	2/10/108/137	-
25	CLA	R	314	22	1/1/14/20	13/31/109/115	-
25	CLA	G	204	13	1/1/11/20	10/13/91/115	-
25	CLA	P	312	22	1/1/13/20	12/25/103/115	-
28	LHG	6	616	-	-	10/50/50/53	-
25	CLA	W	313	-	1/1/10/20	2/11/89/115	-
29	Q6L	U	317	-	-	5/29/67/67	0/2/2/2
25	CLA	O	2003	-	1/1/10/20	0/8/86/115	-
30	BCR	A	850	-	-	1/29/63/63	0/2/2/2
25	CLA	A	814	-	1/1/12/20	7/24/102/115	-
25	CLA	2	610	28	1/1/10/20	3/10/88/115	-
25	CLA	W	310	22	1/1/14/20	9/31/109/115	-
25	CLA	X	311	22	1/1/12/20	8/19/97/115	-
25	CLA	V	310	22	1/1/11/20	8/16/94/115	-
25	CLA	A	842	-	1/1/15/20	14/37/115/115	-
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	W	304	22	3/3/15/26	0/10/108/137	-
26	IWJ	X	318	-	-	6/33/76/76	1/2/2/2
29	Q6L	P	321	-	-	7/29/67/67	0/2/2/2
30	BCR	L	307	-	-	4/29/63/63	0/2/2/2
24	CHL	S	307	-	3/3/15/26	5/10/108/137	-
25	CLA	U	309	22	1/1/11/20	9/15/93/115	-
25	CLA	A	807	-	1/1/14/20	18/36/114/115	-
25	CLA	W	309	22	1/1/14/20	7/36/114/115	-
24	CHL	R	311	-	3/3/15/26	3/13/111/137	-
25	CLA	6	607	6	1/1/11/20	2/13/91/115	-
25	CLA	A	845	28	1/1/12/20	7/19/97/115	-
26	IWJ	4	317	-	-	7/33/76/76	0/2/2/2
25	CLA	A	803	-	1/1/15/20	8/37/115/115	-
26	IWJ	Q	303	-	-	3/33/76/76	0/2/2/2
25	CLA	X	312	-	1/1/12/20	4/21/99/115	-
24	CHL	U	306	-	3/3/15/26	5/13/111/137	-
24	CHL	6	605	-	3/3/15/26	0/10/108/137	-
25	CLA	B	814	-	1/1/15/20	12/37/115/115	-
24	CHL	T	320	-	3/3/17/26	8/23/121/137	-
25	CLA	B	805	-	1/1/15/20	16/37/115/115	-
25	CLA	4	313	4	-	9/28/106/115	-
29	Q6L	X	319	-	-	10/29/67/67	0/2/2/2
25	CLA	3	308	3	1/1/10/20	2/8/86/115	-
26	IWJ	5	611	-	-	5/33/76/76	1/2/2/2
25	CLA	3	303	-	1/1/11/20	0/11/87/115	-
25	CLA	T	313	-	1/1/10/20	4/10/88/115	-
29	Q6L	U	314	-	-	7/29/67/67	0/2/2/2
25	CLA	S	313	-	1/1/10/20	1/8/86/115	-
36	DGD	B	850	-	-	12/48/88/95	0/2/2/2
25	CLA	B	813	-	1/1/15/20	14/37/115/115	-
25	CLA	A	834	-	1/1/13/20	4/27/105/115	-
29	Q6L	X	317	-	-	2/29/67/67	0/2/2/2
30	BCR	A	852	-	-	5/29/63/63	0/2/2/2
25	CLA	B	806	-	1/1/15/20	17/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PQN	A	844	-	-	13/23/43/43	0/2/2/2
25	CLA	Q	314	23	1/1/12/20	12/23/101/115	-
29	Q6L	T	316	-	-	1/29/67/67	0/2/2/2
30	BCR	2	618	-	-	4/29/63/63	0/2/2/2
24	CHL	3	306	-	3/3/16/26	5/13/111/137	-
29	Q6L	P	316	-	-	2/29/67/67	0/2/2/2
25	CLA	A	817	-	-	12/37/115/115	-
25	CLA	K	206	17	1/1/15/20	13/37/115/115	-
25	CLA	Q	306	39	1/1/12/20	9/19/97/115	-
25	CLA	4	304	-	1/1/11/20	6/13/89/115	-
28	LHG	Q	302	-	-	6/39/39/53	-
26	IWJ	1	611	-	-	4/33/76/76	0/2/2/2
25	CLA	1	602	1	1/1/13/20	5/27/105/115	-
30	BCR	3	319	-	-	2/29/63/63	0/2/2/2
24	CHL	Q	308	23	3/3/16/26	4/20/118/137	-
25	CLA	3	312	-	1/1/10/20	0/6/84/115	-
25	CLA	B	802	-	1/1/15/20	13/37/115/115	-
25	CLA	5	607	5	1/1/15/20	13/37/115/115	-
25	CLA	2	603	-	1/1/11/20	3/11/89/115	-
24	CHL	S	305	22	3/3/15/26	4/10/108/137	-
25	CLA	T	301	22	1/1/15/20	13/37/115/115	-
25	CLA	P	313	-	-	4/17/95/115	-
25	CLA	A	806	-	1/1/12/20	7/22/100/115	-
25	CLA	A	833	-	-	5/19/97/115	-
27	XAT	2	617	-	-	0/31/93/93	0/4/4/4
30	BCR	G	205	-	-	2/29/63/63	0/2/2/2
28	LHG	1	614	25	-	12/39/39/53	-
25	CLA	P	310	22	1/1/14/20	10/31/109/115	-
24	CHL	U	305	-	3/3/16/26	6/15/113/137	-
25	CLA	K	204	-	1/1/11/20	7/15/93/115	-
25	CLA	O	2005	-	1/1/10/20	4/8/86/115	-
37	NEX	R	321	-	-	3/27/83/83	0/3/3/3
29	Q6L	X	316	-	-	7/29/63/67	0/2/2/2
30	BCR	K	207	-	-	3/29/63/63	0/2/2/2
26	IWJ	P	320	-	-	2/33/76/76	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	612	2	1/1/15/20	14/37/115/115	-
25	CLA	B	833	-	1/1/10/20	1/11/89/115	-
25	CLA	S	303	-	1/1/12/20	5/19/97/115	-
25	CLA	U	312	-	1/1/10/20	1/8/86/115	-
25	CLA	2	613	-	1/1/10/20	3/9/87/115	-
24	CHL	P	314	22	3/3/15/26	6/13/112/137	-
25	CLA	A	836	-	1/1/15/20	4/37/115/115	-
25	CLA	J	102	16	1/1/10/20	4/10/88/115	-
30	BCR	F	804	-	-	6/29/63/63	0/2/2/2
25	CLA	B	837	-	1/1/10/20	2/10/88/115	-
29	Q6L	W	315	-	-	4/29/67/67	0/2/2/2
29	Q6L	V	315	-	-	11/29/67/67	0/2/2/2
25	CLA	H	304	18	1/1/11/20	4/13/91/115	-
25	CLA	X	313	22	1/1/10/20	3/8/86/115	-
24	CHL	W	307	-	3/3/20/26	13/39/137/137	-
25	CLA	1	606	1	1/1/10/20	5/8/84/115	-
25	CLA	B	820	-	1/1/14/20	10/31/109/115	-
25	CLA	X	304	-	1/1/10/20	5/10/88/115	-
25	CLA	B	804	-	1/1/15/20	15/37/115/115	-
25	CLA	U	301	22	1/1/11/20	7/13/91/115	-
25	CLA	B	827	-	1/1/12/20	4/19/97/115	-
30	BCR	M	101	-	-	6/29/63/63	0/2/2/2
24	CHL	2	615	2	3/3/15/26	5/12/110/137	-
25	CLA	B	823	-	1/1/11/20	6/16/94/115	-
25	CLA	A	839	-	1/1/15/20	17/37/115/115	-
35	SF4	C	102	9	-	-	0/6/5/5
29	Q6L	R	301	-	-	11/29/67/67	0/2/2/2
25	CLA	A	804	39	1/1/15/20	14/37/115/115	-
24	CHL	V	305	22	3/3/15/26	2/12/110/137	-
29	Q6L	W	316	-	-	5/29/67/67	0/2/2/2
25	CLA	P	303	-	1/1/12/20	11/19/97/115	-
38	KC2	S	308	22	-	7/15/71/71	-
25	CLA	B	822	-	1/1/12/20	3/19/97/115	-
29	Q6L	U	315	-	-	2/29/67/67	0/2/2/2
25	CLA	B	828	-	1/1/15/20	5/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Q	301	14	1/1/13/20	14/25/103/115	-
26	IWJ	3	315	-	-	3/33/76/76	1/2/2/2
24	CHL	R	310	-	3/3/17/26	6/23/121/137	-
25	CLA	P	311	-	1/1/14/20	10/31/109/115	-
25	CLA	4	310	4	1/1/12/20	6/24/102/115	-
24	CHL	X	308	-	3/3/15/26	8/13/111/137	-
25	CLA	A	809	-	1/1/12/20	6/19/97/115	-
25	CLA	B	812	-	1/1/15/20	12/37/115/115	-
25	CLA	3	307	3	1/1/14/20	10/33/111/115	-
25	CLA	4	312	4	1/1/10/20	3/8/86/115	-
25	CLA	R	317	-	-	6/17/95/115	-
31	LMG	B	801	-	-	4/33/53/70	0/1/1/1
25	CLA	3	305	3	1/1/10/20	2/10/86/115	-
37	NEX	S	317	-	-	3/27/83/83	0/3/3/3
24	CHL	1	604	1	3/3/15/26	0/8/106/137	-
37	NEX	P	317	-	-	2/27/83/83	0/3/3/3
38	KC2	U	307	22	-	11/15/71/71	-
25	CLA	T	312	22	1/1/13/20	12/25/103/115	-
25	CLA	A	829	-	1/1/15/20	16/37/115/115	-
25	CLA	U	302	-	1/1/13/20	11/27/105/115	-
25	CLA	A	815	-	1/1/15/20	12/37/115/115	-
25	CLA	4	305	-	1/1/11/20	2/11/87/115	-
31	LMG	A	857	-	-	9/41/61/70	0/1/1/1
25	CLA	6	608	6	1/1/10/20	5/10/88/115	-
26	IWJ	S	322	-	-	5/33/76/76	0/2/2/2
24	CHL	S	314	22	3/3/15/26	5/13/112/137	-
25	CLA	6	609	-	1/1/11/20	4/11/89/115	-
25	CLA	A	808	7	1/1/15/20	11/37/115/115	-
29	Q6L	S	320	-	-	7/29/67/67	0/2/2/2
25	CLA	B	825	-	1/1/11/20	6/13/91/115	-
29	Q6L	O	2006	-	-	9/29/67/67	0/2/2/2
25	CLA	X	303	-	1/1/12/20	9/21/99/115	-
25	CLA	W	301	22	1/1/13/20	10/25/103/115	-
28	LHG	3	322	-	-	10/40/40/53	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	3	317	-	-	2/29/63/63	0/2/2/2
25	CLA	5	608	5	1/1/10/20	4/8/86/115	-
25	CLA	O	2004	-	1/1/10/20	5/8/86/115	-
28	LHG	A	847	25	-	9/34/34/53	-
25	CLA	A	827	39	1/1/15/20	9/37/115/115	-
25	CLA	G	202	-	1/1/11/20	7/13/91/115	-
25	CLA	B	807	-	1/1/15/20	12/37/115/115	-
24	CHL	R	302	-	3/3/16/26	5/17/115/137	-
25	CLA	B	838	-	1/1/12/20	0/19/97/115	-
25	CLA	U	308	22	1/1/10/20	1/8/86/115	-
27	XAT	1	612	-	-	6/31/93/93	0/4/4/4
25	CLA	L	301	18	1/1/10/20	3/8/86/115	-
25	CLA	P	301	22	1/1/15/20	9/37/115/115	-
33	CL0	A	802	-	3/3/20/25	8/37/135/135	-
31	LMG	A	855	-	-	4/22/42/70	0/1/1/1
38	KC2	Q	310	23	-	6/15/71/71	-
30	BCR	K	205	-	-	3/29/63/63	0/2/2/2
25	CLA	V	303	-	1/1/12/20	5/19/97/115	-
24	CHL	T	306	-	3/3/17/26	6/23/121/137	-
25	CLA	4	303	4	1/1/14/20	15/31/109/115	-
29	Q6L	S	315	-	-	5/29/67/67	0/2/2/2
25	CLA	A	843	-	1/1/15/20	8/37/115/115	-
25	CLA	2	614	2	1/1/10/20	6/11/90/115	-
25	CLA	T	310	22	1/1/10/20	3/10/88/115	-
30	BCR	F	801	-	-	4/29/63/63	0/2/2/2
25	CLA	A	841	-	1/1/12/20	6/19/97/115	-
25	CLA	1	603	-	1/1/13/20	6/25/103/115	-
25	CLA	1	613	-	1/1/12/20	6/22/100/115	-
25	CLA	A	810	7	1/1/15/20	8/37/115/115	-
25	CLA	3	304	3	1/1/10/20	2/8/86/115	-
25	CLA	4	316	4	1/1/10/20	3/10/88/115	-
24	CHL	U	313	22	3/3/15/26	3/12/110/137	-
25	CLA	A	838	7	-	19/37/115/115	-
29	Q6L	S	321	-	-	11/29/67/67	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	812	-	1/1/14/20	10/36/114/115	-
24	CHL	4	307	-	3/3/15/26	6/12/108/137	-
25	CLA	4	311	-	1/1/10/20	5/10/88/115	-
25	CLA	Q	304	23	1/1/15/20	9/37/115/115	-
24	CHL	P	305	-	3/3/16/26	4/15/113/137	-
27	XAT	5	612	-	-	0/31/93/93	0/4/4/4
31	LMG	L	308	-	-	6/26/46/70	0/1/1/1
25	CLA	V	312	22	-	7/25/103/115	-
29	Q6L	R	323	-	-	9/29/67/67	0/2/2/2
27	XAT	3	316	-	-	3/31/93/93	0/4/4/4
25	CLA	Q	312	23	1/1/10/20	3/10/88/115	-
25	CLA	3	313	-	1/1/10/20	4/8/86/115	-
25	CLA	T	302	-	1/1/15/20	14/37/115/115	-
25	CLA	O	2002	-	1/1/15/20	8/37/115/115	-
25	CLA	A	821	-	1/1/15/20	18/37/115/115	-
25	CLA	S	302	-	1/1/15/20	11/37/115/115	-
25	CLA	A	811	7	1/1/12/20	2/19/97/115	-
24	CHL	4	308	-	3/3/16/26	3/15/113/137	-
25	CLA	B	834	-	1/1/15/20	11/37/115/115	-
25	CLA	2	608	2	1/1/11/20	6/13/91/115	-
27	XAT	4	318	-	-	5/31/93/93	0/4/4/4
25	CLA	A	837	-	1/1/15/20	12/37/115/115	-
24	CHL	U	304	22	3/3/15/26	5/10/108/137	-

The worst 5 of 3027 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	309	CLA	C4B-NB	10.02	1.44	1.35
34	A	844	PQN	C12-C13	9.18	1.55	1.33
34	B	844	PQN	C12-C13	9.06	1.54	1.33
29	V	316	Q6L	C29-C30	8.77	1.53	1.32
38	V	308	KC2	C2A-C3A	8.64	1.54	1.37

The worst 5 of 4503 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	318	XAT	O4-C5-C4	15.74	125.20	113.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	317	NEX	O24-C25-C24	13.84	123.78	113.38
37	R	321	NEX	O24-C25-C24	13.41	123.46	113.38
27	6	615	XAT	O4-C5-C4	13.30	123.38	113.38
37	W	317	NEX	O24-C25-C24	13.18	123.28	113.38

5 of 413 chirality outliers are listed below:

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

5 of 2988 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	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	CHA-CBD-CGD-O1D
24	2	605	CHL	CHA-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

201 monomers are involved in 301 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	F	805	LMG	1	0
25	V	301	CLA	5	0
25	W	312	CLA	2	0
25	A	813	CLA	3	0
25	B	803	CLA	1	0
24	T	307	CHL	1	0
25	R	316	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	R	313	CLA	1	0
25	Q	315	CLA	1	0
24	2	607	CHL	1	0
30	4	319	BCR	2	0
25	V	309	CLA	4	0
25	N	202	CLA	1	0
25	A	826	CLA	1	0
25	K	201	CLA	1	0
30	J	101	BCR	3	0
30	L	305	BCR	3	0
25	S	309	CLA	4	0
30	B	848	BCR	1	0
25	R	307	CLA	1	0
25	B	826	CLA	1	0
25	2	609	CLA	5	0
25	5	609	CLA	3	0
25	B	824	CLA	3	0
25	B	835	CLA	2	0
25	L	303	CLA	1	0
30	G	201	BCR	5	0
26	V	320	IWJ	1	0
29	R	320	Q6L	1	0
30	B	845	BCR	1	0
25	V	302	CLA	1	0
25	6	610	CLA	2	0
25	B	808	CLA	5	0
25	X	310	CLA	1	0
24	Q	307	CHL	1	0
36	A	854	DGD	1	0
25	W	303	CLA	1	0
25	R	305	CLA	4	0
25	A	824	CLA	1	0
24	V	314	CHL	1	0
32	H	303	SQD	1	0
26	4	301	IWJ	1	0
25	B	809	CLA	1	0
25	L	302	CLA	1	0
24	S	304	CHL	2	0
25	F	802	CLA	1	0
24	V	307	CHL	1	0
29	R	319	Q6L	1	0
25	P	309	CLA	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	829	CLA	2	0
26	Q	320	IWJ	1	0
24	W	314	CHL	1	0
29	2	616	Q6L	2	0
38	V	308	KC2	1	0
25	6	602	CLA	2	0
25	5	610	CLA	1	0
25	1	609	CLA	1	0
25	V	311	CLA	3	0
25	B	843	CLA	1	0
27	6	615	XAT	2	0
25	6	612	CLA	2	0
26	R	322	IWJ	1	0
24	R	308	CHL	7	0
24	P	307	CHL	1	0
25	H	301	CLA	1	0
25	A	830	CLA	3	0
30	B	847	BCR	1	0
25	A	820	CLA	1	0
28	2	619	LHG	1	0
25	B	810	CLA	1	0
38	R	312	KC2	2	0
25	4	309	CLA	1	0
25	O	2001	CLA	1	0
25	G	203	CLA	1	0
25	S	310	CLA	3	0
29	Q	319	Q6L	1	0
26	6	614	IWJ	2	0
26	W	318	IWJ	2	0
25	B	841	CLA	1	0
25	B	830	CLA	2	0
24	4	306	CHL	2	0
25	R	306	CLA	1	0
25	X	302	CLA	3	0
25	F	803	CLA	1	0
25	S	301	CLA	6	0
25	1	610	CLA	1	0
25	6	611	CLA	1	0
25	A	822	CLA	1	0
25	1	605	CLA	2	0
38	T	308	KC2	1	0
38	P	308	KC2	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	T	321	IWJ	1	0
25	B	832	CLA	1	0
25	B	815	CLA	4	0
29	V	321	Q6L	1	0
25	A	832	CLA	1	0
30	J	103	BCR	1	0
26	S	319	IWJ	1	0
25	5	602	CLA	2	0
25	1	607	CLA	3	0
25	B	819	CLA	2	0
26	V	317	IWJ	1	0
25	3	301	CLA	3	0
25	B	818	CLA	2	0
25	A	825	CLA	1	0
25	T	311	CLA	1	0
24	1	601	CHL	1	0
26	T	318	IWJ	1	0
25	A	856	CLA	1	0
25	2	602	CLA	1	0
25	B	840	CLA	1	0
26	P	318	IWJ	1	0
25	B	842	CLA	5	0
24	2	601	CHL	1	0
24	X	306	CHL	1	0
25	G	204	CLA	1	0
28	6	616	LHG	1	0
30	A	850	BCR	1	0
25	A	814	CLA	1	0
25	X	311	CLA	3	0
30	A	849	BCR	1	0
24	S	307	CHL	5	0
25	A	807	CLA	2	0
25	W	309	CLA	5	0
24	R	311	CHL	2	0
25	6	607	CLA	3	0
26	4	317	IWJ	2	0
25	A	803	CLA	1	0
29	X	319	Q6L	1	0
25	3	308	CLA	3	0
25	3	303	CLA	1	0
29	U	314	Q6L	2	0
36	B	850	DGD	1	0

*Continued on next page...*

*Continued from previous page...*

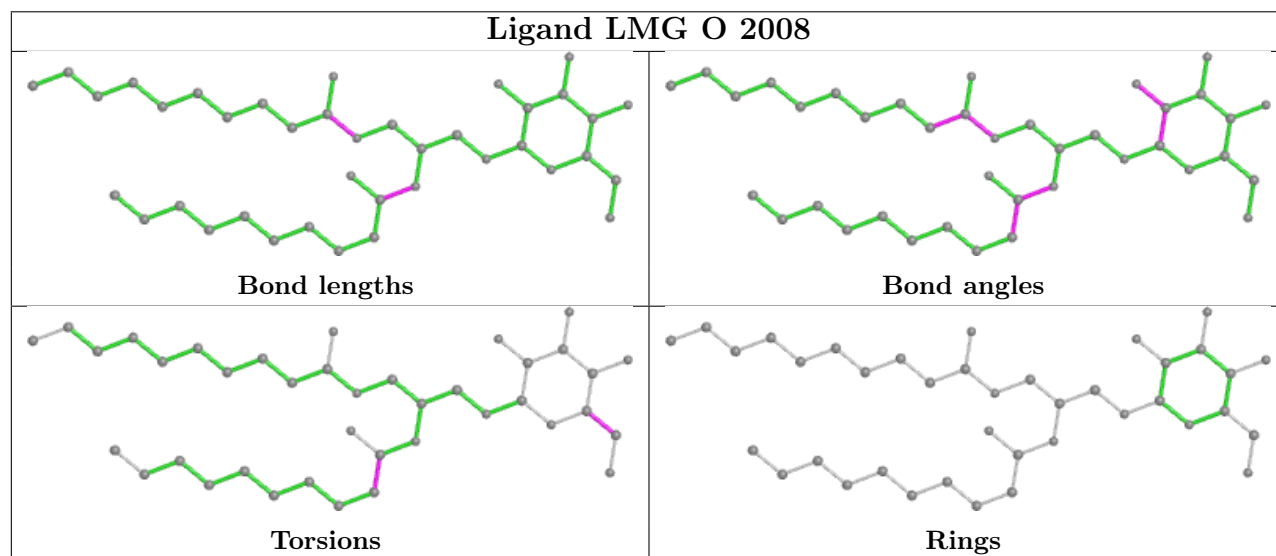
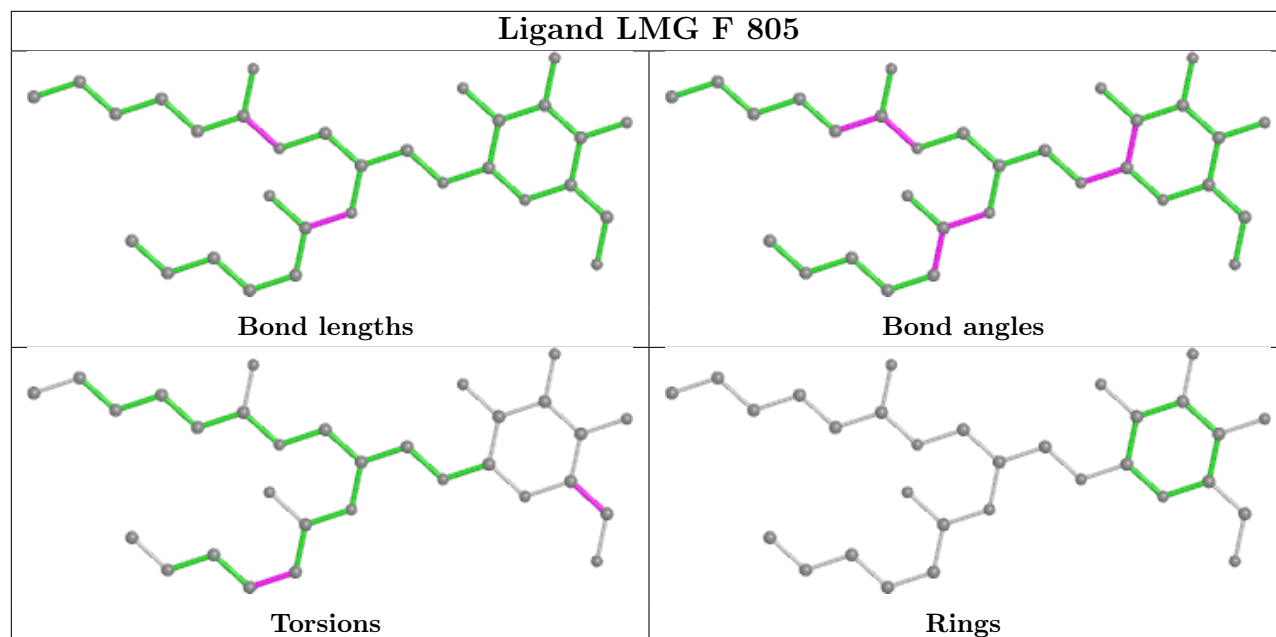
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	813	CLA	1	0
30	A	852	BCR	3	0
25	B	806	CLA	1	0
34	A	844	PQN	1	0
25	Q	314	CLA	2	0
29	T	316	Q6L	1	0
24	3	306	CHL	1	0
29	P	316	Q6L	1	0
25	K	206	CLA	2	0
25	Q	306	CLA	1	0
25	5	607	CLA	2	0
25	A	833	CLA	1	0
27	2	617	XAT	1	0
28	1	614	LHG	1	0
30	K	207	BCR	2	0
26	P	320	IWJ	1	0
25	2	613	CLA	2	0
25	A	836	CLA	1	0
25	J	102	CLA	1	0
29	W	315	Q6L	2	0
25	X	313	CLA	1	0
25	1	606	CLA	2	0
25	X	304	CLA	1	0
25	U	301	CLA	1	0
25	B	827	CLA	1	0
30	M	101	BCR	1	0
25	B	823	CLA	1	0
24	V	305	CHL	1	0
38	S	308	KC2	1	0
26	3	315	IWJ	2	0
25	4	310	CLA	2	0
24	X	308	CHL	1	0
25	A	809	CLA	1	0
25	3	307	CLA	4	0
37	P	317	NEX	1	0
25	T	312	CLA	1	0
25	A	815	CLA	3	0
31	A	857	LMG	1	0
26	S	322	IWJ	1	0
25	A	808	CLA	2	0
25	B	825	CLA	2	0
29	O	2006	Q6L	1	0

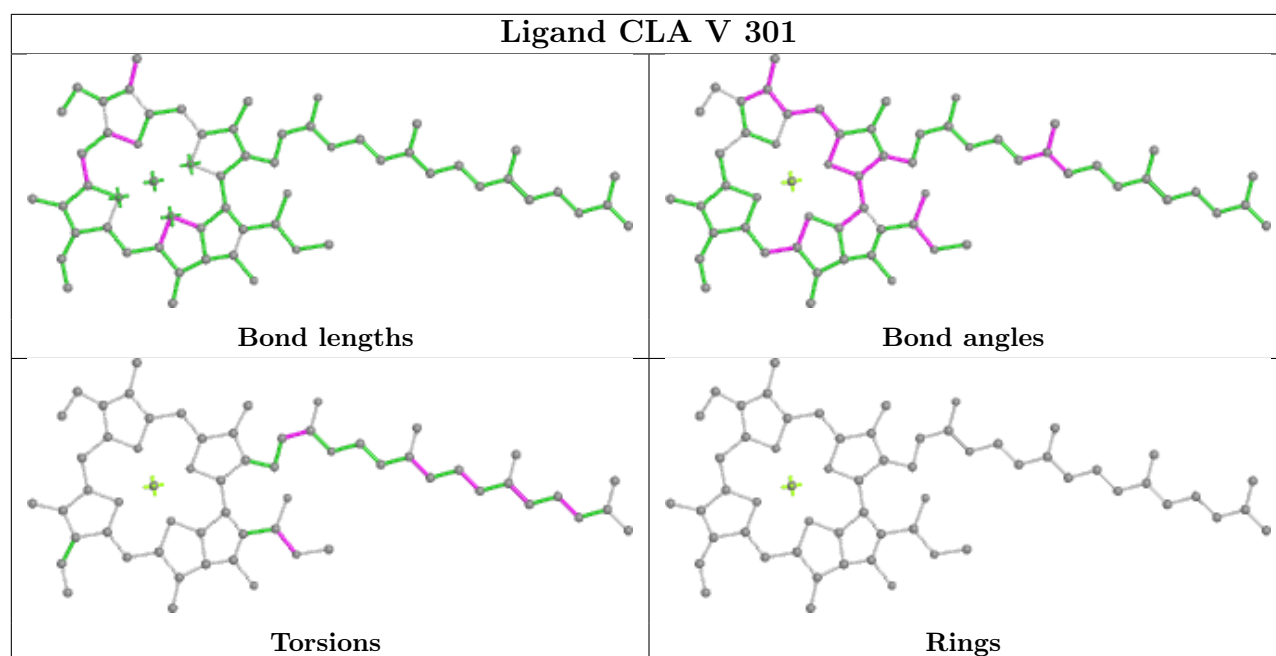
*Continued on next page...*

*Continued from previous page...*

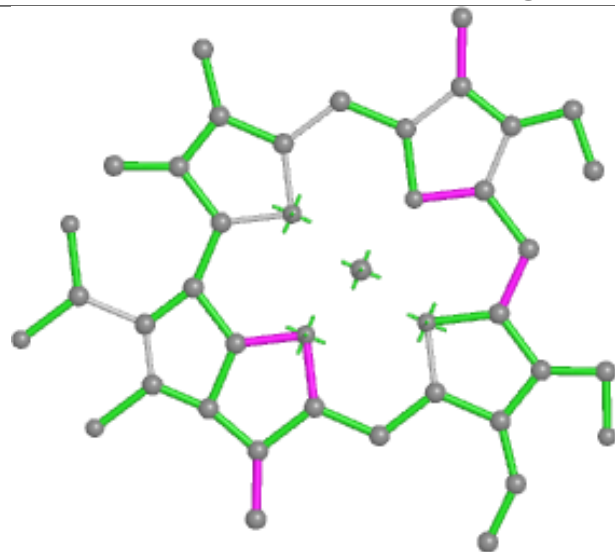
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	W	301	CLA	3	0
30	3	317	BCR	1	0
25	G	202	CLA	1	0
25	B	807	CLA	1	0
25	P	301	CLA	3	0
25	V	303	CLA	1	0
25	4	303	CLA	3	0
29	S	315	Q6L	1	0
25	T	310	CLA	1	0
30	F	801	BCR	1	0
25	A	810	CLA	1	0
25	3	304	CLA	3	0
25	A	812	CLA	1	0
25	Q	304	CLA	6	0
27	5	612	XAT	1	0
25	V	312	CLA	2	0
27	3	316	XAT	2	0
25	Q	312	CLA	1	0
25	3	313	CLA	1	0
25	O	2002	CLA	1	0
25	A	811	CLA	2	0
24	4	308	CHL	1	0
25	B	834	CLA	2	0
25	2	608	CLA	3	0
27	4	318	XAT	1	0
24	U	304	CHL	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.

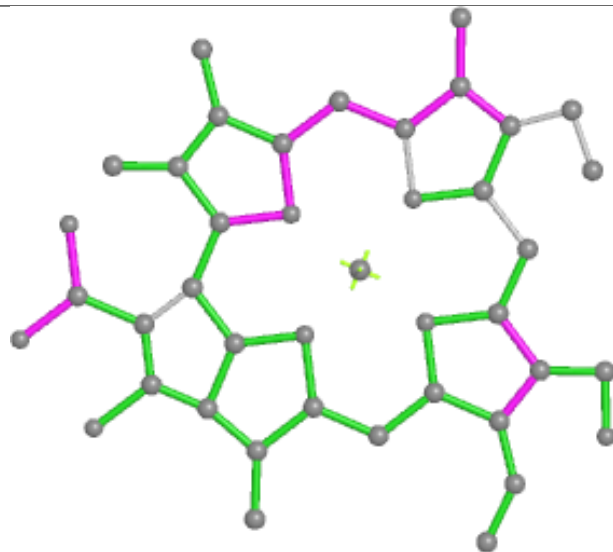




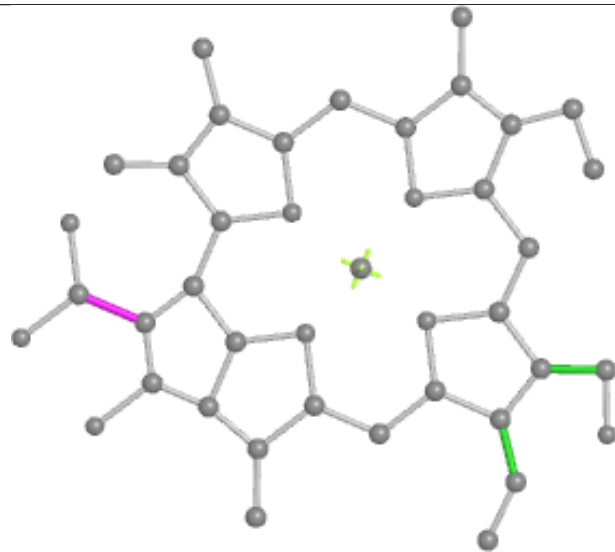
## Ligand CHL 5 605



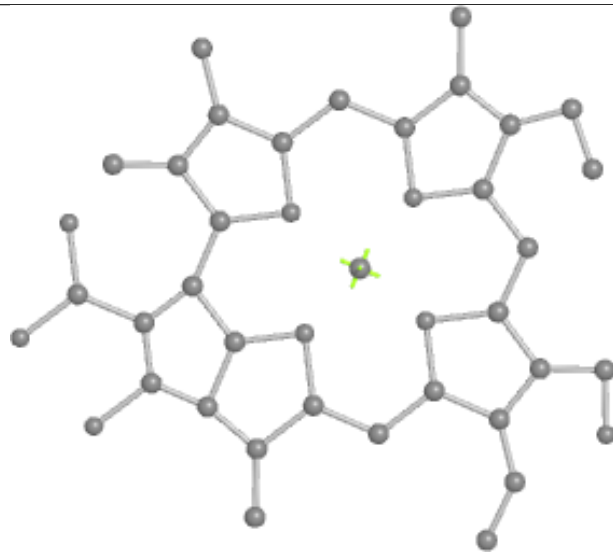
Bond lengths



Bond angles

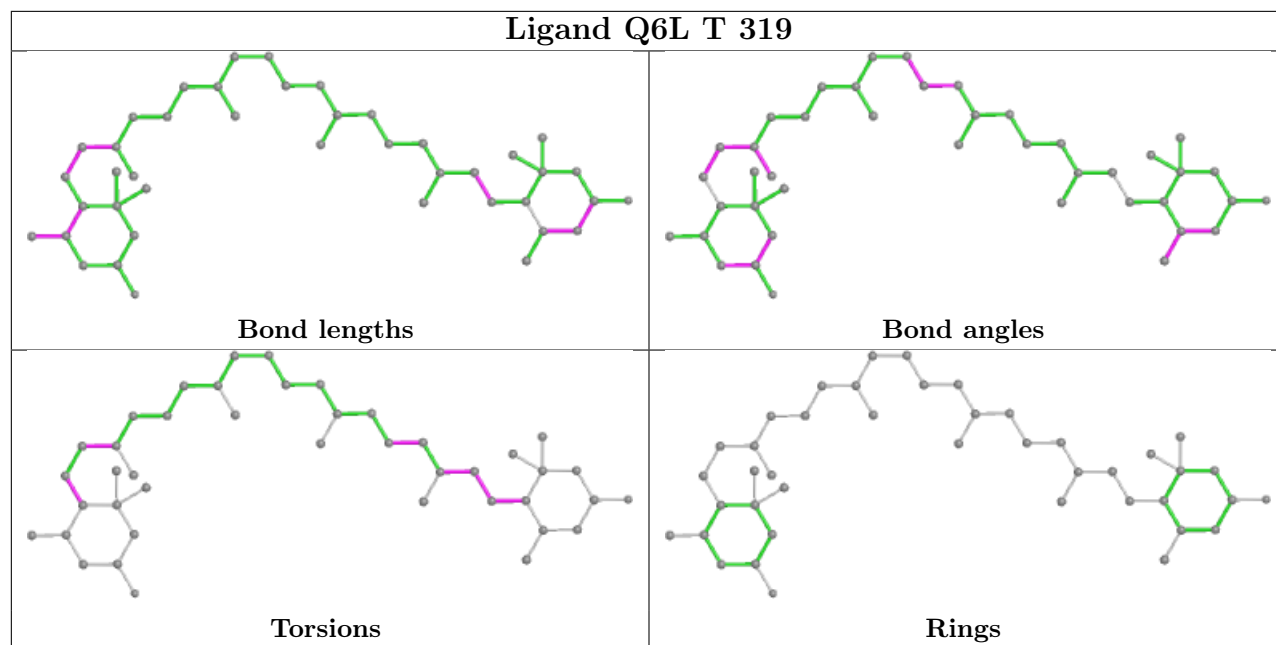


Torsions

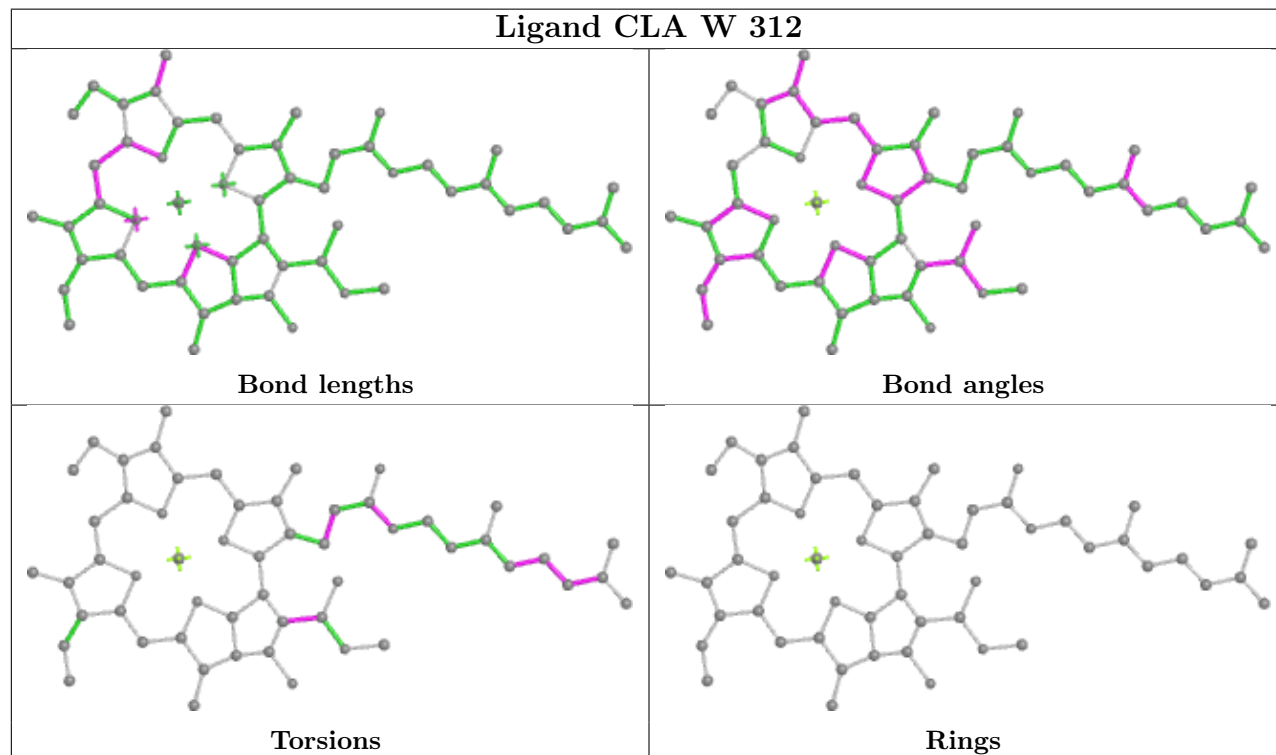


Rings

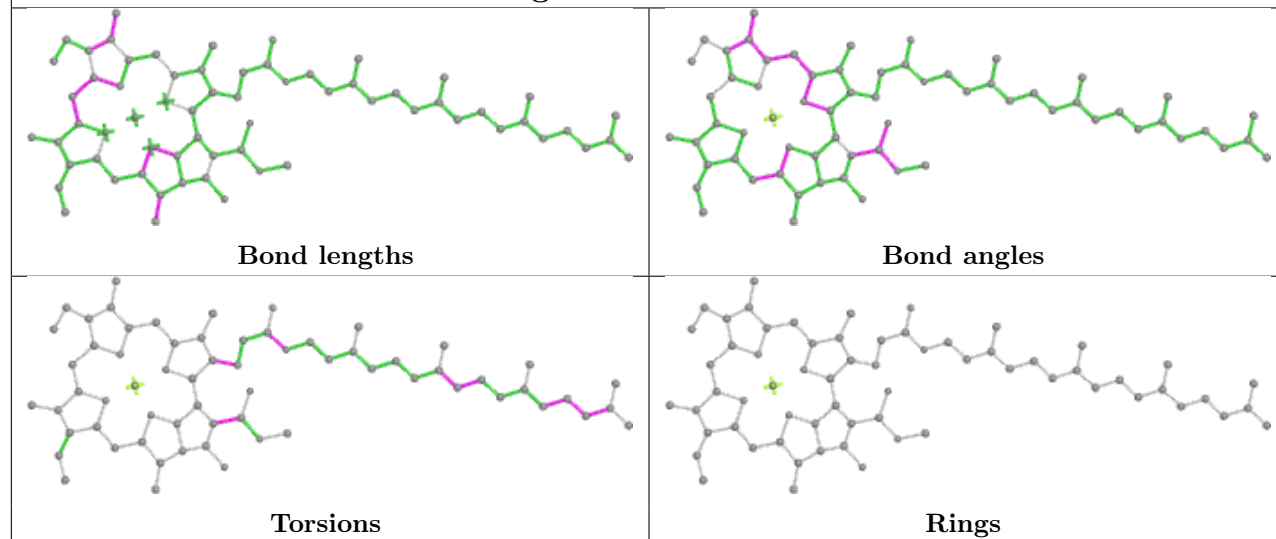
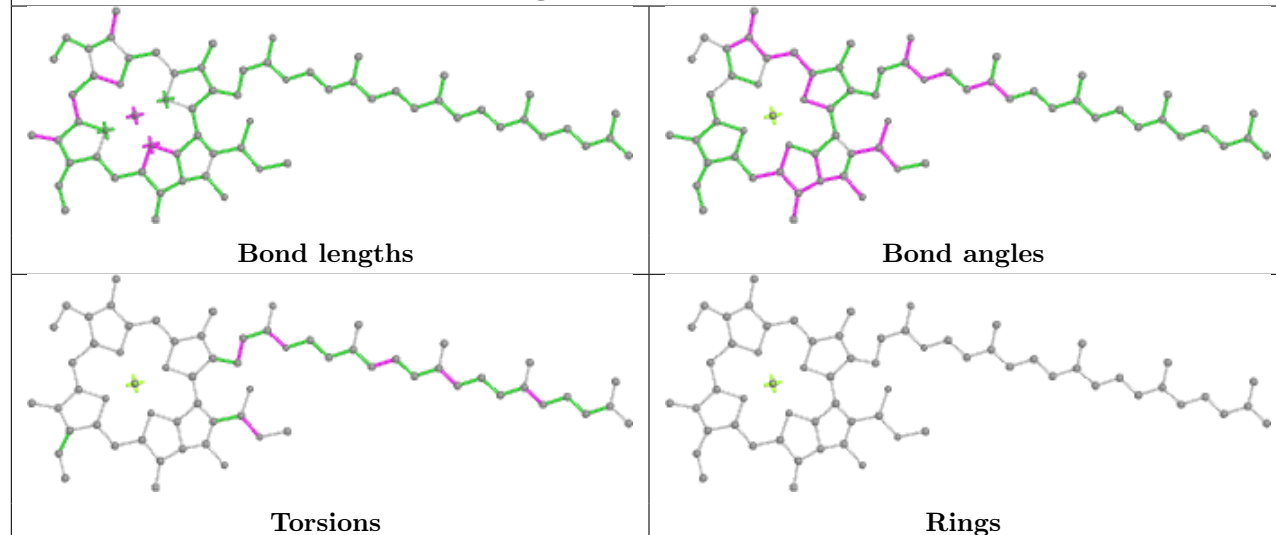
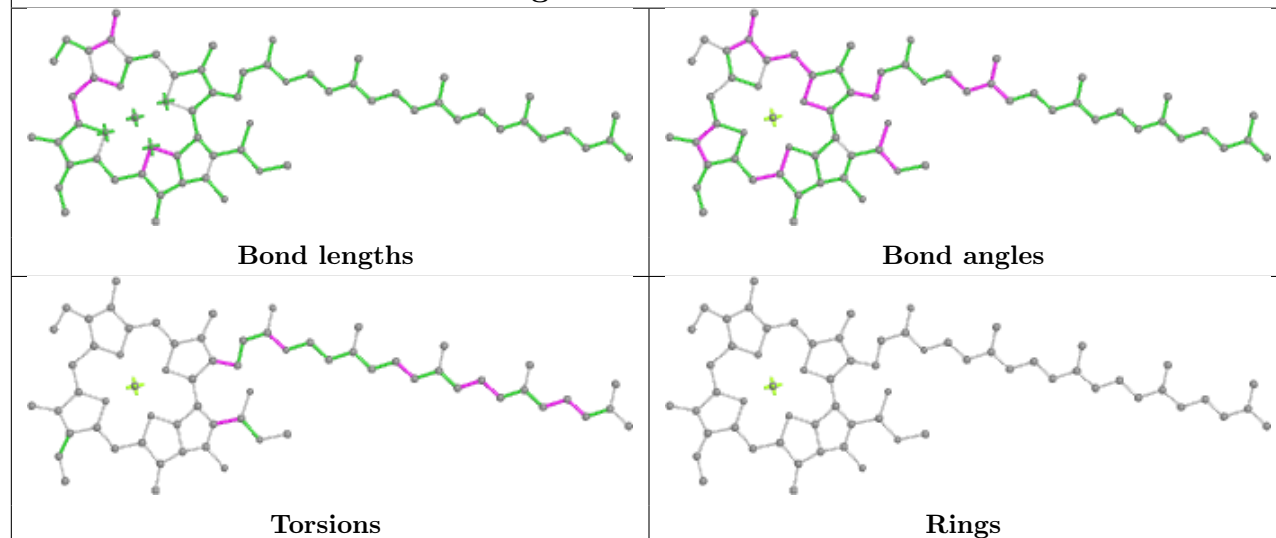
## Ligand Q6L T 319

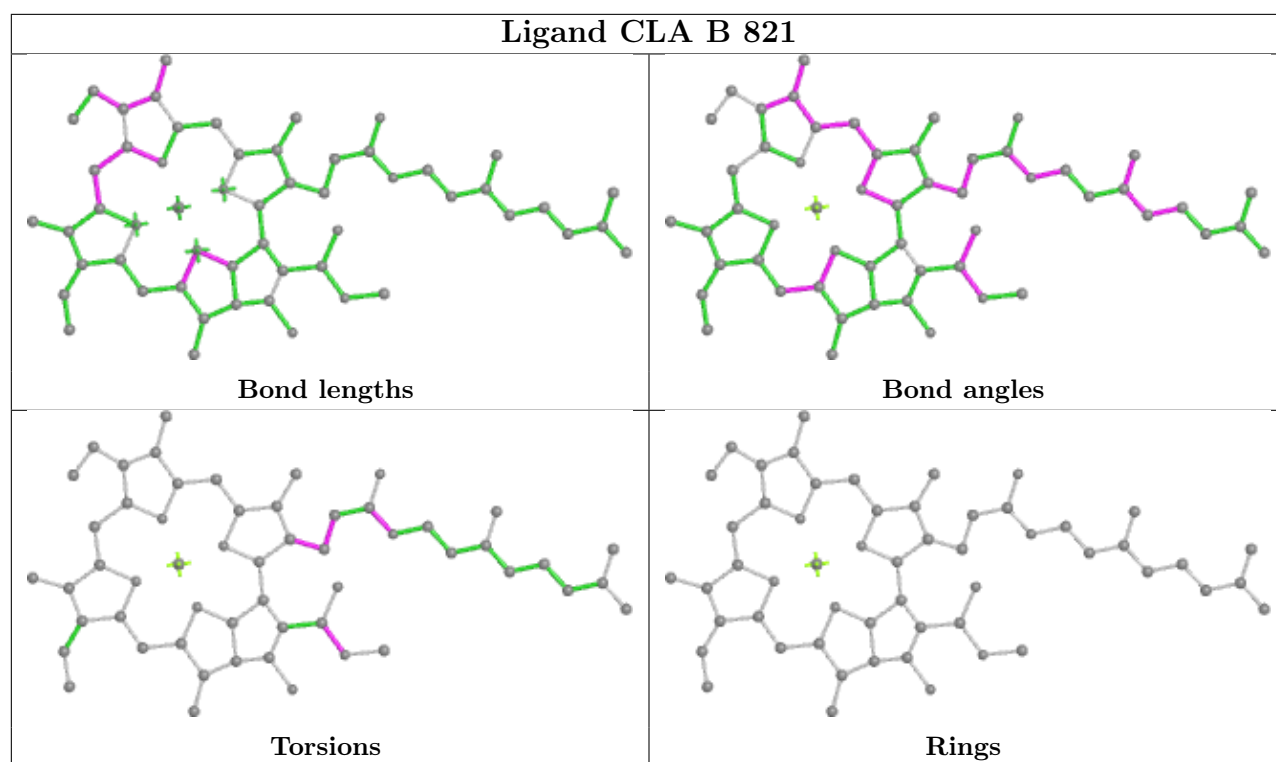


## Ligand CLA W 312

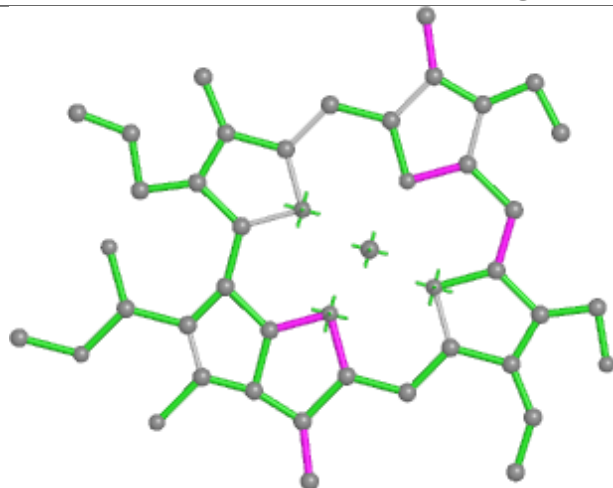




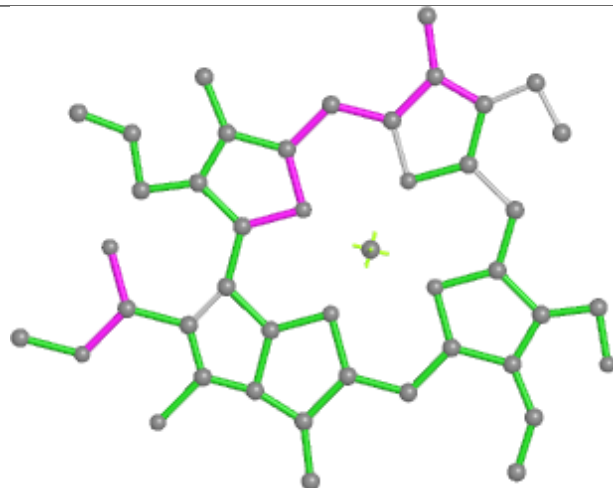
**Ligand CLA A 813****Ligand CLA B 803****Ligand CLA H 302**



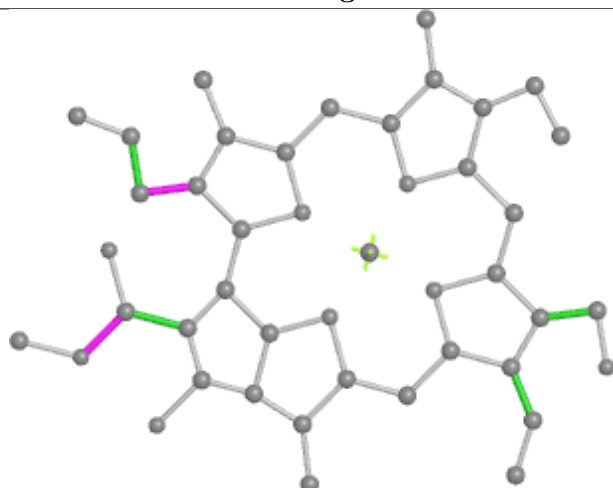
## Ligand CHL T 307



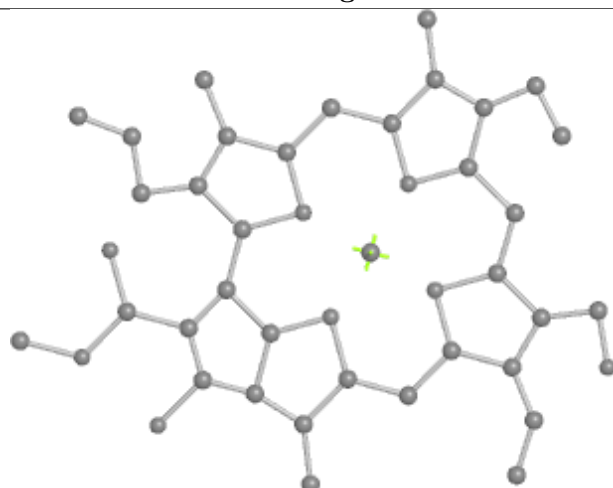
Bond lengths



Bond angles

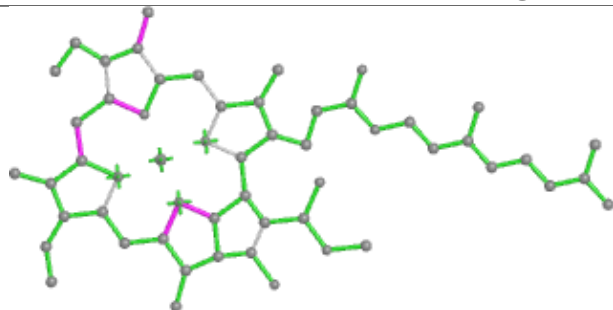


Torsions

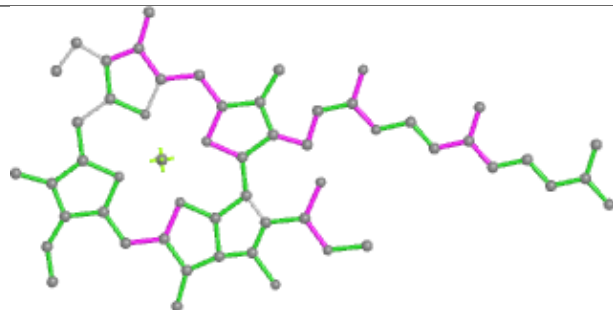


Rings

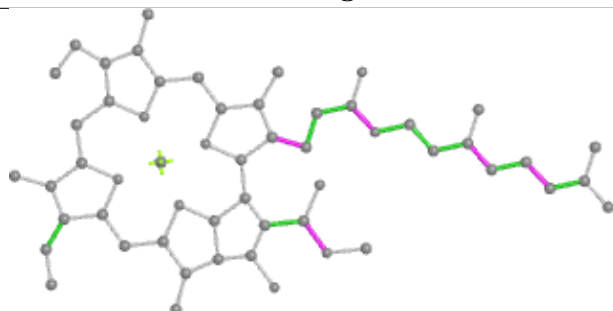
## Ligand CLA R 316



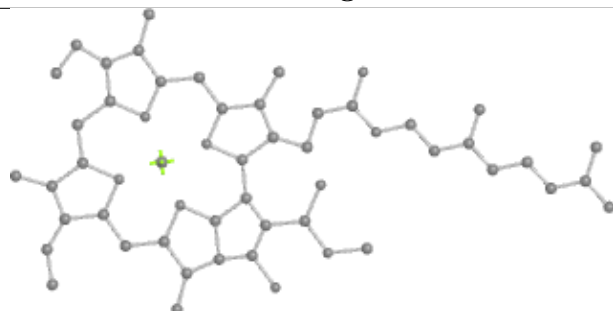
Bond lengths



Bond angles

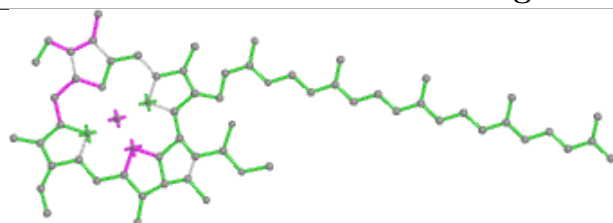


Torsions

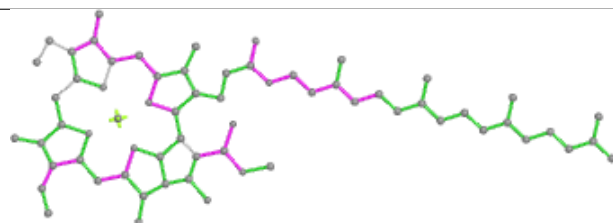


Rings

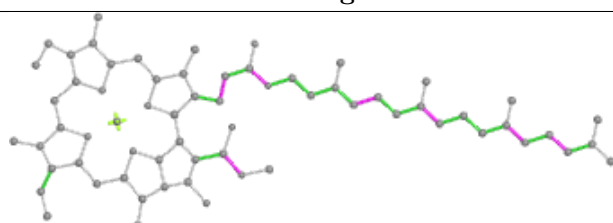
## Ligand CLA A 823



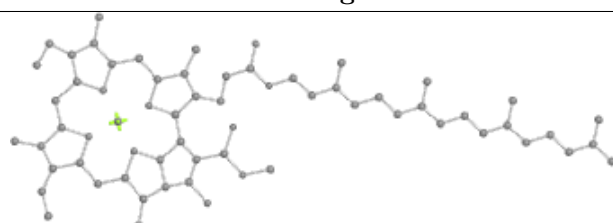
Bond lengths



Bond angles

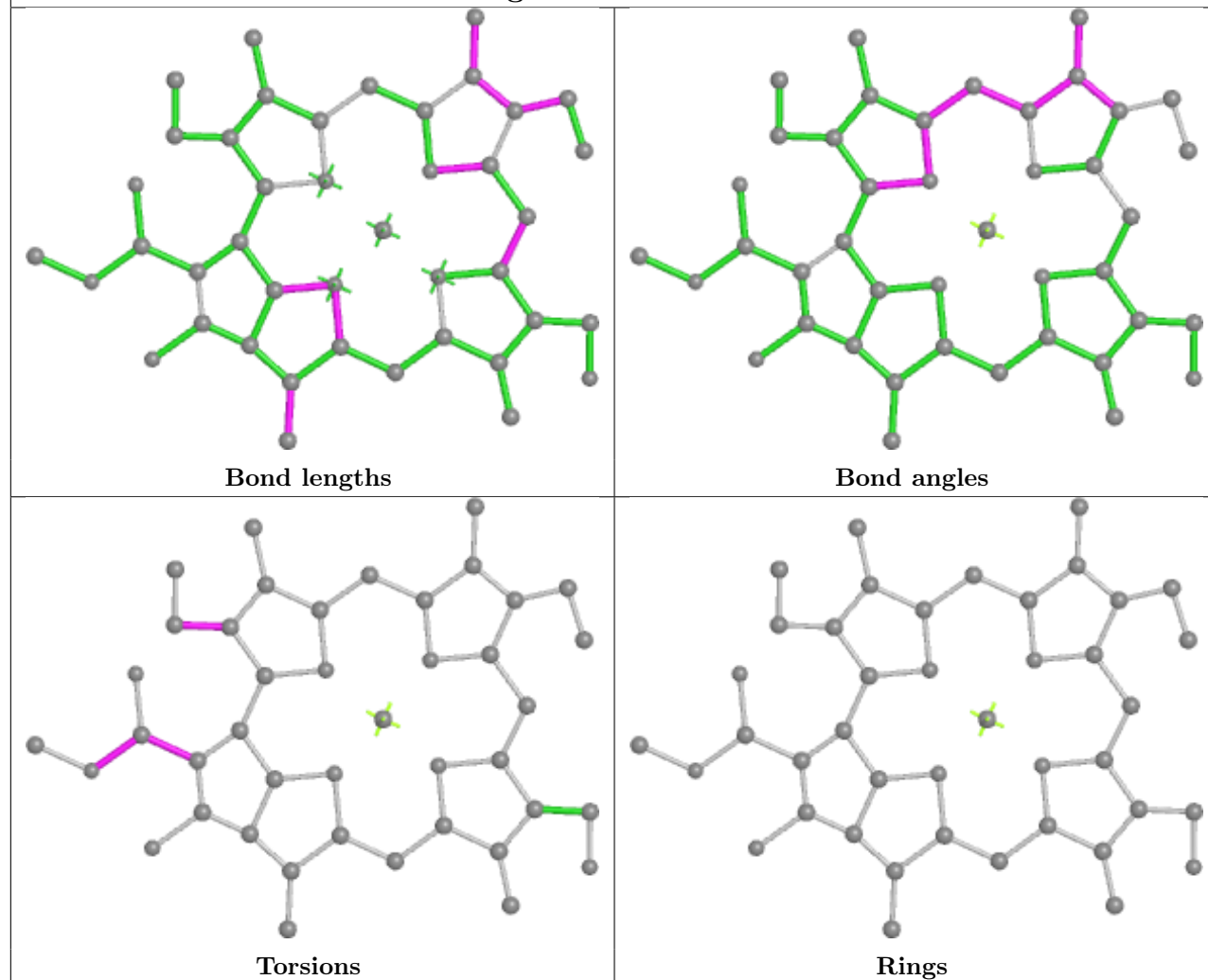


Torsions

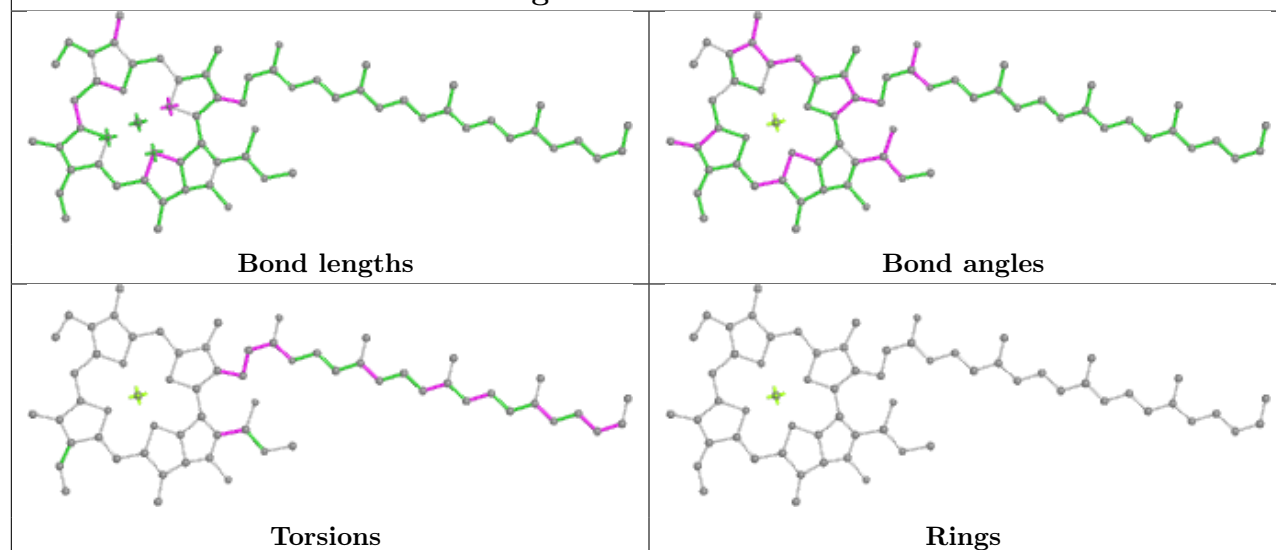


Rings

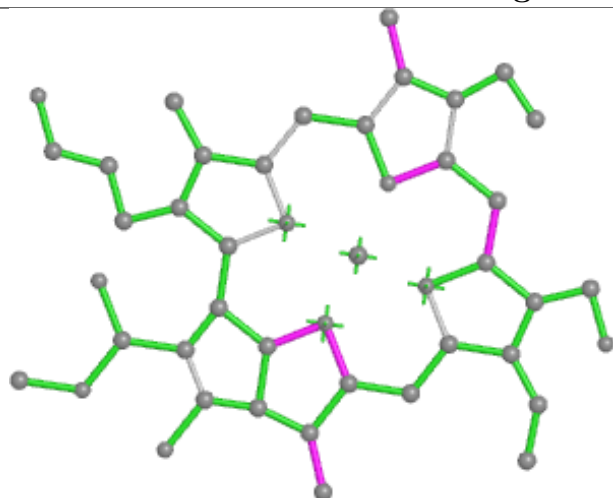
## Ligand CHL 2 605



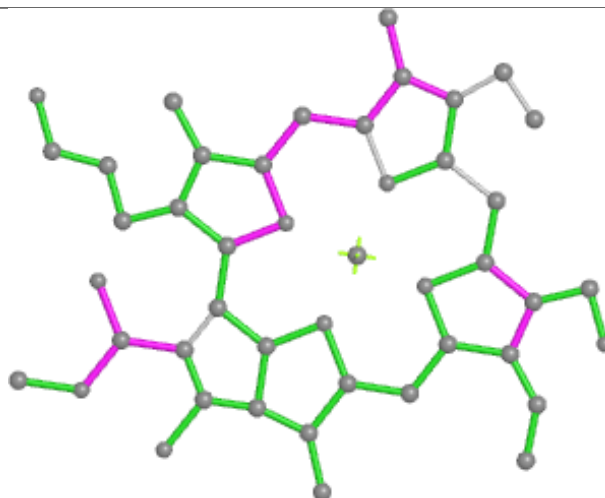
## Ligand CLA R 313



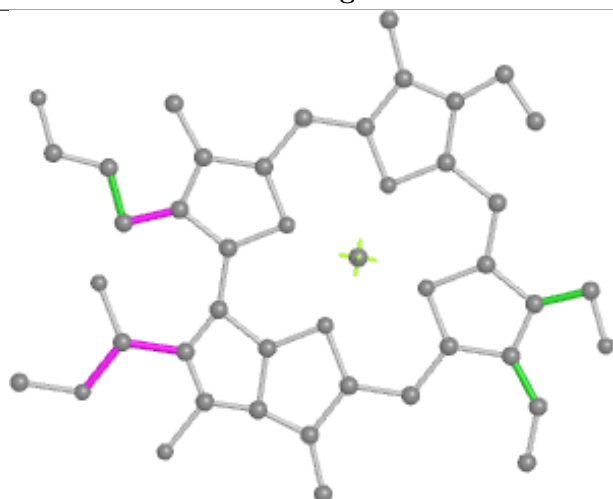
## Ligand CHL R 318



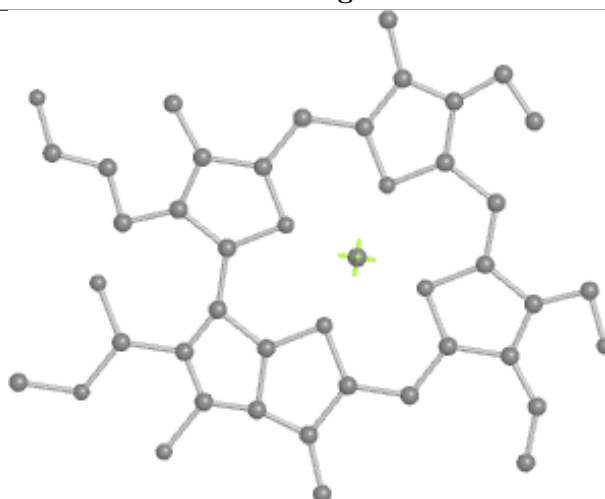
Bond lengths



Bond angles

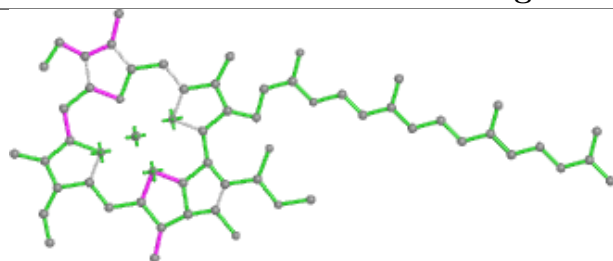


Torsions

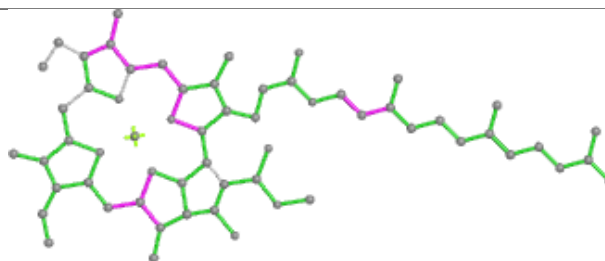


Rings

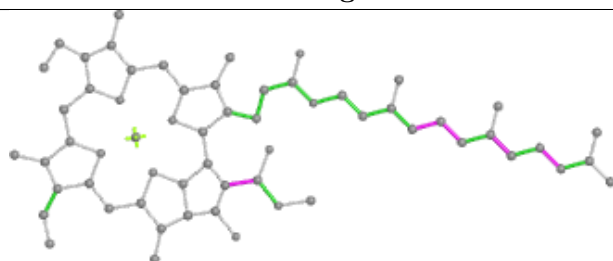
## Ligand CLA B 836



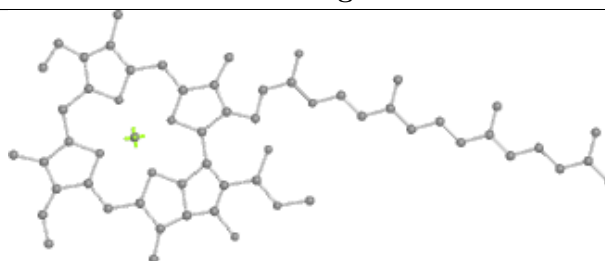
Bond lengths



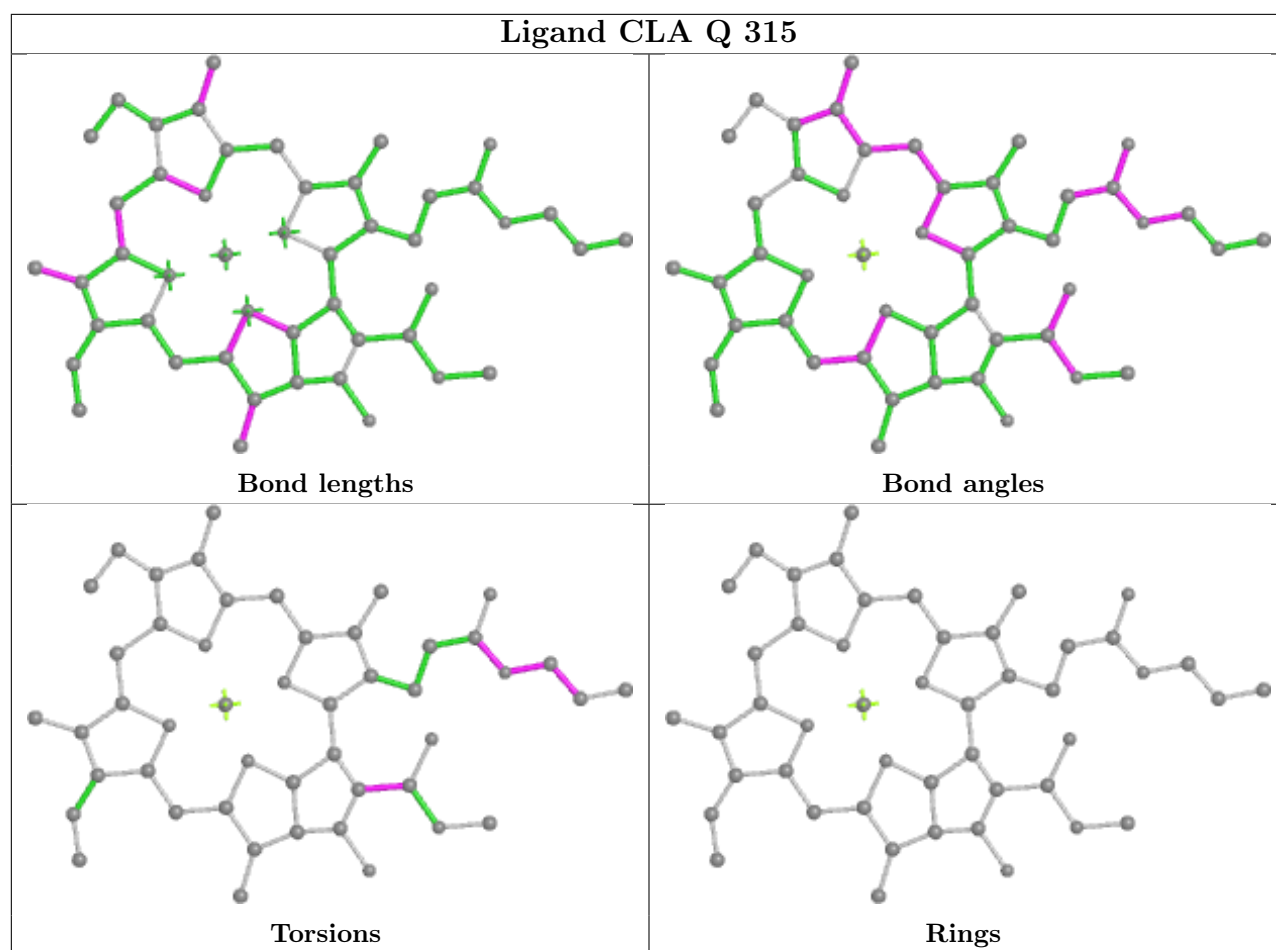
Bond angles



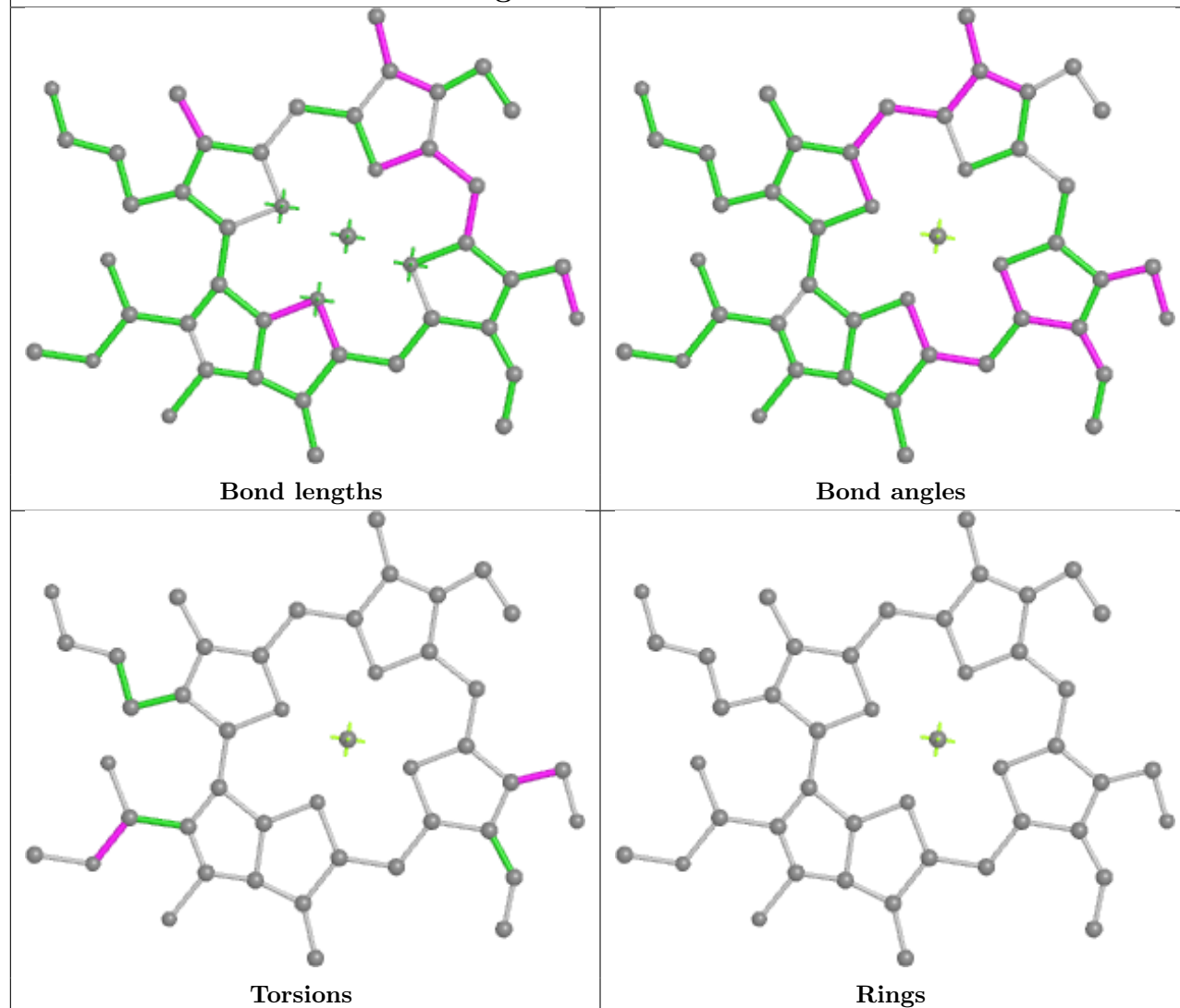
Torsions



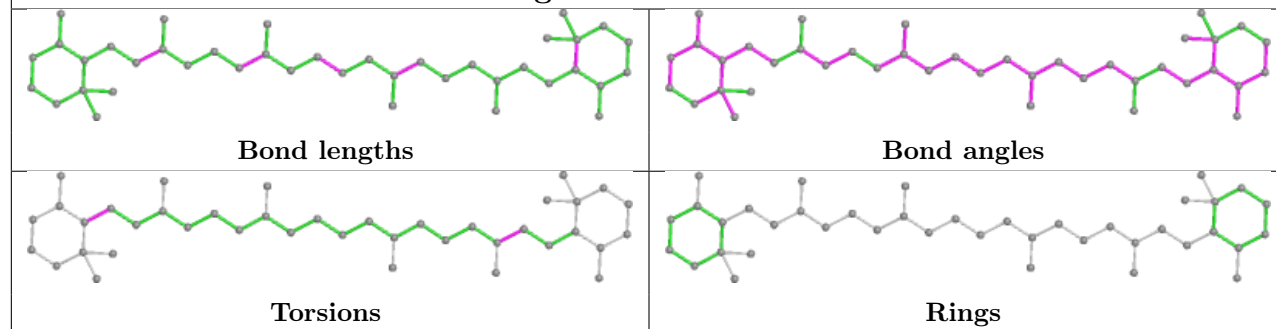
Rings



## Ligand CHL 2 607

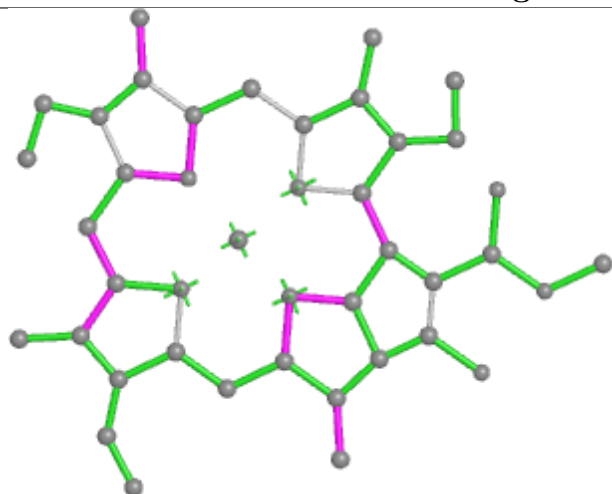


## Ligand BCR 4 319

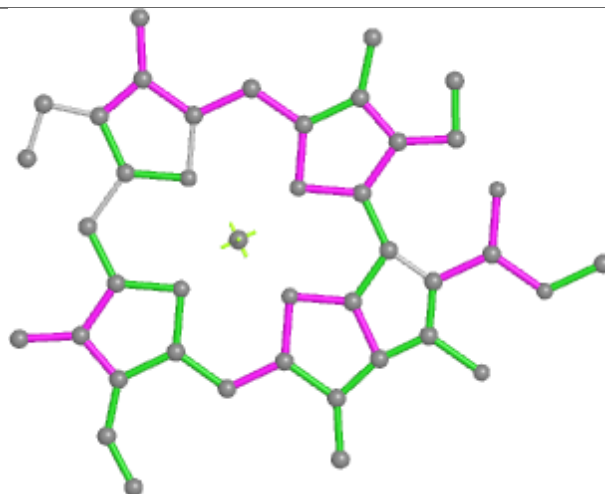




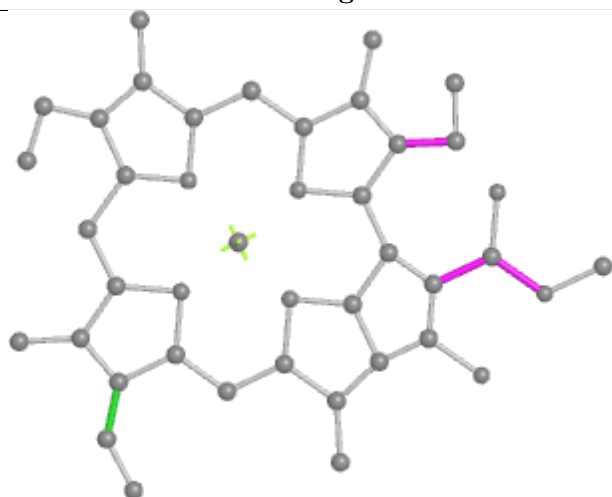
## Ligand CLA V 309



Bond lengths



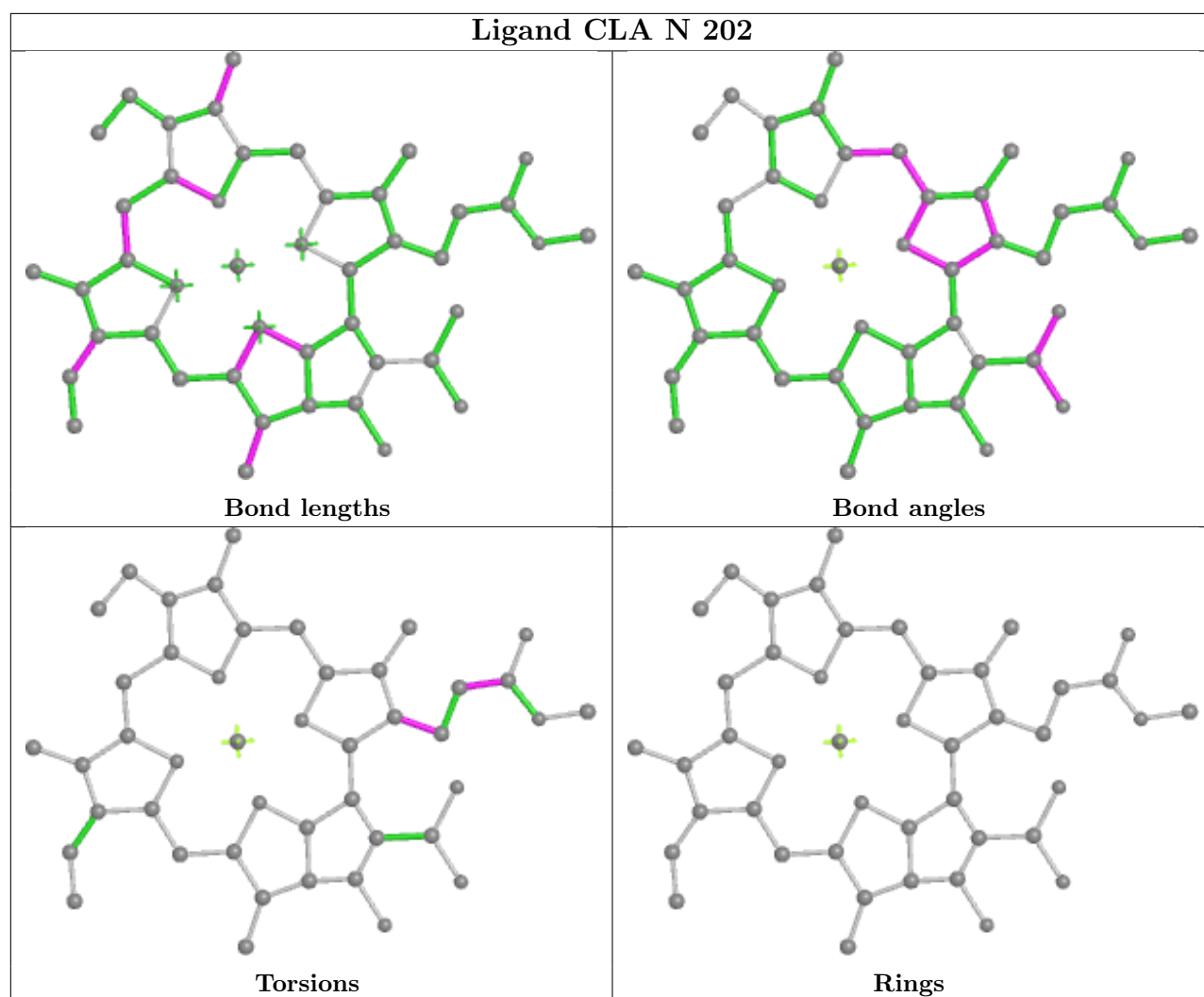
Bond angles



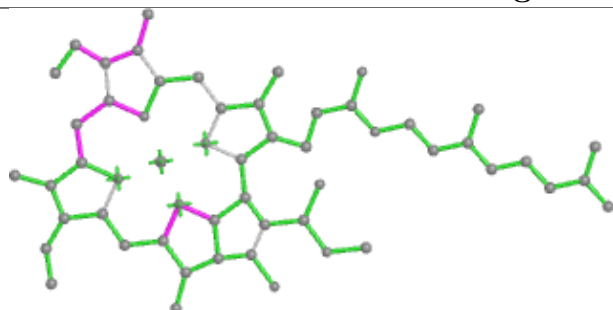
Torsions



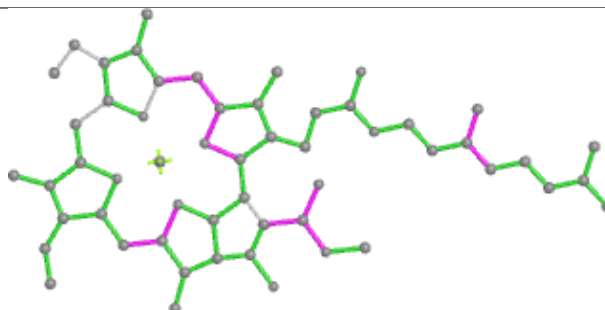
Rings



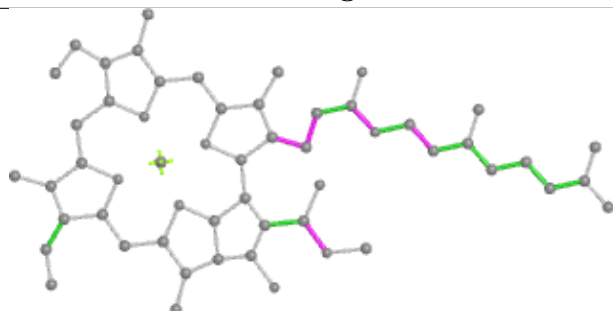
## Ligand CLA A 826



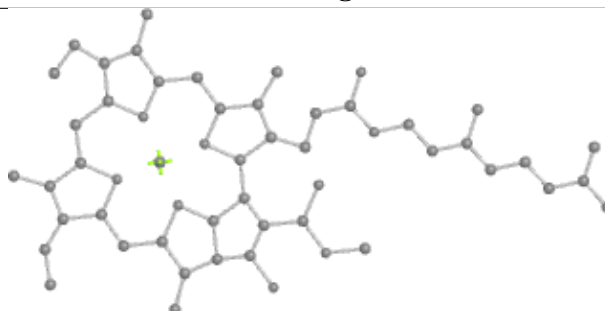
Bond lengths



Bond angles

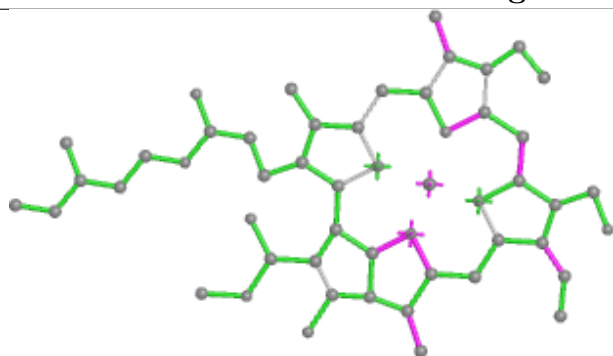


Torsions

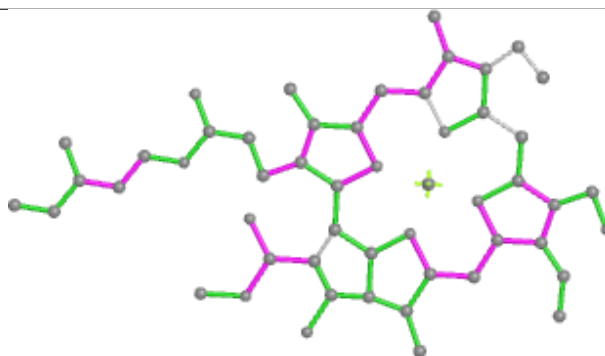


Rings

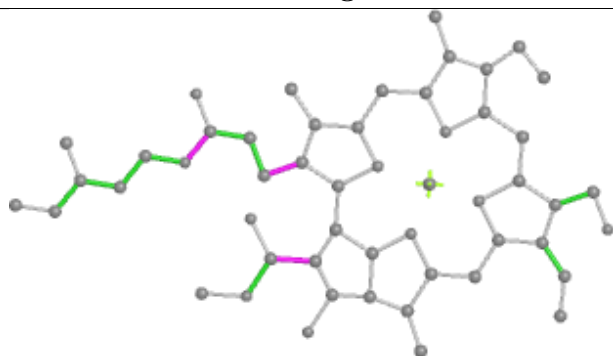
## Ligand CHL W 306



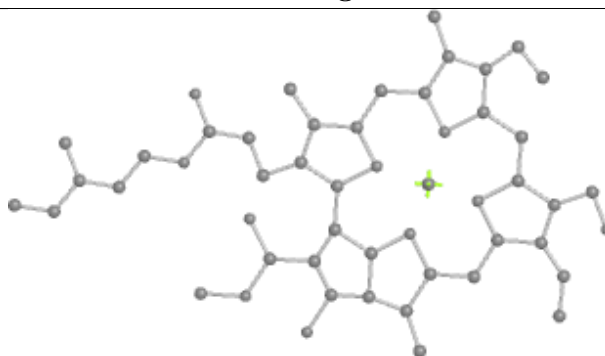
Bond lengths



Bond angles

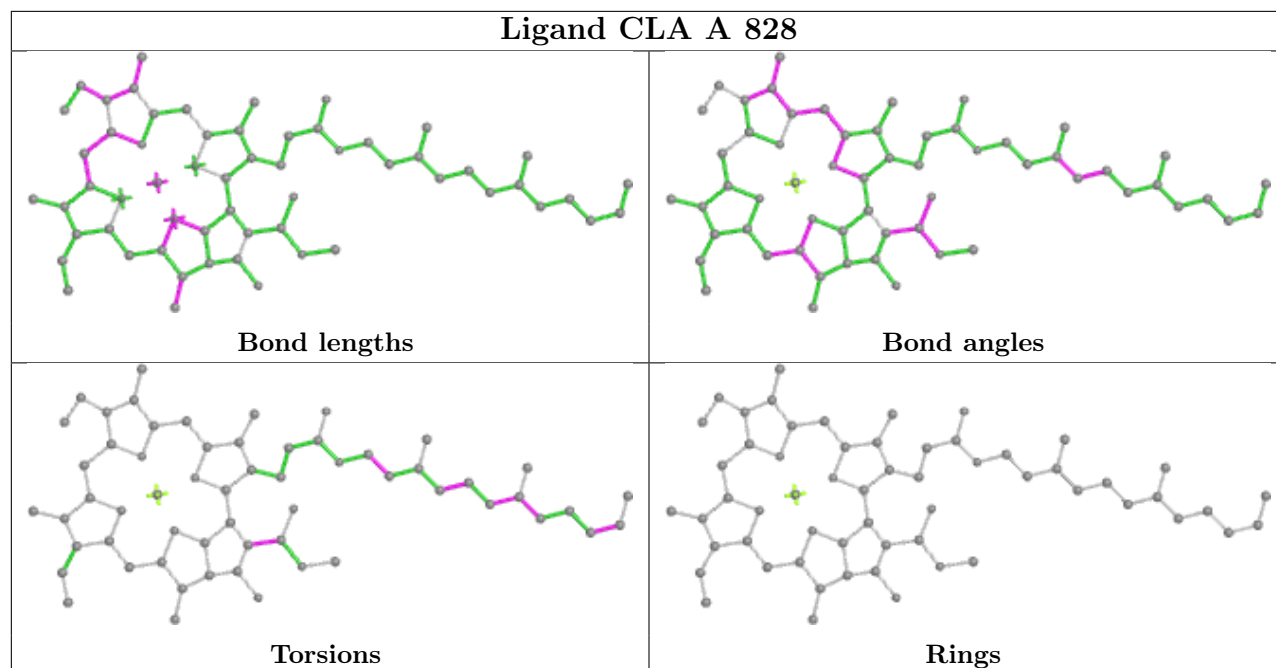


Torsions

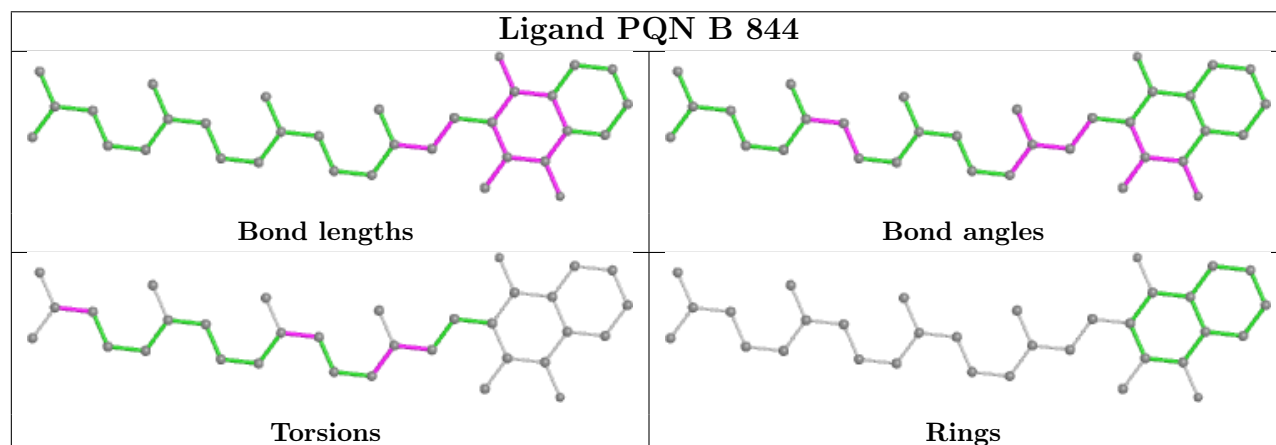


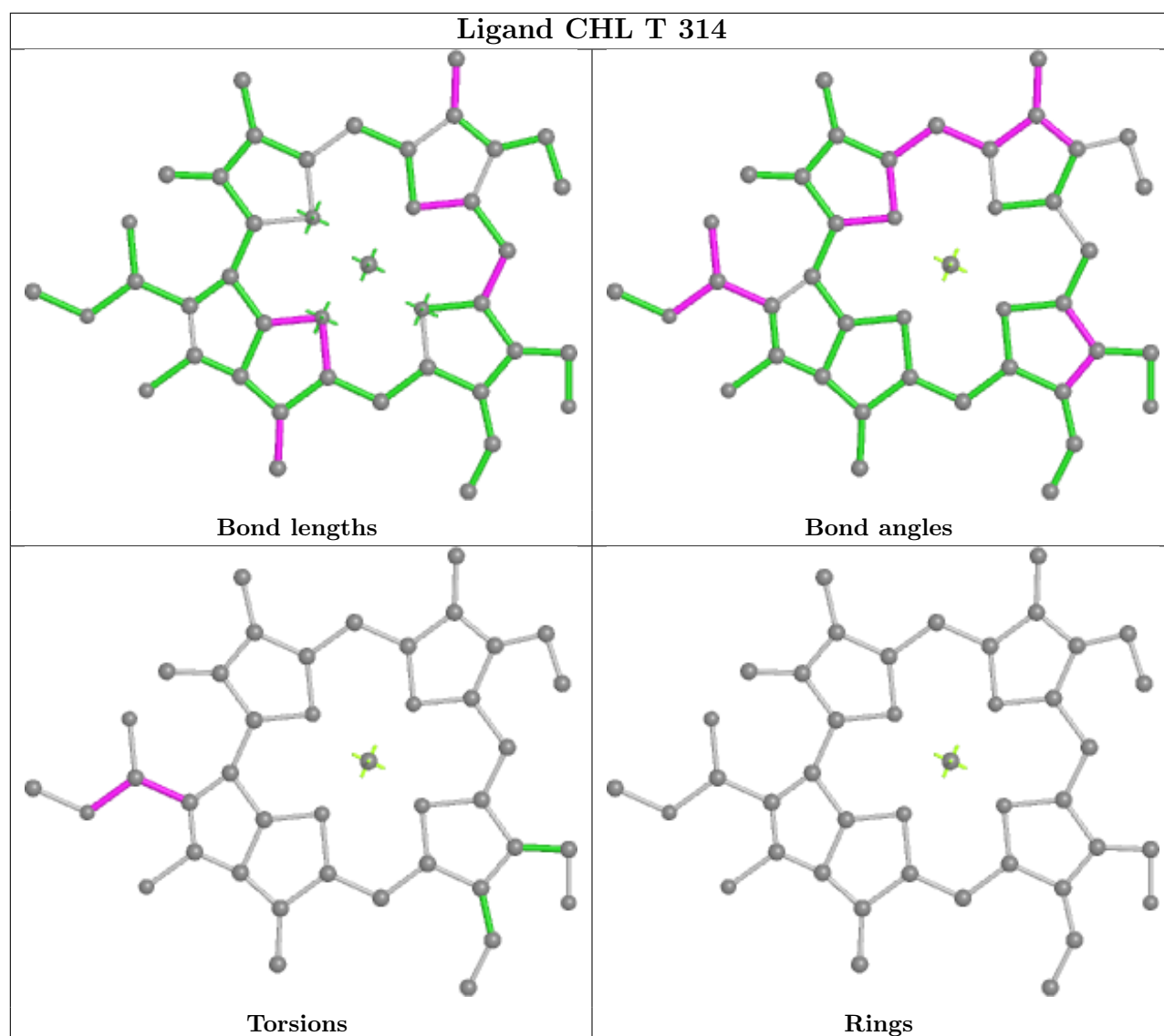
Rings

## Ligand CLA A 828

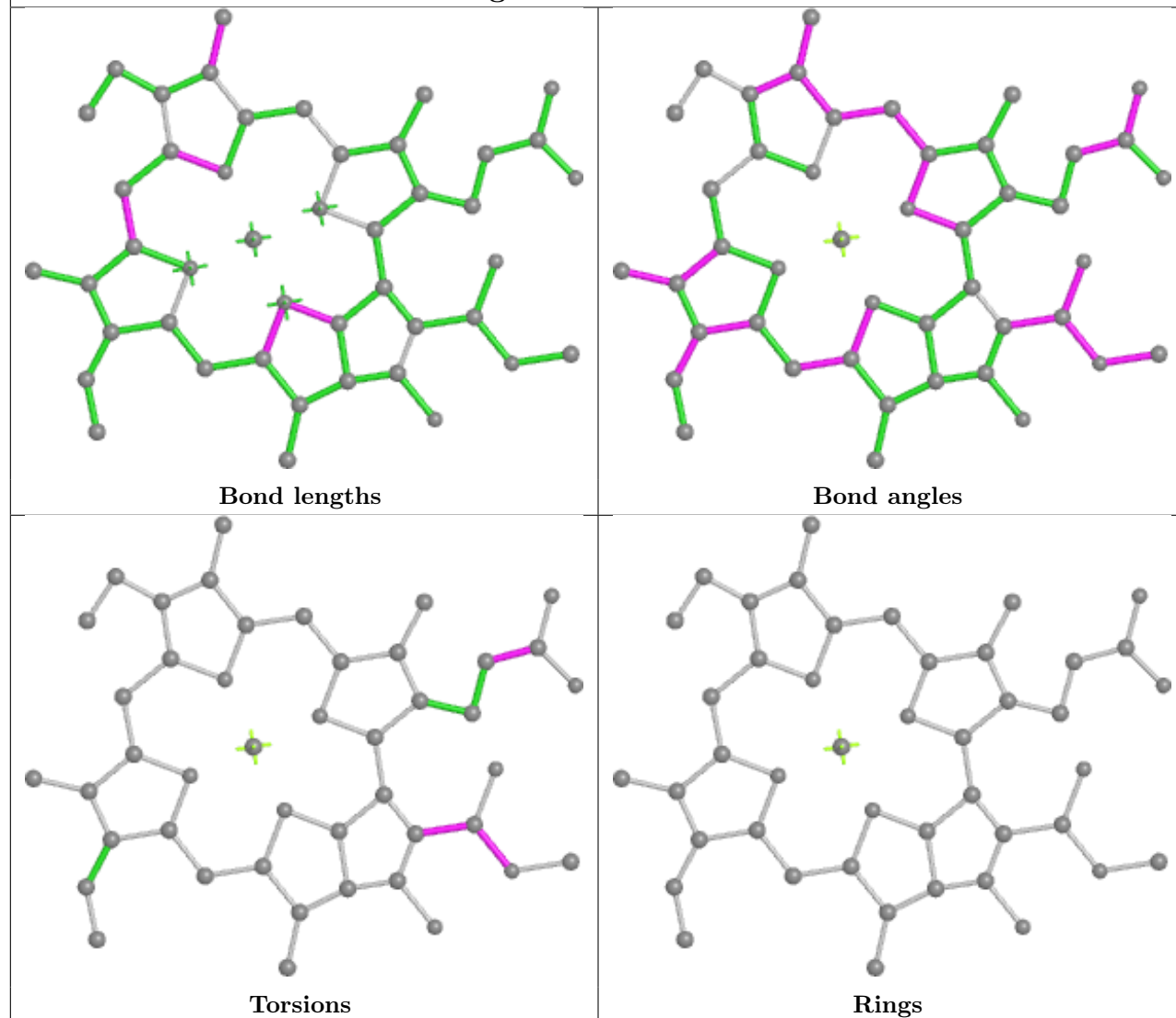


## Ligand PQN B 844

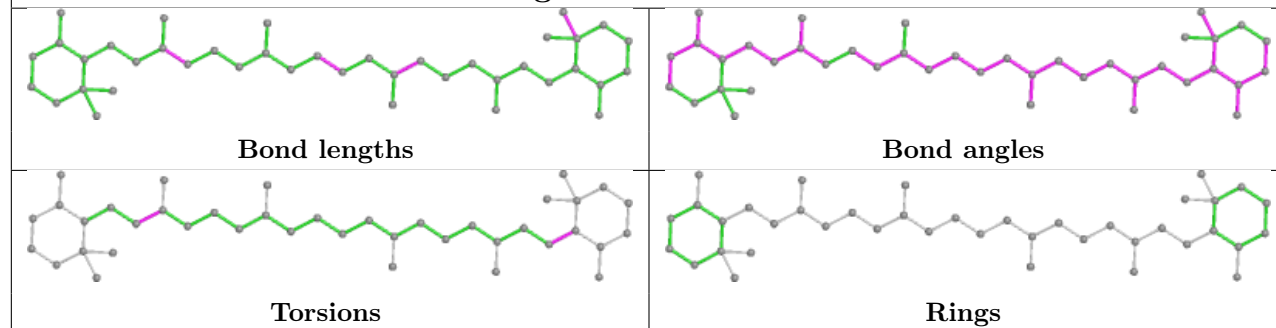


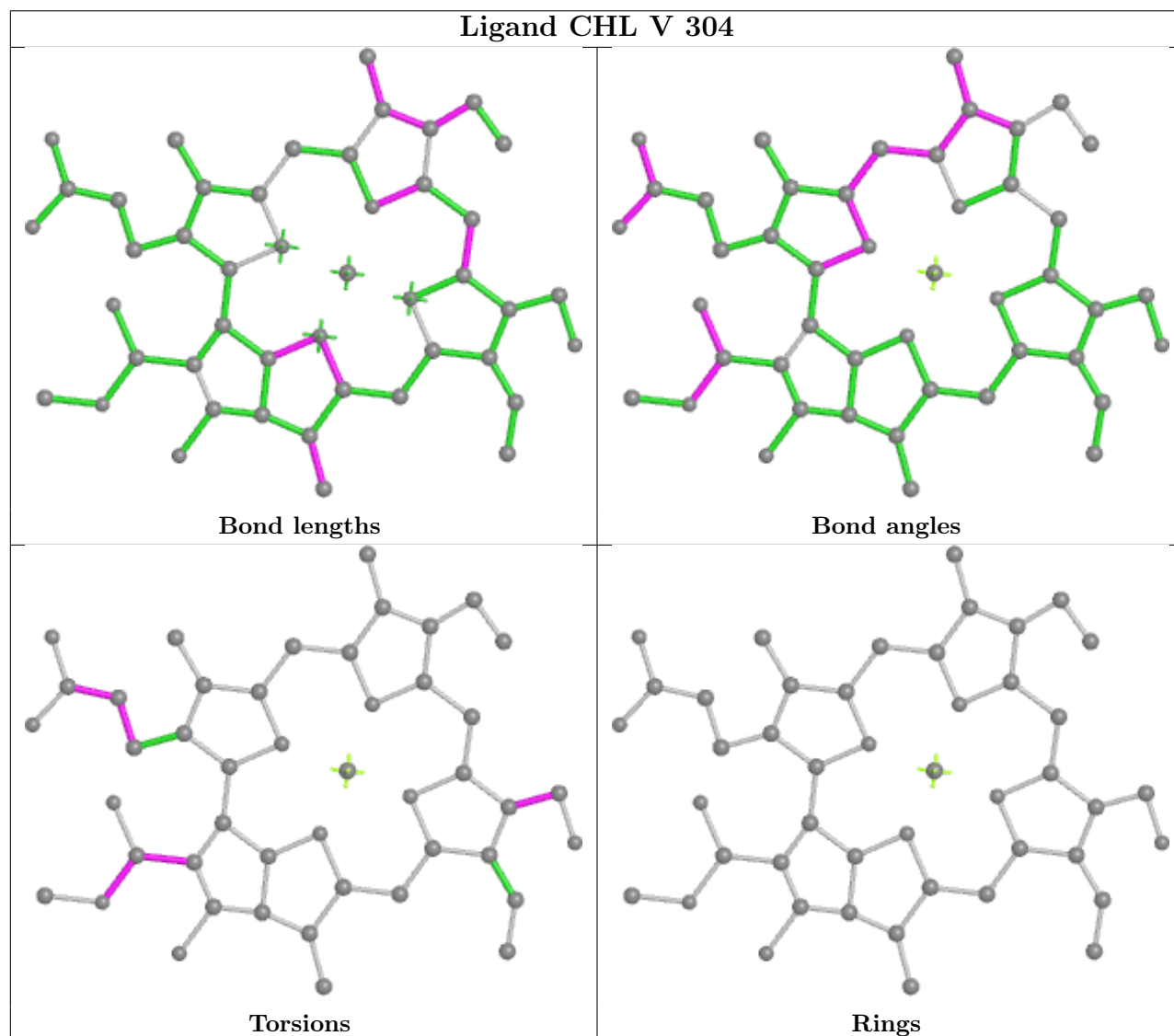
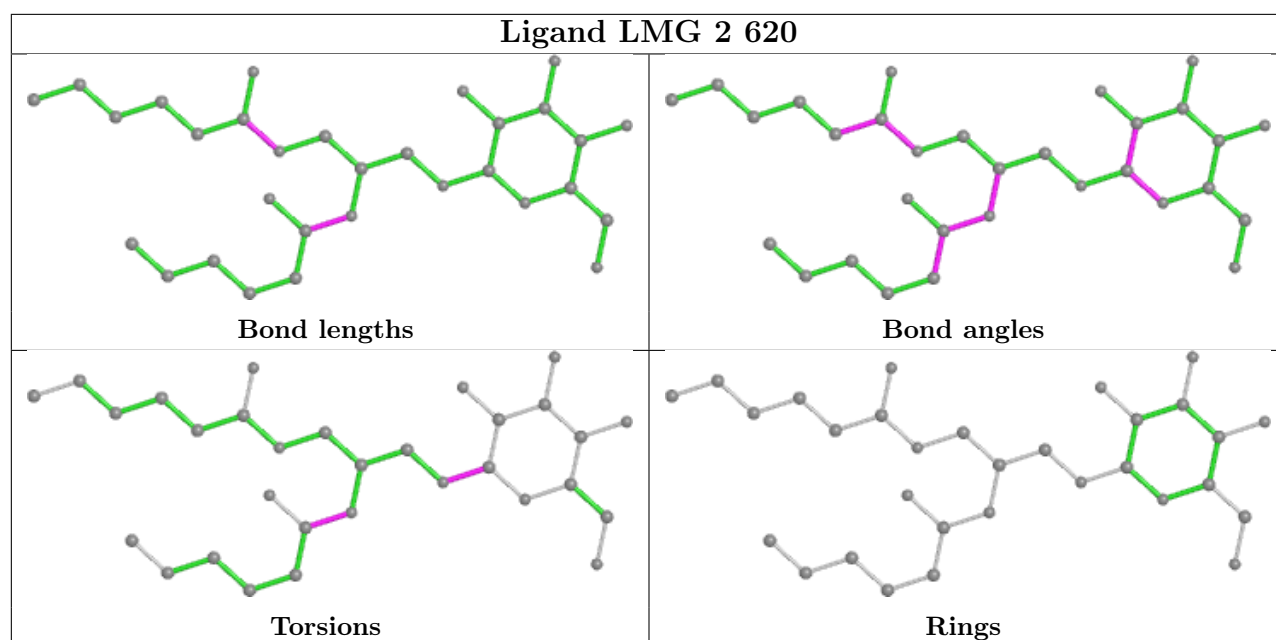


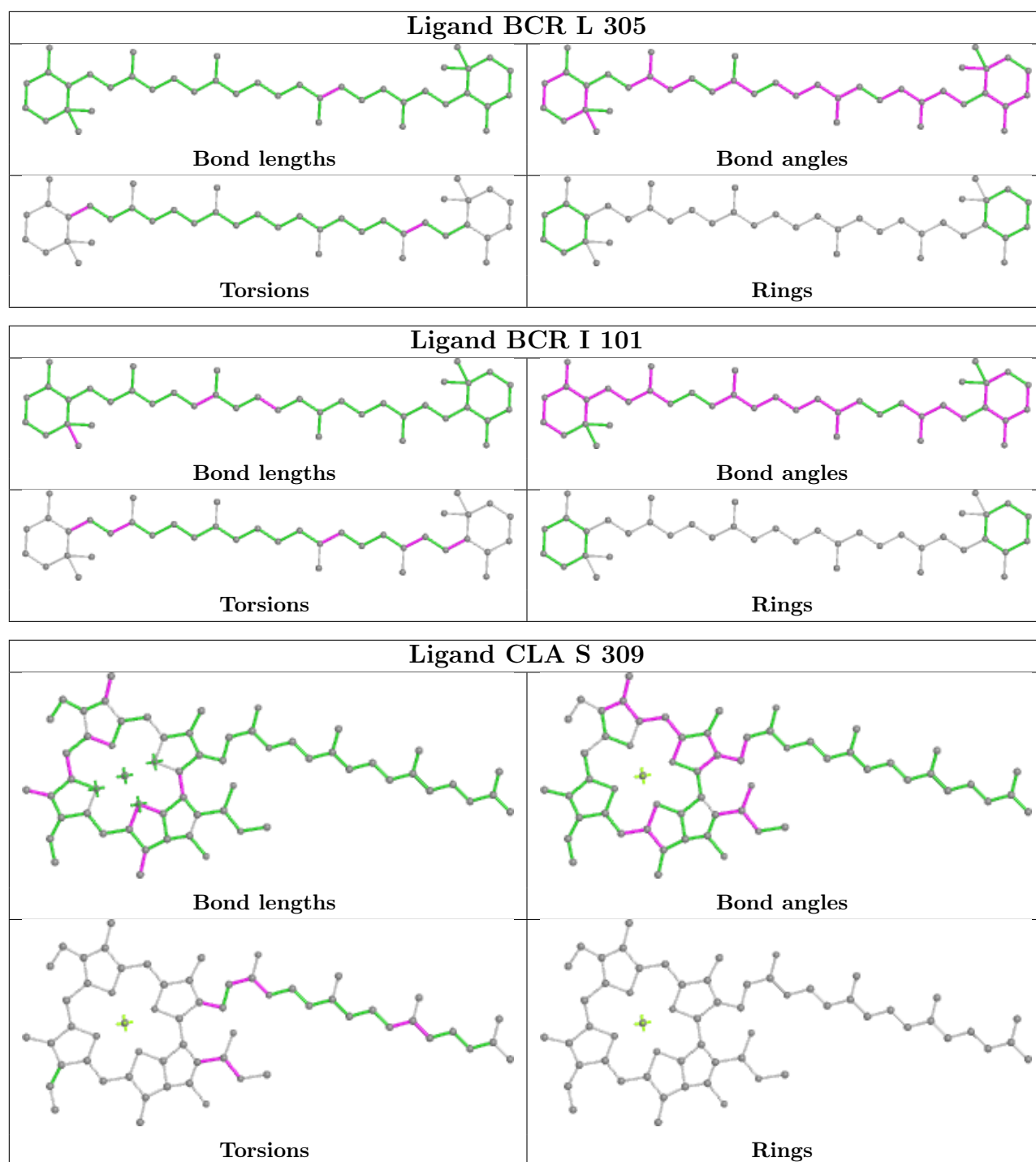
## Ligand CLA K 201



## Ligand BCR J 101

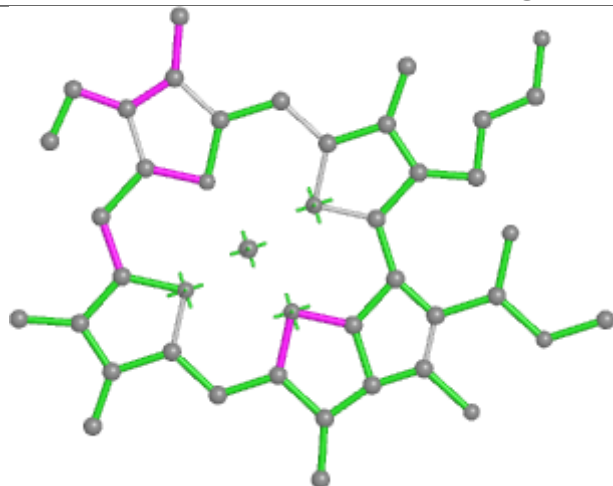




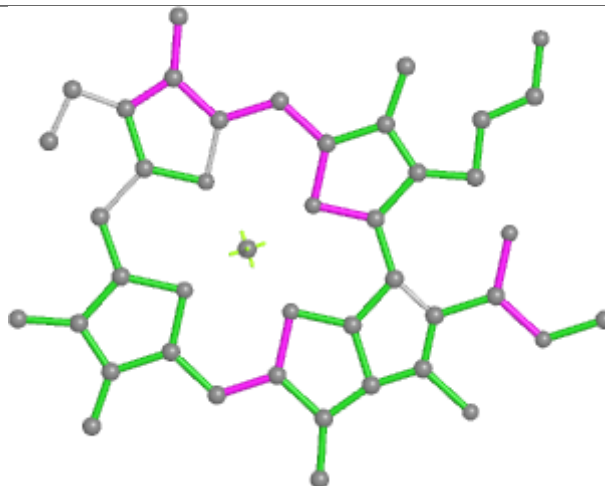




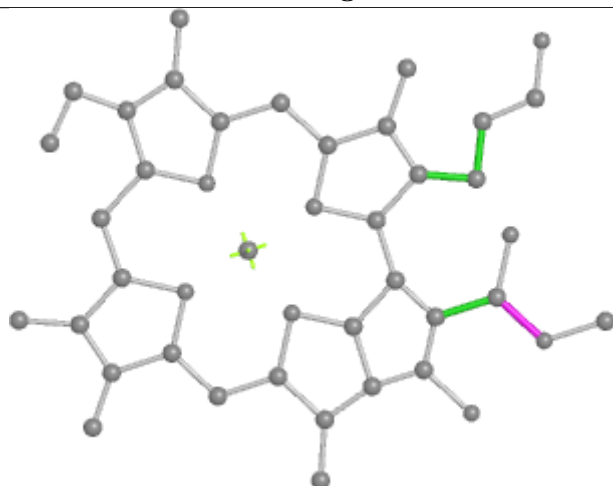
## Ligand CLA 6 604



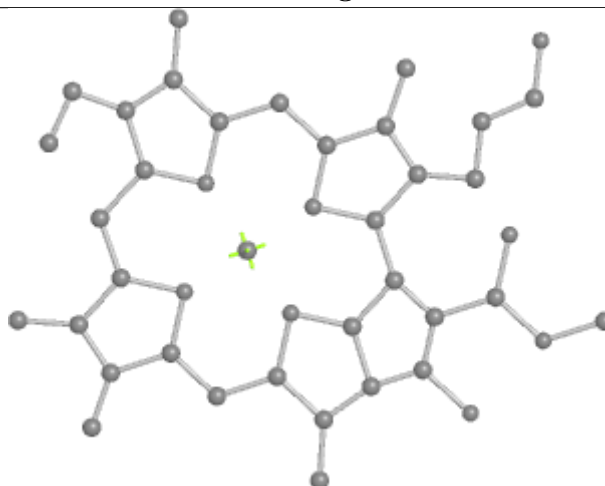
Bond lengths



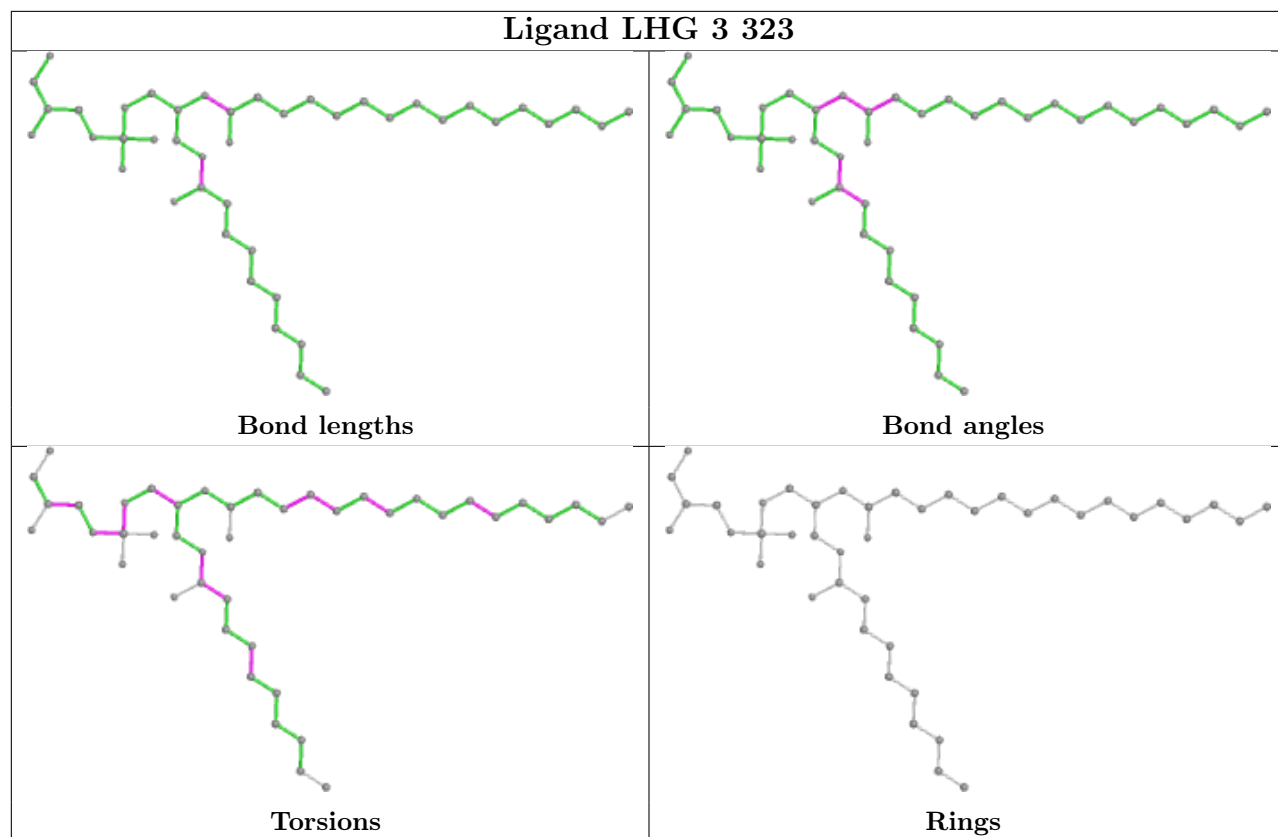
Bond angles



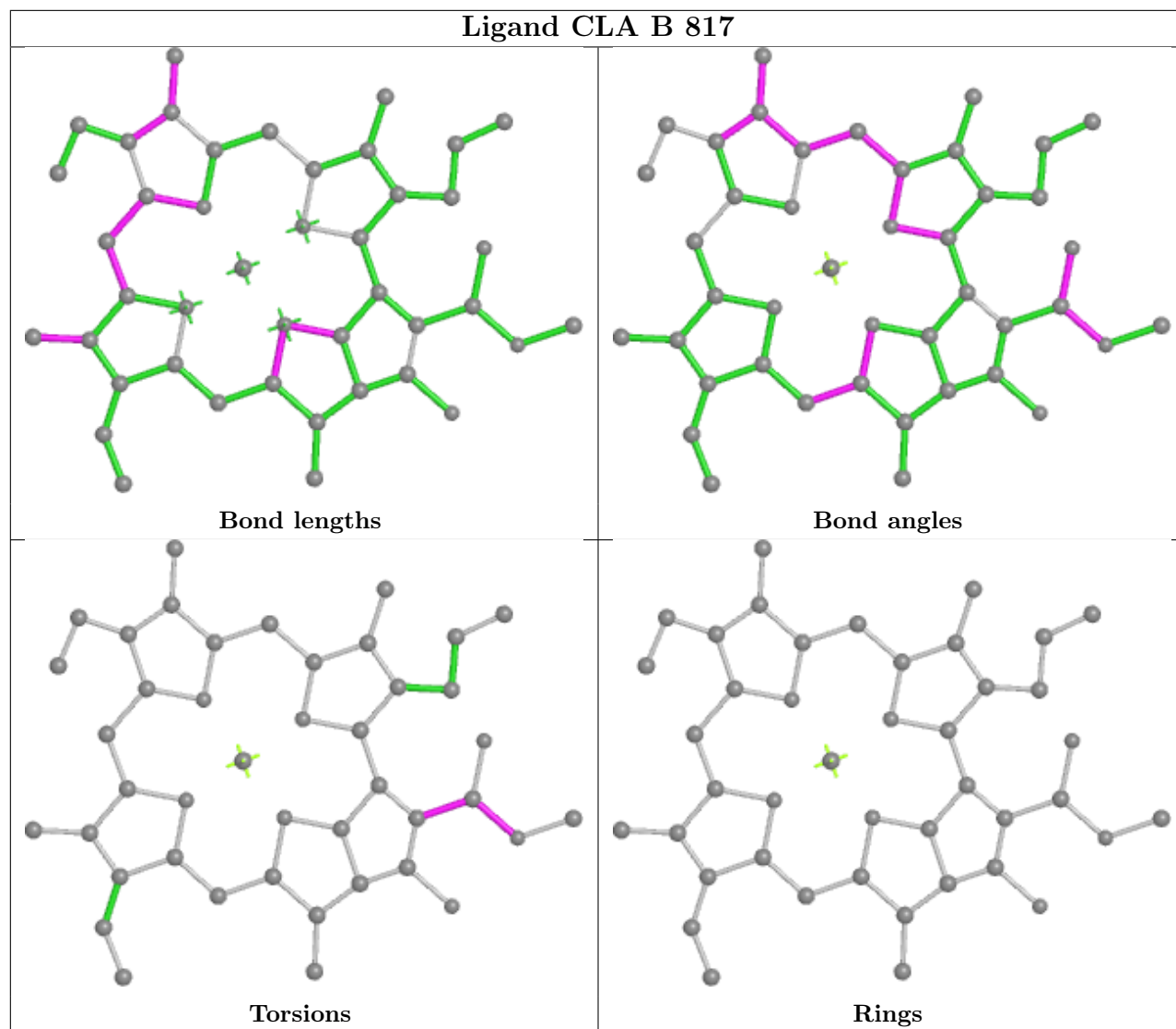
Torsions



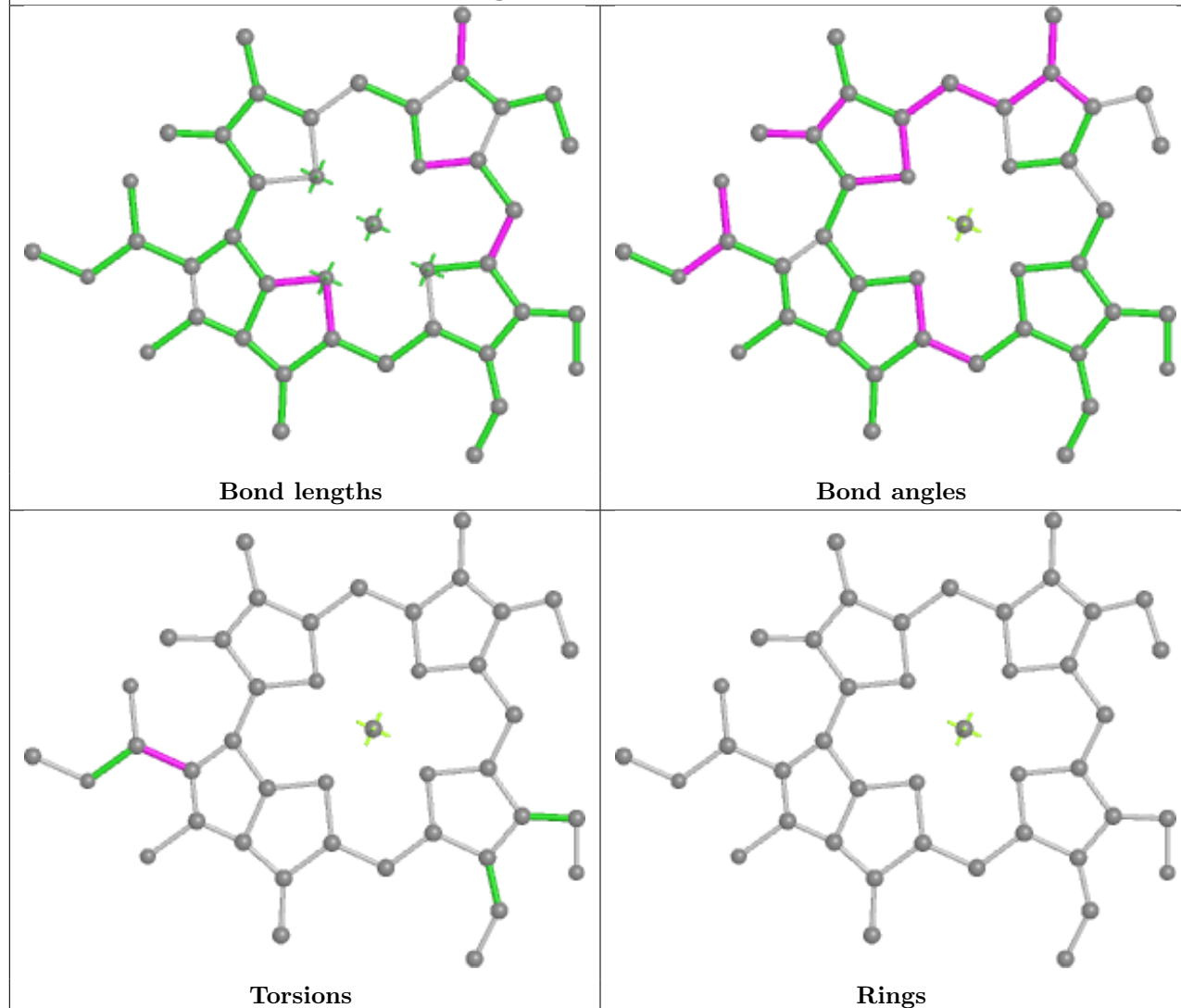
Rings



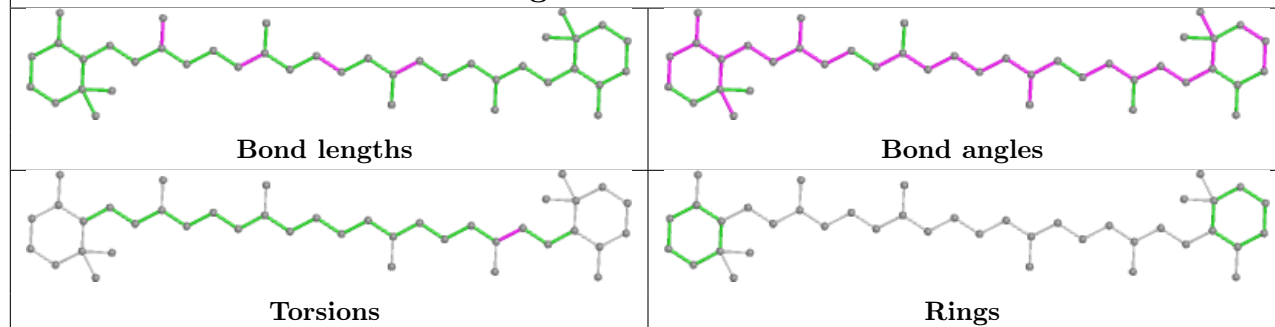
## Ligand CLA B 817

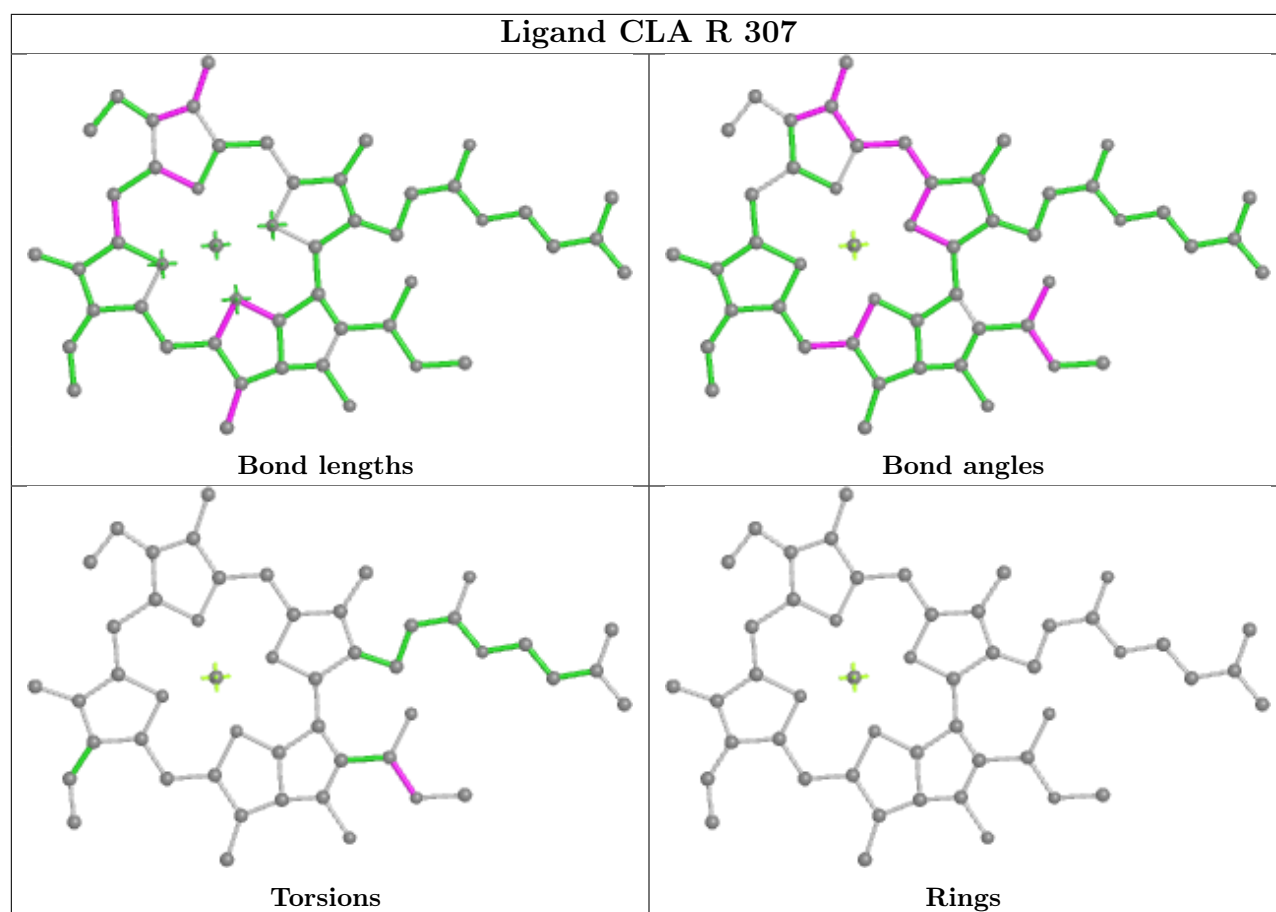


## Ligand CHL X 305

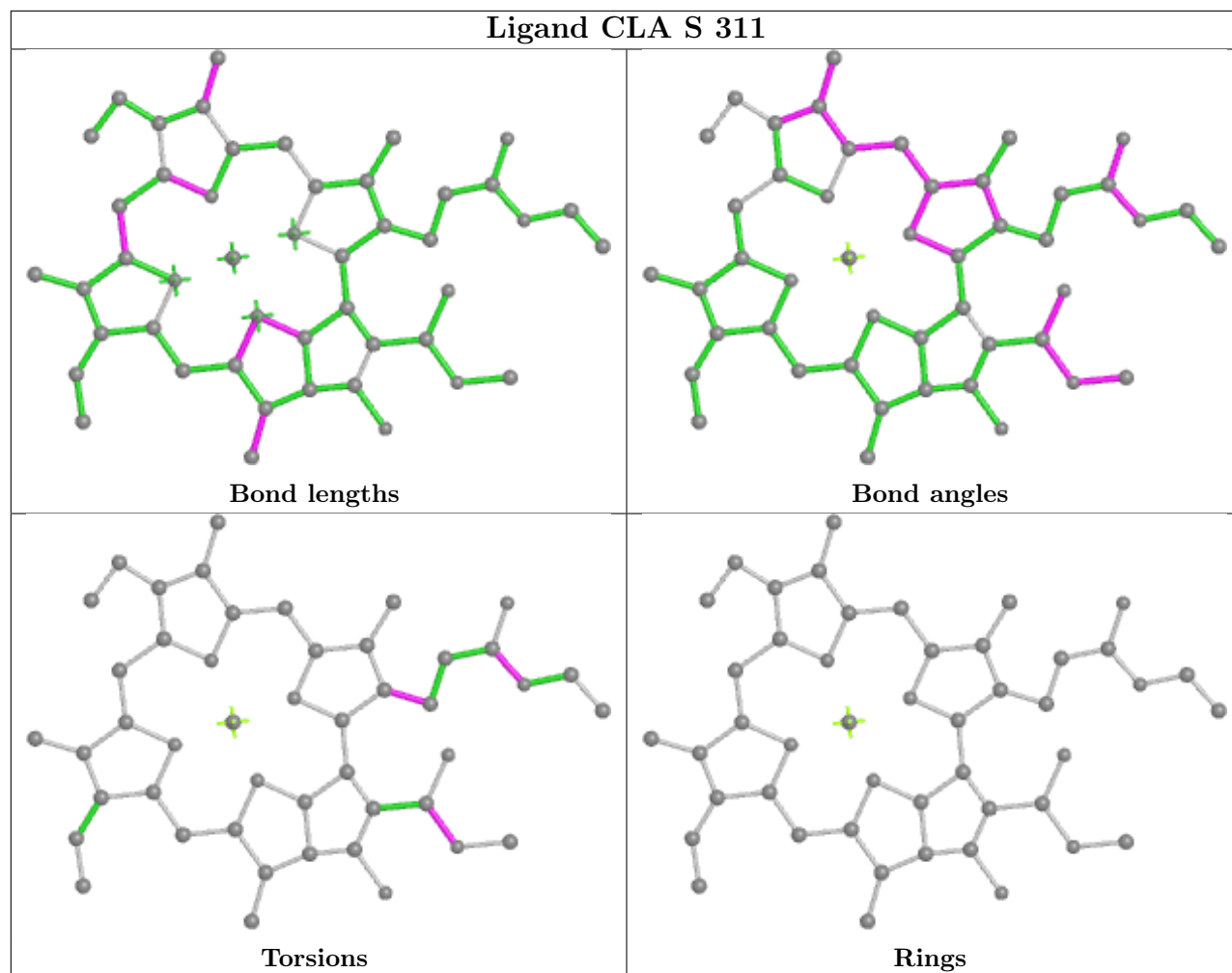


## Ligand BCR B 848

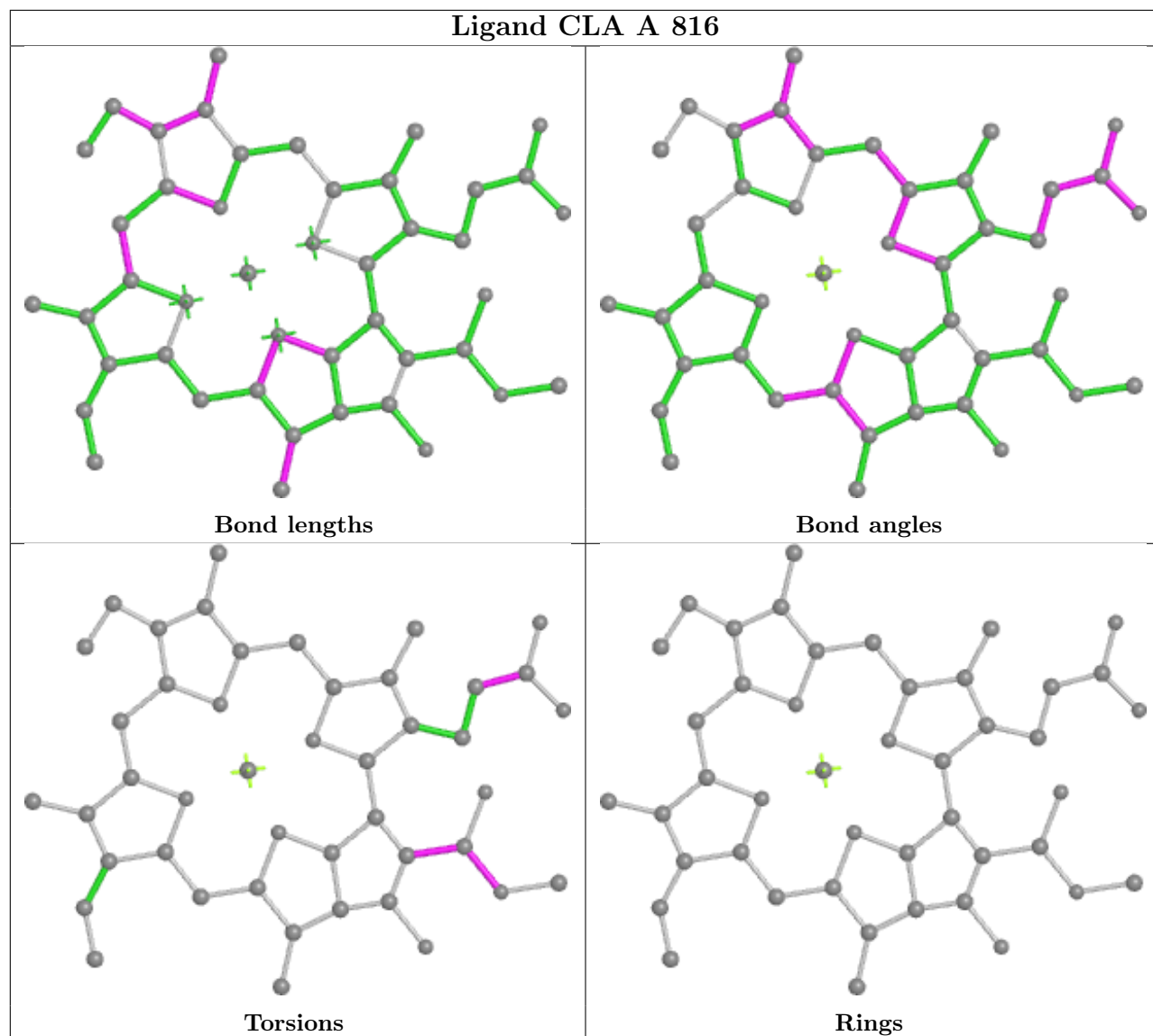




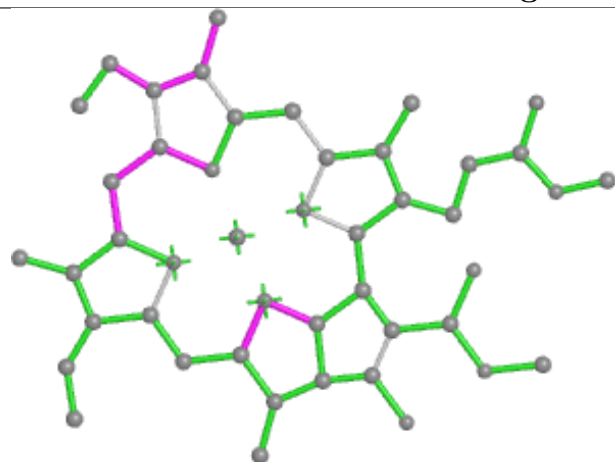
## Ligand CLA S 311



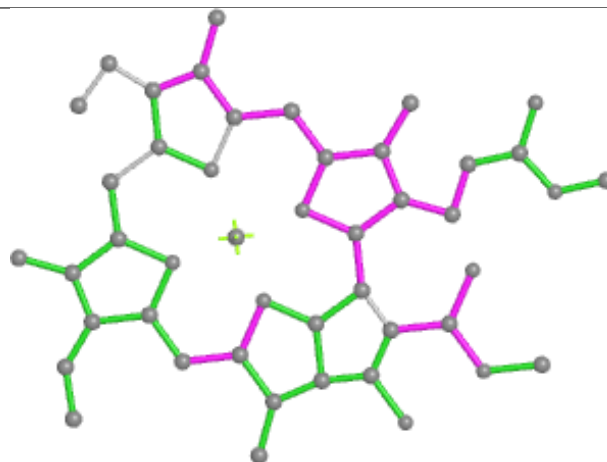
## Ligand CLA A 816



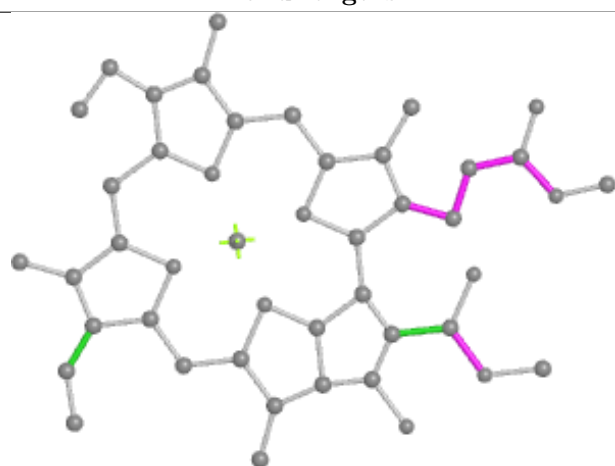
## Ligand CLA 5 601



Bond lengths



Bond angles

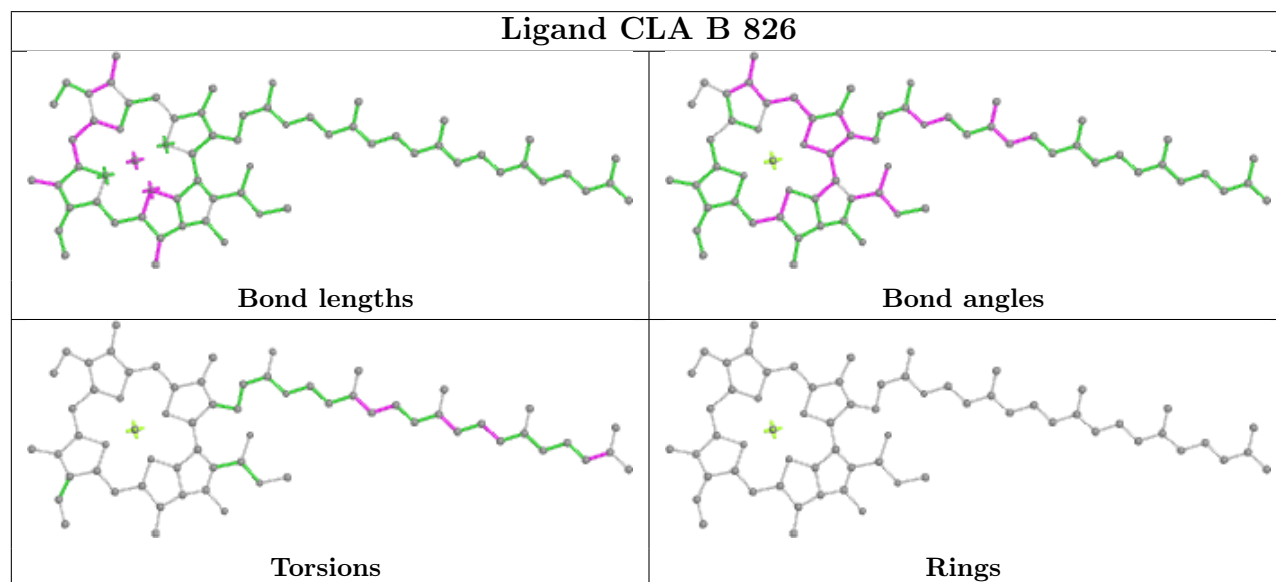
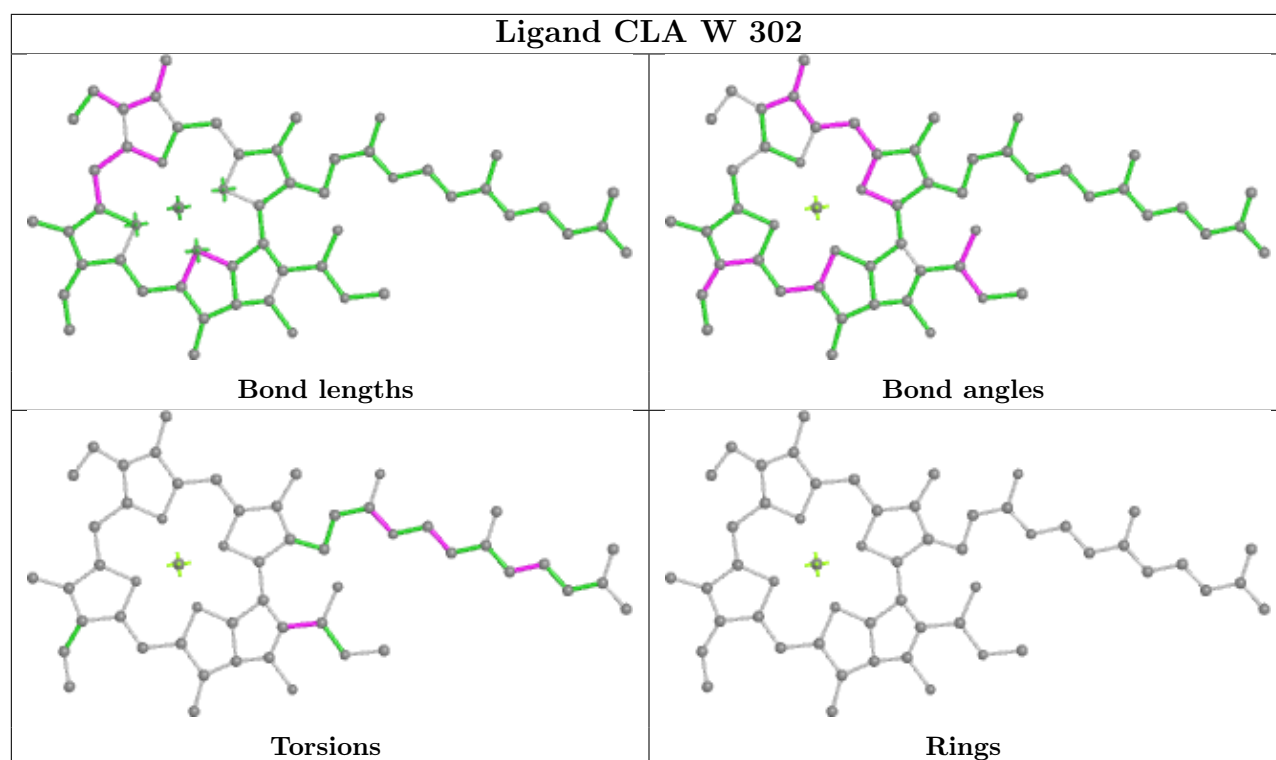


Torsions

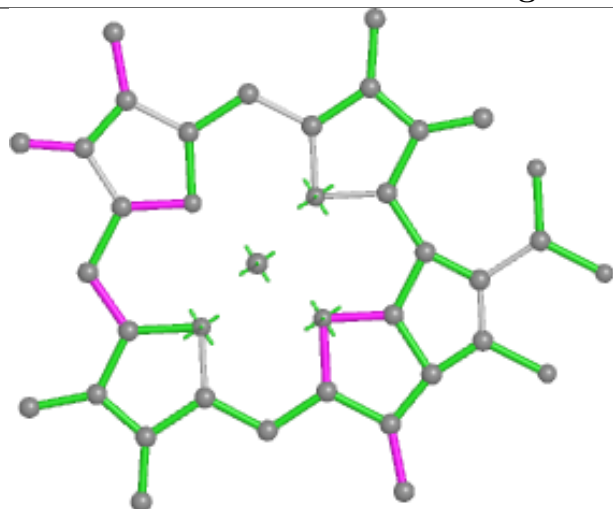


Rings

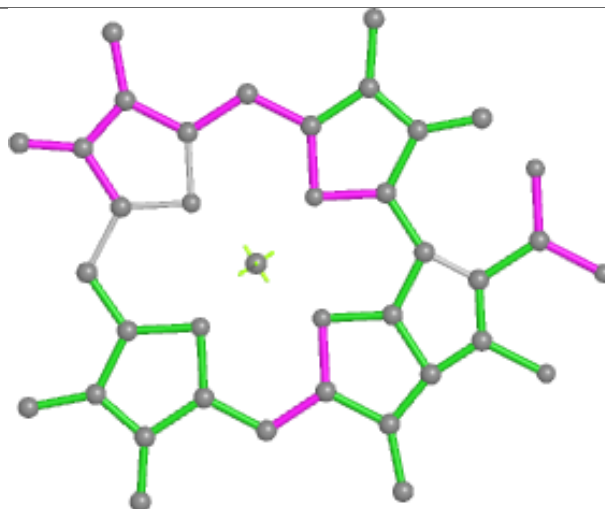




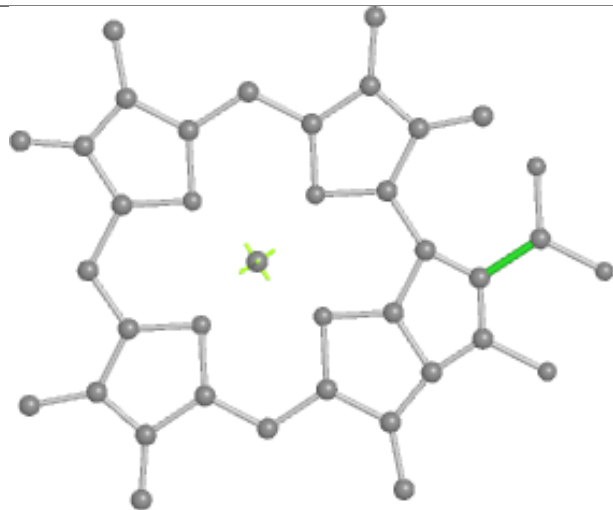
## Ligand CLA 5 604



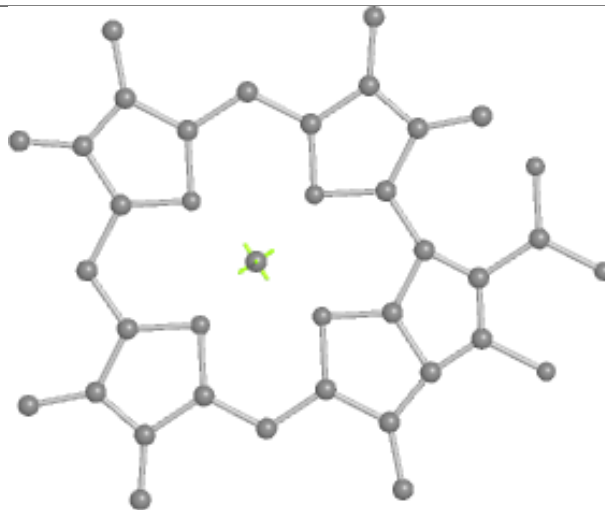
Bond lengths



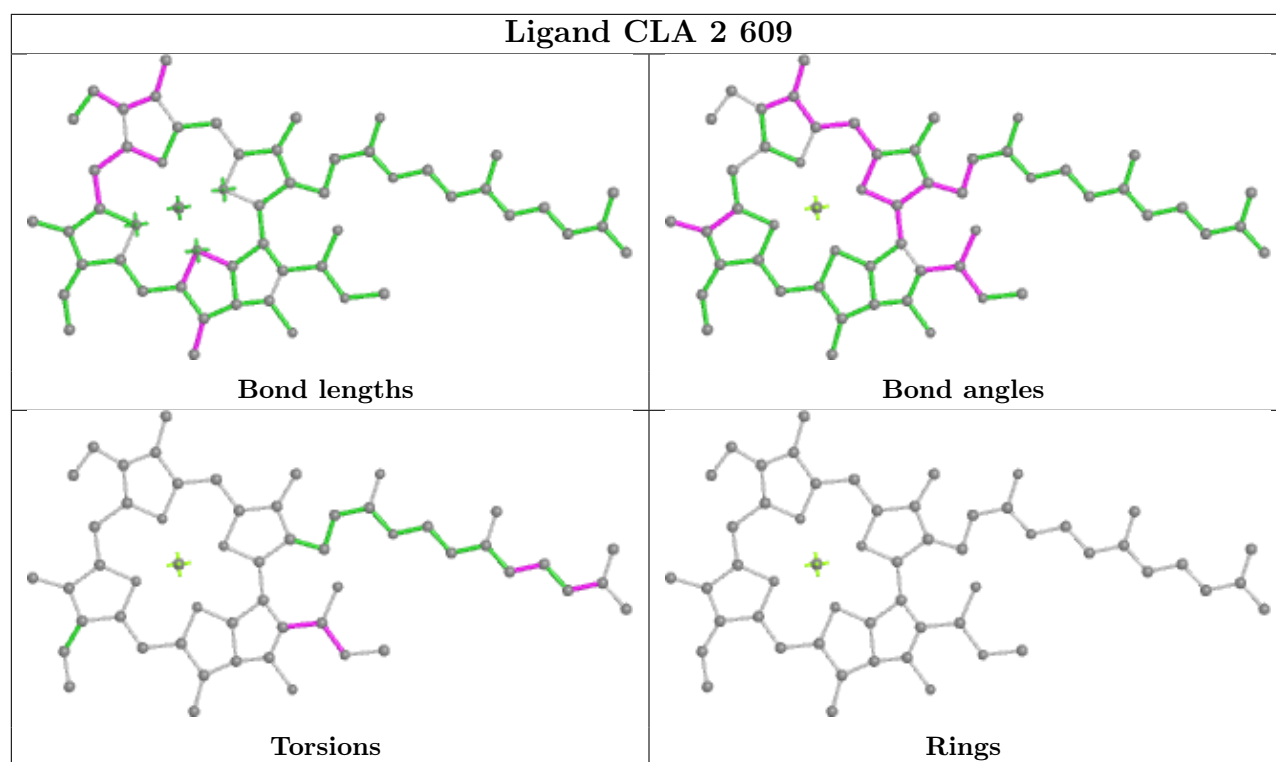
Bond angles



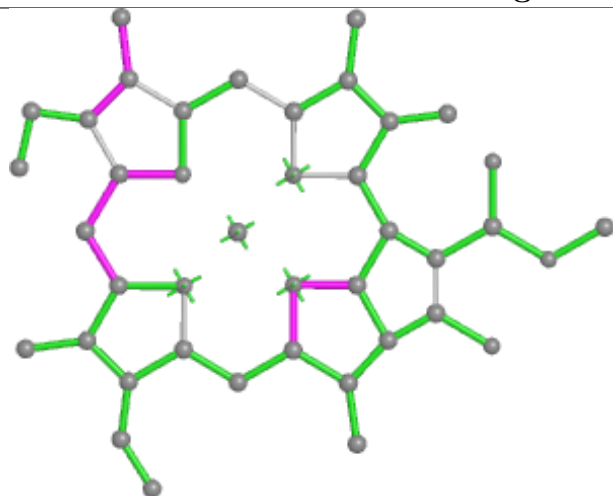
Torsions



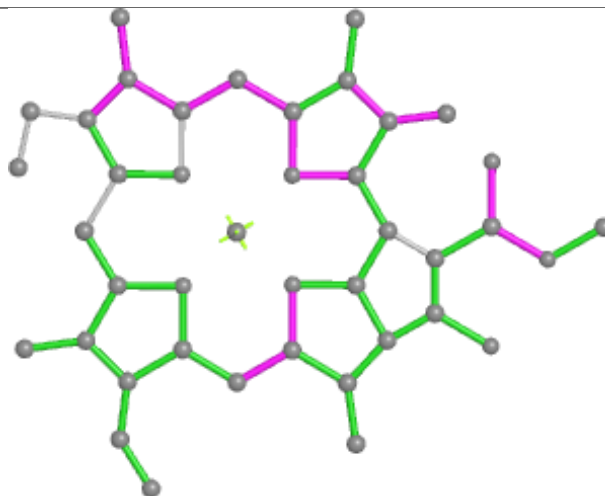
Rings



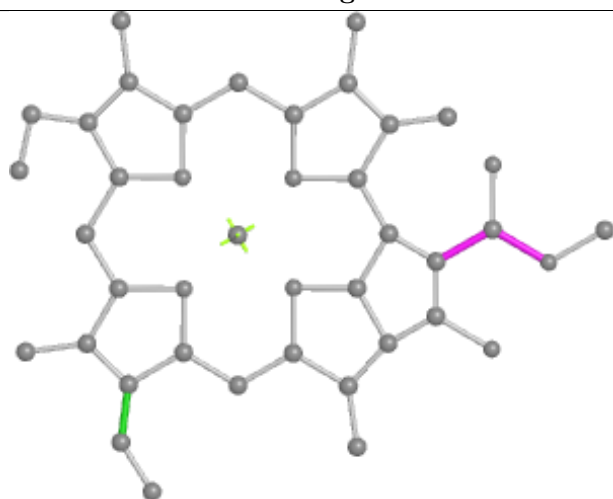
## Ligand CLA X 314



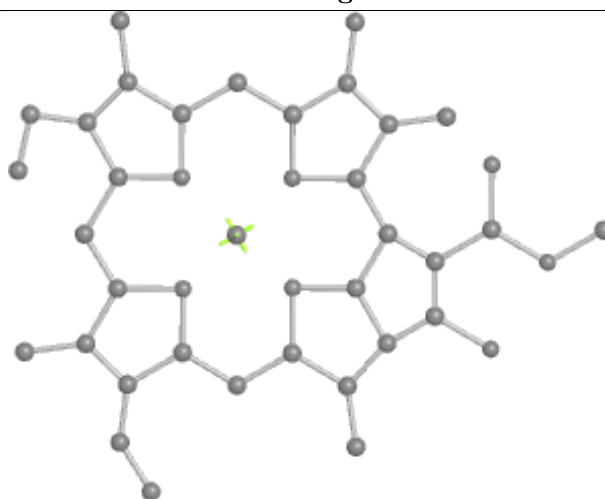
Bond lengths



Bond angles

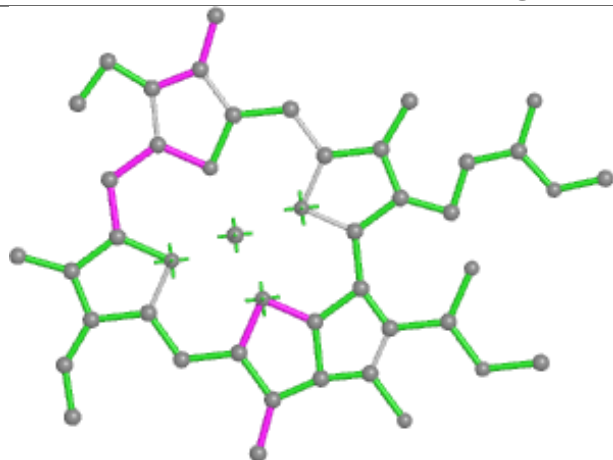


Torsions

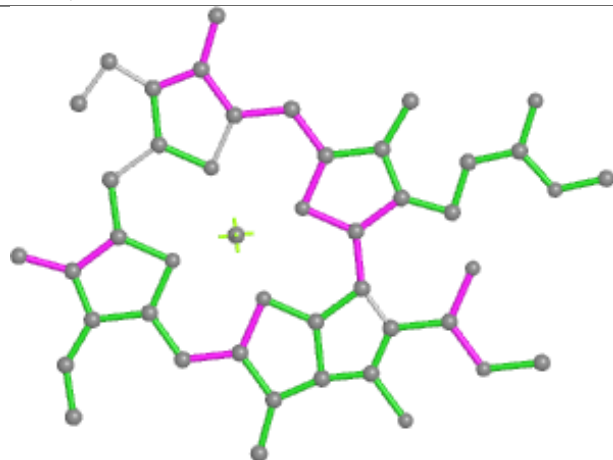


Rings

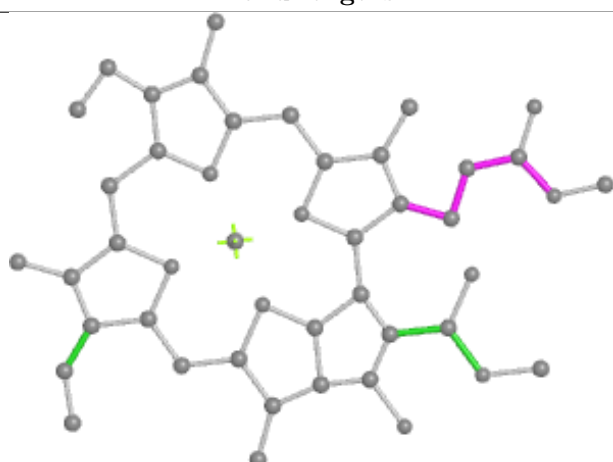
## Ligand CLA Q 313



Bond lengths



Bond angles

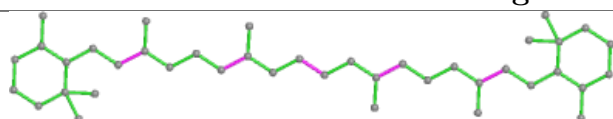


Torsions

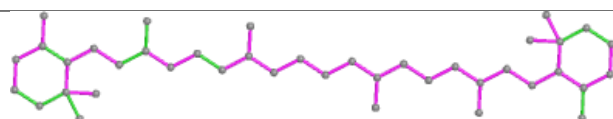


Rings

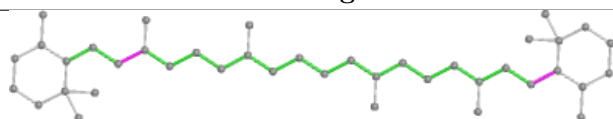
## Ligand BCR A 848



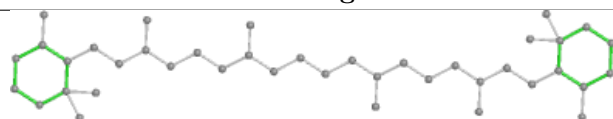
Bond lengths



Bond angles

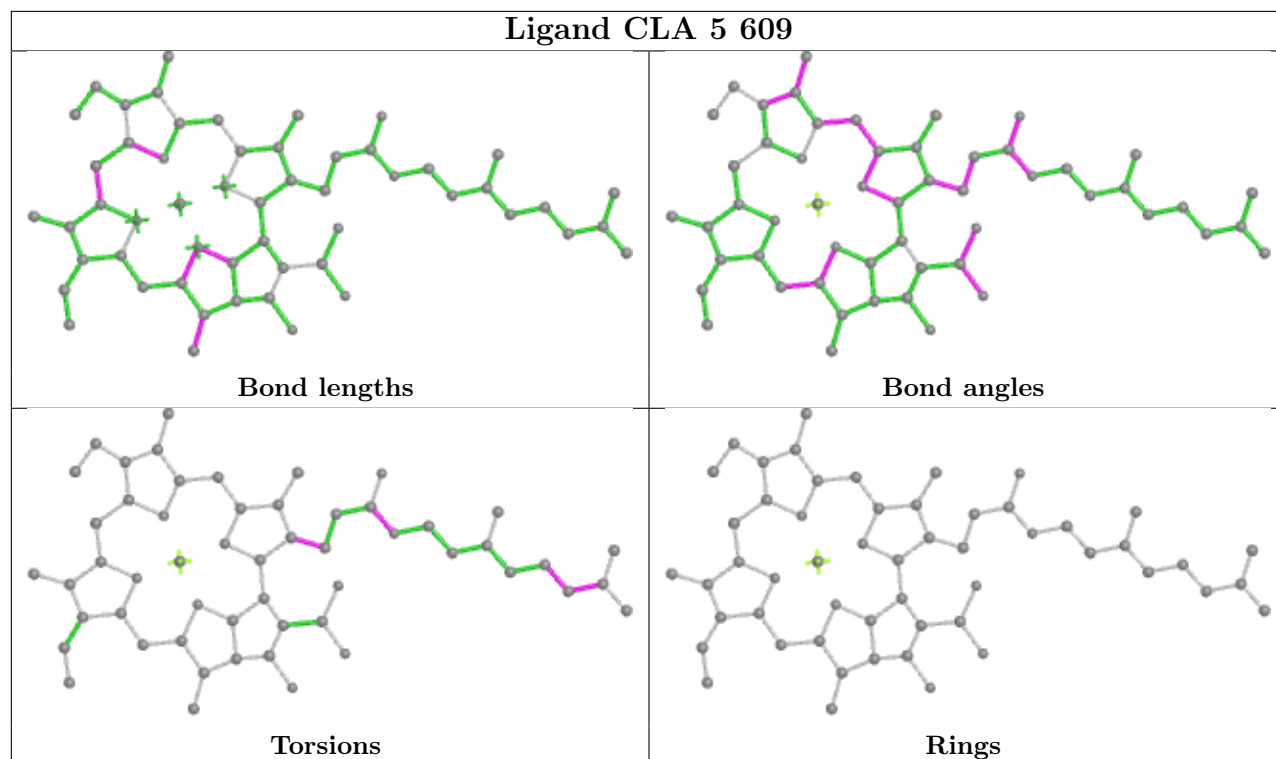


Torsions

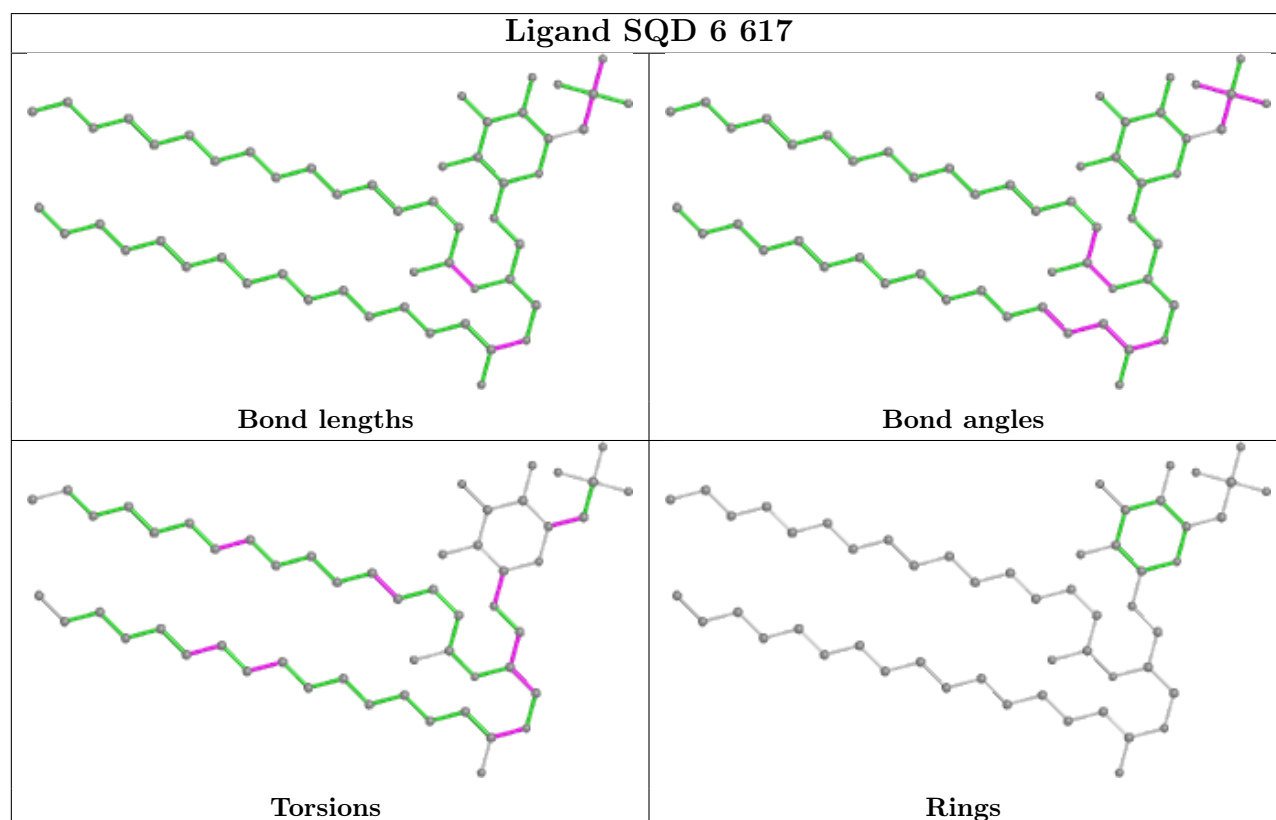


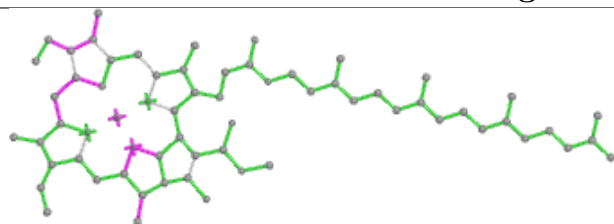
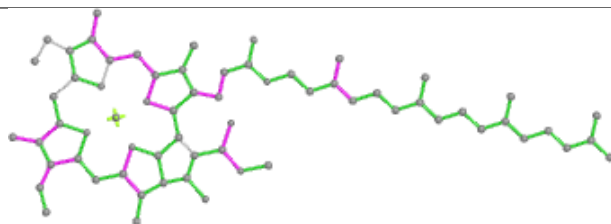
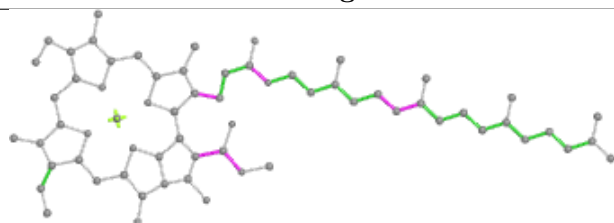
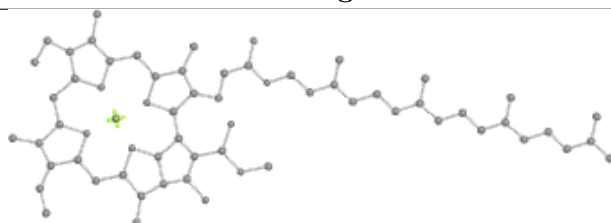
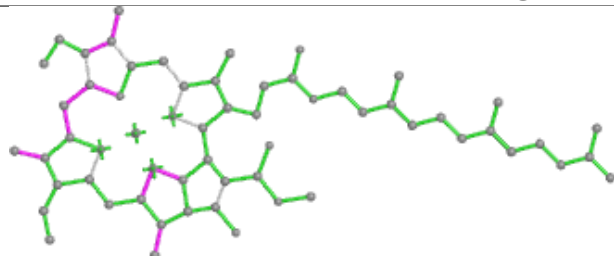
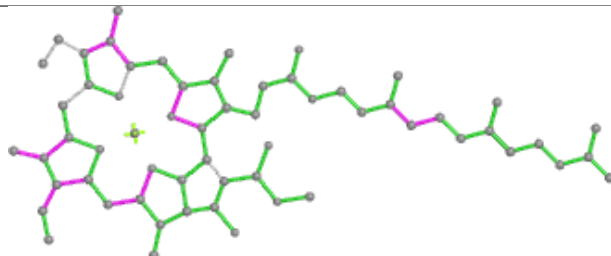
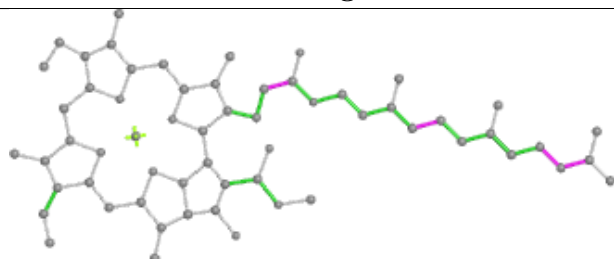
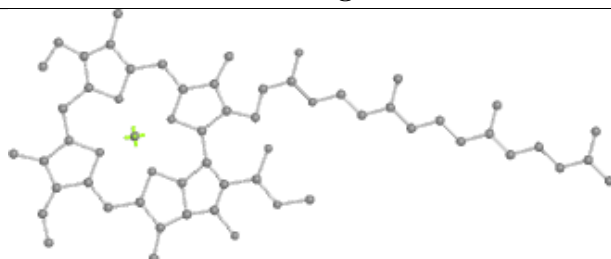
Rings

## Ligand CLA 5 609

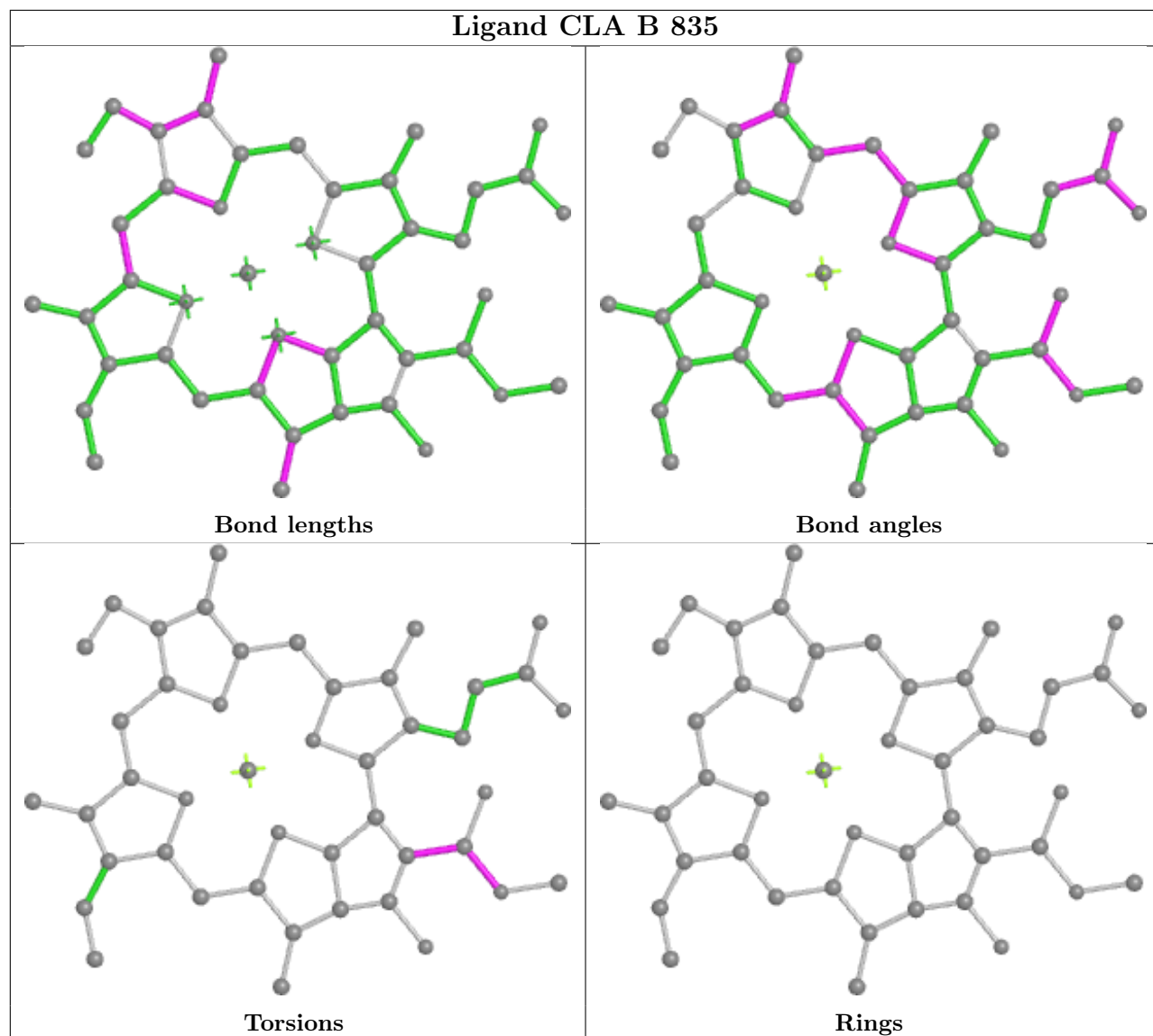


## Ligand SQD 6 617



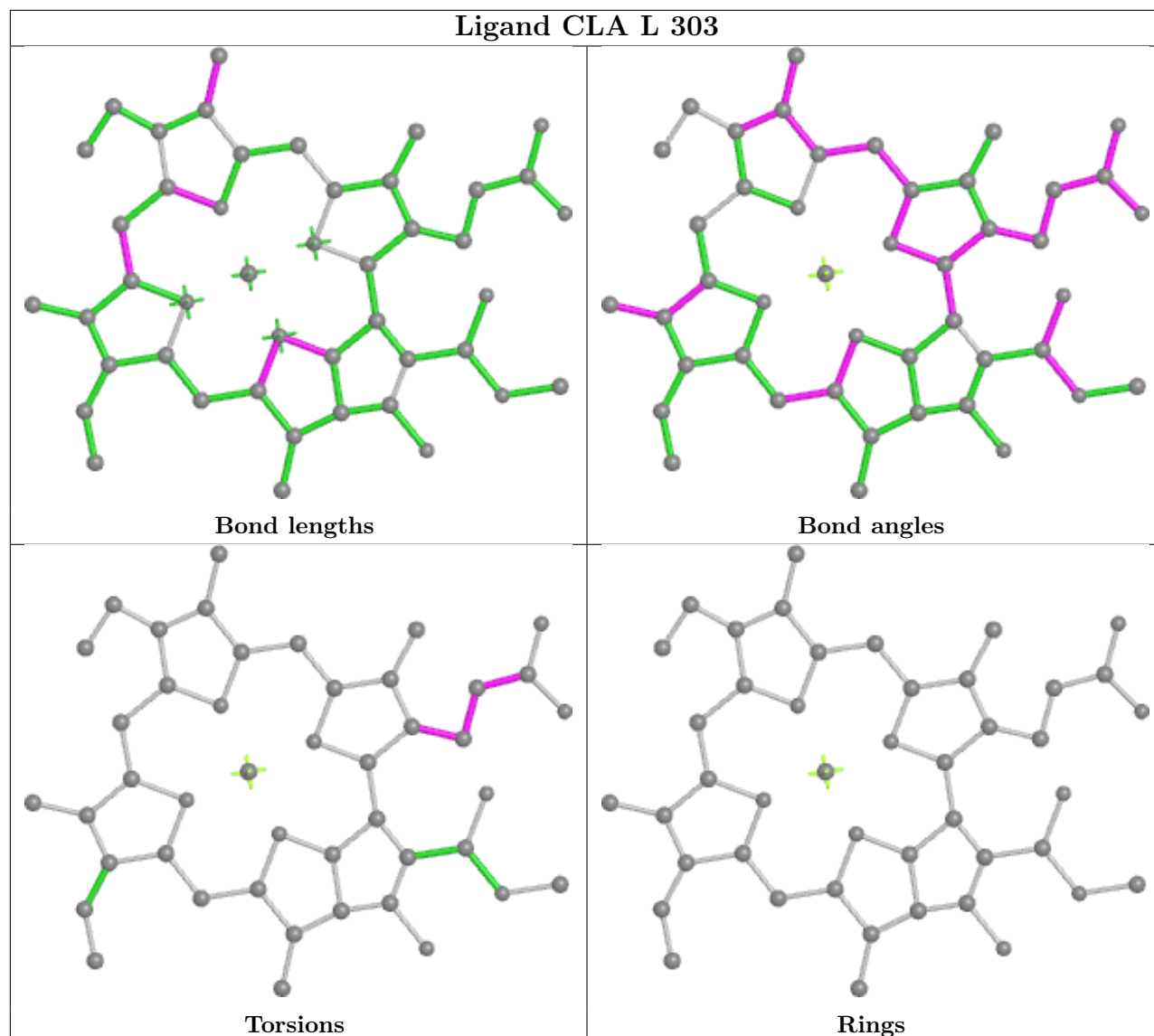
**Ligand CLA 1 608****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 824****Bond lengths****Bond angles****Torsions****Rings**

## Ligand CLA B 835

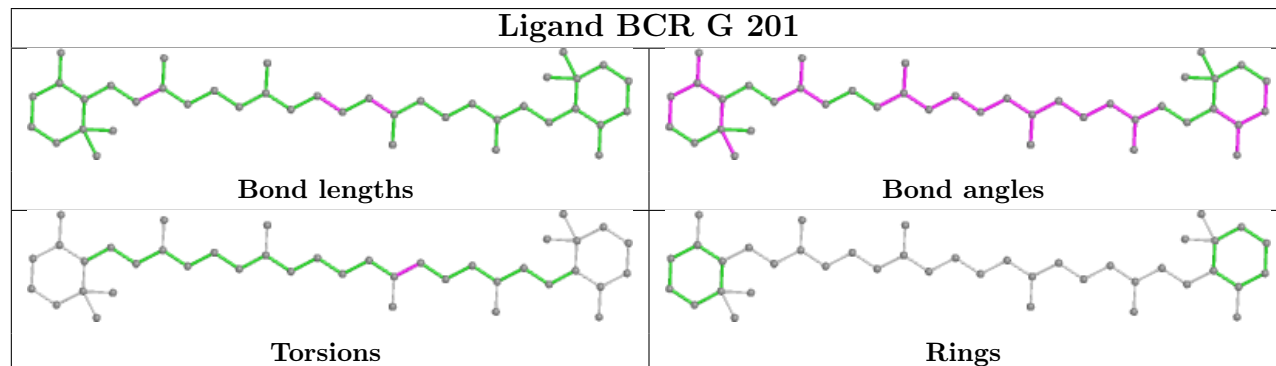


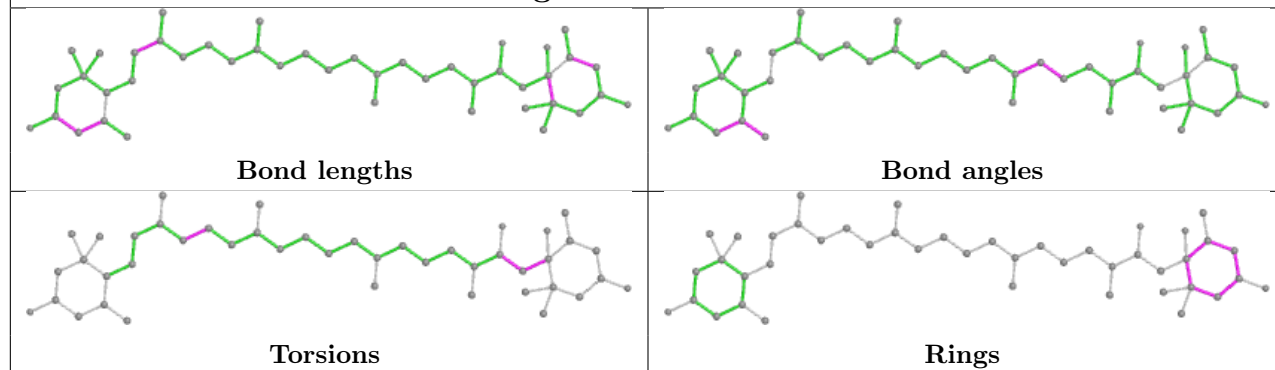
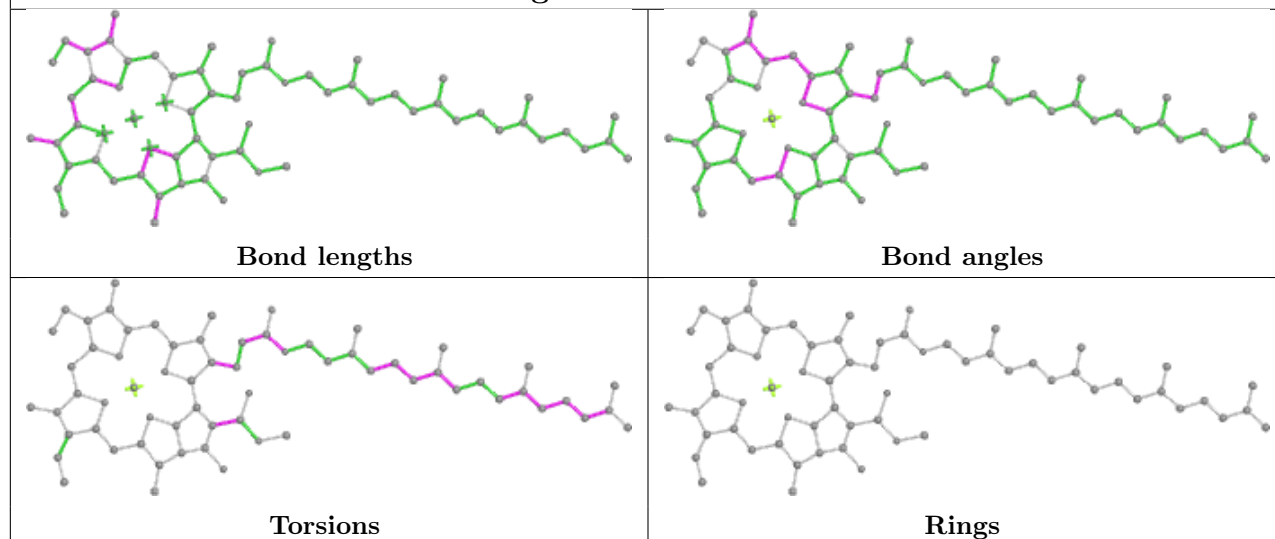
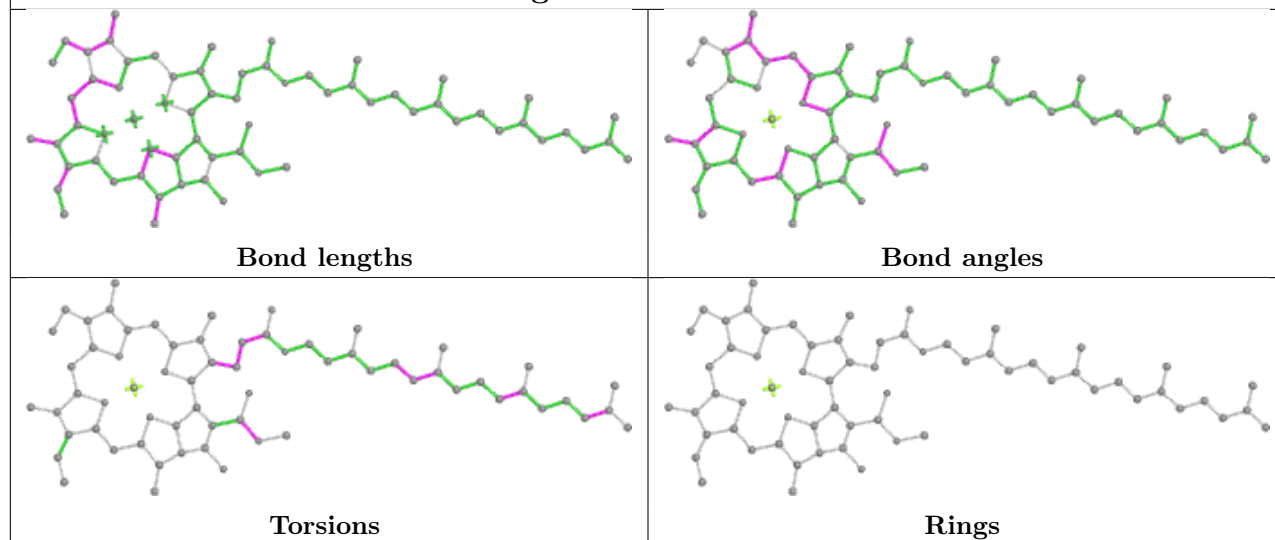


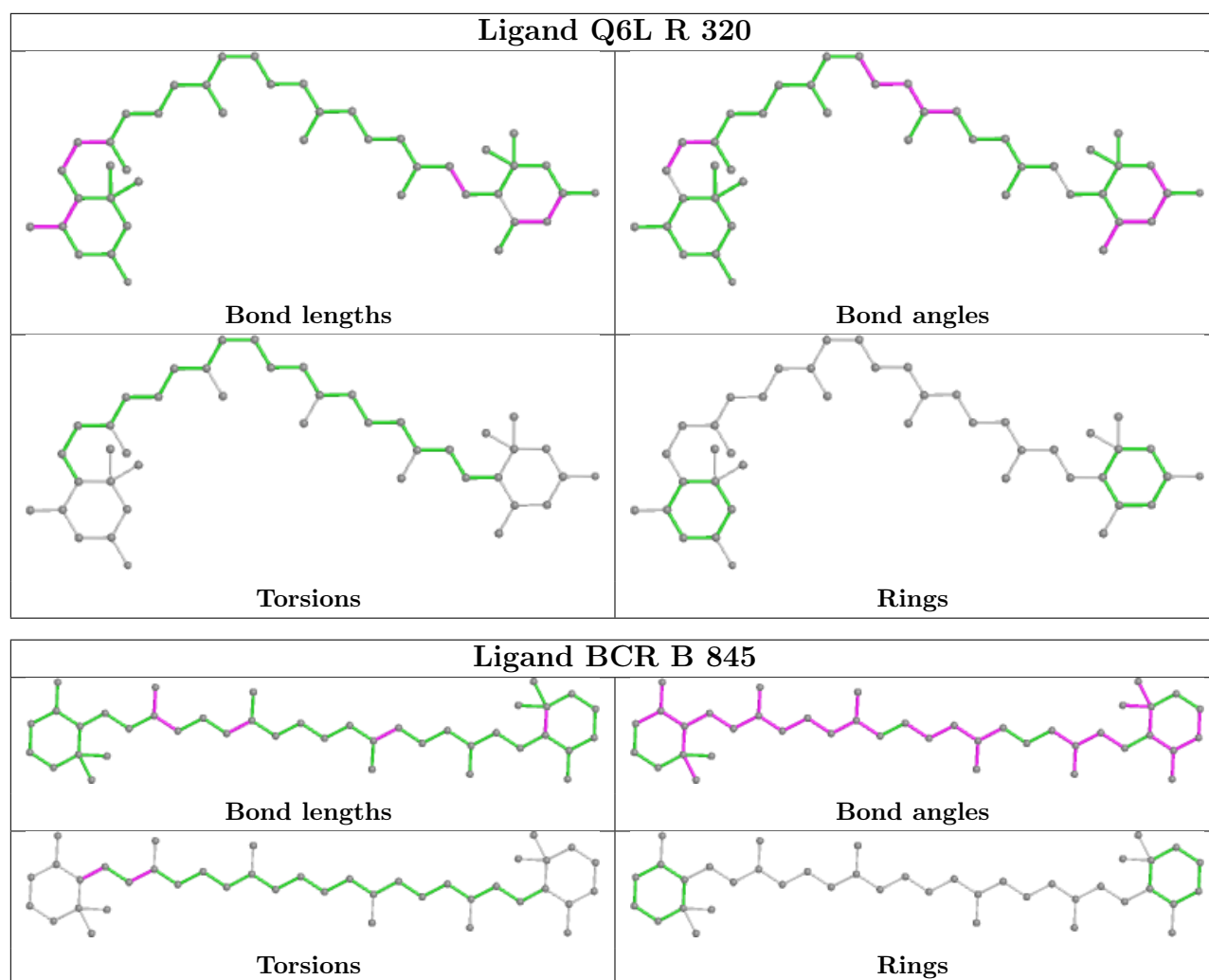
## Ligand CLA L 303



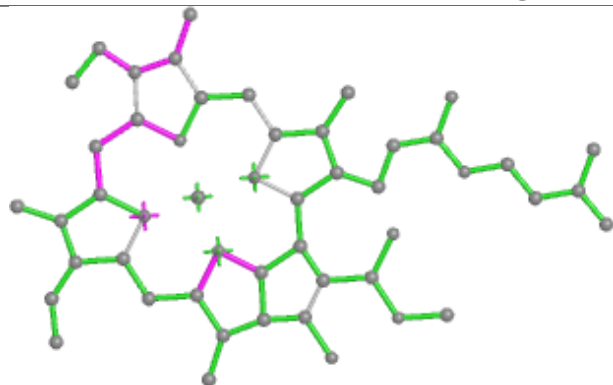
## Ligand BCR G 201



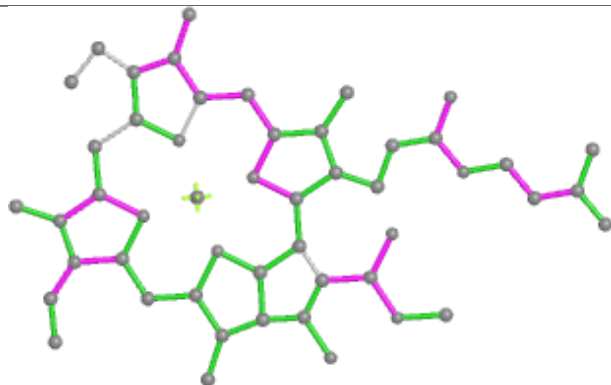
**Ligand IWJ V 320****Ligand CLA B 839****Ligand CLA B 811**



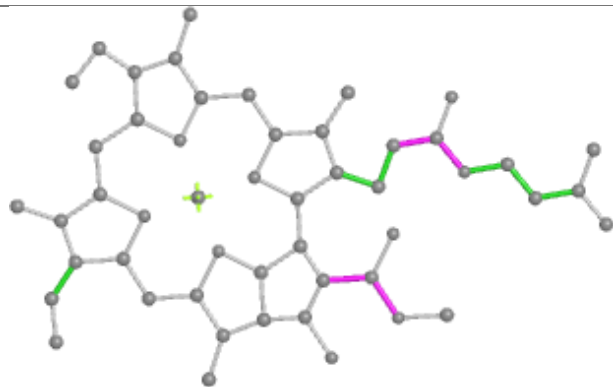
## Ligand CLA V 302



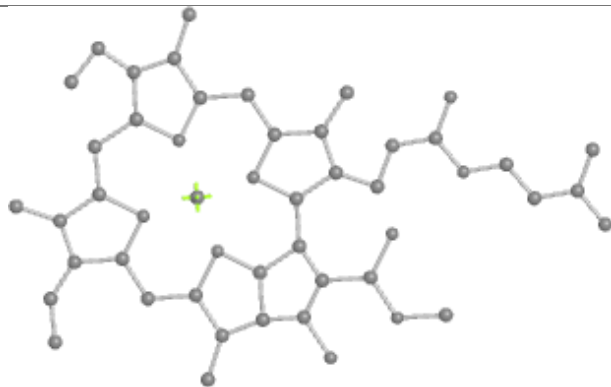
Bond lengths



Bond angles

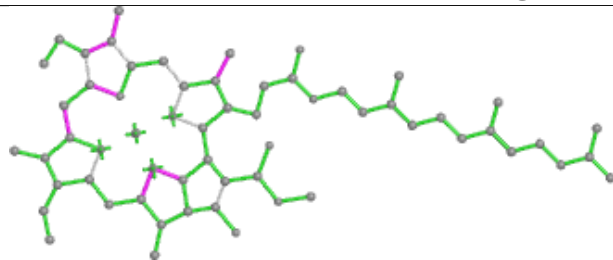


Torsions

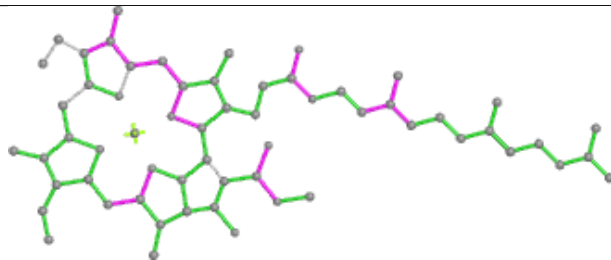


Rings

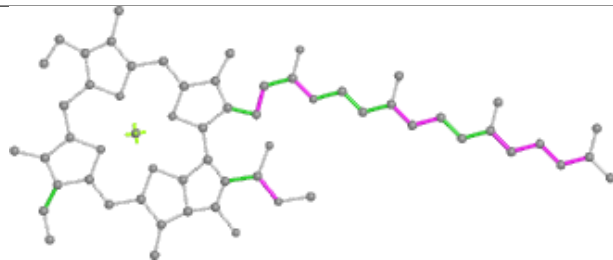
## Ligand CLA A 819



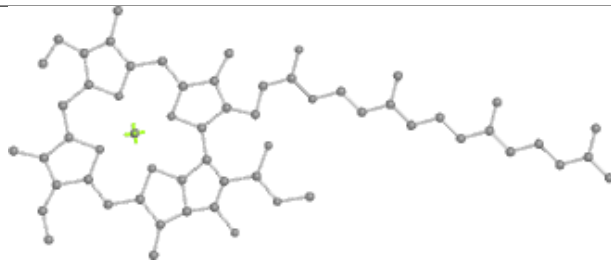
Bond lengths



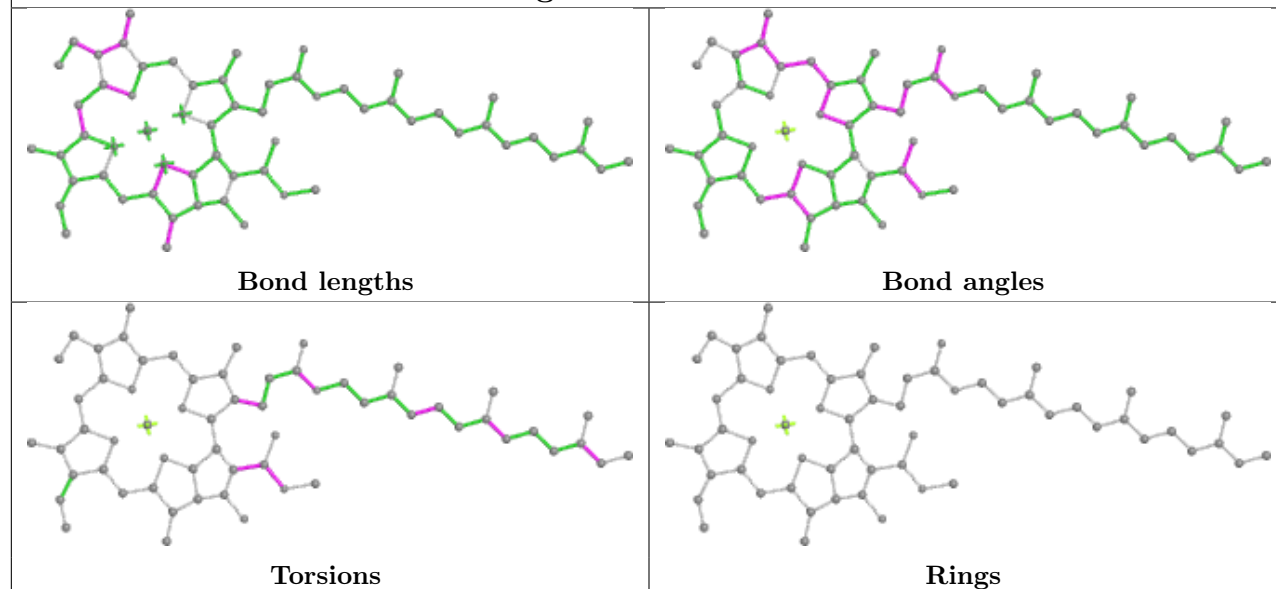
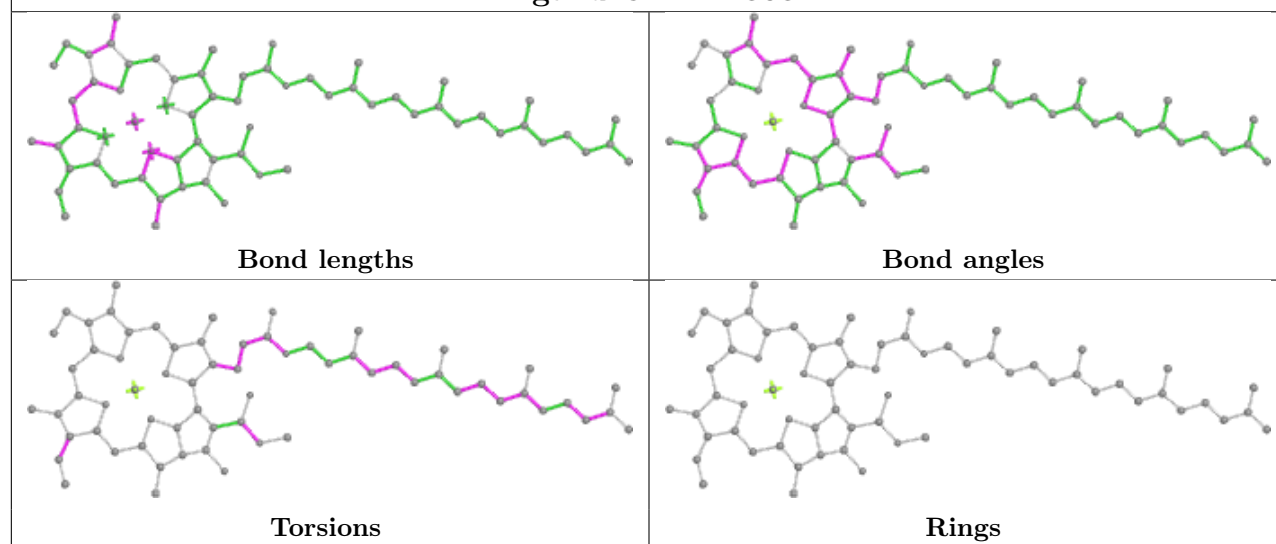
Bond angles



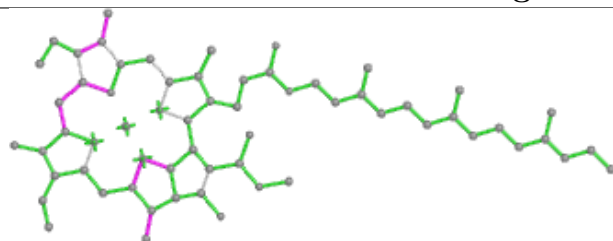
Torsions



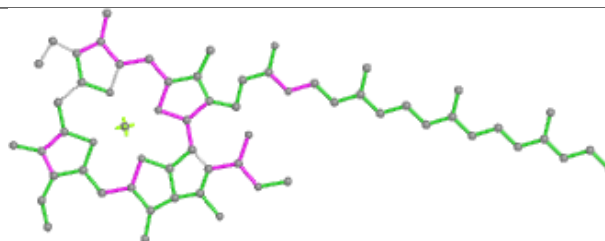
Rings

**Ligand CLA 6 610****Ligand CLA B 808**

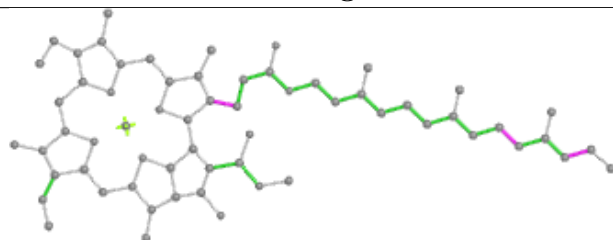
## Ligand CLA K 203



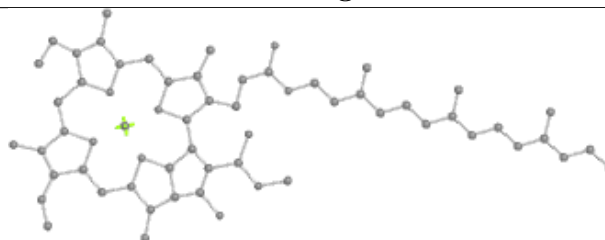
Bond lengths



Bond angles

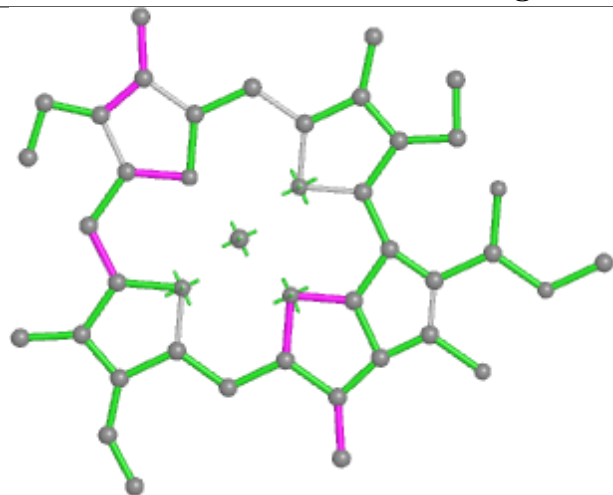


Torsions

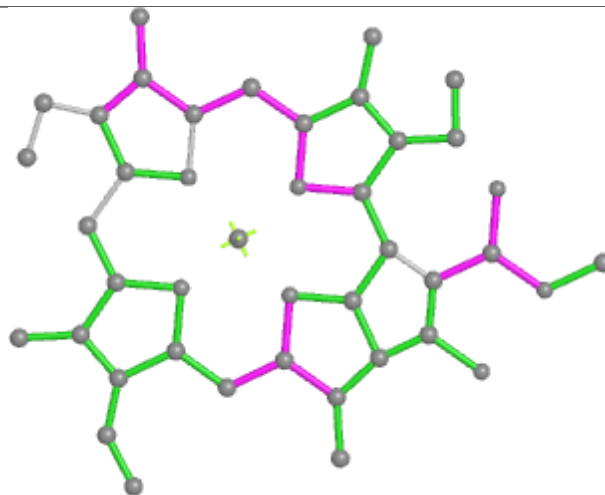


Rings

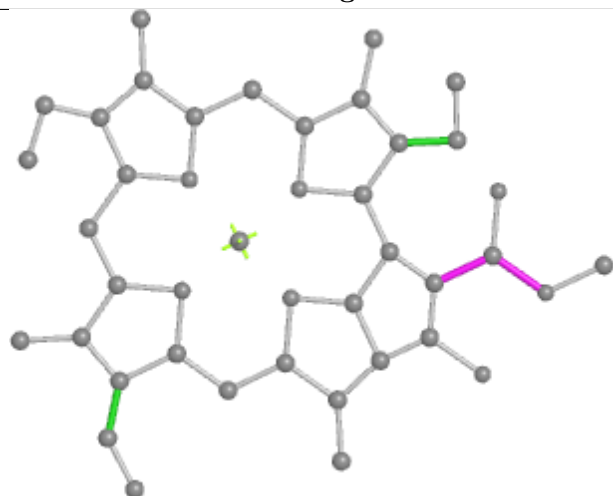
## Ligand CLA X 310



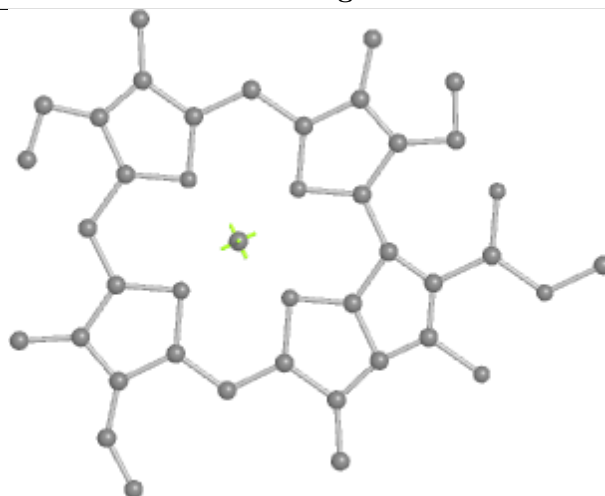
Bond lengths



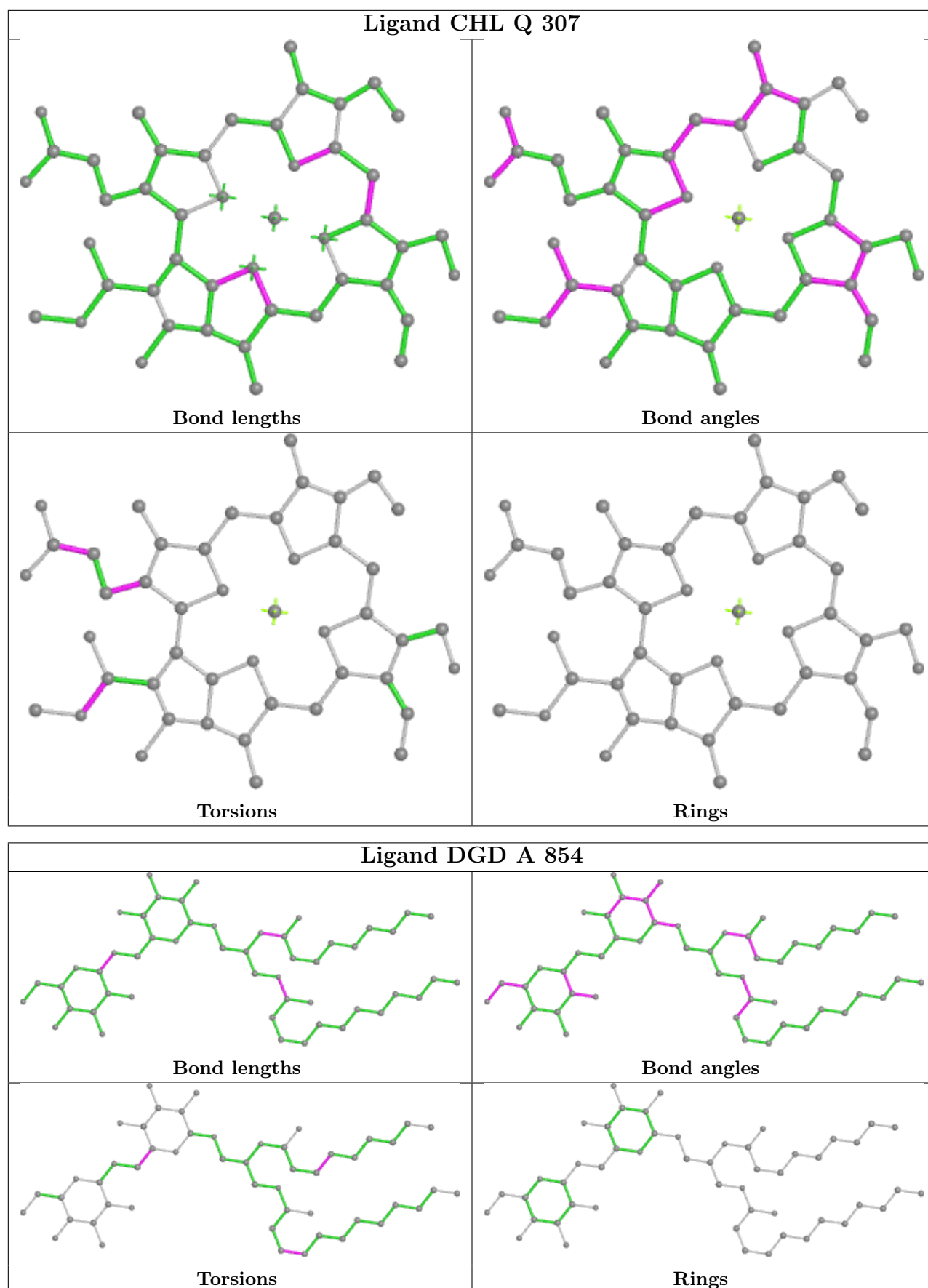
Bond angles



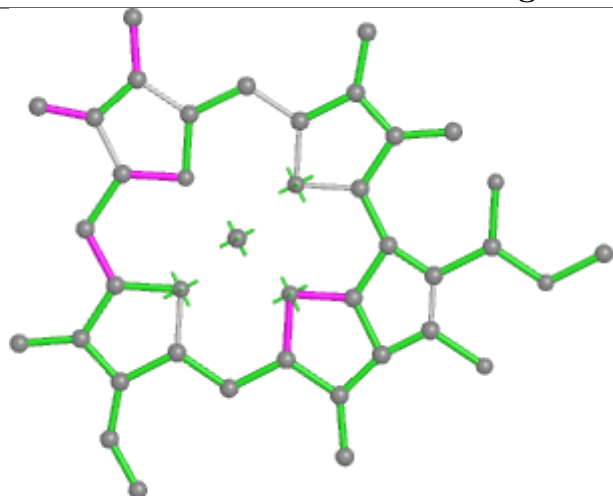
Torsions



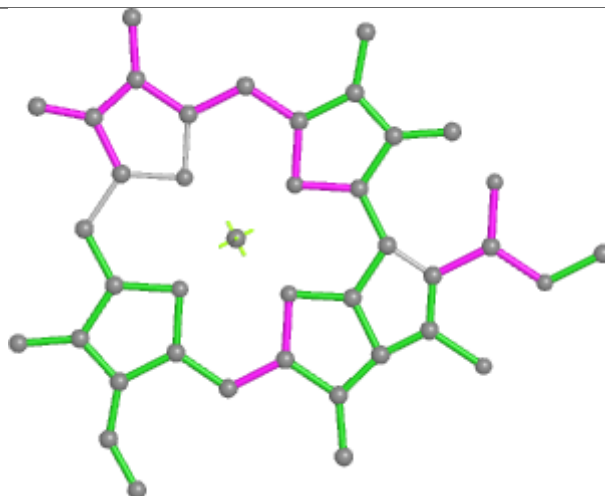
Rings



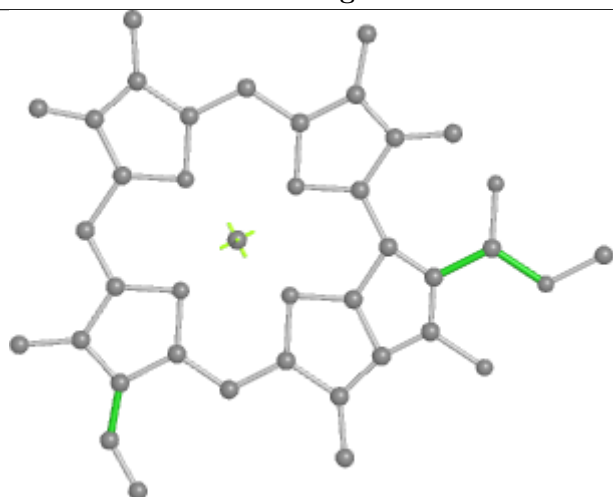
## Ligand CLA 5 606



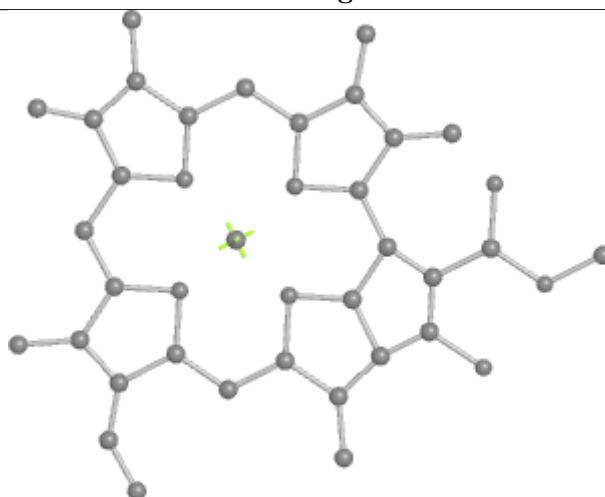
Bond lengths



Bond angles

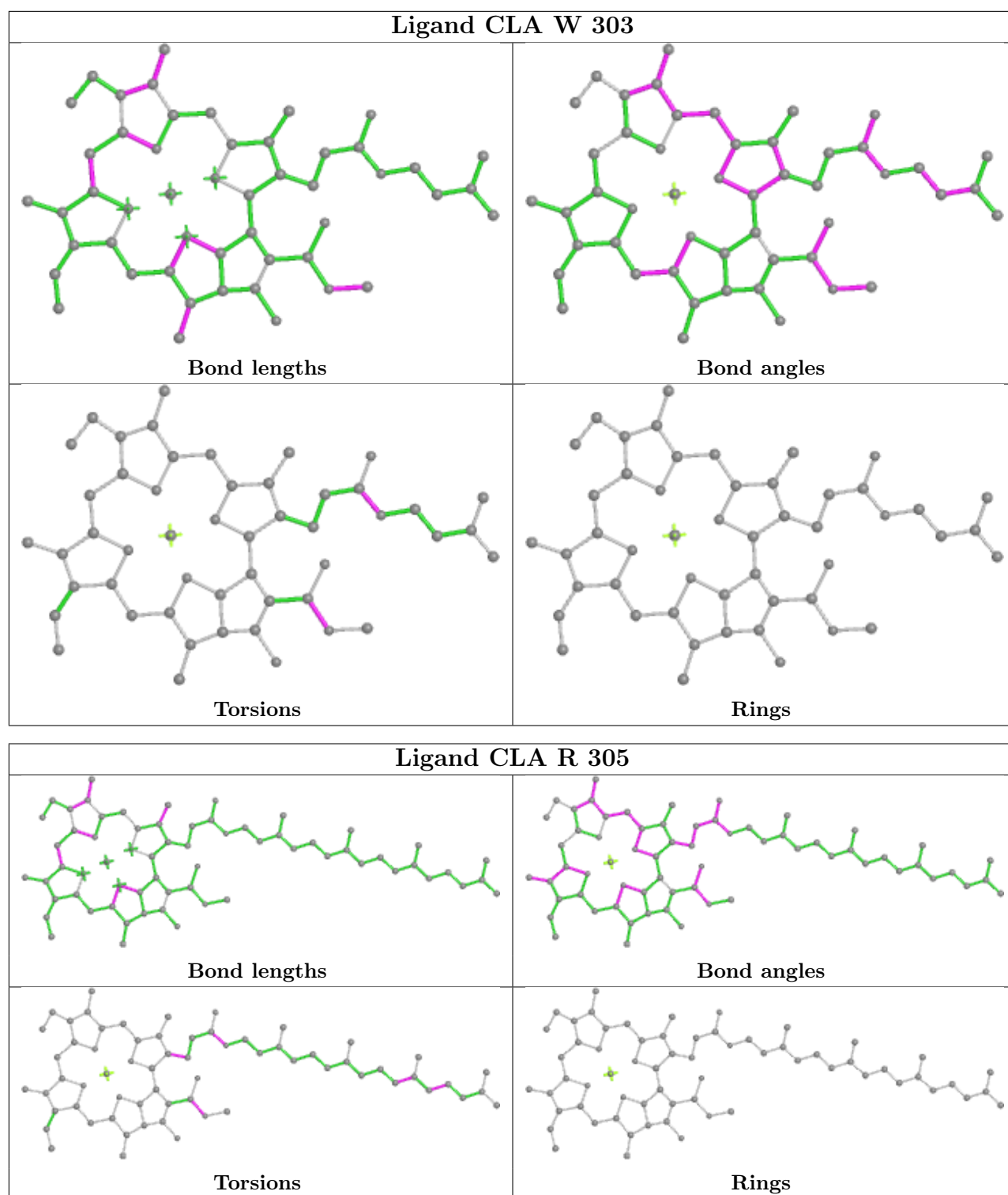


Torsions

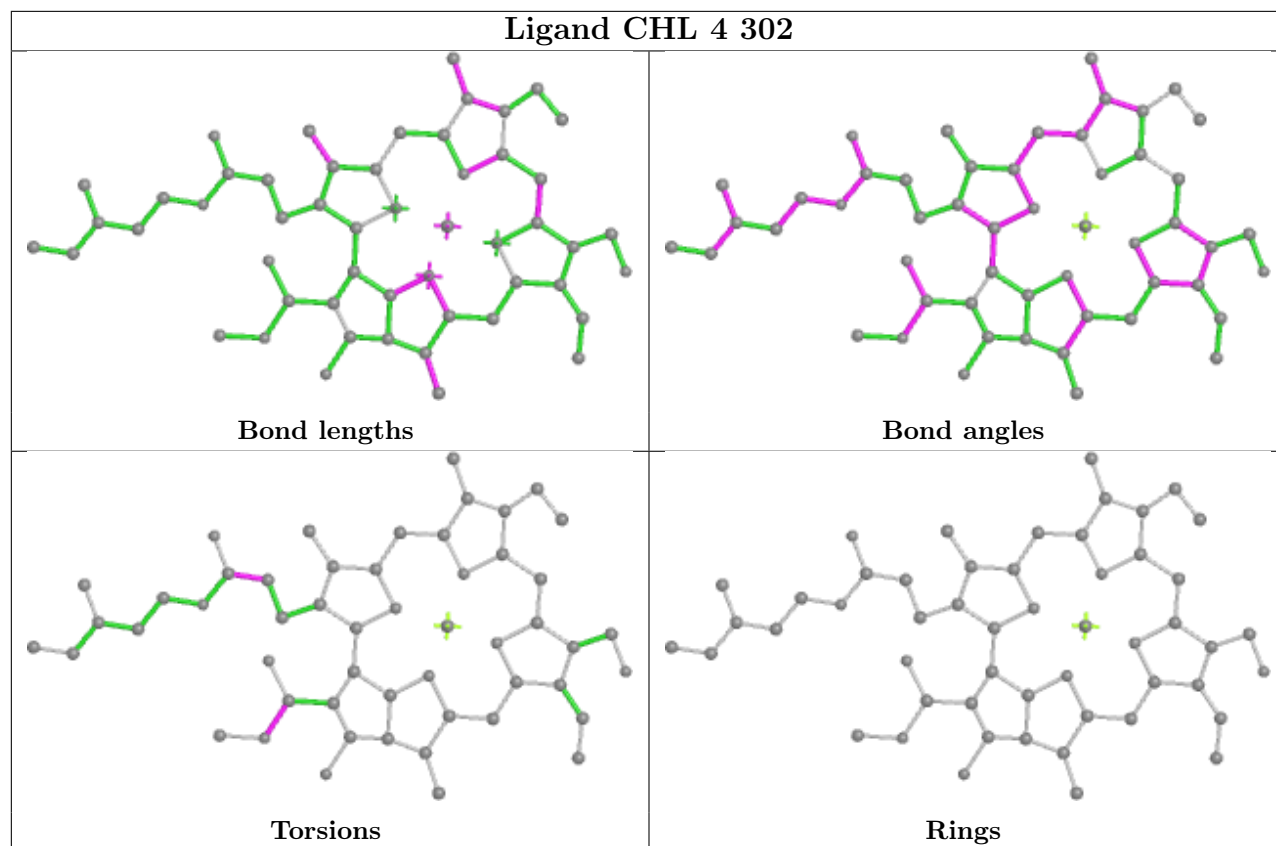


Rings

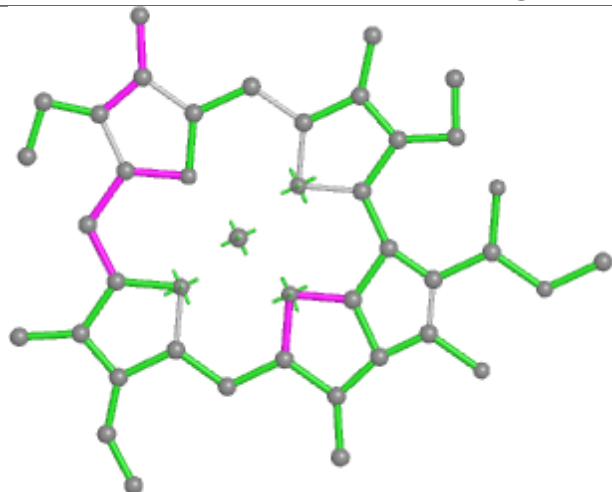




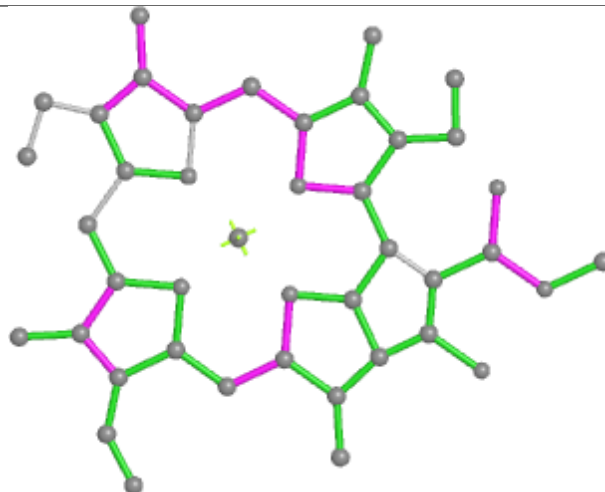
## Ligand CHL 4 302



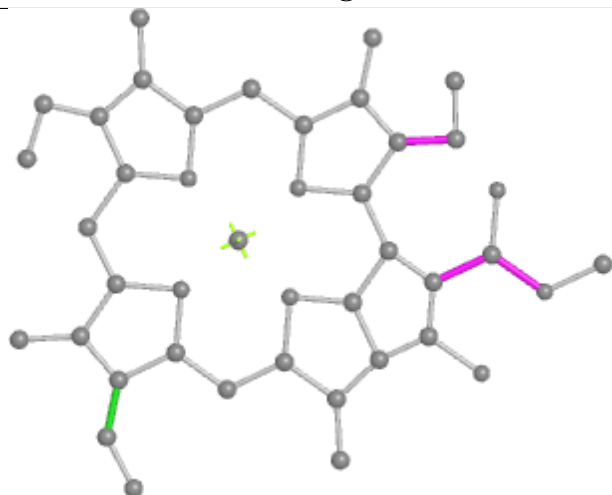
## Ligand CLA A 824



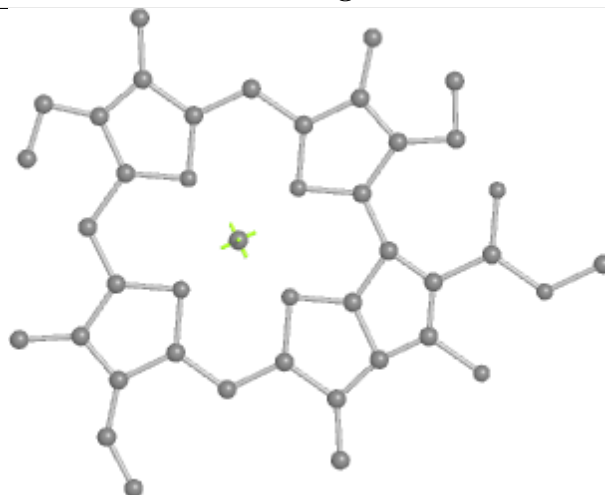
Bond lengths



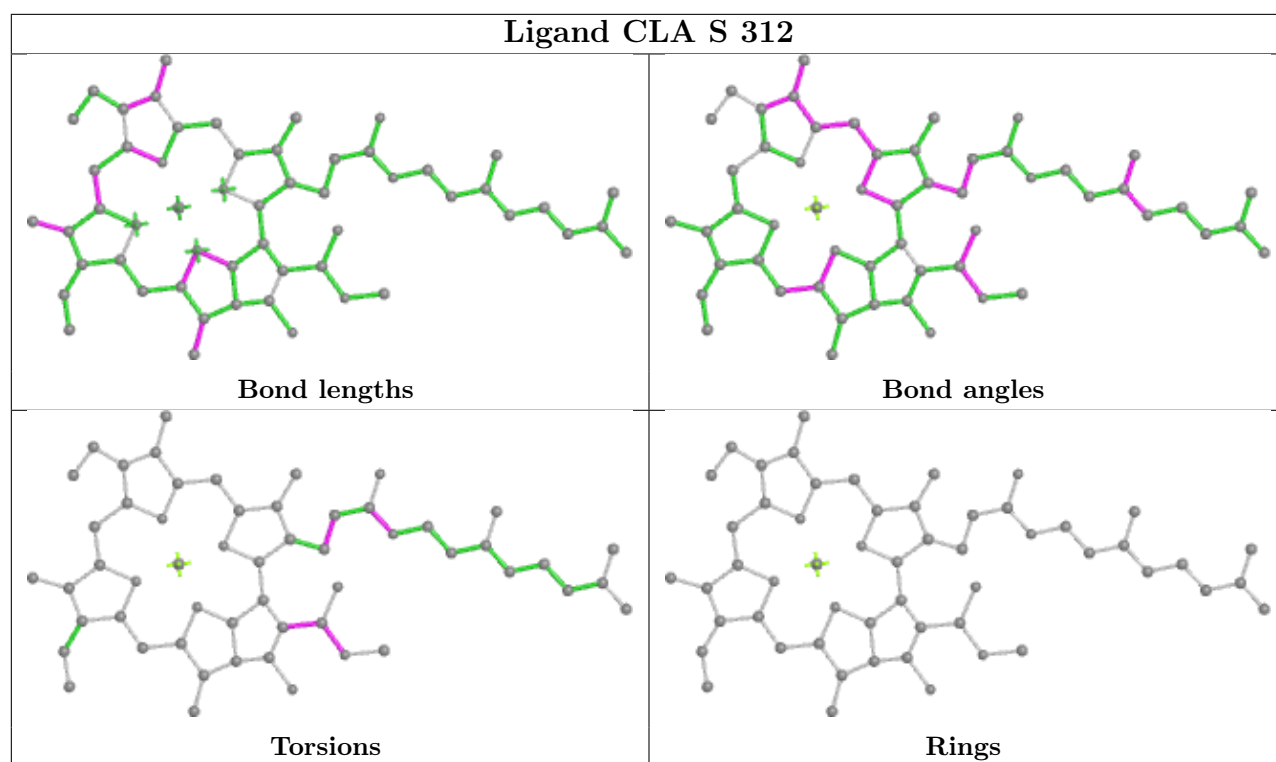
Bond angles



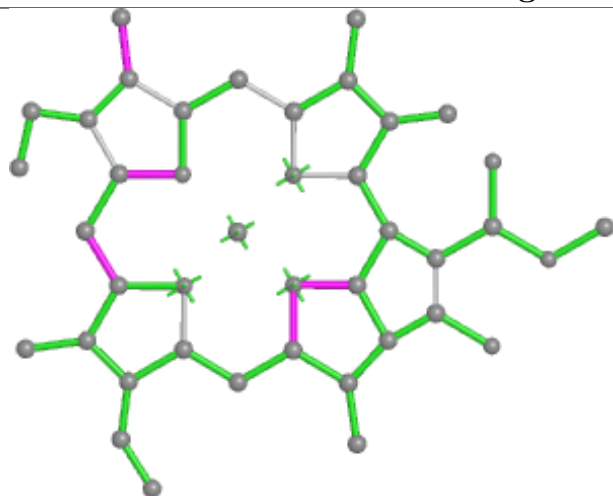
Torsions



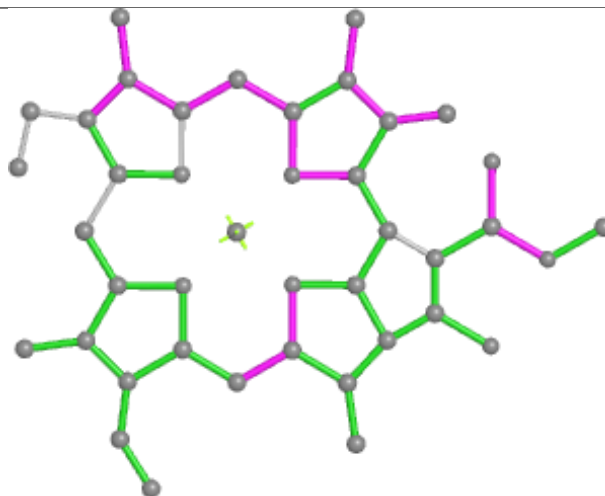
Rings



## Ligand CLA 4 315



Bond lengths



Bond angles

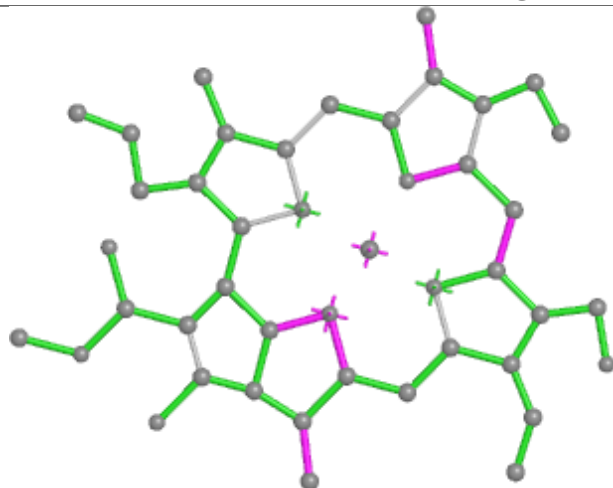


Torsions

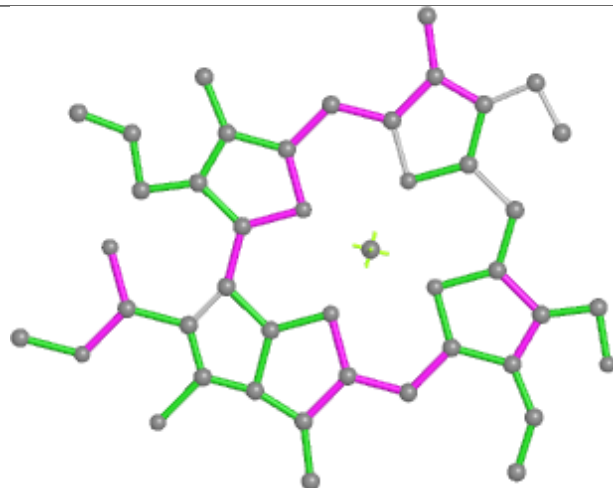


Rings

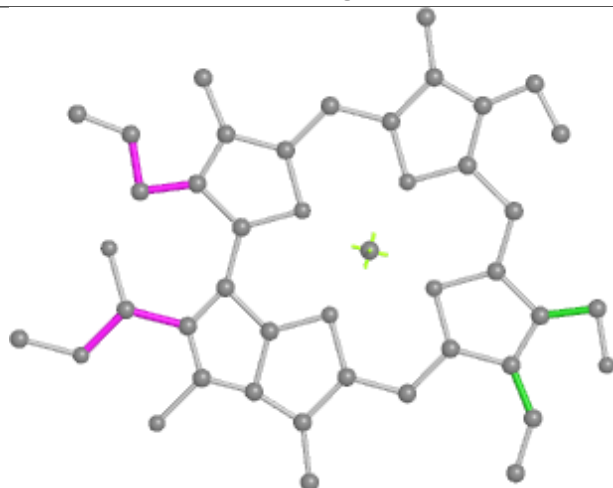
## Ligand CHL V 314



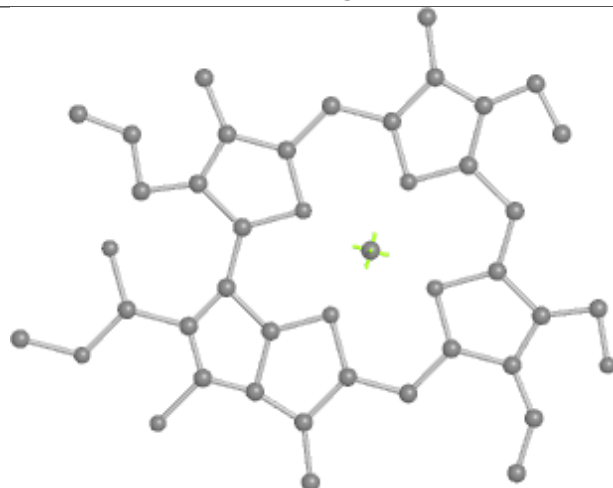
Bond lengths



Bond angles

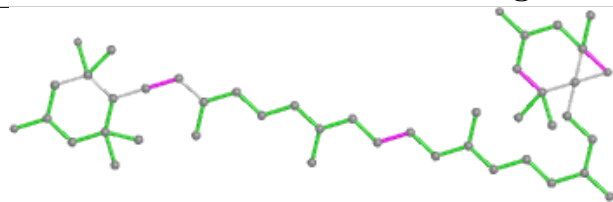


Torsions

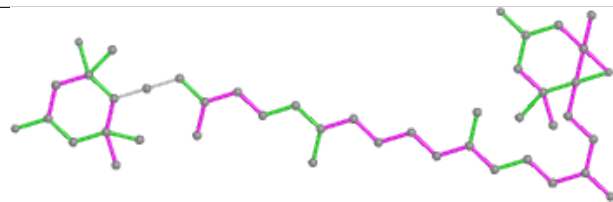


Rings

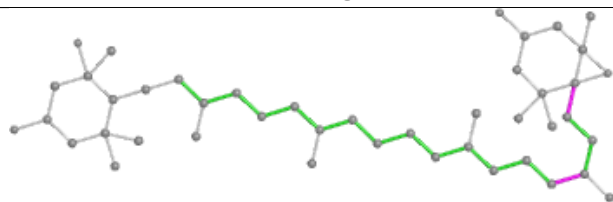
## Ligand NEX T 317



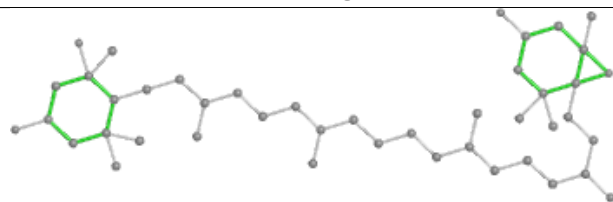
Bond lengths



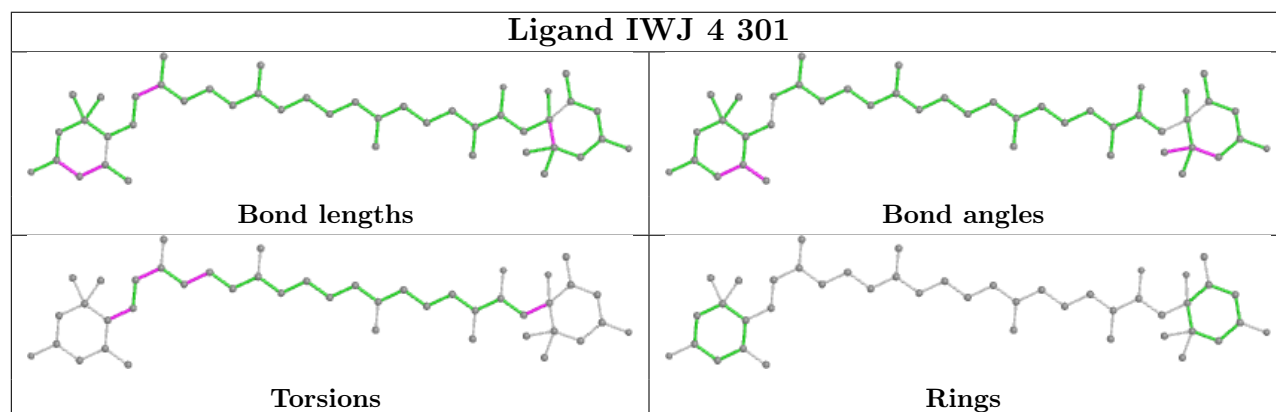
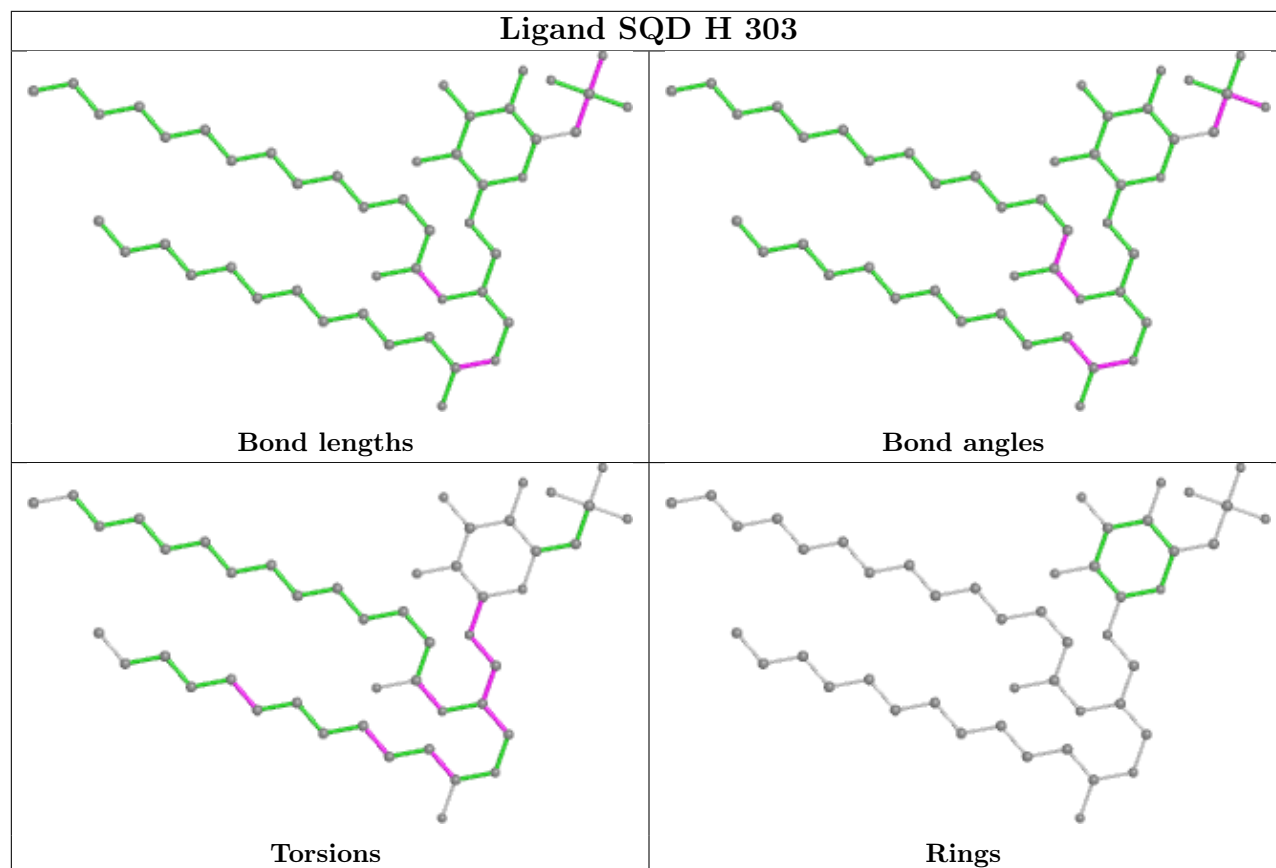
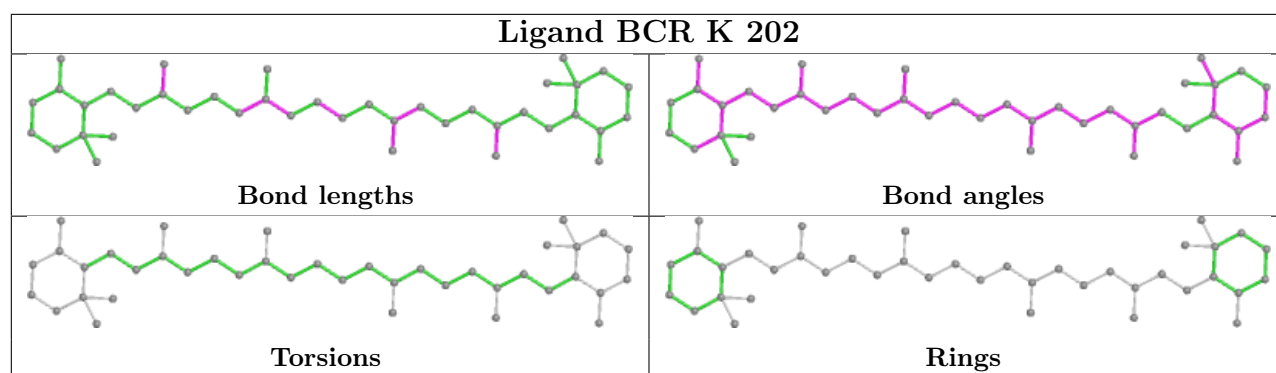
Bond angles

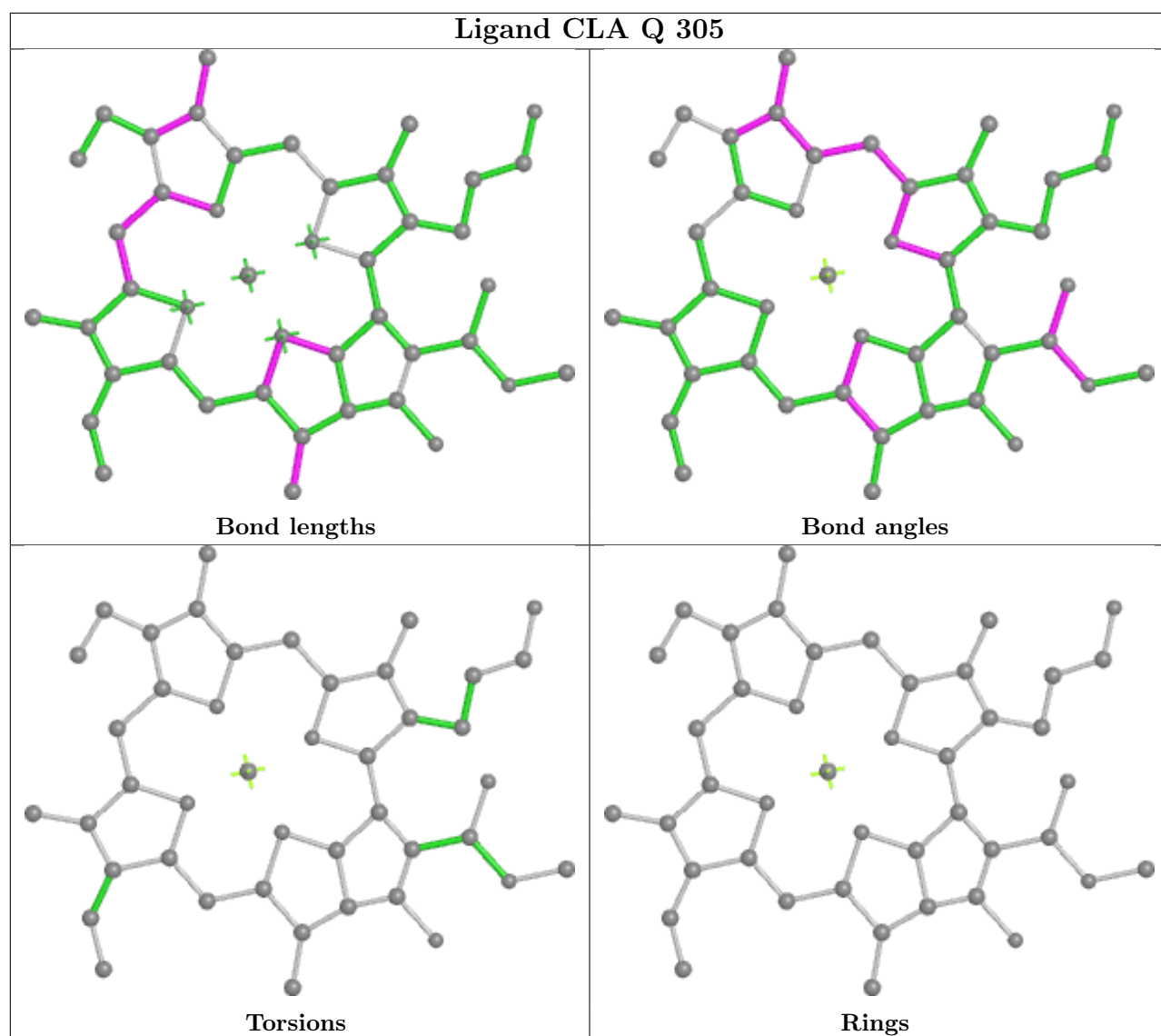


Torsions

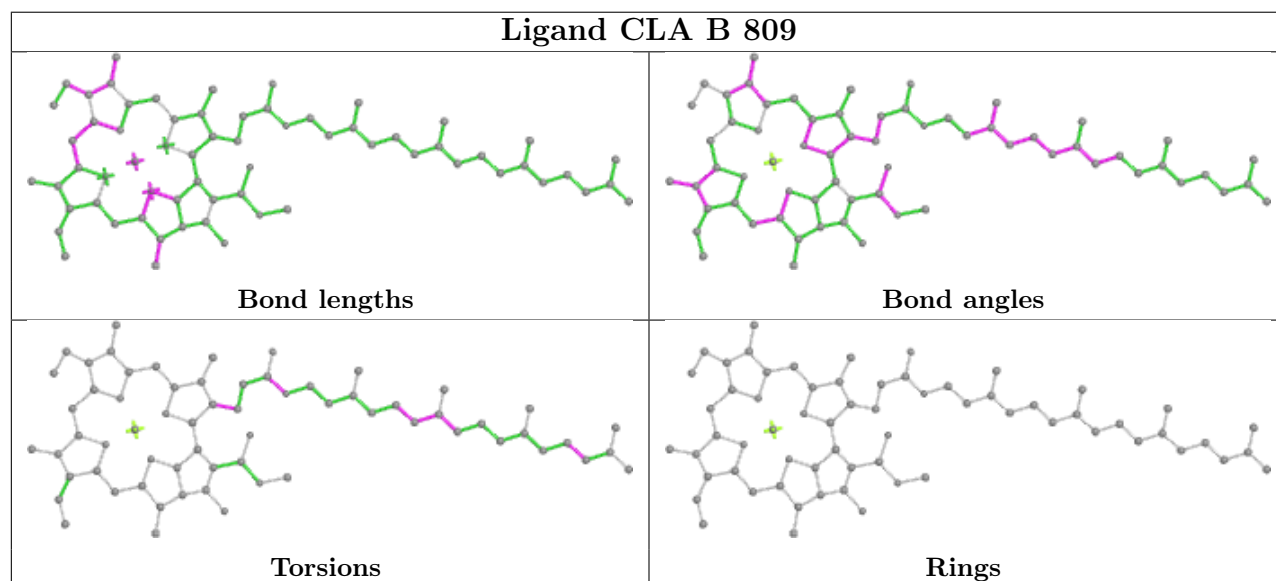
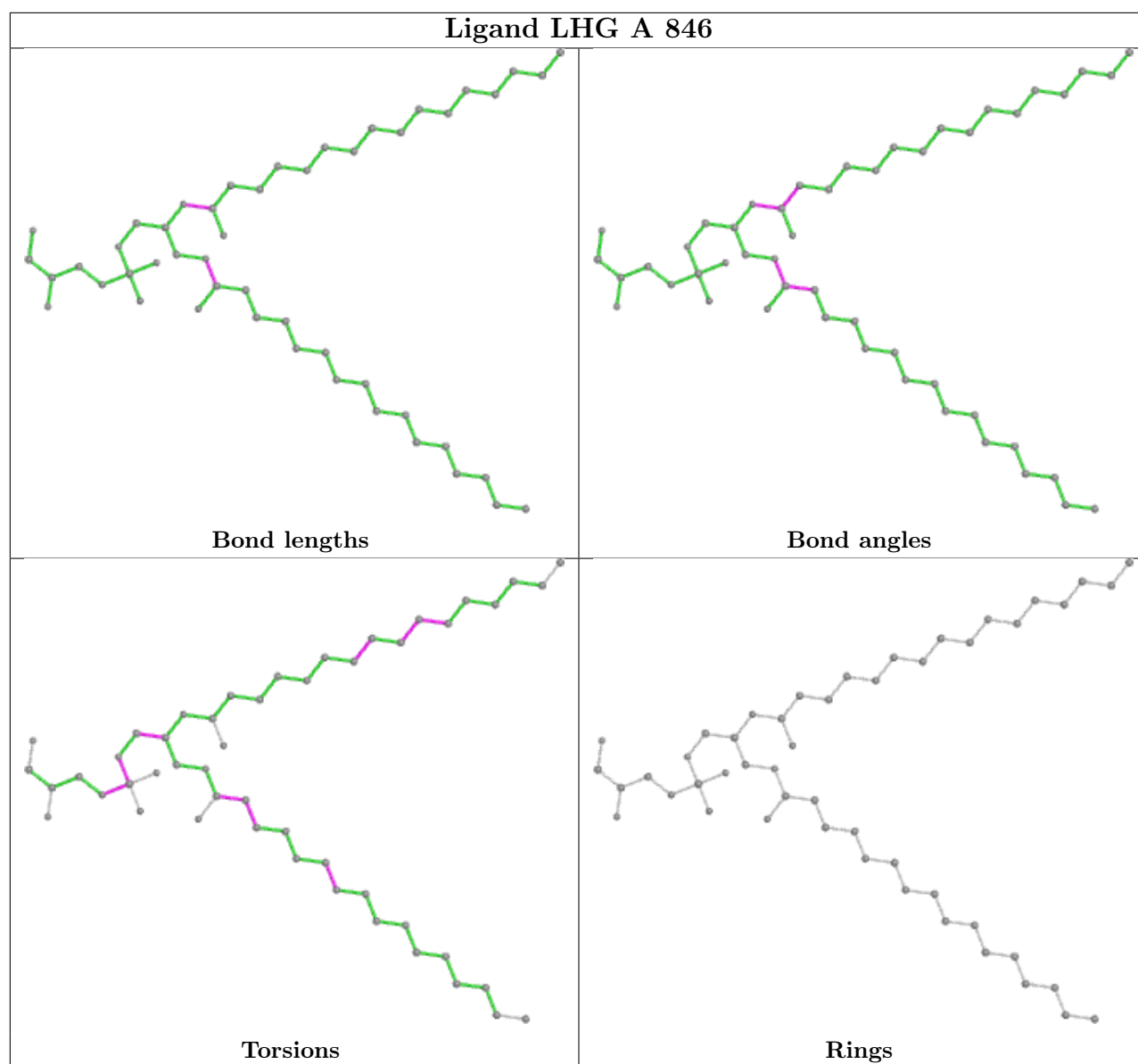


Rings

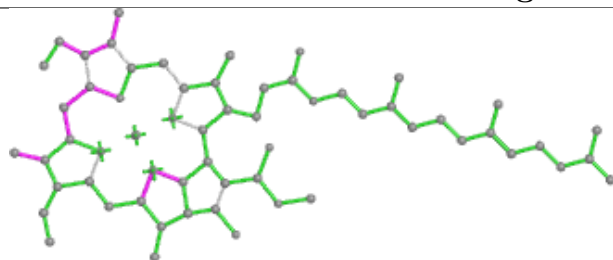




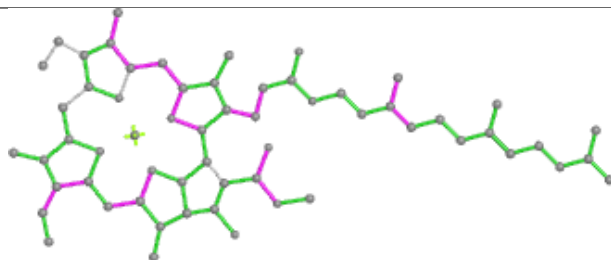




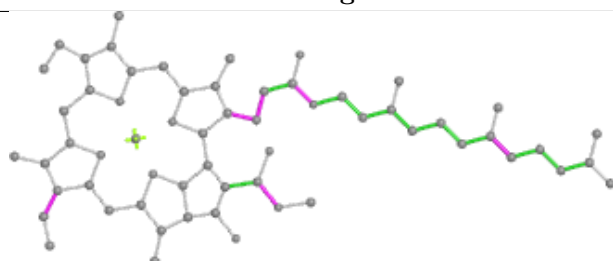
## Ligand CLA L 302



Bond lengths



Bond angles

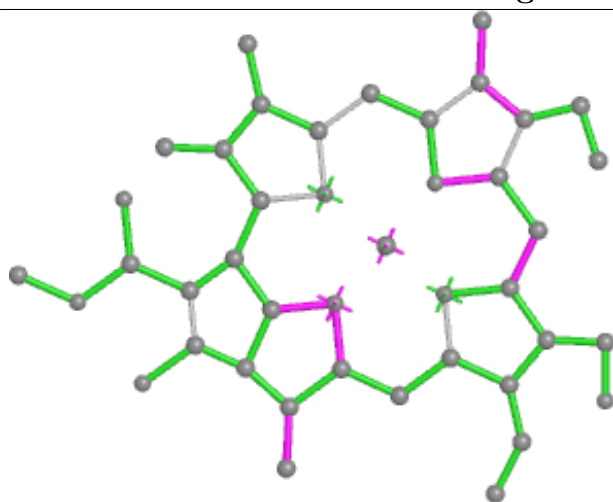


Torsions

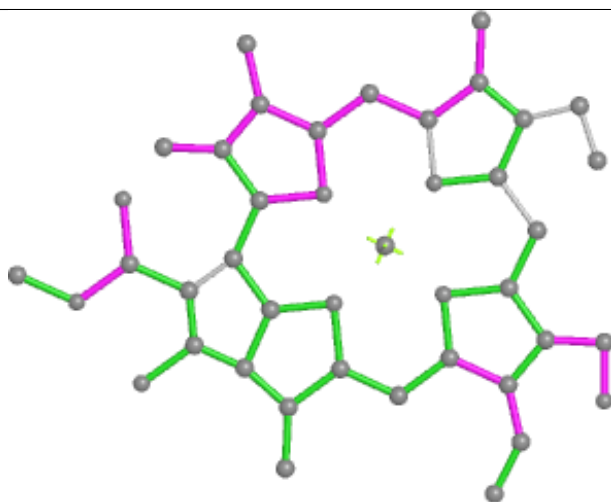


Rings

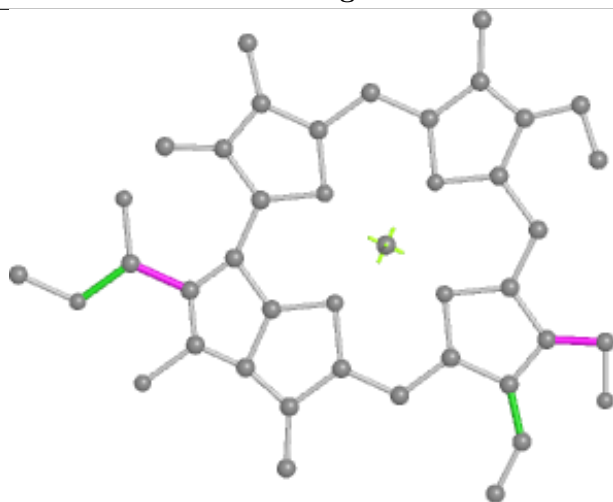
## Ligand CHL S 304



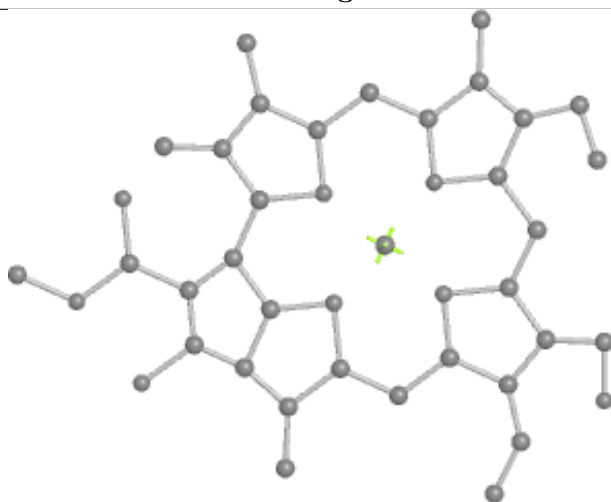
Bond lengths



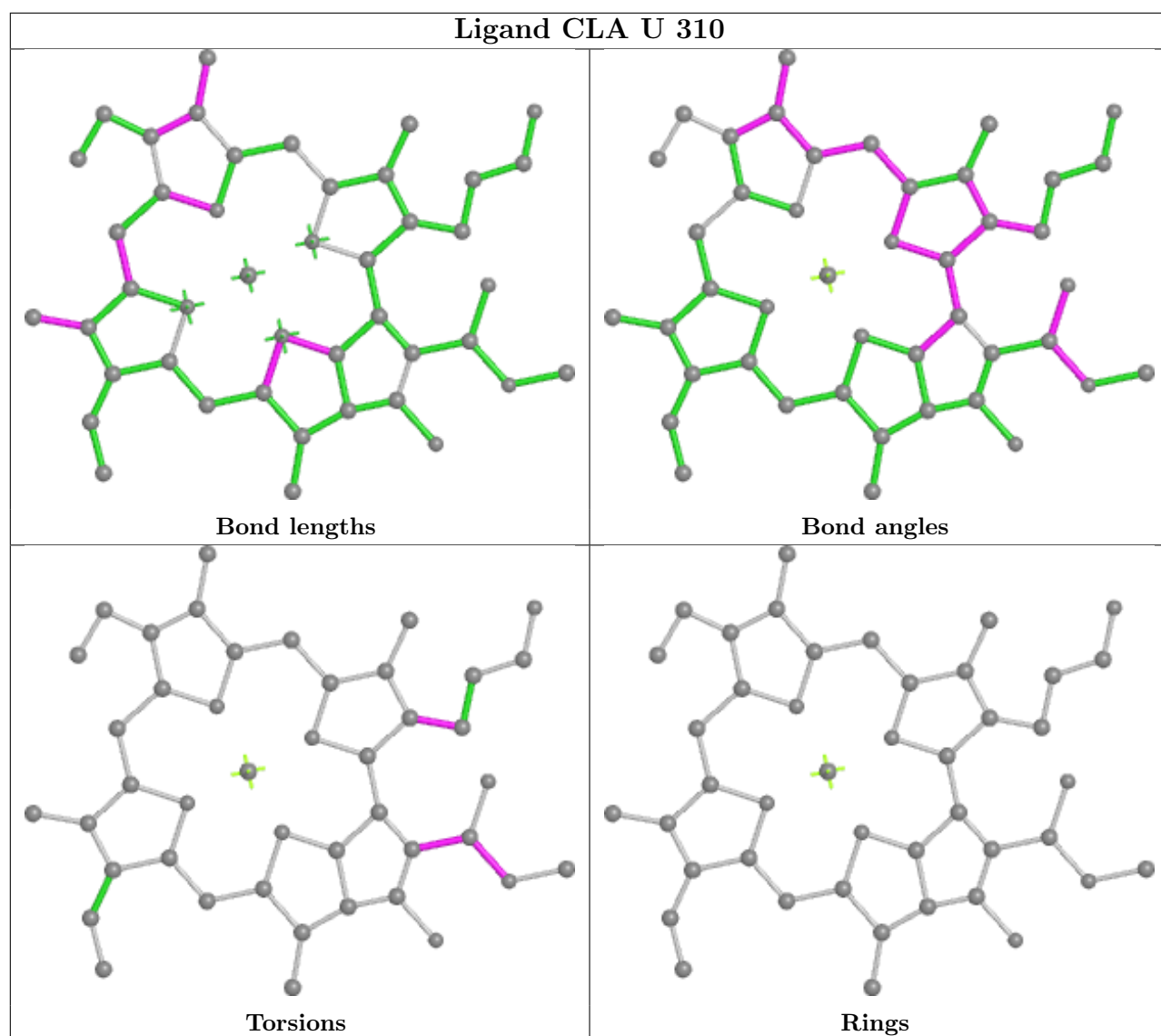
Bond angles



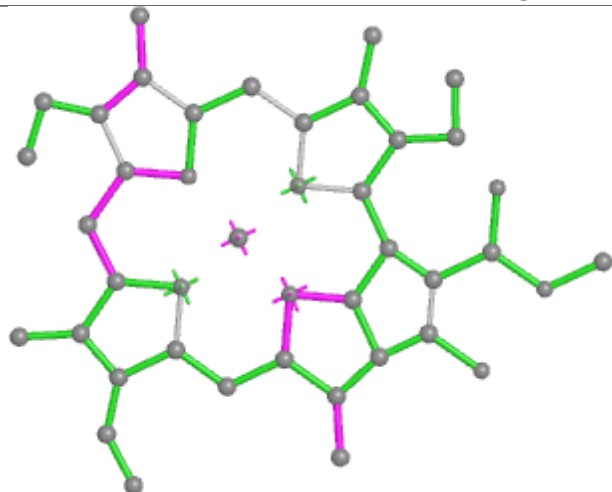
Torsions



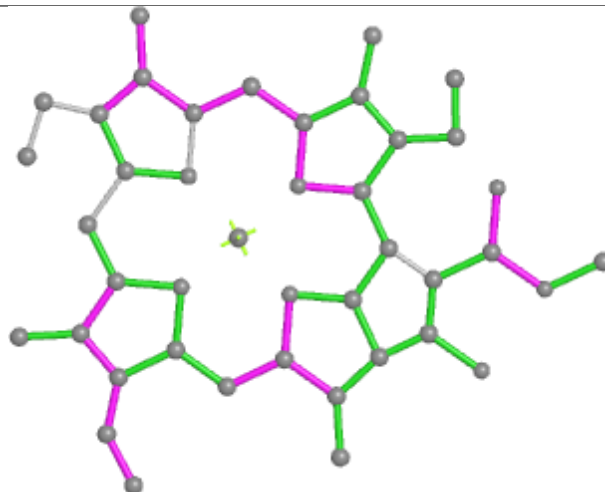
Rings



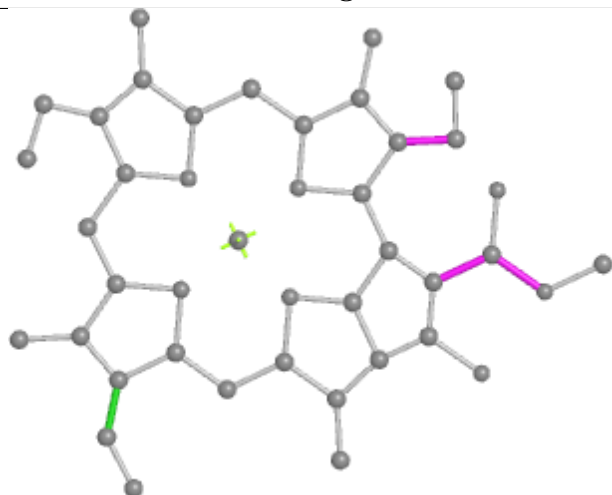
## Ligand CLA F 802



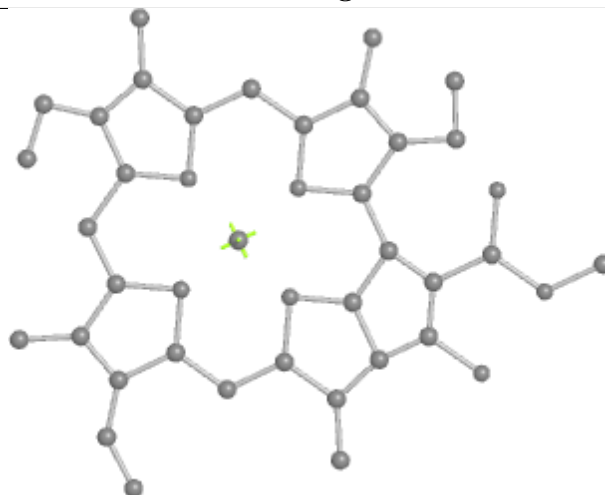
Bond lengths



Bond angles

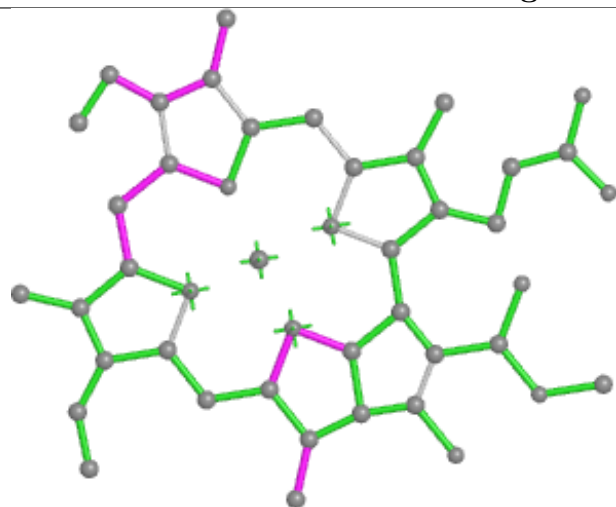


Torsions

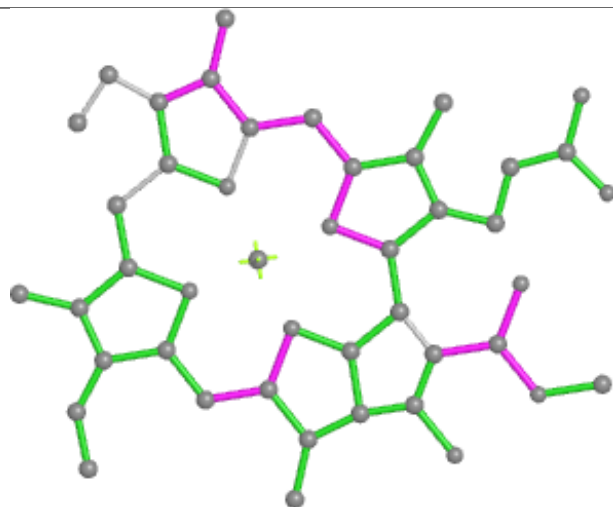


Rings

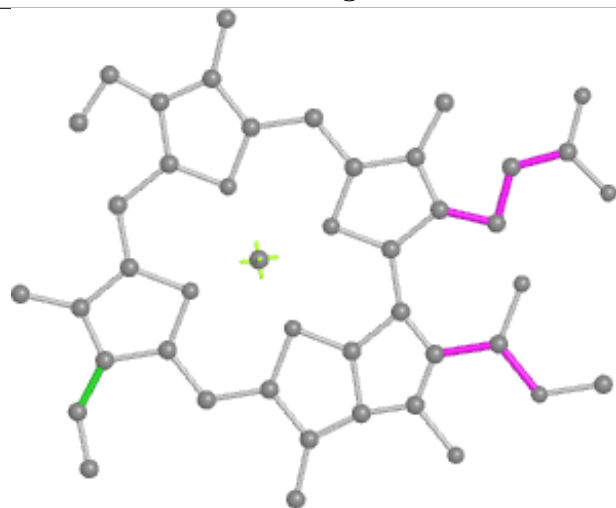
## Ligand CLA 2 606



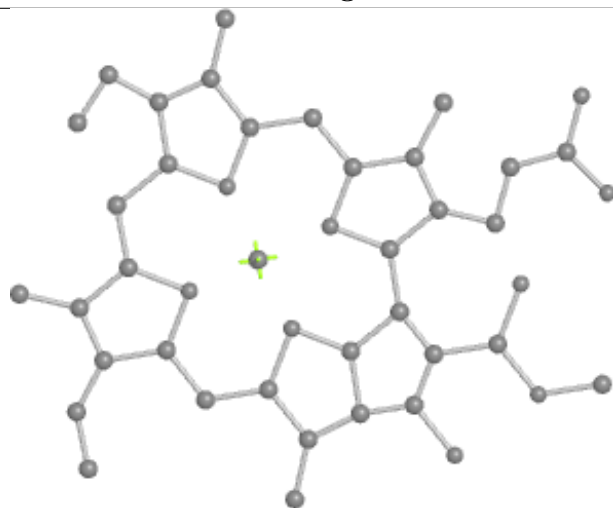
Bond lengths



Bond angles

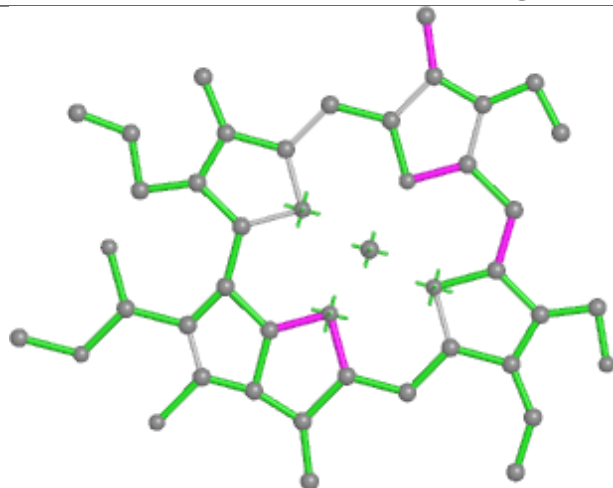


Torsions

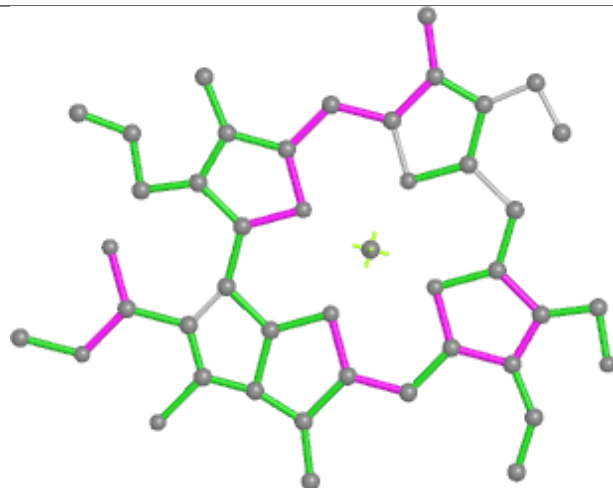


Rings

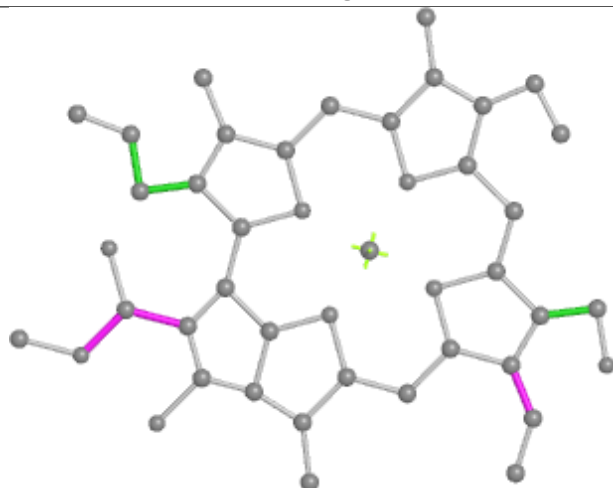
## Ligand CHL V 307



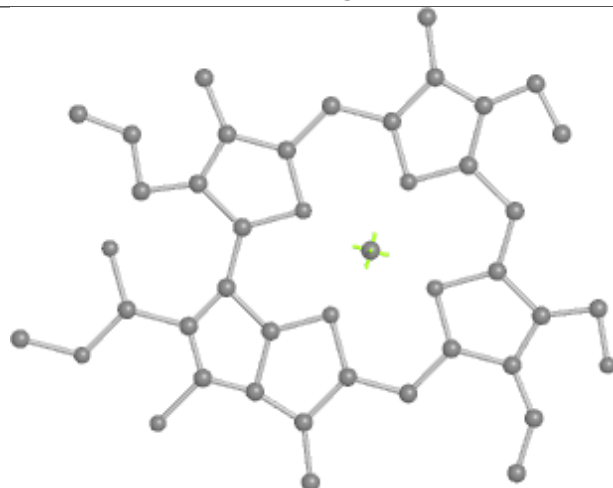
Bond lengths



Bond angles

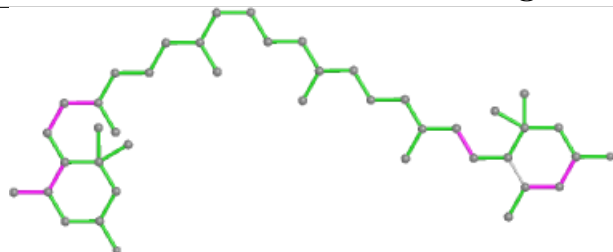


Torsions

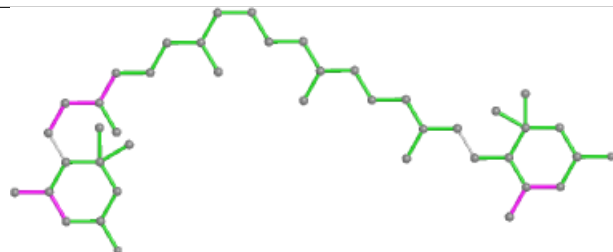


Rings

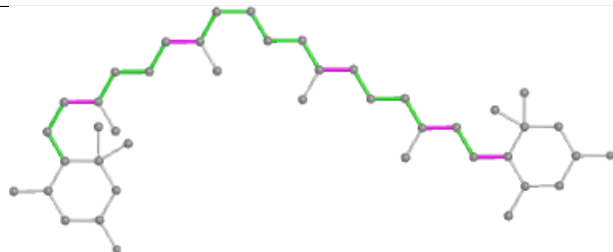
## Ligand Q6L R 319



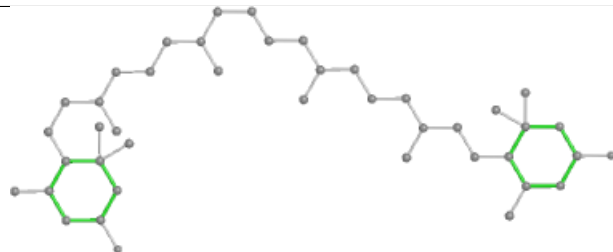
Bond lengths



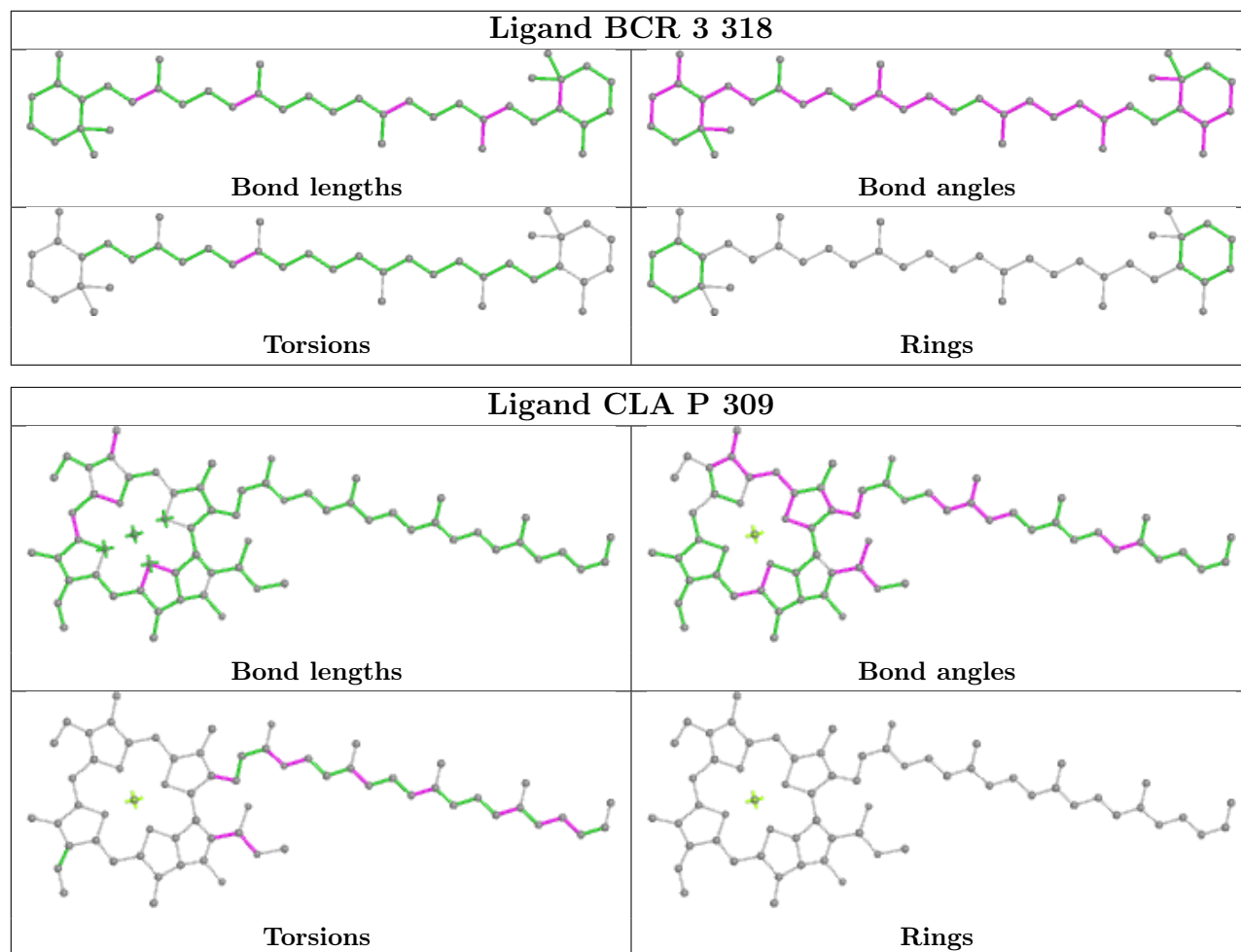
Bond angles



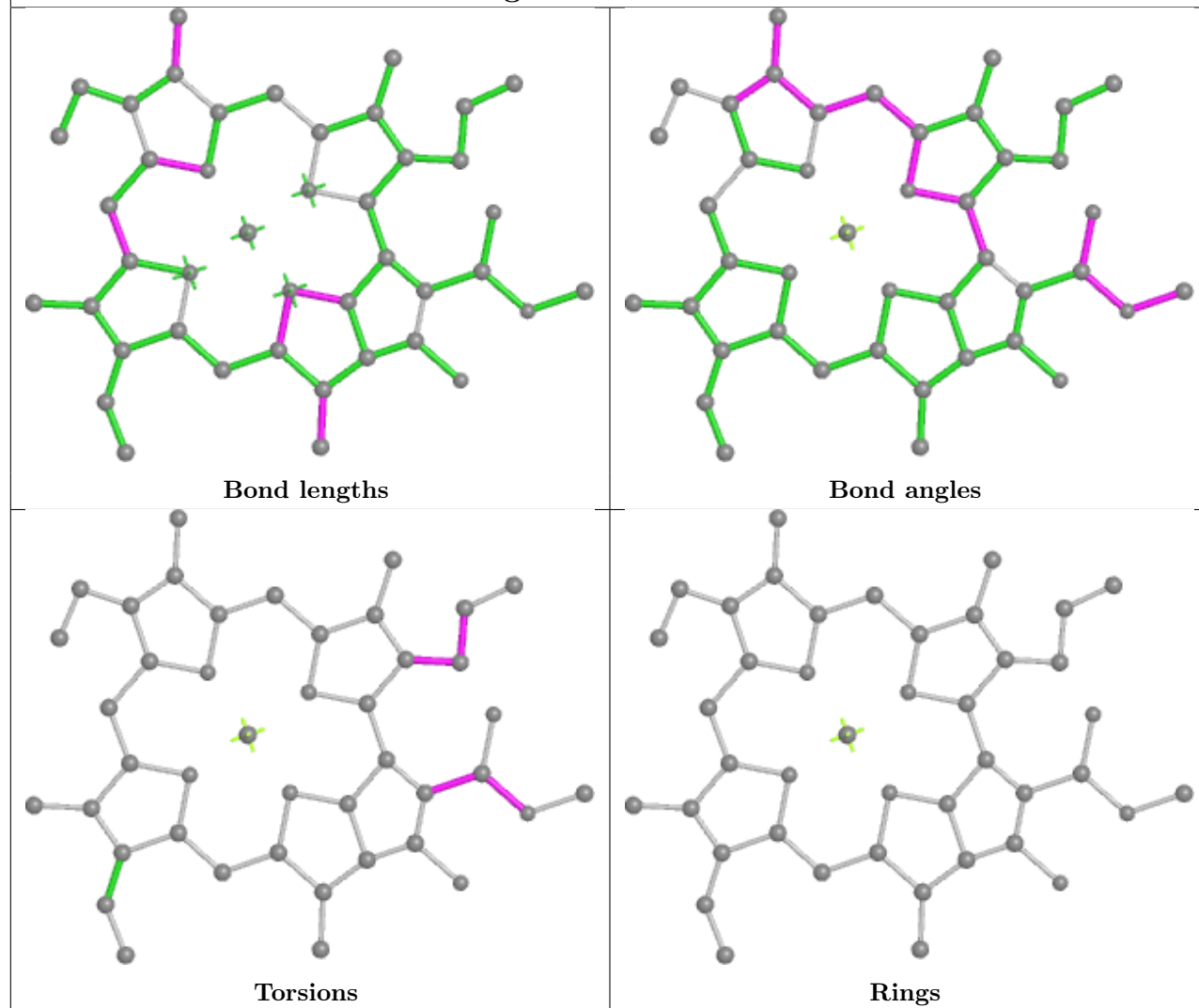
Torsions



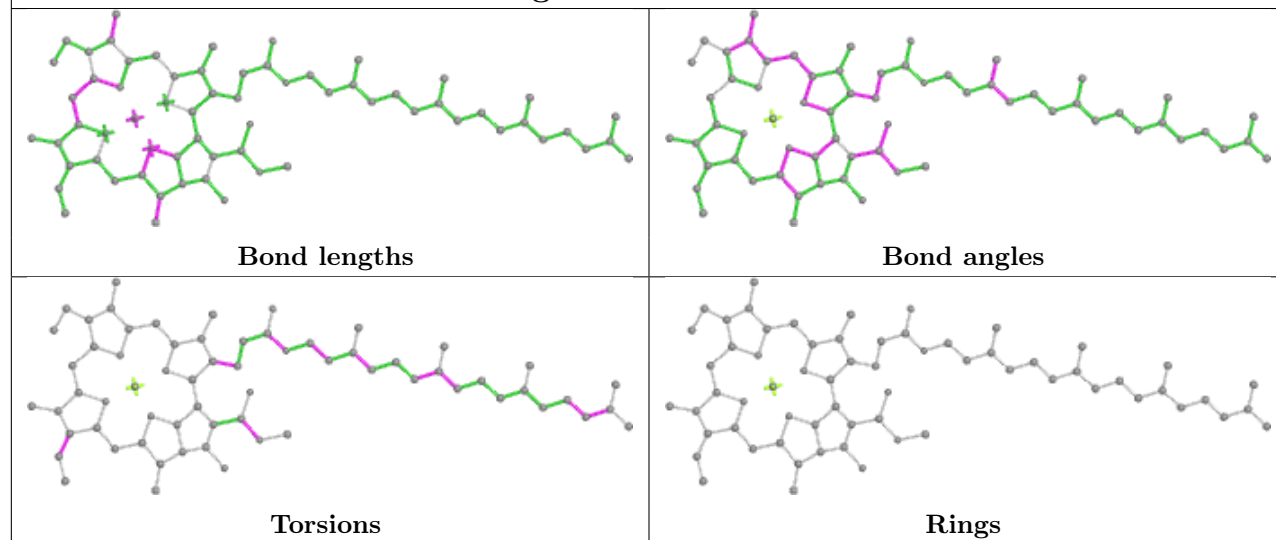
Rings



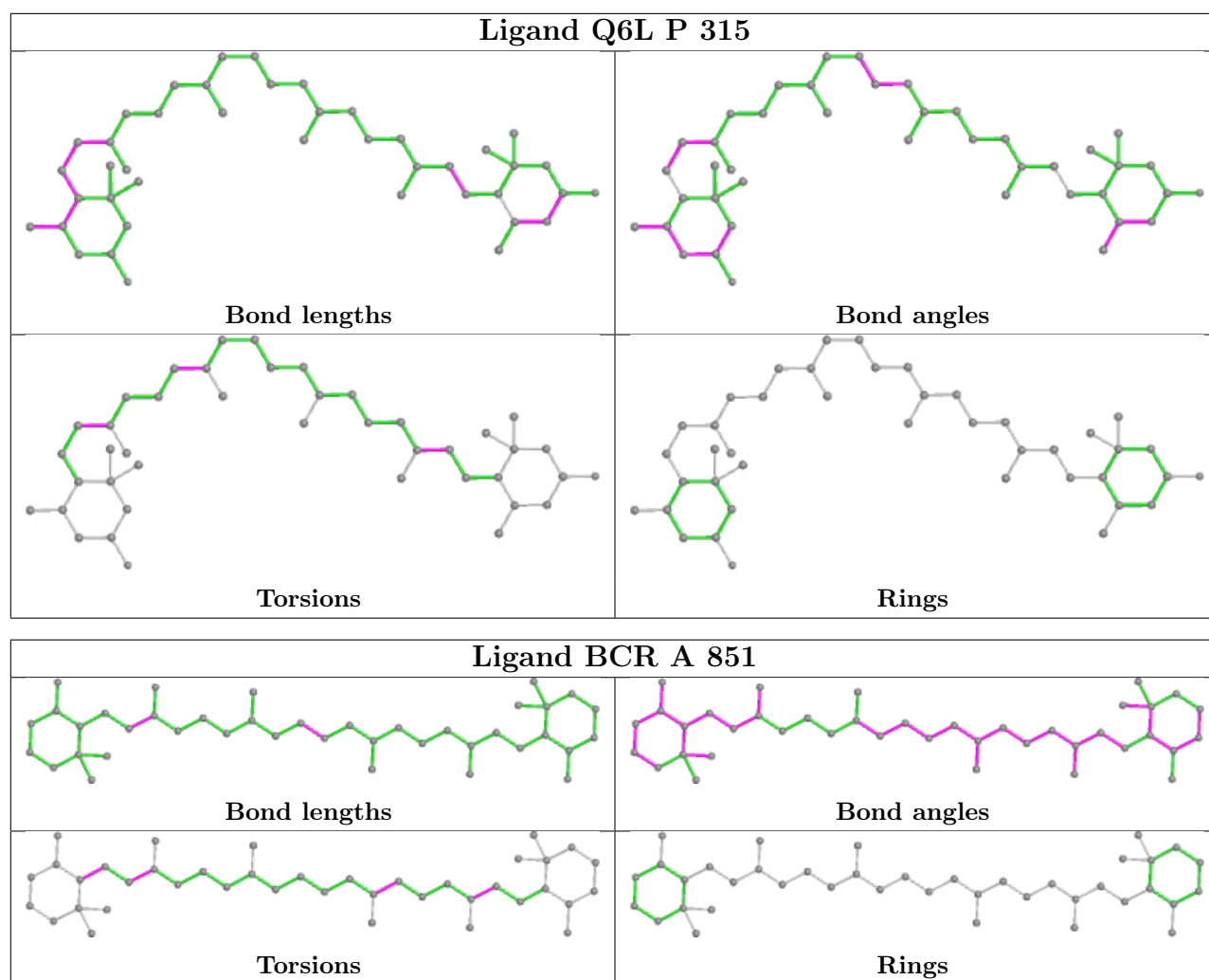
## Ligand CLA 3 310



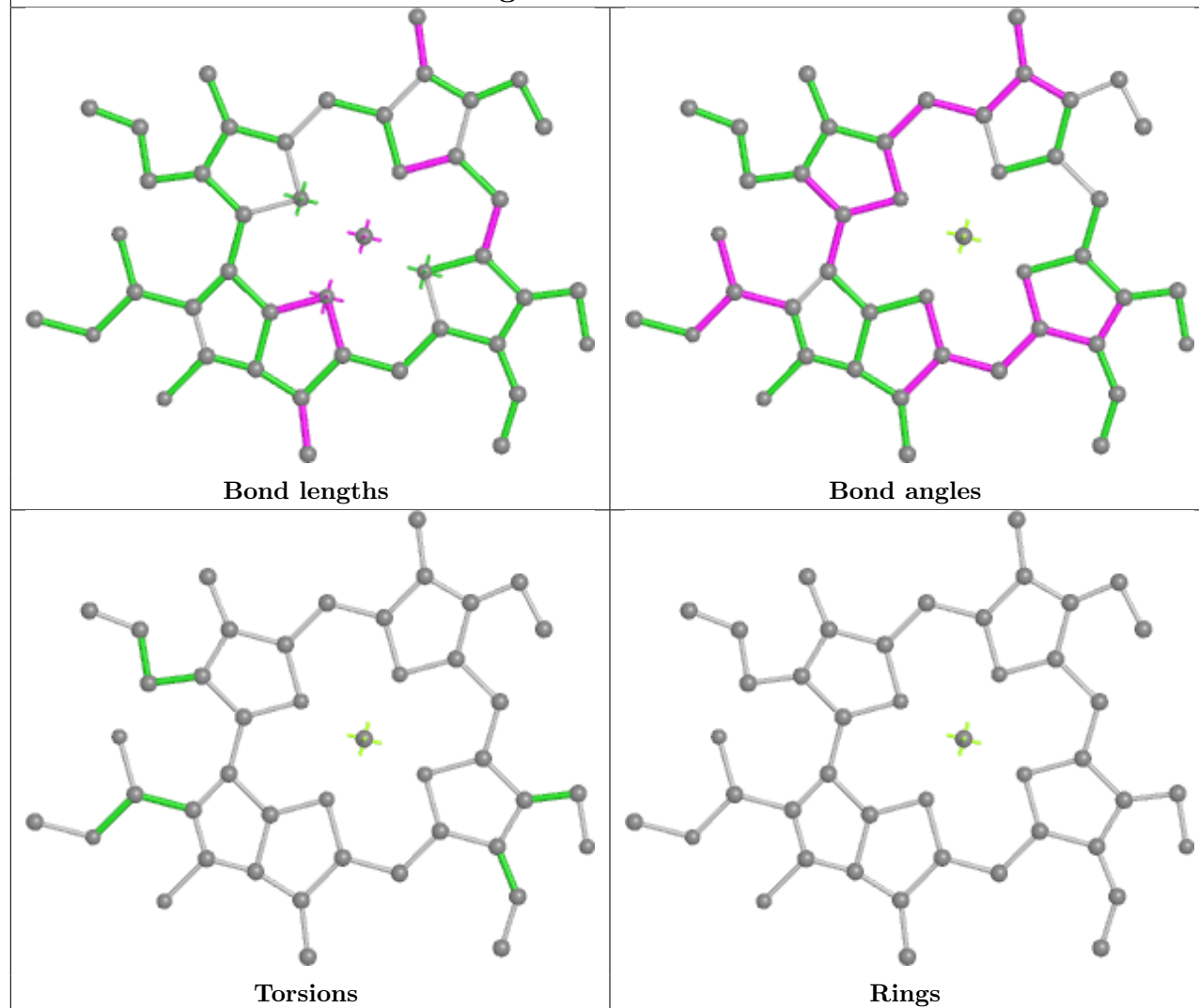
## Ligand CLA B 829



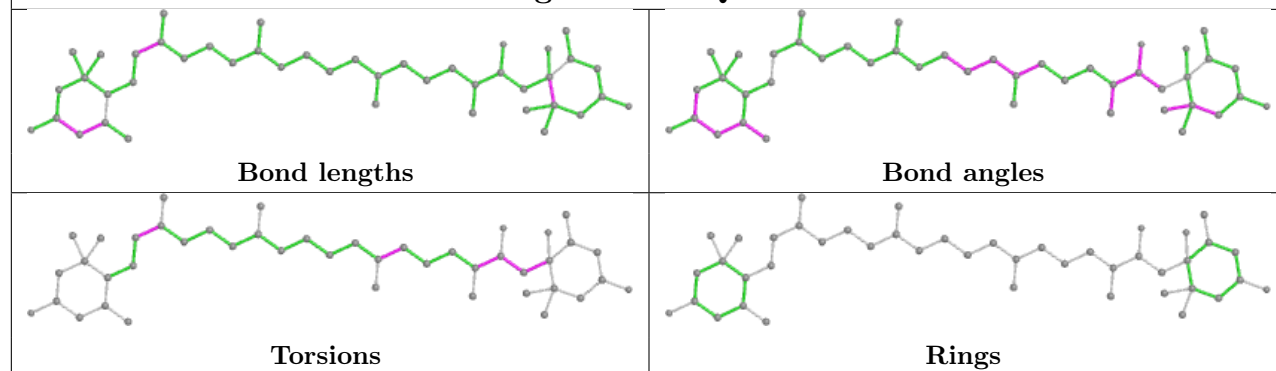




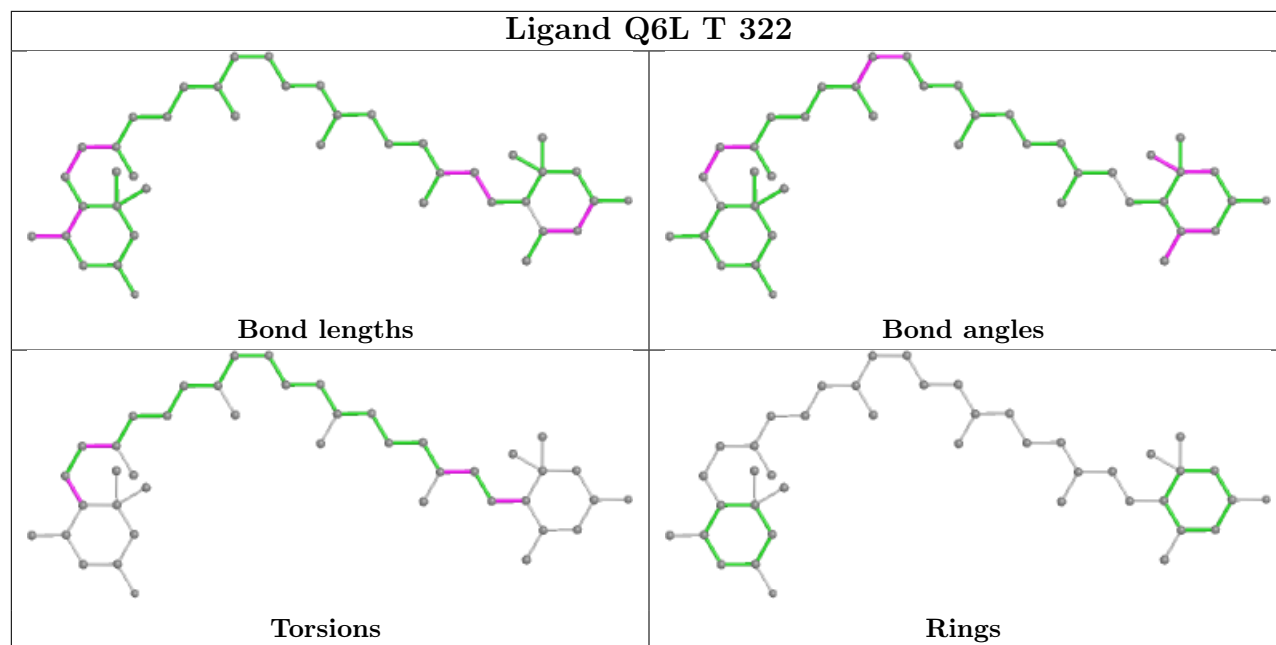
## Ligand CHL V 306



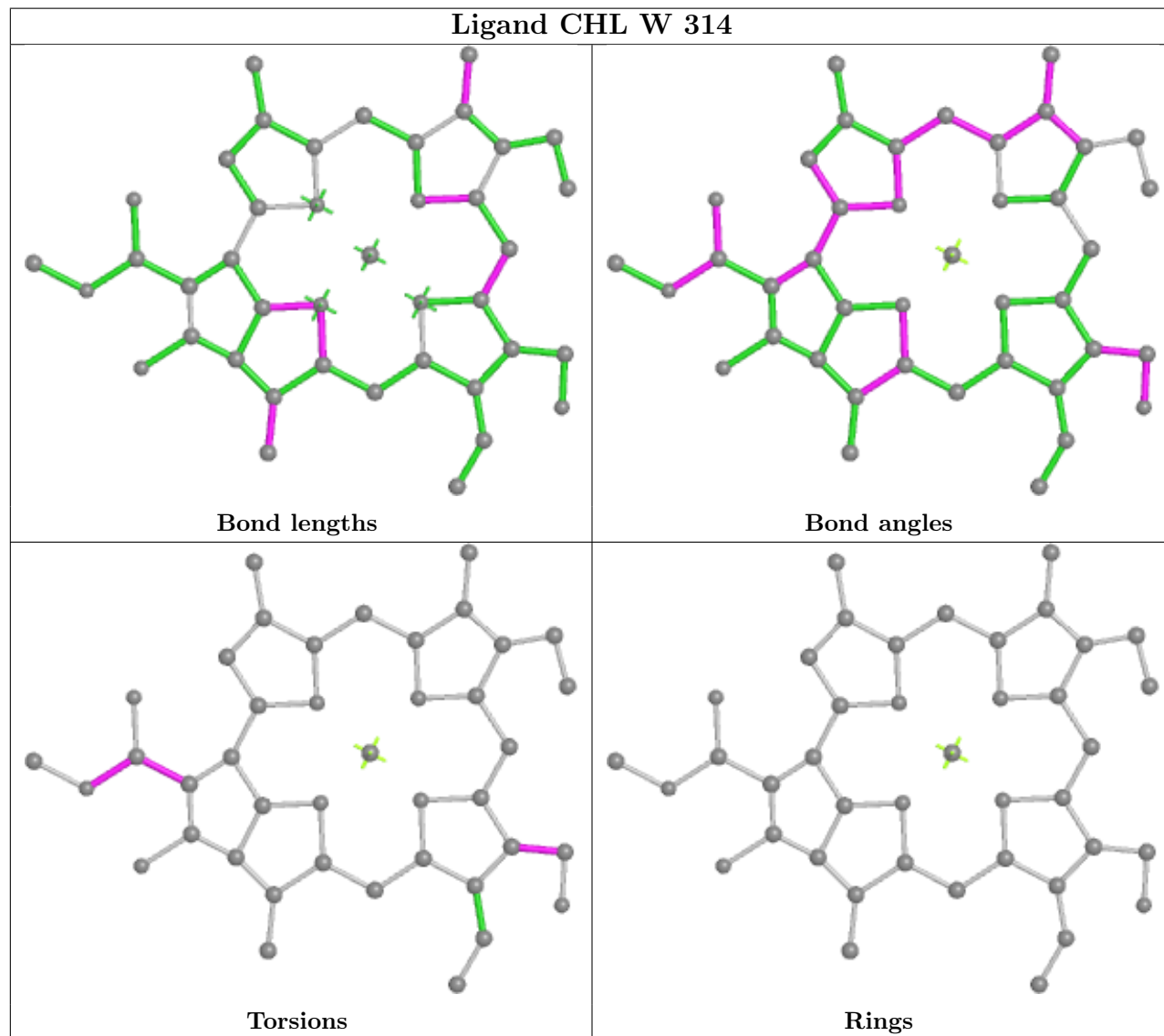
## Ligand IWJ Q 320



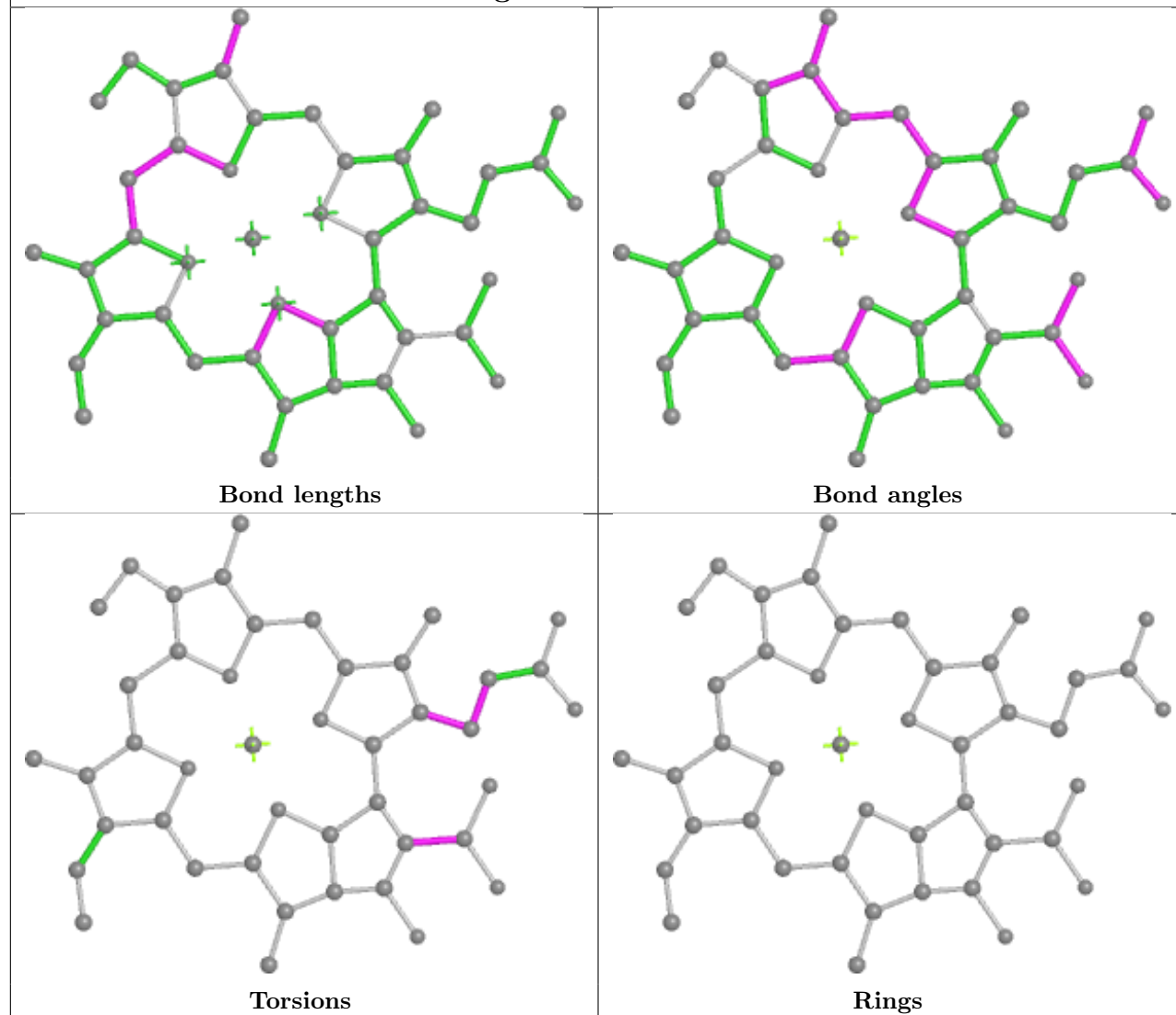
## Ligand Q6L T 322



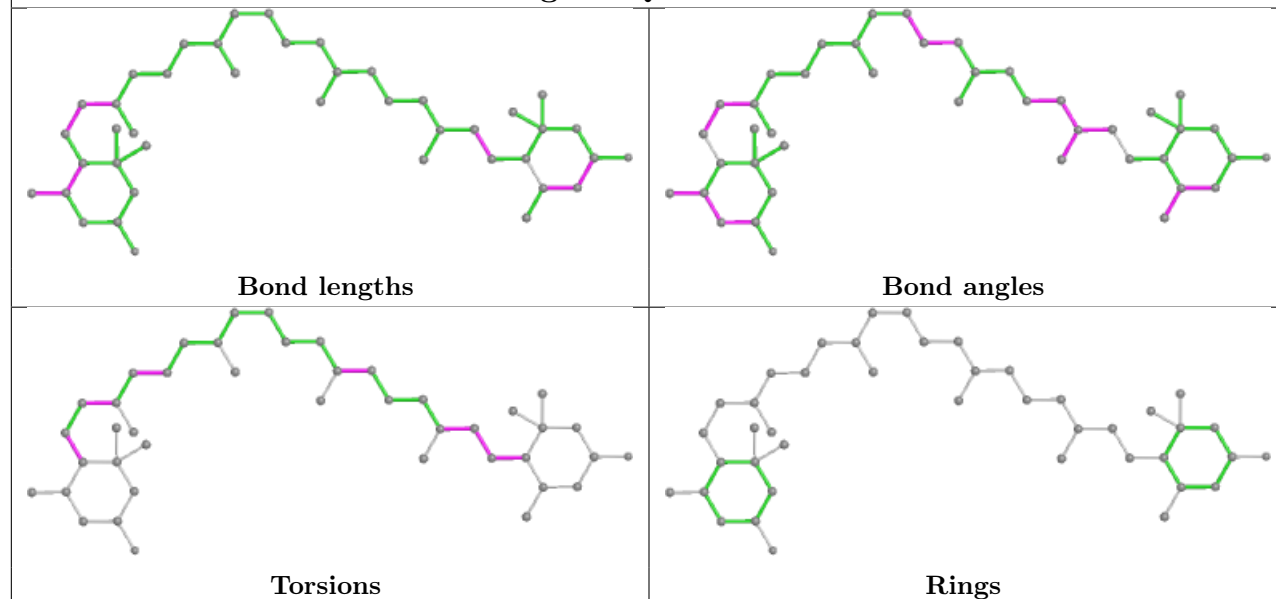
## Ligand CHL W 314

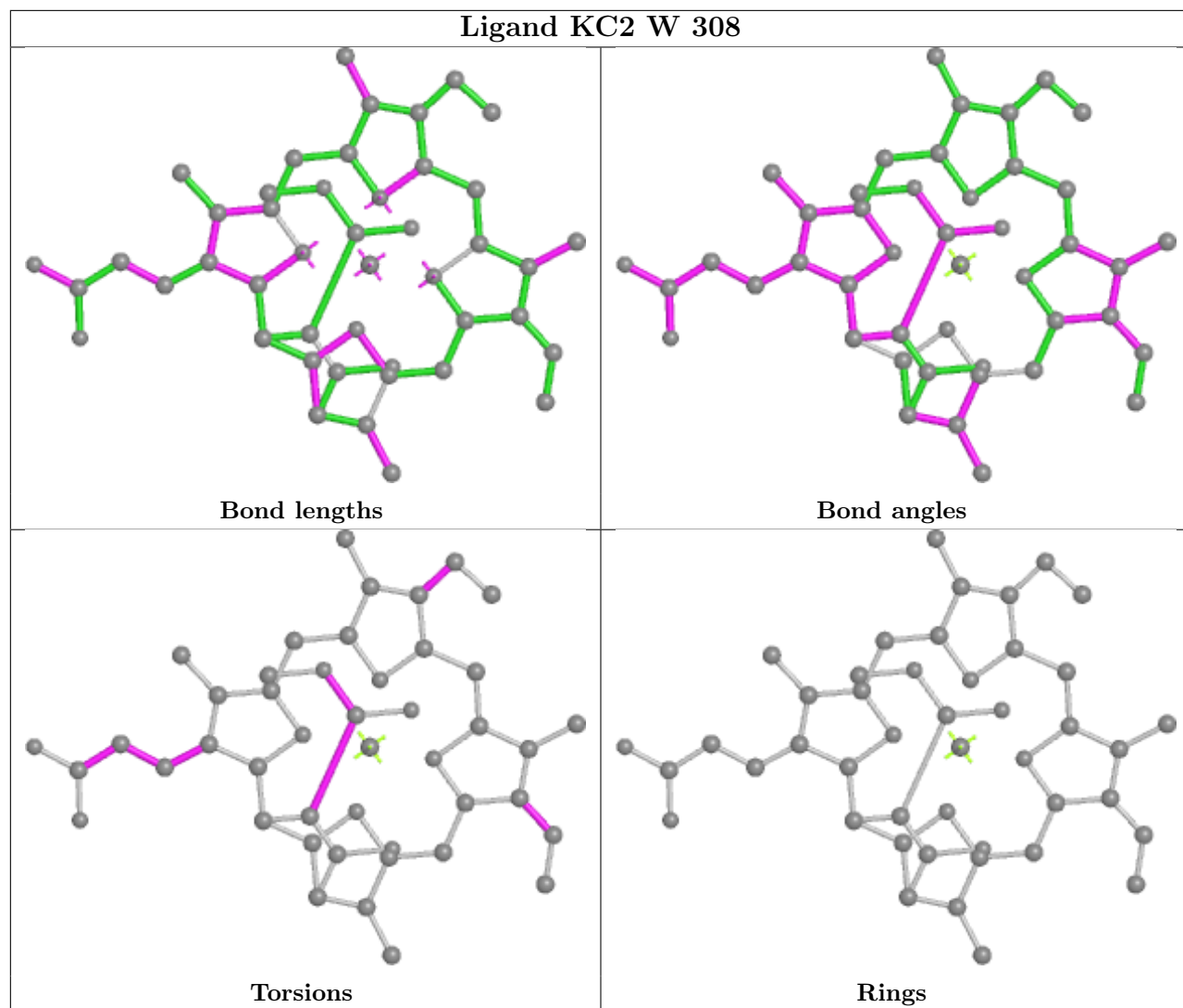


## Ligand CLA 2 611

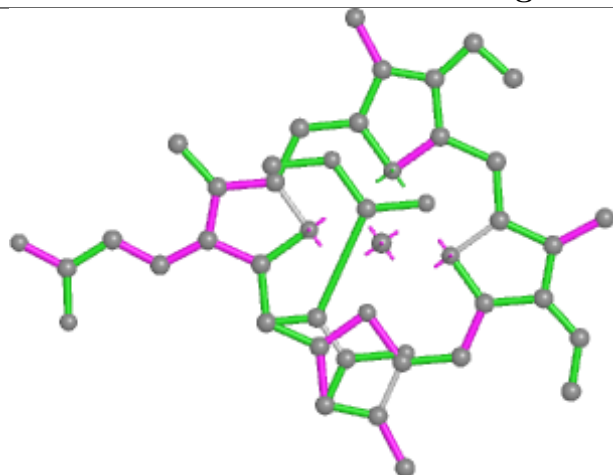


## Ligand Q6L 2 616

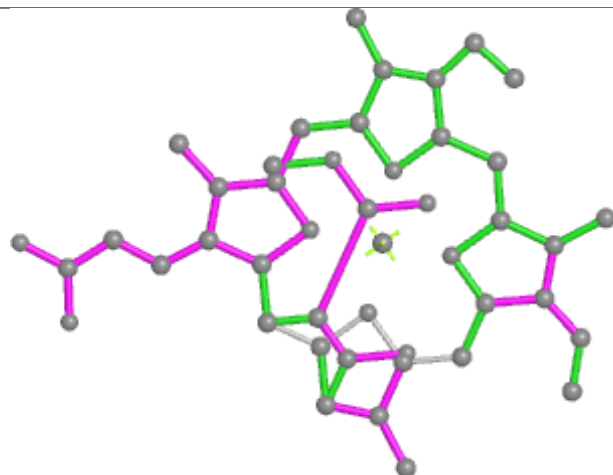




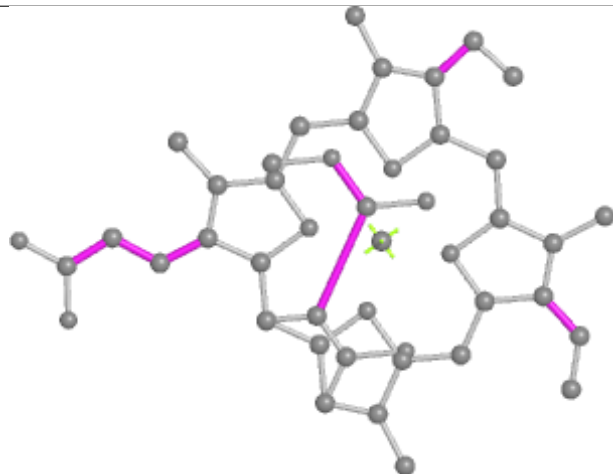
## Ligand KC2 V 308



Bond lengths



Bond angles

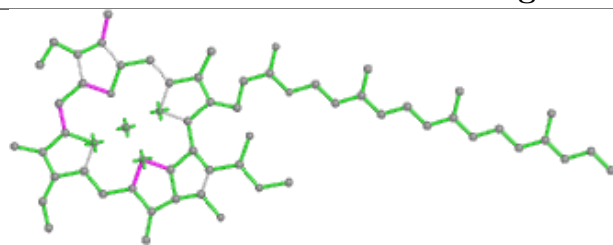


Torsions

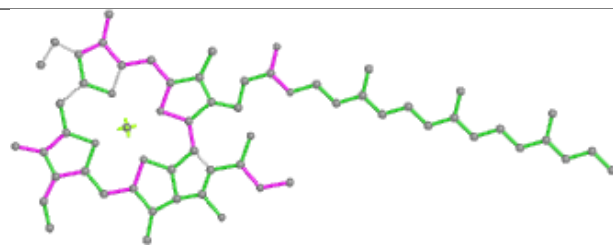


Rings

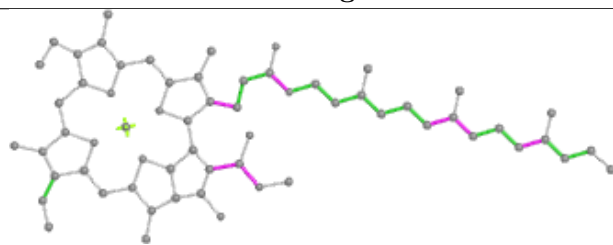
## Ligand CLA 6 602



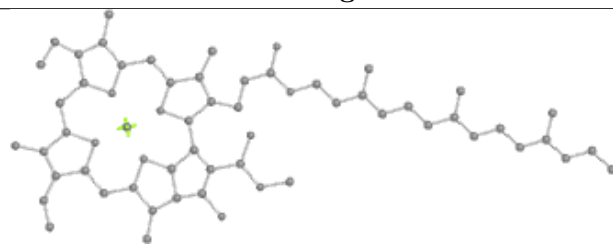
Bond lengths



Bond angles

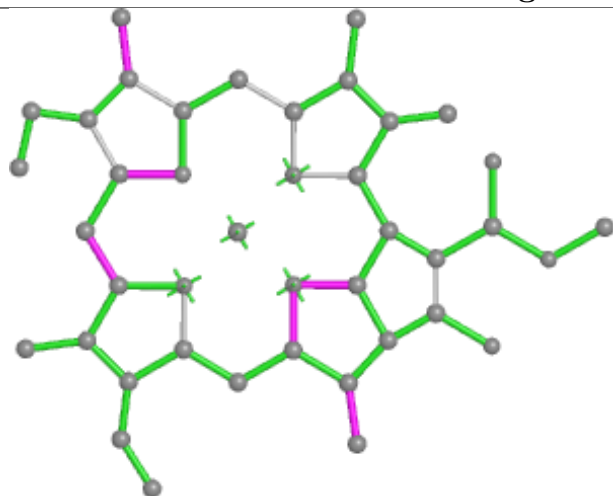


Torsions

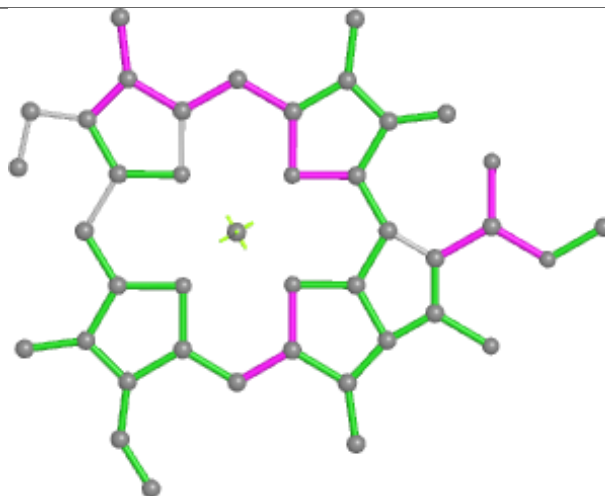


Rings

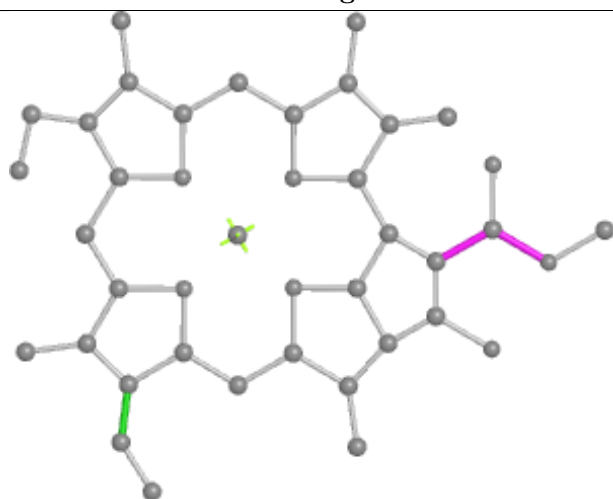
## Ligand CLA 5 610



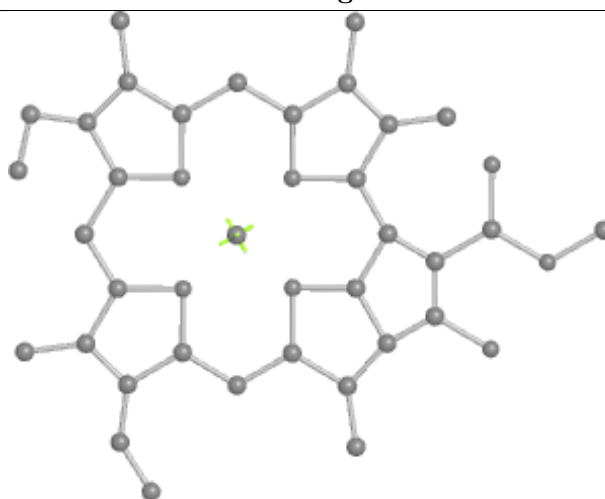
Bond lengths



Bond angles

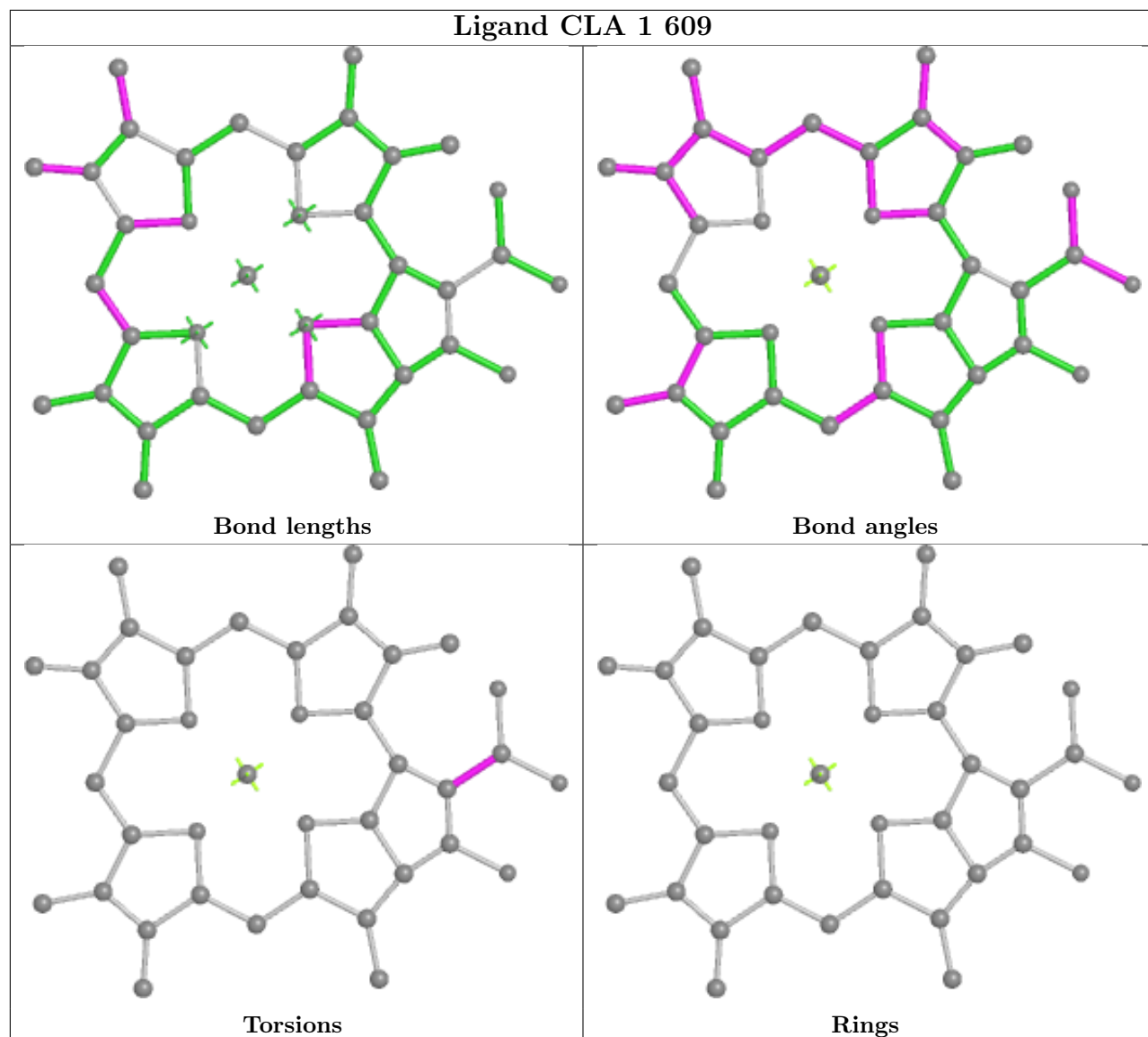


Torsions



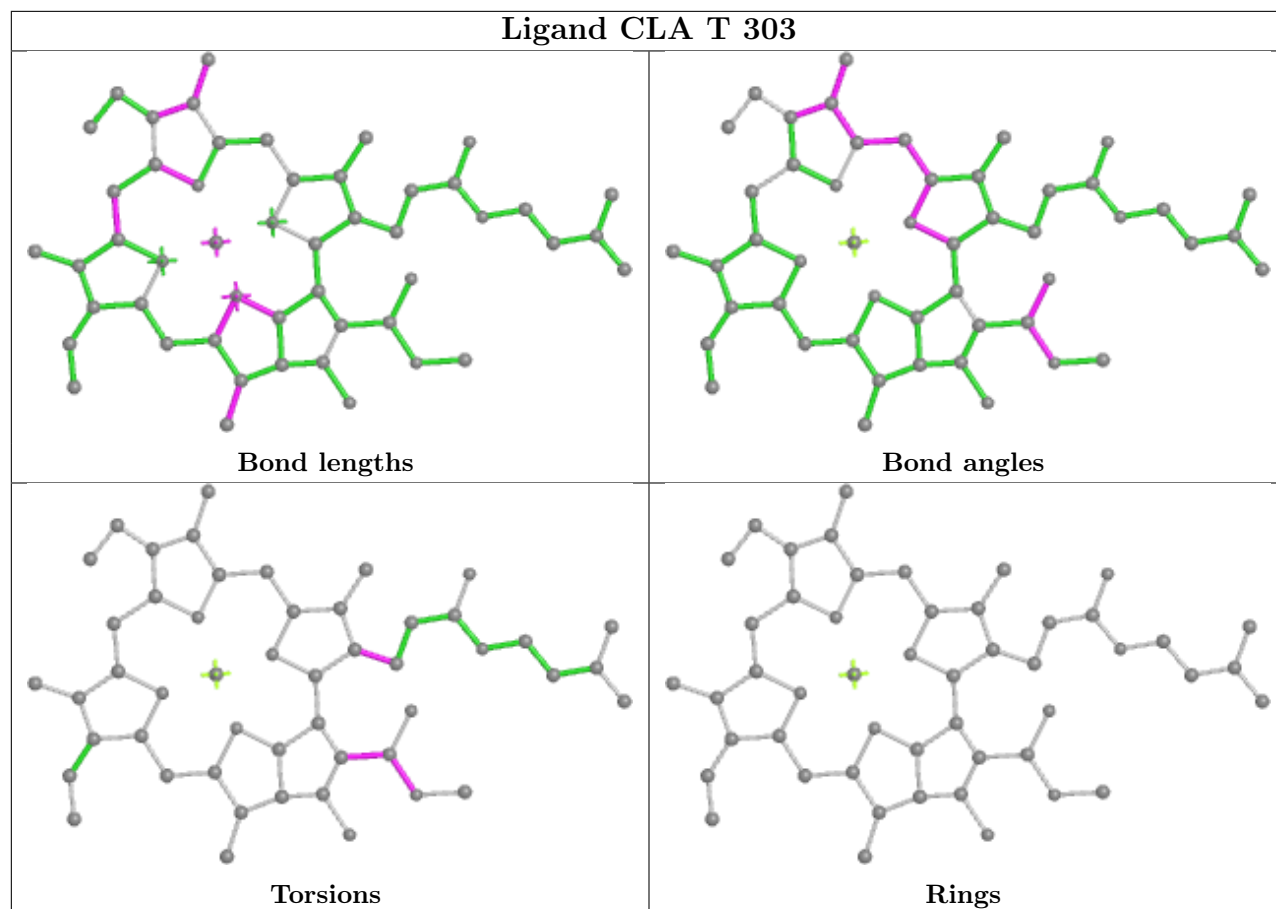
Rings

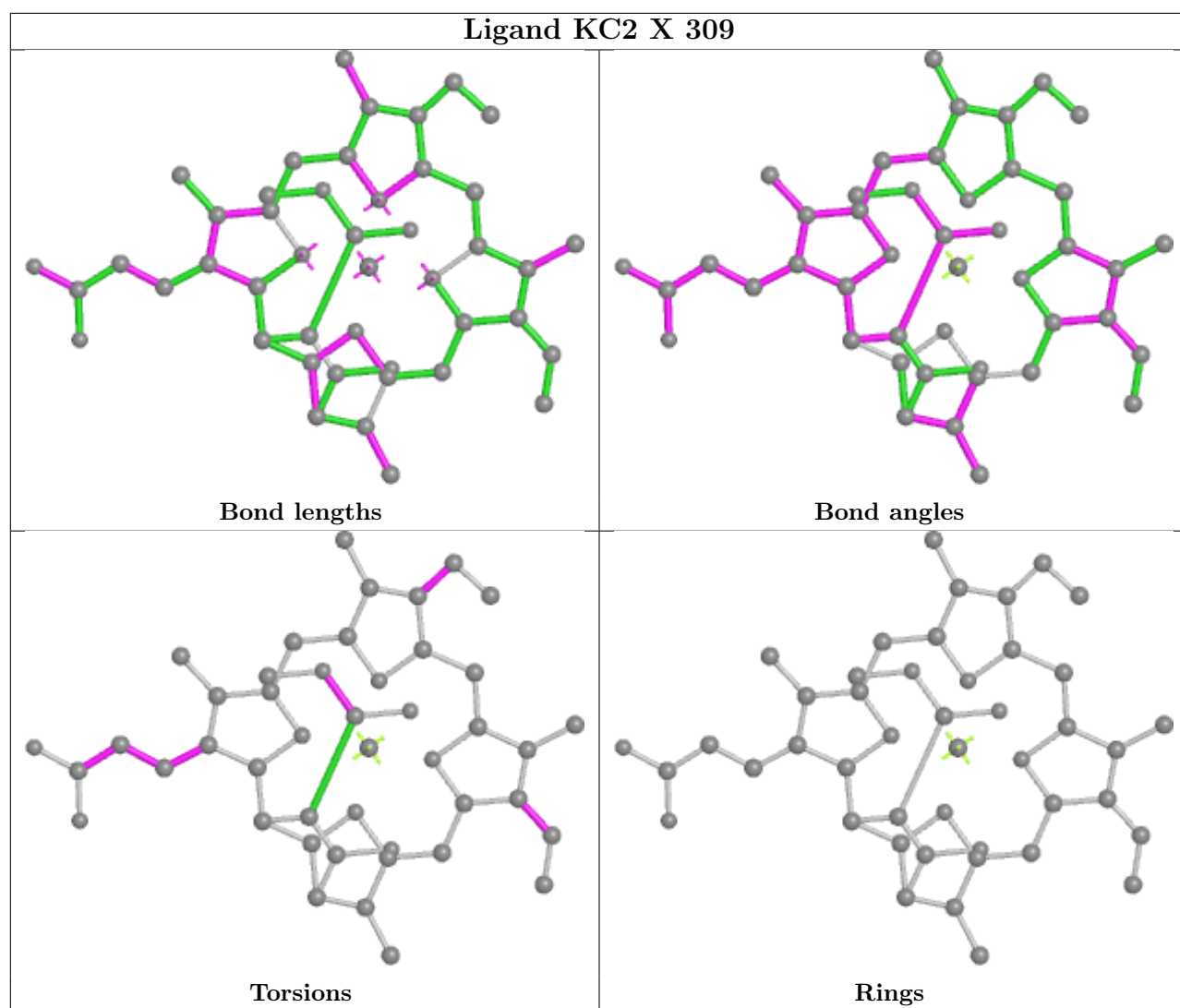
## Ligand CLA 1 609

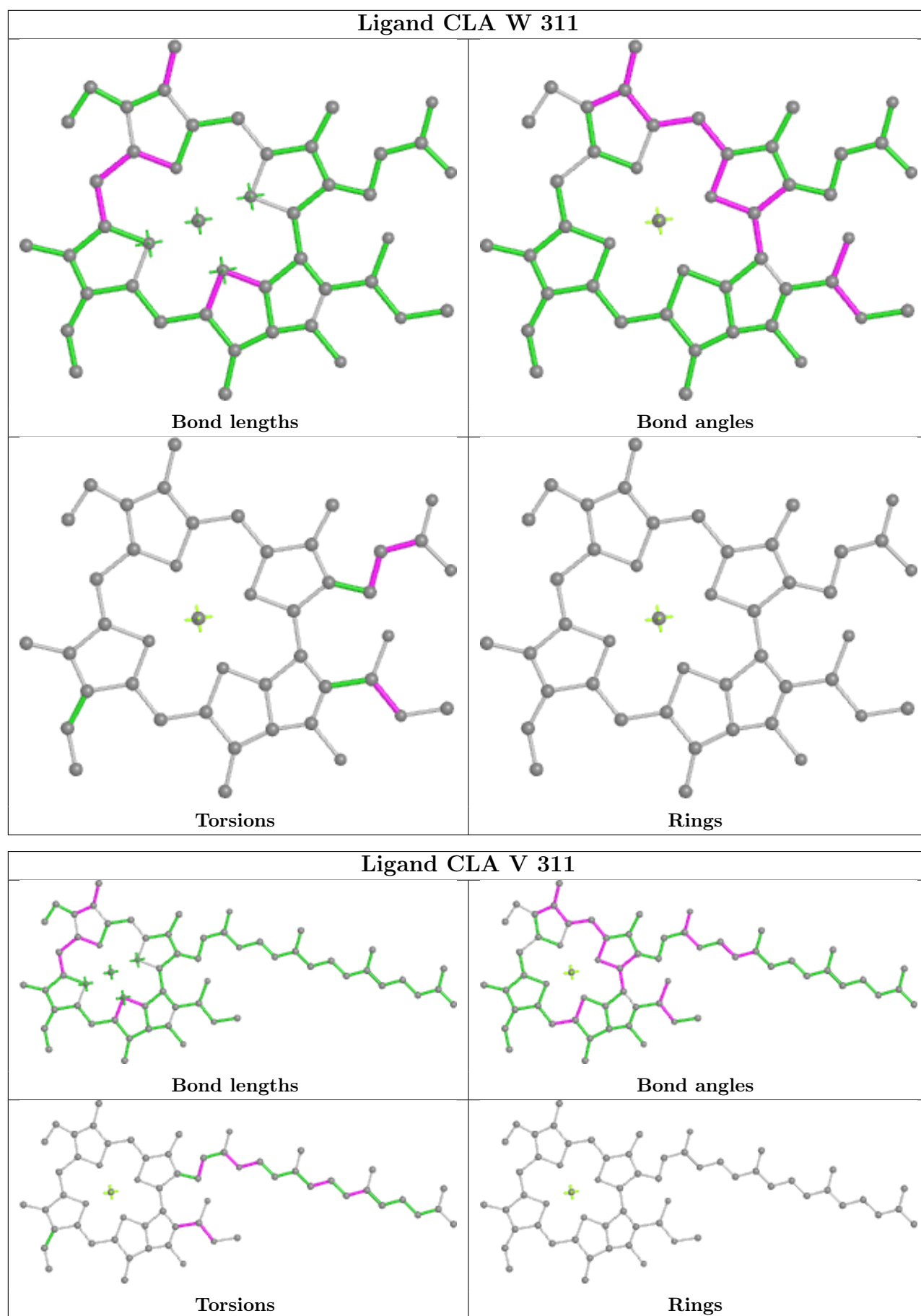




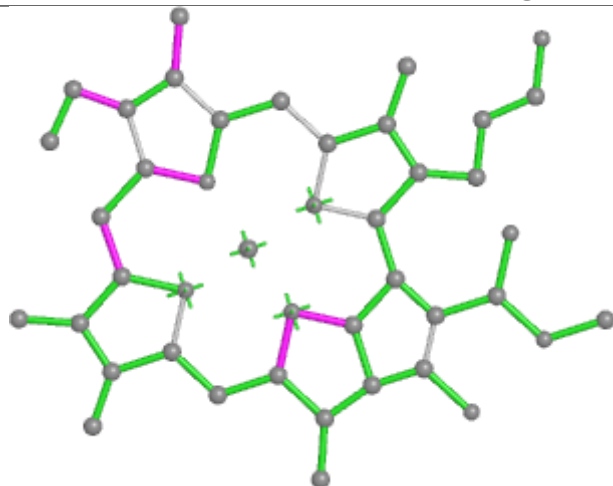
## Ligand CLA T 303



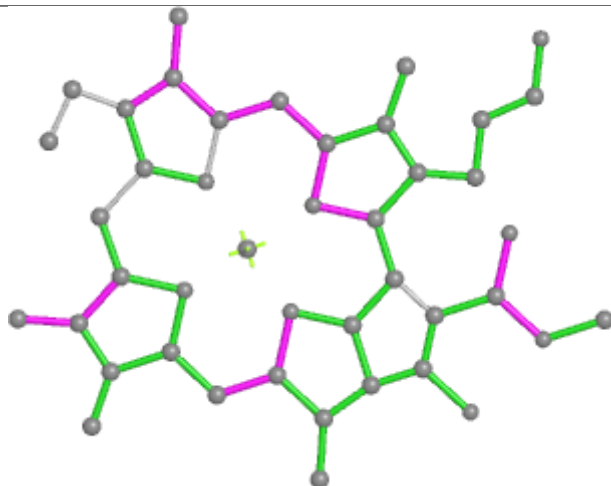




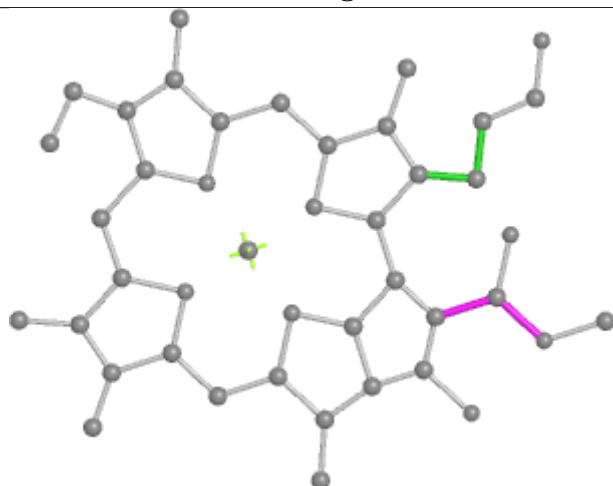
## Ligand CLA 2 604



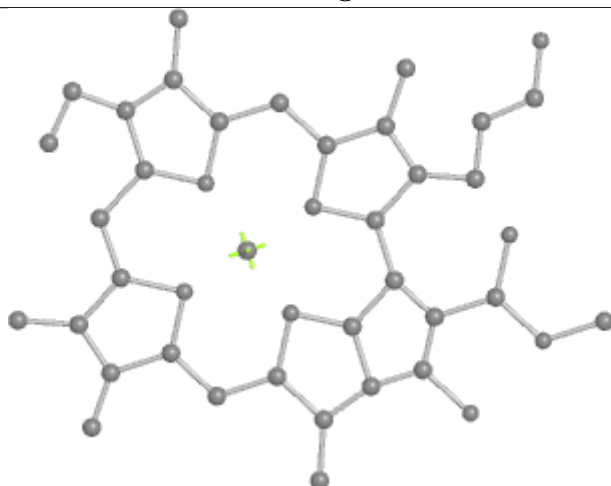
Bond lengths



Bond angles

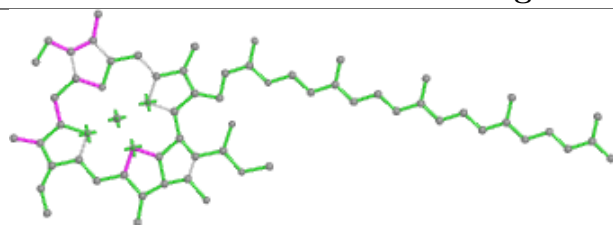


Torsions

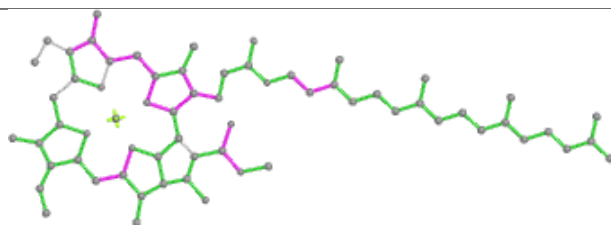


Rings

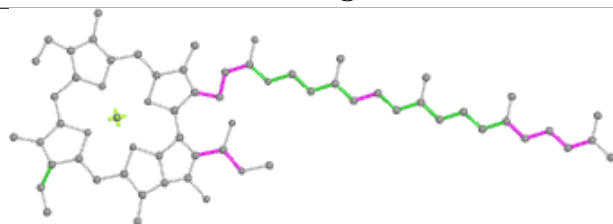
## Ligand CLA B 843



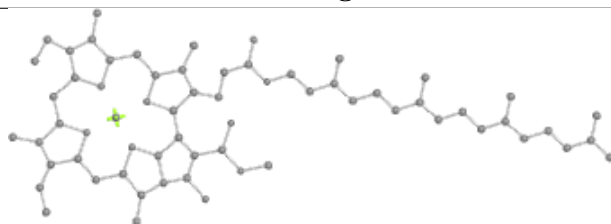
Bond lengths



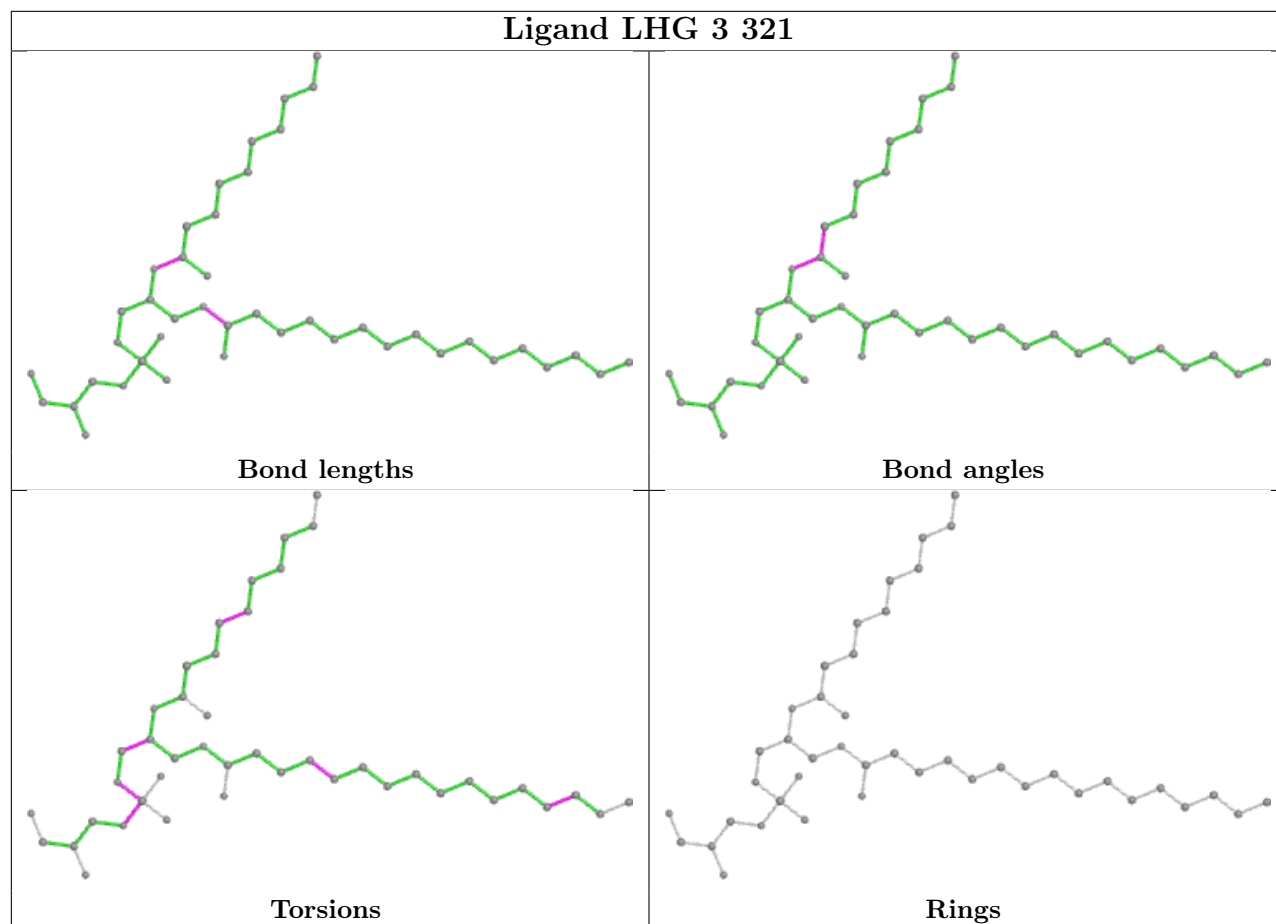
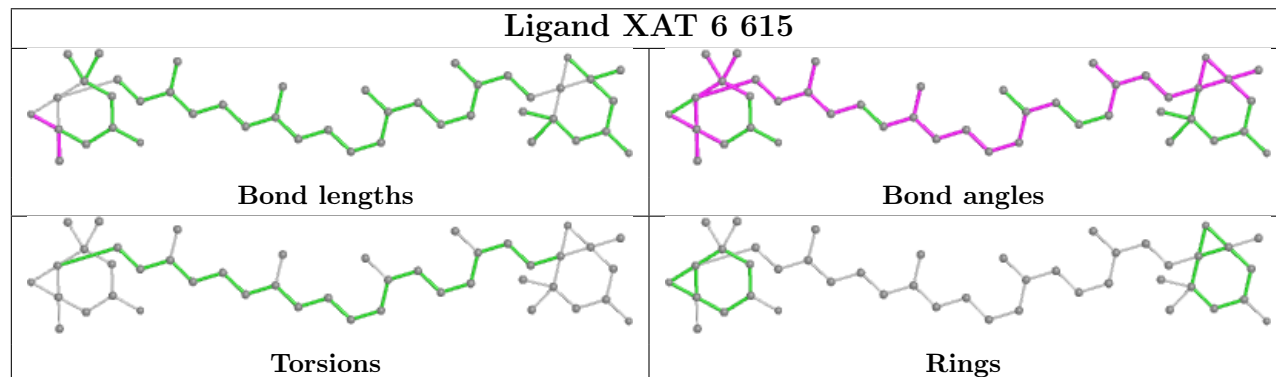
Bond angles

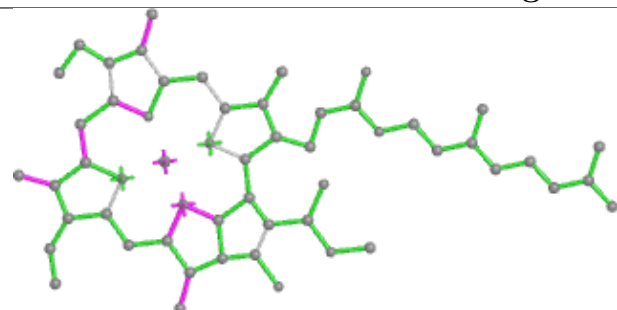


Torsions

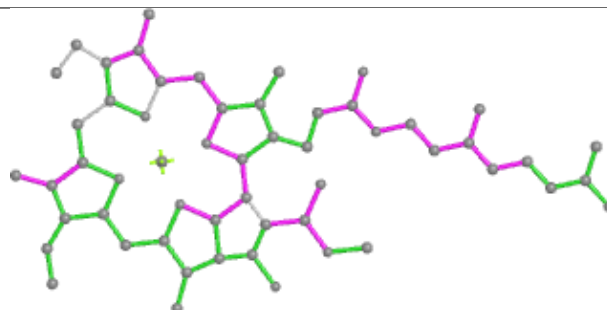


Rings

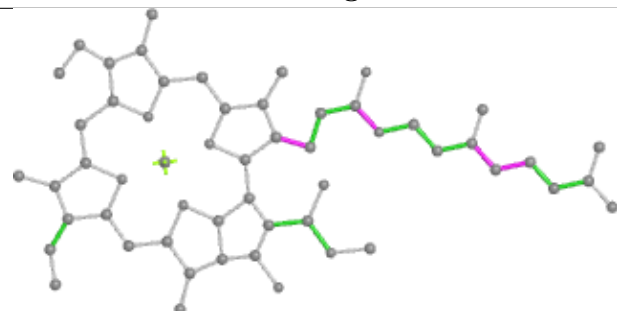
**Ligand LHG 3 321****Ligand XAT 6 615**

**Ligand CLA 3 302**

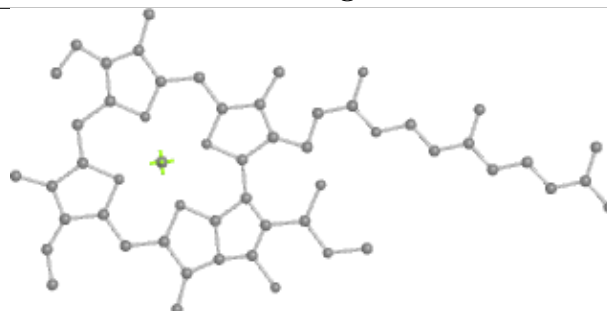
Bond lengths



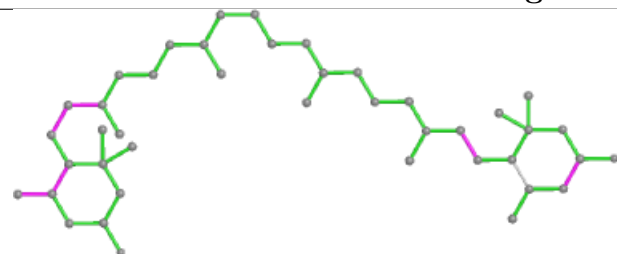
Bond angles



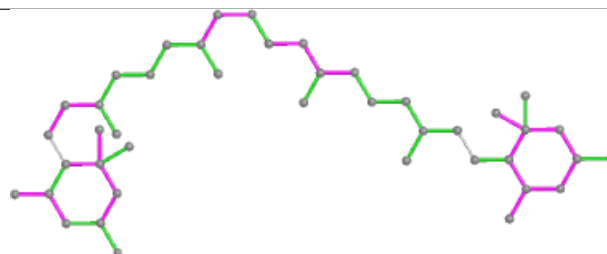
Torsions



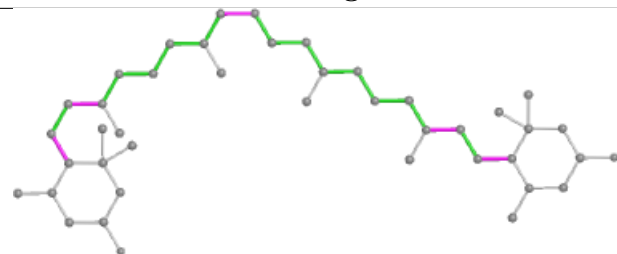
Rings

**Ligand Q6L S 323**

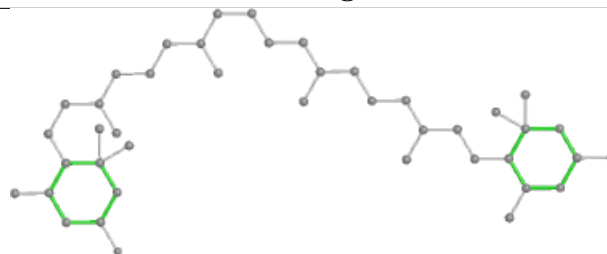
Bond lengths



Bond angles

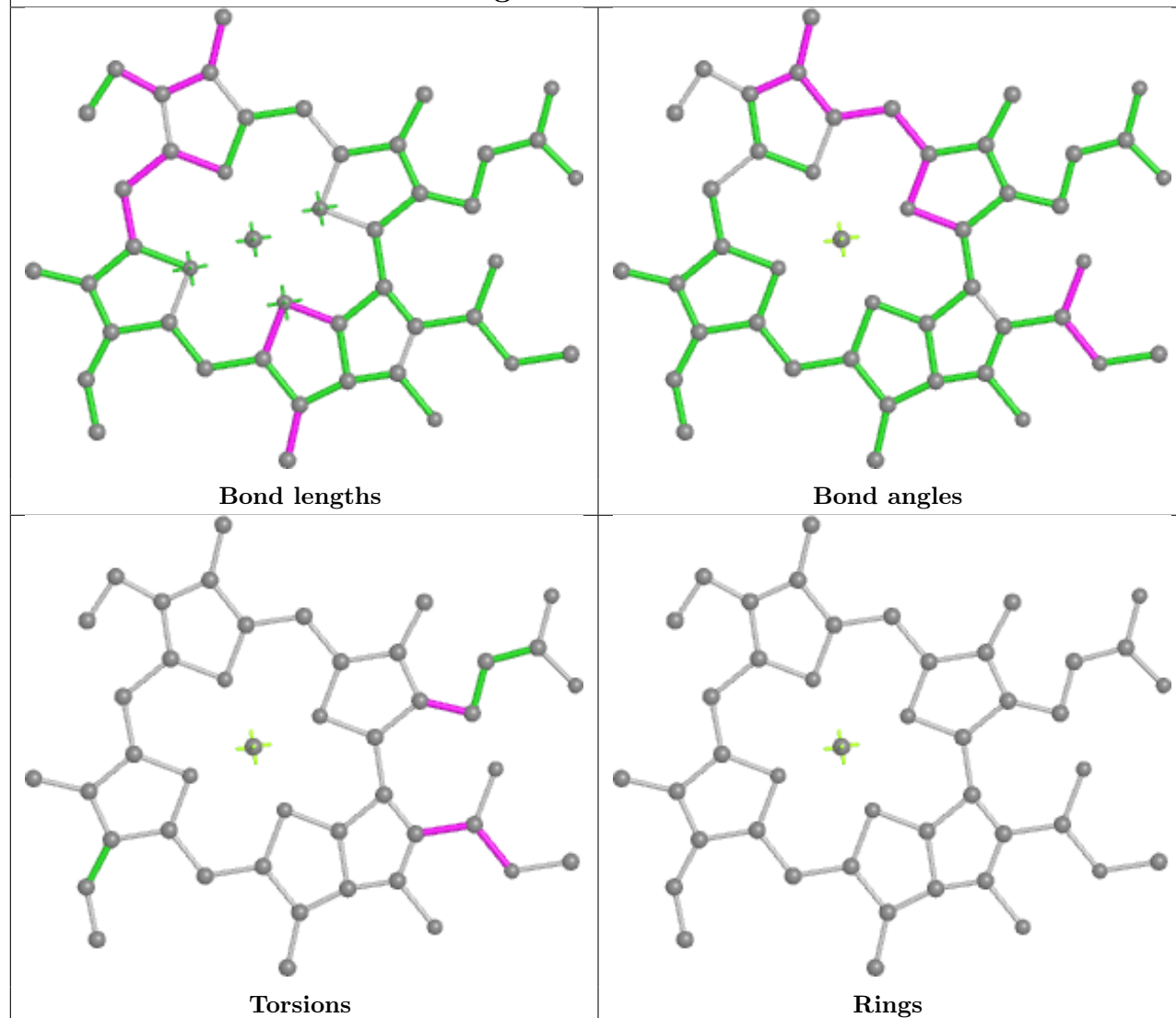


Torsions

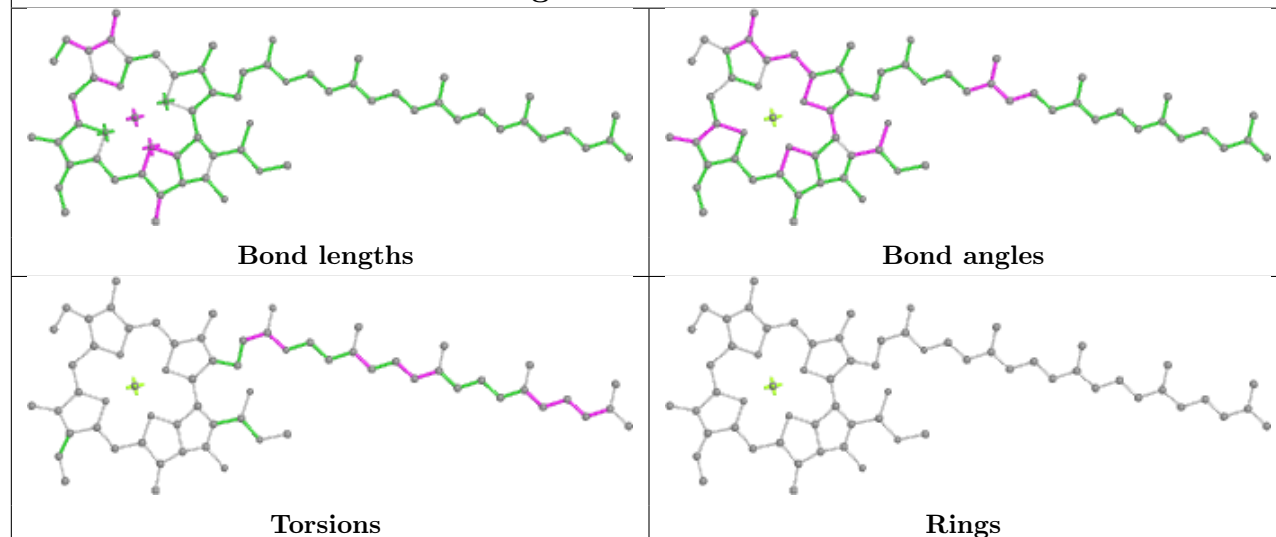


Rings

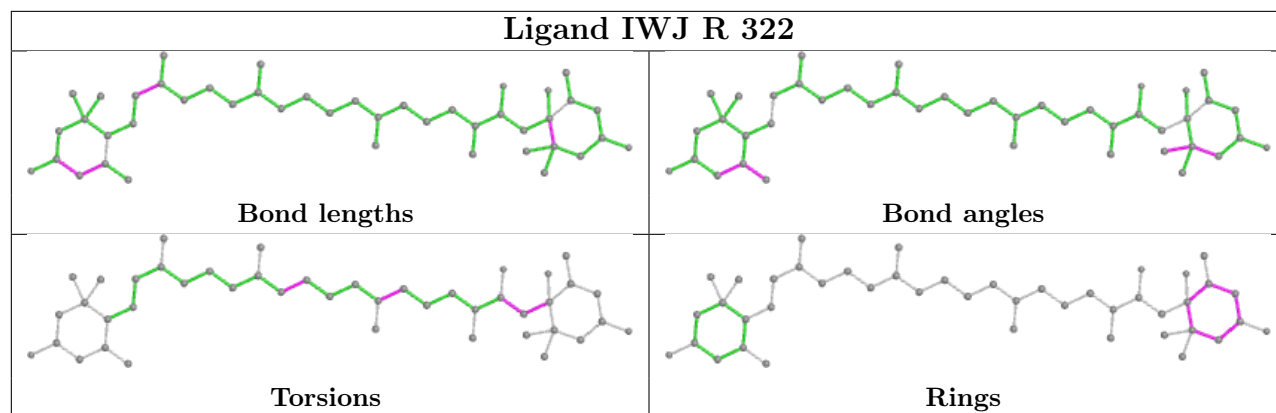
## Ligand CLA 6 612



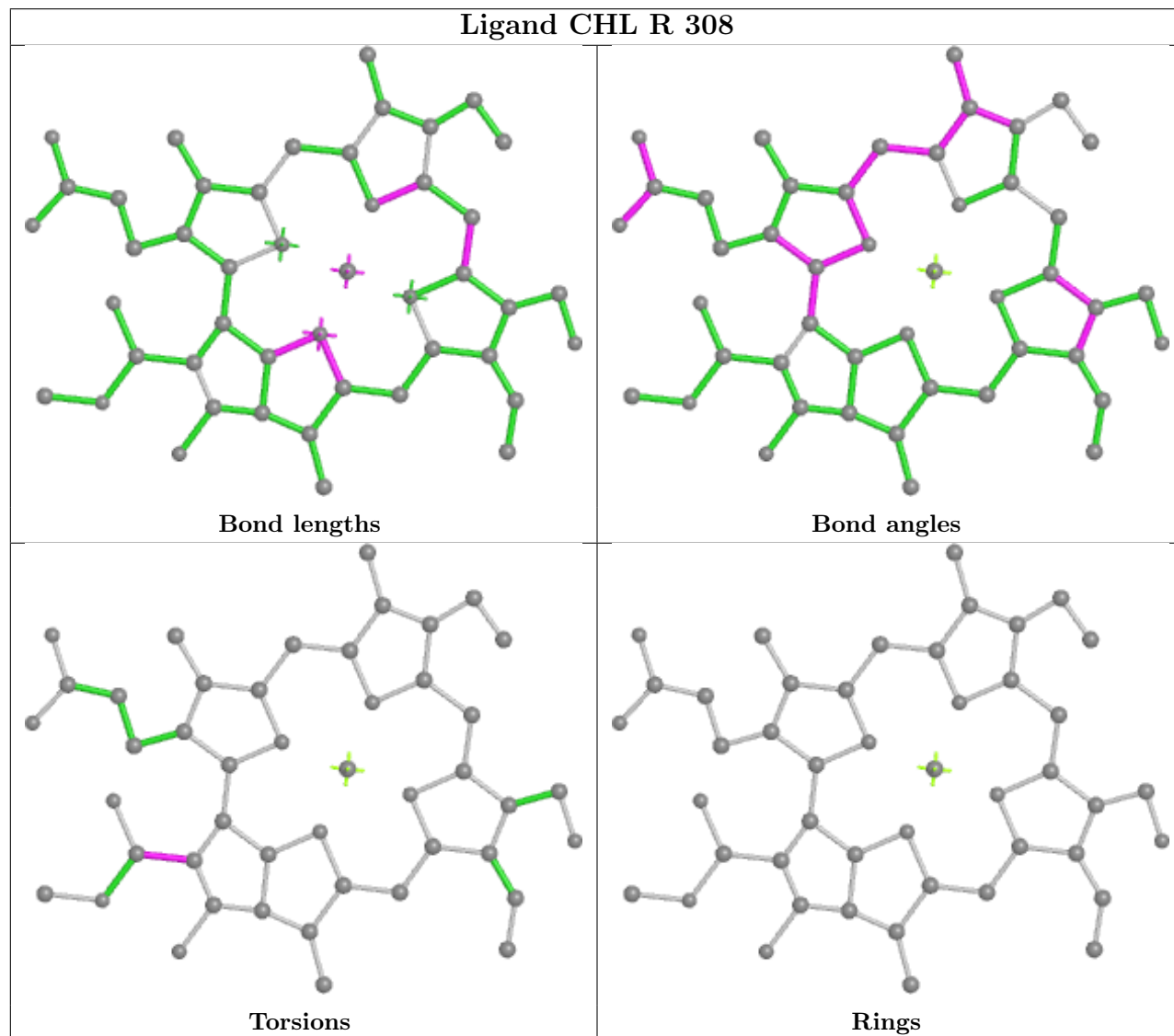
## Ligand CLA A 831



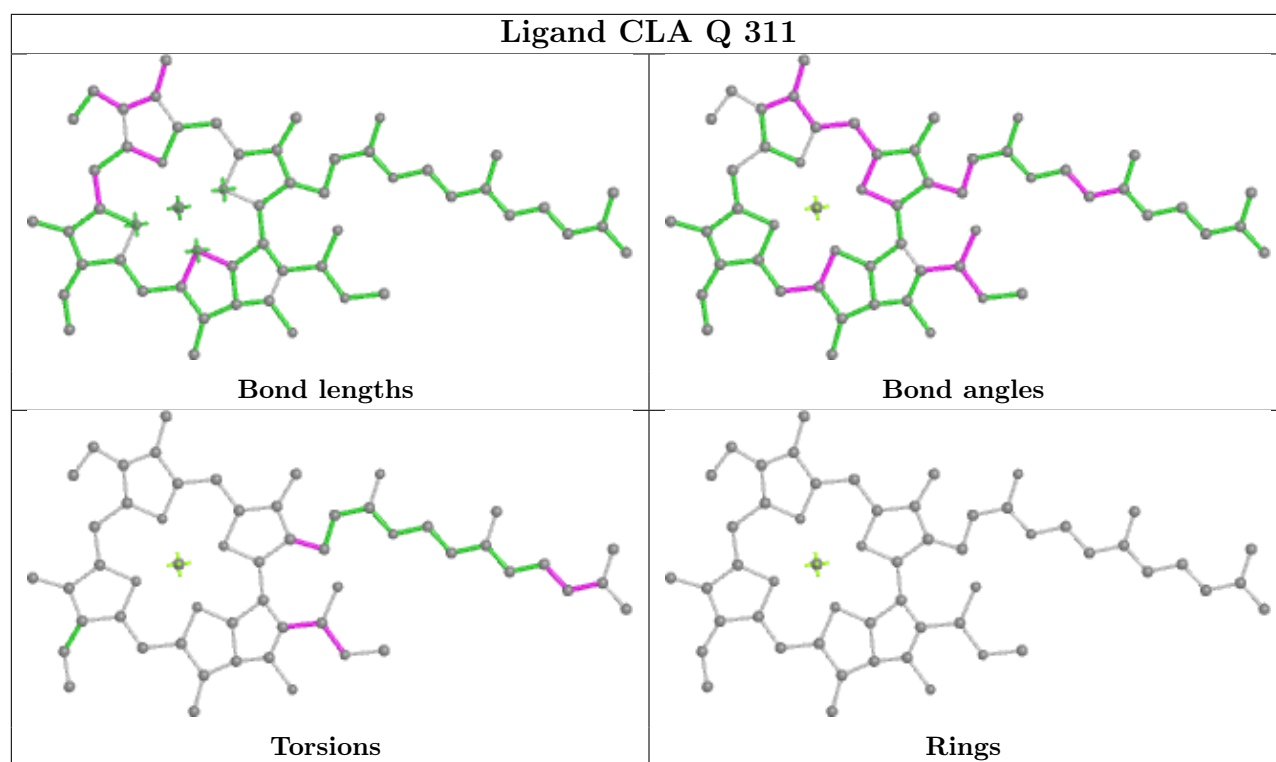
## Ligand IWJ R 322



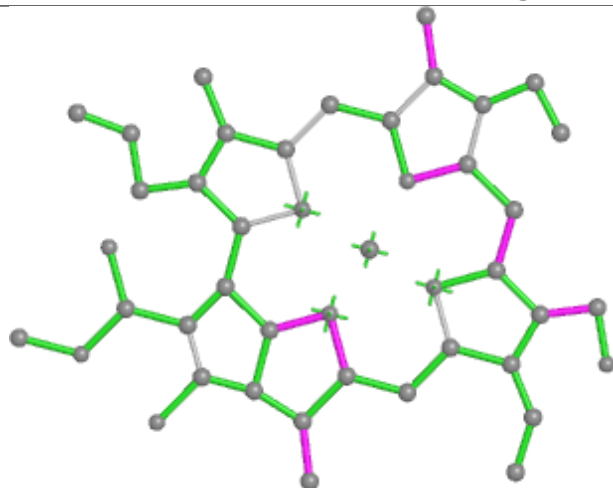
## Ligand CHL R 308



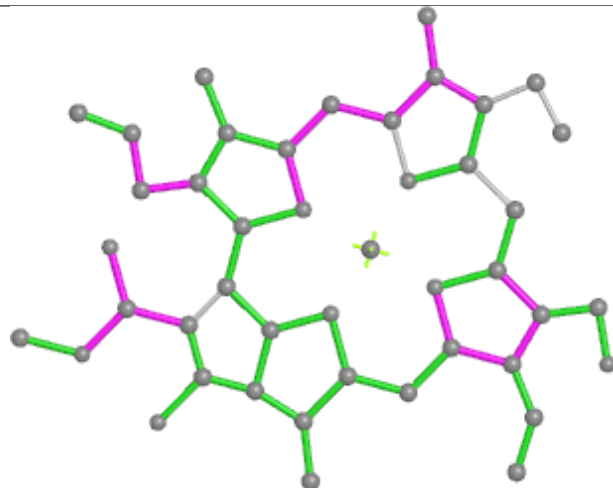




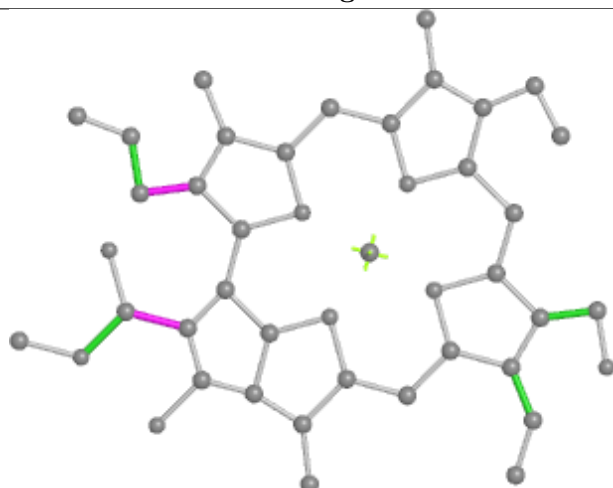
## Ligand CHL P 307



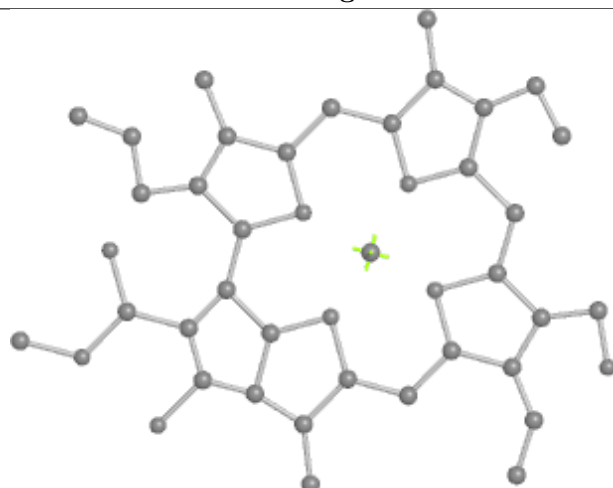
Bond lengths



Bond angles

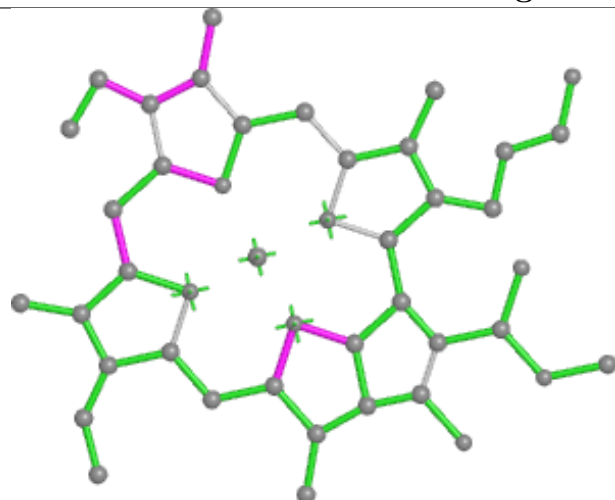


Torsions

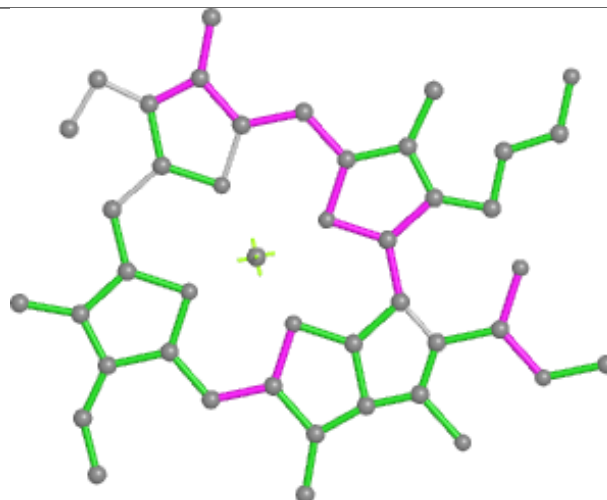


Rings

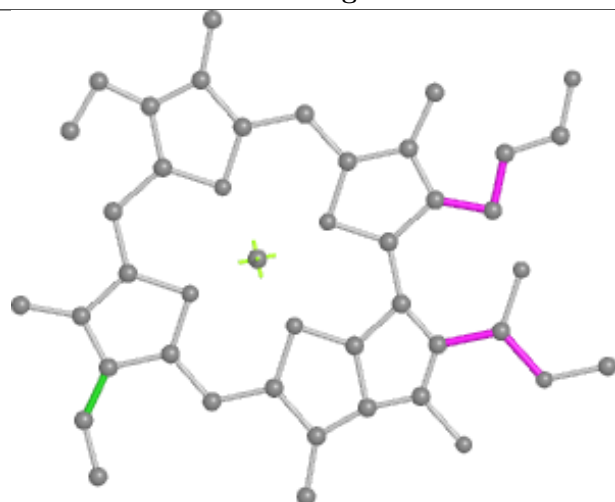
## Ligand CLA H 301



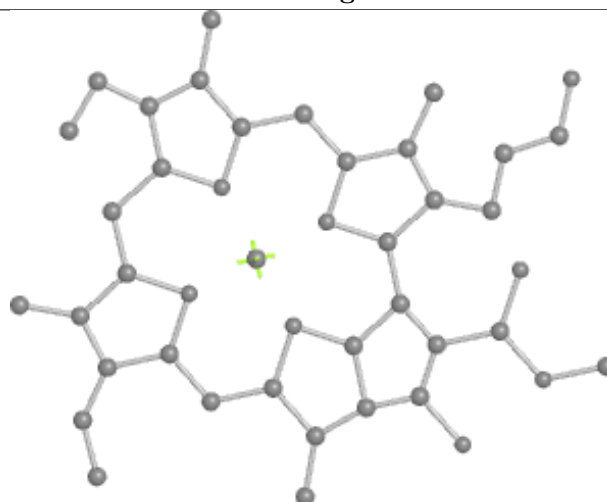
Bond lengths



Bond angles

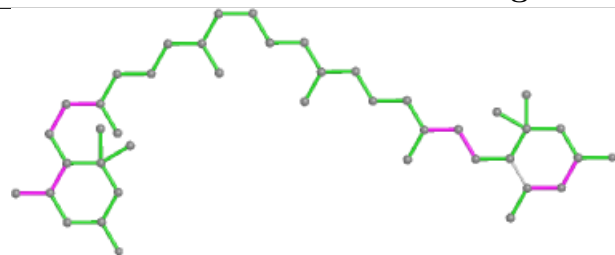


Torsions

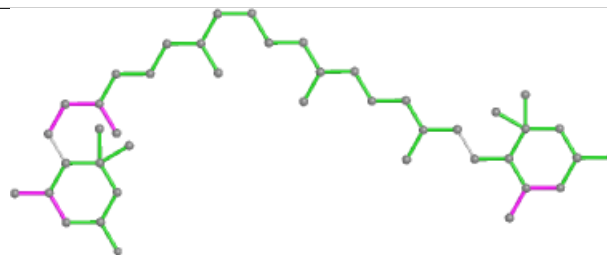


Rings

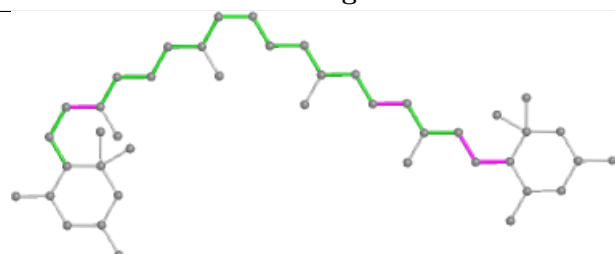
## Ligand Q6L O 2007



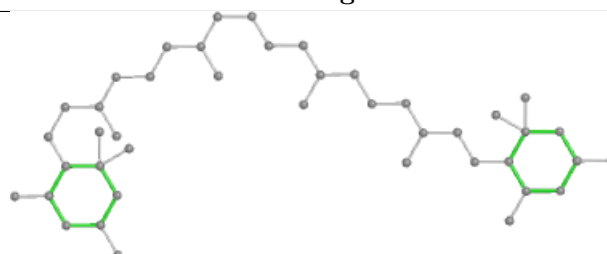
Bond lengths



Bond angles

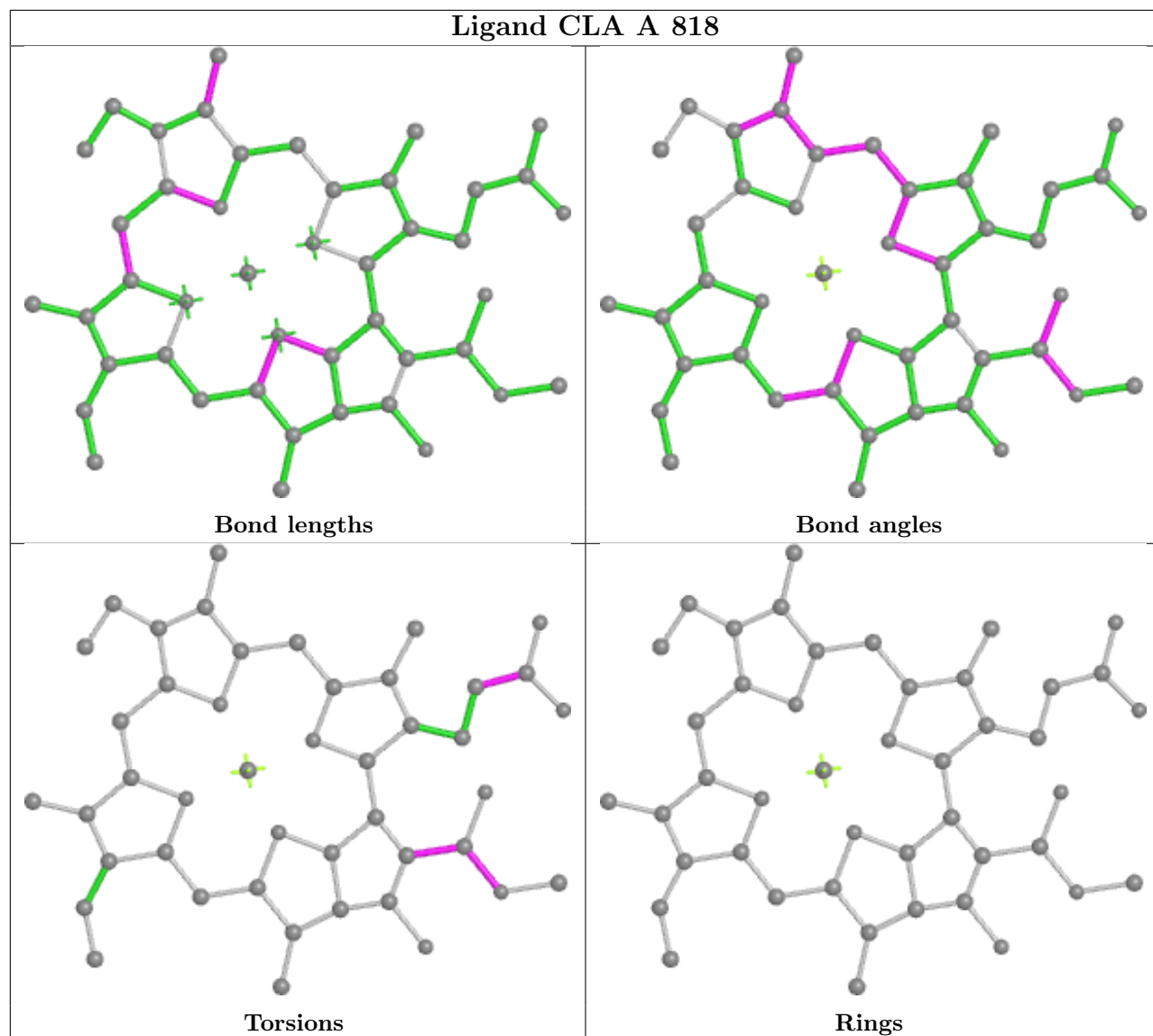


Torsions

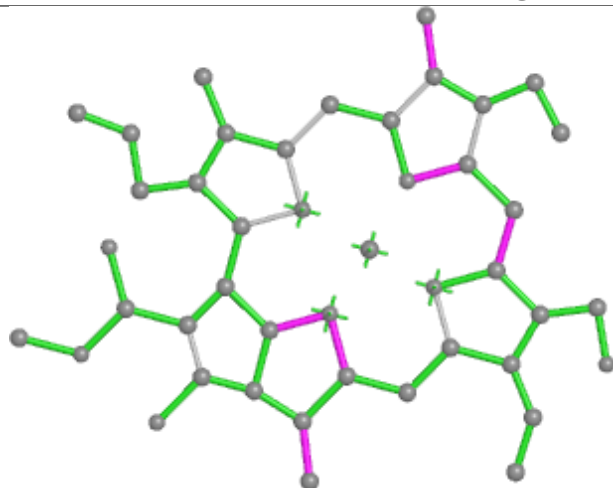


Rings

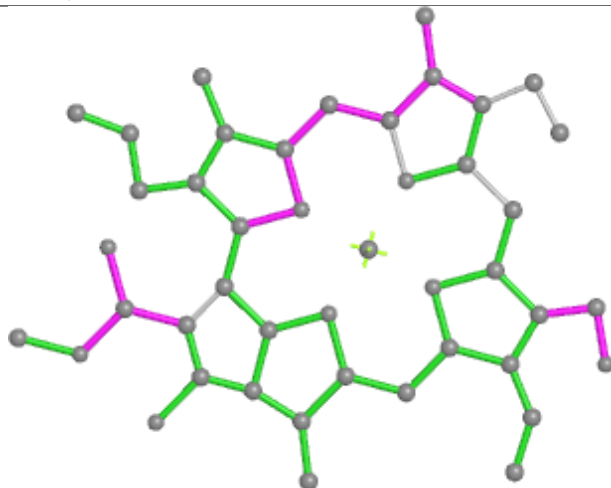
## Ligand CLA A 818



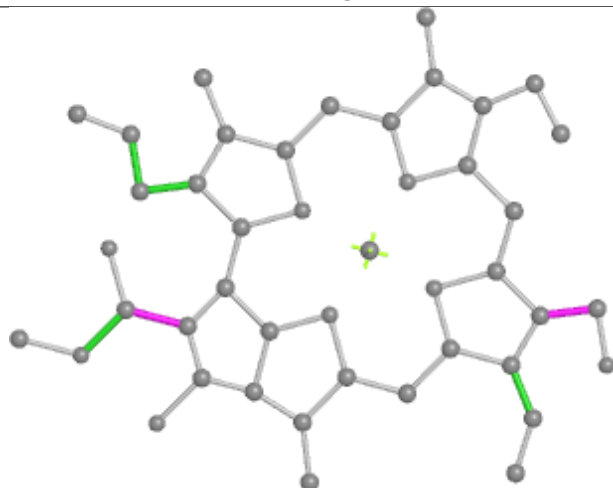
## Ligand CHL Q 309



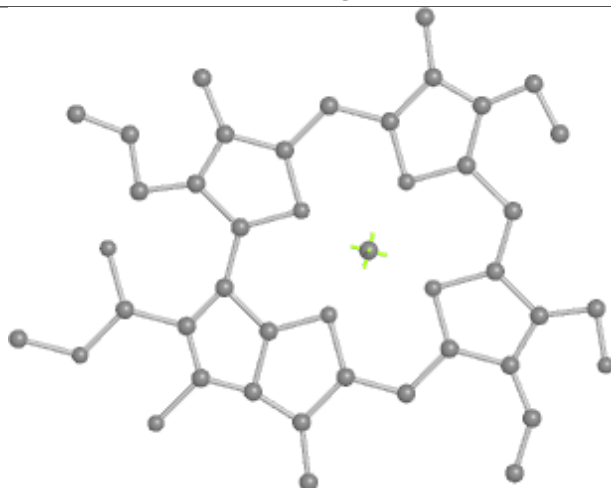
Bond lengths



Bond angles

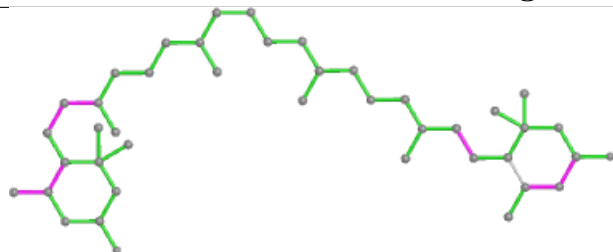


Torsions

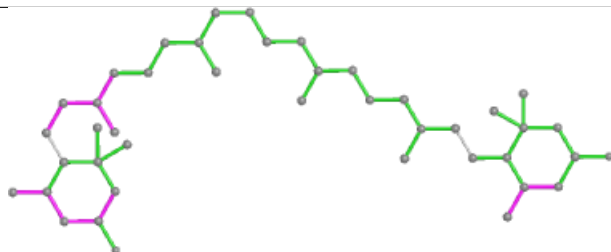


Rings

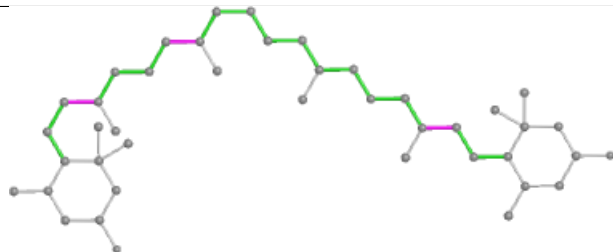
## Ligand Q6L T 315



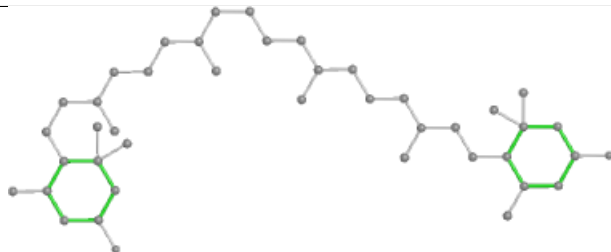
Bond lengths



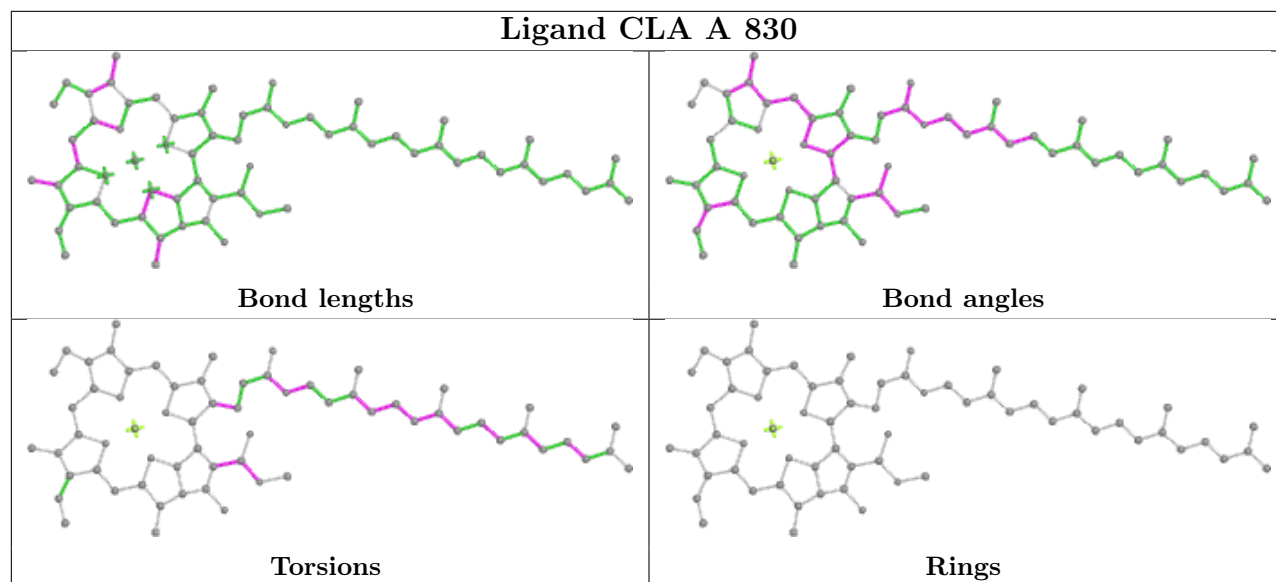
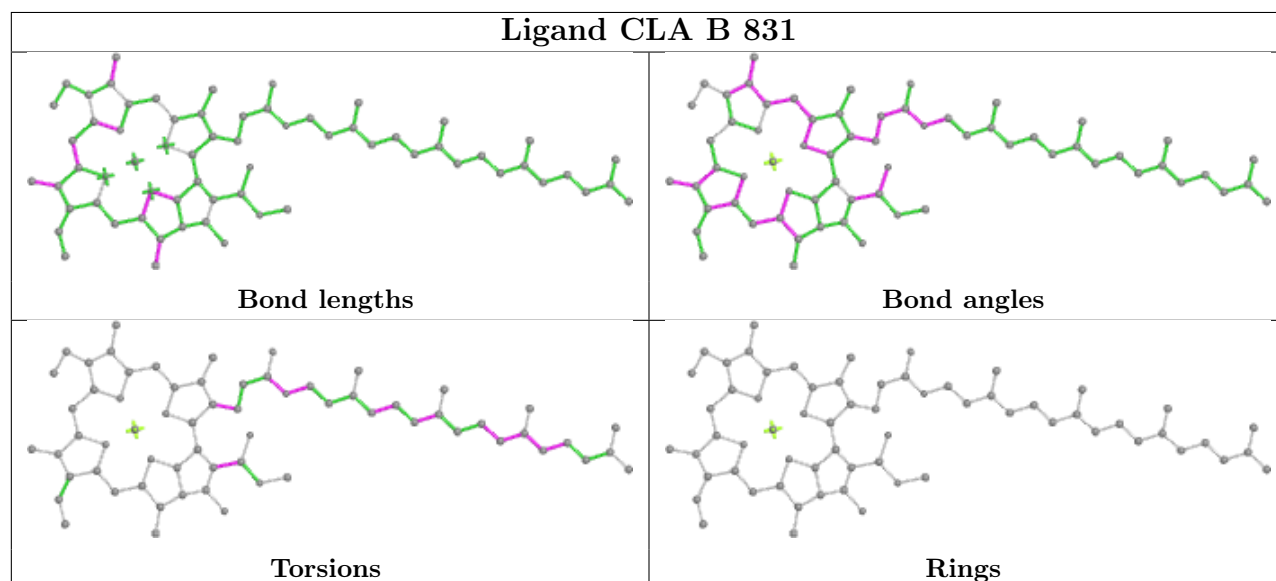
Bond angles



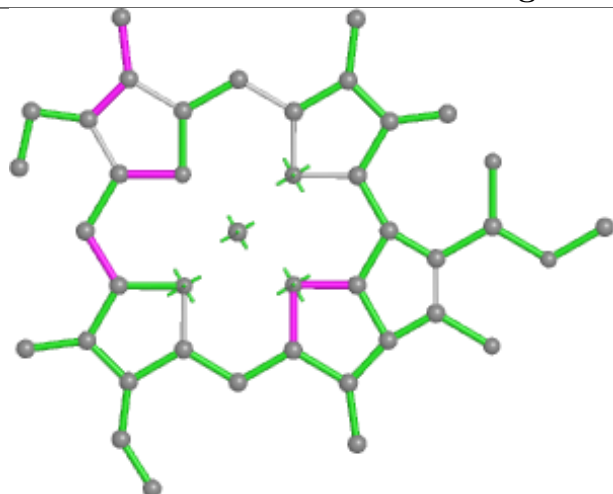
Torsions



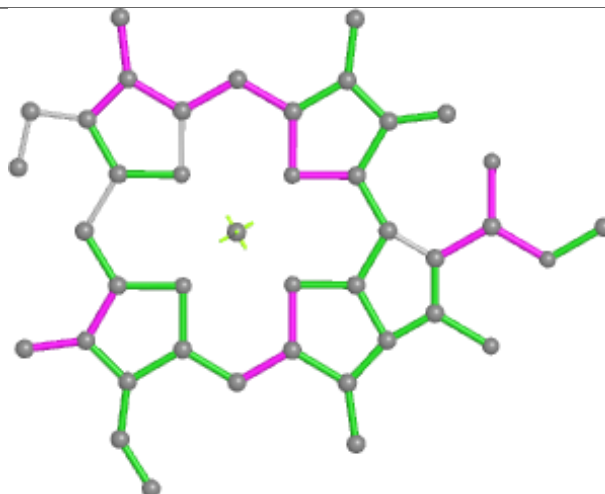
Rings

**Ligand CLA A 830****Ligand CLA B 831**

## Ligand CLA 4 314



Bond lengths



Bond angles

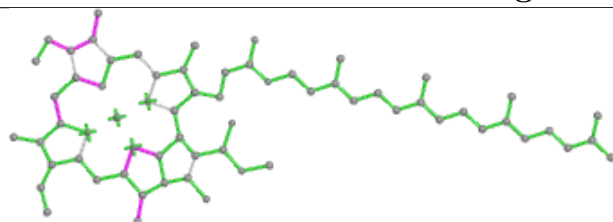


Torsions

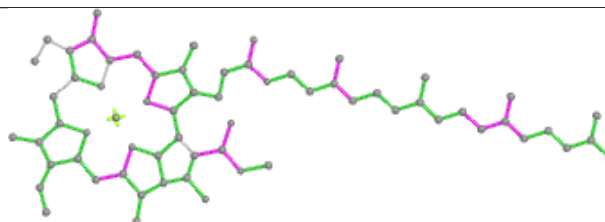


Rings

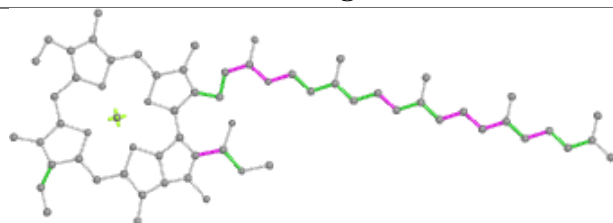
## Ligand CLA P 302



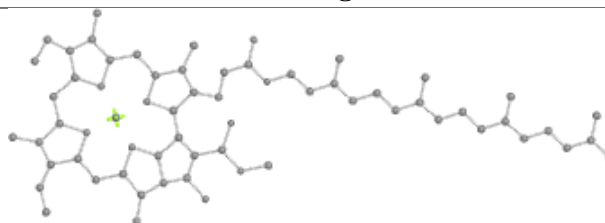
Bond lengths



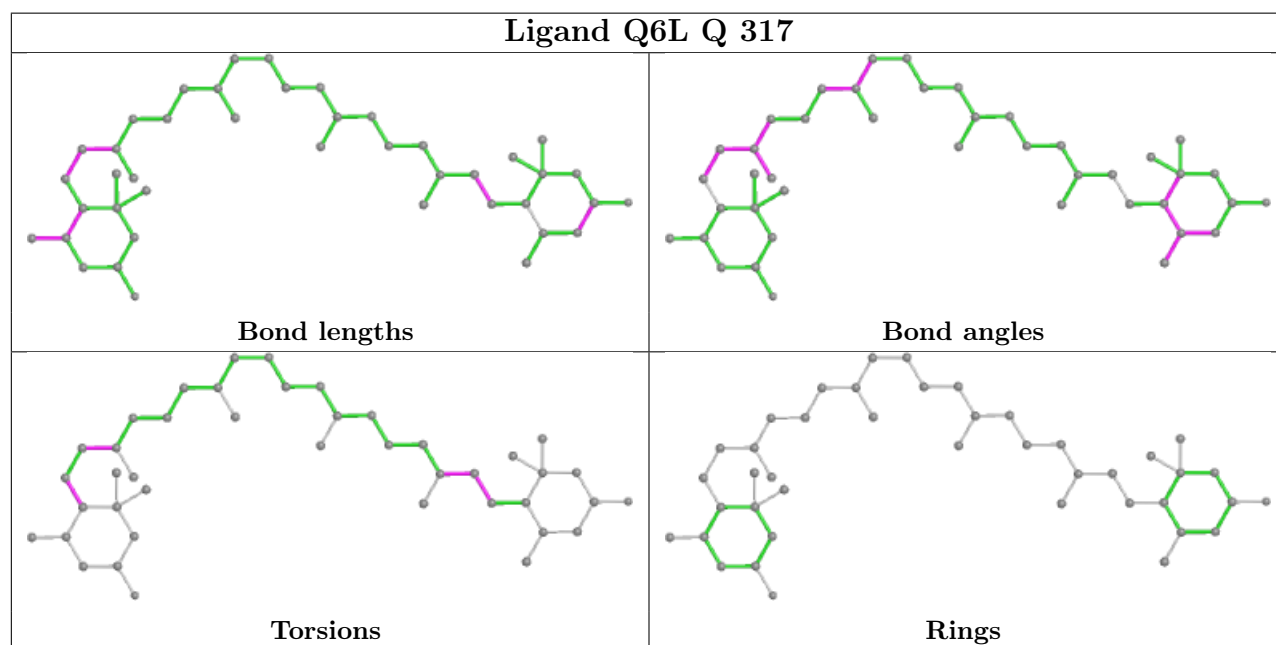
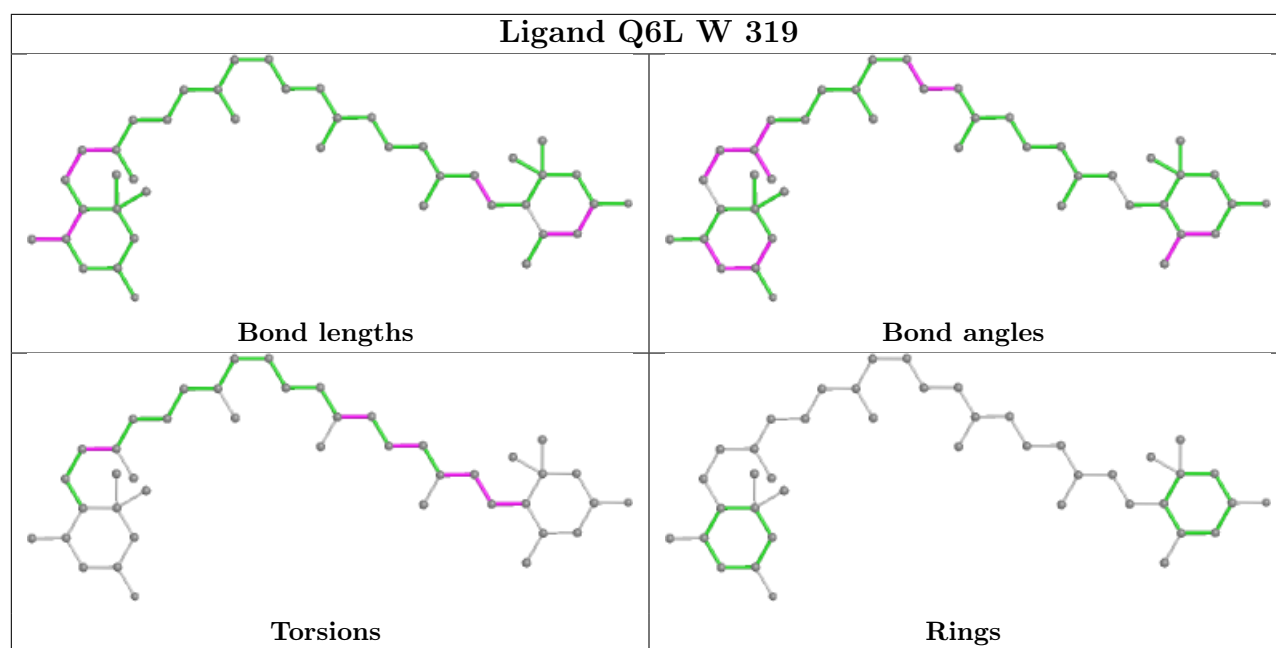
Bond angles



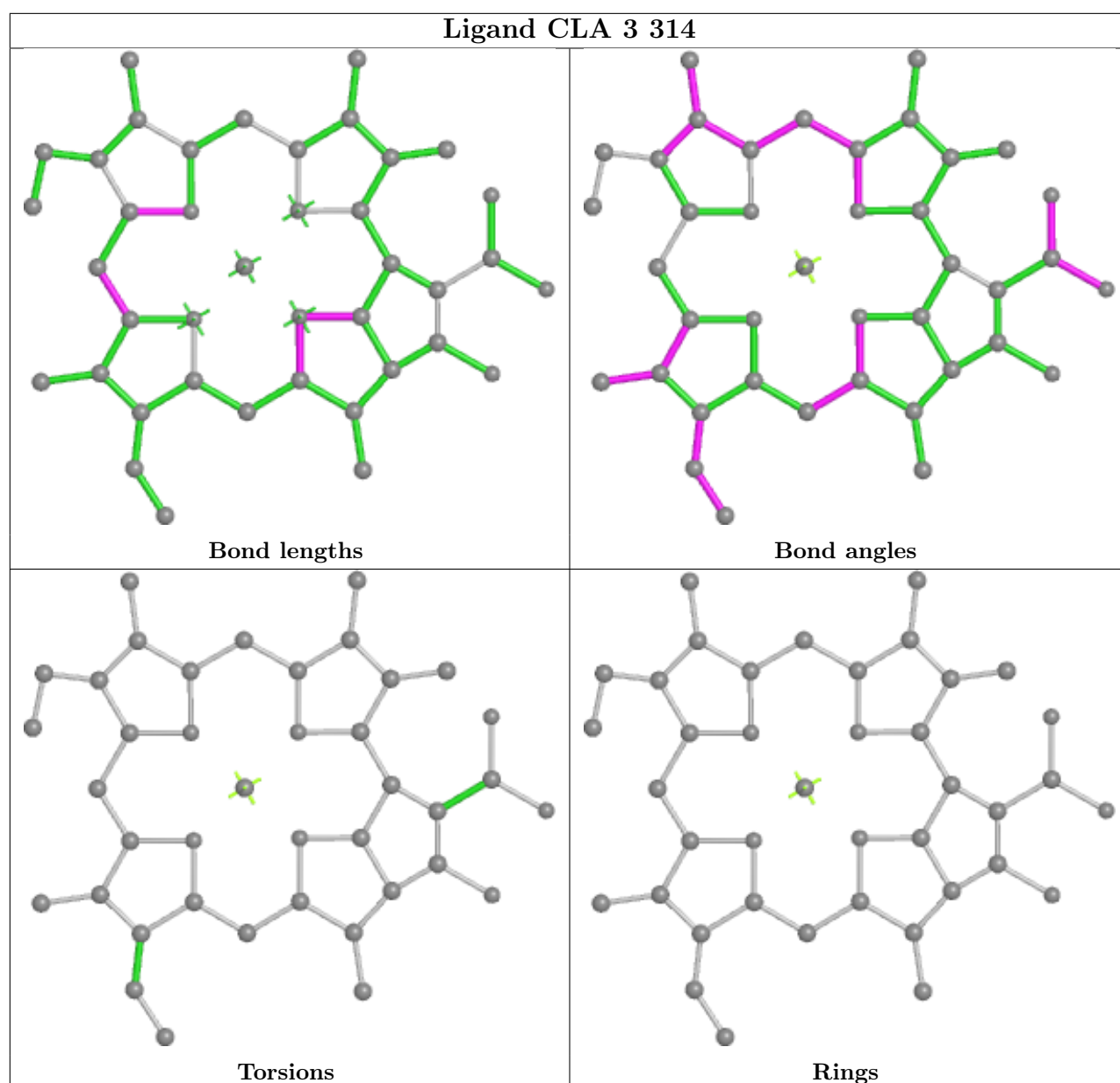
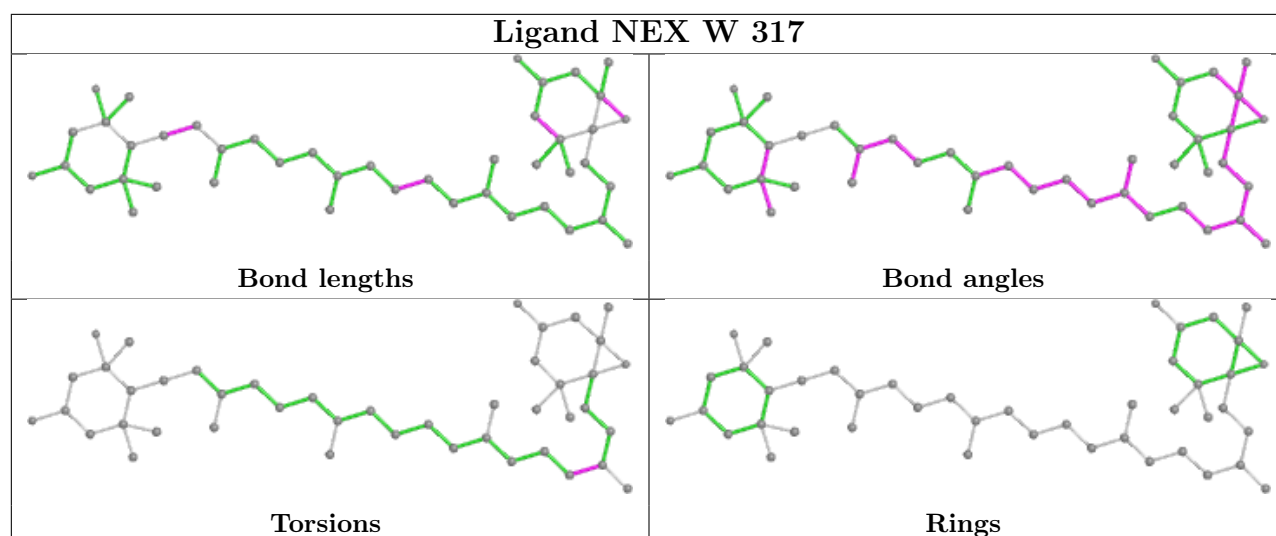
Torsions

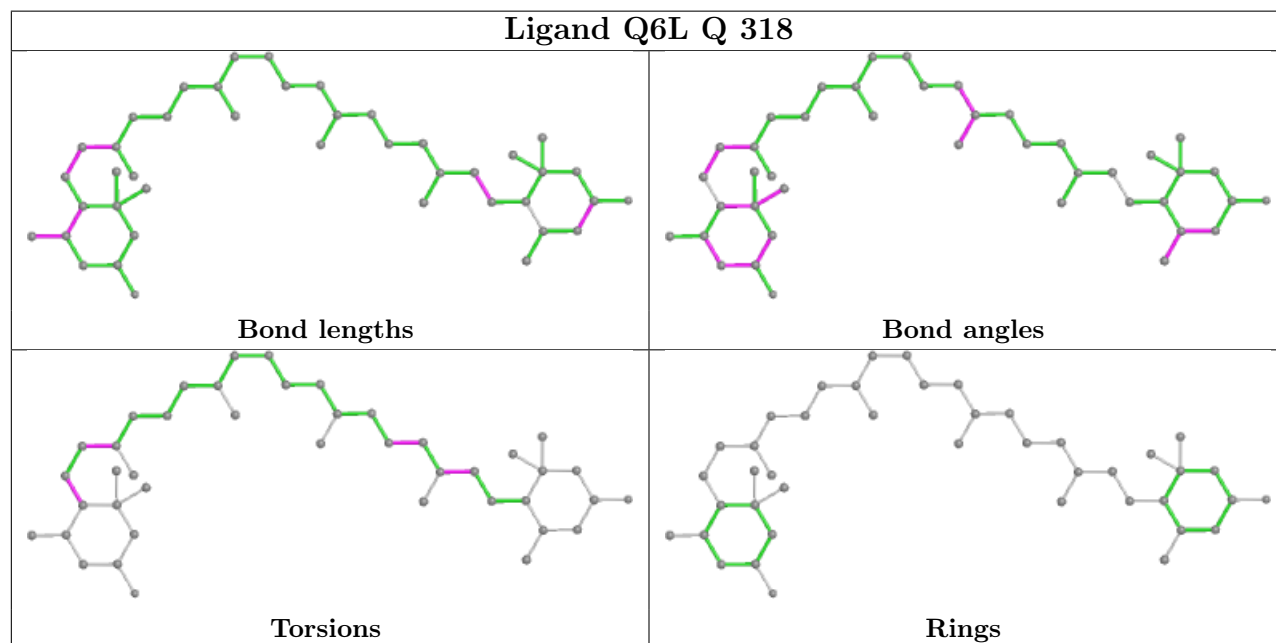
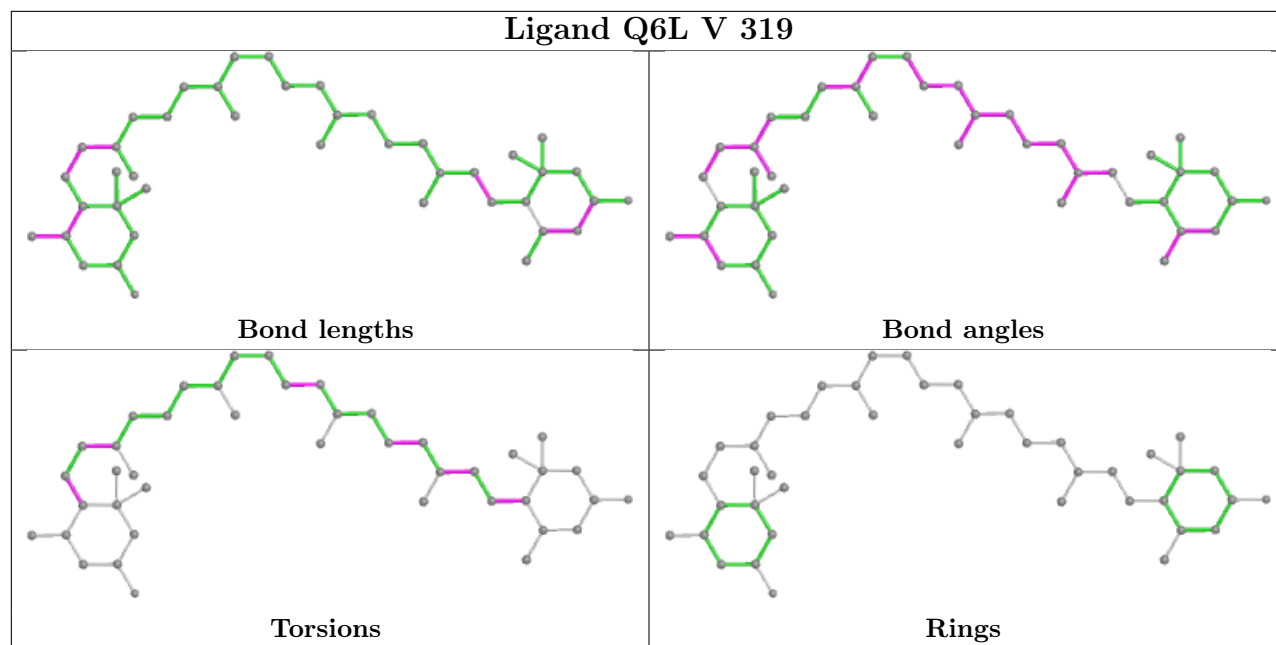


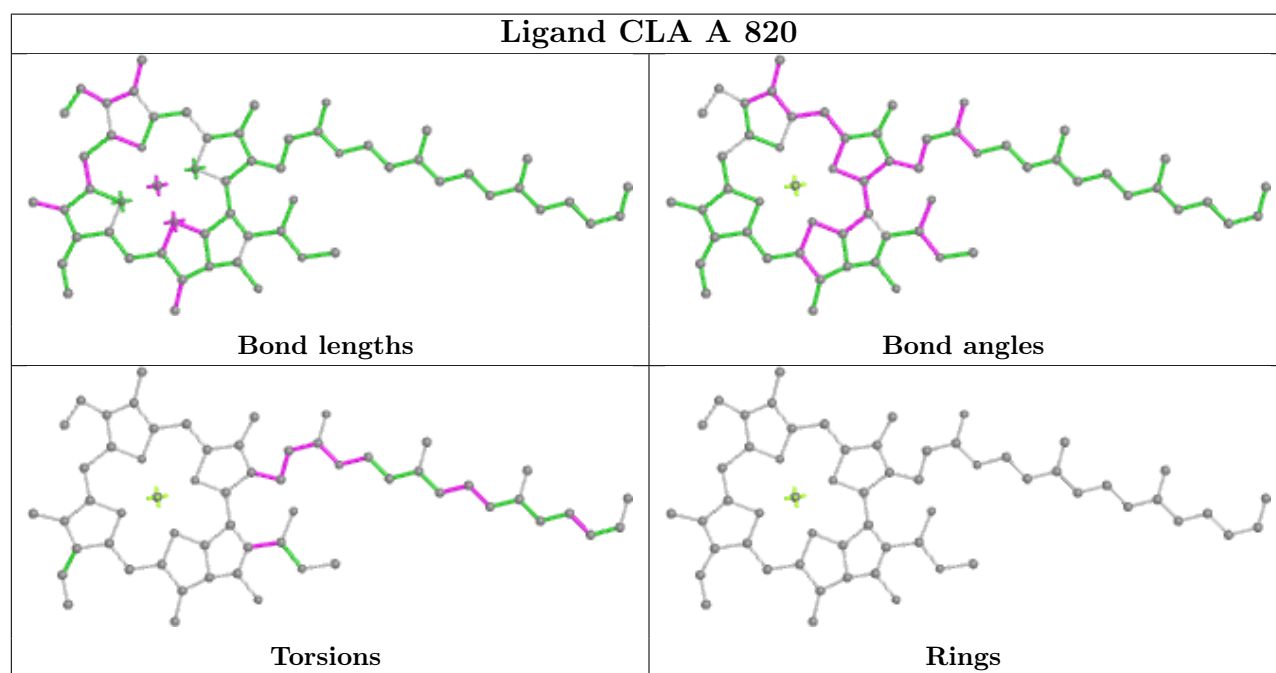
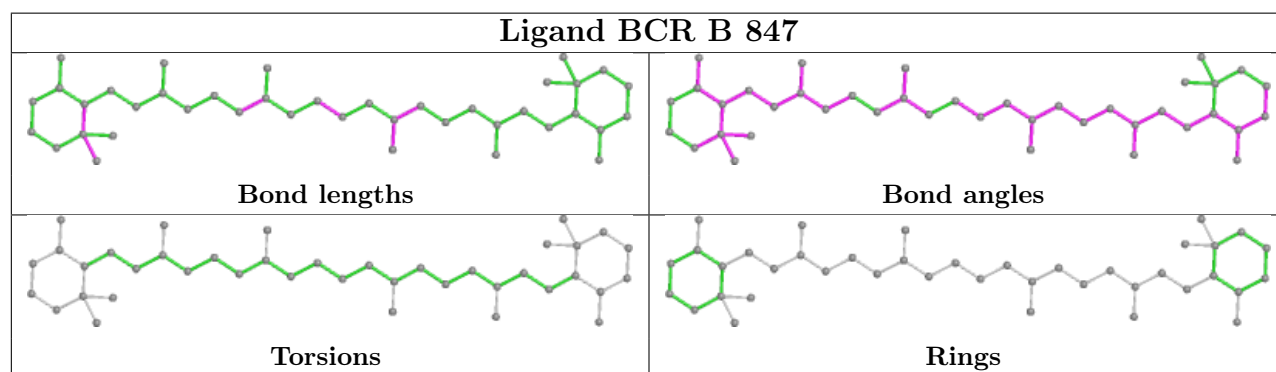
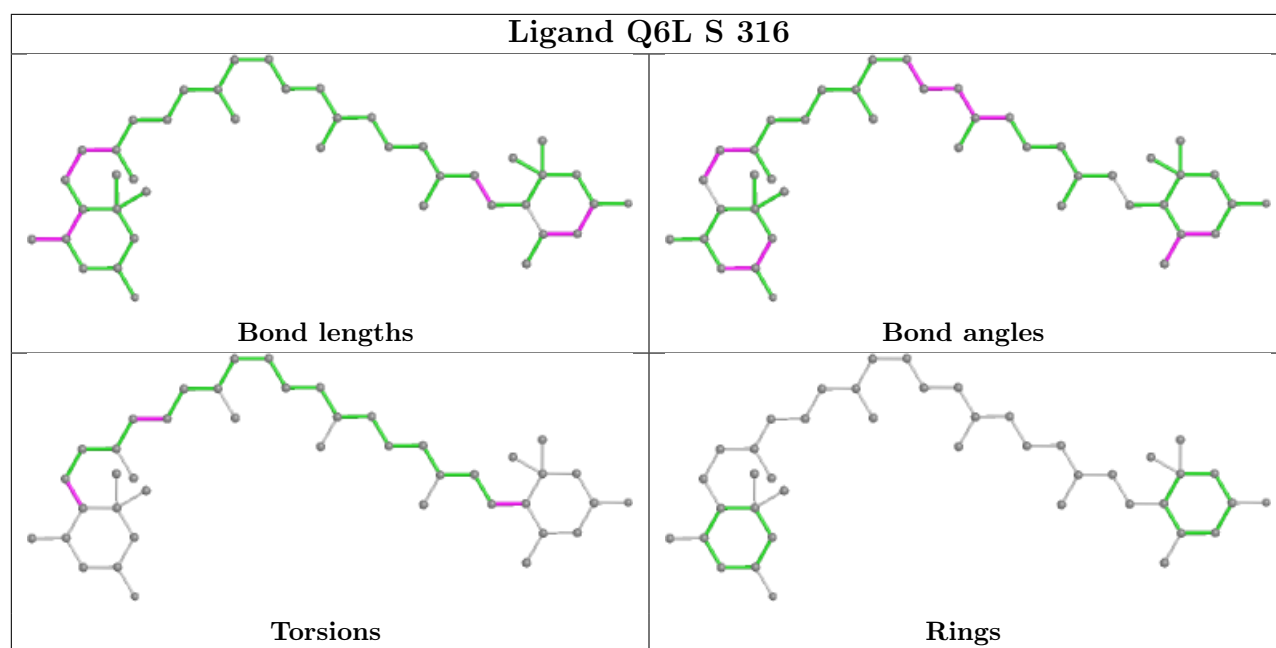
Rings

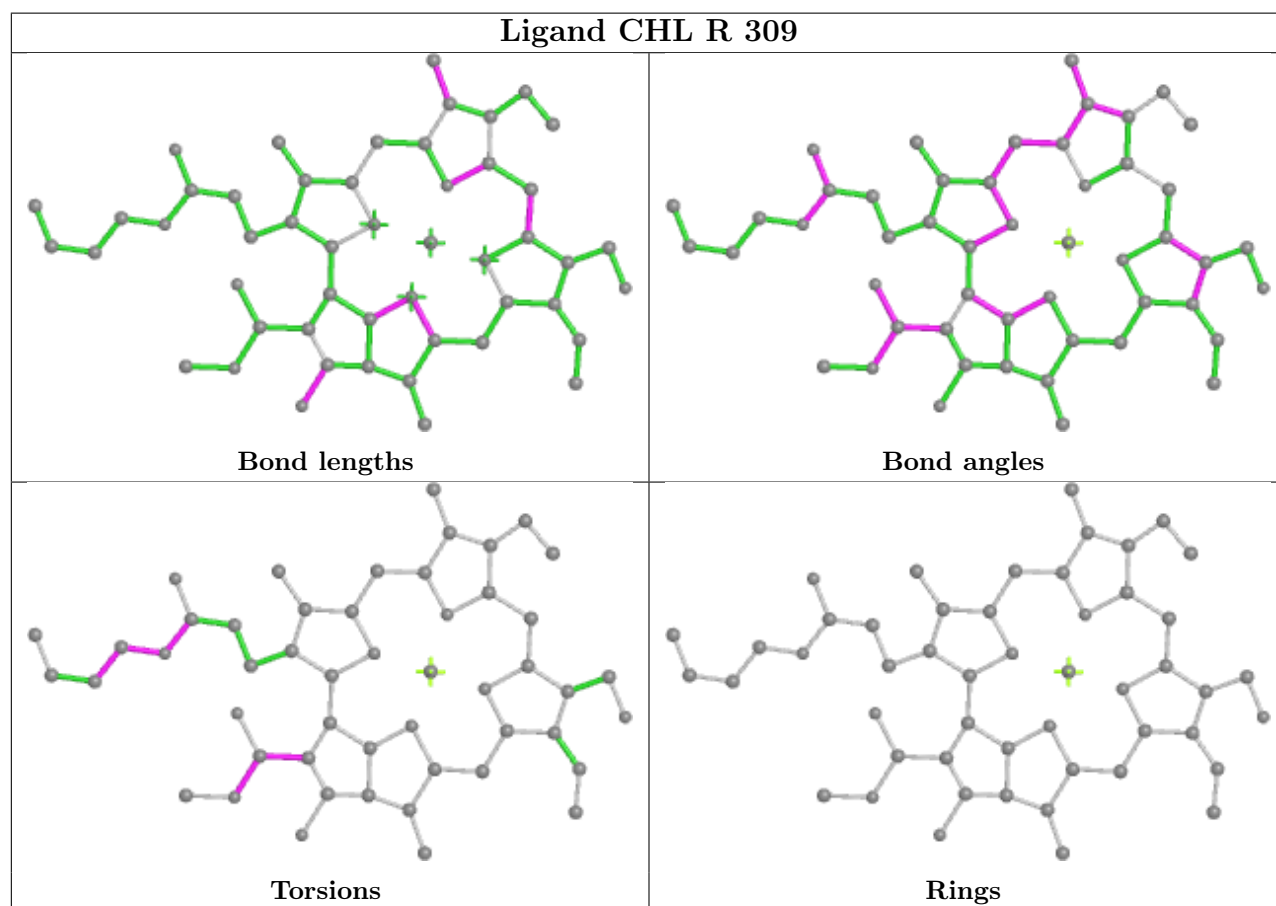
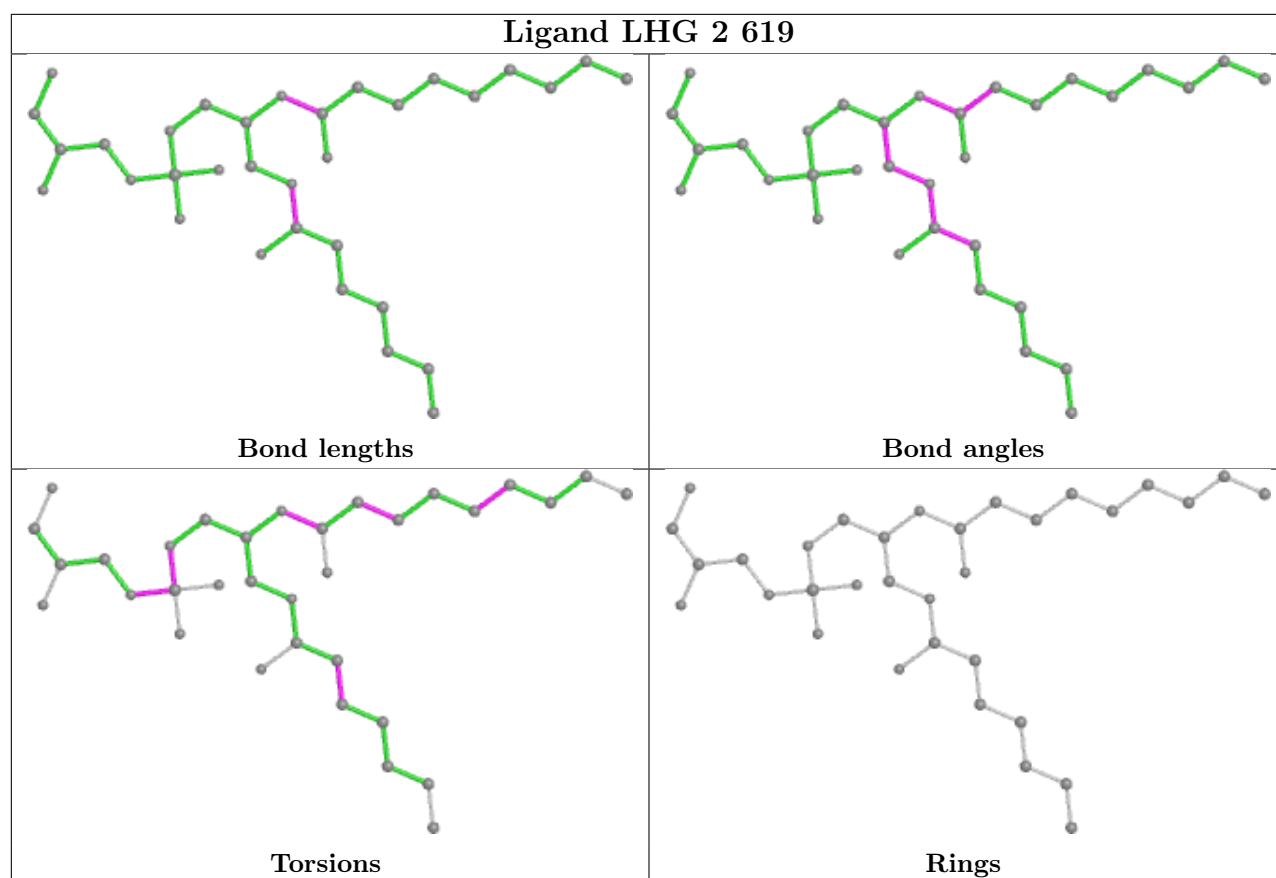




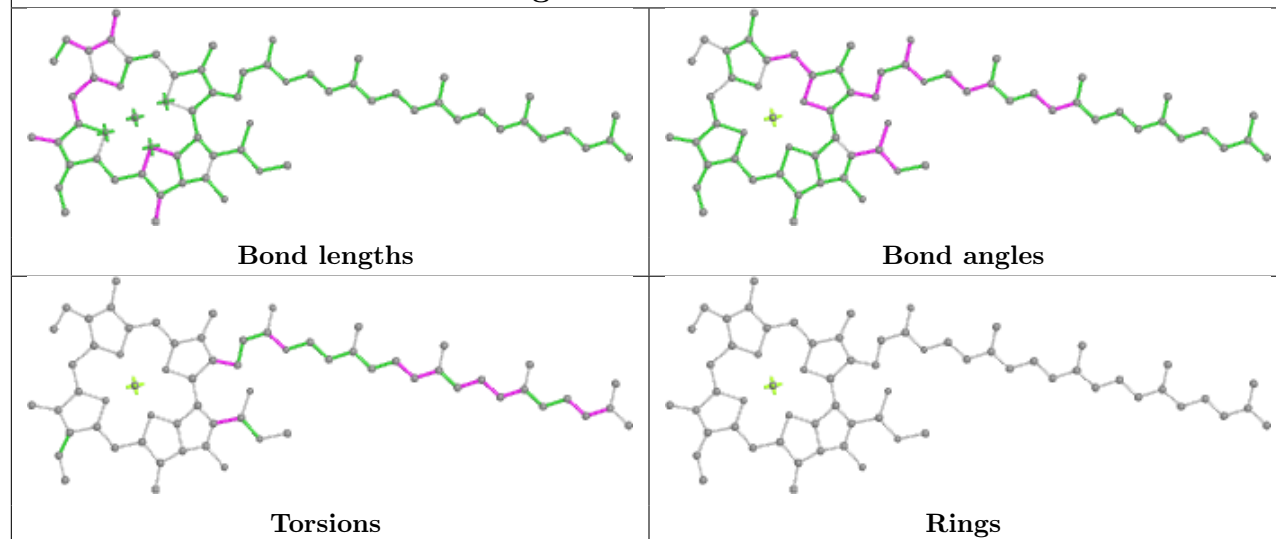




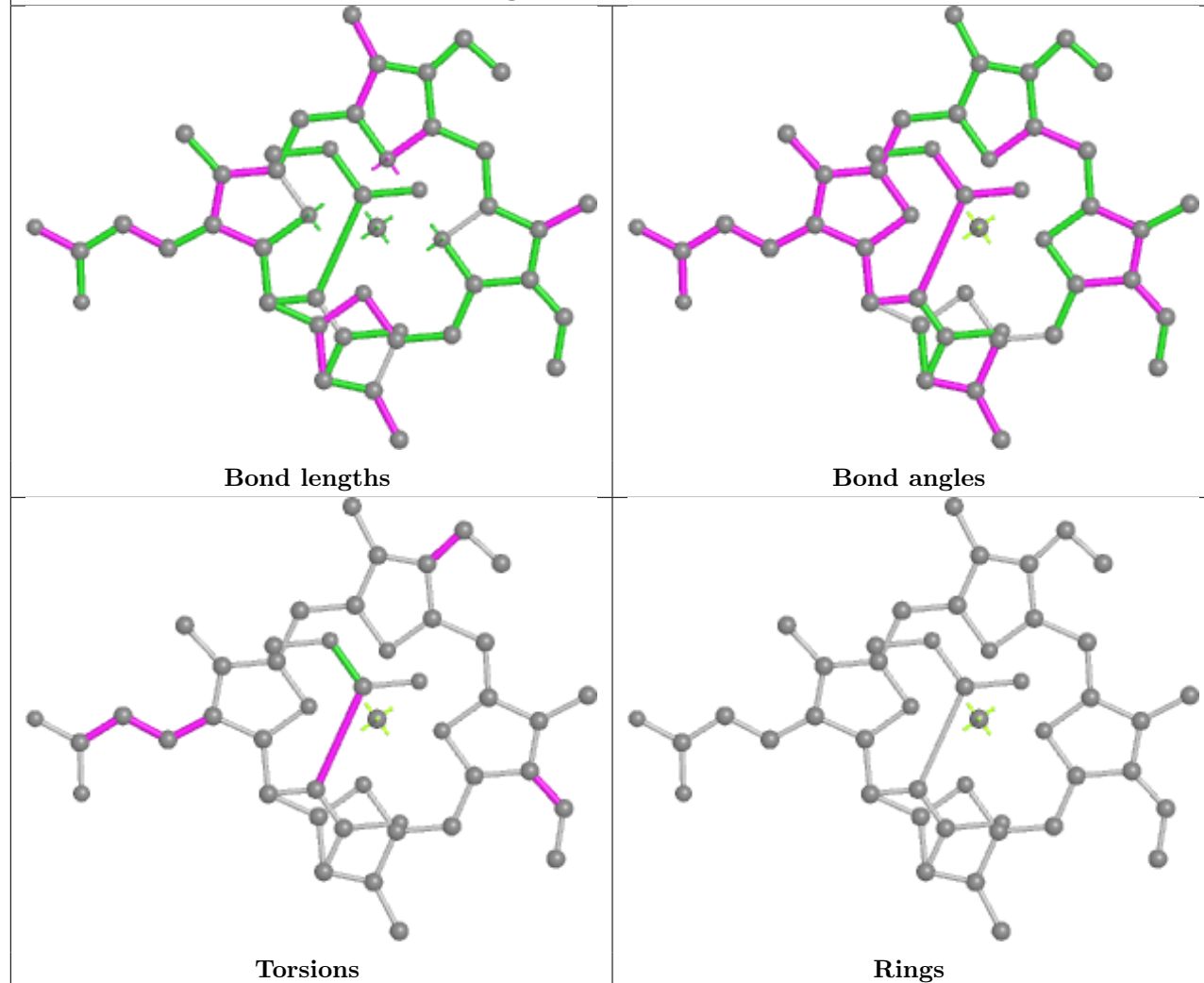




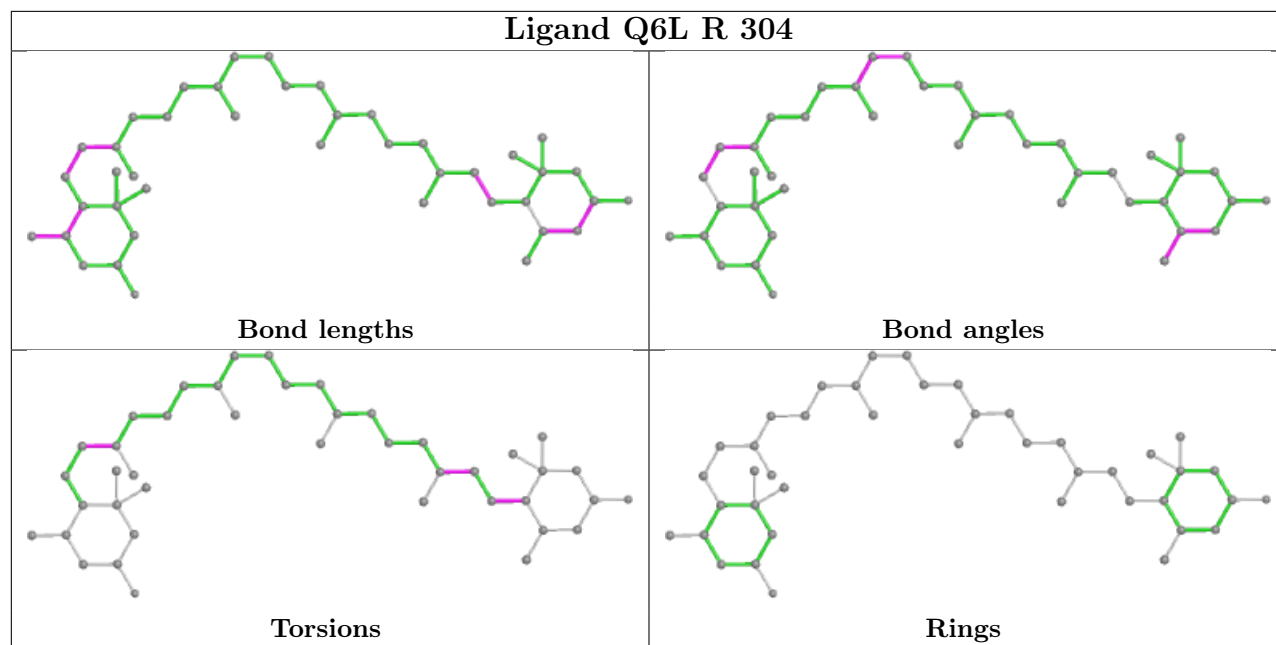
## Ligand CLA B 810



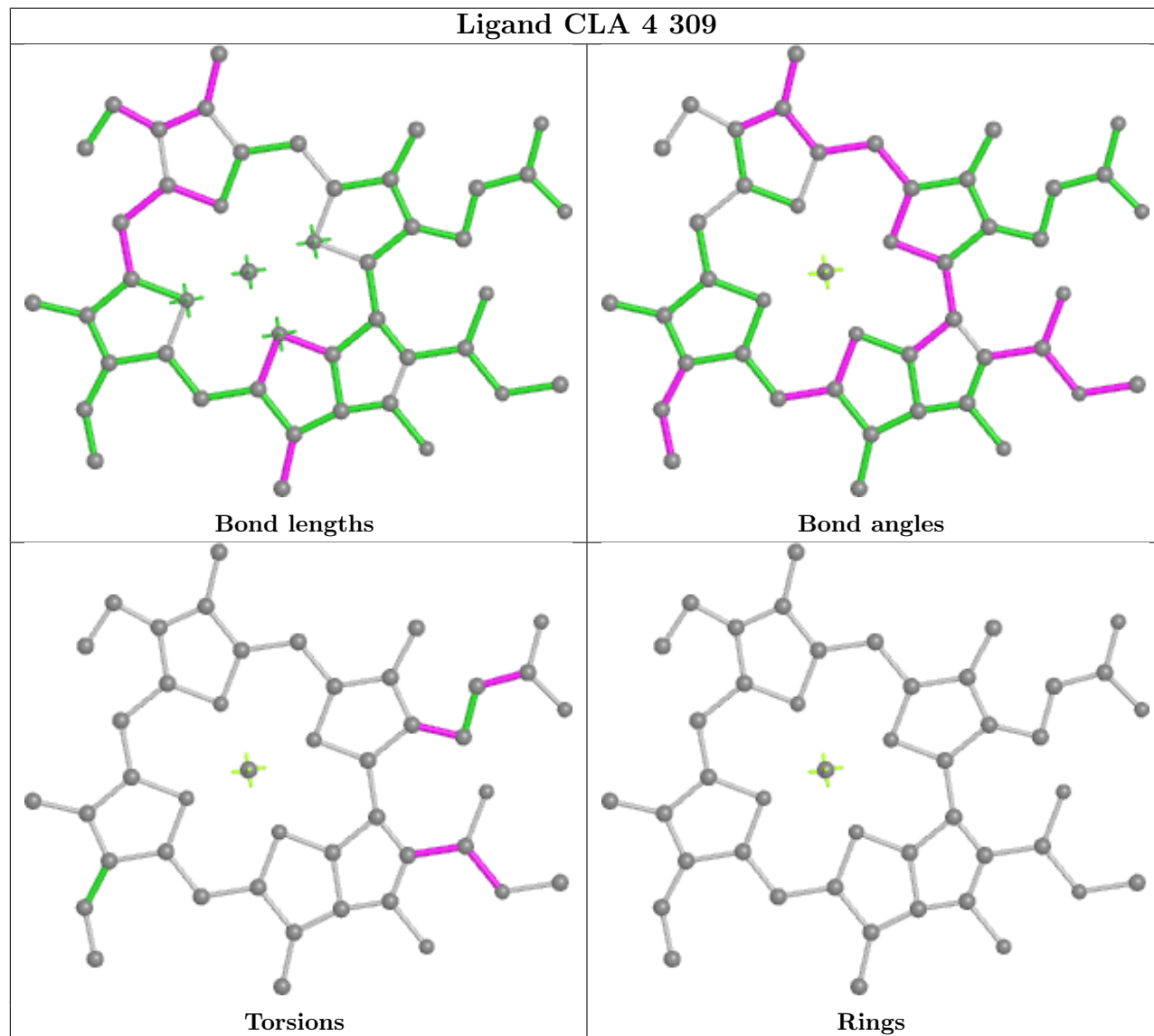
## Ligand KC2 R 312



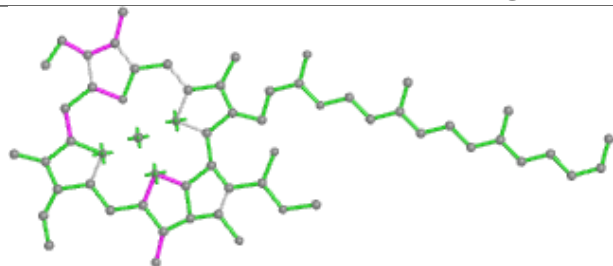
## Ligand Q6L R 304



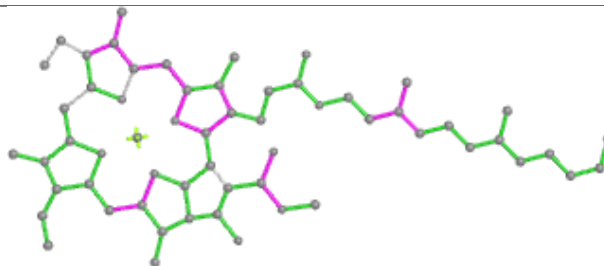
## Ligand CLA 4 309



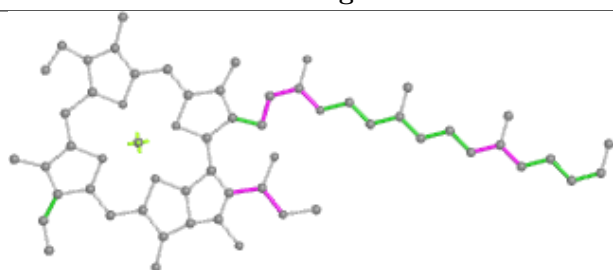
## Ligand CLA O 2001



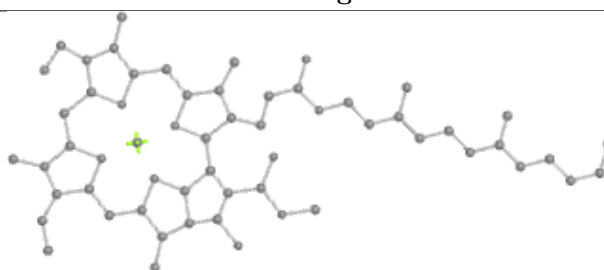
Bond lengths



Bond angles

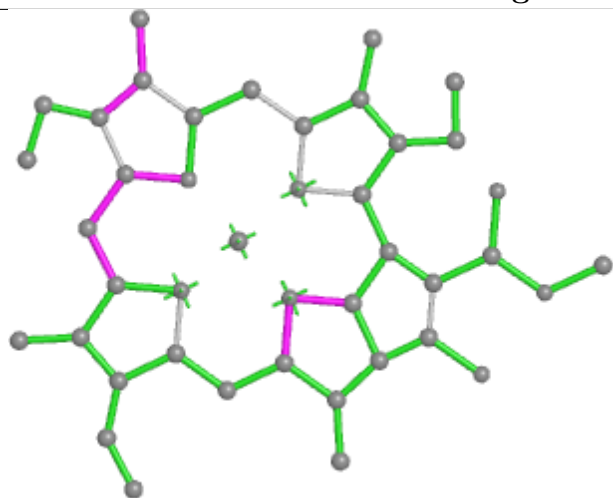


Torsions

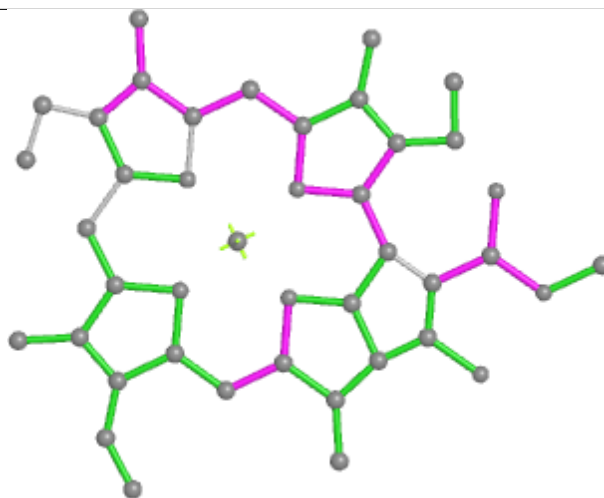


Rings

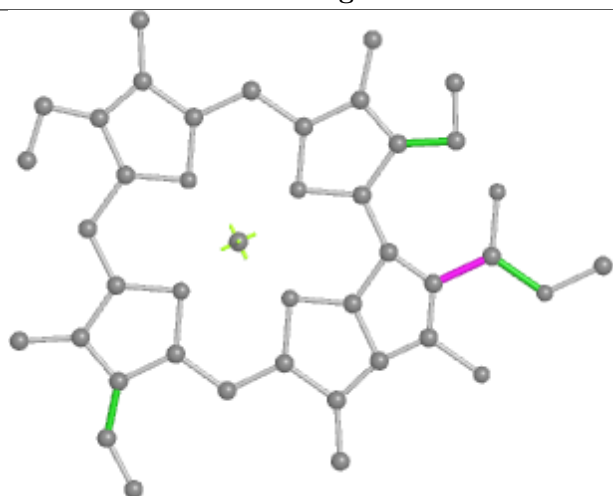
## Ligand CLA G 203



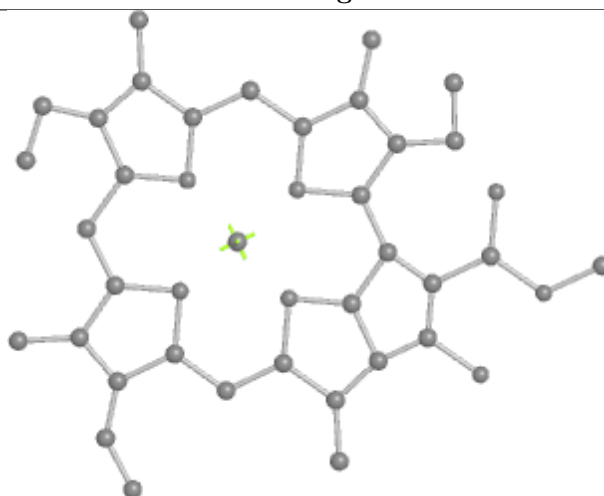
Bond lengths



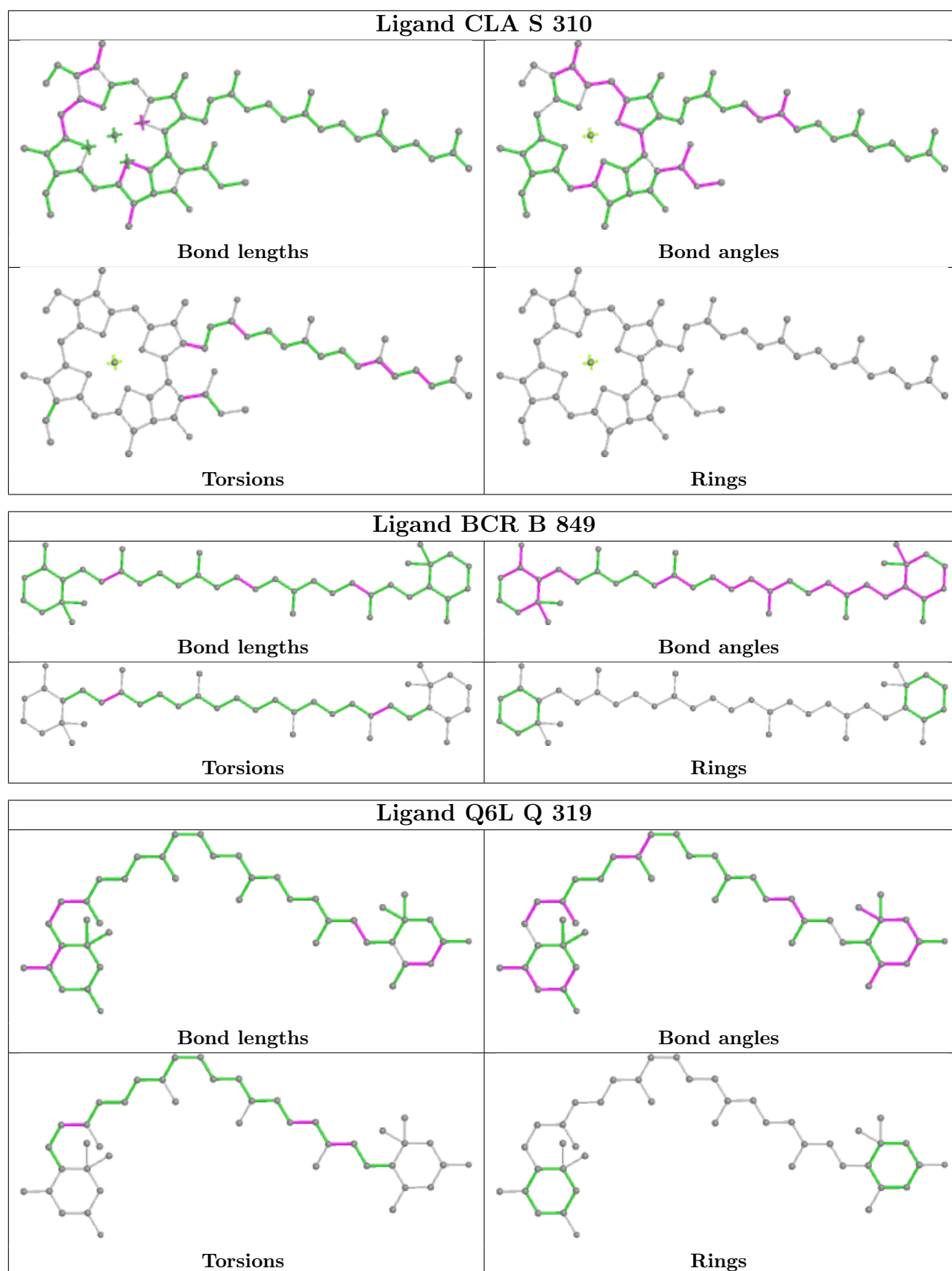
Bond angles



Torsions

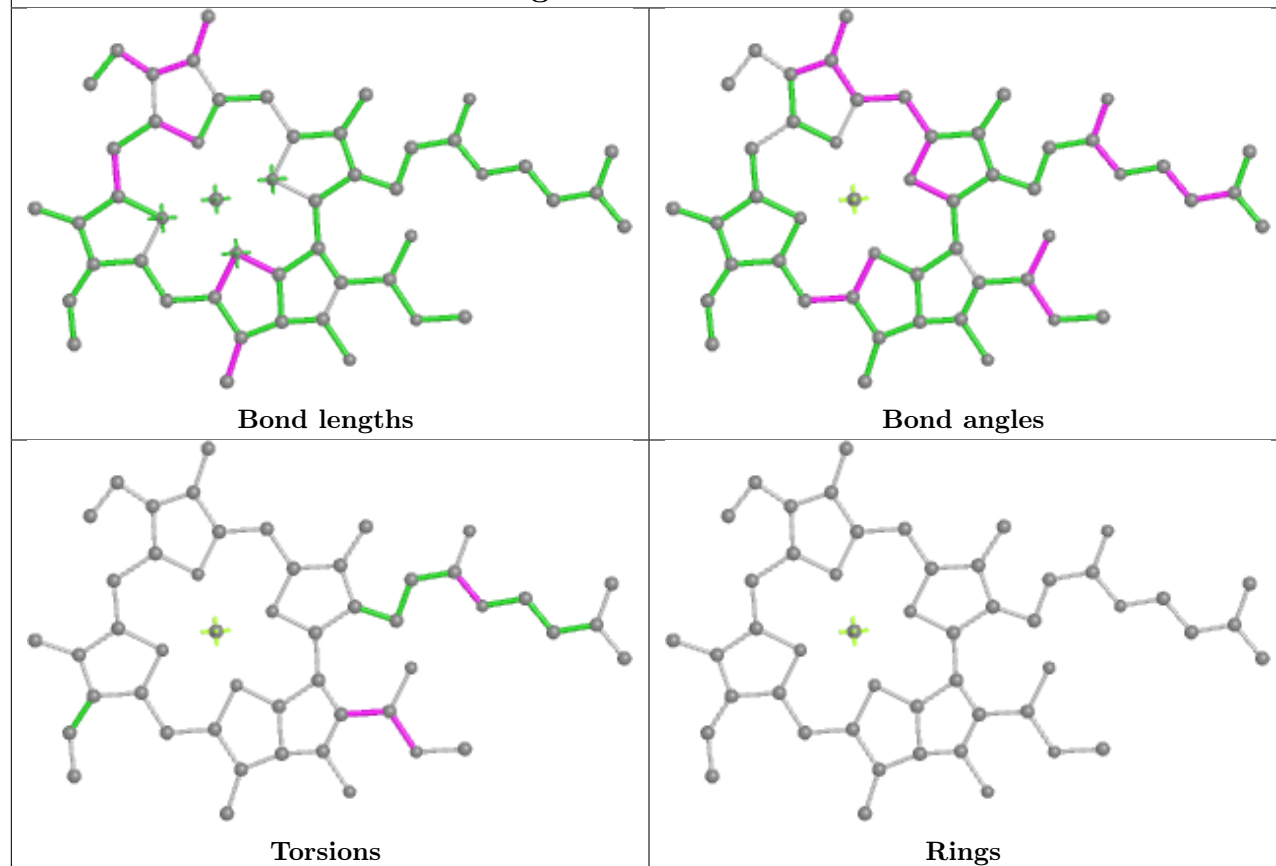


Rings

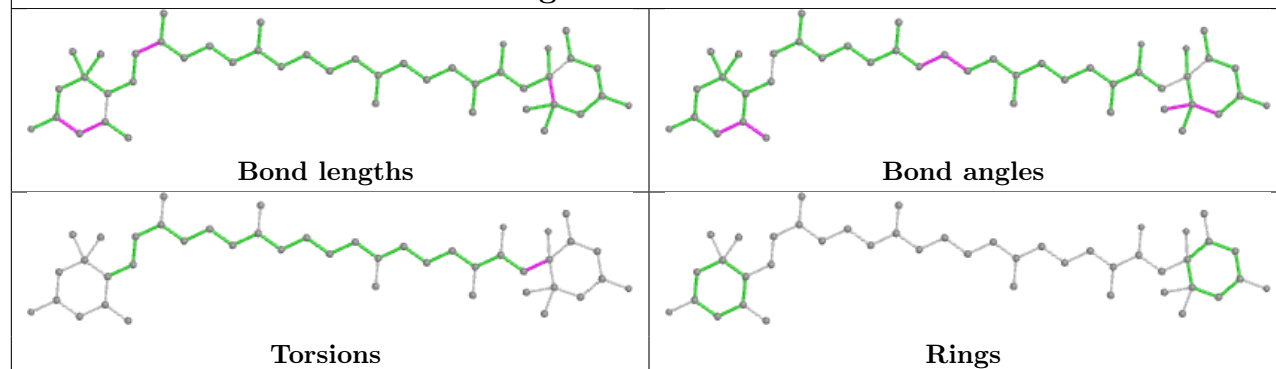




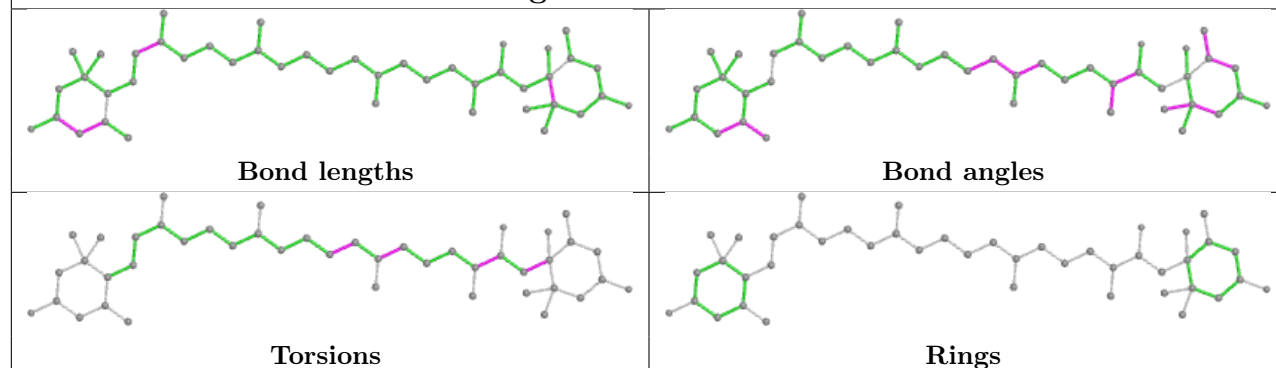
## Ligand CLA U 303



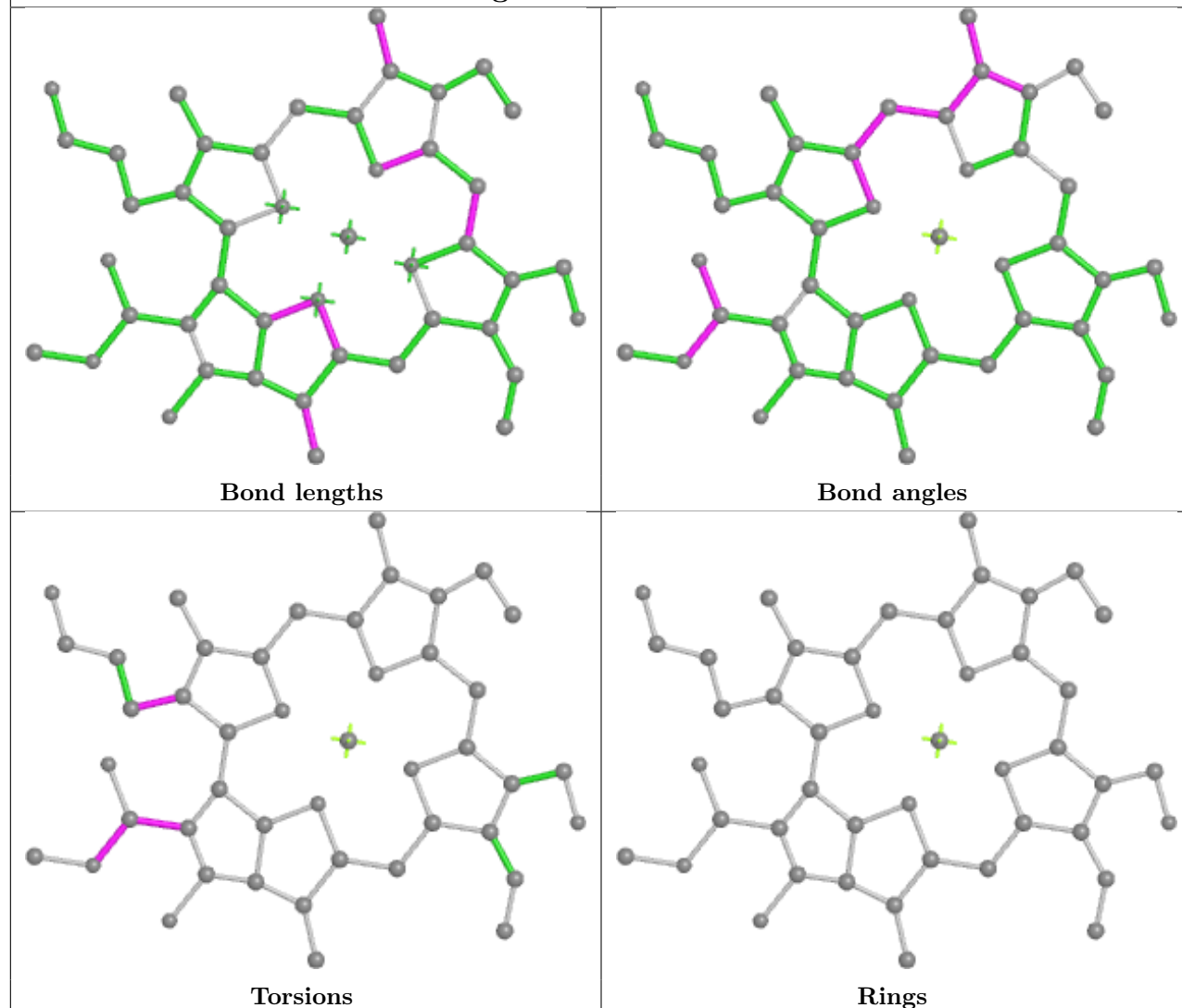
## Ligand IWJ 6 614



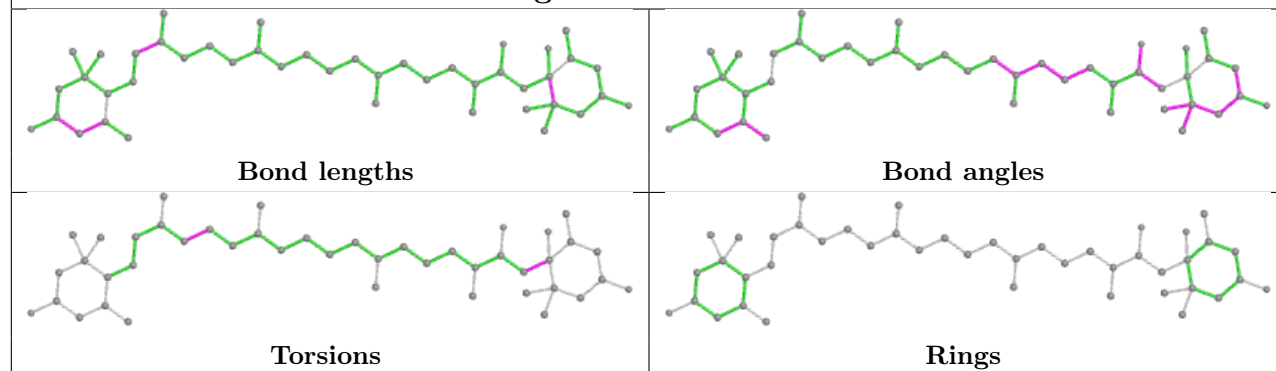
## Ligand IWJ W 318

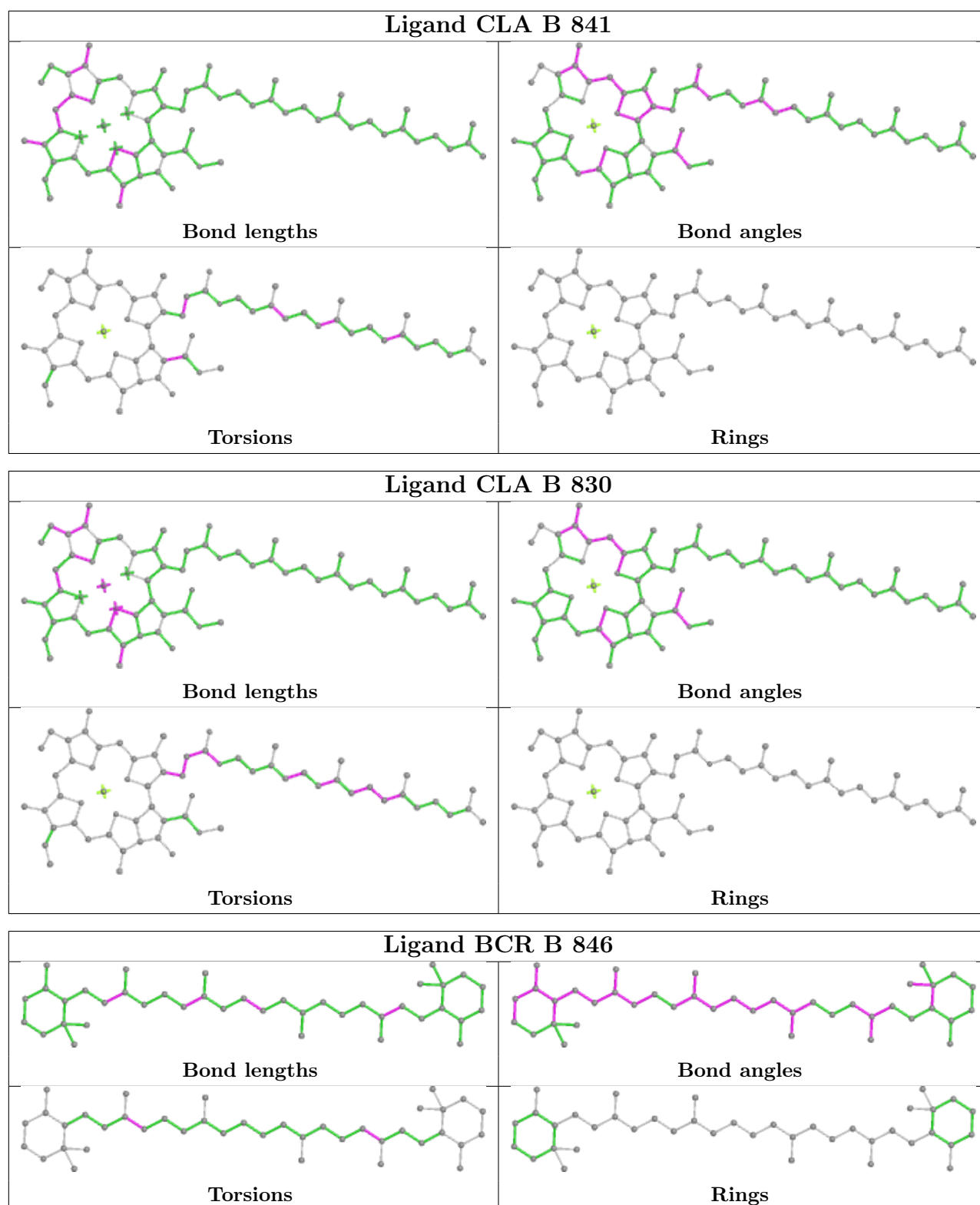


## Ligand CHL X 315

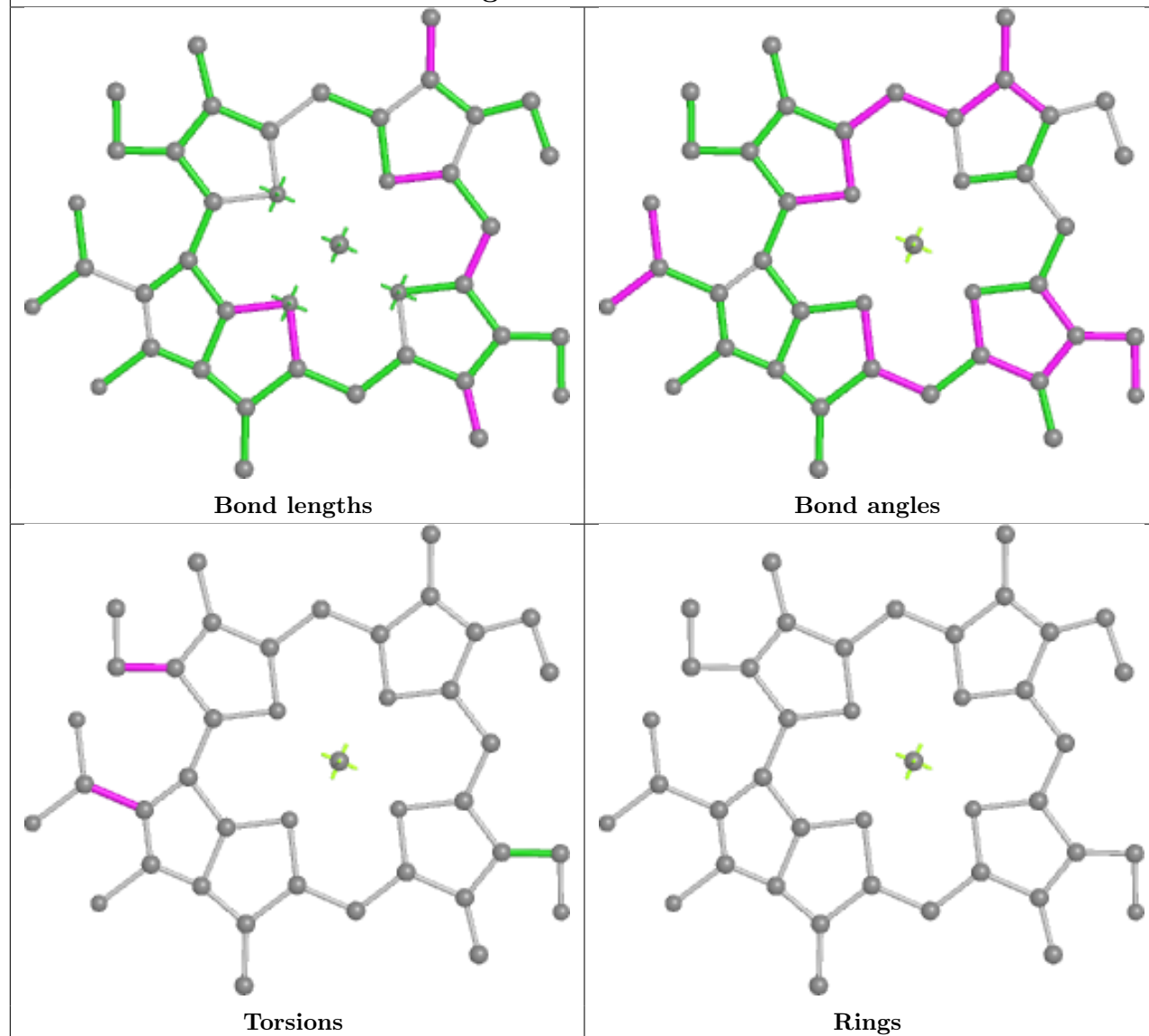


## Ligand IWJ V 318

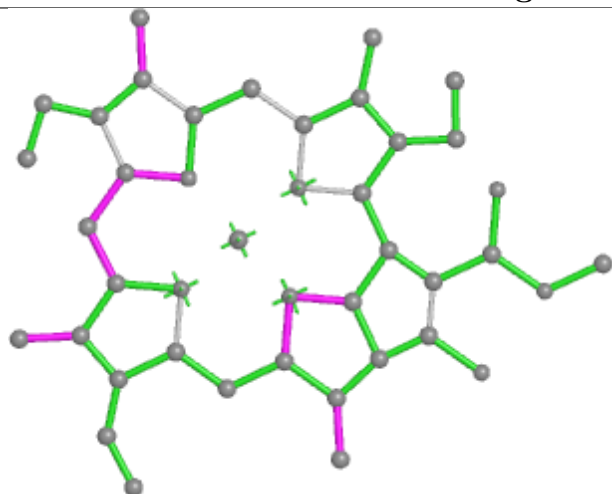




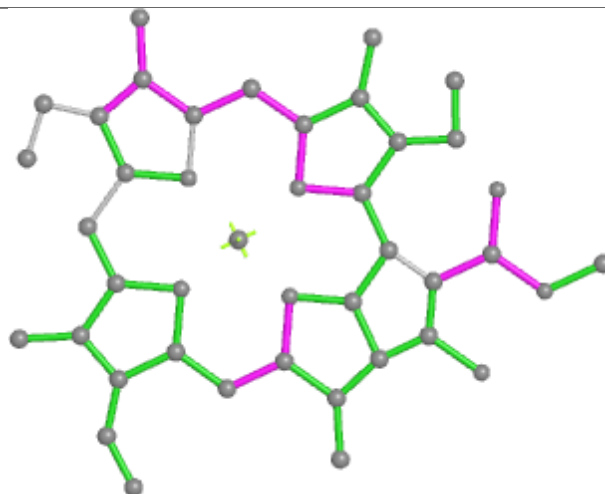
## Ligand CHL 4 306



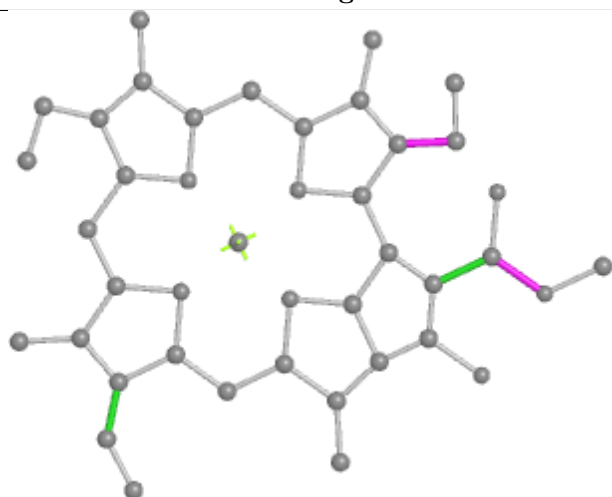
## Ligand CLA L 304



Bond lengths



Bond angles

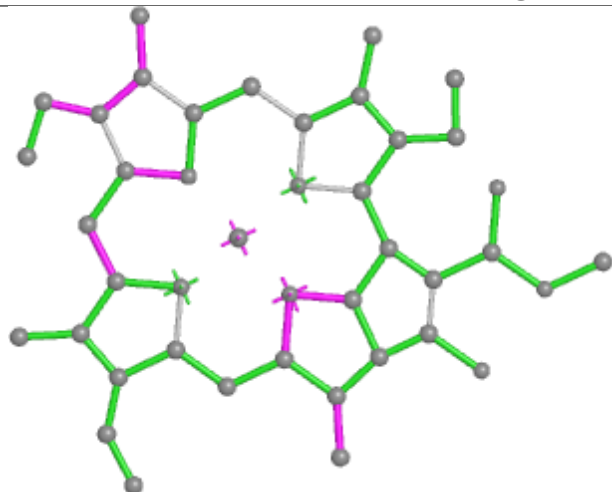


Torsions

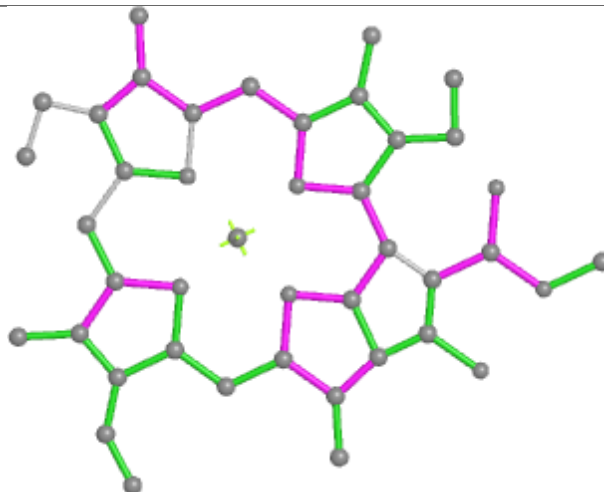


Rings

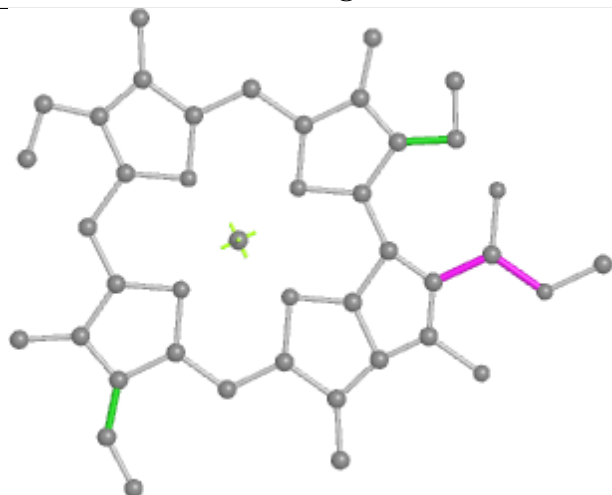
## Ligand CLA N 203



Bond lengths



Bond angles

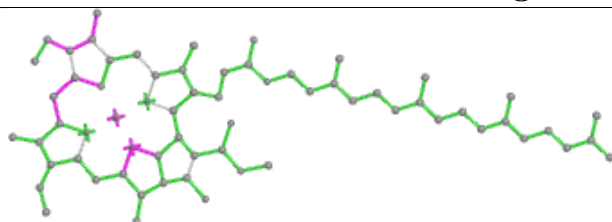


Torsions

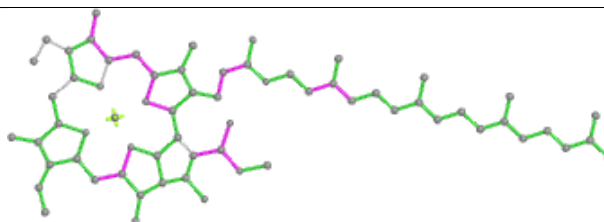


Rings

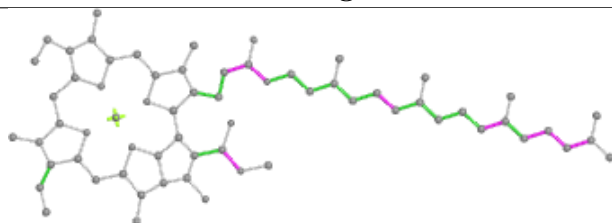
## Ligand CLA A 835



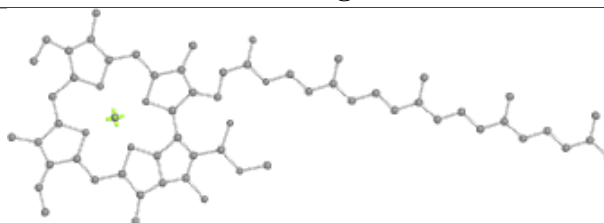
Bond lengths



Bond angles

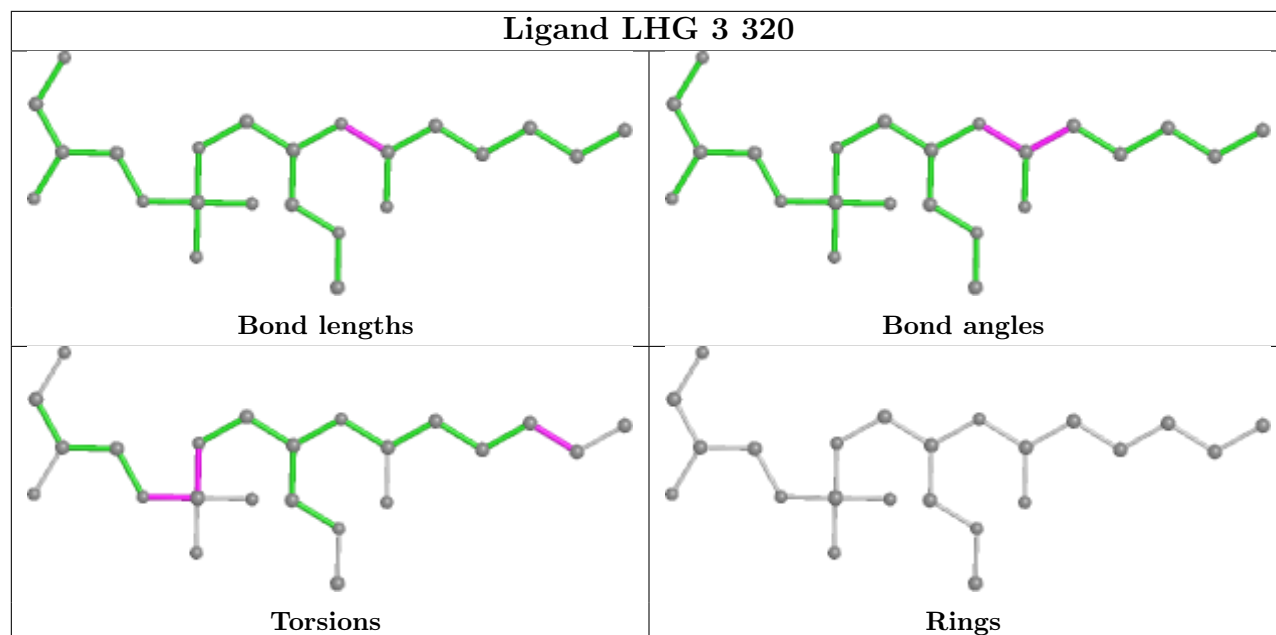


Torsions

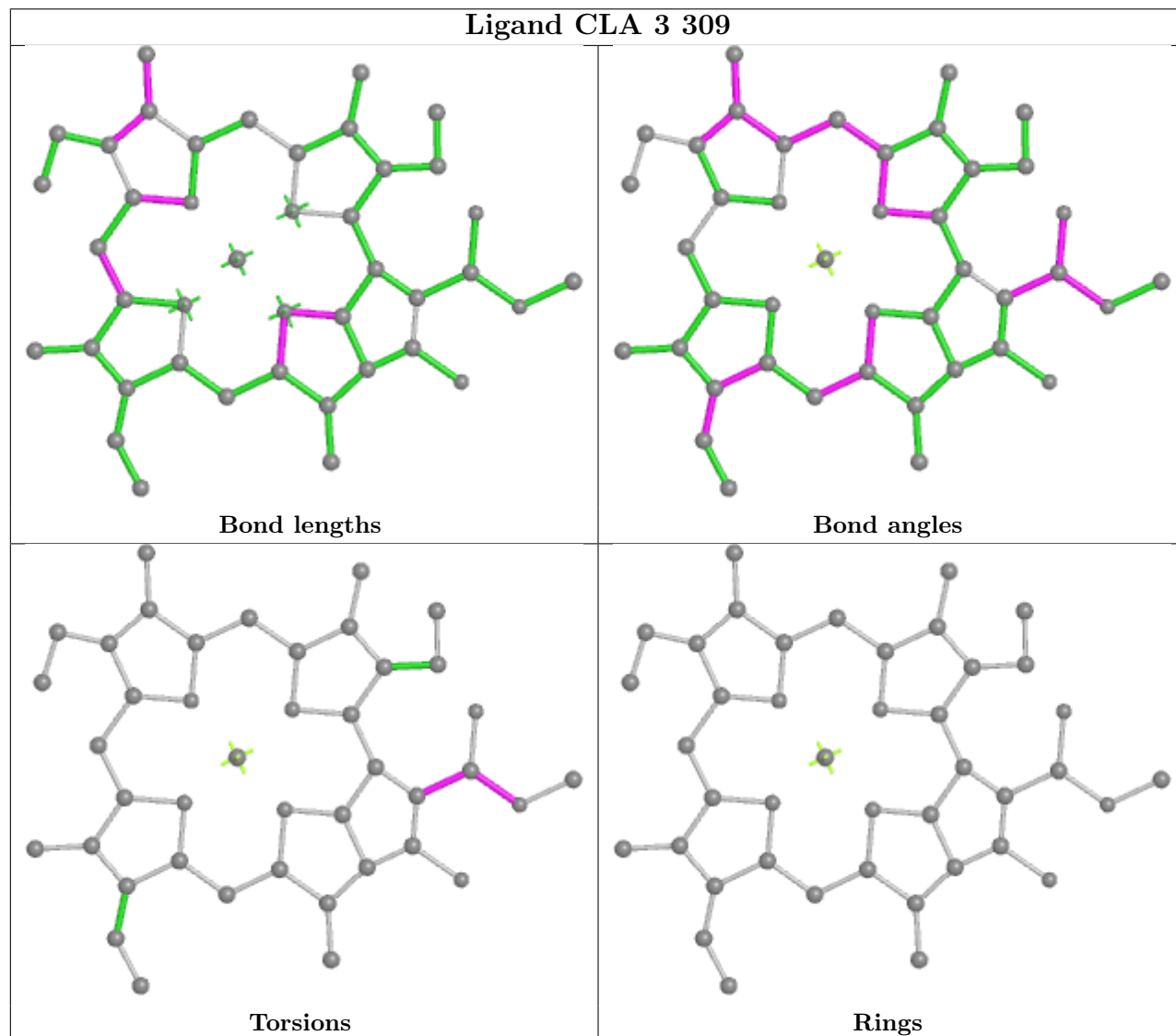


Rings

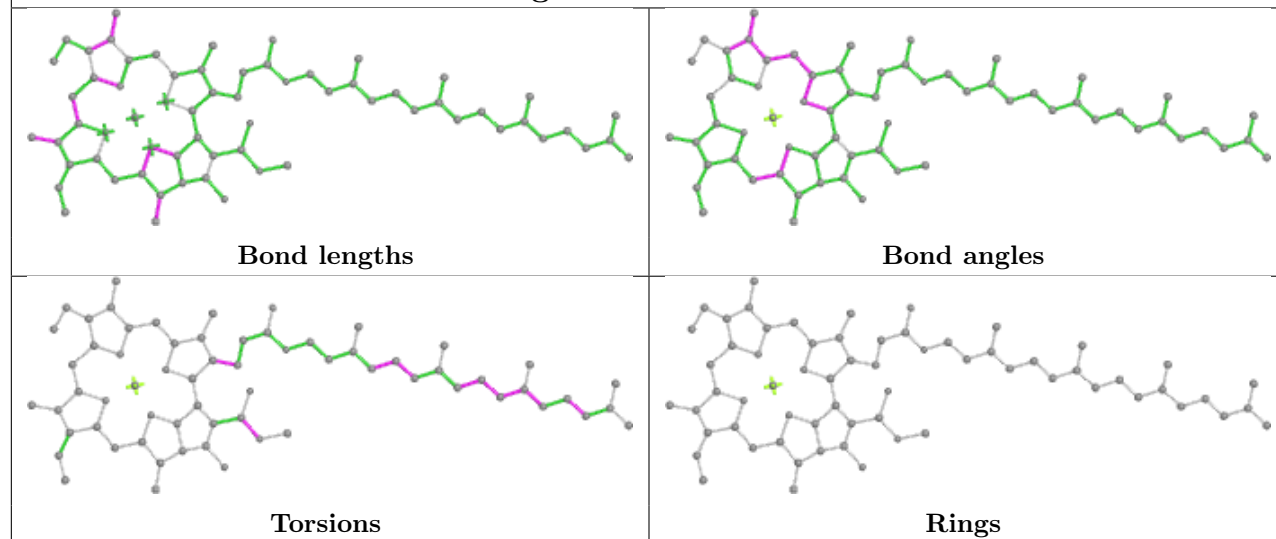
## Ligand LHG 3 320



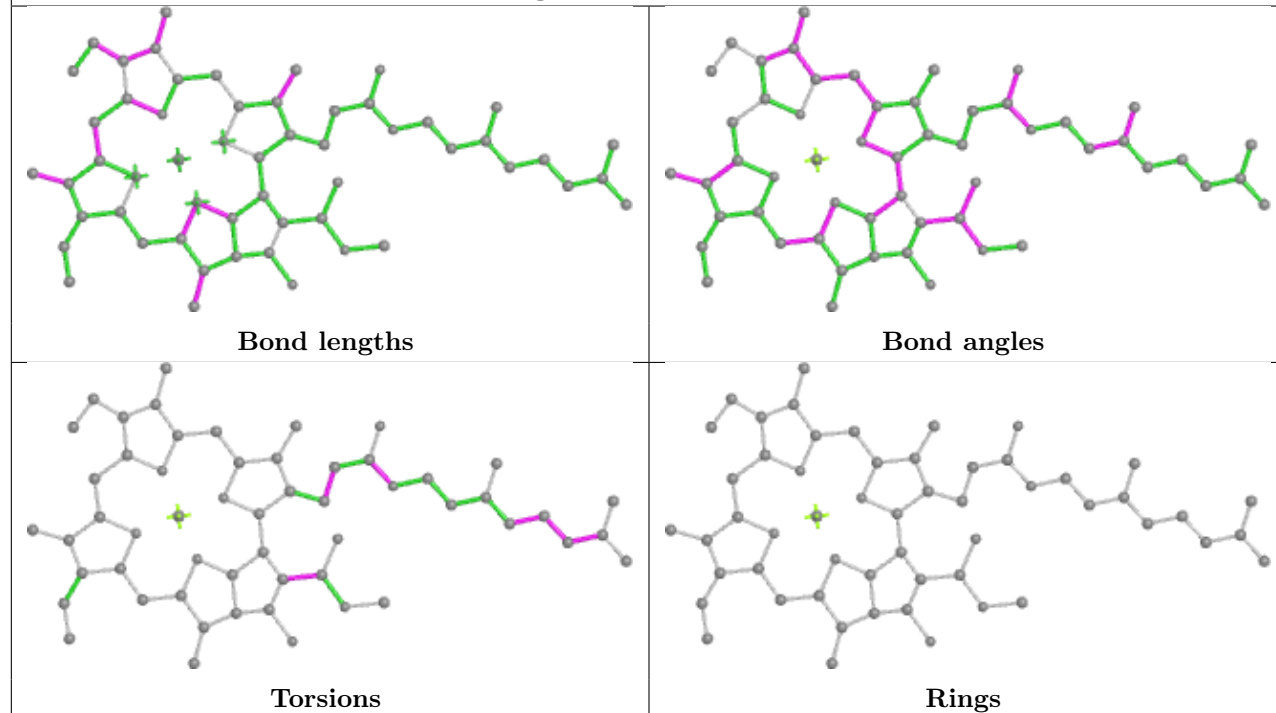
## Ligand CLA 3 309



## Ligand CLA R 306

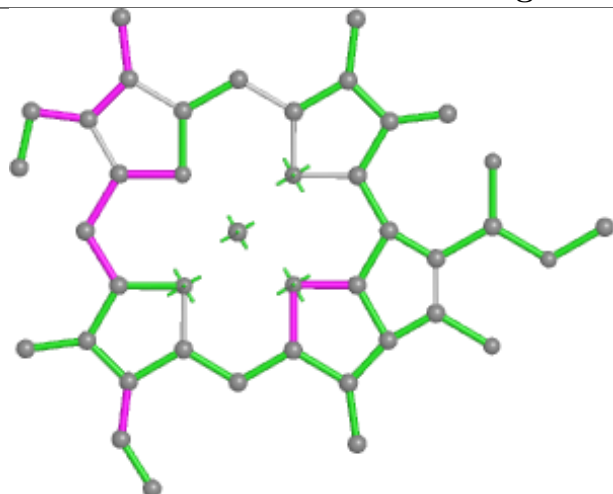


## Ligand CLA X 302

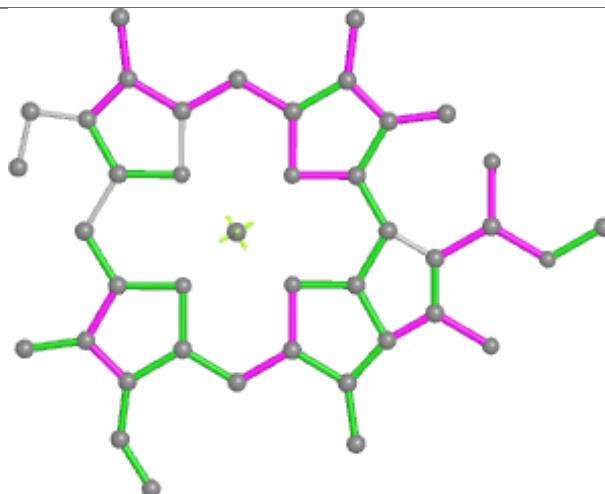




## Ligand CLA F 803



Bond lengths



Bond angles

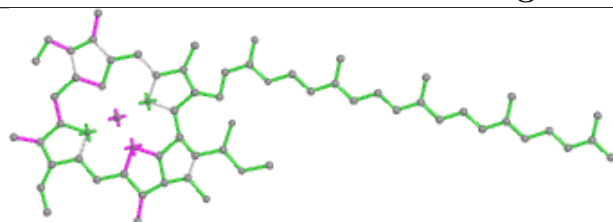


Torsions

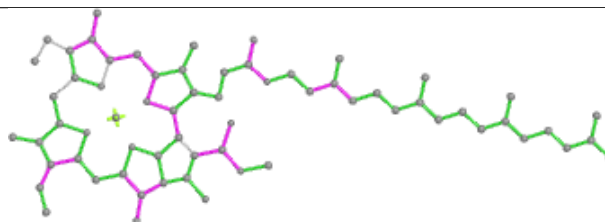


Rings

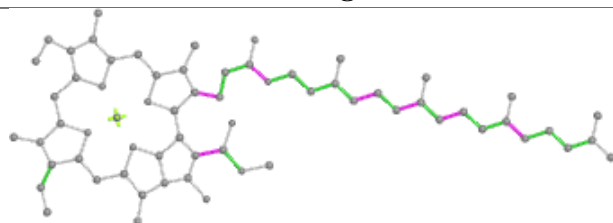
## Ligand CLA S 301



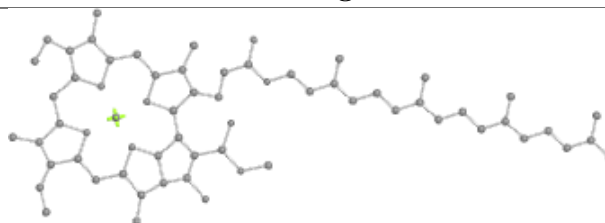
Bond lengths



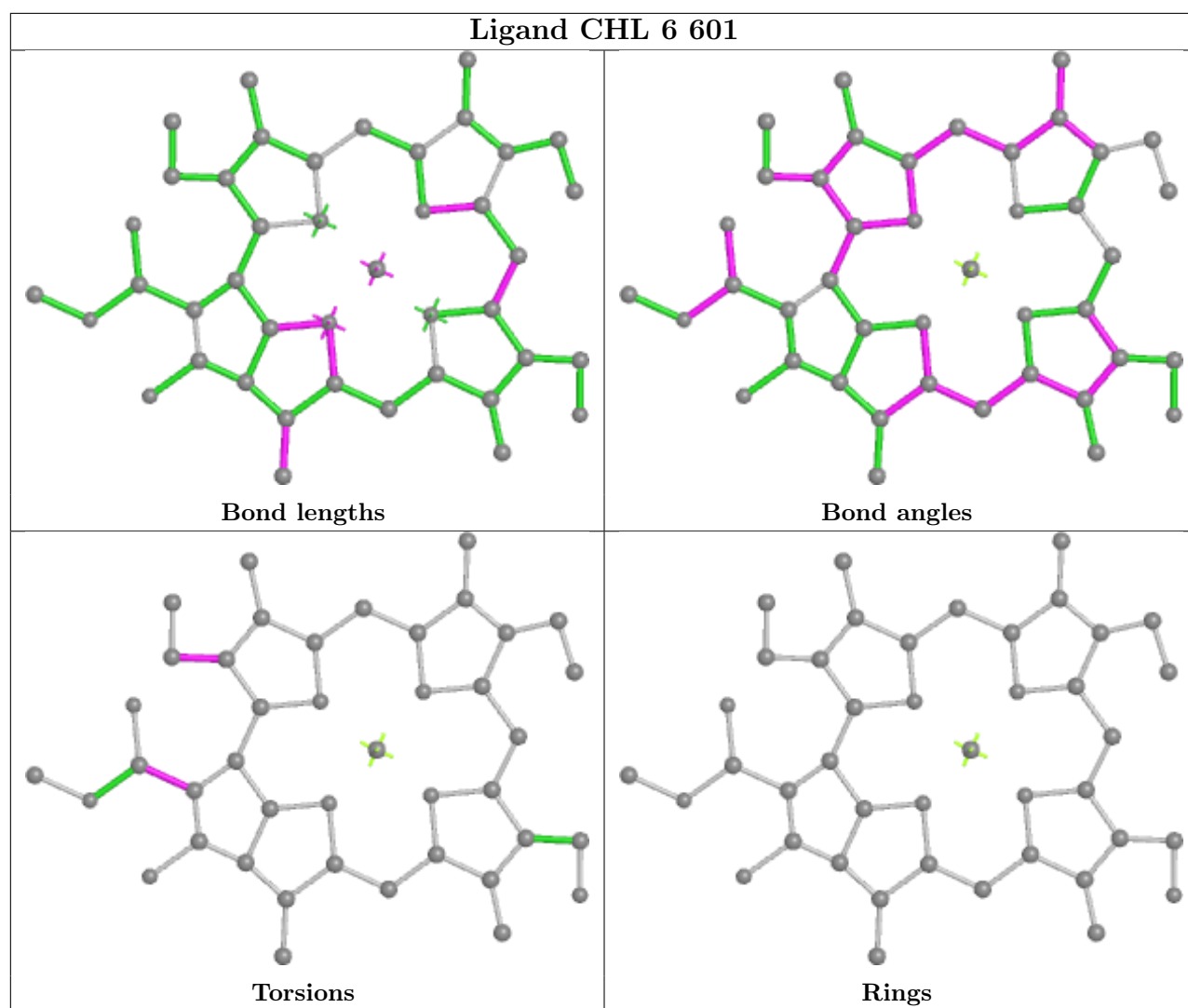
Bond angles

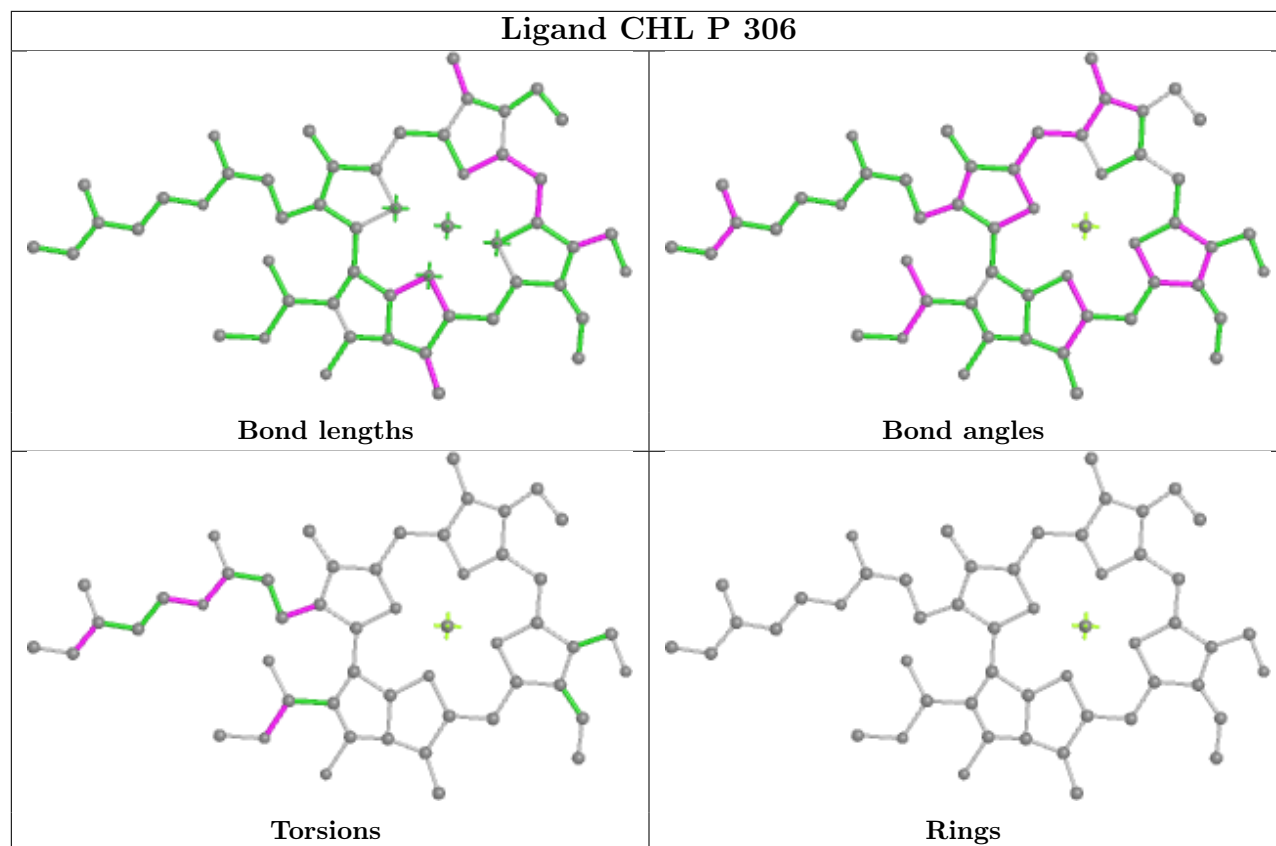


Torsions

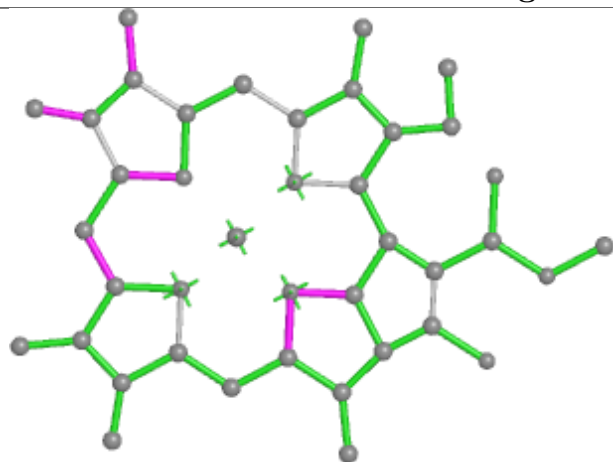


Rings

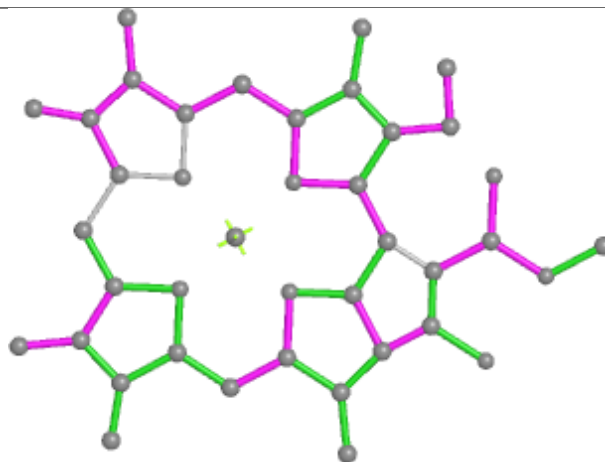




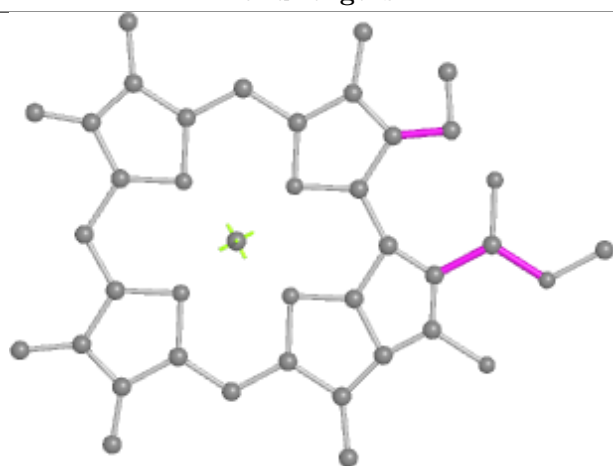
## Ligand CLA 1 610



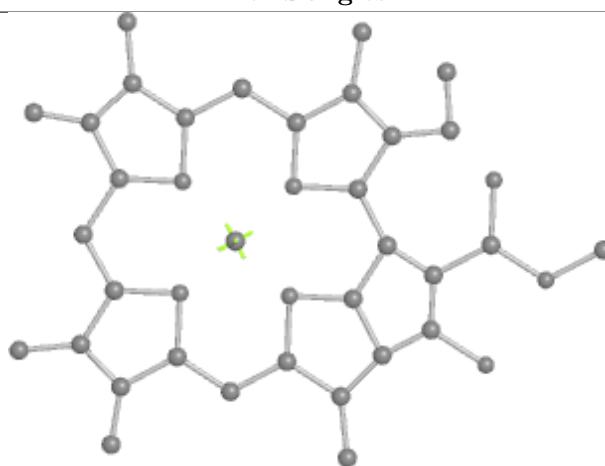
Bond lengths



Bond angles

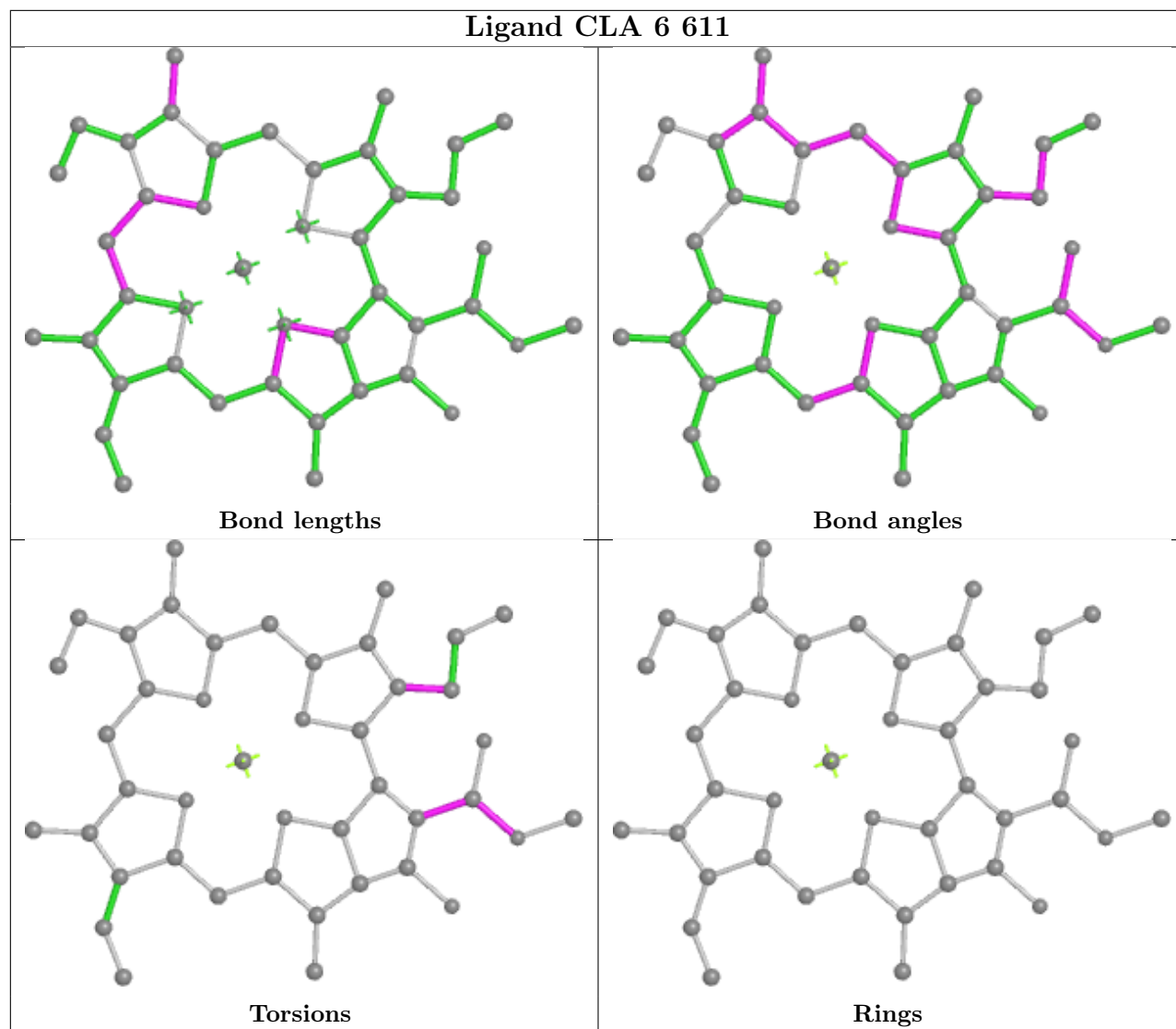


Torsions

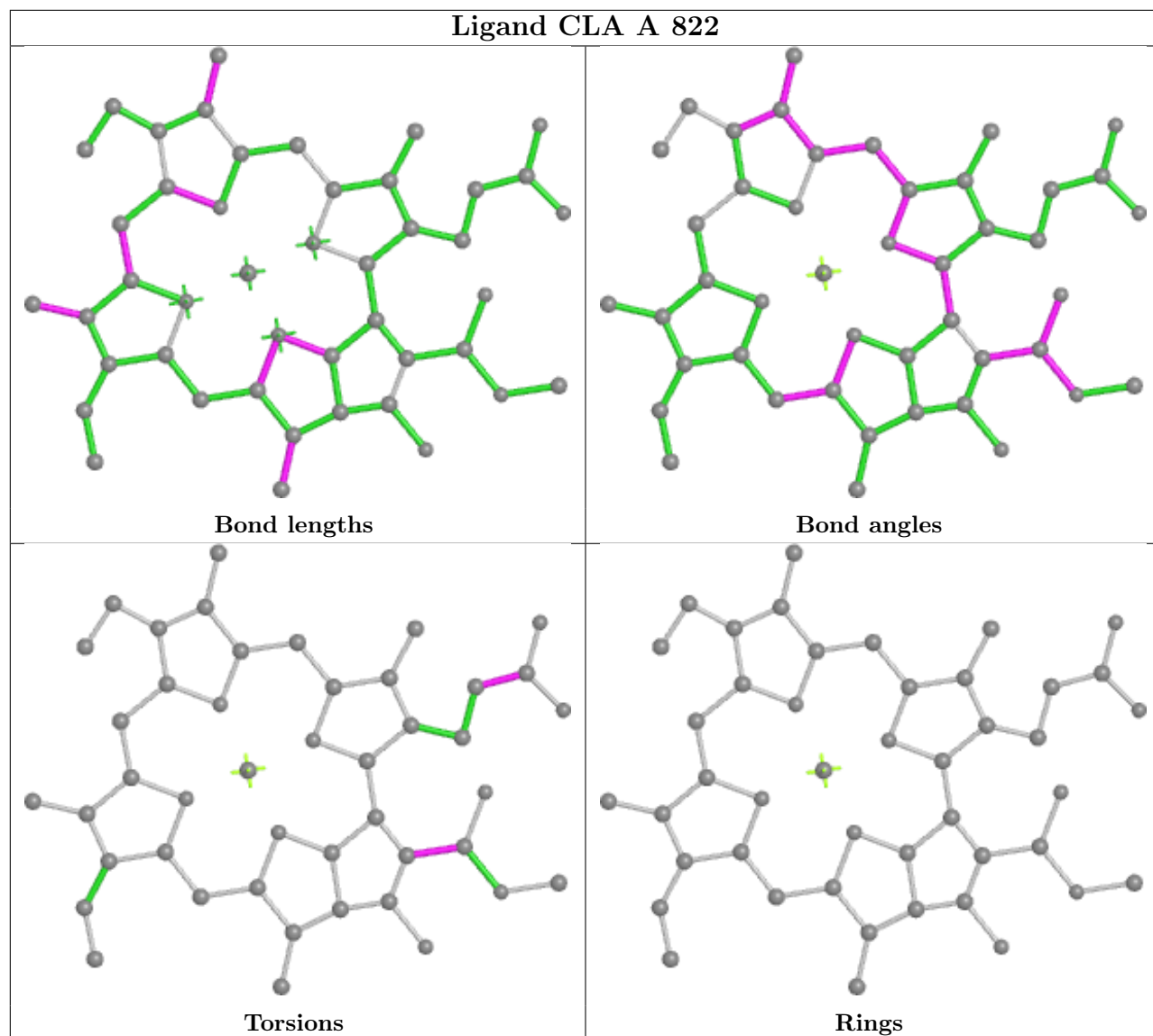


Rings

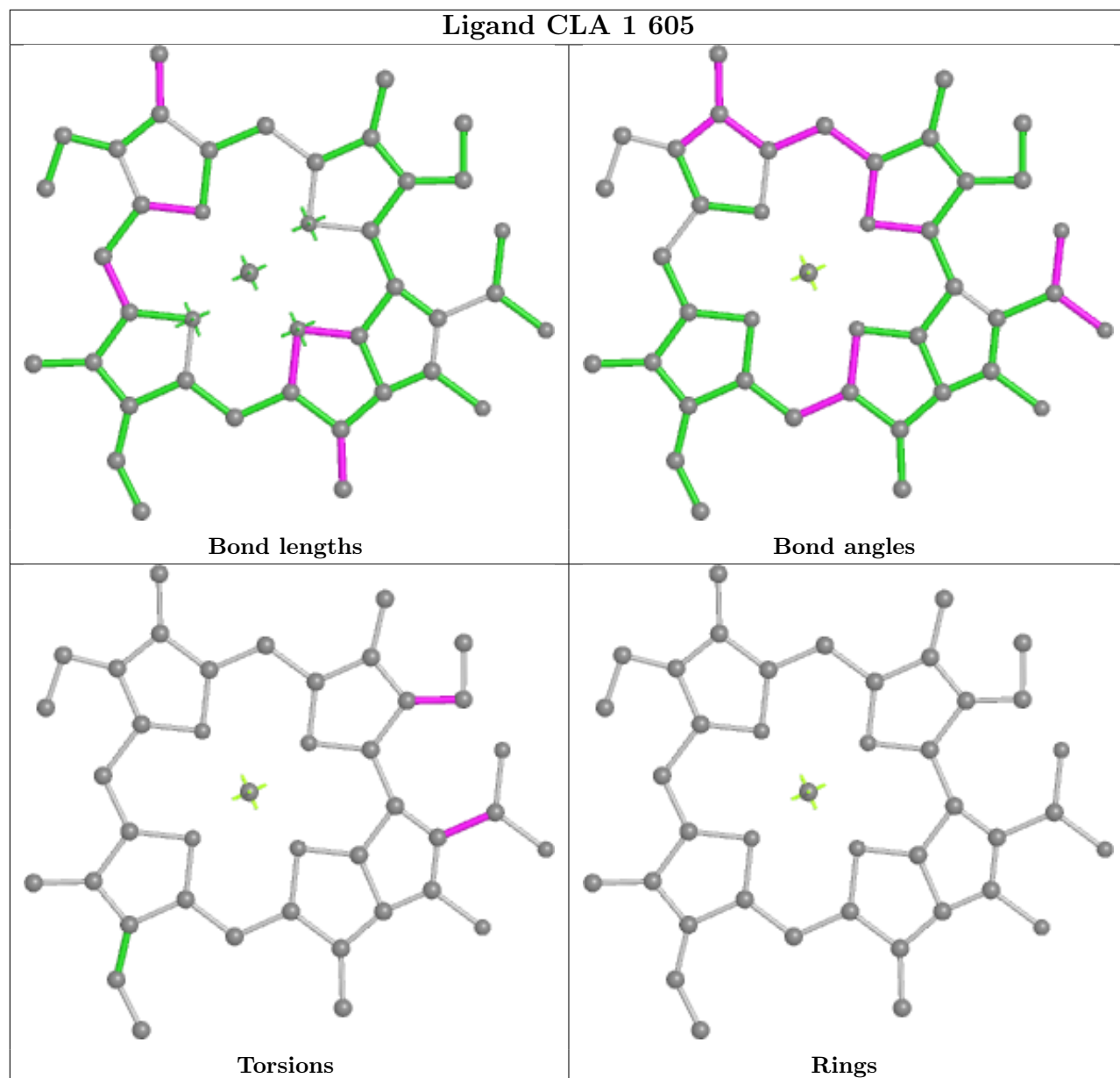
## Ligand CLA 6 611



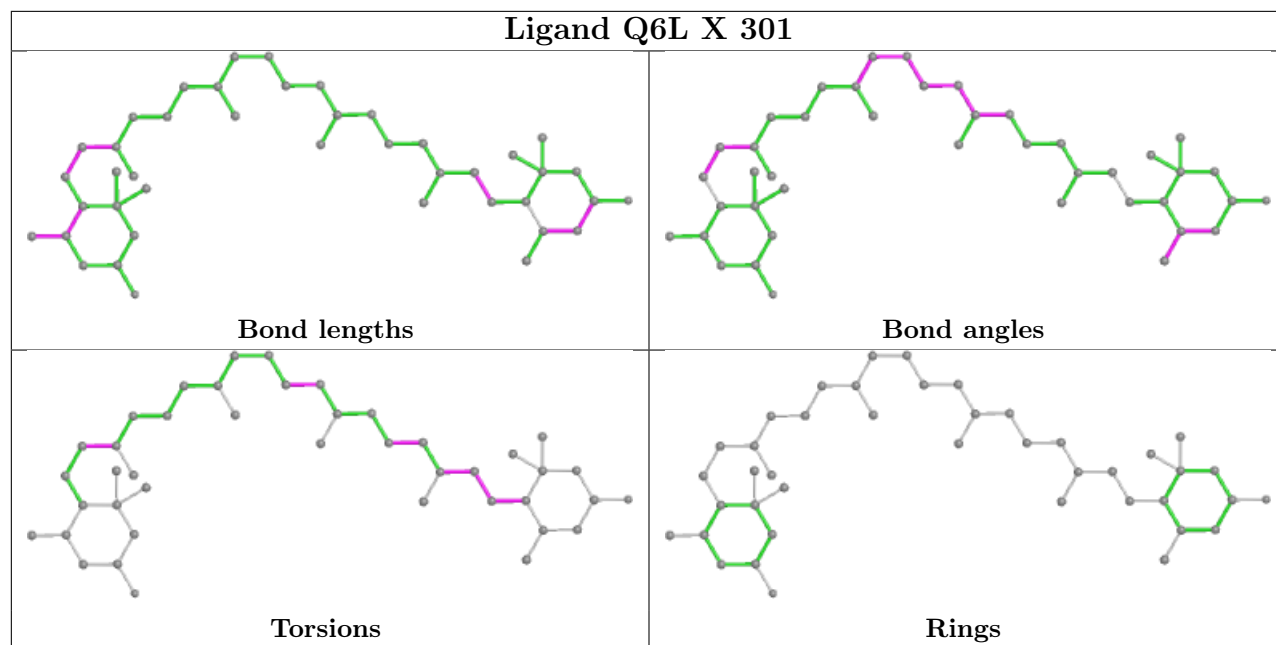
## Ligand CLA A 822



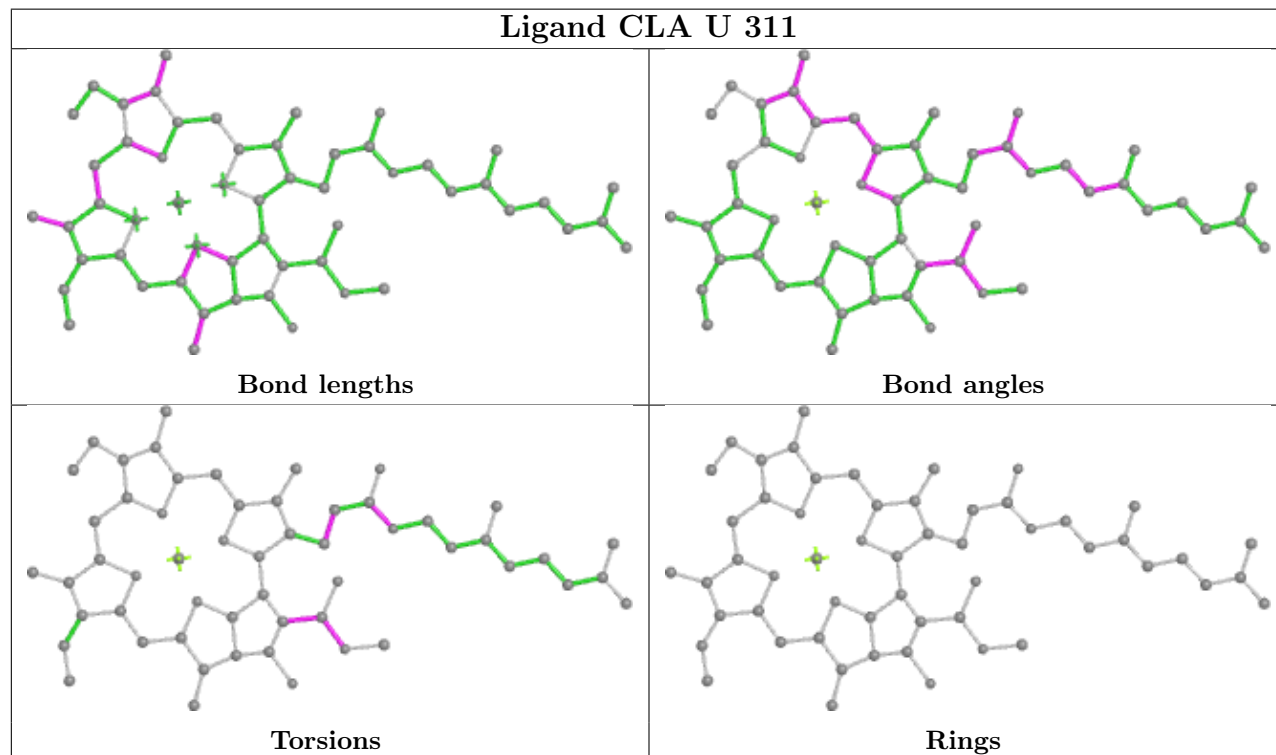
## Ligand CLA 1 605



## Ligand Q6L X 301

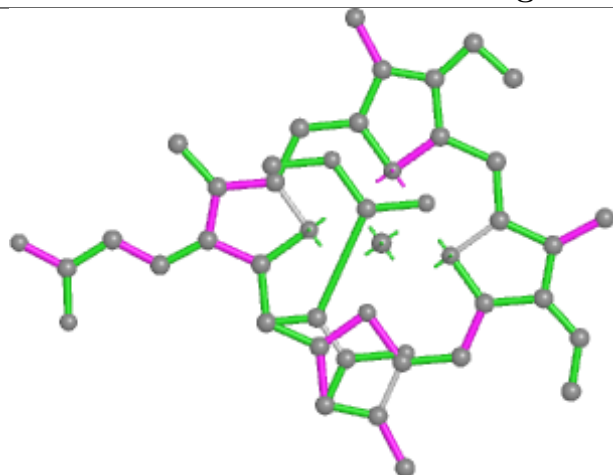


## Ligand CLA U 311

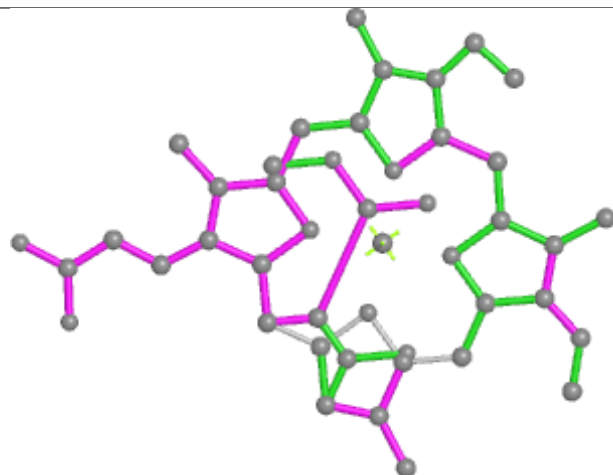




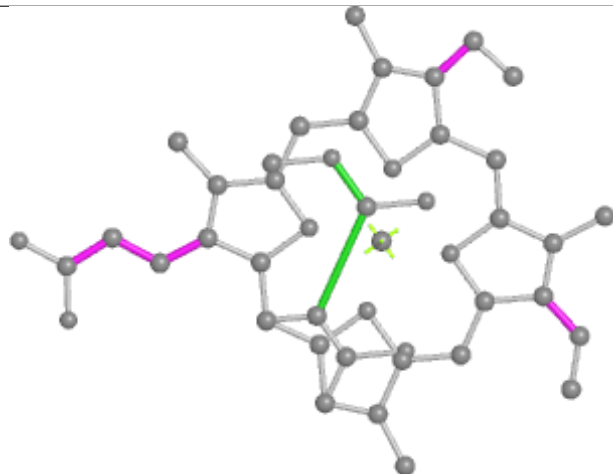
## Ligand KC2 T 308



Bond lengths



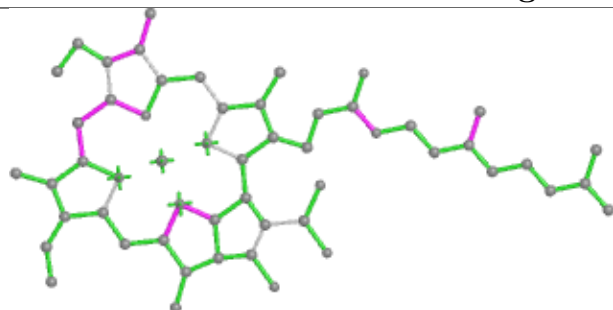
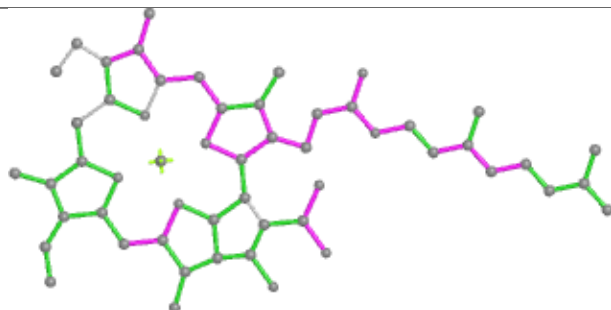
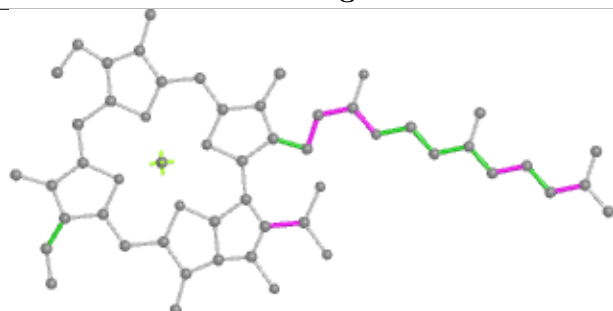
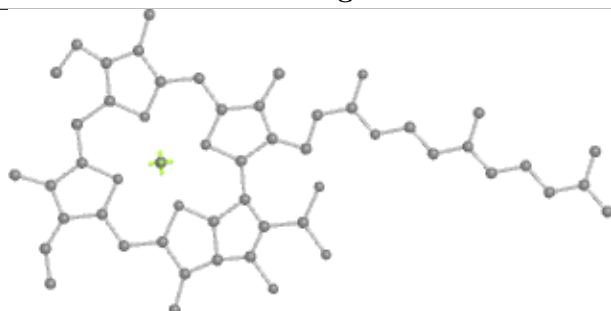
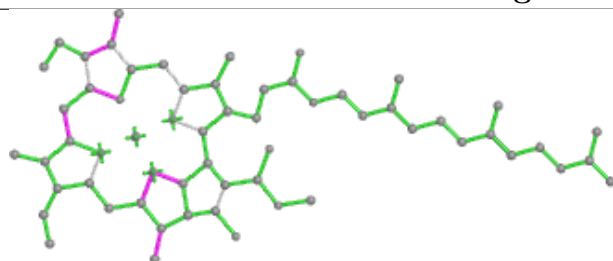
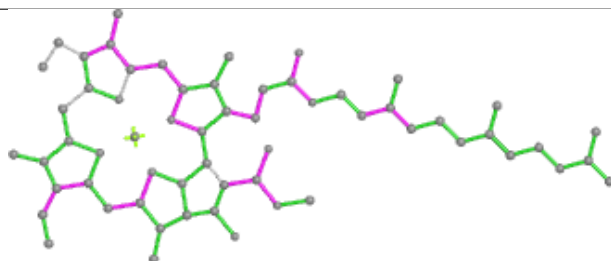
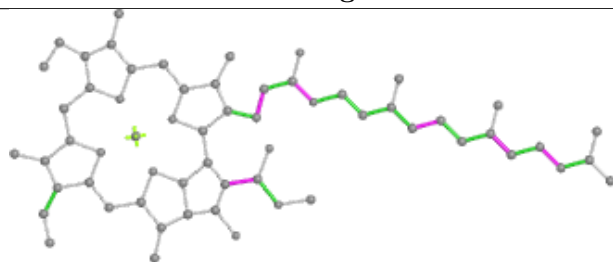
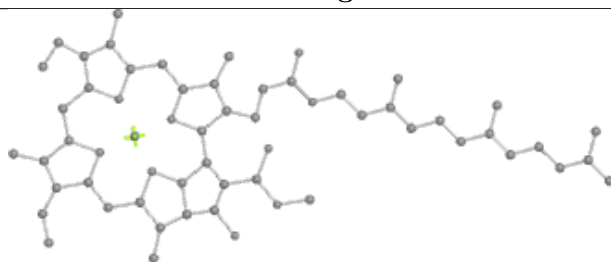
Bond angles



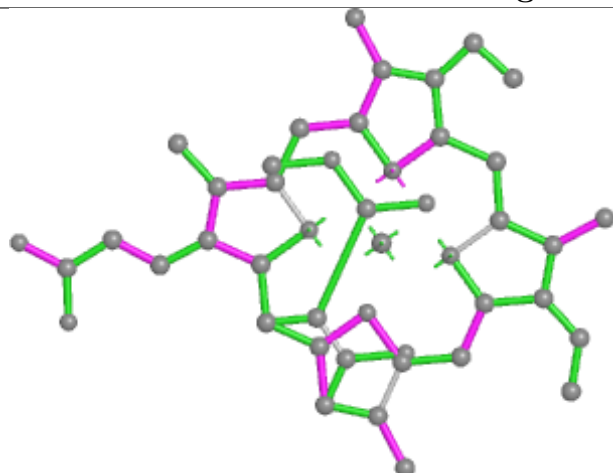
Torsions



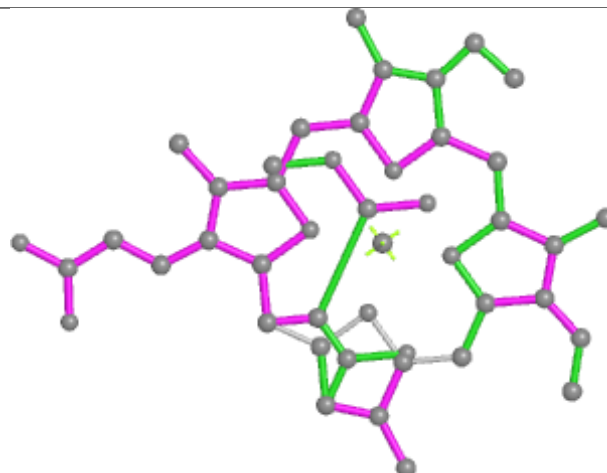
Rings

**Ligand CLA 3 311****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA R 315****Bond lengths****Bond angles****Torsions****Rings**

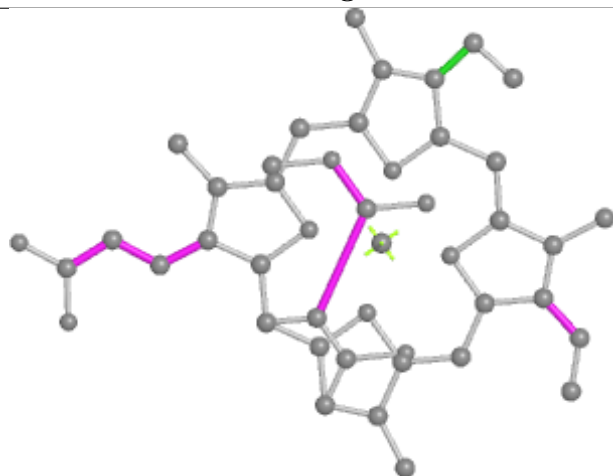
## Ligand KC2 P 308



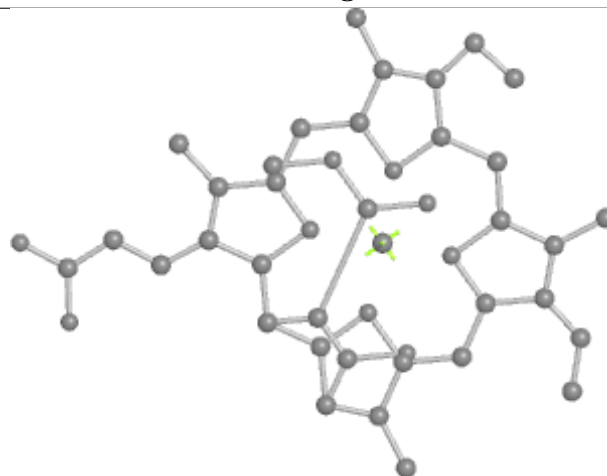
Bond lengths



Bond angles

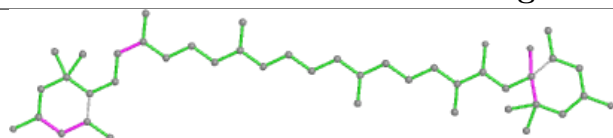


Torsions

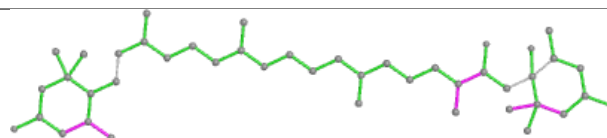


Rings

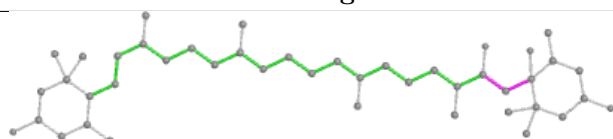
## Ligand IWJ T 321



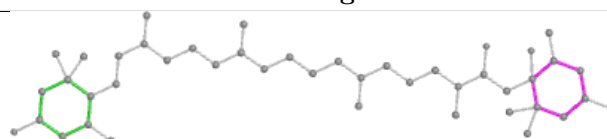
Bond lengths



Bond angles

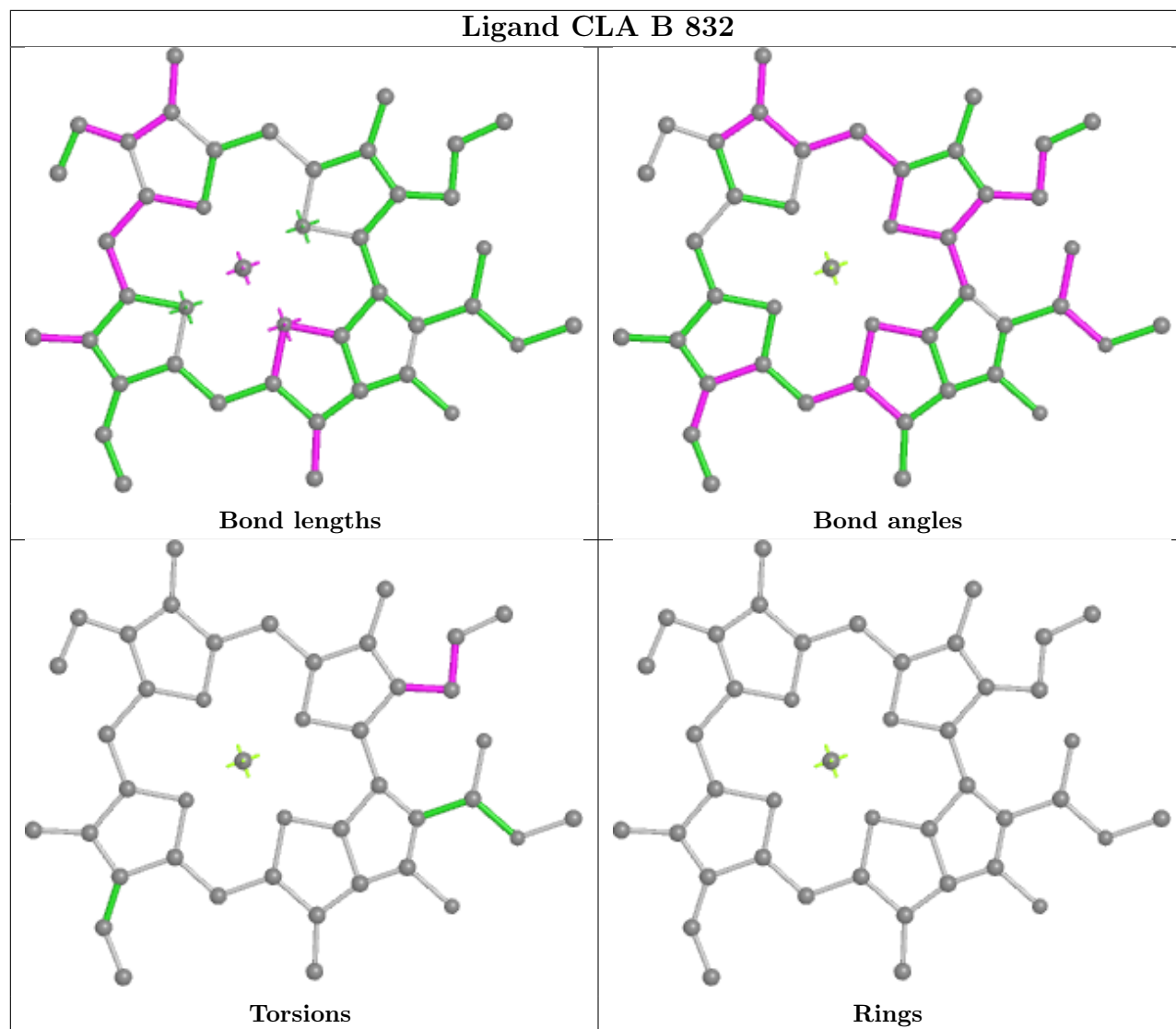


Torsions

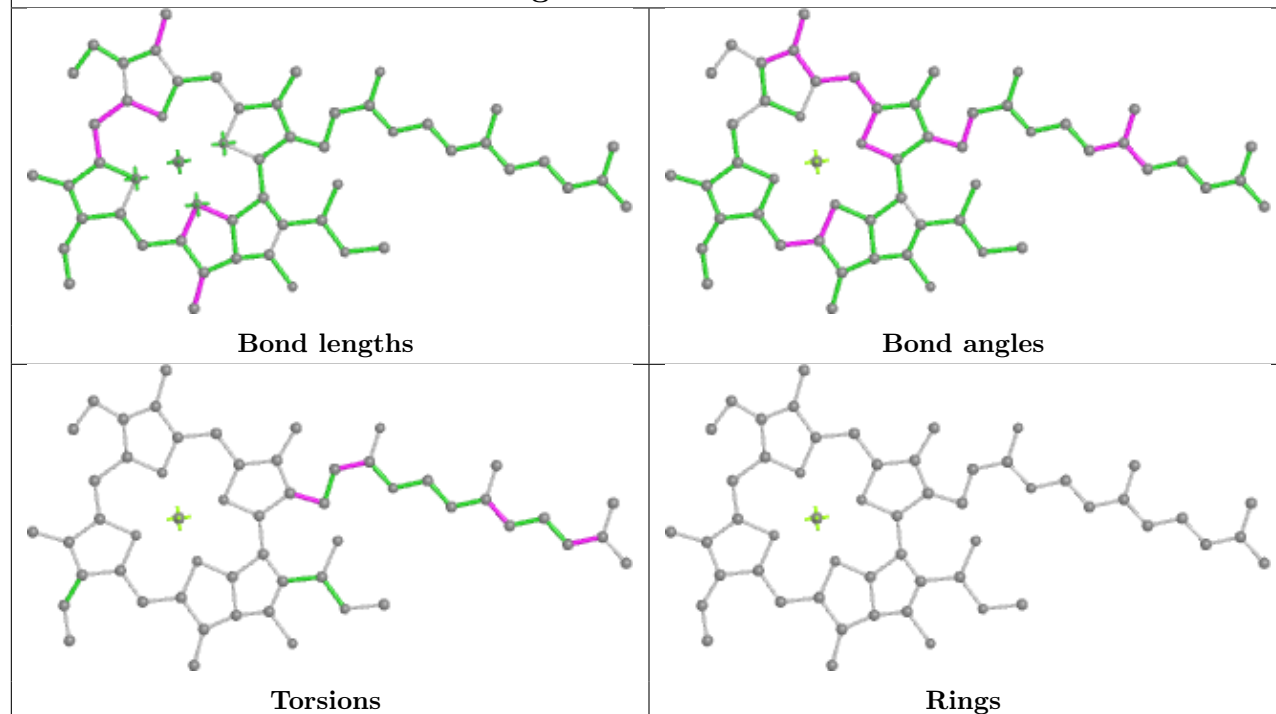


Rings

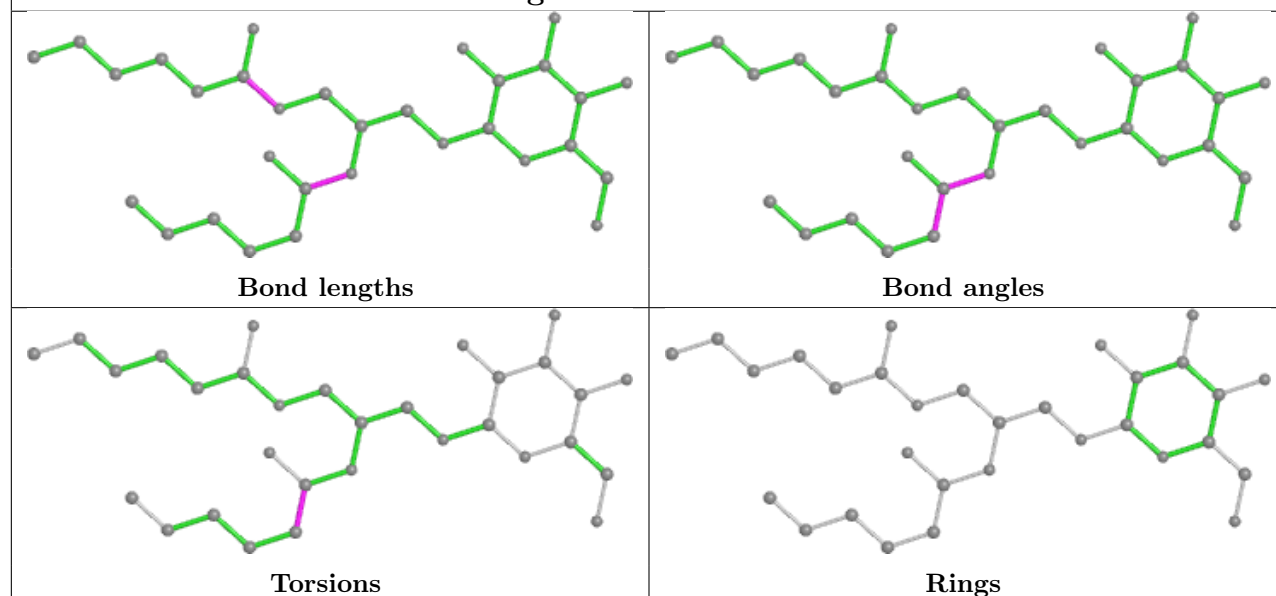
## Ligand CLA B 832



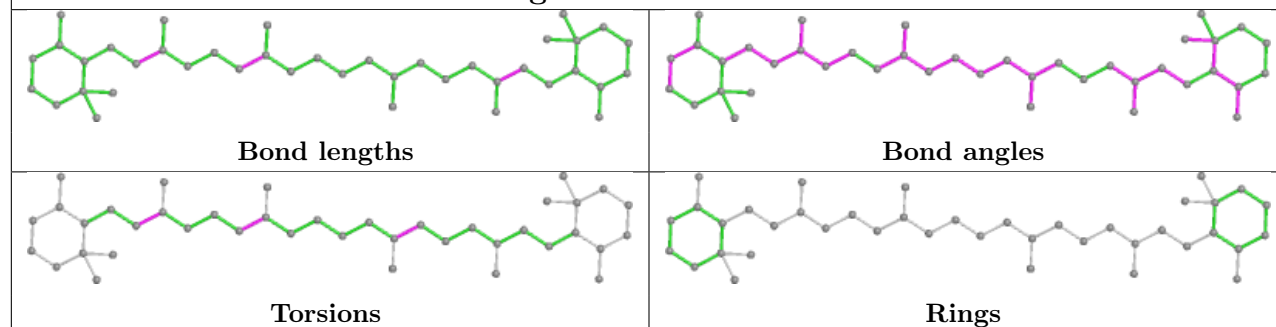
## Ligand CLA A 840

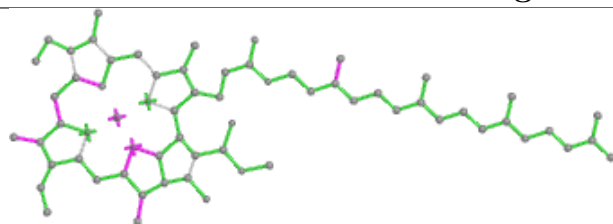
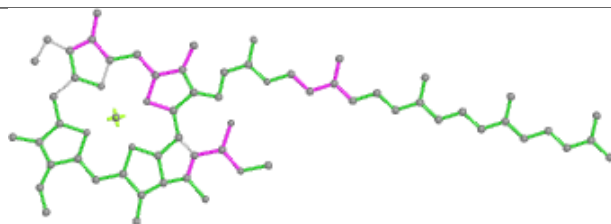
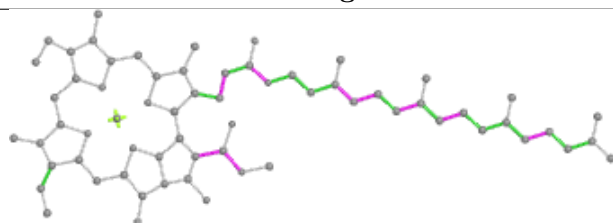
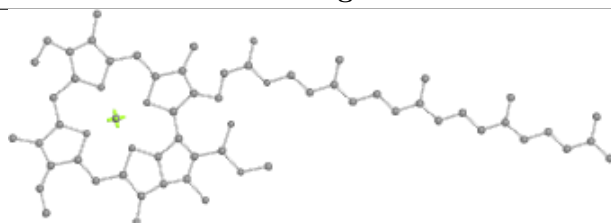
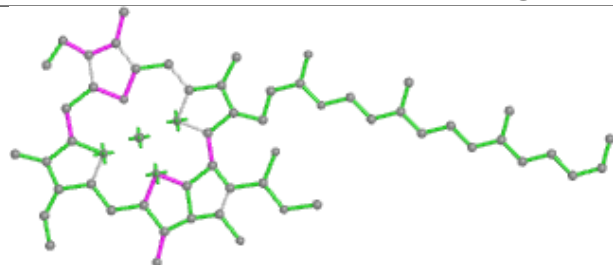
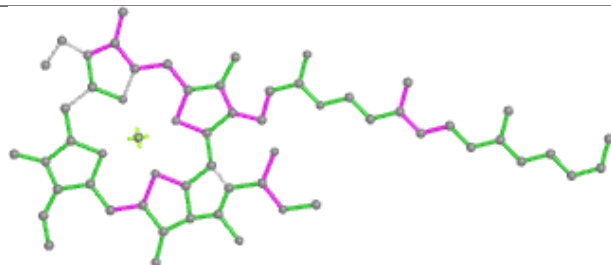
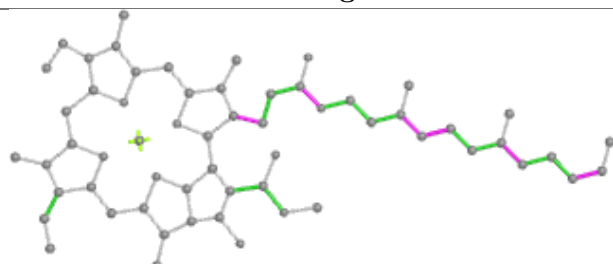
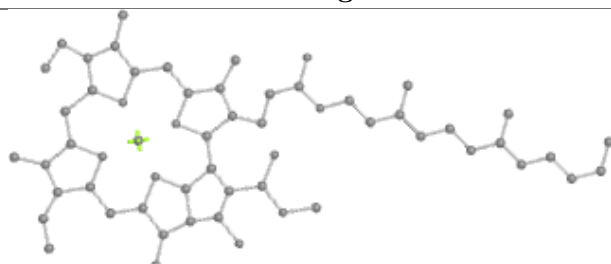


## Ligand LMG A 801

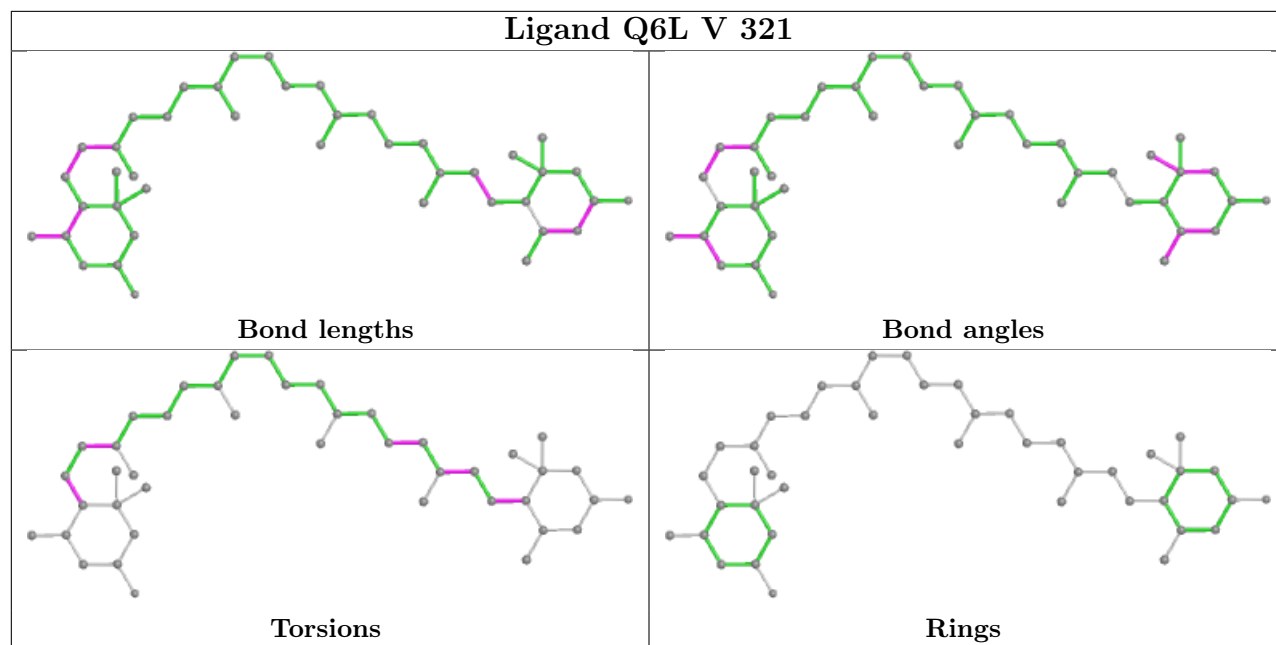


## Ligand BCR H 305

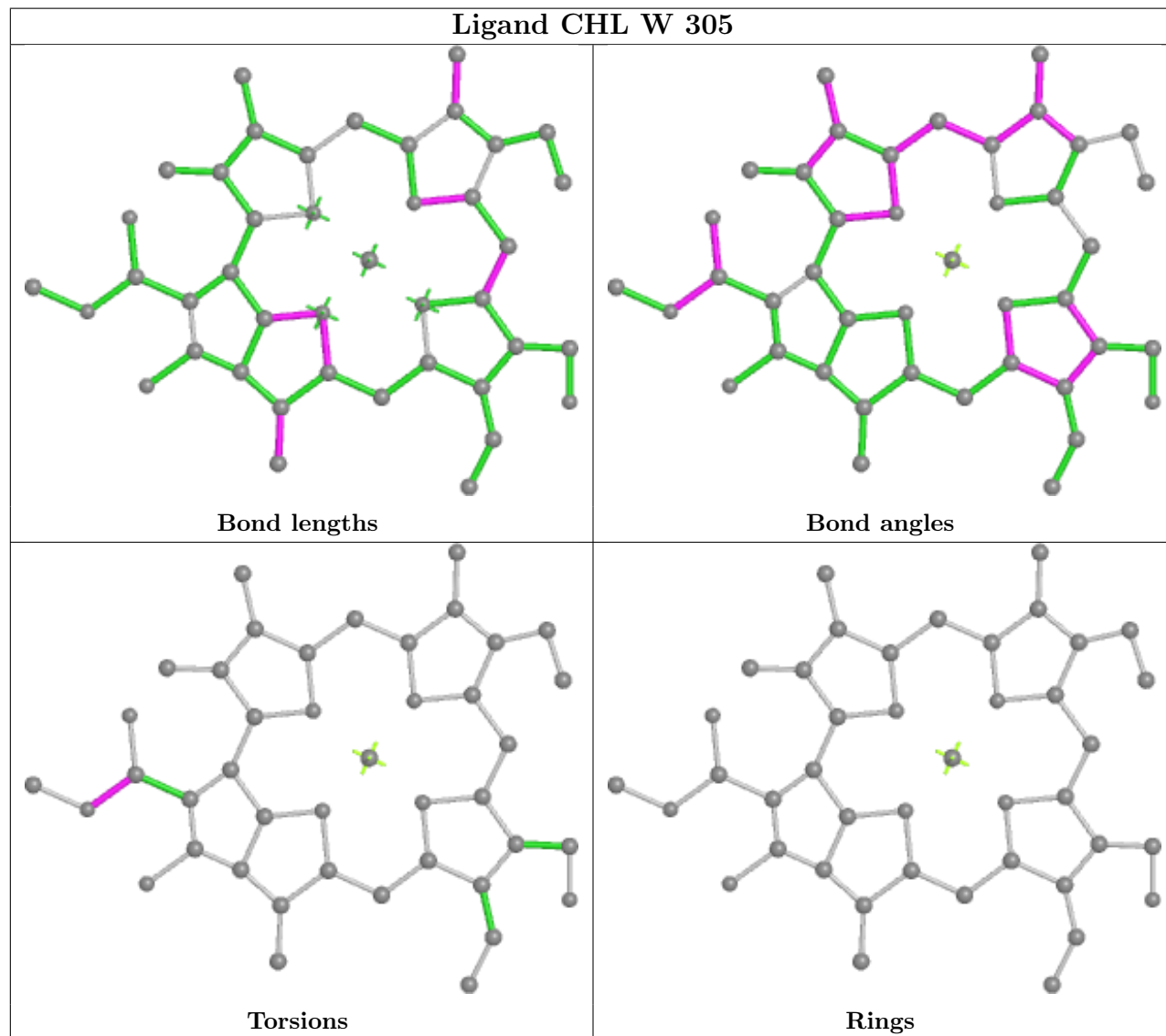


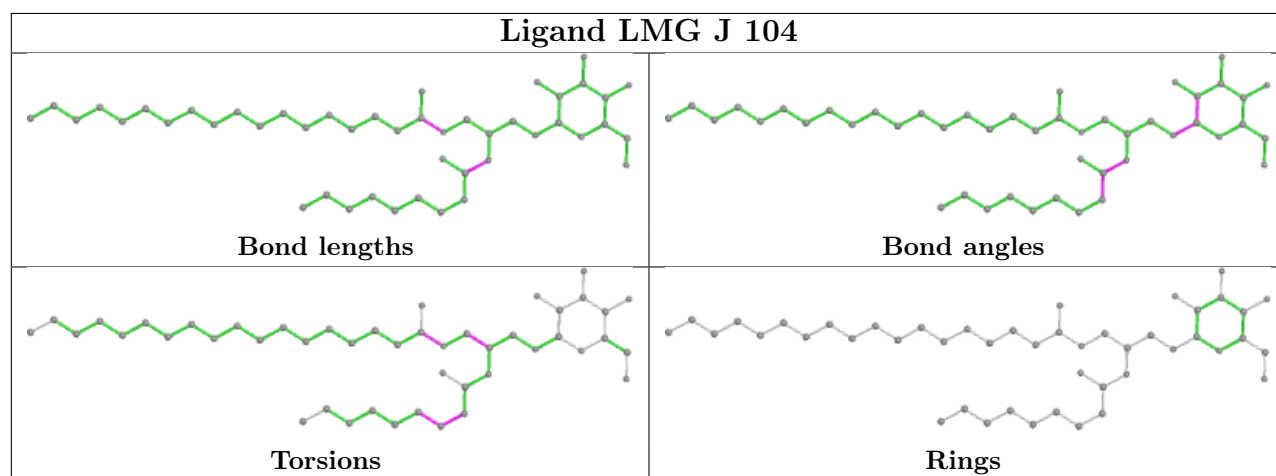
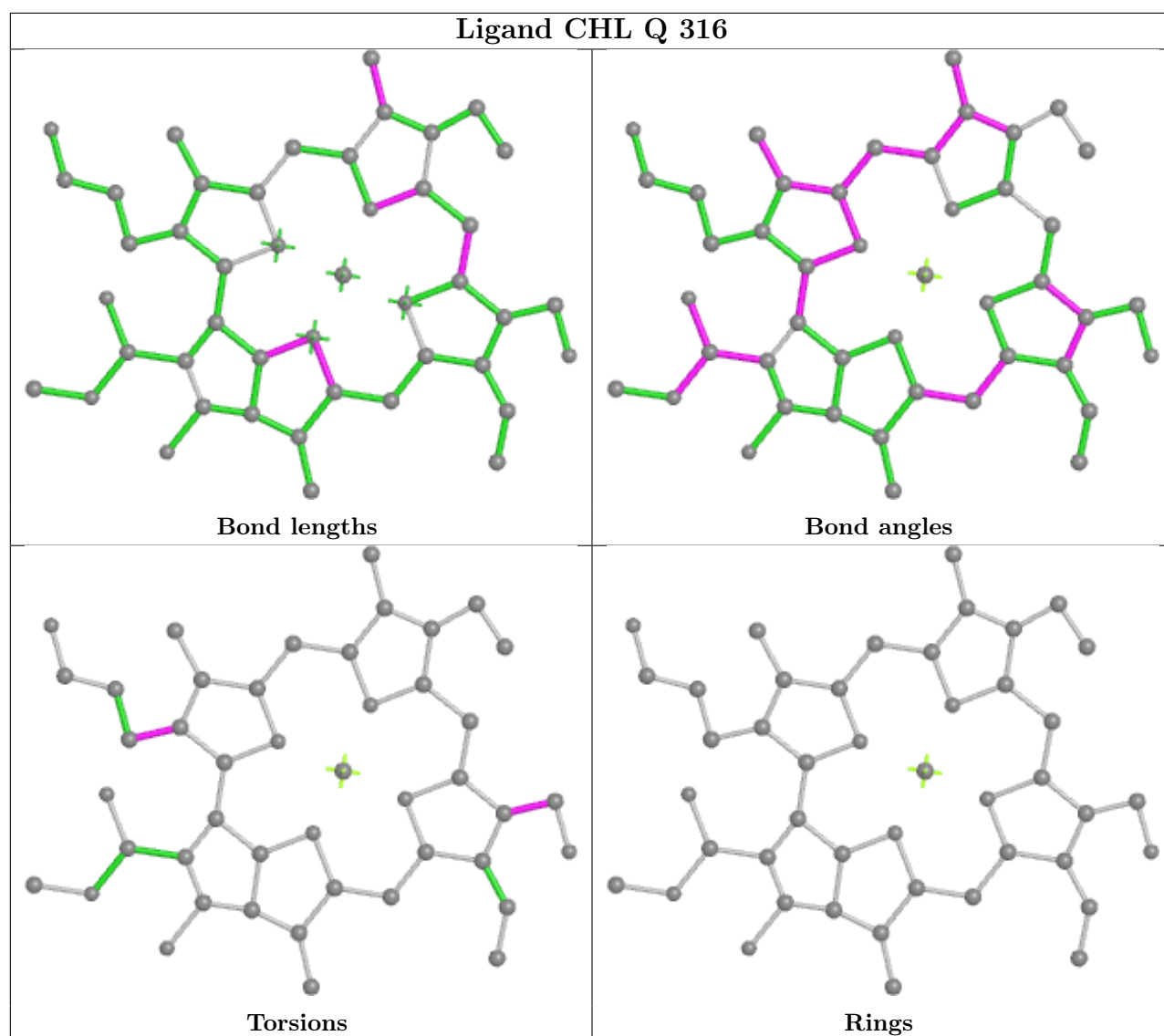
**Ligand CLA B 815****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA T 309****Bond lengths****Bond angles****Torsions****Rings**

## Ligand Q6L V 321

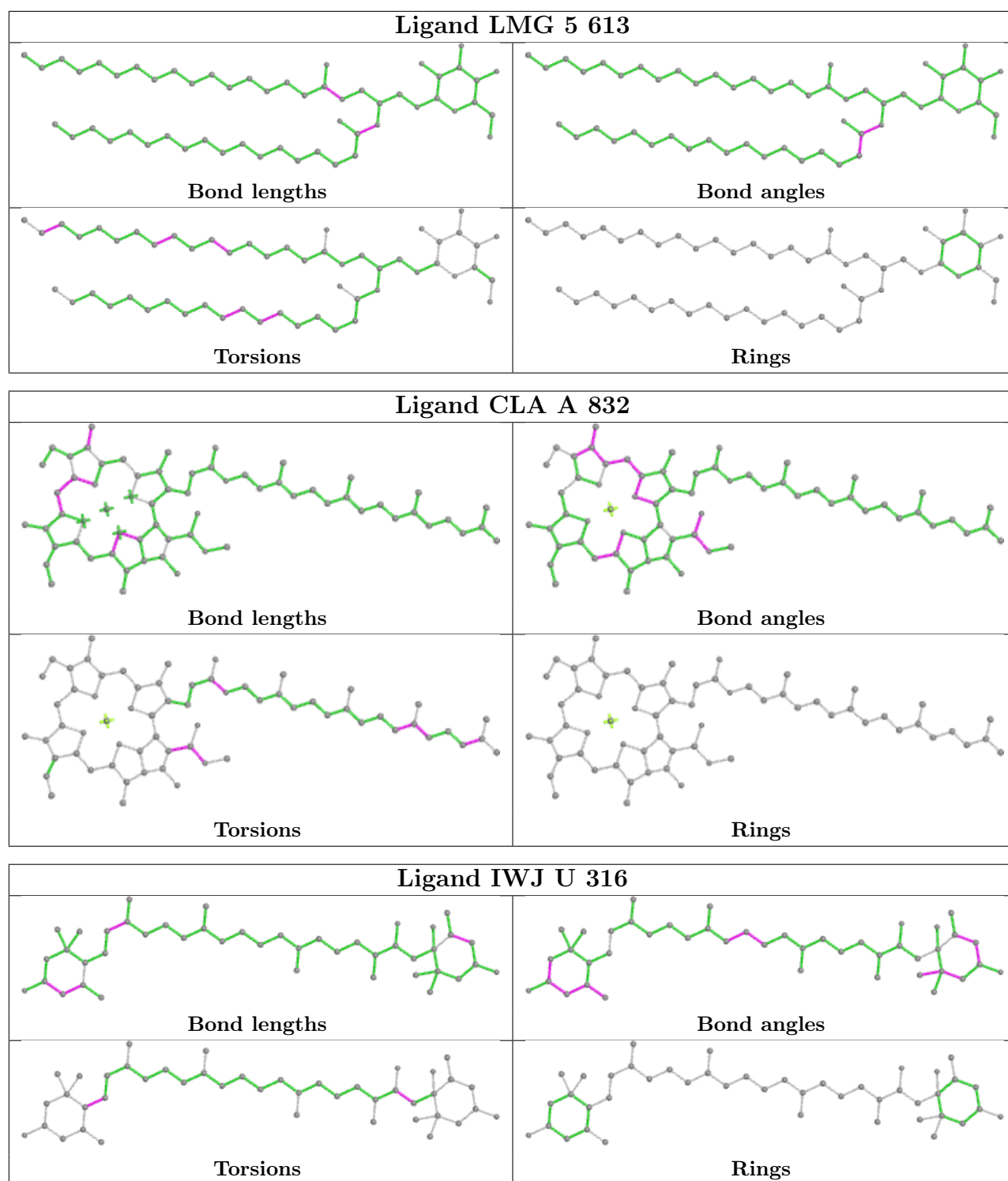


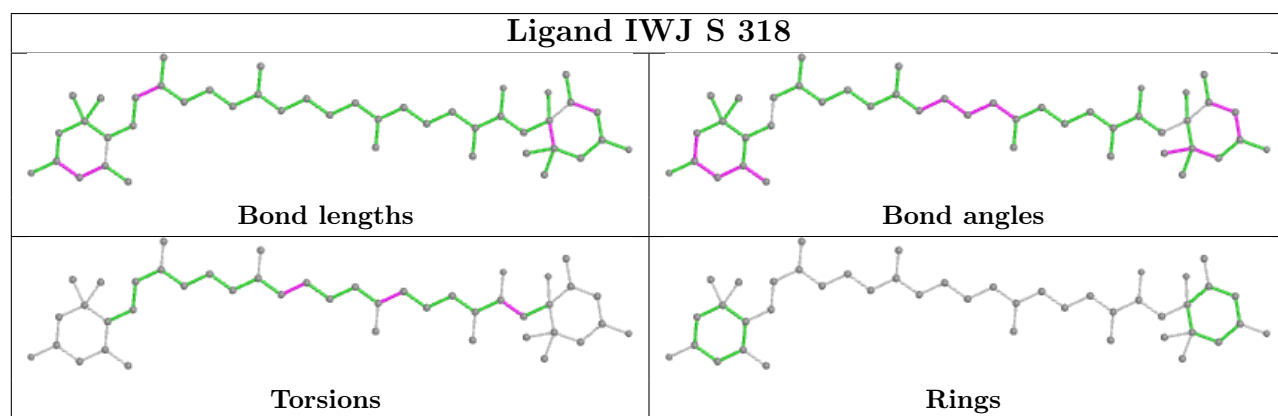
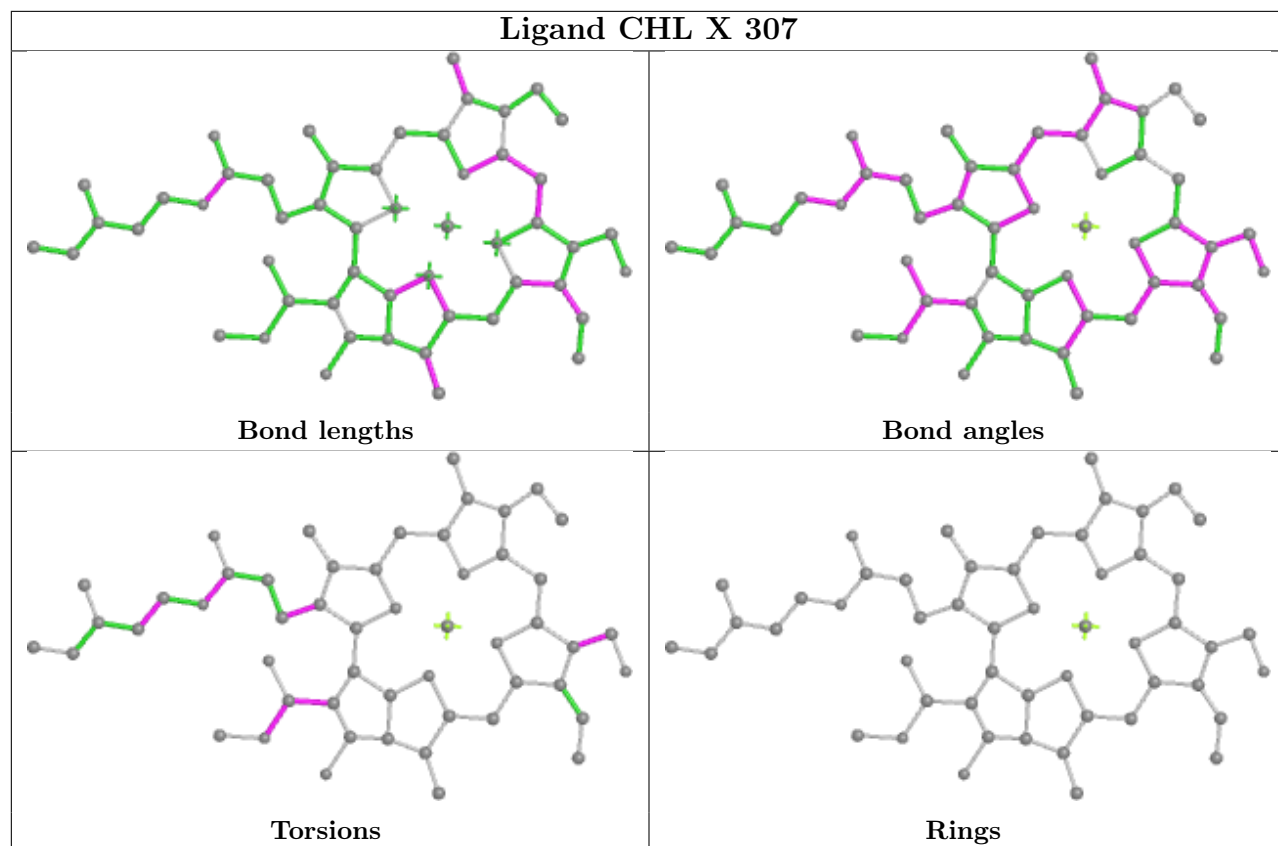
## Ligand CHL W 305



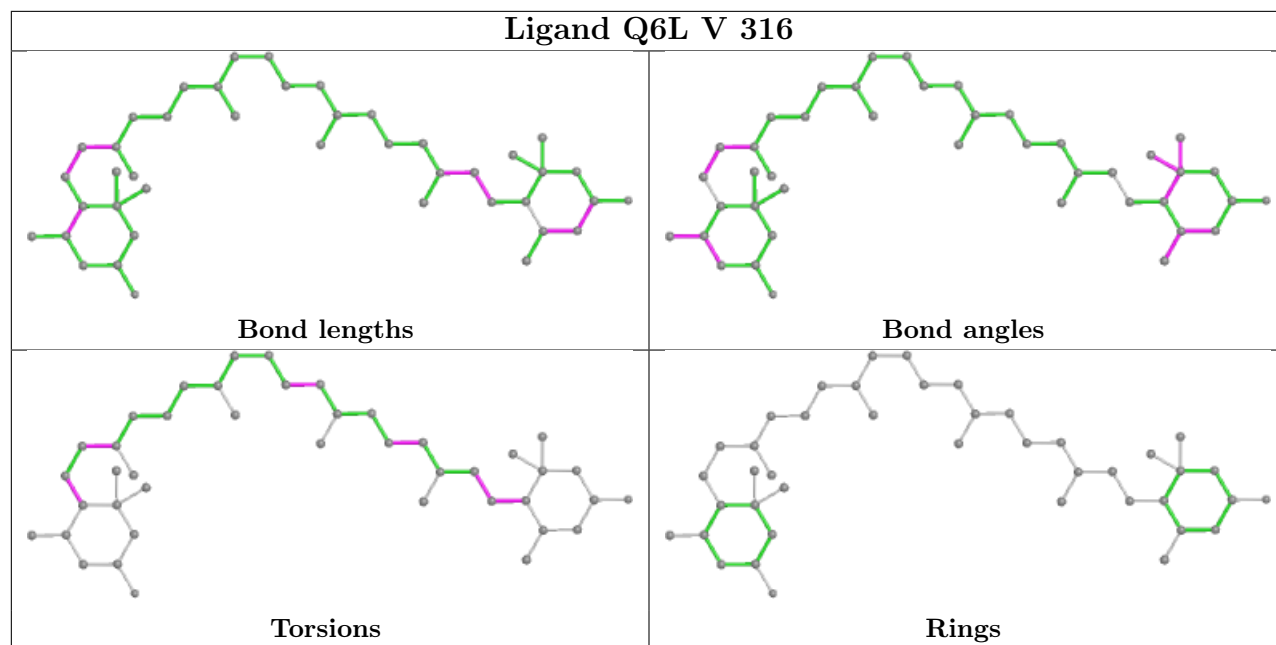




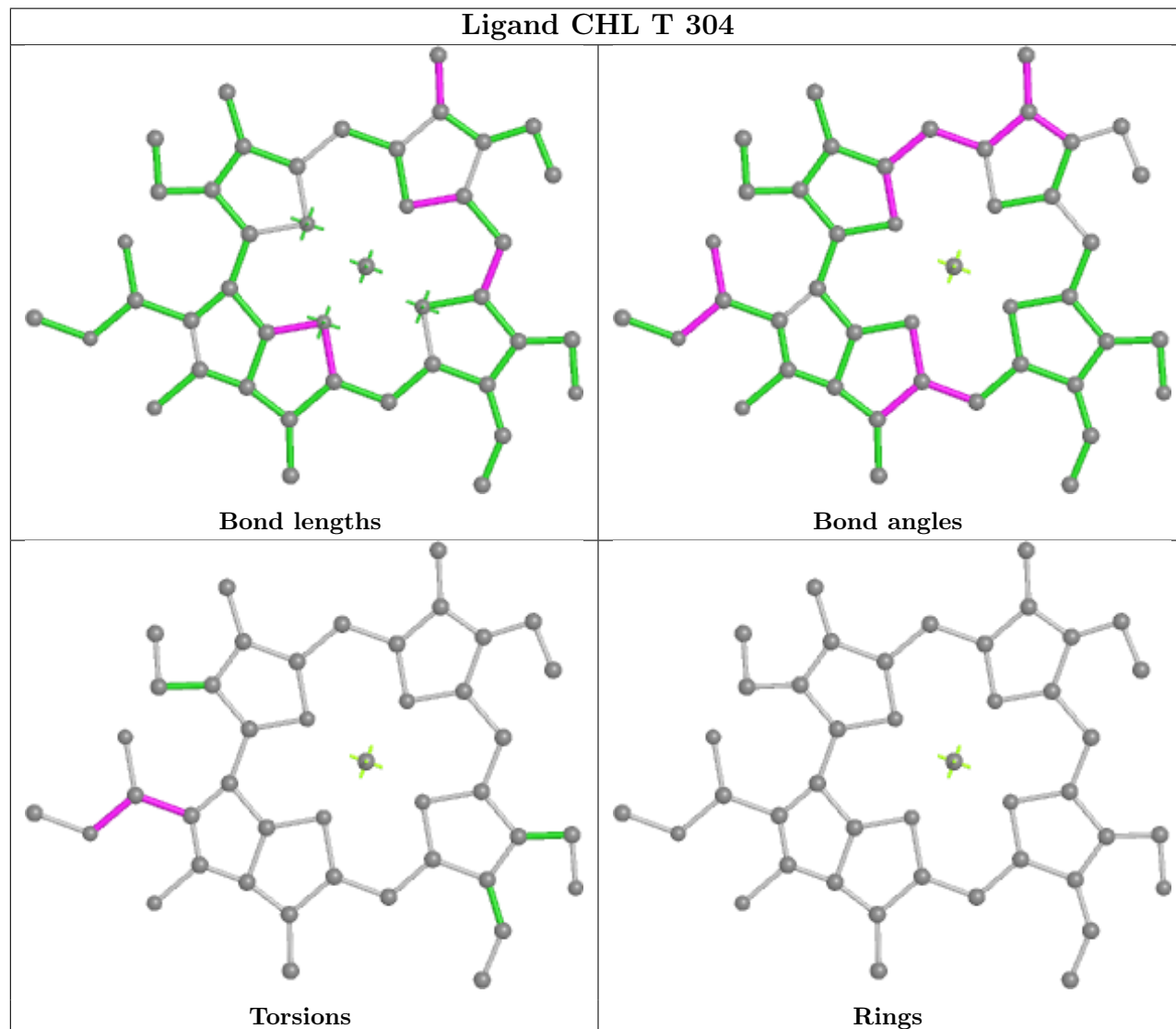


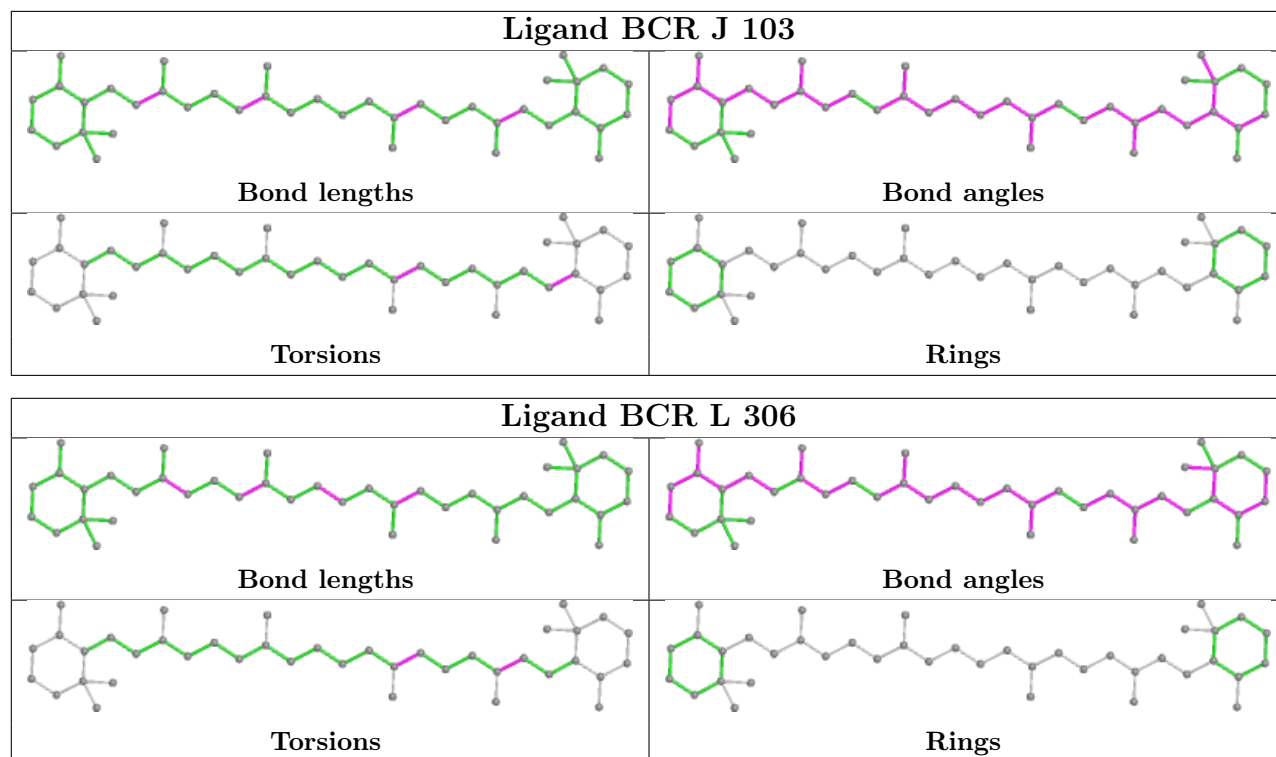


## Ligand Q6L V 316

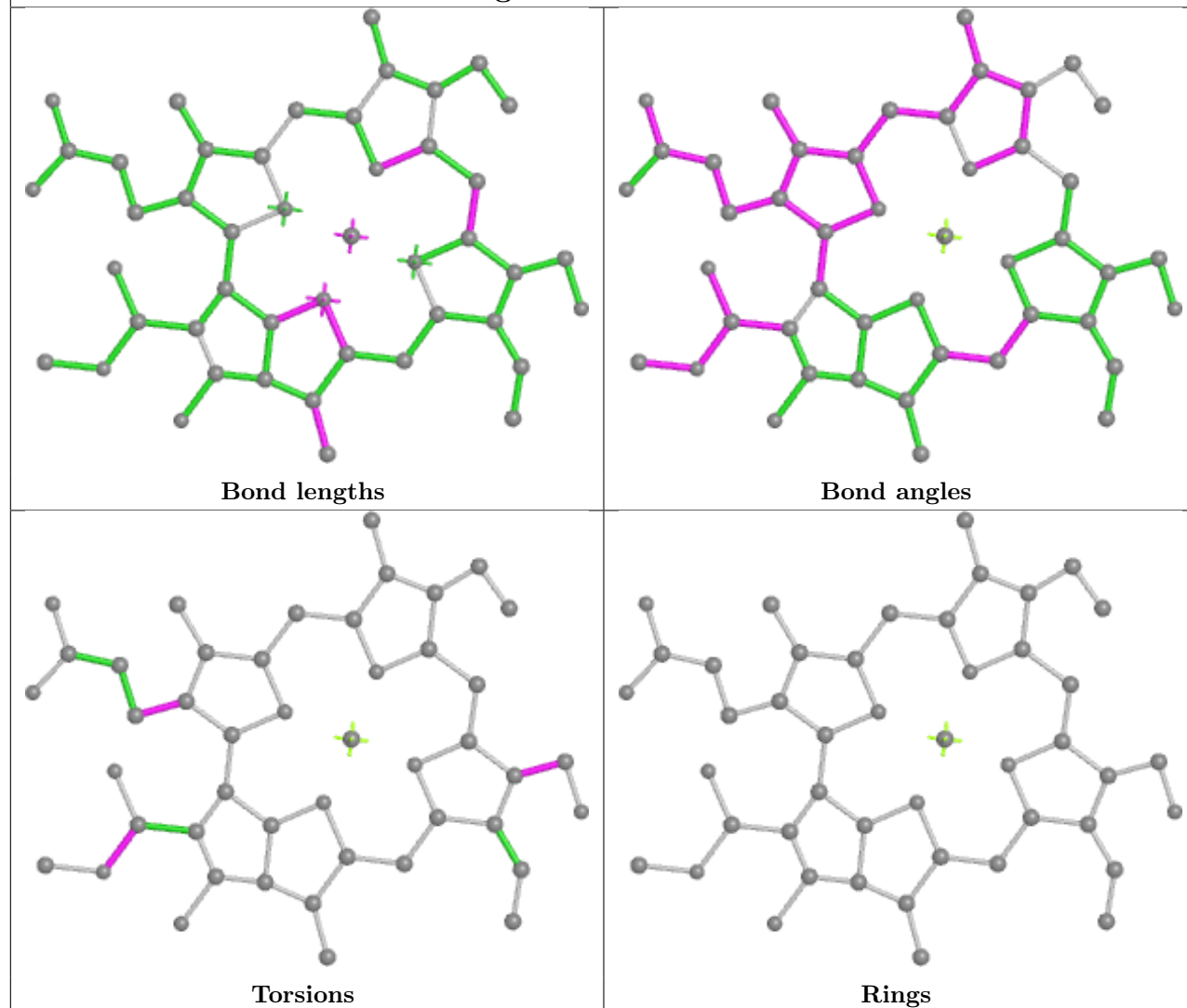


## Ligand CHL T 304

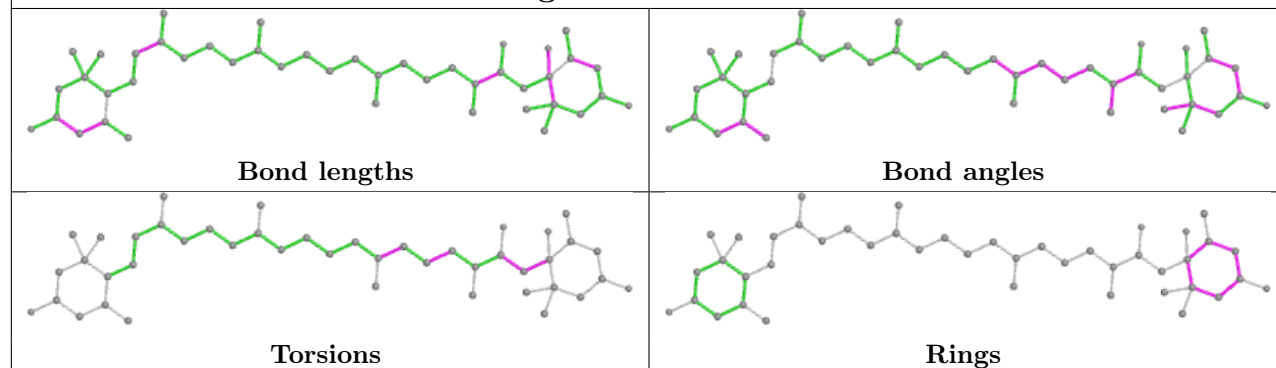


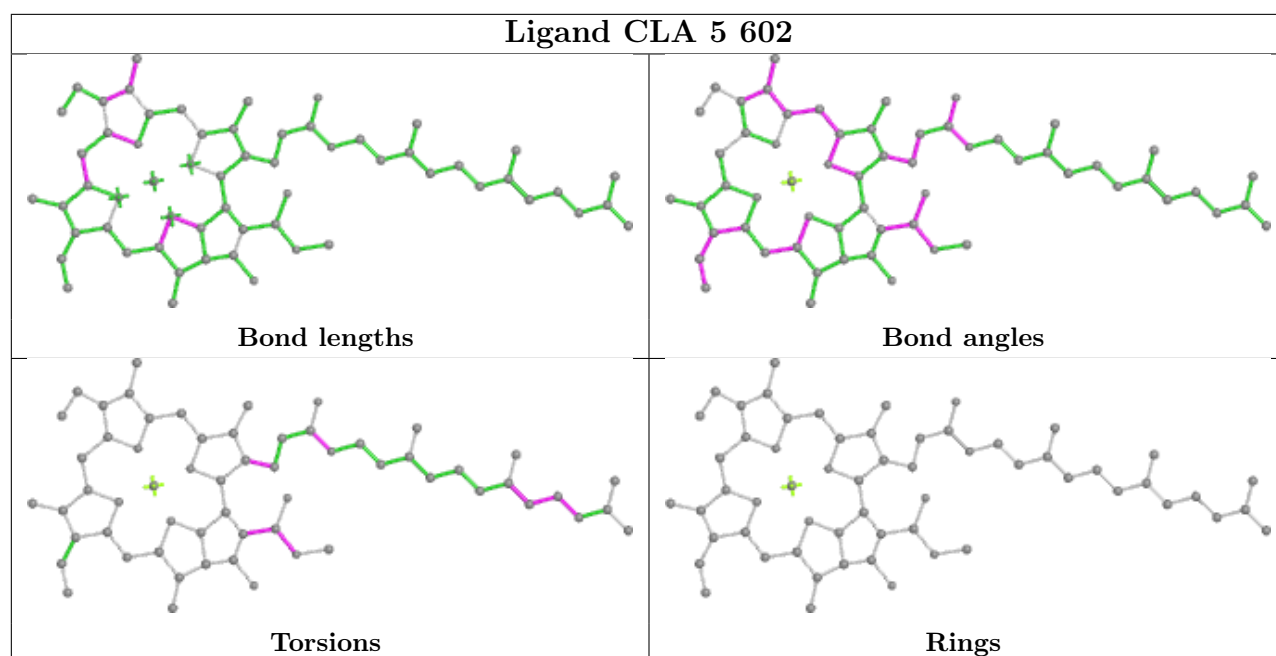


## Ligand CHL P 304

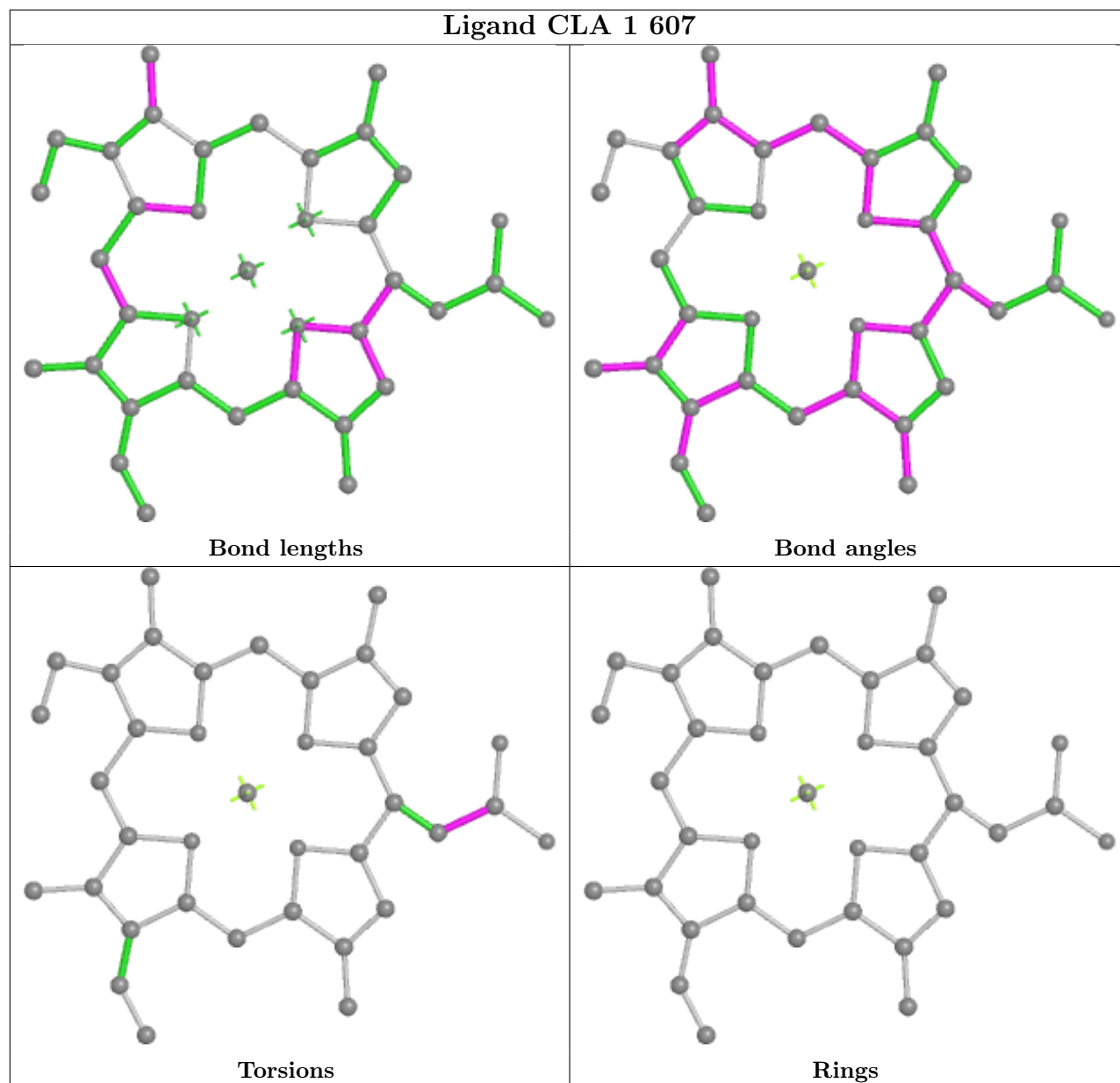


## Ligand IWJ S 319

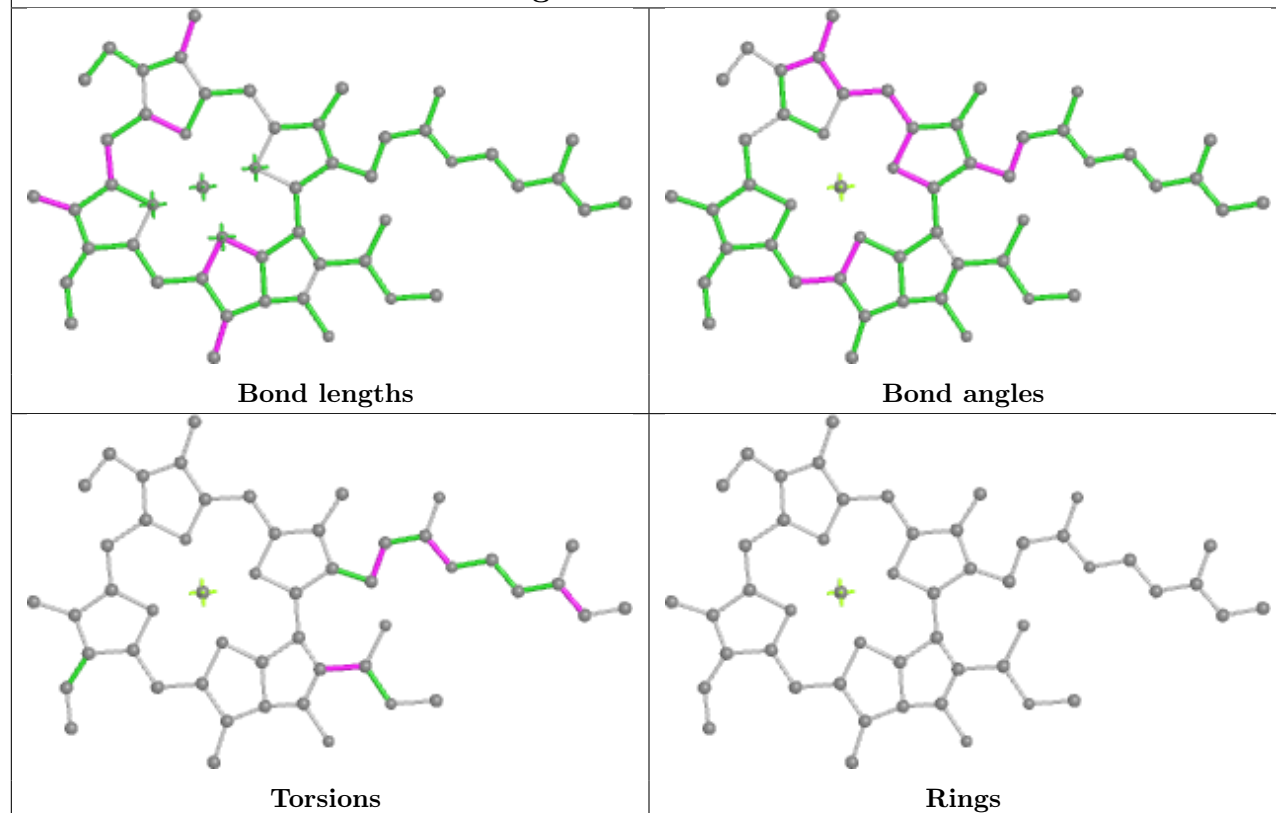




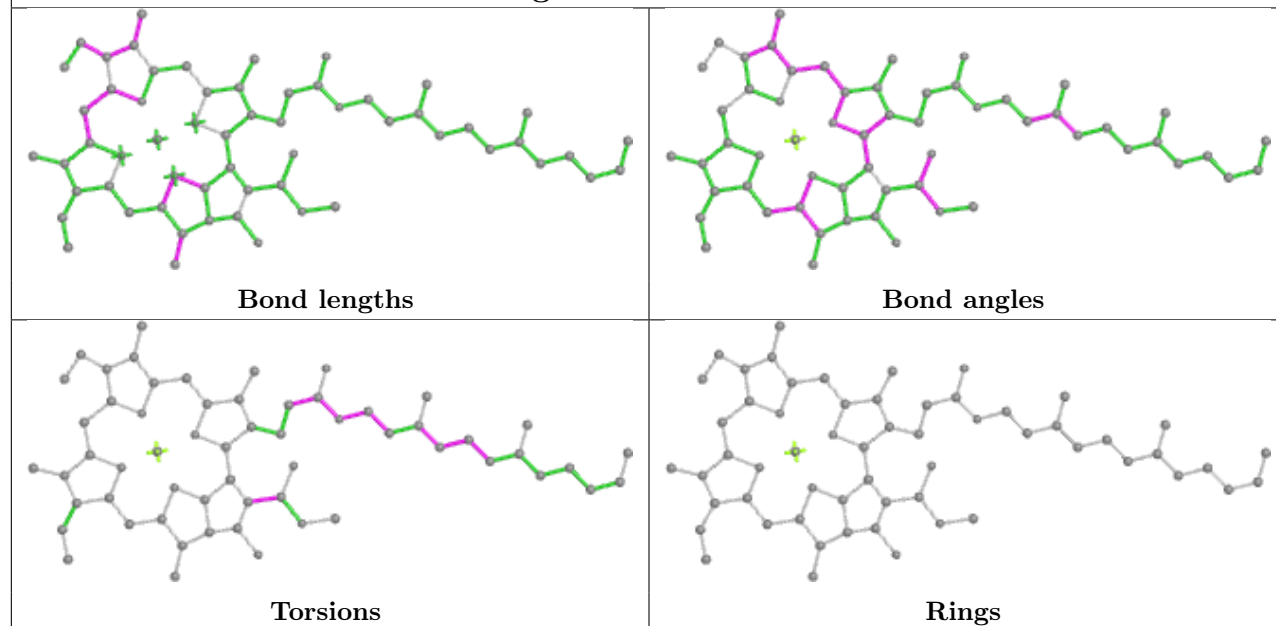
## Ligand CLA 1 607



## Ligand CLA B 816

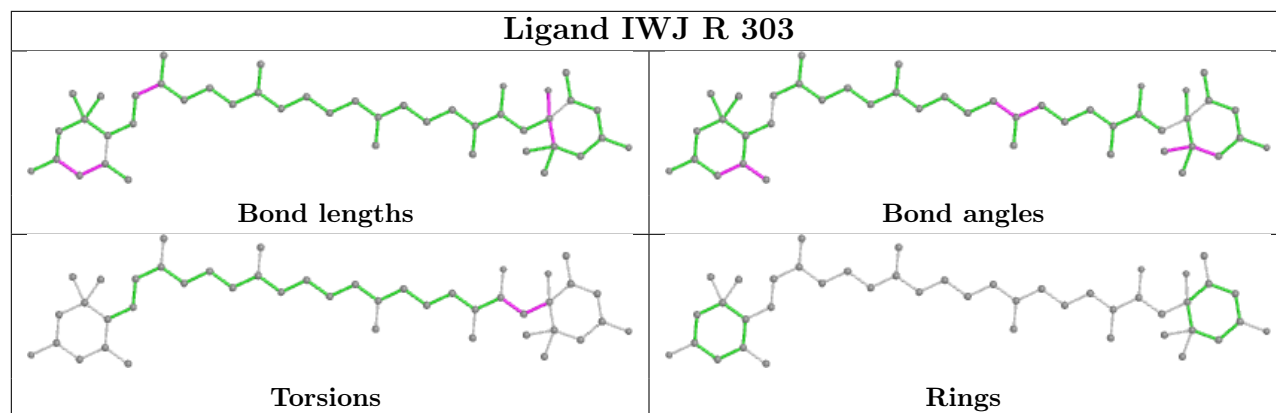


## Ligand CLA B 819

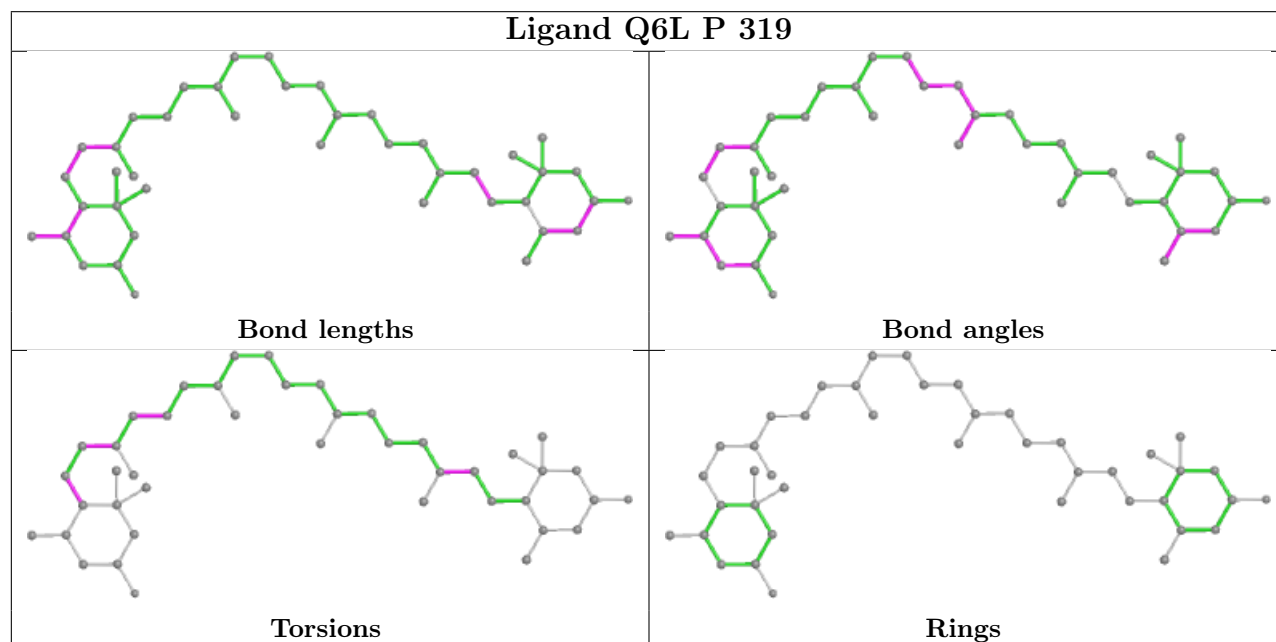




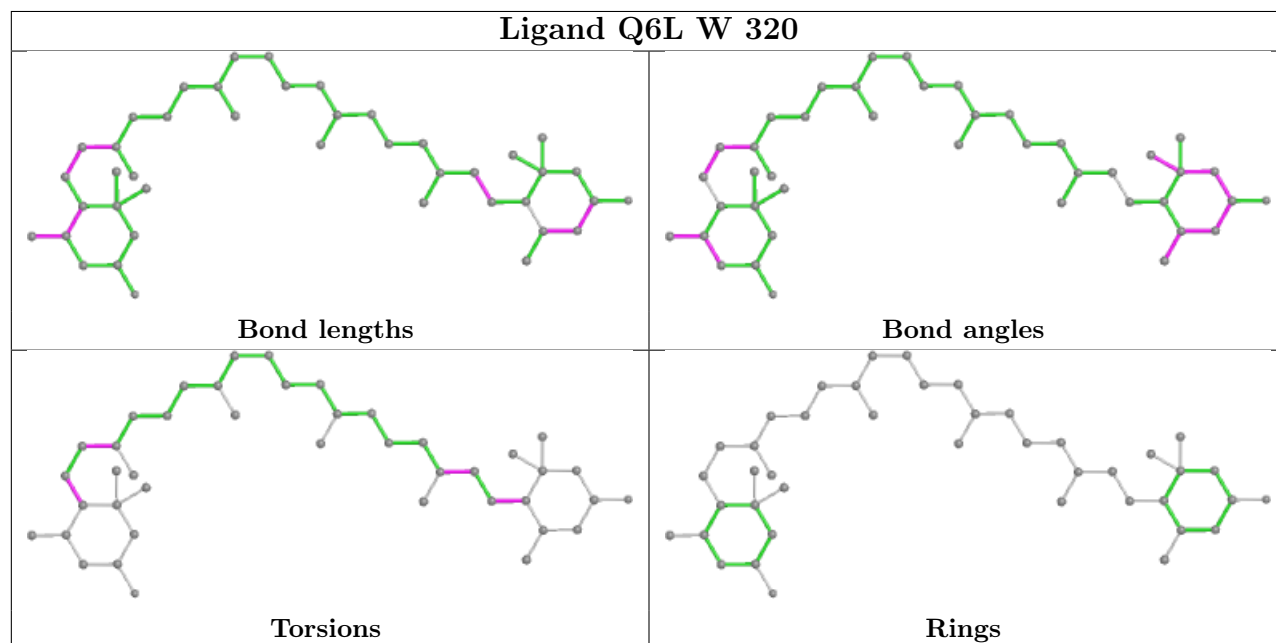
## Ligand IWJ R 303

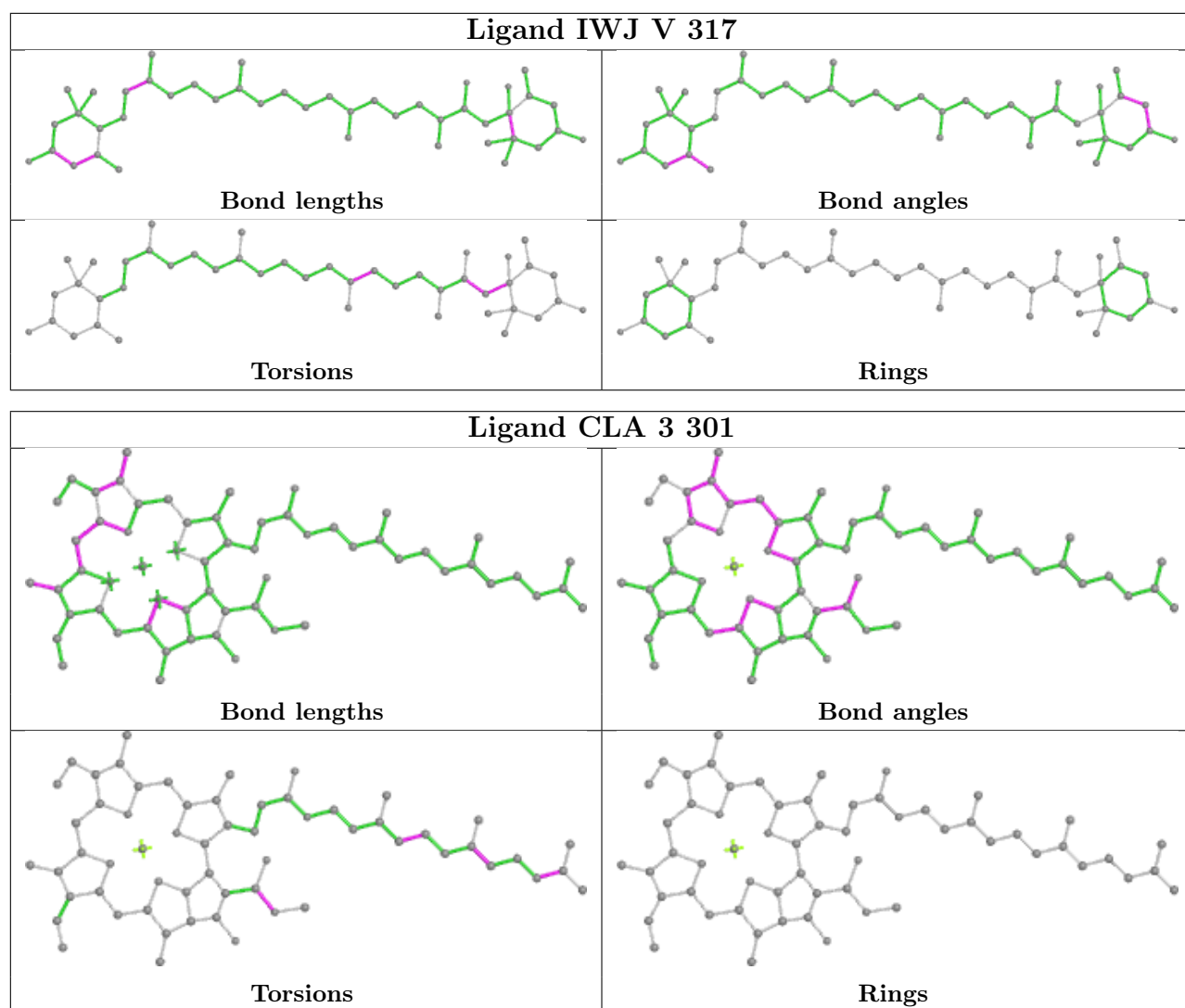


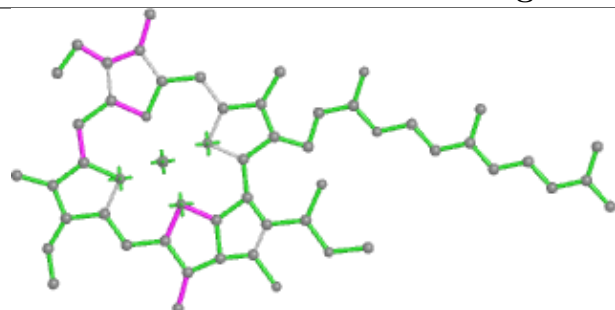
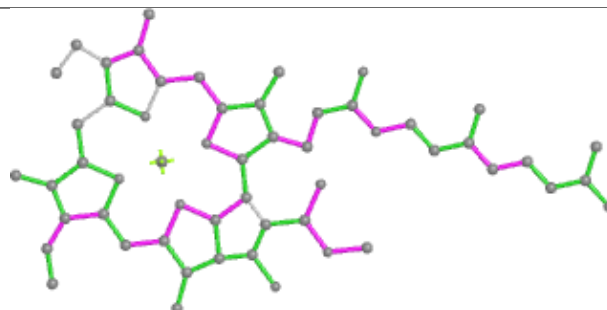
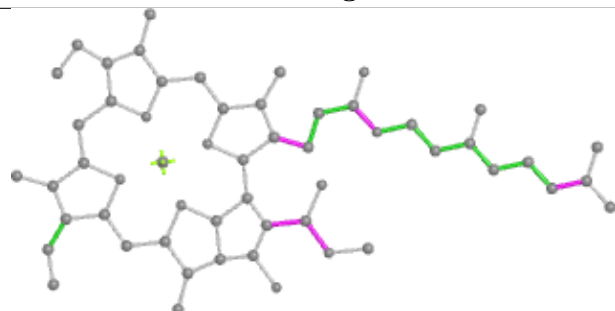
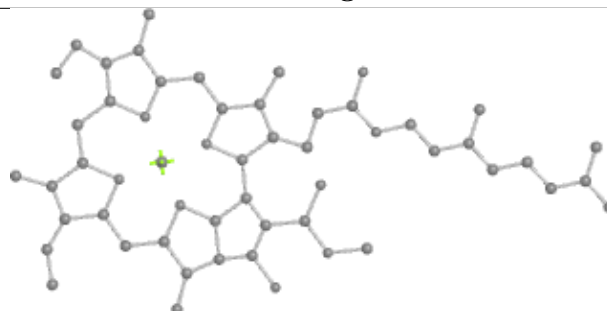
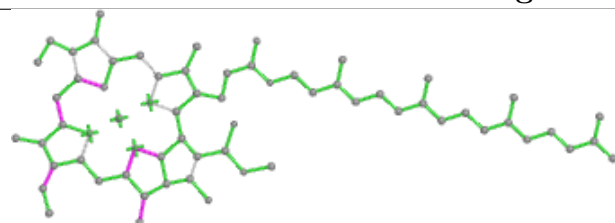
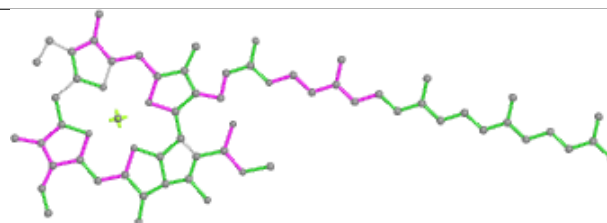
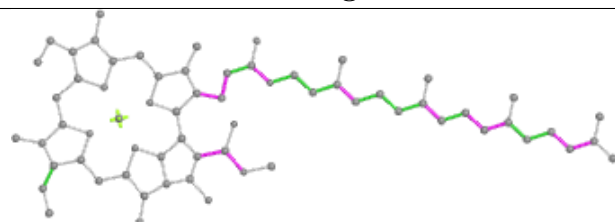
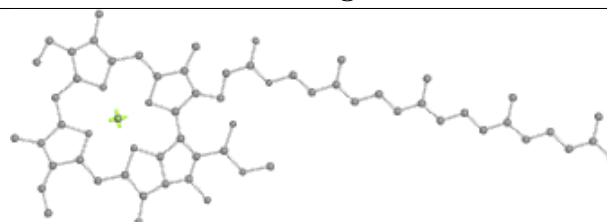
## Ligand Q6L P 319



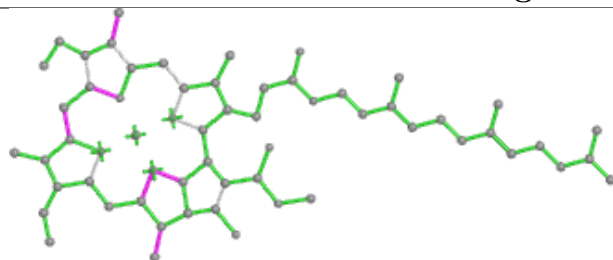
## Ligand Q6L W 320



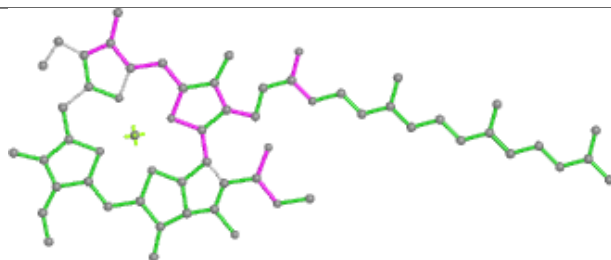


**Ligand CLA B 818****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 825****Bond lengths****Bond angles****Torsions****Rings**

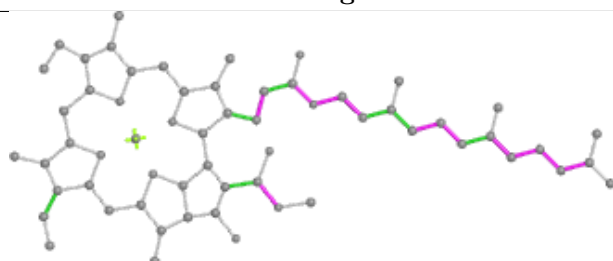
## Ligand CLA T 311



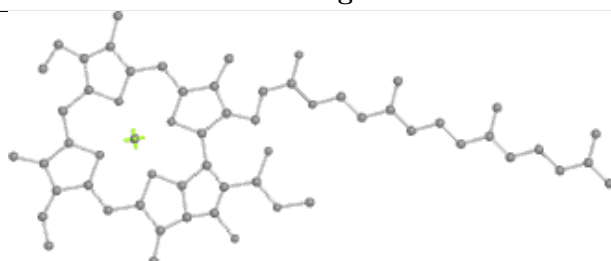
Bond lengths



Bond angles

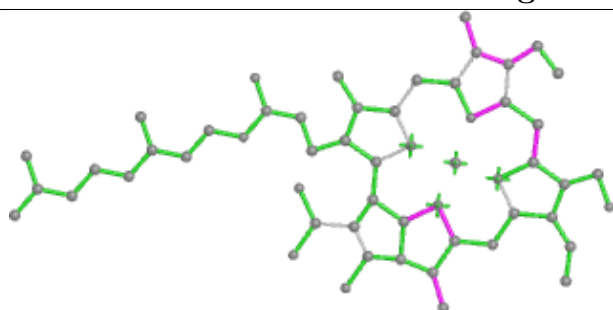


Torsions

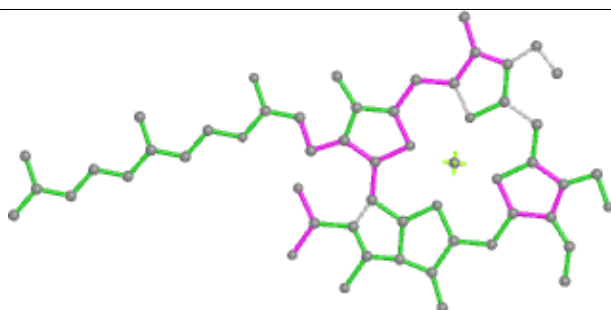


Rings

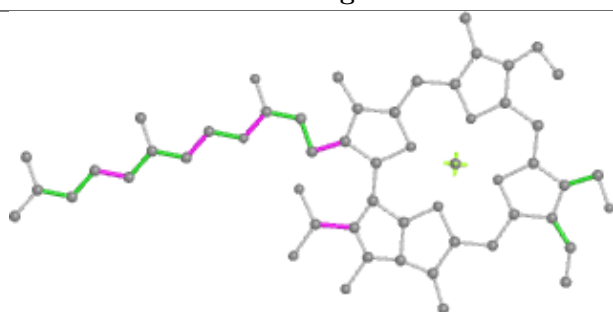
## Ligand CHL 1 601



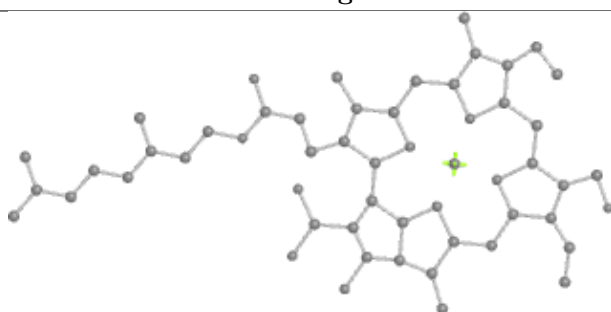
Bond lengths



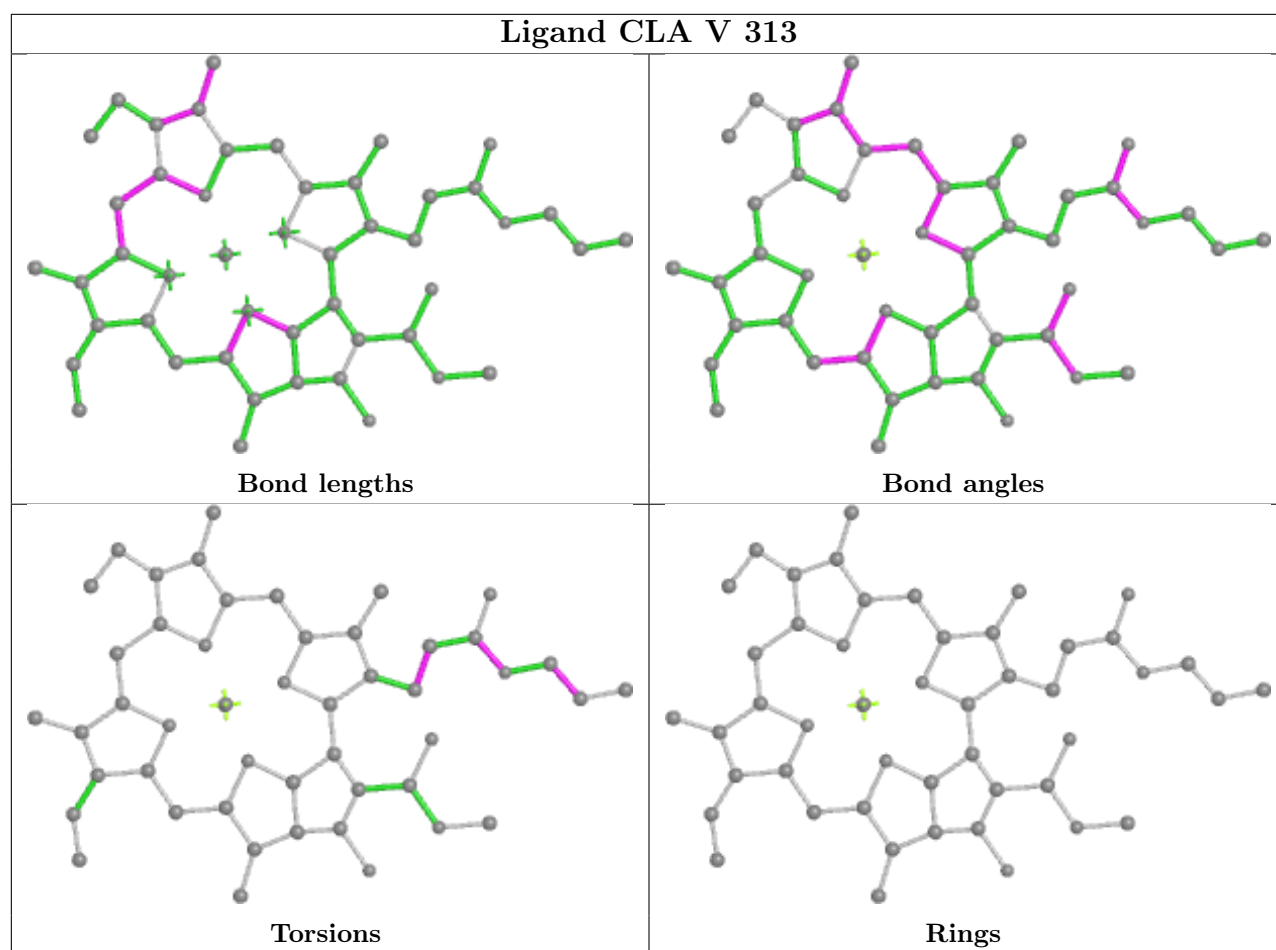
Bond angles



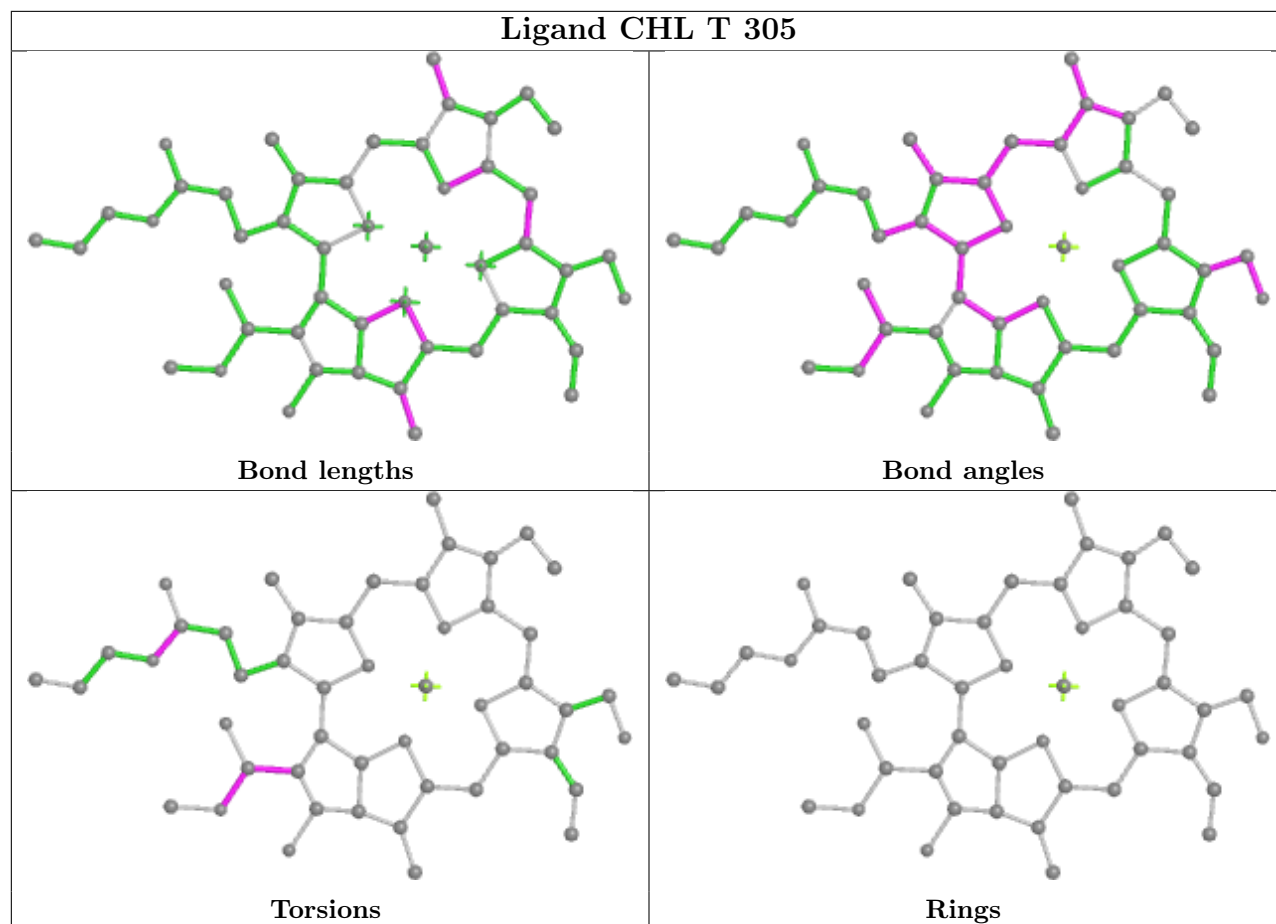
Torsions



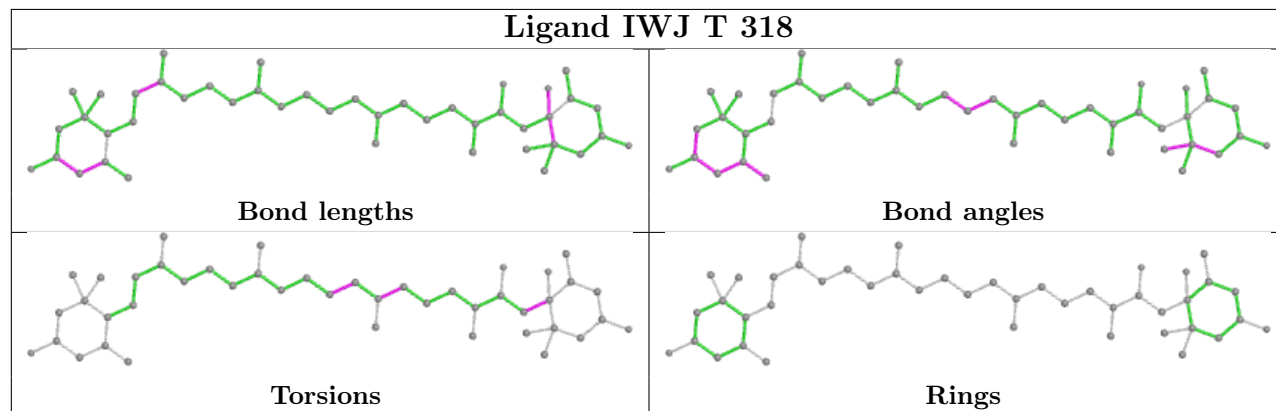
Rings



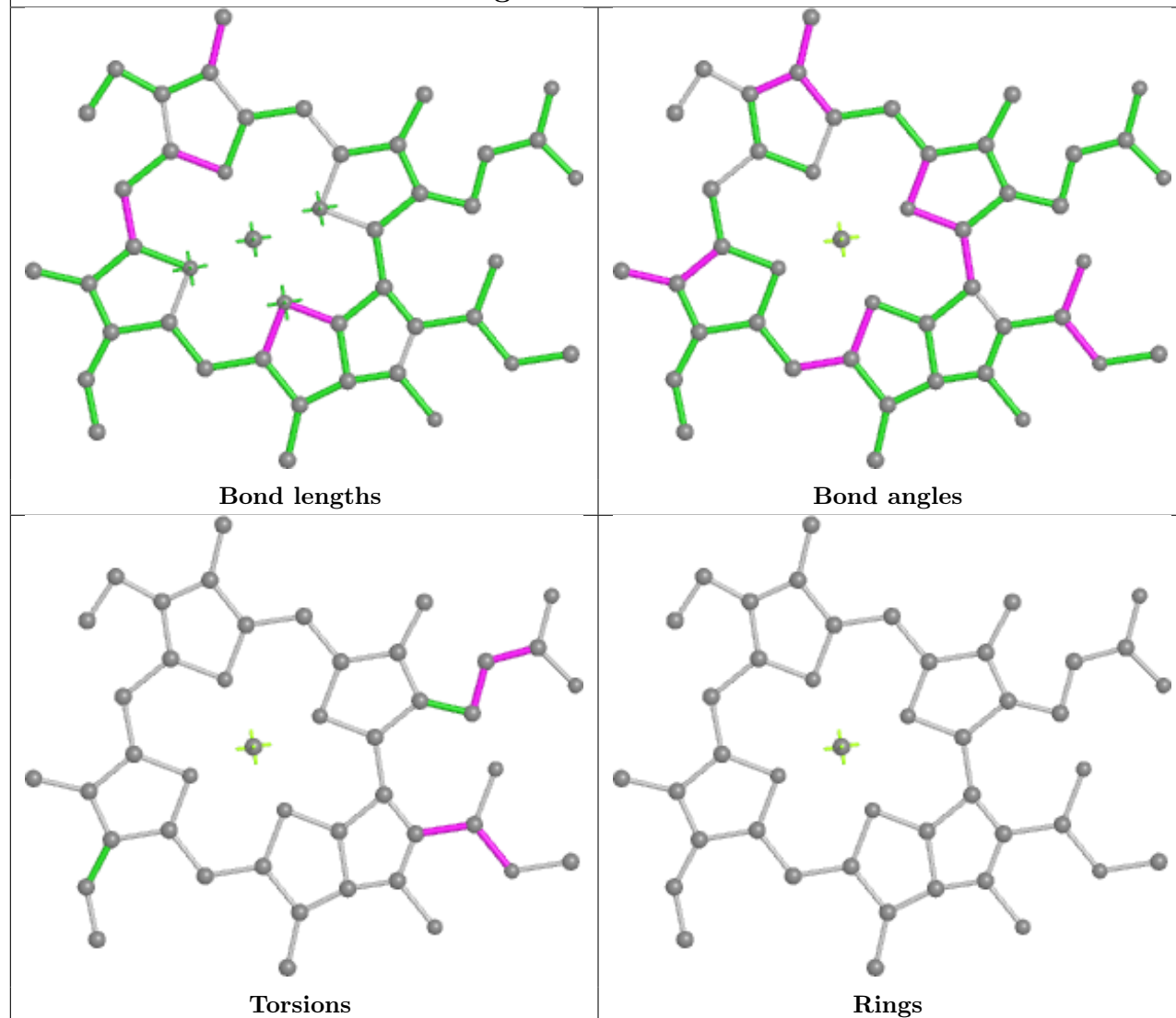
## Ligand CHL T 305



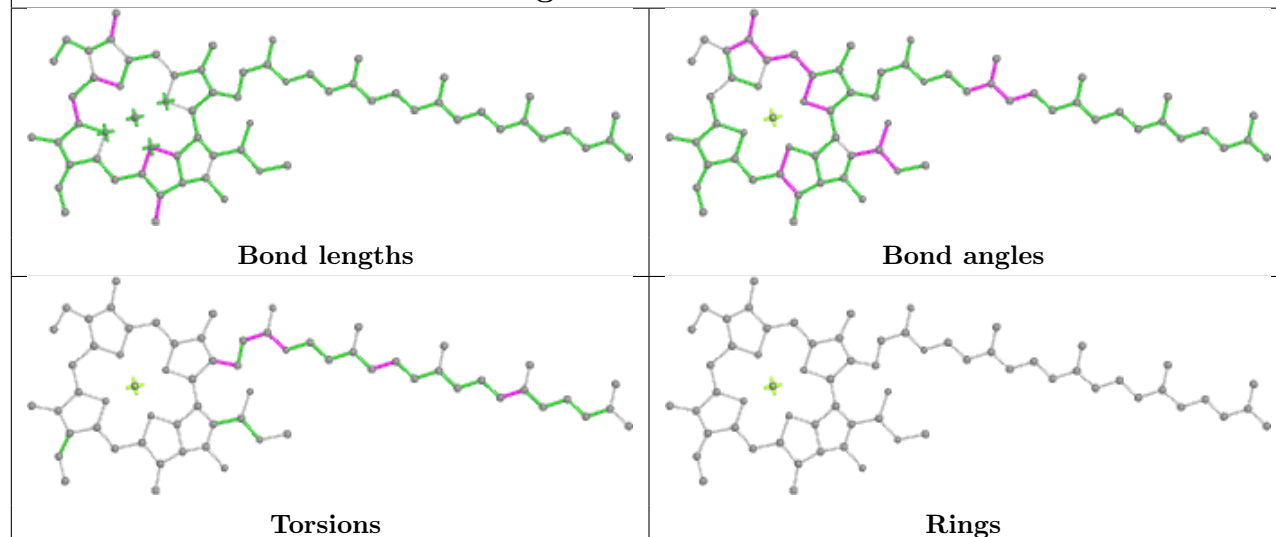
## Ligand IWJ T 318



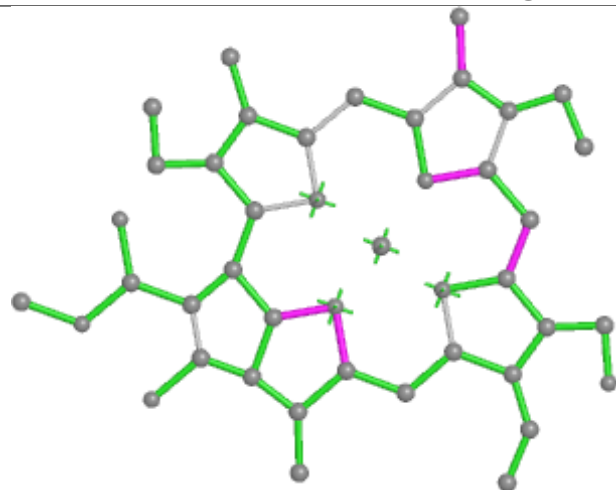
## Ligand CLA 5 603



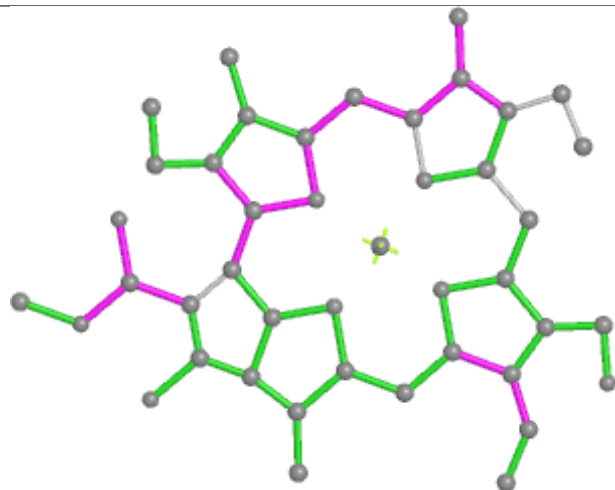
## Ligand CLA 6 613



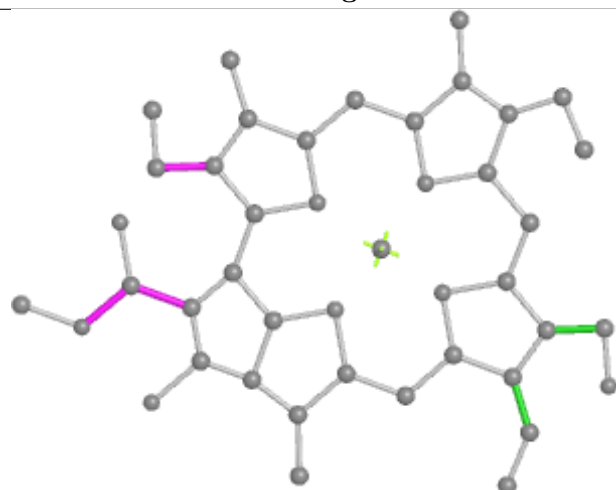
## Ligand CHL 6 606



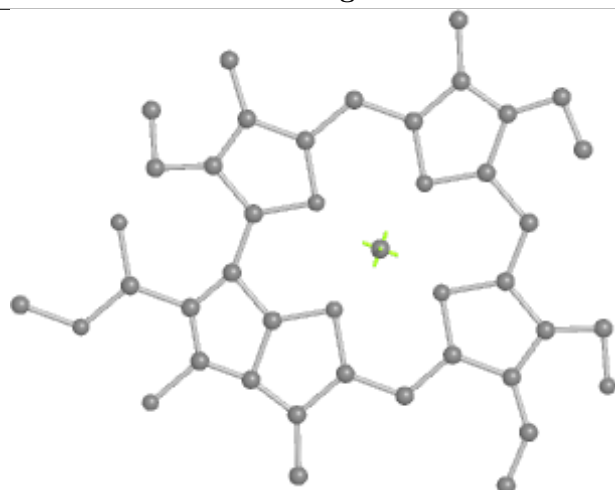
Bond lengths



Bond angles

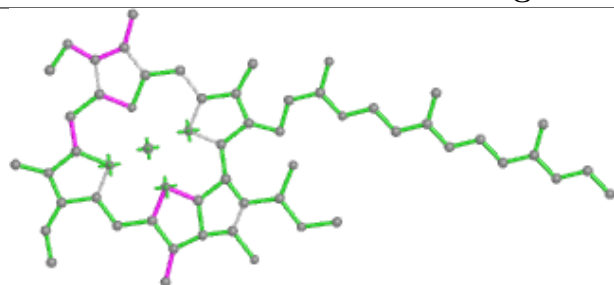
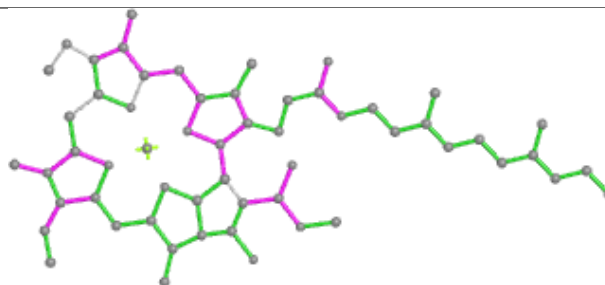
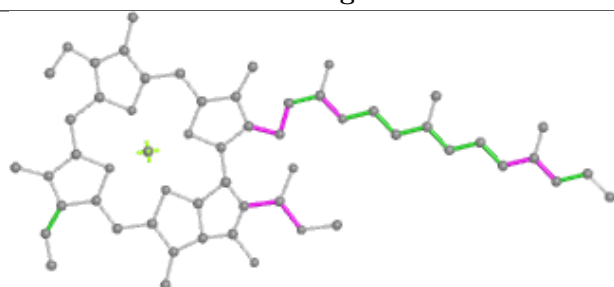
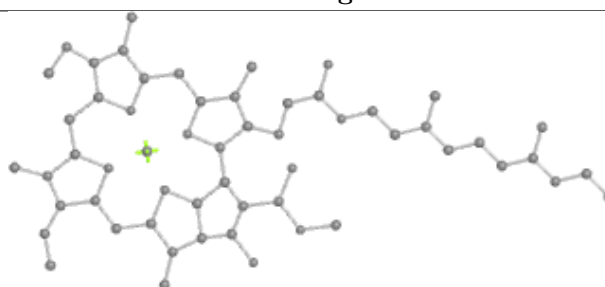
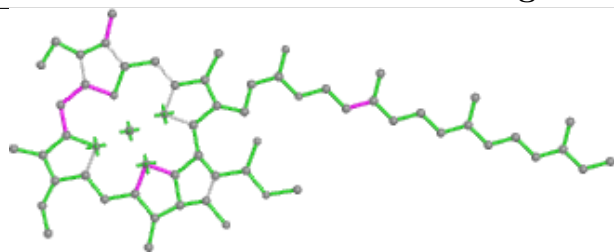
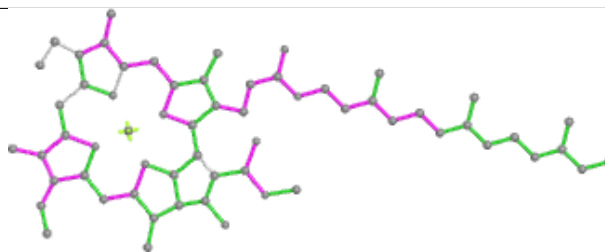
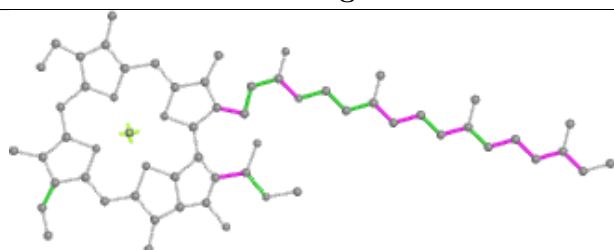
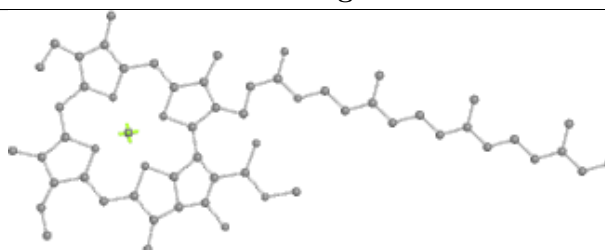


Torsions

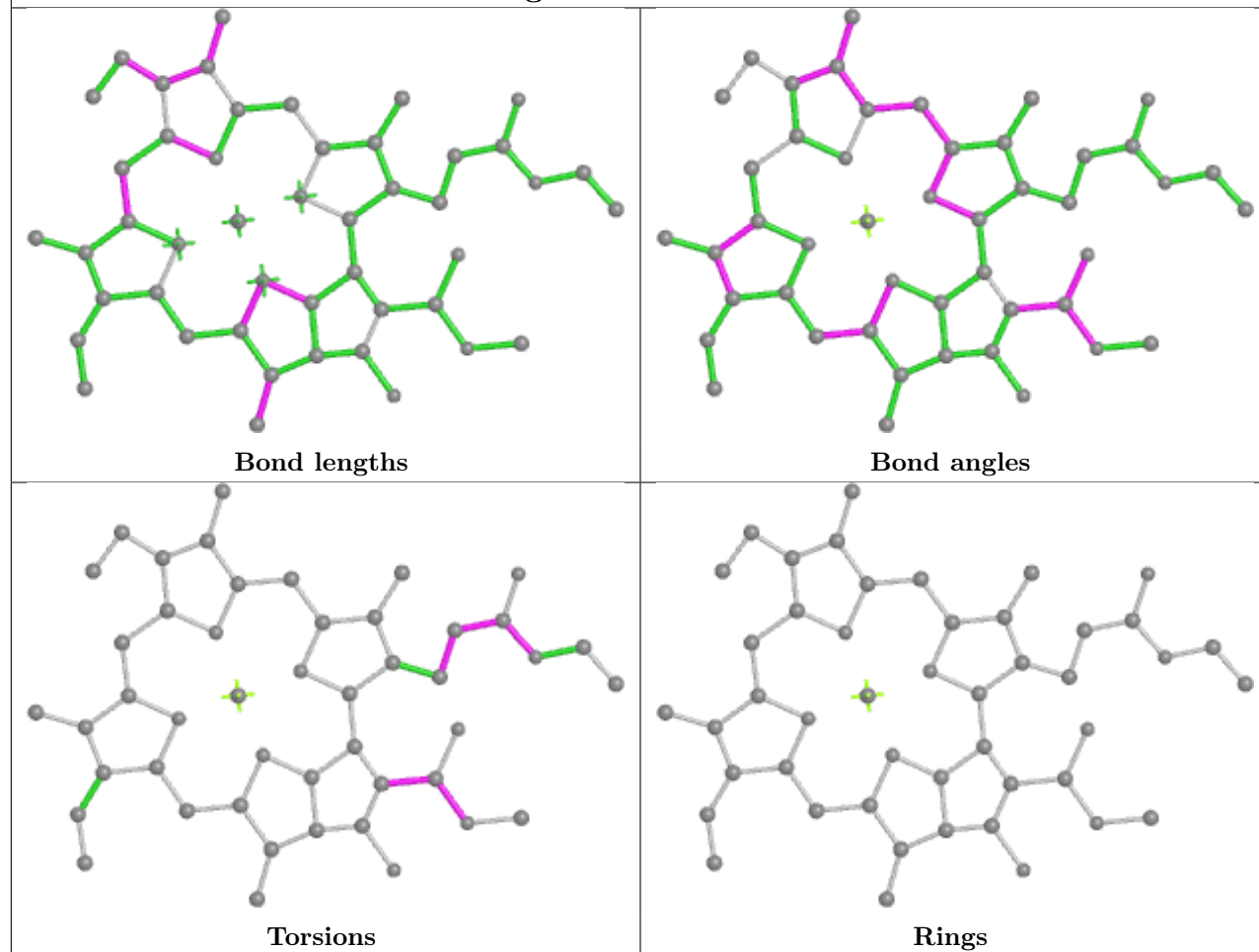


Rings

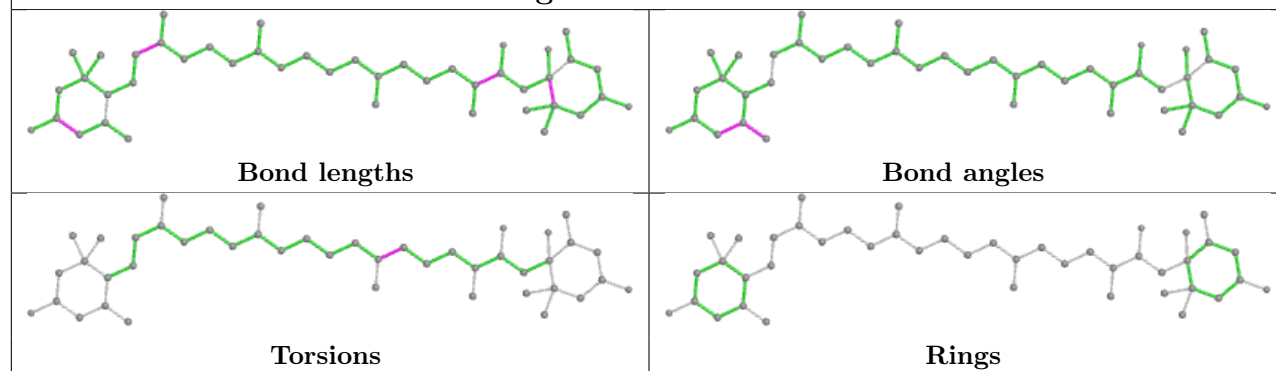


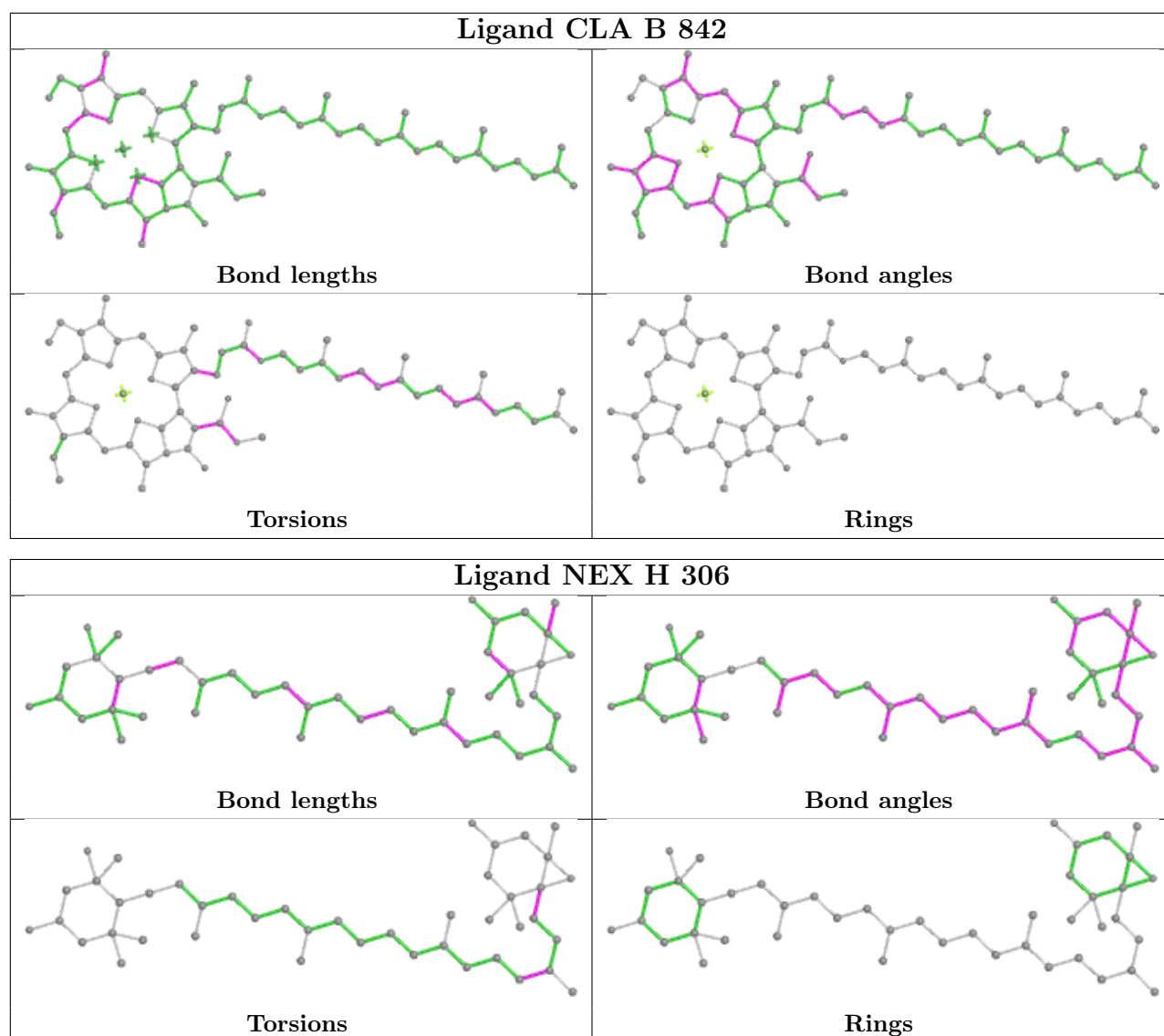
**Ligand CLA A 856****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 2 602****Bond lengths****Bond angles****Torsions****Rings**

## Ligand CLA B 840

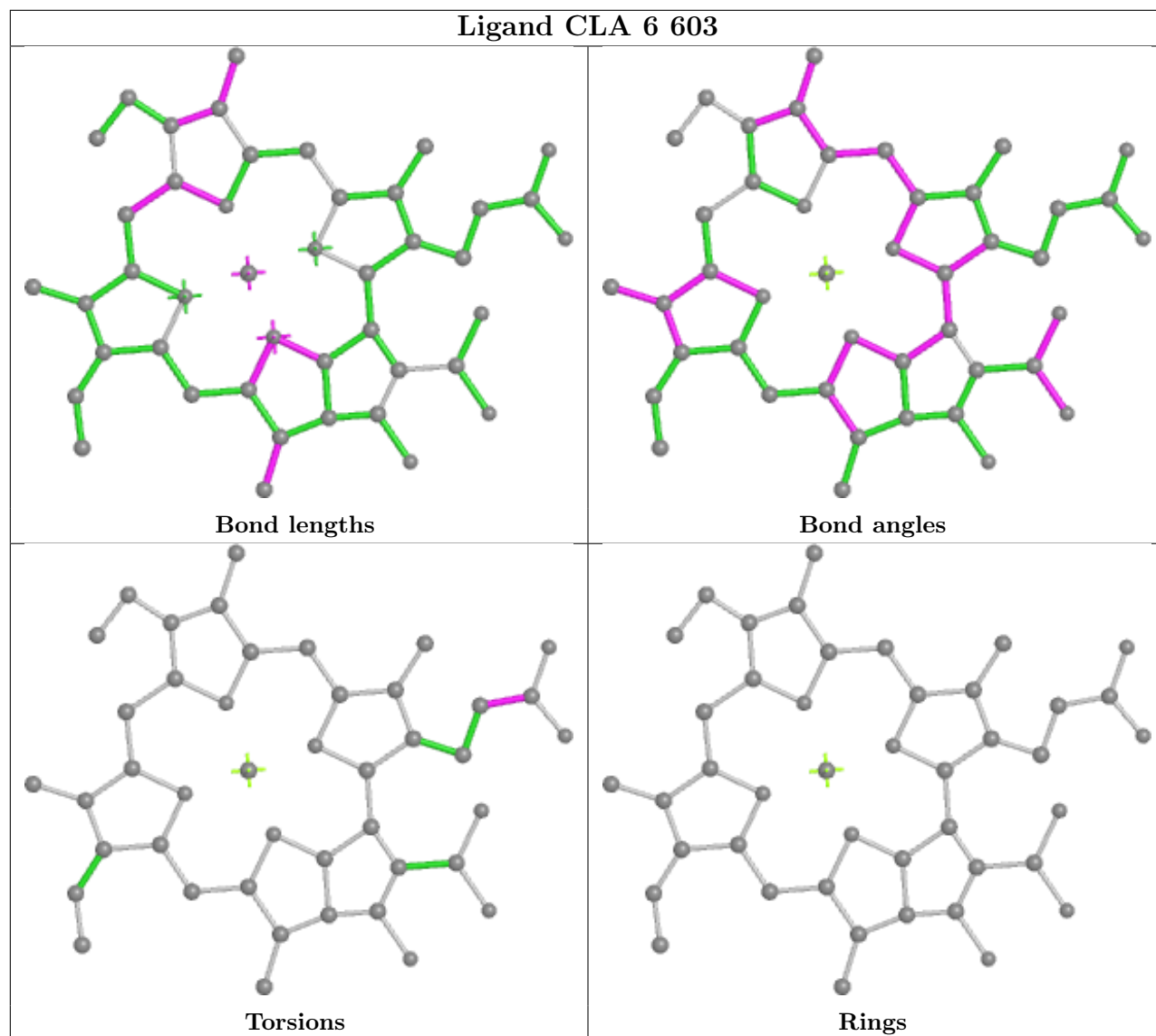


## Ligand IWJ P 318

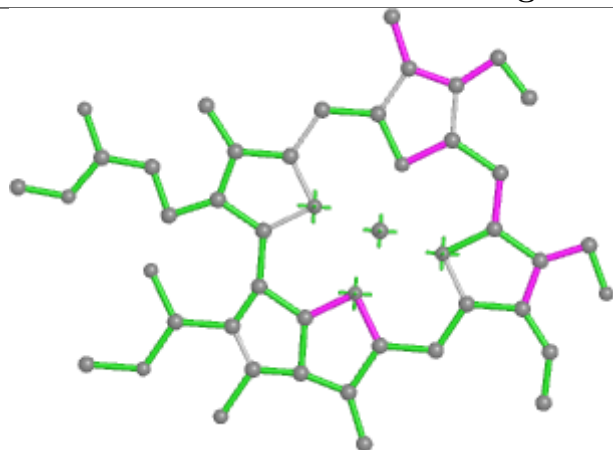




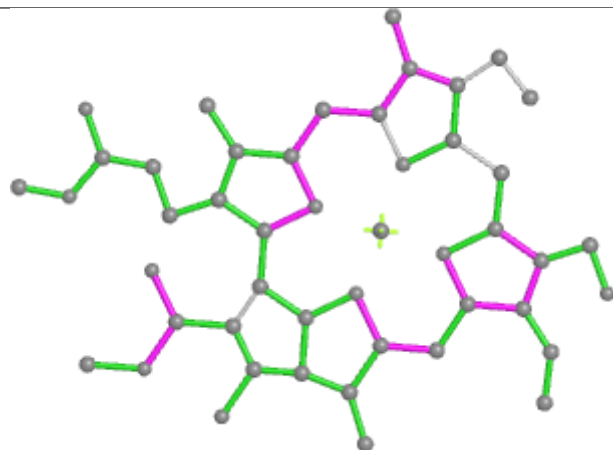
## Ligand CLA 6 603



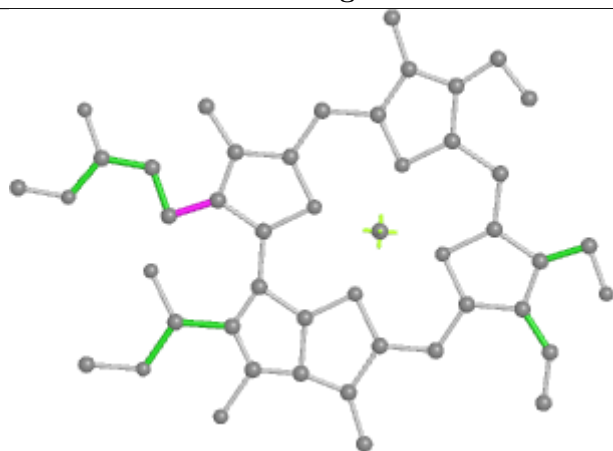
## Ligand CHL 2 601



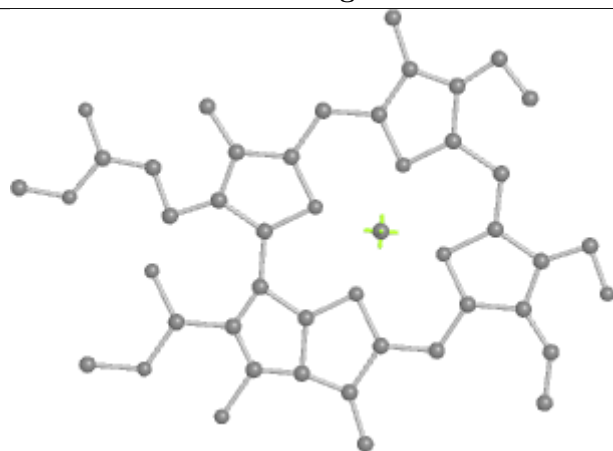
Bond lengths



Bond angles

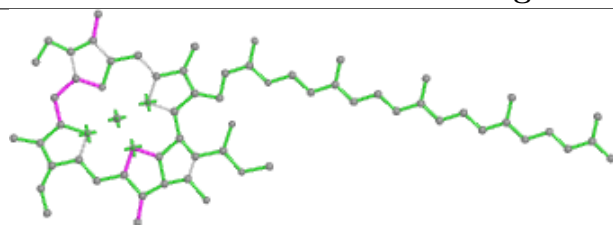


Torsions

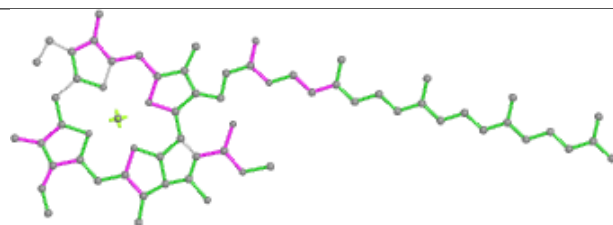


Rings

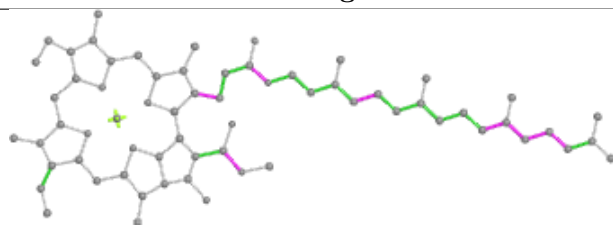
## Ligand CLA A 805



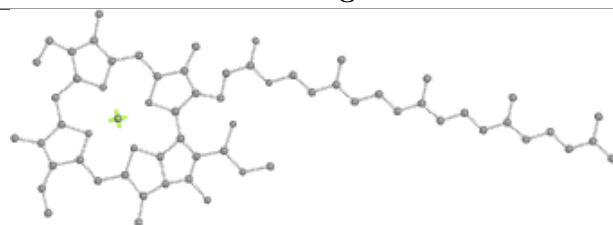
Bond lengths



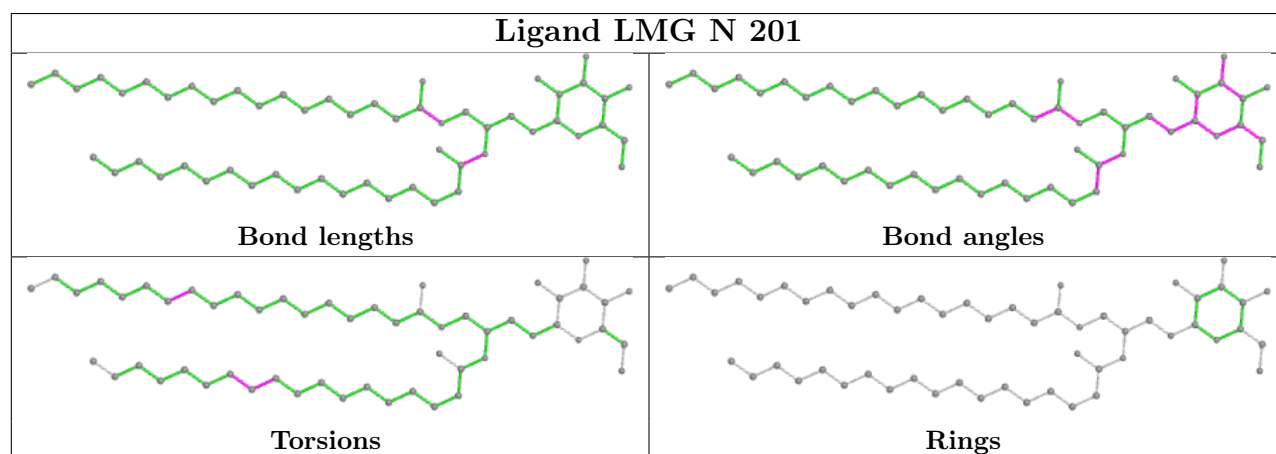
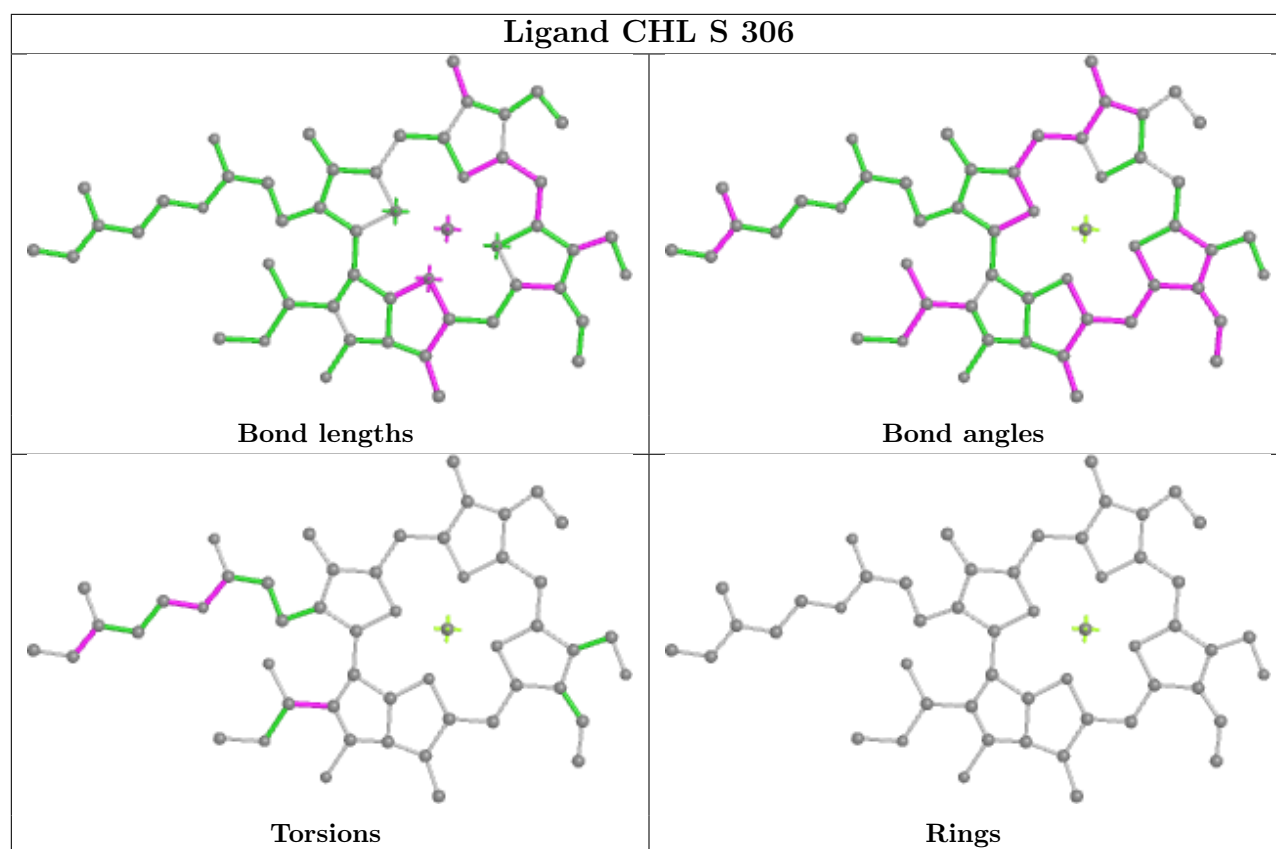
Bond angles



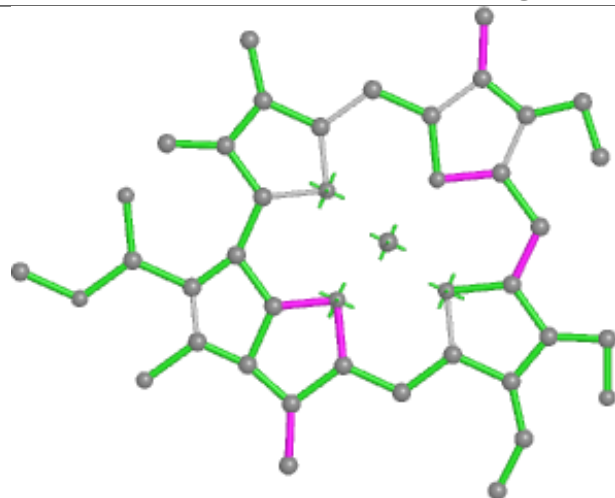
Torsions



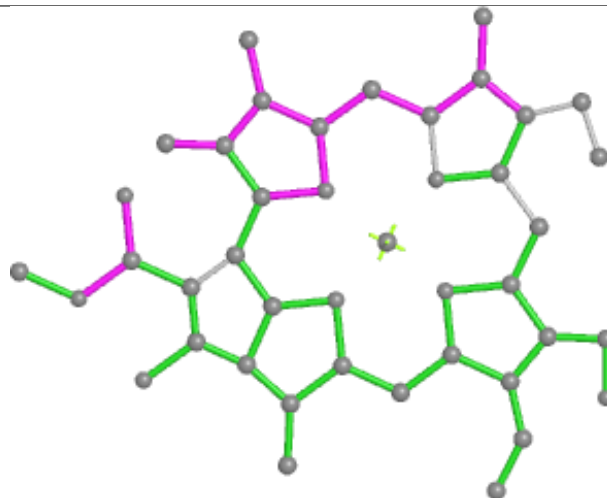
Rings



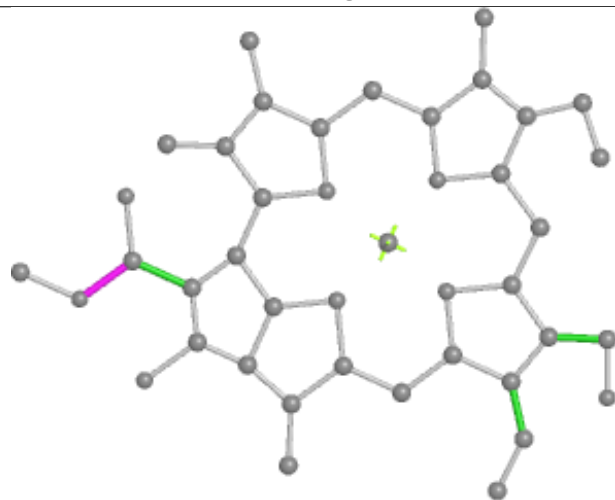
## Ligand CHL X 306



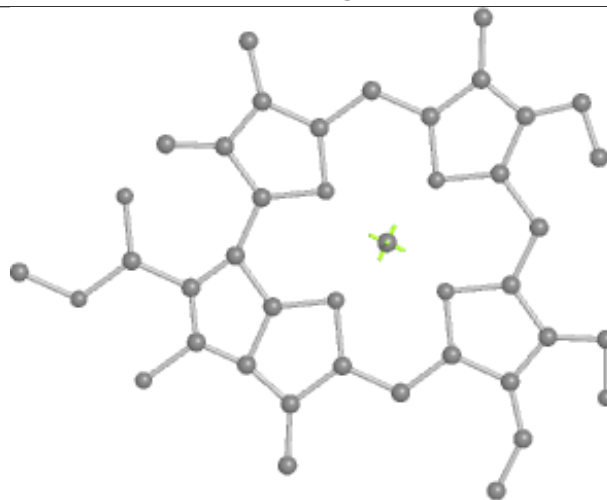
Bond lengths



Bond angles

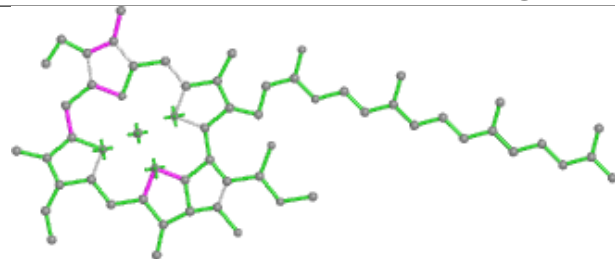


Torsions

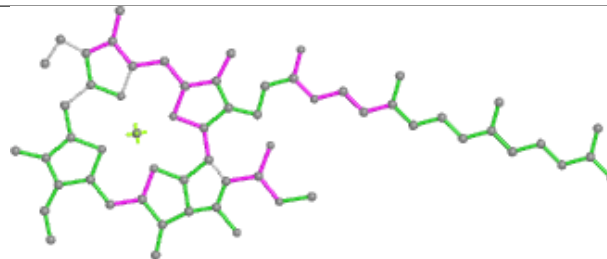


Rings

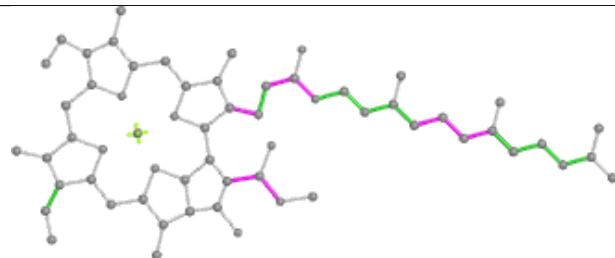
## Ligand CLA R 314



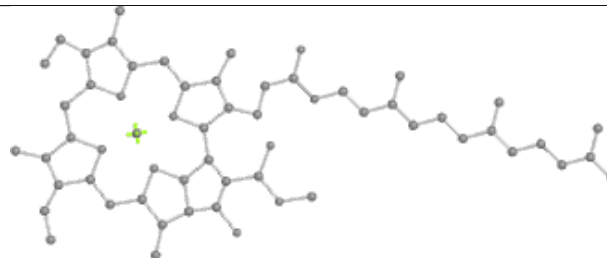
Bond lengths



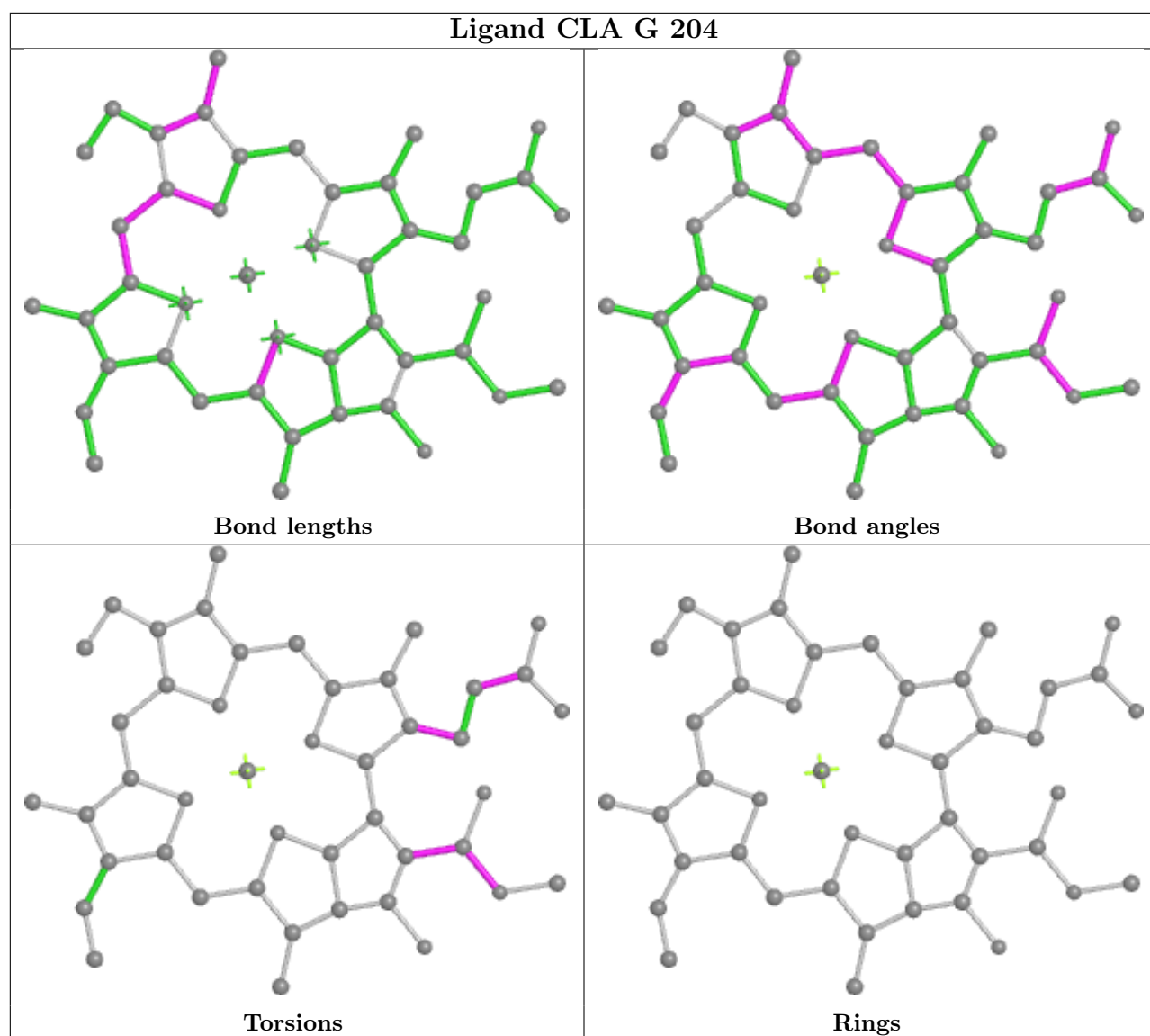
Bond angles



Torsions

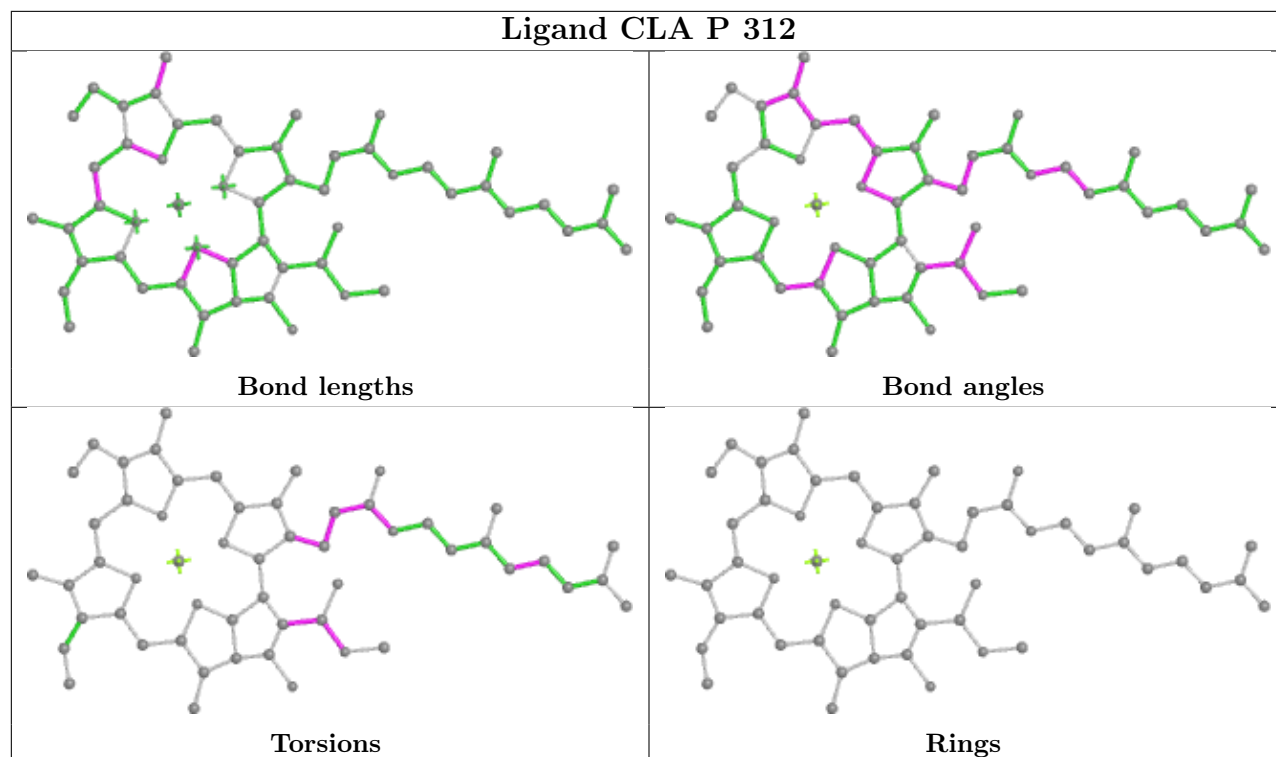


Rings

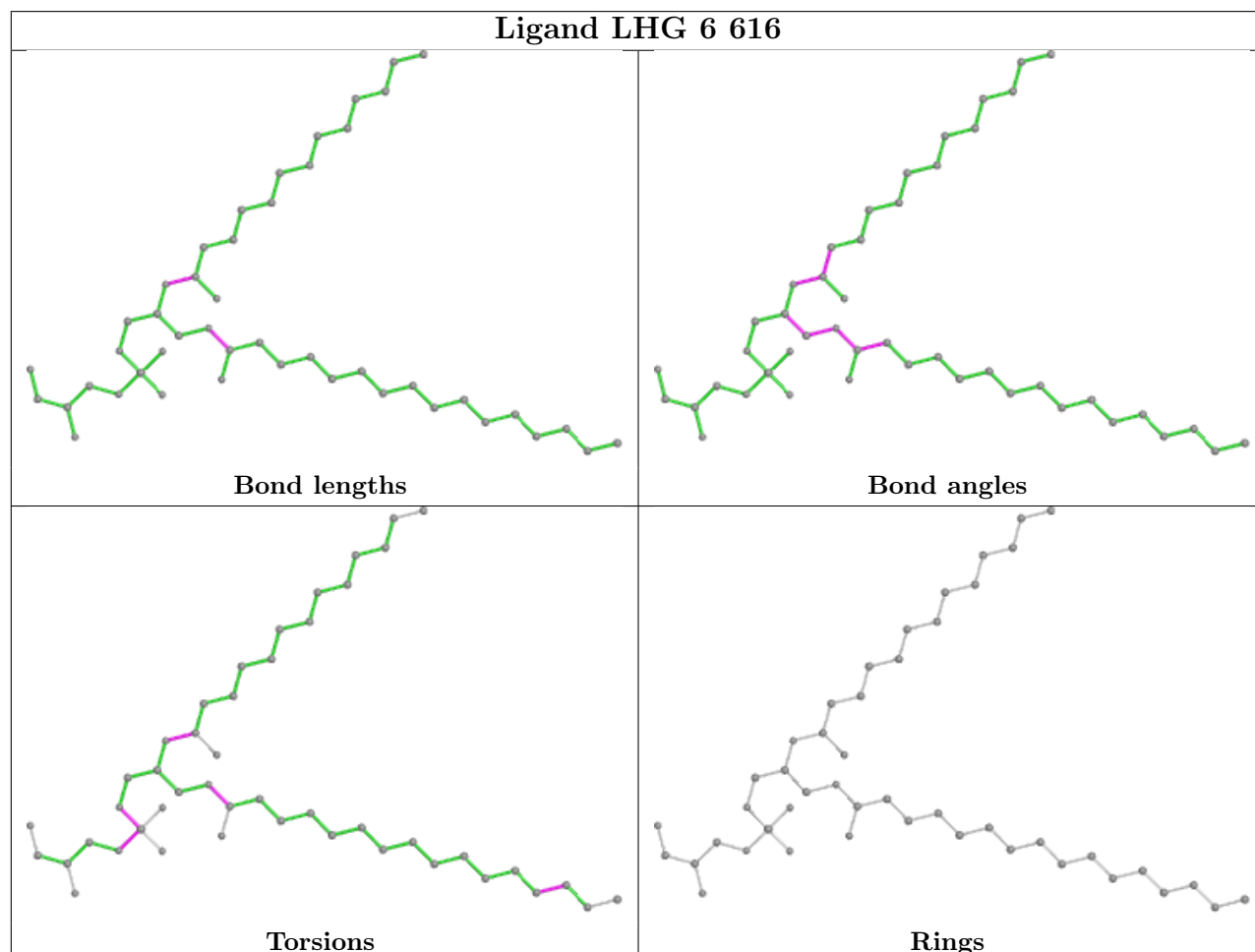


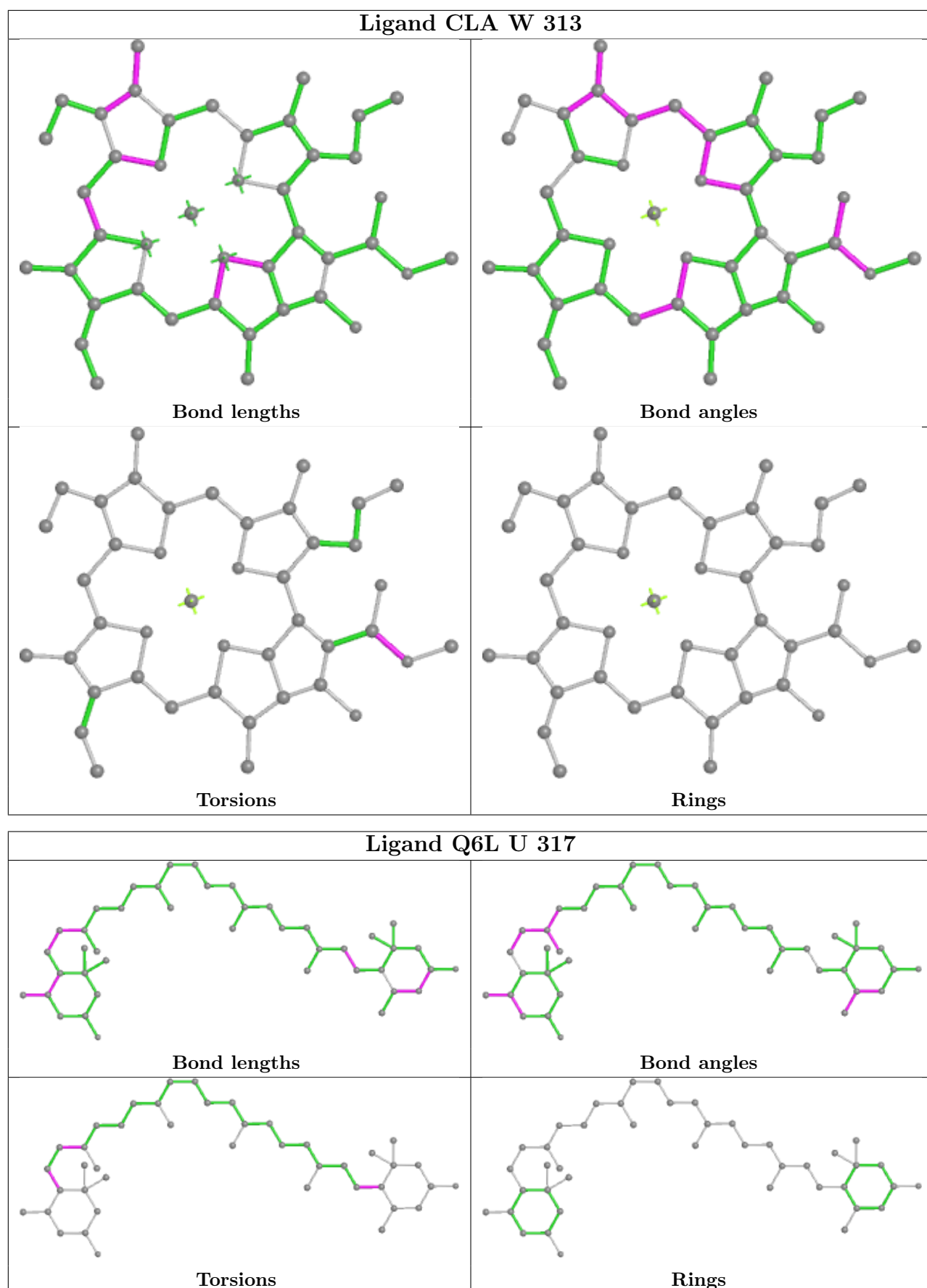


## Ligand CLA P 312

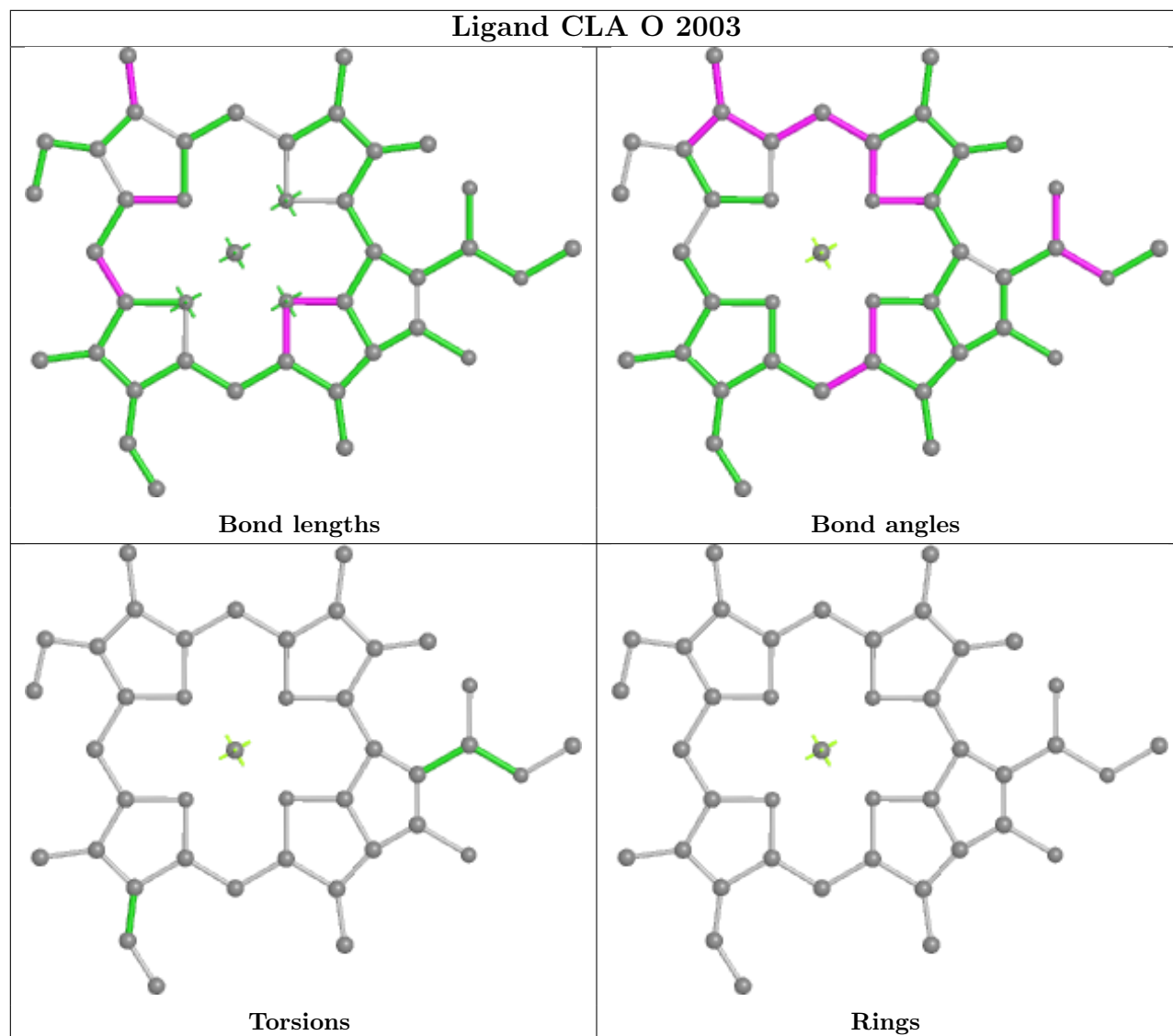


## Ligand LHG 6 616

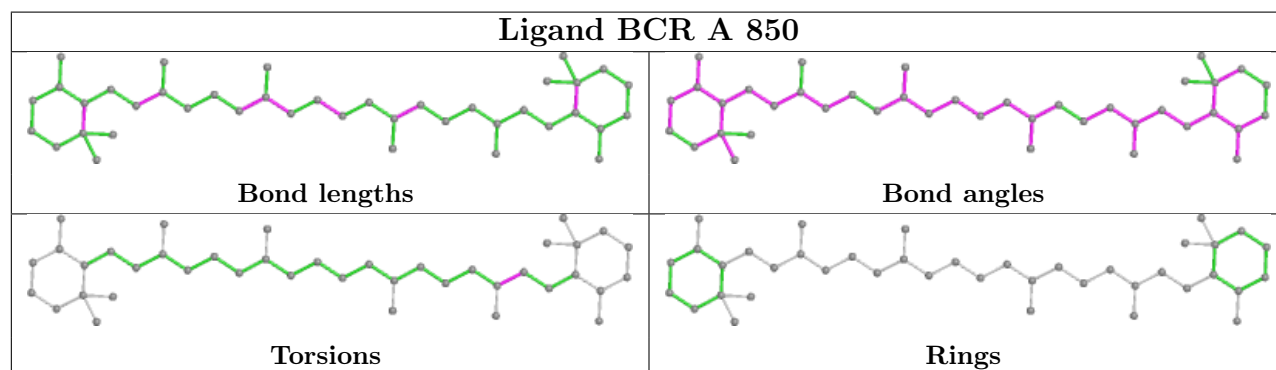


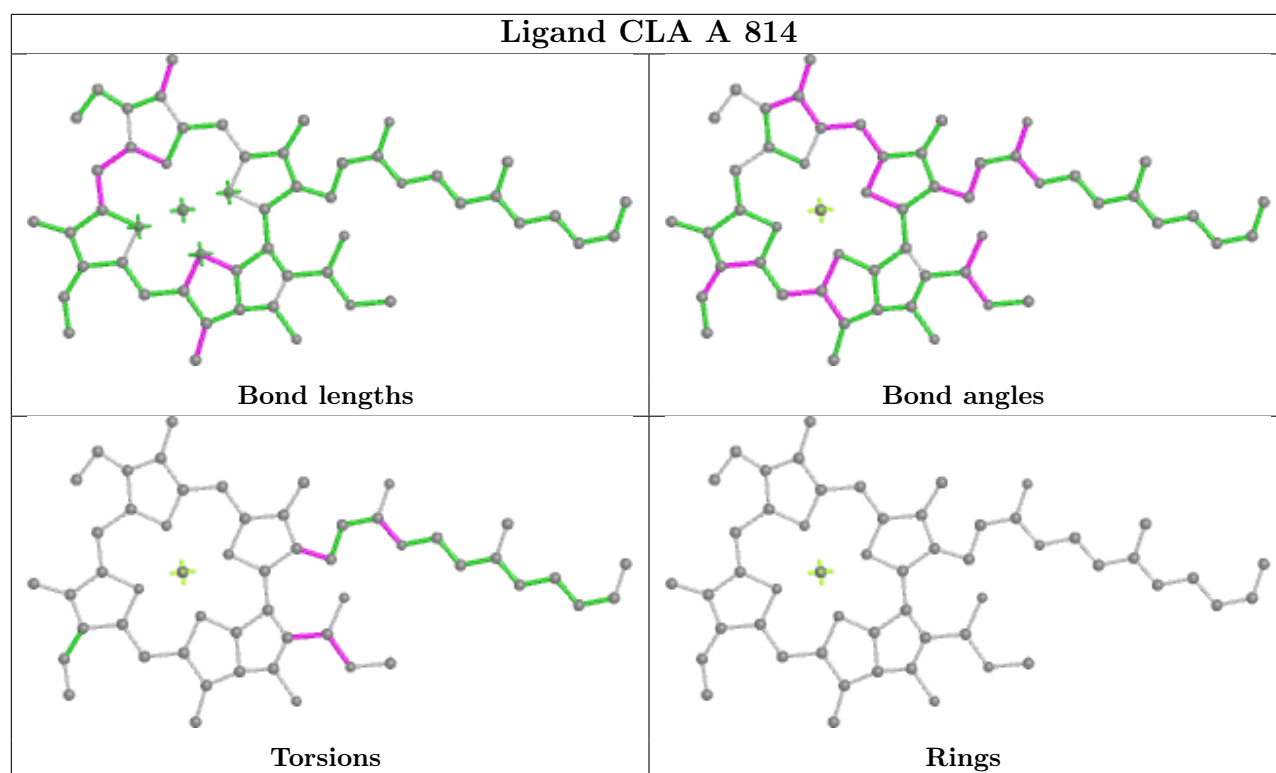


## Ligand CLA O 2003

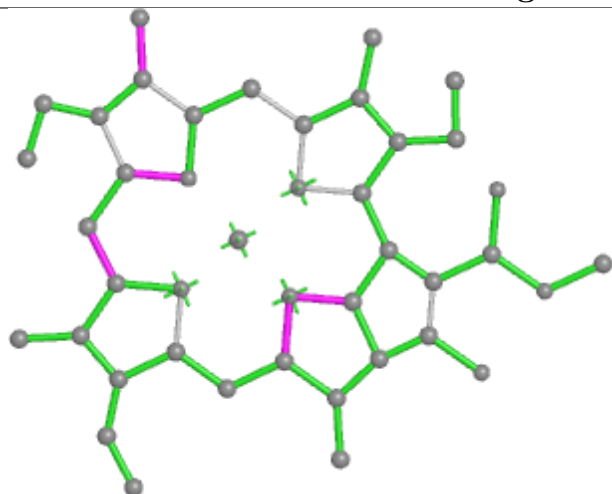


## Ligand BCR A 850

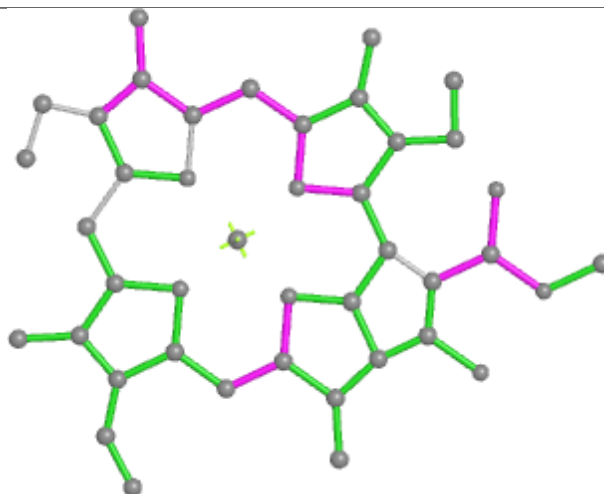




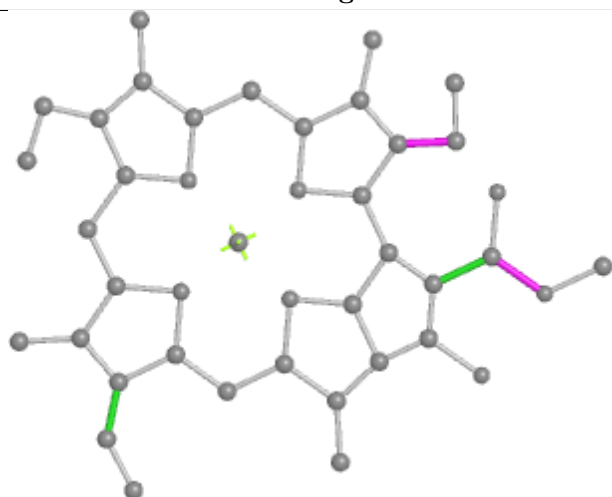
## Ligand CLA 2 610



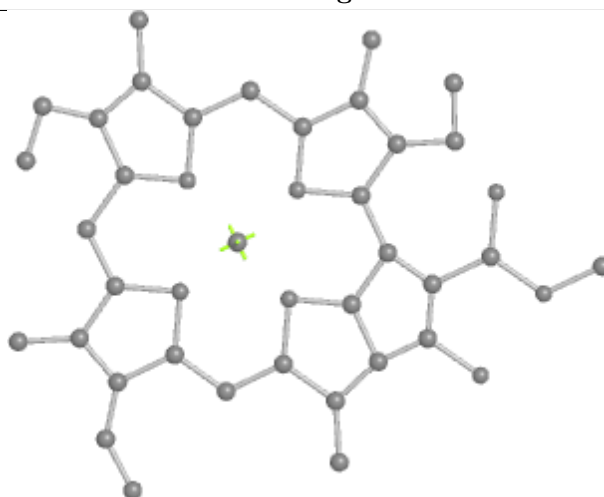
Bond lengths



Bond angles

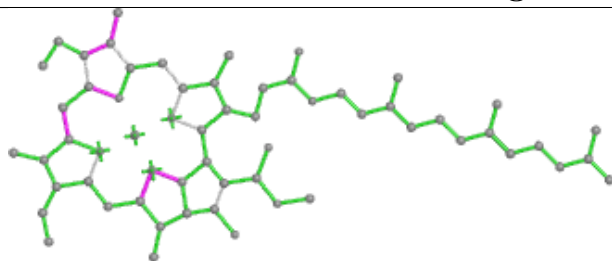


Torsions

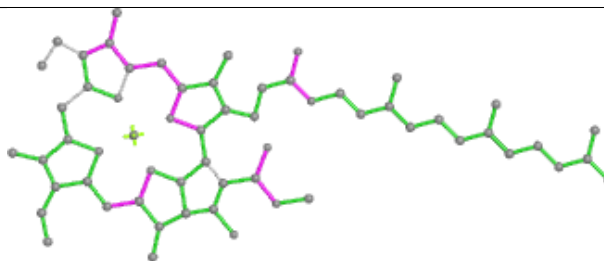


Rings

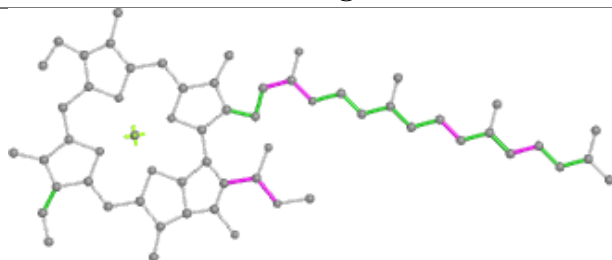
## Ligand CLA W 310



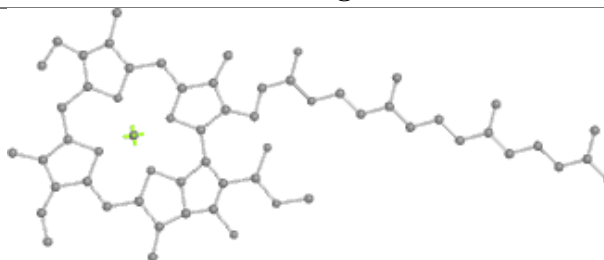
Bond lengths



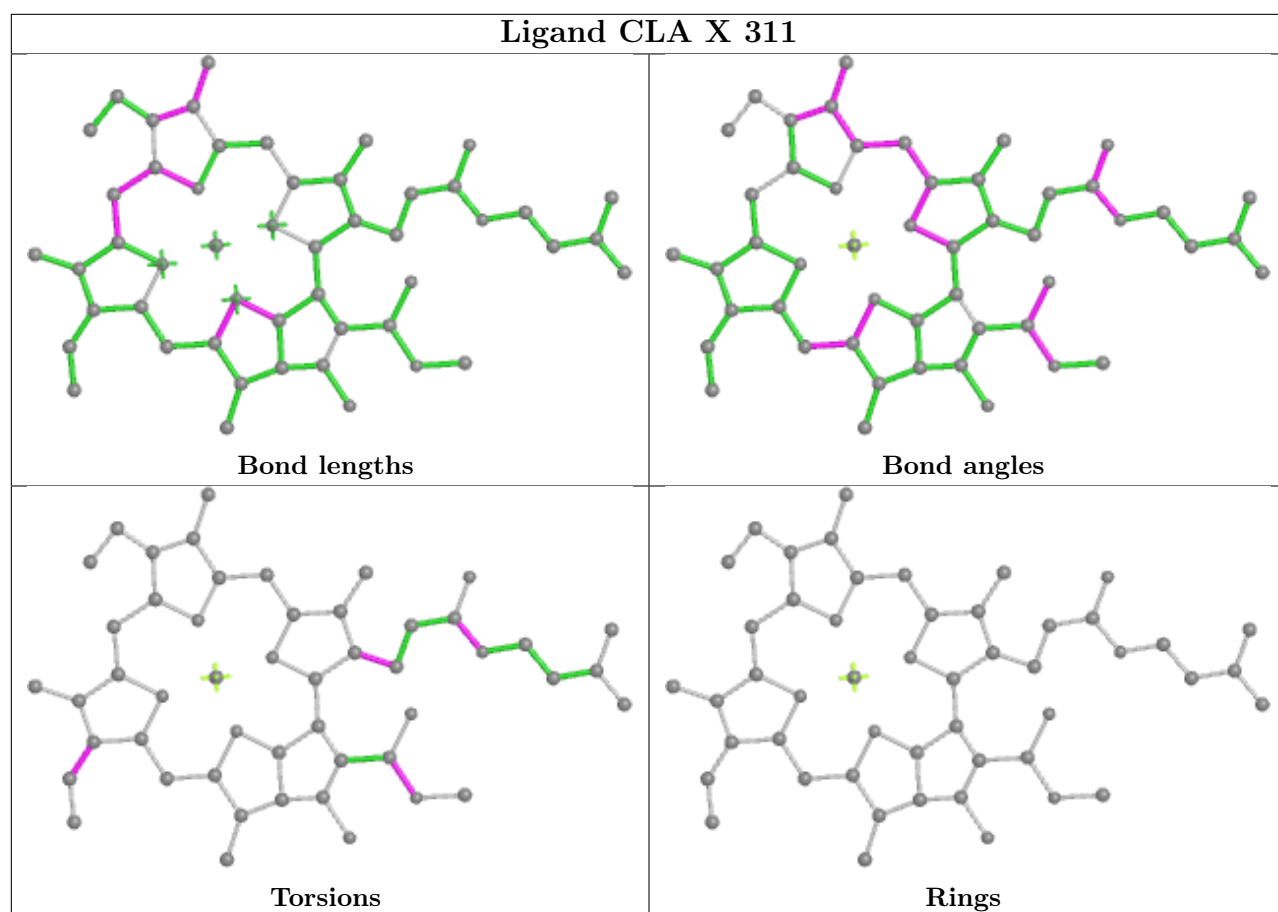
Bond angles



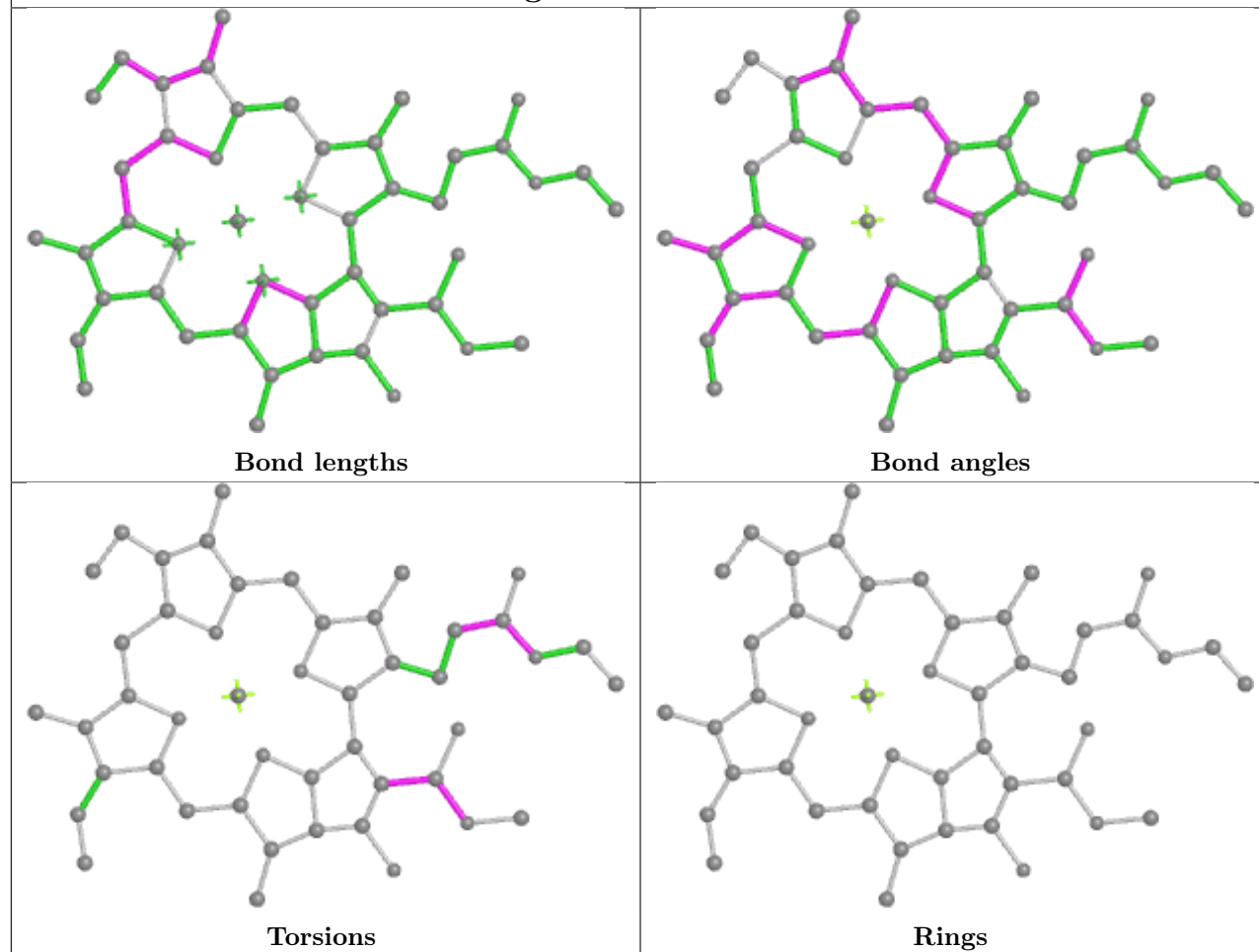
Torsions



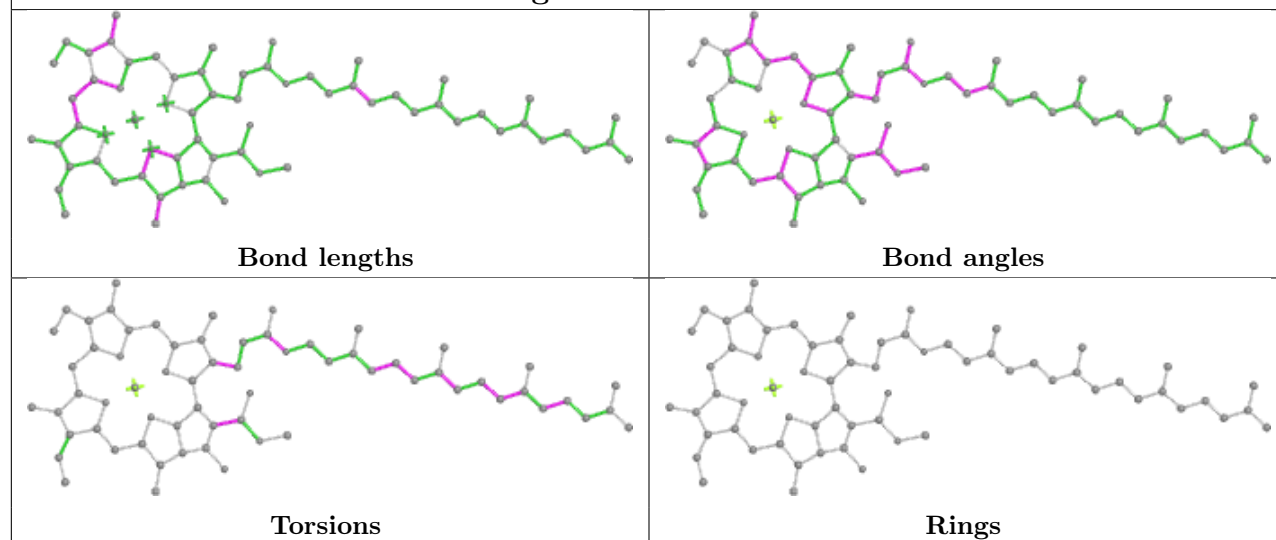
Rings

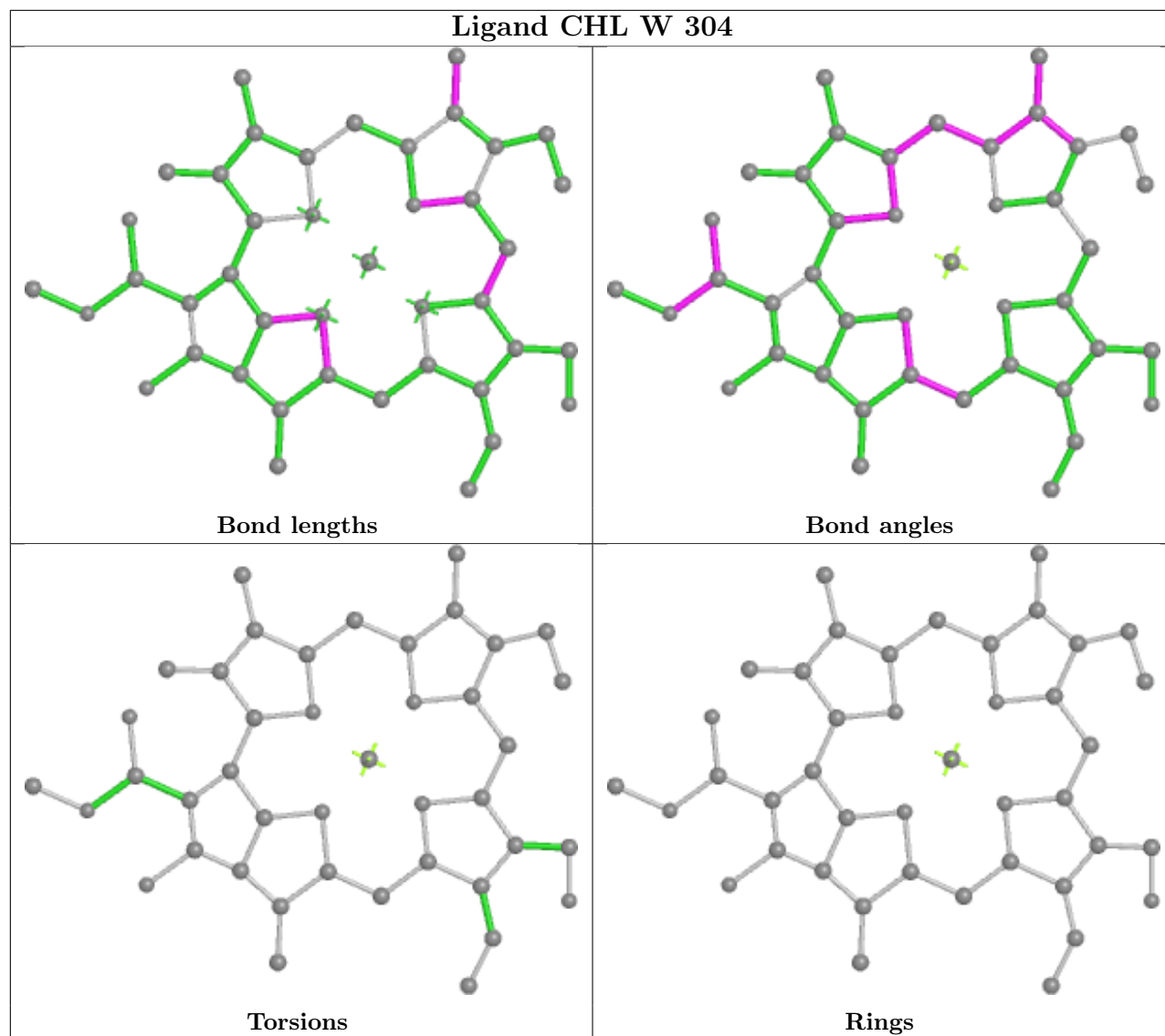
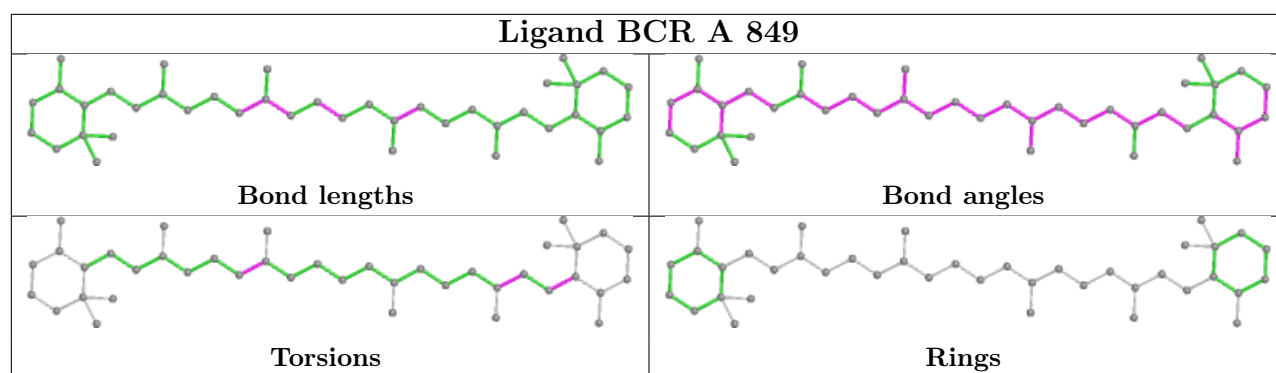


## Ligand CLA V 310



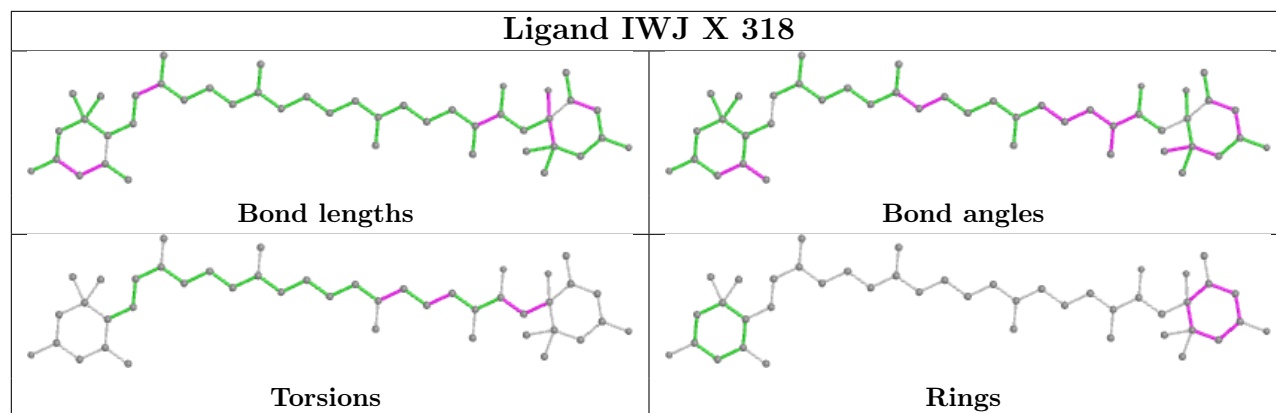
## Ligand CLA A 842



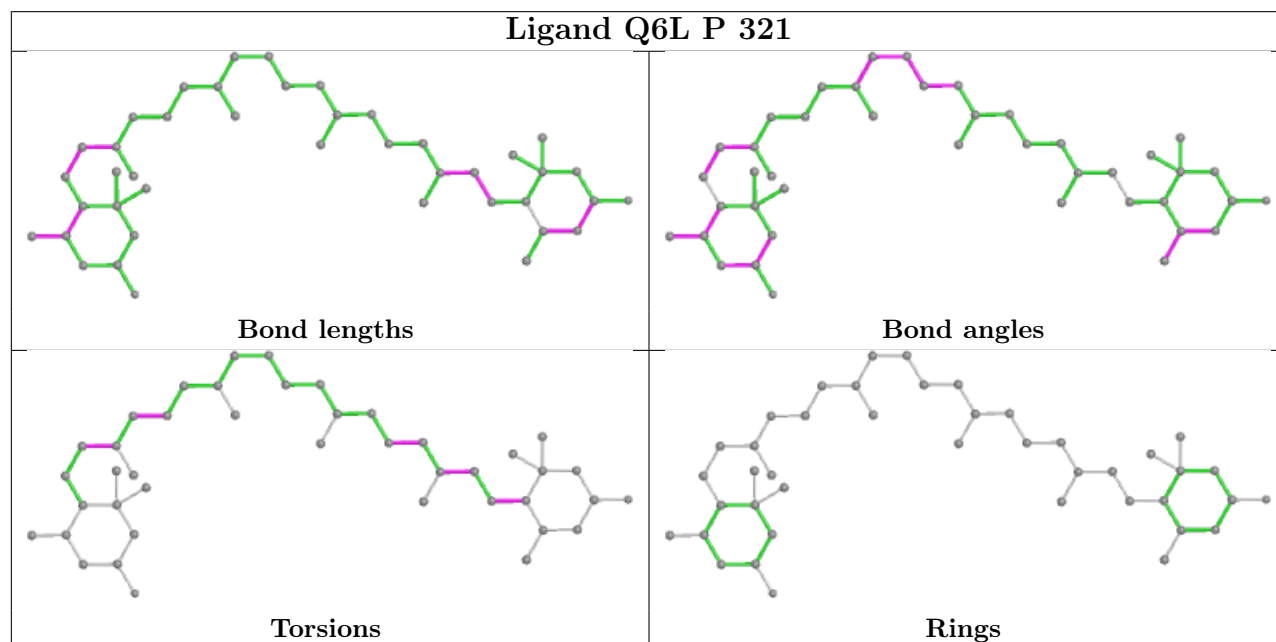




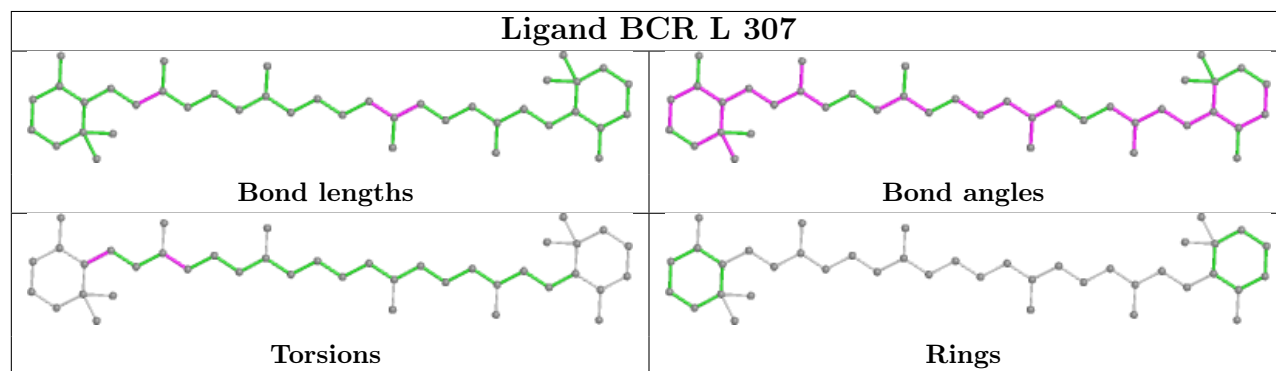
## Ligand IWJ X 318



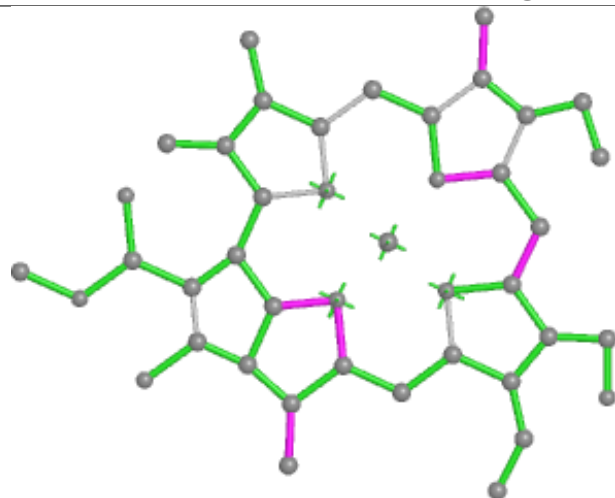
## Ligand Q6L P 321



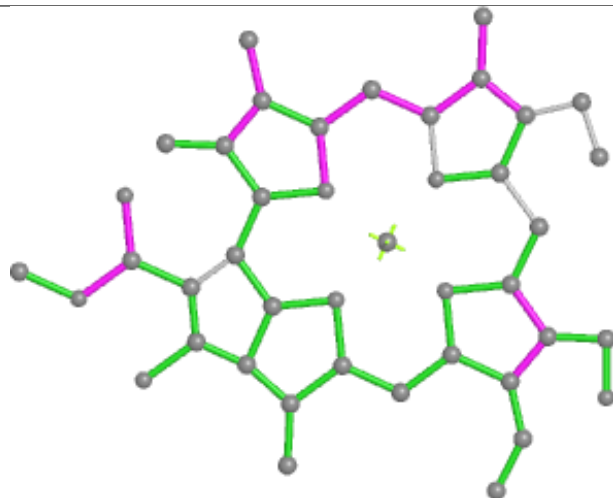
## Ligand BCR L 307



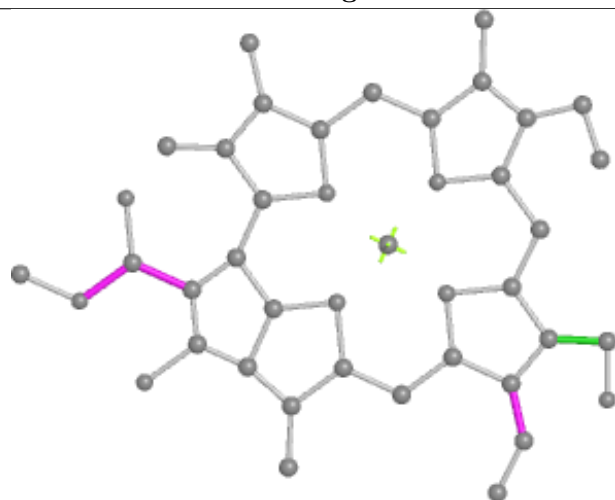
## Ligand CHL S 307



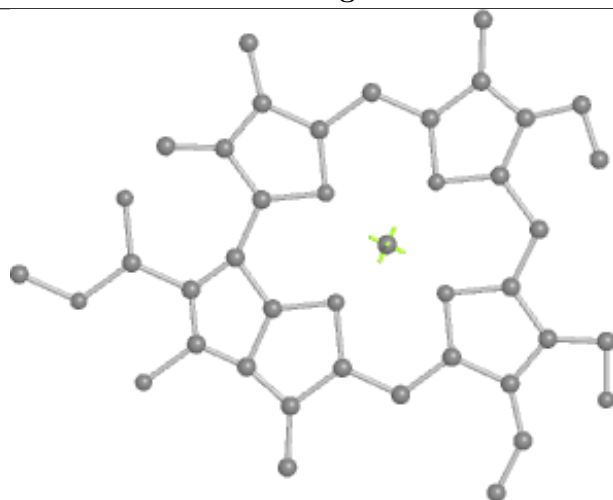
Bond lengths



Bond angles

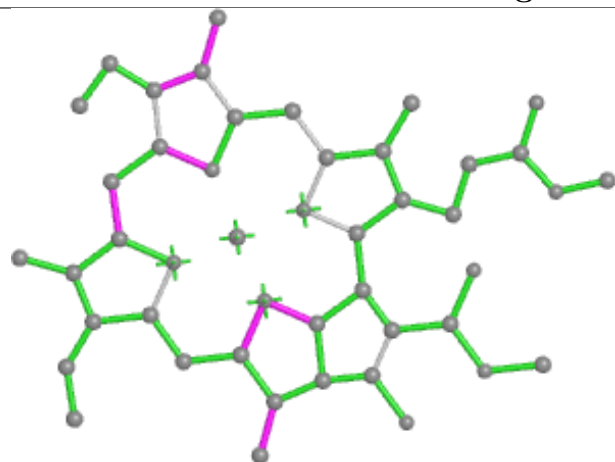


Torsions

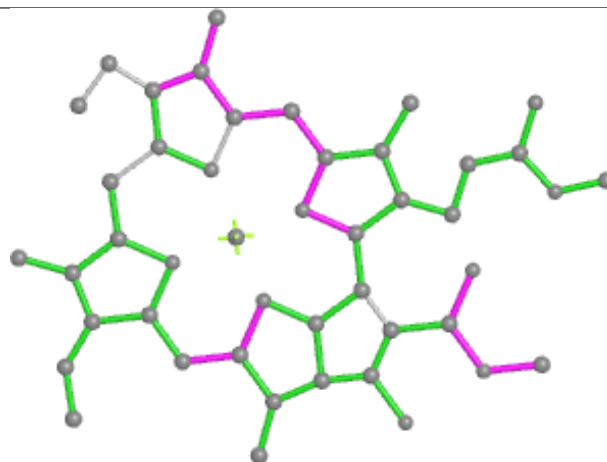


Rings

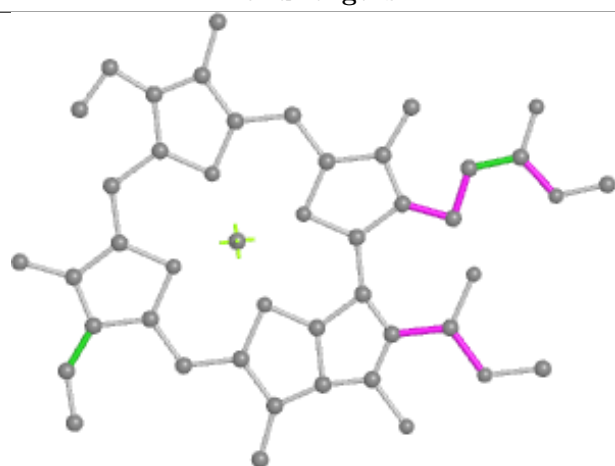
## Ligand CLA U 309



Bond lengths



Bond angles

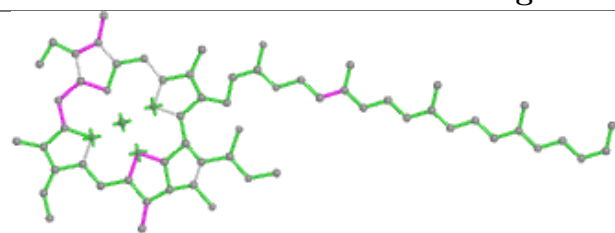


Torsions

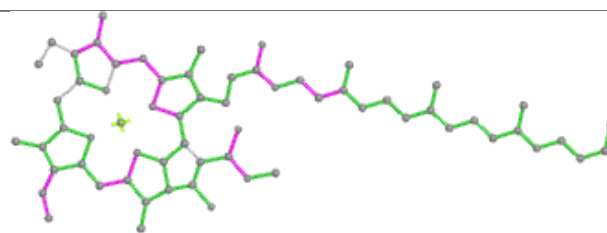


Rings

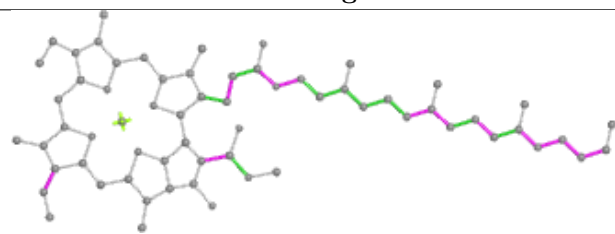
## Ligand CLA A 807



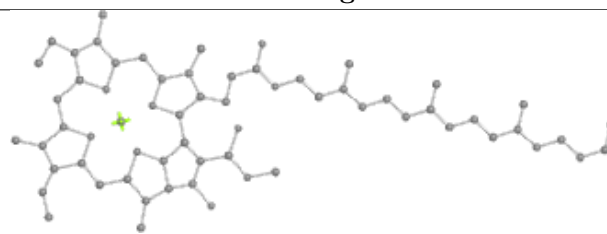
Bond lengths



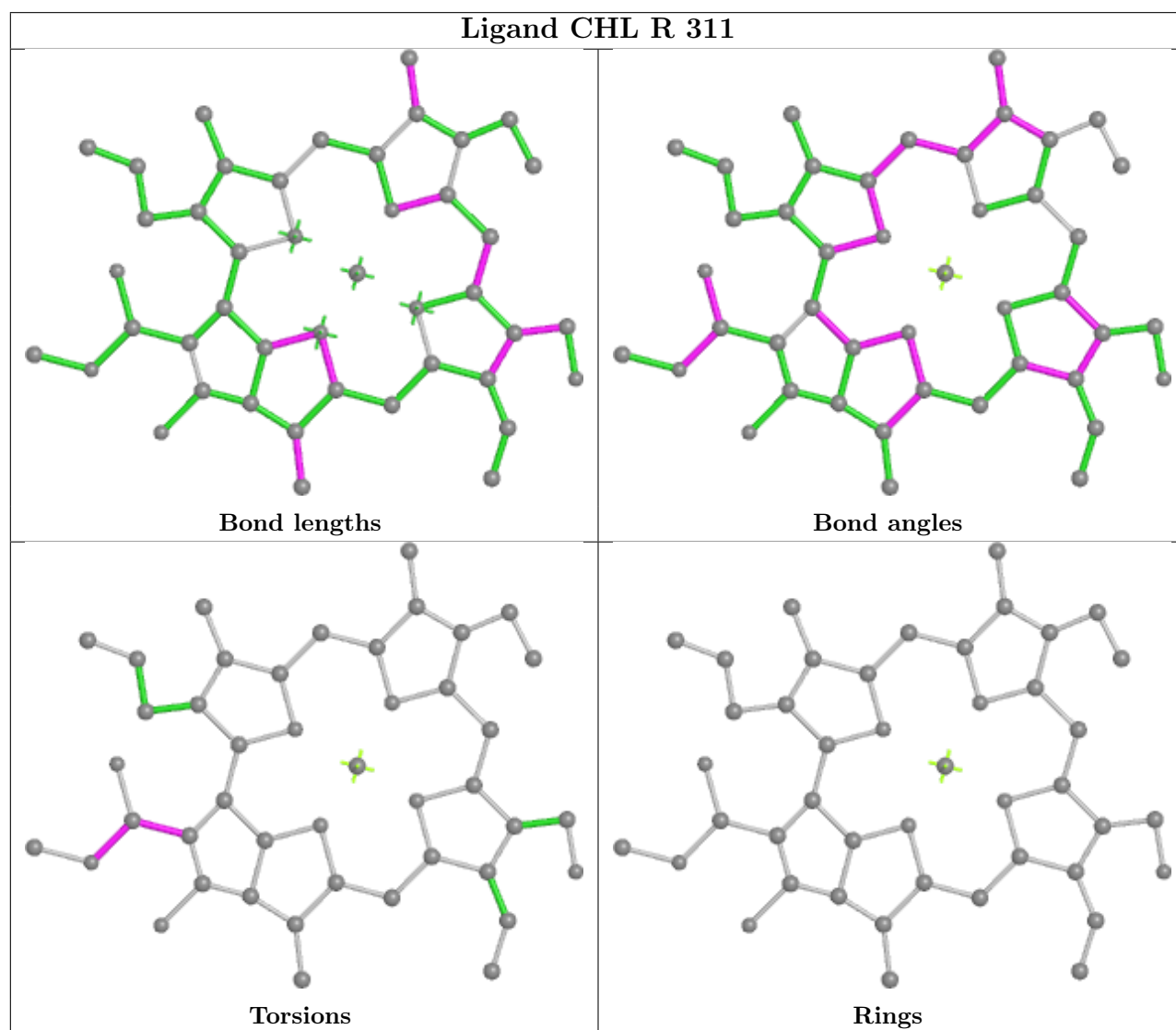
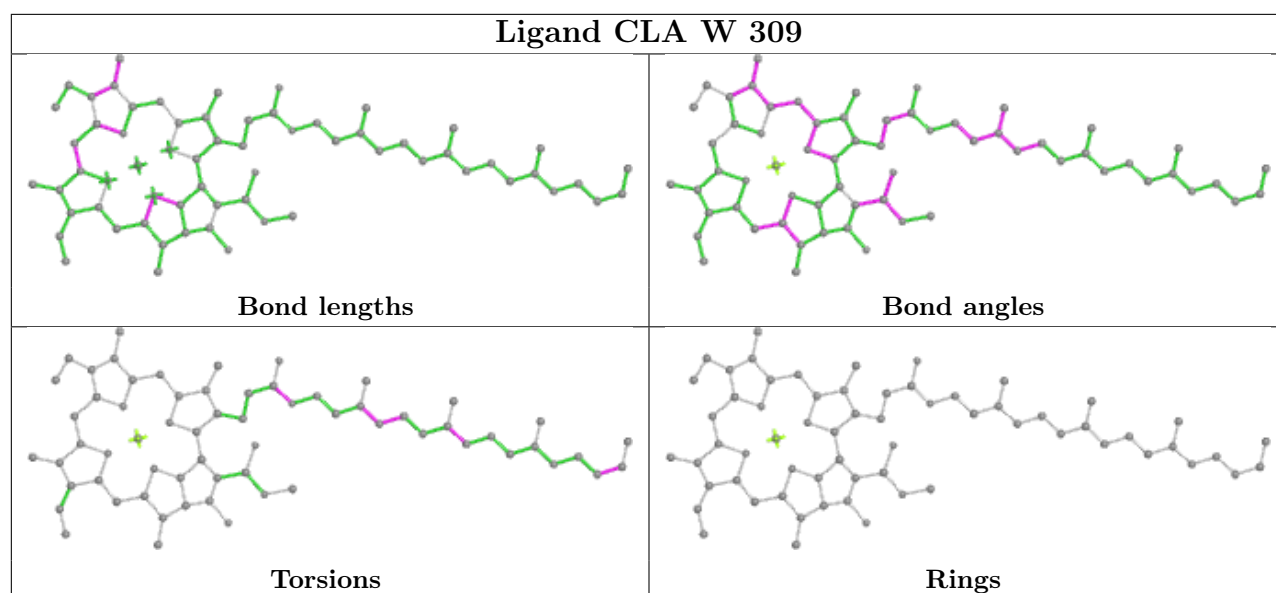
Bond angles



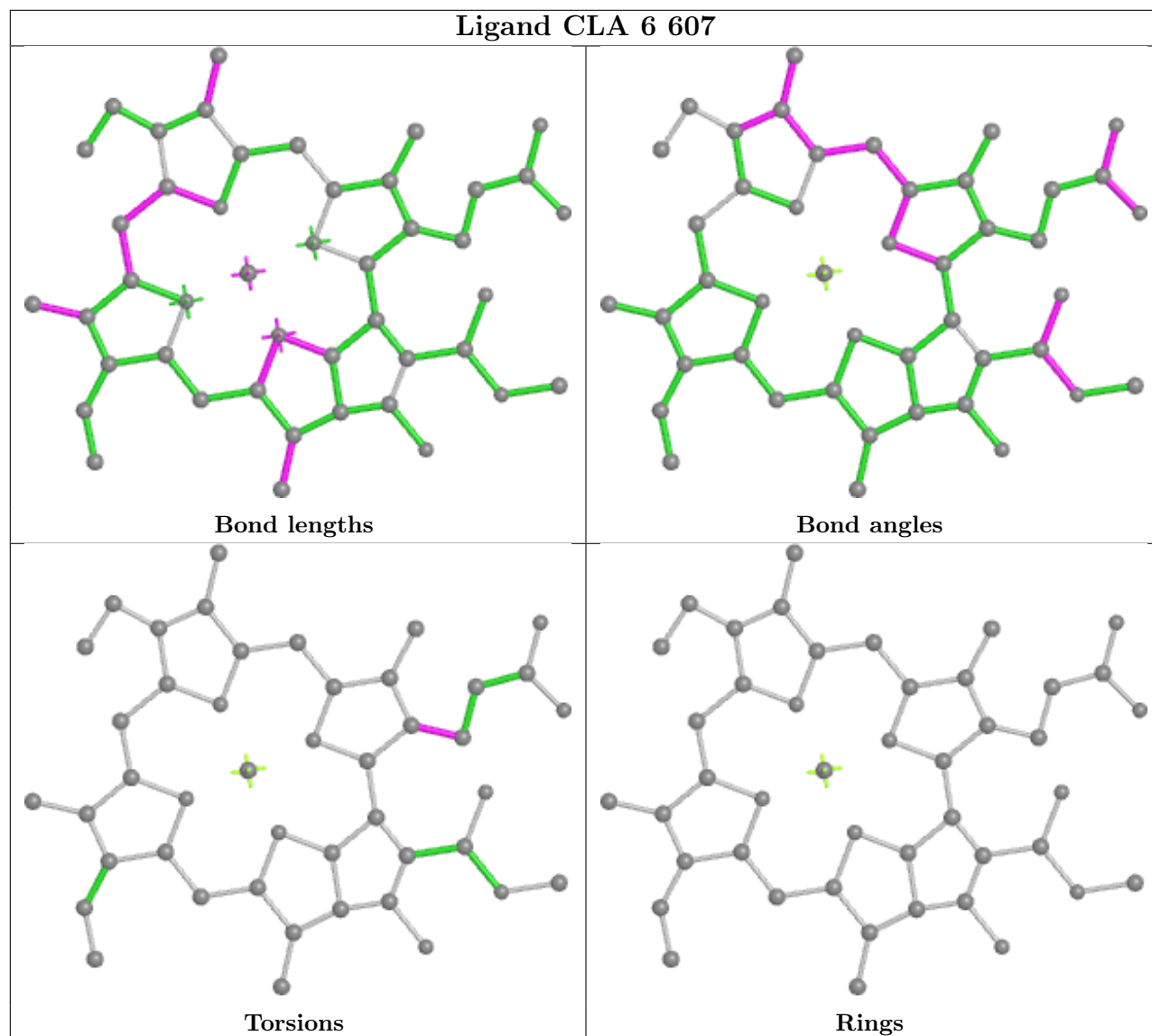
Torsions



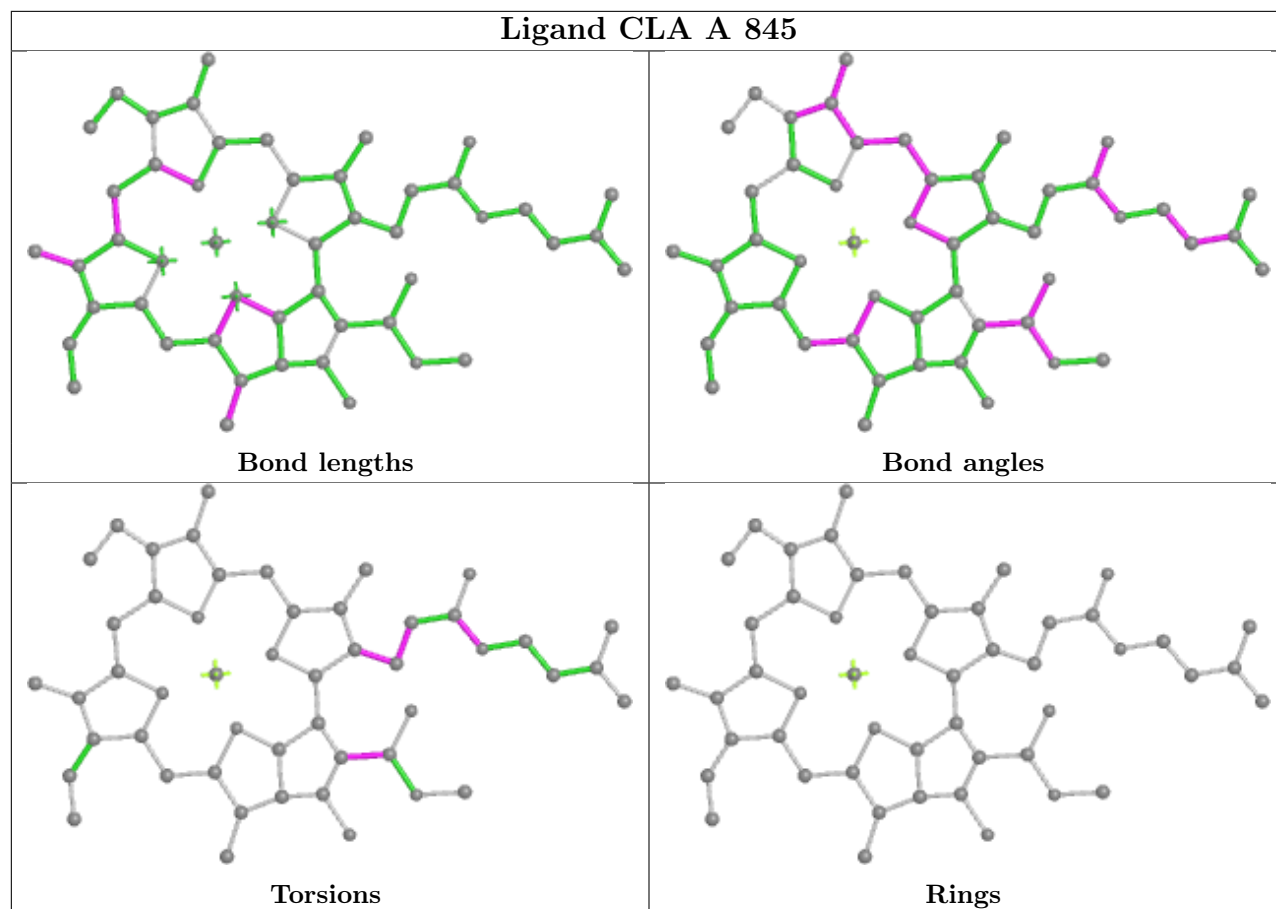
Rings



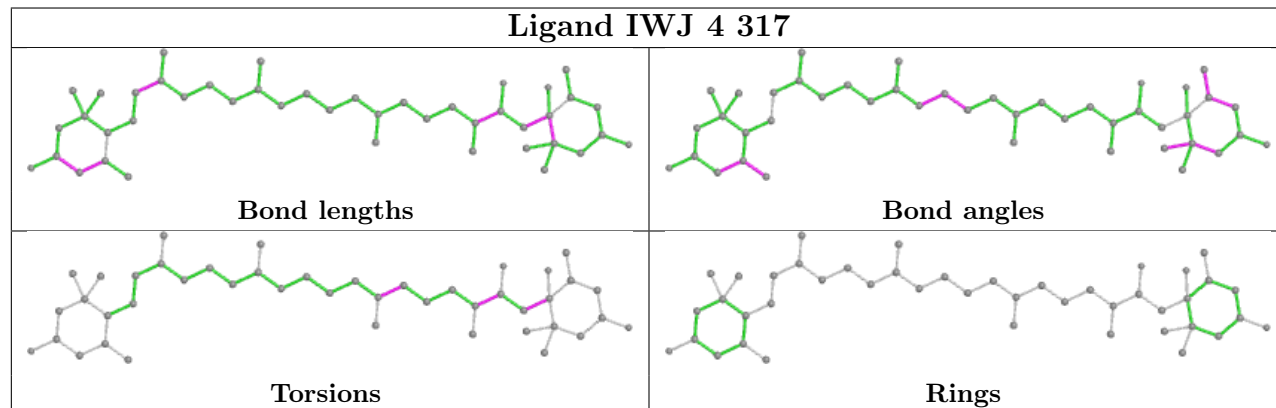
## Ligand CLA 6 607

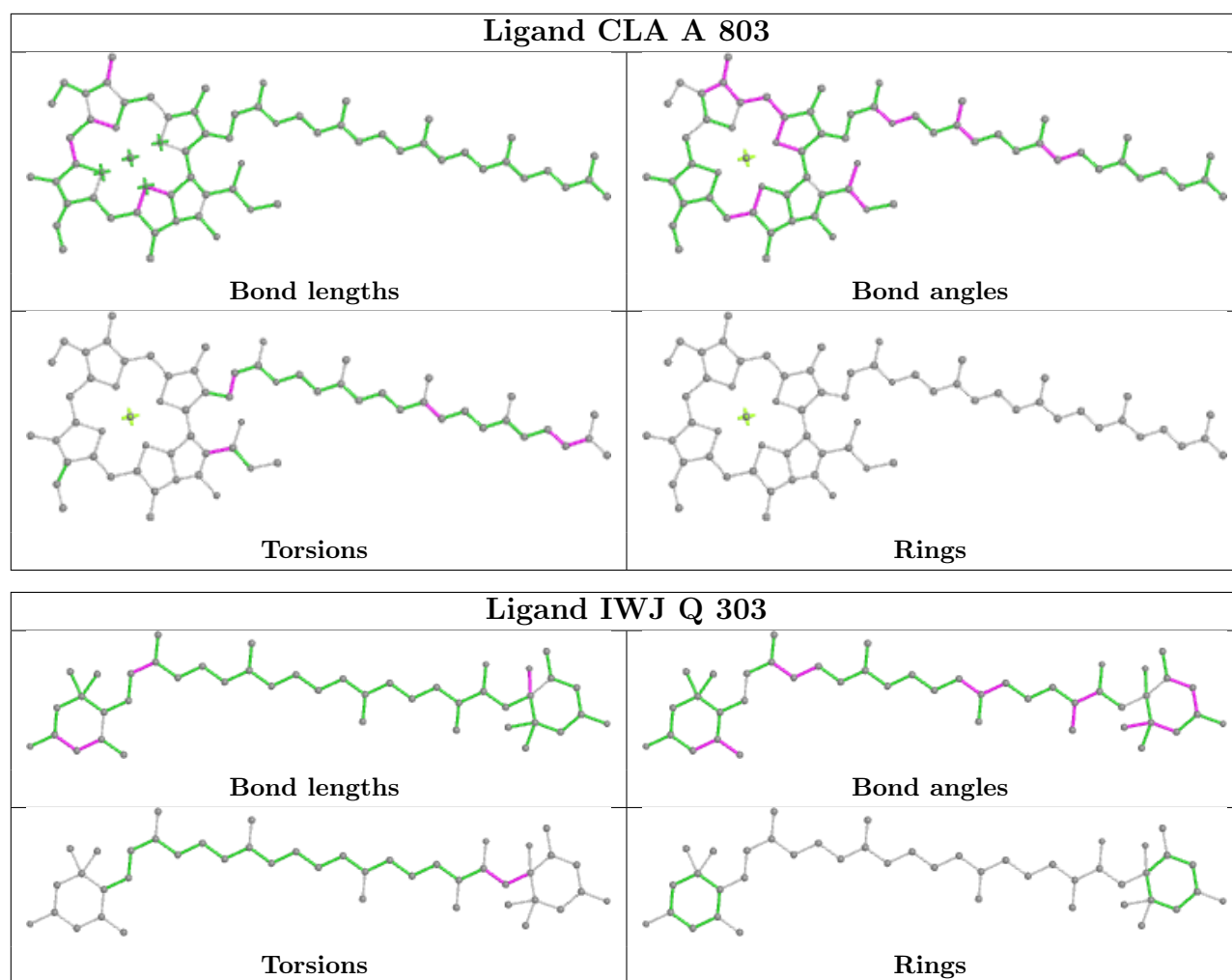


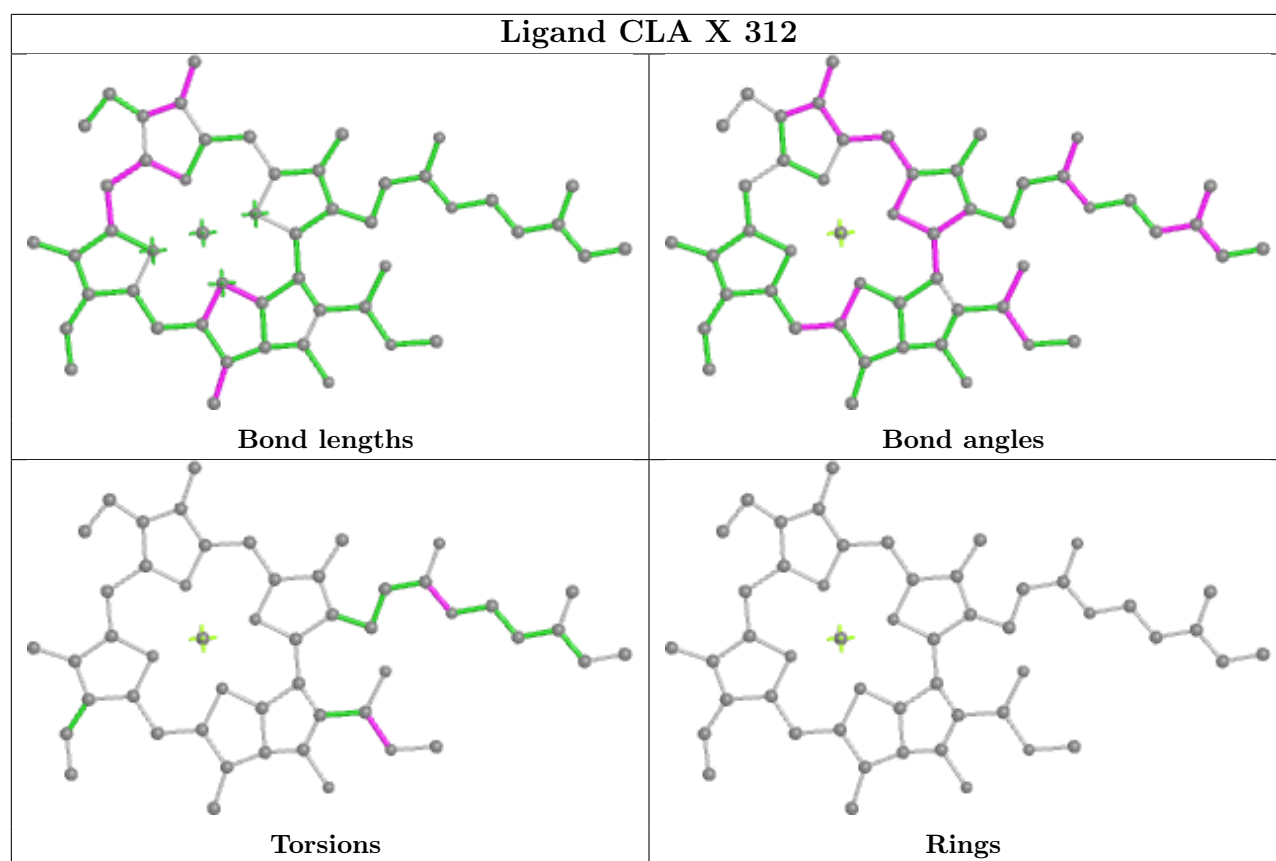
## Ligand CLA A 845



## Ligand IWJ 4 317

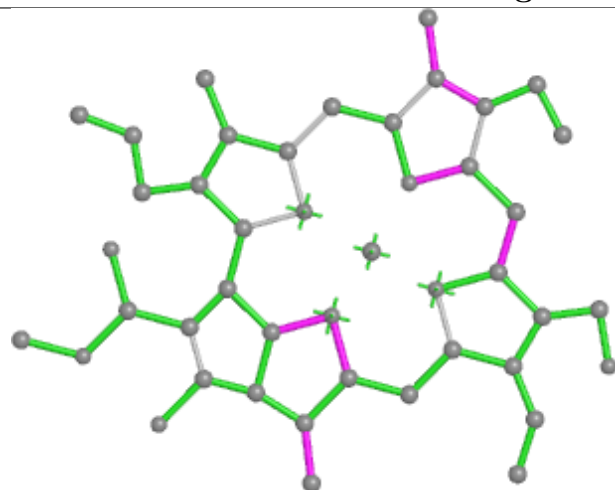




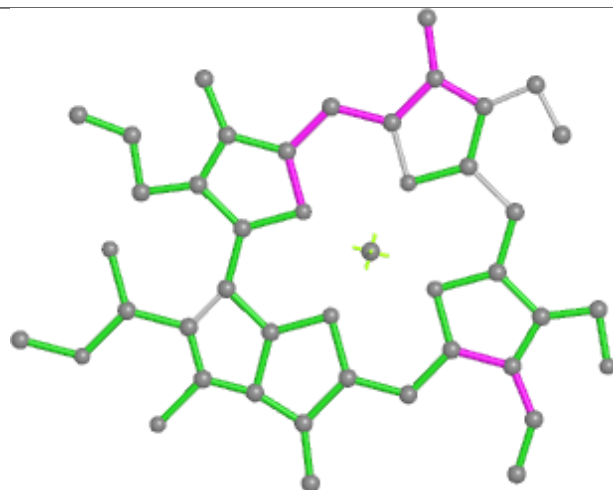




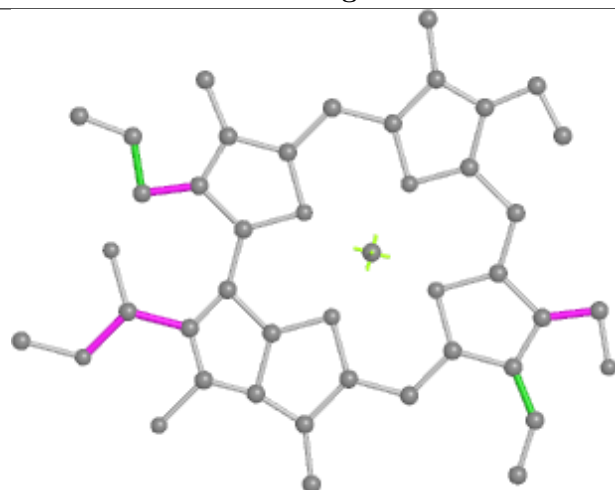
## Ligand CHL U 306



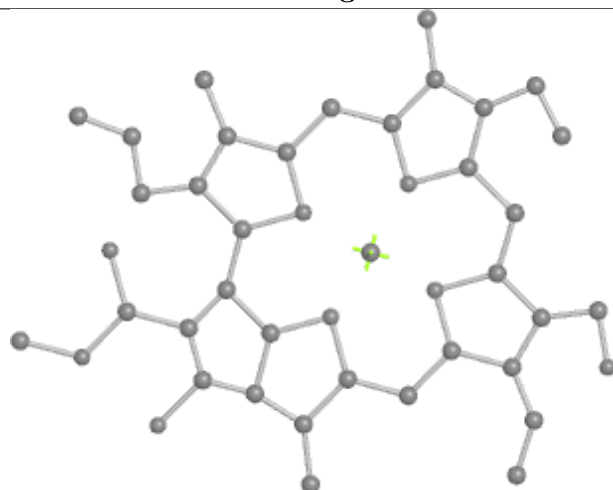
Bond lengths



Bond angles

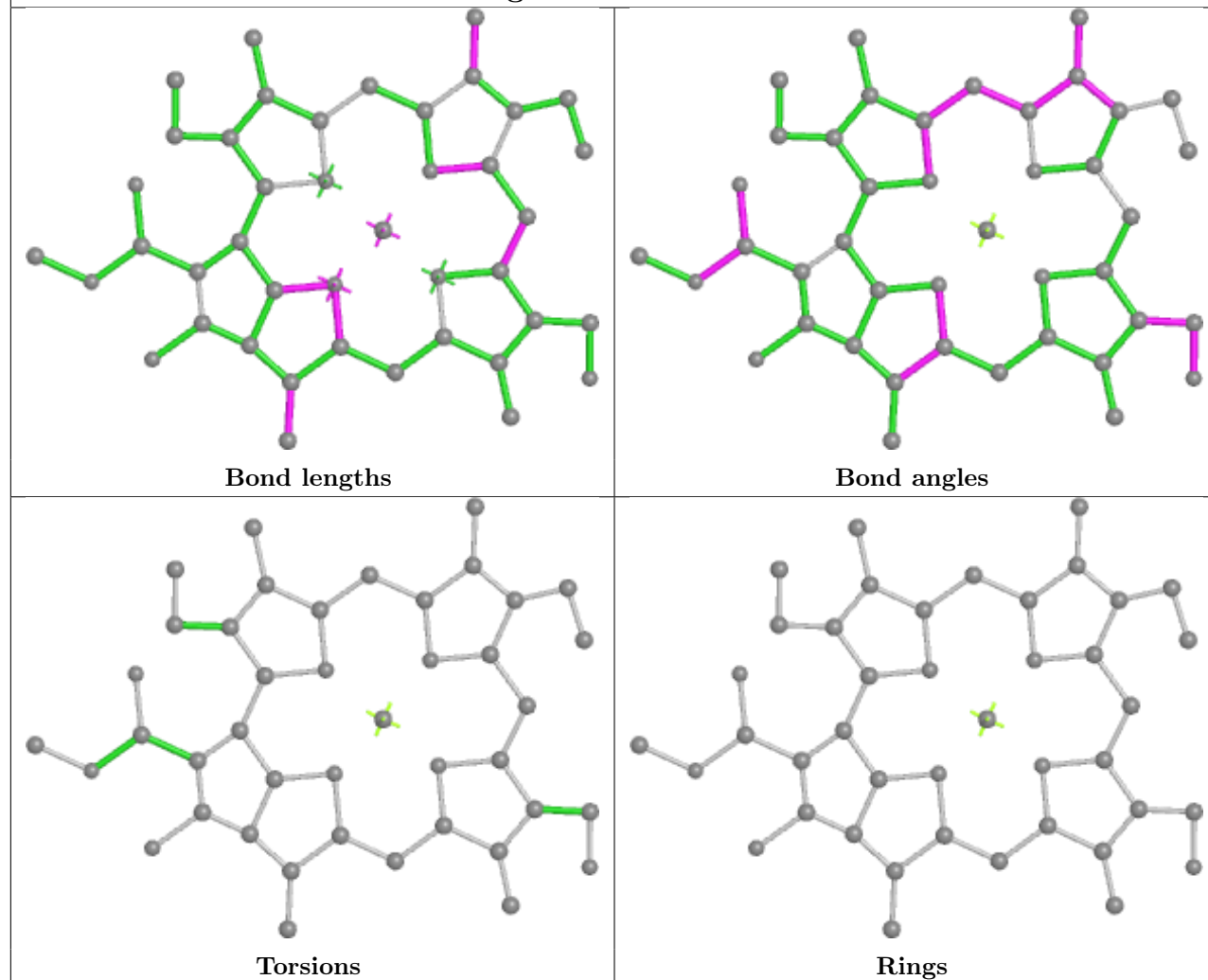


Torsions

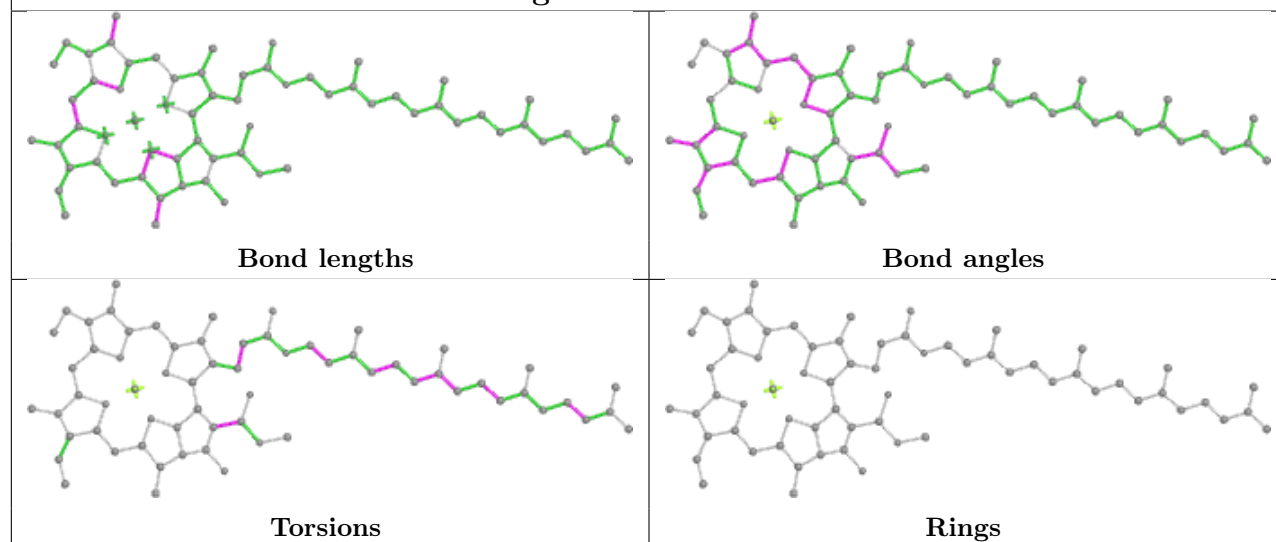


Rings

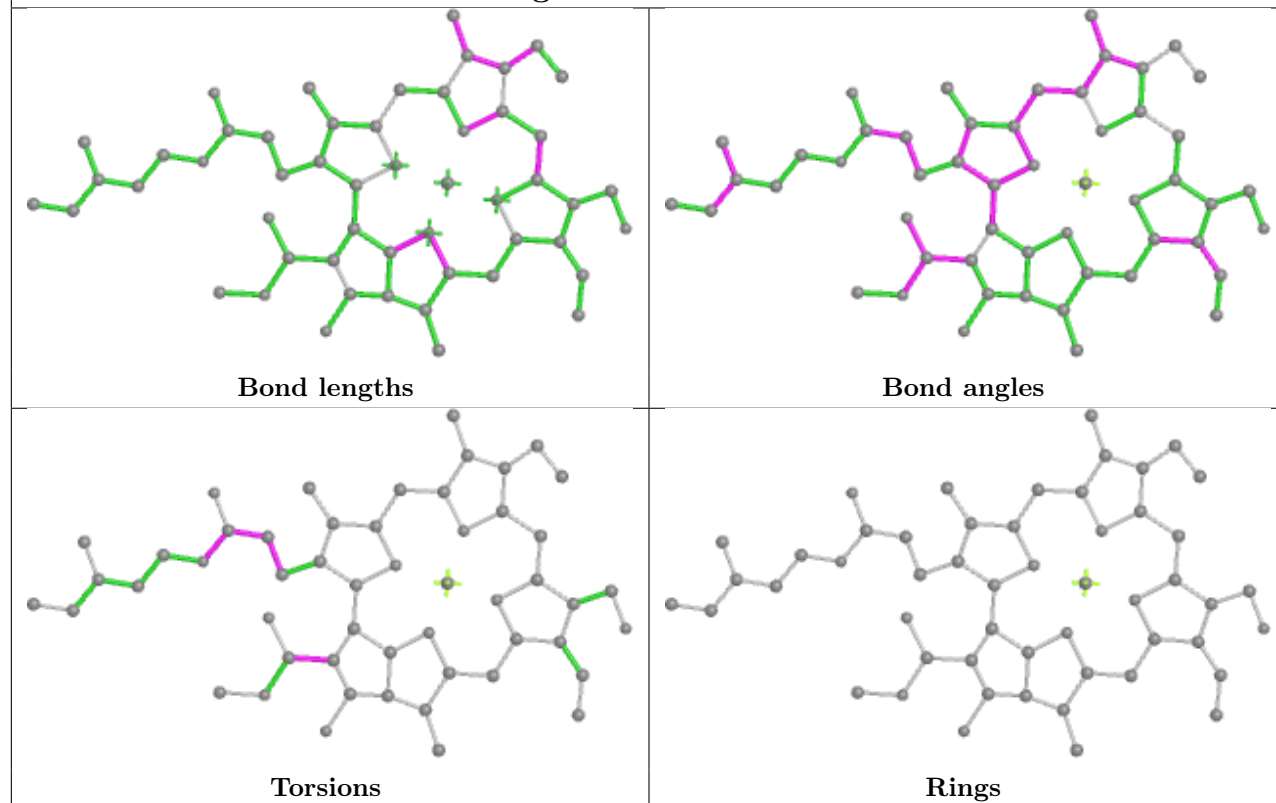
## Ligand CHL 6 605



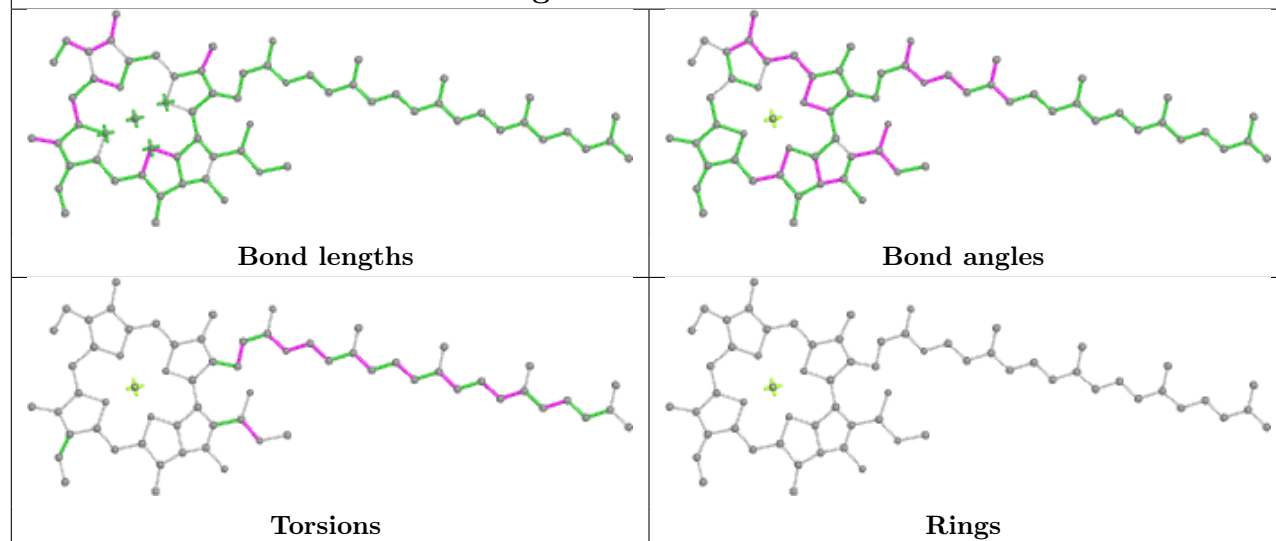
## Ligand CLA B 814

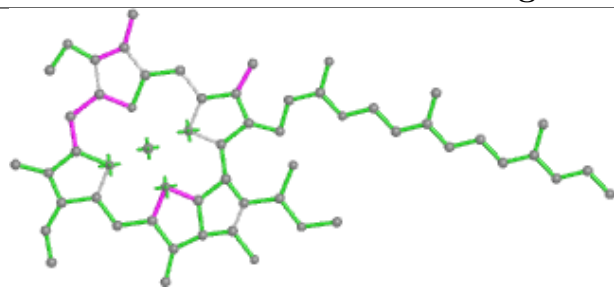


## Ligand CHL T 320

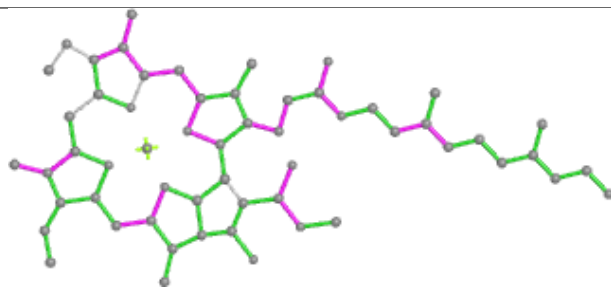


## Ligand CLA B 805

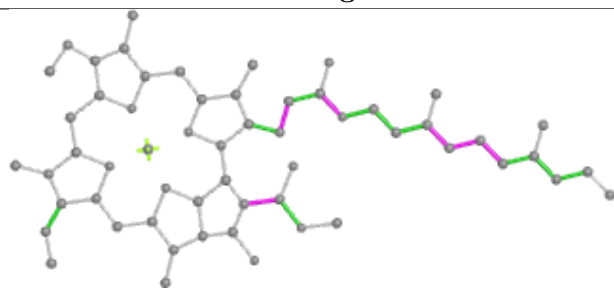


**Ligand CLA 4 313**

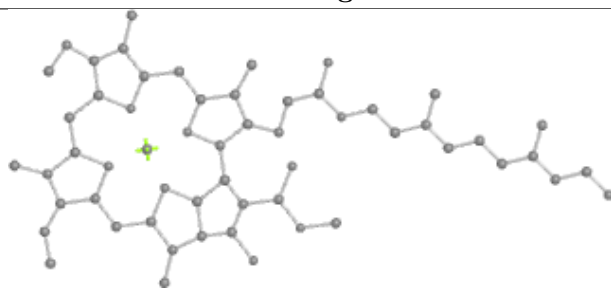
Bond lengths



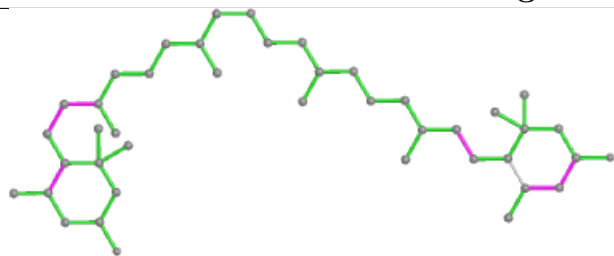
Bond angles



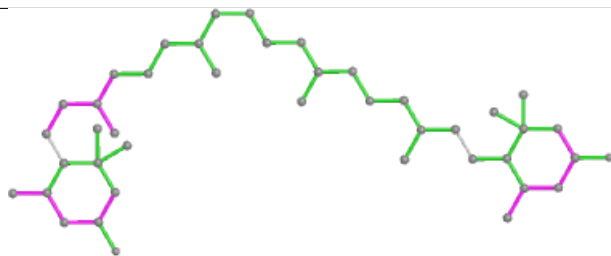
Torsions



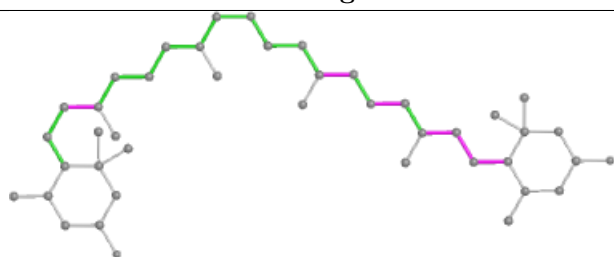
Rings

**Ligand Q6L X 319**

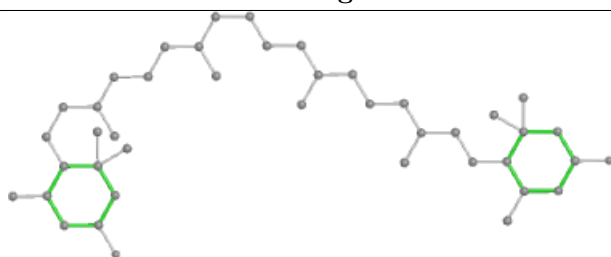
Bond lengths



Bond angles

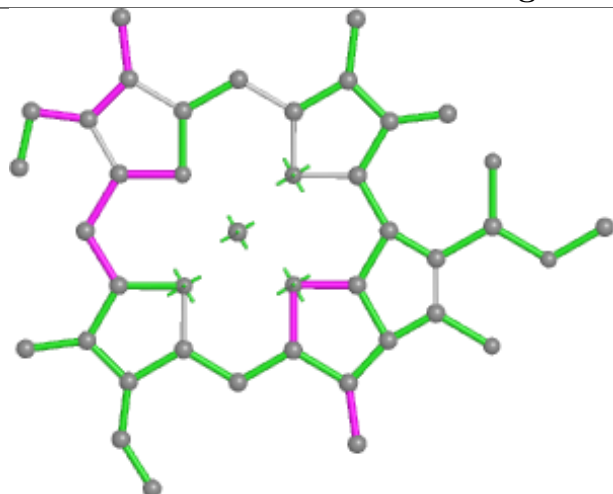


Torsions

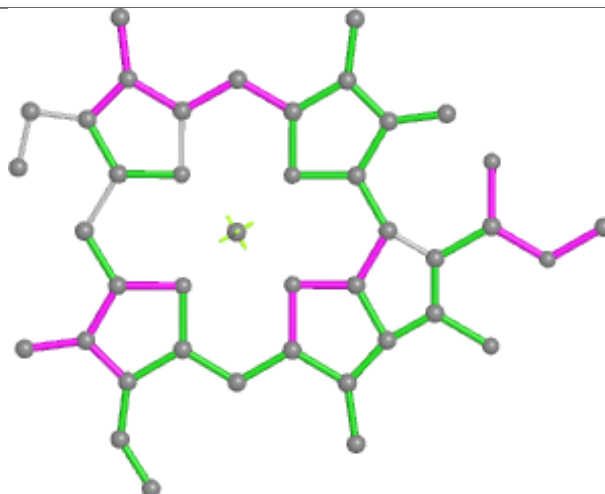


Rings

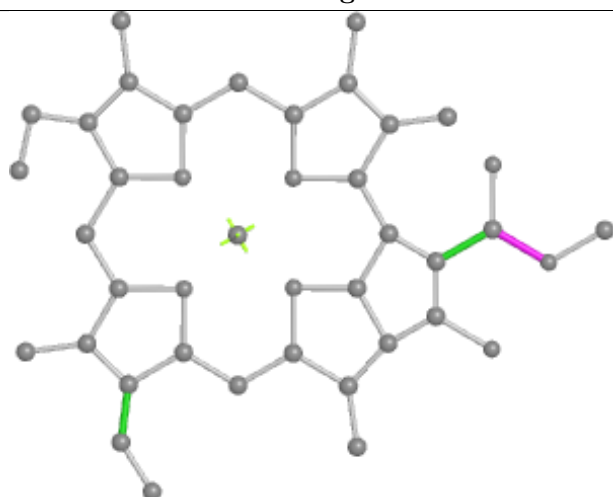
## Ligand CLA 3 308



Bond lengths



Bond angles

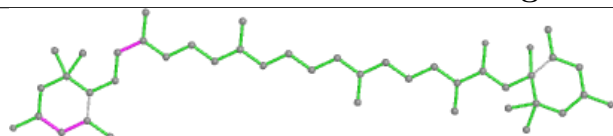


Torsions

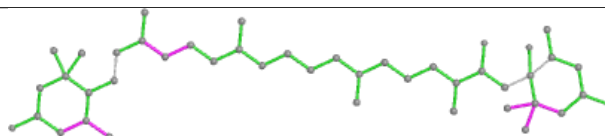


Rings

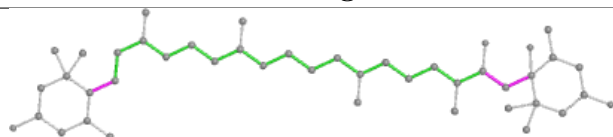
## Ligand IWJ 5 611



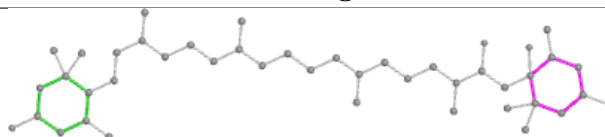
Bond lengths



Bond angles

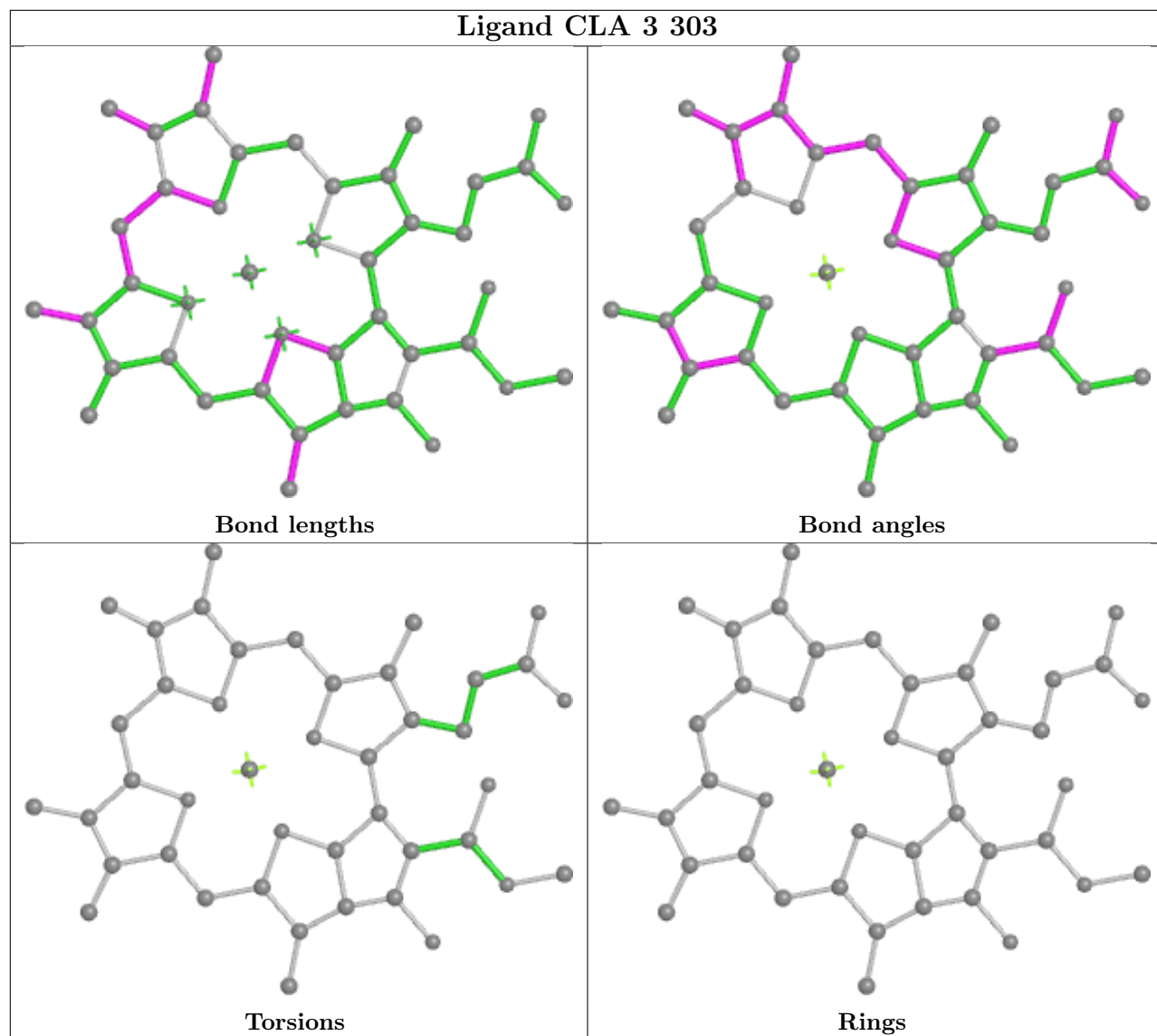


Torsions

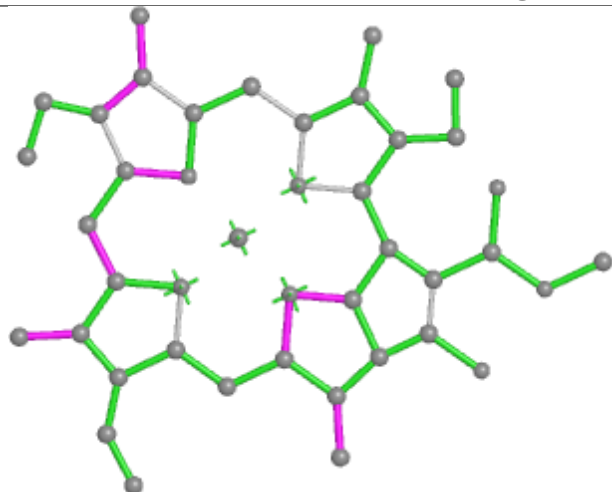


Rings

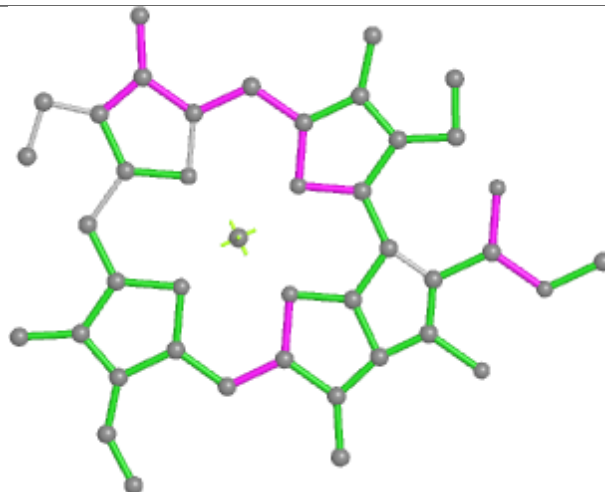
## Ligand CLA 3 303



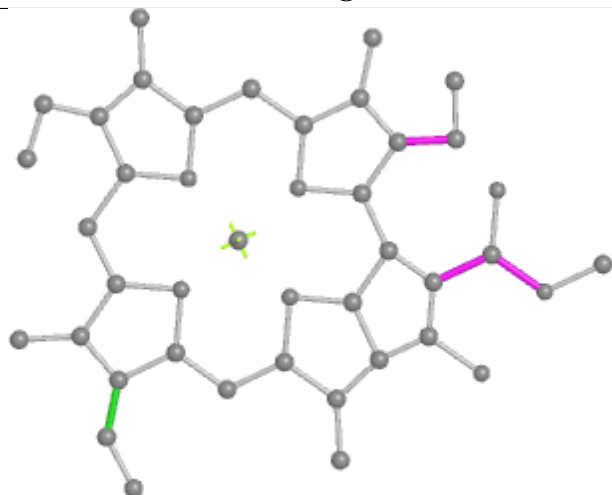
## Ligand CLA T 313



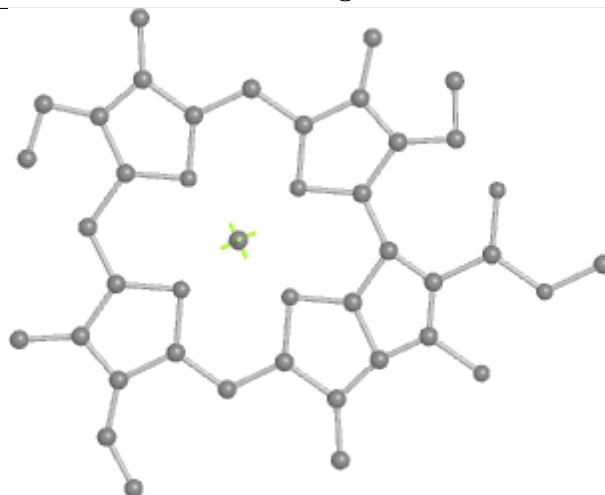
Bond lengths



Bond angles

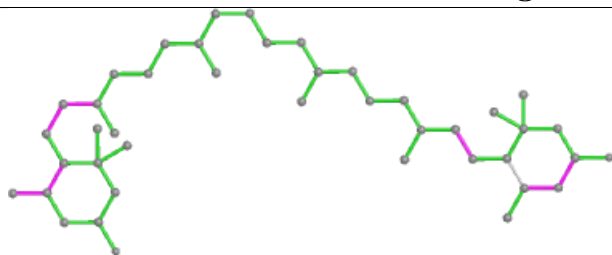


Torsions

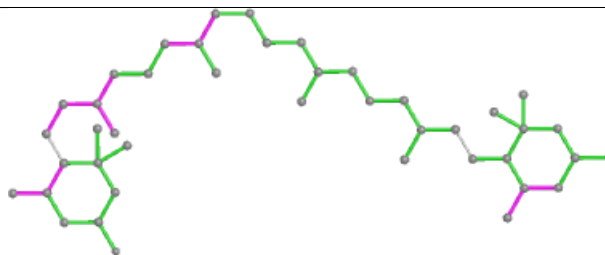


Rings

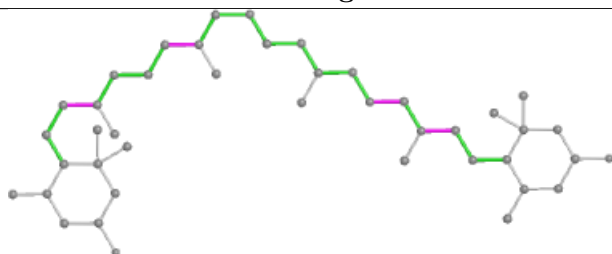
## Ligand Q6L U 314



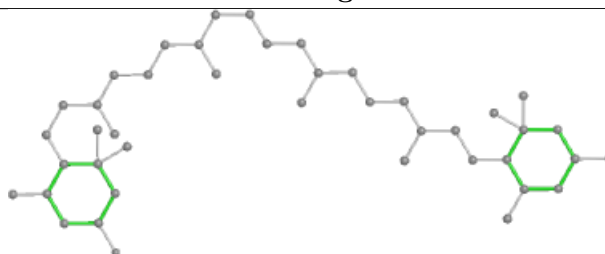
Bond lengths



Bond angles

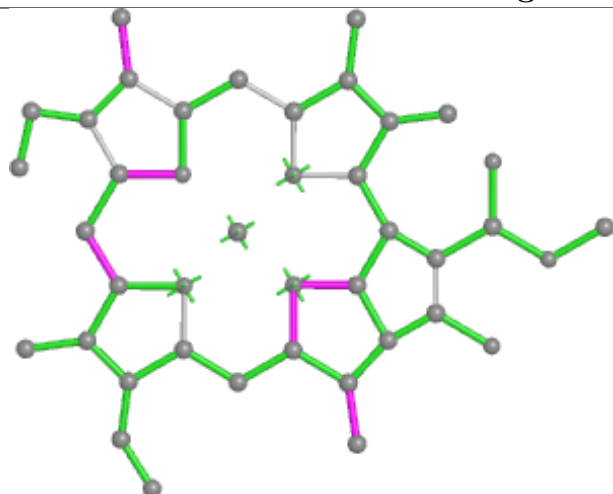


Torsions

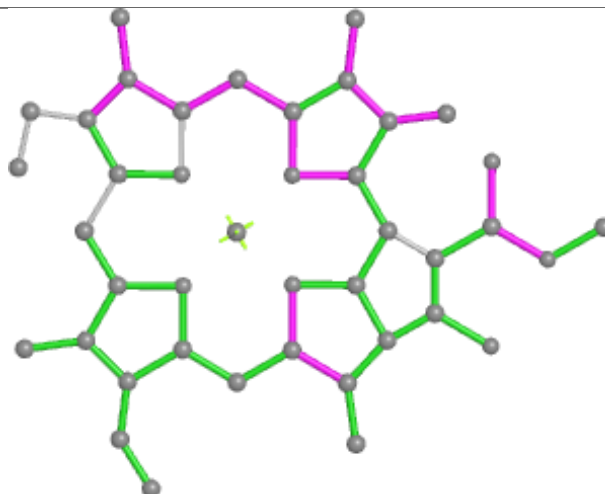


Rings

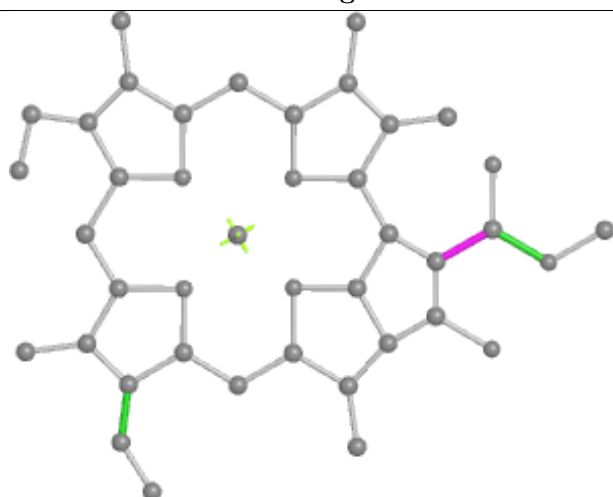
## Ligand CLA S 313



Bond lengths



Bond angles

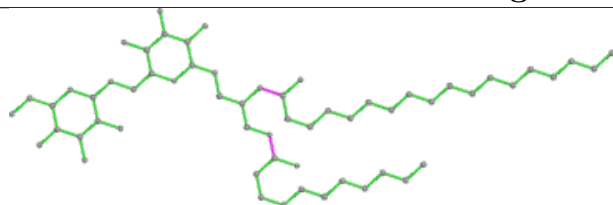


Torsions

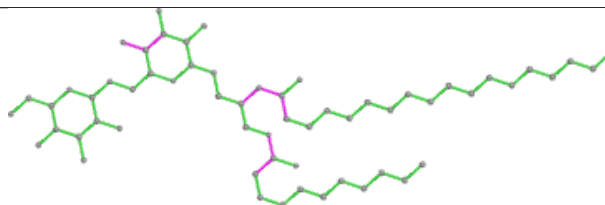


Rings

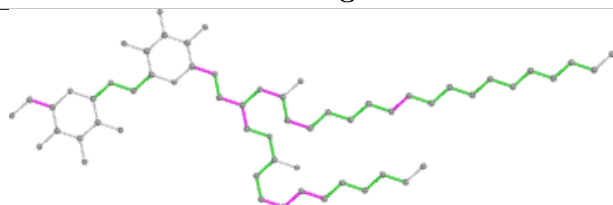
## Ligand DGD B 850



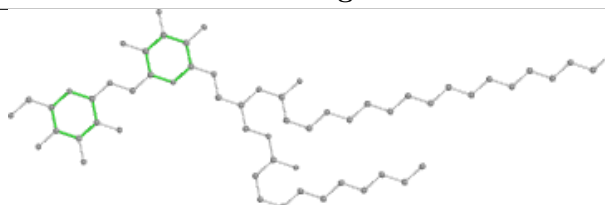
Bond lengths



Bond angles

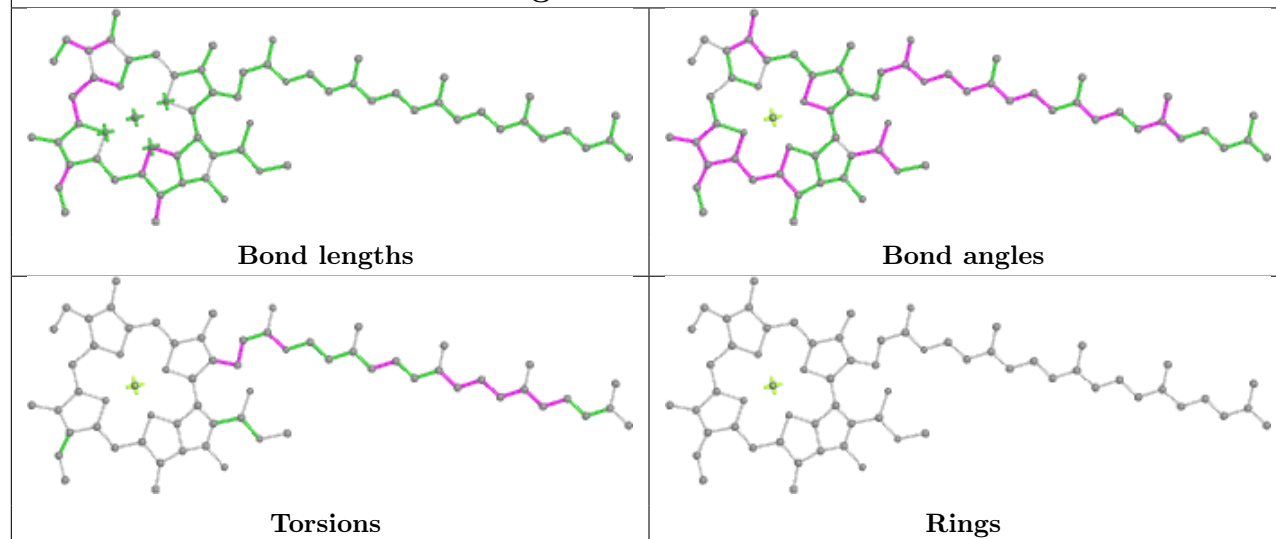
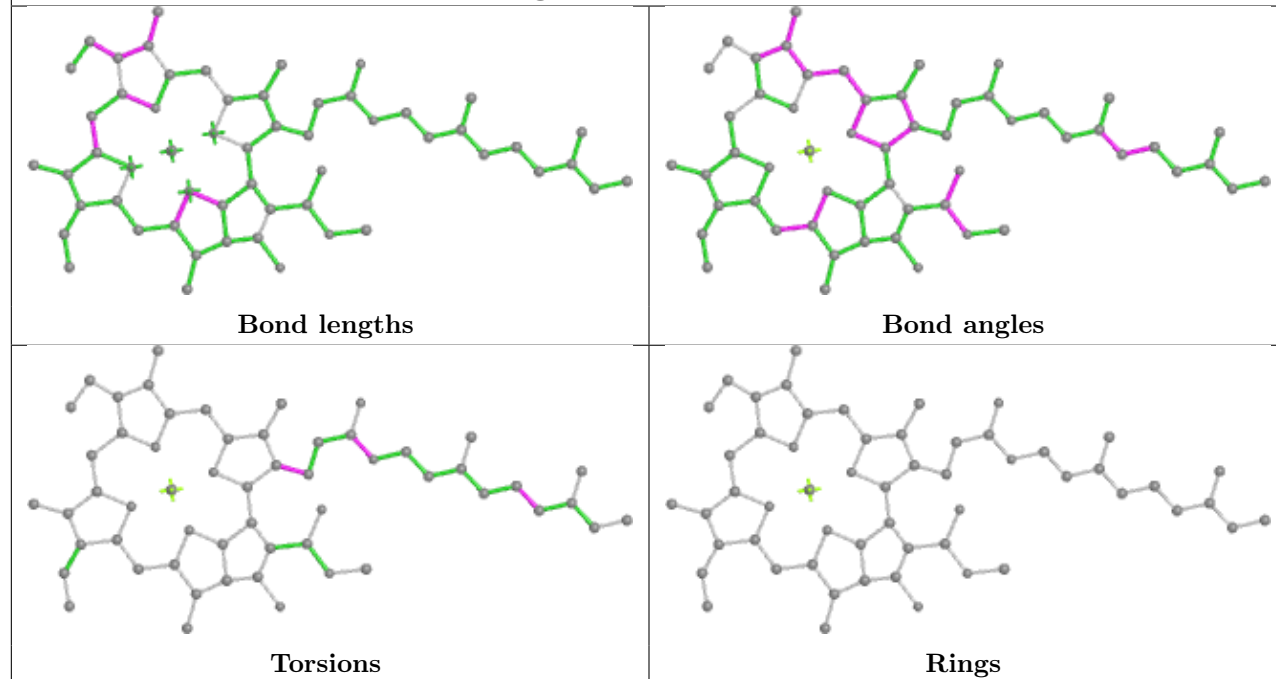


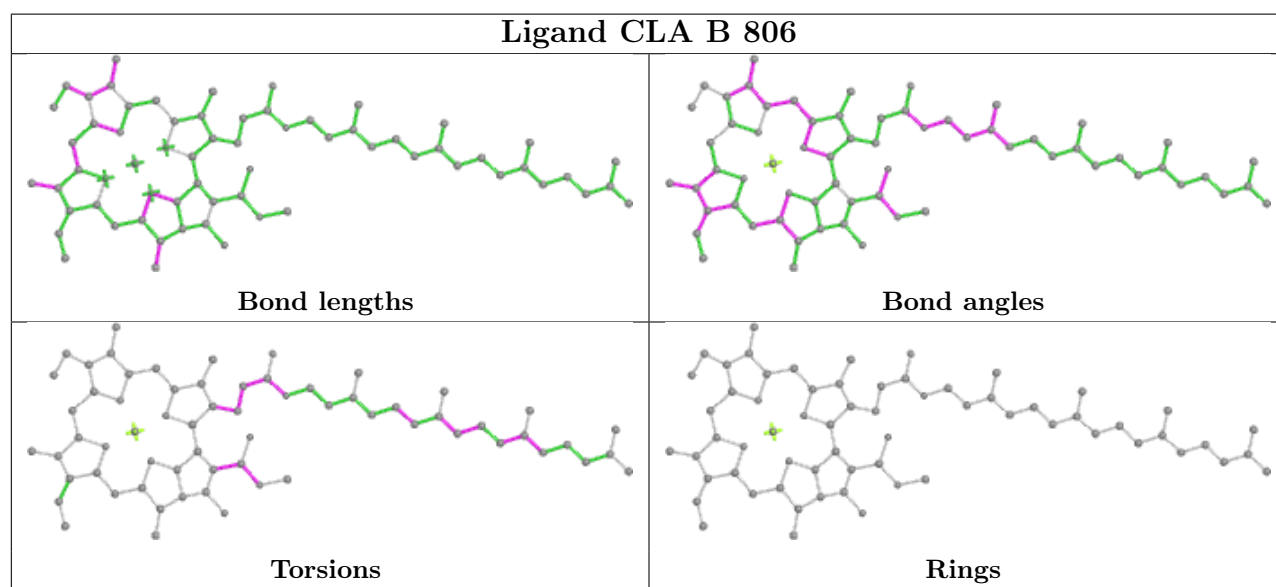
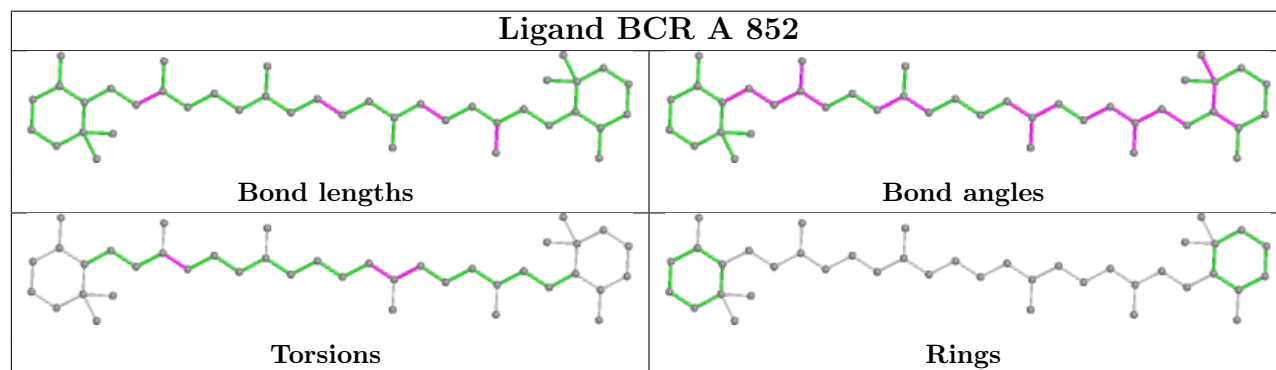
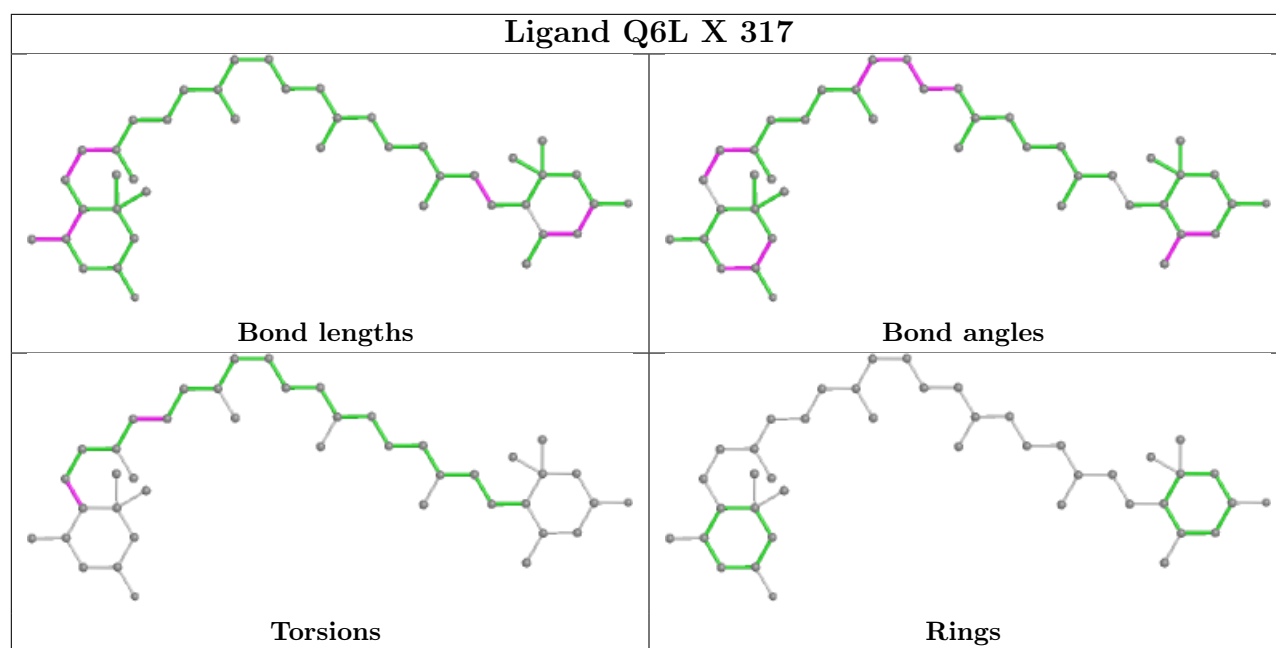
Torsions

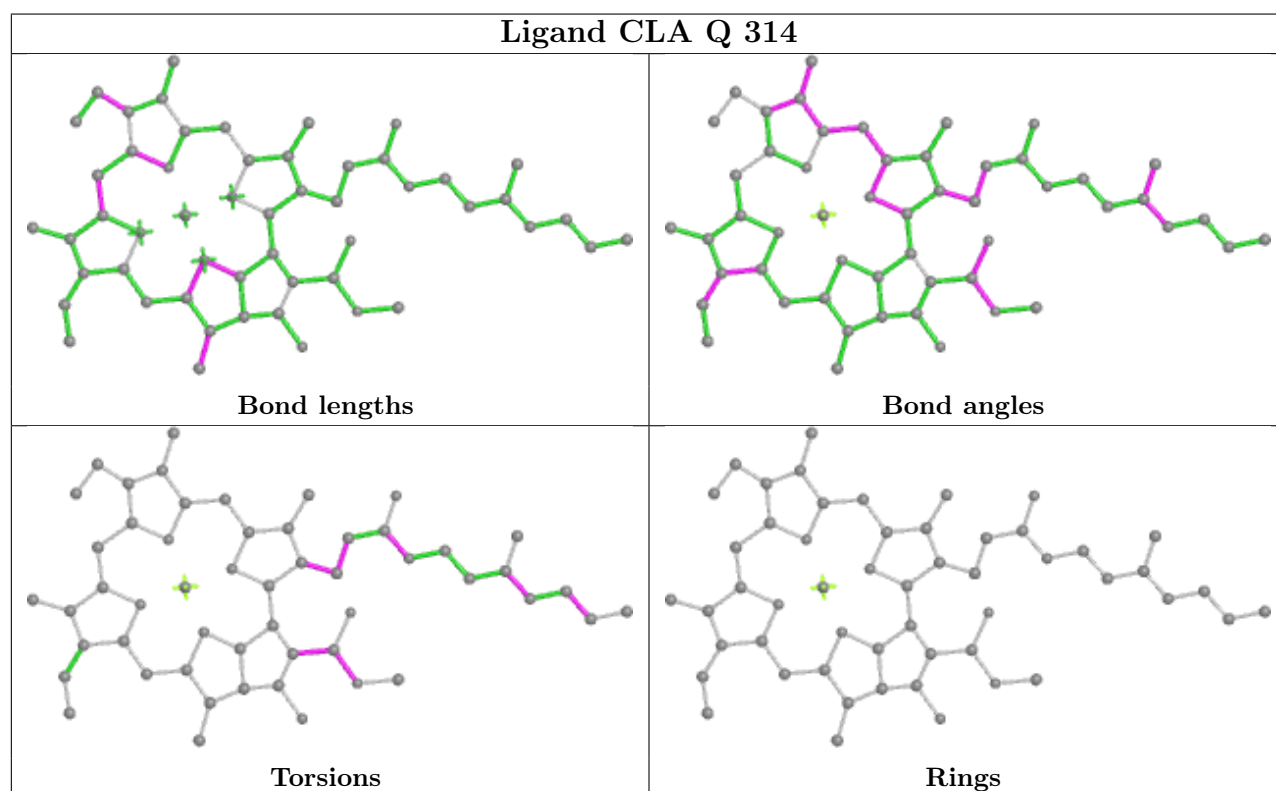
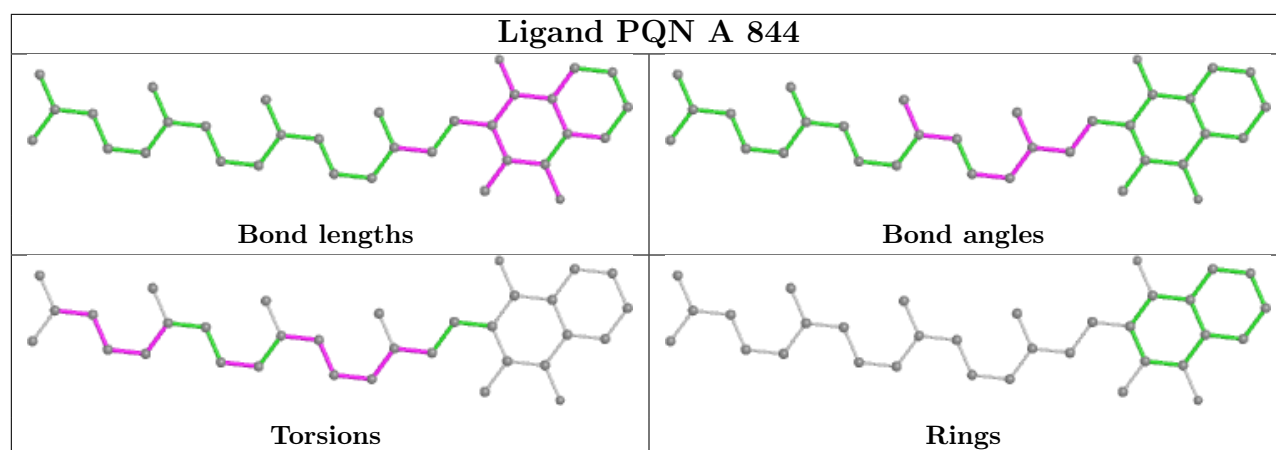


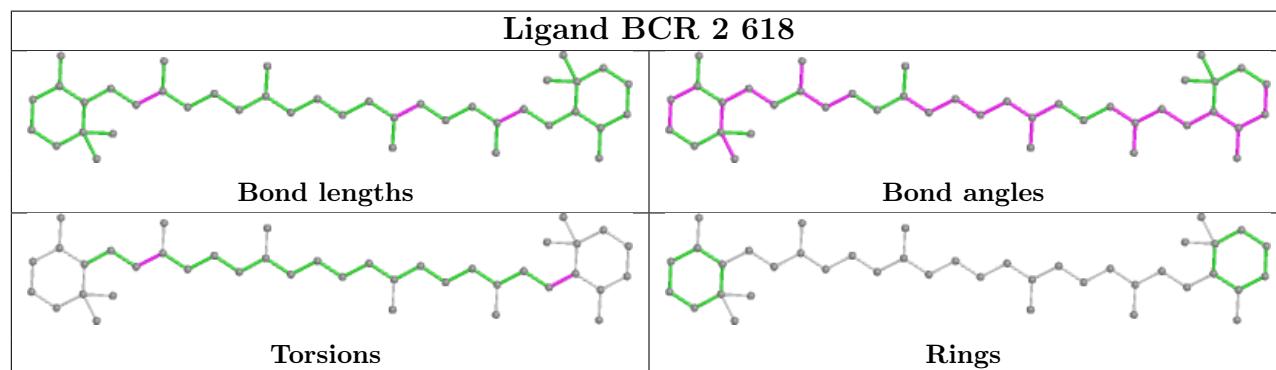
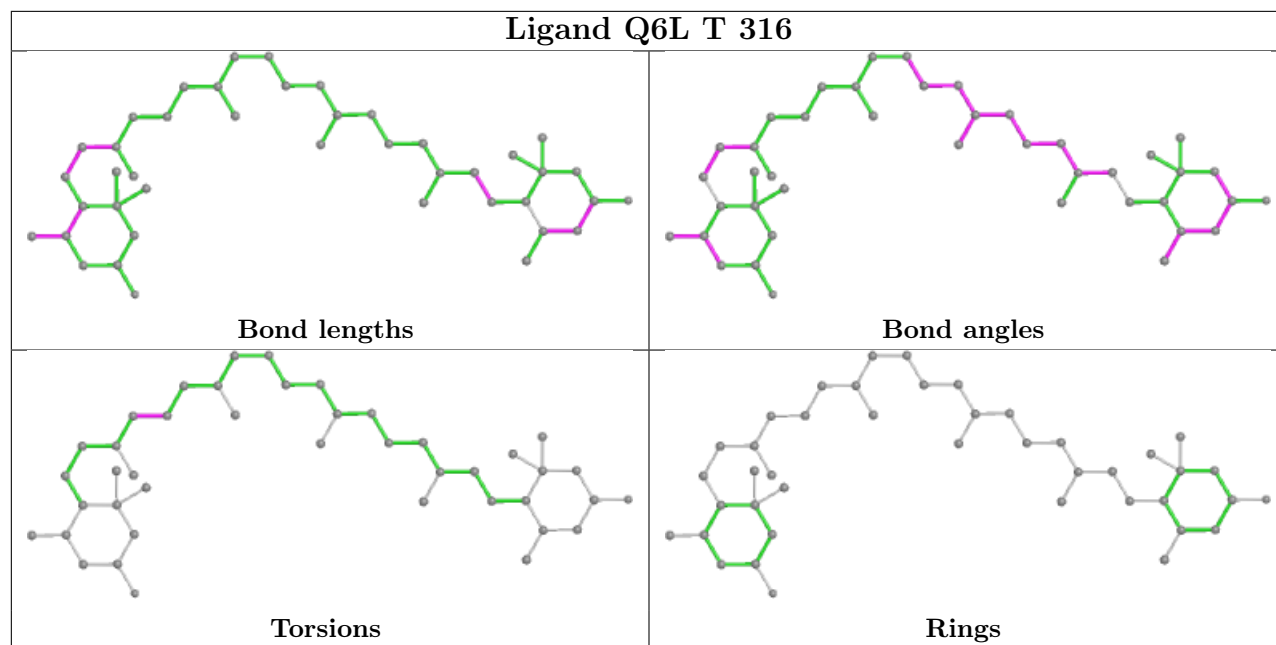
Rings



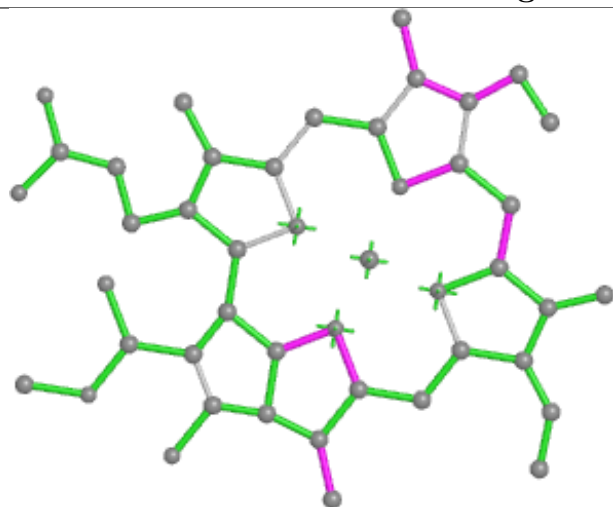
**Ligand CLA B 813****Ligand CLA A 834**



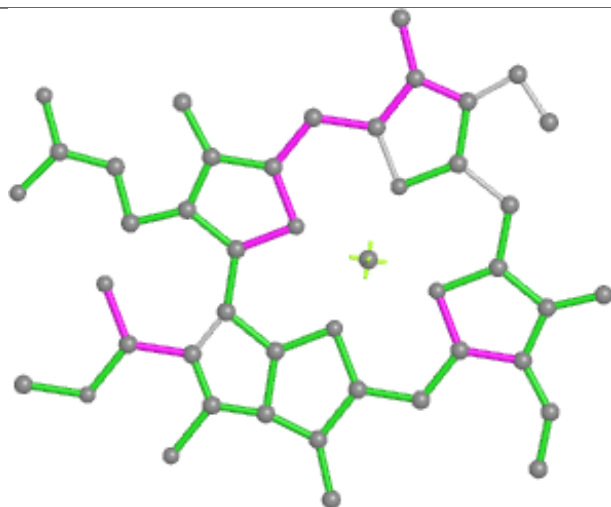




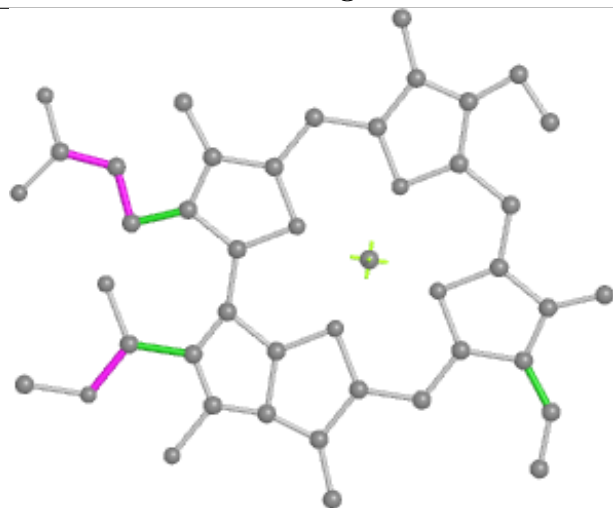
## Ligand CHL 3 306



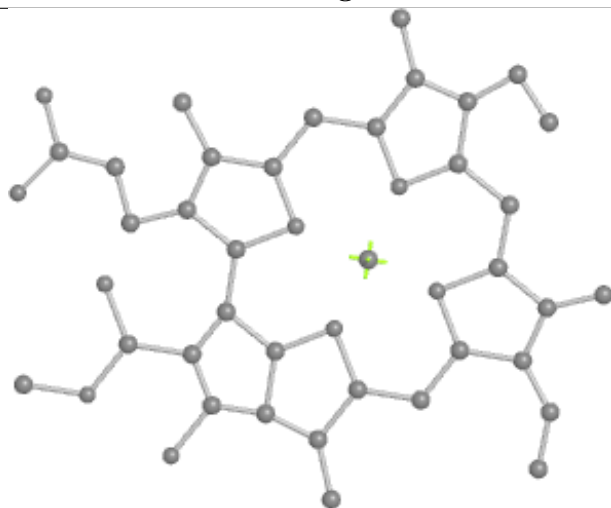
Bond lengths



Bond angles

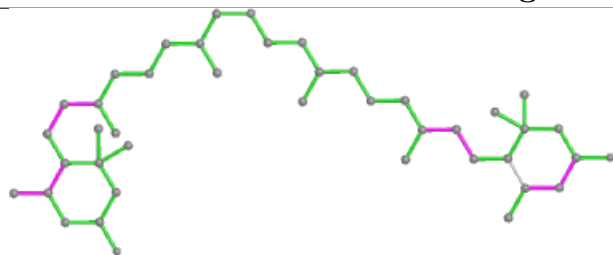


Torsions

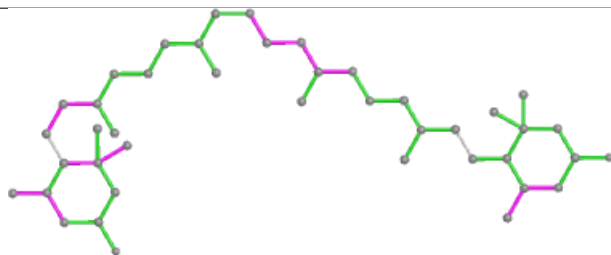


Rings

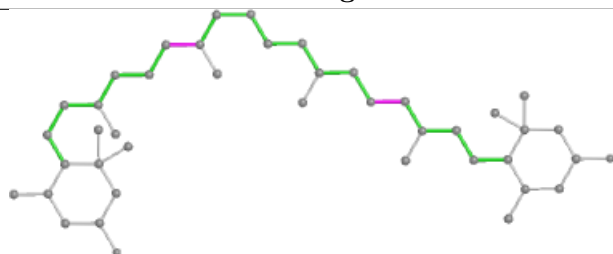
## Ligand Q6L P 316



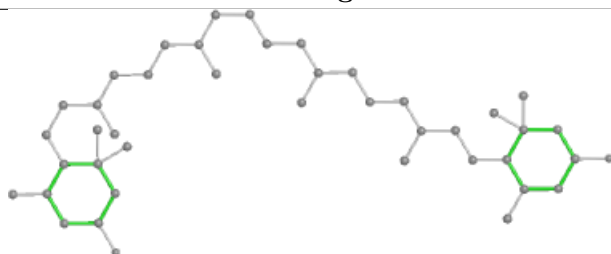
Bond lengths



Bond angles

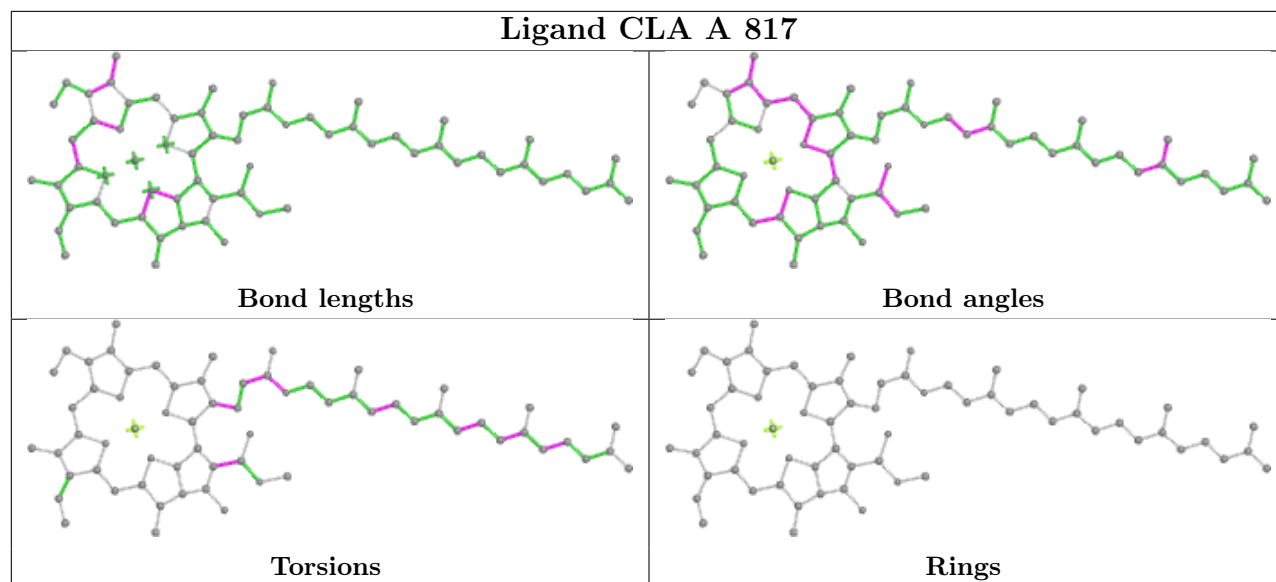


Torsions

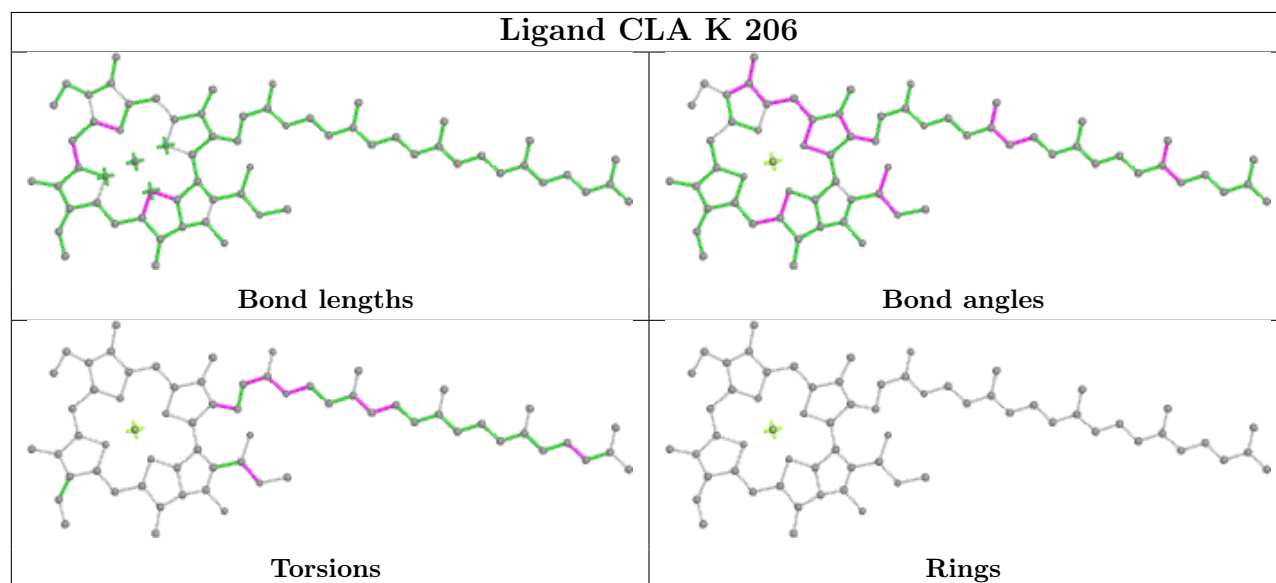


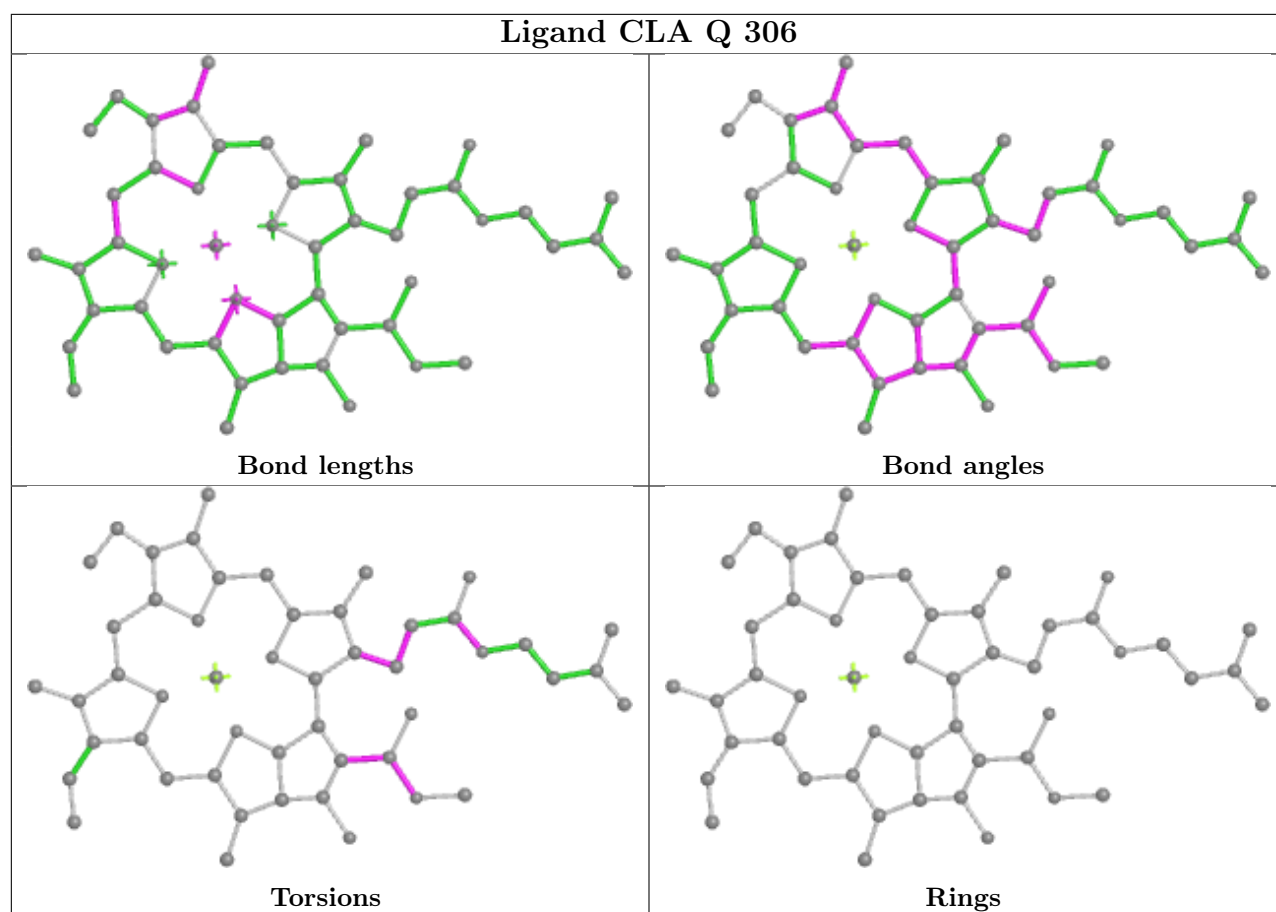
Rings

## Ligand CLA A 817

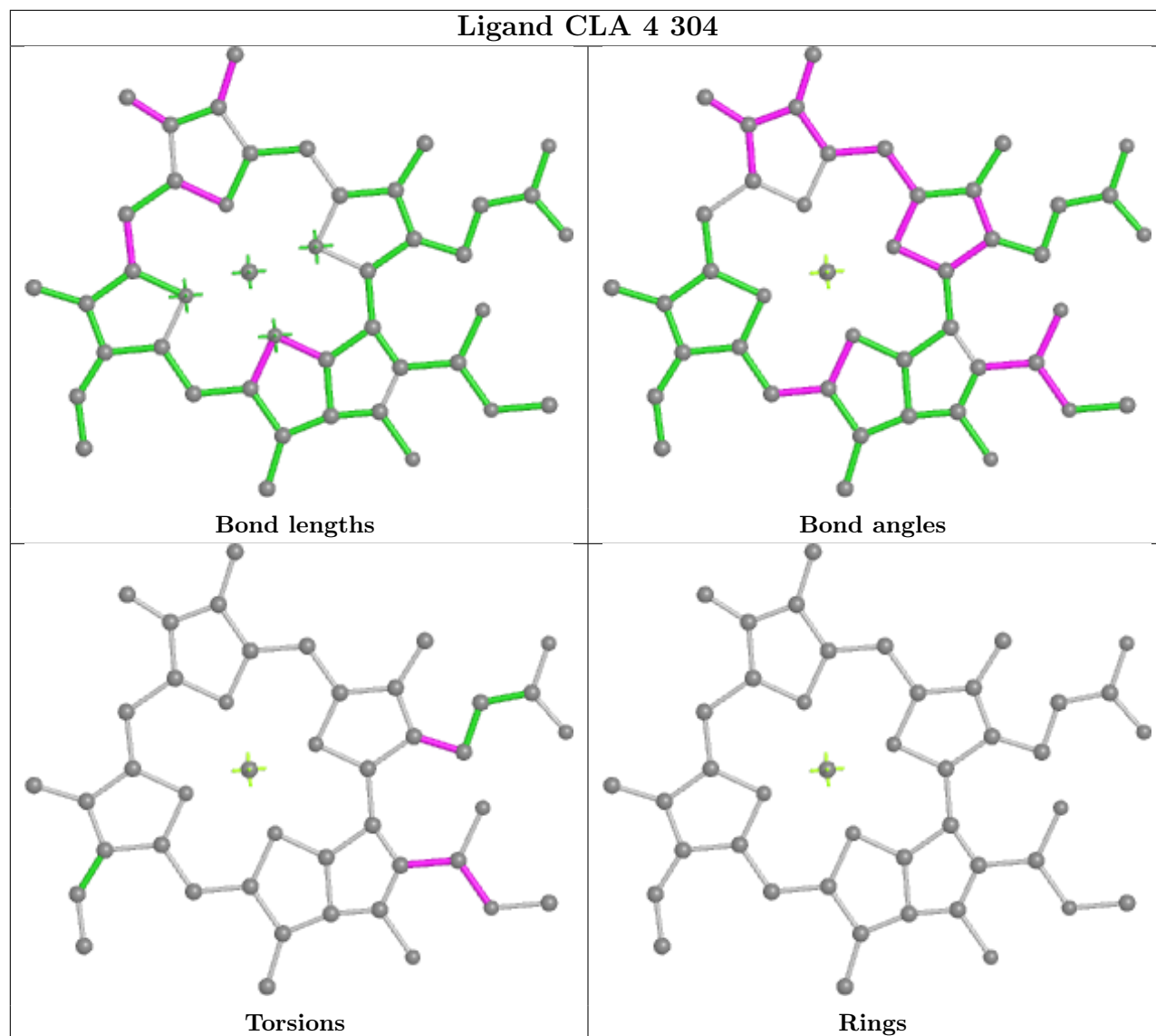


## Ligand CLA K 206

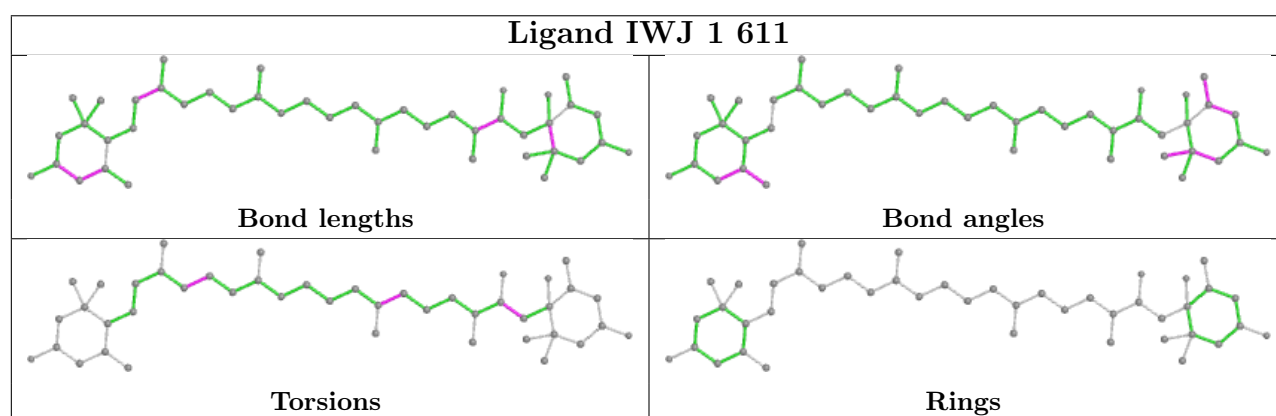
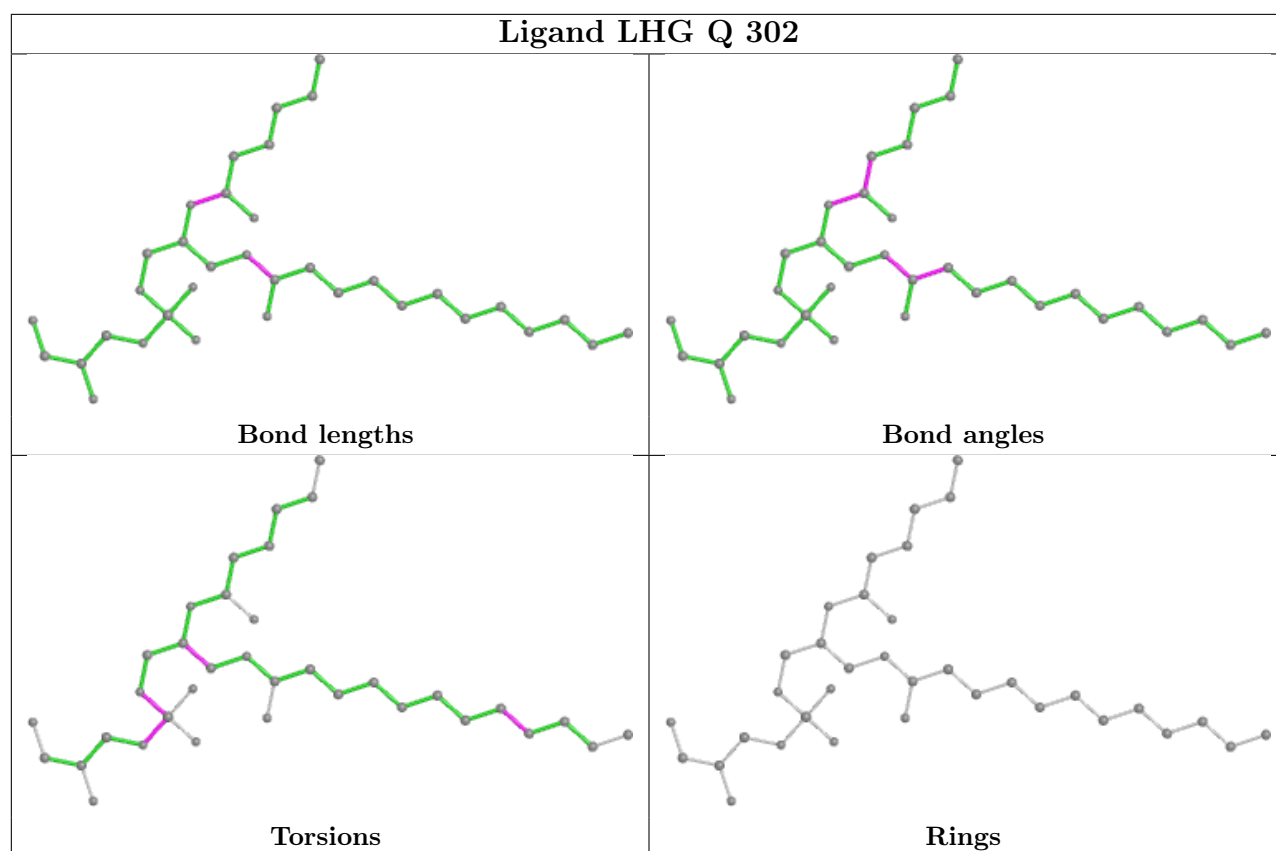


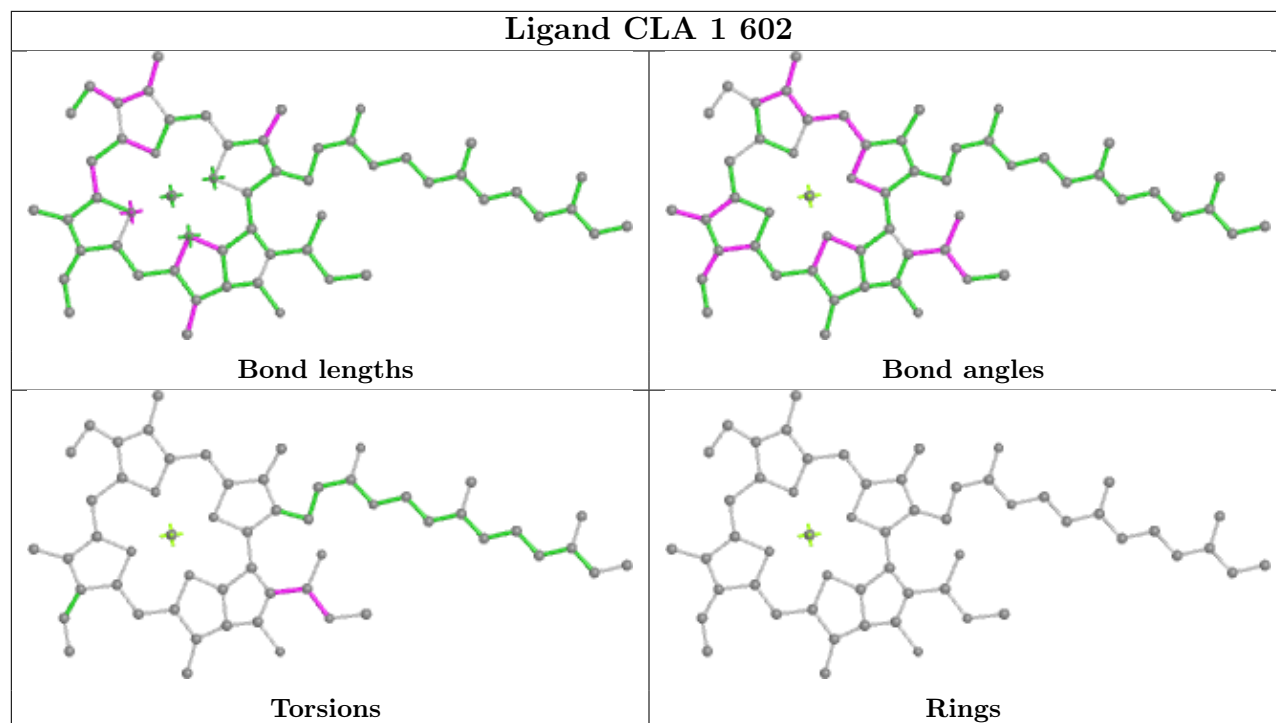
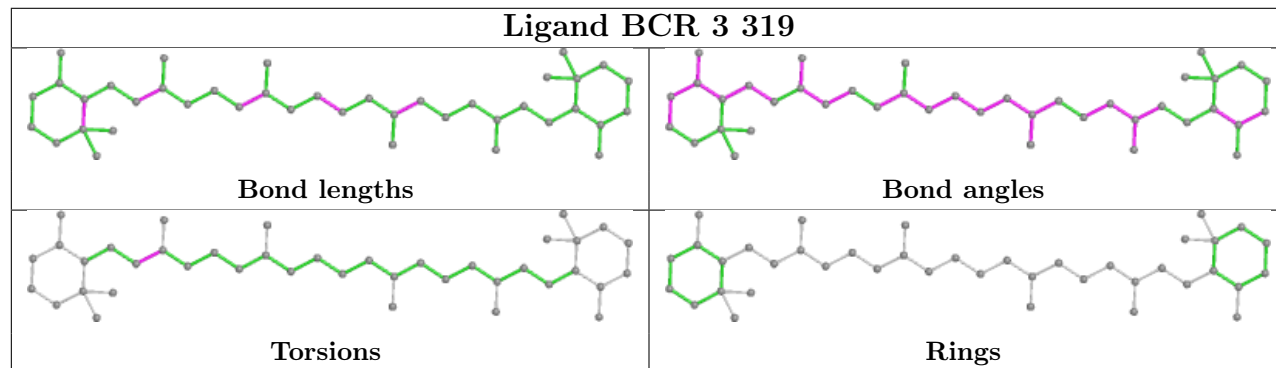


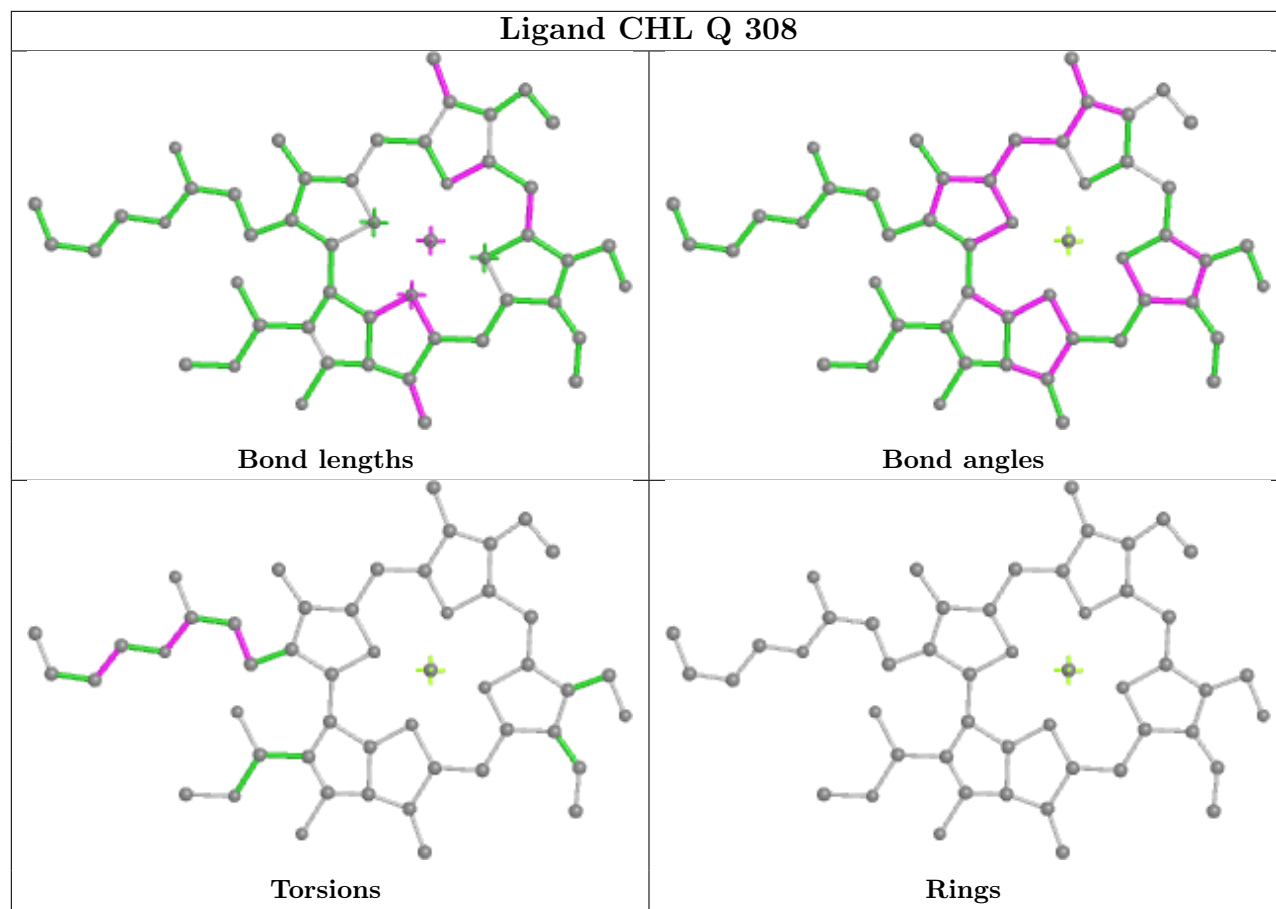
## Ligand CLA 4 304



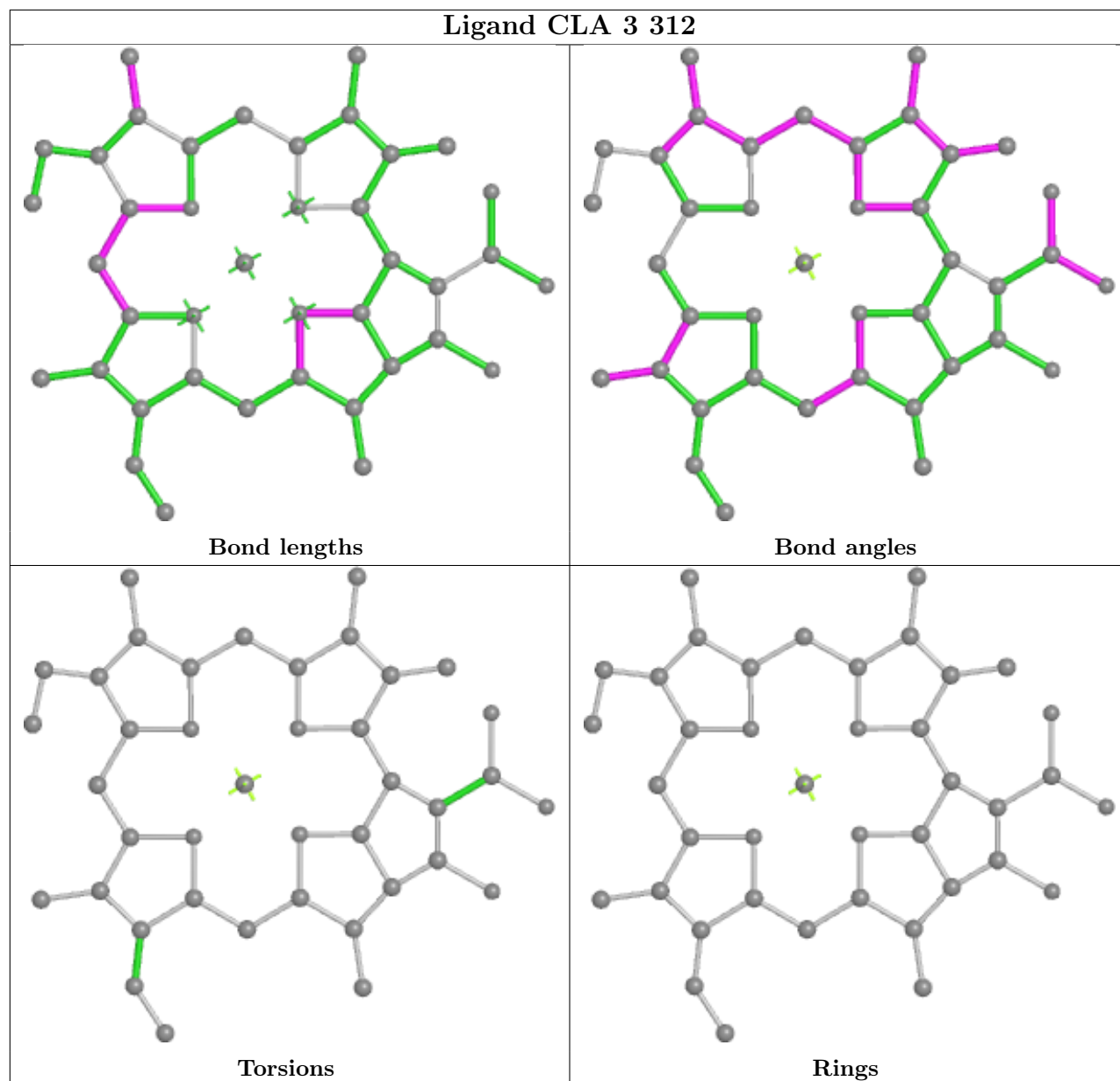


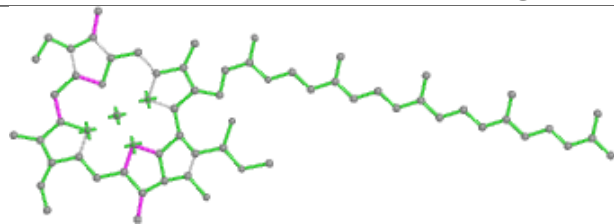
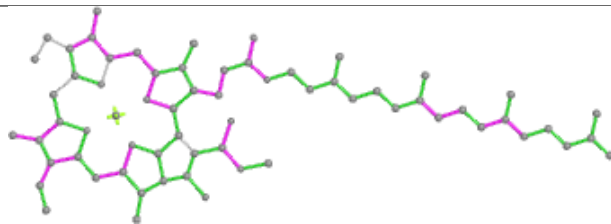
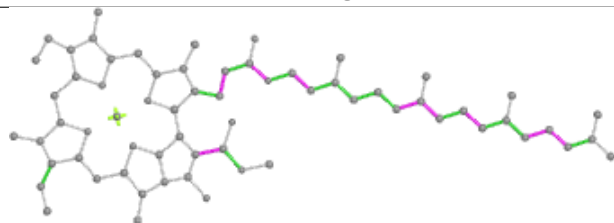
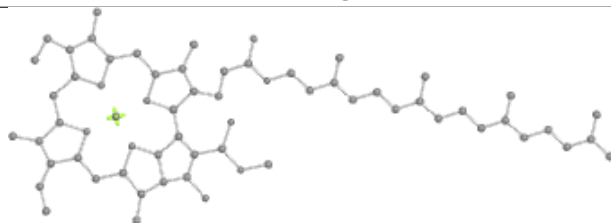
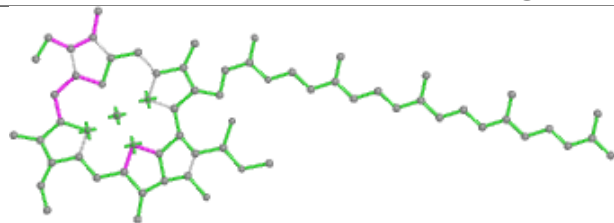
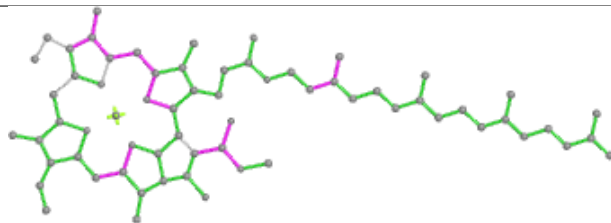
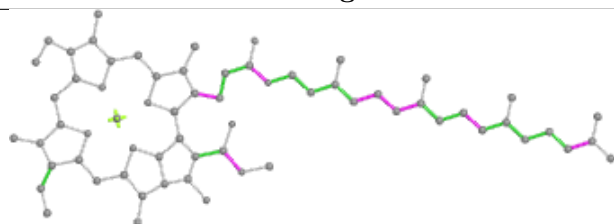
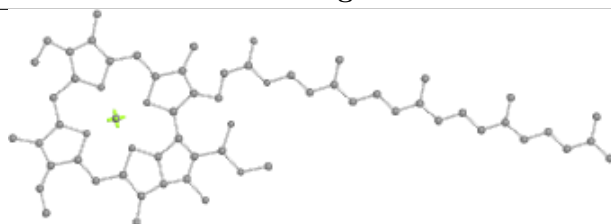


**Ligand CLA 1 602****Ligand BCR 3 319**

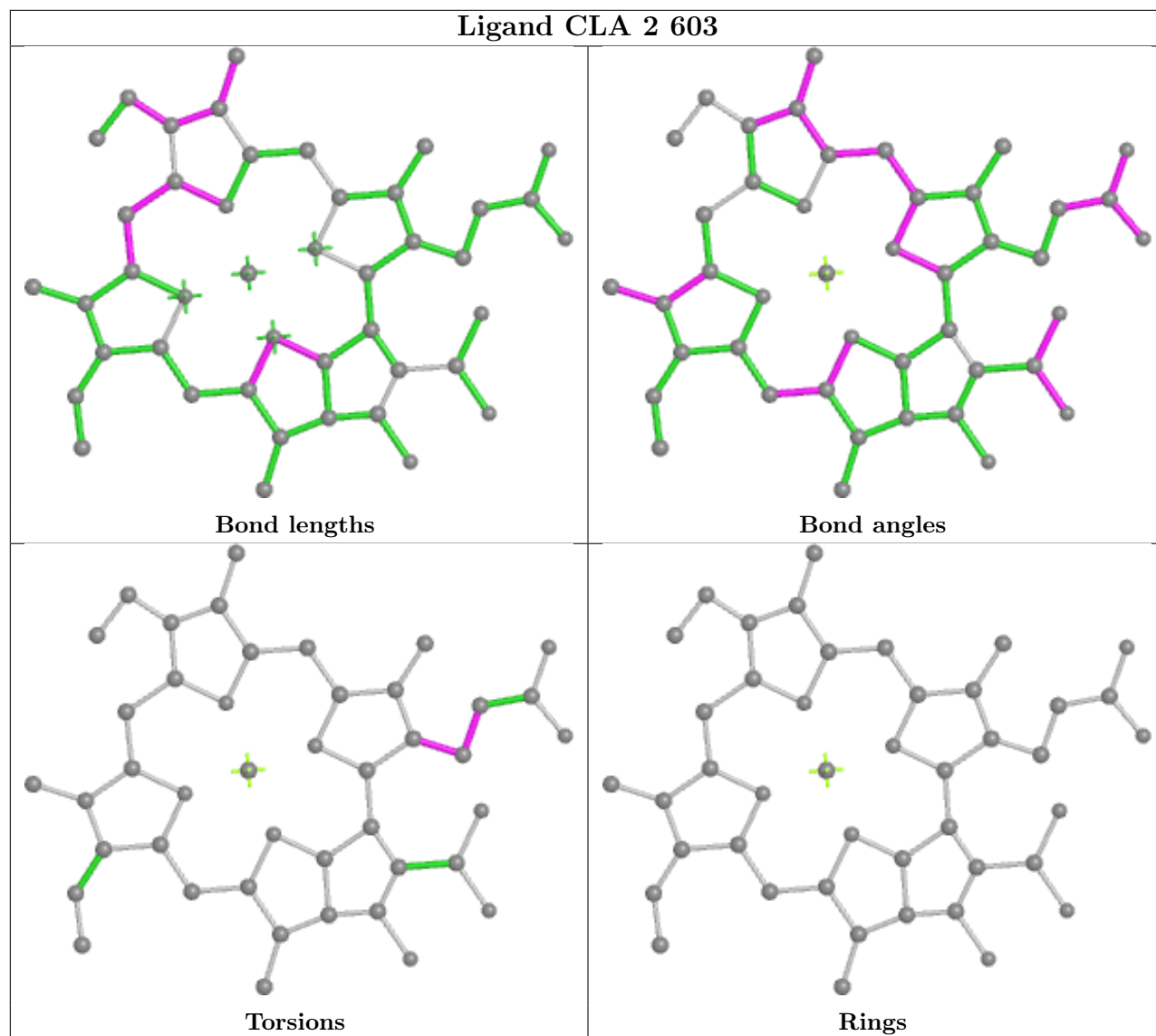


## Ligand CLA 3 312

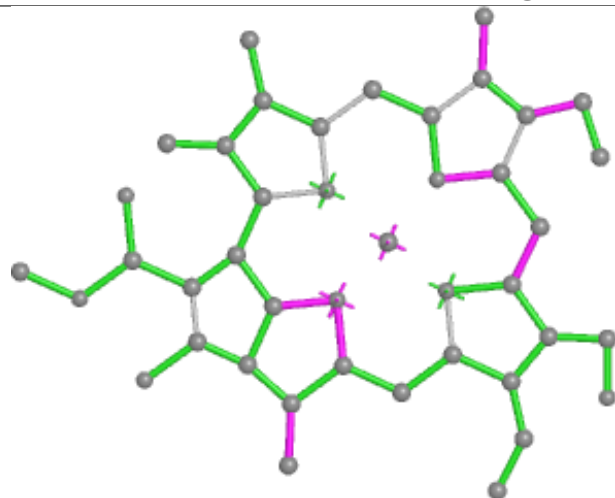


**Ligand CLA B 802****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 5 607****Bond lengths****Bond angles****Torsions****Rings**

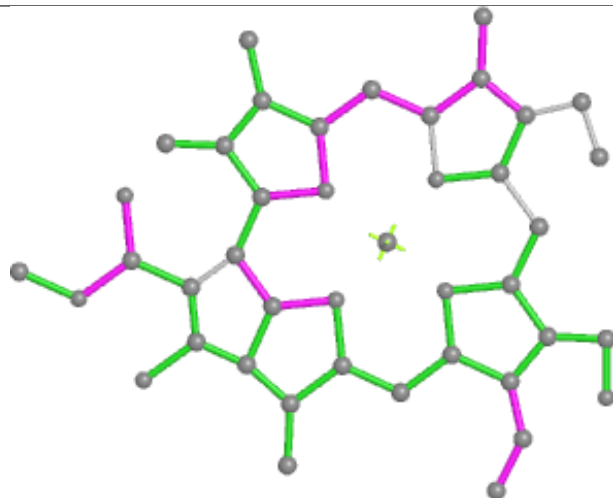
## Ligand CLA 2 603



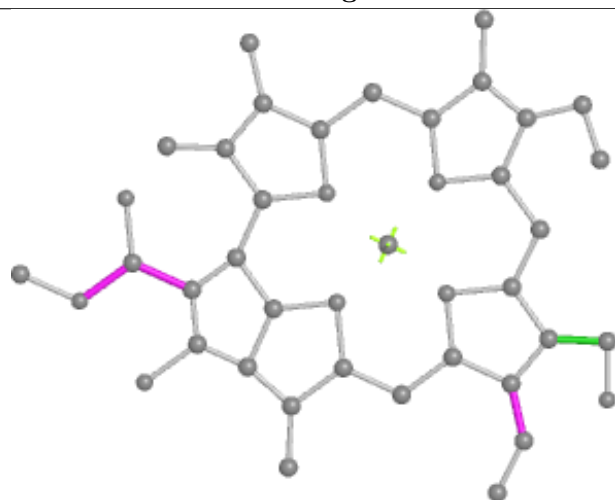
## Ligand CHL S 305



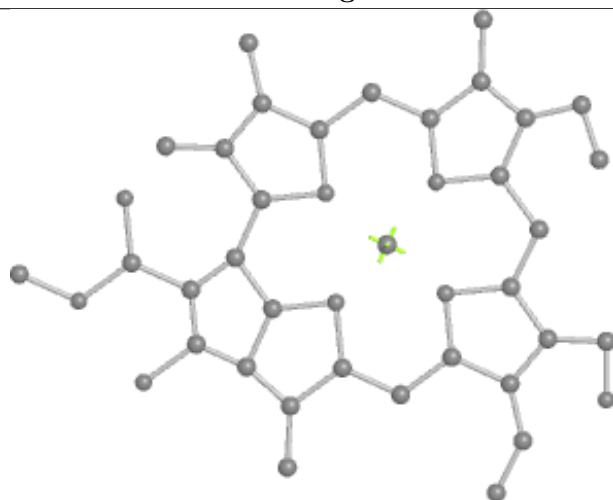
Bond lengths



Bond angles

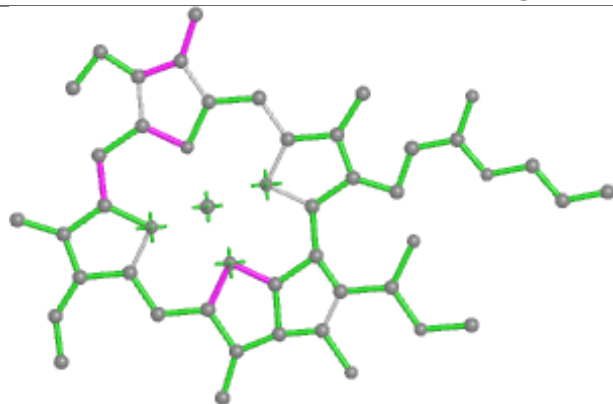


Torsions

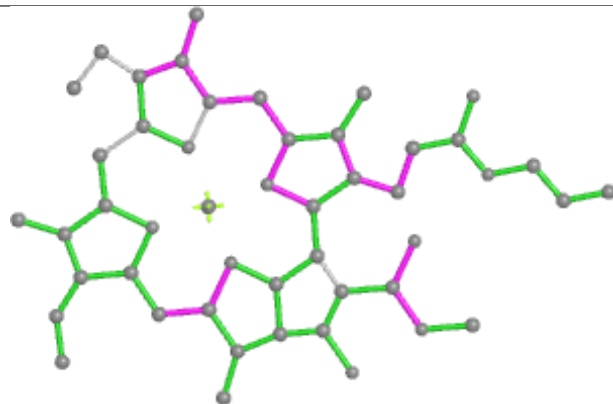


Rings

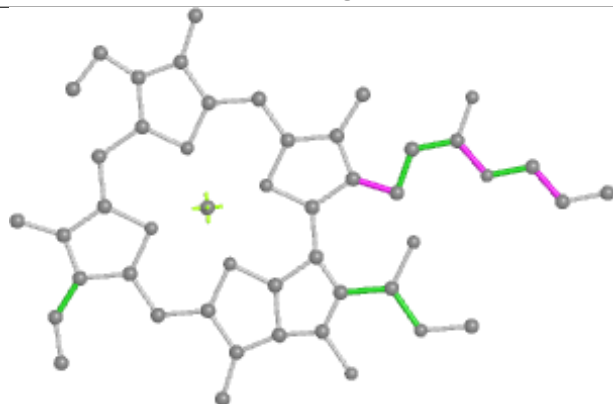
## Ligand CLA P 313



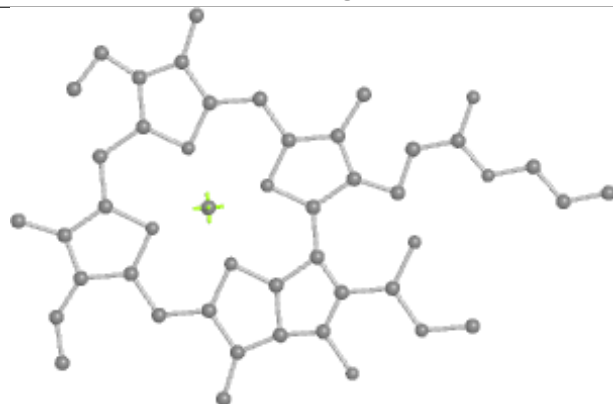
Bond lengths



Bond angles

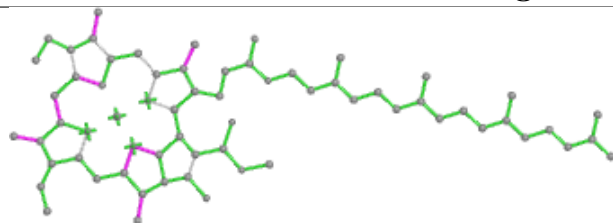


Torsions

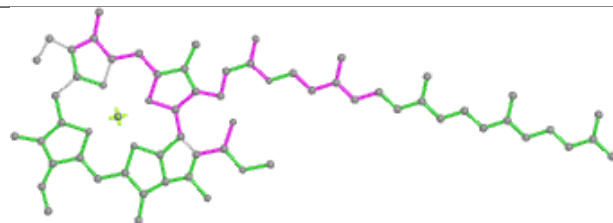


Rings

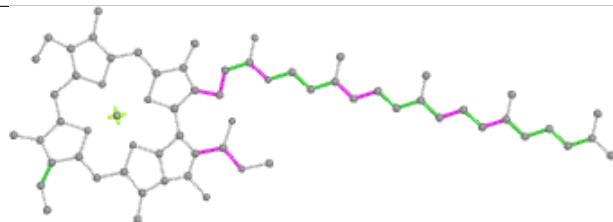
## Ligand CLA T 301



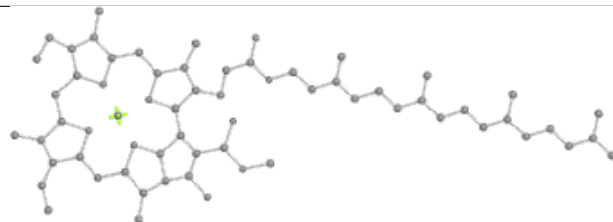
Bond lengths



Bond angles



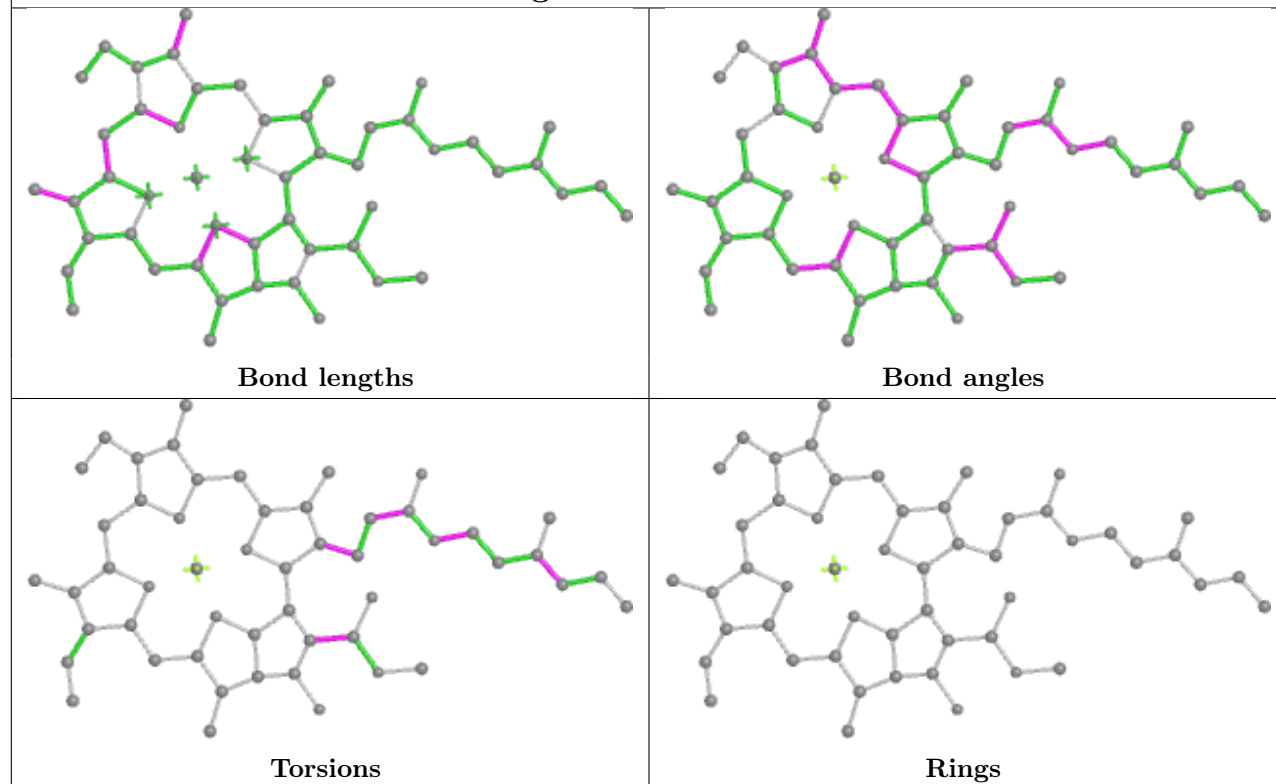
Torsions



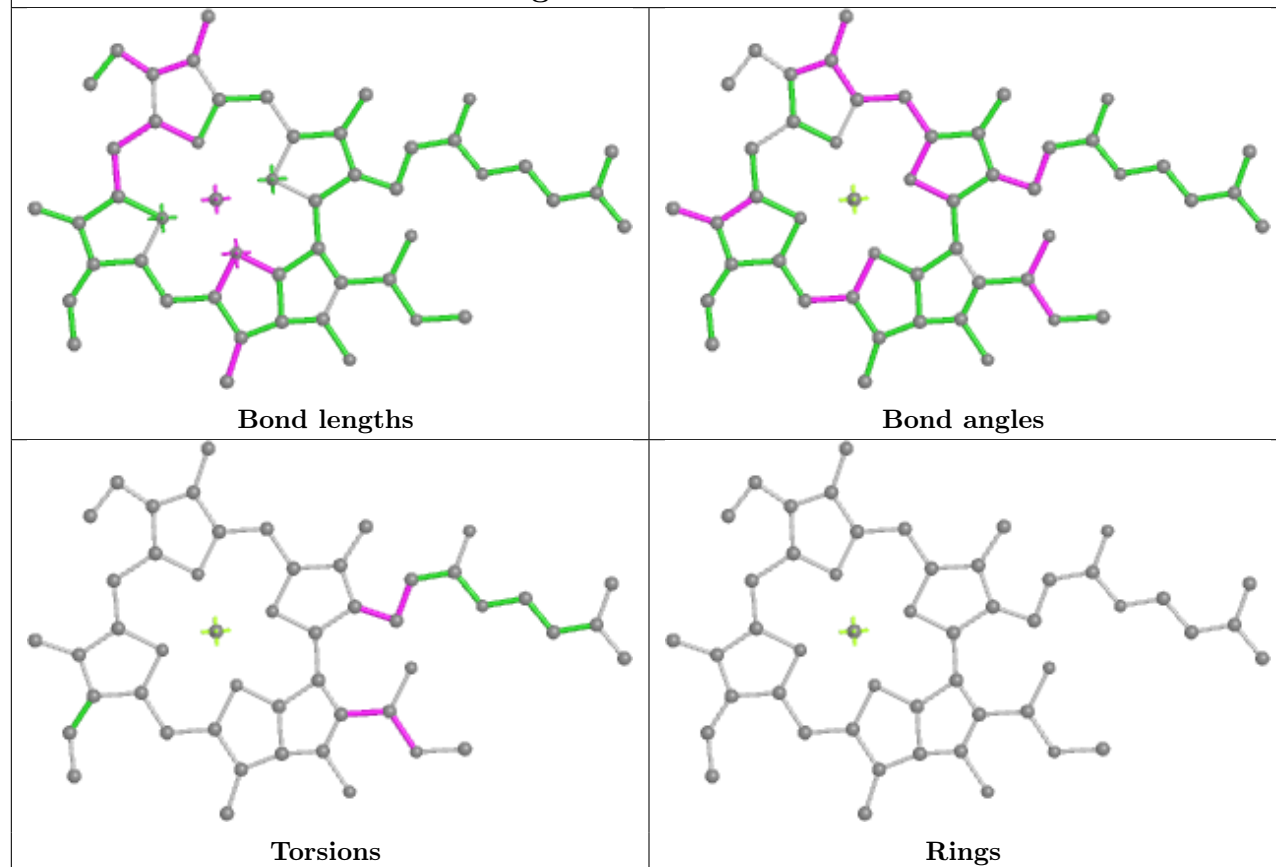
Rings

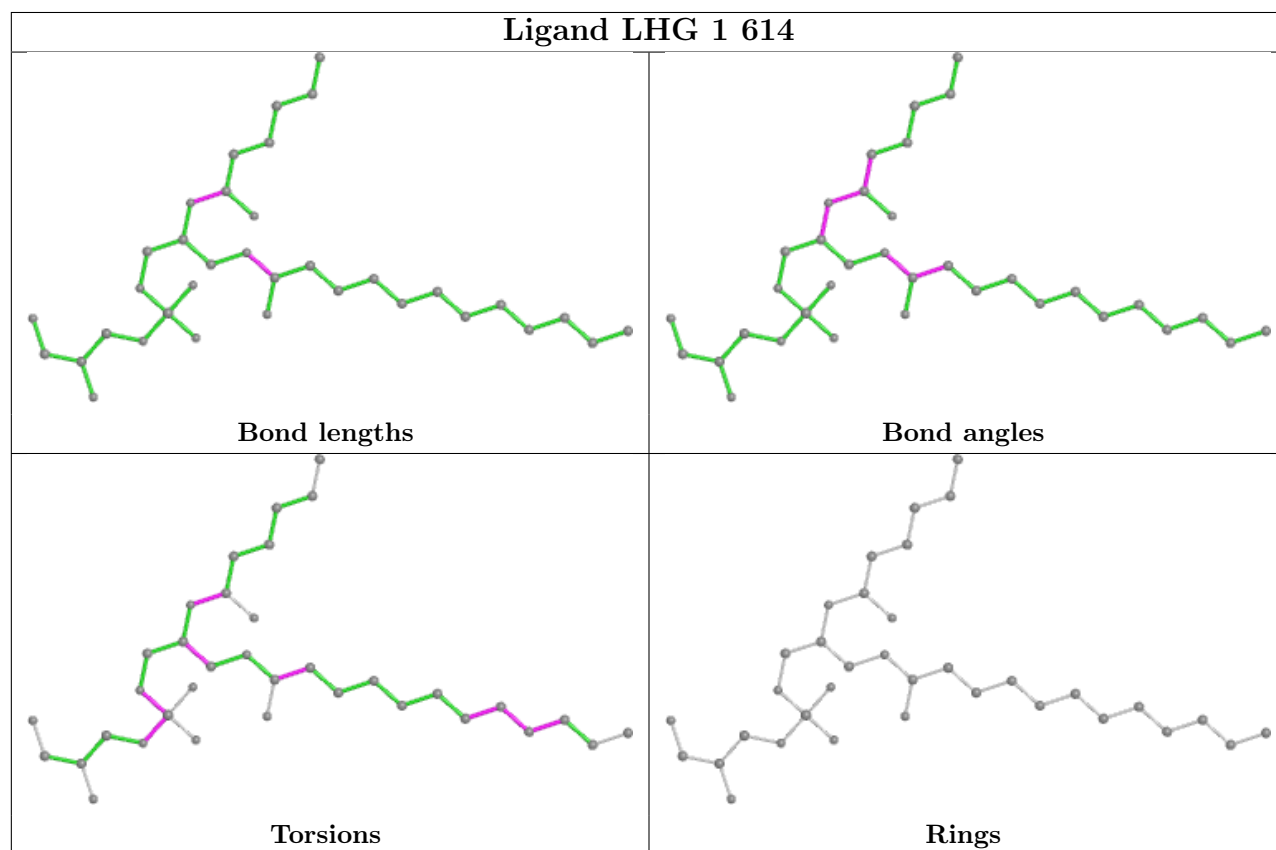
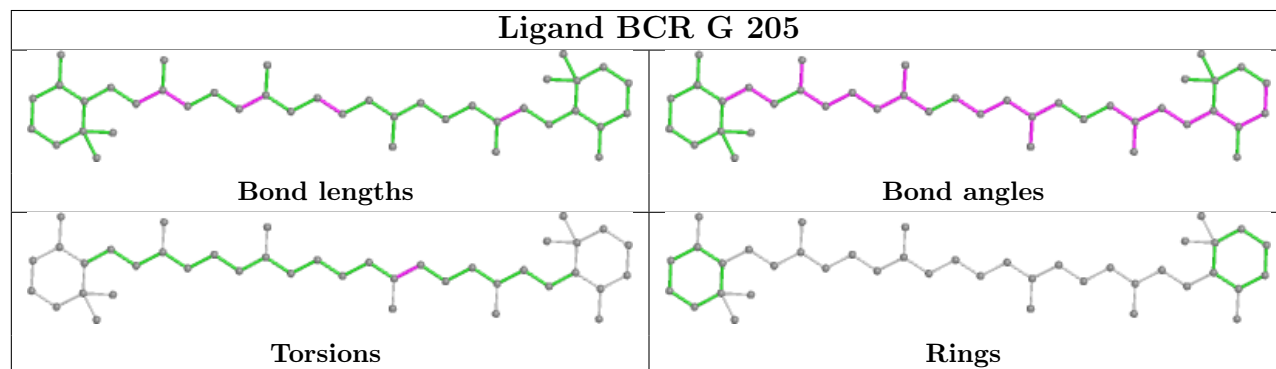
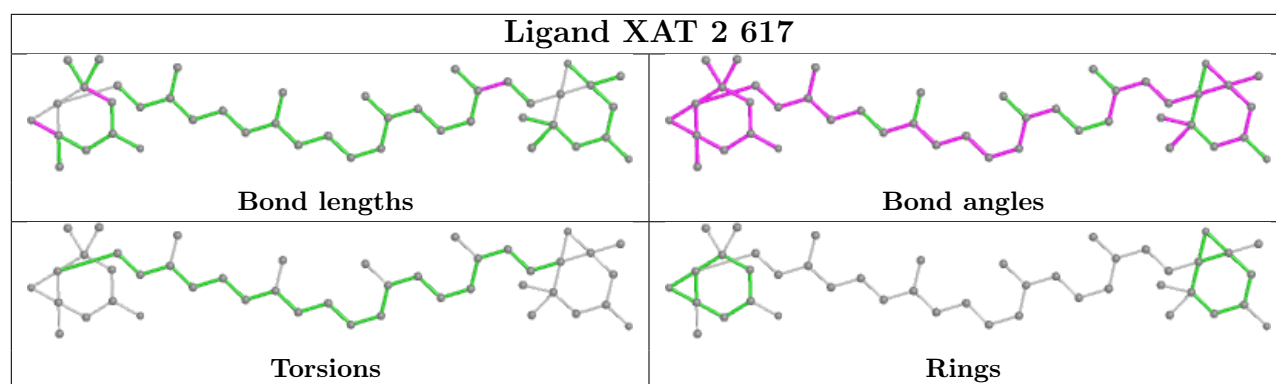


## Ligand CLA A 806

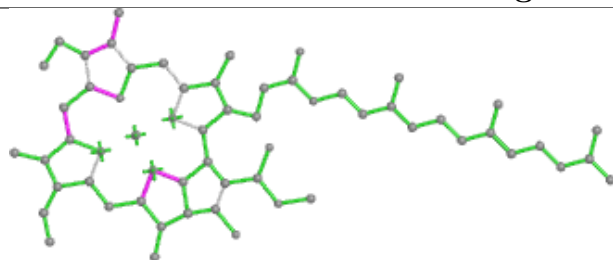


## Ligand CLA A 833

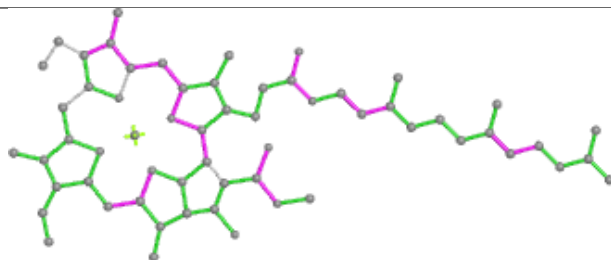




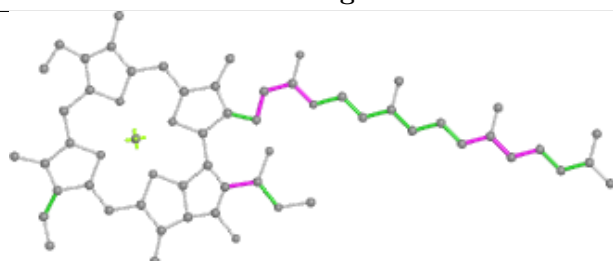
## Ligand CLA P 310



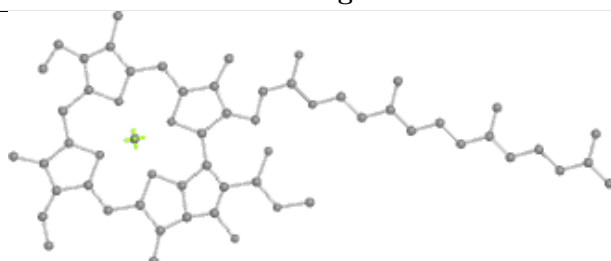
Bond lengths



Bond angles

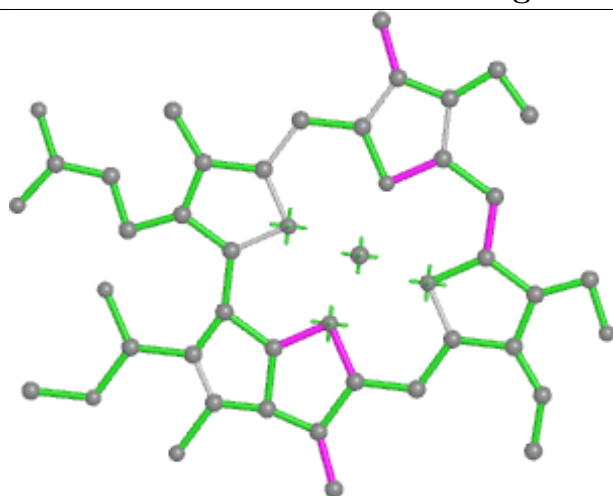


Torsions

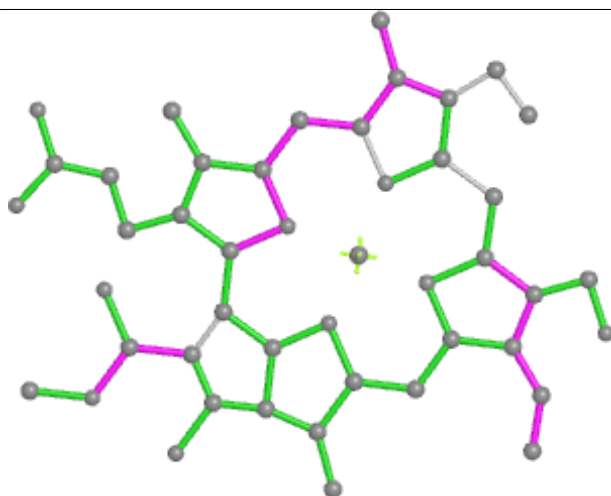


Rings

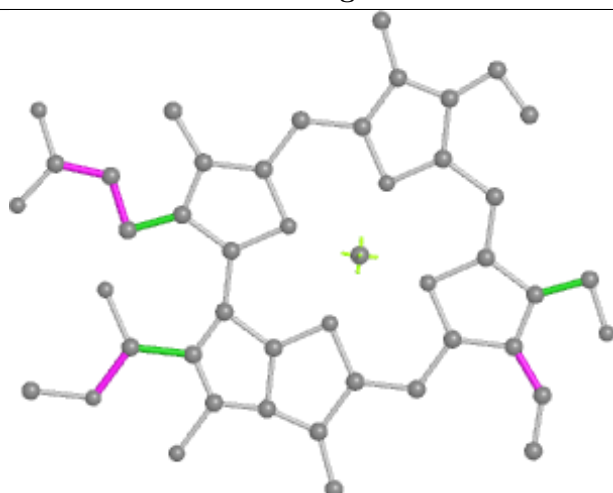
## Ligand CHL U 305



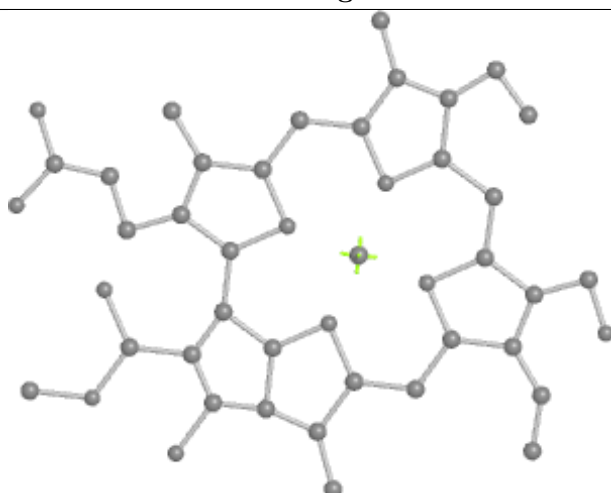
Bond lengths



Bond angles

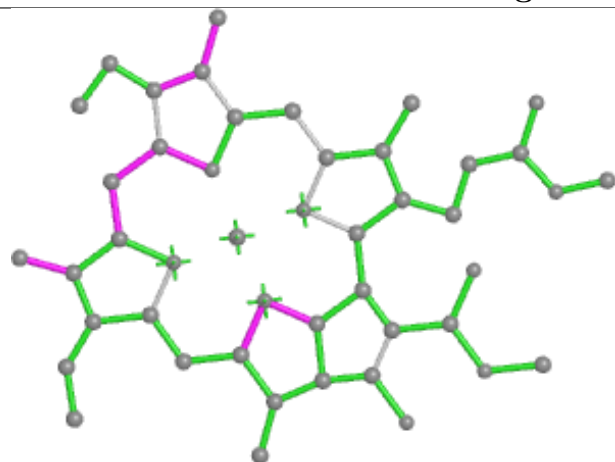


Torsions

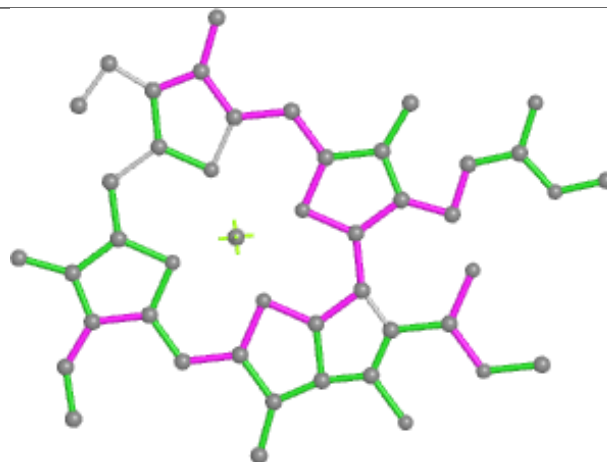


Rings

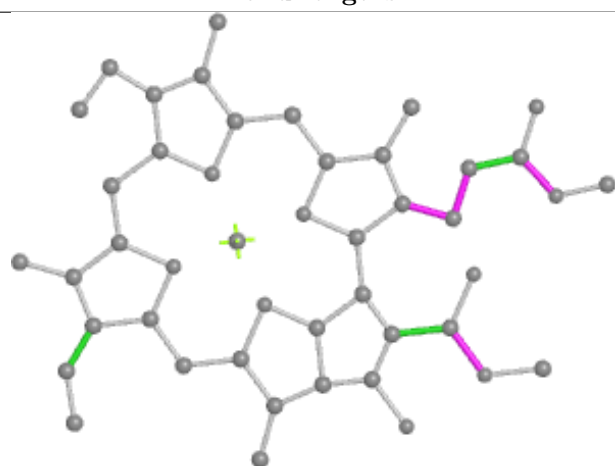
## Ligand CLA K 204



Bond lengths



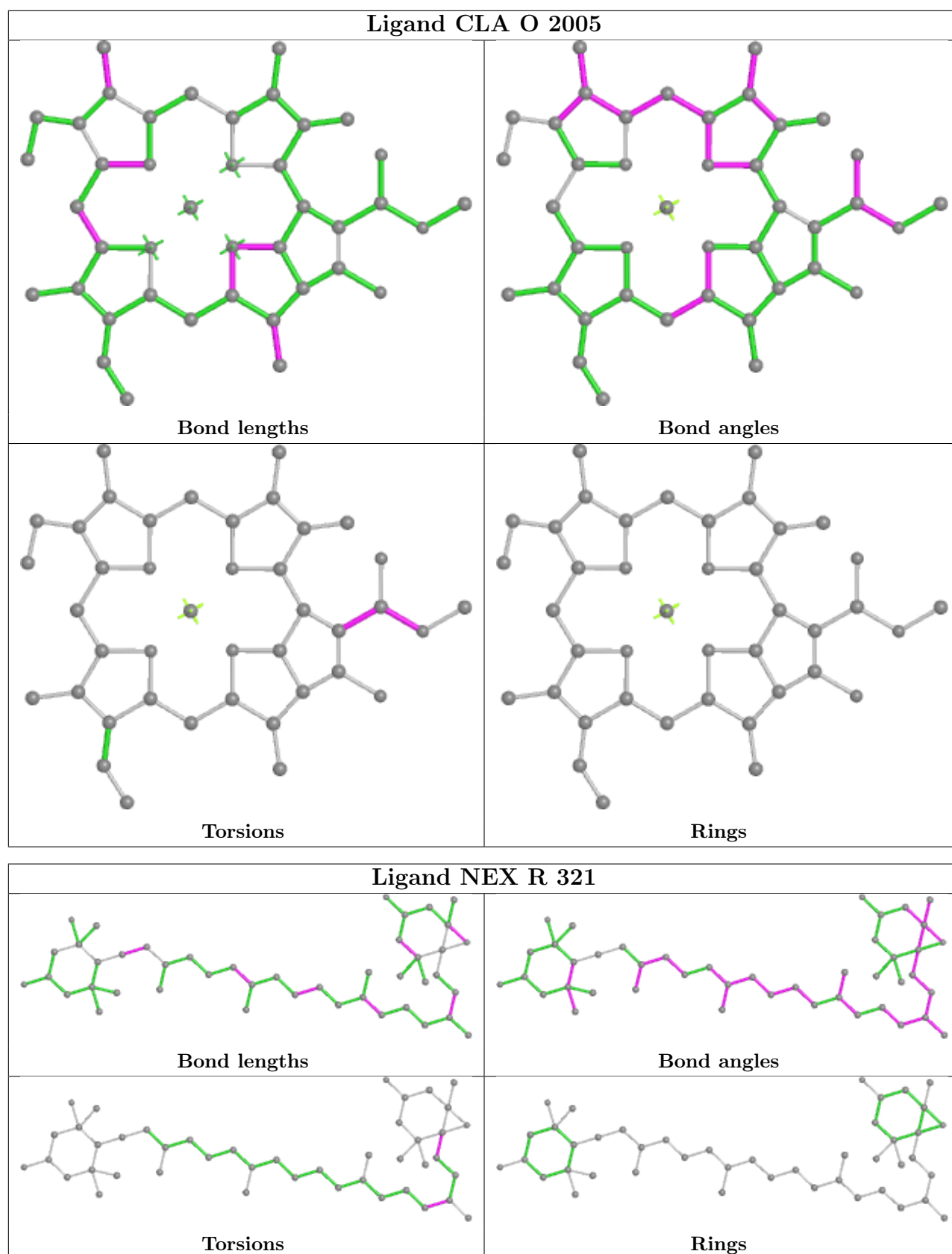
Bond angles

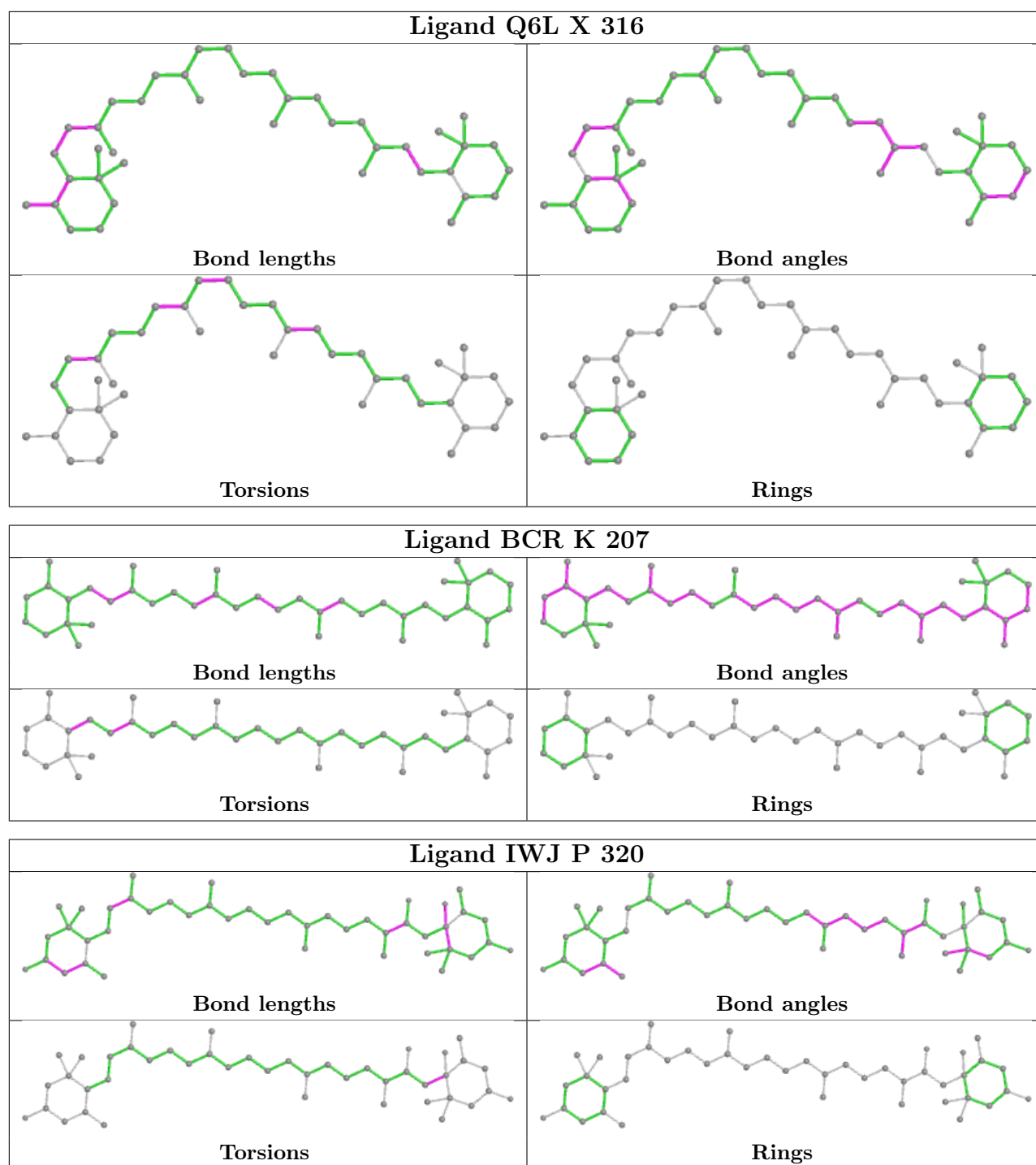


Torsions

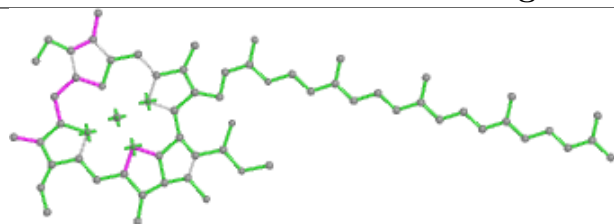


Rings

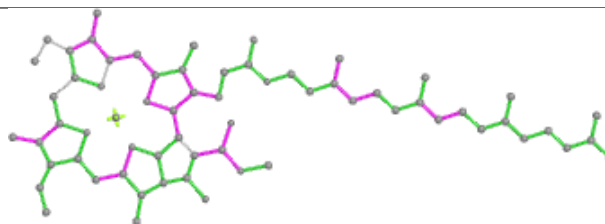




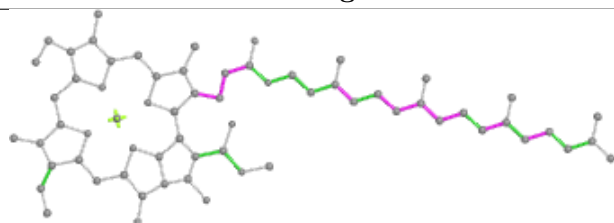
## Ligand CLA 2 612



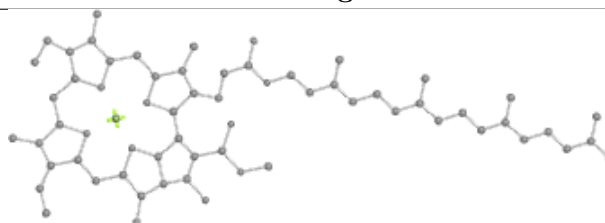
Bond lengths



Bond angles

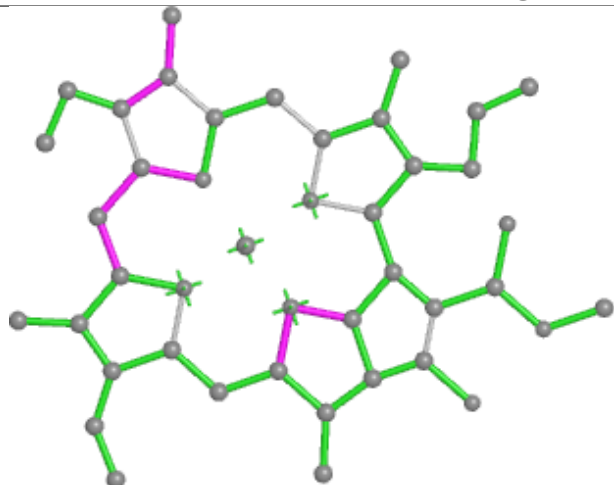


Torsions

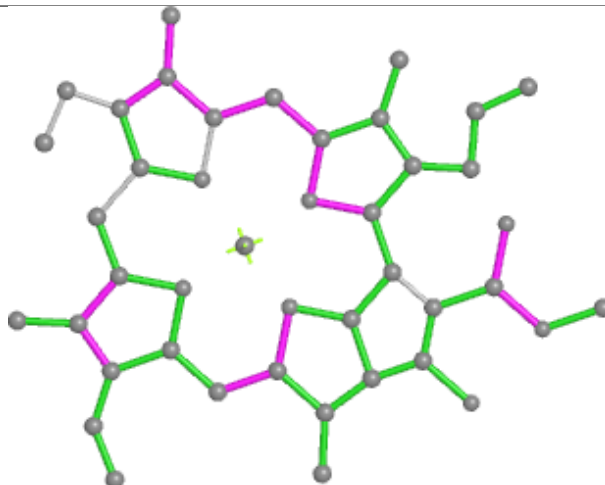


Rings

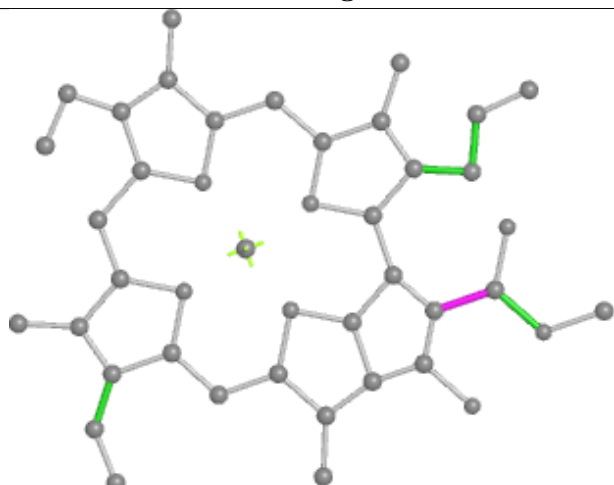
## Ligand CLA B 833



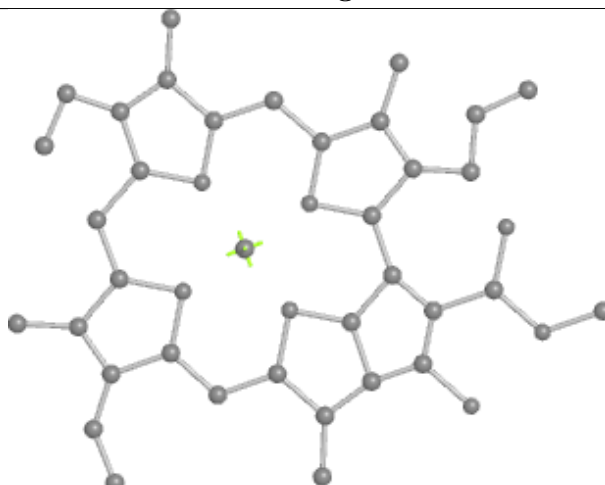
Bond lengths



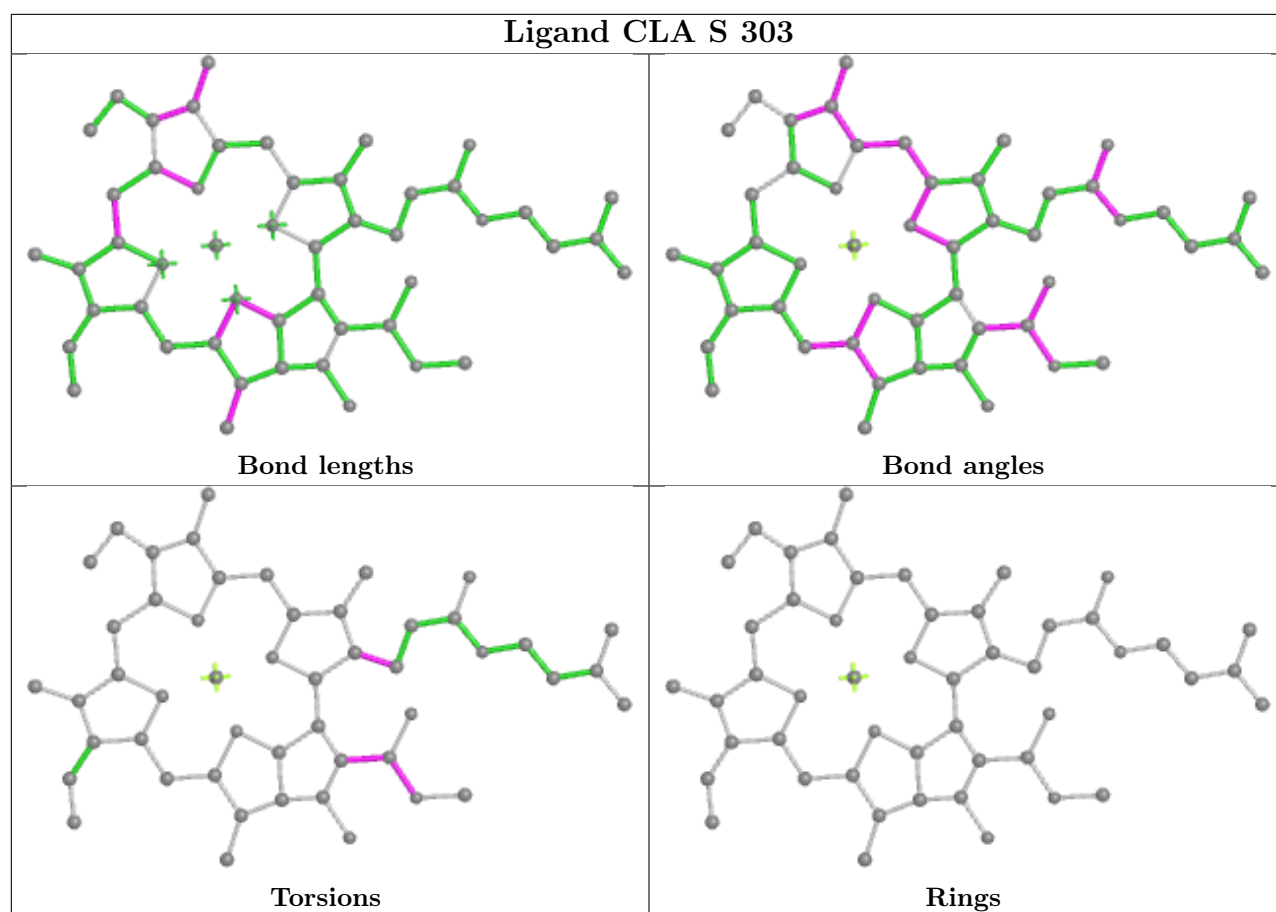
Bond angles



Torsions

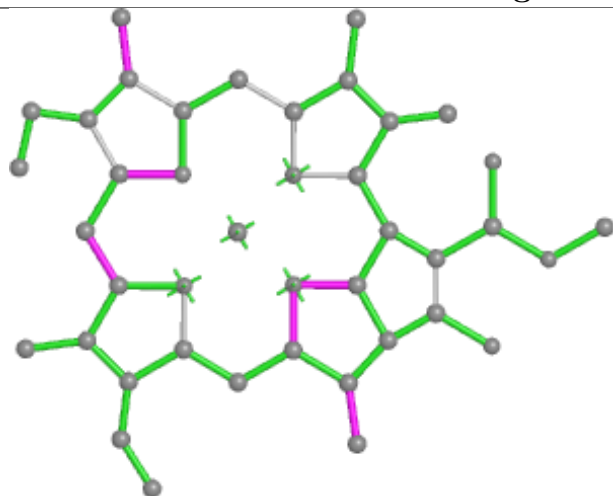


Rings

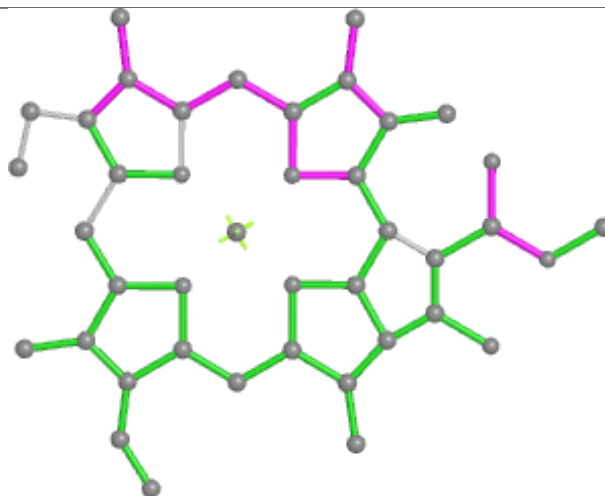




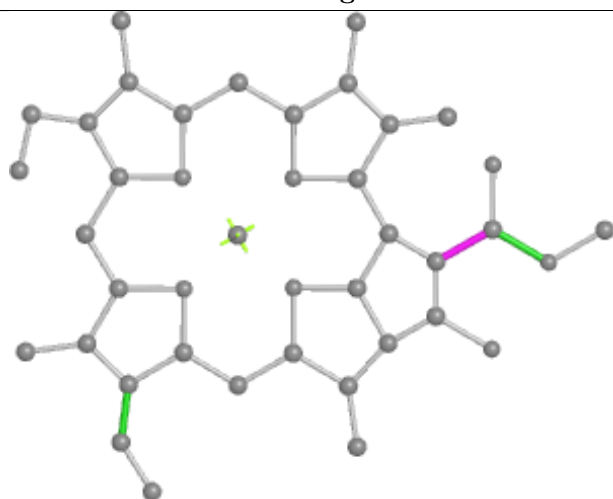
## Ligand CLA U 312



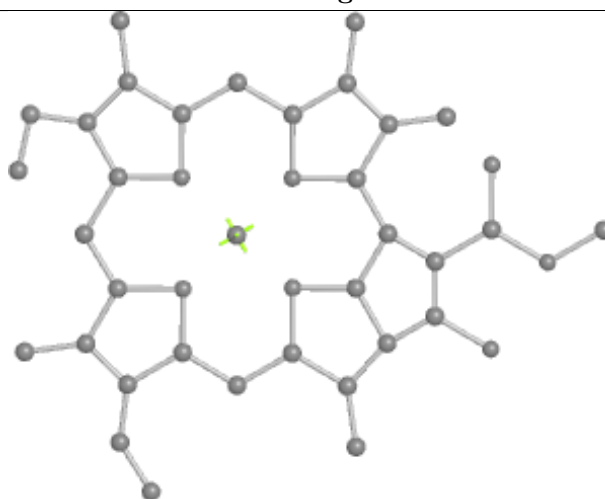
Bond lengths



Bond angles

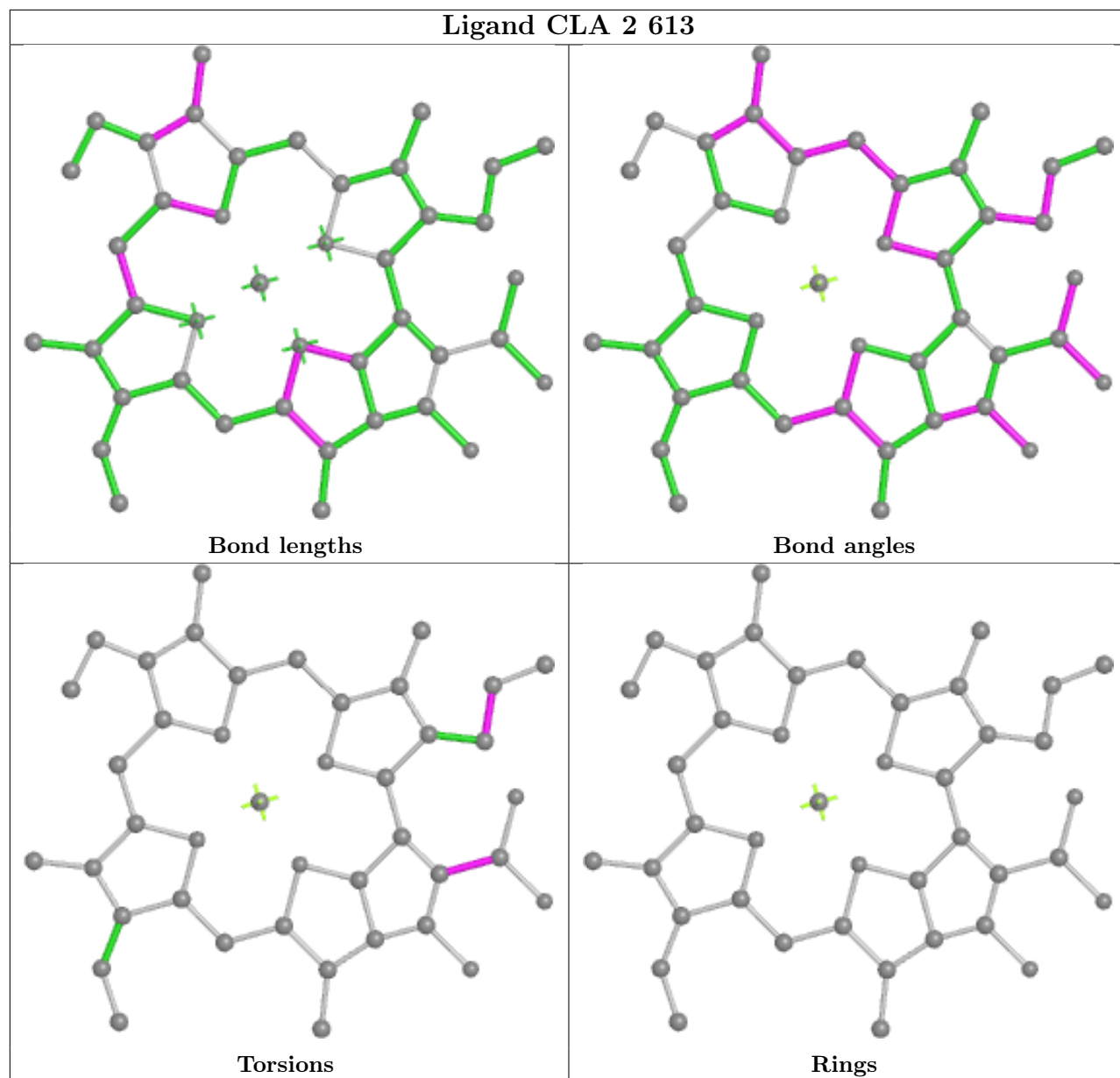


Torsions

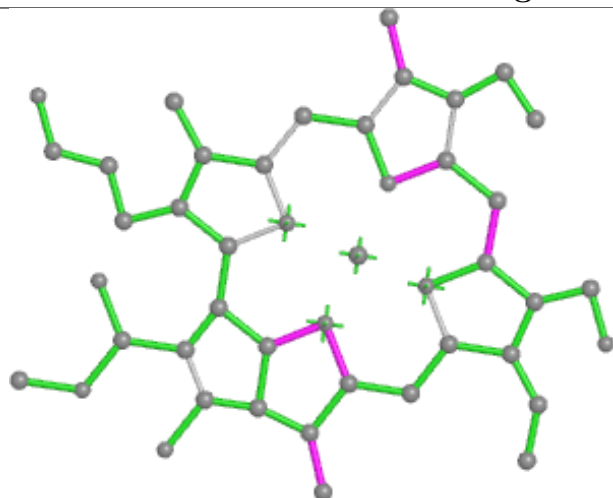


Rings

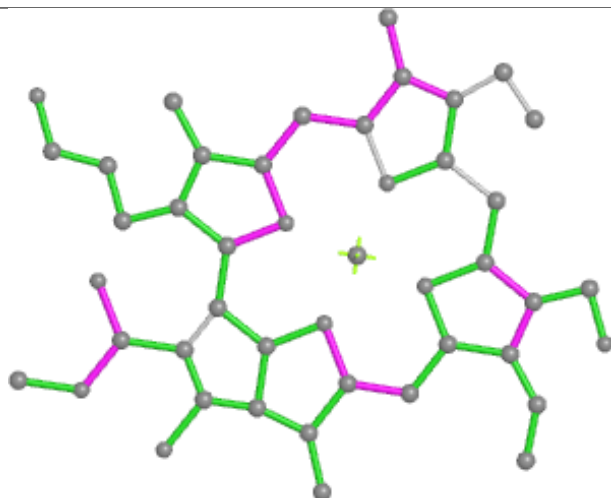
## Ligand CLA 2 613



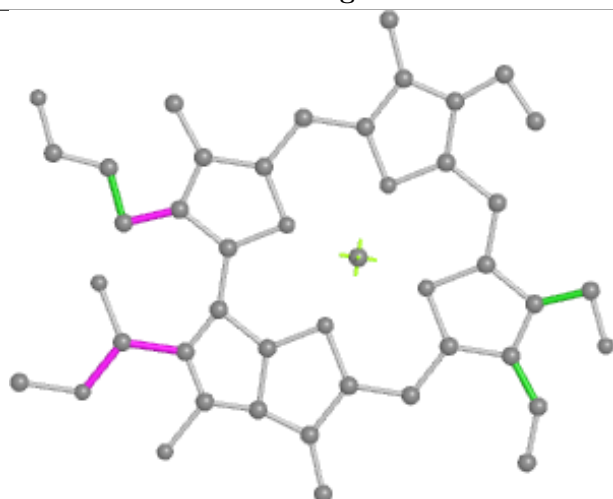
## Ligand CHL P 314



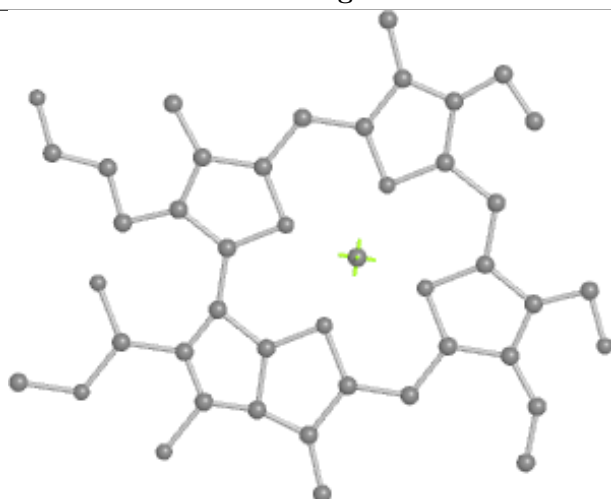
Bond lengths



Bond angles

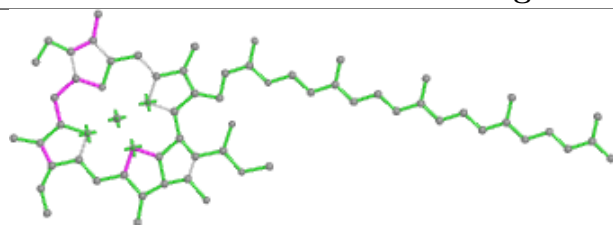


Torsions

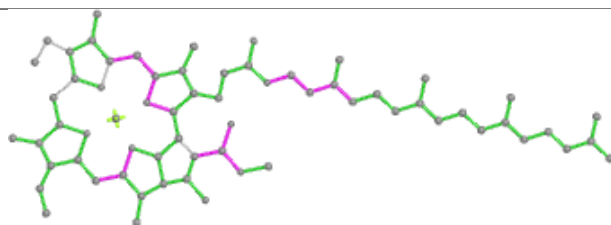


Rings

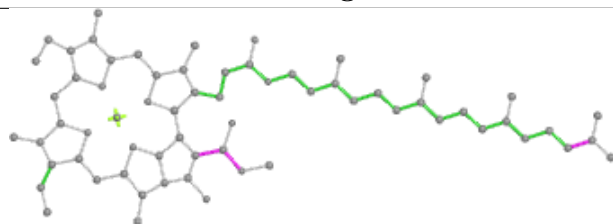
## Ligand CLA A 836



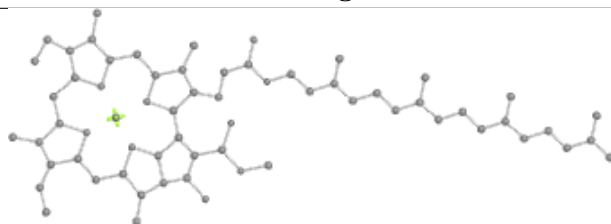
Bond lengths



Bond angles

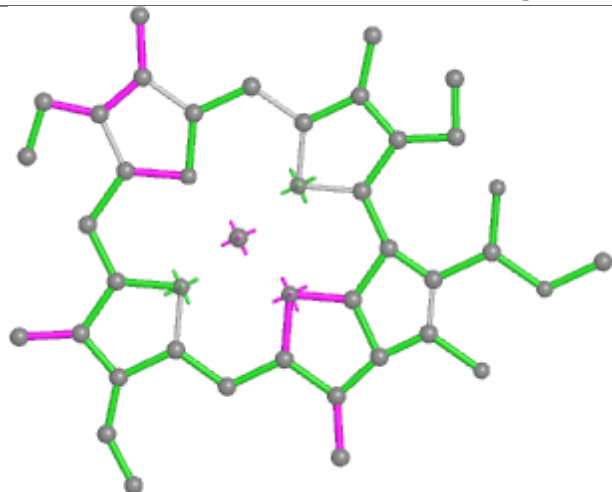


Torsions

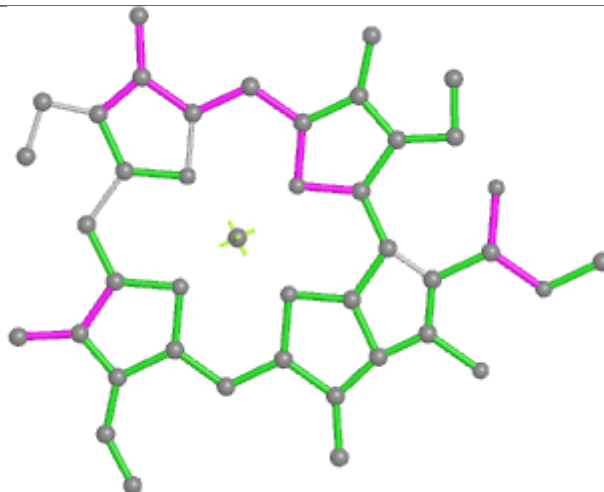


Rings

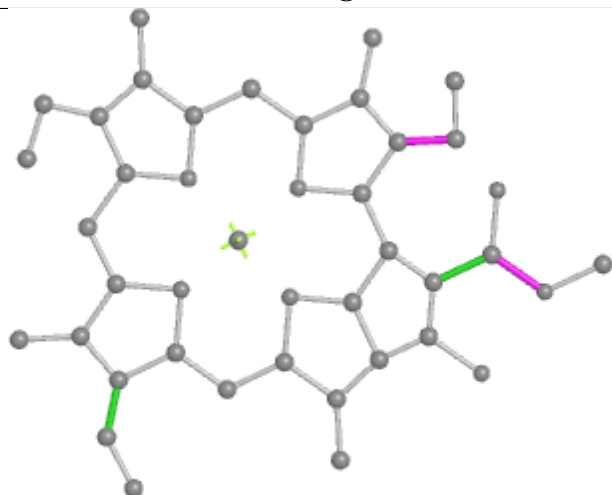
## Ligand CLA J 102



Bond lengths



Bond angles

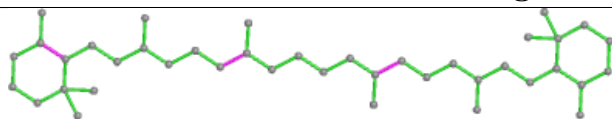


Torsions

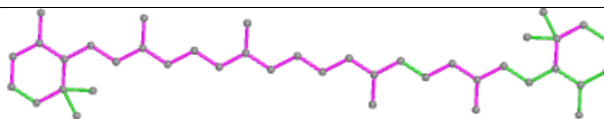


Rings

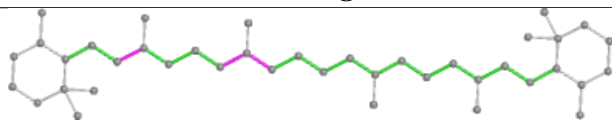
## Ligand BCR F 804



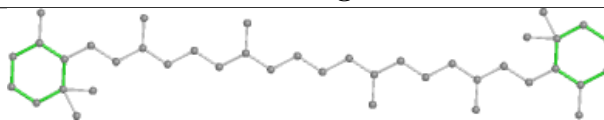
Bond lengths



Bond angles

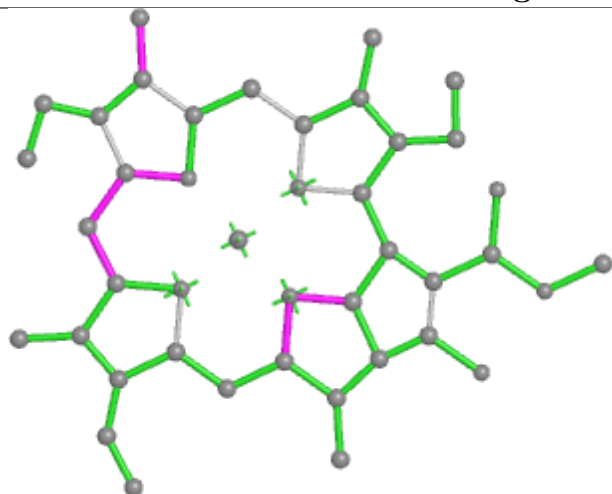


Torsions

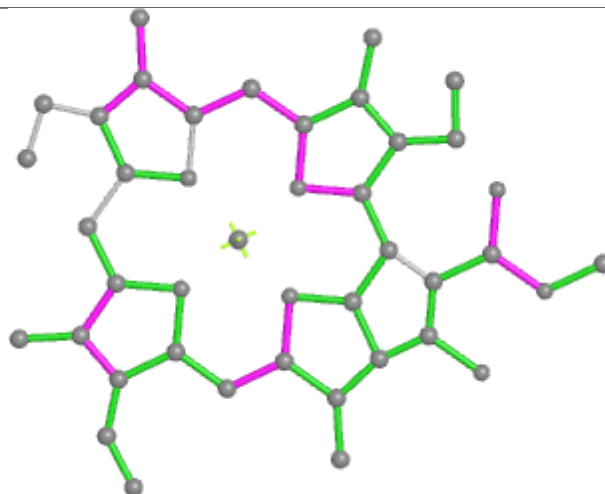


Rings

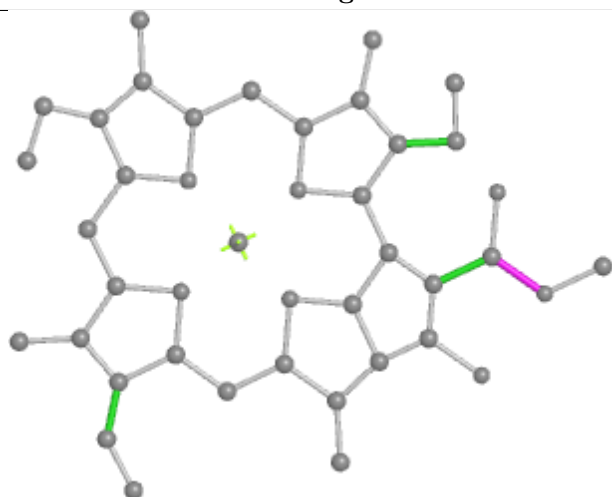
## Ligand CLA B 837



Bond lengths



Bond angles

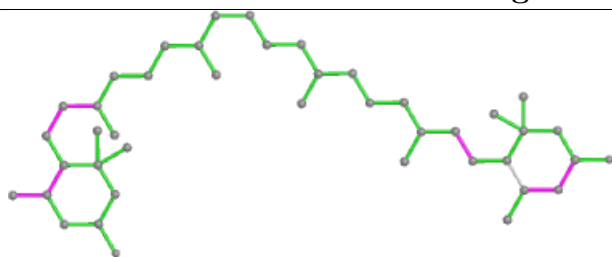


Torsions

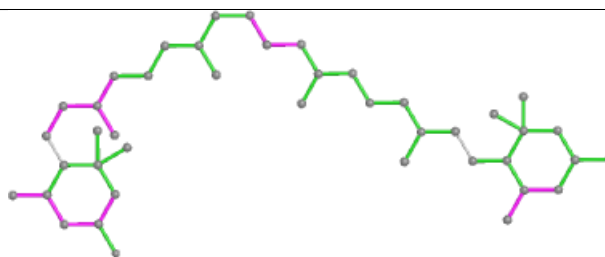


Rings

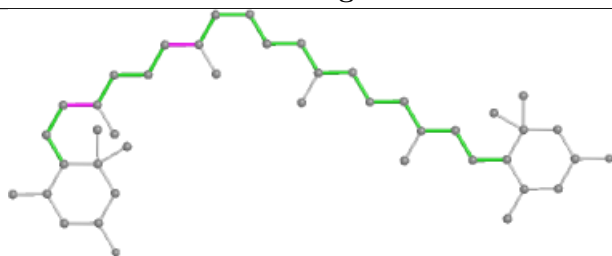
## Ligand Q6L W 315



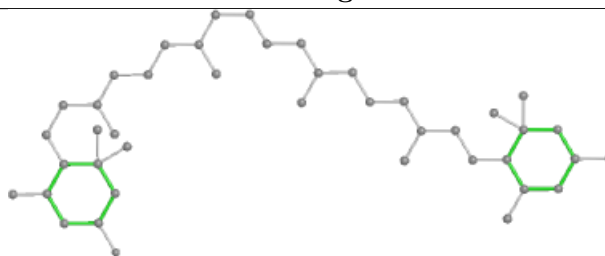
Bond lengths



Bond angles

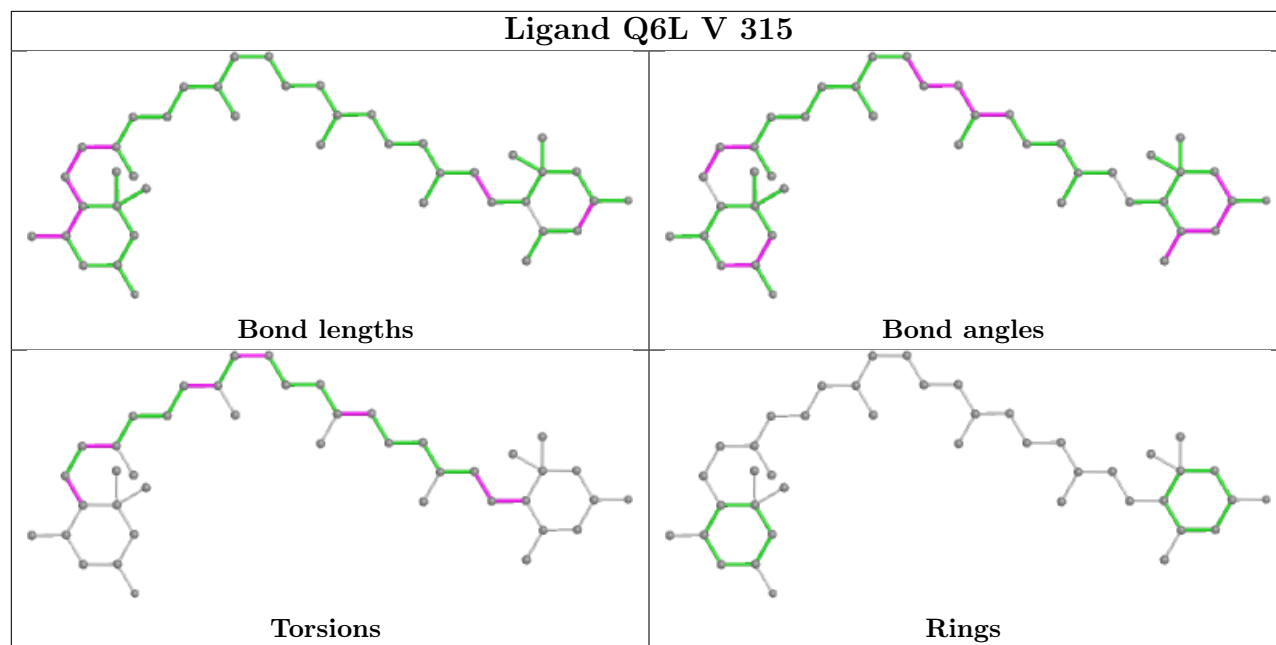


Torsions

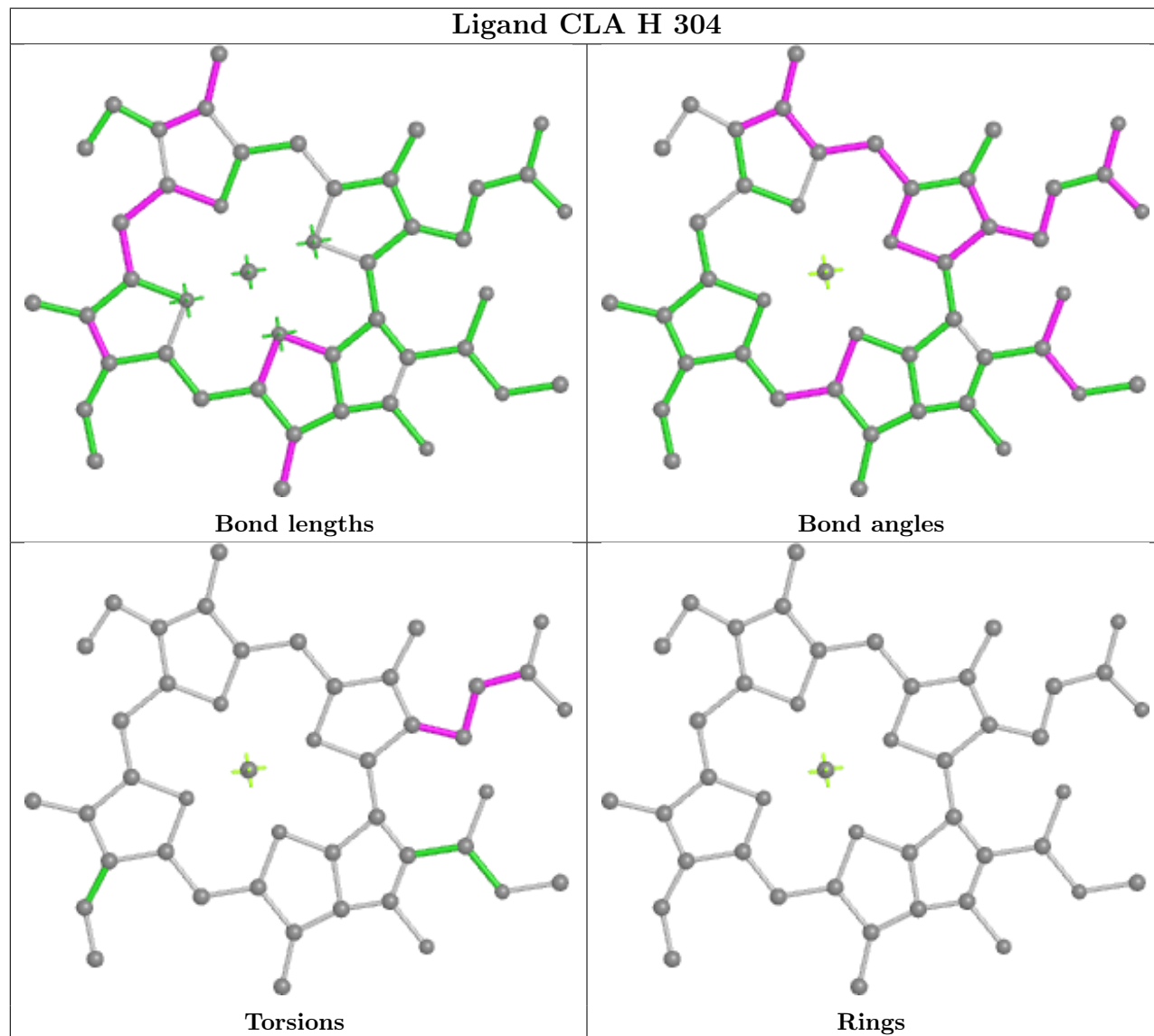


Rings

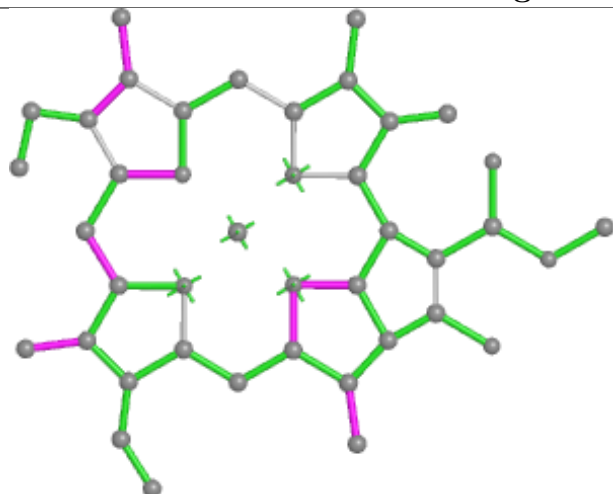
## Ligand Q6L V 315



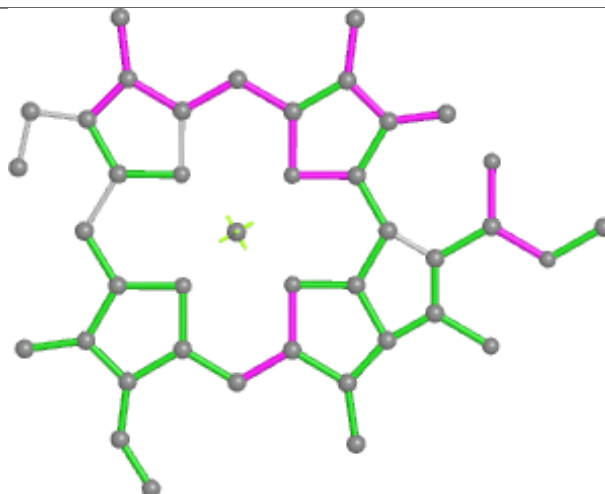
## Ligand CLA H 304



## Ligand CLA X 313



Bond lengths



Bond angles

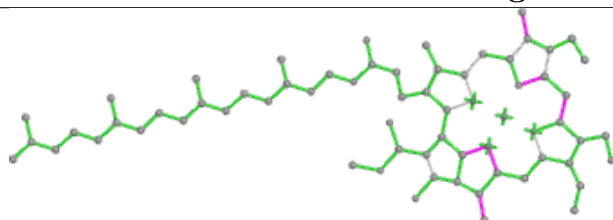


Torsions

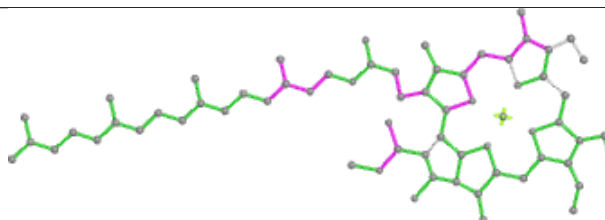


Rings

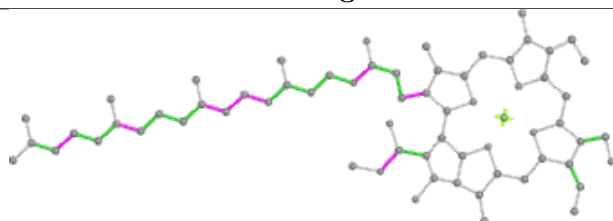
## Ligand CHL W 307



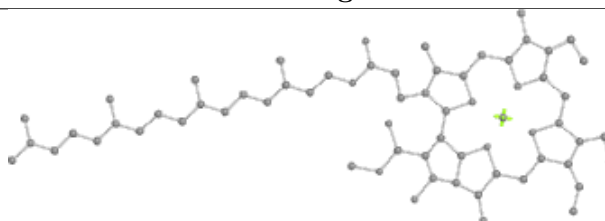
Bond lengths



Bond angles

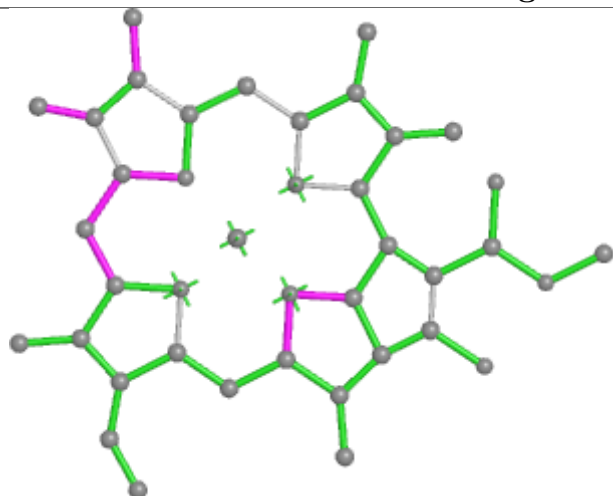


Torsions

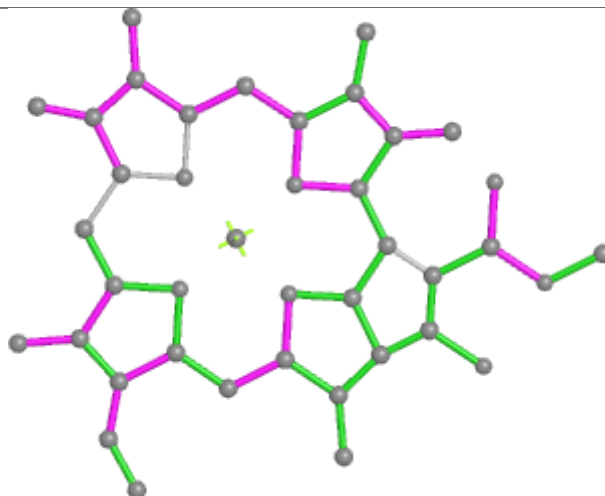


Rings

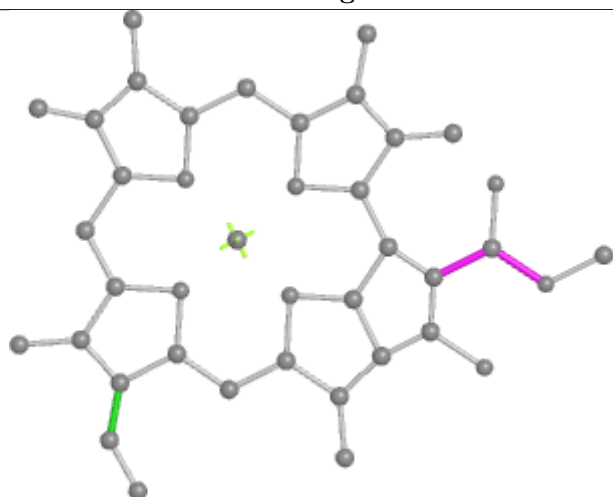
## Ligand CLA 1 606



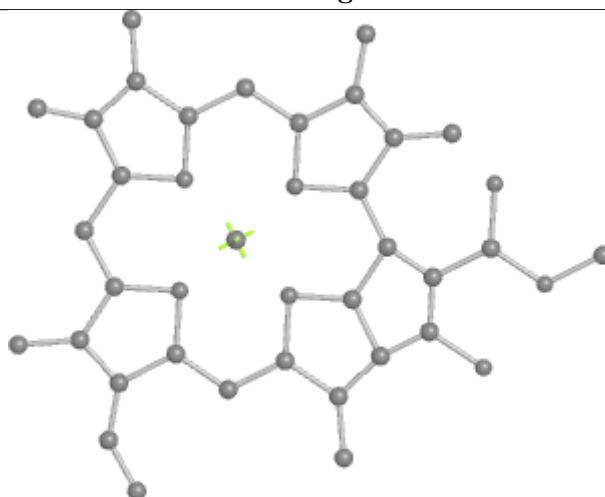
Bond lengths



Bond angles

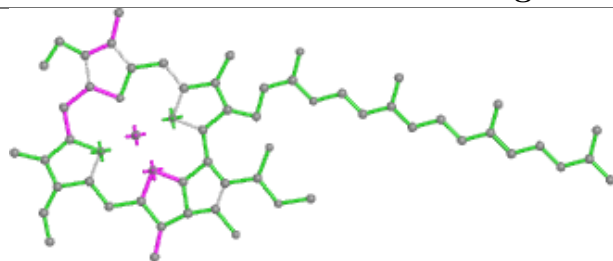


Torsions

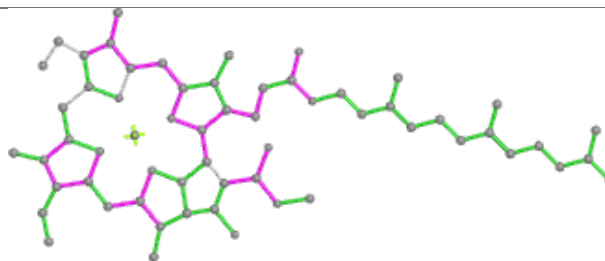


Rings

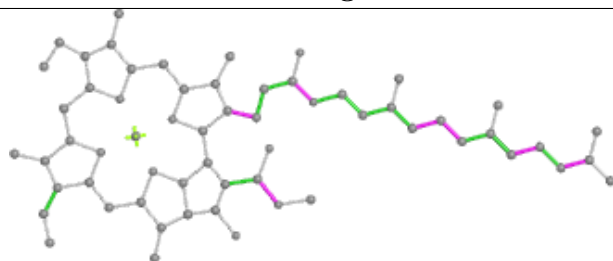
## Ligand CLA B 820



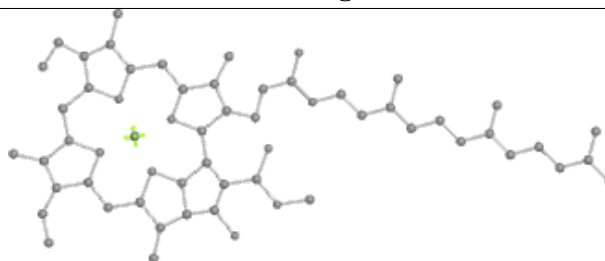
Bond lengths



Bond angles



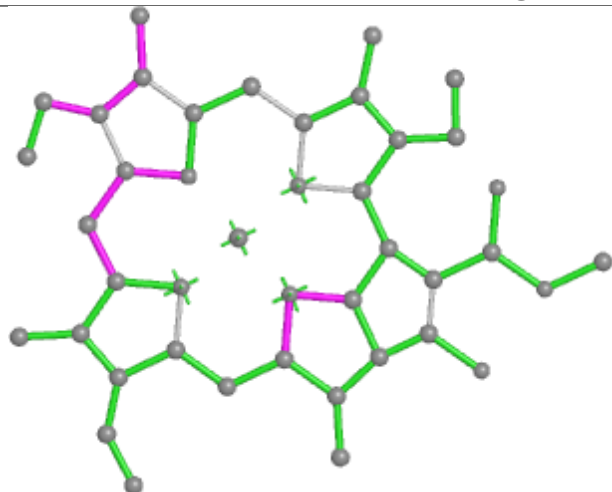
Torsions



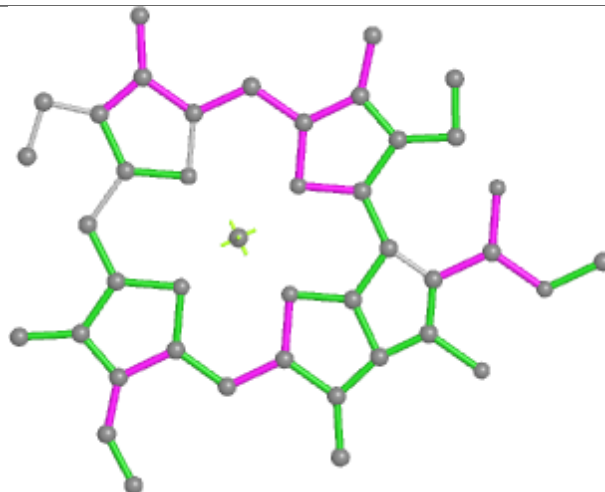
Rings



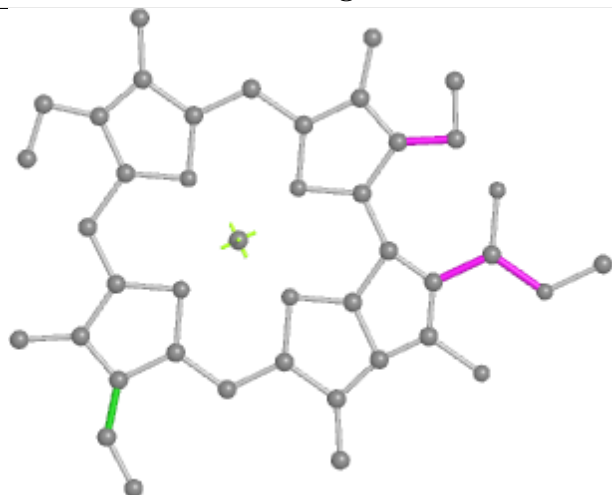
## Ligand CLA X 304



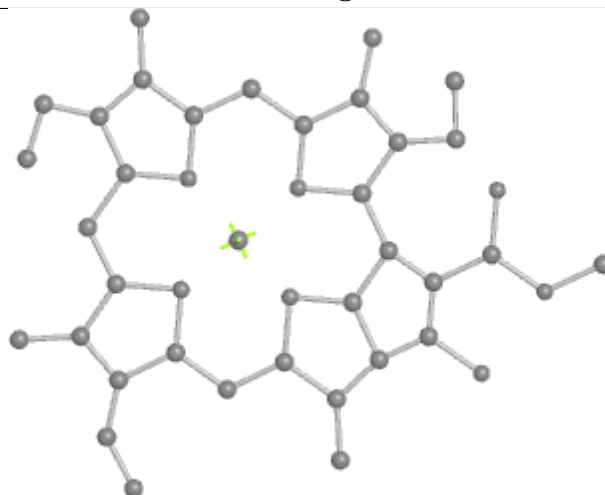
Bond lengths



Bond angles

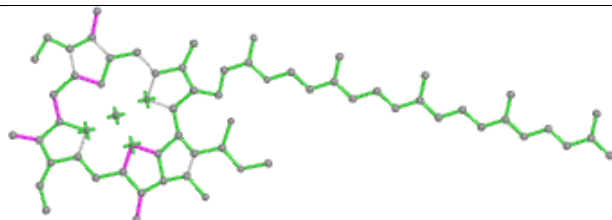


Torsions

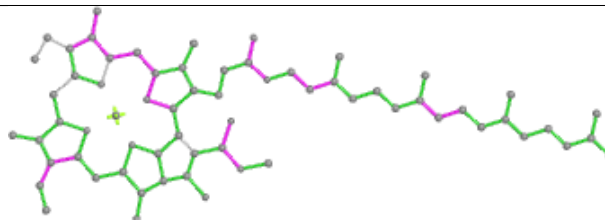


Rings

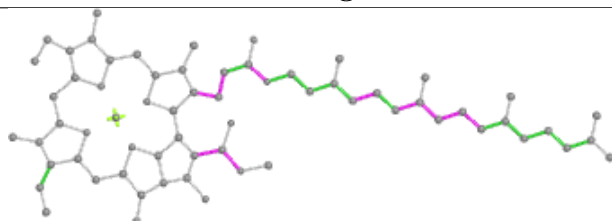
## Ligand CLA B 804



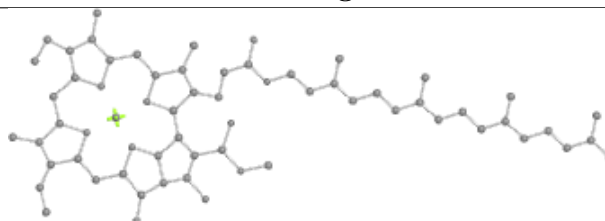
Bond lengths



Bond angles

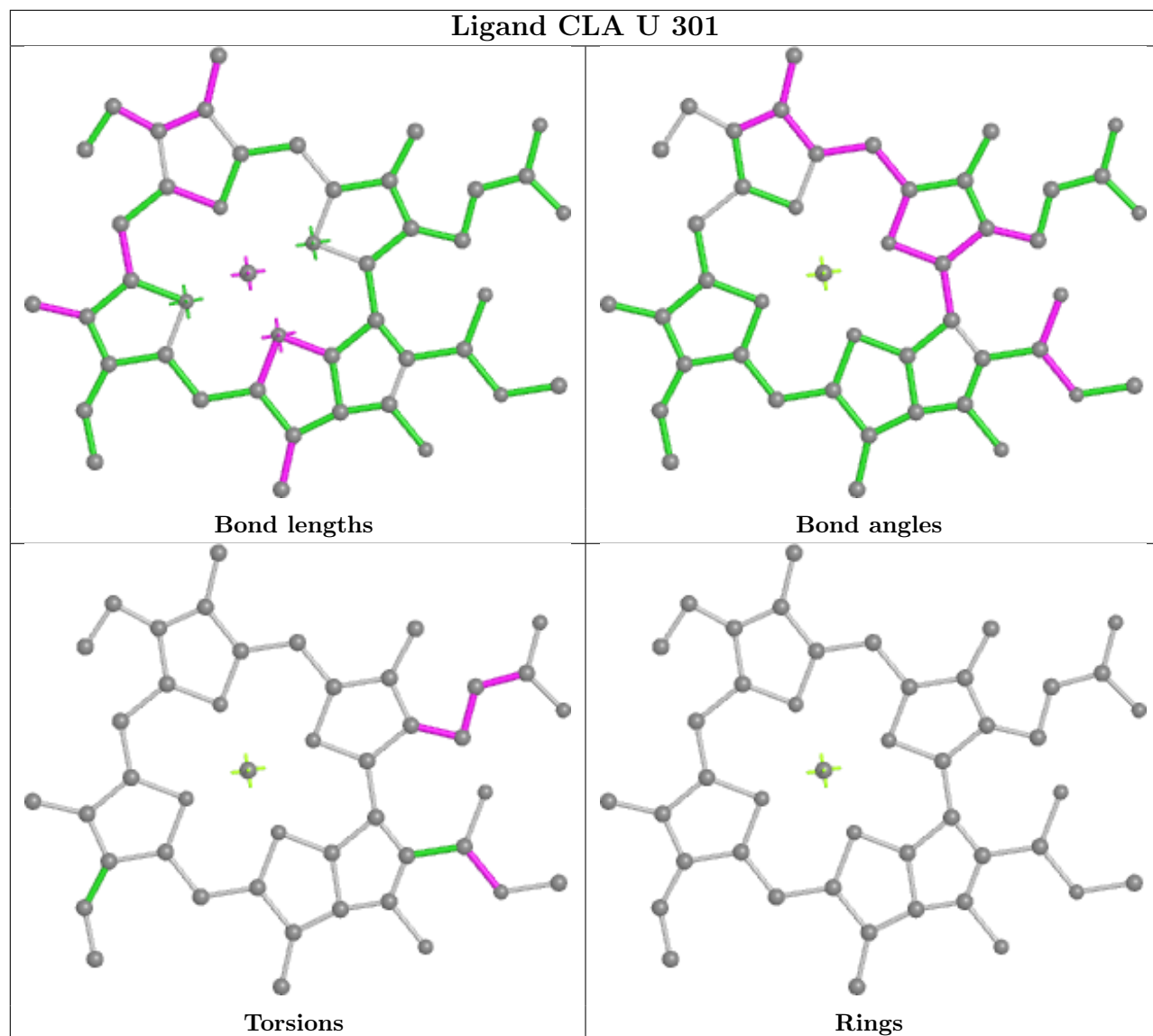


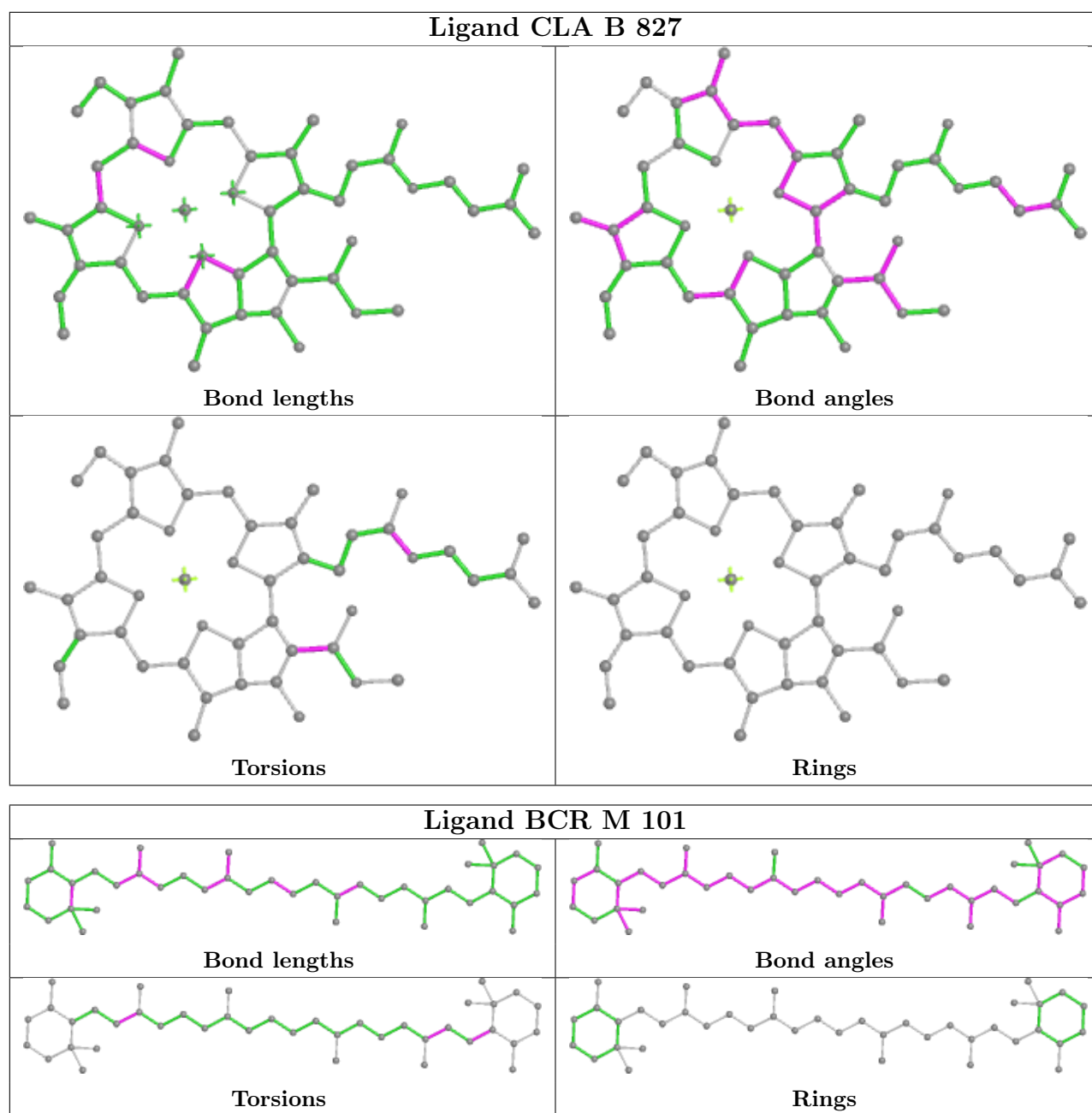
Torsions



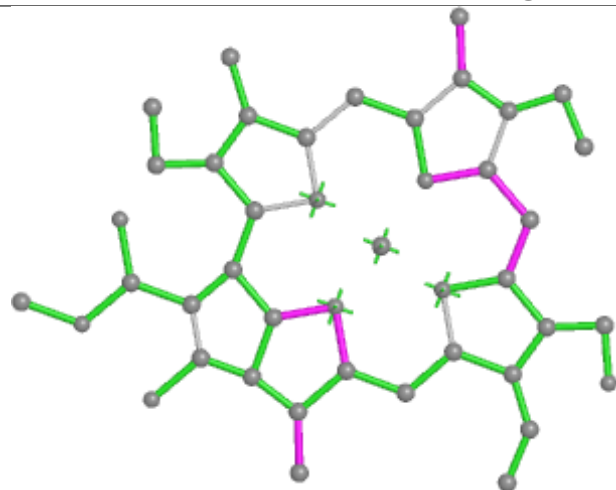
Rings

## Ligand CLA U 301

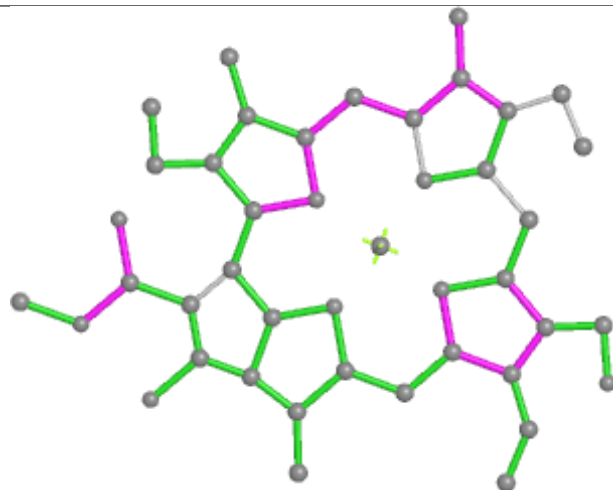




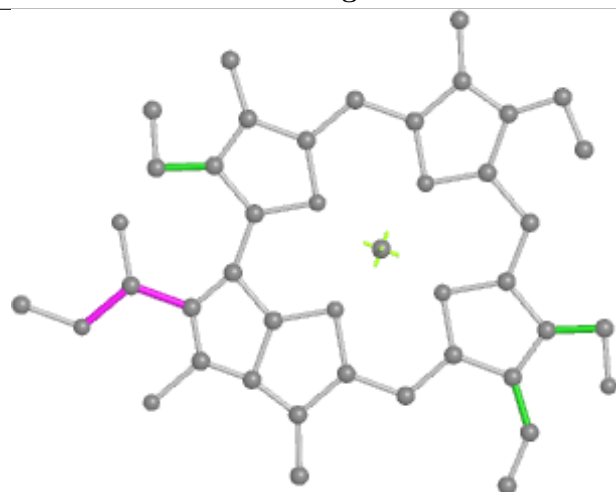
## Ligand CHL 2 615



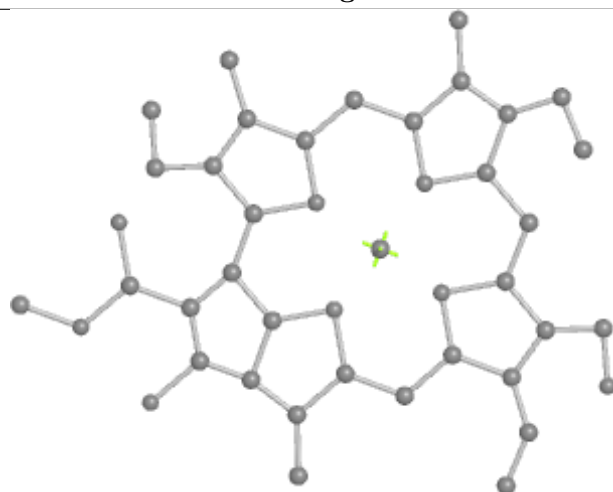
Bond lengths



Bond angles

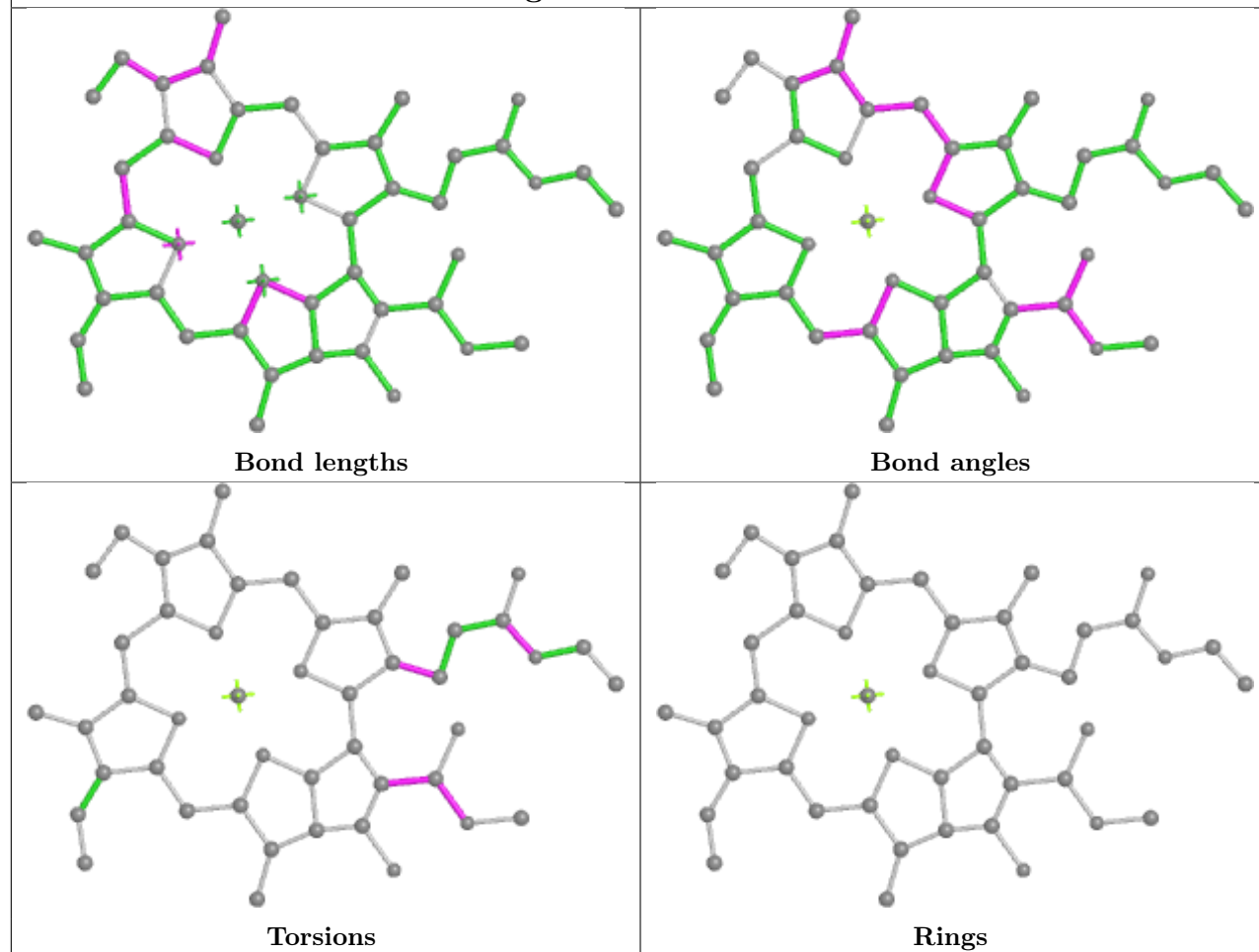


Torsions

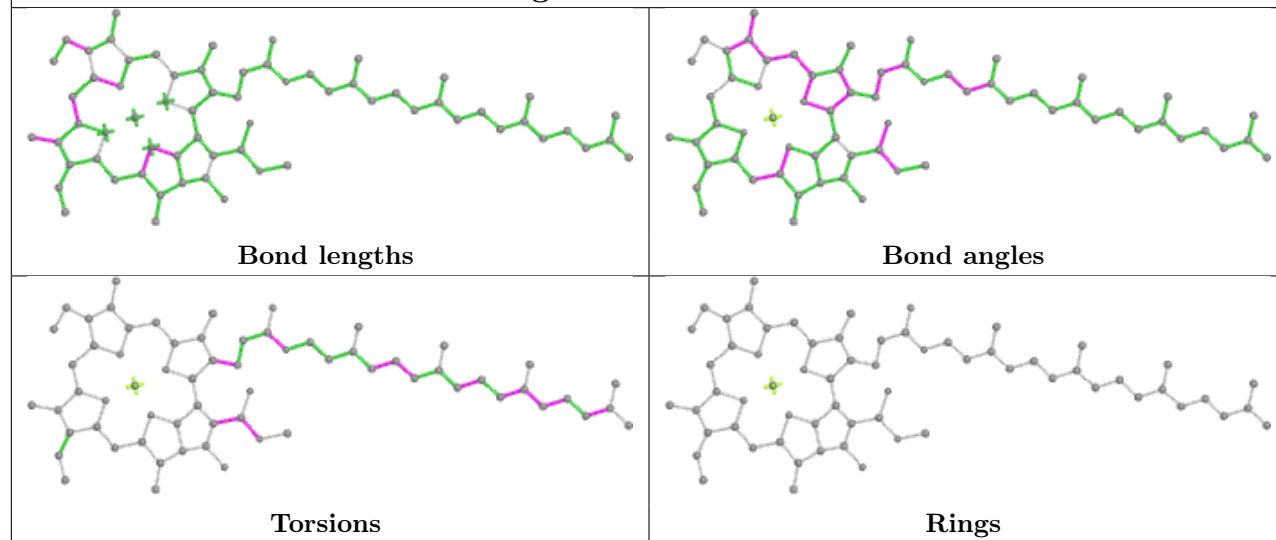


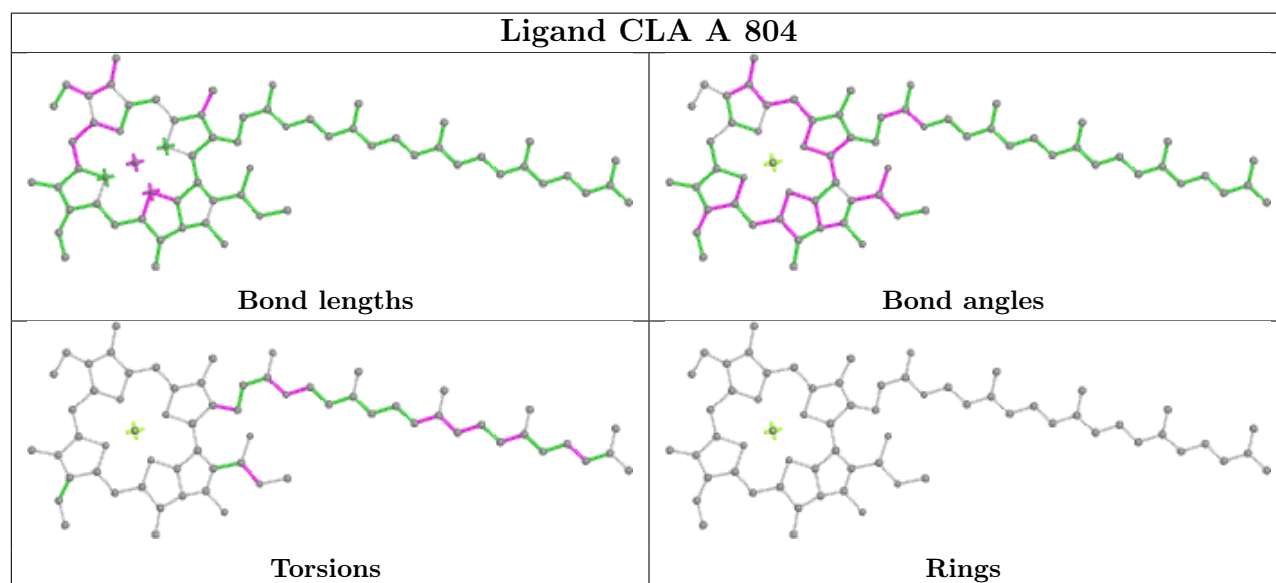
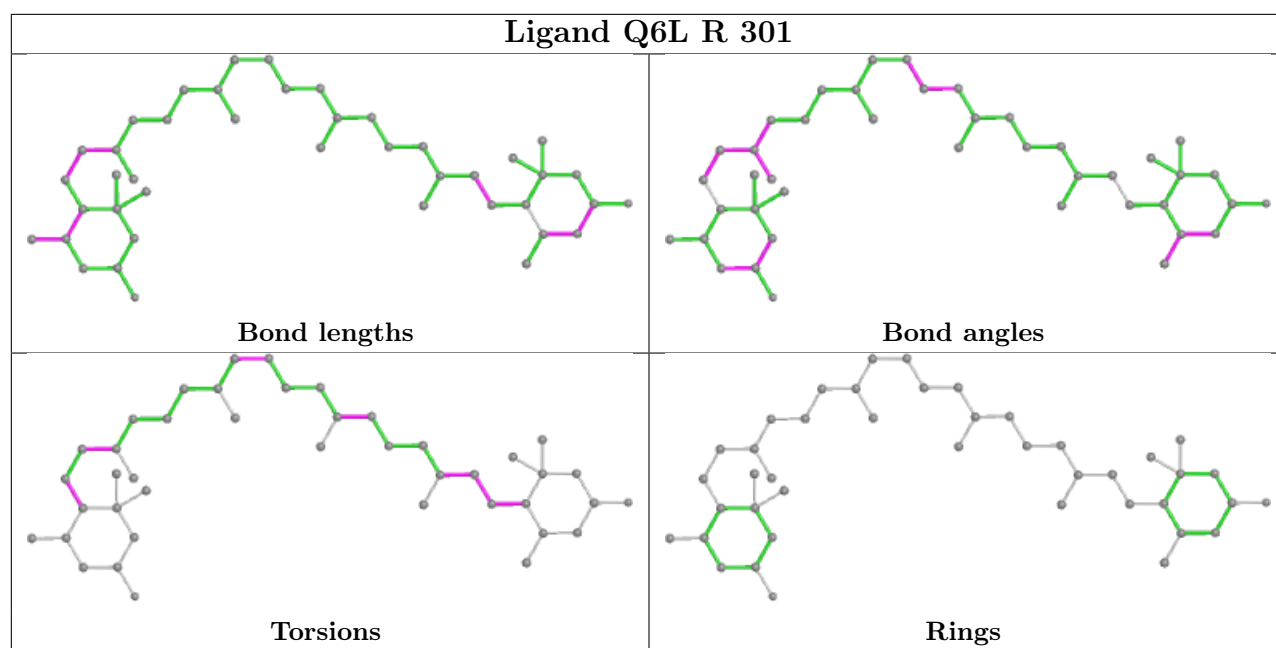
Rings

## Ligand CLA B 823

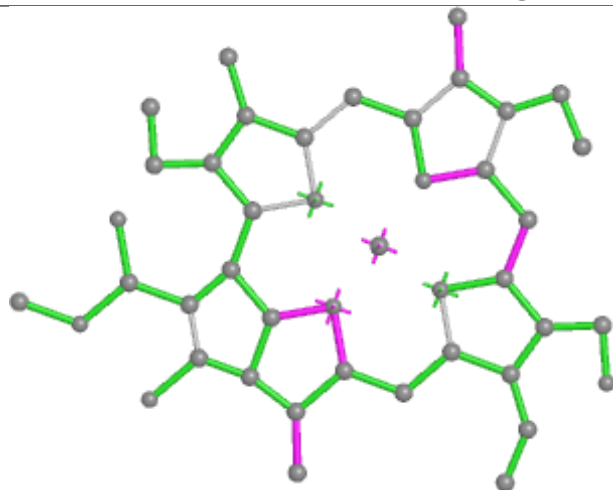


## Ligand CLA A 839

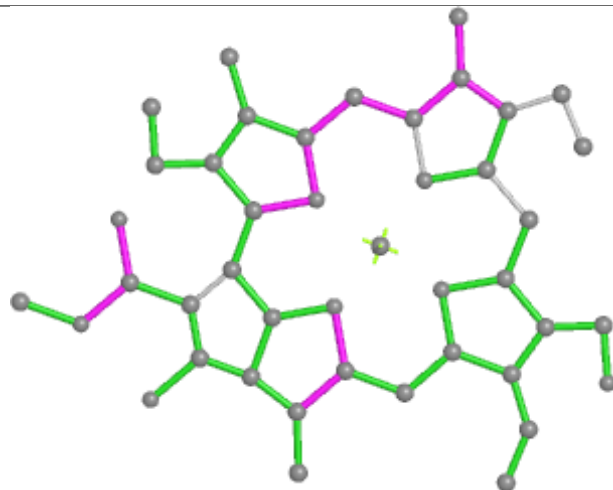




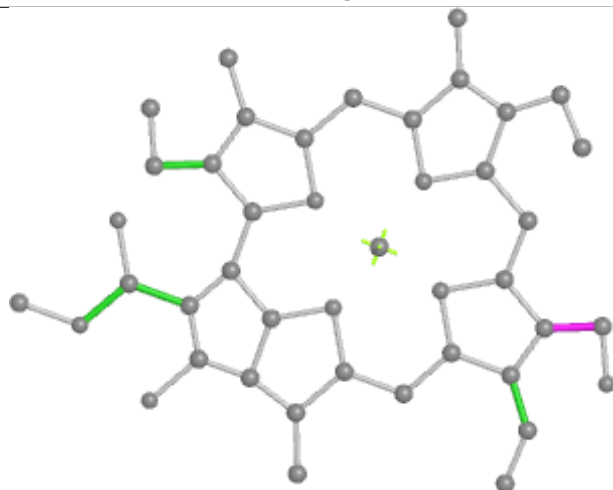
## Ligand CHL V 305



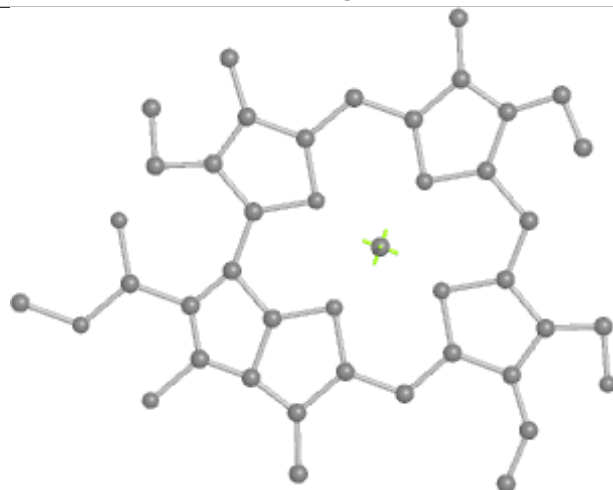
Bond lengths



Bond angles

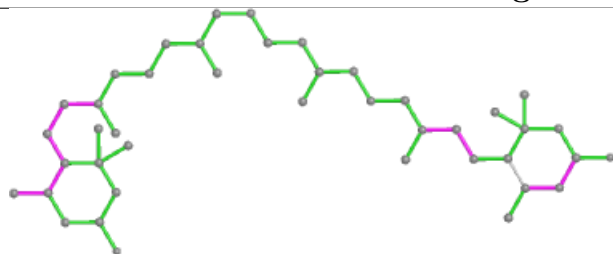


Torsions

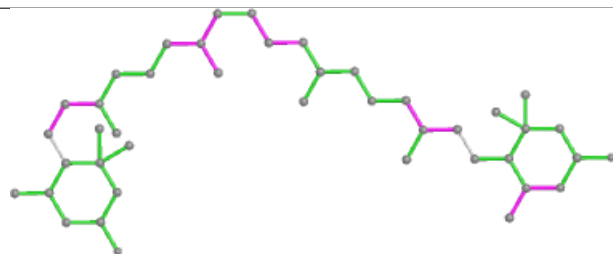


Rings

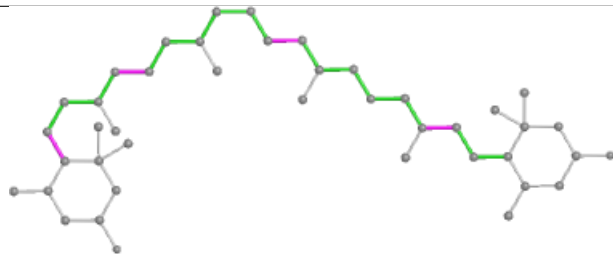
## Ligand Q6L W 316



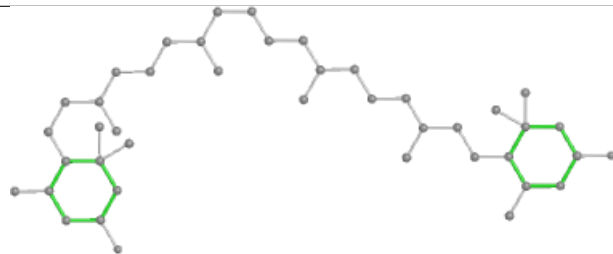
Bond lengths



Bond angles

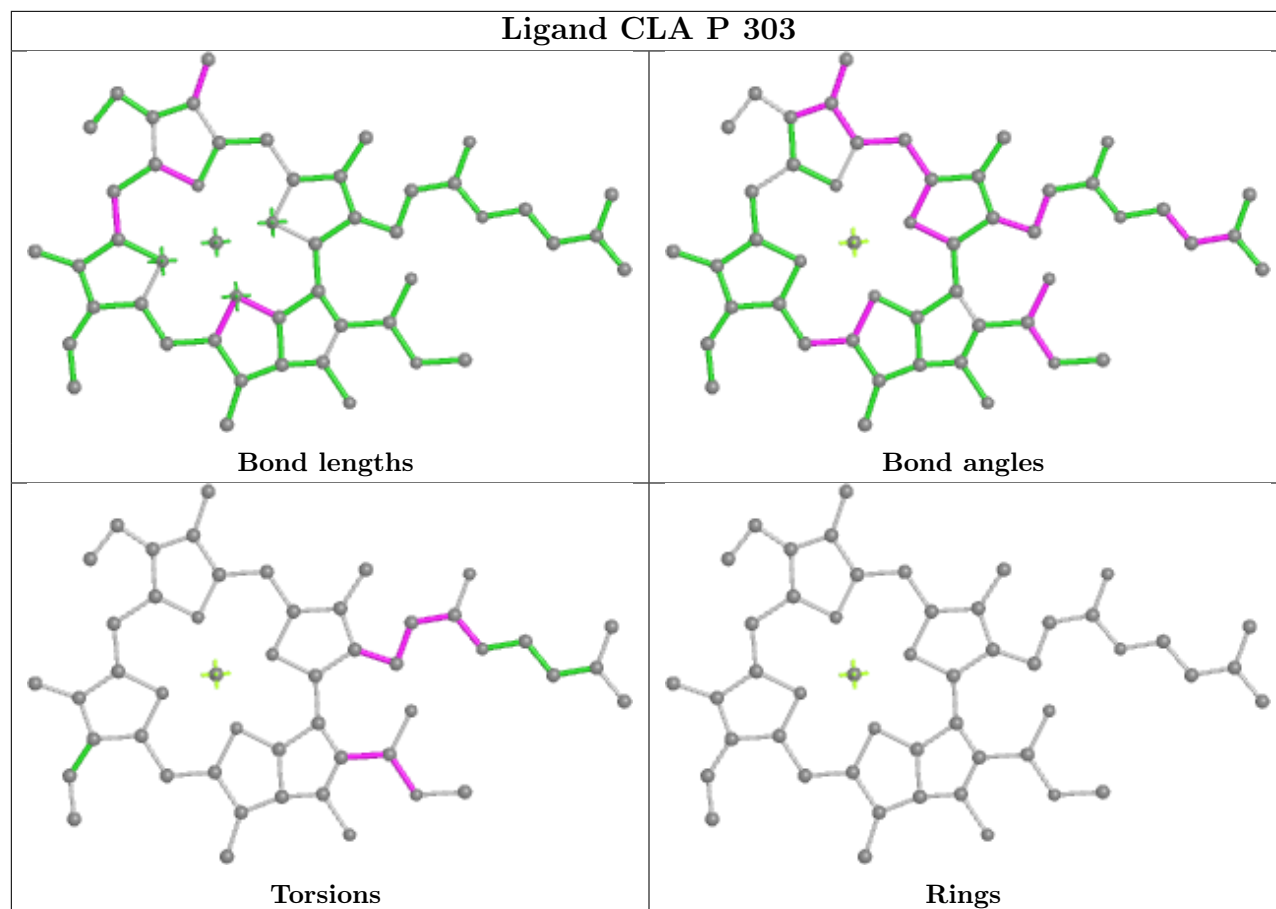


Torsions



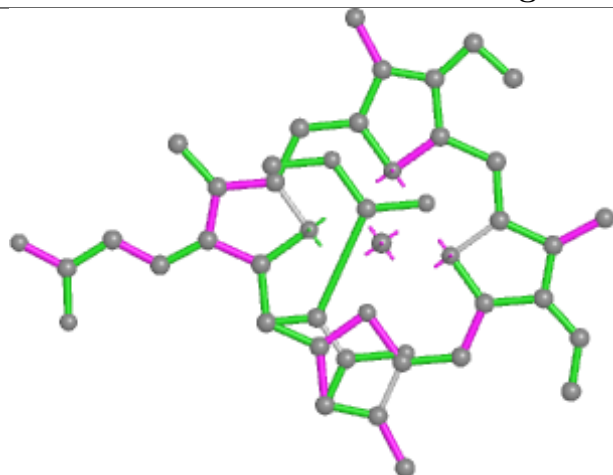
Rings

## Ligand CLA P 303

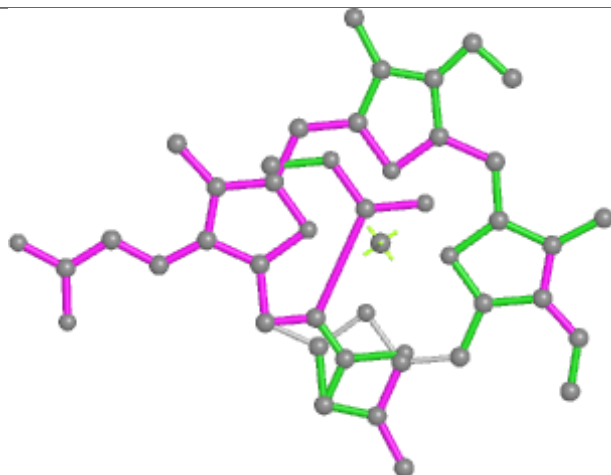




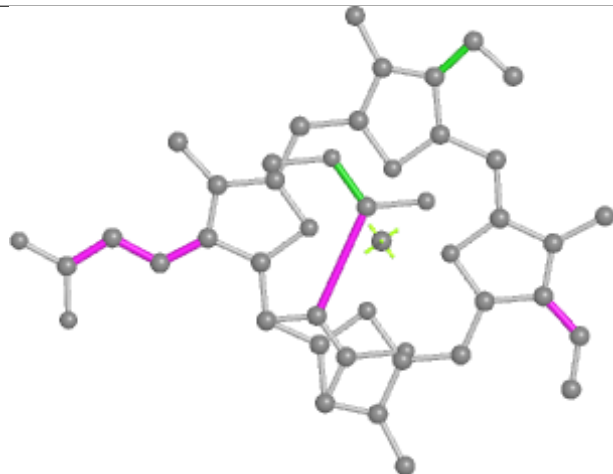
## Ligand KC2 S 308



Bond lengths



Bond angles

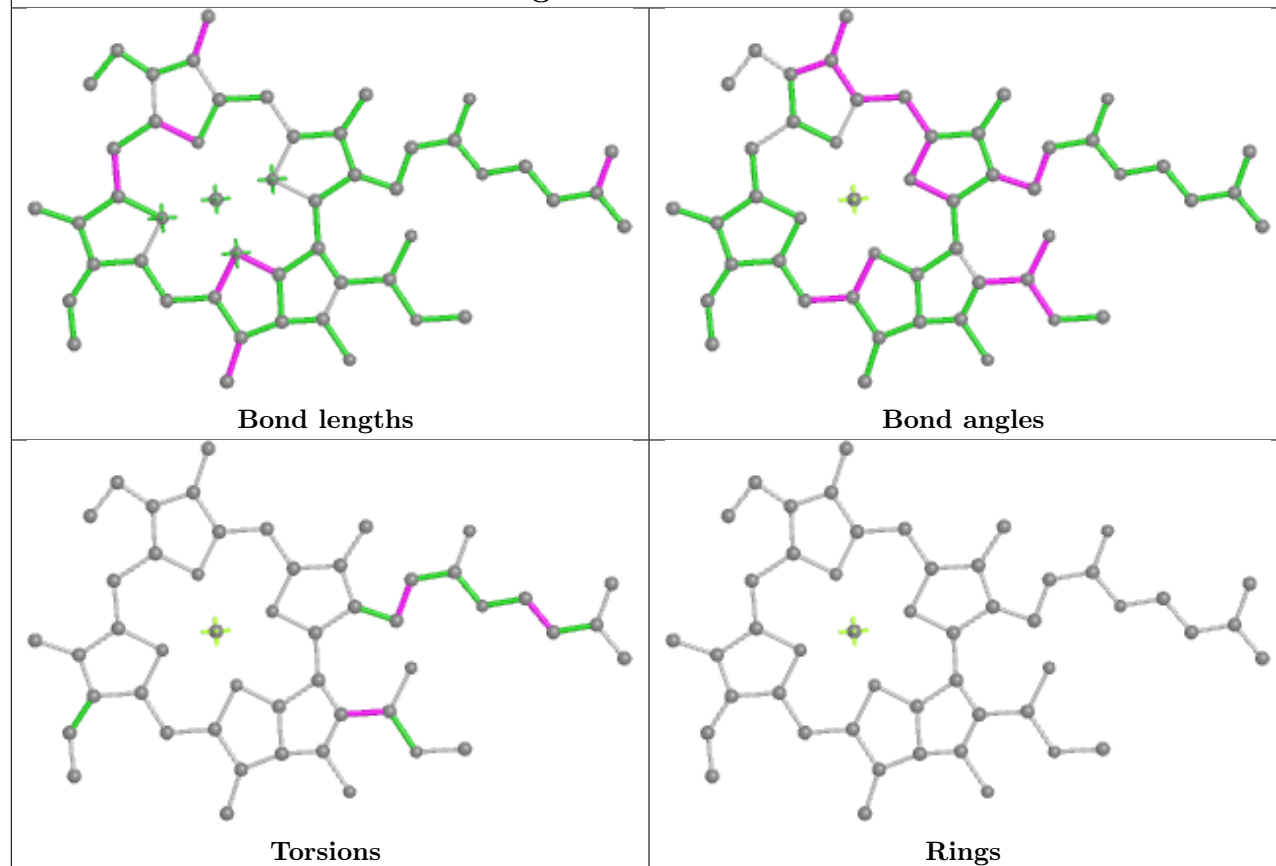


Torsions

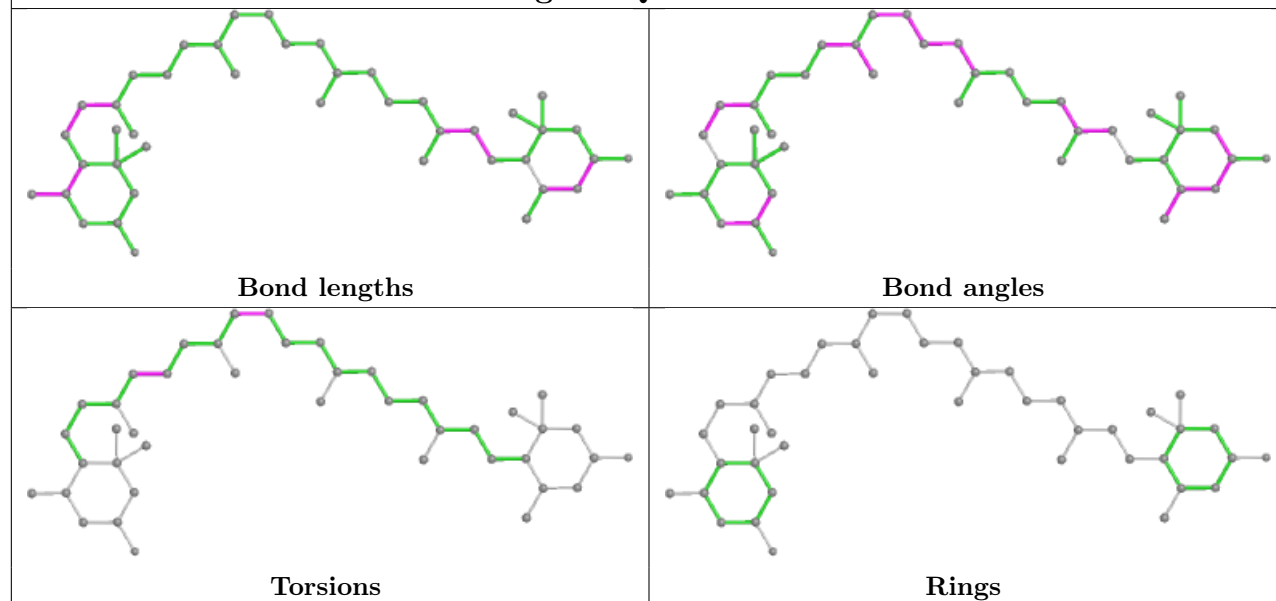


Rings

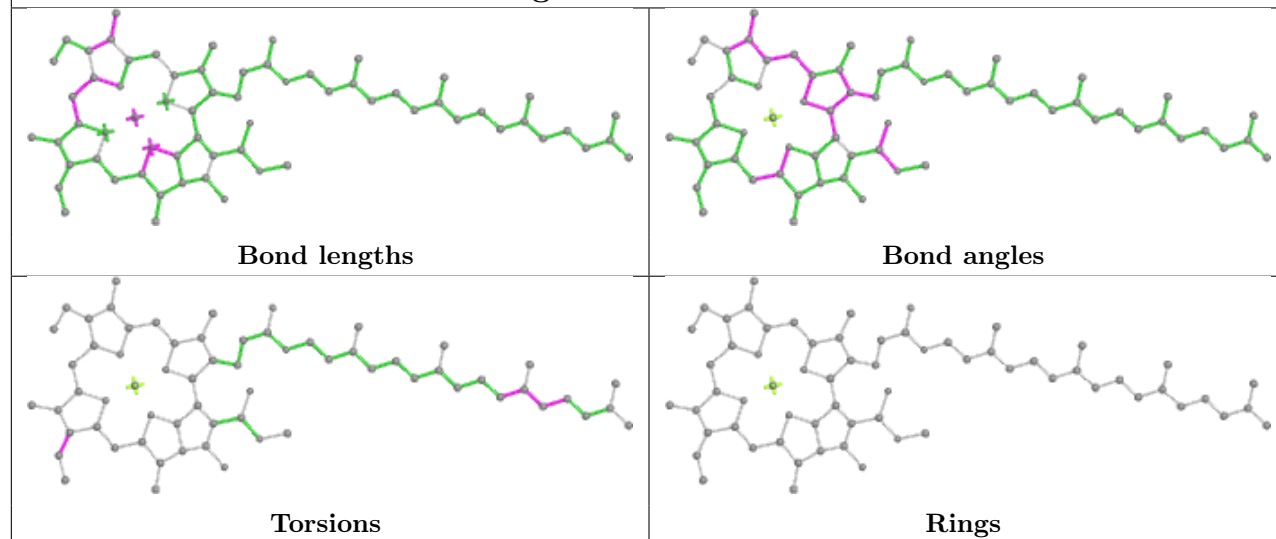
## Ligand CLA B 822



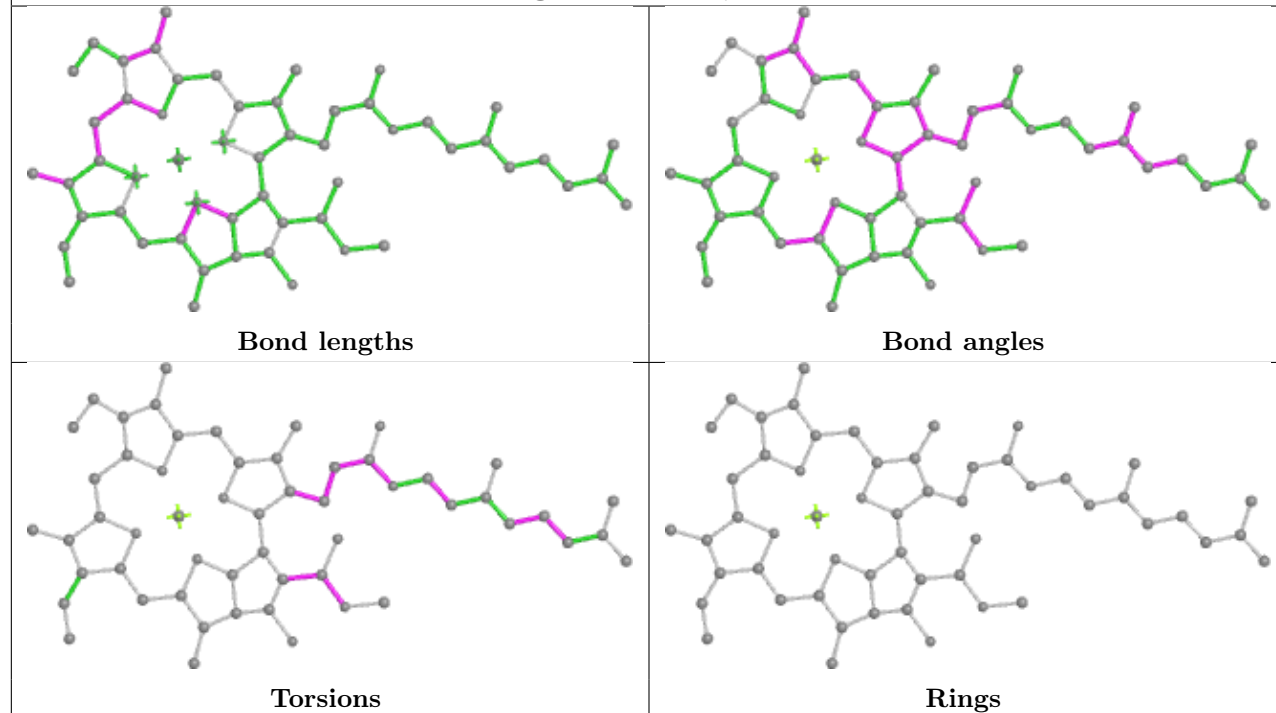
## Ligand Q6L U 315



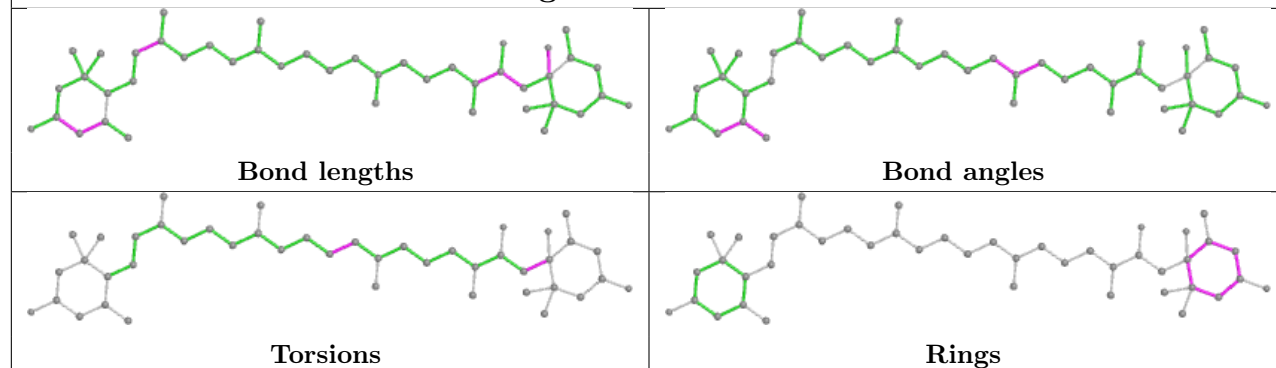
## Ligand CLA B 828



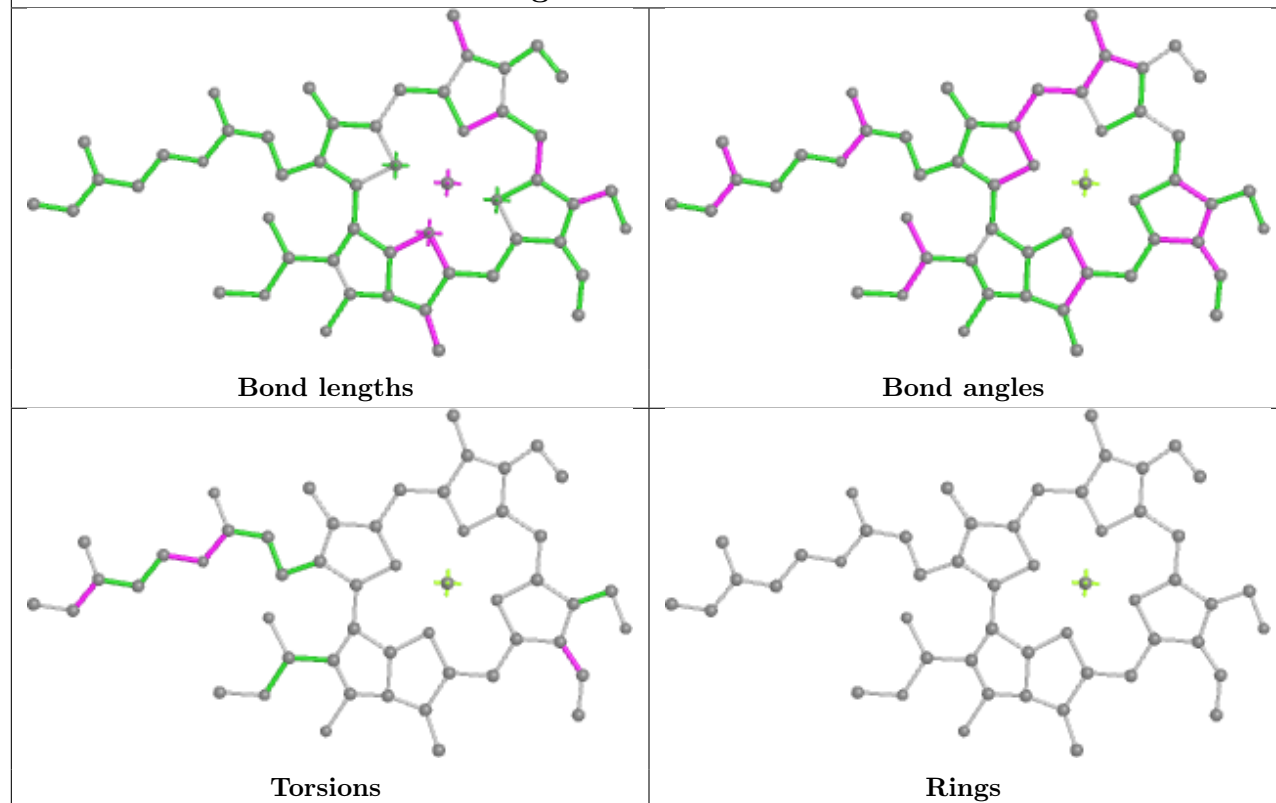
## Ligand CLA Q 301



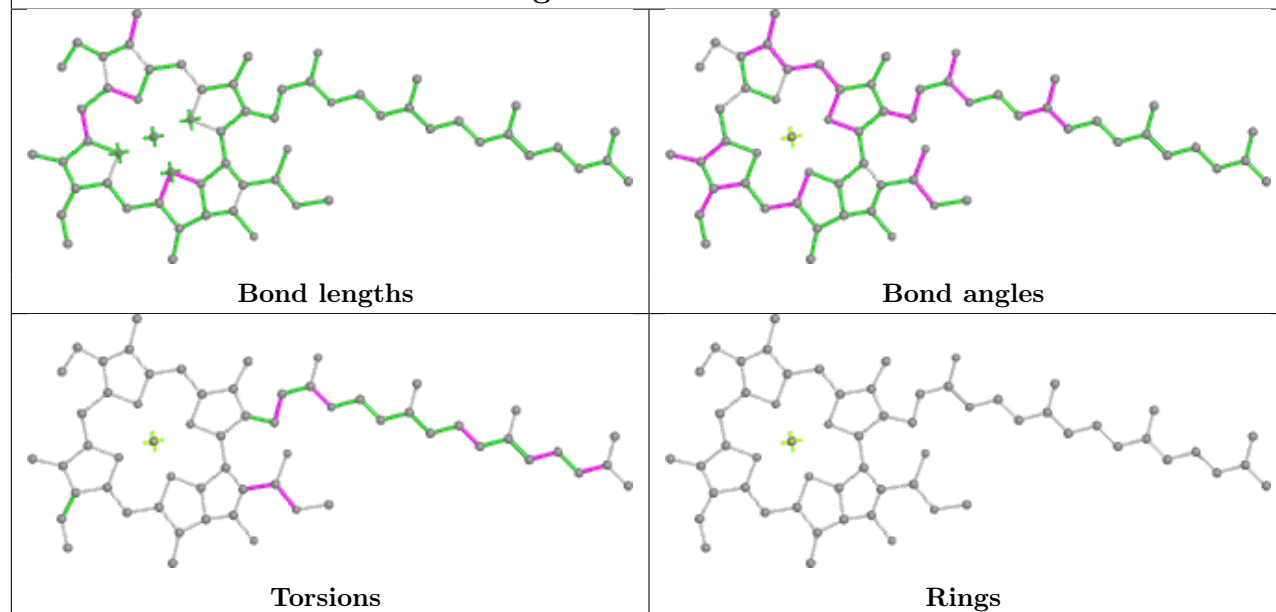
## Ligand IWJ 3 315

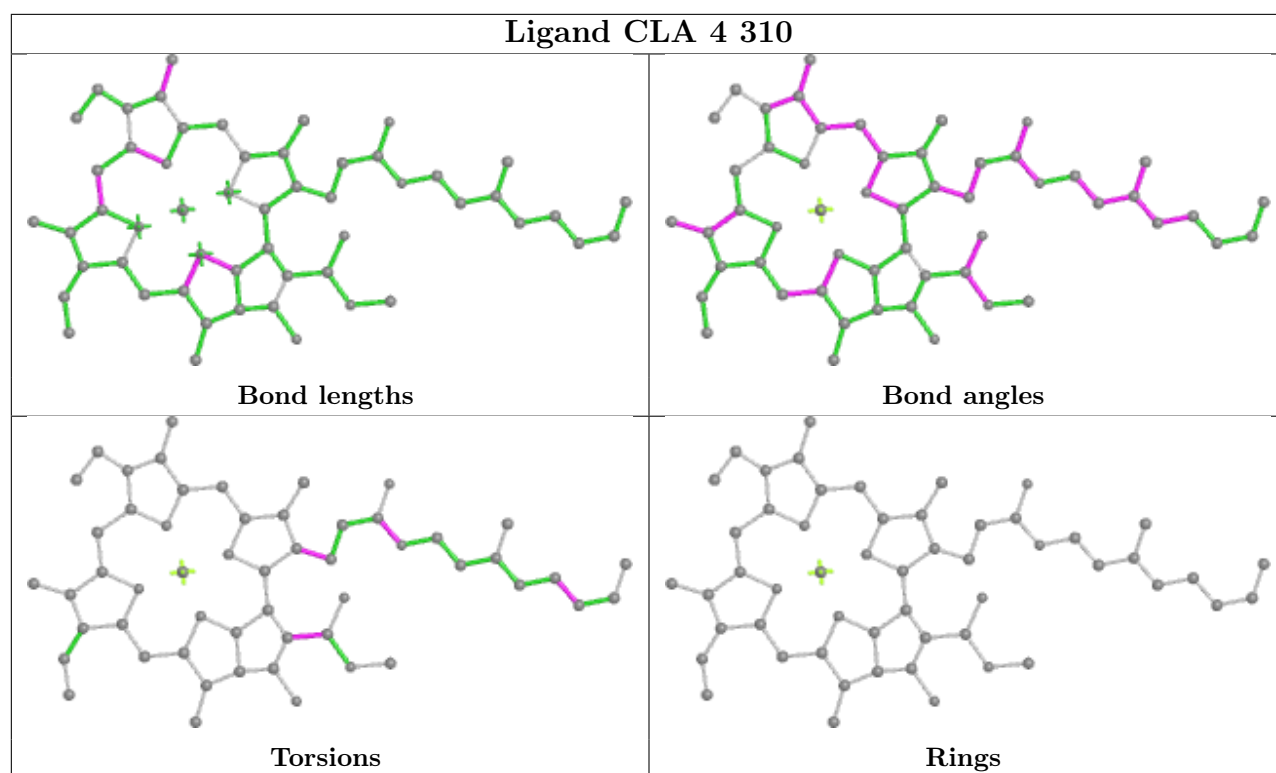


## Ligand CHL R 310

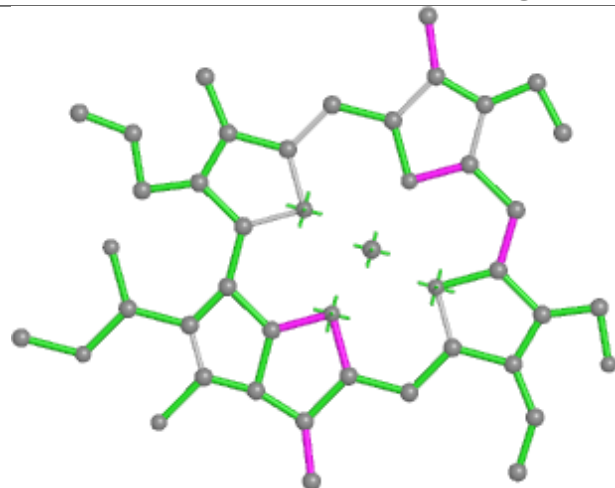


## Ligand CLA P 311

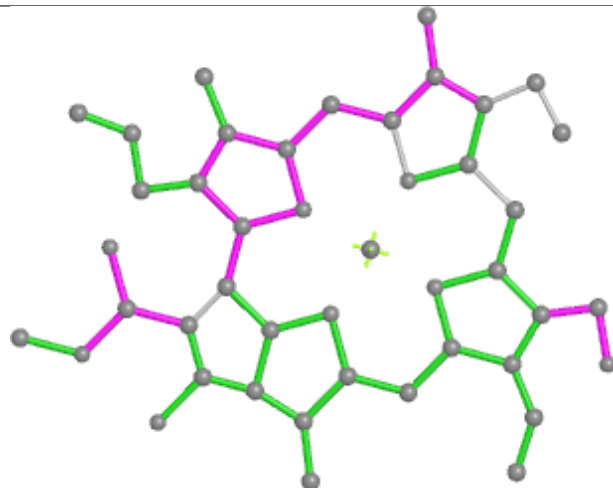




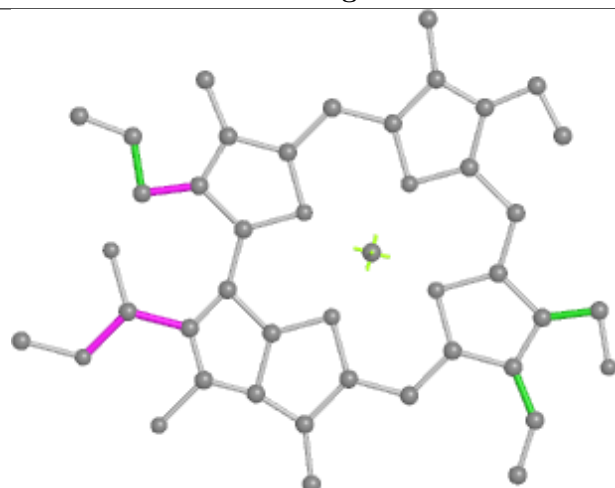
## Ligand CHL X 308



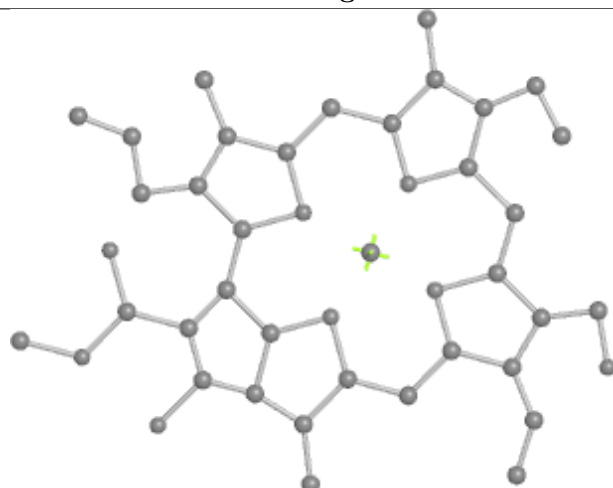
Bond lengths



Bond angles

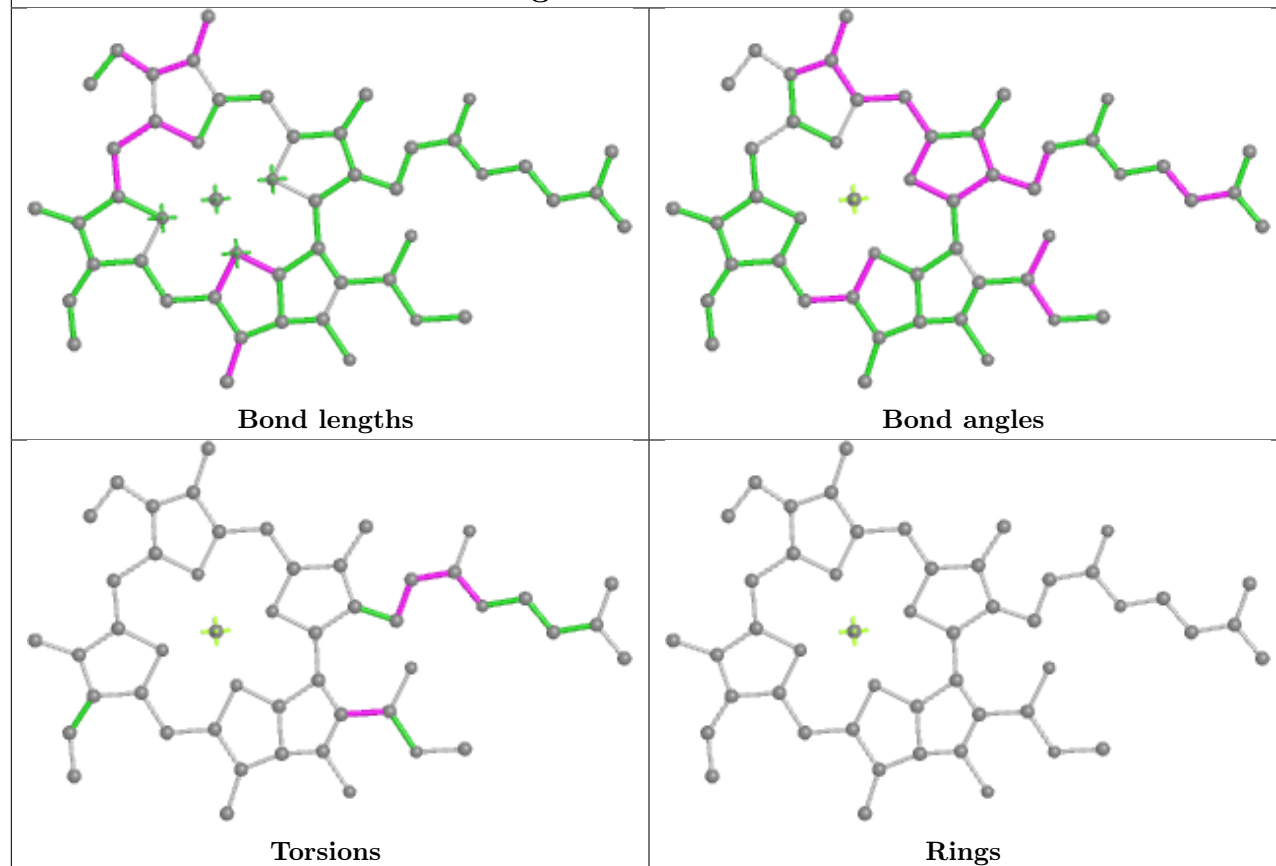


Torsions

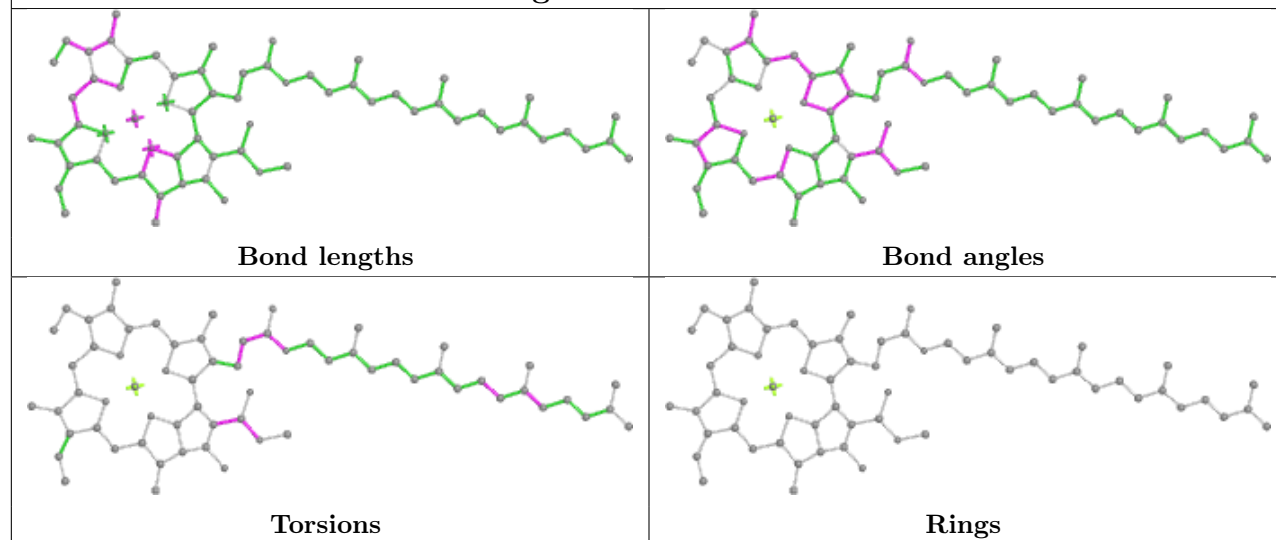


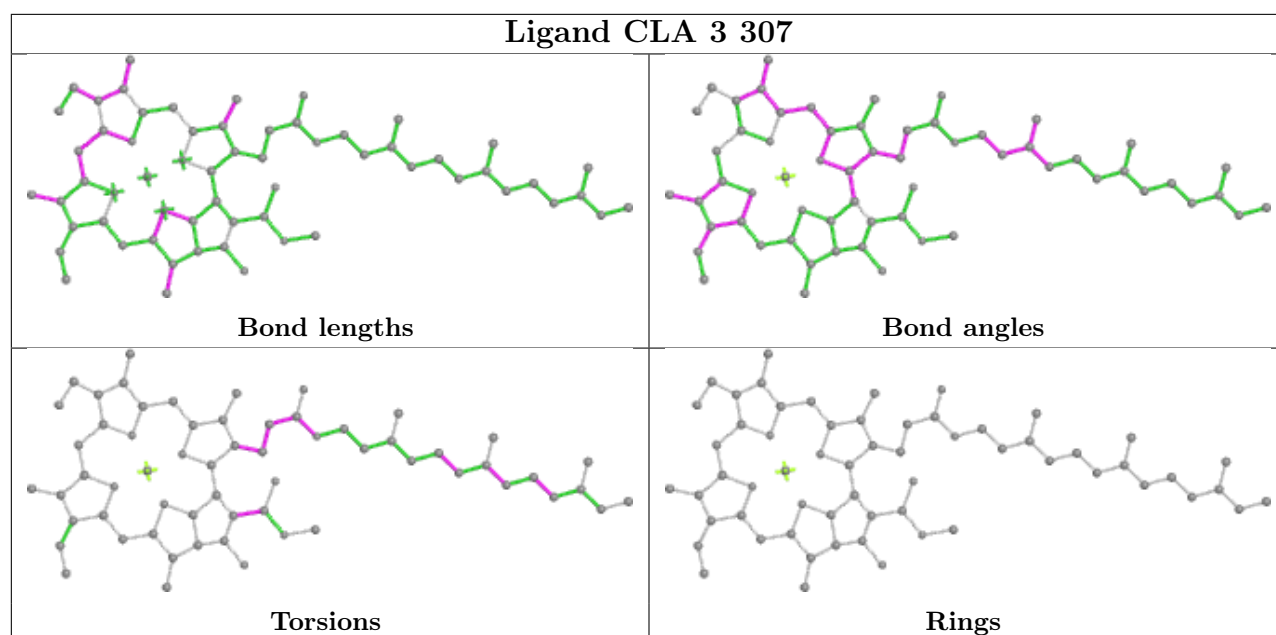
Rings

## Ligand CLA A 809



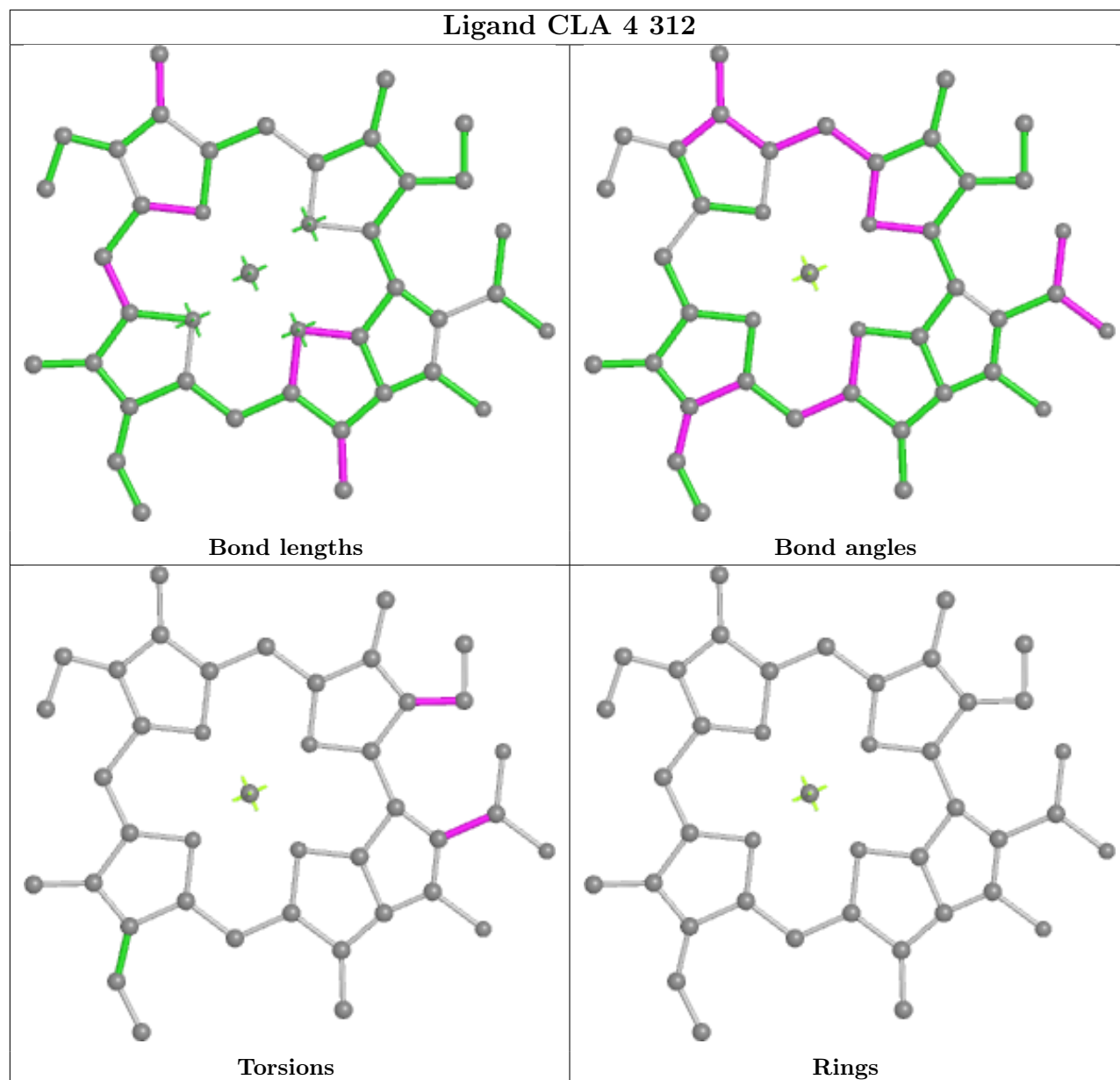
## Ligand CLA B 812



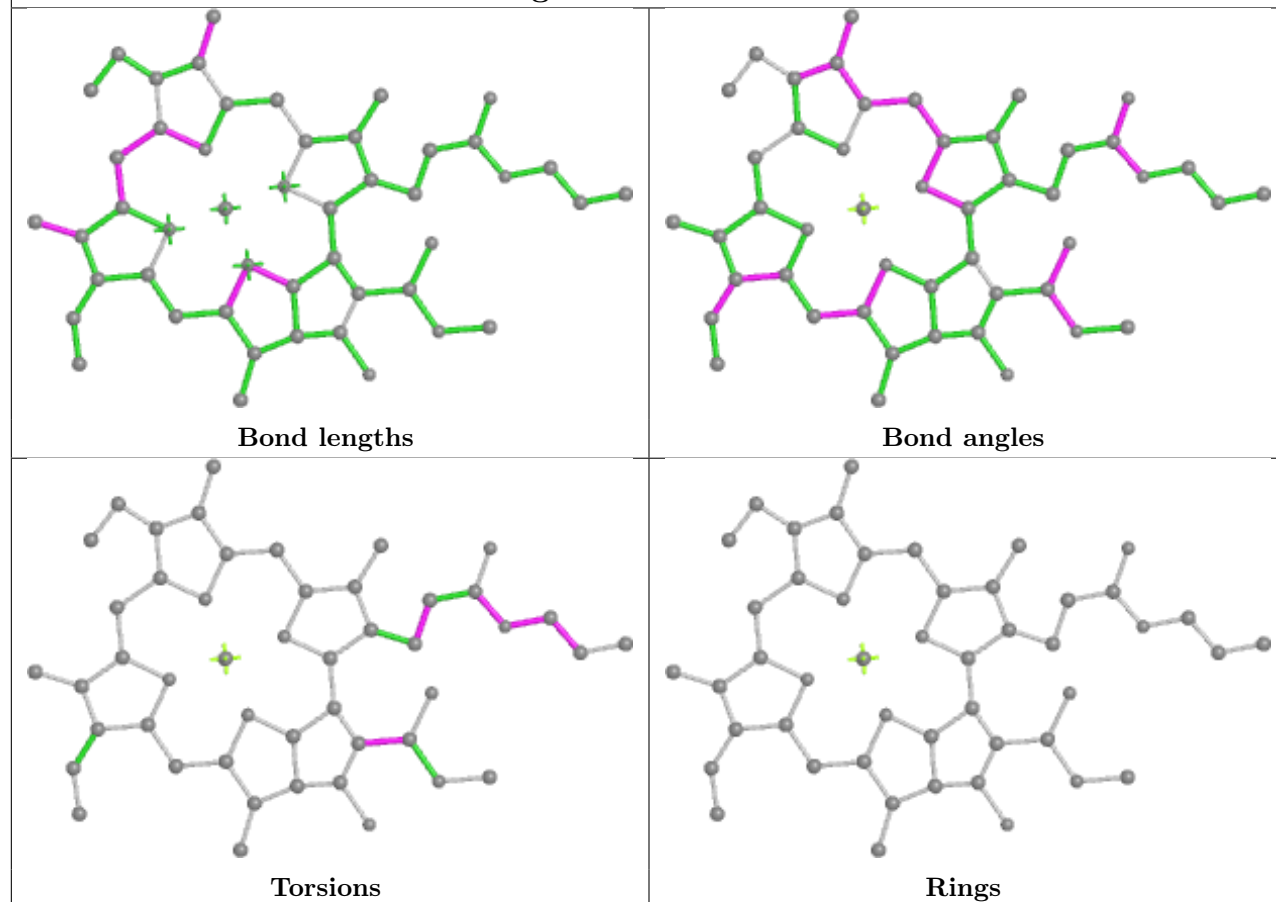




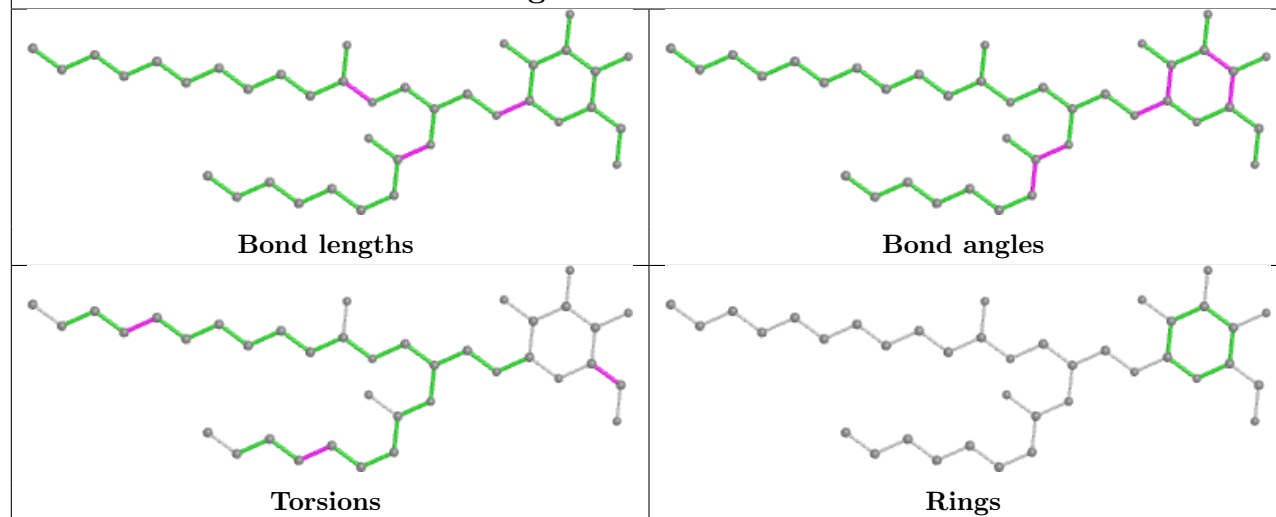
## Ligand CLA 4 312



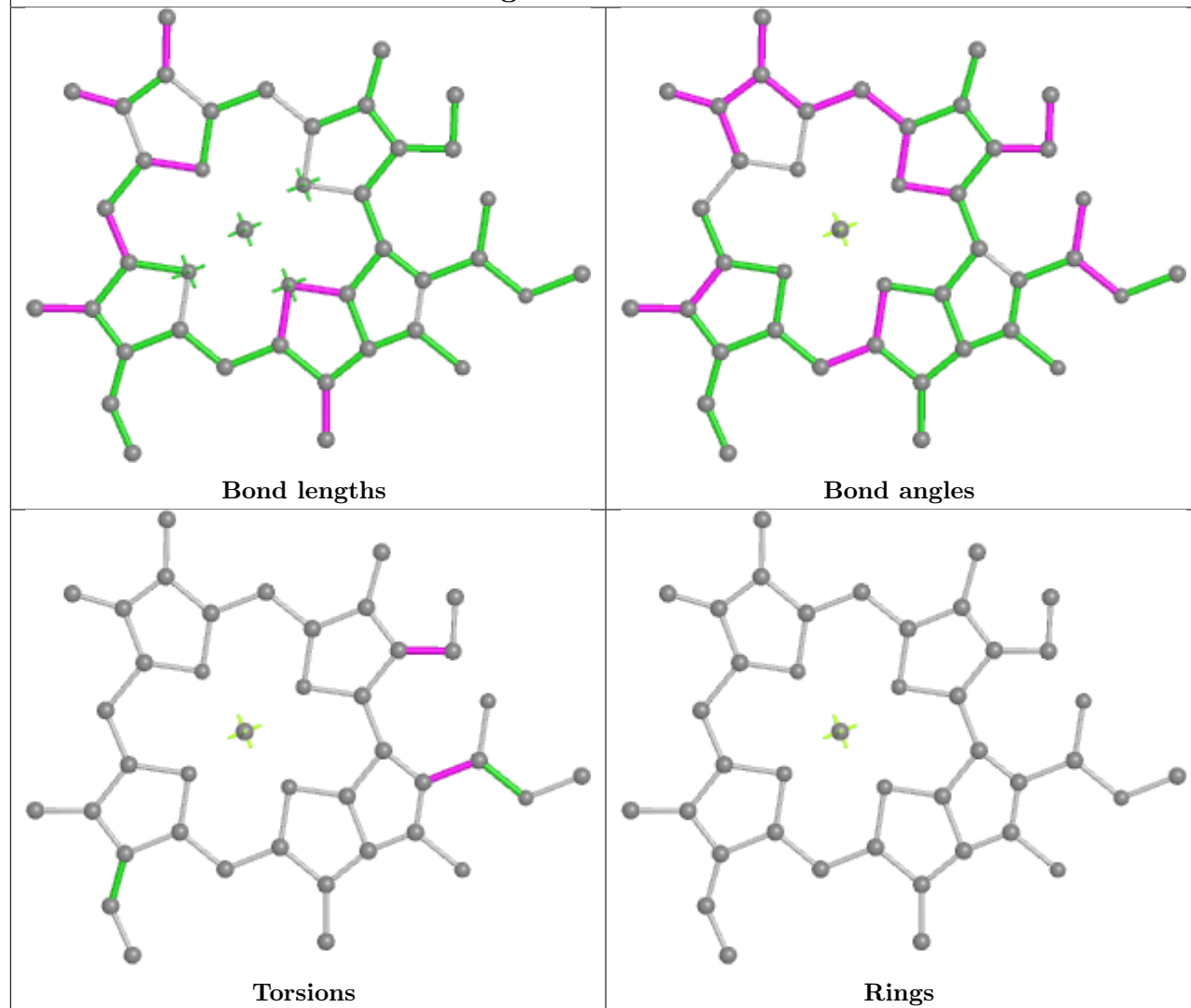
## Ligand CLA R 317



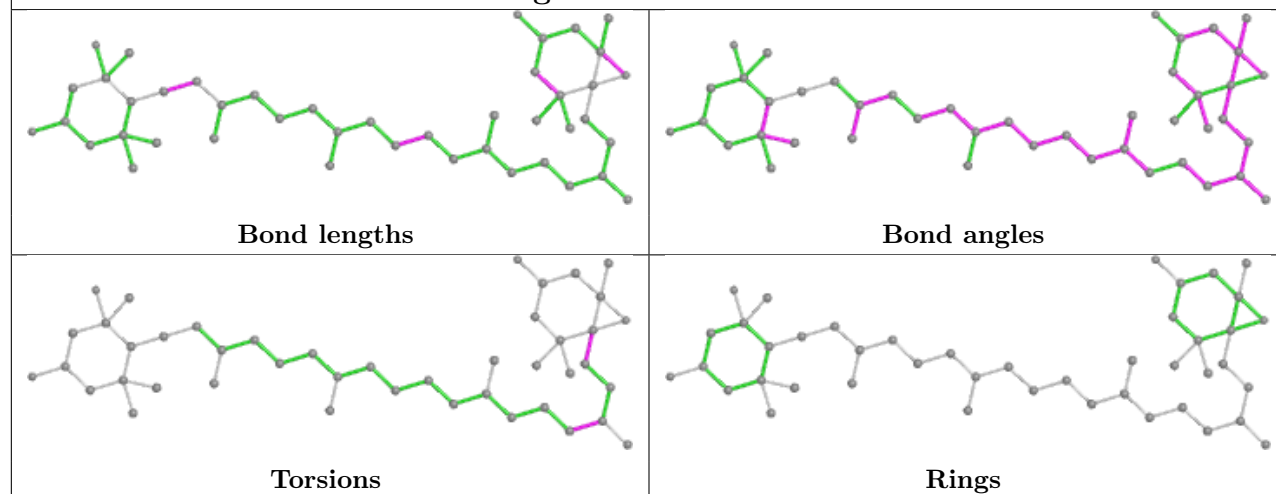
## Ligand LMG B 801



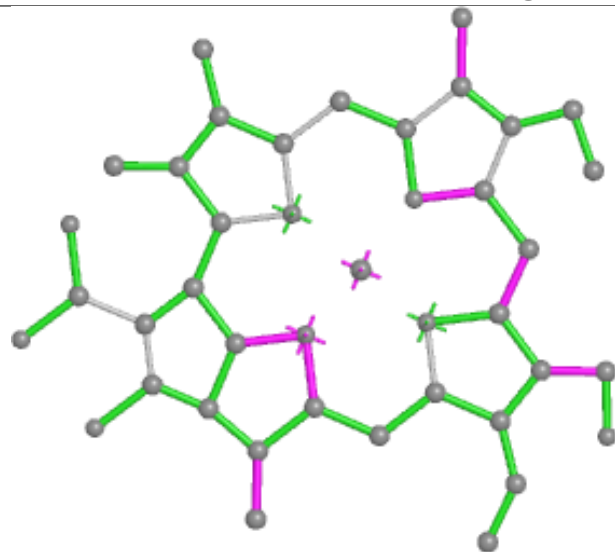
## Ligand CLA 3 305



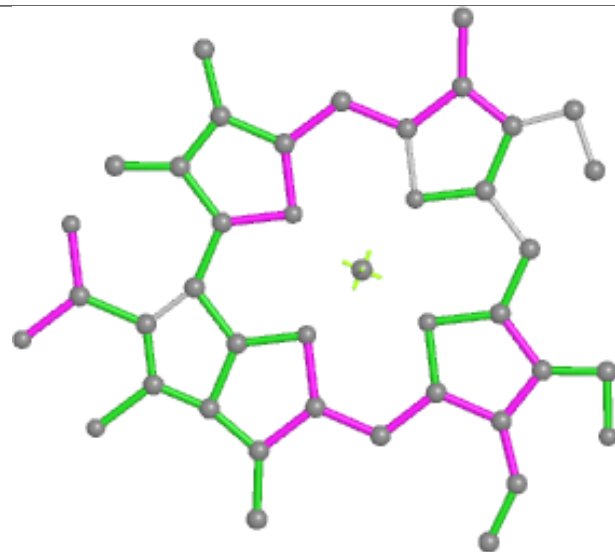
## Ligand NEX S 317



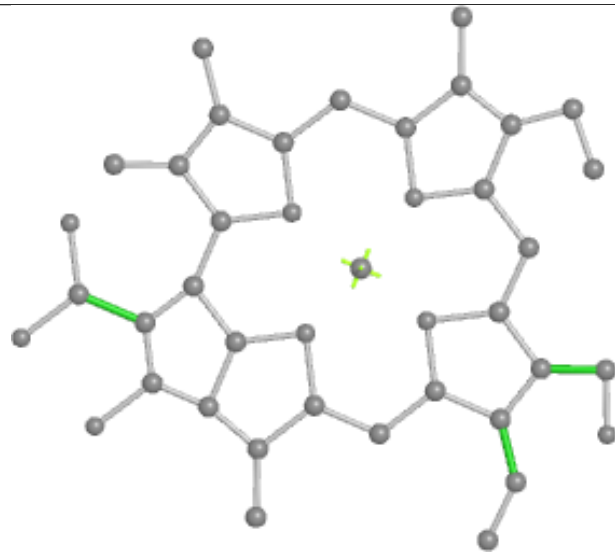
## Ligand CHL 1 604



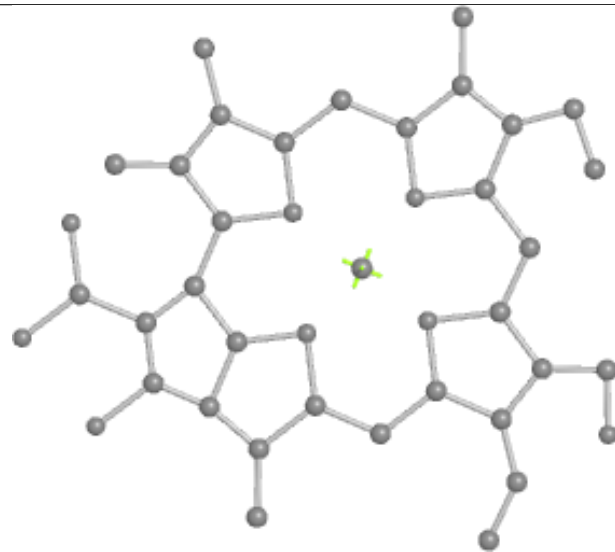
Bond lengths



Bond angles

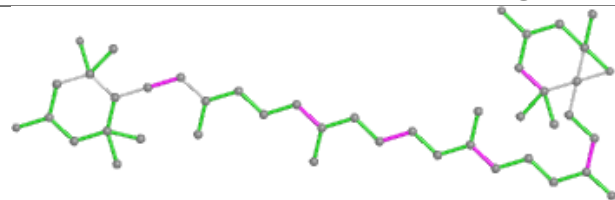


Torsions

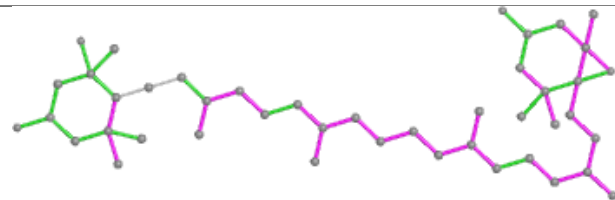


Rings

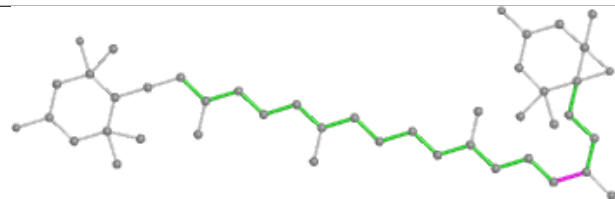
## Ligand NEX P 317



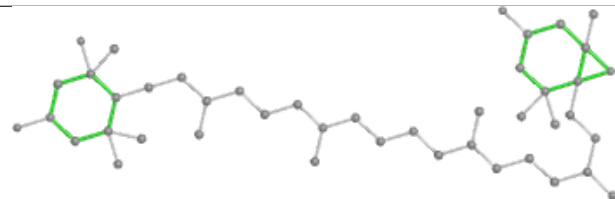
Bond lengths



Bond angles

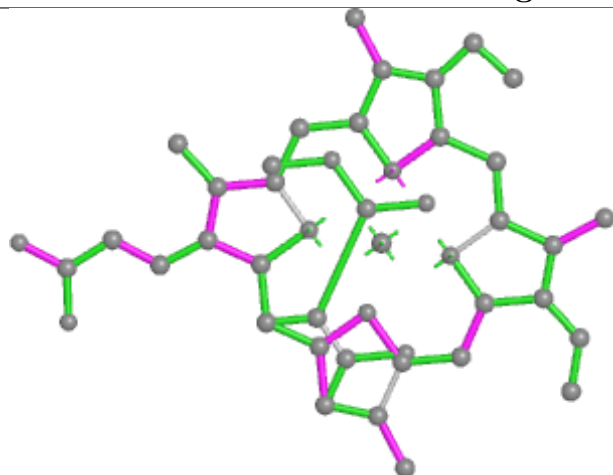


Torsions

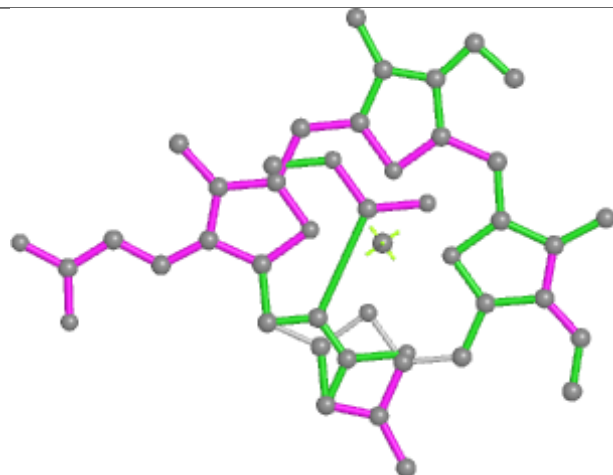


Rings

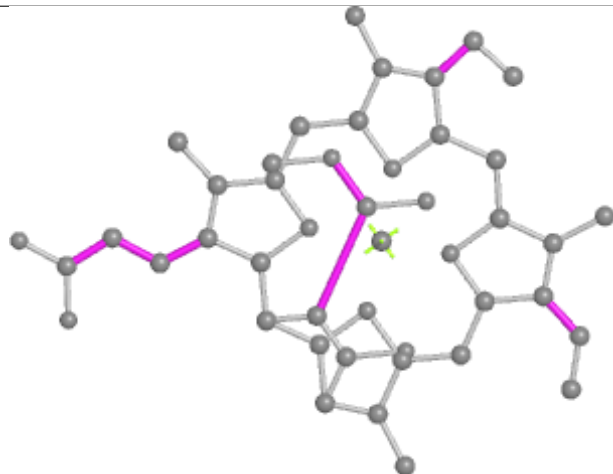
## Ligand KC2 U 307



Bond lengths



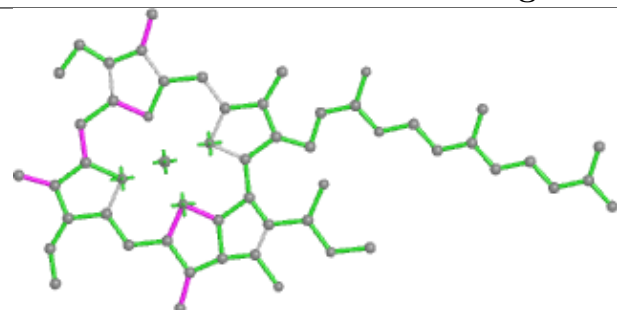
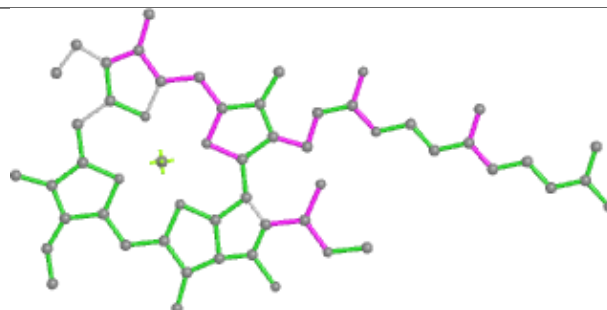
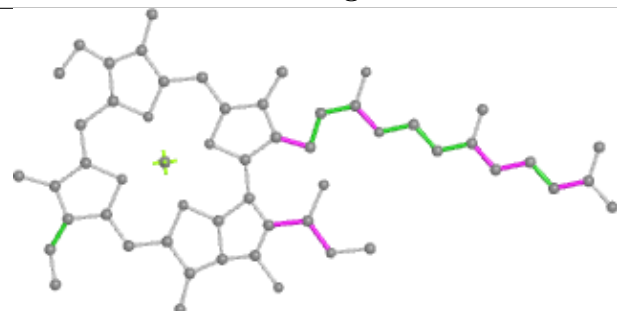
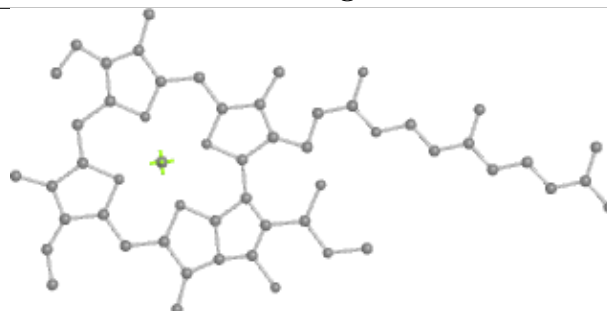
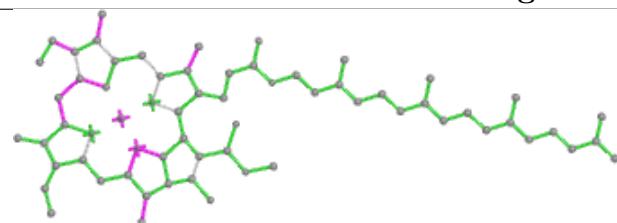
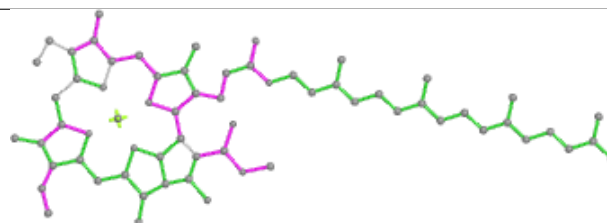
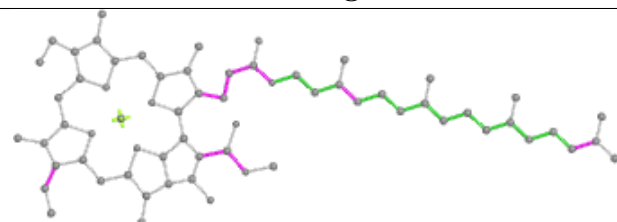
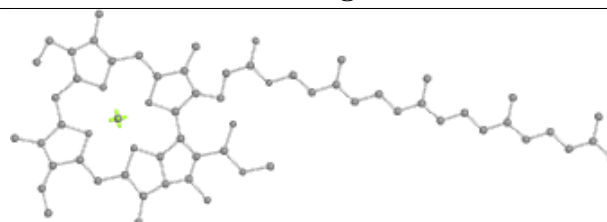
Bond angles

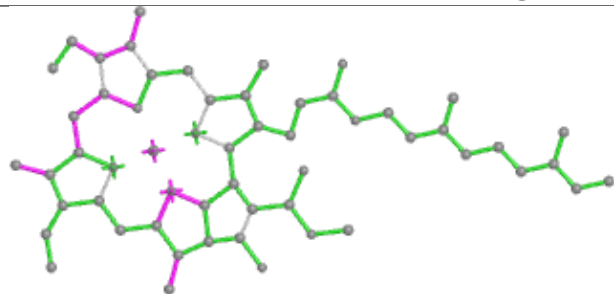


Torsions

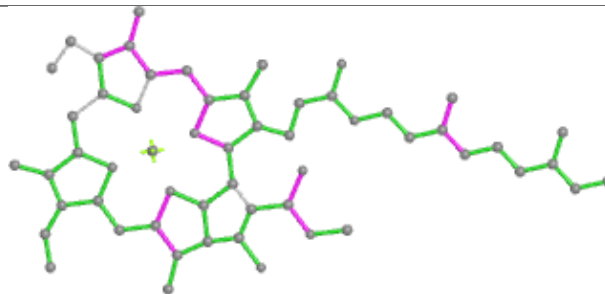


Rings

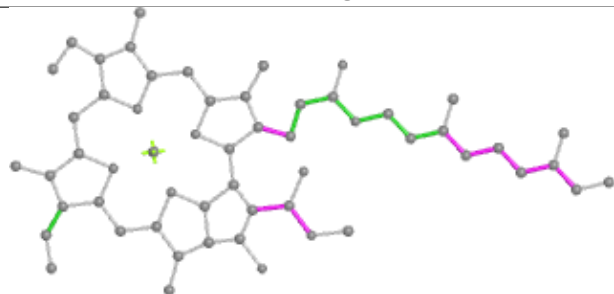
**Ligand CLA T 312****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 829****Bond lengths****Bond angles****Torsions****Rings**

**Ligand CLA U 302**

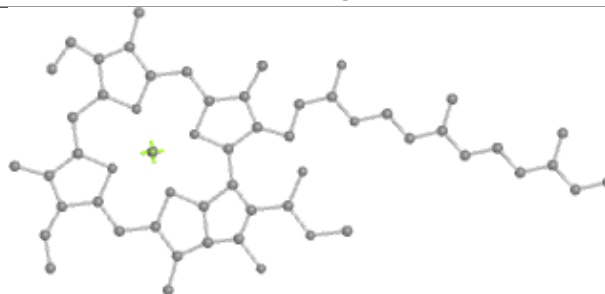
Bond lengths



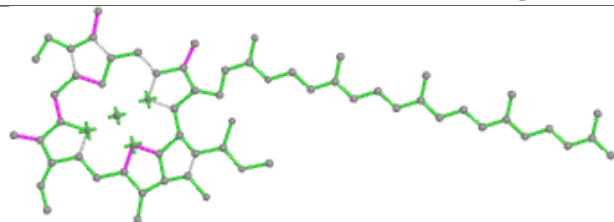
Bond angles



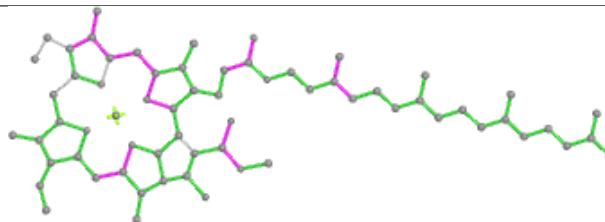
Torsions



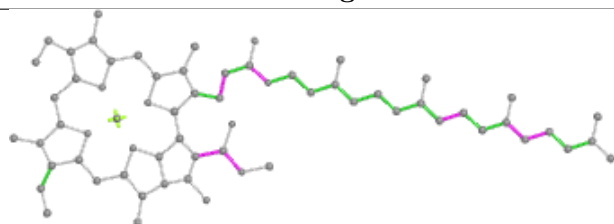
Rings

**Ligand CLA A 815**

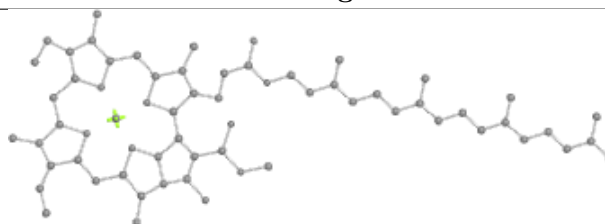
Bond lengths



Bond angles

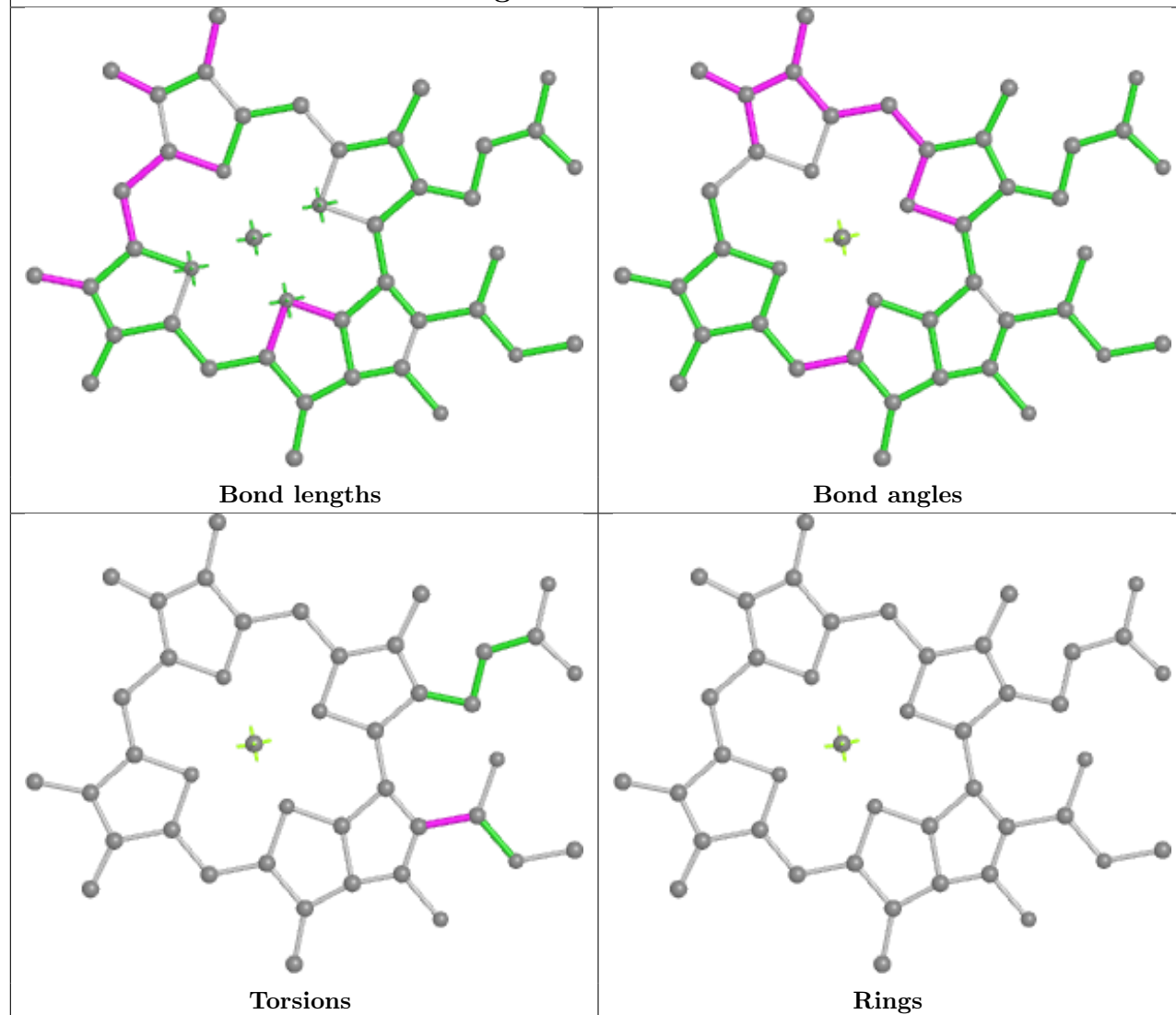


Torsions

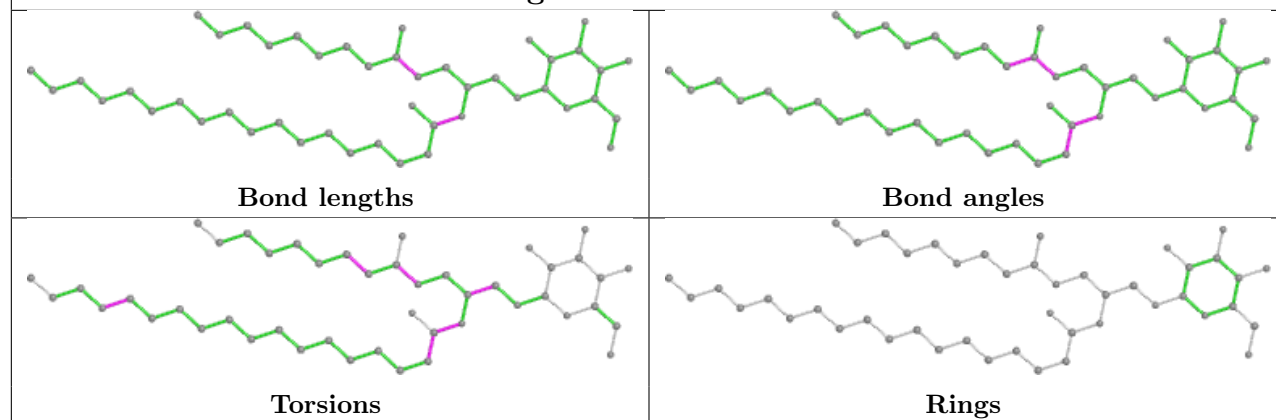


Rings

## Ligand CLA 4 305

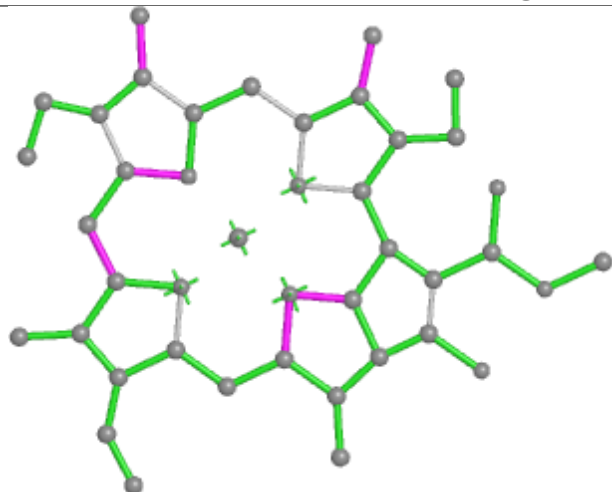


## Ligand LMG A 857

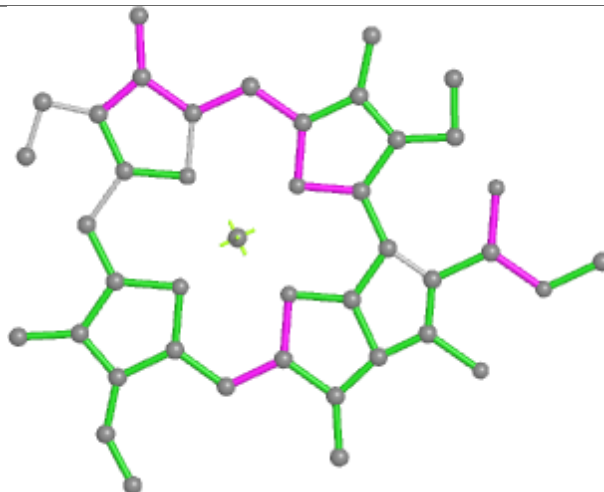




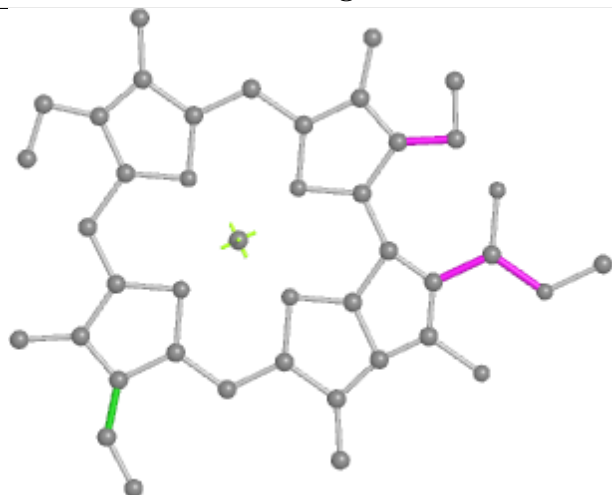
## Ligand CLA 6 608



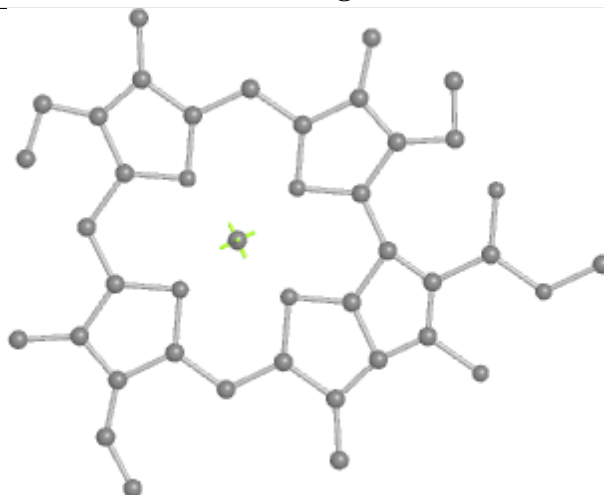
Bond lengths



Bond angles

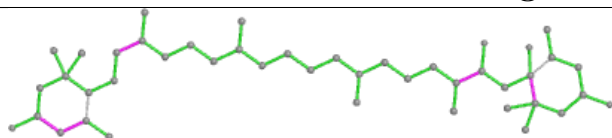


Torsions

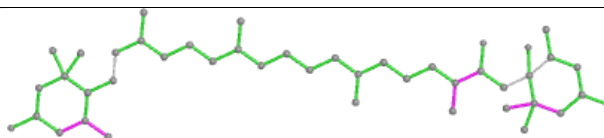


Rings

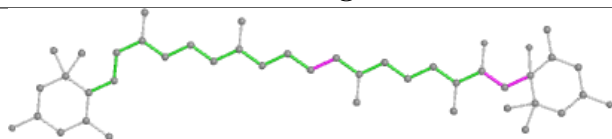
## Ligand IWJ S 322



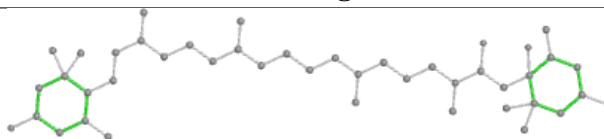
Bond lengths



Bond angles

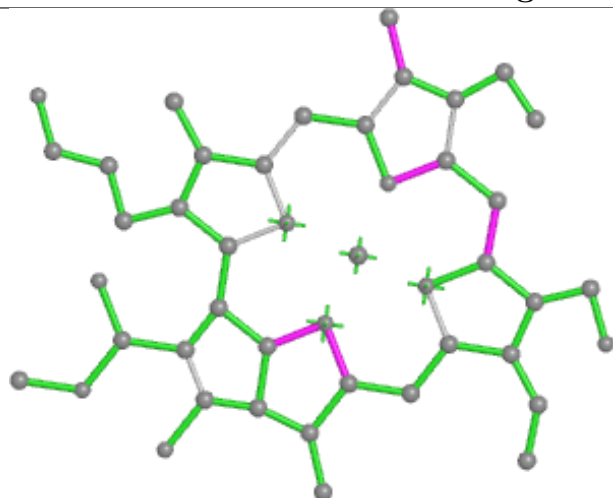


Torsions

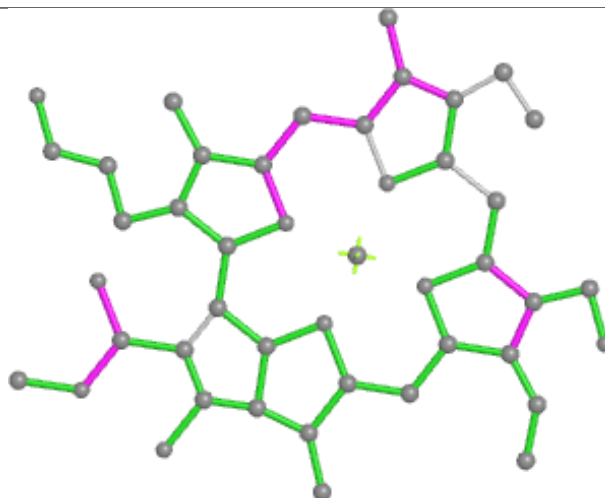


Rings

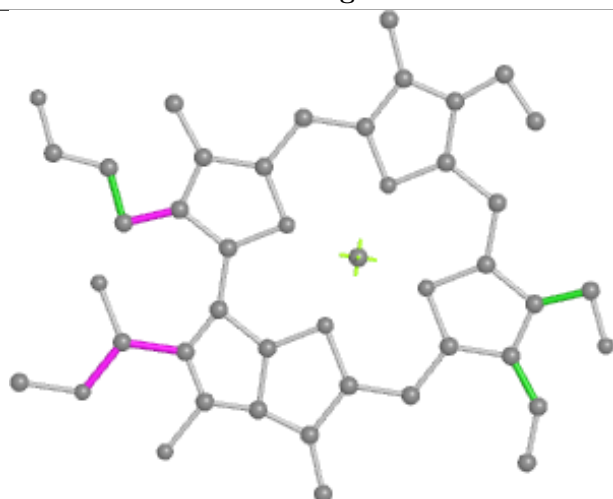
## Ligand CHL S 314



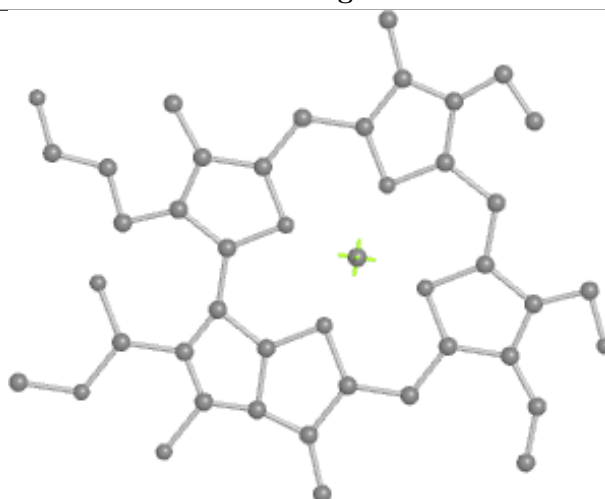
Bond lengths



Bond angles

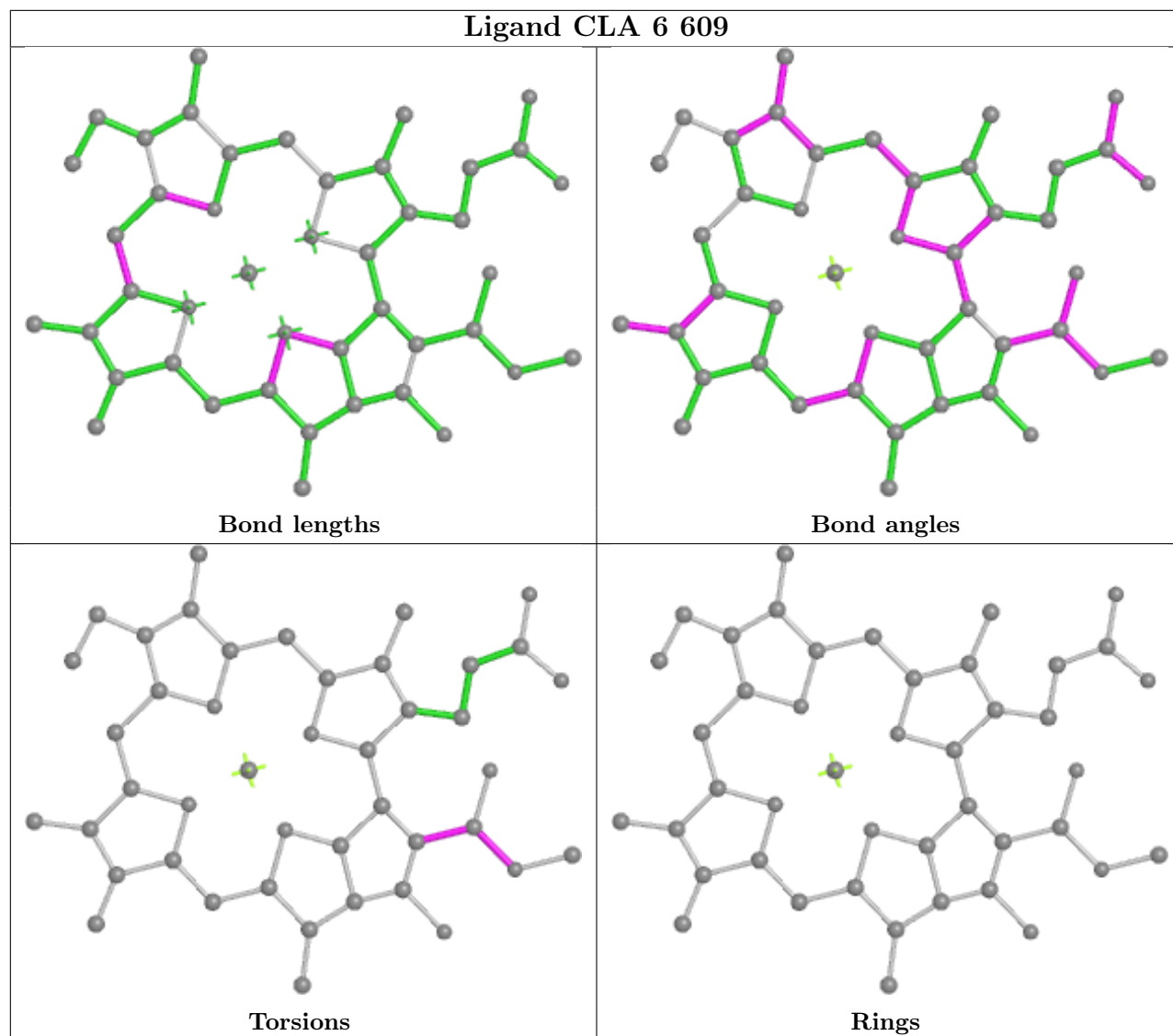


Torsions

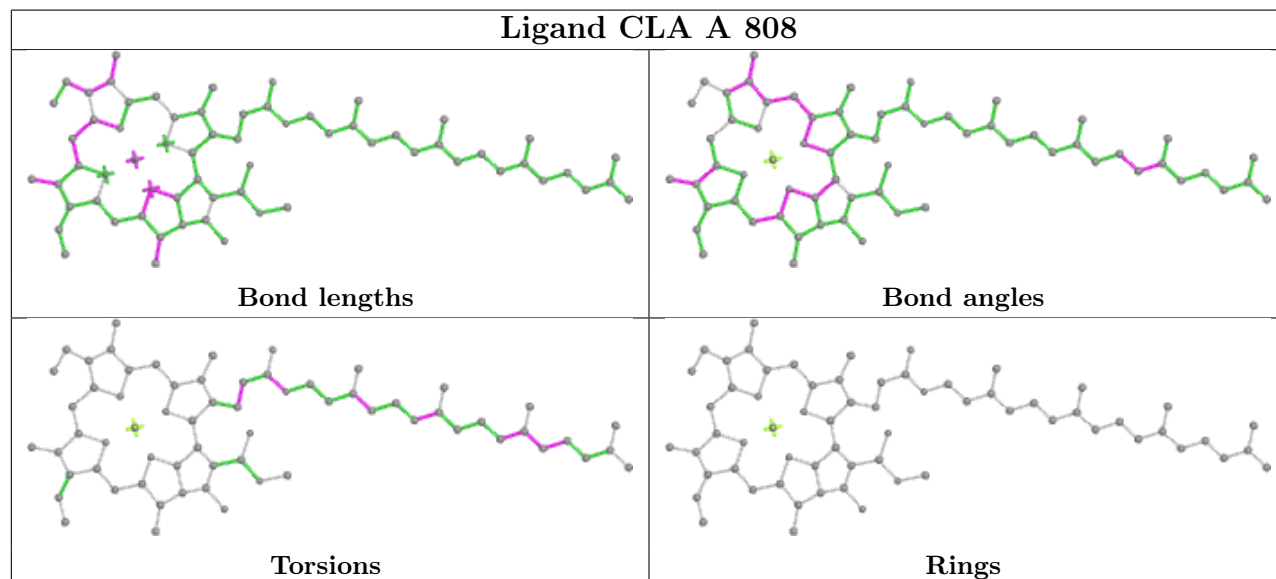


Rings

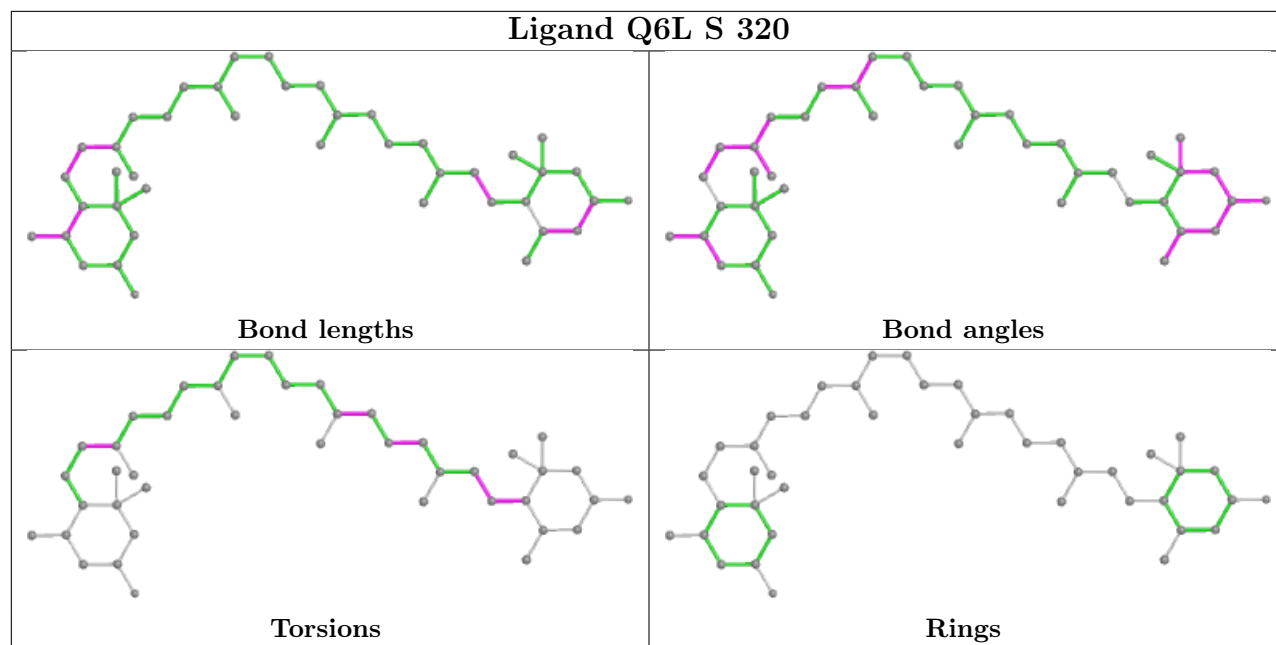
## Ligand CLA 6 609



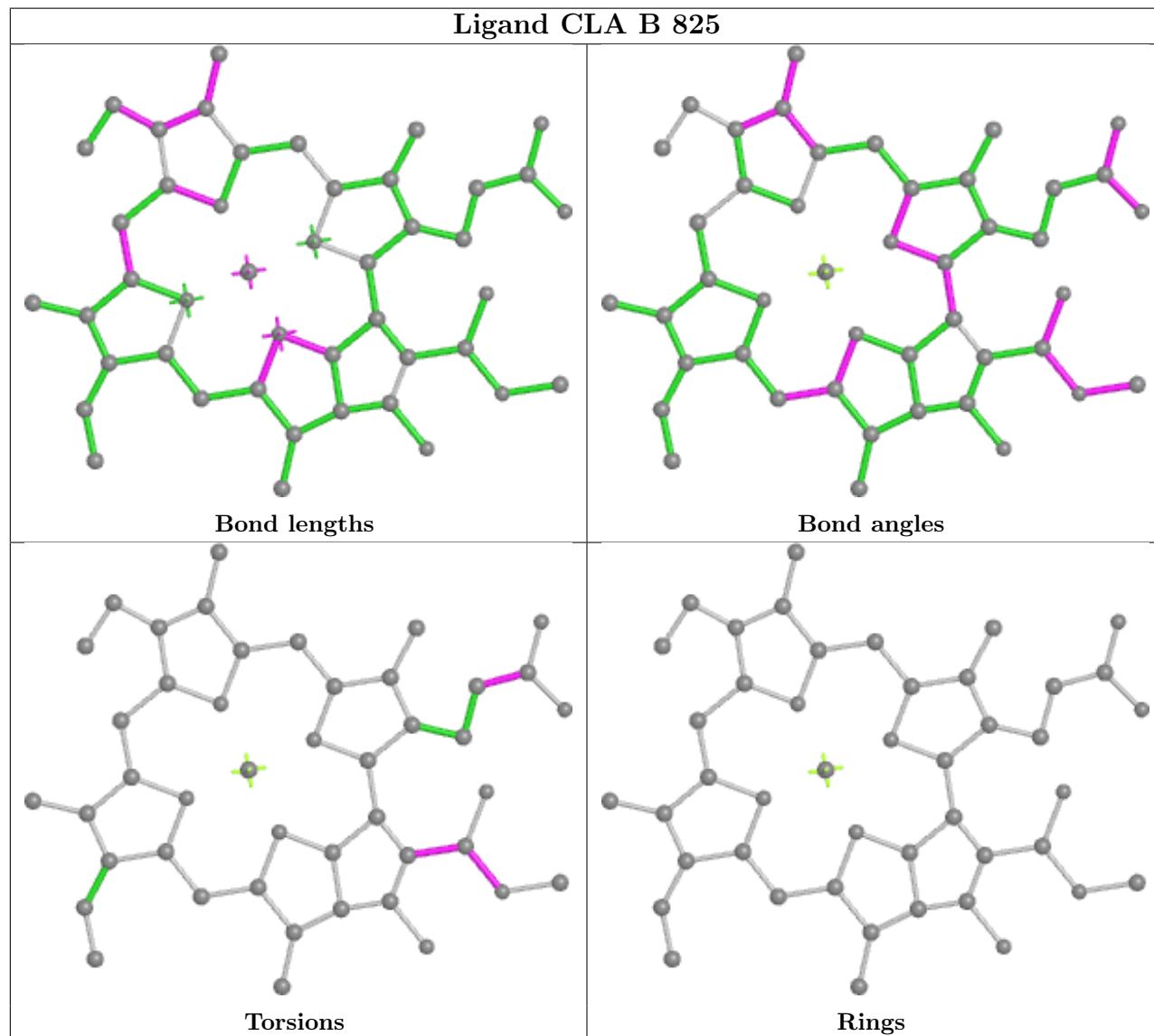
## Ligand CLA A 808

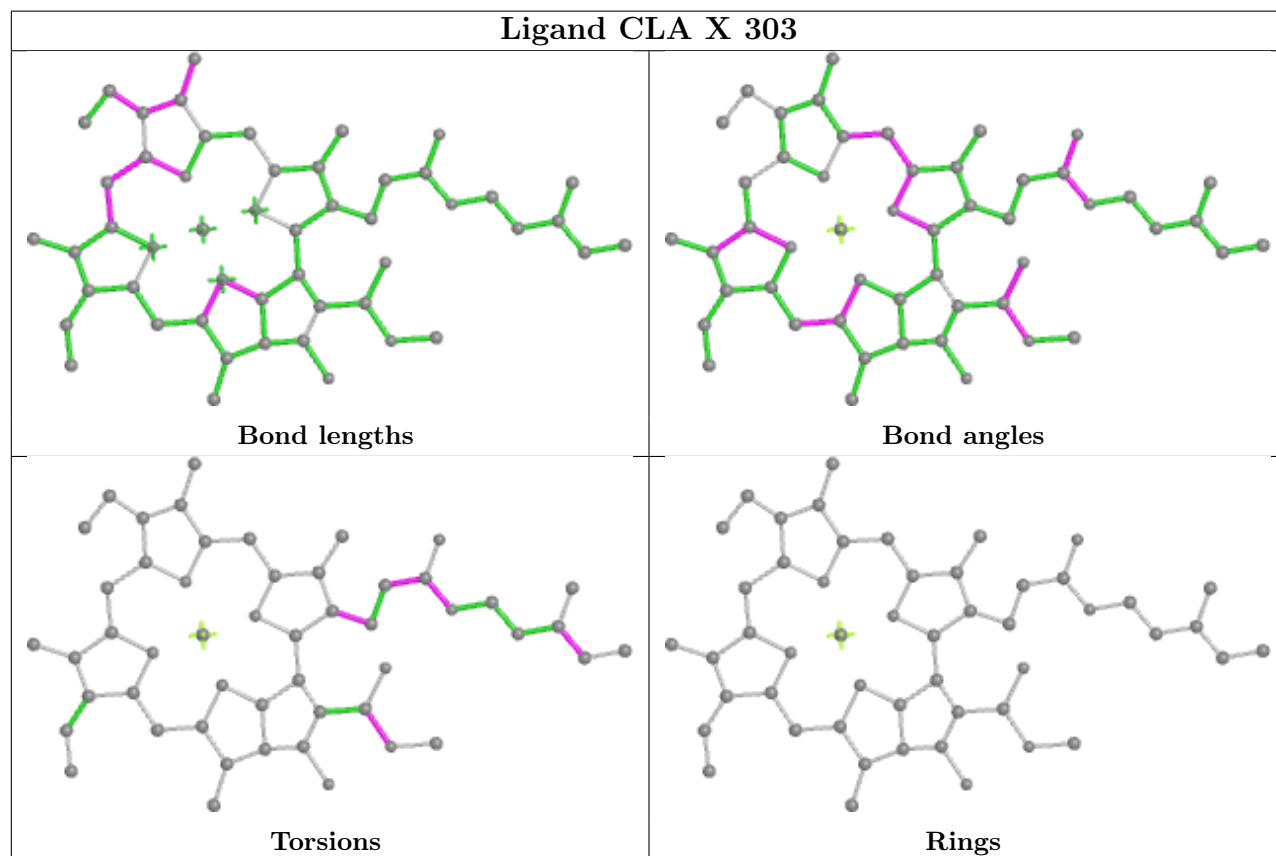
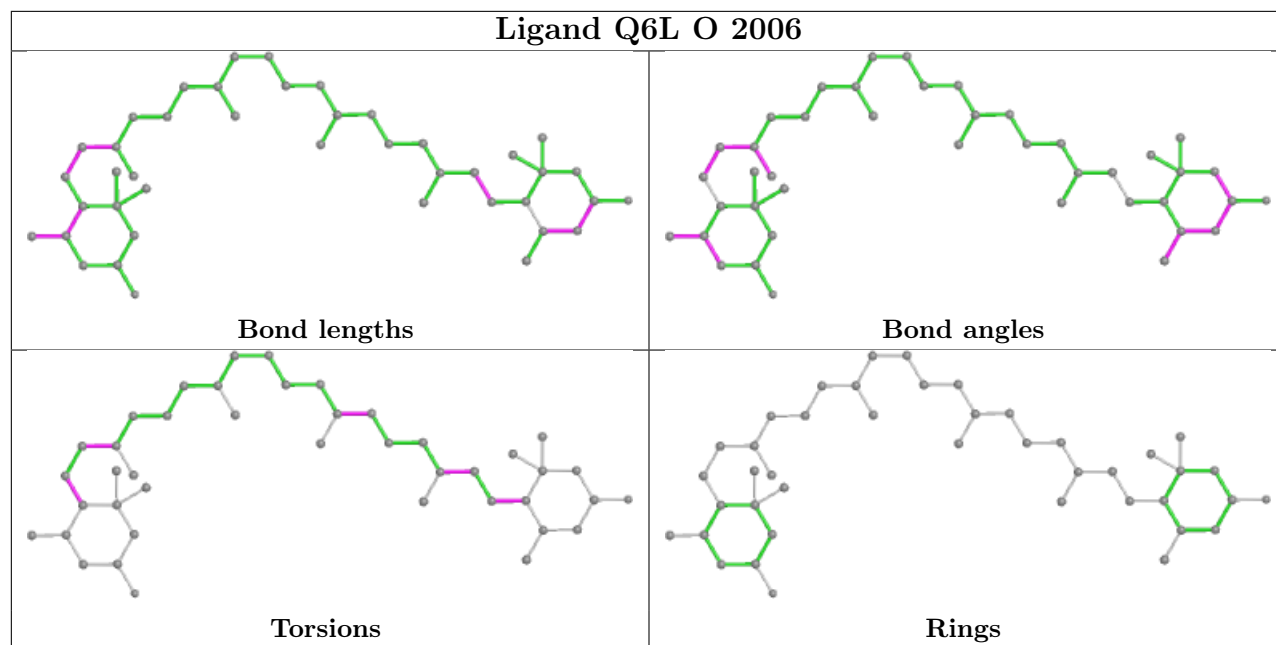


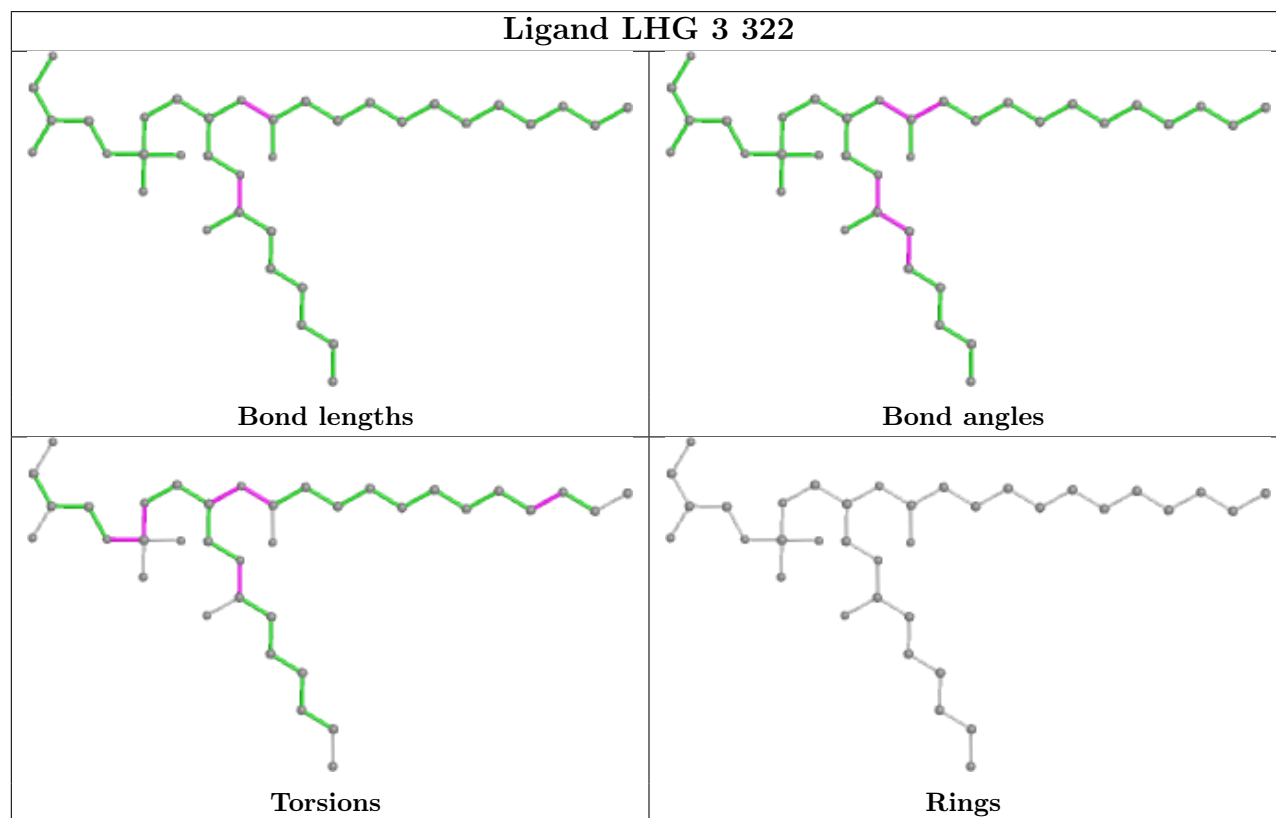
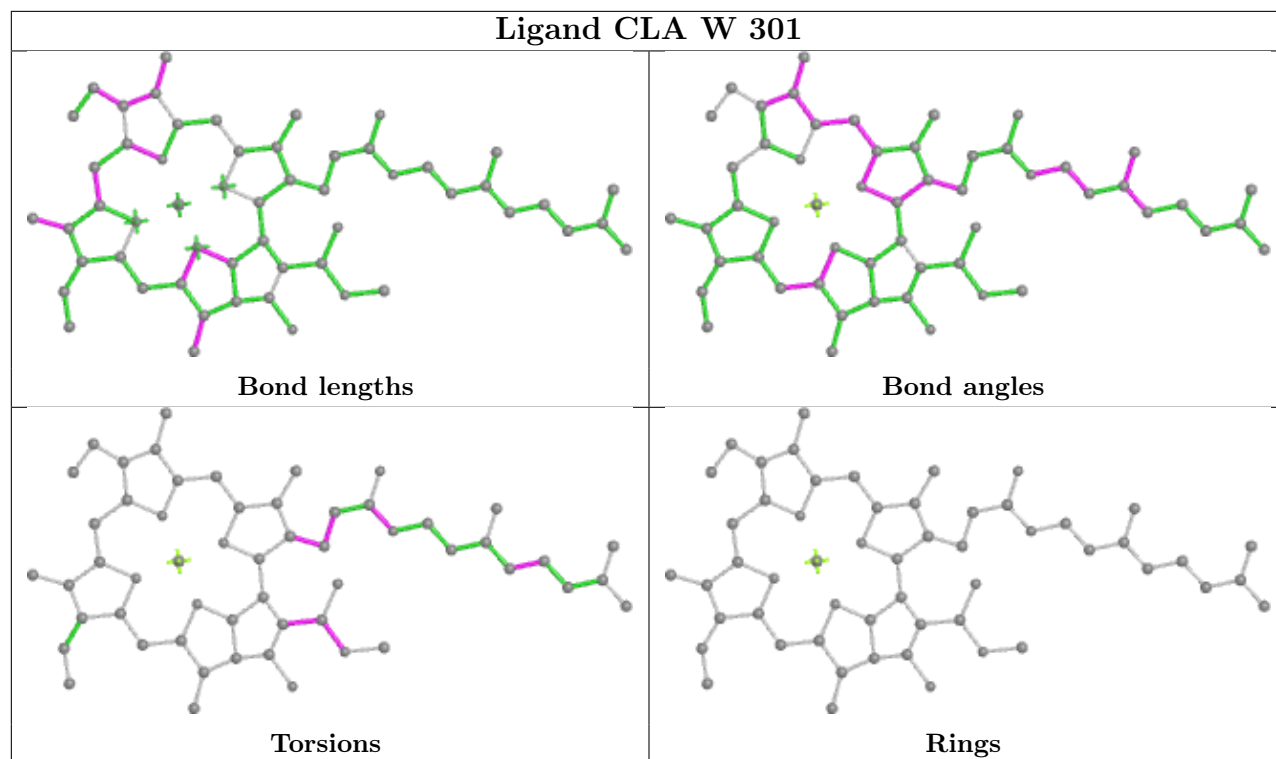
## Ligand Q6L S 320



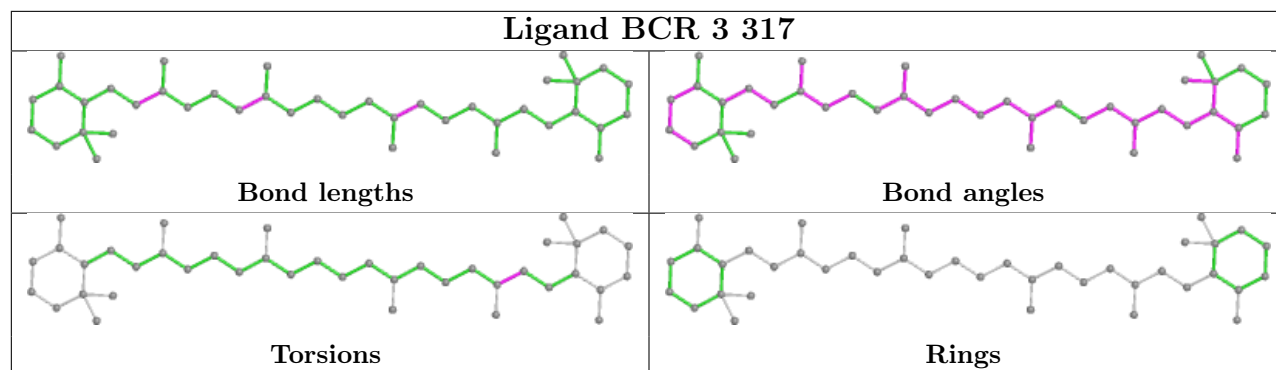
## Ligand CLA B 825



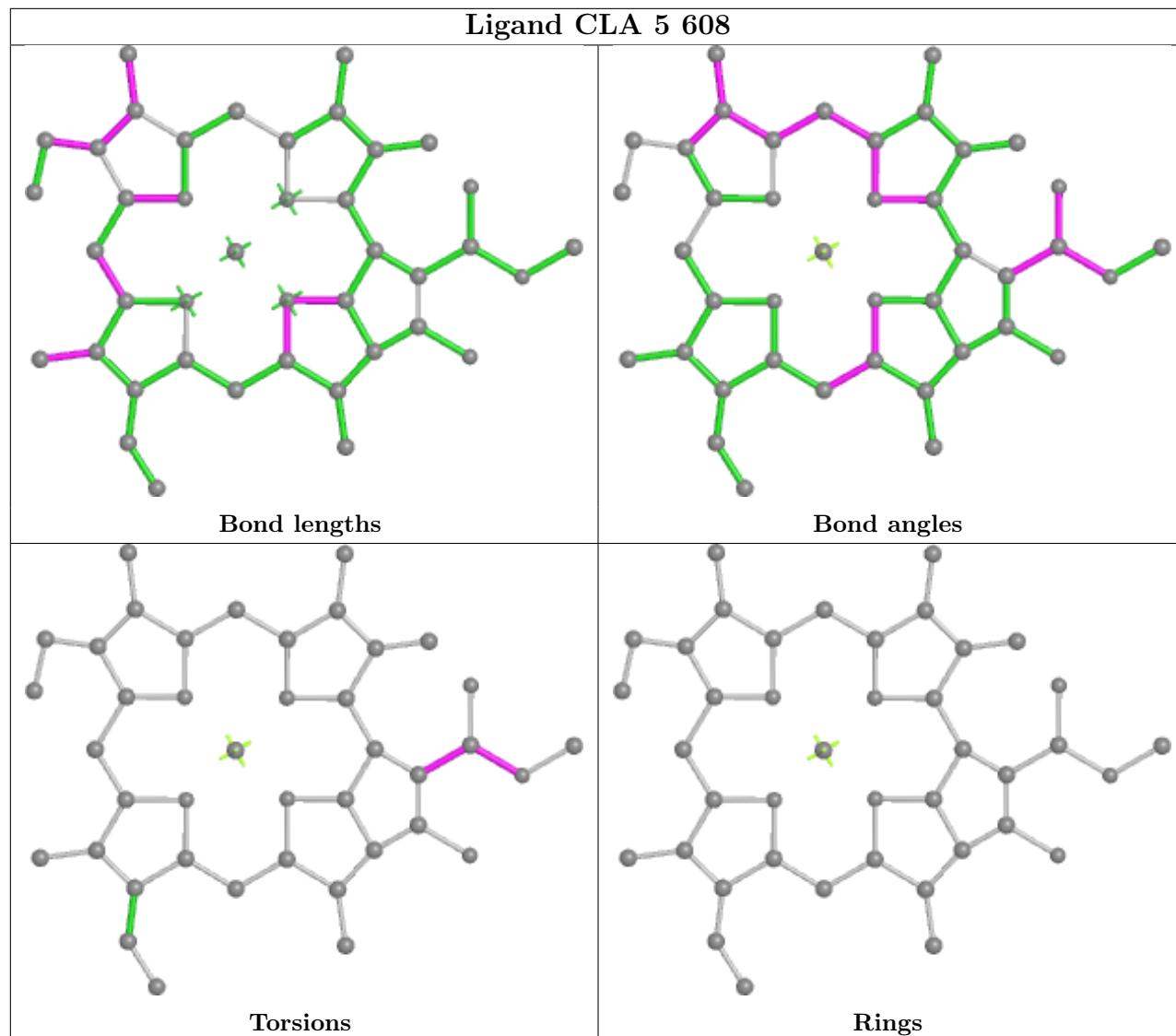


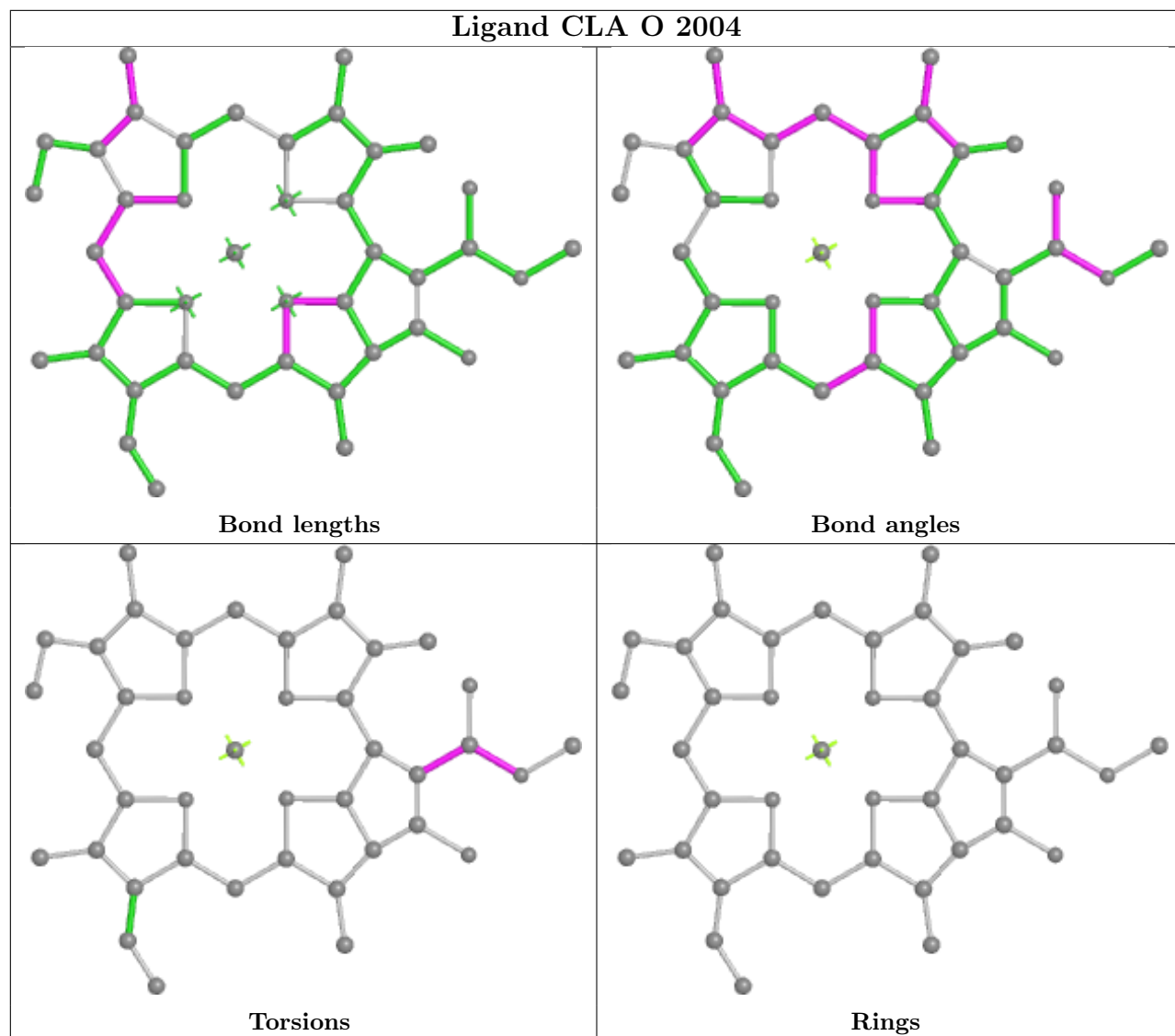


## Ligand BCR 3 317

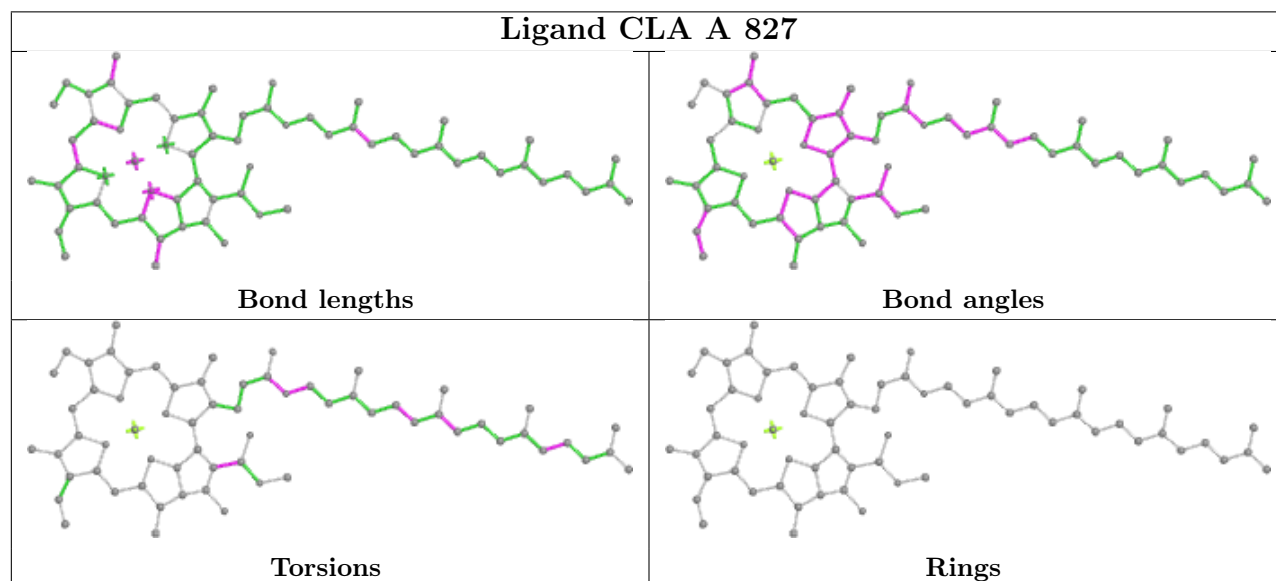
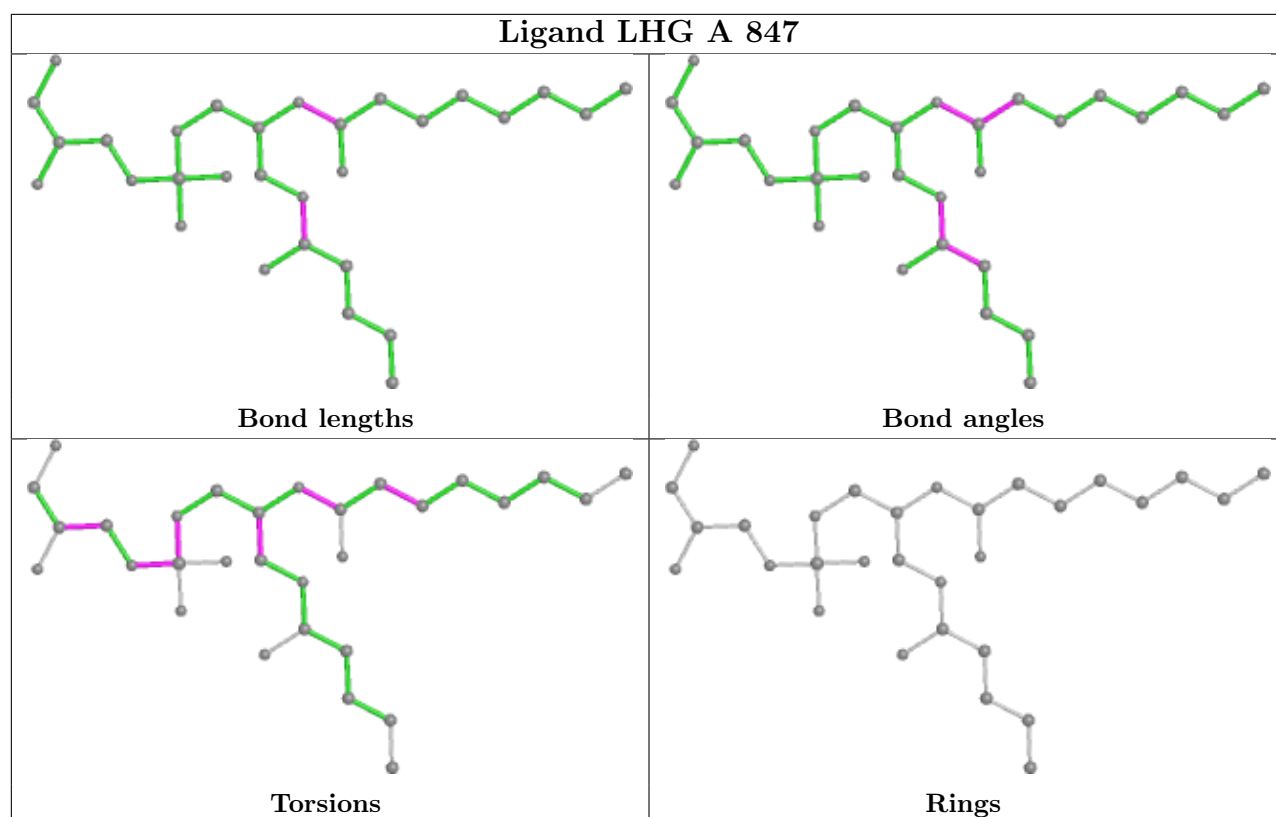


## Ligand CLA 5 608

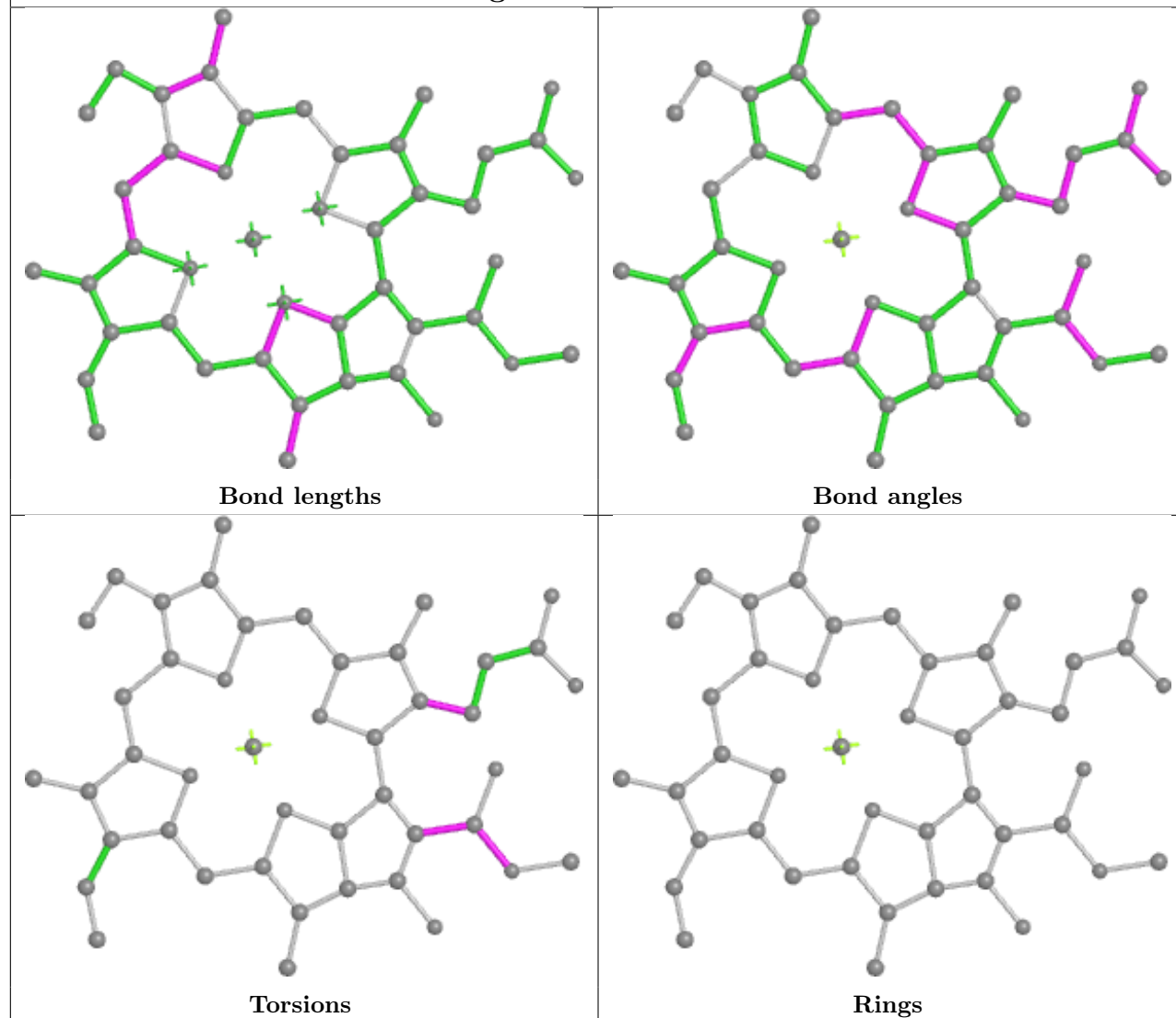




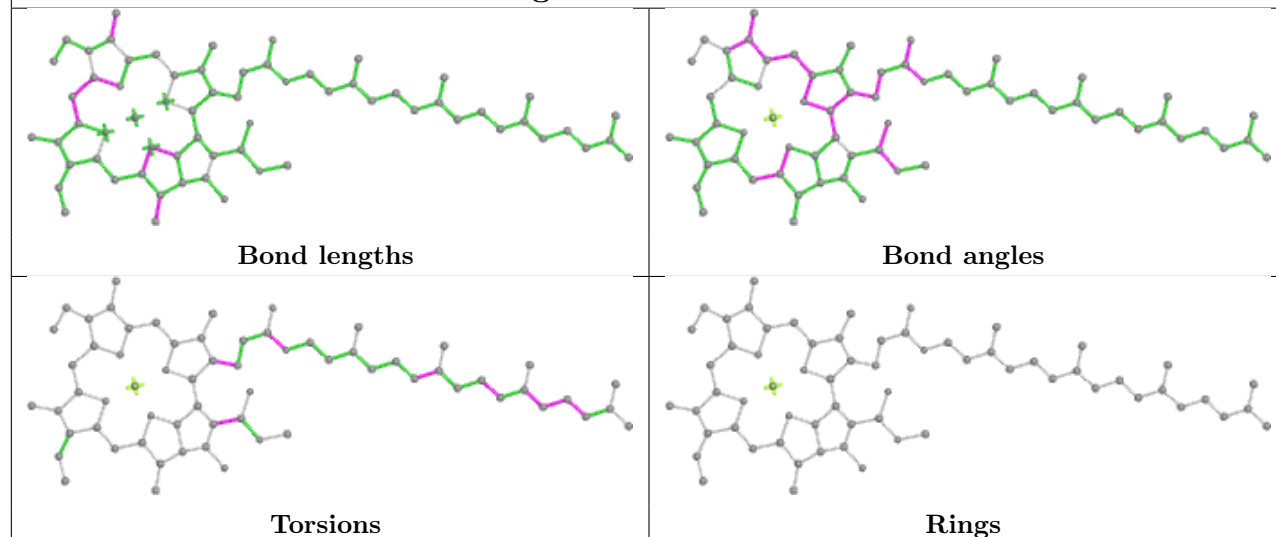




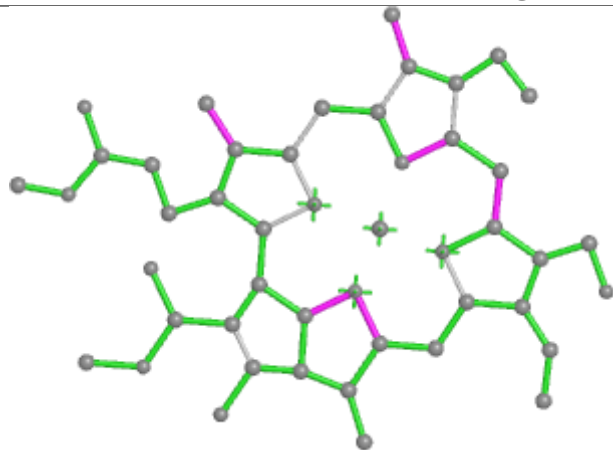
## Ligand CLA G 202



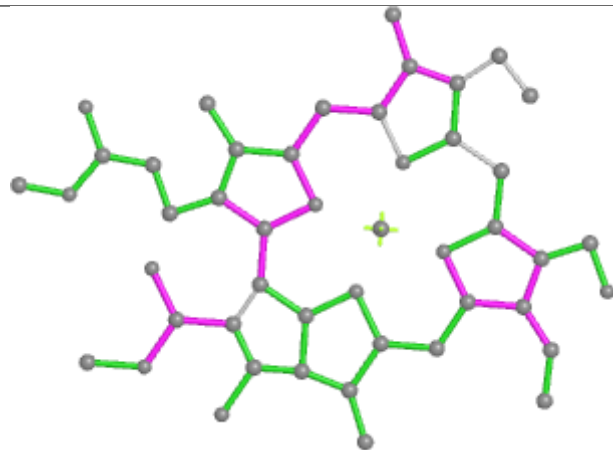
## Ligand CLA B 807



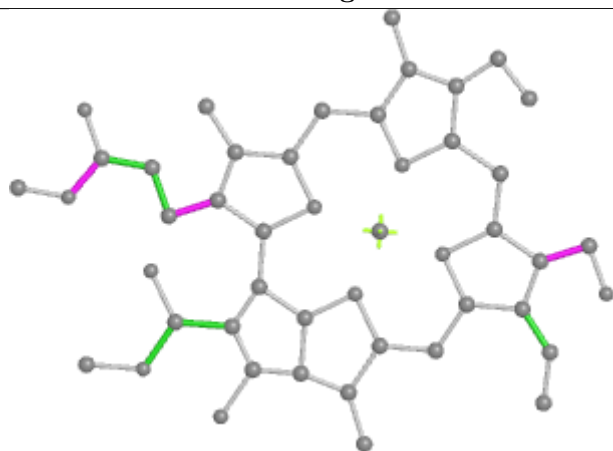
## Ligand CHL R 302



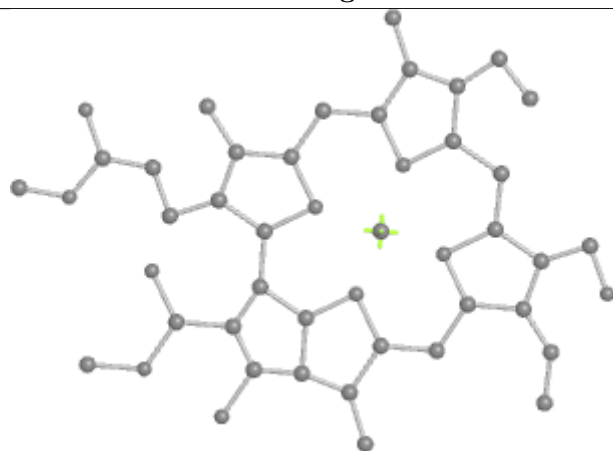
Bond lengths



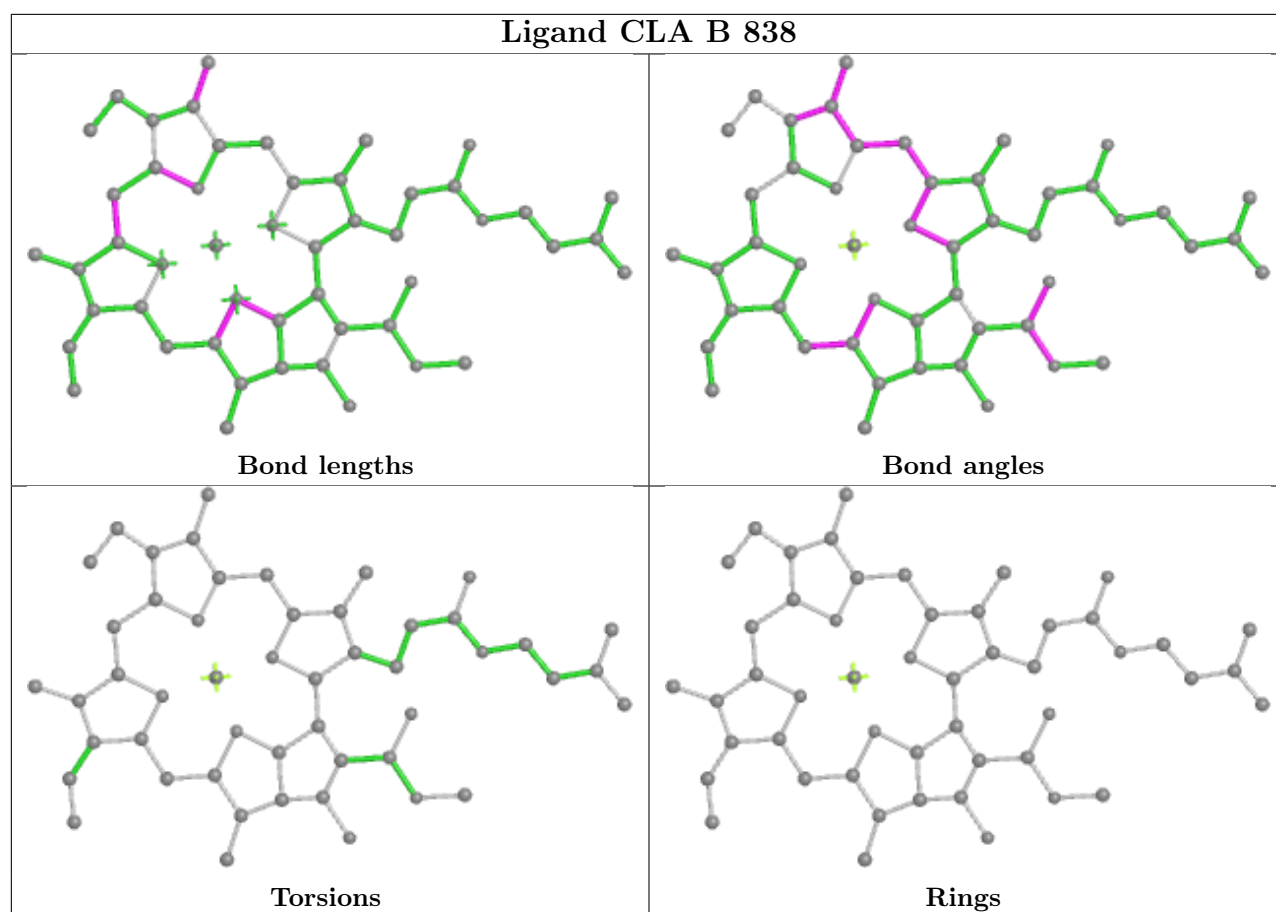
Bond angles



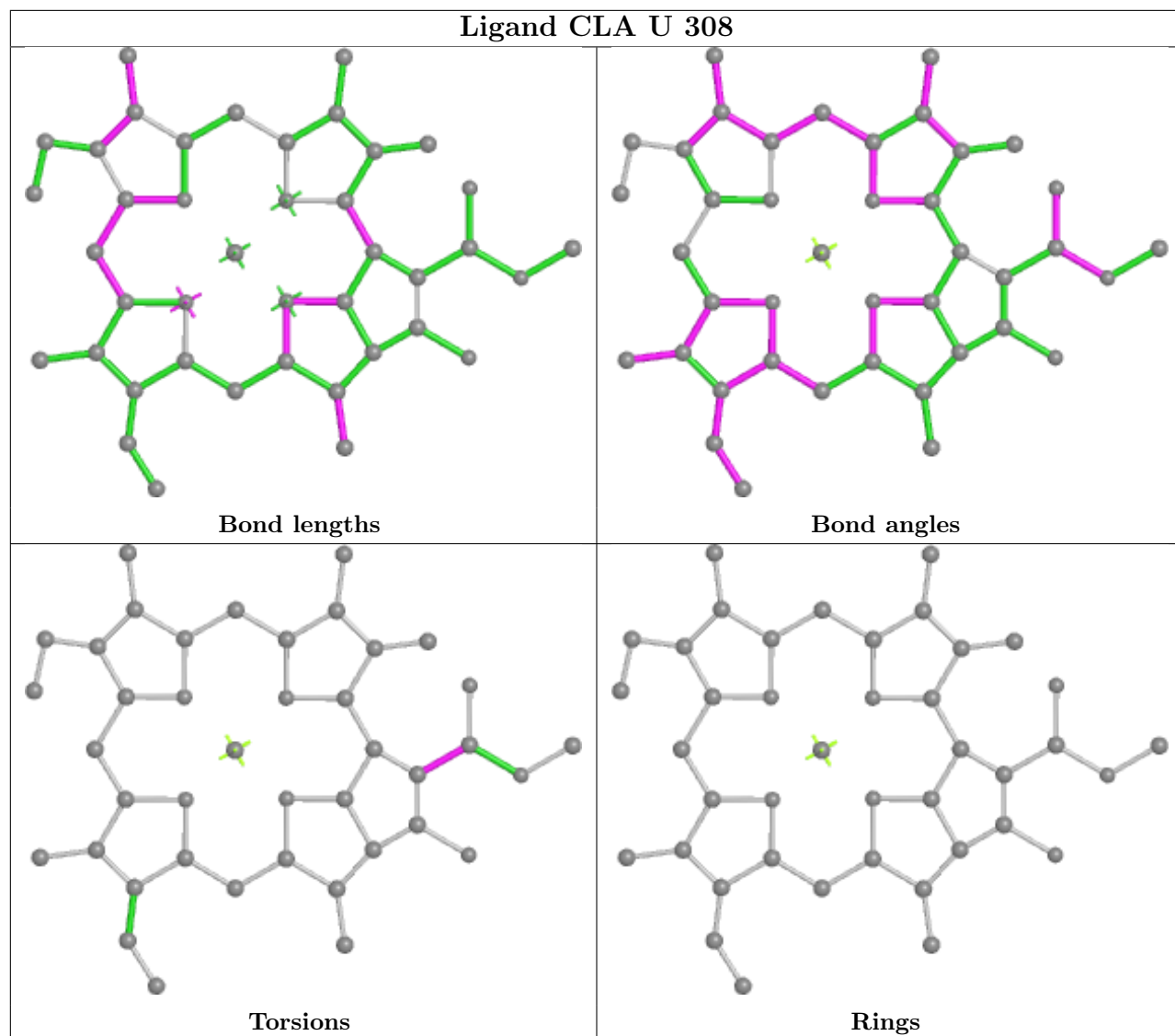
Torsions



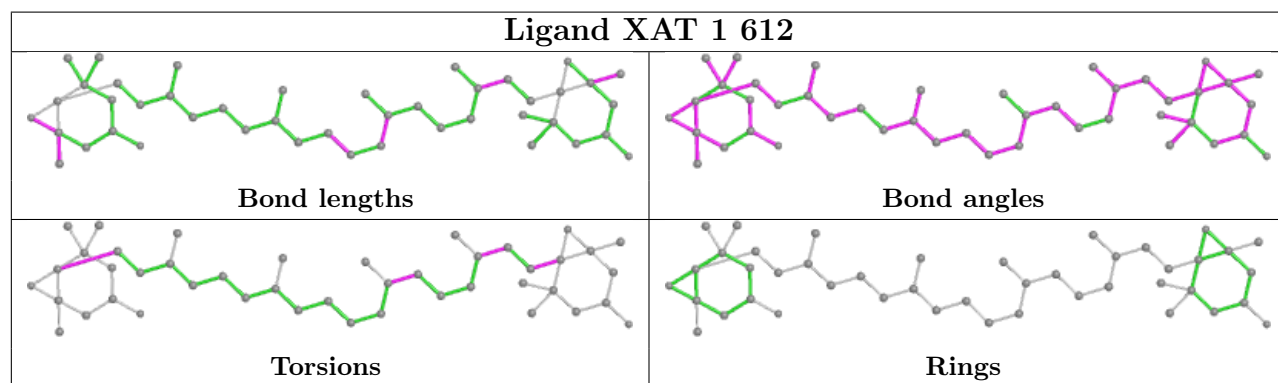
Rings



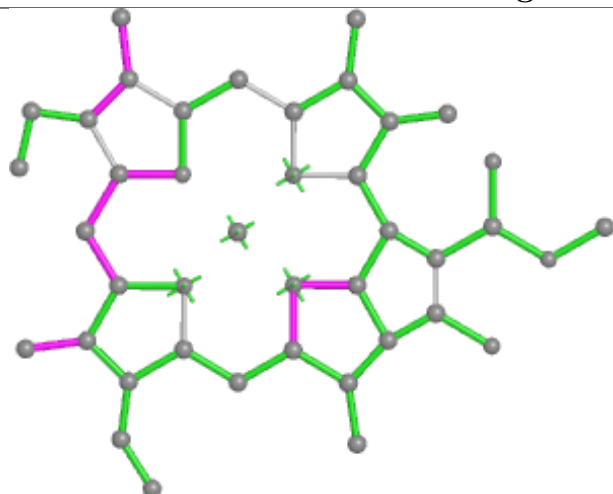
## Ligand CLA U 308



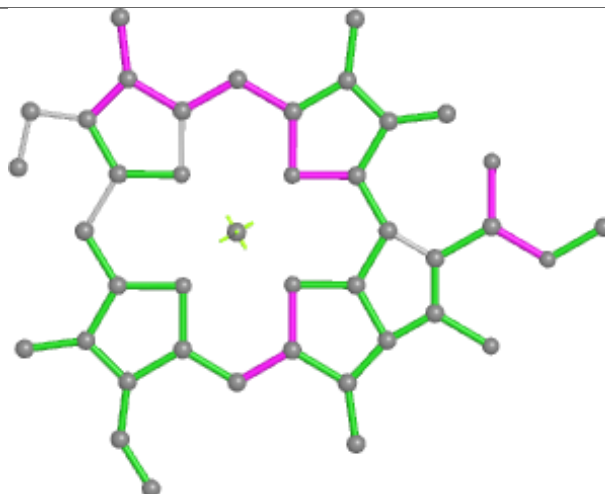
## Ligand XAT 1 612



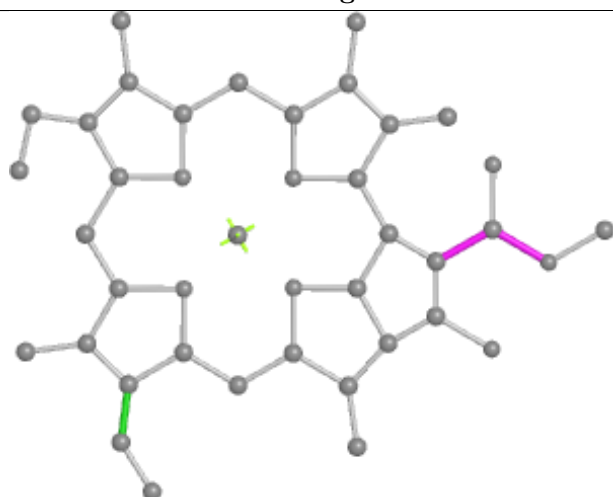
## Ligand CLA L 301



Bond lengths



Bond angles

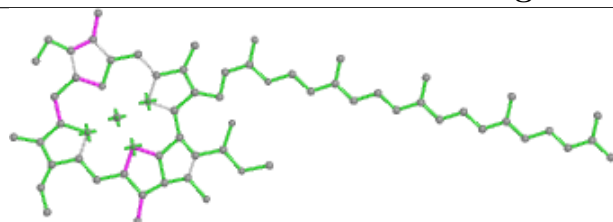


Torsions

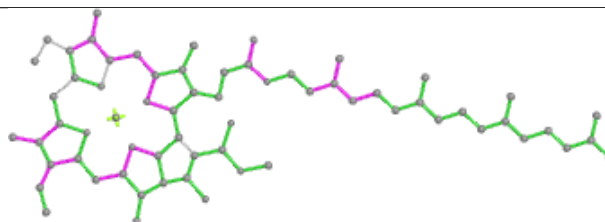


Rings

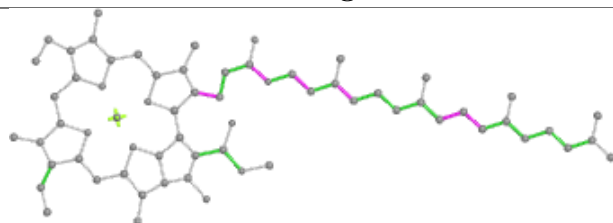
## Ligand CLA P 301



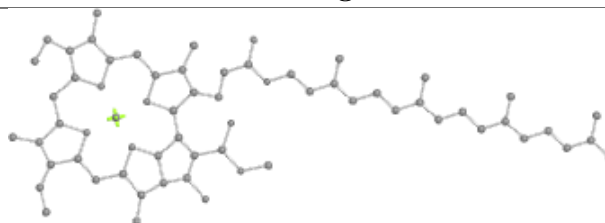
Bond lengths



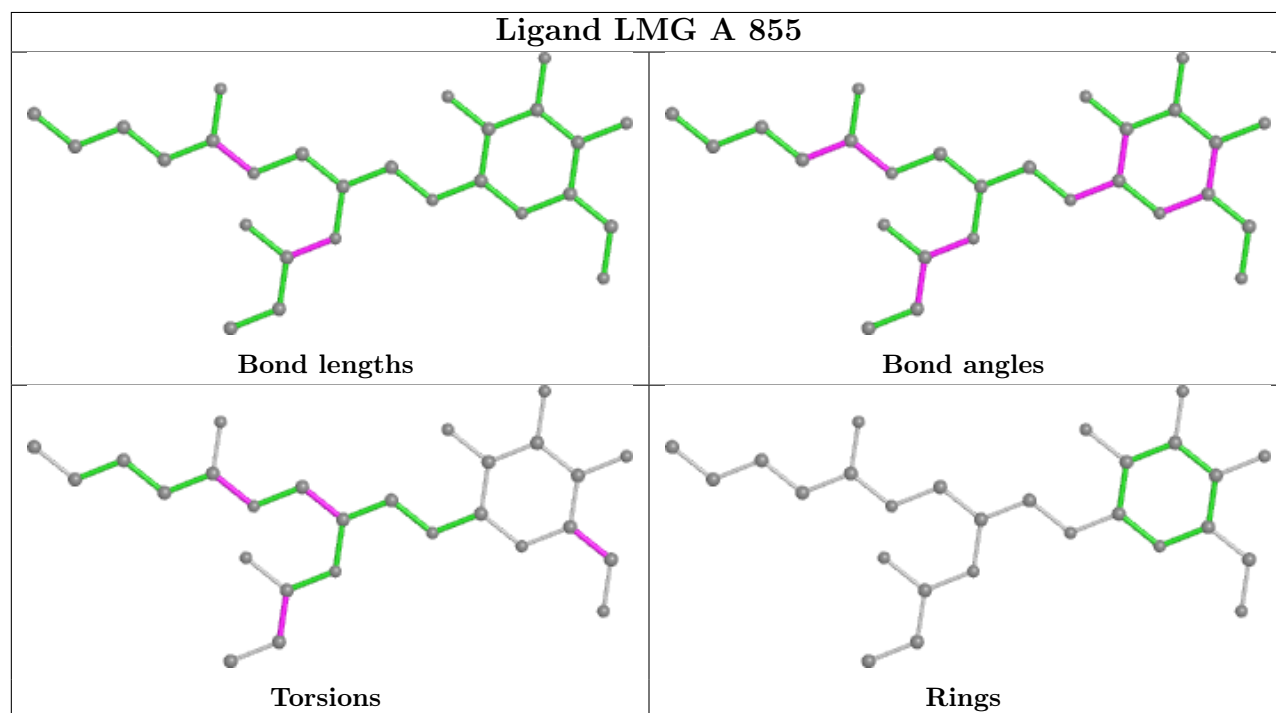
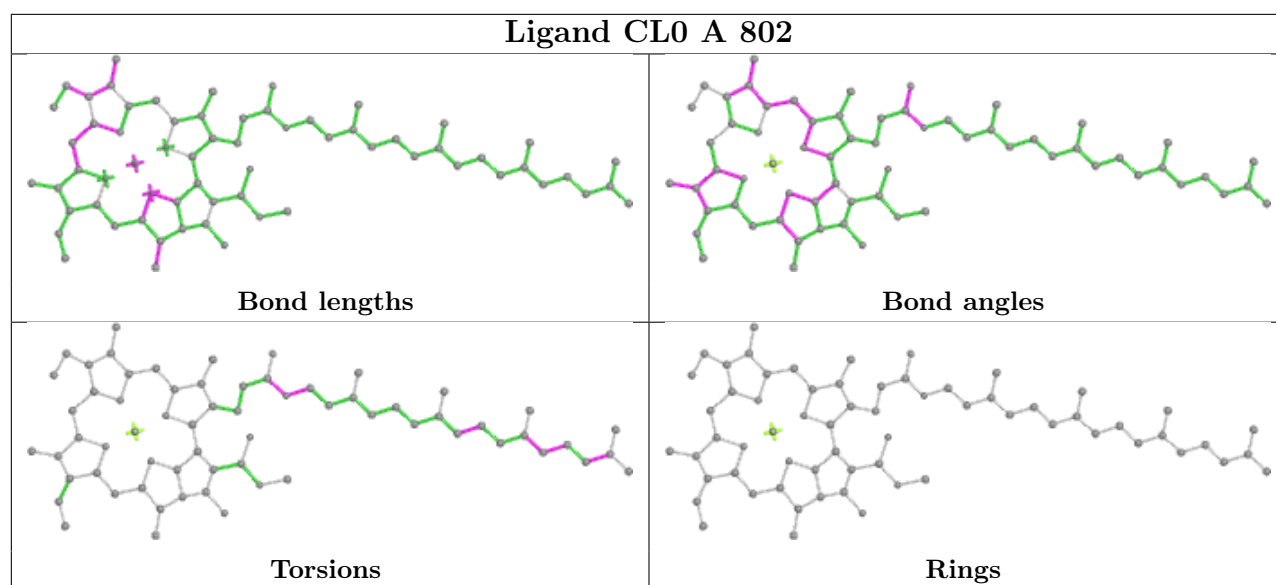
Bond angles



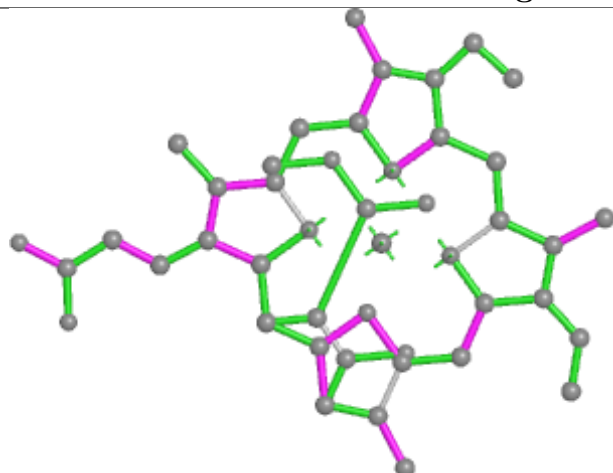
Torsions



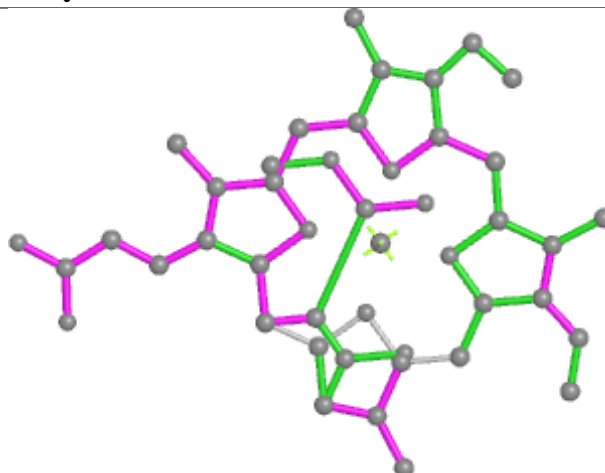
Rings



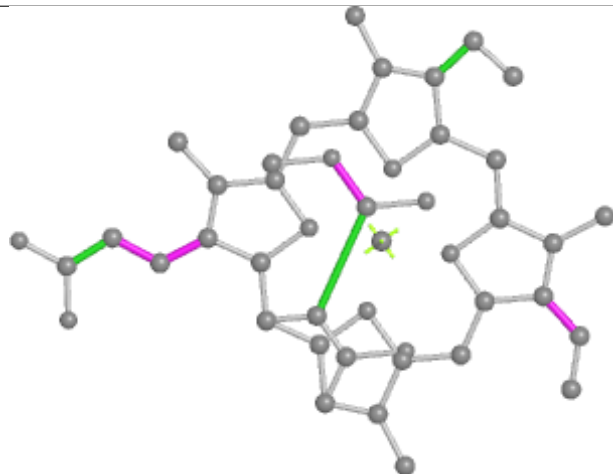
## Ligand KC2 Q 310



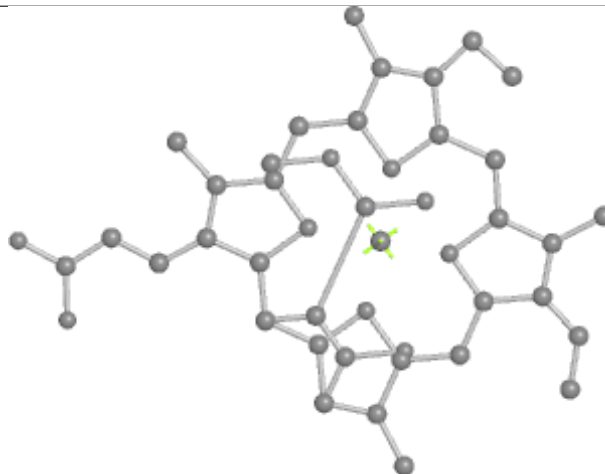
Bond lengths



Bond angles

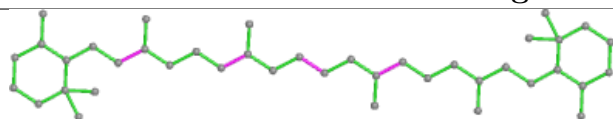


Torsions

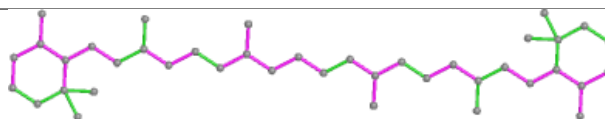


Rings

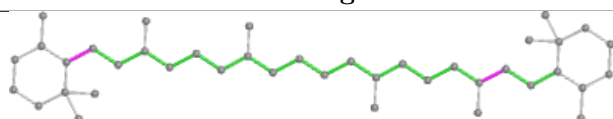
## Ligand BCR K 205



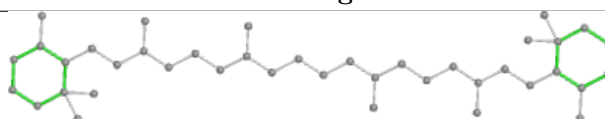
Bond lengths



Bond angles



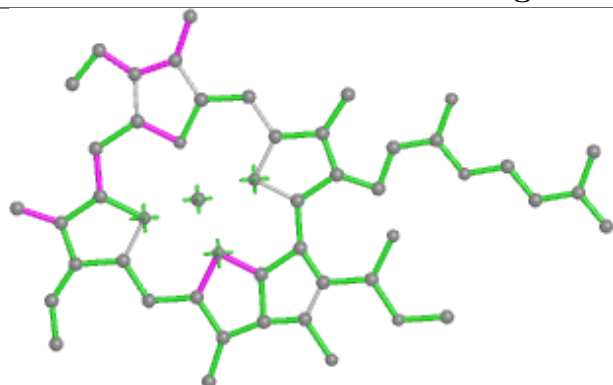
Torsions



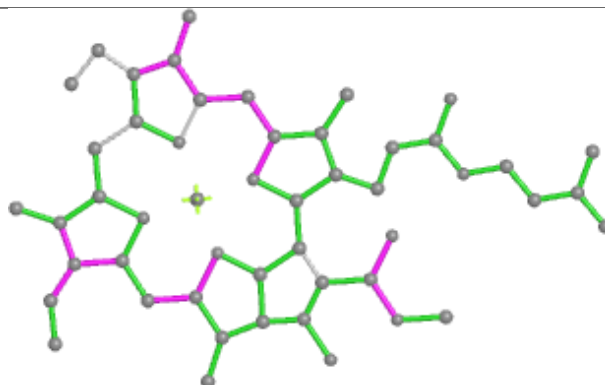
Rings



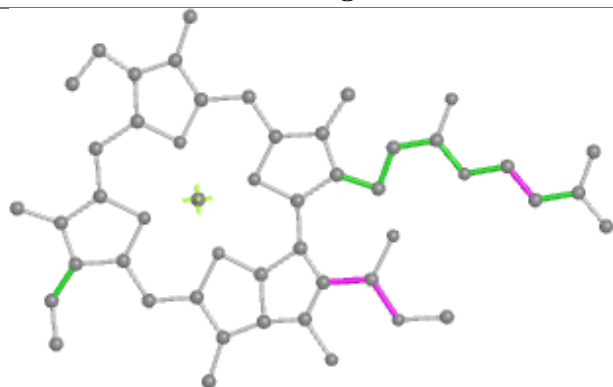
## Ligand CLA V 303



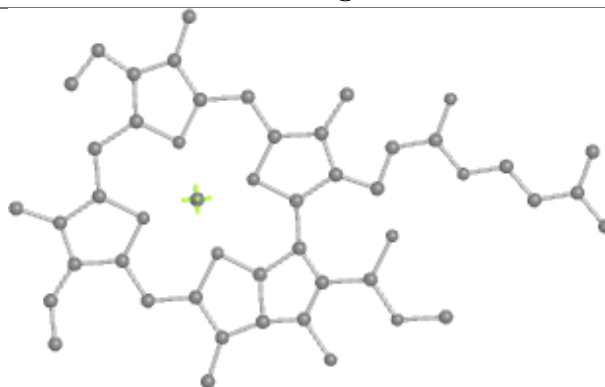
Bond lengths



Bond angles

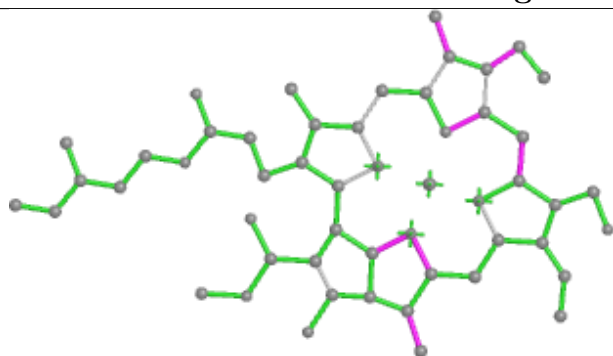


Torsions

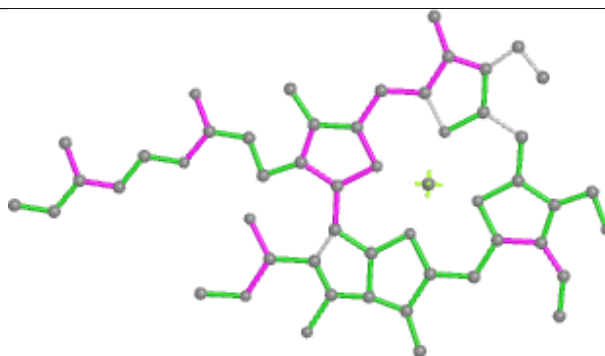


Rings

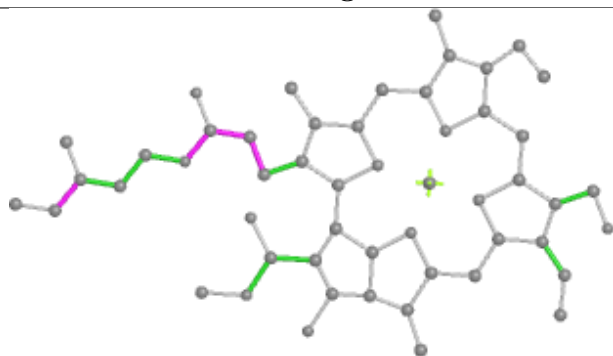
## Ligand CHL T 306



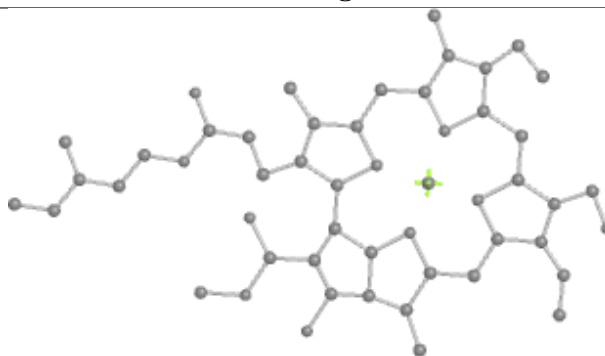
Bond lengths



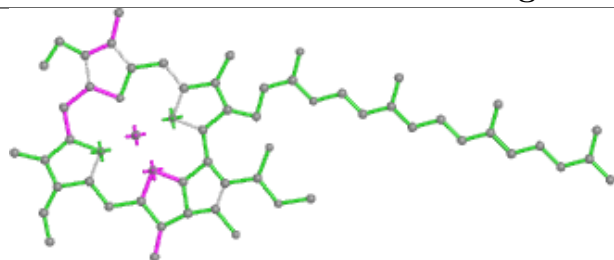
Bond angles



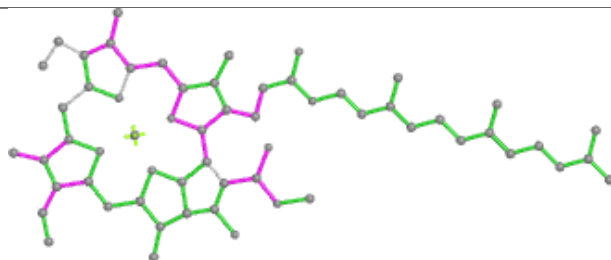
Torsions



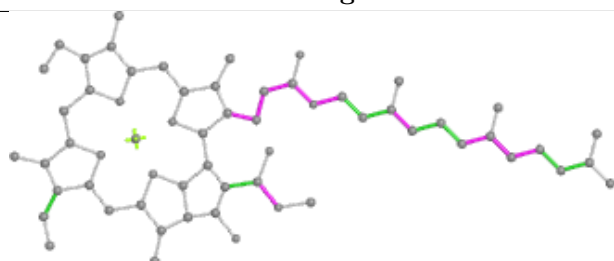
Rings

**Ligand CLA 4 303**

Bond lengths



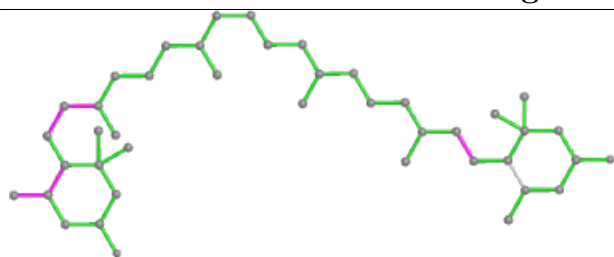
Bond angles



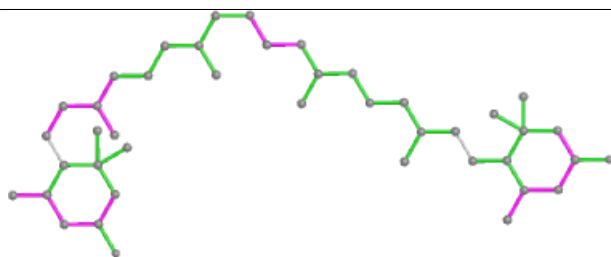
Torsions



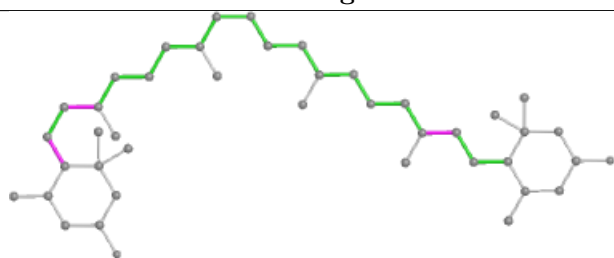
Rings

**Ligand Q6L S 315**

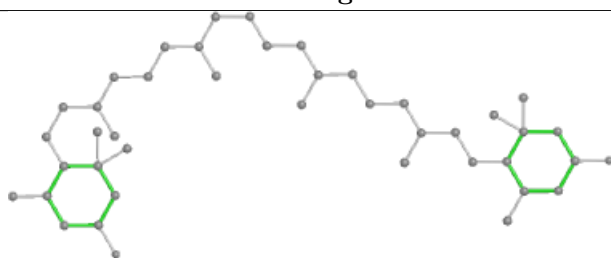
Bond lengths



Bond angles

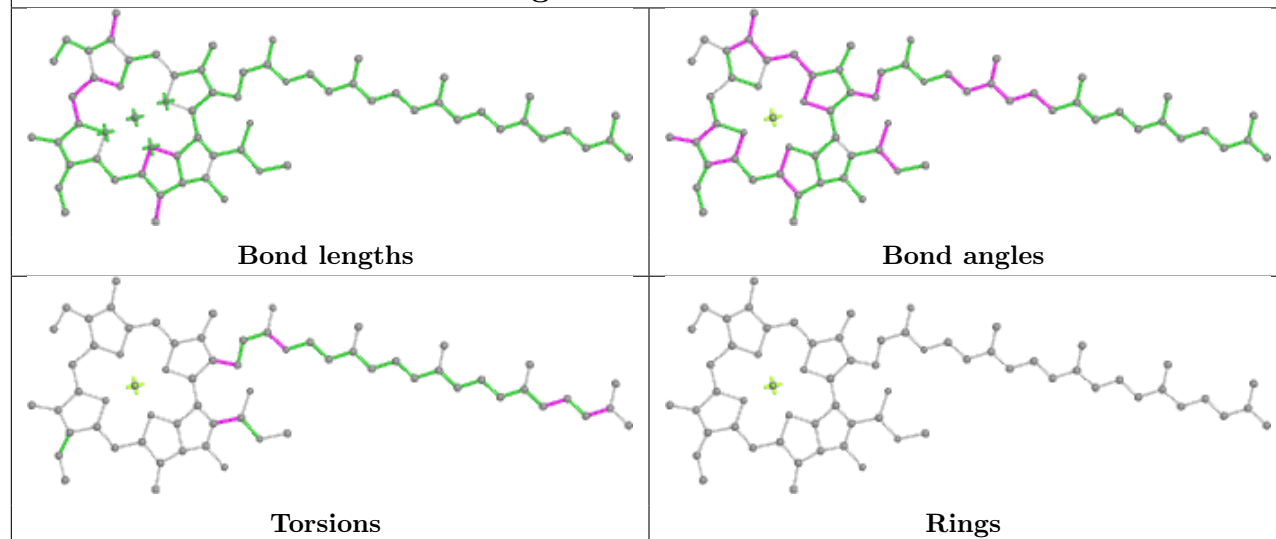


Torsions

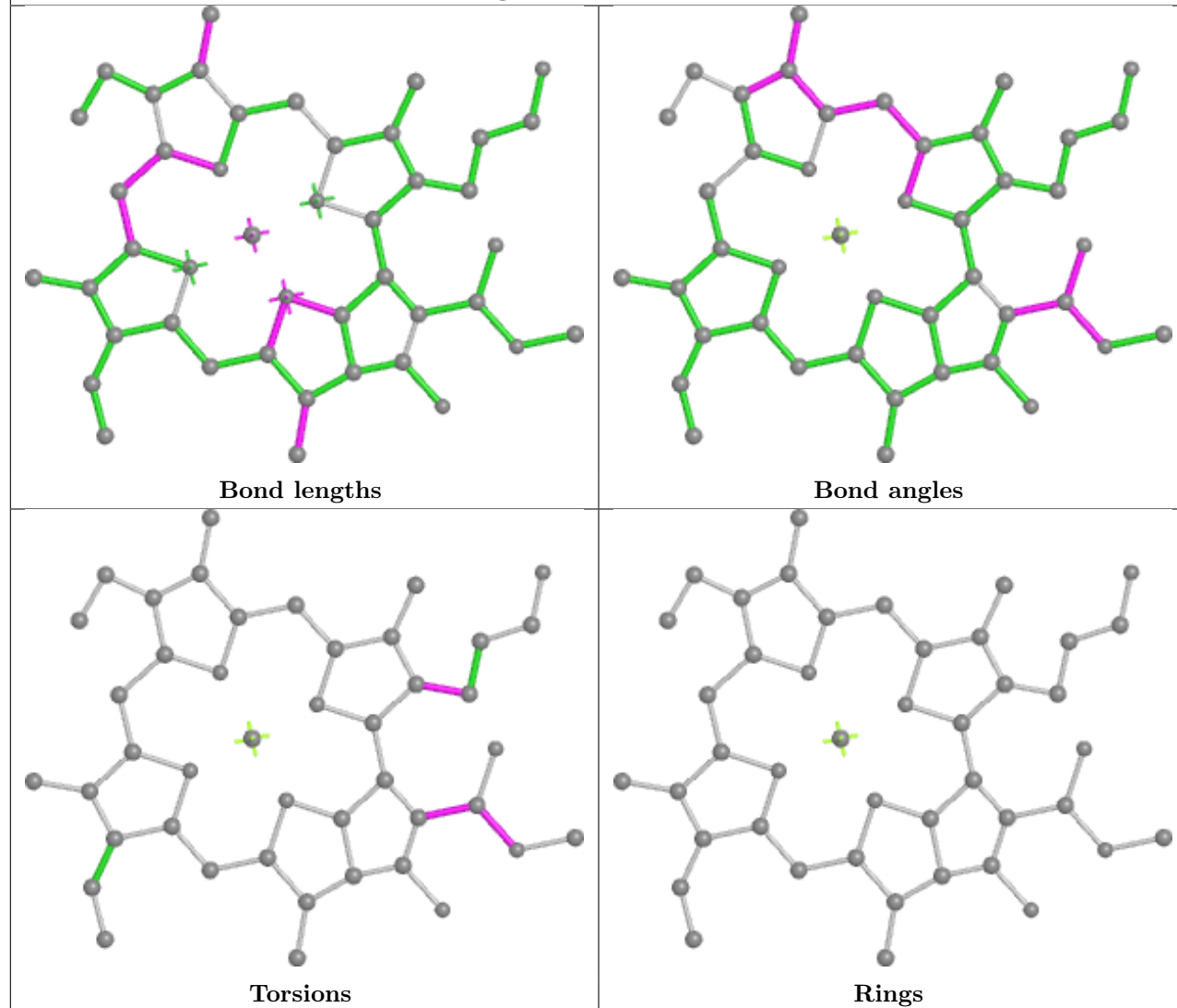


Rings

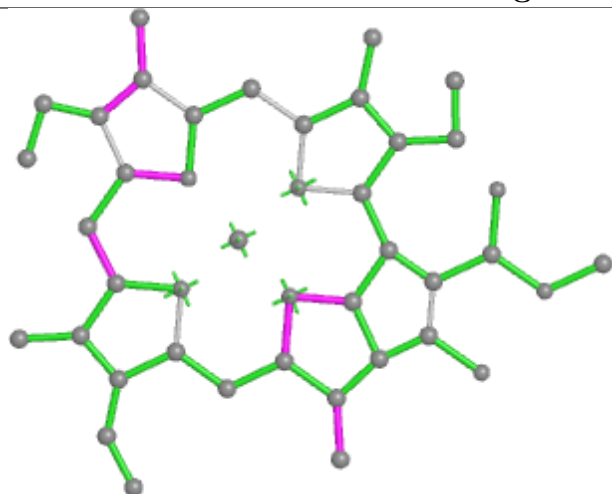
## Ligand CLA A 843



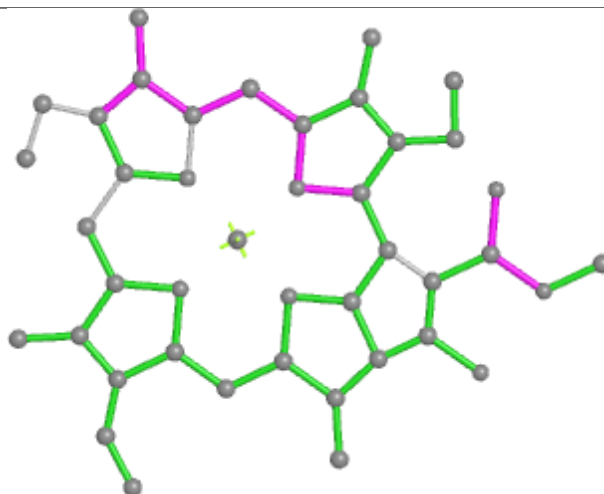
## Ligand CLA 2 614



## Ligand CLA T 310



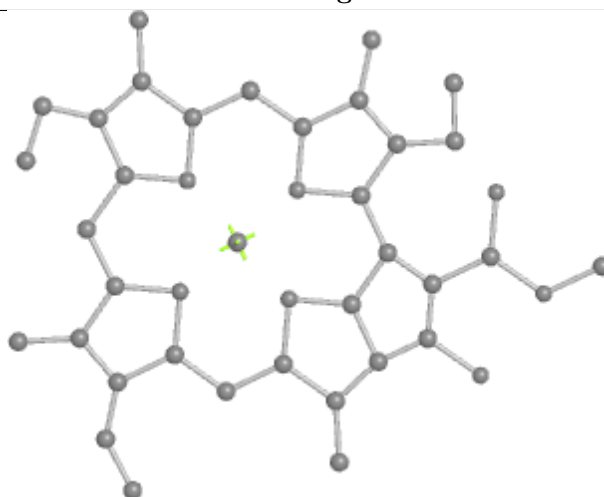
Bond lengths



Bond angles

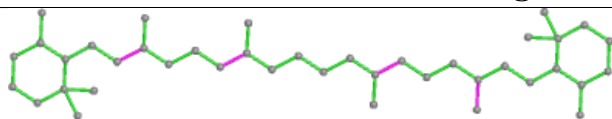


Torsions

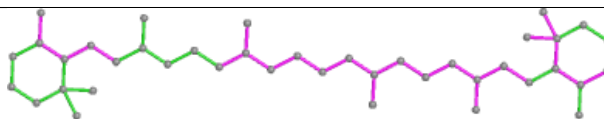


Rings

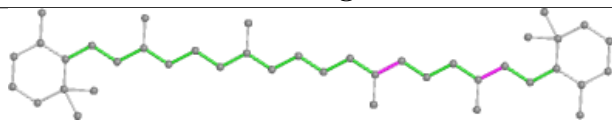
## Ligand BCR F 801



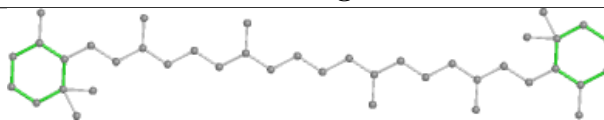
Bond lengths



Bond angles

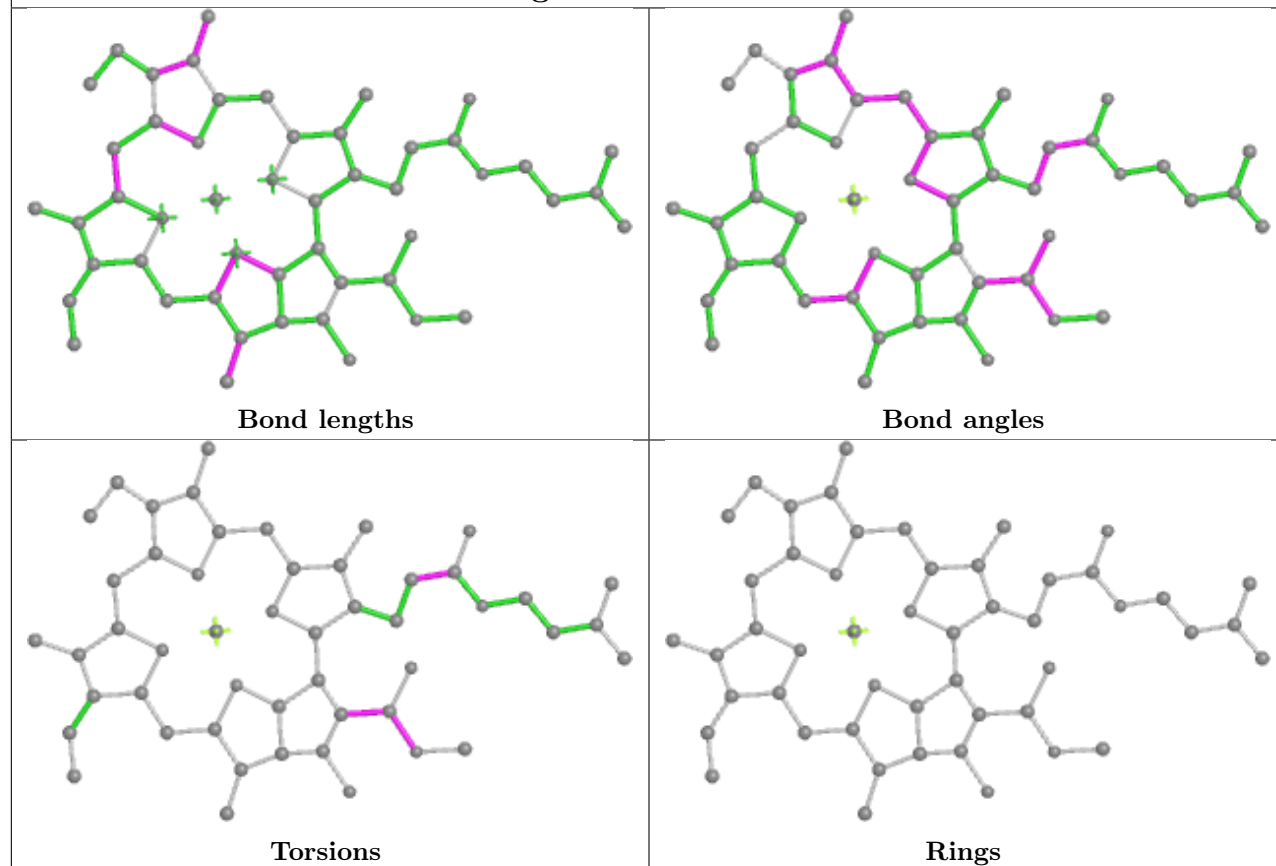


Torsions

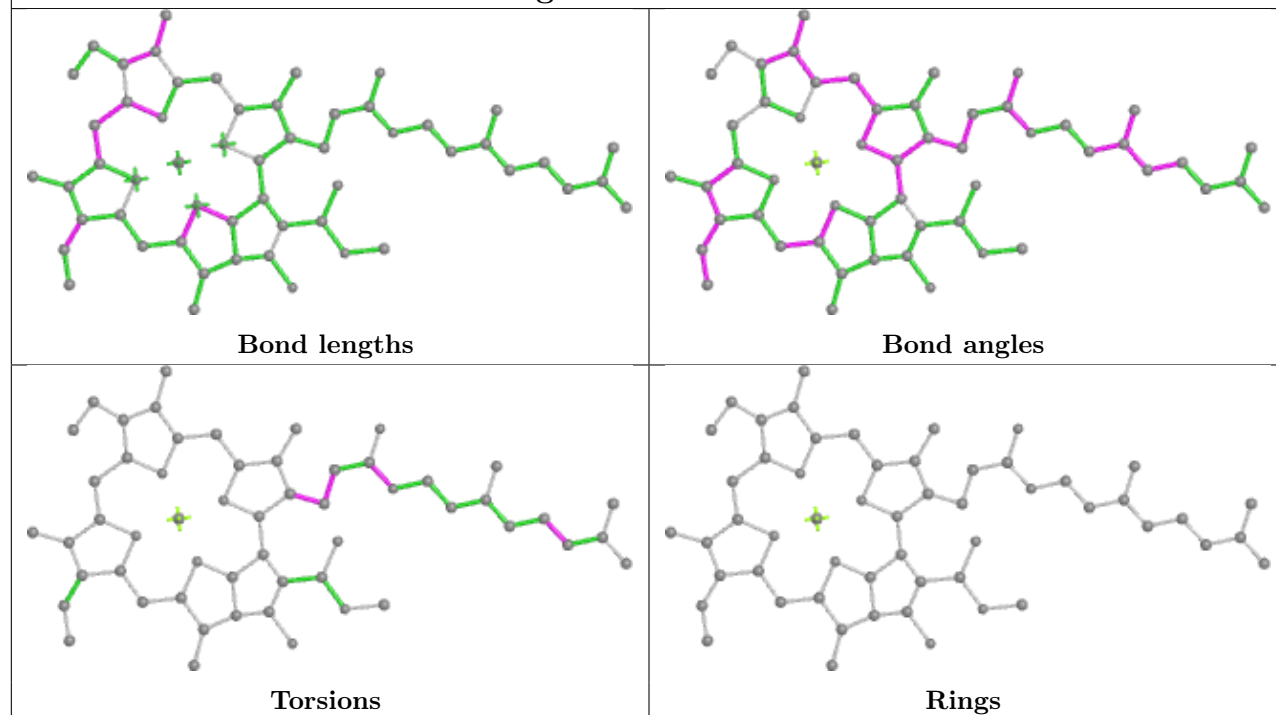


Rings

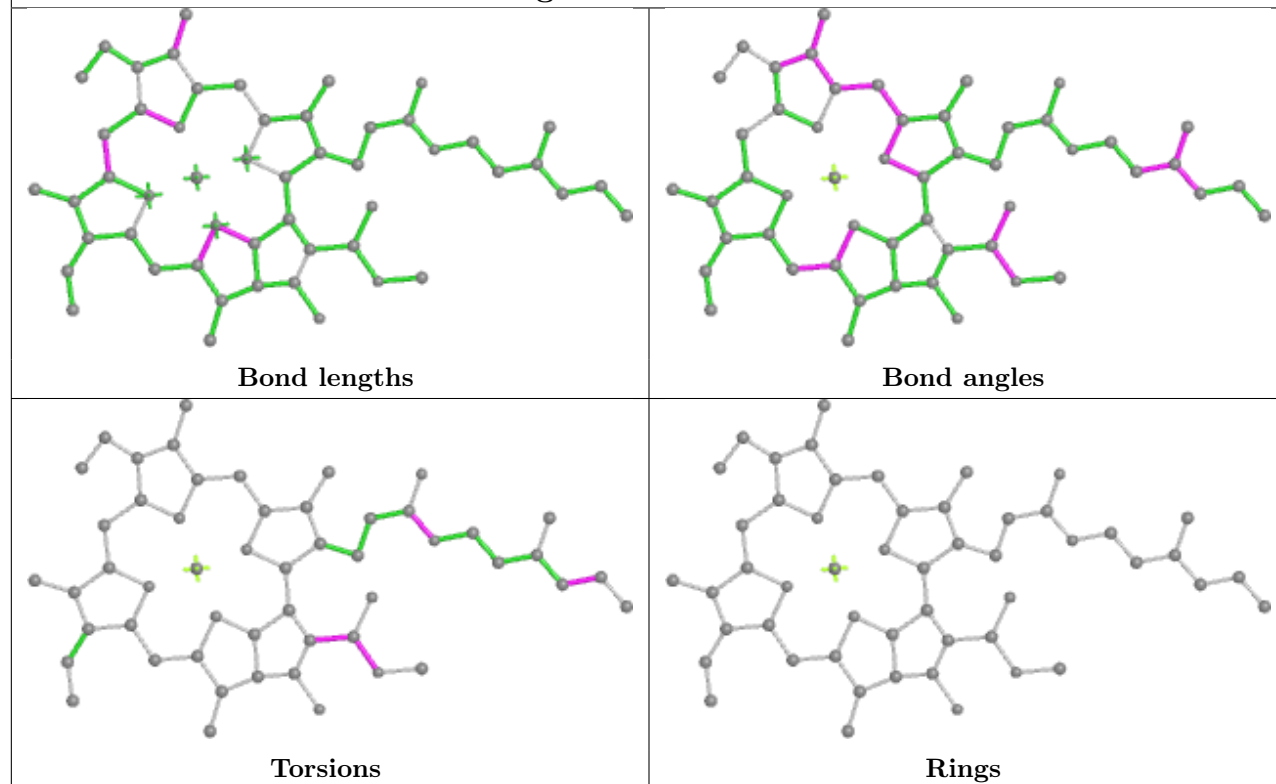
## Ligand CLA A 841



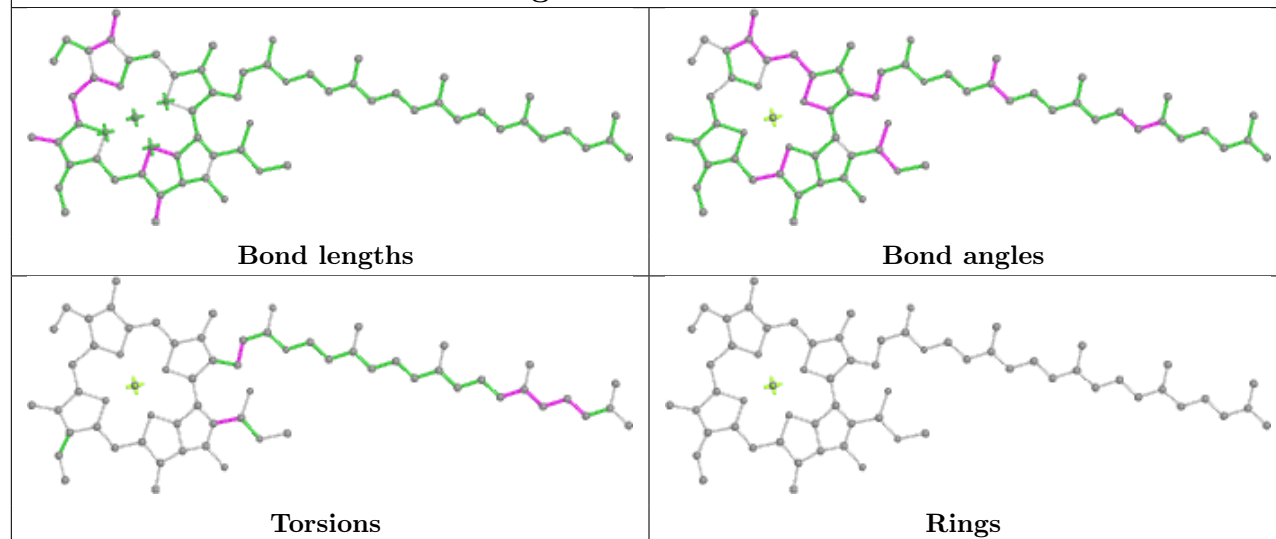
## Ligand CLA 1 603



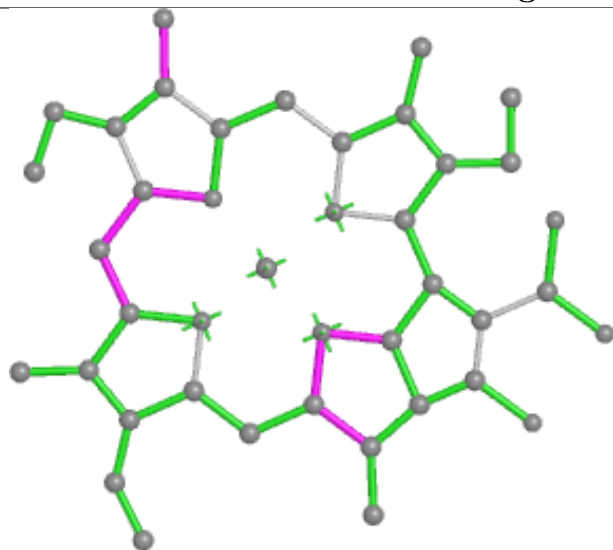
## Ligand CLA 1 613



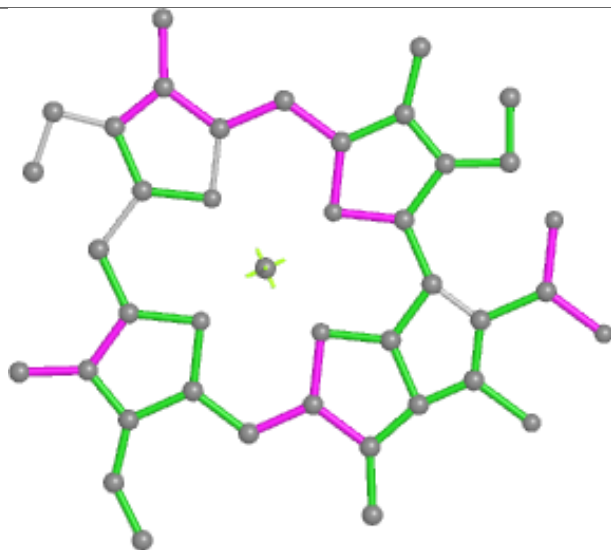
## Ligand CLA A 810



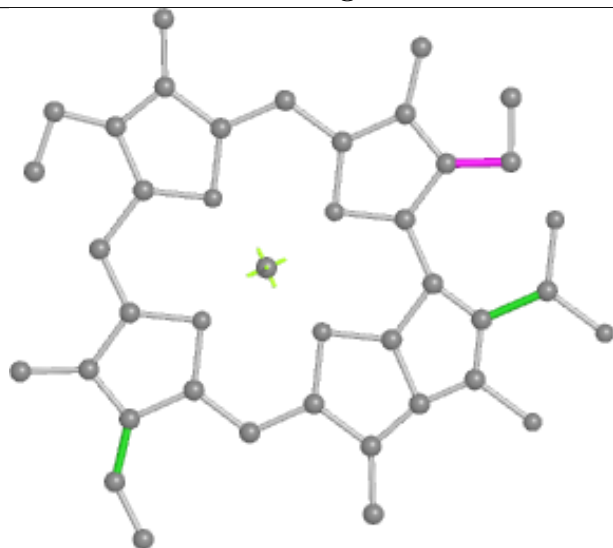
## Ligand CLA 3 304



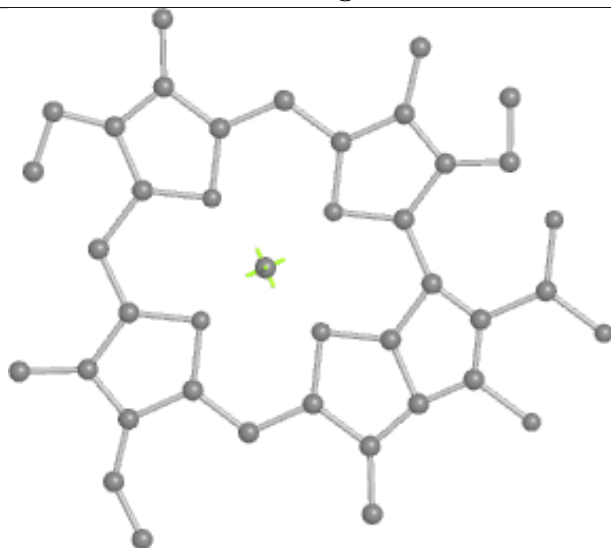
Bond lengths



Bond angles

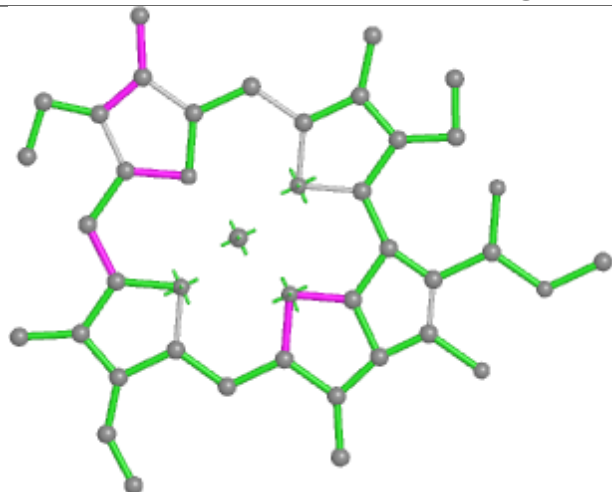


Torsions

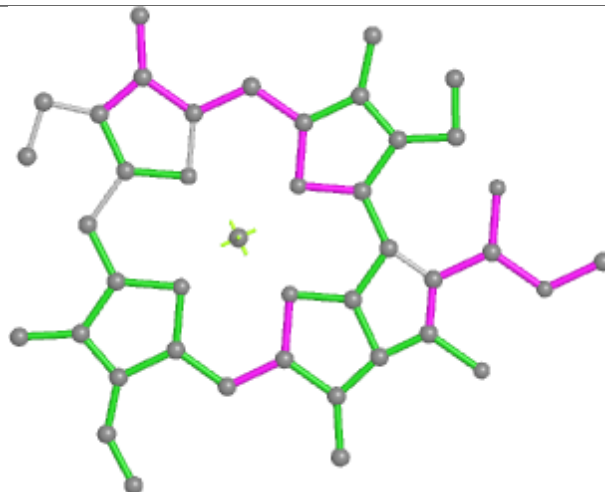


Rings

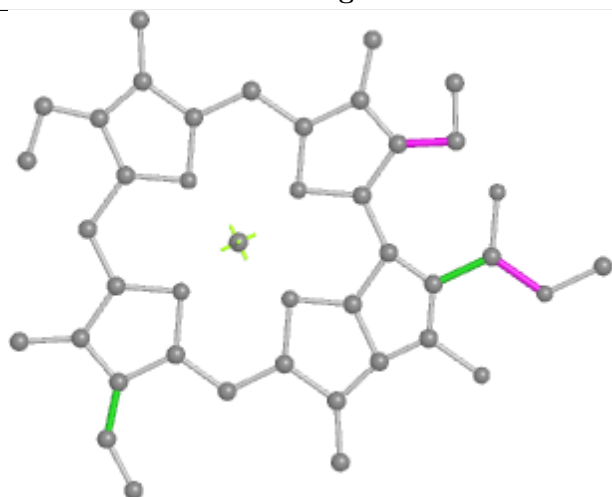
## Ligand CLA 4 316



Bond lengths



Bond angles



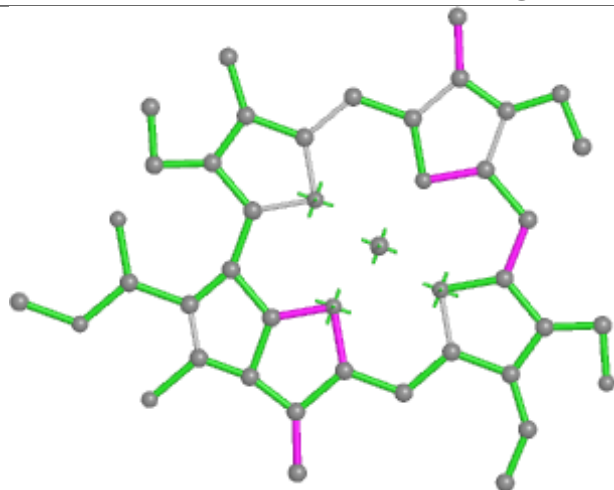
Torsions



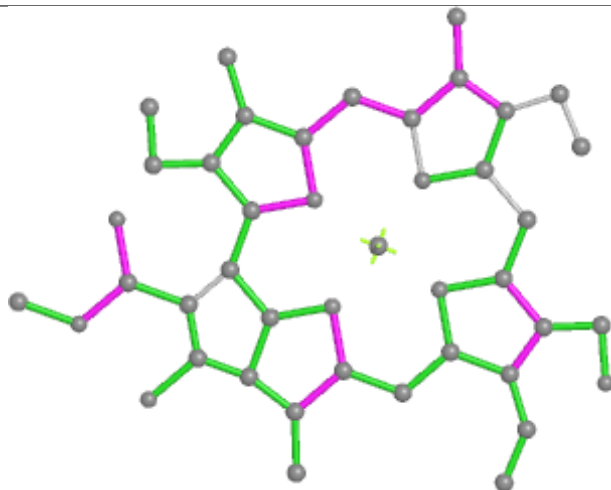
Rings



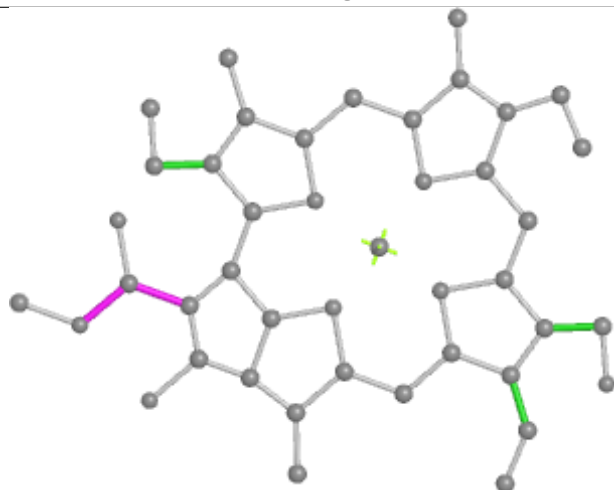
## Ligand CHL U 313



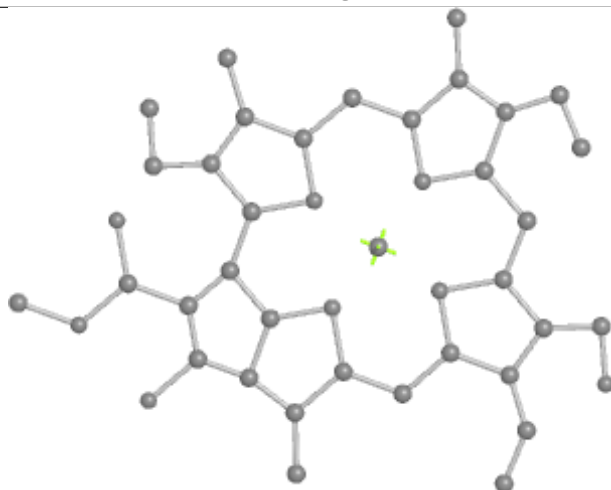
Bond lengths



Bond angles

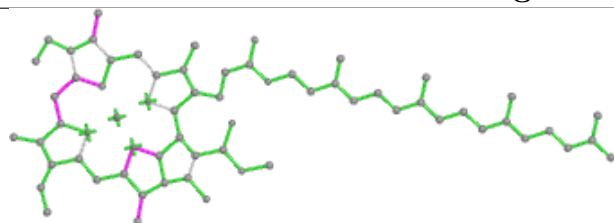


Torsions

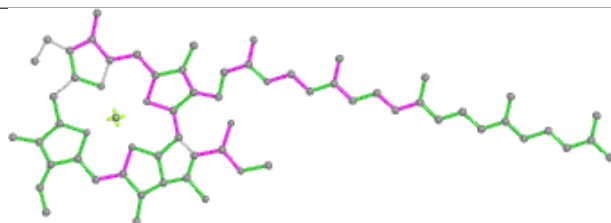


Rings

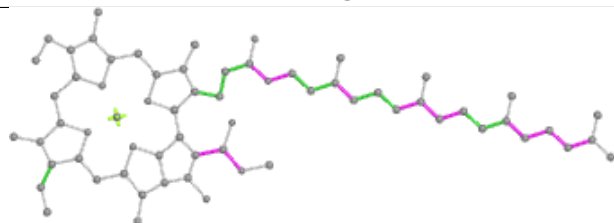
## Ligand CLA A 838



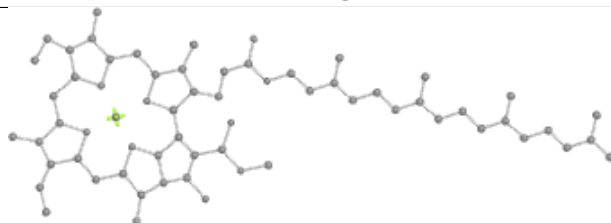
Bond lengths



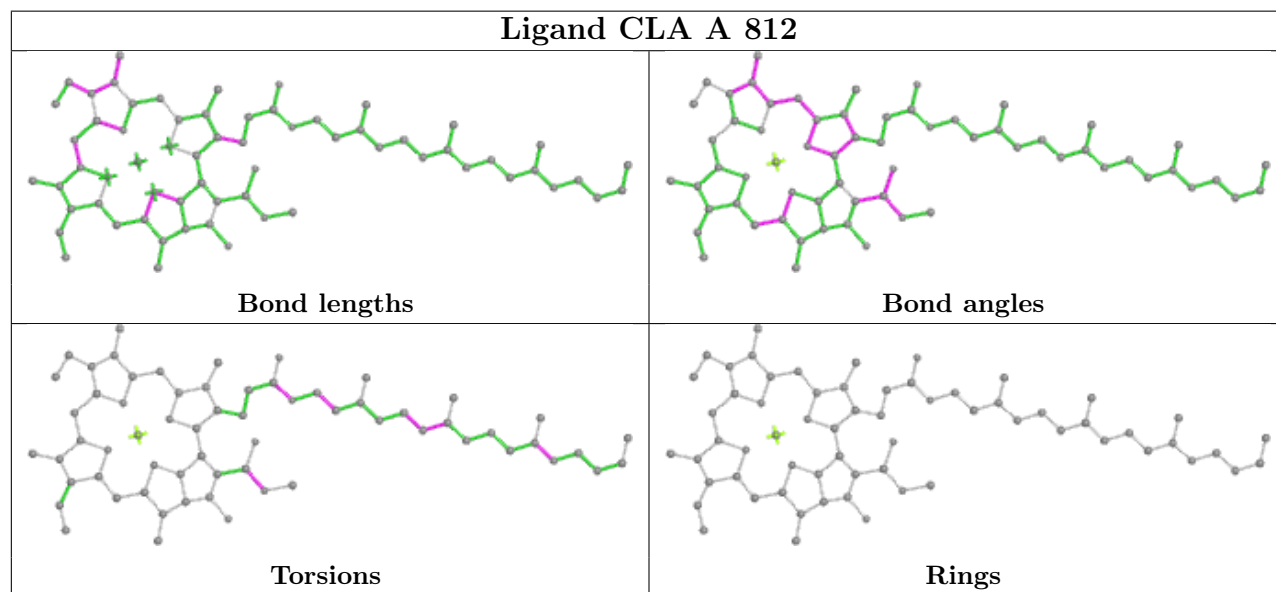
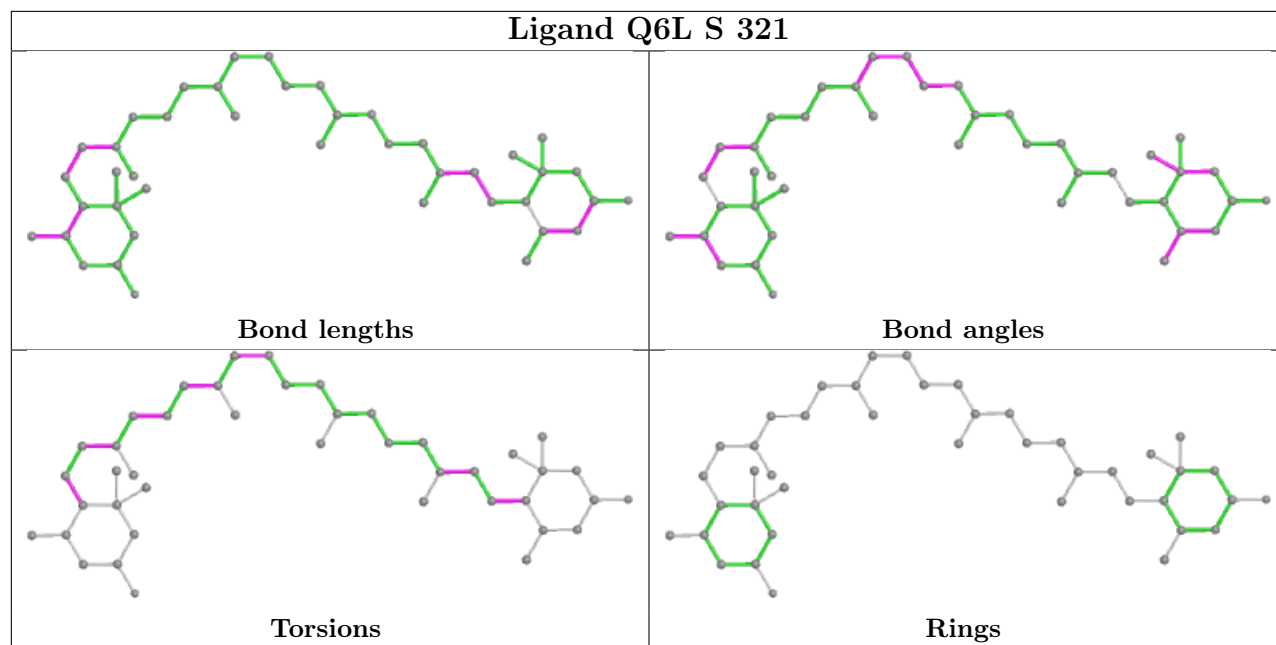
Bond angles



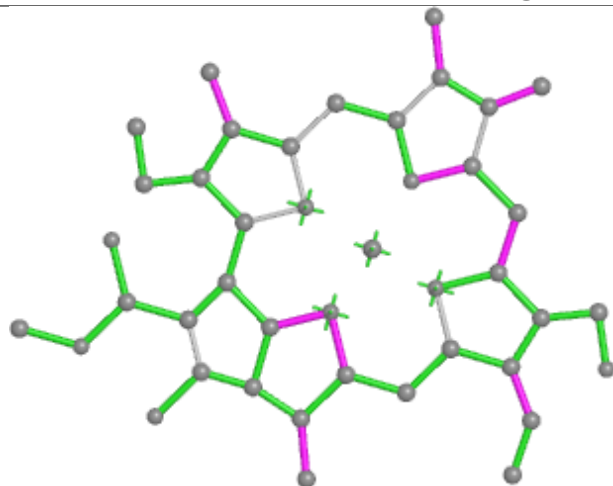
Torsions



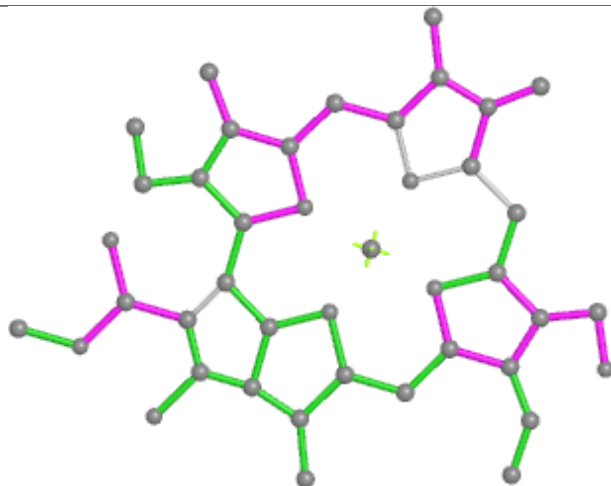
Rings



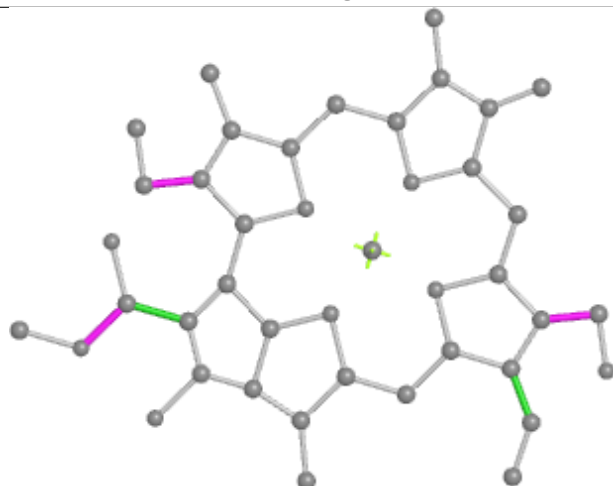
## Ligand CHL 4 307



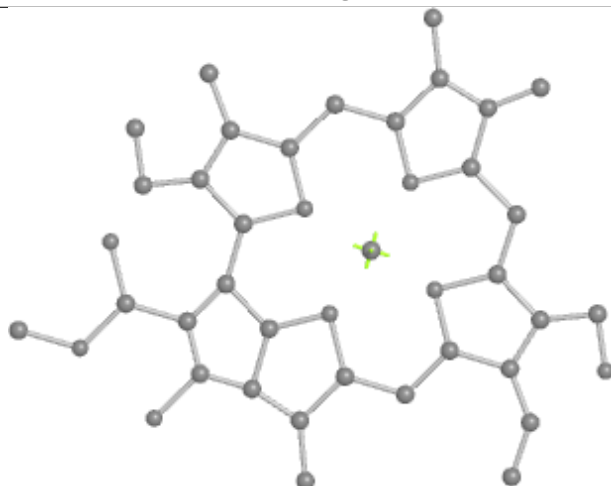
Bond lengths



Bond angles

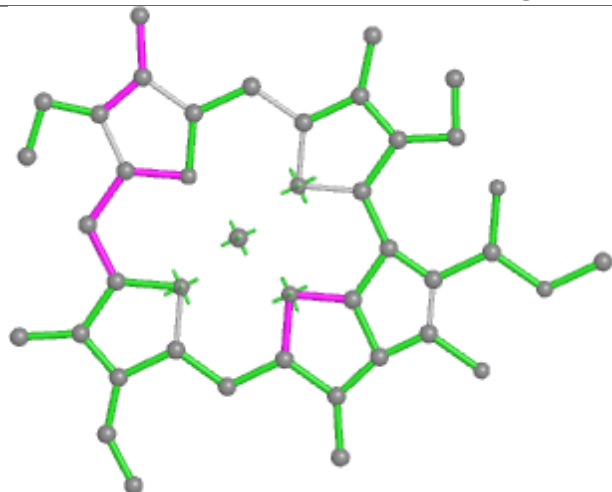


Torsions

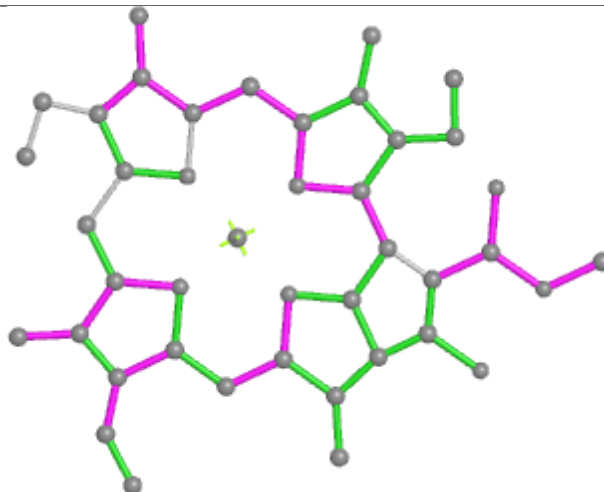


Rings

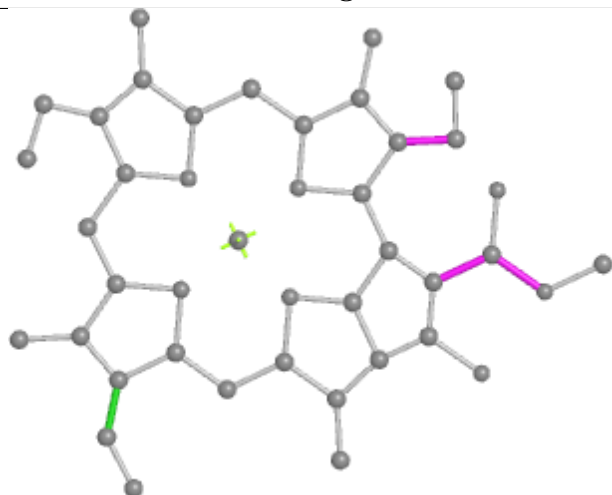
## Ligand CLA 4 311



Bond lengths



Bond angles

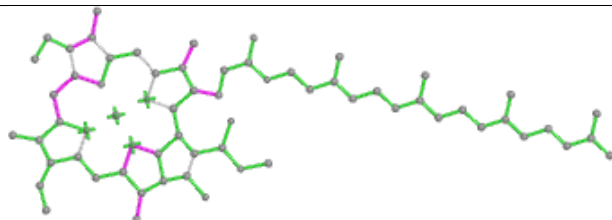


Torsions

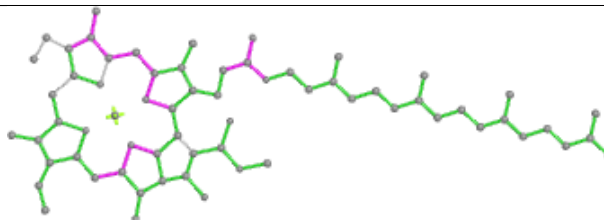


Rings

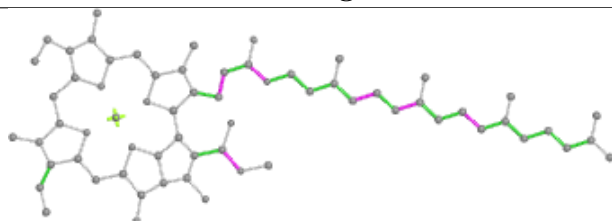
## Ligand CLA Q 304



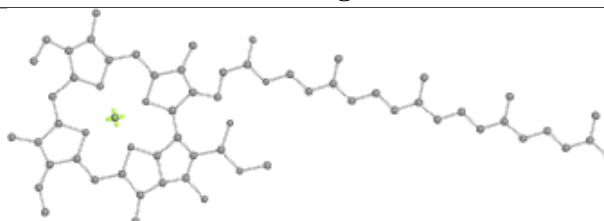
Bond lengths



Bond angles

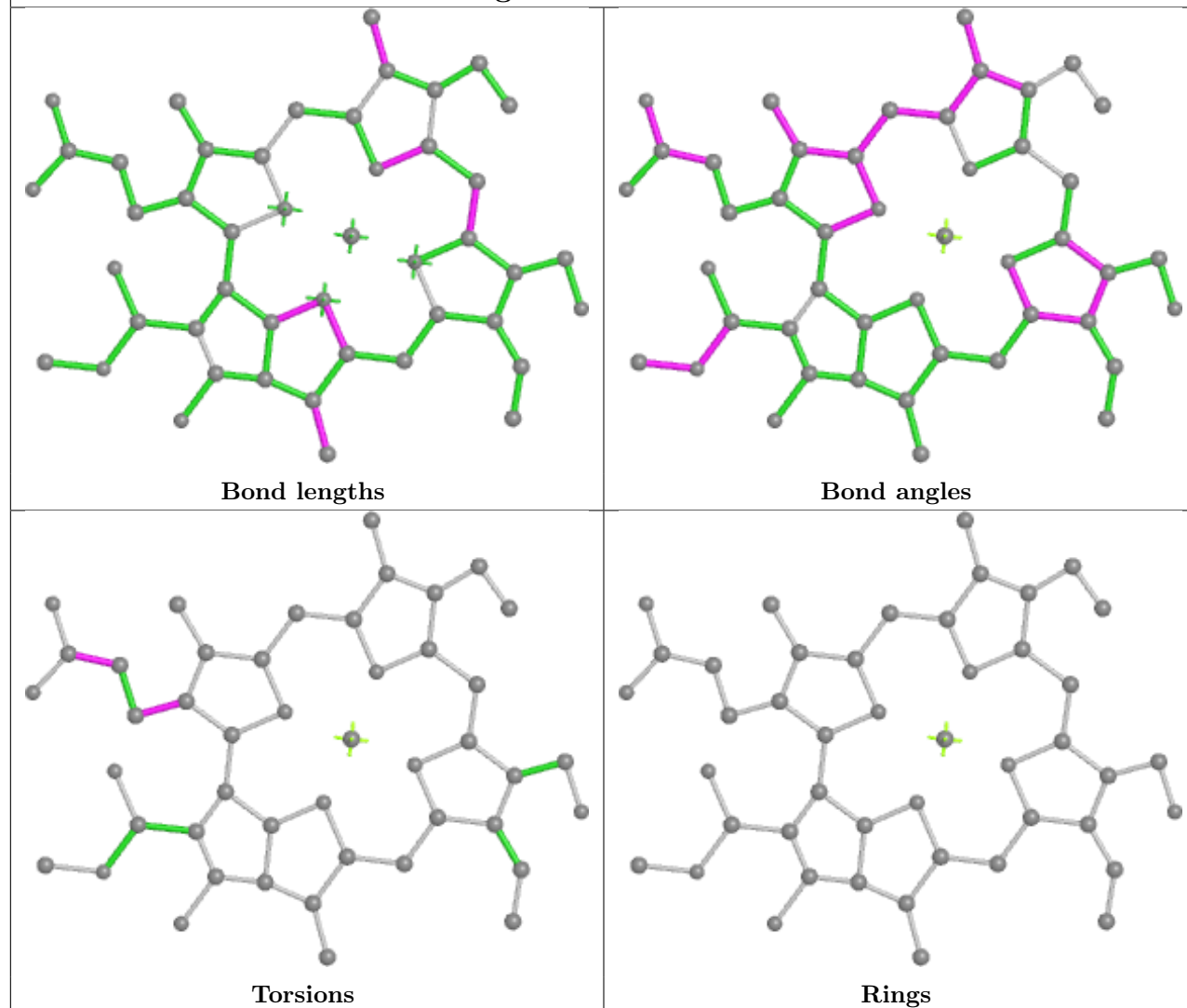


Torsions

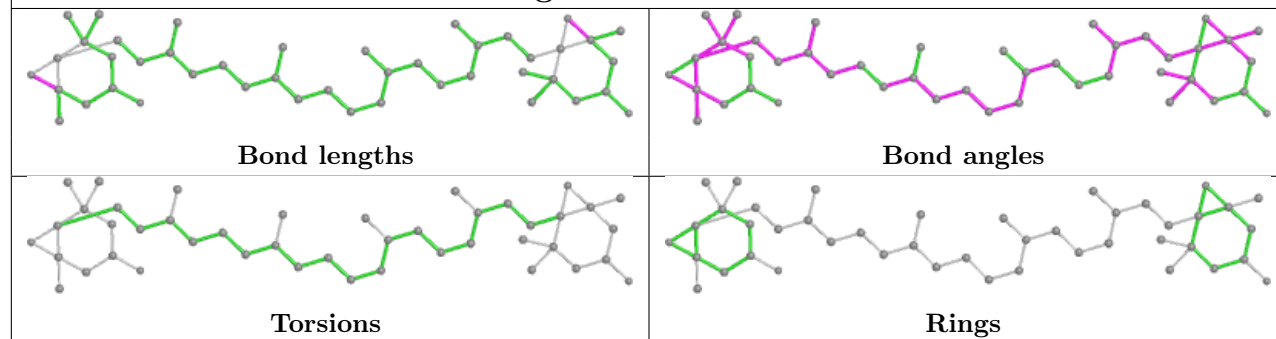


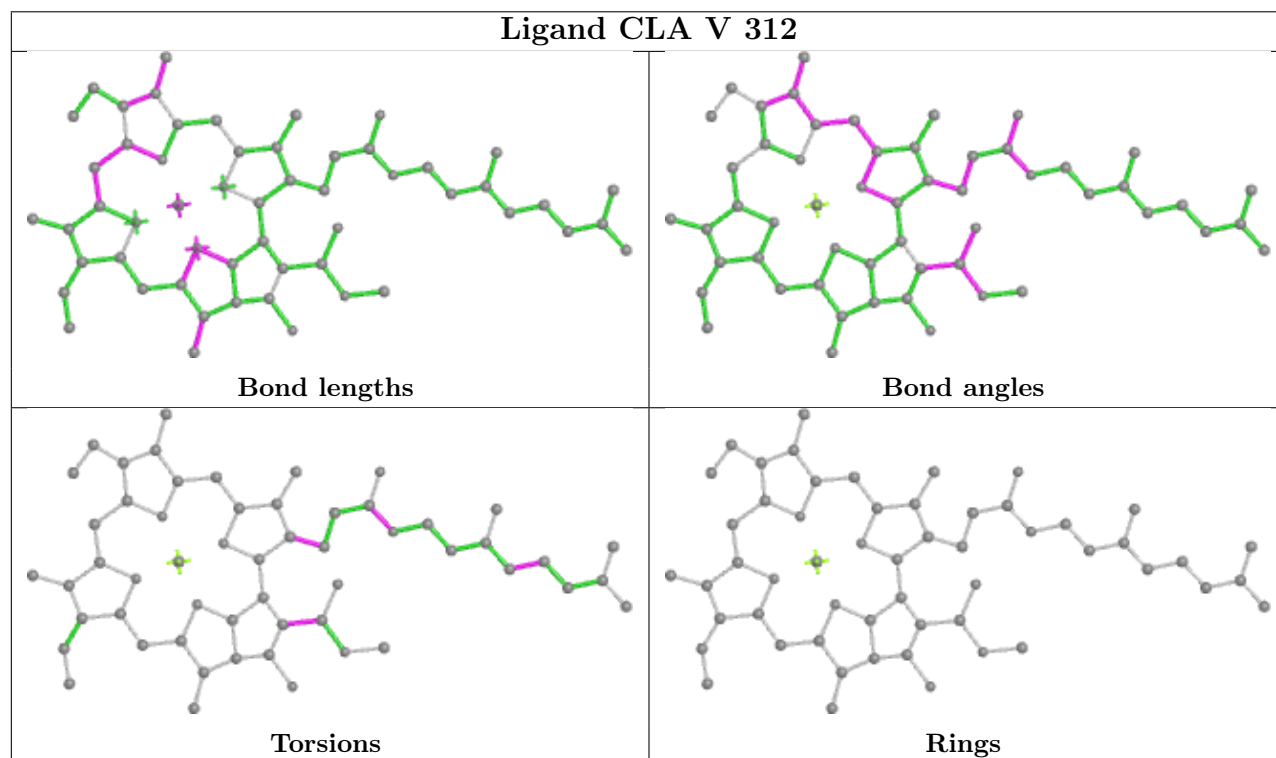
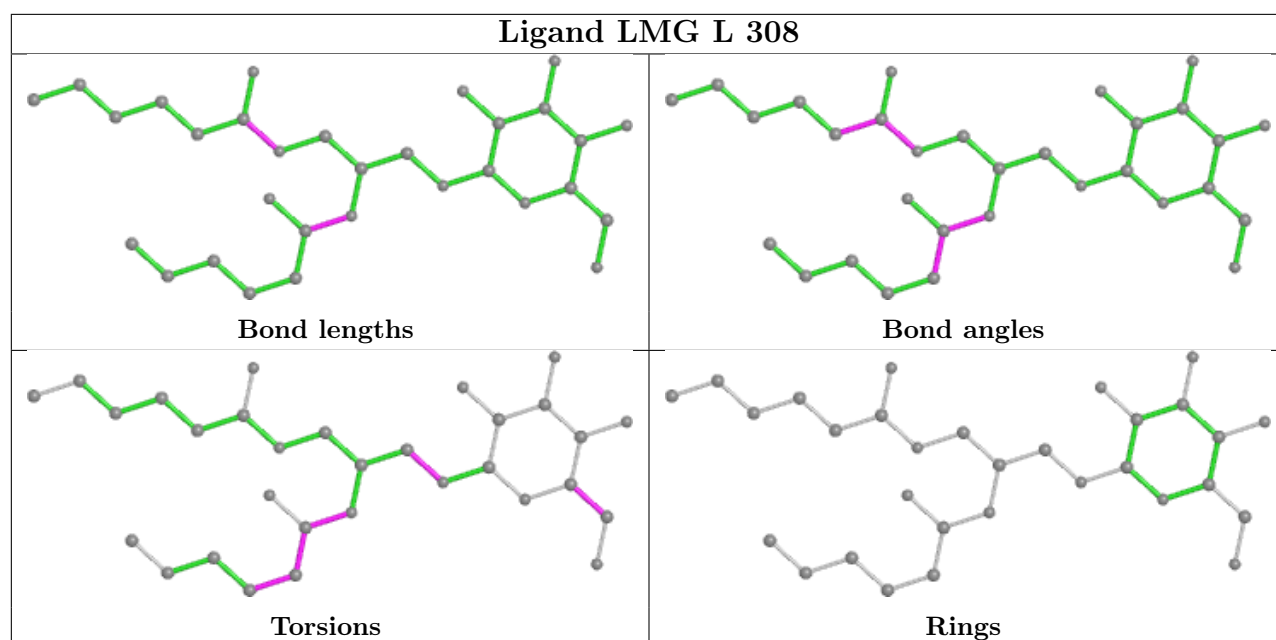
Rings

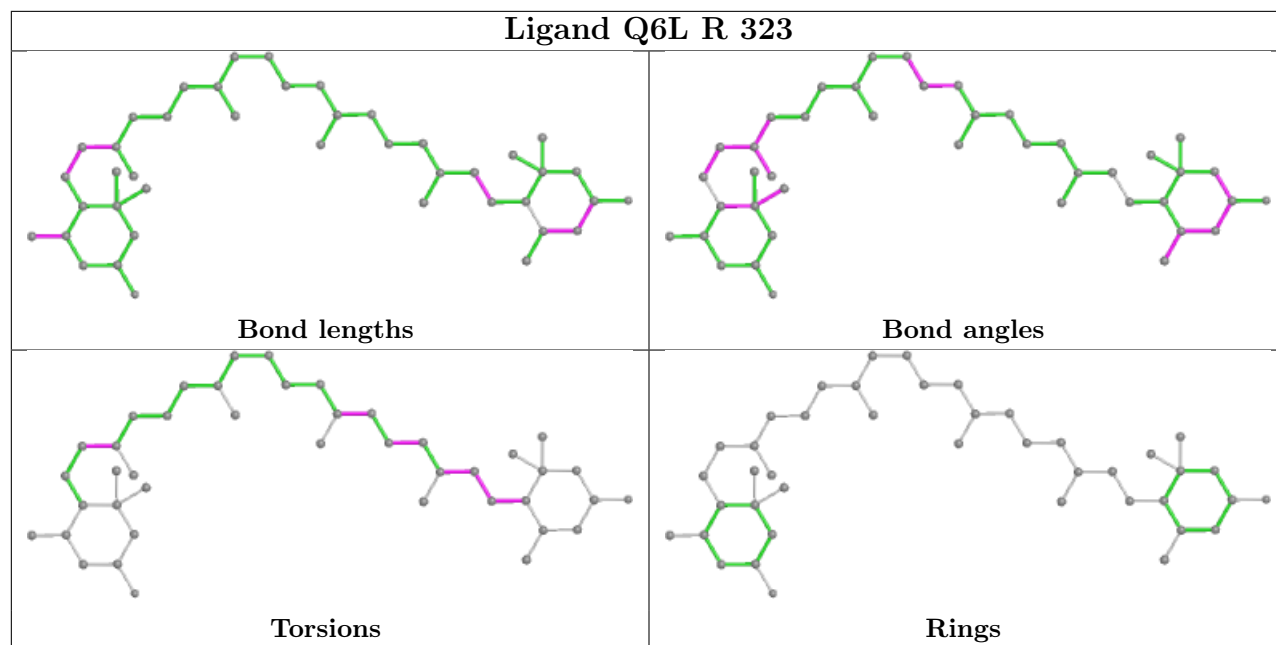
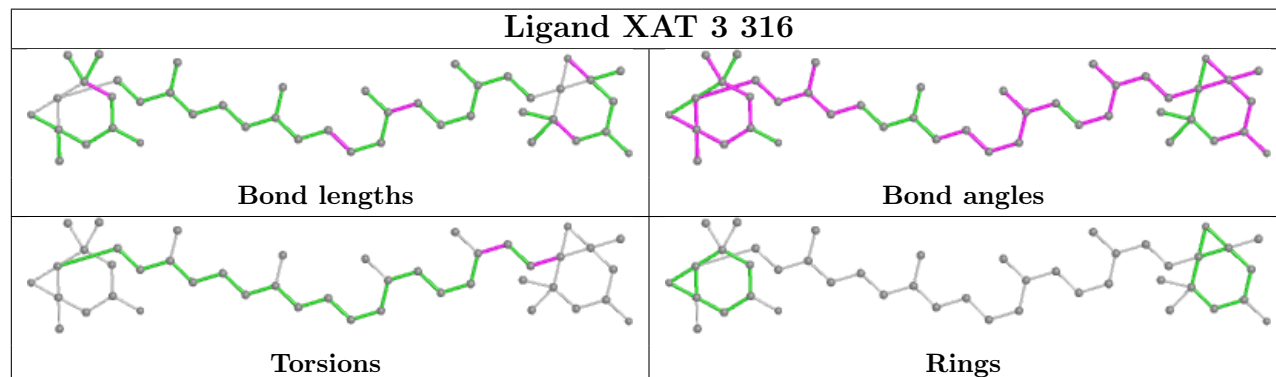
## Ligand CHL P 305



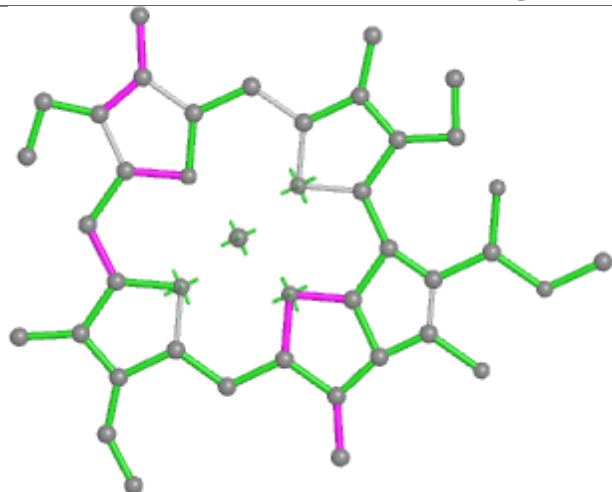
## Ligand XAT 5 612



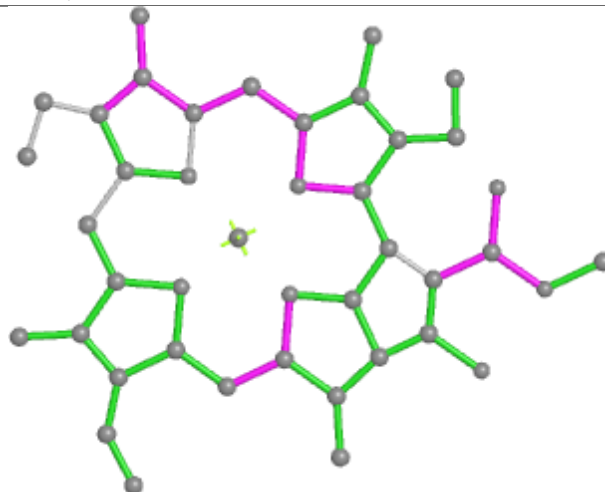


**Ligand Q6L R 323****Ligand XAT 3 316**

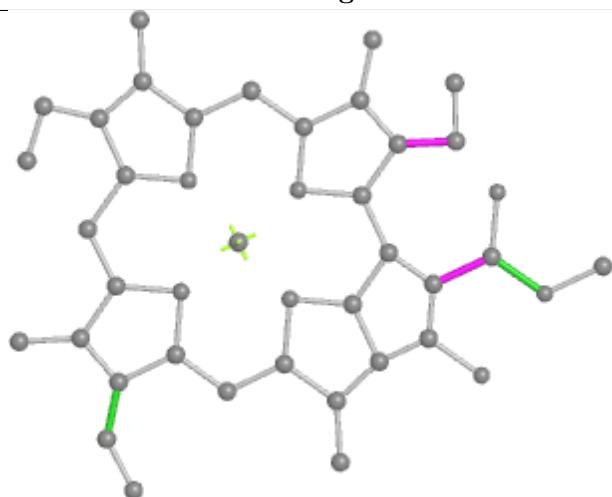
## Ligand CLA Q 312



Bond lengths



Bond angles



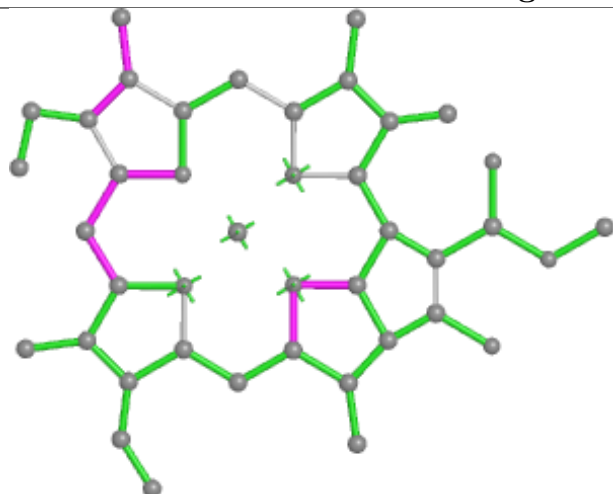
Torsions



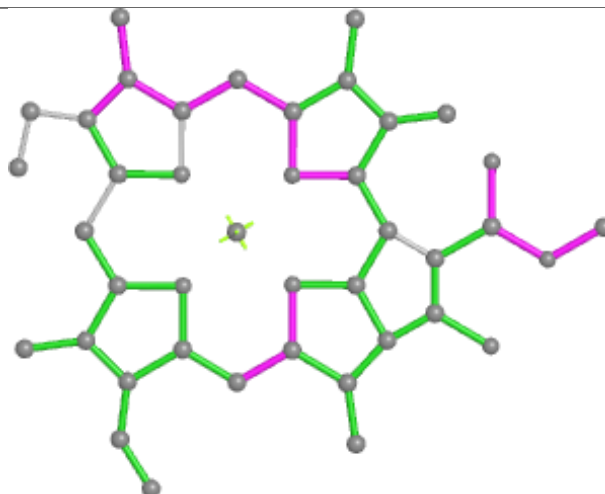
Rings



## Ligand CLA 3 313



Bond lengths



Bond angles

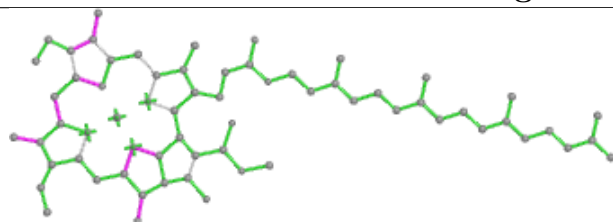


Torsions

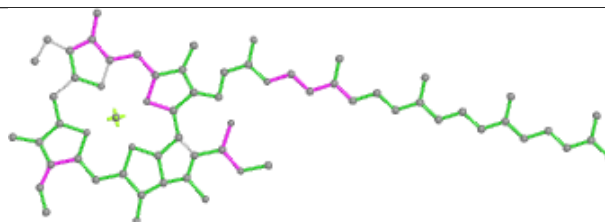


Rings

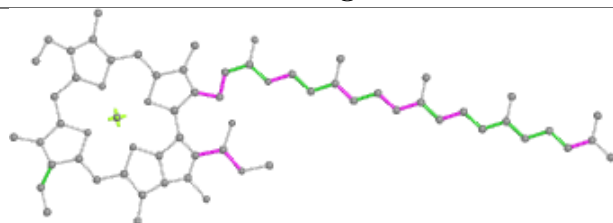
## Ligand CLA T 302



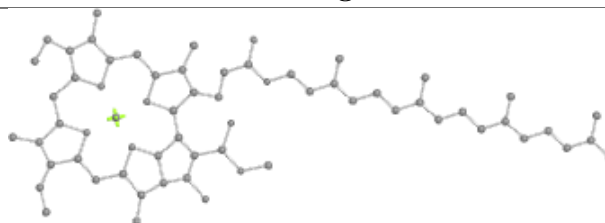
Bond lengths



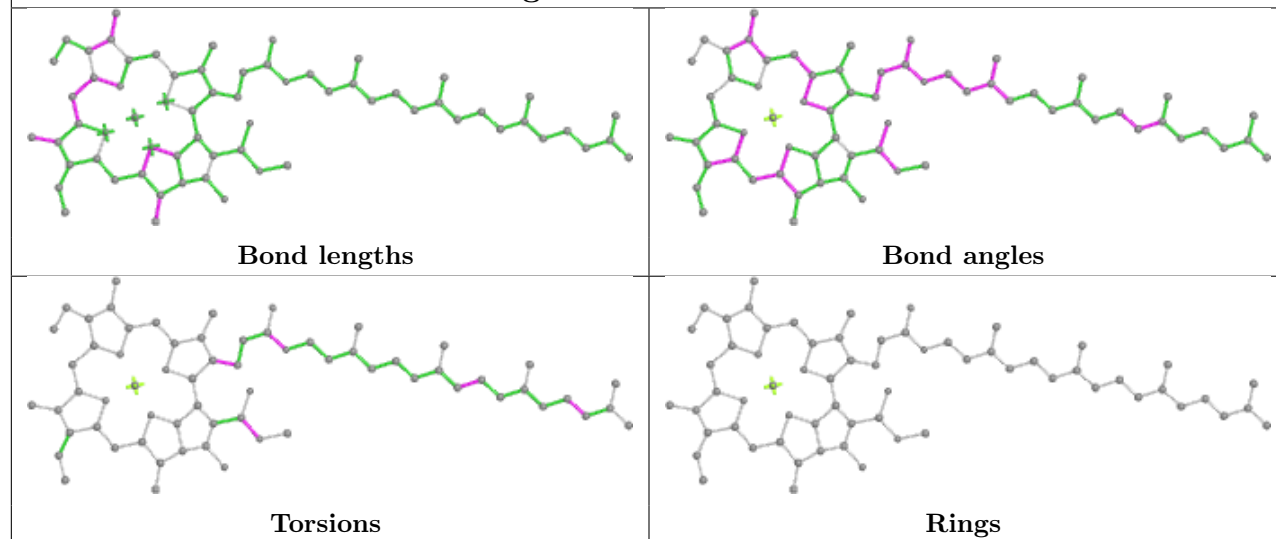
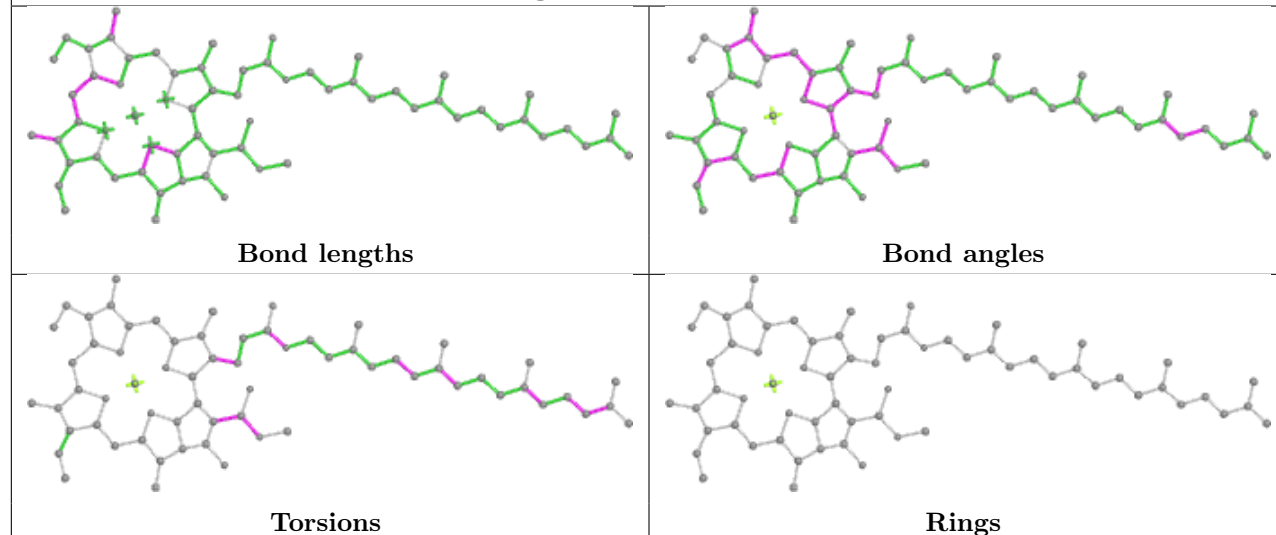
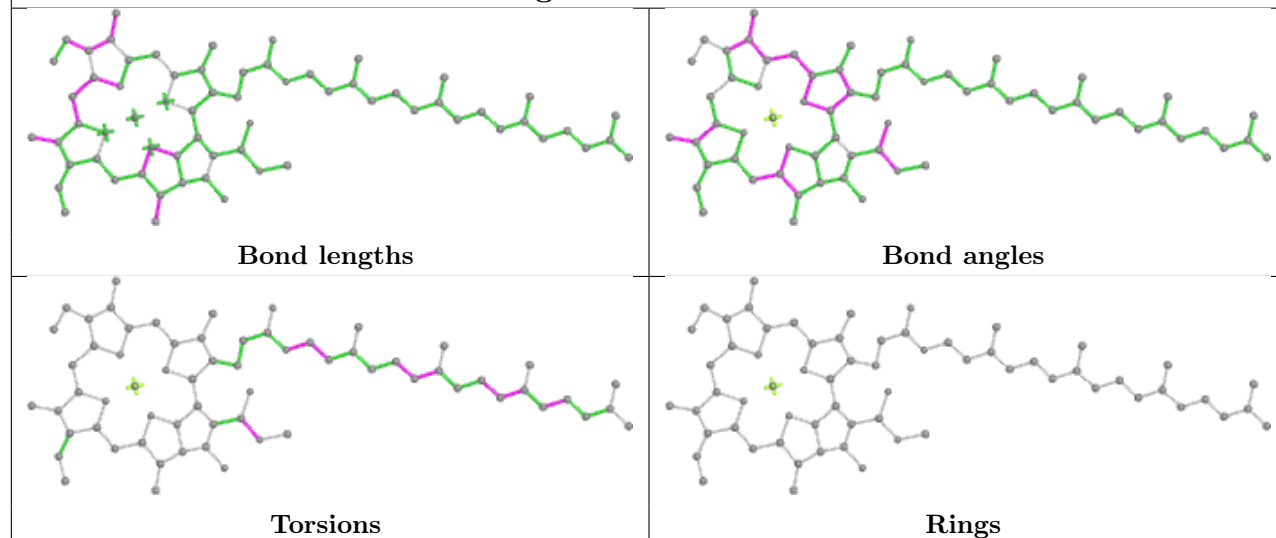
Bond angles

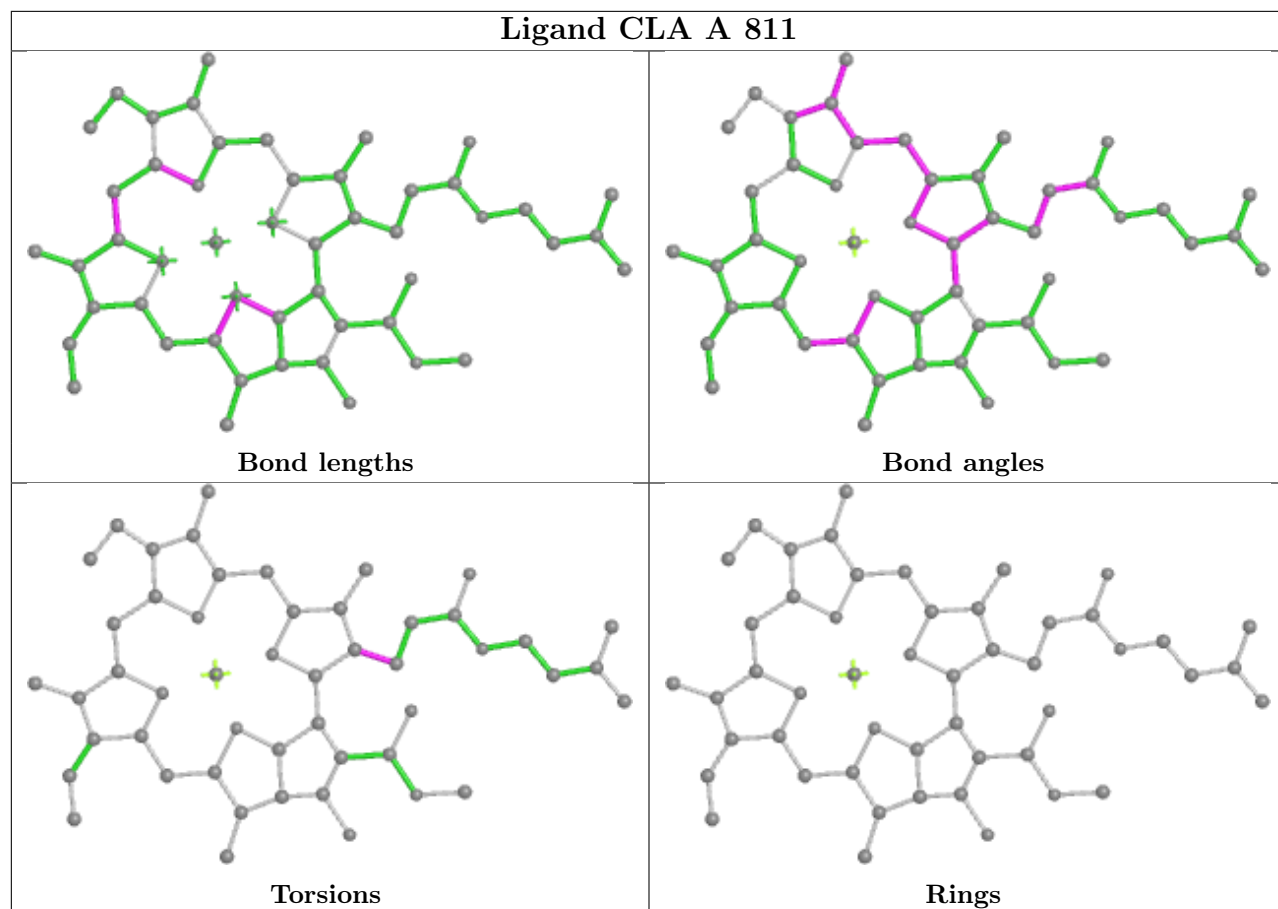


Torsions

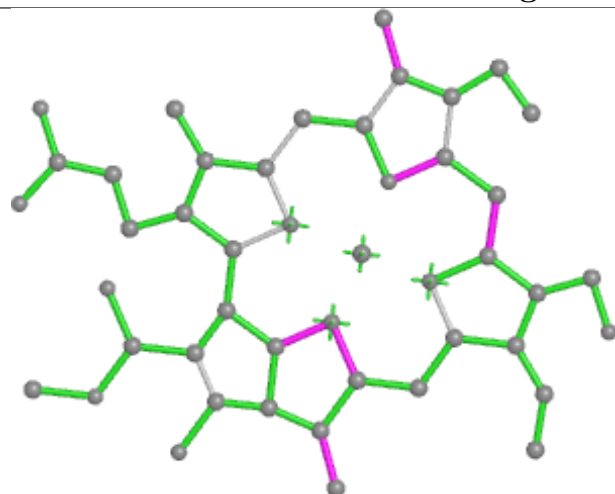


Rings

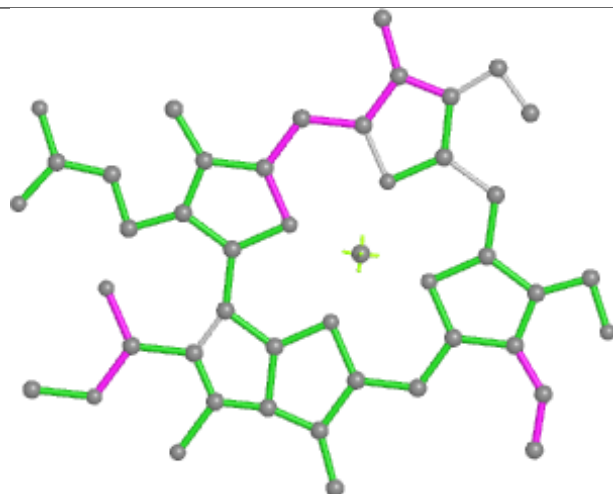
**Ligand CLA O 2002****Ligand CLA A 821****Ligand CLA S 302**



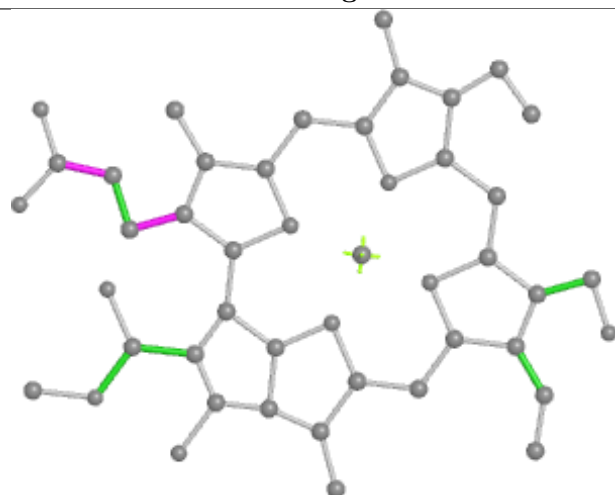
## Ligand CHL 4 308



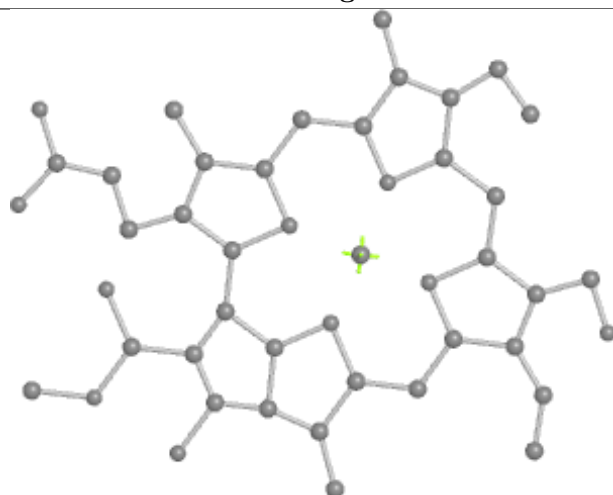
Bond lengths



Bond angles

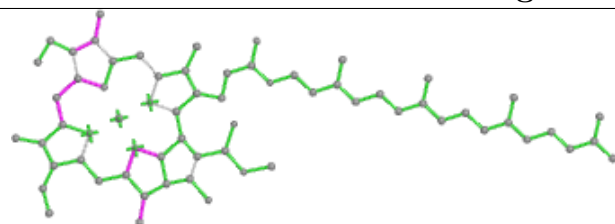


Torsions

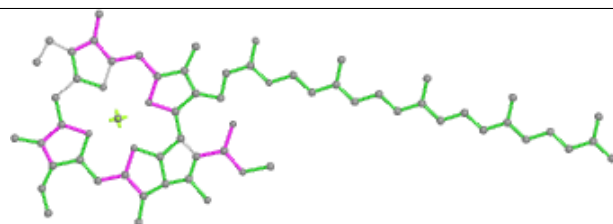


Rings

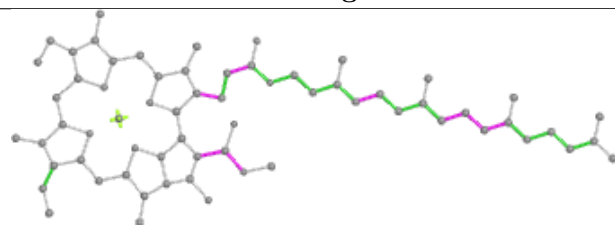
## Ligand CLA B 834



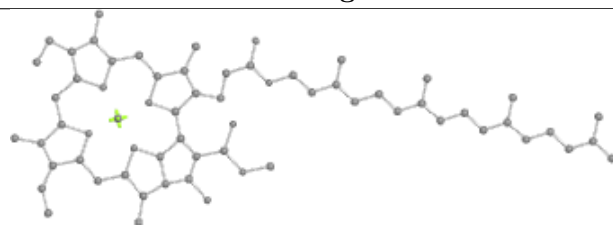
Bond lengths



Bond angles

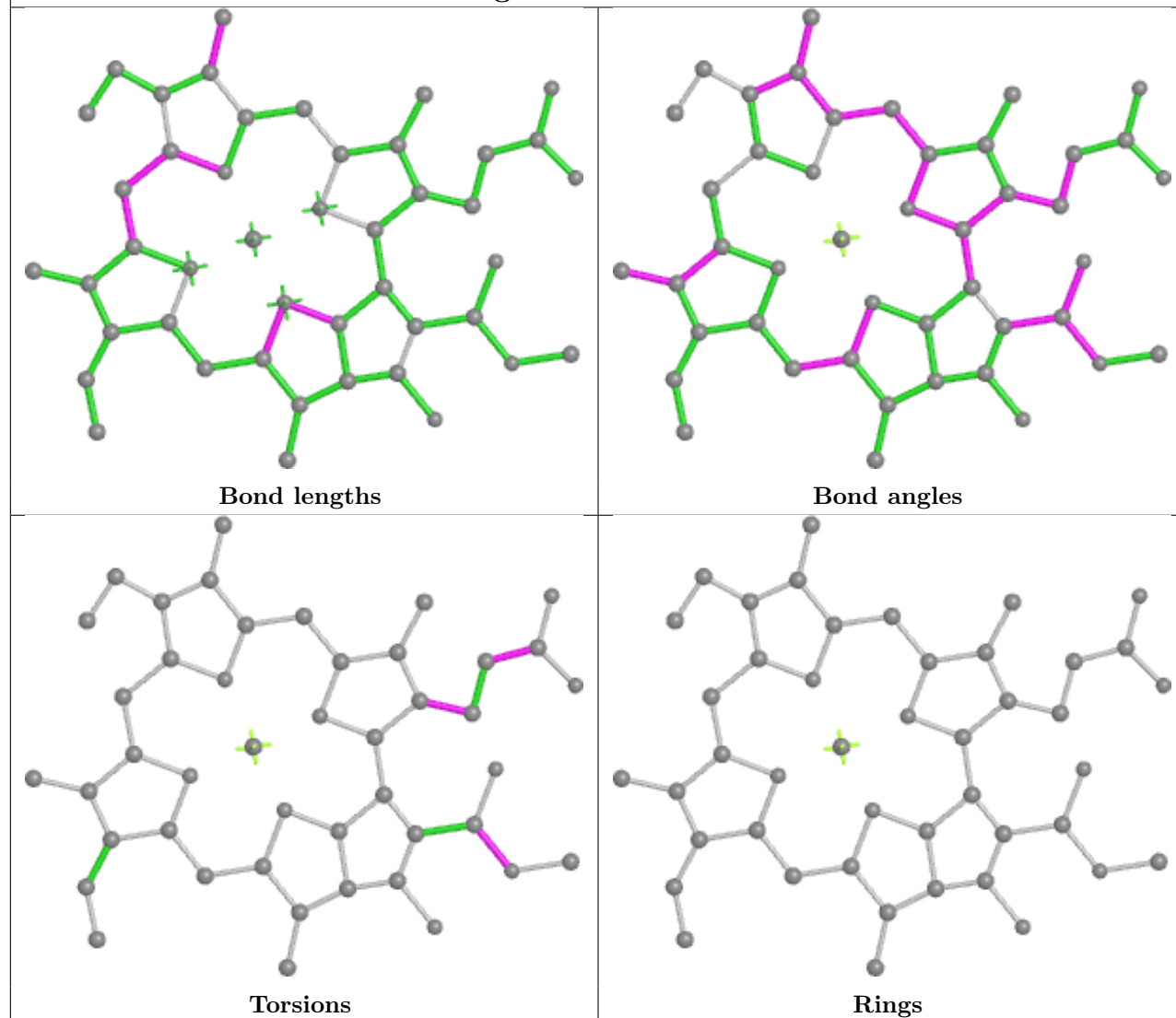


Torsions

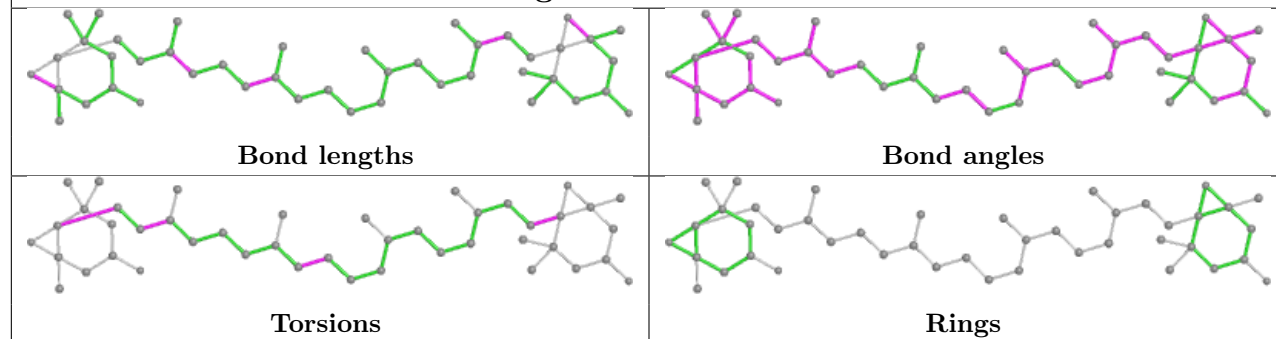


Rings

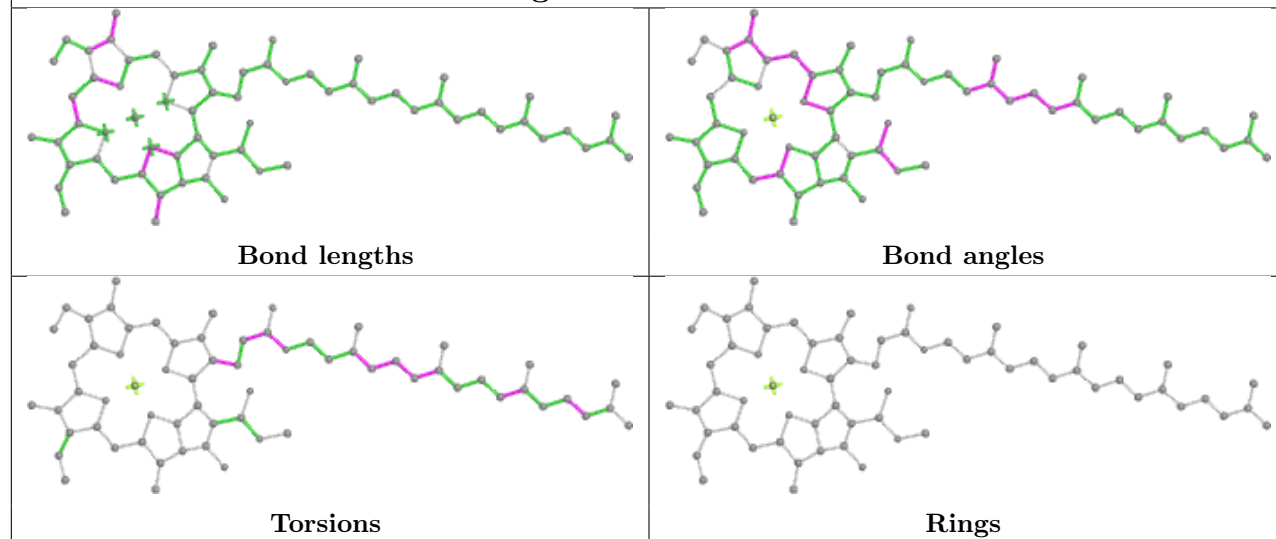
## Ligand CLA 2 608



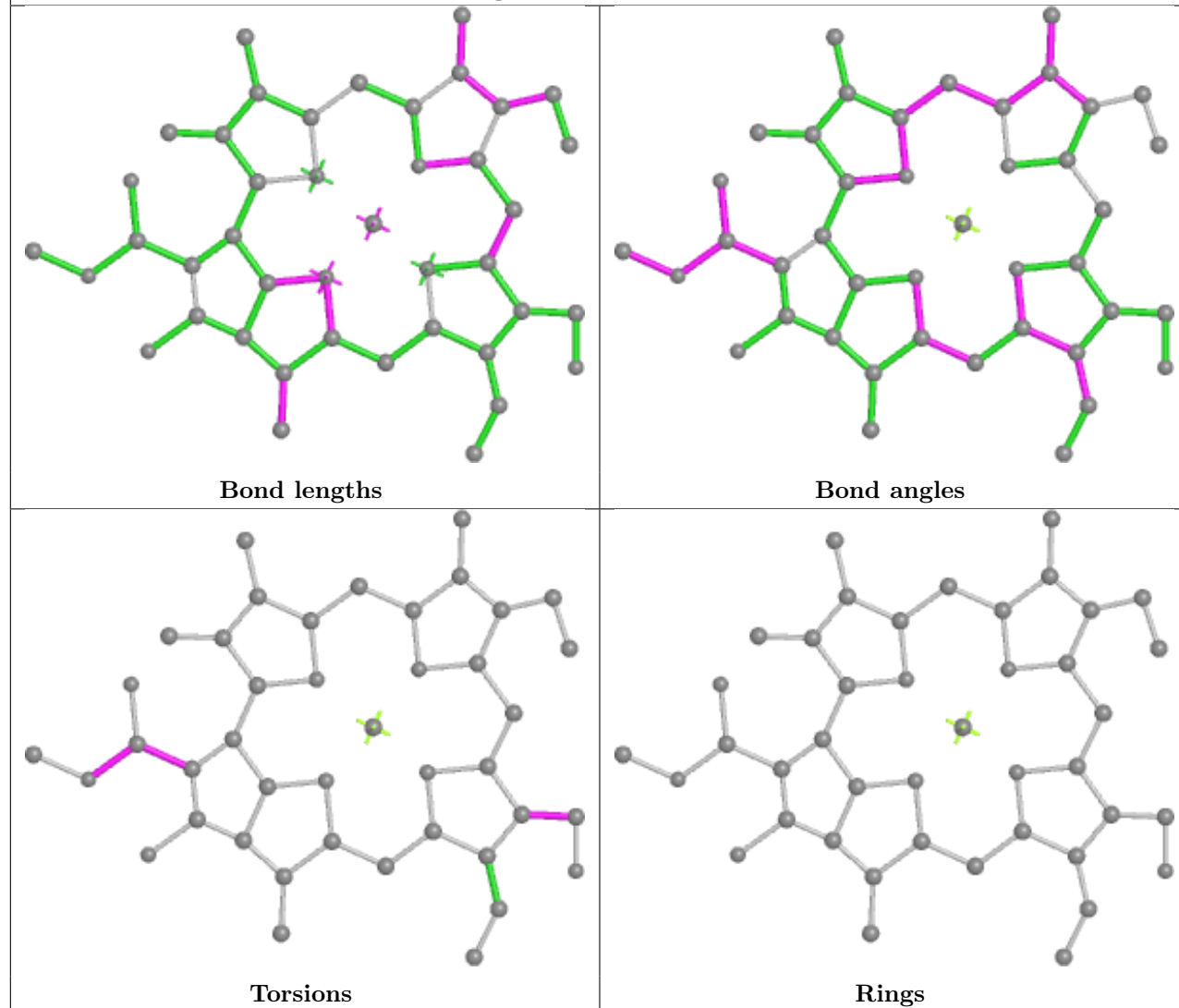
## Ligand XAT 4 318



## Ligand CLA A 837



## Ligand CHL U 304



## 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.

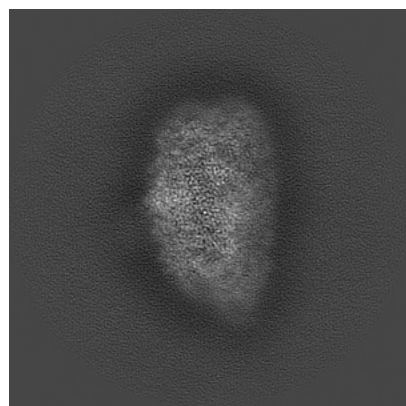
## 6 Map visualisation [i](#)

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.

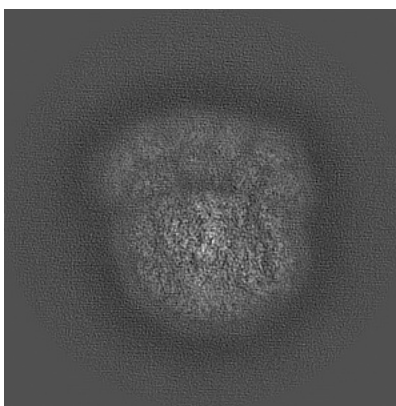
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

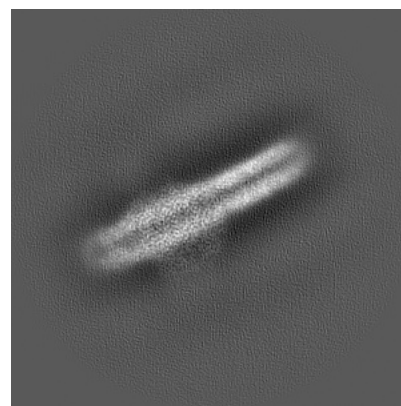
#### 6.1.1 Primary map



X

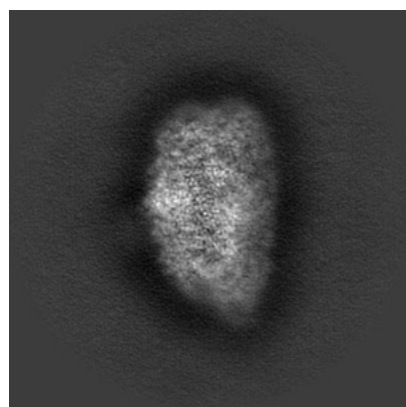


Y

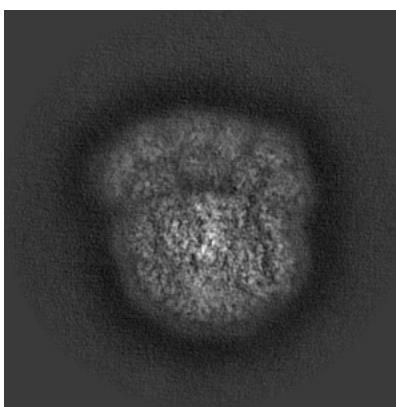


Z

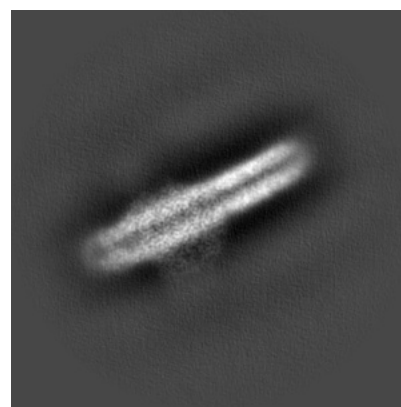
#### 6.1.2 Raw map



X



Y



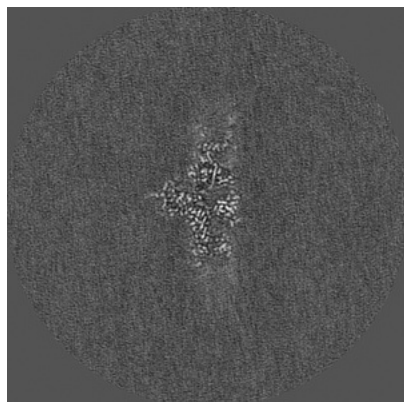
Z

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

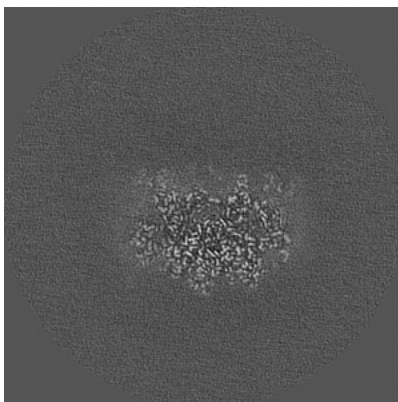


## 6.2 Central slices [i](#)

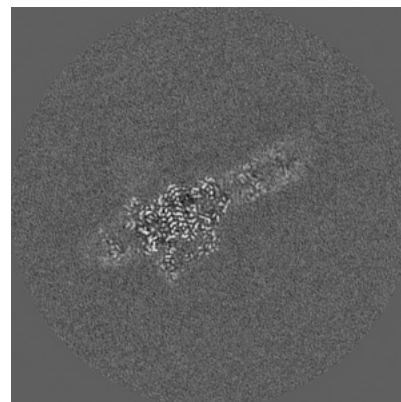
### 6.2.1 Primary map



X Index: 192

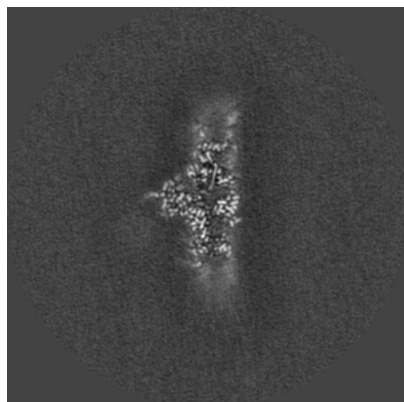


Y Index: 192

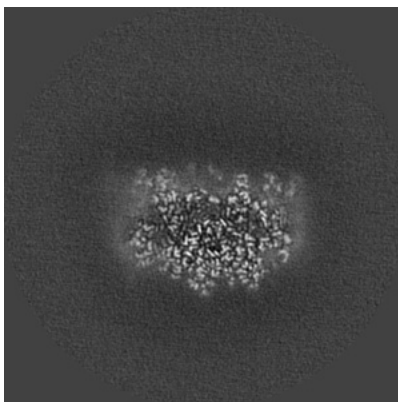


Z Index: 192

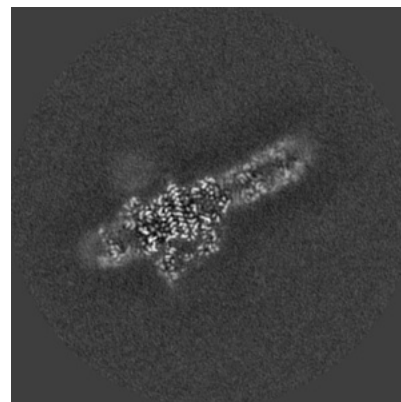
### 6.2.2 Raw map



X Index: 192



Y Index: 192

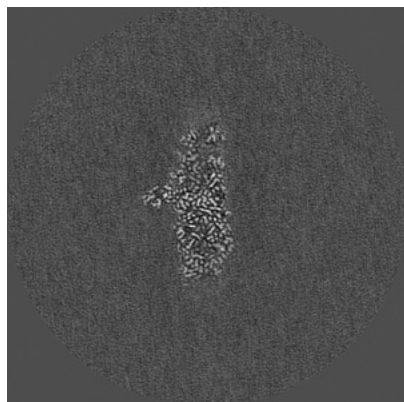


Z Index: 192

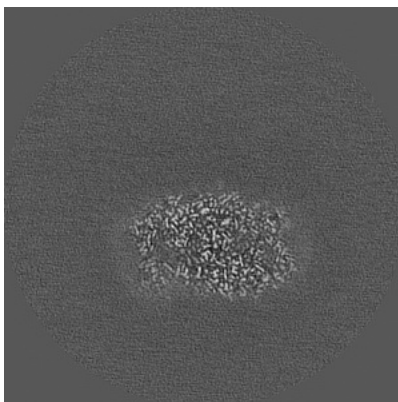
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

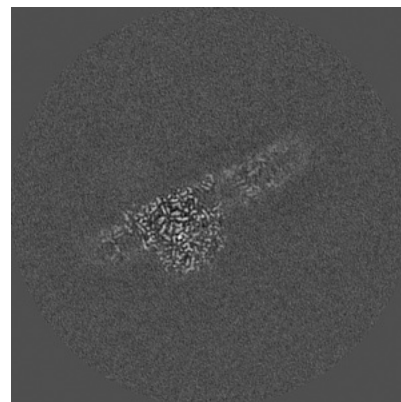
### 6.3.1 Primary map



X Index: 169

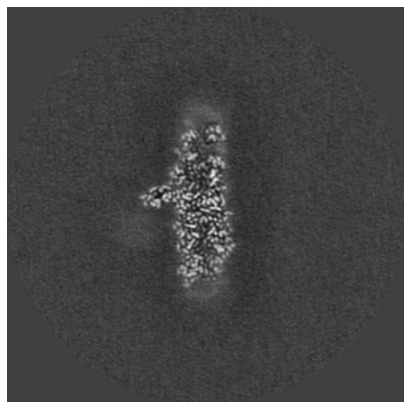


Y Index: 180

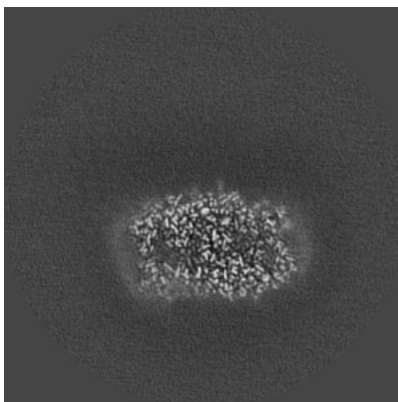


Z Index: 201

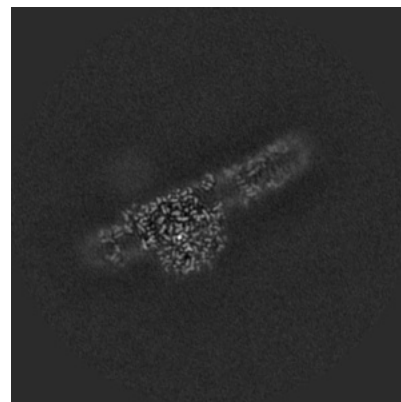
### 6.3.2 Raw map



X Index: 168



Y Index: 180

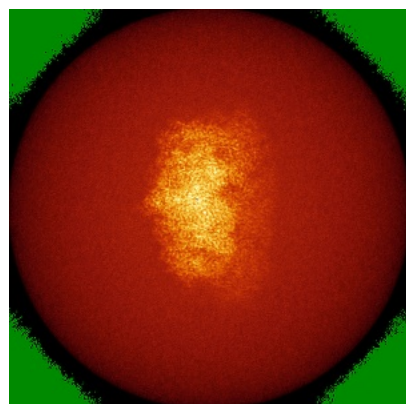


Z Index: 201

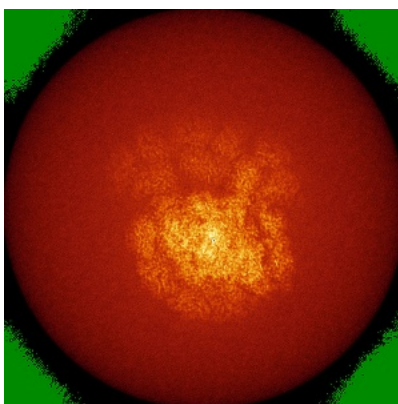
The images above show the largest variance slices of the map in three orthogonal directions.

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

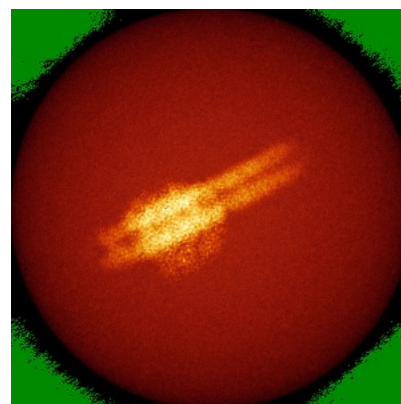
### 6.4.1 Primary map



X

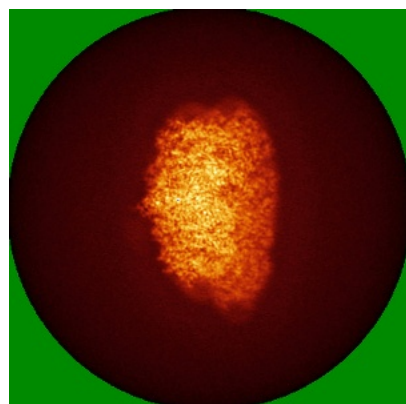


Y

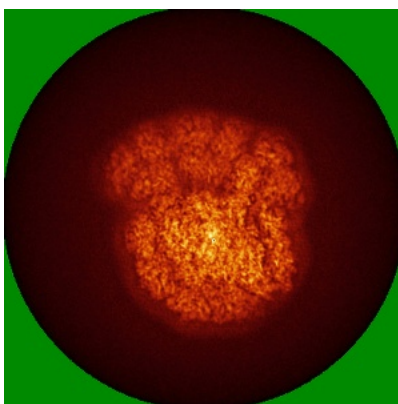


Z

### 6.4.2 Raw map



X



Y

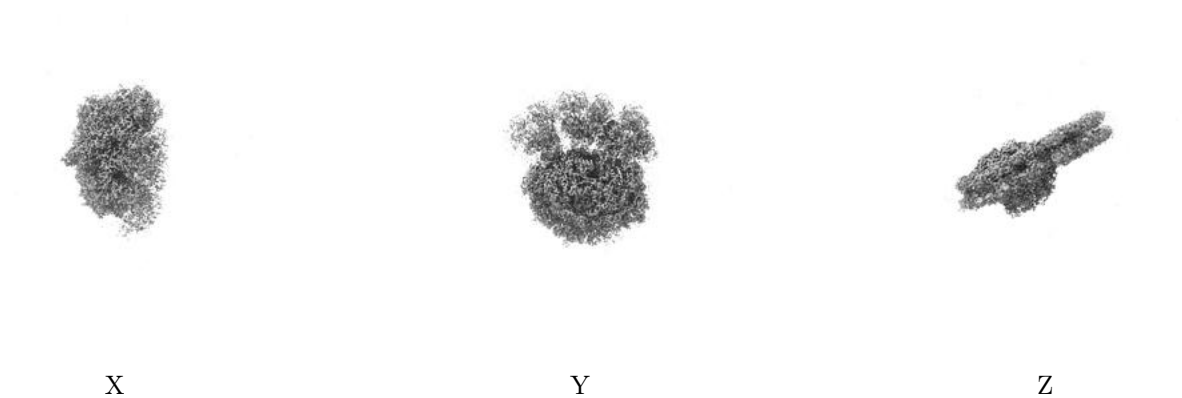


Z

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.

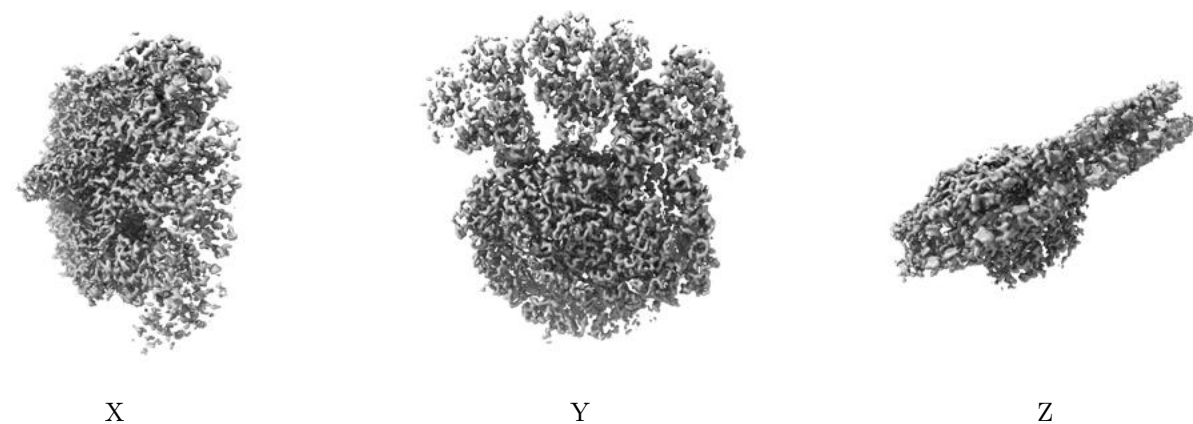
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

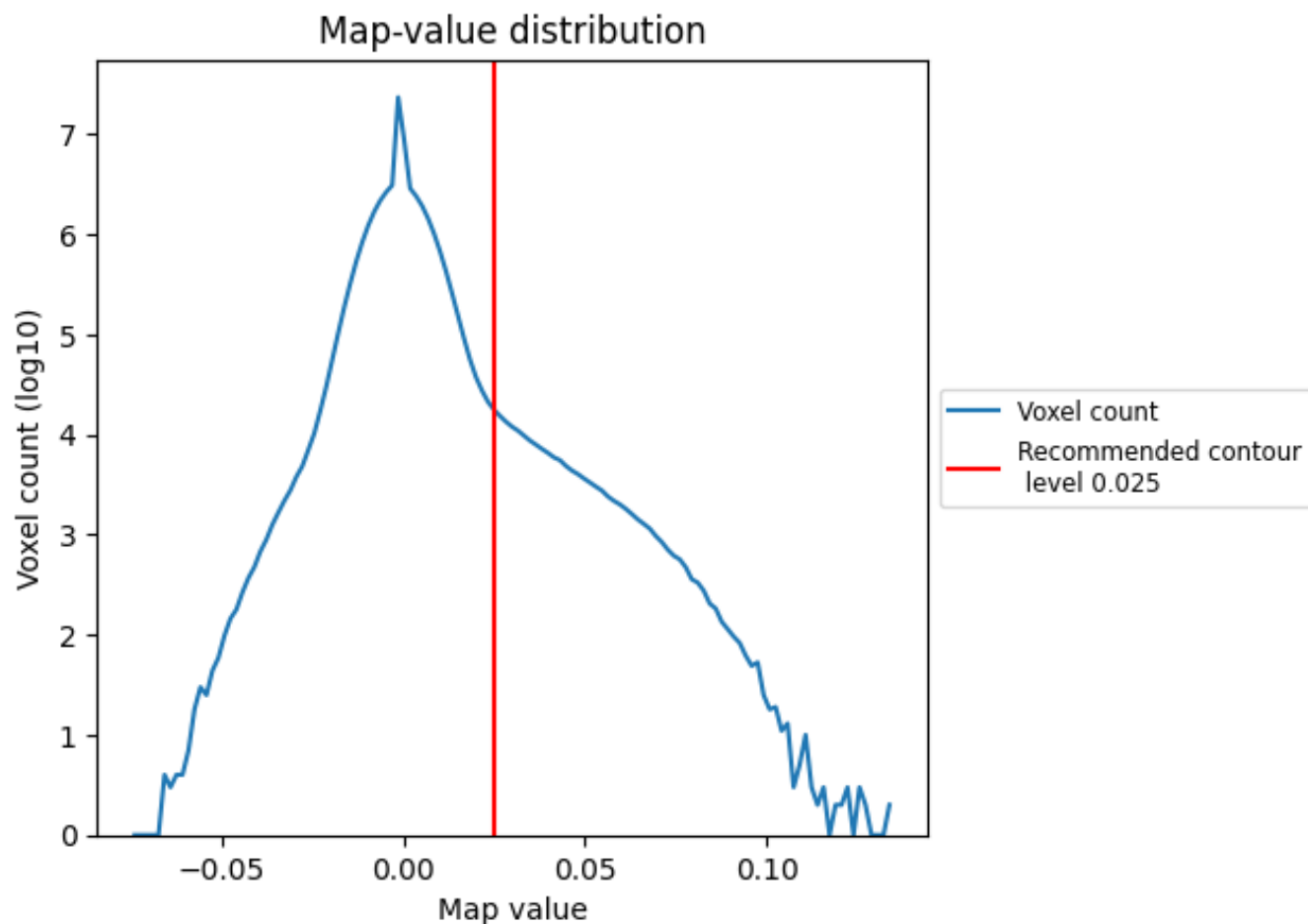
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

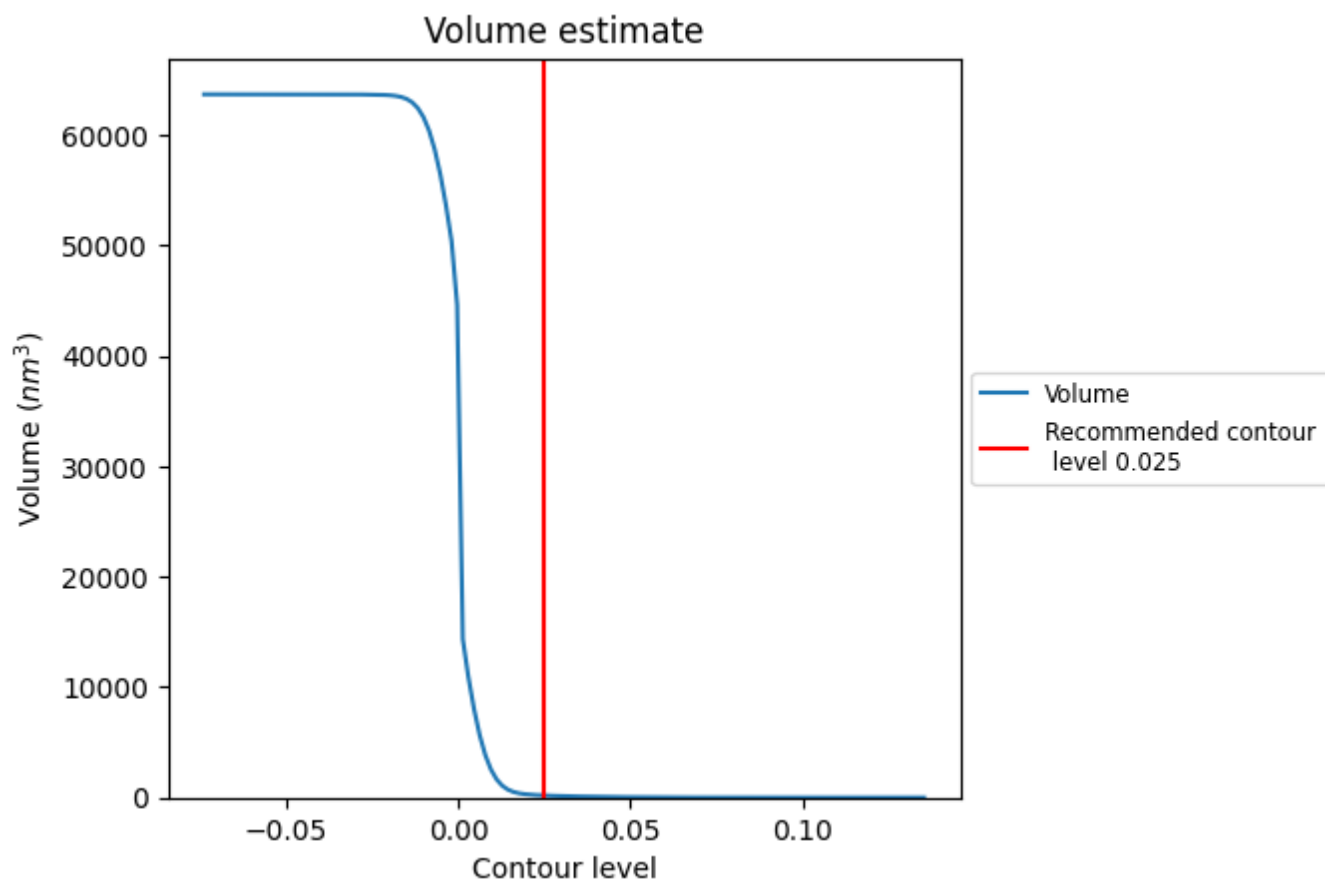
This section contains the results of statistical analysis of the map.

### 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](#)

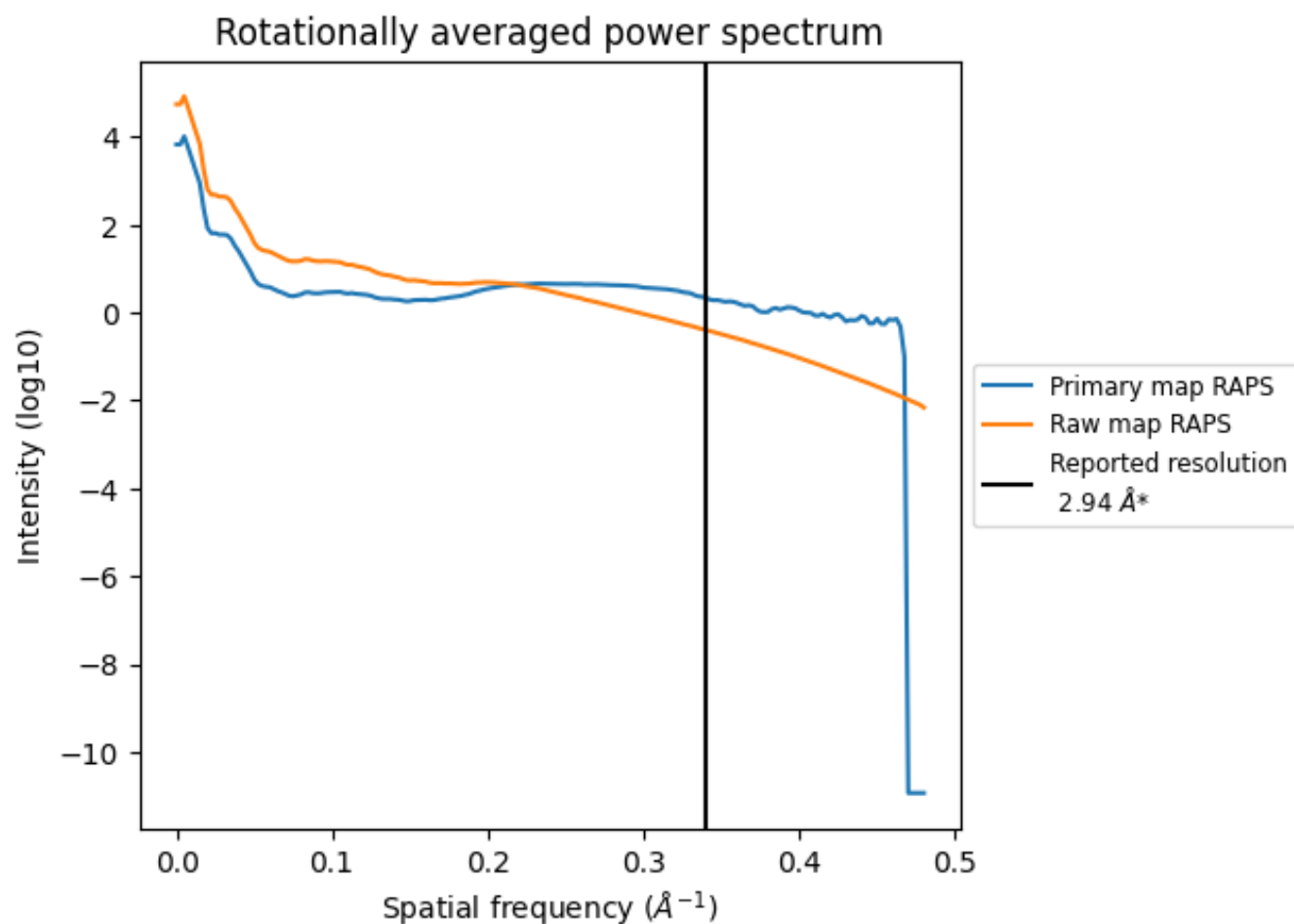


The volume at the recommended contour level is 188 nm<sup>3</sup>; this corresponds to an approximate mass of 169 kDa.

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 ⓘ

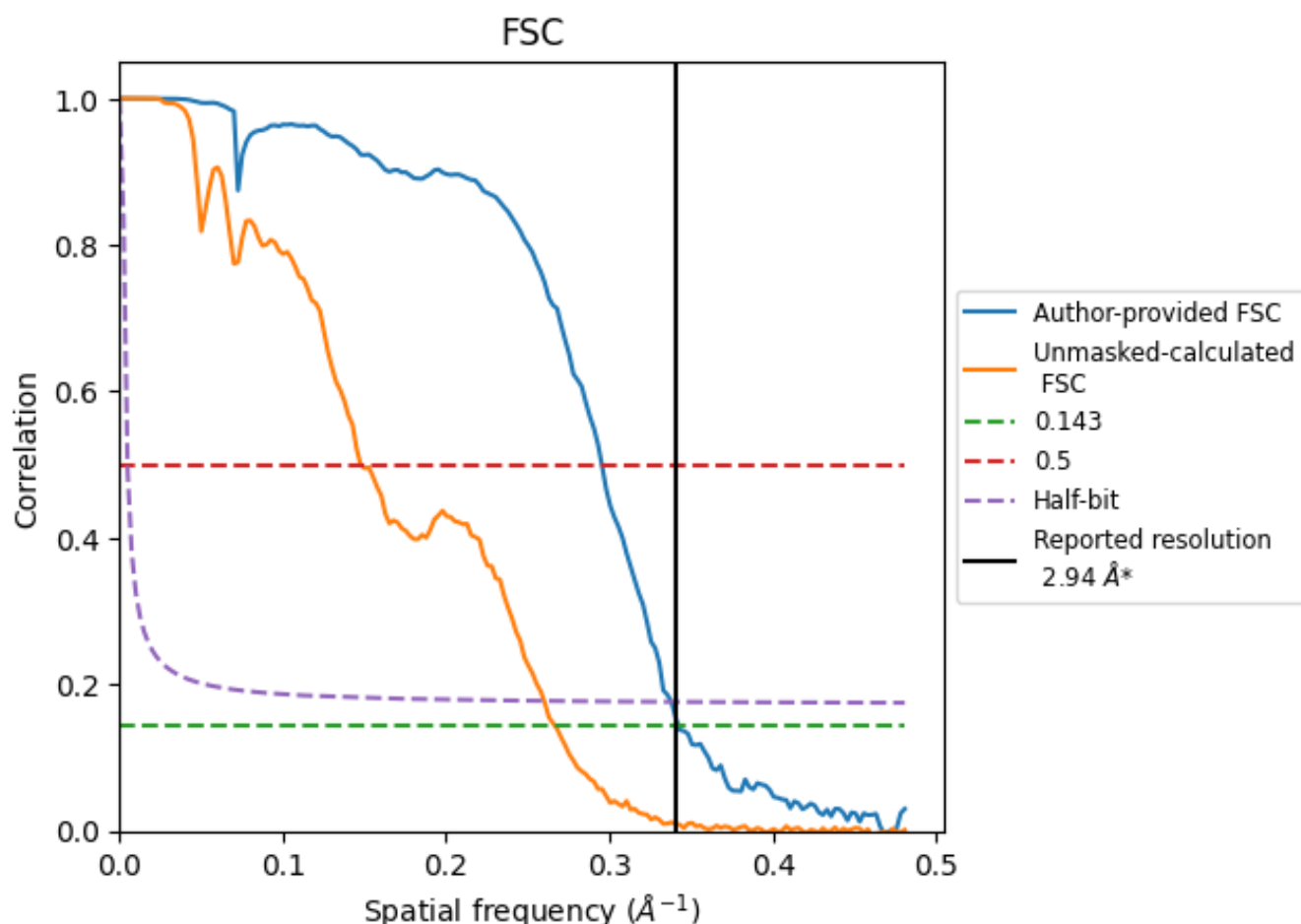


\*Reported resolution corresponds to spatial frequency of 0.340 Å<sup>-1</sup>

## 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 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

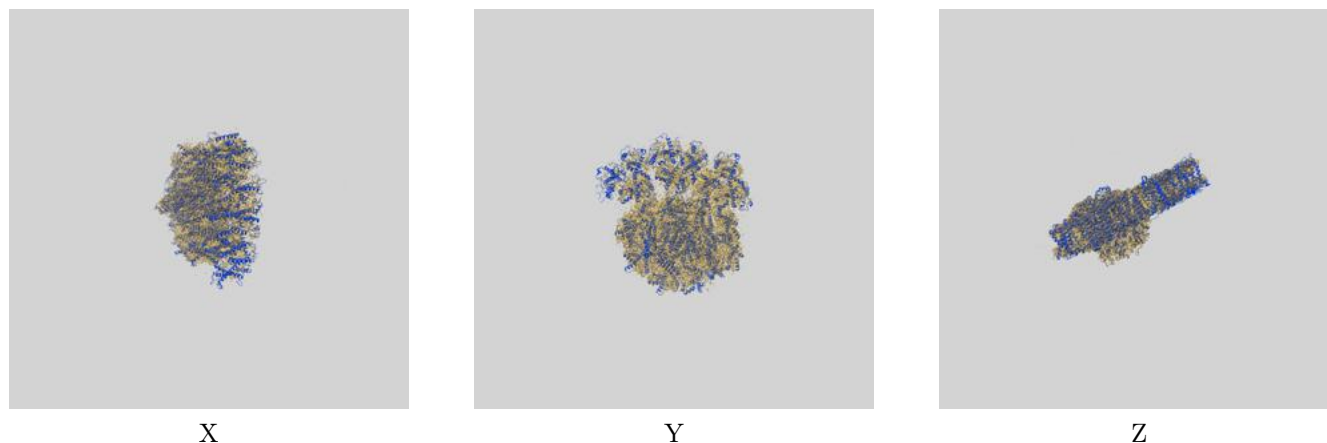
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.39	2.96
Unmasked-calculated*	3.75	6.77	3.85

\*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](#)

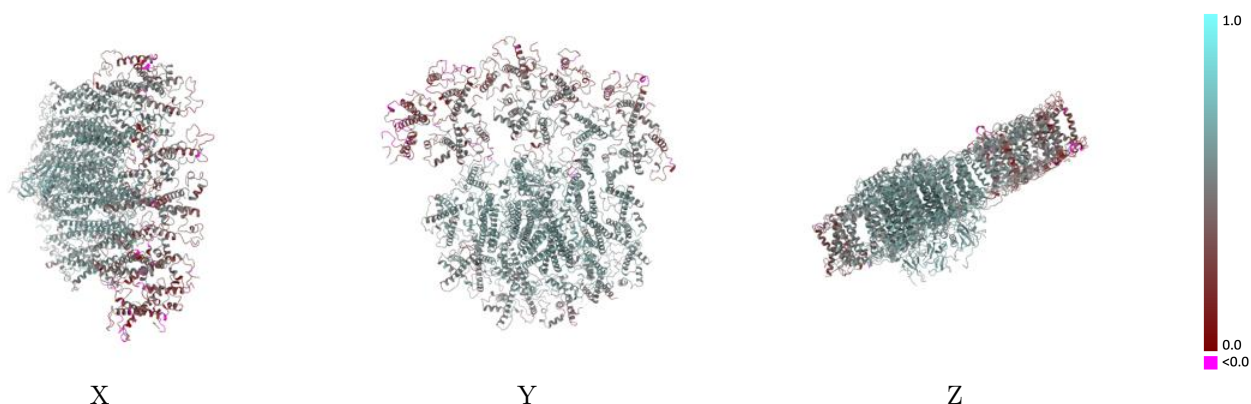
This section contains information regarding the fit between EMDB map EMD-33737 and PDB model 7YCA. Per-residue inclusion information can be found in [section 3](#) on [page 44](#).

### 9.1 Map-model overlay [i](#)



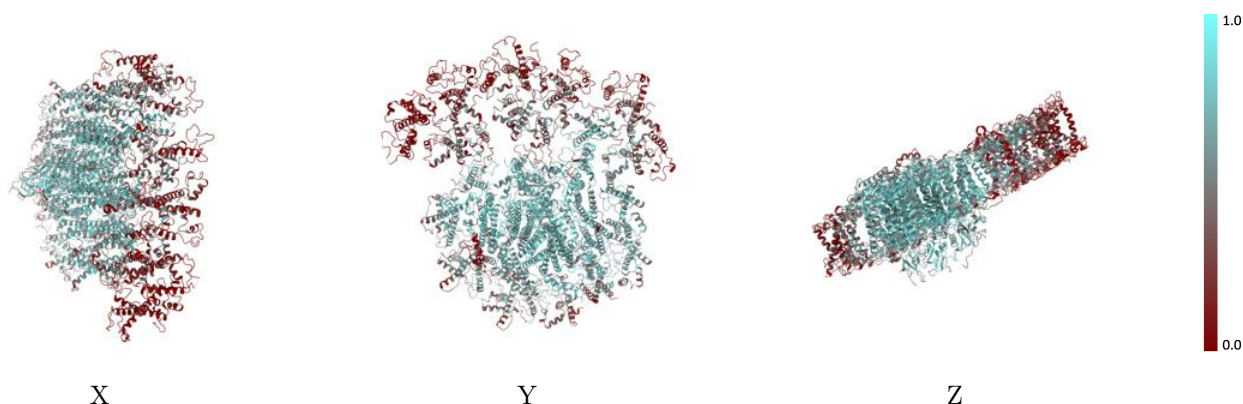
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



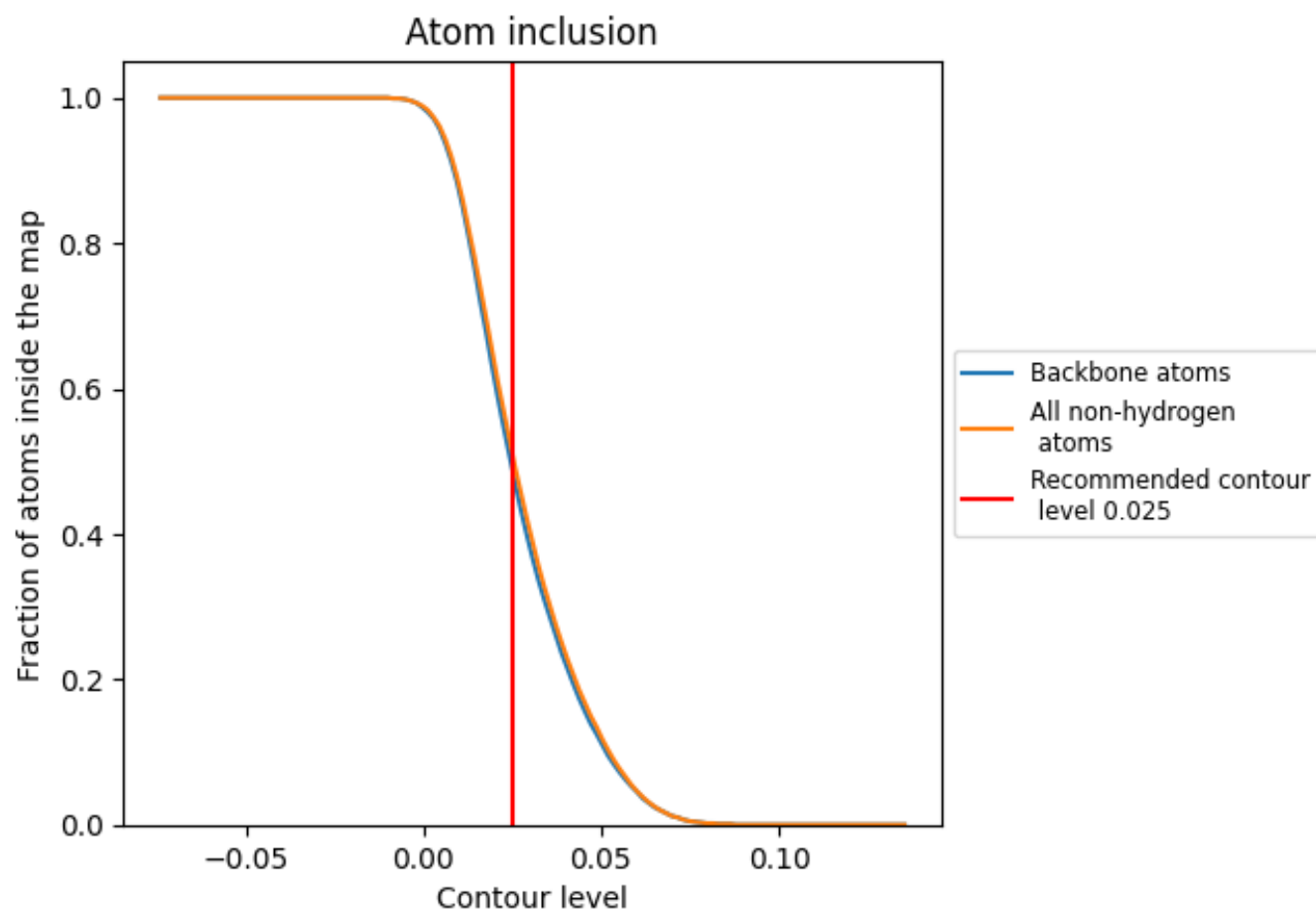
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

