



wwPDB EM Validation Summary Report ⓘ

Dec 1, 2025 – 09:42 PM JST

PDB ID : 8ZOC / pdb_00008zoc
EMDB ID : EMD-60288
Title : Structure of the canthaxanthin mutant PSI-9VCPI supercomplex in Nan-
nochloropsis oceanica
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

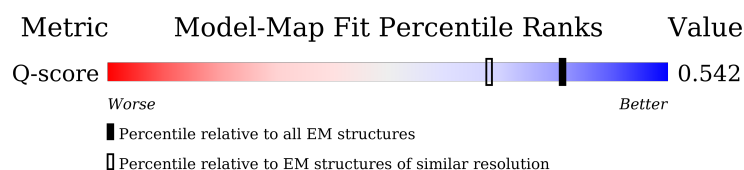
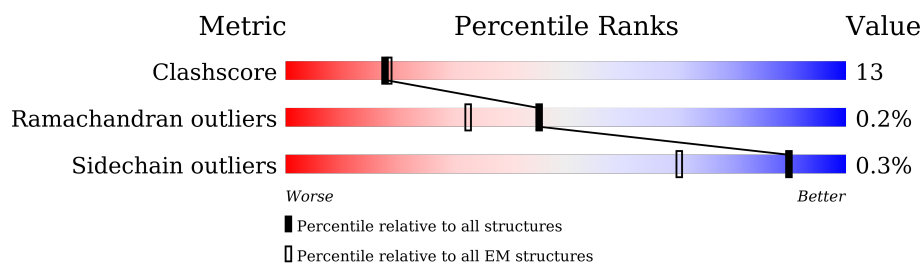
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11965 (2.35 - 3.35)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	5	244	
2	9	232	
3	8	200	
4	4	202	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	7	202	
5	3	220	
6	6	259	
7	2	223	
8	1	208	
9	a	745	
10	b	737	
11	d	136	
12	e	67	
13	f	185	
14	h	128	
15	i	45	
16	j	41	
17	l	172	
18	m	30	
19	g	55	
20	c	81	

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
23	CLA	1	305	X	-	-	-
23	CLA	1	306	X	-	-	-
23	CLA	1	307	X	-	-	-
23	CLA	1	308	X	-	-	-
23	CLA	1	309	X	-	-	-
23	CLA	1	310	X	-	-	-
23	CLA	1	311	X	-	-	-
23	CLA	1	312	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	1	313	X	-	-	-
23	CLA	1	314	X	-	-	-
23	CLA	2	306	X	-	-	-
23	CLA	2	307	X	-	-	-
23	CLA	2	308	X	-	-	-
23	CLA	2	309	X	-	-	-
23	CLA	2	310	X	-	-	-
23	CLA	2	311	X	-	-	-
23	CLA	2	312	X	-	-	-
23	CLA	2	313	X	-	-	-
23	CLA	2	314	X	-	-	-
23	CLA	2	315	X	-	-	-
23	CLA	2	316	X	-	-	-
23	CLA	3	307	X	-	-	-
23	CLA	3	308	X	-	-	-
23	CLA	3	309	X	-	-	-
23	CLA	3	310	X	-	-	-
23	CLA	3	311	X	-	-	-
23	CLA	3	312	X	-	-	-
23	CLA	3	313	X	-	-	-
23	CLA	3	314	X	-	-	-
23	CLA	3	315	X	-	-	-
23	CLA	4	306	X	-	-	-
23	CLA	4	307	X	-	-	-
23	CLA	4	308	X	-	-	-
23	CLA	4	309	X	-	-	-
23	CLA	4	310	X	-	-	-
23	CLA	4	311	X	-	-	-
23	CLA	4	312	X	-	-	-
23	CLA	4	313	X	-	-	-
23	CLA	4	314	X	-	-	-
23	CLA	4	315	X	-	-	-
23	CLA	4	316	X	-	-	-
23	CLA	4	317	X	-	-	-
23	CLA	5	305	X	-	-	-
23	CLA	5	306	X	-	-	-
23	CLA	5	307	X	-	-	-
23	CLA	5	308	X	-	-	-
23	CLA	5	309	X	-	-	-
23	CLA	5	310	X	-	-	-
23	CLA	5	311	X	-	-	-
23	CLA	5	312	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	5	313	X	-	-	-
23	CLA	5	314	X	-	-	-
23	CLA	5	315	X	-	-	-
23	CLA	6	307	X	-	-	-
23	CLA	6	308	X	-	-	-
23	CLA	6	309	X	-	-	-
23	CLA	6	310	X	-	-	-
23	CLA	6	311	X	-	-	-
23	CLA	6	312	X	-	-	-
23	CLA	6	313	X	-	-	-
23	CLA	6	314	X	-	-	-
23	CLA	6	315	X	-	-	-
23	CLA	6	316	X	-	-	-
23	CLA	6	317	X	-	-	-
23	CLA	7	306	X	-	-	-
23	CLA	7	307	X	-	-	-
23	CLA	7	308	X	-	-	-
23	CLA	7	309	X	-	-	-
23	CLA	7	310	X	-	-	-
23	CLA	7	311	X	-	-	-
23	CLA	7	312	X	-	-	-
23	CLA	7	313	X	-	-	-
23	CLA	7	314	X	-	-	-
23	CLA	7	315	X	-	-	-
23	CLA	7	316	X	-	-	-
23	CLA	7	317	X	-	-	-
23	CLA	8	305	X	-	-	-
23	CLA	8	306	X	-	-	-
23	CLA	8	307	X	-	-	-
23	CLA	8	308	X	-	-	-
23	CLA	8	309	X	-	-	-
23	CLA	8	310	X	-	-	-
23	CLA	8	311	X	-	-	-
23	CLA	8	312	X	-	-	-
23	CLA	8	313	X	-	-	-
23	CLA	8	314	X	-	-	-
23	CLA	9	308	X	-	-	-
23	CLA	9	309	X	-	-	-
23	CLA	9	310	X	-	-	-
23	CLA	9	311	X	-	-	-
23	CLA	9	312	X	-	-	-
23	CLA	9	313	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	9	314	X	-	-	-
23	CLA	9	315	X	-	-	-
23	CLA	9	316	X	-	-	-
23	CLA	9	318	X	-	-	-
23	CLA	a	801	X	-	-	-
23	CLA	a	802	X	-	-	-
23	CLA	a	803	X	-	-	-
23	CLA	a	804	X	-	-	-
23	CLA	a	805	X	-	-	-
23	CLA	a	806	X	-	-	-
23	CLA	a	807	X	-	-	-
23	CLA	a	808	X	-	-	-
23	CLA	a	809	X	-	-	-
23	CLA	a	810	X	-	-	-
23	CLA	a	811	X	-	-	-
23	CLA	a	812	X	-	-	-
23	CLA	a	813	X	-	-	-
23	CLA	a	814	X	-	-	-
23	CLA	a	815	X	-	-	-
23	CLA	a	816	X	-	-	-
23	CLA	a	817	X	-	-	-
23	CLA	a	818	X	-	-	-
23	CLA	a	819	X	-	-	-
23	CLA	a	820	X	-	-	-
23	CLA	a	821	X	-	-	-
23	CLA	a	822	X	-	-	-
23	CLA	a	823	X	-	-	-
23	CLA	a	824	X	-	-	-
23	CLA	a	825	X	-	-	-
23	CLA	a	826	X	-	-	-
23	CLA	a	827	X	-	-	-
23	CLA	a	828	X	-	-	-
23	CLA	a	829	X	-	-	-
23	CLA	a	830	X	-	-	-
23	CLA	a	831	X	-	-	-
23	CLA	a	832	X	-	-	-
23	CLA	a	833	X	-	-	-
23	CLA	a	834	X	-	-	-
23	CLA	a	835	X	-	-	-
23	CLA	a	836	X	-	-	-
23	CLA	a	837	X	-	-	-
23	CLA	a	838	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	a	839	X	-	-	-
23	CLA	a	840	X	-	-	-
23	CLA	a	841	X	-	-	-
23	CLA	a	842	X	-	-	-
23	CLA	a	844	X	-	-	-
23	CLA	a	854	X	-	-	-
23	CLA	b	801	X	-	-	-
23	CLA	b	802	X	-	-	-
23	CLA	b	803	X	-	-	-
23	CLA	b	804	X	-	-	-
23	CLA	b	805	X	-	-	-
23	CLA	b	806	X	-	-	-
23	CLA	b	807	X	-	-	-
23	CLA	b	808	X	-	-	-
23	CLA	b	809	X	-	-	-
23	CLA	b	810	X	-	-	-
23	CLA	b	811	X	-	-	-
23	CLA	b	812	X	-	-	-
23	CLA	b	813	X	-	-	-
23	CLA	b	814	X	-	-	-
23	CLA	b	815	X	-	-	-
23	CLA	b	816	X	-	-	-
23	CLA	b	817	X	-	-	-
23	CLA	b	818	X	-	-	-
23	CLA	b	819	X	-	-	-
23	CLA	b	820	X	-	-	-
23	CLA	b	821	X	-	-	-
23	CLA	b	822	X	-	-	-
23	CLA	b	823	X	-	-	-
23	CLA	b	824	X	-	-	-
23	CLA	b	825	X	-	-	-
23	CLA	b	826	X	-	-	-
23	CLA	b	827	X	-	-	-
23	CLA	b	828	X	-	-	-
23	CLA	b	829	X	-	-	-
23	CLA	b	830	X	-	-	-
23	CLA	b	831	X	-	-	-
23	CLA	b	832	X	-	-	-
23	CLA	b	833	X	-	-	-
23	CLA	b	834	X	-	-	-
23	CLA	b	835	X	-	-	-
23	CLA	b	836	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	b	837	X	-	-	-
23	CLA	b	838	X	-	-	-
23	CLA	b	839	X	-	-	-
23	CLA	b	840	X	-	-	-
23	CLA	f	802	X	-	-	-
23	CLA	f	803	X	-	-	-
23	CLA	h	204	X	-	-	-
23	CLA	j	102	X	-	-	-
23	CLA	j	103	X	-	-	-
23	CLA	l	202	X	-	-	-
23	CLA	l	203	X	-	-	-
23	CLA	l	204	X	-	-	-
32	SF4	c	102	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 43772 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 VCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	169	Total	C	N	O	S	0	0
			1317	867	222	222	6		

- Molecule 2 is a protein called VCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	201	Total	C	N	O	S	0	0
			1466	936	256	269	5		

- Molecule 3 is a protein called VCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	164	Total	C	N	O	S	0	0
			1258	822	203	227	6		

- Molecule 4 is a protein called VCPI-4/7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	168	Total	C	N	O	S	0	0
			1268	822	211	229	6		
4	7	166	Total	C	N	O	S	0	0
			1220	791	202	222	5		

- Molecule 5 is a protein called VCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	177	Total	C	N	O	S	0	0
			1324	846	225	245	8		

- Molecule 6 is a protein called VCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	180	Total	C	N	O	S	0	0
			1352	880	223	244	5		

- Molecule 7 is a protein called VCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	185	Total	C	N	O	S	0	0
			1372	892	224	249	7		

- Molecule 8 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	739	Total	C	N	O	S	0	0
			5827	3828	982	1000	17		

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	735	Total	C	N	O	S	0	0
			5865	3874	985	989	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	130	Total	C	N	O	S	0	0
			1014	652	175	184	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	61	Total	C	N	O	0	0
			494	314	86	94		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	f	160	Total	C	N	O	S	0	0
			1266	815	213	235	3		

- Molecule 14 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	85	Total	C	N	O	S	0	0
			646	427	100	117	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	i	34	Total	C	N	O	S	0	0
			271	189	36	45	1		

- 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
			339	233	48	57	1		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	l	171	Total	C	N	O		0	0
			1283	848	203	232			

- Molecule 18 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	m	30	Total	C	N	O		0	0
			210	137	35	38			

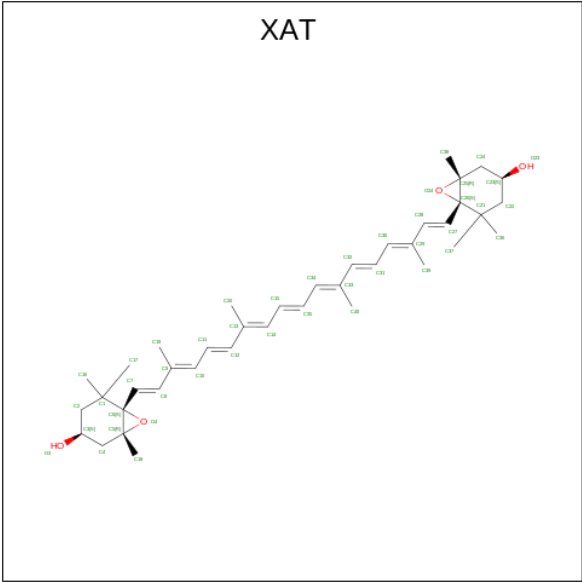
- Molecule 19 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	55	Total	C	N	O		0	0
			275	165	55	55			

- Molecule 20 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	80	Total	C	N	O	S	0	0
			596	366	103	117	10		

- Molecule 21 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	5	1	Total	C	O	0
			44	40	4	
21	5	1	Total	C	O	0
			44	40	4	
21	5	1	Total	C	O	0
			44	40	4	
21	9	1	Total	C	O	0
			44	40	4	
21	9	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

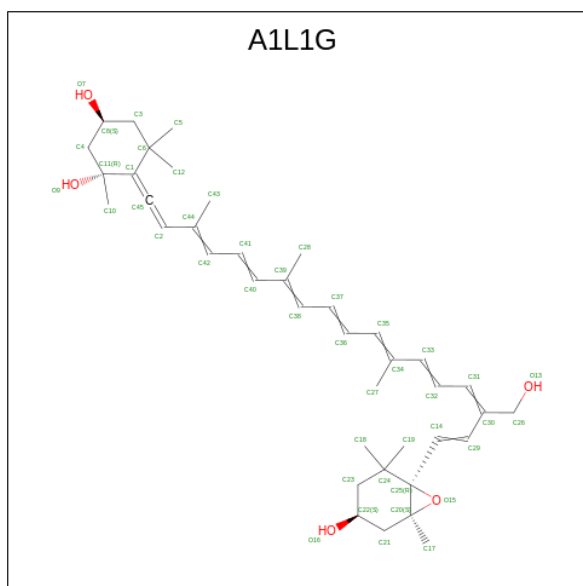
Mol	Chain	Residues	Atoms			AltConf
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	1	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	a	1	Total	C	O	0
			44	40	4	
21	j	1	Total	C	O	0
			44	40	4	

- Molecule 22 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



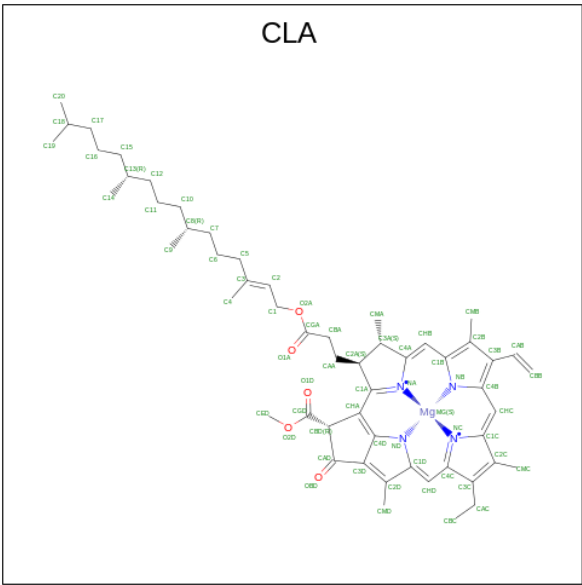
Mol	Chain	Residues	Atoms			AltConf
22	5	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	
22	7	1	Total	C	O	0
			45	40	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			45	40	5	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	4	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	2	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	2	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	2	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
23	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
23	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
23	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	1	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	1	1	Total 52	C 42	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	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
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	b	1	Total 59	C 49	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

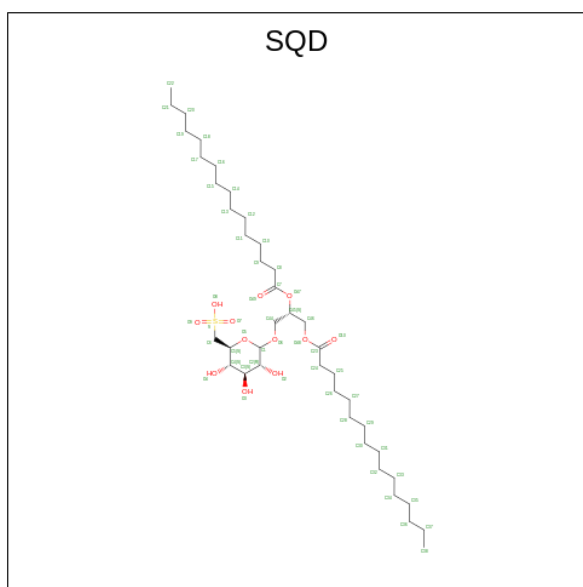
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

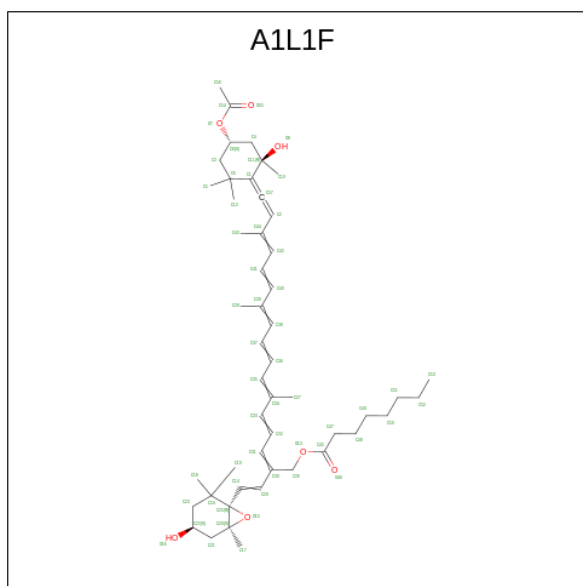
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



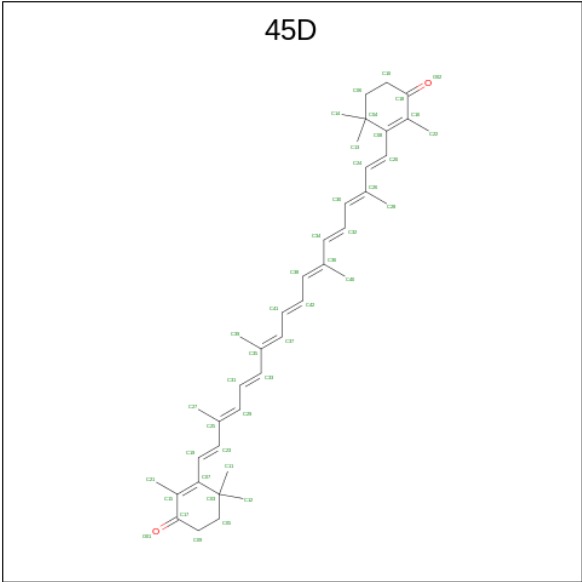
Mol	Chain	Residues	Atoms				AltConf
24	5	1	Total	C	O	S	0
			35	22	12	1	
24	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 25 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: C₅₀H₇₂O₇) (labeled as "Ligand of Interest" by depositor).



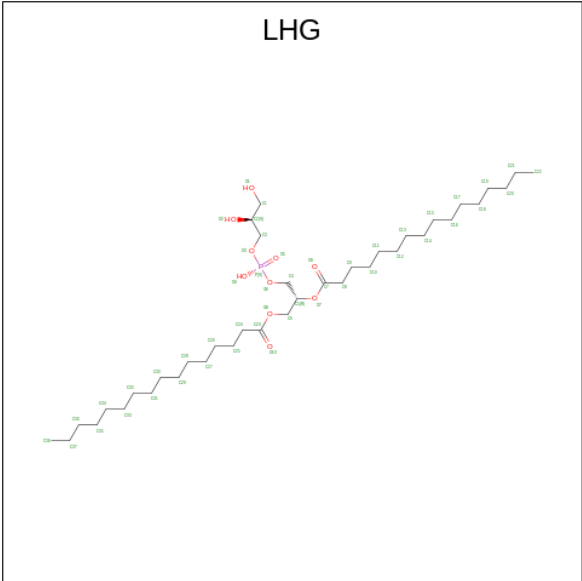
Mol	Chain	Residues	Atoms				AltConf
25	9	1	Total	C	O		0
			57	50	7		
25	8	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			53	46	7		
25	1	1	Total	C	O		0
			57	50	7		
25	h	1	Total	C	O		0
			57	50	7		

- Molecule 26 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	9	1	Total	C	O	0
			42	40	2	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



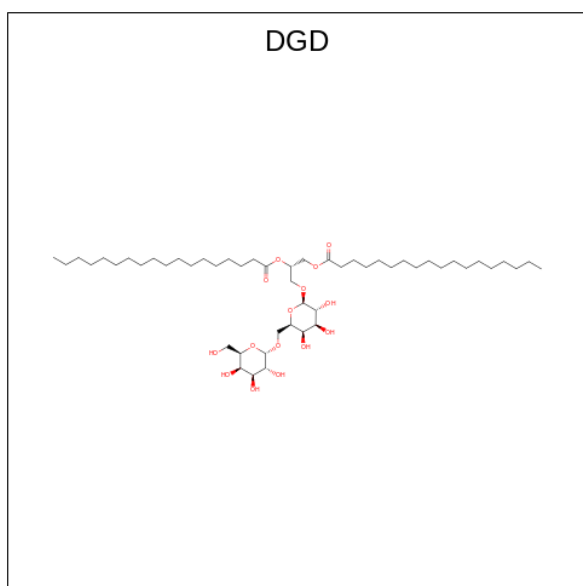
Mol	Chain	Residues	Atoms				AltConf
27	9	1	Total	C	O	P	0
			36	25	10	1	
27	9	1	Total	C	O	P	0
			46	35	10	1	

Continued on next page...

Continued from previous page...

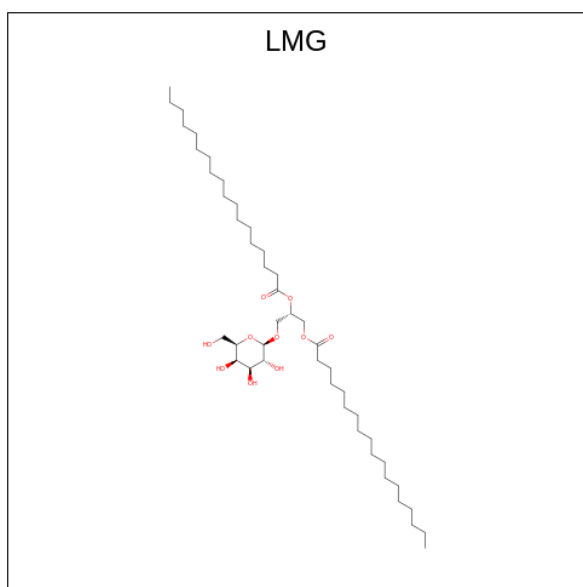
Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	C	O	P	0
			48	37	10	1	
27	a	1	Total	C	O	P	0
			27	16	10	1	
27	b	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



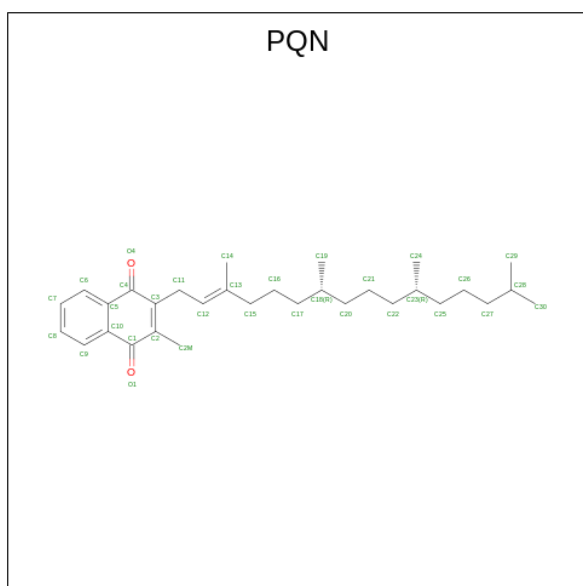
Mol	Chain	Residues	Atoms			AltConf
28	8	1	Total	C	O	0
			40	25	15	
28	4	1	Total	C	O	0
			40	25	15	
28	b	1	Total	C	O	0
			57	42	15	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



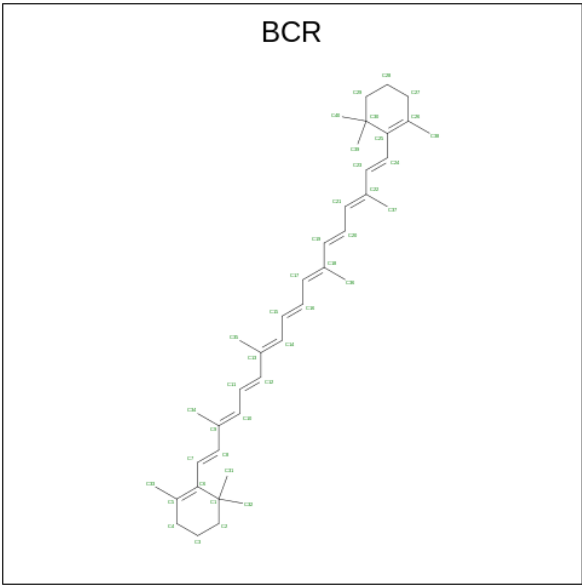
Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			35	25	10	
29	a	1	Total	C	O	0
			34	24	10	
29	j	1	Total	C	O	0
			32	22	10	

- Molecule 30 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	a	1	Total	C	O	0
			33	31	2	
30	b	1	Total	C	O	0
			33	31	2	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



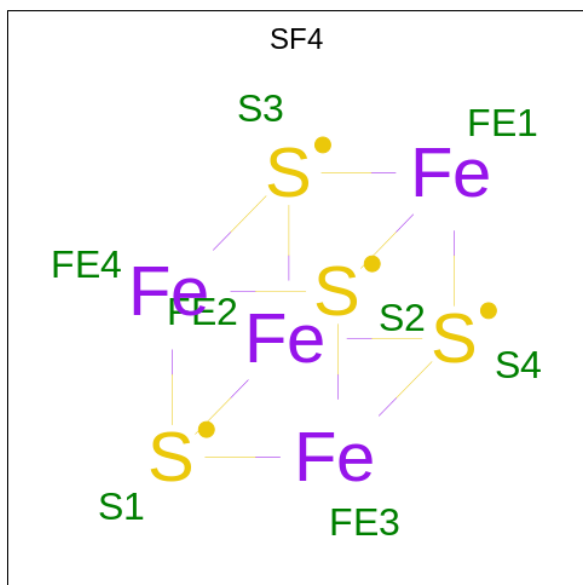
Mol	Chain	Residues	Atoms		AltConf
31	a	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C 40 40	0
31	f	1	Total C 40 40	0
31	f	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	i	1	Total C 40 40	0
31	j	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	m	1	Total C 40 40	0

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



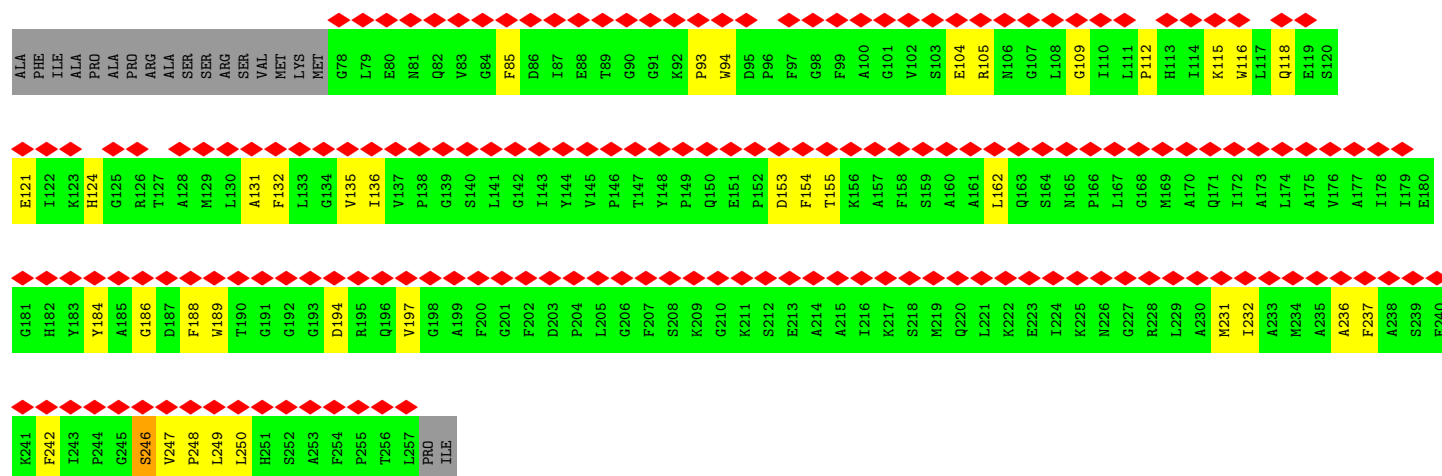
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total Fe S 8 4 4	0

Continued on next page...

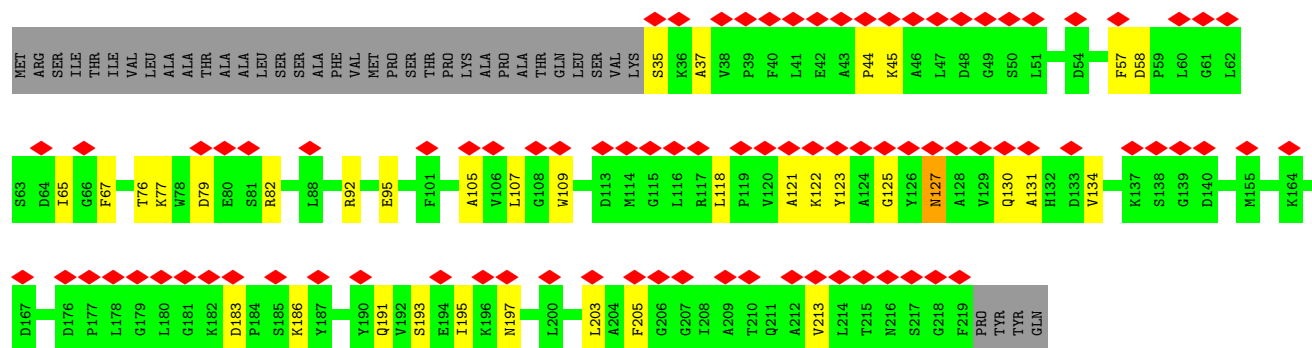
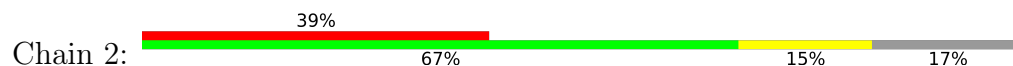
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
32	c	1	Total	Fe	S	0
			8	4	4	
32	c	1	Total	Fe	S	0
			8	4	4	

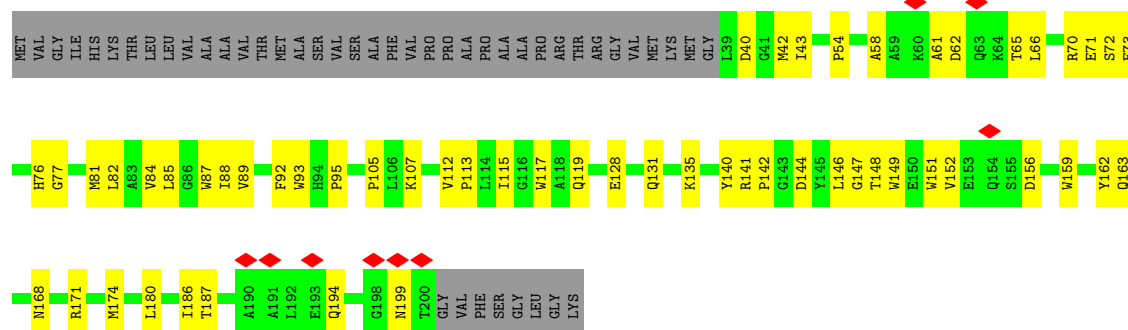




- Molecule 7: VCPI-2

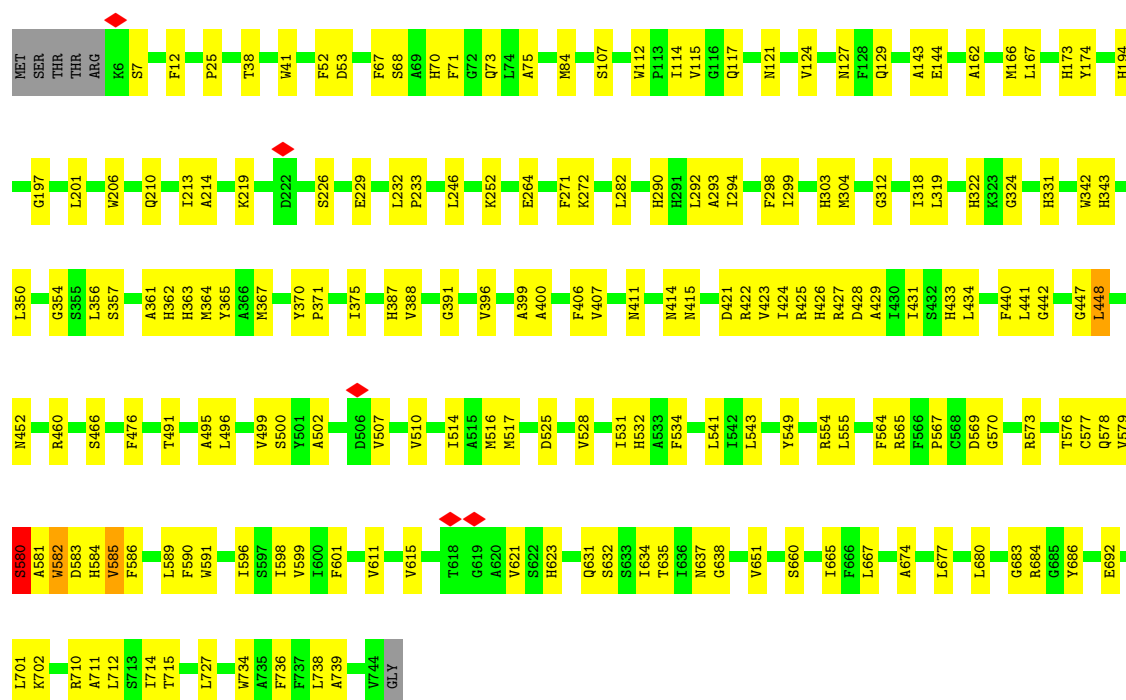


- Molecule 8: VCPI-1



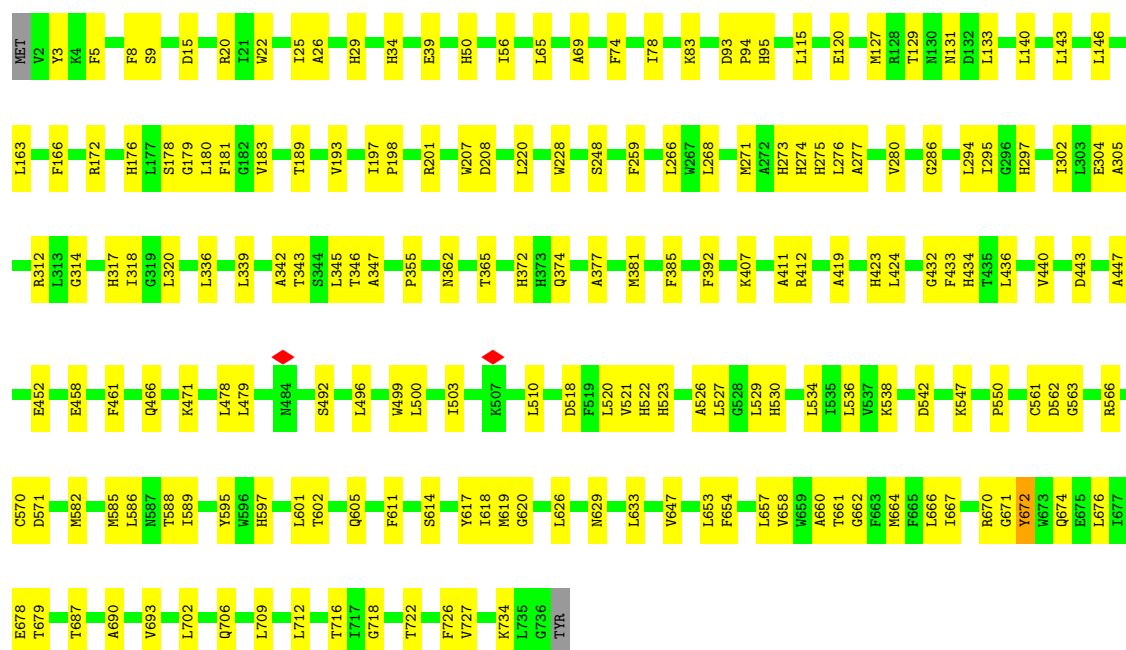
- Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1





• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 75% 25%

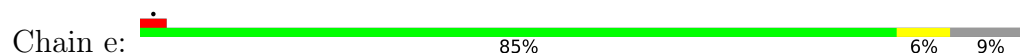


• Molecule 11: Photosystem I reaction center subunit II

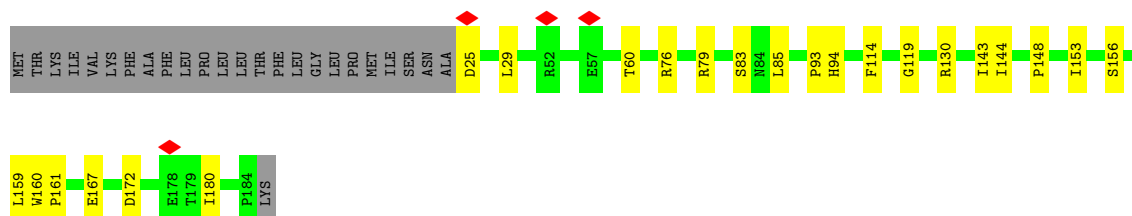
Chain d: 77% 18%



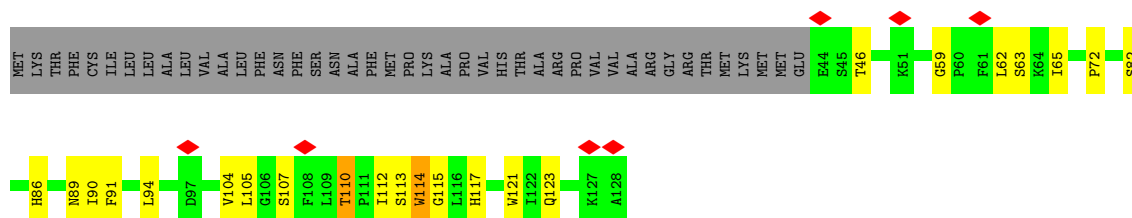
- Molecule 12: Photosystem I reaction center subunit IV



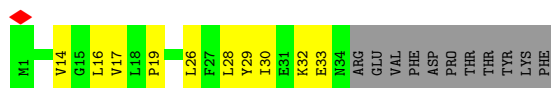
- Molecule 13: Photosystem I reaction center subunit III



- Molecule 14: Psar



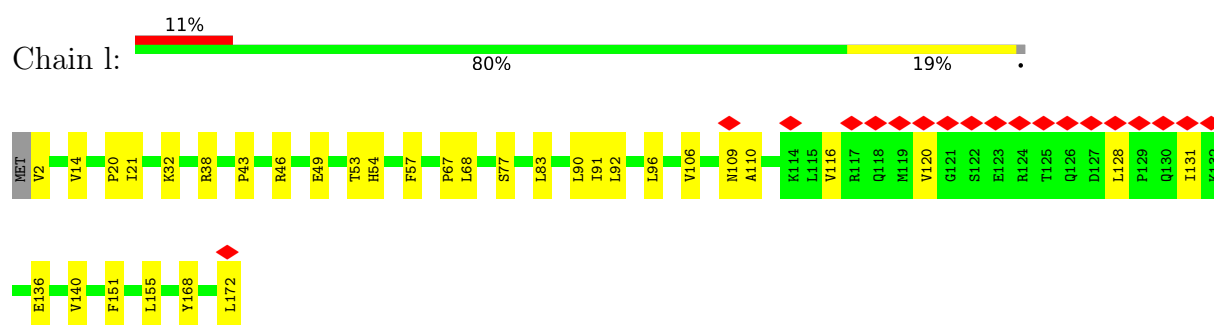
- Molecule 15: Photosystem I reaction center subunit VIII



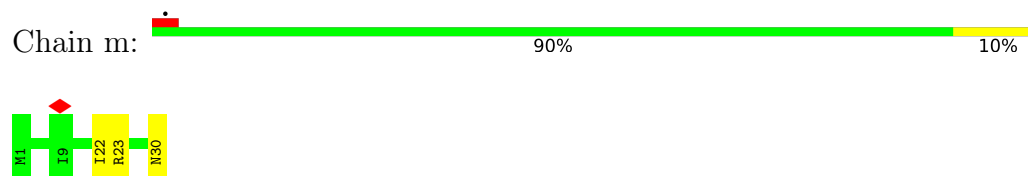
- Molecule 16: Photosystem I reaction center subunit IX



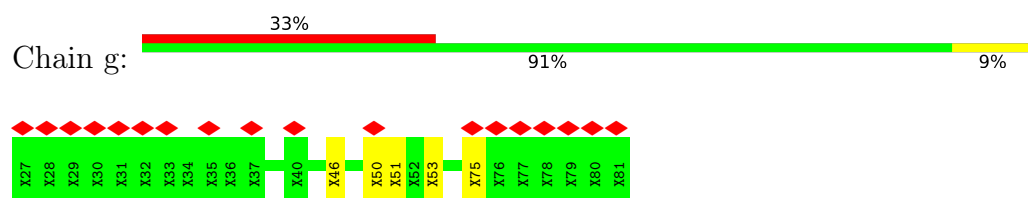
- Molecule 17: PSI subunit V



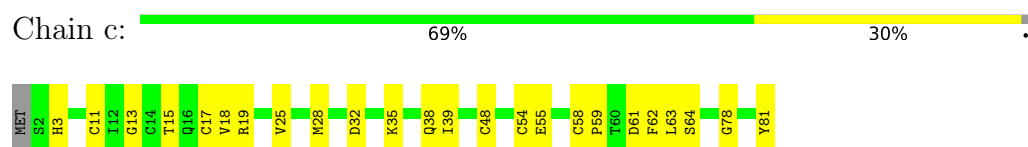
- Molecule 18: PsaM



- Molecule 19: PsaS



- Molecule 20: Photosystem I iron-sulfur center



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.811	Depositor
Minimum map value	-0.420	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.287	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1L1F, SF4, BCR, XAT, LMG, CLA, LHG, A1L1G, SQD, 45D, DGD, PQN

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	5	0.14	0/1353	0.29	0/1823
2	9	0.35	0/1496	0.33	0/2032
3	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
4	4	0.17	0/1298	0.32	0/1761
4	7	0.18	0/1248	0.37	0/1700
5	3	0.12	0/1350	0.27	0/1821
6	6	0.17	0/1390	0.31	0/1883
7	2	0.14	0/1405	0.36	0/1904
8	1	0.13	0/1293	0.33	0/1759
9	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
10	b	0.20	0/6080	0.32	1/8302 (0.0%)
11	d	0.12	0/1040	0.32	0/1402
12	e	0.09	0/502	0.20	0/681
13	f	0.14	0/1297	0.31	0/1762
14	h	0.51	1/667 (0.1%)	0.52	0/915
15	i	0.14	0/278	0.33	0/378
16	j	0.15	0/351	0.35	0/478
17	l	0.14	0/1315	0.31	0/1796
18	m	0.09	0/210	0.28	0/288
20	c	0.13	0/606	0.34	0/822
All	All	0.23	5/30489 (0.0%)	0.33	8/41469 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	580	SER	CA-C	-7.04	1.43	1.52
3	8	44	LEU	C-O	-6.11	1.15	1.23
9	a	581	ALA	CA-C	-5.46	1.45	1.52
14	h	114	TRP	C-O	-5.26	1.18	1.24
9	a	582	TRP	CA-C	-5.03	1.45	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	581	ALA	N-CA-C	-8.62	102.51	113.72
9	a	448	LEU	N-CA-C	-6.08	104.22	111.69
3	8	39	LYS	N-CA-C	-6.06	105.72	113.23
9	a	584	HIS	N-CA-C	-5.82	106.53	113.97
10	b	672	TYR	N-CA-C	-5.56	106.33	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1317	0	1318	39	0
2	9	1466	0	1470	52	0
3	8	1258	0	1280	32	0
4	4	1268	0	1288	23	0
4	7	1220	0	1209	43	0
5	3	1324	0	1340	23	0
6	6	1352	0	1334	30	0
7	2	1372	0	1347	23	0
8	1	1262	0	1237	42	0
9	a	5827	0	5697	141	0
10	b	5865	0	5710	151	0
11	d	1014	0	1015	19	0
12	e	494	0	495	4	0
13	f	1266	0	1262	21	0
14	h	646	0	649	19	0
15	i	271	0	292	12	0
16	j	339	0	342	21	0
17	l	1283	0	1278	26	0
18	m	210	0	226	3	0
19	g	275	0	62	3	0
20	c	596	0	583	20	0
21	1	88	0	112	5	0
21	2	220	0	280	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	3	176	0	224	19	0
21	4	220	0	280	26	0
21	5	132	0	168	18	0
21	6	176	0	224	20	0
21	7	176	0	224	29	0
21	8	132	0	168	16	0
21	9	88	0	112	14	0
21	a	44	0	56	4	0
21	j	44	0	56	7	0
22	1	45	0	0	1	0
22	3	90	0	0	0	0
22	5	45	0	0	1	0
22	7	45	0	0	2	0
22	9	90	0	0	3	0
23	1	547	0	508	14	0
23	2	544	0	452	12	0
23	3	458	0	378	8	0
23	4	613	0	522	33	0
23	5	563	0	472	23	0
23	6	564	0	485	15	0
23	7	576	0	444	22	0
23	8	507	0	429	23	0
23	9	519	0	452	37	0
23	a	2579	0	2562	144	0
23	b	2410	0	2464	136	0
23	f	117	0	115	2	0
23	h	55	0	49	3	0
23	j	100	0	86	10	0
23	l	148	0	123	3	0
24	1	45	0	54	2	0
24	5	35	0	34	1	0
25	1	57	0	0	2	0
25	6	110	0	0	6	0
25	8	57	0	0	2	0
25	9	57	0	0	2	0
25	h	57	0	0	4	0
26	9	42	0	52	8	0
27	9	82	0	110	5	0
27	a	75	0	93	7	0
27	b	31	0	32	1	0
28	4	40	0	38	11	0
28	8	40	0	38	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	57	0	72	6	0
29	2	35	0	40	3	0
29	a	34	0	38	10	0
29	j	32	0	34	6	0
30	a	33	0	46	5	0
30	b	33	0	46	3	0
31	a	160	0	224	15	0
31	b	240	0	336	26	0
31	f	80	0	112	15	0
31	h	80	0	112	8	0
31	i	40	0	56	2	0
31	j	40	0	56	9	0
31	l	80	0	112	14	0
31	m	40	0	56	1	0
32	a	8	0	0	0	0
32	c	16	0	0	3	0
All	All	43772	0	42670	1138	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 13.

The worst 5 of 1138 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)
4:4:193:ALA:HB1	28:4:318:DGD:HE62	1.13	1.13
4:4:193:ALA:HB1	28:4:318:DGD:C6E	1.85	1.05
28:4:318:DGD:O4E	28:4:318:DGD:O5E	1.61	1.02
21:2:303:XAT:H32	23:2:308:CLA:HAB	1.52	0.90
21:5:302:XAT:H12	23:5:307:CLA:HAB	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	25	43
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	22	40
4	7	164/202 (81%)	144 (88%)	20 (12%)	0	100	100
5	3	175/220 (80%)	166 (95%)	9 (5%)	0	100	100
6	6	178/259 (69%)	158 (89%)	20 (11%)	0	100	100
7	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	8	18
8	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
9	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	69
10	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
11	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
12	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
13	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
14	h	83/128 (65%)	76 (92%)	6 (7%)	1 (1%)	11	23
15	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
16	j	39/41 (95%)	39 (100%)	0	0	100	100
17	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	11	23
18	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
20	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3798/4357 (87%)	3551 (94%)	238 (6%)	9 (0%)	45	63

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	9	32	THR
7	2	45	LYS
17	1	120	VAL
7	2	127	ASN
7	2	213	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	133/182 (73%)	133 (100%)	0	100	100
2	9	141/167 (84%)	139 (99%)	2 (1%)	62	82
3	8	132/160 (82%)	131 (99%)	1 (1%)	79	90
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	122/159 (77%)	121 (99%)	1 (1%)	79	90
5	3	136/164 (83%)	136 (100%)	0	100	100
6	6	135/201 (67%)	134 (99%)	1 (1%)	81	91
7	2	134/172 (78%)	134 (100%)	0	100	100
8	1	128/165 (78%)	128 (100%)	0	100	100
9	a	607/613 (99%)	603 (99%)	4 (1%)	81	91
10	b	599/602 (100%)	599 (100%)	0	100	100
11	d	107/113 (95%)	107 (100%)	0	100	100
12	e	56/62 (90%)	56 (100%)	0	100	100
13	f	138/162 (85%)	138 (100%)	0	100	100
14	h	71/107 (66%)	70 (99%)	1 (1%)	62	82
15	i	32/43 (74%)	32 (100%)	0	100	100
16	j	36/36 (100%)	36 (100%)	0	100	100
17	l	130/141 (92%)	130 (100%)	0	100	100
18	m	21/24 (88%)	21 (100%)	0	100	100
20	c	67/68 (98%)	67 (100%)	0	100	100
All	All	3058/3500 (87%)	3048 (100%)	10 (0%)	90	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	a	579	VAL
9	a	580	SER
14	h	110	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	6	246	SER
4	7	95	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
10	b	605	GLN
13	f	166	GLN
11	d	7	GLN
8	1	194	GLN
10	b	326	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

273 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	$\# Z > 2$
23	CLA	4	310	-	65,73,73	1.49	5 (7%)	76,113,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	820	-	50,58,73	1.70	6 (12%)	58,95,113	1.60	10 (17%)
22	A1L1G	7	302	-	38,47,47	1.44	6 (15%)	49,71,71	1.50	9 (18%)
23	CLA	a	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
21	XAT	3	301	-	39,47,47	0.90	1 (2%)	54,74,74	2.55	18 (33%)
23	CLA	7	311	-	46,54,73	1.79	6 (13%)	53,90,113	1.57	7 (13%)
23	CLA	7	313	-	54,62,73	1.66	5 (9%)	62,99,113	1.50	9 (14%)
31	BCR	1	205	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
23	CLA	3	308	-	47,55,73	1.76	5 (10%)	54,91,113	1.57	8 (14%)
23	CLA	5	312	-	52,60,73	1.66	5 (9%)	60,97,113	1.56	9 (15%)
22	A1L1G	9	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.57	10 (20%)
23	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	a	804	-	55,63,73	1.62	6 (10%)	64,101,113	1.55	9 (14%)
21	XAT	5	301	-	39,47,47	0.94	1 (2%)	54,74,74	2.57	19 (35%)
23	CLA	a	825	-	55,63,73	1.61	5 (9%)	64,101,113	1.45	8 (12%)
23	CLA	j	102	-	58,66,73	1.59	6 (10%)	67,104,113	1.42	8 (11%)
21	XAT	7	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.63	20 (37%)
28	DGD	b	848	-	58,58,67	1.15	7 (12%)	72,72,81	1.53	10 (13%)
31	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.05	16 (28%)
21	XAT	6	302	-	39,47,47	0.91	0	54,74,74	2.81	20 (37%)
21	XAT	7	304	-	39,47,47	0.91	1 (2%)	54,74,74	2.67	21 (38%)
23	CLA	1	309	8	46,54,73	1.78	6 (13%)	53,90,113	1.50	7 (13%)
31	BCR	b	844	-	41,41,41	0.68	0	56,56,56	2.10	16 (28%)
23	CLA	7	308	-	60,68,73	1.53	5 (8%)	70,107,113	1.44	7 (10%)
25	A1L1F	6	301	-	50,59,59	1.30	5 (10%)	62,85,85	2.50	20 (32%)
23	CLA	3	314	5	47,55,73	1.74	5 (10%)	54,91,113	1.54	6 (11%)
31	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
25	A1L1F	6	304	-	46,55,59	1.32	4 (8%)	58,81,85	2.56	20 (34%)
23	CLA	8	307	3	65,73,73	1.47	5 (7%)	76,113,113	1.38	8 (10%)
23	CLA	2	307	-	47,55,73	1.73	5 (10%)	54,91,113	1.64	7 (12%)
23	CLA	a	840	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	8 (10%)
21	XAT	8	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.66	20 (37%)
21	XAT	8	301	-	39,47,47	0.91	1 (2%)	54,74,74	2.53	19 (35%)
23	CLA	b	802	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
23	CLA	6	312	6	51,59,73	1.68	6 (11%)	59,96,113	1.52	6 (10%)
23	CLA	b	832	-	65,73,73	1.46	5 (7%)	76,113,113	1.39	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	b	842	-	41,41,41	0.71	0	56,56,56	2.29	20 (35%)
23	CLA	a	821	-	45,53,73	1.77	6 (13%)	52,89,113	1.64	6 (11%)
23	CLA	b	826	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	6 (7%)
23	CLA	a	820	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	9 (11%)
21	XAT	9	303	-	39,47,47	0.94	1 (2%)	54,74,74	2.61	19 (35%)
23	CLA	8	312	3	52,60,73	1.65	5 (9%)	60,97,113	1.52	8 (13%)
23	CLA	1	313	-	41,49,73	1.85	6 (14%)	47,84,113	1.64	7 (14%)
23	CLA	a	841	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	9 (11%)
23	CLA	2	306	-	41,50,73	1.86	6 (14%)	46,85,113	1.56	6 (13%)
23	CLA	a	801	-	65,73,73	1.50	8 (12%)	76,113,113	1.38	7 (9%)
21	XAT	4	301	-	39,47,47	0.94	2 (5%)	54,74,74	2.63	19 (35%)
23	CLA	a	822	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
23	CLA	a	817	-	45,53,73	1.80	5 (11%)	52,89,113	1.58	6 (11%)
23	CLA	4	308	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	9 (11%)
23	CLA	1	310	8	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
23	CLA	b	812	-	53,61,73	1.64	5 (9%)	61,98,113	1.49	8 (13%)
31	BCR	f	801	-	41,41,41	0.68	0	56,56,56	2.14	16 (28%)
23	CLA	4	316	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
23	CLA	b	806	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	7 (9%)
23	CLA	3	309	5	56,64,73	1.60	6 (10%)	65,102,113	1.46	7 (10%)
30	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.09	3 (7%)
23	CLA	1	203	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	7 (10%)
23	CLA	6	310	-	52,60,73	1.66	5 (9%)	60,97,113	1.53	8 (13%)
23	CLA	a	816	-	50,58,73	1.68	6 (12%)	58,95,113	1.58	8 (13%)
23	CLA	5	311	-	51,59,73	1.65	5 (9%)	59,96,113	1.53	9 (15%)
21	XAT	4	302	-	39,47,47	0.91	0	54,74,74	2.57	20 (37%)
21	XAT	6	305	-	39,47,47	0.90	1 (2%)	54,74,74	2.73	19 (35%)
23	CLA	2	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.56	7 (13%)
23	CLA	7	310	-	46,54,73	1.76	5 (10%)	53,90,113	1.56	6 (11%)
23	CLA	5	314	-	52,60,73	1.66	6 (11%)	60,97,113	1.54	8 (13%)
23	CLA	a	831	-	65,73,73	1.50	5 (7%)	76,113,113	1.47	8 (10%)
23	CLA	4	313	-	53,61,73	1.65	5 (9%)	61,98,113	1.49	8 (13%)
23	CLA	a	836	-	50,58,73	1.69	5 (10%)	58,95,113	1.51	9 (15%)
23	CLA	b	824	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	7 (9%)
25	A1L1F	9	302	-	50,59,59	1.37	5 (10%)	62,85,85	2.71	19 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	A1L1F	8	304	-	50,59,59	1.30	4 (8%)	62,85,85	2.79	23 (37%)
29	LMG	a	853	-	34,34,55	1.13	2 (5%)	42,42,63	1.16	3 (7%)
31	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.13	14 (25%)
31	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
23	CLA	b	805	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	a	803	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	6 (7%)
21	XAT	8	303	-	39,47,47	0.88	1 (2%)	54,74,74	2.64	18 (33%)
21	XAT	9	304	-	39,47,47	0.94	1 (2%)	54,74,74	2.42	19 (35%)
23	CLA	b	816	-	55,63,73	1.62	5 (9%)	64,101,113	1.48	9 (14%)
29	LMG	j	105	-	32,32,55	1.12	2 (6%)	40,40,63	1.14	3 (7%)
23	CLA	4	312	-	46,54,73	1.78	5 (10%)	53,90,113	1.52	7 (13%)
23	CLA	b	813	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	8 (10%)
23	CLA	8	311	-	56,64,73	1.58	5 (8%)	65,102,113	1.51	8 (12%)
23	CLA	4	306	4	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
23	CLA	a	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	9 (11%)
23	CLA	b	829	-	65,73,73	1.51	6 (9%)	76,113,113	1.44	10 (13%)
23	CLA	a	818	-	56,64,73	1.62	5 (8%)	65,102,113	1.43	8 (12%)
23	CLA	b	835	-	58,66,73	1.56	5 (8%)	67,104,113	1.53	8 (11%)
23	CLA	7	307	-	45,53,73	1.79	5 (11%)	52,89,113	1.57	7 (13%)
30	PQN	b	841	-	34,34,34	1.55	2 (5%)	42,45,45	1.20	4 (9%)
23	CLA	a	819	-	54,62,73	1.63	5 (9%)	62,99,113	1.45	7 (11%)
23	CLA	a	802	-	58,66,73	1.55	5 (8%)	67,104,113	1.49	7 (10%)
23	CLA	b	819	-	55,63,73	1.63	6 (10%)	64,101,113	1.44	8 (12%)
23	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	9	316	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
23	CLA	h	204	-	55,63,73	1.62	6 (10%)	64,101,113	1.48	9 (14%)
23	CLA	3	312	5	59,67,73	1.57	6 (10%)	68,105,113	1.43	7 (10%)
31	BCR	l	201	-	41,41,41	0.71	0	56,56,56	1.96	17 (30%)
23	CLA	2	315	-	42,50,73	1.86	5 (11%)	48,85,113	1.56	7 (14%)
23	CLA	a	823	-	49,57,73	1.68	5 (10%)	55,93,113	1.60	7 (12%)
23	CLA	b	814	-	55,63,73	1.61	6 (10%)	64,101,113	1.55	8 (12%)
23	CLA	7	314	-	45,53,73	1.80	6 (13%)	52,89,113	1.65	7 (13%)
31	BCR	b	849	-	41,41,41	0.73	0	56,56,56	2.06	15 (26%)
23	CLA	8	314	-	41,49,73	1.87	5 (12%)	47,84,113	1.65	7 (14%)
23	CLA	2	314	-	56,64,73	1.61	6 (10%)	65,102,113	1.44	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	4	317	-	55,63,73	1.63	5 (9%)	64,101,113	1.47	7 (10%)
23	CLA	b	823	-	53,61,73	1.63	6 (11%)	61,98,113	1.47	8 (13%)
27	LHG	b	847	23	30,30,48	1.33	6 (20%)	33,36,54	1.15	2 (6%)
23	CLA	a	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
23	CLA	a	808	-	51,59,73	1.71	6 (11%)	59,96,113	1.50	8 (13%)
23	CLA	a	832	-	50,58,73	1.70	6 (12%)	58,95,113	1.54	8 (13%)
31	BCR	b	846	-	41,41,41	0.75	0	56,56,56	1.78	15 (26%)
23	CLA	a	811	-	56,64,73	1.59	5 (8%)	65,102,113	1.48	8 (12%)
23	CLA	l	202	-	42,50,73	1.83	6 (14%)	48,85,113	1.64	7 (14%)
31	BCR	m	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	6 (10%)
23	CLA	a	813	-	54,62,73	1.63	5 (9%)	62,99,113	1.44	7 (11%)
23	CLA	b	838	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	6	309	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	6 (7%)
23	CLA	1	308	8	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
23	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	8 (10%)
21	XAT	4	303	-	39,47,47	0.89	0	54,74,74	2.57	18 (33%)
23	CLA	6	316	6	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
23	CLA	l	204	-	46,54,73	1.75	6 (13%)	53,90,113	1.56	7 (13%)
23	CLA	6	308	-	58,66,73	1.60	6 (10%)	67,104,113	1.42	6 (8%)
29	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.31	4 (9%)
22	A1L1G	5	303	-	38,47,47	1.41	6 (15%)	49,71,71	1.46	7 (14%)
24	SQD	5	316	23	34,35,54	1.47	4 (11%)	43,46,65	1.34	7 (16%)
22	A1L1G	9	306	-	38,47,47	1.41	6 (15%)	49,71,71	1.53	8 (16%)
23	CLA	9	311	-	46,54,73	1.75	5 (10%)	53,90,113	1.61	8 (15%)
25	A1L1F	h	203	-	50,59,59	1.38	5 (10%)	62,85,85	2.60	22 (35%)
23	CLA	9	314	-	55,63,73	1.61	6 (10%)	64,101,113	1.50	8 (12%)
23	CLA	1	305	-	61,69,73	1.55	5 (8%)	71,108,113	1.39	7 (9%)
28	DGD	8	315	23	41,41,67	1.05	2 (4%)	55,55,81	1.11	5 (9%)
23	CLA	2	316	7	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
23	CLA	6	315	6	41,49,73	1.86	5 (12%)	47,84,113	1.63	6 (12%)
21	XAT	7	303	-	39,47,47	0.97	1 (2%)	54,74,74	2.59	19 (35%)
23	CLA	a	806	-	65,73,73	1.49	11 (16%)	76,113,113	1.67	13 (17%)
21	XAT	j	101	-	39,47,47	0.89	0	54,74,74	2.72	18 (33%)
23	CLA	3	313	-	52,60,73	1.66	5 (9%)	60,97,113	1.52	9 (15%)
23	CLA	4	311	-	46,54,73	1.78	6 (13%)	53,90,113	1.55	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	2	313	7	41,49,73	1.84	5 (12%)	47,84,113	1.68	8 (17%)
23	CLA	7	309	-	46,55,73	1.76	5 (10%)	52,91,113	1.53	7 (13%)
23	CLA	4	314	4	45,53,73	1.81	5 (11%)	52,89,113	1.56	7 (13%)
23	CLA	7	312	-	48,56,73	1.71	6 (12%)	55,92,113	1.55	8 (14%)
32	SF4	c	102	-	0,12,12	-	-	-	-	-
23	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.54	7 (10%)
23	CLA	1	306	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	10 (13%)
23	CLA	b	809	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	8 (10%)
23	CLA	b	810	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	7 (9%)
21	XAT	4	304	-	39,47,47	0.89	1 (2%)	54,74,74	2.56	16 (29%)
23	CLA	2	308	7	54,62,73	1.65	5 (9%)	62,99,113	1.45	8 (12%)
23	CLA	a	826	-	65,73,73	1.47	6 (9%)	76,113,113	1.45	6 (7%)
23	CLA	b	839	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	8 (10%)
24	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	5 (9%)
32	SF4	c	101	-	0,12,12	-	-	-	-	-
23	CLA	a	838	-	51,59,73	1.66	6 (11%)	59,96,113	1.56	9 (15%)
23	CLA	1	312	8	52,60,73	1.70	5 (9%)	60,97,113	1.48	8 (13%)
21	XAT	2	301	-	39,47,47	0.93	1 (2%)	54,74,74	2.71	19 (35%)
23	CLA	a	828	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
23	CLA	5	310	-	46,54,73	1.76	5 (10%)	53,90,113	1.54	7 (13%)
23	CLA	9	312	-	46,54,73	1.74	6 (13%)	53,90,113	1.68	8 (15%)
23	CLA	b	834	-	53,61,73	1.68	6 (11%)	61,98,113	1.51	8 (13%)
23	CLA	b	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	7 (9%)
23	CLA	a	837	9	45,53,73	1.79	6 (13%)	52,89,113	1.58	7 (13%)
31	BCR	b	845	-	41,41,41	0.76	0	56,56,56	2.19	22 (39%)
21	XAT	2	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.50	18 (33%)
23	CLA	b	808	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	9 (11%)
23	CLA	a	814	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	5	315	-	46,54,73	1.75	5 (10%)	53,90,113	1.56	7 (13%)
23	CLA	7	315	4	41,49,73	1.86	5 (12%)	47,84,113	1.65	7 (14%)
21	XAT	6	303	-	39,47,47	0.89	1 (2%)	54,74,74	2.65	20 (37%)
23	CLA	7	316	-	51,59,73	1.64	6 (11%)	59,96,113	1.60	8 (13%)
23	CLA	7	317	-	45,53,73	1.80	5 (11%)	52,89,113	1.59	6 (11%)
21	XAT	3	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.62	19 (35%)
32	SF4	a	851	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	8	310	-	46,54,73	1.77	6 (13%)	53,90,113	1.55	7 (13%)
23	CLA	2	310	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
23	CLA	a	842	-	65,73,73	1.51	6 (9%)	76,113,113	1.38	7 (9%)
31	BCR	h	202	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
23	CLA	b	825	-	64,72,73	1.48	6 (9%)	74,111,113	1.45	8 (10%)
23	CLA	1	307	-	54,62,73	1.62	5 (9%)	62,99,113	1.51	8 (12%)
21	XAT	3	303	-	39,47,47	0.90	1 (2%)	54,74,74	2.59	21 (38%)
23	CLA	9	318	-	62,70,73	1.55	6 (9%)	72,109,113	1.38	8 (11%)
23	CLA	6	307	-	46,54,73	1.77	5 (10%)	53,90,113	1.54	7 (13%)
23	CLA	1	311	-	53,61,73	1.63	5 (9%)	61,98,113	1.51	9 (14%)
23	CLA	6	317	-	65,73,73	1.50	5 (7%)	76,113,113	1.45	7 (9%)
23	CLA	a	844	27	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)
23	CLA	5	309	1	65,73,73	1.49	5 (7%)	76,113,113	1.37	7 (9%)
23	CLA	9	315	2	42,50,73	1.82	5 (11%)	48,85,113	1.60	7 (14%)
23	CLA	a	824	-	46,54,73	1.77	6 (13%)	53,90,113	1.50	7 (13%)
23	CLA	5	308	-	55,63,73	1.63	6 (10%)	64,101,113	1.47	7 (10%)
23	CLA	9	310	-	46,54,73	1.74	5 (10%)	53,90,113	1.65	6 (11%)
21	XAT	a	852	-	39,47,47	0.95	2 (5%)	54,74,74	2.69	20 (37%)
23	CLA	4	307	-	56,64,73	1.62	5 (8%)	65,102,113	1.44	7 (10%)
23	CLA	a	812	23	62,70,73	1.51	6 (9%)	72,109,113	1.44	8 (11%)
23	CLA	6	313	-	52,60,73	1.65	5 (9%)	60,97,113	1.50	7 (11%)
31	BCR	a	849	-	41,41,41	0.72	0	56,56,56	2.17	20 (35%)
31	BCR	j	104	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
23	CLA	3	311	-	50,58,73	1.70	5 (10%)	58,95,113	1.55	9 (15%)
23	CLA	b	828	-	65,73,73	1.51	6 (9%)	76,113,113	1.32	7 (9%)
23	CLA	2	311	-	58,66,73	1.59	5 (8%)	67,104,113	1.42	7 (10%)
27	LHG	9	317	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
23	CLA	5	313	1	45,53,73	1.81	5 (11%)	52,89,113	1.57	6 (11%)
23	CLA	b	831	-	49,57,73	1.70	5 (10%)	55,93,113	1.56	8 (14%)
23	CLA	5	305	1	46,54,73	1.77	6 (13%)	53,90,113	1.54	8 (15%)
28	DGD	4	318	-	41,41,67	1.07	2 (4%)	55,55,81	1.82	6 (10%)
23	CLA	8	309	-	57,65,73	1.59	5 (8%)	66,103,113	1.45	9 (13%)
21	XAT	7	305	-	39,47,47	0.86	0	54,74,74	2.65	20 (37%)
21	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	15 (27%)
21	XAT	2	304	-	39,47,47	0.88	0	54,74,74	2.54	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	XAT	2	305	-	39,47,47	0.91	1 (2%)	54,74,74	2.43	18 (33%)
22	A1L1G	3	302	-	38,47,47	1.47	6 (15%)	49,71,71	1.39	7 (14%)
25	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
23	CLA	j	103	16	42,50,73	1.82	5 (11%)	48,85,113	1.65	6 (12%)
22	A1L1G	3	306	-	38,47,47	1.43	6 (15%)	49,71,71	1.50	9 (18%)
21	XAT	1	303	-	39,47,47	0.90	0	54,74,74	2.52	19 (35%)
23	CLA	5	306	24	45,53,73	1.79	5 (11%)	52,89,113	1.57	6 (11%)
23	CLA	b	811	-	54,62,73	1.67	7 (12%)	67,100,113	1.49	9 (13%)
23	CLA	8	313	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	6 (11%)
23	CLA	b	822	-	60,68,73	1.54	6 (10%)	70,107,113	1.38	8 (11%)
23	CLA	b	840	27	65,73,73	1.52	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	7	306	4	48,56,73	1.73	6 (12%)	55,92,113	1.52	7 (12%)
23	CLA	3	310	-	56,64,73	1.59	5 (8%)	65,102,113	1.45	7 (10%)
26	45D	9	305	-	43,43,43	1.10	4 (9%)	54,60,60	2.17	18 (33%)
27	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
23	CLA	b	830	-	41,49,73	1.83	6 (14%)	47,84,113	1.64	8 (17%)
23	CLA	a	810	9	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	f	803	13	52,60,73	1.67	5 (9%)	60,97,113	1.50	8 (13%)
23	CLA	b	833	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
23	CLA	a	854	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
23	CLA	8	308	-	55,63,73	1.62	5 (9%)	64,101,113	1.50	9 (14%)
23	CLA	a	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.59	7 (13%)
23	CLA	b	817	-	59,67,73	1.56	6 (10%)	68,105,113	1.51	9 (13%)
23	CLA	b	821	-	51,59,73	1.64	5 (9%)	59,96,113	1.56	9 (15%)
23	CLA	4	315	4	41,49,73	1.87	5 (12%)	47,84,113	1.65	8 (17%)
23	CLA	3	307	5	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
23	CLA	2	312	-	47,55,73	1.75	5 (10%)	54,91,113	1.57	7 (12%)
22	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.58	11 (22%)
23	CLA	8	305	3	43,51,73	1.78	5 (11%)	49,86,113	1.64	7 (14%)
23	CLA	b	818	-	60,68,73	1.57	5 (8%)	70,107,113	1.41	7 (10%)
23	CLA	b	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	9 (11%)
27	LHG	a	846	23	26,26,48	1.28	5 (19%)	29,32,54	1.21	2 (6%)
31	BCR	a	850	-	41,41,41	0.73	0	56,56,56	2.16	14 (25%)
23	CLA	a	809	9	65,73,73	1.44	5 (7%)	76,113,113	1.43	9 (11%)
23	CLA	9	309	2	46,54,73	1.76	6 (13%)	53,90,113	1.54	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	804	-	65,73,73	1.45	6 (9%)	76,113,113	1.55	12 (15%)
23	CLA	1	314	-	45,53,73	1.80	5 (11%)	52,89,113	1.55	6 (11%)
21	XAT	2	303	-	39,47,47	0.97	1 (2%)	54,74,74	2.63	20 (37%)
21	XAT	4	305	-	39,47,47	0.91	1 (2%)	54,74,74	2.75	19 (35%)
23	CLA	9	308	2	65,73,73	1.50	7 (10%)	76,113,113	1.42	9 (11%)
23	CLA	3	315	5	46,54,73	1.79	6 (13%)	53,90,113	1.52	7 (13%)
23	CLA	b	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
23	CLA	6	311	6	42,50,73	1.84	5 (11%)	48,85,113	1.57	7 (14%)
23	CLA	6	314	-	46,54,73	1.73	5 (10%)	53,90,113	1.62	6 (11%)
23	CLA	b	837	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	8 (10%)
23	CLA	b	836	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	9 (11%)
27	LHG	9	307	-	35,35,48	1.22	6 (17%)	38,41,54	0.97	2 (5%)
23	CLA	a	829	-	62,70,73	1.52	5 (8%)	72,109,113	1.41	8 (11%)
23	CLA	b	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.60	7 (13%)
23	CLA	8	306	28	46,54,73	1.76	5 (10%)	53,90,113	1.54	7 (13%)
23	CLA	5	307	1	60,68,73	1.53	5 (8%)	70,107,113	1.42	8 (11%)
23	CLA	4	309	-	50,58,73	1.69	5 (10%)	58,95,113	1.56	8 (13%)
21	XAT	6	306	-	39,47,47	0.94	2 (5%)	54,74,74	2.60	19 (35%)
21	XAT	5	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.58	20 (37%)
23	CLA	a	830	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	8 (10%)
31	BCR	b	843	-	41,41,41	0.71	0	56,56,56	1.92	16 (28%)
23	CLA	9	313	2	46,54,73	1.76	5 (10%)	53,90,113	1.62	7 (13%)
21	XAT	3	305	-	39,47,47	0.88	1 (2%)	54,74,74	2.57	16 (29%)
23	CLA	a	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	9 (11%)
23	CLA	a	805	23	55,63,73	1.61	5 (9%)	64,101,113	1.51	8 (12%)
31	BCR	h	201	-	41,41,41	0.71	0	56,56,56	1.97	21 (37%)
21	XAT	5	304	-	39,47,47	0.89	0	54,74,74	2.86	22 (40%)

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	CLA	4	310	-	1/1/15/20	16/37/115/115	-
23	CLA	b	820	-	1/1/12/20	7/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
23	CLA	a	839	-	1/1/15/20	15/37/115/115	-
23	CLA	7	313	-	1/1/12/20	7/24/102/115	-
23	CLA	7	311	-	1/1/11/20	5/15/93/115	-
21	XAT	3	301	-	-	3/31/93/93	0/4/4/4
31	BCR	1	205	-	-	8/29/63/63	0/2/2/2
23	CLA	3	308	-	1/1/11/20	5/16/94/115	-
23	CLA	5	312	-	1/1/12/20	0/22/100/115	-
22	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
23	CLA	f	802	-	1/1/15/20	13/37/115/115	-
23	CLA	a	804	-	1/1/13/20	10/25/103/115	-
23	CLA	j	102	-	1/1/13/20	16/29/107/115	-
23	CLA	a	825	-	1/1/13/20	8/25/103/115	-
21	XAT	5	301	-	-	3/31/93/93	0/4/4/4
21	XAT	7	301	-	-	6/31/93/93	0/4/4/4
28	DGD	b	848	-	-	20/46/86/95	0/2/2/2
31	BCR	f	804	-	-	4/29/63/63	0/2/2/2
21	XAT	6	302	-	-	7/31/93/93	0/4/4/4
21	XAT	7	304	-	-	6/31/93/93	0/4/4/4
23	CLA	1	309	8	1/1/11/20	6/15/93/115	-
31	BCR	b	844	-	-	6/29/63/63	0/2/2/2
23	CLA	7	308	-	1/1/14/20	14/31/109/115	-
25	A1L1F	6	301	-	-	11/43/99/99	0/3/3/3
23	CLA	3	314	5	1/1/11/20	7/16/94/115	-
31	BCR	a	847	-	-	0/29/63/63	0/2/2/2
25	A1L1F	6	304	-	-	12/39/95/99	0/3/3/3
23	CLA	8	307	3	1/1/15/20	13/37/115/115	-
23	CLA	2	307	-	1/1/11/20	6/16/94/115	-
23	CLA	a	840	-	1/1/15/20	8/37/115/115	-
21	XAT	8	302	-	-	4/31/93/93	0/4/4/4
23	CLA	b	802	-	1/1/15/20	17/37/115/115	-
21	XAT	8	301	-	-	3/31/93/93	0/4/4/4
23	CLA	6	312	6	1/1/12/20	5/21/99/115	-
23	CLA	b	832	-	1/1/15/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	b	842	-	-	2/29/63/63	0/2/2/2
23	CLA	a	821	-	1/1/11/20	2/13/91/115	-
23	CLA	b	826	-	1/1/15/20	5/37/115/115	-
23	CLA	a	820	-	1/1/15/20	15/37/115/115	-
21	XAT	9	303	-	-	4/31/93/93	0/4/4/4
23	CLA	8	312	3	1/1/12/20	2/22/100/115	-
23	CLA	1	313	-	1/1/10/20	3/8/86/115	-
23	CLA	a	841	-	1/1/15/20	15/37/115/115	-
23	CLA	2	306	-	1/1/10/20	2/9/87/115	-
23	CLA	a	801	-	1/1/15/20	22/37/115/115	-
21	XAT	4	301	-	-	4/31/93/93	0/4/4/4
23	CLA	a	822	-	1/1/15/20	5/37/115/115	-
23	CLA	a	817	-	1/1/11/20	6/13/91/115	-
23	CLA	4	308	-	1/1/15/20	14/37/115/115	-
23	CLA	1	310	8	1/1/15/20	18/37/115/115	-
23	CLA	b	812	-	1/1/12/20	6/23/101/115	-
31	BCR	f	801	-	-	3/29/63/63	0/2/2/2
23	CLA	4	316	-	1/1/11/20	7/15/93/115	-
23	CLA	b	806	-	1/1/15/20	16/37/115/115	-
23	CLA	3	309	5	1/1/13/20	5/27/105/115	-
30	PQN	a	843	-	-	5/23/43/43	0/2/2/2
23	CLA	1	203	-	1/1/14/20	6/31/109/115	-
23	CLA	6	310	-	1/1/12/20	7/22/100/115	-
23	CLA	a	816	-	1/1/12/20	5/19/97/115	-
23	CLA	5	311	-	1/1/12/20	8/21/99/115	-
23	CLA	2	309	-	1/1/11/20	4/15/93/115	-
23	CLA	a	836	-	1/1/12/20	6/19/97/115	-
21	XAT	4	302	-	-	0/31/93/93	0/4/4/4
23	CLA	7	310	-	1/1/11/20	6/15/93/115	-
23	CLA	5	314	-	1/1/12/20	4/22/100/115	-
23	CLA	a	831	-	1/1/15/20	11/37/115/115	-
23	CLA	4	313	-	1/1/12/20	6/23/101/115	-
23	CLA	b	824	-	1/1/15/20	14/37/115/115	-
21	XAT	6	305	-	-	4/31/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
25	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
29	LMG	a	853	-	-	13/29/49/70	0/1/1/1
31	BCR	i	101	-	-	3/29/63/63	0/2/2/2
31	BCR	a	848	-	-	0/29/63/63	0/2/2/2
23	CLA	b	805	-	1/1/15/20	12/37/115/115	-
23	CLA	a	803	-	1/1/15/20	3/37/115/115	-
21	XAT	8	303	-	-	0/31/93/93	0/4/4/4
21	XAT	9	304	-	-	1/31/93/93	0/4/4/4
23	CLA	b	816	-	1/1/13/20	4/25/103/115	-
29	LMG	j	105	-	-	11/27/47/70	0/1/1/1
23	CLA	4	312	-	1/1/11/20	4/15/93/115	-
23	CLA	b	813	-	1/1/15/20	14/37/115/115	-
23	CLA	8	311	-	1/1/13/20	8/27/105/115	-
23	CLA	4	306	4	1/1/11/20	7/13/91/115	-
23	CLA	a	827	-	1/1/15/20	8/37/115/115	-
23	CLA	b	829	-	1/1/15/20	10/37/115/115	-
23	CLA	a	818	-	1/1/13/20	11/27/105/115	-
23	CLA	b	835	-	1/1/13/20	11/29/107/115	-
23	CLA	7	307	-	1/1/11/20	5/13/91/115	-
30	PQN	b	841	-	-	1/23/43/43	0/2/2/2
23	CLA	a	819	-	1/1/12/20	4/24/102/115	-
23	CLA	a	802	-	1/1/13/20	7/29/107/115	-
23	CLA	b	819	-	1/1/13/20	3/25/103/115	-
23	CLA	b	801	-	1/1/15/20	20/37/115/115	-
23	CLA	9	316	-	1/1/15/20	17/37/115/115	-
23	CLA	h	204	-	1/1/13/20	9/25/103/115	-
23	CLA	3	312	5	1/1/13/20	9/30/108/115	-
31	BCR	l	201	-	-	4/29/63/63	0/2/2/2
23	CLA	2	315	-	1/1/10/20	1/10/88/115	-
23	CLA	a	823	-	1/1/11/20	7/18/96/115	-
23	CLA	b	814	-	1/1/13/20	13/25/103/115	-
23	CLA	7	314	-	1/1/11/20	4/13/91/115	-
31	BCR	b	849	-	-	5/29/63/63	0/2/2/2
23	CLA	8	314	-	1/1/10/20	5/8/86/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	2	314	-	1/1/13/20	13/27/105/115	-
23	CLA	4	317	-	1/1/13/20	7/25/103/115	-
23	CLA	b	823	-	1/1/12/20	8/23/101/115	-
27	LHG	b	847	23	-	20/35/35/53	-
23	CLA	a	807	-	1/1/15/20	18/37/115/115	-
23	CLA	a	808	-	1/1/12/20	3/21/99/115	-
23	CLA	a	832	-	1/1/12/20	5/19/97/115	-
31	BCR	b	846	-	-	2/29/63/63	0/2/2/2
23	CLA	a	811	-	1/1/13/20	8/27/105/115	-
23	CLA	l	202	-	1/1/10/20	2/10/88/115	-
31	BCR	m	101	-	-	9/29/63/63	0/2/2/2
23	CLA	a	813	-	1/1/12/20	9/24/102/115	-
23	CLA	b	838	-	1/1/15/20	13/37/115/115	-
23	CLA	6	309	-	1/1/15/20	10/37/115/115	-
23	CLA	1	308	8	1/1/15/20	13/37/115/115	-
23	CLA	a	835	-	1/1/15/20	12/37/115/115	-
23	CLA	6	316	6	1/1/11/20	7/15/93/115	-
23	CLA	l	204	-	1/1/11/20	4/15/93/115	-
21	XAT	4	303	-	-	3/31/93/93	0/4/4/4
23	CLA	6	308	-	1/1/13/20	4/29/107/115	-
29	LMG	2	317	-	-	11/30/50/70	0/1/1/1
22	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
24	SQD	5	316	23	-	11/30/50/69	0/1/1/1
23	CLA	9	311	-	1/1/11/20	7/15/93/115	-
22	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
25	A1L1F	h	203	-	-	11/43/99/99	1/3/3/3
23	CLA	9	314	-	1/1/13/20	9/25/103/115	-
23	CLA	1	305	-	1/1/14/20	10/33/111/115	-
28	DGD	8	315	23	-	11/29/69/95	0/2/2/2
23	CLA	2	316	7	1/1/11/20	5/15/93/115	-
23	CLA	6	315	6	1/1/10/20	3/8/86/115	-
23	CLA	a	806	-	1/1/15/20	12/37/115/115	-
21	XAT	7	303	-	-	8/31/93/93	0/4/4/4
21	XAT	j	101	-	-	5/31/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	3	313	-	1/1/12/20	1/22/100/115	-
23	CLA	4	311	-	1/1/11/20	8/15/93/115	-
23	CLA	2	313	7	1/1/10/20	4/8/86/115	-
23	CLA	7	309	-	1/1/11/20	5/15/93/115	-
23	CLA	4	314	4	1/1/11/20	3/13/91/115	-
23	CLA	7	312	-	1/1/11/20	3/17/95/115	-
32	SF4	c	102	-	-	-	0/6/5/5
23	CLA	a	833	-	1/1/13/20	2/25/103/115	-
23	CLA	1	306	-	1/1/15/20	15/37/115/115	-
23	CLA	b	809	-	1/1/15/20	11/37/115/115	-
23	CLA	b	810	-	1/1/15/20	16/37/115/115	-
21	XAT	4	304	-	-	0/31/93/93	0/4/4/4
23	CLA	2	308	7	1/1/12/20	5/24/102/115	-
23	CLA	a	826	-	1/1/15/20	9/37/115/115	-
23	CLA	b	839	-	1/1/15/20	17/37/115/115	-
24	SQD	1	315	-	-	19/40/60/69	0/1/1/1
32	SF4	c	101	-	-	-	0/6/5/5
23	CLA	a	838	-	1/1/12/20	6/21/99/115	-
23	CLA	1	312	8	1/1/12/20	3/22/100/115	-
21	XAT	2	301	-	-	3/31/93/93	0/4/4/4
23	CLA	a	828	-	1/1/15/20	9/37/115/115	-
23	CLA	5	310	-	1/1/11/20	6/15/93/115	-
23	CLA	9	312	-	1/1/11/20	9/15/93/115	-
23	CLA	b	834	-	1/1/12/20	8/23/101/115	-
23	CLA	b	803	-	1/1/15/20	18/37/115/115	-
23	CLA	a	837	9	1/1/11/20	4/13/91/115	-
31	BCR	b	845	-	-	1/29/63/63	0/2/2/2
23	CLA	b	808	-	1/1/15/20	12/37/115/115	-
21	XAT	2	302	-	-	0/31/93/93	0/4/4/4
23	CLA	a	814	-	1/1/15/20	20/37/115/115	-
23	CLA	5	315	-	1/1/11/20	5/15/93/115	-
23	CLA	7	315	4	1/1/10/20	4/8/86/115	-
23	CLA	7	317	-	1/1/11/20	5/13/91/115	-
23	CLA	7	316	-	1/1/12/20	11/21/99/115	-
21	XAT	6	303	-	-	5/31/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	XAT	3	304	-	-	3/31/93/93	0/4/4/4
32	SF4	a	851	-	-	-	0/6/5/5
23	CLA	8	310	-	1/1/11/20	5/15/93/115	-
23	CLA	2	310	-	1/1/15/20	14/37/115/115	-
23	CLA	a	842	-	1/1/15/20	9/37/115/115	-
31	BCR	h	202	-	-	2/29/63/63	0/2/2/2
23	CLA	b	825	-	1/1/14/20	6/36/114/115	-
23	CLA	1	307	-	1/1/12/20	6/24/102/115	-
21	XAT	3	303	-	-	3/31/93/93	0/4/4/4
23	CLA	9	318	-	1/1/14/20	9/34/112/115	-
23	CLA	6	307	-	1/1/11/20	1/15/93/115	-
23	CLA	1	311	-	1/1/12/20	6/23/101/115	-
23	CLA	6	317	-	1/1/15/20	9/37/115/115	-
23	CLA	a	844	27	1/1/15/20	16/37/115/115	-
23	CLA	5	309	1	1/1/15/20	14/37/115/115	-
23	CLA	9	315	2	1/1/10/20	6/10/88/115	-
23	CLA	a	824	-	1/1/11/20	4/15/93/115	-
23	CLA	5	308	-	1/1/13/20	4/25/103/115	-
23	CLA	9	310	-	1/1/11/20	6/15/93/115	-
23	CLA	4	307	-	1/1/13/20	7/27/105/115	-
23	CLA	a	812	23	1/1/14/20	9/34/112/115	-
21	XAT	a	852	-	-	7/31/93/93	0/4/4/4
23	CLA	6	313	-	1/1/12/20	2/22/100/115	-
31	BCR	a	849	-	-	0/29/63/63	0/2/2/2
31	BCR	j	104	-	-	4/29/63/63	0/2/2/2
23	CLA	3	311	-	1/1/12/20	4/19/97/115	-
23	CLA	b	828	-	1/1/15/20	11/37/115/115	-
23	CLA	2	311	-	1/1/13/20	5/29/107/115	-
27	LHG	9	317	-	-	28/50/50/53	-
23	CLA	5	313	1	1/1/11/20	4/13/91/115	-
23	CLA	b	831	-	1/1/11/20	6/18/96/115	-
23	CLA	5	305	1	1/1/11/20	4/15/93/115	-
28	DGD	4	318	-	-	10/29/69/95	0/2/2/2
23	CLA	8	309	-	1/1/13/20	8/28/106/115	-
21	XAT	7	305	-	-	2/31/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	XAT	1	302	-	-	0/31/93/93	0/4/4/4
21	XAT	2	304	-	-	3/31/93/93	0/4/4/4
21	XAT	2	305	-	-	2/31/93/93	0/4/4/4
22	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
25	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
23	CLA	j	103	16	1/1/10/20	5/10/88/115	-
22	A1L1G	3	306	-	-	18/29/85/85	0/3/3/3
21	XAT	1	303	-	-	0/31/93/93	0/4/4/4
23	CLA	5	306	24	1/1/11/20	7/13/91/115	-
23	CLA	b	811	-	1/1/13/20	5/25/101/115	-
23	CLA	8	313	-	1/1/11/20	3/15/93/115	-
23	CLA	b	822	-	1/1/14/20	7/31/109/115	-
23	CLA	b	840	27	1/1/15/20	9/37/115/115	-
23	CLA	7	306	4	1/1/11/20	10/17/95/115	-
23	CLA	3	310	-	1/1/13/20	4/27/105/115	-
26	45D	9	305	-	-	9/29/69/69	0/2/2/2
27	LHG	a	845	-	-	27/52/52/53	-
23	CLA	b	830	-	1/1/10/20	1/8/86/115	-
23	CLA	a	810	9	1/1/15/20	13/37/115/115	-
23	CLA	f	803	13	1/1/12/20	2/22/100/115	-
23	CLA	b	833	-	1/1/15/20	14/37/115/115	-
23	CLA	a	854	-	1/1/15/20	13/37/115/115	-
23	CLA	8	308	-	1/1/13/20	7/25/103/115	-
23	CLA	a	815	-	1/1/11/20	2/13/91/115	-
23	CLA	b	817	-	1/1/13/20	10/30/108/115	-
23	CLA	b	821	-	1/1/12/20	2/21/99/115	-
23	CLA	4	315	4	1/1/10/20	5/8/86/115	-
23	CLA	3	307	5	1/1/11/20	1/13/91/115	-
23	CLA	2	312	-	1/1/11/20	4/16/94/115	-
23	CLA	b	818	-	1/1/14/20	14/31/109/115	-
23	CLA	8	305	3	1/1/10/20	2/11/89/115	-
22	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
23	CLA	b	807	-	1/1/15/20	19/37/115/115	-
27	LHG	a	846	23	-	16/31/31/53	-
31	BCR	a	850	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	809	9	1/1/15/20	15/37/115/115	-
23	CLA	9	309	2	1/1/11/20	3/15/93/115	-
23	CLA	b	804	-	1/1/15/20	10/37/115/115	-
23	CLA	1	314	-	1/1/11/20	5/13/91/115	-
23	CLA	3	315	5	1/1/11/20	8/15/93/115	-
21	XAT	4	305	-	-	4/31/93/93	0/4/4/4
23	CLA	9	308	2	1/1/15/20	15/37/115/115	-
21	XAT	2	303	-	-	6/31/93/93	0/4/4/4
23	CLA	b	827	-	1/1/15/20	14/37/115/115	-
23	CLA	6	311	6	1/1/10/20	2/10/88/115	-
23	CLA	6	314	-	1/1/11/20	6/15/93/115	-
23	CLA	b	837	-	1/1/15/20	8/37/115/115	-
23	CLA	b	836	-	1/1/15/20	8/37/115/115	-
27	LHG	9	307	-	-	21/40/40/53	-
23	CLA	a	829	-	1/1/14/20	15/34/112/115	-
23	CLA	b	815	-	1/1/11/20	3/13/91/115	-
23	CLA	8	306	28	1/1/11/20	2/15/93/115	-
23	CLA	5	307	1	1/1/14/20	7/31/109/115	-
23	CLA	4	309	-	1/1/12/20	7/19/97/115	-
23	CLA	a	830	-	1/1/15/20	15/37/115/115	-
21	XAT	5	302	-	-	3/31/93/93	0/4/4/4
21	XAT	6	306	-	-	4/31/93/93	0/4/4/4
31	BCR	b	843	-	-	2/29/63/63	0/2/2/2
23	CLA	9	313	2	1/1/11/20	9/15/93/115	-
21	XAT	3	305	-	-	0/31/93/93	0/4/4/4
23	CLA	a	834	-	1/1/15/20	7/37/115/115	-
23	CLA	a	805	23	1/1/13/20	6/25/103/115	-
31	BCR	h	201	-	-	0/29/63/63	0/2/2/2
21	XAT	5	304	-	-	1/31/93/93	0/4/4/4

The worst 5 of 1196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	312	CLA	C4B-NB	7.88	1.42	1.35
23	a	840	CLA	C4B-NB	7.78	1.42	1.35
23	3	315	CLA	C4B-NB	7.76	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	818	CLA	C4B-NB	7.74	1.42	1.35
23	a	842	CLA	C4B-NB	7.72	1.42	1.35

The worst 5 of 2650 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	9	302	A1L1F	O15-C20-C21	13.19	123.29	113.38
28	4	318	DGD	C6E-C5E-C4E	-9.41	90.97	113.00
25	6	301	A1L1F	O15-C20-C21	8.71	119.92	113.38
25	6	304	A1L1F	O15-C20-C21	8.65	119.88	113.38
25	8	304	A1L1F	O15-C20-C21	8.49	119.76	113.38

5 of 188 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	5	305	CLA	ND
23	5	306	CLA	ND
23	5	307	CLA	ND
23	5	308	CLA	ND
23	5	309	CLA	ND

5 of 2081 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	5	302	XAT	O4-C6-C7-C8
21	5	302	XAT	C7-C8-C9-C10
21	5	302	XAT	C7-C8-C9-C19
21	9	303	XAT	O4-C6-C7-C8
21	9	304	XAT	O24-C26-C27-C28

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	h	203	A1L1F	C1-C11-C3-C4-C6-C8

235 monomers are involved in 722 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	310	CLA	6	0
23	b	820	CLA	3	0
22	7	302	A1L1G	2	0
23	a	839	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	301	XAT	8	0
23	7	311	CLA	3	0
23	7	313	CLA	4	0
31	1	205	BCR	10	0
23	3	308	CLA	2	0
23	5	312	CLA	3	0
22	9	301	A1L1G	2	0
23	f	802	CLA	2	0
23	a	804	CLA	5	0
21	5	301	XAT	4	0
23	a	825	CLA	5	0
23	j	102	CLA	8	0
21	7	301	XAT	3	0
28	b	848	DGD	6	0
31	f	804	BCR	6	0
21	6	302	XAT	3	0
21	7	304	XAT	11	0
31	b	844	BCR	5	0
23	7	308	CLA	6	0
25	6	301	A1L1F	2	0
31	a	847	BCR	3	0
25	6	304	A1L1F	4	0
23	8	307	CLA	6	0
23	2	307	CLA	1	0
23	a	840	CLA	6	0
21	8	302	XAT	6	0
21	8	301	XAT	3	0
23	b	802	CLA	3	0
23	b	832	CLA	3	0
31	b	842	BCR	4	0
23	b	826	CLA	5	0
23	a	820	CLA	5	0
21	9	303	XAT	6	0
23	8	312	CLA	3	0
23	a	841	CLA	7	0
23	a	801	CLA	6	0
21	4	301	XAT	3	0
23	a	822	CLA	5	0
23	4	308	CLA	7	0
23	1	310	CLA	1	0
23	b	812	CLA	4	0
31	f	801	BCR	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	316	CLA	1	0
23	b	806	CLA	2	0
23	3	309	CLA	1	0
30	a	843	PQN	5	0
23	l	203	CLA	2	0
23	a	816	CLA	2	0
23	5	311	CLA	1	0
21	4	302	XAT	4	0
21	6	305	XAT	5	0
23	5	314	CLA	1	0
23	a	831	CLA	5	0
23	4	313	CLA	4	0
23	a	836	CLA	1	0
23	b	824	CLA	5	0
25	9	302	A1L1F	2	0
25	8	304	A1L1F	2	0
29	a	853	LMG	10	0
31	i	101	BCR	2	0
31	a	848	BCR	7	0
23	b	805	CLA	3	0
23	a	803	CLA	4	0
21	8	303	XAT	7	0
21	9	304	XAT	8	0
23	b	816	CLA	6	0
29	j	105	LMG	6	0
23	4	312	CLA	1	0
23	b	813	CLA	7	0
23	8	311	CLA	3	0
23	4	306	CLA	2	0
23	a	827	CLA	3	0
23	b	829	CLA	4	0
23	a	818	CLA	11	0
23	b	835	CLA	5	0
23	7	307	CLA	1	0
30	b	841	PQN	3	0
23	a	819	CLA	6	0
23	a	802	CLA	5	0
23	b	819	CLA	1	0
23	b	801	CLA	5	0
23	9	316	CLA	7	0
23	h	204	CLA	3	0
23	3	312	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	l	201	BCR	4	0
23	a	823	CLA	3	0
23	b	814	CLA	3	0
23	7	314	CLA	2	0
31	b	849	BCR	7	0
23	8	314	CLA	1	0
23	2	314	CLA	1	0
23	4	317	CLA	7	0
23	b	823	CLA	6	0
27	b	847	LHG	1	0
23	a	807	CLA	4	0
23	a	808	CLA	1	0
23	a	832	CLA	2	0
31	b	846	BCR	3	0
23	l	202	CLA	1	0
31	m	101	BCR	1	0
23	a	813	CLA	1	0
23	b	838	CLA	6	0
23	6	309	CLA	1	0
23	1	308	CLA	3	0
23	a	835	CLA	5	0
21	4	303	XAT	10	0
23	6	308	CLA	4	0
29	2	317	LMG	3	0
22	5	303	A1L1G	1	0
24	5	316	SQD	1	0
22	9	306	A1L1G	1	0
23	9	311	CLA	3	0
25	h	203	A1L1F	4	0
23	9	314	CLA	7	0
28	8	315	DGD	2	0
23	2	316	CLA	2	0
23	6	315	CLA	3	0
21	7	303	XAT	13	0
23	a	806	CLA	9	0
21	j	101	XAT	7	0
23	3	313	CLA	3	0
23	4	311	CLA	1	0
23	4	314	CLA	1	0
23	7	312	CLA	1	0
32	c	102	SF4	3	0
23	a	833	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	1	306	CLA	5	0
23	b	809	CLA	4	0
23	b	810	CLA	1	0
21	4	304	XAT	5	0
23	2	308	CLA	4	0
23	a	826	CLA	6	0
23	b	839	CLA	5	0
24	1	315	SQD	2	0
23	a	838	CLA	1	0
23	1	312	CLA	2	0
21	2	301	XAT	3	0
23	a	828	CLA	6	0
23	5	310	CLA	1	0
23	9	312	CLA	3	0
23	b	803	CLA	3	0
23	a	837	CLA	1	0
31	b	845	BCR	6	0
21	2	302	XAT	1	0
23	b	808	CLA	1	0
23	a	814	CLA	3	0
23	5	315	CLA	2	0
23	7	315	CLA	2	0
21	6	303	XAT	9	0
23	7	316	CLA	2	0
21	3	304	XAT	4	0
23	2	310	CLA	4	0
23	a	842	CLA	4	0
31	h	202	BCR	6	0
23	b	825	CLA	3	0
21	3	303	XAT	3	0
23	9	318	CLA	5	0
23	1	311	CLA	2	0
23	6	317	CLA	4	0
23	a	844	CLA	5	0
23	5	309	CLA	4	0
23	9	315	CLA	1	0
23	a	824	CLA	1	0
23	5	308	CLA	2	0
23	9	310	CLA	2	0
21	a	852	XAT	4	0
23	4	307	CLA	1	0
23	a	812	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	6	313	CLA	2	0
31	a	849	BCR	4	0
31	j	104	BCR	9	0
23	3	311	CLA	1	0
23	b	828	CLA	4	0
27	9	317	LHG	3	0
23	b	831	CLA	2	0
23	5	305	CLA	3	0
28	4	318	DGD	11	0
21	7	305	XAT	2	0
21	1	302	XAT	2	0
21	2	304	XAT	3	0
21	2	305	XAT	5	0
25	1	304	A1L1F	2	0
23	j	103	CLA	2	0
21	1	303	XAT	3	0
23	b	811	CLA	3	0
23	8	313	CLA	3	0
23	b	822	CLA	6	0
23	b	840	CLA	5	0
23	7	306	CLA	2	0
26	9	305	45D	8	0
27	a	845	LHG	4	0
23	b	830	CLA	5	0
23	a	810	CLA	4	0
23	b	833	CLA	6	0
23	a	854	CLA	3	0
23	8	308	CLA	1	0
23	b	817	CLA	9	0
23	b	821	CLA	2	0
23	4	315	CLA	1	0
22	1	301	A1L1G	1	0
23	8	305	CLA	5	0
23	b	818	CLA	3	0
23	b	807	CLA	6	0
27	a	846	LHG	3	0
31	a	850	BCR	2	0
23	a	809	CLA	2	0
23	9	309	CLA	1	0
23	b	804	CLA	5	0
23	1	314	CLA	1	0
21	2	303	XAT	11	0

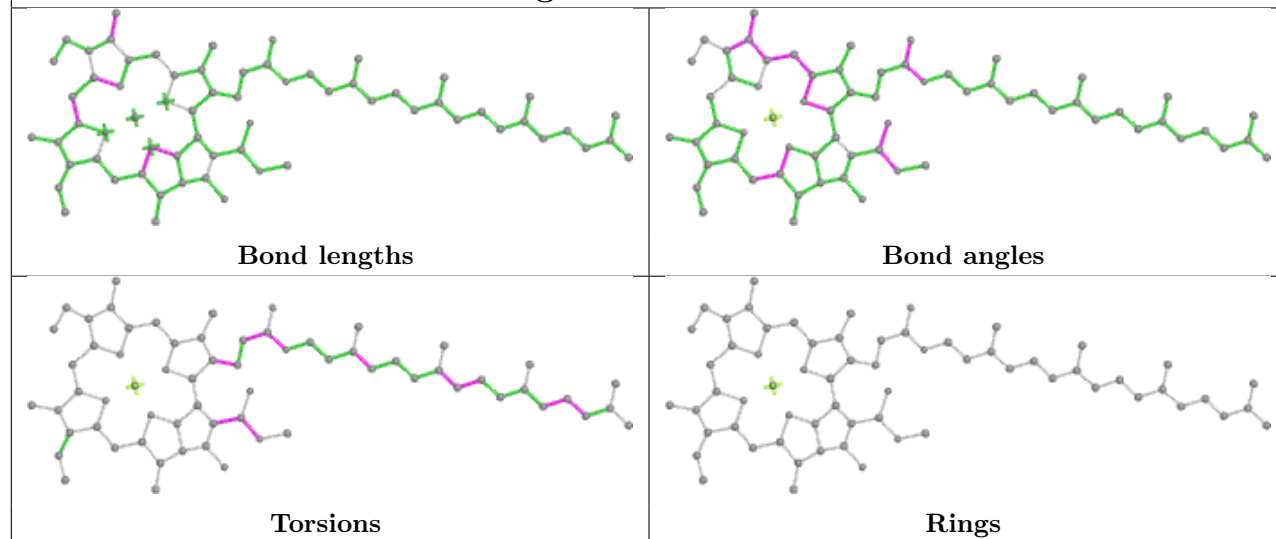
Continued on next page...

Continued from previous page...

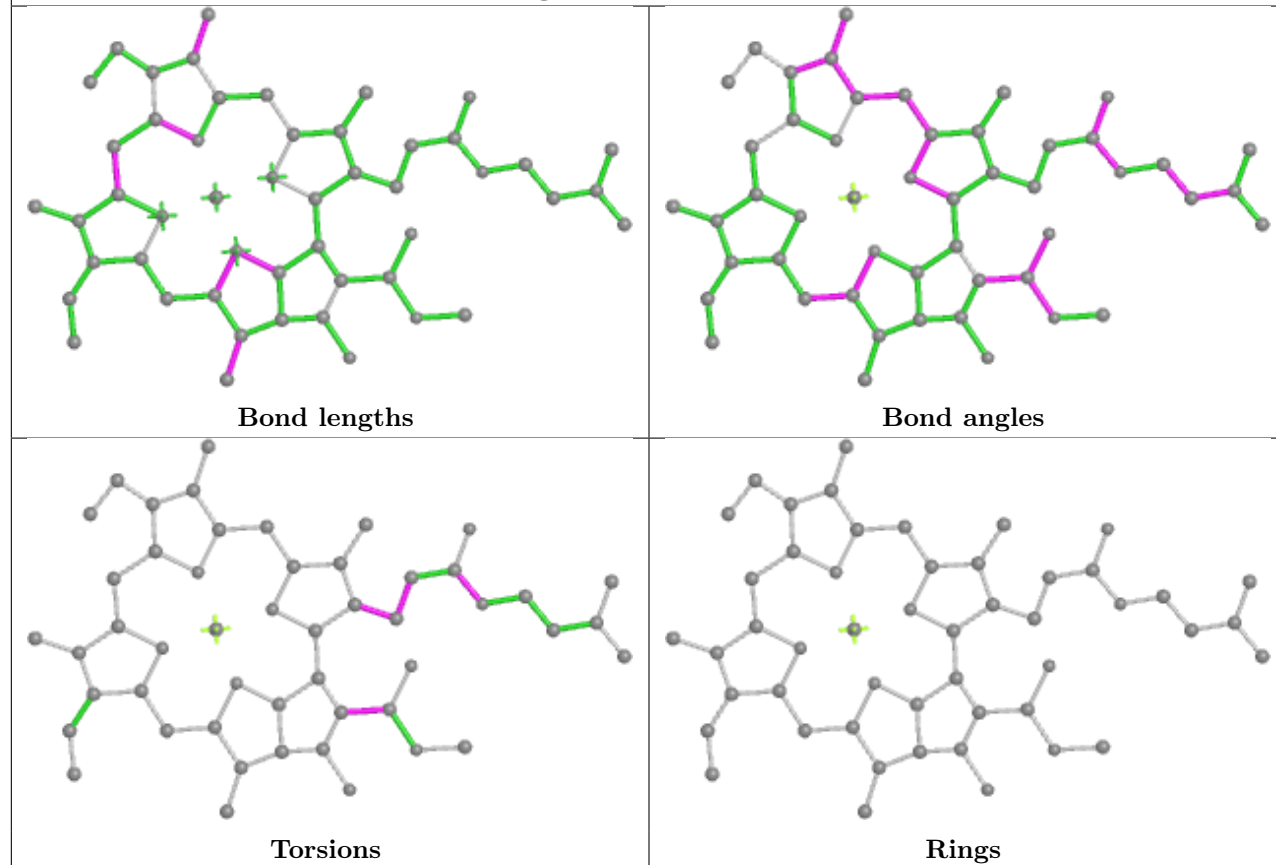
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4	305	XAT	4	0
23	9	308	CLA	7	0
23	b	827	CLA	5	0
23	6	314	CLA	1	0
23	b	837	CLA	5	0
23	b	836	CLA	6	0
27	9	307	LHG	2	0
23	a	829	CLA	8	0
23	8	306	CLA	1	0
23	5	307	CLA	7	0
23	4	309	CLA	3	0
21	6	306	XAT	3	0
21	5	302	XAT	9	0
23	a	830	CLA	7	0
31	b	843	BCR	1	0
23	9	313	CLA	2	0
21	3	305	XAT	4	0
23	a	834	CLA	6	0
23	a	805	CLA	1	0
31	h	201	BCR	2	0
21	5	304	XAT	5	0

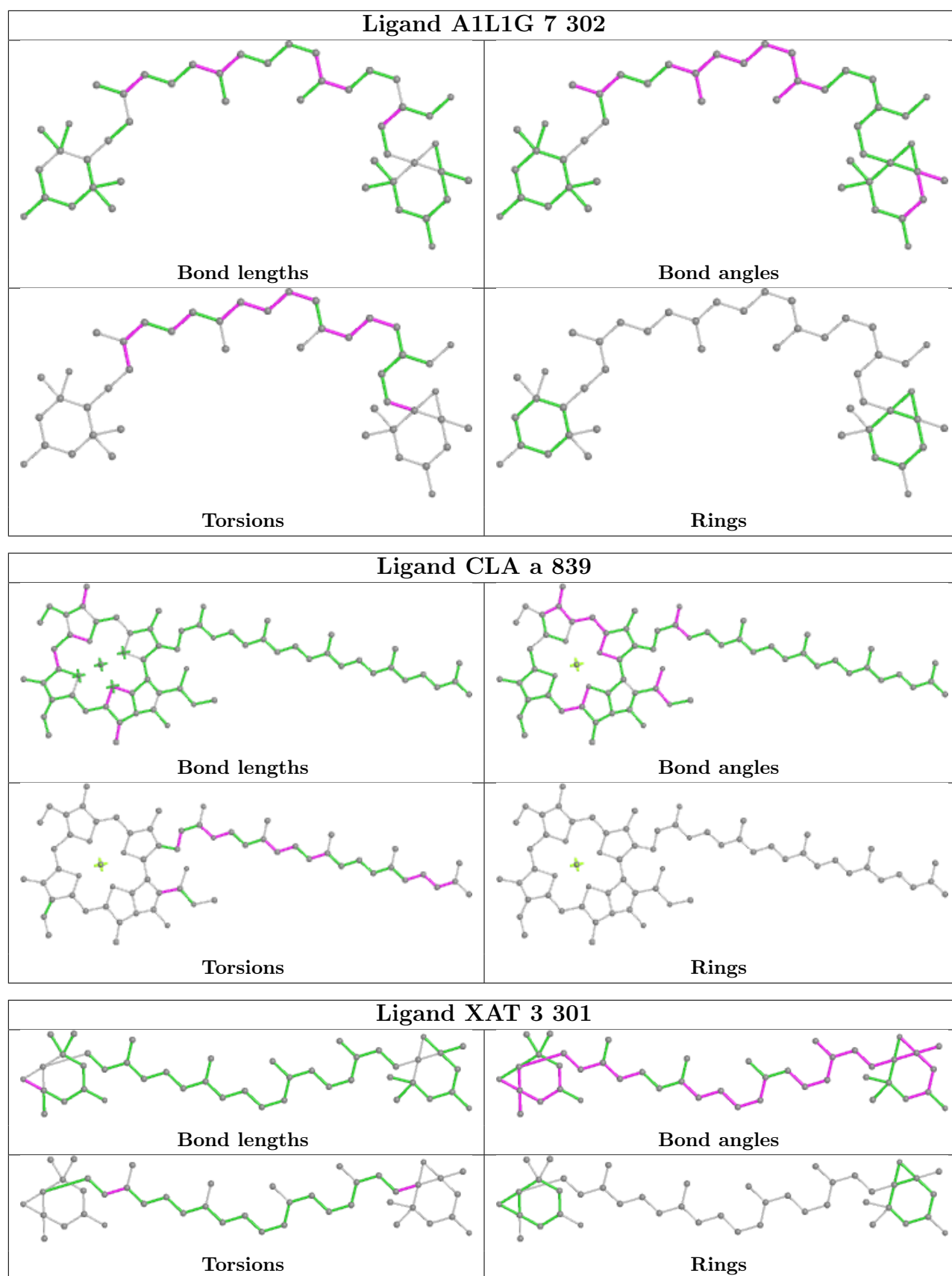
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA 4 310

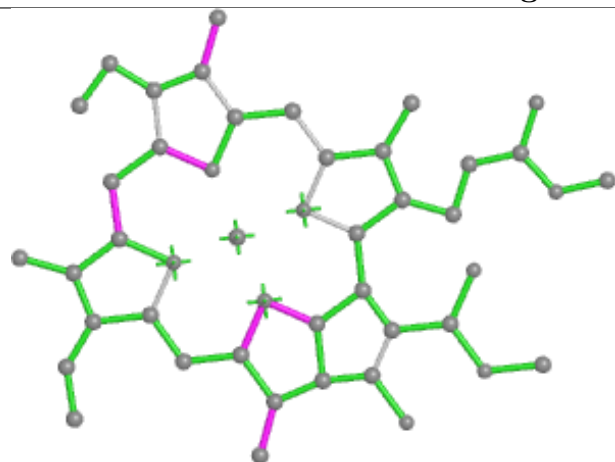


Ligand CLA b 820

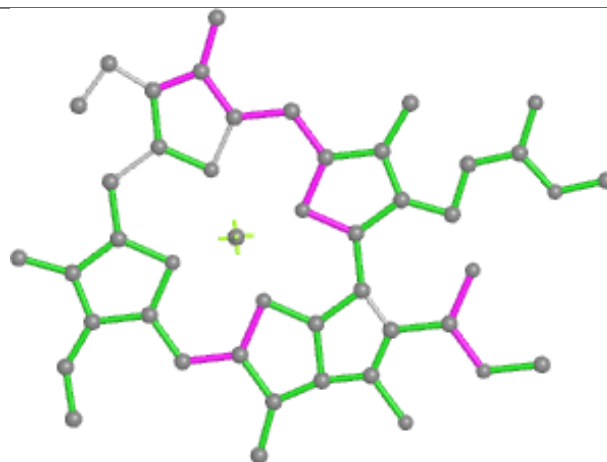




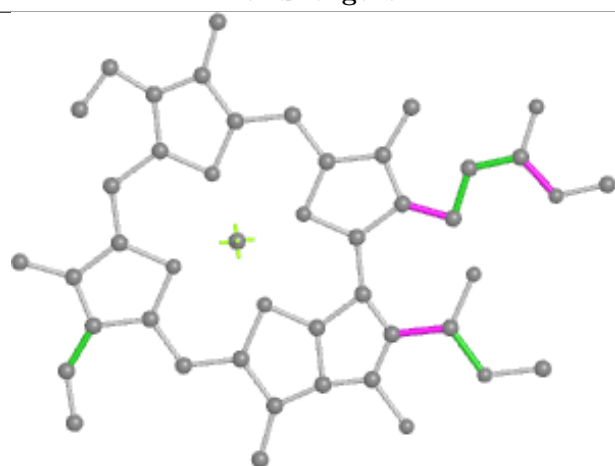
Ligand CLA 7 311



Bond lengths



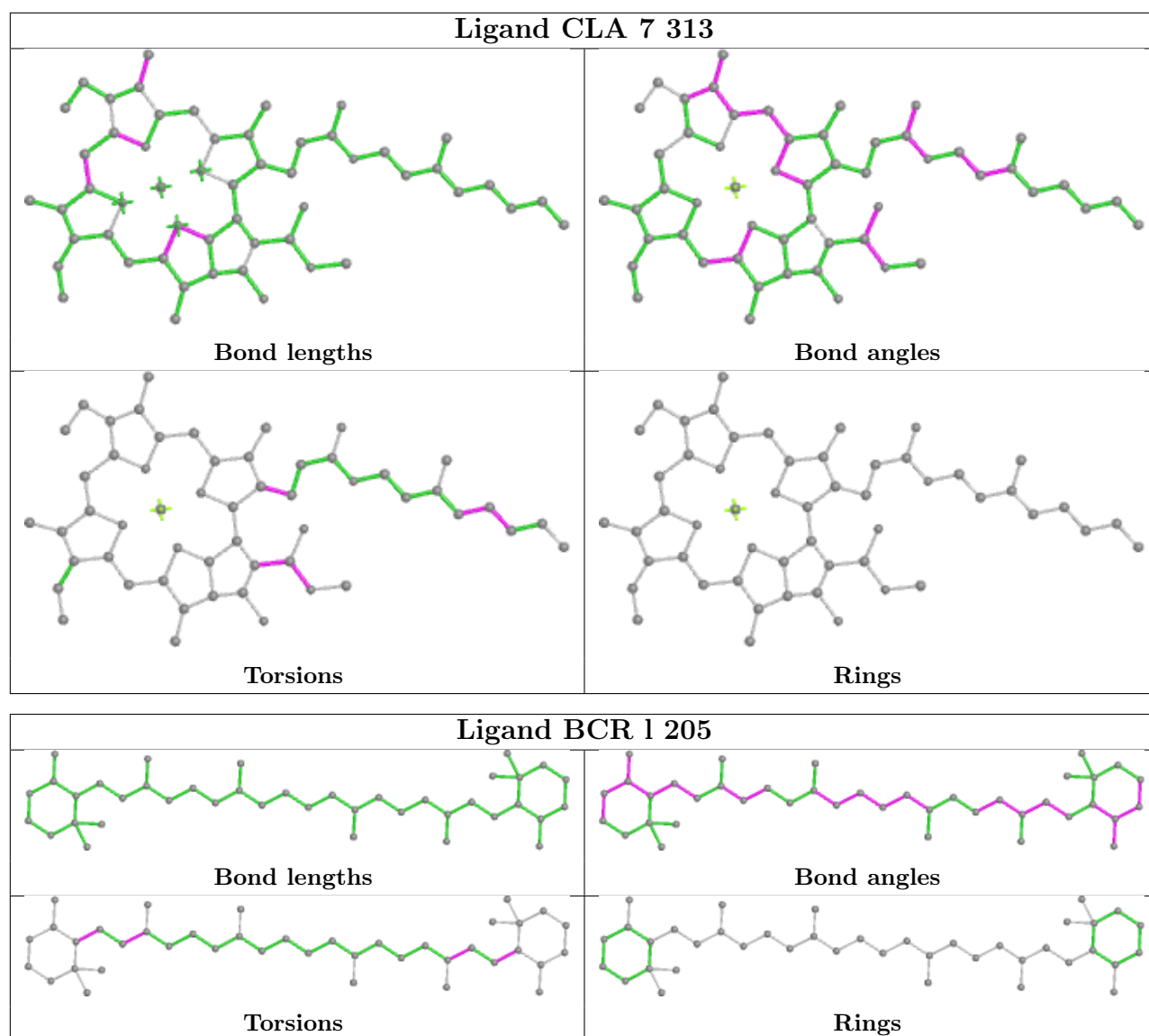
Bond angles



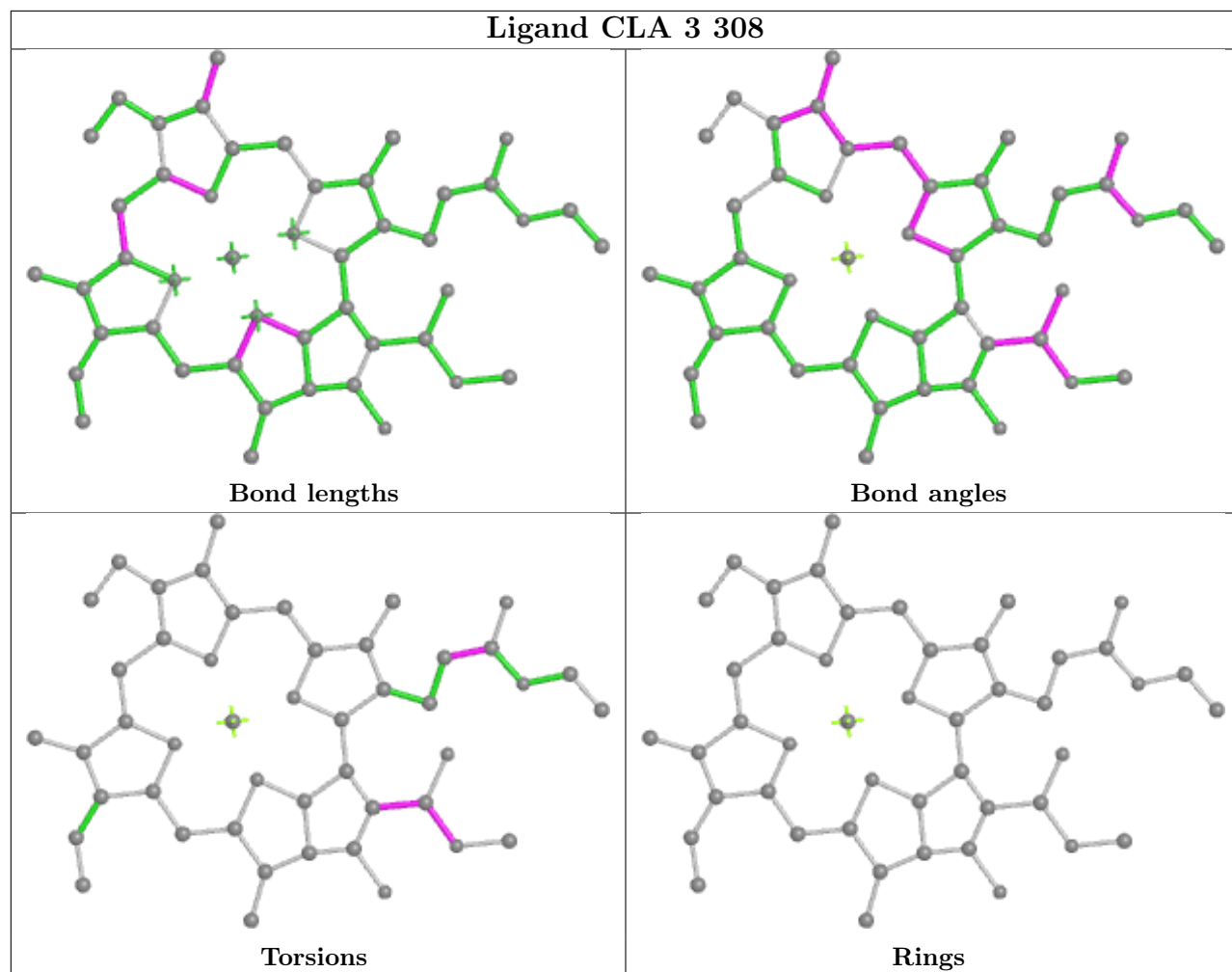
Torsions

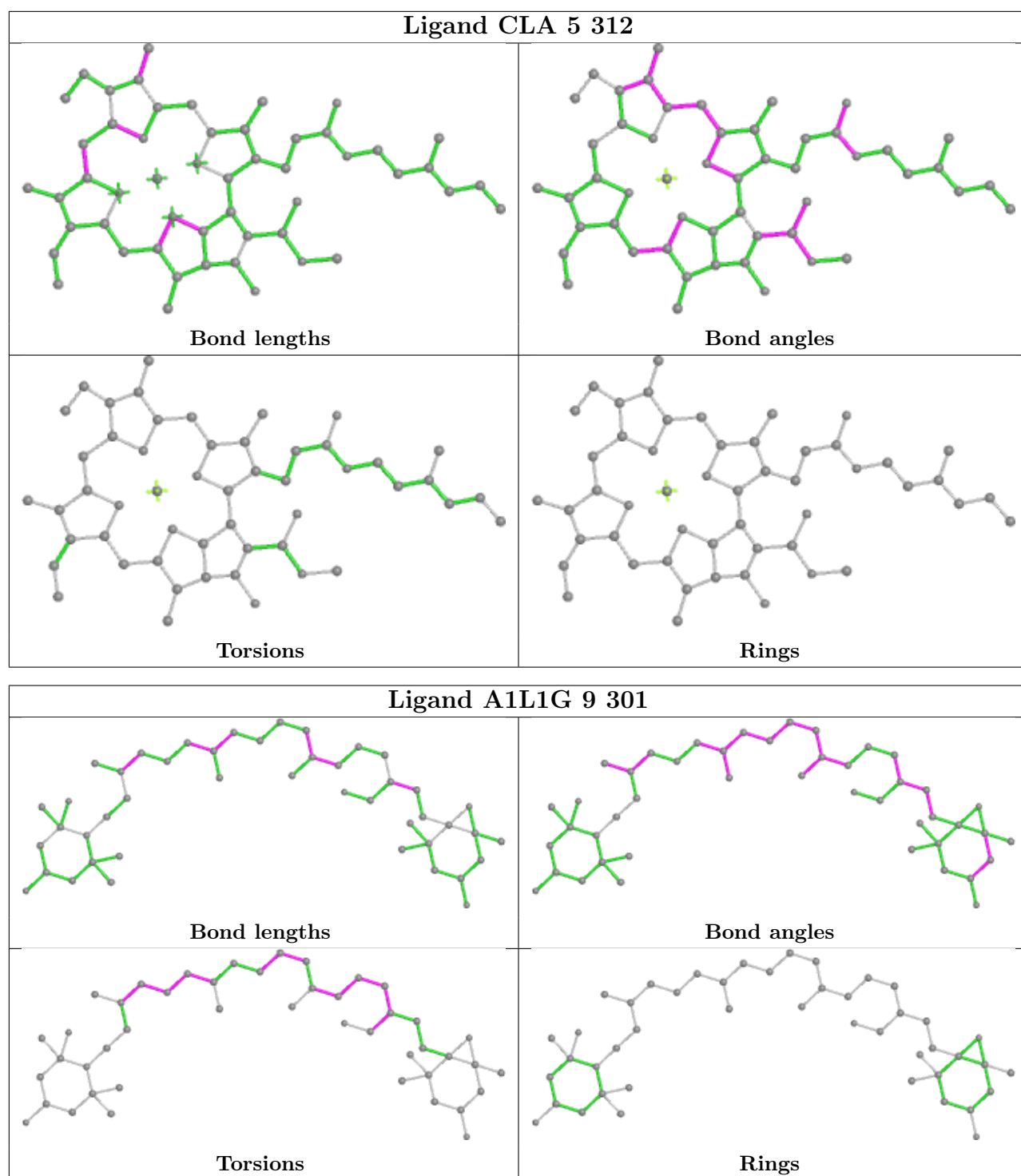


Rings

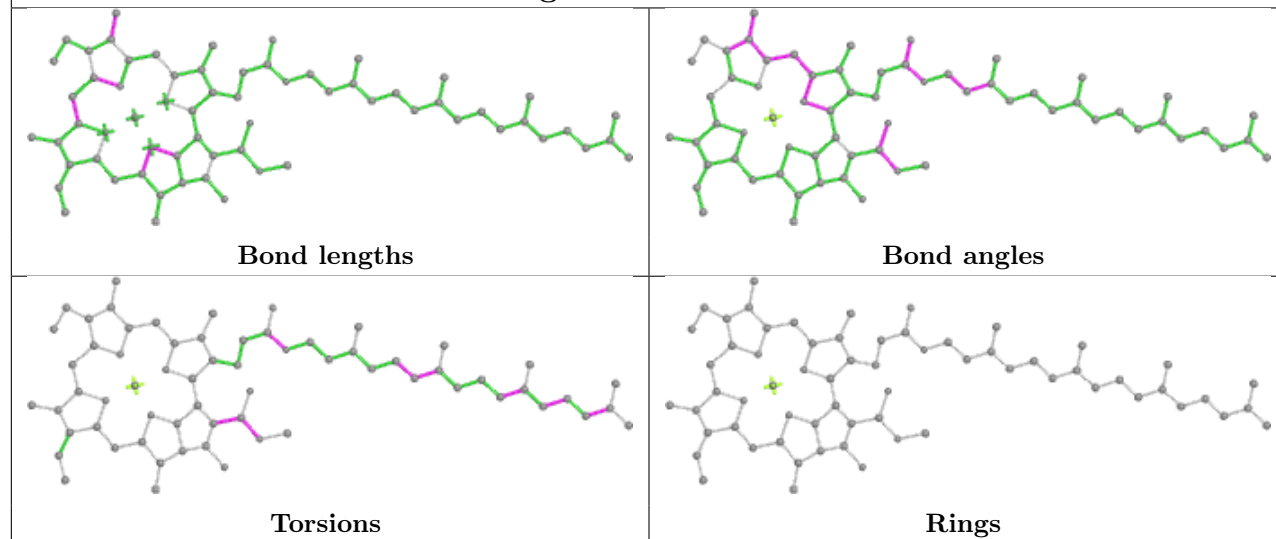


Ligand CLA 3 308

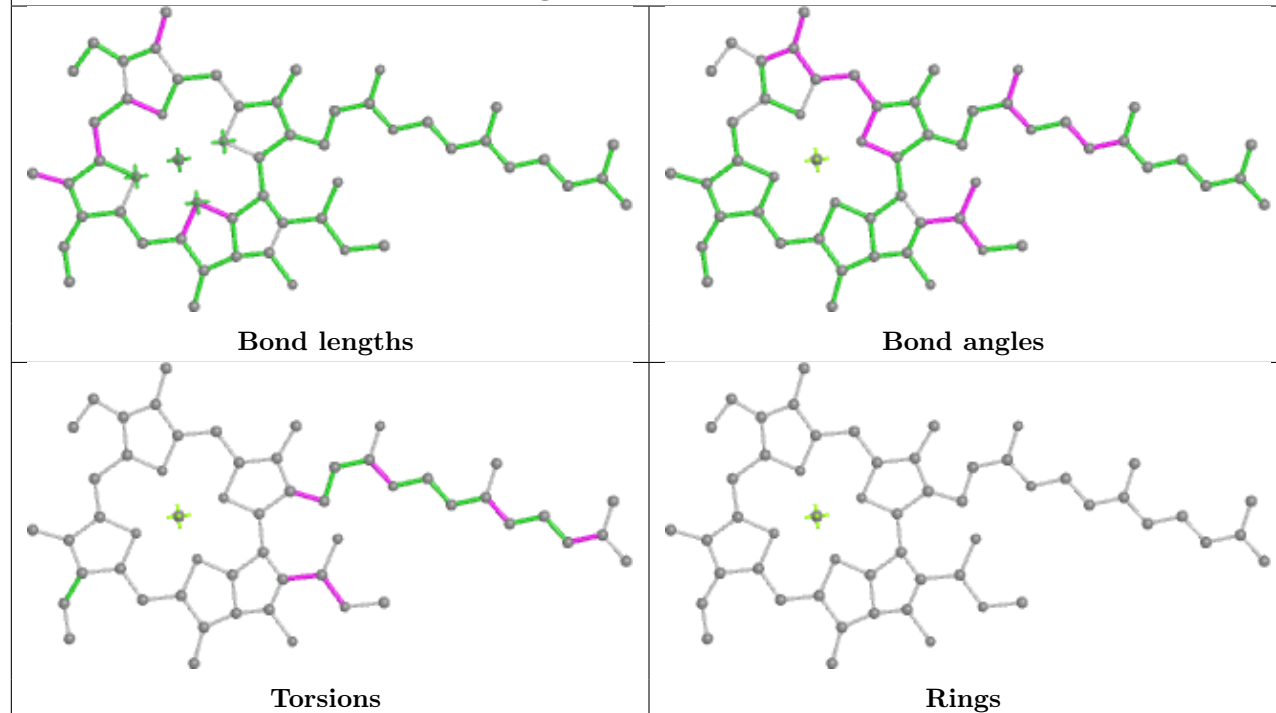




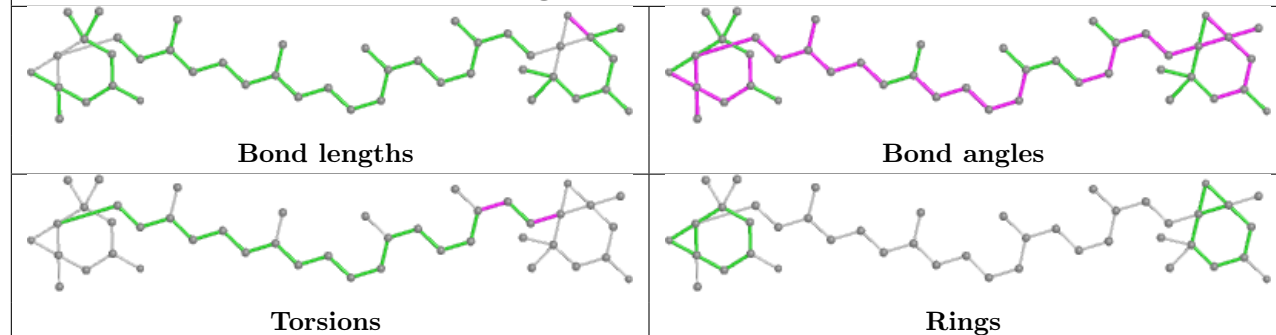
Ligand CLA f 802



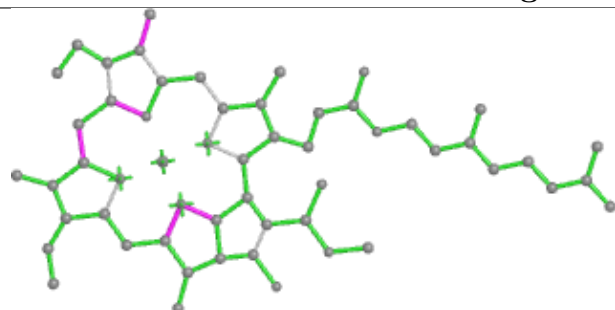
Ligand CLA a 804



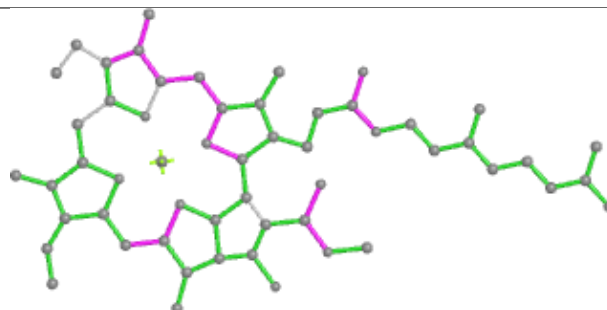
Ligand XAT 5 301



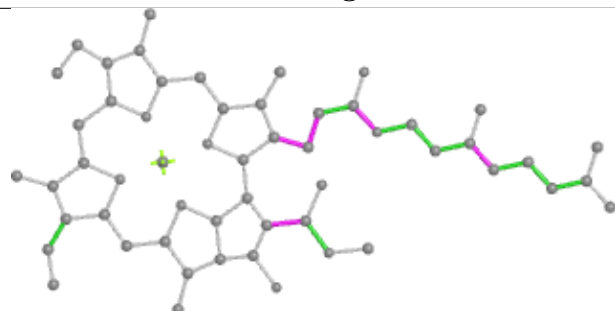
Ligand CLA a 825



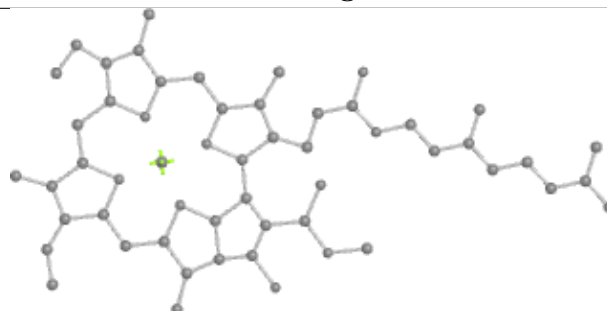
Bond lengths



Bond angles

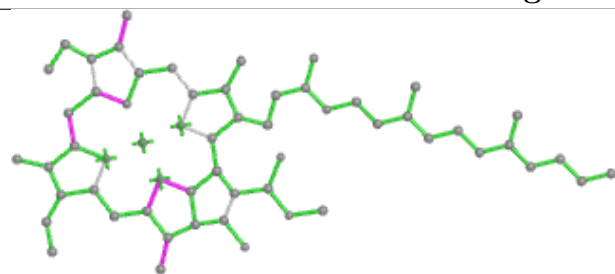


Torsions

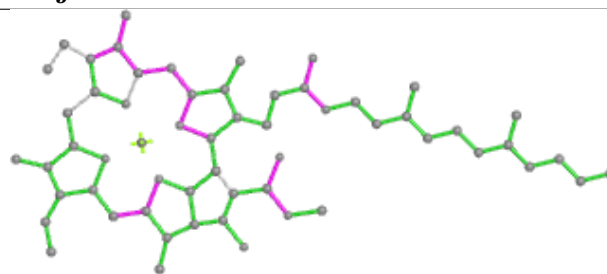


Rings

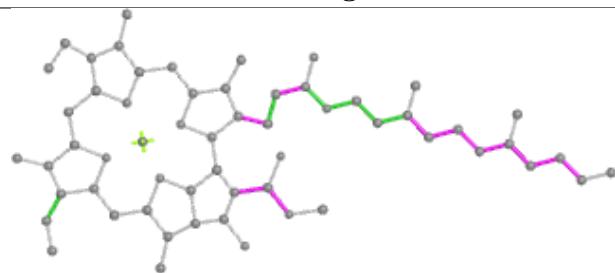
Ligand CLA j 102



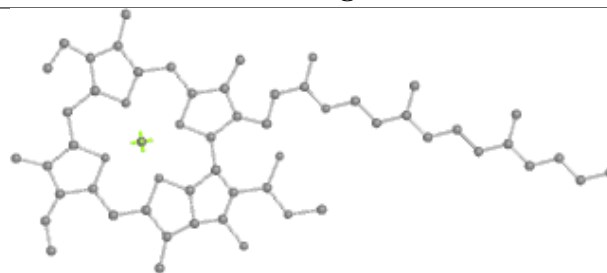
Bond lengths



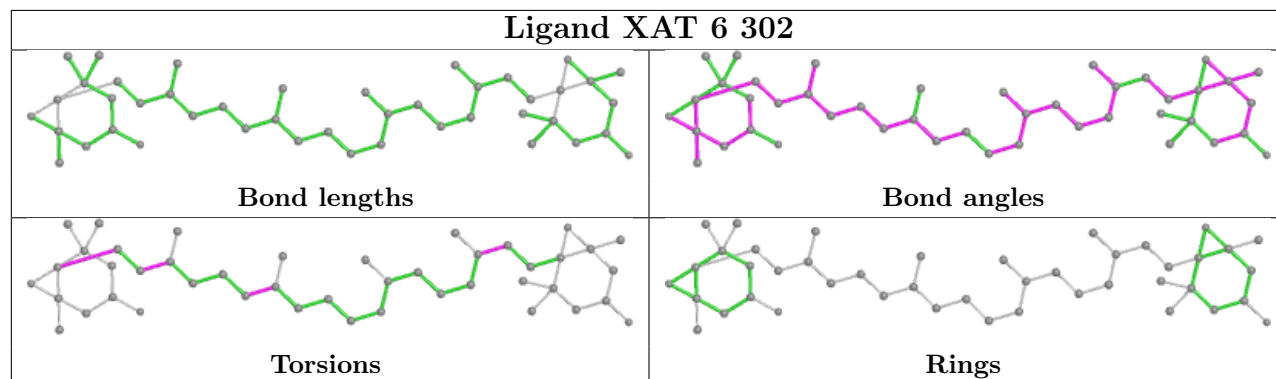
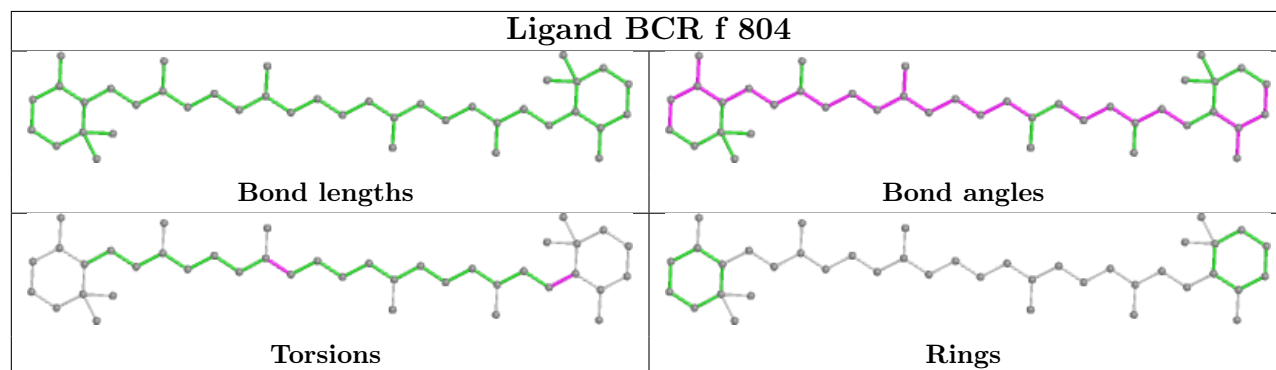
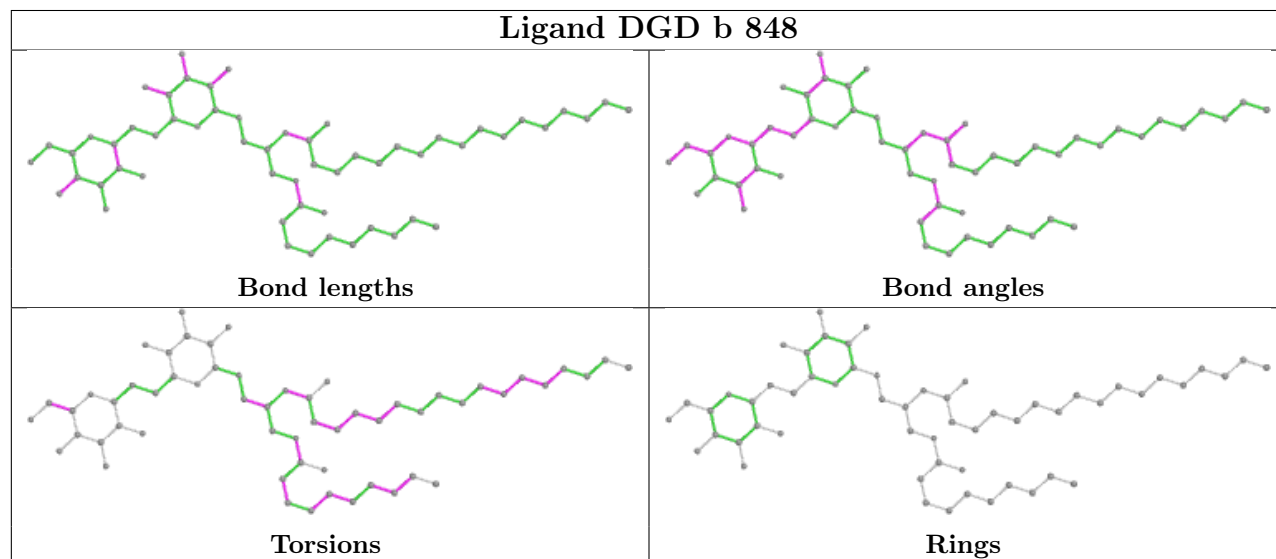
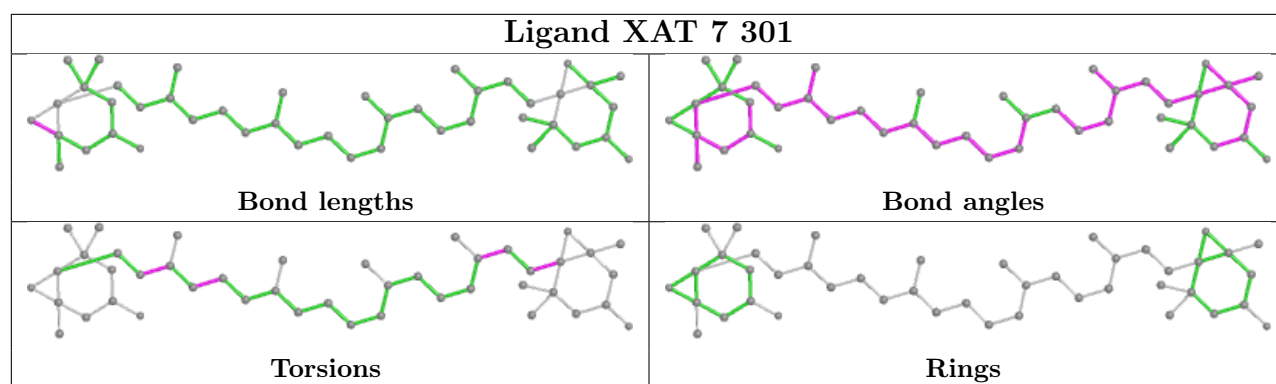
Bond angles

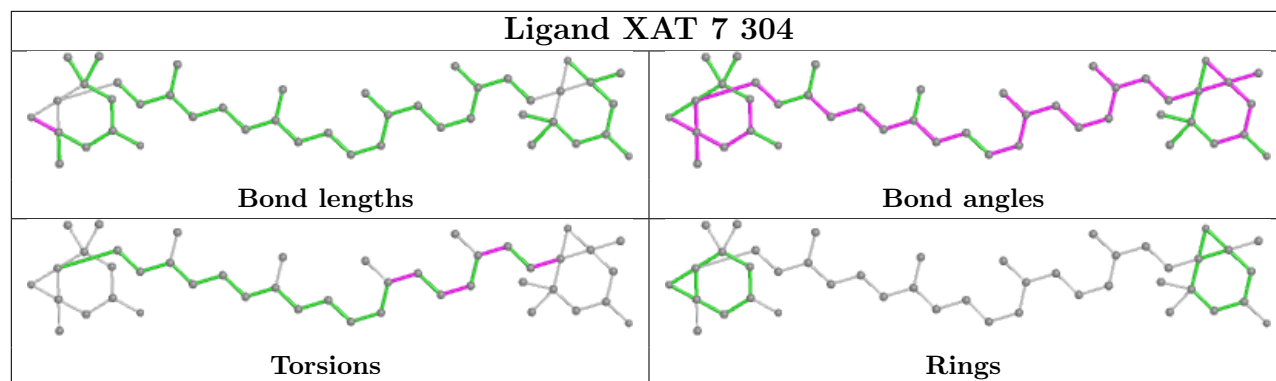
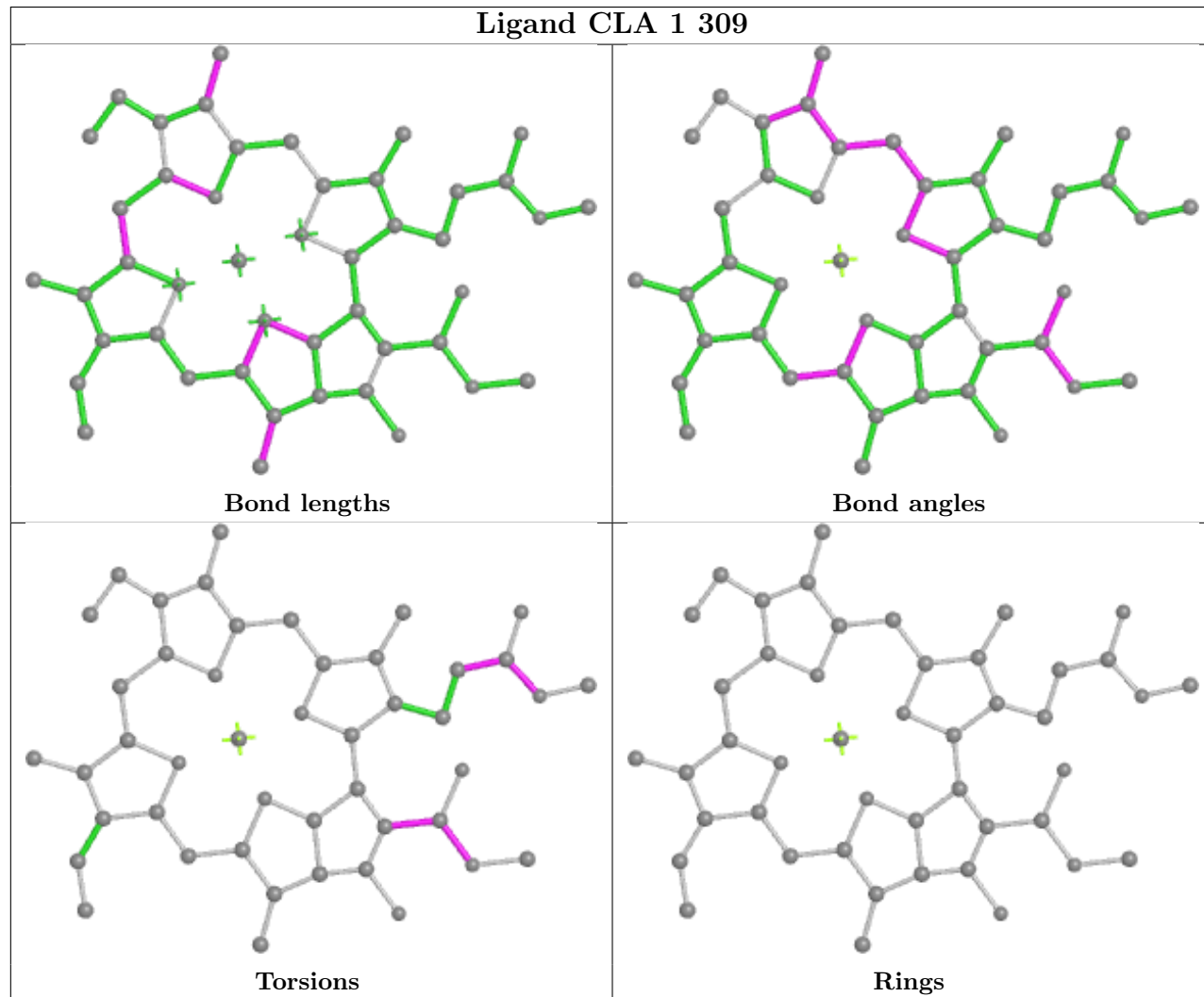


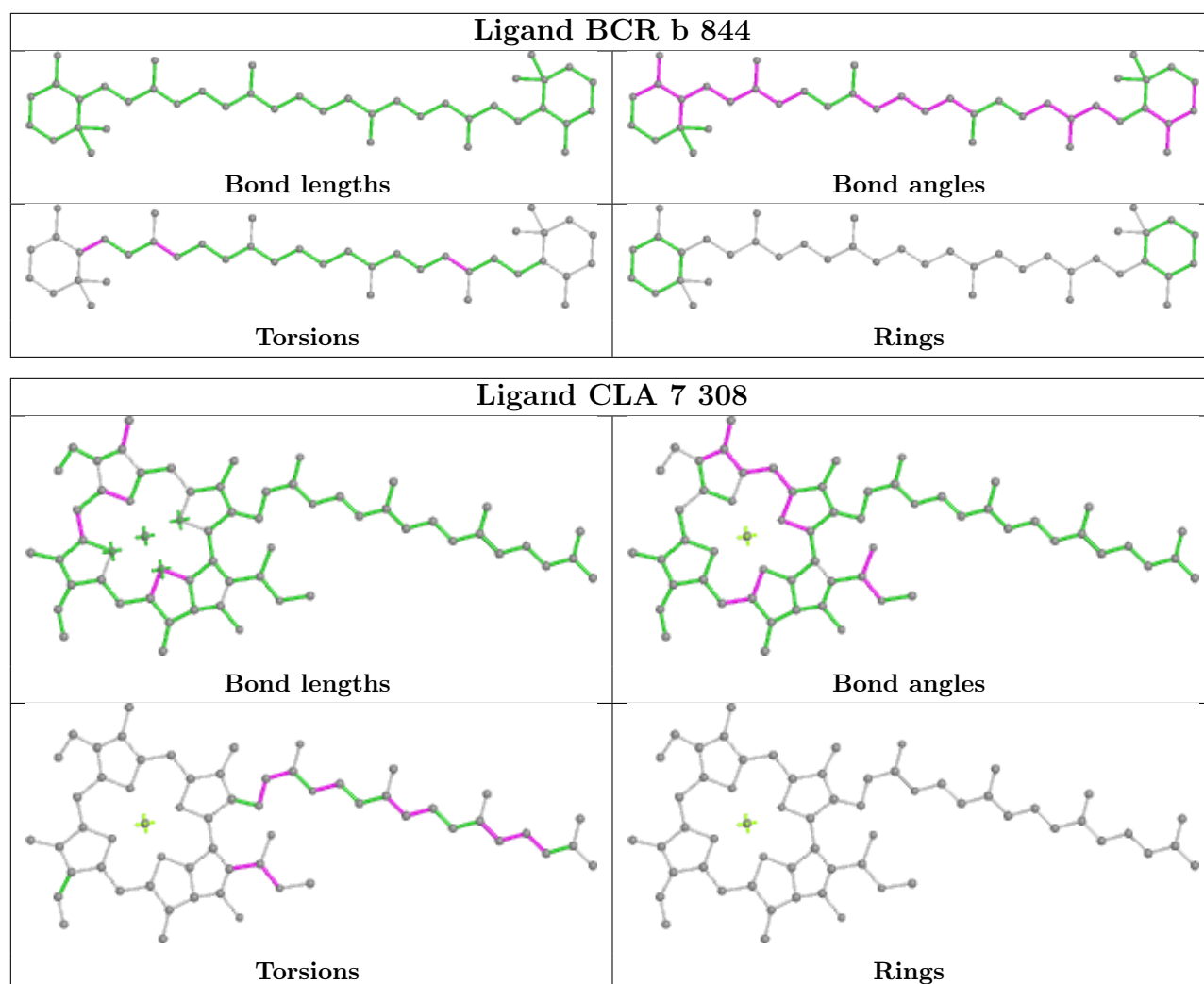
Torsions



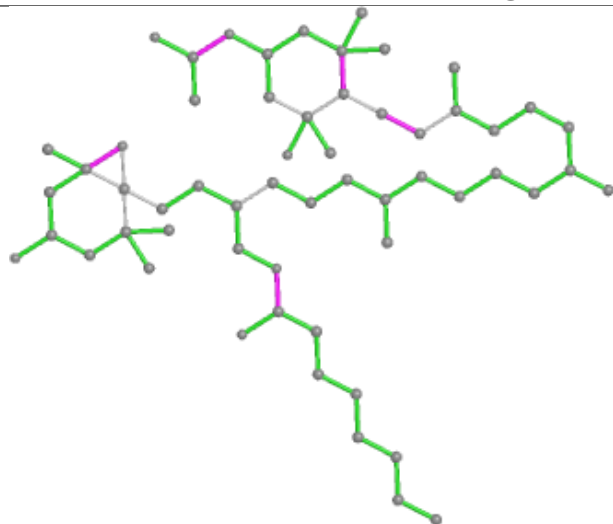
Rings



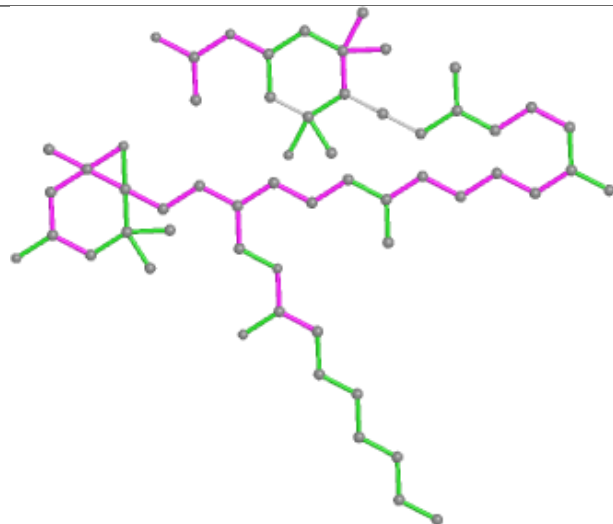
Ligand XAT 7 304**Ligand CLA 1 309**



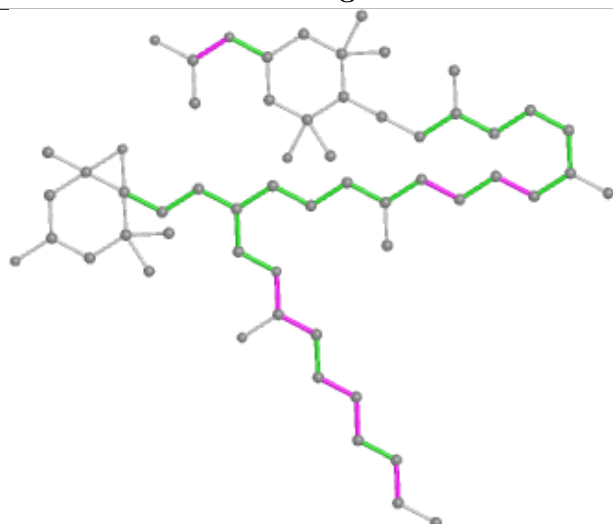
Ligand A1L1F 6 301



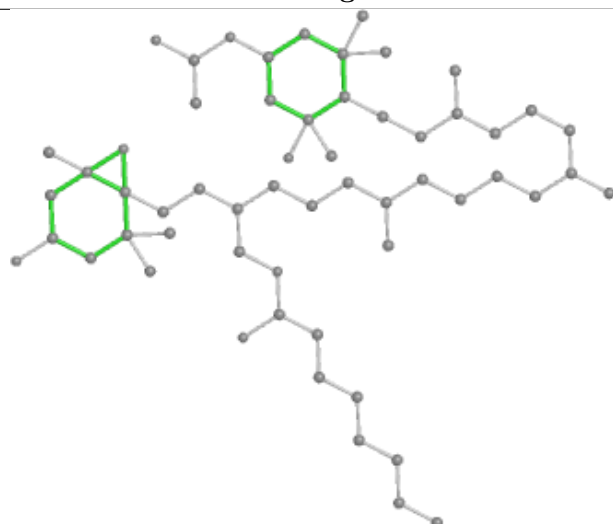
Bond lengths



Bond angles

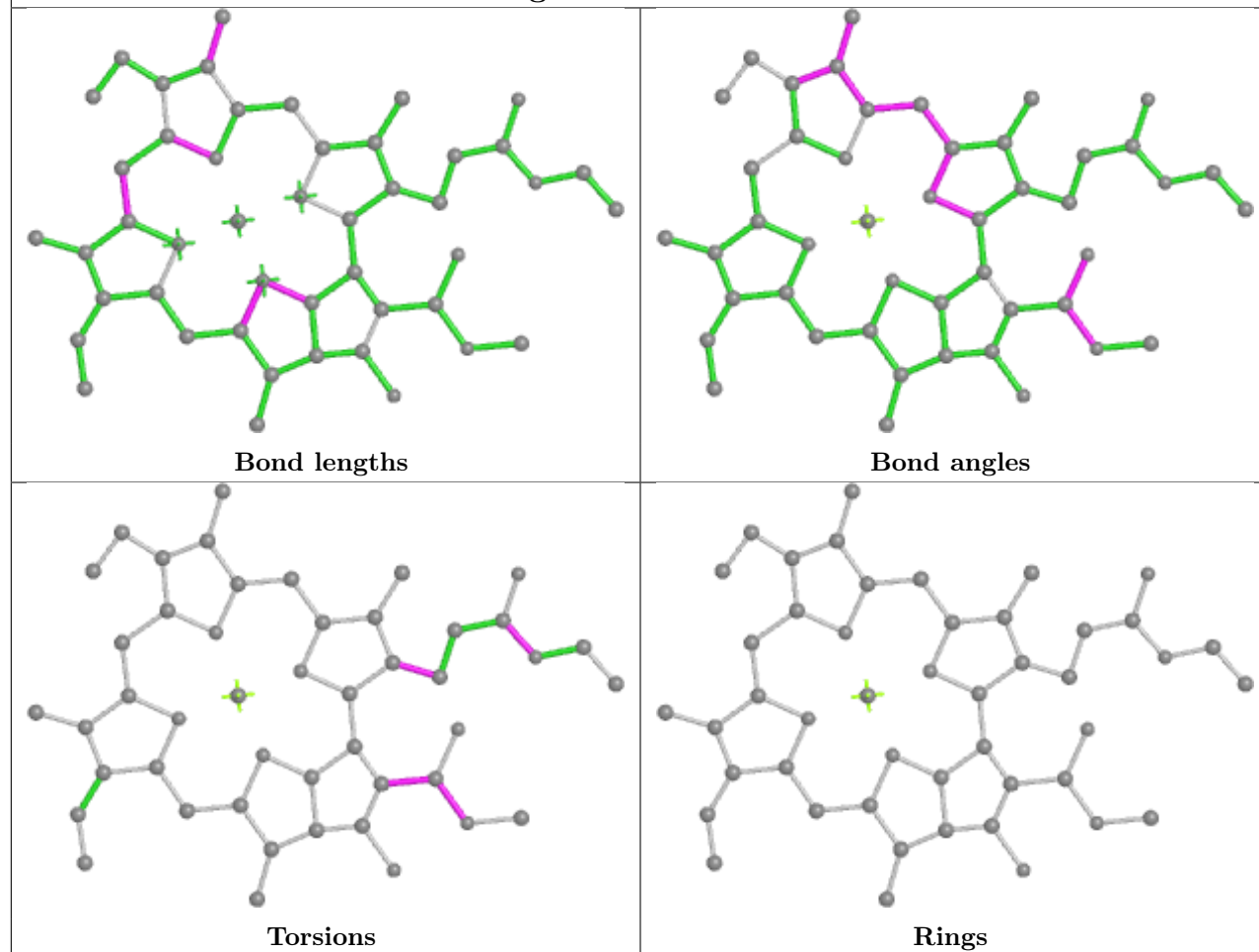


Torsions

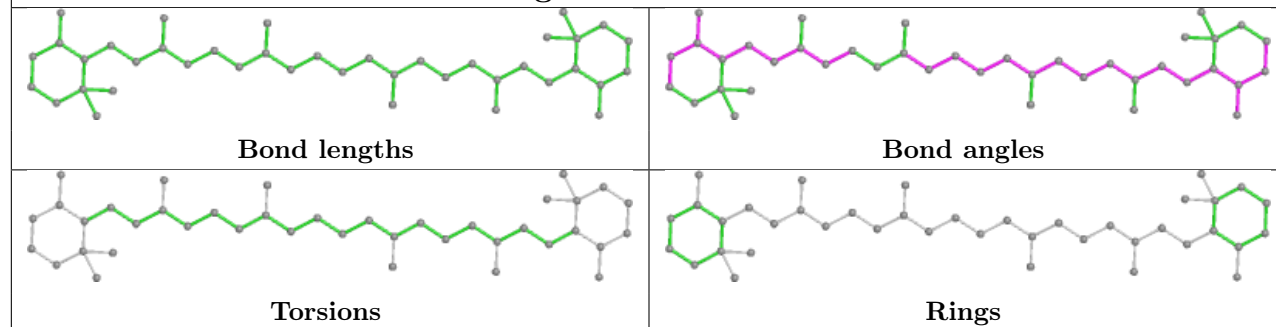


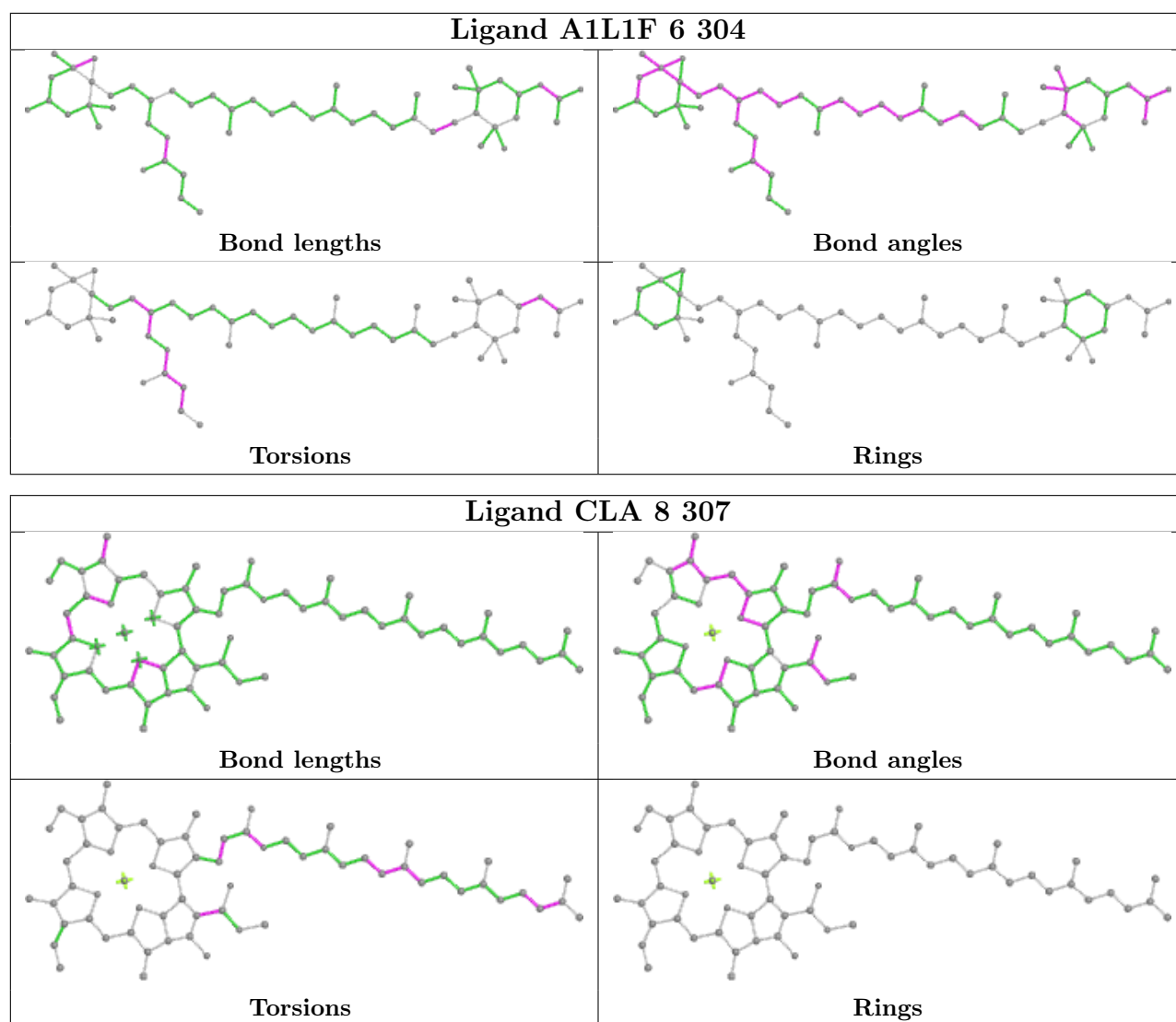
Rings

Ligand CLA 3 314

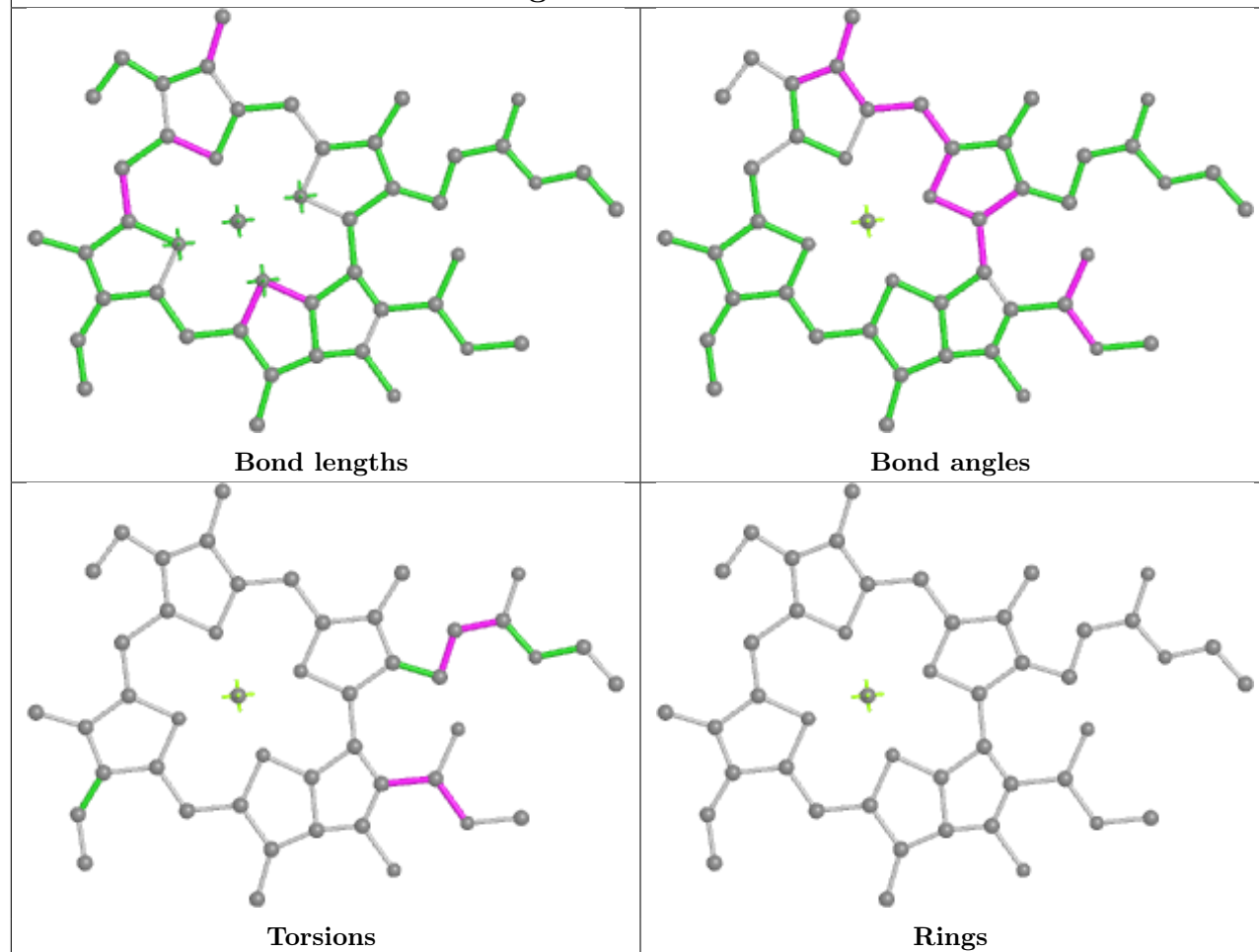


Ligand BCR a 847

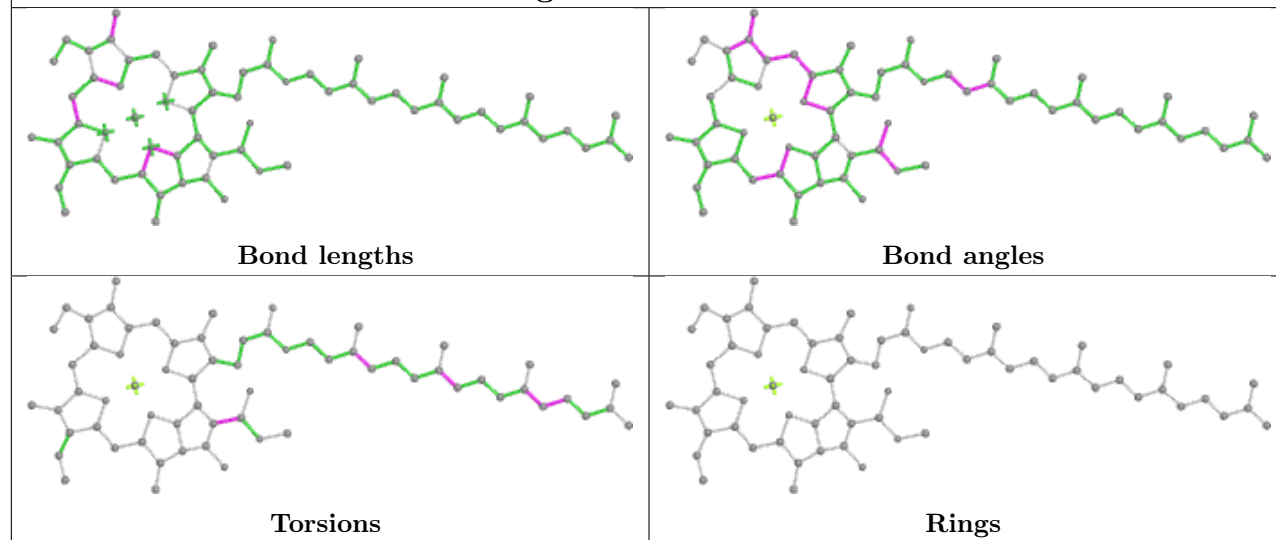


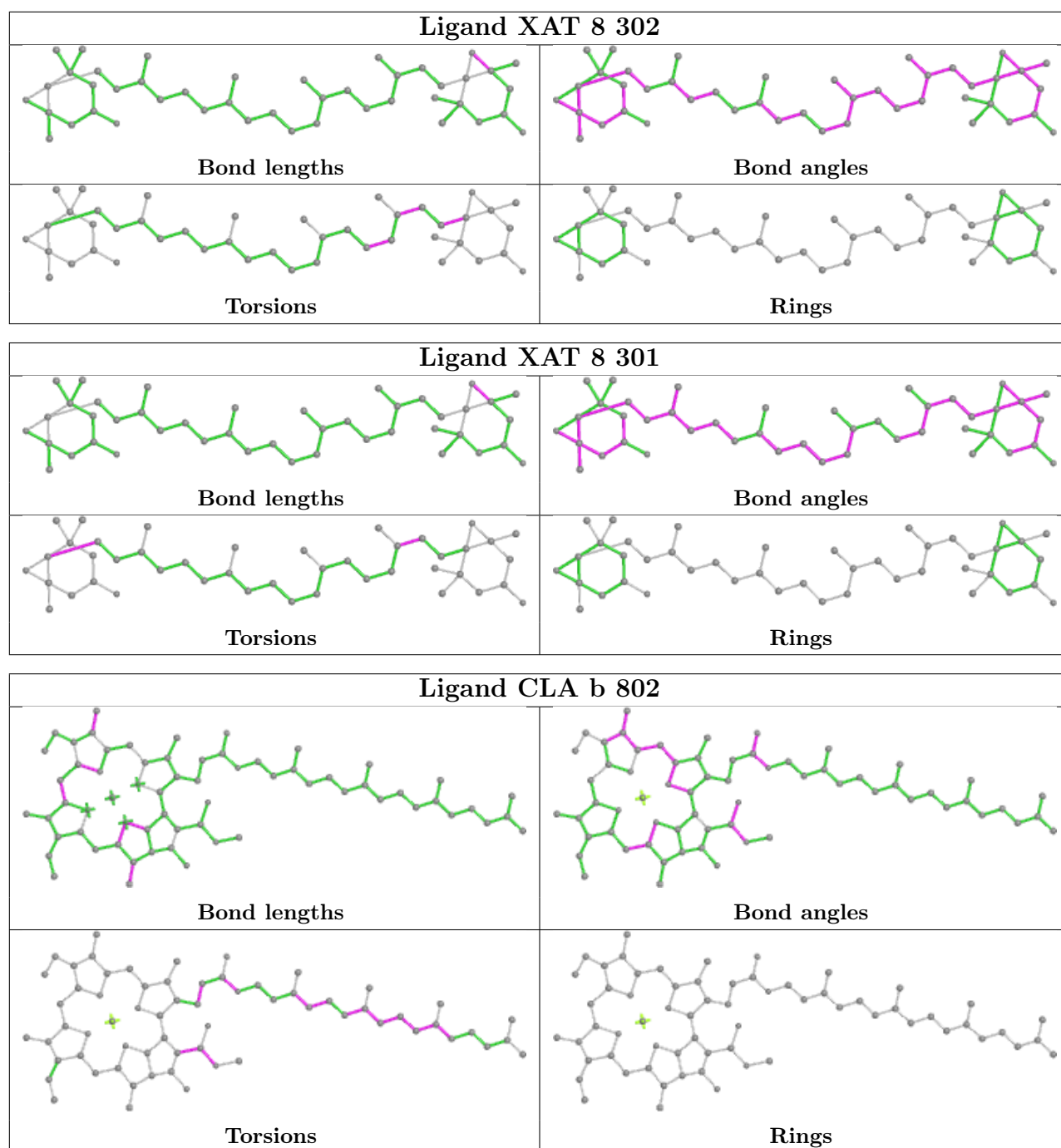


Ligand CLA 2 307

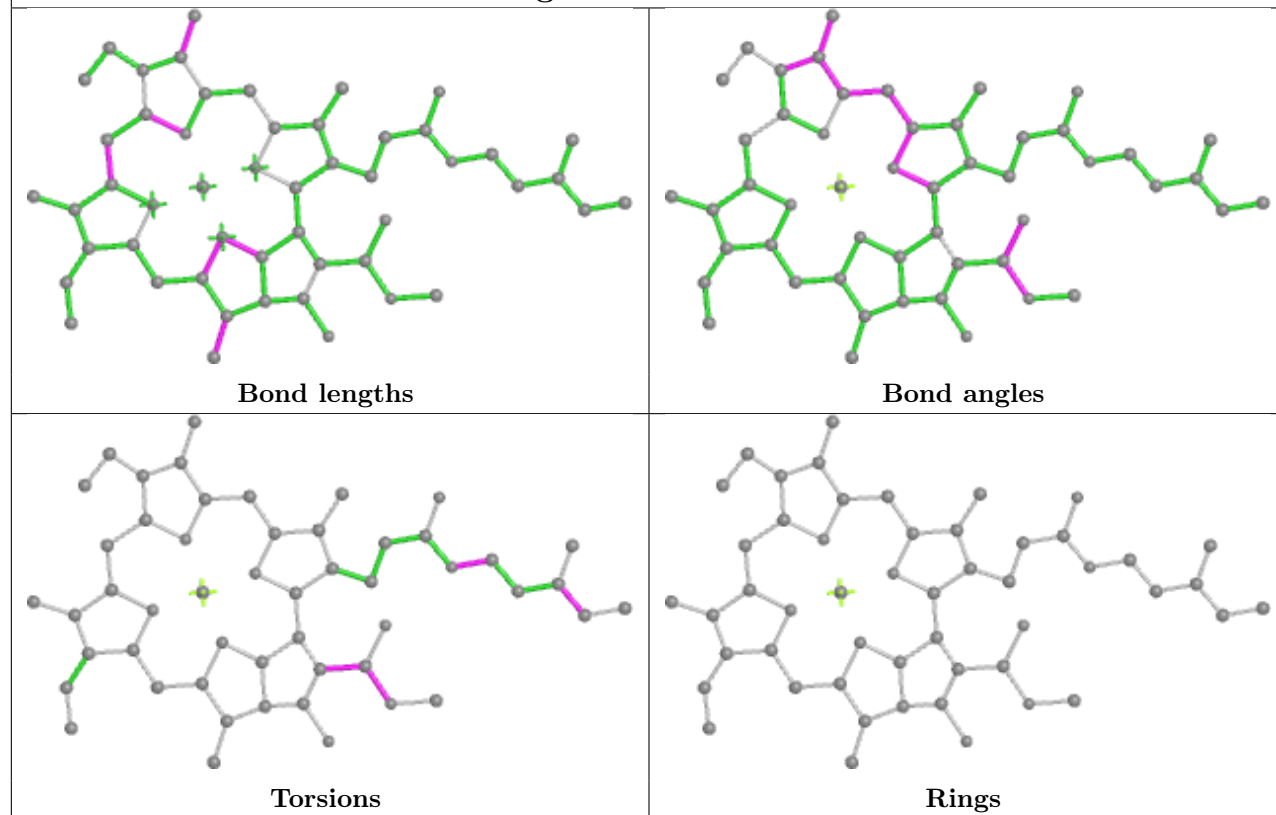


Ligand CLA a 840

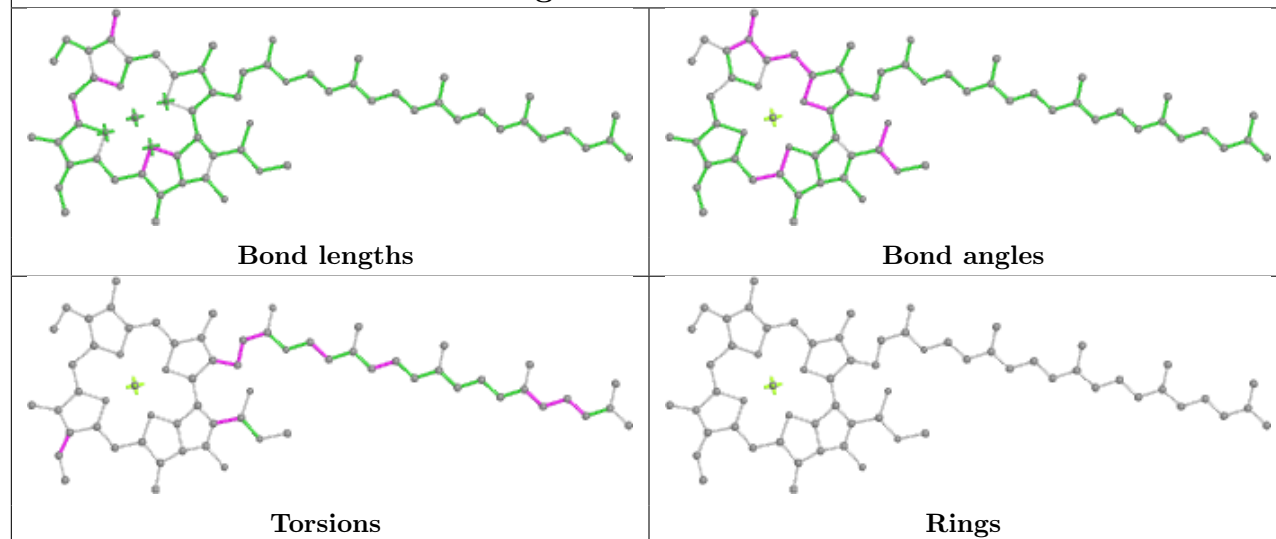


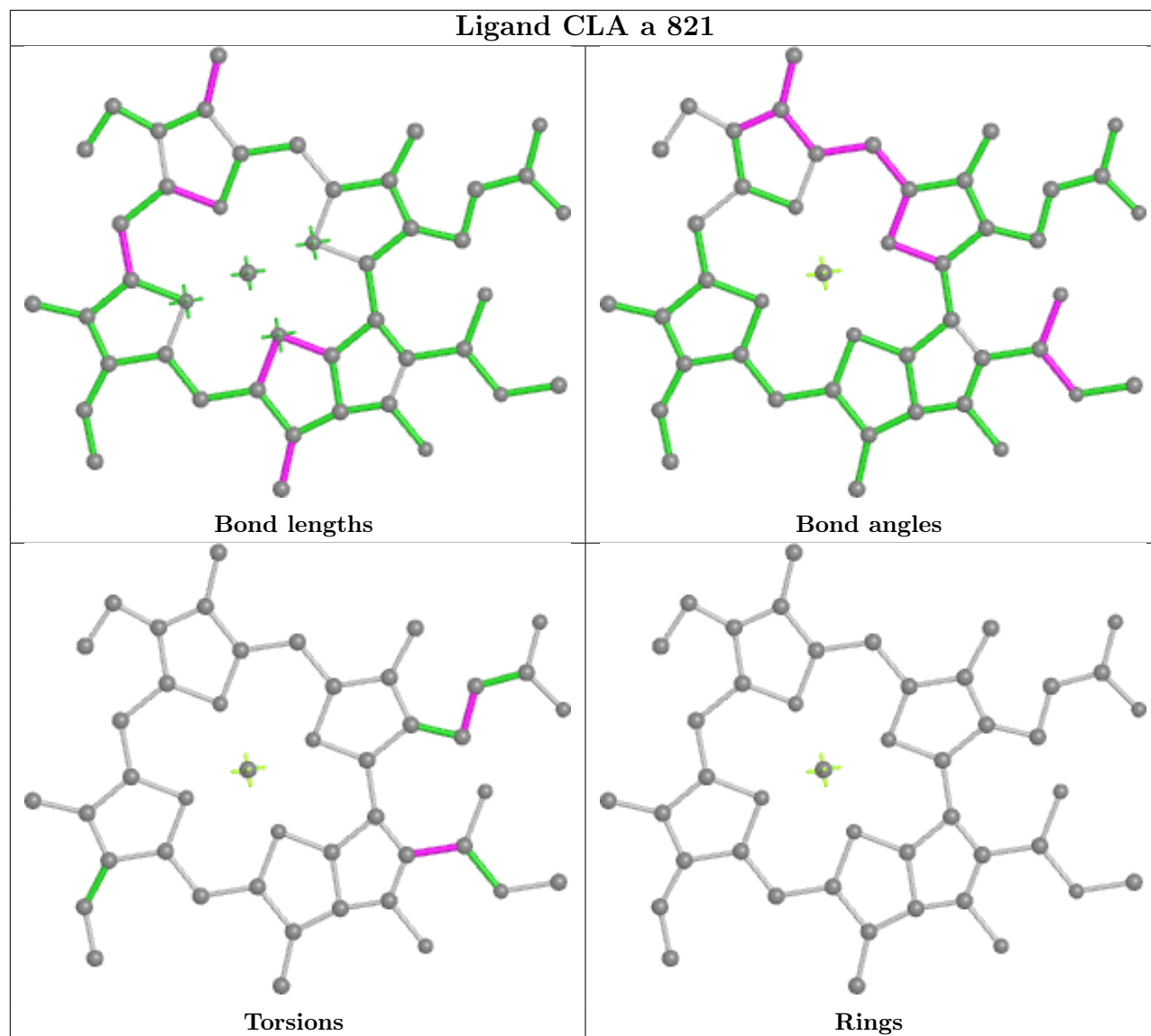
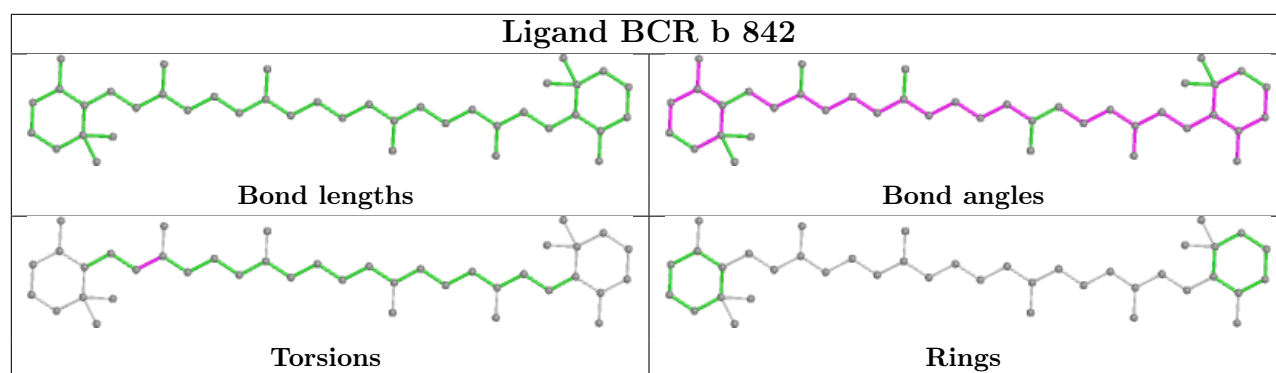


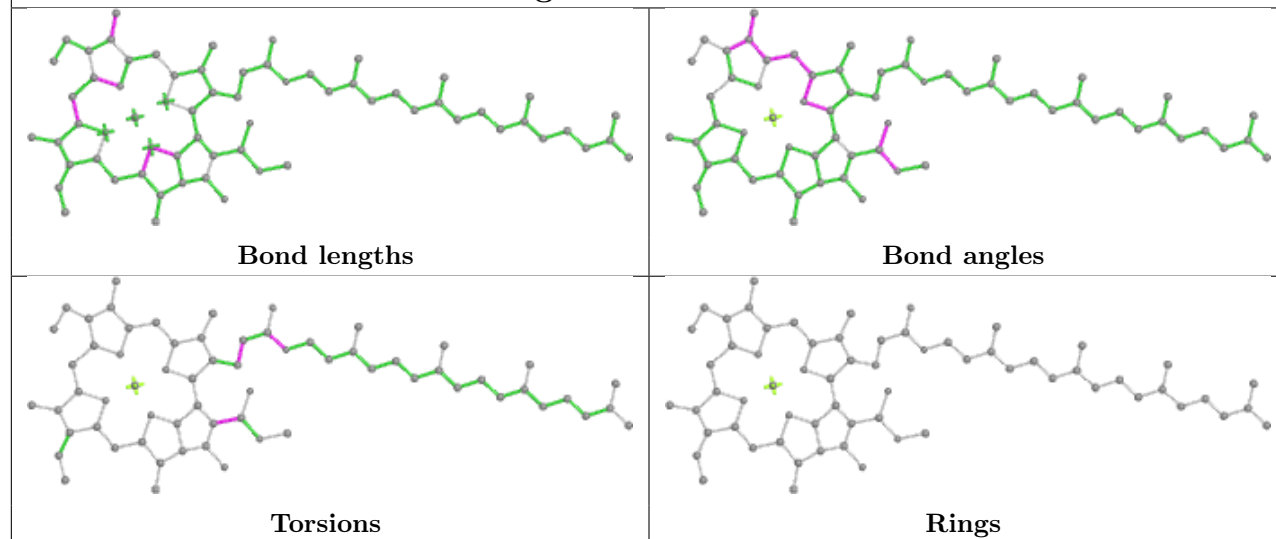
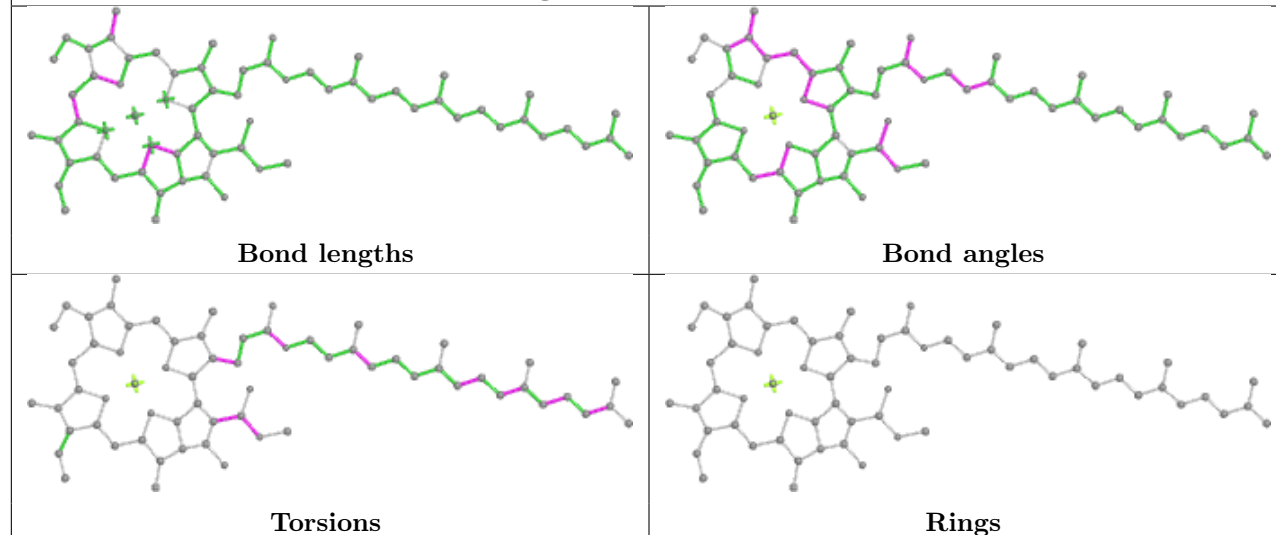
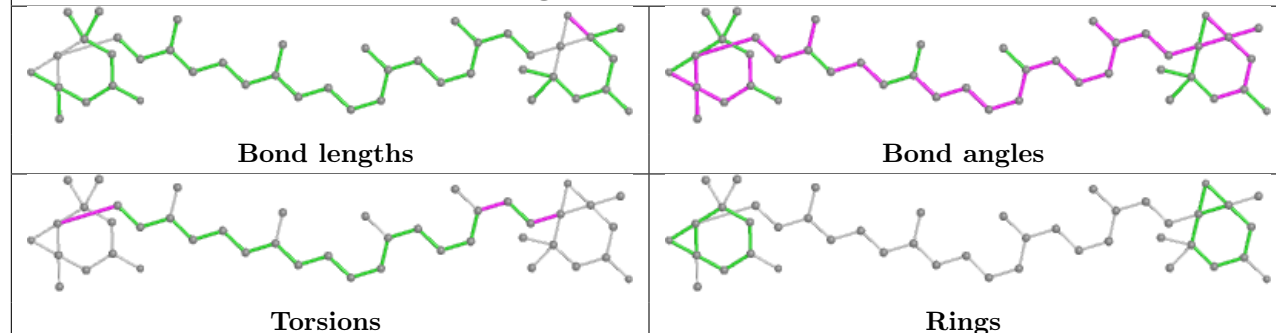
Ligand CLA 6 312

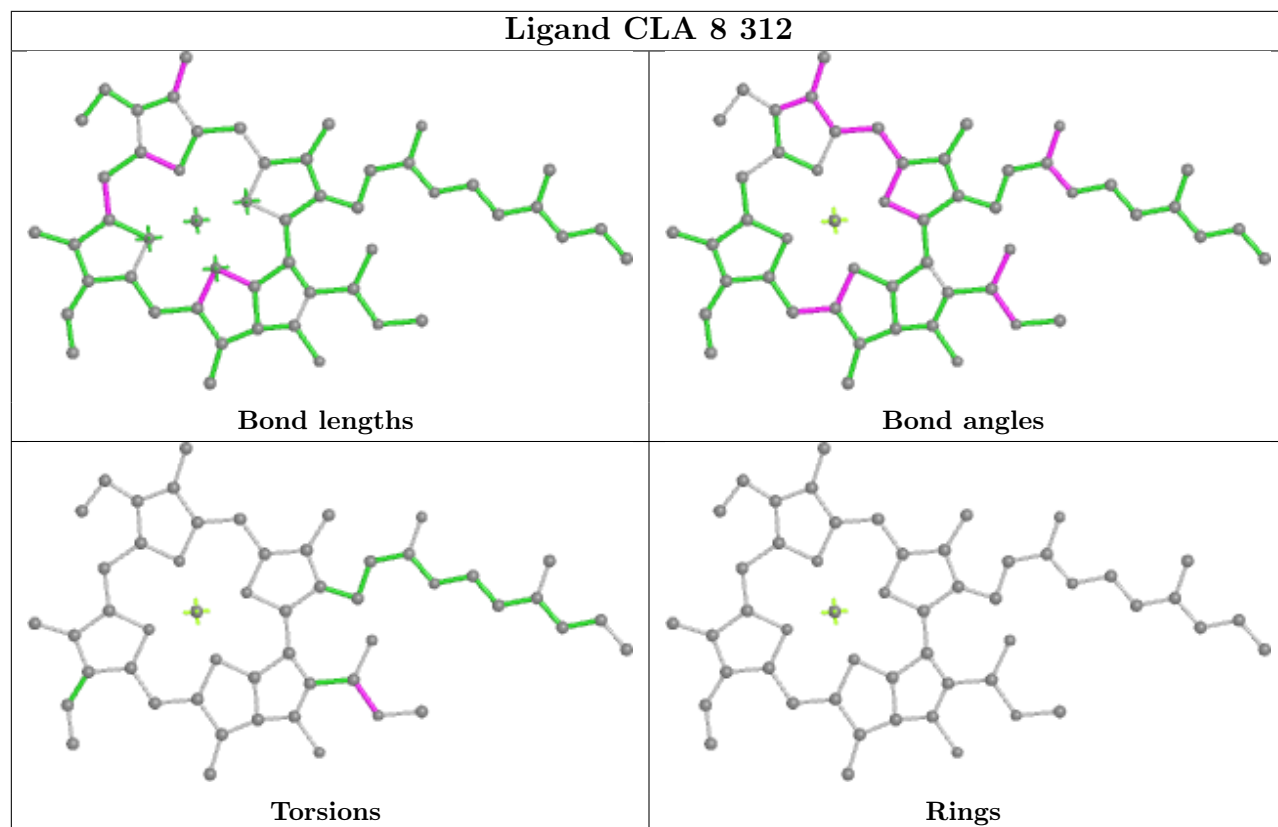


Ligand CLA b 832

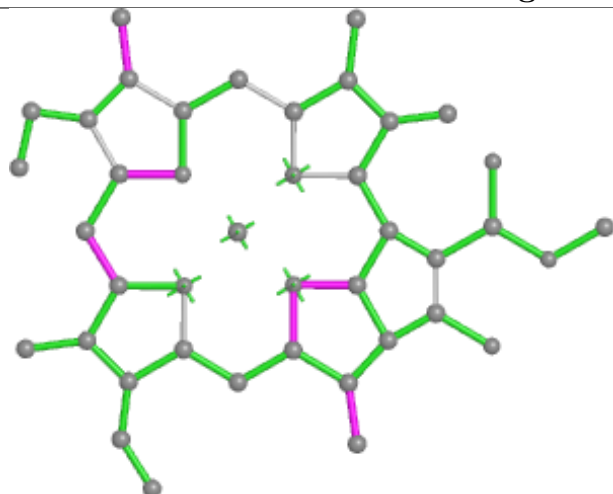




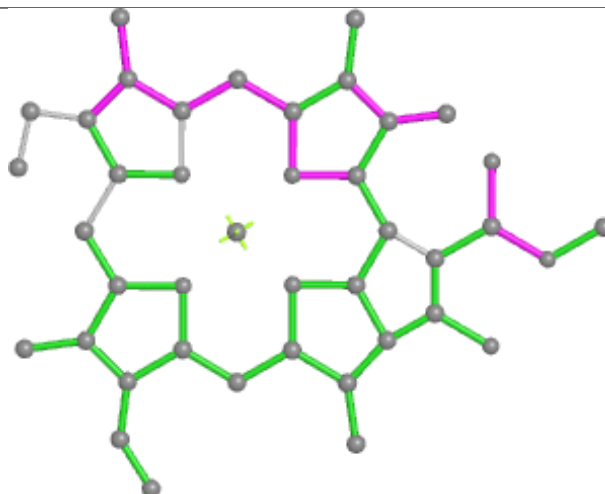
Ligand CLA b 826**Ligand CLA a 820****Ligand XAT 9 303**



Ligand CLA 1 313



Bond lengths



Bond angles

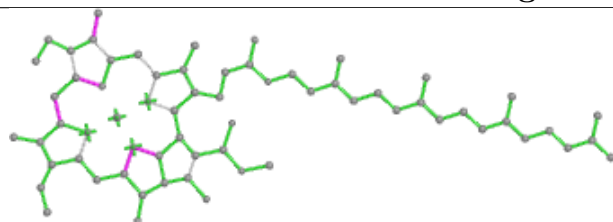


Torsions

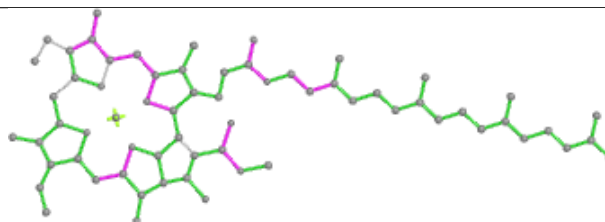


Rings

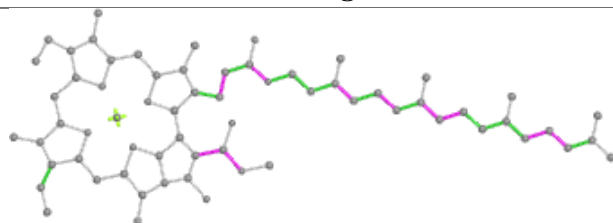
Ligand CLA a 841



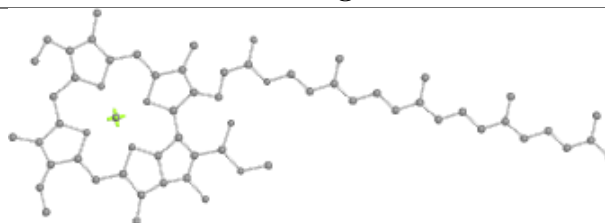
Bond lengths



Bond angles

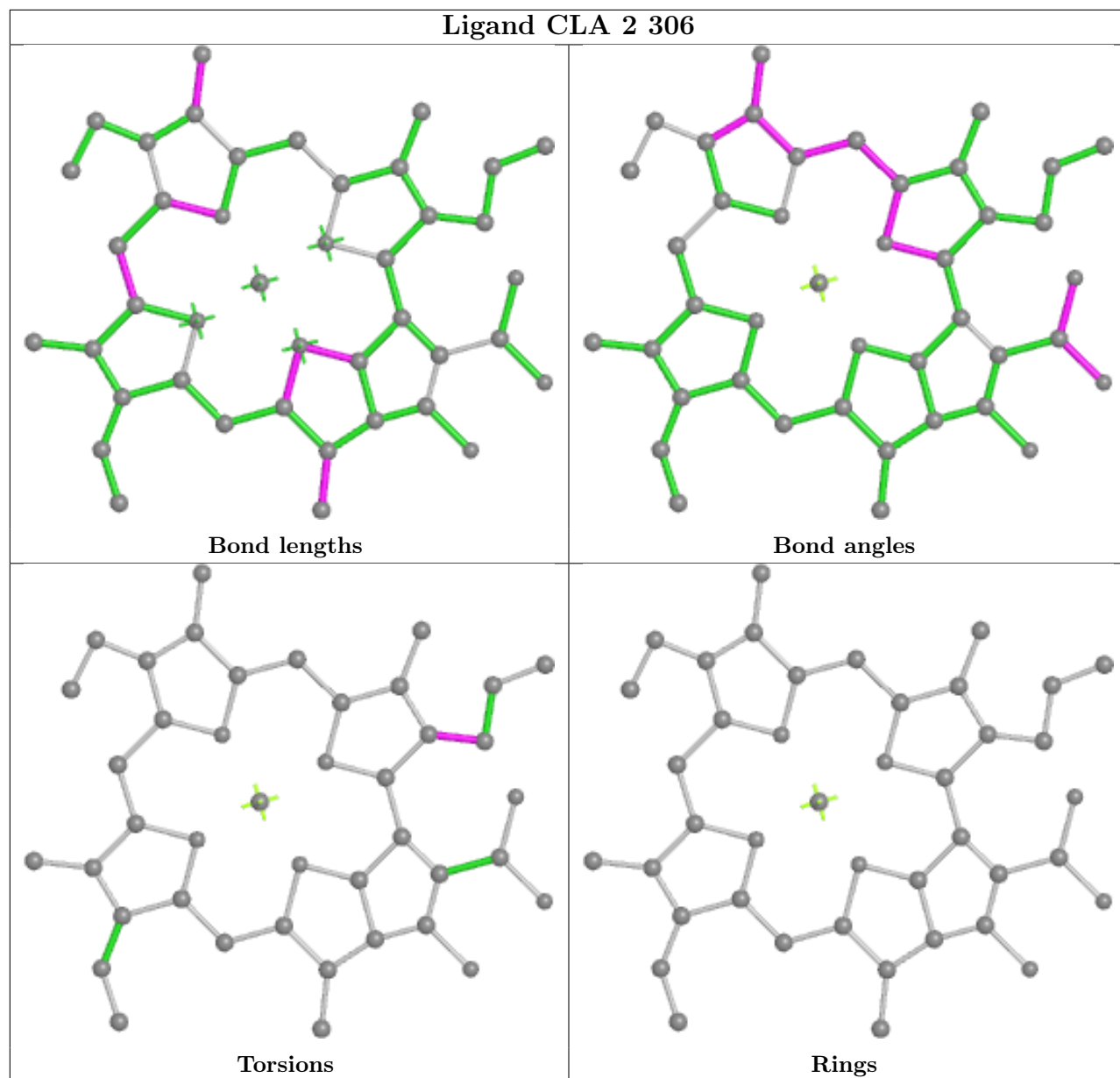


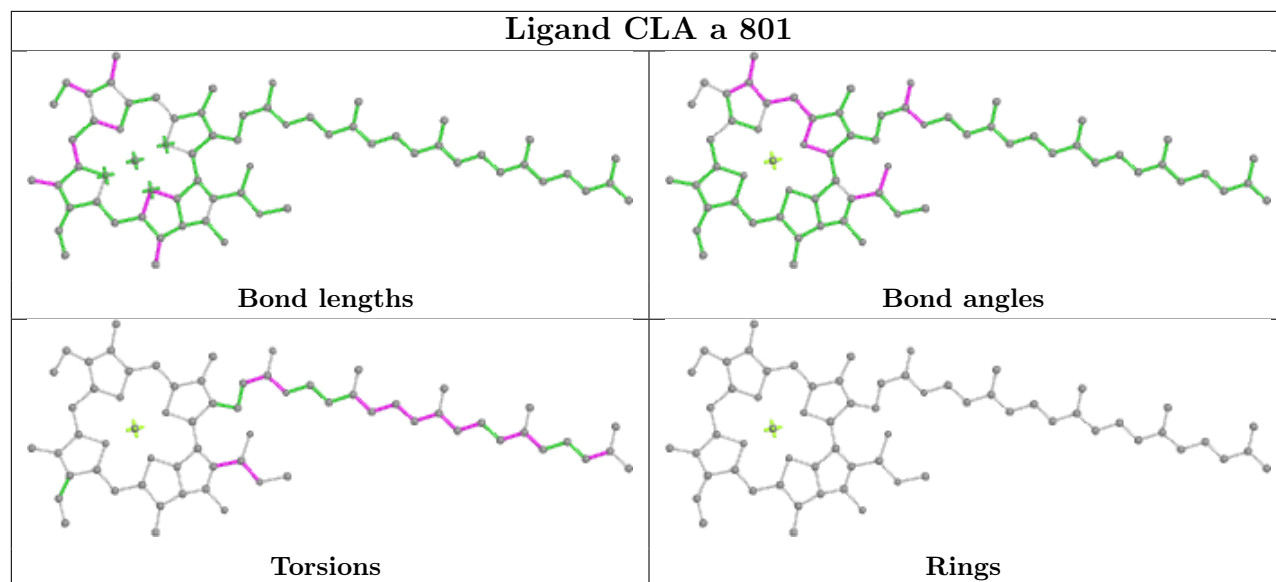
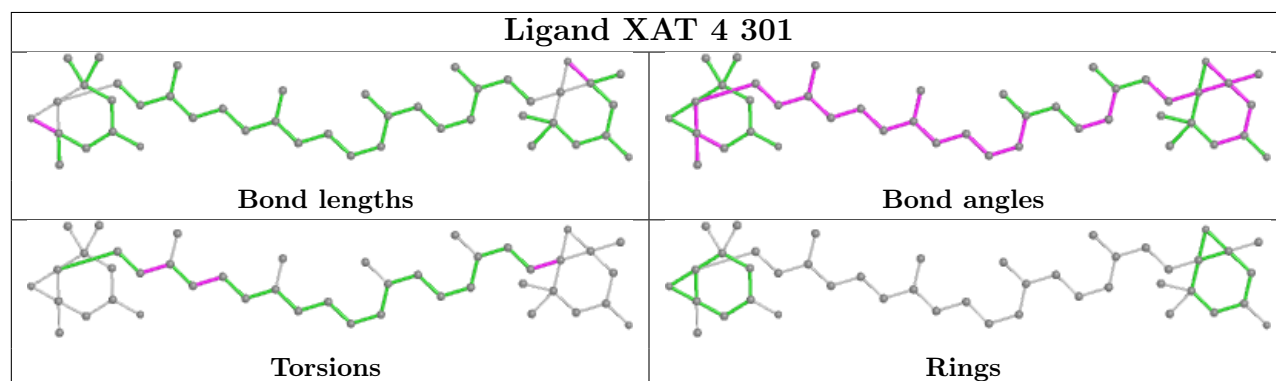
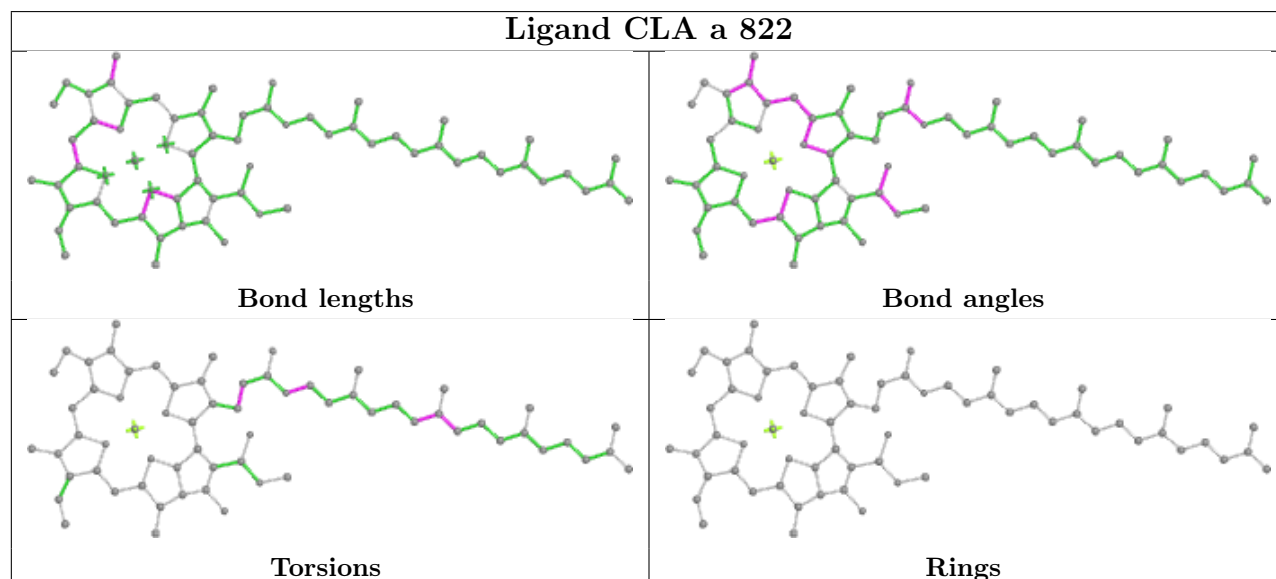
Torsions



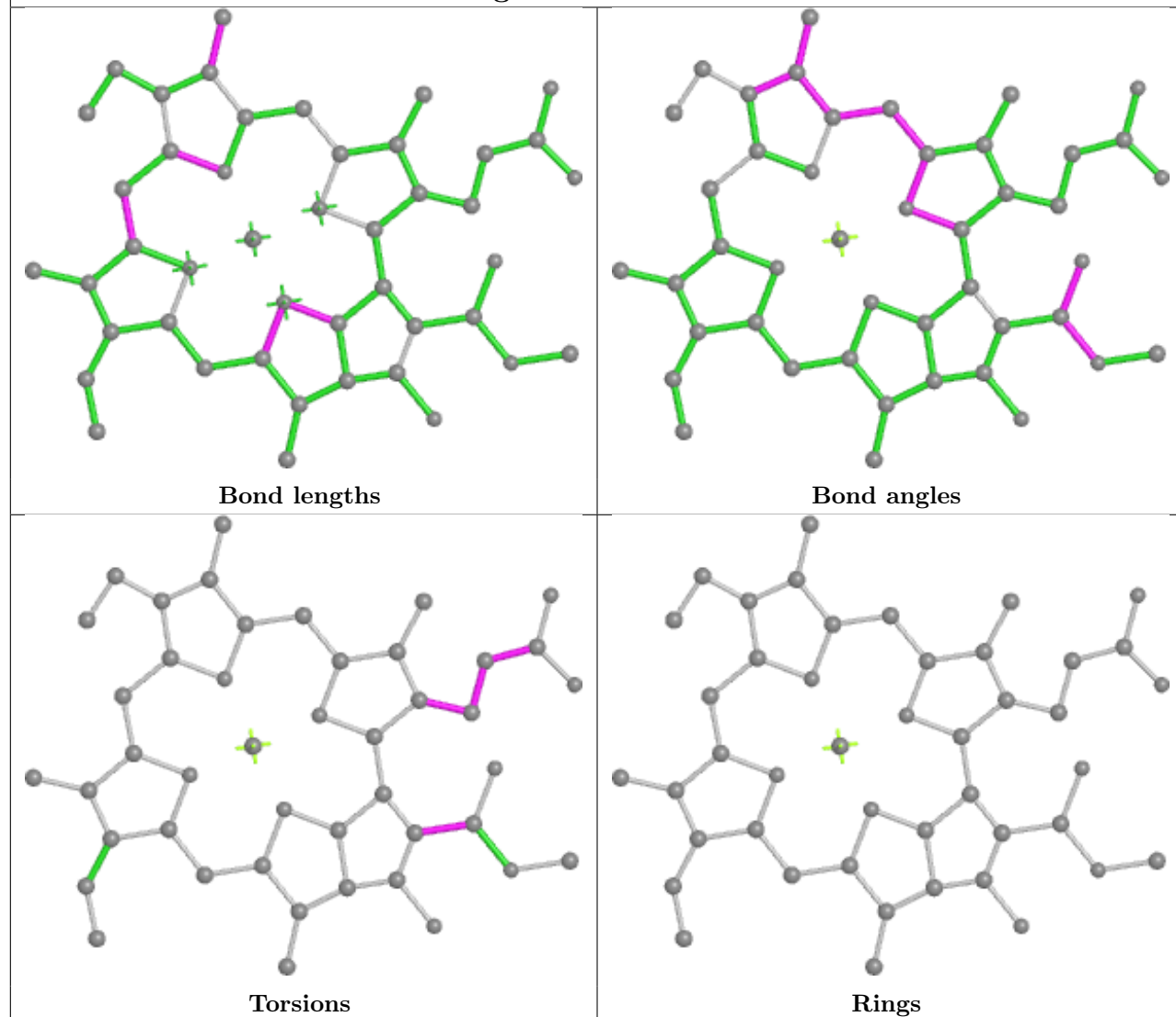
Rings

Ligand CLA 2 306

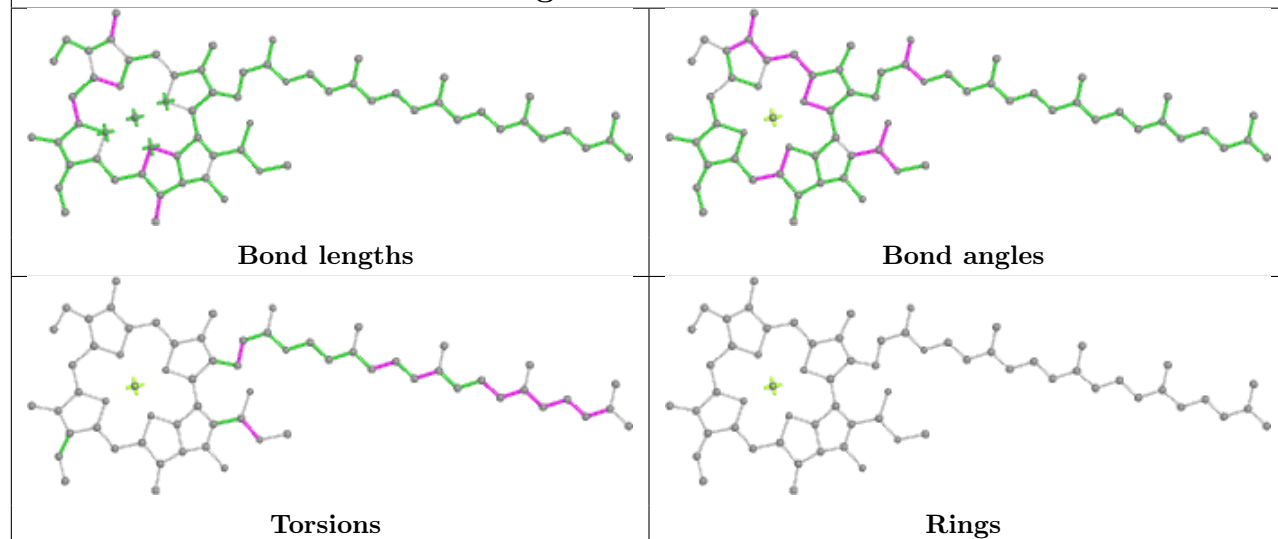


Ligand CLA a 801**Ligand XAT 4 301****Ligand CLA a 822**

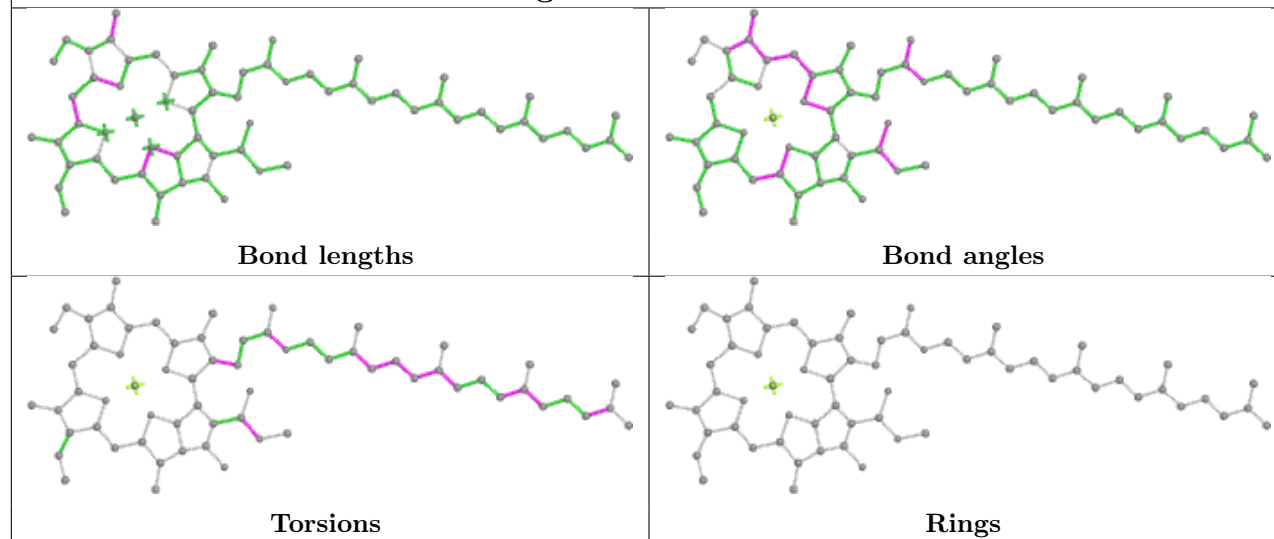
Ligand CLA a 817



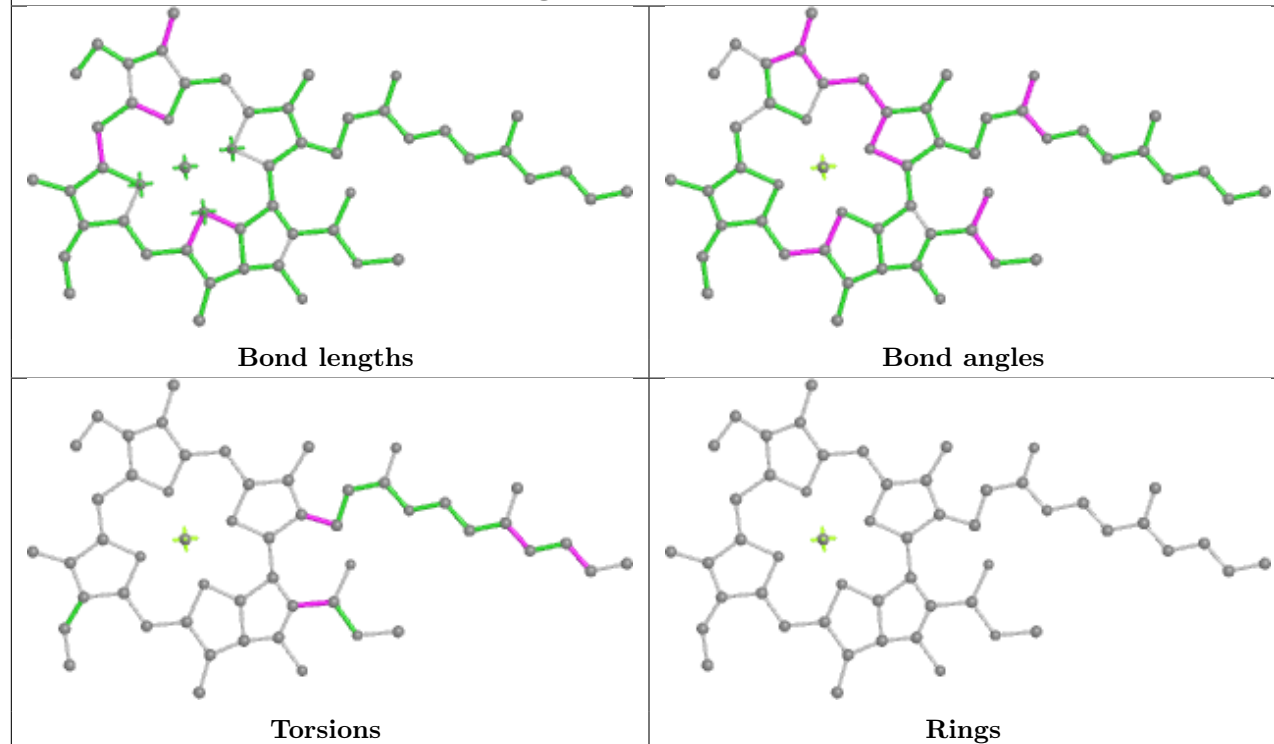
Ligand CLA 4 308



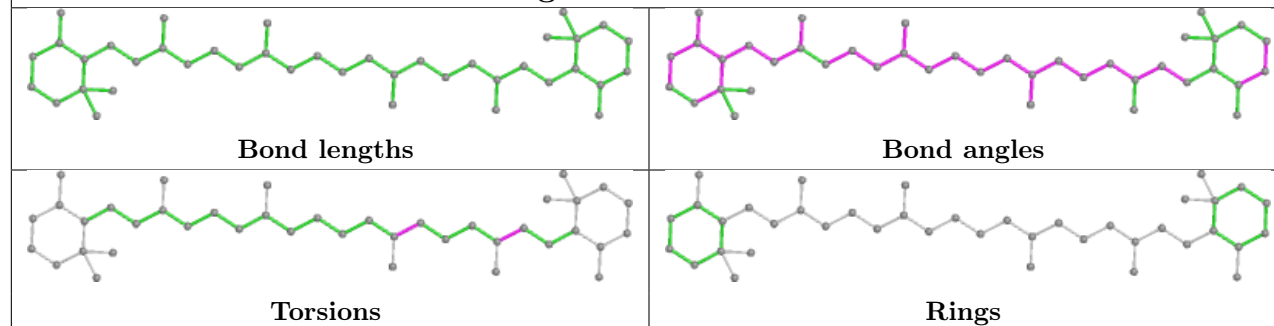
Ligand CLA 1 310



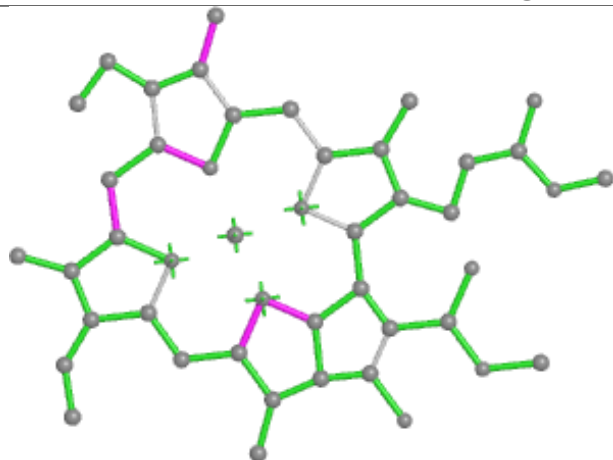
Ligand CLA b 812



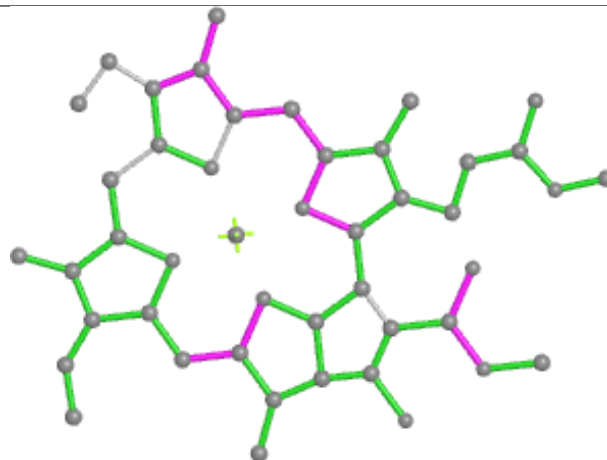
Ligand BCR f 801



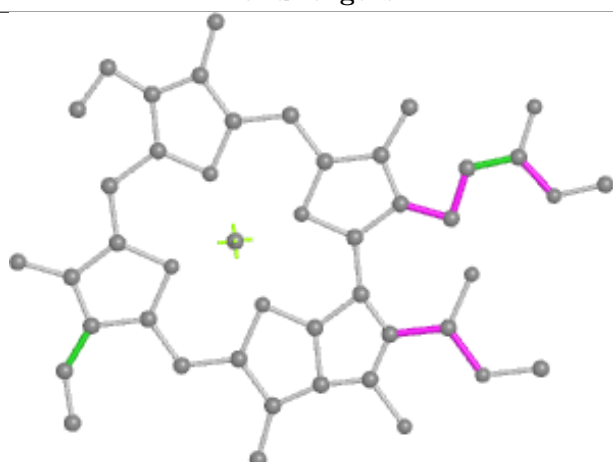
Ligand CLA 4 316



Bond lengths



Bond angles

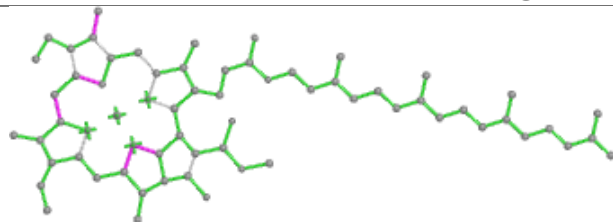


Torsions

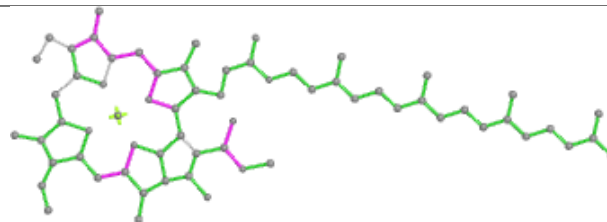


Rings

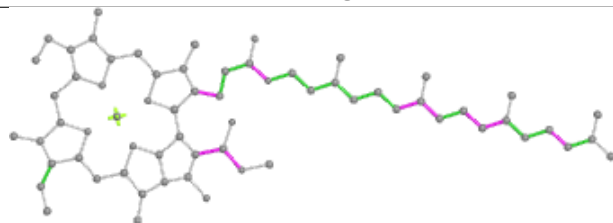
Ligand CLA b 806



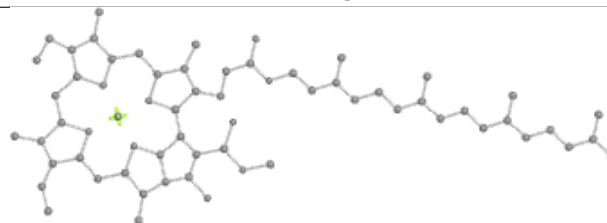
Bond lengths



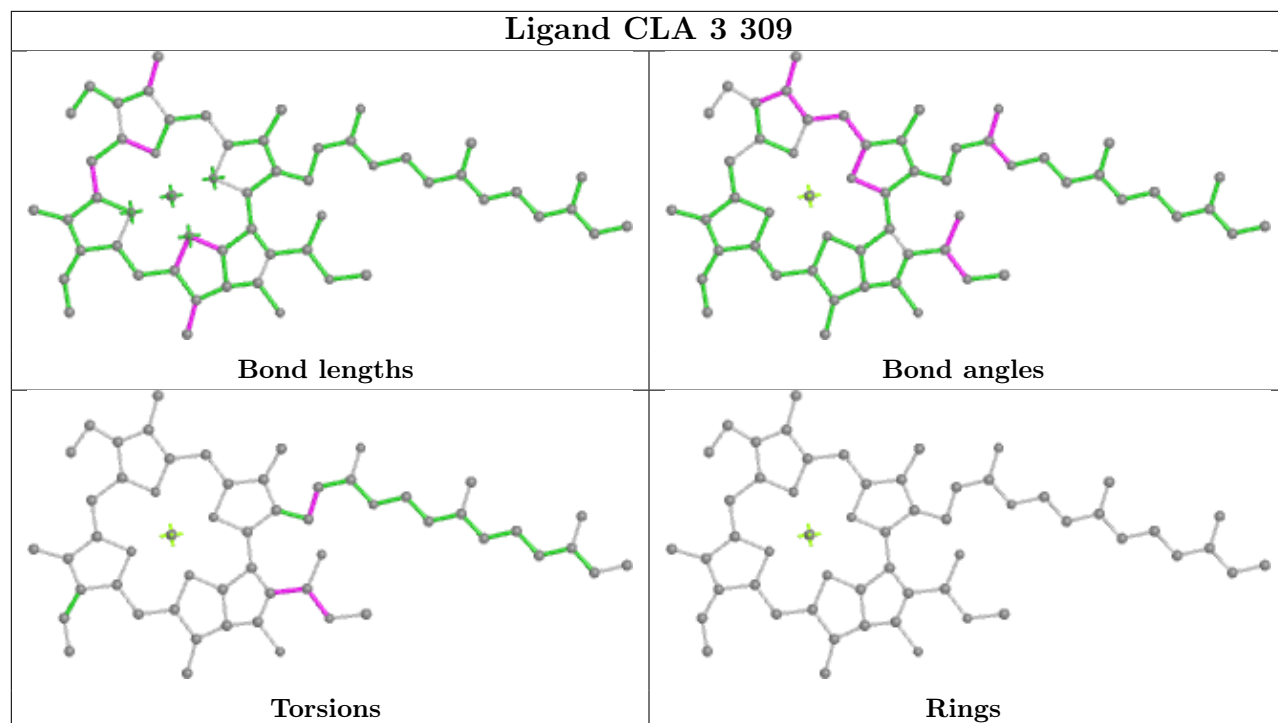
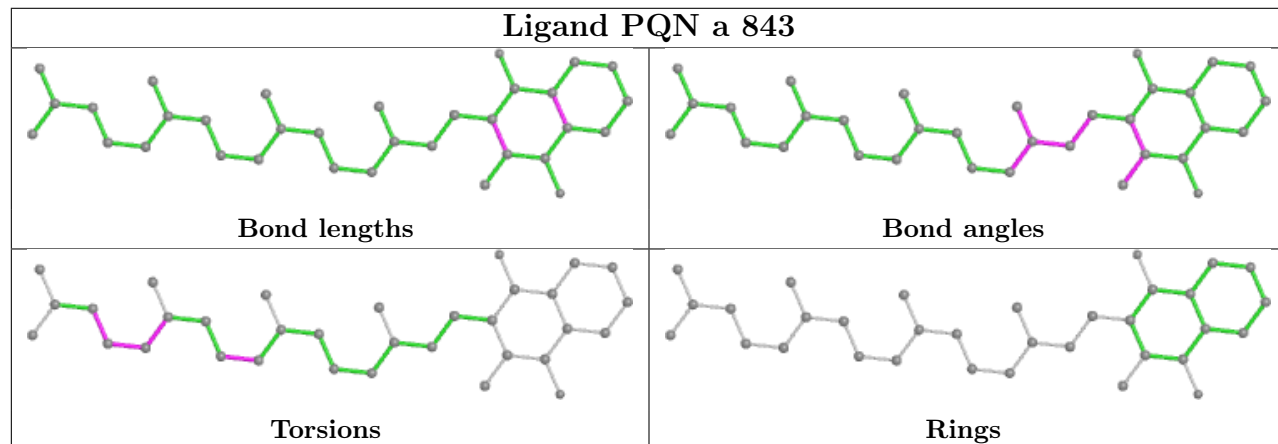
Bond angles



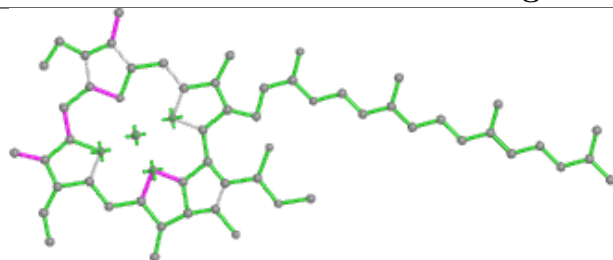
Torsions



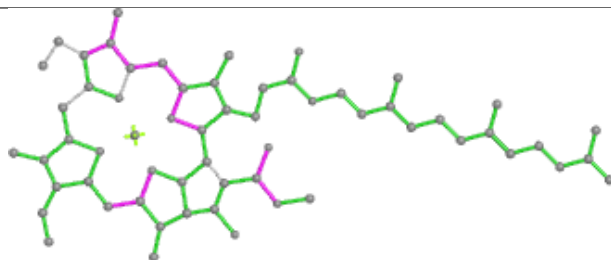
Rings

Ligand CLA 3 309**Ligand PQN a 843**

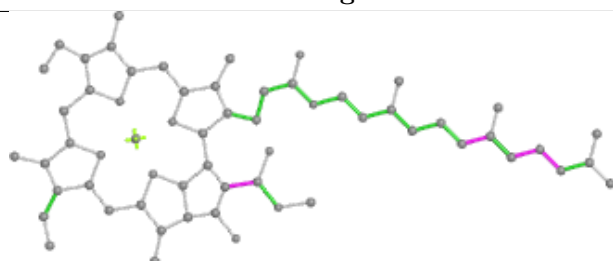
Ligand CLA 1 203



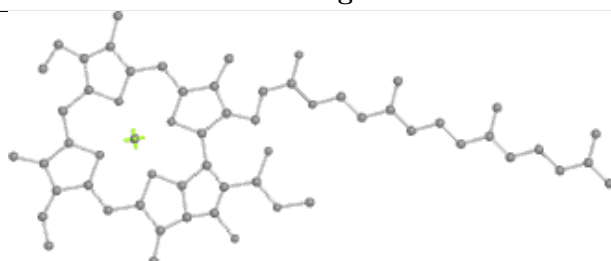
Bond lengths



Bond angles

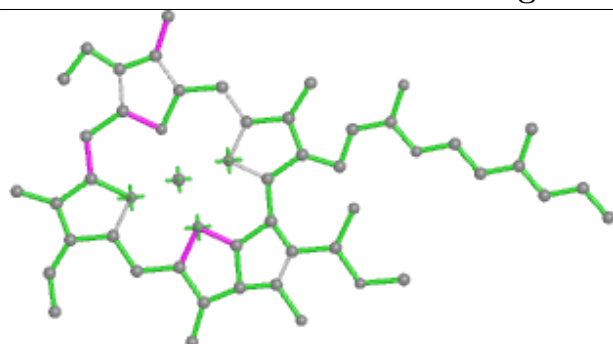


Torsions

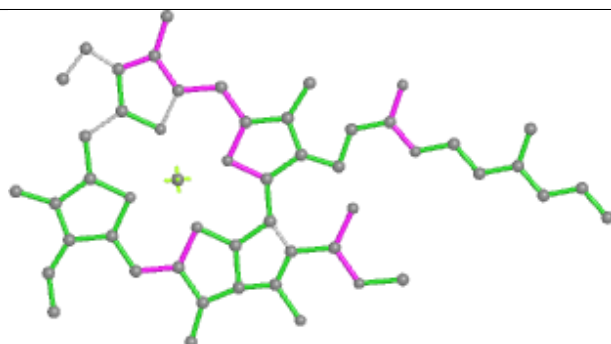


Rings

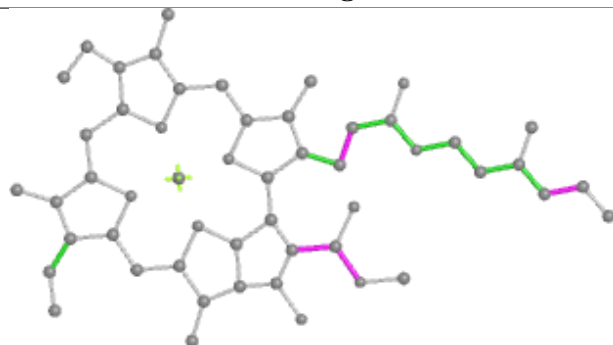
Ligand CLA 6 310



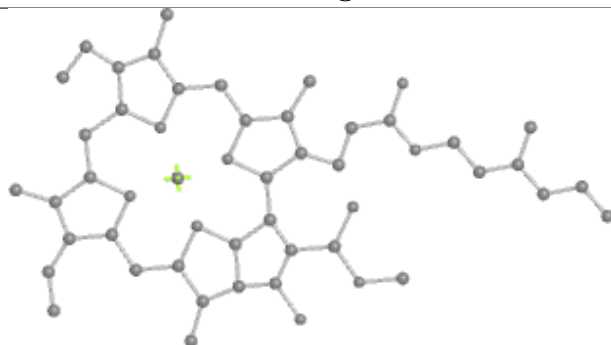
Bond lengths



Bond angles

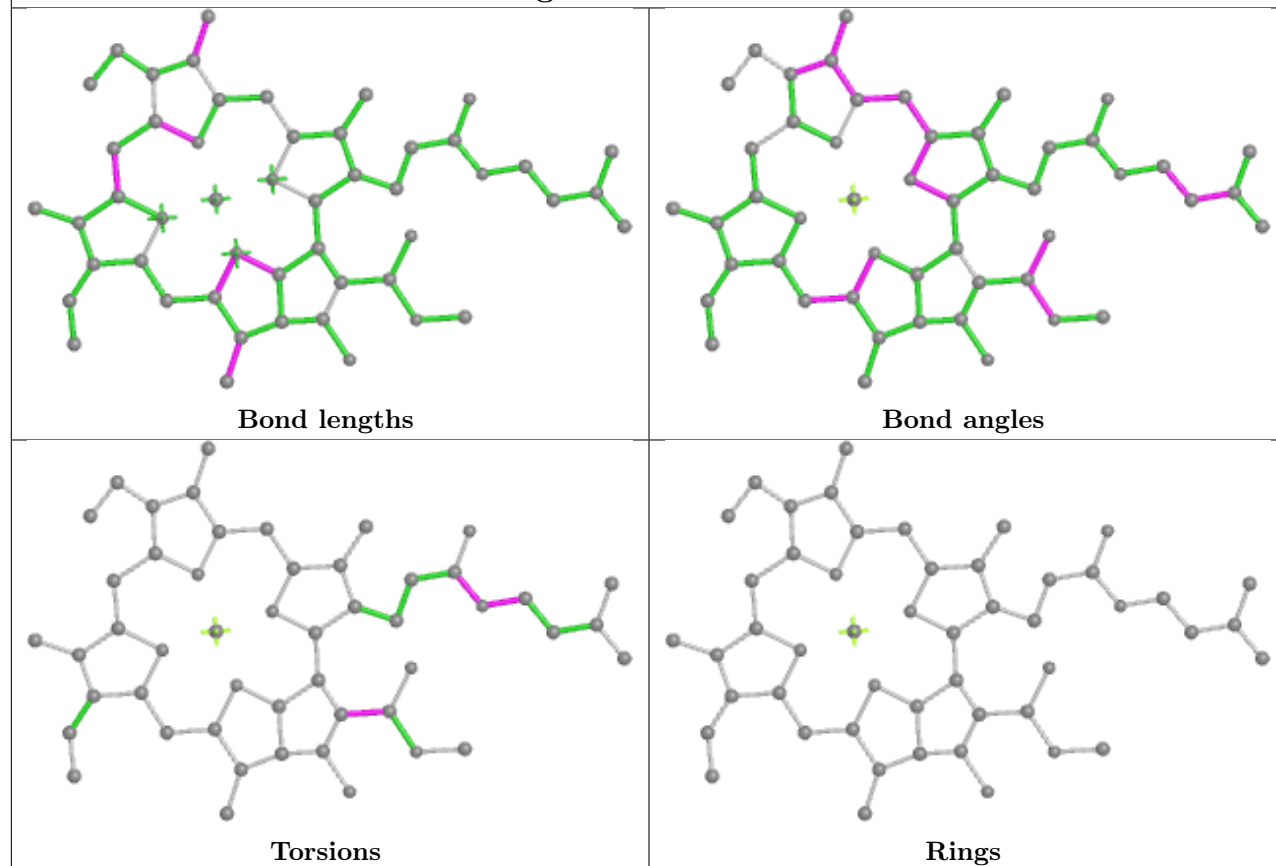


Torsions

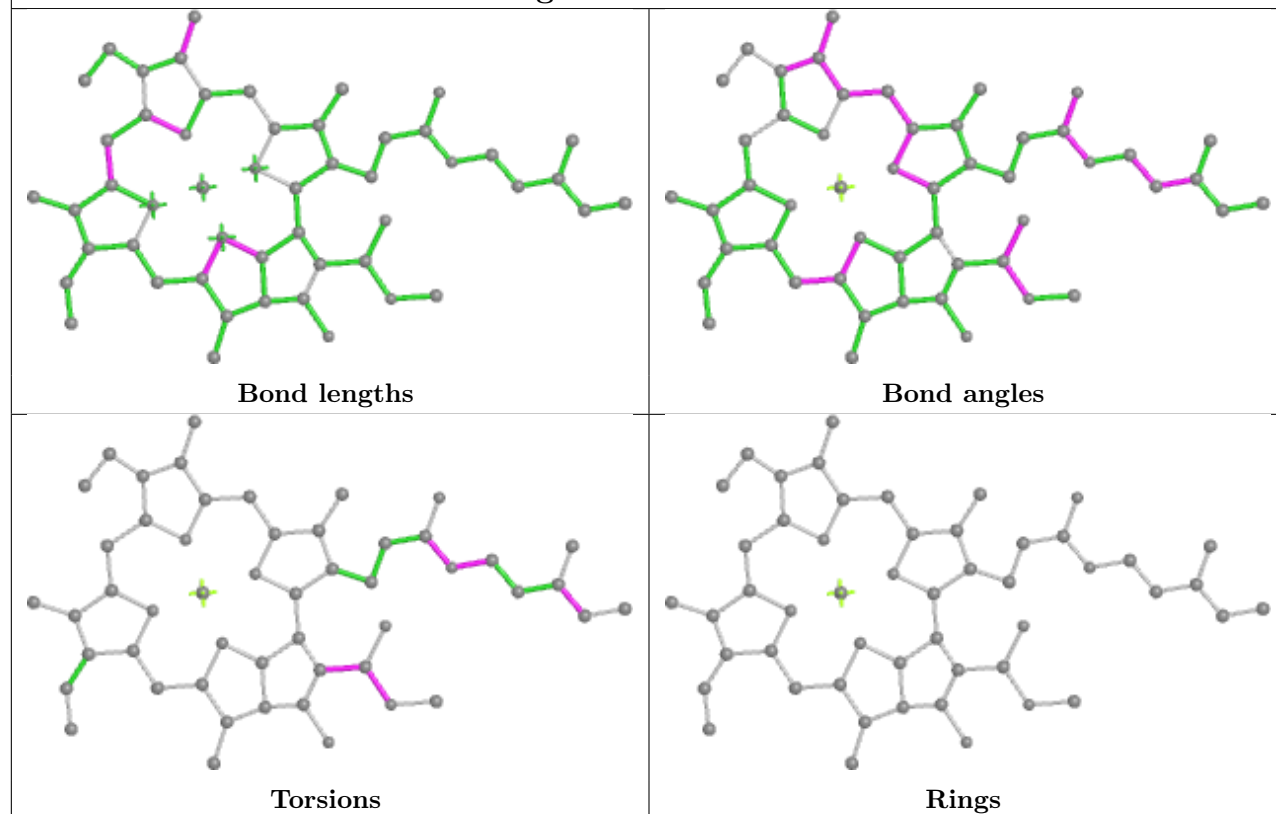


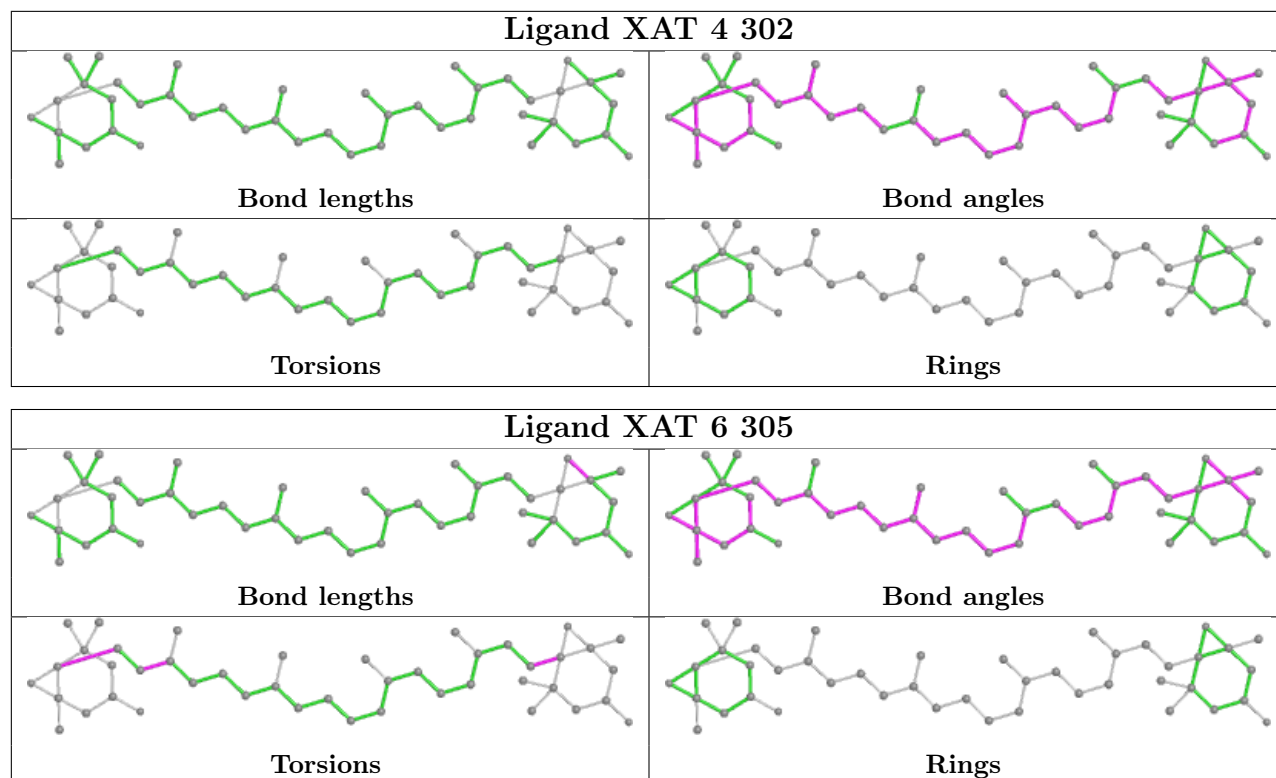
Rings

Ligand CLA a 816

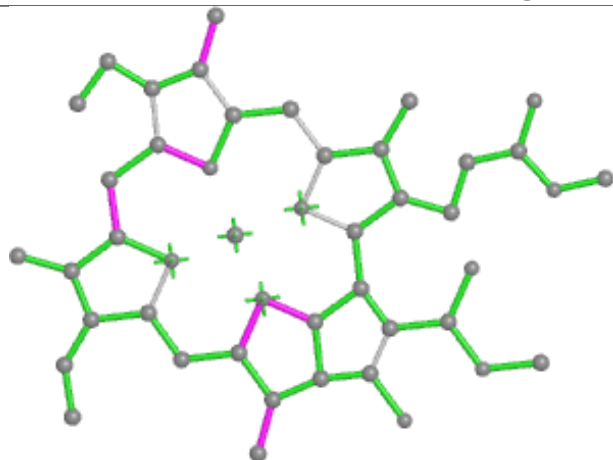


Ligand CLA 5 311

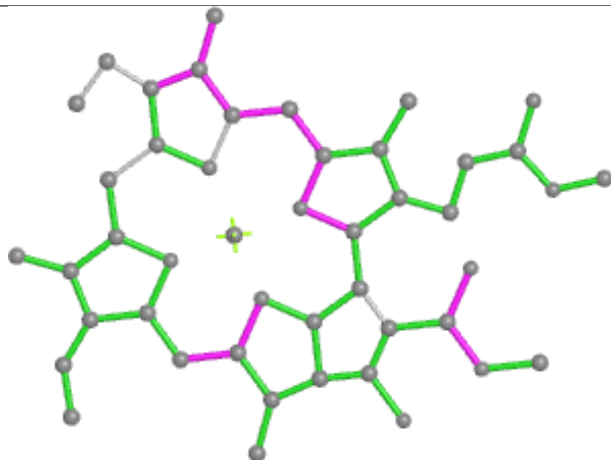




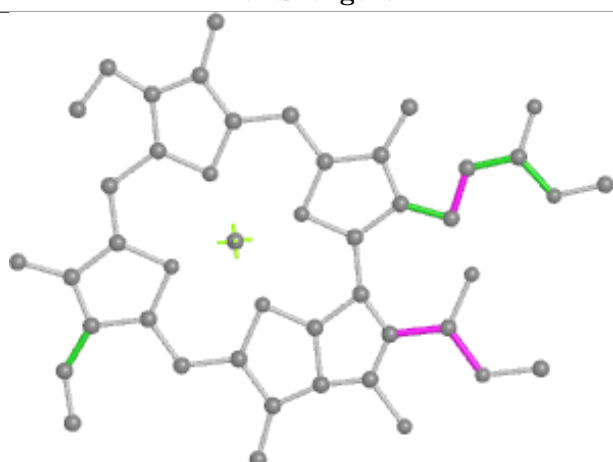
Ligand CLA 2 309



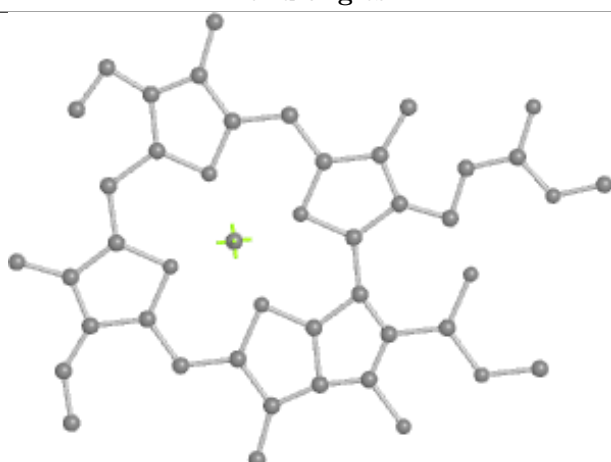
Bond lengths



Bond angles

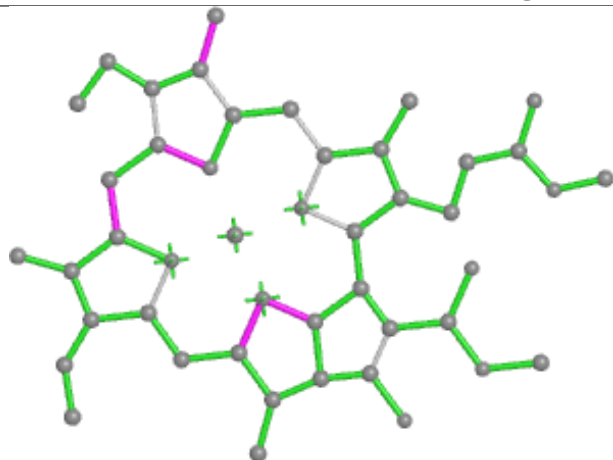


Torsions

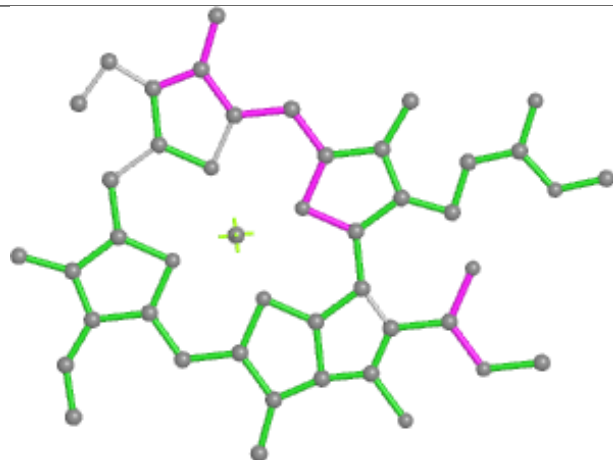


Rings

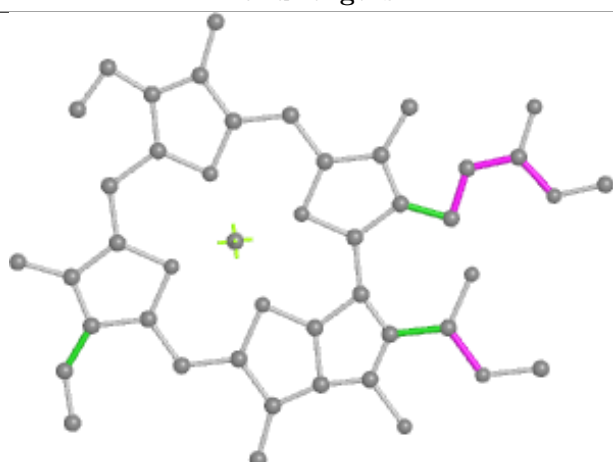
Ligand CLA 7 310



Bond lengths



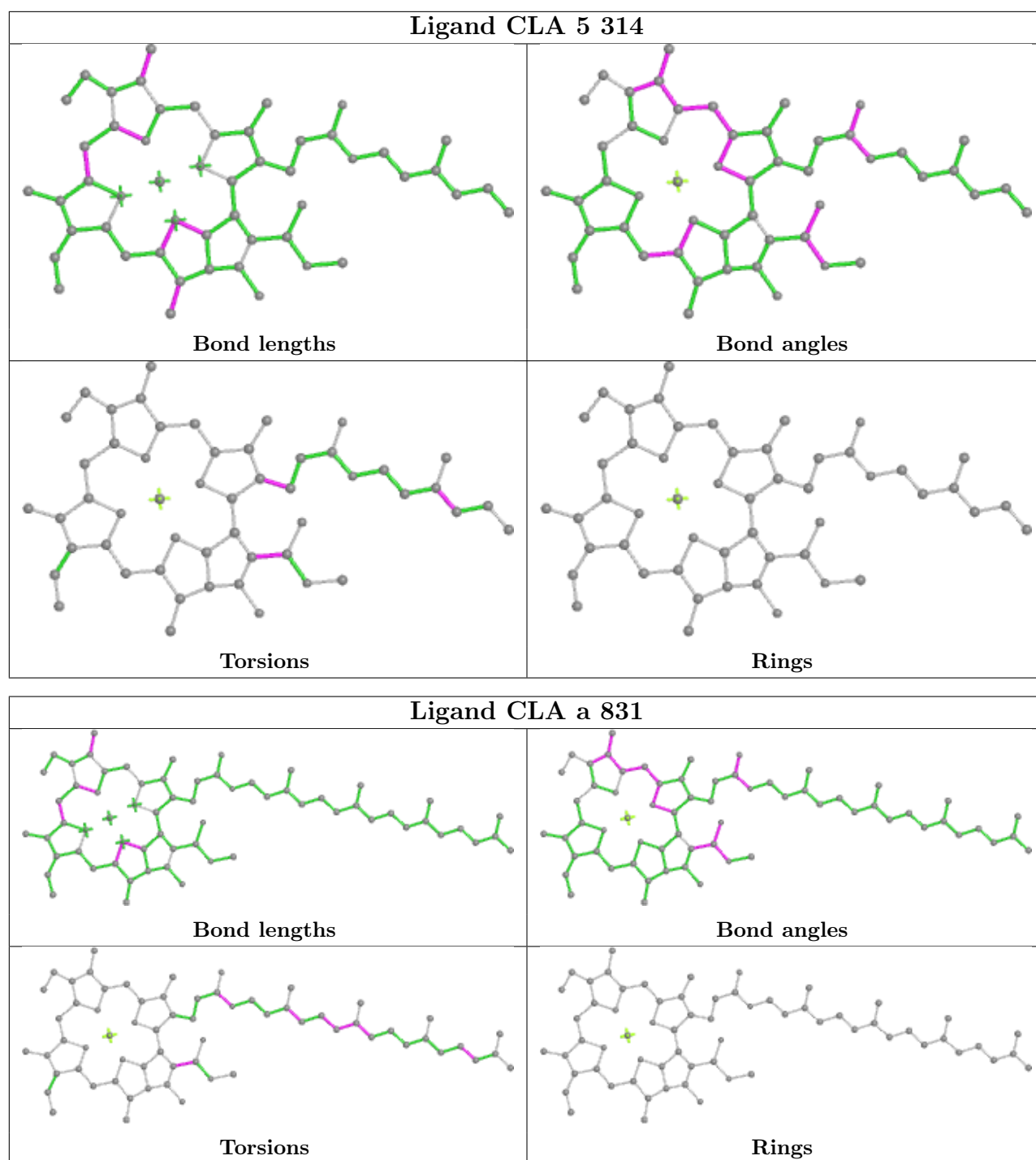
Bond angles



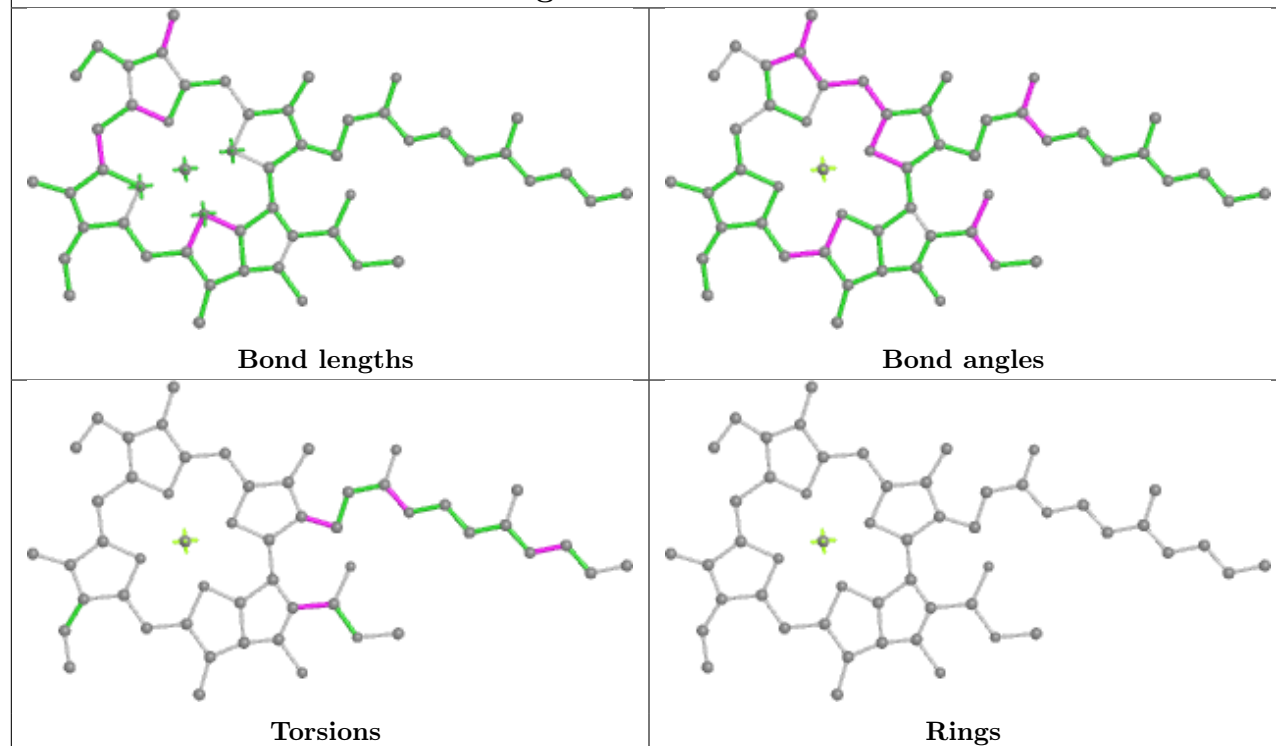
Torsions



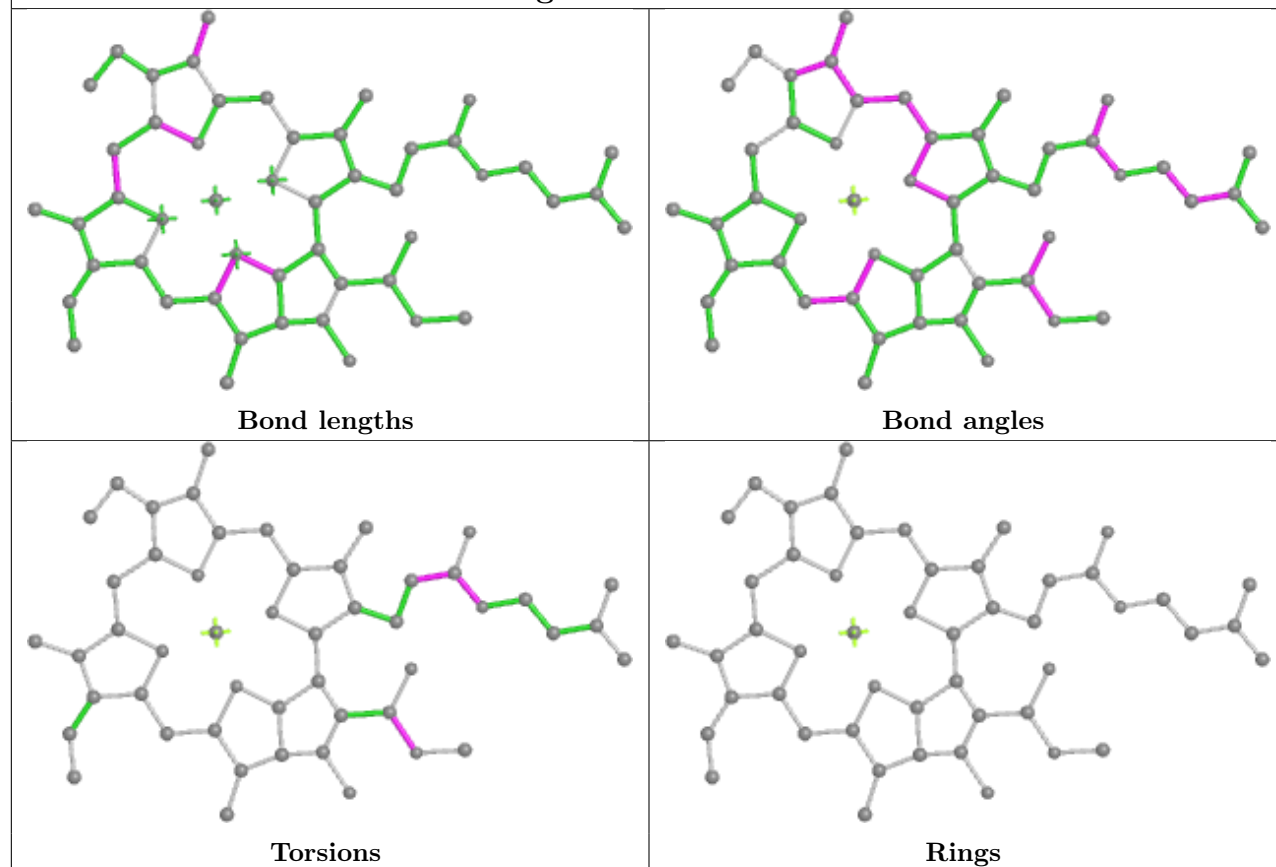
Rings

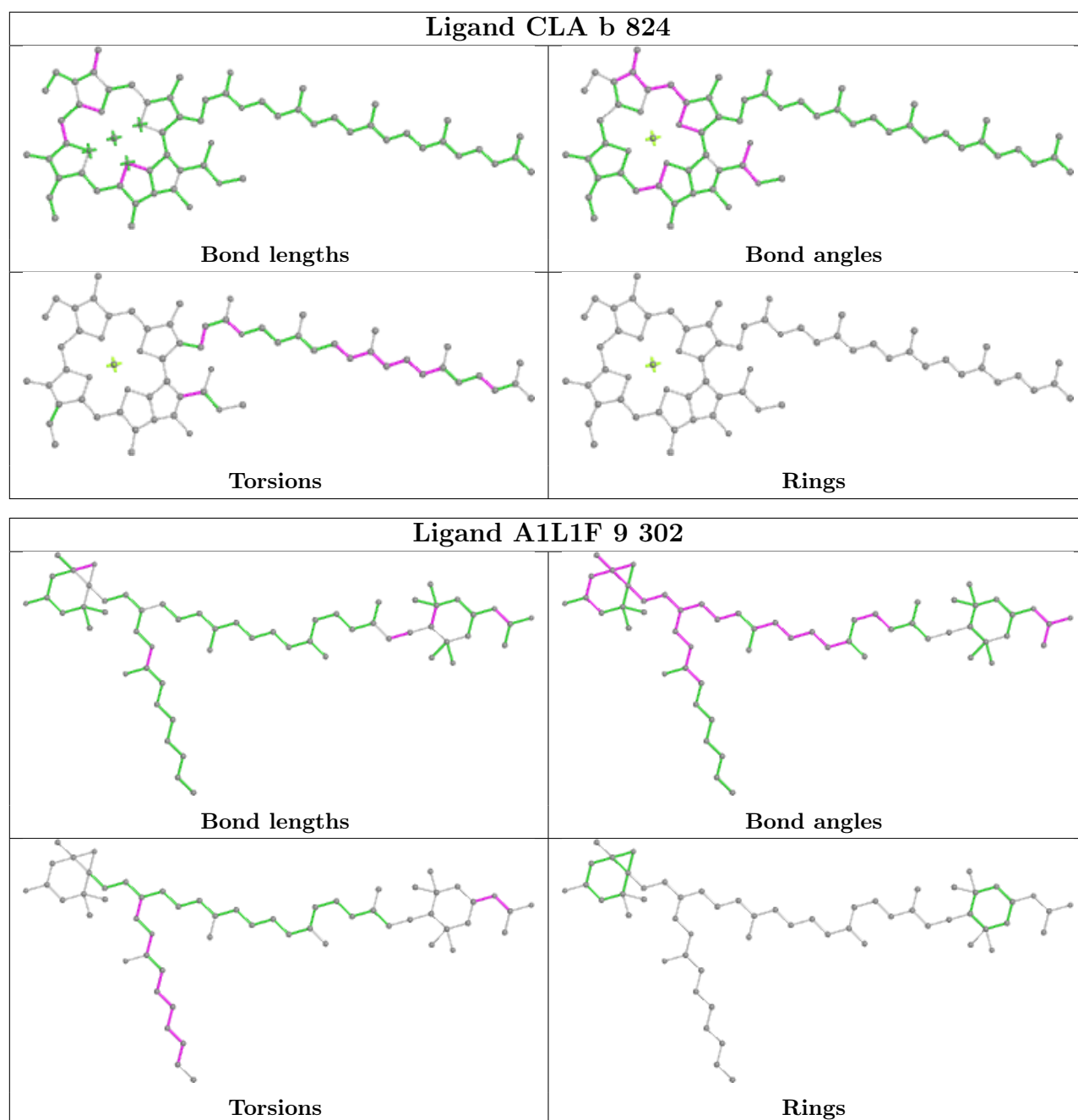


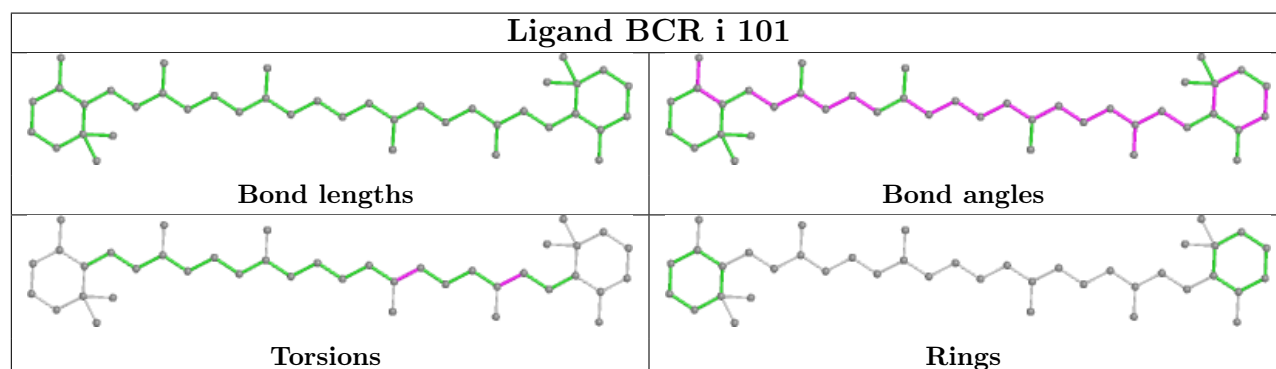
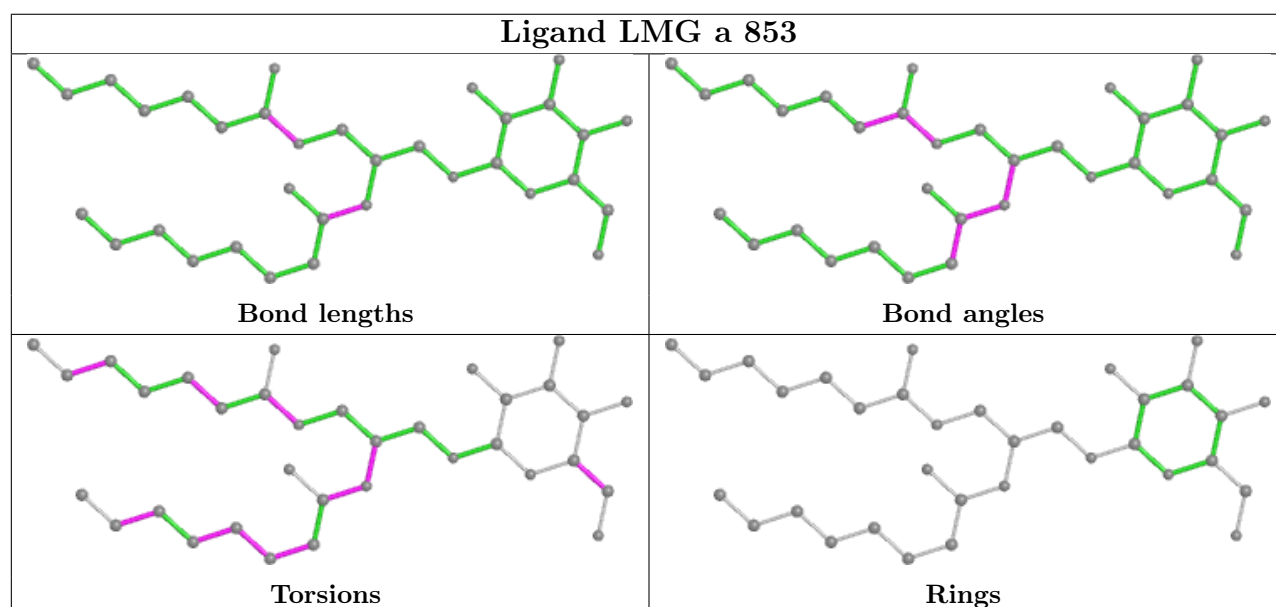
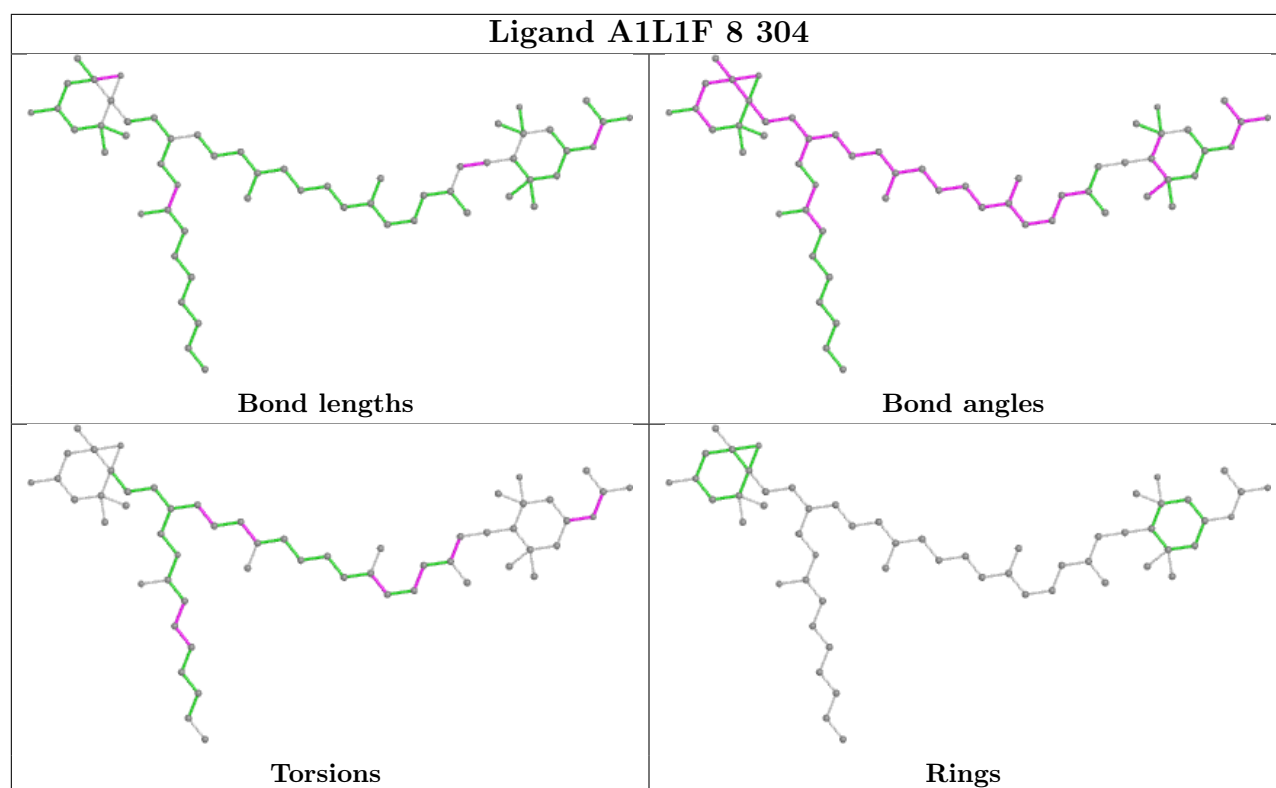
Ligand CLA 4 313

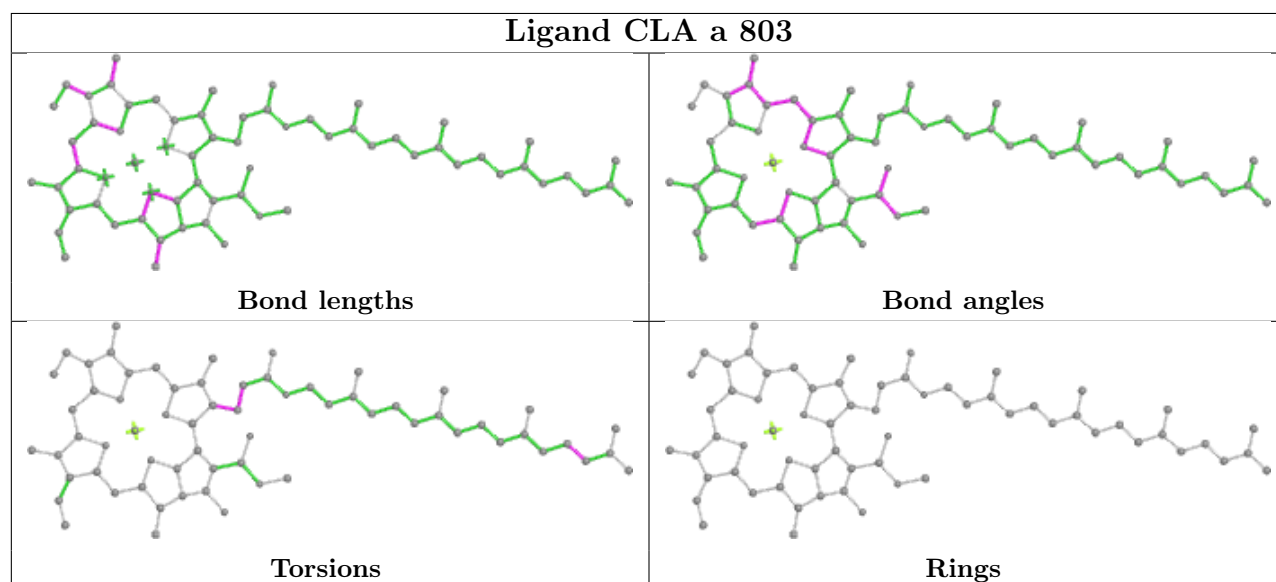
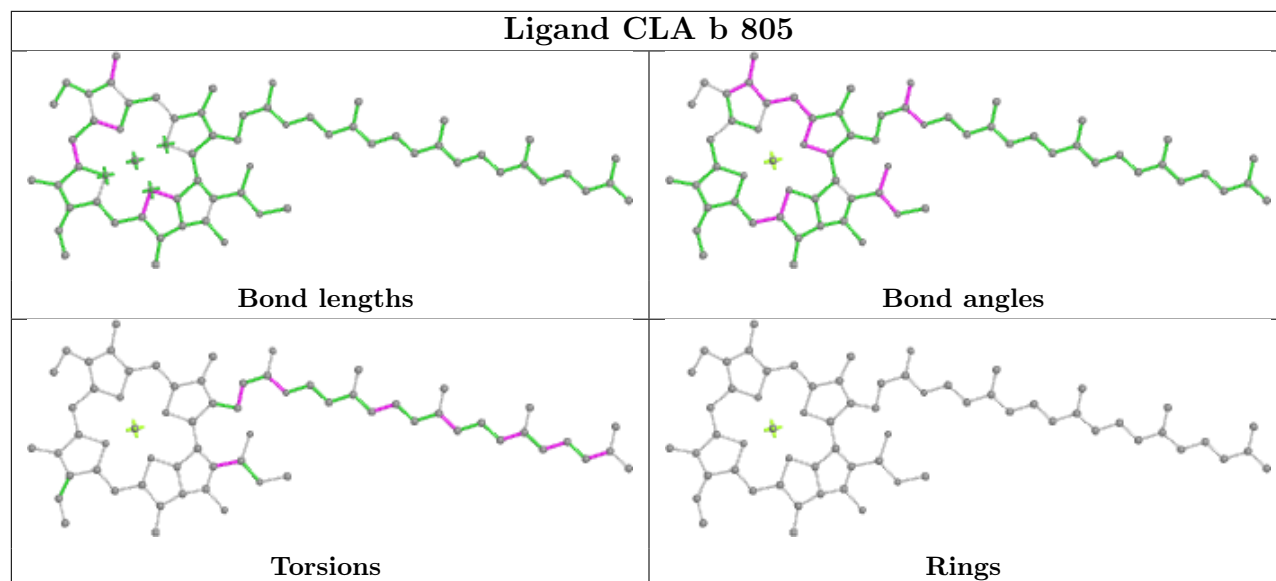
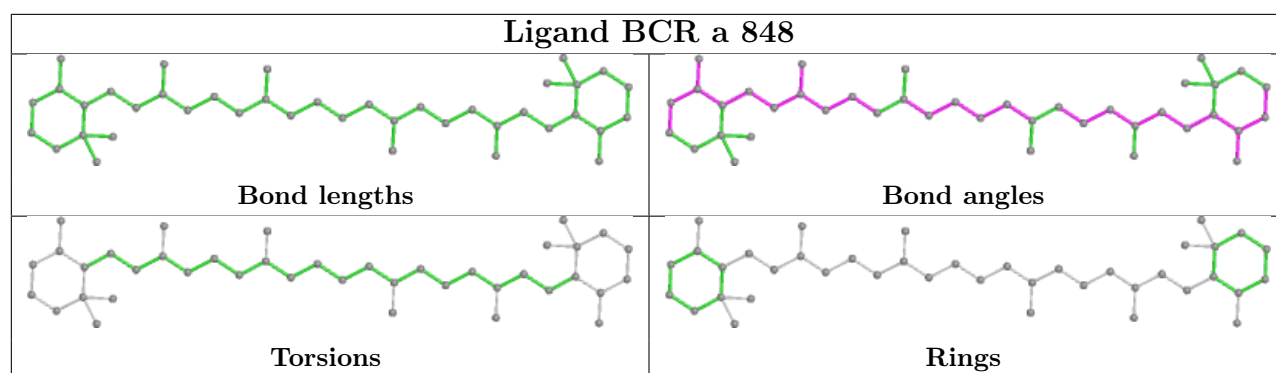


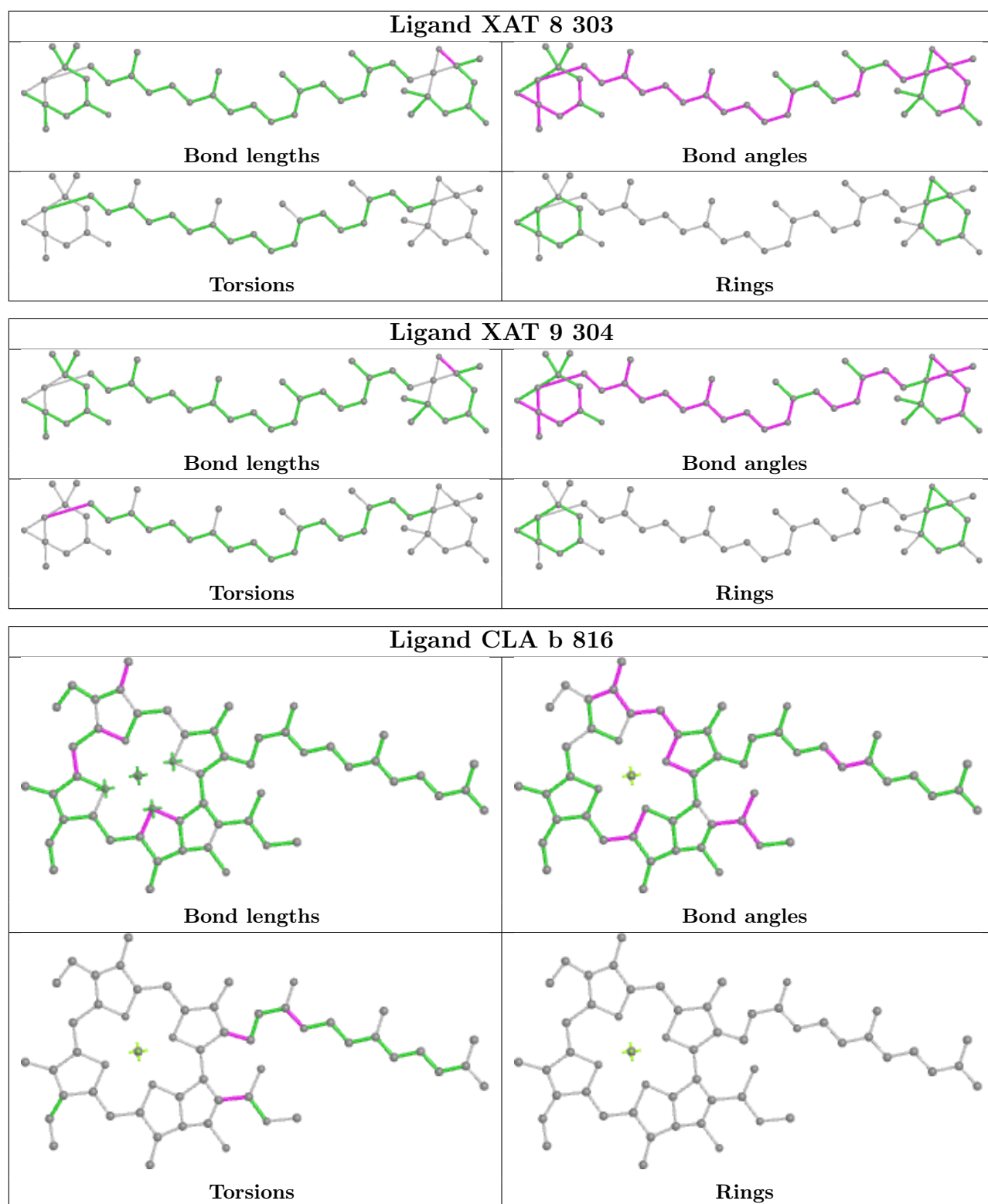
Ligand CLA a 836



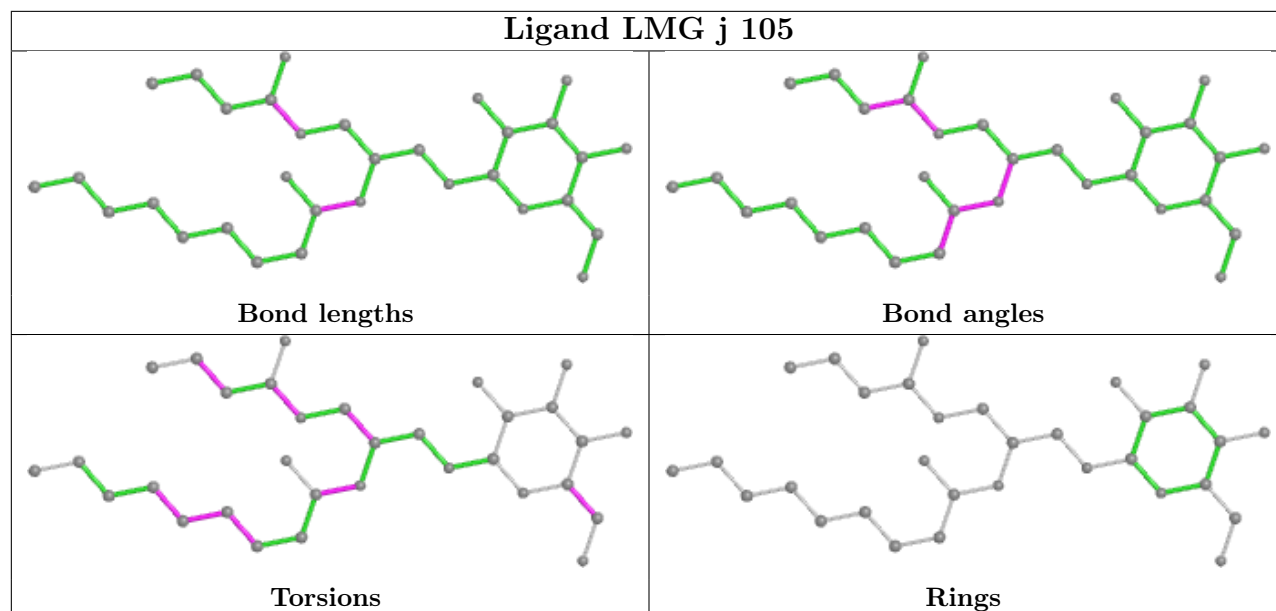




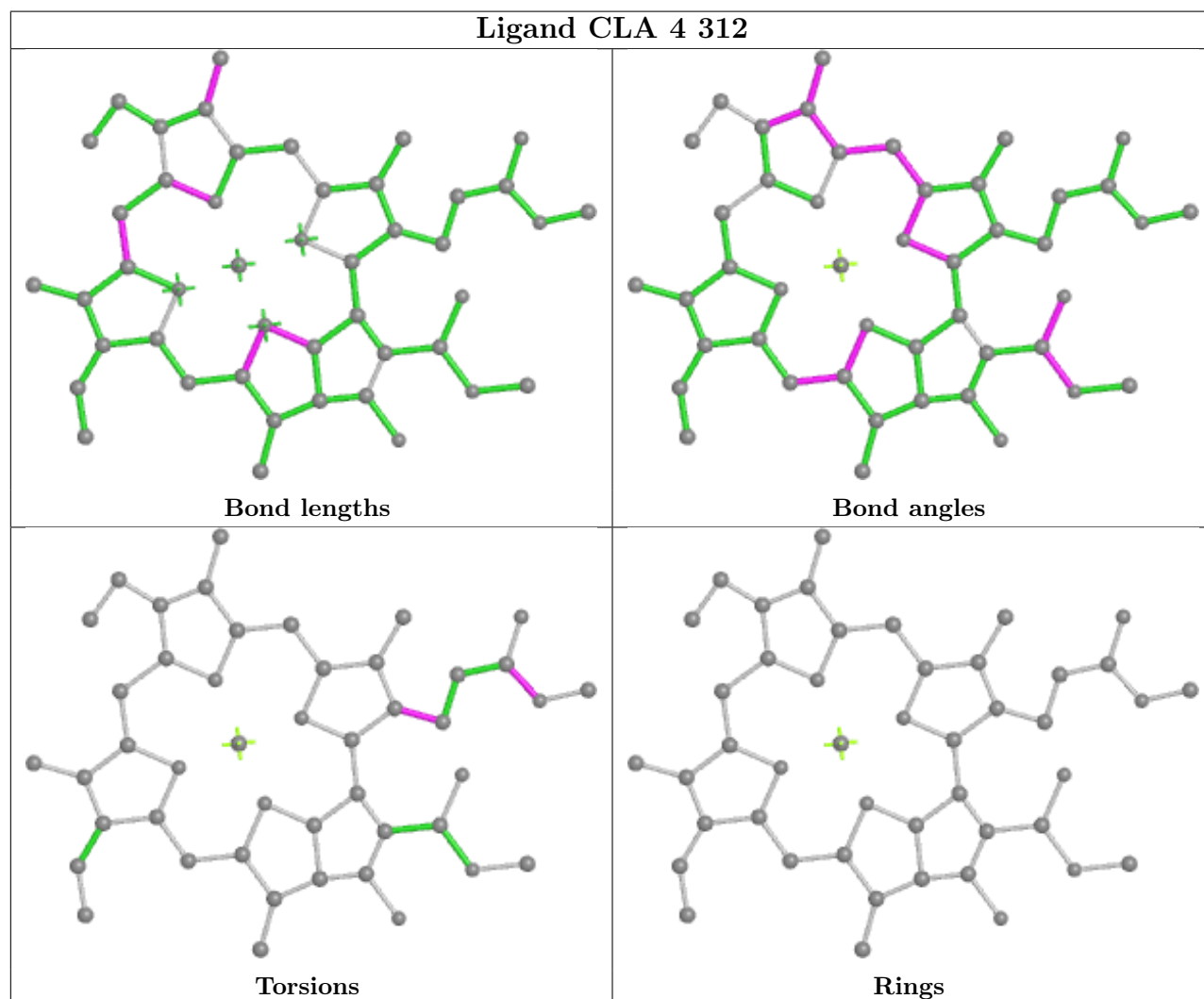




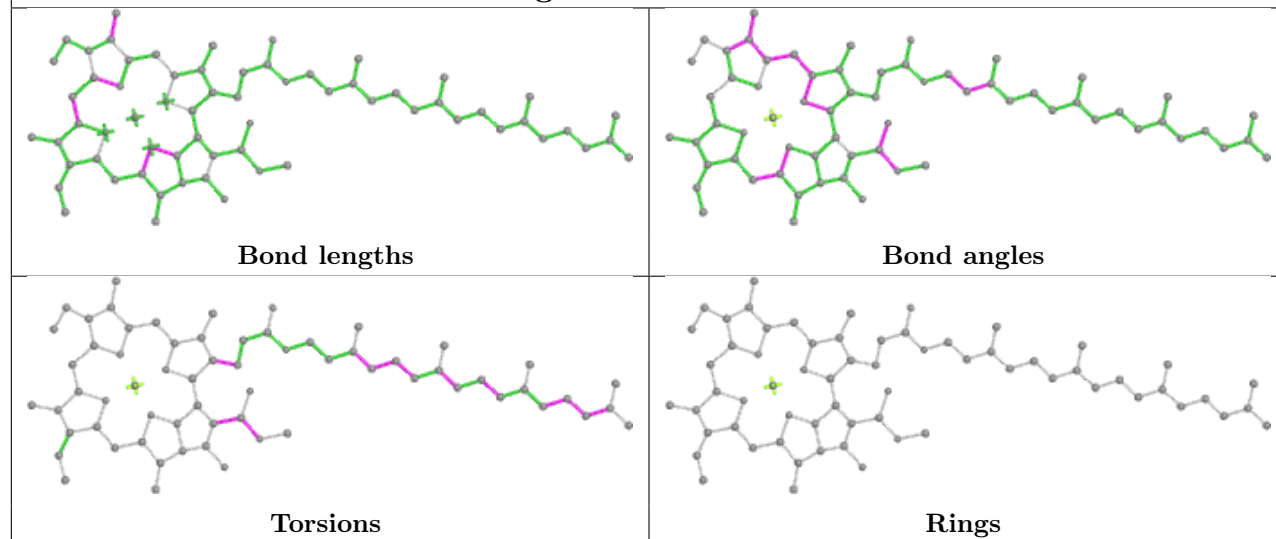
Ligand LMG j 105



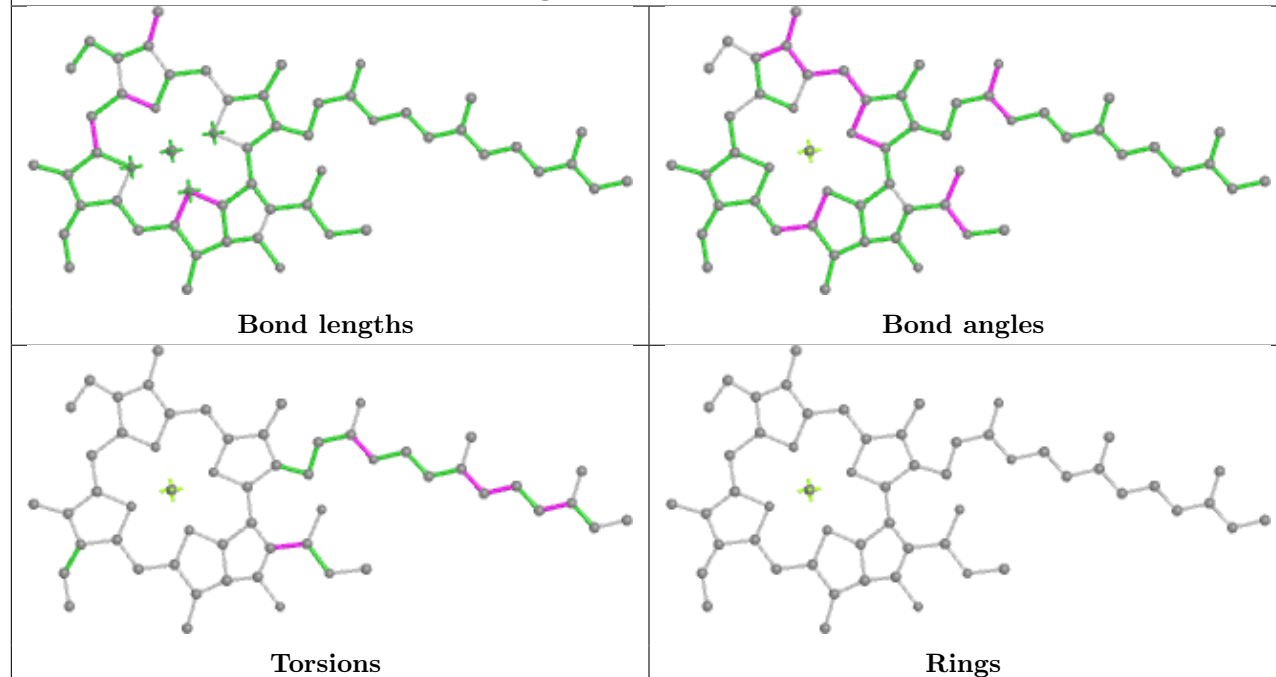
Ligand CLA 4 312



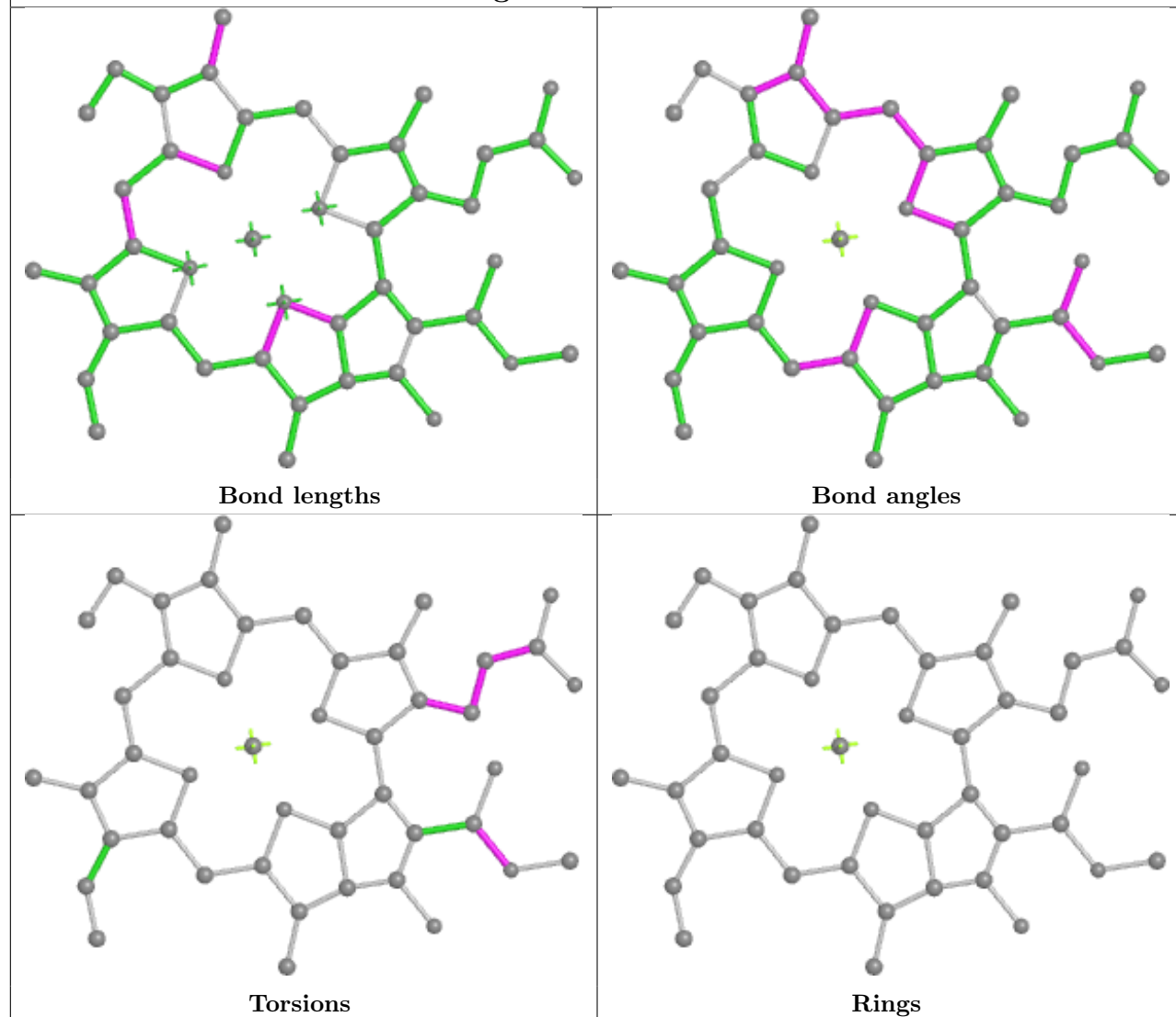
Ligand CLA b 813



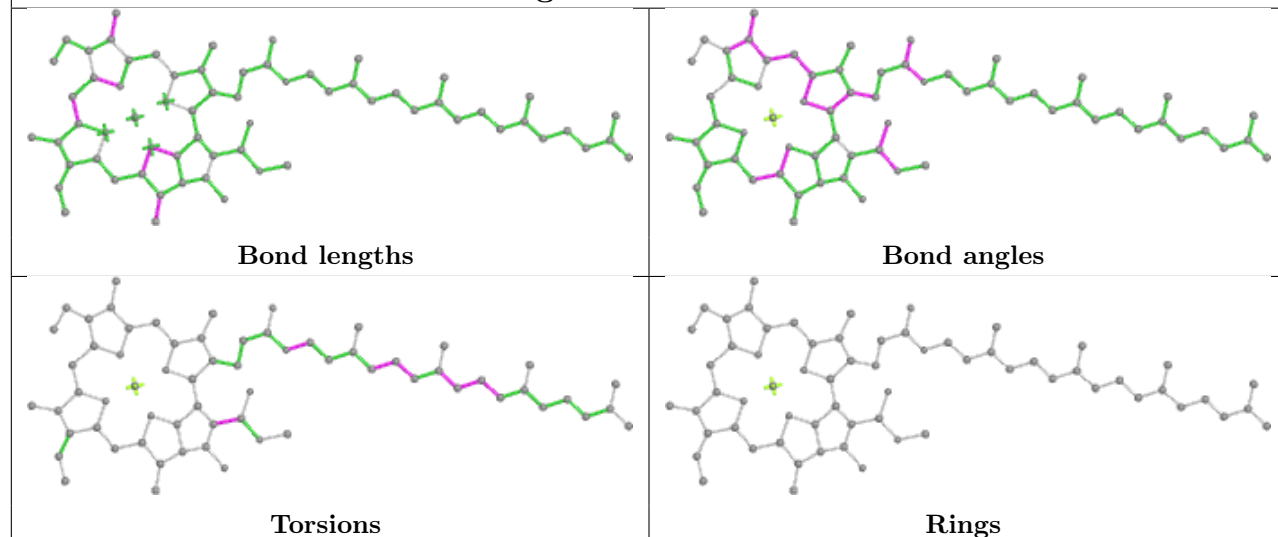
Ligand CLA 8 311



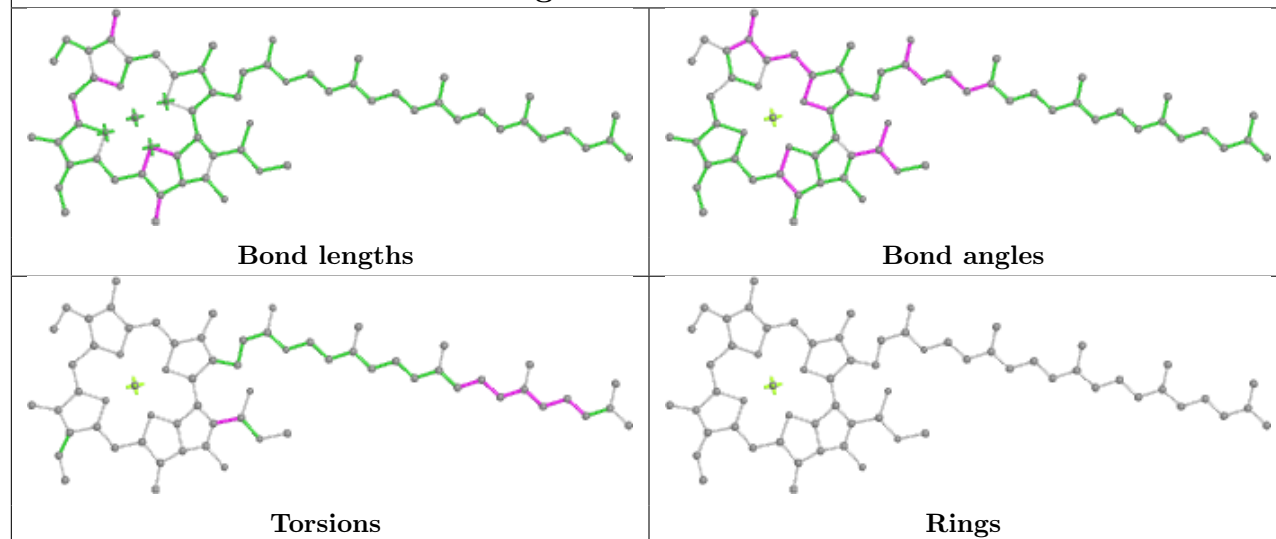
Ligand CLA 4 306



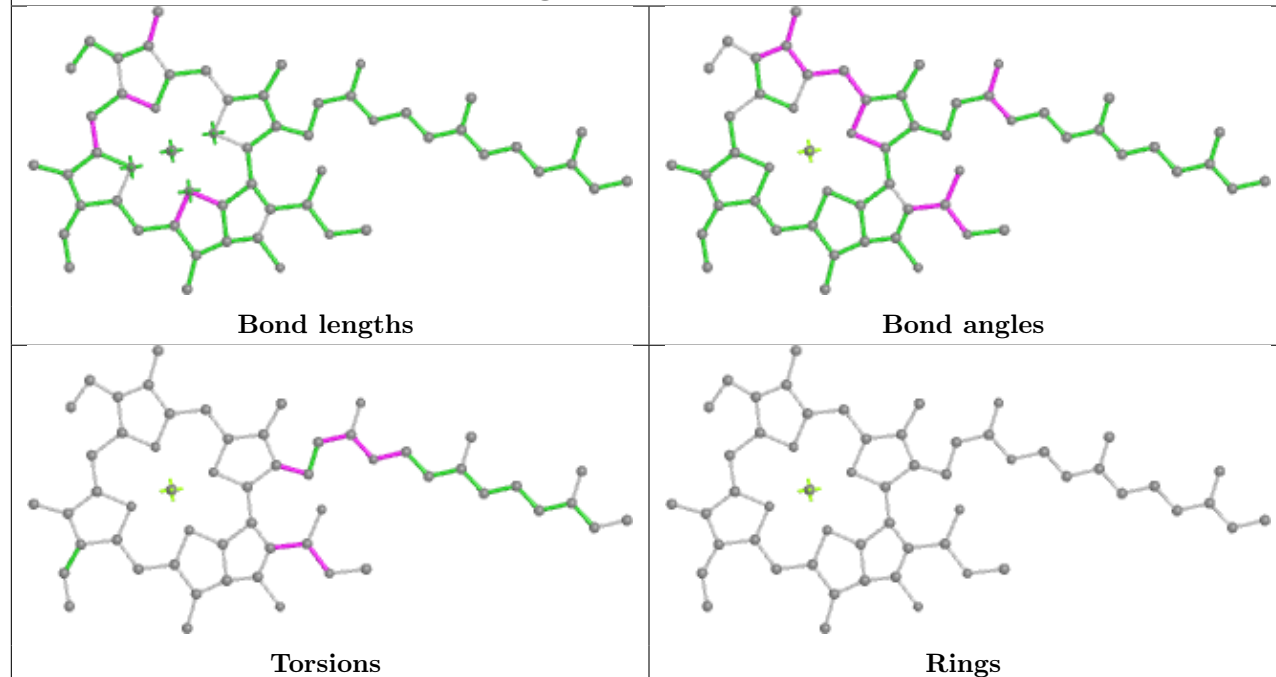
Ligand CLA a 827

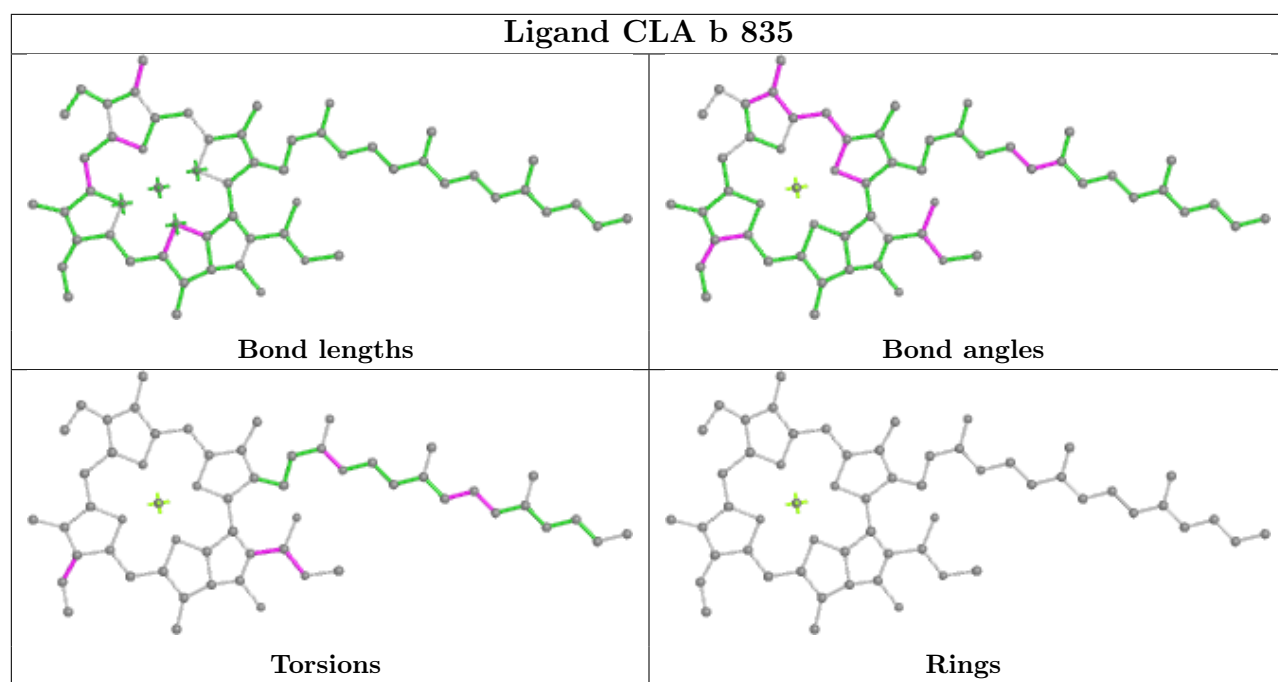


Ligand CLA b 829

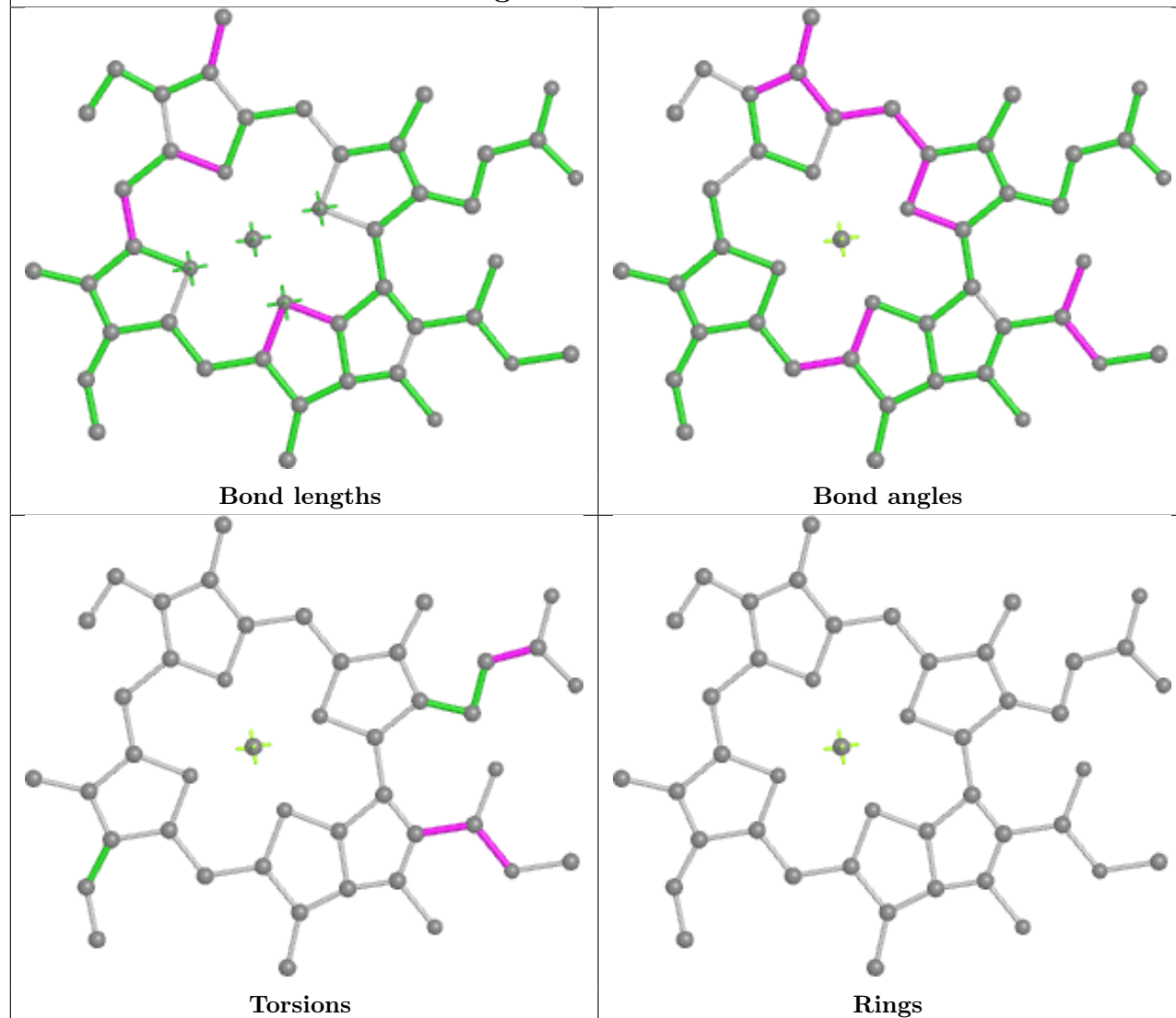


Ligand CLA a 818

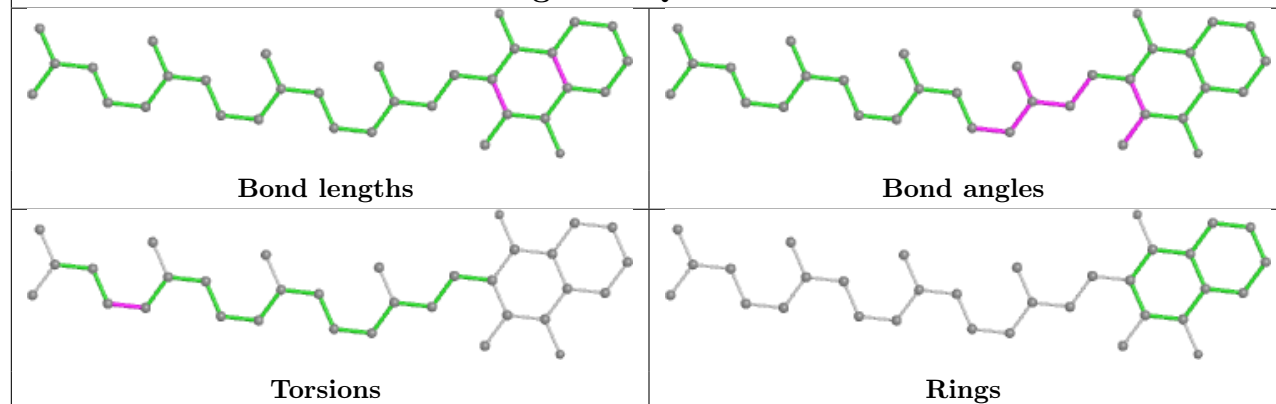




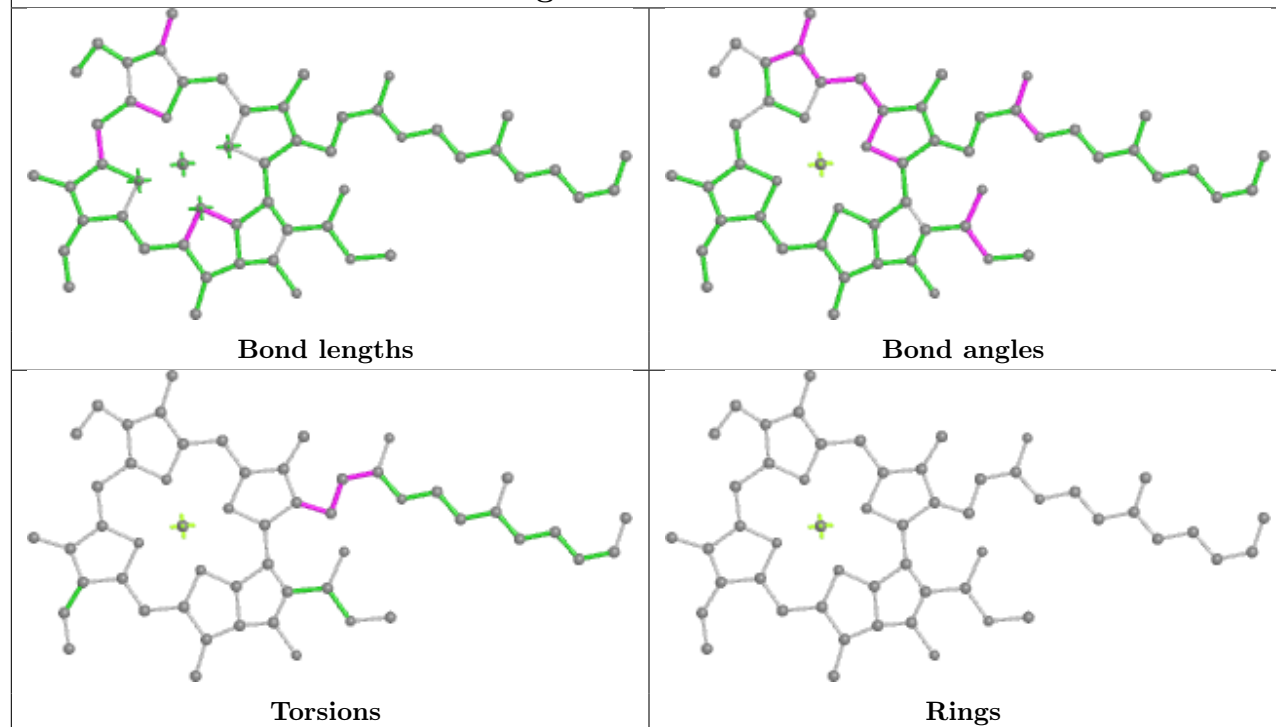
Ligand CLA 7 307



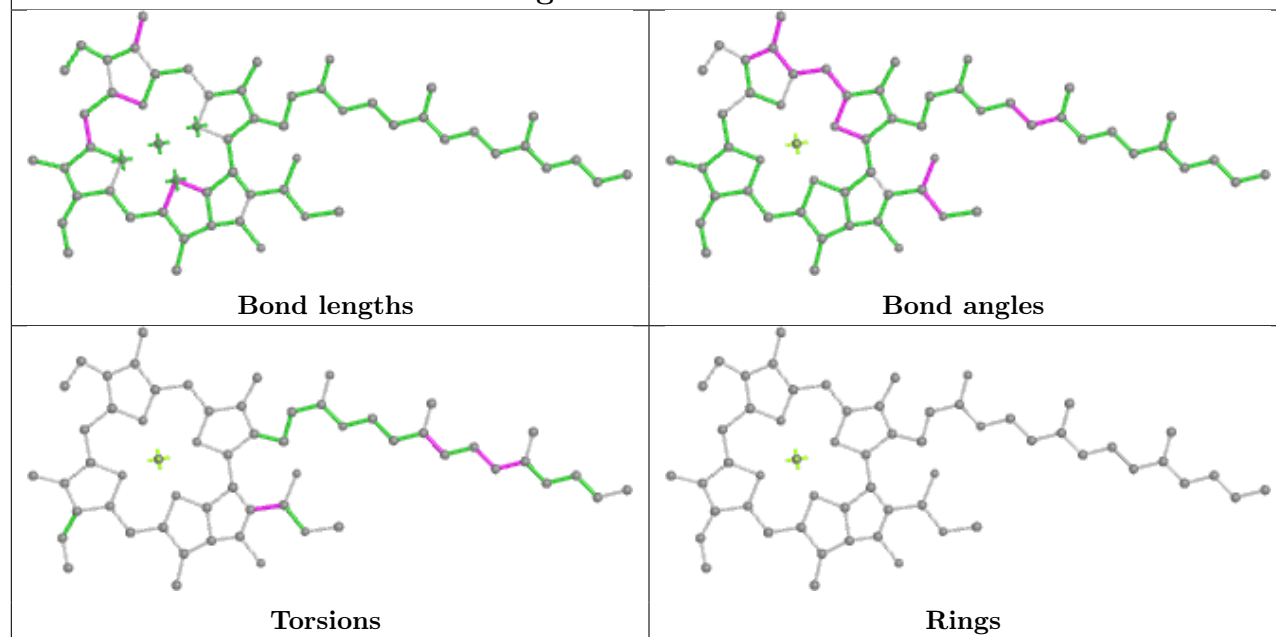
Ligand PQN b 841



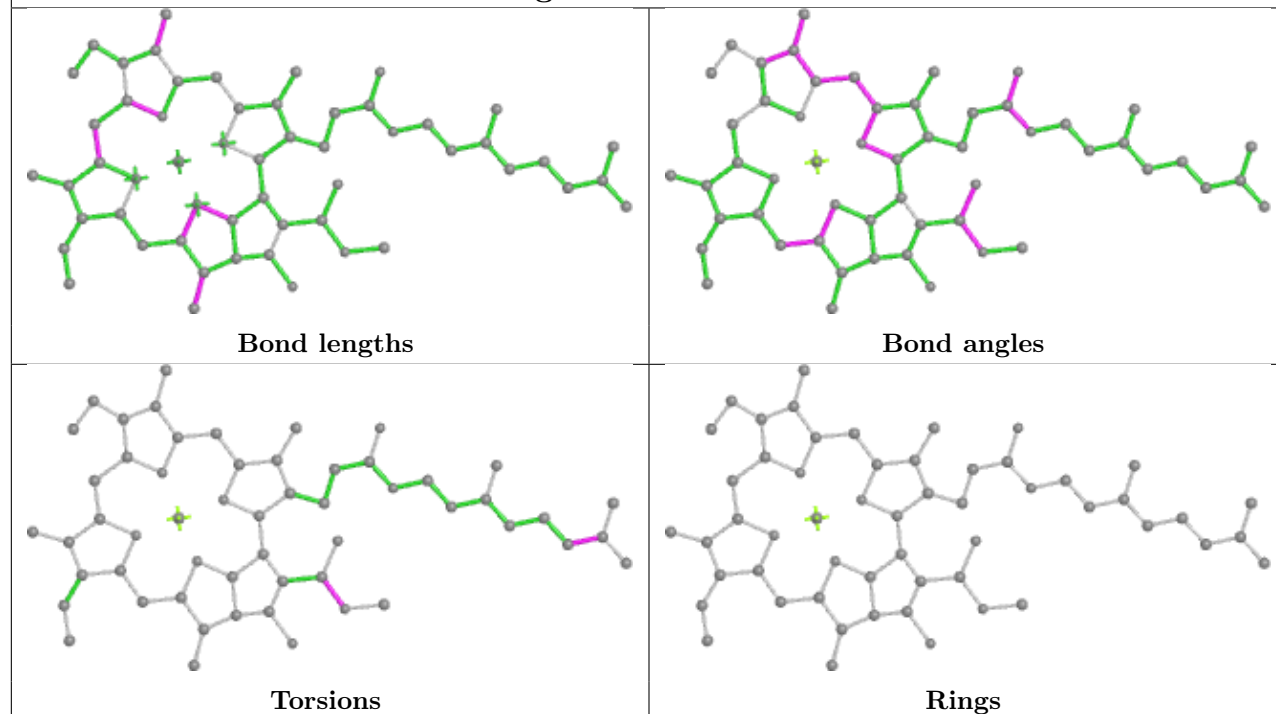
Ligand CLA a 819



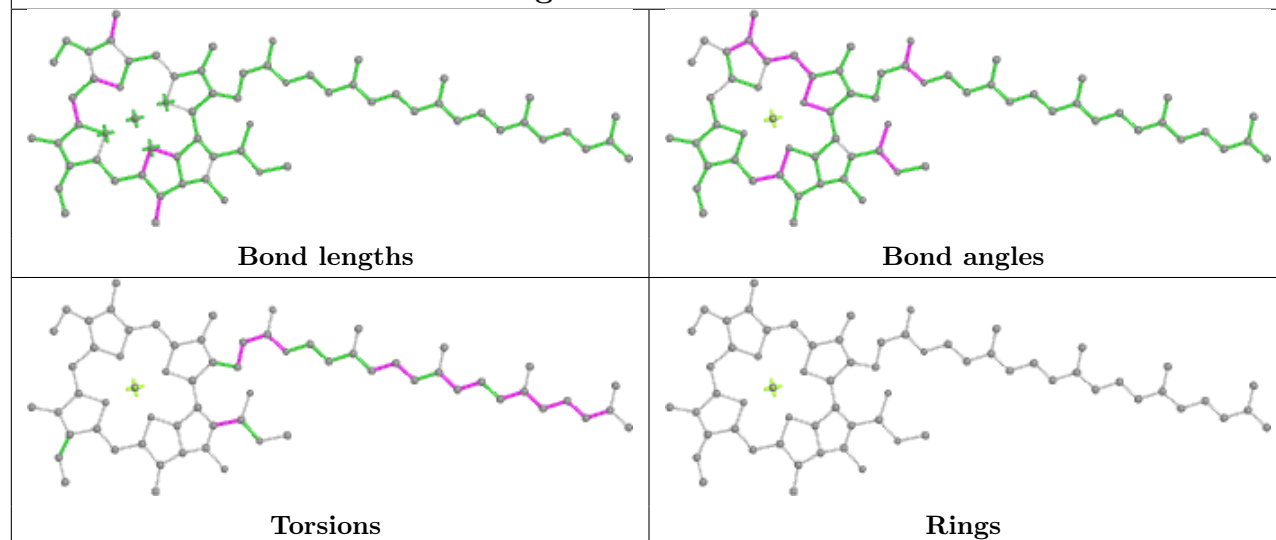
Ligand CLA a 802

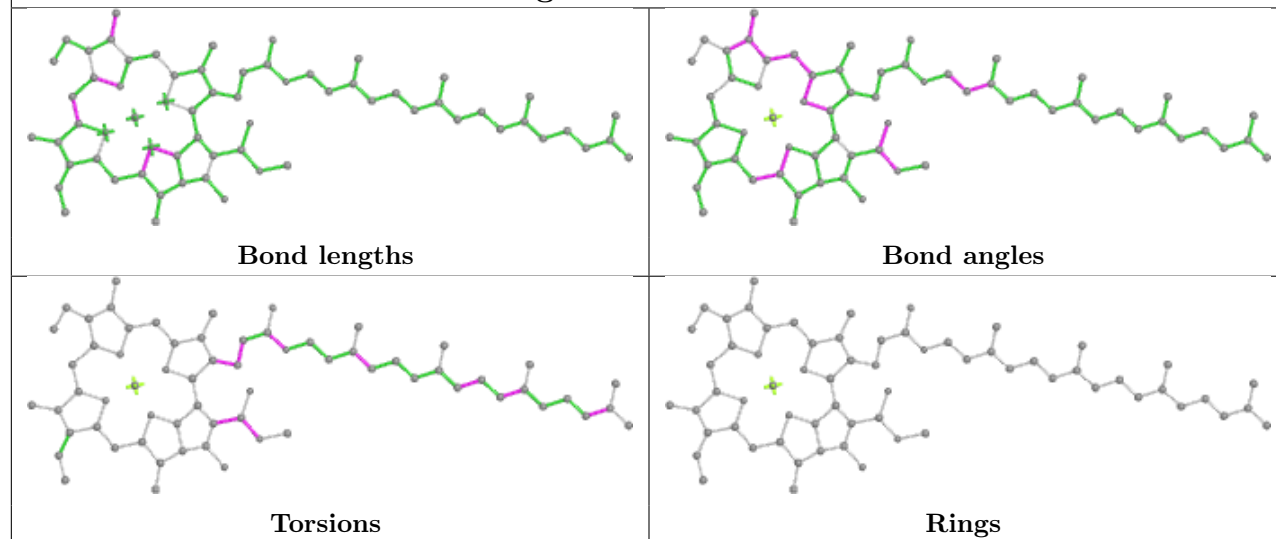
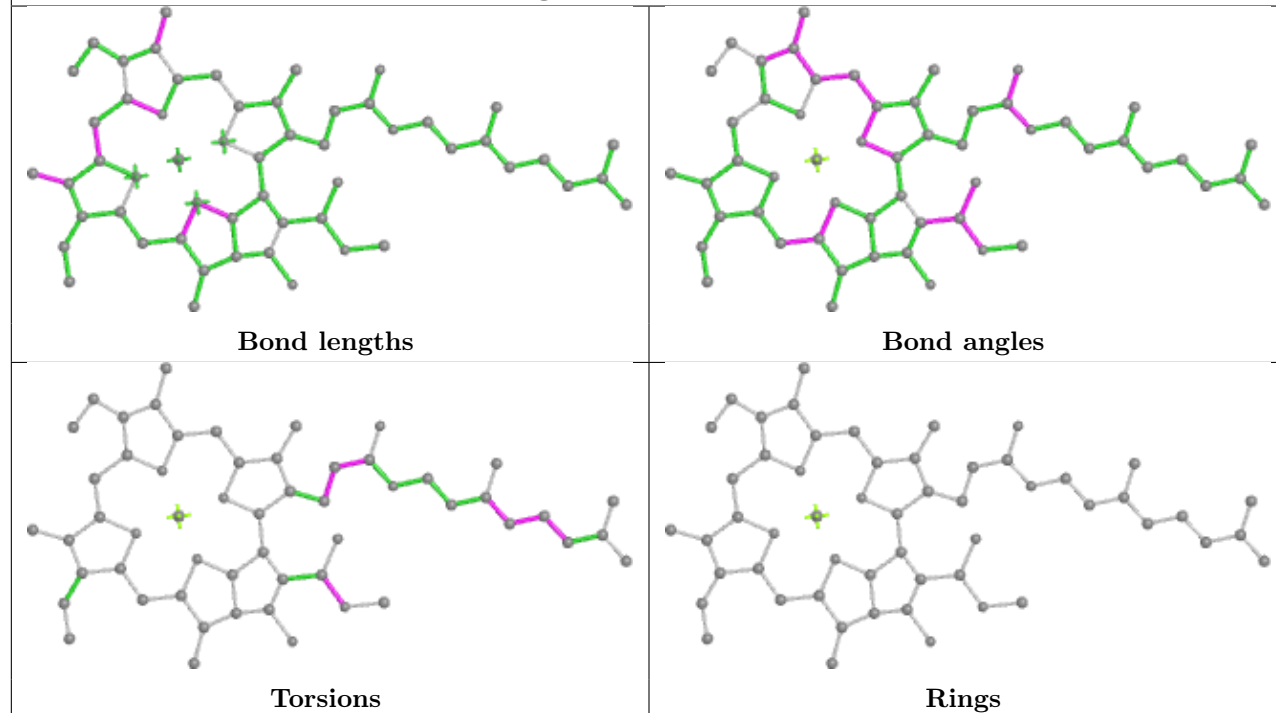


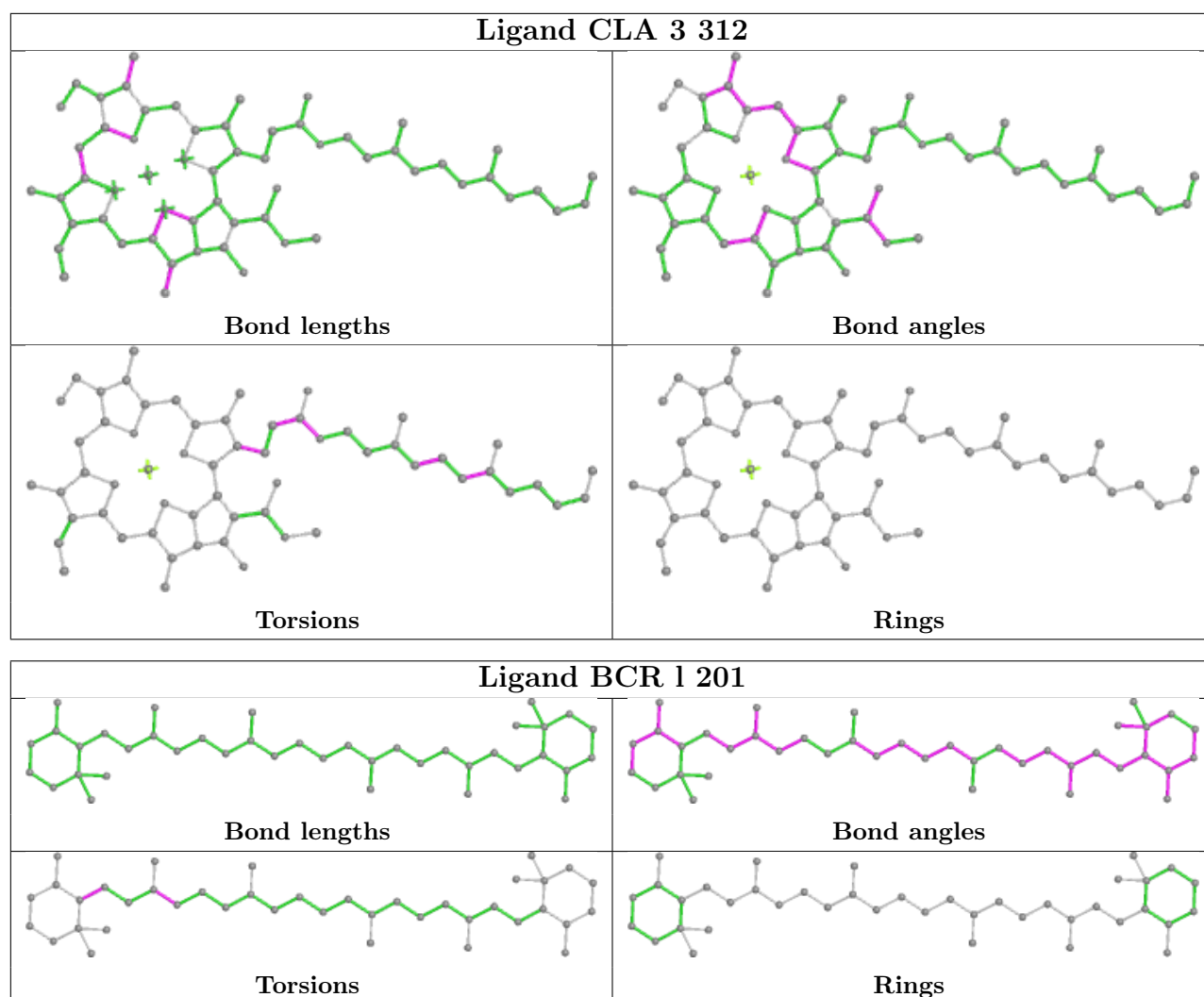
Ligand CLA b 819



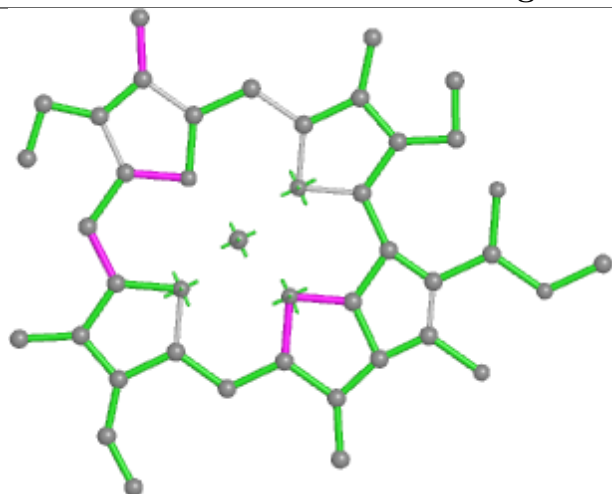
Ligand CLA b 801



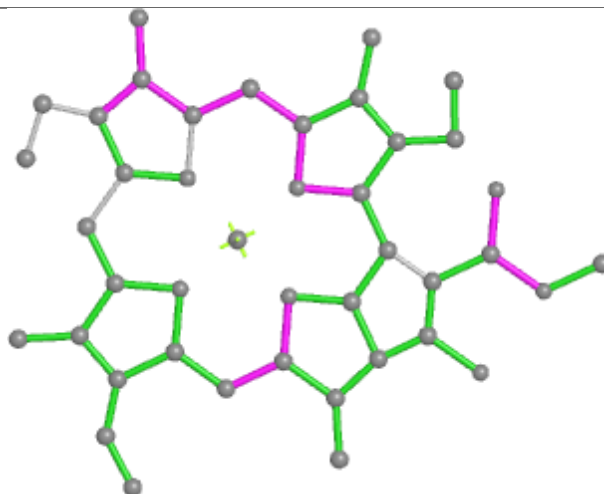
Ligand CLA 9 316**Ligand CLA h 204**



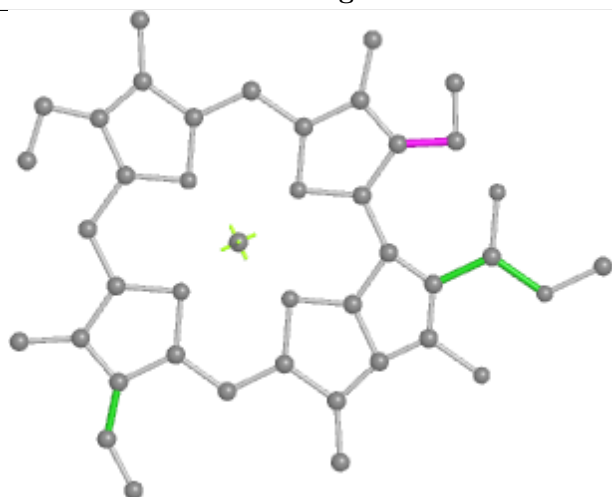
Ligand CLA 2 315



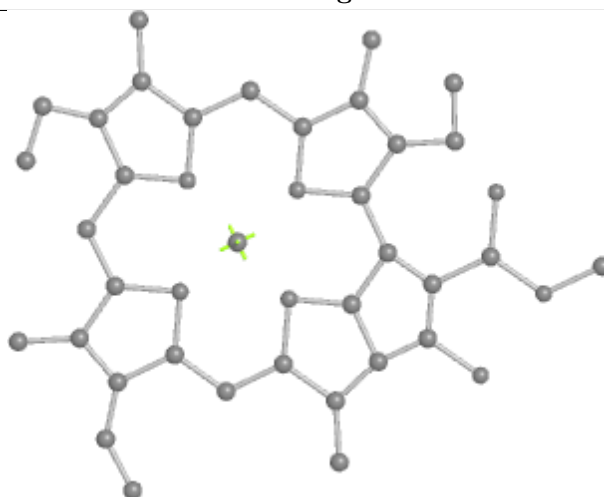
Bond lengths



Bond angles

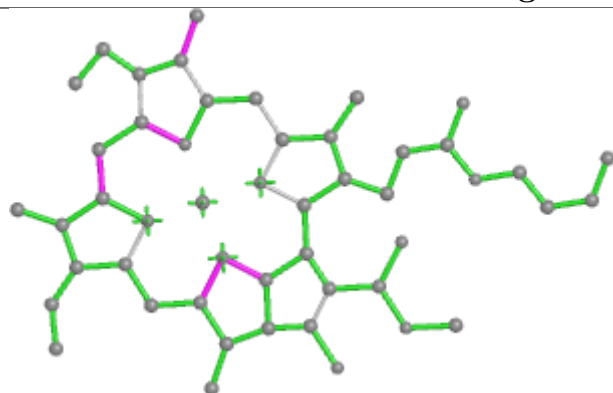


Torsions

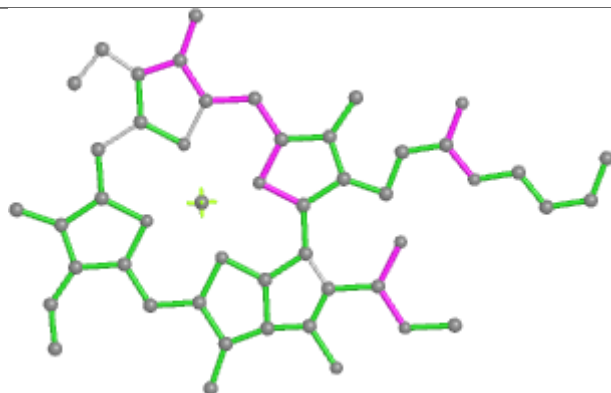


Rings

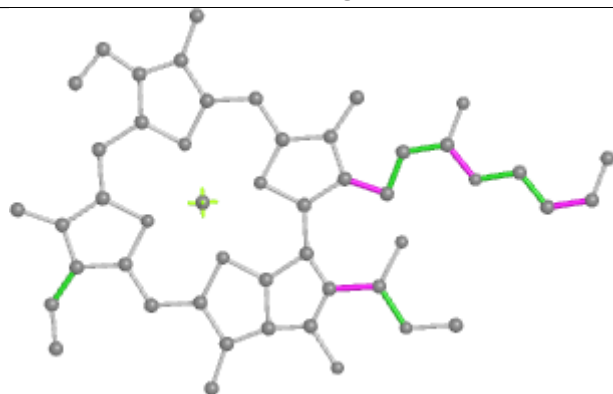
Ligand CLA a 823



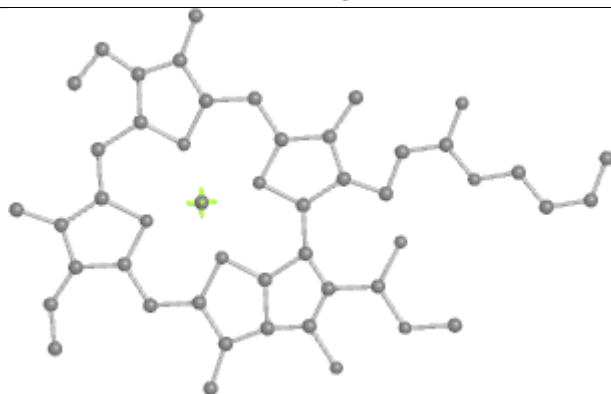
Bond lengths



Bond angles

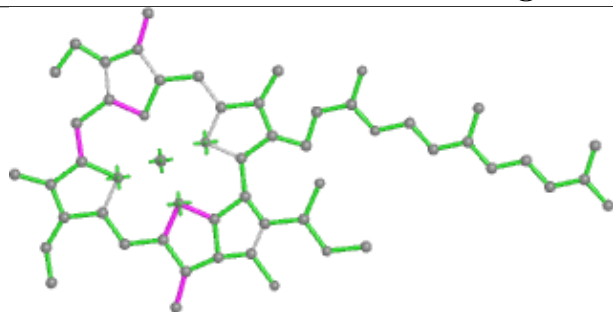


Torsions

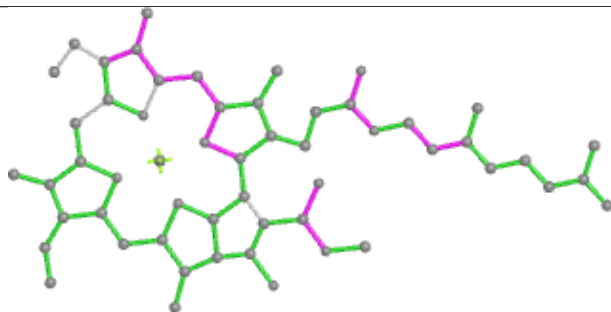


Rings

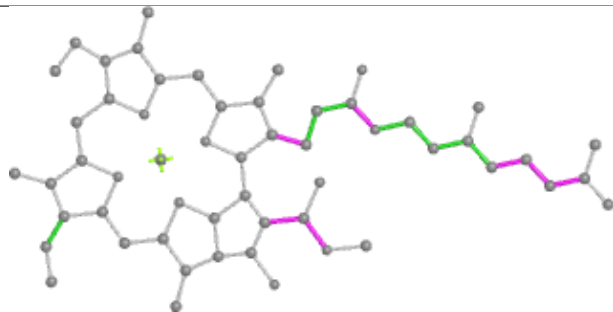
Ligand CLA b 814



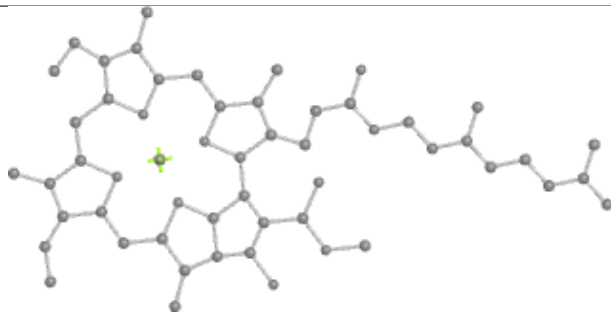
Bond lengths



Bond angles

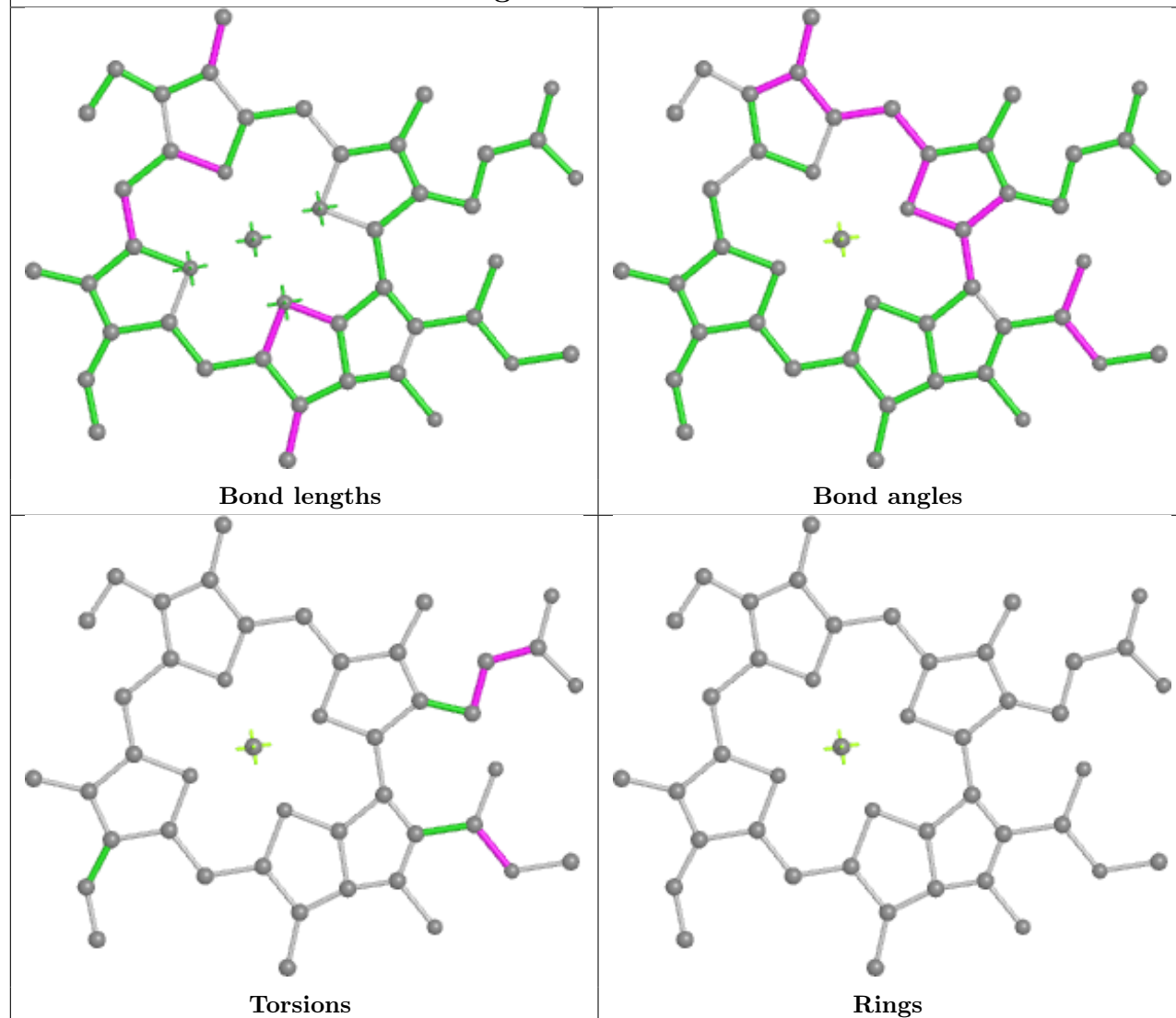


Torsions

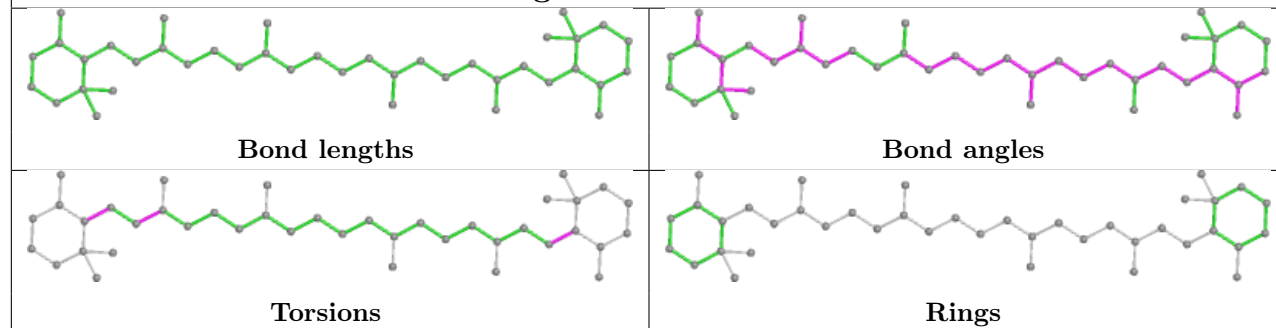


Rings

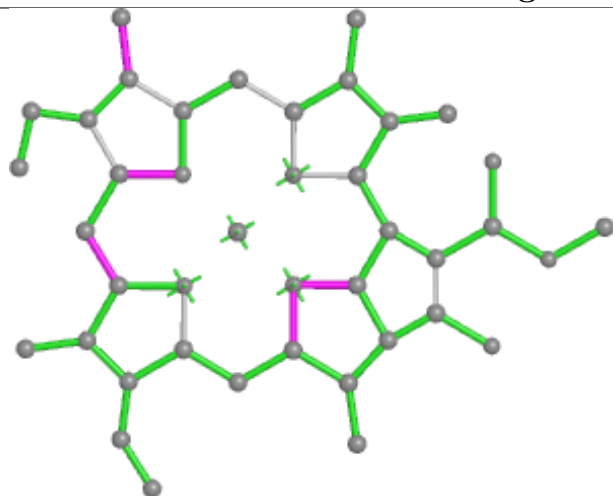
Ligand CLA 7 314



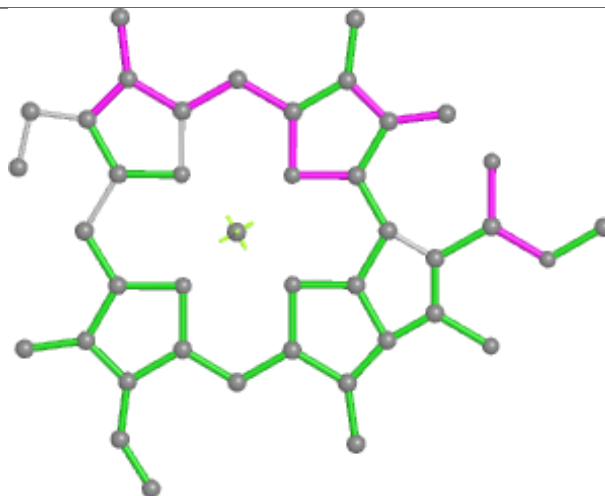
Ligand BCR b 849



Ligand CLA 8 314



Bond lengths



Bond angles

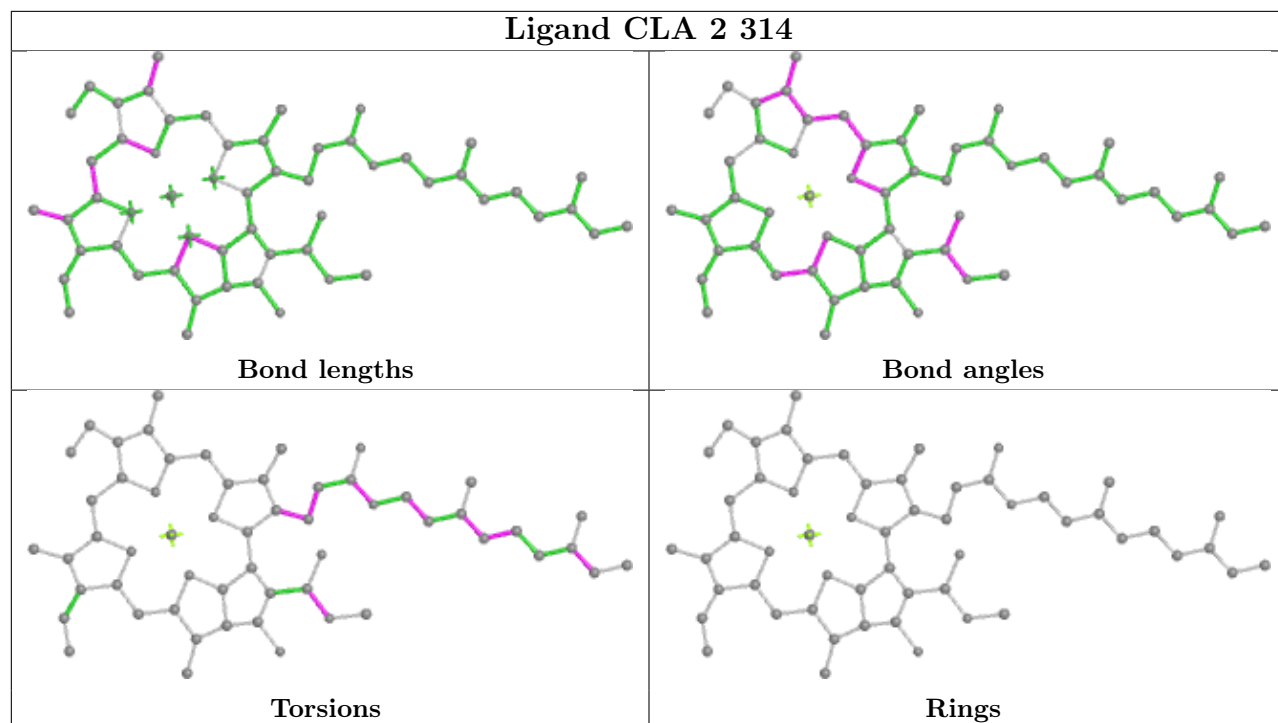


Torsions

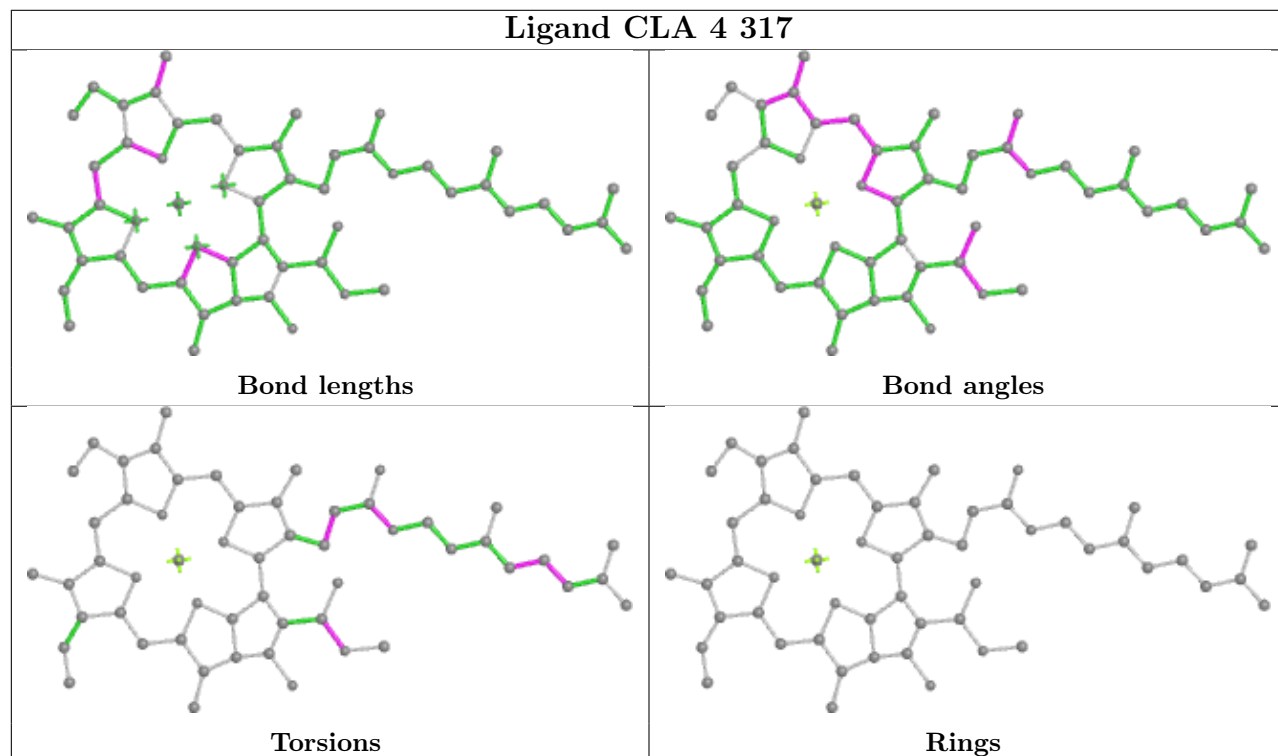


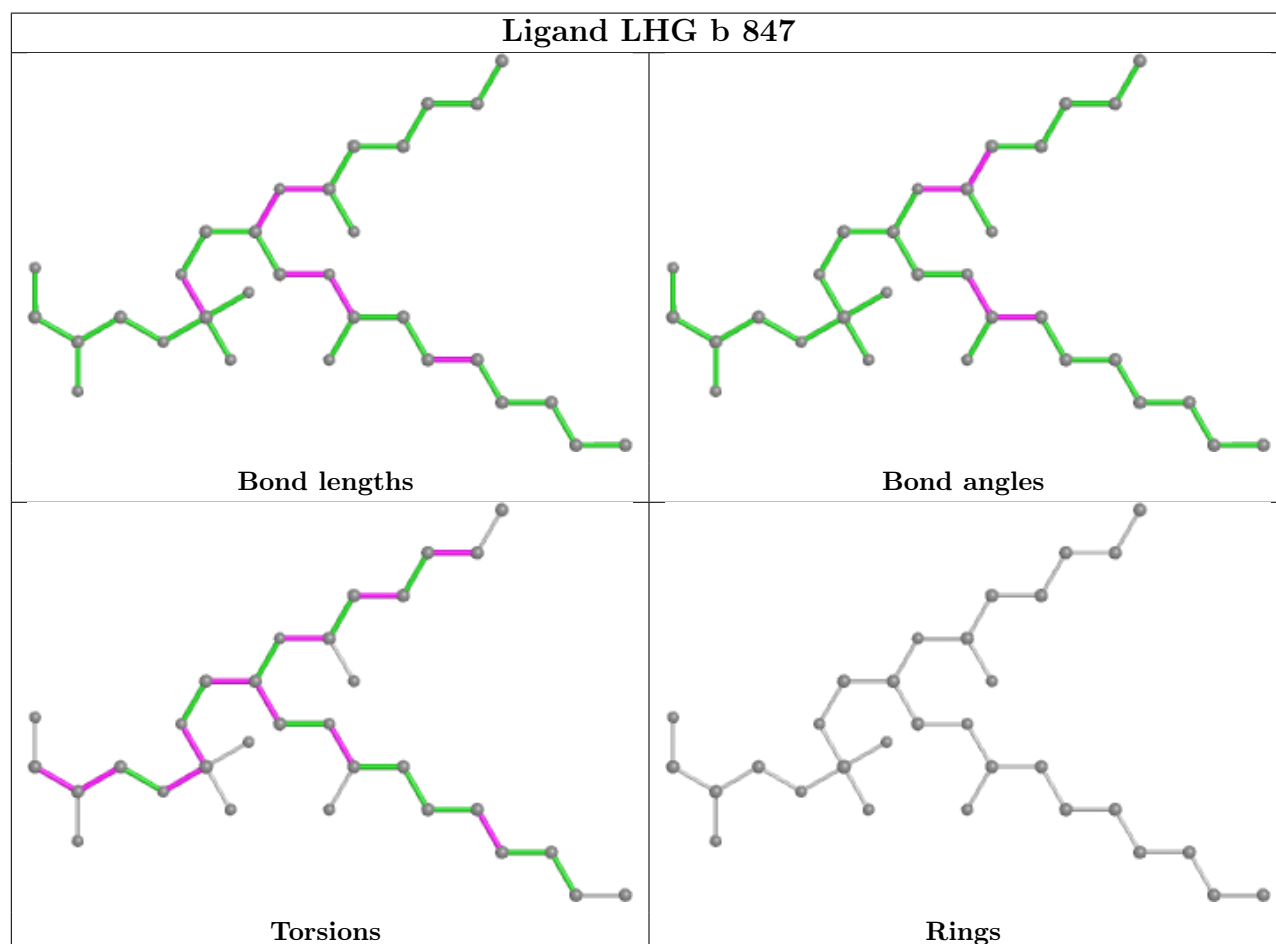
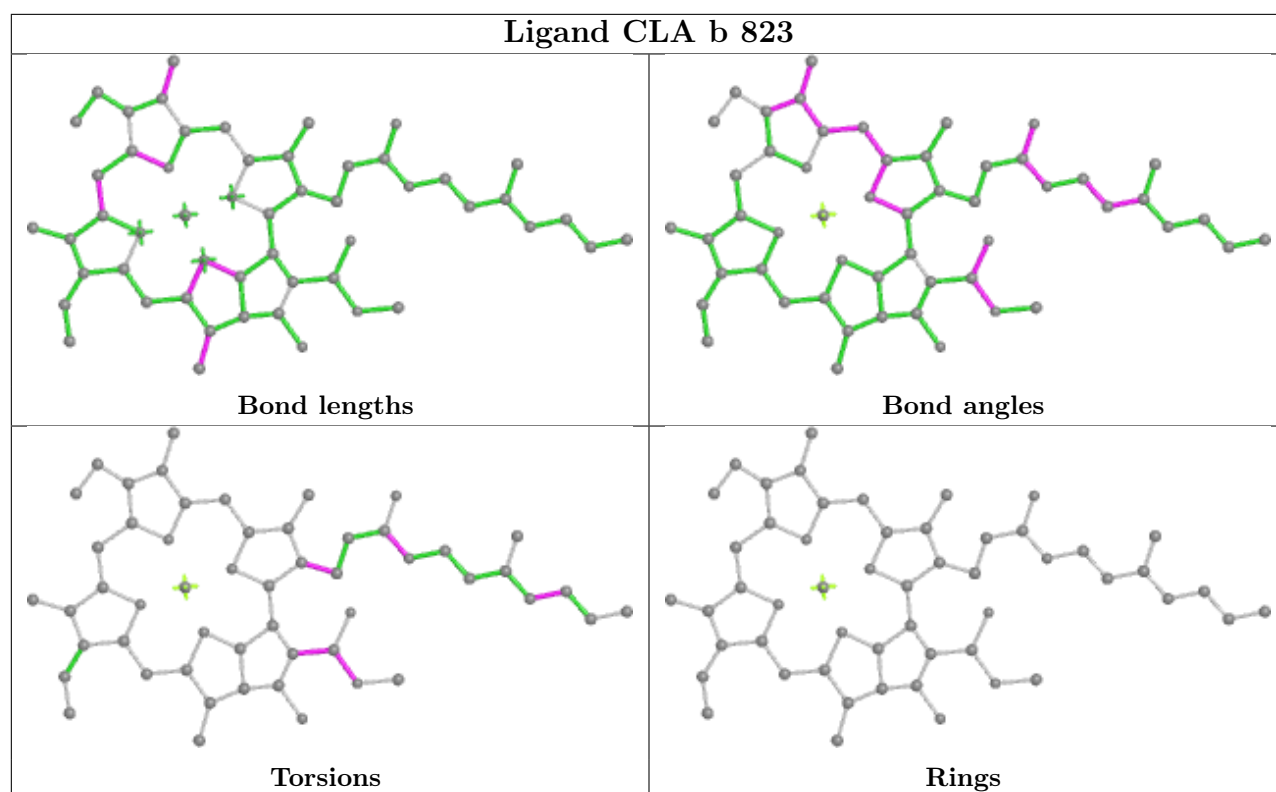
Rings

Ligand CLA 2 314

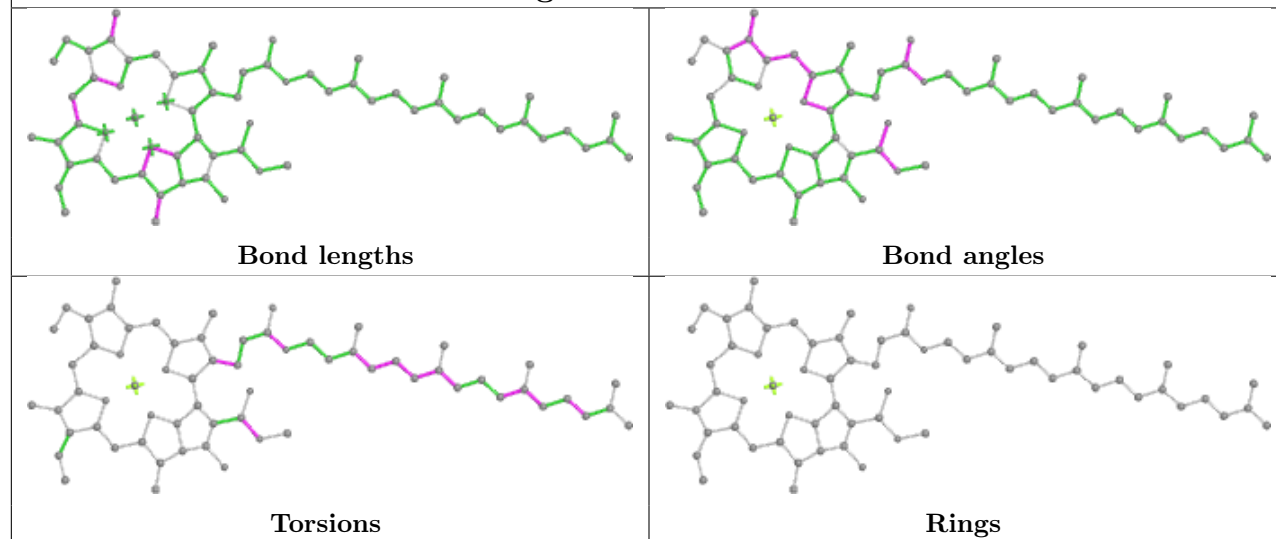


Ligand CLA 4 317

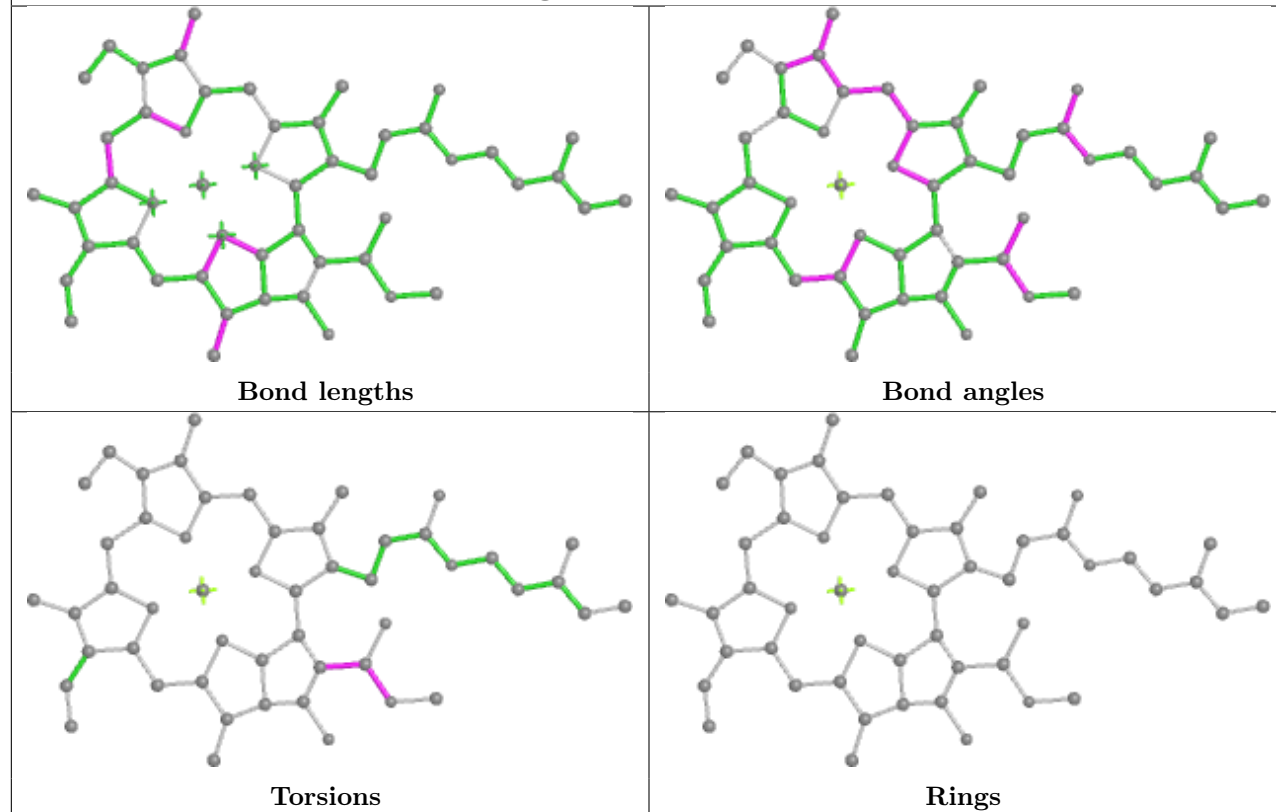


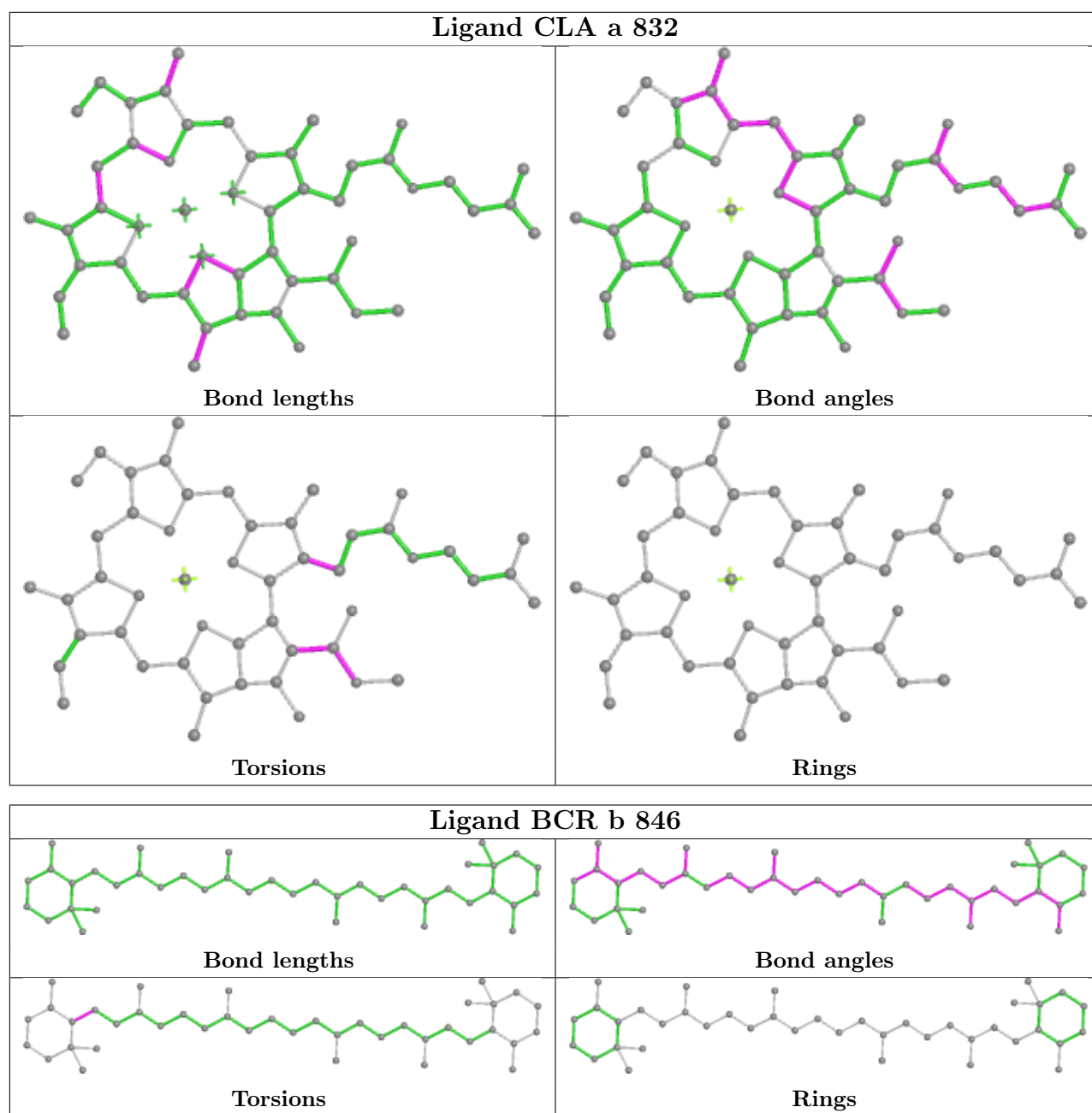


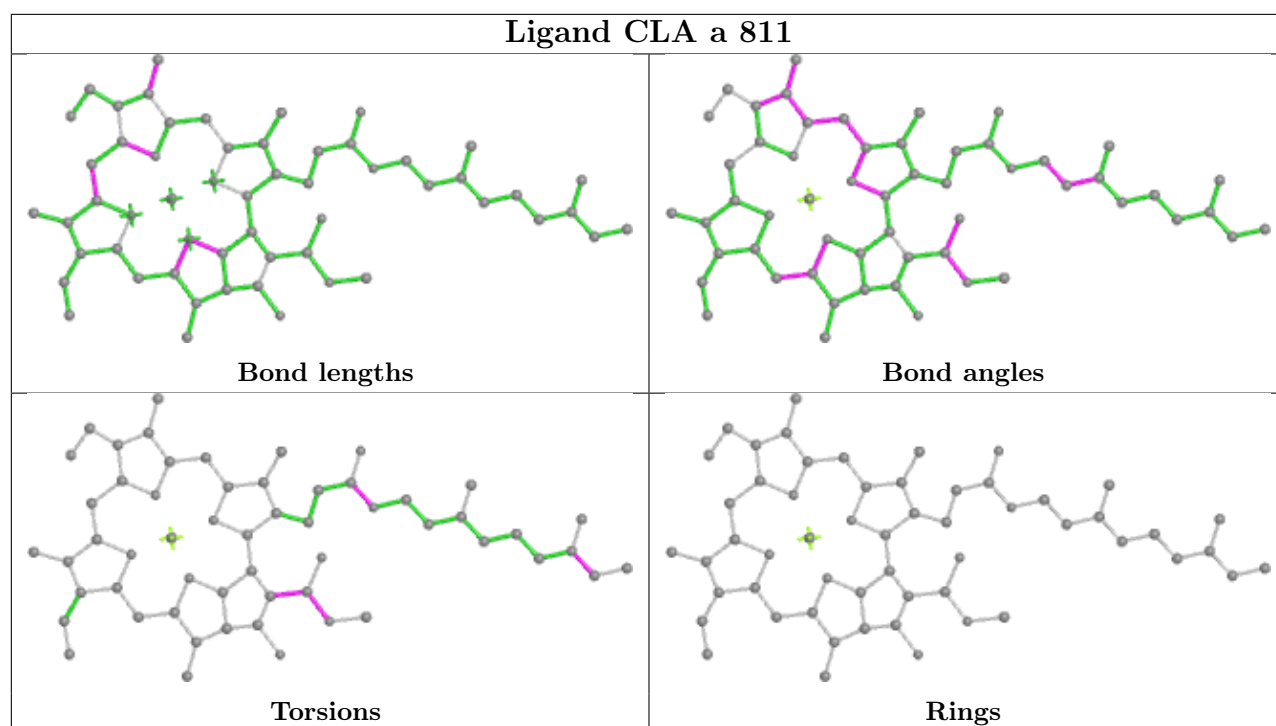
Ligand CLA a 807



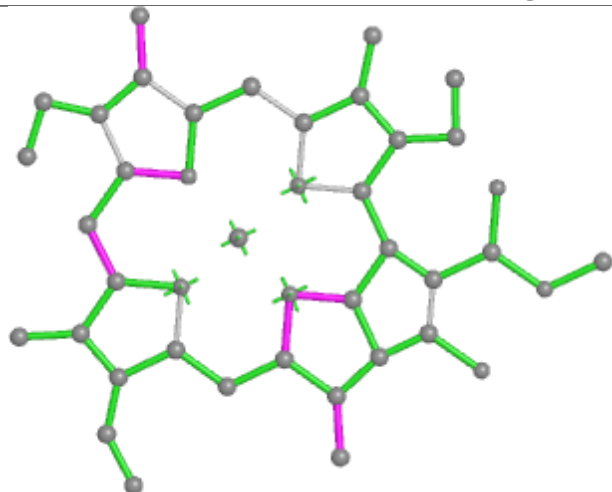
Ligand CLA a 808



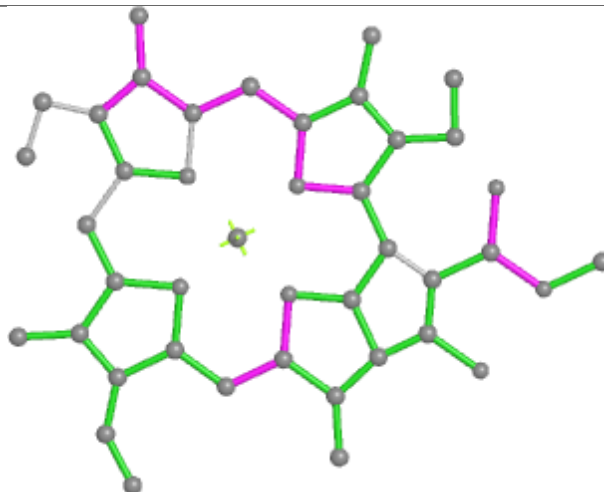




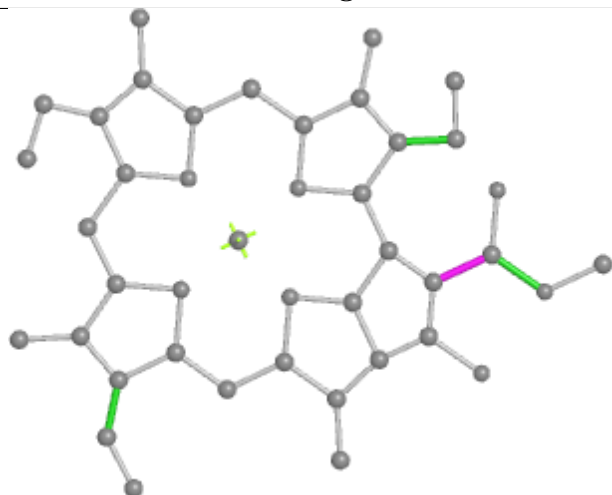
Ligand CLA 1 202



Bond lengths



Bond angles

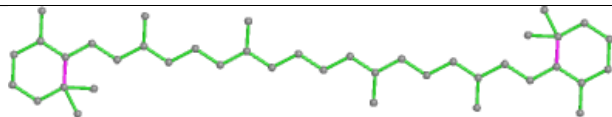


Torsions

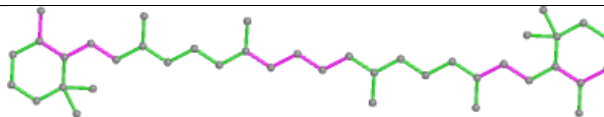


Rings

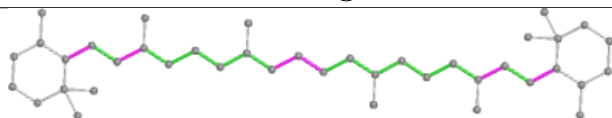
Ligand BCR m 101



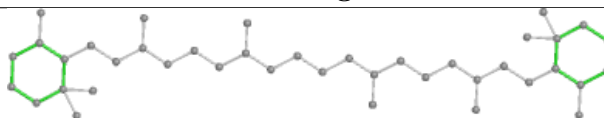
Bond lengths



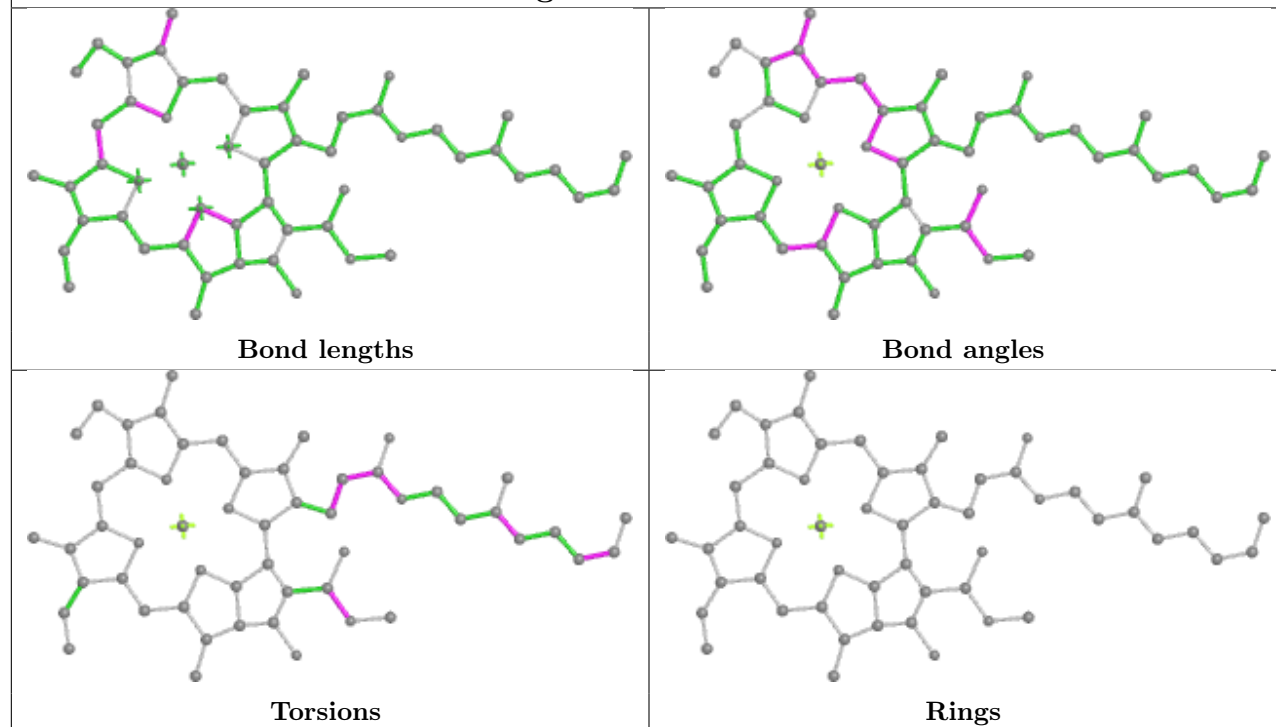
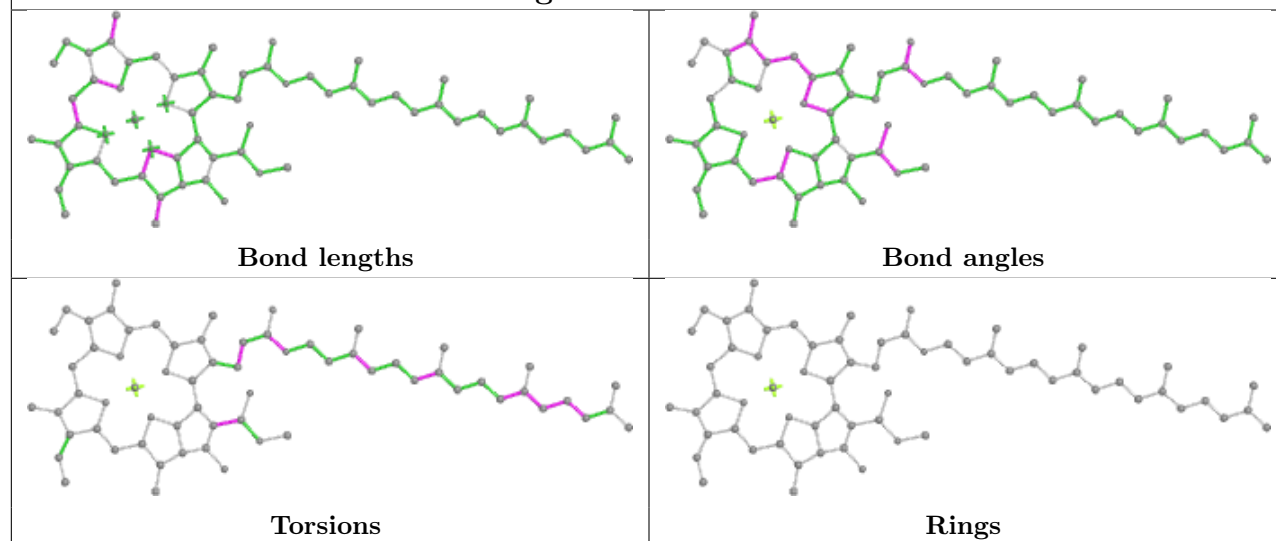
Bond angles

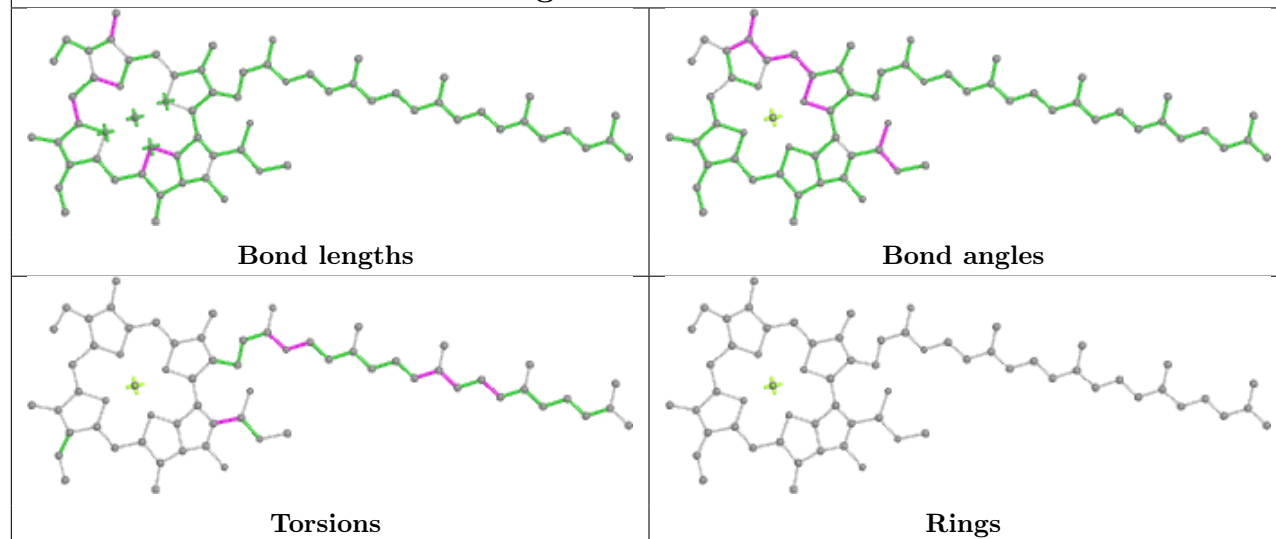
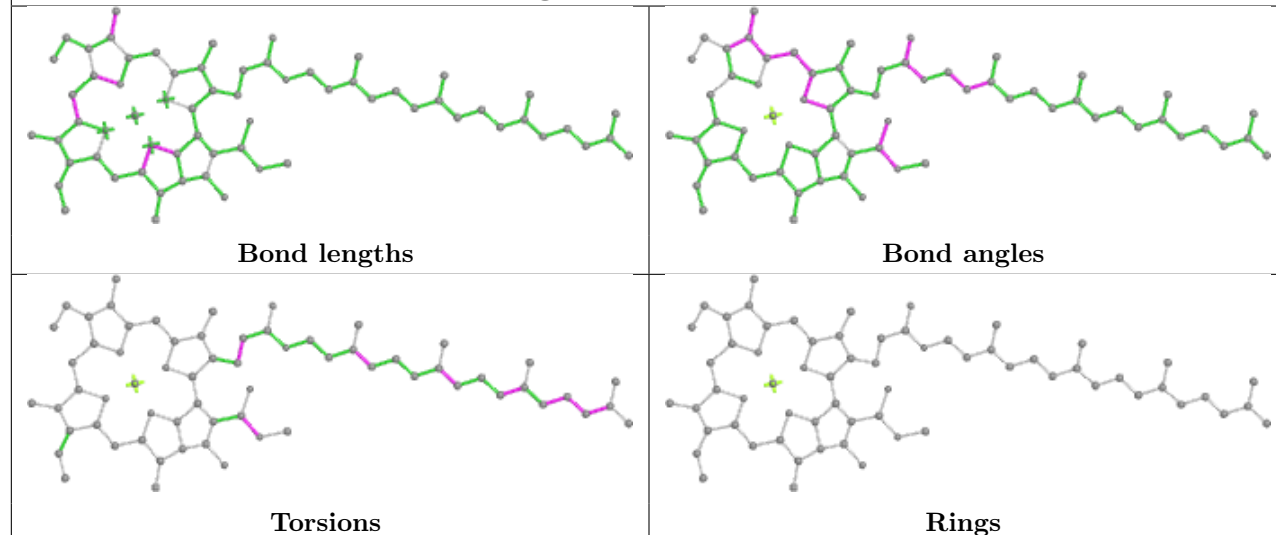
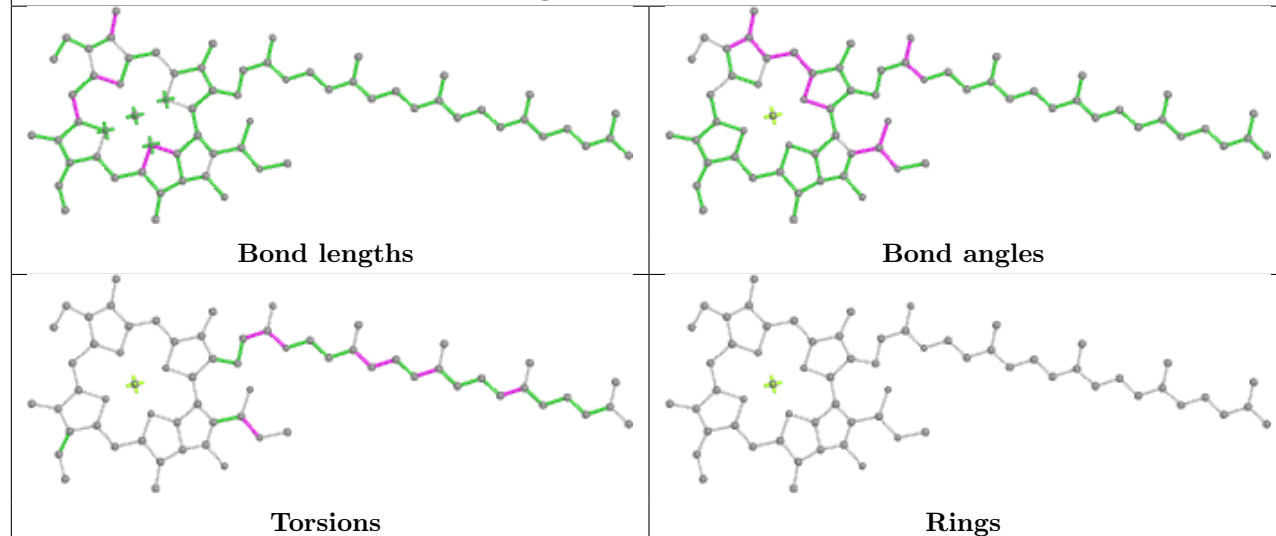


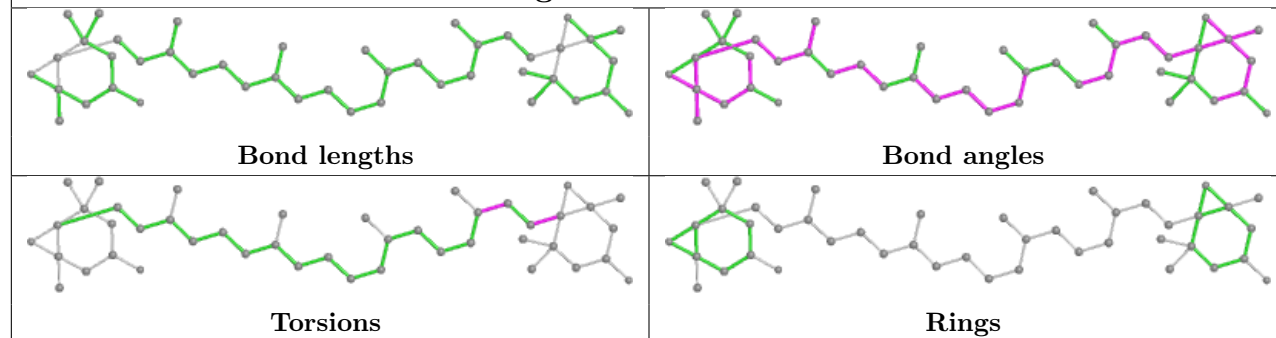
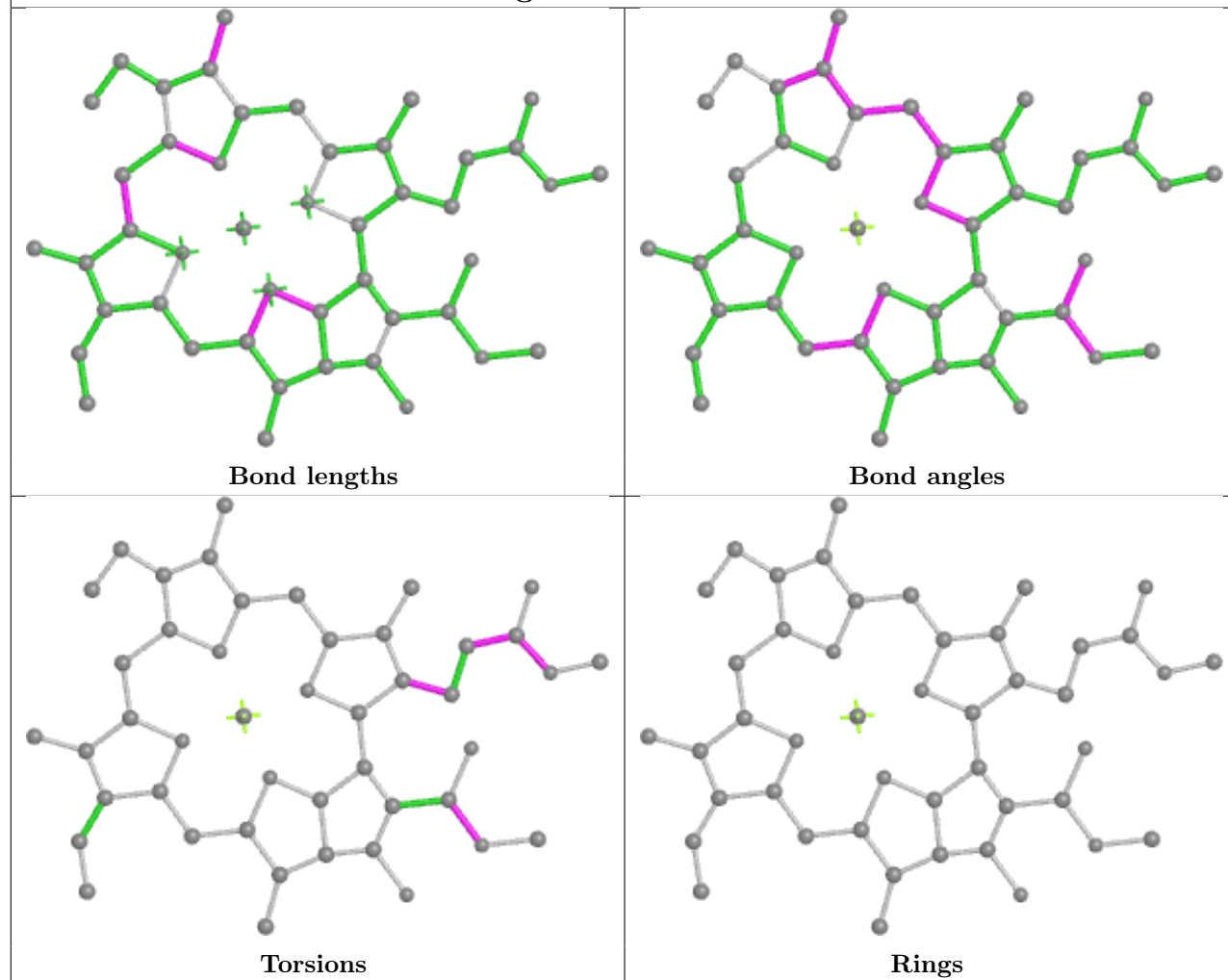
Torsions



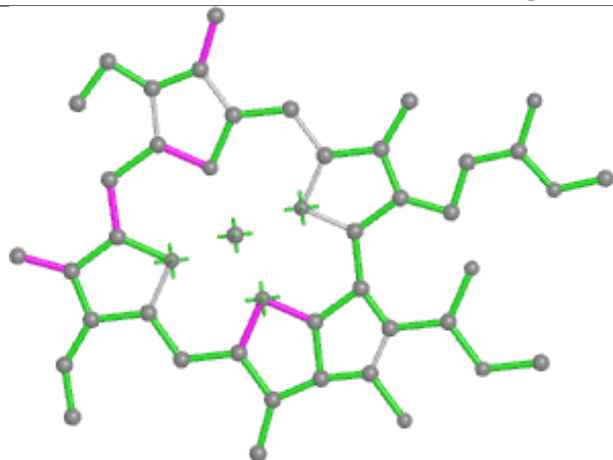
Rings

Ligand CLA a 813**Ligand CLA b 838**

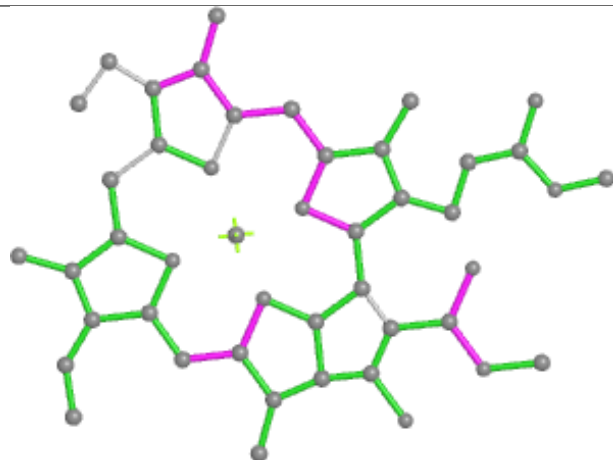
Ligand CLA 6 309**Ligand CLA 1 308****Ligand CLA a 835**

Ligand XAT 4 303**Ligand CLA 6 316**

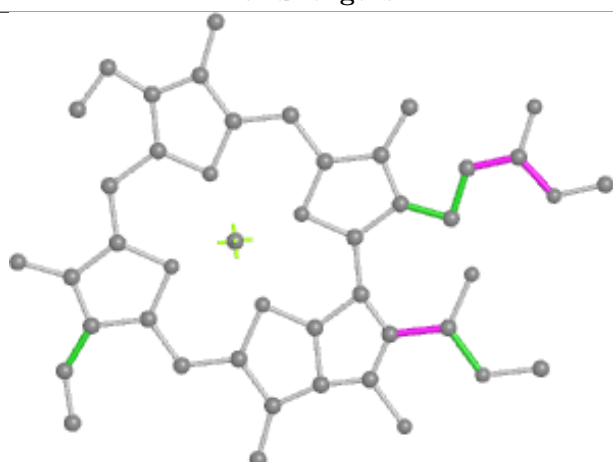
Ligand CLA 1 204



Bond lengths



Bond angles

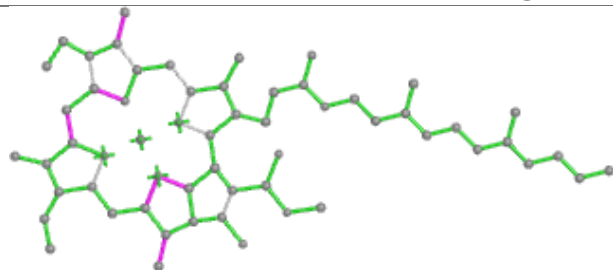


Torsions

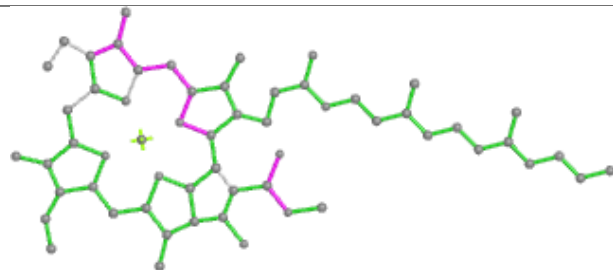


Rings

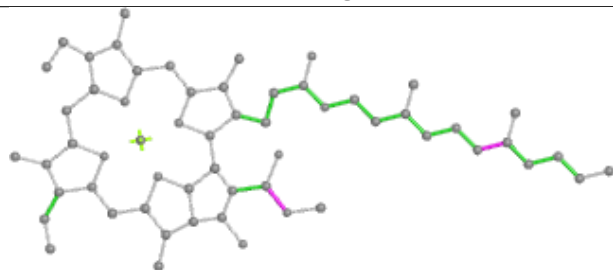
Ligand CLA 6 308



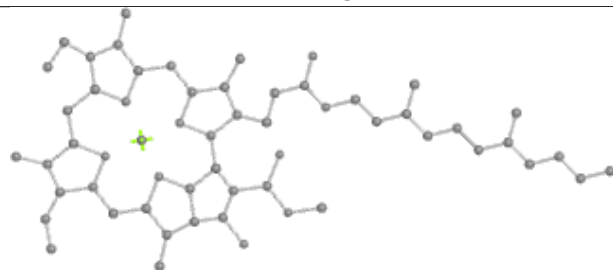
Bond lengths



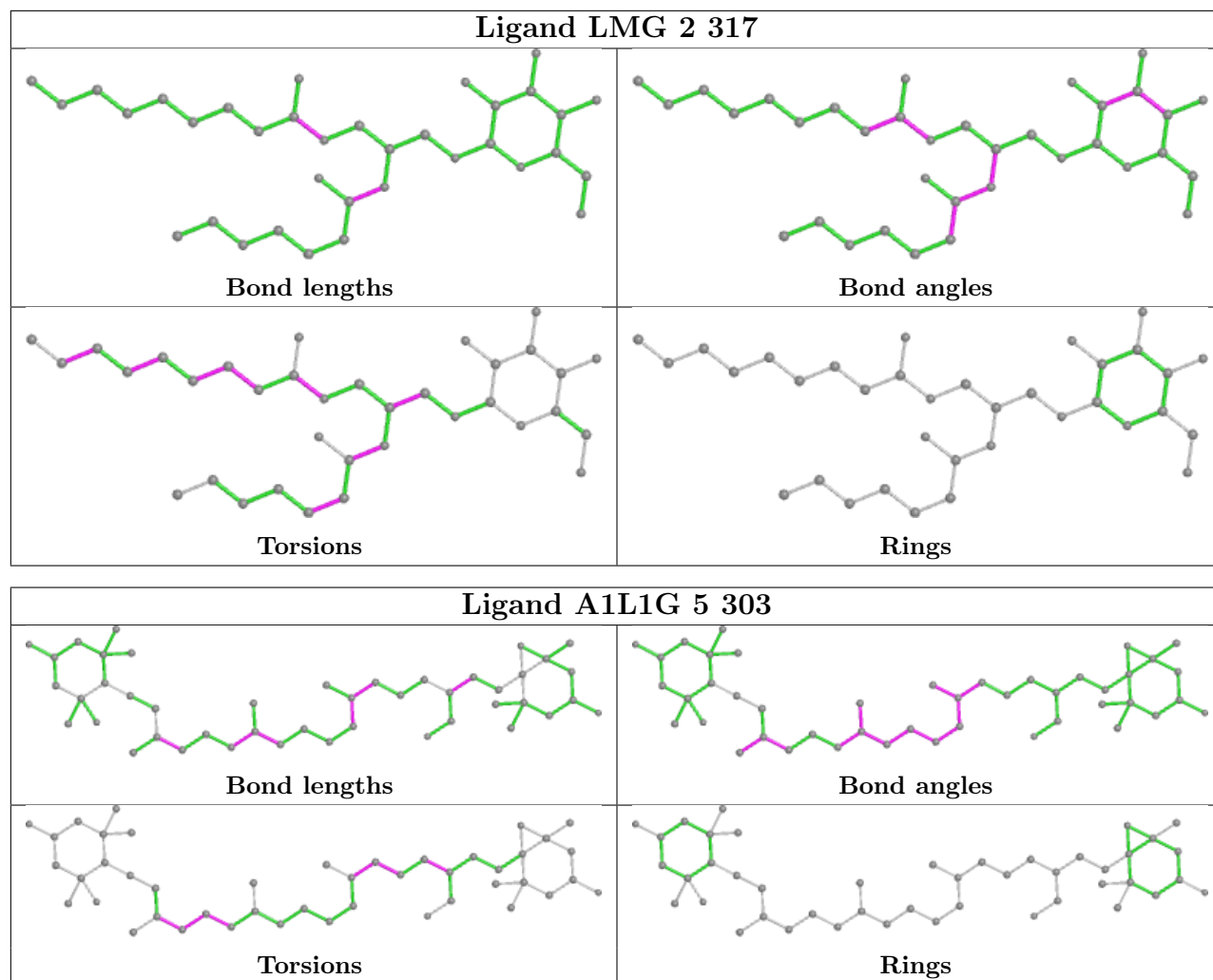
Bond angles



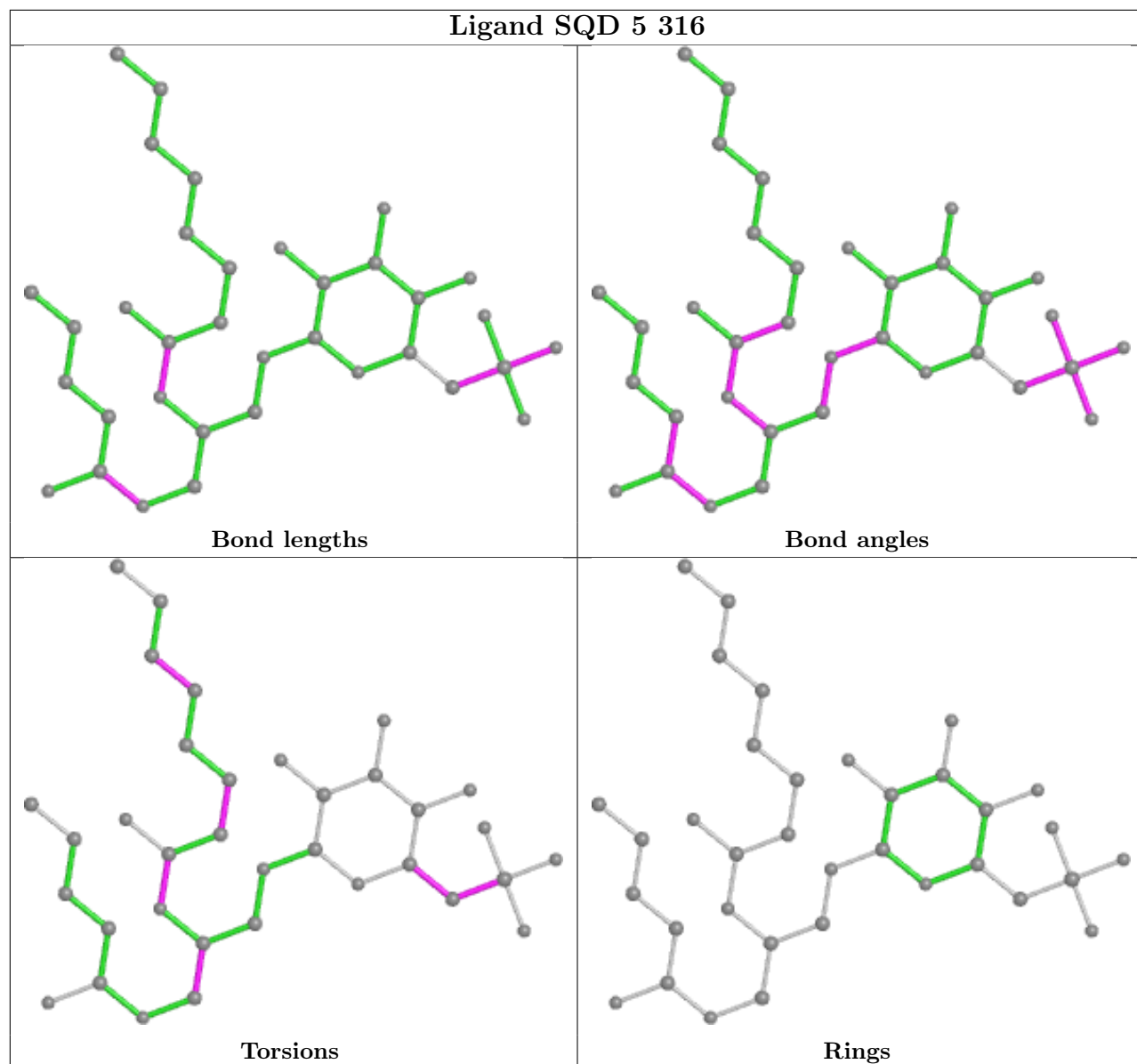
Torsions



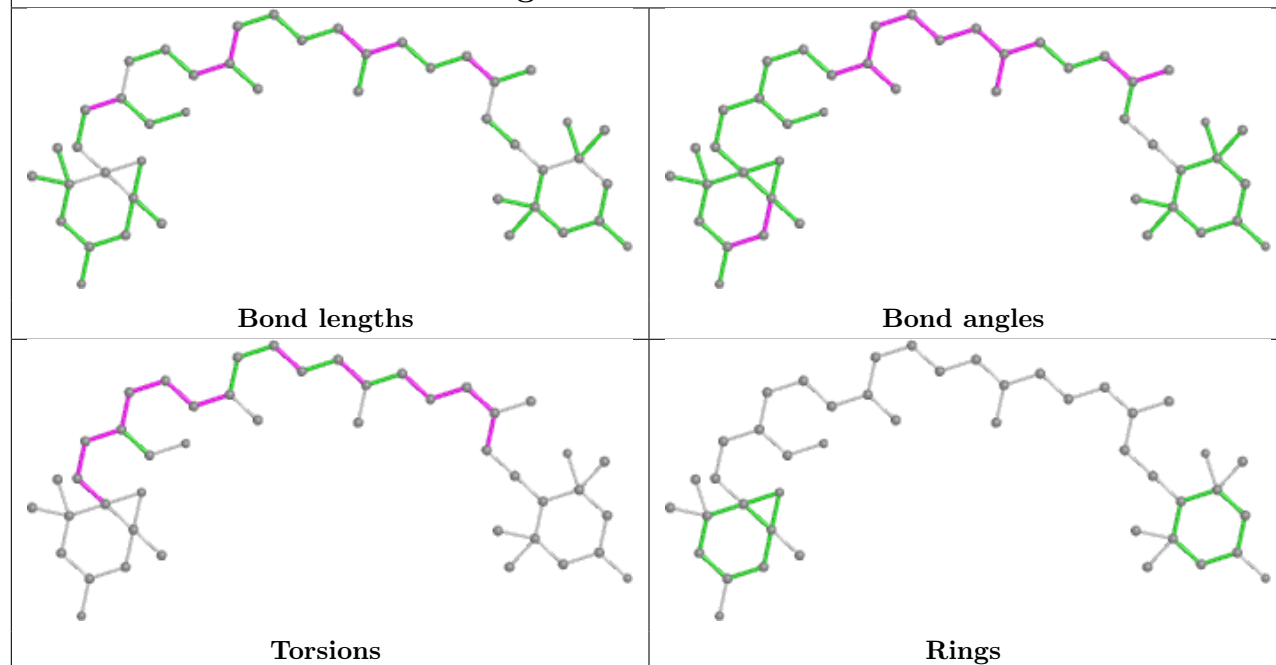
Rings



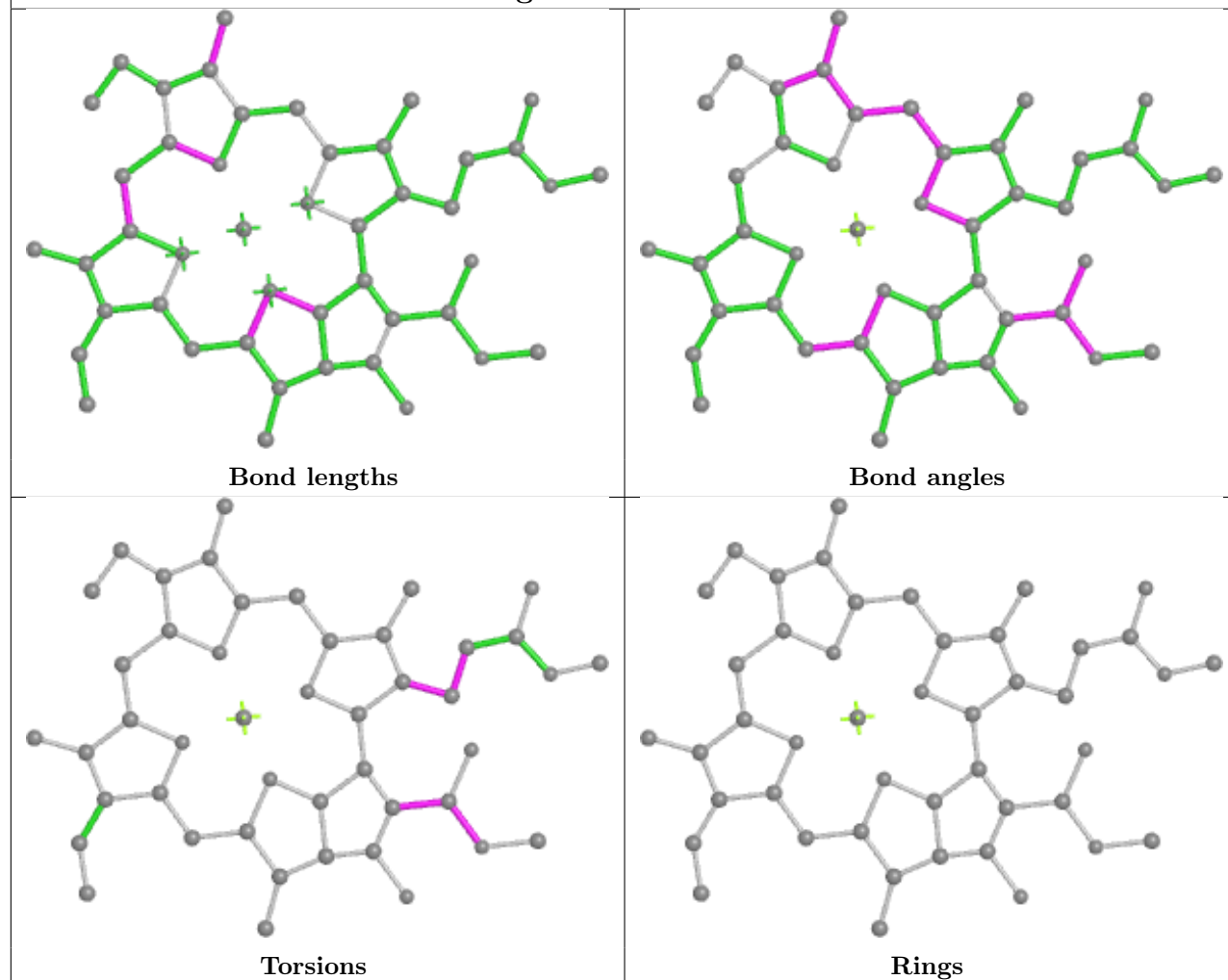
Ligand SQD 5 316

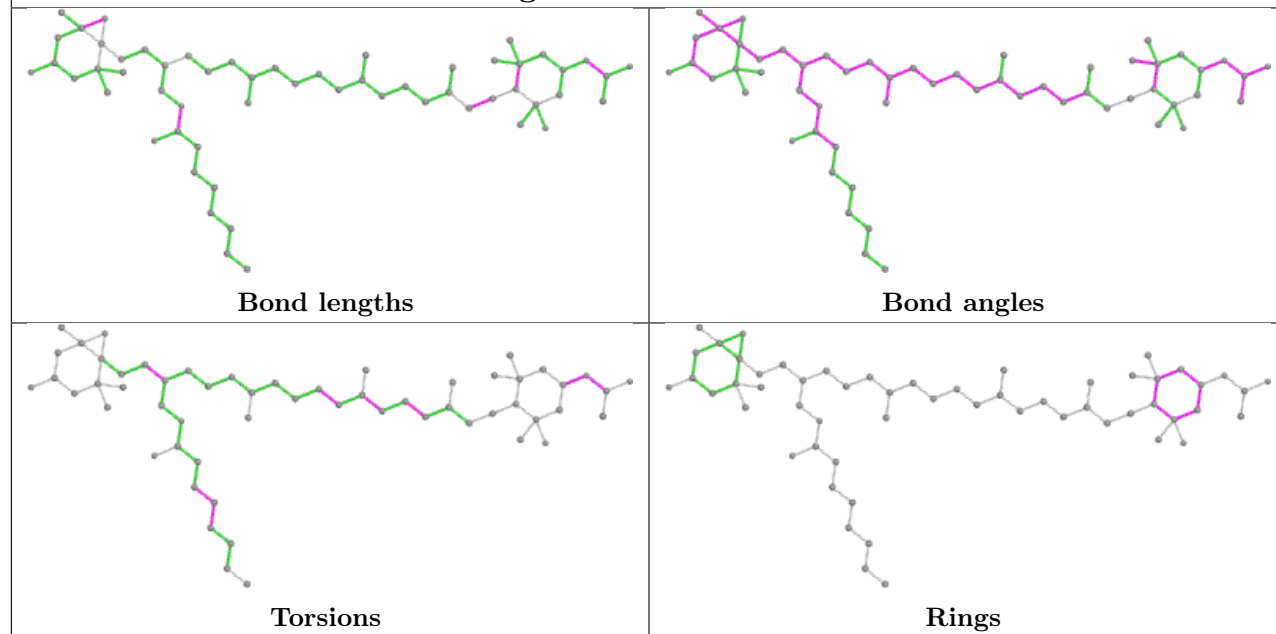
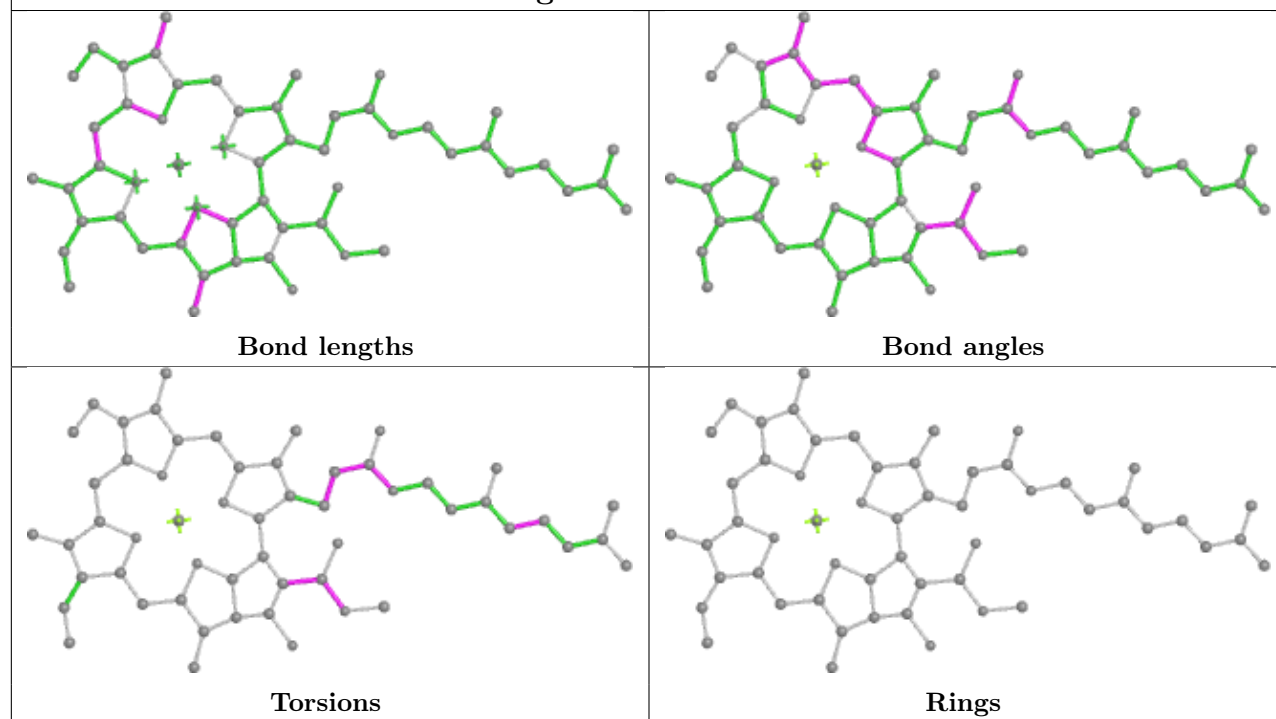


Ligand A1L1G 9 306

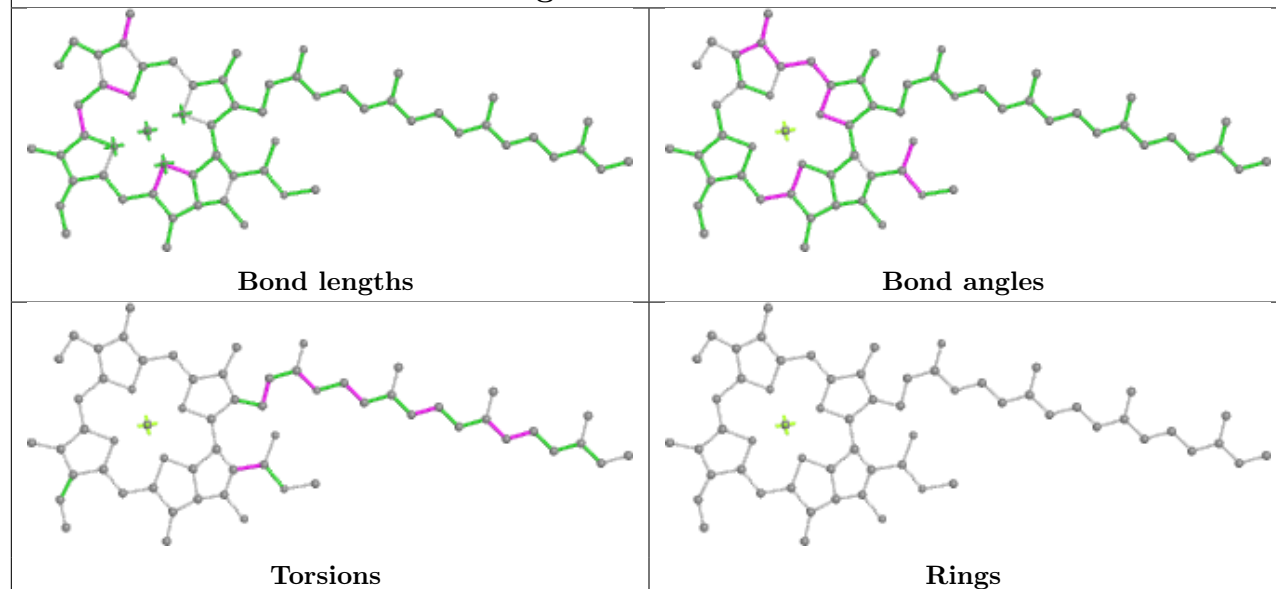


Ligand CLA 9 311

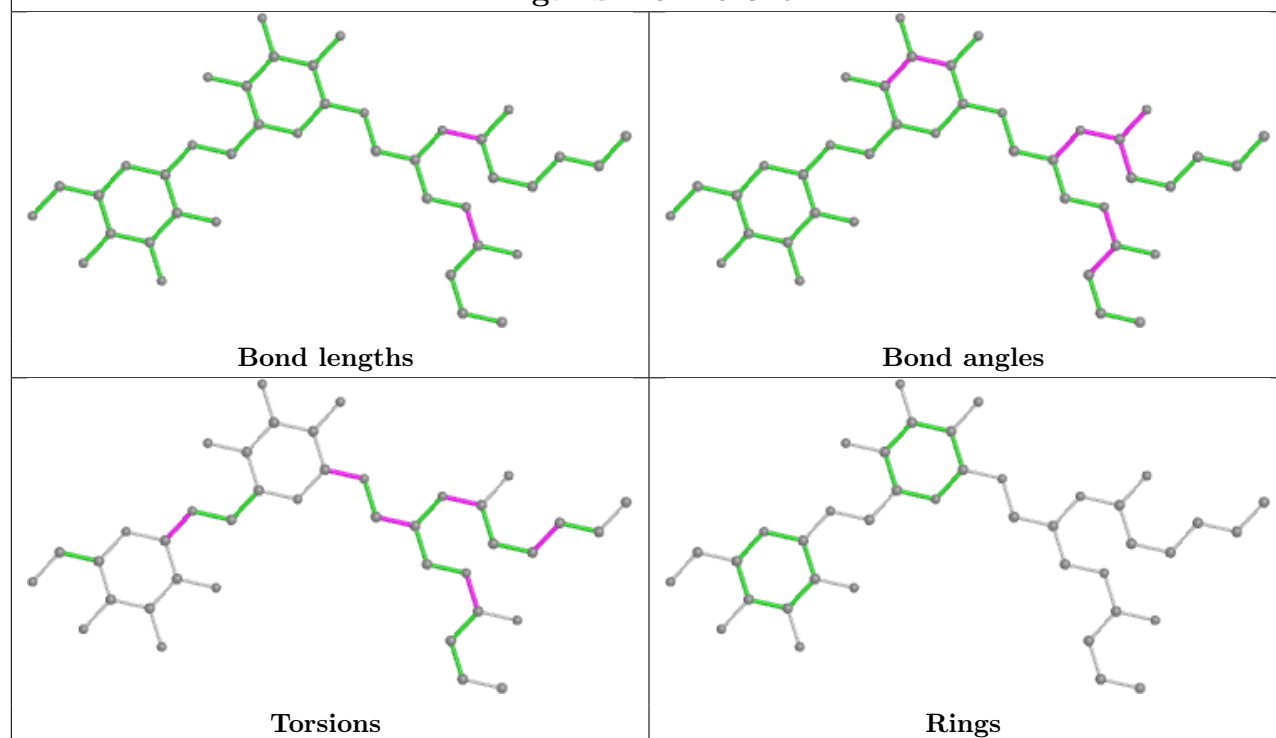


Ligand A1L1F h 203**Ligand CLA 9 314**

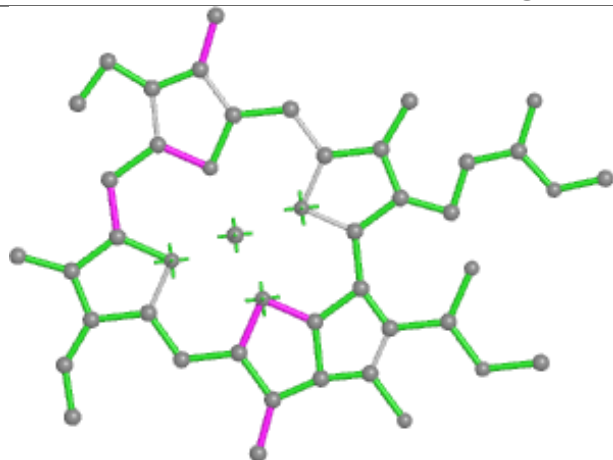
Ligand CLA 1 305



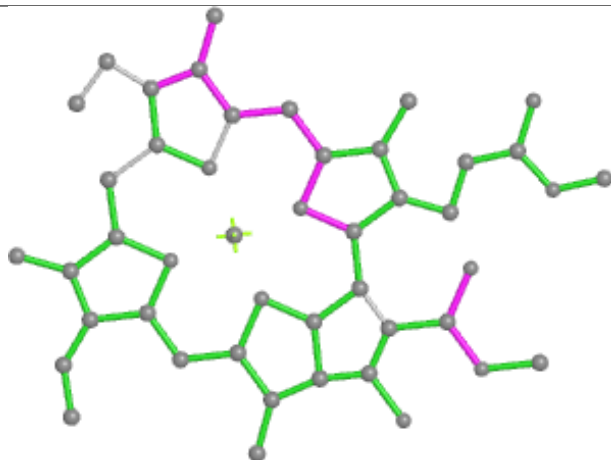
Ligand DGD 8 315



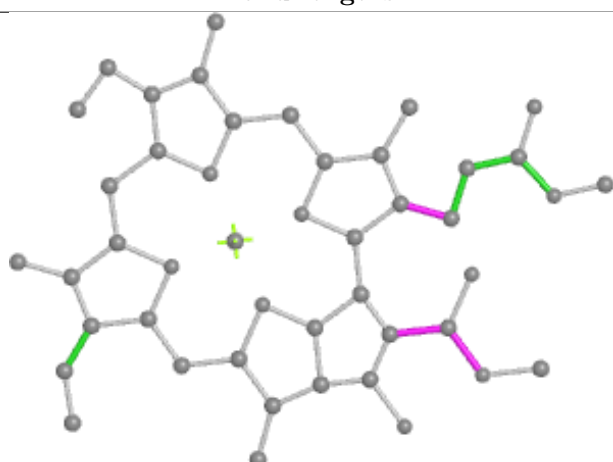
Ligand CLA 2 316



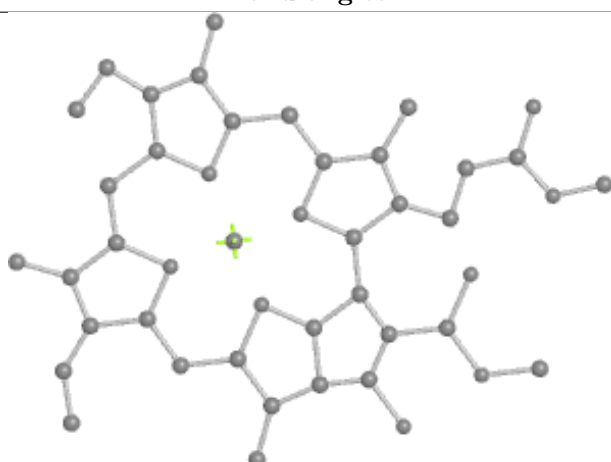
Bond lengths



Bond angles

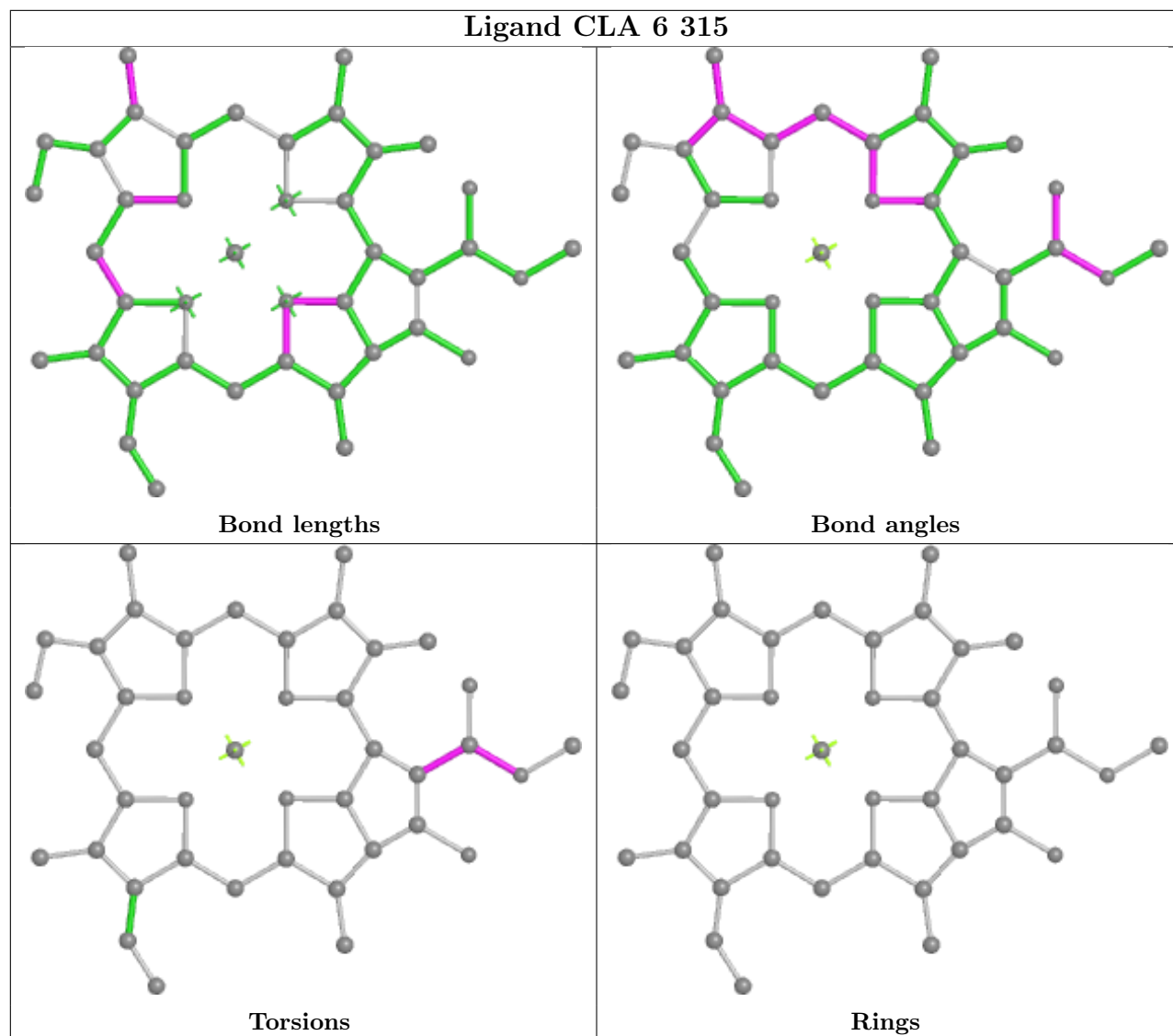


Torsions

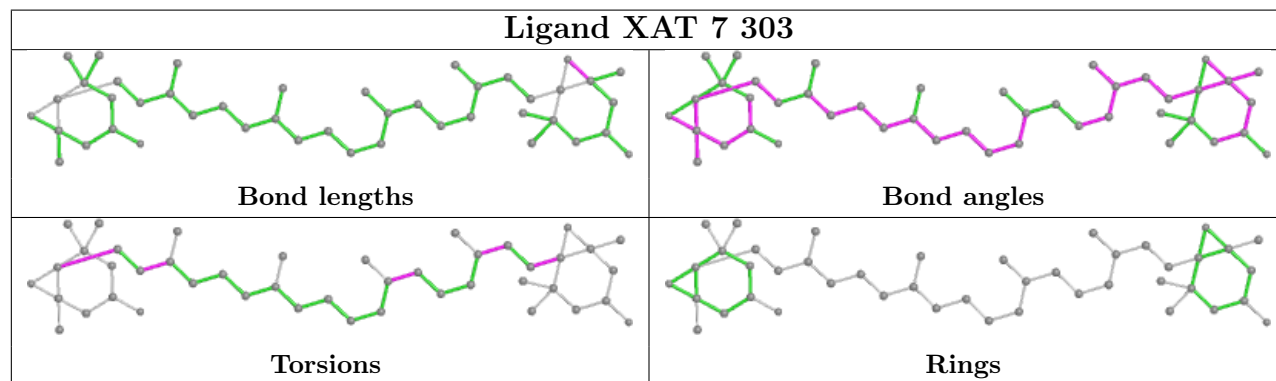


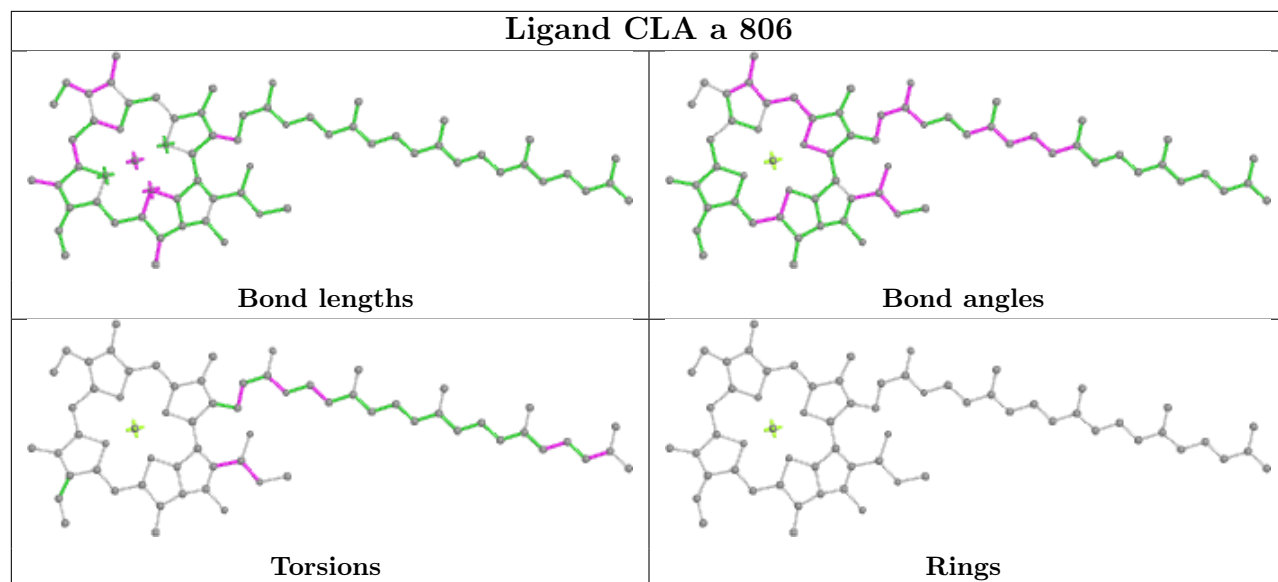
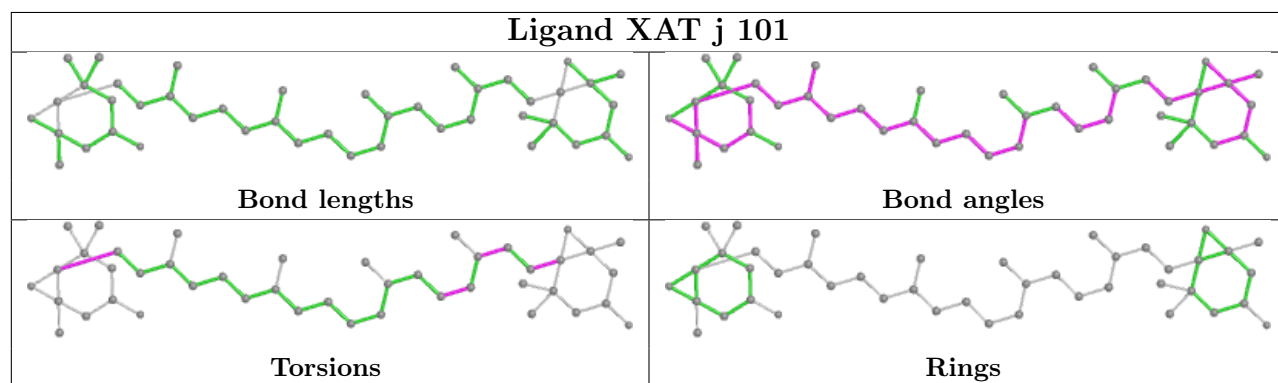
Rings

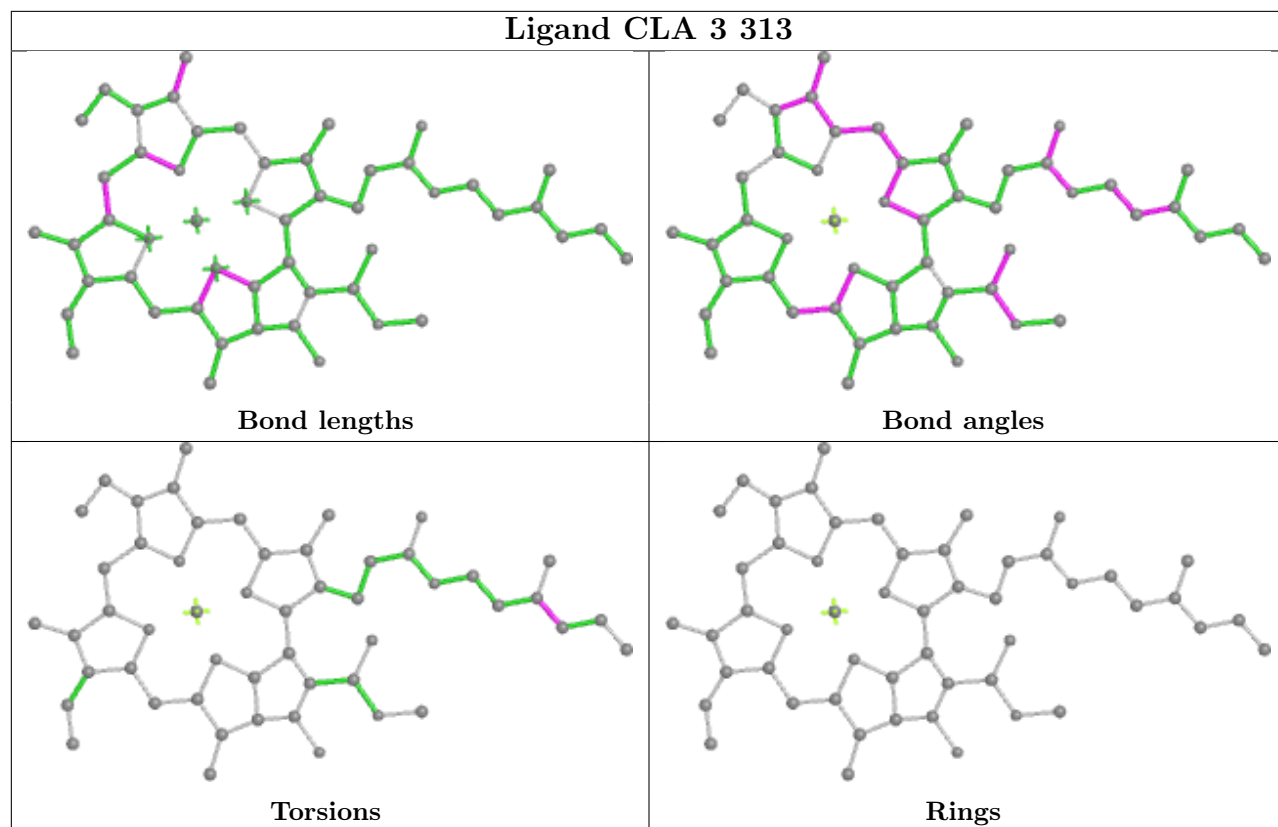
Ligand CLA 6 315



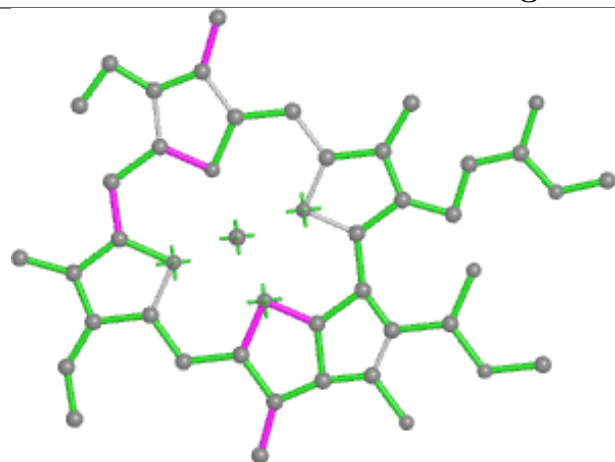
Ligand XAT 7 303



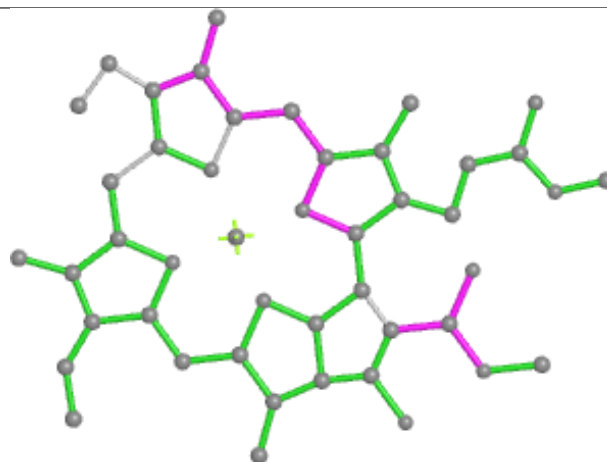
Ligand CLA a 806**Ligand XAT j 101**



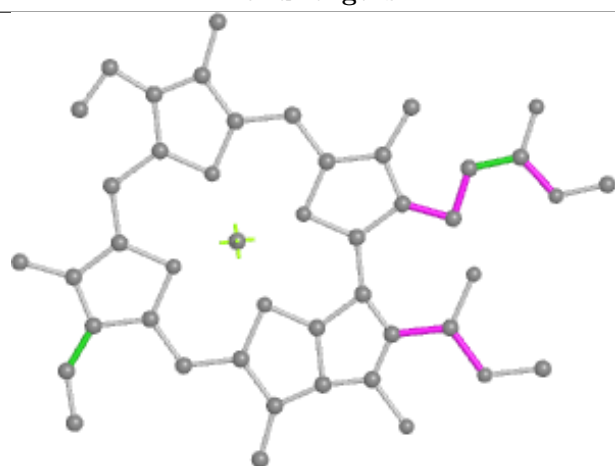
Ligand CLA 4 311



Bond lengths



Bond angles

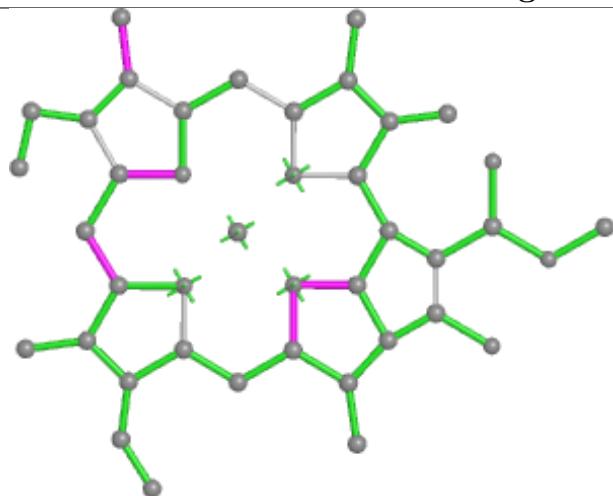


Torsions

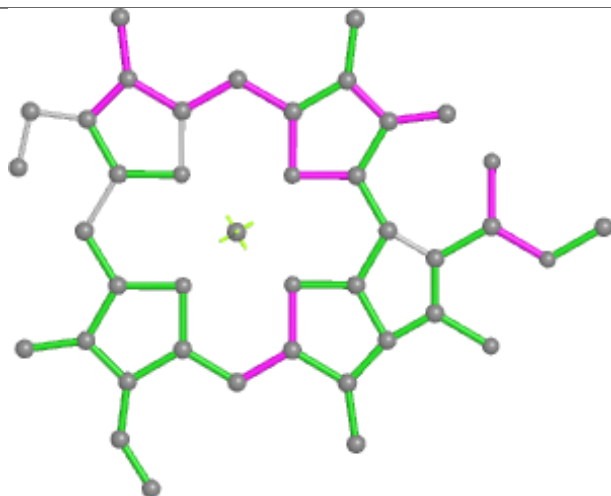


Rings

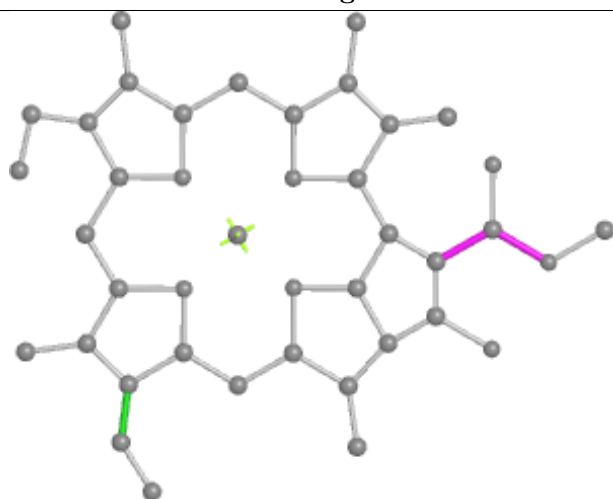
Ligand CLA 2 313



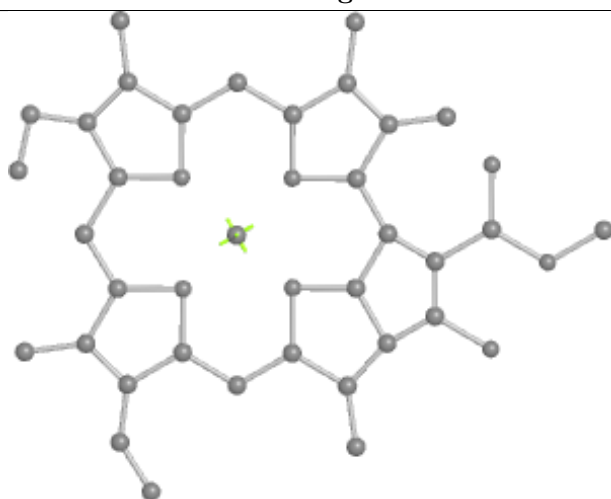
Bond lengths



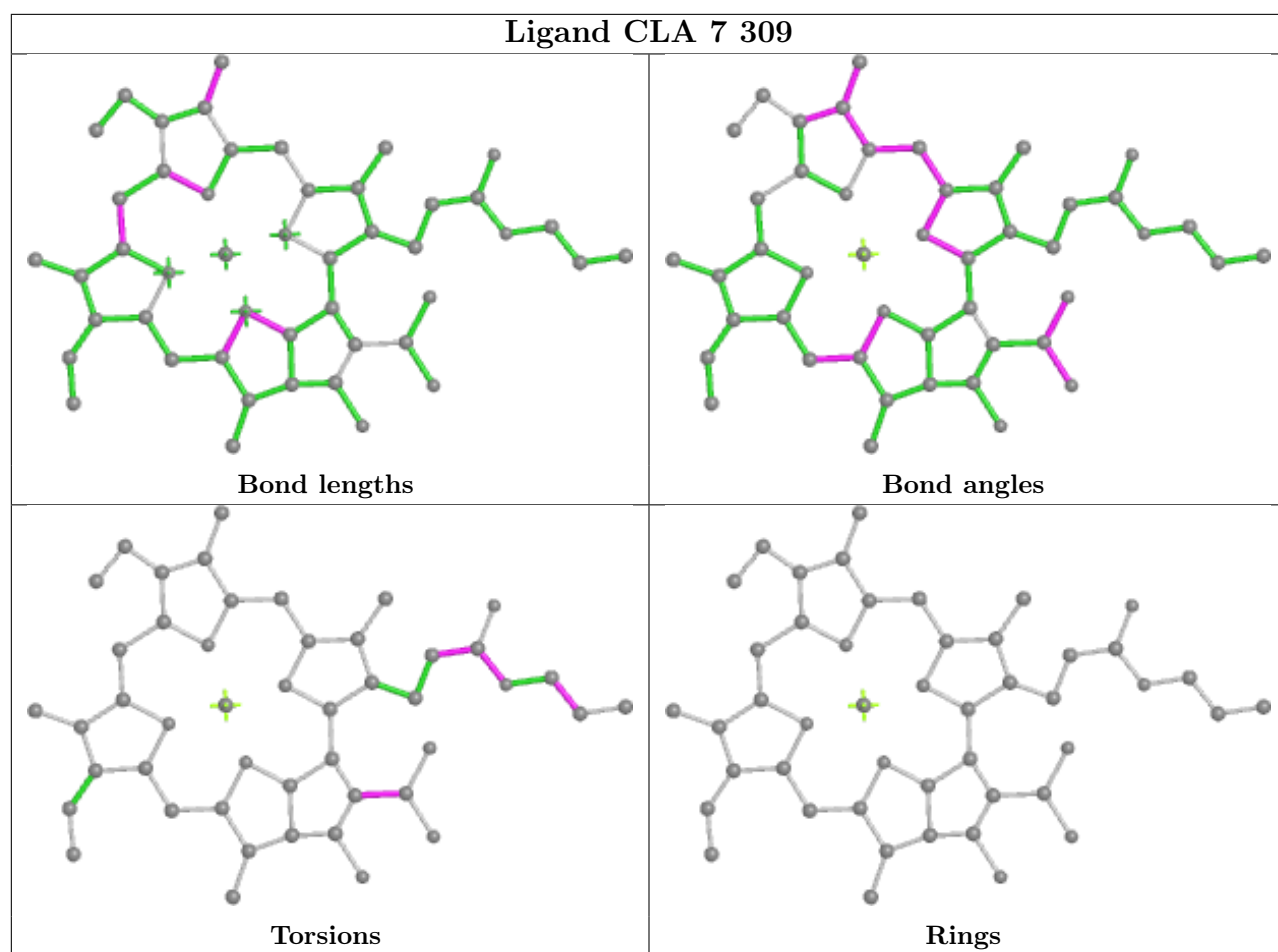
Bond angles



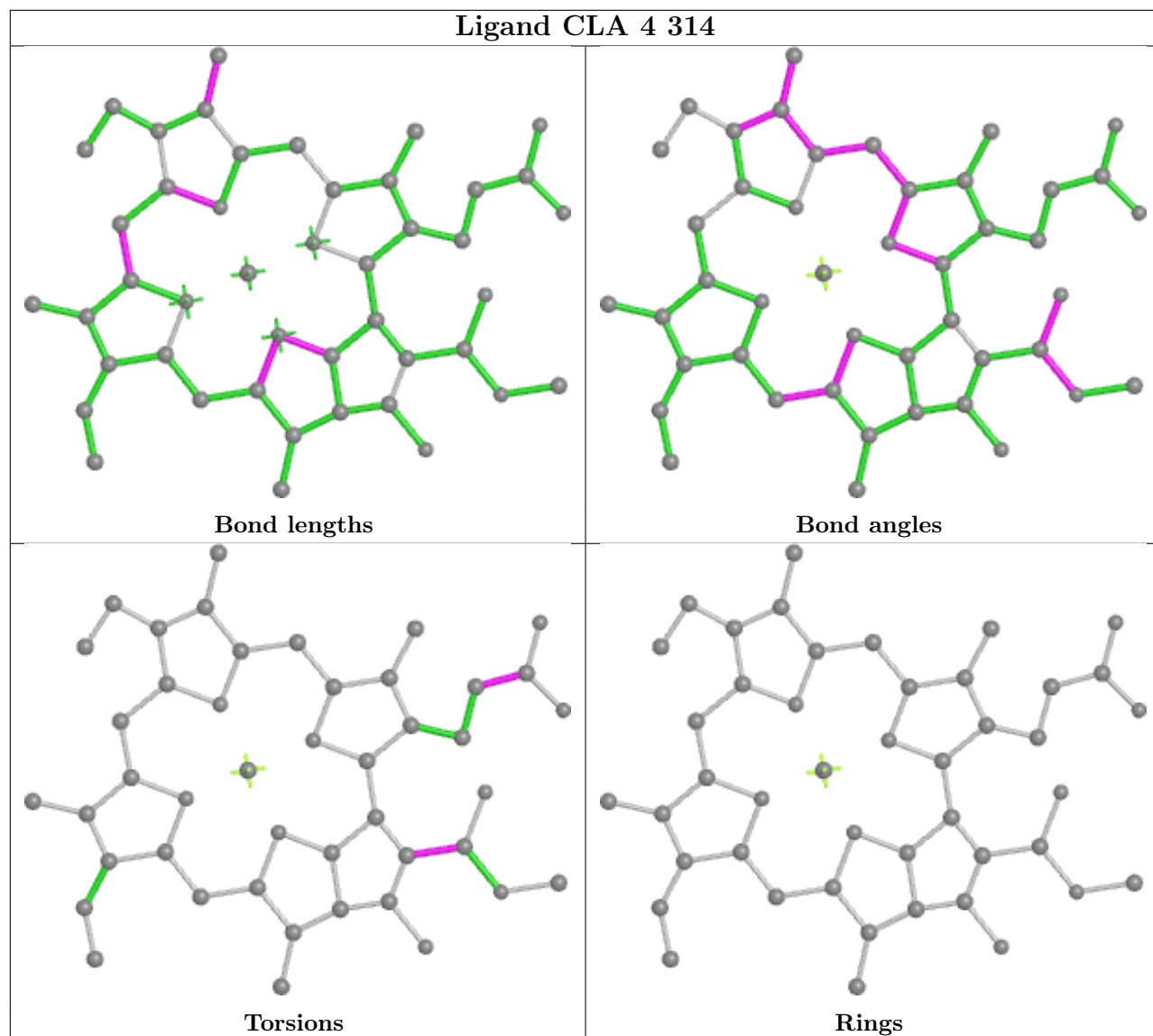
Torsions

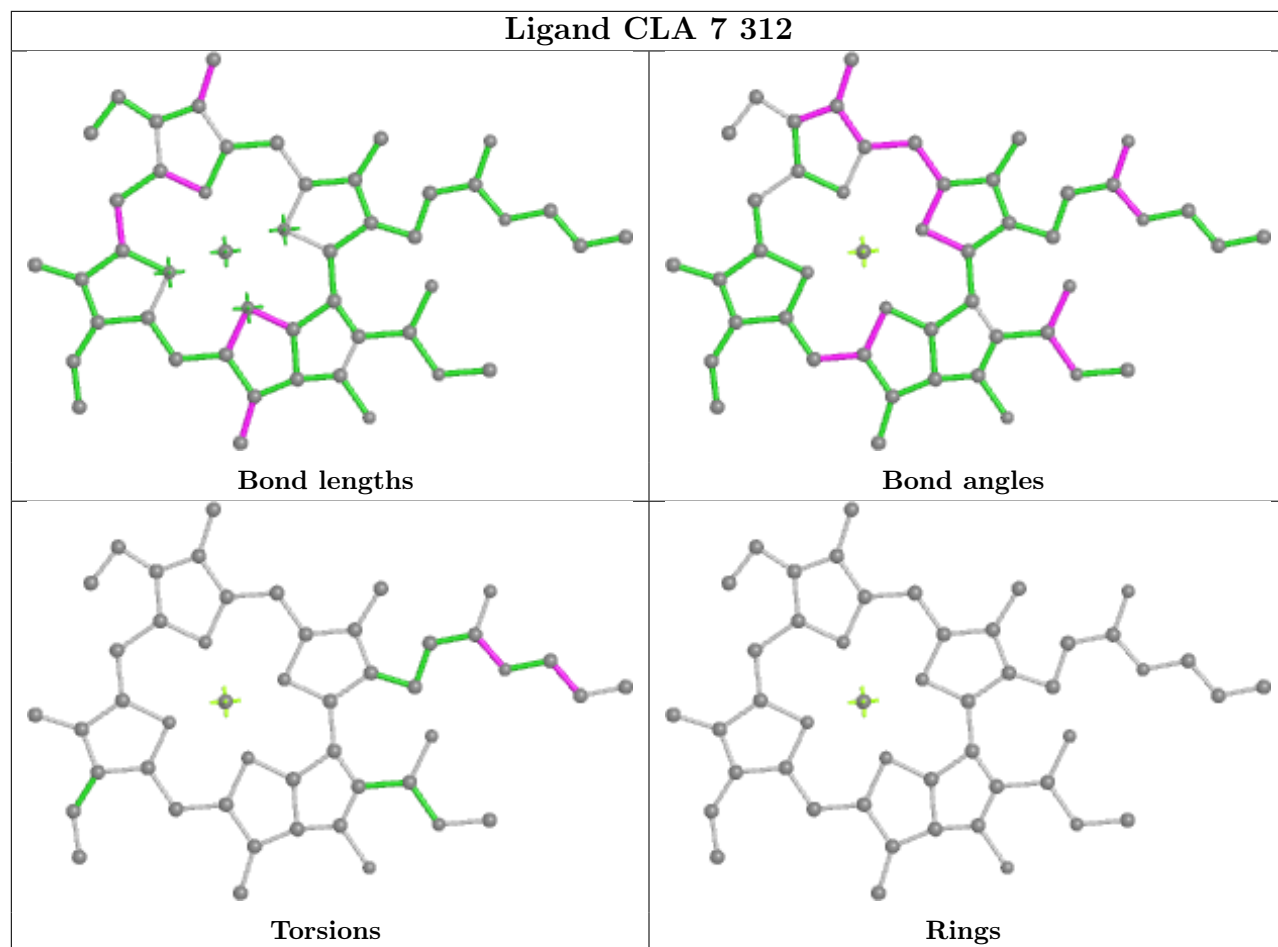


Rings

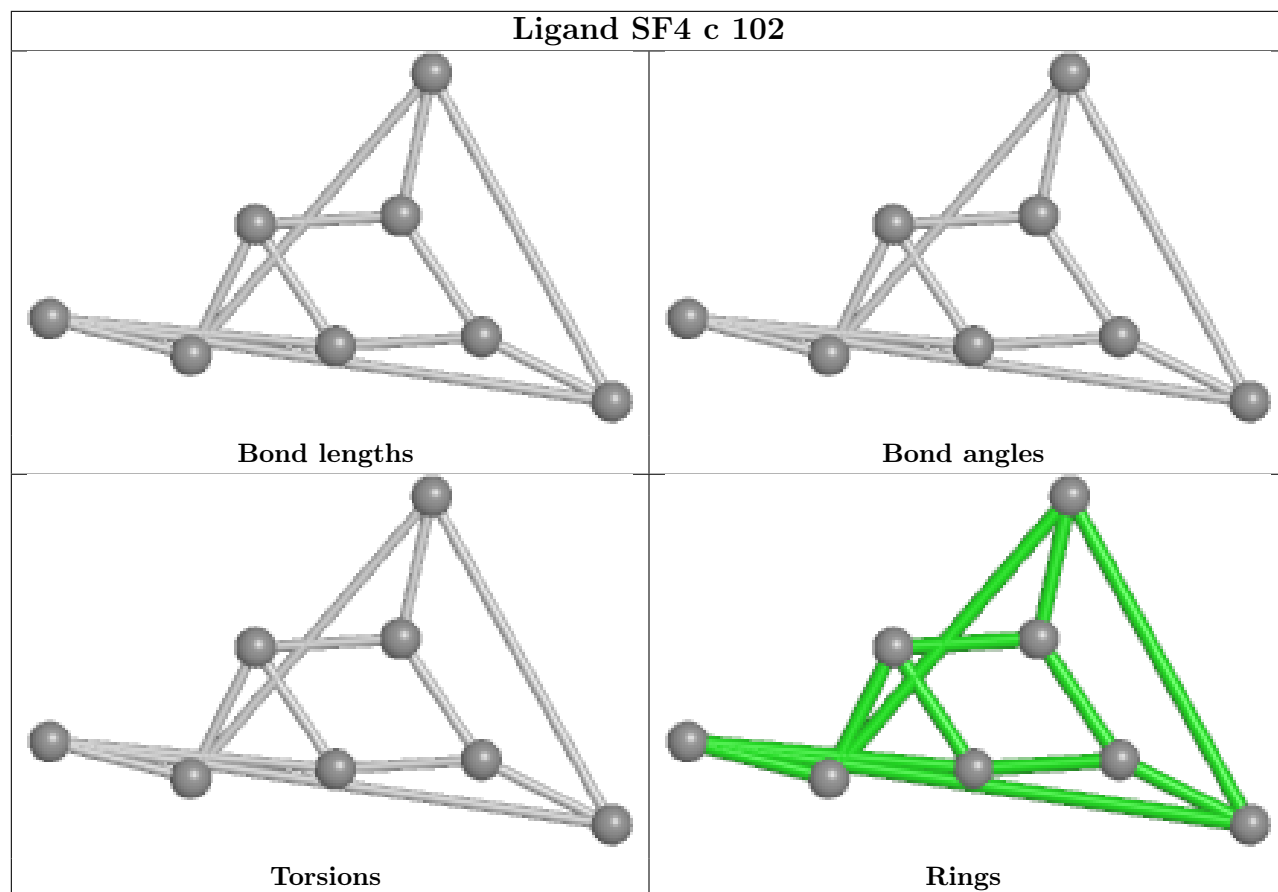


Ligand CLA 4 314

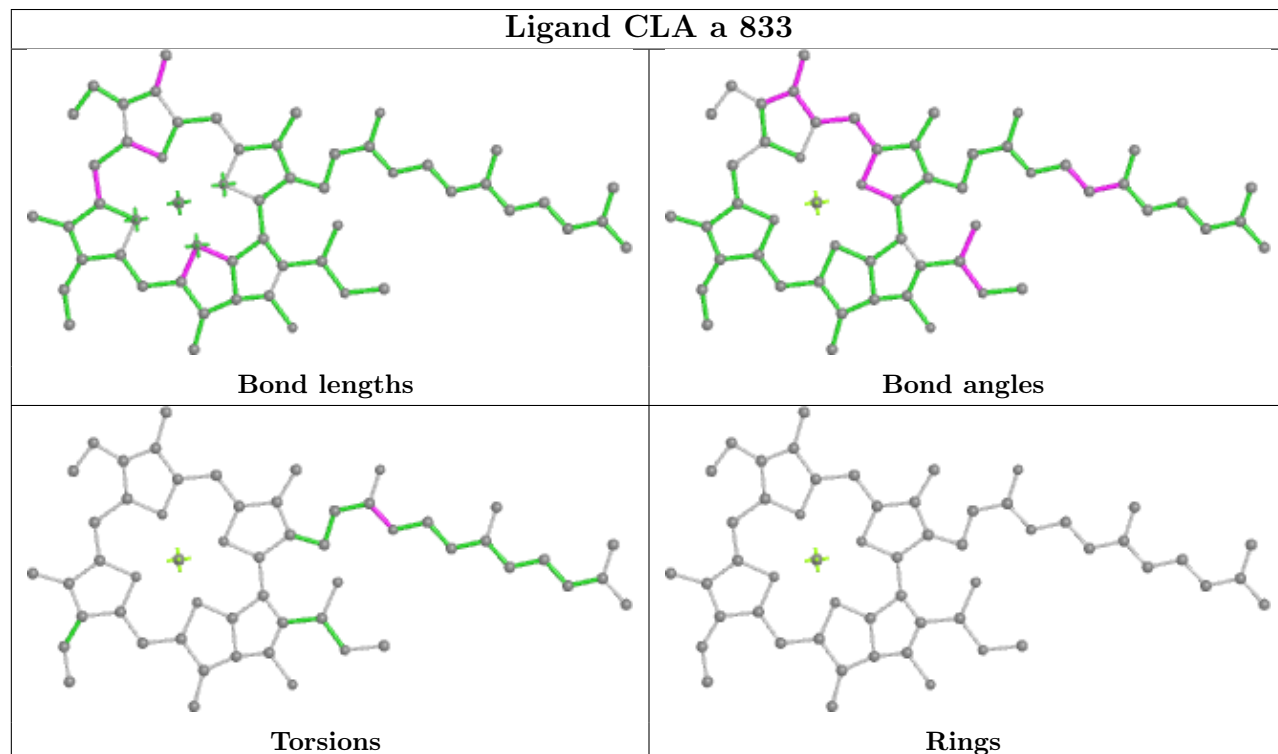


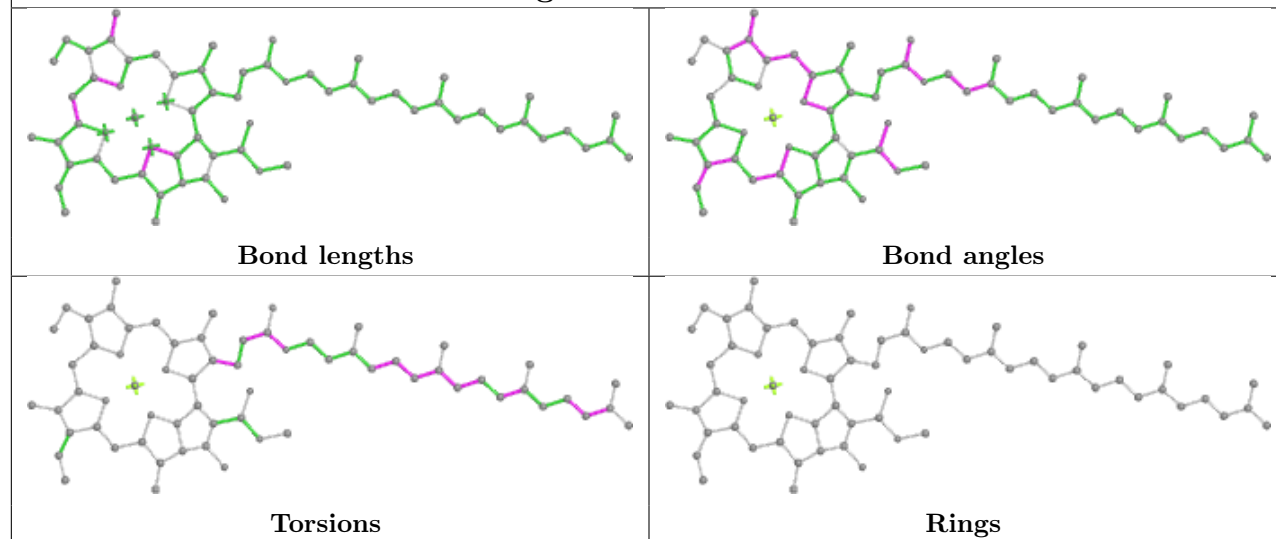
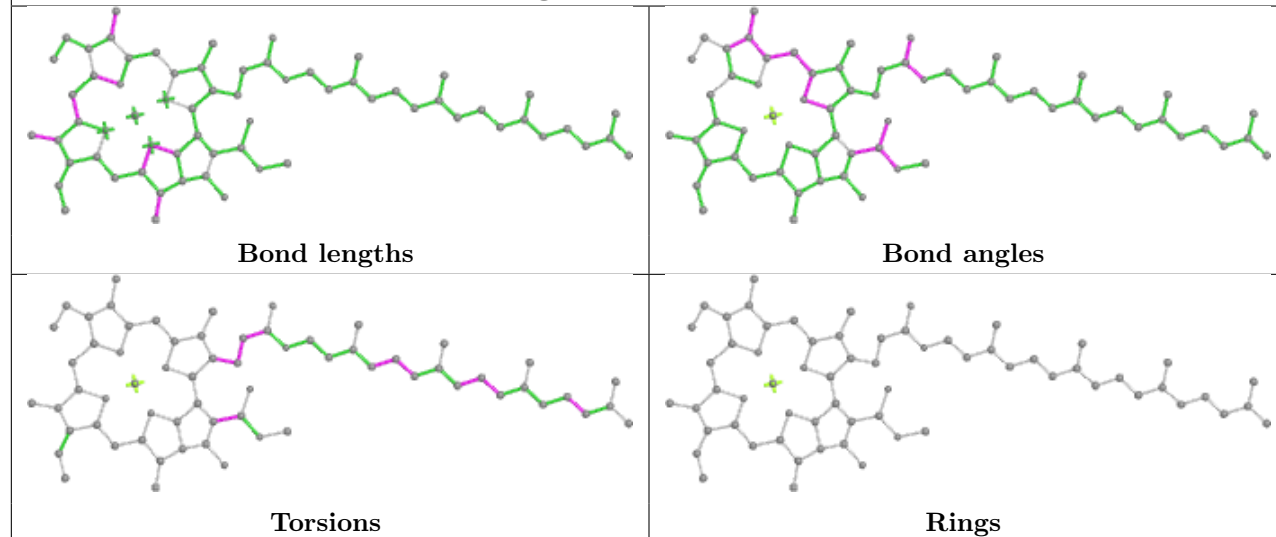
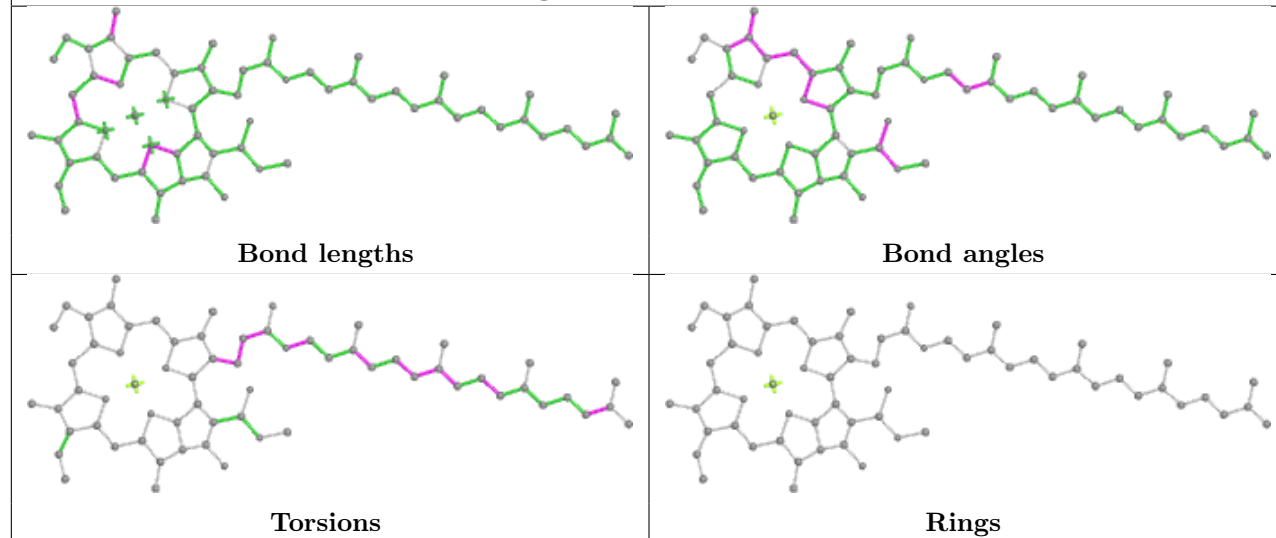


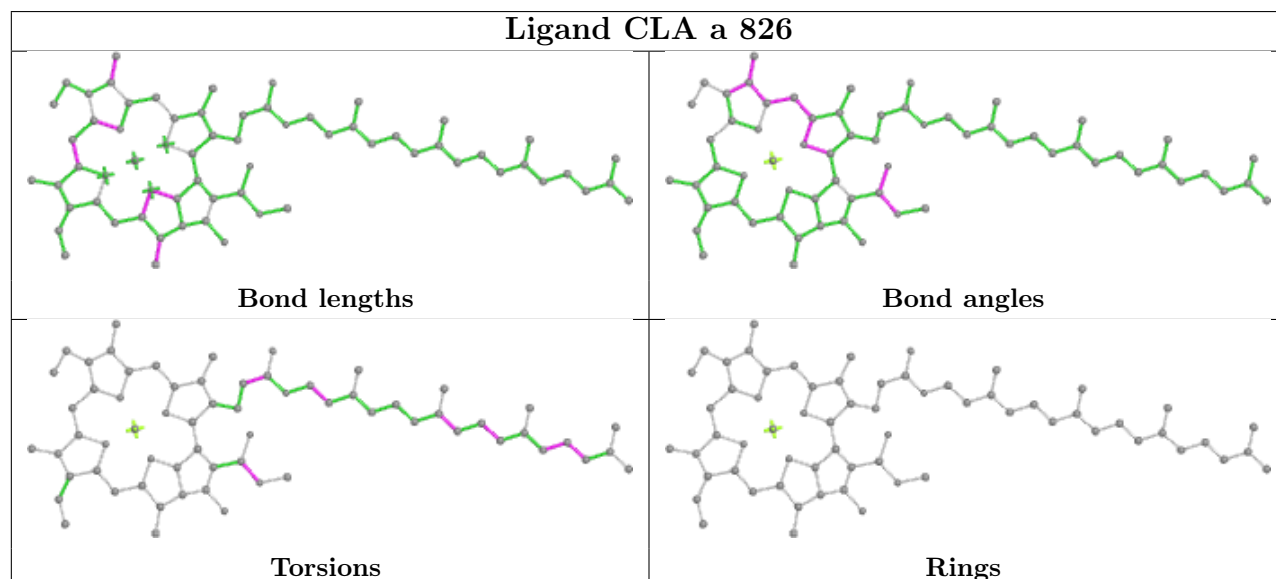
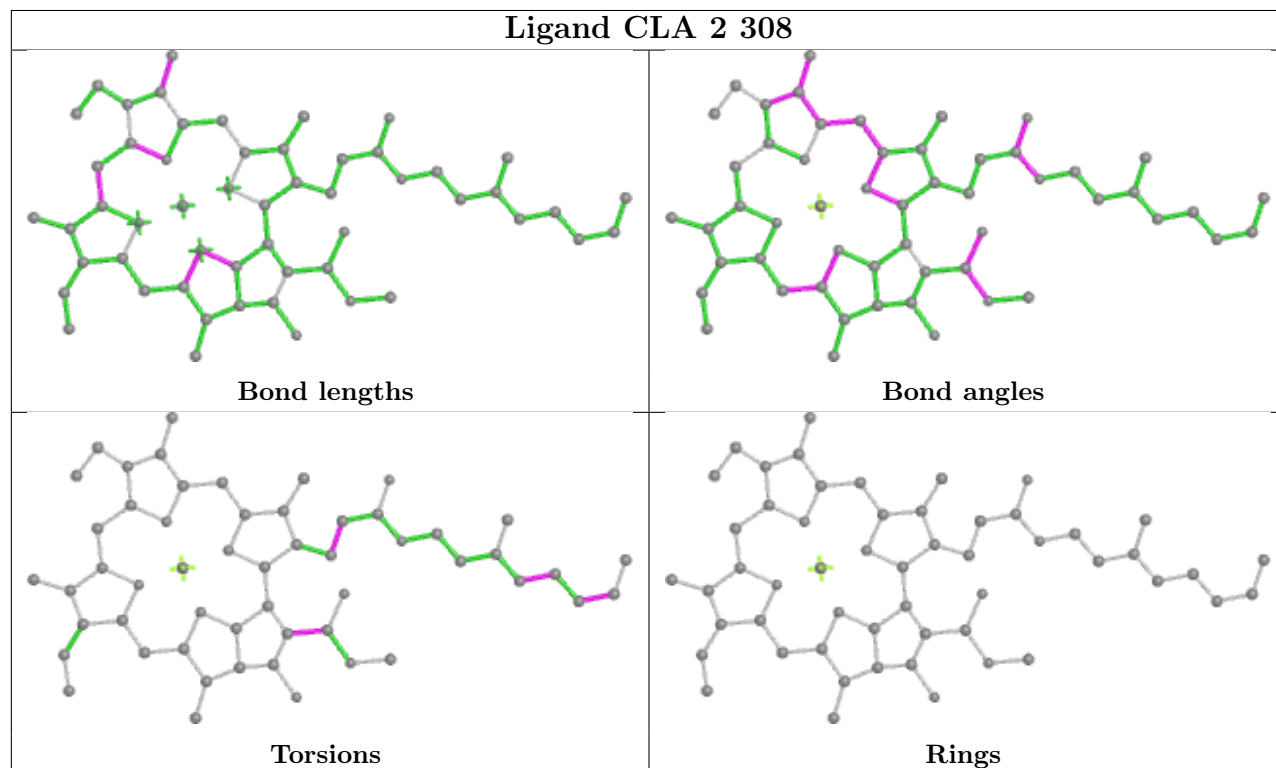
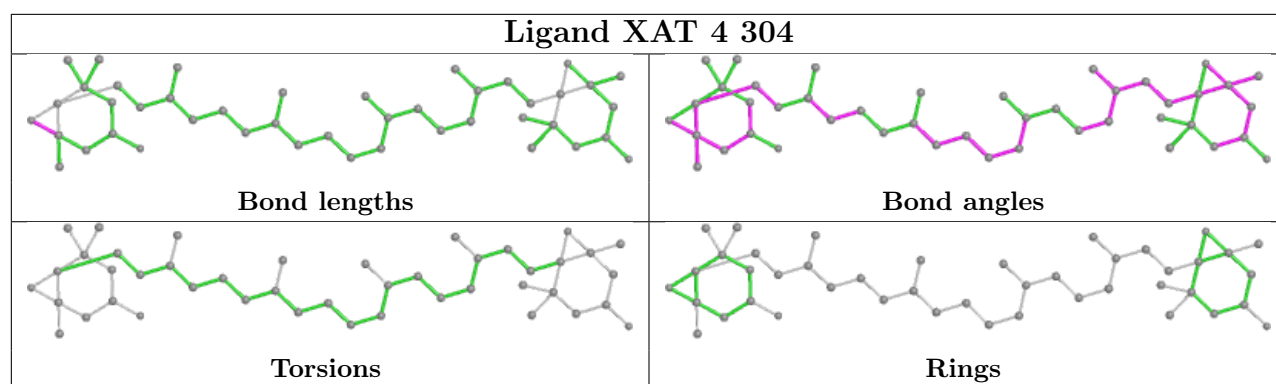
Ligand SF4 c 102



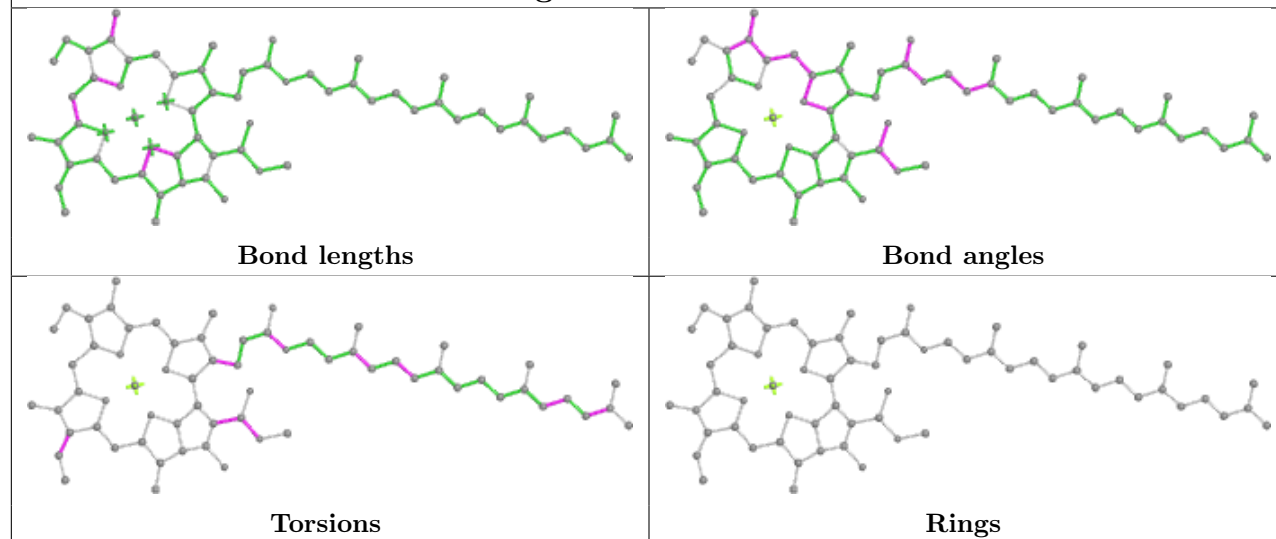
Ligand CLA a 833



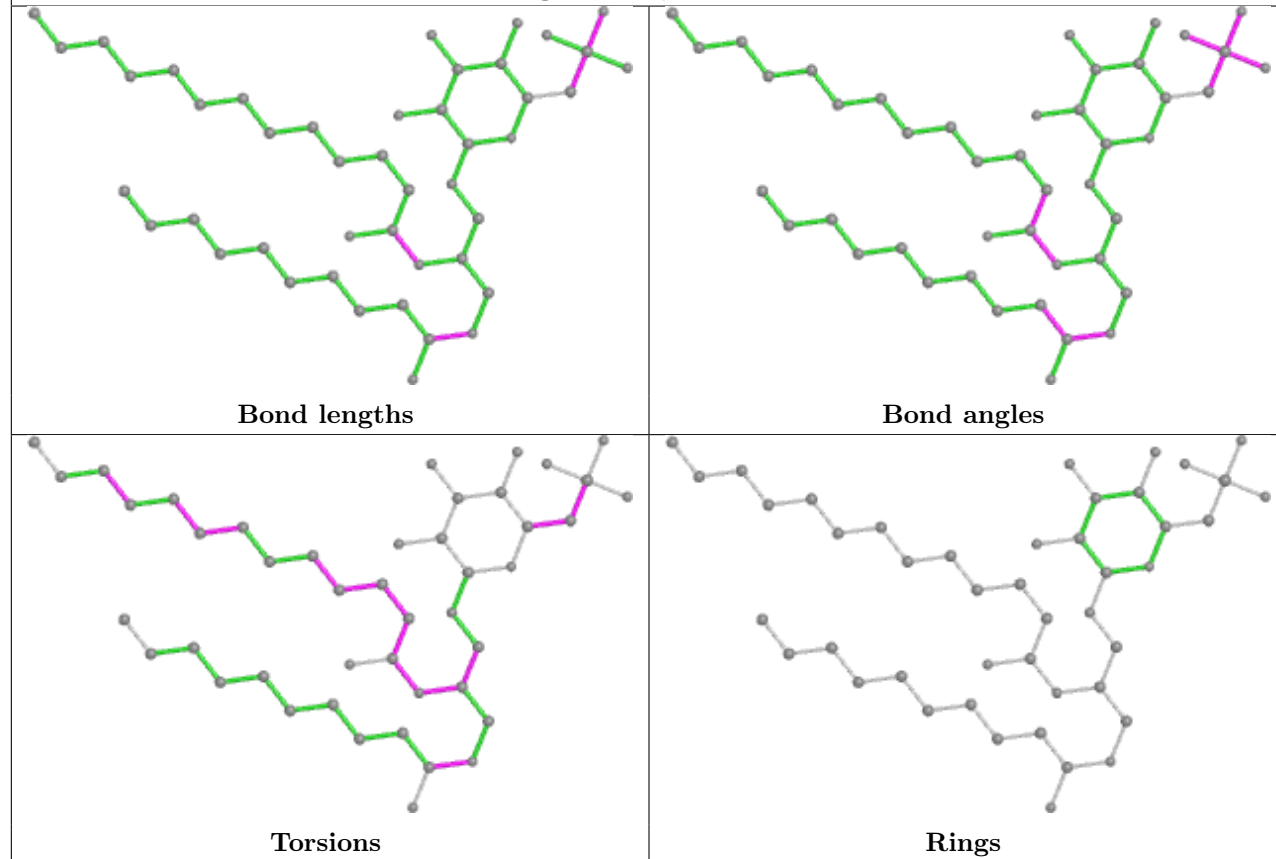
Ligand CLA 1 306**Ligand CLA b 809****Ligand CLA b 810**



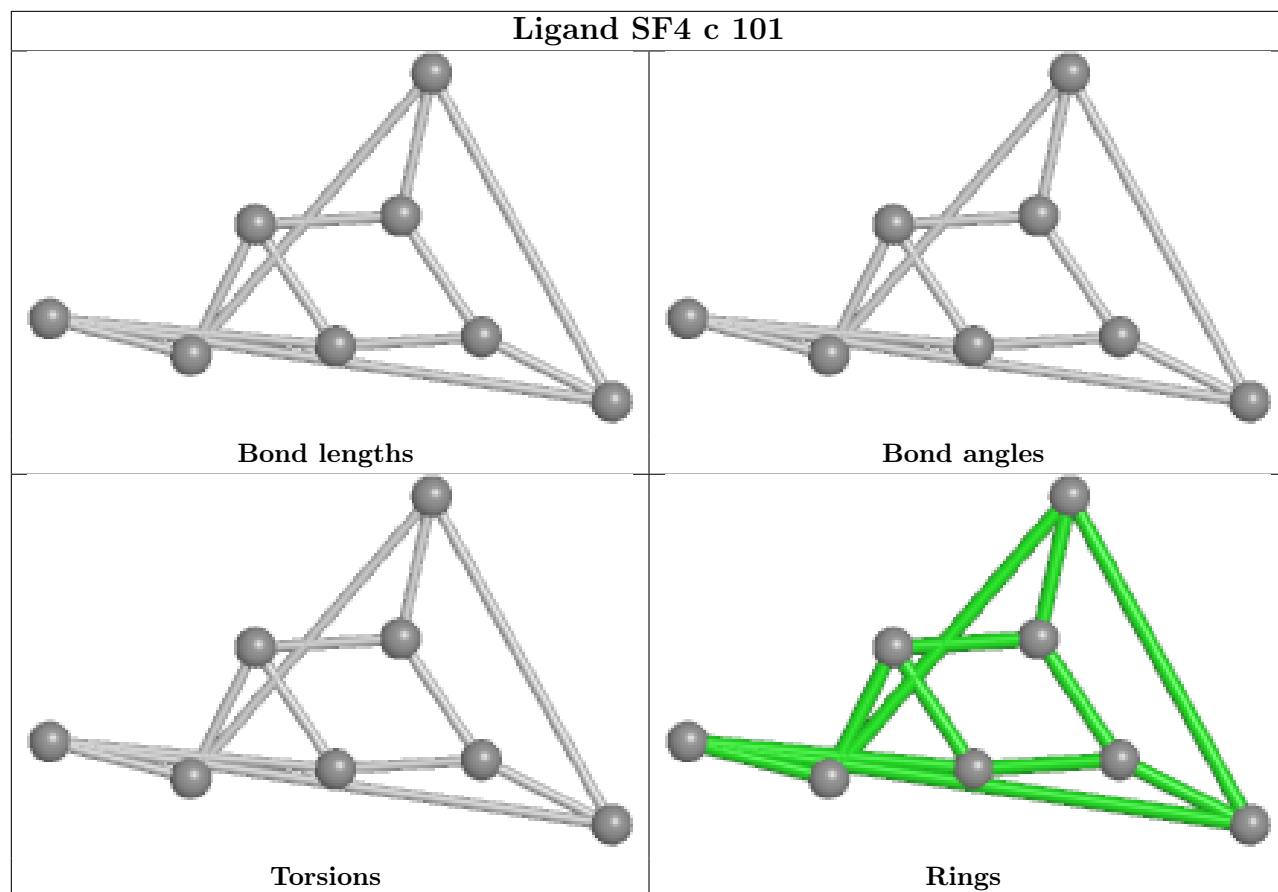
Ligand CLA b 839



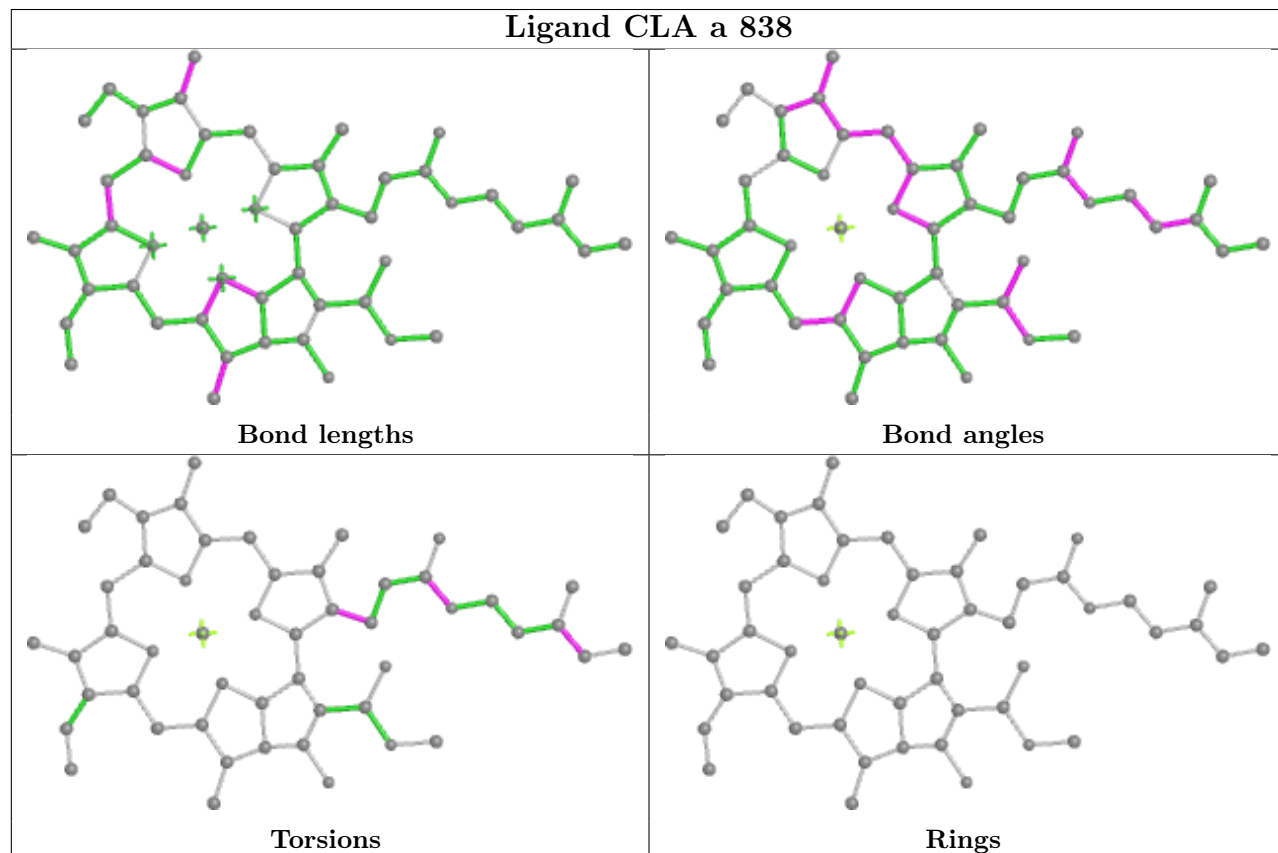
Ligand SQD 1 315

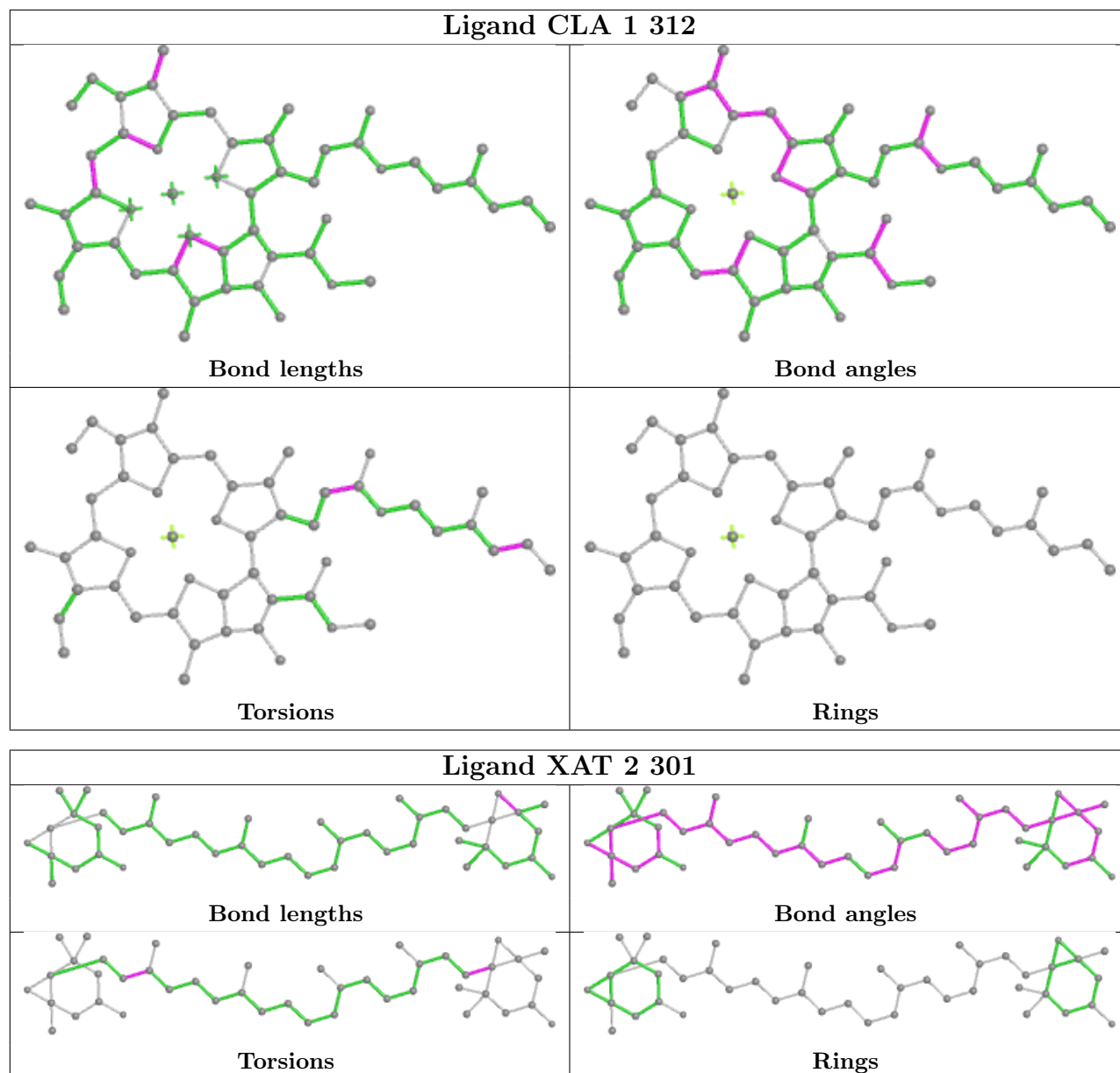


Ligand SF4 c 101

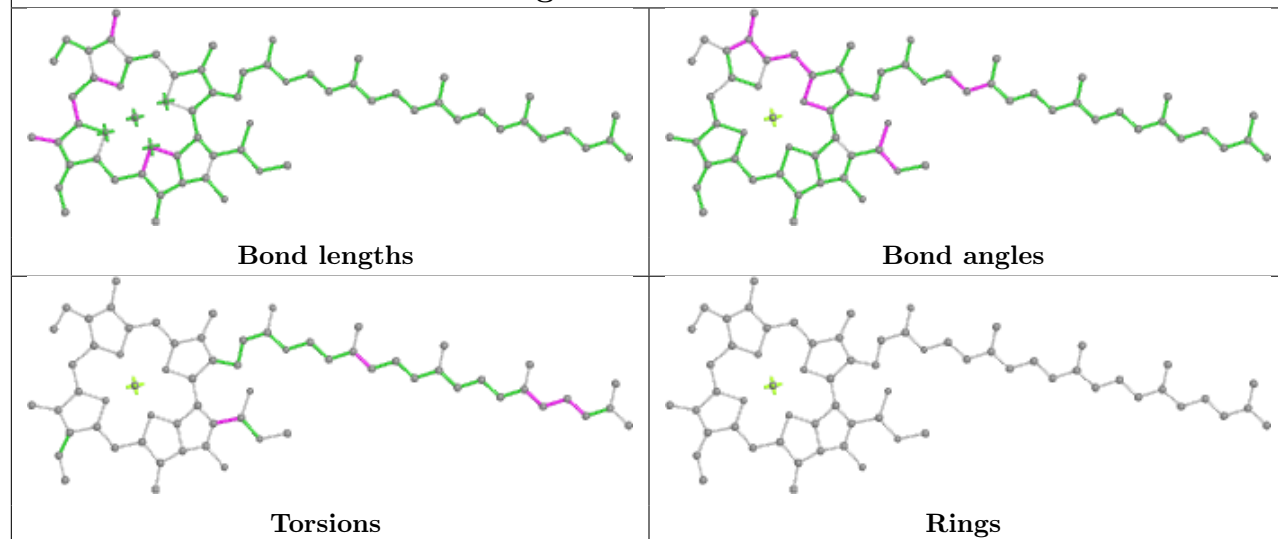


Ligand CLA a 838

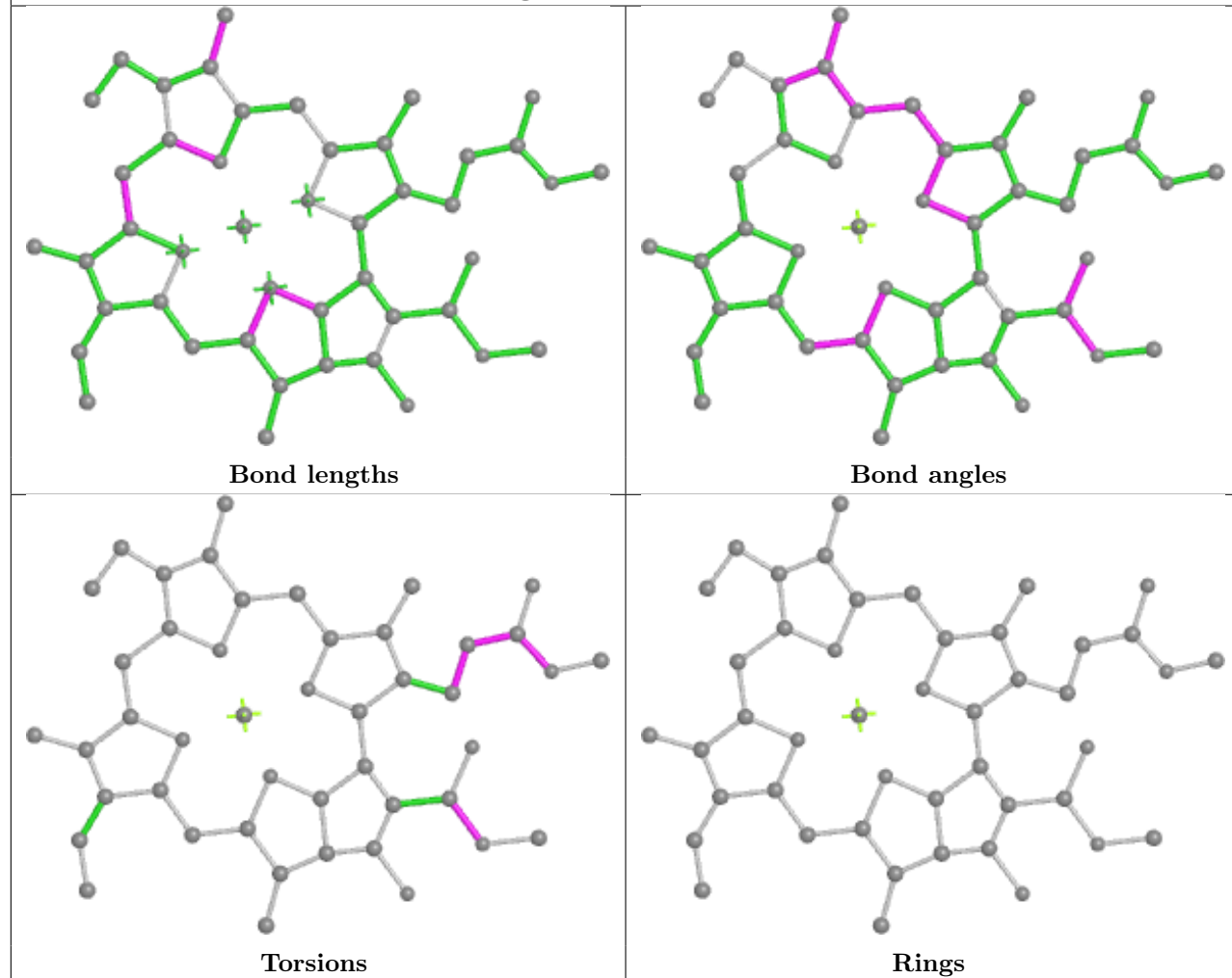




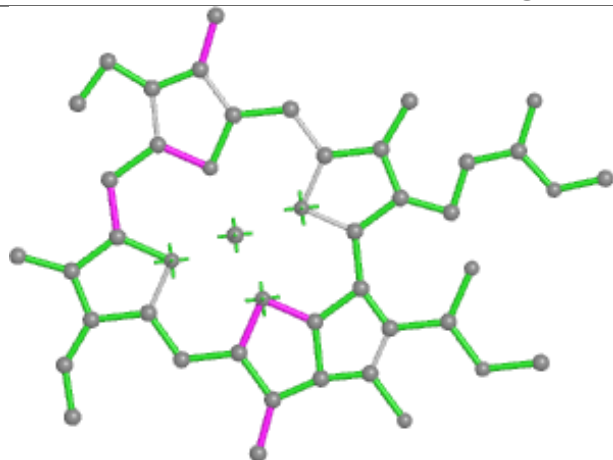
Ligand CLA a 828



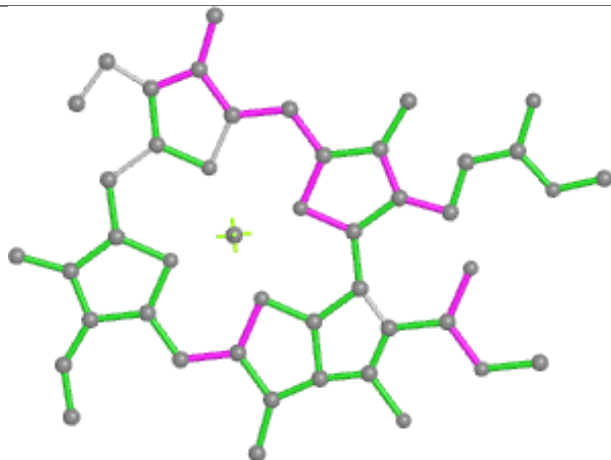
Ligand CLA 5 310



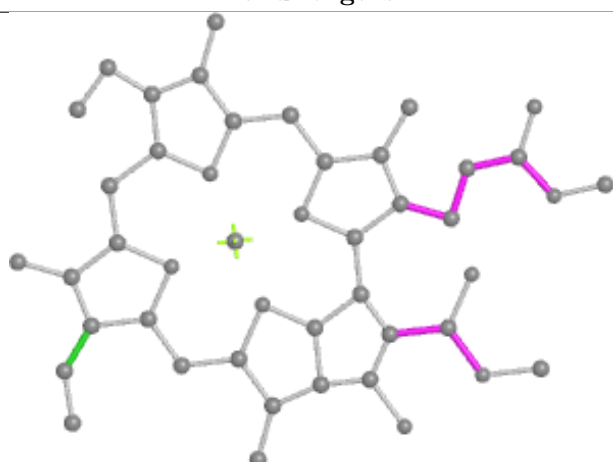
Ligand CLA 9 312



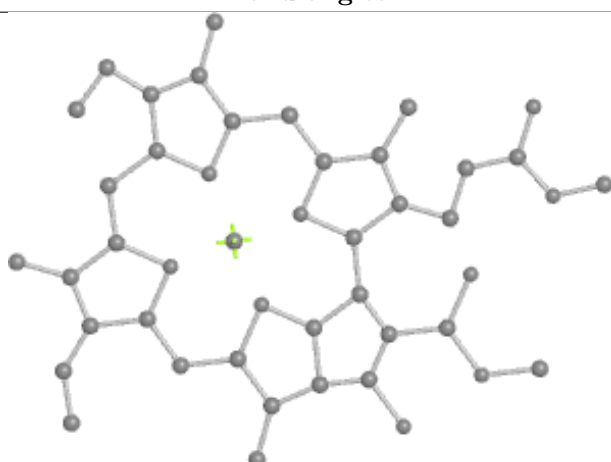
Bond lengths



Bond angles

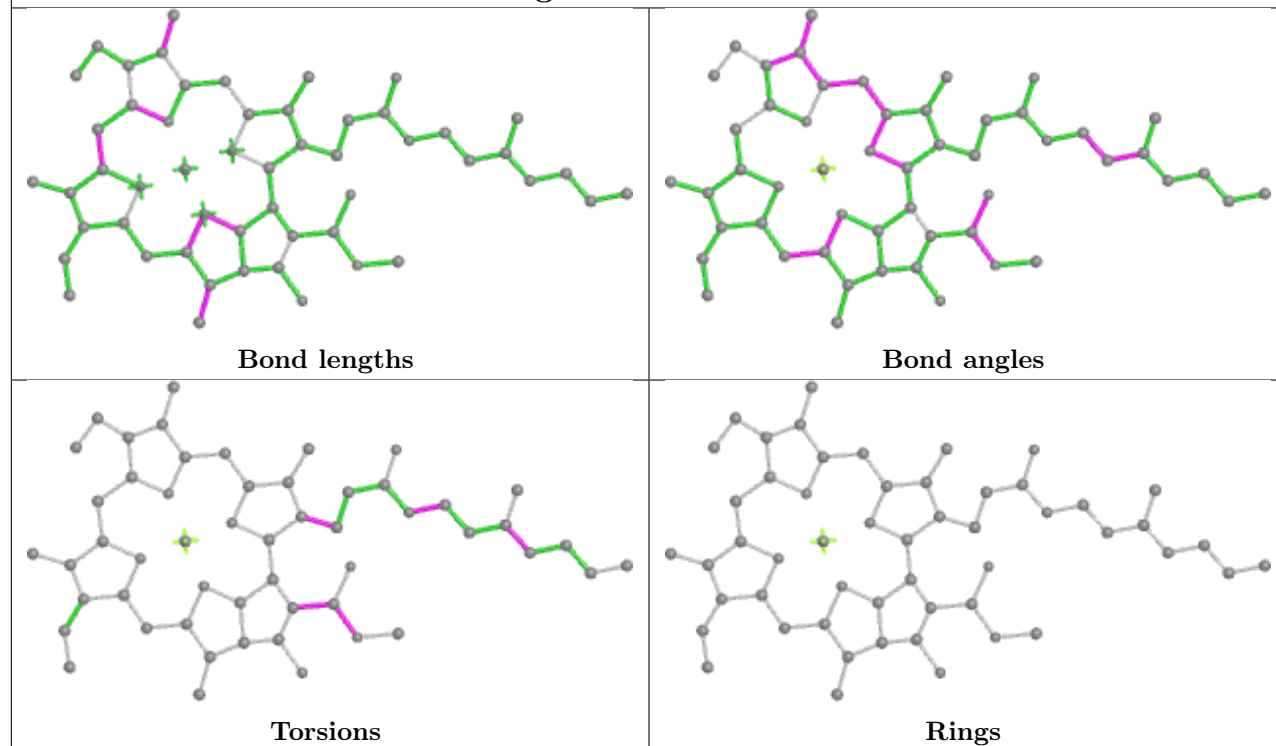


Torsions

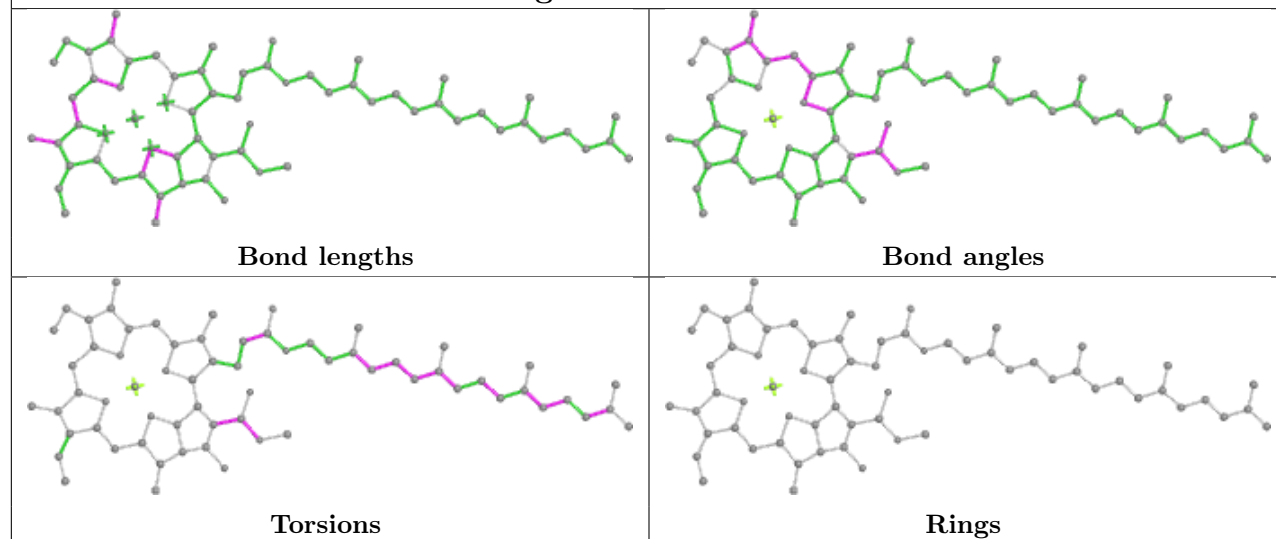


Rings

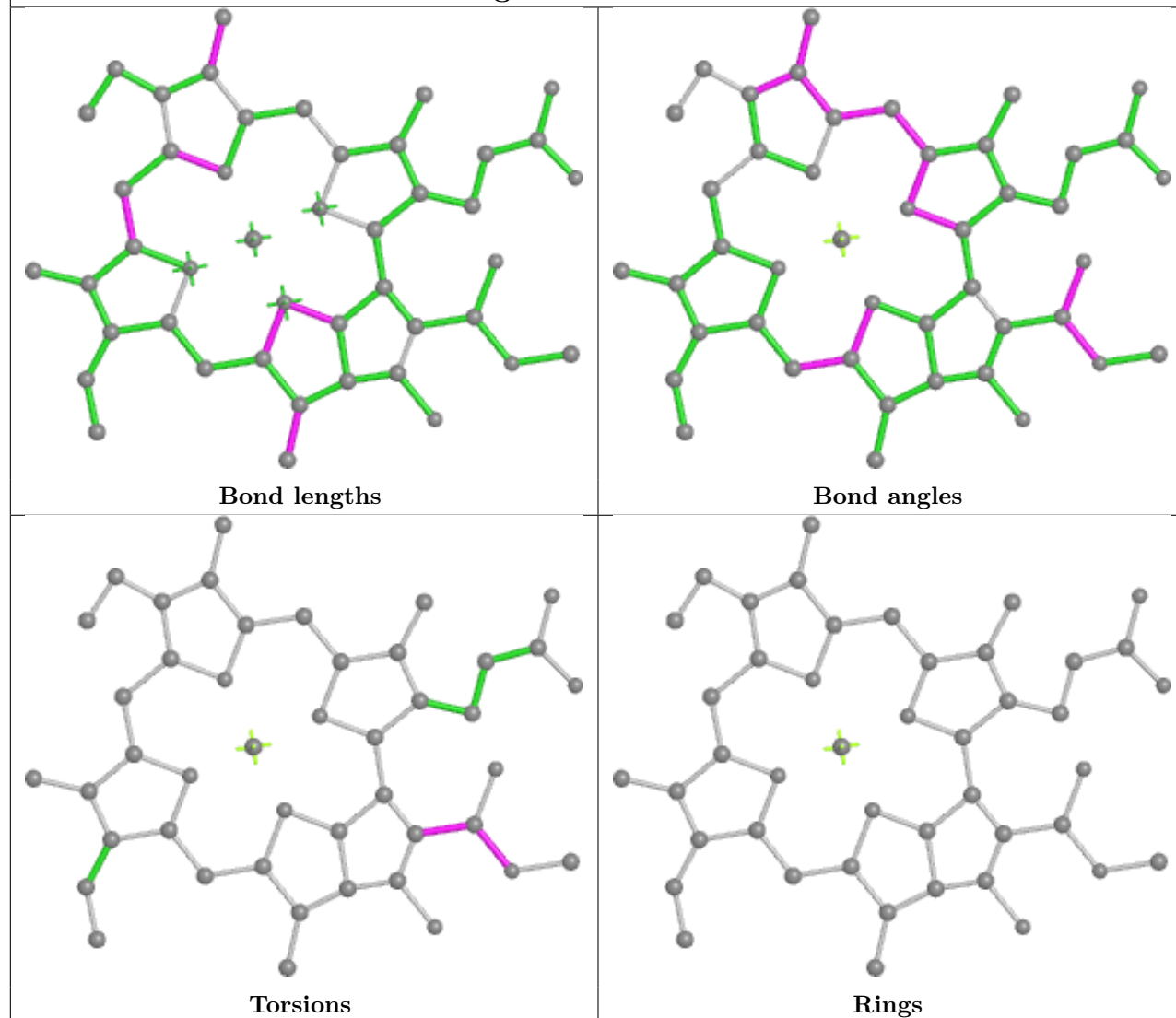
Ligand CLA b 834



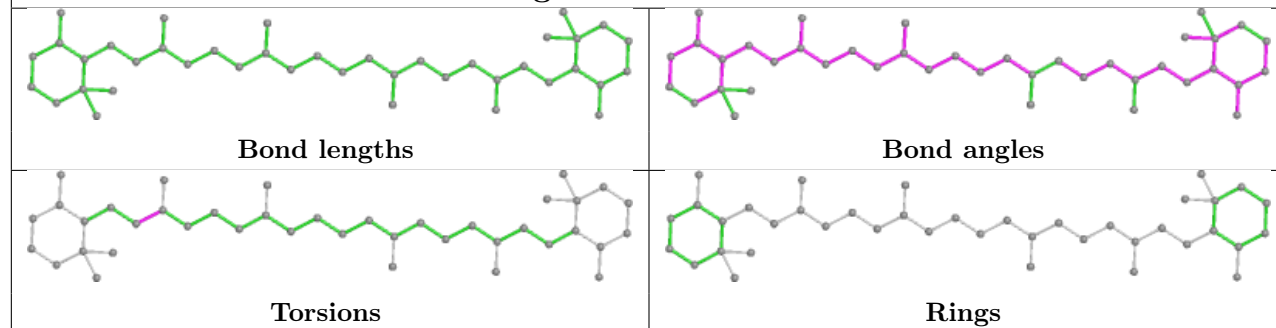
Ligand CLA b 803

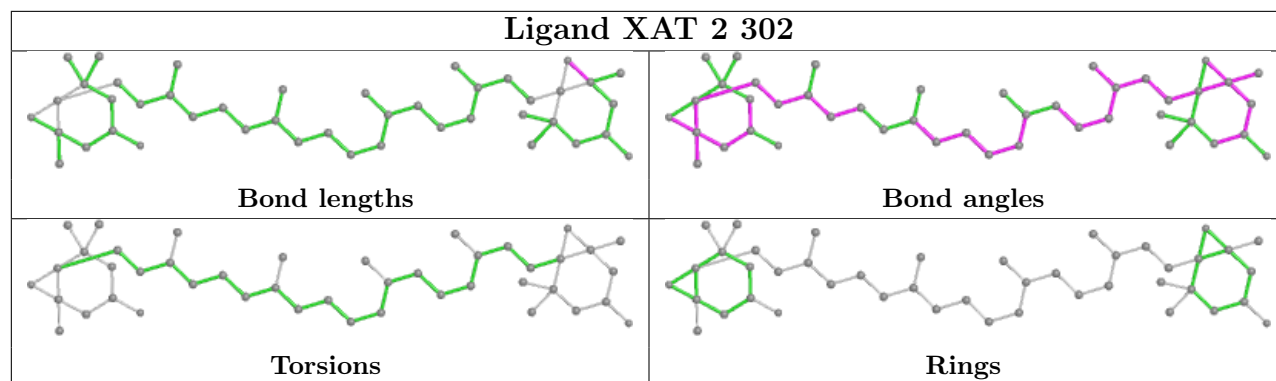
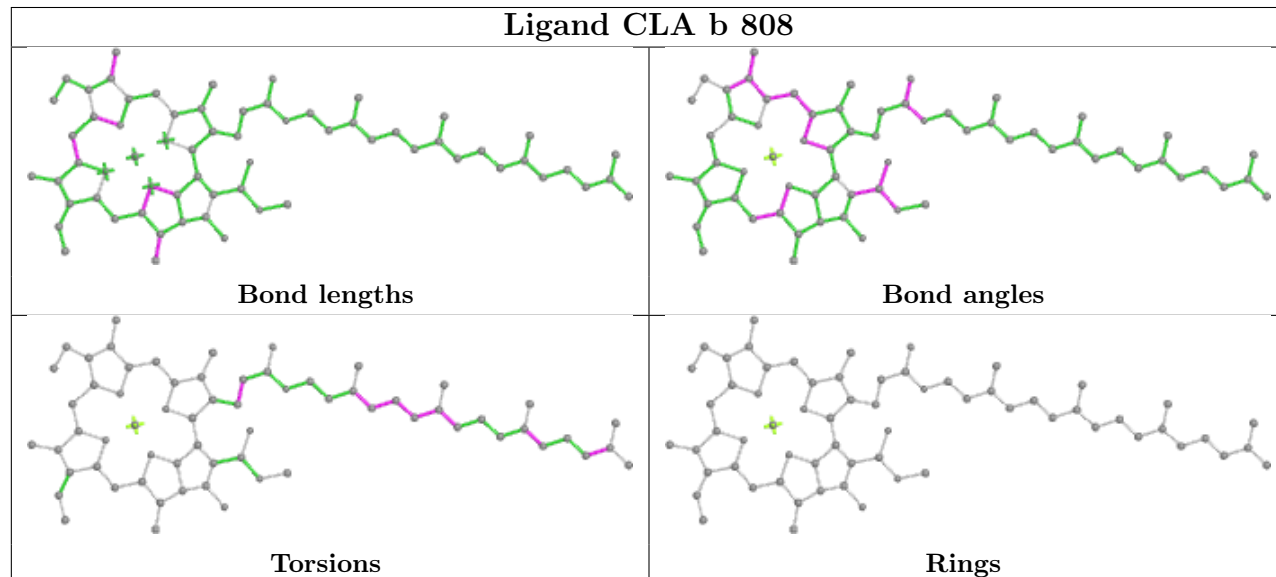
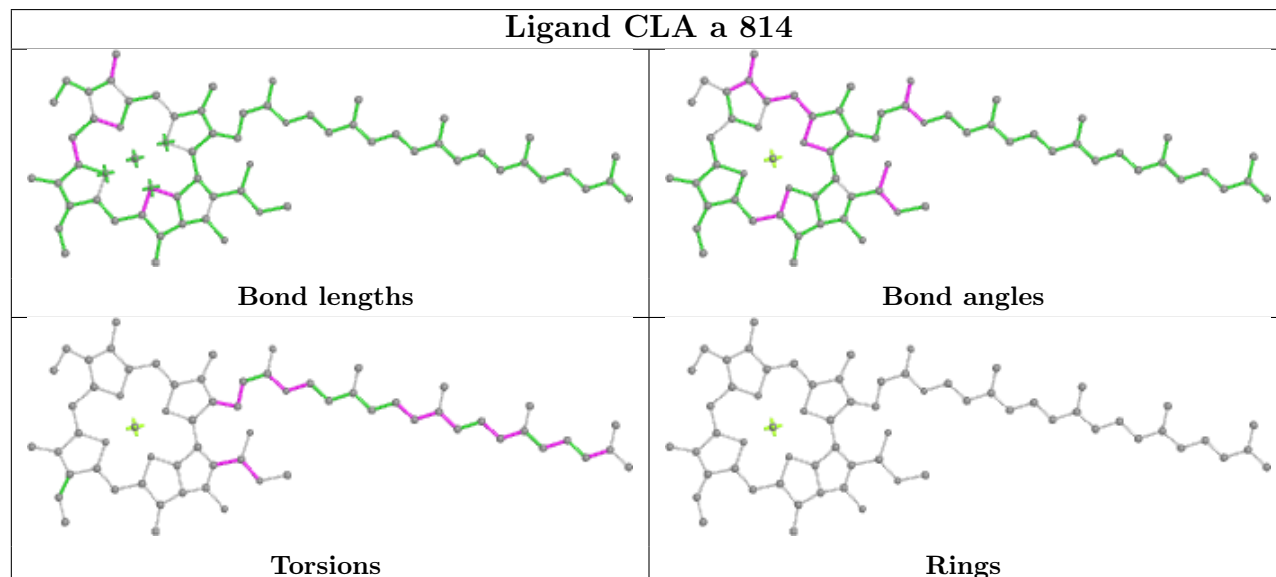


Ligand CLA a 837

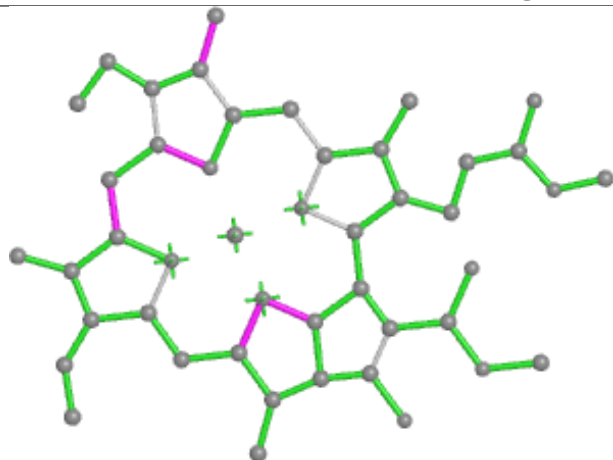


Ligand BCR b 845

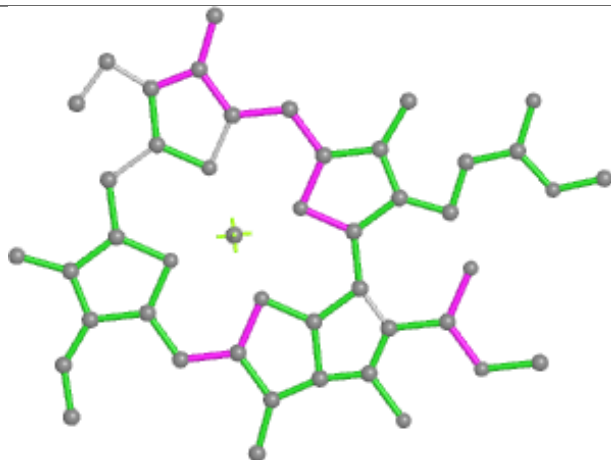


Ligand XAT 2 302**Ligand CLA b 808****Ligand CLA a 814**

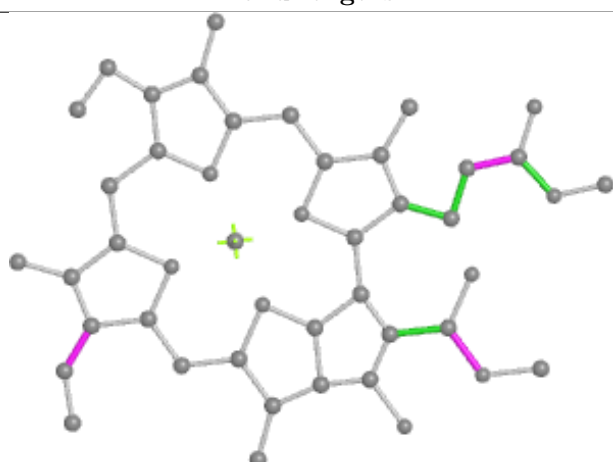
Ligand CLA 5 315



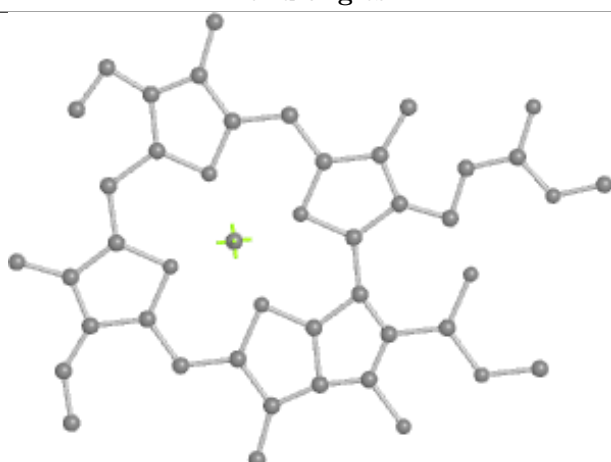
Bond lengths



Bond angles

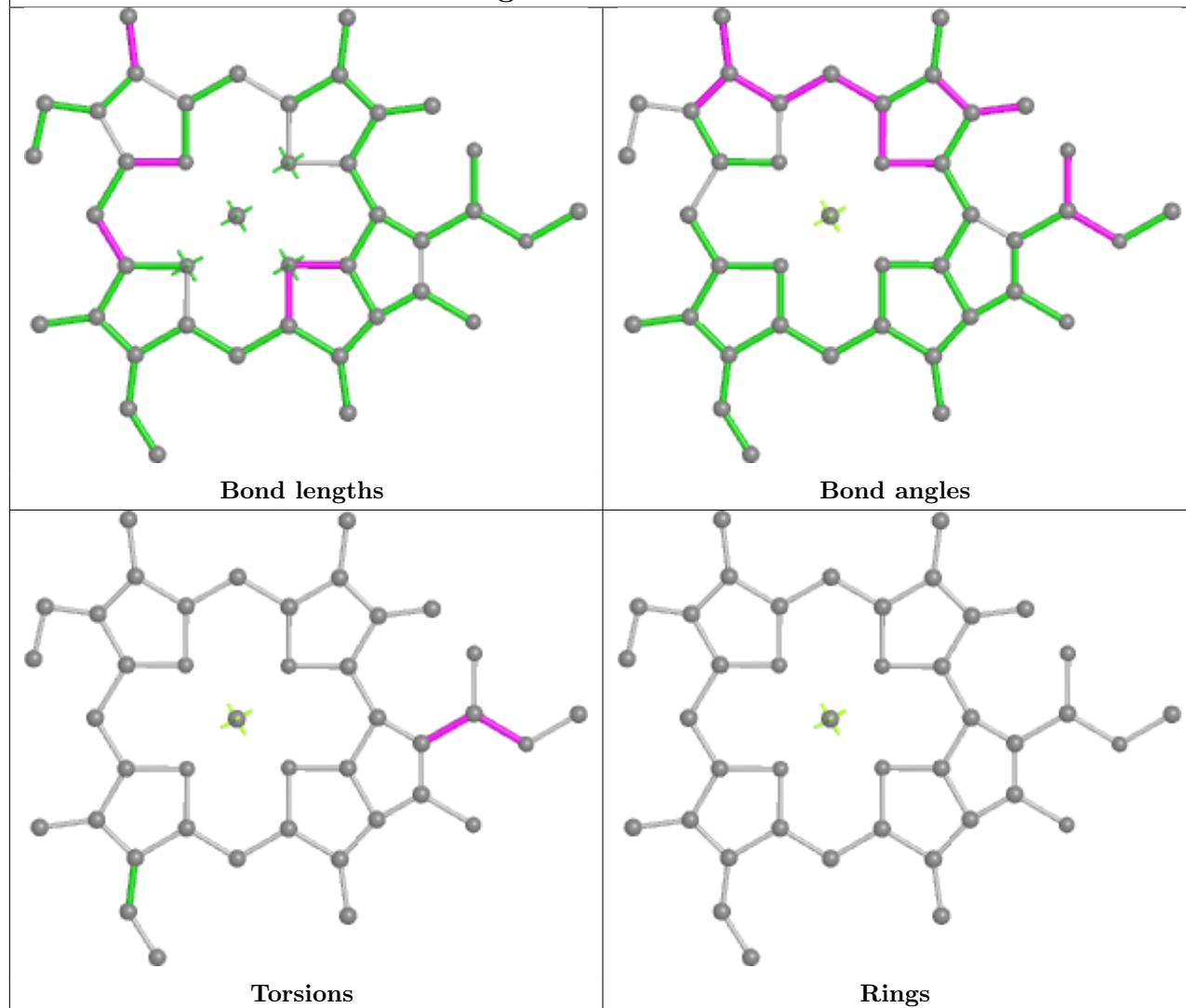


Torsions

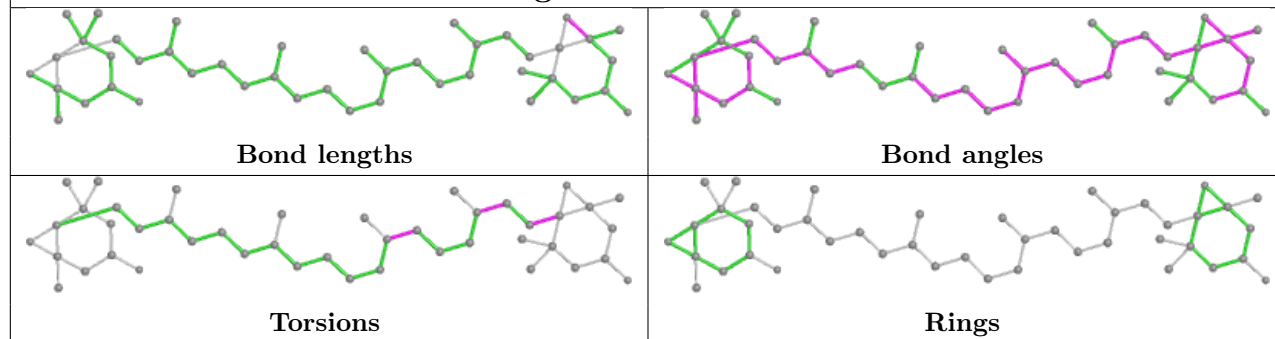


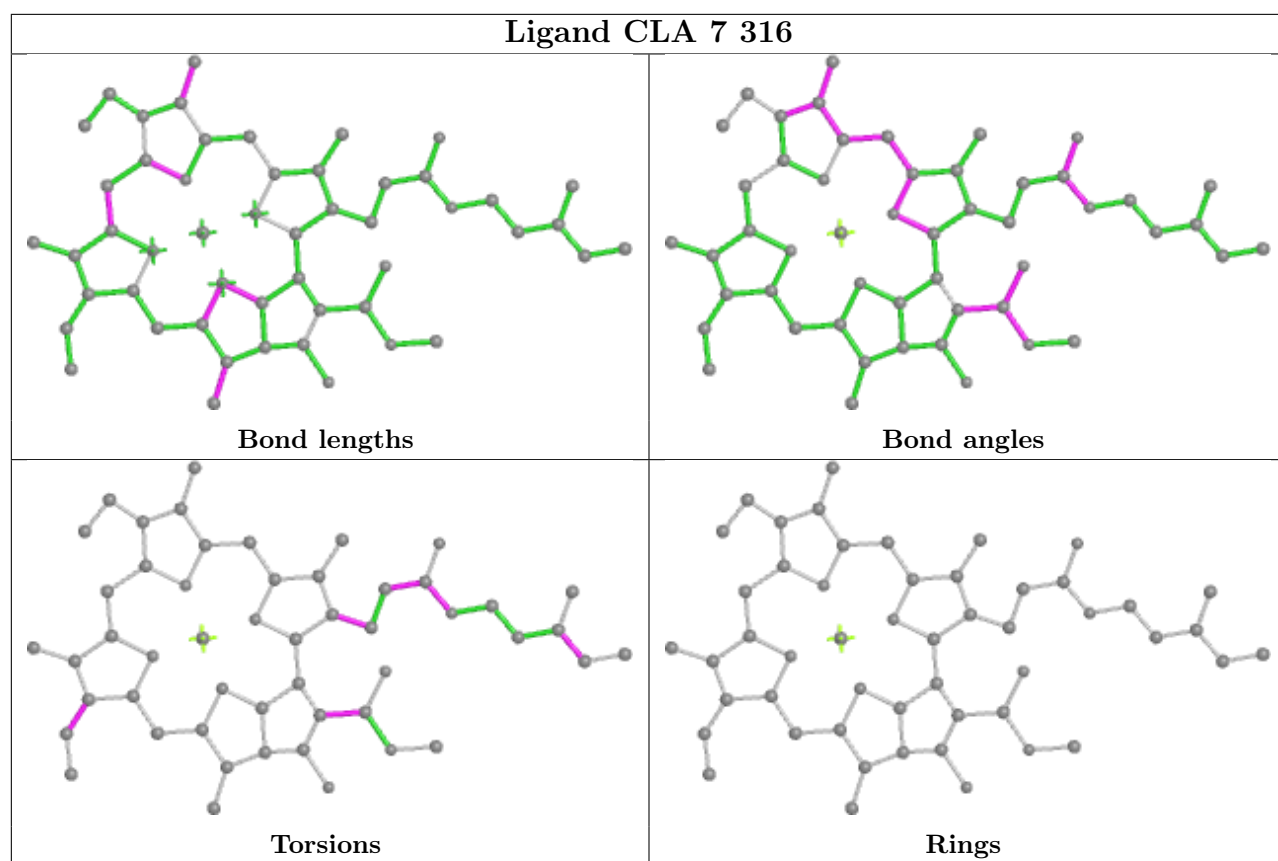
Rings

Ligand CLA 7 315

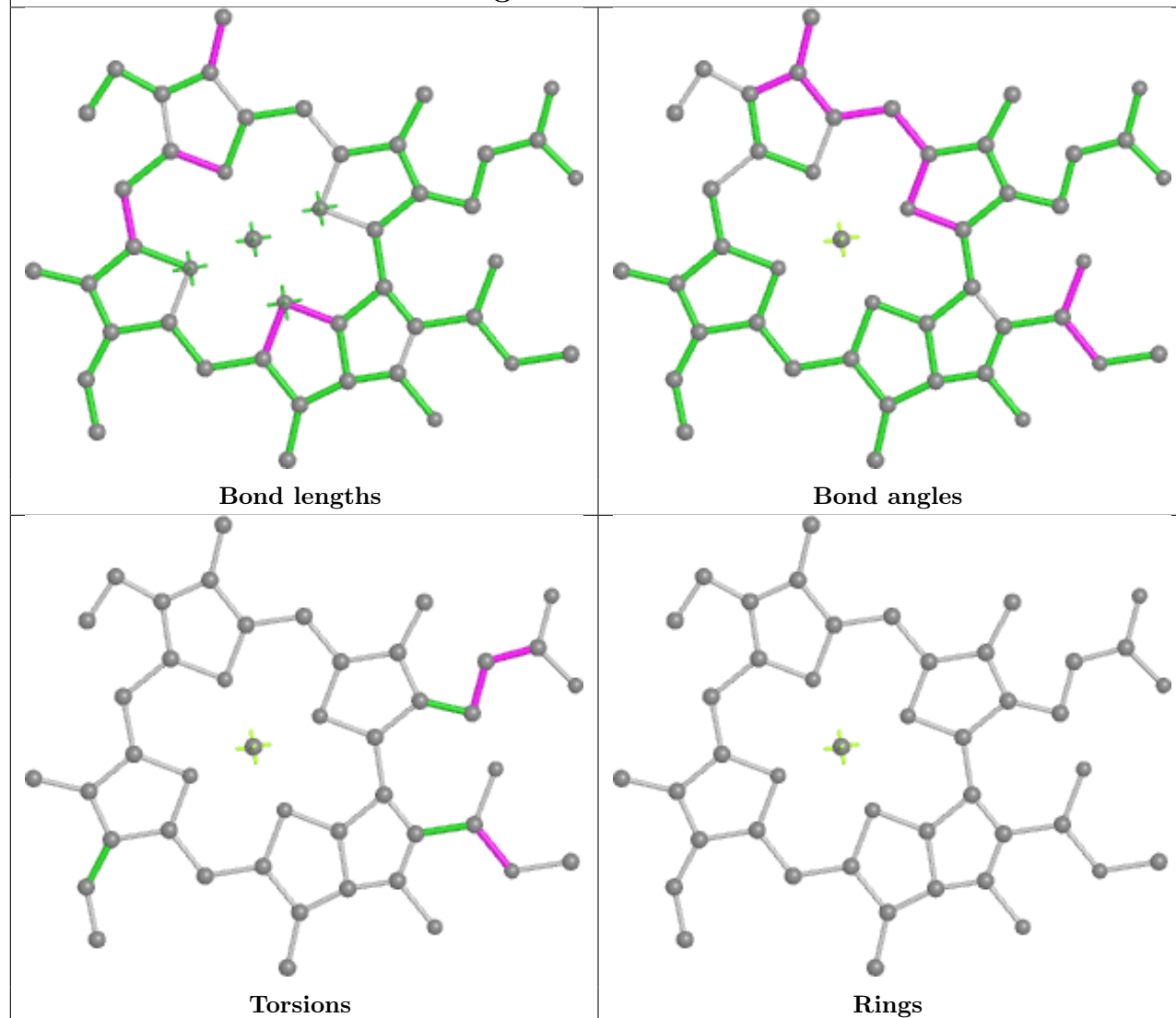


Ligand XAT 6 303

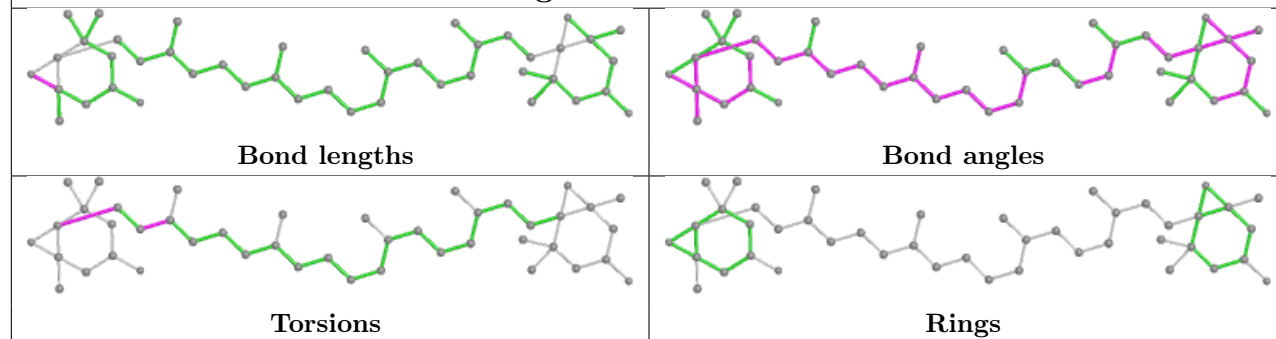


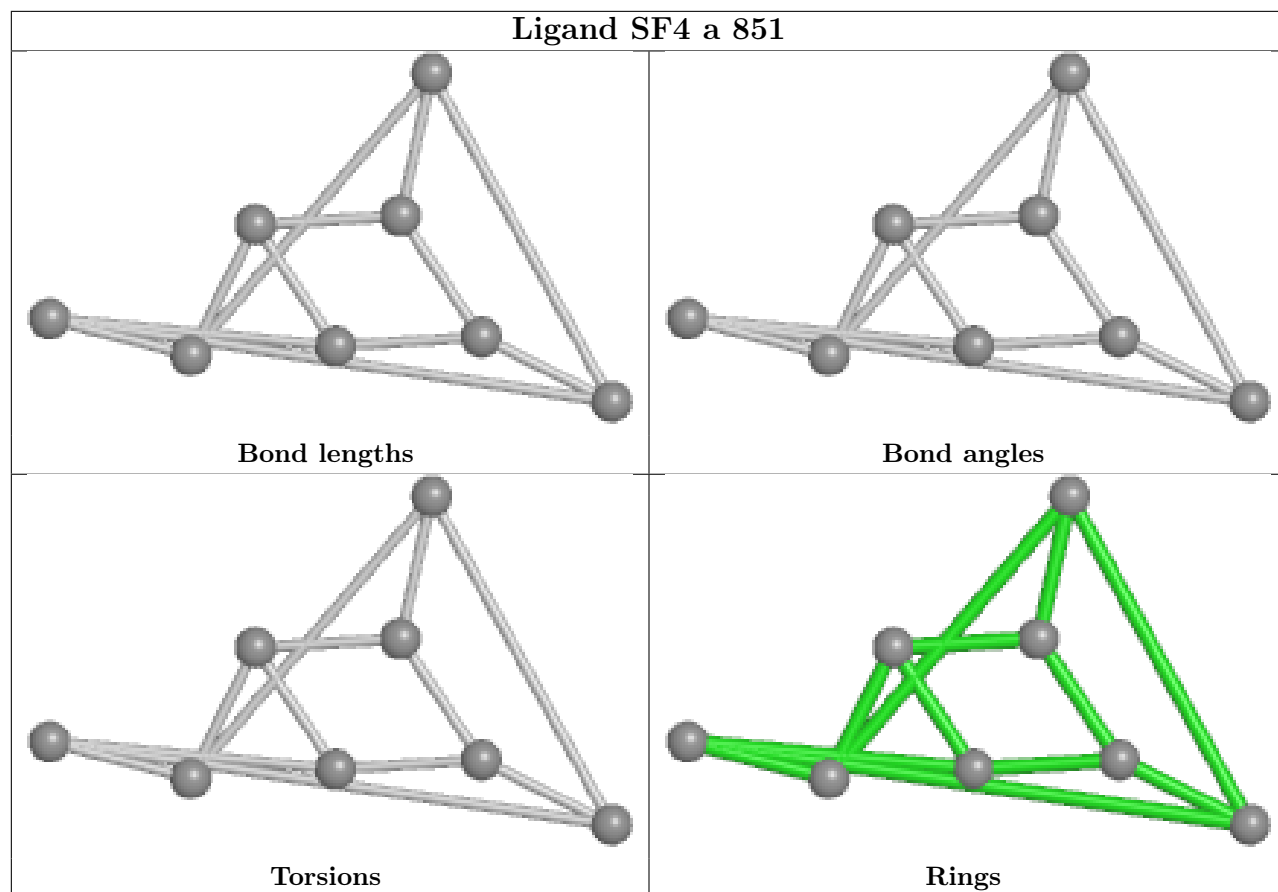


Ligand CLA 7 317

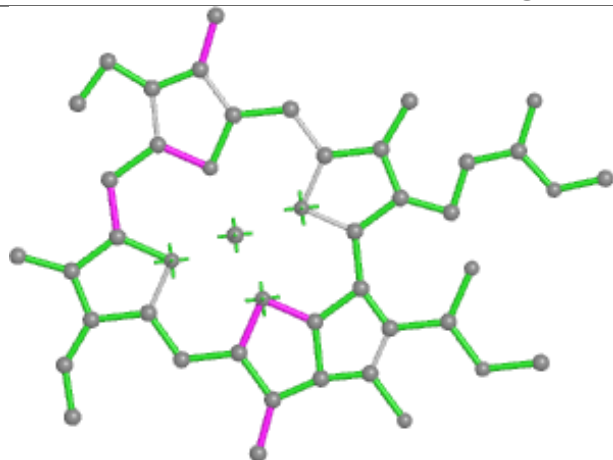


Ligand XAT 3 304

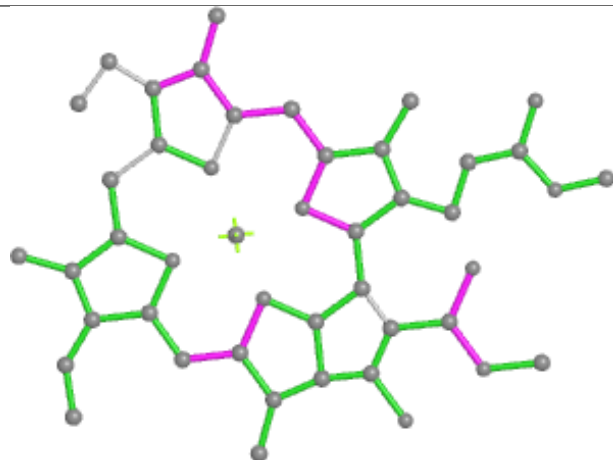




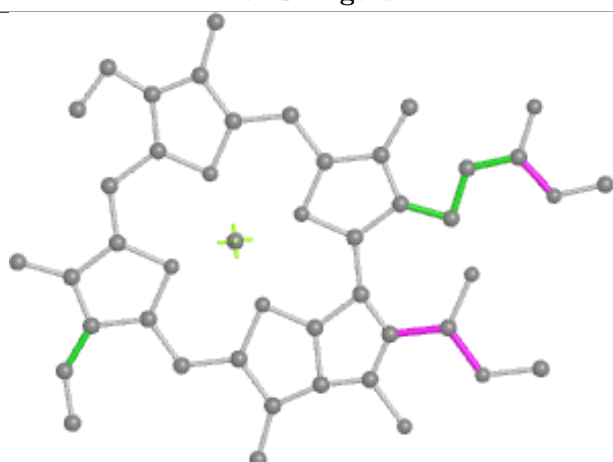
Ligand CLA 8 310



Bond lengths



Bond angles

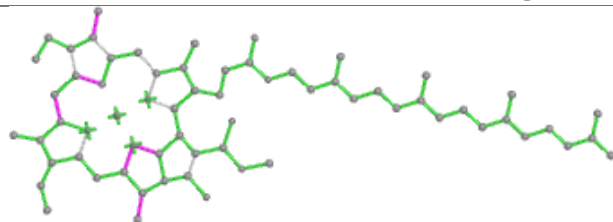


Torsions

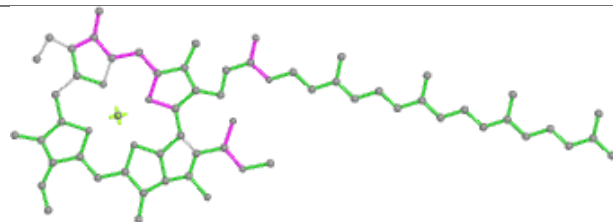


Rings

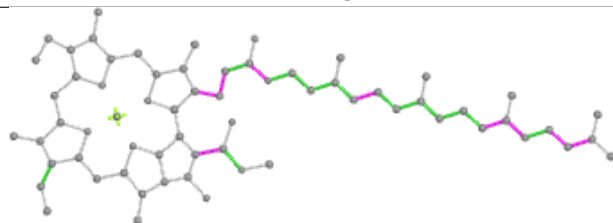
Ligand CLA 2 310



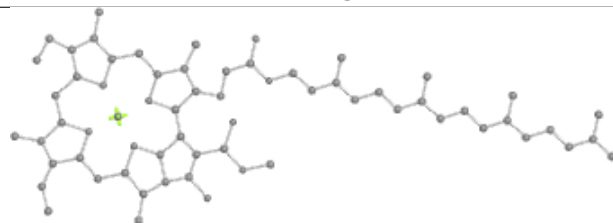
Bond lengths



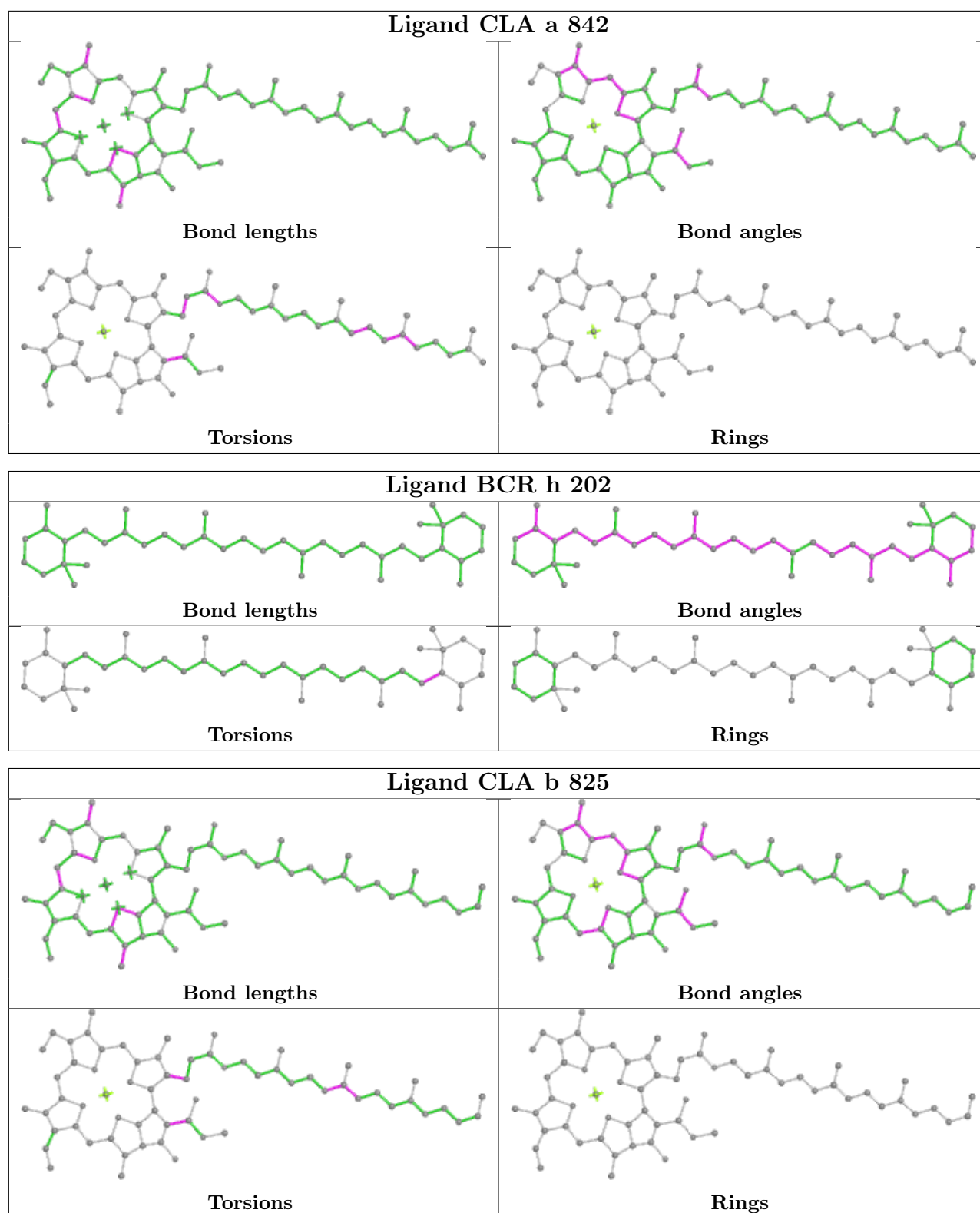
Bond angles



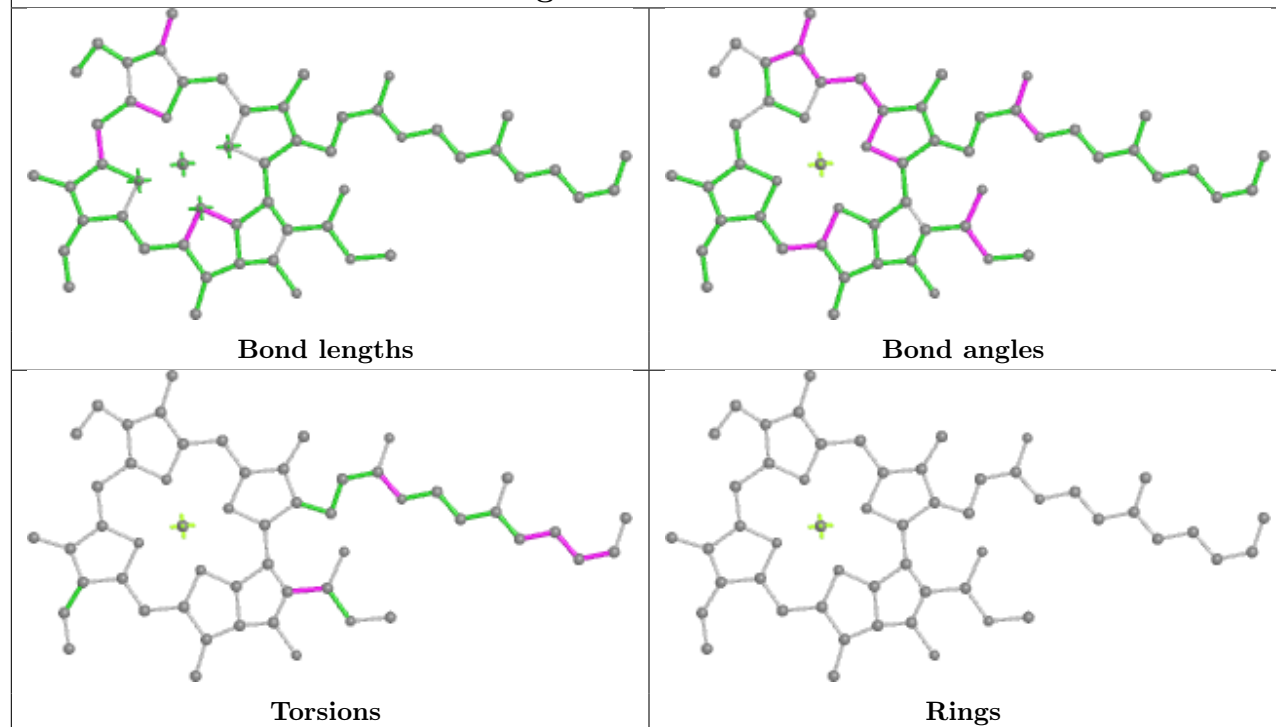
Torsions



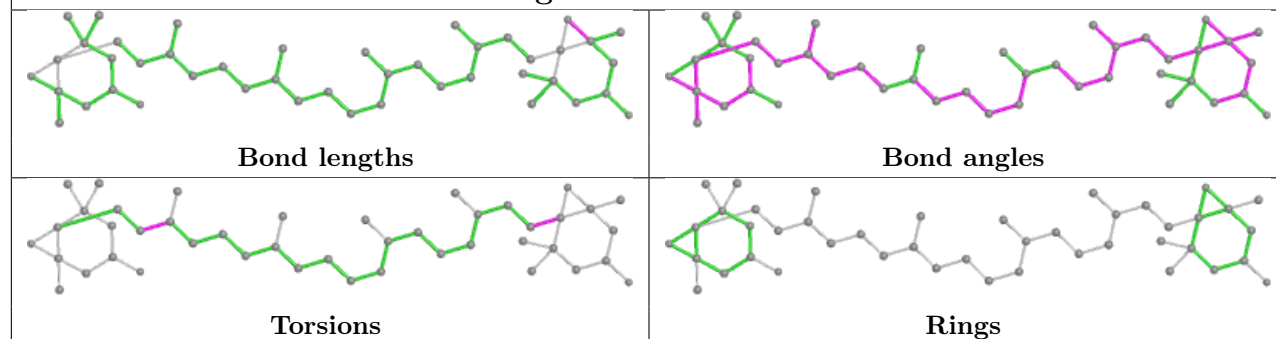
Rings



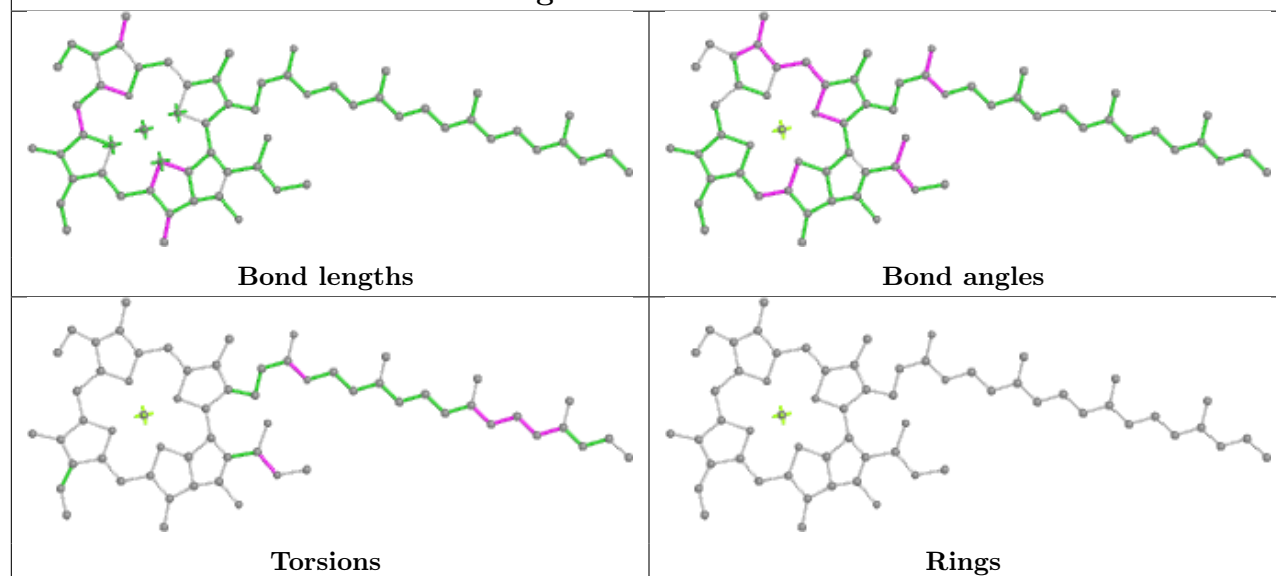
Ligand CLA 1 307



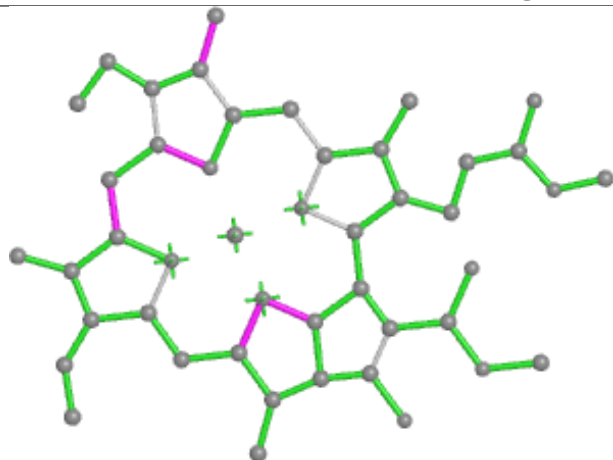
Ligand XAT 3 303



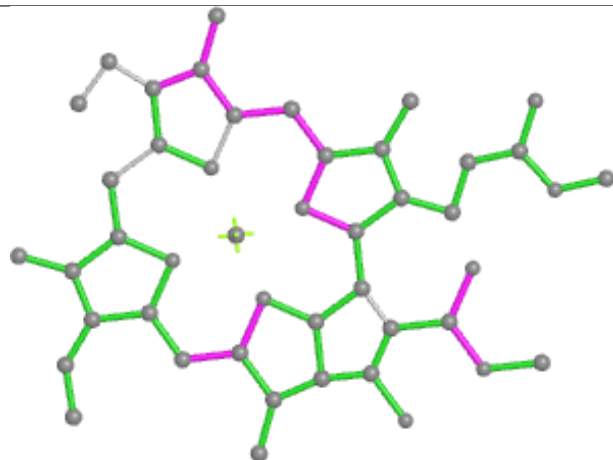
Ligand CLA 9 318



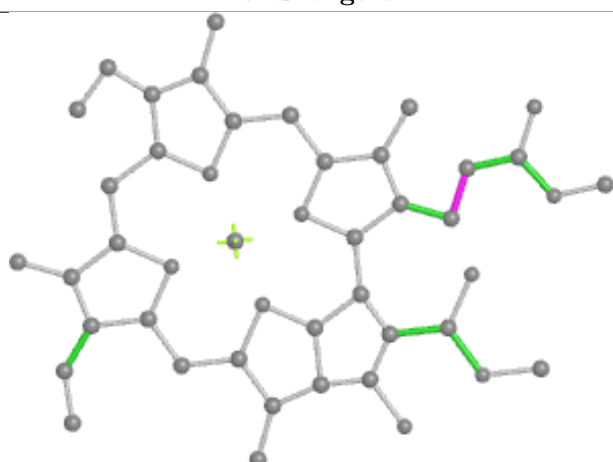
Ligand CLA 6 307



Bond lengths



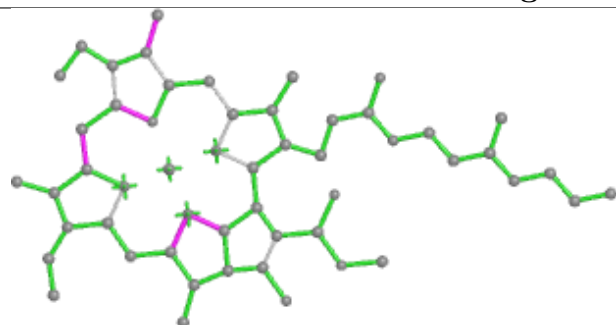
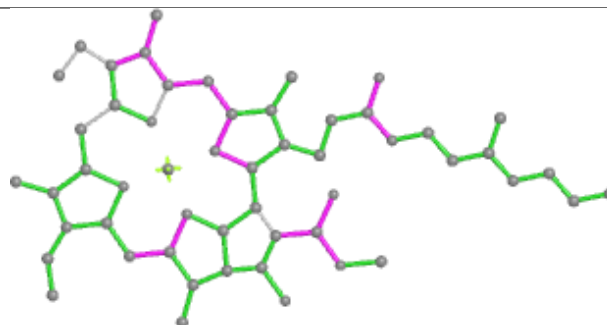
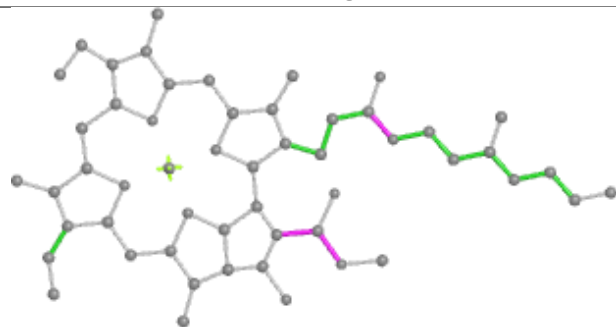
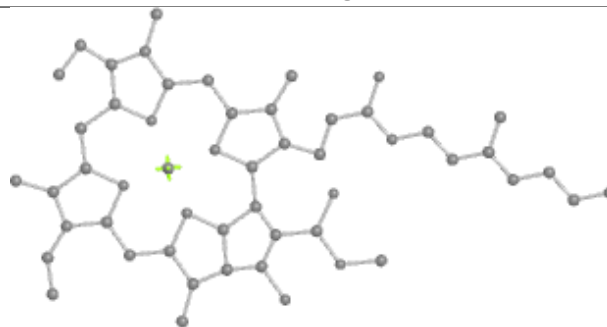
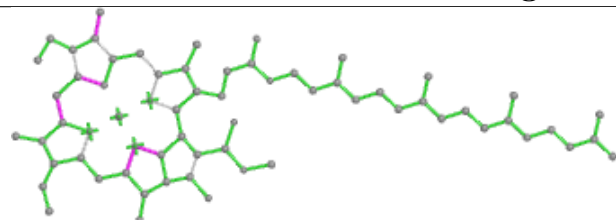
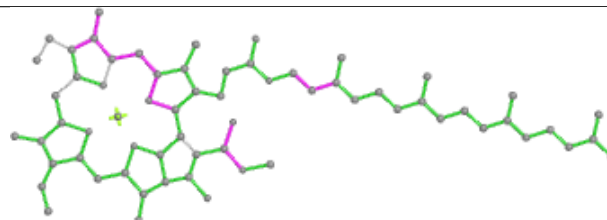
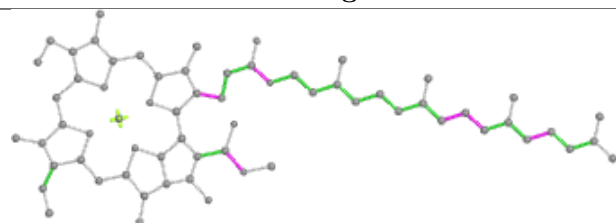
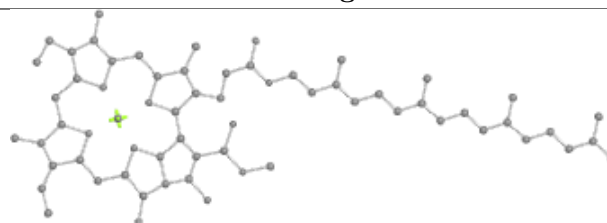
Bond angles

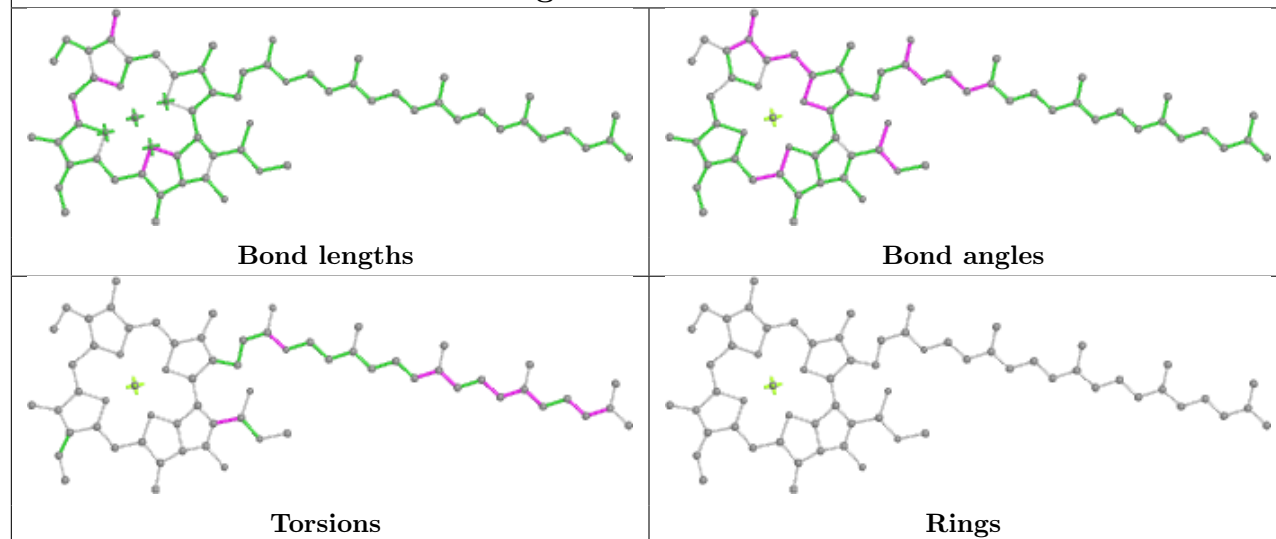
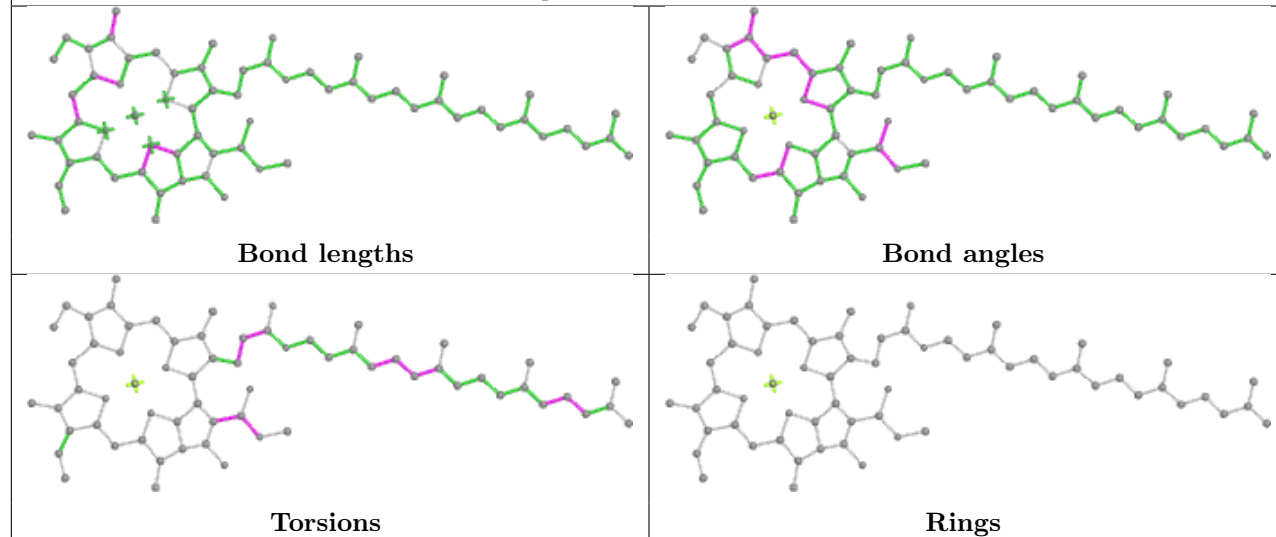


Torsions

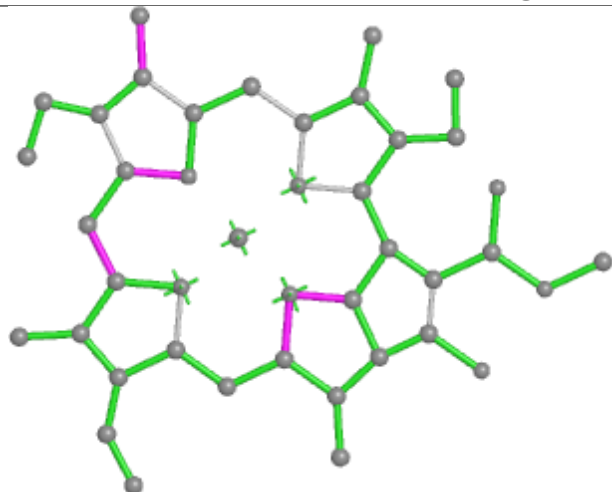


Rings

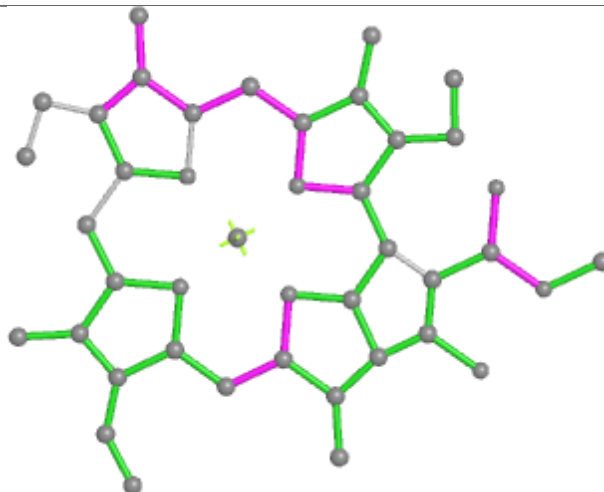
Ligand CLA 1 311**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 6 317****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA a 844**Ligand CLA 5 309**

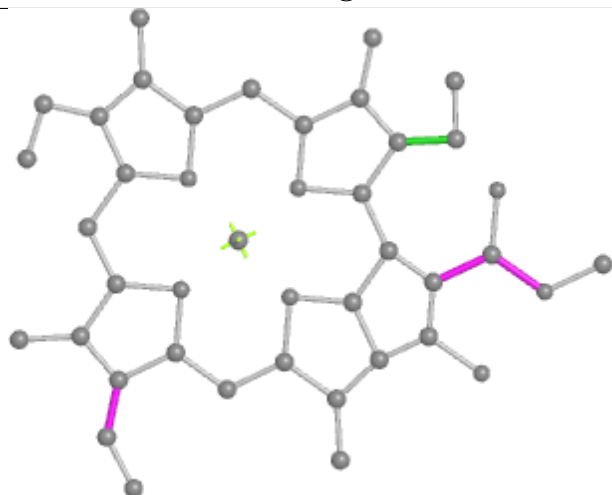
Ligand CLA 9 315



Bond lengths



Bond angles

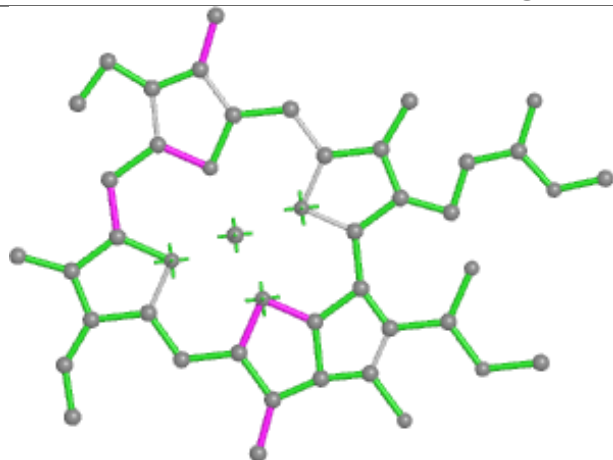


Torsions

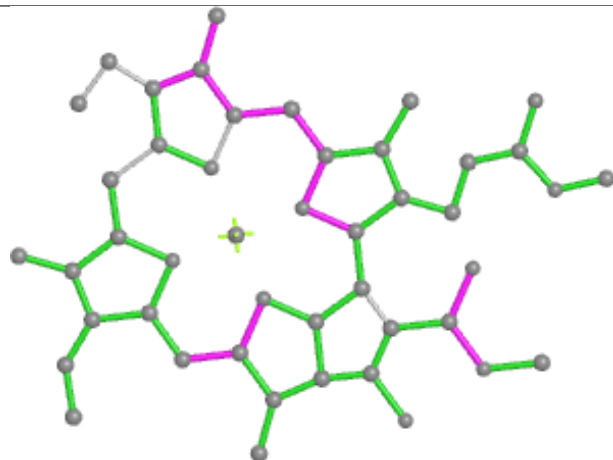


Rings

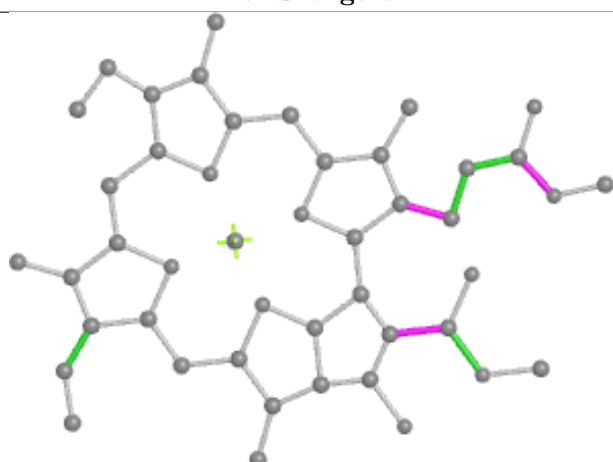
Ligand CLA a 824



Bond lengths



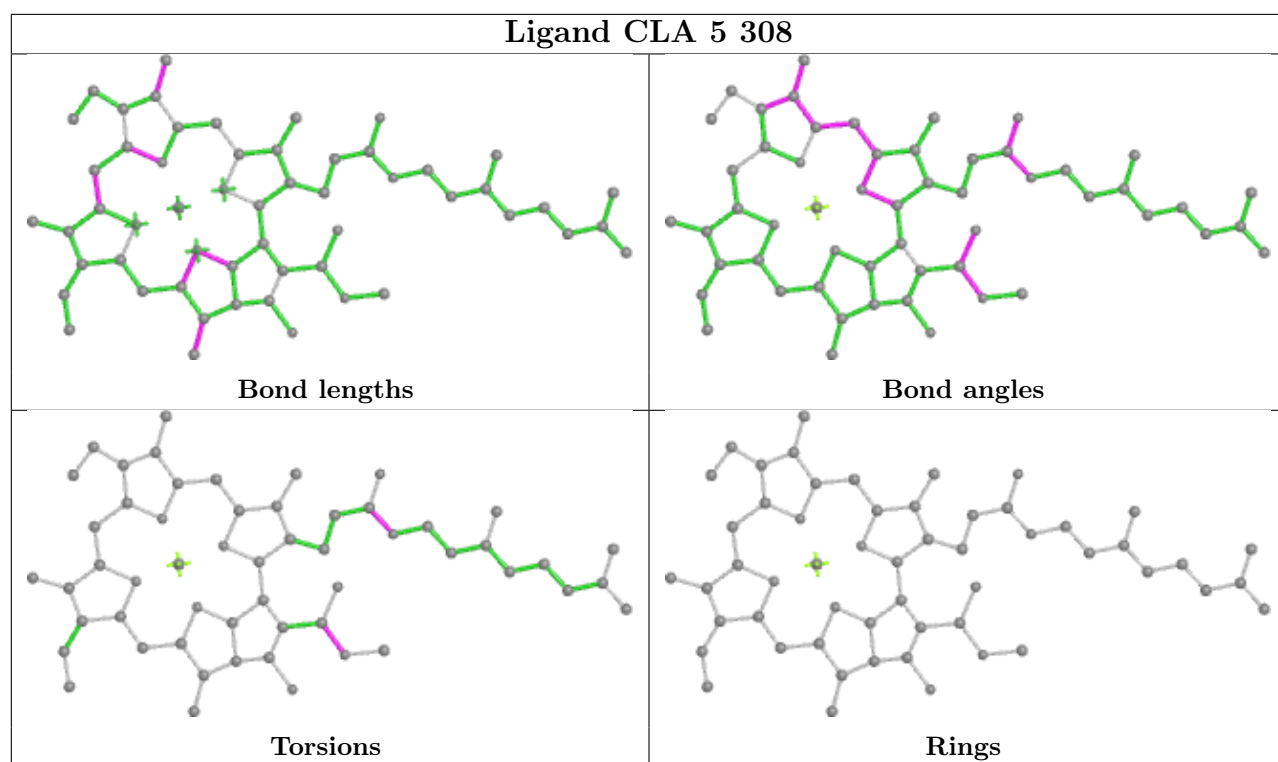
Bond angles



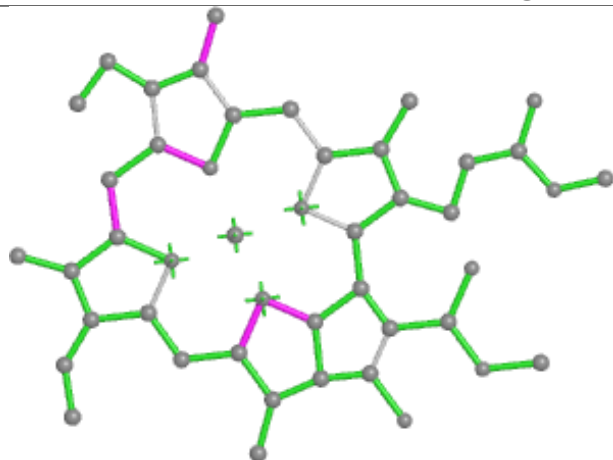
Torsions



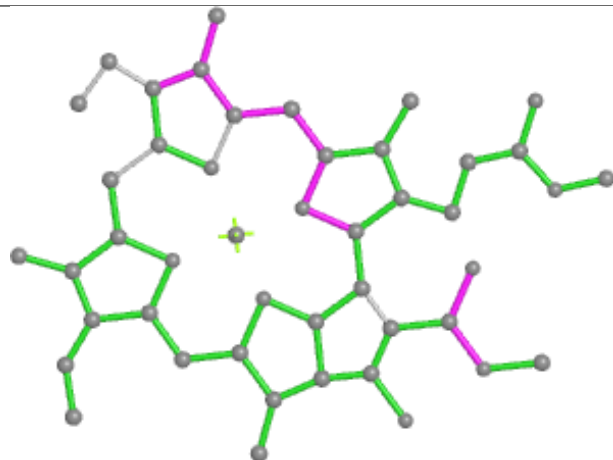
Rings



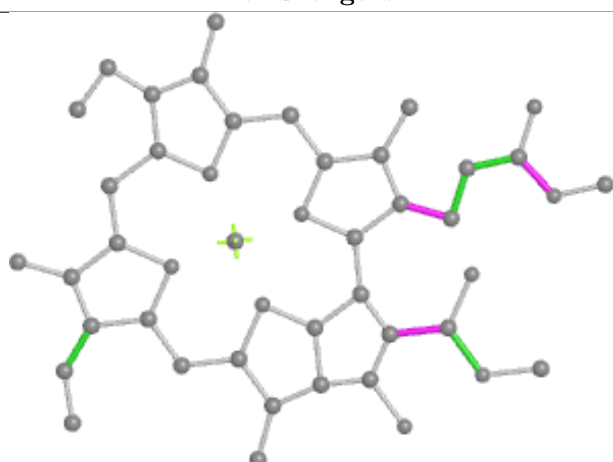
Ligand CLA 9 310



Bond lengths



Bond angles

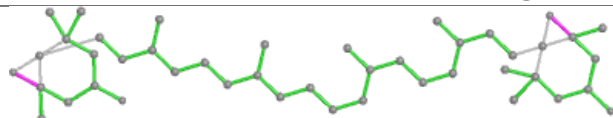


Torsions

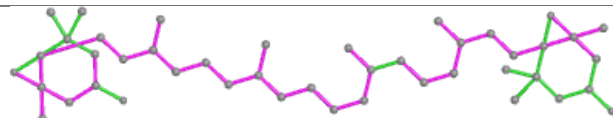


Rings

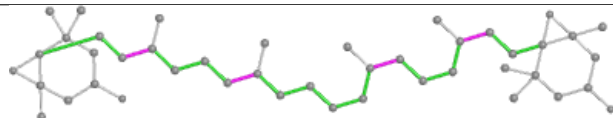
Ligand XAT a 852



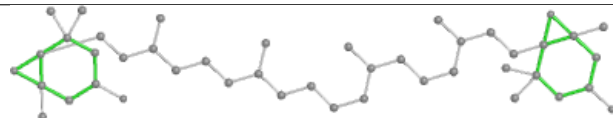
Bond lengths



Bond angles

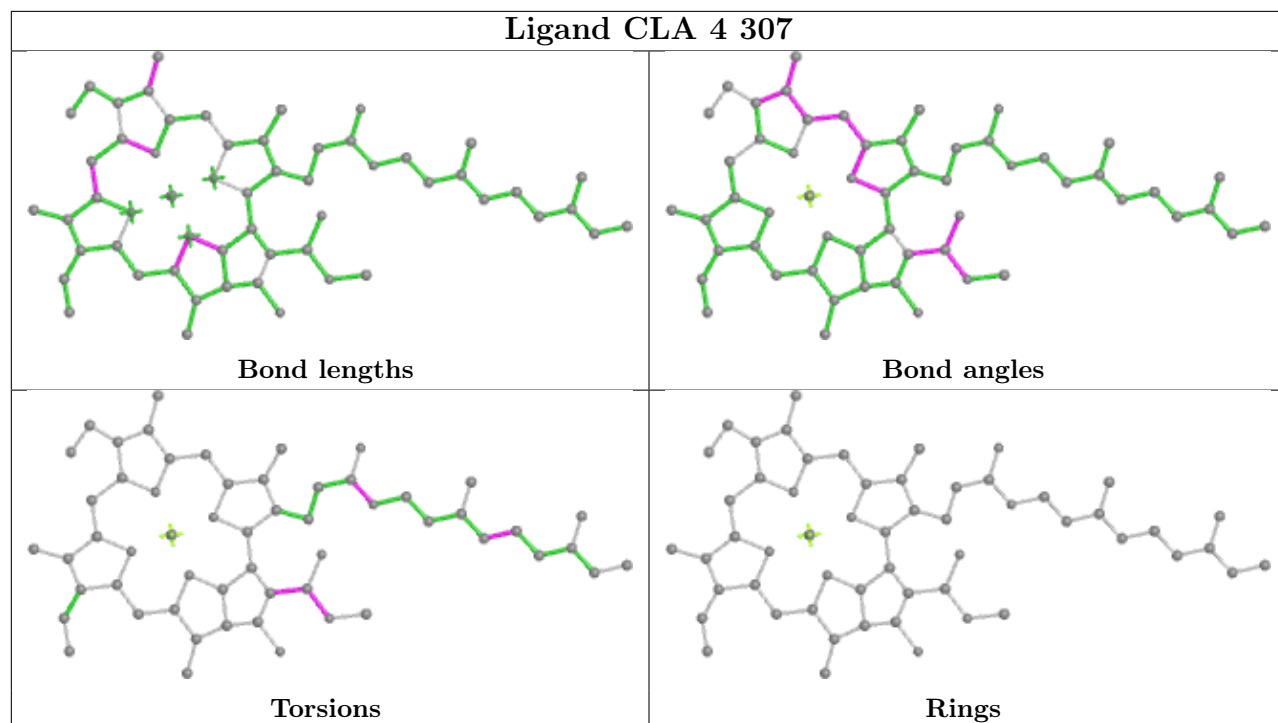


Torsions

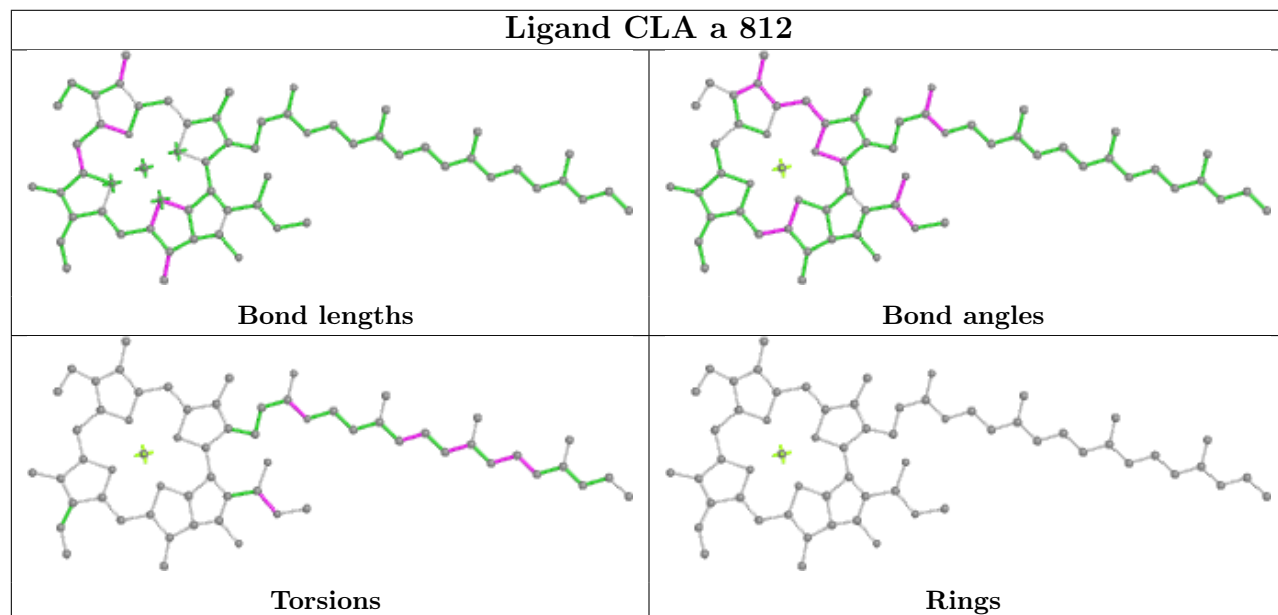


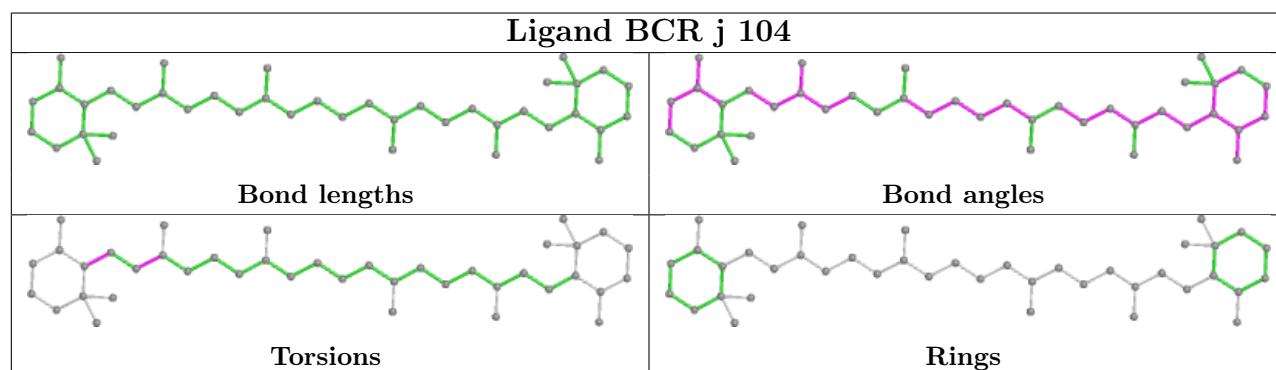
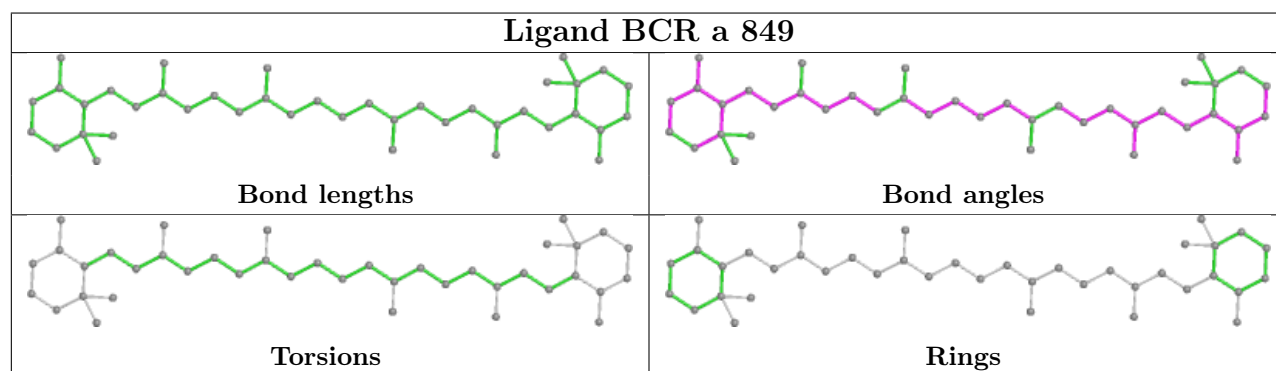
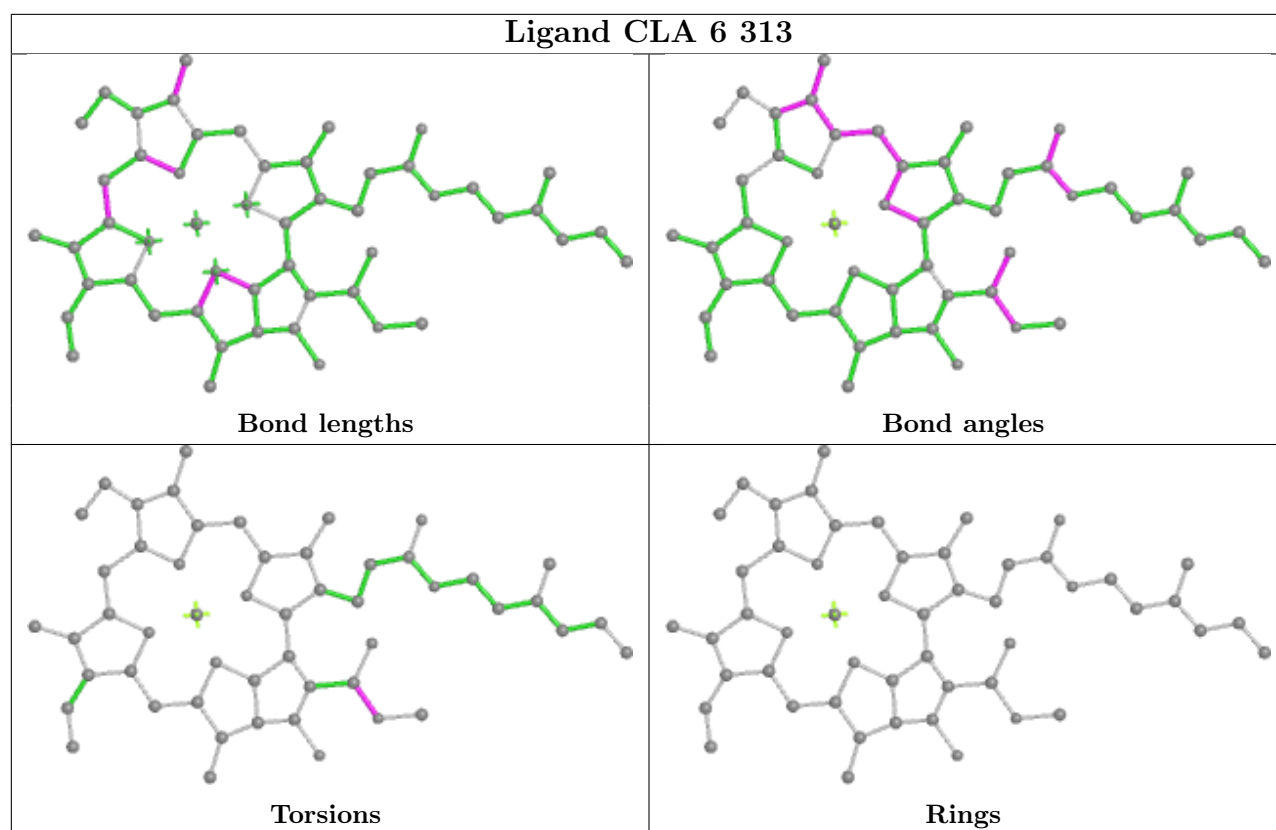
Rings

Ligand CLA 4 307

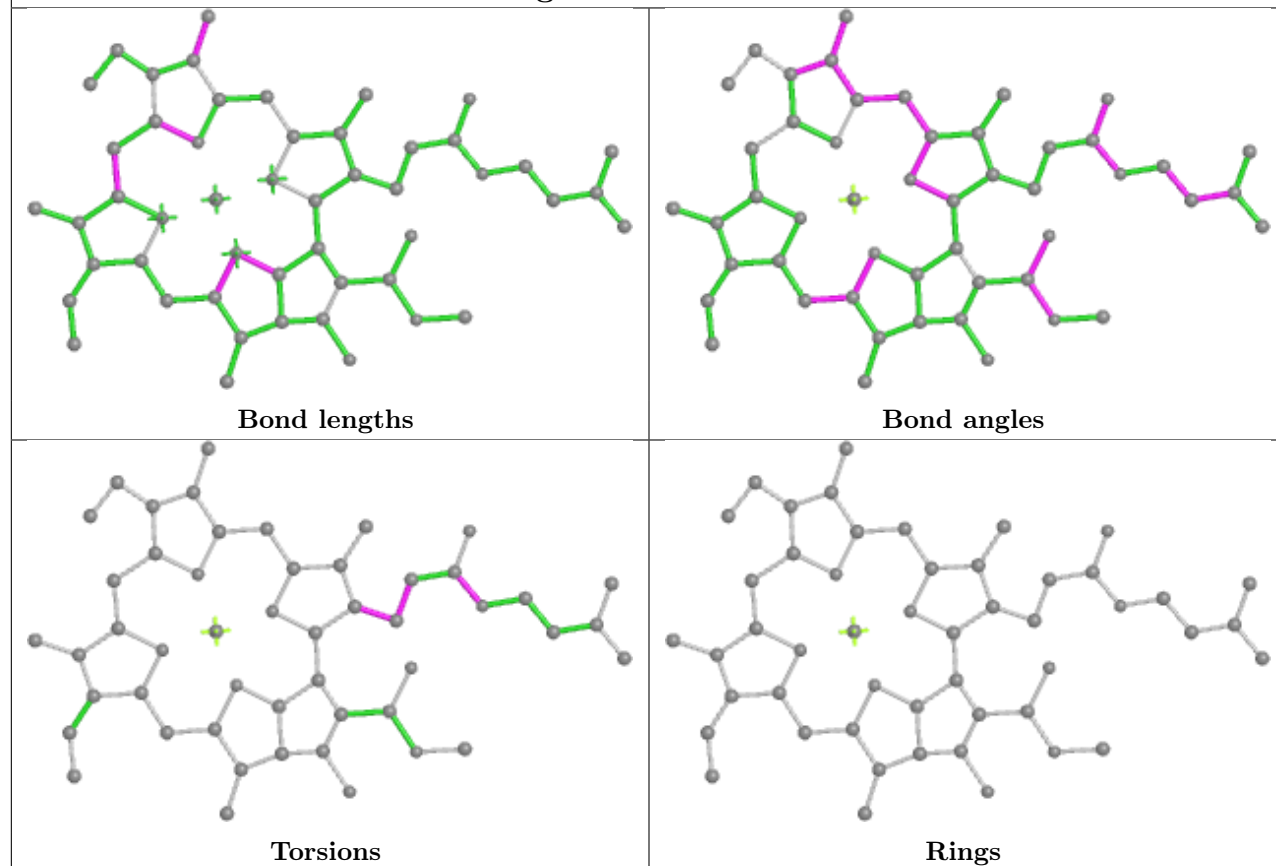


Ligand CLA a 812

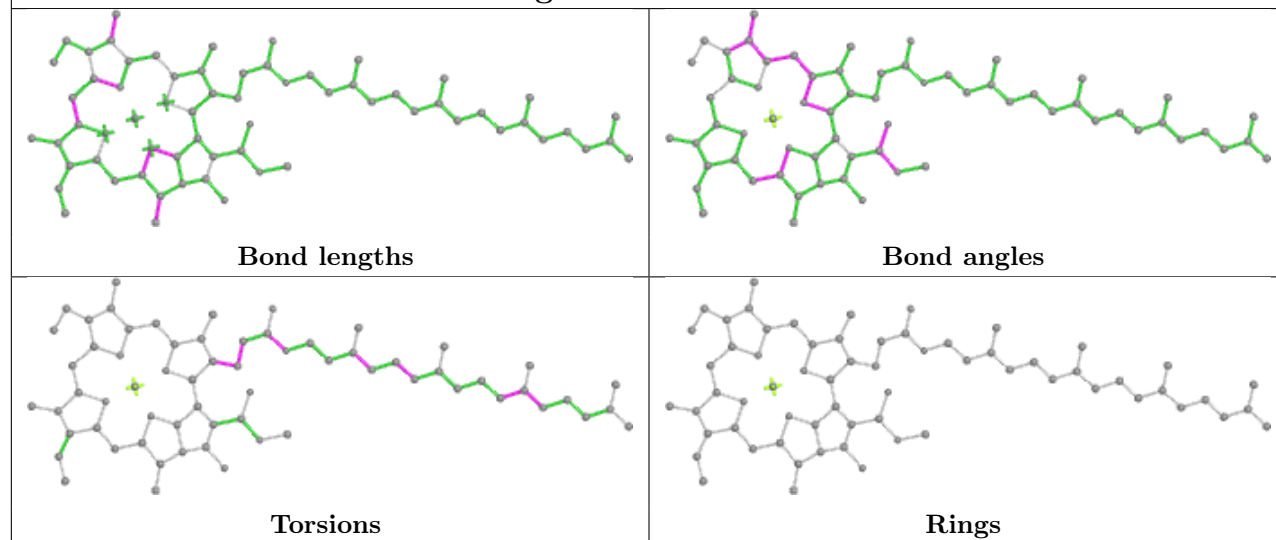




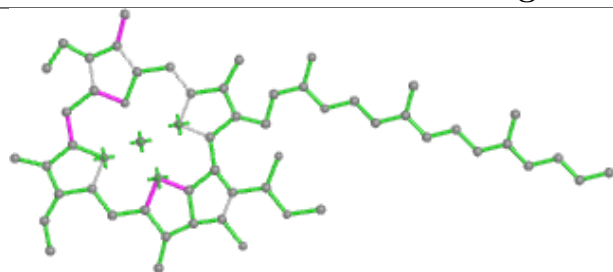
Ligand CLA 3 311



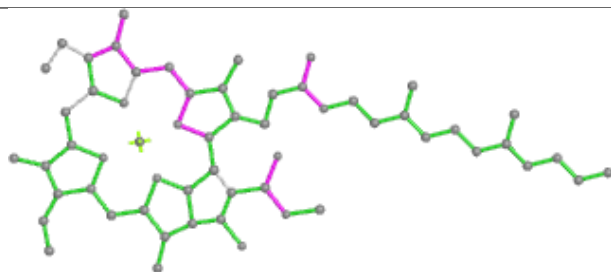
Ligand CLA b 828



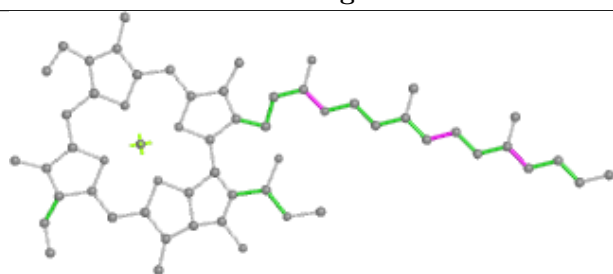
Ligand CLA 2 311



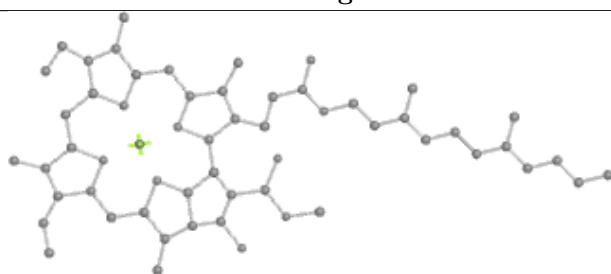
Bond lengths



Bond angles

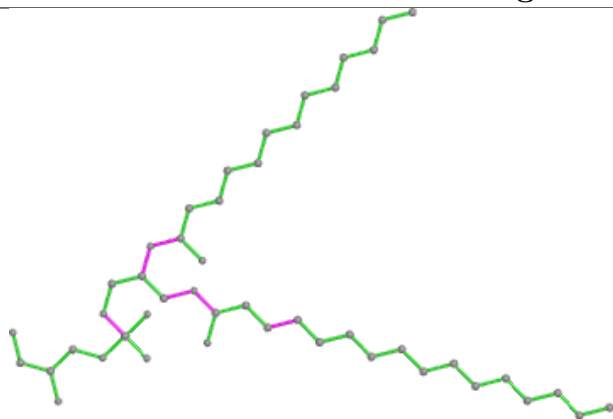


Torsions

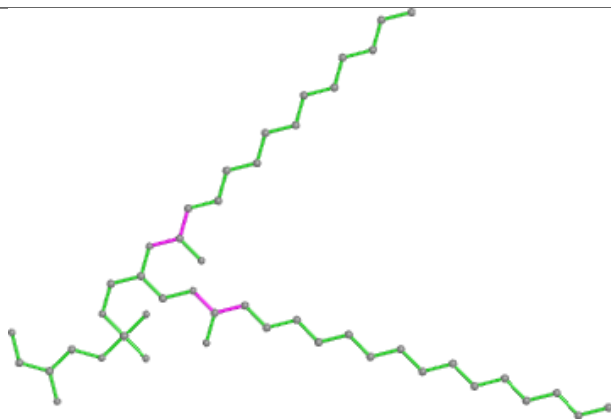


Rings

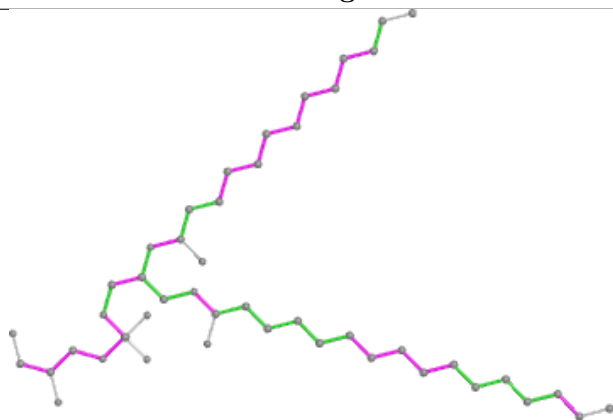
Ligand LHG 9 317



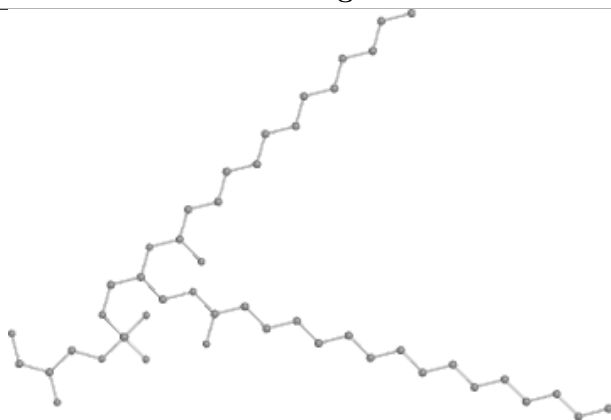
Bond lengths



Bond angles

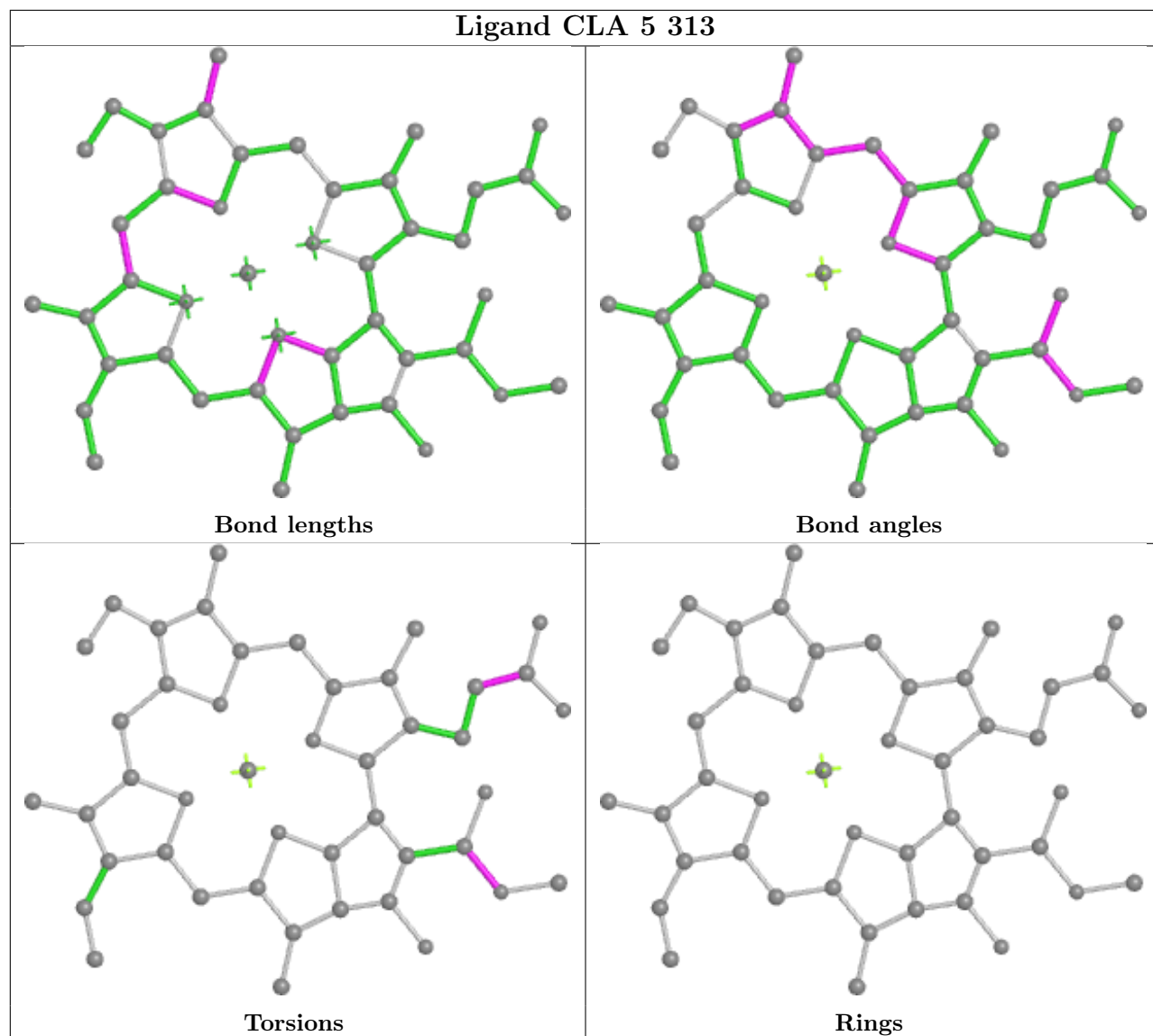


Torsions

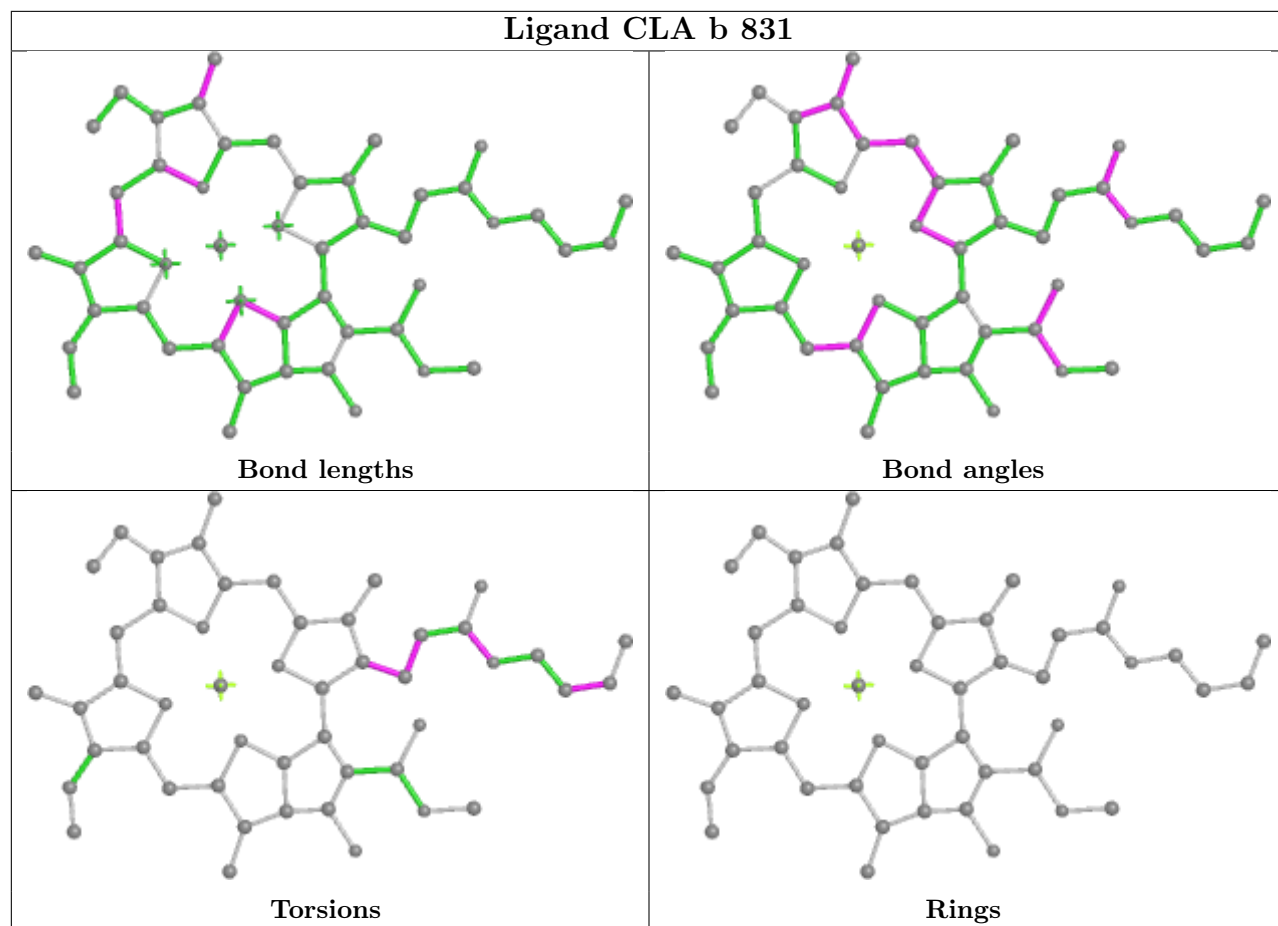


Rings

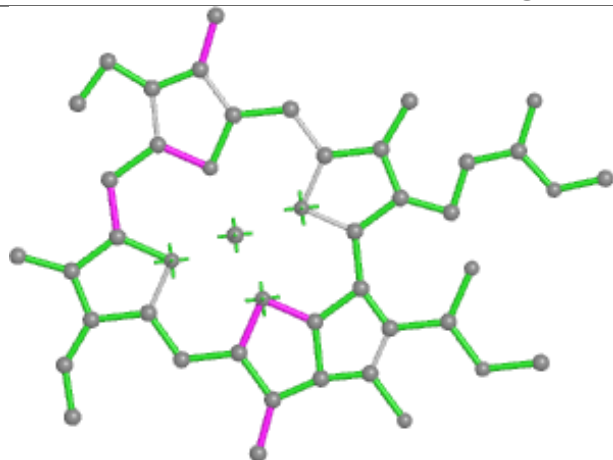
Ligand CLA 5 313



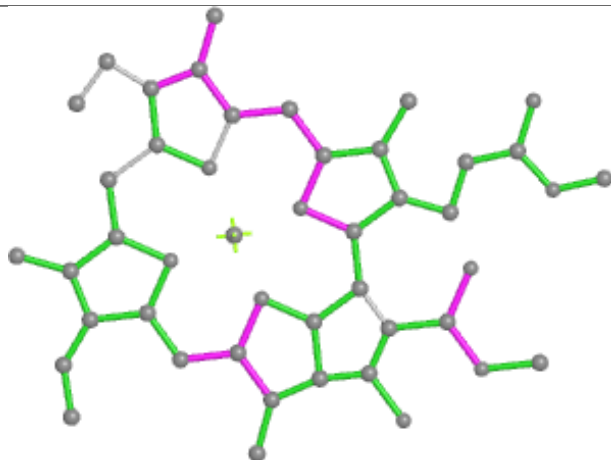
Ligand CLA b 831



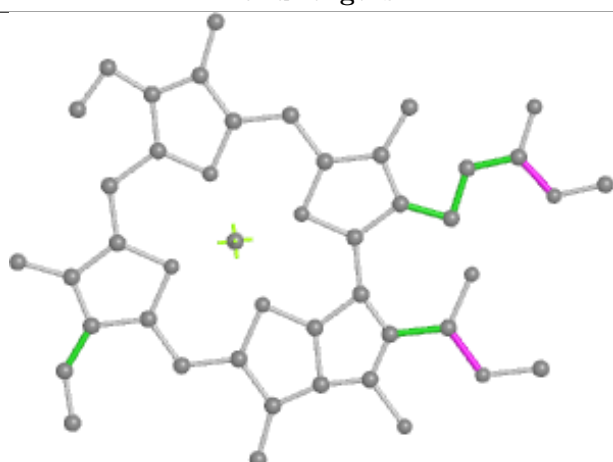
Ligand CLA 5 305



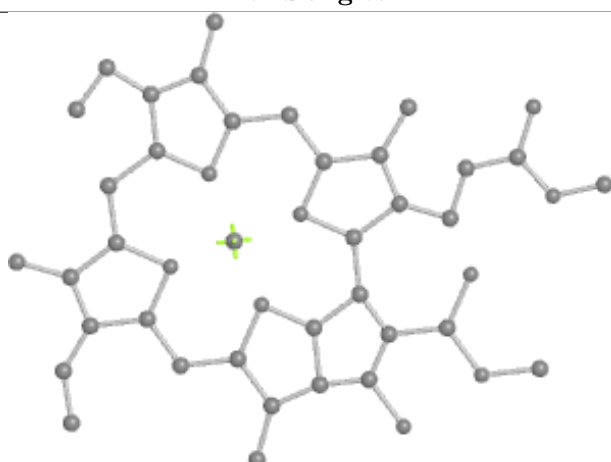
Bond lengths



Bond angles

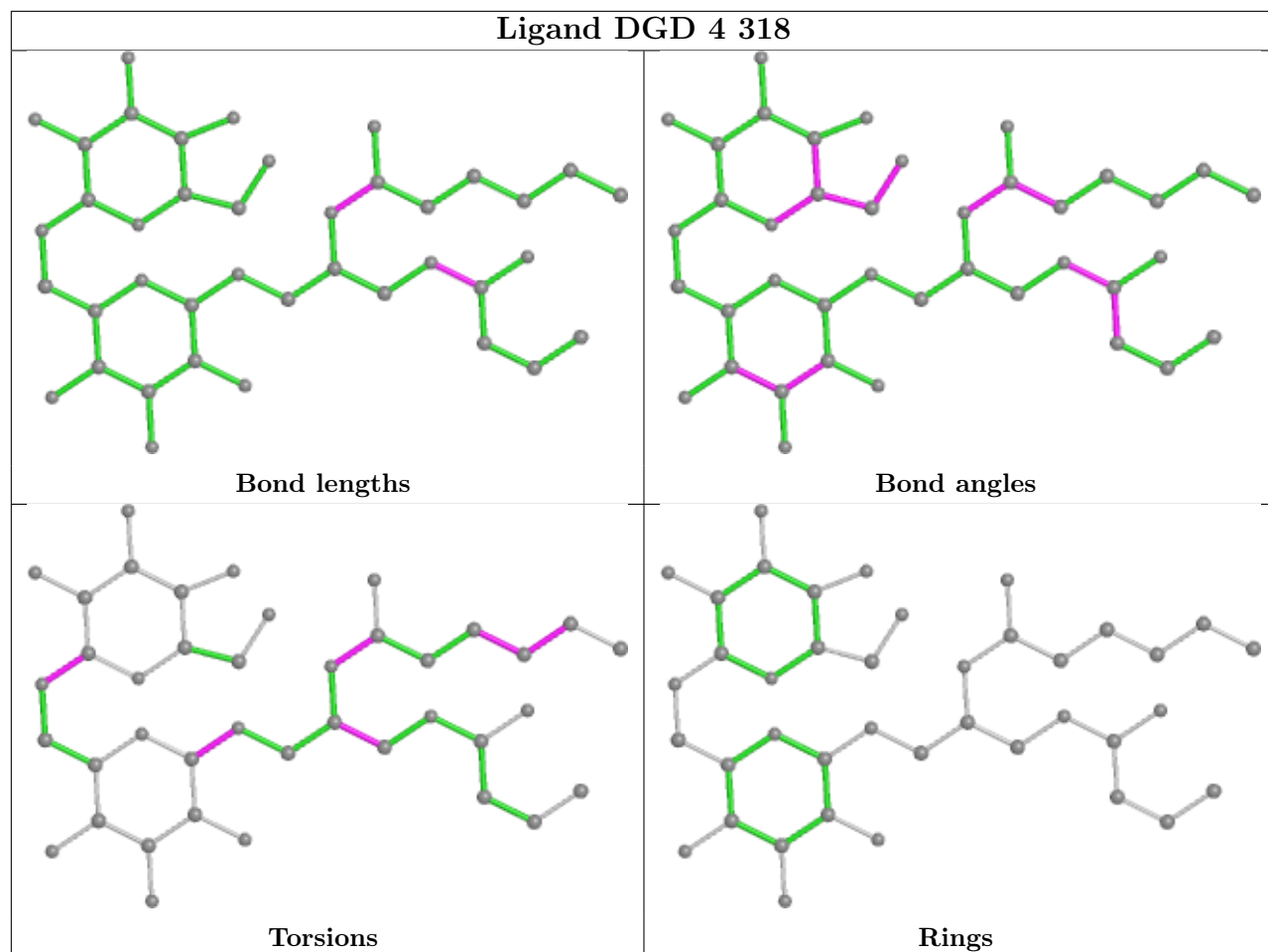


Torsions

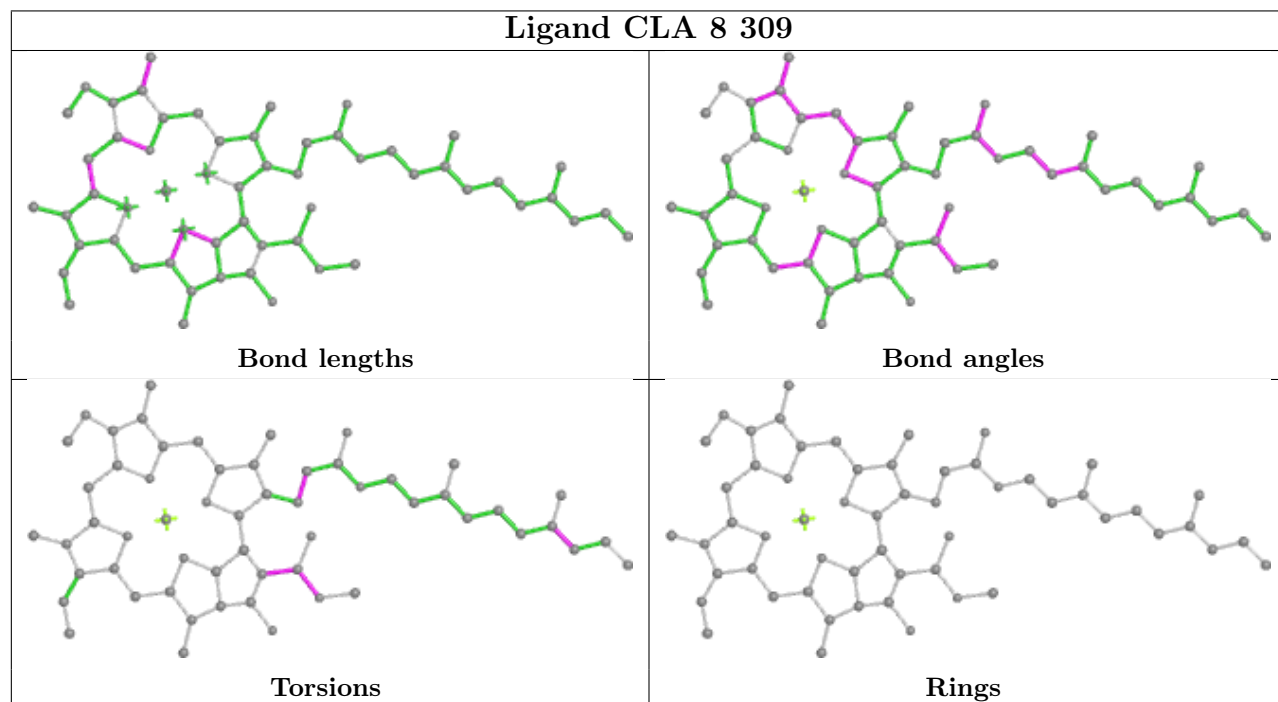


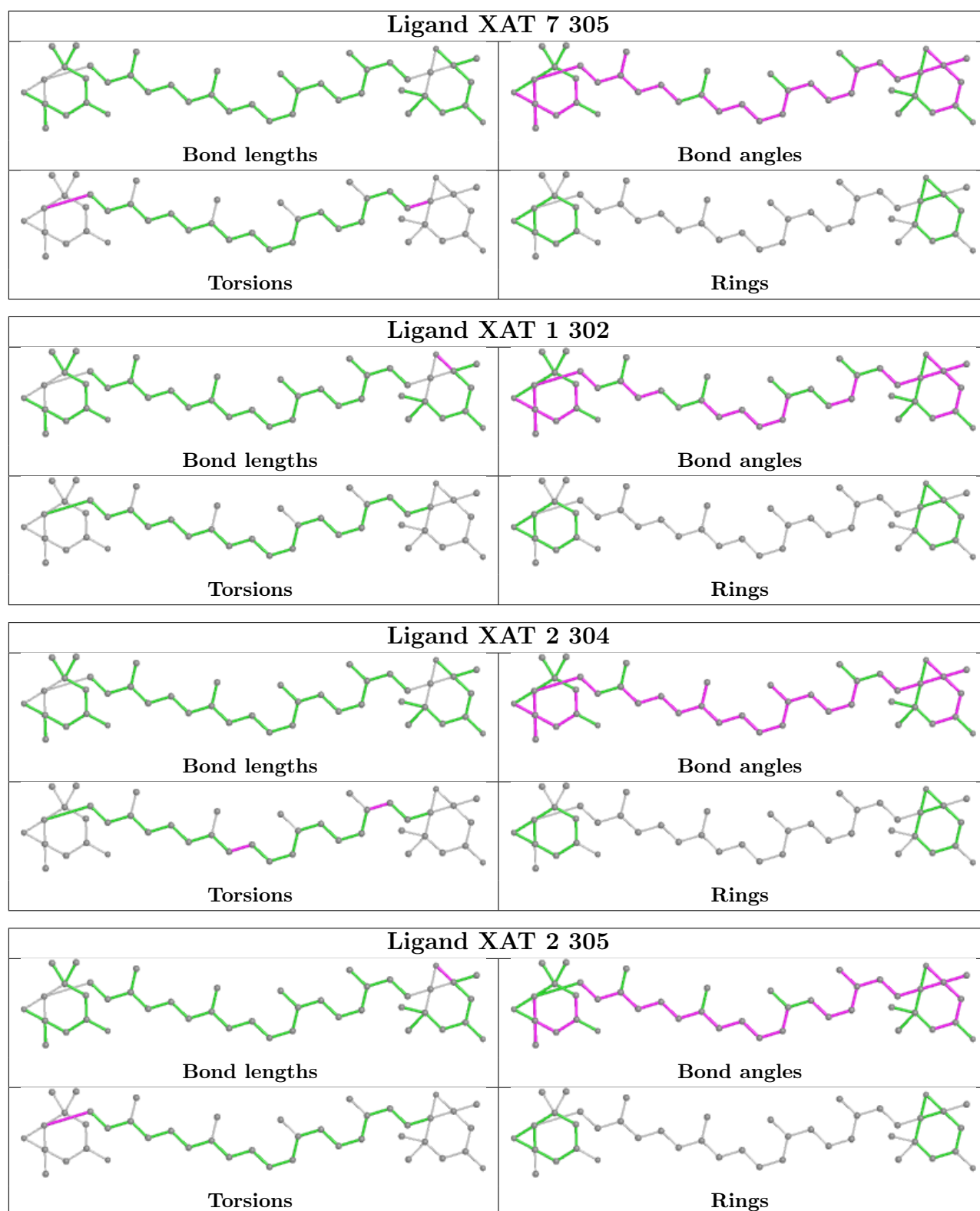
Rings

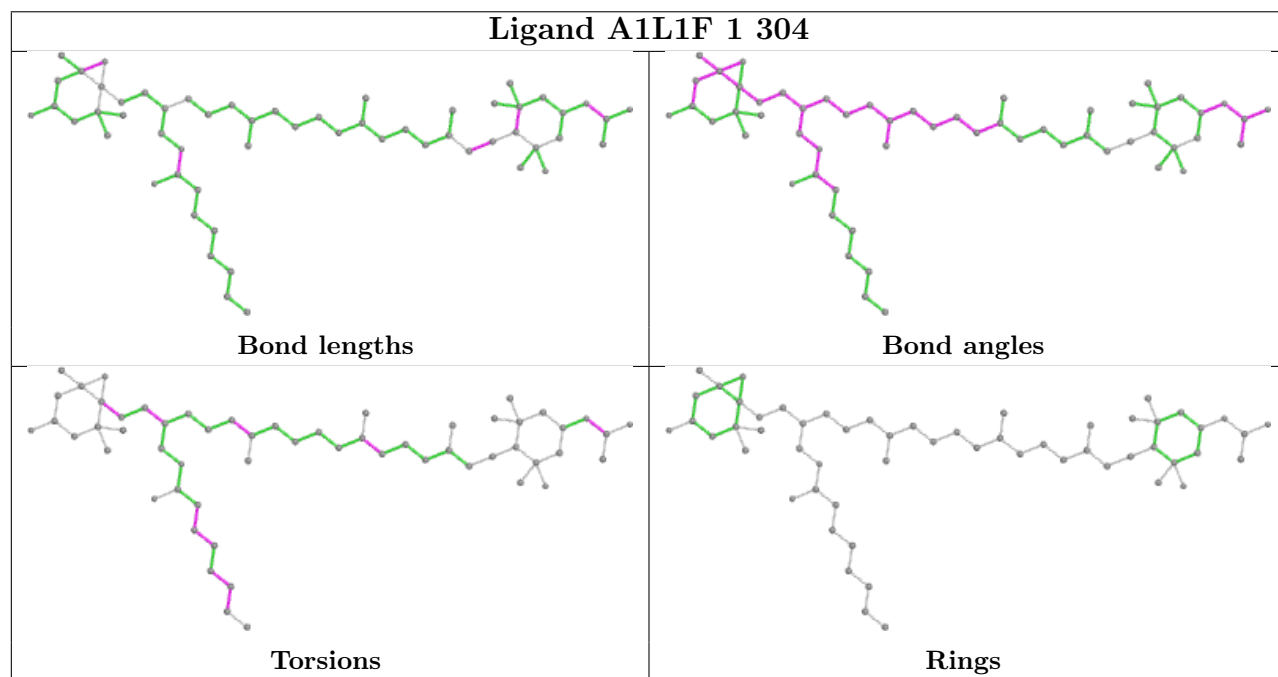
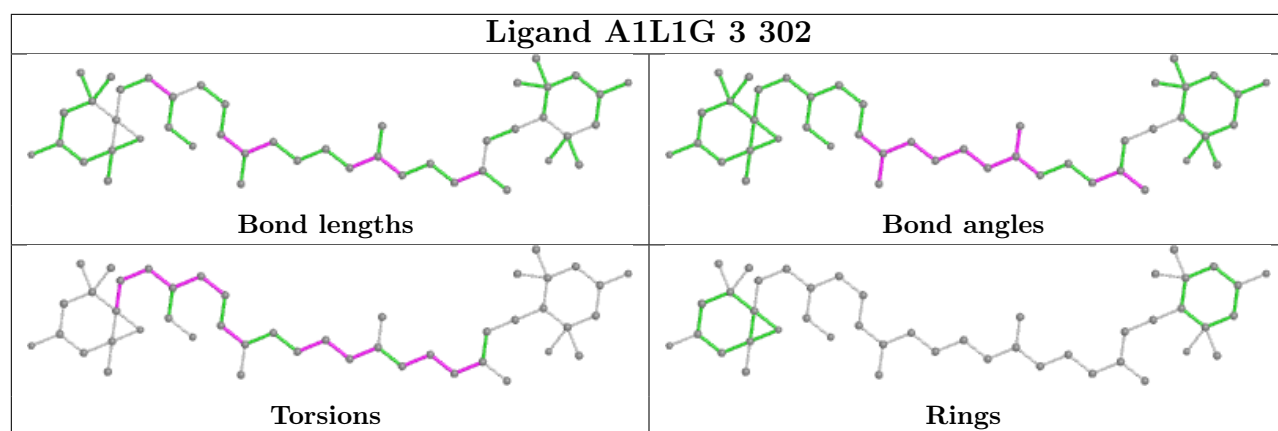
Ligand DGD 4 318



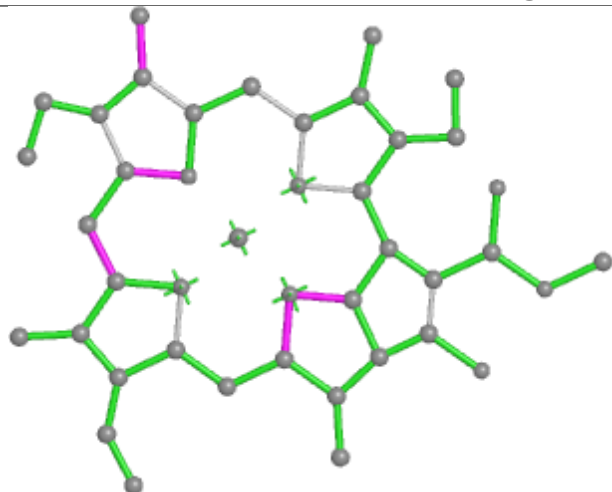
Ligand CLA 8 309



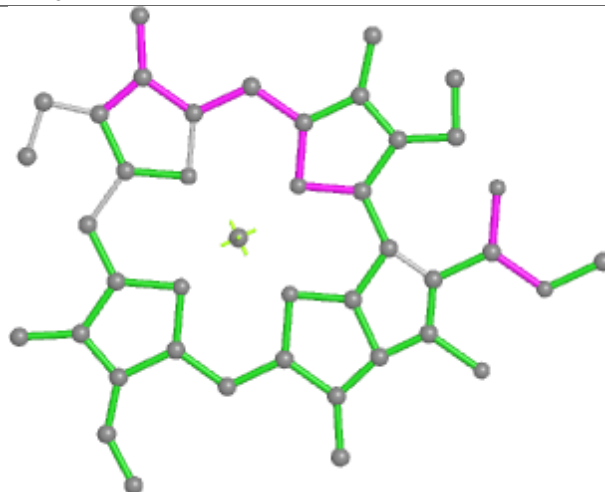




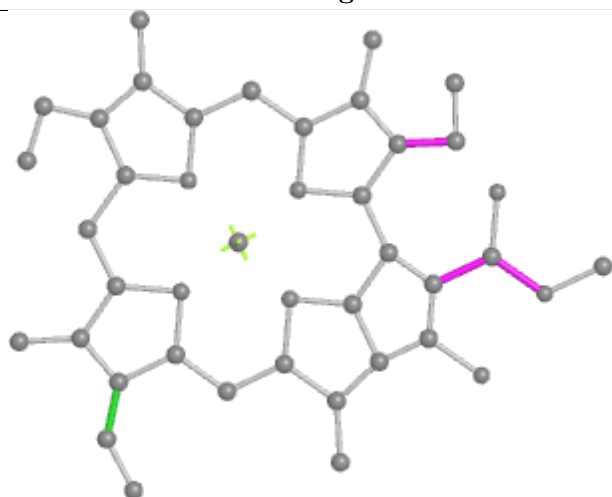
Ligand CLA j 103



Bond lengths



Bond angles

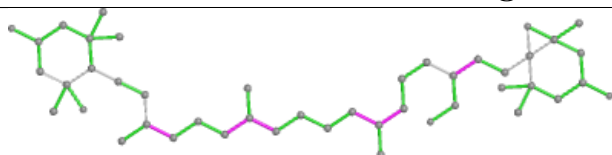


Torsions

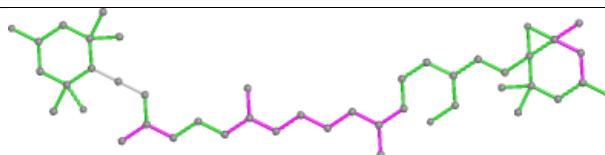


Rings

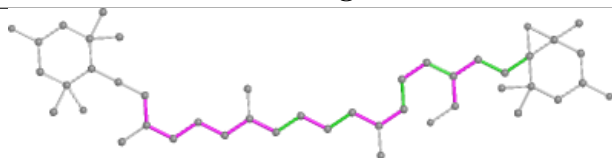
Ligand A1L1G 3 306



Bond lengths



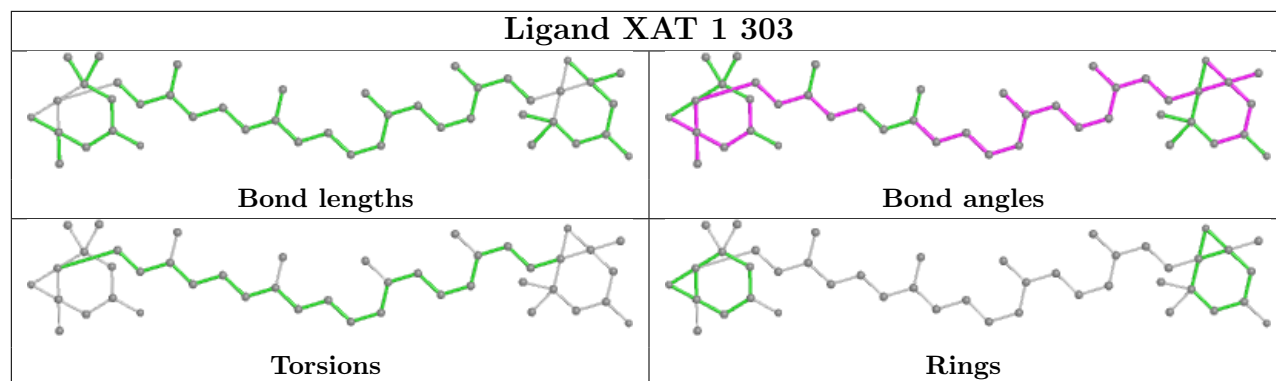
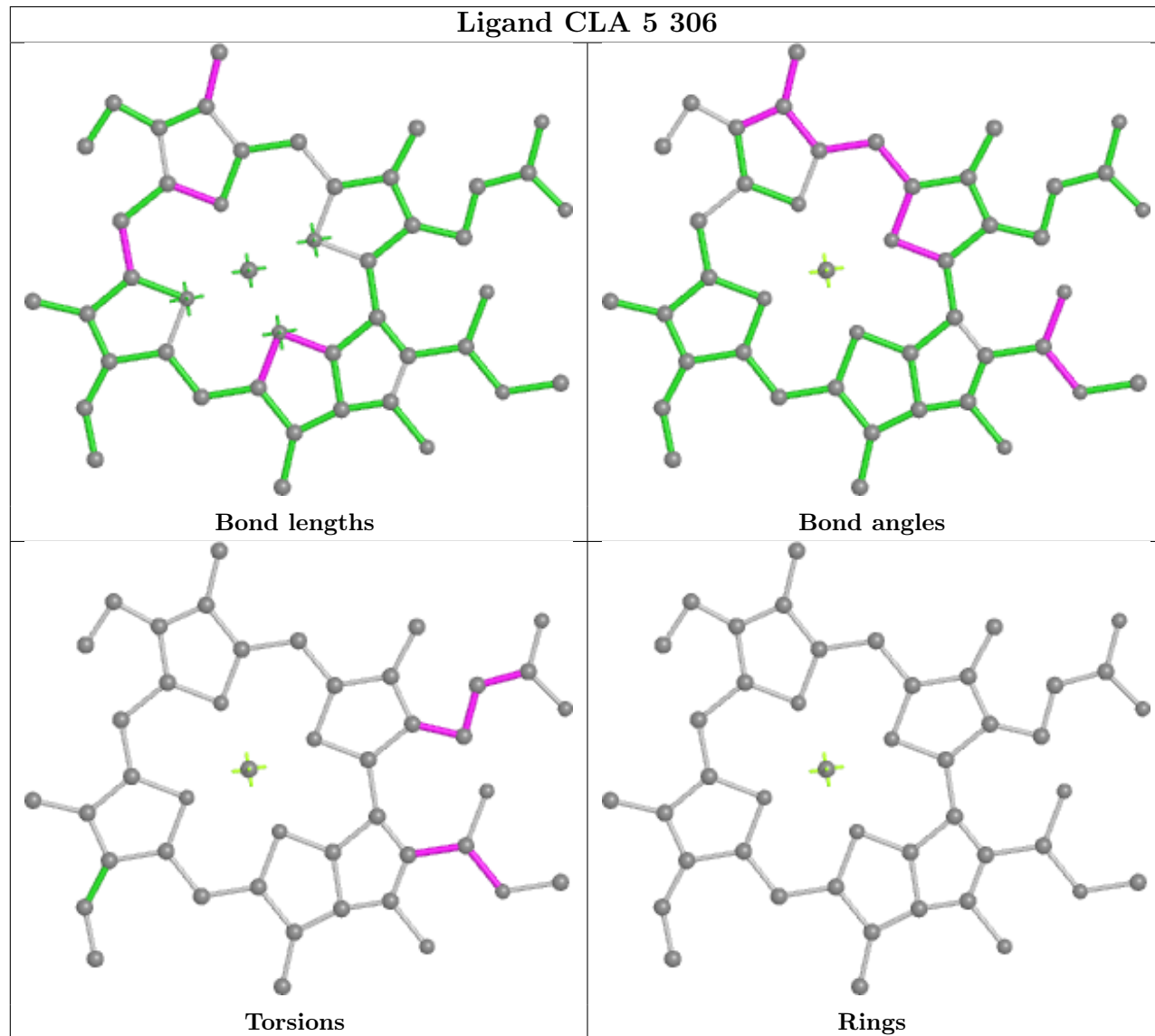
Bond angles

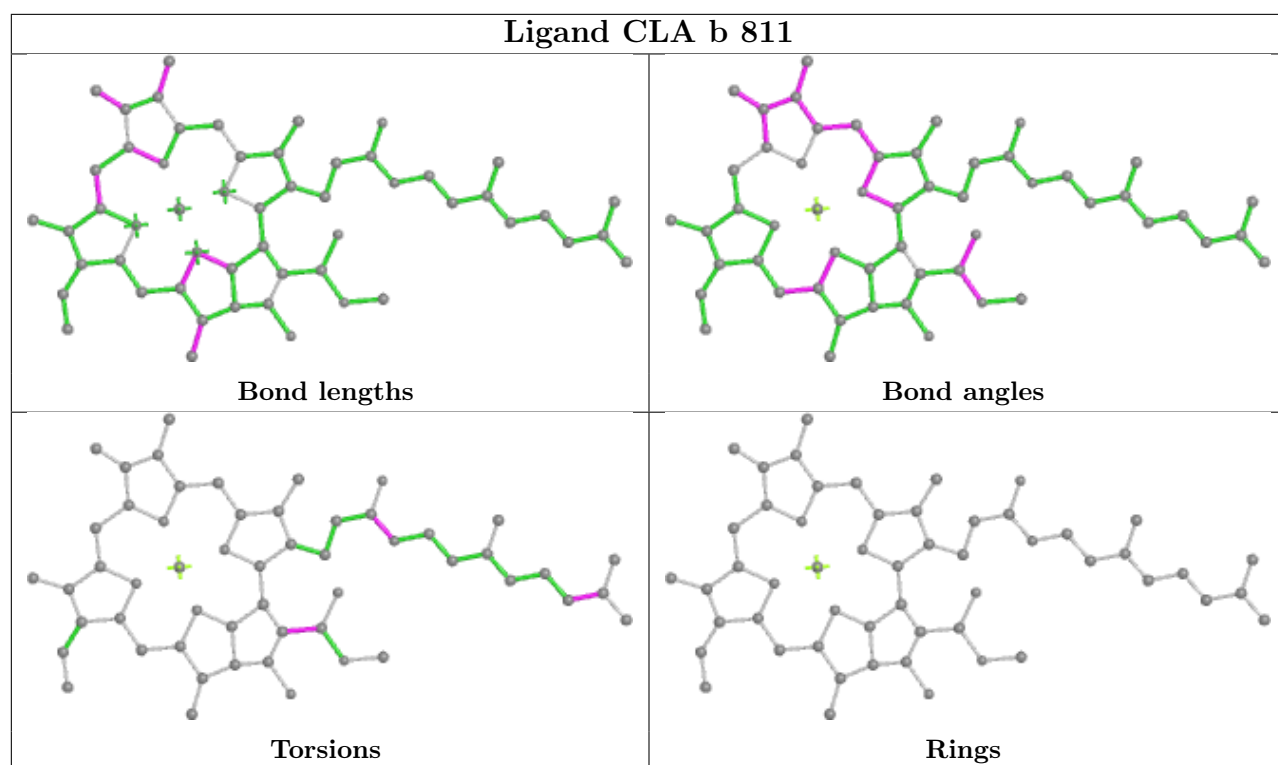


Torsions

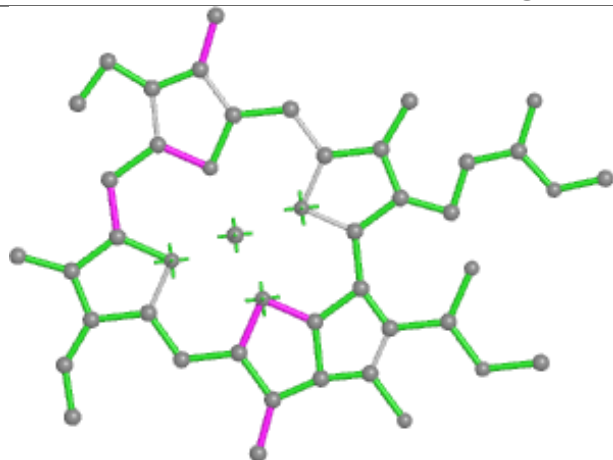


Rings

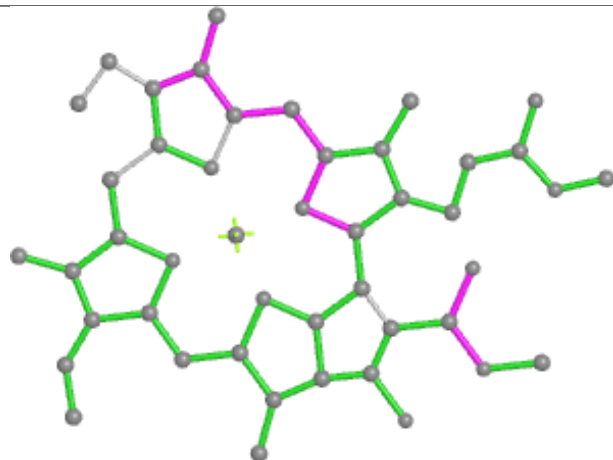
Ligand XAT 1 303**Ligand CLA 5 306**



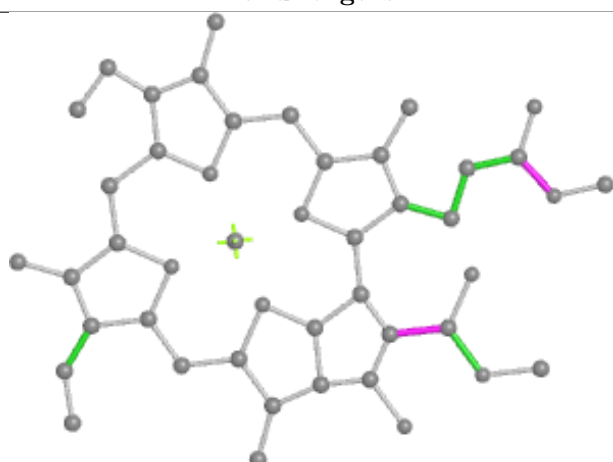
Ligand CLA 8 313



Bond lengths



Bond angles

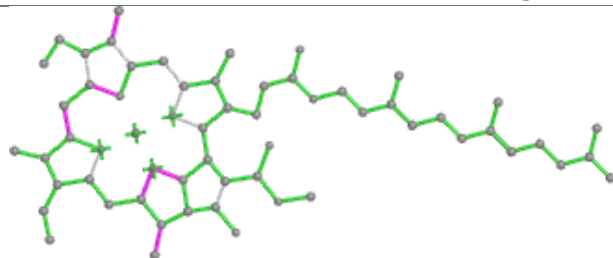


Torsions

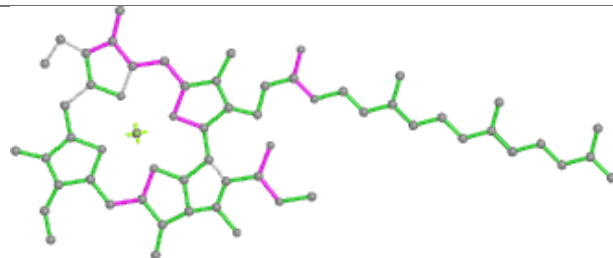


Rings

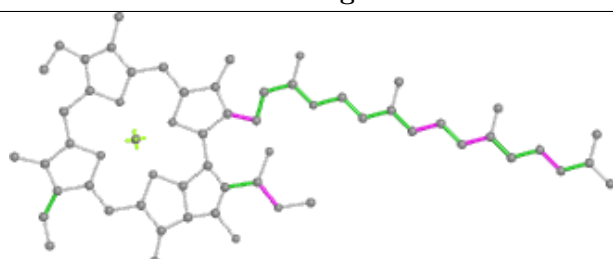
Ligand CLA b 822



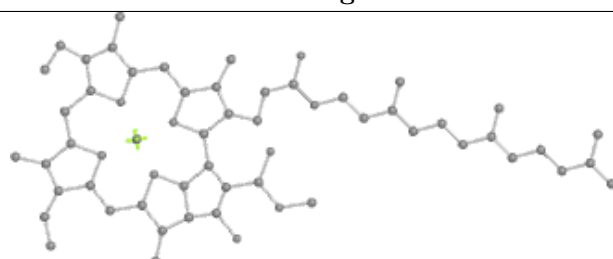
Bond lengths



Bond angles

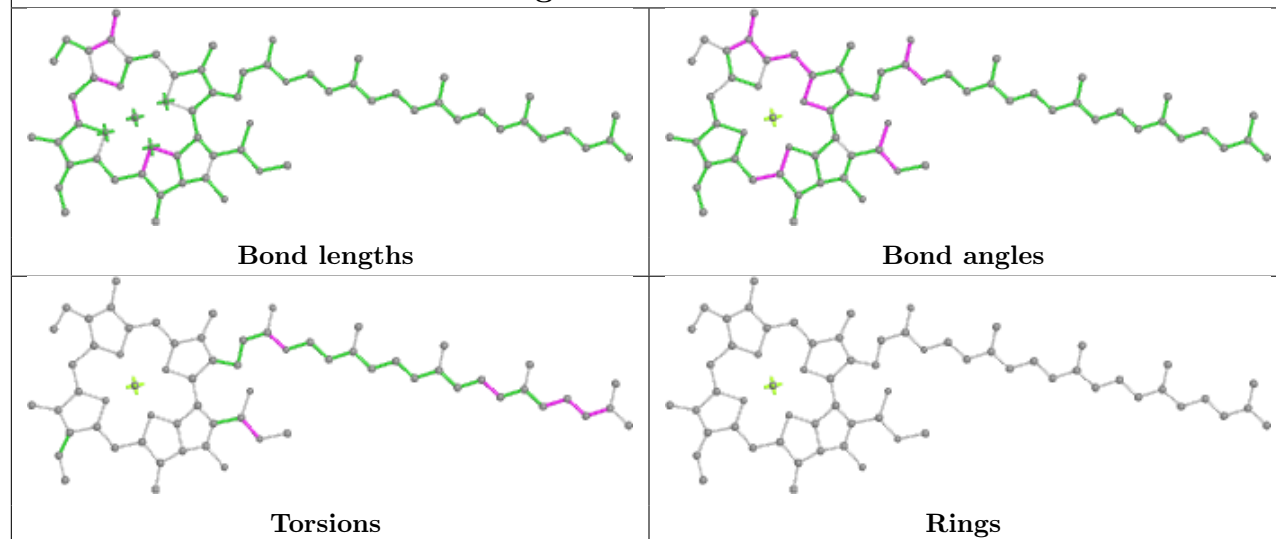


Torsions

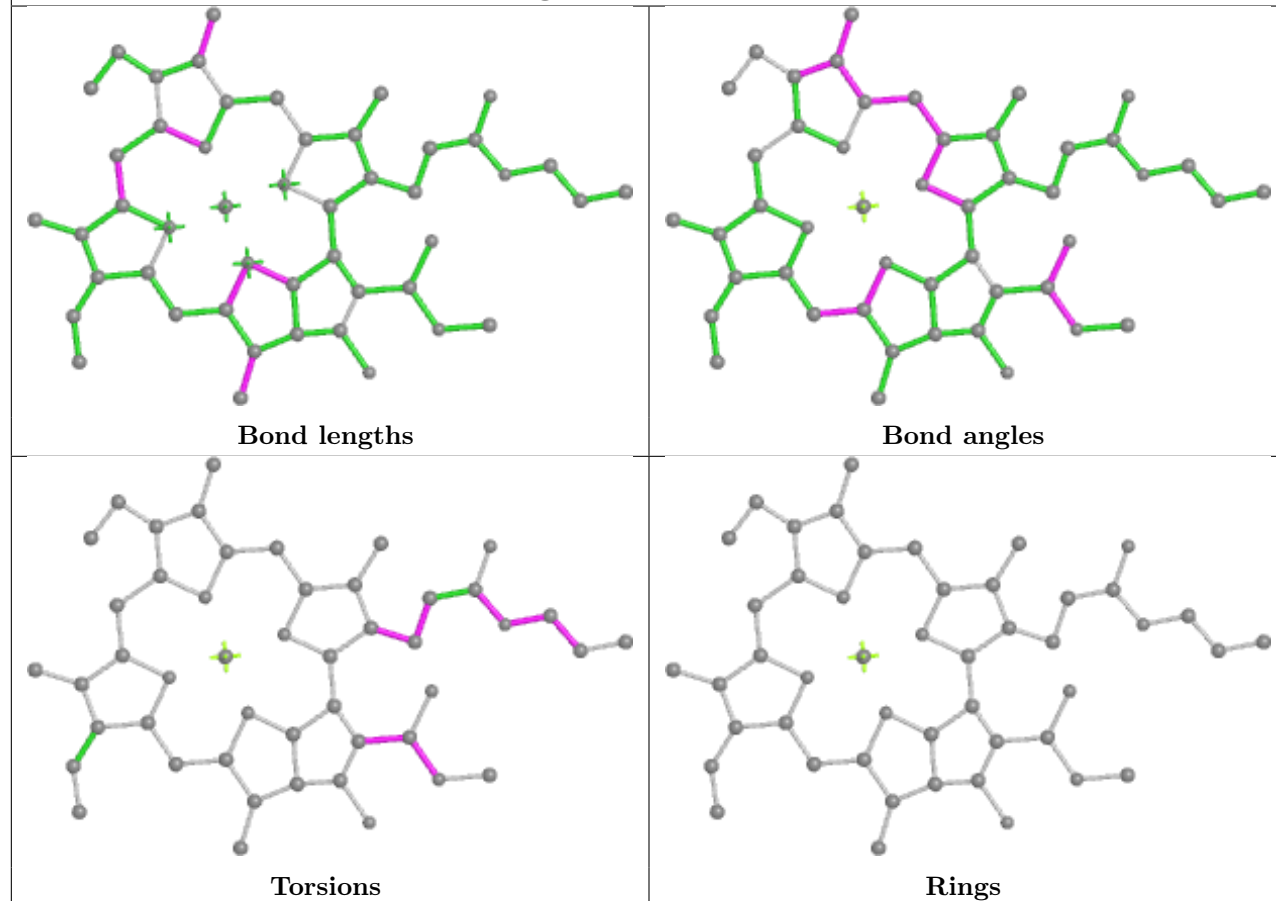


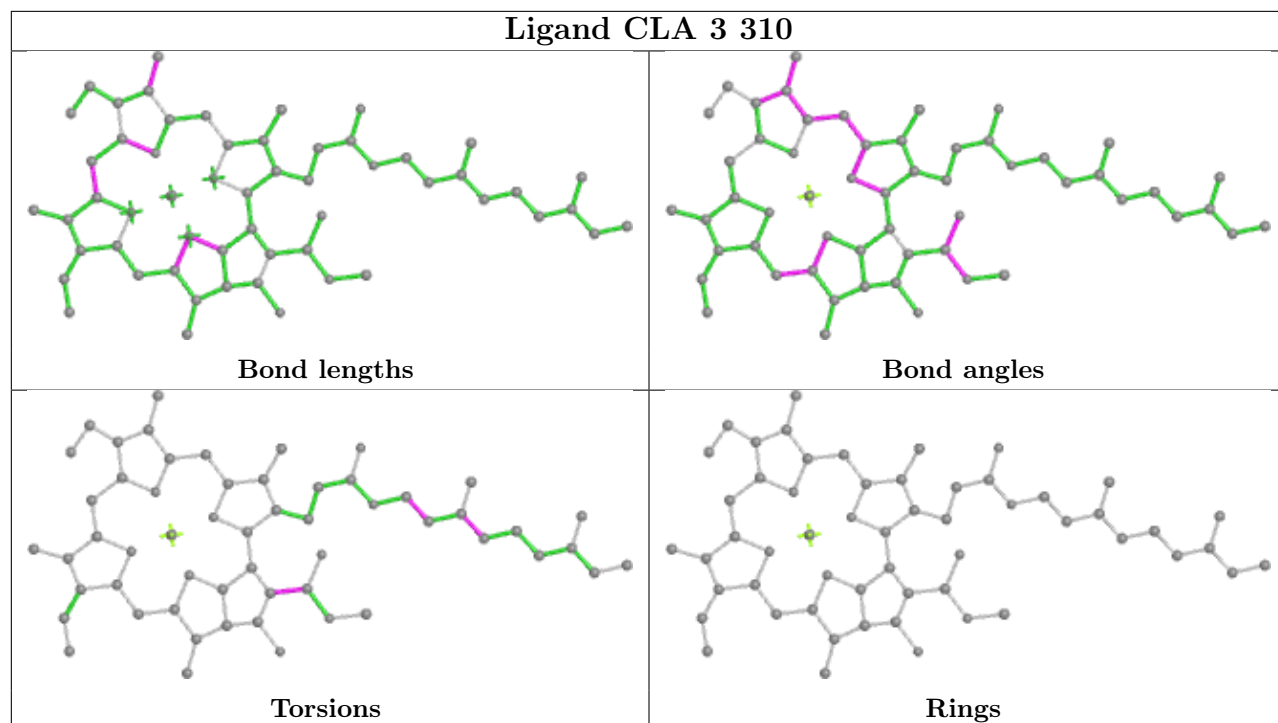
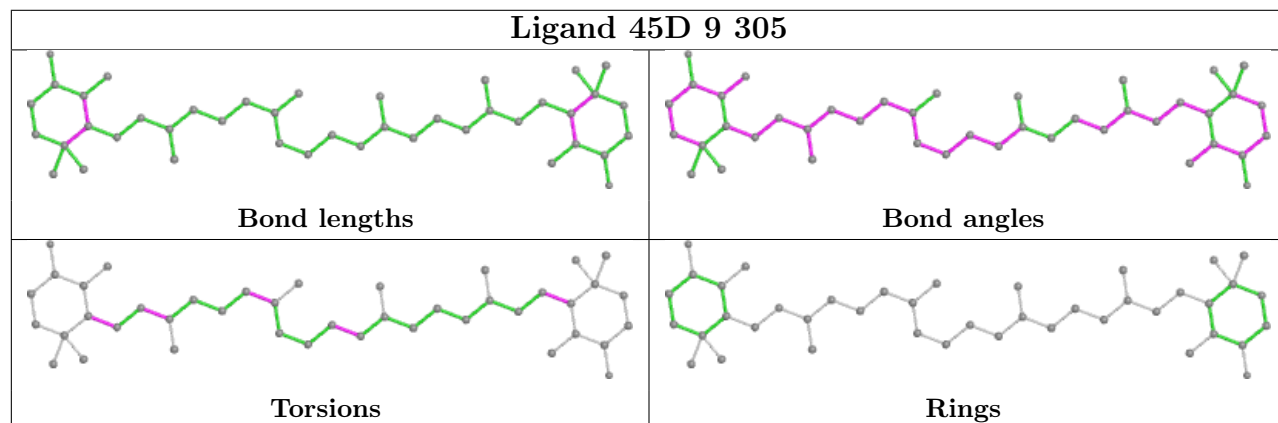
Rings

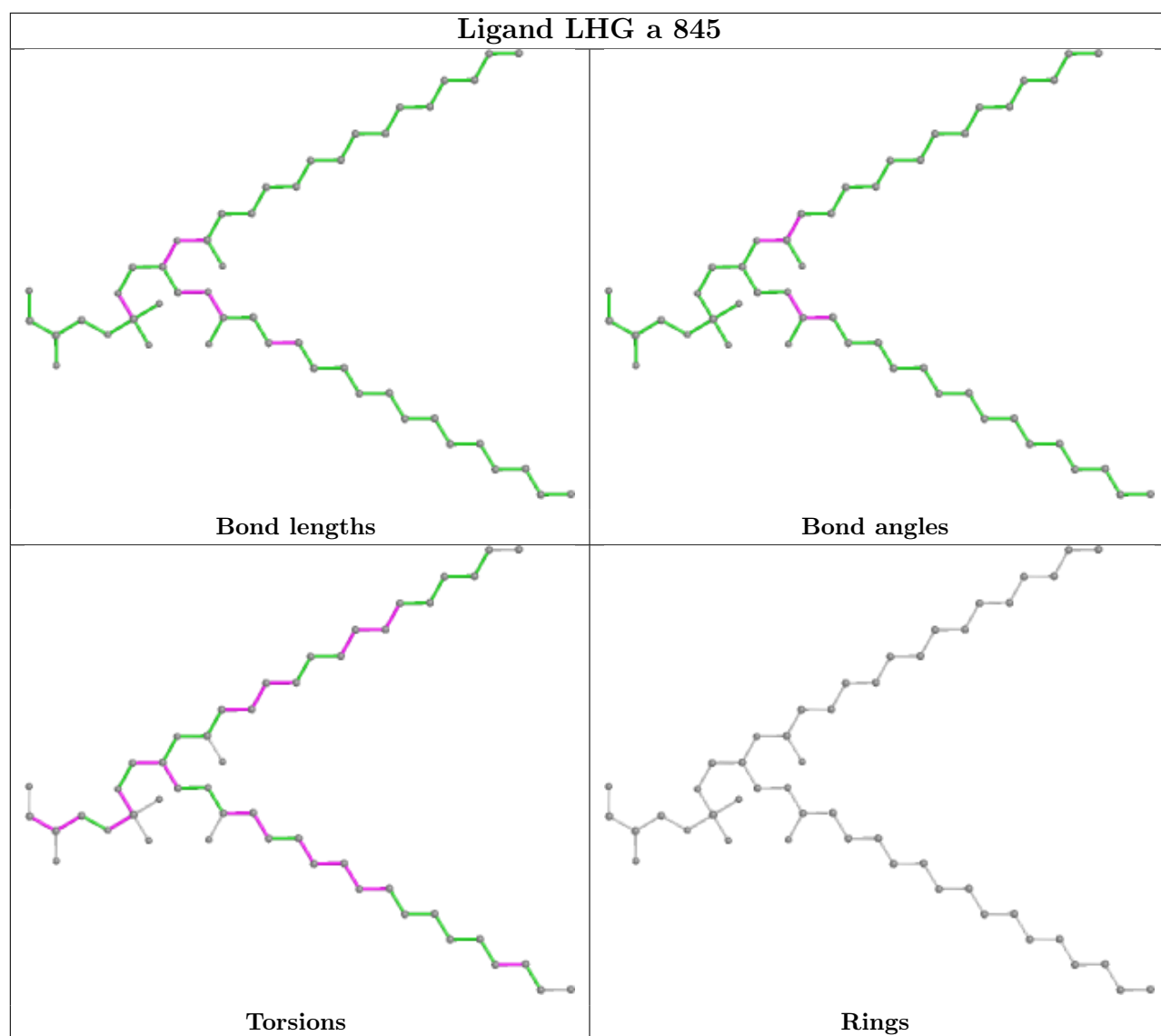
Ligand CLA b 840



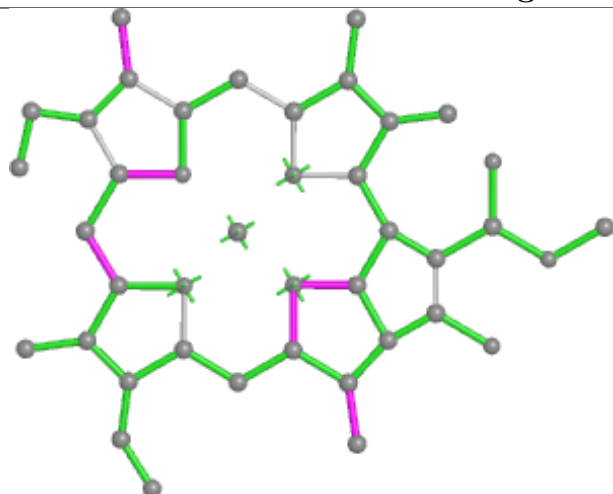
Ligand CLA 7 306



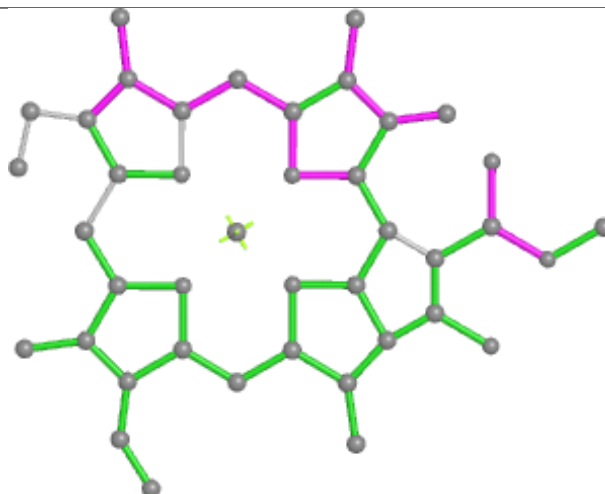
Ligand CLA 3 310**Ligand 45D 9 305**



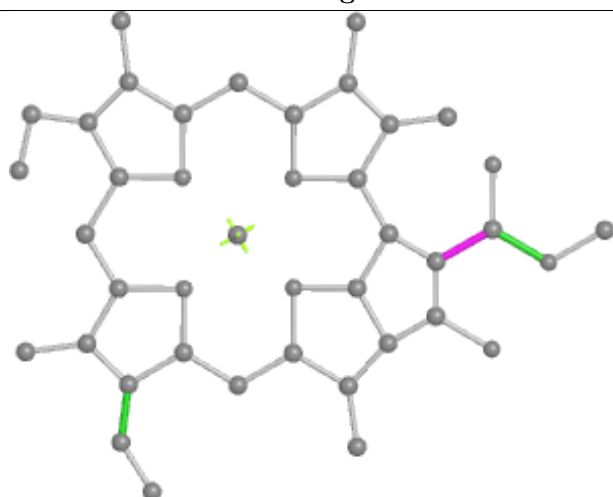
Ligand CLA b 830



Bond lengths



Bond angles

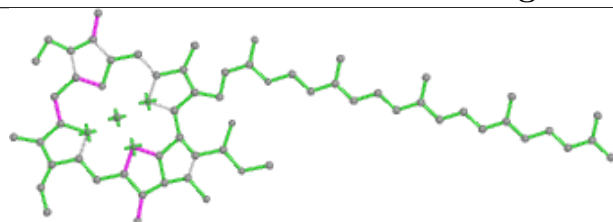


Torsions

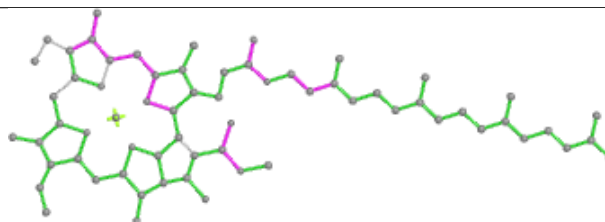


Rings

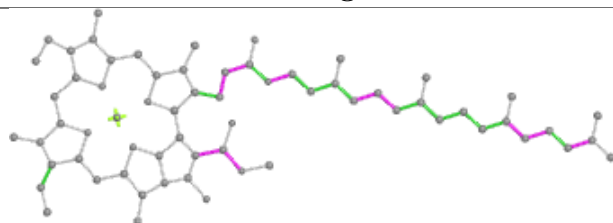
Ligand CLA a 810



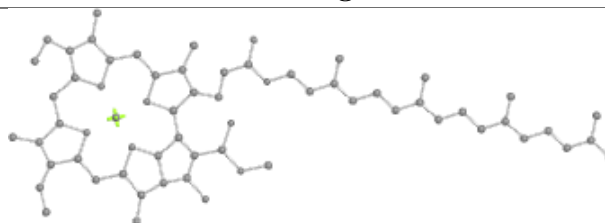
Bond lengths



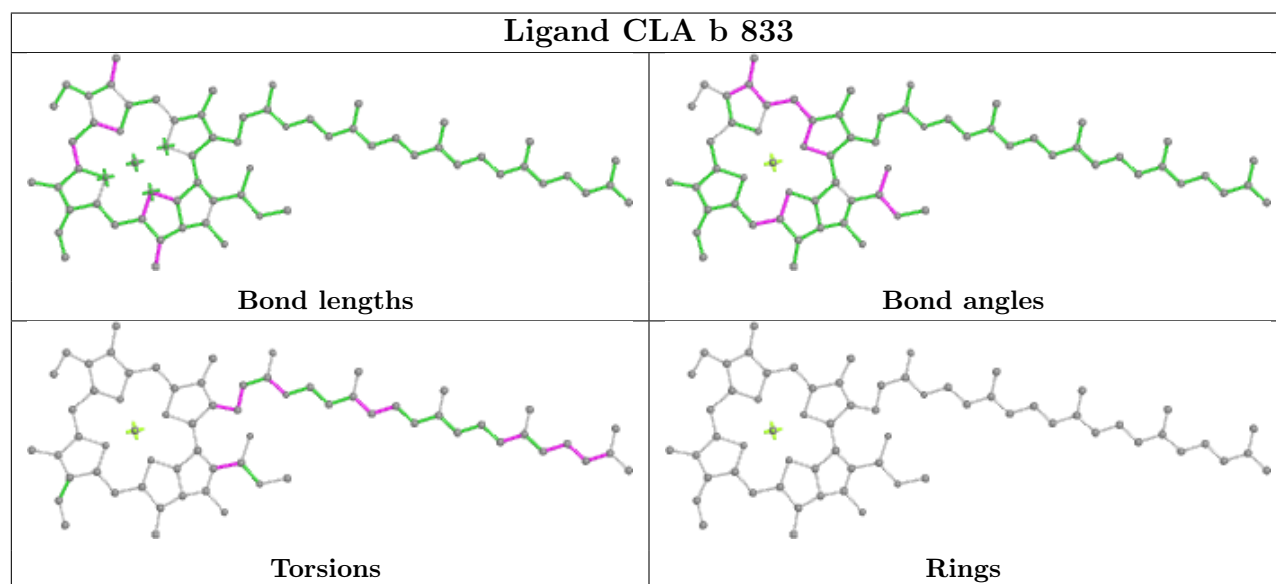
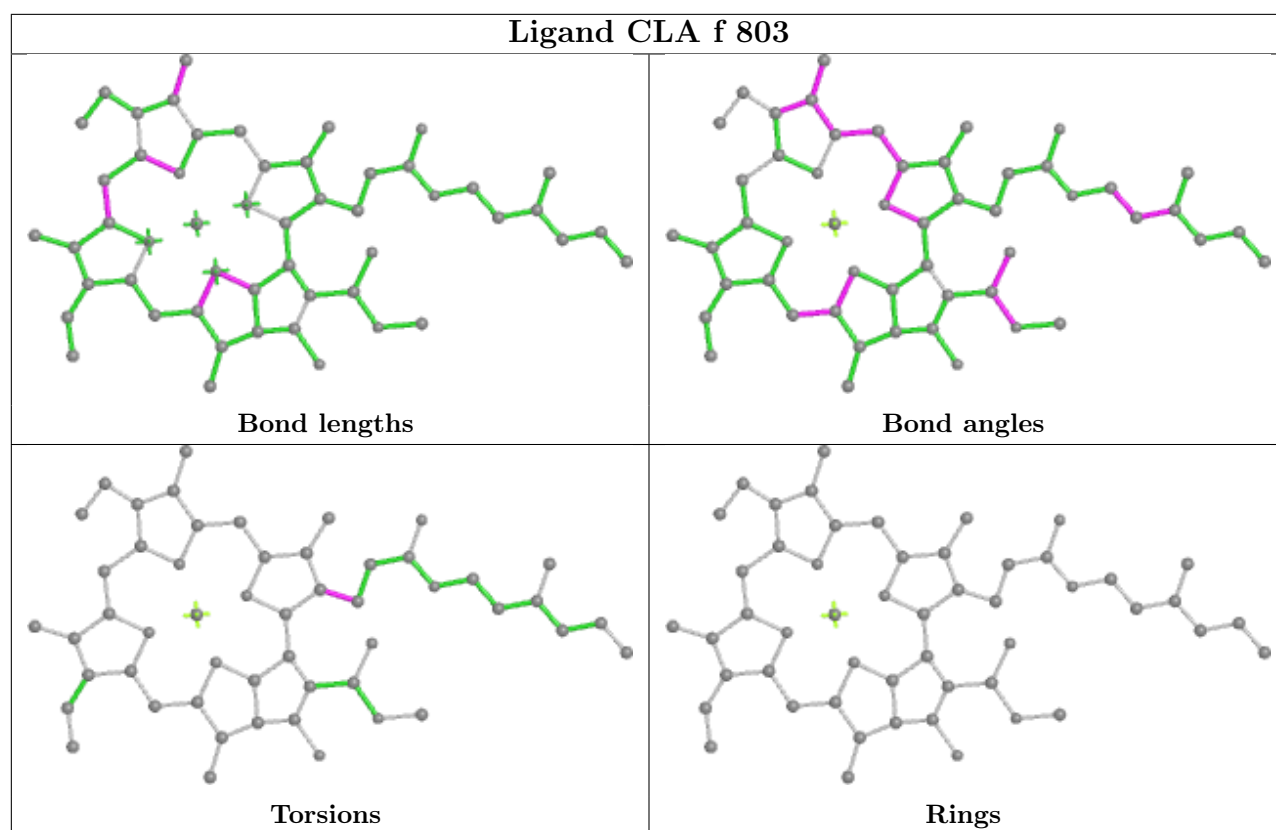
Bond angles

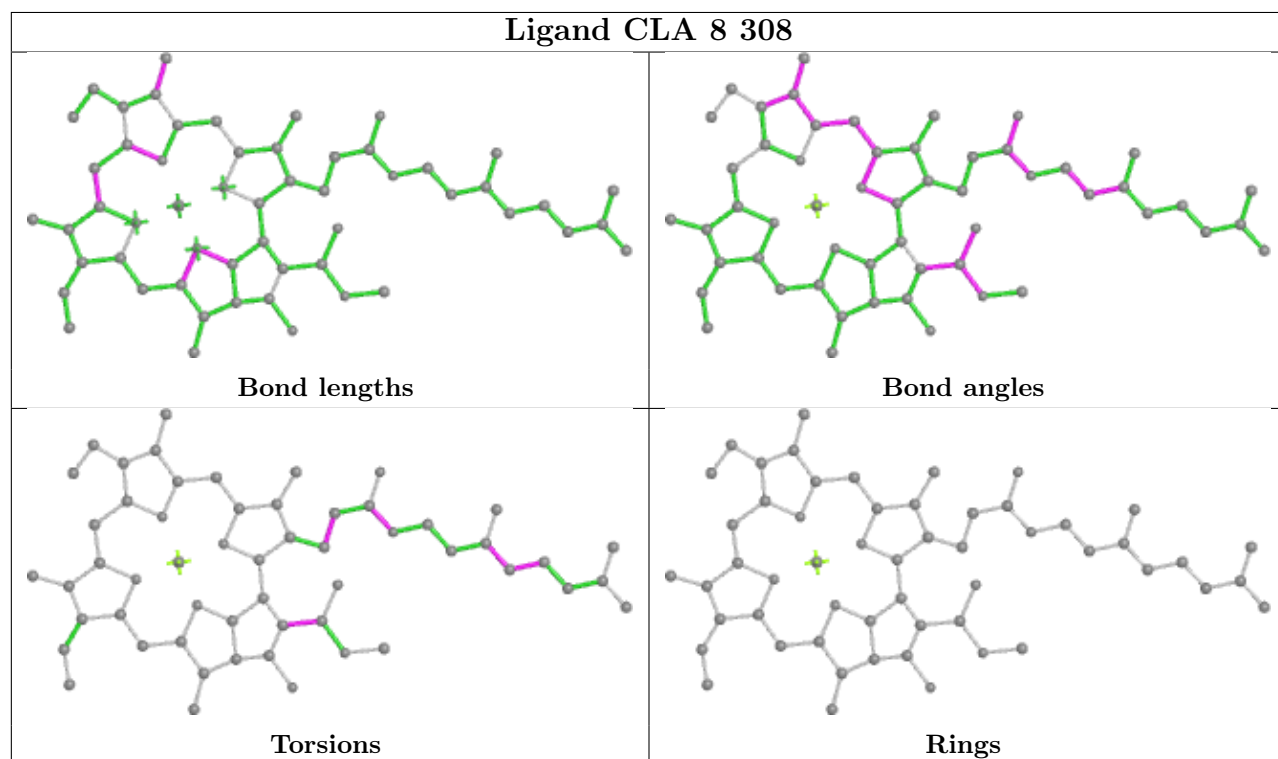
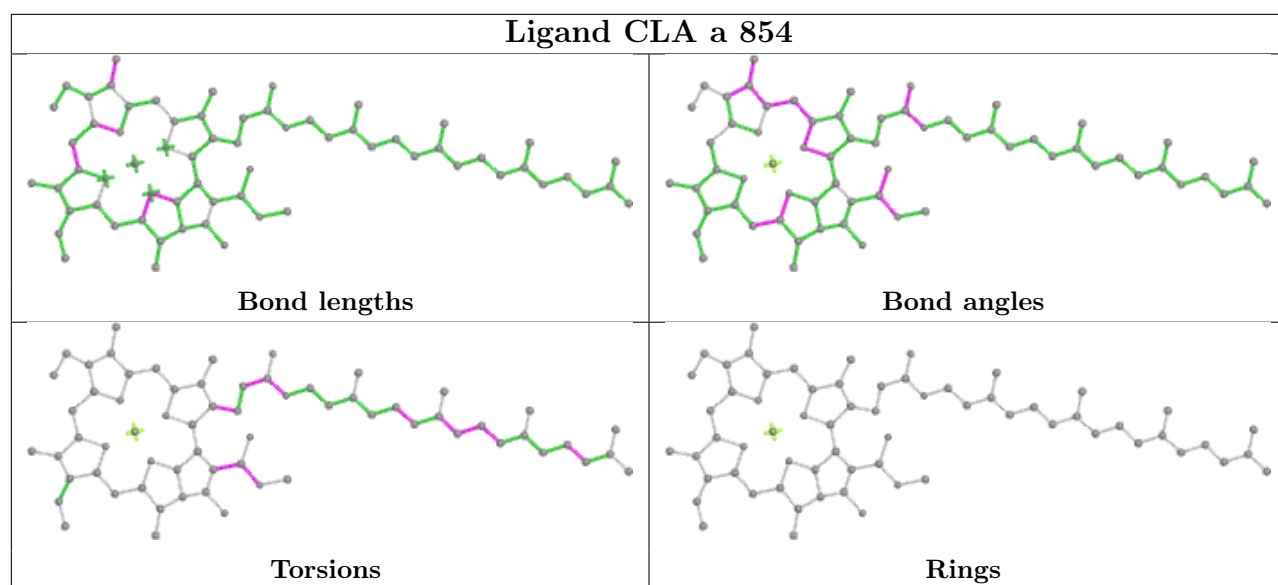


Torsions

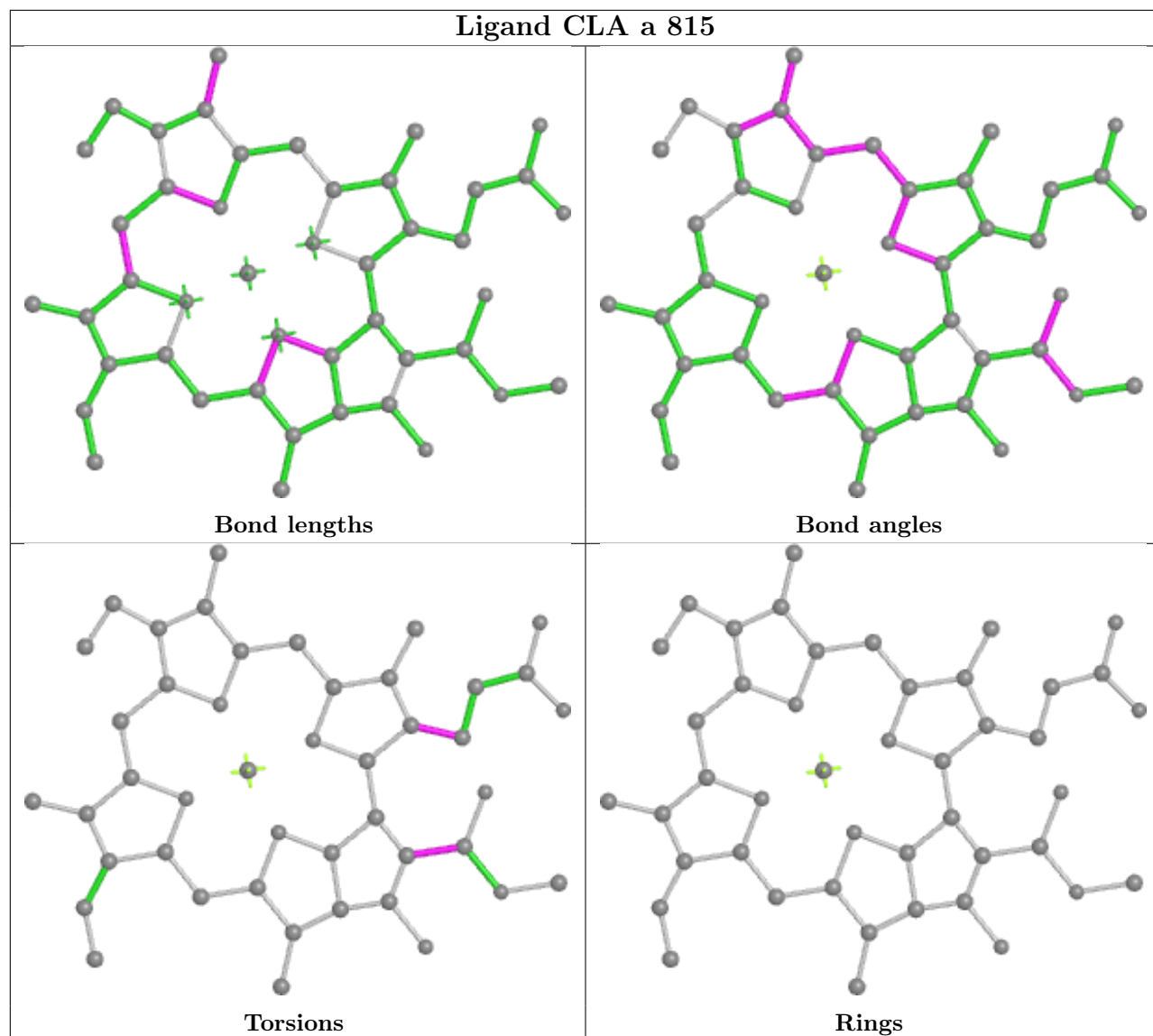


Rings

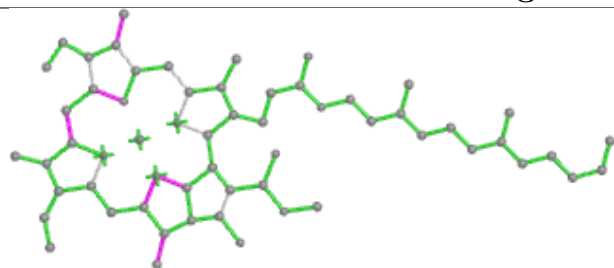




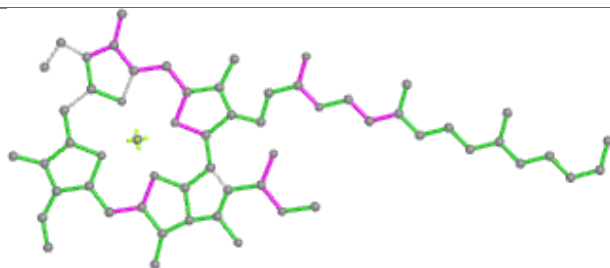
Ligand CLA a 815



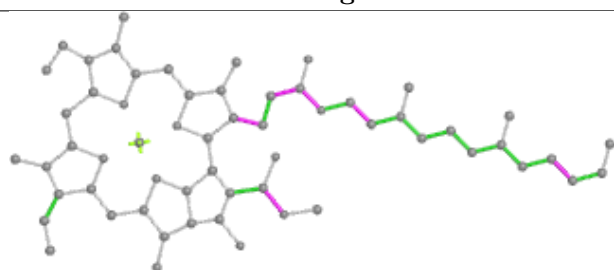
Ligand CLA b 817



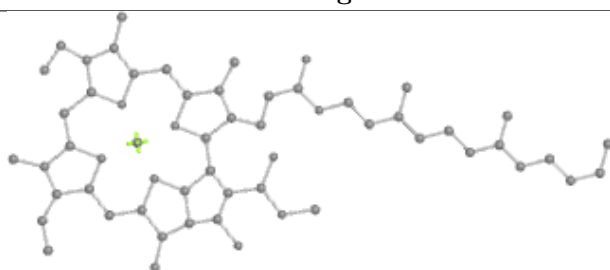
Bond lengths



Bond angles

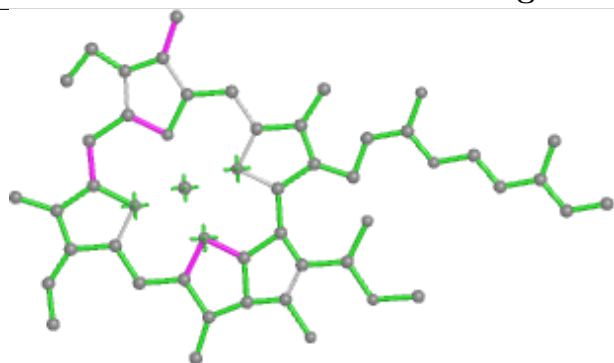


Torsions

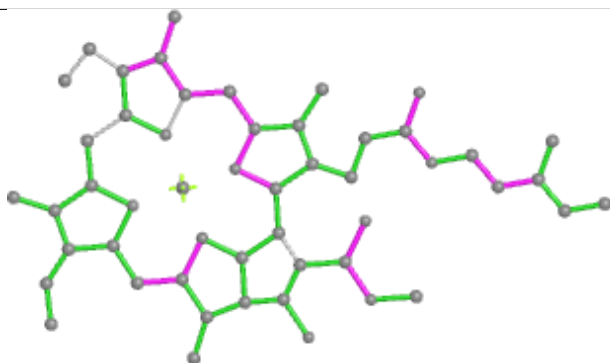


Rings

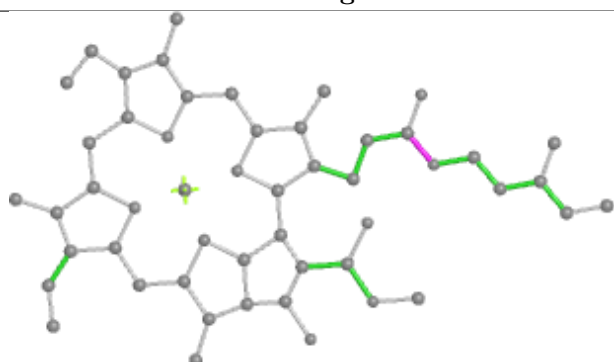
Ligand CLA b 821



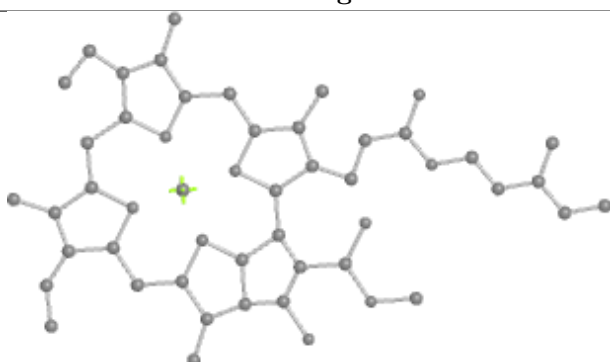
Bond lengths



Bond angles

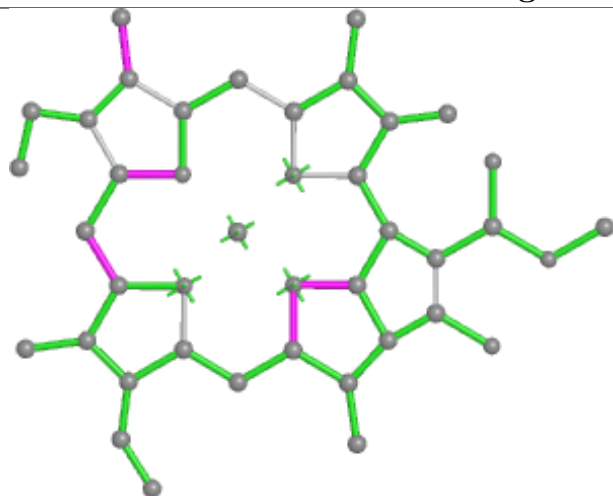


Torsions

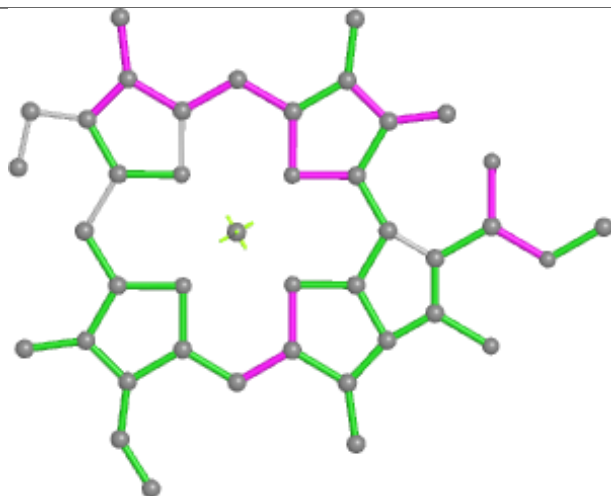


Rings

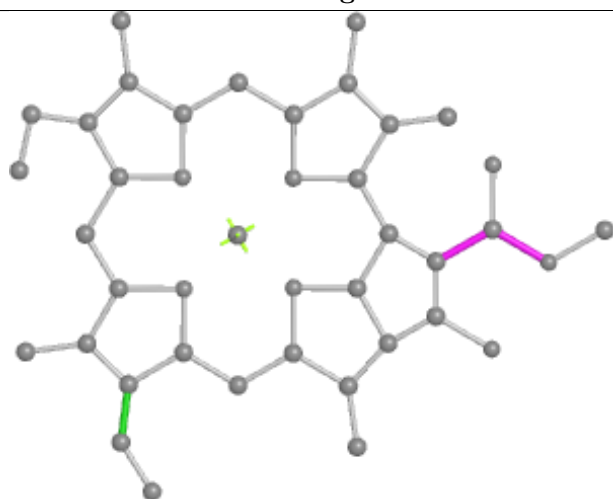
Ligand CLA 4 315



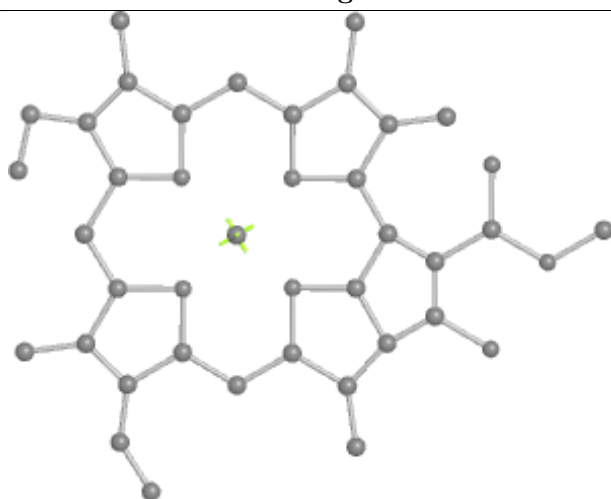
Bond lengths



Bond angles

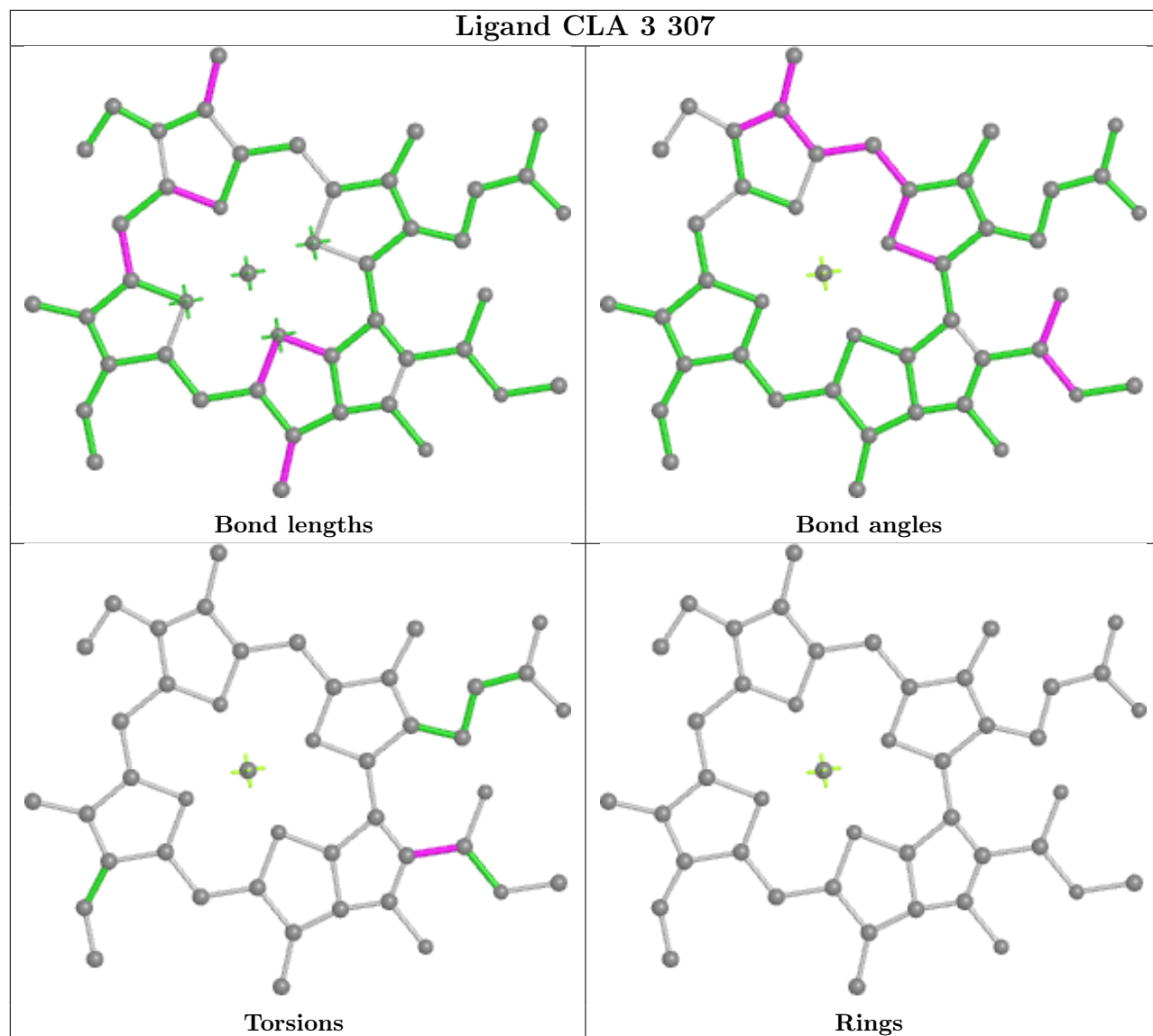


Torsions

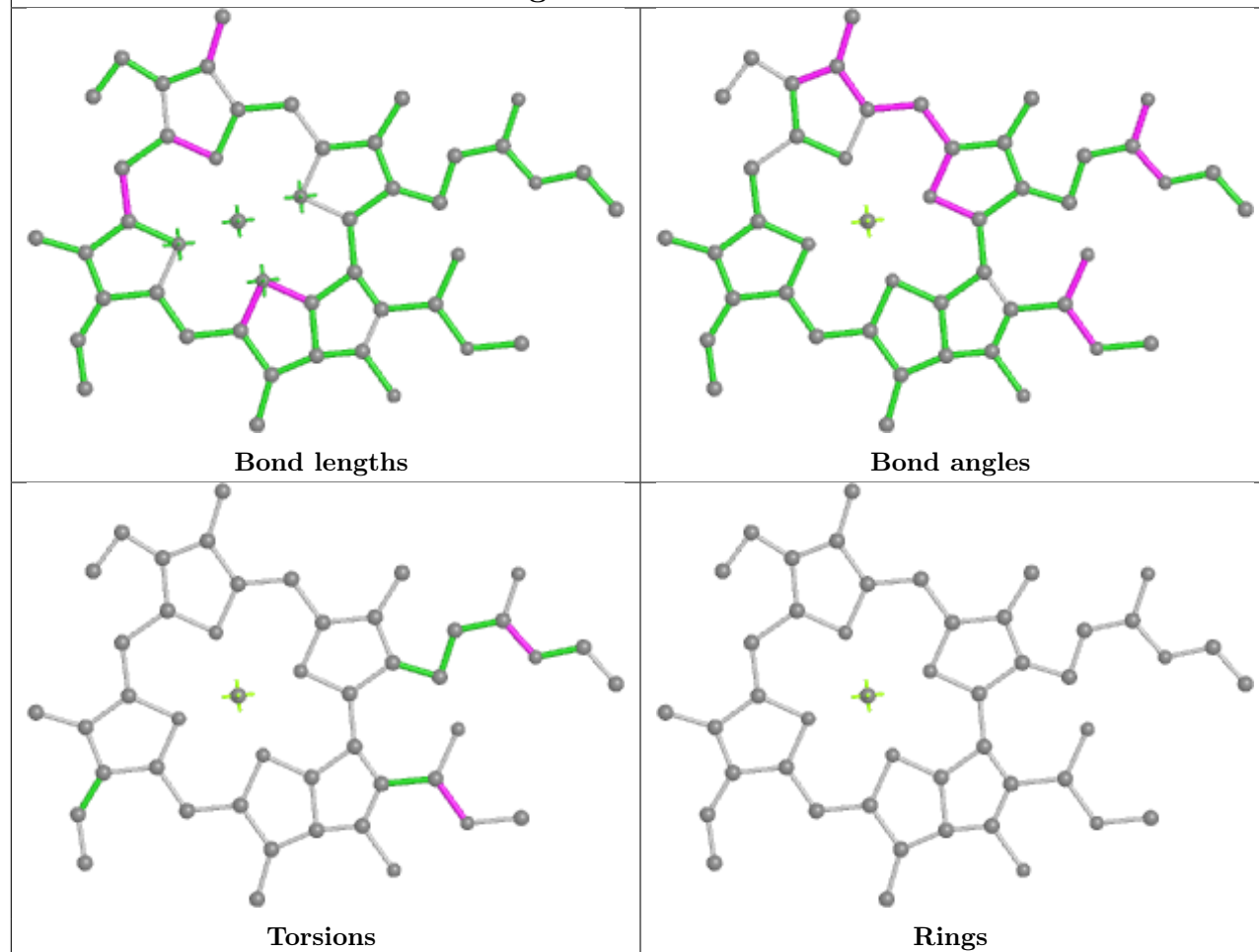


Rings

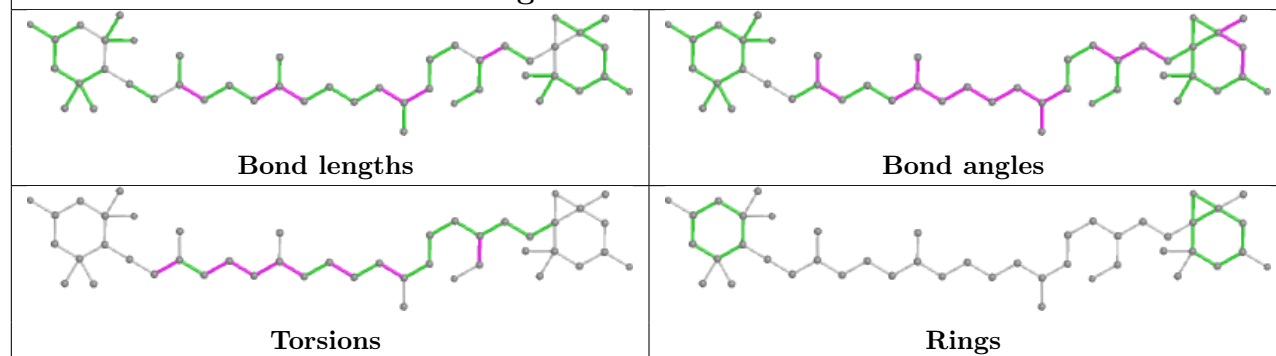
Ligand CLA 3 307



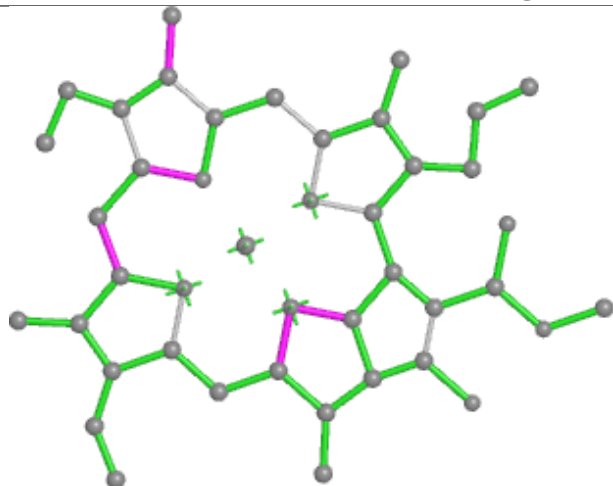
Ligand CLA 2 312



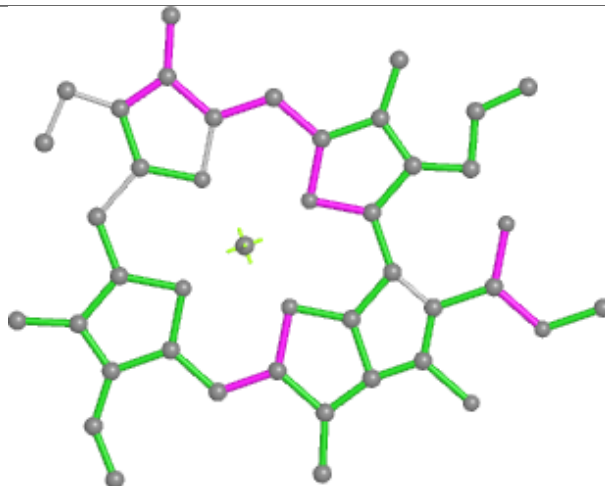
Ligand A1L1G 1 301



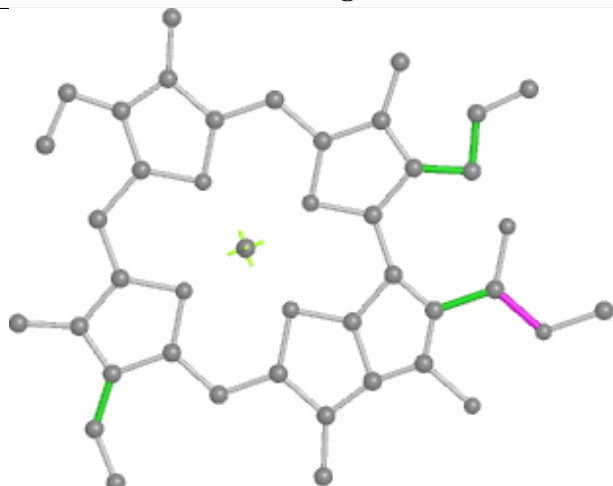
Ligand CLA 8 305



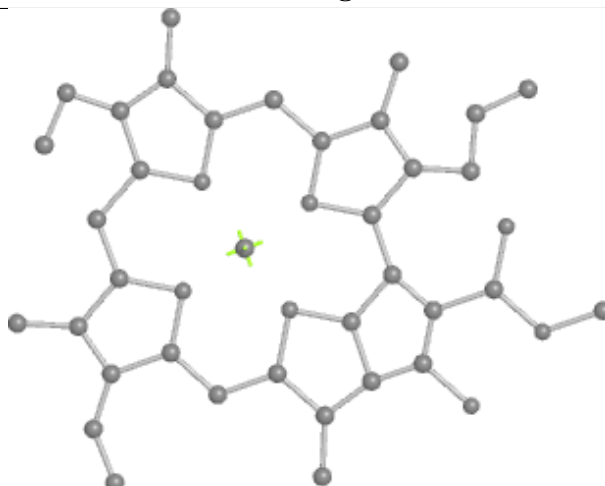
Bond lengths



Bond angles

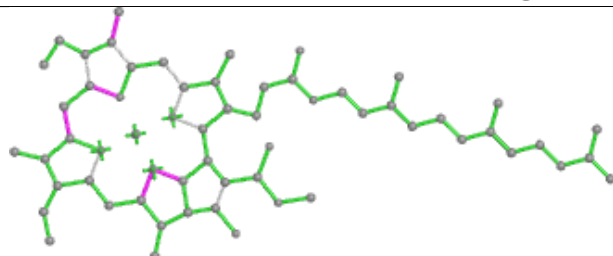


Torsions

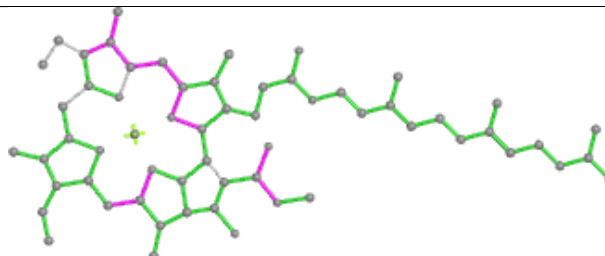


Rings

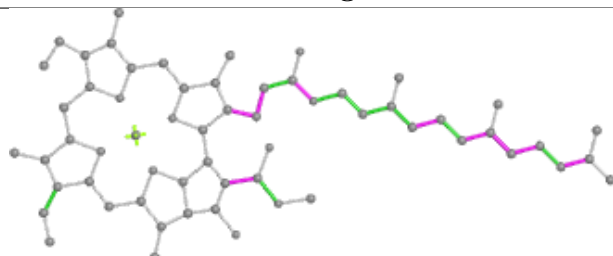
Ligand CLA b 818



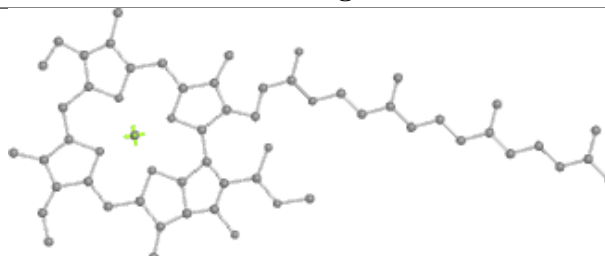
Bond lengths



Bond angles

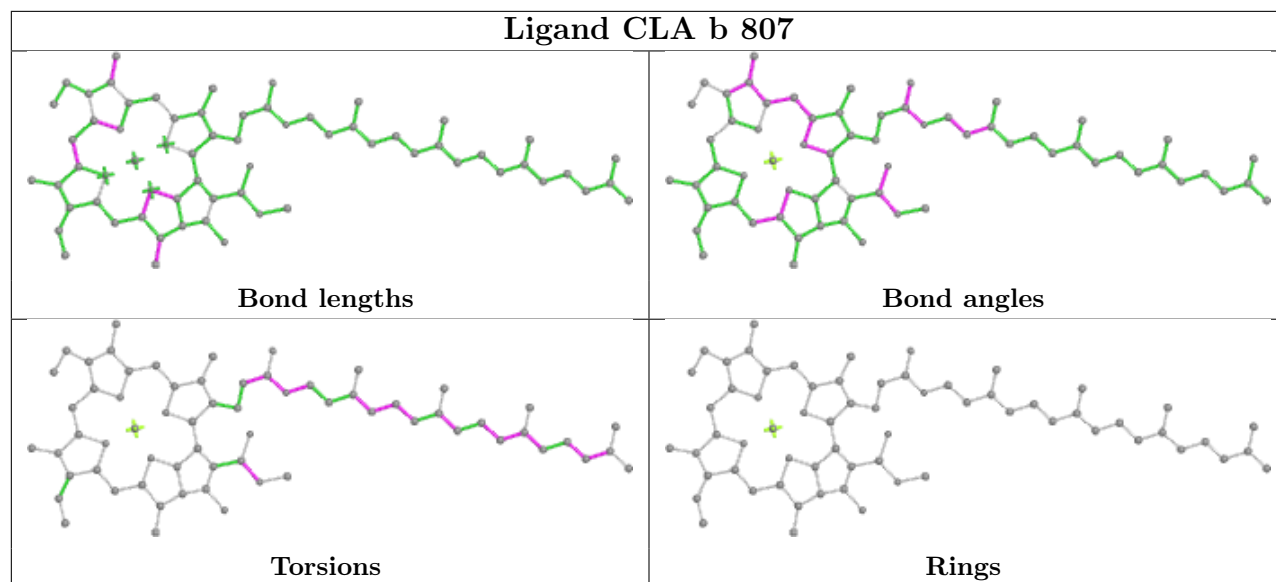


Torsions

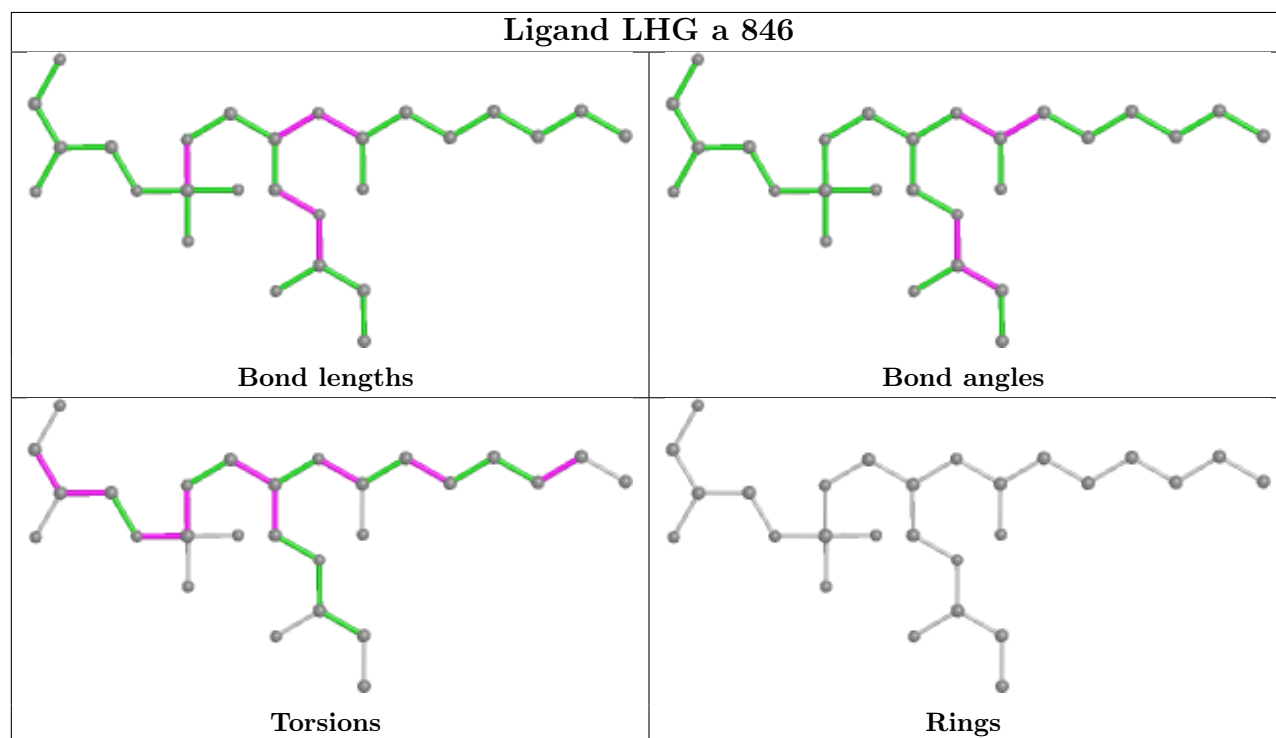


Rings

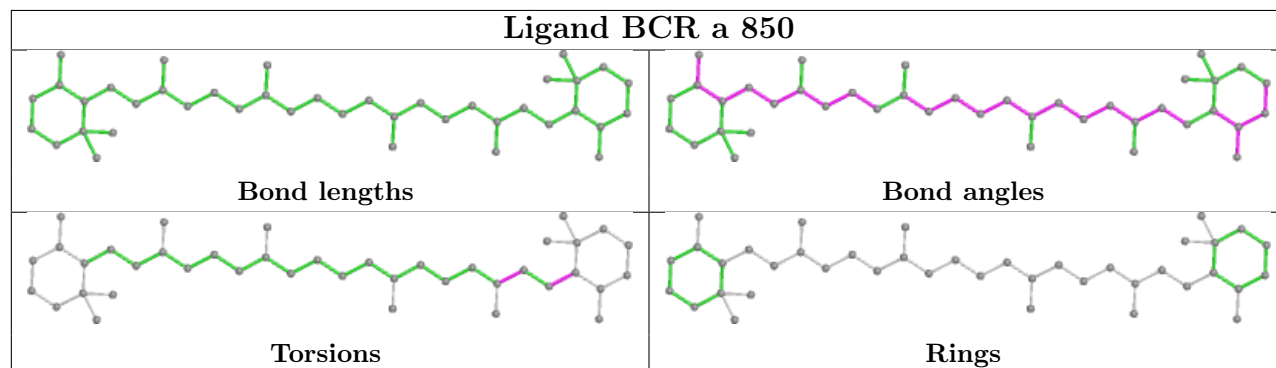
Ligand CLA b 807



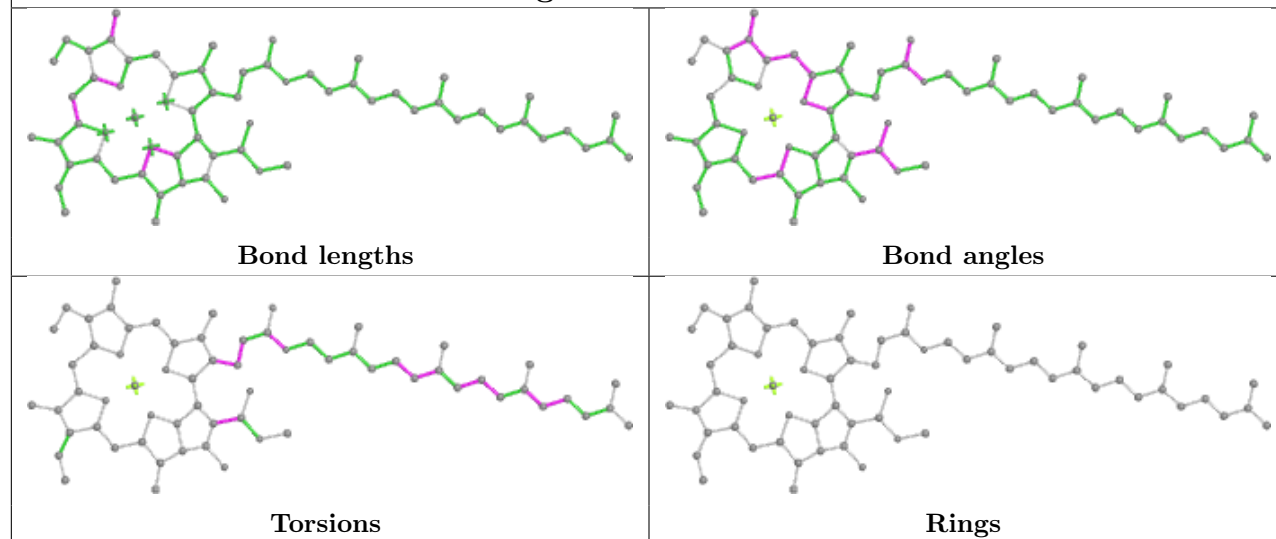
Ligand LHG a 846



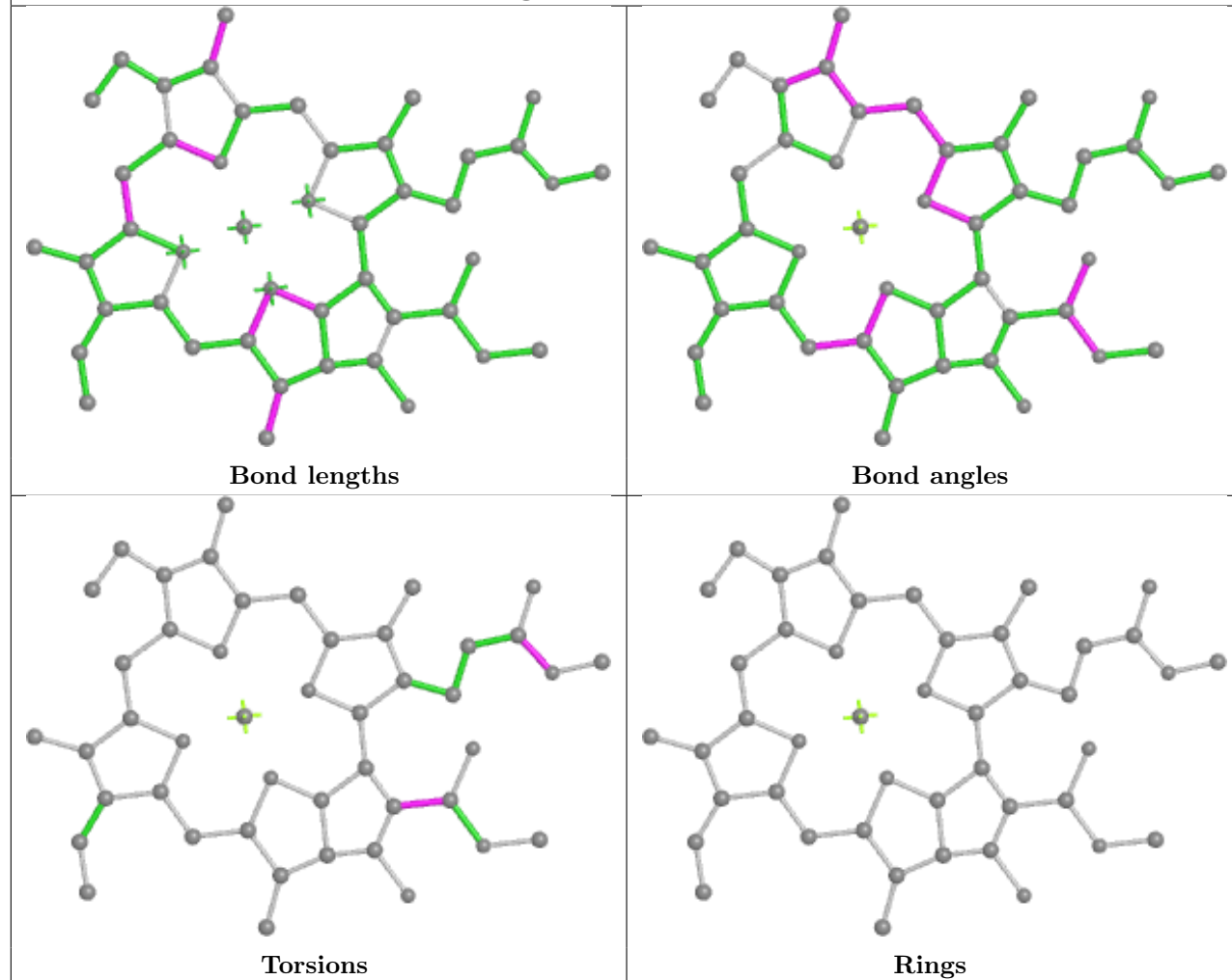
Ligand BCR a 850



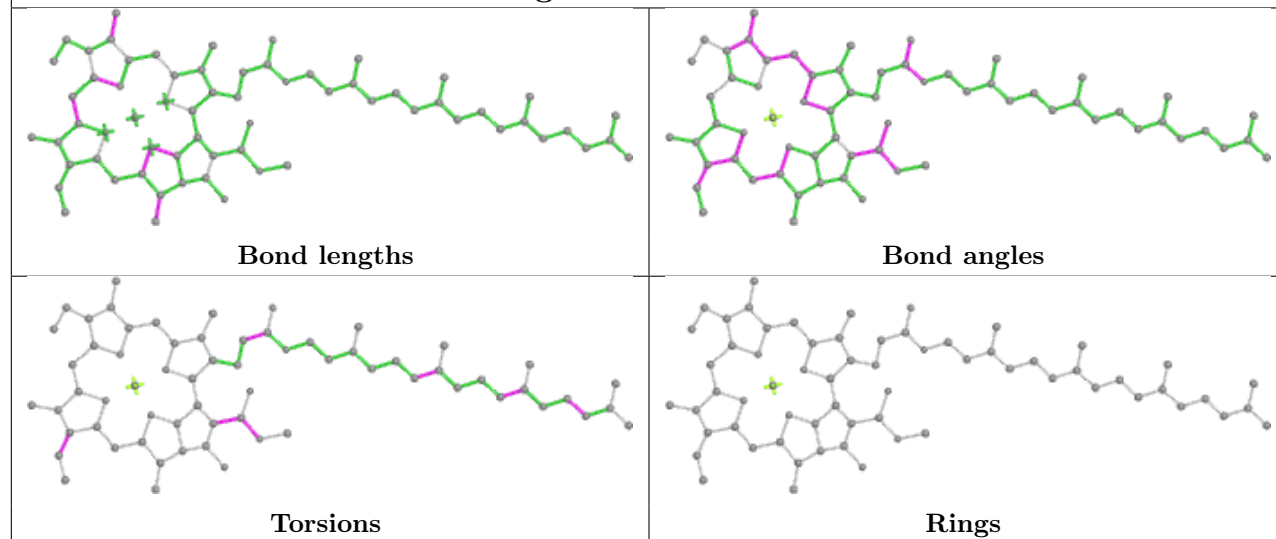
Ligand CLA a 809



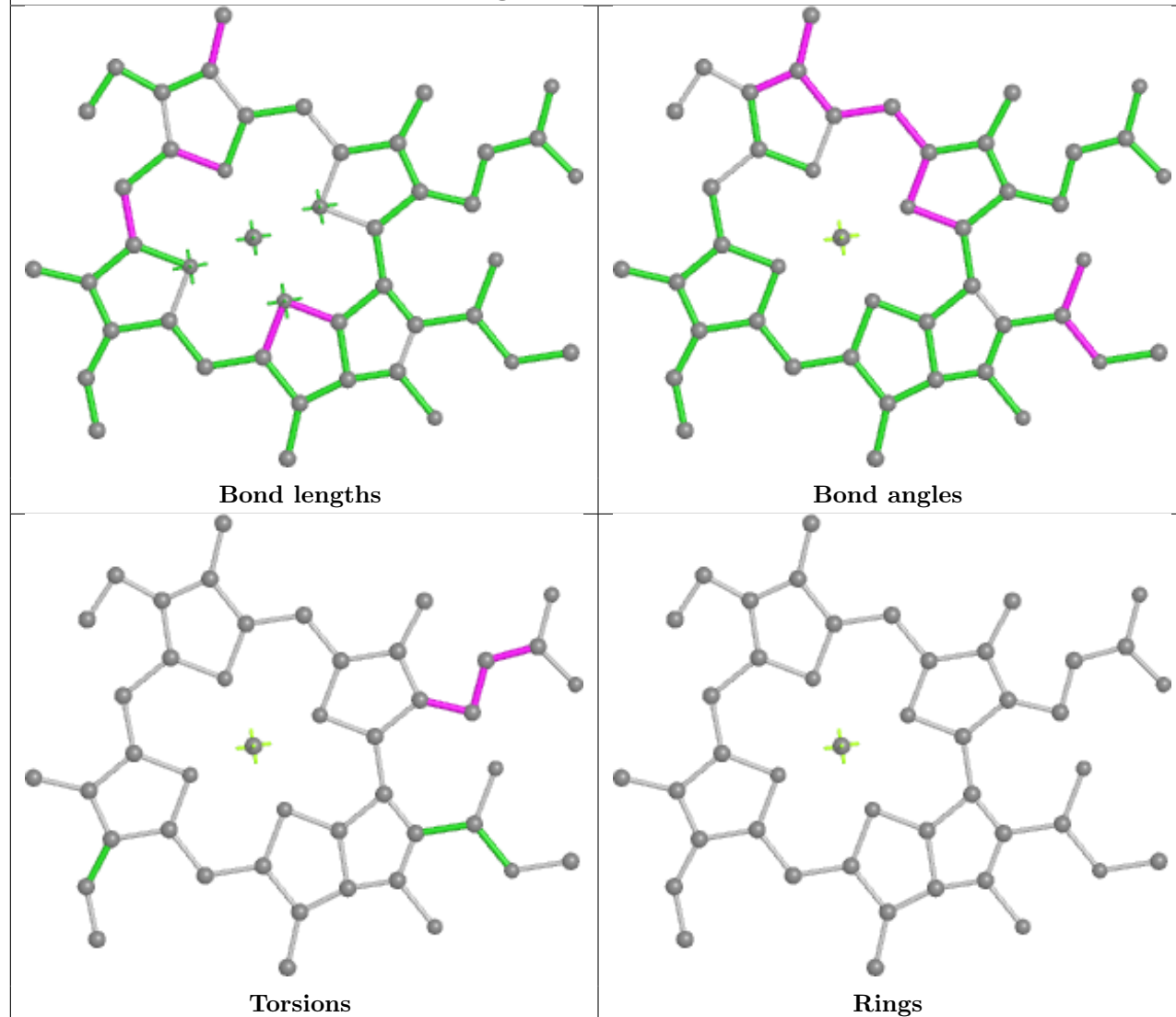
Ligand CLA 9 309

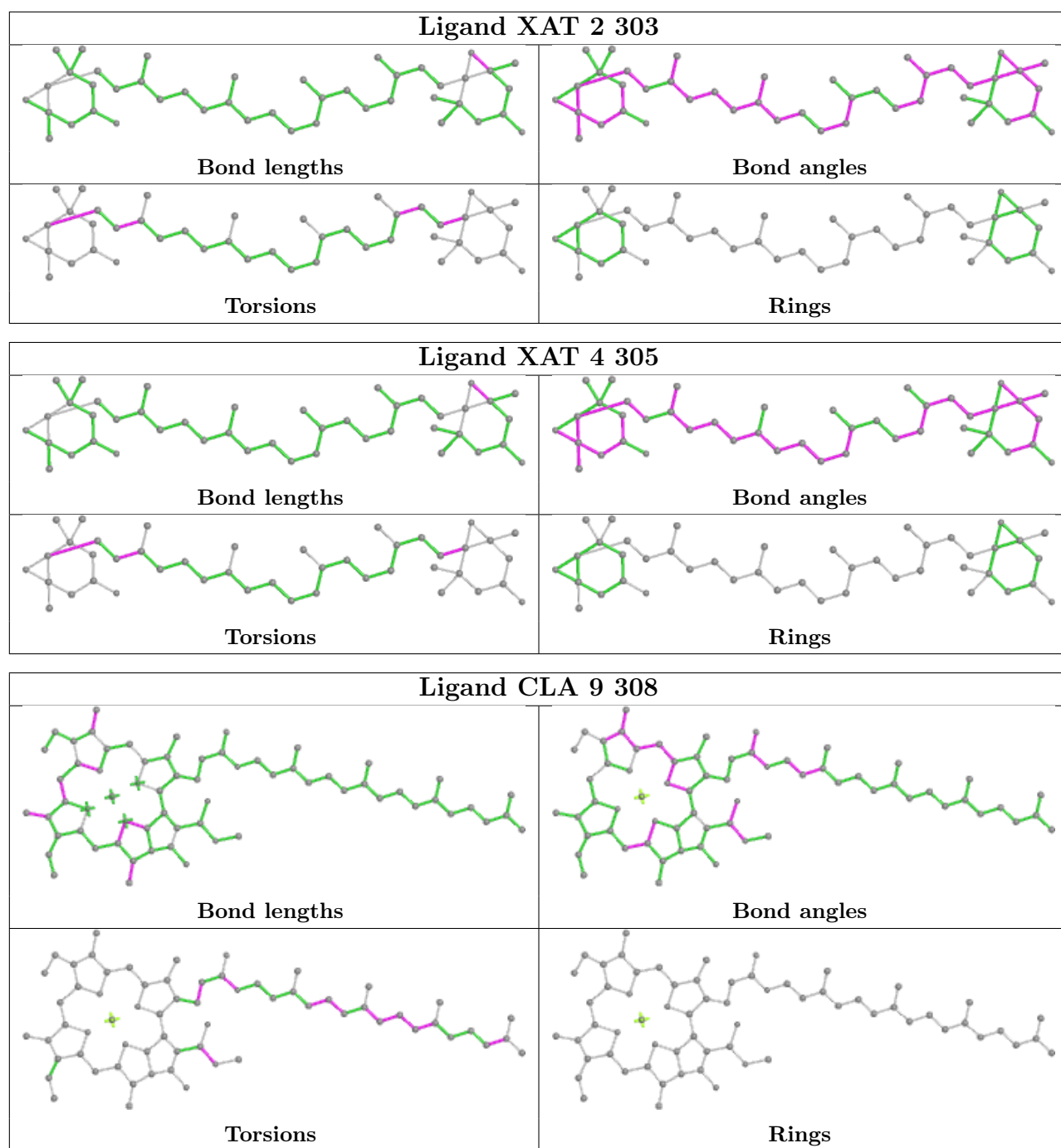


Ligand CLA b 804

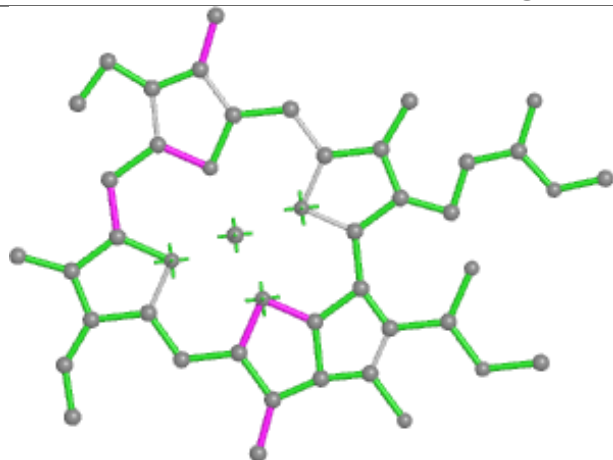


Ligand CLA 1 314

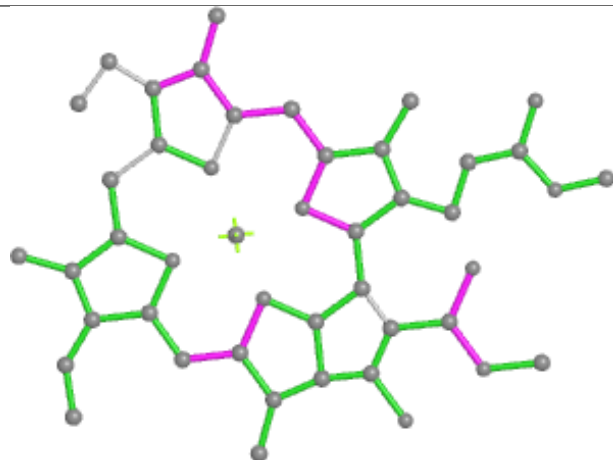




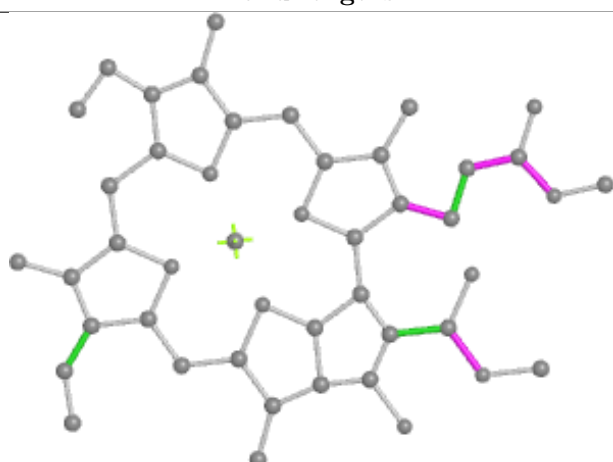
Ligand CLA 3 315



Bond lengths



Bond angles

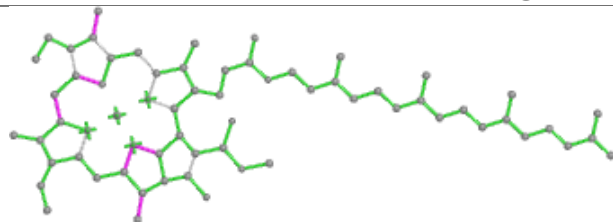


Torsions

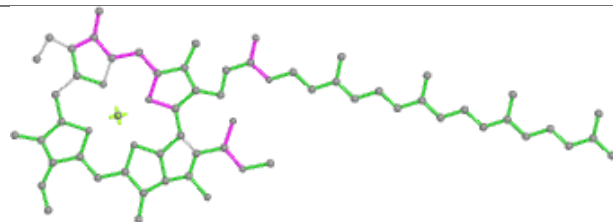


Rings

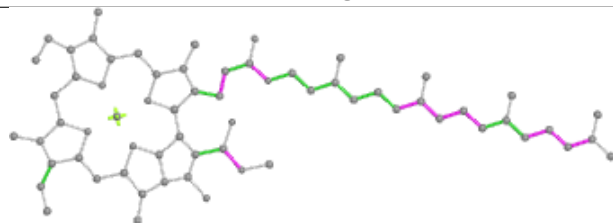
Ligand CLA b 827



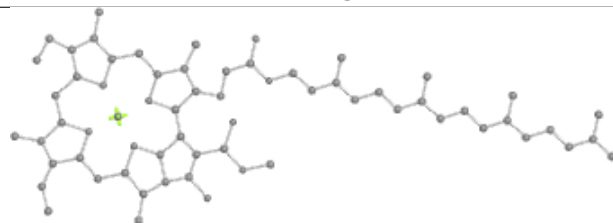
Bond lengths



Bond angles

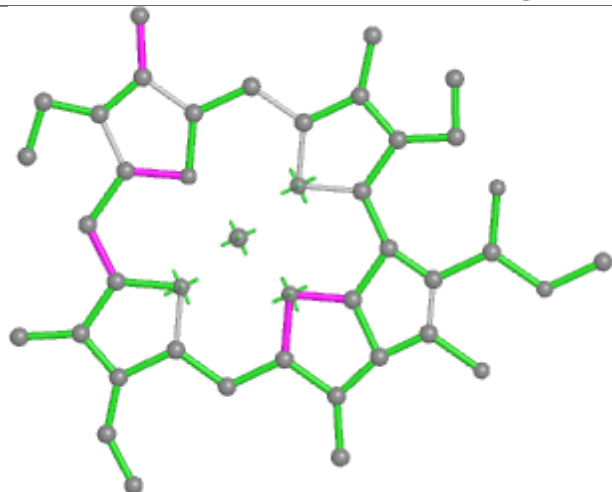


Torsions

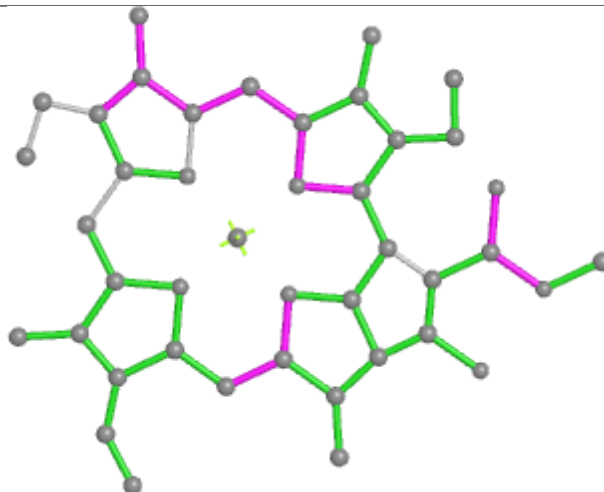


Rings

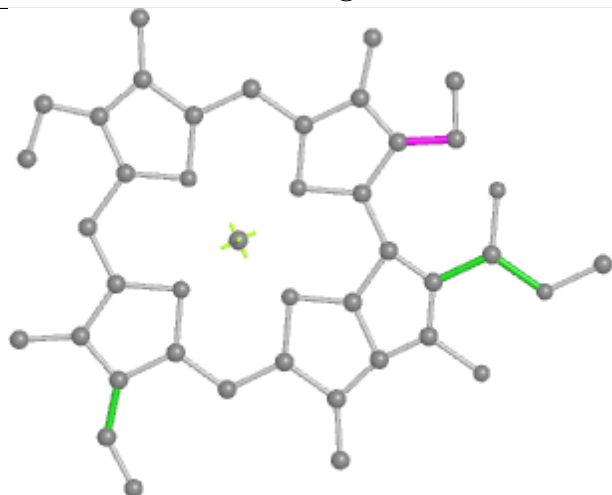
Ligand CLA 6 311



Bond lengths



Bond angles

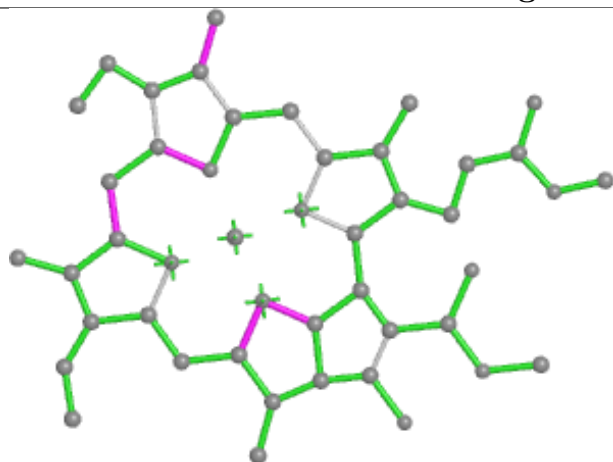


Torsions

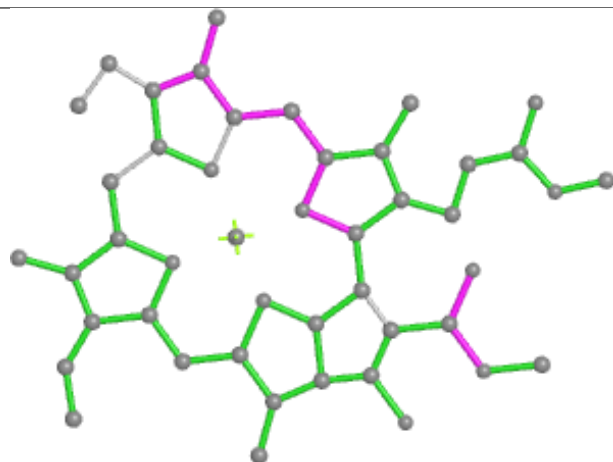


Rings

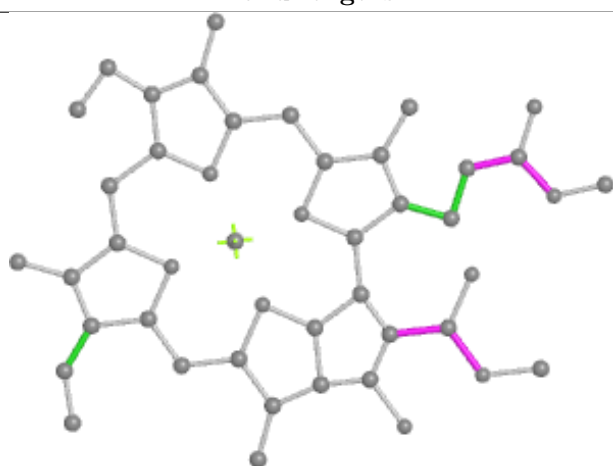
Ligand CLA 6 314



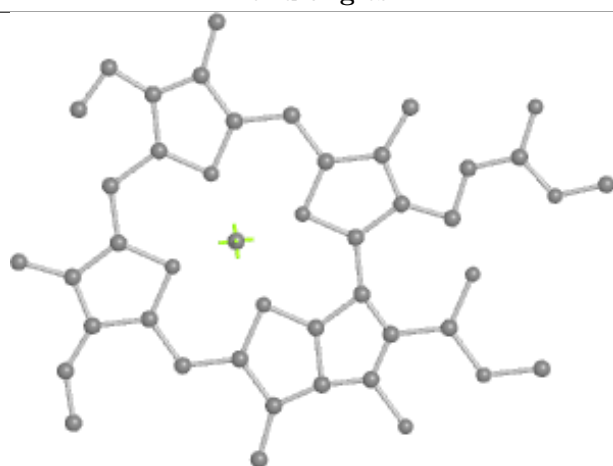
Bond lengths



Bond angles

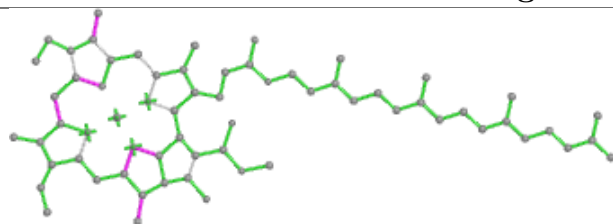


Torsions

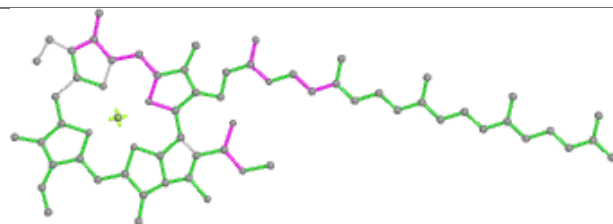


Rings

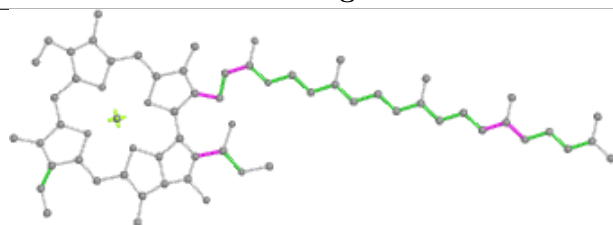
Ligand CLA b 837



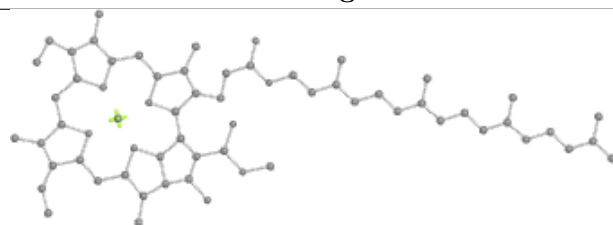
Bond lengths



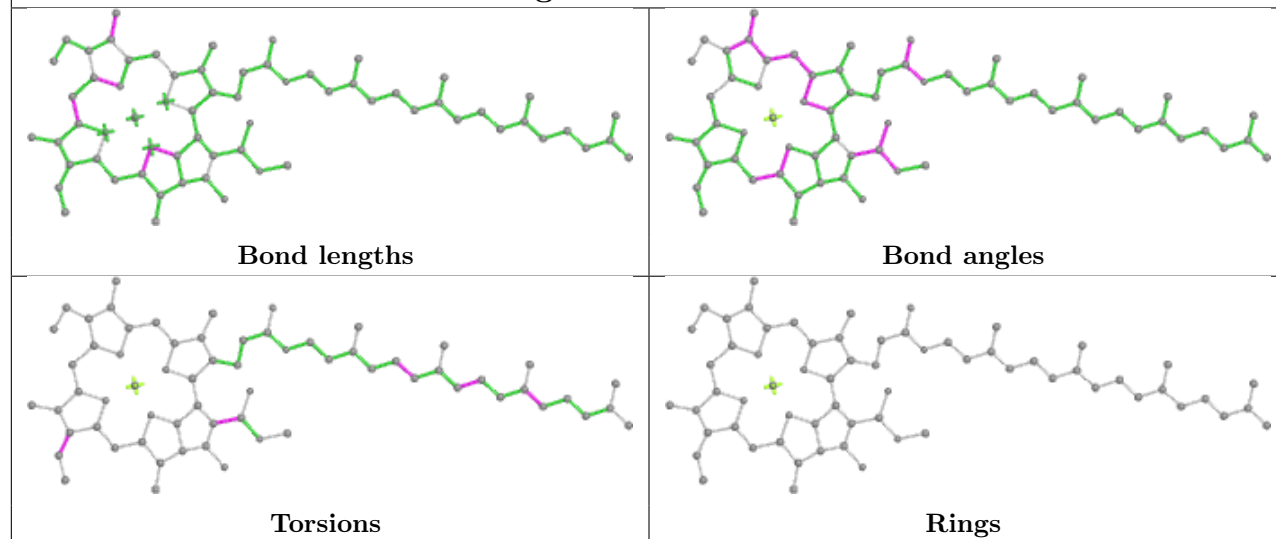
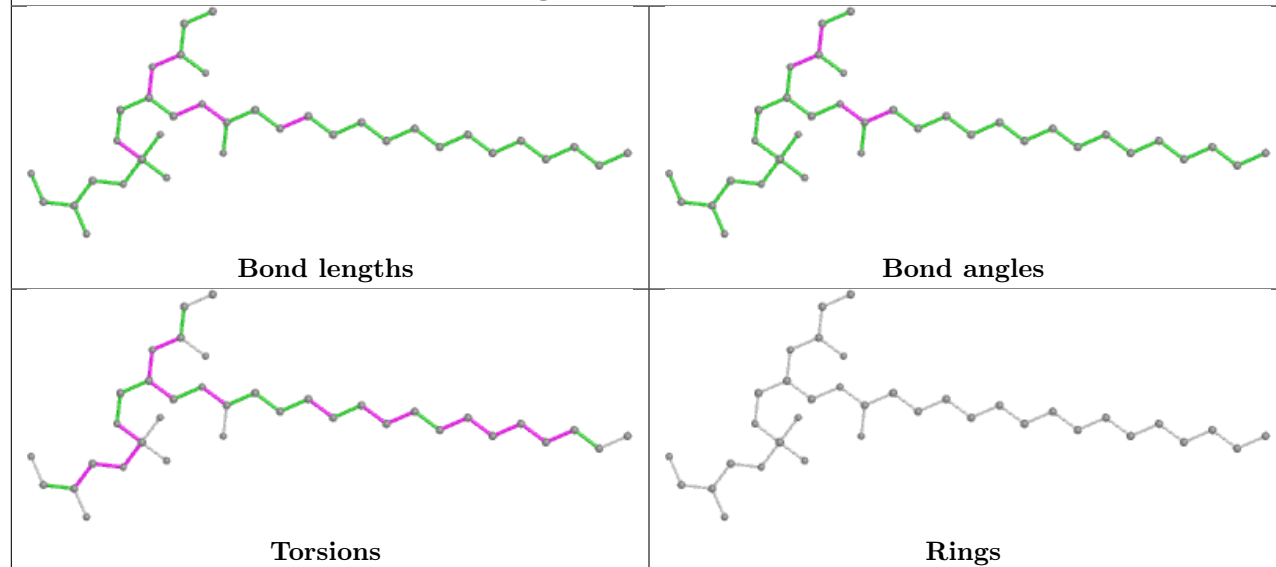
Bond angles



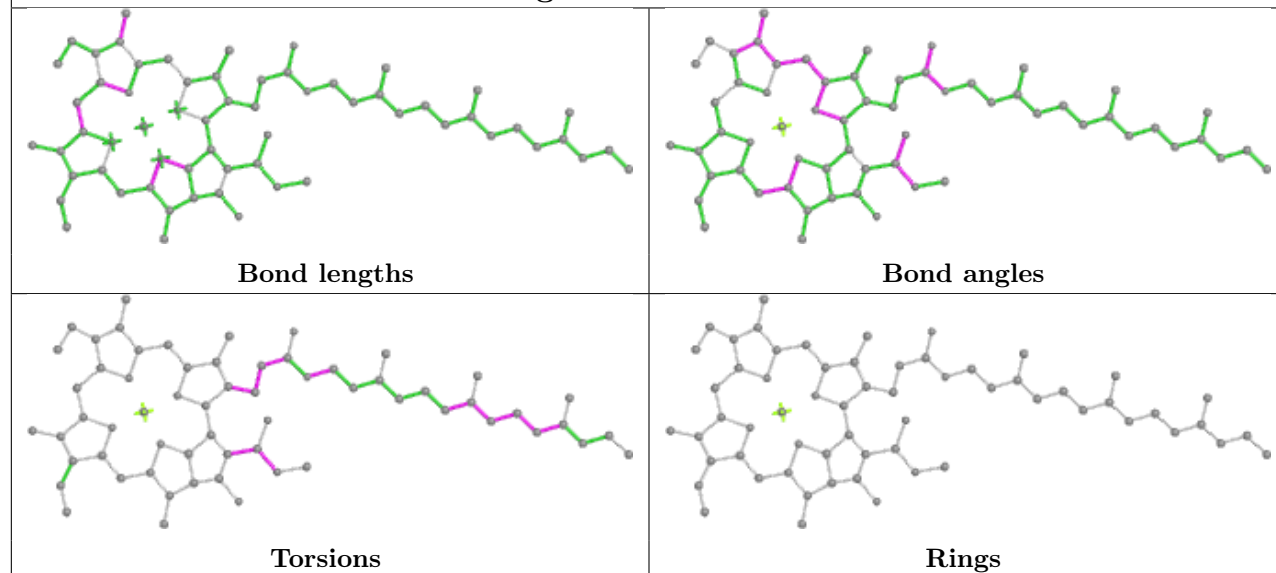
Torsions



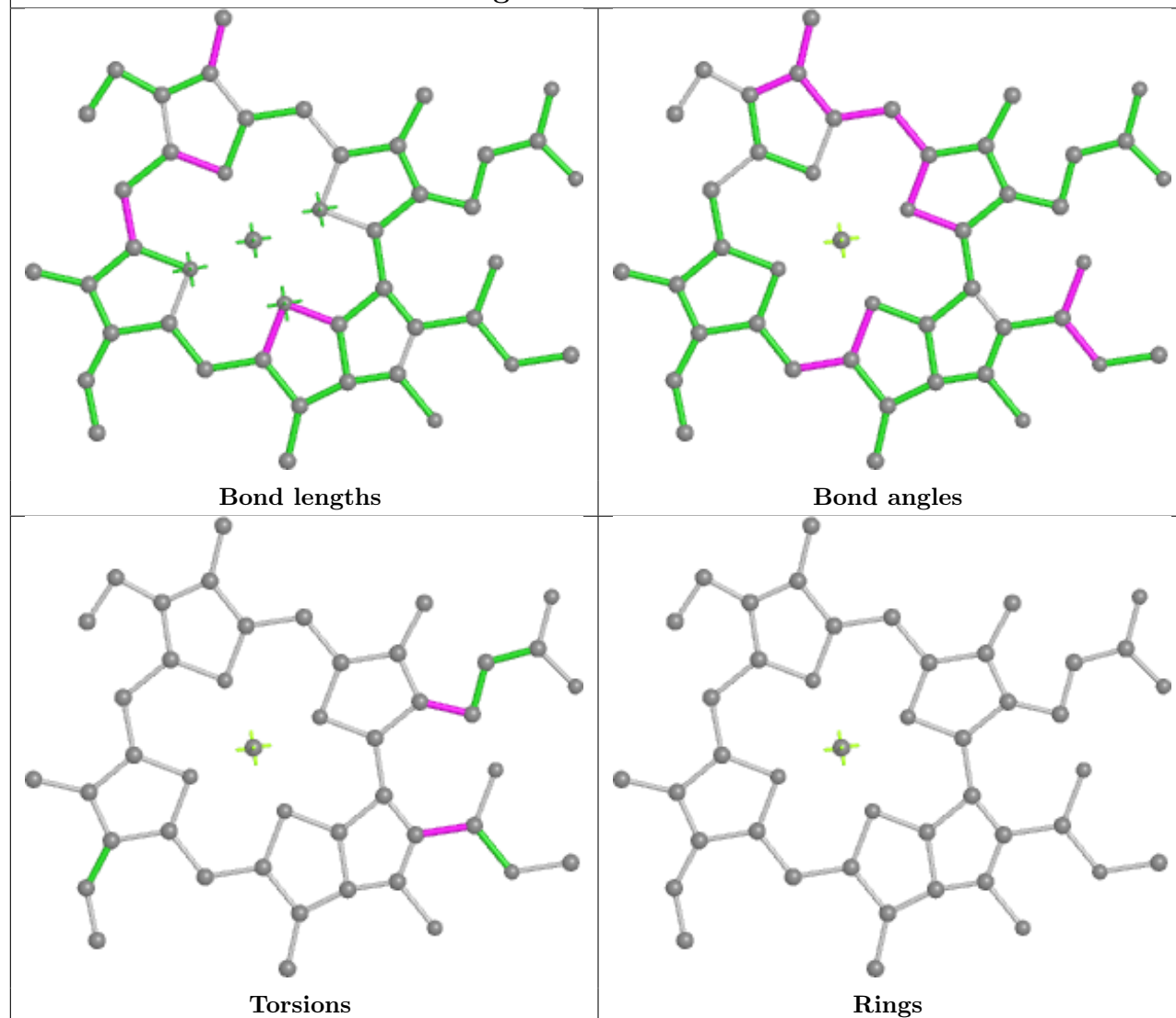
Rings

Ligand CLA b 836**Ligand LHG 9 307**

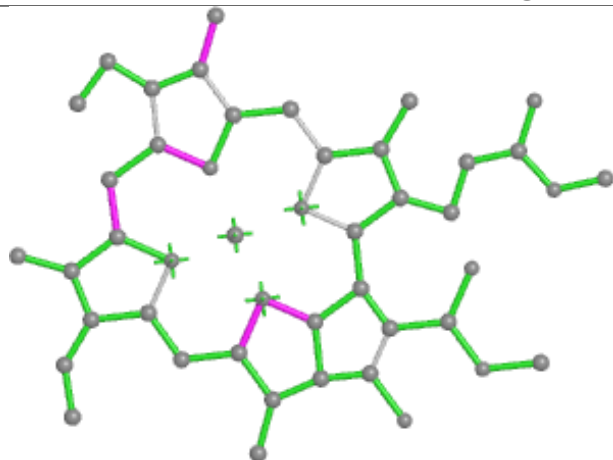
Ligand CLA a 829



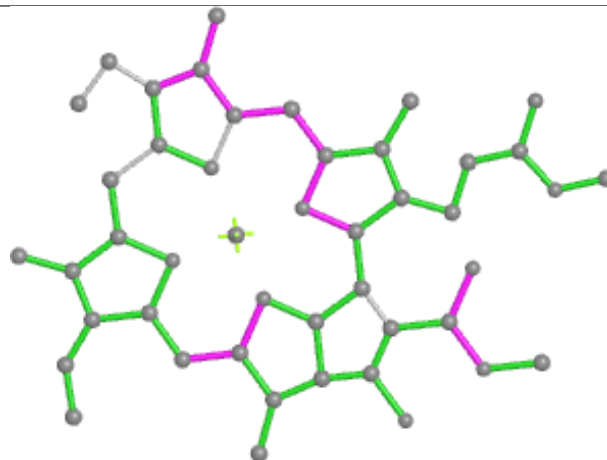
Ligand CLA b 815



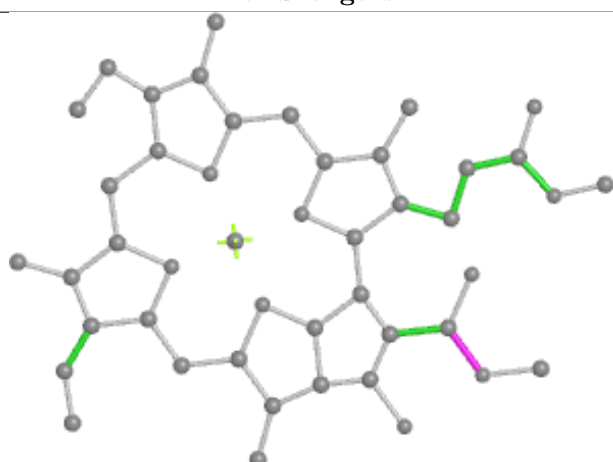
Ligand CLA 8 306



Bond lengths



Bond angles

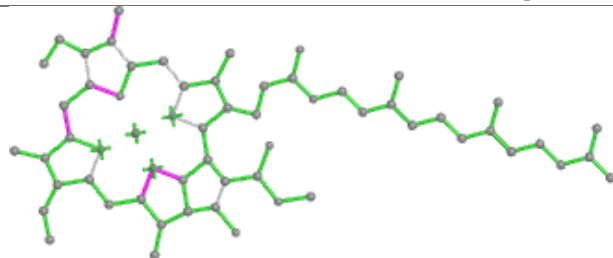


Torsions

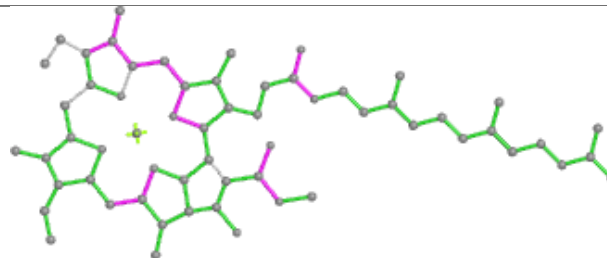


Rings

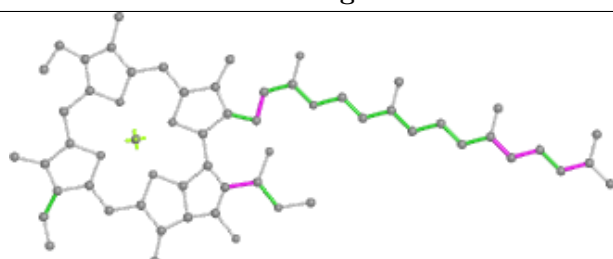
Ligand CLA 5 307



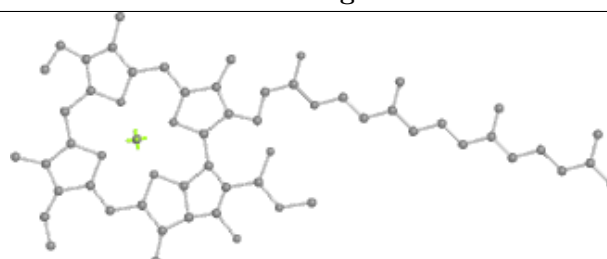
Bond lengths



Bond angles

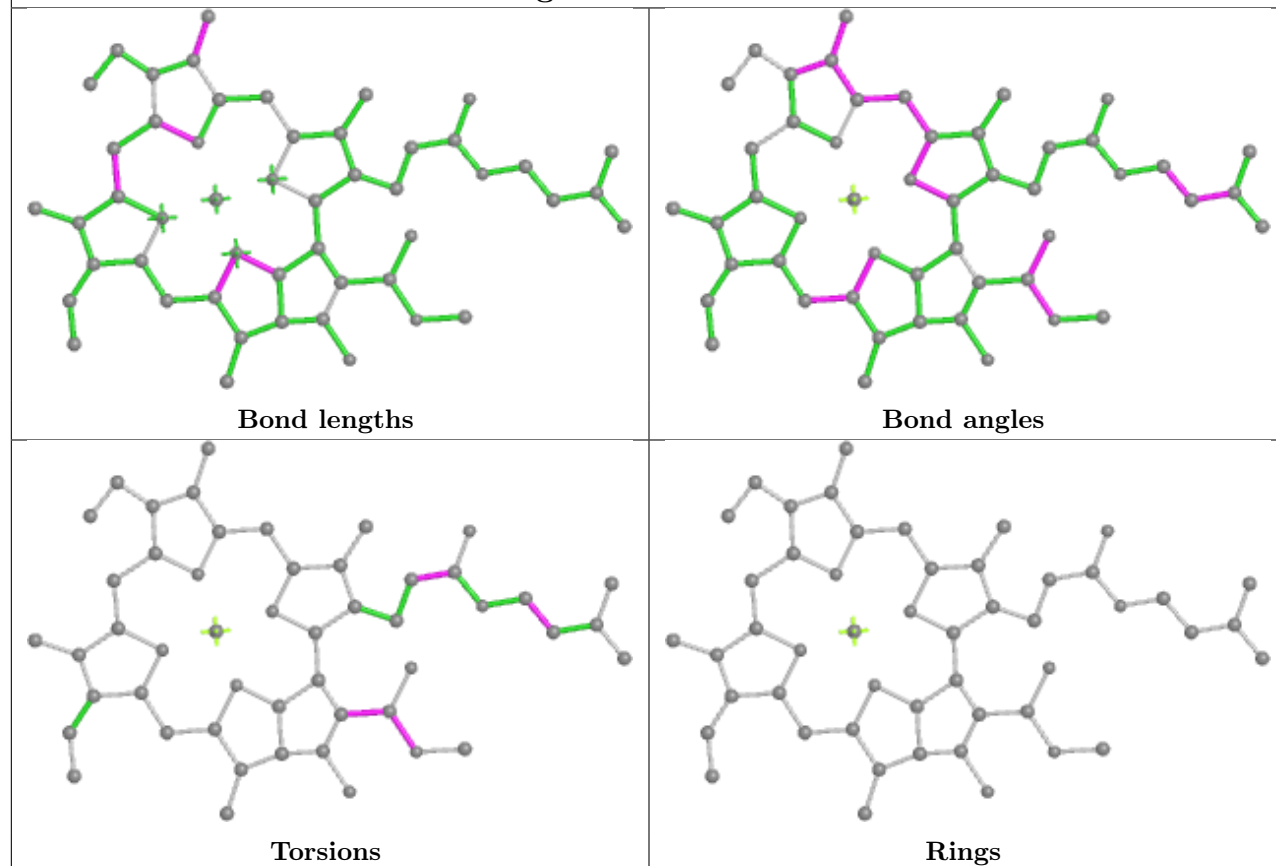


Torsions

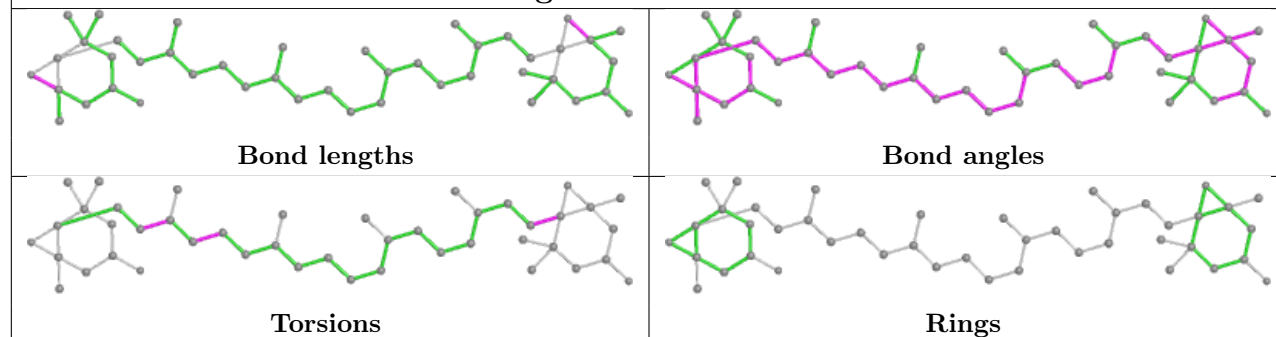


Rings

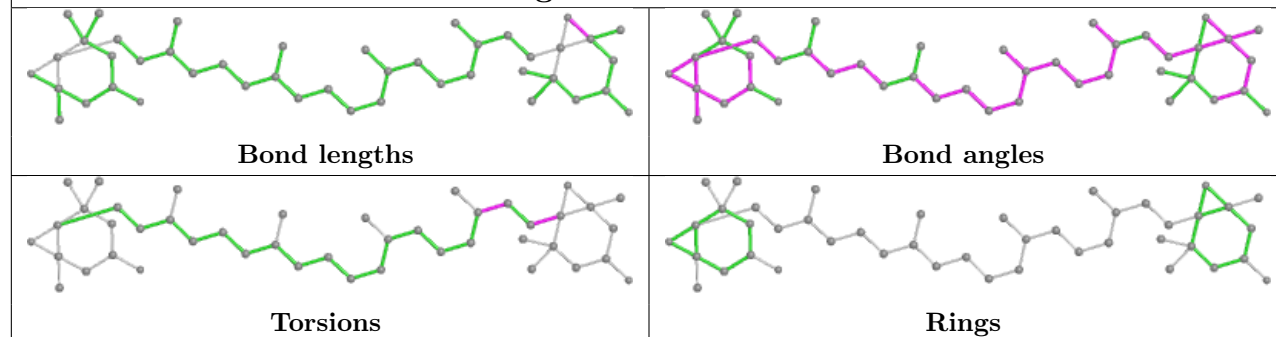
Ligand CLA 4 309

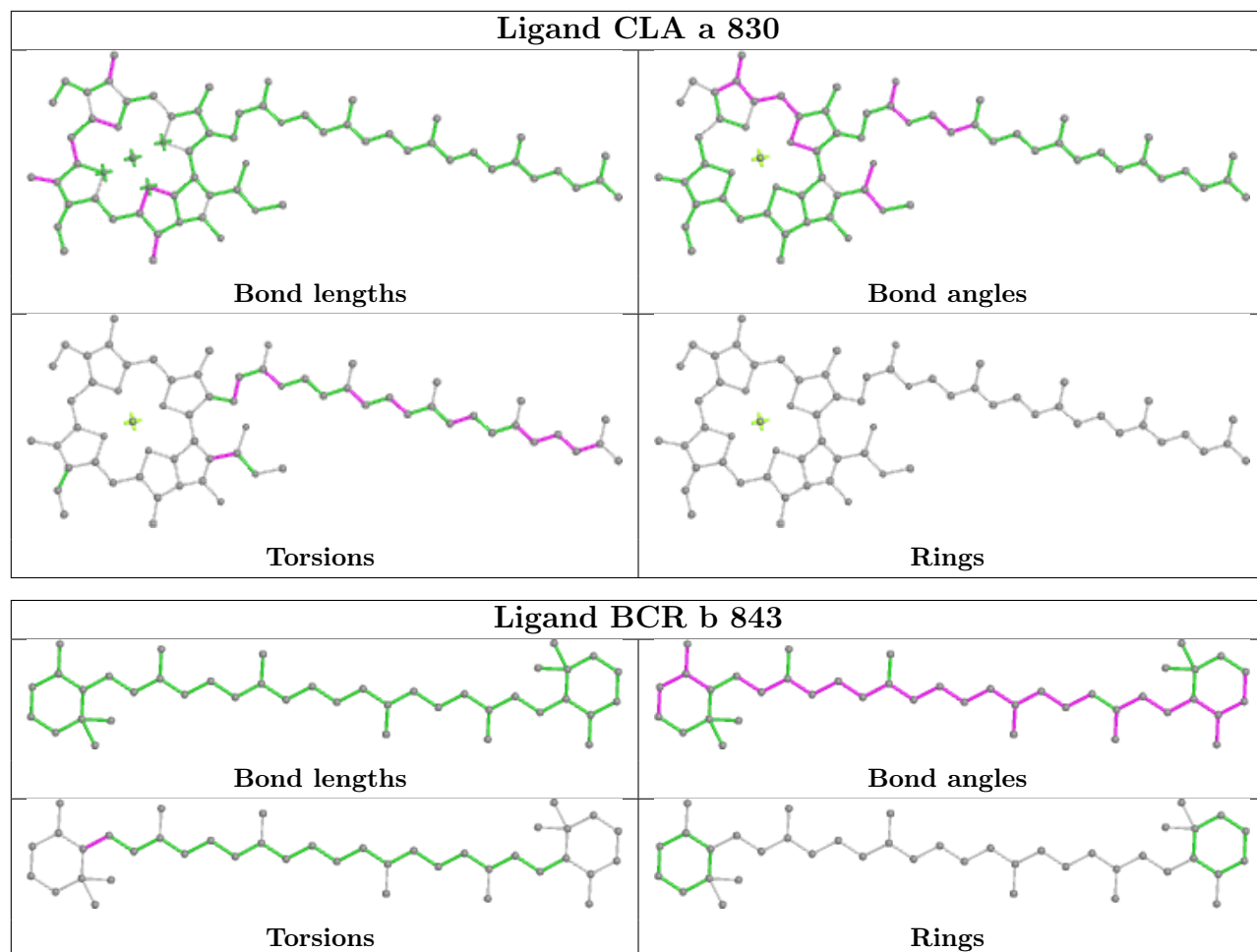


Ligand XAT 6 306

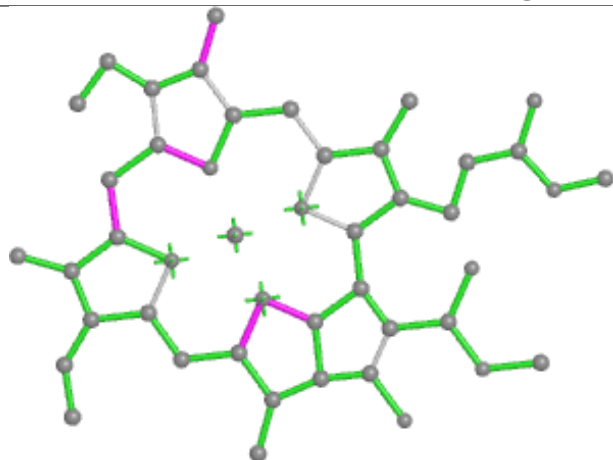


Ligand XAT 5 302

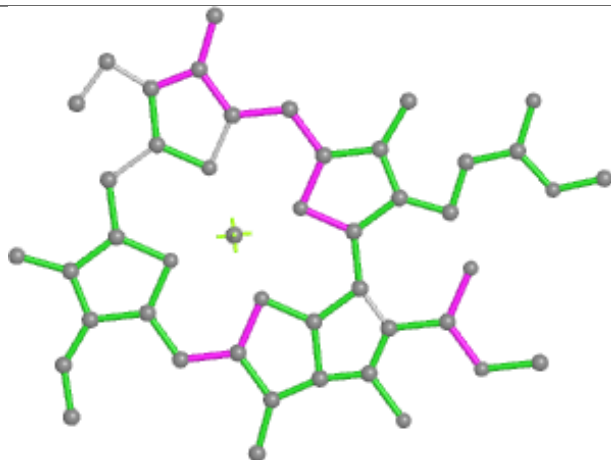




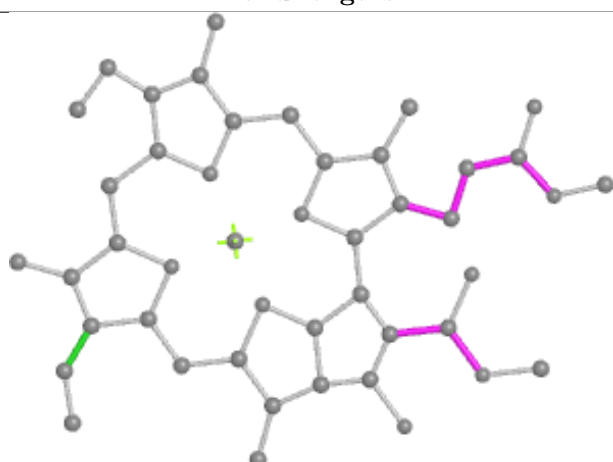
Ligand CLA 9 313



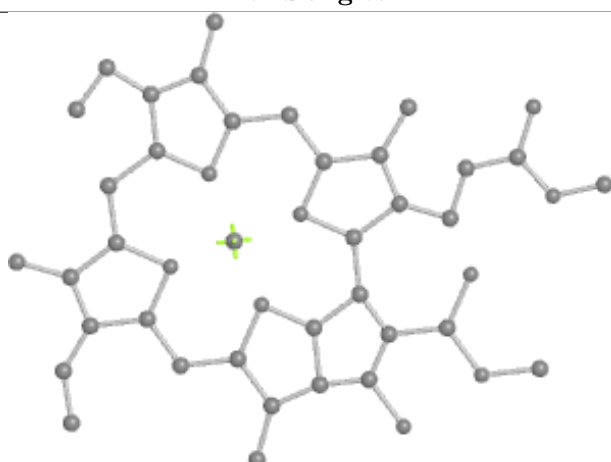
Bond lengths



Bond angles

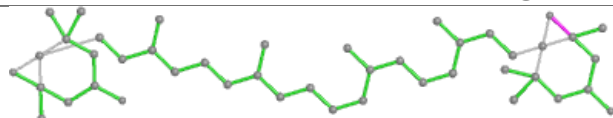


Torsions

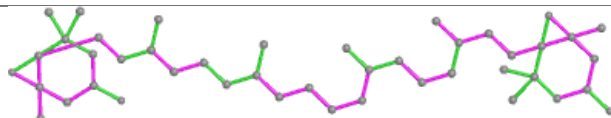


Rings

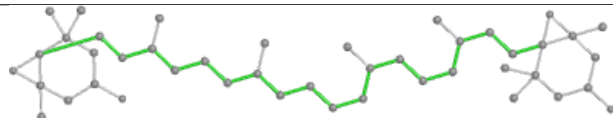
Ligand XAT 3 305



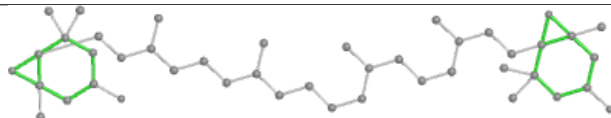
Bond lengths



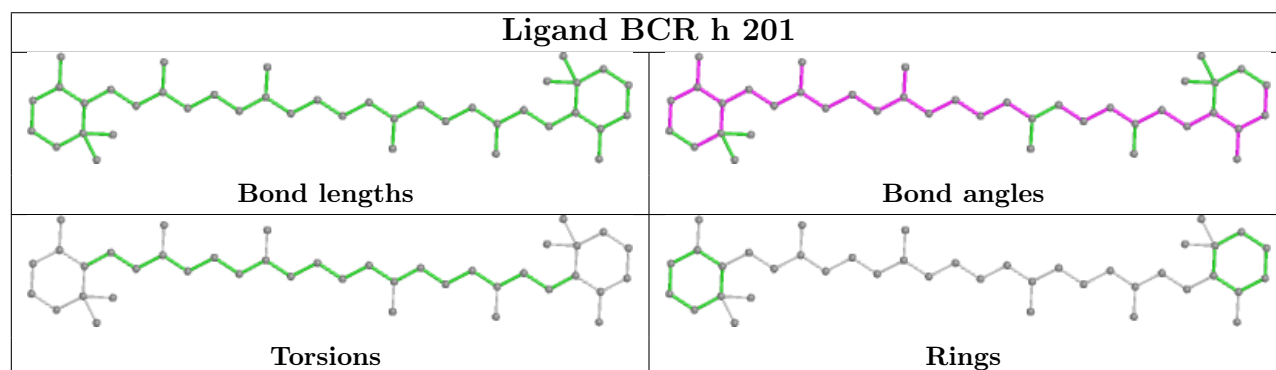
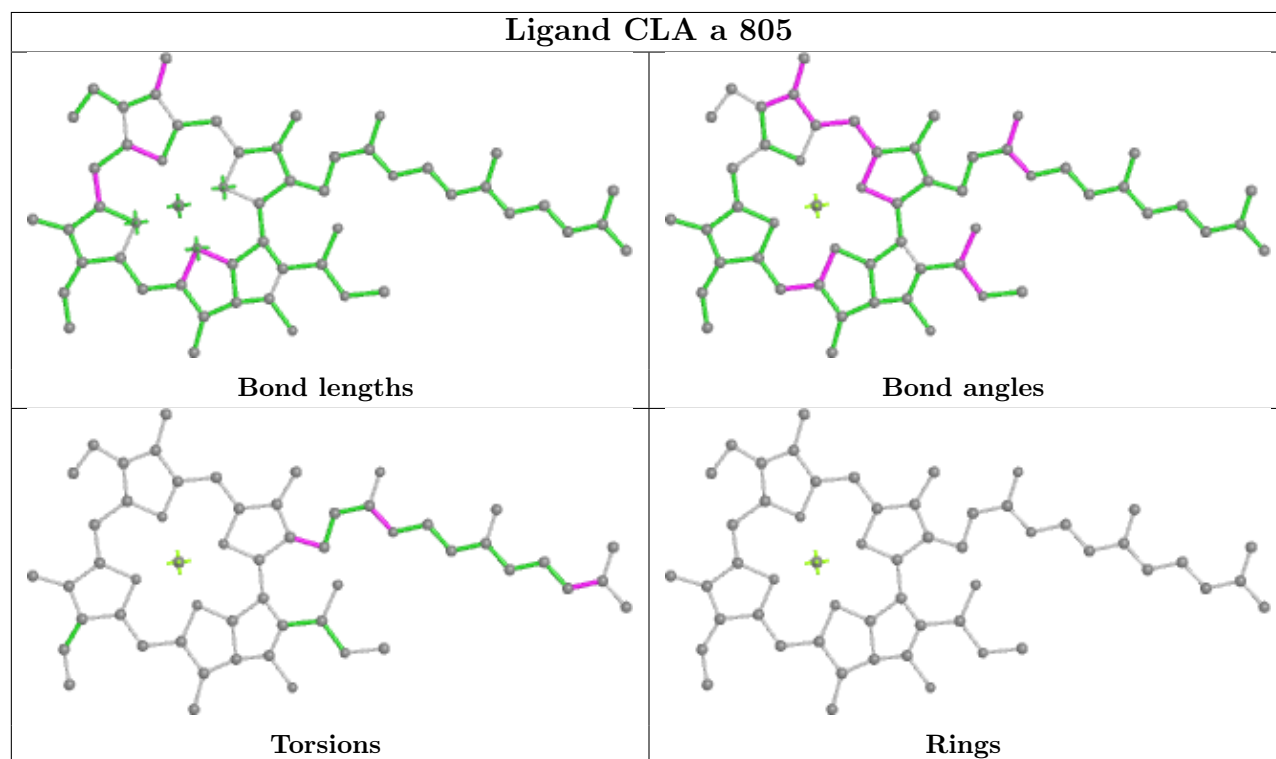
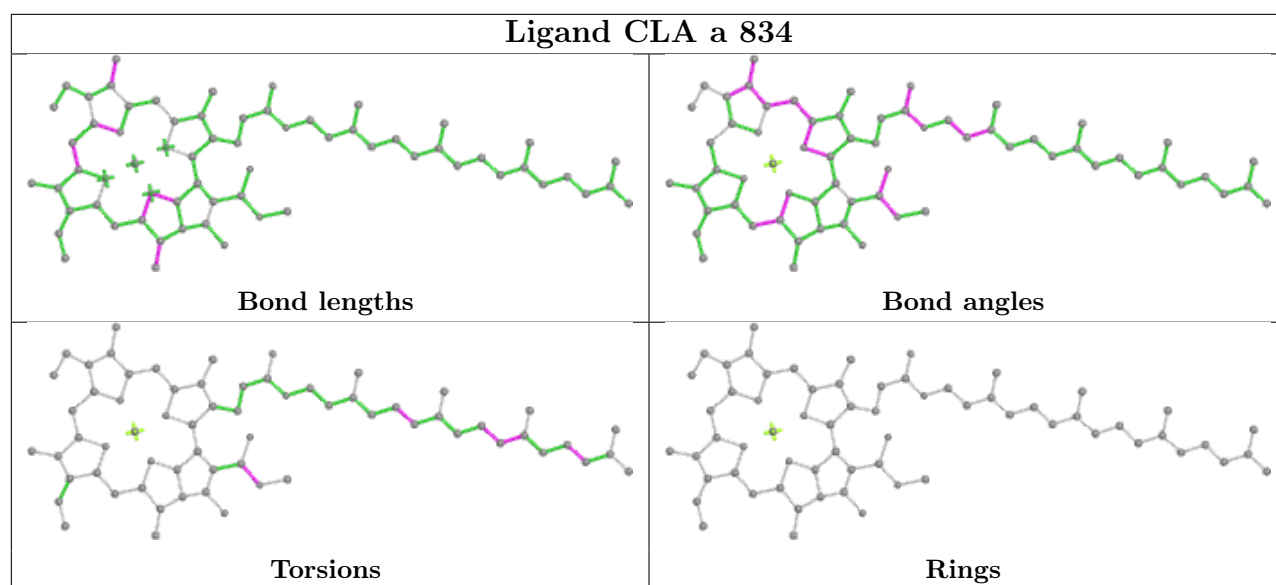
Bond angles

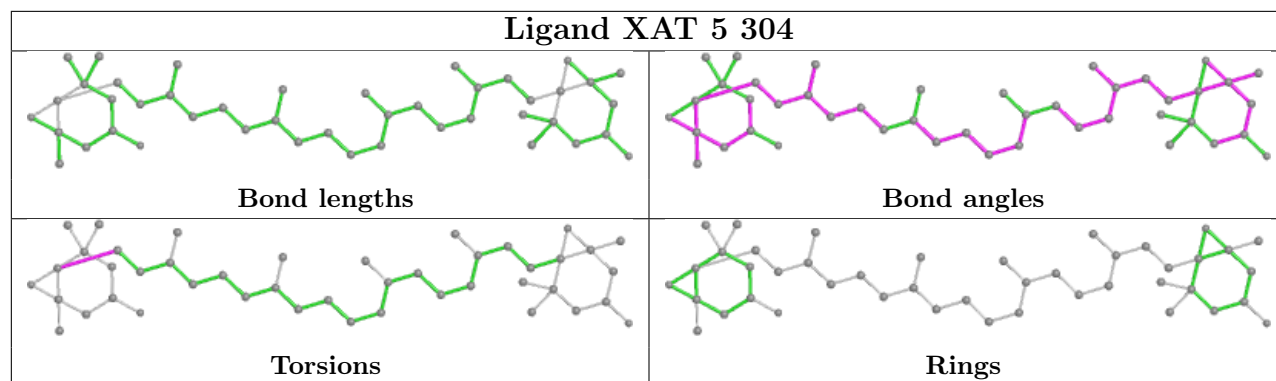


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

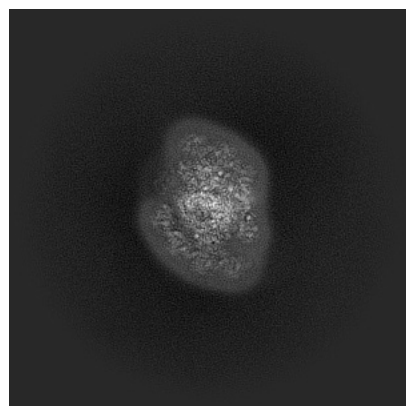
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60288. These allow visual inspection of the internal detail of the map and identification of artifacts.

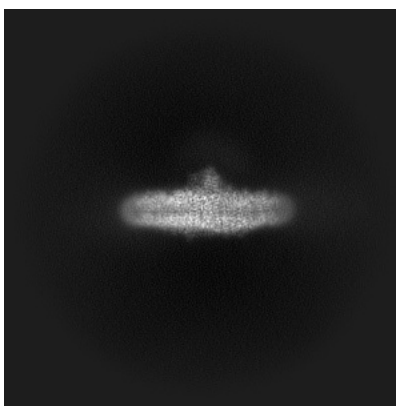
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

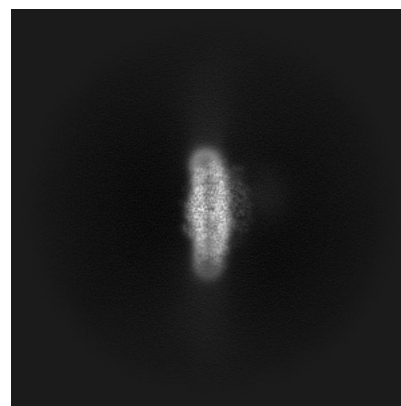
6.1.1 Primary map



X

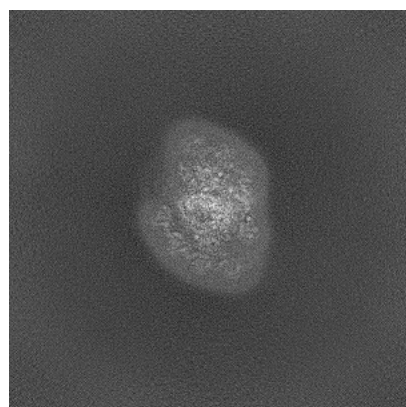


Y

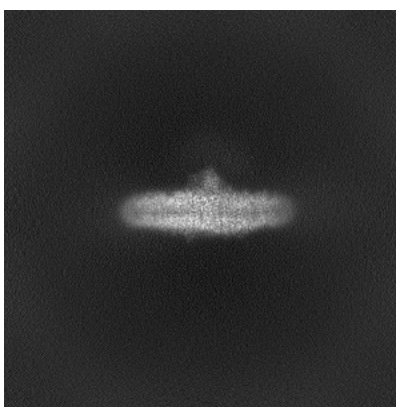


Z

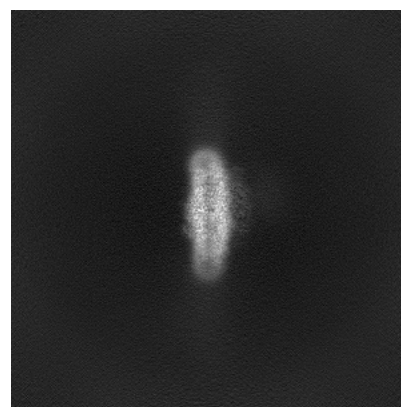
6.1.2 Raw map



X



Y

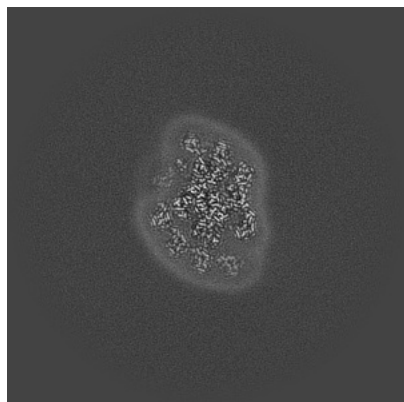


Z

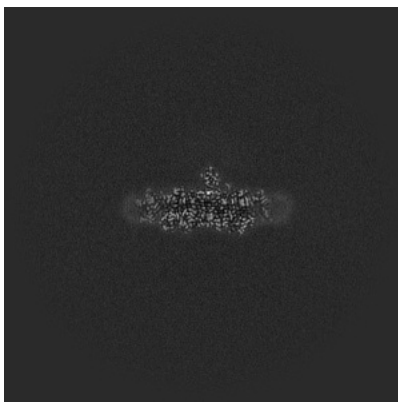
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

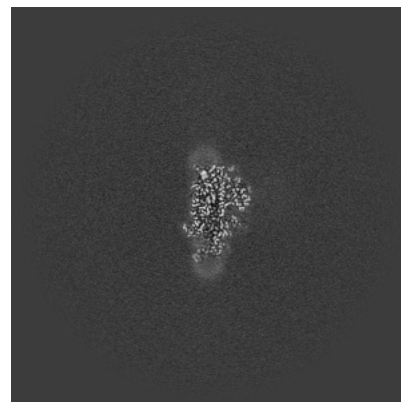
6.2.1 Primary map



X Index: 256

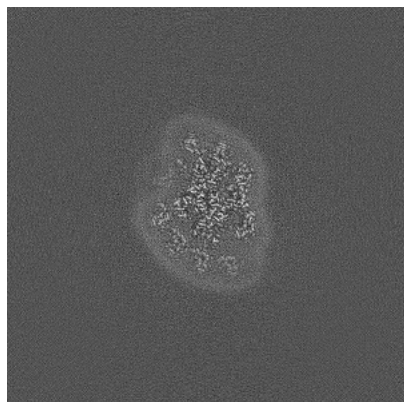


Y Index: 256

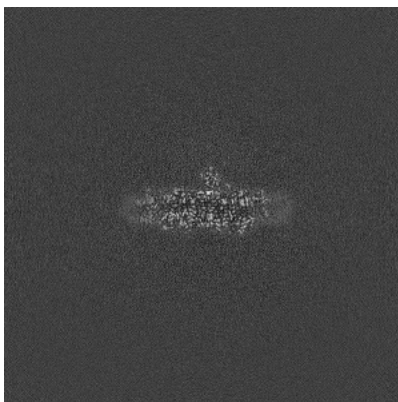


Z Index: 256

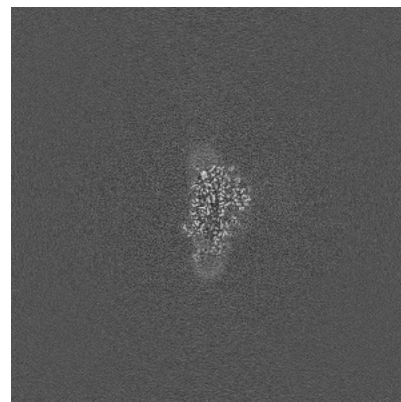
6.2.2 Raw map



X Index: 256



Y Index: 256

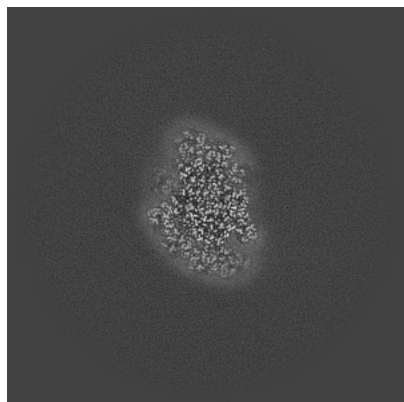


Z Index: 256

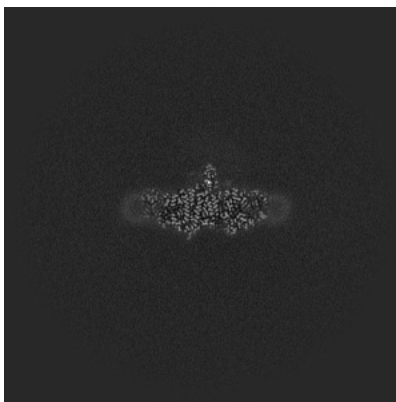
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

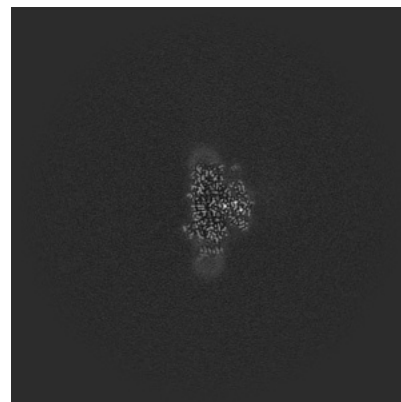
6.3.1 Primary map



X Index: 268

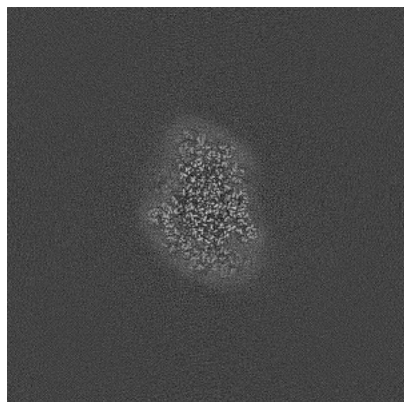


Y Index: 262

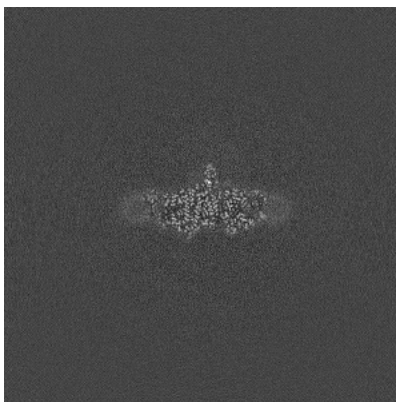


Z Index: 261

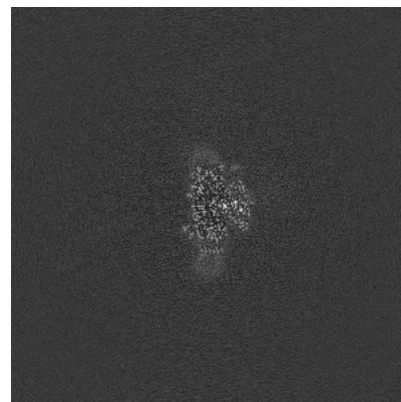
6.3.2 Raw map



X Index: 268



Y Index: 262

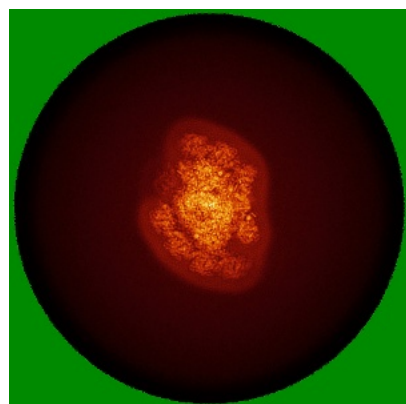


Z Index: 261

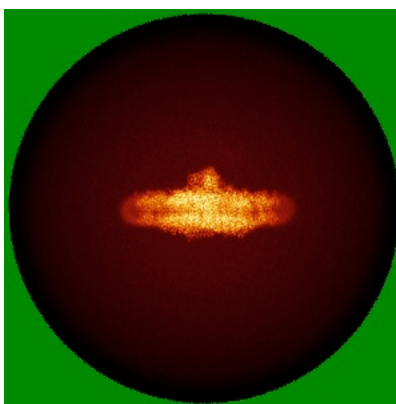
The images above show the largest variance slices of the map in three orthogonal directions.

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

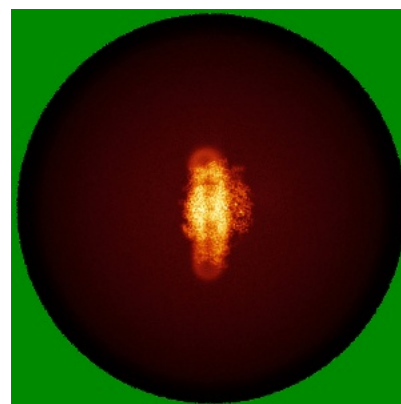
6.4.1 Primary map



X

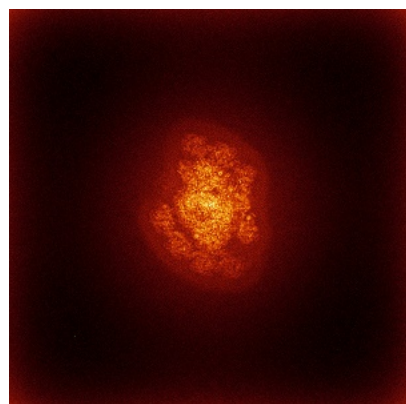


Y

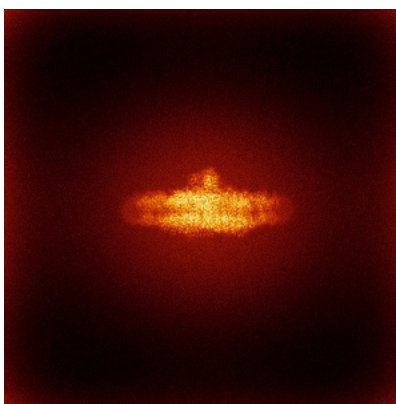


Z

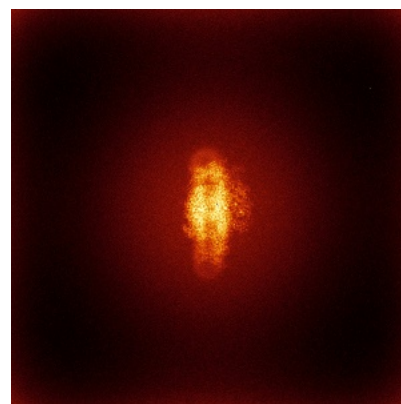
6.4.2 Raw map



X



Y

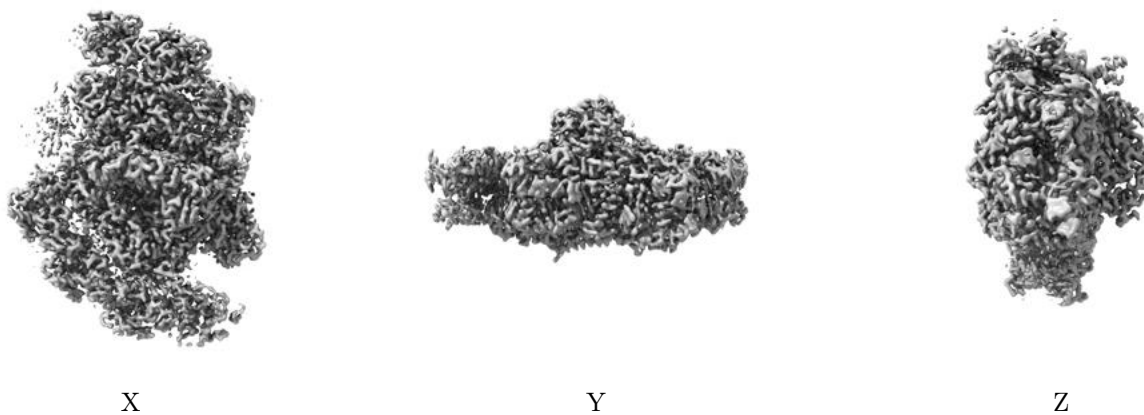


Z

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

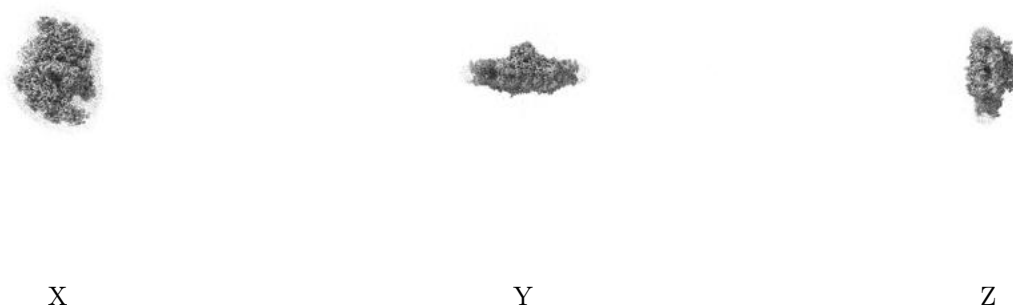
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.287. 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.

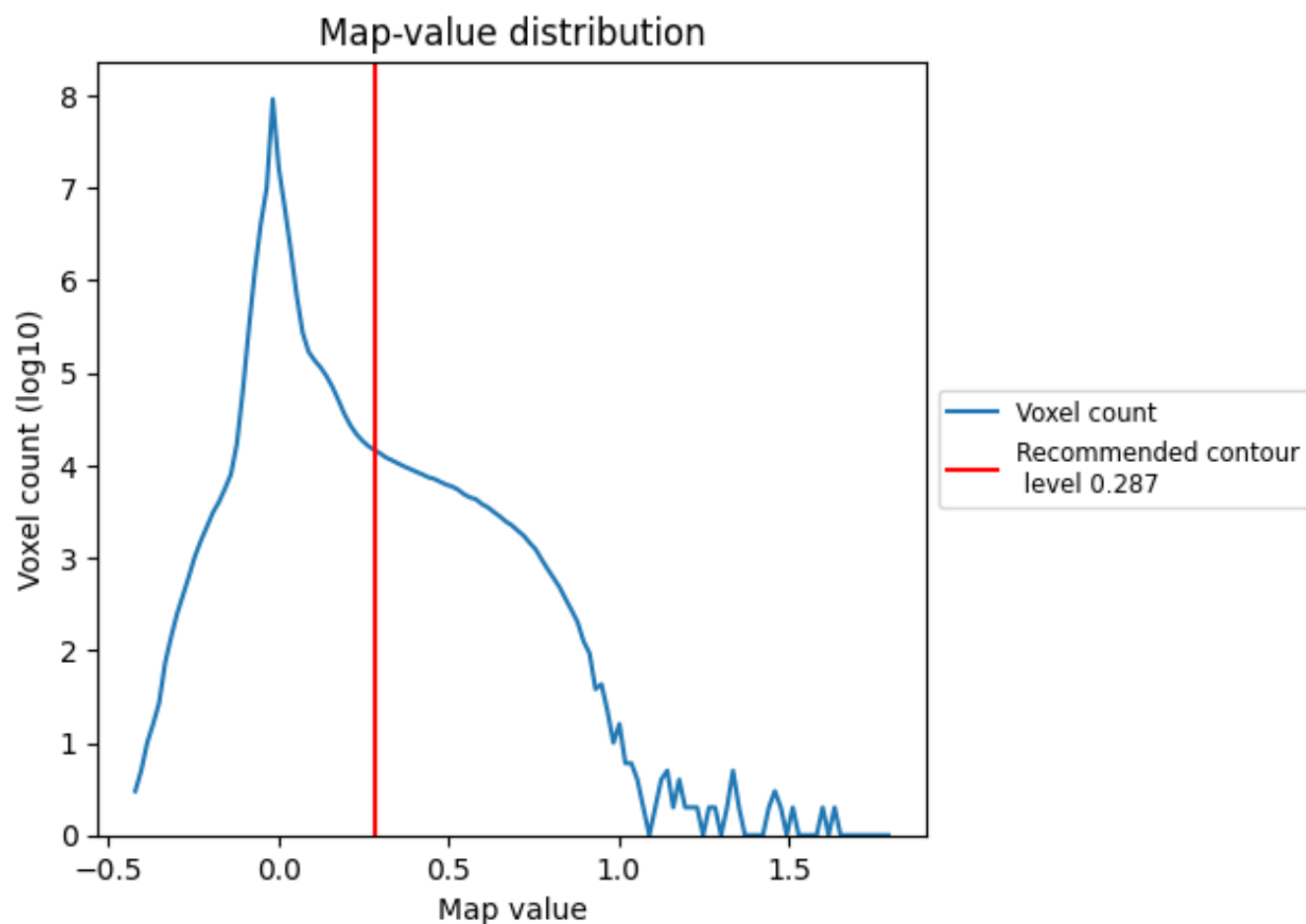
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

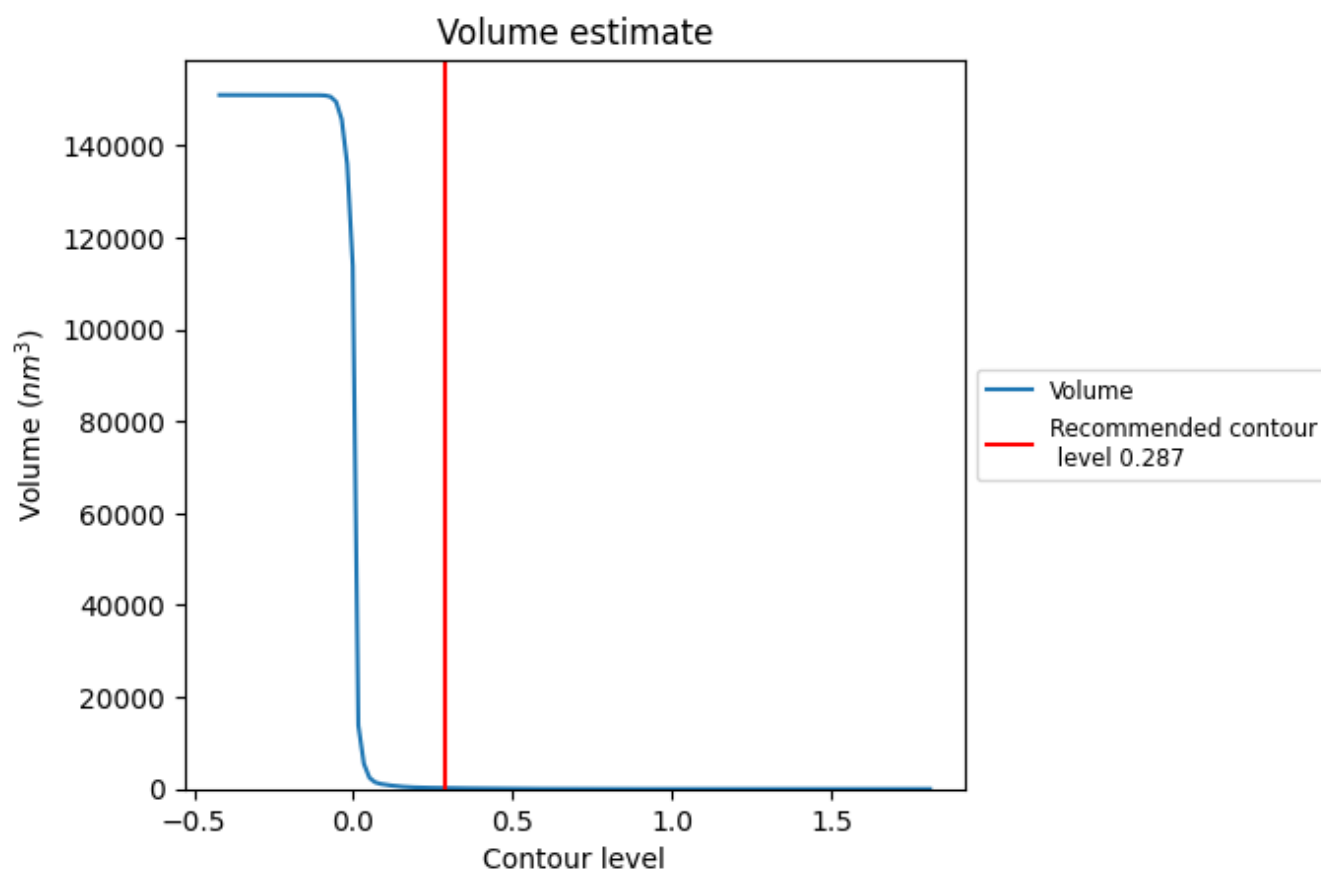
This section contains the results of statistical analysis of the map.

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.

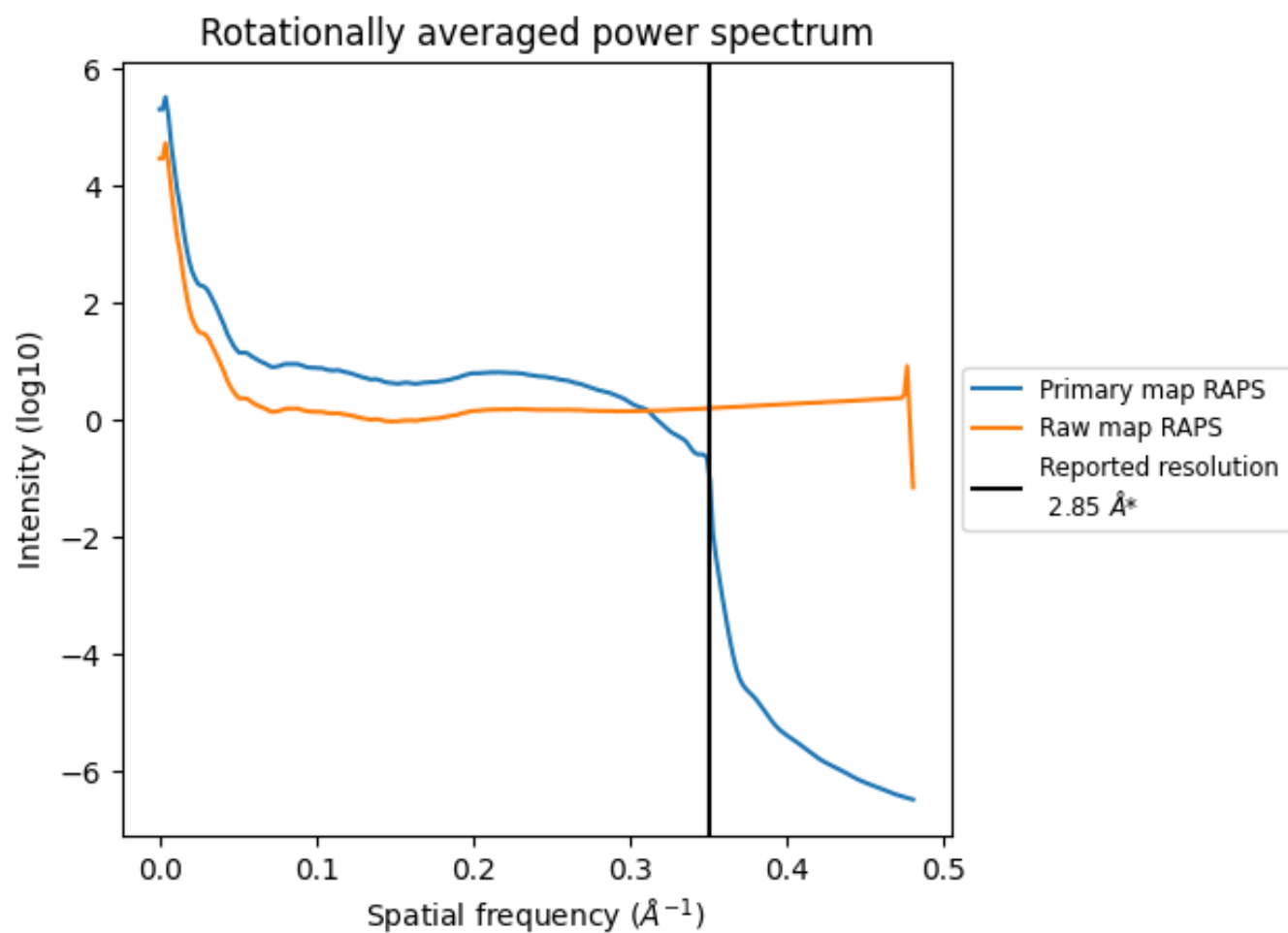
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm^3 ; this corresponds to an approximate mass of 178 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 ⓘ

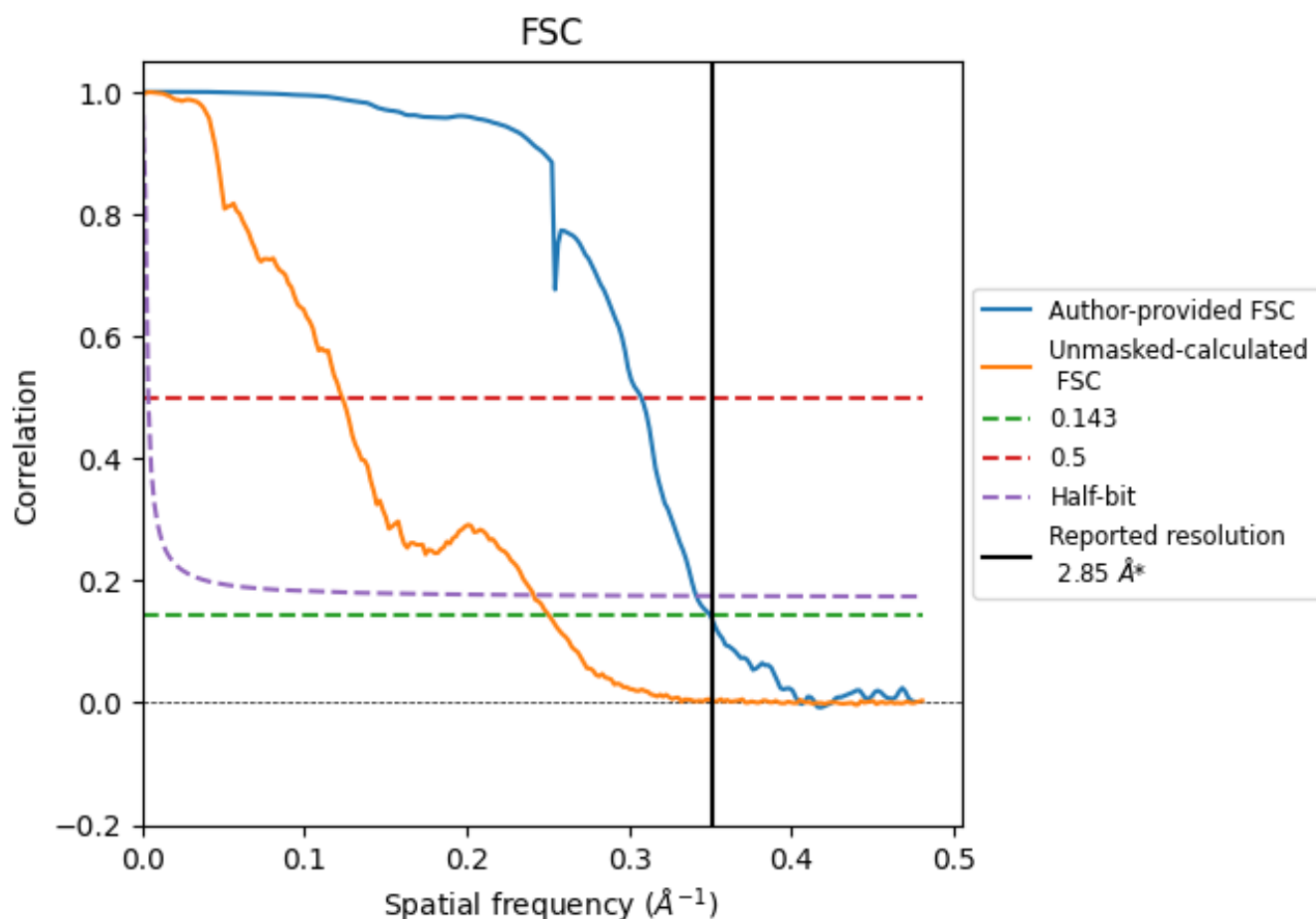


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.351 \AA^{-1}

8.2 Resolution estimates [i](#)

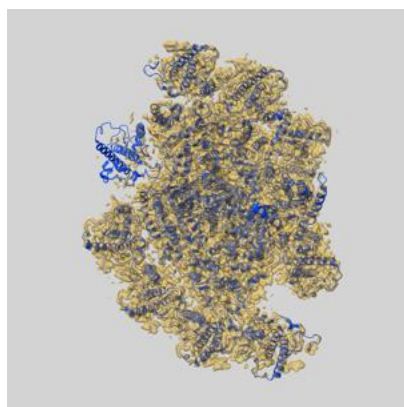
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.25	2.93
Unmasked-calculated*	3.99	8.12	4.15

*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 3.99 differs from the reported value 2.85 by more than 10 %

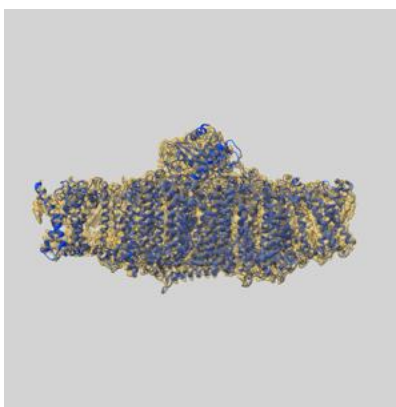
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60288 and PDB model 8ZOC. Per-residue inclusion information can be found in section 3 on page 32.

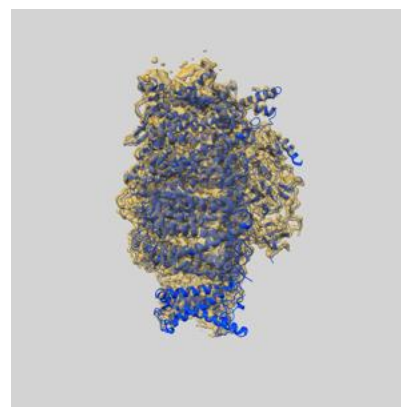
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.287 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](#)



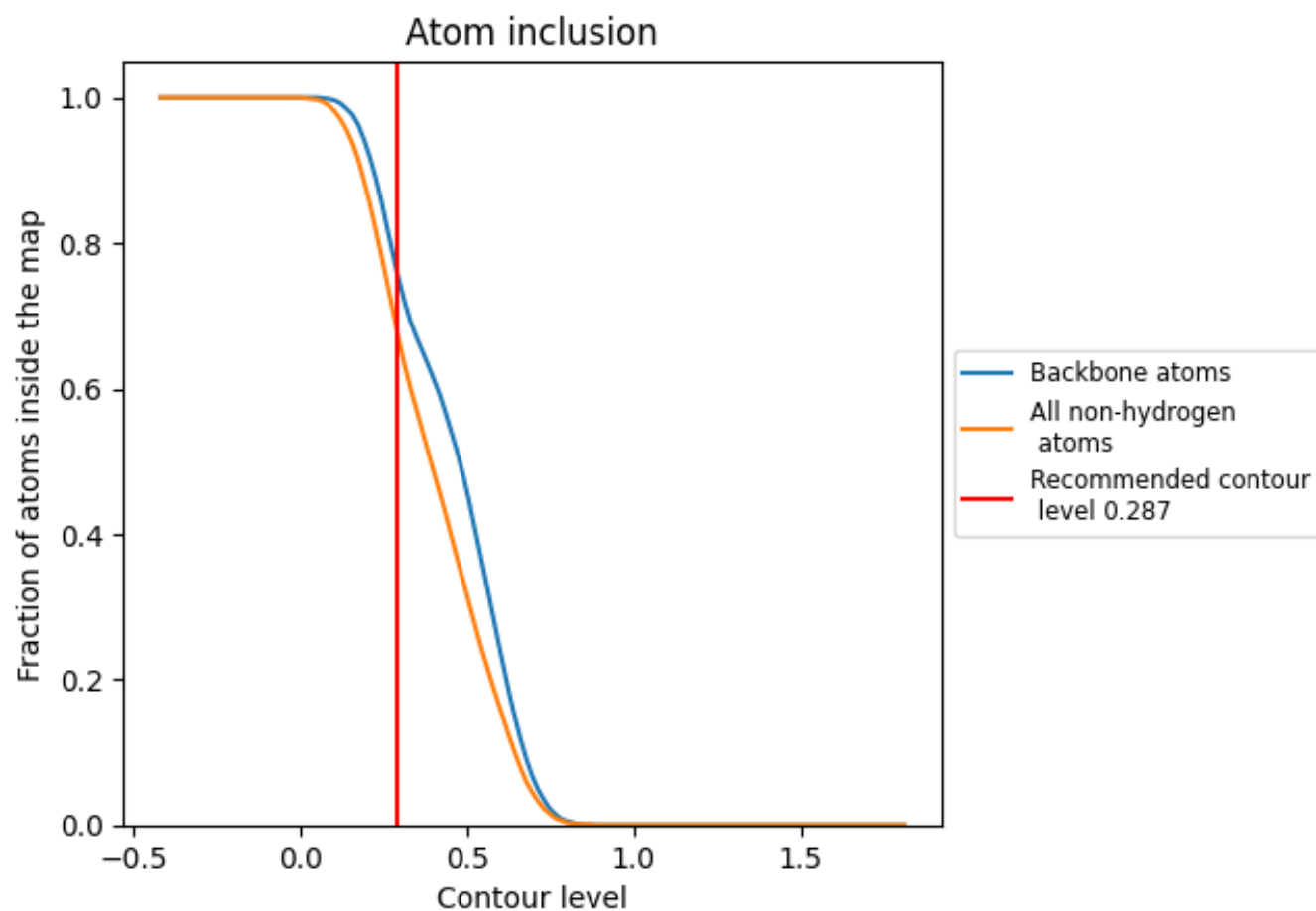
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.287).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.287) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6840	<div></div> 0.5420
1	<div></div> 0.6930	<div></div> 0.5420
2	<div></div> 0.4040	<div></div> 0.4440
3	<div></div> 0.6100	<div></div> 0.5280
4	<div></div> 0.6630	<div></div> 0.5280
5	<div></div> 0.6730	<div></div> 0.5220
6	<div></div> 0.0880	<div></div> 0.4270
7	<div></div> 0.5460	<div></div> 0.4920
8	<div></div> 0.6920	<div></div> 0.5440
9	<div></div> 0.6930	<div></div> 0.5420
a	<div></div> 0.8030	<div></div> 0.5800
b	<div></div> 0.8030	<div></div> 0.5790
c	<div></div> 0.8380	<div></div> 0.5620
d	<div></div> 0.7520	<div></div> 0.5590
e	<div></div> 0.7320	<div></div> 0.5630
f	<div></div> 0.7270	<div></div> 0.5470
g	<div></div> 0.5380	<div></div> 0.4440
h	<div></div> 0.6160	<div></div> 0.5330
i	<div></div> 0.7580	<div></div> 0.5460
j	<div></div> 0.7420	<div></div> 0.5680
l	<div></div> 0.7230	<div></div> 0.5360
m	<div></div> 0.7530	<div></div> 0.5310

