



## wwPDB EM Validation Summary Report ⓘ

Dec 2, 2025 – 12:05 AM JST

PDB ID : 8ZOG / pdb\_00008zog  
EMDB ID : EMD-60292  
Title : Structure of the astaxanthin mutant PSI-9VCPI supercomplex in *Nanochloropsis oceanica*  
Authors : Shen, L.L.; Shen, J.R.; Wang, W.D.  
Deposited on : 2024-05-28  
Resolution : 3.16 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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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

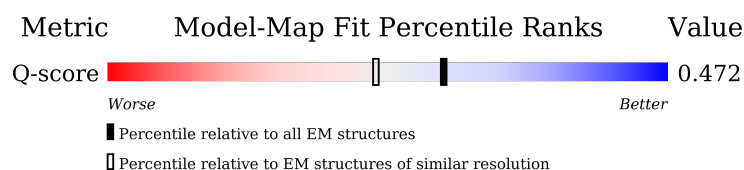
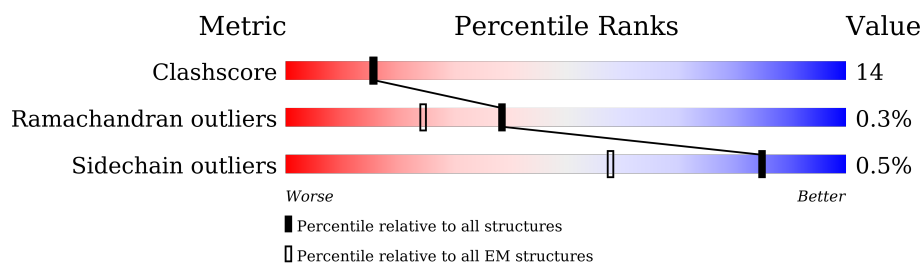
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.16 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	14474 ( 2.66 - 3.66 )

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

Mol	Chain	Length	Quality of chain
1	5	244	<div> <div>11%</div> <div> <div></div> <div>52%</div> <div>17%</div> <div>31%</div> </div> </div>
2	9	232	<div> <div>21%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>13%</div> </div> </div>
3	8	200	<div> <div>12%</div> <div> <div></div> <div>62%</div> <div>18%</div> <div>18%</div> </div> </div>
4	4	202	<div> <div>11%</div> <div> <div></div> <div>71%</div> <div>12%</div> <div>17%</div> </div> </div>

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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	-	-	-

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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	305	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	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	-	-	-
23	CLA	5	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	5	314	X	-	-	-
23	CLA	5	315	X	-	-	-
23	CLA	5	316	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	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	-	-	-
23	CLA	9	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	9	315	X	-	-	-
23	CLA	9	316	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	-	-	-
23	CLA	a	839	X	-	-	-
23	CLA	a	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	a	841	X	-	-	-
23	CLA	a	842	X	-	-	-
23	CLA	a	844	X	-	-	-
23	CLA	a	852	X	-	-	-
23	CLA	a	856	X	-	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	-	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	-	-	-
23	CLA	b	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	b	838	X	-	-	-
23	CLA	b	839	X	-	-	-
23	CLA	b	840	X	-	-	-
23	CLA	b	841	X	-	-	-
23	CLA	f	802	X	-	-	-
23	CLA	f	803	X	-	-	-
23	CLA	h	201	X	-	-	-
23	CLA	h	203	X	-	-	-
23	CLA	j	101	X	-	-	-
23	CLA	l	201	X	-	-	-
23	CLA	l	202	X	-	-	-
23	CLA	l	203	X	-	-	-
30	BCR	f	801	-	-	X	-
31	SF4	c	102	-	-	X	-

## 2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 43749 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			

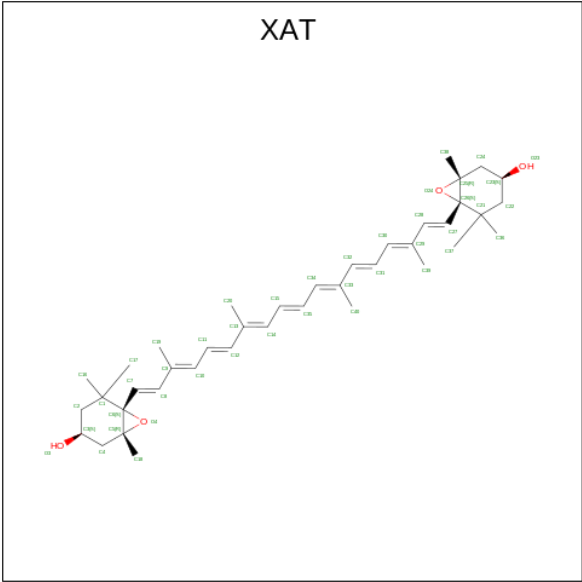
- Molecule 19 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	50	Total	C	N	O		0	0
			250	150	50	50			

- 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: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (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	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	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	

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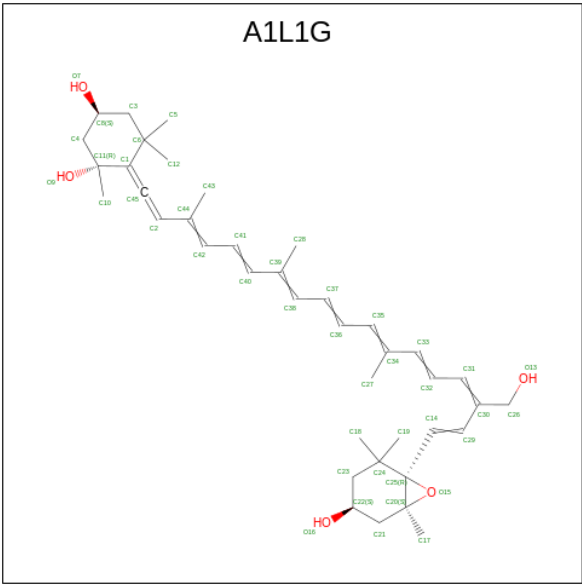
Mol	Chain	Residues	Atoms			AltConf
21	4	1	Total 44	C 40	O 4	0
21	4	1	Total 44	C 40	O 4	0
21	4	1	Total 44	C 40	O 4	0
21	4	1	Total 44	C 40	O 4	0
21	3	1	Total 44	C 40	O 4	0
21	3	1	Total 44	C 40	O 4	0
21	3	1	Total 44	C 40	O 4	0
21	3	1	Total 44	C 40	O 4	0
21	6	1	Total 44	C 40	O 4	0
21	6	1	Total 44	C 40	O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

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Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	1	1	Total	C	O	0
			44	40	4	
21	a	1	Total	C	O	0
			44	40	4	
21	a	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-oxa bicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclo hexane-1,3-diol (CCD ID: A1L1G) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



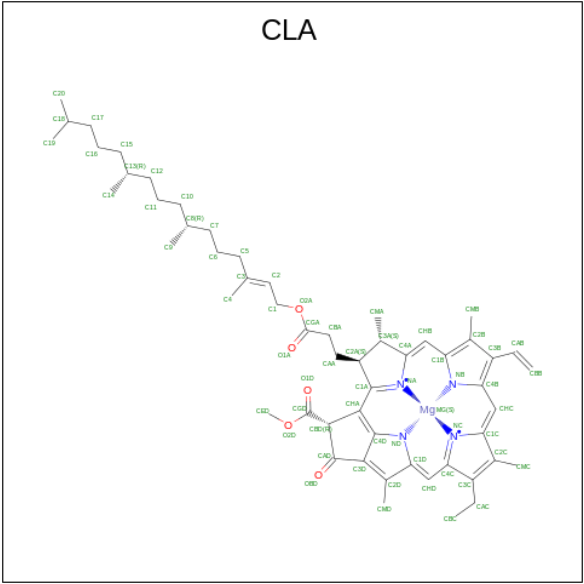
Mol	Chain	Residues	Atoms			AltConf
22	5	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (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	

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Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
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
			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	

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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

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Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
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
23	1	1	Total 41	C 33	Mg 1	N 4	O 3	0

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

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

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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

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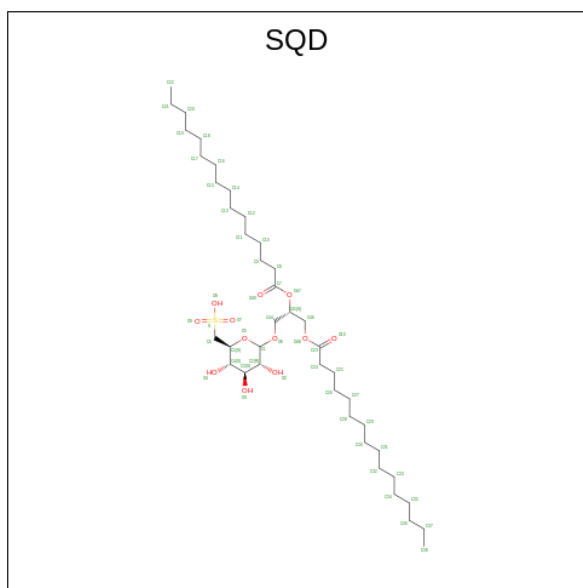
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			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
			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
			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	

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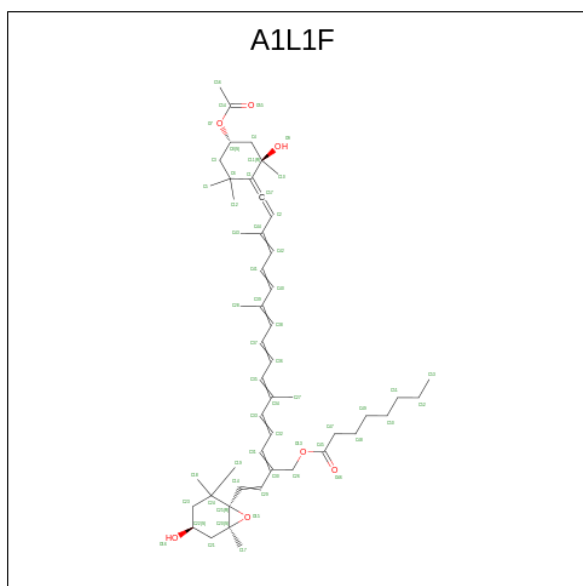
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	j	1	Total	C	Mg	N	O	0
			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).



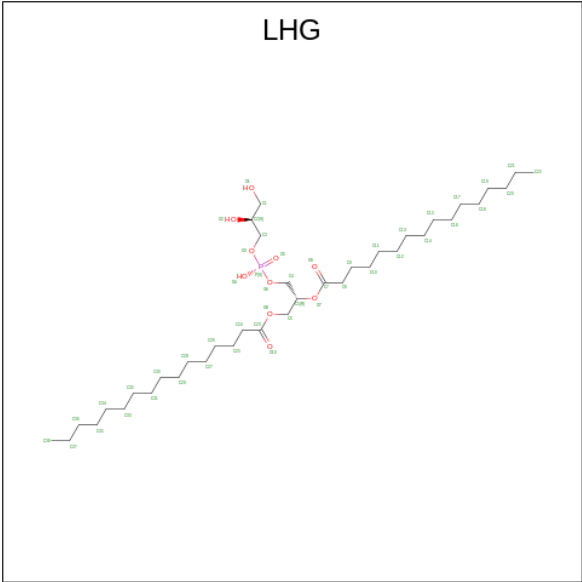
Mol	Chain	Residues	Atoms				AltConf
24	5	1	Total	C	O	S	0
			35	22	12	1	
24	1	1	Total	C	O	S	0
			45	32	12	1	

- 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: C<sub>50</sub>H<sub>72</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



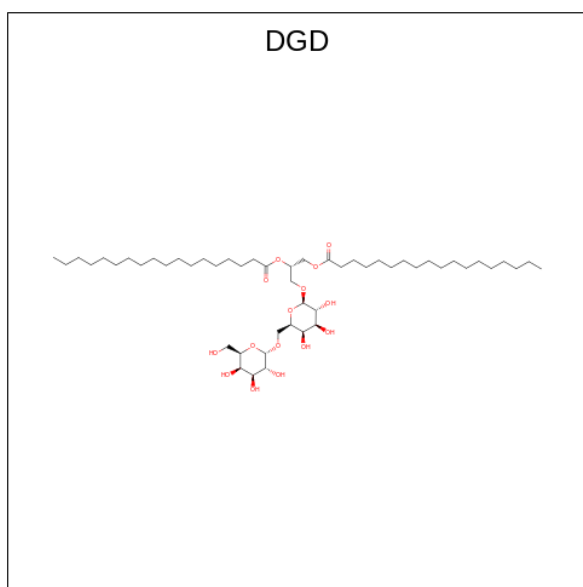
Mol	Chain	Residues	Atoms				AltConf
25	9	1	Total	C	O		0
			57	50	7		
25	8	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			53	46	7		
25	1	1	Total	C	O		0
			57	50	7		
25	h	1	Total	C	O		0
			57	50	7		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



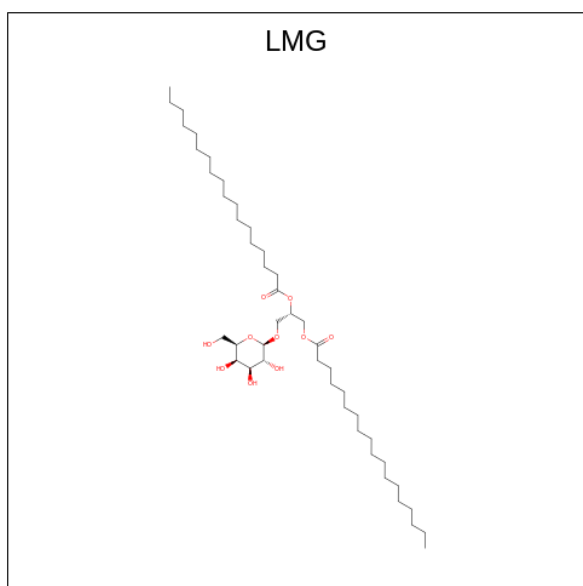
Mol	Chain	Residues	Atoms				AltConf
26	9	1	Total	C	O	P	0
			36	25	10	1	
26	a	1	Total	C	O	P	0
			48	37	10	1	
26	a	1	Total	C	O	P	0
			27	16	10	1	
26	b	1	Total	C	O	P	0
			31	20	10	1	
26	m	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>) (labeled as "Ligand of Interest" by depositor).



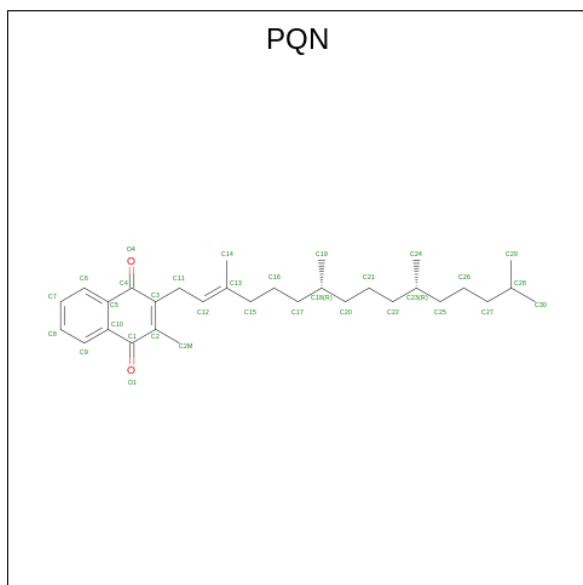
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	8	1	40	25	15	0
27	4	1	40	25	15	0
27	b	1	57	42	15	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



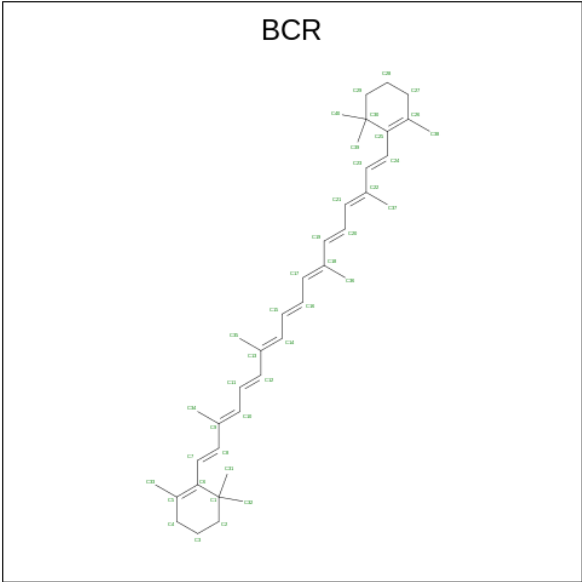
Mol	Chain	Residues	Atoms			AltConf
28	2	1	Total	C	O	0
			35	25	10	
28	a	1	Total	C	O	0
			34	24	10	
28	j	1	Total	C	O	0
			32	22	10	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



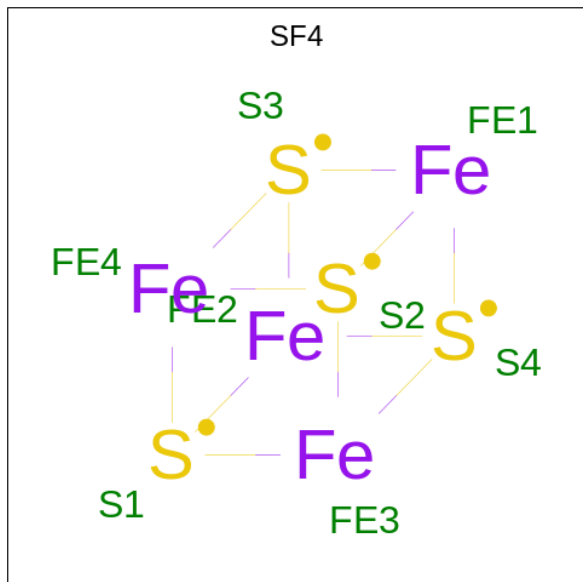
Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C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

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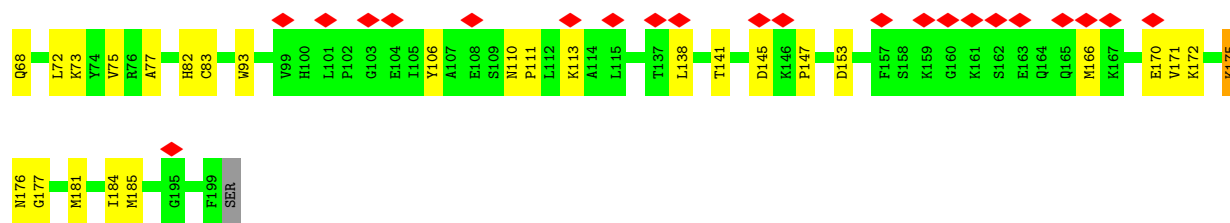
Mol	Chain	Residues	Atoms	AltConf
30	f	1	Total C 40 40	0
30	i	1	Total C 40 40	0
30	i	1	Total C 40 40	0
30	j	1	Total C 40 40	0
30	m	1	Total C 40 40	0

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).

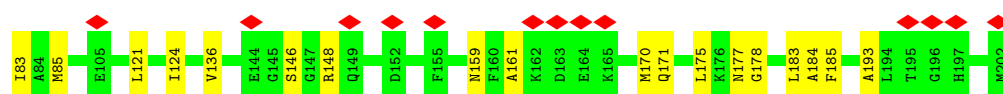
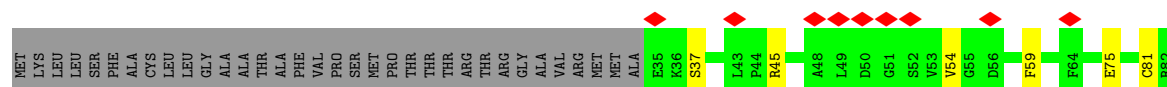


Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total Fe S 8 4 4	0
31	c	1	Total Fe S 8 4 4	0
31	c	1	Total Fe S 8 4 4	0

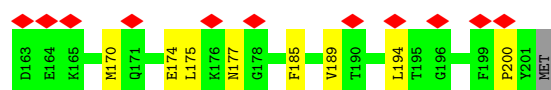
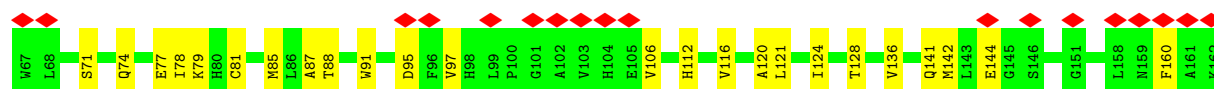
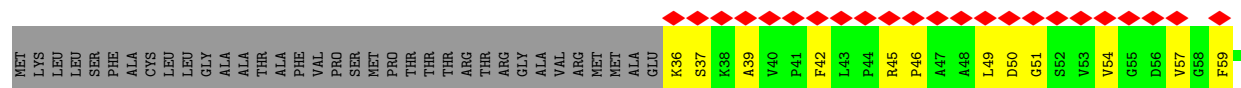




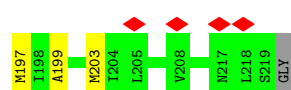
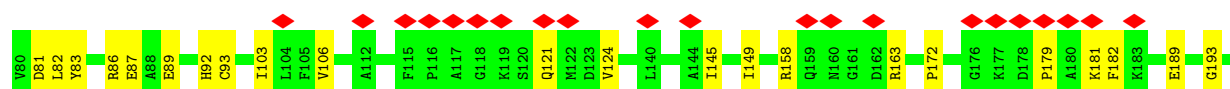
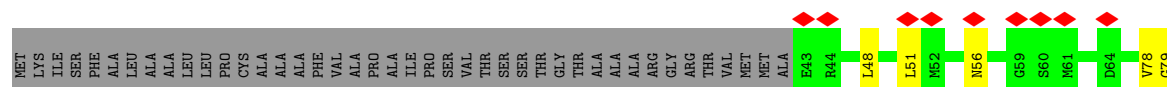
• Molecule 4: VCPI-4/7



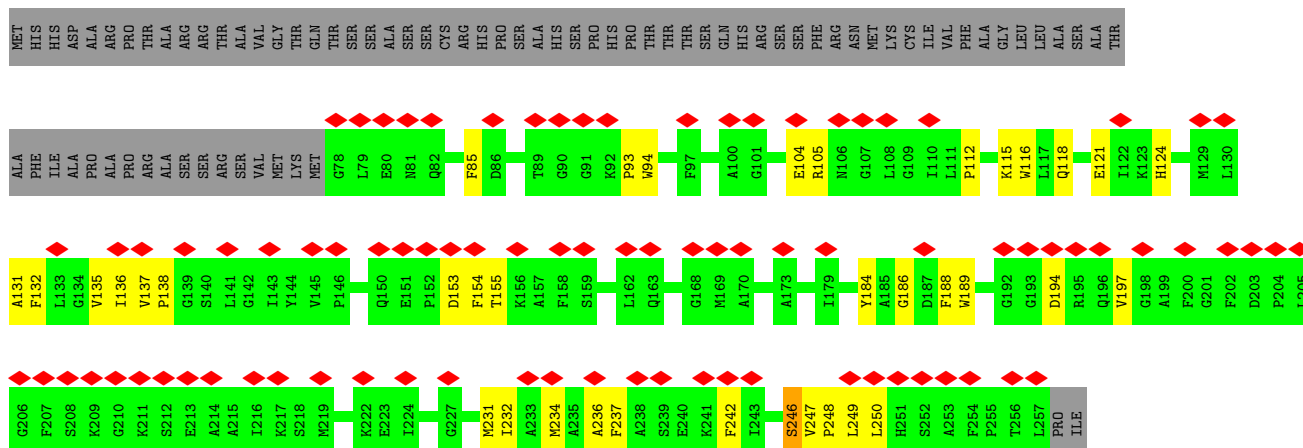
• Molecule 4: VCPI-4/7



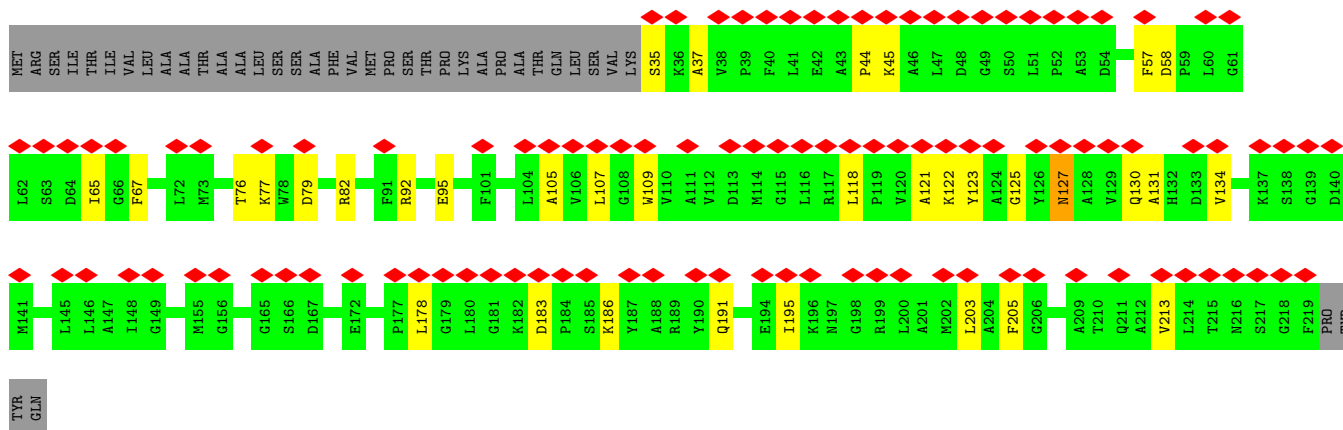
• Molecule 5: VCPI-3



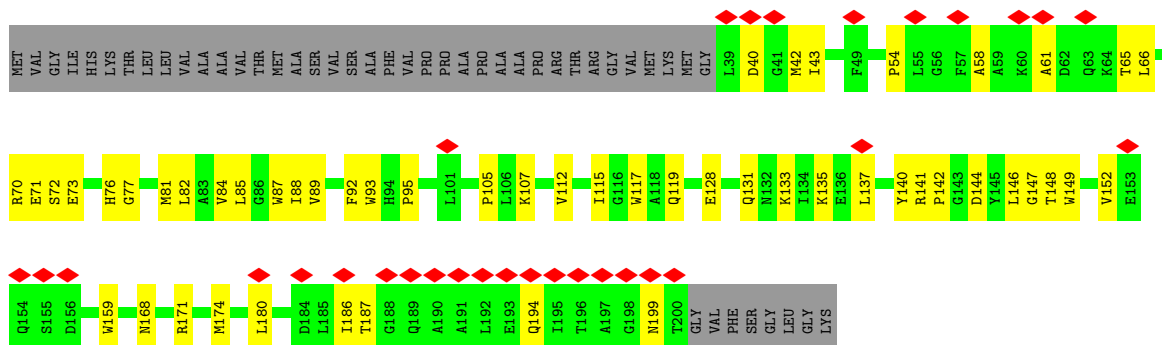
• Molecule 6: VCPI-6



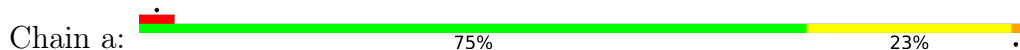
• Molecule 7: VCPI-2

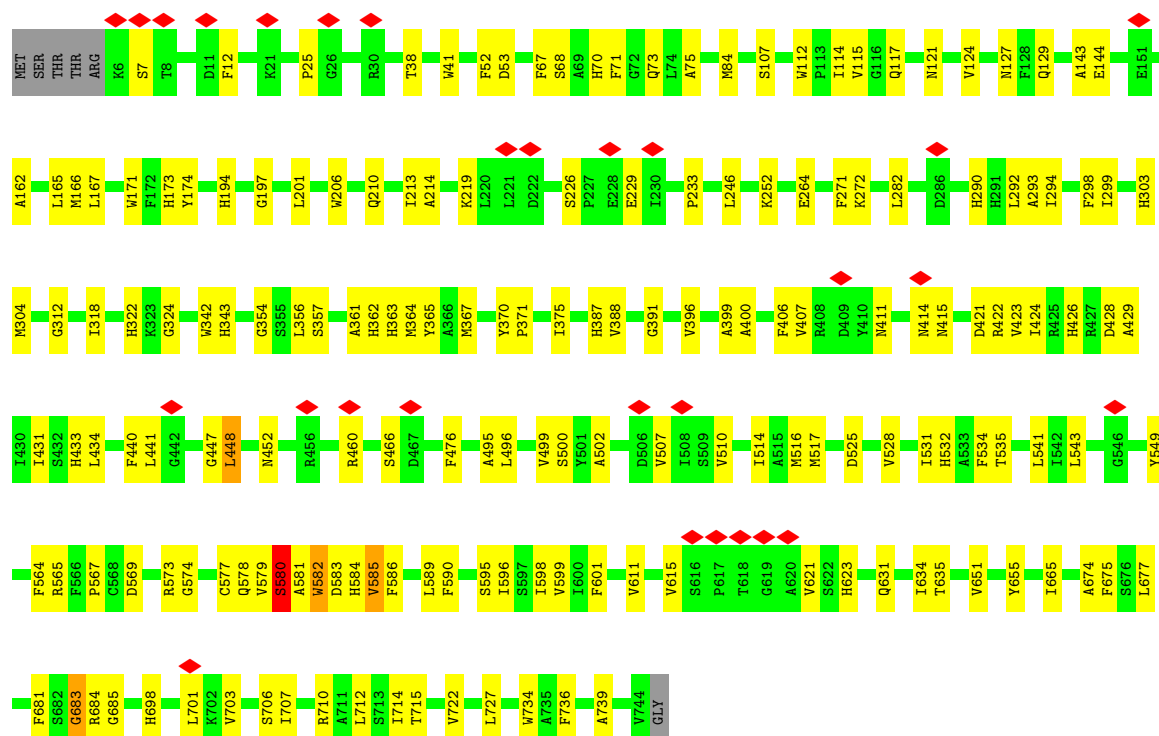


• Molecule 8: VCPI-1



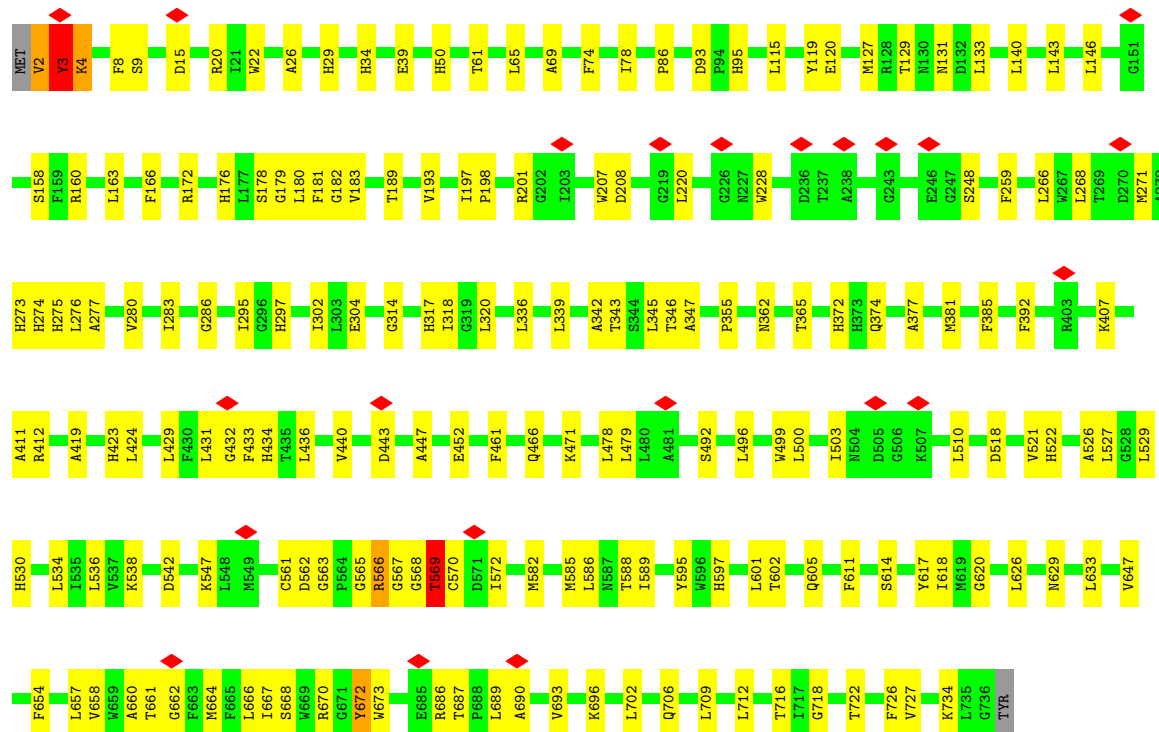
• Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1



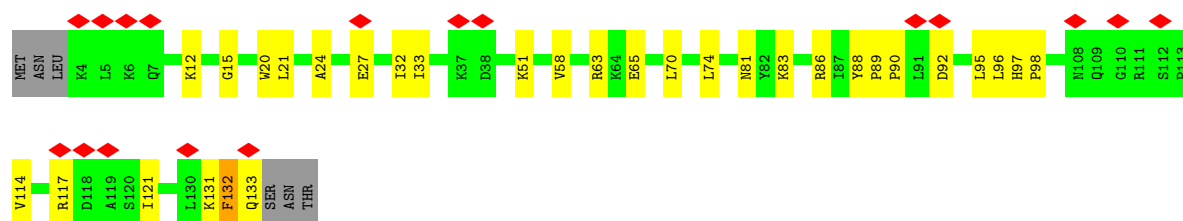
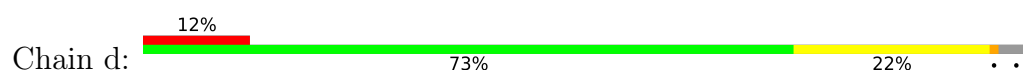


• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A2

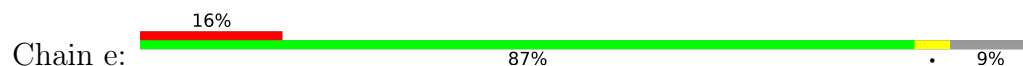
Chain b: 74% 24%



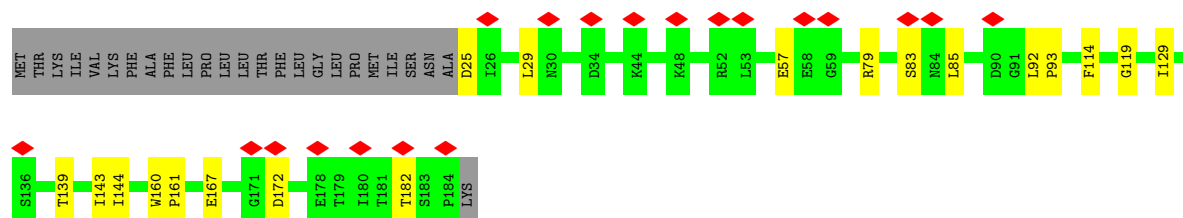
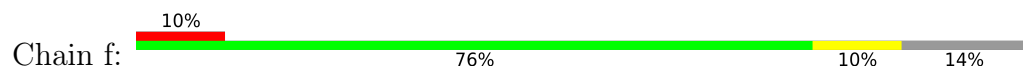
• Molecule 11: Photosystem I reaction center subunit II



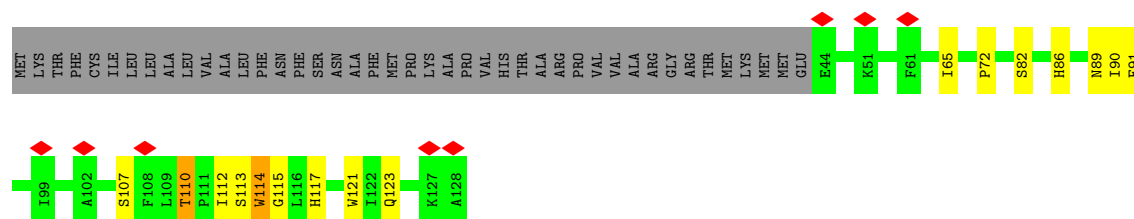
- Molecule 12: Photosystem I reaction center subunit IV



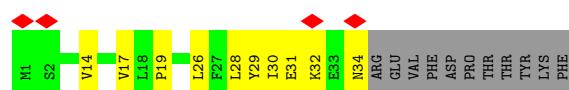
- Molecule 13: Photosystem I reaction center subunit III



- Molecule 14: PsaR

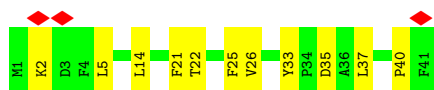


- Molecule 15: Photosystem I reaction center subunit VIII

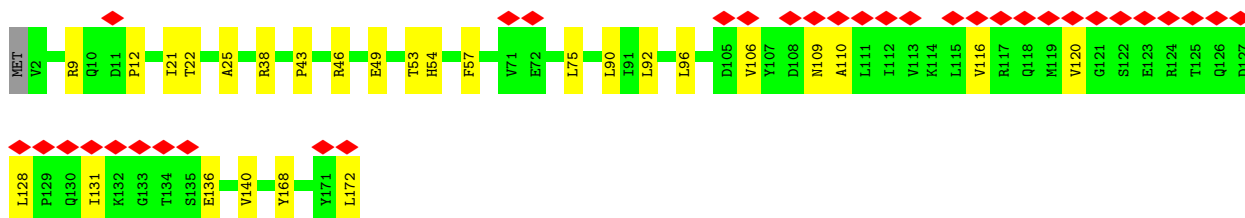
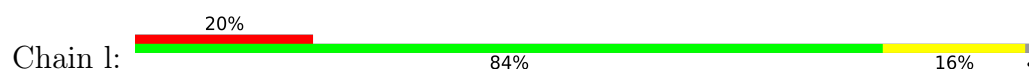


- Molecule 16: Photosystem I reaction center subunit IX





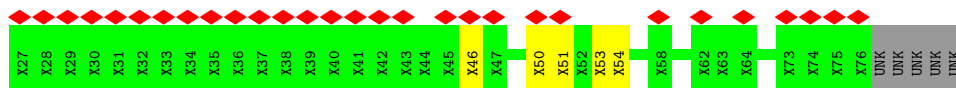
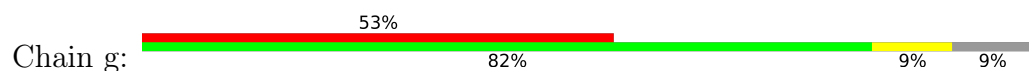
- Molecule 17: PSI subunit V



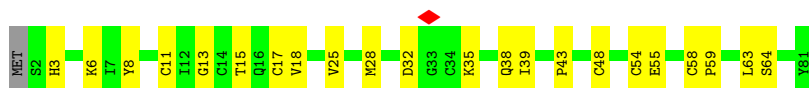
- Molecule 18: PsaM



- 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	31137	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 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.682	Depositor
Minimum map value	-0.465	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.293	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: A1L1G, BCR, SQD, A1L1F, DGD, PQN, CLA, LMG, SF4, XAT, LHG

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	0.34	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	0.19	0/1248	0.37	0/1700
5	3	0.12	0/1350	0.28	0/1821
6	6	0.17	0/1390	0.32	0/1883
7	2	0.14	0/1405	0.36	0/1904
8	1	0.14	0/1293	0.33	0/1759
9	a	0.30	3/6024 (0.0%)	0.35	5/8219 (0.1%)
10	b	0.26	0/6080	0.35	2/8302 (0.0%)
11	d	0.18	0/1040	0.36	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	0.15	0/278	0.33	0/378
16	j	0.16	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	0.25	5/30489 (0.0%)	0.35	10/41469 (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	-7.00	1.43	1.52
3	8	44	LEU	C-O	-6.14	1.15	1.23
9	a	581	ALA	CA-C	-5.39	1.45	1.52
14	h	114	TRP	C-O	-5.33	1.18	1.24
9	a	582	TRP	CA-C	-5.06	1.45	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	581	ALA	N-CA-C	-8.65	102.47	113.72
9	a	683	GLY	O-C-N	-8.45	116.29	123.73
10	b	568	GLY	N-CA-C	-7.50	100.71	110.69
3	8	39	LYS	N-CA-C	-6.12	105.65	113.23
9	a	448	LEU	N-CA-C	-6.06	104.24	111.69

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	36	0
2	9	1466	0	1470	56	0
3	8	1258	0	1280	32	0
4	4	1268	0	1288	24	0
4	7	1220	0	1209	40	0
5	3	1324	0	1340	20	0
6	6	1352	0	1334	30	0
7	2	1372	0	1347	23	0
8	1	1262	0	1237	37	0
9	a	5827	0	5697	156	0
10	b	5865	0	5711	202	0
11	d	1014	0	1015	29	0
12	e	494	0	495	3	0
13	f	1266	0	1262	29	0
14	h	646	0	649	11	0
15	i	271	0	292	19	0
16	j	339	0	342	15	0
17	l	1283	0	1278	26	0
18	m	210	0	226	2	0
19	g	250	0	57	4	0
20	c	596	0	583	23	0
21	1	88	0	112	7	0
21	2	220	0	280	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	3	176	0	224	14	0
21	4	176	0	224	24	0
21	5	176	0	224	24	0
21	6	176	0	224	18	0
21	7	176	0	224	28	0
21	8	132	0	168	15	0
21	9	132	0	168	16	0
21	a	88	0	112	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	15	0
23	2	544	0	452	10	0
23	3	458	0	378	8	0
23	4	613	0	522	30	0
23	5	563	0	472	26	0
23	6	499	0	413	12	0
23	7	576	0	444	24	0
23	8	507	0	429	22	0
23	9	454	0	380	35	0
23	a	2644	0	2634	215	0
23	b	2468	0	2519	173	0
23	f	117	0	115	2	0
23	h	120	0	121	7	0
23	j	42	0	31	2	0
23	l	148	0	123	10	0
24	1	45	0	54	3	0
24	5	35	0	34	1	0
25	1	57	0	0	11	0
25	6	110	0	0	5	0
25	8	57	0	0	2	0
25	9	57	0	0	1	0
25	h	57	0	0	4	0
26	9	36	0	45	1	0
26	a	75	0	93	5	0
26	b	31	0	32	2	0
26	m	46	0	65	2	0
27	4	40	0	38	11	0
27	8	40	0	38	2	0
27	b	57	0	72	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	2	35	0	40	3	0
28	a	34	0	38	10	0
28	j	32	0	34	6	0
29	a	33	0	46	4	0
29	b	33	0	46	6	0
30	a	160	0	224	13	0
30	b	360	0	504	57	0
30	f	80	0	112	31	0
30	i	80	0	112	17	0
30	j	40	0	56	14	0
30	m	40	0	56	0	0
31	a	8	0	0	0	0
31	c	16	0	0	3	0
All	All	43749	0	42670	1242	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 14.

The worst 5 of 1242 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)
9:a:698:HIS:NE2	23:a:856:CLA:HAC1	1.52	1.25
23:a:834:CLA:H151	29:b:842:PQN:H202	1.21	1.21
23:a:803:CLA:H151	23:b:810:CLA:HBC3	1.24	1.15
25:l:304:A1L1F:C2	23:a:844:CLA:H42	1.80	1.11
23:a:802:CLA:HED3	30:f:801:BCR:C40	1.80	1.10

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	25	57
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	22	54
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	33
8	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
9	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	77
10	b	733/737 (100%)	697 (95%)	33 (4%)	3 (0%)	30	61
11	d	128/136 (94%)	112 (88%)	15 (12%)	1 (1%)	16	47
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%)	77 (93%)	5 (6%)	1 (1%)	11	39
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	39
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%)	3546 (93%)	239 (6%)	13 (0%)	38	66

5 of 13 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	80
3	8	132/160 (82%)	131 (99%)	1 (1%)	79	89
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	122/159 (77%)	121 (99%)	1 (1%)	79	89
5	3	136/164 (83%)	136 (100%)	0	100	100
6	6	135/201 (67%)	134 (99%)	1 (1%)	81	90
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	90
10	b	599/602 (100%)	595 (99%)	4 (1%)	81	90
11	d	107/113 (95%)	106 (99%)	1 (1%)	75	87
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	80
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%)	3043 (100%)	15 (0%)	85	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	a	579	VAL
11	d	133	GLN
9	a	580	SER
14	h	110	THR
10	b	4	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
10	b	373	HIS
10	b	605	GLN
18	m	6	GLN
10	b	587	ASN
10	b	629	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	1	307	-	54,62,73	1.63	5 (9%)	62,99,113	1.52	7 (11%)
23	CLA	4	315	-	46,54,73	1.77	5 (10%)	53,90,113	1.57	7 (13%)
23	CLA	3	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.57	8 (14%)
23	CLA	a	856	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	8 (10%)
21	XAT	2	305	-	39,47,47	0.92	0	54,74,74	2.43	18 (33%)
23	CLA	5	310	1	65,73,73	1.49	5 (7%)	76,113,113	1.37	7 (9%)
23	CLA	b	840	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	6	308	-	58,66,73	1.61	6 (10%)	67,104,113	1.43	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	XAT	2	301	-	39,47,47	0.91	0	54,74,74	2.71	19 (35%)
23	CLA	a	830	-	65,73,73	1.48	7 (10%)	76,113,113	1.40	8 (10%)
21	XAT	3	303	-	39,47,47	0.90	0	54,74,74	2.59	20 (37%)
25	A1L1F	6	301	-	50,59,59	1.30	5 (10%)	62,85,85	2.49	20 (32%)
26	LHG	b	849	23	30,30,48	1.34	6 (20%)	33,36,54	1.14	2 (6%)
23	CLA	a	813	-	54,62,73	1.65	6 (11%)	62,99,113	1.45	7 (11%)
23	CLA	b	836	-	58,66,73	1.56	6 (10%)	67,104,113	1.53	8 (11%)
23	CLA	4	308	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	8 (13%)
28	LMG	a	855	-	34,34,55	1.14	2 (5%)	42,42,63	1.15	3 (7%)
23	CLA	2	313	7	41,49,73	1.85	5 (12%)	47,84,113	1.70	8 (17%)
23	CLA	a	812	23	62,70,73	1.51	6 (9%)	72,109,113	1.45	8 (11%)
21	XAT	2	303	-	39,47,47	0.98	1 (2%)	54,74,74	2.63	20 (37%)
23	CLA	8	313	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	7 (13%)
23	CLA	1	312	8	52,60,73	1.71	5 (9%)	60,97,113	1.48	8 (13%)
21	XAT	9	305	-	39,47,47	0.96	1 (2%)	54,74,74	2.36	18 (33%)
23	CLA	b	833	-	58,66,73	1.58	6 (10%)	67,104,113	1.42	8 (11%)
23	CLA	b	837	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	8 (10%)
21	XAT	6	305	-	39,47,47	0.89	1 (2%)	54,74,74	2.73	19 (35%)
30	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
23	CLA	5	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
23	CLA	4	313	4	45,53,73	1.80	6 (13%)	52,89,113	1.56	7 (13%)
28	LMG	j	103	-	32,32,55	1.13	2 (6%)	40,40,63	1.14	3 (7%)
23	CLA	b	809	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	9 (11%)
21	XAT	5	301	-	39,47,47	0.95	2 (5%)	54,74,74	2.62	19 (35%)
25	A1L1F	8	304	-	50,59,59	1.30	4 (8%)	62,85,85	2.79	23 (37%)
30	BCR	f	801	-	41,41,41	0.69	0	56,56,56	2.14	15 (26%)
23	CLA	a	822	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
23	CLA	8	312	3	52,60,73	1.65	5 (9%)	60,97,113	1.53	8 (13%)
23	CLA	6	313	-	52,60,73	1.66	5 (9%)	60,97,113	1.51	7 (11%)
23	CLA	9	308	2	65,73,73	1.49	7 (10%)	76,113,113	1.42	9 (11%)
23	CLA	a	810	9	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)
21	XAT	8	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.66	20 (37%)
22	A1L1G	9	301	-	38,47,47	1.46	6 (15%)	49,71,71	1.57	10 (20%)
23	CLA	a	801	-	65,73,73	1.51	8 (12%)	76,113,113	1.38	7 (9%)
23	CLA	b	831	-	49,57,73	1.69	5 (10%)	55,93,113	1.55	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	DGD	4	317	-	41,41,67	1.06	2 (4%)	55,55,81	1.81	5 (9%)
30	BCR	b	844	-	41,41,41	0.71	0	56,56,56	1.92	16 (28%)
31	SF4	a	851	-	0,12,12	-	-	-		
23	CLA	1	306	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	9 (11%)
23	CLA	b	806	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	b	832	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
21	XAT	9	303	-	39,47,47	0.94	1 (2%)	54,74,74	2.61	19 (35%)
30	BCR	b	846	-	41,41,41	0.71	0	56,56,56	1.97	21 (37%)
23	CLA	2	312	-	47,55,73	1.75	6 (12%)	54,91,113	1.56	7 (12%)
23	CLA	5	308	1	60,68,73	1.55	5 (8%)	70,107,113	1.42	8 (11%)
23	CLA	a	811	-	56,64,73	1.59	6 (10%)	65,102,113	1.47	9 (13%)
23	CLA	3	314	5	47,55,73	1.74	5 (10%)	54,91,113	1.55	7 (12%)
23	CLA	a	808	-	51,59,73	1.70	5 (9%)	59,96,113	1.51	8 (13%)
30	BCR	b	845	-	41,41,41	0.68	0	56,56,56	2.10	16 (28%)
26	LHG	a	846	23	26,26,48	1.27	4 (15%)	29,32,54	1.20	2 (6%)
21	XAT	6	303	-	39,47,47	0.89	0	54,74,74	2.65	19 (35%)
23	CLA	5	313	-	52,60,73	1.65	5 (9%)	60,97,113	1.54	9 (15%)
23	CLA	6	314	-	46,54,73	1.73	5 (10%)	53,90,113	1.61	6 (11%)
23	CLA	b	816	-	55,63,73	1.63	5 (9%)	64,101,113	1.48	9 (14%)
23	CLA	2	307	-	47,55,73	1.74	5 (10%)	54,91,113	1.64	8 (14%)
23	CLA	1	313	-	41,49,73	1.84	6 (14%)	47,84,113	1.65	7 (14%)
23	CLA	b	819	-	55,63,73	1.62	6 (10%)	64,101,113	1.44	8 (12%)
21	XAT	8	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.53	19 (35%)
21	XAT	5	305	-	39,47,47	0.90	0	54,74,74	2.86	22 (40%)
23	CLA	2	310	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
23	CLA	b	820	-	50,58,73	1.69	6 (12%)	58,95,113	1.60	10 (17%)
23	CLA	2	316	7	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
30	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.13	14 (25%)
23	CLA	b	823	-	53,61,73	1.63	6 (11%)	61,98,113	1.46	8 (13%)
27	DGD	8	315	23	41,41,67	1.05	2 (4%)	55,55,81	1.11	4 (7%)
23	CLA	a	834	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	9 (11%)
23	CLA	b	828	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
23	CLA	6	316	6	46,54,73	1.75	5 (10%)	53,90,113	1.58	6 (11%)
23	CLA	3	307	5	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
23	CLA	2	309	-	46,54,73	1.76	5 (10%)	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	j	101	16	42,50,73	1.81	5 (11%)	48,85,113	1.64	6 (12%)
23	CLA	4	316	-	55,63,73	1.63	6 (10%)	64,101,113	1.45	7 (10%)
23	CLA	3	310	-	56,64,73	1.60	5 (8%)	65,102,113	1.45	7 (10%)
23	CLA	4	309	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
24	SQD	5	317	23	34,35,54	1.47	4 (11%)	43,46,65	1.35	7 (16%)
23	CLA	7	317	-	45,53,73	1.80	5 (11%)	52,89,113	1.59	6 (11%)
23	CLA	a	806	-	65,73,73	1.50	11 (16%)	76,113,113	1.67	13 (17%)
23	CLA	7	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.58	7 (13%)
23	CLA	3	309	5	56,64,73	1.59	6 (10%)	65,102,113	1.45	7 (10%)
22	A1L1G	9	306	-	38,47,47	1.41	6 (15%)	49,71,71	1.54	8 (16%)
23	CLA	a	837	9	45,53,73	1.79	5 (11%)	52,89,113	1.58	7 (13%)
23	CLA	b	839	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
23	CLA	b	825	-	64,72,73	1.49	6 (9%)	74,111,113	1.44	7 (9%)
23	CLA	7	313	-	54,62,73	1.65	5 (9%)	62,99,113	1.49	9 (14%)
23	CLA	a	838	-	51,59,73	1.66	5 (9%)	59,96,113	1.55	8 (13%)
26	LHG	9	307	-	35,35,48	1.22	6 (17%)	38,41,54	0.97	2 (5%)
21	XAT	2	304	-	39,47,47	0.88	0	54,74,74	2.54	20 (37%)
23	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	9	316	-	62,70,73	1.55	6 (9%)	72,109,113	1.37	8 (11%)
23	CLA	a	817	-	45,53,73	1.79	5 (11%)	52,89,113	1.58	6 (11%)
23	CLA	b	808	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	8 (10%)
23	CLA	9	309	2	46,54,73	1.77	6 (13%)	53,90,113	1.55	7 (13%)
23	CLA	a	816	-	50,58,73	1.69	6 (12%)	58,95,113	1.57	9 (15%)
23	CLA	a	829	-	62,70,73	1.51	5 (8%)	72,109,113	1.39	8 (11%)
23	CLA	9	315	2	42,50,73	1.83	5 (11%)	48,85,113	1.61	7 (14%)
22	A1L1G	3	306	-	38,47,47	1.45	6 (15%)	49,71,71	1.49	9 (18%)
23	CLA	a	821	-	45,53,73	1.77	6 (13%)	52,89,113	1.61	7 (13%)
23	CLA	b	815	-	45,53,73	1.76	6 (13%)	52,89,113	1.58	7 (13%)
23	CLA	8	305	3	43,51,73	1.79	5 (11%)	49,86,113	1.65	7 (14%)
23	CLA	h	201	-	65,73,73	1.51	6 (9%)	76,113,113	1.46	7 (9%)
30	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
23	CLA	4	307	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
23	CLA	7	308	-	60,68,73	1.53	5 (8%)	70,107,113	1.44	7 (10%)
23	CLA	b	817	-	59,67,73	1.56	5 (8%)	68,105,113	1.51	9 (13%)
30	BCR	b	850	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	SF4	c	101	-	0,12,12	-	-	-		
23	CLA	5	309	-	55,63,73	1.63	6 (10%)	64,101,113	1.48	7 (10%)
23	CLA	b	813	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	8 (10%)
21	XAT	8	303	-	39,47,47	0.87	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	a	825	-	55,63,73	1.62	5 (9%)	64,101,113	1.46	8 (12%)
21	XAT	7	305	-	39,47,47	0.86	0	54,74,74	2.65	19 (35%)
23	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.54	8 (12%)
21	XAT	3	304	-	39,47,47	0.90	2 (5%)	54,74,74	2.62	19 (35%)
23	CLA	5	307	24	45,53,73	1.80	5 (11%)	52,89,113	1.56	6 (11%)
23	CLA	6	310	-	52,60,73	1.65	5 (9%)	60,97,113	1.53	7 (11%)
25	A1L1F	9	302	-	50,59,59	1.37	5 (10%)	62,85,85	2.71	19 (30%)
23	CLA	b	824	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	5	314	1	45,53,73	1.81	5 (11%)	52,89,113	1.58	6 (11%)
23	CLA	a	809	9	65,73,73	1.45	6 (9%)	76,113,113	1.44	9 (11%)
23	CLA	a	827	-	65,73,73	1.49	6 (9%)	76,113,113	1.45	9 (11%)
30	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.04	17 (30%)
30	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.79	16 (28%)
23	CLA	9	313	2	46,54,73	1.77	5 (10%)	53,90,113	1.62	7 (13%)
21	XAT	4	302	-	39,47,47	0.90	2 (5%)	54,74,74	2.57	17 (31%)
29	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.09	3 (7%)
23	CLA	7	310	-	46,54,73	1.77	5 (10%)	53,90,113	1.57	6 (11%)
21	XAT	7	303	-	39,47,47	0.96	1 (2%)	54,74,74	2.60	17 (31%)
21	XAT	a	854	-	39,47,47	0.94	2 (5%)	54,74,74	2.70	20 (37%)
23	CLA	1	305	-	61,69,73	1.55	6 (9%)	71,108,113	1.39	7 (9%)
21	XAT	a	853	-	39,47,47	0.88	1 (2%)	54,74,74	2.72	18 (33%)
23	CLA	a	804	-	55,63,73	1.63	6 (10%)	64,101,113	1.55	10 (15%)
23	CLA	b	841	26	65,73,73	1.53	5 (7%)	76,113,113	1.36	8 (10%)
23	CLA	6	307	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
30	BCR	b	847	-	41,41,41	0.76	0	56,56,56	2.19	22 (39%)
23	CLA	7	312	-	48,56,73	1.71	5 (10%)	55,92,113	1.56	8 (14%)
23	CLA	a	818	-	56,64,73	1.62	6 (10%)	65,102,113	1.44	8 (12%)
23	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	7 (9%)
23	CLA	b	818	-	60,68,73	1.56	5 (8%)	70,107,113	1.40	7 (10%)
23	CLA	l	202	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
26	LHG	m	101	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
23	CLA	3	312	5	59,67,73	1.57	5 (8%)	68,105,113	1.43	7 (10%)
23	CLA	a	852	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
23	CLA	b	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
23	CLA	b	822	-	60,68,73	1.55	6 (10%)	70,107,113	1.37	7 (10%)
23	CLA	7	306	4	48,56,73	1.73	6 (12%)	55,92,113	1.53	6 (10%)
23	CLA	8	311	-	56,64,73	1.58	5 (8%)	65,102,113	1.50	8 (12%)
30	BCR	j	102	-	41,41,41	0.73	0	56,56,56	2.08	17 (30%)
24	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	4 (7%)
23	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	b	802	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	8 (10%)
30	BCR	b	852	-	41,41,41	0.72	0	56,56,56	2.06	15 (26%)
23	CLA	4	305	4	45,53,73	1.80	6 (13%)	52,89,113	1.57	7 (13%)
25	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
23	CLA	4	314	4	41,49,73	1.86	6 (14%)	47,84,113	1.64	7 (14%)
23	CLA	4	312	-	53,61,73	1.65	5 (9%)	61,98,113	1.48	8 (13%)
23	CLA	7	315	4	41,49,73	1.86	5 (12%)	47,84,113	1.65	8 (17%)
23	CLA	3	315	5	46,54,73	1.78	6 (13%)	53,90,113	1.53	7 (13%)
23	CLA	a	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.59	8 (15%)
23	CLA	1	308	8	65,73,73	1.48	5 (7%)	76,113,113	1.43	9 (11%)
23	CLA	8	308	-	55,63,73	1.61	6 (10%)	64,101,113	1.51	9 (14%)
23	CLA	a	831	-	65,73,73	1.51	5 (7%)	76,113,113	1.47	8 (10%)
23	CLA	7	307	-	45,53,73	1.81	5 (11%)	52,89,113	1.58	6 (11%)
31	SF4	c	102	-	0,12,12	-	-	-		
23	CLA	5	315	-	52,60,73	1.66	5 (9%)	60,97,113	1.54	8 (13%)
23	CLA	6	311	6	42,50,73	1.84	5 (11%)	48,85,113	1.58	7 (14%)
23	CLA	b	811	-	54,62,73	1.66	7 (12%)	67,100,113	1.50	9 (13%)
23	CLA	b	830	-	41,49,73	1.83	6 (14%)	47,84,113	1.64	9 (19%)
23	CLA	b	838	-	65,73,73	1.52	6 (9%)	76,113,113	1.34	8 (10%)
21	XAT	1	303	-	39,47,47	0.89	1 (2%)	54,74,74	2.52	20 (37%)
23	CLA	a	844	26	65,73,73	1.46	5 (7%)	76,113,113	1.39	9 (11%)
23	CLA	5	316	-	46,54,73	1.74	5 (10%)	53,90,113	1.57	7 (13%)
23	CLA	1	314	-	45,53,73	1.79	5 (11%)	52,89,113	1.56	6 (11%)
21	XAT	7	301	-	39,47,47	0.93	1 (2%)	54,74,74	2.62	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	XAT	3	301	-	39,47,47	0.92	2 (5%)	54,74,74	2.54	19 (35%)
21	XAT	7	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.68	21 (38%)
23	CLA	b	804	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	b	812	-	53,61,73	1.65	5 (9%)	61,98,113	1.49	8 (13%)
23	CLA	l	201	-	42,50,73	1.82	6 (14%)	48,85,113	1.64	7 (14%)
30	BCR	b	843	-	41,41,41	0.70	0	56,56,56	2.29	21 (37%)
23	CLA	a	840	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	7 (9%)
23	CLA	9	312	-	46,54,73	1.75	6 (13%)	53,90,113	1.68	8 (15%)
23	CLA	b	803	-	65,73,73	1.45	6 (9%)	76,113,113	1.54	12 (15%)
23	CLA	6	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	6 (7%)
23	CLA	b	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
25	A1L1F	6	304	-	46,55,59	1.33	4 (8%)	58,81,85	2.55	20 (34%)
23	CLA	a	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
29	PQN	b	842	-	34,34,34	1.55	2 (5%)	42,45,45	1.21	4 (9%)
23	CLA	1	309	8	46,54,73	1.79	5 (10%)	53,90,113	1.51	7 (13%)
23	CLA	b	810	-	65,73,73	1.46	5 (7%)	76,113,113	1.45	8 (10%)
30	BCR	a	849	-	41,41,41	0.74	0	56,56,56	2.16	19 (33%)
23	CLA	a	823	-	49,57,73	1.69	6 (12%)	55,93,113	1.61	7 (12%)
23	CLA	8	314	-	41,49,73	1.85	5 (12%)	47,84,113	1.63	7 (14%)
23	CLA	5	312	-	51,59,73	1.65	5 (9%)	59,96,113	1.52	9 (15%)
23	CLA	h	203	-	55,63,73	1.62	6 (10%)	64,101,113	1.47	9 (14%)
23	CLA	b	821	-	51,59,73	1.66	6 (11%)	59,96,113	1.57	9 (15%)
23	CLA	3	311	-	50,58,73	1.71	5 (10%)	58,95,113	1.54	9 (15%)
27	DGD	b	851	-	58,58,67	1.15	7 (12%)	72,72,81	1.53	10 (13%)
23	CLA	8	306	27	46,54,73	1.75	5 (10%)	53,90,113	1.54	7 (13%)
30	BCR	b	853	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
23	CLA	b	814	-	55,63,73	1.61	6 (10%)	64,101,113	1.56	8 (12%)
21	XAT	6	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.81	20 (37%)
21	XAT	5	302	-	39,47,47	0.94	1 (2%)	54,74,74	2.57	19 (35%)
23	CLA	l	203	-	46,54,73	1.75	6 (13%)	53,90,113	1.57	7 (13%)
23	CLA	a	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
22	A1L1G	7	302	-	38,47,47	1.42	6 (15%)	49,71,71	1.51	9 (18%)
23	CLA	a	803	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	6 (7%)
23	CLA	a	832	-	50,58,73	1.68	6 (12%)	58,95,113	1.54	9 (15%)
23	CLA	a	824	-	46,54,73	1.77	6 (13%)	53,90,113	1.49	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	829	-	65,73,73	1.52	6 (9%)	76,113,113	1.44	10 (13%)
23	CLA	a	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	6 (7%)
23	CLA	a	802	-	58,66,73	1.55	6 (10%)	67,104,113	1.50	8 (11%)
23	CLA	b	805	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	7 (9%)
21	XAT	4	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.75	19 (35%)
22	A1L1G	5	304	-	38,47,47	1.41	6 (15%)	49,71,71	1.44	7 (14%)
23	CLA	7	314	-	45,53,73	1.80	6 (13%)	52,89,113	1.64	7 (13%)
25	A1L1F	h	202	-	50,59,59	1.39	5 (10%)	62,85,85	2.60	22 (35%)
23	CLA	2	314	-	56,64,73	1.63	7 (12%)	65,102,113	1.45	7 (10%)
21	XAT	6	306	-	39,47,47	0.93	1 (2%)	54,74,74	2.61	19 (35%)
21	XAT	3	305	-	39,47,47	0.87	1 (2%)	54,74,74	2.57	17 (31%)
23	CLA	7	316	-	51,59,73	1.64	6 (11%)	59,96,113	1.58	8 (13%)
21	XAT	4	303	-	39,47,47	0.88	0	54,74,74	2.56	15 (27%)
23	CLA	b	826	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	6 (7%)
23	CLA	2	315	-	42,50,73	1.86	6 (14%)	48,85,113	1.55	7 (14%)
23	CLA	f	803	13	52,60,73	1.67	5 (9%)	60,97,113	1.49	8 (13%)
23	CLA	a	819	-	54,62,73	1.63	7 (12%)	62,99,113	1.46	7 (11%)
23	CLA	8	307	3	65,73,73	1.47	5 (7%)	76,113,113	1.39	8 (10%)
23	CLA	2	311	-	58,66,73	1.58	5 (8%)	67,104,113	1.41	7 (10%)
23	CLA	7	309	-	46,55,73	1.75	5 (10%)	52,91,113	1.52	7 (13%)
28	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.30	4 (9%)
22	A1L1G	3	302	-	38,47,47	1.46	6 (15%)	49,71,71	1.38	7 (14%)
30	BCR	i	102	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
23	CLA	8	309	-	57,65,73	1.60	5 (8%)	66,103,113	1.45	9 (13%)
23	CLA	1	310	8	65,73,73	1.50	5 (7%)	76,113,113	1.33	8 (10%)
23	CLA	a	842	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
23	CLA	b	835	-	53,61,73	1.67	5 (9%)	61,98,113	1.50	8 (13%)
23	CLA	3	313	-	52,60,73	1.65	6 (11%)	60,97,113	1.52	9 (15%)
23	CLA	2	306	-	41,50,73	1.85	6 (14%)	46,85,113	1.57	6 (13%)
23	CLA	1	311	-	53,61,73	1.63	5 (9%)	61,98,113	1.50	9 (14%)
23	CLA	8	310	-	46,54,73	1.76	6 (13%)	53,90,113	1.54	7 (13%)
21	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.60	16 (29%)
23	CLA	6	315	6	41,49,73	1.87	6 (14%)	47,84,113	1.62	6 (12%)
23	CLA	a	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	a	841	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	2	308	7	54,62,73	1.64	6 (11%)	62,99,113	1.46	8 (12%)
22	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.57	11 (22%)
21	XAT	5	303	-	39,47,47	0.93	1 (2%)	54,74,74	2.59	20 (37%)
23	CLA	4	310	-	46,54,73	1.78	6 (13%)	53,90,113	1.55	7 (13%)
23	CLA	a	814	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	6	312	6	51,59,73	1.67	6 (11%)	59,96,113	1.52	6 (10%)
23	CLA	a	820	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	9 (11%)
30	BCR	m	102	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	6 (10%)
21	XAT	2	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.50	18 (33%)
23	CLA	9	314	-	55,63,73	1.62	6 (10%)	64,101,113	1.50	8 (12%)
30	BCR	a	850	-	41,41,41	0.74	0	56,56,56	2.16	14 (25%)
23	CLA	9	311	-	46,54,73	1.77	5 (10%)	53,90,113	1.62	8 (15%)
23	CLA	5	306	1	46,54,73	1.78	6 (13%)	53,90,113	1.55	8 (15%)
23	CLA	b	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	4	306	-	56,64,73	1.61	5 (8%)	65,102,113	1.44	9 (13%)
23	CLA	4	311	-	46,54,73	1.79	6 (13%)	53,90,113	1.51	7 (13%)
23	CLA	a	805	23	55,63,73	1.61	6 (10%)	64,101,113	1.51	8 (12%)
23	CLA	a	836	-	50,58,73	1.70	6 (12%)	58,95,113	1.50	9 (15%)
23	CLA	9	310	-	46,54,73	1.75	5 (10%)	53,90,113	1.64	6 (11%)
21	XAT	4	301	-	39,47,47	0.91	1 (2%)	54,74,74	2.57	19 (35%)

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	1	307	-	1/1/12/20	6/24/102/115	-
23	CLA	4	315	-	1/1/11/20	7/15/93/115	-
23	CLA	3	308	-	1/1/11/20	5/16/94/115	-
23	CLA	a	856	-	1/1/15/20	13/37/115/115	-
21	XAT	2	305	-	-	2/31/93/93	0/4/4/4
23	CLA	5	310	1	1/1/15/20	14/37/115/115	-
23	CLA	b	840	-	1/1/15/20	17/37/115/115	-
23	CLA	6	308	-	1/1/13/20	4/29/107/115	-
21	XAT	2	301	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	830	-	1/1/15/20	15/37/115/115	-
21	XAT	3	303	-	-	3/31/93/93	0/4/4/4
25	A1L1F	6	301	-	-	11/43/99/99	0/3/3/3
26	LHG	b	849	23	-	20/35/35/53	-
23	CLA	a	813	-	1/1/12/20	10/24/102/115	-
23	CLA	b	836	-	1/1/13/20	11/29/107/115	-
23	CLA	4	308	-	1/1/12/20	7/19/97/115	-
28	LMG	a	855	-	-	13/29/49/70	0/1/1/1
23	CLA	2	313	7	1/1/10/20	4/8/86/115	-
23	CLA	a	812	23	1/1/14/20	9/34/112/115	-
23	CLA	8	313	-	1/1/11/20	3/15/93/115	-
23	CLA	b	833	-	1/1/13/20	16/29/107/115	-
23	CLA	1	312	8	1/1/12/20	3/22/100/115	-
23	CLA	b	837	-	1/1/15/20	8/37/115/115	-
21	XAT	9	305	-	-	3/31/93/93	0/4/4/4
21	XAT	2	303	-	-	6/31/93/93	0/4/4/4
21	XAT	6	305	-	-	4/31/93/93	0/4/4/4
30	BCR	a	847	-	-	0/29/63/63	0/2/2/2
23	CLA	5	311	-	1/1/11/20	6/15/93/115	-
23	CLA	4	313	4	1/1/11/20	3/13/91/115	-
28	LMG	j	103	-	-	11/27/47/70	0/1/1/1
23	CLA	b	809	-	1/1/15/20	16/37/115/115	-
21	XAT	5	301	-	-	4/31/93/93	0/4/4/4
25	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
30	BCR	f	801	-	-	3/29/63/63	0/2/2/2
23	CLA	a	822	-	1/1/15/20	5/37/115/115	-
23	CLA	8	312	3	1/1/12/20	2/22/100/115	-
23	CLA	6	313	-	1/1/12/20	2/22/100/115	-
23	CLA	9	308	2	1/1/15/20	15/37/115/115	-
23	CLA	a	810	9	1/1/15/20	13/37/115/115	-
23	CLA	b	831	-	1/1/11/20	6/18/96/115	-
21	XAT	8	302	-	-	4/31/93/93	0/4/4/4
23	CLA	a	801	-	1/1/15/20	22/37/115/115	-
22	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DGD	4	317	-	-	10/29/69/95	0/2/2/2
30	BCR	b	844	-	-	2/29/63/63	0/2/2/2
31	SF4	a	851	-	-	-	0/6/5/5
23	CLA	1	306	-	1/1/15/20	15/37/115/115	-
23	CLA	b	806	-	1/1/15/20	19/37/115/115	-
23	CLA	b	832	-	1/1/15/20	13/37/115/115	-
21	XAT	9	303	-	-	4/31/93/93	0/4/4/4
30	BCR	b	846	-	-	0/29/63/63	0/2/2/2
23	CLA	2	312	-	1/1/11/20	4/16/94/115	-
23	CLA	5	308	1	1/1/14/20	7/31/109/115	-
23	CLA	a	811	-	1/1/13/20	8/27/105/115	-
23	CLA	3	314	5	1/1/11/20	7/16/94/115	-
23	CLA	a	808	-	1/1/12/20	3/21/99/115	-
30	BCR	b	845	-	-	6/29/63/63	0/2/2/2
26	LHG	a	846	23	-	16/31/31/53	-
21	XAT	6	303	-	-	5/31/93/93	0/4/4/4
23	CLA	5	313	-	1/1/12/20	0/22/100/115	-
23	CLA	6	314	-	1/1/11/20	6/15/93/115	-
23	CLA	b	816	-	1/1/13/20	4/25/103/115	-
23	CLA	2	307	-	1/1/11/20	6/16/94/115	-
23	CLA	1	313	-	1/1/10/20	3/8/86/115	-
23	CLA	b	819	-	1/1/13/20	3/25/103/115	-
21	XAT	8	301	-	-	3/31/93/93	0/4/4/4
23	CLA	2	310	-	1/1/15/20	14/37/115/115	-
21	XAT	5	305	-	-	1/31/93/93	0/4/4/4
23	CLA	b	820	-	1/1/12/20	7/19/97/115	-
23	CLA	2	316	7	1/1/11/20	5/15/93/115	-
30	BCR	i	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	823	-	1/1/12/20	8/23/101/115	-
27	DGD	8	315	23	-	11/29/69/95	0/2/2/2
23	CLA	a	834	-	1/1/15/20	7/37/115/115	-
23	CLA	b	828	-	1/1/15/20	11/37/115/115	-
23	CLA	6	316	6	1/1/11/20	7/15/93/115	-
23	CLA	3	307	5	1/1/11/20	1/13/91/115	-
23	CLA	2	309	-	1/1/11/20	4/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	j	101	16	1/1/10/20	5/10/88/115	-
23	CLA	4	316	-	1/1/13/20	7/25/103/115	-
23	CLA	3	310	-	1/1/13/20	4/27/105/115	-
23	CLA	4	309	-	1/1/15/20	16/37/115/115	-
24	SQD	5	317	23	-	11/30/50/69	0/1/1/1
23	CLA	7	317	-	1/1/11/20	5/13/91/115	-
23	CLA	a	806	-	1/1/15/20	12/37/115/115	-
23	CLA	7	311	-	1/1/11/20	5/15/93/115	-
23	CLA	3	309	5	1/1/13/20	5/27/105/115	-
22	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
23	CLA	a	837	9	1/1/11/20	4/13/91/115	-
23	CLA	b	839	-	1/1/15/20	13/37/115/115	-
23	CLA	b	825	-	1/1/14/20	6/36/114/115	-
23	CLA	7	313	-	1/1/12/20	7/24/102/115	-
23	CLA	a	838	-	1/1/12/20	6/21/99/115	-
26	LHG	9	307	-	-	21/40/40/53	-
21	XAT	2	304	-	-	3/31/93/93	0/4/4/4
23	CLA	f	802	-	1/1/15/20	13/37/115/115	-
23	CLA	9	316	-	1/1/14/20	9/34/112/115	-
23	CLA	a	817	-	1/1/11/20	6/13/91/115	-
23	CLA	b	808	-	1/1/15/20	11/37/115/115	-
23	CLA	9	309	2	1/1/11/20	3/15/93/115	-
23	CLA	a	816	-	1/1/12/20	5/19/97/115	-
23	CLA	a	829	-	1/1/14/20	15/34/112/115	-
23	CLA	9	315	2	1/1/10/20	6/10/88/115	-
22	A1L1G	3	306	-	-	18/29/85/85	0/3/3/3
23	CLA	a	821	-	1/1/11/20	2/13/91/115	-
23	CLA	b	815	-	1/1/11/20	3/13/91/115	-
23	CLA	8	305	3	1/1/10/20	2/11/89/115	-
23	CLA	h	201	-	1/1/15/20	9/37/115/115	-
30	BCR	a	848	-	-	0/29/63/63	0/2/2/2
23	CLA	4	307	-	1/1/15/20	14/37/115/115	-
23	CLA	7	308	-	1/1/14/20	14/31/109/115	-
23	CLA	b	817	-	1/1/13/20	10/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	b	850	-	-	2/29/63/63	0/2/2/2
31	SF4	c	101	-	-	-	0/6/5/5
23	CLA	5	309	-	1/1/13/20	4/25/103/115	-
23	CLA	b	813	-	1/1/15/20	14/37/115/115	-
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	a	825	-	1/1/13/20	8/25/103/115	-
21	XAT	7	305	-	-	2/31/93/93	0/4/4/4
23	CLA	a	833	-	1/1/13/20	2/25/103/115	-
21	XAT	3	304	-	-	3/31/93/93	0/4/4/4
23	CLA	5	307	24	1/1/11/20	7/13/91/115	-
23	CLA	6	310	-	1/1/12/20	7/22/100/115	-
25	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
23	CLA	b	824	-	1/1/15/20	14/37/115/115	-
23	CLA	5	314	1	1/1/11/20	5/13/91/115	-
23	CLA	a	809	9	1/1/15/20	15/37/115/115	-
23	CLA	a	827	-	1/1/15/20	8/37/115/115	-
30	BCR	f	804	-	-	4/29/63/63	0/2/2/2
30	BCR	b	848	-	-	2/29/63/63	0/2/2/2
23	CLA	9	313	2	1/1/11/20	9/15/93/115	-
21	XAT	4	302	-	-	3/31/93/93	0/4/4/4
29	PQN	a	843	-	-	5/23/43/43	0/2/2/2
23	CLA	7	310	-	1/1/11/20	6/15/93/115	-
21	XAT	7	303	-	-	8/31/93/93	0/4/4/4
23	CLA	1	305	-	1/1/14/20	10/33/111/115	-
23	CLA	a	804	-	1/1/13/20	10/25/103/115	-
23	CLA	b	841	26	1/1/15/20	9/37/115/115	-
21	XAT	a	853	-	-	5/31/93/93	0/4/4/4
21	XAT	a	854	-	-	7/31/93/93	0/4/4/4
23	CLA	6	307	-	1/1/11/20	1/15/93/115	-
30	BCR	b	847	-	-	1/29/63/63	0/2/2/2
23	CLA	7	312	-	1/1/11/20	3/17/95/115	-
23	CLA	a	818	-	1/1/13/20	11/27/105/115	-
23	CLA	a	835	-	1/1/15/20	12/37/115/115	-
23	CLA	b	818	-	1/1/14/20	14/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	l	202	-	1/1/14/20	6/31/109/115	-
26	LHG	a	845	-	-	27/52/52/53	-
26	LHG	m	101	-	-	28/50/50/53	-
23	CLA	3	312	5	1/1/13/20	9/30/108/115	-
23	CLA	a	852	-	1/1/15/20	17/37/115/115	-
23	CLA	b	807	-	1/1/15/20	12/37/115/115	-
23	CLA	b	822	-	1/1/14/20	7/31/109/115	-
23	CLA	7	306	4	1/1/11/20	10/17/95/115	-
23	CLA	8	311	-	1/1/13/20	8/27/105/115	-
30	BCR	j	102	-	-	4/29/63/63	0/2/2/2
24	SQD	1	315	-	-	19/40/60/69	0/1/1/1
23	CLA	b	801	-	1/1/15/20	20/37/115/115	-
23	CLA	b	802	-	1/1/15/20	18/37/115/115	-
30	BCR	b	852	-	-	5/29/63/63	0/2/2/2
23	CLA	4	305	4	1/1/11/20	7/13/91/115	-
25	A1L1F	1	304	-	-	11/43/99/99	0/3/3/3
23	CLA	4	314	4	1/1/10/20	5/8/86/115	-
23	CLA	4	312	-	1/1/12/20	6/23/101/115	-
23	CLA	7	315	4	1/1/10/20	4/8/86/115	-
23	CLA	3	315	5	1/1/11/20	8/15/93/115	-
23	CLA	a	815	-	1/1/11/20	2/13/91/115	-
23	CLA	1	308	8	1/1/15/20	13/37/115/115	-
23	CLA	8	308	-	1/1/13/20	7/25/103/115	-
23	CLA	a	831	-	1/1/15/20	11/37/115/115	-
23	CLA	7	307	-	1/1/11/20	5/13/91/115	-
31	SF4	c	102	-	-	-	0/6/5/5
23	CLA	5	315	-	1/1/12/20	4/22/100/115	-
23	CLA	6	311	6	1/1/10/20	2/10/88/115	-
23	CLA	b	811	-	1/1/13/20	5/25/101/115	-
23	CLA	b	830	-	1/1/10/20	1/8/86/115	-
23	CLA	b	838	-	1/1/15/20	8/37/115/115	-
21	XAT	1	303	-	-	0/31/93/93	0/4/4/4
23	CLA	a	844	26	1/1/15/20	16/37/115/115	-
23	CLA	5	316	-	1/1/11/20	5/15/93/115	-
23	CLA	1	314	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	804	-	1/1/15/20	12/37/115/115	-
23	CLA	b	812	-	1/1/12/20	6/23/101/115	-
23	CLA	l	201	-	1/1/10/20	2/10/88/115	-
21	XAT	3	301	-	-	3/31/93/93	0/4/4/4
21	XAT	7	301	-	-	6/31/93/93	0/4/4/4
21	XAT	7	304	-	-	6/31/93/93	0/4/4/4
30	BCR	b	843	-	-	2/29/63/63	0/2/2/2
23	CLA	a	840	-	1/1/15/20	8/37/115/115	-
23	CLA	9	312	-	1/1/11/20	9/15/93/115	-
23	CLA	b	803	-	1/1/15/20	10/37/115/115	-
23	CLA	6	309	-	1/1/15/20	10/37/115/115	-
23	CLA	b	834	-	1/1/15/20	14/37/115/115	-
25	A1L1F	6	304	-	-	12/39/95/99	0/3/3/3
23	CLA	a	828	-	1/1/15/20	9/37/115/115	-
29	PQN	b	842	-	-	1/23/43/43	0/2/2/2
23	CLA	1	309	8	1/1/11/20	6/15/93/115	-
23	CLA	b	810	-	1/1/15/20	17/37/115/115	-
30	BCR	a	849	-	-	0/29/63/63	0/2/2/2
23	CLA	a	823	-	1/1/11/20	7/18/96/115	-
23	CLA	8	314	-	1/1/10/20	5/8/86/115	-
23	CLA	5	312	-	1/1/12/20	8/21/99/115	-
23	CLA	h	203	-	1/1/13/20	9/25/103/115	-
23	CLA	b	821	-	1/1/12/20	2/21/99/115	-
23	CLA	3	311	-	1/1/12/20	4/19/97/115	-
27	DGD	b	851	-	-	20/46/86/95	0/2/2/2
23	CLA	8	306	27	1/1/11/20	2/15/93/115	-
30	BCR	b	853	-	-	4/29/63/63	0/2/2/2
23	CLA	b	814	-	1/1/13/20	13/25/103/115	-
21	XAT	6	302	-	-	7/31/93/93	0/4/4/4
23	CLA	l	203	-	1/1/11/20	4/15/93/115	-
21	XAT	5	302	-	-	3/31/93/93	0/4/4/4
23	CLA	a	807	-	1/1/15/20	18/37/115/115	-
23	CLA	a	832	-	1/1/12/20	5/19/97/115	-
23	CLA	a	803	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	829	-	1/1/15/20	11/37/115/115	-
23	CLA	a	824	-	1/1/11/20	4/15/93/115	-
22	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
23	CLA	a	826	-	1/1/15/20	9/37/115/115	-
23	CLA	a	802	-	1/1/13/20	7/29/107/115	-
23	CLA	b	805	-	1/1/15/20	16/37/115/115	-
23	CLA	7	314	-	1/1/11/20	4/13/91/115	-
21	XAT	4	304	-	-	4/31/93/93	0/4/4/4
22	A1L1G	5	304	-	-	9/29/85/85	0/3/3/3
25	A1L1F	h	202	-	-	11/43/99/99	1/3/3/3
23	CLA	2	314	-	1/1/13/20	13/27/105/115	-
21	XAT	6	306	-	-	4/31/93/93	0/4/4/4
21	XAT	3	305	-	-	0/31/93/93	0/4/4/4
23	CLA	7	316	-	1/1/12/20	11/21/99/115	-
21	XAT	4	303	-	-	0/31/93/93	0/4/4/4
23	CLA	b	826	-	1/1/15/20	5/37/115/115	-
23	CLA	2	315	-	1/1/10/20	1/10/88/115	-
23	CLA	f	803	13	1/1/12/20	2/22/100/115	-
23	CLA	a	819	-	1/1/12/20	4/24/102/115	-
23	CLA	8	307	3	1/1/15/20	13/37/115/115	-
23	CLA	2	311	-	1/1/13/20	5/29/107/115	-
23	CLA	7	309	-	1/1/11/20	5/15/93/115	-
28	LMG	2	317	-	-	11/30/50/70	0/1/1/1
22	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
30	BCR	i	102	-	-	8/29/63/63	0/2/2/2
23	CLA	8	309	-	1/1/13/20	8/28/106/115	-
23	CLA	1	310	8	1/1/15/20	18/37/115/115	-
23	CLA	a	842	-	1/1/15/20	9/37/115/115	-
23	CLA	b	835	-	1/1/12/20	8/23/101/115	-
23	CLA	3	313	-	1/1/12/20	1/22/100/115	-
23	CLA	2	306	-	1/1/10/20	2/9/87/115	-
23	CLA	1	311	-	1/1/12/20	6/23/101/115	-
23	CLA	8	310	-	1/1/11/20	5/15/93/115	-
21	XAT	1	302	-	-	0/31/93/93	0/4/4/4
23	CLA	6	315	6	1/1/10/20	3/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	839	-	1/1/15/20	15/37/115/115	-
23	CLA	a	841	-	1/1/15/20	15/37/115/115	-
23	CLA	2	308	7	1/1/12/20	5/24/102/115	-
22	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
23	CLA	4	310	-	1/1/11/20	8/15/93/115	-
21	XAT	5	303	-	-	3/31/93/93	0/4/4/4
23	CLA	a	814	-	1/1/15/20	20/37/115/115	-
23	CLA	6	312	6	1/1/12/20	5/21/99/115	-
23	CLA	a	820	-	1/1/15/20	16/37/115/115	-
30	BCR	m	102	-	-	9/29/63/63	0/2/2/2
21	XAT	2	302	-	-	0/31/93/93	0/4/4/4
23	CLA	9	314	-	1/1/13/20	9/25/103/115	-
30	BCR	a	850	-	-	4/29/63/63	0/2/2/2
23	CLA	9	311	-	1/1/11/20	7/15/93/115	-
23	CLA	5	306	1	1/1/11/20	4/15/93/115	-
23	CLA	b	827	-	1/1/15/20	14/37/115/115	-
23	CLA	4	306	-	1/1/13/20	7/27/105/115	-
23	CLA	4	311	-	1/1/11/20	4/15/93/115	-
23	CLA	a	805	23	1/1/13/20	6/25/103/115	-
23	CLA	a	836	-	1/1/12/20	6/19/97/115	-
23	CLA	9	310	-	1/1/11/20	6/15/93/115	-
21	XAT	4	301	-	-	0/31/93/93	0/4/4/4

The worst 5 of 1214 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	312	CLA	C4B-NB	7.98	1.42	1.35
23	a	818	CLA	C4B-NB	7.78	1.42	1.35
23	a	840	CLA	C4B-NB	7.78	1.42	1.35
23	a	842	CLA	C4B-NB	7.76	1.42	1.35
23	b	838	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	13.14	123.26	113.38
27	4	317	DGD	C6E-C5E-C4E	-9.39	91.00	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	301	A1L1F	O15-C20-C21	8.72	119.94	113.38
25	6	304	A1L1F	O15-C20-C21	8.65	119.88	113.38
25	8	304	A1L1F	O15-C20-C21	8.52	119.78	113.38

5 of 188 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	5	306	CLA	ND
23	5	307	CLA	ND
23	5	308	CLA	ND
23	5	309	CLA	ND
23	5	310	CLA	ND

5 of 2078 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	5	301	XAT	C27-C28-C29-C30
21	5	301	XAT	C27-C28-C29-C39
21	5	303	XAT	O4-C6-C7-C8
21	5	303	XAT	C7-C8-C9-C10
21	5	303	XAT	C7-C8-C9-C19

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	h	202	A1L1F	C1-C11-C3-C4-C6-C8

234 monomers are involved in 806 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	315	CLA	1	0
23	3	308	CLA	2	0
23	a	856	CLA	23	0
21	2	305	XAT	4	0
23	5	310	CLA	6	0
23	b	840	CLA	5	0
23	6	308	CLA	5	0
21	2	301	XAT	3	0
23	a	830	CLA	7	0
21	3	303	XAT	2	0
25	6	301	A1L1F	2	0
26	b	849	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	813	CLA	1	0
23	b	836	CLA	5	0
23	4	308	CLA	3	0
28	a	855	LMG	10	0
23	a	812	CLA	2	0
21	2	303	XAT	11	0
23	8	313	CLA	3	0
23	1	312	CLA	2	0
21	9	305	XAT	3	0
23	b	833	CLA	5	0
23	b	837	CLA	7	0
21	6	305	XAT	3	0
30	a	847	BCR	3	0
23	5	311	CLA	2	0
23	4	313	CLA	1	0
28	j	103	LMG	6	0
23	b	809	CLA	1	0
21	5	301	XAT	4	0
25	8	304	A1L1F	2	0
30	f	801	BCR	24	0
23	a	822	CLA	5	0
23	8	312	CLA	2	0
23	6	313	CLA	1	0
23	9	308	CLA	5	0
23	a	810	CLA	9	0
21	8	302	XAT	6	0
22	9	301	A1L1G	2	0
23	a	801	CLA	6	0
23	b	831	CLA	1	0
27	4	317	DGD	11	0
30	b	844	BCR	2	0
23	1	306	CLA	5	0
23	b	806	CLA	5	0
23	b	832	CLA	11	0
21	9	303	XAT	6	0
30	b	846	BCR	2	0
23	5	308	CLA	7	0
23	a	808	CLA	1	0
30	b	845	BCR	6	0
26	a	846	LHG	2	0
21	6	303	XAT	10	0
23	5	313	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	6	314	CLA	1	0
23	b	816	CLA	4	0
23	b	819	CLA	1	0
21	8	301	XAT	3	0
21	5	305	XAT	5	0
23	2	310	CLA	3	0
23	b	820	CLA	2	0
23	2	316	CLA	2	0
30	i	101	BCR	4	0
23	b	823	CLA	6	0
27	8	315	DGD	2	0
23	a	834	CLA	7	0
23	b	828	CLA	3	0
23	j	101	CLA	2	0
23	4	316	CLA	7	0
23	4	309	CLA	4	0
24	5	317	SQD	1	0
23	a	806	CLA	10	0
23	7	311	CLA	3	0
23	3	309	CLA	1	0
22	9	306	A1L1G	1	0
23	a	837	CLA	1	0
23	b	839	CLA	15	0
23	b	825	CLA	3	0
23	7	313	CLA	4	0
23	a	838	CLA	1	0
26	9	307	LHG	1	0
21	2	304	XAT	3	0
23	f	802	CLA	1	0
23	9	316	CLA	12	0
23	b	808	CLA	3	0
23	9	309	CLA	1	0
23	a	816	CLA	2	0
23	a	829	CLA	7	0
23	9	315	CLA	1	0
23	8	305	CLA	4	0
23	h	201	CLA	5	0
30	a	848	BCR	5	0
23	4	307	CLA	6	0
23	7	308	CLA	7	0
23	b	817	CLA	8	0
30	b	850	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	5	309	CLA	1	0
23	b	813	CLA	6	0
21	8	303	XAT	6	0
21	9	304	XAT	7	0
23	a	825	CLA	5	0
21	7	305	XAT	2	0
23	a	833	CLA	11	0
21	3	304	XAT	4	0
25	9	302	A1L1F	1	0
23	b	824	CLA	6	0
23	a	809	CLA	2	0
23	a	827	CLA	3	0
30	f	804	BCR	7	0
30	b	848	BCR	6	0
23	9	313	CLA	2	0
21	4	302	XAT	9	0
29	a	843	PQN	4	0
23	7	310	CLA	1	0
21	7	303	XAT	12	0
21	a	854	XAT	3	0
21	a	853	XAT	4	0
23	a	804	CLA	2	0
23	b	841	CLA	4	0
30	b	847	BCR	6	0
23	7	312	CLA	1	0
23	a	818	CLA	12	0
23	a	835	CLA	4	0
23	b	818	CLA	3	0
23	l	202	CLA	9	0
26	a	845	LHG	3	0
26	m	101	LHG	2	0
23	3	312	CLA	1	0
23	a	852	CLA	4	0
23	b	807	CLA	2	0
23	b	822	CLA	5	0
23	7	306	CLA	2	0
23	8	311	CLA	3	0
30	j	102	BCR	14	0
24	1	315	SQD	3	0
23	b	801	CLA	16	0
23	b	802	CLA	3	0
30	b	852	BCR	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	305	CLA	2	0
25	1	304	A1L1F	11	0
23	4	314	CLA	1	0
23	4	312	CLA	3	0
23	7	315	CLA	2	0
23	1	308	CLA	4	0
23	8	308	CLA	2	0
23	a	831	CLA	5	0
23	7	307	CLA	2	0
31	c	102	SF4	3	0
23	5	315	CLA	3	0
23	b	811	CLA	2	0
23	b	830	CLA	5	0
23	b	838	CLA	5	0
21	1	303	XAT	4	0
23	a	844	CLA	17	0
23	5	316	CLA	1	0
21	7	301	XAT	3	0
21	3	301	XAT	4	0
21	7	304	XAT	11	0
23	b	804	CLA	3	0
23	b	812	CLA	5	0
23	l	201	CLA	1	0
30	b	843	BCR	4	0
23	a	840	CLA	6	0
23	9	312	CLA	4	0
23	b	803	CLA	4	0
23	6	309	CLA	2	0
23	b	834	CLA	4	0
25	6	304	A1L1F	3	0
23	a	828	CLA	5	0
29	b	842	PQN	6	0
23	b	810	CLA	22	0
30	a	849	BCR	4	0
23	a	823	CLA	3	0
23	8	314	CLA	1	0
23	5	312	CLA	1	0
23	h	203	CLA	2	0
23	b	821	CLA	3	0
23	3	311	CLA	1	0
27	b	851	DGD	6	0
23	8	306	CLA	1	0

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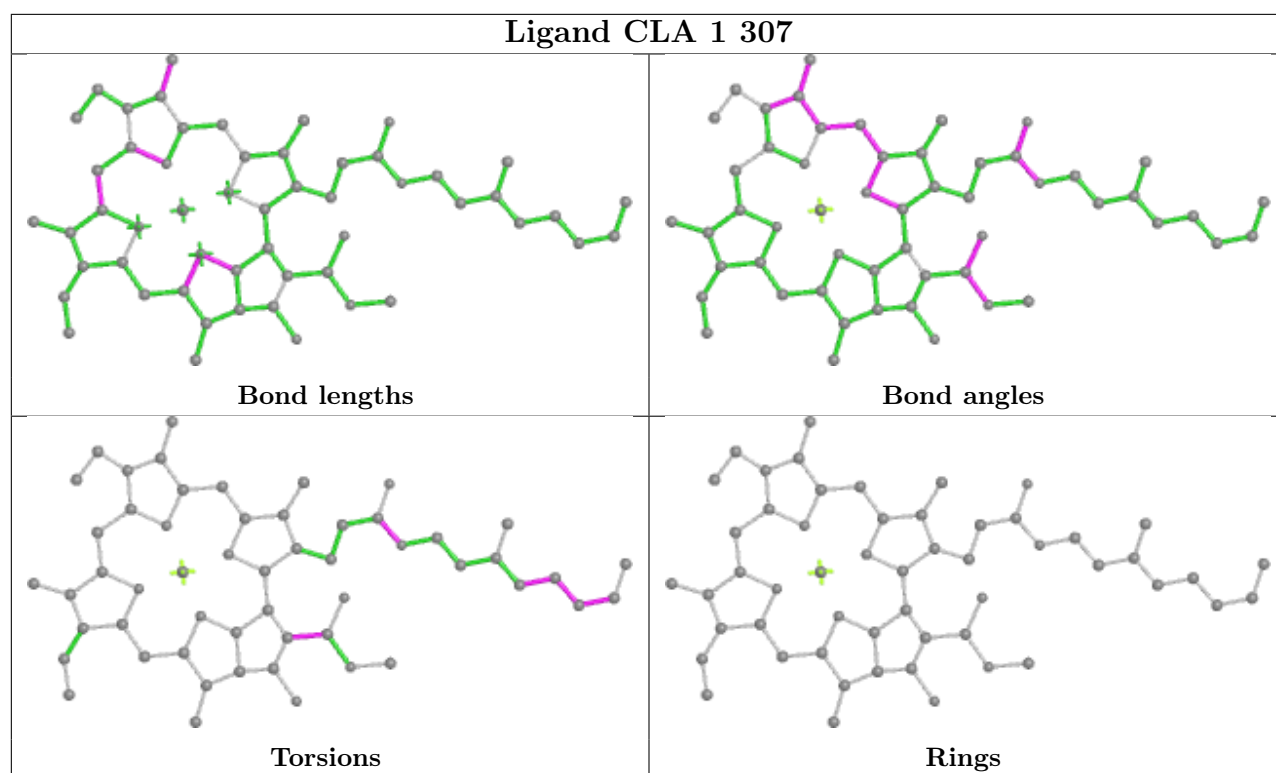
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	b	853	BCR	16	0
23	b	814	CLA	3	0
21	6	302	XAT	3	0
21	5	302	XAT	6	0
23	a	807	CLA	4	0
22	7	302	A1L1G	2	0
23	a	803	CLA	13	0
23	a	832	CLA	2	0
23	a	824	CLA	1	0
23	b	829	CLA	4	0
23	a	826	CLA	8	0
23	a	802	CLA	14	0
23	b	805	CLA	2	0
21	4	304	XAT	6	0
22	5	304	A1L1G	1	0
23	7	314	CLA	3	0
25	h	202	A1L1F	4	0
23	2	314	CLA	1	0
21	6	306	XAT	2	0
21	3	305	XAT	4	0
23	7	316	CLA	1	0
21	4	303	XAT	3	0
23	b	826	CLA	5	0
23	f	803	CLA	1	0
23	a	819	CLA	5	0
23	8	307	CLA	5	0
28	2	317	LMG	3	0
30	i	102	BCR	13	0
23	a	842	CLA	4	0
23	b	835	CLA	1	0
23	3	313	CLA	3	0
23	1	311	CLA	4	0
23	8	310	CLA	1	0
21	1	302	XAT	3	0
23	6	315	CLA	3	0
23	a	839	CLA	3	0
23	a	841	CLA	17	0
23	2	308	CLA	4	0
22	1	301	A1L1G	1	0
21	5	303	XAT	9	0
23	4	310	CLA	2	0
23	a	814	CLA	3	0

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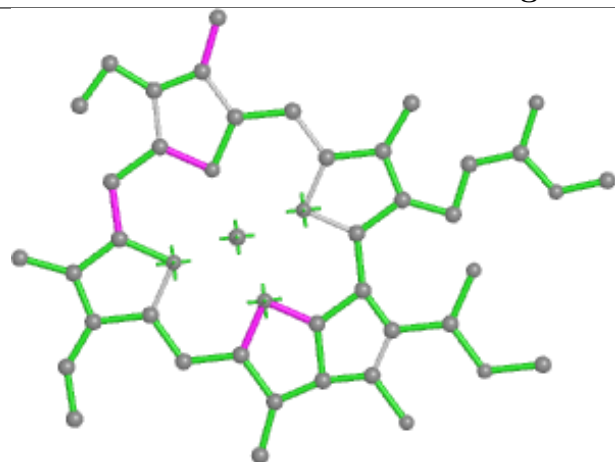
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	820	CLA	6	0
21	2	302	XAT	3	0
23	9	314	CLA	7	0
30	a	850	BCR	2	0
23	9	311	CLA	2	0
23	5	306	CLA	2	0
23	b	827	CLA	4	0
23	4	306	CLA	1	0
23	4	311	CLA	1	0
23	a	805	CLA	1	0
23	9	310	CLA	1	0
21	4	301	XAT	6	0

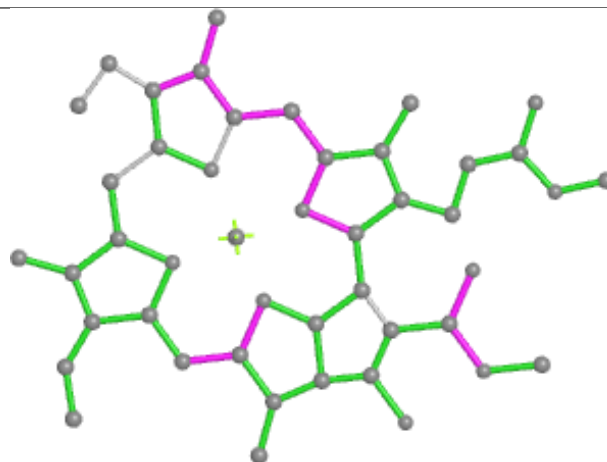
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



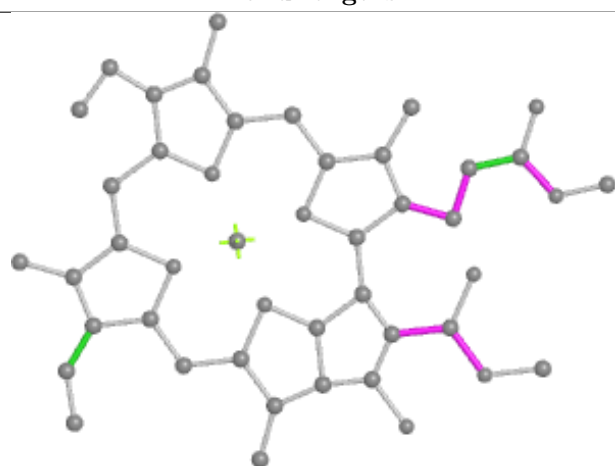
## Ligand CLA 4 315



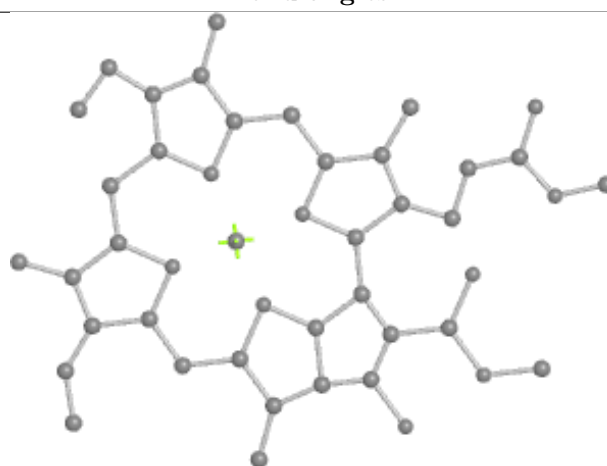
Bond lengths



Bond angles

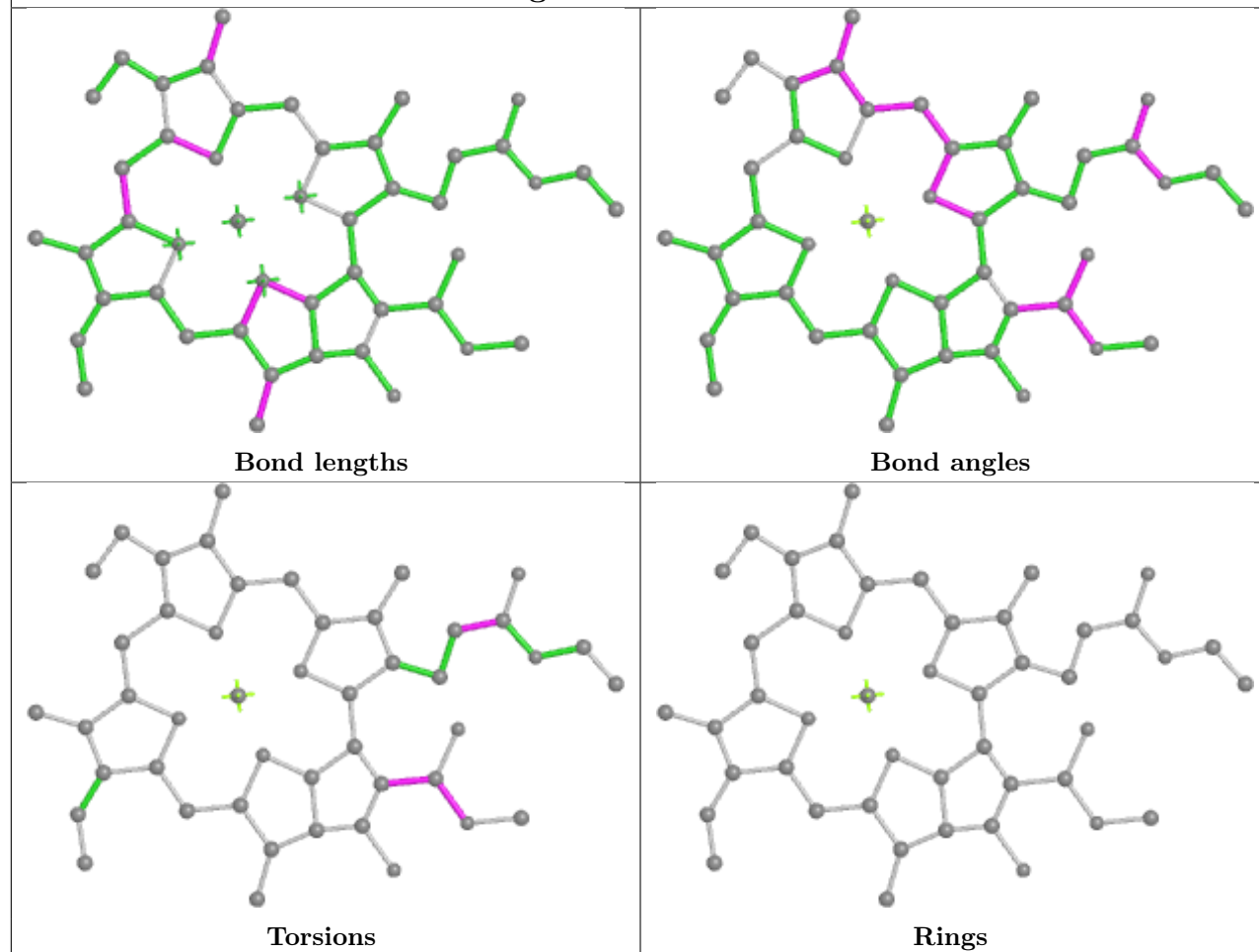


Torsions

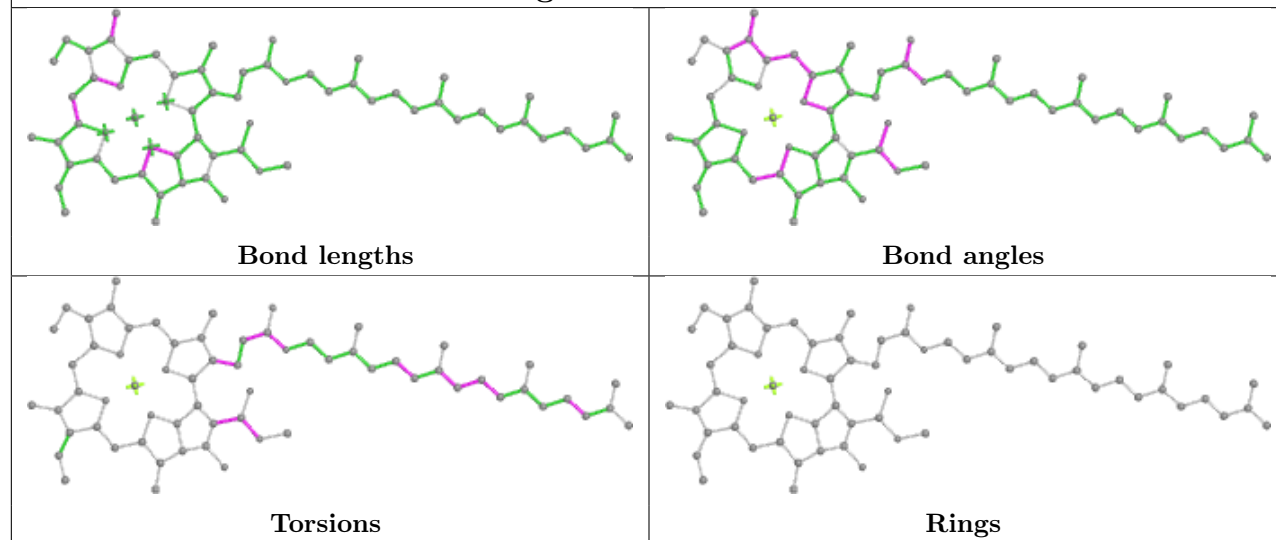


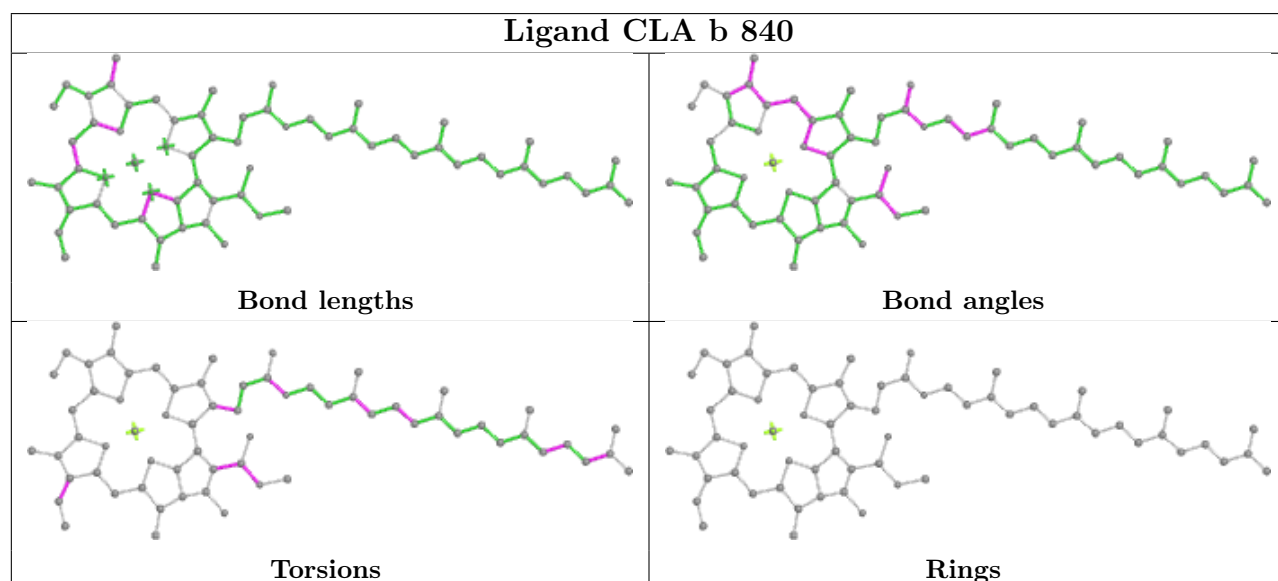
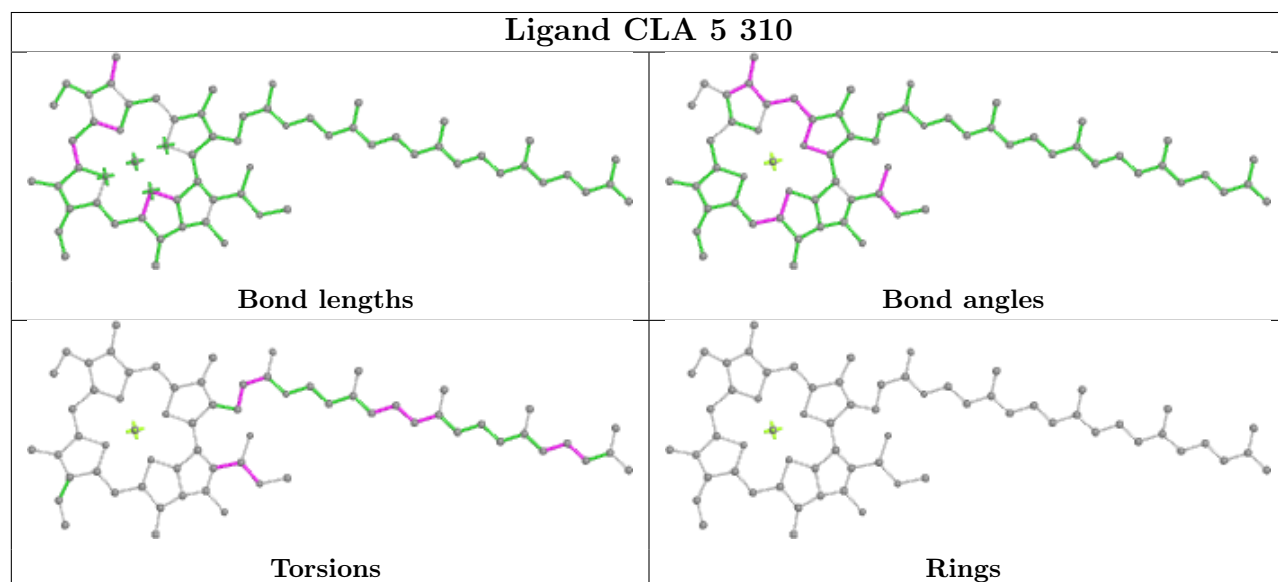
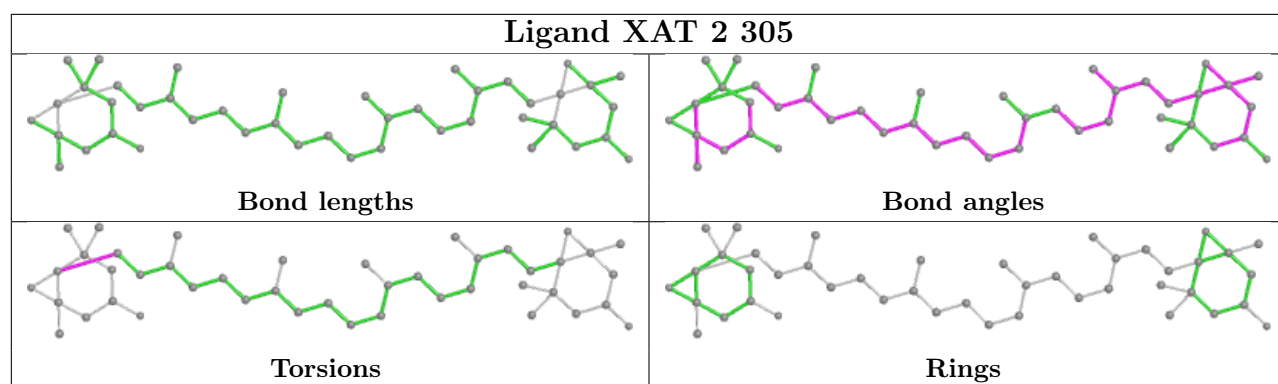
Rings

## Ligand CLA 3 308

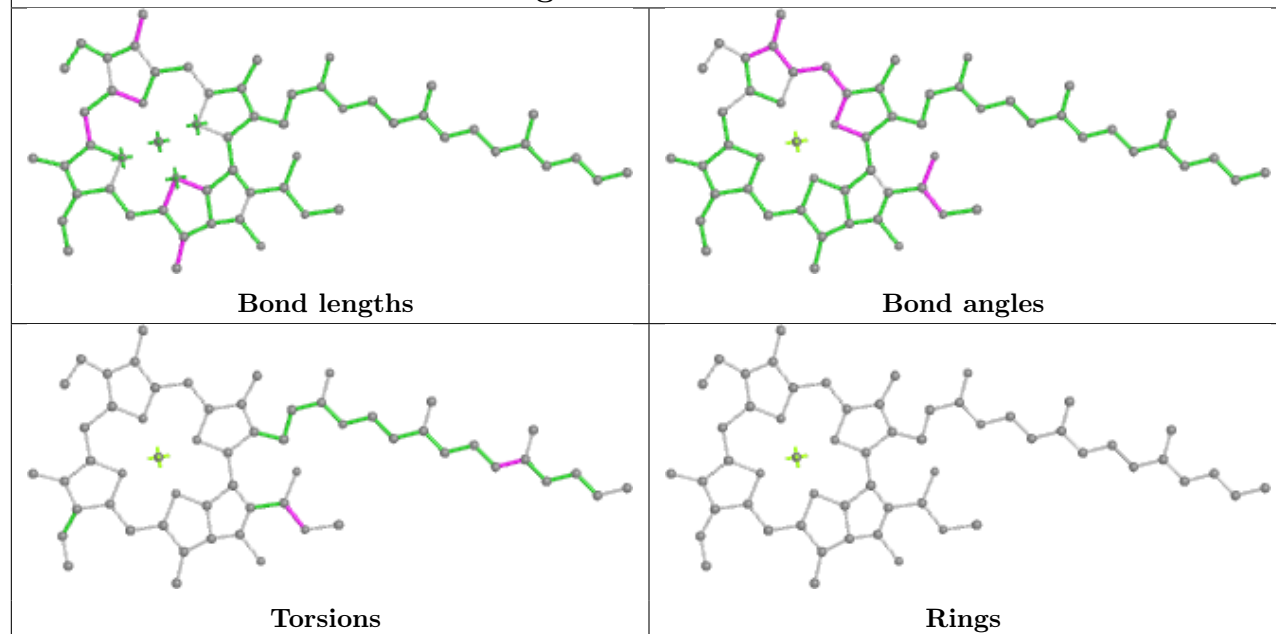


## Ligand CLA a 856

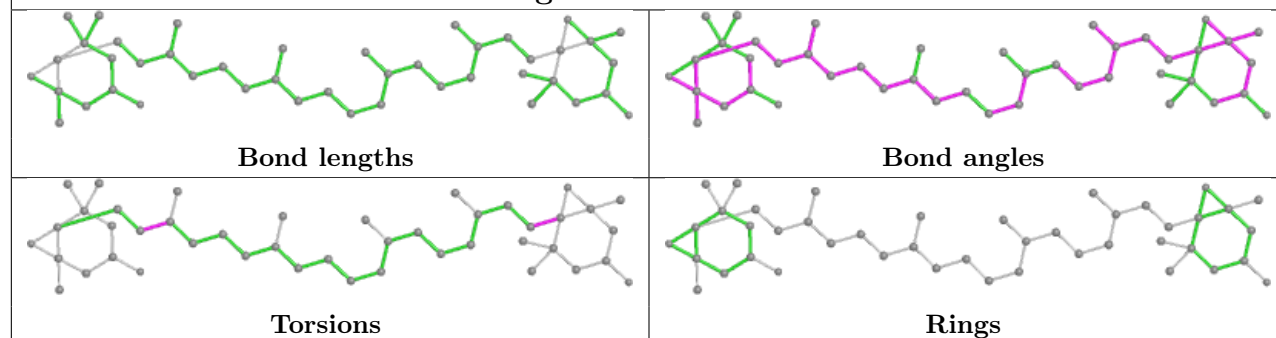




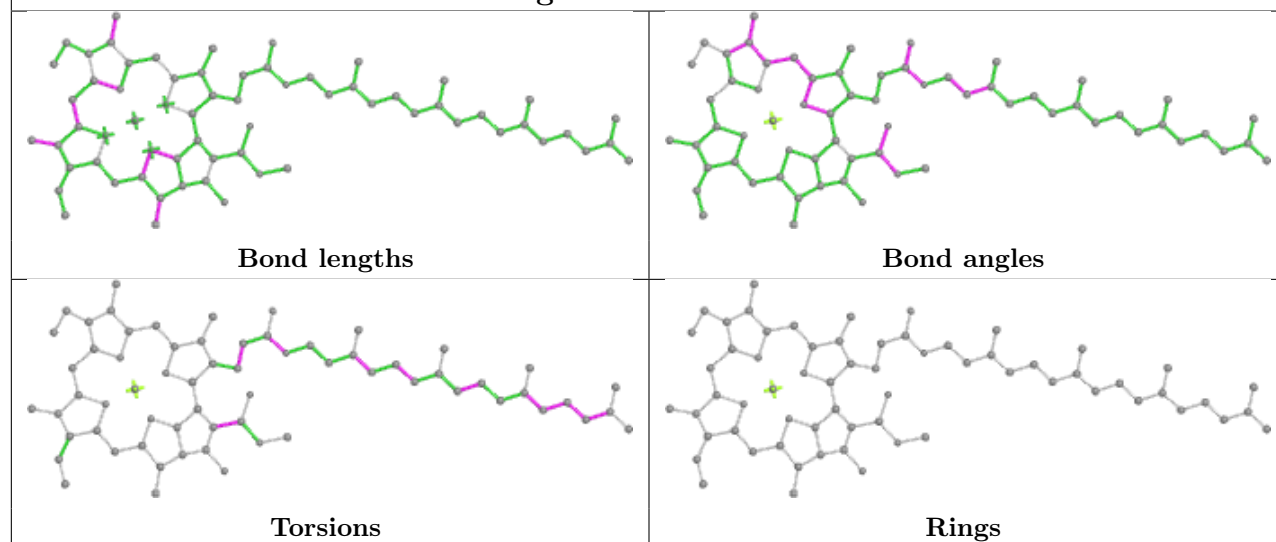
## Ligand CLA 6 308

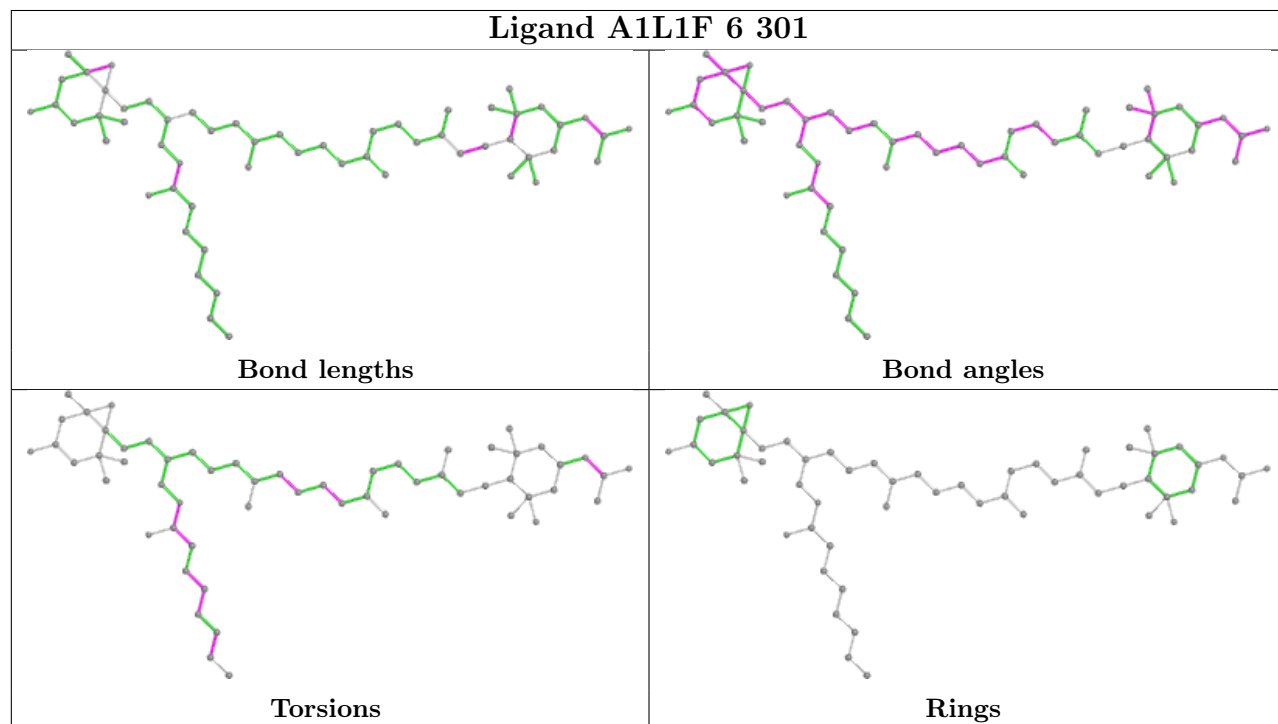
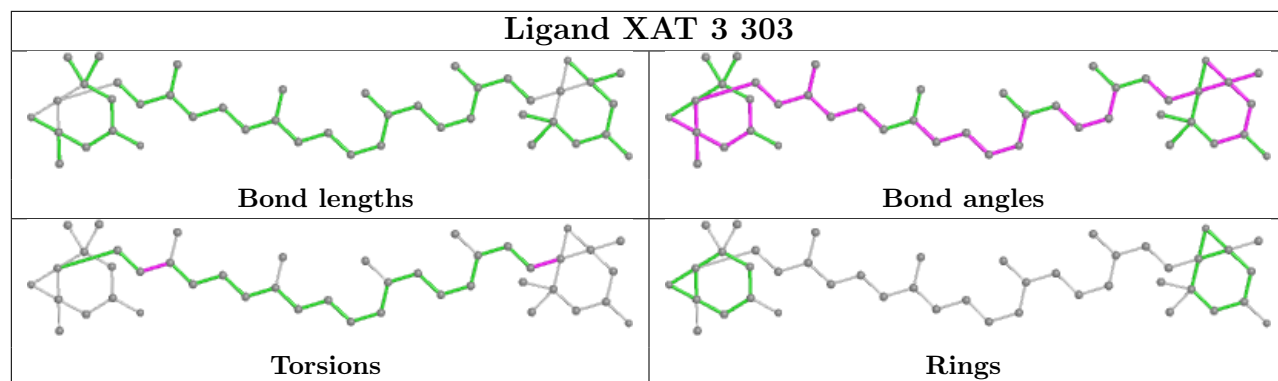


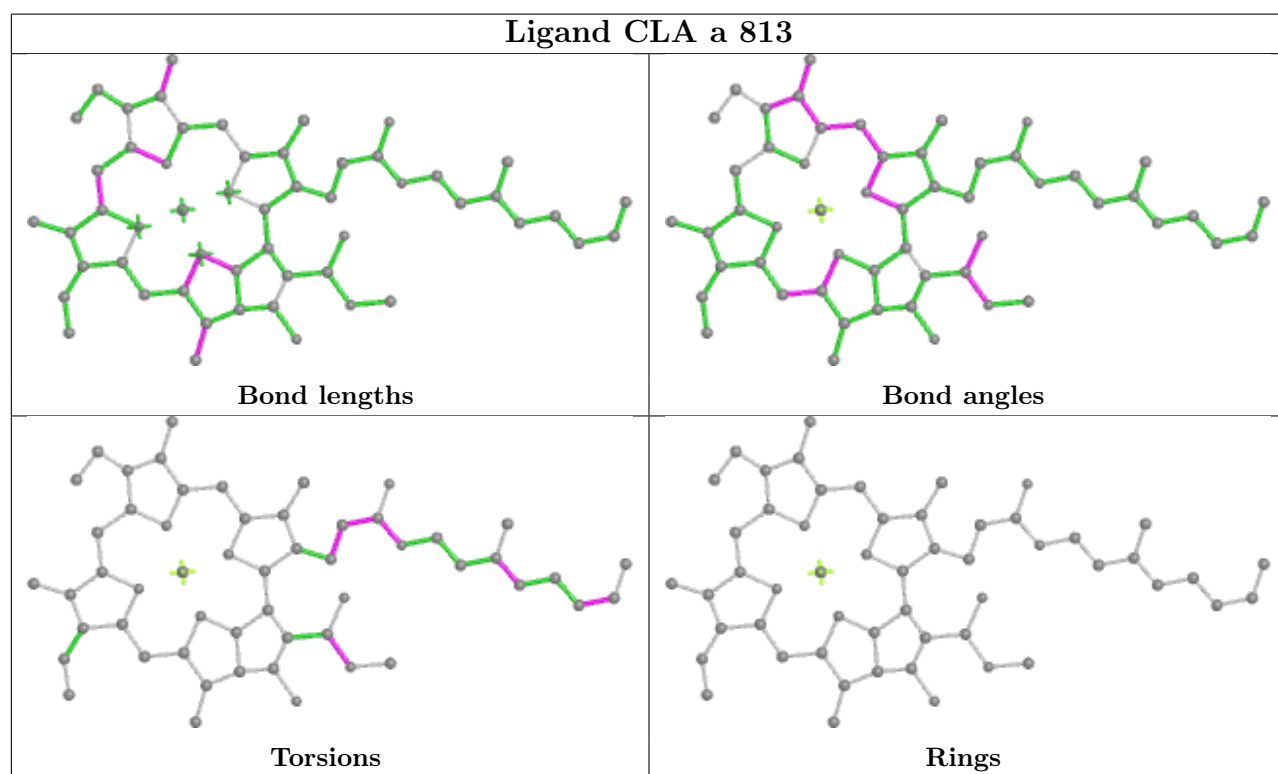
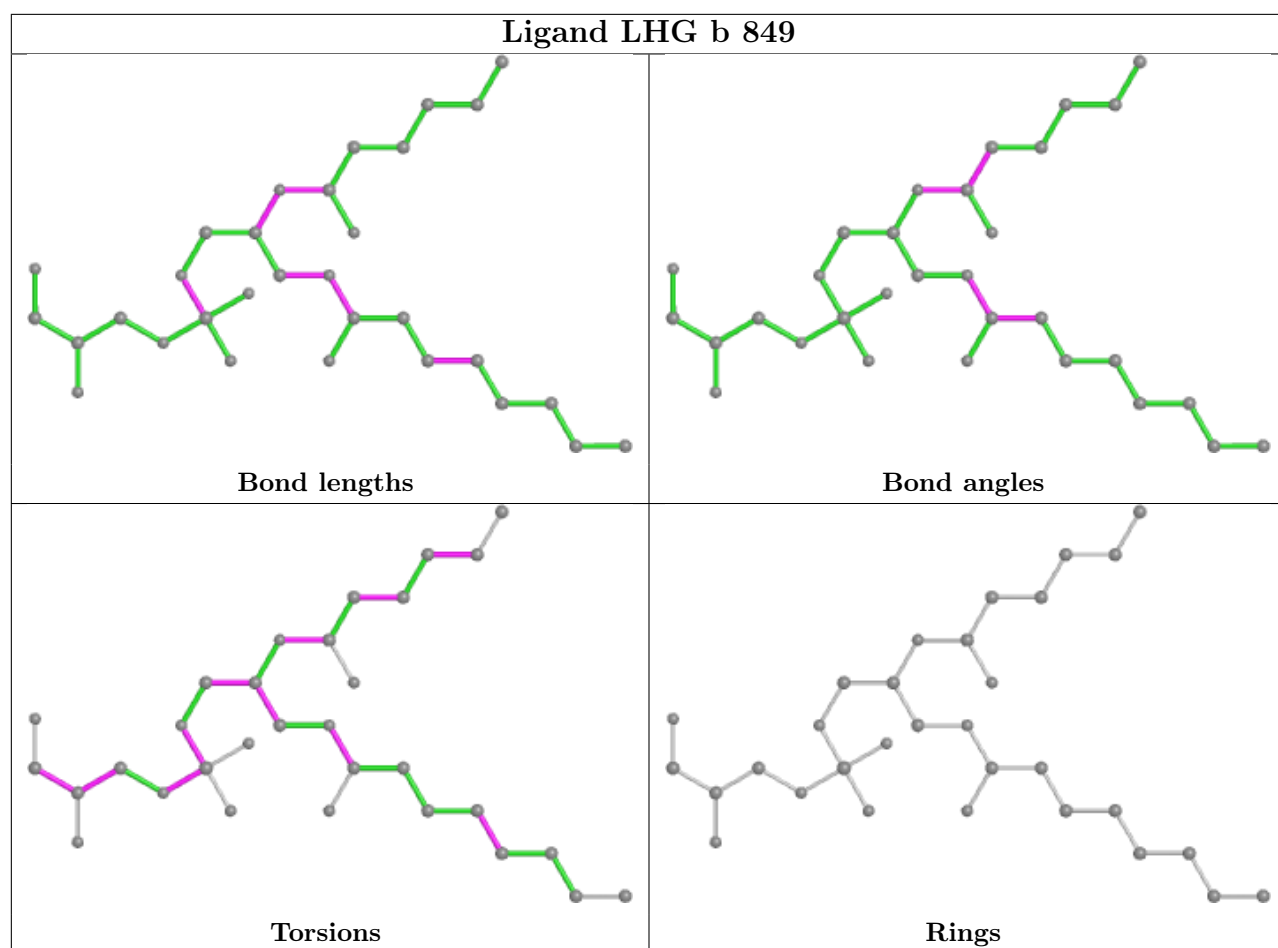
## Ligand XAT 2 301



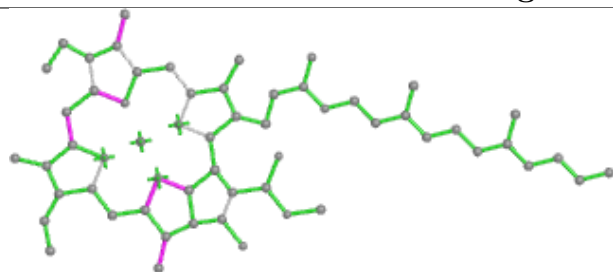
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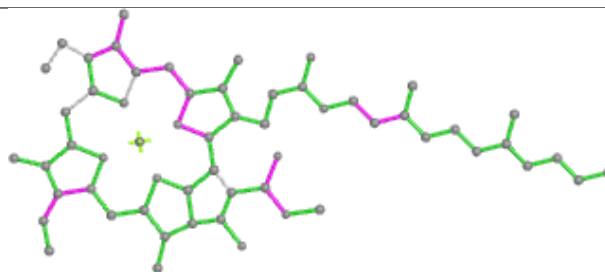




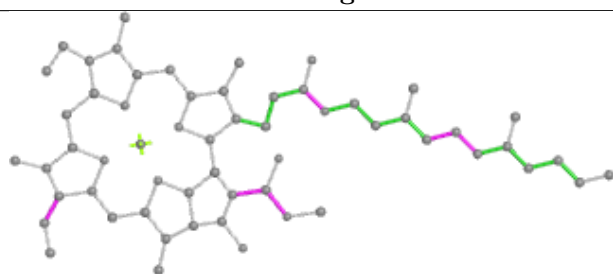
## Ligand CLA b 836



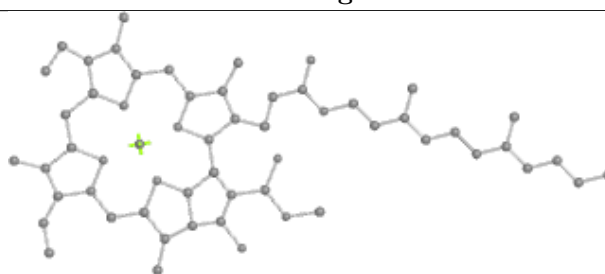
Bond lengths



Bond angles

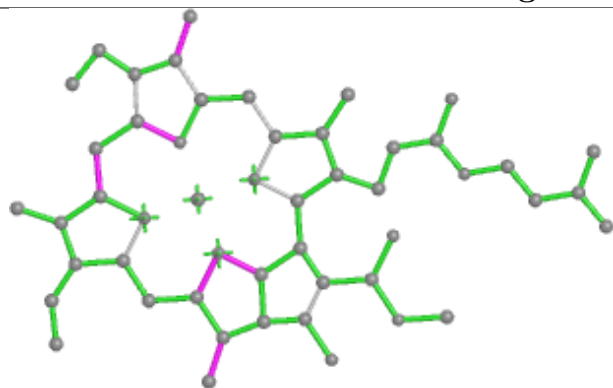


Torsions

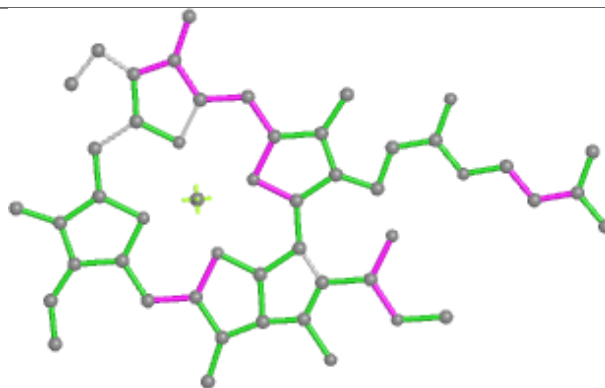


Rings

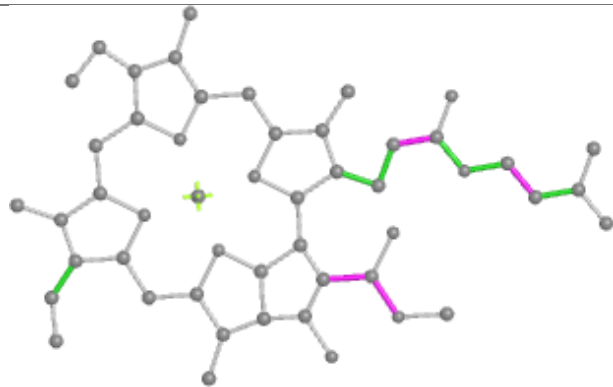
## Ligand CLA 4 308



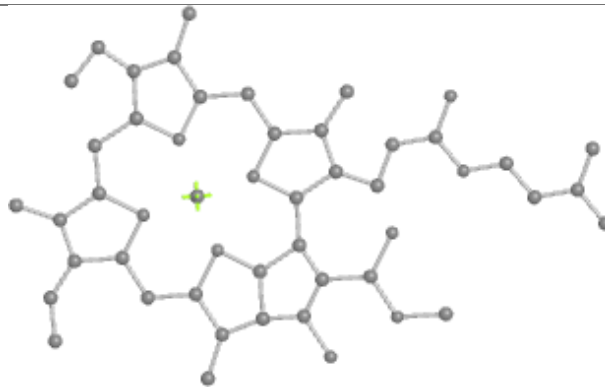
Bond lengths



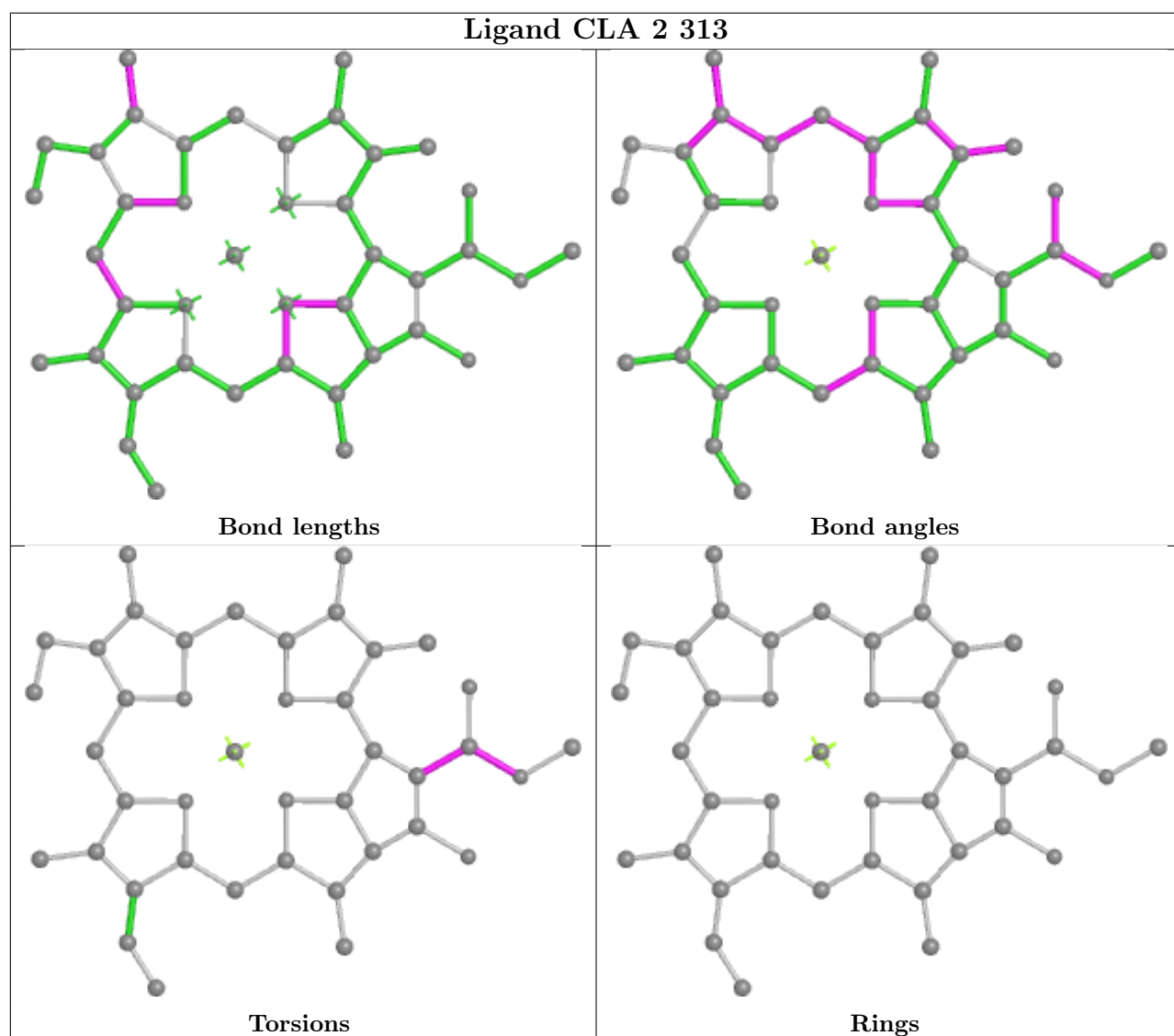
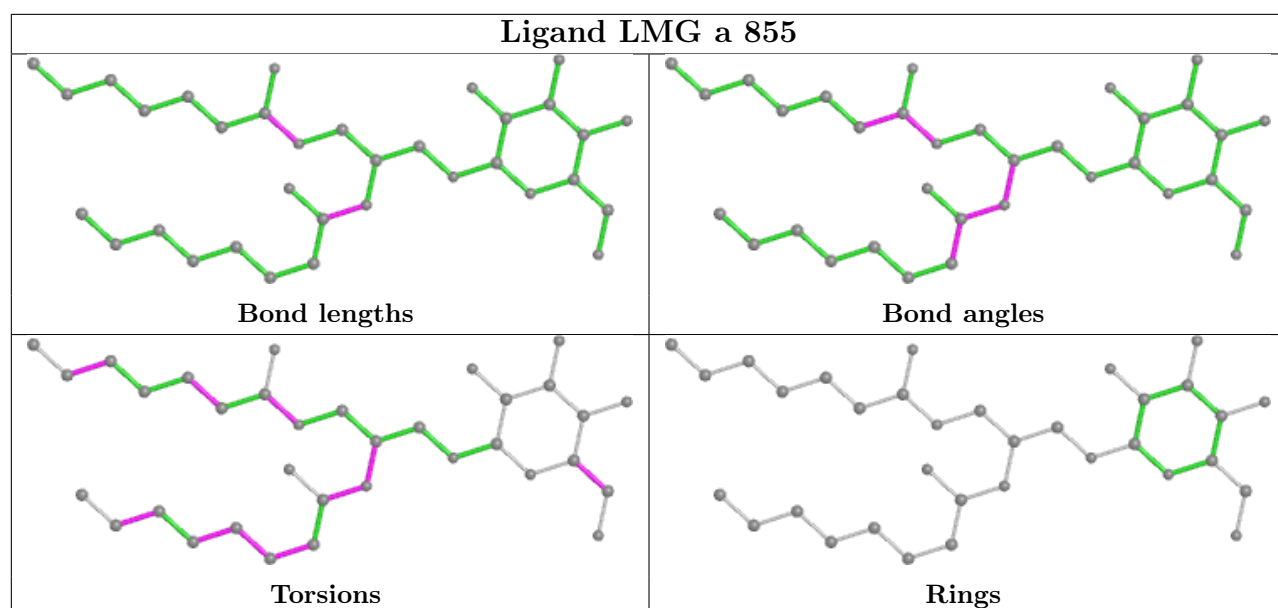
Bond angles

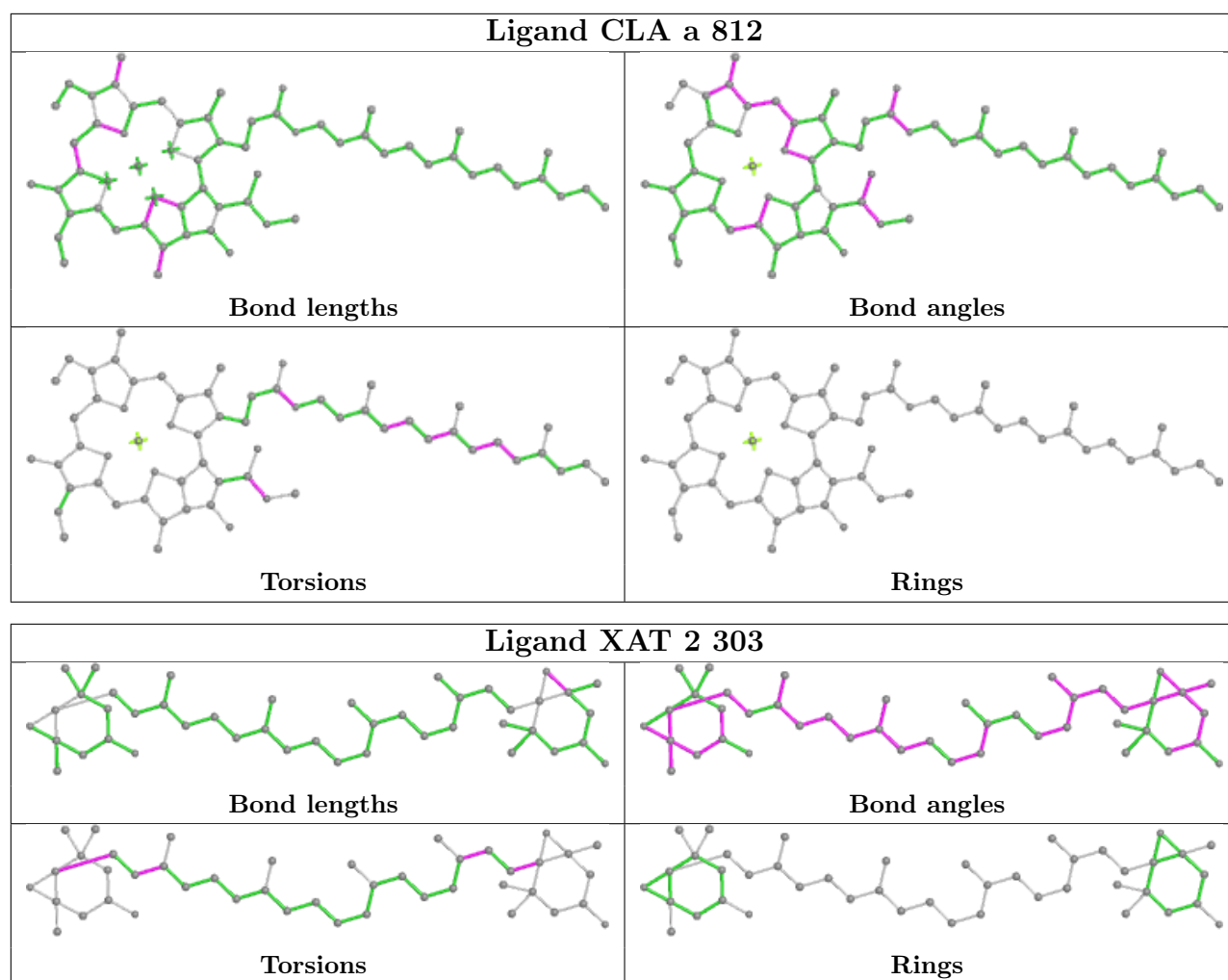


Torsions

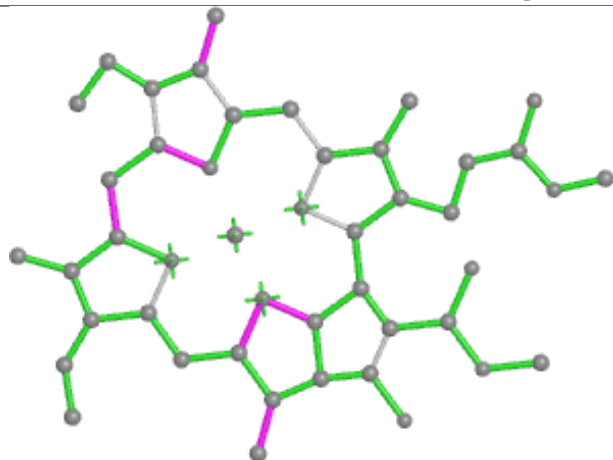


Rings

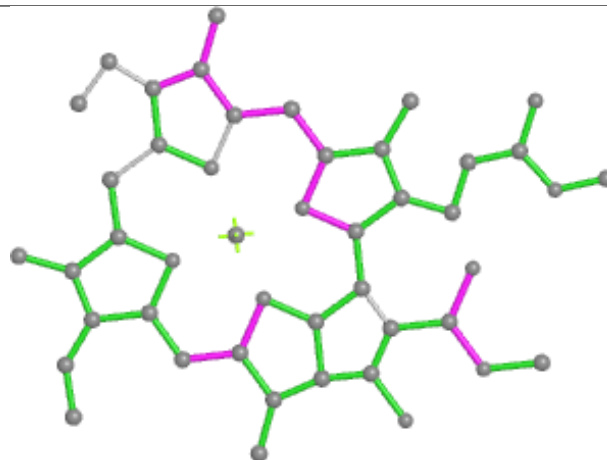




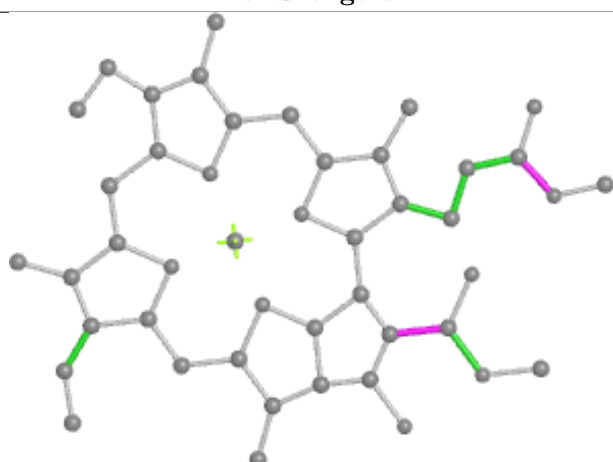
## Ligand CLA 8 313



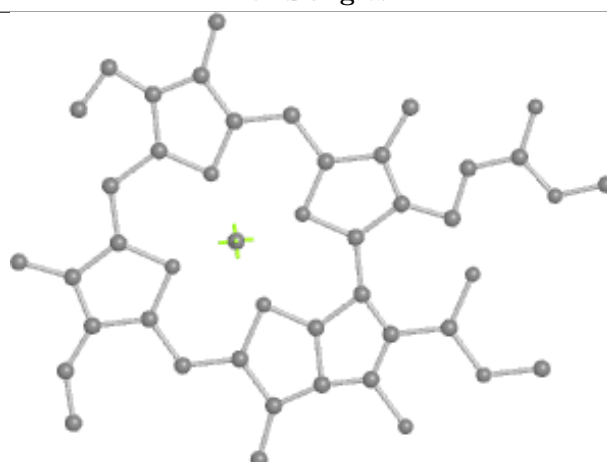
Bond lengths



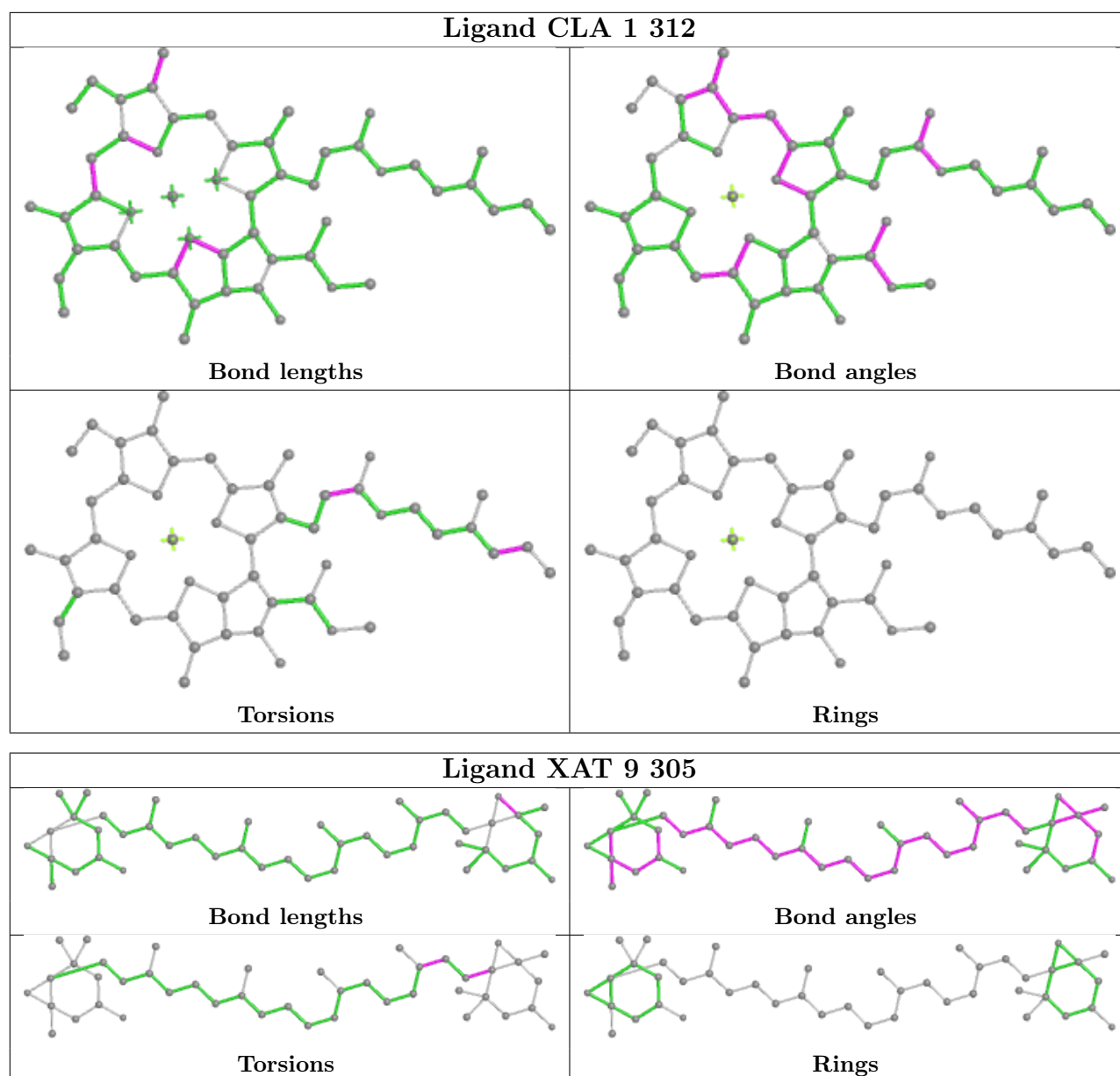
Bond angles

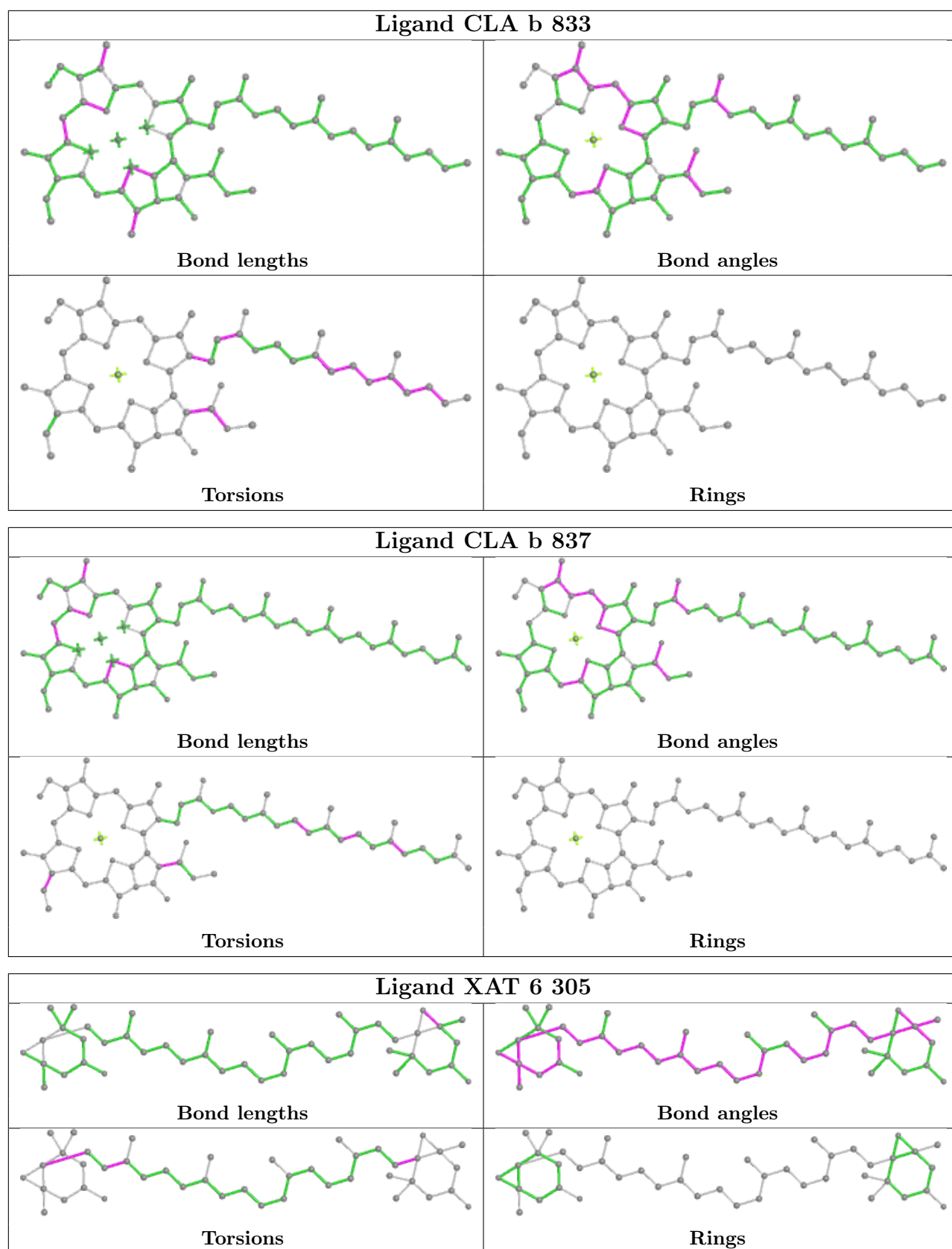


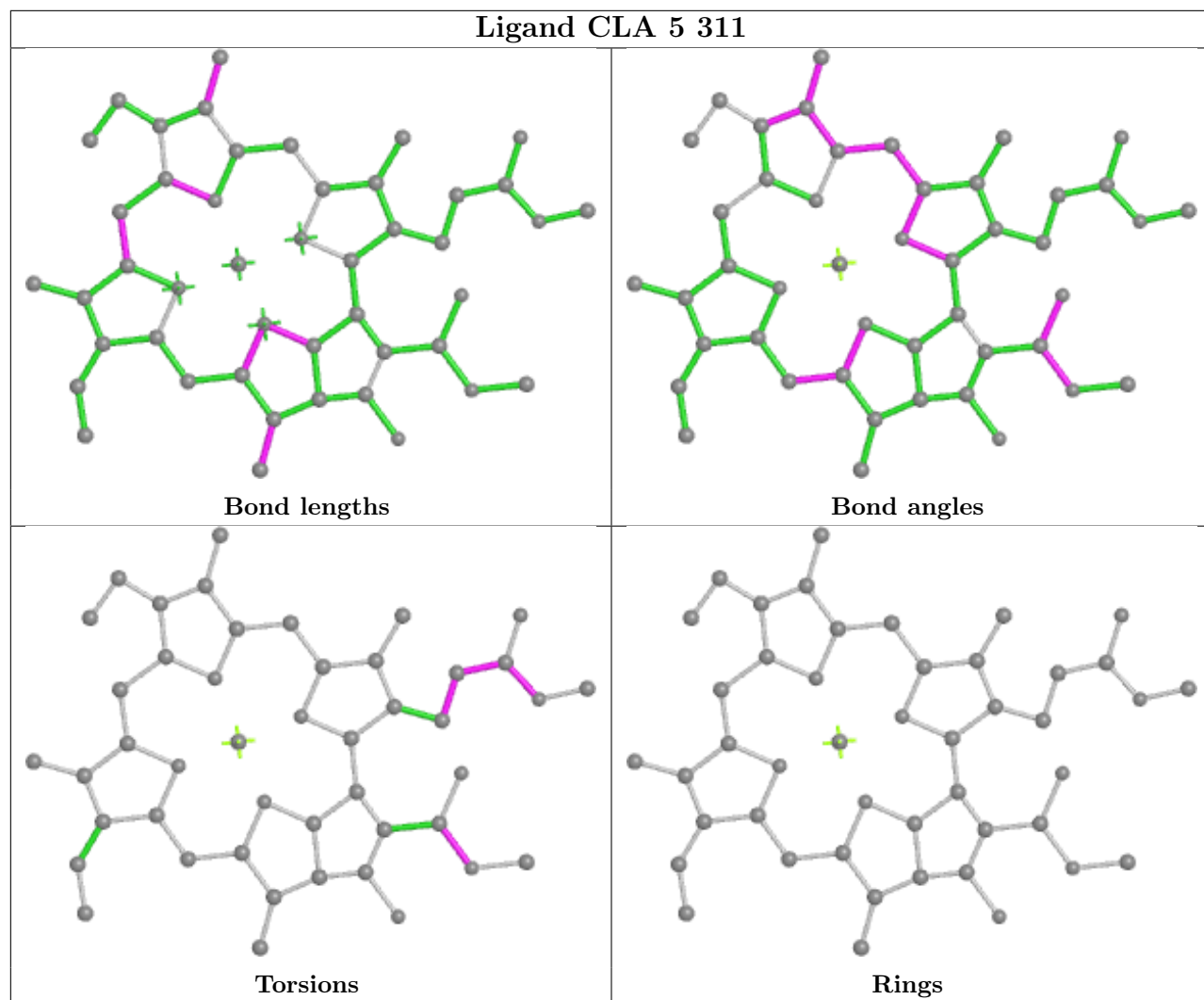
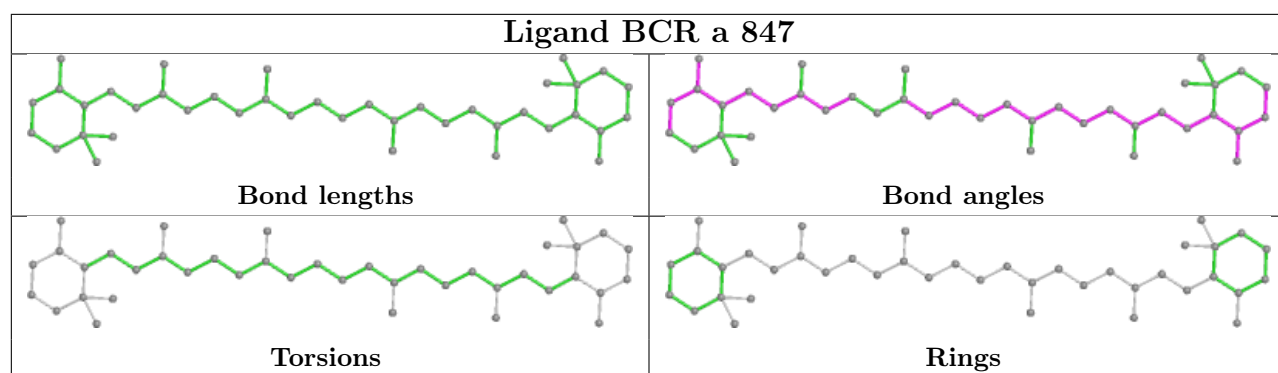
Torsions



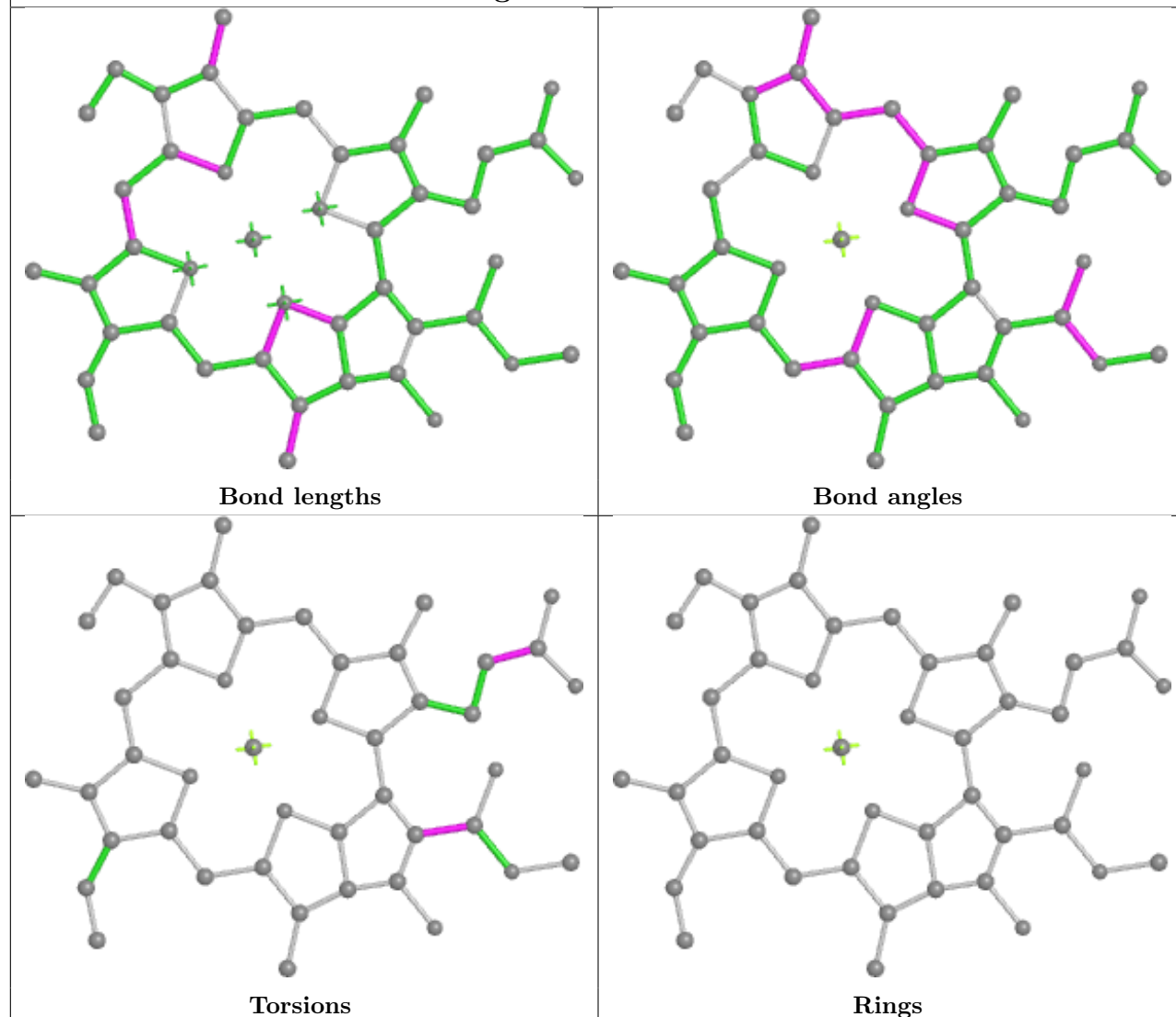
Rings



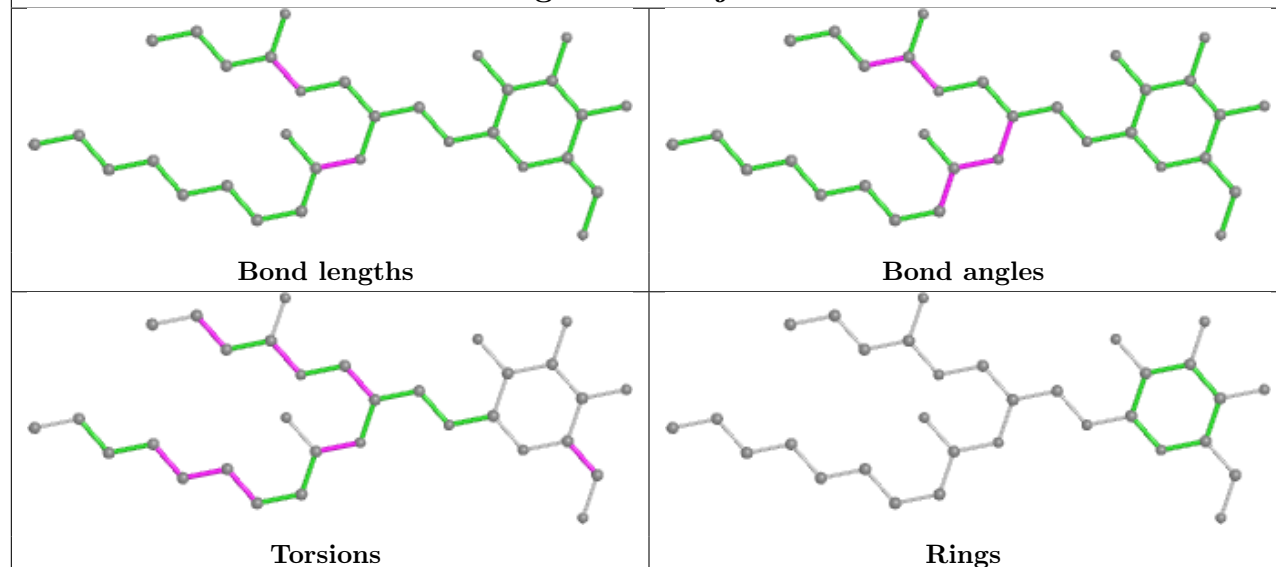


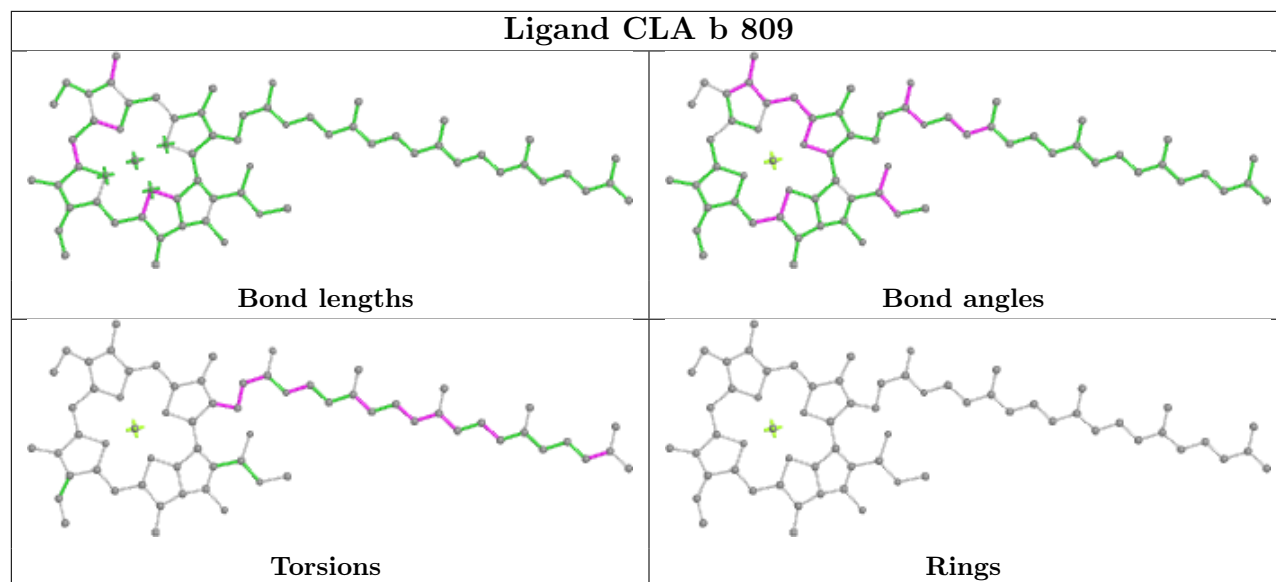
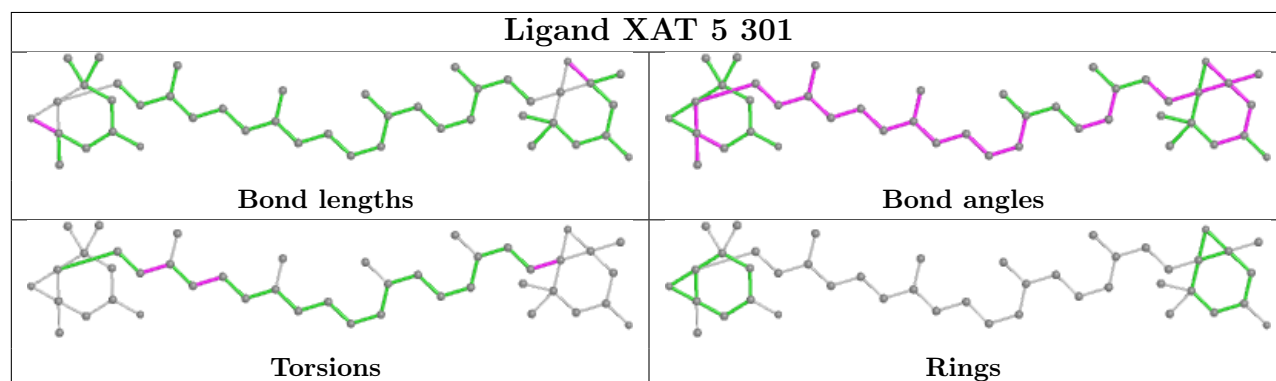
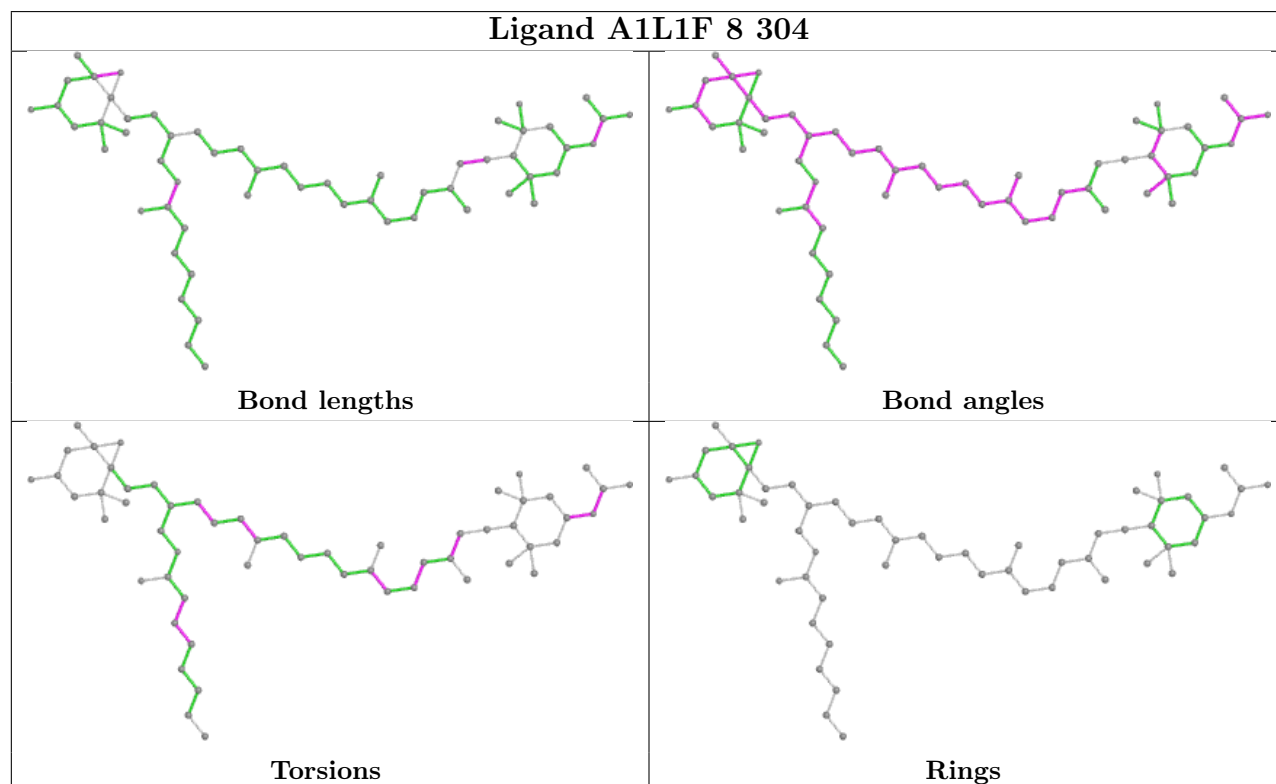


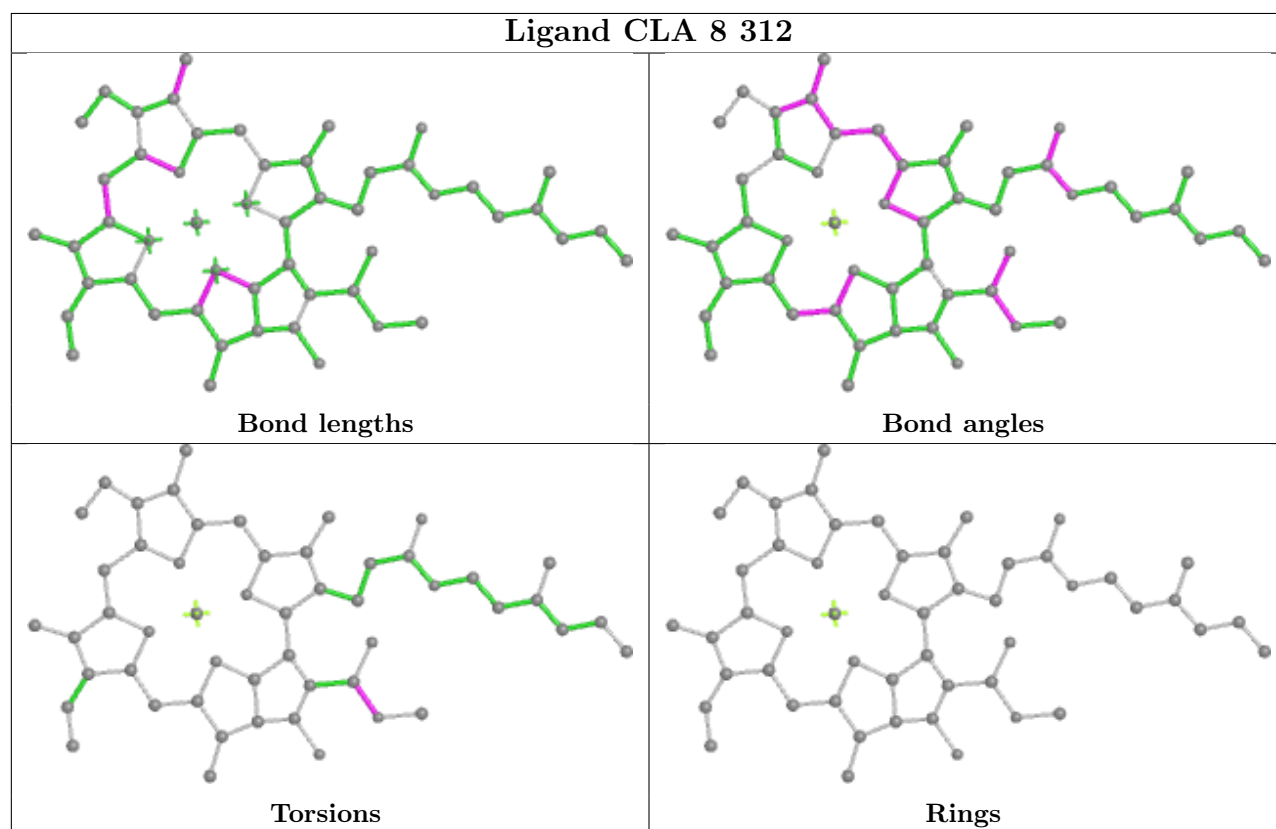
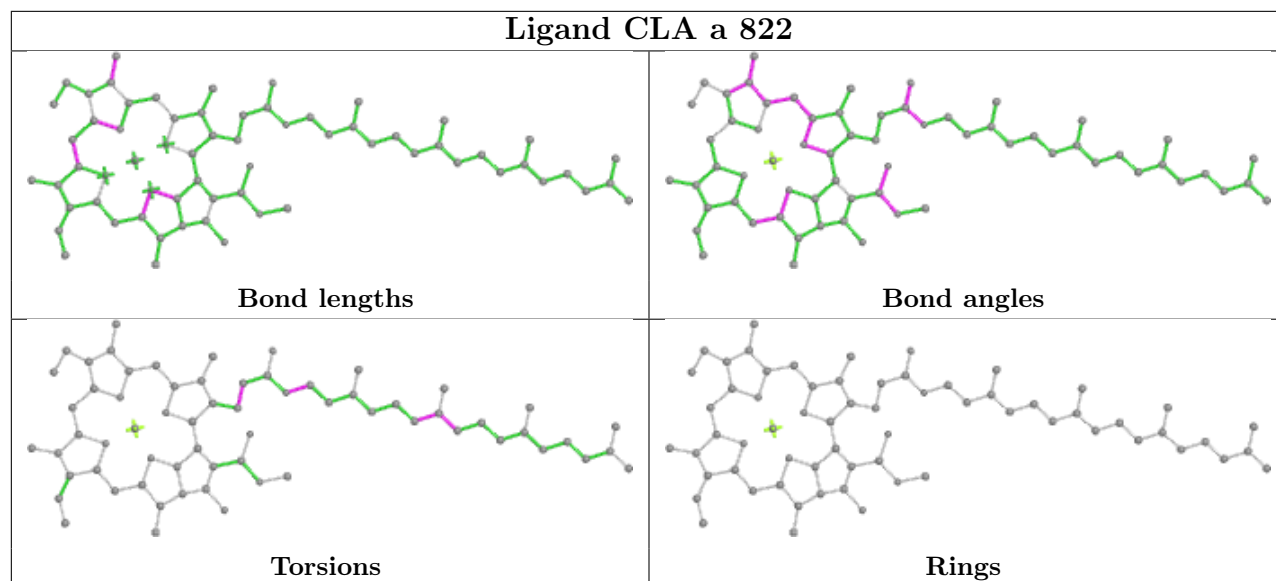
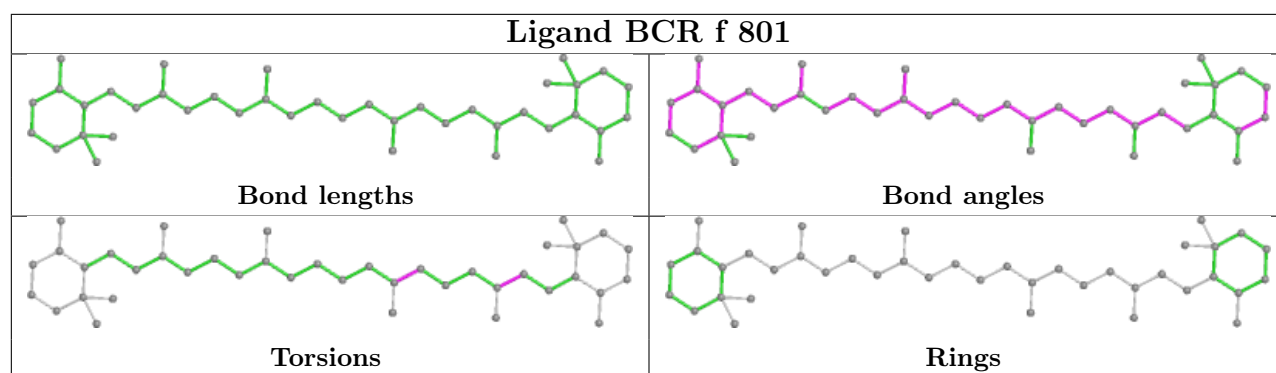
## Ligand CLA 4 313

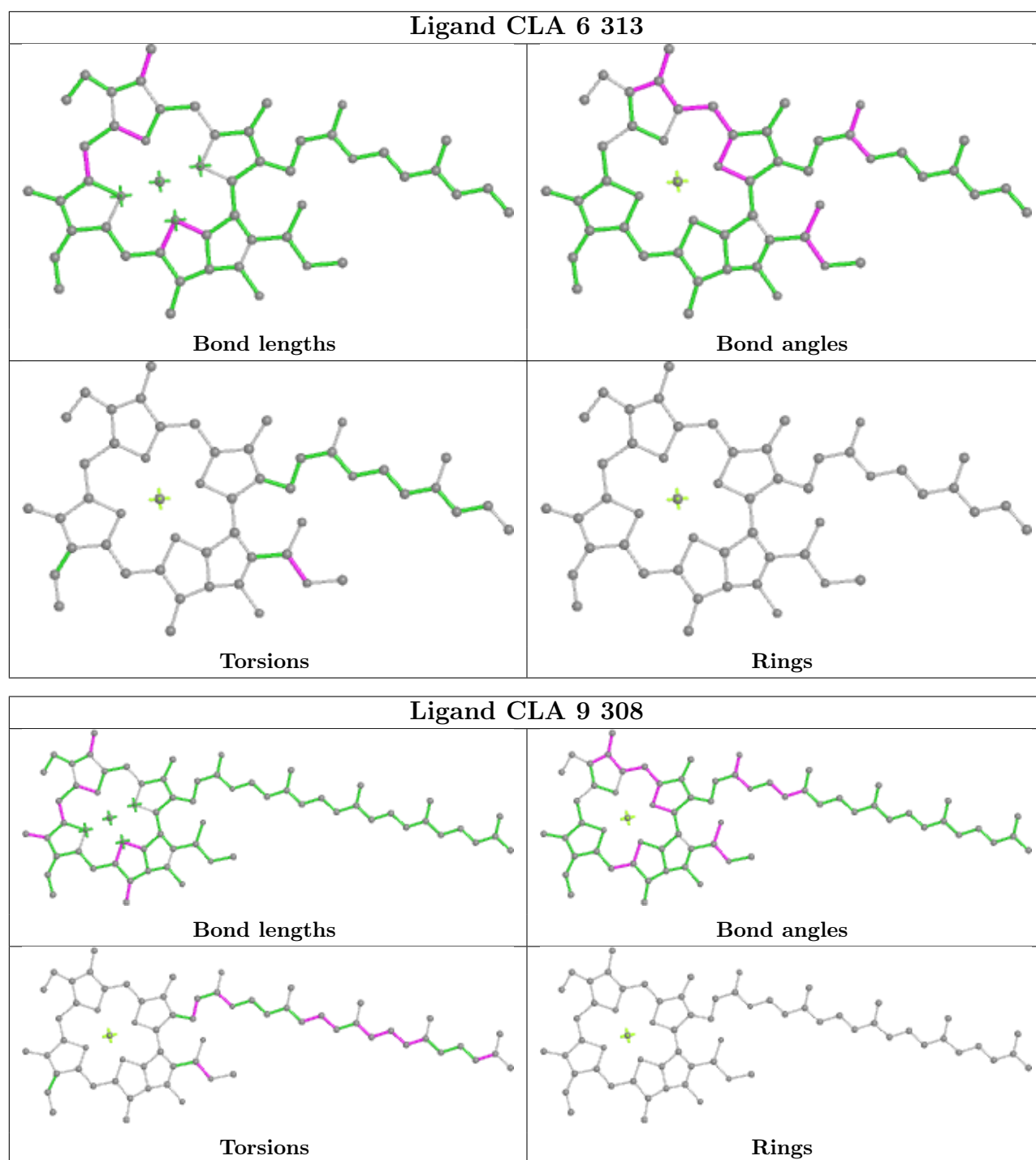


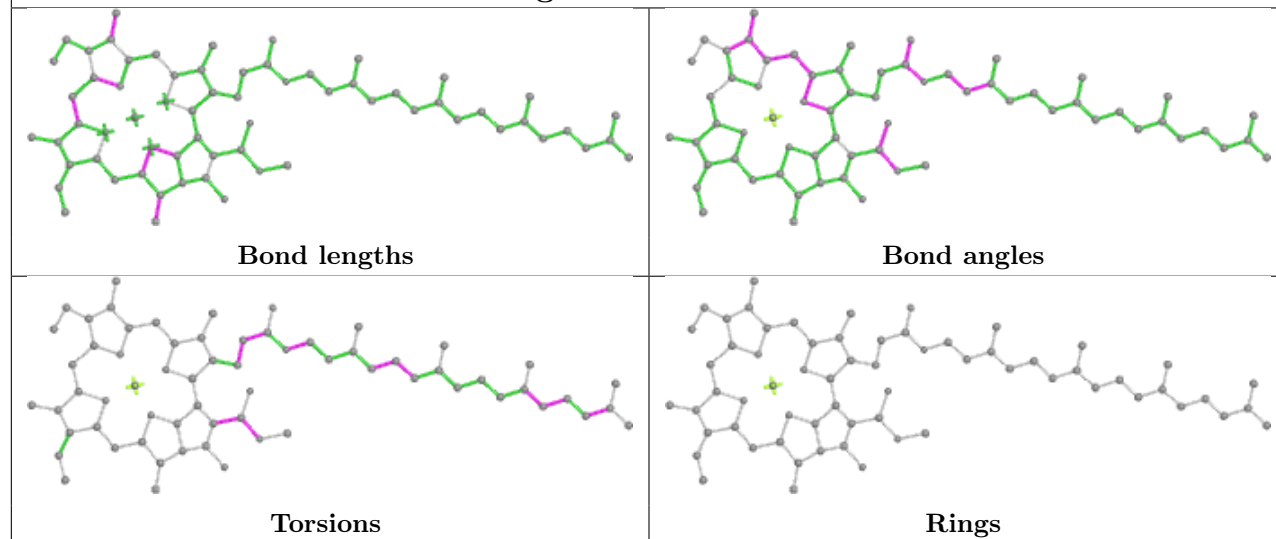
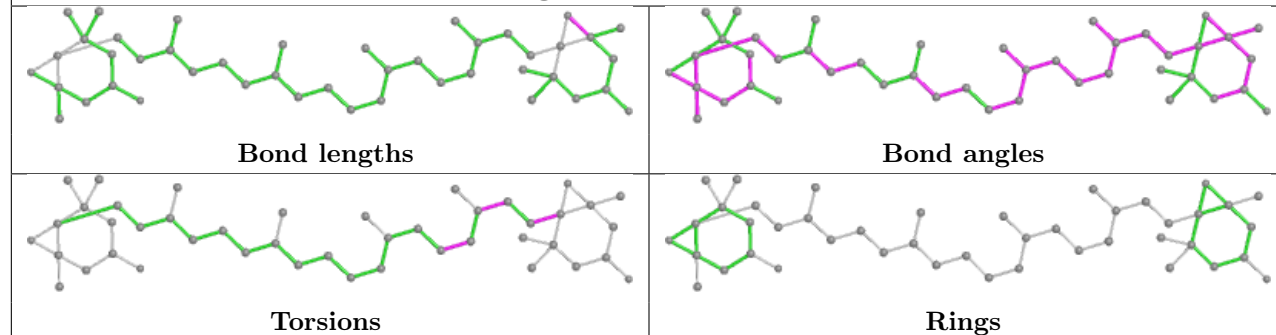
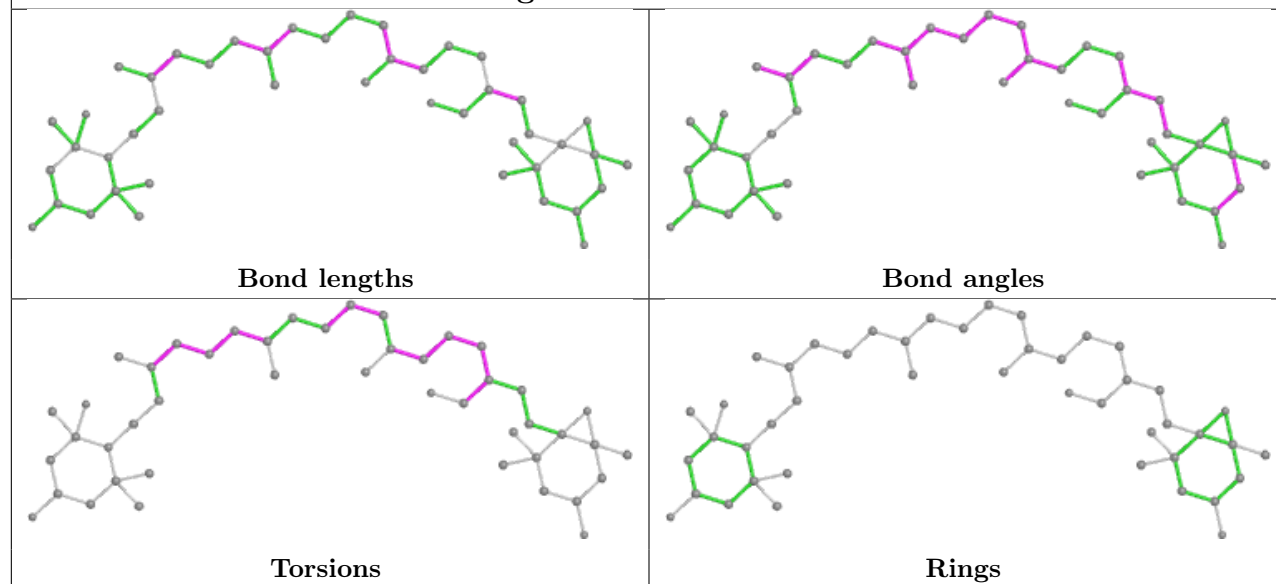
## Ligand LMG j 103



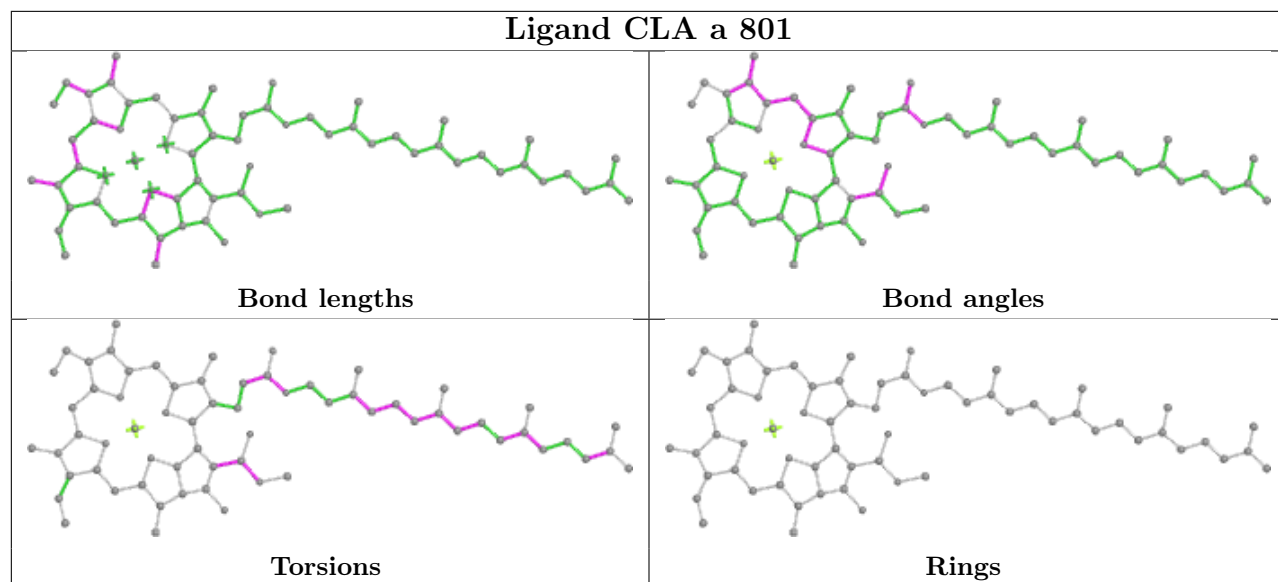
**Ligand CLA b 809****Ligand XAT 5 301****Ligand A1L1F 8 304**



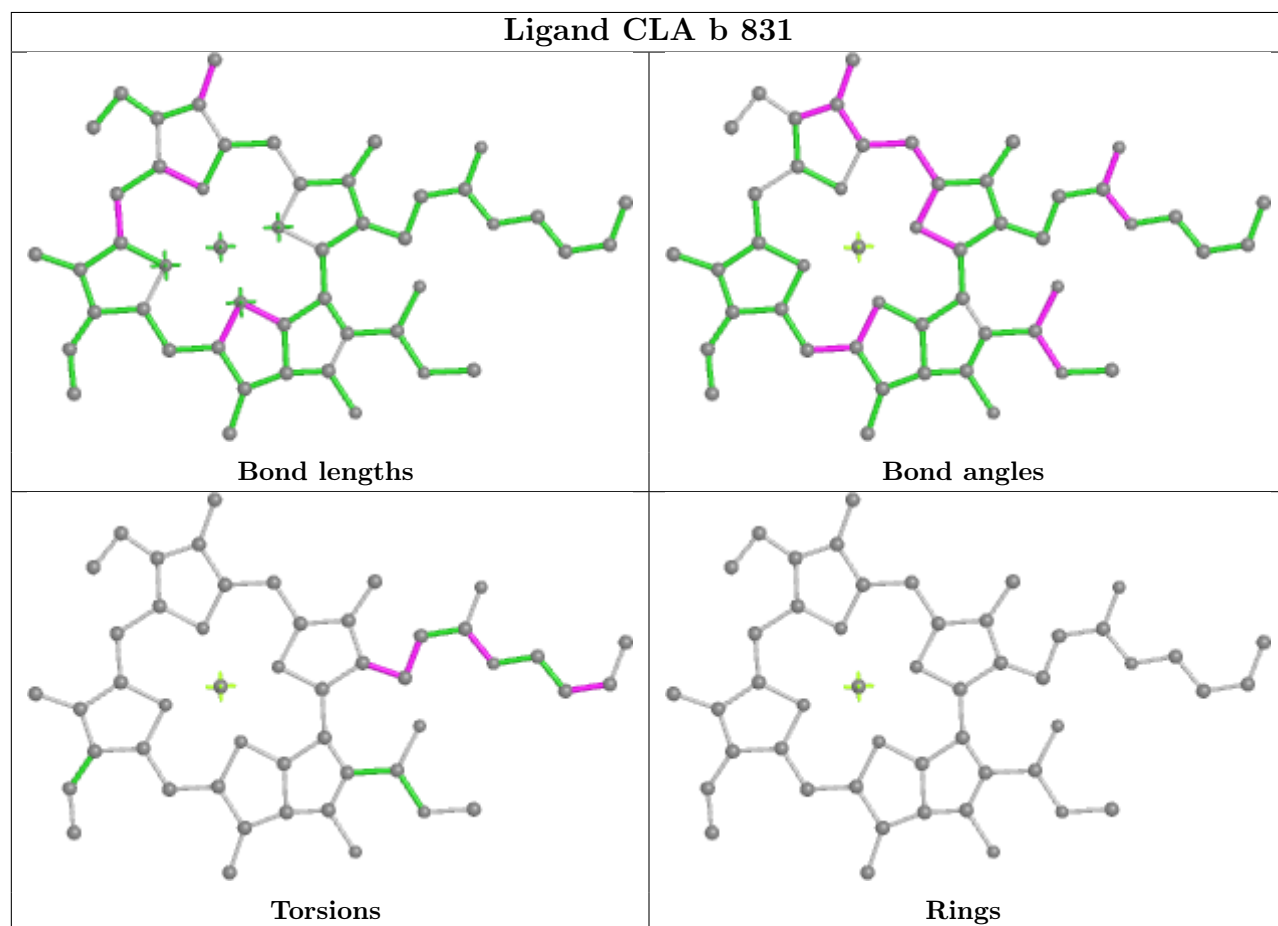


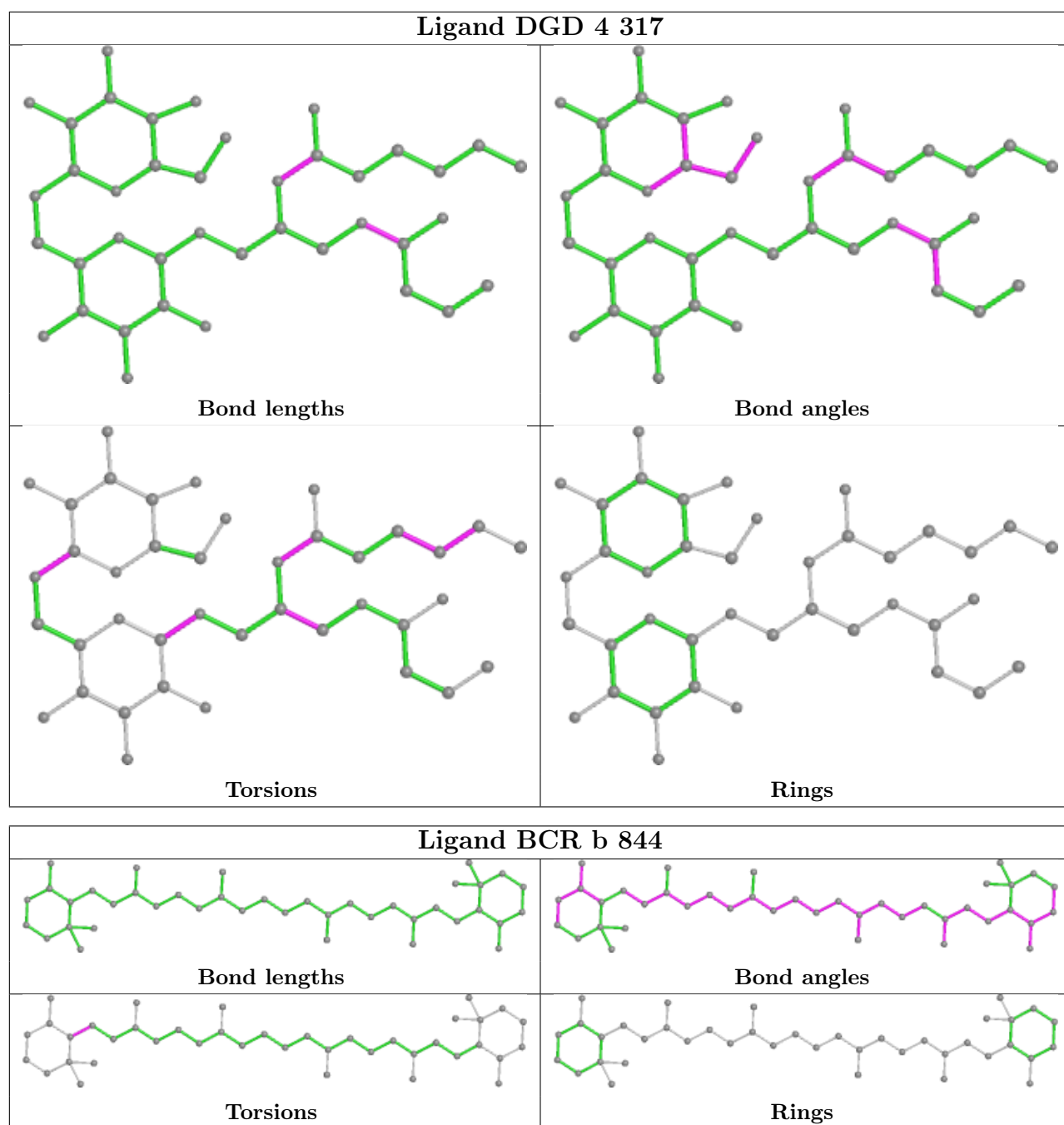
**Ligand CLA a 810****Ligand XAT 8 302****Ligand A1L1G 9 301**

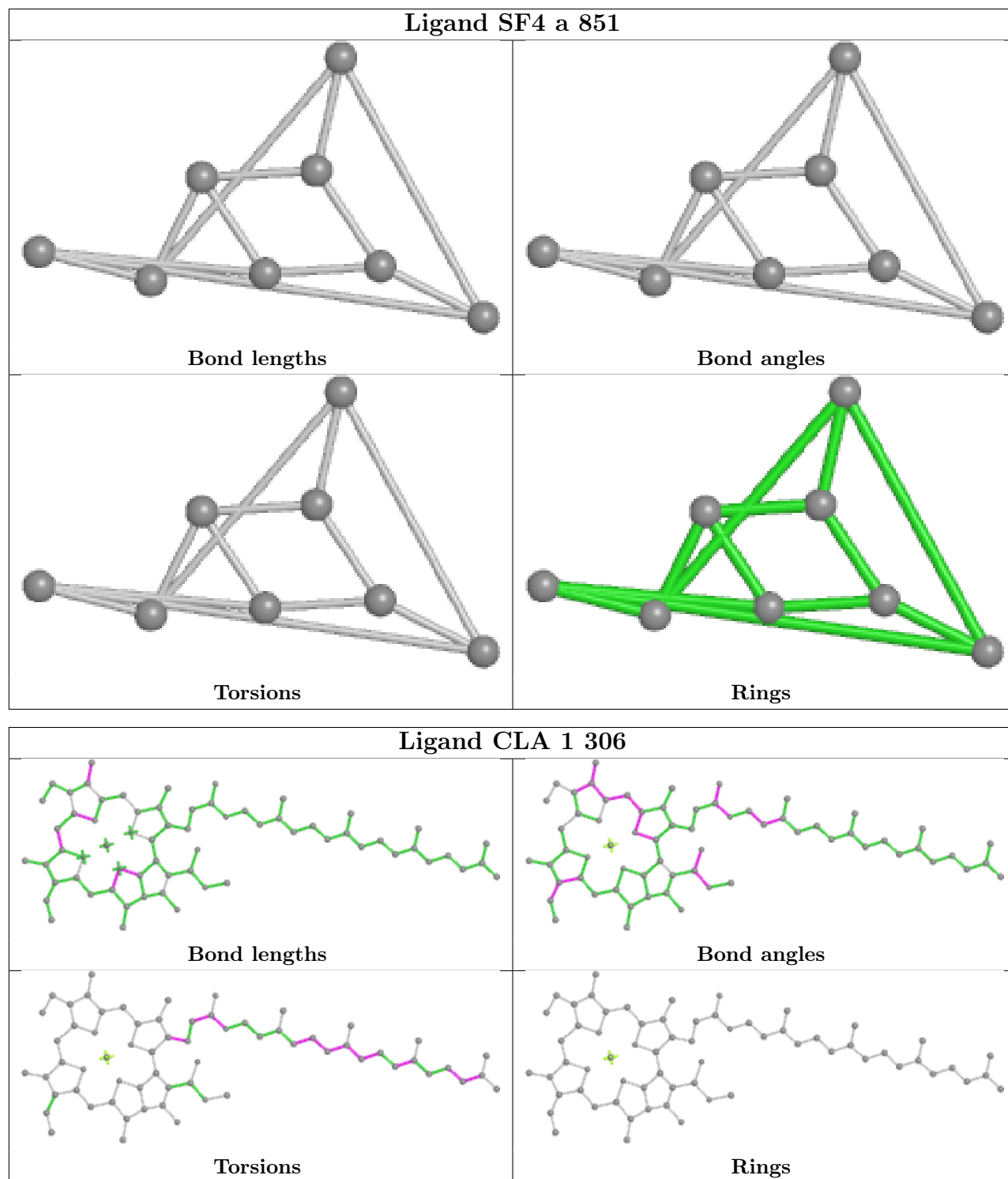
## Ligand CLA a 801

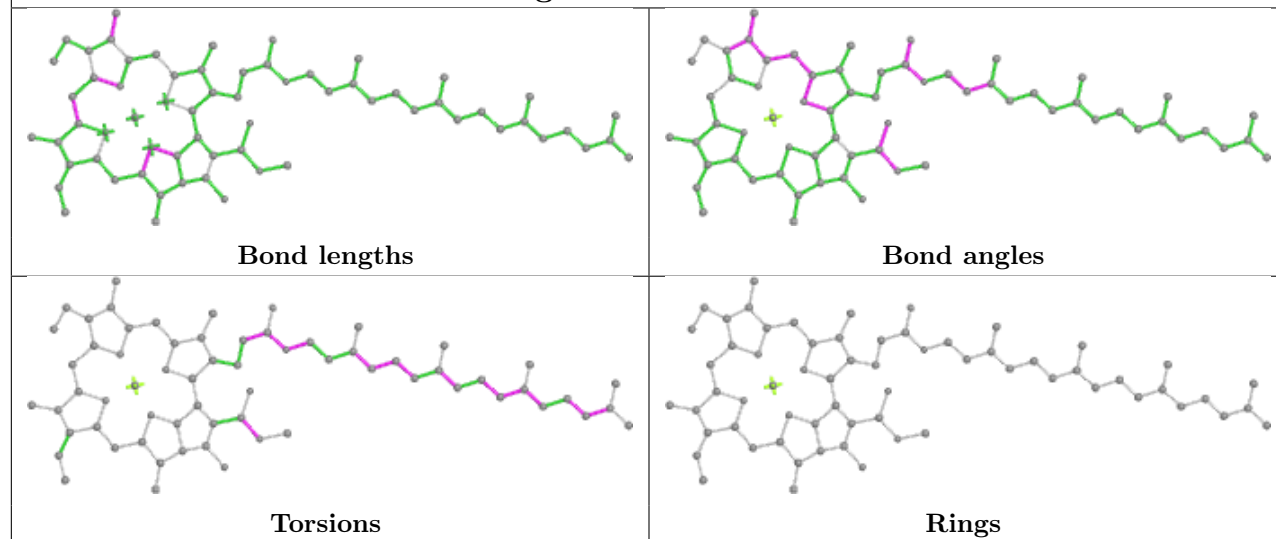
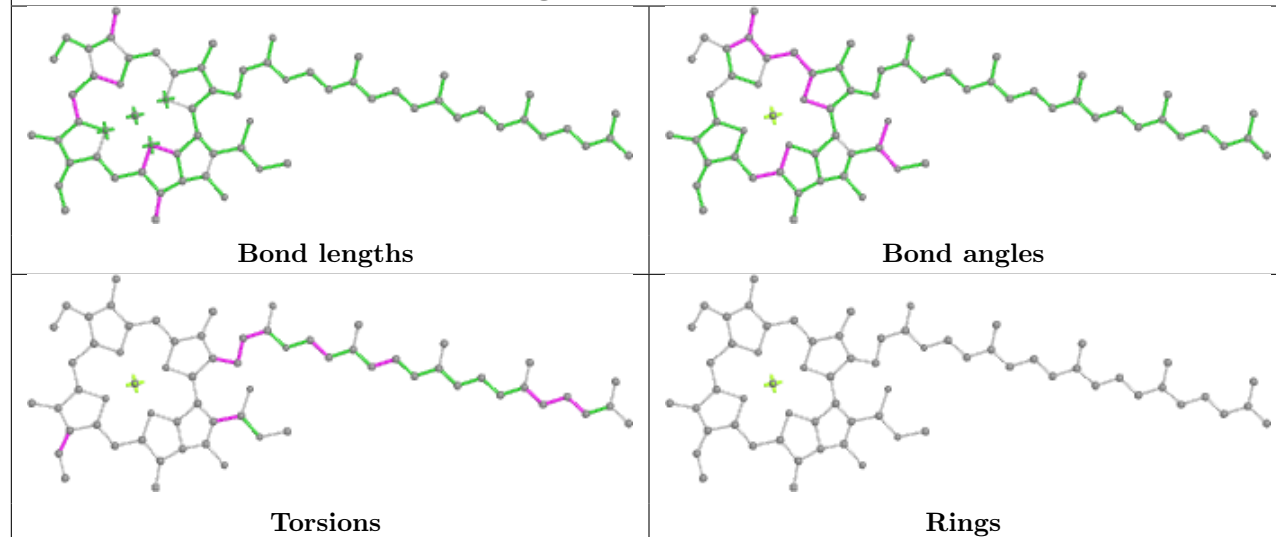
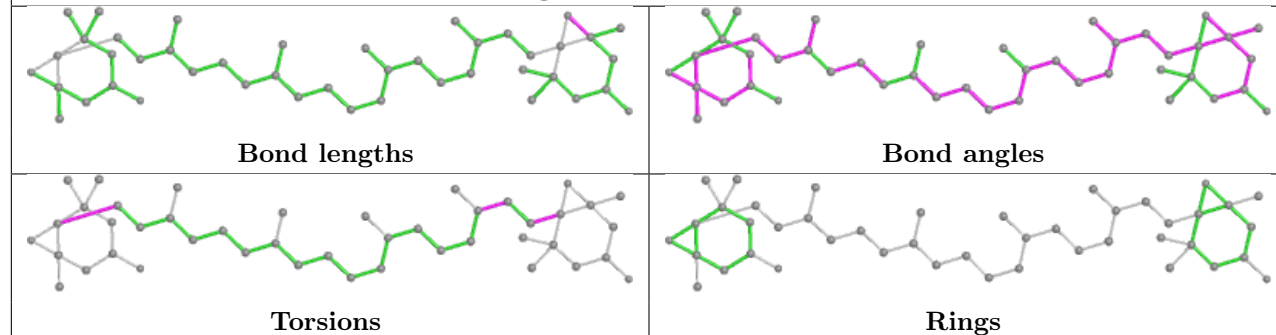


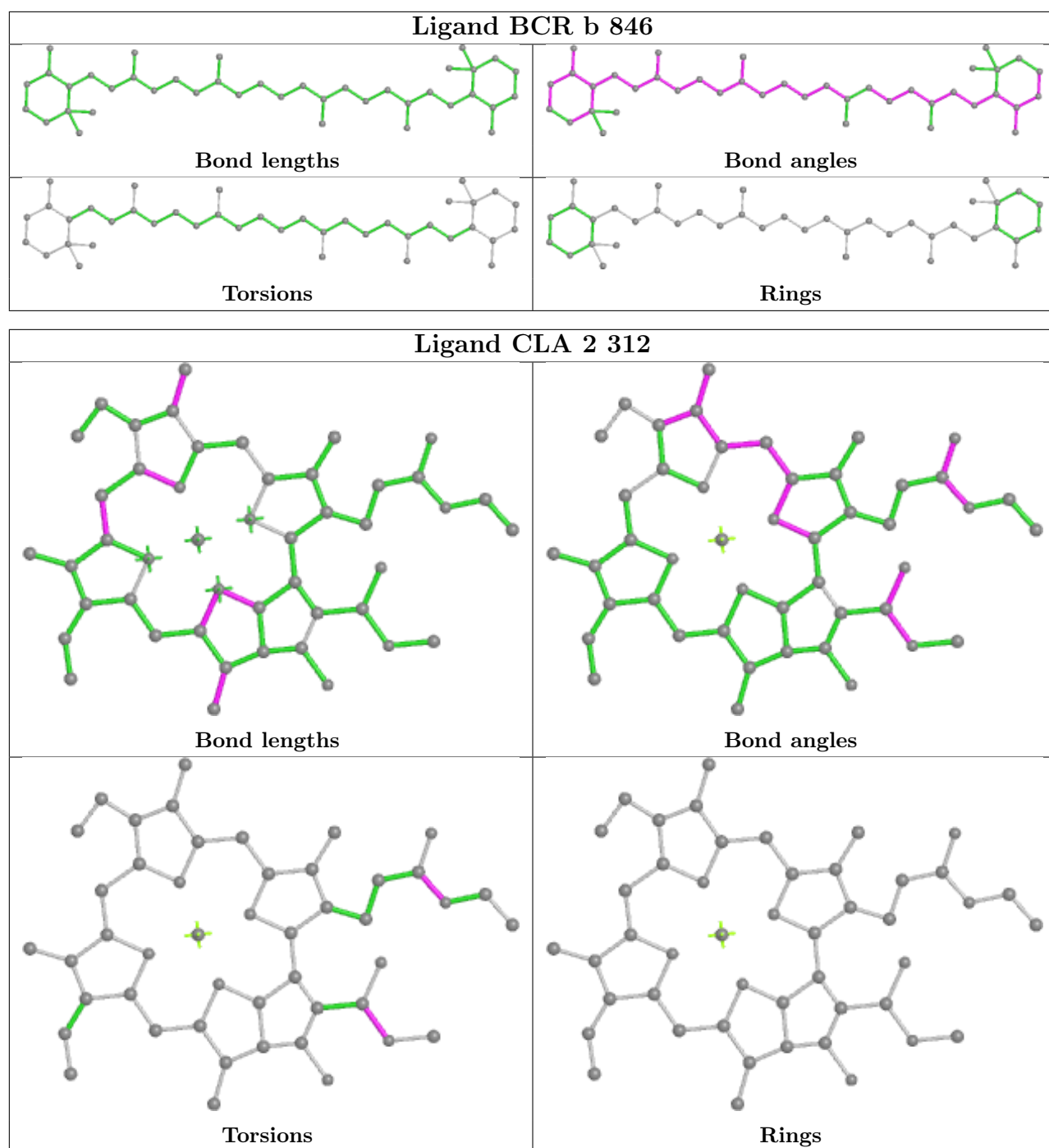
## Ligand CLA b 831

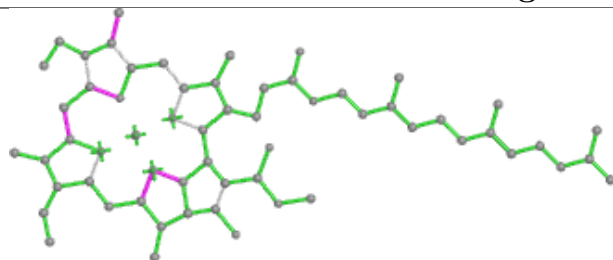




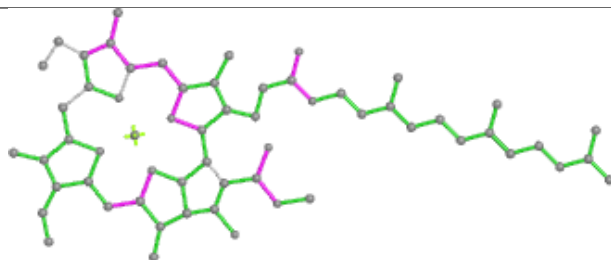


**Ligand CLA b 806****Ligand CLA b 832****Ligand XAT 9 303**

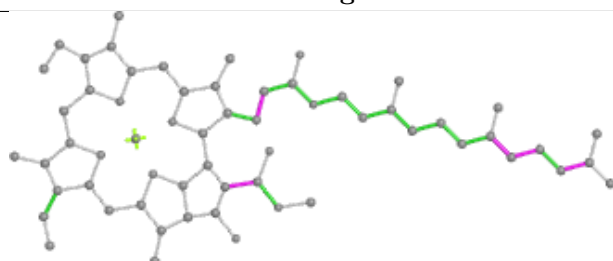


**Ligand CLA 5 308**

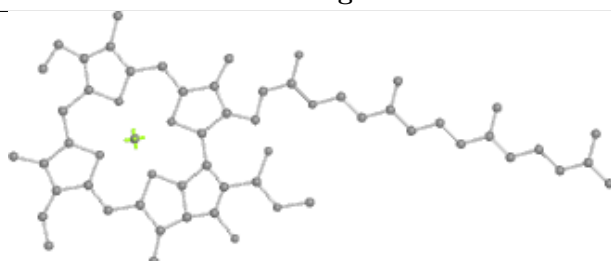
Bond lengths



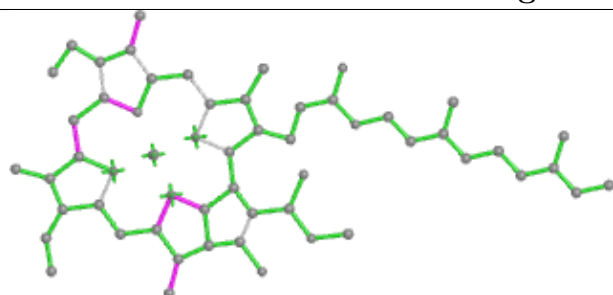
Bond angles



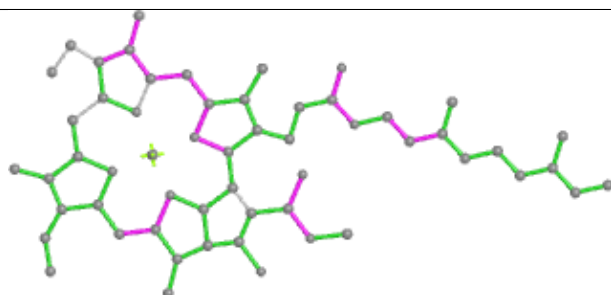
Torsions



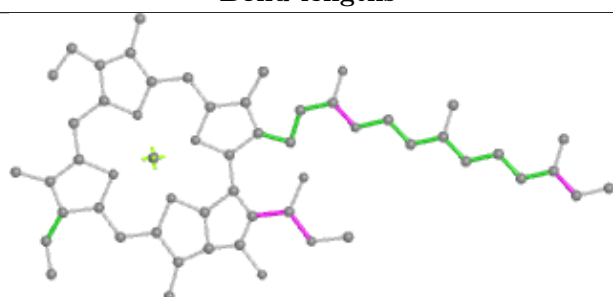
Rings

**Ligand CLA a 811**

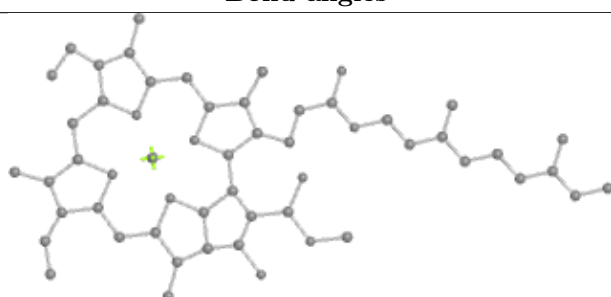
Bond lengths



Bond angles

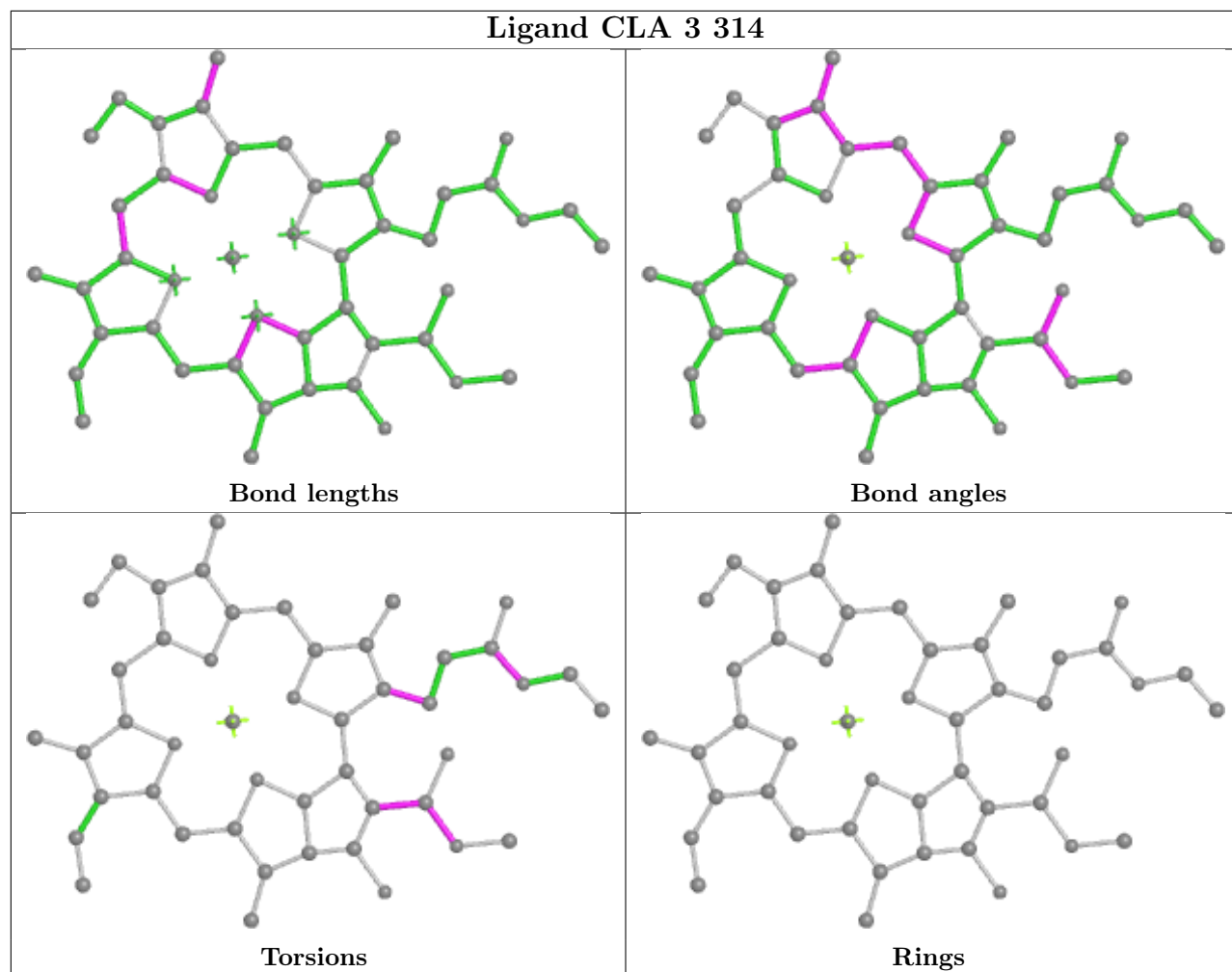


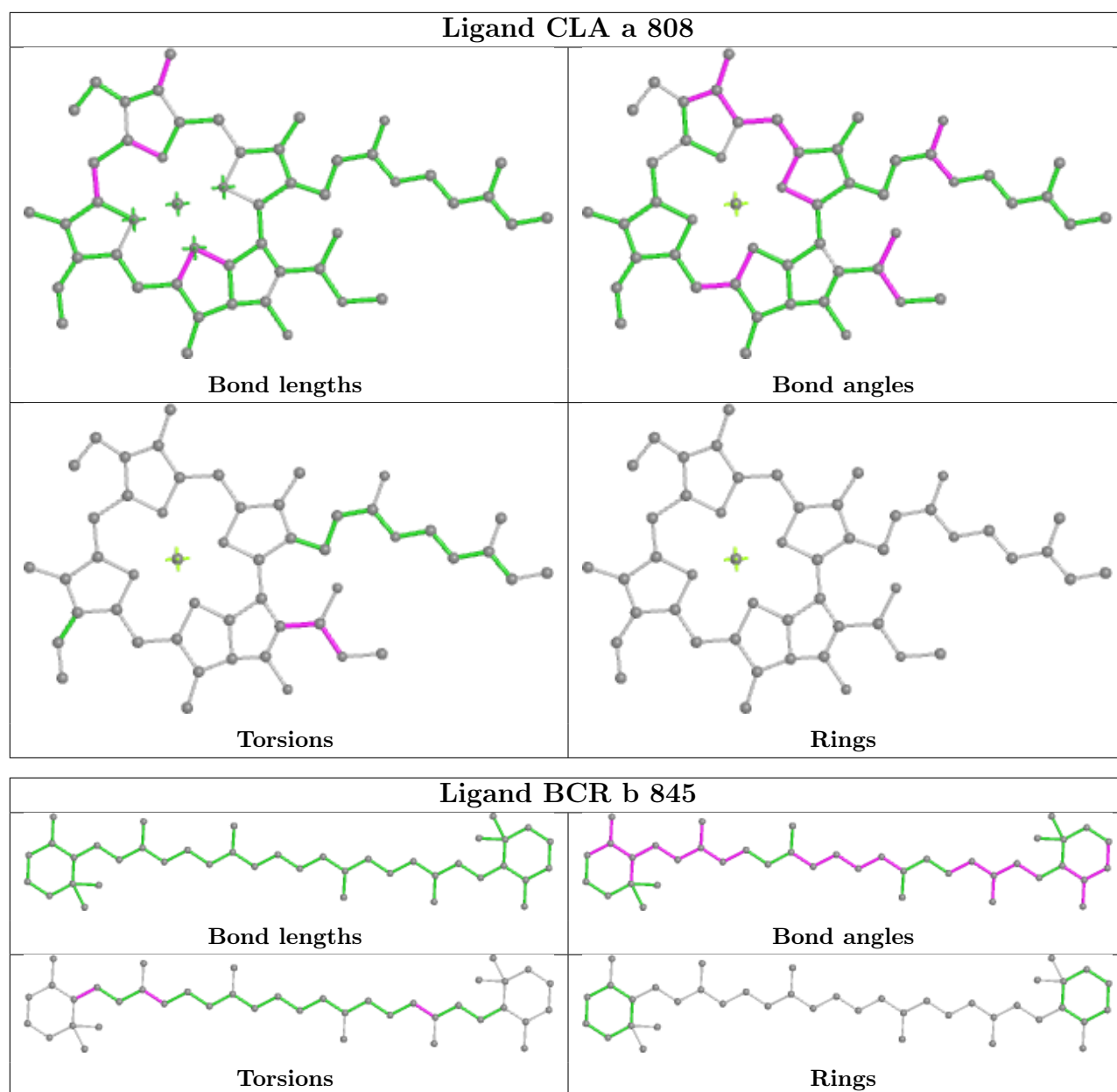
Torsions

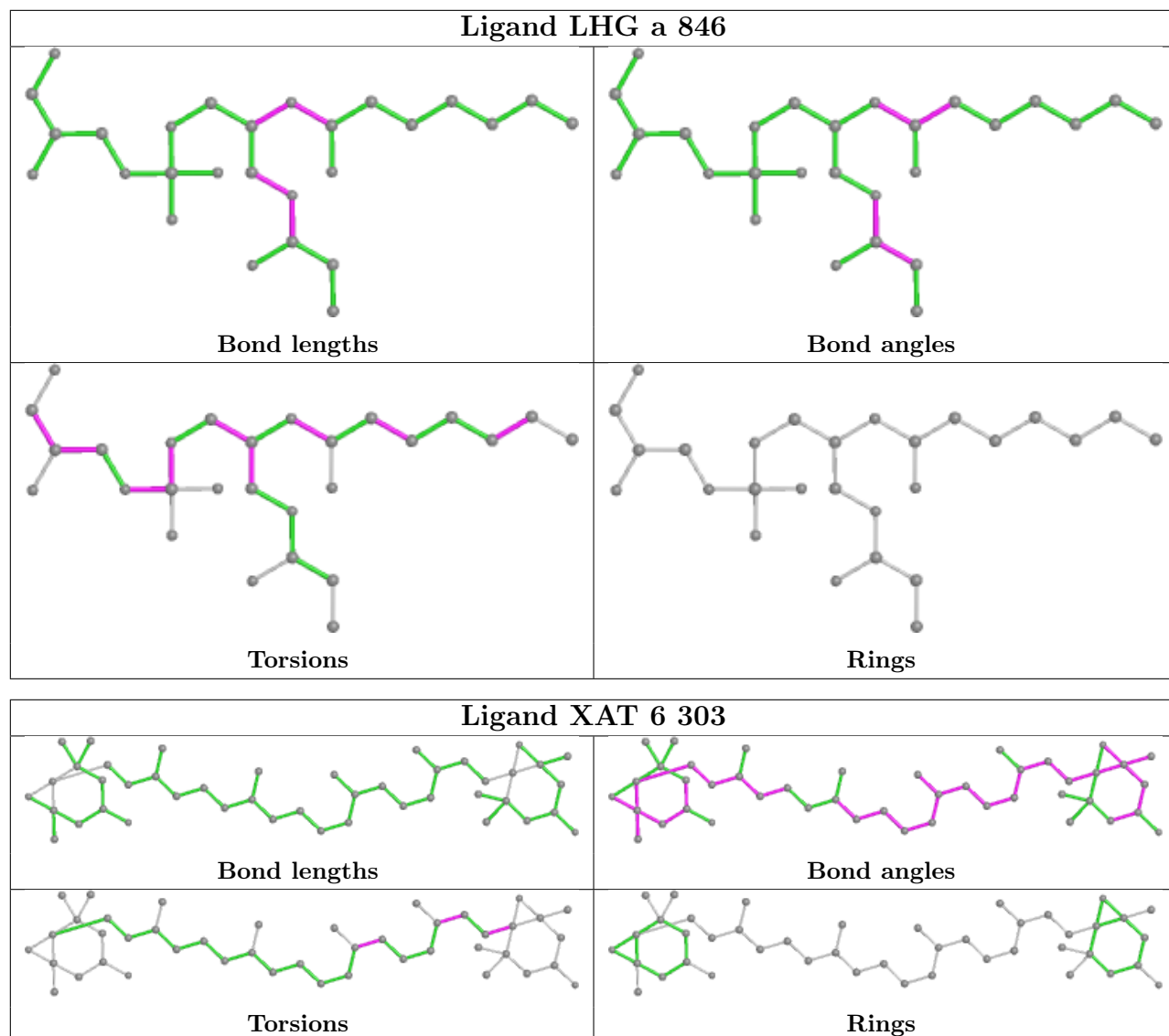


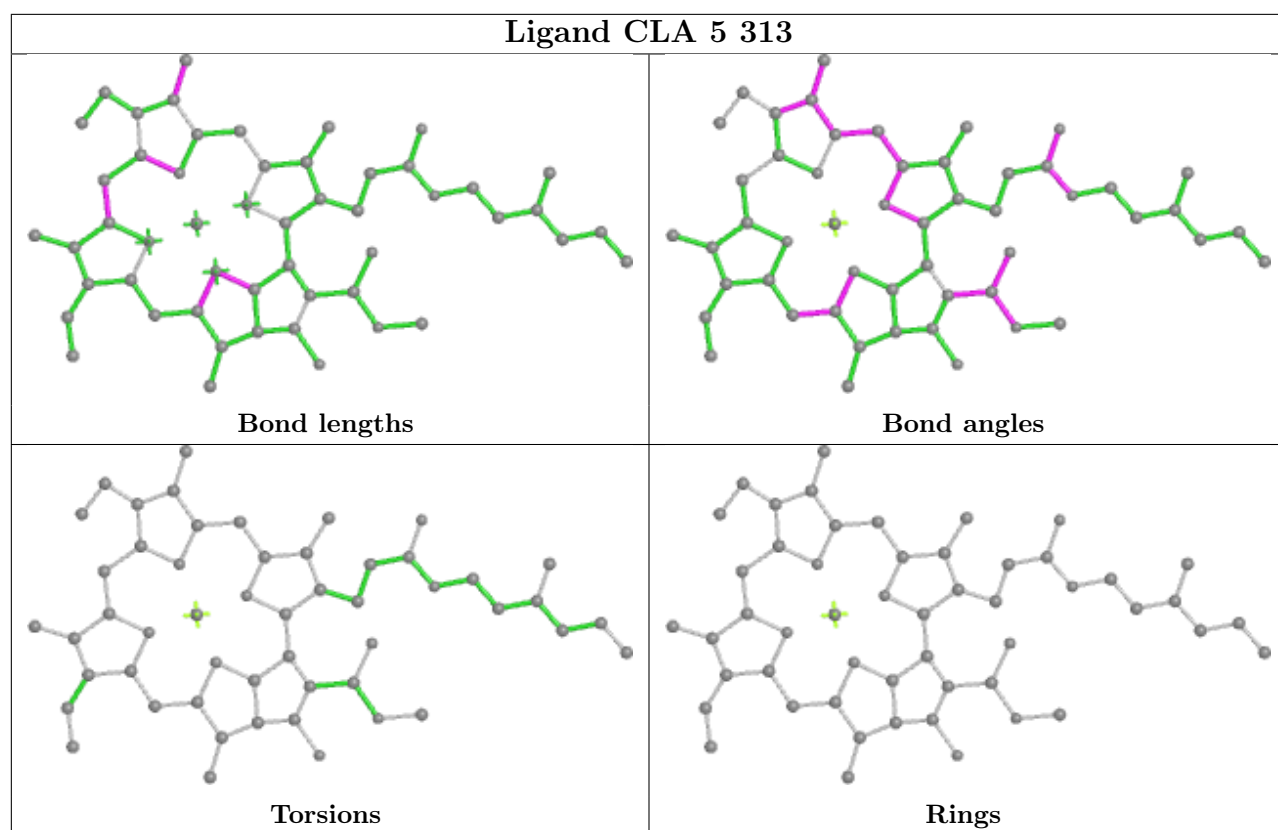
Rings

## Ligand CLA 3 314

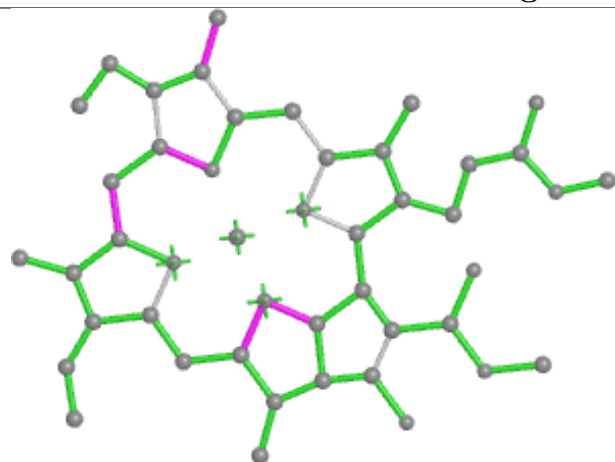




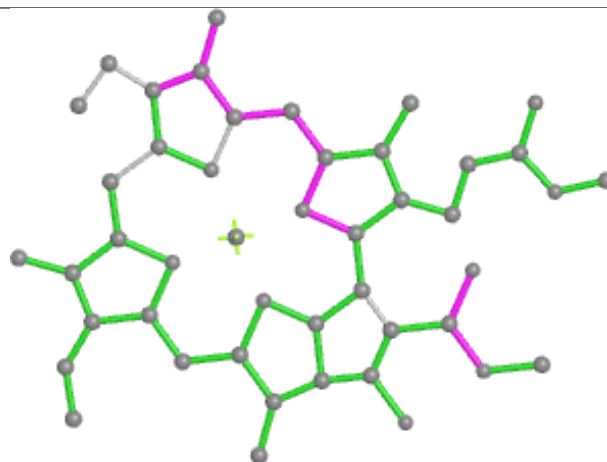




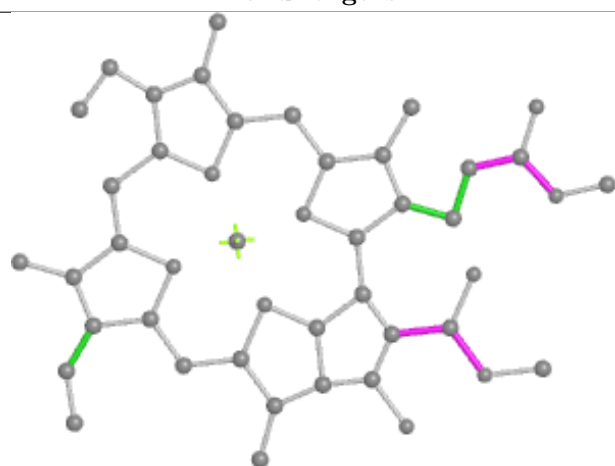
## Ligand CLA 6 314



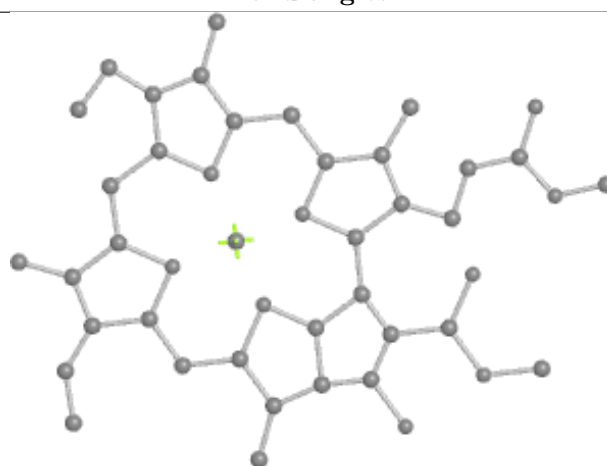
Bond lengths



Bond angles

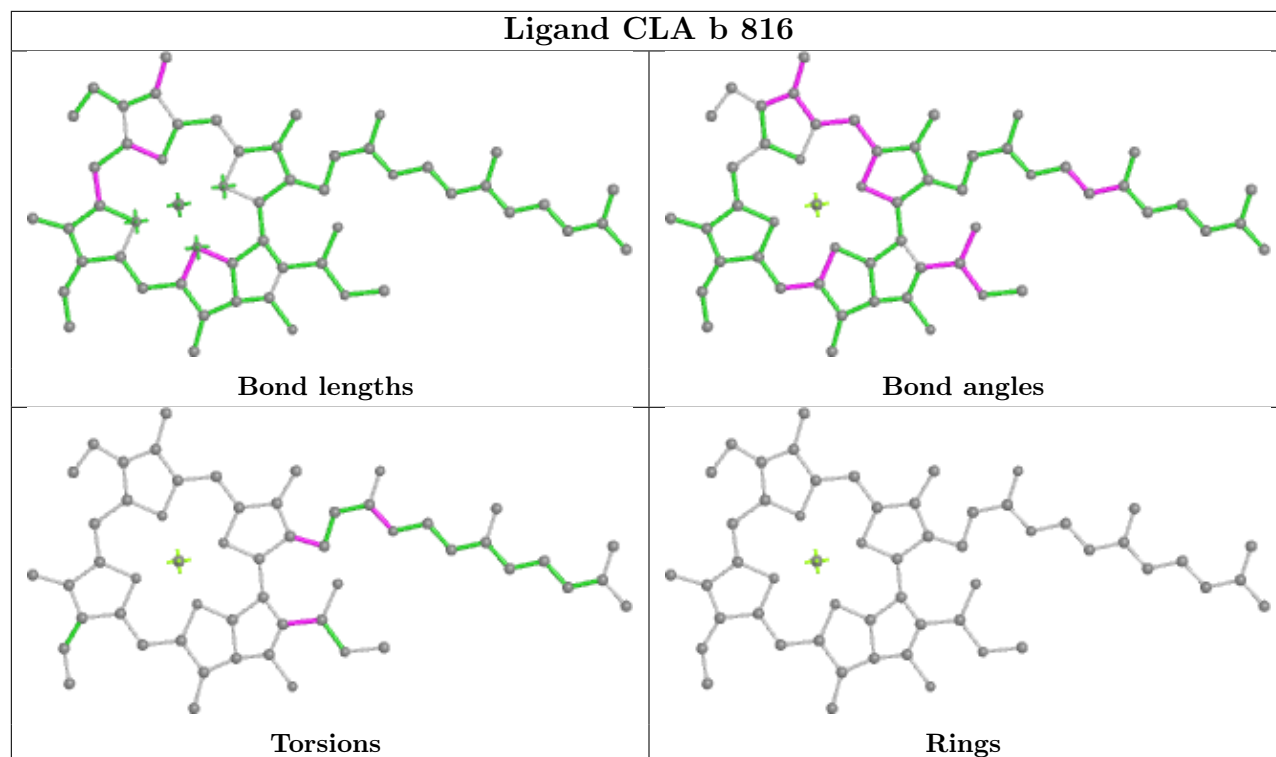


Torsions

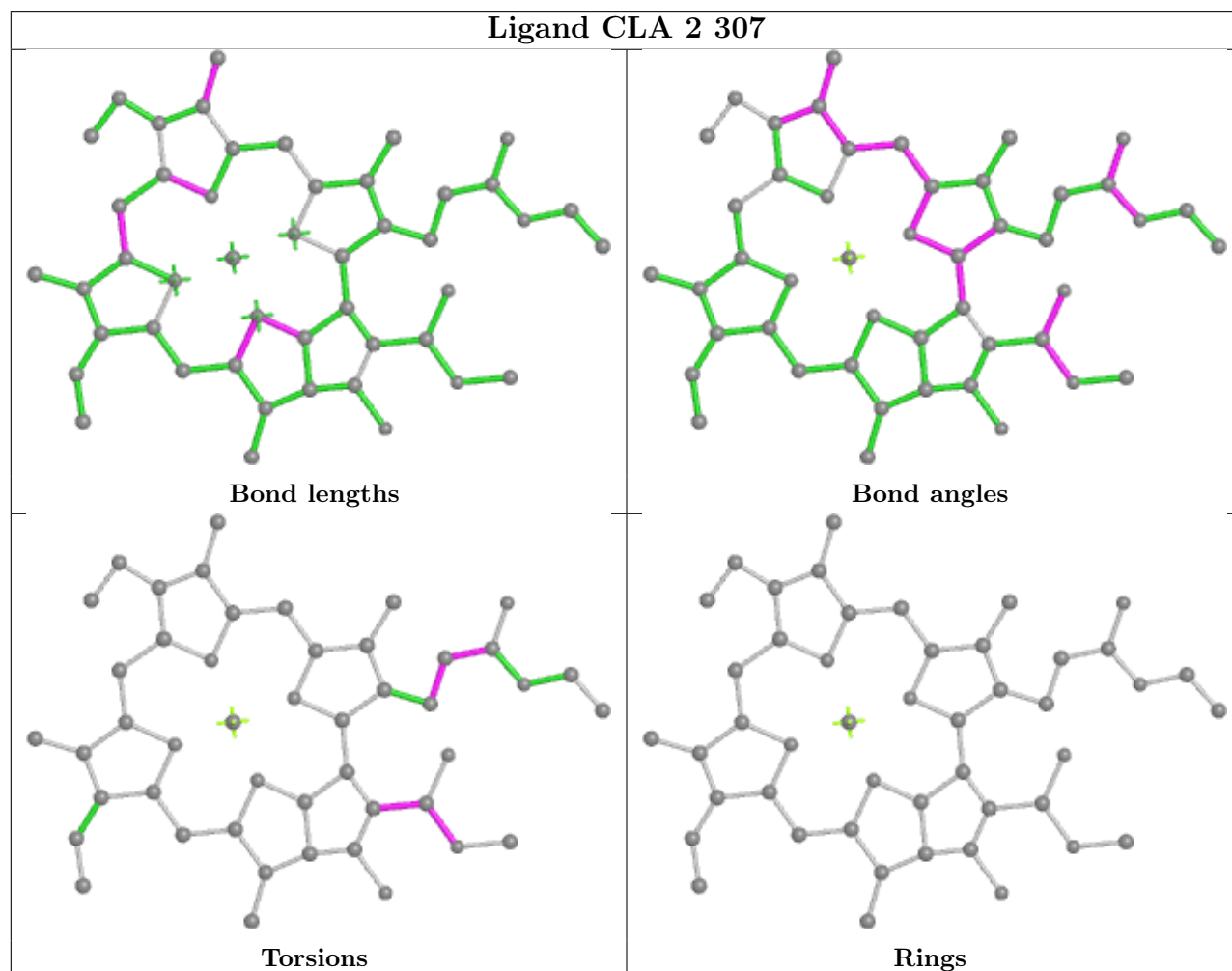


Rings

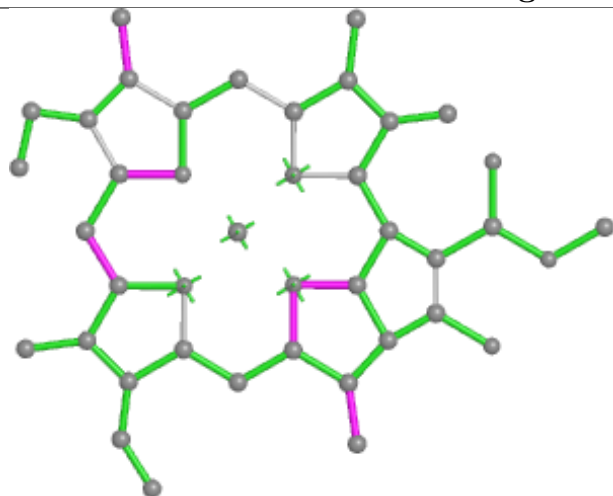
## Ligand CLA b 816



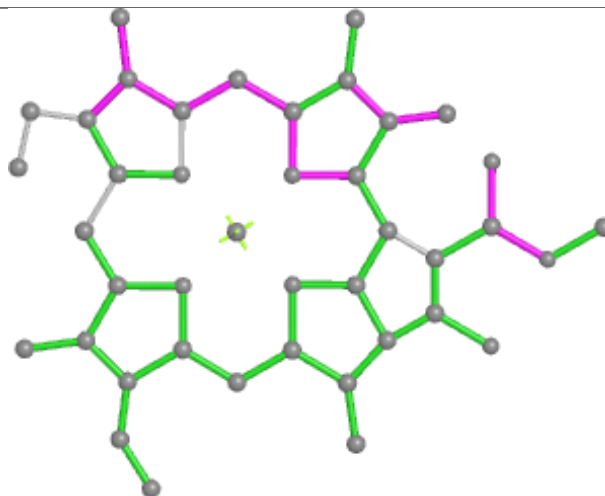
## Ligand CLA 2 307



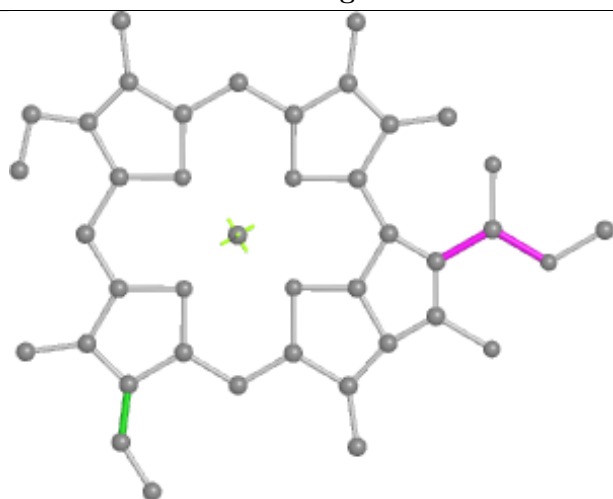
## Ligand CLA 1 313



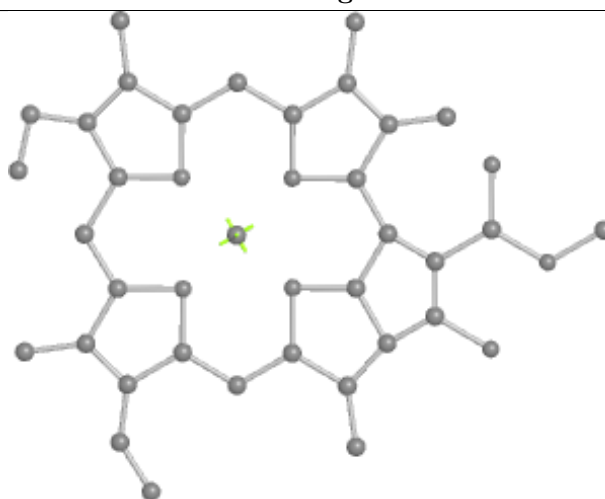
Bond lengths



Bond angles

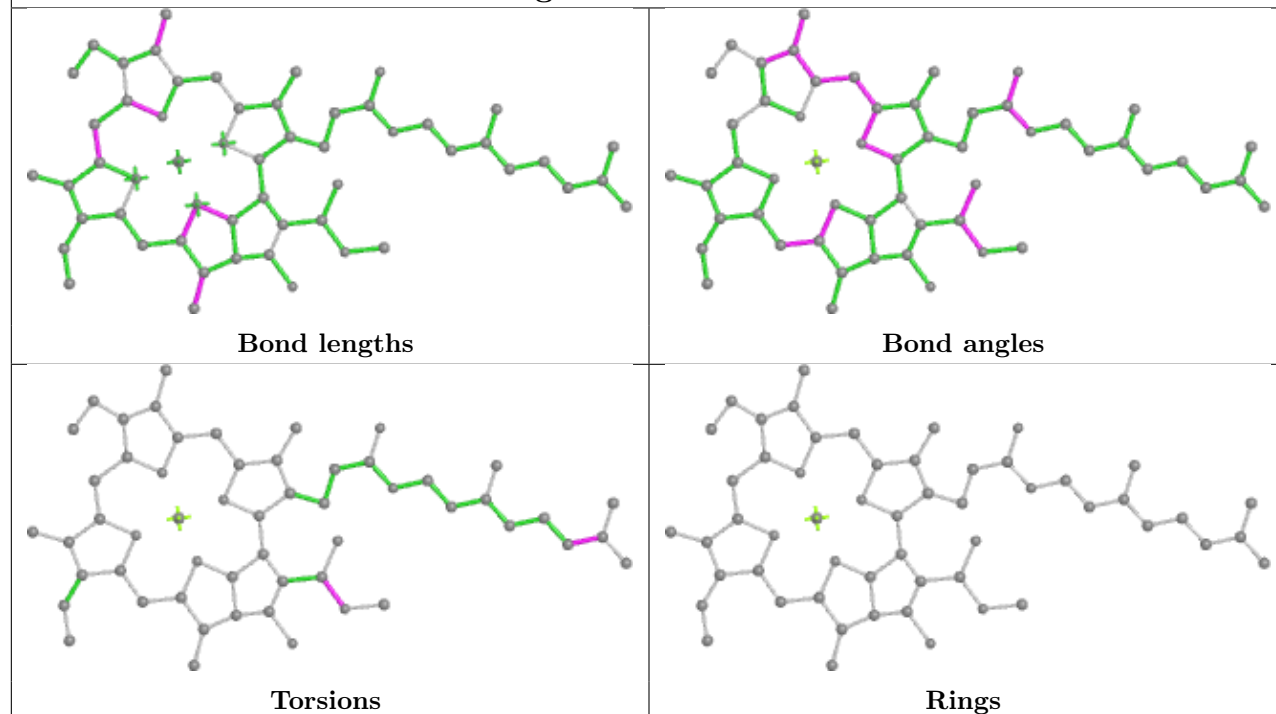


Torsions

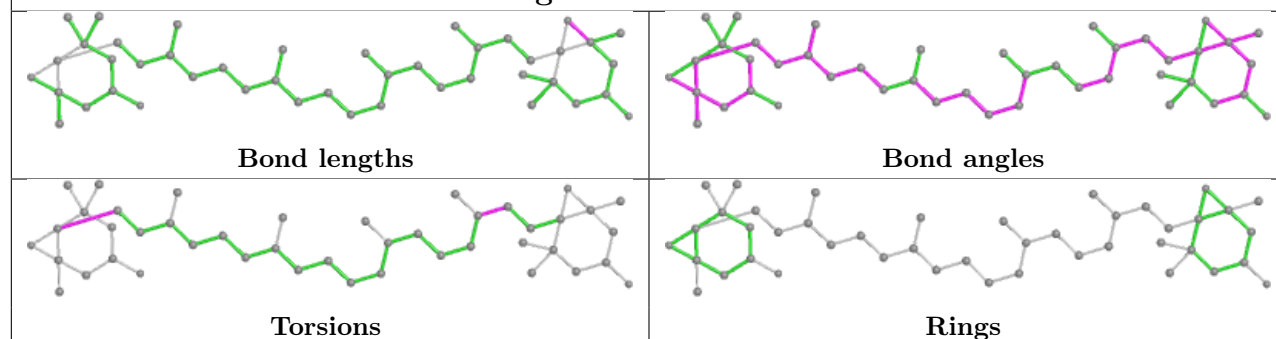


Rings

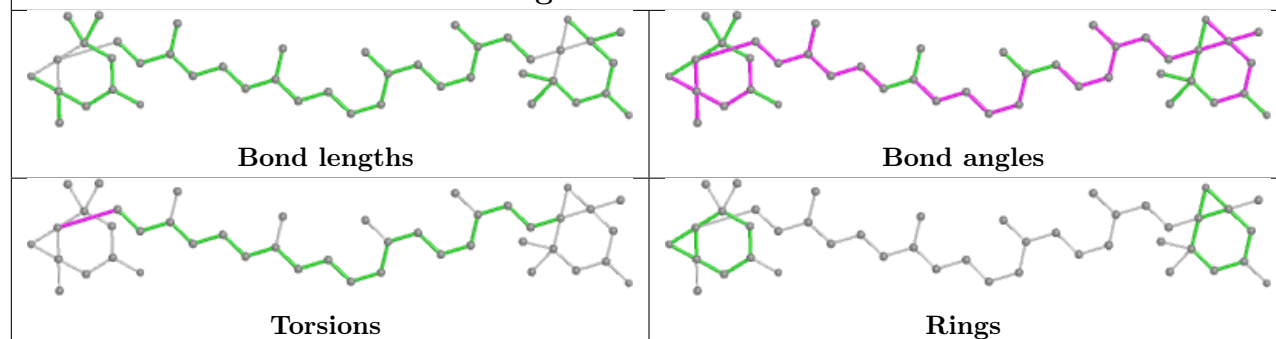
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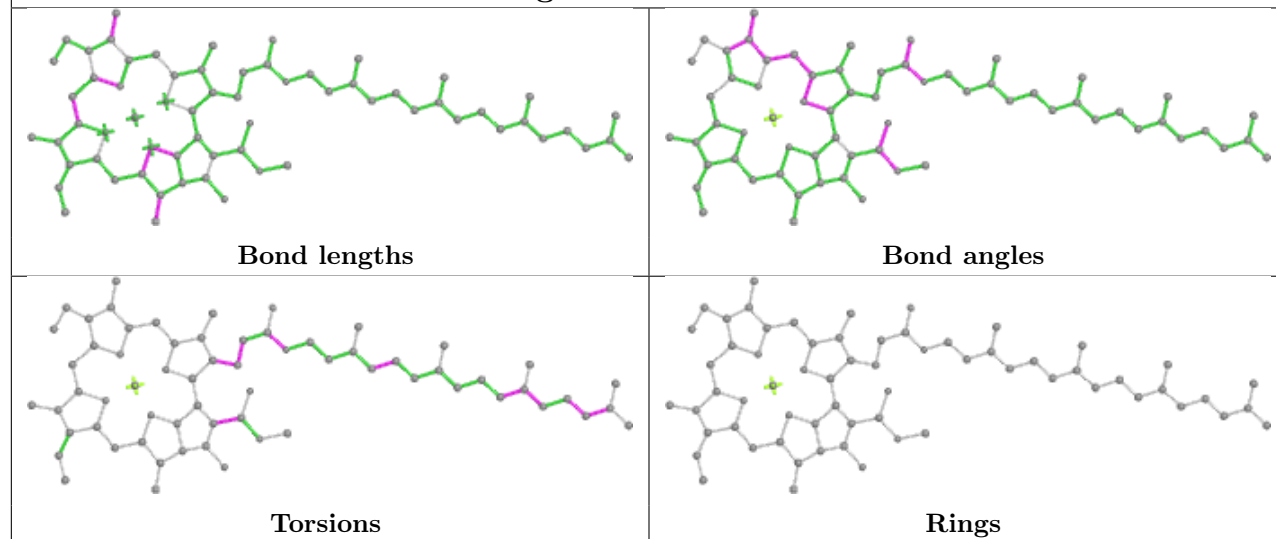
## Ligand XAT 8 301



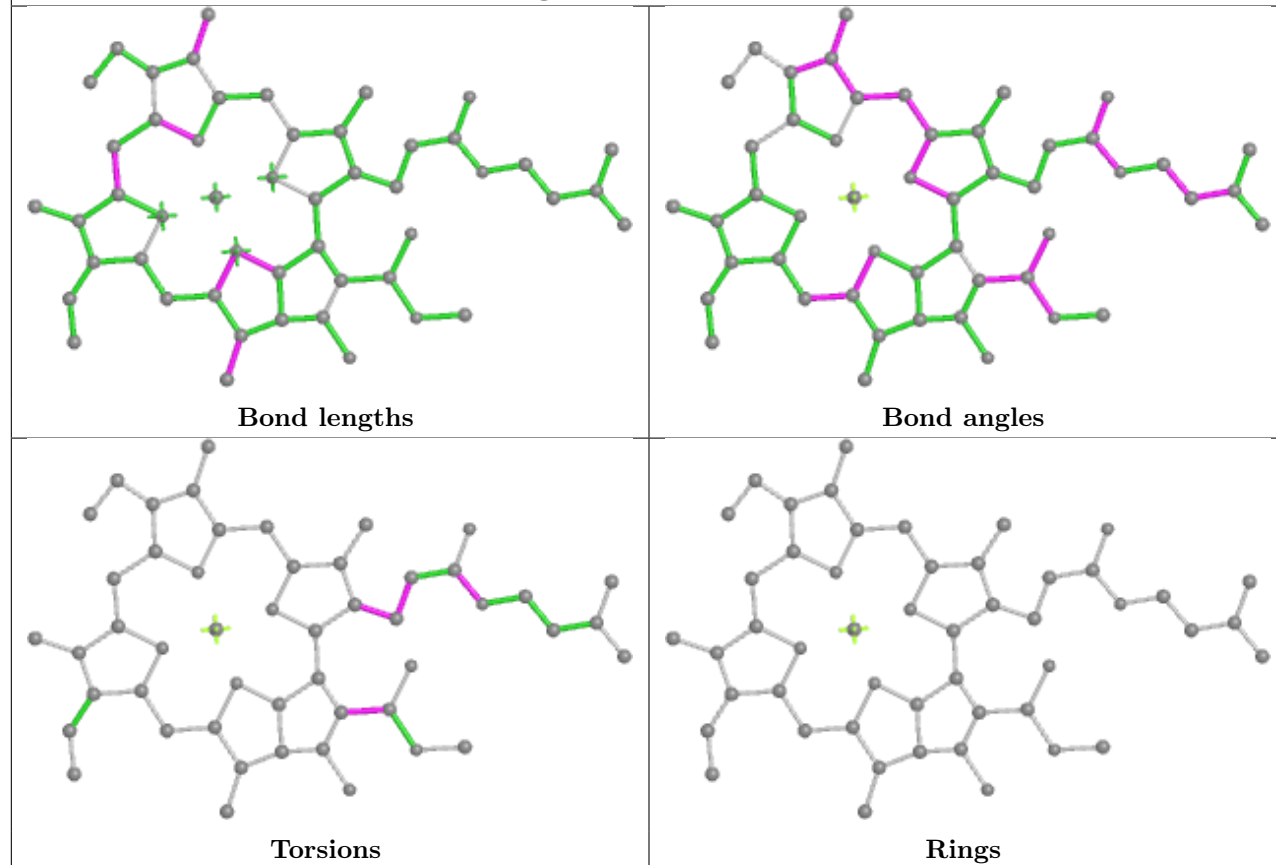
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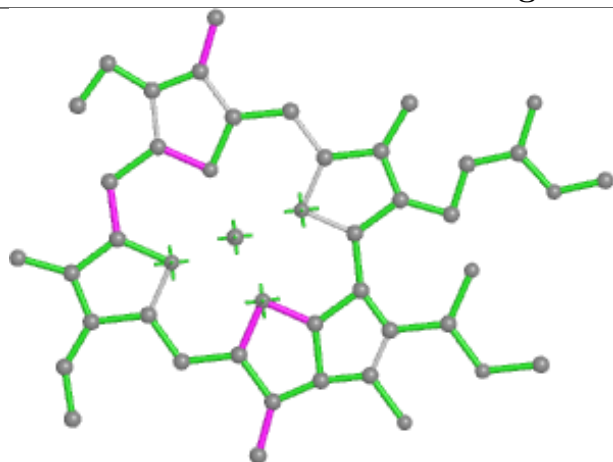
## Ligand CLA 2 310



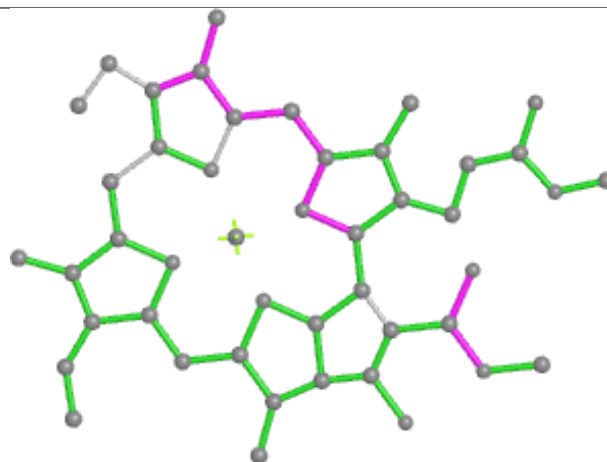
## Ligand CLA b 820



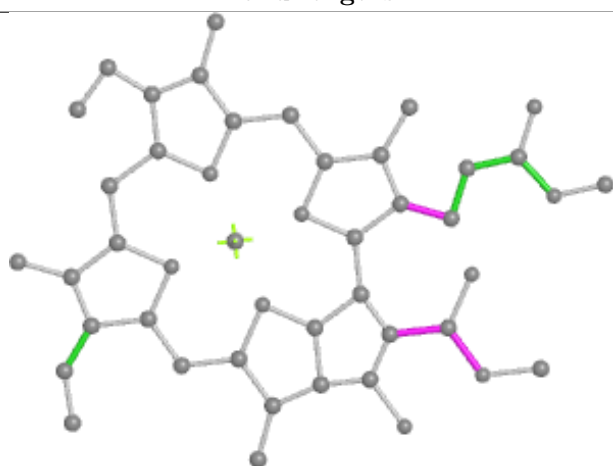
## Ligand CLA 2 316



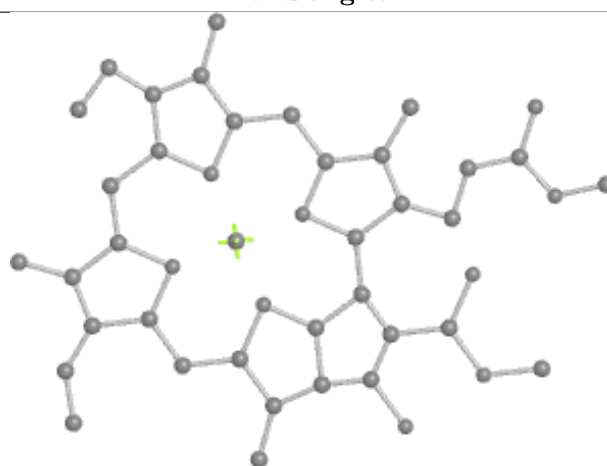
Bond lengths



Bond angles

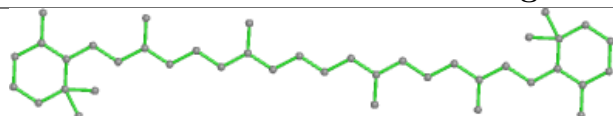


Torsions

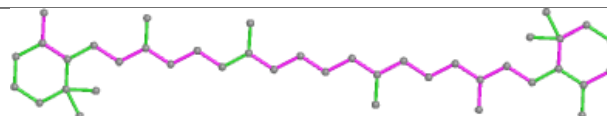


Rings

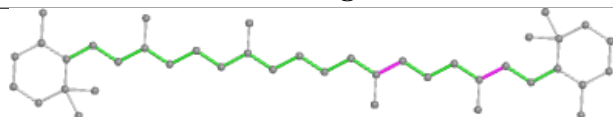
## Ligand BCR i 101



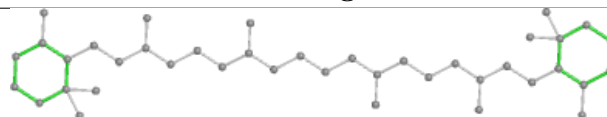
Bond lengths



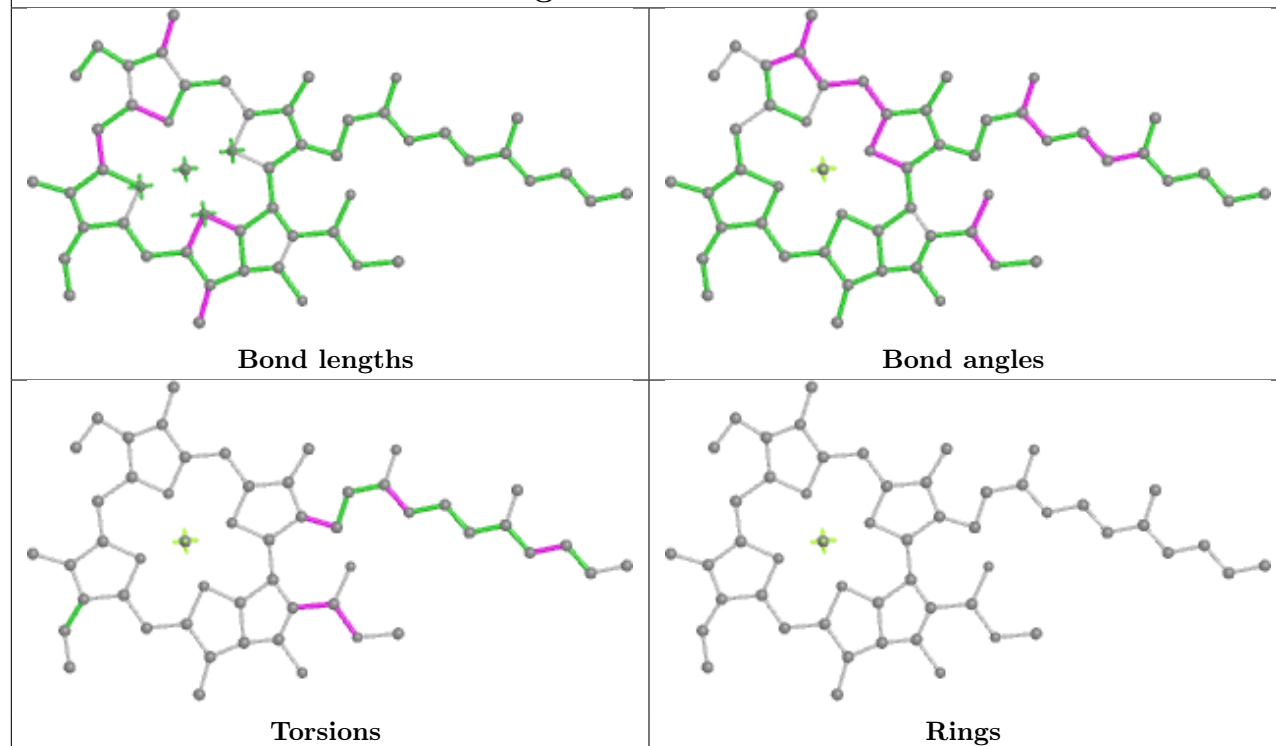
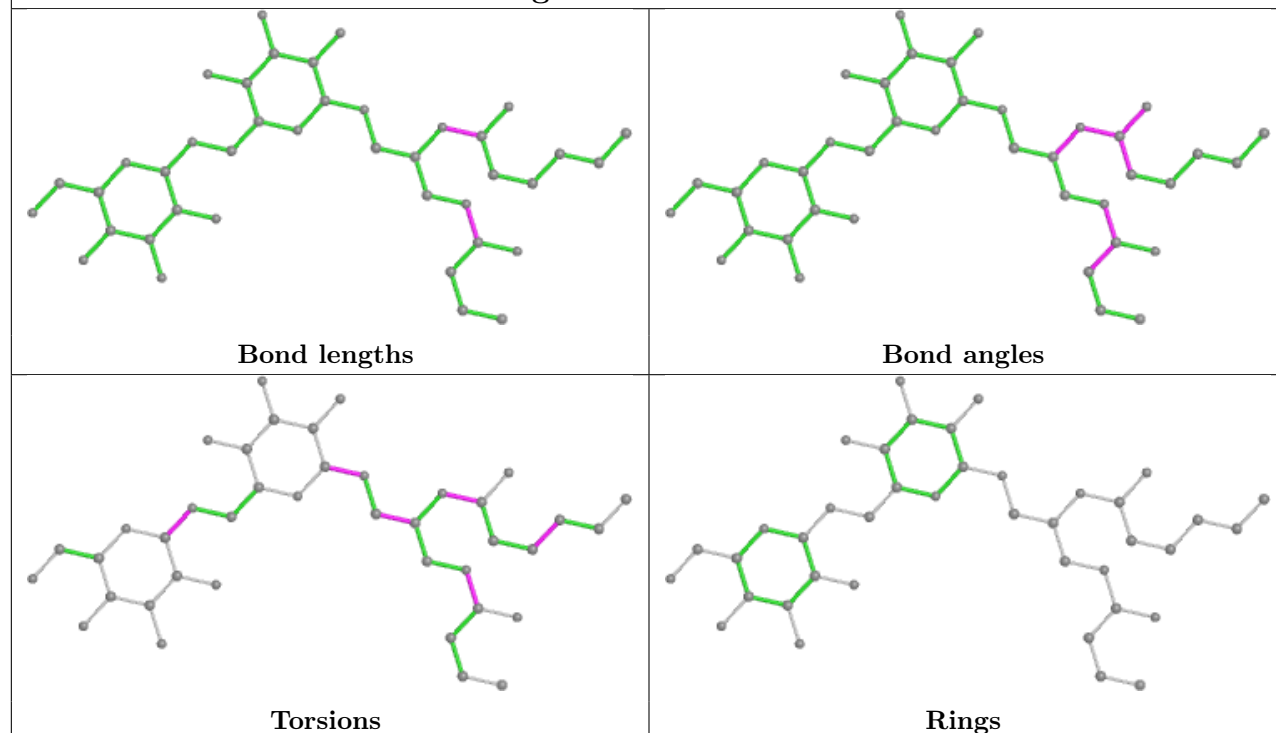
Bond angles

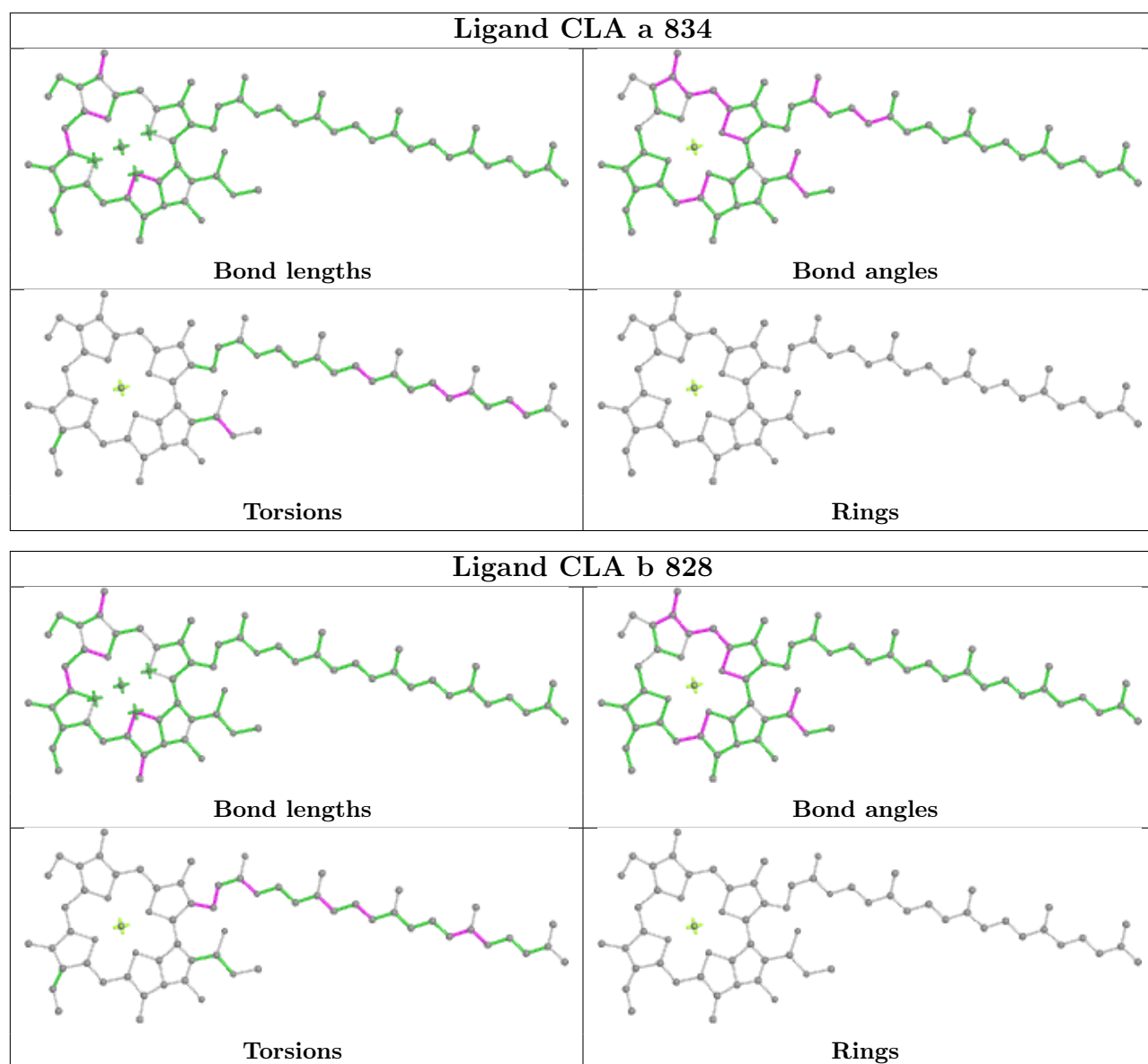


Torsions

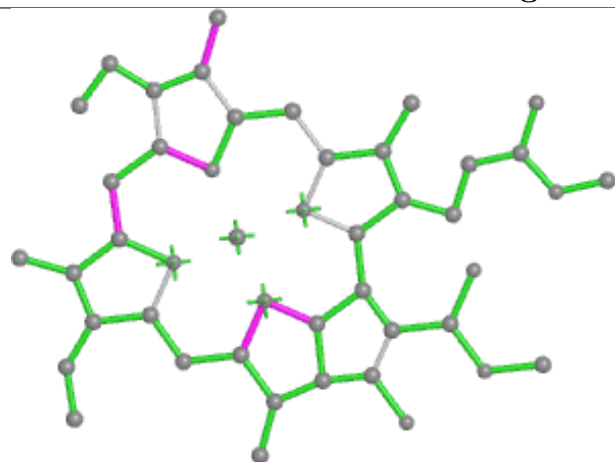


Rings

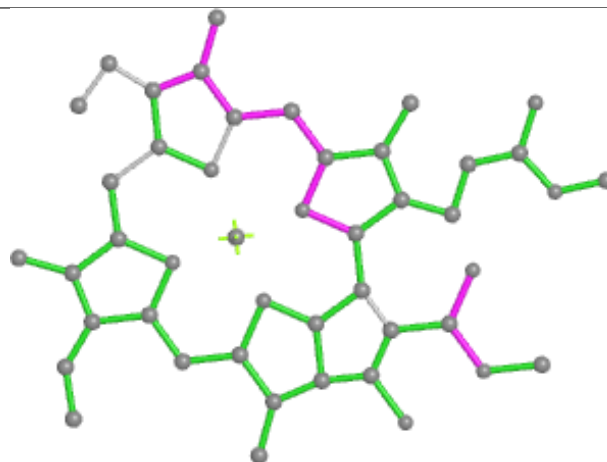
**Ligand CLA b 823****Ligand DGD 8 315**



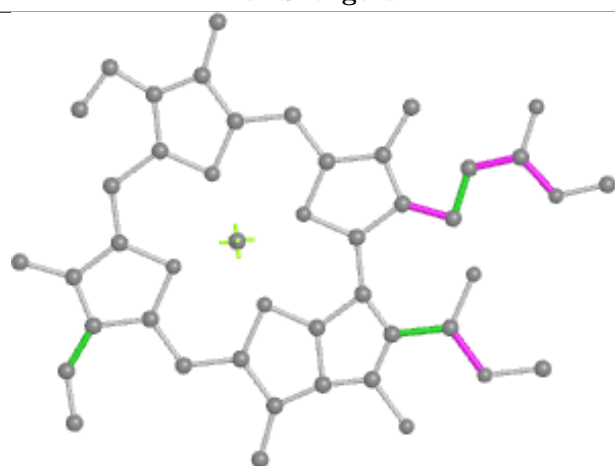
## Ligand CLA 6 316



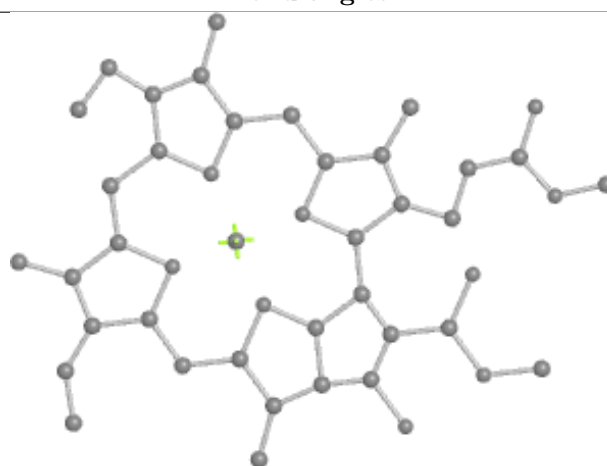
Bond lengths



Bond angles

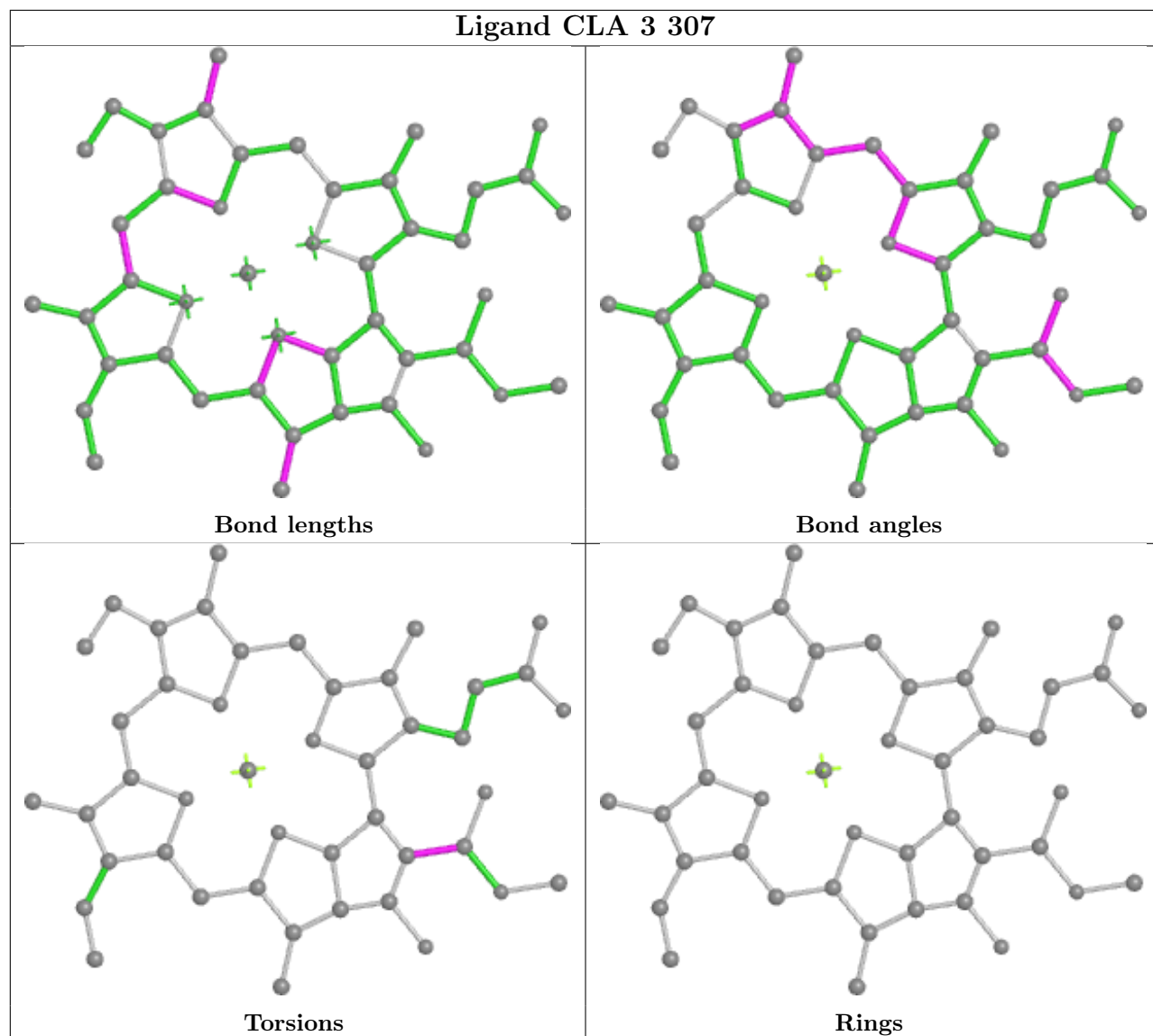


Torsions

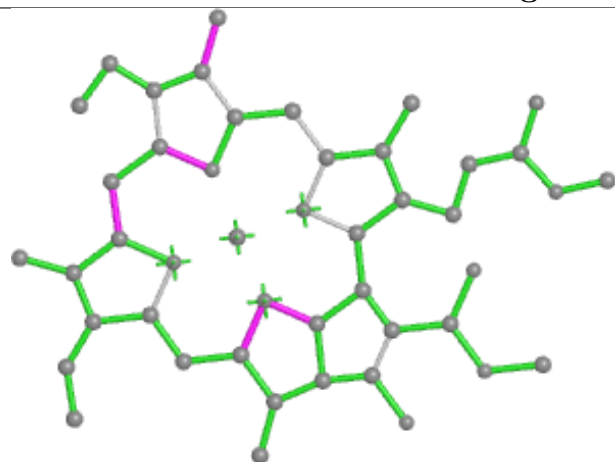


Rings

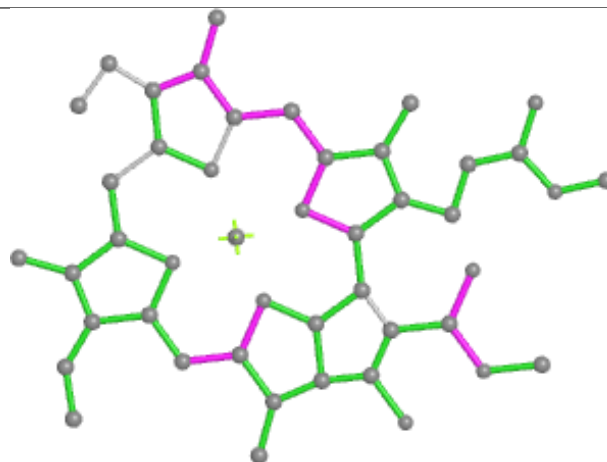
## Ligand CLA 3 307



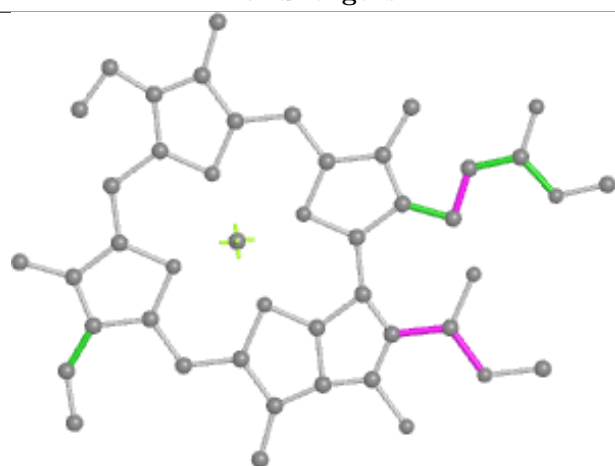
## Ligand CLA 2 309



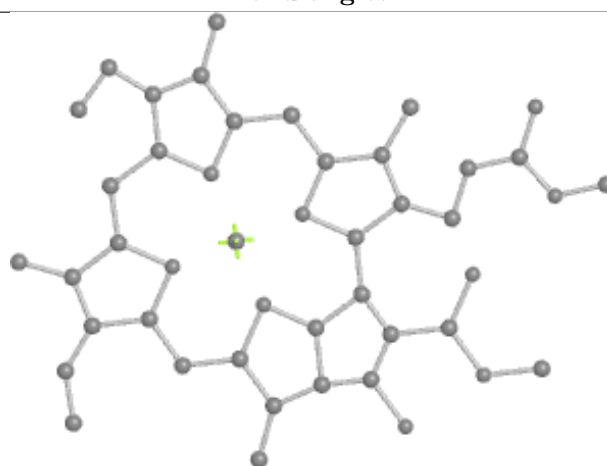
Bond lengths



Bond angles

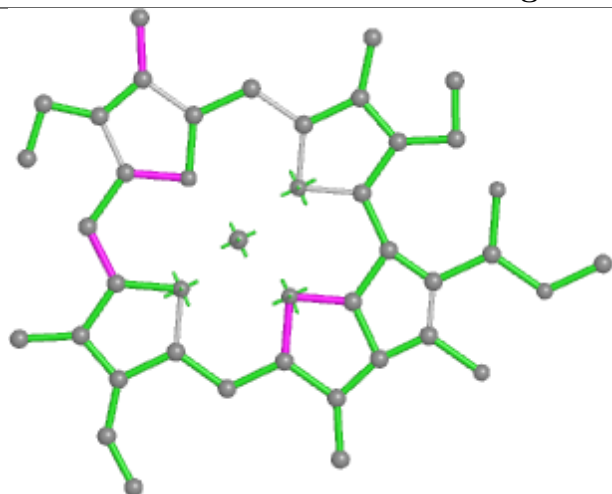


Torsions

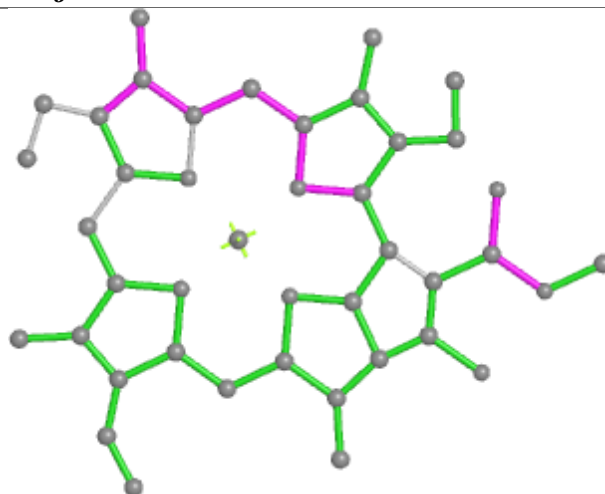


Rings

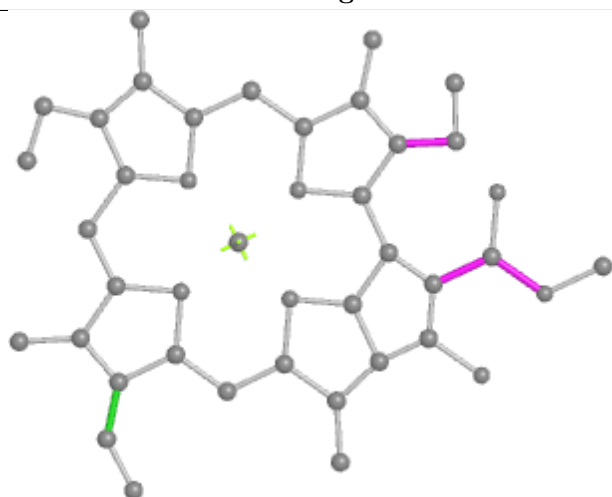
## Ligand CLA j 101



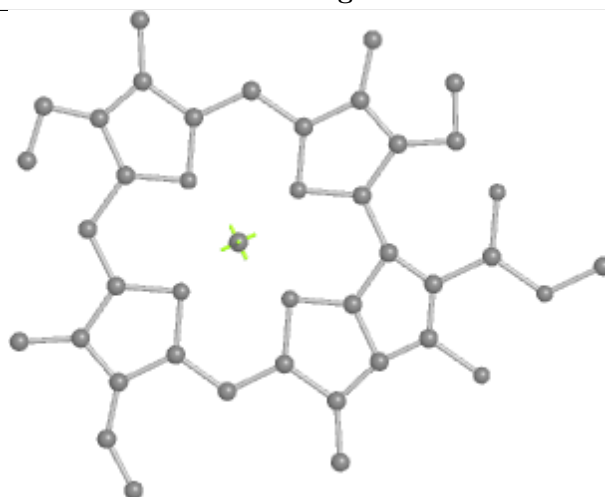
Bond lengths



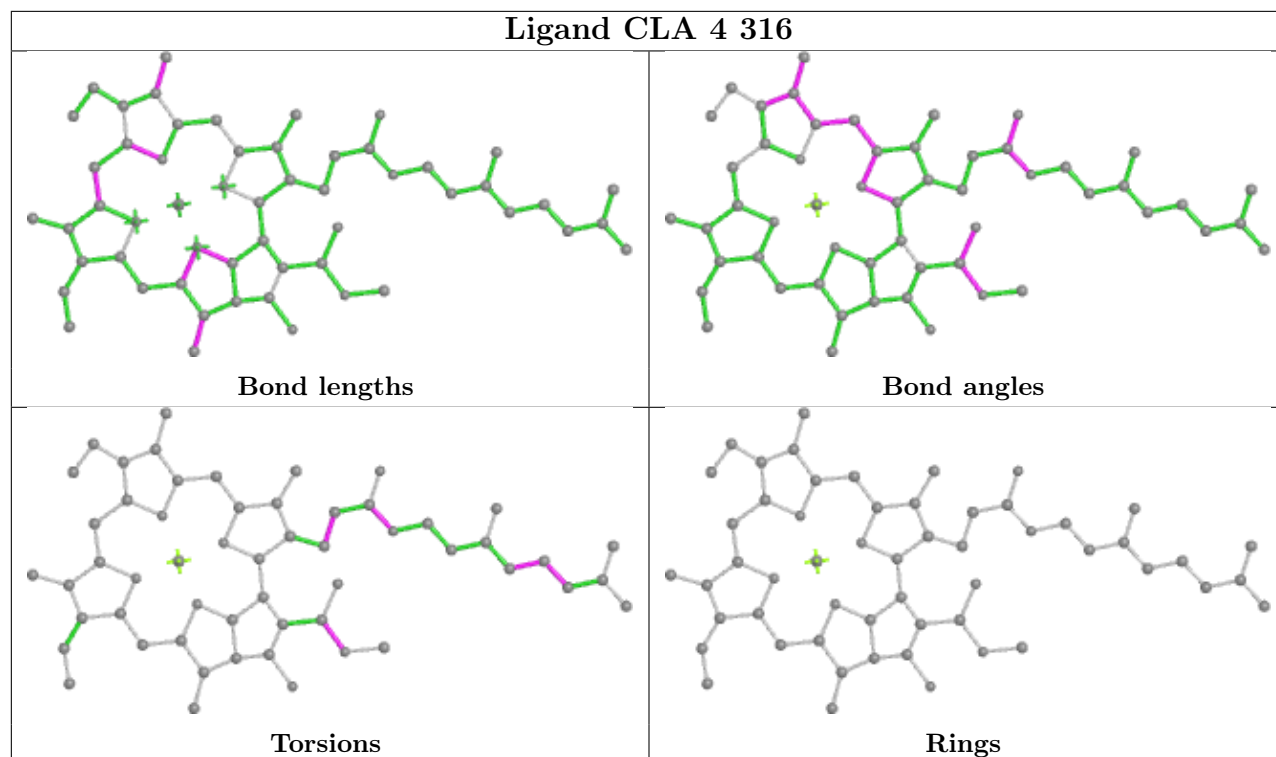
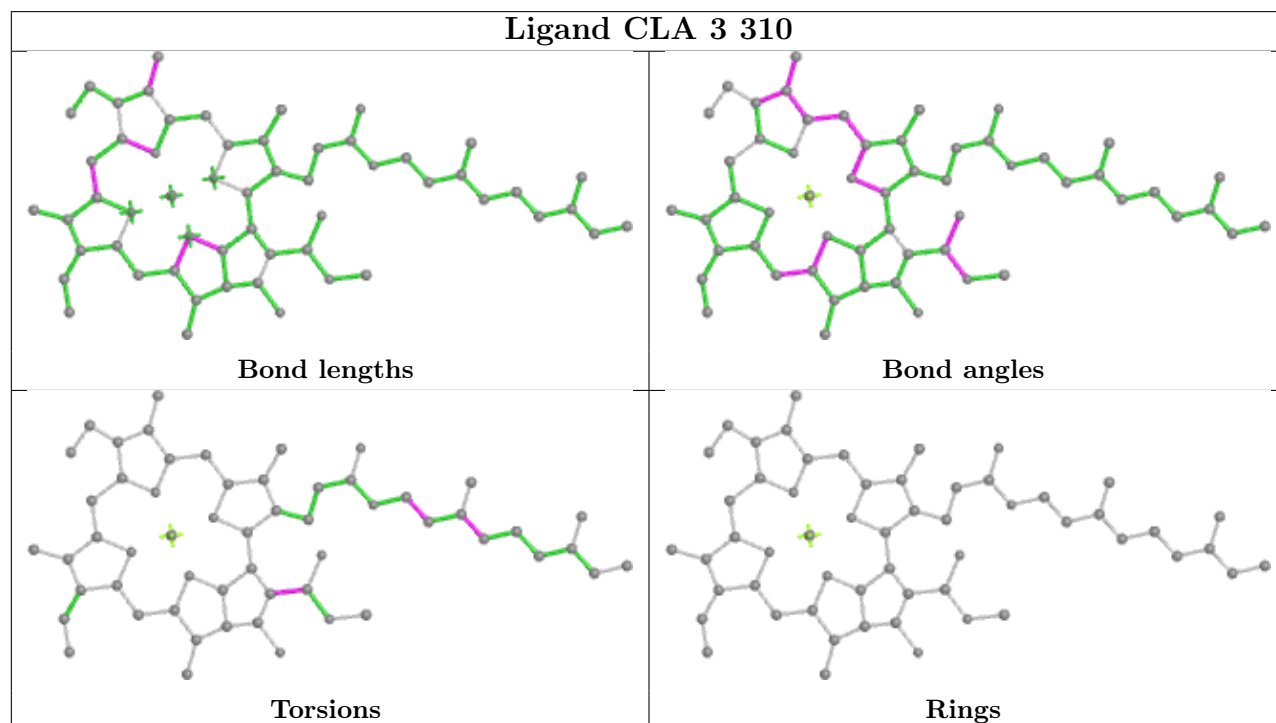
Bond angles



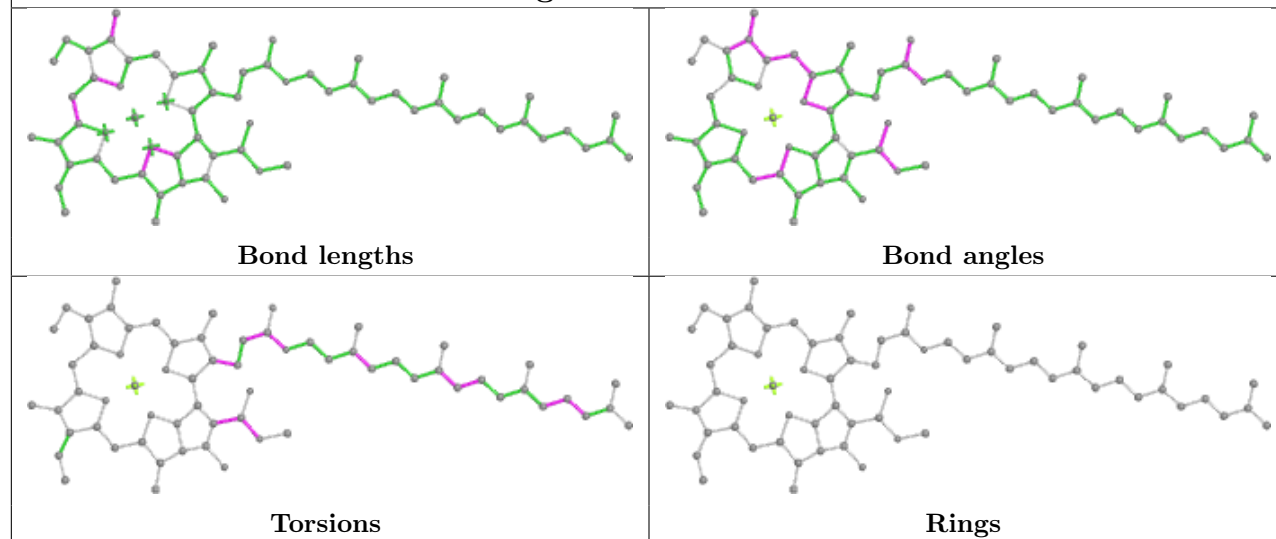
Torsions



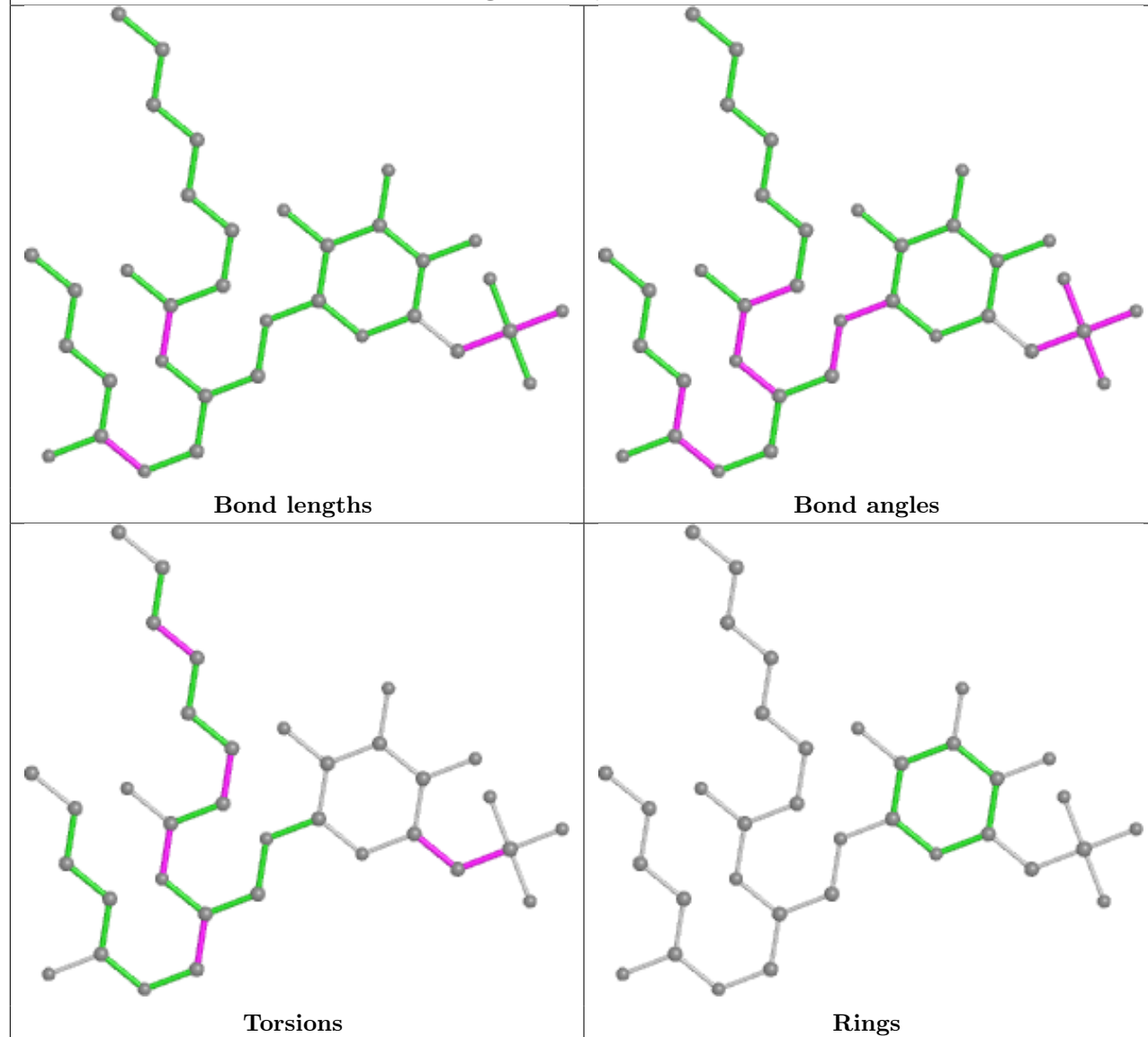
Rings

**Ligand CLA 4 316****Ligand CLA 3 310**

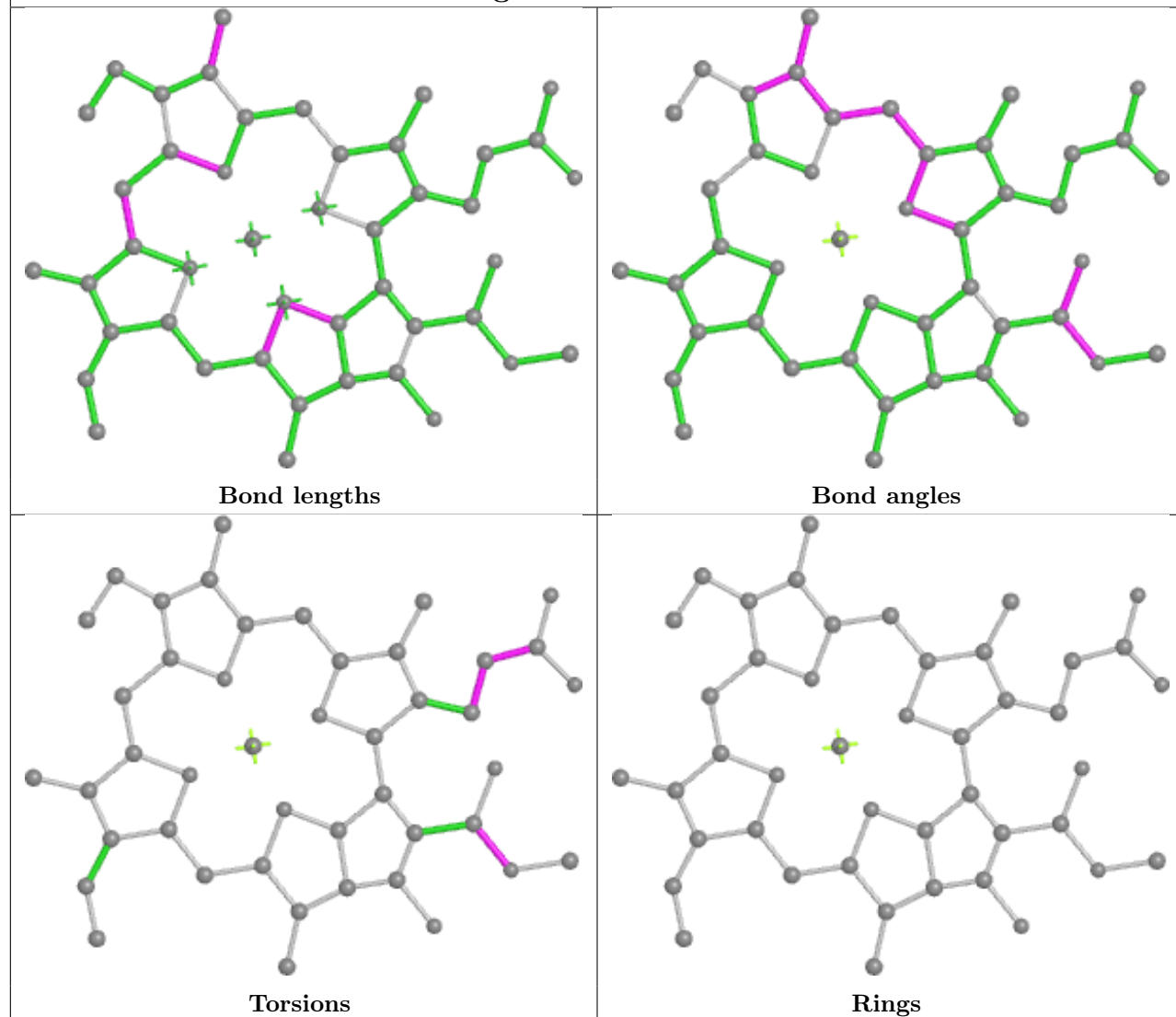
## Ligand CLA 4 309



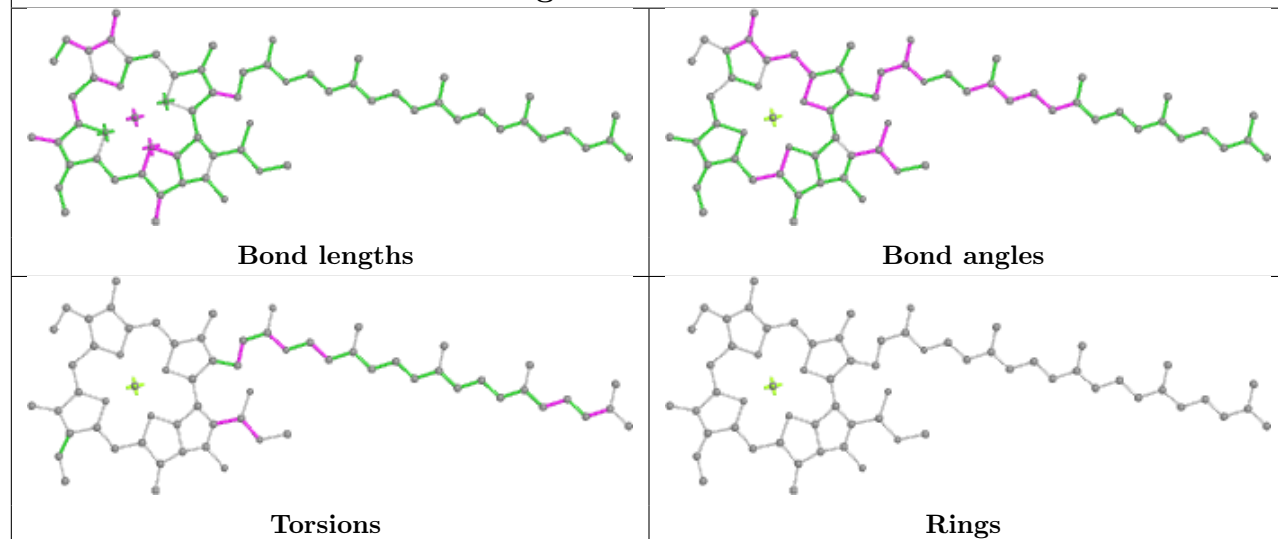
## Ligand SQD 5 317



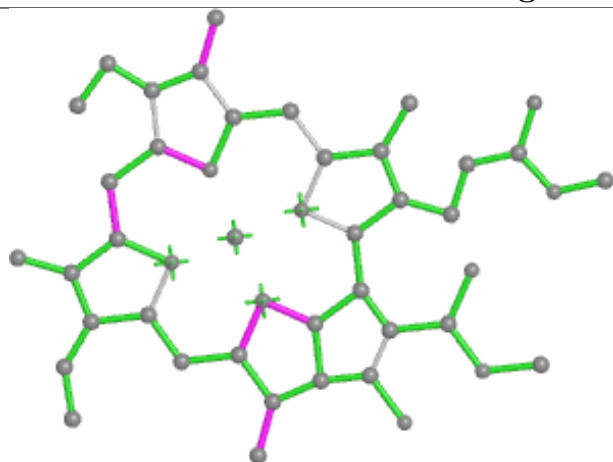
## Ligand CLA 7 317



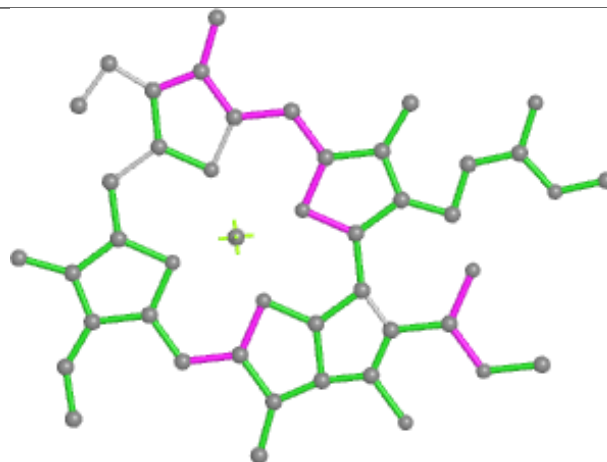
## Ligand CLA a 806



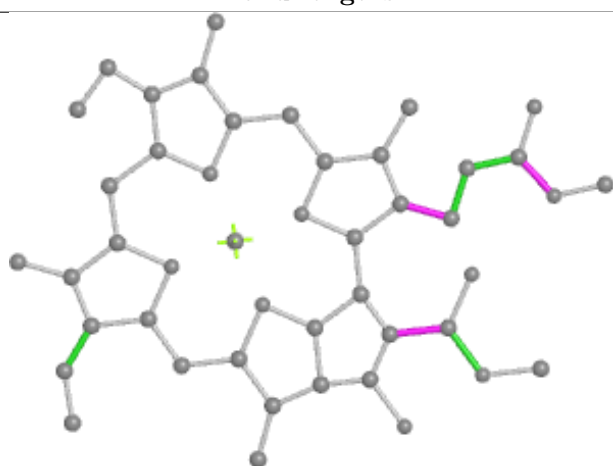
## Ligand CLA 7 311



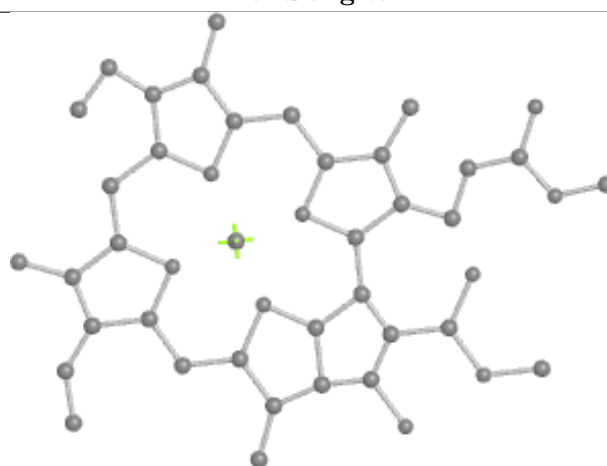
Bond lengths



Bond angles

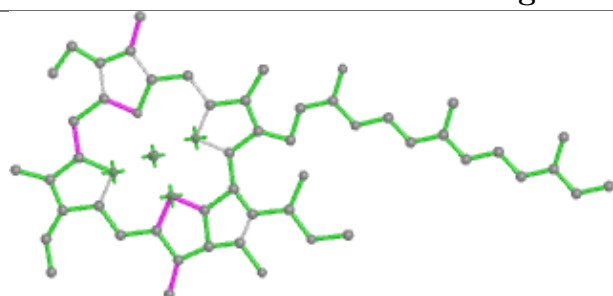


Torsions

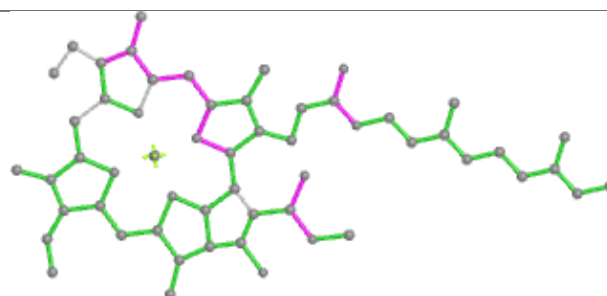


Rings

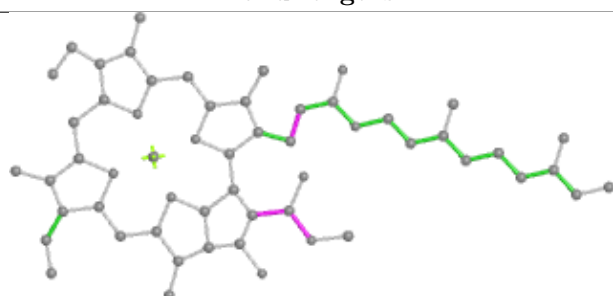
## Ligand CLA 3 309



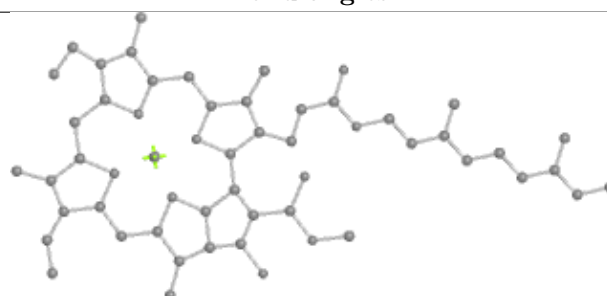
Bond lengths



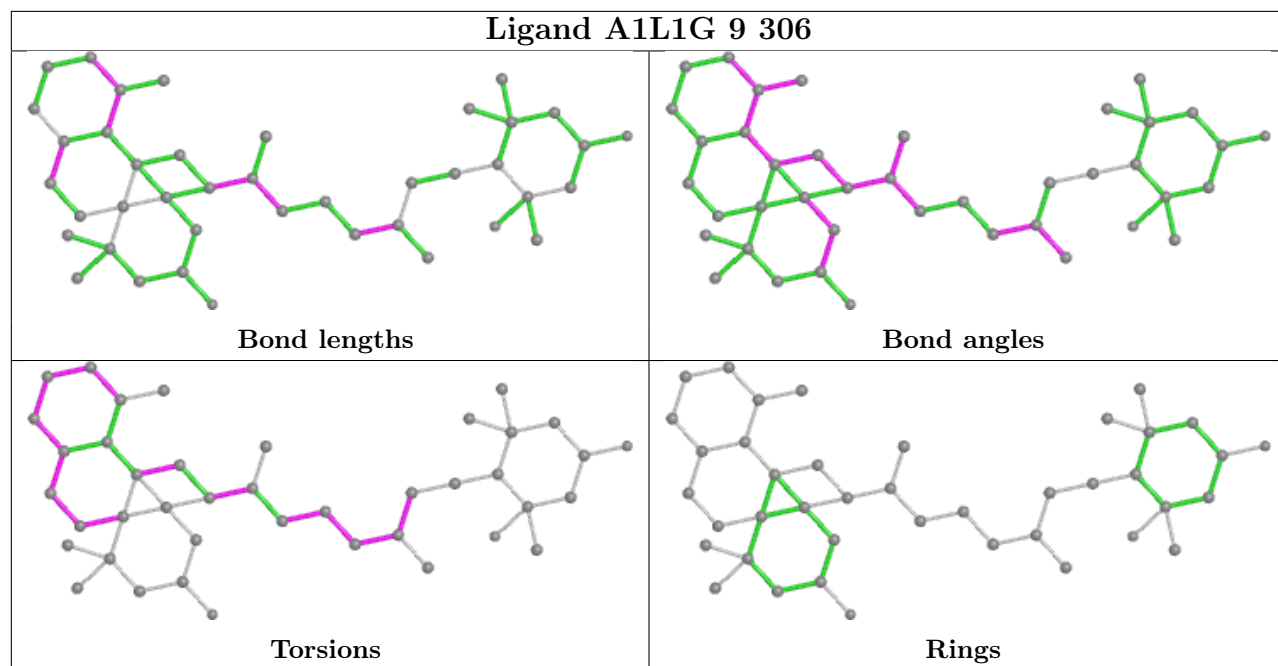
Bond angles



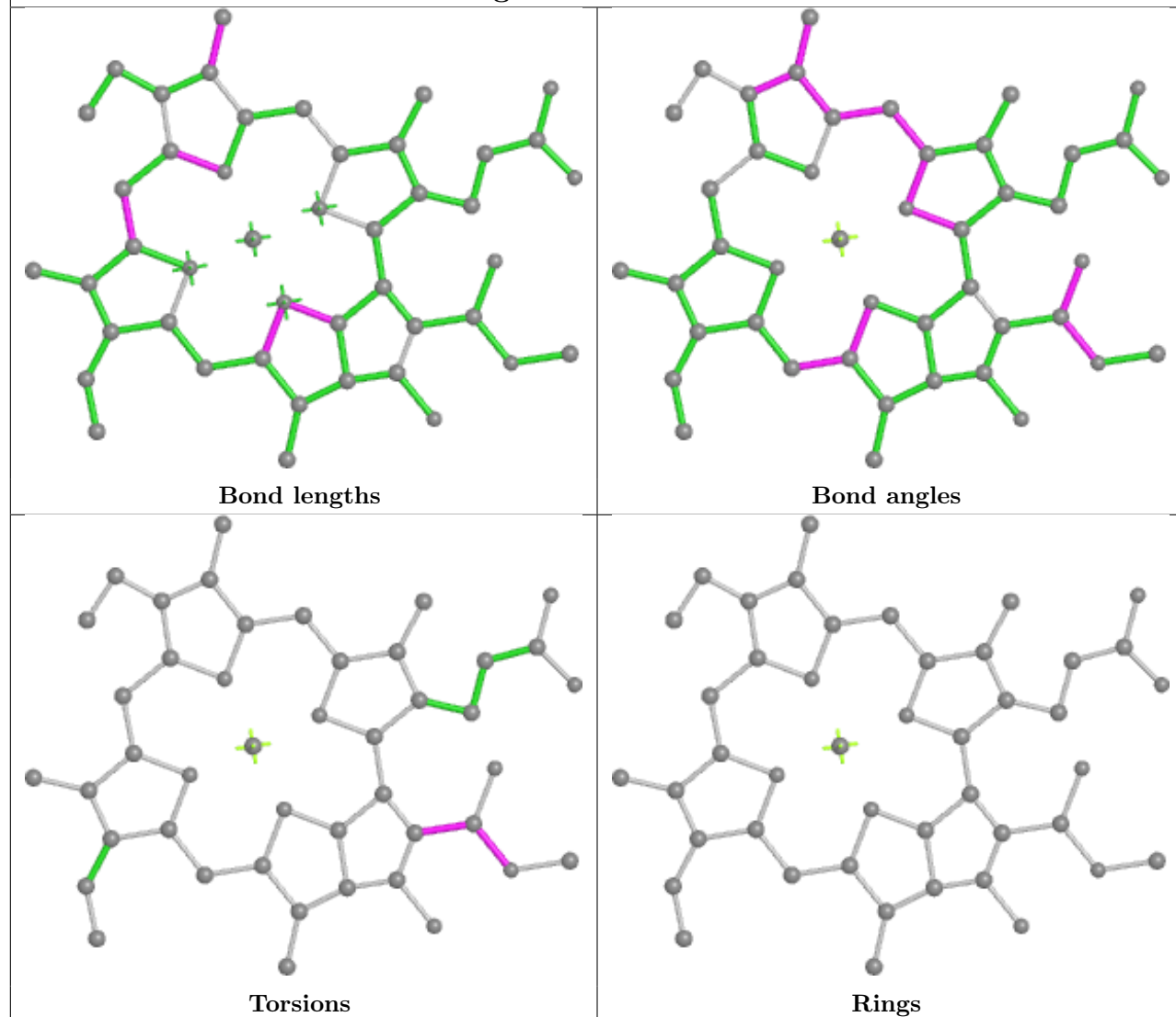
Torsions



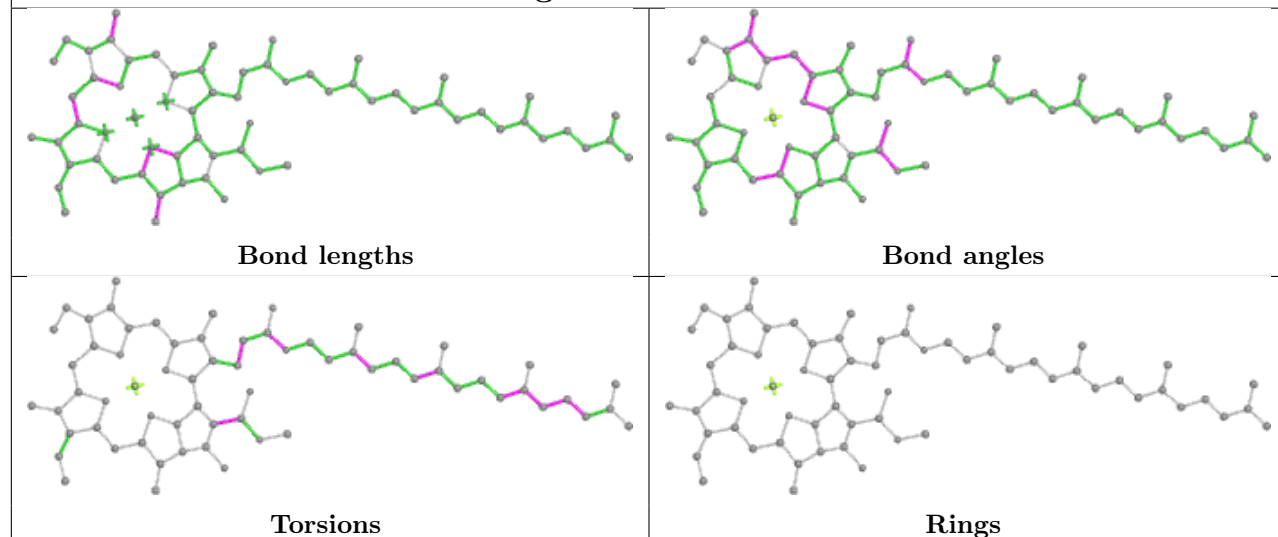
Rings

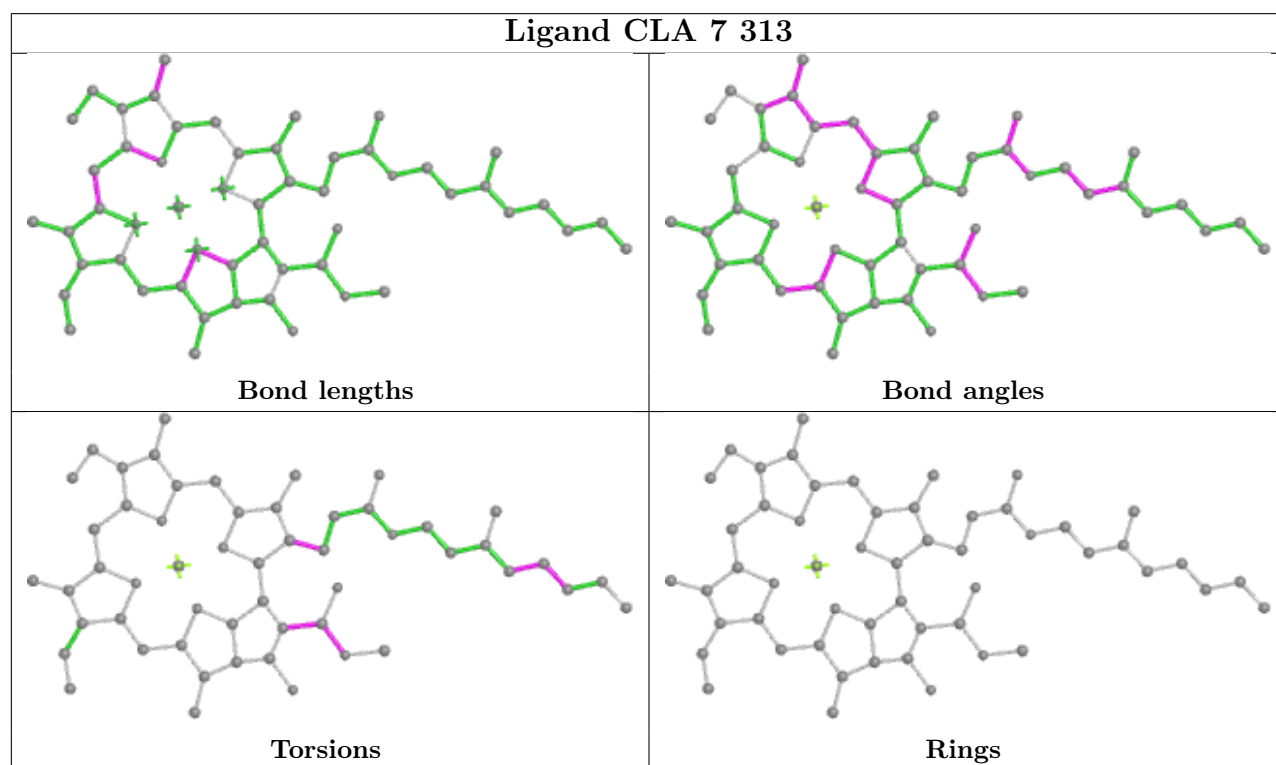
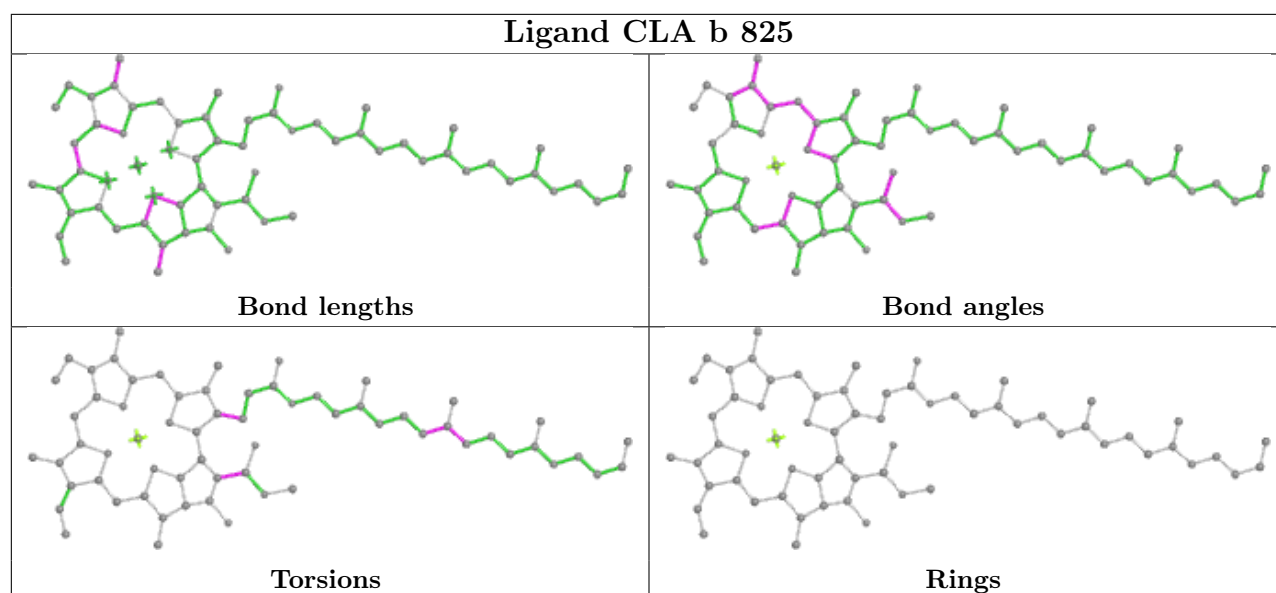


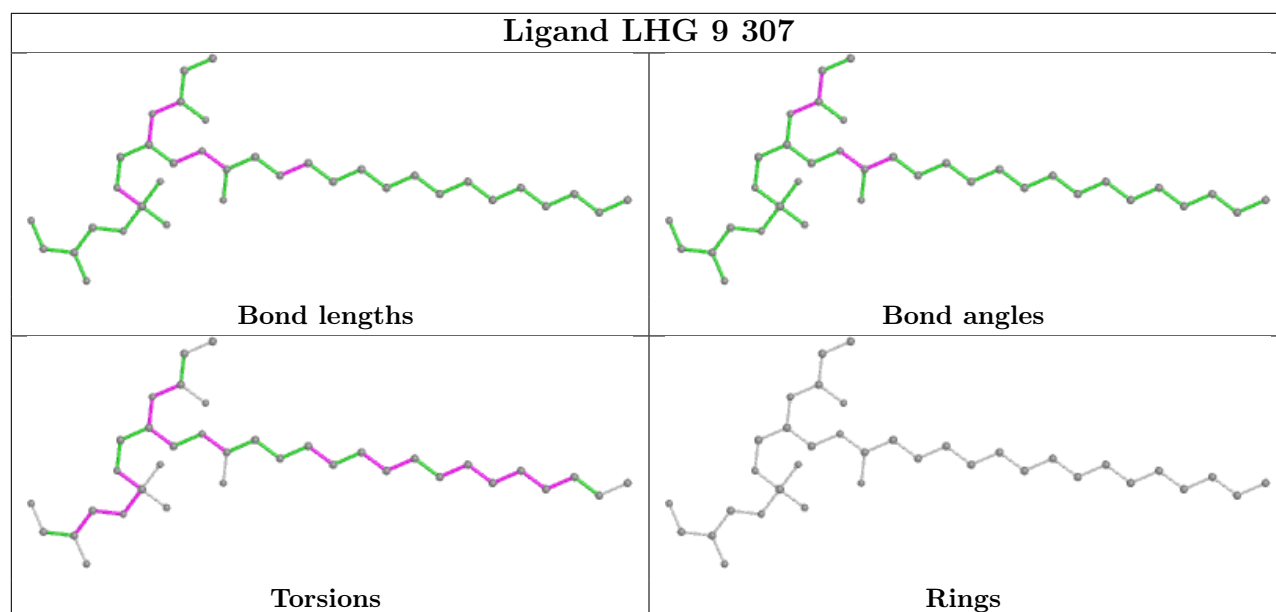
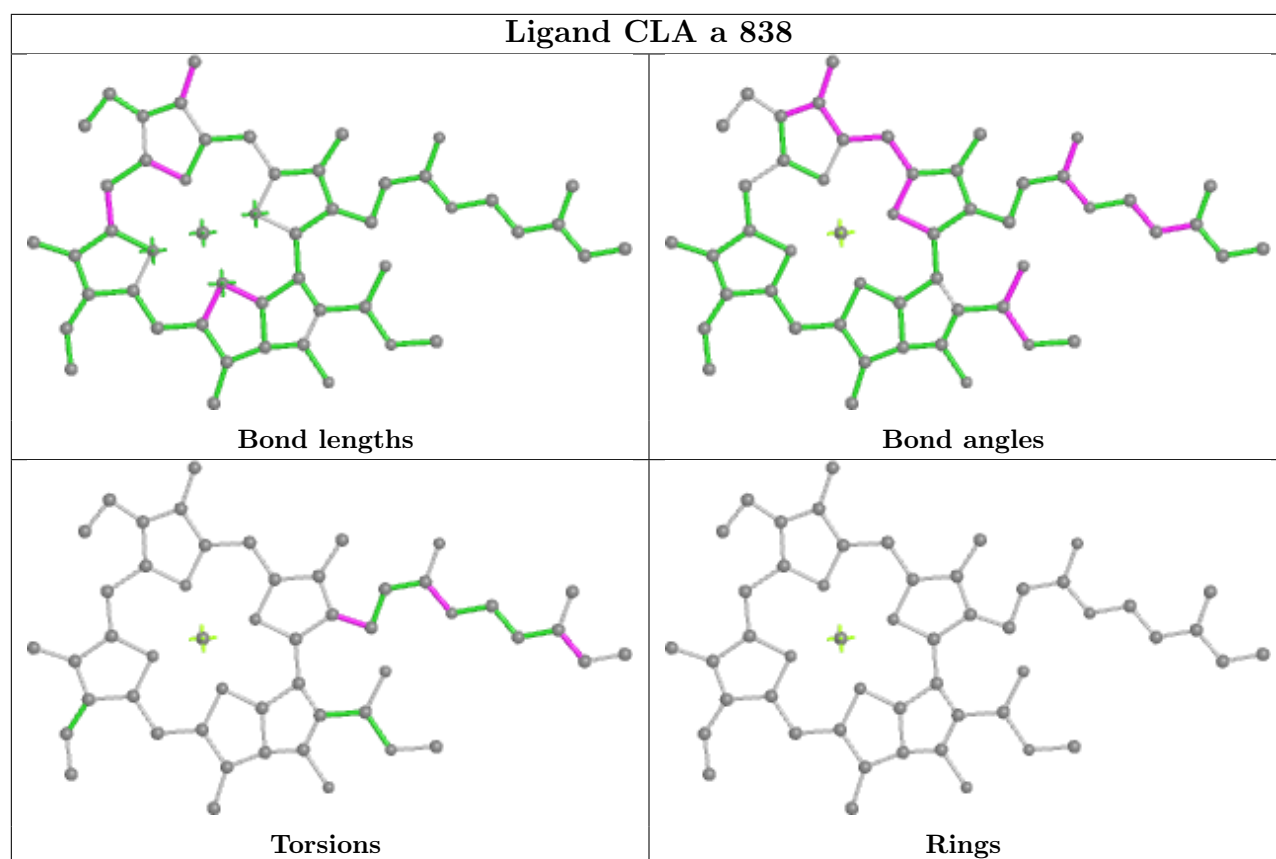
## Ligand CLA a 837

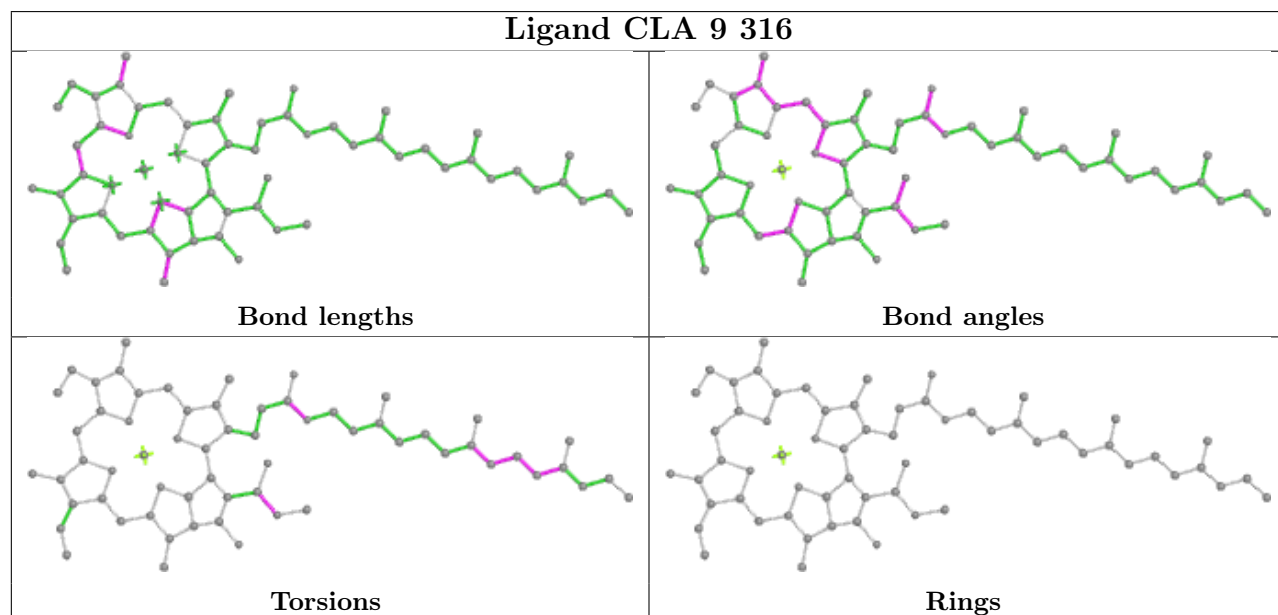
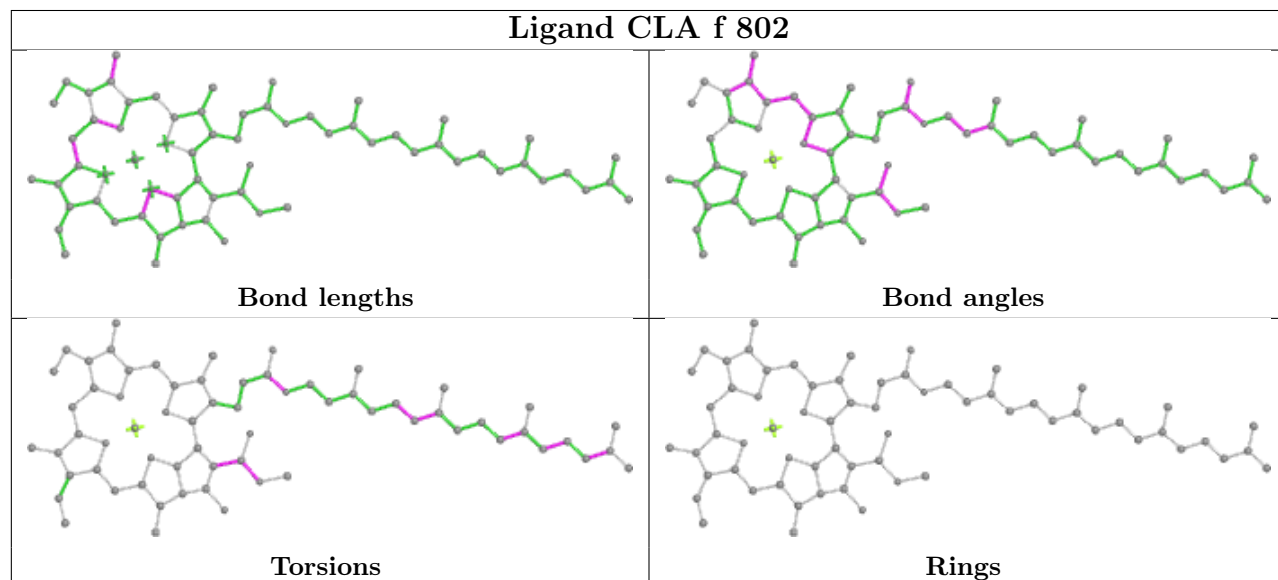
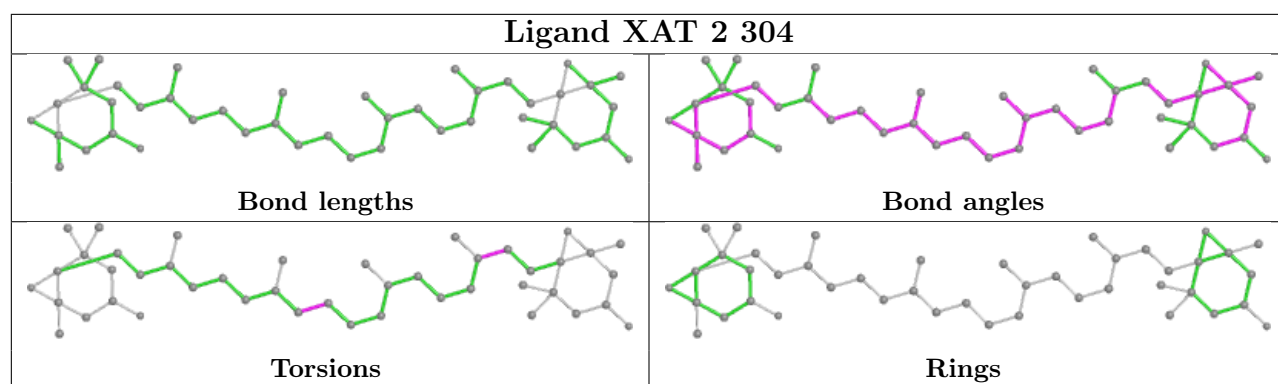


## Ligand CLA b 839

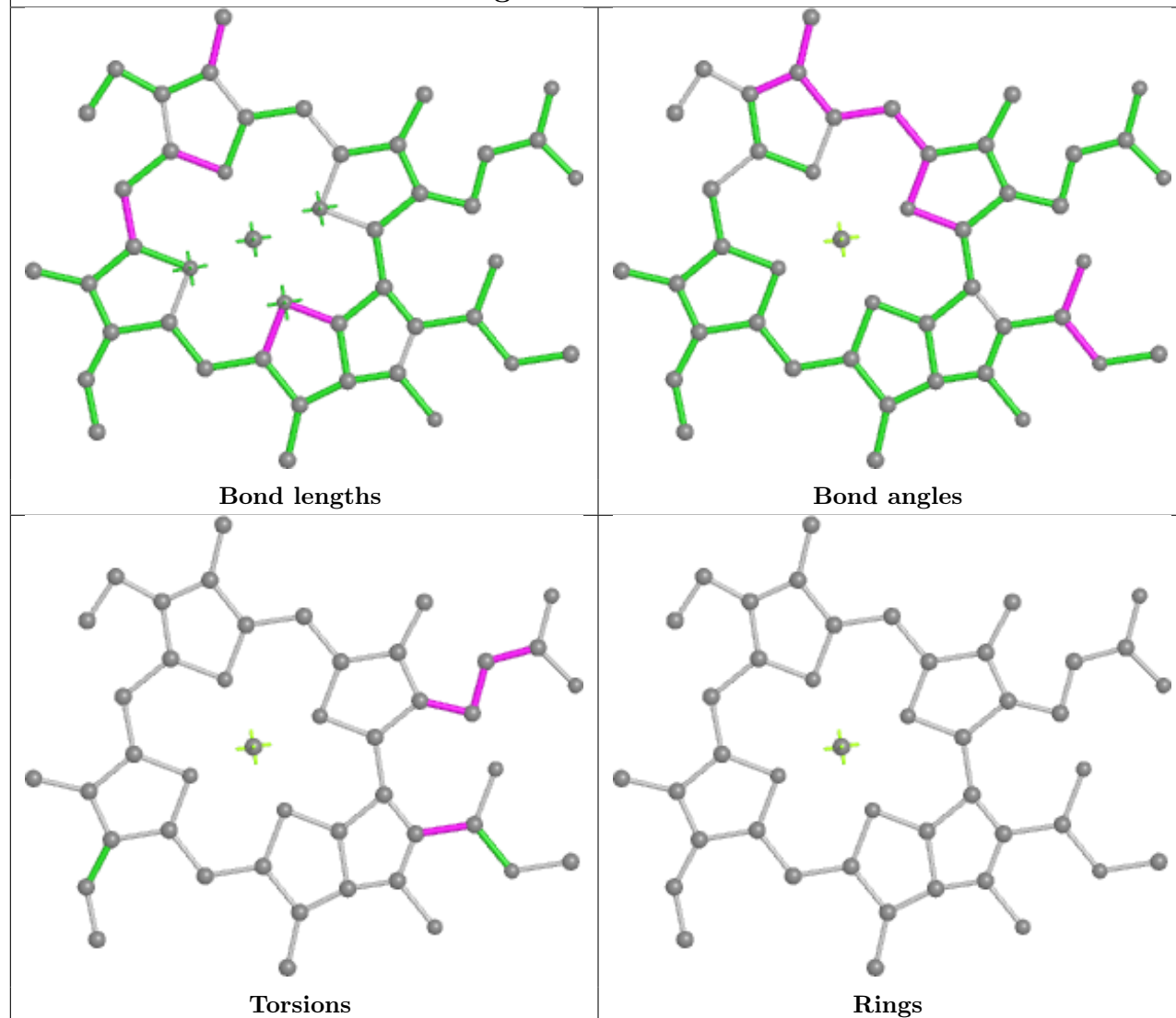




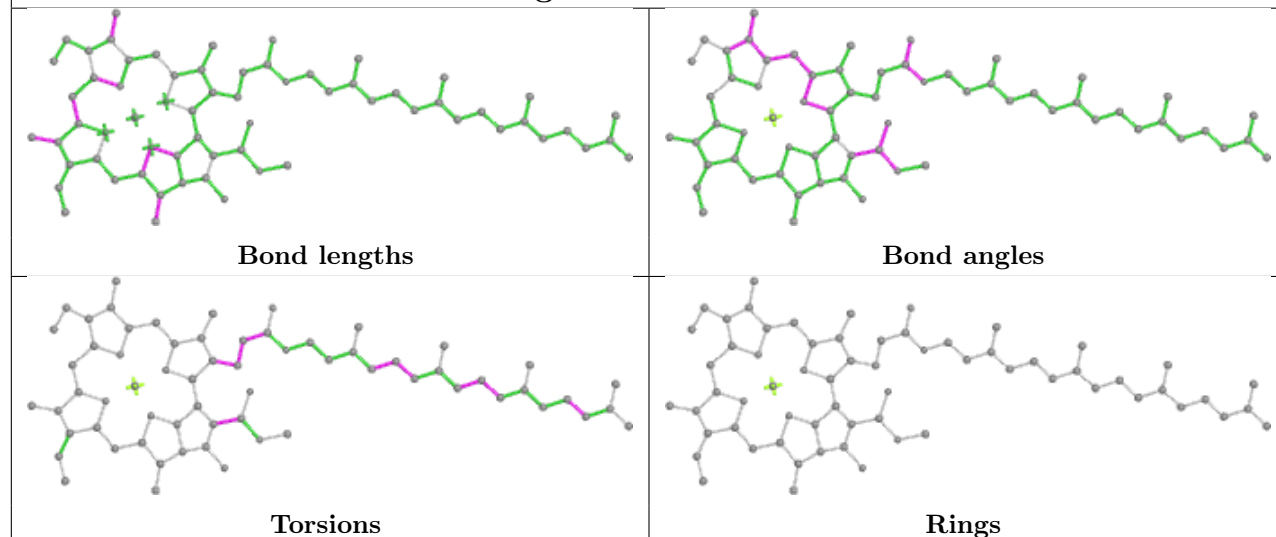




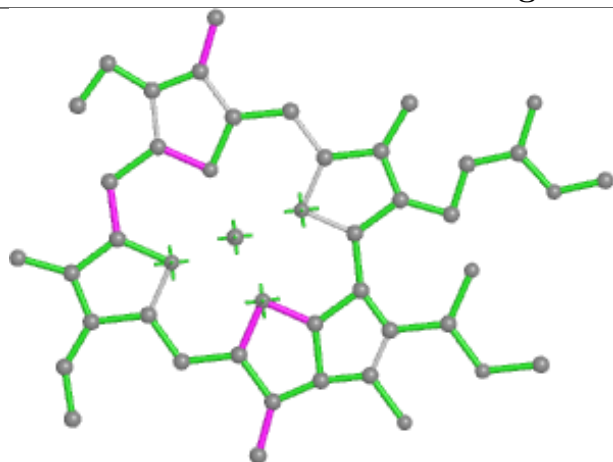
## Ligand CLA a 817



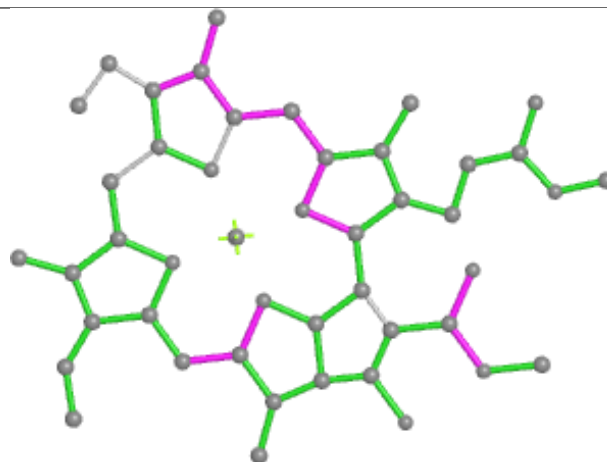
## Ligand CLA b 808



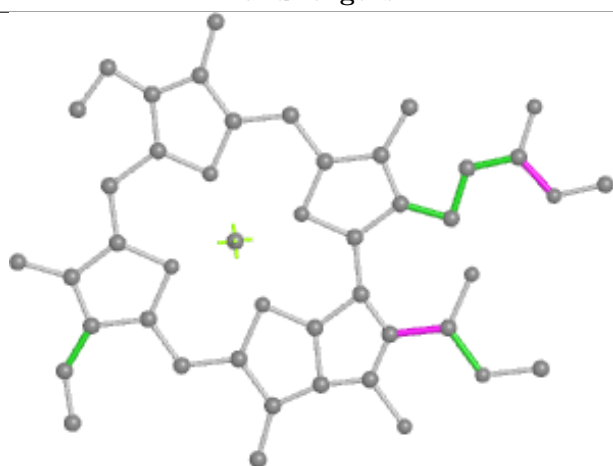
## Ligand CLA 9 309



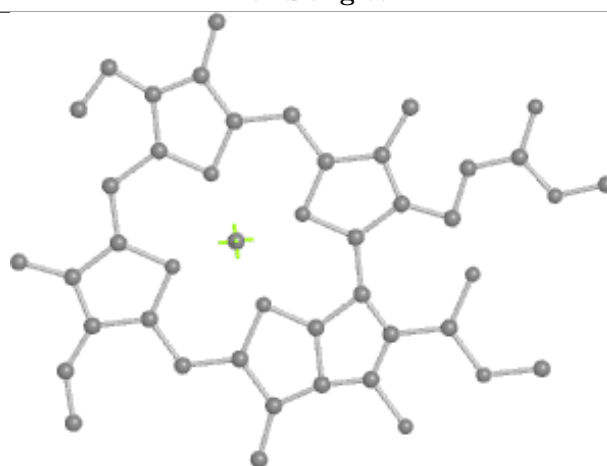
Bond lengths



Bond angles

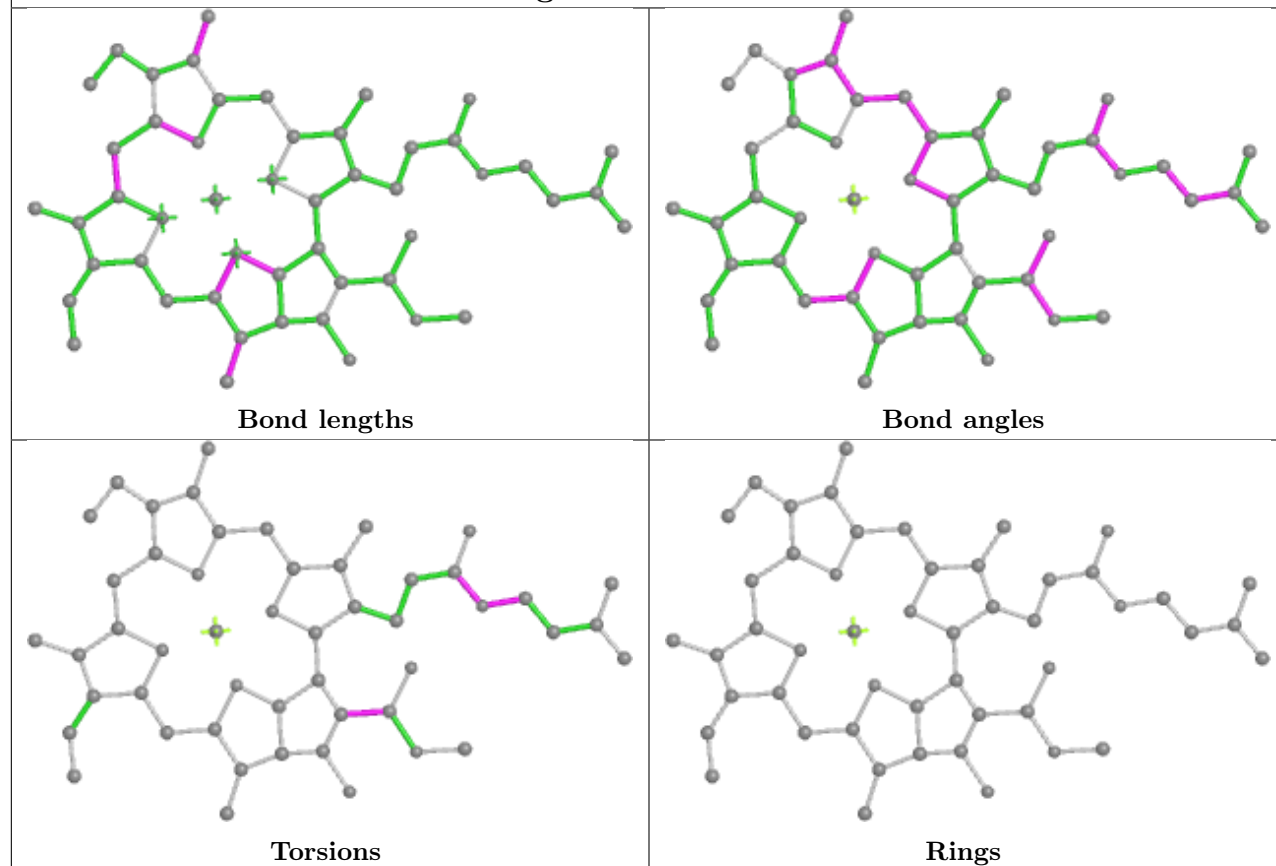


Torsions

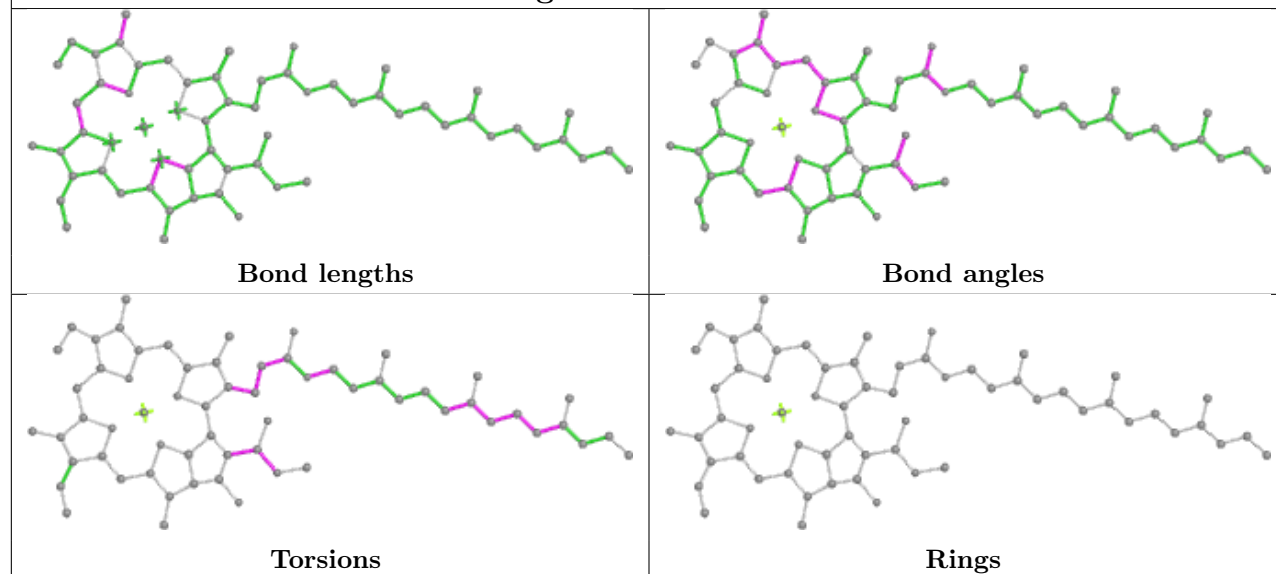


Rings

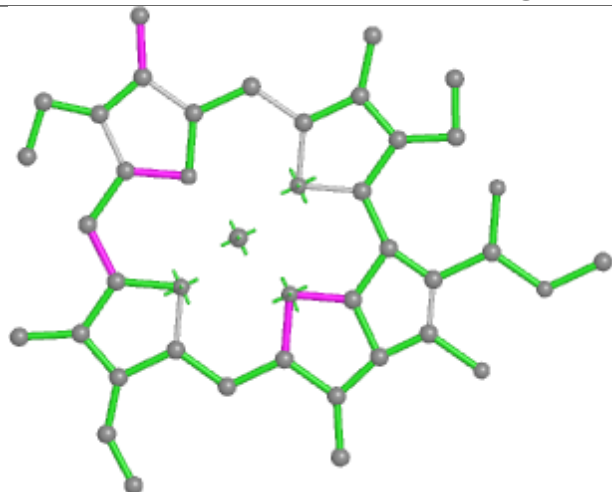
## Ligand CLA a 816



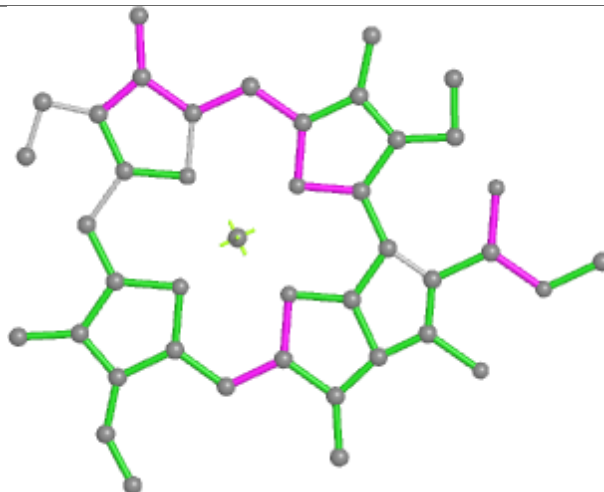
## Ligand CLA a 829



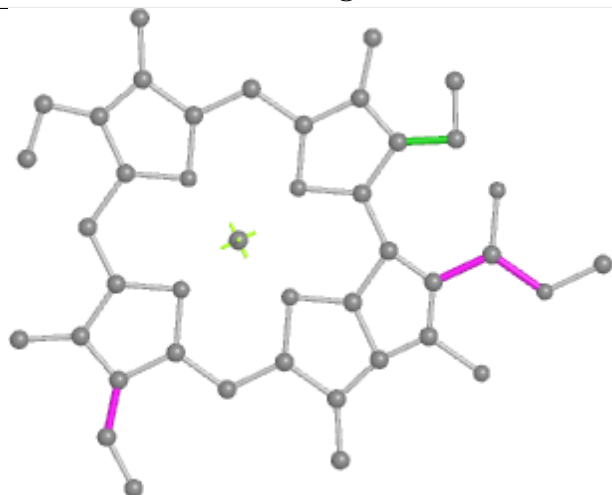
## Ligand CLA 9 315



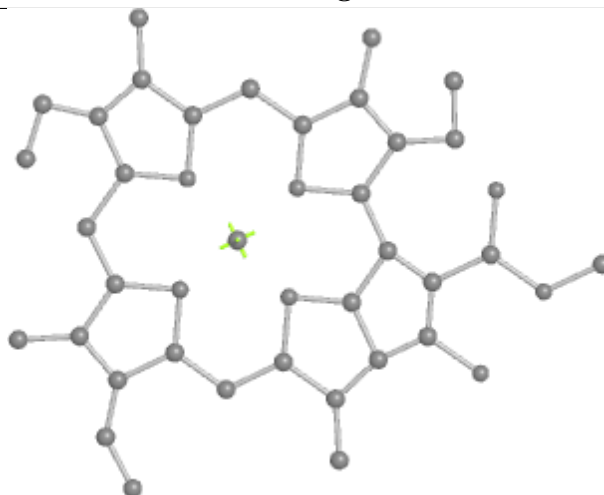
Bond lengths



Bond angles

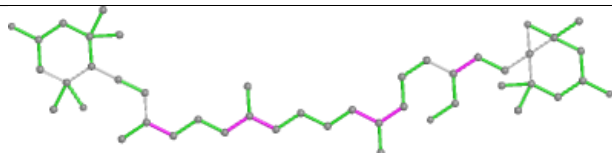


Torsions

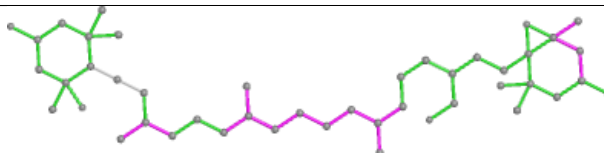


Rings

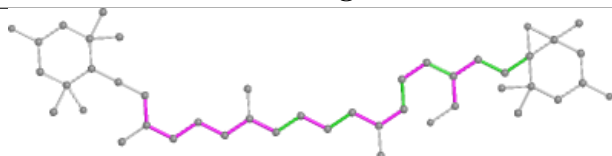
## Ligand A1L1G 3 306



Bond lengths



Bond angles

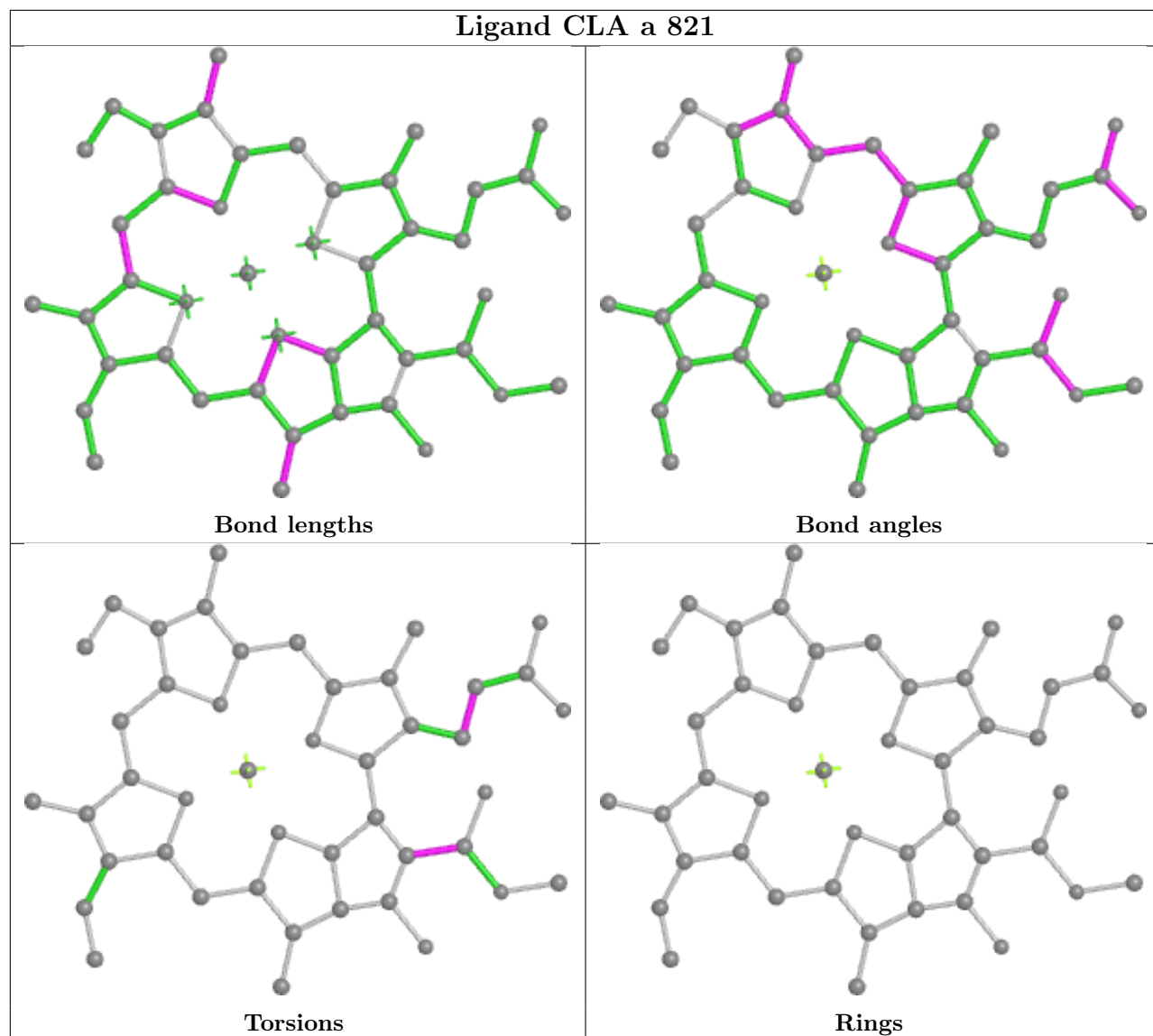


Torsions

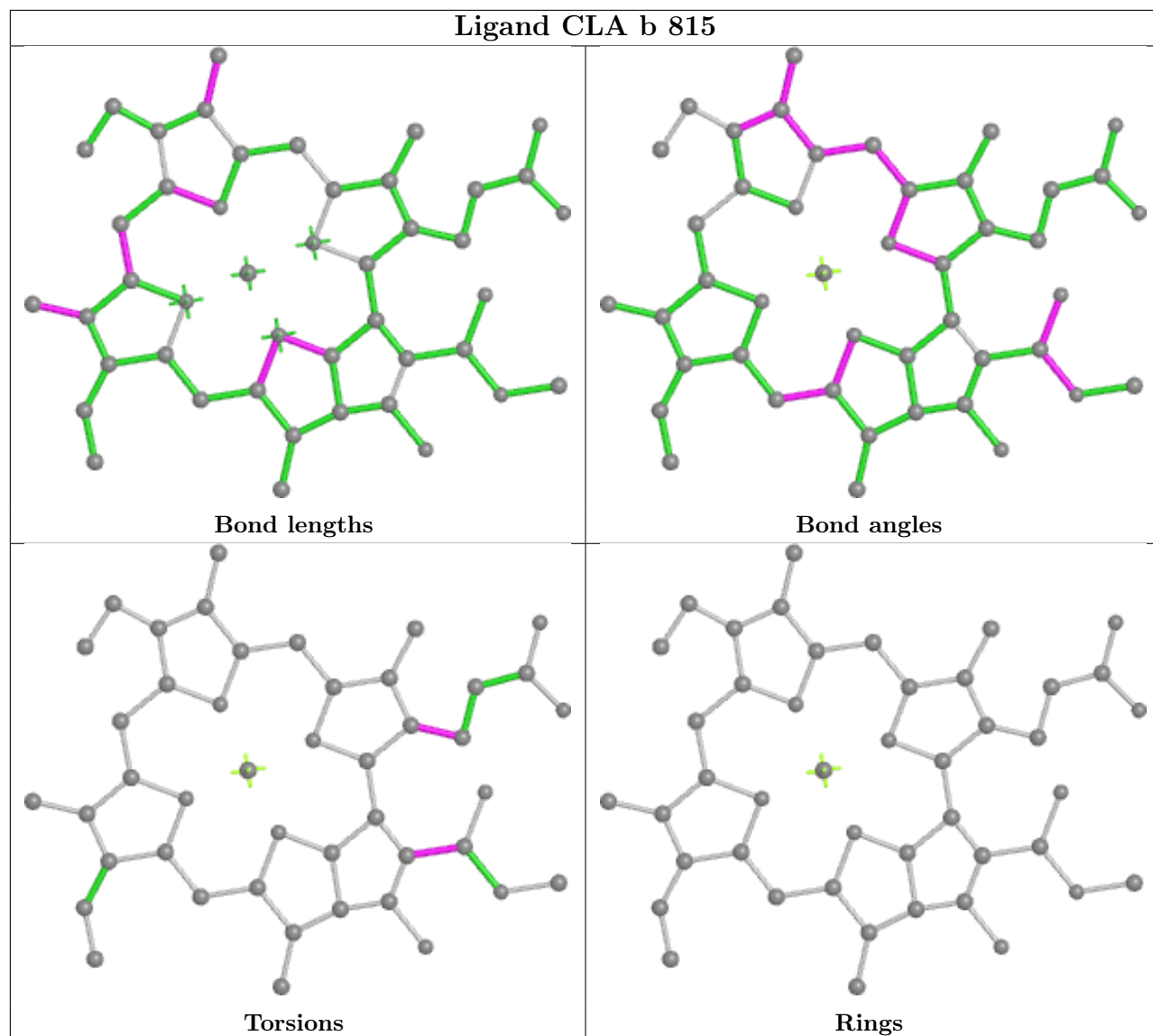


Rings

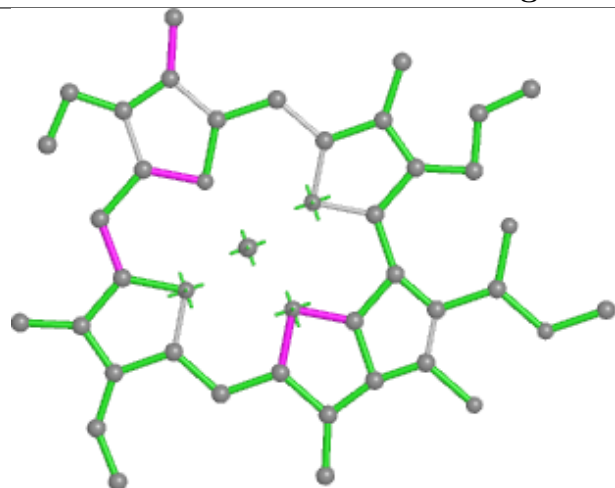
## Ligand CLA a 821



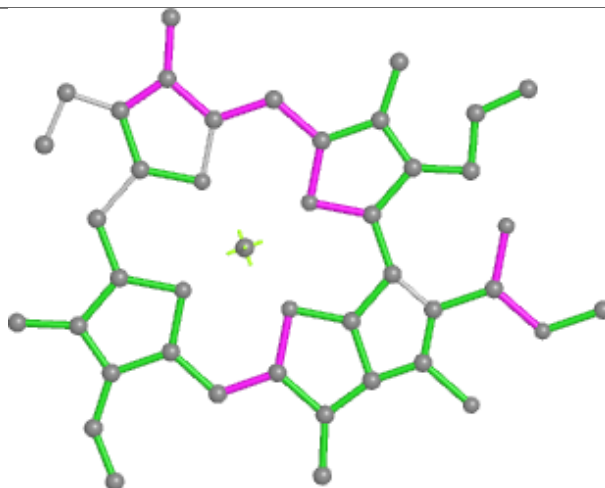
## Ligand CLA b 815



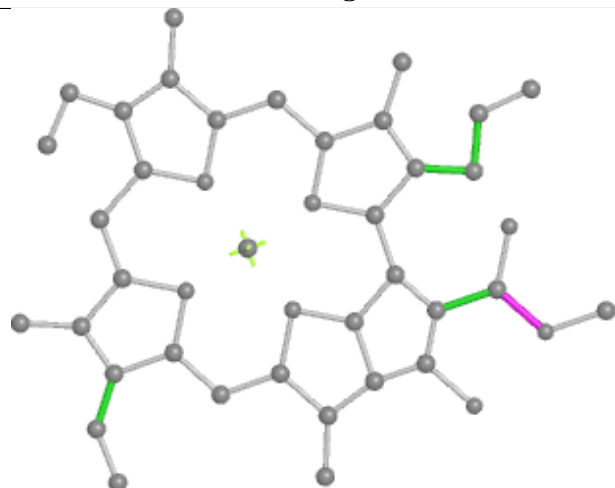
## Ligand CLA 8 305



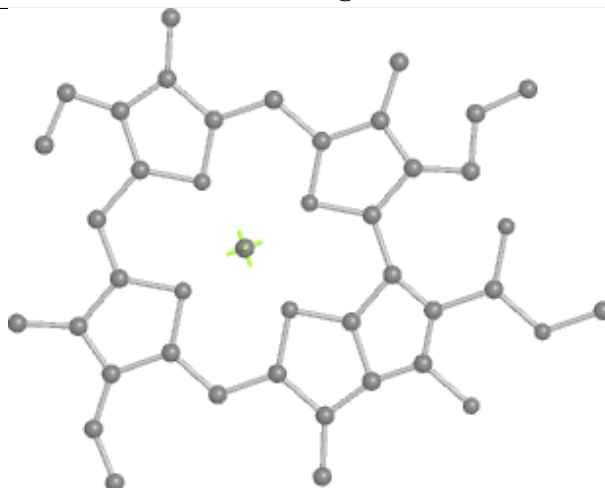
Bond lengths



Bond angles

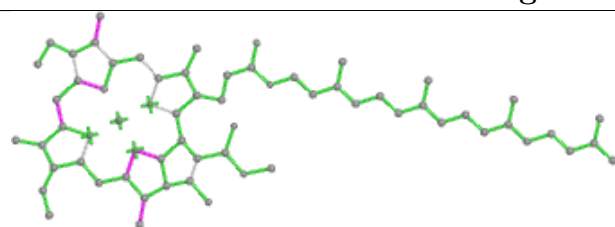


Torsions

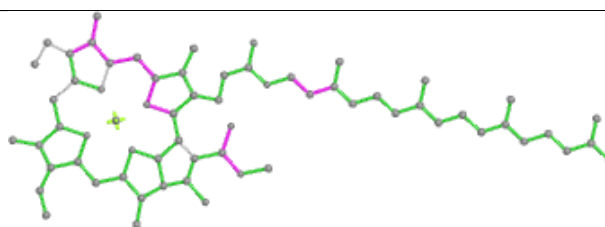


Rings

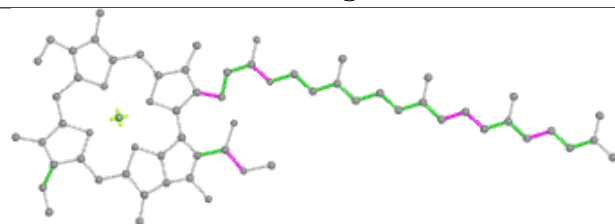
## Ligand CLA h 201



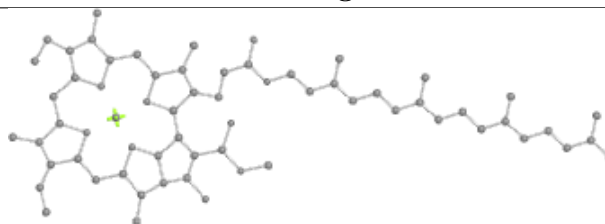
Bond lengths



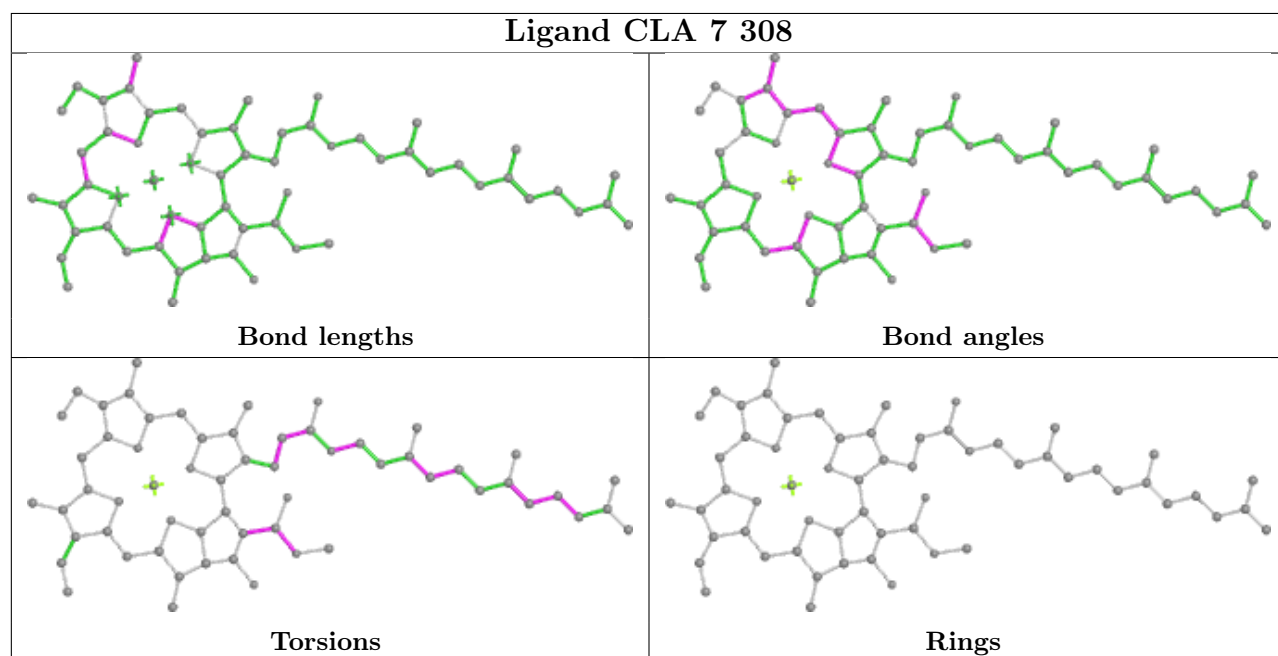
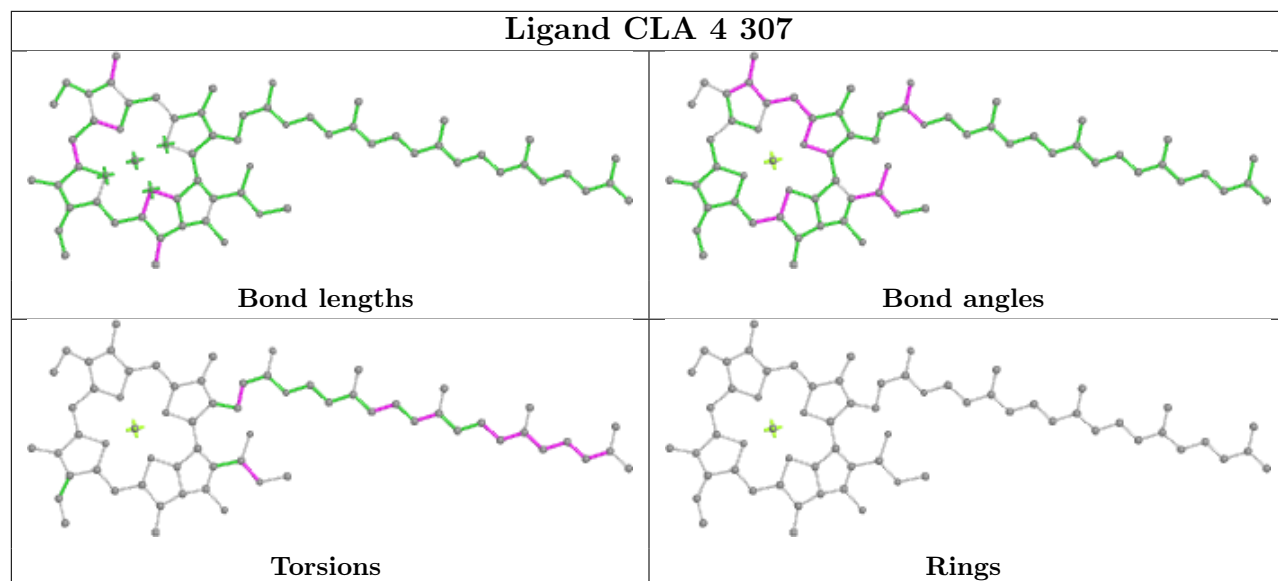
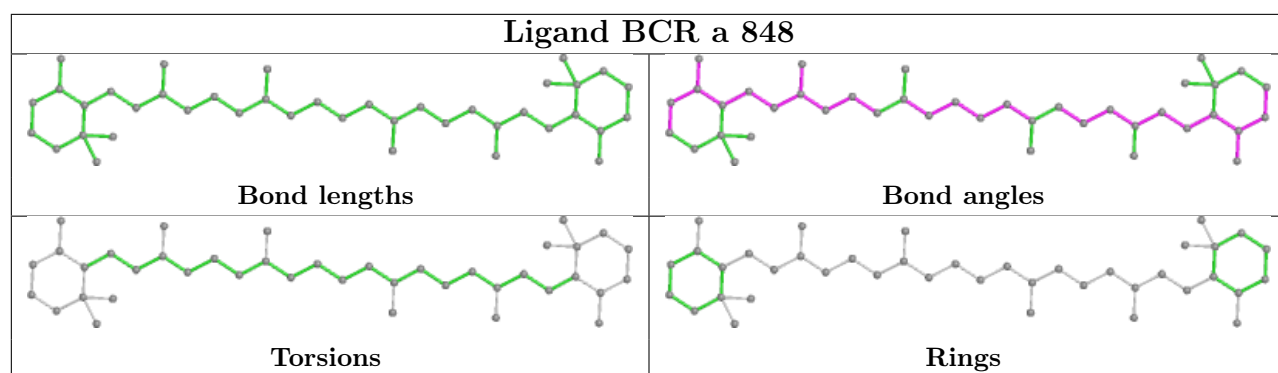
Bond angles

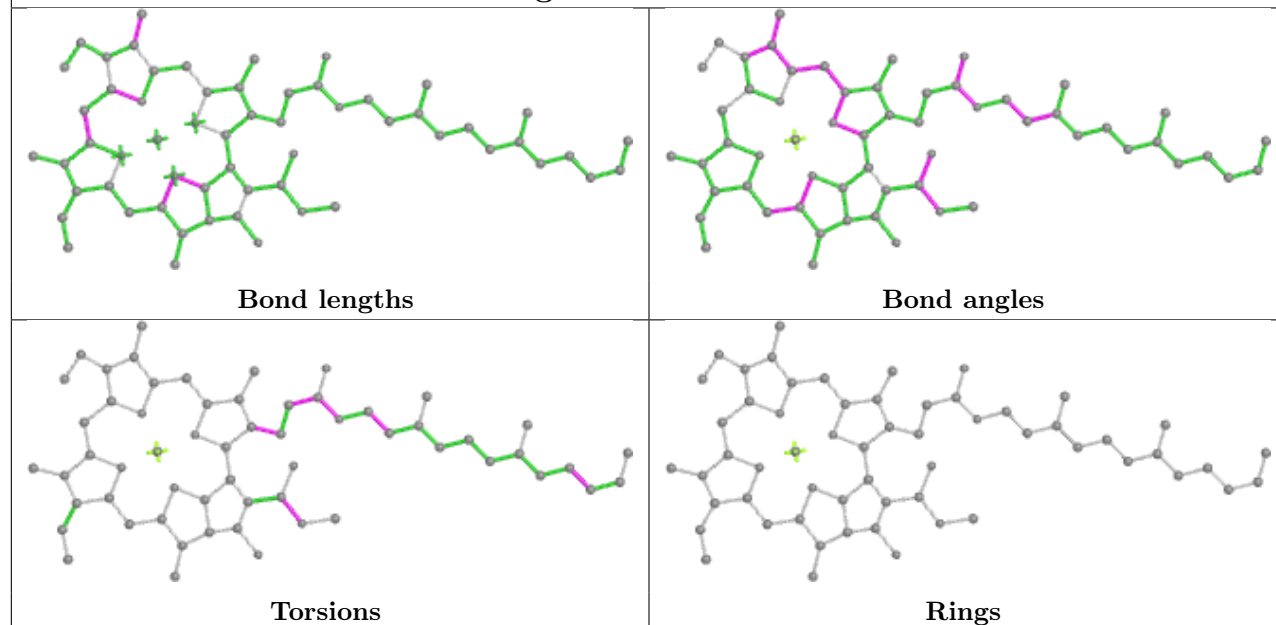
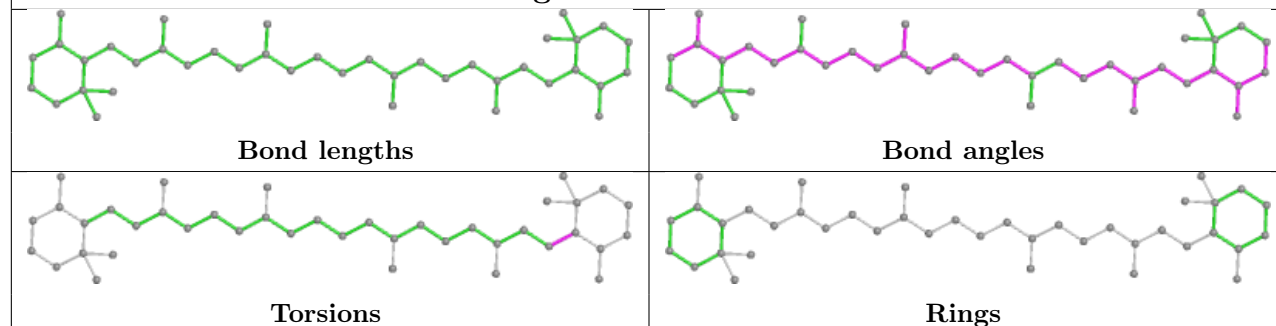


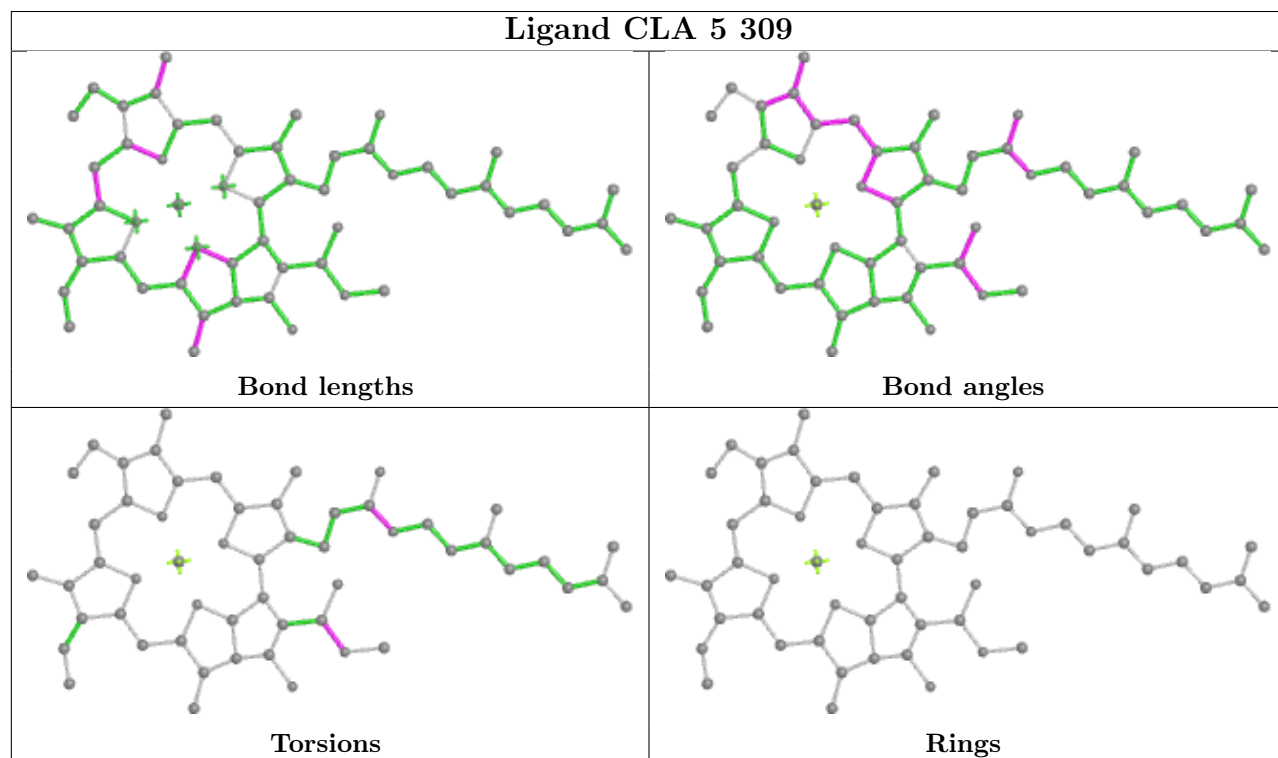
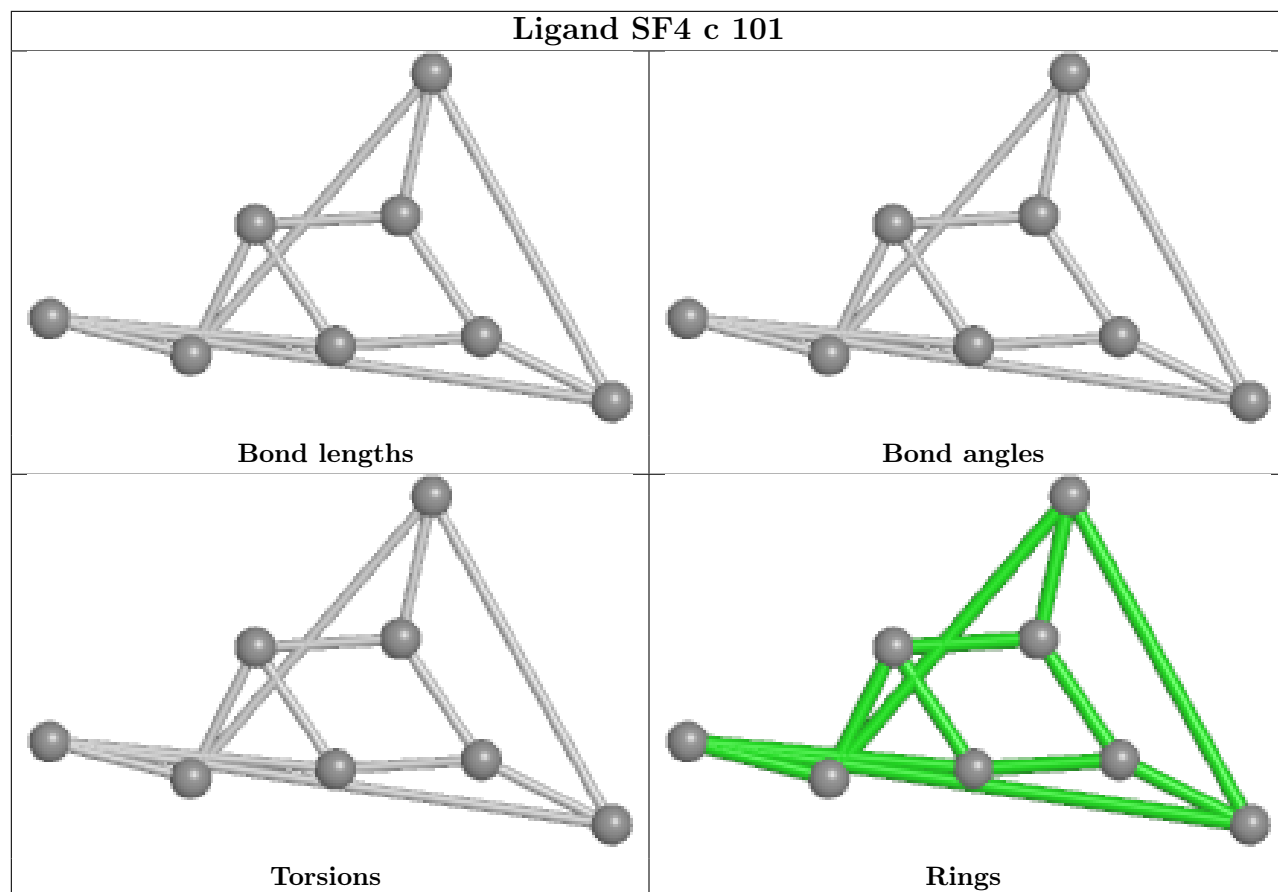
Torsions

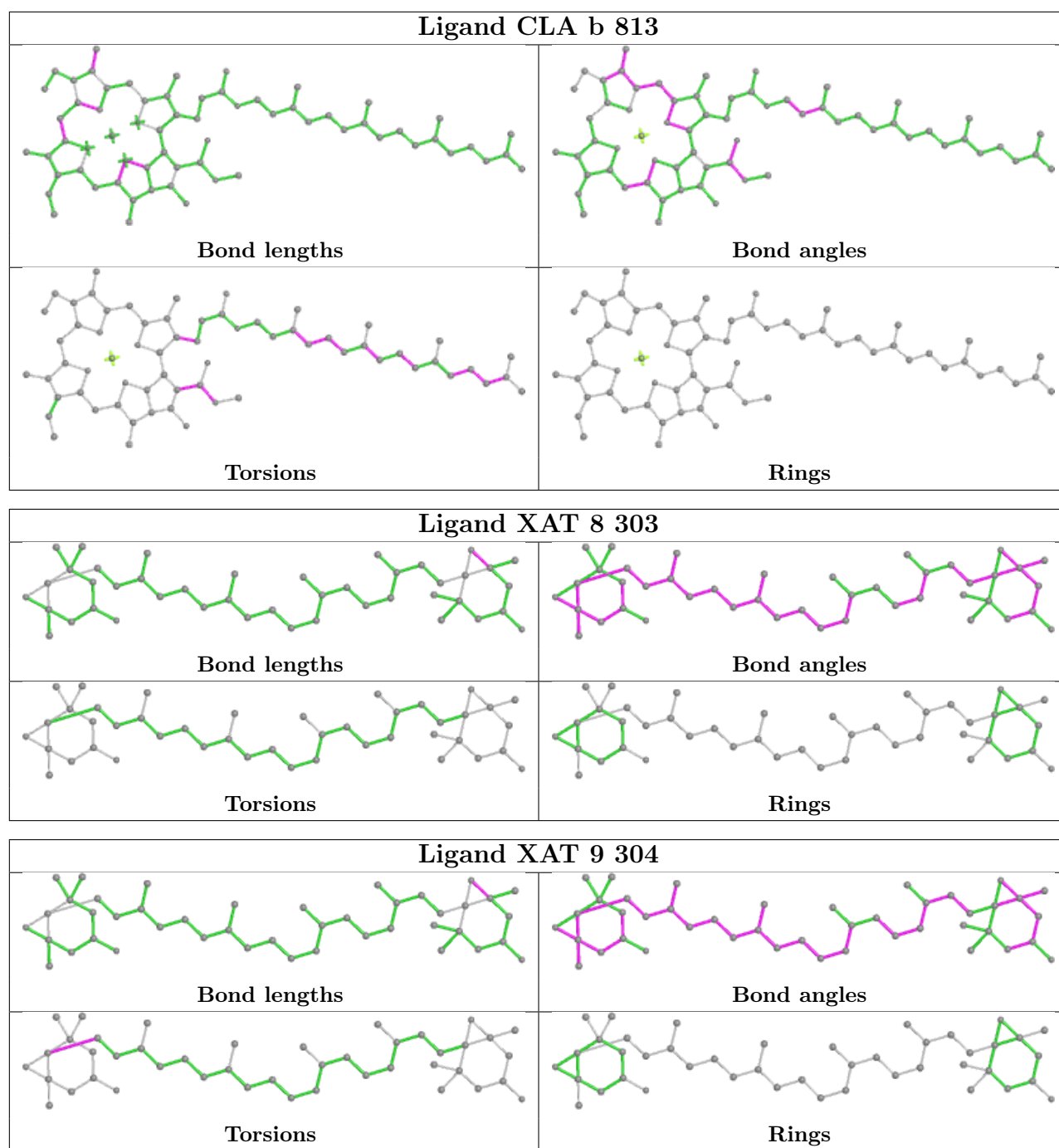


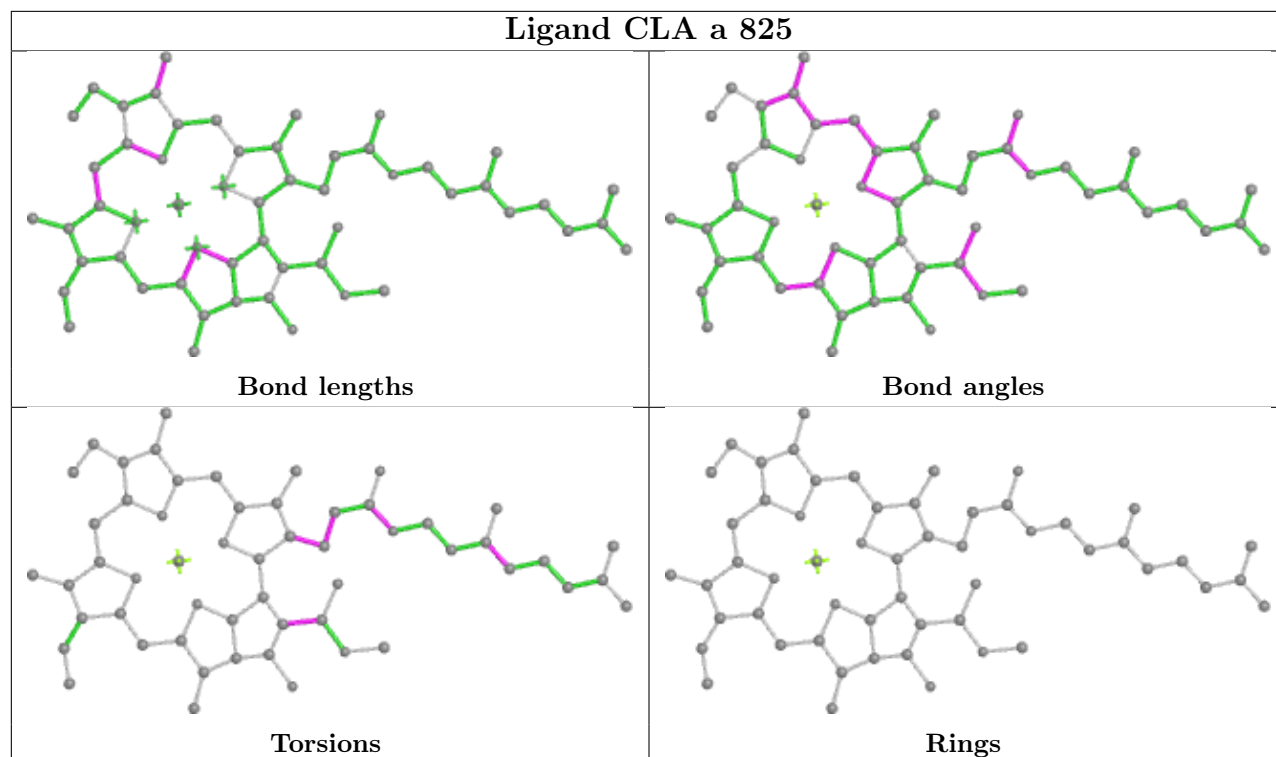
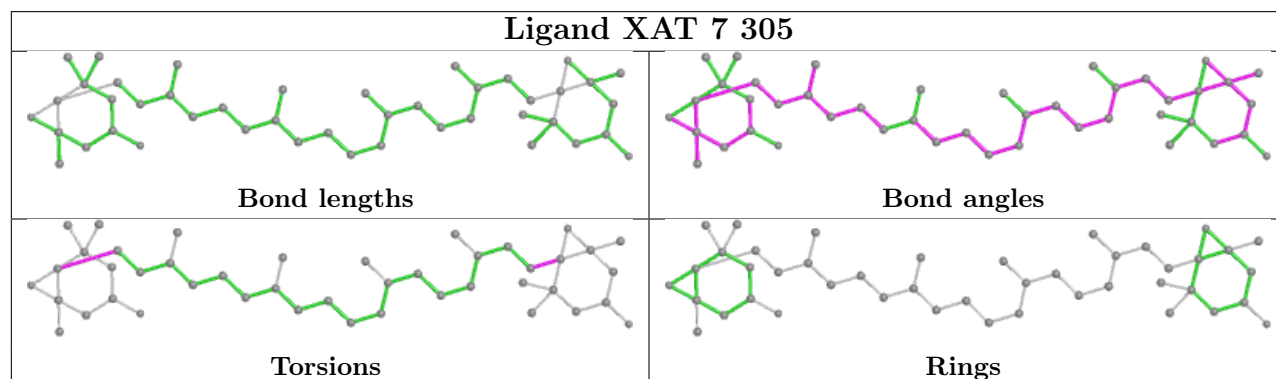
Rings

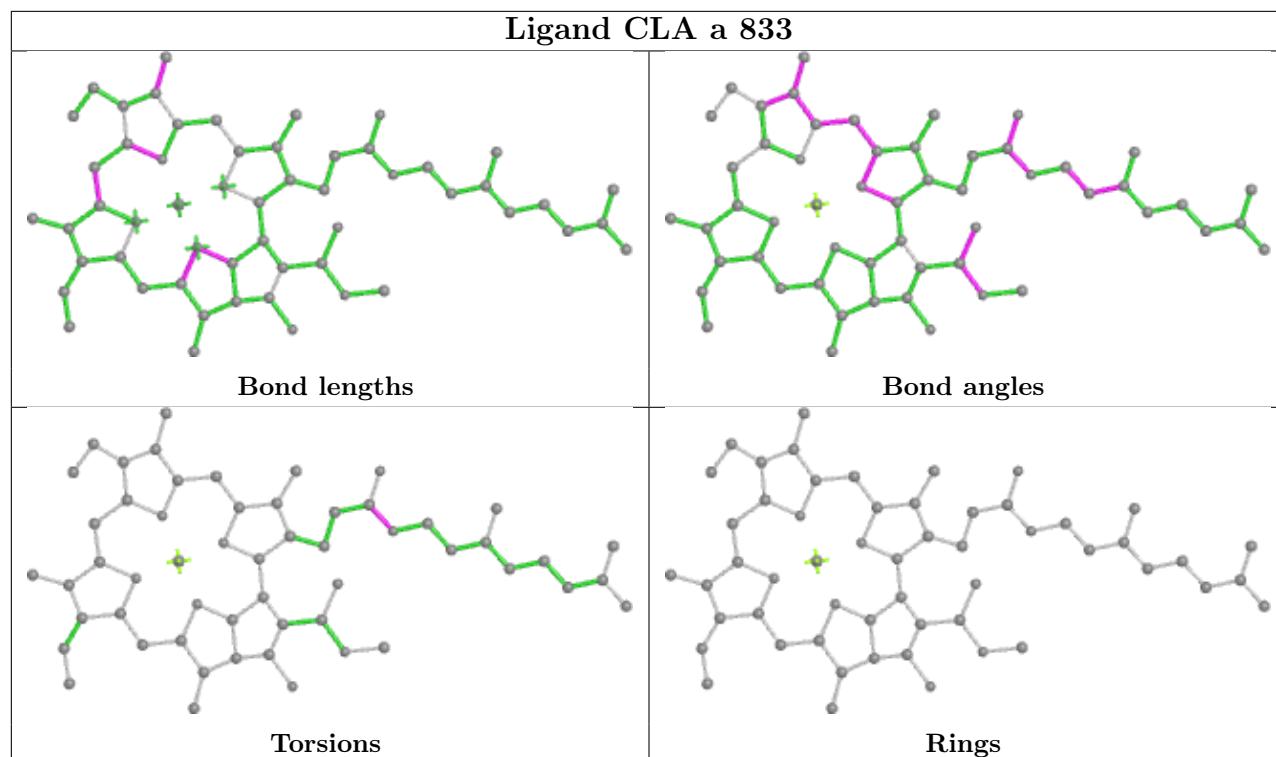
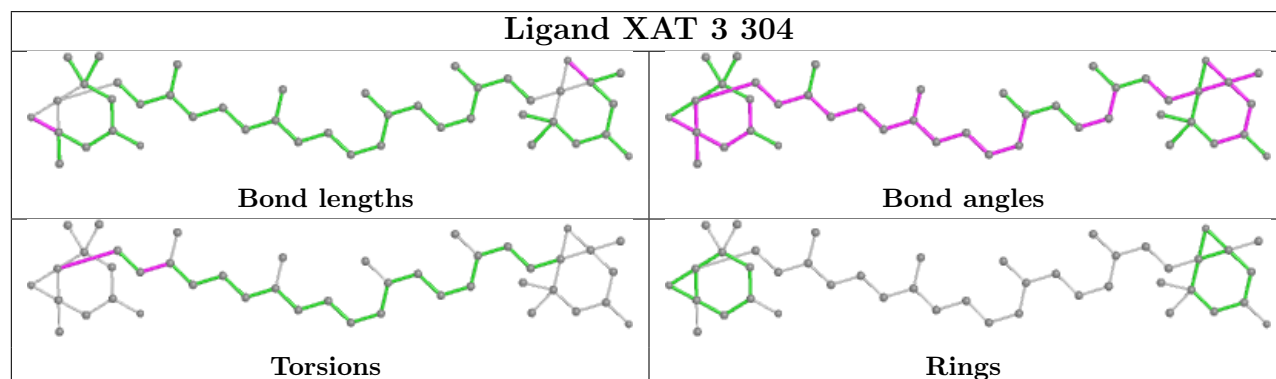


**Ligand CLA b 817****Ligand BCR b 850**

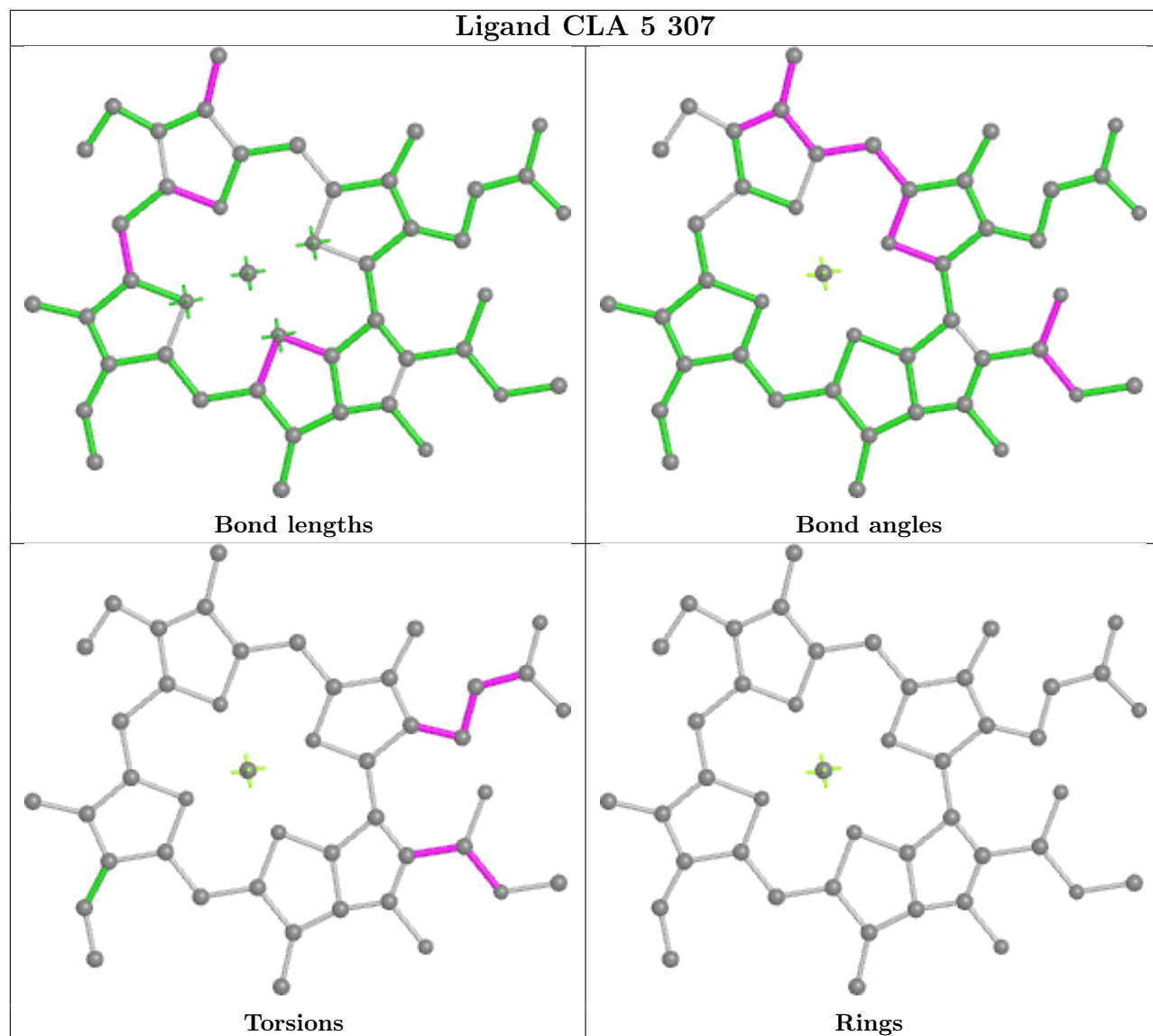


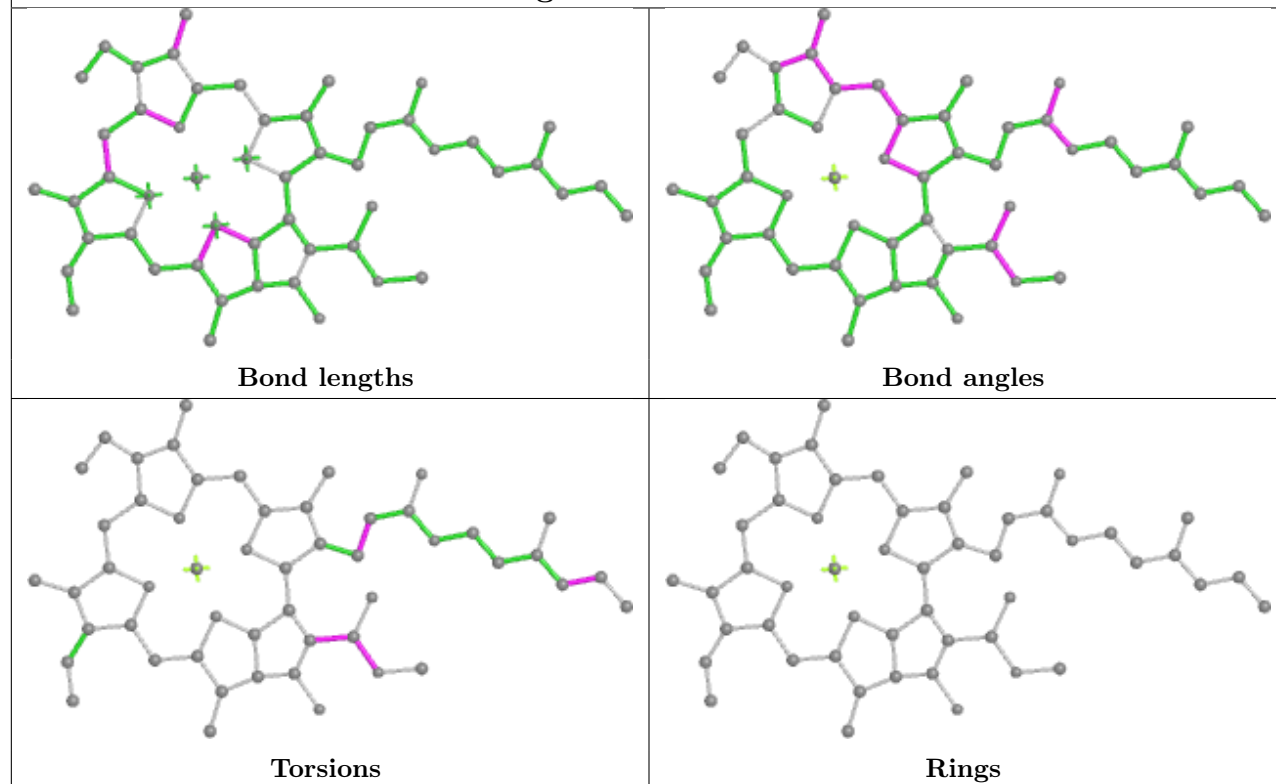
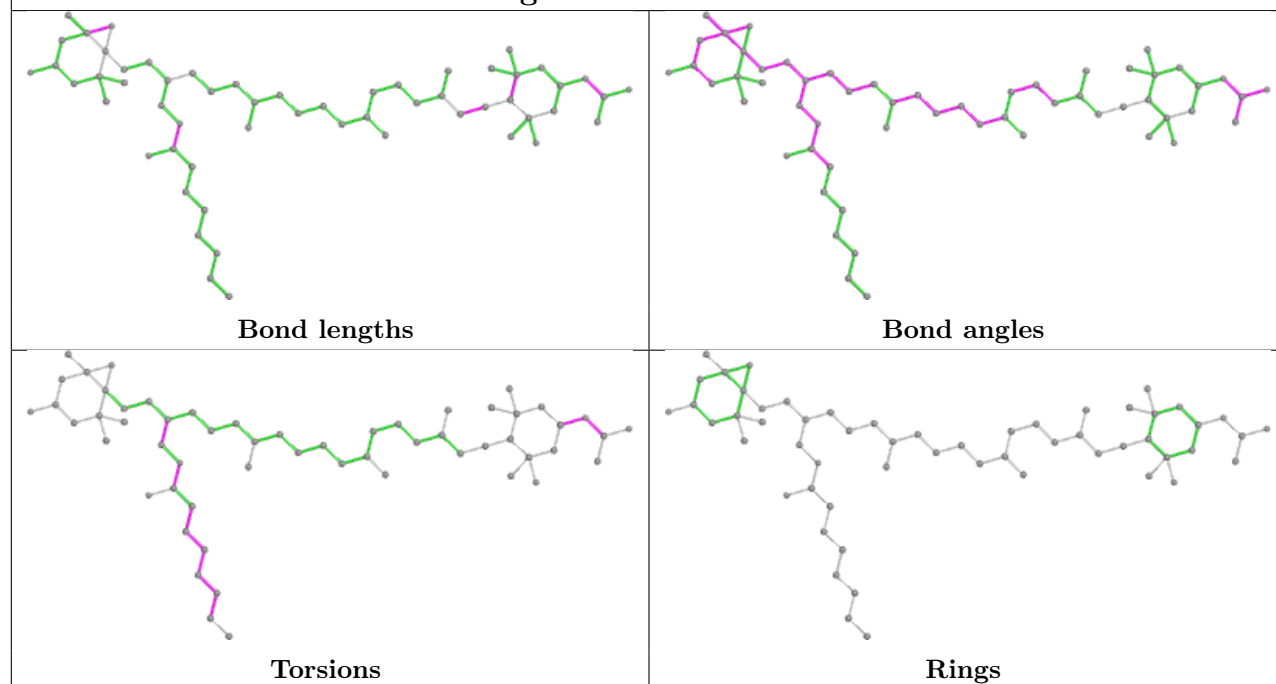


**Ligand CLA a 825****Ligand XAT 7 305**

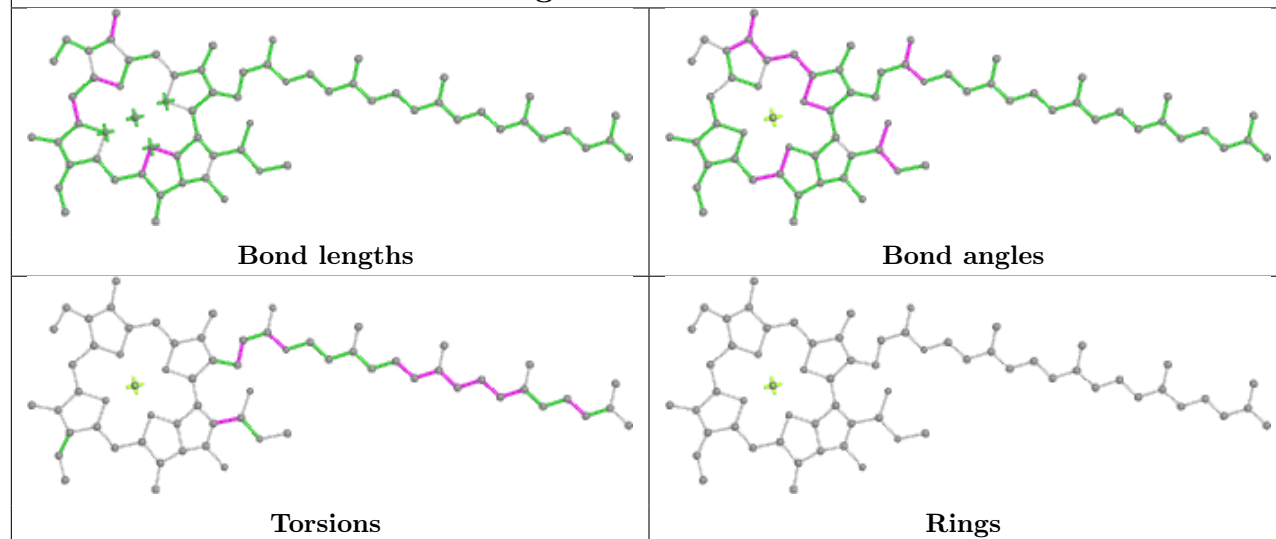
**Ligand CLA a 833****Ligand XAT 3 304**

## Ligand CLA 5 307

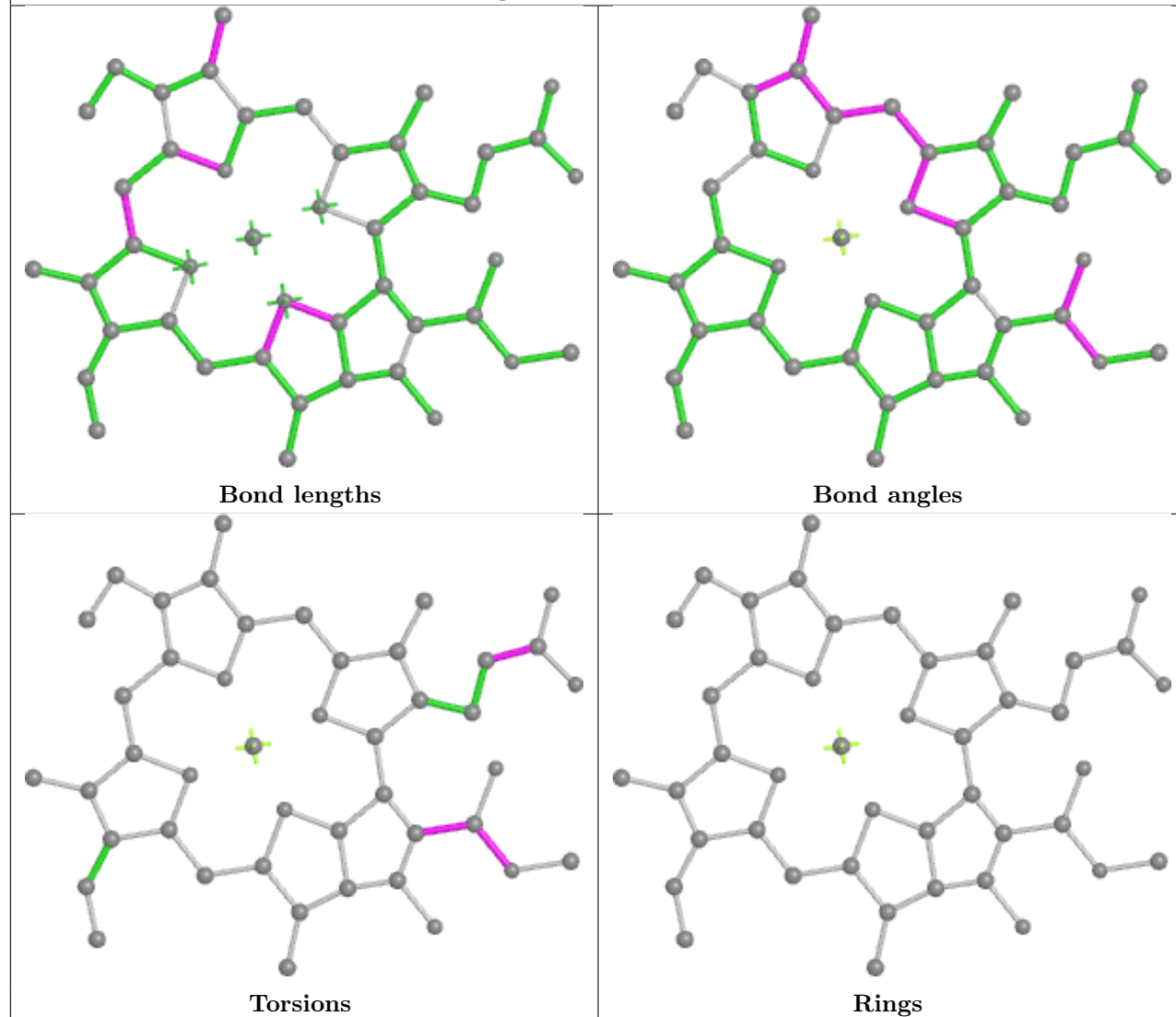


**Ligand CLA 6 310****Ligand A1L1F 9 302**

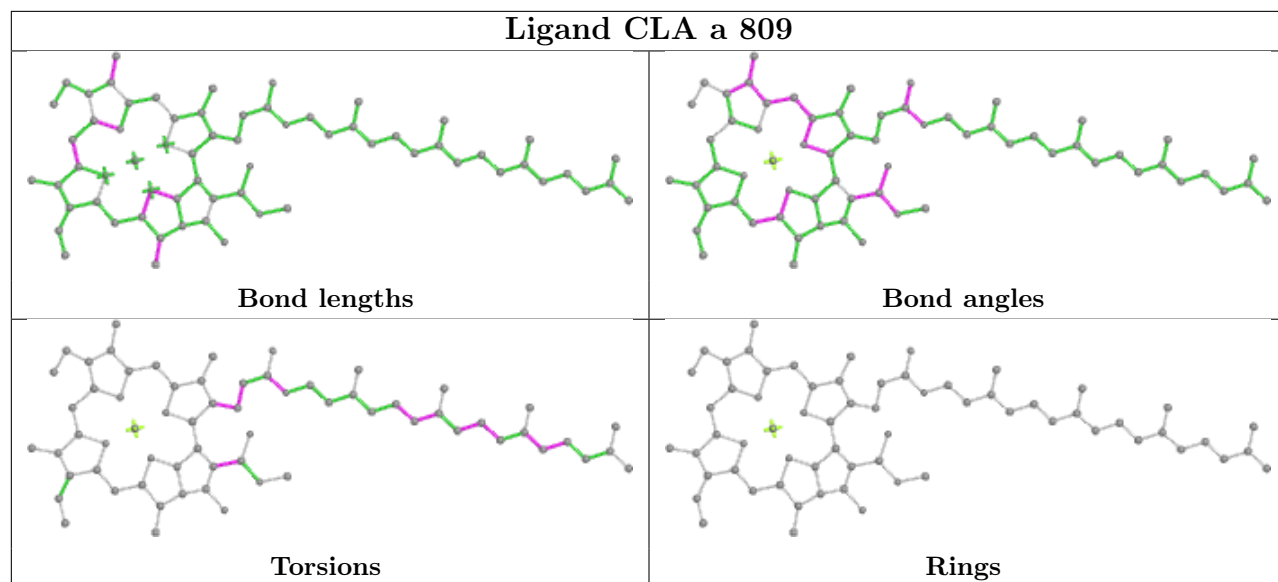
## Ligand CLA b 824



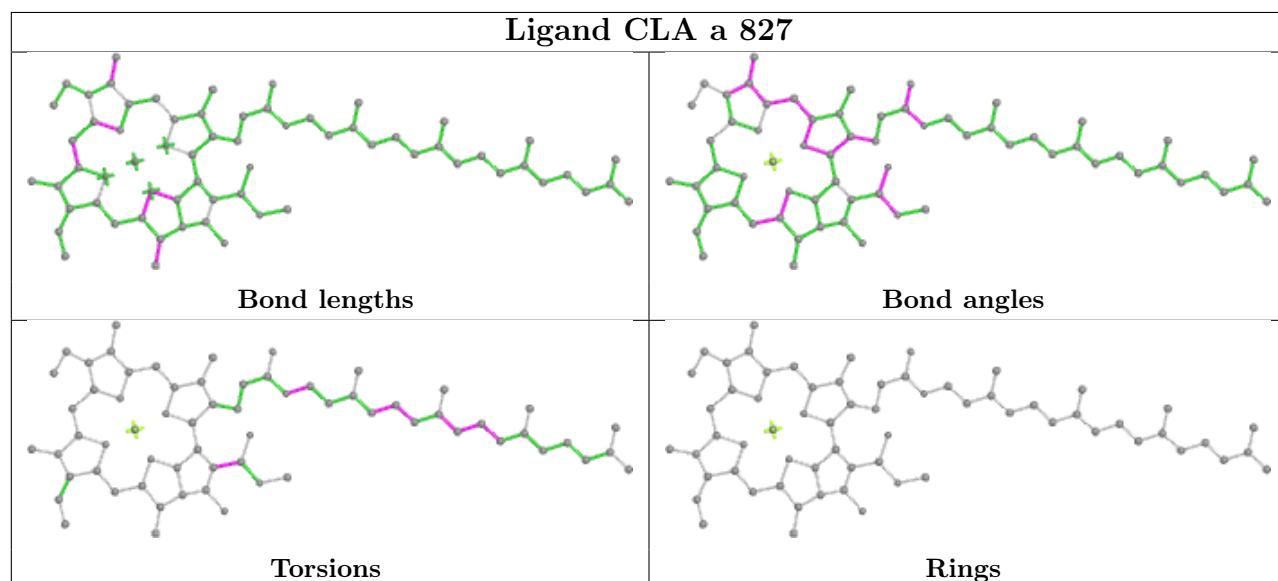
## Ligand CLA 5 314



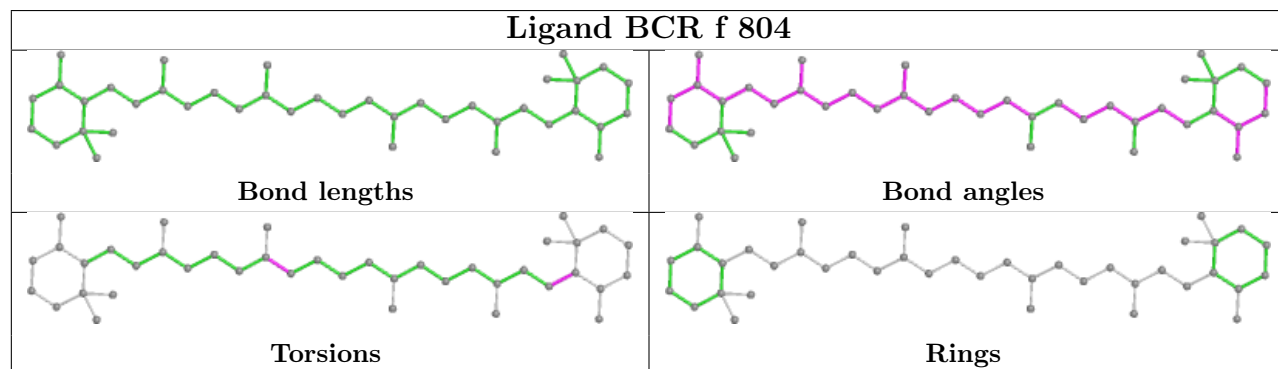
## Ligand CLA a 809

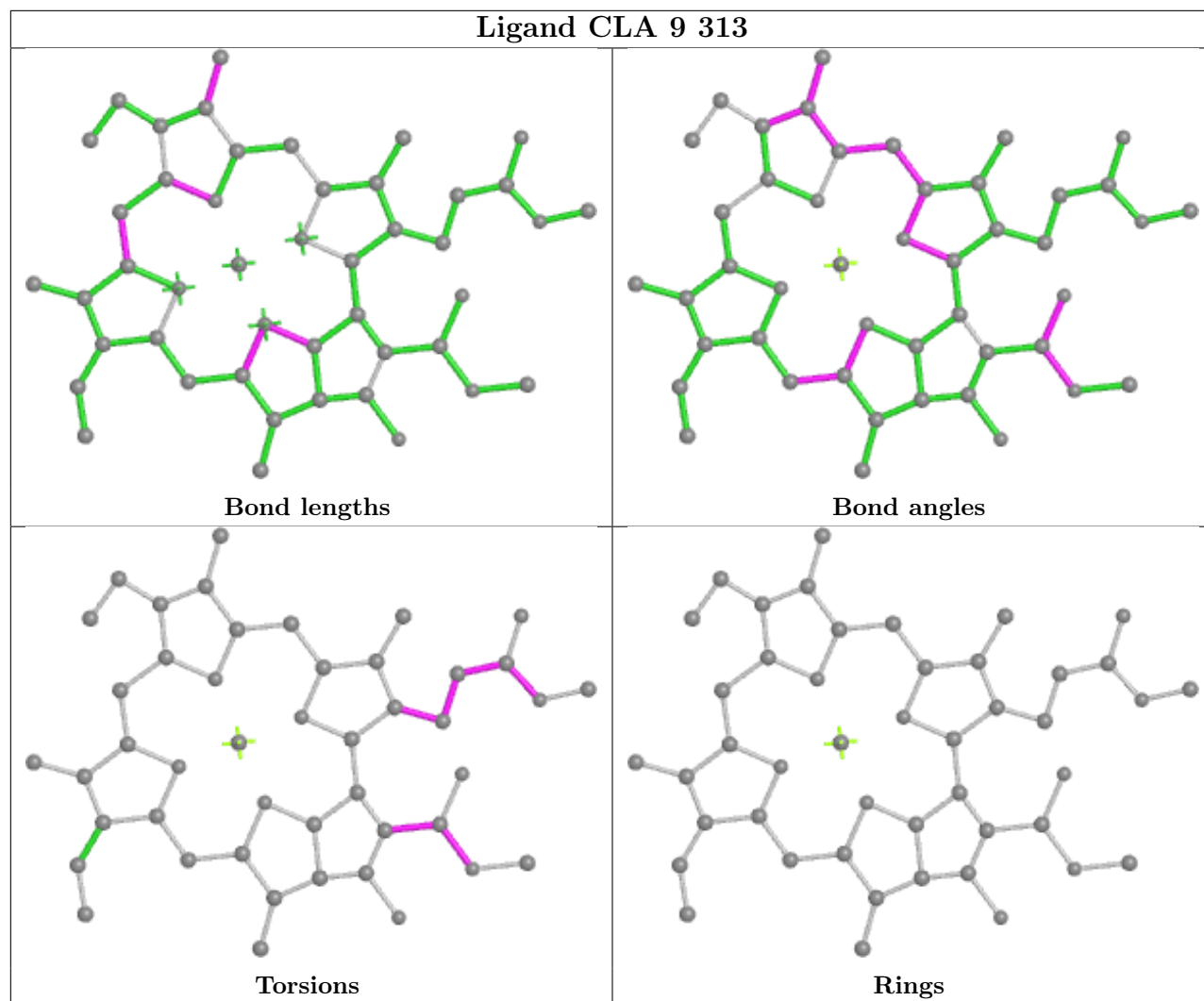
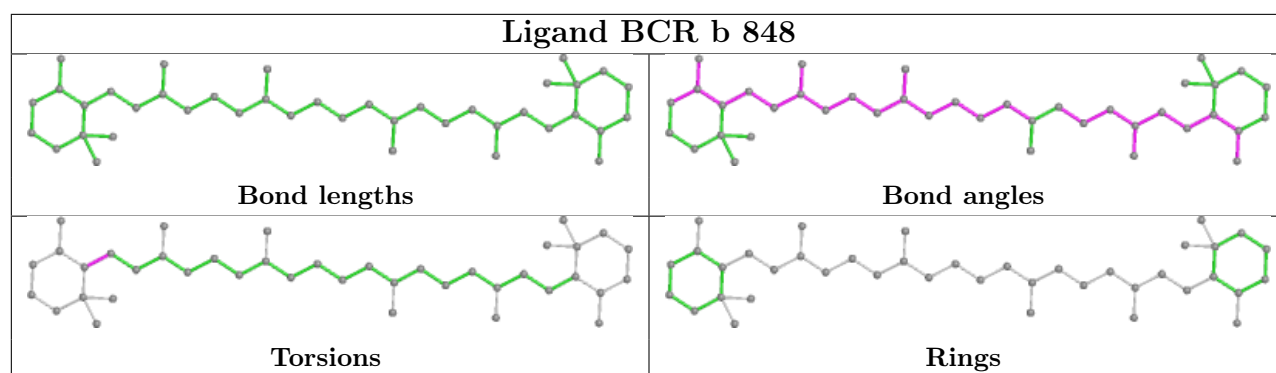


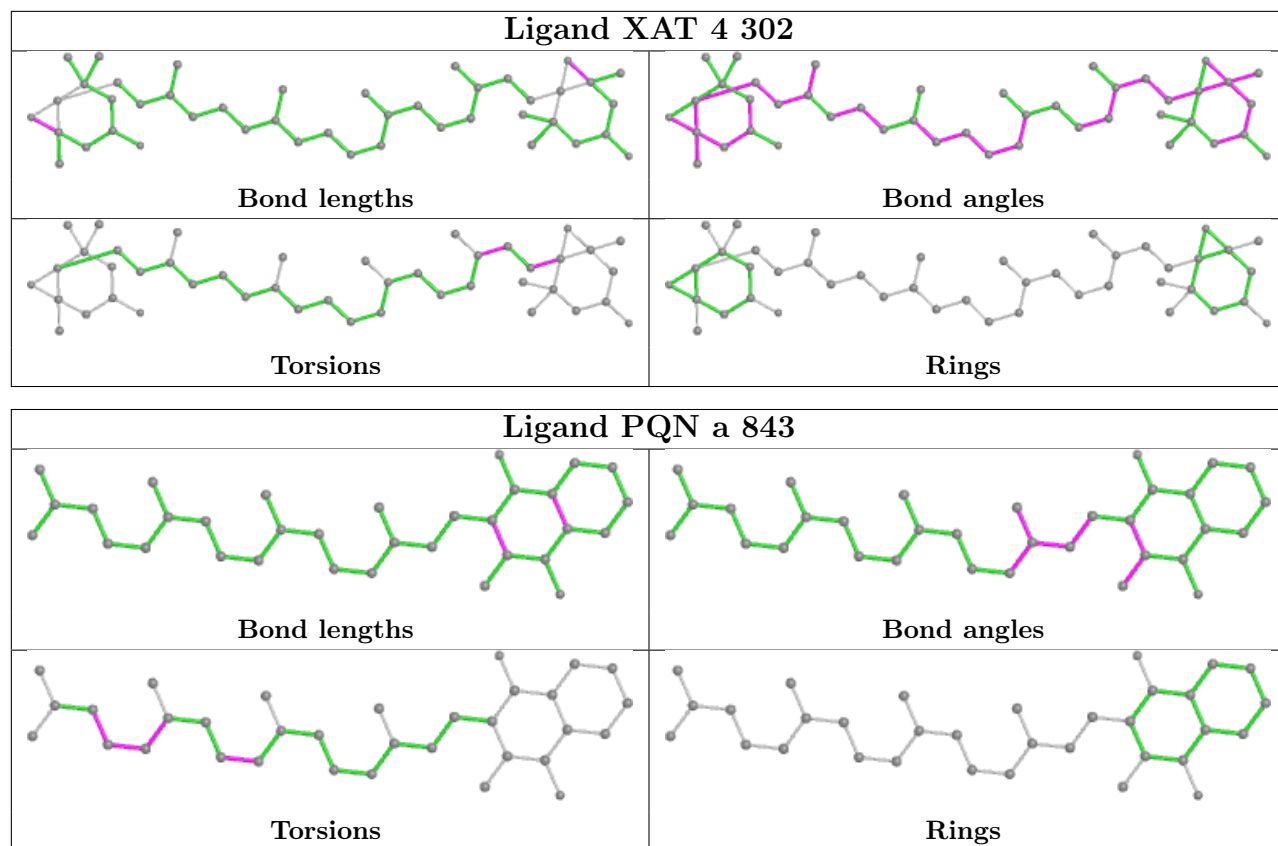
## Ligand CLA a 827



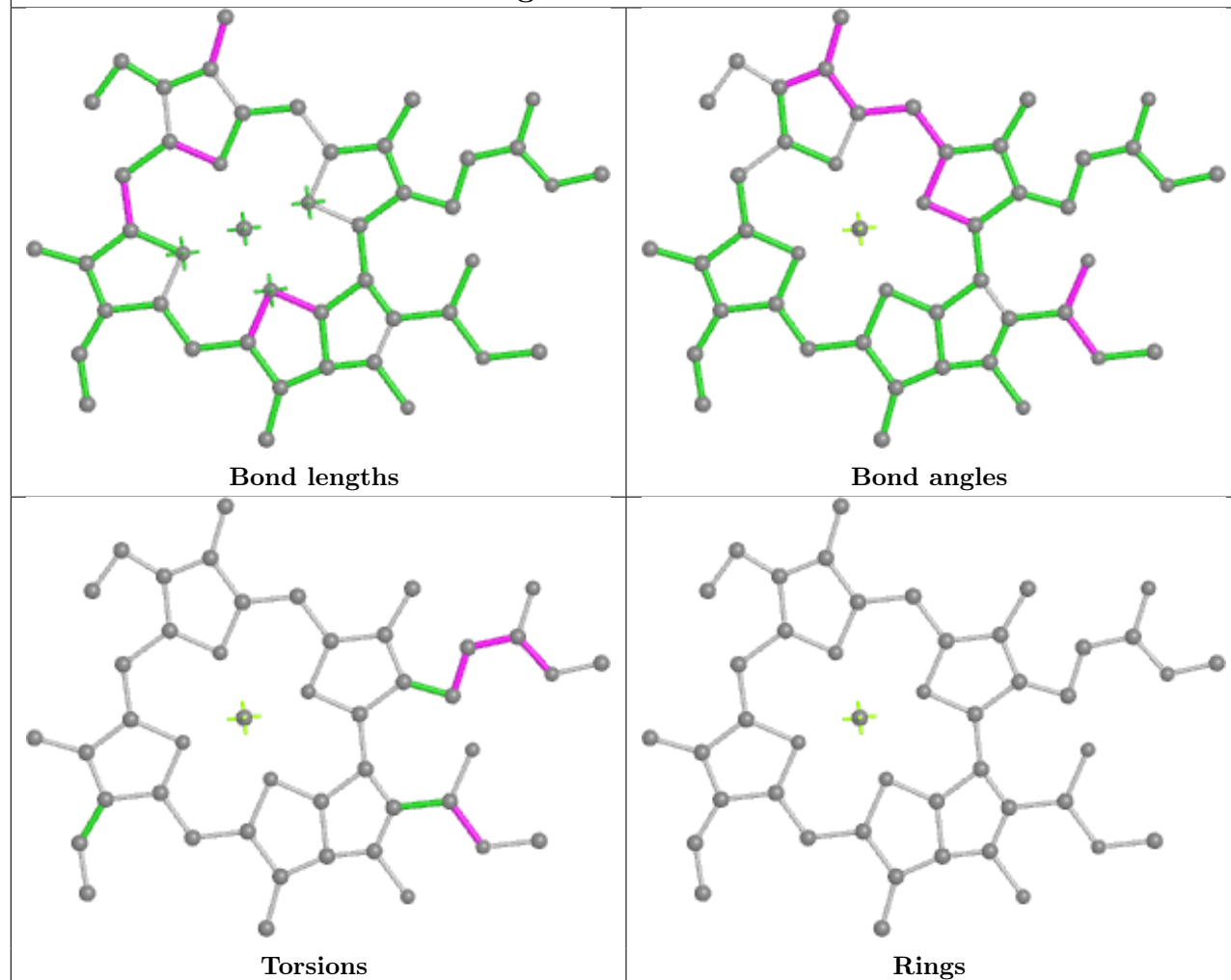
## Ligand BCR f 804



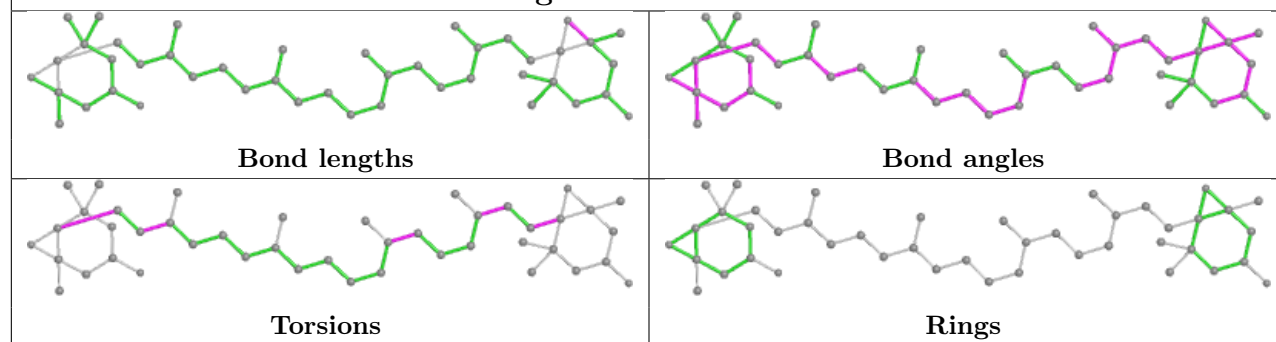


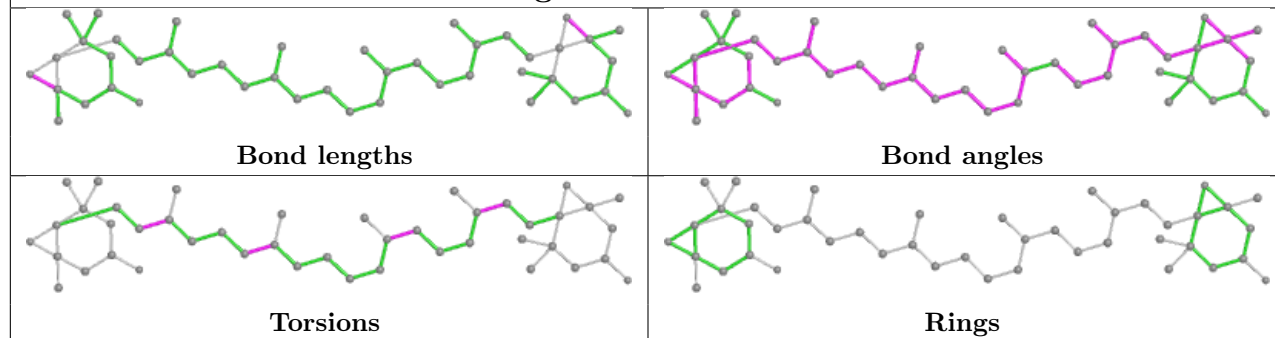
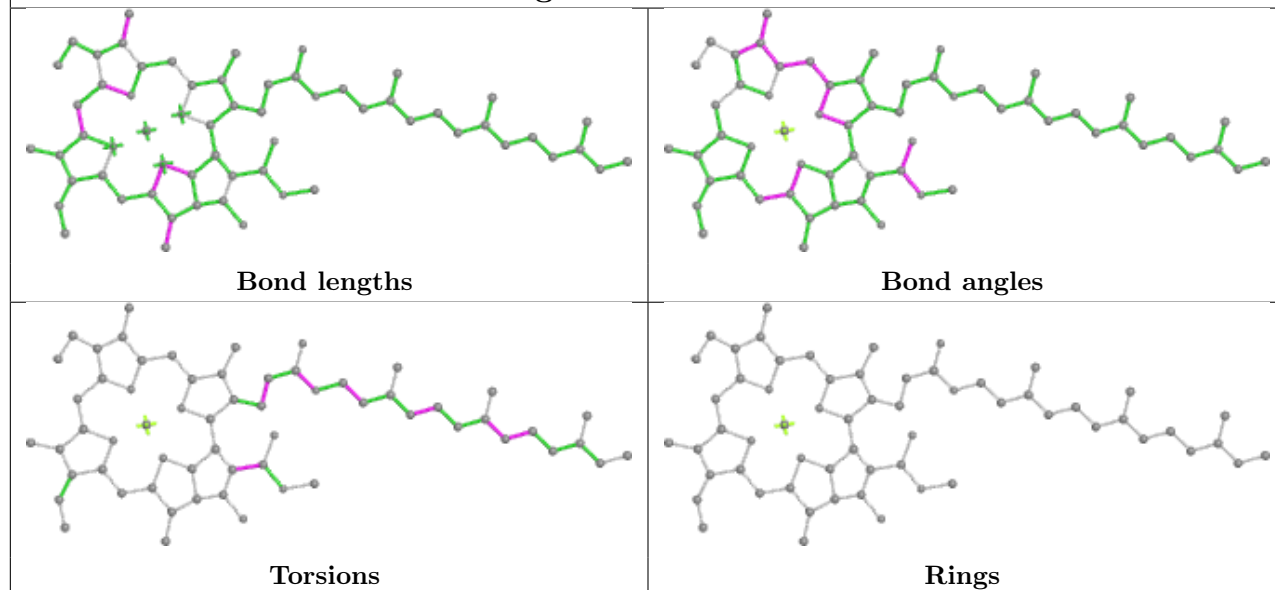
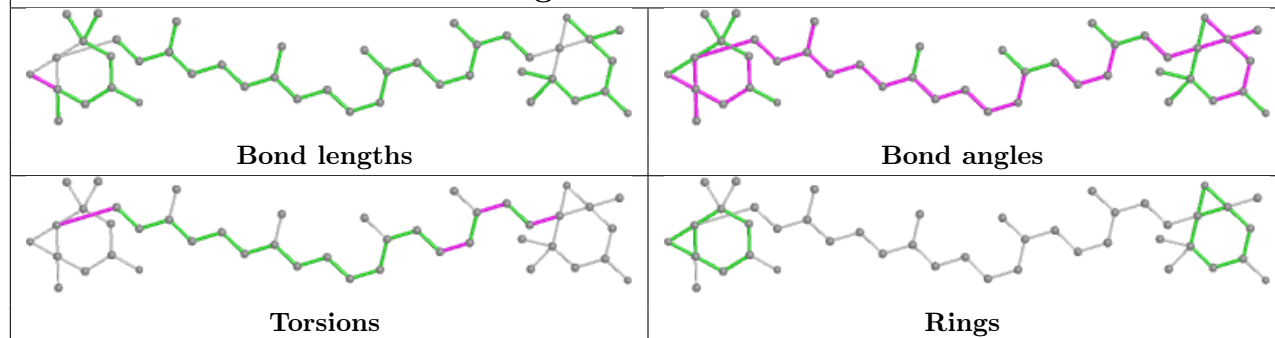


## Ligand CLA 7 310

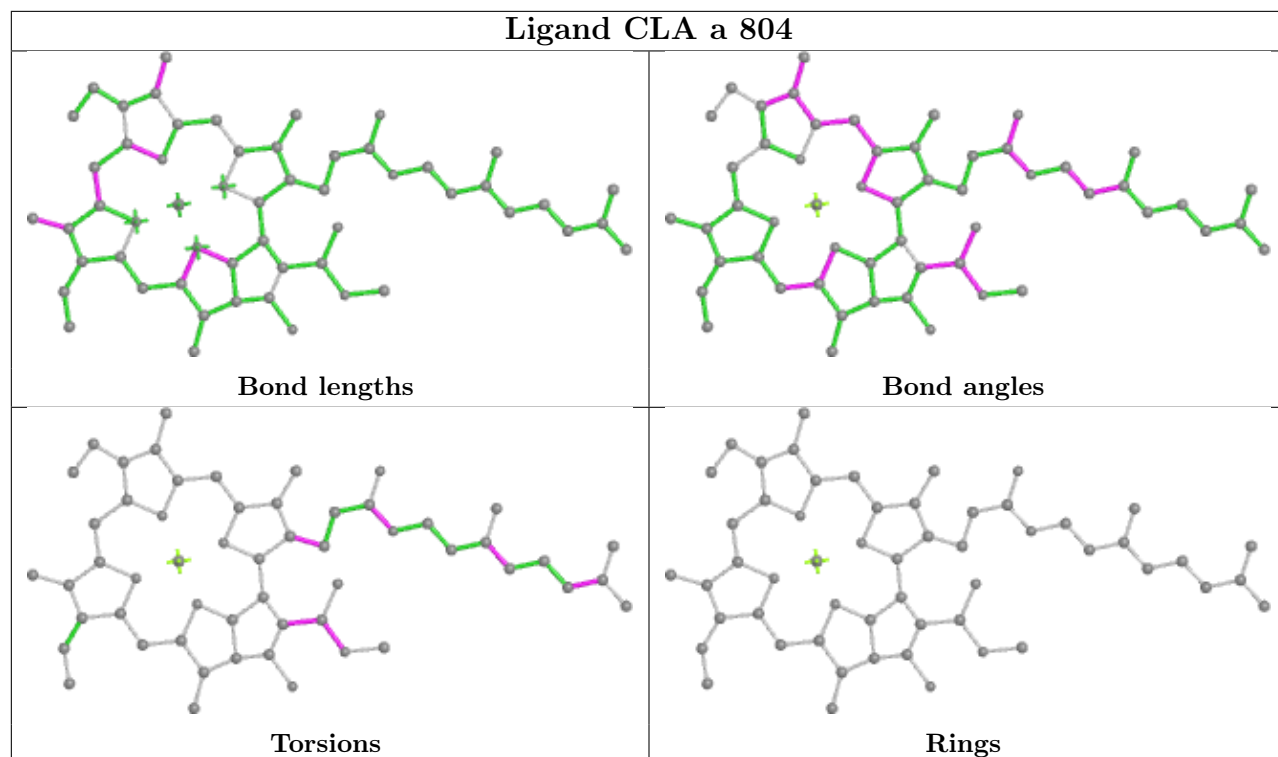


## Ligand XAT 7 303

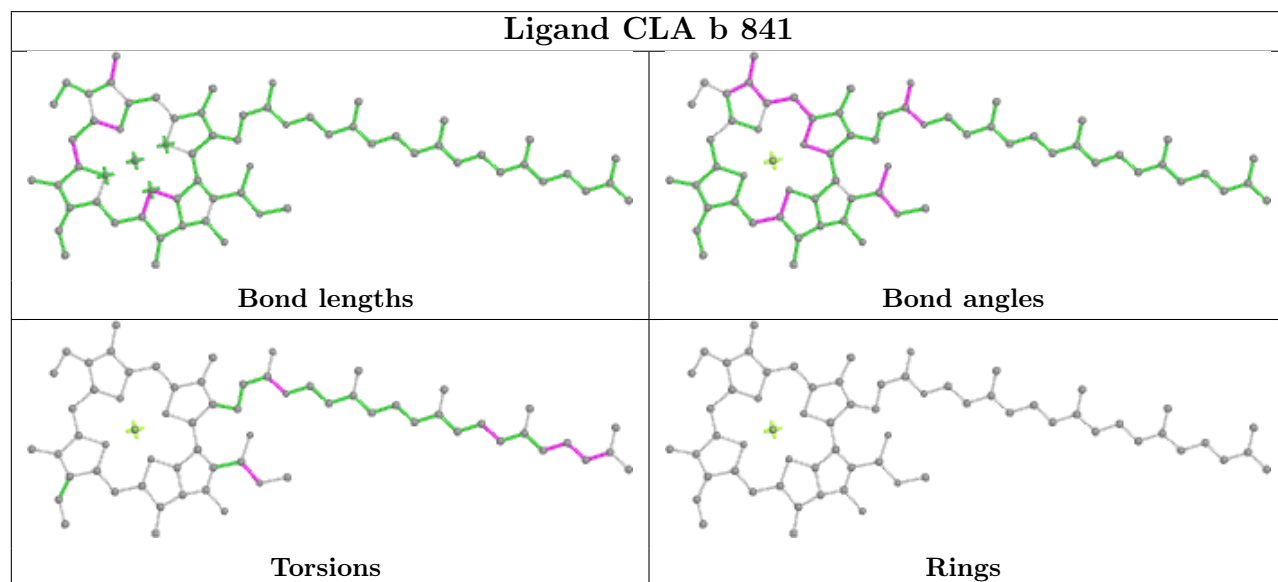


**Ligand XAT a 854****Ligand CLA 1 305****Ligand XAT a 853**

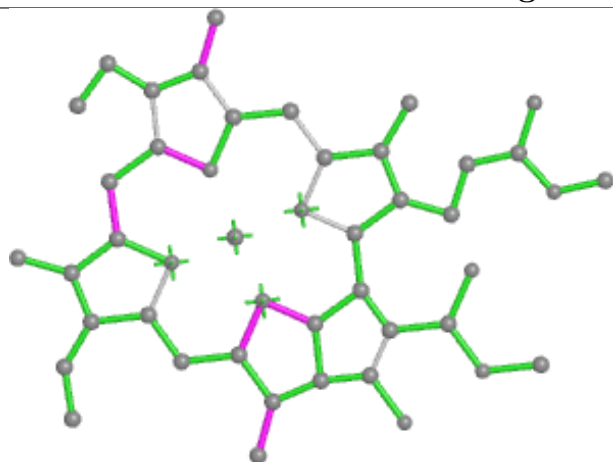
## Ligand CLA a 804



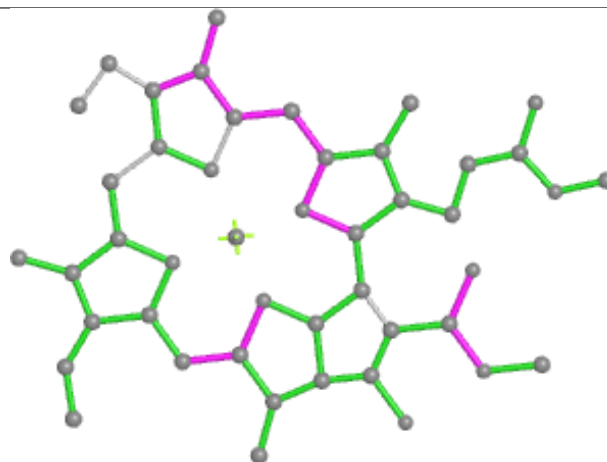
## Ligand CLA b 841



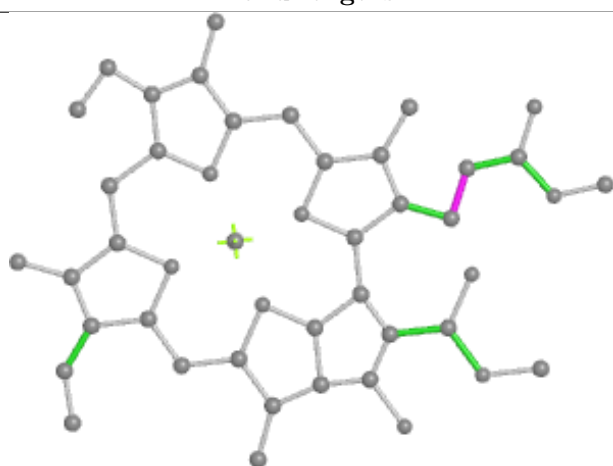
## Ligand CLA 6 307



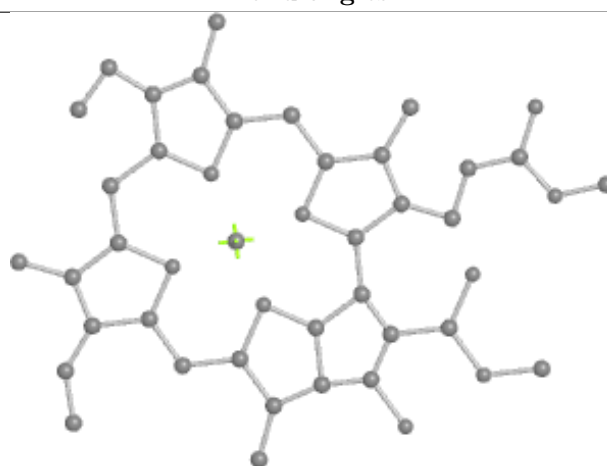
Bond lengths



Bond angles

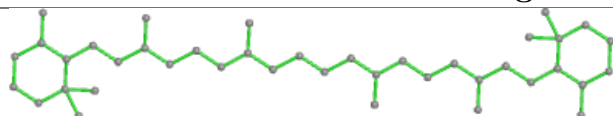


Torsions

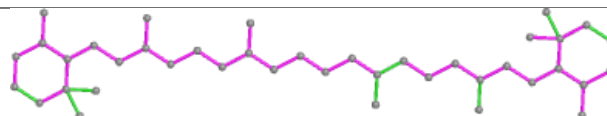


Rings

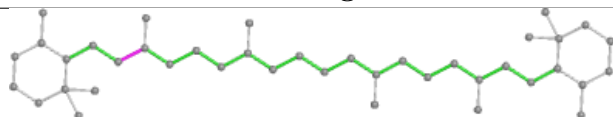
## Ligand BCR b 847



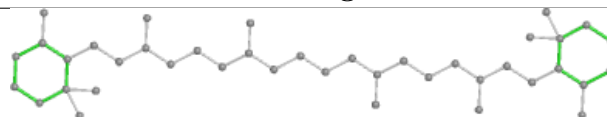
Bond lengths



Bond angles

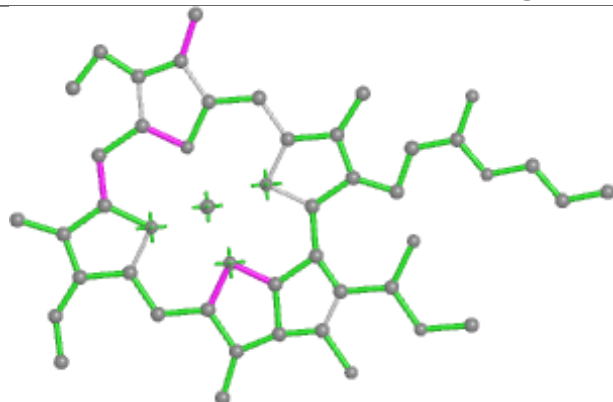


Torsions

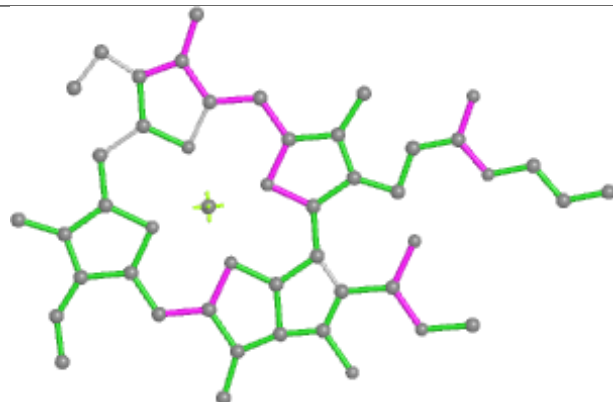


Rings

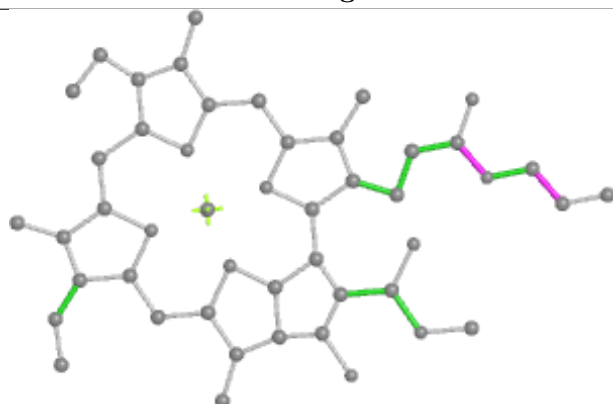
## Ligand CLA 7 312



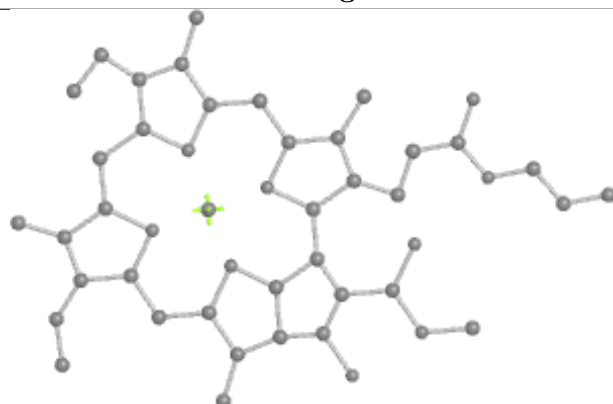
Bond lengths



Bond angles

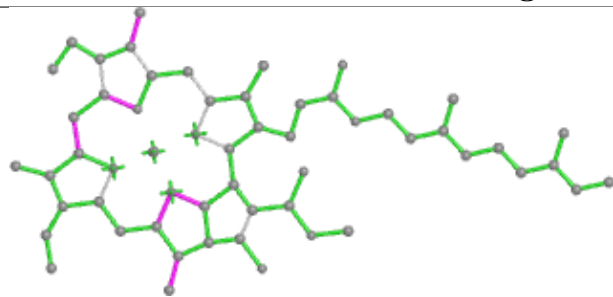


Torsions

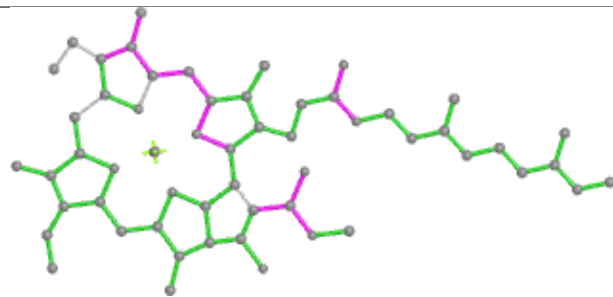


Rings

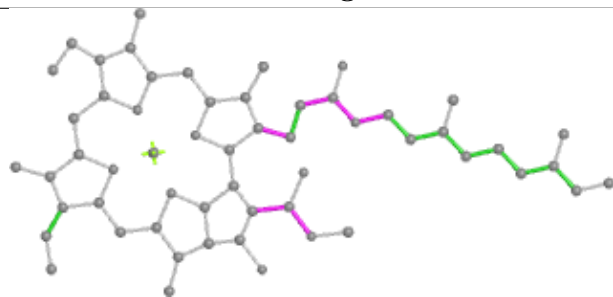
## Ligand CLA a 818



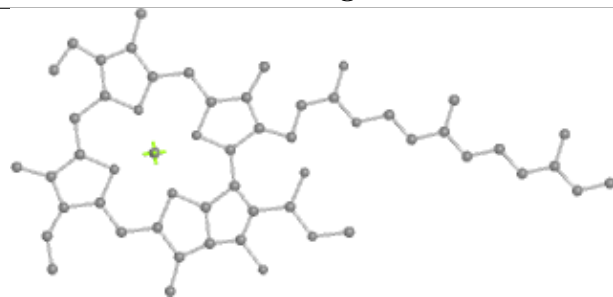
Bond lengths



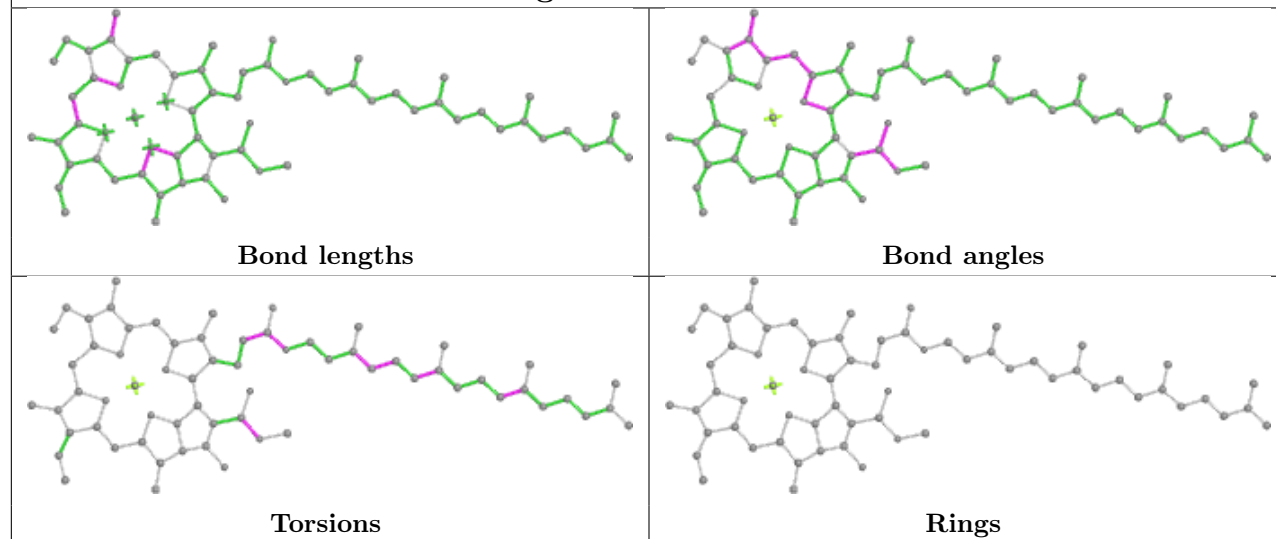
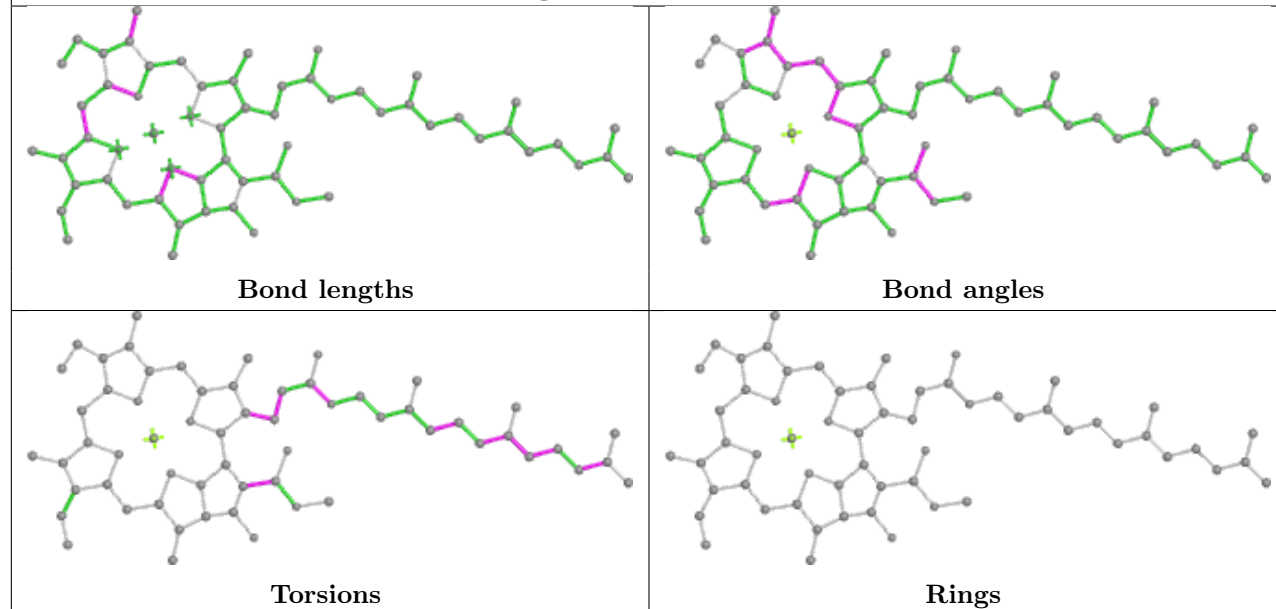
Bond angles

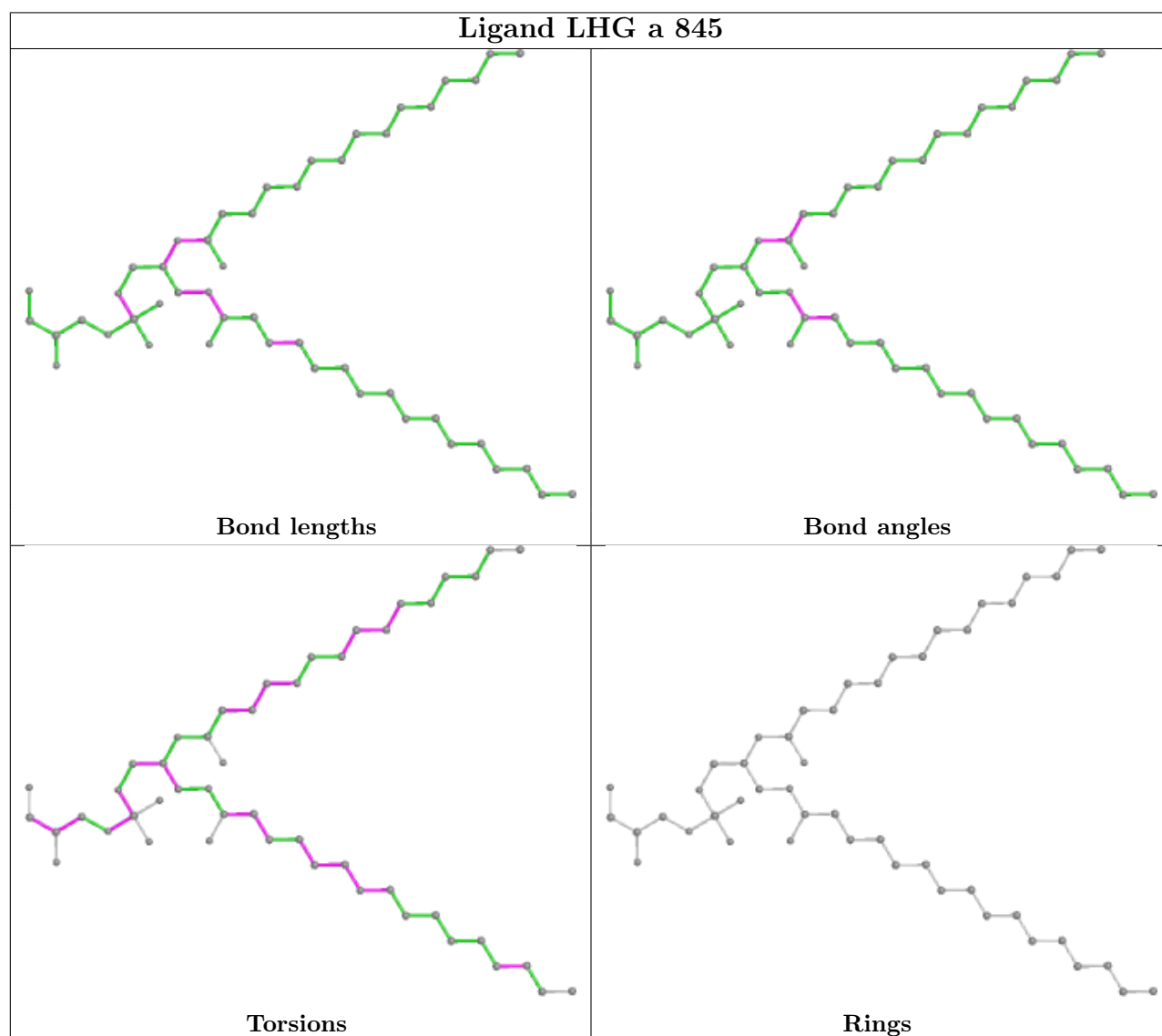
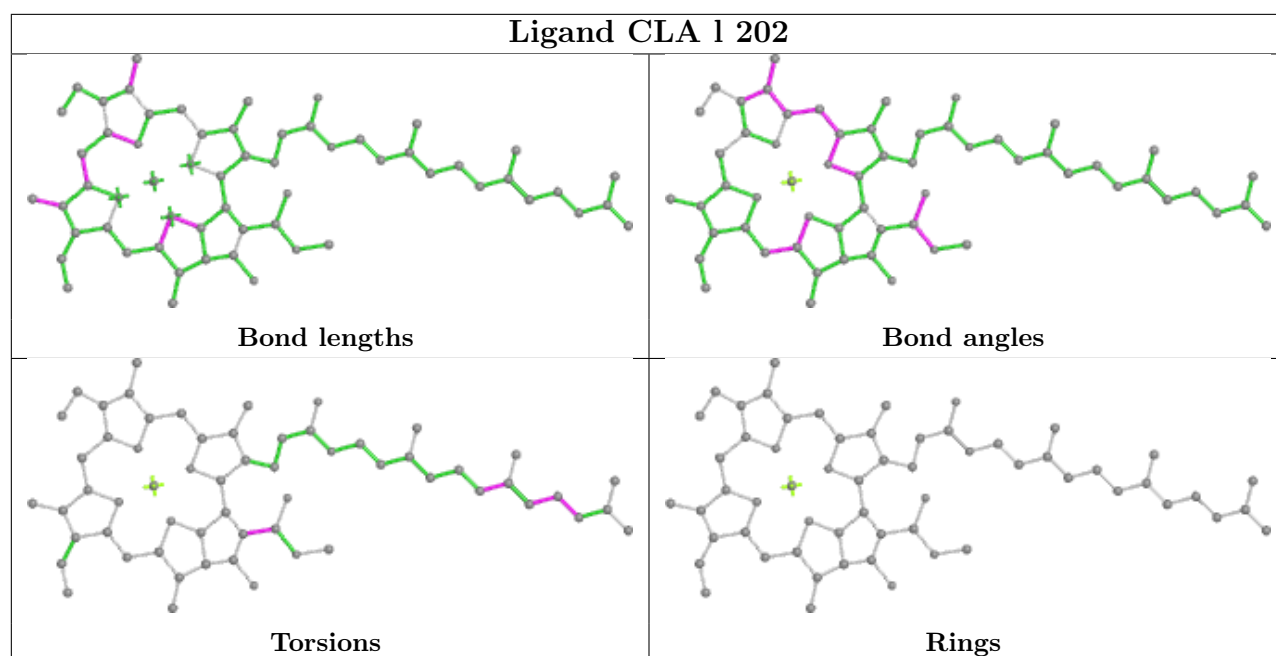


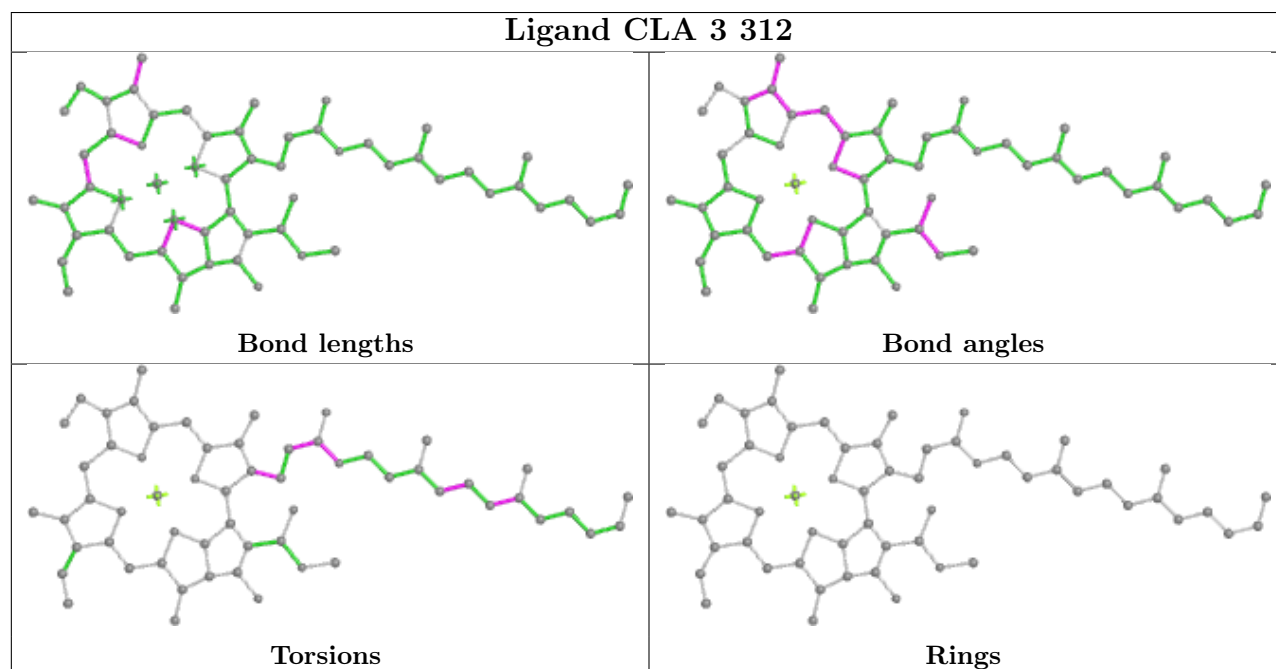
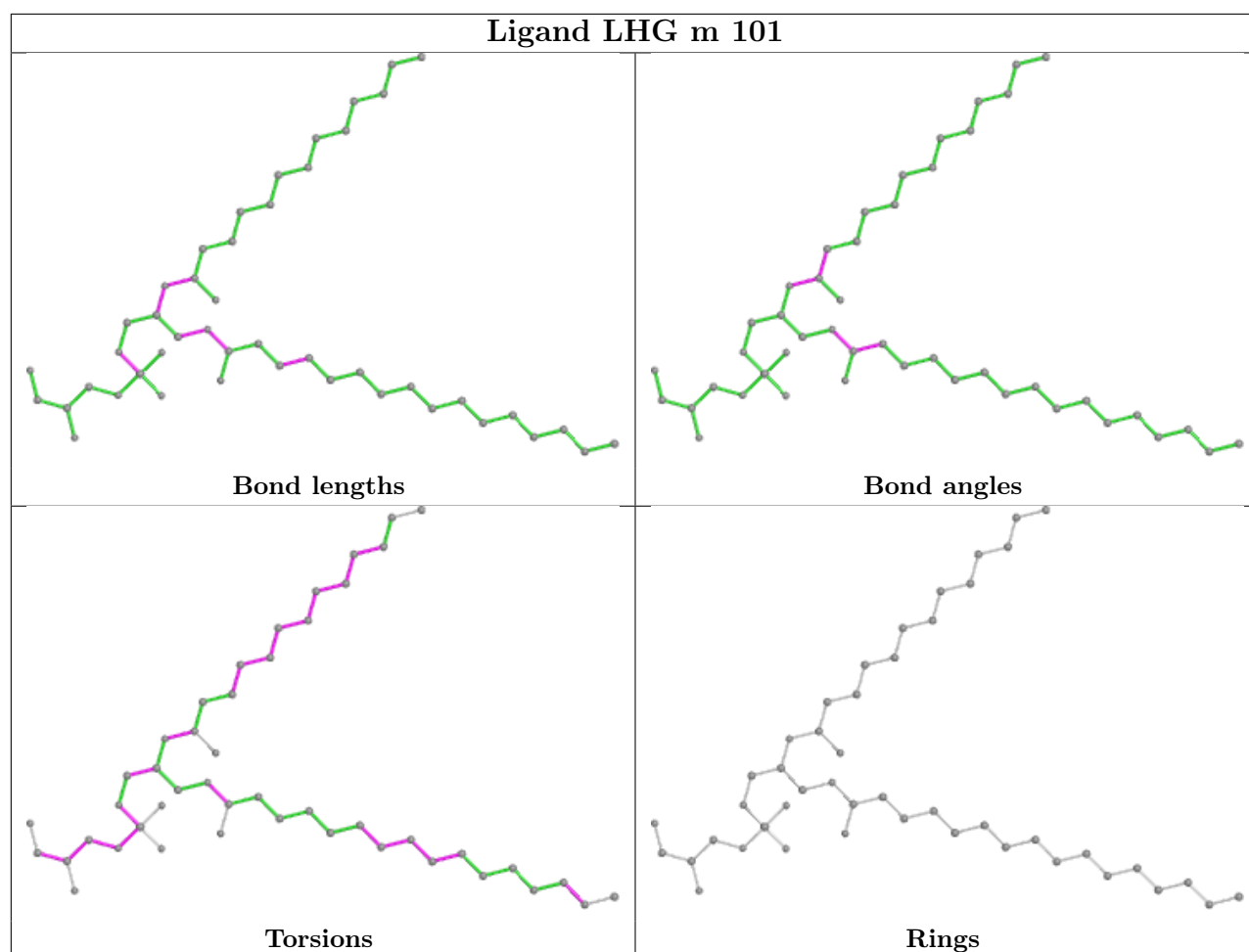
Torsions

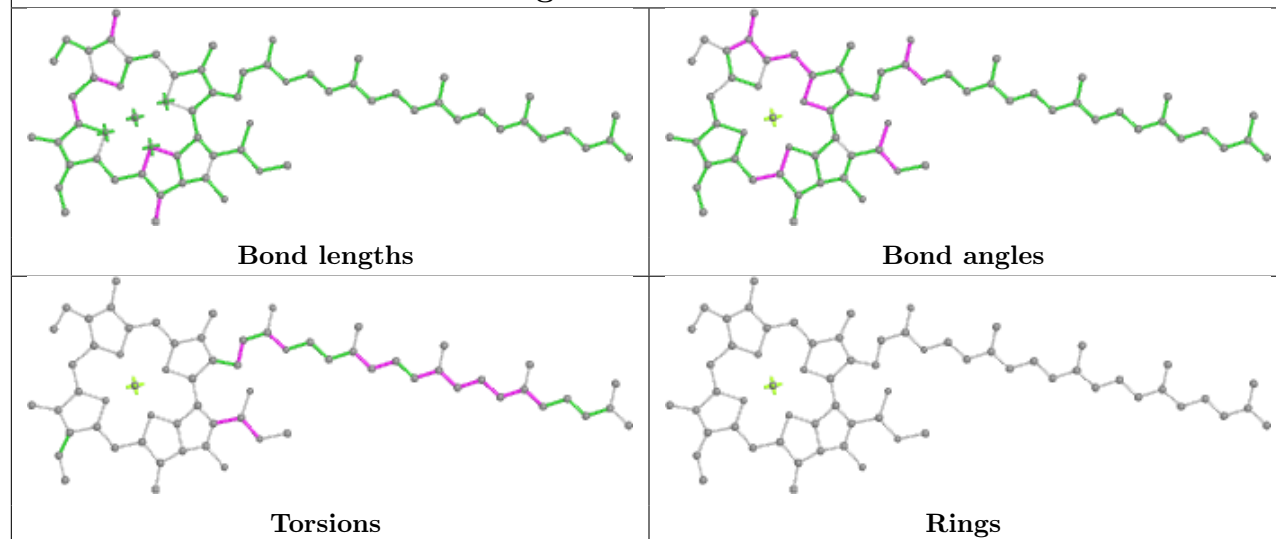
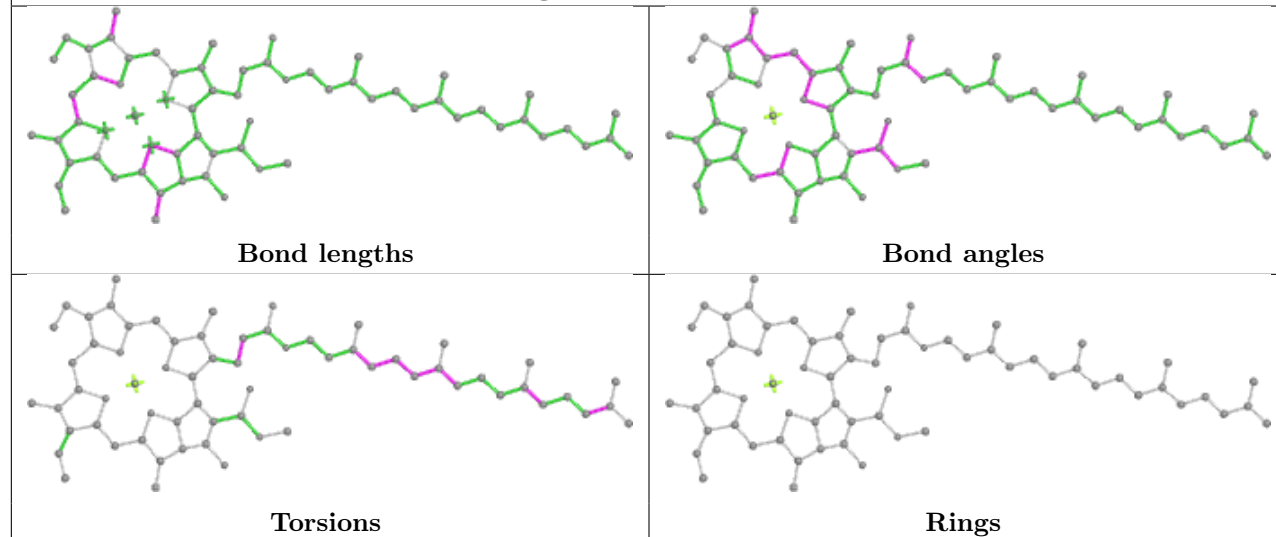


Rings

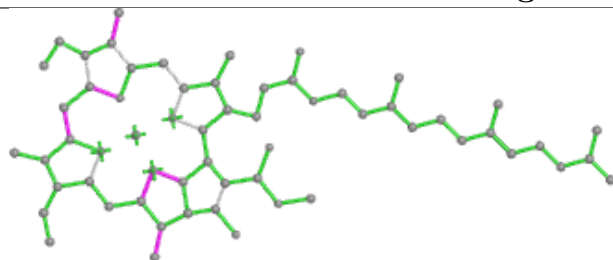
**Ligand CLA a 835****Ligand CLA b 818**



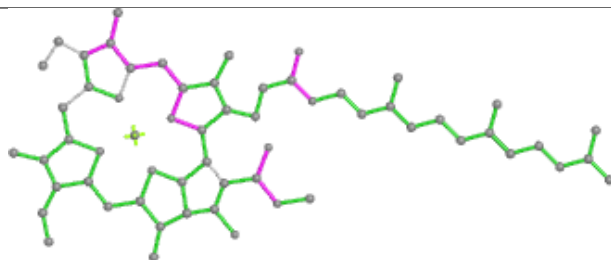


**Ligand CLA a 852****Ligand CLA b 807**

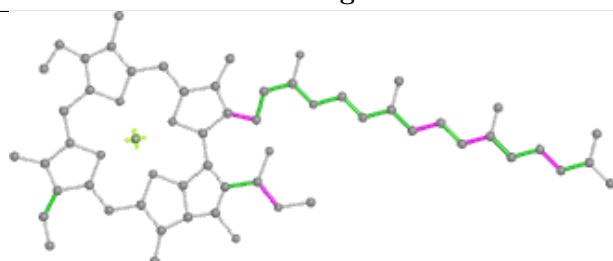
## Ligand CLA b 822



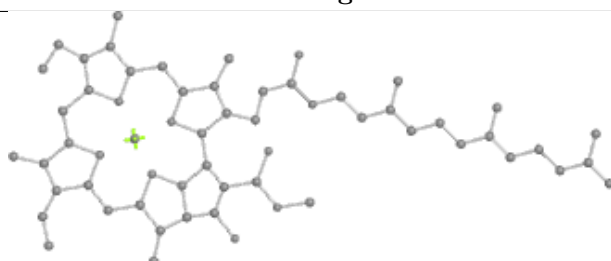
Bond lengths



Bond angles

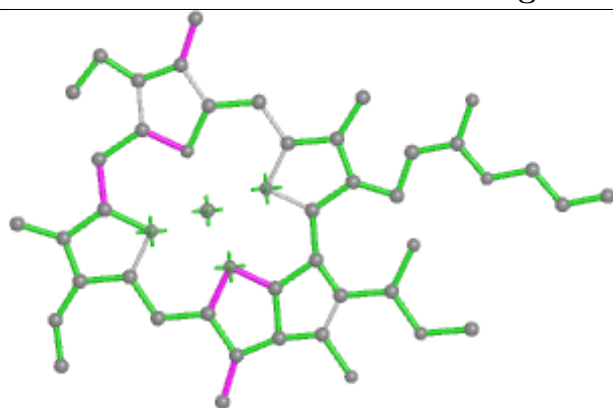


Torsions

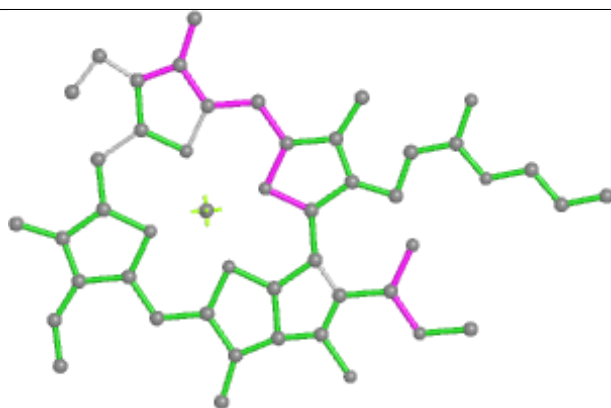


Rings

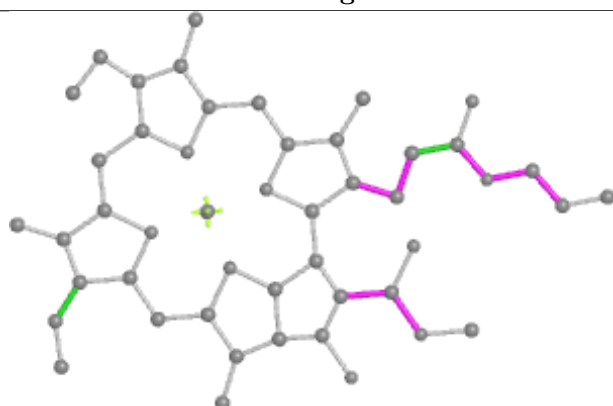
## Ligand CLA 7 306



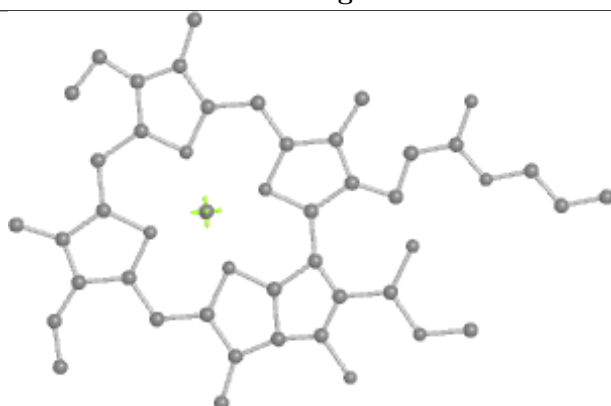
Bond lengths



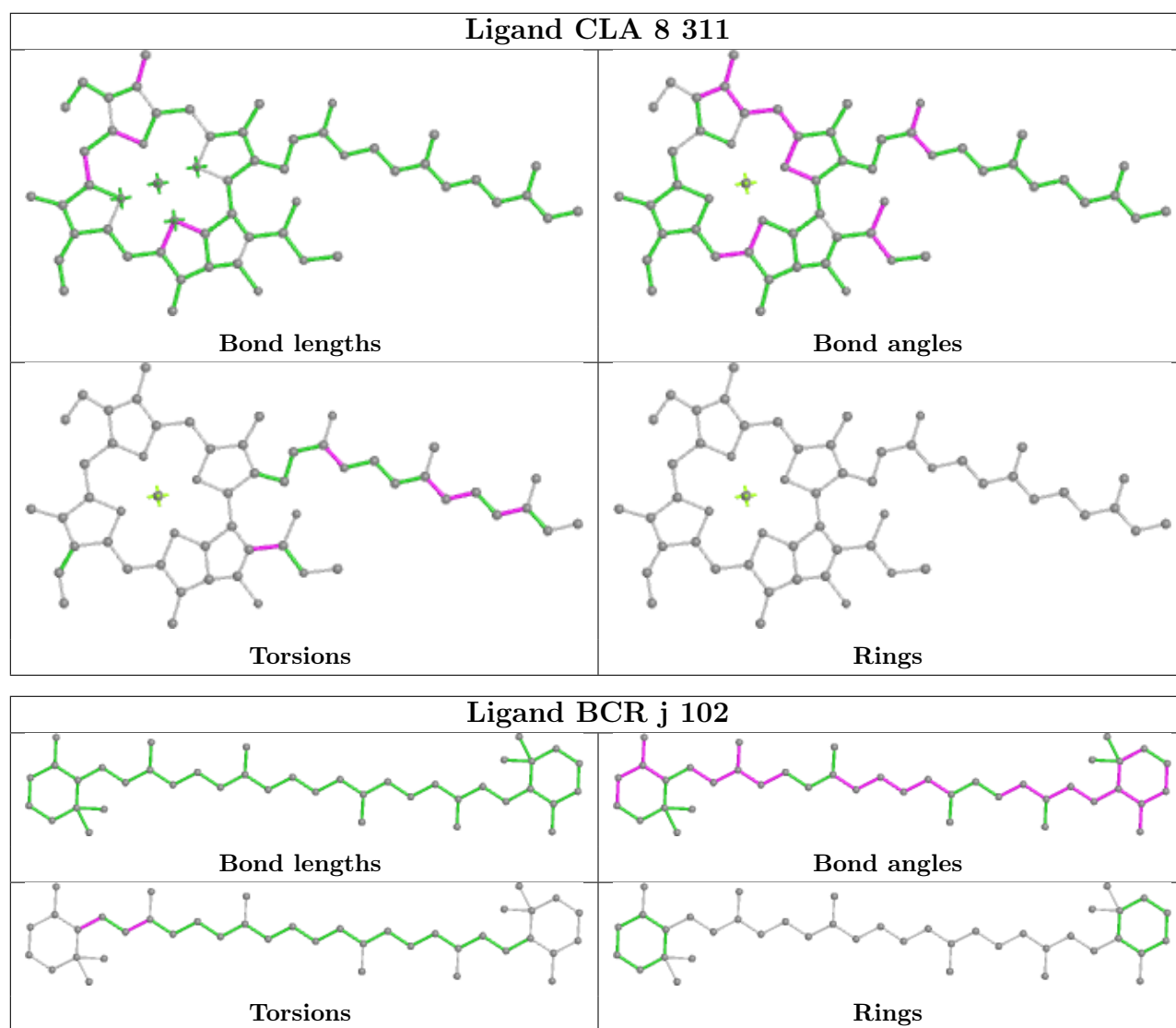
Bond angles

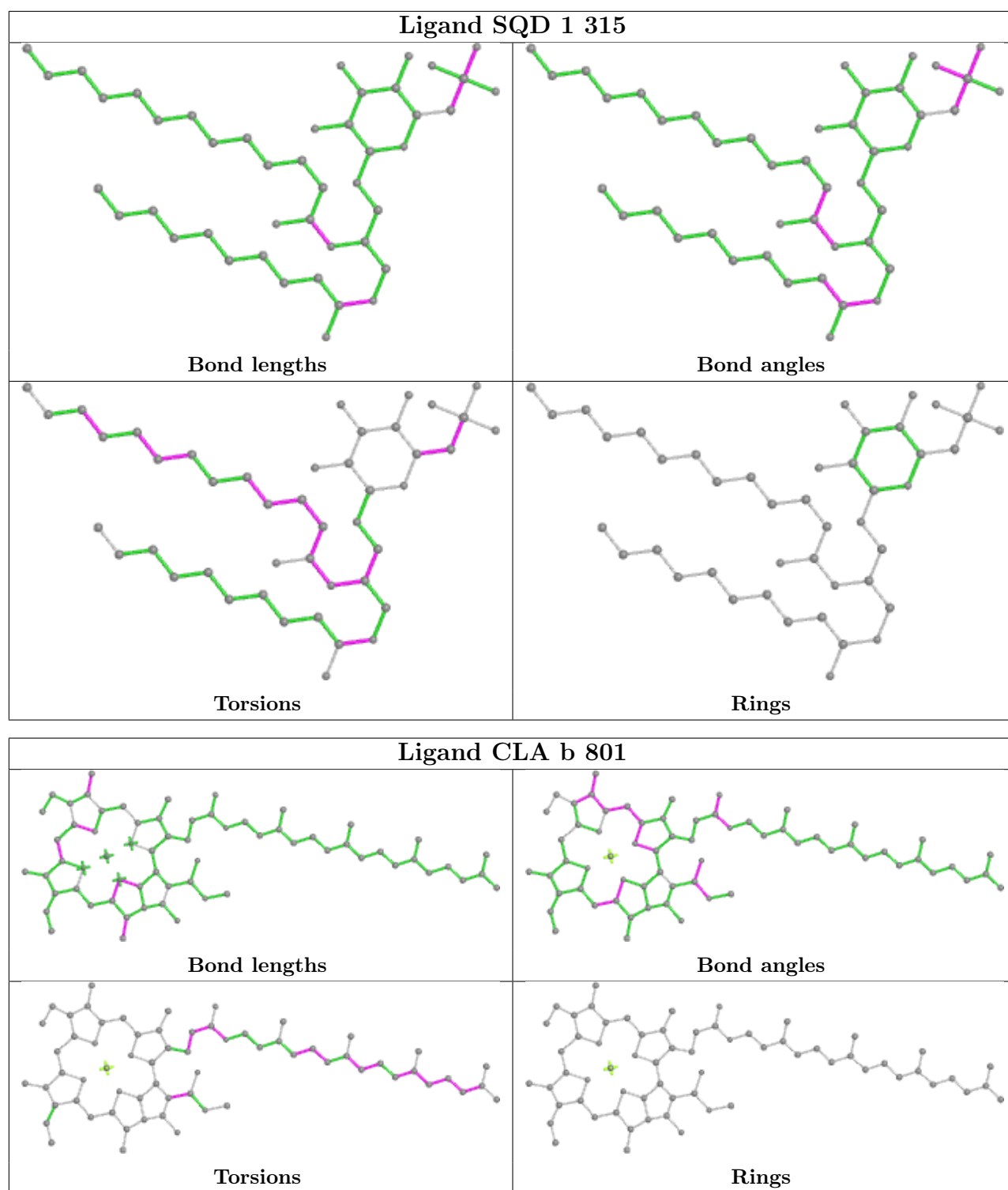


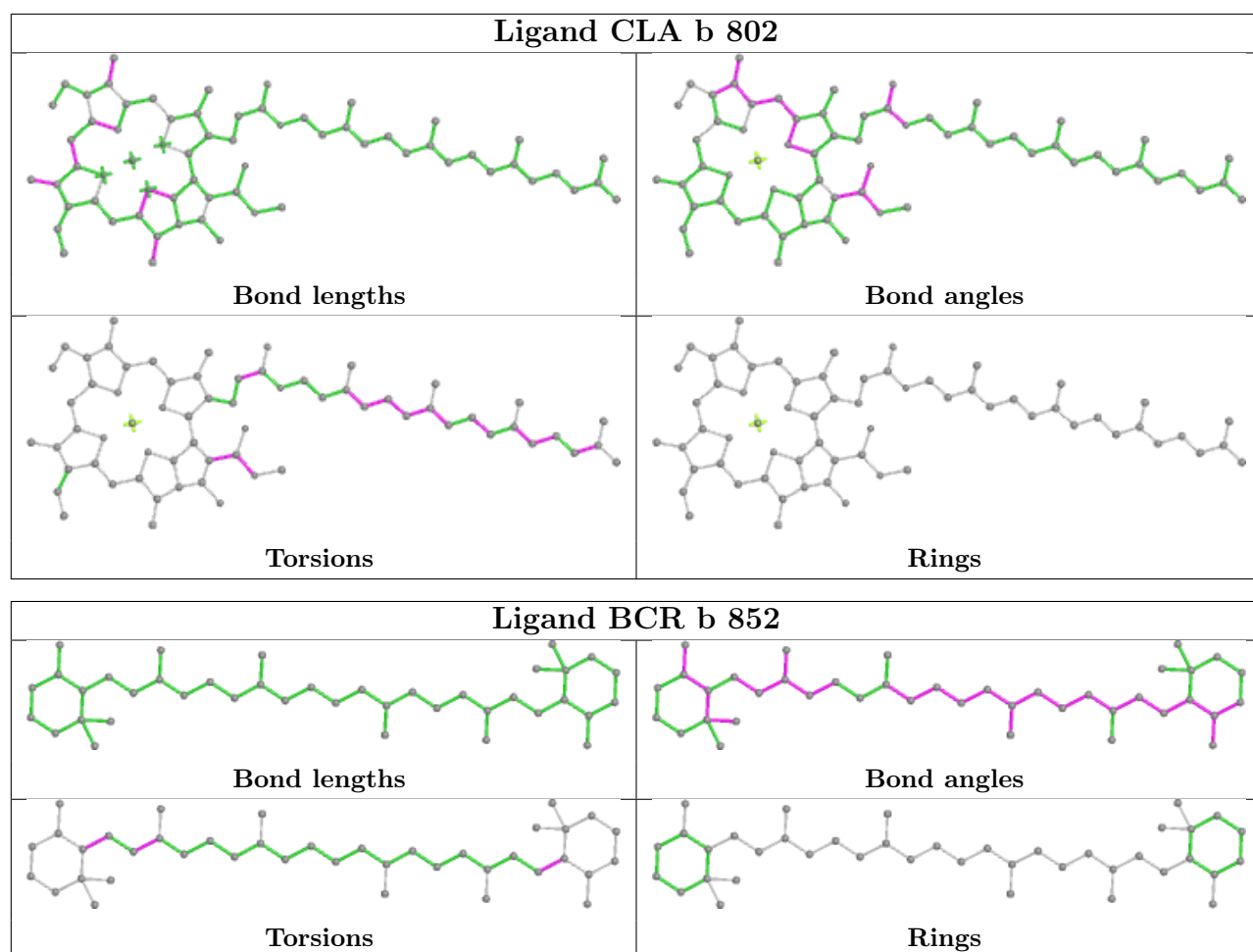
Torsions



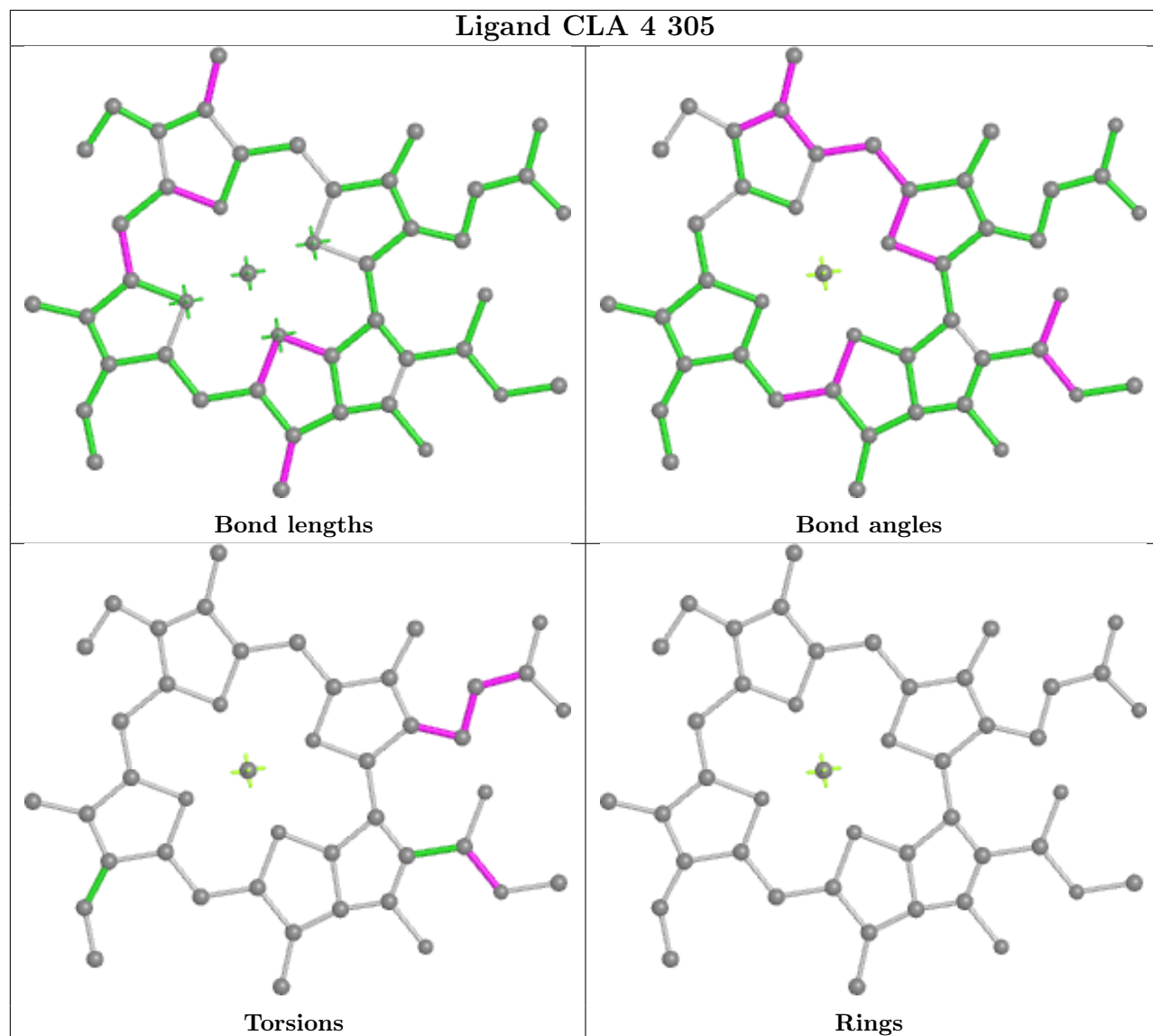
Rings



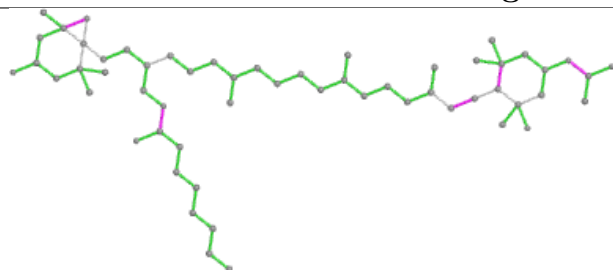




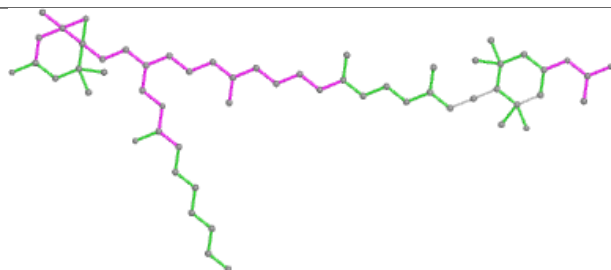
## Ligand CLA 4 305



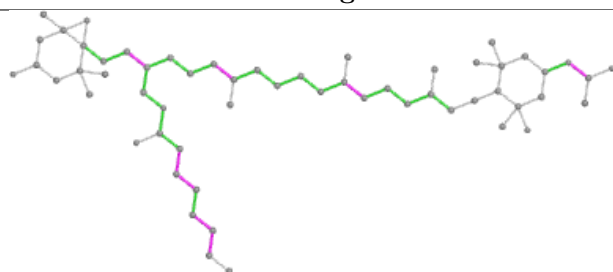
## Ligand A1L1F 1 304



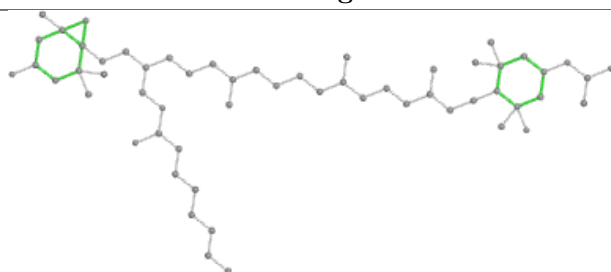
Bond lengths



Bond angles

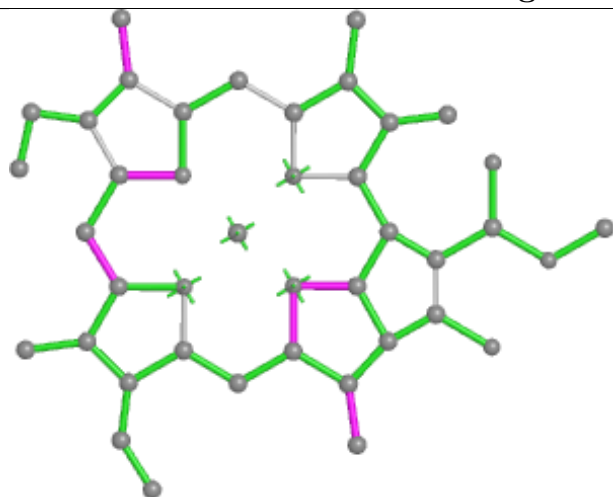


Torsions

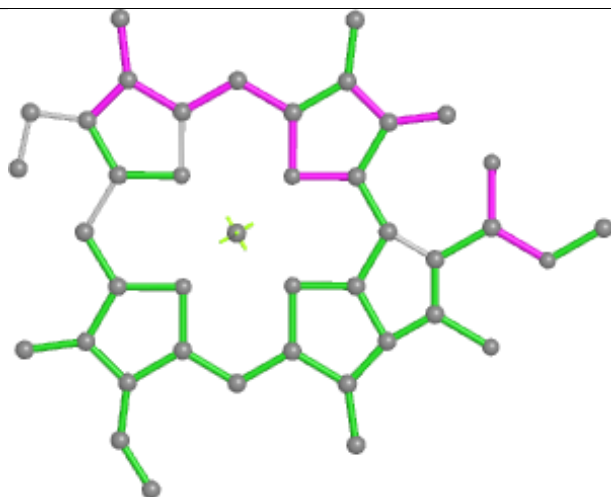


Rings

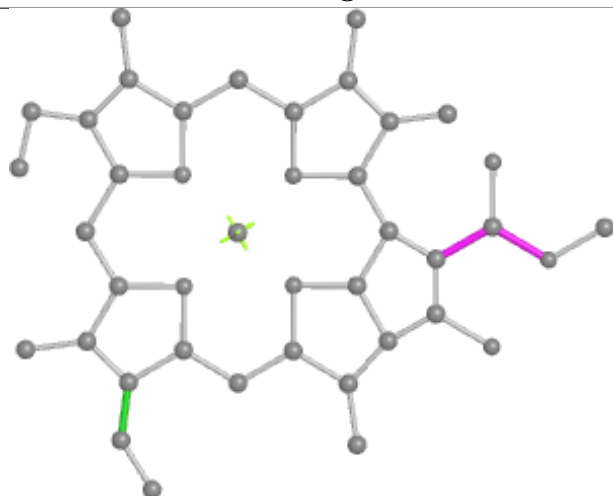
## Ligand CLA 4 314



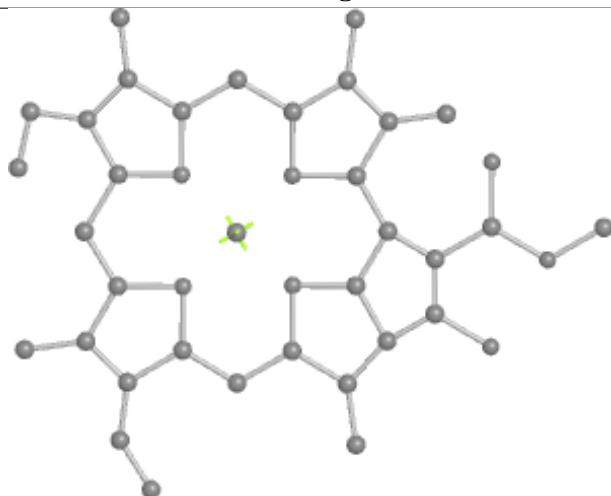
Bond lengths



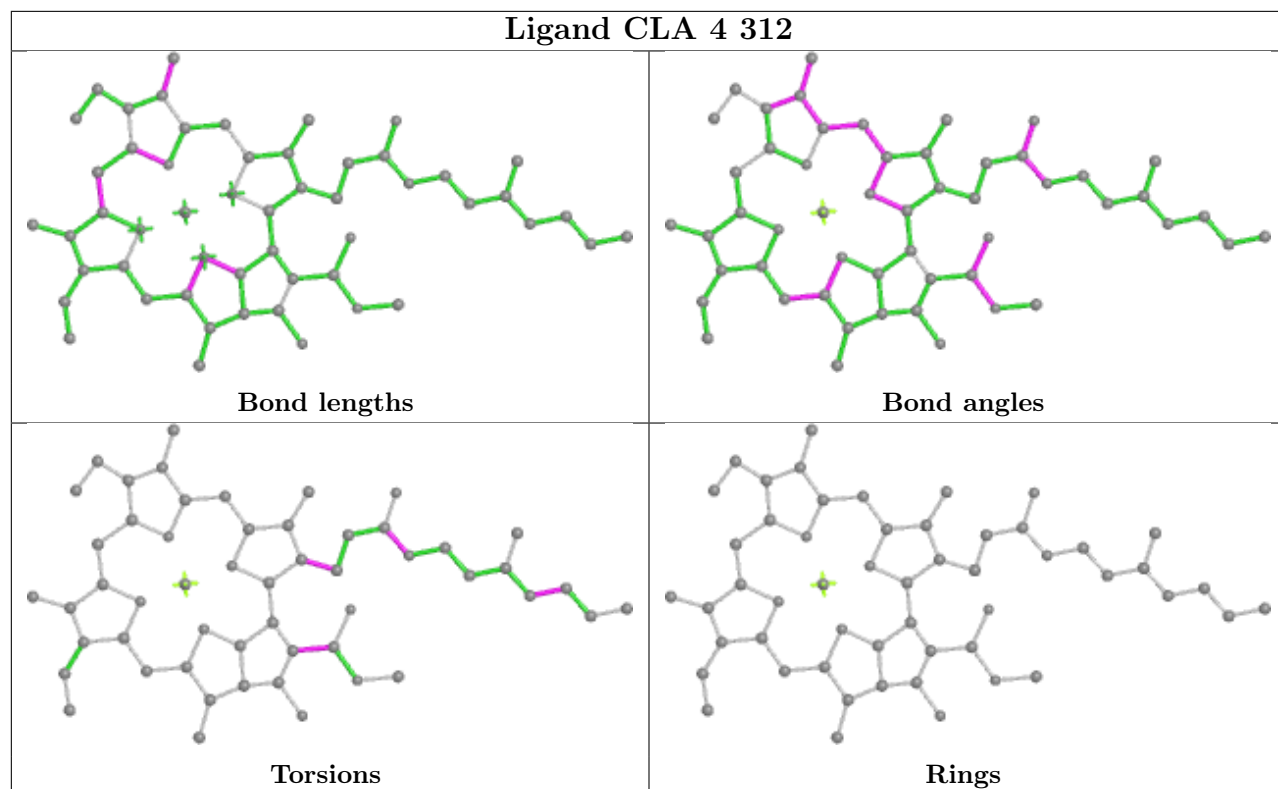
Bond angles



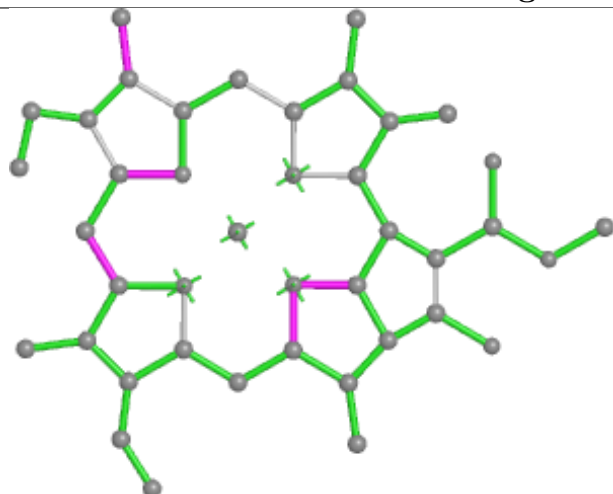
Torsions



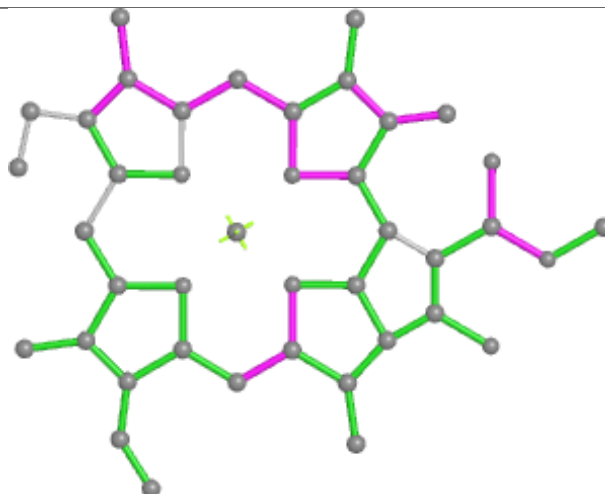
Rings



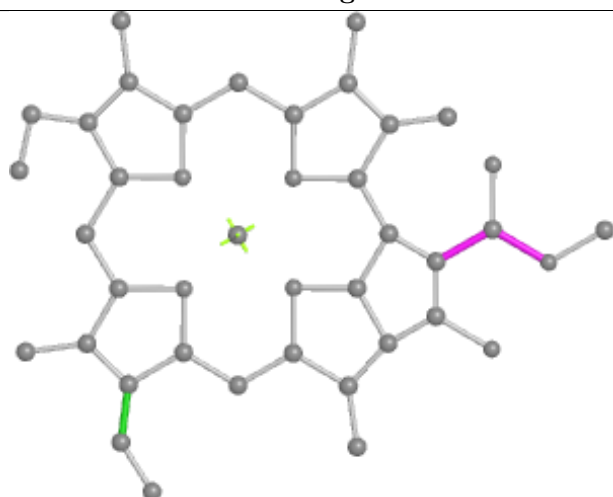
## Ligand CLA 7 315



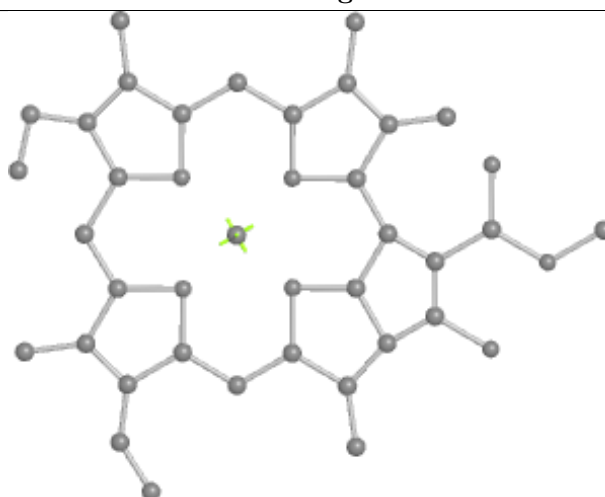
Bond lengths



Bond angles

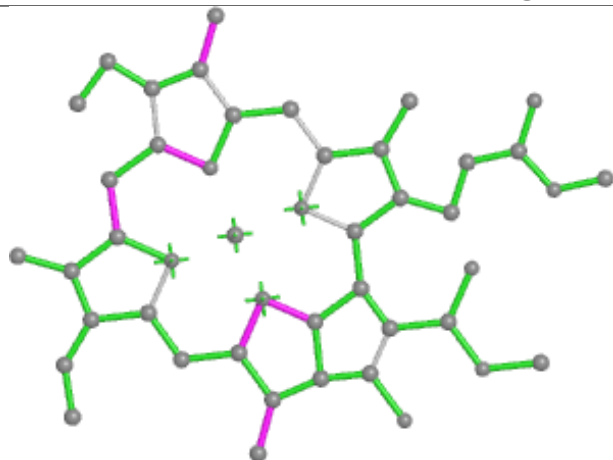


Torsions

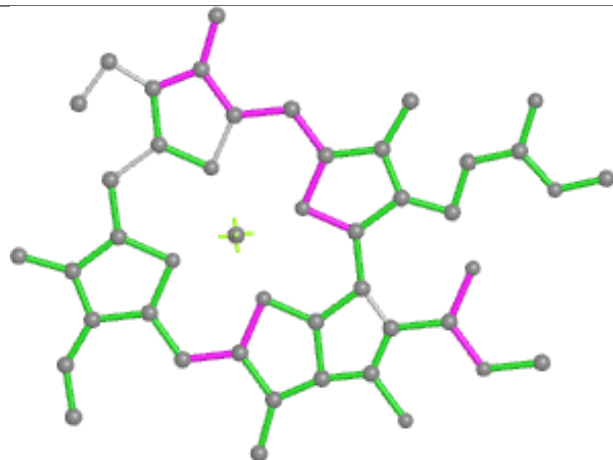


Rings

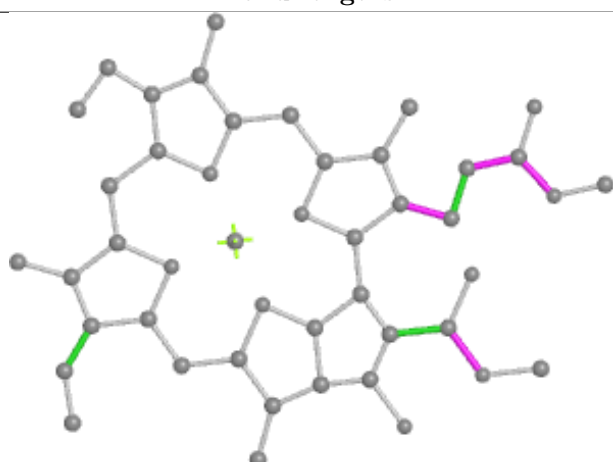
## Ligand CLA 3 315



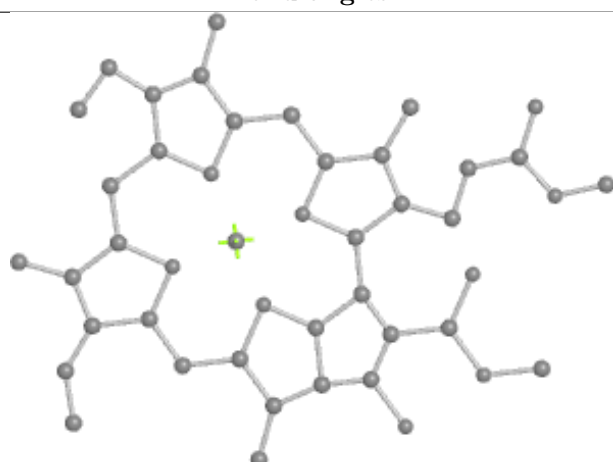
Bond lengths



Bond angles

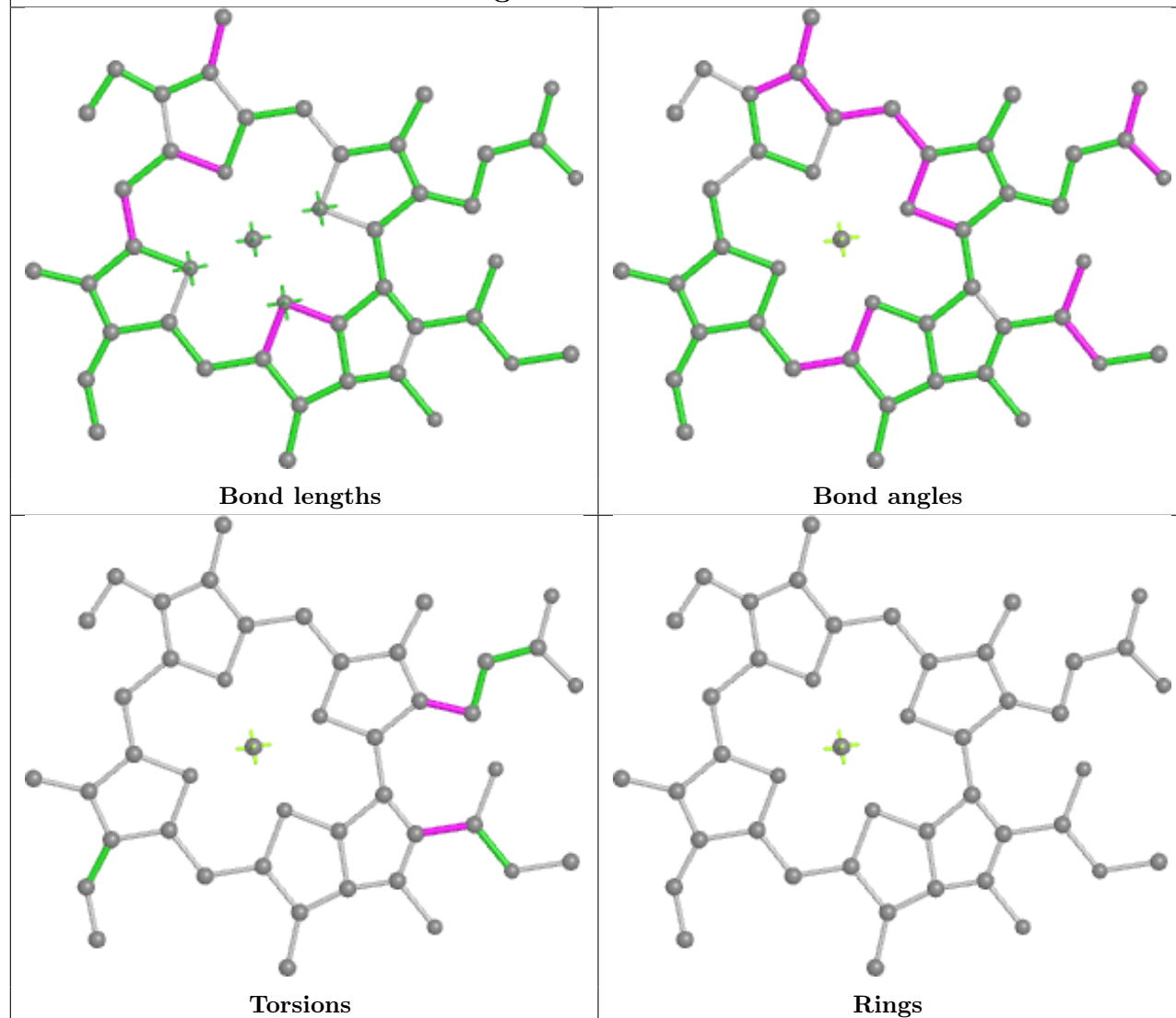


Torsions

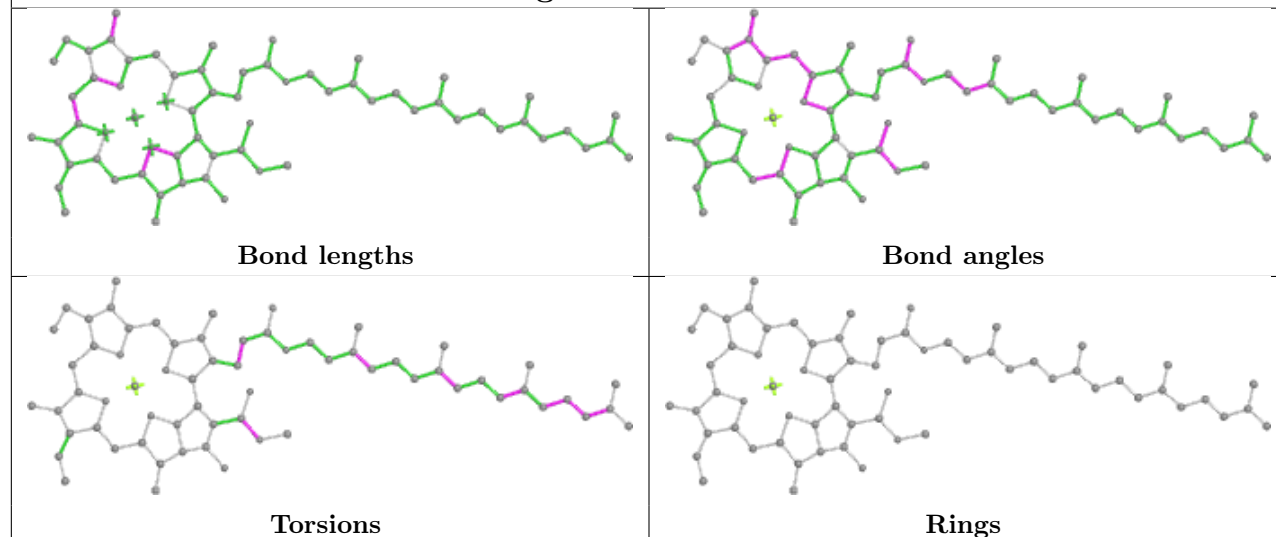


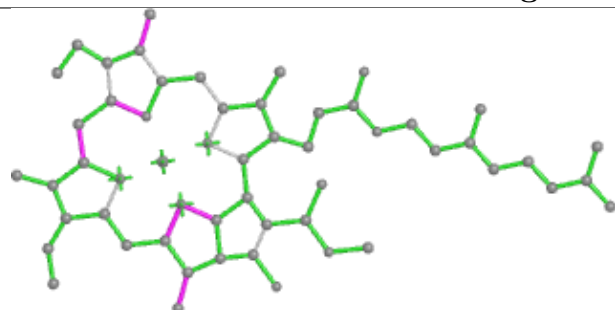
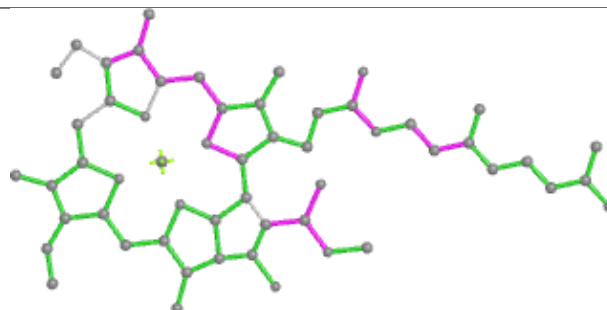
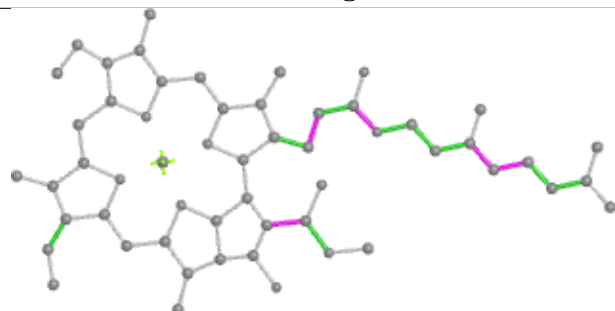
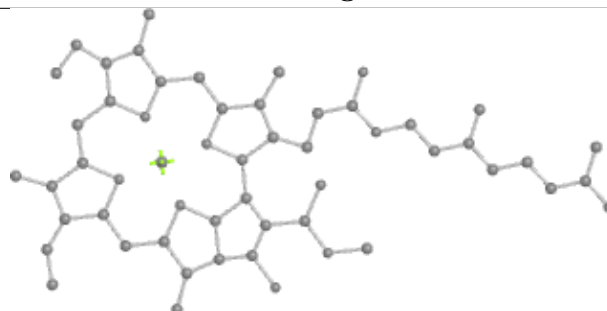
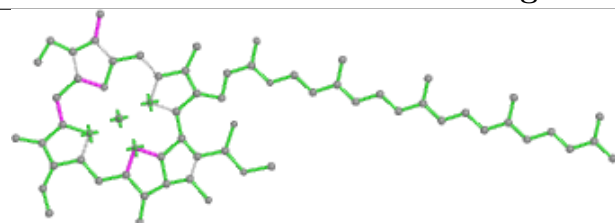
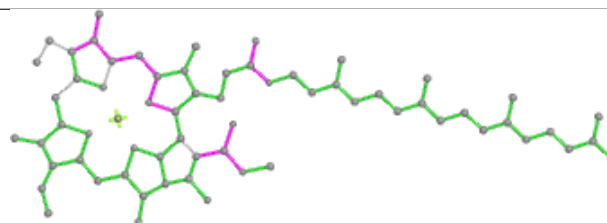
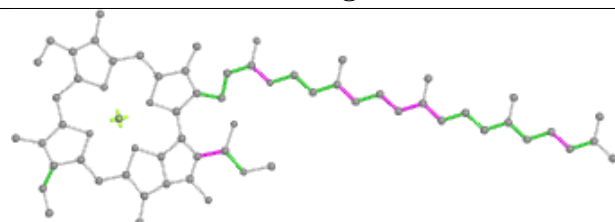
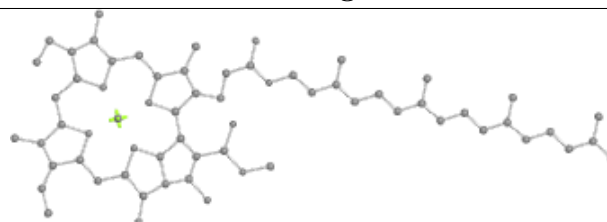
Rings

## Ligand CLA a 815

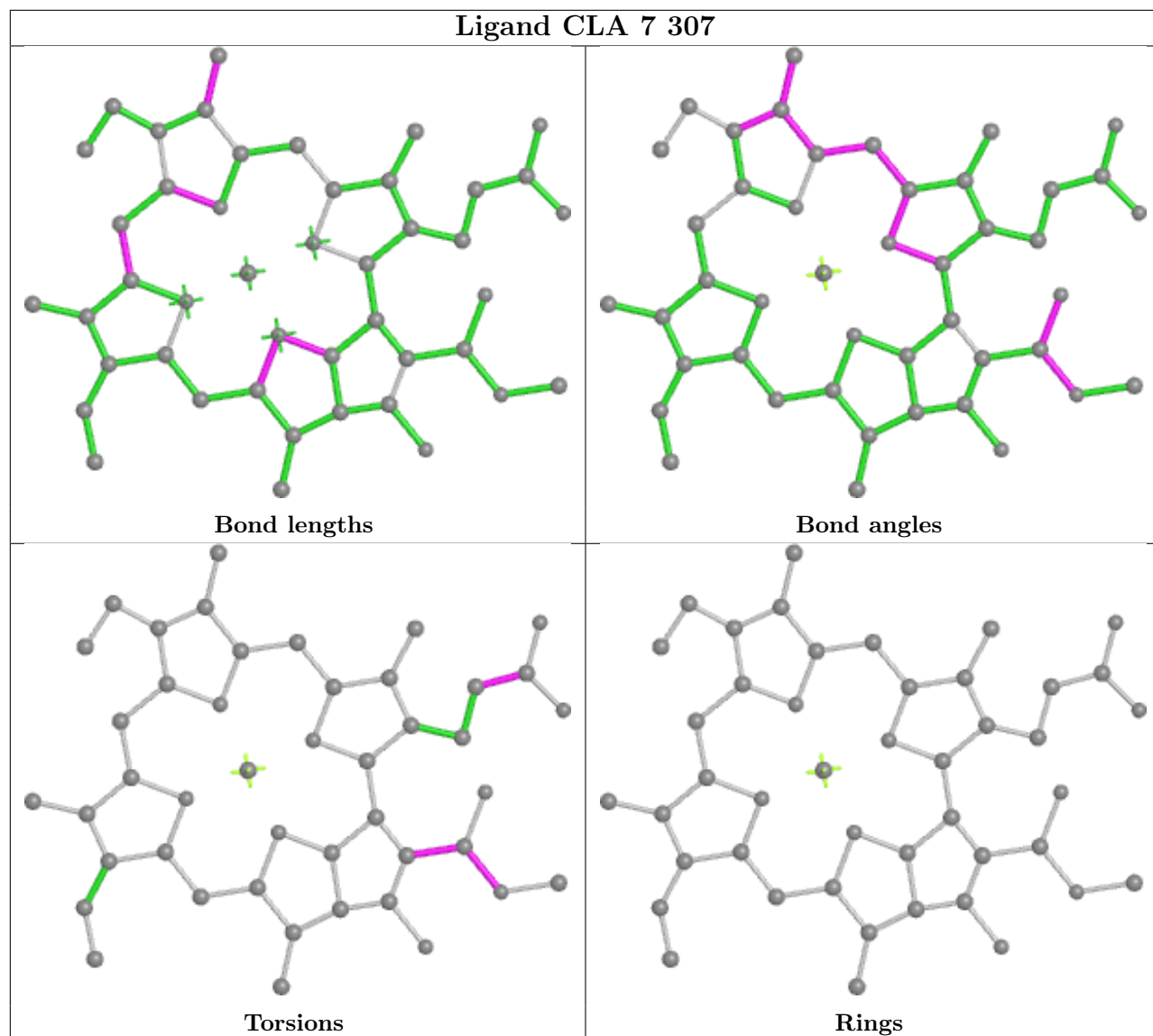


## Ligand CLA 1 308

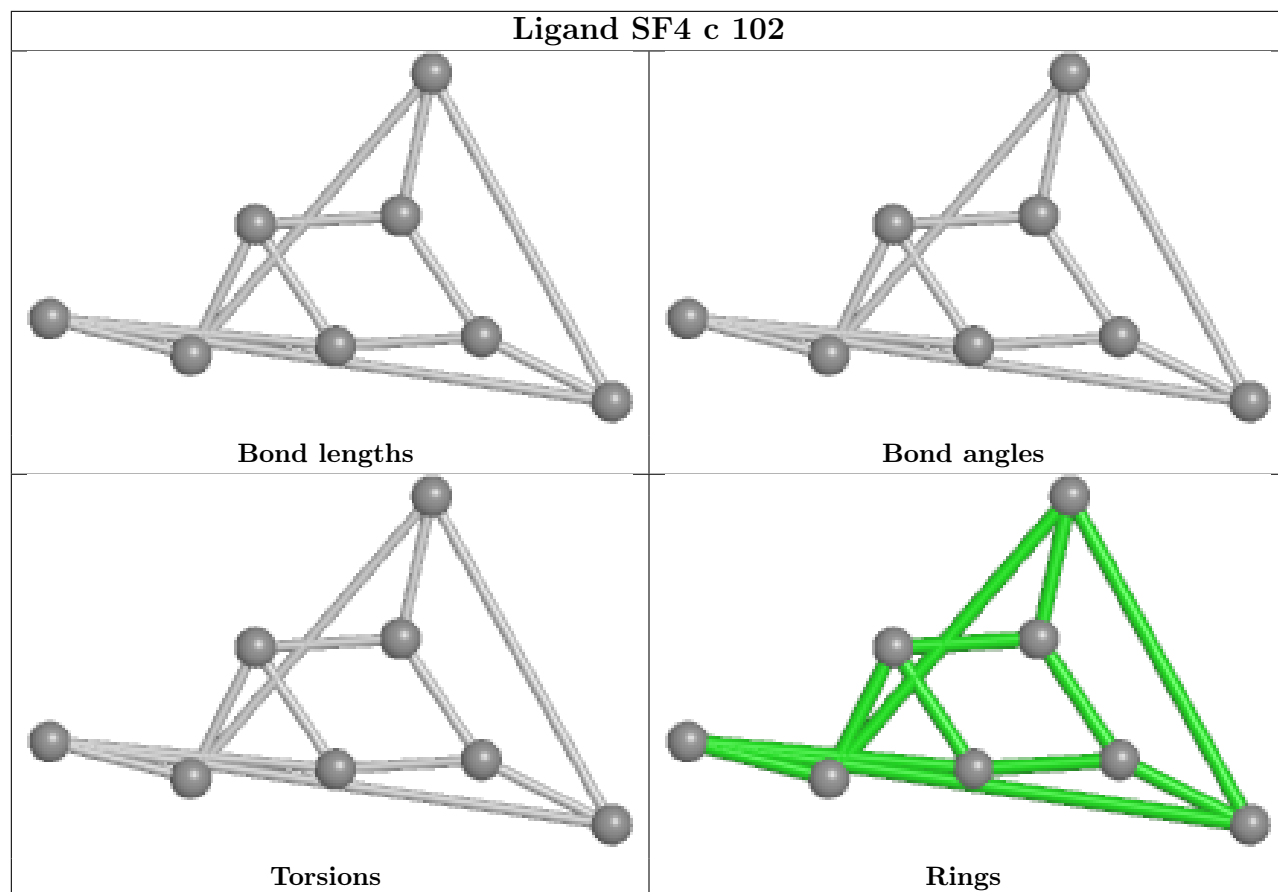


**Ligand CLA 8 308****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA a 831****Bond lengths****Bond angles****Torsions****Rings**

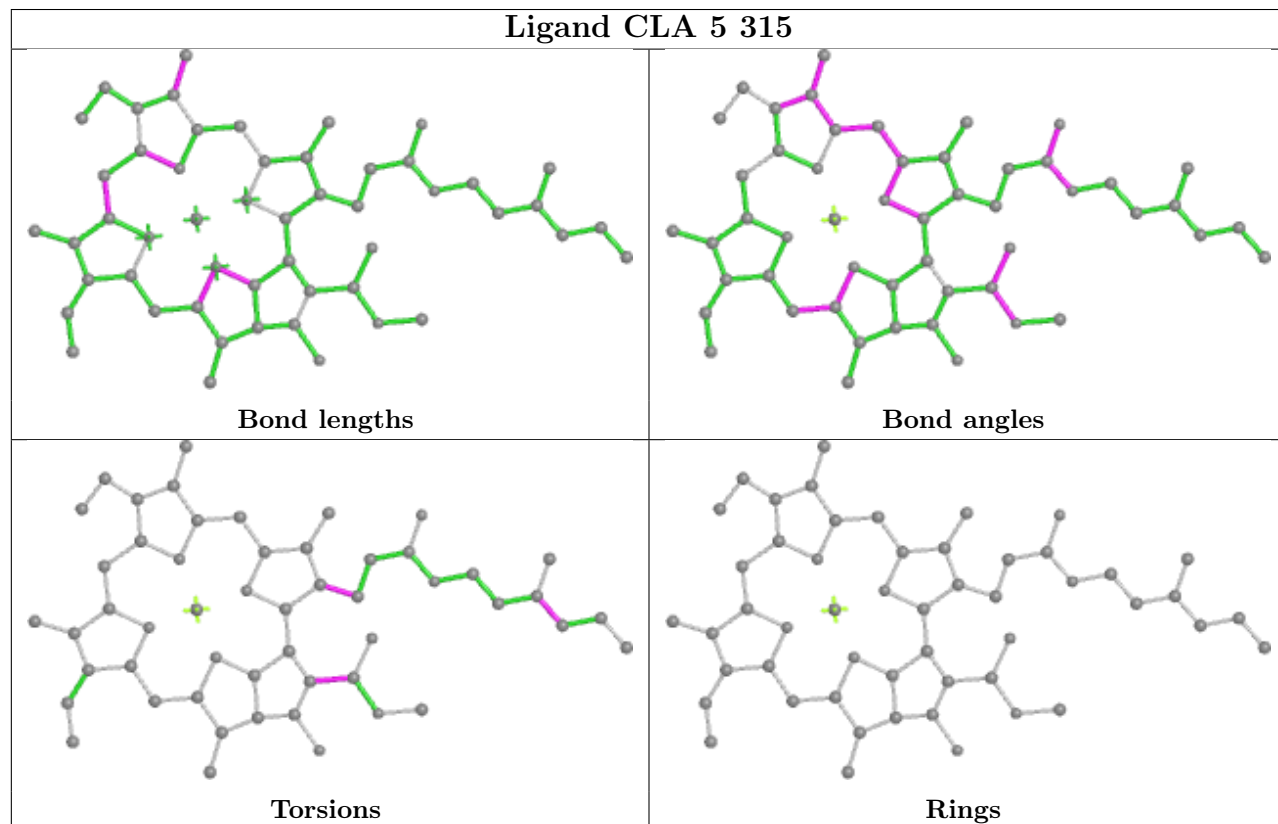
## Ligand CLA 7 307



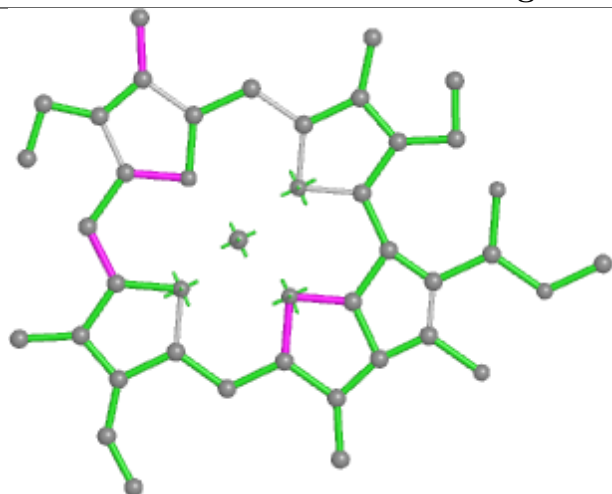
## Ligand SF4 c 102



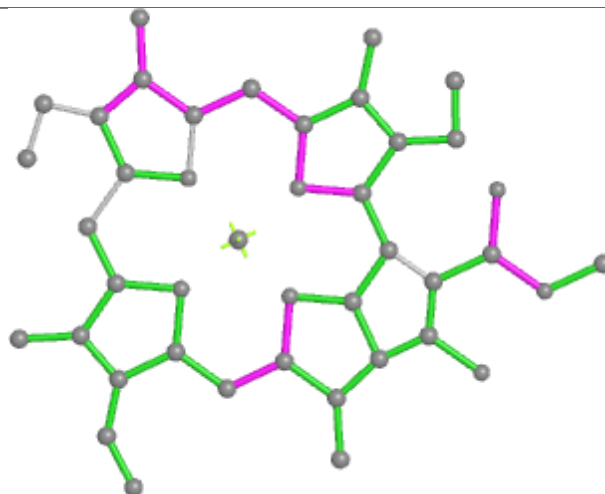
## Ligand CLA 5 315



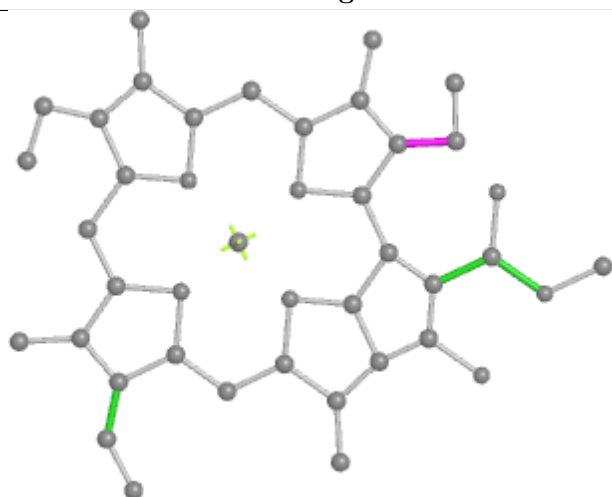
## Ligand CLA 6 311



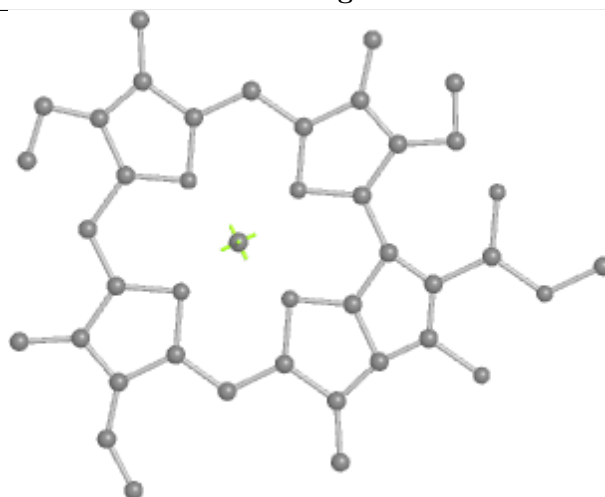
Bond lengths



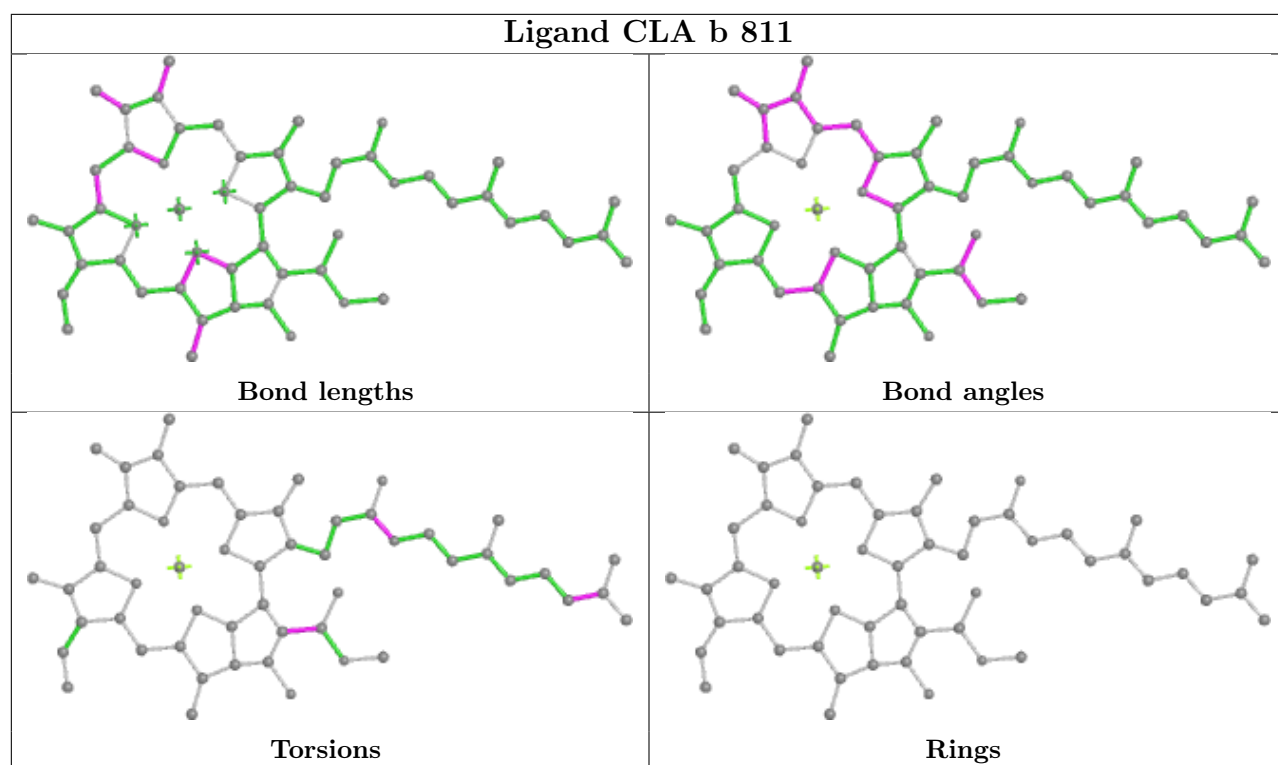
Bond angles



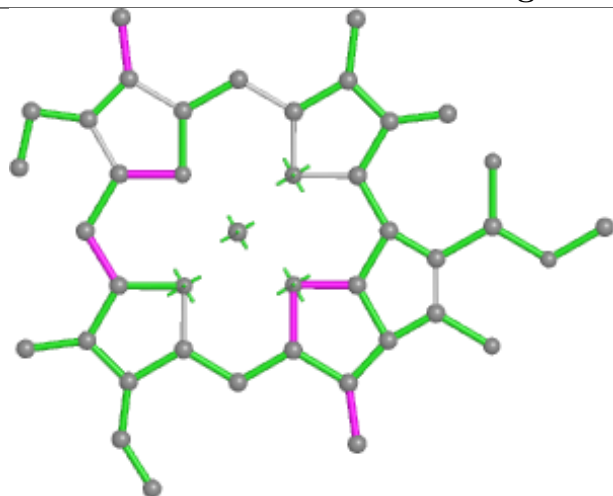
Torsions



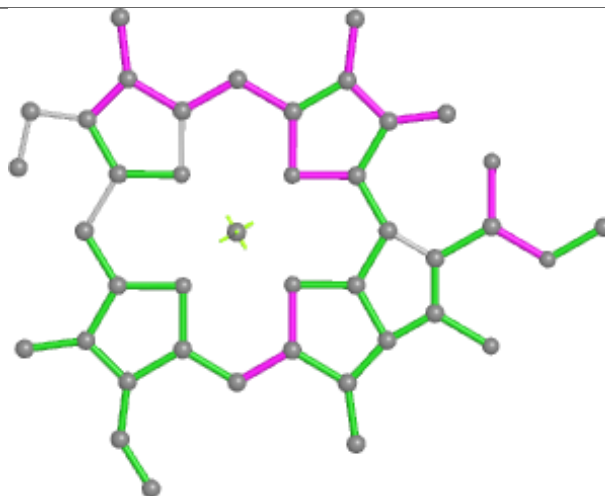
Rings



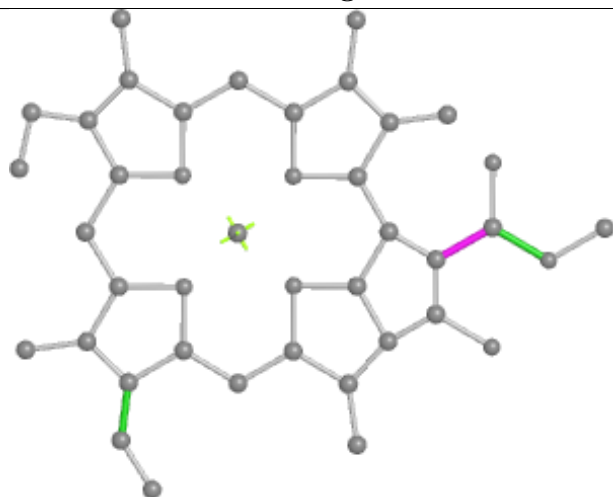
## Ligand CLA b 830



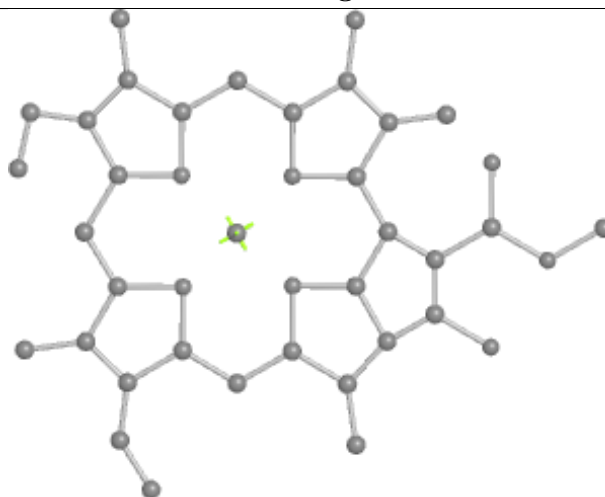
Bond lengths



Bond angles

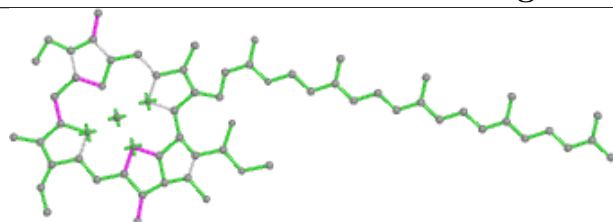


Torsions

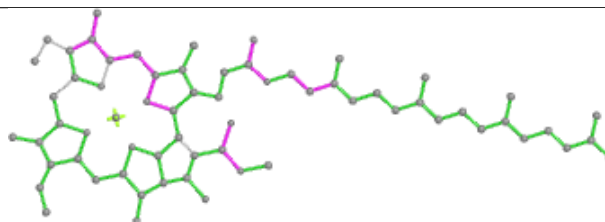


Rings

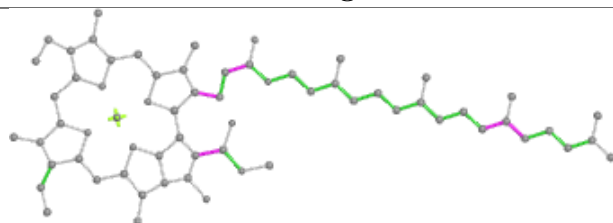
## Ligand CLA b 838



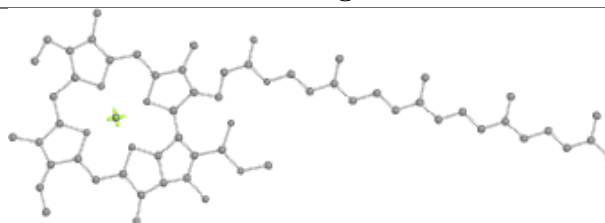
Bond lengths



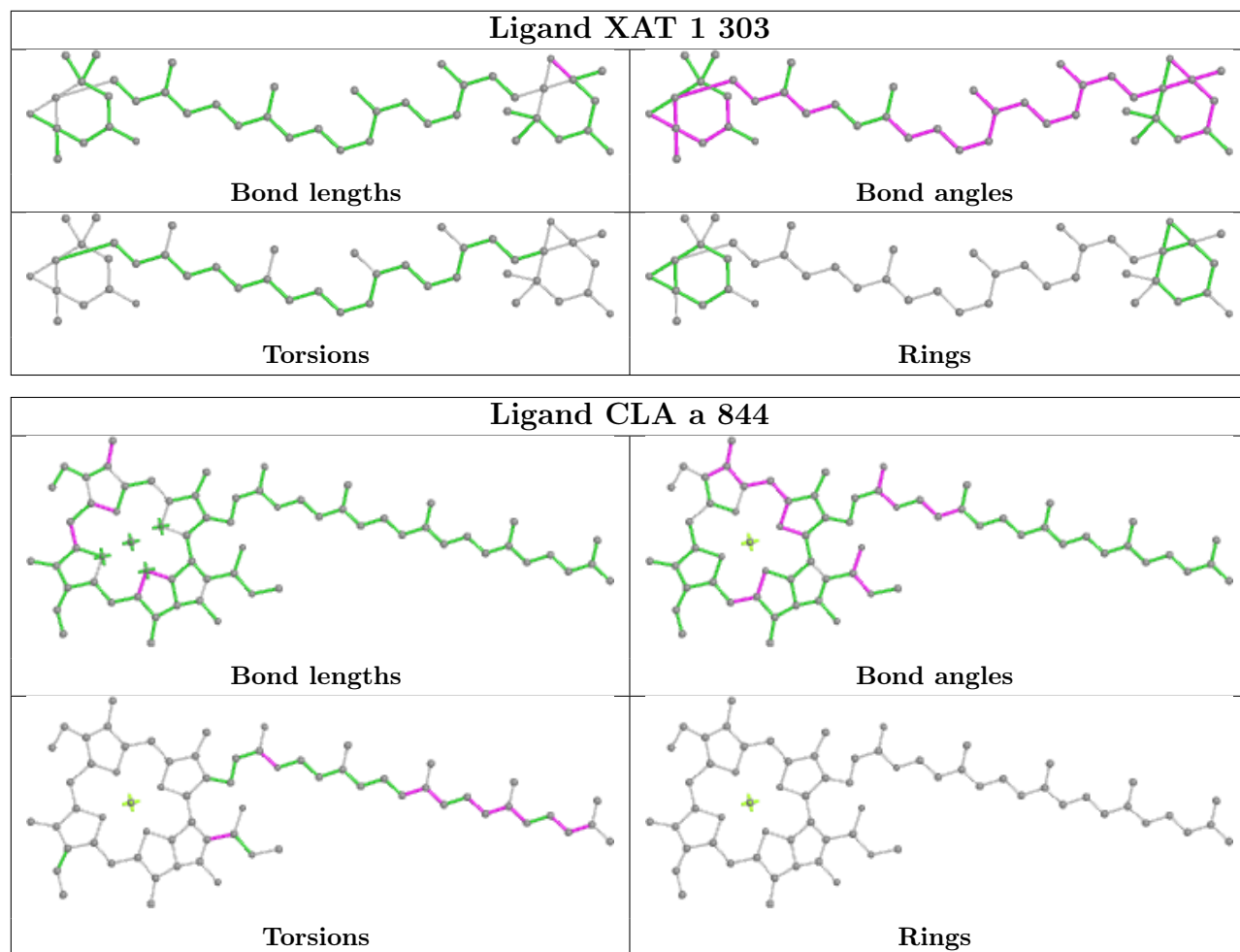
Bond angles



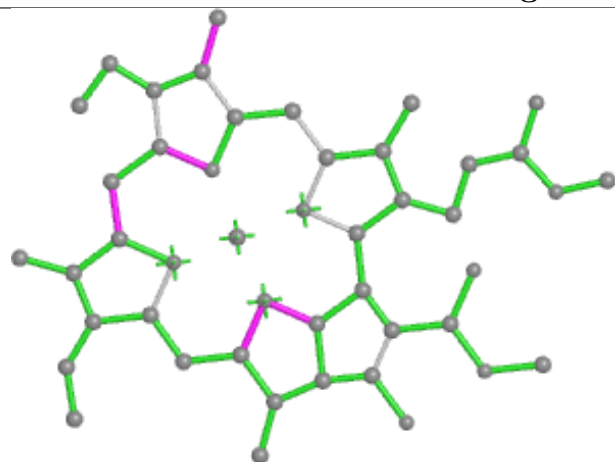
Torsions



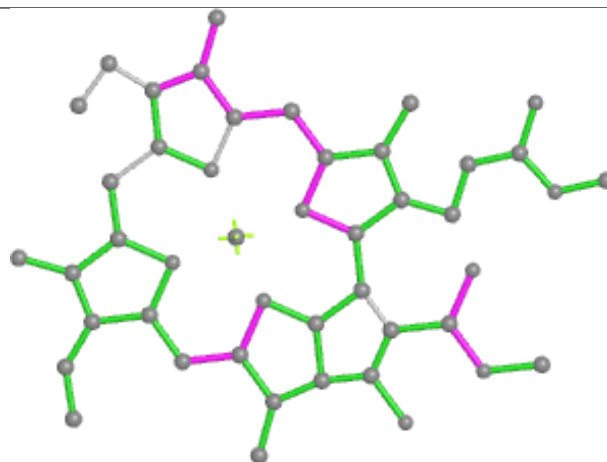
Rings



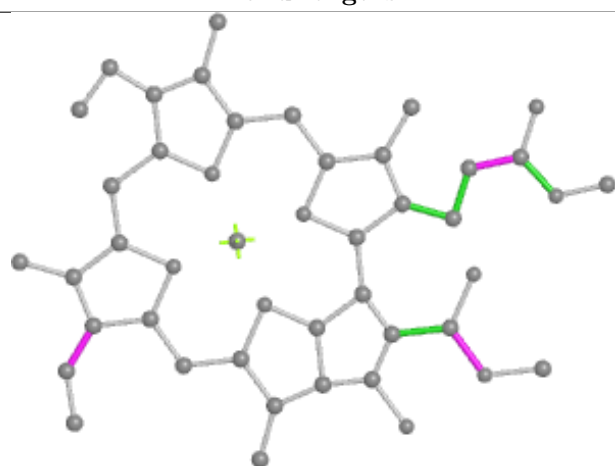
## Ligand CLA 5 316



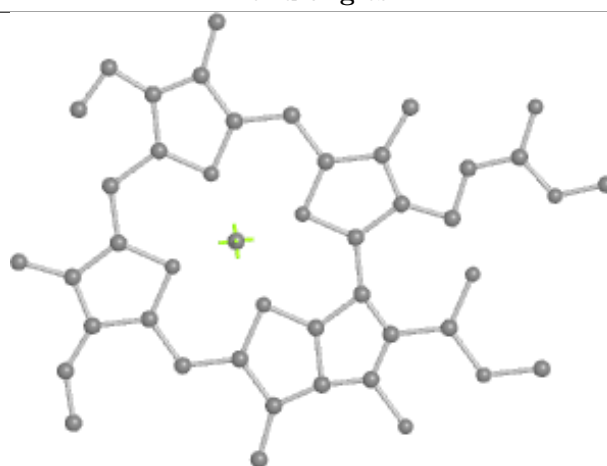
Bond lengths



Bond angles

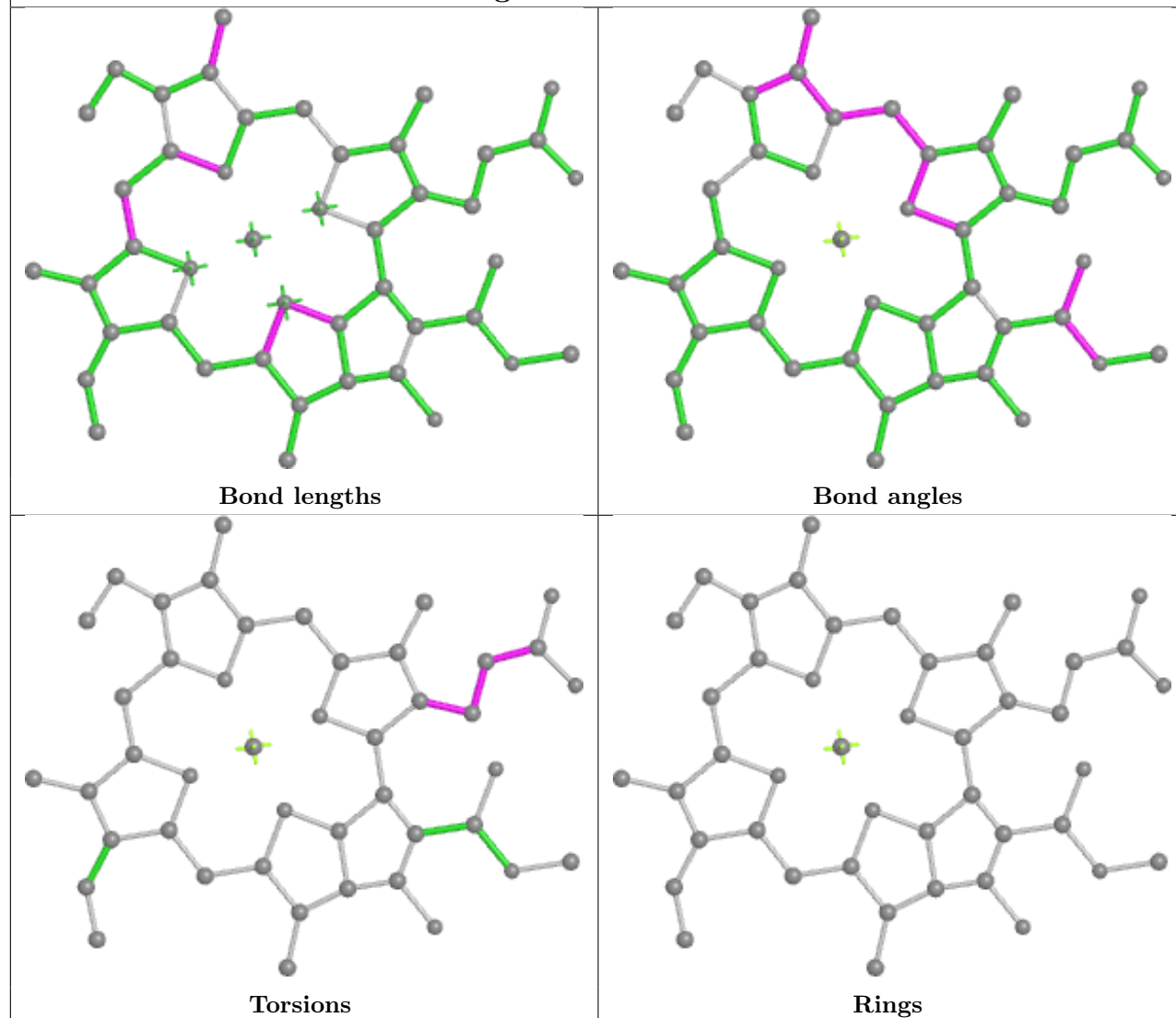


Torsions

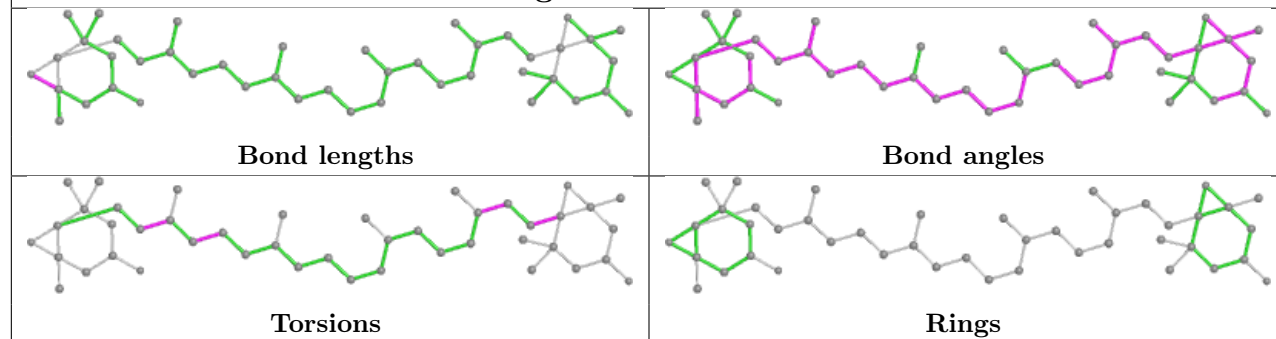


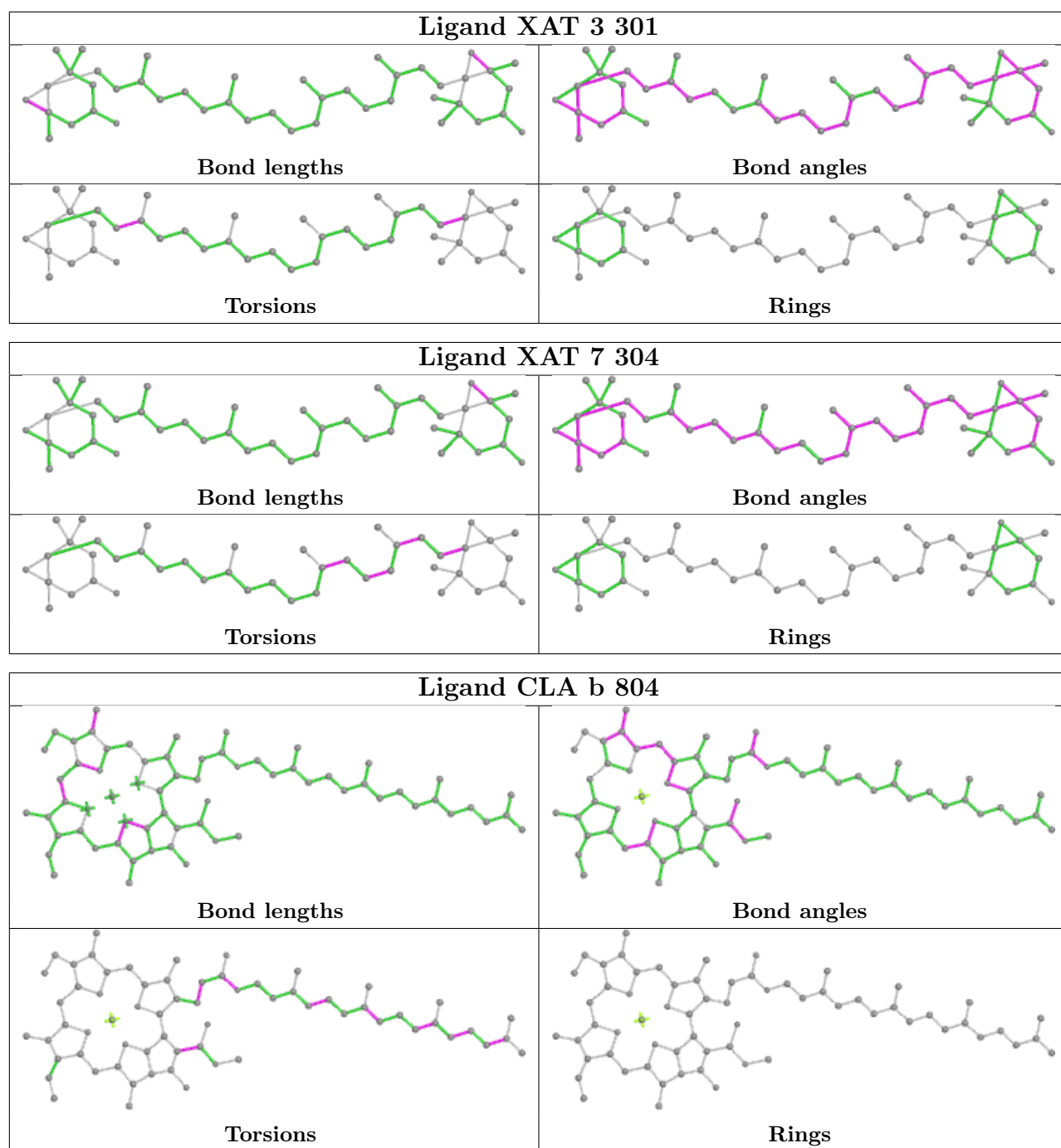
Rings

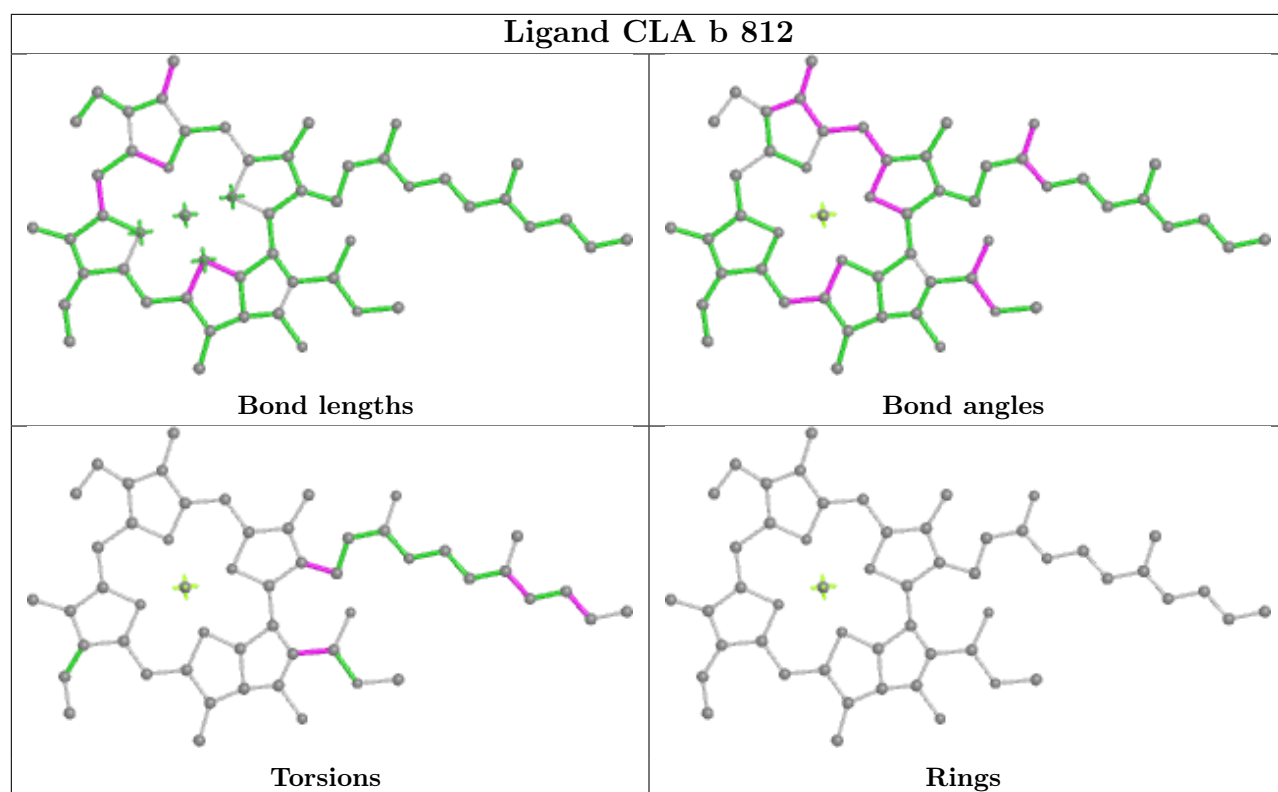
## Ligand CLA 1 314



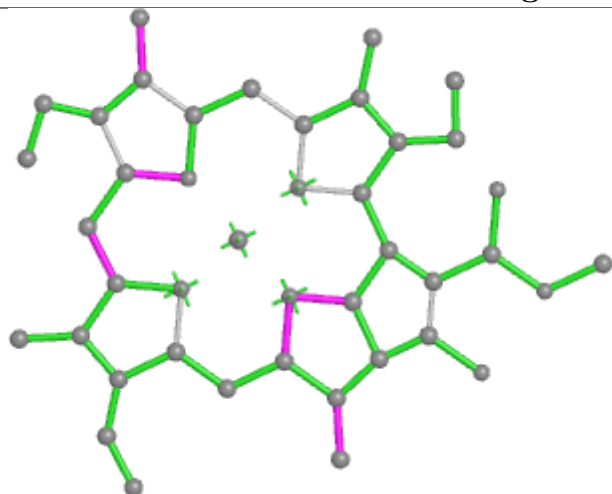
## Ligand XAT 7 301



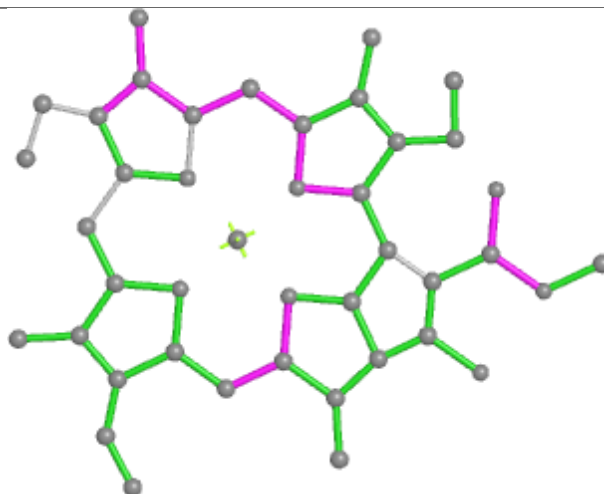




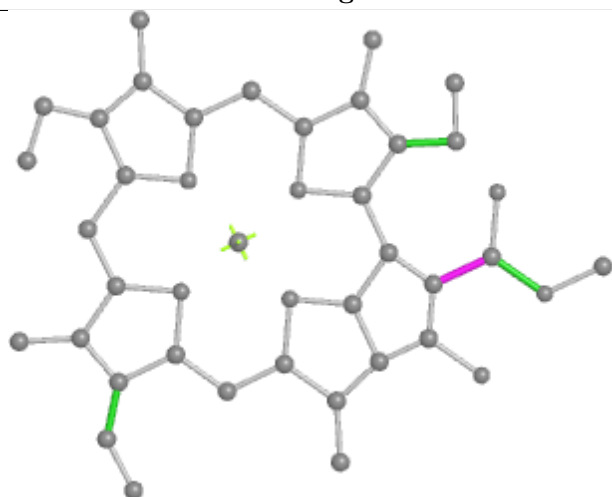
## Ligand CLA l 201



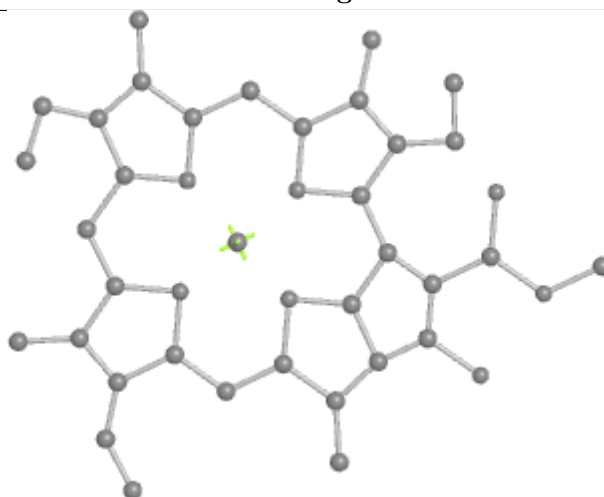
Bond lengths



Bond angles

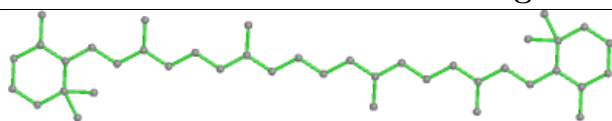


Torsions

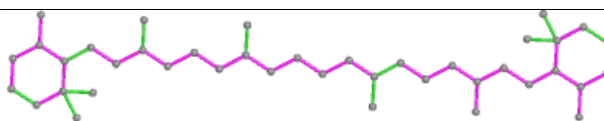


Rings

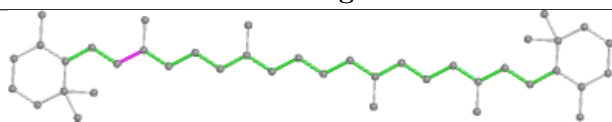
## Ligand BCR b 843



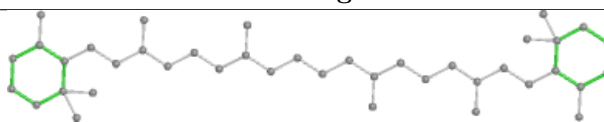
Bond lengths



Bond angles

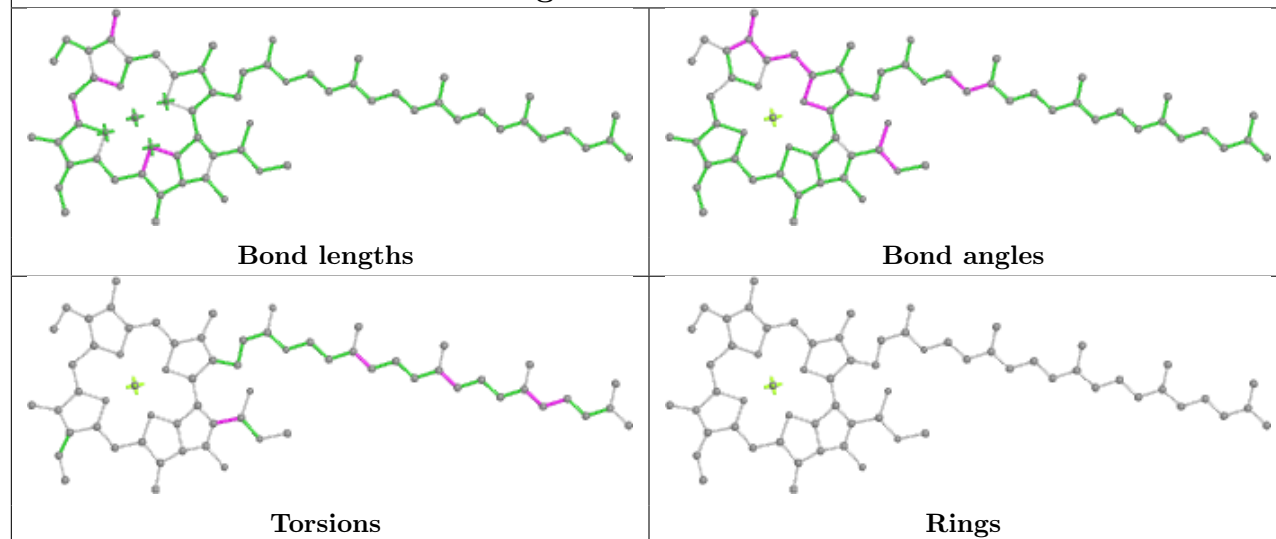


Torsions

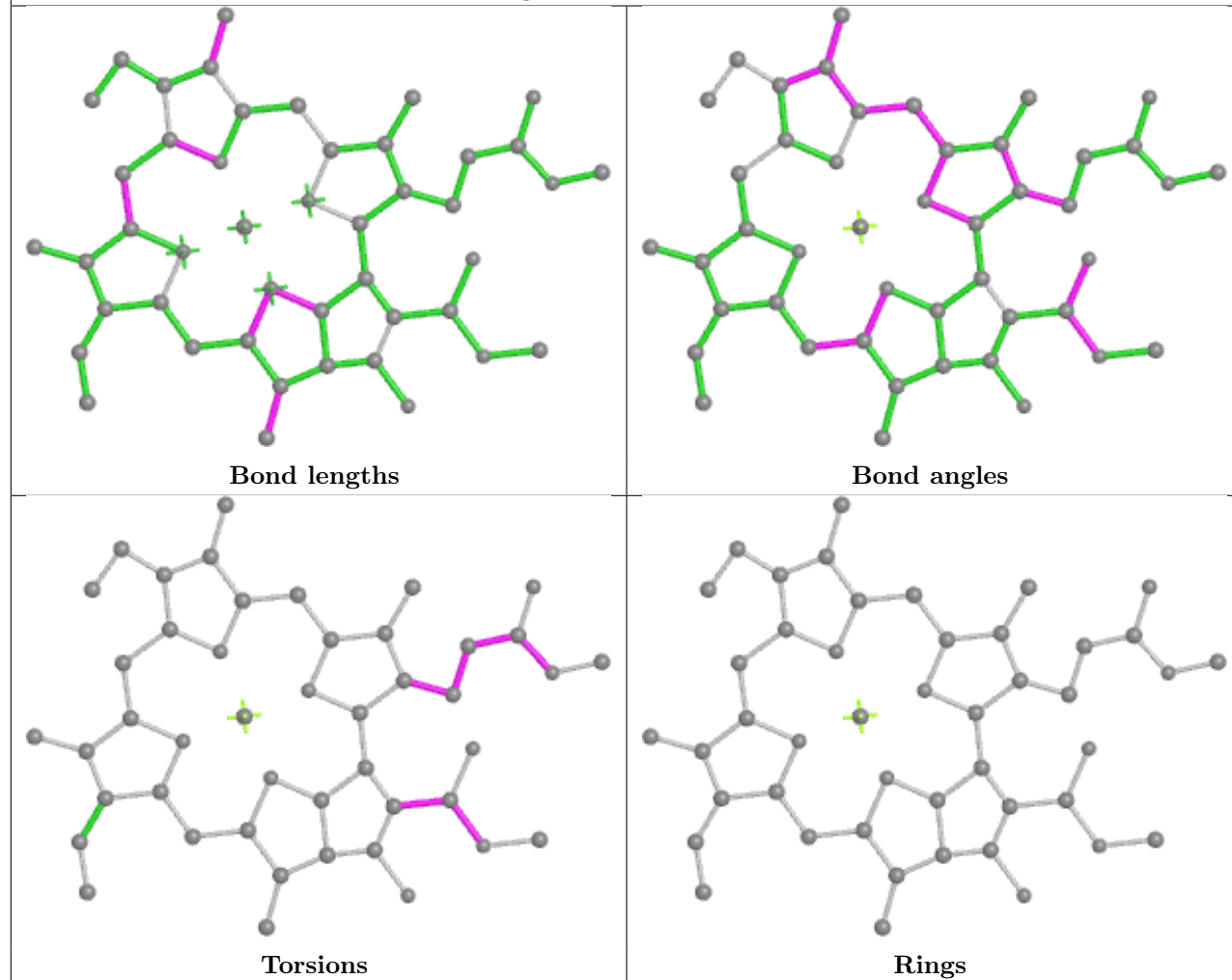


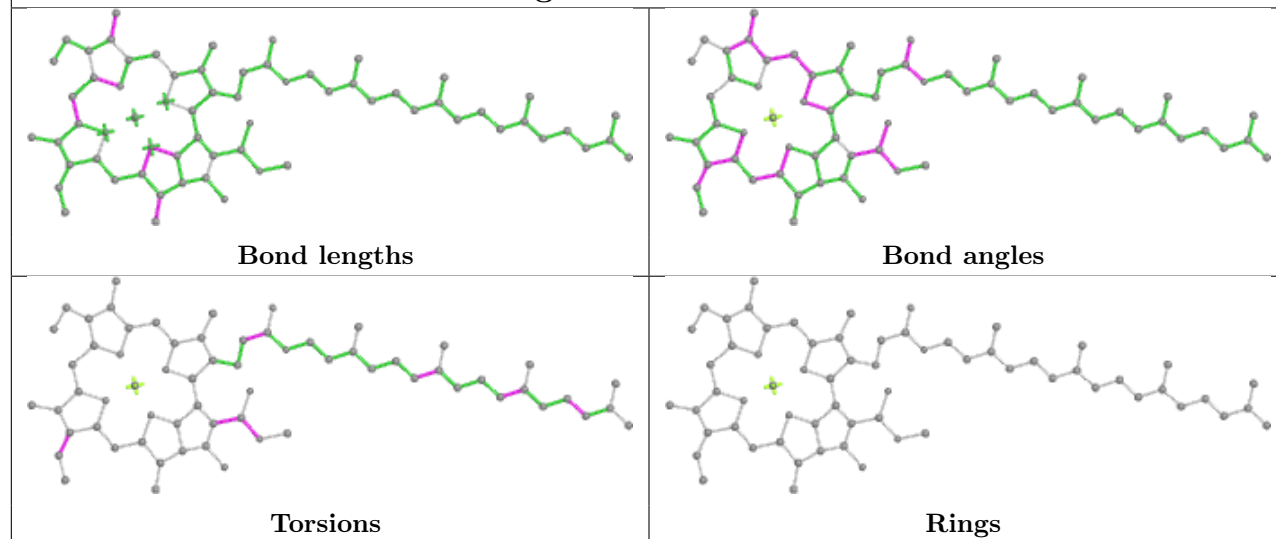
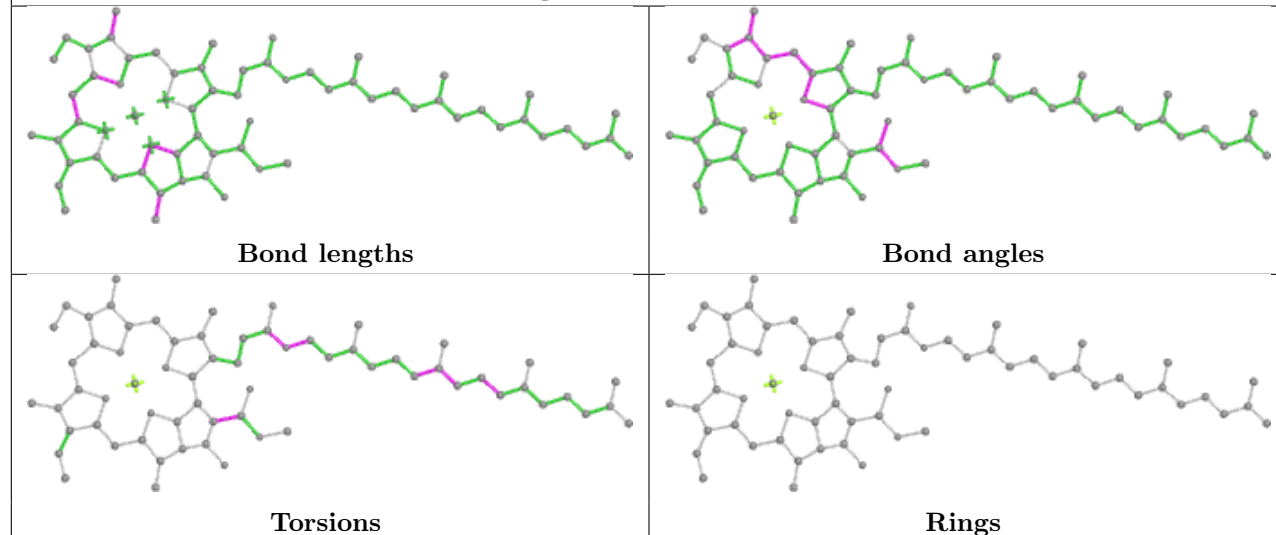
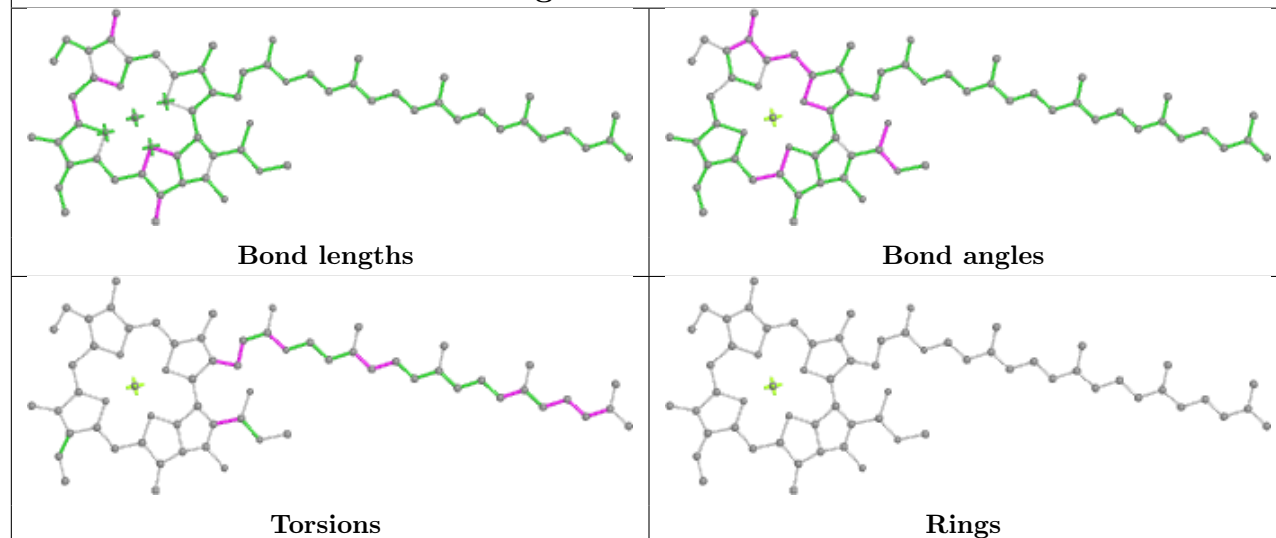
Rings

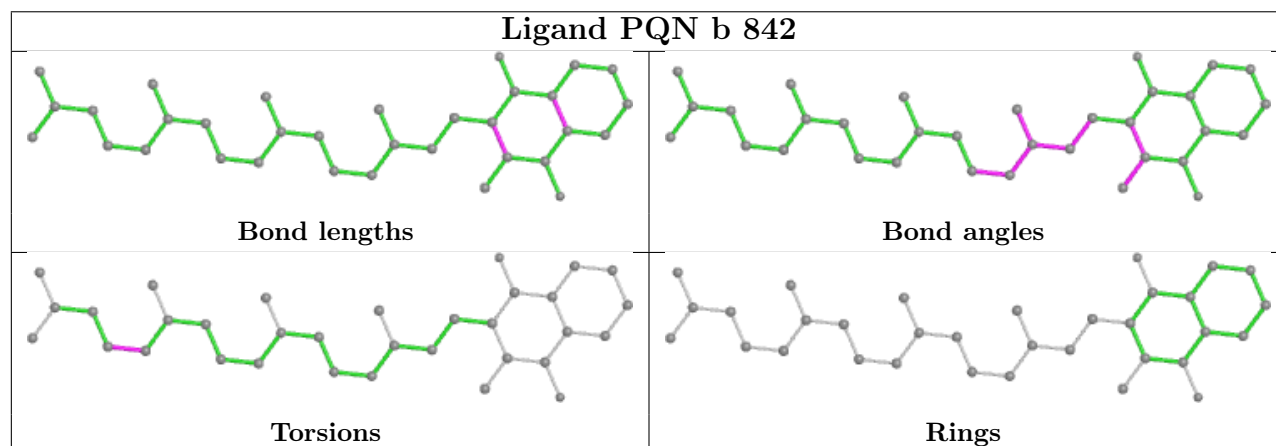
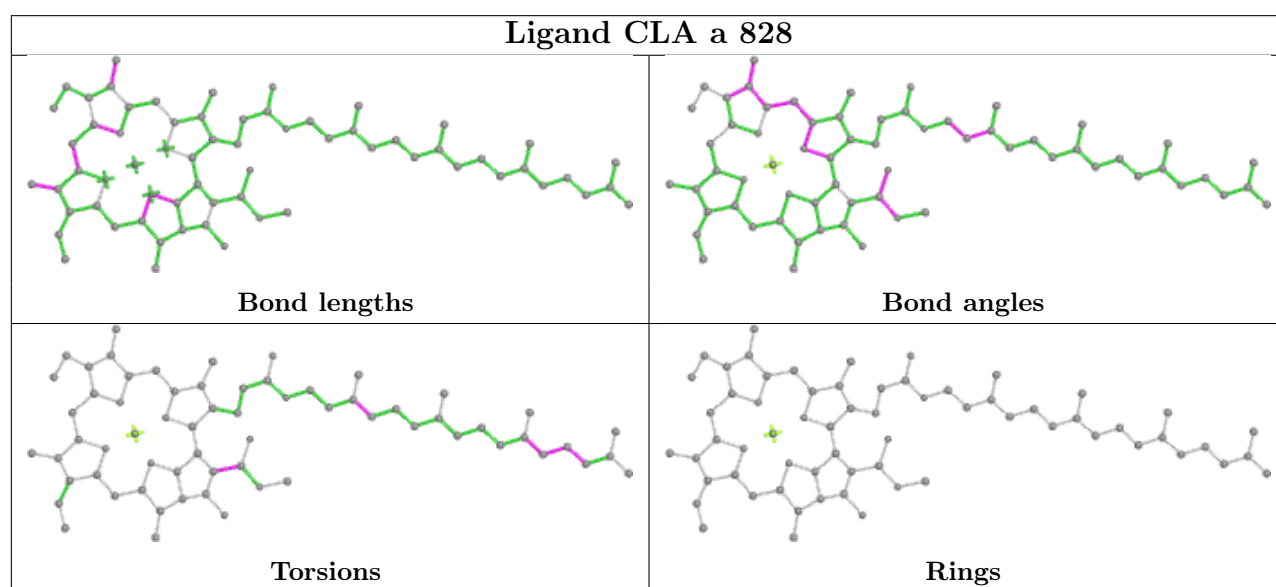
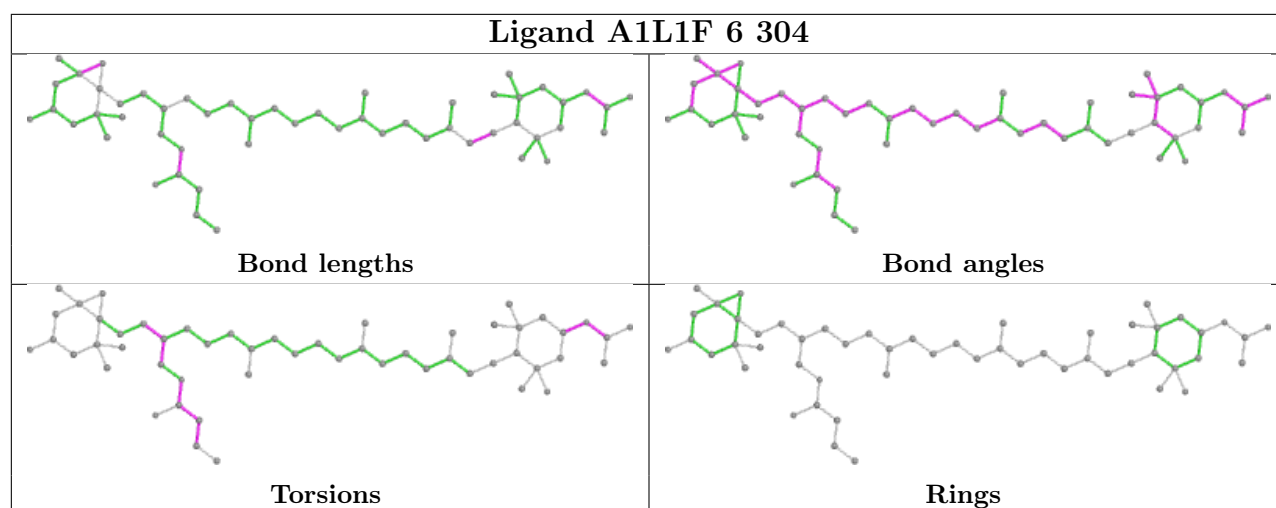
## Ligand CLA a 840



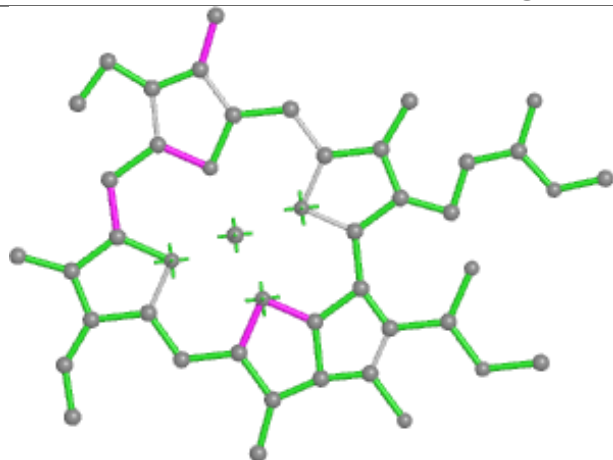
## Ligand CLA 9 312



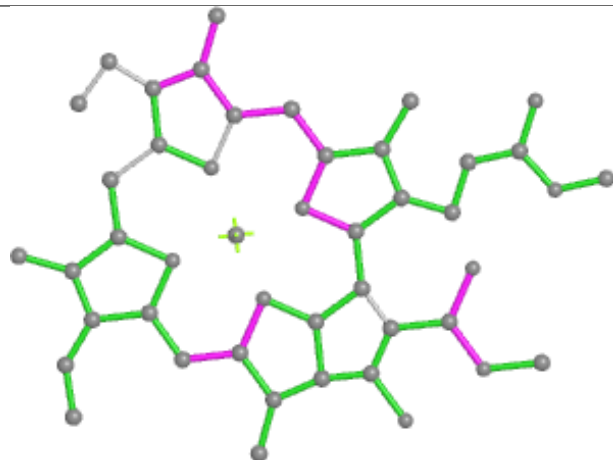
**Ligand CLA b 803****Ligand CLA 6 309****Ligand CLA b 834**



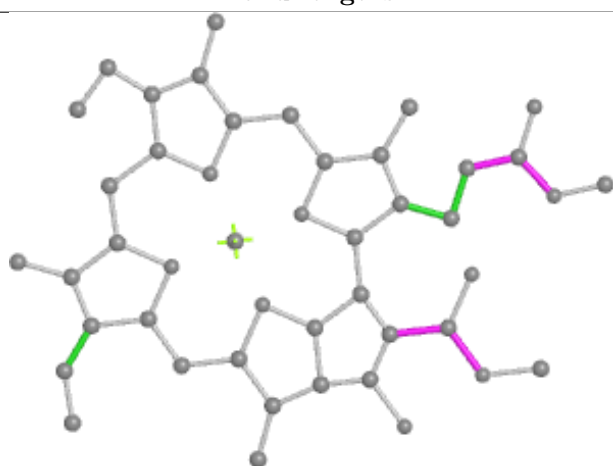
## Ligand CLA 1 309



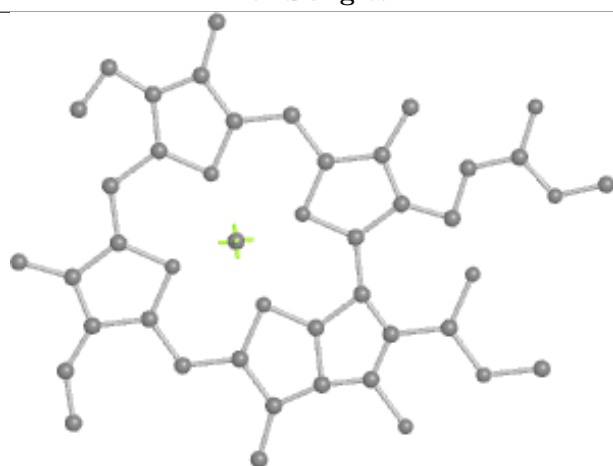
Bond lengths



Bond angles

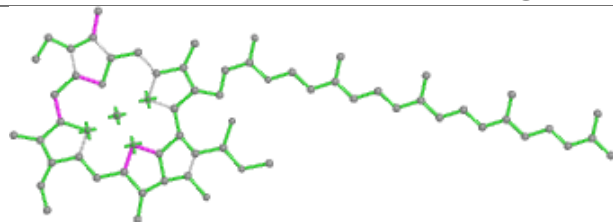


Torsions

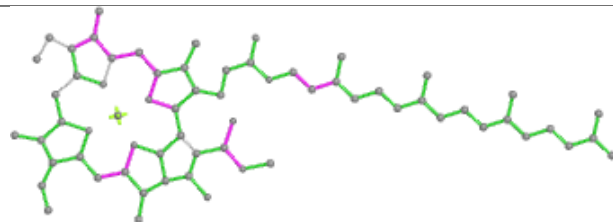


Rings

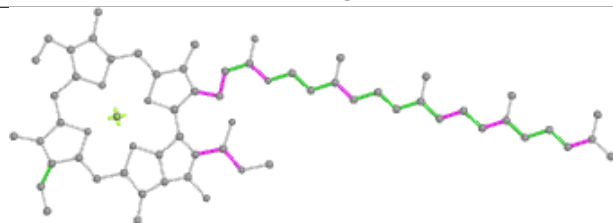
## Ligand CLA b 810



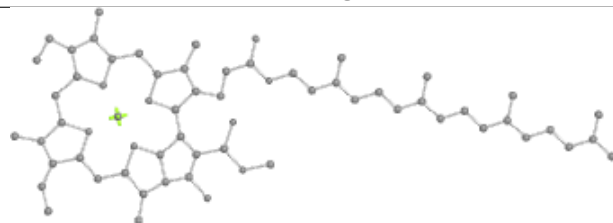
Bond lengths



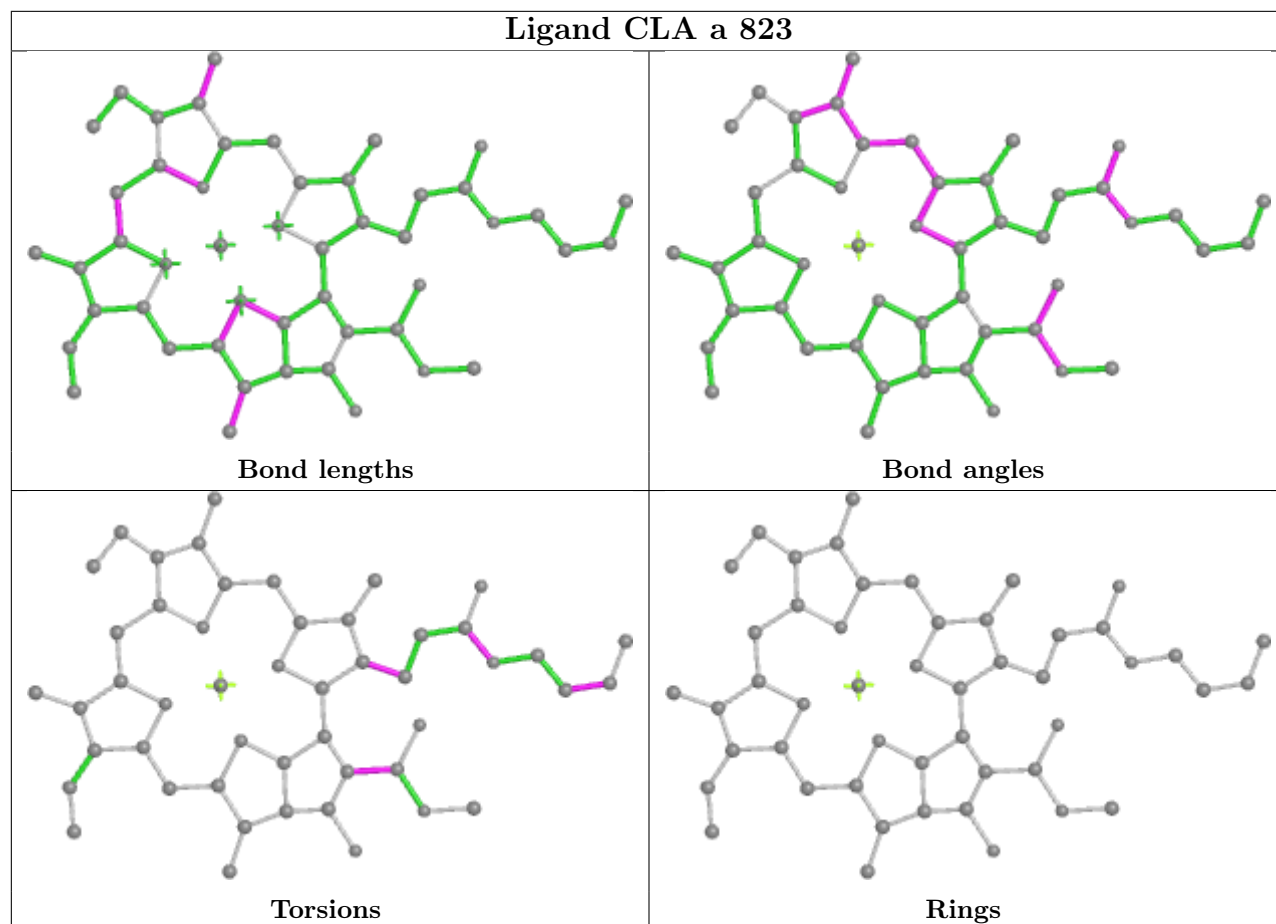
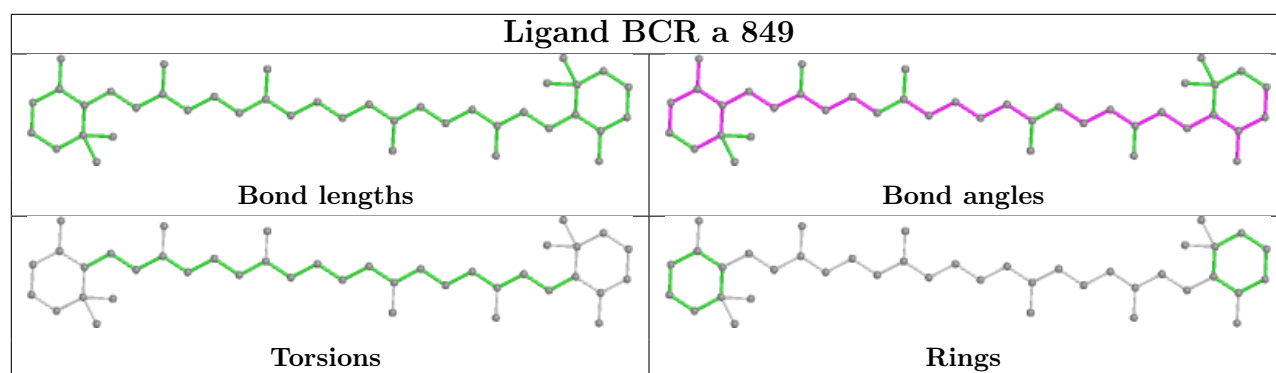
Bond angles



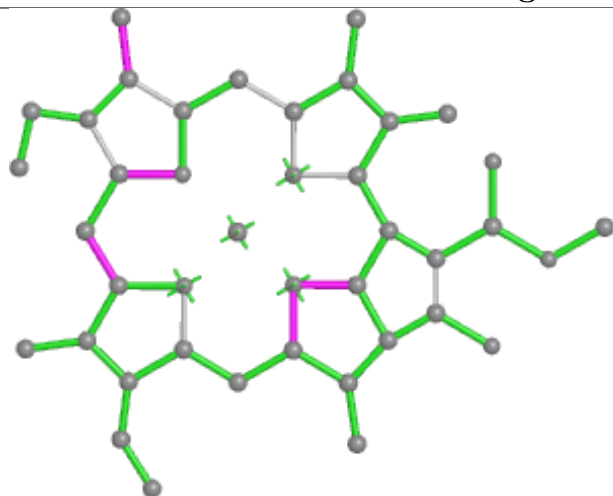
Torsions



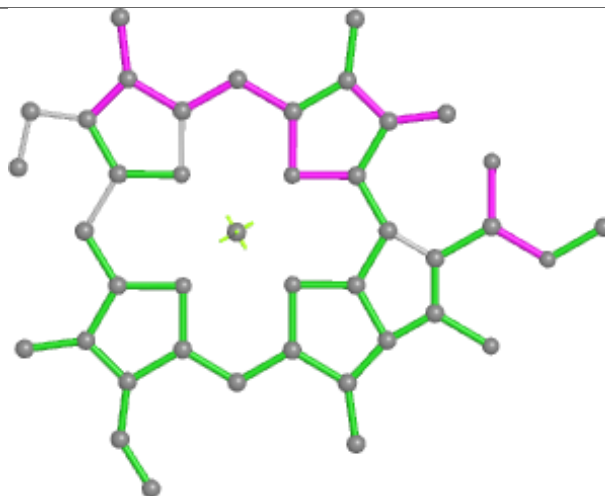
Rings



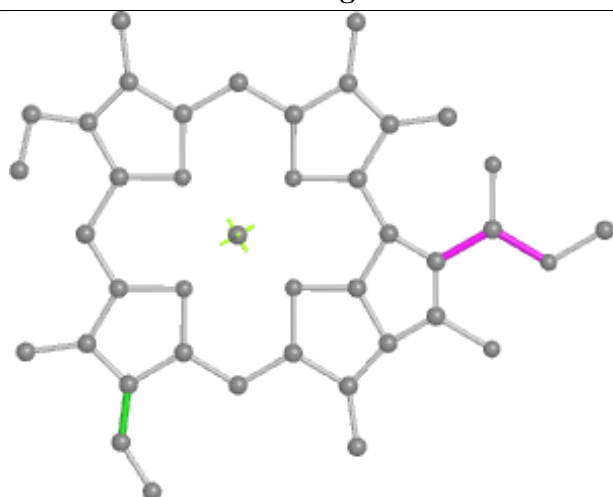
## Ligand CLA 8 314



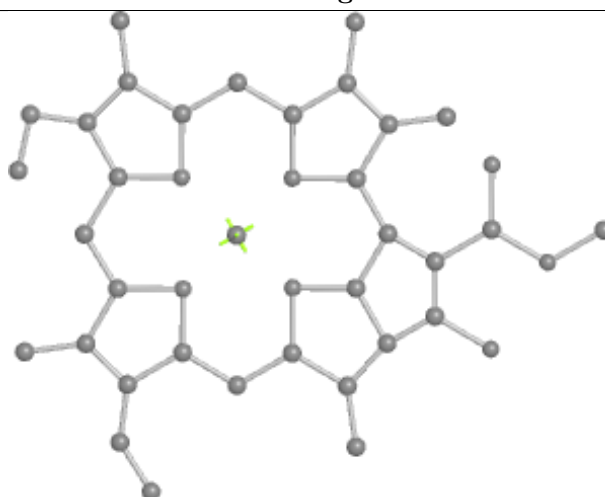
Bond lengths



Bond angles

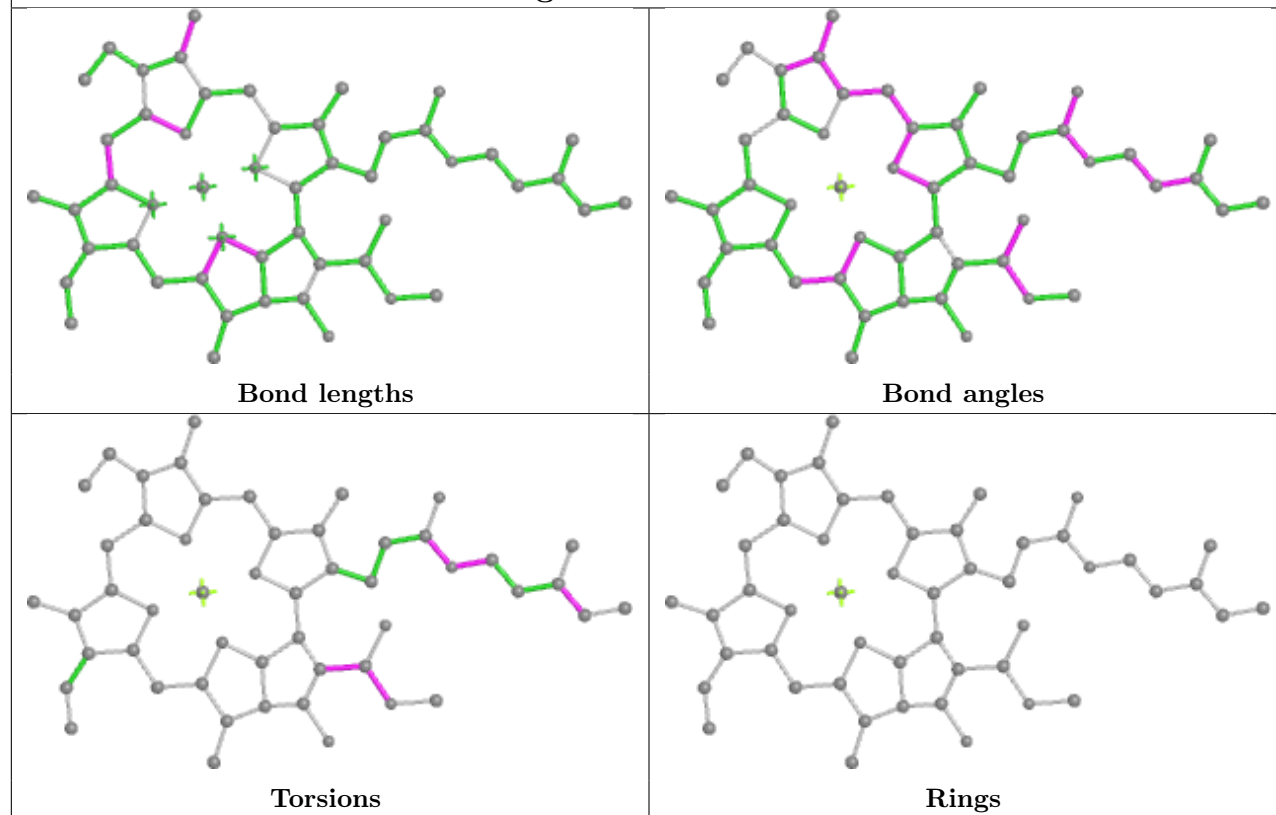


Torsions

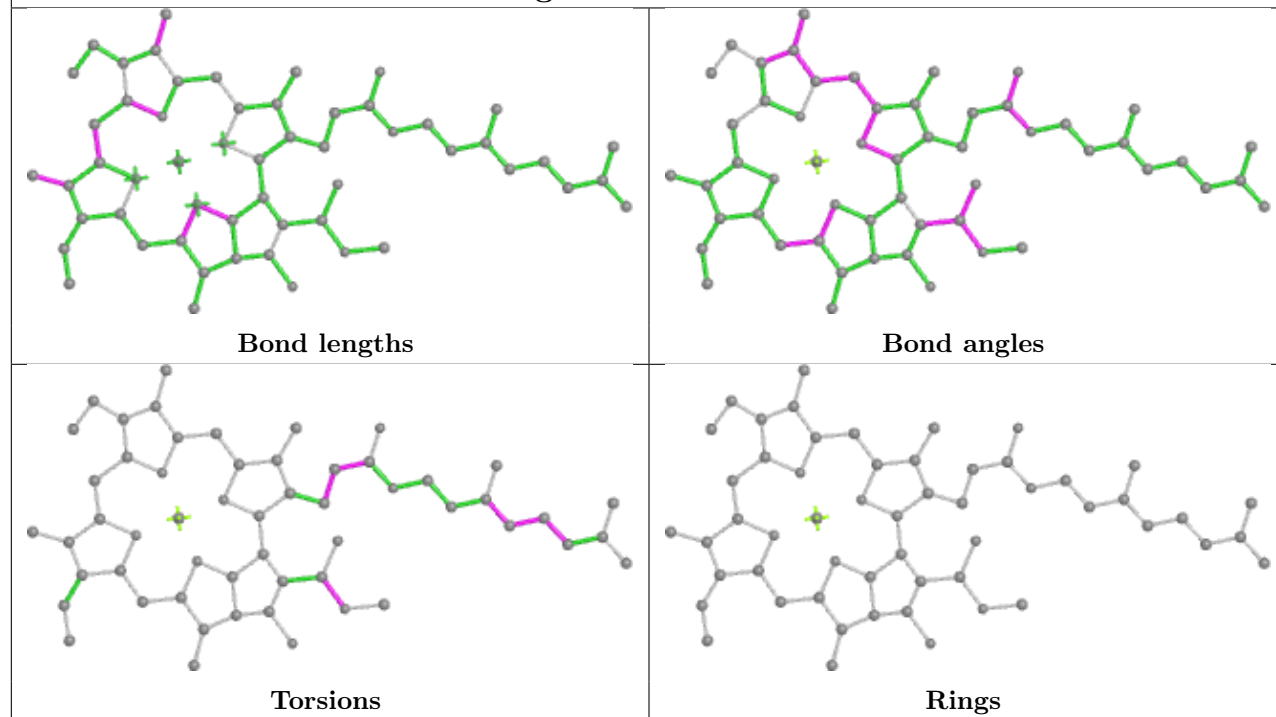


Rings

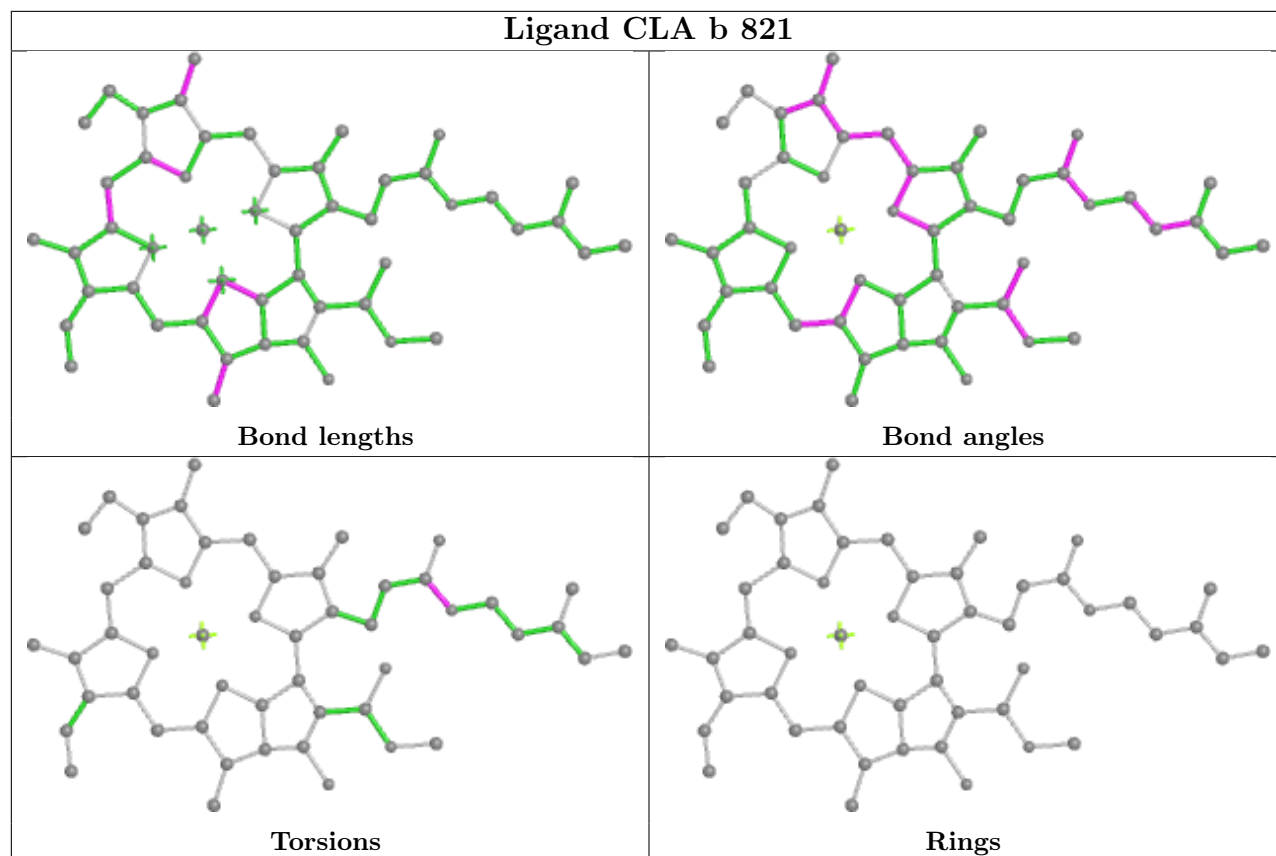
## Ligand CLA 5 312



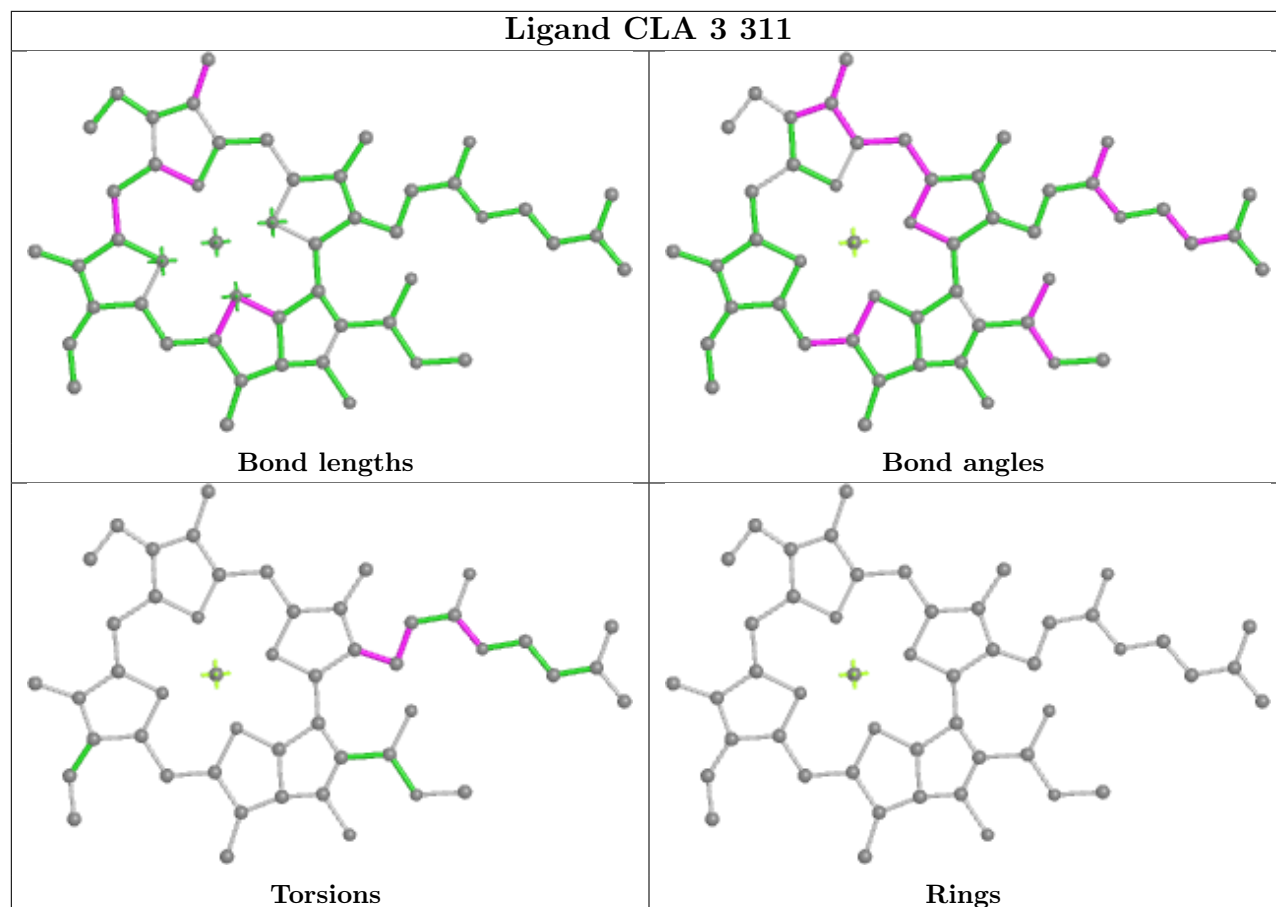
## Ligand CLA h 203

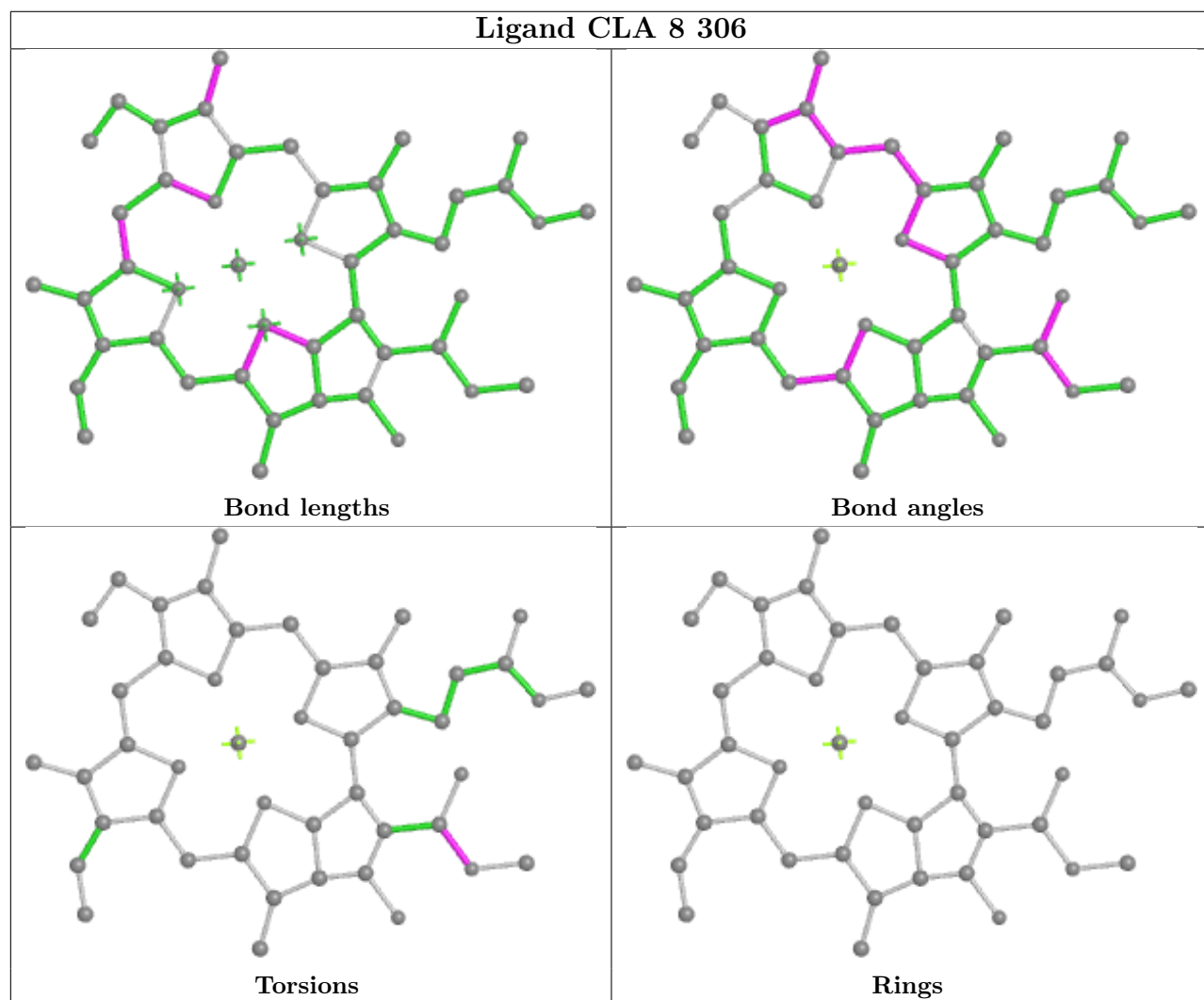
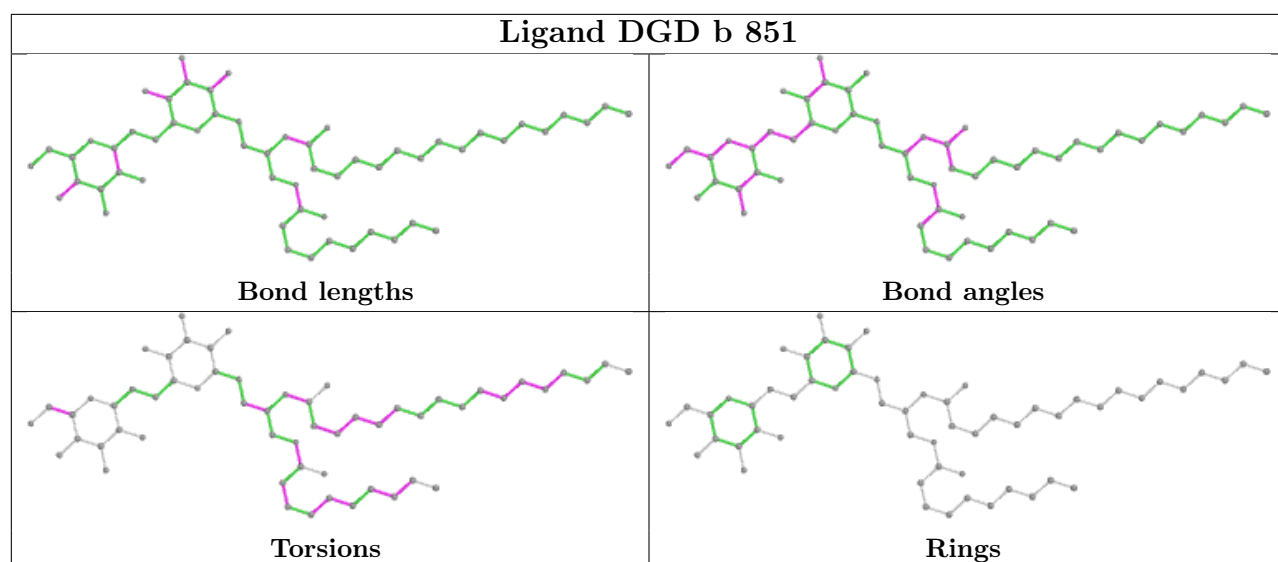


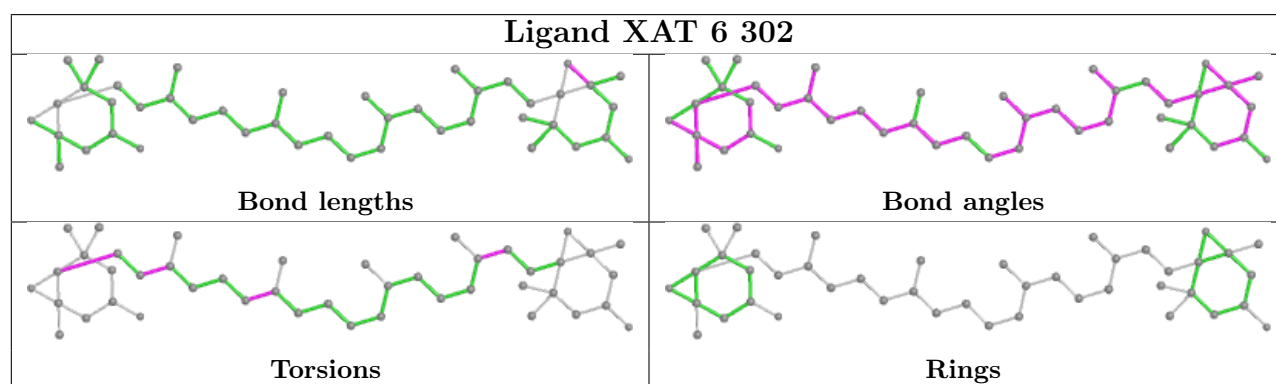
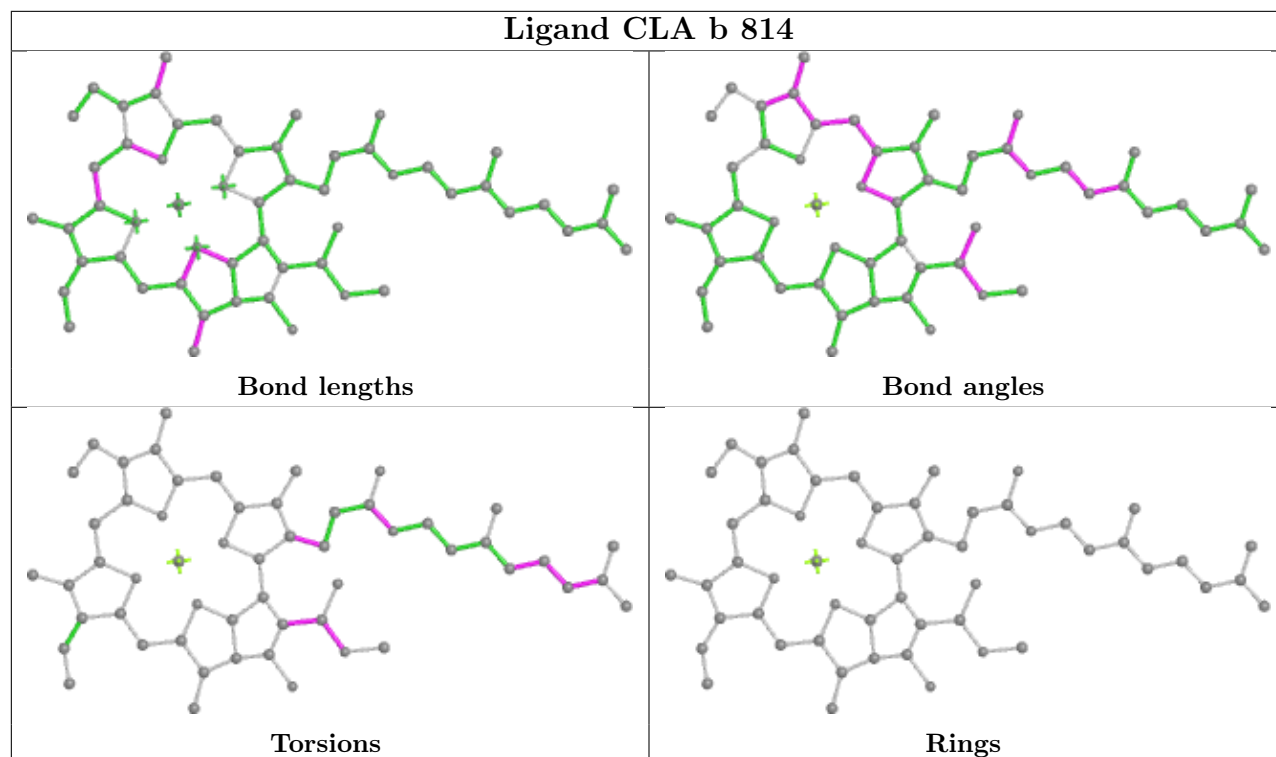
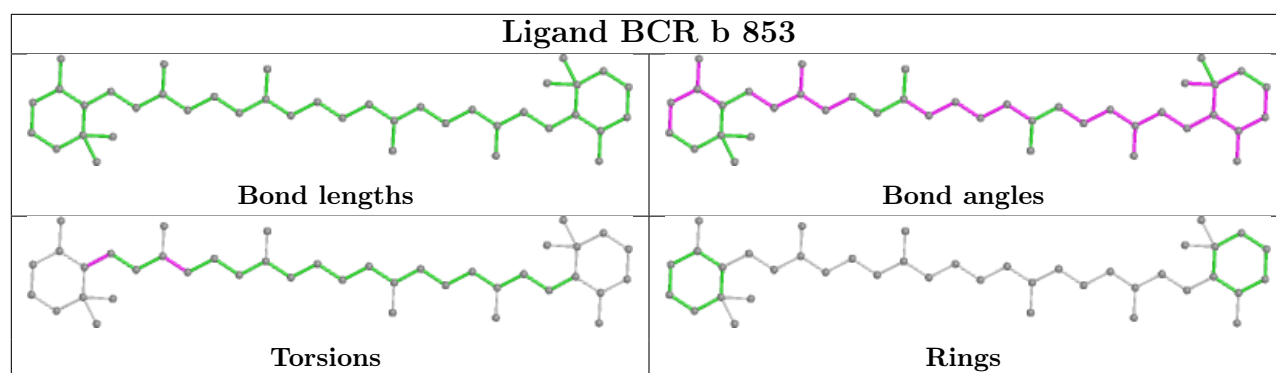
## Ligand CLA b 821

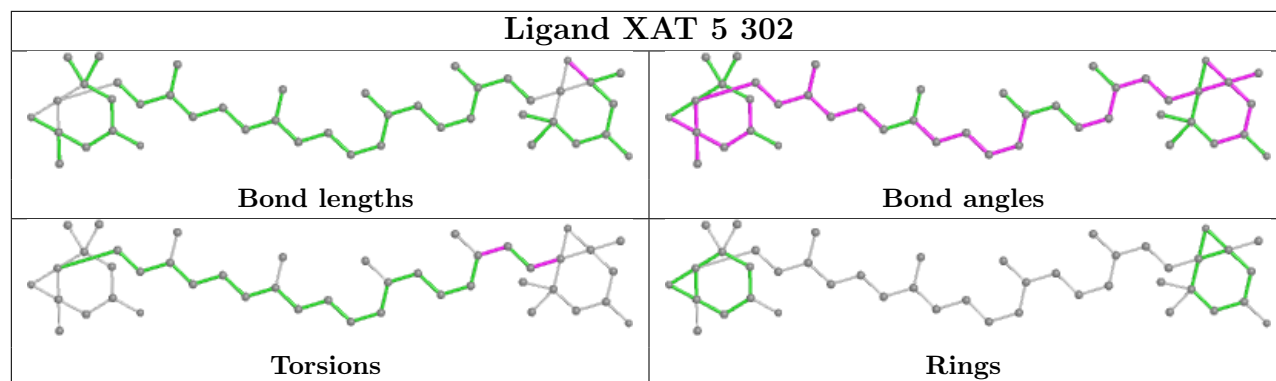
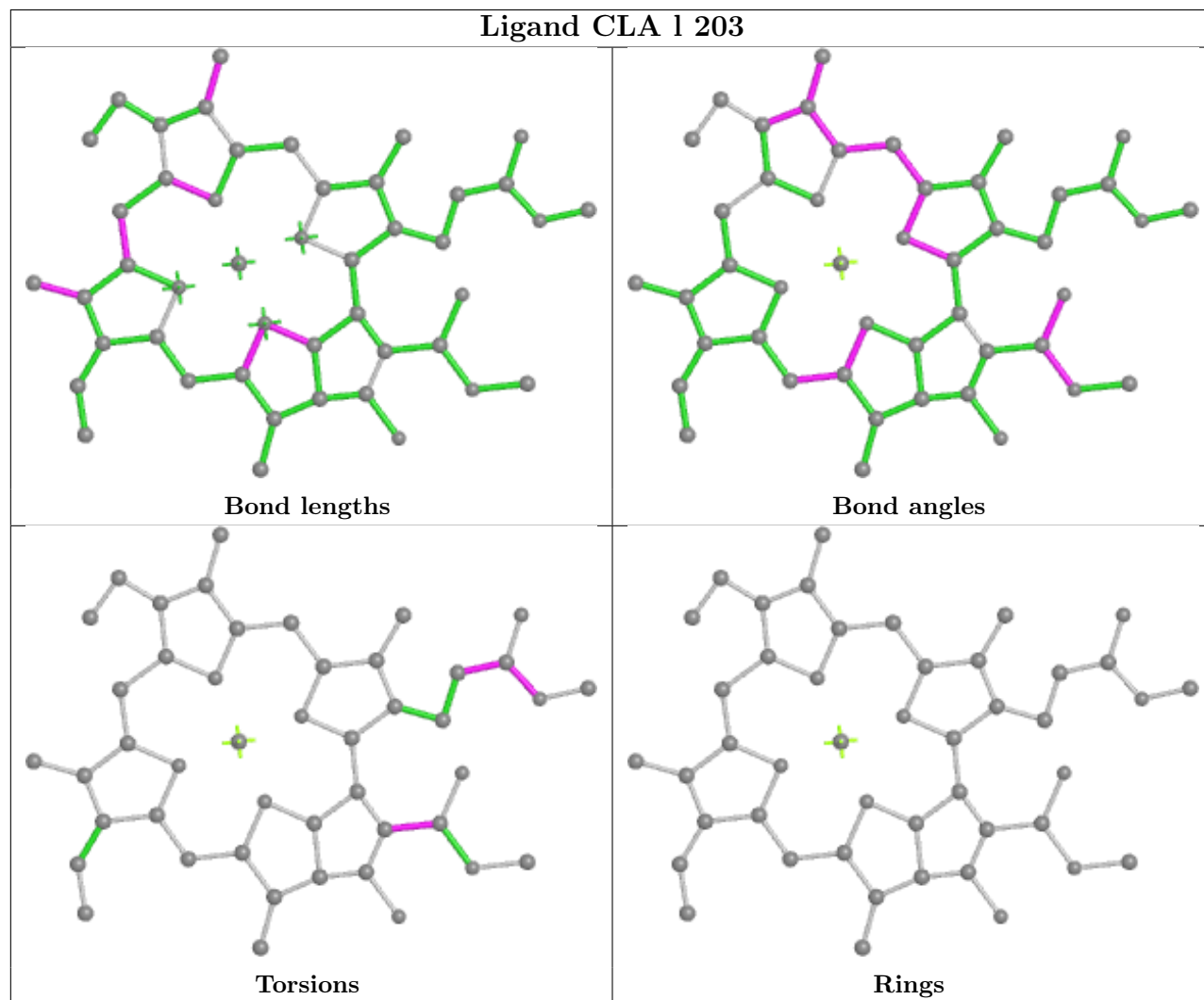


## Ligand CLA 3 311

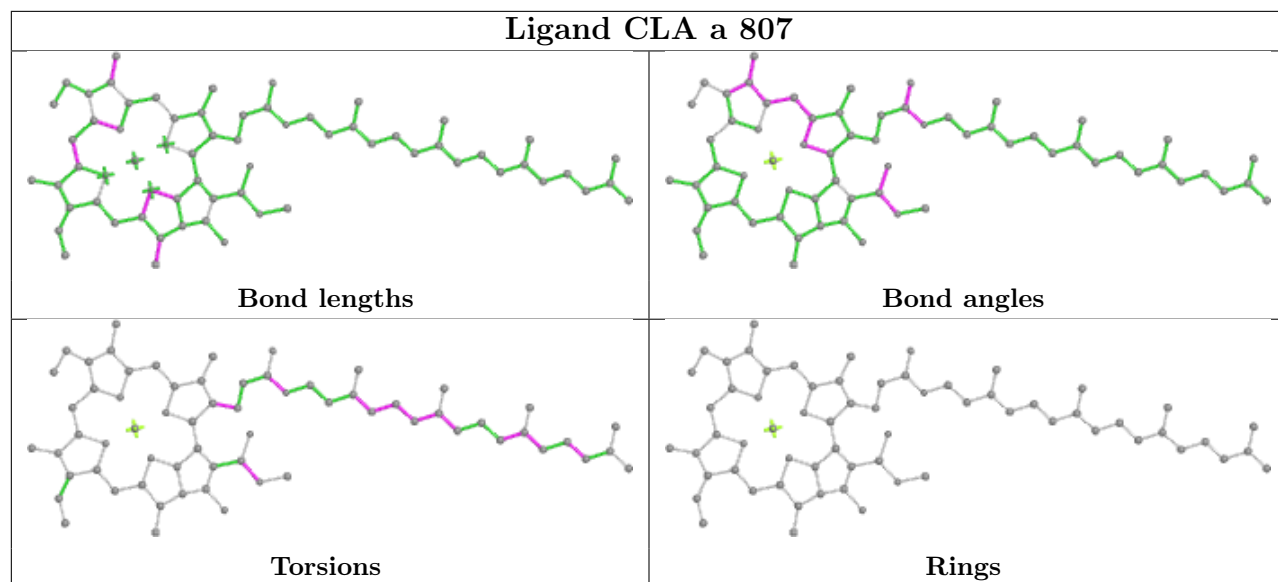




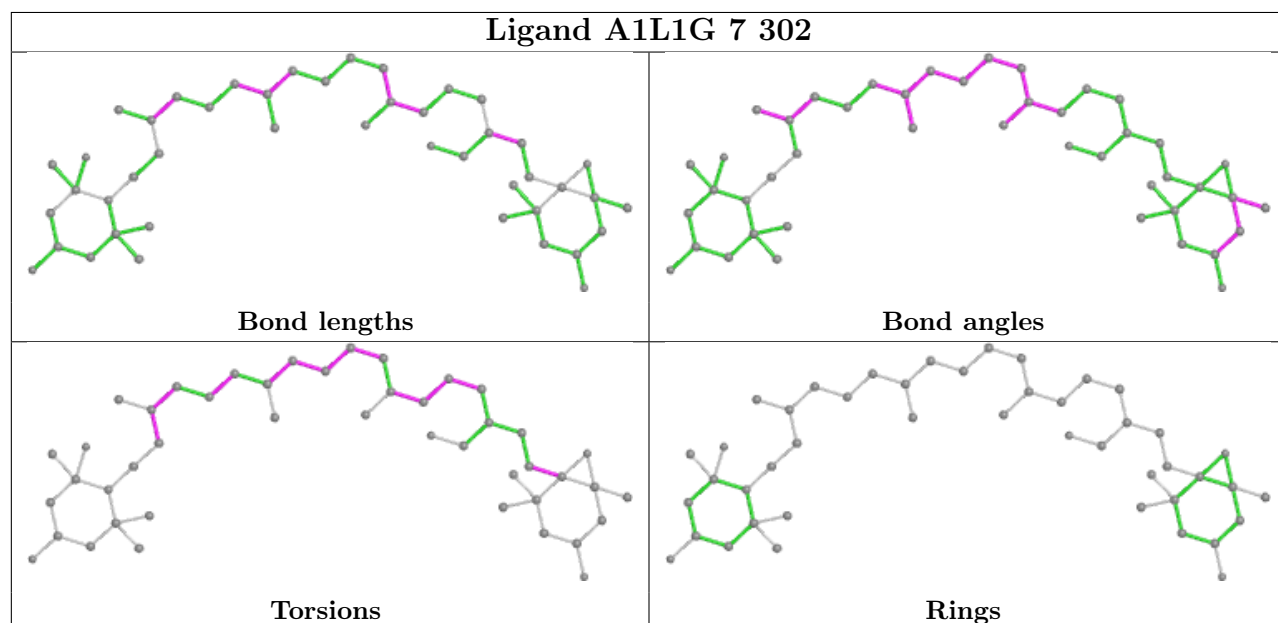


**Ligand XAT 5 302****Ligand CLA 1 203**

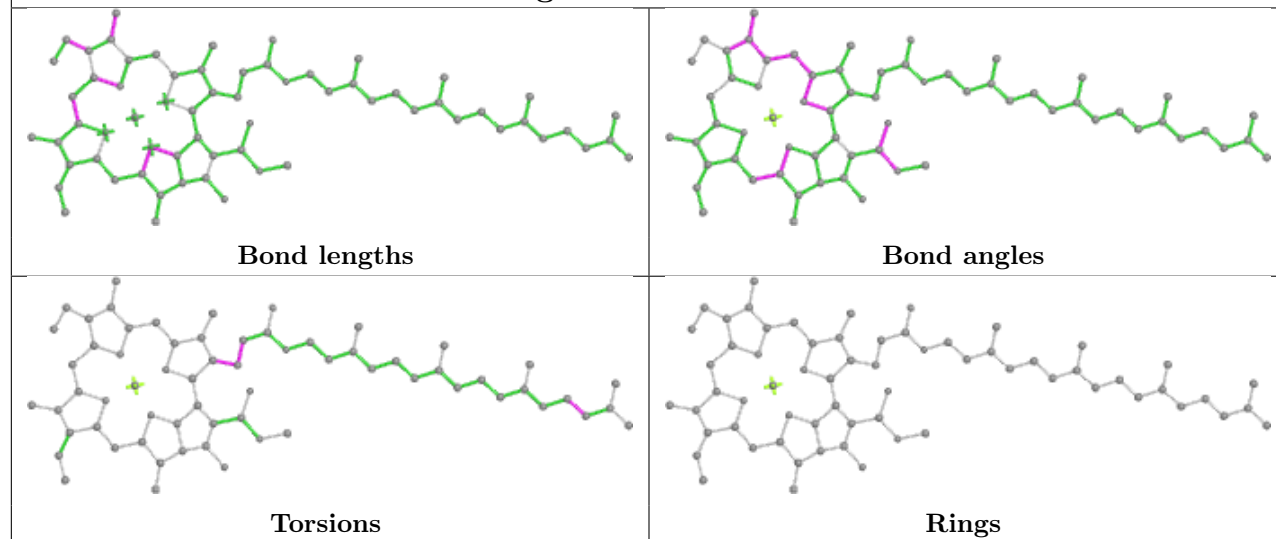
## Ligand CLA a 807



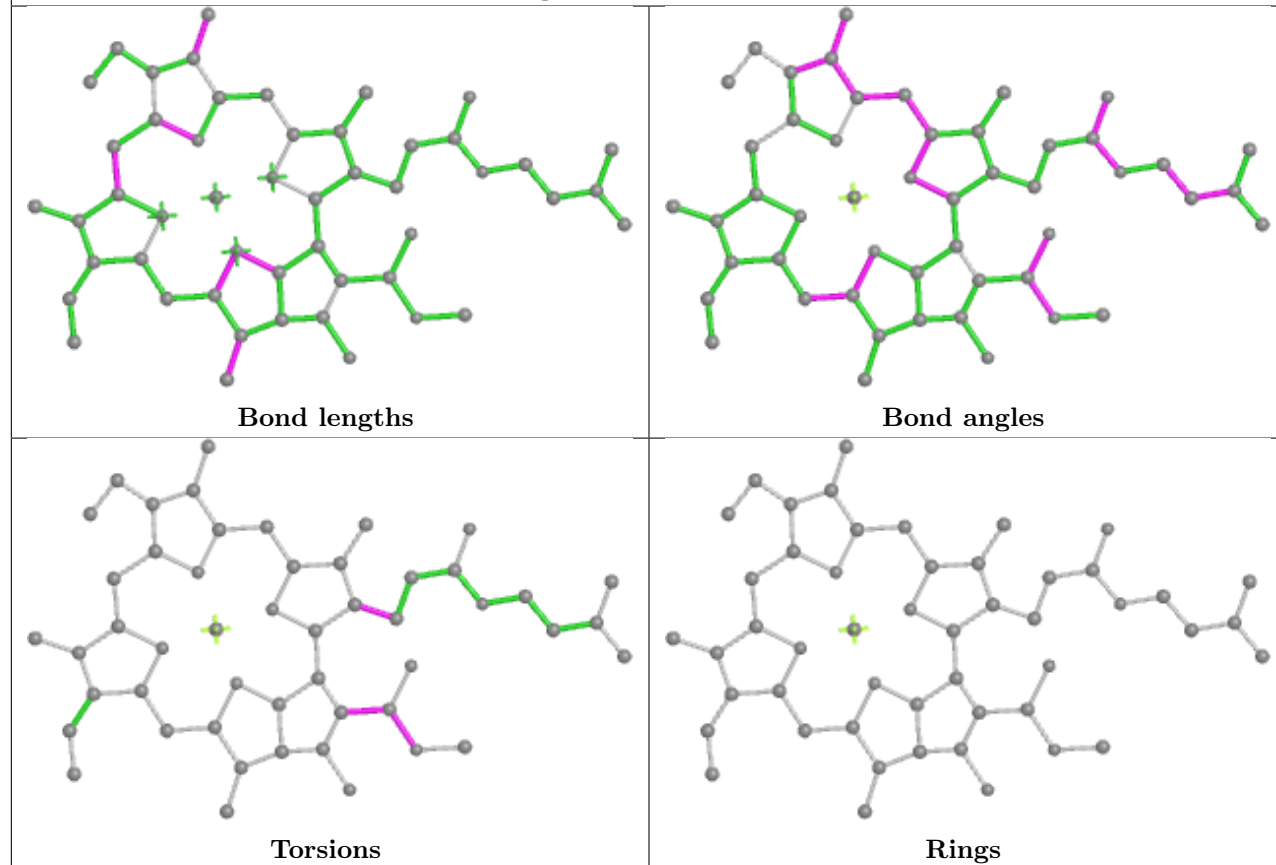
## Ligand A1L1G 7 302



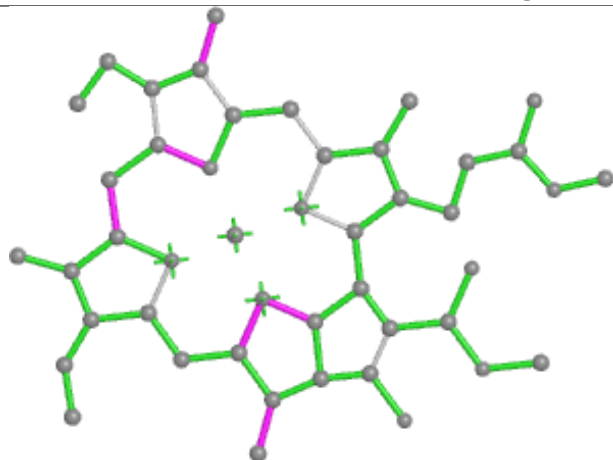
## Ligand CLA a 803



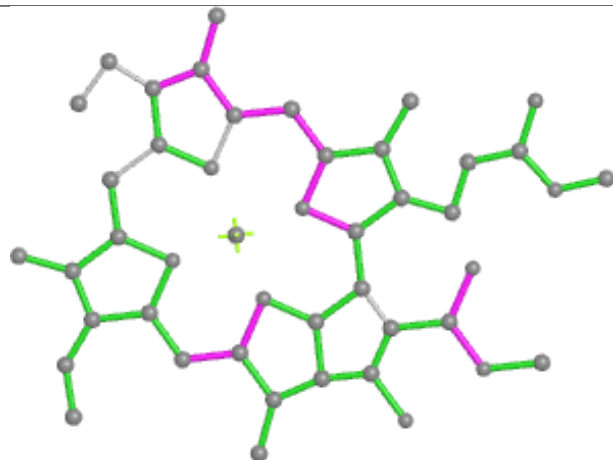
## Ligand CLA a 832



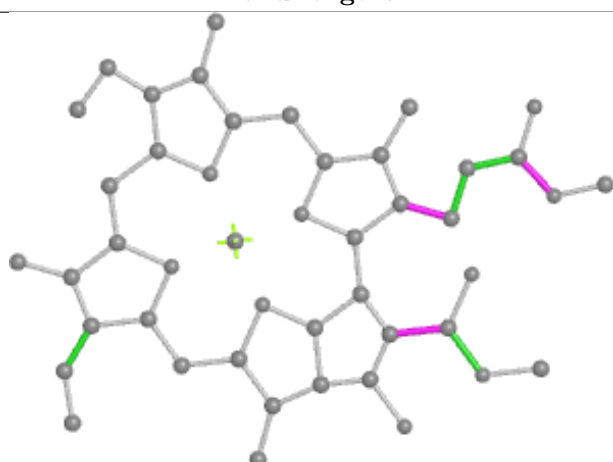
## Ligand CLA a 824



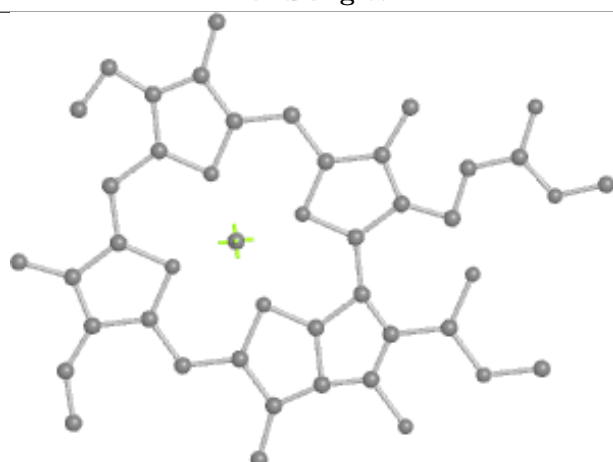
Bond lengths



Bond angles

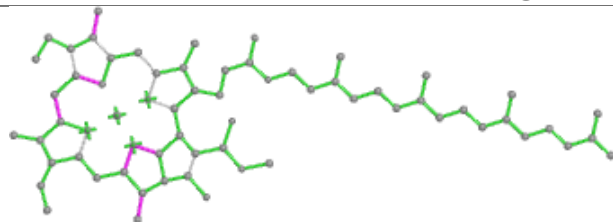


Torsions

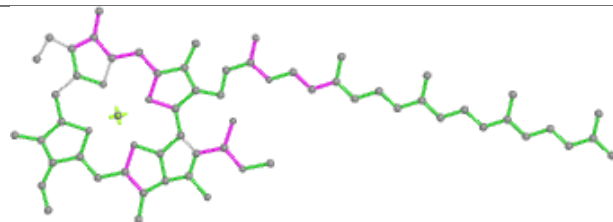


Rings

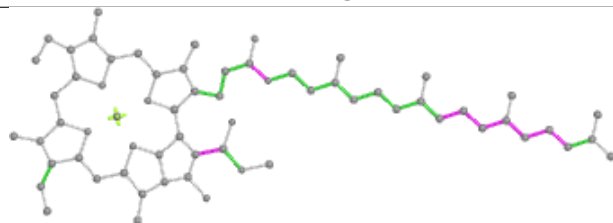
## Ligand CLA b 829



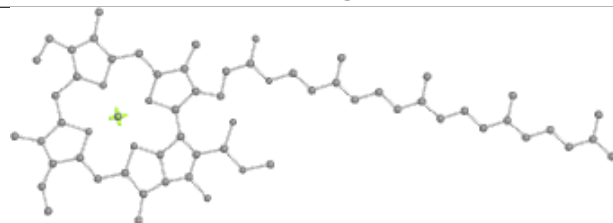
Bond lengths



Bond angles

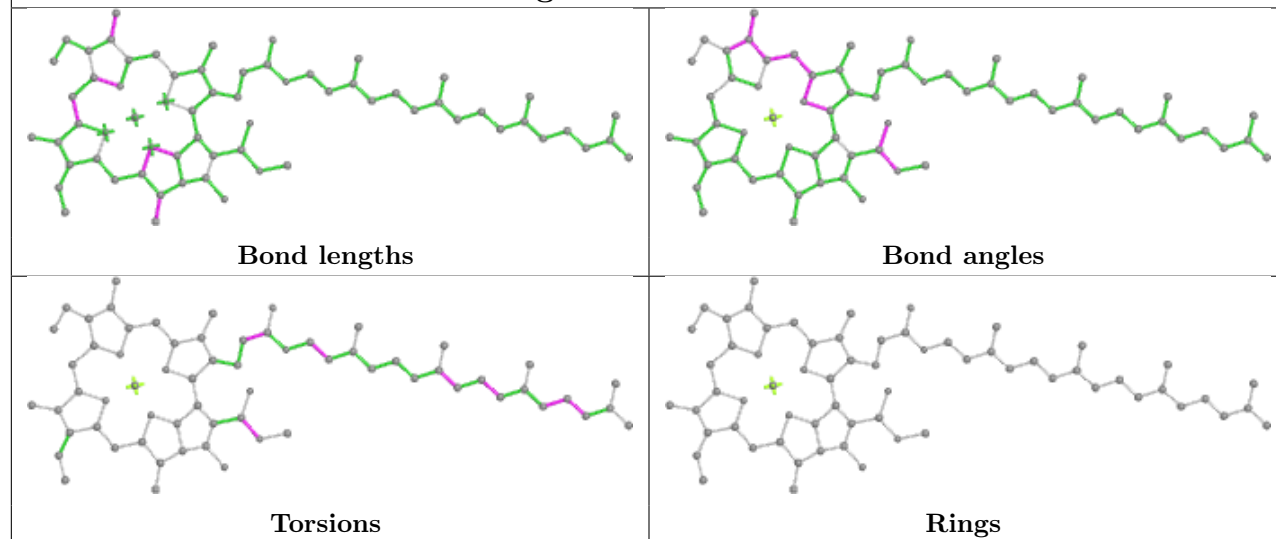


Torsions

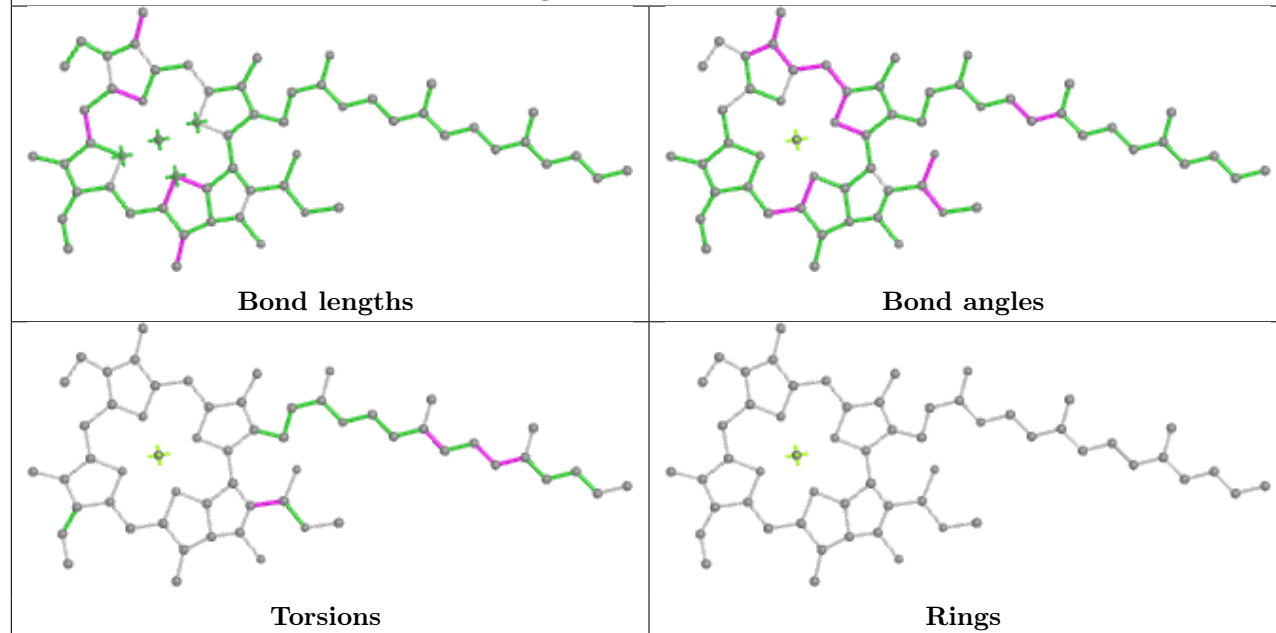


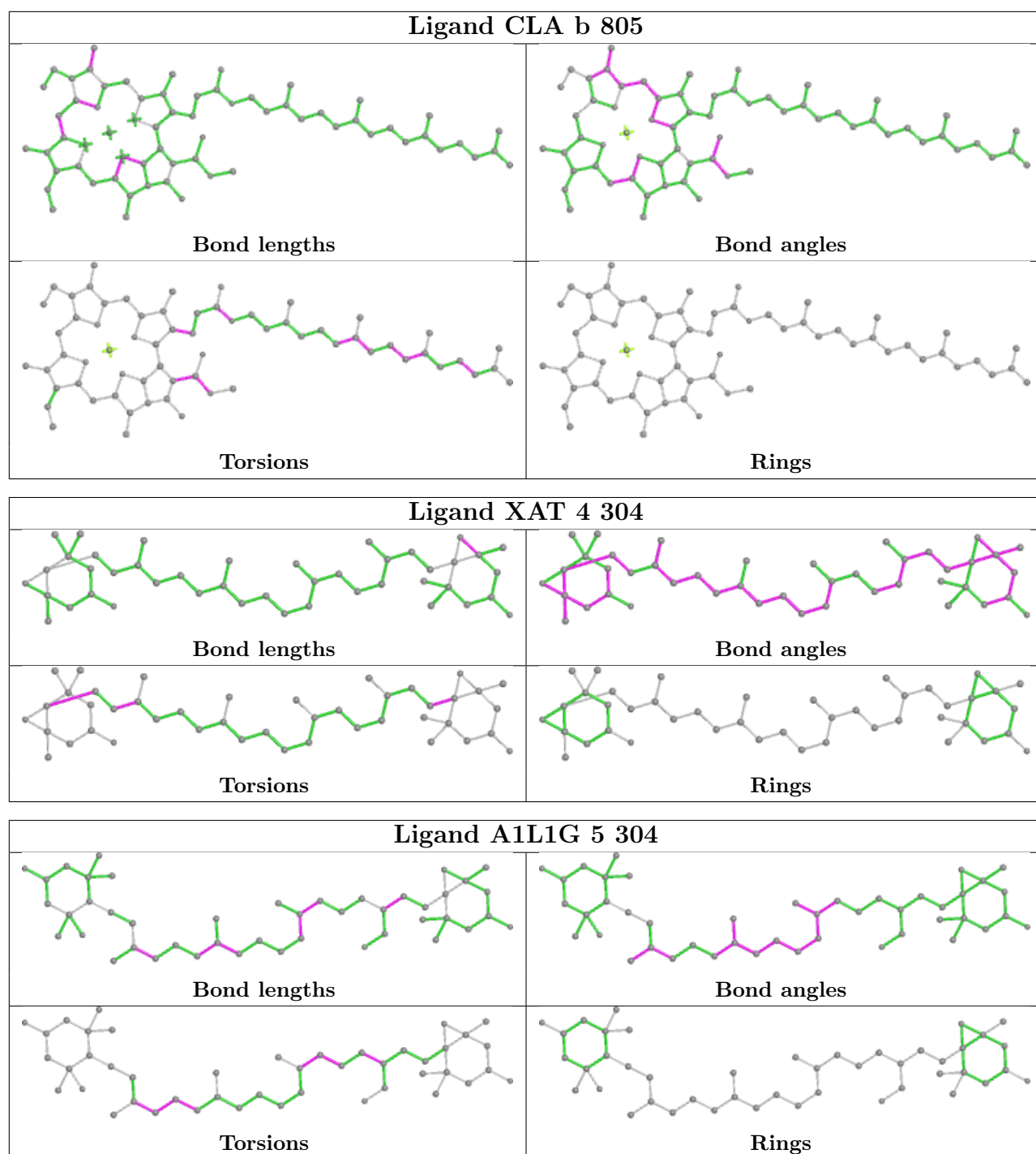
Rings

## Ligand CLA a 826

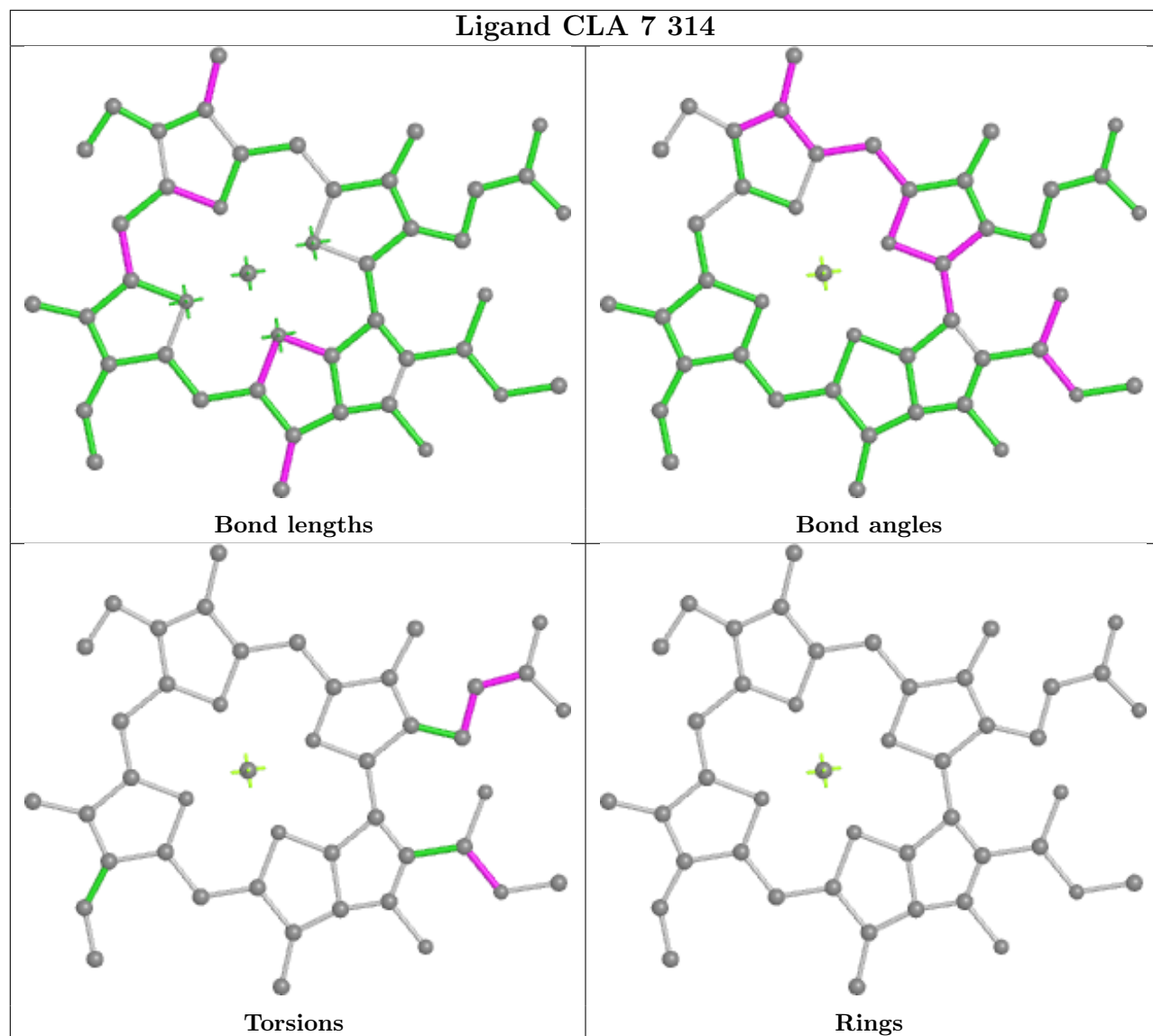


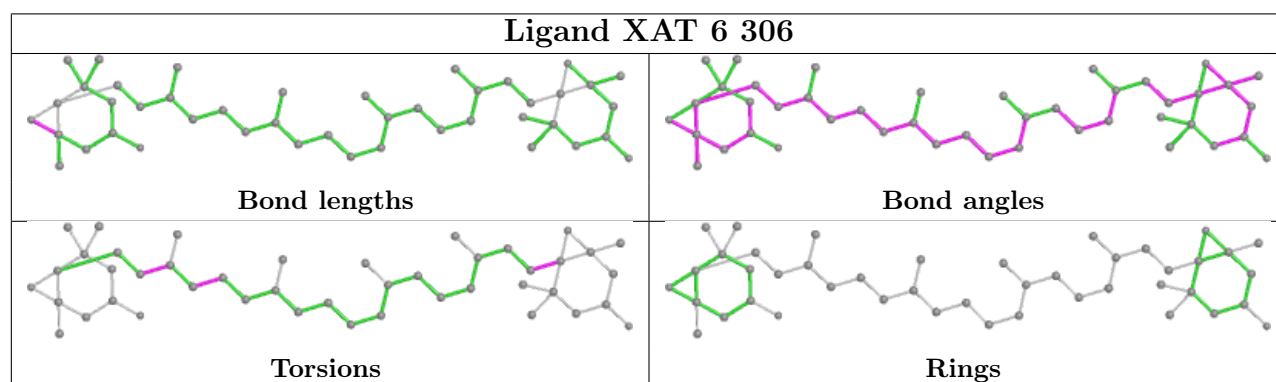
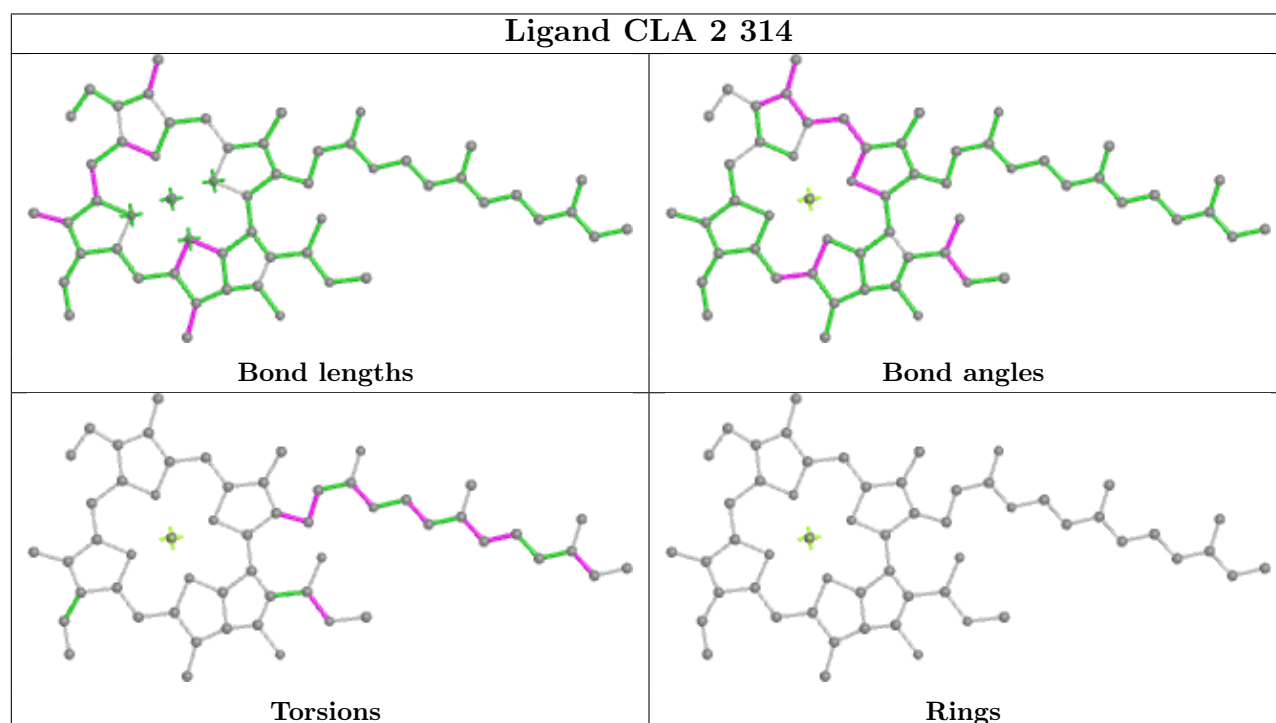
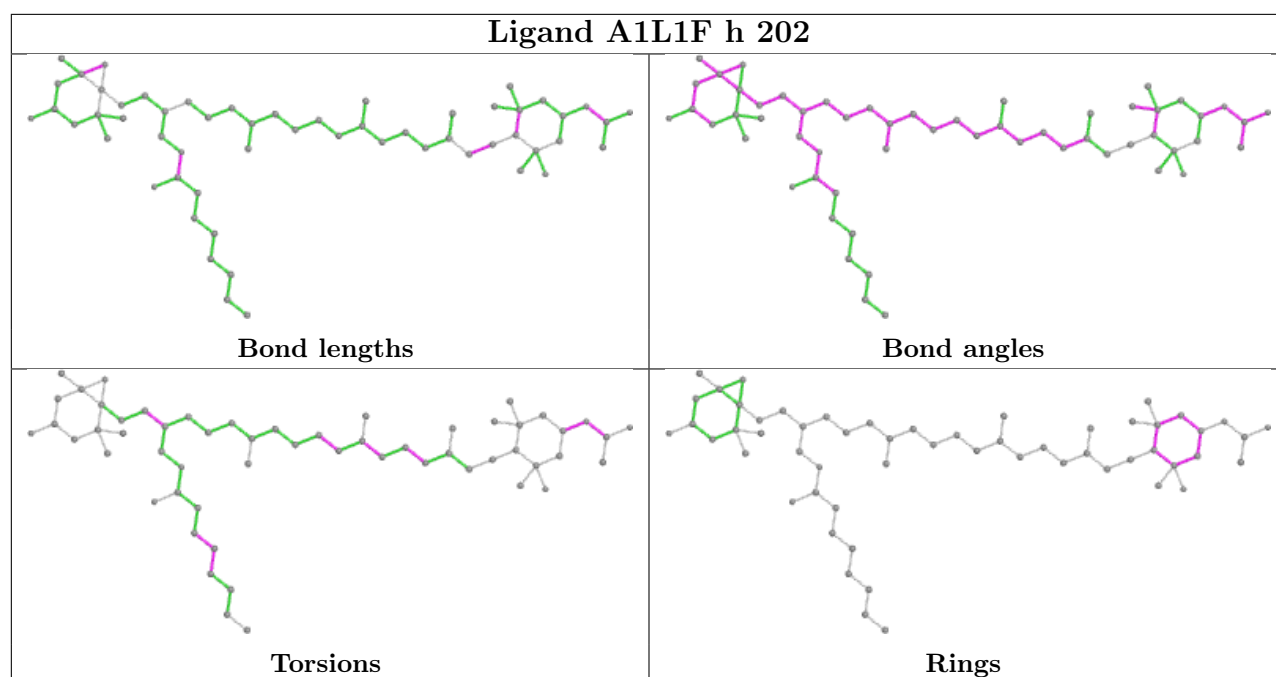
## Ligand CLA a 802

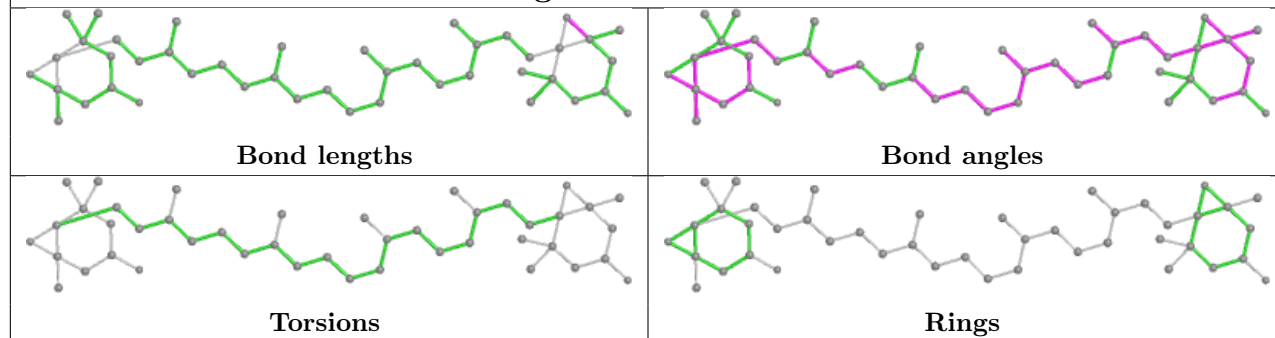
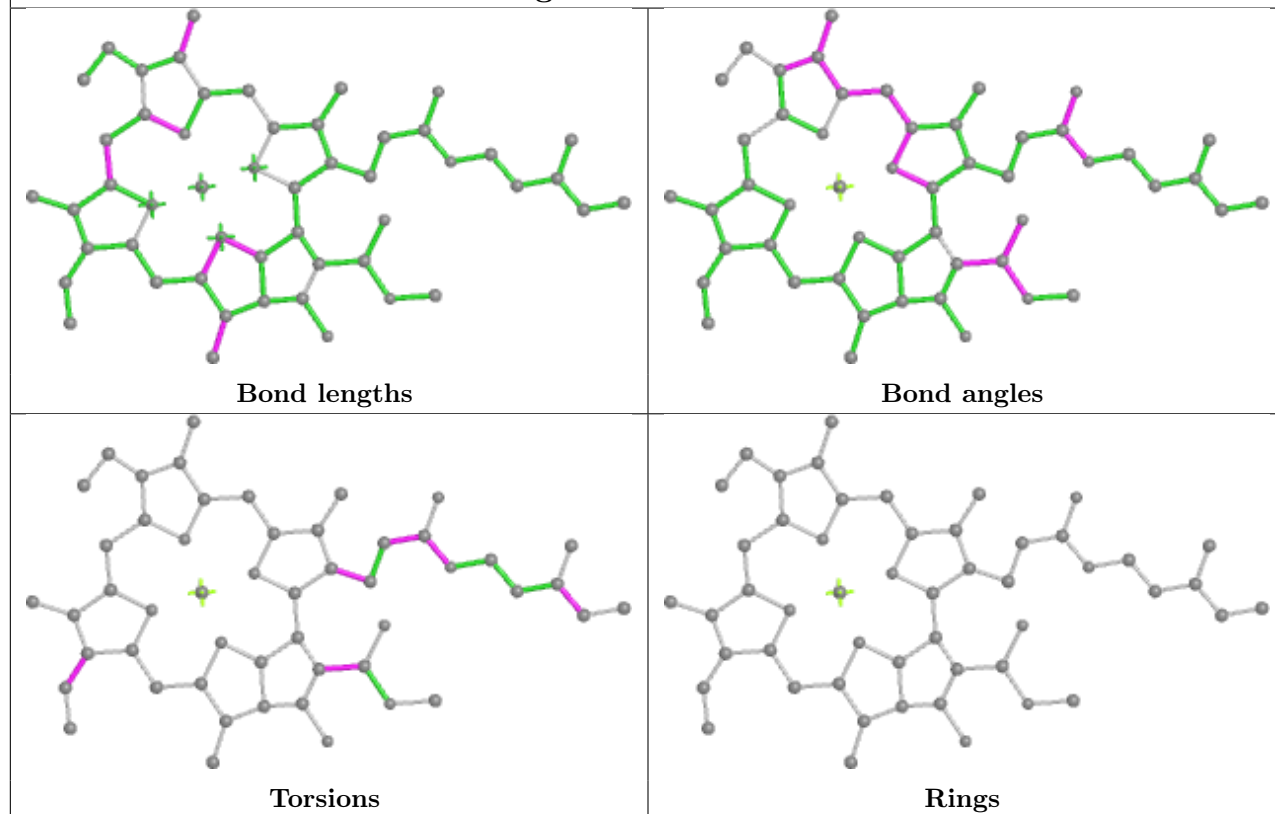
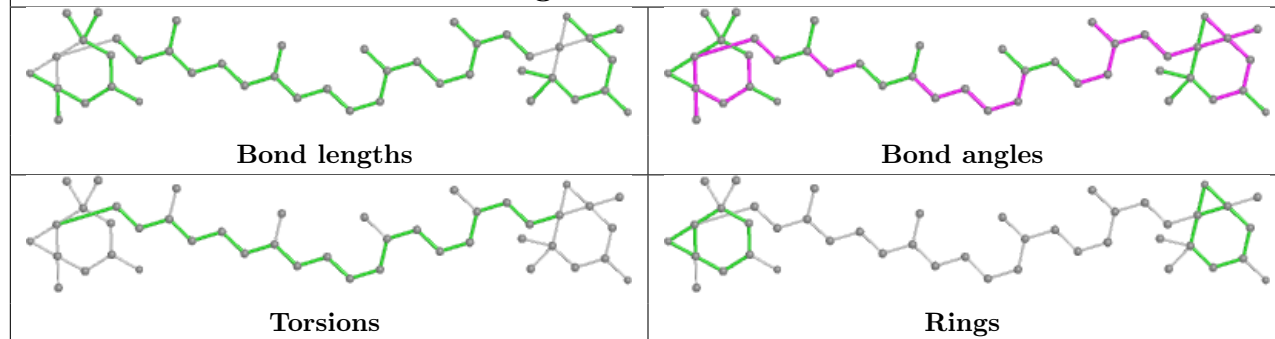




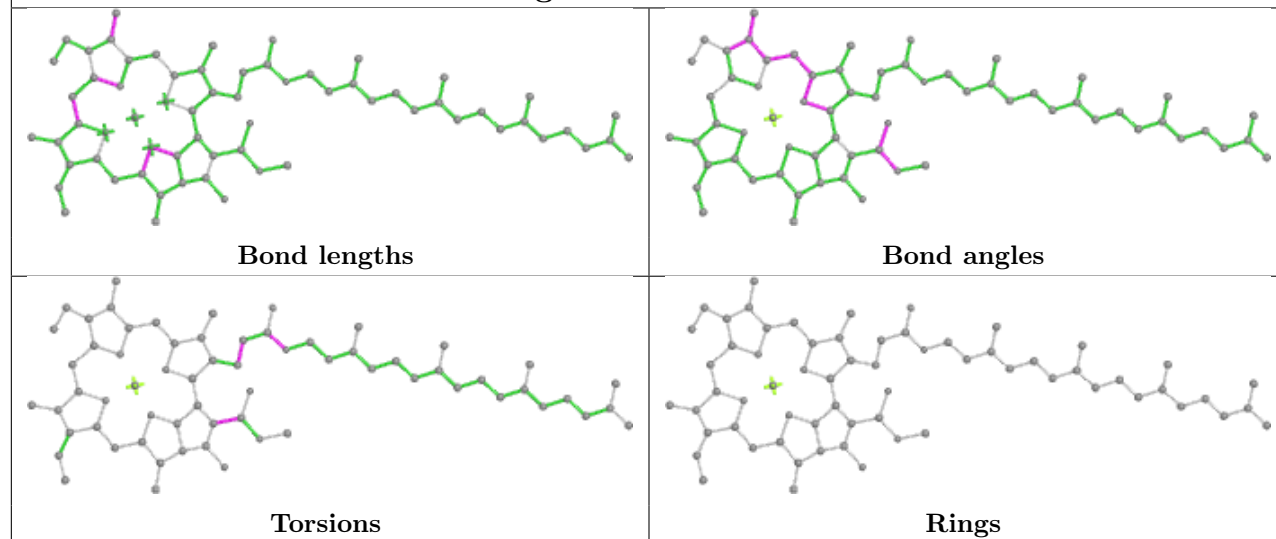
## Ligand CLA 7 314



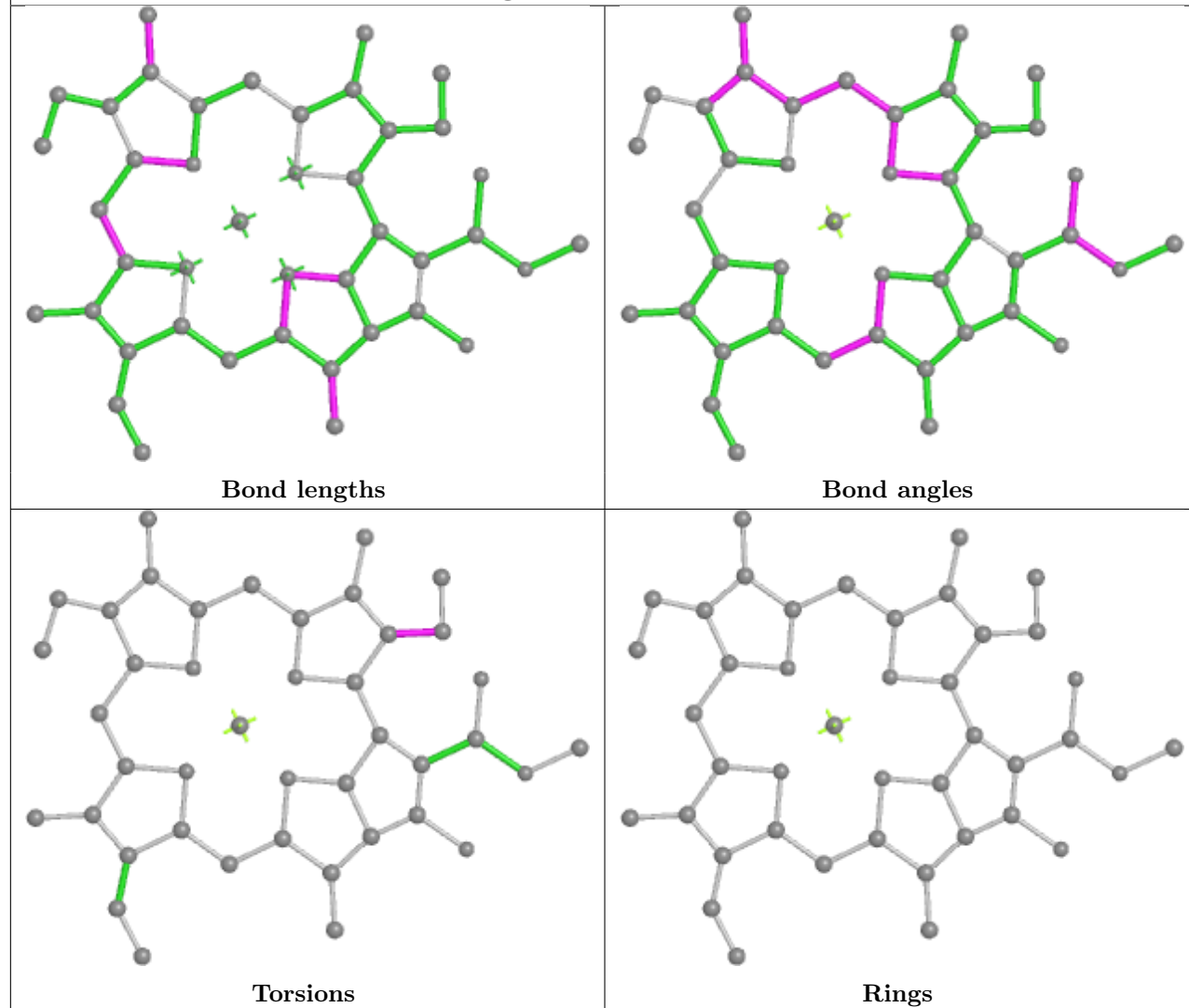


**Ligand XAT 3 305****Ligand CLA 7 316****Ligand XAT 4 303**

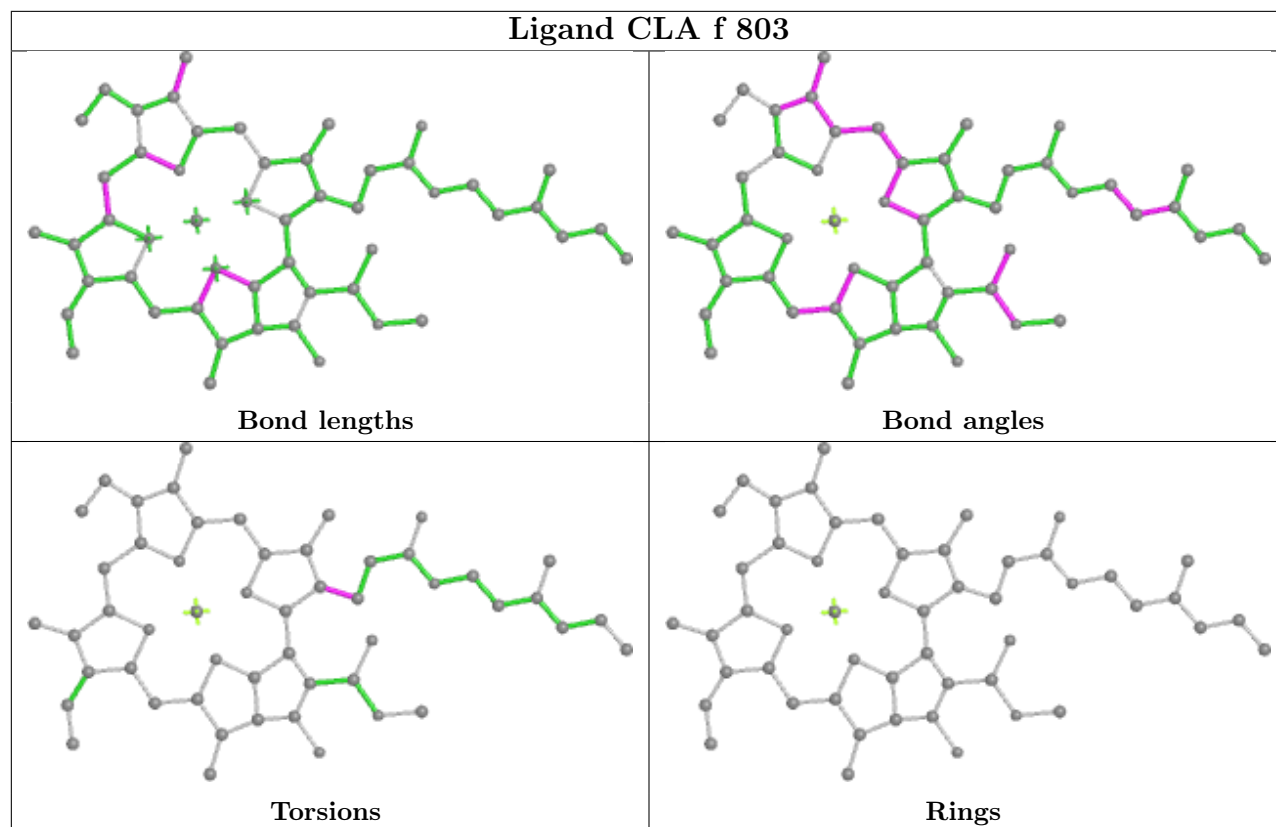
## Ligand CLA b 826



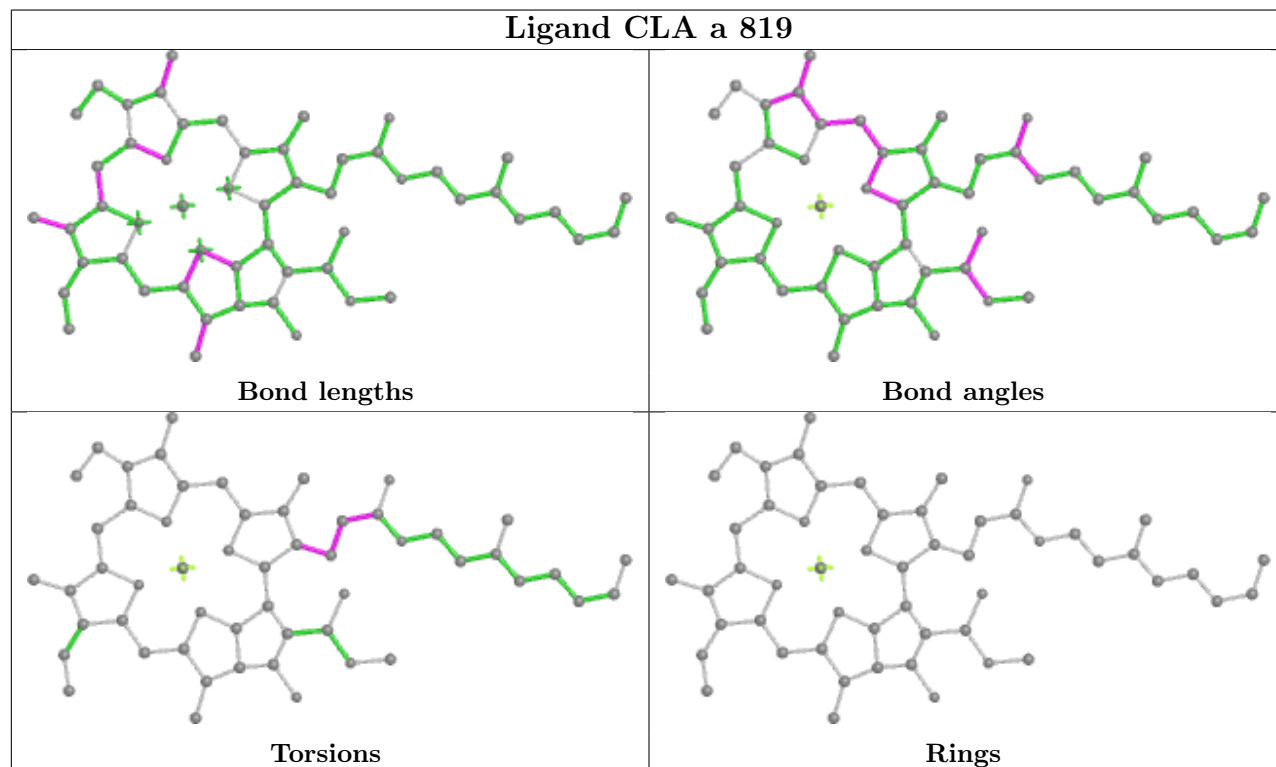
## Ligand CLA 2 315

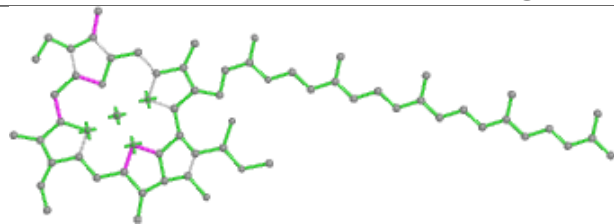
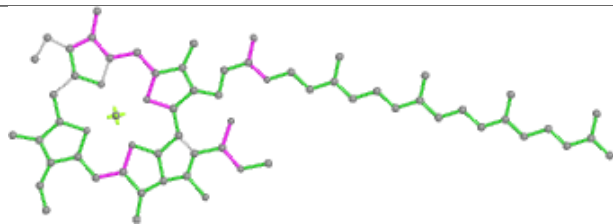
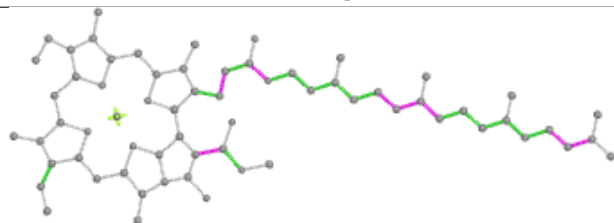
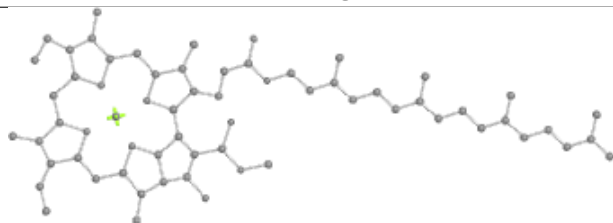
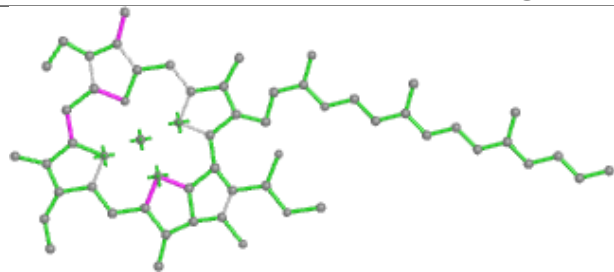
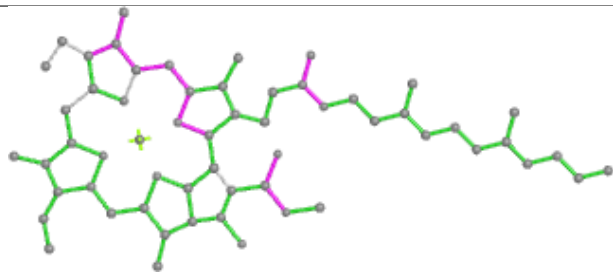
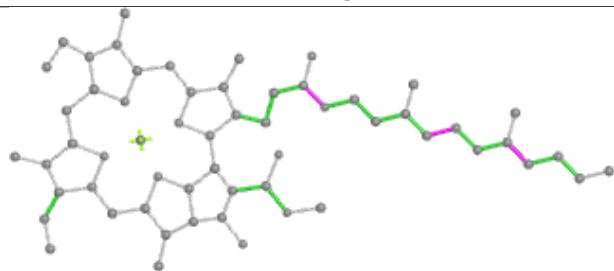
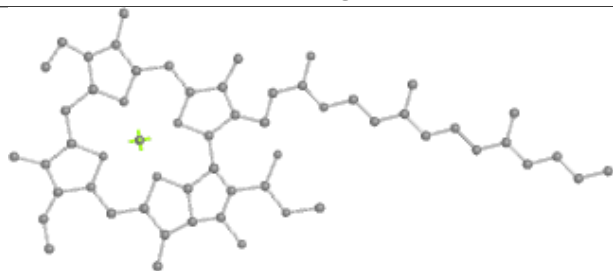


## Ligand CLA f 803

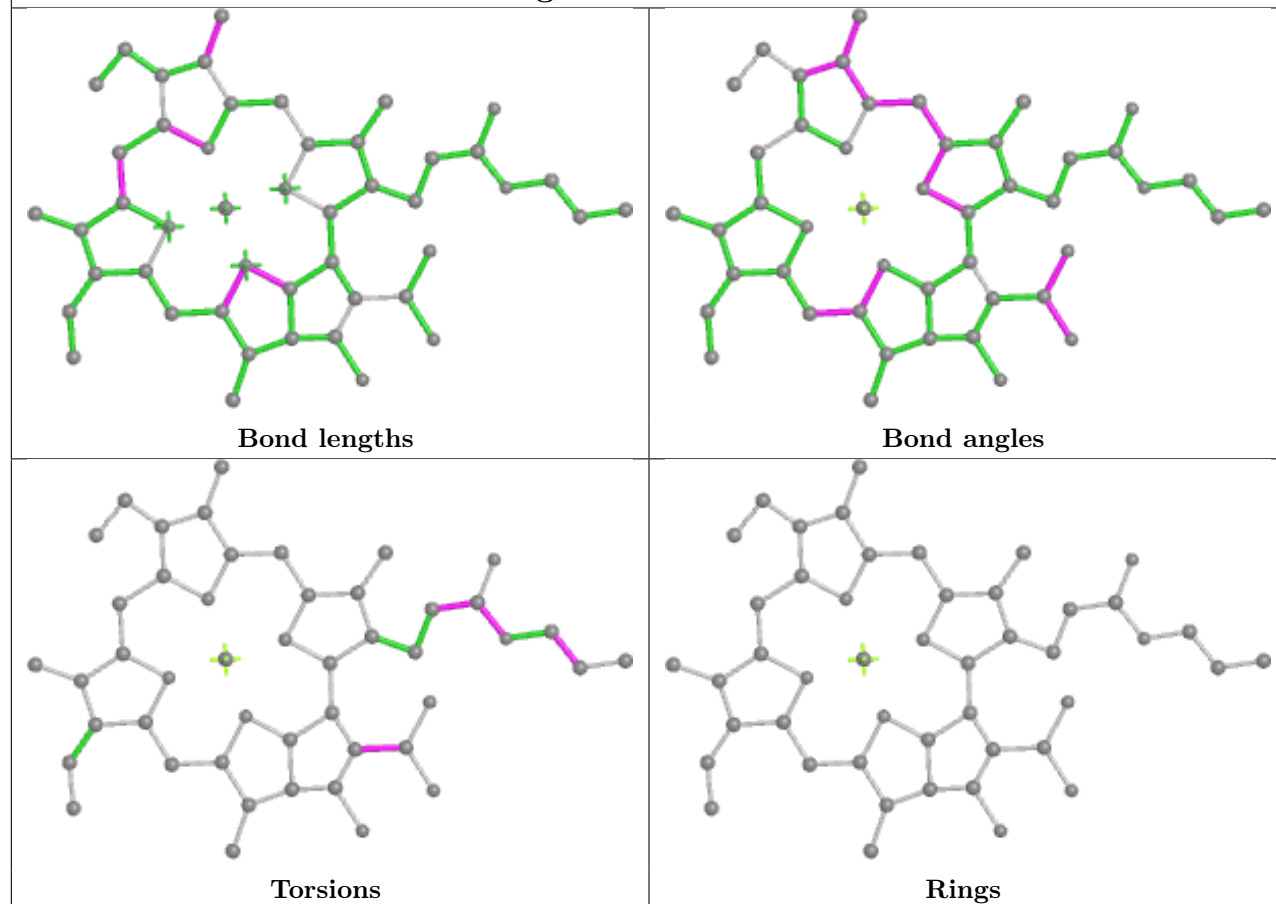


## Ligand CLA a 819

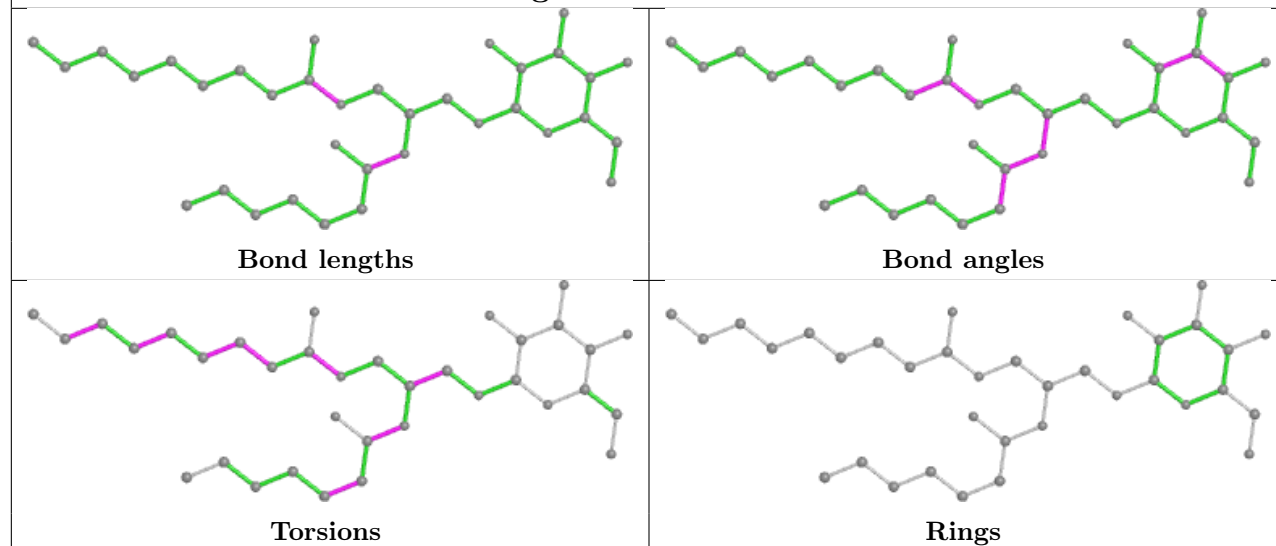


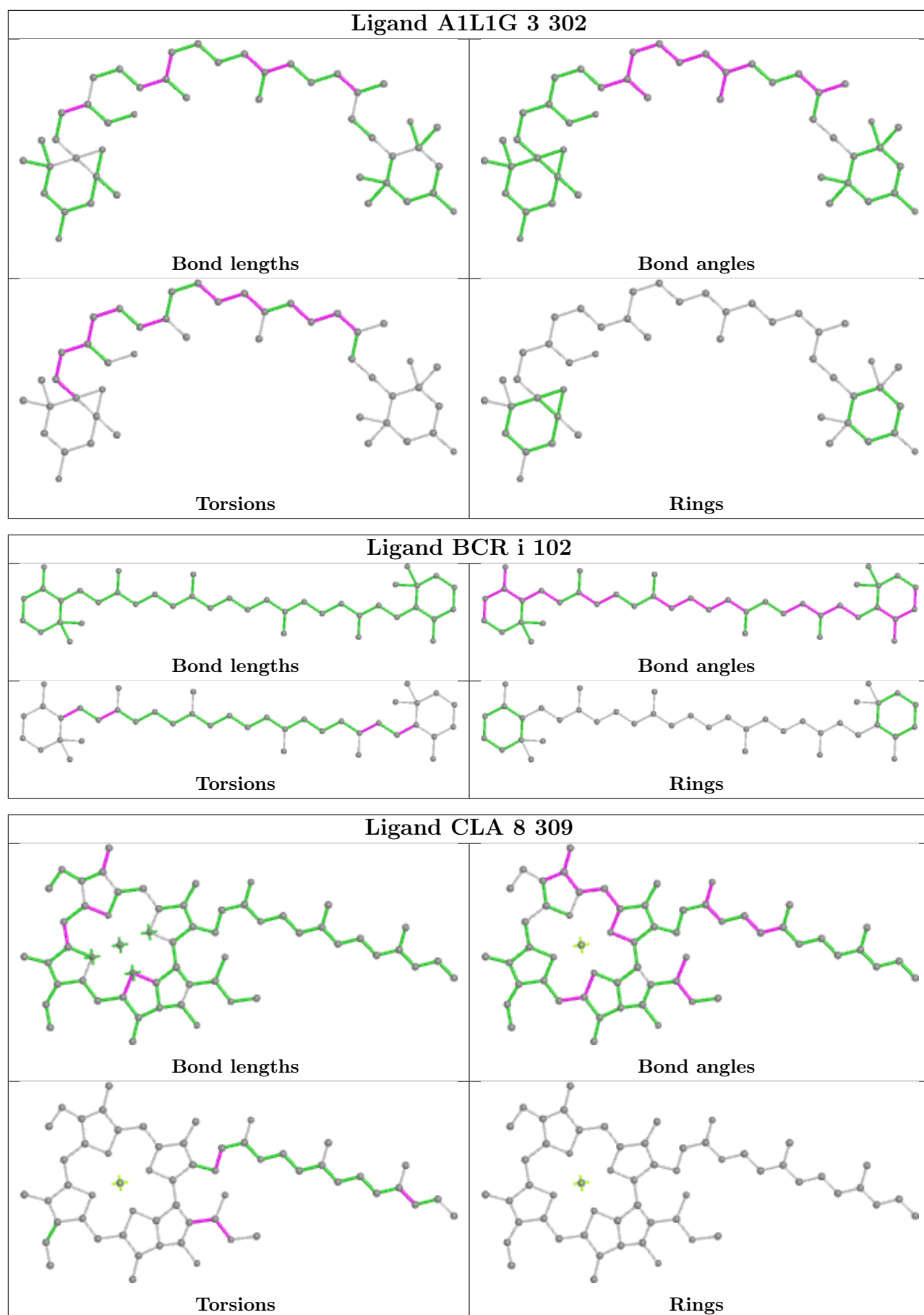
**Ligand CLA 8 307****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 2 311****Bond lengths****Bond angles****Torsions****Rings**

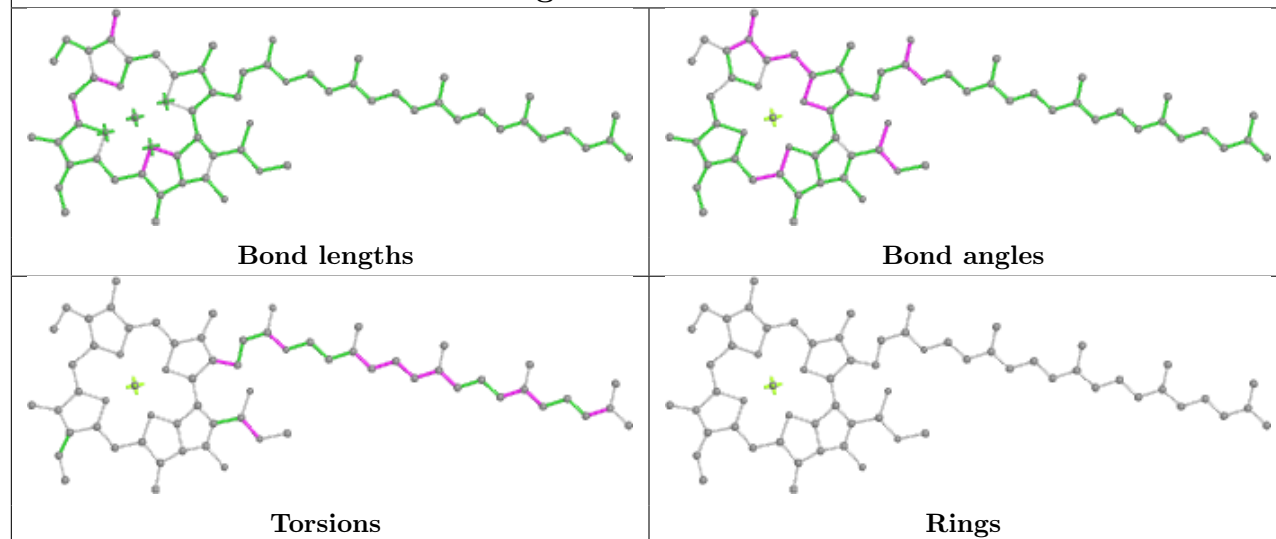
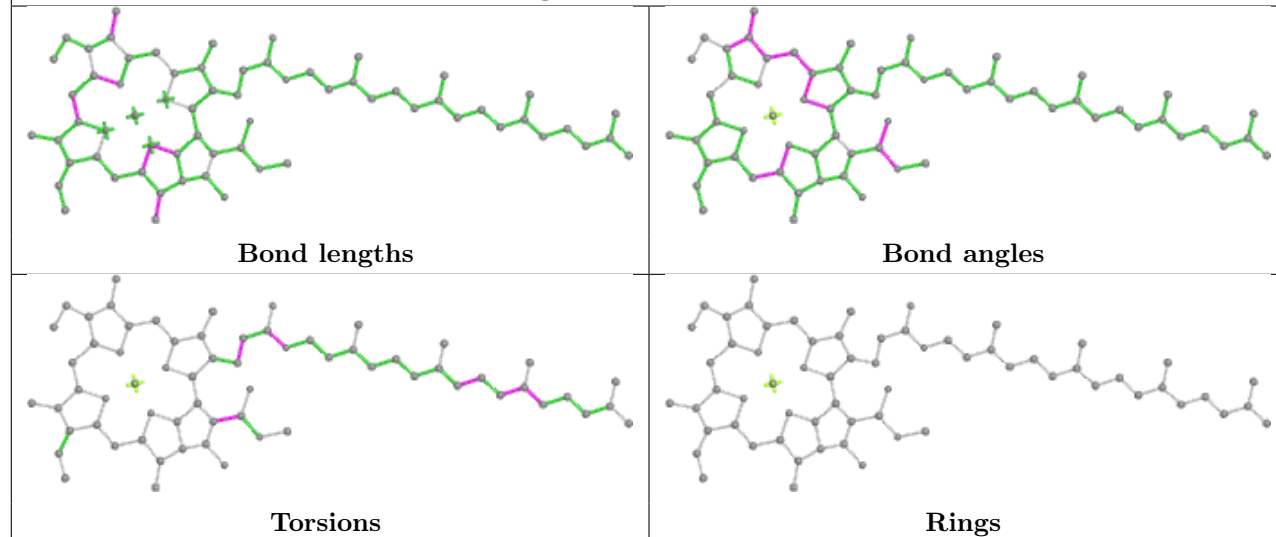
## Ligand CLA 7 309



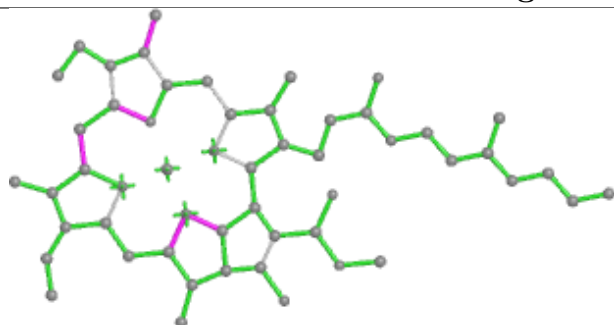
## Ligand LMG 2 317



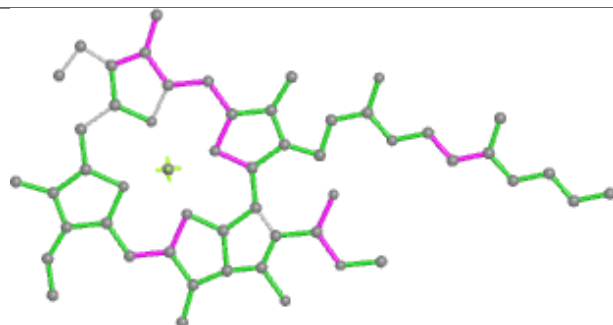


**Ligand CLA 1 310****Ligand CLA a 842**

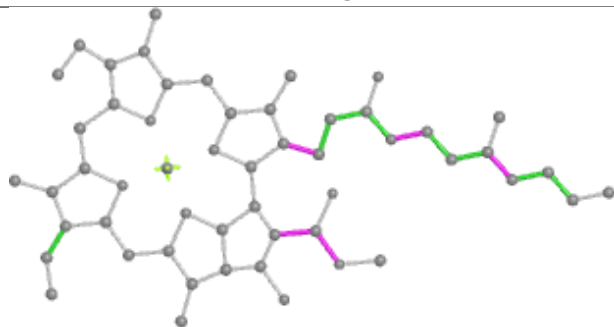
## Ligand CLA b 835



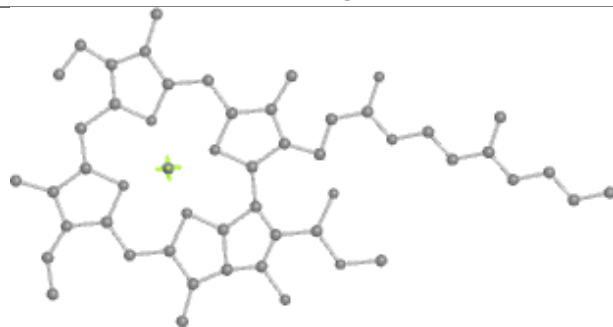
Bond lengths



Bond angles

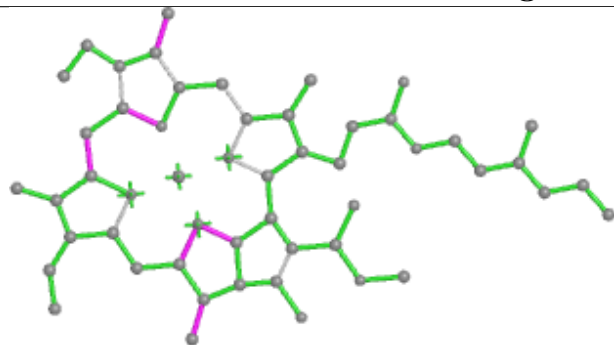


Torsions

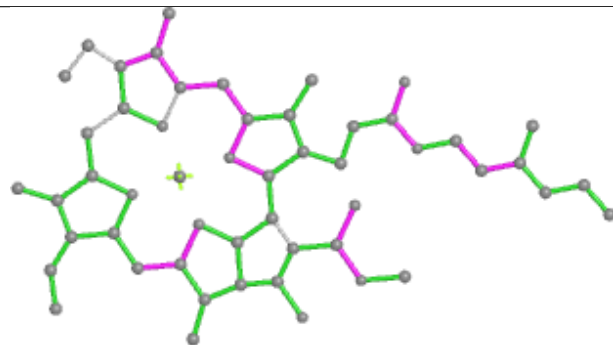


Rings

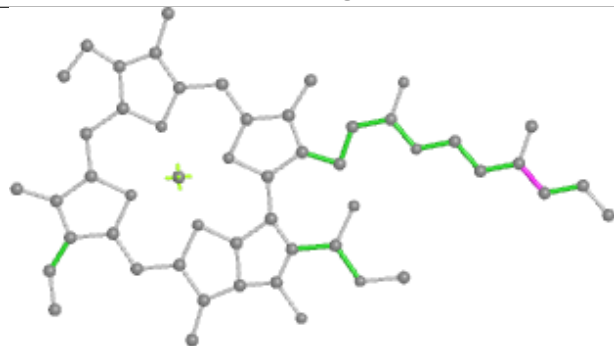
## Ligand CLA 3 313



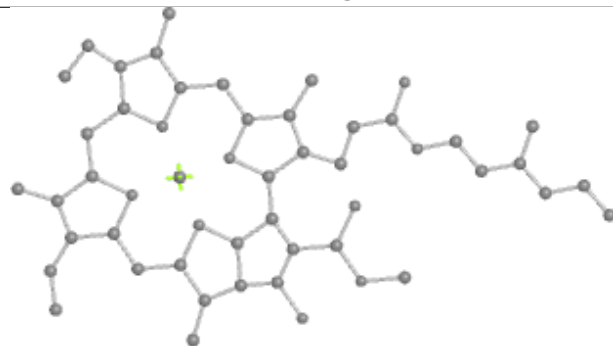
Bond lengths



Bond angles

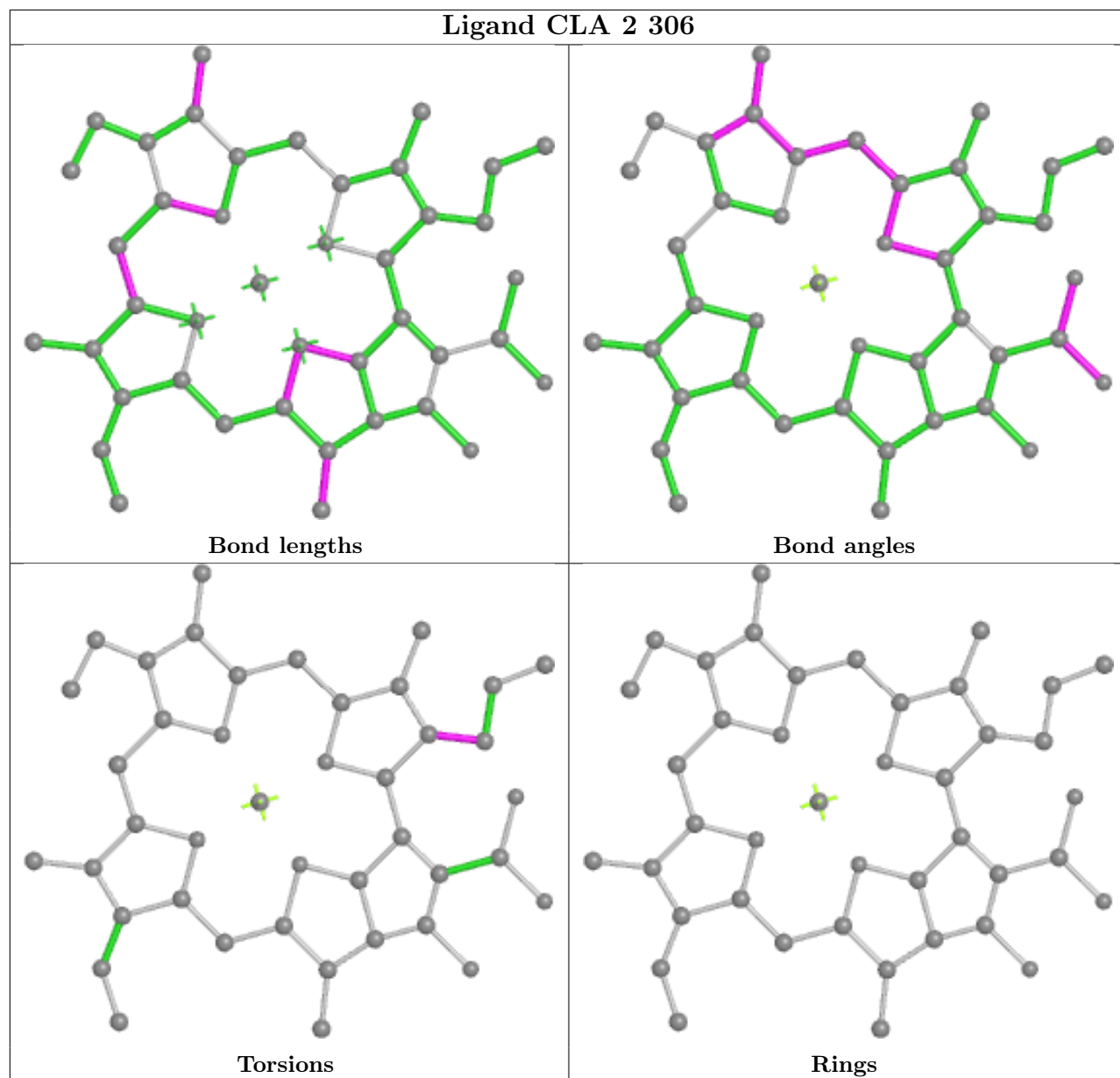


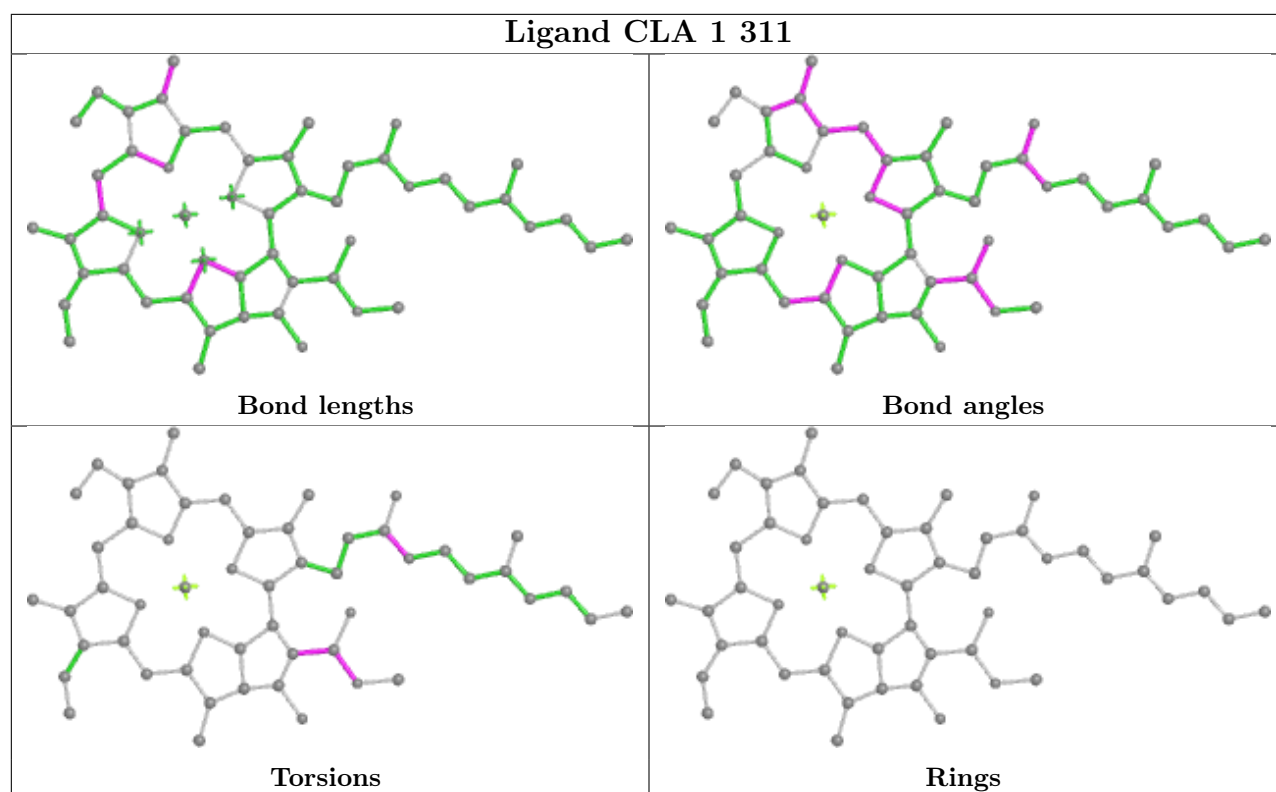
Torsions



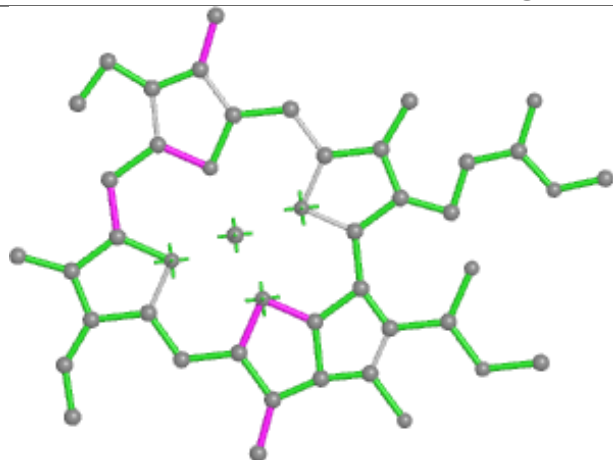
Rings

## Ligand CLA 2 306

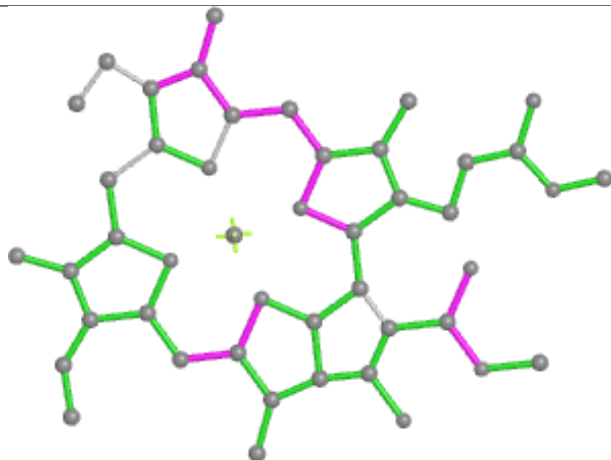




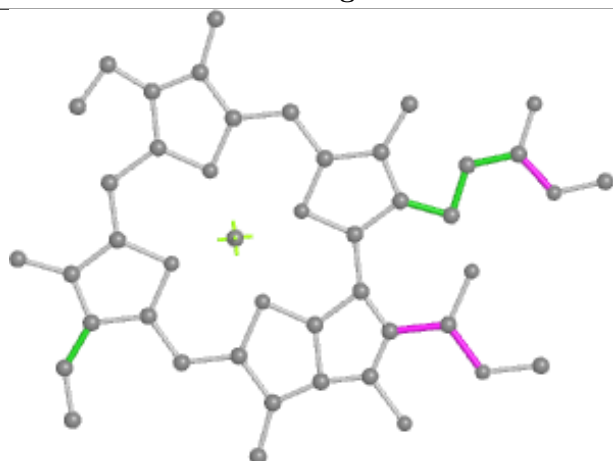
## Ligand CLA 8 310



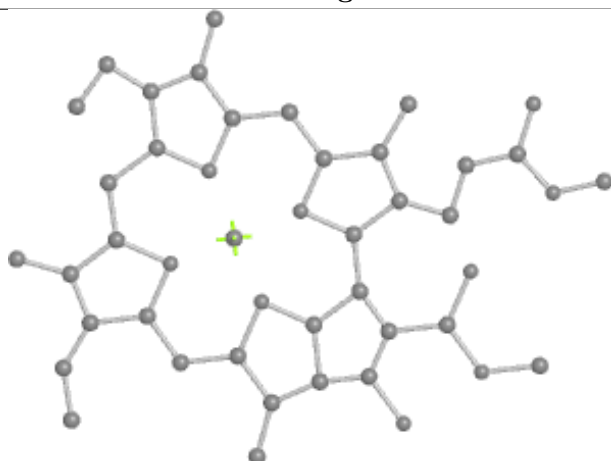
Bond lengths



Bond angles

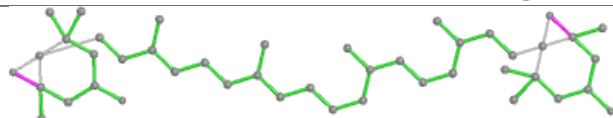


Torsions

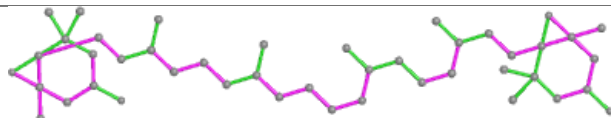


Rings

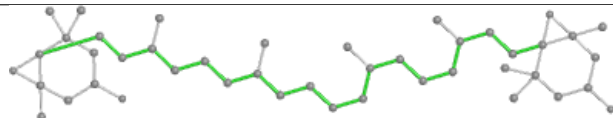
## Ligand XAT 1 302



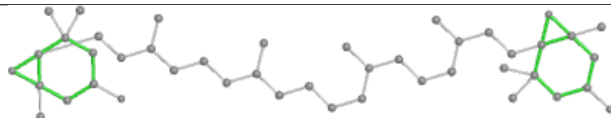
Bond lengths



Bond angles

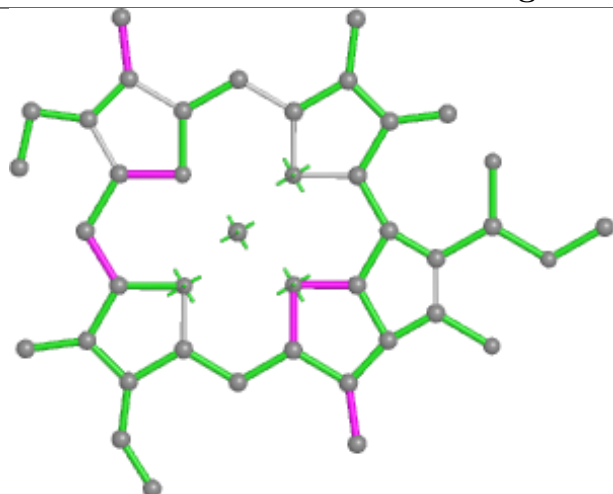


Torsions

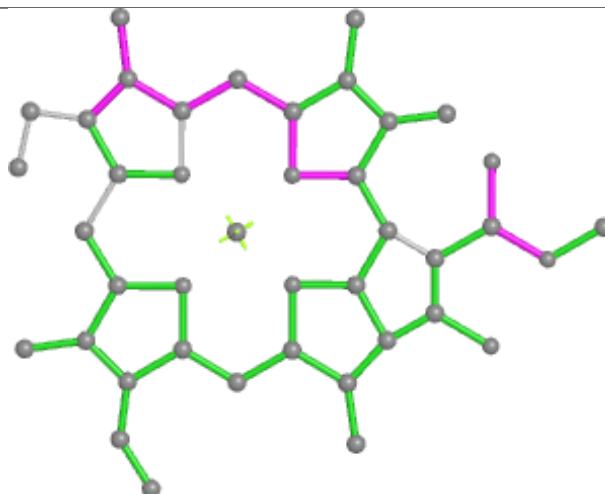


Rings

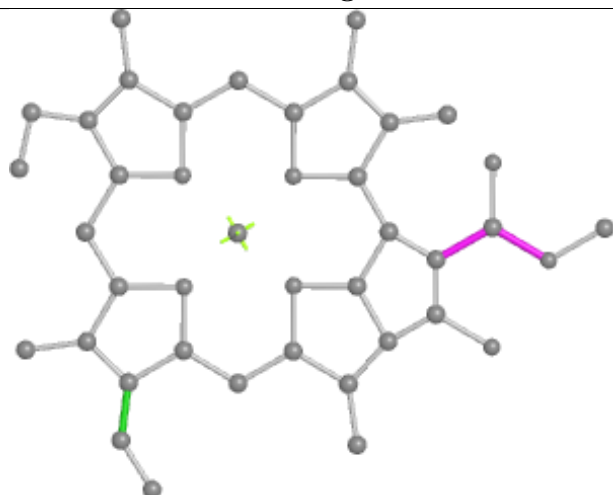
## Ligand CLA 6 315



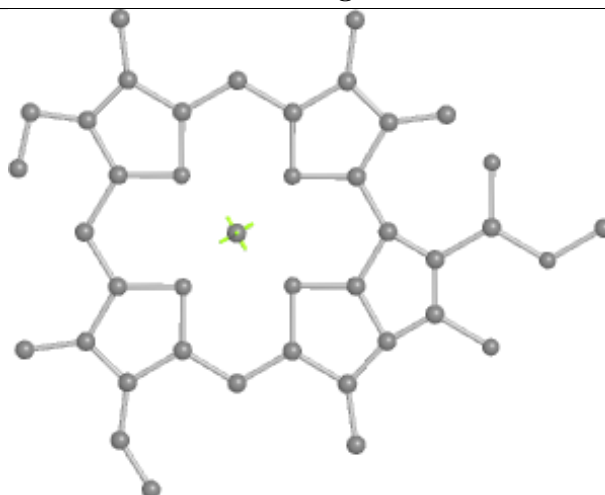
Bond lengths



Bond angles

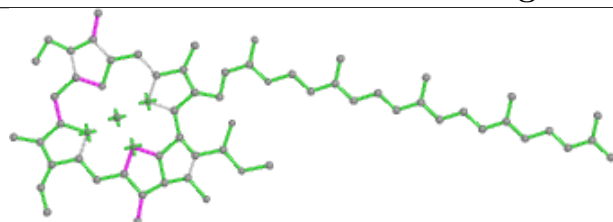


Torsions

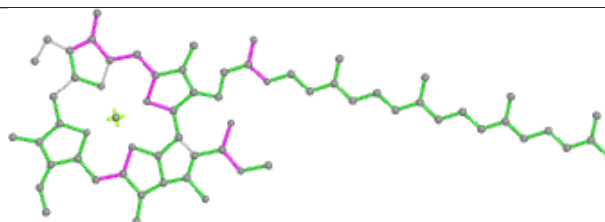


Rings

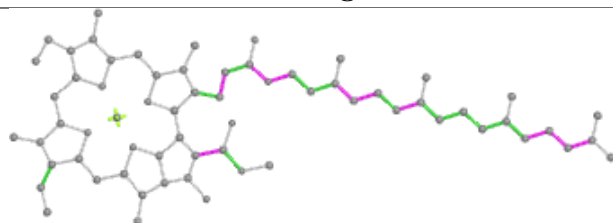
## Ligand CLA a 839



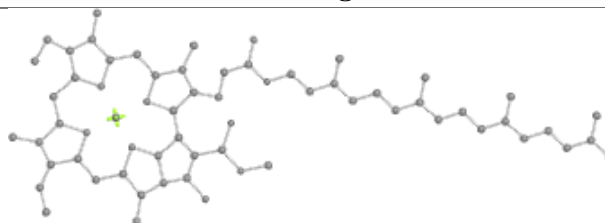
Bond lengths



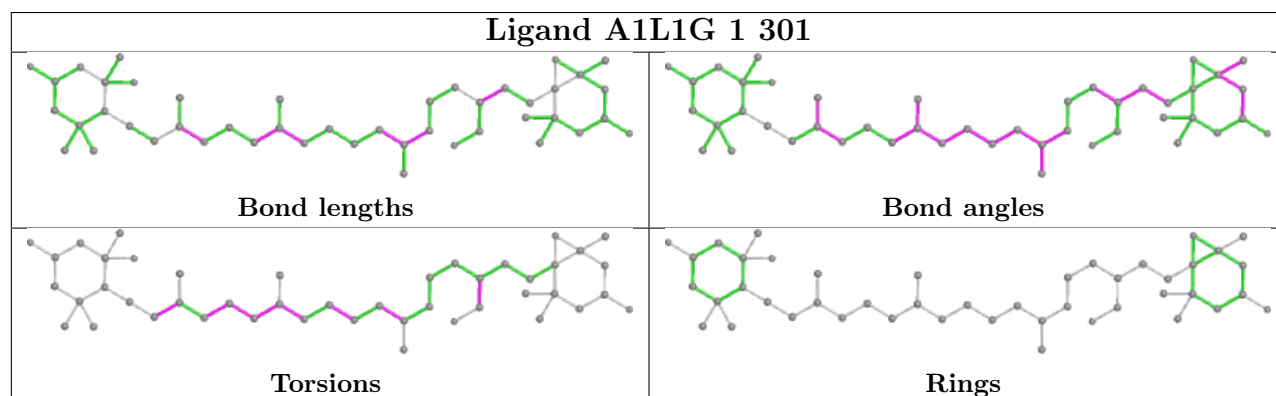
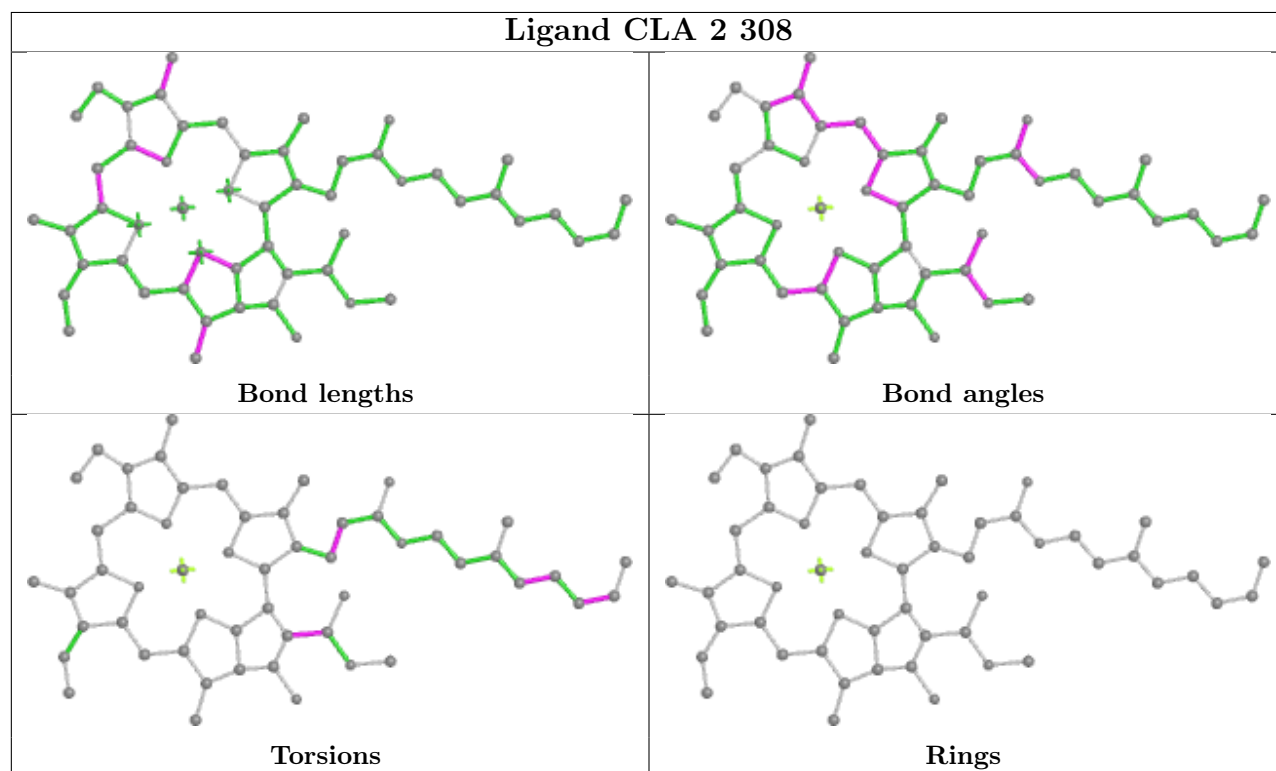
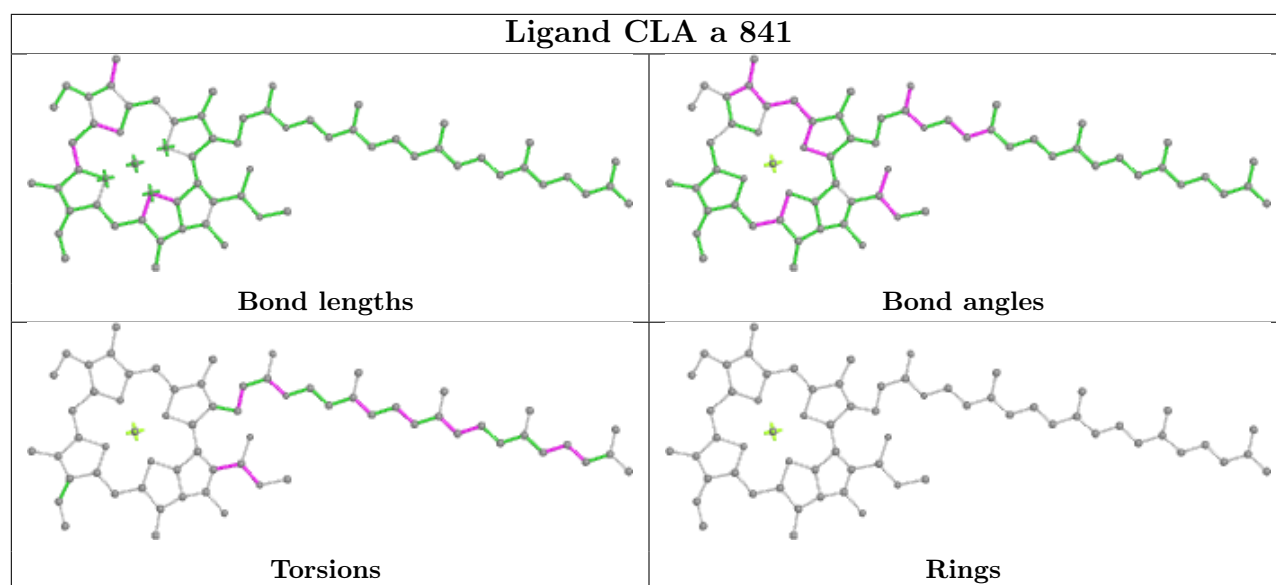
Bond angles

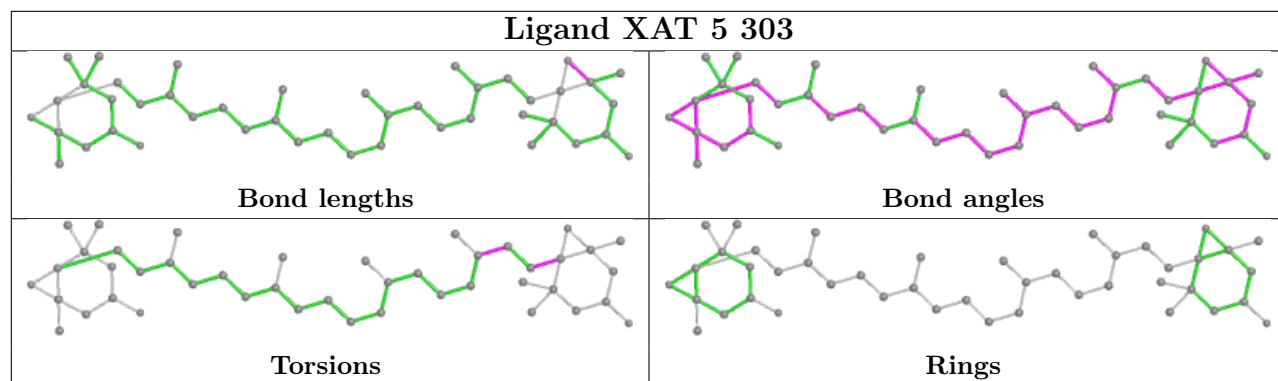
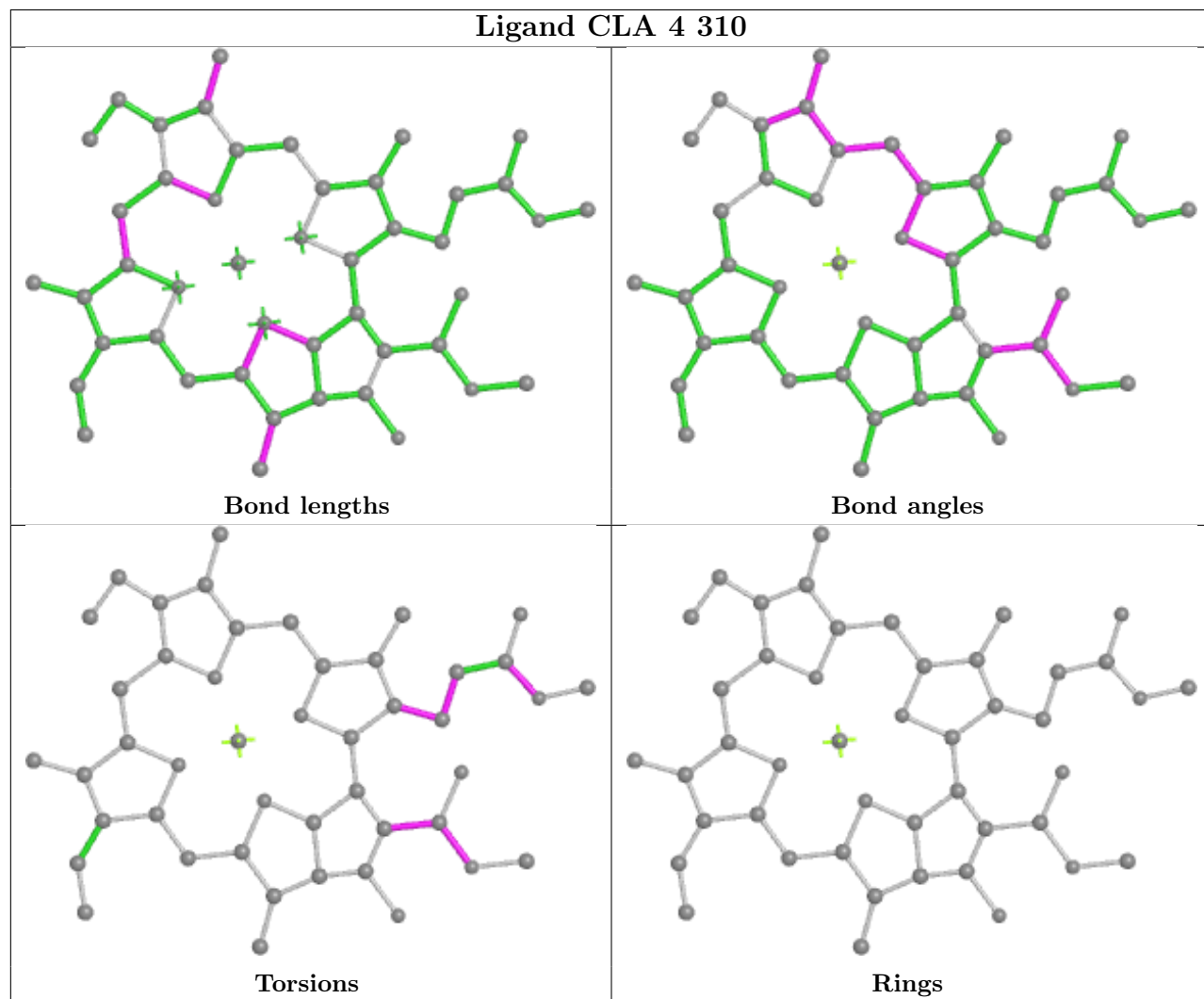


Torsions

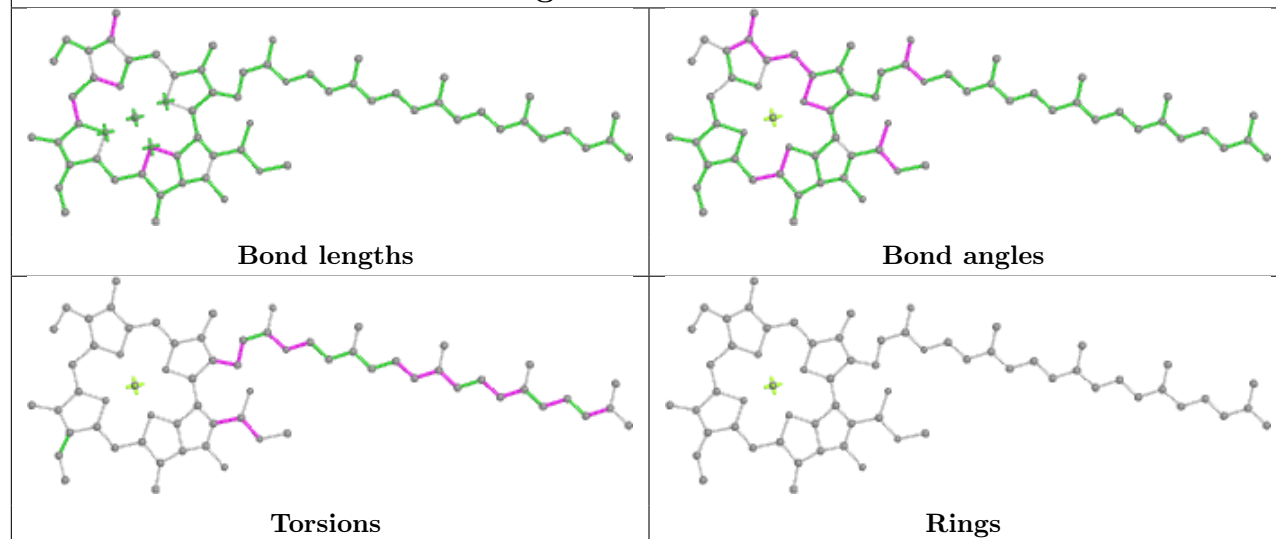


Rings

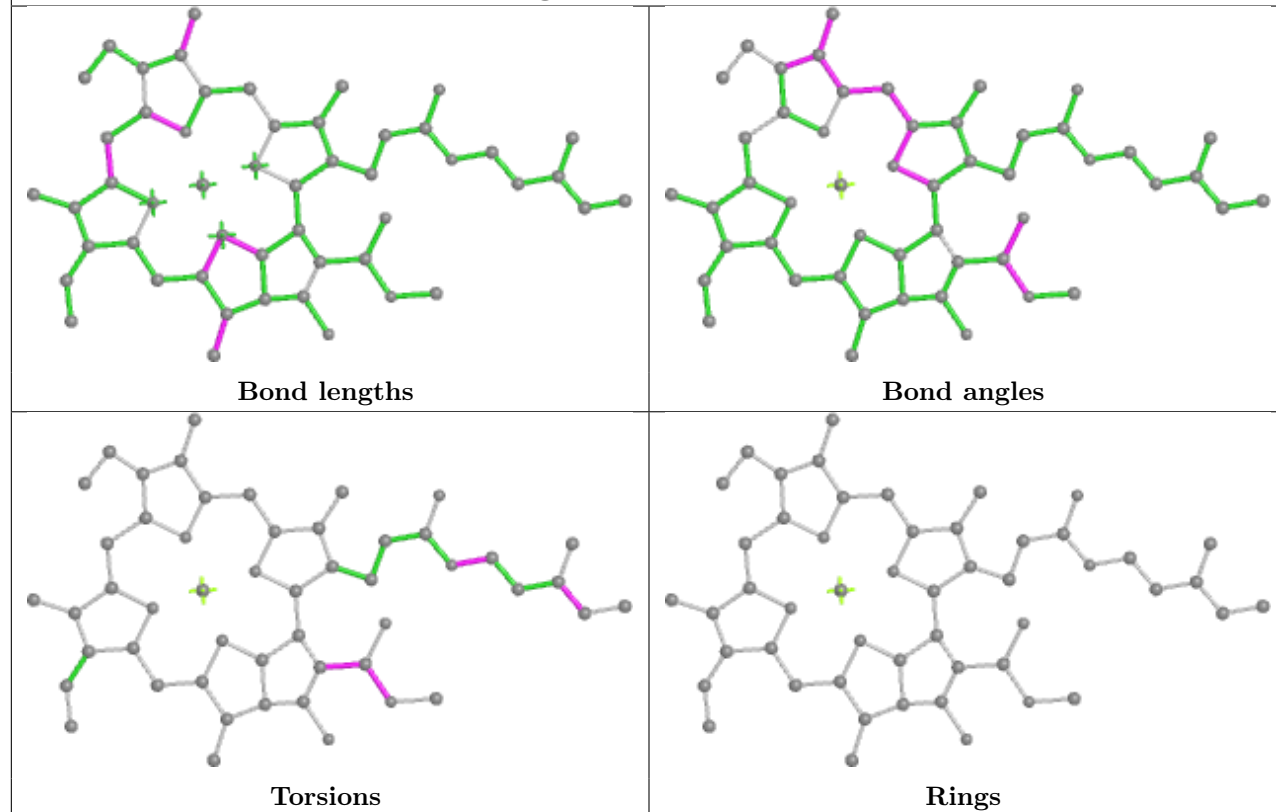


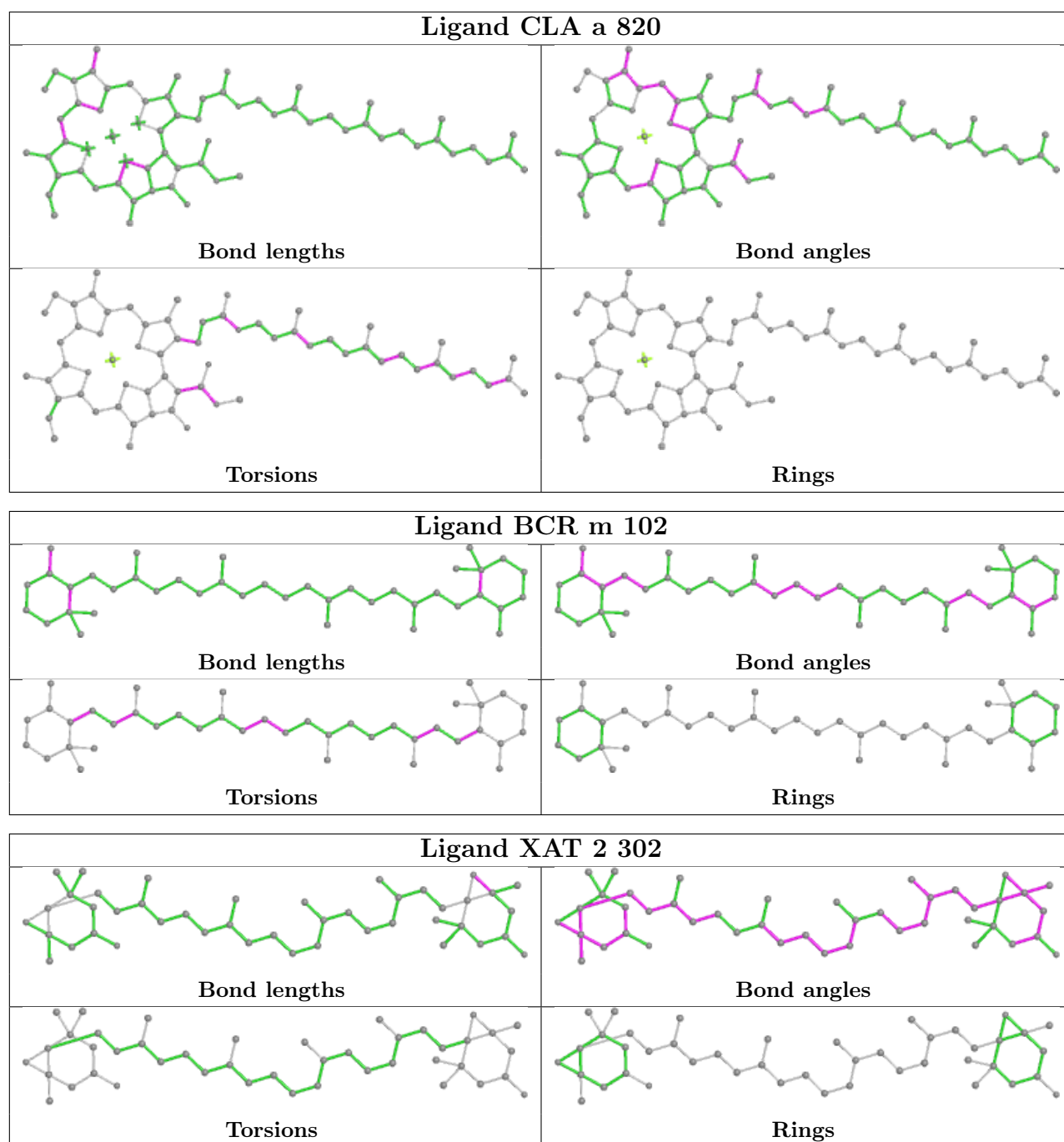
**Ligand XAT 5 303****Ligand CLA 4 310**

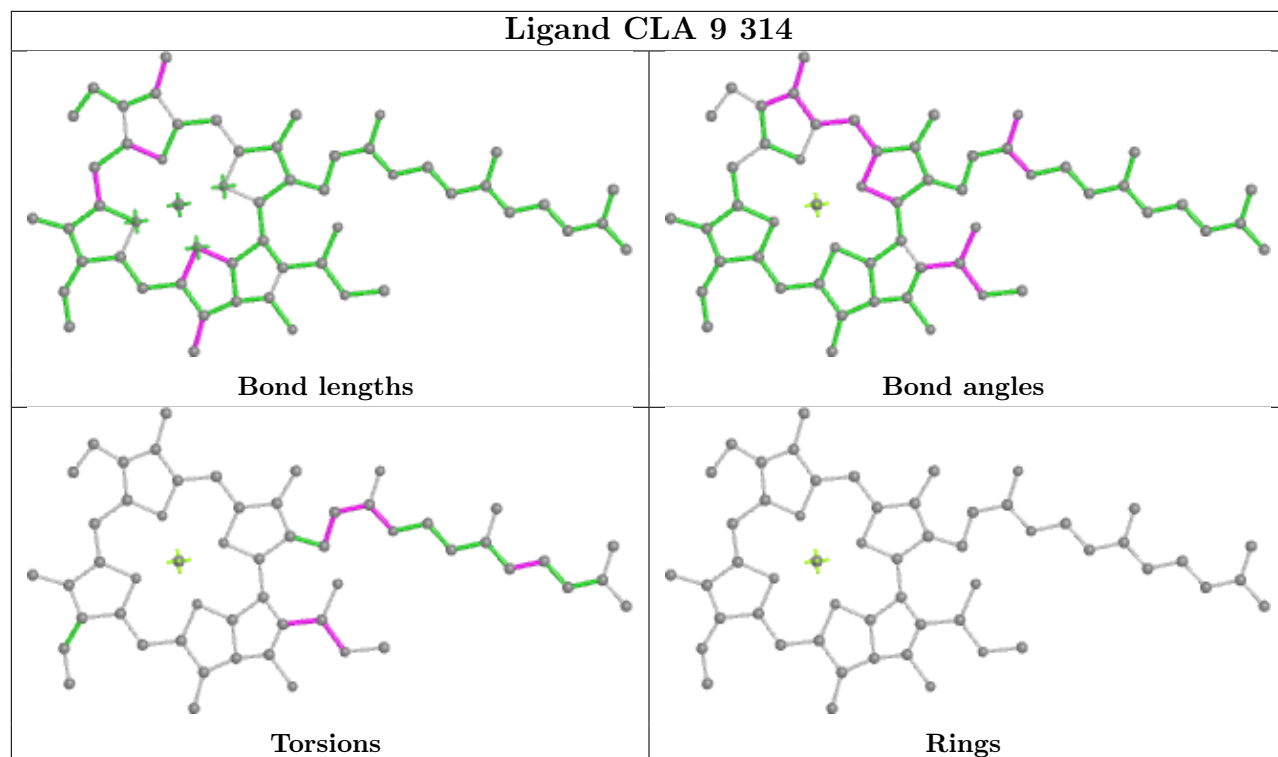
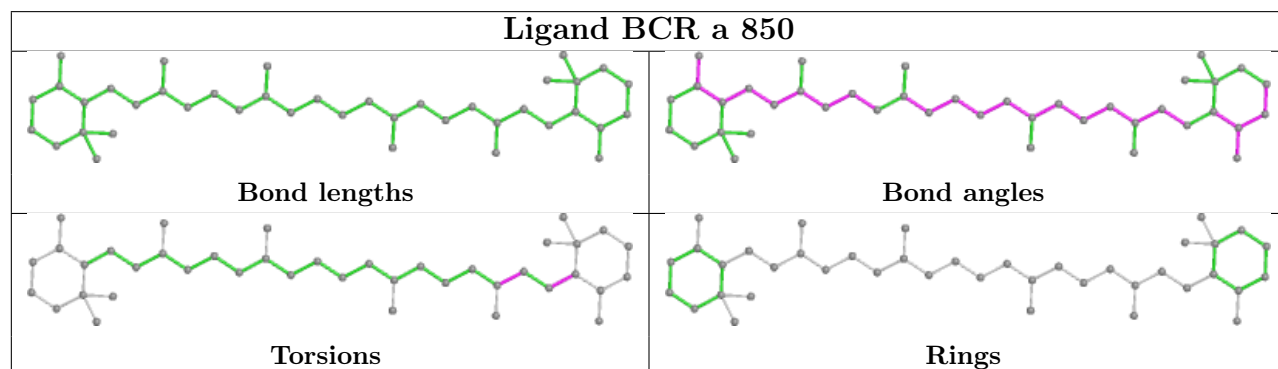
## Ligand CLA a 814



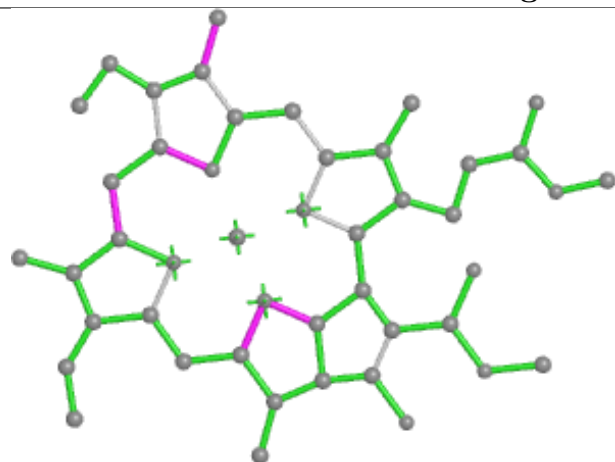
## Ligand CLA 6 312



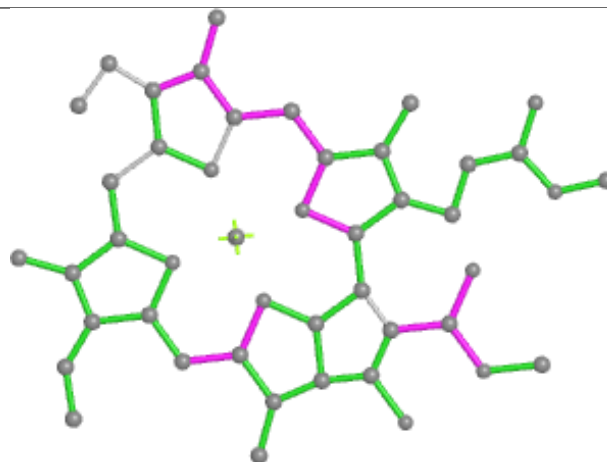


**Ligand CLA 9 314****Ligand BCR a 850**

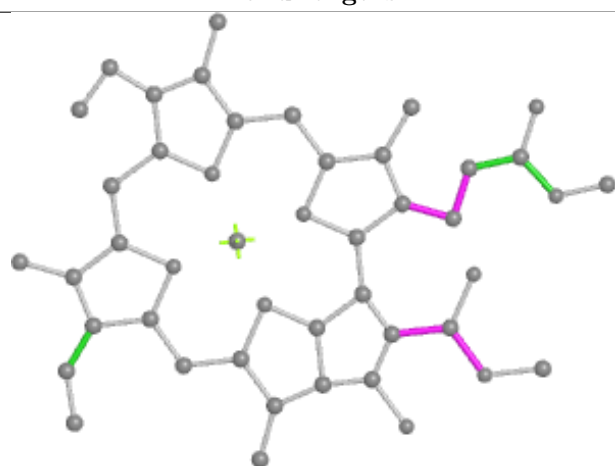
## Ligand CLA 9 311



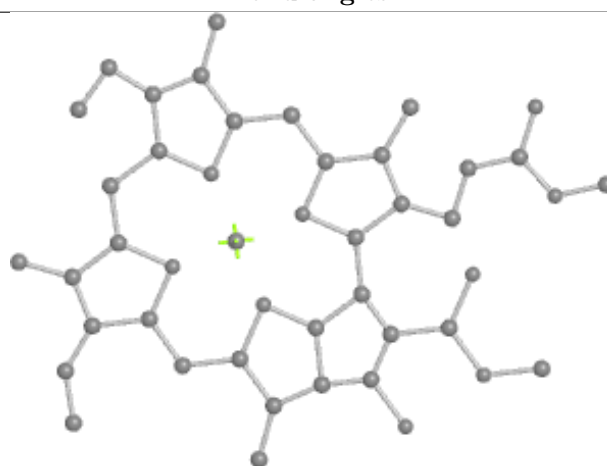
Bond lengths



Bond angles

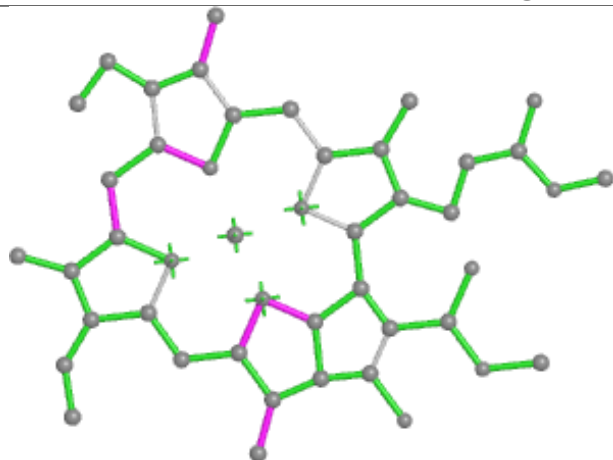


Torsions

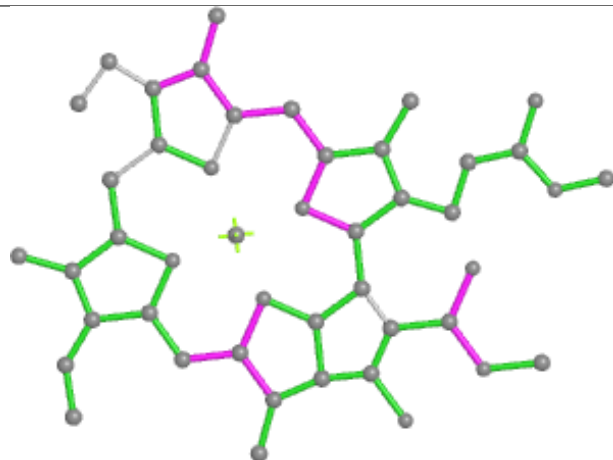


Rings

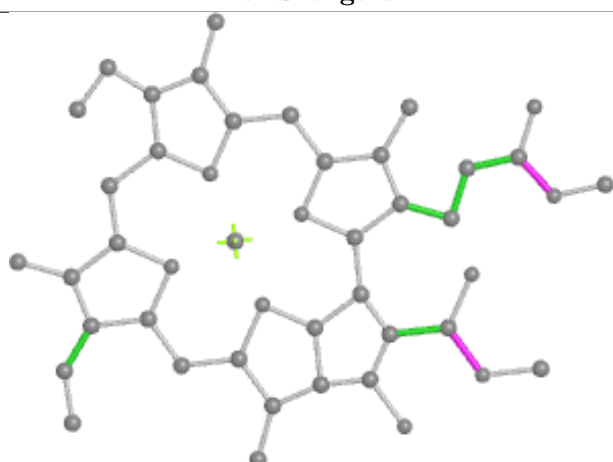
## Ligand CLA 5 306



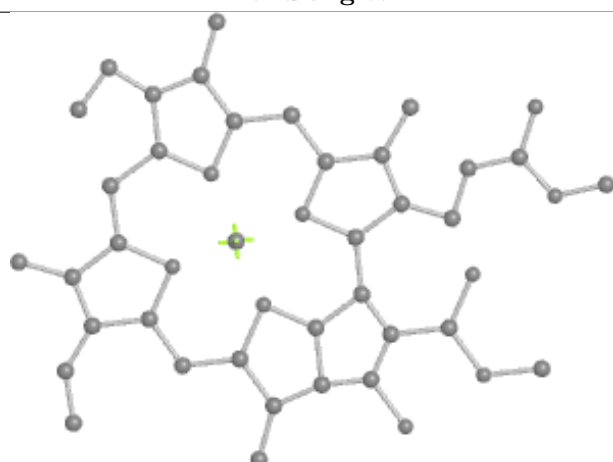
Bond lengths



Bond angles

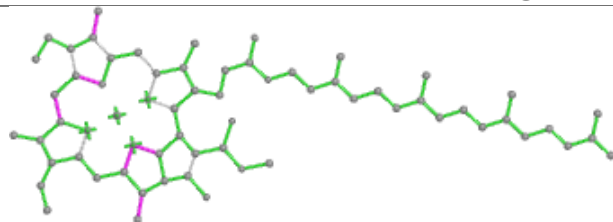


Torsions

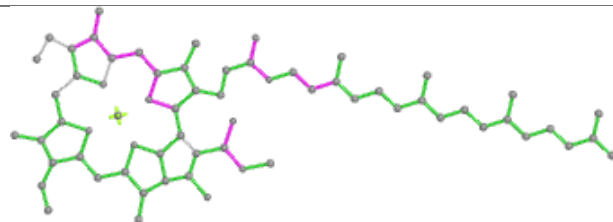


Rings

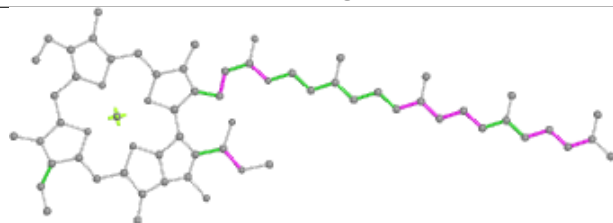
## Ligand CLA b 827



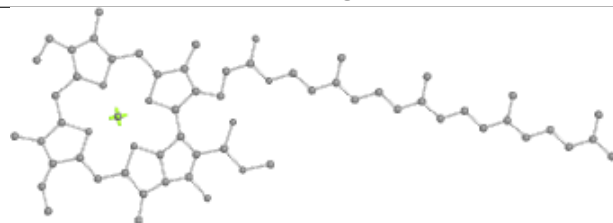
Bond lengths



Bond angles

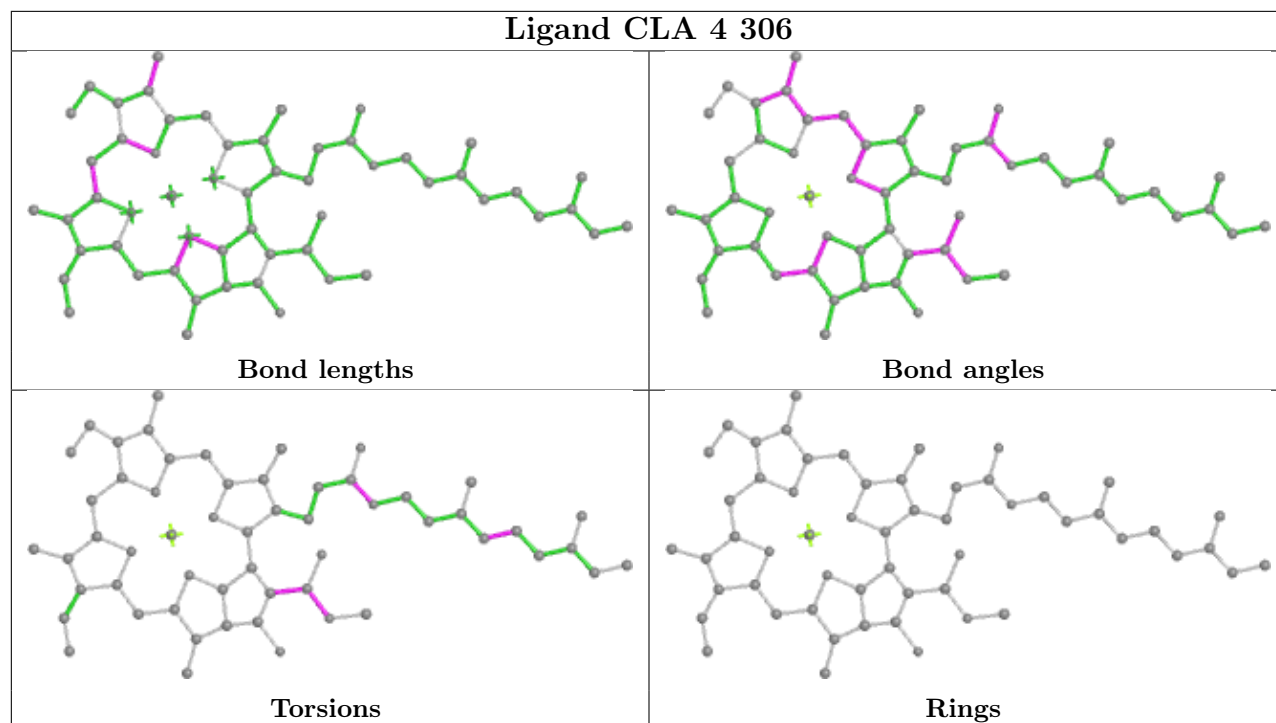


Torsions

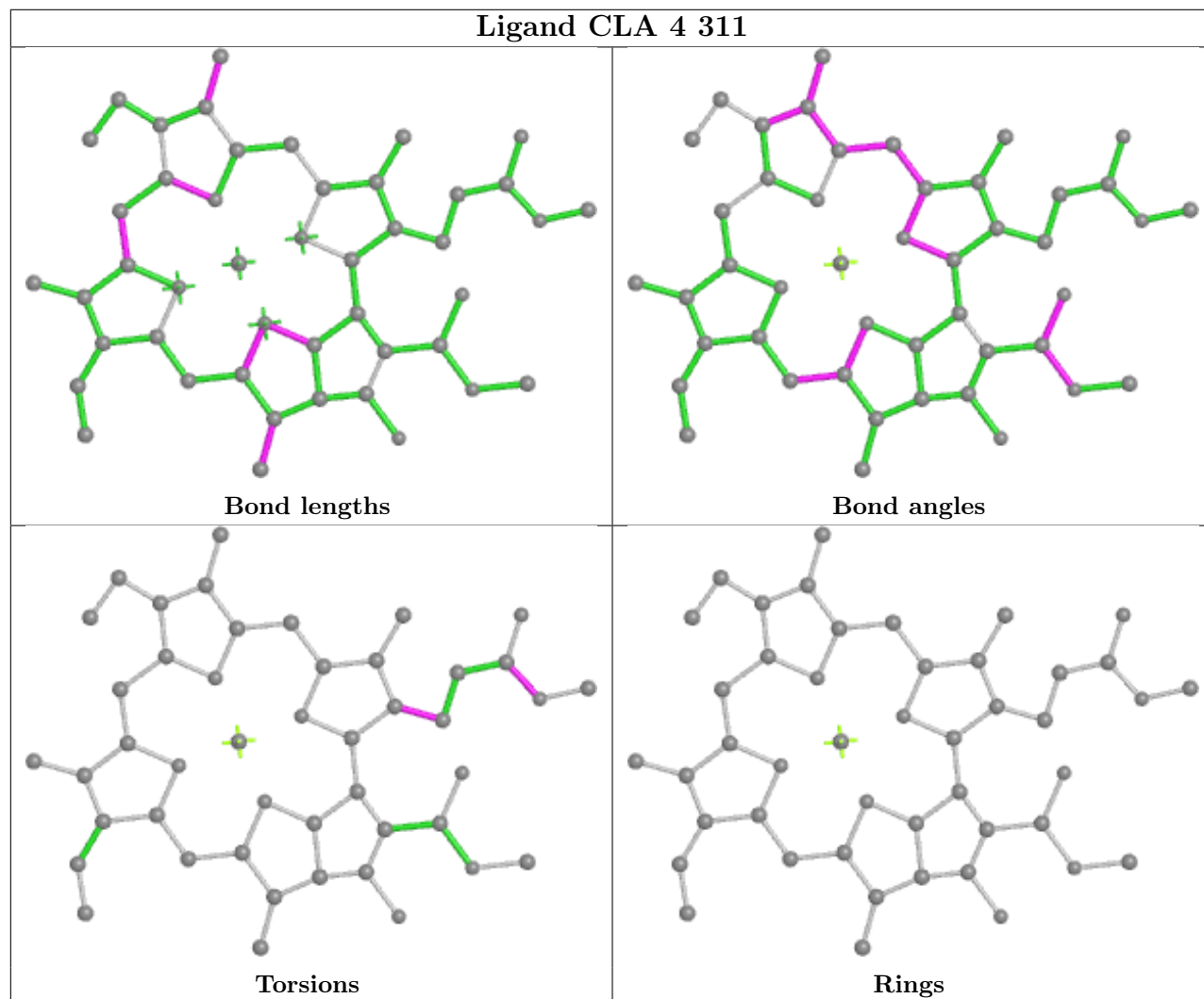


Rings

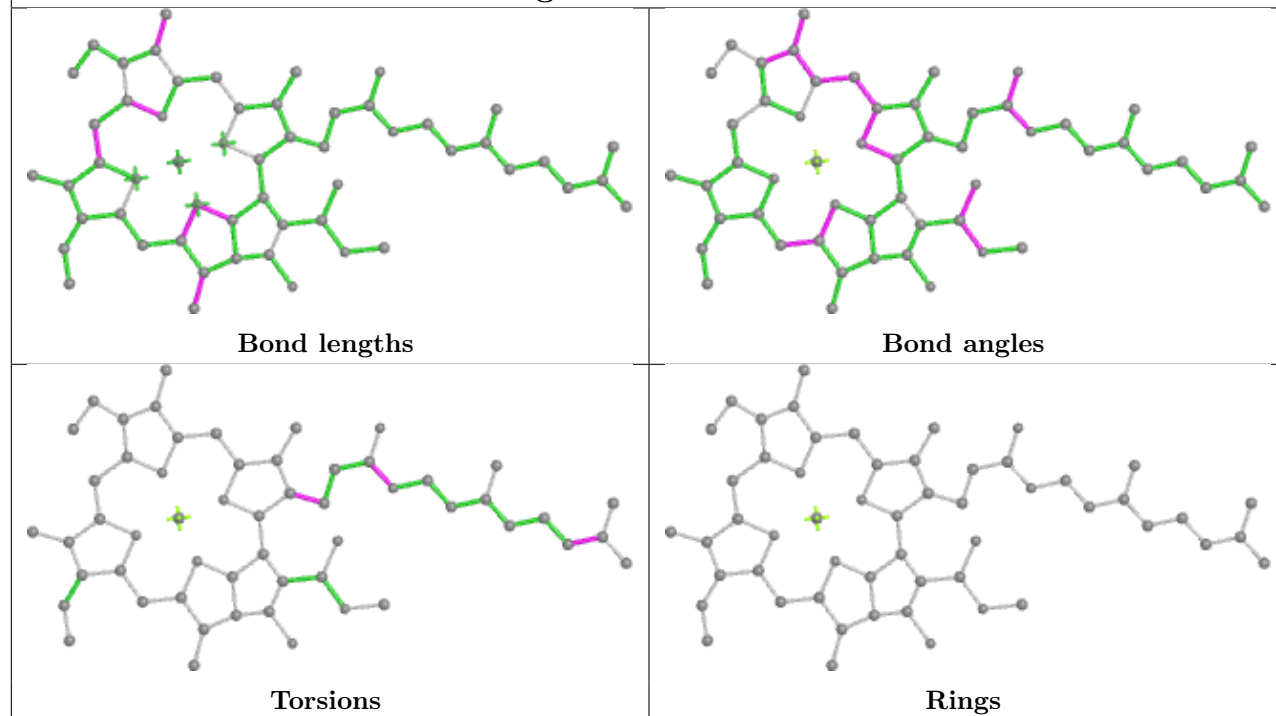
## Ligand CLA 4 306



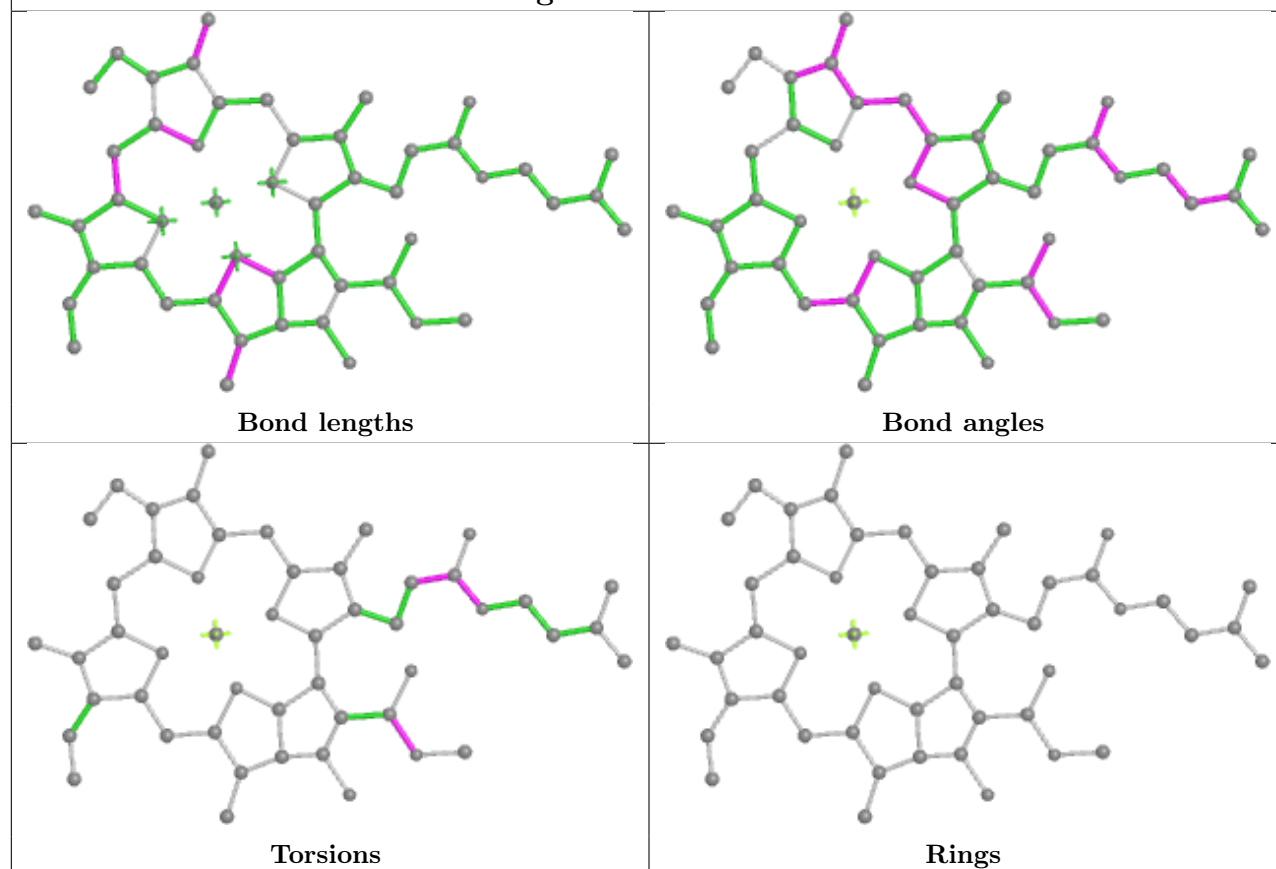
## Ligand CLA 4 311

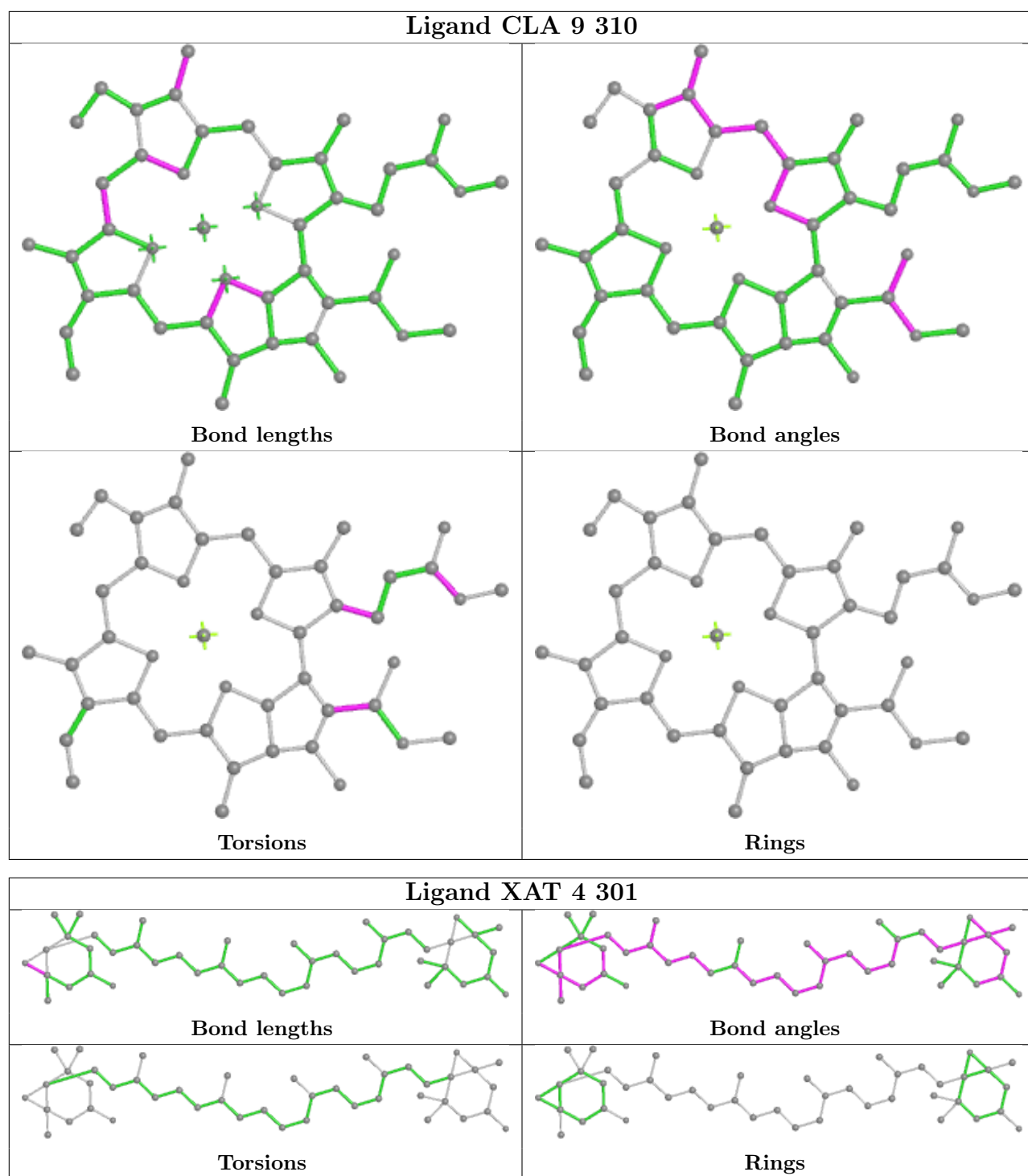


## Ligand CLA a 805



## Ligand CLA a 836





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

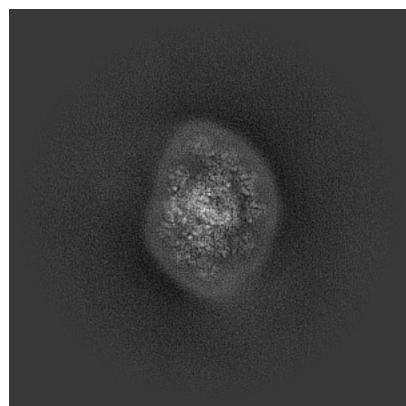
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60292. These allow visual inspection of the internal detail of the map and identification of artifacts.

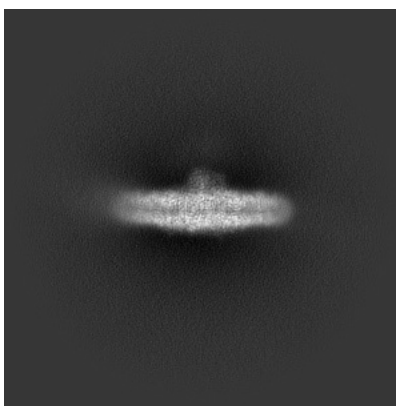
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

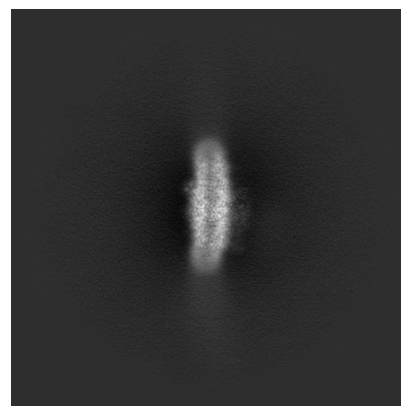
#### 6.1.1 Primary map



X

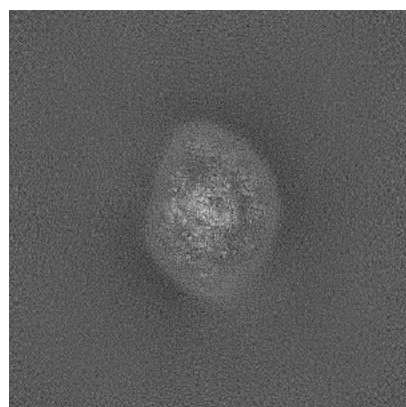


Y

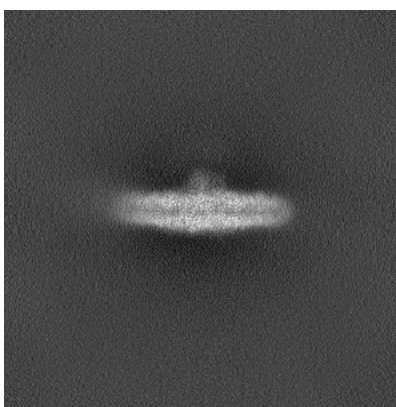


Z

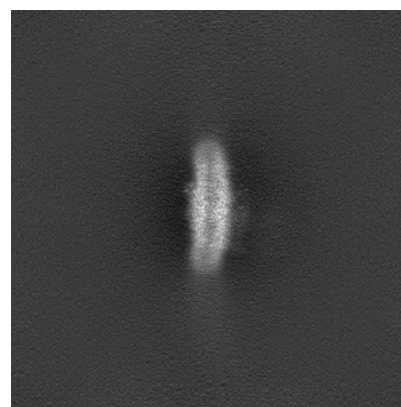
#### 6.1.2 Raw map



X



Y

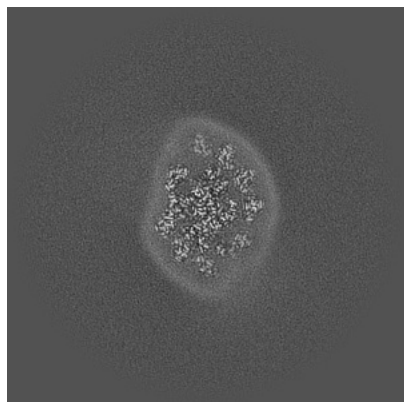


Z

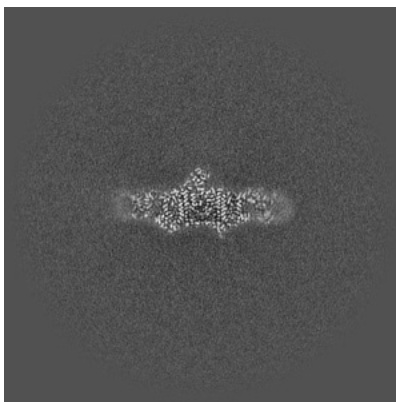
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

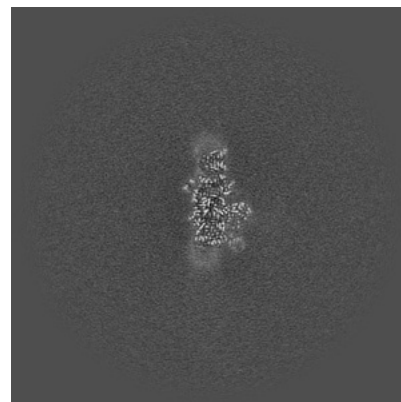
### 6.2.1 Primary map



X Index: 256

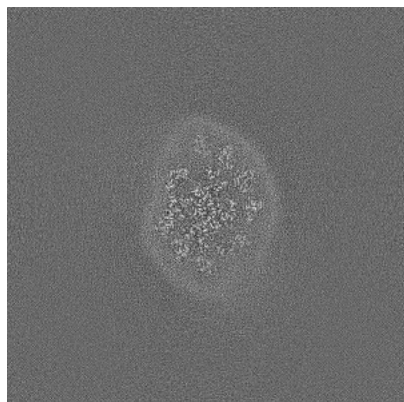


Y Index: 256

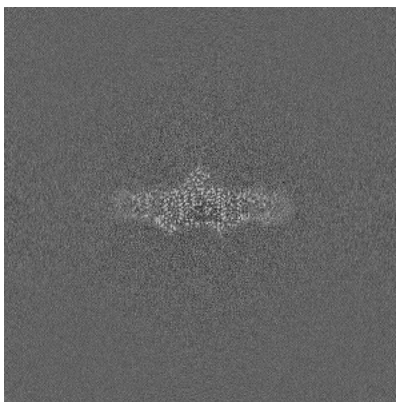


Z Index: 256

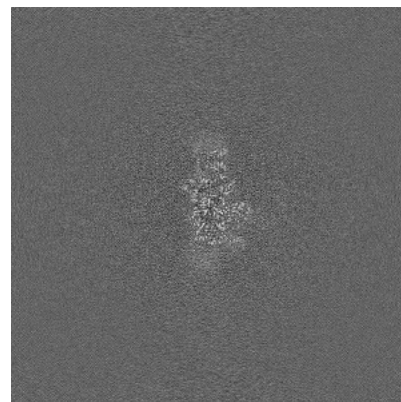
### 6.2.2 Raw map



X Index: 256



Y Index: 256

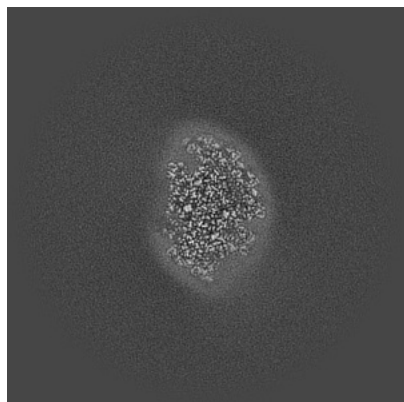


Z Index: 256

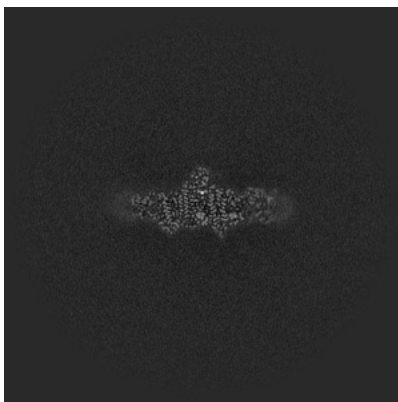
The images above show central slices of the map in three orthogonal directions.

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

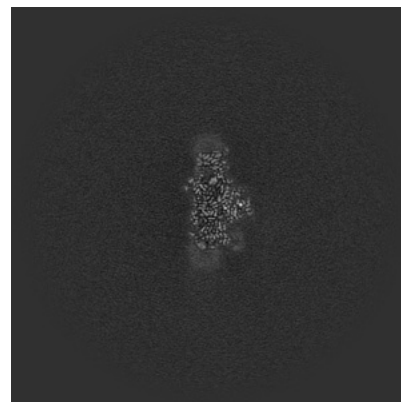
### 6.3.1 Primary map



X Index: 267

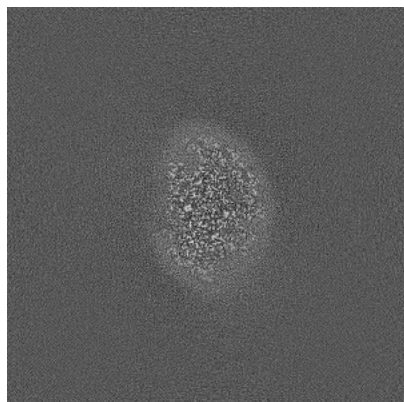


Y Index: 254

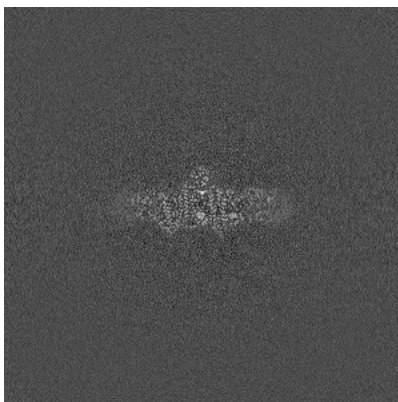


Z Index: 252

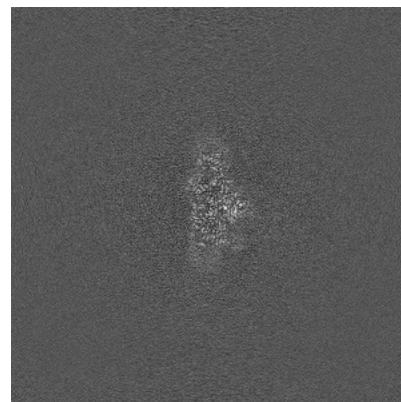
### 6.3.2 Raw map



X Index: 267



Y Index: 254

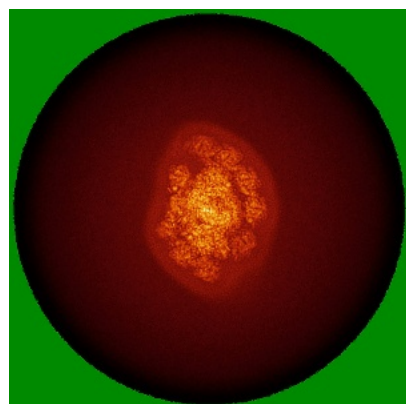


Z Index: 253

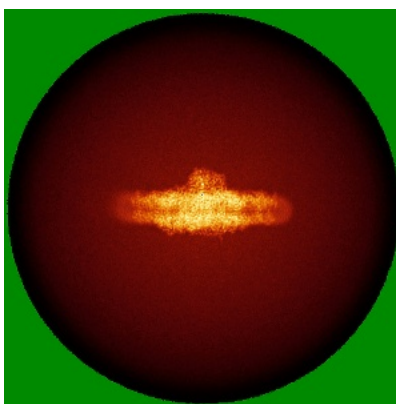
The images above show the largest variance slices of the map in three orthogonal directions.

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

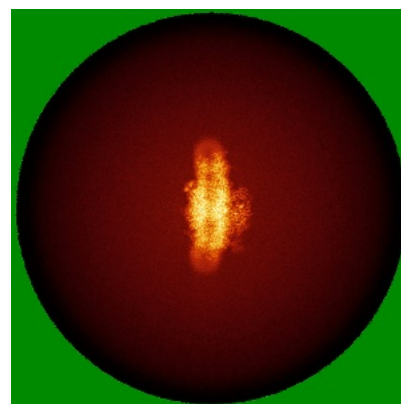
### 6.4.1 Primary map



X

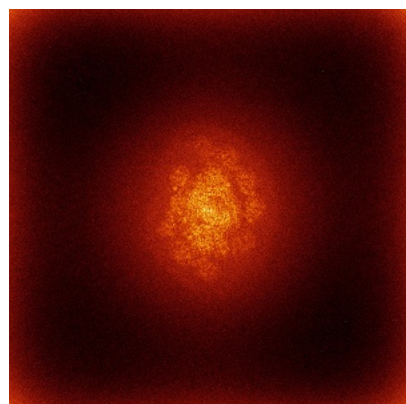


Y

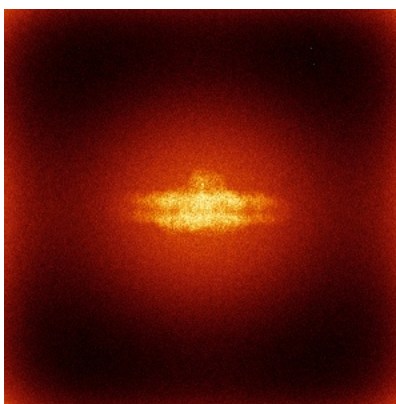


Z

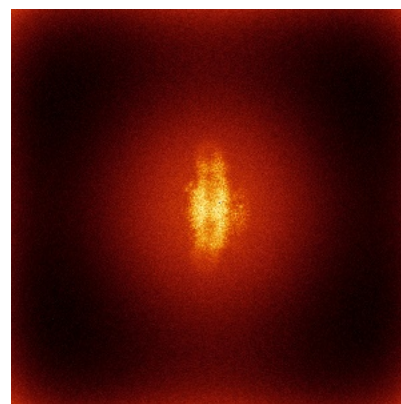
### 6.4.2 Raw map



X



Y

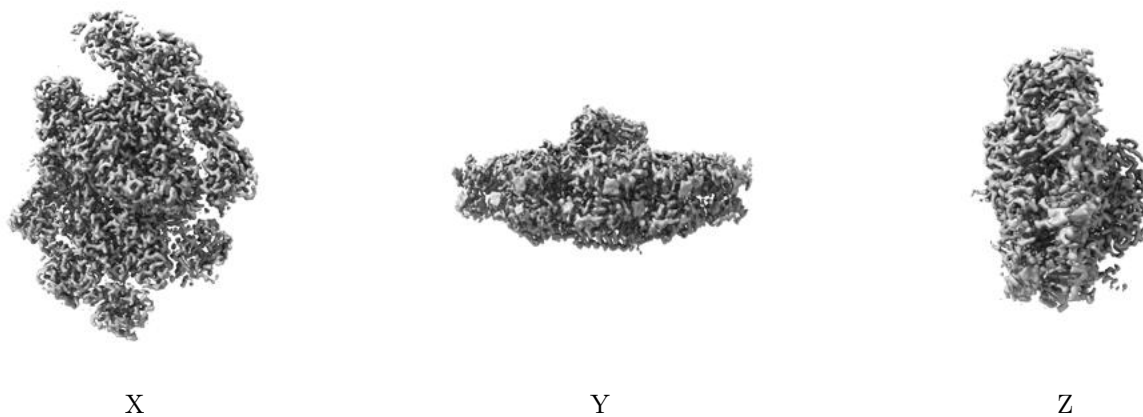


Z

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.

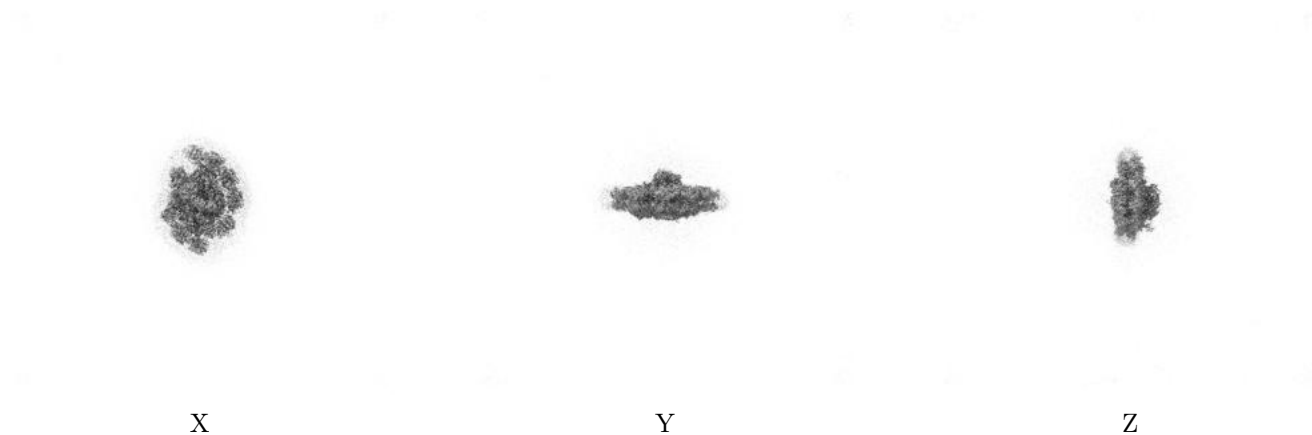
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.293. 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.

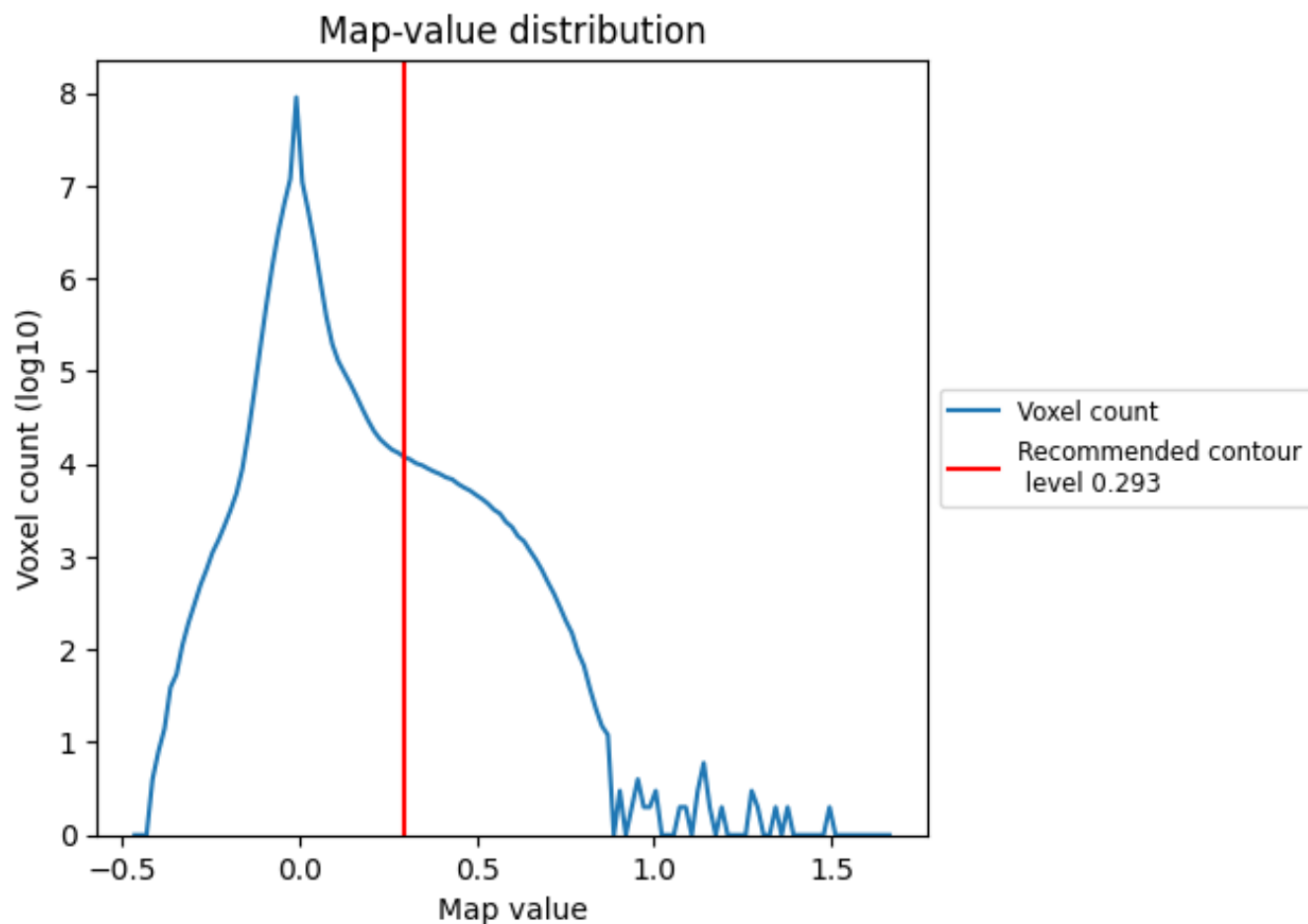
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

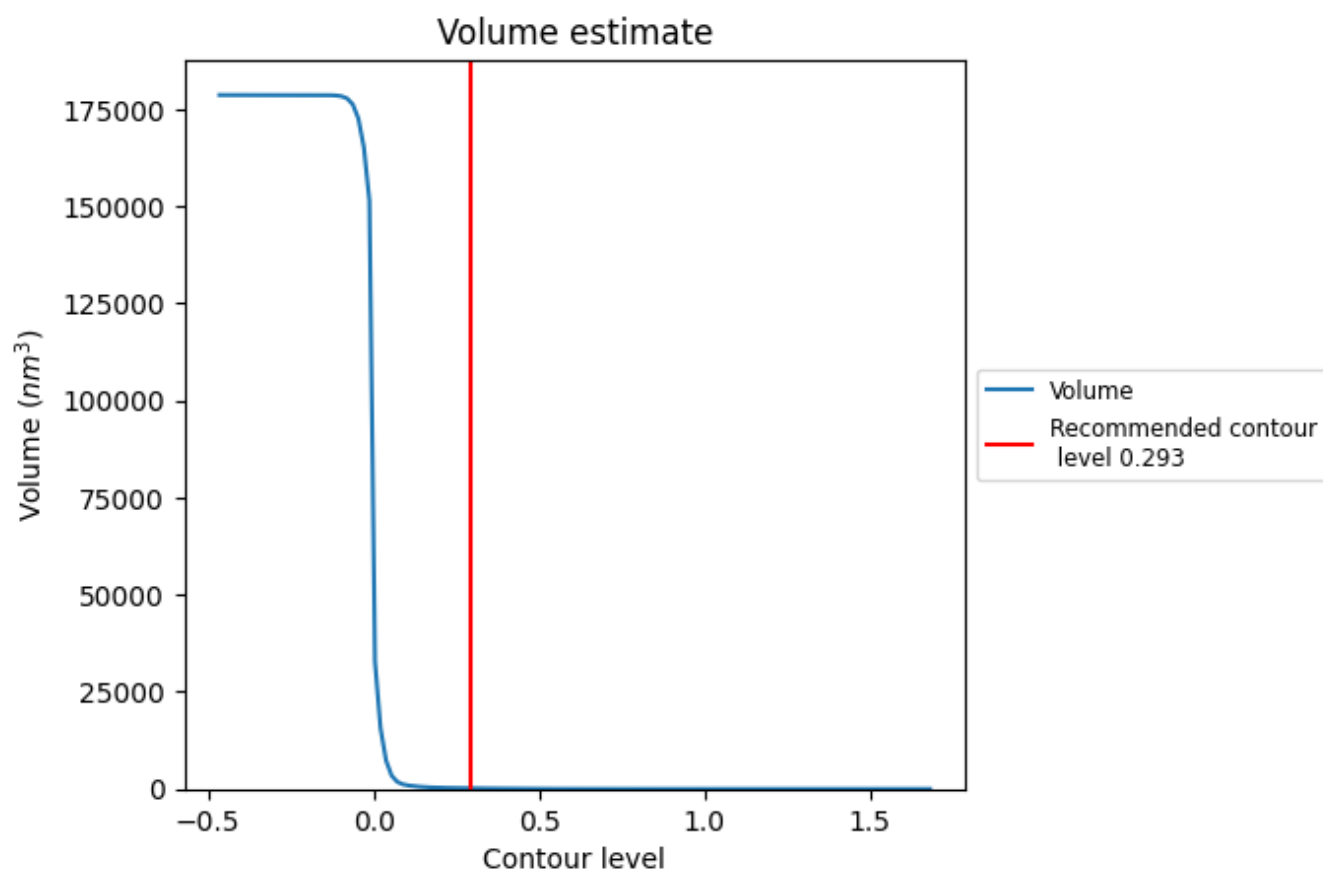
This section contains the results of statistical analysis of the map.

### 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.

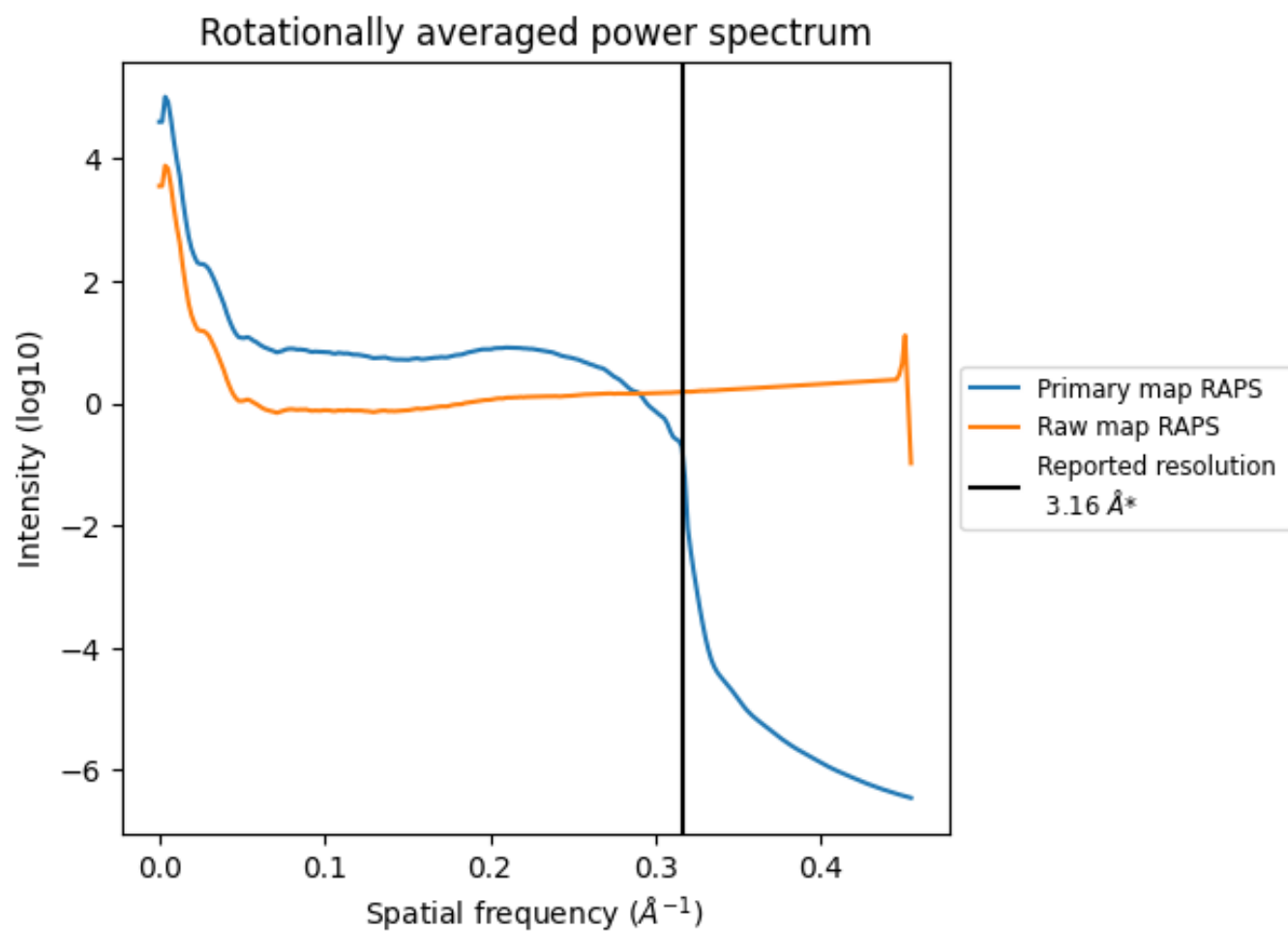
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176  $\text{nm}^3$ ; this corresponds to an approximate mass of 159 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 ⓘ

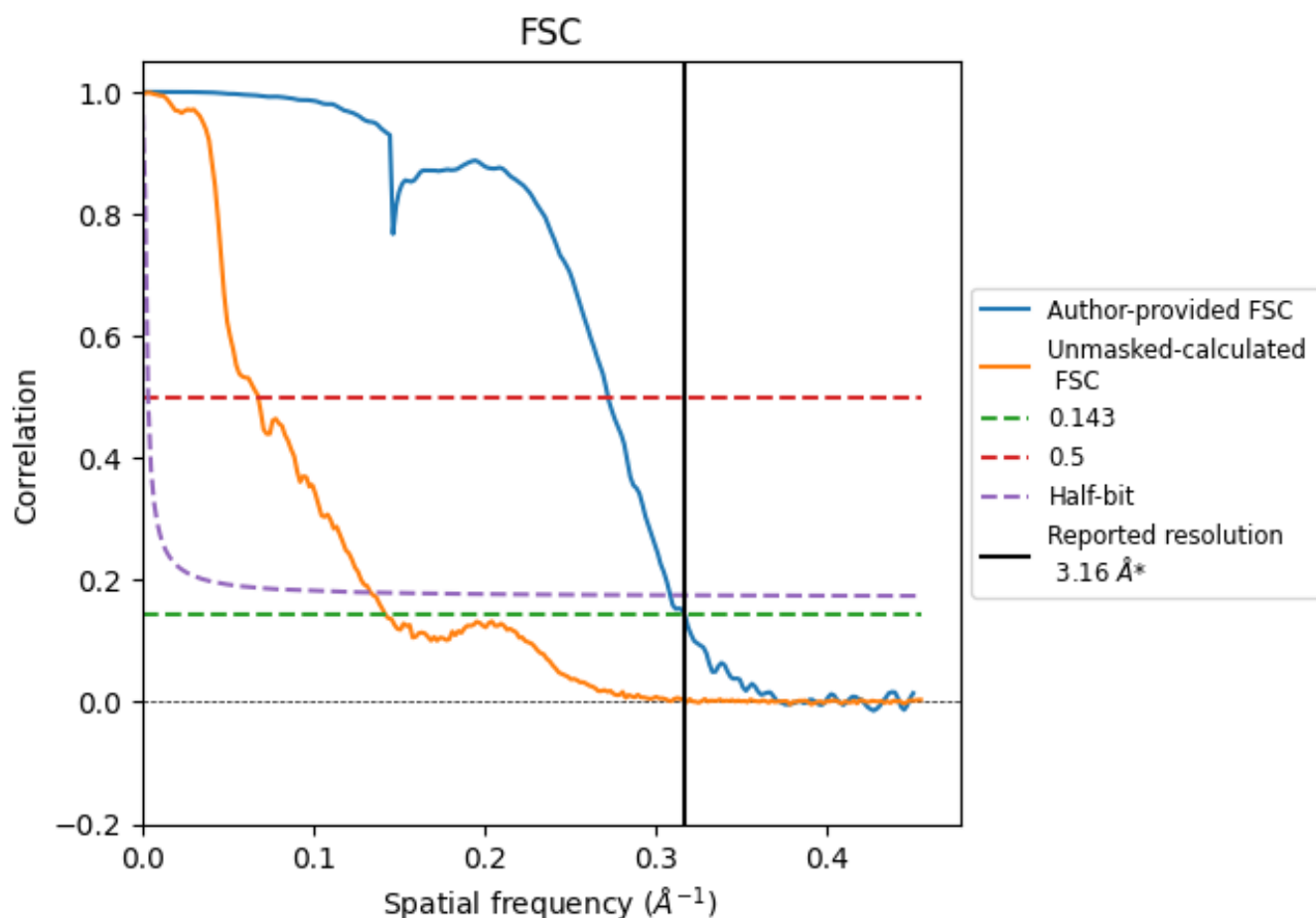


\*Reported resolution corresponds to spatial frequency of 0.316  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.316  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

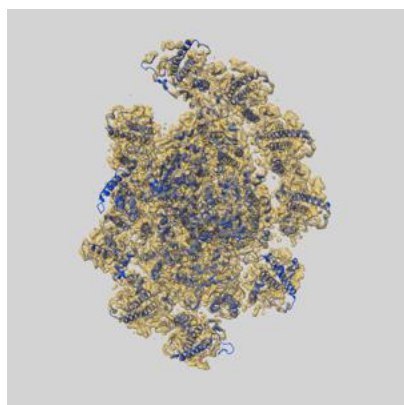
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.68	3.24
Unmasked-calculated*	7.04	14.77	7.49

\*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 7.04 differs from the reported value 3.16 by more than 10 %

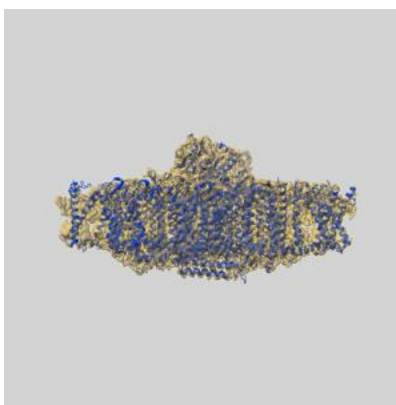
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60292 and PDB model 8ZOG. Per-residue inclusion information can be found in section 3 on page 31.

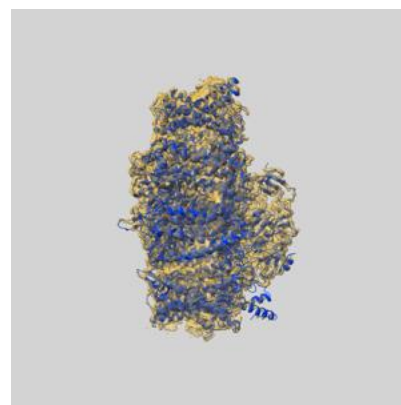
### 9.1 Map-model overlay [i](#)



X



Y



Z

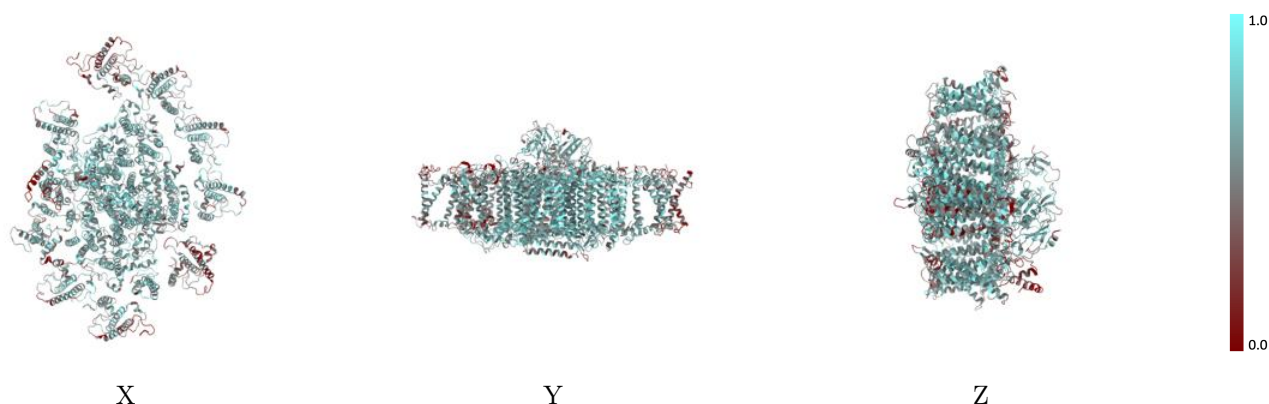
The images above show the 3D surface view of the map at the recommended contour level 0.293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



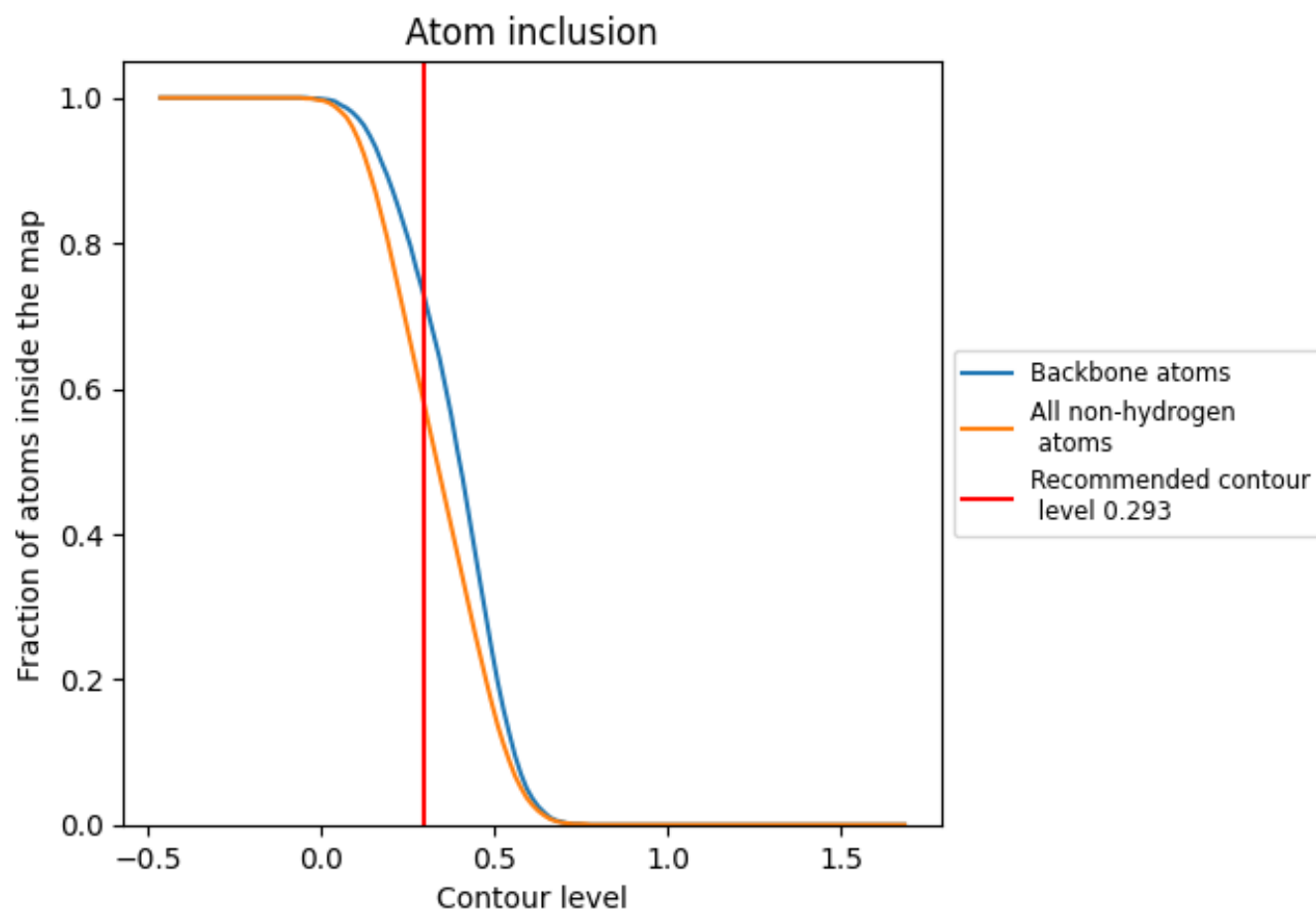
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.293).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 58% 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 (0.293) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5850	 0.4720
1	 0.5640	 0.4770
2	 0.3310	 0.3980
3	 0.5440	 0.4740
4	 0.5870	 0.4750
5	 0.5840	 0.4770
6	 0.3990	 0.4320
7	 0.4560	 0.4360
8	 0.5790	 0.4770
9	 0.5250	 0.4670
a	 0.6600	 0.4850
b	 0.6580	 0.4860
c	 0.7320	 0.5180
d	 0.6210	 0.5030
e	 0.6050	 0.5020
f	 0.5980	 0.4580
g	 0.3840	 0.4000
h	 0.5930	 0.4870
i	 0.6260	 0.5090
j	 0.6150	 0.5000
l	 0.6110	 0.4600
m	 0.5600	 0.4880

