



## wwPDB EM Validation Summary Report ⓘ

Dec 1, 2025 – 06:50 PM JST

PDB ID : 8ZOE / pdb\_00008zoe  
EMDB ID : EMD-60290  
Title : Structure of the canthaxanthin mutant PSI-4VCPI supercomplex in *Nanochloropsis oceanica*  
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.  
Deposited on : 2024-05-28  
Resolution : 3.02 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:

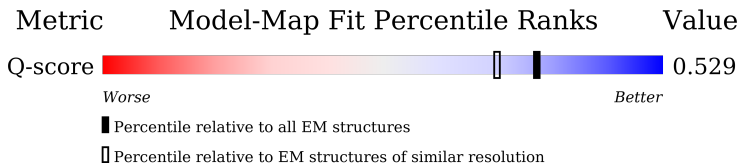
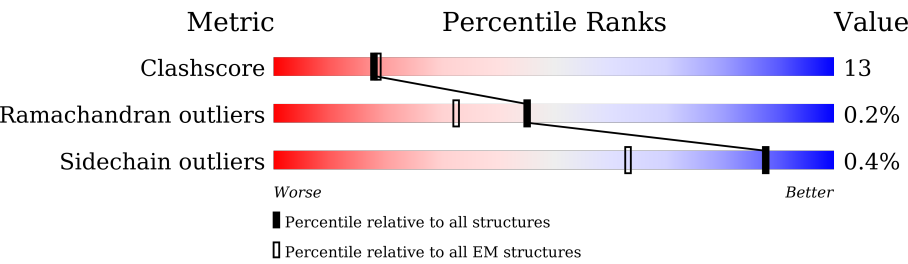
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the 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 3.02 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.





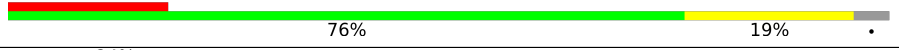



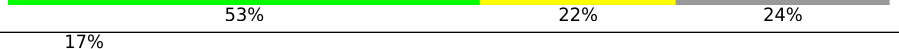
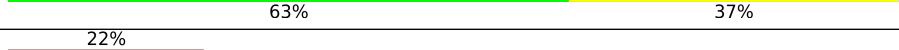
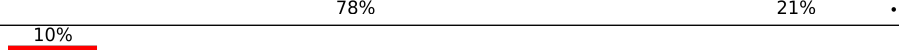


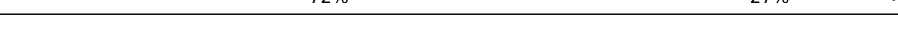
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13913 ( 2.52 - 3.52 )

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	9	232	<div><div>26%</div><div>65%</div><div>21%</div><div>13%</div></div>
2	8	200	<div><div>29%</div><div>62%</div><div>19%</div><div>18%</div></div>
3	7	202	<div><div>56%</div><div>59%</div><div>23%</div><div>18%</div></div>
4	1	208	<div><div>15%</div><div>51%</div><div>26%</div><div>22%</div></div>

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Mol	Chain	Length	Quality of chain
5	a	745	
6	b	737	
7	d	136	
8	e	67	
9	f	185	
10	h	128	
11	i	45	
12	j	41	
13	l	172	
14	m	30	
15	g	55	
16	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
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	1	311	X	-	-	-
22	CLA	1	312	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	1	314	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	308	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	7	313	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-
22	CLA	8	305	X	-	-	-
22	CLA	8	306	X	-	-	-
22	CLA	8	307	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	8	311	X	-	-	-
22	CLA	8	312	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	314	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	312	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	9	314	X	-	-	-
22	CLA	9	315	X	-	-	-
22	CLA	9	316	X	-	-	-
22	CLA	9	318	X	-	-	-
22	CLA	a	801	X	-	-	-
22	CLA	a	802	X	-	-	-
22	CLA	a	803	X	-	-	-
22	CLA	a	804	X	-	-	-
22	CLA	a	805	X	-	-	-
22	CLA	a	806	X	-	-	-
22	CLA	a	807	X	-	-	-
22	CLA	a	808	X	-	-	-
22	CLA	a	809	X	-	-	-
22	CLA	a	810	X	-	-	-
22	CLA	a	811	X	-	-	-
22	CLA	a	812	X	-	-	-
22	CLA	a	813	X	-	-	-
22	CLA	a	814	X	-	-	-
22	CLA	a	815	X	-	-	-
22	CLA	a	816	X	-	-	-
22	CLA	a	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	818	X	-	-	-
22	CLA	a	819	X	-	-	-
22	CLA	a	820	X	-	-	-
22	CLA	a	821	X	-	-	-
22	CLA	a	822	X	-	-	-
22	CLA	a	823	X	-	-	-
22	CLA	a	824	X	-	-	-
22	CLA	a	825	X	-	-	-
22	CLA	a	826	X	-	-	-
22	CLA	a	827	X	-	-	-
22	CLA	a	828	X	-	-	-
22	CLA	a	829	X	-	-	-
22	CLA	a	830	X	-	-	-
22	CLA	a	831	X	-	-	-
22	CLA	a	832	X	-	-	-
22	CLA	a	833	X	-	-	-
22	CLA	a	834	X	-	-	-
22	CLA	a	835	X	-	-	-
22	CLA	a	836	X	-	-	-
22	CLA	a	837	X	-	-	-
22	CLA	a	838	X	-	-	-
22	CLA	a	839	X	-	-	-
22	CLA	a	840	X	-	-	-
22	CLA	a	841	X	-	-	-
22	CLA	a	842	X	-	-	-
22	CLA	a	844	X	-	-	-
22	CLA	a	854	X	-	-	-
22	CLA	b	801	X	-	-	-
22	CLA	b	802	X	-	-	-
22	CLA	b	803	X	-	-	-
22	CLA	b	804	X	-	-	-
22	CLA	b	805	X	-	-	-
22	CLA	b	806	X	-	-	-
22	CLA	b	807	X	-	-	-
22	CLA	b	808	X	-	-	-
22	CLA	b	809	X	-	-	-
22	CLA	b	810	X	-	-	-
22	CLA	b	811	X	-	-	-
22	CLA	b	812	X	-	-	-
22	CLA	b	813	X	-	-	-
22	CLA	b	814	X	-	-	-
22	CLA	b	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	b	816	X	-	-	-
22	CLA	b	817	X	-	-	-
22	CLA	b	818	X	-	-	-
22	CLA	b	819	X	-	-	-
22	CLA	b	820	X	-	-	-
22	CLA	b	821	X	-	-	-
22	CLA	b	822	X	-	-	-
22	CLA	b	823	X	-	-	-
22	CLA	b	824	X	-	-	-
22	CLA	b	825	X	-	-	-
22	CLA	b	826	X	-	-	-
22	CLA	b	827	X	-	-	-
22	CLA	b	828	X	-	-	-
22	CLA	b	829	X	-	-	-
22	CLA	b	830	X	-	-	-
22	CLA	b	831	X	-	-	-
22	CLA	b	832	X	-	-	-
22	CLA	b	833	X	-	-	-
22	CLA	b	834	X	-	-	-
22	CLA	b	835	X	-	-	-
22	CLA	b	836	X	-	-	-
22	CLA	b	837	X	-	-	-
22	CLA	b	838	X	-	-	-
22	CLA	b	839	X	-	-	-
22	CLA	b	840	X	-	-	-
22	CLA	f	802	X	-	-	-
22	CLA	f	803	X	-	-	-
22	CLA	h	203	X	-	-	-
22	CLA	h	205	X	-	-	-
22	CLA	j	102	X	-	-	-
22	CLA	j	103	X	-	-	-
22	CLA	l	202	X	-	-	-
22	CLA	l	203	X	-	-	-
22	CLA	l	204	X	-	-	-
27	SF4	c	102	-	-	X	-

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33183 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-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	9	201	Total	C	N	O	S	0	0
			1466	936	256	269	5		

- Molecule 2 is a protein called VCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	8	164	Total	C	N	O	S	0	0
			1258	822	203	227	6		

- Molecule 3 is a protein called VCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	166	Total	C	N	O	S	0	0
			1220	791	202	222	5		

- Molecule 4 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

- Molecule 7 is a protein called Photosystem I reaction center subunit II.

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

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

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

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

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

- Molecule 10 is a protein called Psar.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	j	41	Total	C	N	O	S	0	0
			339	233	48	57	1		

- Molecule 13 is a protein called PSI subunit V.

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

- Molecule 14 is a protein called Psam.

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

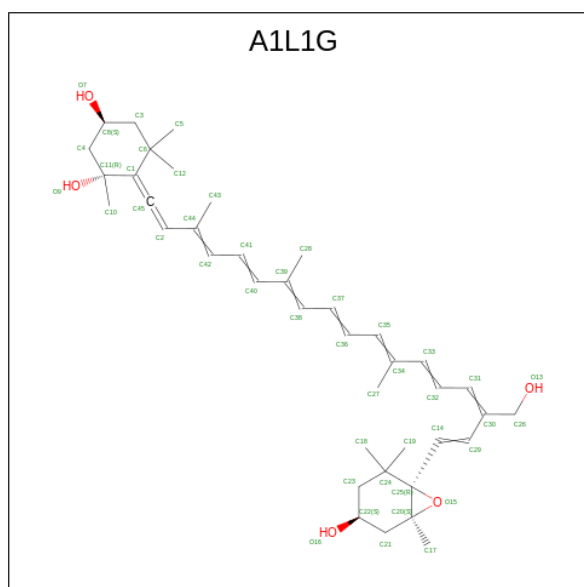
- Molecule 15 is a protein called PsaS.

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

- Molecule 16 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 17 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-cyclohexane-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).



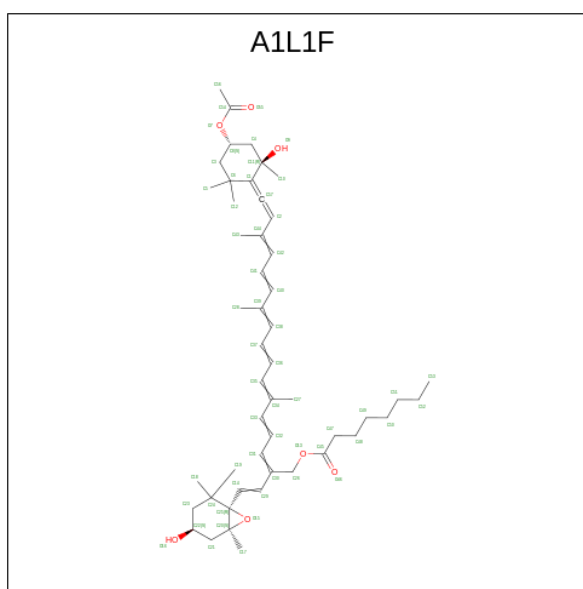
Mol	Chain	Residues	Atoms			AltConf
17	9	1	Total	C	O	0
			45	40	5	
17	9	1	Total	C	O	0
			45	40	5	

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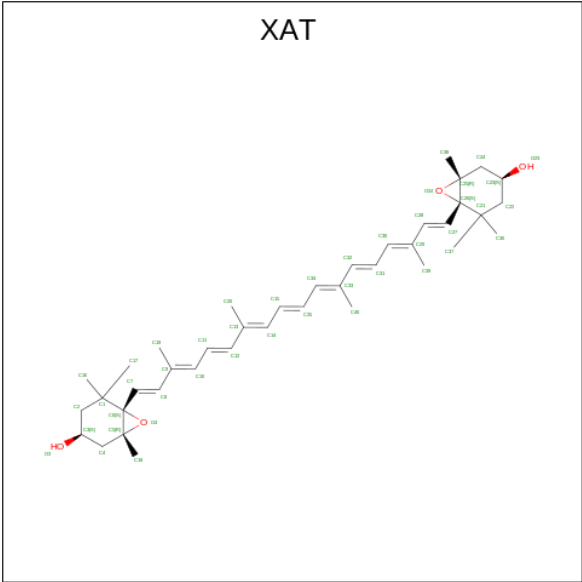
Mol	Chain	Residues	Atoms			AltConf
17	7	1	Total	C	O	0
			45	40	5	
17	1	1	Total	C	O	0
			45	40	5	

- Molecule 18 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
18	9	1	Total	C	O	0
			57	50	7	
18	8	1	Total	C	O	0
			57	50	7	
18	1	1	Total	C	O	0
			57	50	7	
18	h	1	Total	C	O	0
			57	50	7	

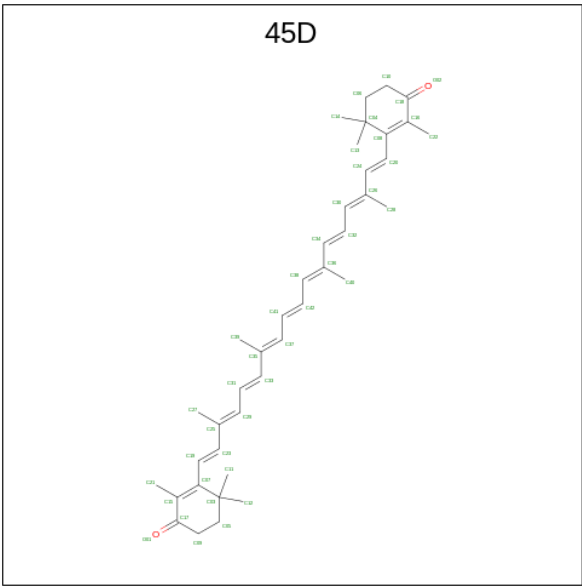
- Molecule 19 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	9	1	Total	C	O	0
			44	40	4	
19	9	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	1	1	Total	C	O	0
			44	40	4	
19	1	1	Total	C	O	0
			44	40	4	
19	a	1	Total	C	O	0
			44	40	4	
19	j	1	Total	C	O	0
			44	40	4	

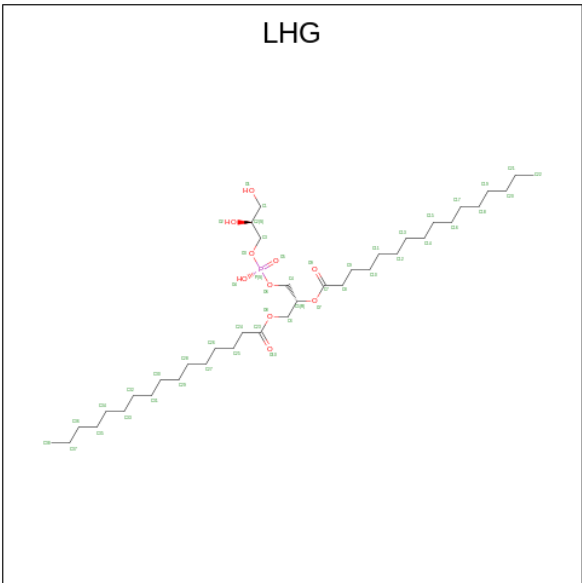
- Molecule 20 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>2</sub>) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
20	9	1	Total	C	O	0
			42	40	2	

- Molecule 21 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
21	9	1	Total	C	O	P	0
			36	25	10	1	

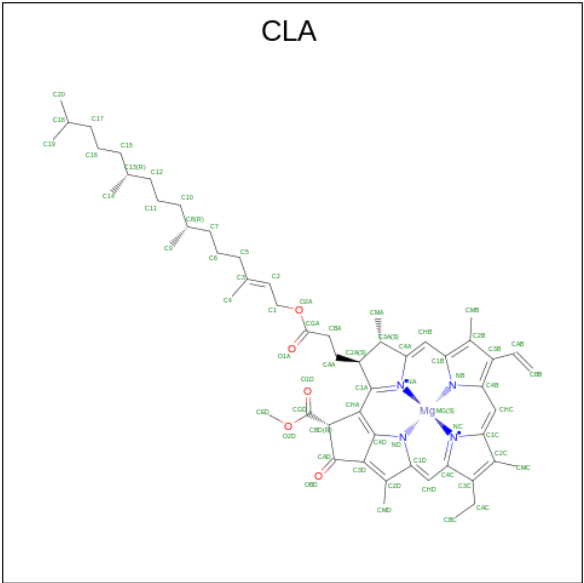
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Mol	Chain	Residues	Atoms				AltConf
21	9	1	Total	C	O	P	0
			46	35	10	1	
21	a	1	Total	C	O	P	0
			48	37	10	1	
21	a	1	Total	C	O	P	0
			27	16	10	1	
21	b	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 22 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
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	9	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	7	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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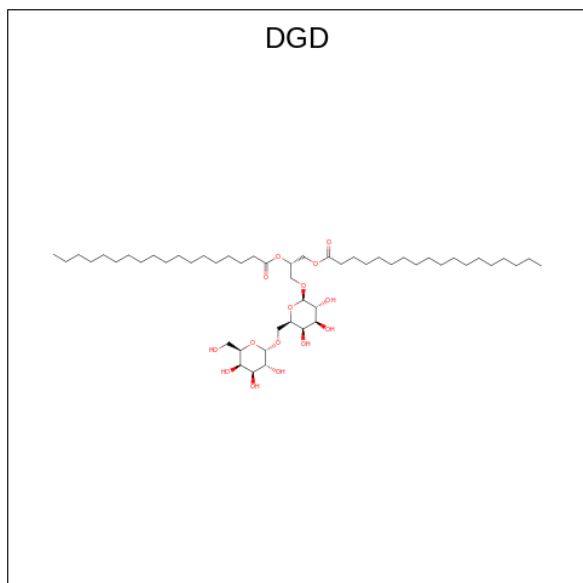
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	f	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	j	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	l	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

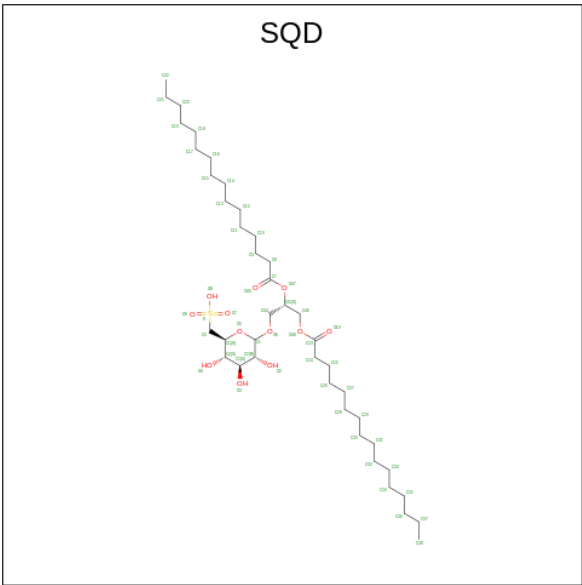
- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	8	1	Total	C	O	0
			40	25	15	
23	b	1	Total	C	O	0
			57	42	15	

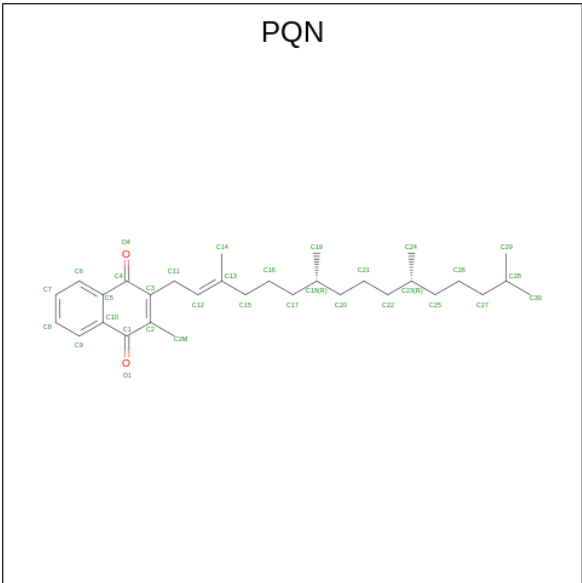
- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).





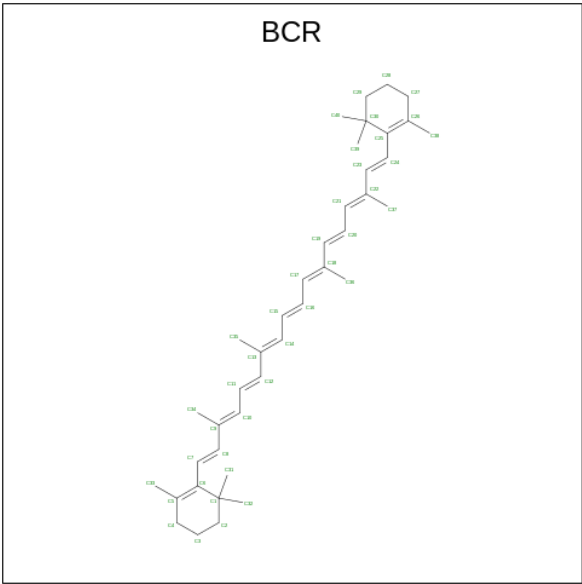
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



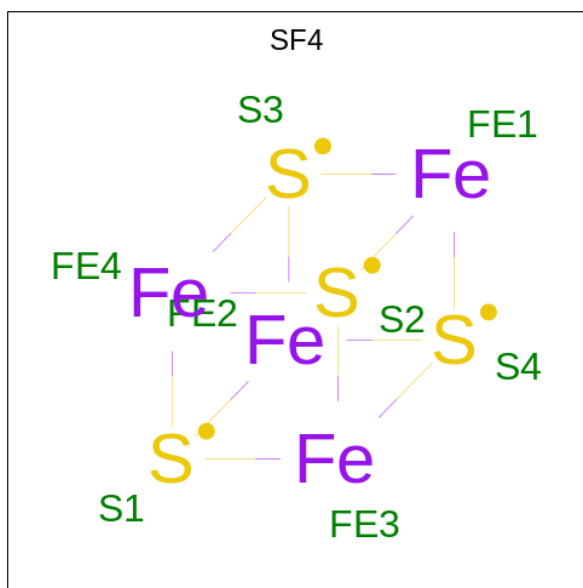
Mol	Chain	Residues	Atoms	AltConf
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	f	1	Total C 40 40	0
26	f	1	Total C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

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Mol	Chain	Residues	Atoms	AltConf
26	h	1	Total C 40 40	0
26	h	1	Total C 40 40	0
26	i	1	Total C 40 40	0
26	j	1	Total C 40 40	0
26	l	1	Total C 40 40	0
26	l	1	Total C 40 40	0
26	m	1	Total C 40 40	0

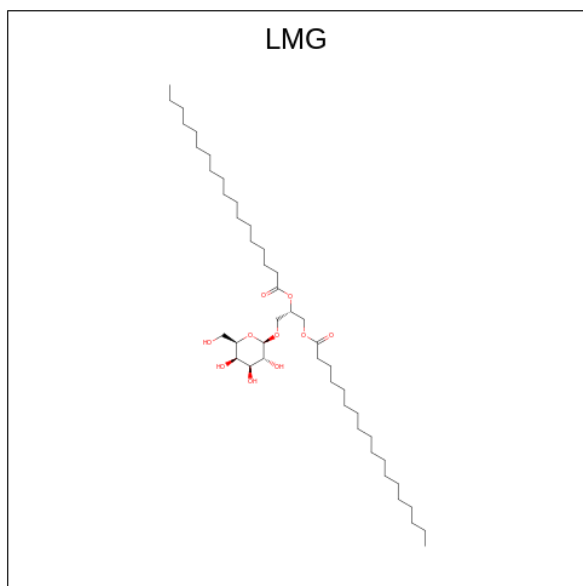
- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



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

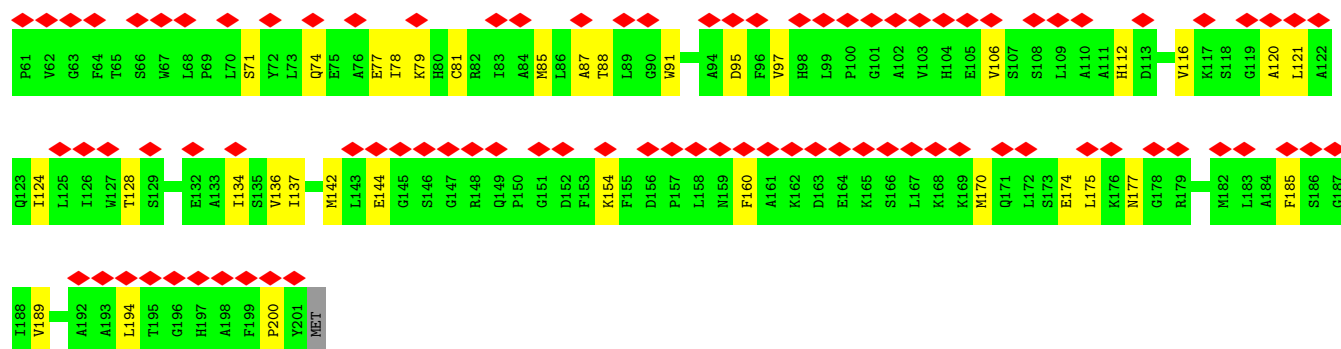
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).

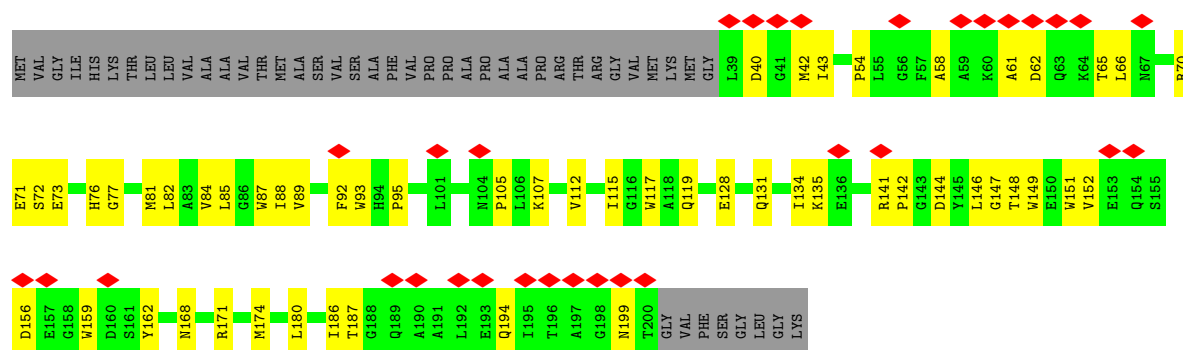


Mol	Chain	Residues	Atoms			AltConf
28	a	1	Total	C	O	0
			34	24	10	
28	j	1	Total	C	O	0
			32	22	10	

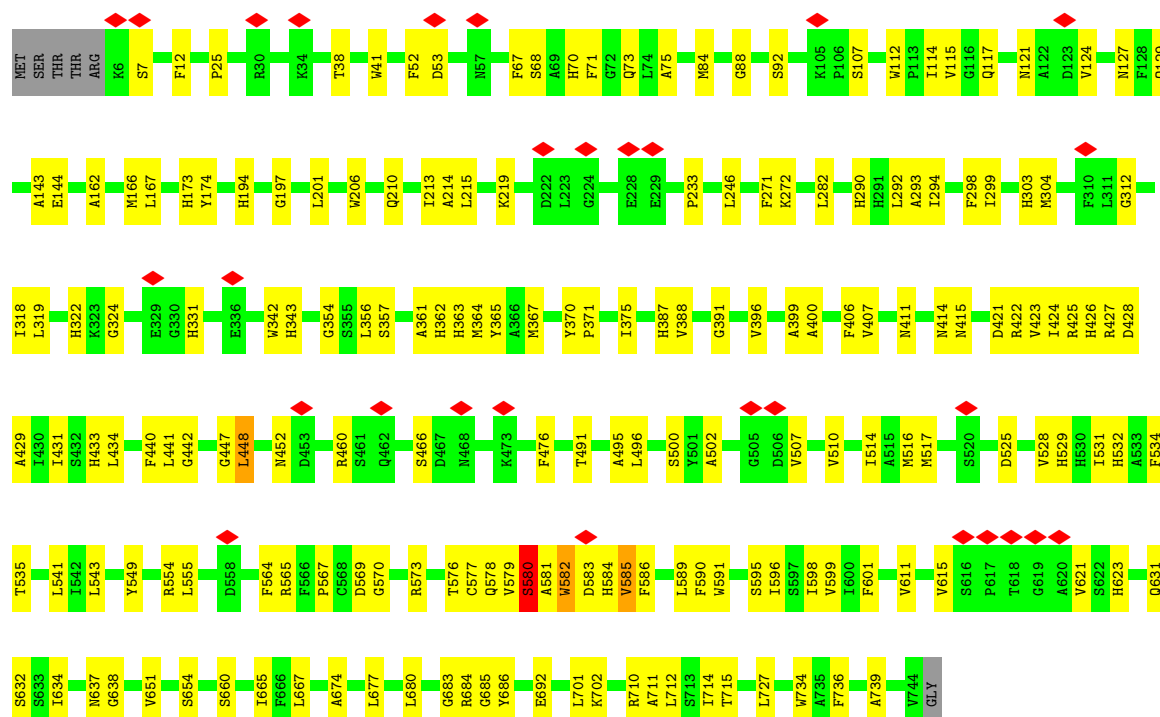
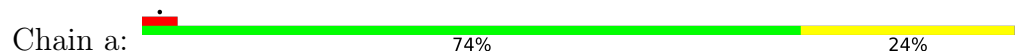




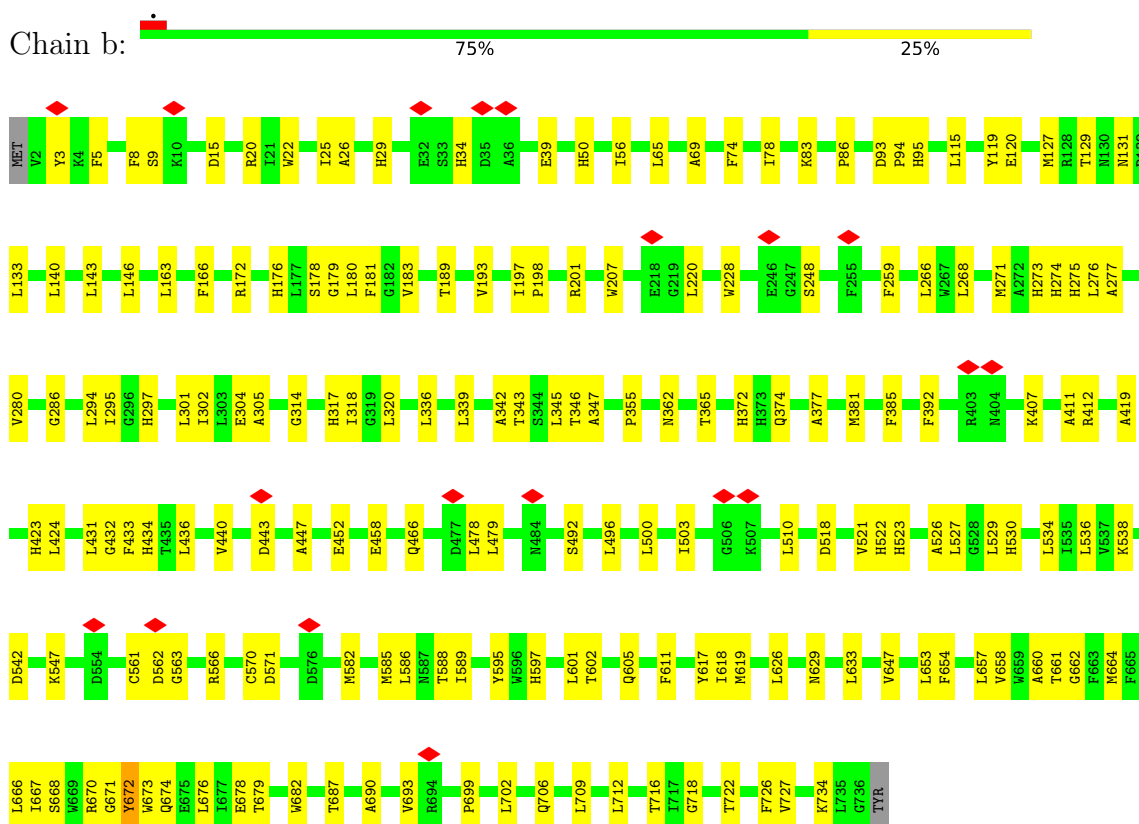
• Molecule 4: VCPI-1



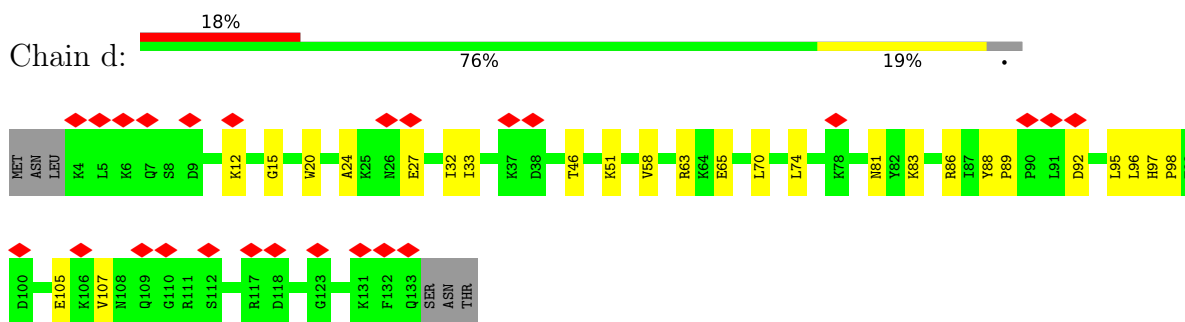
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



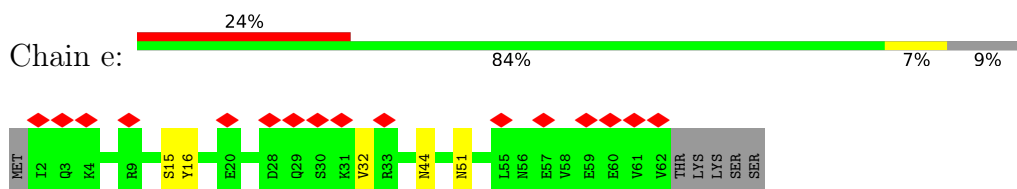
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 7: Photosystem I reaction center subunit II

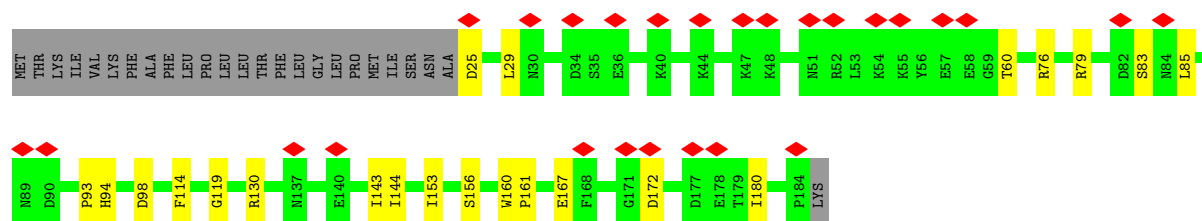


- Molecule 8: Photosystem I reaction center subunit IV

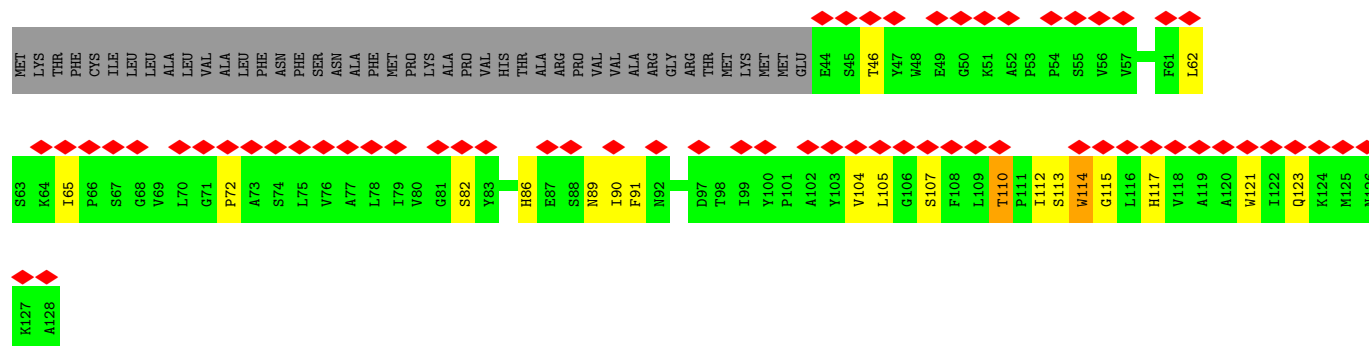


- Molecule 9: Photosystem I reaction center subunit III





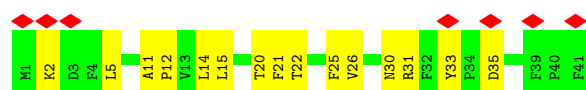
- Molecule 10: Psar



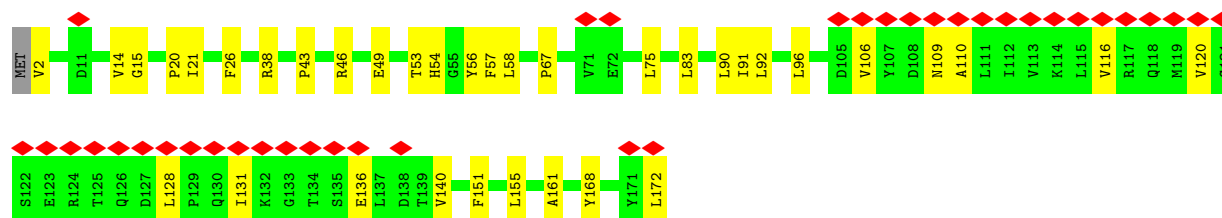
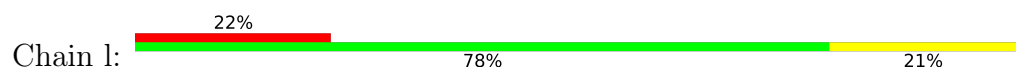
- Molecule 11: Photosystem I reaction center subunit VIII



- Molecule 12: Photosystem I reaction center subunit IX

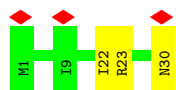
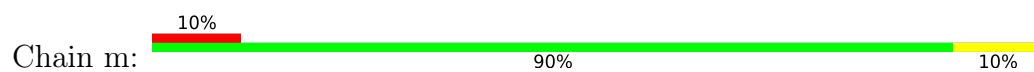


- Molecule 13: PSI subunit V

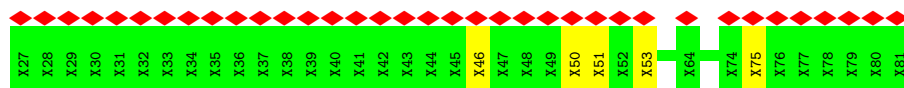
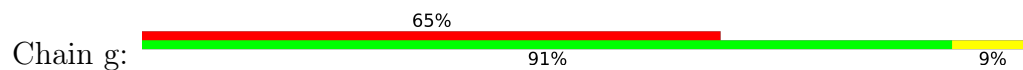


- Molecule 14: PsaM

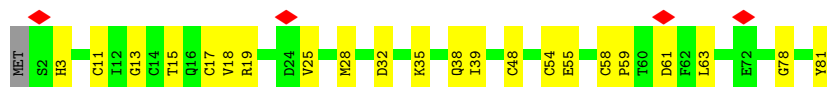




- Molecule 15: PsaS



- Molecule 16: 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	41262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.615	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.343	Depositor
Map size ( $\text{\AA}$ )	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	9	0.35	0/1496	0.33	0/2032
2	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
3	7	0.18	0/1248	0.37	0/1700
4	1	0.14	0/1293	0.33	0/1759
5	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
6	b	0.20	0/6080	0.32	1/8302 (0.0%)
7	d	0.12	0/1040	0.32	0/1402
8	e	0.09	0/502	0.20	0/681
9	f	0.14	0/1297	0.31	0/1762
10	h	0.51	1/667 (0.1%)	0.52	0/915
11	i	0.14	0/278	0.33	0/378
12	j	0.16	0/351	0.36	0/478
13	l	0.14	0/1315	0.31	0/1796
14	m	0.09	0/210	0.28	0/288
16	c	0.13	0/606	0.34	0/822
All	All	0.25	5/23693 (0.0%)	0.34	8/32277 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	580	SER	CA-C	-7.05	1.43	1.52
2	8	44	LEU	C-O	-6.16	1.15	1.23
5	a	581	ALA	CA-C	-5.45	1.45	1.52
10	h	114	TRP	C-O	-5.25	1.18	1.24
5	a	582	TRP	CA-C	-5.03	1.45	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	581	ALA	N-CA-C	-8.63	102.50	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	448	LEU	N-CA-C	-6.10	104.18	111.69
2	8	39	LYS	N-CA-C	-6.09	105.68	113.23
5	a	584	HIS	N-CA-C	-5.82	106.52	113.97
6	b	672	TYR	N-CA-C	-5.58	106.31	113.23

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9	1466	0	1470	49	0
2	8	1258	0	1280	33	0
3	7	1220	0	1209	44	0
4	1	1262	0	1237	39	0
5	a	5827	0	5697	140	0
6	b	5865	0	5710	149	0
7	d	1014	0	1015	20	0
8	e	494	0	495	5	0
9	f	1266	0	1262	20	0
10	h	646	0	649	18	0
11	i	271	0	292	12	0
12	j	339	0	342	21	0
13	l	1283	0	1278	29	0
14	m	210	0	226	3	0
15	g	275	0	62	3	0
16	c	596	0	583	19	0
17	1	45	0	0	1	0
17	7	45	0	0	2	0
17	9	90	0	0	3	0
18	1	57	0	0	2	0
18	8	57	0	0	2	0
18	9	57	0	0	2	0
18	h	57	0	0	4	0
19	1	88	0	112	6	0
19	7	176	0	224	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	8	132	0	168	17	0
19	9	88	0	112	14	0
19	a	44	0	56	6	0
19	j	44	0	56	6	0
20	9	42	0	52	8	0
21	9	82	0	110	5	0
21	a	75	0	93	7	0
21	b	31	0	32	0	0
22	1	547	0	508	14	0
22	7	576	0	444	25	0
22	8	507	0	429	24	0
22	9	519	0	452	35	0
22	a	2579	0	2562	140	0
22	b	2410	0	2464	129	0
22	f	117	0	115	1	0
22	h	120	0	121	6	0
22	j	100	0	86	9	0
22	l	148	0	123	3	0
23	8	40	0	38	2	0
23	b	57	0	72	6	0
24	1	45	0	54	3	0
25	a	33	0	46	3	0
25	b	33	0	46	2	0
26	a	160	0	224	13	0
26	b	240	0	336	25	0
26	f	80	0	112	15	0
26	h	80	0	112	5	0
26	i	40	0	56	2	0
26	j	40	0	56	9	0
26	l	80	0	112	12	0
26	m	40	0	56	1	0
27	a	8	0	0	0	0
27	c	16	0	0	2	0
28	a	34	0	38	10	0
28	j	32	0	34	7	0
All	All	33183	0	32518	863	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 863 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)
22:a:806:CLA:O1A	22:a:814:CLA:HBA1	1.81	0.81
5:a:531:ILE:HD12	22:a:801:CLA:H172	1.63	0.80
19:8:303:XAT:H12	22:8:312:CLA:HAB	1.67	0.77
22:b:825:CLA:HMA1	26:b:845:BCR:H17C	1.66	0.77
22:1:312:CLA:HHC	22:1:312:CLA:HBB1	1.69	0.73

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	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	25	59
2	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
3	7	164/202 (81%)	144 (88%)	20 (12%)	0	100	100
4	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
5	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	80
6	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
7	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
8	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
9	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
10	h	83/128 (65%)	76 (92%)	6 (7%)	1 (1%)	11	39
11	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
12	j	39/41 (95%)	39 (100%)	0	0	100	100
13	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	11	39
14	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	2929/3209 (91%)	2765 (94%)	159 (5%)	5 (0%)	45	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	9	32	THR
13	l	120	VAL
5	a	580	SER
13	l	131	ILE
10	h	90	ILE

### 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	9	141/167 (84%)	139 (99%)	2 (1%)	62	83
2	8	132/160 (82%)	131 (99%)	1 (1%)	79	90
3	7	122/159 (77%)	121 (99%)	1 (1%)	79	90
4	1	128/165 (78%)	128 (100%)	0	100	100
5	a	607/613 (99%)	603 (99%)	4 (1%)	81	91
6	b	599/602 (100%)	599 (100%)	0	100	100
7	d	107/113 (95%)	107 (100%)	0	100	100
8	e	56/62 (90%)	56 (100%)	0	100	100
9	f	138/162 (85%)	138 (100%)	0	100	100
10	h	71/107 (66%)	70 (99%)	1 (1%)	62	83
11	i	32/43 (74%)	32 (100%)	0	100	100
12	j	36/36 (100%)	36 (100%)	0	100	100
13	l	130/141 (92%)	130 (100%)	0	100	100
14	m	21/24 (88%)	21 (100%)	0	100	100
16	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2387/2622 (91%)	2378 (100%)	9 (0%)	88	95

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	a	580	SER
10	h	110	THR
3	7	95	ASP
5	a	428	ASP
5	a	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
6	b	605	GLN
9	f	166	GLN
13	l	144	GLN
7	d	7	GLN
5	a	239	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](#)

191 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
22	CLA	b	838	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	a	803	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	6 (7%)
19	XAT	8	303	-	39,47,47	0.87	1 (2%)	54,74,74	2.64	18 (33%)
22	CLA	7	311	-	46,54,73	1.79	6 (13%)	53,90,113	1.57	7 (13%)
22	CLA	b	832	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
25	PQN	a	843	-	34,34,34	1.59	2 (5%)	42,45,45	1.10	3 (7%)
22	CLA	7	309	-	46,55,73	1.76	5 (10%)	52,91,113	1.54	7 (13%)
26	BCR	h	202	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
22	CLA	b	813	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	b	814	-	55,63,73	1.61	6 (10%)	64,101,113	1.56	8 (12%)
22	CLA	j	102	-	58,66,73	1.60	6 (10%)	67,104,113	1.41	8 (11%)
22	CLA	8	311	-	56,64,73	1.58	5 (8%)	65,102,113	1.52	8 (12%)
26	BCR	f	801	-	41,41,41	0.68	0	56,56,56	2.14	16 (28%)
22	CLA	a	827	-	65,73,73	1.48	5 (7%)	76,113,113	1.46	9 (11%)
22	CLA	b	804	-	65,73,73	1.45	6 (9%)	76,113,113	1.54	11 (14%)
22	CLA	a	831	-	65,73,73	1.50	5 (7%)	76,113,113	1.47	8 (10%)
22	CLA	b	819	-	55,63,73	1.63	6 (10%)	64,101,113	1.44	8 (12%)
22	CLA	7	315	3	41,49,73	1.85	6 (14%)	47,84,113	1.64	7 (14%)
22	CLA	b	820	-	50,58,73	1.70	6 (12%)	58,95,113	1.59	10 (17%)
22	CLA	9	318	-	62,70,73	1.55	6 (9%)	72,109,113	1.37	8 (11%)
22	CLA	7	316	-	51,59,73	1.65	6 (11%)	59,96,113	1.60	8 (13%)
22	CLA	b	836	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	9 (11%)
26	BCR	b	849	-	41,41,41	0.73	0	56,56,56	2.05	15 (26%)
22	CLA	a	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
22	CLA	l	203	-	60,68,73	1.55	6 (10%)	70,107,113	1.47	7 (10%)
22	CLA	b	808	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	9 (11%)
22	CLA	1	308	4	65,73,73	1.47	5 (7%)	76,113,113	1.41	8 (10%)
28	LMG	j	105	-	32,32,55	1.12	2 (6%)	40,40,63	1.14	3 (7%)
22	CLA	7	307	-	45,53,73	1.79	5 (11%)	52,89,113	1.56	7 (13%)
21	LHG	b	847	22	30,30,48	1.33	6 (20%)	33,36,54	1.15	2 (6%)
22	CLA	a	832	-	50,58,73	1.69	6 (12%)	58,95,113	1.53	8 (13%)
26	BCR	a	848	-	41,41,41	0.75	0	56,56,56	1.94	18 (32%)
22	CLA	b	810	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
22	CLA	a	806	-	65,73,73	1.49	11 (16%)	76,113,113	1.67	13 (17%)
22	CLA	9	313	1	46,54,73	1.76	5 (10%)	53,90,113	1.62	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	a	837	5	45,53,73	1.79	6 (13%)	52,89,113	1.59	7 (13%)
20	45D	9	305	-	43,43,43	1.10	4 (9%)	54,60,60	2.16	18 (33%)
22	CLA	b	821	-	51,59,73	1.64	5 (9%)	59,96,113	1.56	9 (15%)
22	CLA	1	314	-	45,53,73	1.79	5 (11%)	52,89,113	1.56	6 (11%)
17	A1L1G	9	306	-	38,47,47	1.41	6 (15%)	49,71,71	1.54	8 (16%)
22	CLA	b	833	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
22	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	9 (11%)
22	CLA	a	819	-	54,62,73	1.62	6 (11%)	62,99,113	1.45	7 (11%)
22	CLA	a	823	-	49,57,73	1.68	6 (12%)	55,93,113	1.61	7 (12%)
26	BCR	l	205	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
22	CLA	b	839	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
25	PQN	b	841	-	34,34,34	1.55	2 (5%)	42,45,45	1.20	4 (9%)
22	CLA	b	840	21	65,73,73	1.53	6 (9%)	76,113,113	1.36	8 (10%)
22	CLA	b	830	-	41,49,73	1.83	6 (14%)	47,84,113	1.64	8 (17%)
22	CLA	b	824	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	7 (9%)
27	SF4	a	851	-	0,12,12	-	-	-	-	-
22	CLA	9	315	1	42,50,73	1.82	5 (11%)	48,85,113	1.59	7 (14%)
22	CLA	a	801	-	65,73,73	1.50	8 (12%)	76,113,113	1.38	7 (9%)
22	CLA	9	314	-	55,63,73	1.62	6 (10%)	64,101,113	1.50	8 (12%)
26	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
22	CLA	8	305	2	43,51,73	1.77	5 (11%)	49,86,113	1.65	7 (14%)
26	BCR	b	843	-	41,41,41	0.71	0	56,56,56	1.92	16 (28%)
19	XAT	7	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.62	20 (37%)
26	BCR	b	846	-	41,41,41	0.75	0	56,56,56	1.78	15 (26%)
26	BCR	m	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	9 (11%)
22	CLA	9	309	1	46,54,73	1.75	6 (13%)	53,90,113	1.54	7 (13%)
22	CLA	8	313	-	46,54,73	1.78	6 (13%)	53,90,113	1.53	6 (11%)
22	CLA	a	854	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
22	CLA	b	834	-	53,61,73	1.69	6 (11%)	61,98,113	1.52	9 (14%)
22	CLA	a	826	-	65,73,73	1.47	6 (9%)	76,113,113	1.45	6 (7%)
19	XAT	7	304	-	39,47,47	0.92	1 (2%)	54,74,74	2.68	21 (38%)
22	CLA	a	838	-	51,59,73	1.66	5 (9%)	59,96,113	1.56	8 (13%)
22	CLA	b	805	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
22	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	XAT	7	303	-	39,47,47	0.98	1 (2%)	54,74,74	2.59	19 (35%)
18	A1L1F	h	204	-	50,59,59	1.38	5 (10%)	62,85,85	2.61	22 (35%)
22	CLA	a	816	-	50,58,73	1.69	6 (12%)	58,95,113	1.58	8 (13%)
22	CLA	a	821	-	45,53,73	1.78	6 (13%)	52,89,113	1.64	6 (11%)
22	CLA	l	204	-	46,54,73	1.75	6 (13%)	53,90,113	1.57	7 (13%)
22	CLA	b	822	-	60,68,73	1.54	6 (10%)	70,107,113	1.38	8 (11%)
26	BCR	a	849	-	41,41,41	0.73	0	56,56,56	2.17	20 (35%)
22	CLA	7	310	-	46,54,73	1.77	6 (13%)	53,90,113	1.56	6 (11%)
27	SF4	c	102	-	0,12,12	-	-	-	-	-
18	A1L1F	9	302	-	50,59,59	1.37	5 (10%)	62,85,85	2.71	19 (30%)
26	BCR	a	850	-	41,41,41	0.74	0	56,56,56	2.16	14 (25%)
22	CLA	b	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	9 (11%)
22	CLA	8	307	2	65,73,73	1.47	5 (7%)	76,113,113	1.38	8 (10%)
22	CLA	9	310	-	46,54,73	1.75	5 (10%)	53,90,113	1.65	6 (11%)
22	CLA	b	817	-	59,67,73	1.56	6 (10%)	68,105,113	1.51	9 (13%)
22	CLA	b	823	-	53,61,73	1.63	6 (11%)	61,98,113	1.47	8 (13%)
22	CLA	8	309	-	57,65,73	1.59	5 (8%)	66,103,113	1.45	9 (13%)
22	CLA	b	809	-	65,73,73	1.47	7 (10%)	76,113,113	1.43	8 (10%)
26	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.04	17 (30%)
22	CLA	7	308	-	60,68,73	1.53	6 (10%)	70,107,113	1.45	7 (10%)
22	CLA	a	822	-	65,73,73	1.50	5 (7%)	76,113,113	1.39	8 (10%)
18	A1L1F	8	304	-	50,59,59	1.31	4 (8%)	62,85,85	2.79	23 (37%)
22	CLA	a	842	-	65,73,73	1.52	6 (9%)	76,113,113	1.37	7 (9%)
21	LHG	9	317	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
22	CLA	a	812	22	62,70,73	1.51	6 (9%)	72,109,113	1.44	8 (11%)
22	CLA	a	841	-	65,73,73	1.49	5 (7%)	76,113,113	1.42	9 (11%)
22	CLA	a	813	-	54,62,73	1.64	6 (11%)	62,99,113	1.44	7 (11%)
22	CLA	1	312	4	52,60,73	1.70	6 (11%)	60,97,113	1.48	8 (13%)
19	XAT	1	303	-	39,47,47	0.91	0	54,74,74	2.53	18 (33%)
22	CLA	a	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	9 (11%)
26	BCR	l	201	-	41,41,41	0.71	0	56,56,56	1.96	18 (32%)
28	LMG	a	853	-	34,34,55	1.14	2 (5%)	42,42,63	1.16	3 (7%)
22	CLA	a	814	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	7 (9%)
27	SF4	c	101	-	0,12,12	-	-	-	-	-
22	CLA	a	810	5	65,73,73	1.50	6 (9%)	76,113,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	b	802	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
26	BCR	b	844	-	41,41,41	0.69	0	56,56,56	2.10	16 (28%)
19	XAT	a	852	-	39,47,47	0.95	2 (5%)	54,74,74	2.69	20 (37%)
22	CLA	9	312	-	46,54,73	1.75	6 (13%)	53,90,113	1.68	8 (15%)
23	DGD	b	848	-	58,58,67	1.15	6 (10%)	72,72,81	1.53	10 (13%)
22	CLA	b	811	-	54,62,73	1.68	7 (12%)	67,100,113	1.49	9 (13%)
22	CLA	1	305	-	61,69,73	1.54	5 (8%)	71,108,113	1.39	7 (9%)
22	CLA	b	837	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	8 (10%)
22	CLA	8	308	-	55,63,73	1.62	5 (9%)	64,101,113	1.50	9 (14%)
22	CLA	b	818	-	60,68,73	1.57	5 (8%)	70,107,113	1.41	7 (10%)
22	CLA	a	805	22	55,63,73	1.61	5 (9%)	64,101,113	1.52	8 (12%)
17	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.57	11 (22%)
22	CLA	1	306	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	10 (13%)
22	CLA	a	817	-	45,53,73	1.80	5 (11%)	52,89,113	1.58	7 (13%)
19	XAT	j	101	-	39,47,47	0.88	0	54,74,74	2.72	18 (33%)
22	CLA	h	203	-	65,73,73	1.50	5 (7%)	76,113,113	1.45	7 (9%)
22	CLA	a	829	-	62,70,73	1.53	5 (8%)	72,109,113	1.40	8 (11%)
24	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	5 (9%)
22	CLA	8	312	2	52,60,73	1.65	5 (9%)	60,97,113	1.52	8 (13%)
22	CLA	a	825	-	55,63,73	1.61	5 (9%)	64,101,113	1.46	8 (12%)
22	CLA	b	827	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
22	CLA	7	314	-	45,53,73	1.80	6 (13%)	52,89,113	1.65	7 (13%)
26	BCR	b	845	-	41,41,41	0.77	0	56,56,56	2.19	22 (39%)
19	XAT	8	301	-	39,47,47	0.91	1 (2%)	54,74,74	2.53	18 (33%)
22	CLA	h	205	-	55,63,73	1.63	6 (10%)	64,101,113	1.48	9 (14%)
22	CLA	8	310	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
22	CLA	a	802	-	58,66,73	1.54	5 (8%)	67,104,113	1.49	7 (10%)
22	CLA	9	308	1	65,73,73	1.50	7 (10%)	76,113,113	1.42	9 (11%)
17	A1L1G	9	301	-	38,47,47	1.46	6 (15%)	49,71,71	1.57	10 (20%)
22	CLA	7	312	-	48,56,73	1.71	6 (12%)	55,92,113	1.56	8 (14%)
22	CLA	b	816	-	55,63,73	1.62	5 (9%)	64,101,113	1.47	8 (12%)
21	LHG	a	845	-	47,47,48	1.12	6 (12%)	50,53,54	0.97	2 (4%)
22	CLA	9	316	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
22	CLA	b	806	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	7 (9%)
22	CLA	b	826	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	j	103	12	42,50,73	1.81	5 (11%)	48,85,113	1.66	6 (12%)
22	CLA	a	824	-	46,54,73	1.77	6 (13%)	53,90,113	1.51	7 (13%)
22	CLA	8	306	23	46,54,73	1.76	5 (10%)	53,90,113	1.54	6 (11%)
21	LHG	9	307	-	35,35,48	1.22	6 (17%)	38,41,54	0.96	2 (5%)
22	CLA	a	830	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	8 (10%)
22	CLA	7	317	-	45,53,73	1.79	5 (11%)	52,89,113	1.59	7 (13%)
22	CLA	b	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	7 (9%)
22	CLA	b	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.59	7 (13%)
22	CLA	1	310	4	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
22	CLA	a	828	-	65,73,73	1.45	6 (9%)	76,113,113	1.39	7 (9%)
22	CLA	a	808	-	51,59,73	1.71	6 (11%)	59,96,113	1.51	8 (13%)
22	CLA	b	835	-	58,66,73	1.57	5 (8%)	67,104,113	1.53	8 (11%)
22	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.54	8 (12%)
22	CLA	a	807	-	65,73,73	1.47	5 (7%)	76,113,113	1.37	7 (9%)
19	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	16 (29%)
19	XAT	7	305	-	39,47,47	0.86	0	54,74,74	2.65	19 (35%)
23	DGD	8	315	22	41,41,67	1.05	2 (4%)	55,55,81	1.11	5 (9%)
22	CLA	7	313	-	54,62,73	1.67	6 (11%)	62,99,113	1.50	9 (14%)
22	CLA	a	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.59	7 (13%)
18	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
22	CLA	a	811	-	56,64,73	1.59	6 (10%)	65,102,113	1.48	8 (12%)
22	CLA	7	306	3	48,56,73	1.73	5 (10%)	55,92,113	1.53	7 (12%)
22	CLA	a	818	-	56,64,73	1.63	5 (8%)	65,102,113	1.43	8 (12%)
22	CLA	b	825	-	64,72,73	1.48	6 (9%)	74,111,113	1.44	8 (10%)
26	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.13	14 (25%)
22	CLA	a	804	-	55,63,73	1.62	6 (10%)	64,101,113	1.55	10 (15%)
22	CLA	a	809	5	65,73,73	1.44	5 (7%)	76,113,113	1.43	8 (10%)
17	A1L1G	7	302	-	38,47,47	1.44	6 (15%)	49,71,71	1.50	9 (18%)
22	CLA	8	314	-	41,49,73	1.87	5 (12%)	47,84,113	1.64	7 (14%)
22	CLA	1	313	-	41,49,73	1.84	6 (14%)	47,84,113	1.64	7 (14%)
22	CLA	b	829	-	65,73,73	1.52	6 (9%)	76,113,113	1.44	10 (13%)
22	CLA	b	831	-	49,57,73	1.70	5 (10%)	55,93,113	1.57	8 (14%)
21	LHG	a	846	22	26,26,48	1.28	5 (19%)	29,32,54	1.20	2 (6%)
19	XAT	9	304	-	39,47,47	0.94	1 (2%)	54,74,74	2.42	19 (35%)
22	CLA	1	307	-	54,62,73	1.63	5 (9%)	62,99,113	1.51	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	a	840	-	65,73,73	1.52	6 (9%)	76,113,113	1.37	8 (10%)
22	CLA	a	820	-	65,73,73	1.48	5 (7%)	76,113,113	1.44	9 (11%)
22	CLA	f	803	9	52,60,73	1.66	5 (9%)	60,97,113	1.50	8 (13%)
19	XAT	8	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.66	20 (37%)
22	CLA	a	836	-	50,58,73	1.69	5 (10%)	58,95,113	1.51	9 (15%)
22	CLA	1	309	4	46,54,73	1.78	6 (13%)	53,90,113	1.50	7 (13%)
26	BCR	b	842	-	41,41,41	0.71	0	56,56,56	2.29	21 (37%)
26	BCR	h	201	-	41,41,41	0.71	0	56,56,56	1.98	21 (37%)
22	CLA	1	311	-	53,61,73	1.64	5 (9%)	61,98,113	1.51	9 (14%)
22	CLA	b	828	-	65,73,73	1.51	6 (9%)	76,113,113	1.32	7 (9%)
26	BCR	j	104	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
22	CLA	b	812	-	53,61,73	1.63	5 (9%)	61,98,113	1.50	8 (13%)
22	CLA	9	311	-	46,54,73	1.75	5 (10%)	53,90,113	1.63	8 (15%)
22	CLA	l	202	-	42,50,73	1.83	6 (14%)	48,85,113	1.64	7 (14%)
19	XAT	9	303	-	39,47,47	0.95	1 (2%)	54,74,74	2.61	19 (35%)
22	CLA	a	844	21	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)

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
22	CLA	b	838	-	1/1/15/20	13/37/115/115	-
22	CLA	a	803	-	1/1/15/20	3/37/115/115	-
19	XAT	8	303	-	-	0/31/93/93	0/4/4/4
22	CLA	7	311	-	1/1/11/20	5/15/93/115	-
22	CLA	b	832	-	1/1/15/20	13/37/115/115	-
25	PQN	a	843	-	-	5/23/43/43	0/2/2/2
22	CLA	7	309	-	1/1/11/20	5/15/93/115	-
26	BCR	h	202	-	-	2/29/63/63	0/2/2/2
22	CLA	b	813	-	1/1/15/20	14/37/115/115	-
22	CLA	b	814	-	1/1/13/20	13/25/103/115	-
22	CLA	j	102	-	1/1/13/20	16/29/107/115	-
22	CLA	8	311	-	1/1/13/20	8/27/105/115	-
26	BCR	f	801	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	827	-	1/1/15/20	8/37/115/115	-
22	CLA	b	804	-	1/1/15/20	10/37/115/115	-
22	CLA	a	831	-	1/1/15/20	11/37/115/115	-
22	CLA	b	819	-	1/1/13/20	3/25/103/115	-
22	CLA	7	315	3	1/1/10/20	4/8/86/115	-
22	CLA	b	820	-	1/1/12/20	7/19/97/115	-
22	CLA	9	318	-	1/1/14/20	9/34/112/115	-
22	CLA	7	316	-	1/1/12/20	11/21/99/115	-
22	CLA	b	836	-	1/1/15/20	8/37/115/115	-
26	BCR	b	849	-	-	5/29/63/63	0/2/2/2
22	CLA	a	839	-	1/1/15/20	15/37/115/115	-
22	CLA	l	203	-	1/1/14/20	6/31/109/115	-
22	CLA	b	808	-	1/1/15/20	12/37/115/115	-
22	CLA	1	308	4	1/1/15/20	13/37/115/115	-
28	LMG	j	105	-	-	11/27/47/70	0/1/1/1
22	CLA	7	307	-	1/1/11/20	5/13/91/115	-
21	LHG	b	847	22	-	20/35/35/53	-
22	CLA	a	832	-	1/1/12/20	5/19/97/115	-
26	BCR	a	848	-	-	0/29/63/63	0/2/2/2
22	CLA	b	810	-	1/1/15/20	16/37/115/115	-
22	CLA	a	806	-	1/1/15/20	12/37/115/115	-
22	CLA	9	313	1	1/1/11/20	9/15/93/115	-
22	CLA	a	837	5	1/1/11/20	4/13/91/115	-
20	45D	9	305	-	-	9/29/69/69	0/2/2/2
22	CLA	b	821	-	1/1/12/20	2/21/99/115	-
22	CLA	1	314	-	1/1/11/20	5/13/91/115	-
17	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
22	CLA	b	833	-	1/1/15/20	14/37/115/115	-
22	CLA	a	835	-	1/1/15/20	12/37/115/115	-
22	CLA	a	819	-	1/1/12/20	4/24/102/115	-
22	CLA	a	823	-	1/1/11/20	7/18/96/115	-
26	BCR	l	205	-	-	8/29/63/63	0/2/2/2
22	CLA	b	839	-	1/1/15/20	17/37/115/115	-
25	PQN	b	841	-	-	1/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	840	21	1/1/15/20	9/37/115/115	-
22	CLA	b	830	-	1/1/10/20	1/8/86/115	-
22	CLA	b	824	-	1/1/15/20	14/37/115/115	-
27	SF4	a	851	-	-	-	0/6/5/5
22	CLA	9	315	1	1/1/10/20	6/10/88/115	-
22	CLA	a	801	-	1/1/15/20	22/37/115/115	-
22	CLA	9	314	-	1/1/13/20	9/25/103/115	-
26	BCR	a	847	-	-	0/29/63/63	0/2/2/2
22	CLA	8	305	2	1/1/10/20	2/11/89/115	-
26	BCR	b	843	-	-	2/29/63/63	0/2/2/2
19	XAT	7	301	-	-	6/31/93/93	0/4/4/4
26	BCR	b	846	-	-	2/29/63/63	0/2/2/2
26	BCR	m	101	-	-	9/29/63/63	0/2/2/2
22	CLA	f	802	-	1/1/15/20	13/37/115/115	-
22	CLA	9	309	1	1/1/11/20	3/15/93/115	-
22	CLA	8	313	-	1/1/11/20	3/15/93/115	-
22	CLA	a	854	-	1/1/15/20	13/37/115/115	-
22	CLA	b	834	-	1/1/12/20	8/23/101/115	-
22	CLA	a	826	-	1/1/15/20	10/37/115/115	-
19	XAT	7	304	-	-	6/31/93/93	0/4/4/4
22	CLA	a	838	-	1/1/12/20	6/21/99/115	-
22	CLA	b	805	-	1/1/15/20	12/37/115/115	-
22	CLA	b	801	-	1/1/15/20	20/37/115/115	-
19	XAT	7	303	-	-	8/31/93/93	0/4/4/4
22	CLA	a	816	-	1/1/12/20	5/19/97/115	-
18	A1L1F	h	204	-	-	11/43/99/99	1/3/3/3
22	CLA	a	821	-	1/1/11/20	2/13/91/115	-
22	CLA	l	204	-	1/1/11/20	4/15/93/115	-
22	CLA	b	822	-	1/1/14/20	7/31/109/115	-
26	BCR	a	849	-	-	0/29/63/63	0/2/2/2
22	CLA	7	310	-	1/1/11/20	6/15/93/115	-
27	SF4	c	102	-	-	-	0/6/5/5
18	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
26	BCR	a	850	-	-	4/29/63/63	0/2/2/2
22	CLA	b	807	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	8	307	2	1/1/15/20	13/37/115/115	-
22	CLA	9	310	-	1/1/11/20	6/15/93/115	-
22	CLA	b	817	-	1/1/13/20	10/30/108/115	-
22	CLA	b	823	-	1/1/12/20	8/23/101/115	-
22	CLA	8	309	-	1/1/13/20	8/28/106/115	-
22	CLA	b	809	-	1/1/15/20	11/37/115/115	-
26	BCR	f	804	-	-	4/29/63/63	0/2/2/2
22	CLA	7	308	-	1/1/14/20	14/31/109/115	-
22	CLA	a	822	-	1/1/15/20	5/37/115/115	-
18	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
22	CLA	a	842	-	1/1/15/20	9/37/115/115	-
21	LHG	9	317	-	-	28/50/50/53	-
22	CLA	a	812	22	1/1/14/20	9/34/112/115	-
22	CLA	a	841	-	1/1/15/20	15/37/115/115	-
22	CLA	a	813	-	1/1/12/20	9/24/102/115	-
22	CLA	1	312	4	1/1/12/20	3/22/100/115	-
19	XAT	1	303	-	-	0/31/93/93	0/4/4/4
22	CLA	a	834	-	1/1/15/20	7/37/115/115	-
26	BCR	l	201	-	-	4/29/63/63	0/2/2/2
28	LMG	a	853	-	-	13/29/49/70	0/1/1/1
22	CLA	a	814	-	1/1/15/20	20/37/115/115	-
27	SF4	c	101	-	-	-	0/6/5/5
22	CLA	a	810	5	1/1/15/20	13/37/115/115	-
22	CLA	b	802	-	1/1/15/20	17/37/115/115	-
26	BCR	b	844	-	-	6/29/63/63	0/2/2/2
19	XAT	a	852	-	-	7/31/93/93	0/4/4/4
22	CLA	9	312	-	1/1/11/20	9/15/93/115	-
23	DGD	b	848	-	-	20/46/86/95	0/2/2/2
22	CLA	b	811	-	1/1/13/20	5/25/101/115	-
22	CLA	1	305	-	1/1/14/20	10/33/111/115	-
22	CLA	b	837	-	1/1/15/20	8/37/115/115	-
22	CLA	8	308	-	1/1/13/20	7/25/103/115	-
22	CLA	b	818	-	1/1/14/20	14/31/109/115	-
22	CLA	a	805	22	1/1/13/20	6/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	306	-	1/1/15/20	15/37/115/115	-
17	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
22	CLA	a	817	-	1/1/11/20	6/13/91/115	-
19	XAT	j	101	-	-	5/31/93/93	0/4/4/4
22	CLA	h	203	-	1/1/15/20	9/37/115/115	-
22	CLA	a	829	-	1/1/14/20	15/34/112/115	-
24	SQD	1	315	-	-	19/40/60/69	0/1/1/1
22	CLA	8	312	2	1/1/12/20	2/22/100/115	-
22	CLA	a	825	-	1/1/13/20	8/25/103/115	-
22	CLA	b	827	-	1/1/15/20	14/37/115/115	-
22	CLA	7	314	-	1/1/11/20	4/13/91/115	-
26	BCR	b	845	-	-	1/29/63/63	0/2/2/2
19	XAT	8	301	-	-	3/31/93/93	0/4/4/4
22	CLA	h	205	-	1/1/13/20	9/25/103/115	-
22	CLA	8	310	-	1/1/11/20	5/15/93/115	-
22	CLA	a	802	-	1/1/13/20	7/29/107/115	-
22	CLA	9	308	1	1/1/15/20	15/37/115/115	-
22	CLA	b	816	-	1/1/13/20	4/25/103/115	-
22	CLA	7	312	-	1/1/11/20	3/17/95/115	-
22	CLA	b	826	-	1/1/15/20	5/37/115/115	-
22	CLA	9	316	-	1/1/15/20	17/37/115/115	-
22	CLA	j	103	12	1/1/10/20	5/10/88/115	-
22	CLA	b	806	-	1/1/15/20	16/37/115/115	-
17	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
21	LHG	a	845	-	-	27/52/52/53	-
22	CLA	a	824	-	1/1/11/20	4/15/93/115	-
22	CLA	8	306	23	1/1/11/20	2/15/93/115	-
22	CLA	a	830	-	1/1/15/20	15/37/115/115	-
22	CLA	b	815	-	1/1/11/20	3/13/91/115	-
22	CLA	7	317	-	1/1/11/20	5/13/91/115	-
22	CLA	b	803	-	1/1/15/20	18/37/115/115	-
22	CLA	b	835	-	1/1/13/20	11/29/107/115	-
22	CLA	1	310	4	1/1/15/20	18/37/115/115	-
22	CLA	a	828	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	808	-	1/1/12/20	3/21/99/115	-
21	LHG	9	307	-	-	21/40/40/53	-
22	CLA	a	833	-	1/1/13/20	2/25/103/115	-
22	CLA	a	807	-	1/1/15/20	18/37/115/115	-
19	XAT	1	302	-	-	0/31/93/93	0/4/4/4
19	XAT	7	305	-	-	2/31/93/93	0/4/4/4
23	DGD	8	315	22	-	11/29/69/95	0/2/2/2
22	CLA	7	313	-	1/1/12/20	7/24/102/115	-
22	CLA	a	815	-	1/1/11/20	2/13/91/115	-
22	CLA	a	811	-	1/1/13/20	8/27/105/115	-
22	CLA	a	818	-	1/1/13/20	11/27/105/115	-
22	CLA	7	306	3	1/1/11/20	10/17/95/115	-
22	CLA	b	825	-	1/1/14/20	6/36/114/115	-
18	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
26	BCR	i	101	-	-	3/29/63/63	0/2/2/2
22	CLA	a	804	-	1/1/13/20	10/25/103/115	-
22	CLA	a	809	5	1/1/15/20	15/37/115/115	-
17	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
22	CLA	8	314	-	1/1/10/20	5/8/86/115	-
22	CLA	1	313	-	1/1/10/20	3/8/86/115	-
22	CLA	b	829	-	1/1/15/20	11/37/115/115	-
22	CLA	b	831	-	1/1/11/20	6/18/96/115	-
21	LHG	a	846	22	-	16/31/31/53	-
19	XAT	9	304	-	-	1/31/93/93	0/4/4/4
22	CLA	1	307	-	1/1/12/20	6/24/102/115	-
22	CLA	a	840	-	1/1/15/20	8/37/115/115	-
22	CLA	a	820	-	1/1/15/20	15/37/115/115	-
22	CLA	f	803	9	1/1/12/20	2/22/100/115	-
19	XAT	8	302	-	-	4/31/93/93	0/4/4/4
22	CLA	a	836	-	1/1/12/20	6/19/97/115	-
22	CLA	1	309	4	1/1/11/20	6/15/93/115	-
26	BCR	b	842	-	-	2/29/63/63	0/2/2/2
26	BCR	h	201	-	-	0/29/63/63	0/2/2/2
22	CLA	1	311	-	1/1/12/20	6/23/101/115	-
22	CLA	b	828	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	j	104	-	-	4/29/63/63	0/2/2/2
22	CLA	b	812	-	1/1/12/20	6/23/101/115	-
22	CLA	9	311	-	1/1/11/20	7/15/93/115	-
22	CLA	l	202	-	1/1/10/20	2/10/88/115	-
19	XAT	9	303	-	-	4/31/93/93	0/4/4/4
22	CLA	a	844	21	1/1/15/20	16/37/115/115	-

The worst 5 of 869 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	l	312	CLA	C4B-NB	7.91	1.42	1.35
22	a	818	CLA	C4B-NB	7.82	1.42	1.35
22	a	840	CLA	C4B-NB	7.78	1.42	1.35
22	a	842	CLA	C4B-NB	7.78	1.42	1.35
22	b	834	CLA	C4B-NB	7.72	1.42	1.35

The worst 5 of 1792 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	9	302	A1L1F	O15-C20-C21	13.20	123.30	113.38
18	8	304	A1L1F	O15-C20-C21	8.53	119.79	113.38
18	9	302	A1L1F	C17-C20-C25	-8.46	108.08	122.26
18	h	204	A1L1F	O15-C20-C21	8.43	119.72	113.38
18	h	204	A1L1F	C17-C20-C25	-8.37	108.23	122.26

5 of 135 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	9	308	CLA	ND
22	9	309	CLA	ND
22	9	310	CLA	ND
22	9	311	CLA	ND
22	9	312	CLA	ND

5 of 1615 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	9	301	A1L1G	O13-C26-C30-C29
17	9	301	A1L1G	C26-C30-C31-C32
17	9	301	A1L1G	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
17	9	301	A1L1G	C28-C39-C40-C41
17	9	301	A1L1G	C38-C39-C40-C41

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	h	204	A1L1F	C1-C11-C3-C4-C6-C8

170 monomers are involved in 528 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	838	CLA	4	0
22	a	803	CLA	5	0
19	8	303	XAT	7	0
22	7	311	CLA	3	0
22	b	832	CLA	3	0
25	a	843	PQN	3	0
26	h	202	BCR	4	0
22	b	813	CLA	7	0
22	b	814	CLA	3	0
22	j	102	CLA	7	0
22	8	311	CLA	3	0
26	f	801	BCR	9	0
22	a	827	CLA	3	0
22	b	804	CLA	4	0
22	a	831	CLA	4	0
22	b	819	CLA	1	0
22	7	315	CLA	2	0
22	b	820	CLA	2	0
22	9	318	CLA	6	0
22	7	316	CLA	2	0
22	b	836	CLA	5	0
26	b	849	BCR	6	0
22	a	839	CLA	6	0
22	l	203	CLA	2	0
22	b	808	CLA	2	0
22	1	308	CLA	3	0
28	j	105	LMG	7	0
22	7	307	CLA	2	0
22	a	832	CLA	2	0
26	a	848	BCR	5	0
22	b	810	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	806	CLA	9	0
22	9	313	CLA	2	0
22	a	837	CLA	1	0
20	9	305	45D	8	0
22	b	821	CLA	2	0
17	9	306	A1L1G	1	0
22	b	833	CLA	3	0
22	a	835	CLA	5	0
22	a	819	CLA	5	0
22	a	823	CLA	3	0
26	l	205	BCR	9	0
22	b	839	CLA	5	0
25	b	841	PQN	2	0
22	b	840	CLA	6	0
22	b	830	CLA	5	0
22	b	824	CLA	8	0
22	9	315	CLA	1	0
22	a	801	CLA	7	0
22	9	314	CLA	7	0
26	a	847	BCR	4	0
22	8	305	CLA	5	0
26	b	843	BCR	2	0
19	7	301	XAT	3	0
26	b	846	BCR	3	0
26	m	101	BCR	1	0
22	f	802	CLA	1	0
22	9	309	CLA	1	0
22	8	313	CLA	3	0
22	a	854	CLA	3	0
22	a	826	CLA	6	0
19	7	304	XAT	12	0
22	a	838	CLA	1	0
22	b	805	CLA	4	0
22	b	801	CLA	5	0
19	7	303	XAT	11	0
18	h	204	A1L1F	4	0
22	a	816	CLA	2	0
22	b	822	CLA	6	0
26	a	849	BCR	3	0
22	7	310	CLA	1	0
27	c	102	SF4	2	0
18	9	302	A1L1F	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	a	850	BCR	2	0
22	b	807	CLA	7	0
22	8	307	CLA	6	0
22	9	310	CLA	2	0
22	b	817	CLA	8	0
22	b	823	CLA	6	0
22	8	309	CLA	1	0
22	b	809	CLA	3	0
26	f	804	BCR	6	0
22	7	308	CLA	7	0
22	a	822	CLA	5	0
18	8	304	A1L1F	2	0
22	a	842	CLA	3	0
21	9	317	LHG	3	0
22	a	841	CLA	7	0
22	1	312	CLA	2	0
19	1	303	XAT	3	0
22	a	834	CLA	5	0
26	l	201	BCR	3	0
28	a	853	LMG	10	0
22	a	814	CLA	3	0
22	a	810	CLA	4	0
22	b	802	CLA	4	0
26	b	844	BCR	5	0
19	a	852	XAT	6	0
22	9	312	CLA	3	0
23	b	848	DGD	6	0
22	b	811	CLA	3	0
22	b	837	CLA	6	0
22	8	308	CLA	1	0
22	b	818	CLA	3	0
22	a	805	CLA	1	0
17	1	301	A1L1G	1	0
22	1	306	CLA	5	0
19	j	101	XAT	6	0
22	h	203	CLA	4	0
22	a	829	CLA	6	0
24	1	315	SQD	3	0
22	8	312	CLA	3	0
22	a	825	CLA	4	0
22	b	827	CLA	3	0
22	7	314	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	845	BCR	5	0
19	8	301	XAT	2	0
22	h	205	CLA	2	0
22	a	802	CLA	5	0
22	9	308	CLA	6	0
17	9	301	A1L1G	2	0
22	7	312	CLA	1	0
22	b	816	CLA	6	0
21	a	845	LHG	4	0
22	9	316	CLA	6	0
22	b	806	CLA	2	0
22	b	826	CLA	3	0
22	j	103	CLA	2	0
22	a	824	CLA	1	0
22	8	306	CLA	1	0
21	9	307	LHG	2	0
22	a	830	CLA	7	0
22	b	803	CLA	3	0
22	1	310	CLA	2	0
22	a	828	CLA	4	0
22	a	808	CLA	1	0
22	b	835	CLA	4	0
22	a	833	CLA	2	0
22	a	807	CLA	4	0
19	1	302	XAT	3	0
19	7	305	XAT	2	0
23	8	315	DGD	2	0
22	7	313	CLA	4	0
18	1	304	A1L1F	2	0
22	7	306	CLA	2	0
22	a	818	CLA	11	0
22	b	825	CLA	2	0
26	i	101	BCR	2	0
22	a	804	CLA	4	0
22	a	809	CLA	3	0
17	7	302	A1L1G	2	0
22	8	314	CLA	1	0
22	b	829	CLA	4	0
22	b	831	CLA	2	0
21	a	846	LHG	3	0
19	9	304	XAT	6	0
22	a	840	CLA	6	0

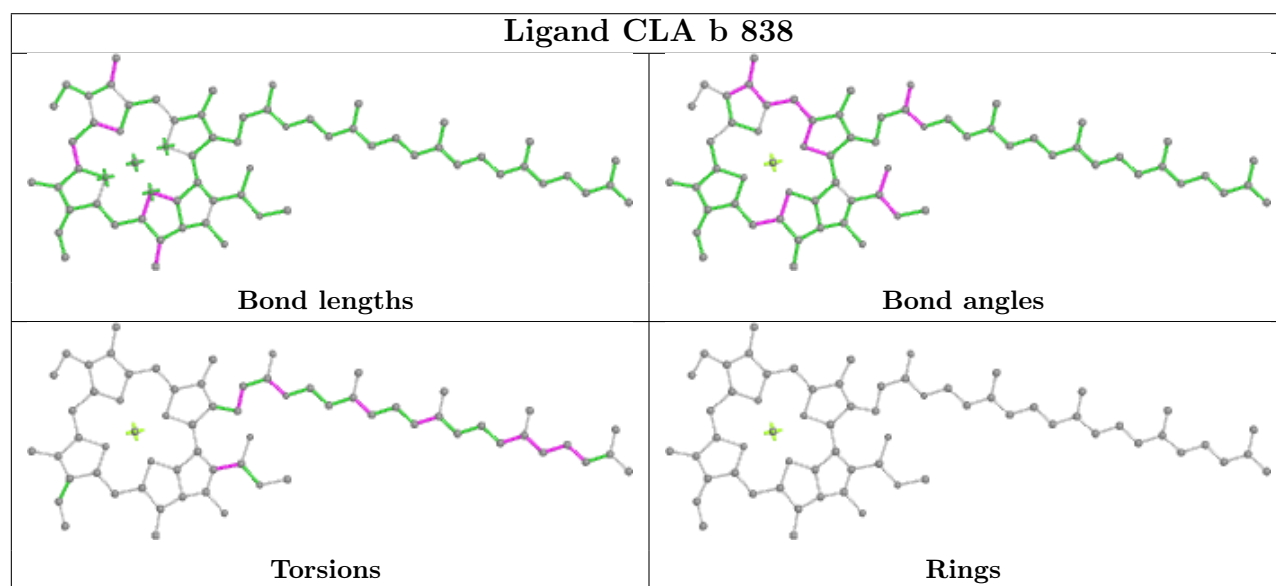
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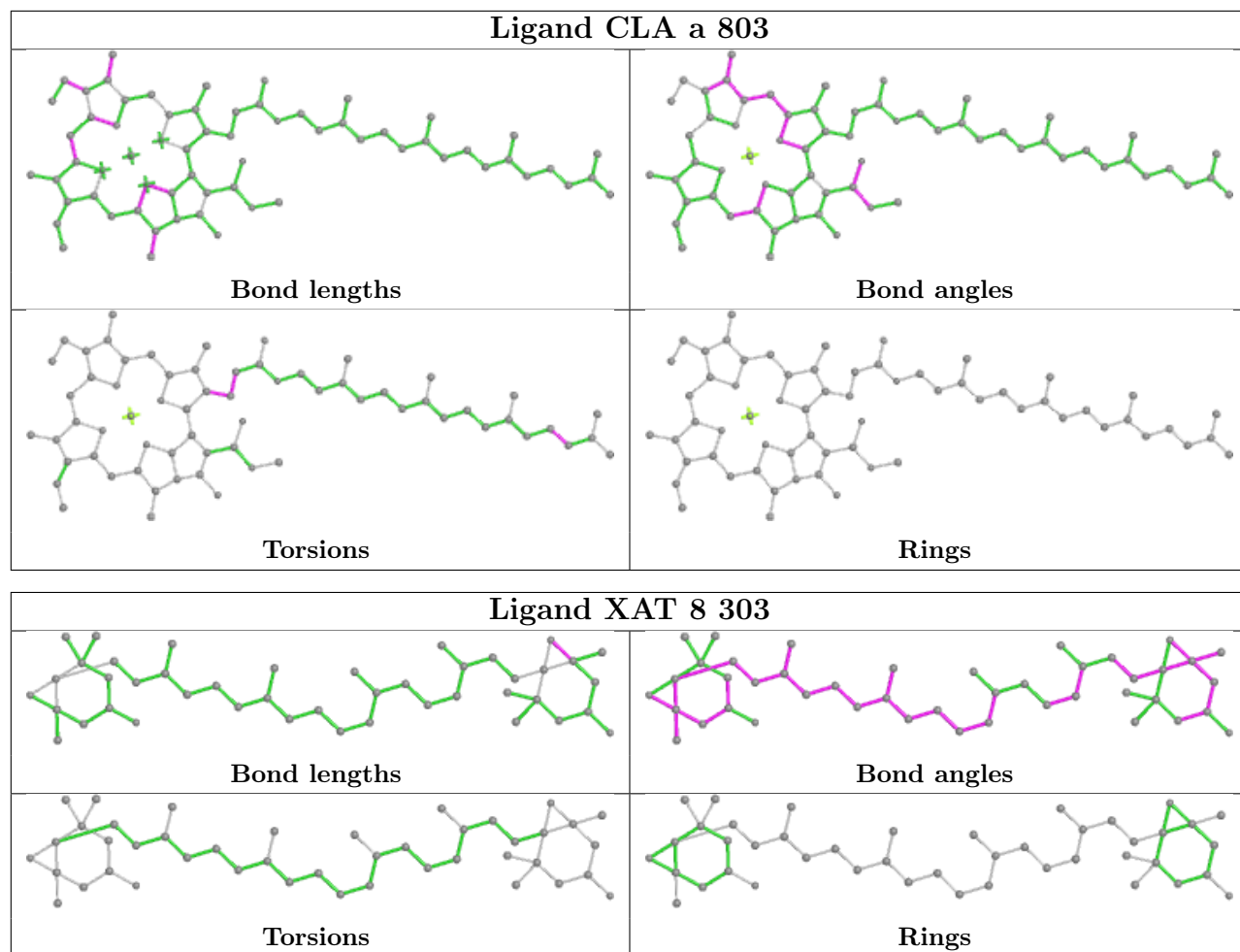


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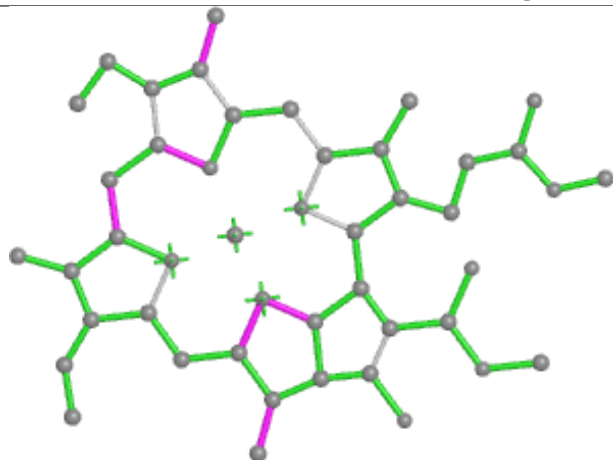
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	820	CLA	6	0
19	8	302	XAT	8	0
22	a	836	CLA	1	0
26	b	842	BCR	4	0
26	h	201	BCR	1	0
22	l	311	CLA	2	0
22	b	828	CLA	3	0
26	j	104	BCR	9	0
22	b	812	CLA	4	0
22	9	311	CLA	2	0
22	l	202	CLA	1	0
19	9	303	XAT	8	0
22	a	844	CLA	6	0

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.

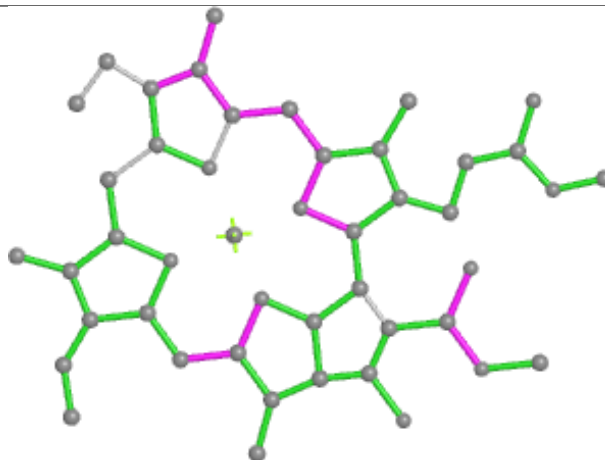




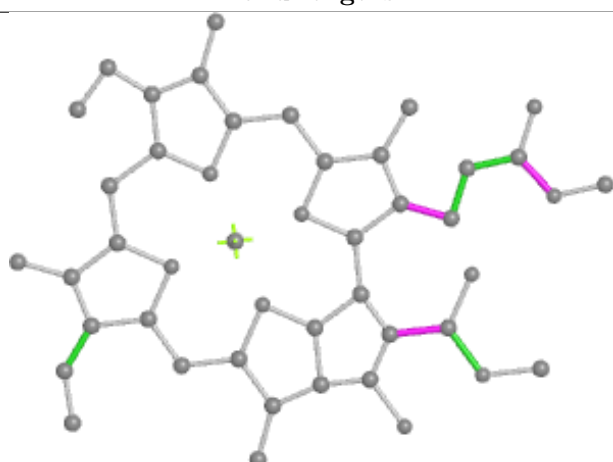
## Ligand CLA 7 311



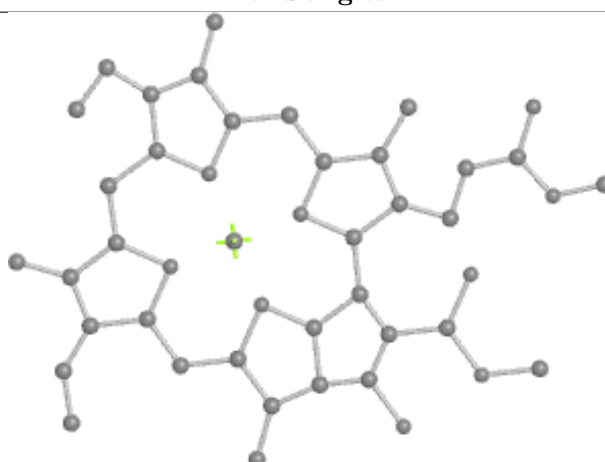
Bond lengths



Bond angles

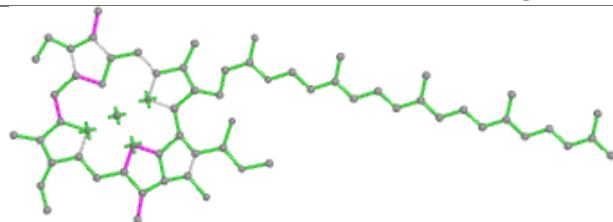


Torsions

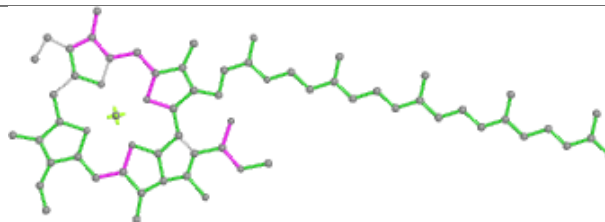


Rings

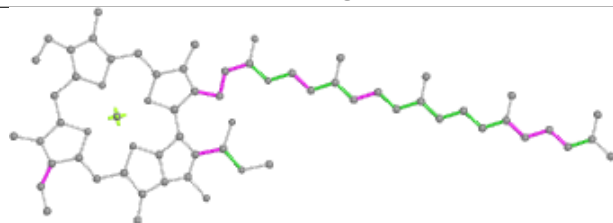
## Ligand CLA b 832



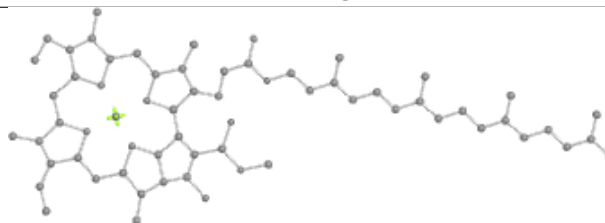
Bond lengths



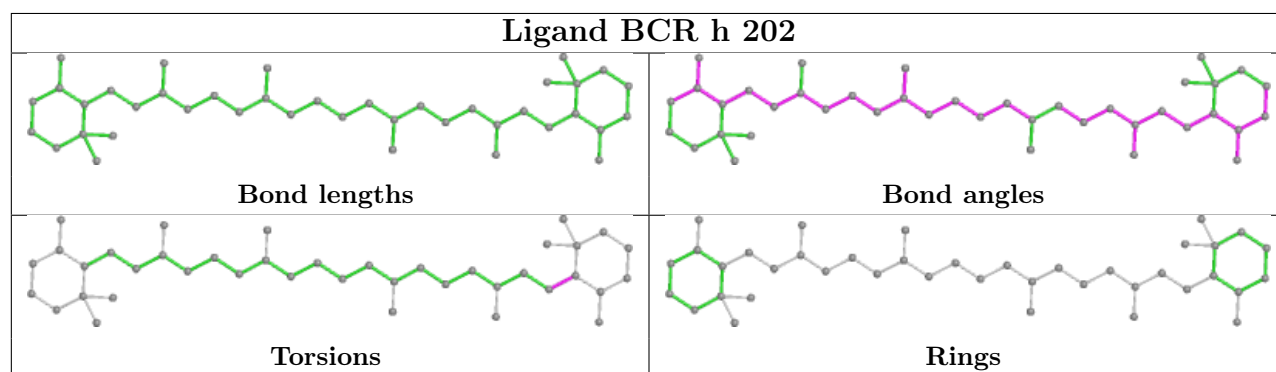
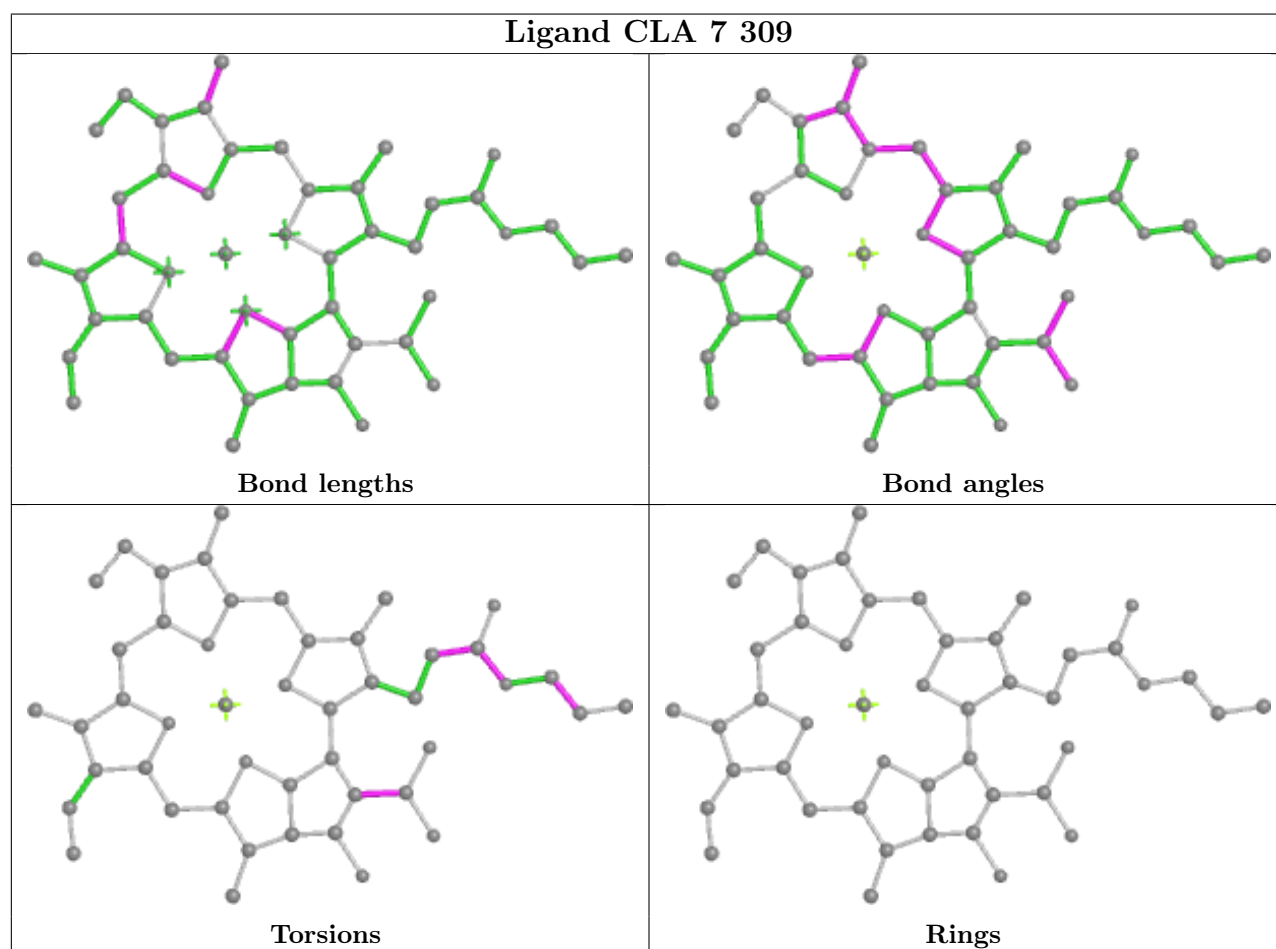
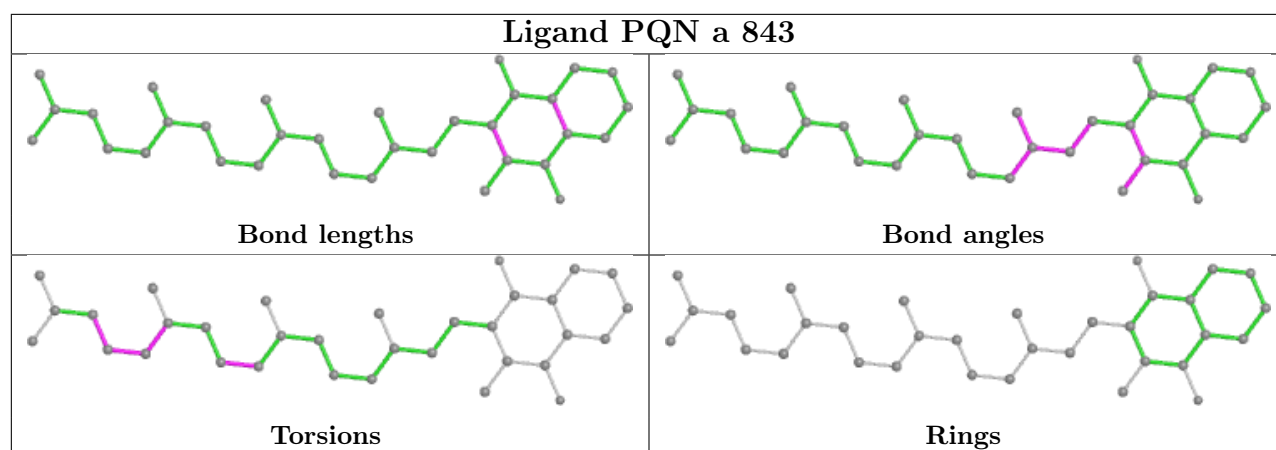
Bond angles



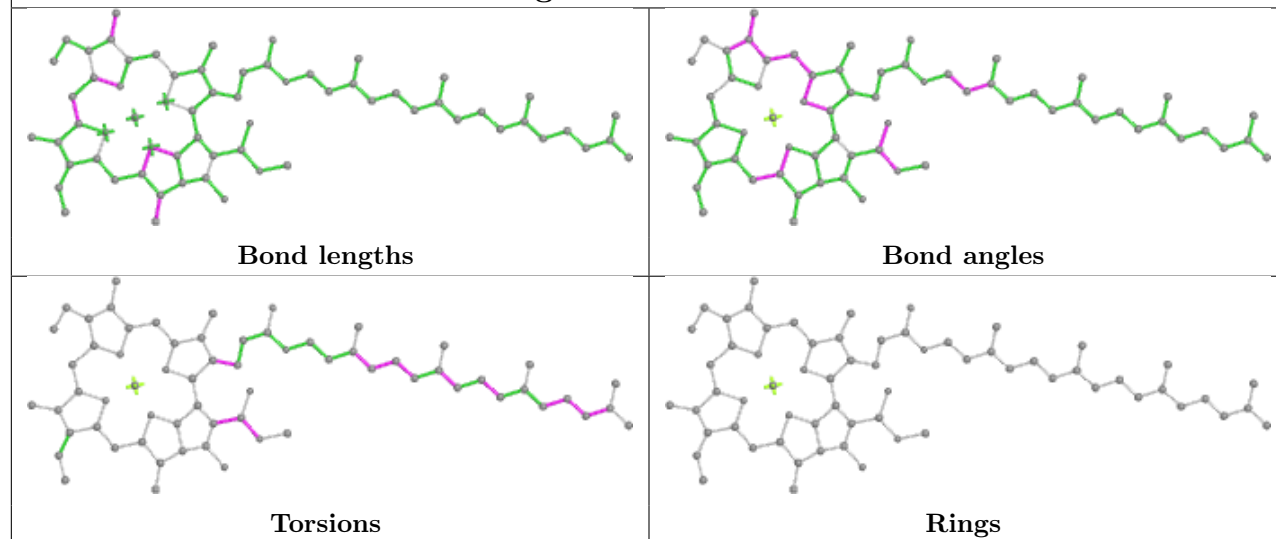
Torsions



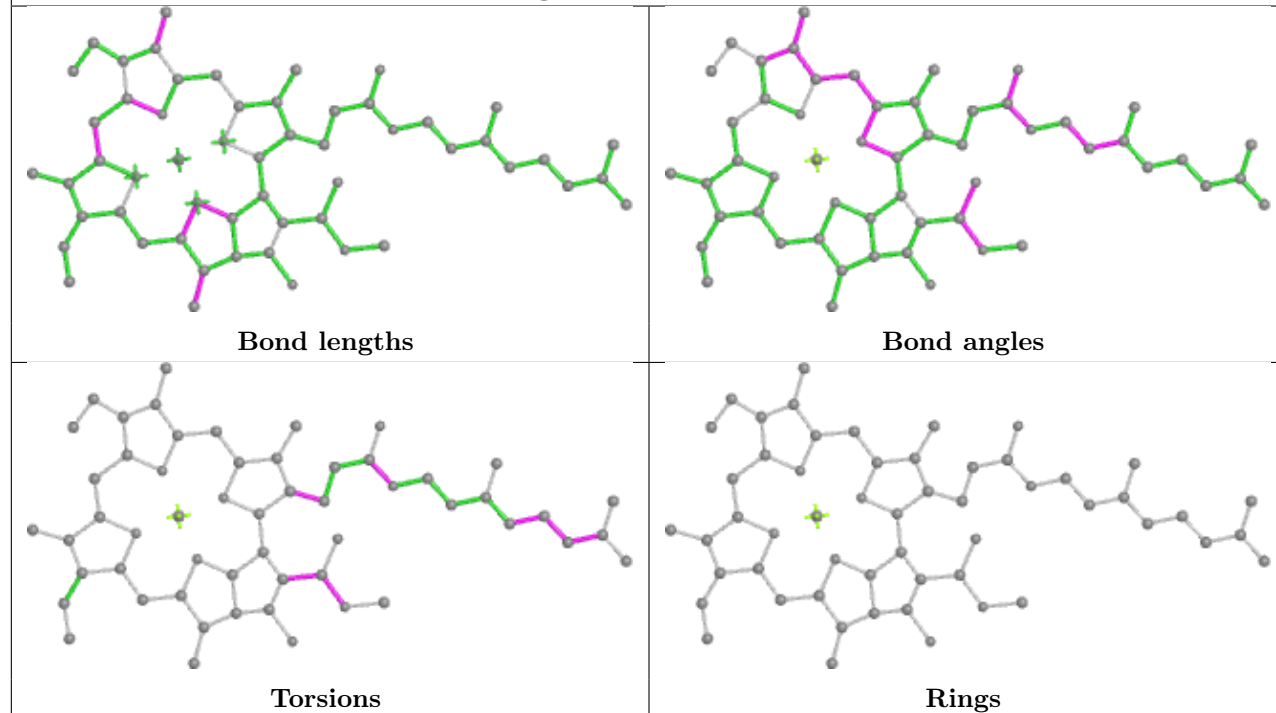
Rings

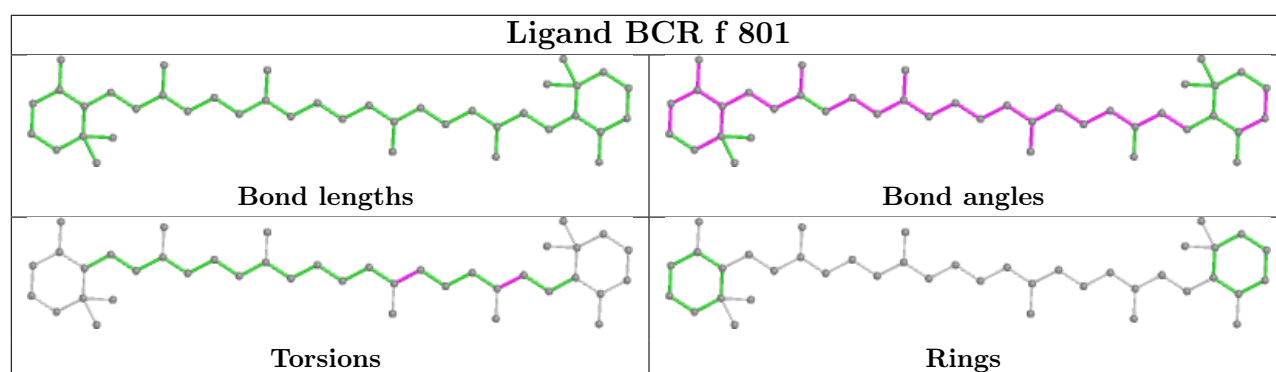
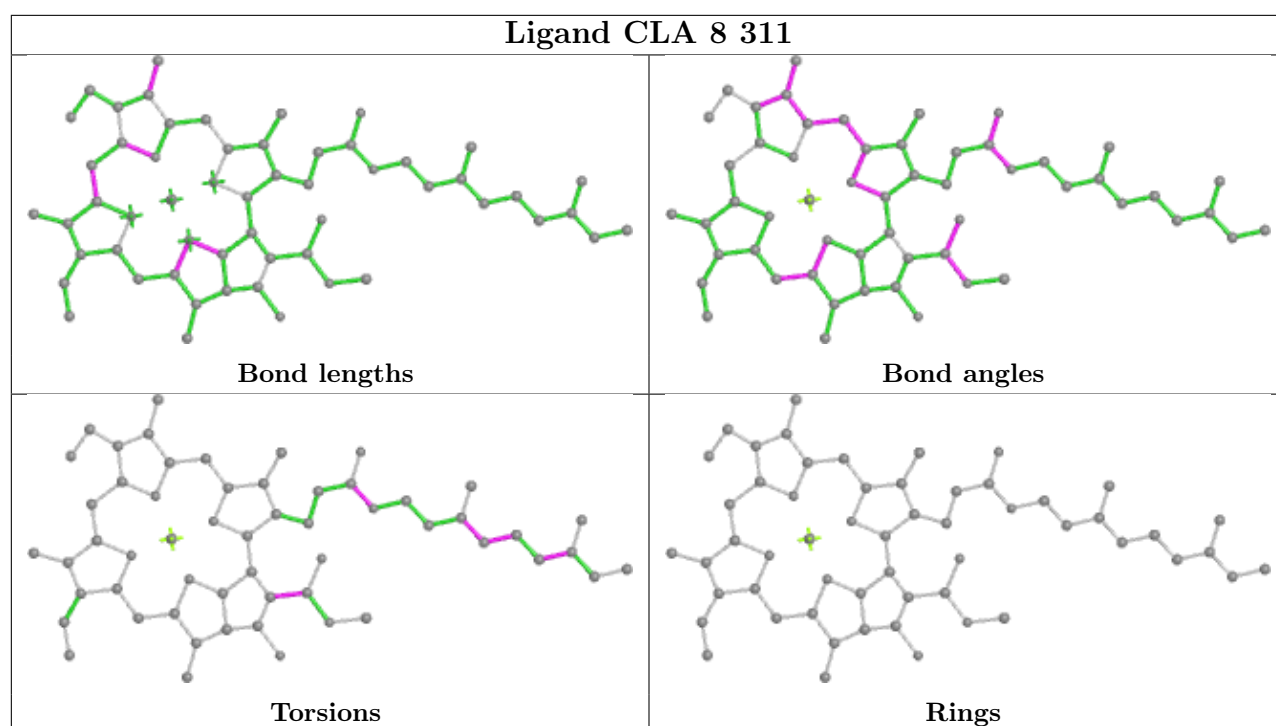
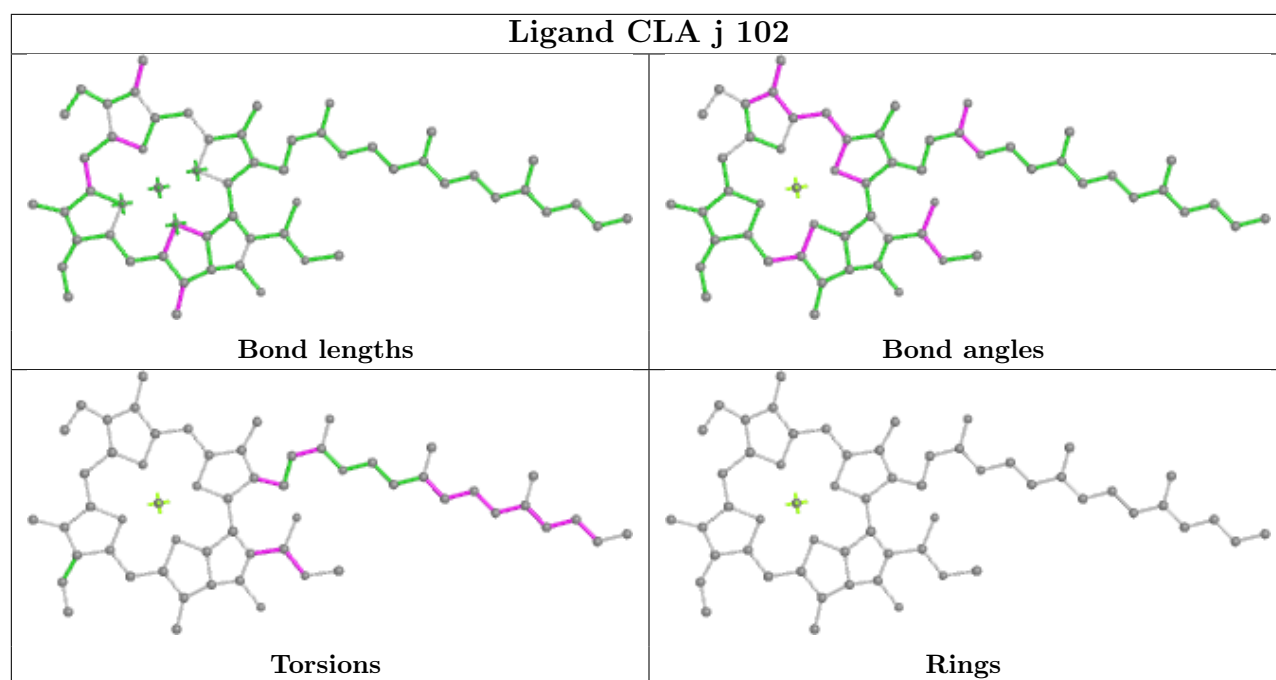


## Ligand CLA b 813

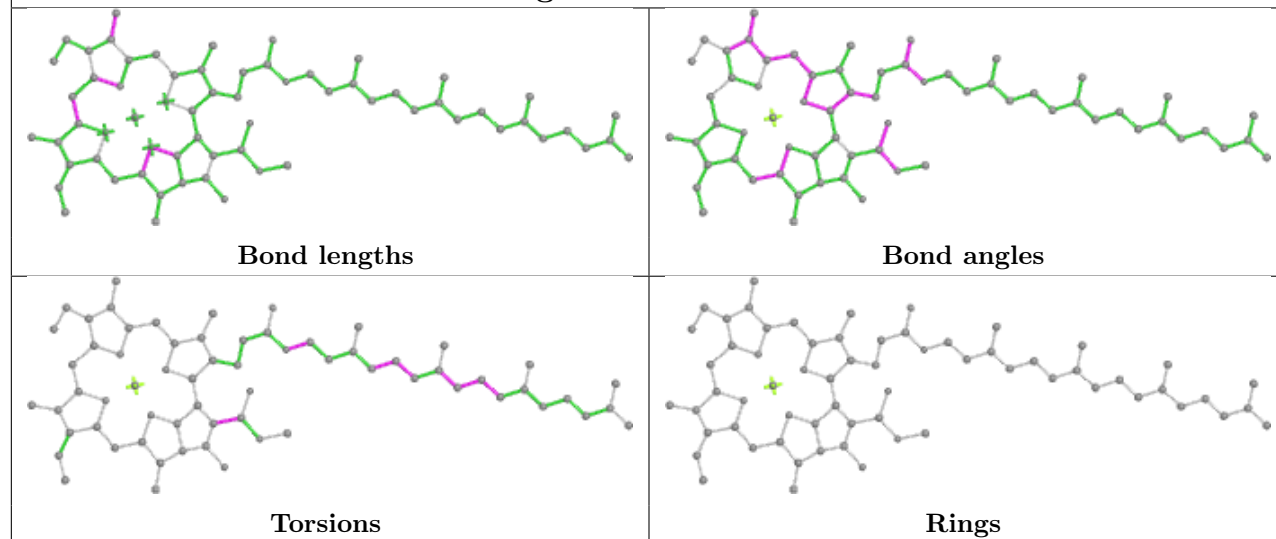


## Ligand CLA b 814

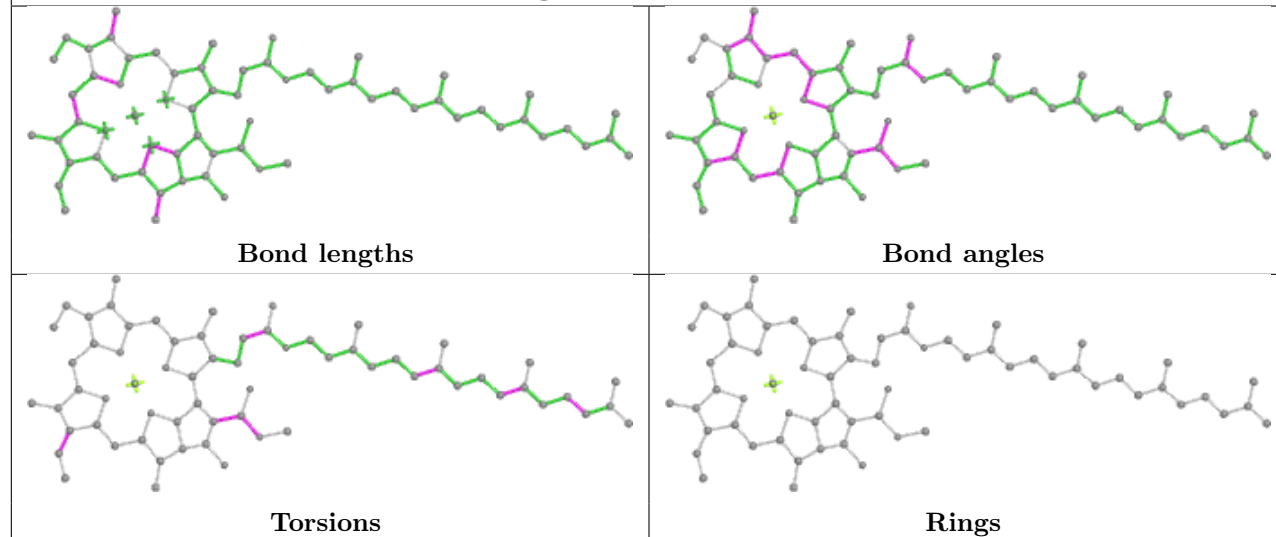




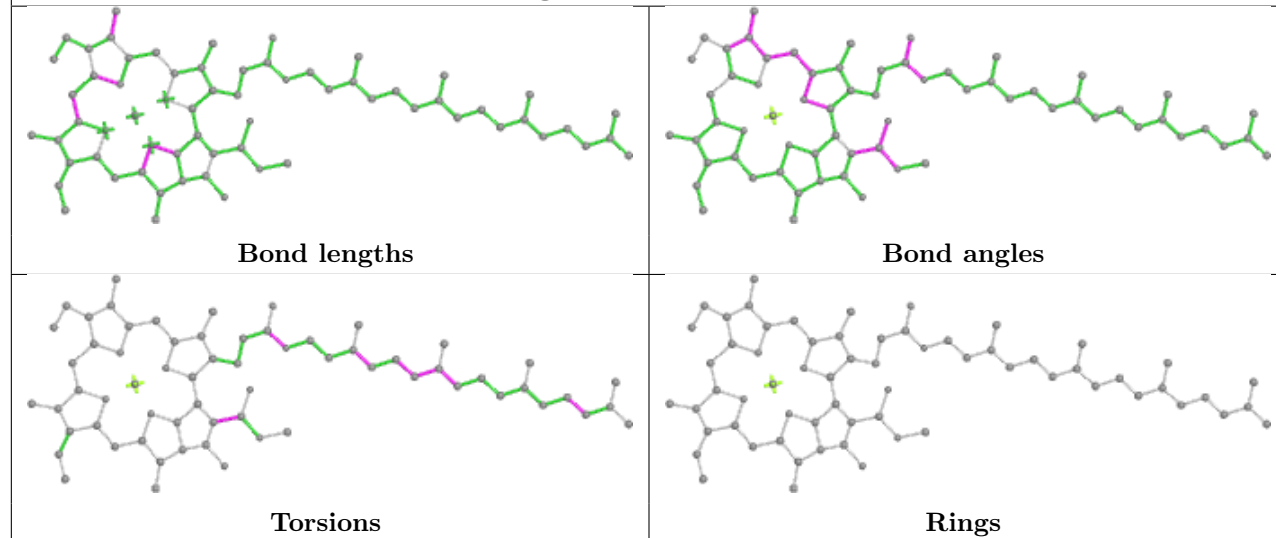
## Ligand CLA a 827

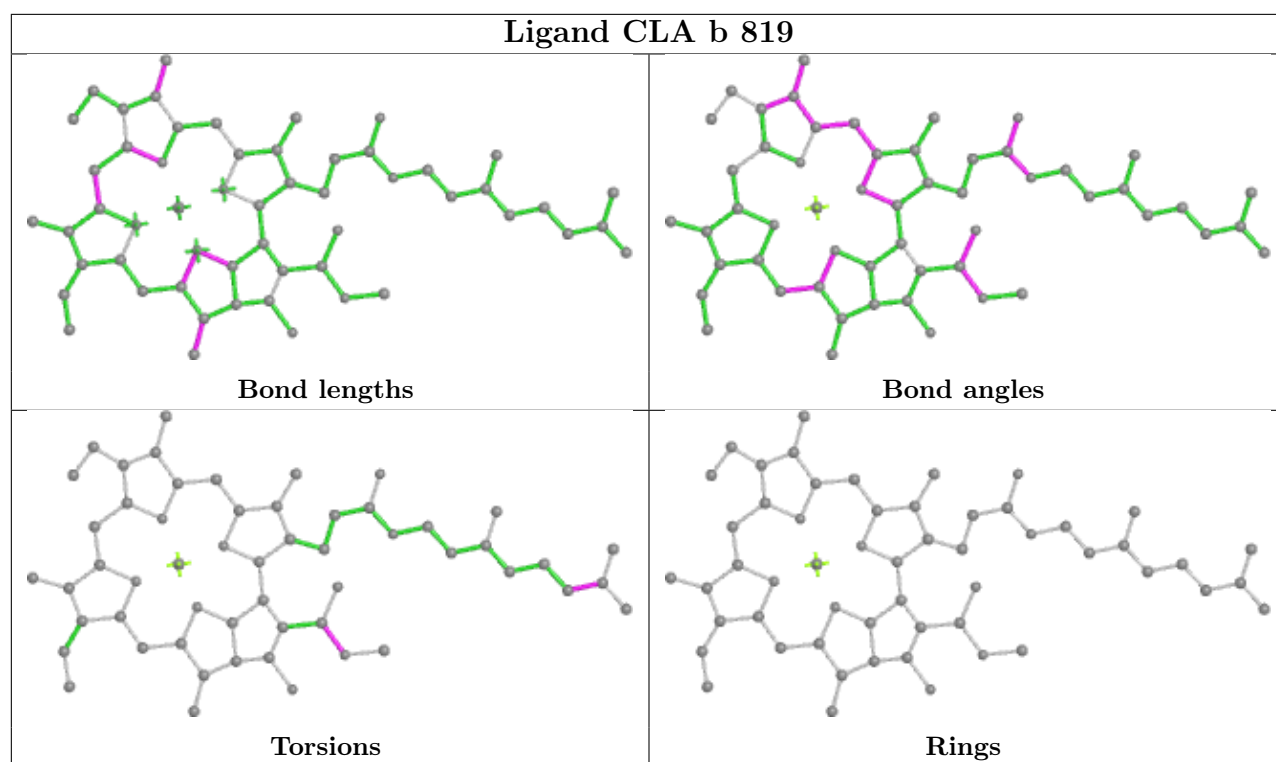


## Ligand CLA b 804



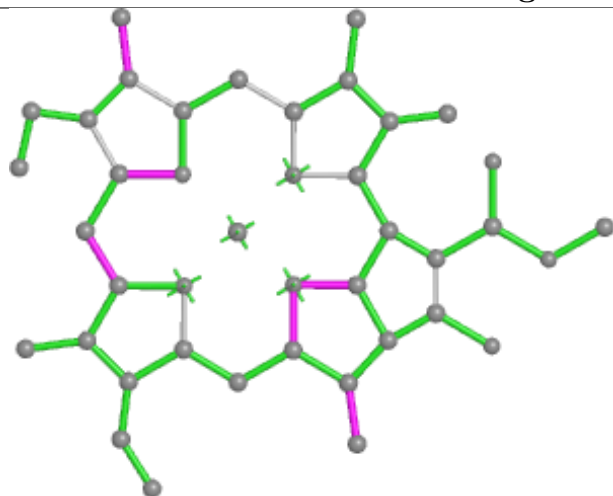
## Ligand CLA a 831



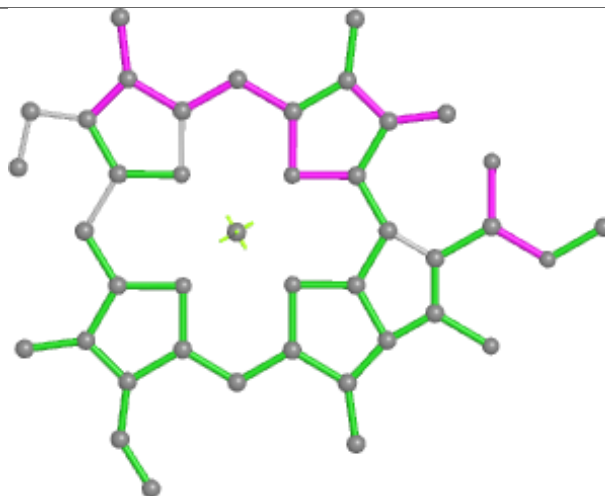




## Ligand CLA 7 315



Bond lengths



Bond angles

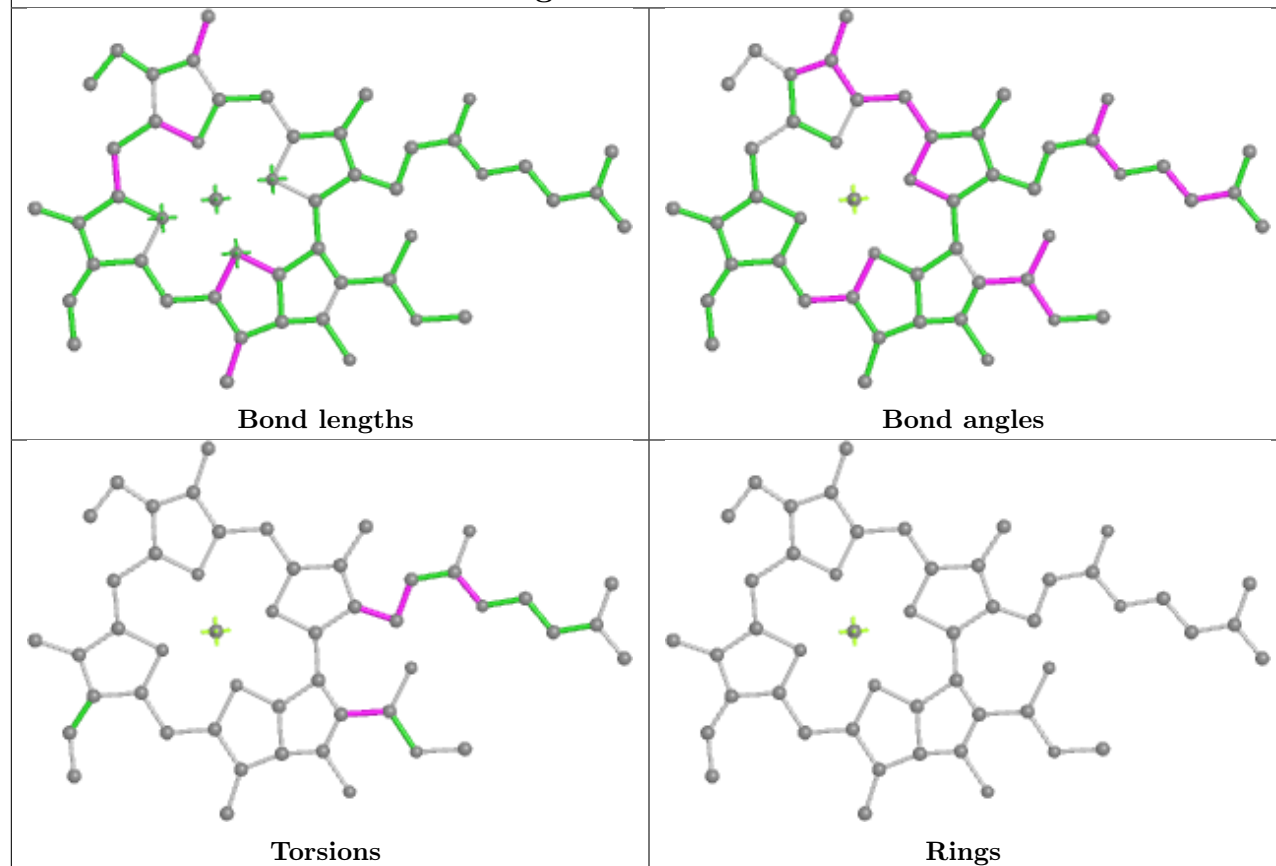


Torsions

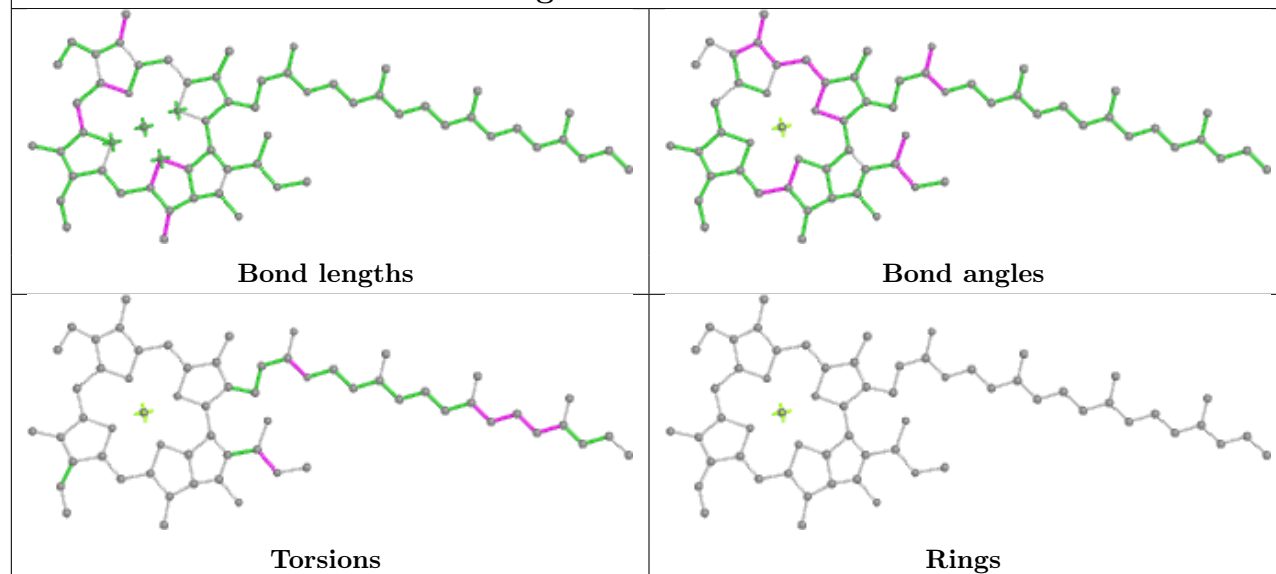


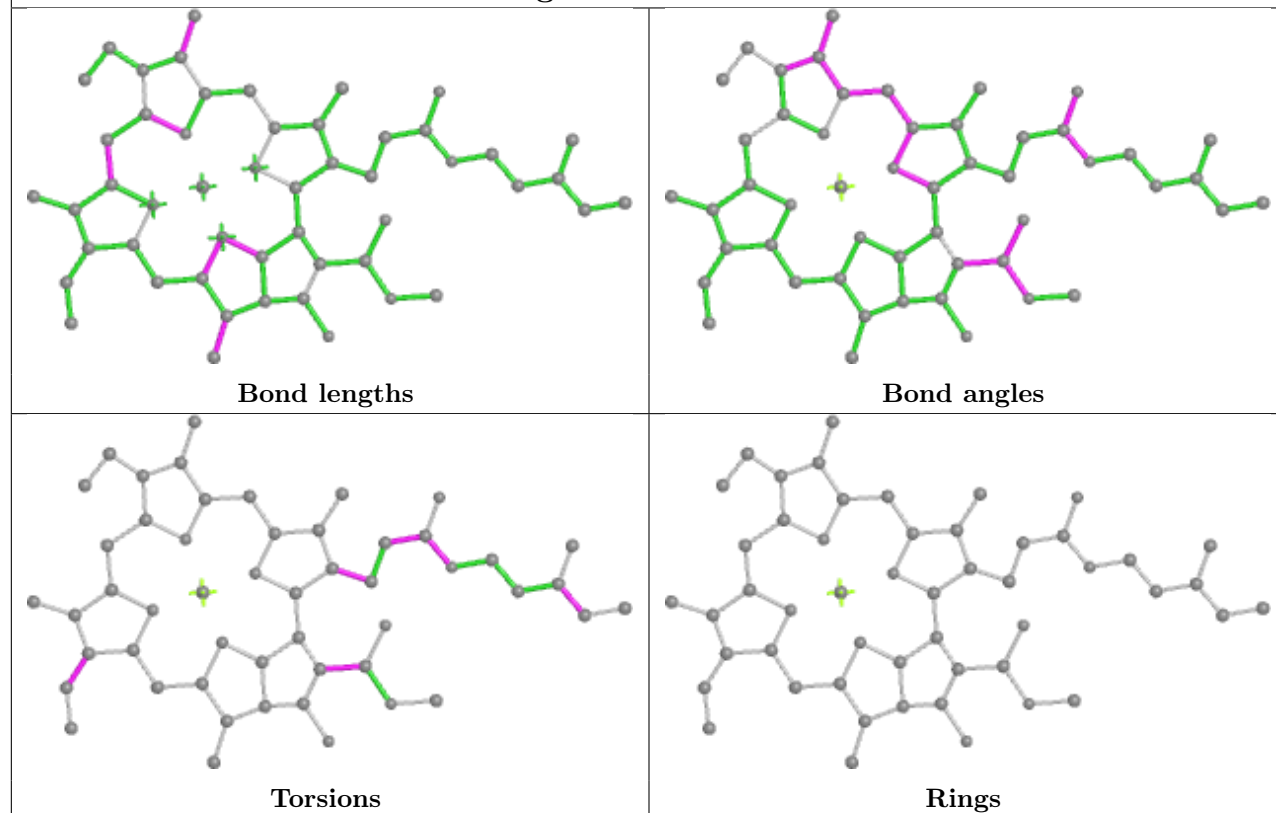
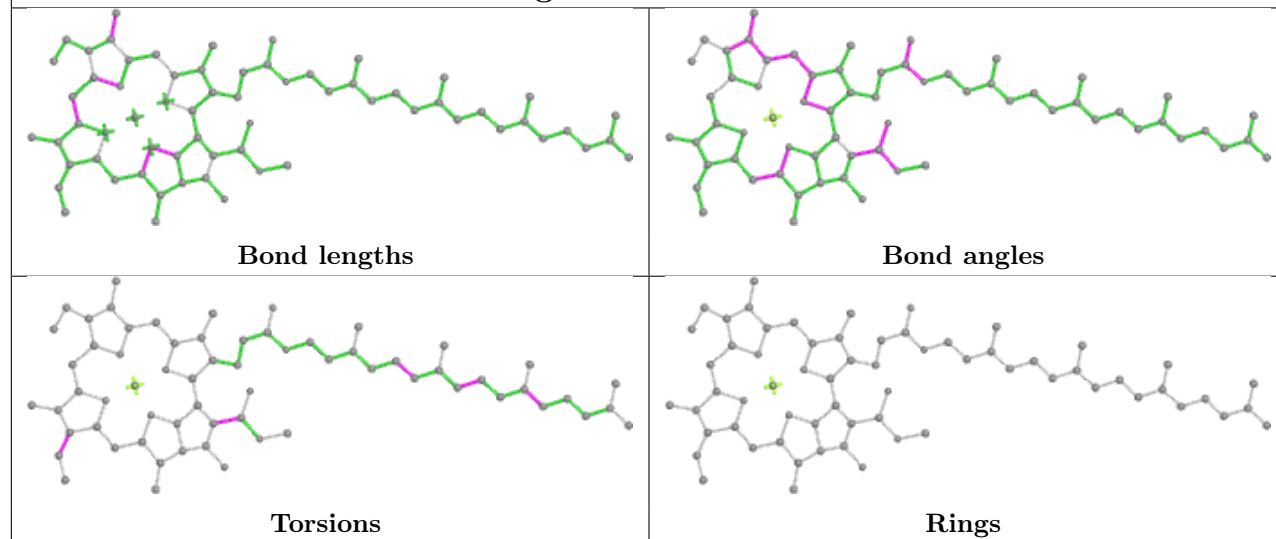
Rings

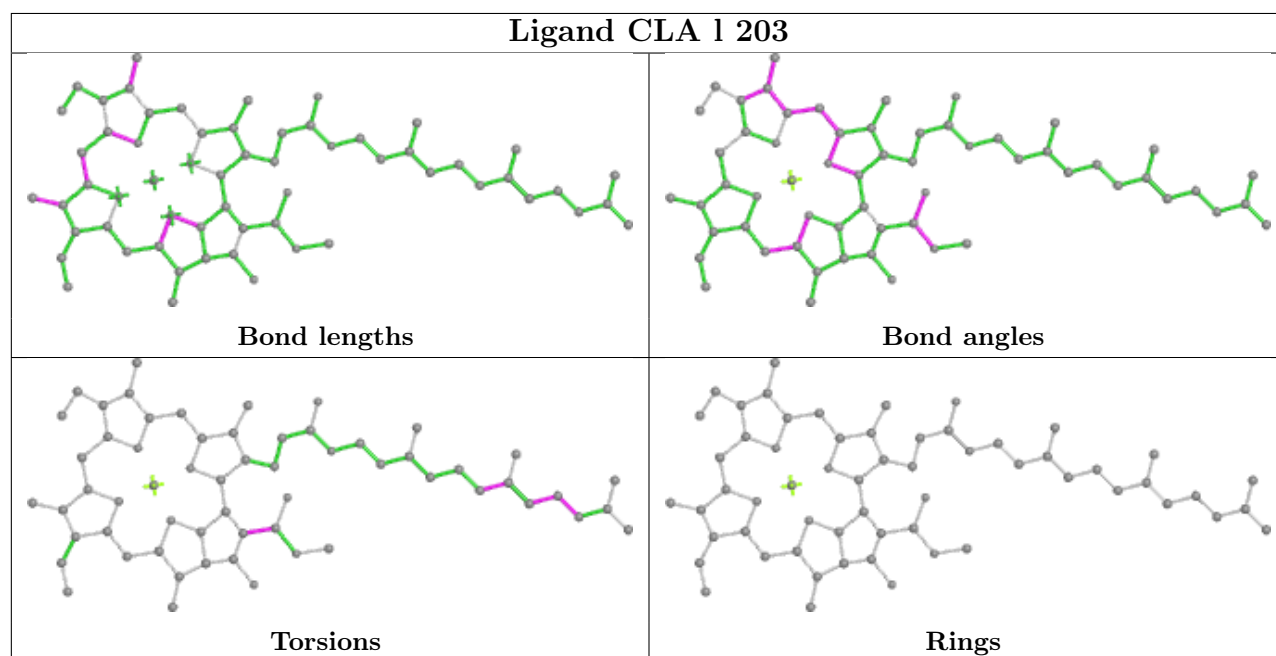
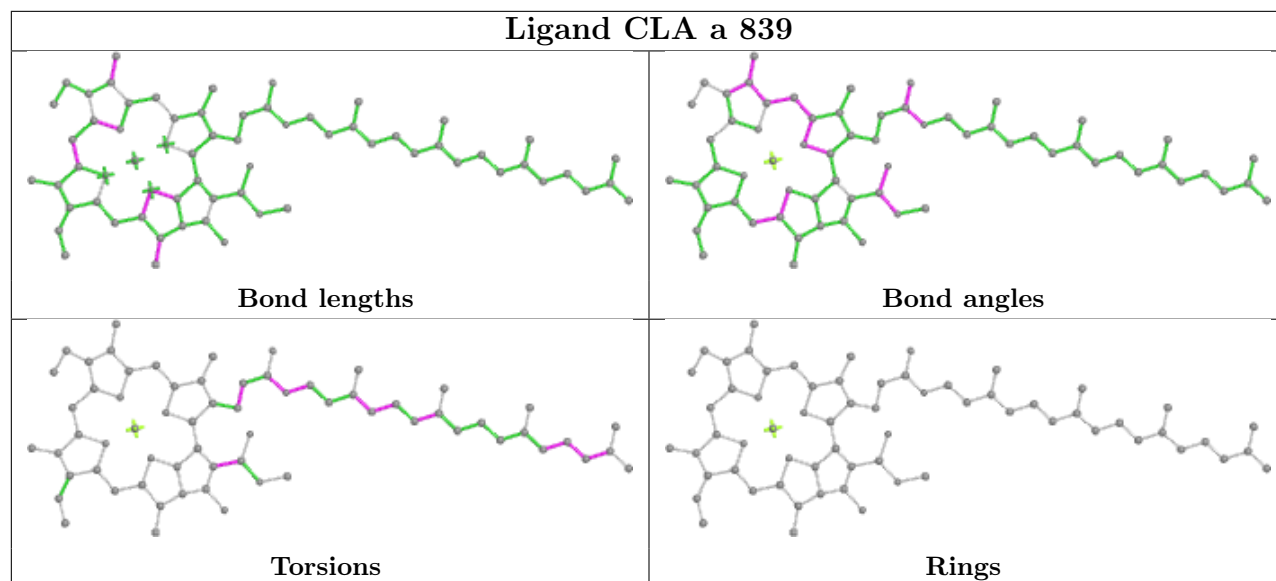
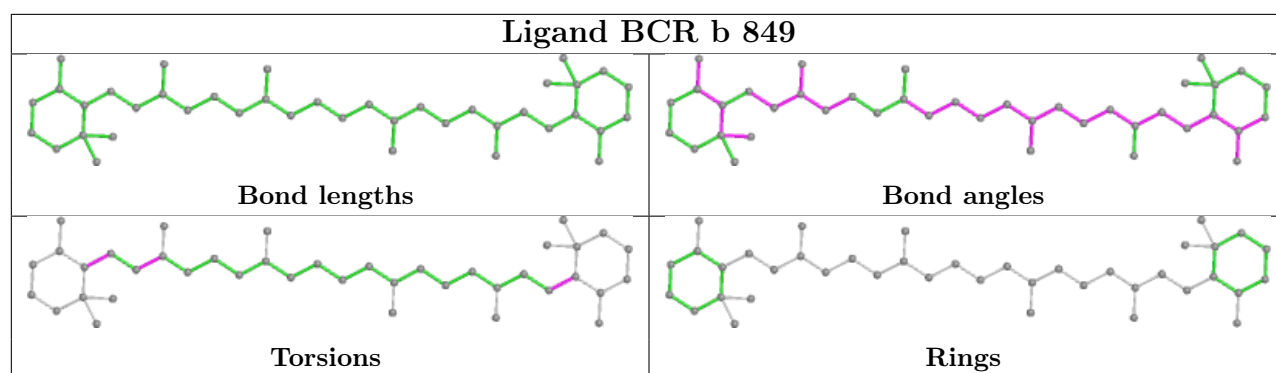
## Ligand CLA b 820



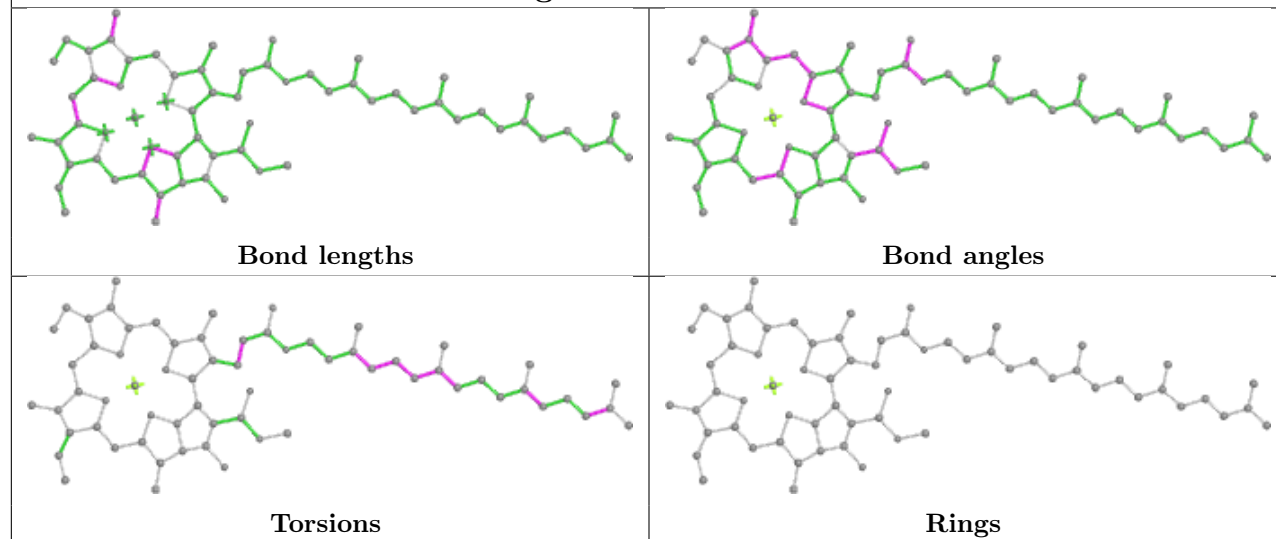
## Ligand CLA 9 318



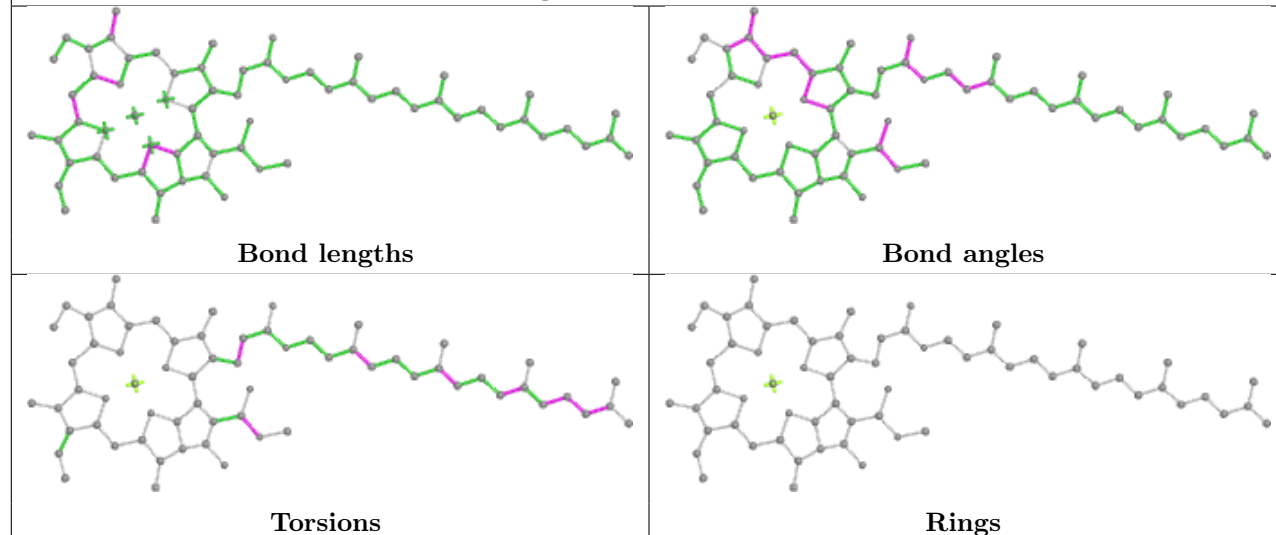
**Ligand CLA 7 316****Ligand CLA b 836**



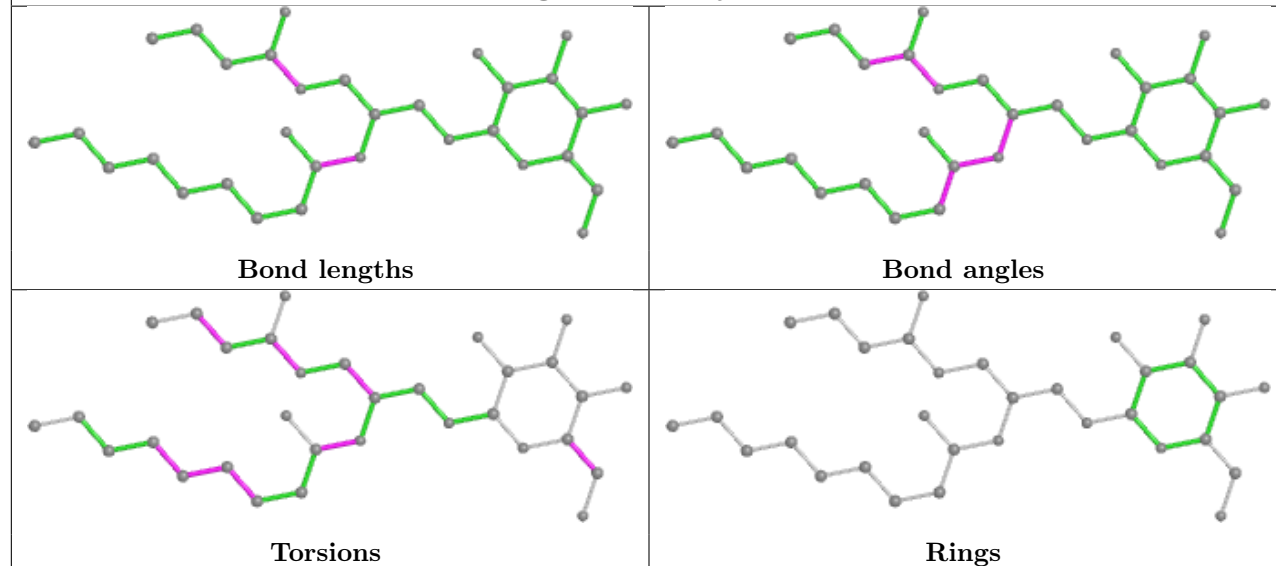
## Ligand CLA b 808



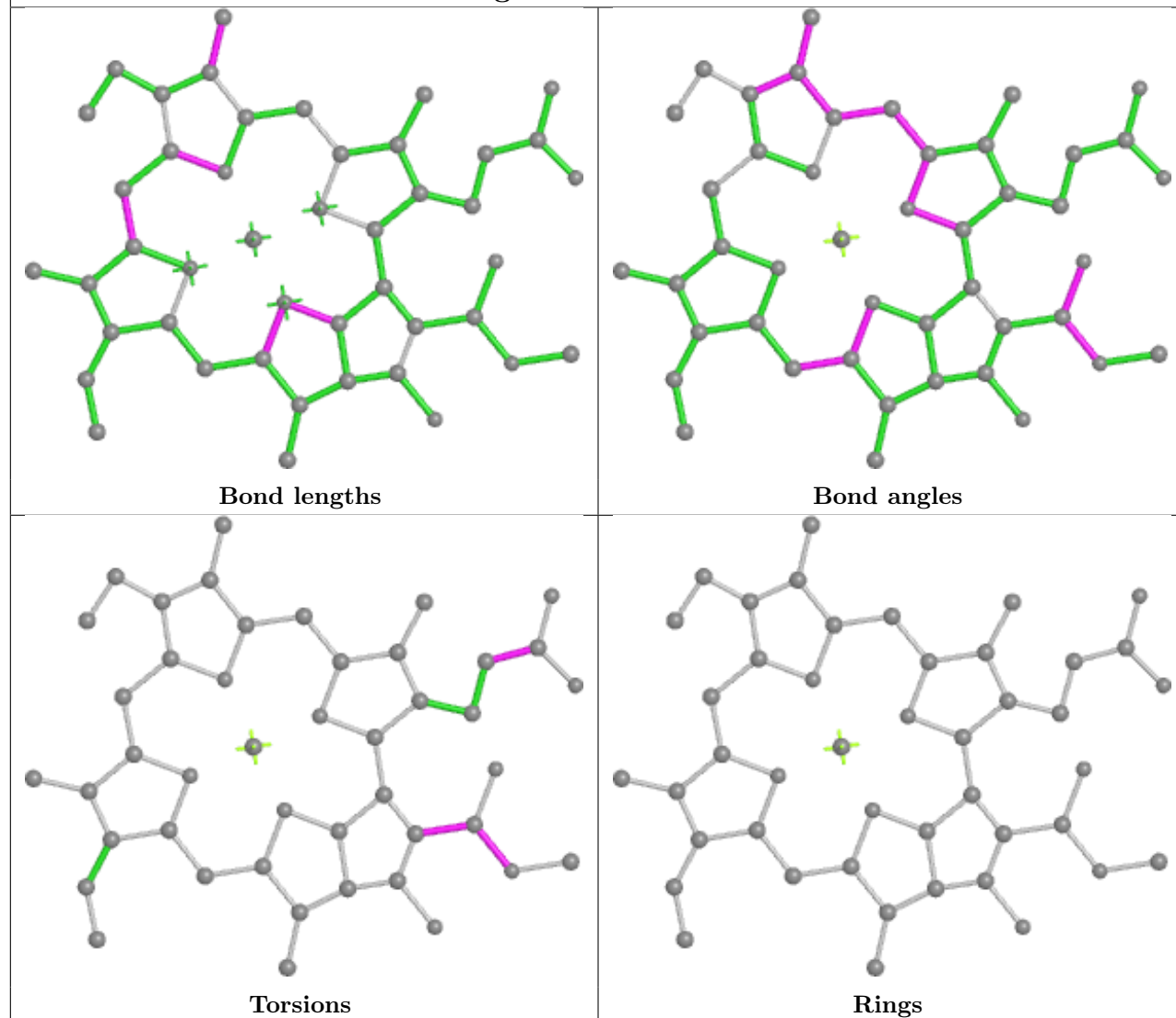
## Ligand CLA 1 308

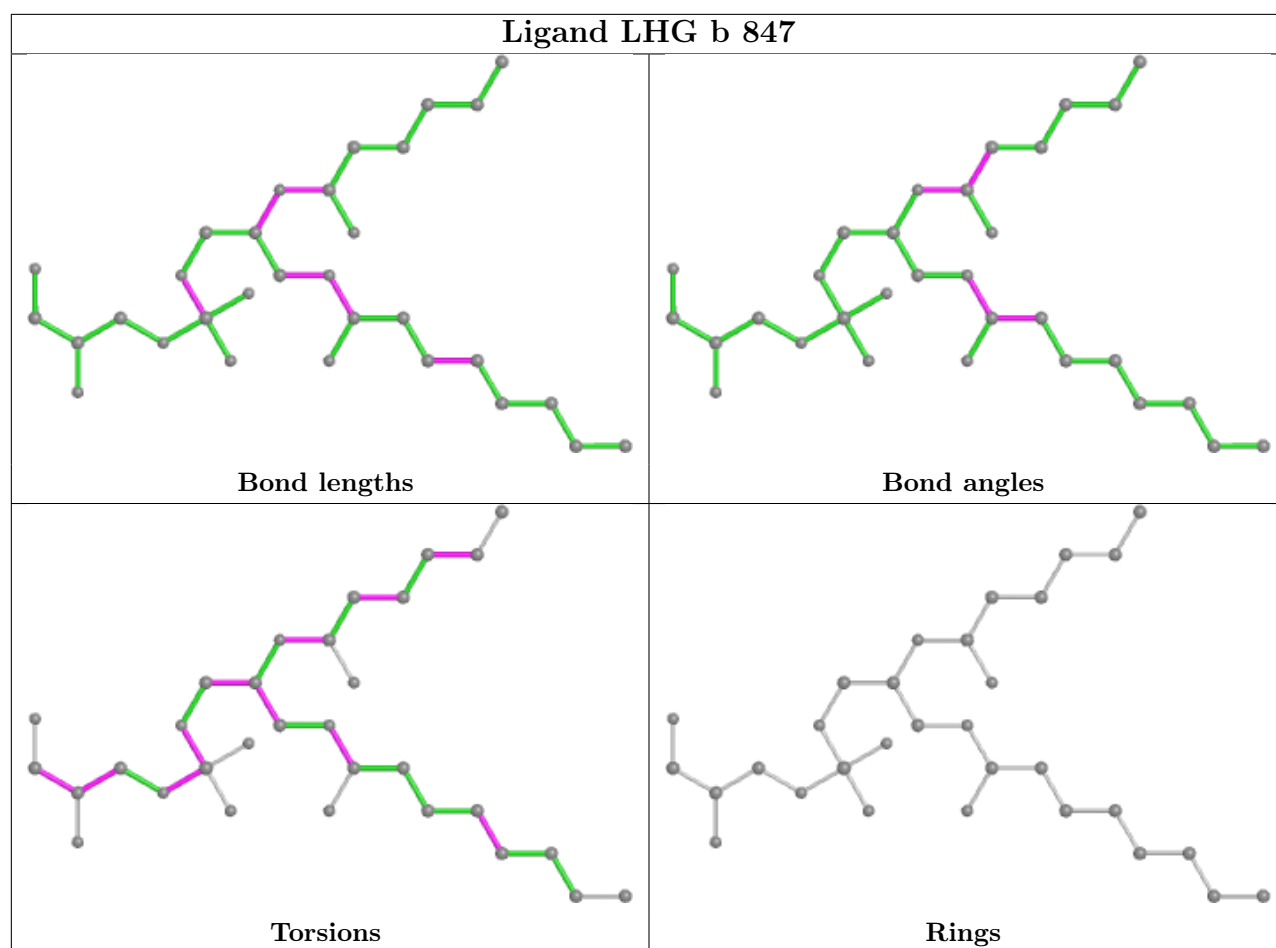


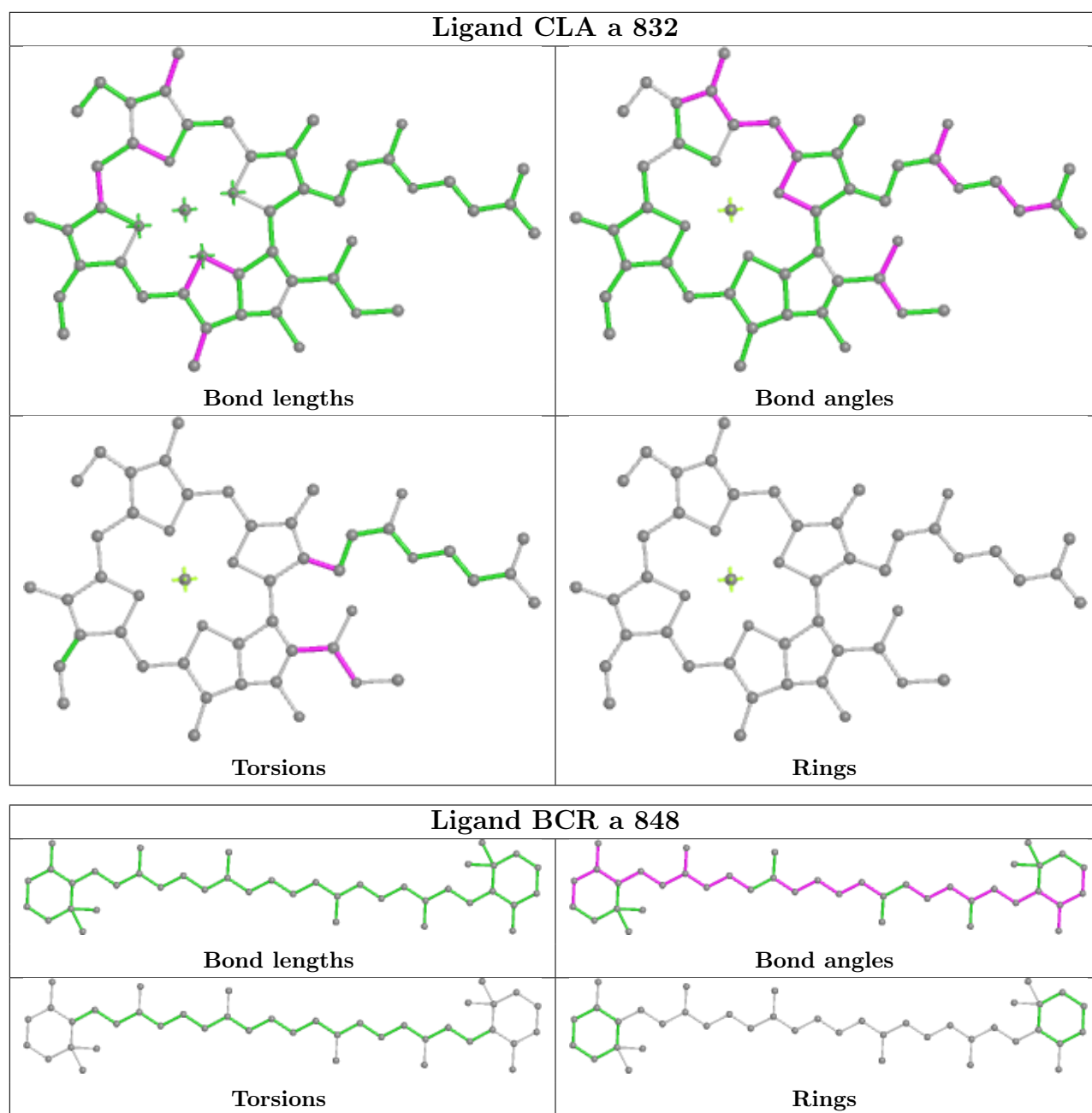
## Ligand LMG j 105



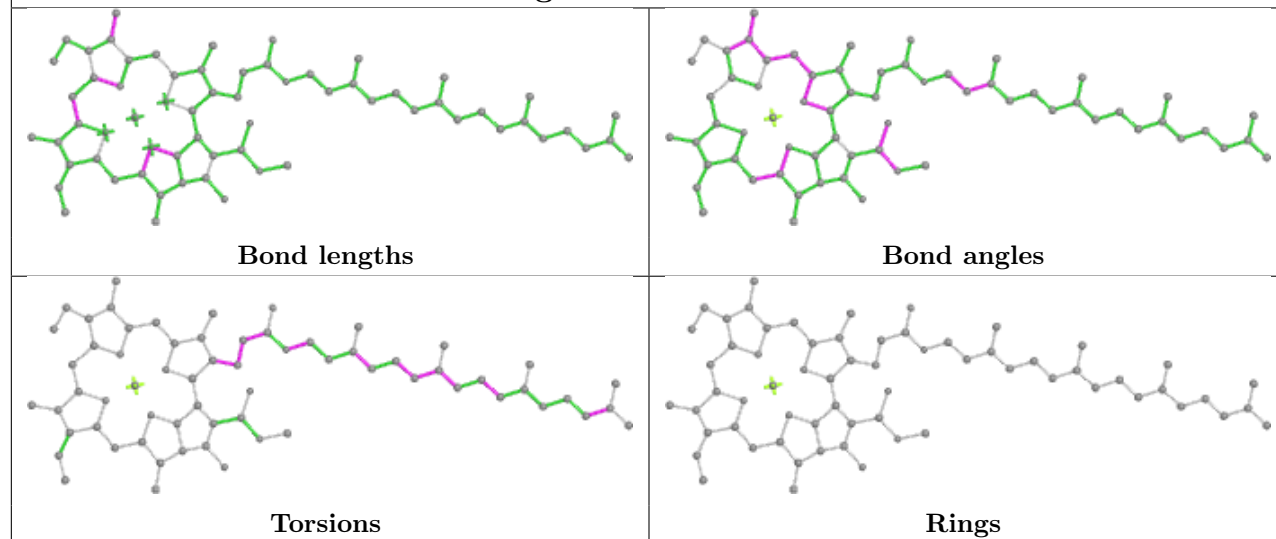
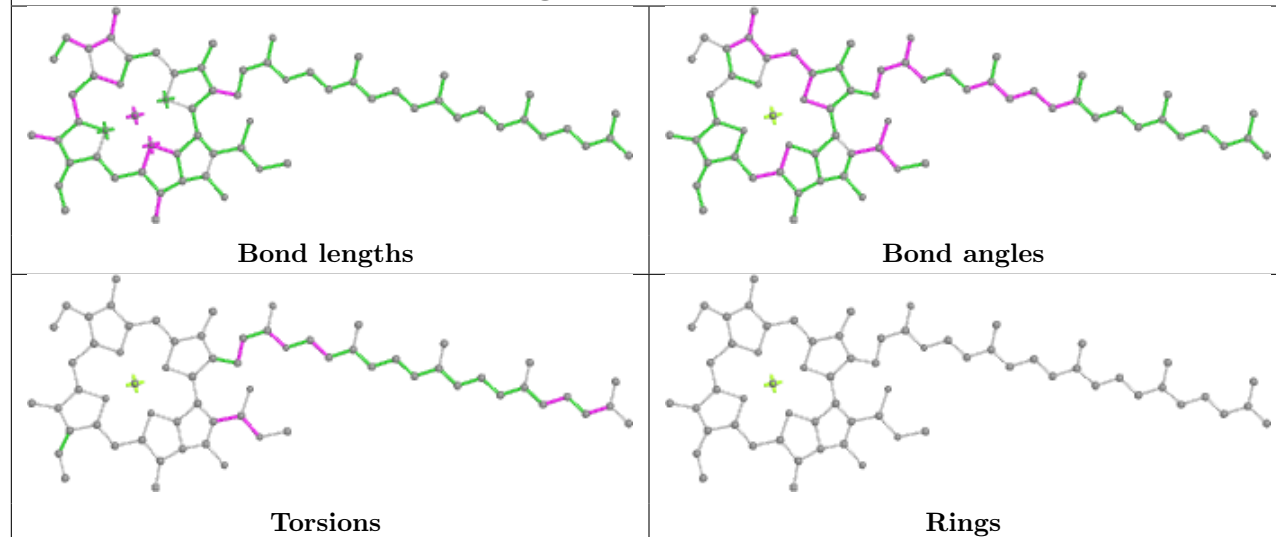
## Ligand CLA 7 307



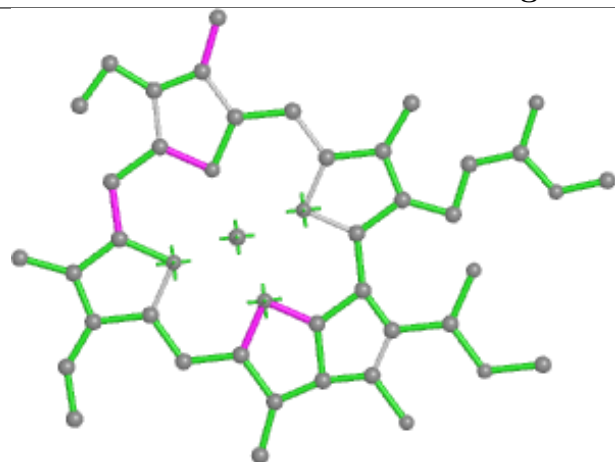




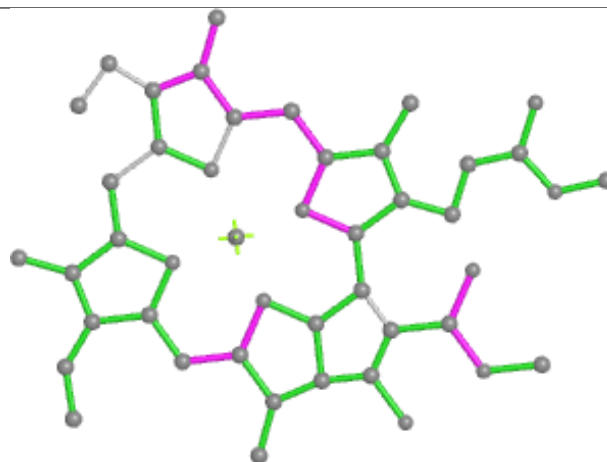


**Ligand CLA b 810****Ligand CLA a 806**

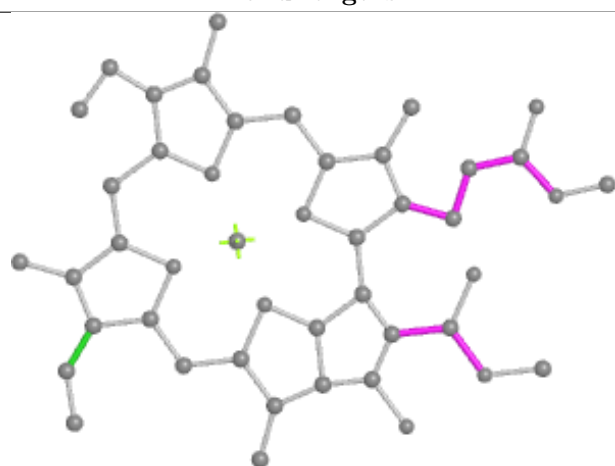
## Ligand CLA 9 313



Bond lengths



Bond angles

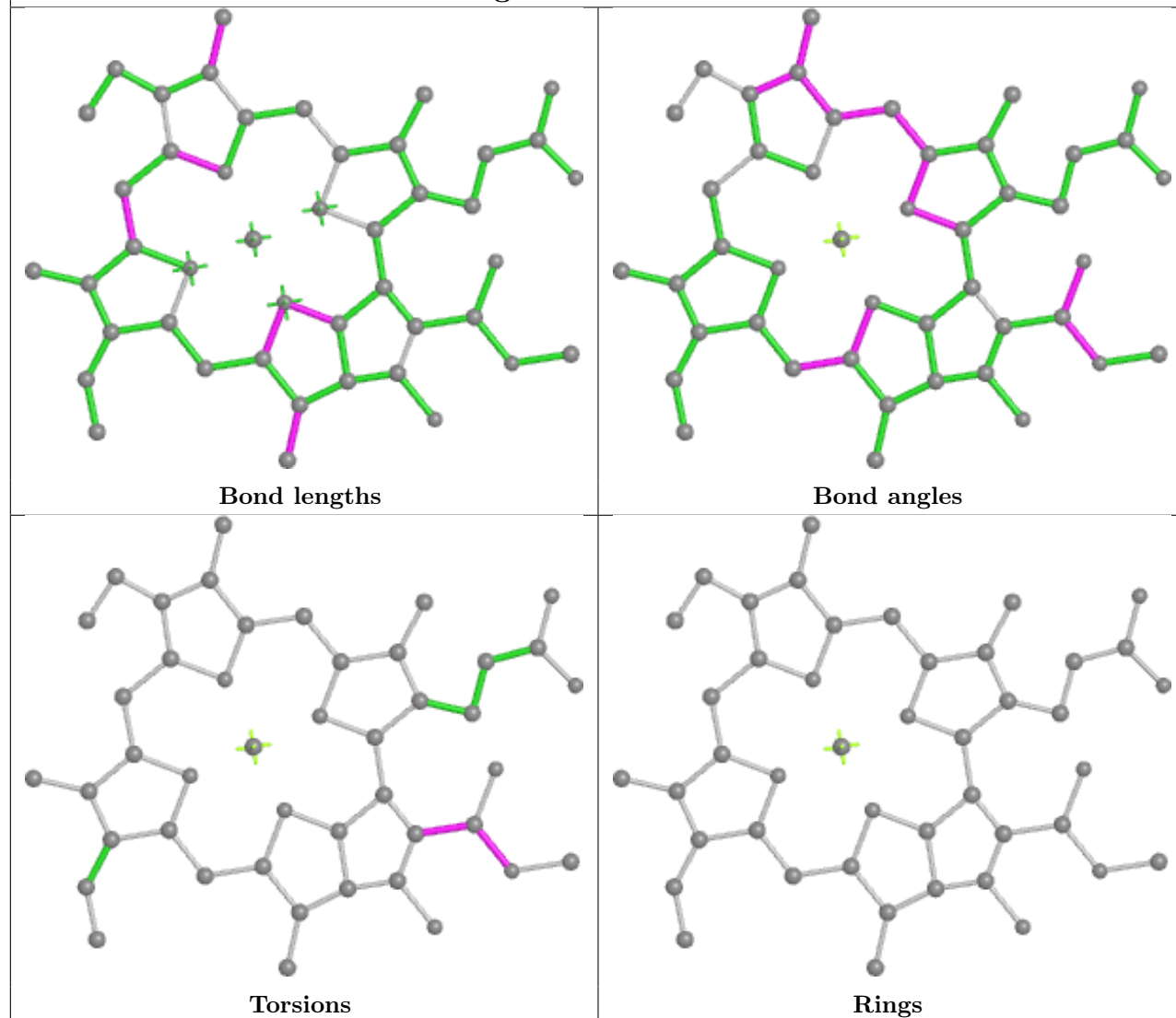


Torsions

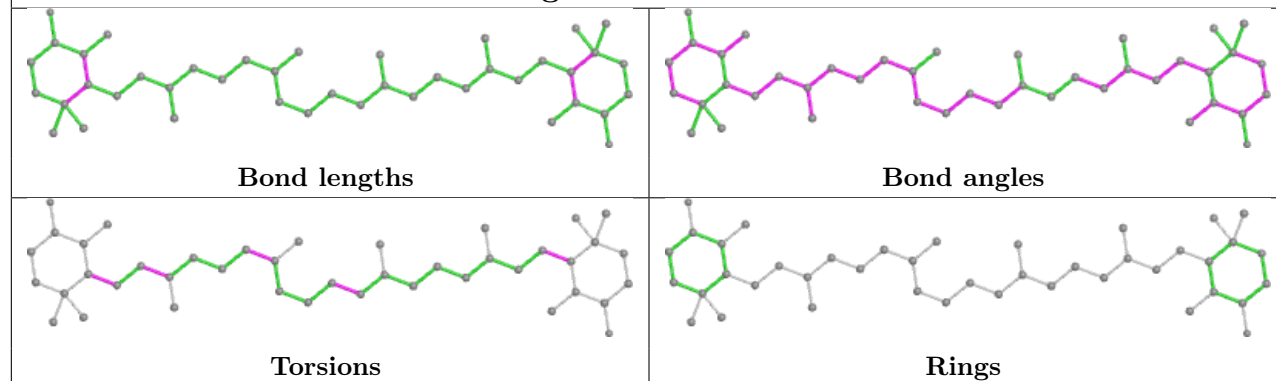


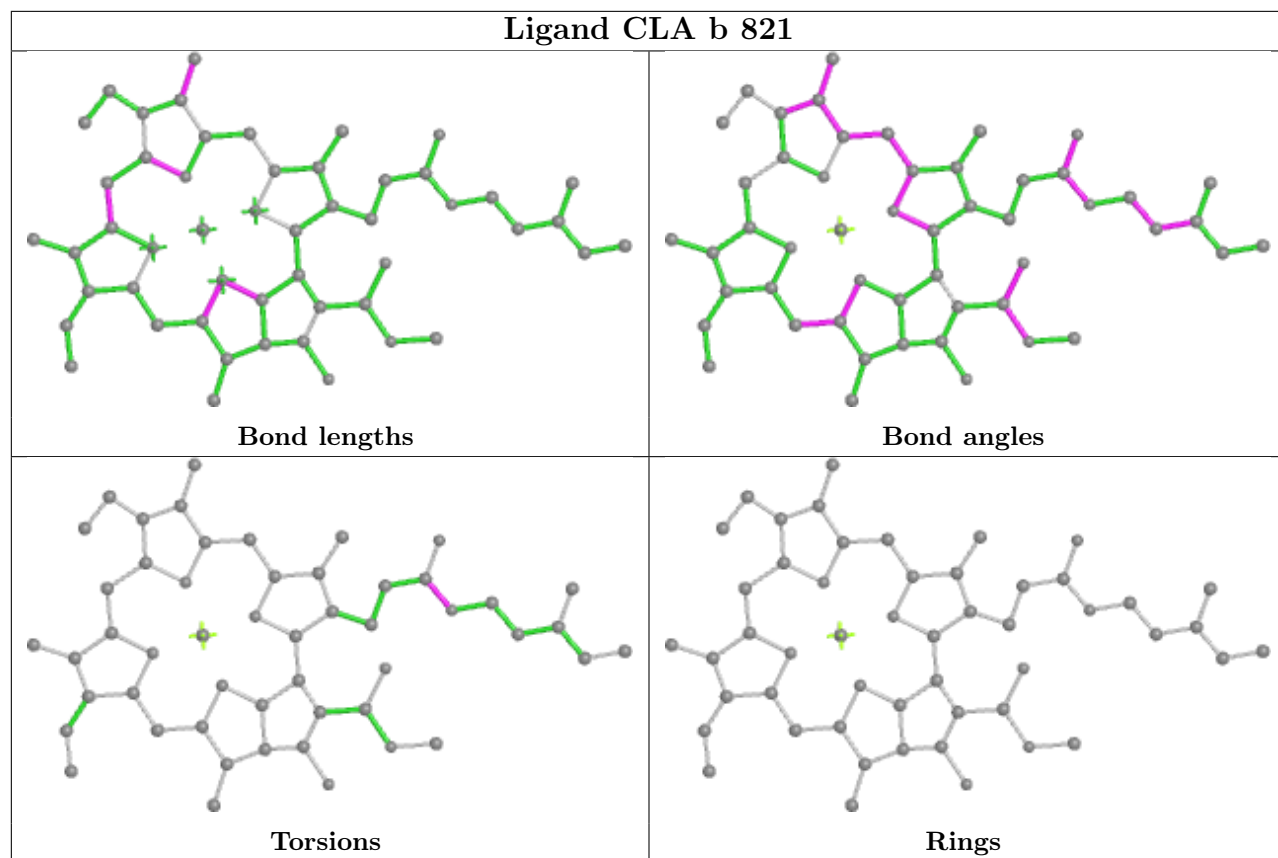
Rings

## Ligand CLA a 837

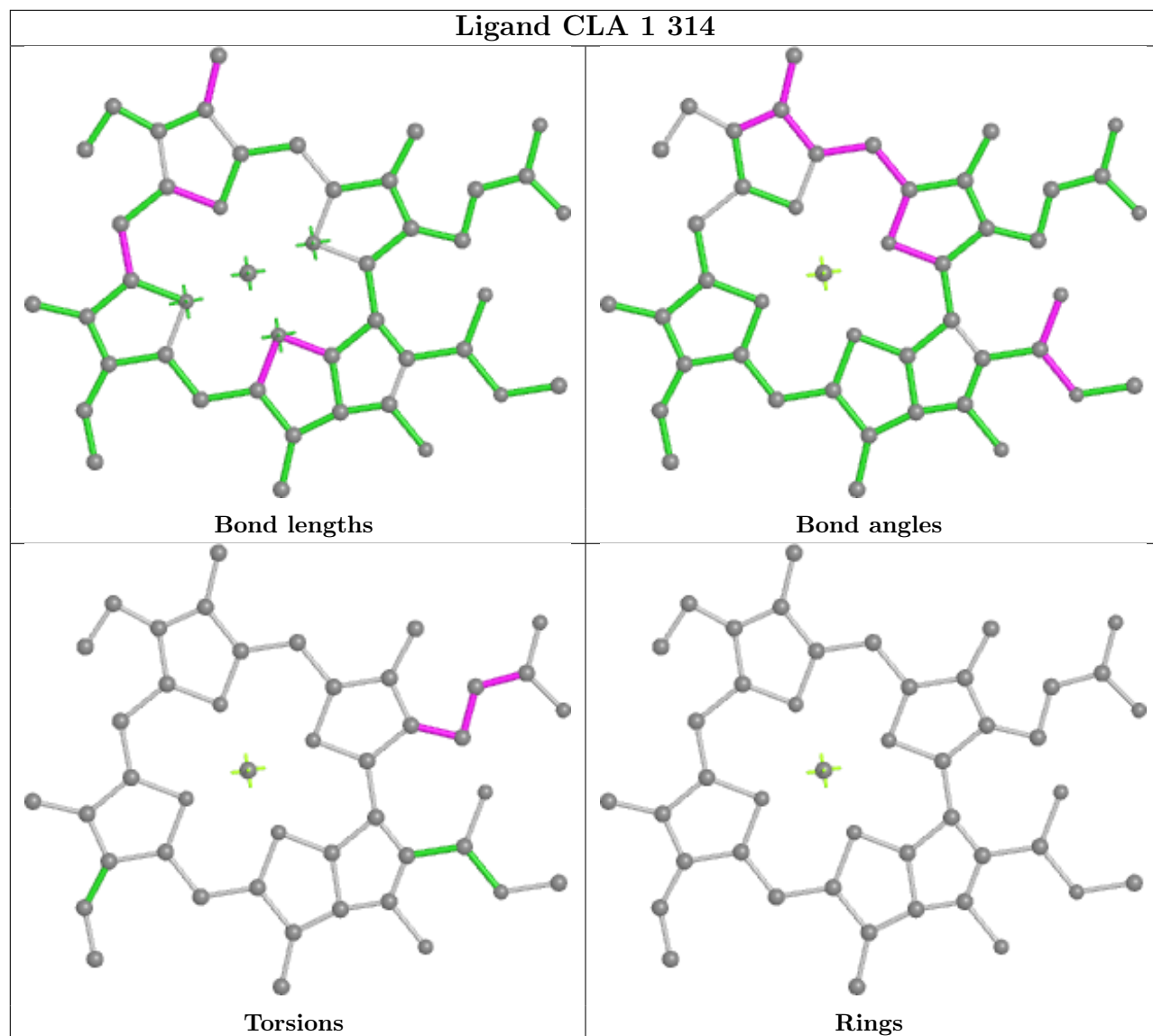


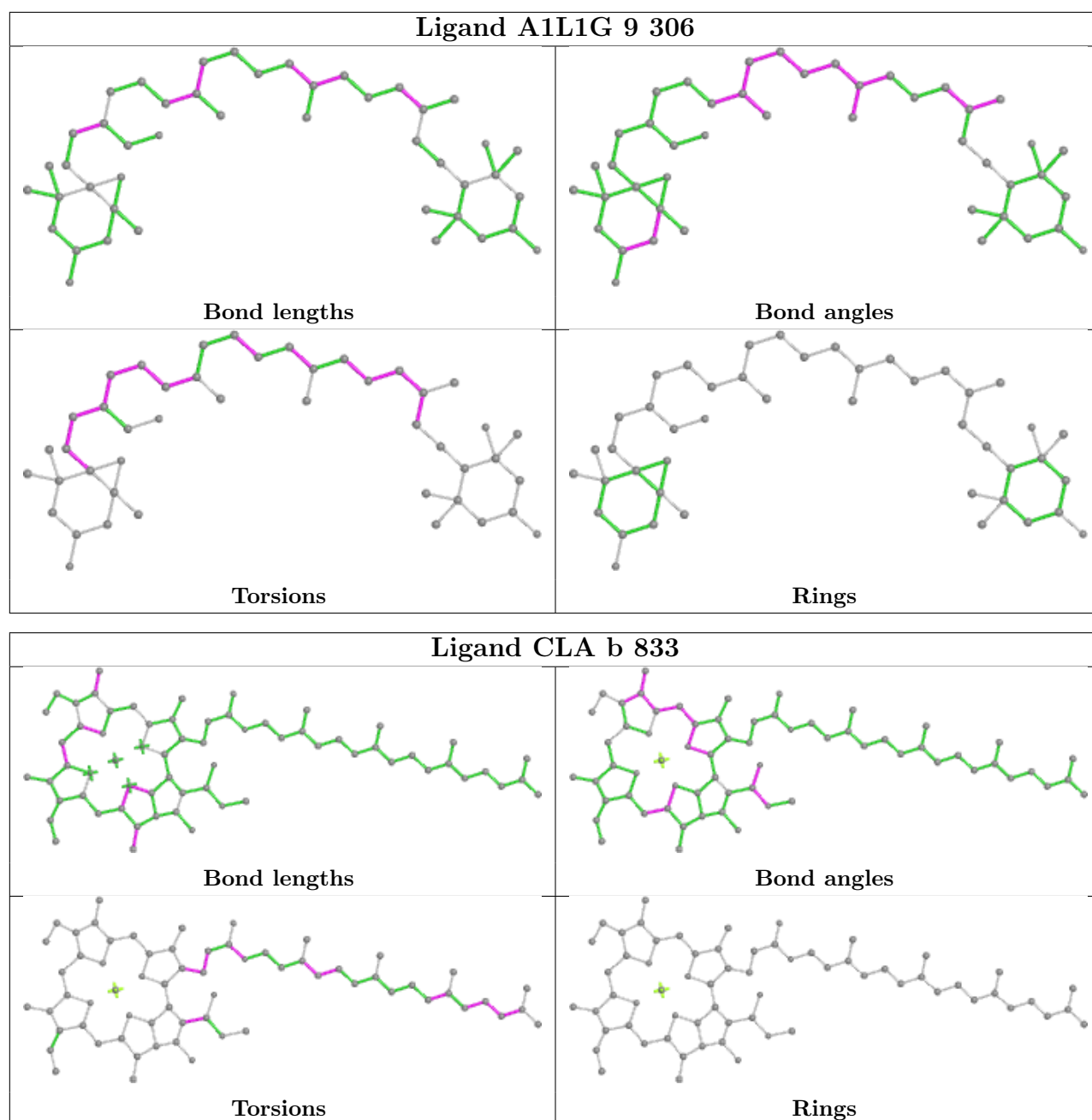
## Ligand 45D 9 305

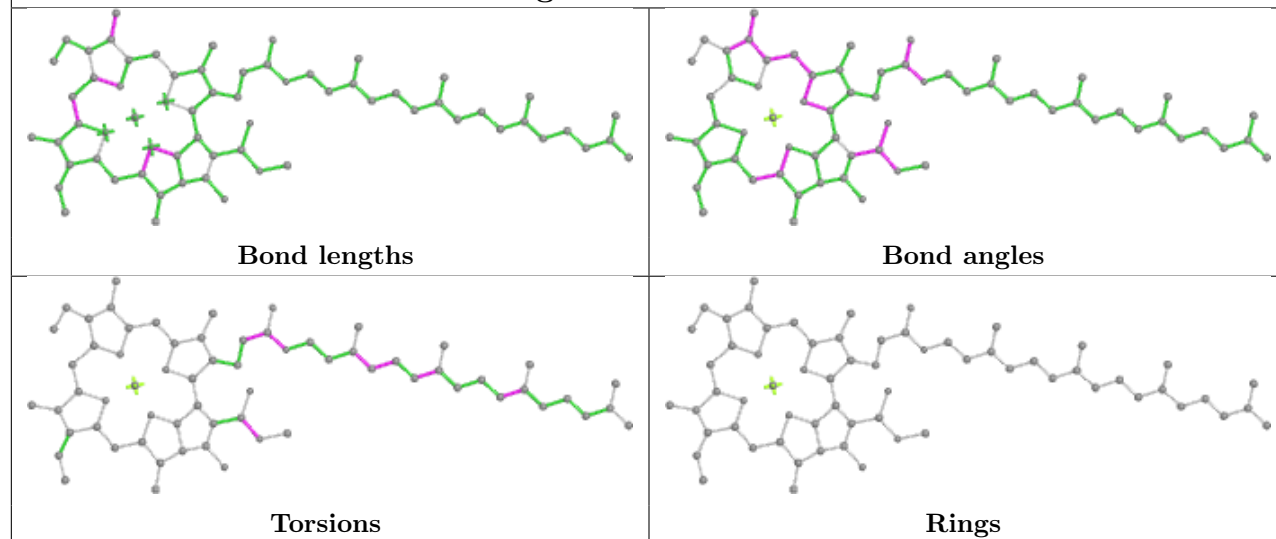
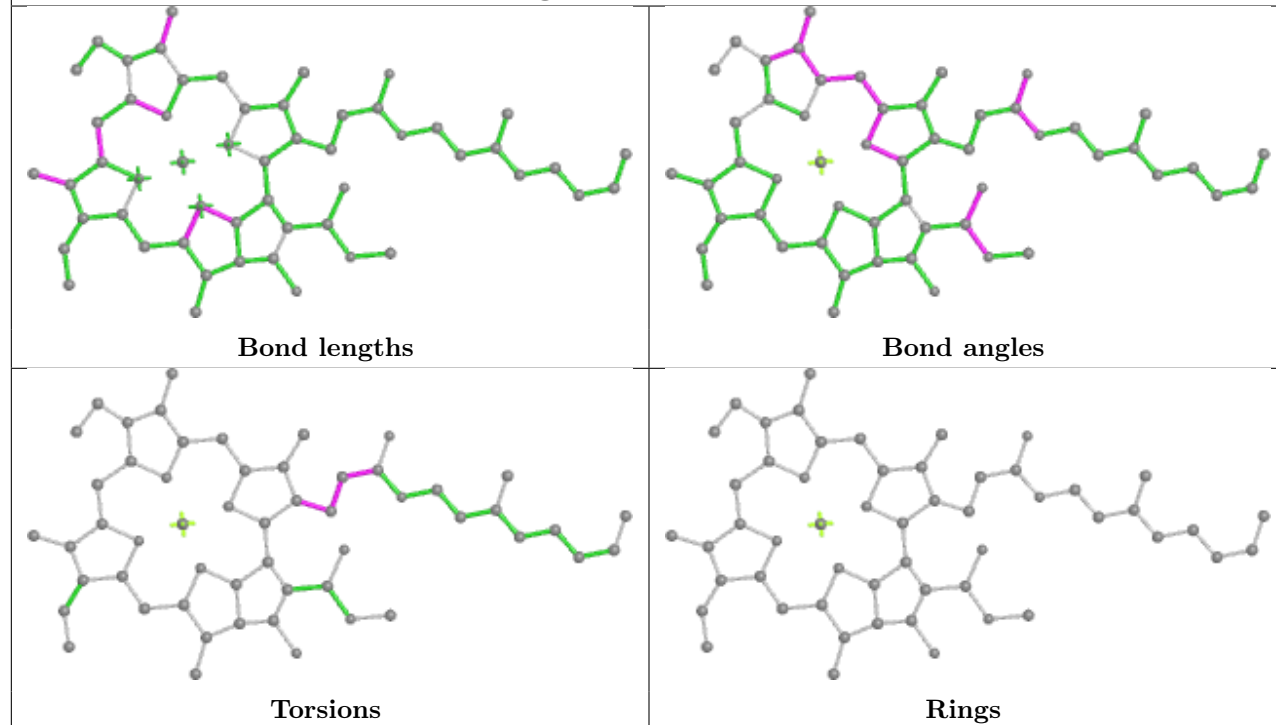




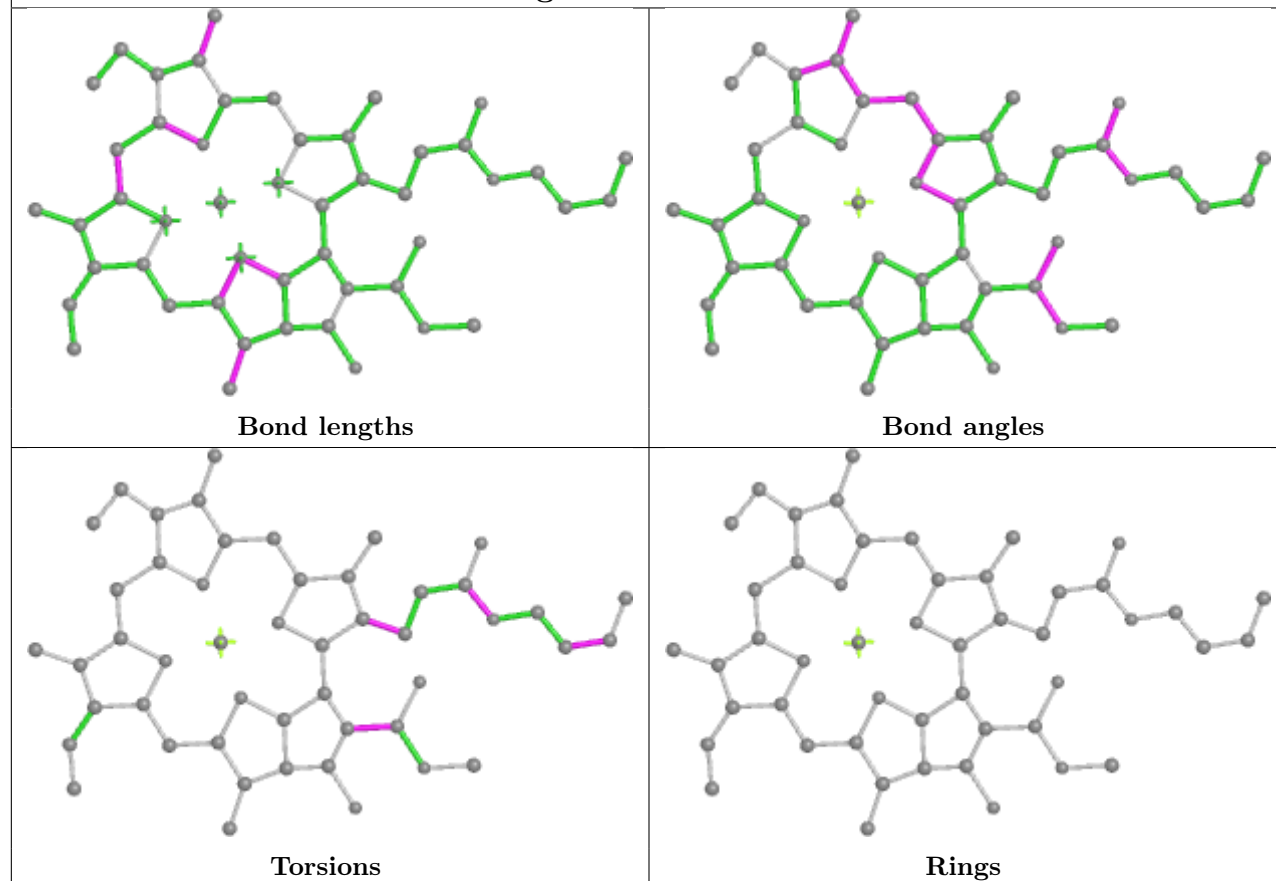
## Ligand CLA 1 314



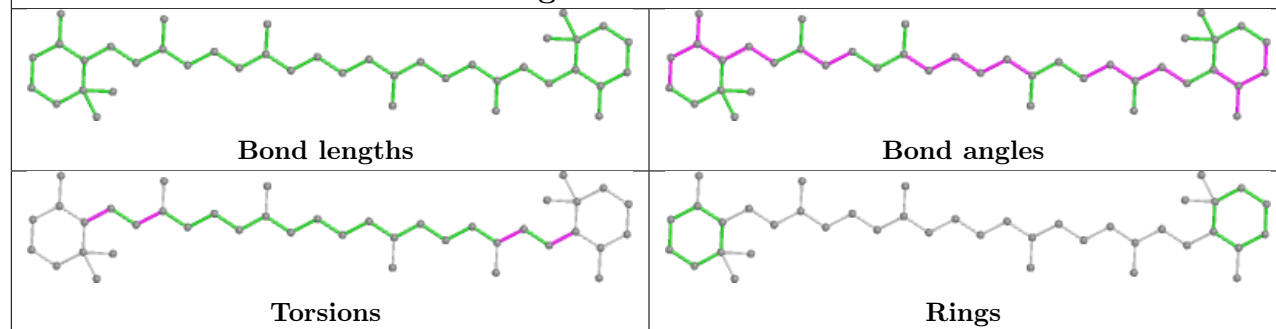


**Ligand CLA a 835****Ligand CLA a 819**

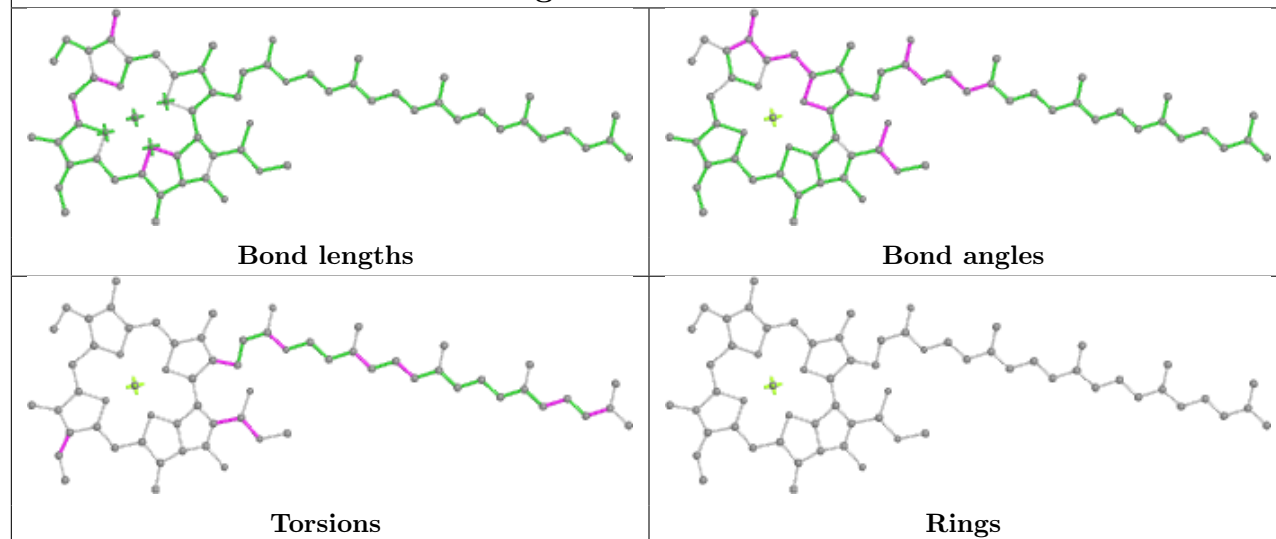
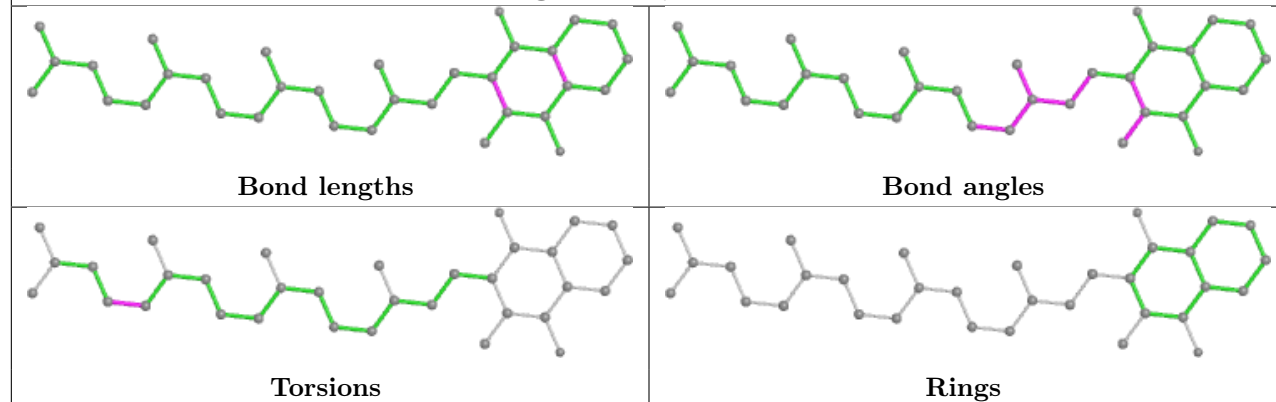
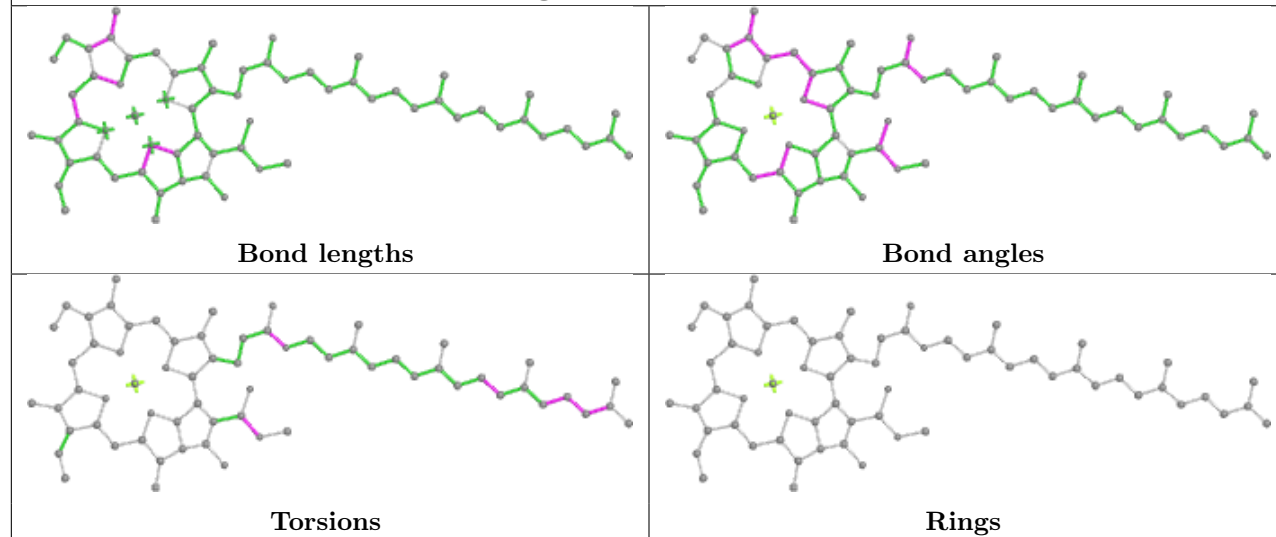
## Ligand CLA a 823



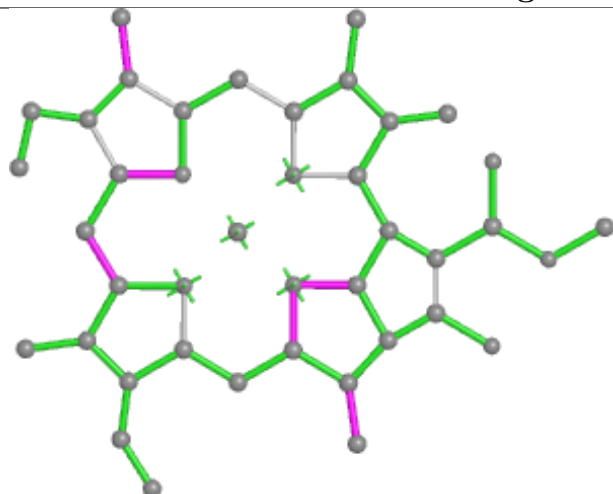
## Ligand BCR 1 205



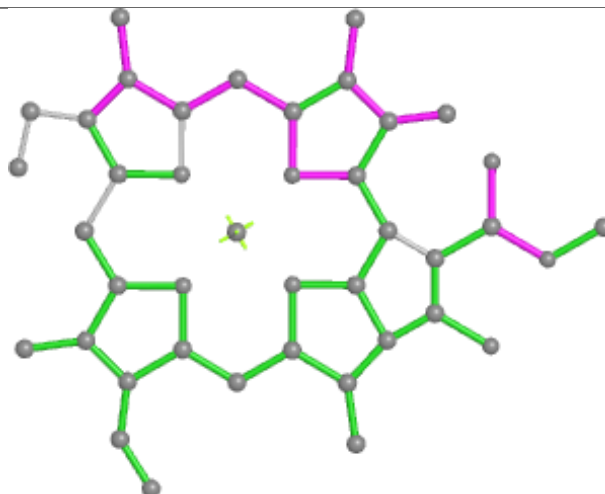


**Ligand CLA b 839****Ligand PQN b 841****Ligand CLA b 840**

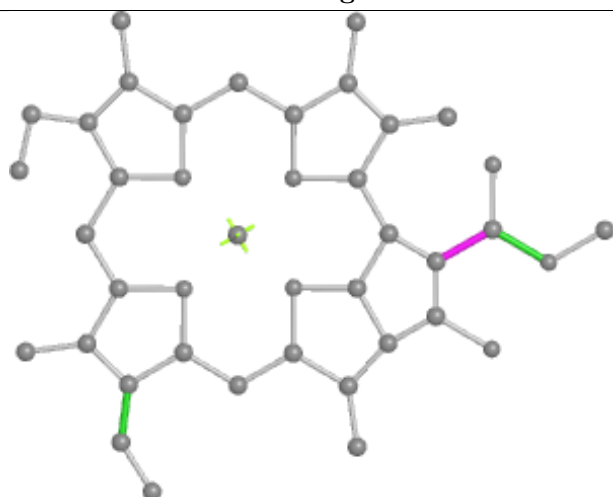
## Ligand CLA b 830



Bond lengths



Bond angles

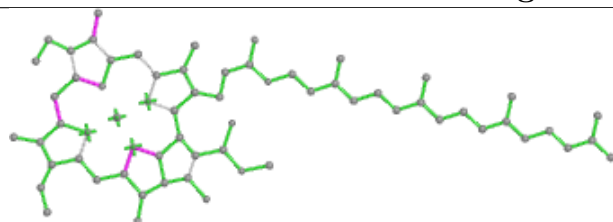


Torsions

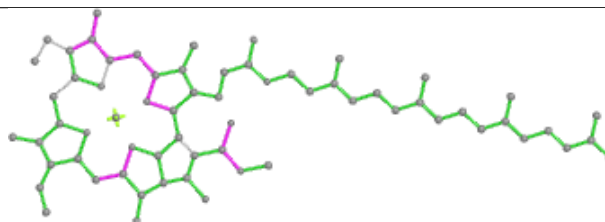


Rings

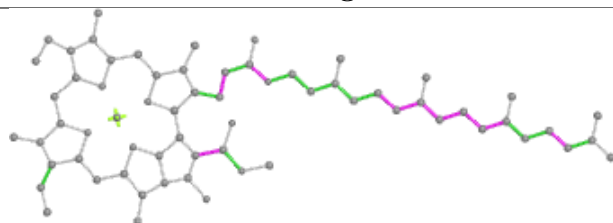
## Ligand CLA b 824



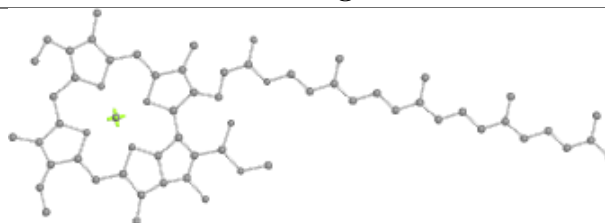
Bond lengths



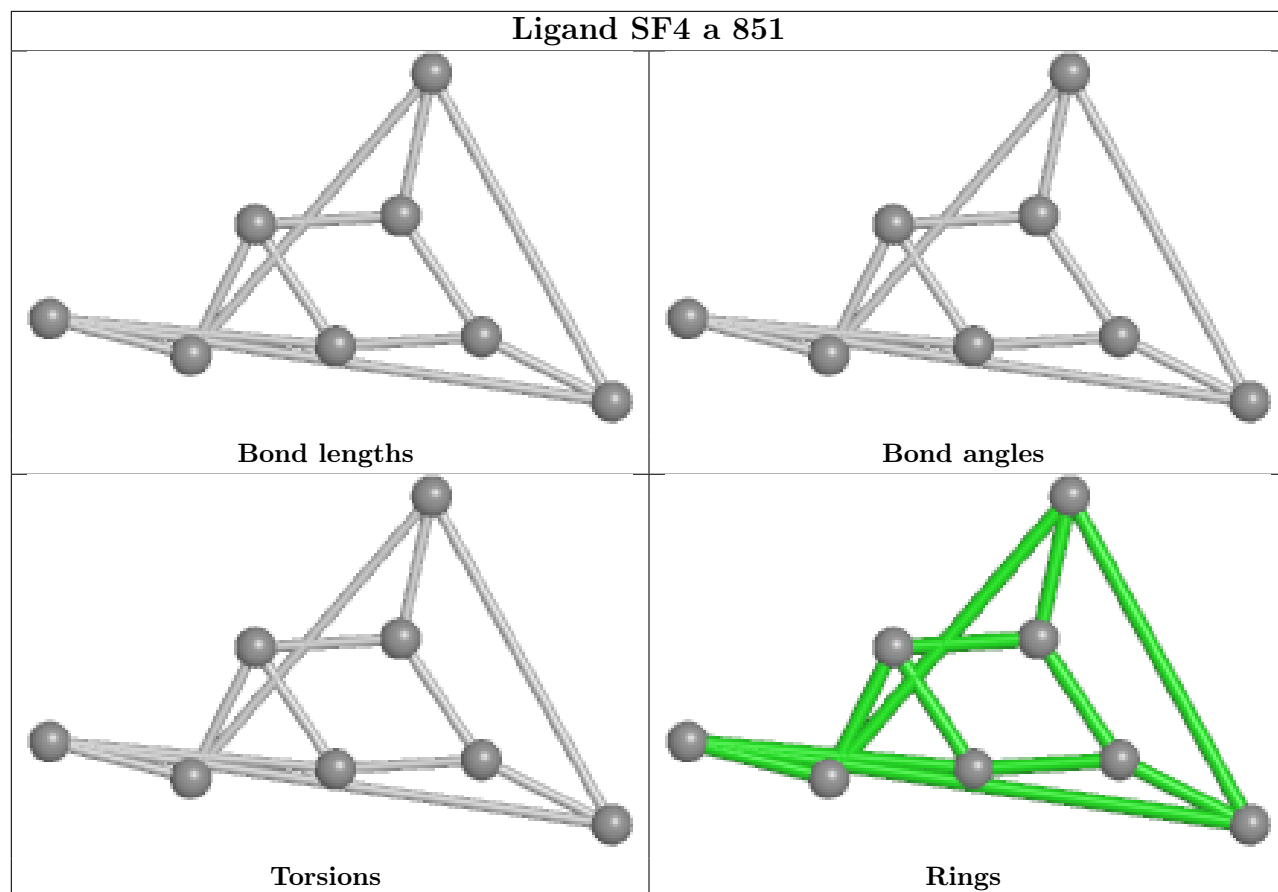
Bond angles



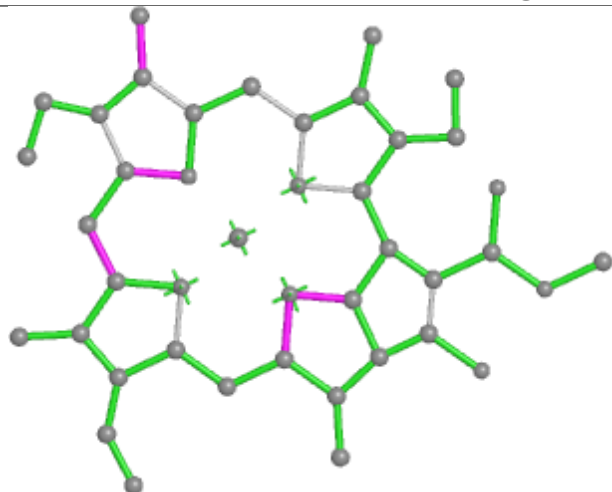
Torsions



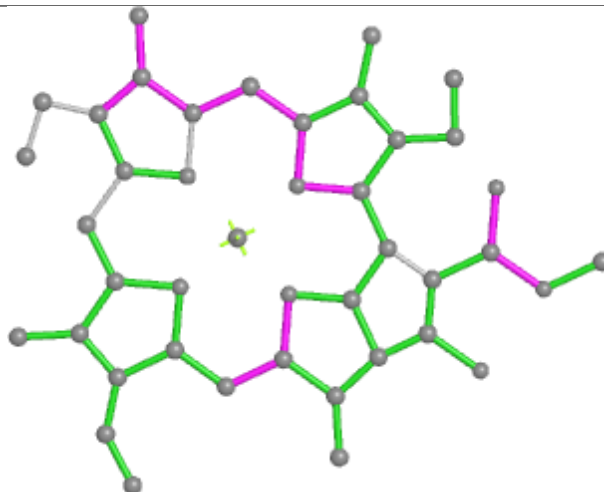
Rings



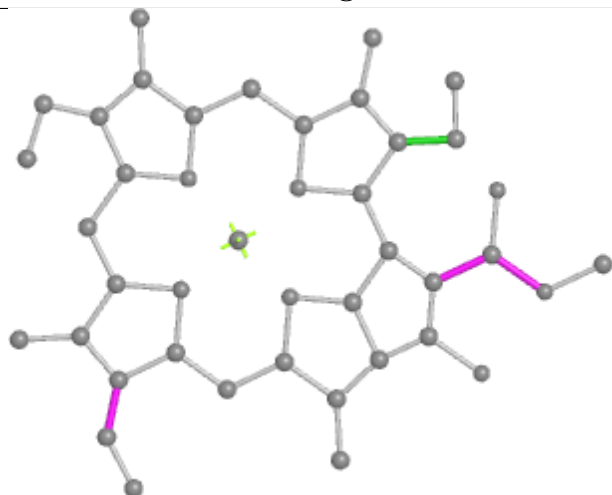
## Ligand CLA 9 315



Bond lengths



Bond angles

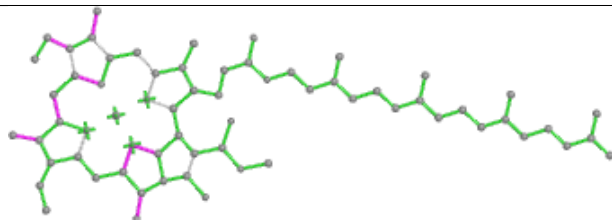


Torsions

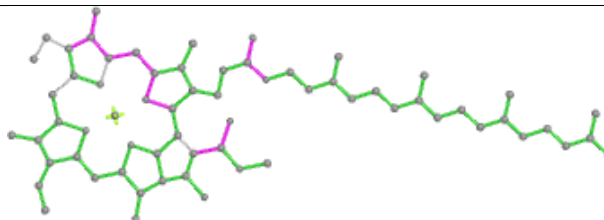


Rings

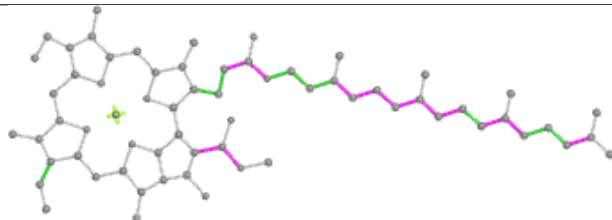
## Ligand CLA a 801



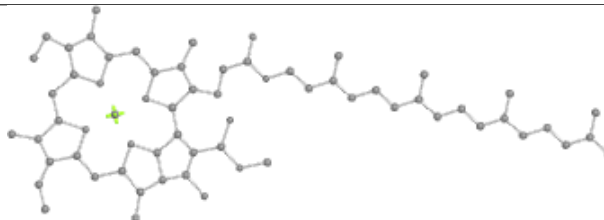
Bond lengths



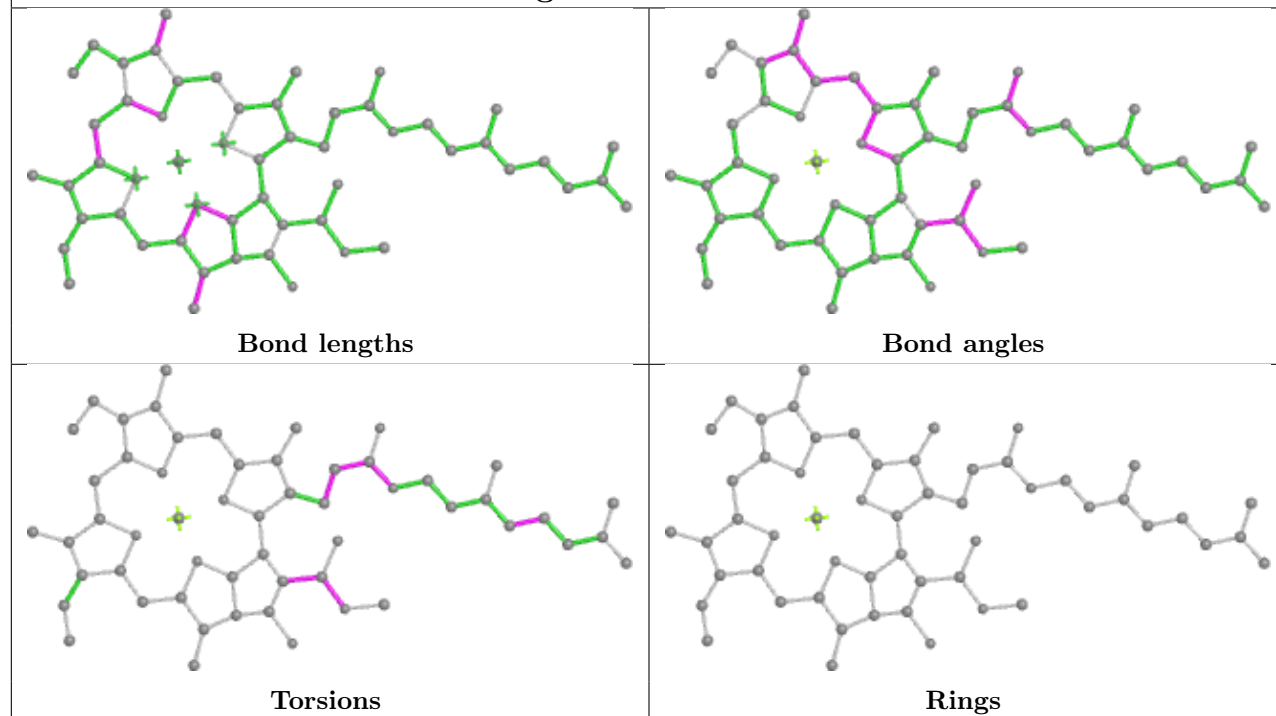
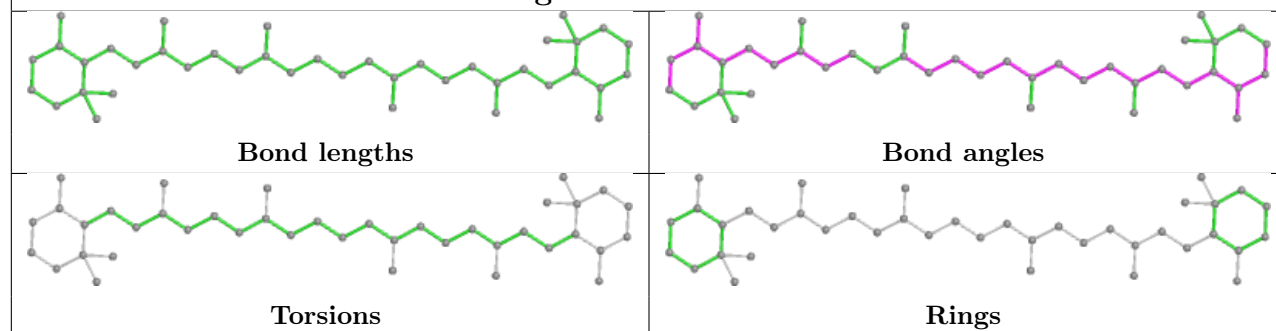
Bond angles



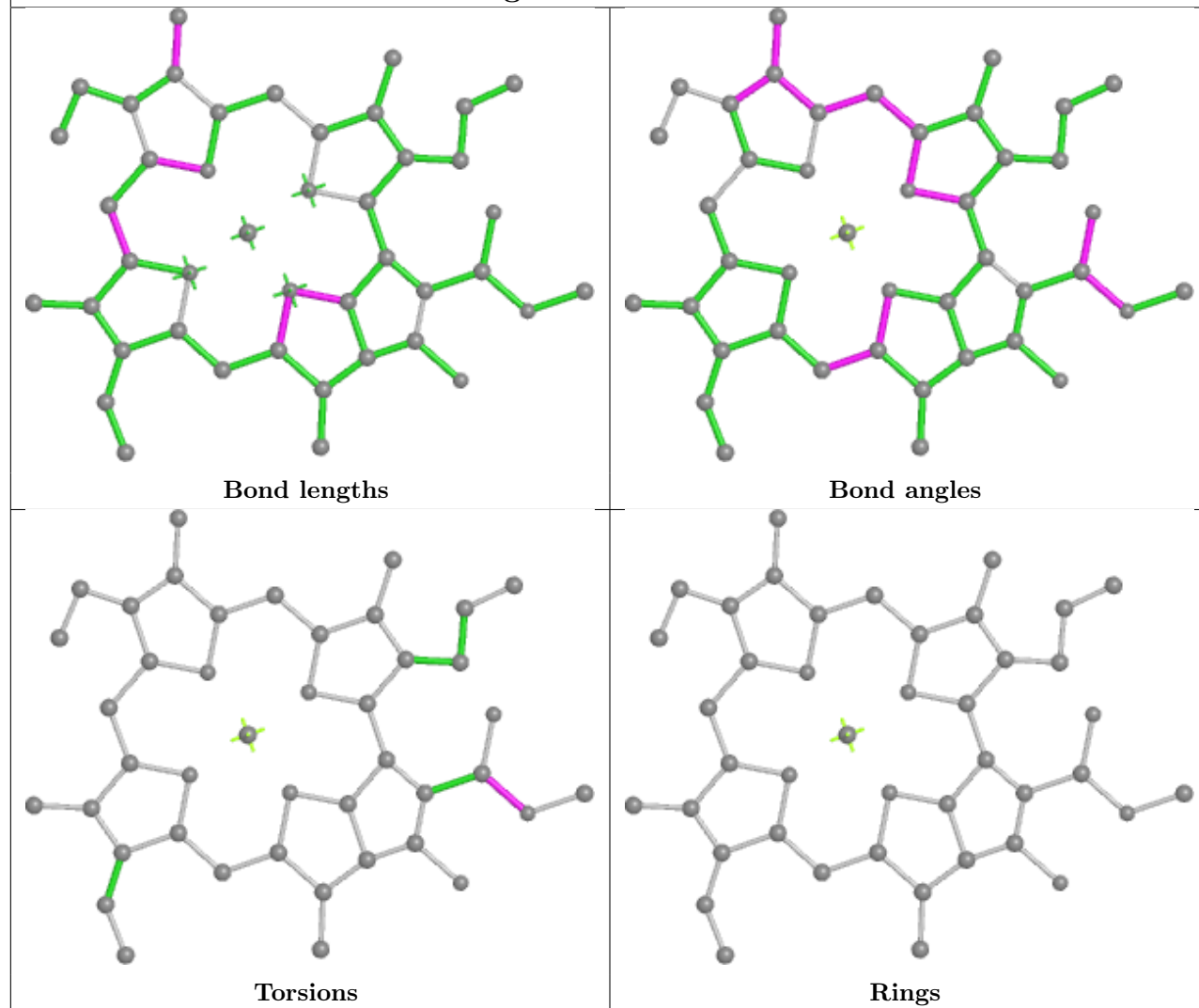
Torsions



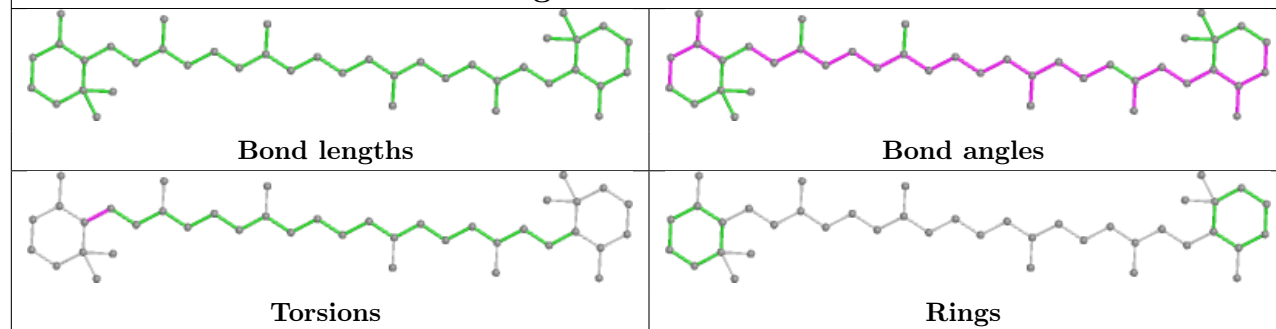
Rings

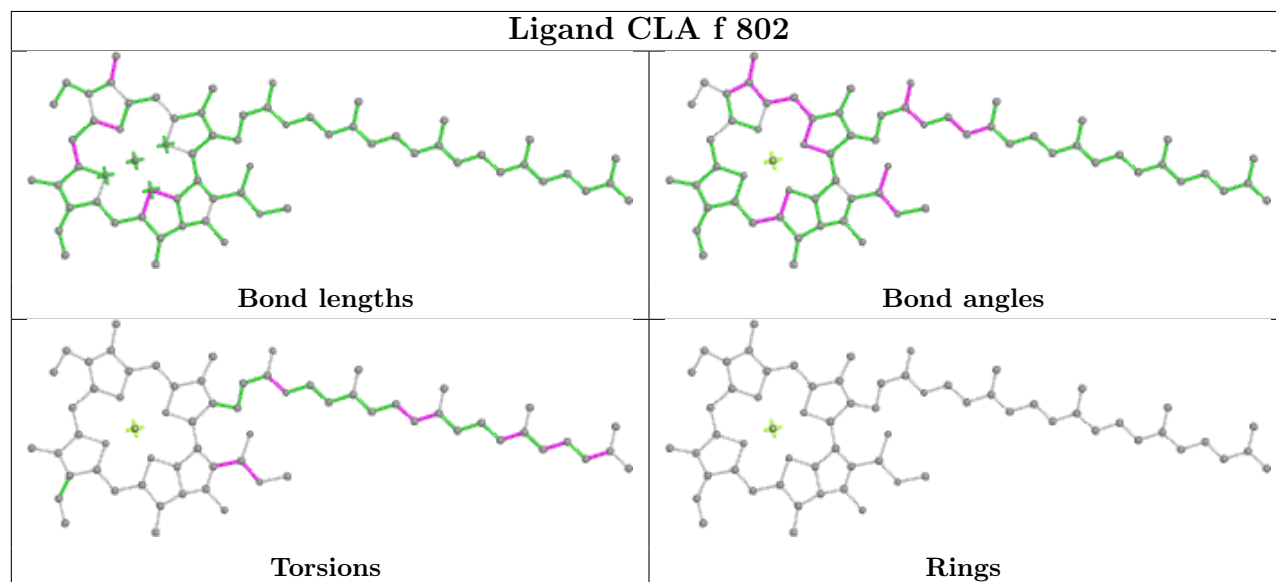
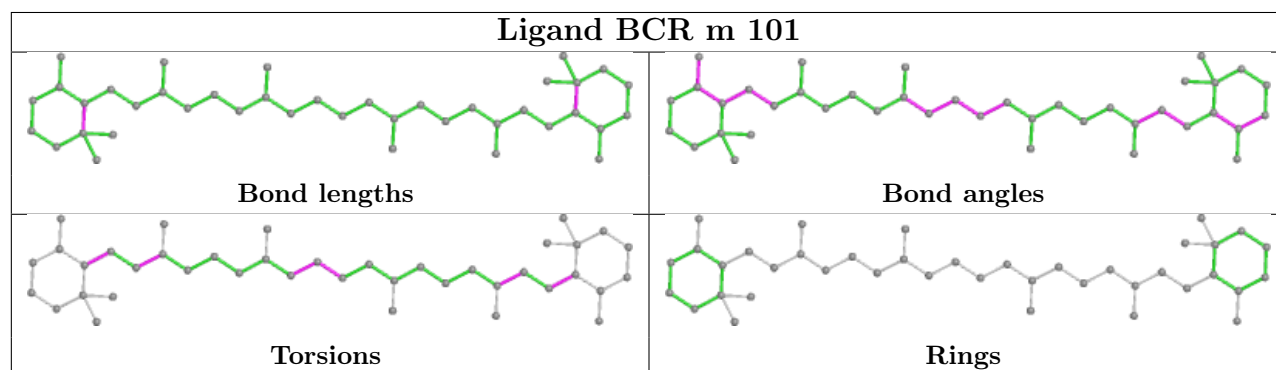
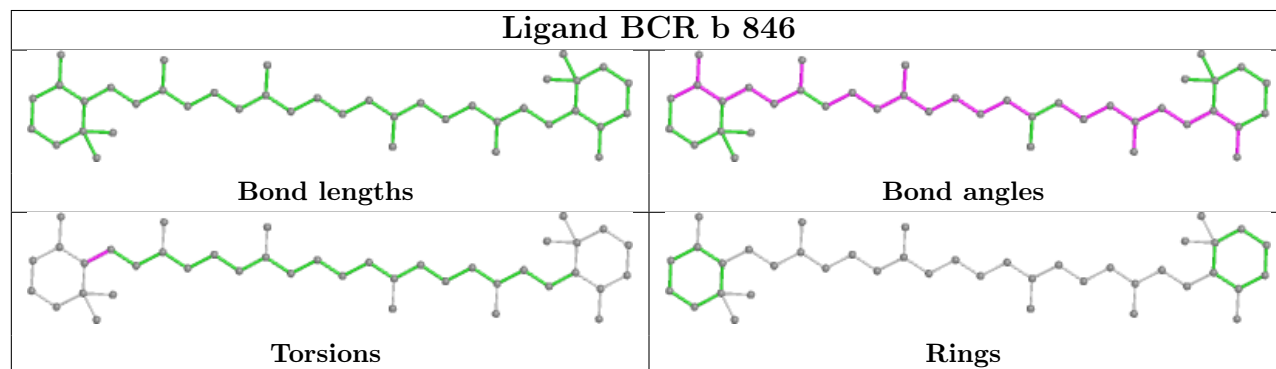
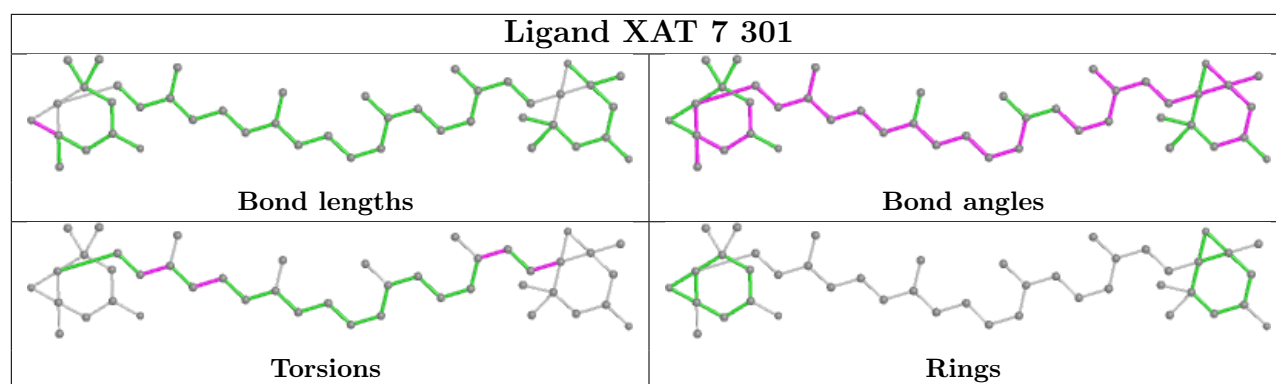
**Ligand CLA 9 314****Ligand BCR a 847**

## Ligand CLA 8 305

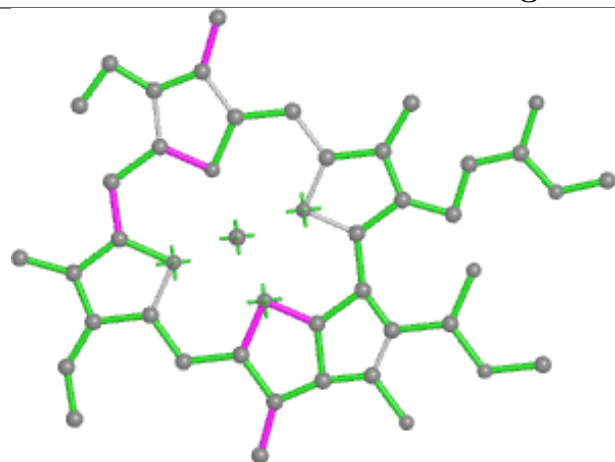


## Ligand BCR b 843

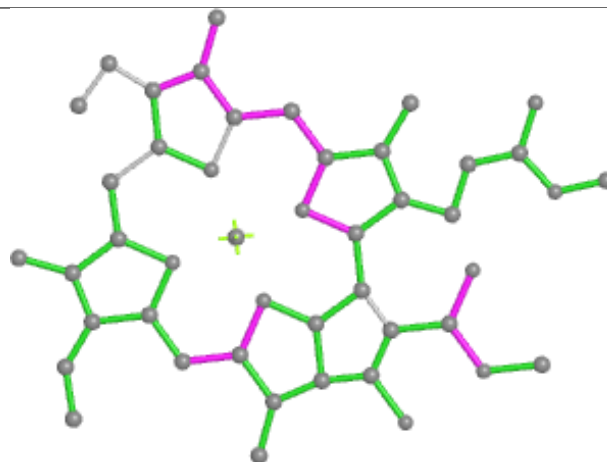




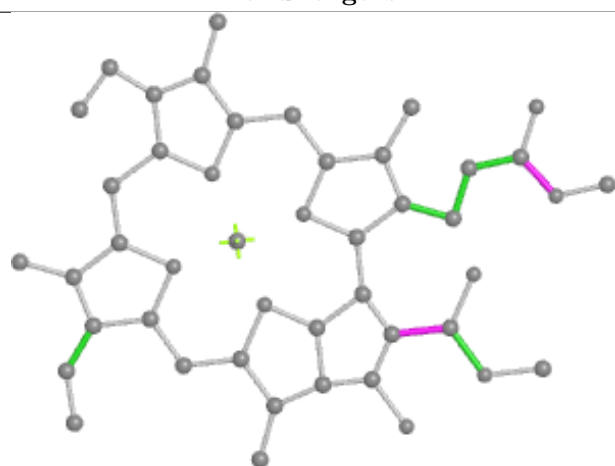
## Ligand CLA 9 309



Bond lengths



Bond angles



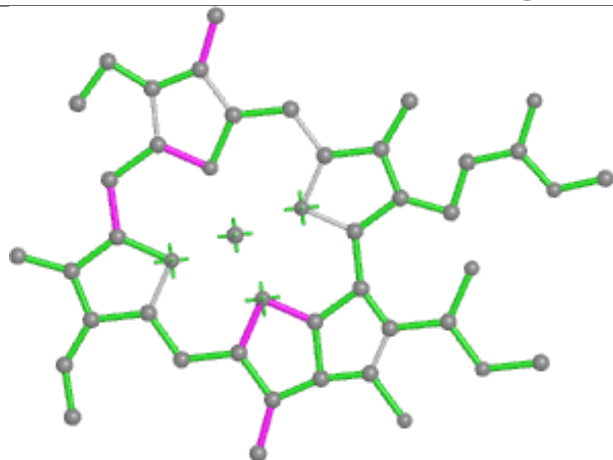
Torsions



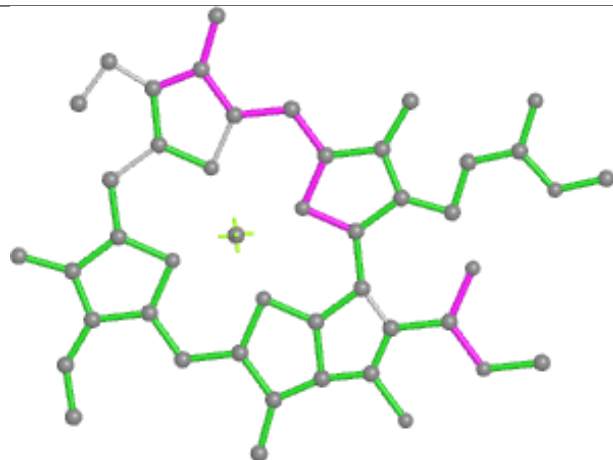
Rings



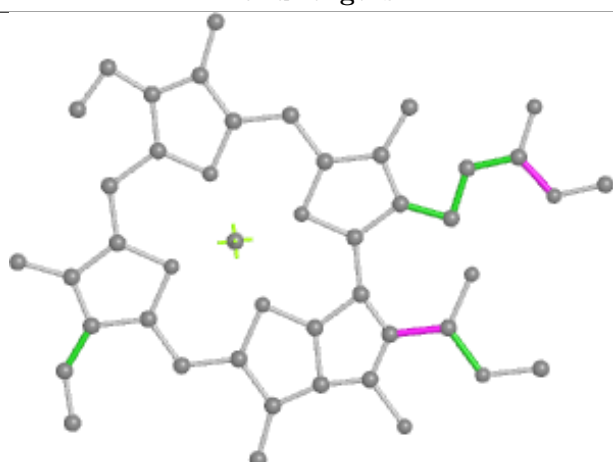
## Ligand CLA 8 313



Bond lengths



Bond angles

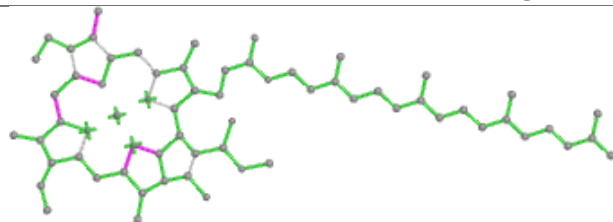


Torsions

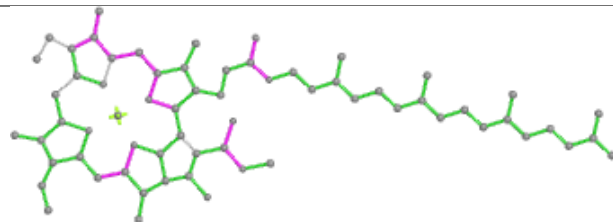


Rings

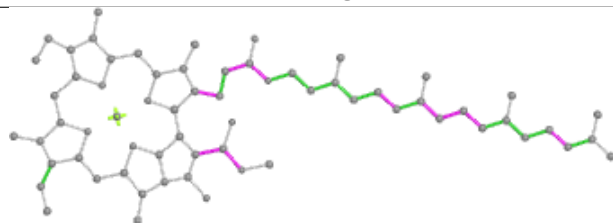
## Ligand CLA a 854



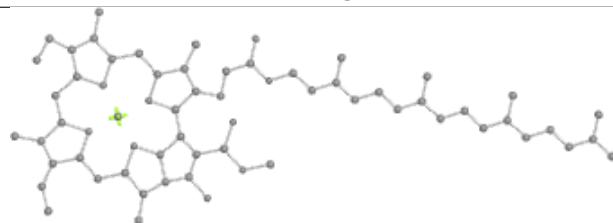
Bond lengths



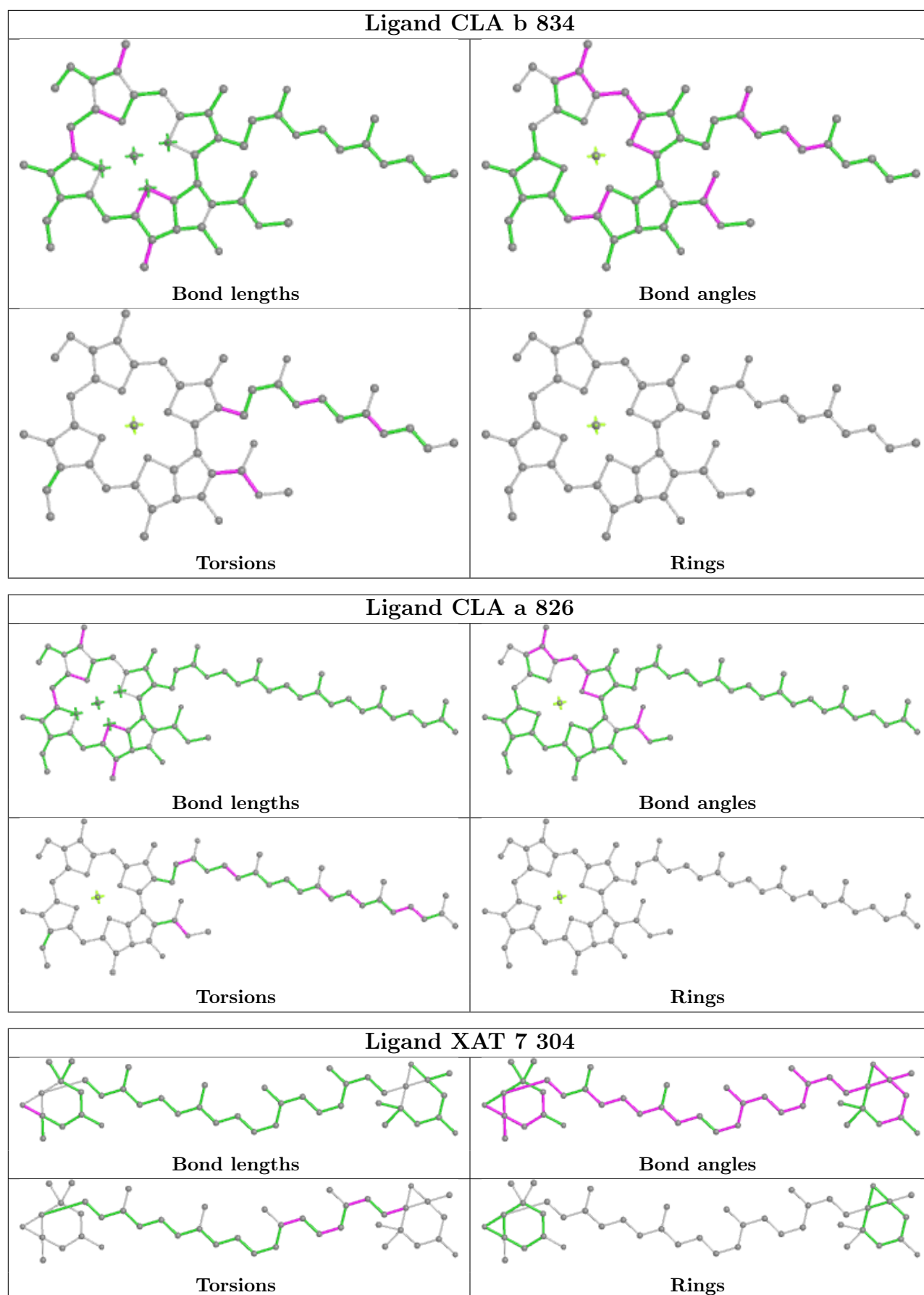
Bond angles

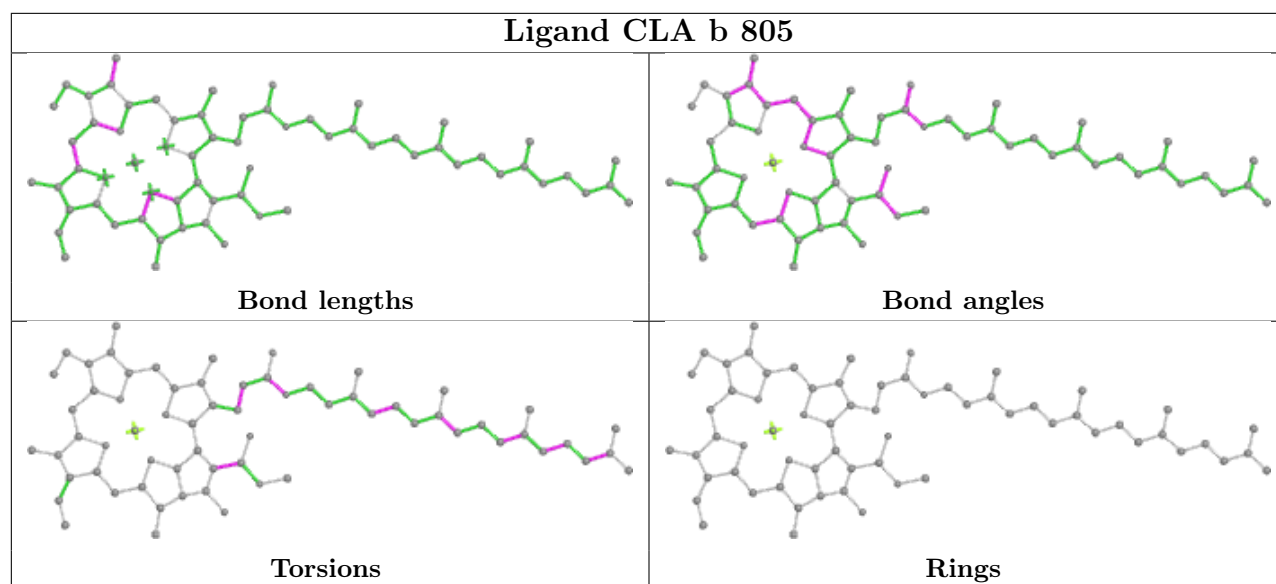
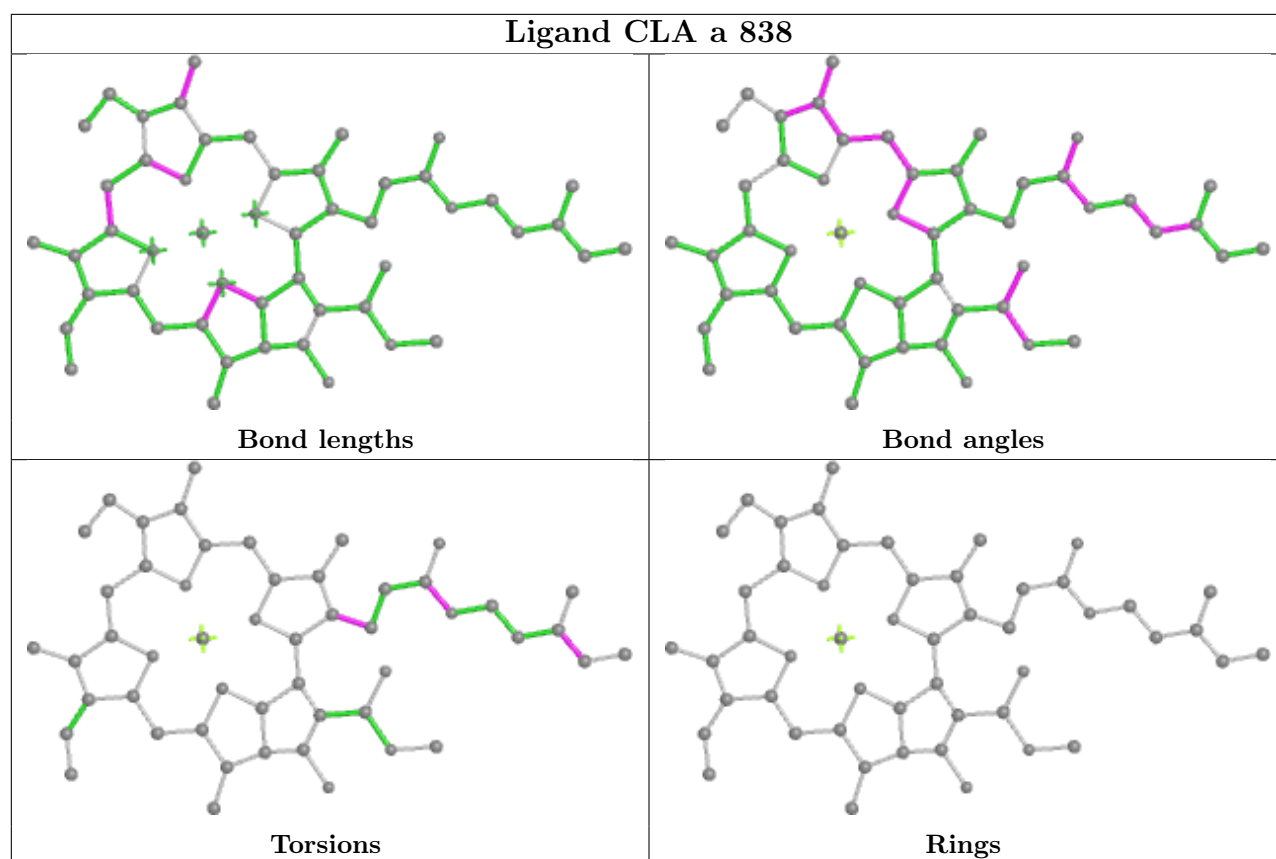


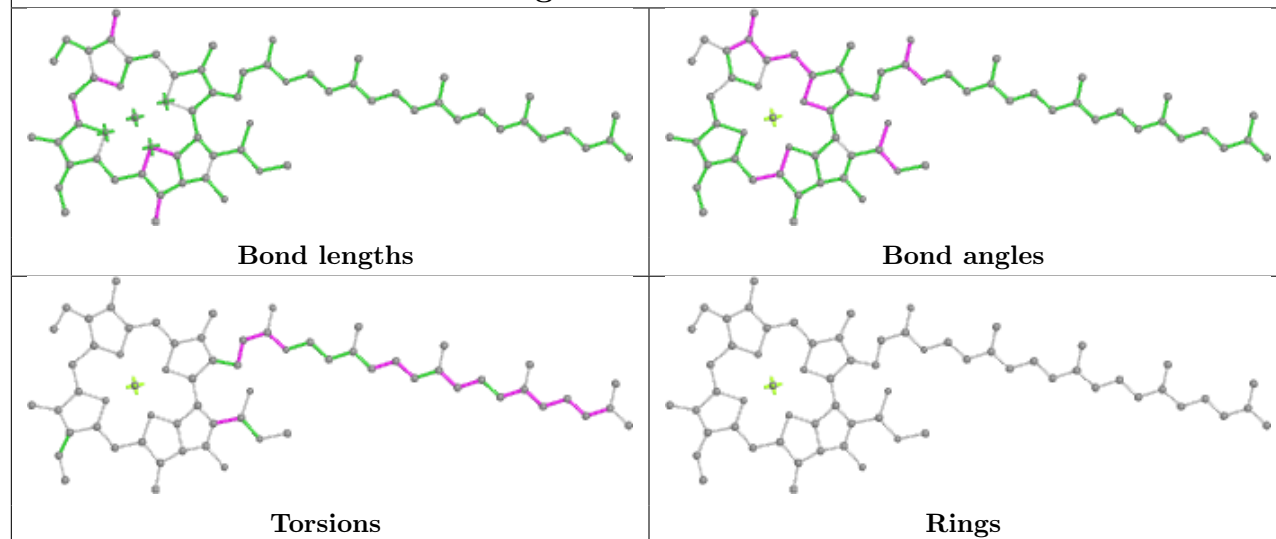
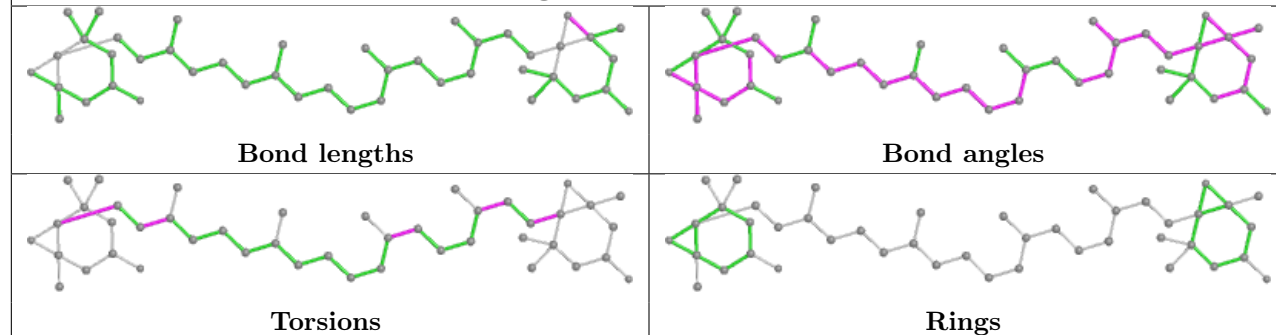
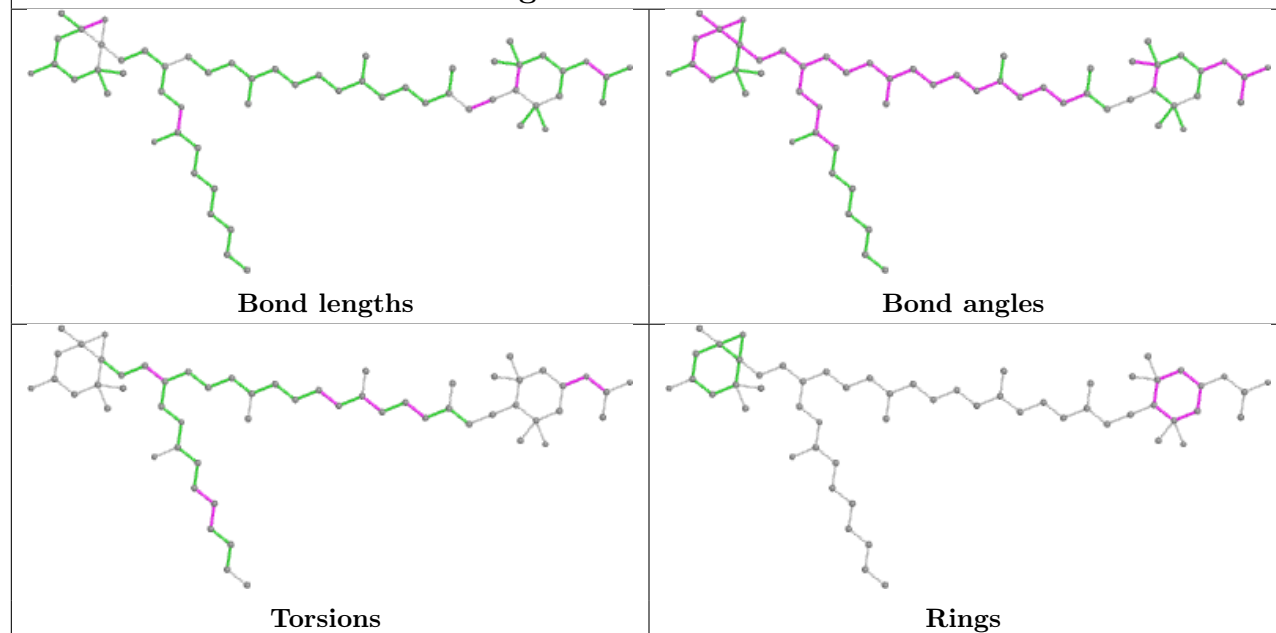
Torsions

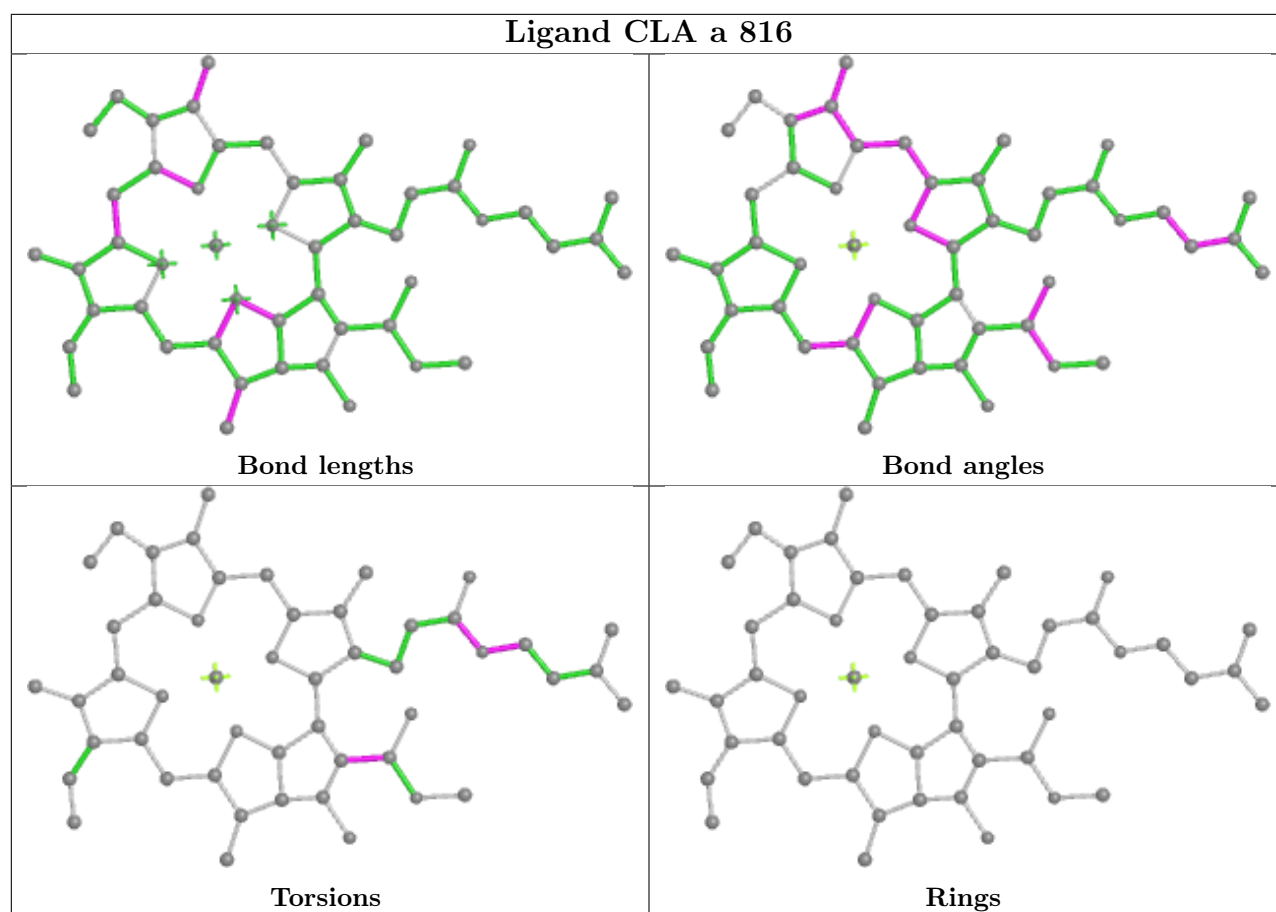


Rings

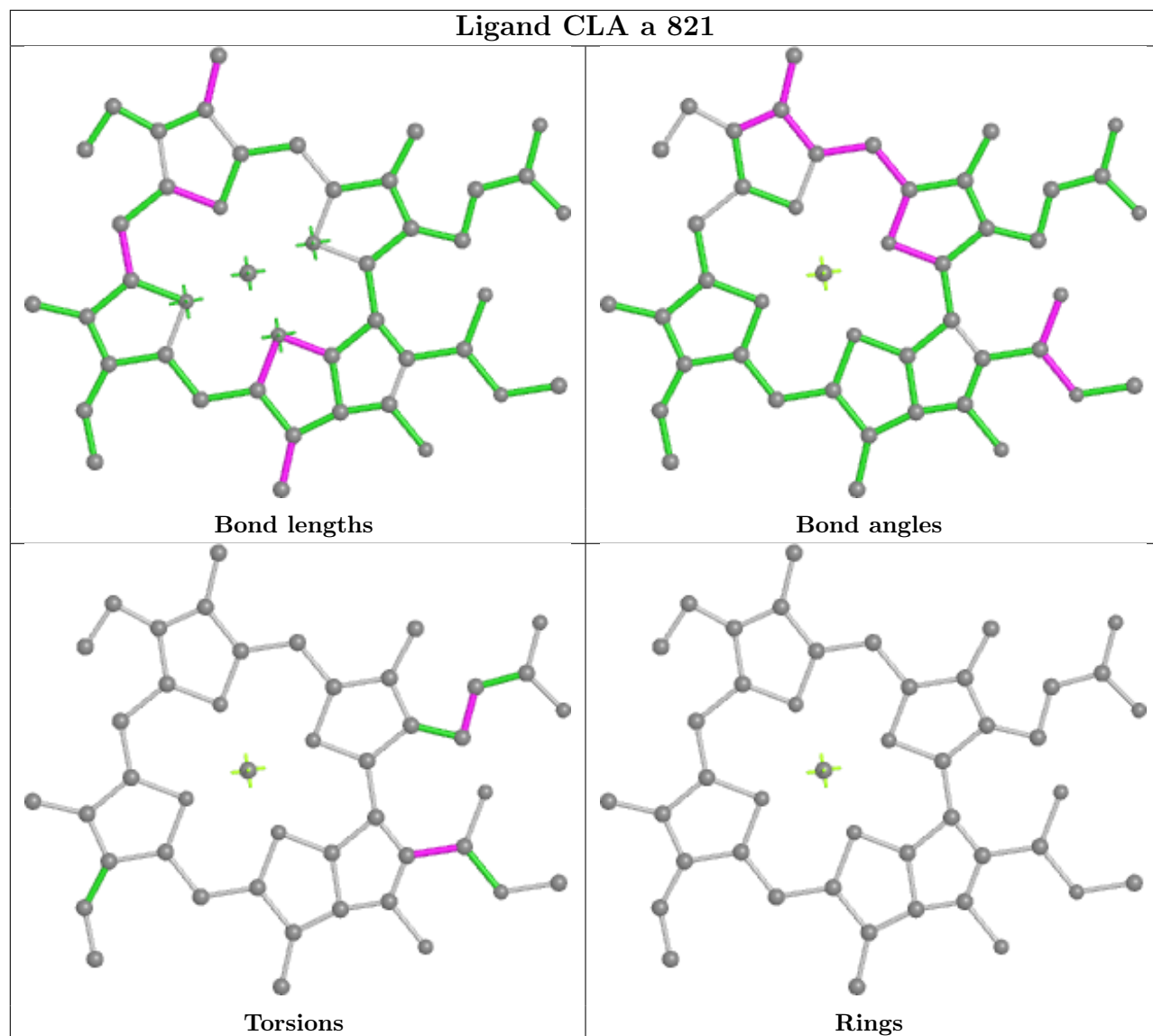




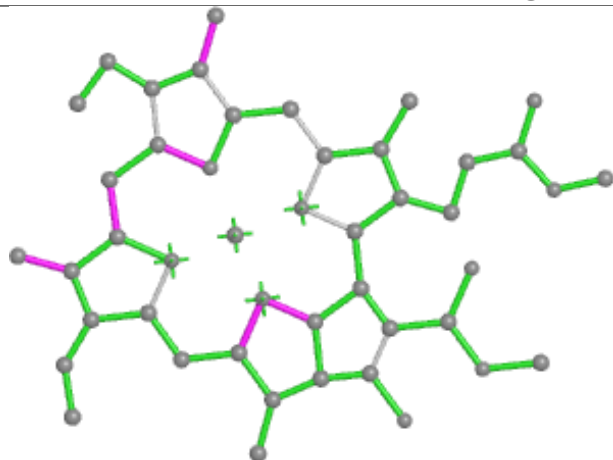
**Ligand CLA b 801****Ligand XAT 7 303****Ligand A1L1F h 204**



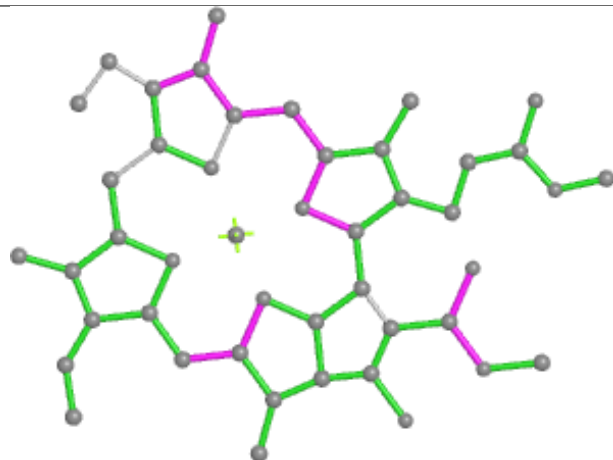
## Ligand CLA a 821



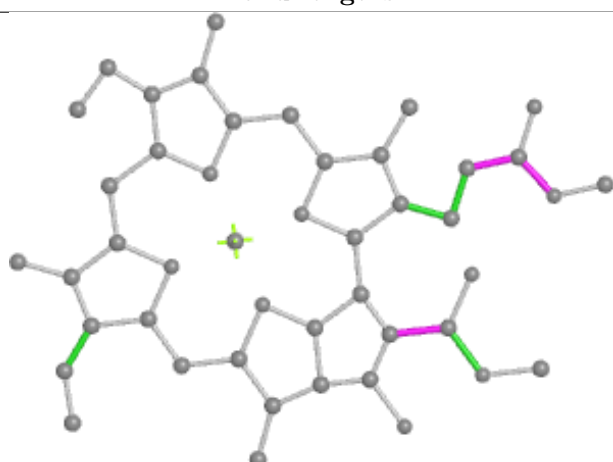
## Ligand CLA l 204



Bond lengths



Bond angles

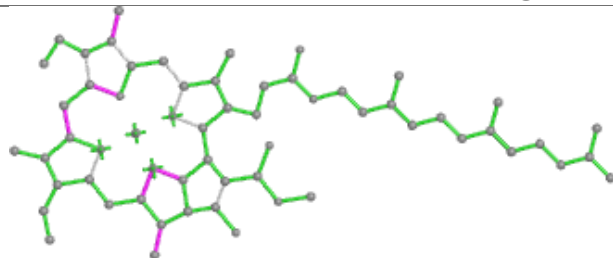


Torsions

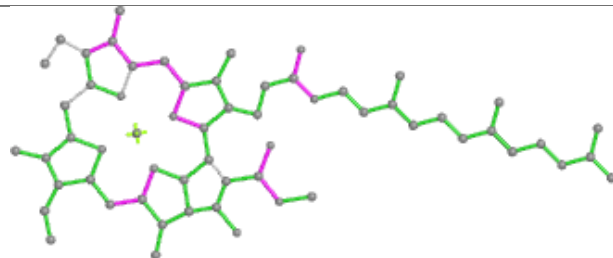


Rings

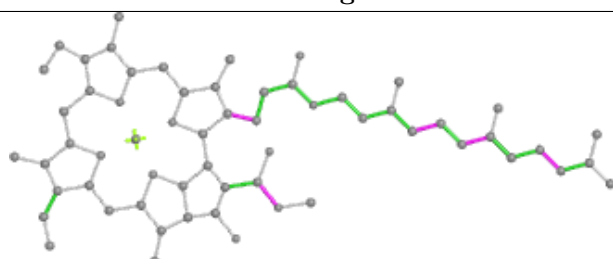
## Ligand CLA b 822



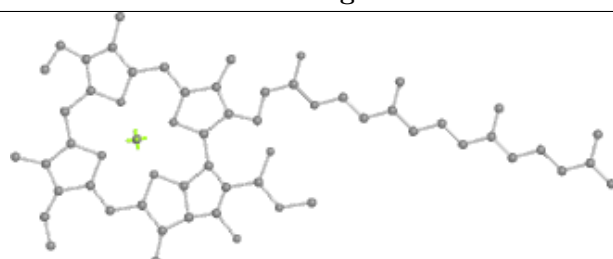
Bond lengths



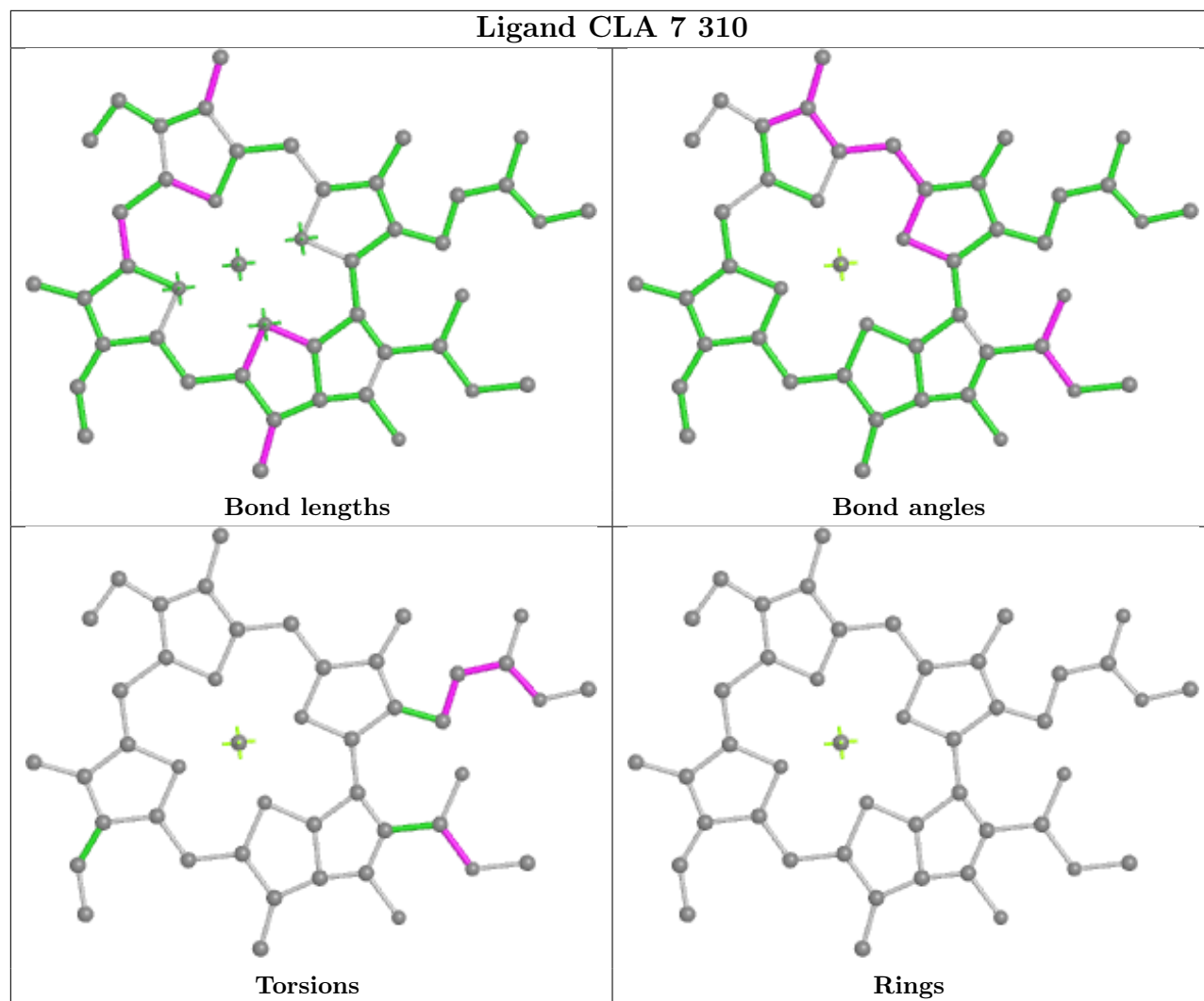
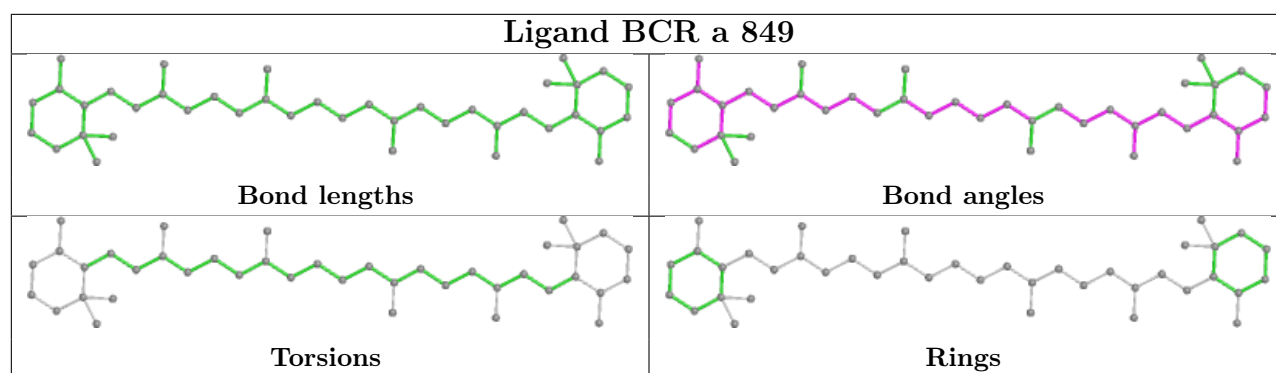
Bond angles



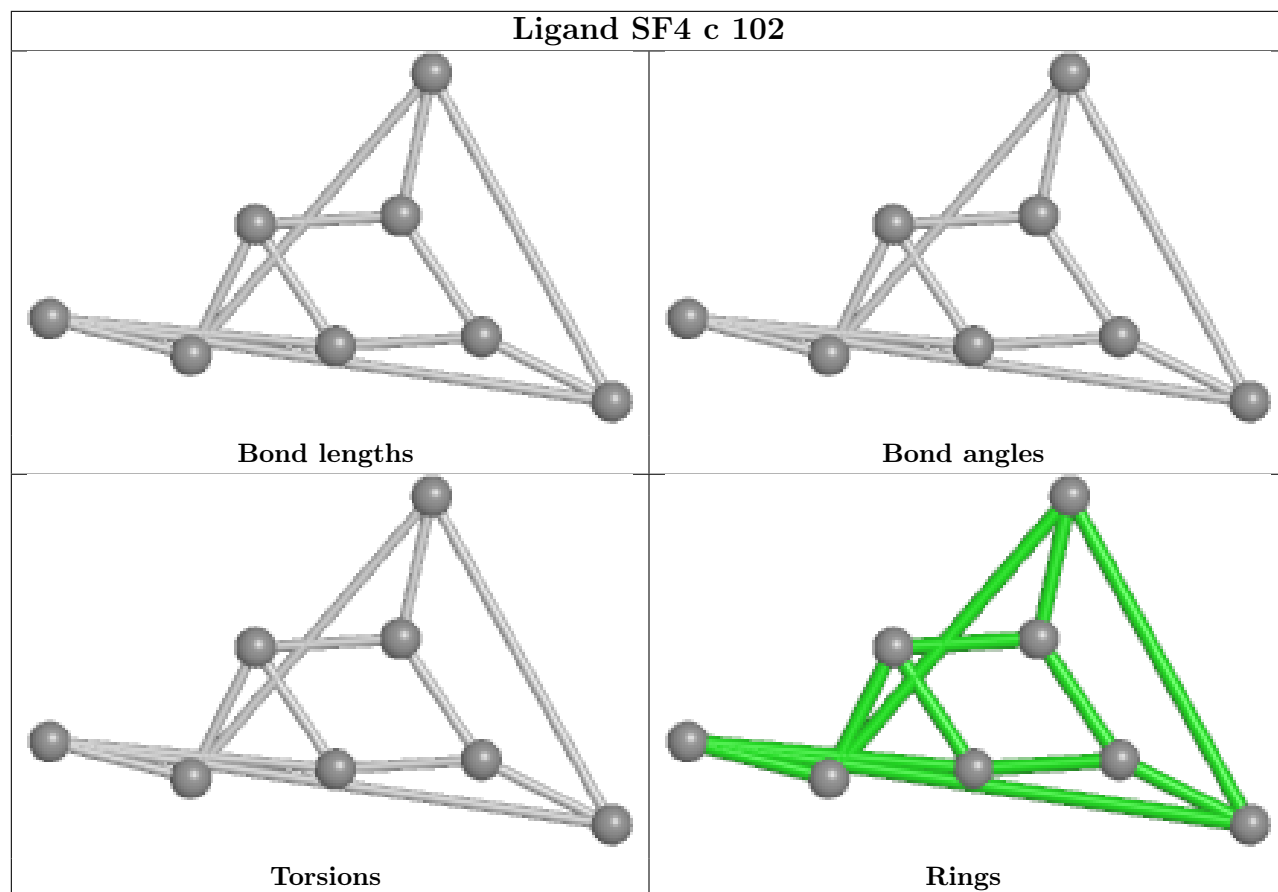
Torsions



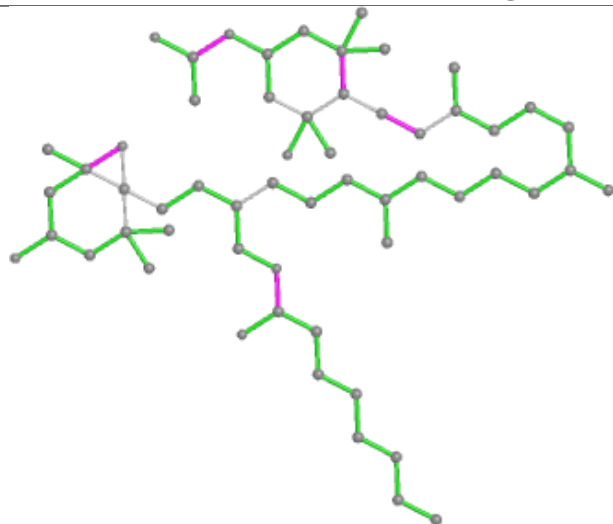
Rings



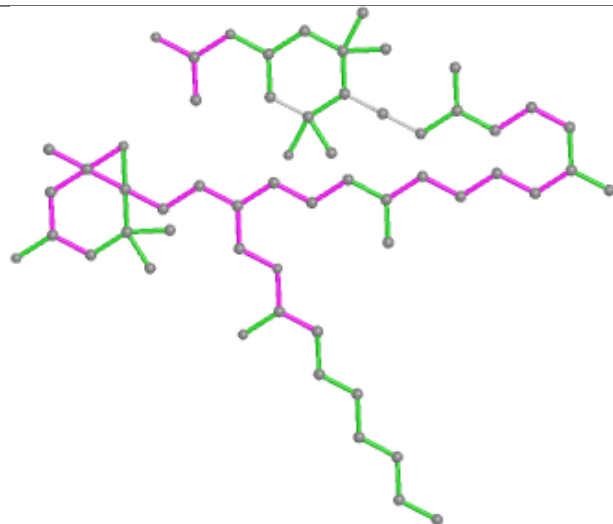




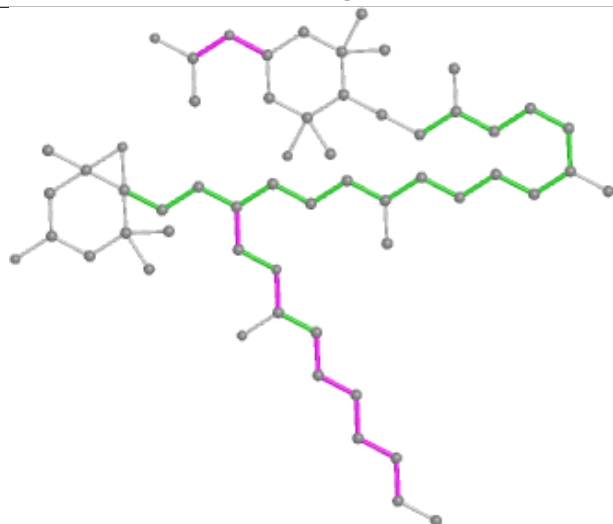
## Ligand A1L1F 9 302



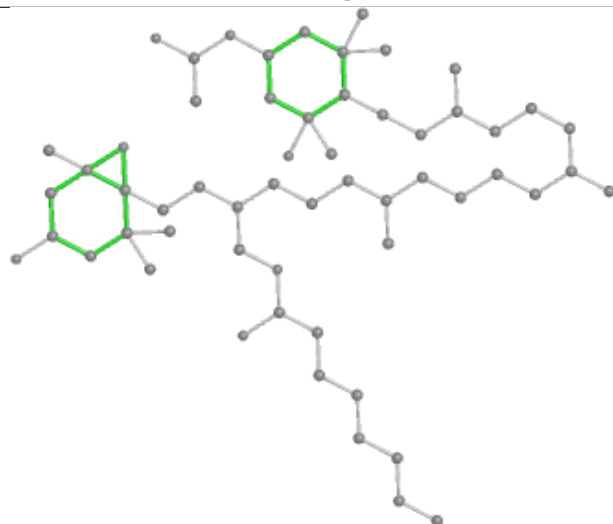
Bond lengths



Bond angles

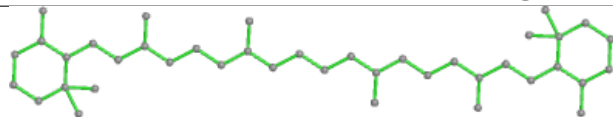


Torsions

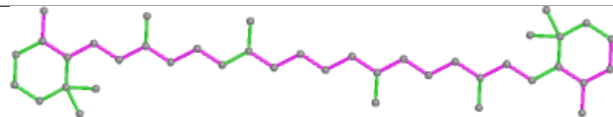


Rings

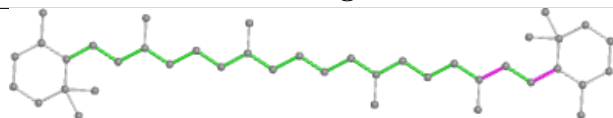
## Ligand BCR a 850



Bond lengths



Bond angles

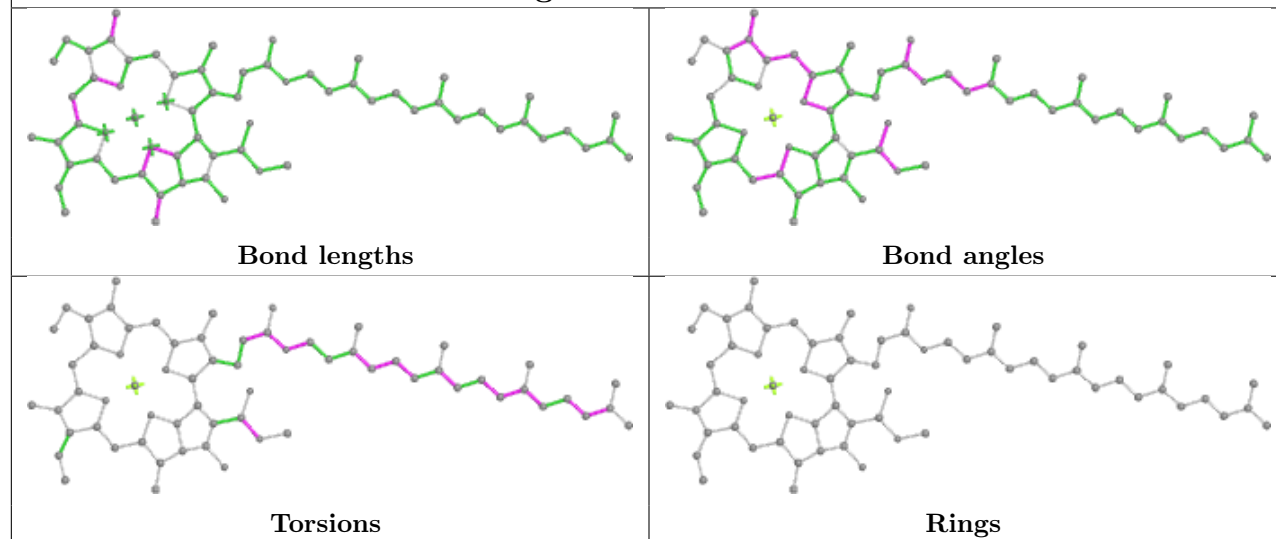


Torsions

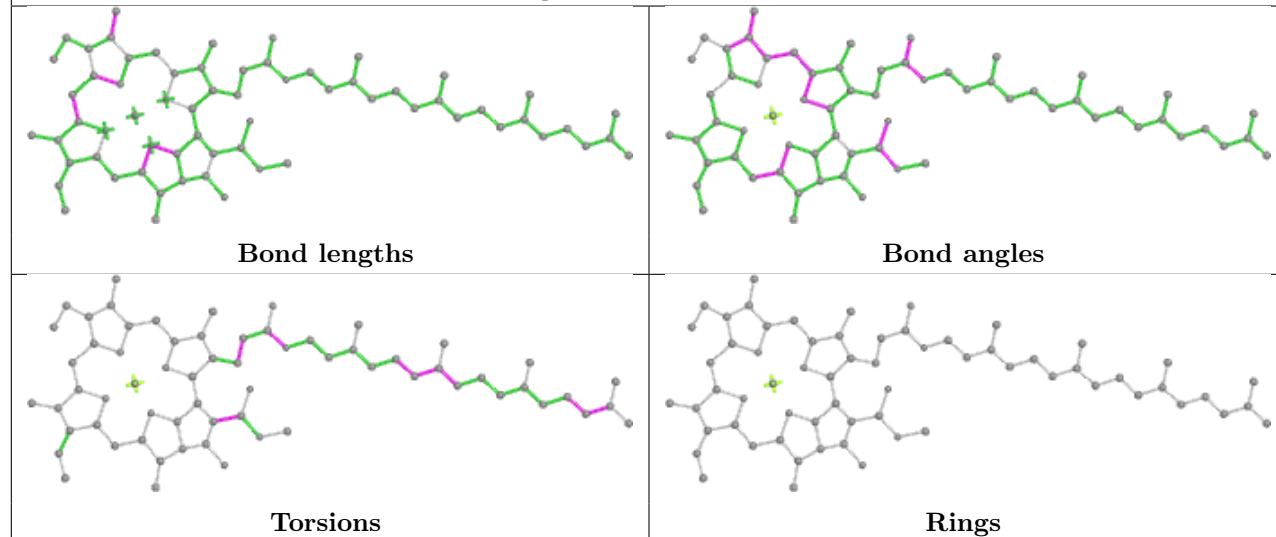


Rings

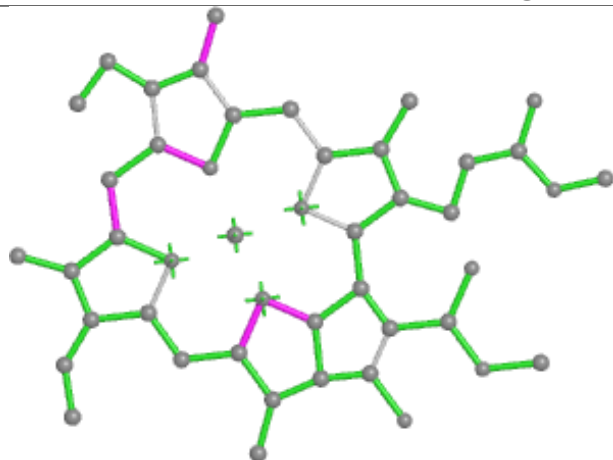
## Ligand CLA b 807



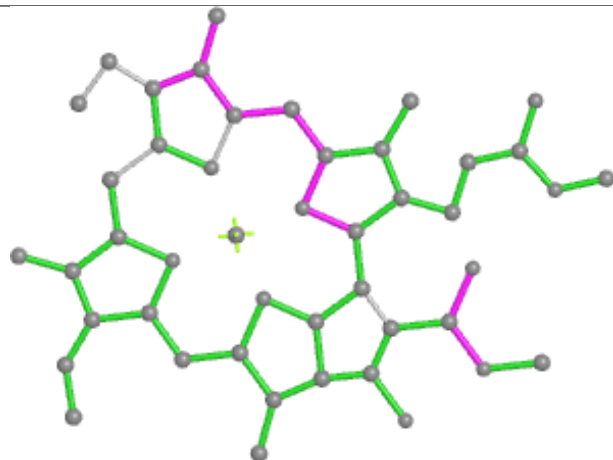
## Ligand CLA 8 307



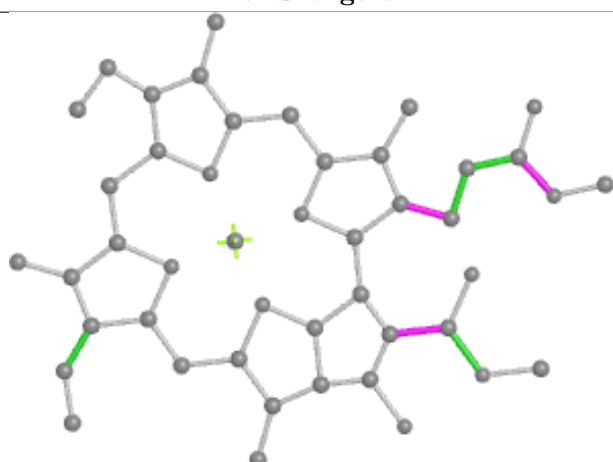
## Ligand CLA 9 310



Bond lengths



Bond angles

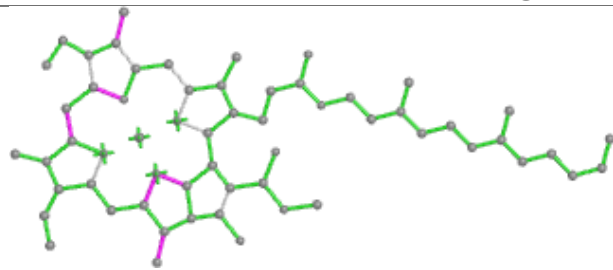


Torsions

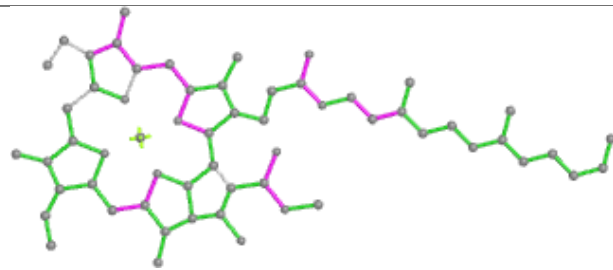


Rings

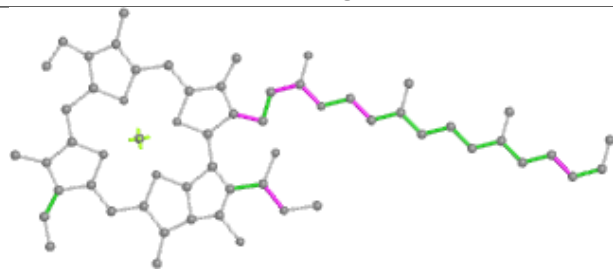
## Ligand CLA b 817



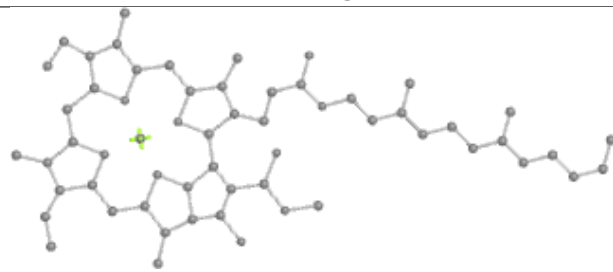
Bond lengths



Bond angles

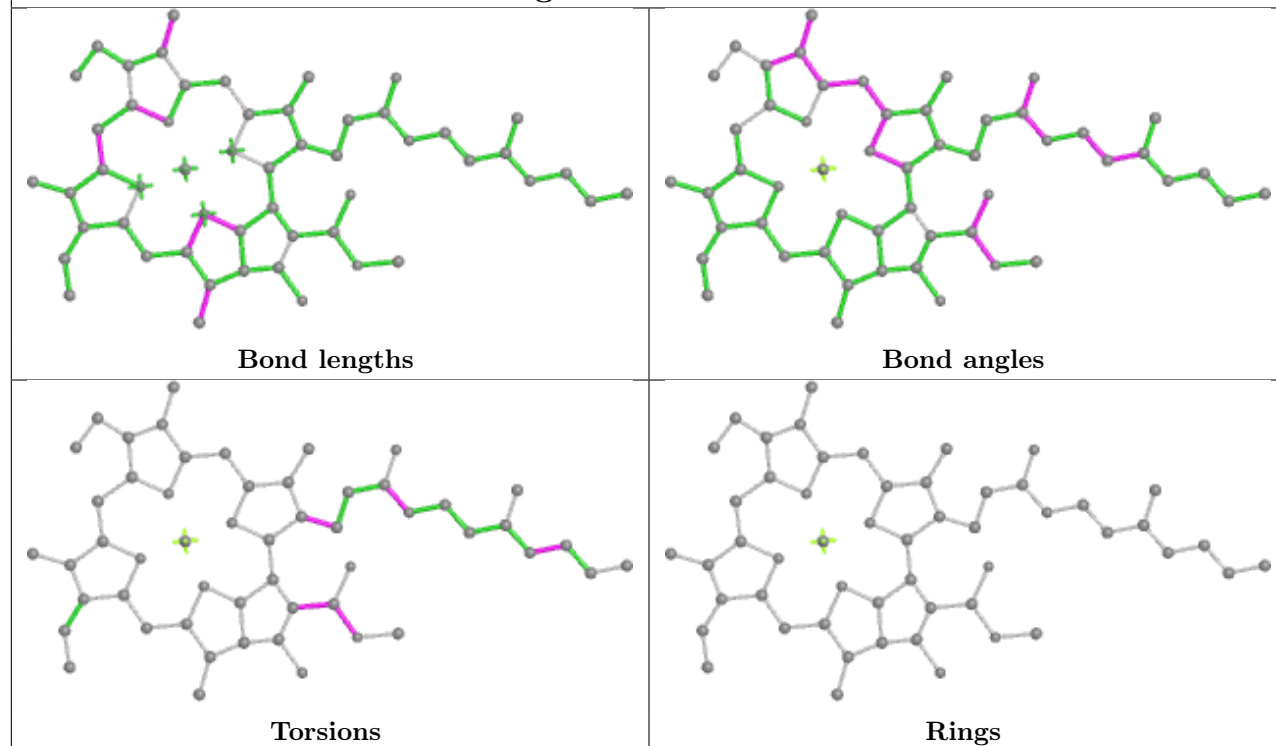


Torsions

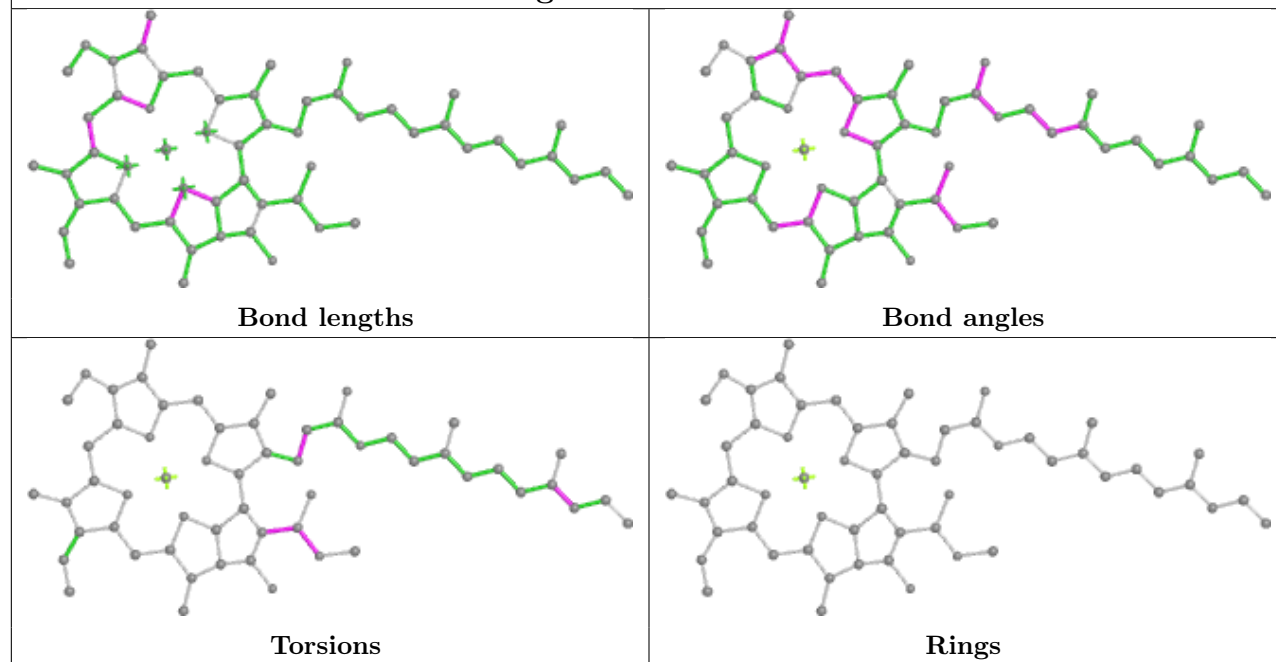


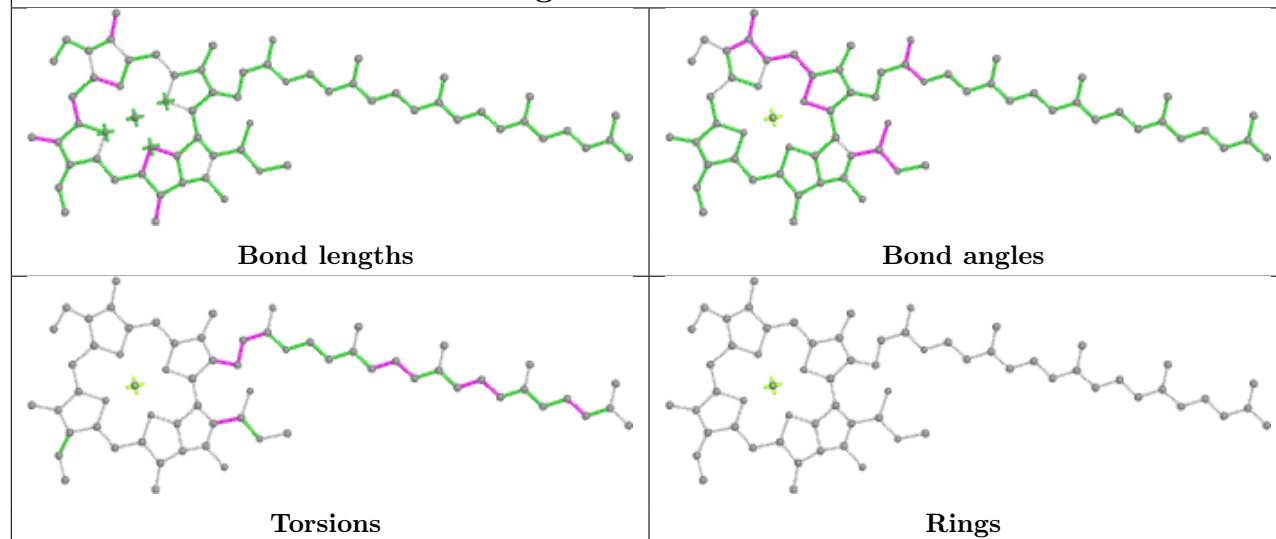
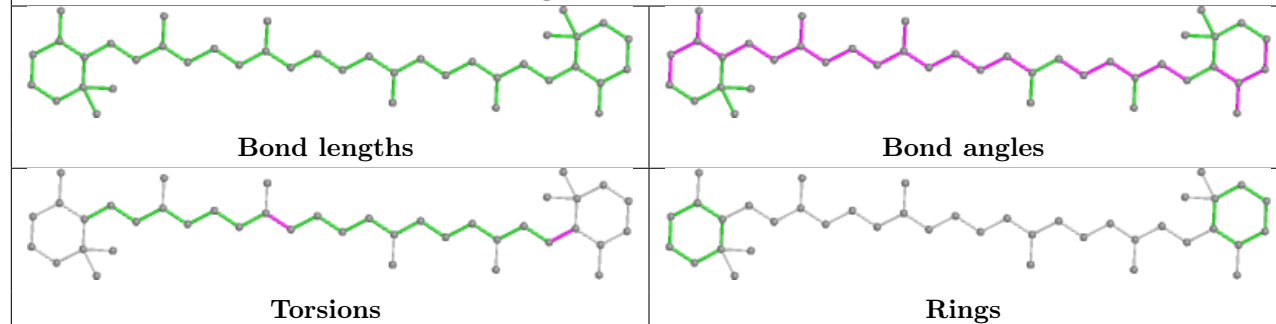
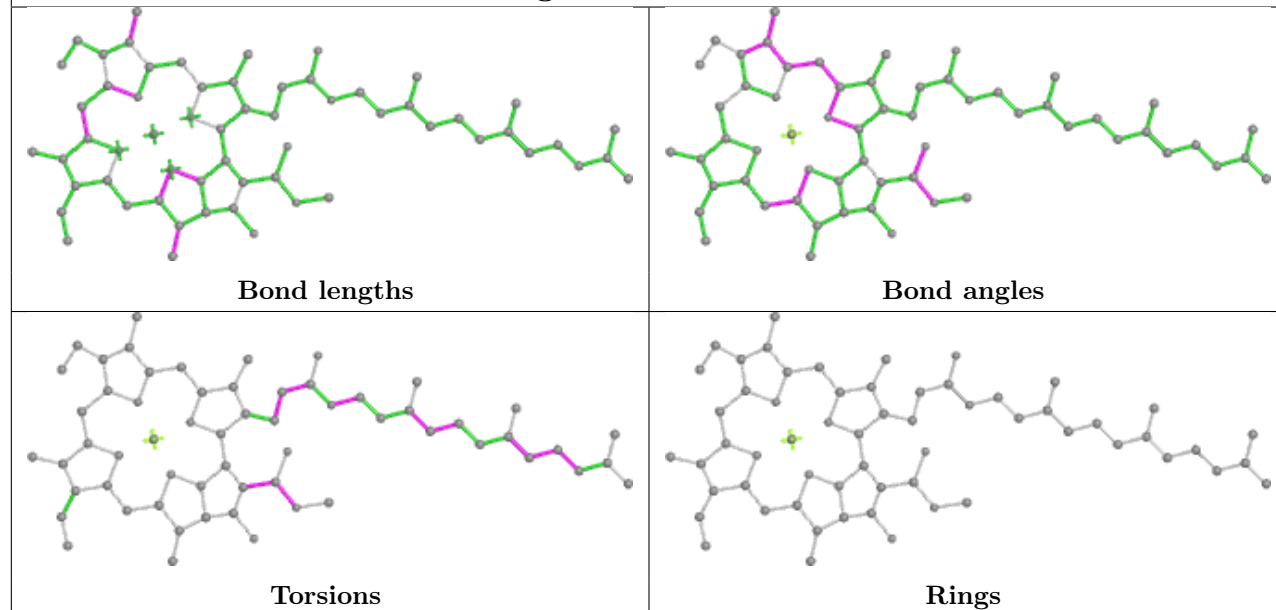
Rings

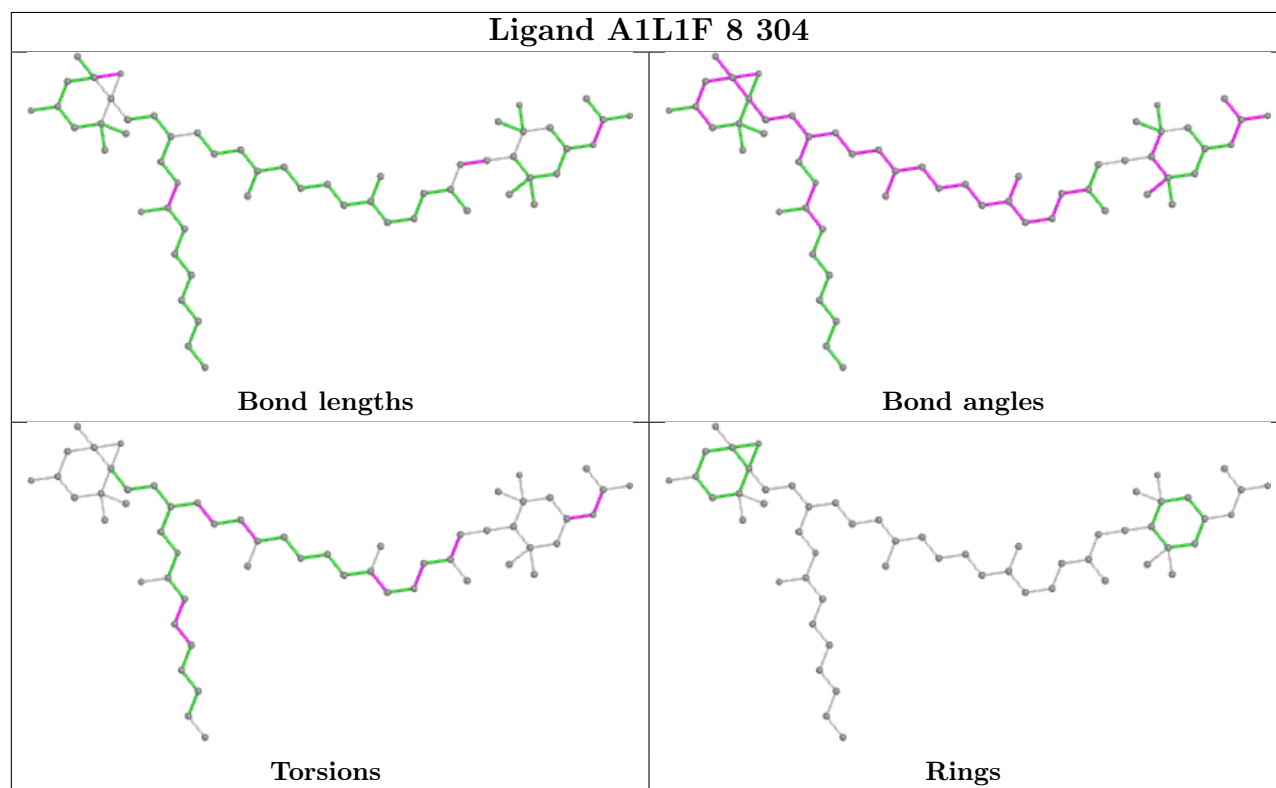
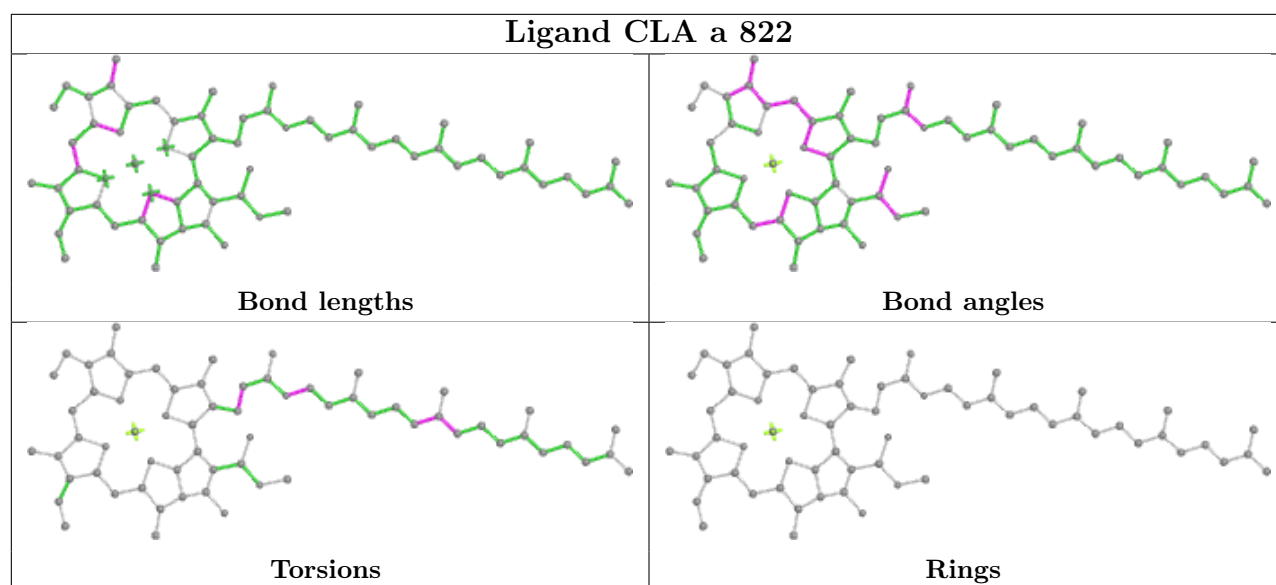
## Ligand CLA b 823

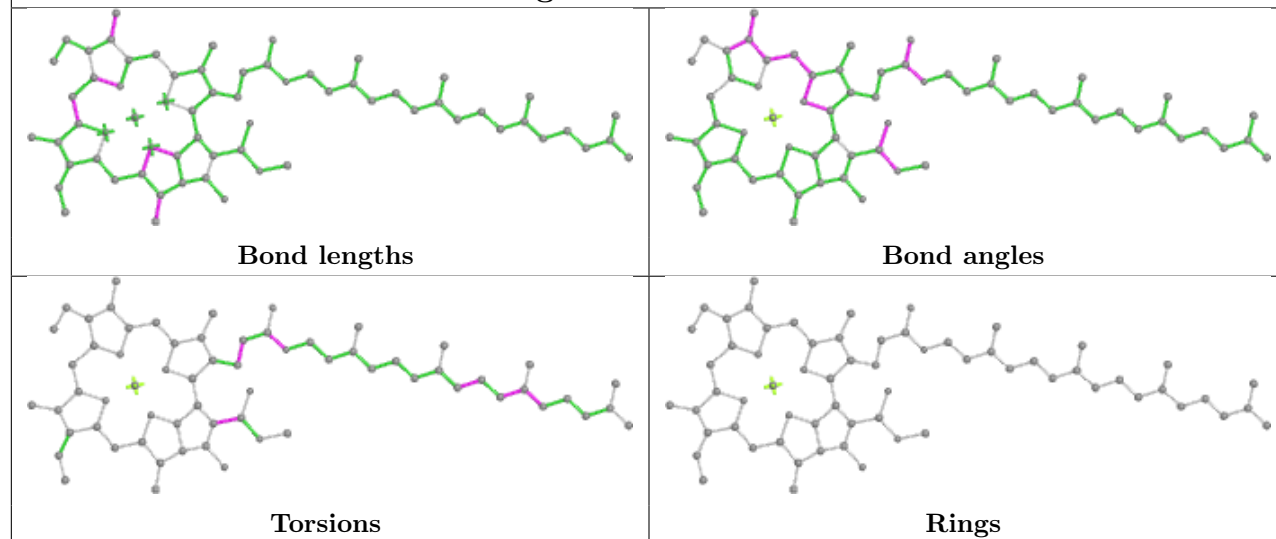
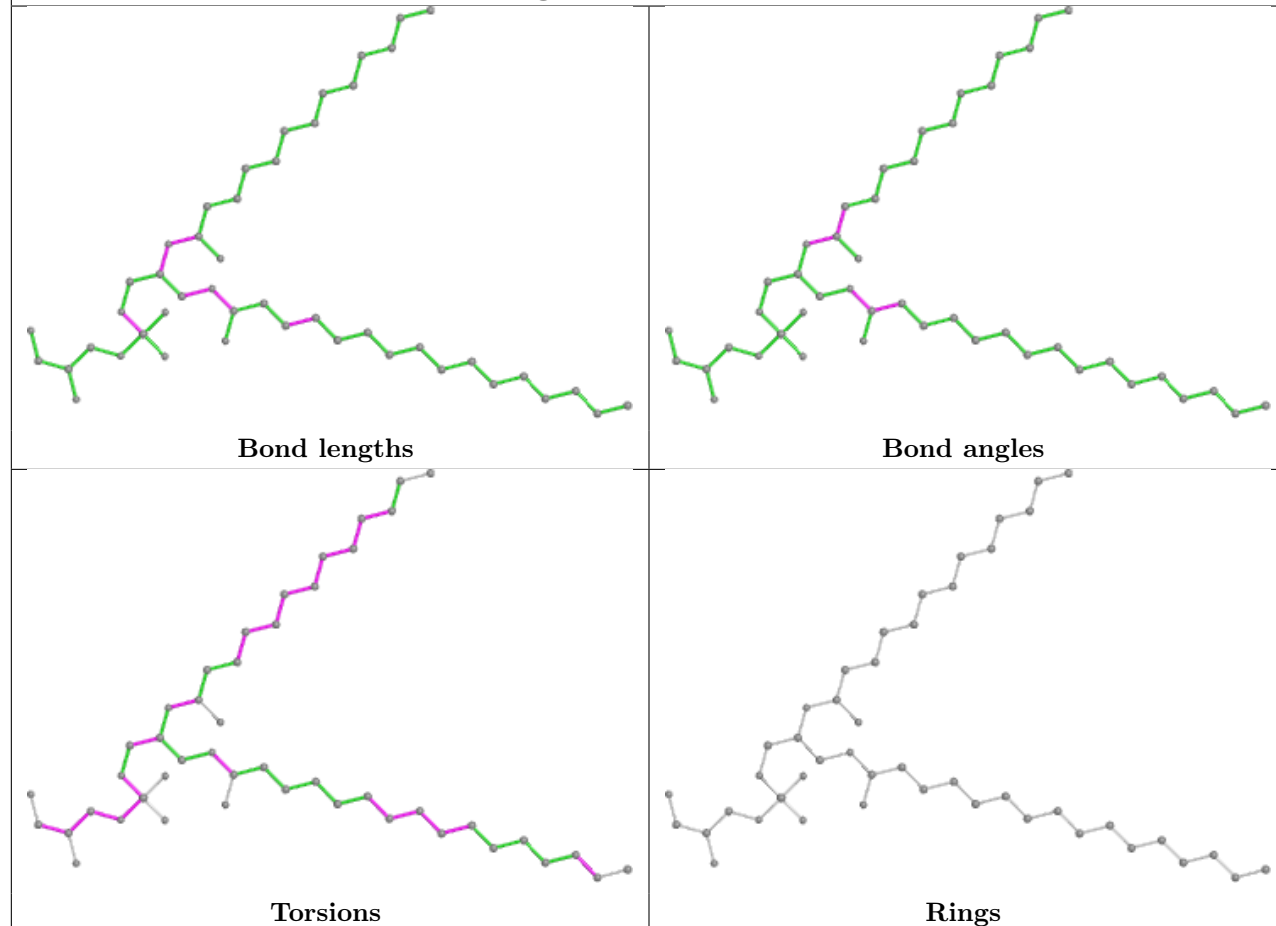


## Ligand CLA 8 309

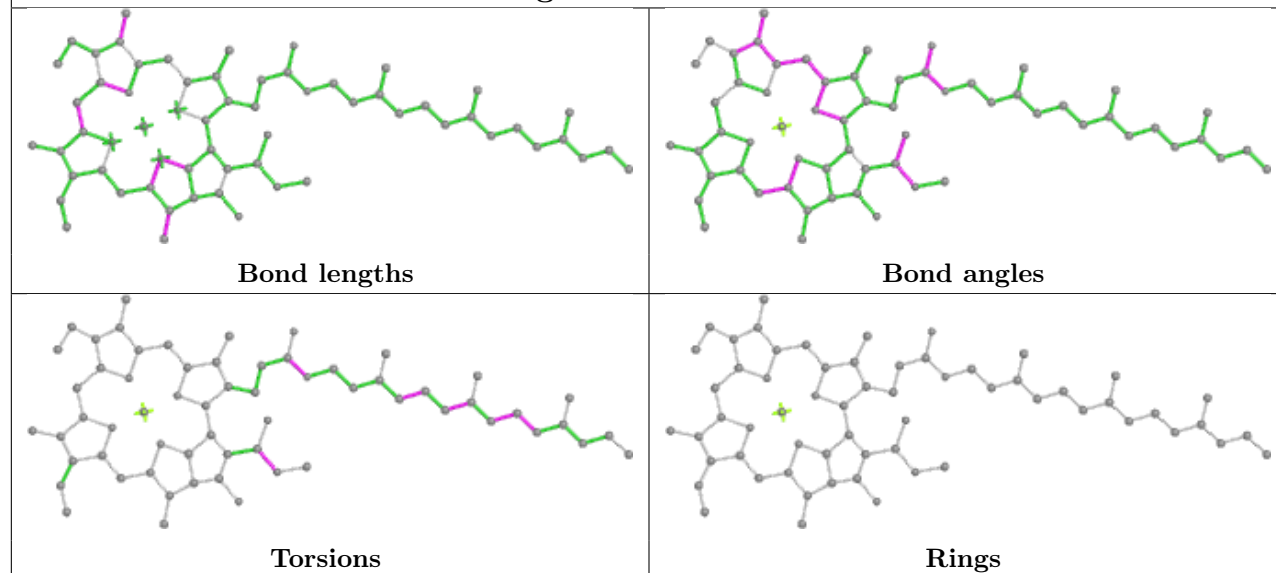
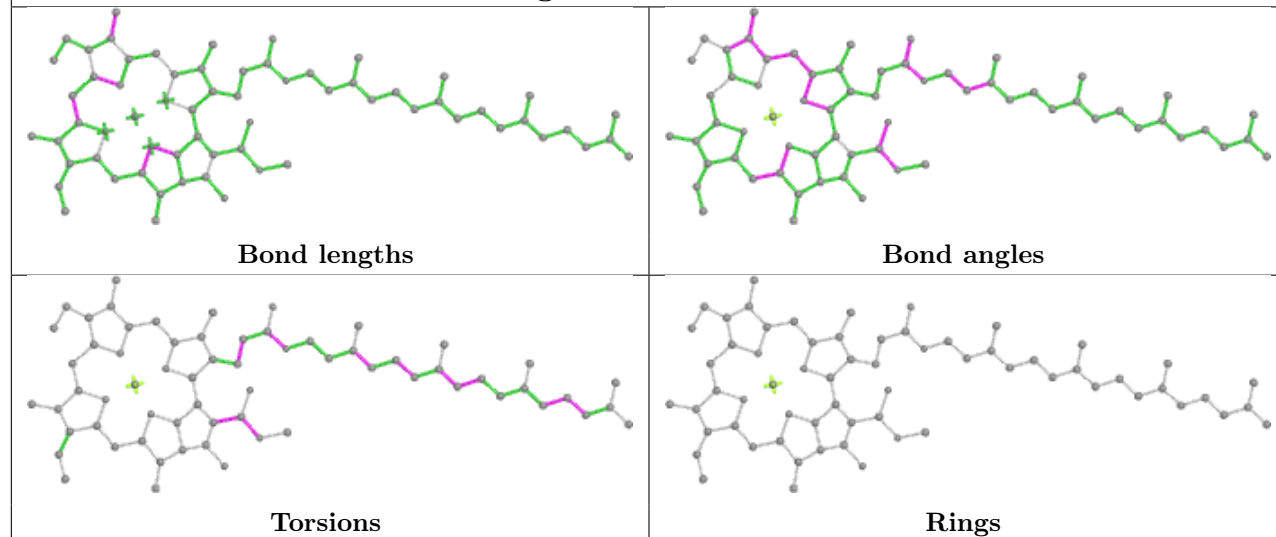


**Ligand CLA b 809****Ligand BCR f 804****Ligand CLA 7 308**

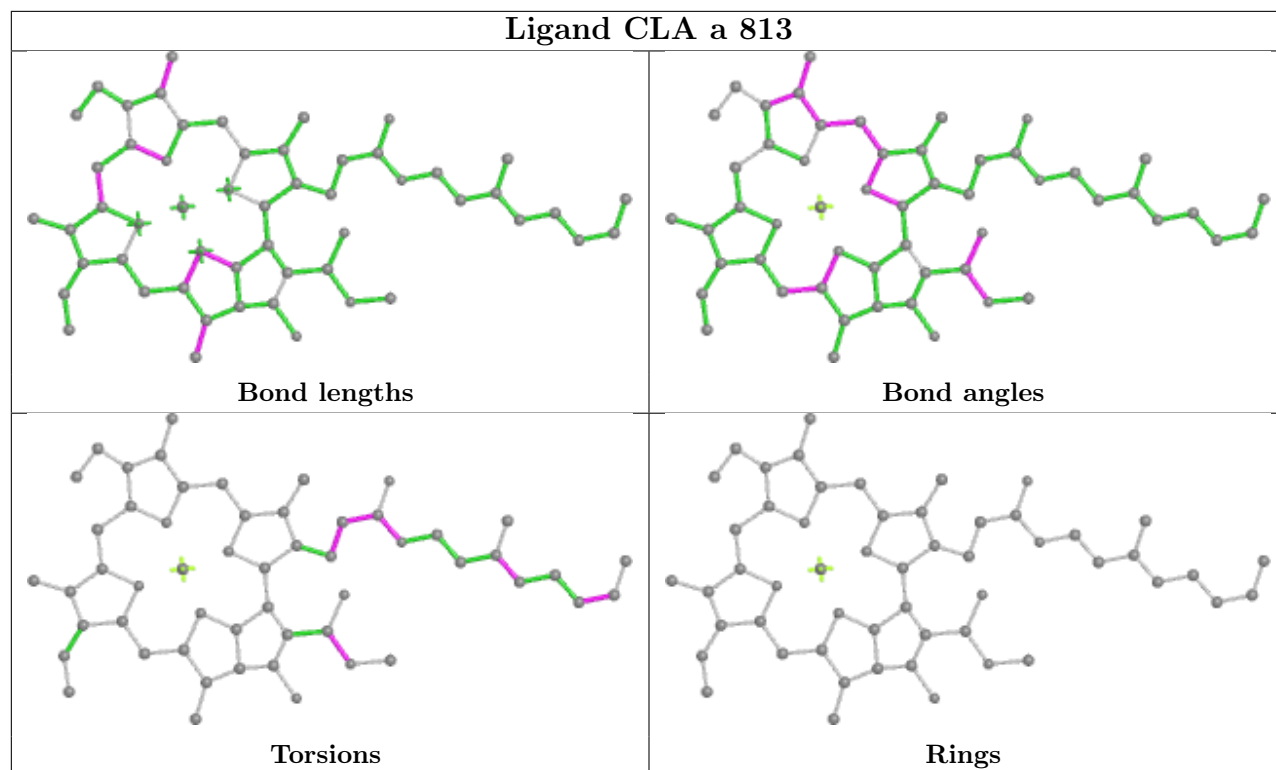


**Ligand CLA a 842****Ligand LHG 9 317**

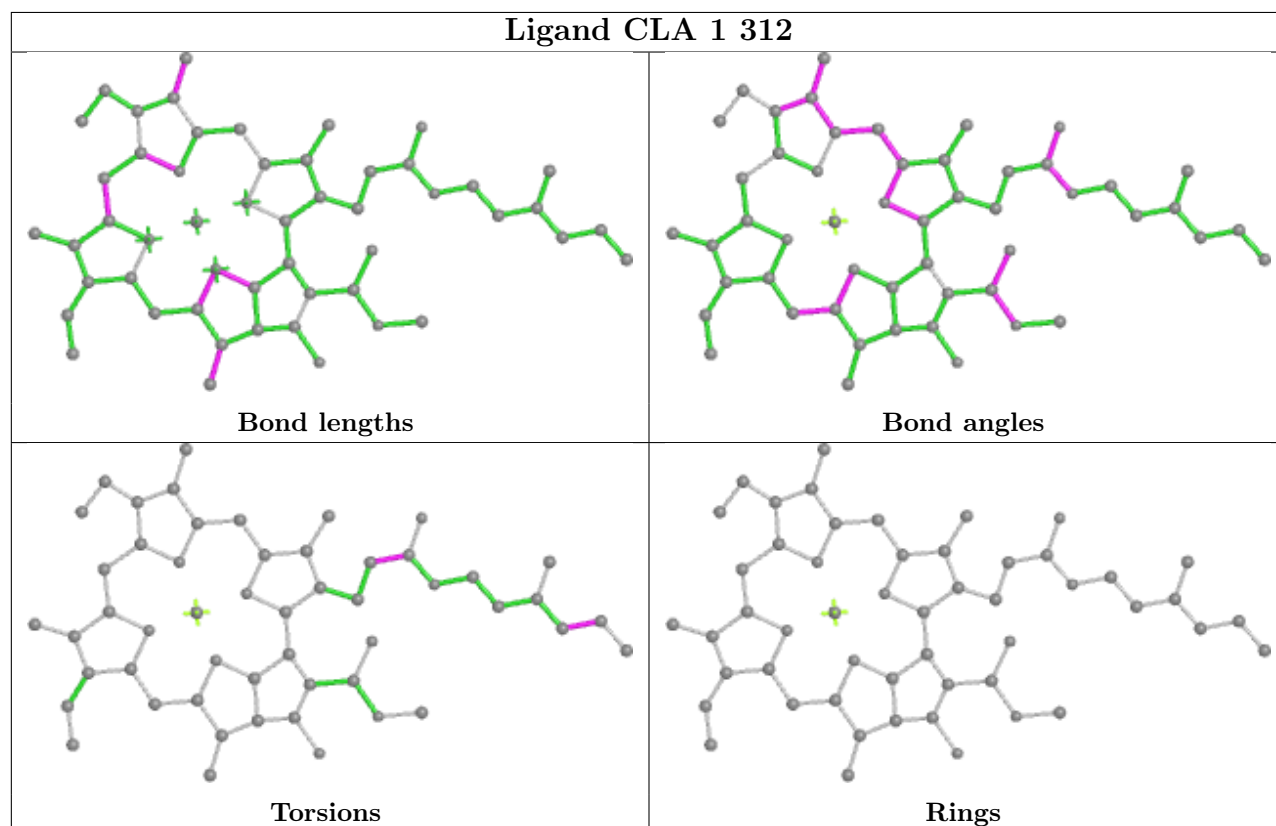


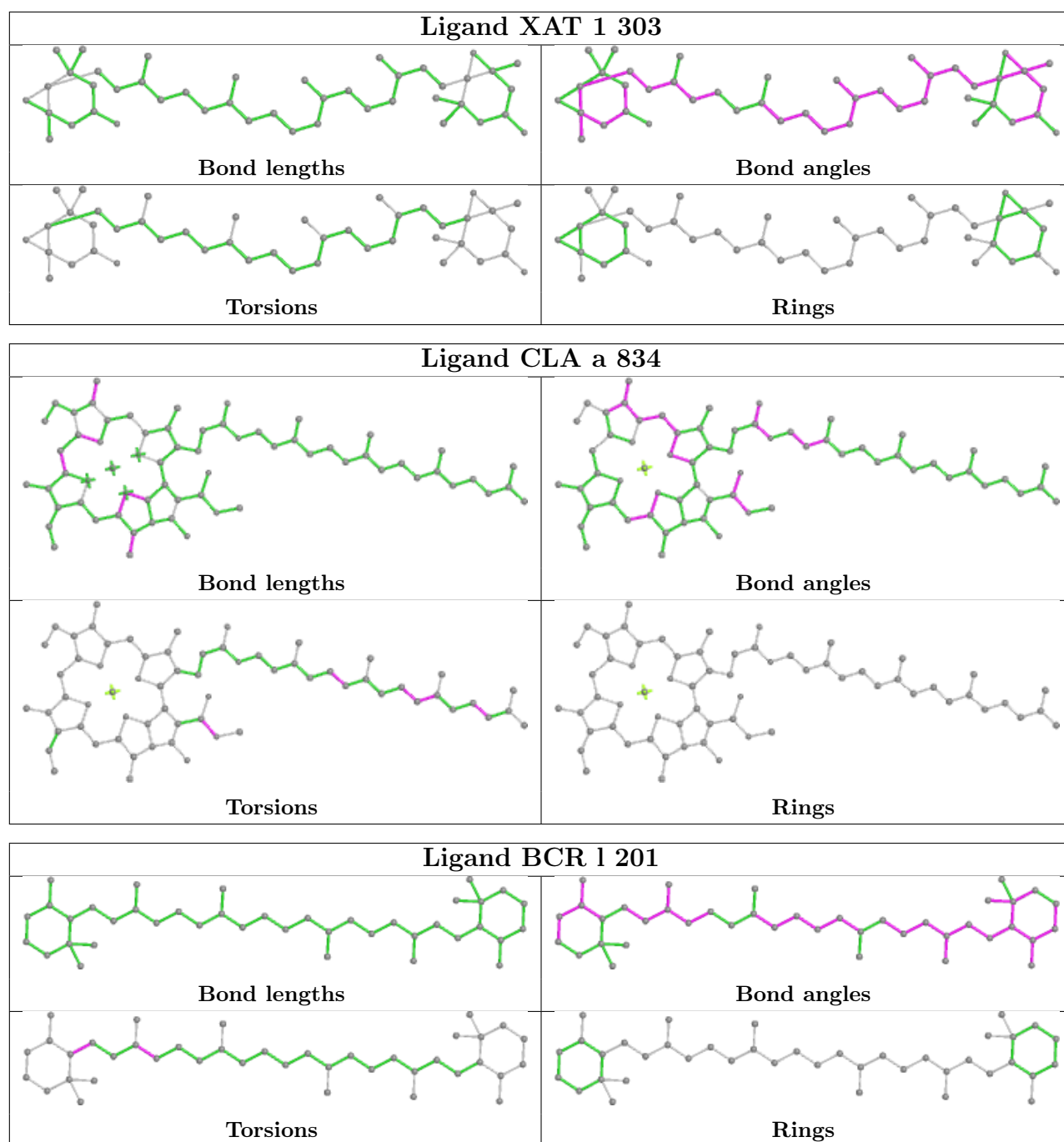
**Ligand CLA a 812****Ligand CLA a 841**

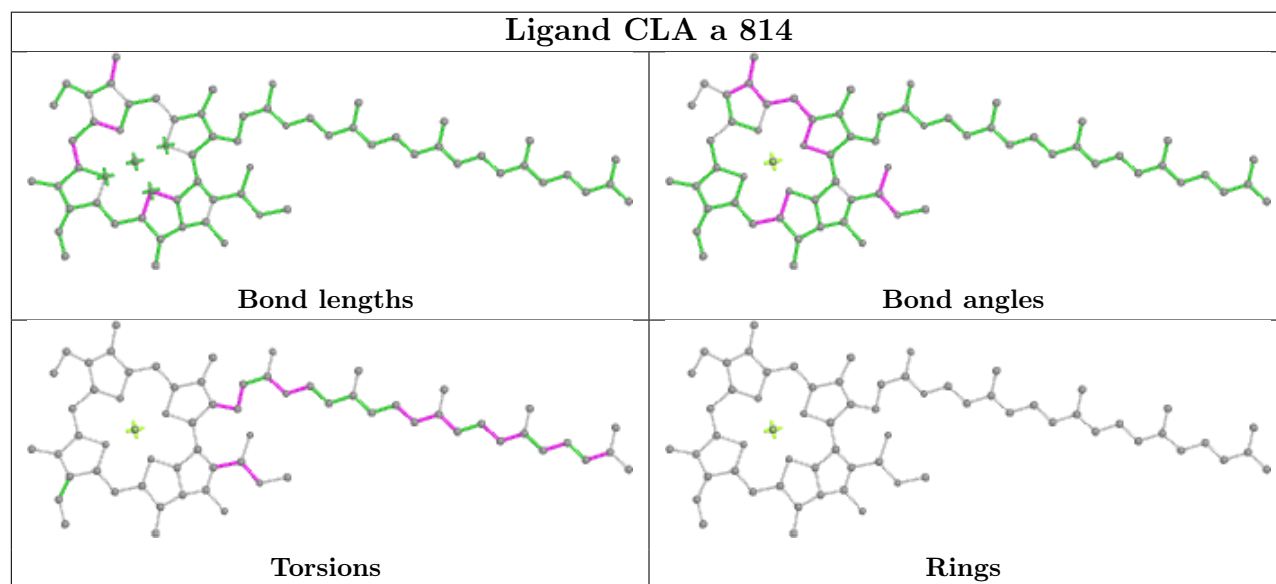
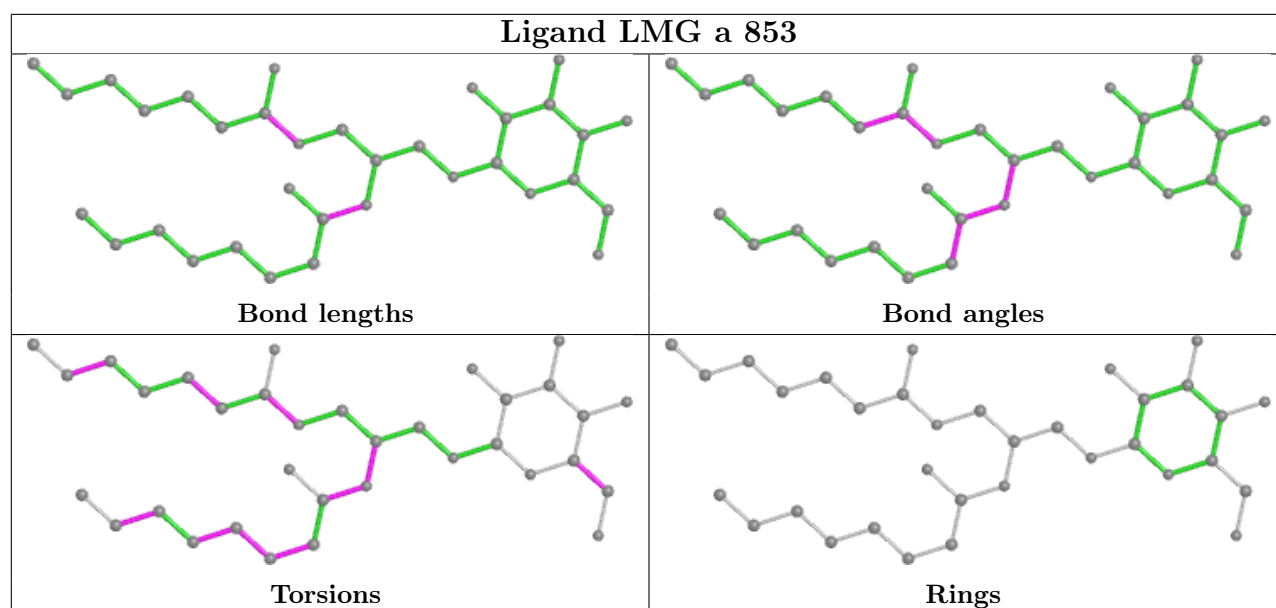
## Ligand CLA a 813

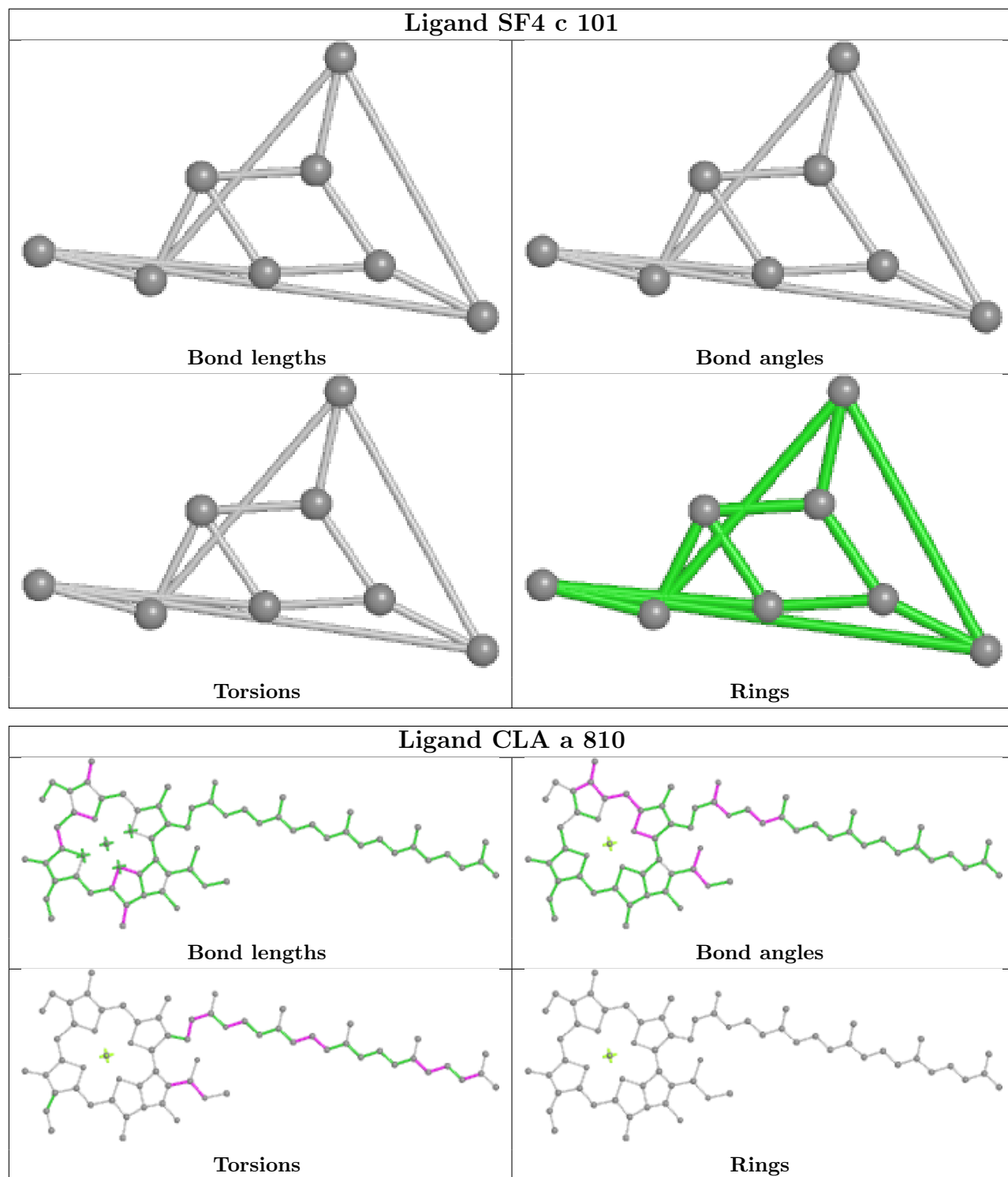


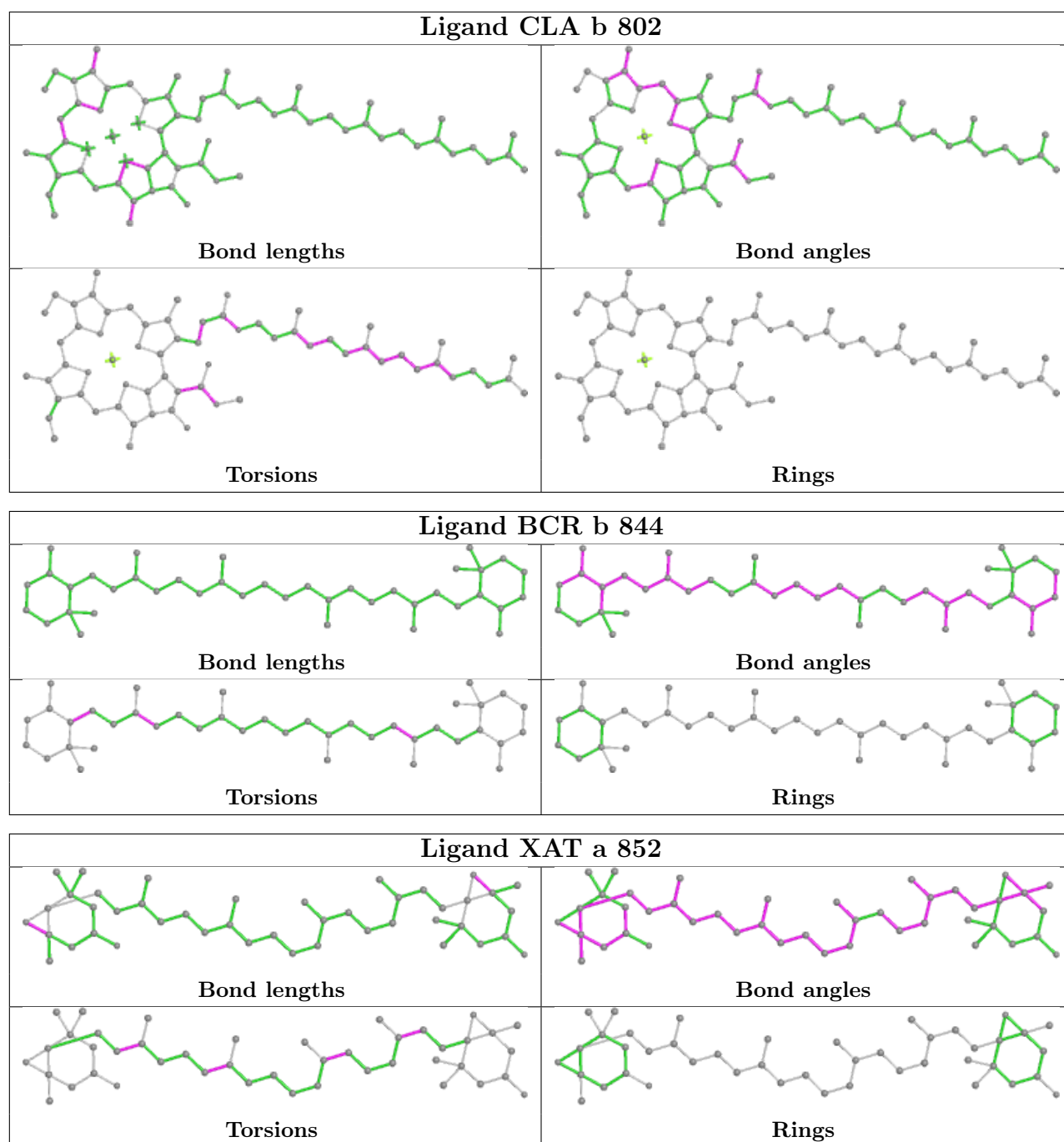
## Ligand CLA 1 312



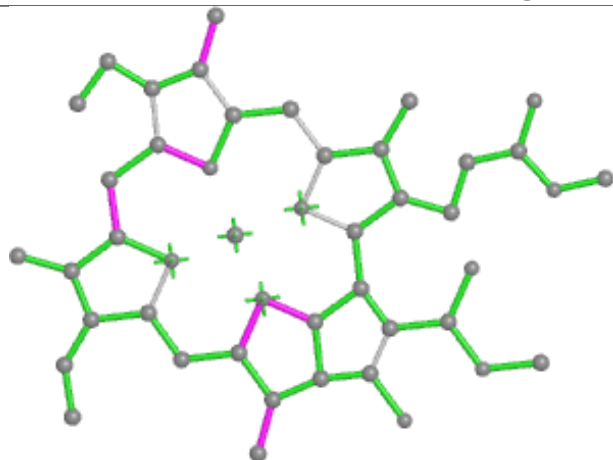




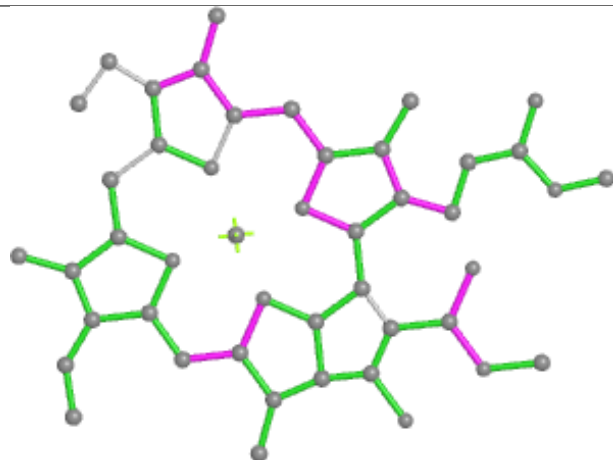




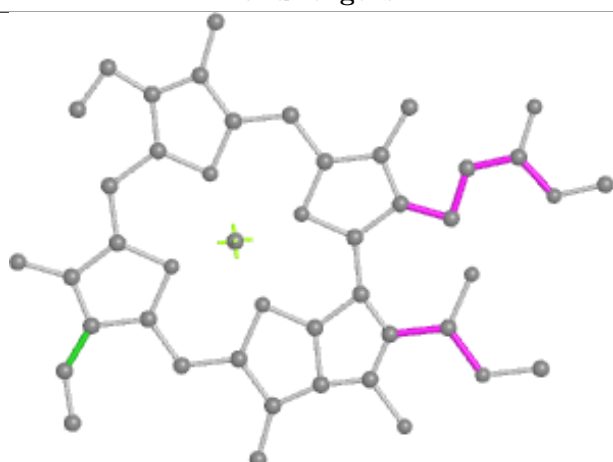
## Ligand CLA 9 312



Bond lengths



Bond angles

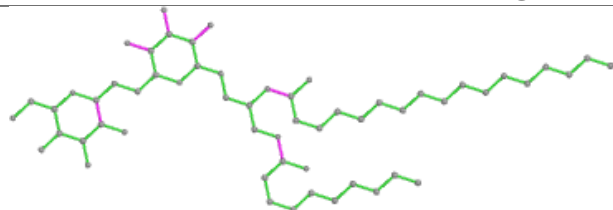


Torsions

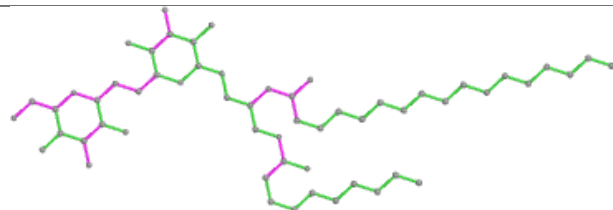


Rings

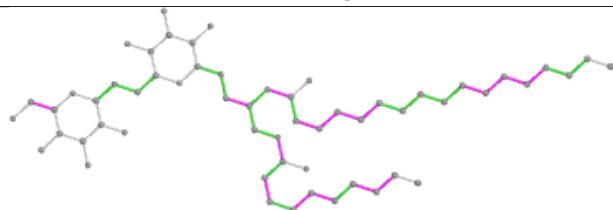
## Ligand DGD b 848



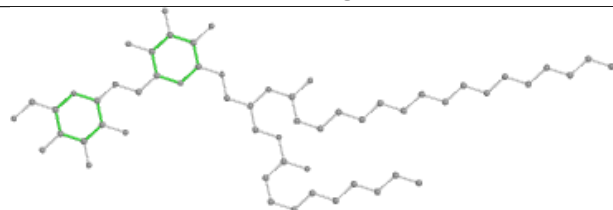
Bond lengths



Bond angles

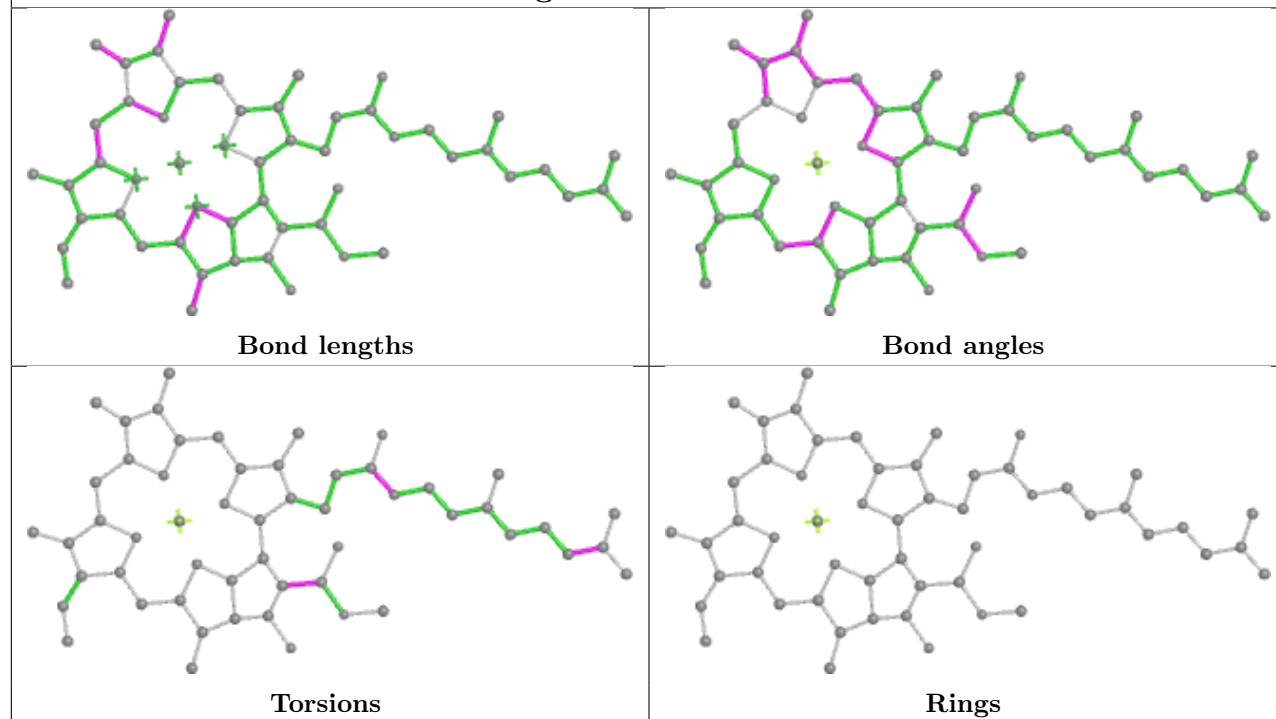


Torsions

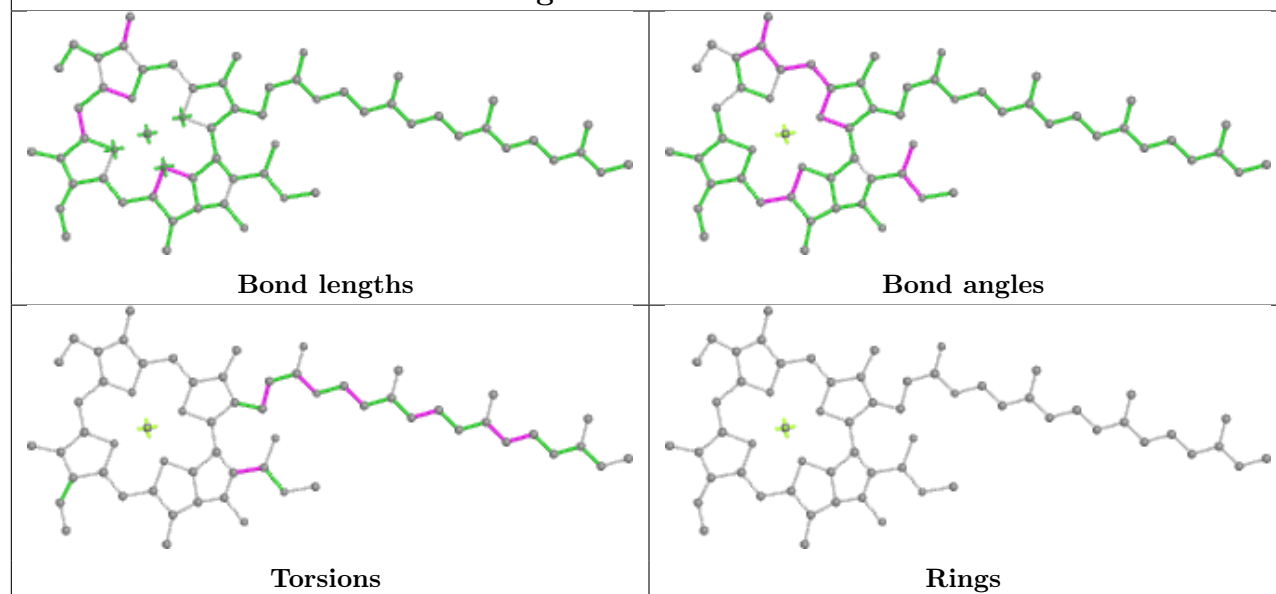


Rings

## Ligand CLA b 811

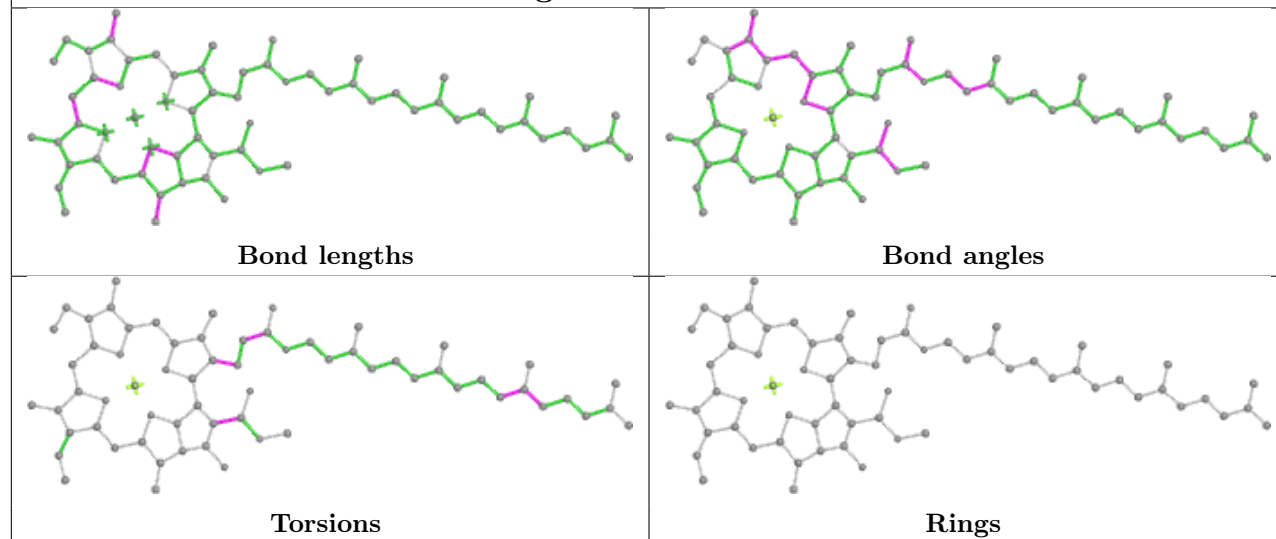


## Ligand CLA 1 305

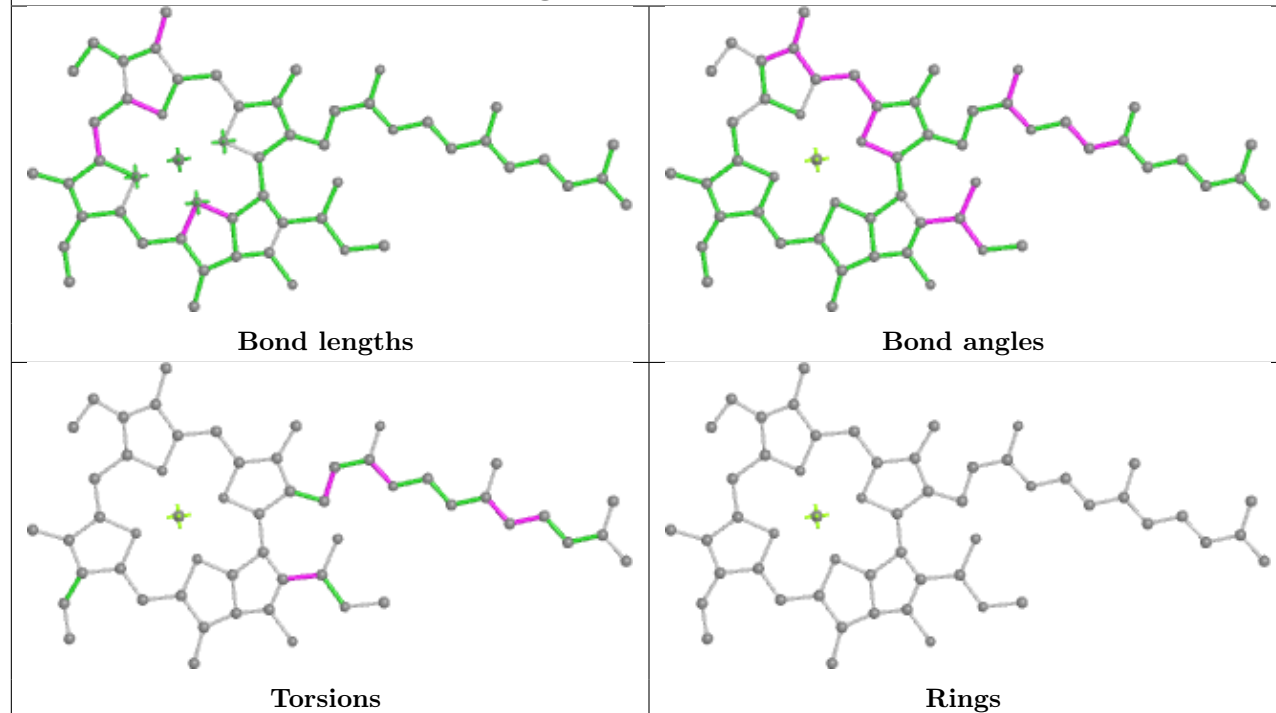




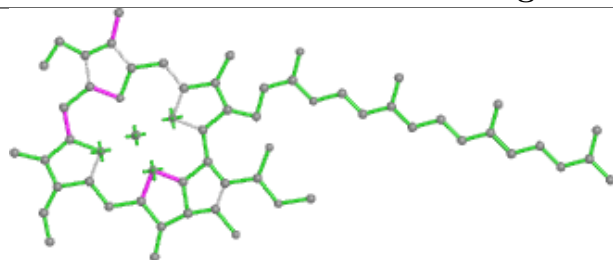
## Ligand CLA b 837



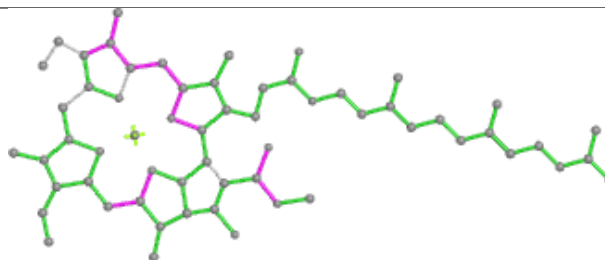
## Ligand CLA 8 308



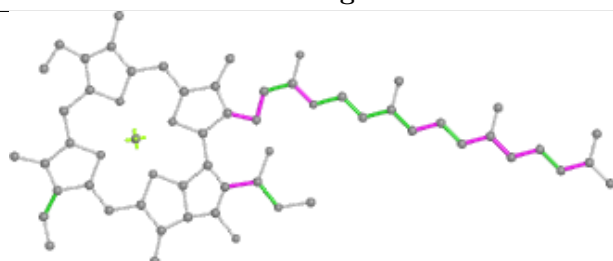
## Ligand CLA b 818



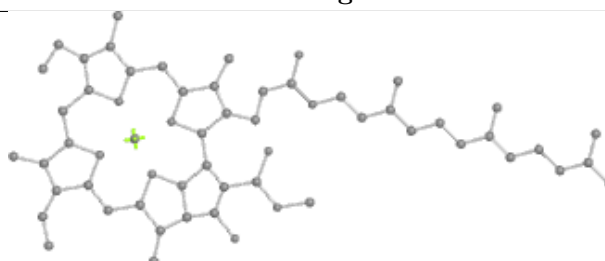
Bond lengths



Bond angles

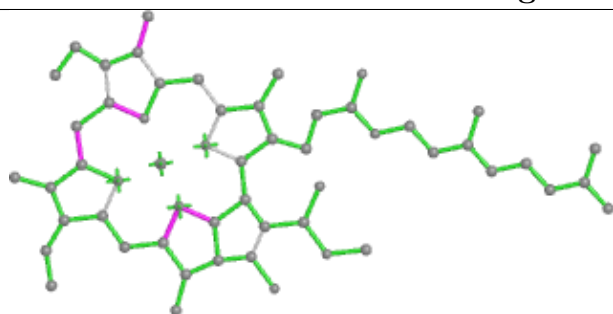


Torsions

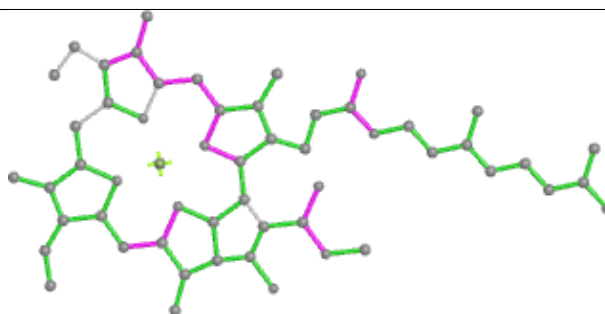


Rings

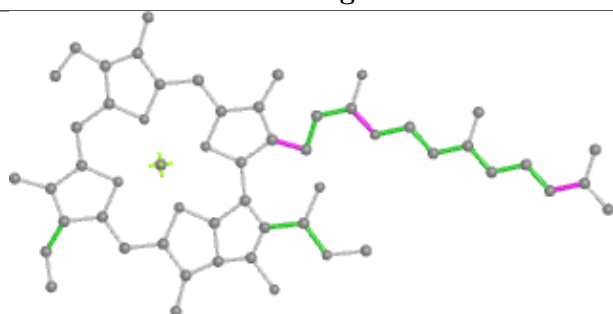
## Ligand CLA a 805



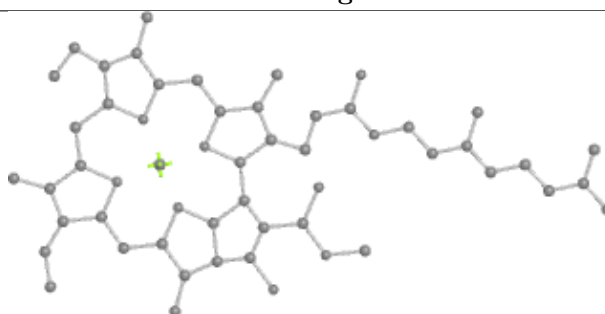
Bond lengths



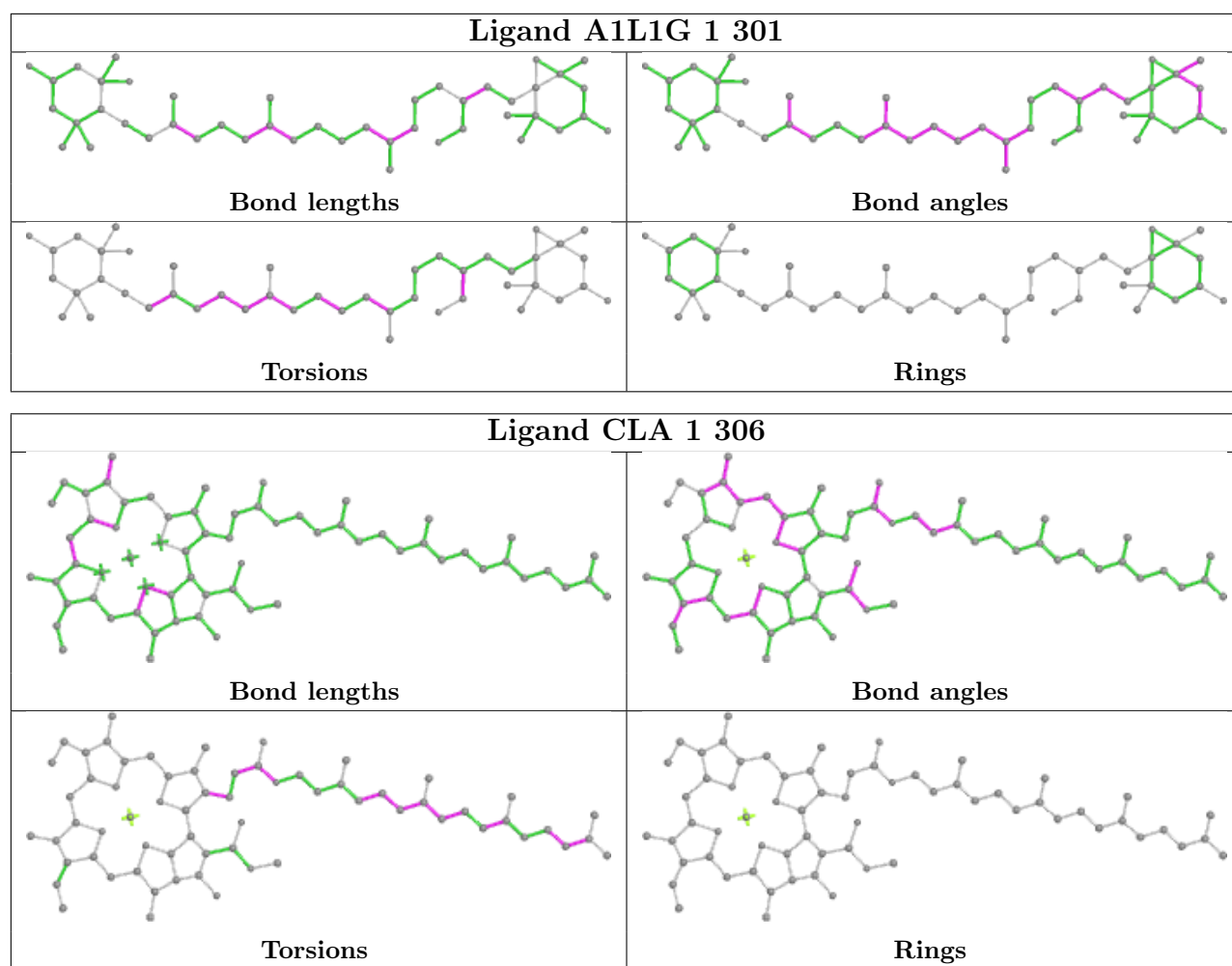
Bond angles



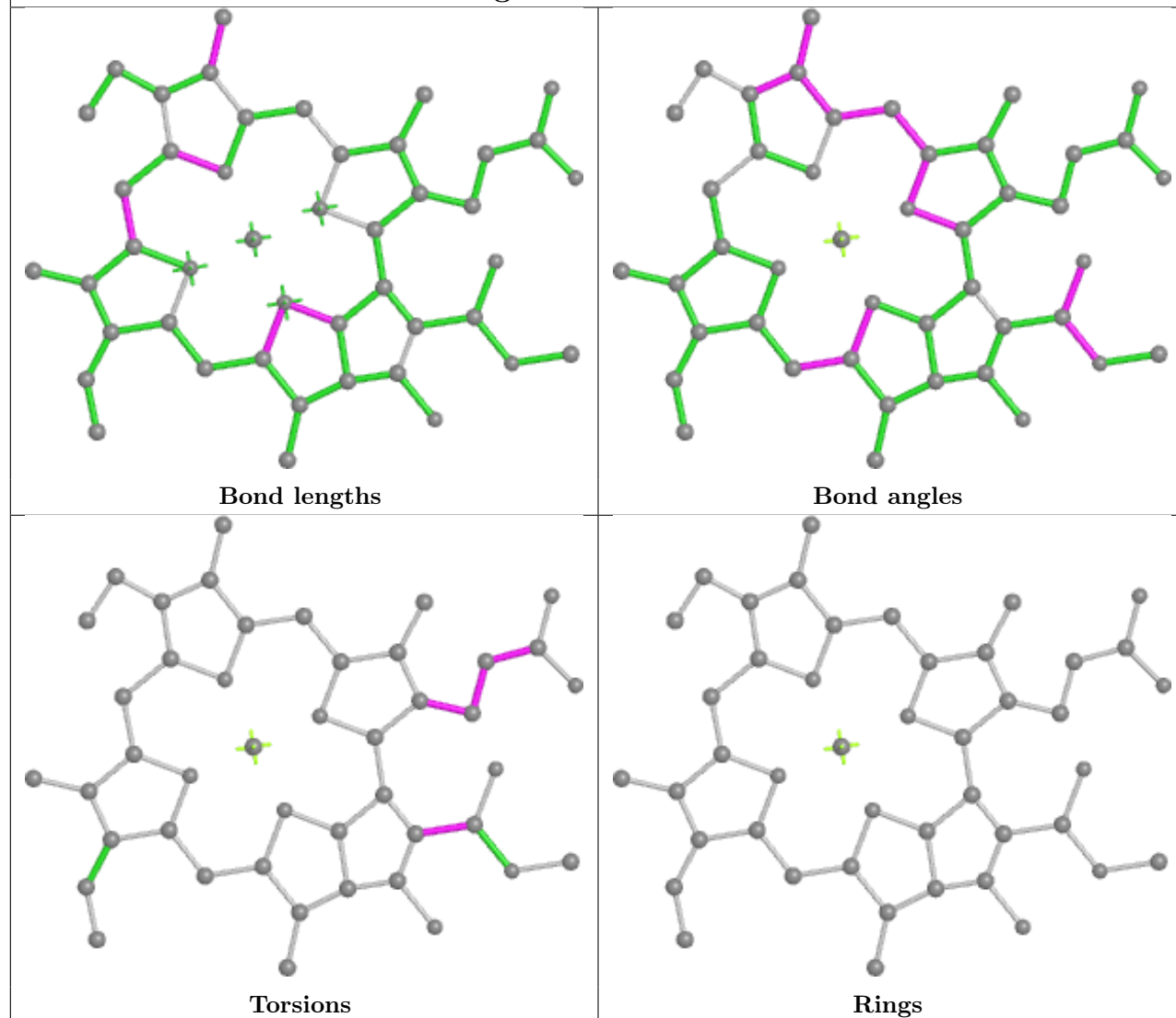
Torsions



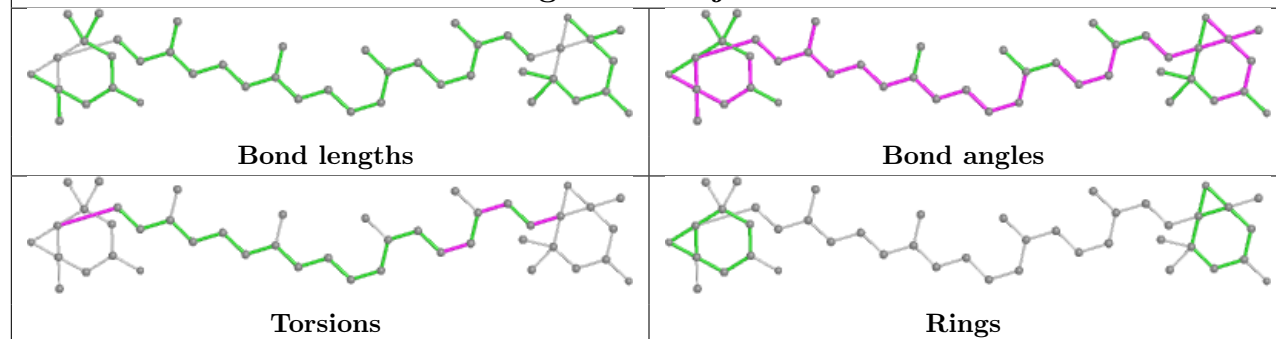
Rings



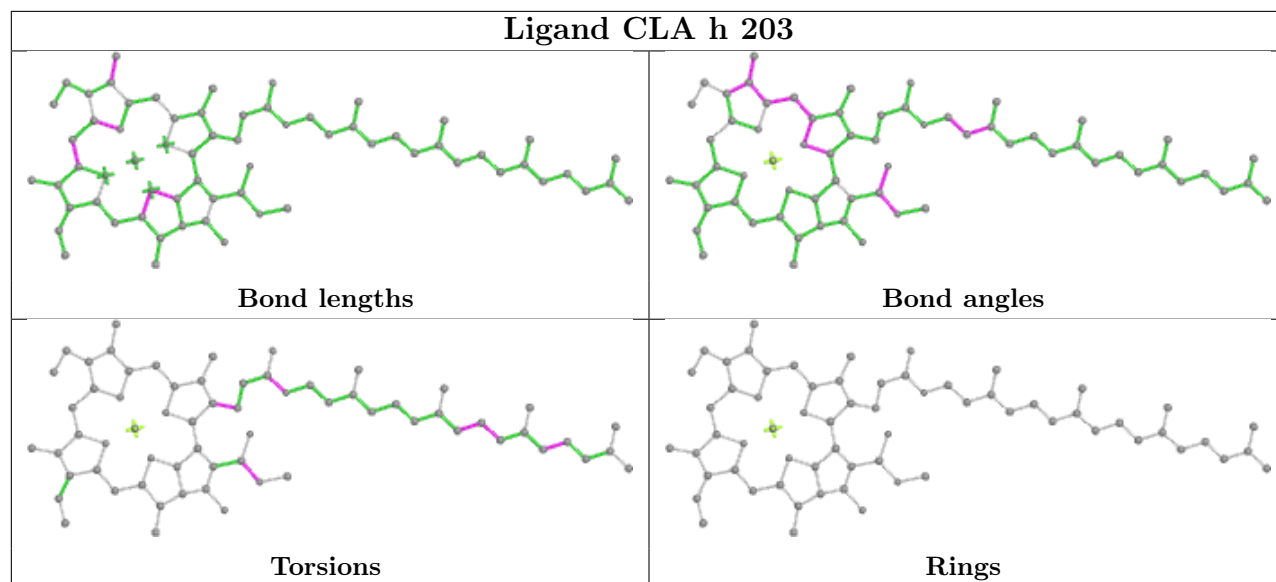
## Ligand CLA a 817



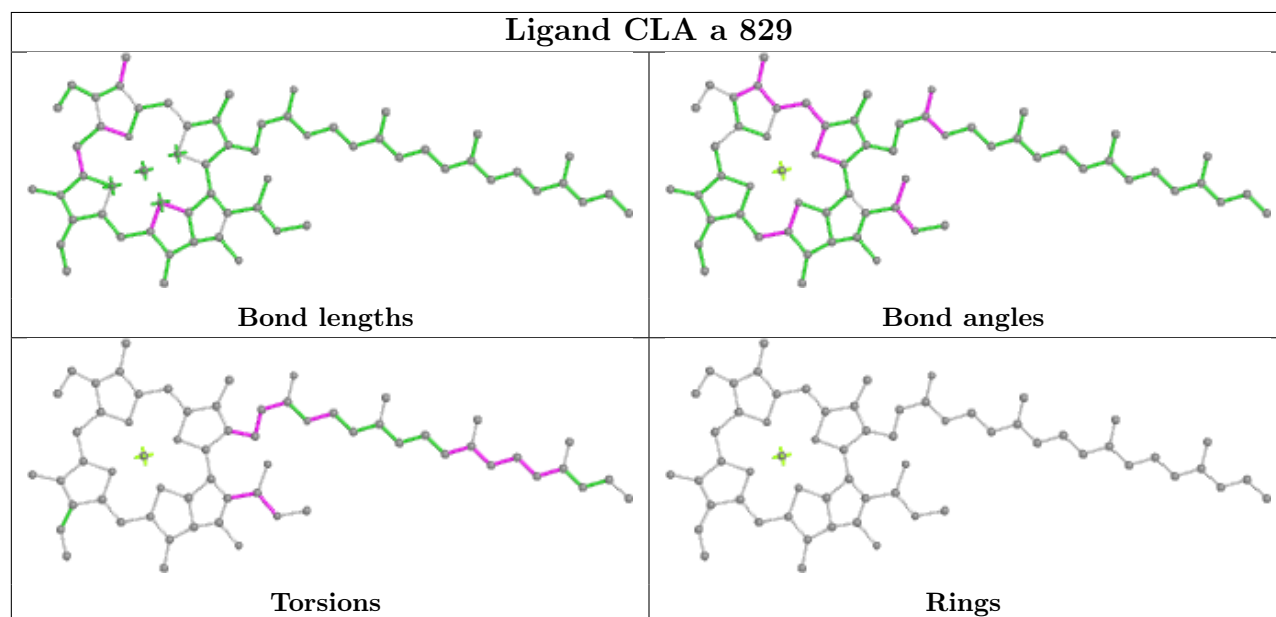
## Ligand XAT j 101

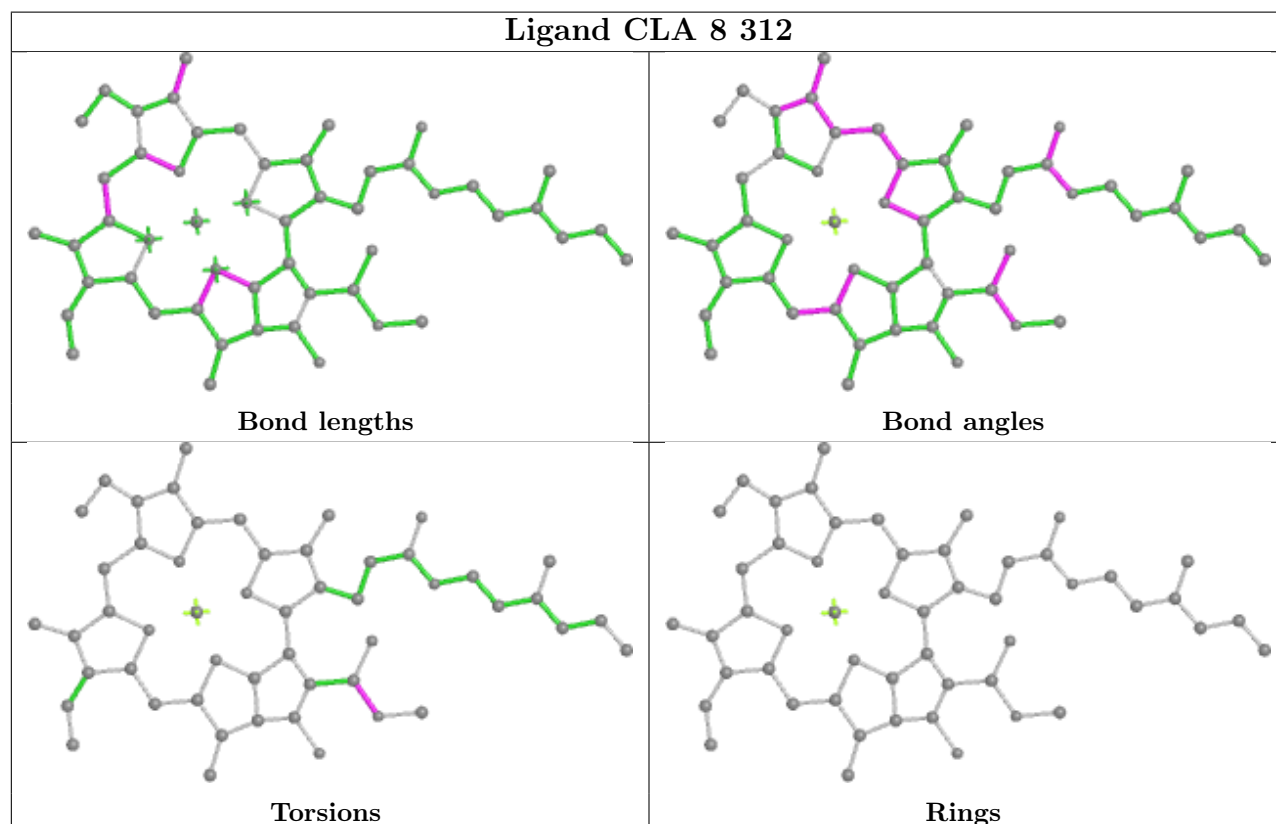
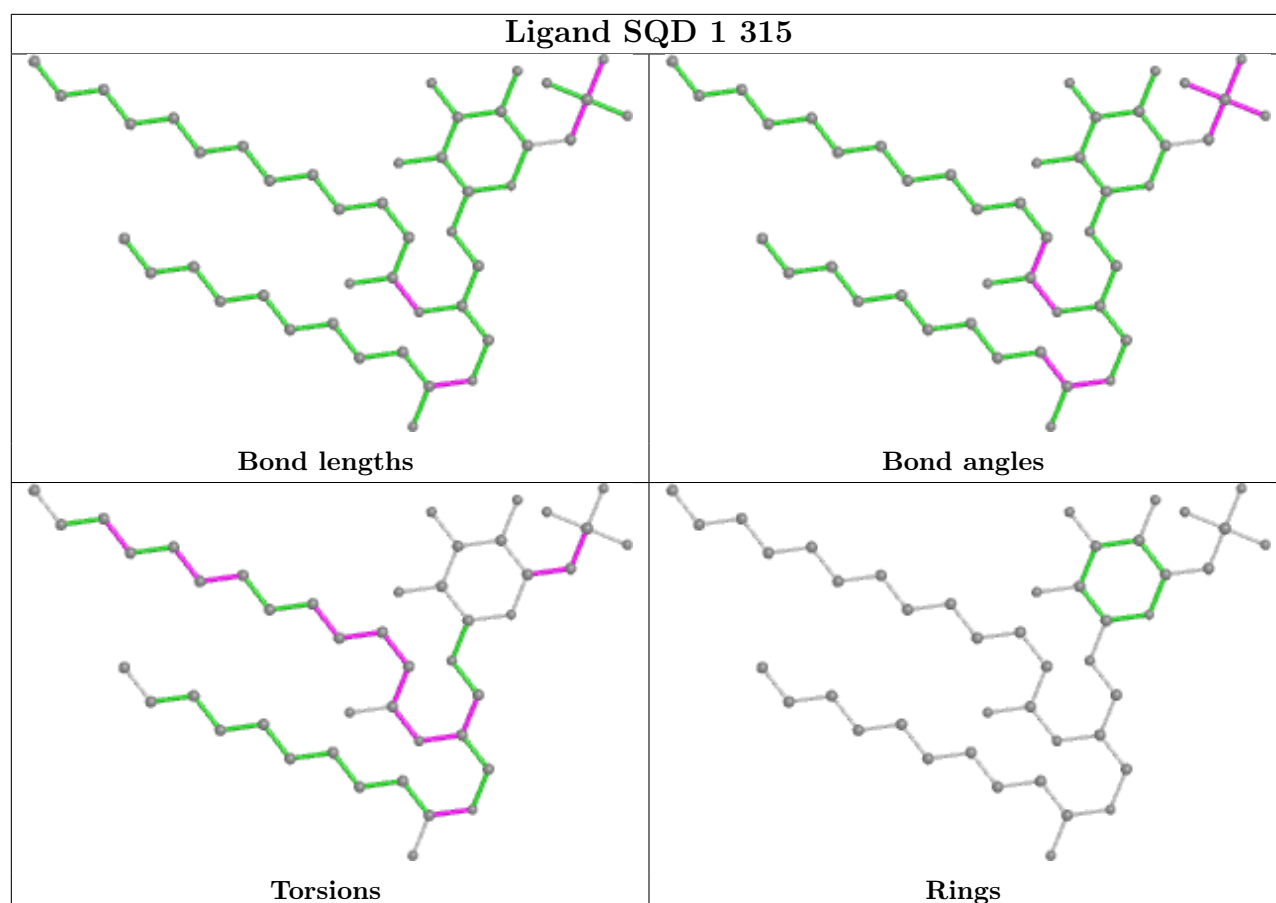


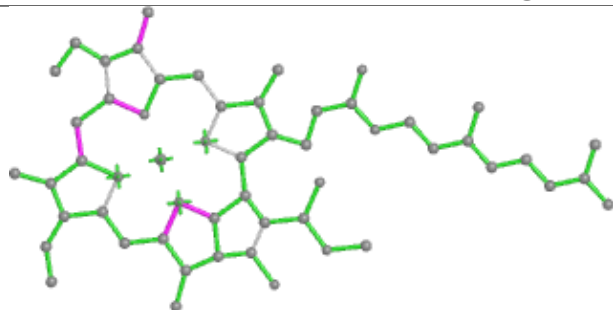
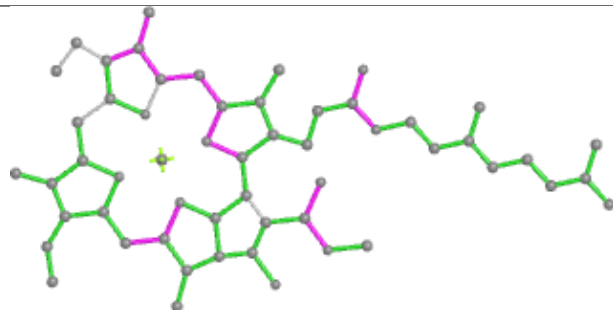
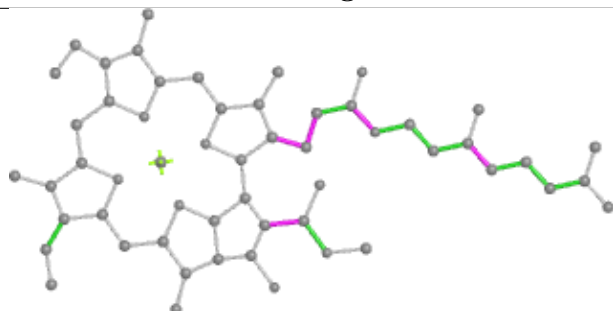
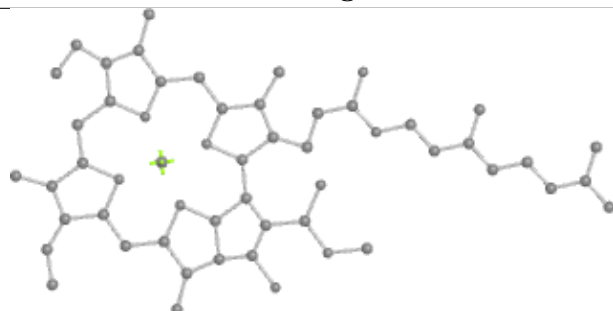
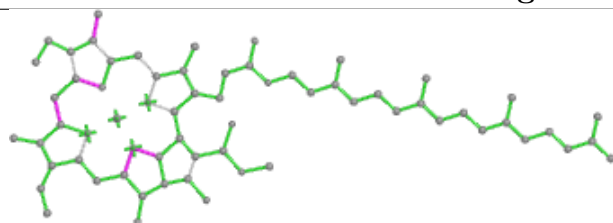
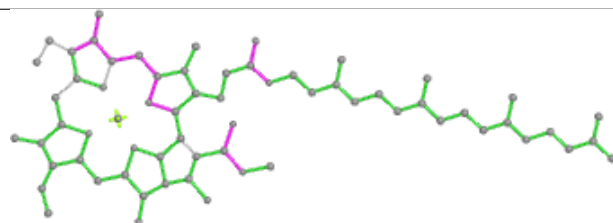
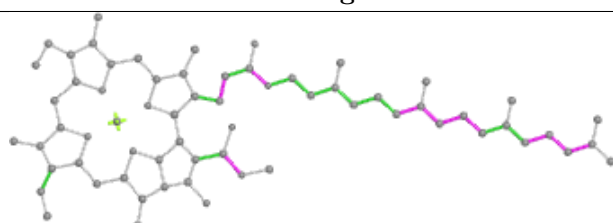
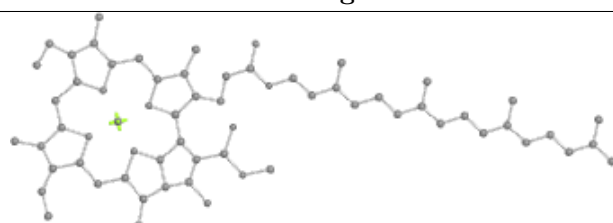
## Ligand CLA h 203



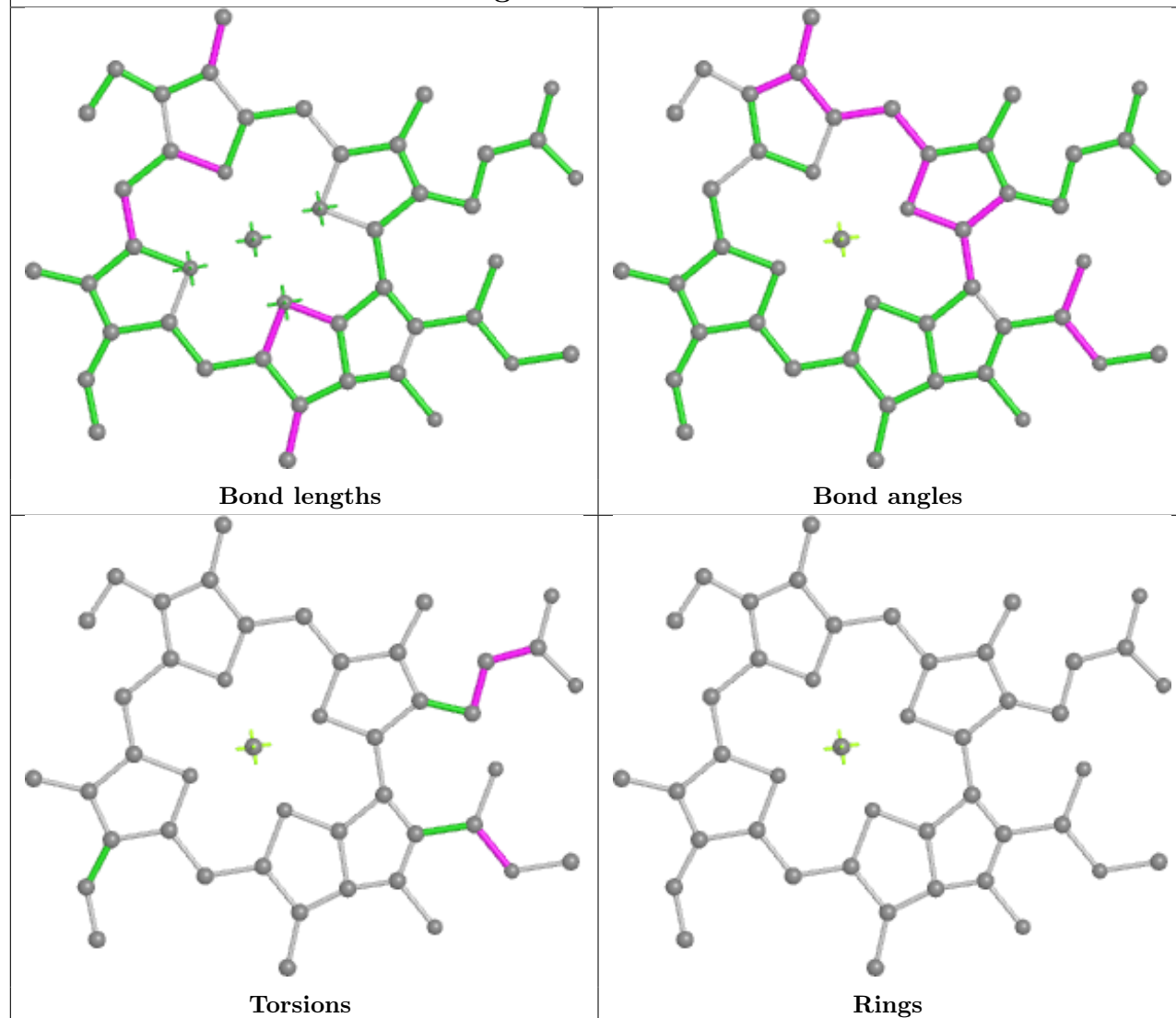
## Ligand CLA a 829



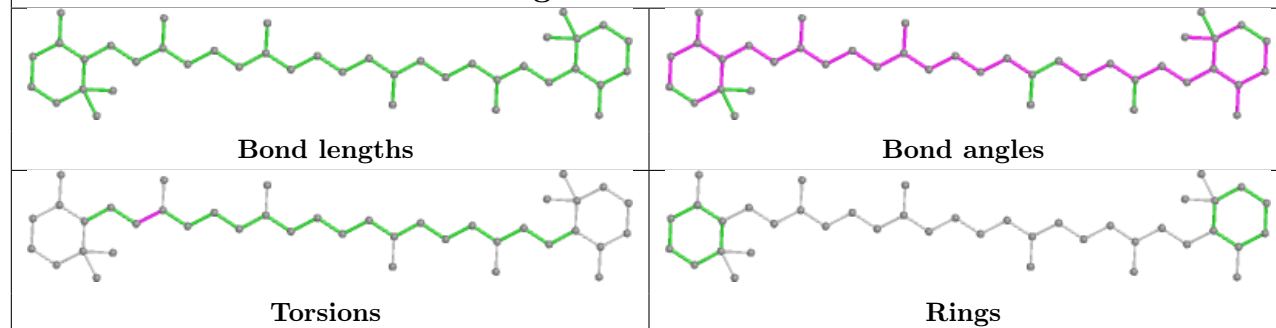


**Ligand CLA a 825****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA b 827****Bond lengths****Bond angles****Torsions****Rings**

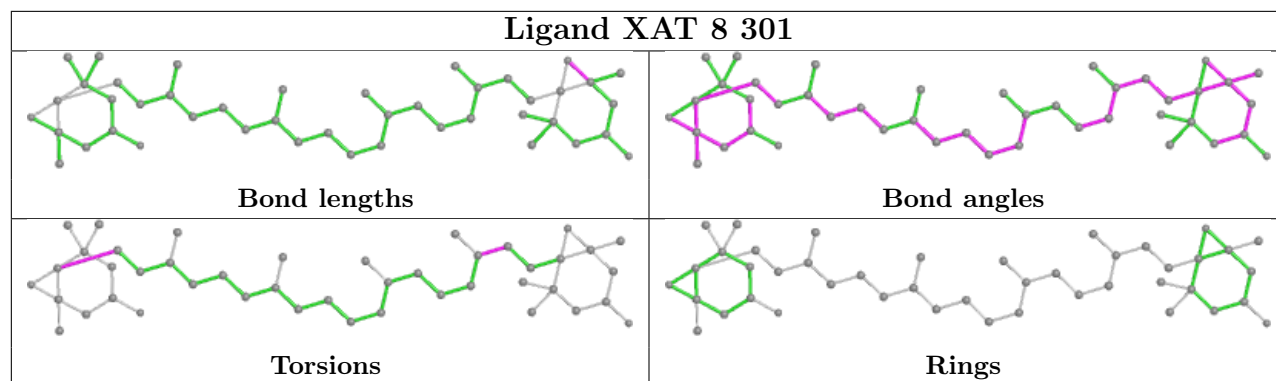
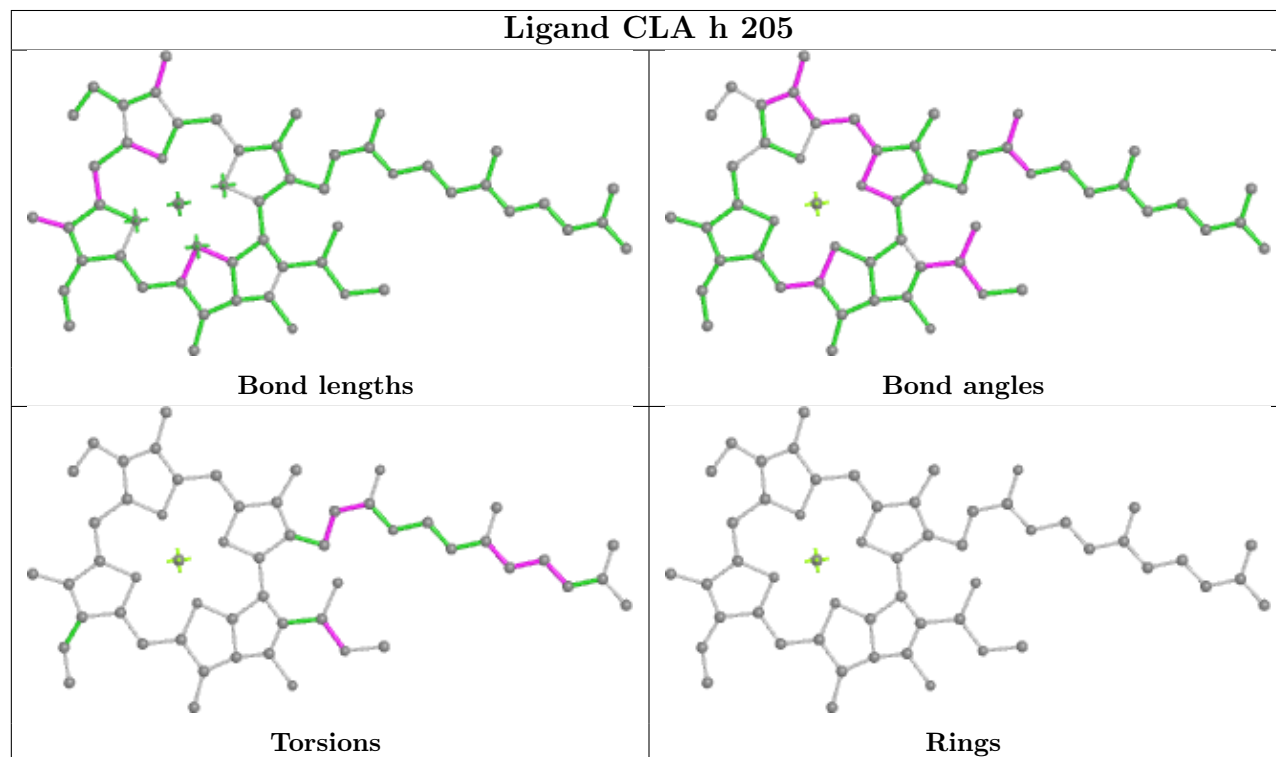
## Ligand CLA 7 314



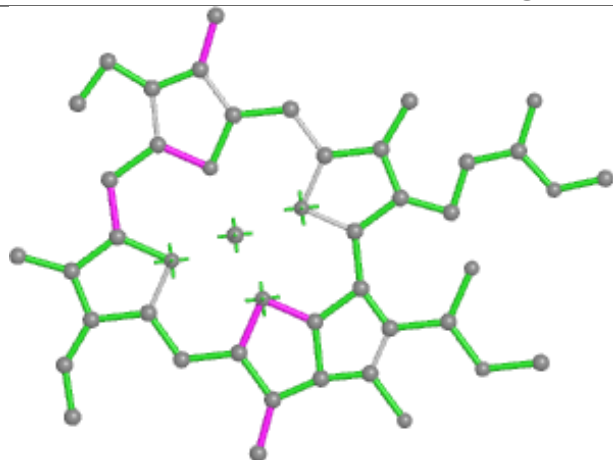
## Ligand BCR b 845



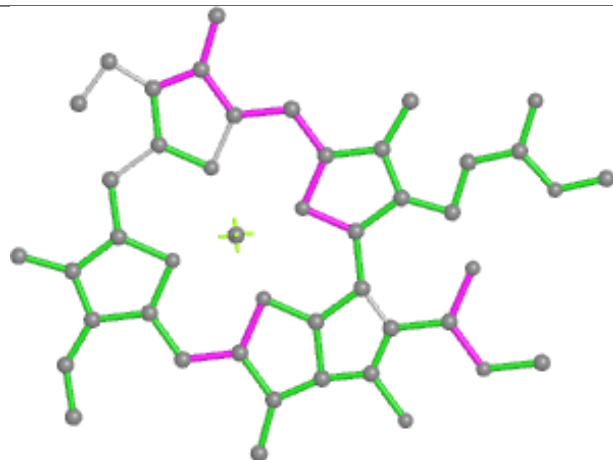


**Ligand XAT 8 301****Ligand CLA h 205**

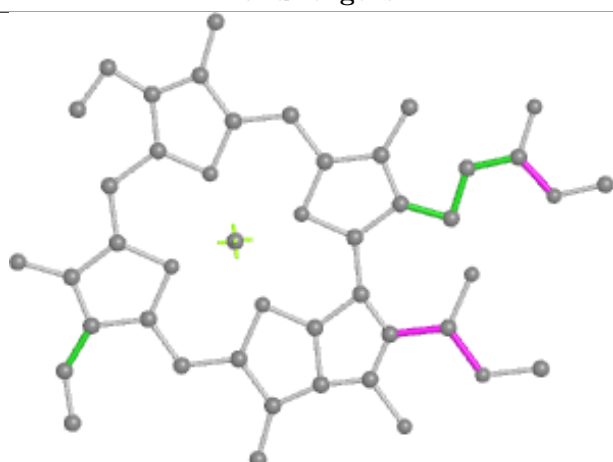
## Ligand CLA 8 310



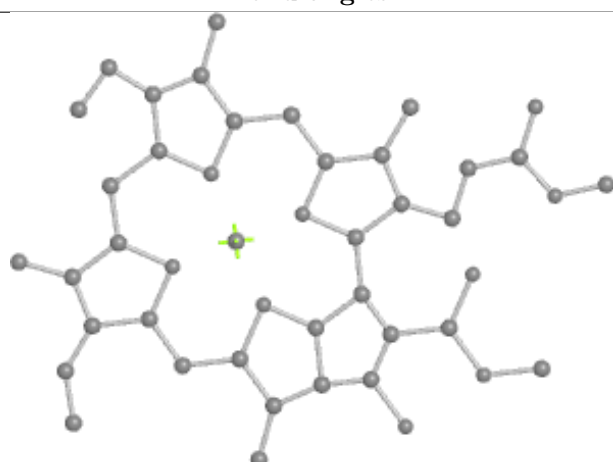
Bond lengths



Bond angles

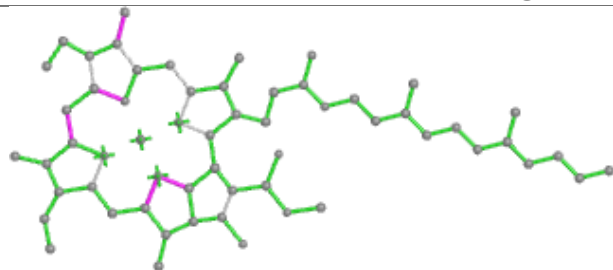


Torsions

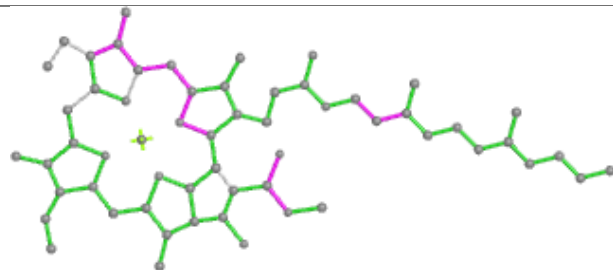


Rings

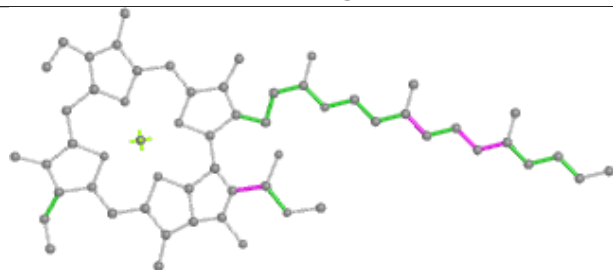
## Ligand CLA a 802



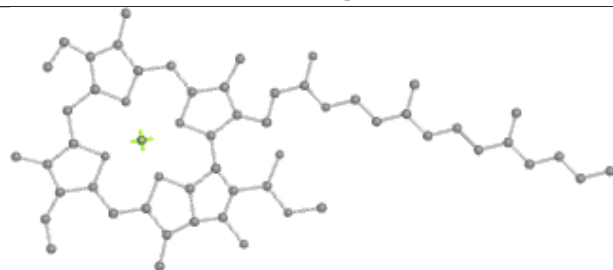
Bond lengths



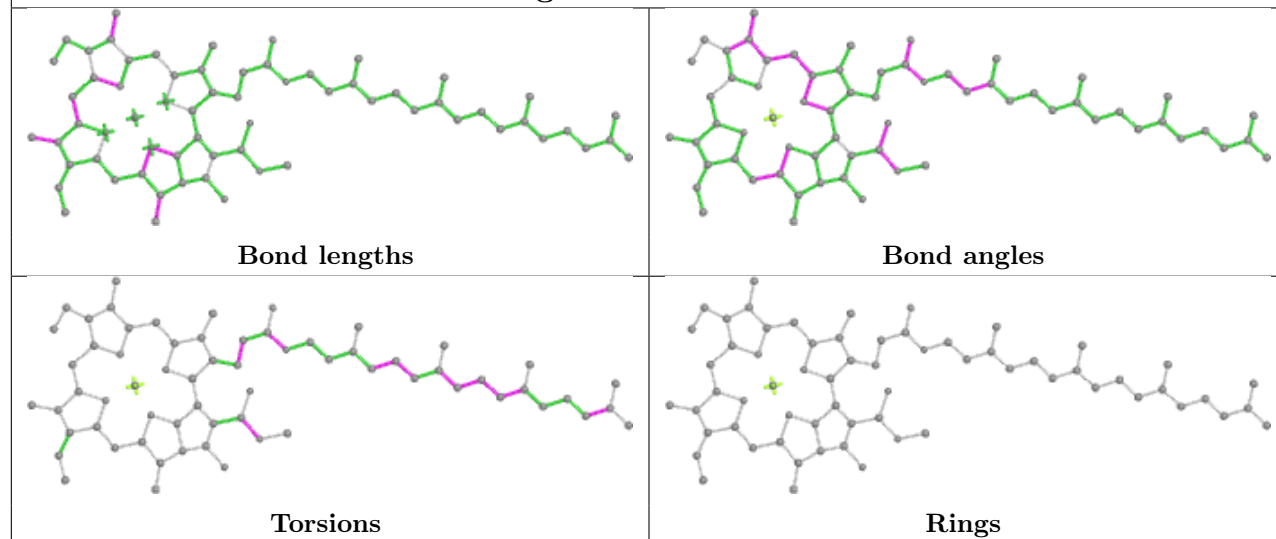
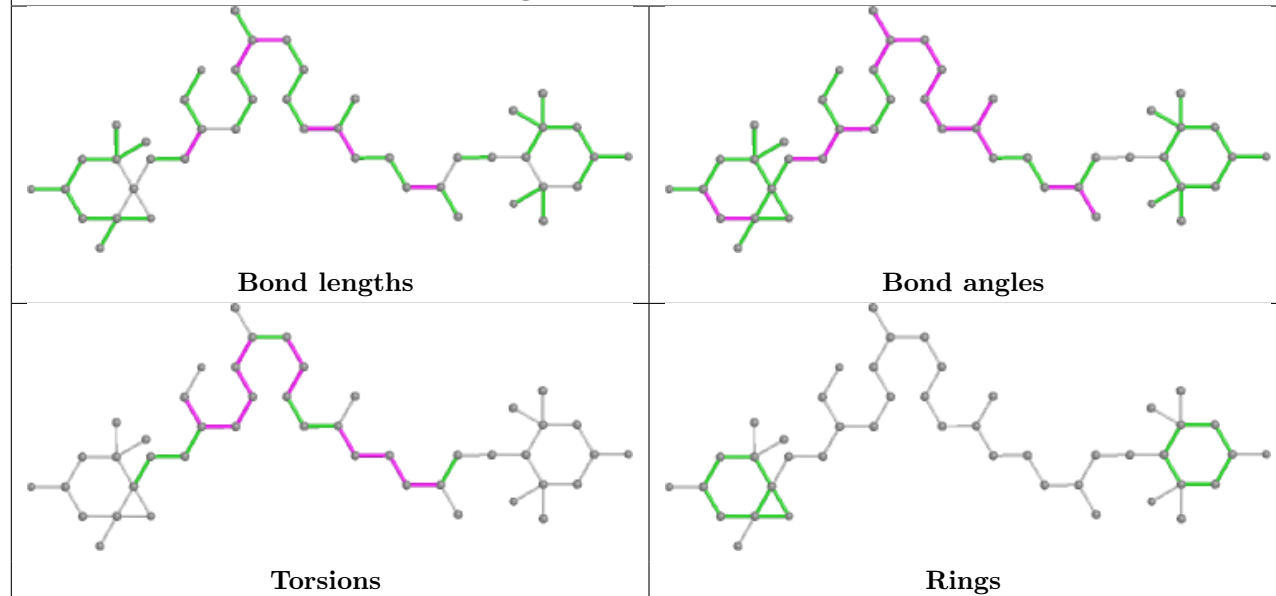
Bond angles



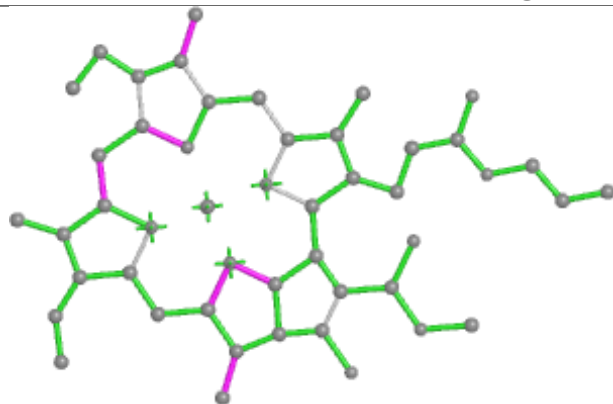
Torsions



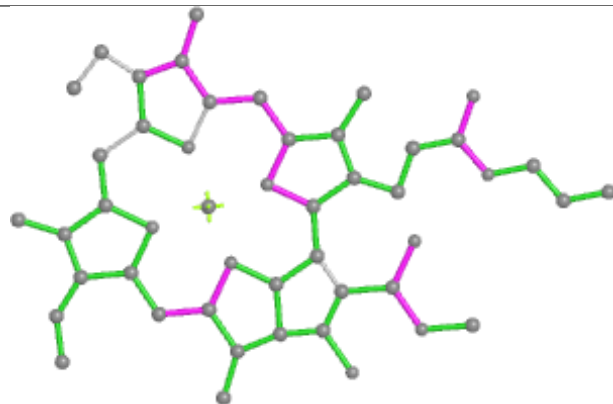
Rings

**Ligand CLA 9 308****Ligand A1L1G 9 301**

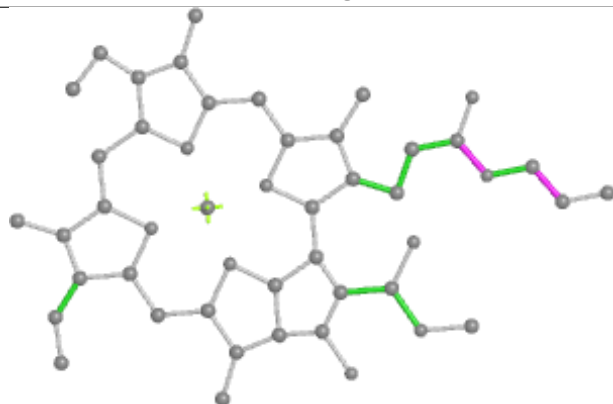
## Ligand CLA 7 312



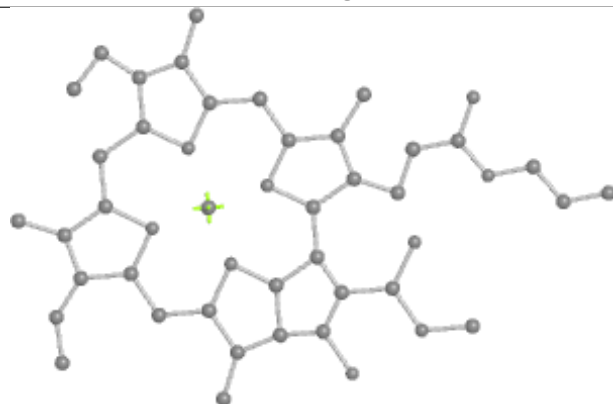
Bond lengths



Bond angles

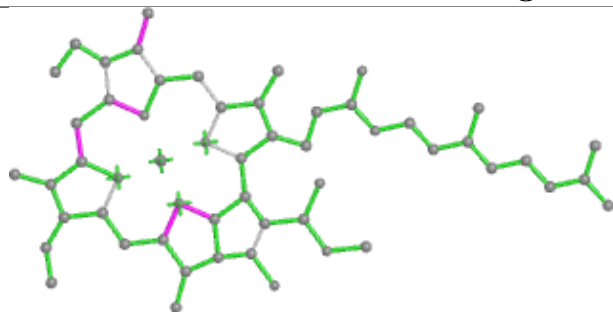


Torsions

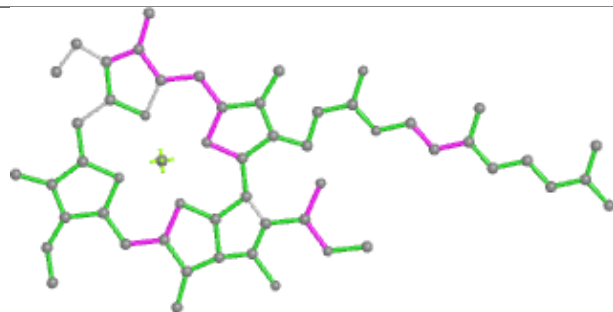


Rings

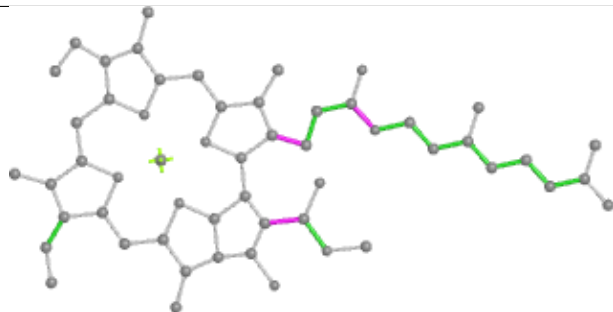
## Ligand CLA b 816



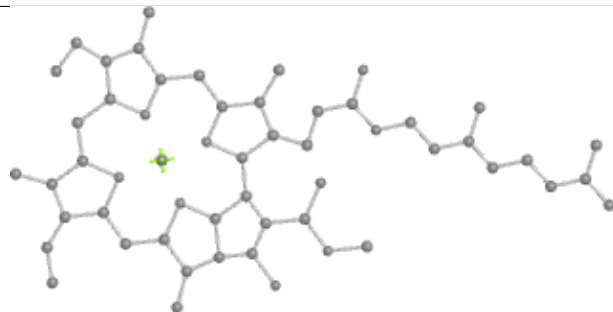
Bond lengths



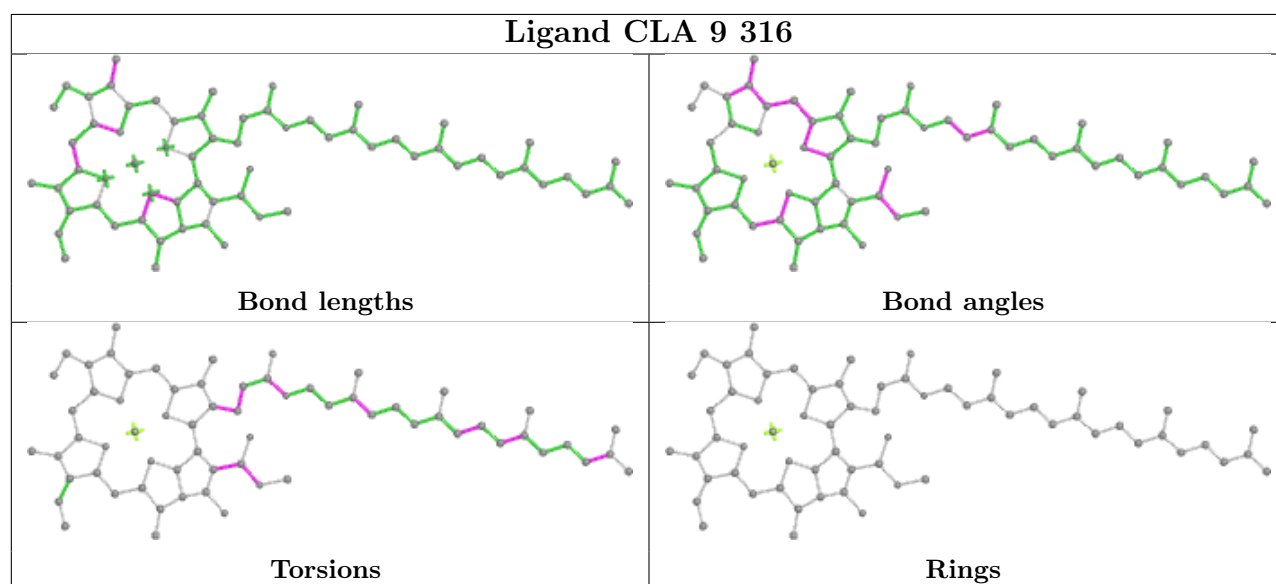
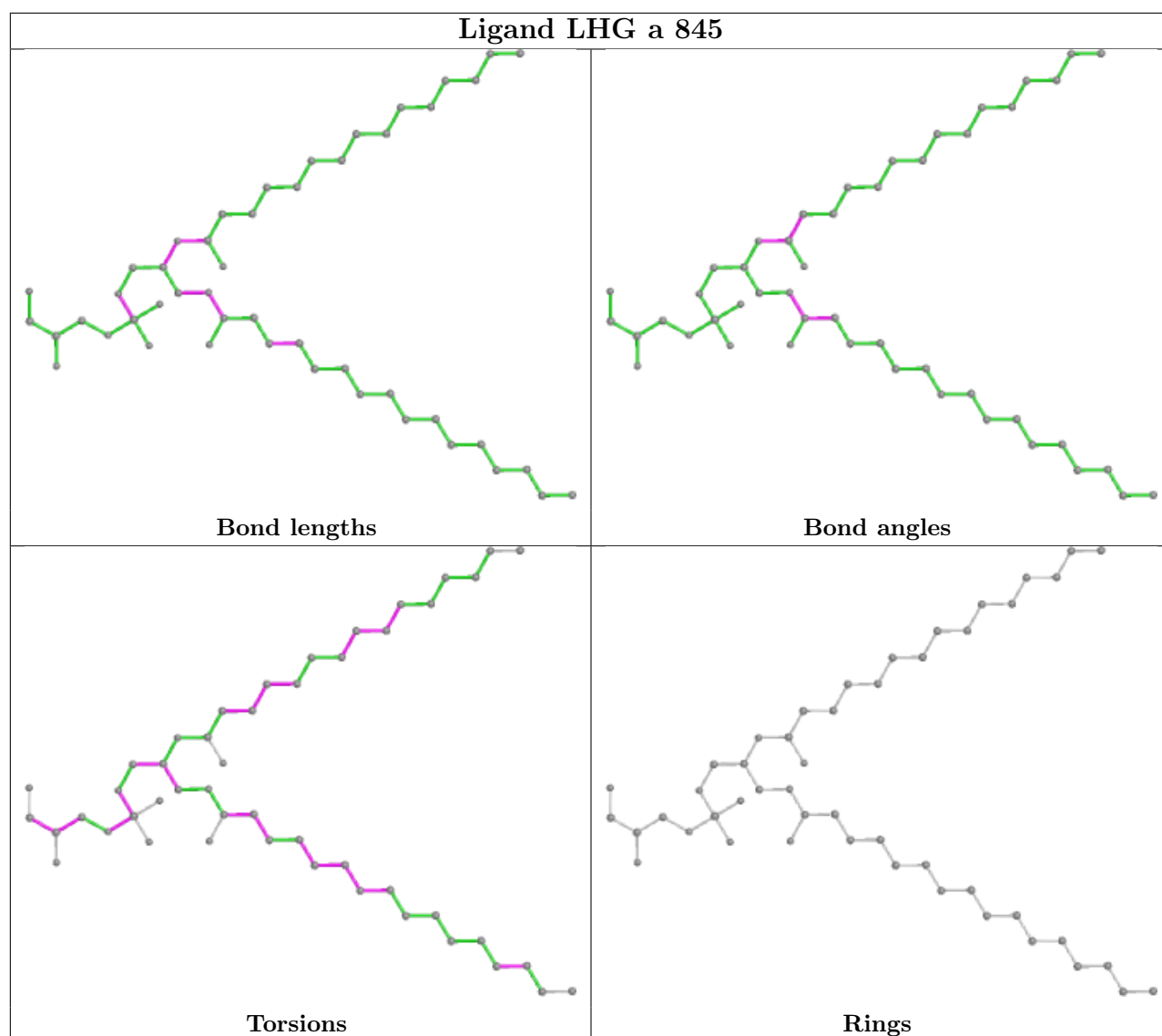
Bond angles

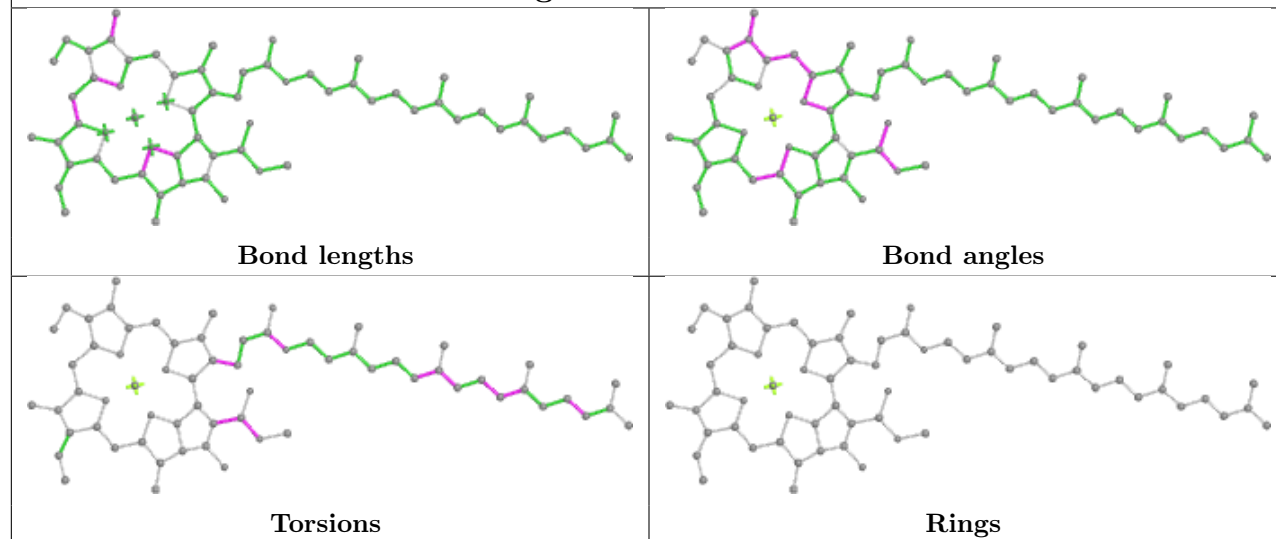
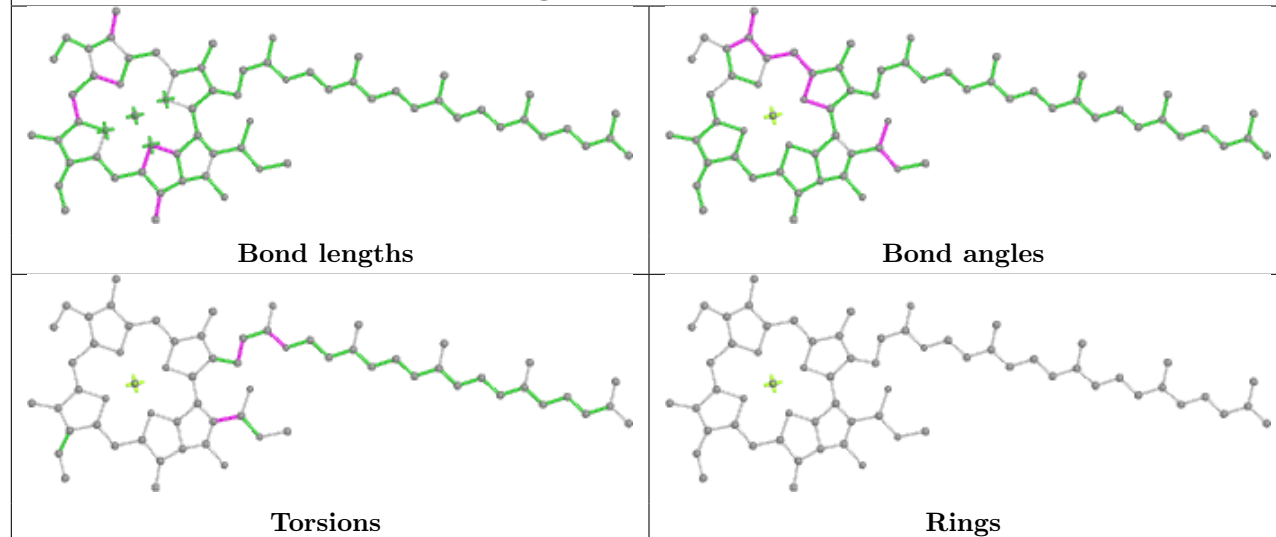


Torsions

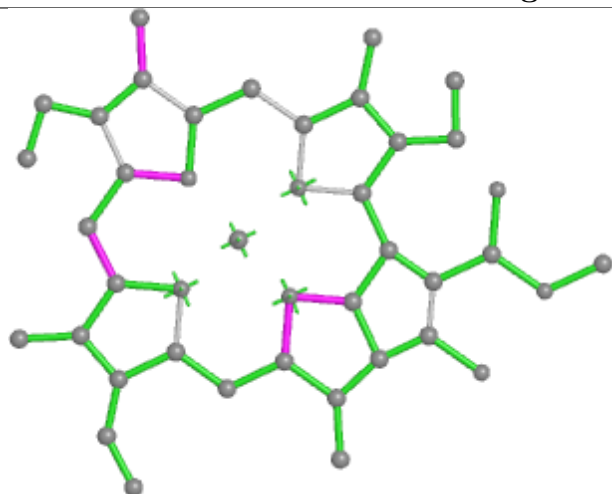


Rings

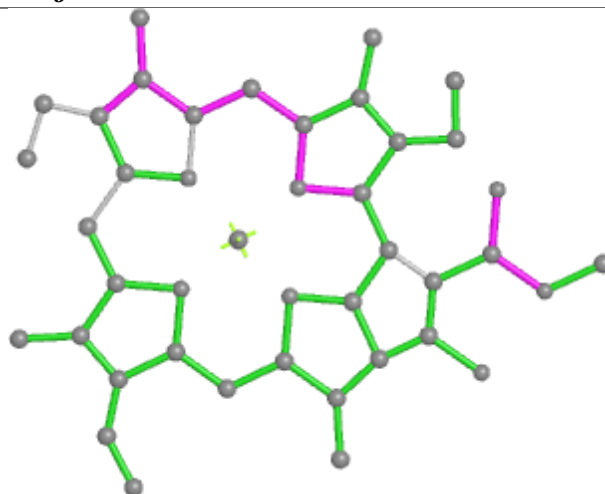


**Ligand CLA b 806****Ligand CLA b 826**

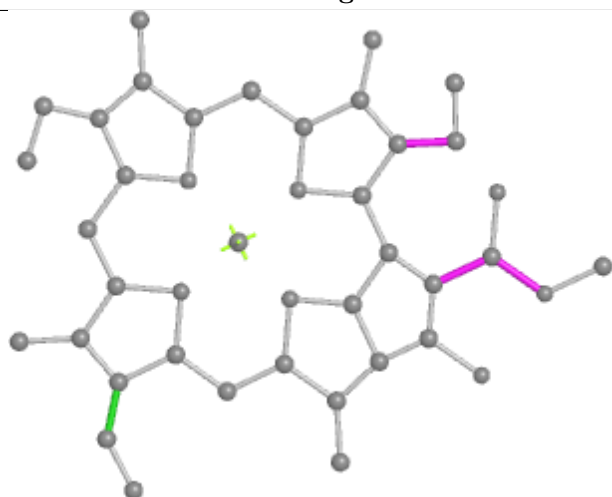
## Ligand CLA j 103



Bond lengths



Bond angles

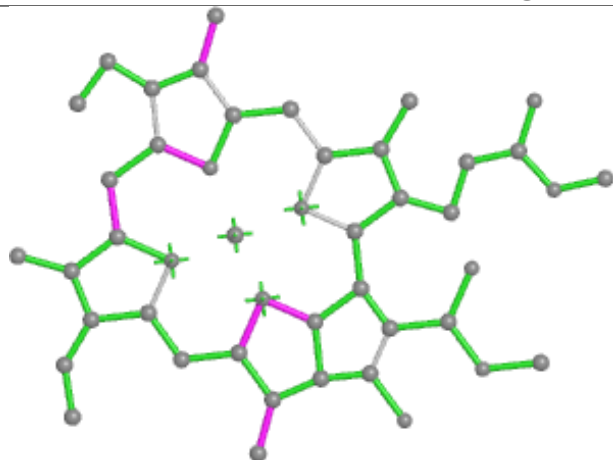


Torsions

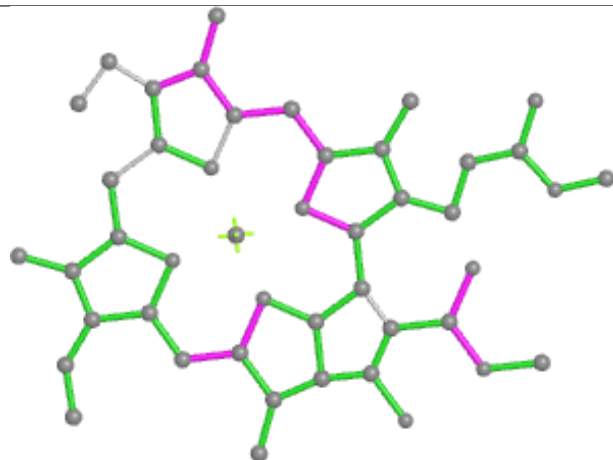


Rings

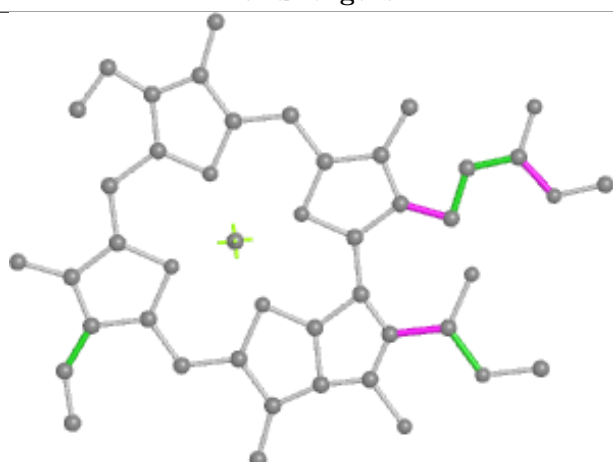
## Ligand CLA a 824



Bond lengths



Bond angles



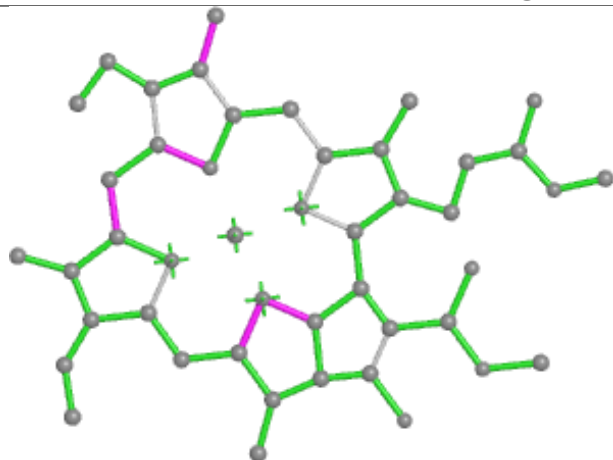
Torsions



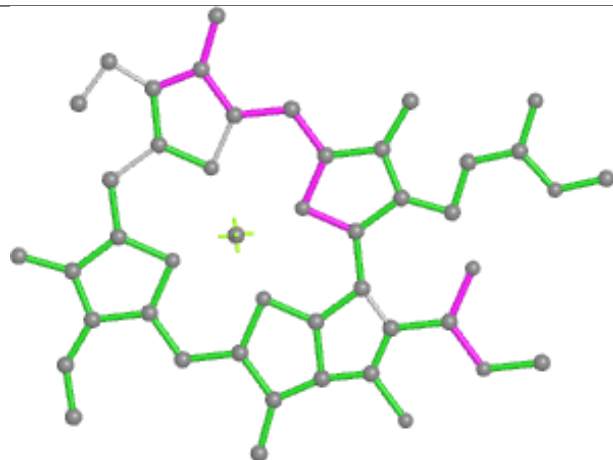
Rings



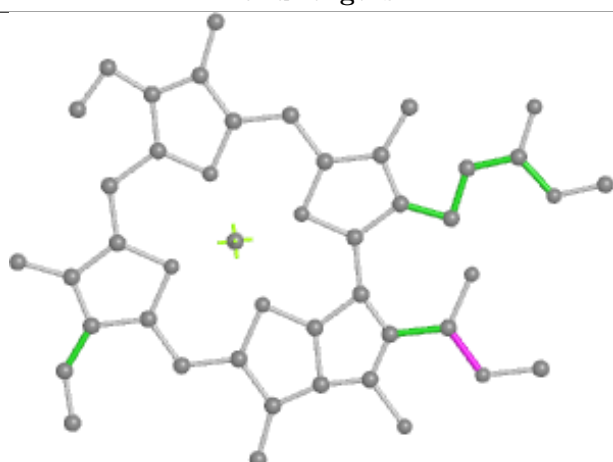
## Ligand CLA 8 306



Bond lengths



Bond angles

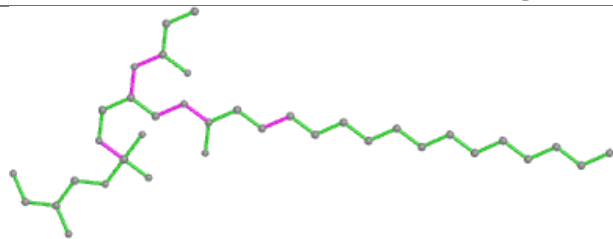


Torsions

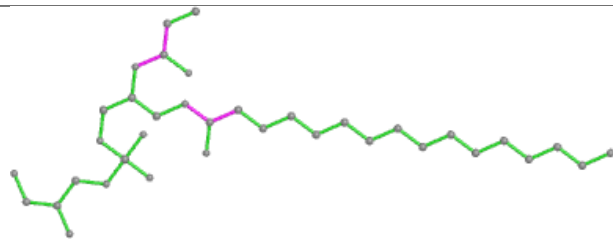


Rings

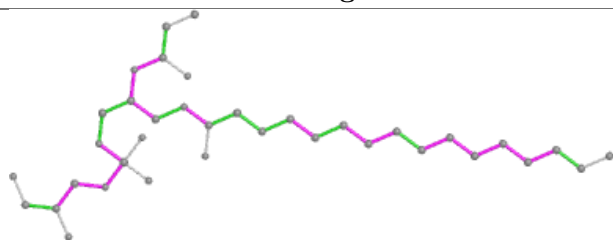
## Ligand LHG 9 307



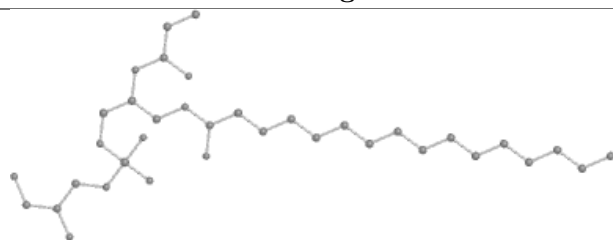
Bond lengths



Bond angles

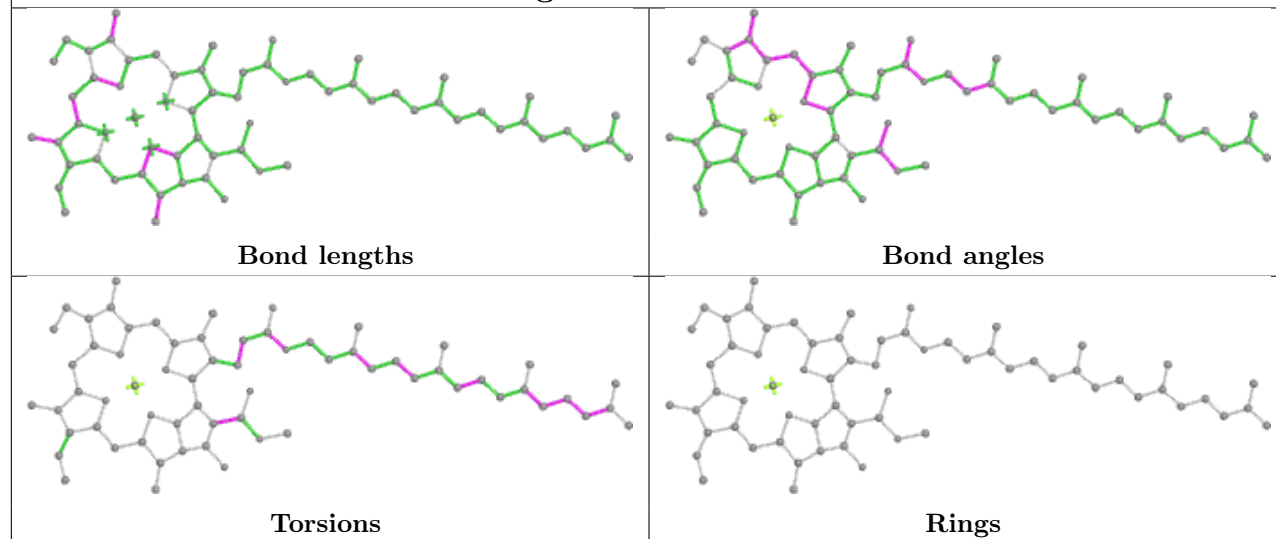


Torsions

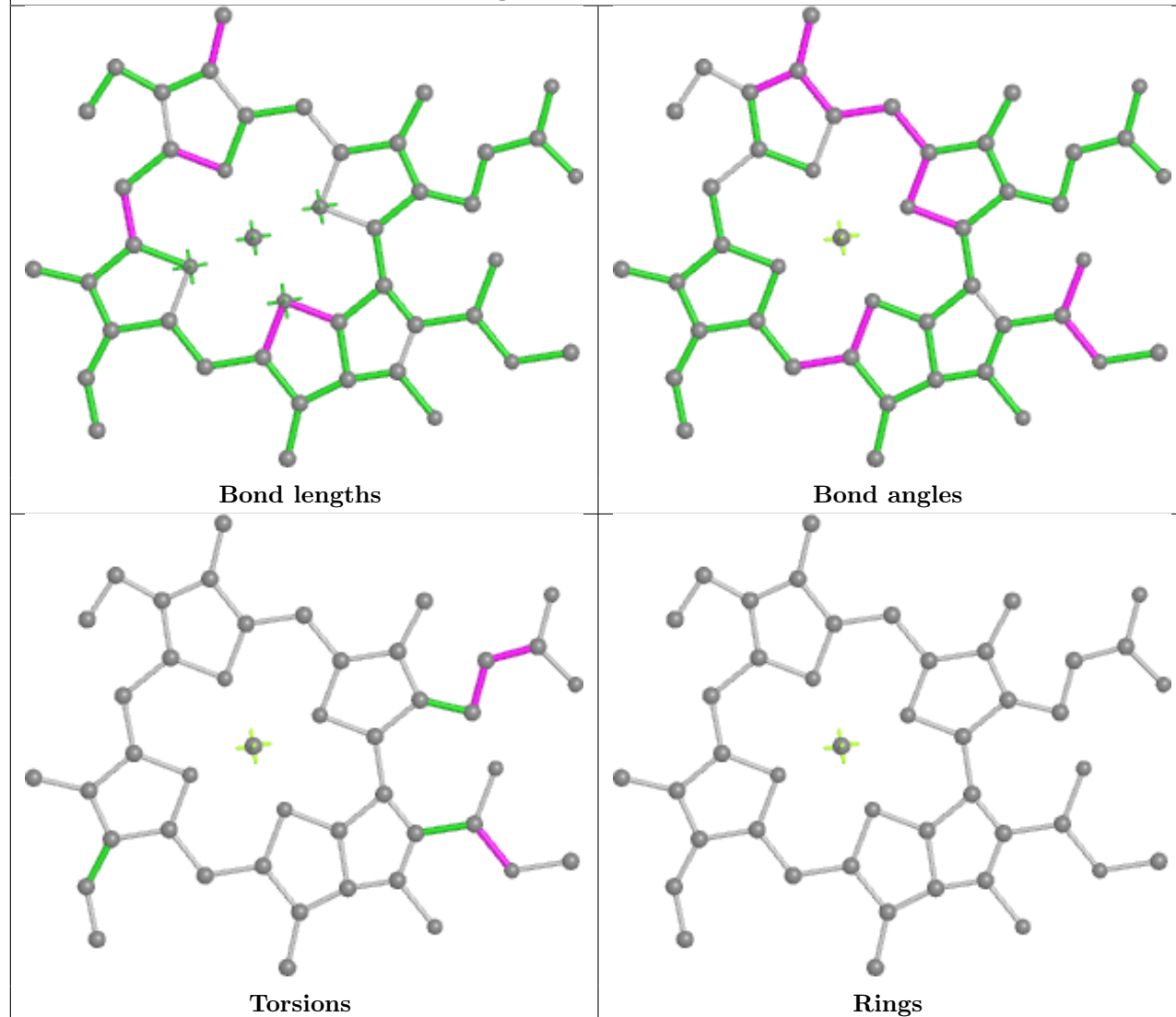


Rings

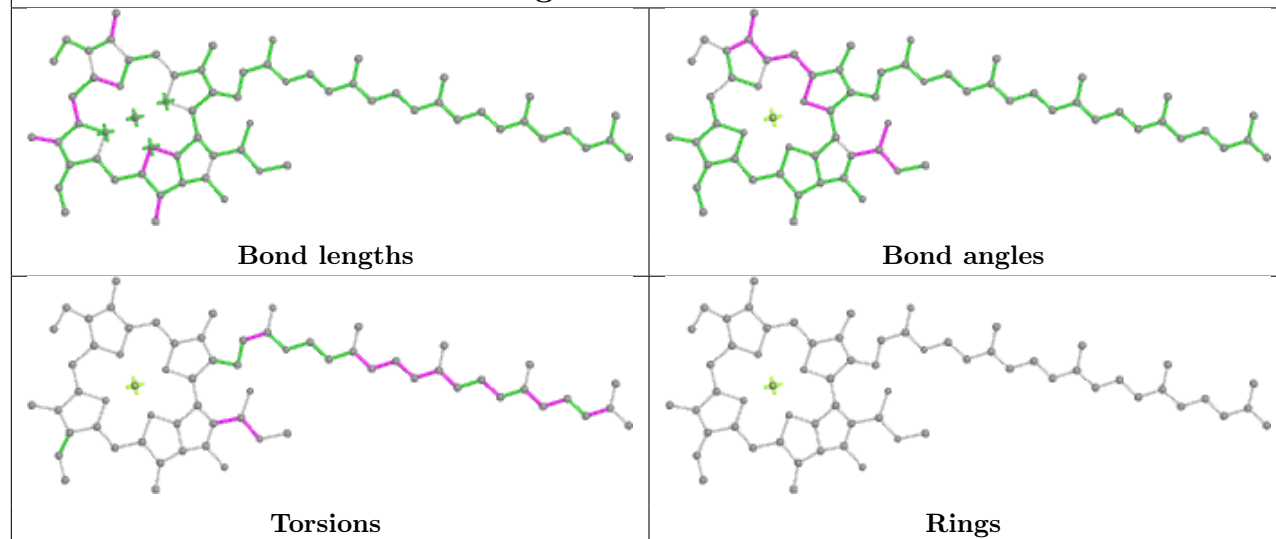
## Ligand CLA a 830



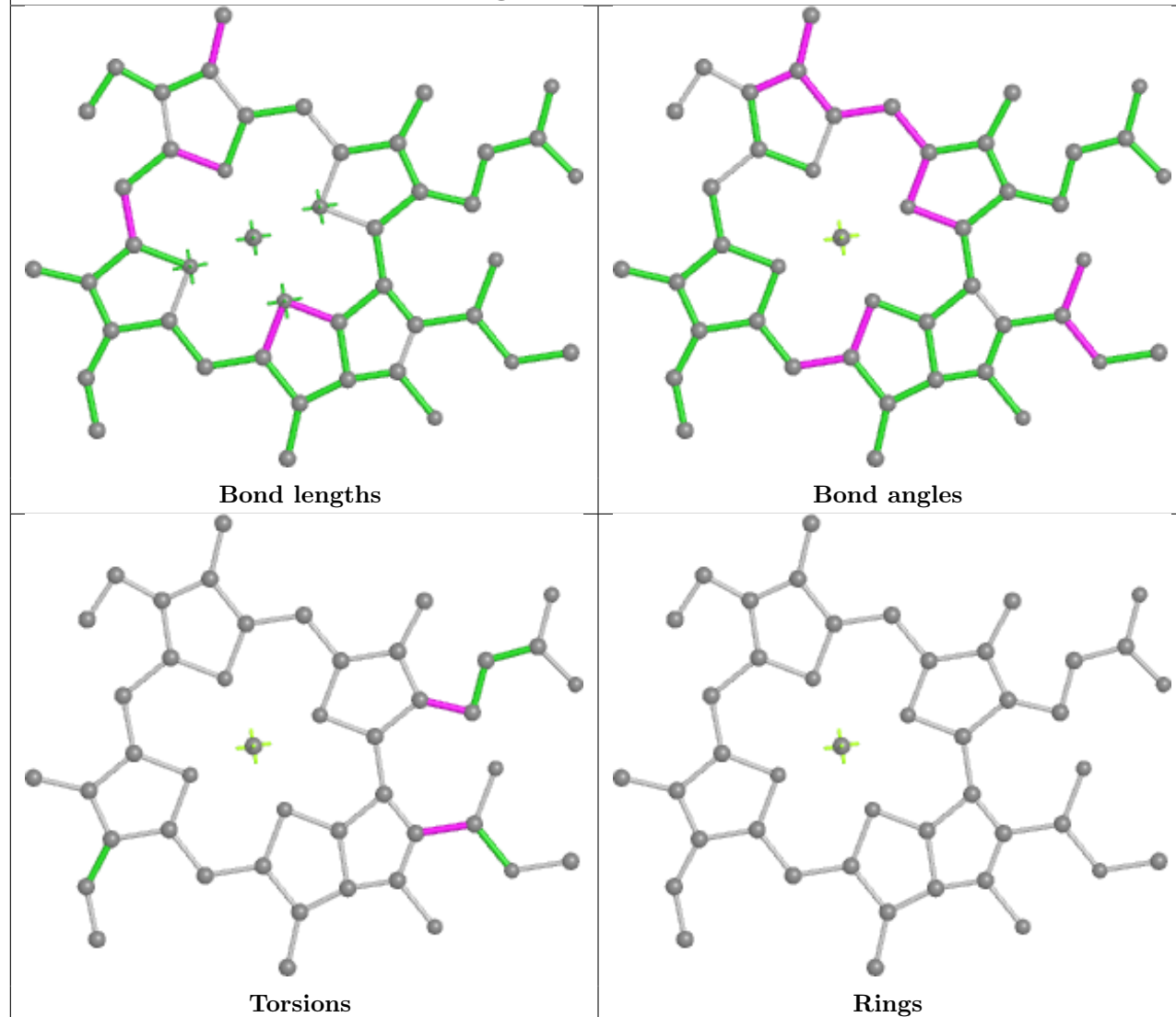
## Ligand CLA 7 317

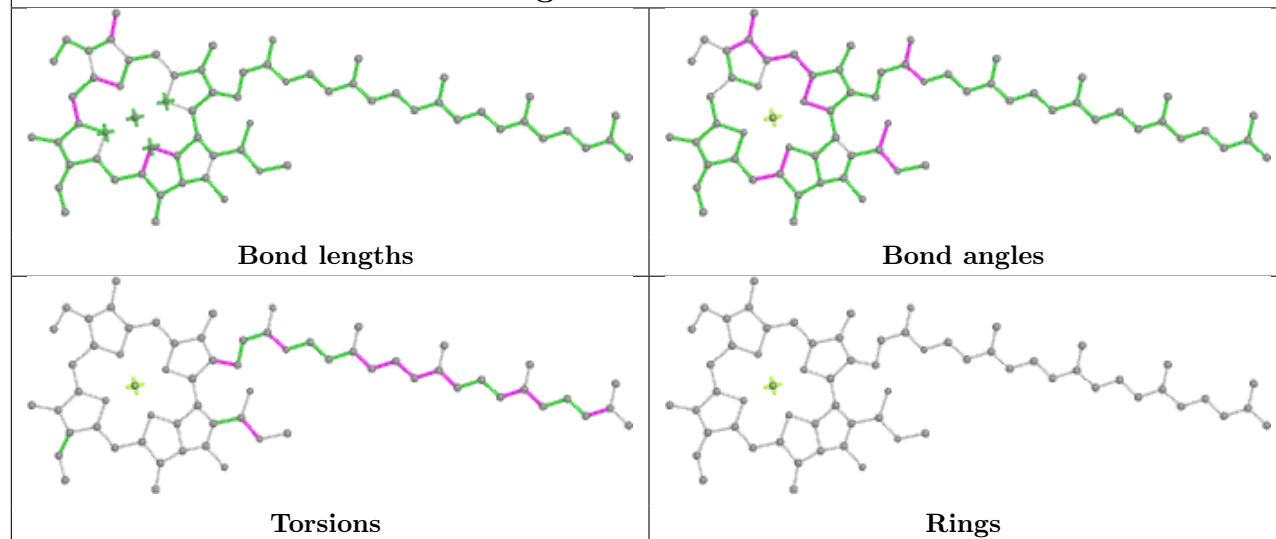
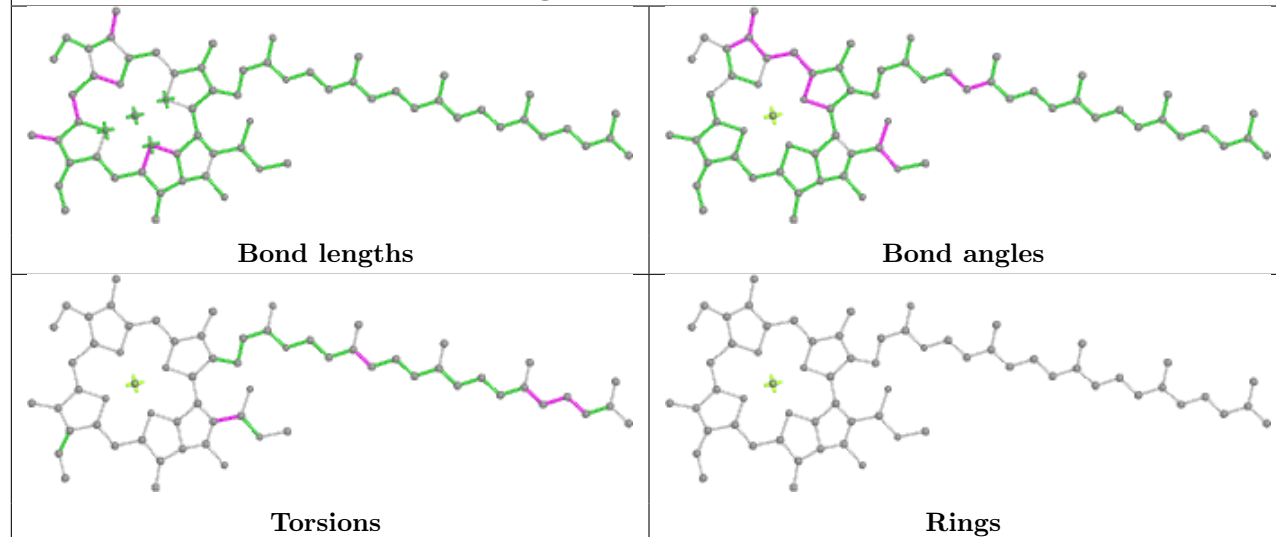


## Ligand CLA b 803

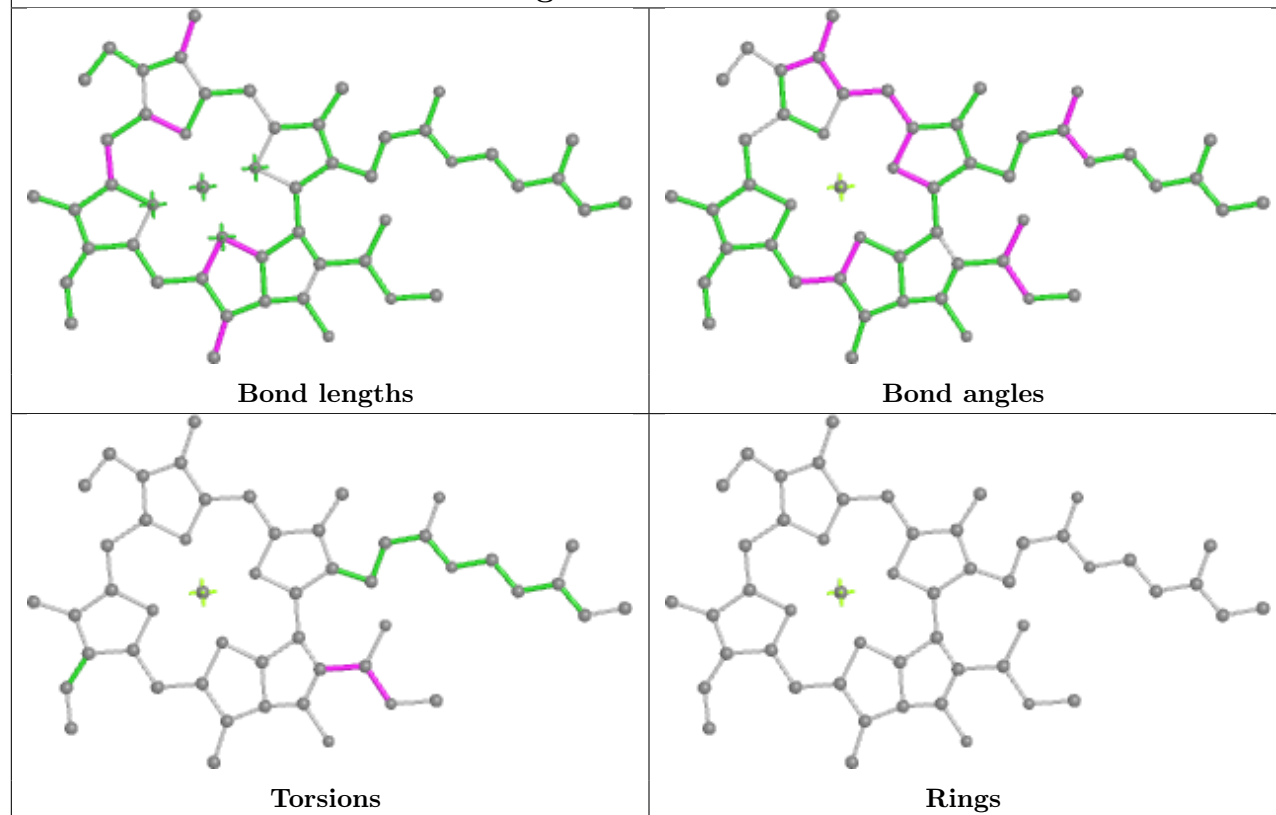


## Ligand CLA b 815

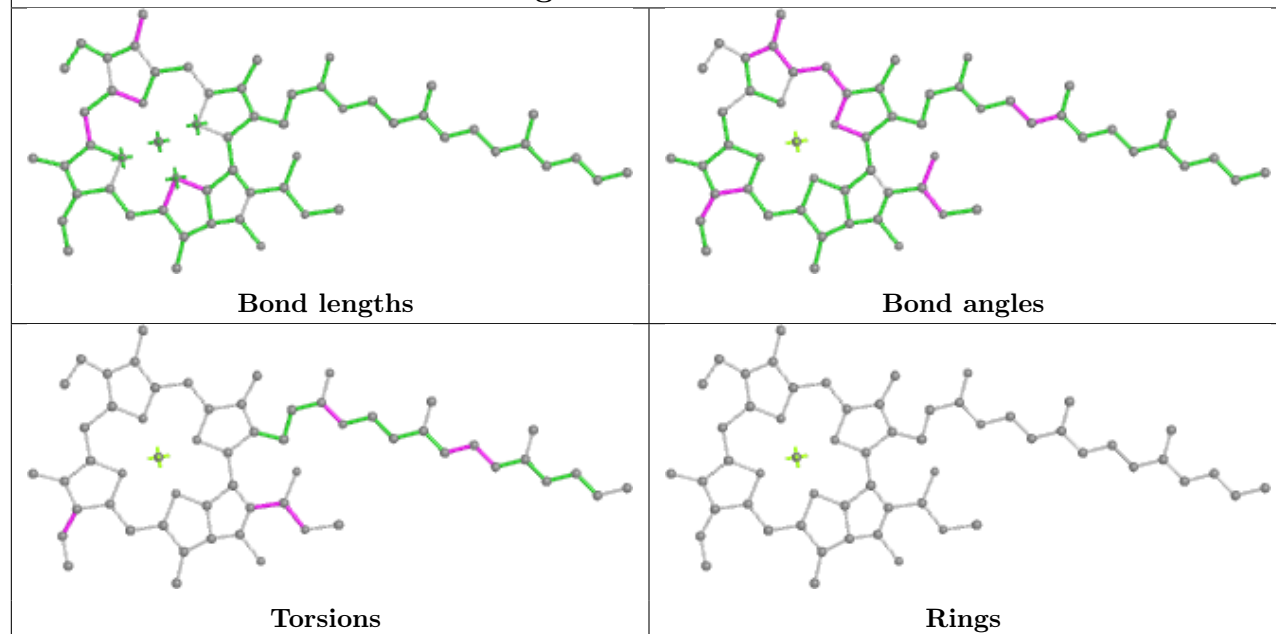


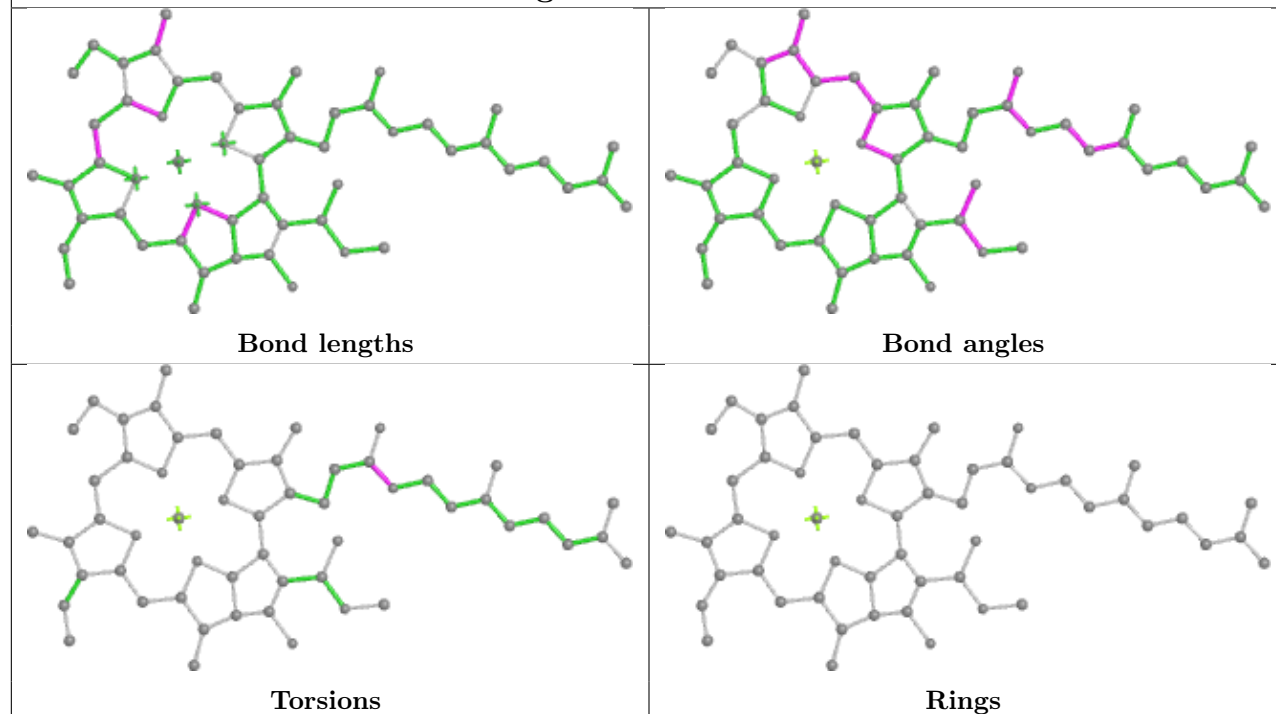
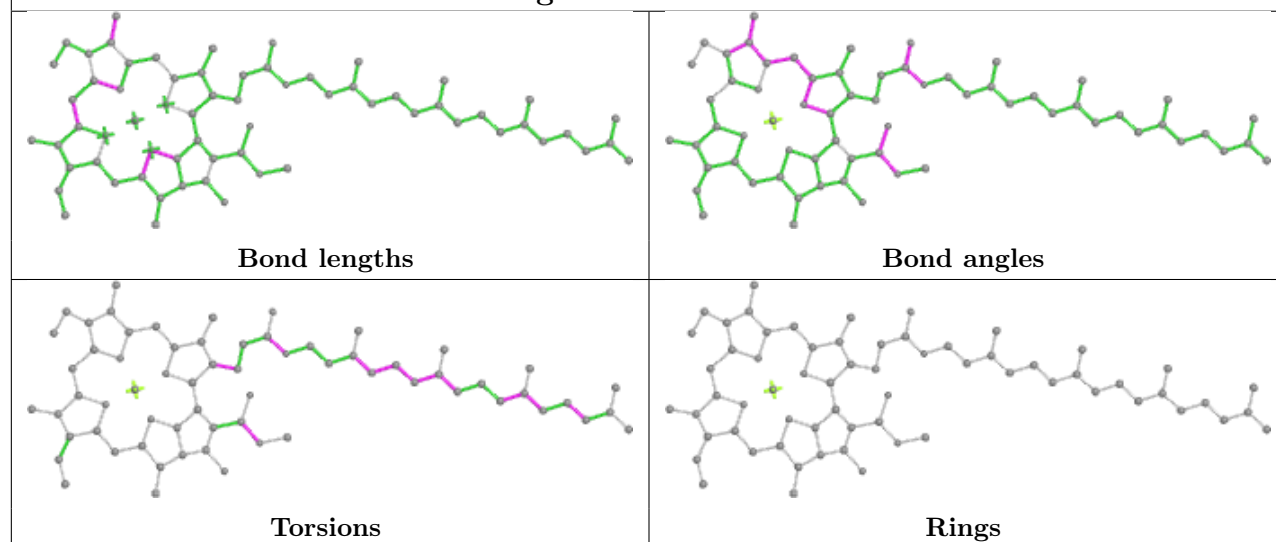
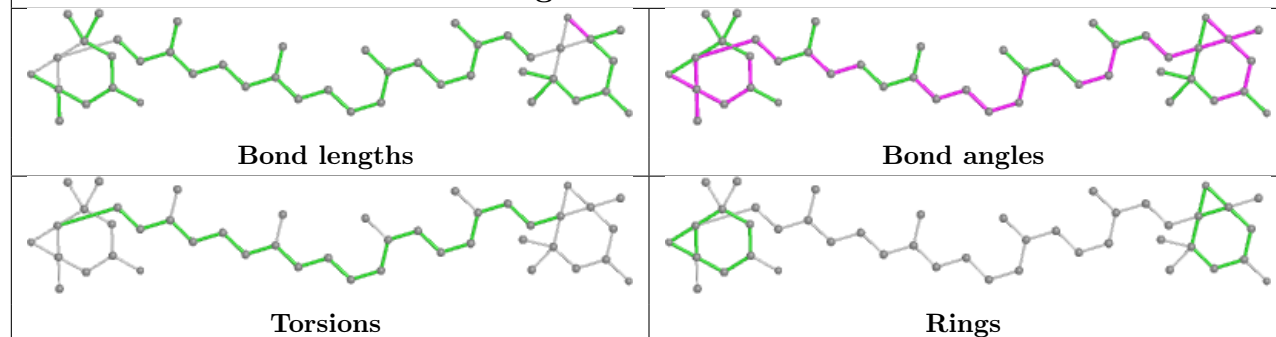
**Ligand CLA 1 310****Ligand CLA a 828**

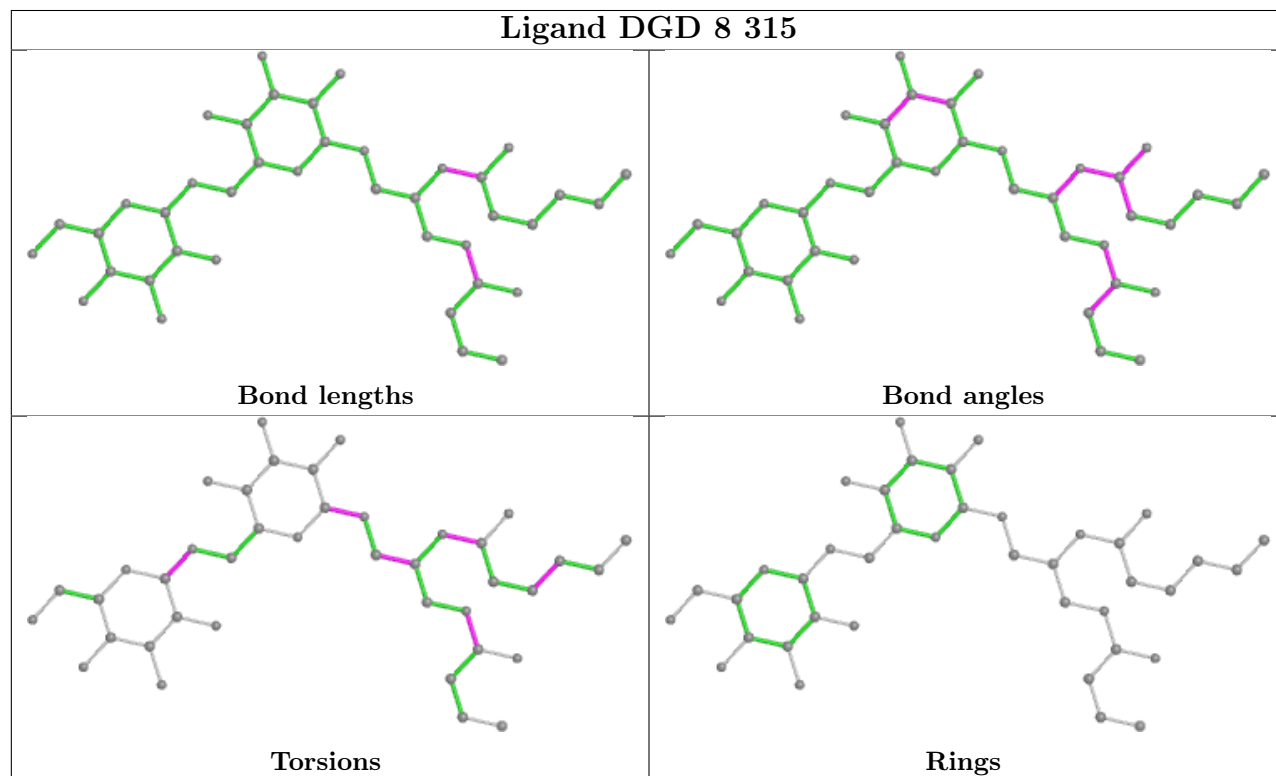
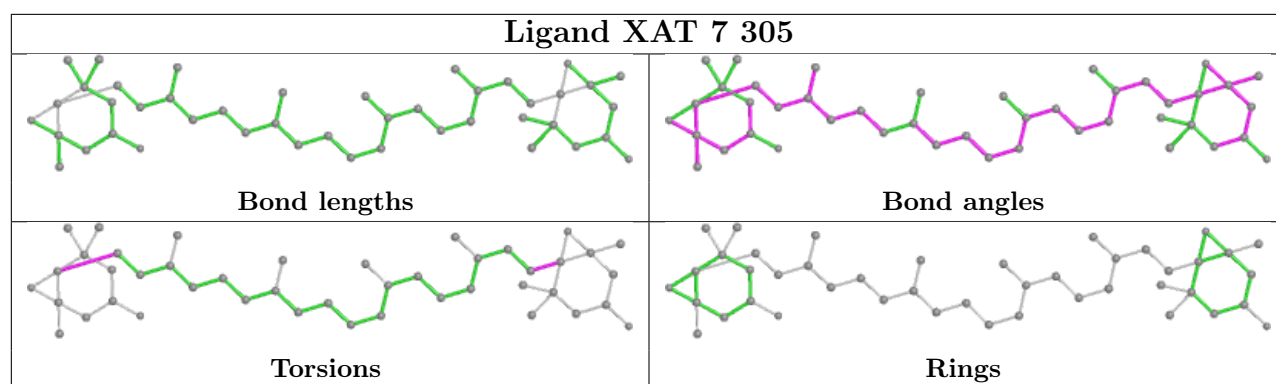
## Ligand CLA a 808

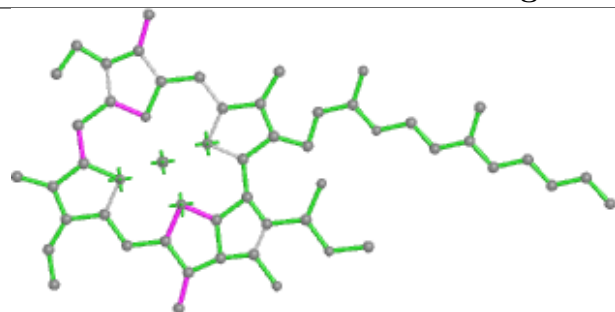


## Ligand CLA b 835

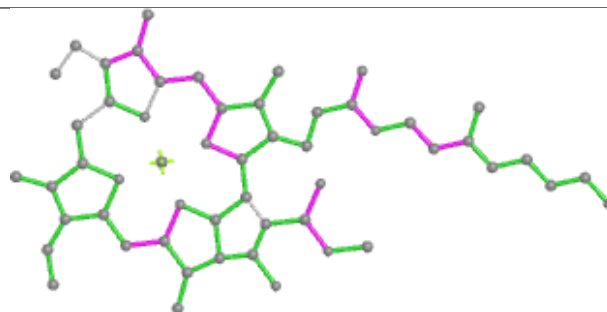


**Ligand CLA a 833****Ligand CLA a 807****Ligand XAT 1 302**

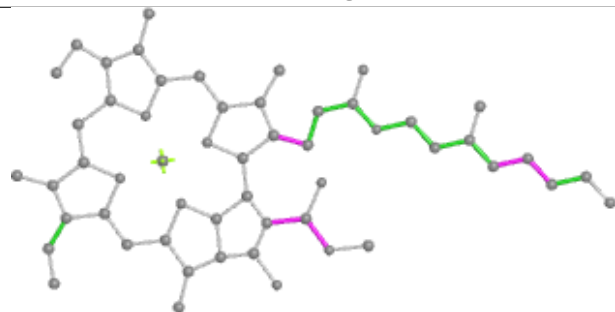


**Ligand CLA 7 313**

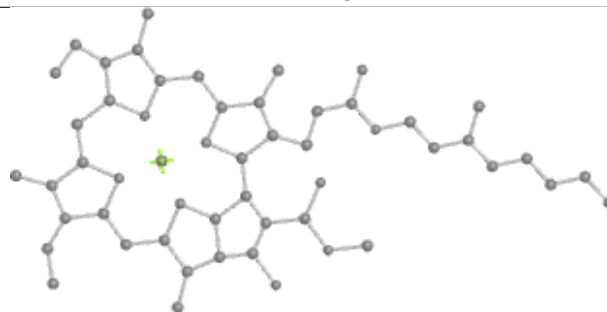
Bond lengths



Bond angles



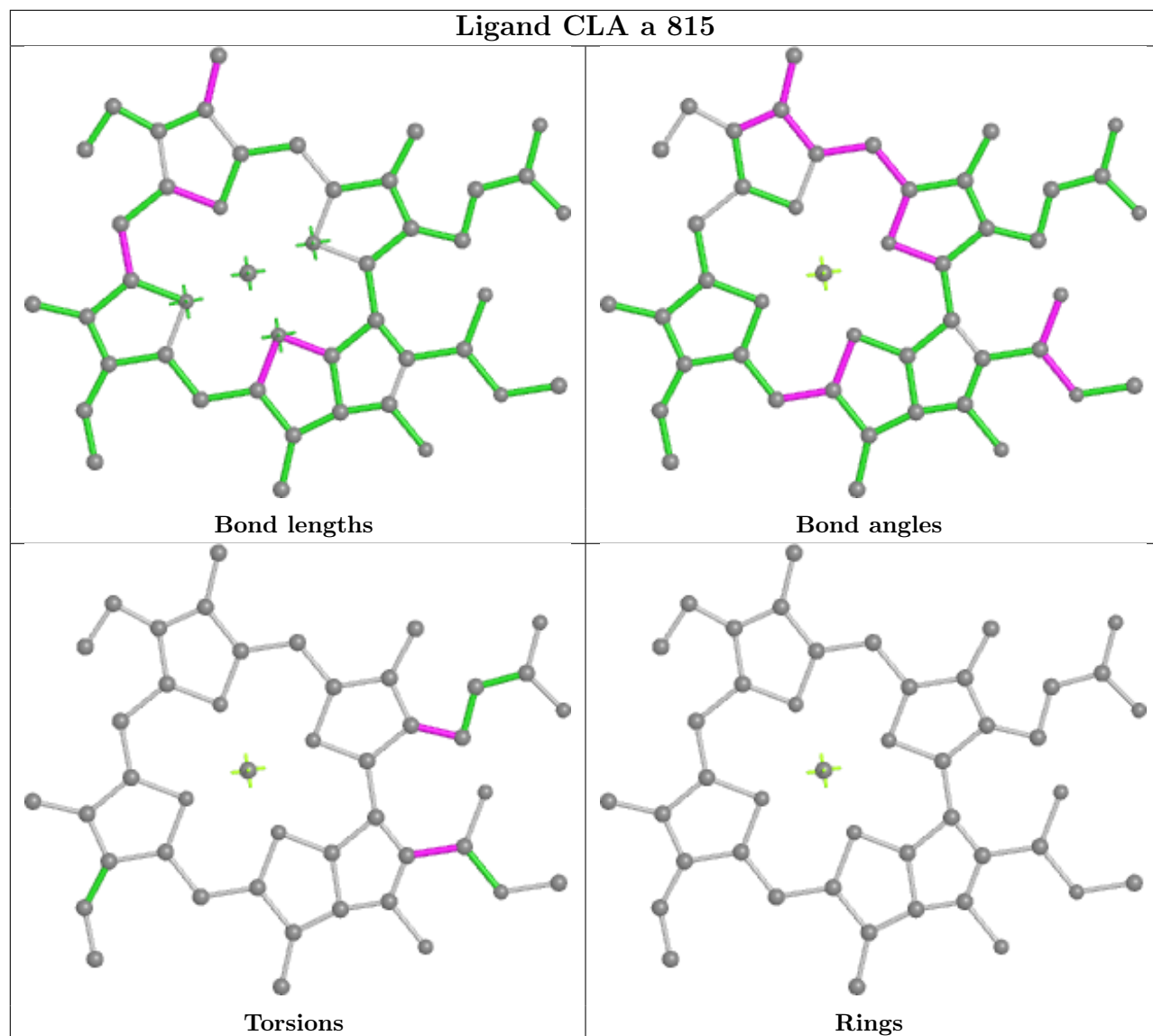
Torsions



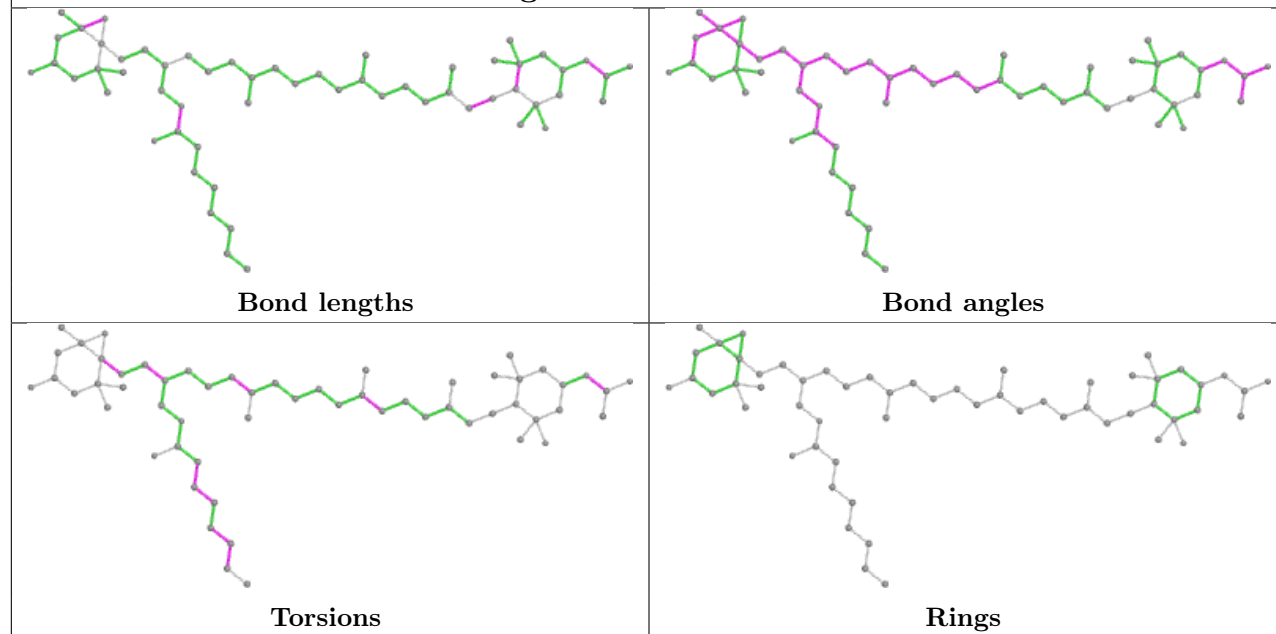
Rings



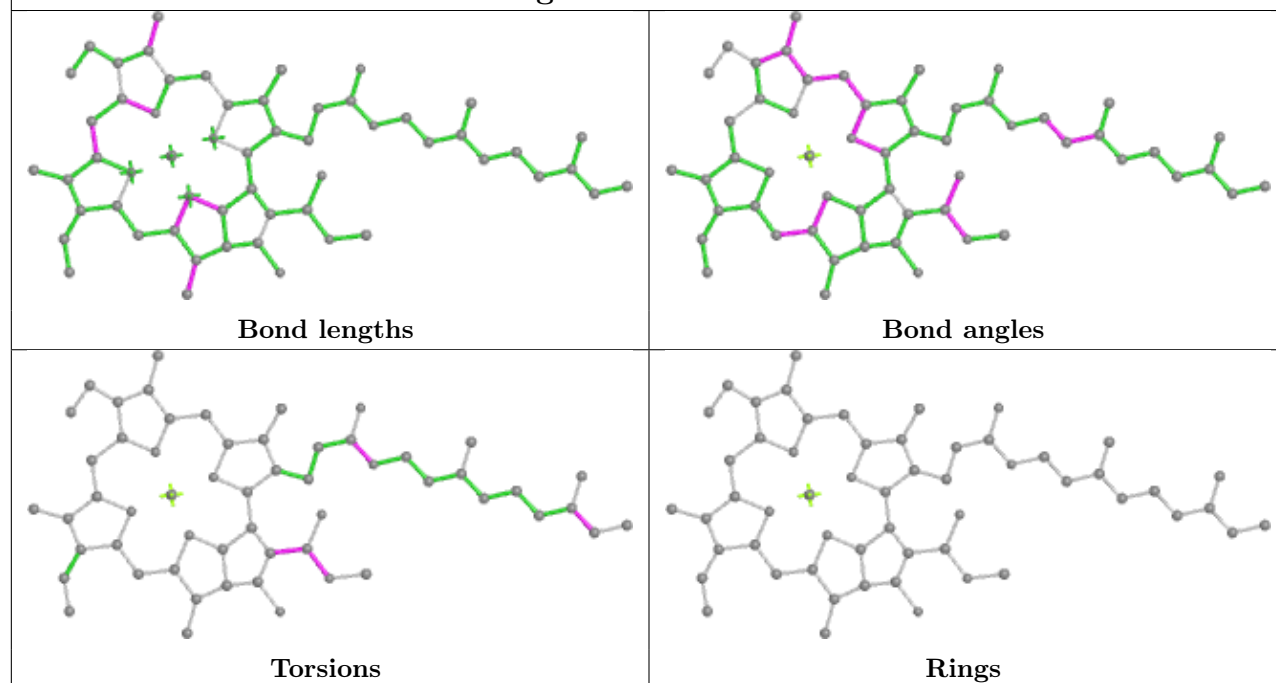
## Ligand CLA a 815



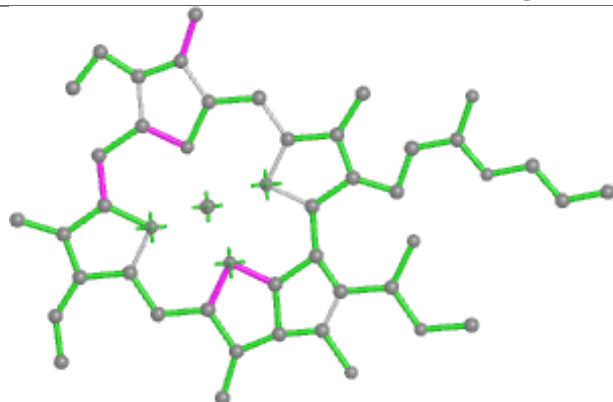
## Ligand A1L1F 1 304



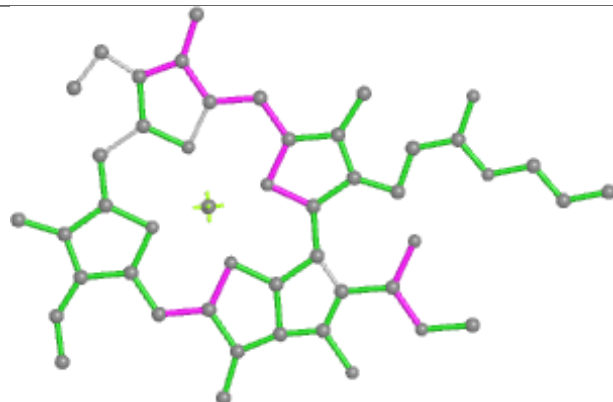
## Ligand CLA a 811



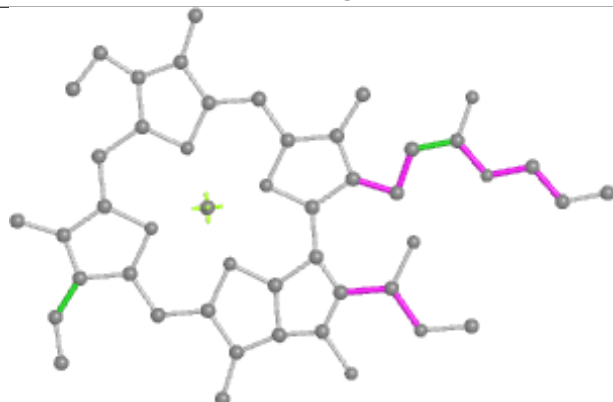
## Ligand CLA 7 306



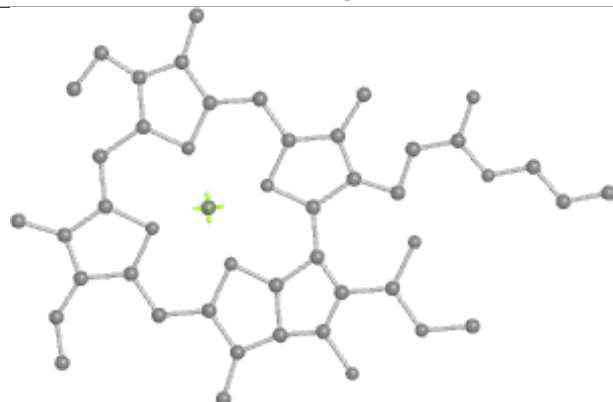
Bond lengths



Bond angles

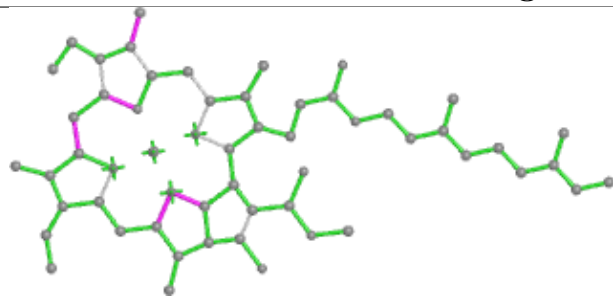


Torsions

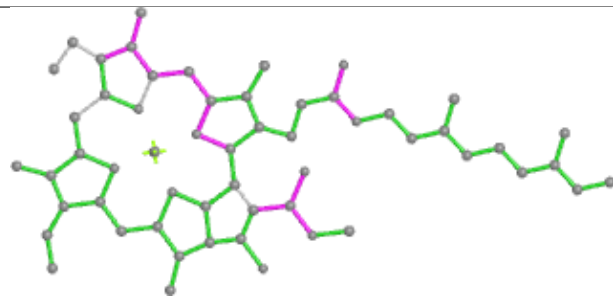


Rings

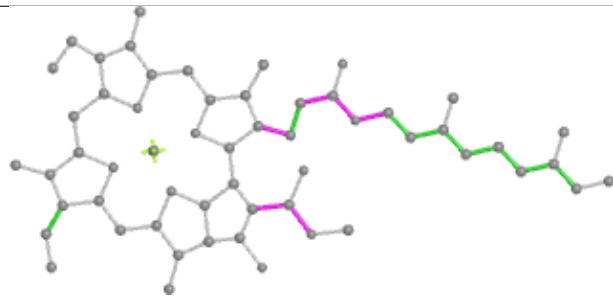
## Ligand CLA a 818



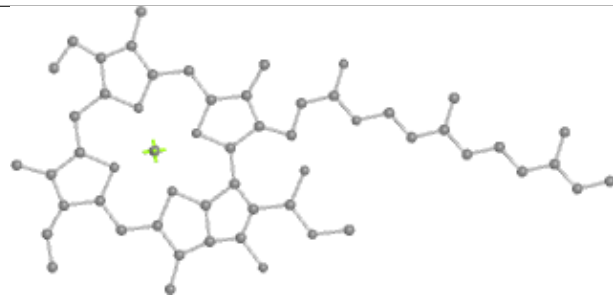
Bond lengths



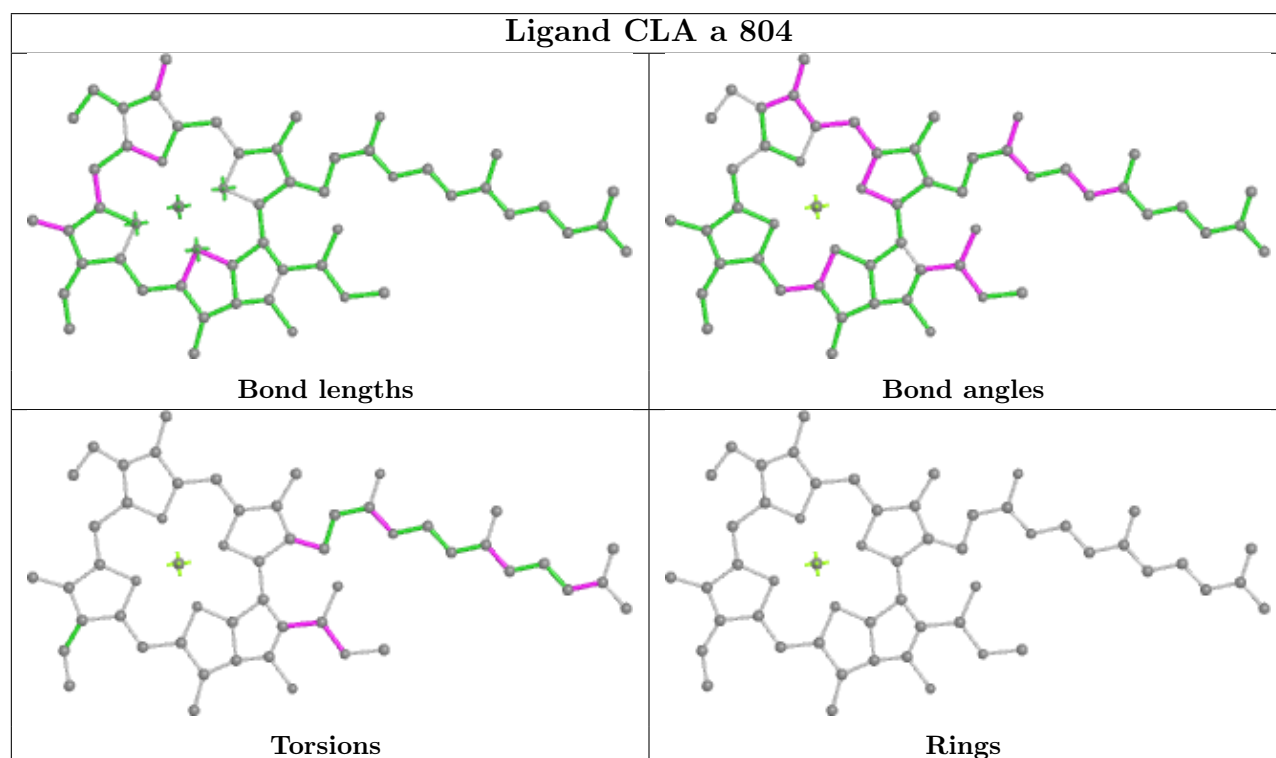
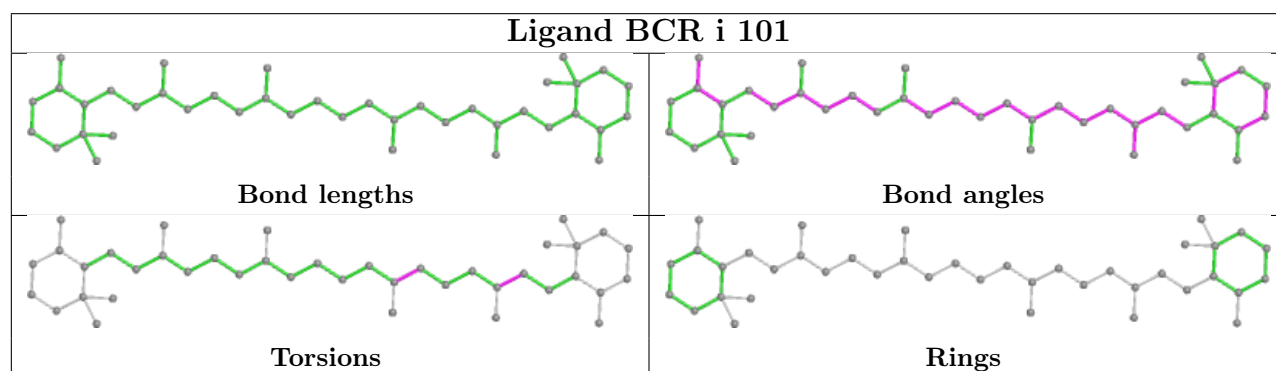
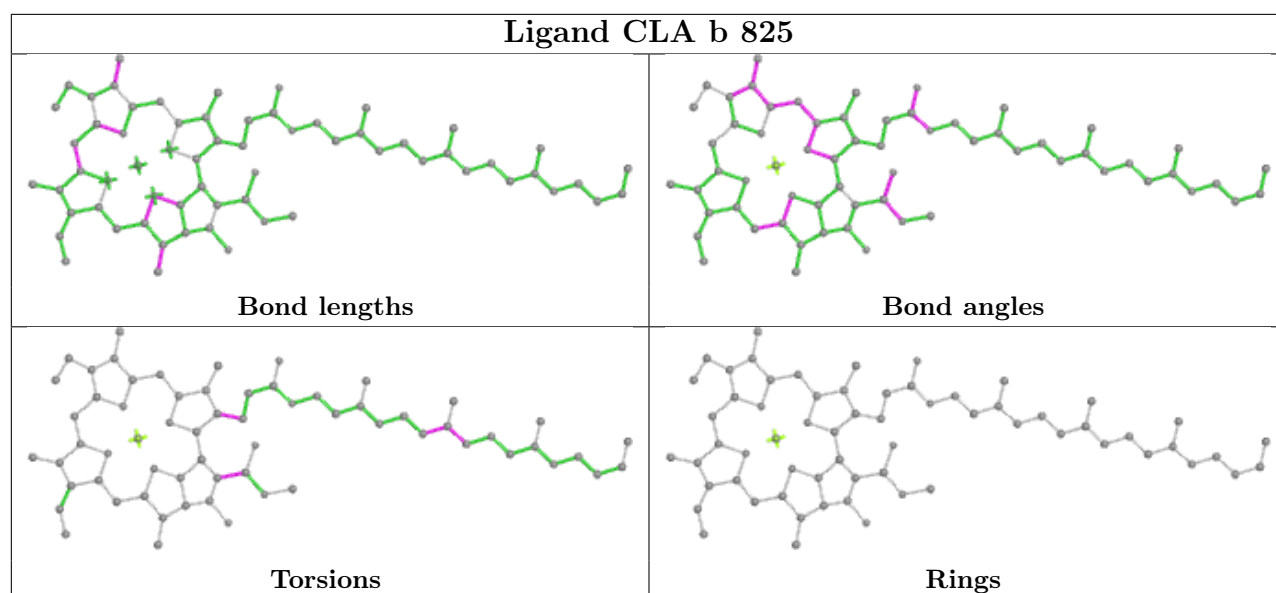
Bond angles



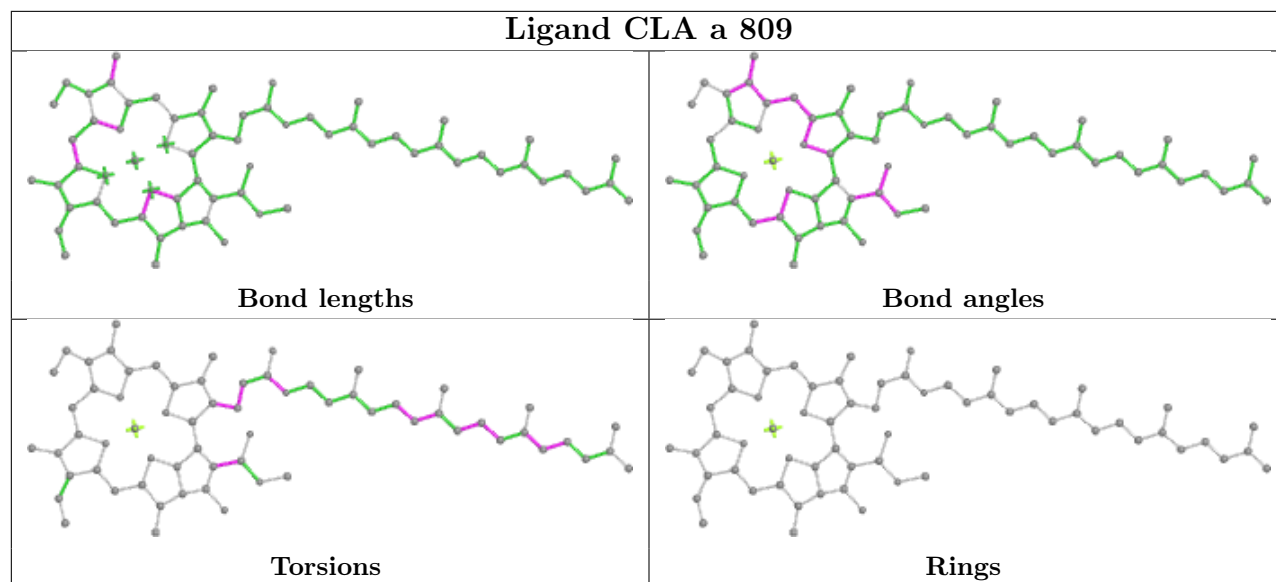
Torsions



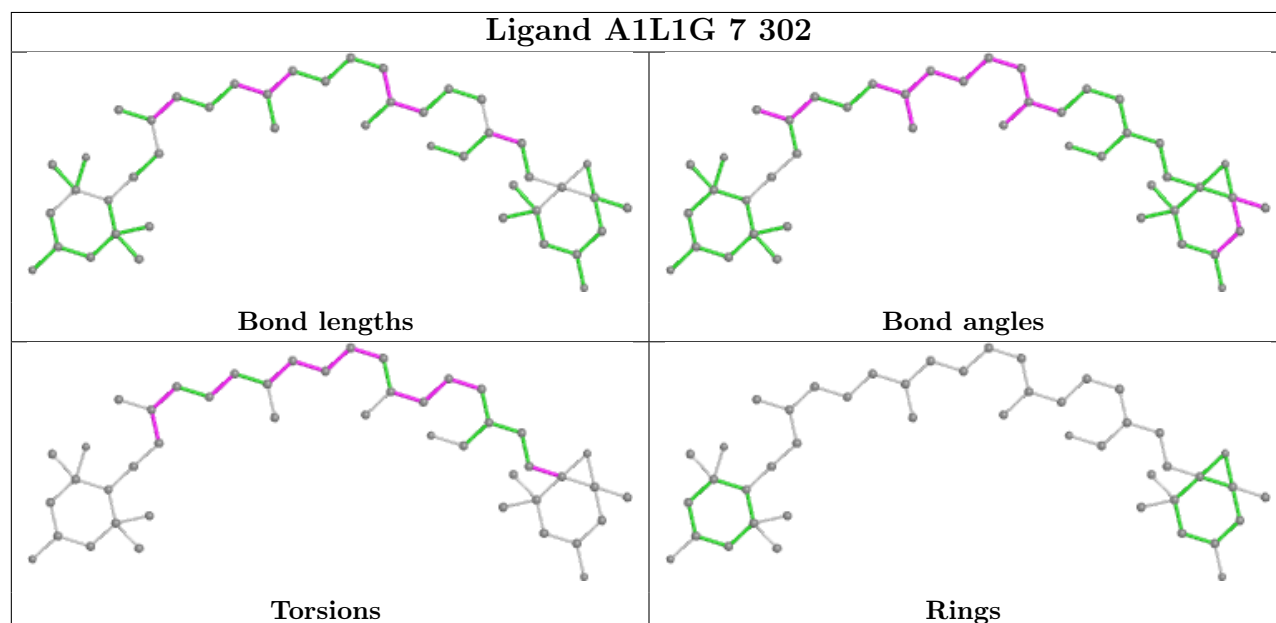
Rings



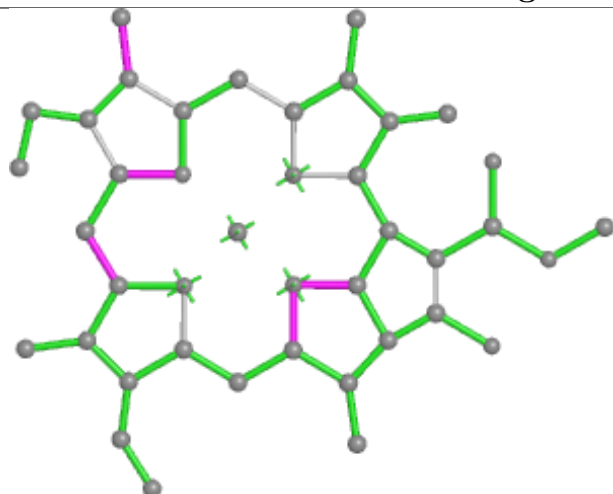
## Ligand CLA a 809



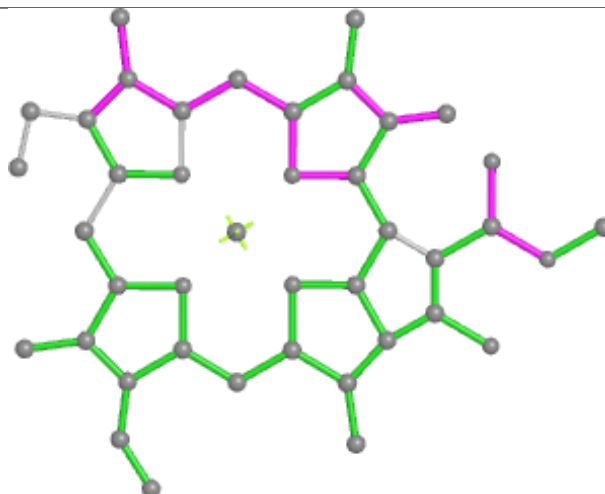
## Ligand A1L1G 7 302



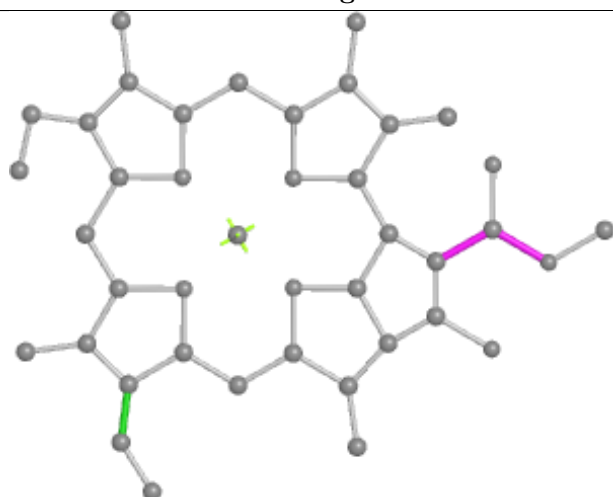
## Ligand CLA 8 314



Bond lengths



Bond angles

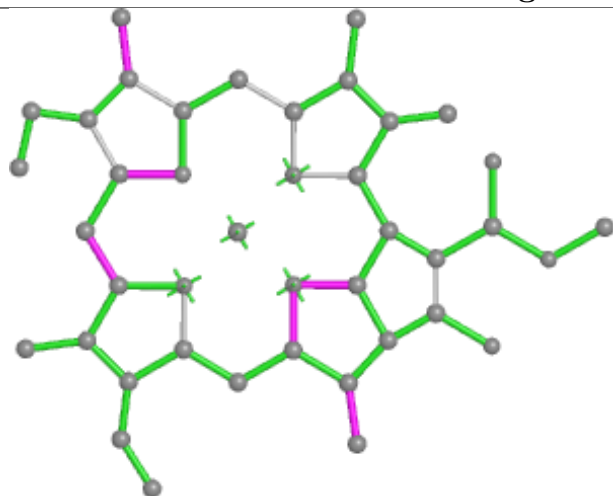


Torsions

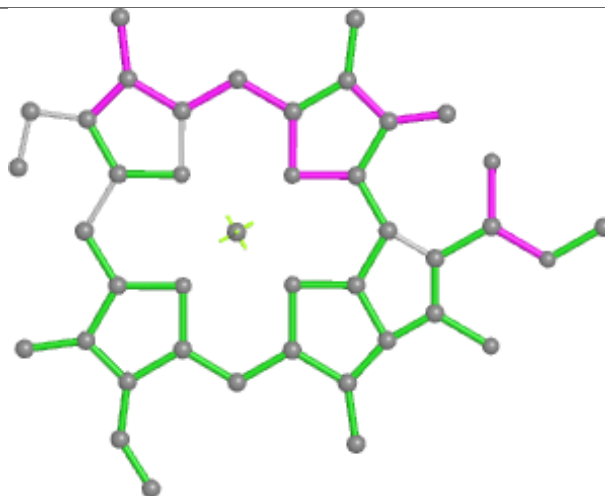


Rings

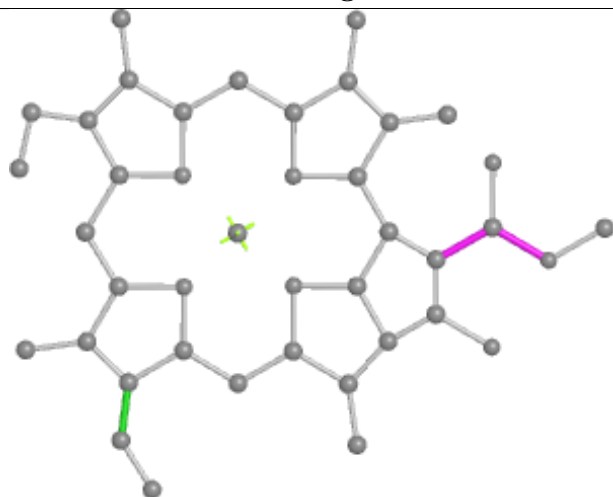
## Ligand CLA 1 313



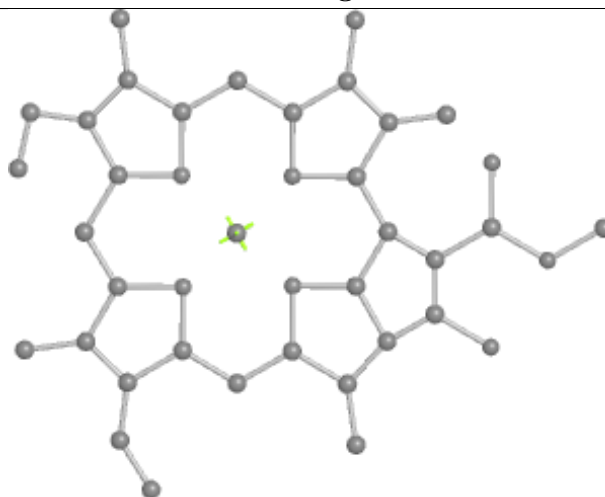
Bond lengths



Bond angles

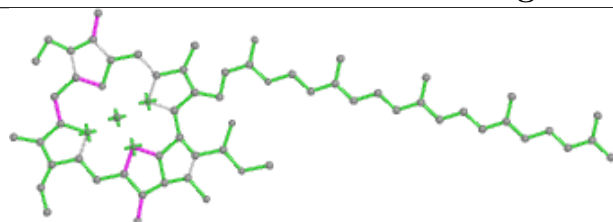


Torsions

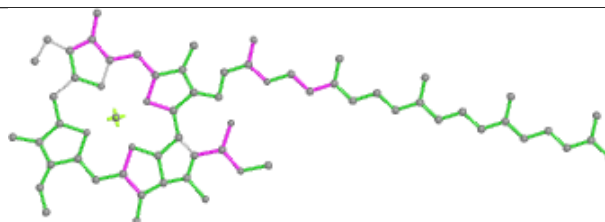


Rings

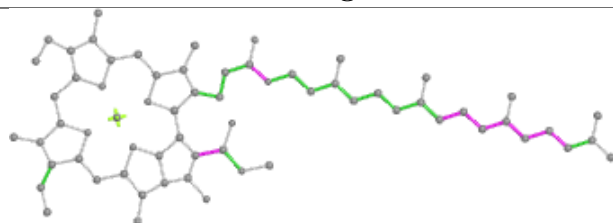
## Ligand CLA b 829



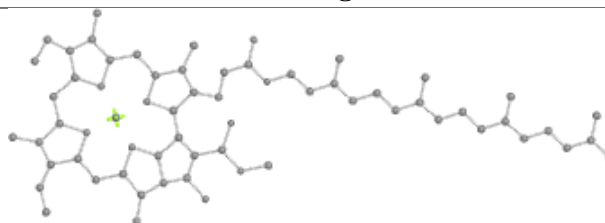
Bond lengths



Bond angles

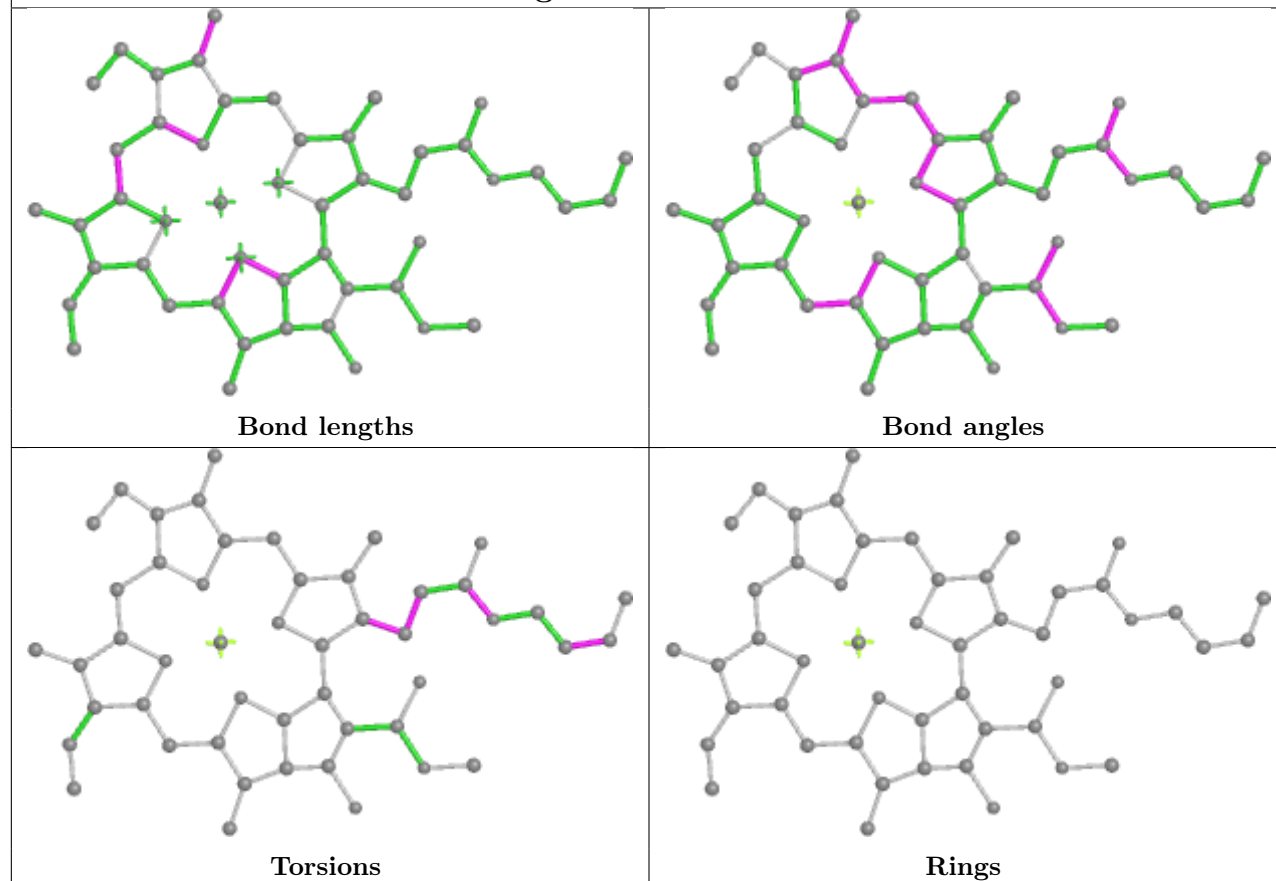


Torsions

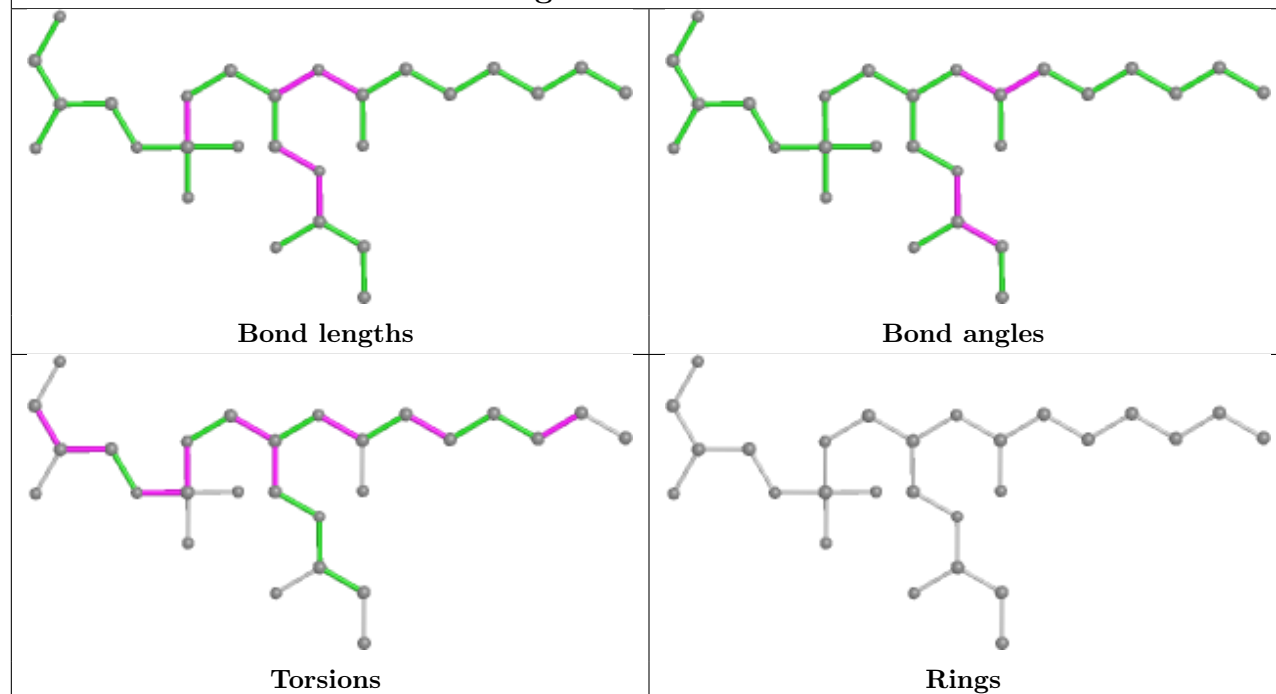


Rings

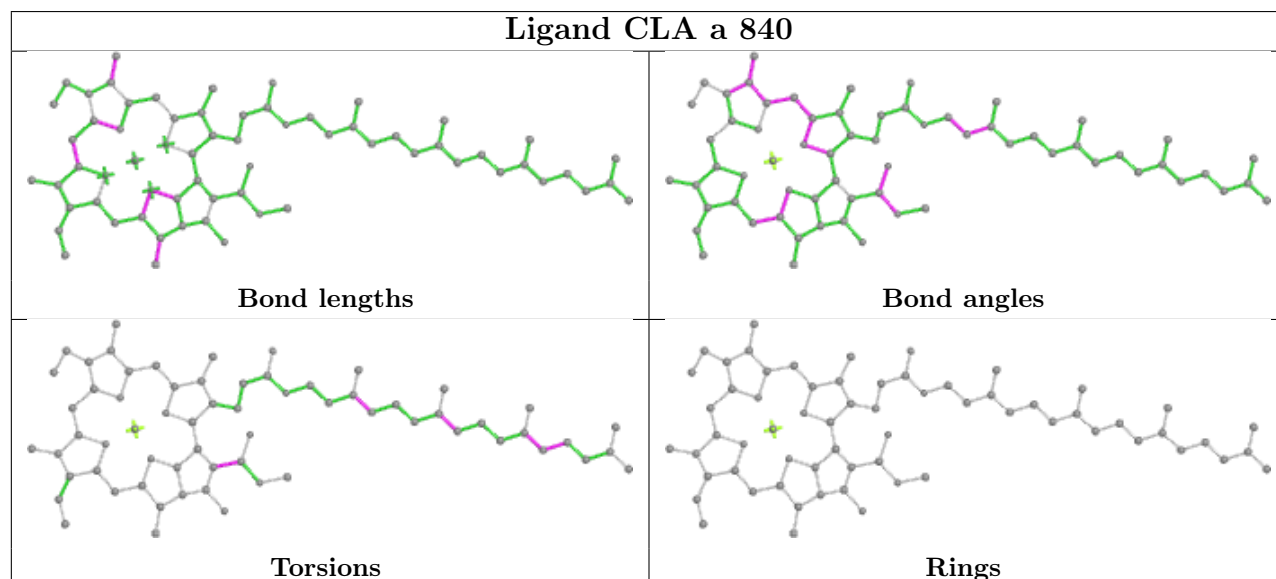
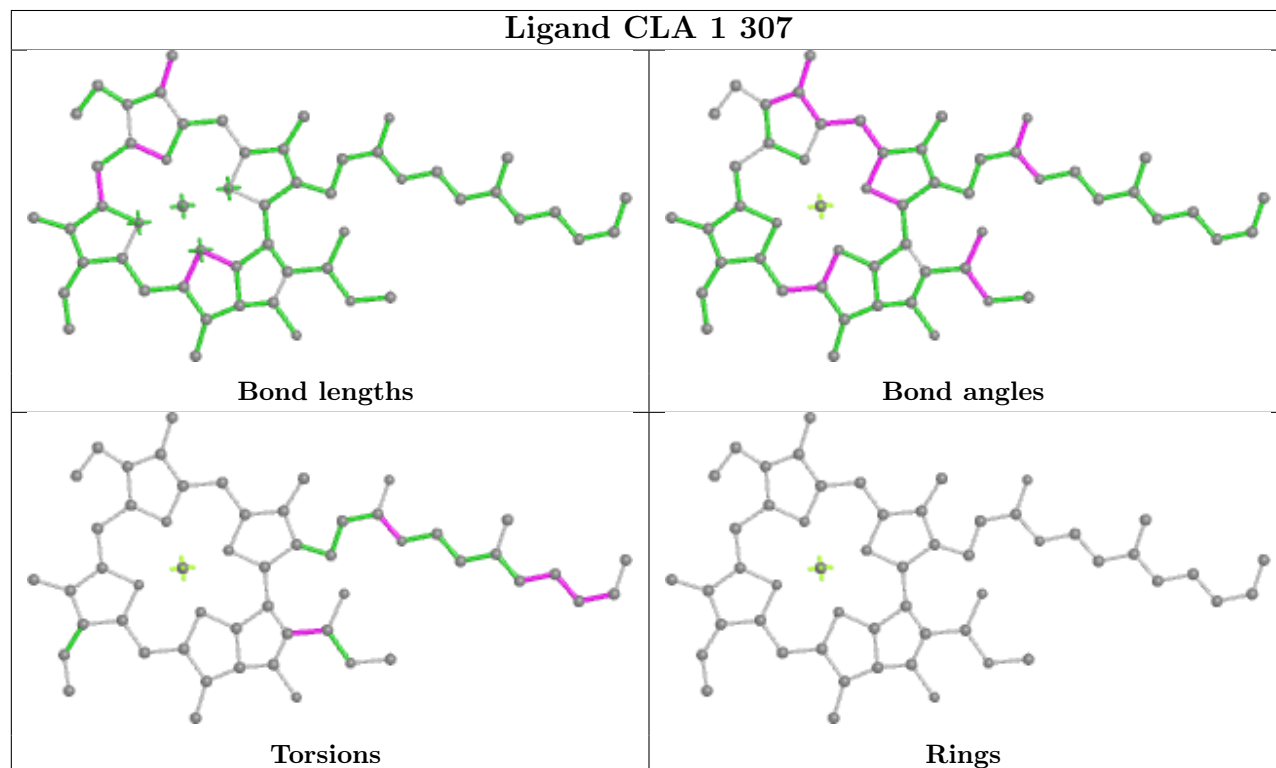
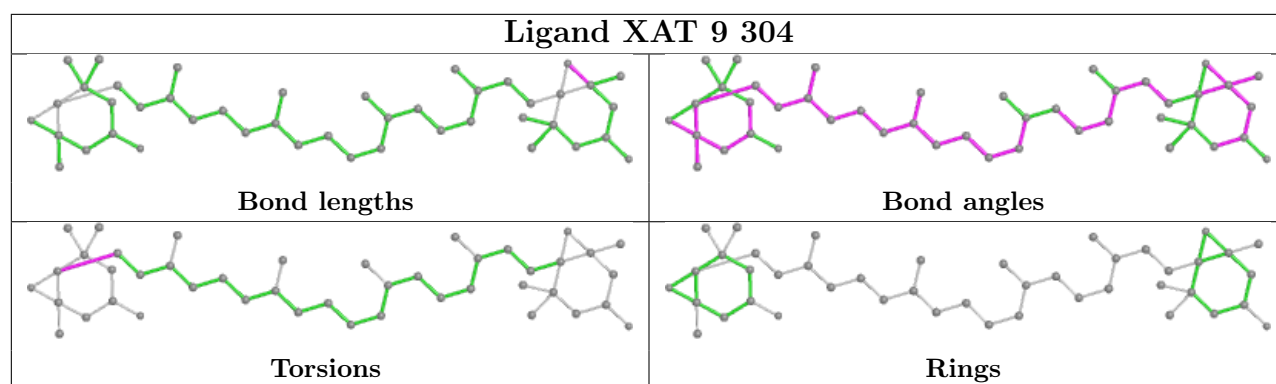
## Ligand CLA b 831



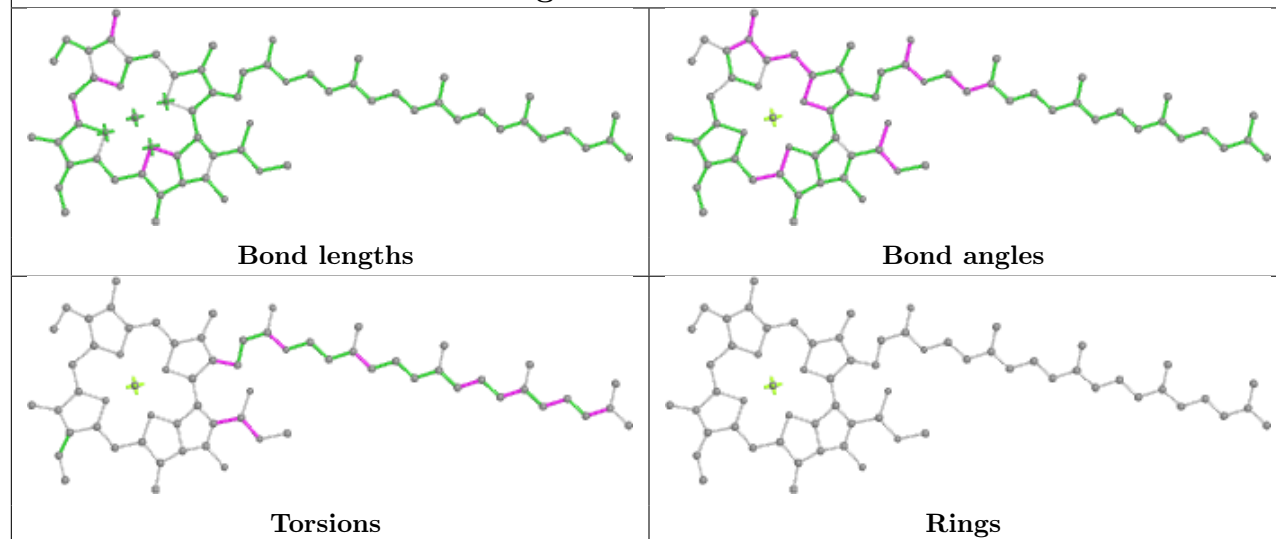
## Ligand LHG a 846



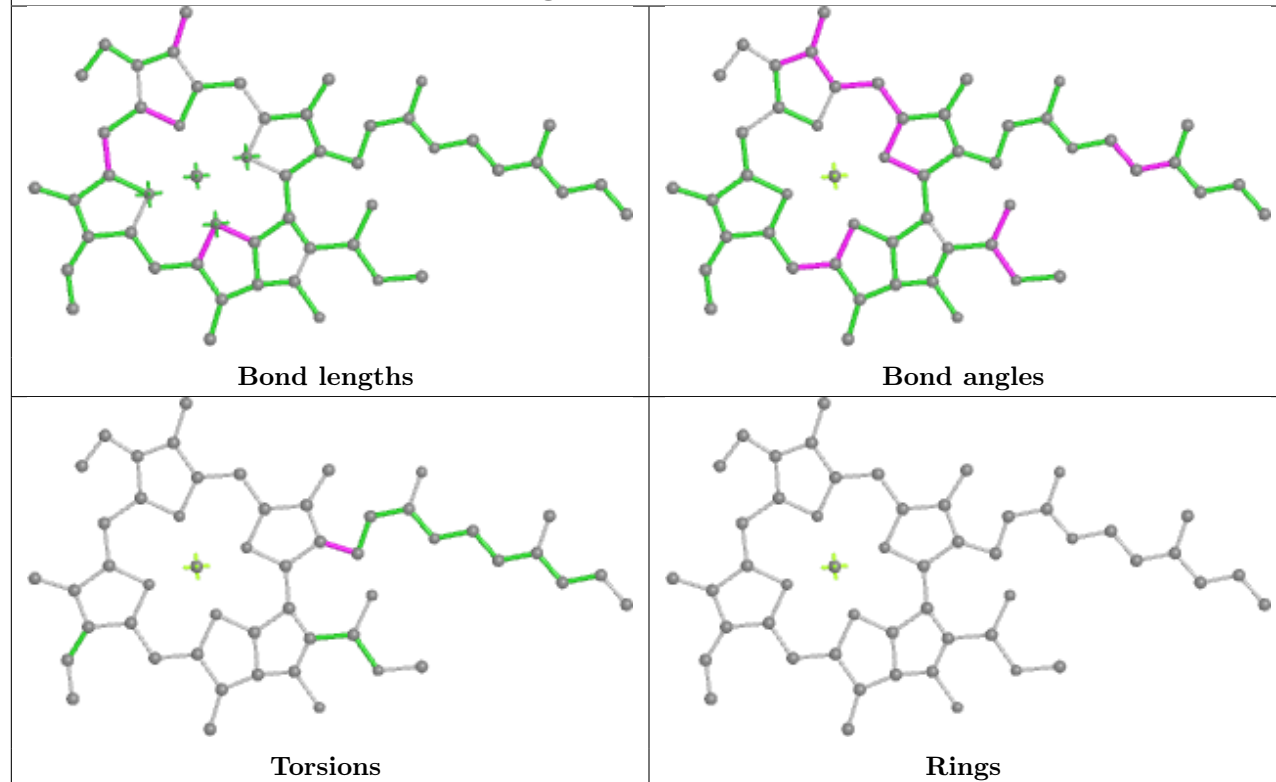


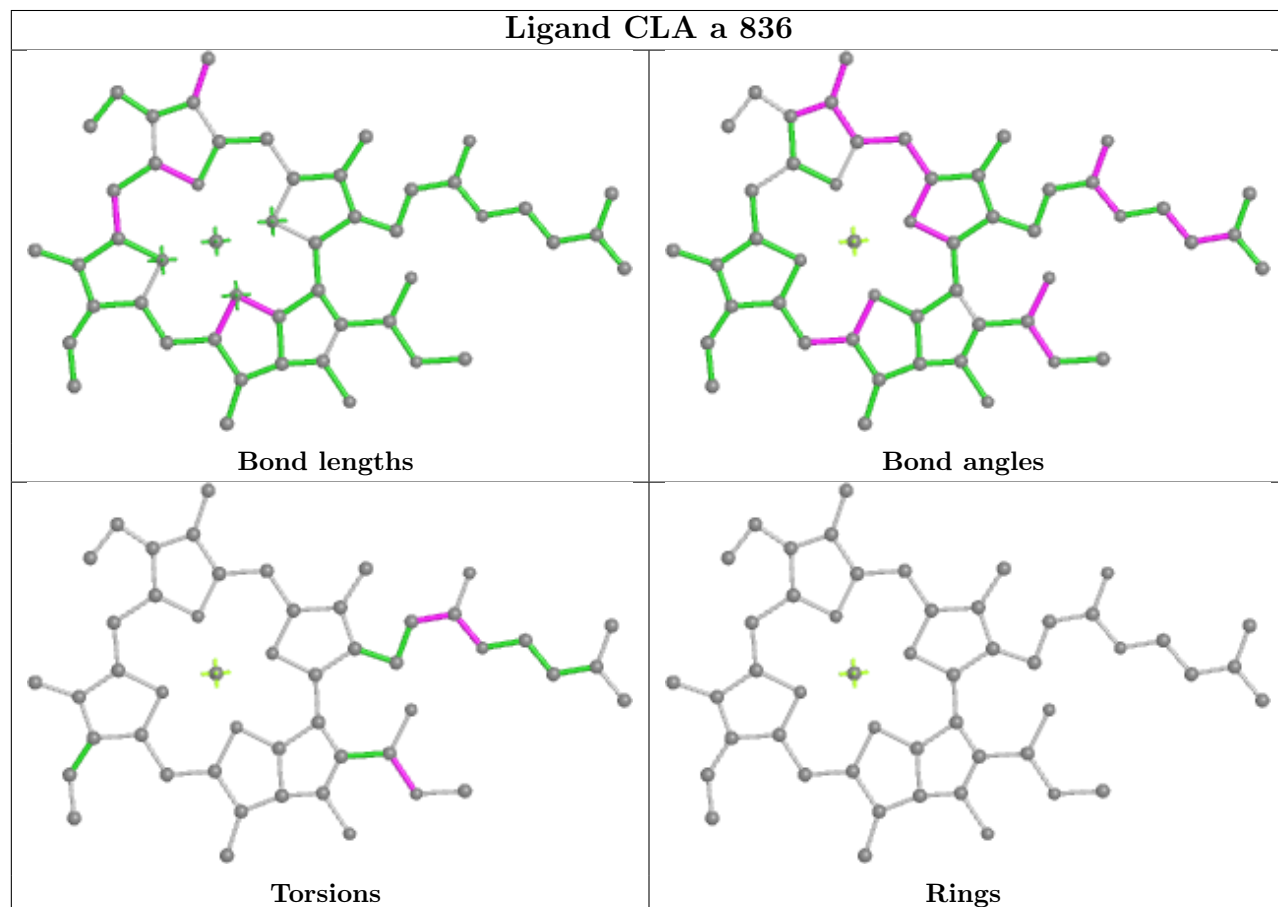
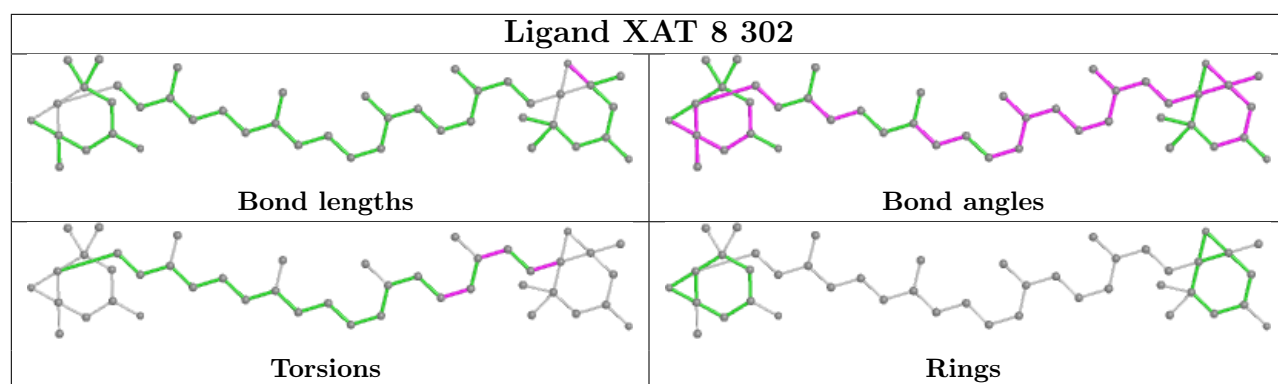


## Ligand CLA a 820

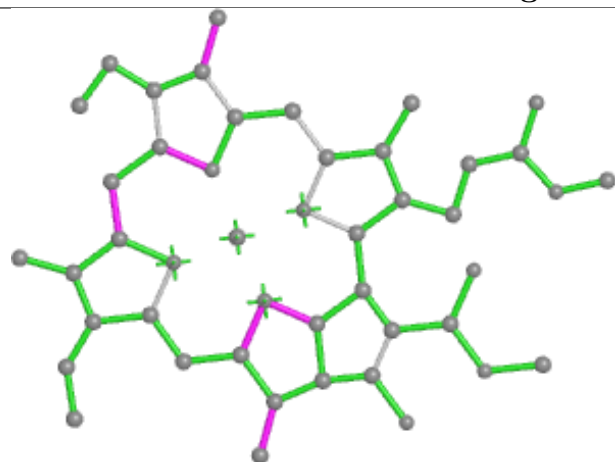


## Ligand CLA f 803

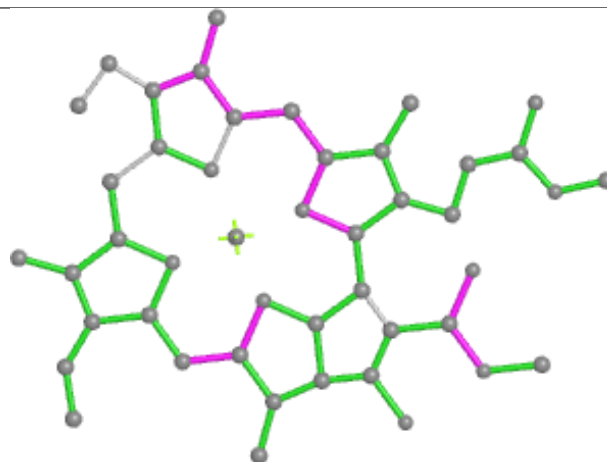




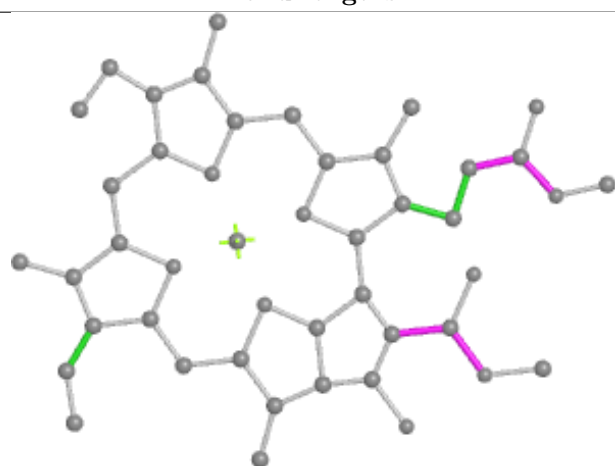
## Ligand CLA 1 309



Bond lengths



Bond angles

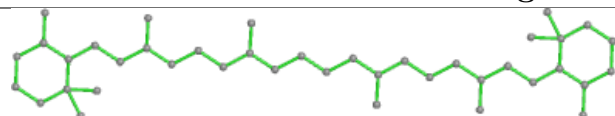


Torsions

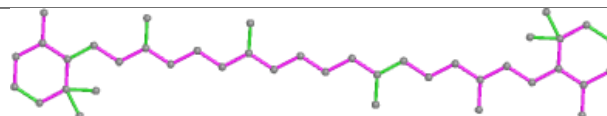


Rings

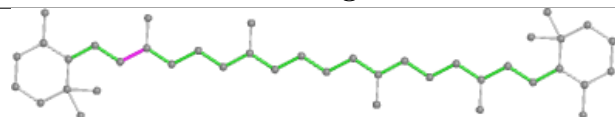
## Ligand BCR b 842



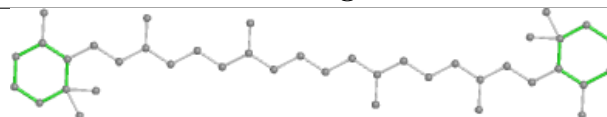
Bond lengths



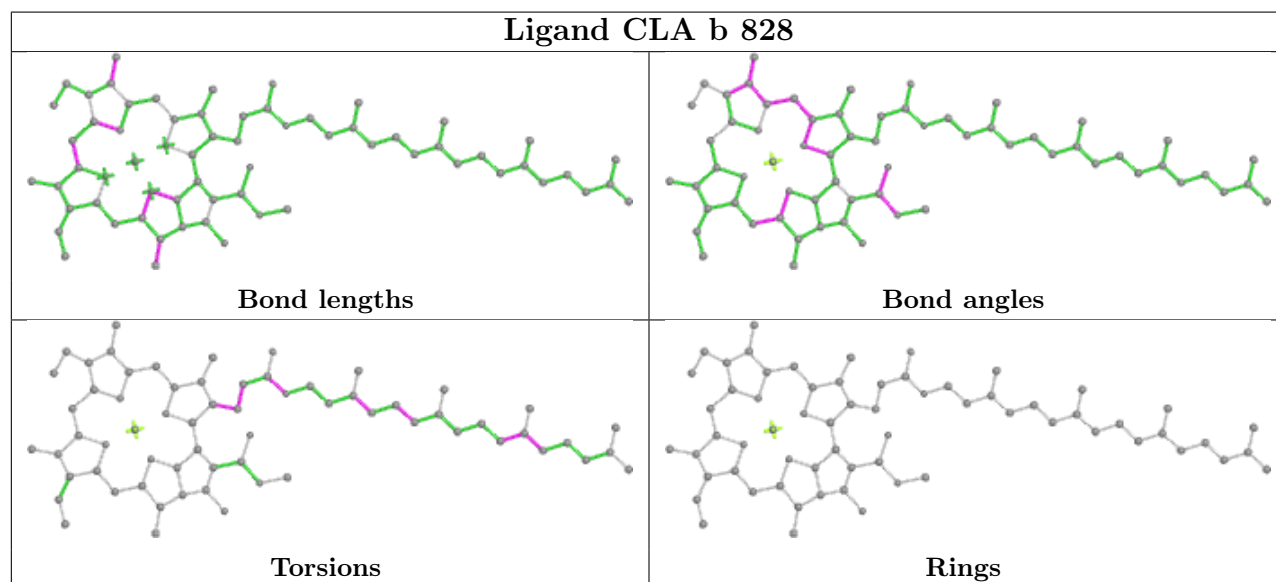
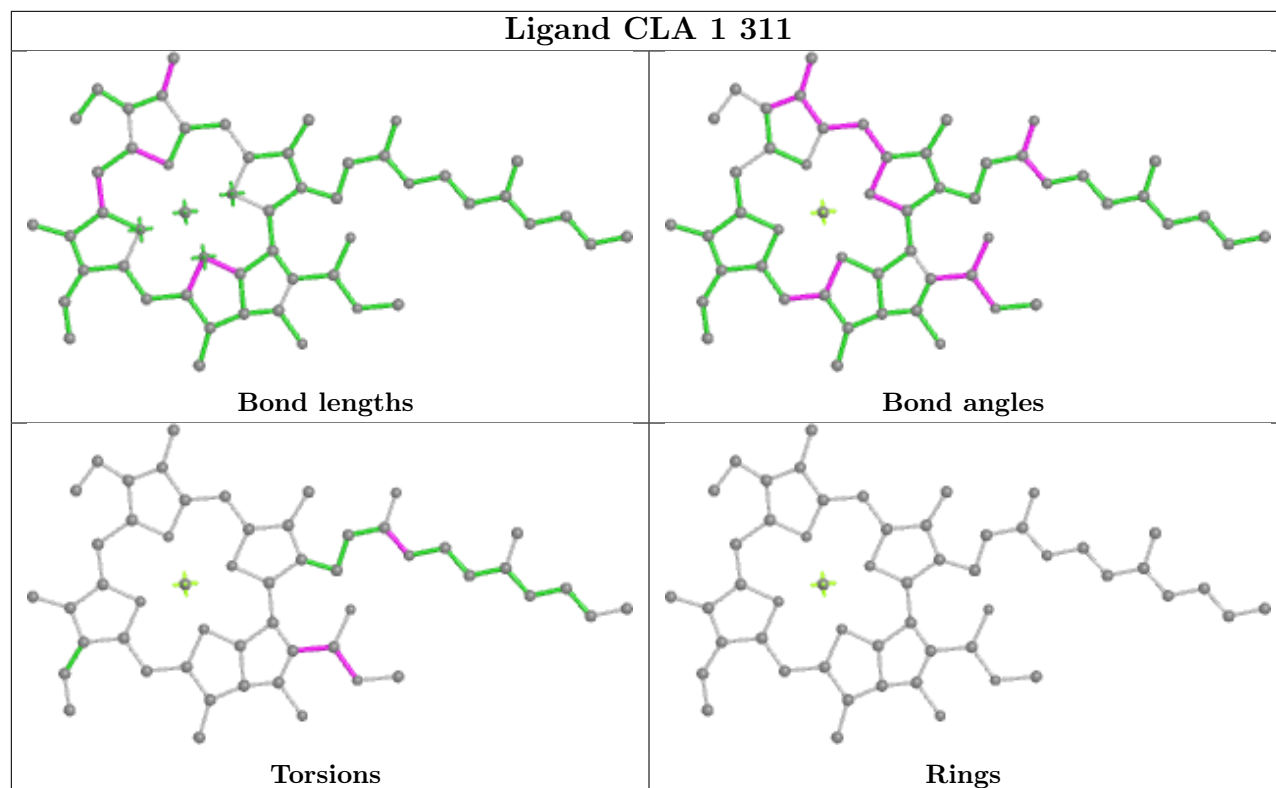
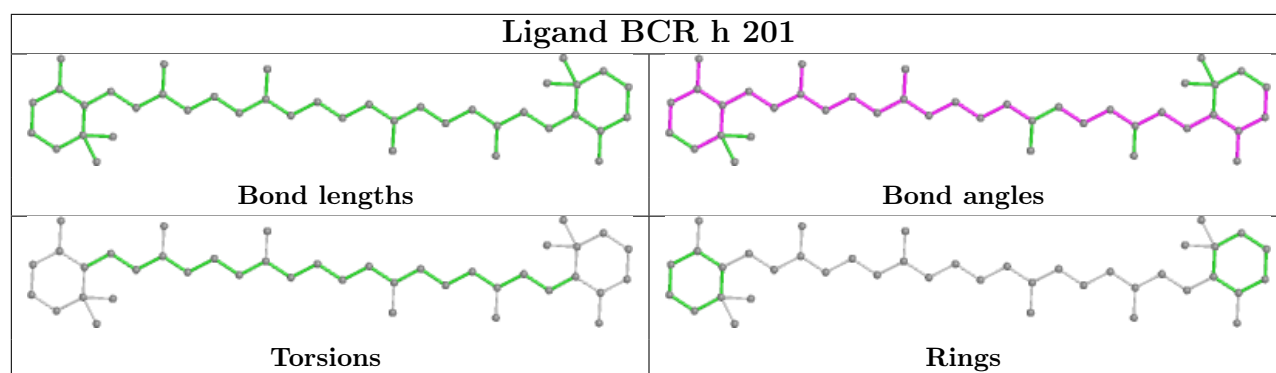
Bond angles

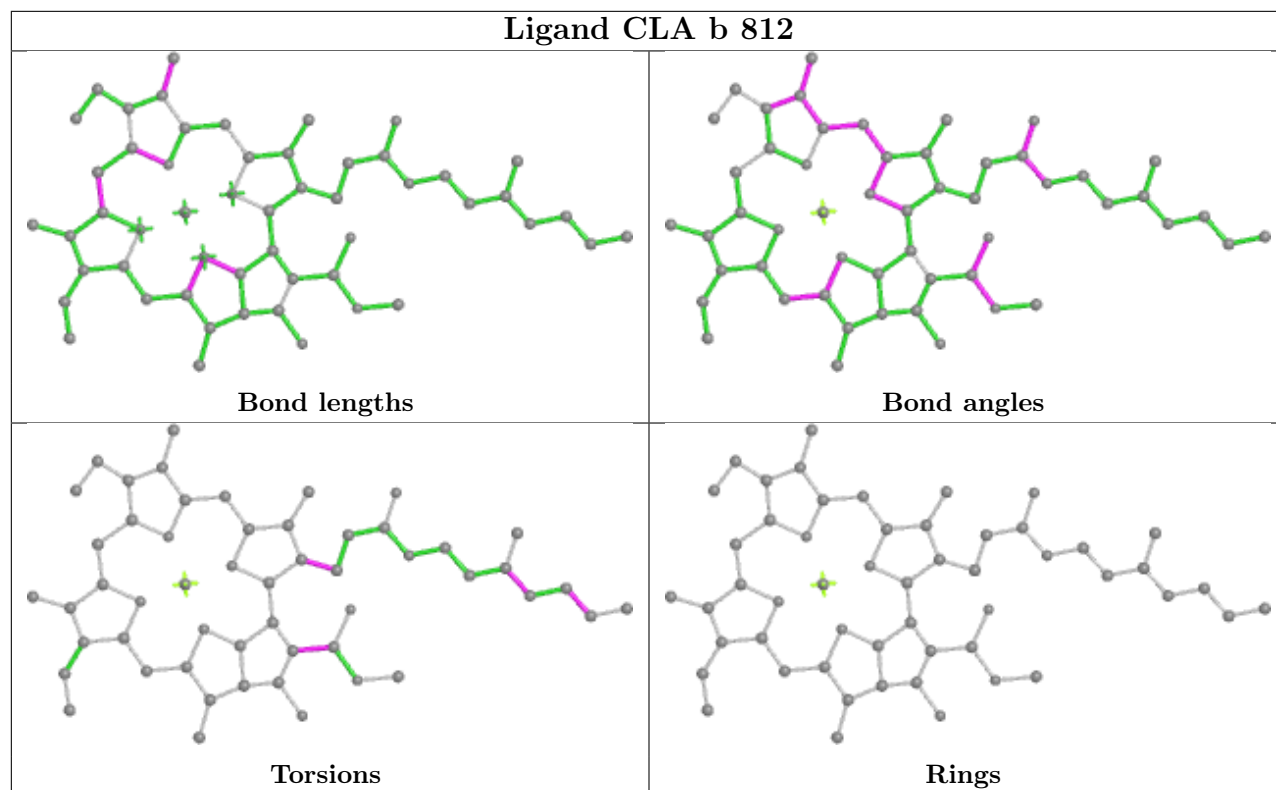
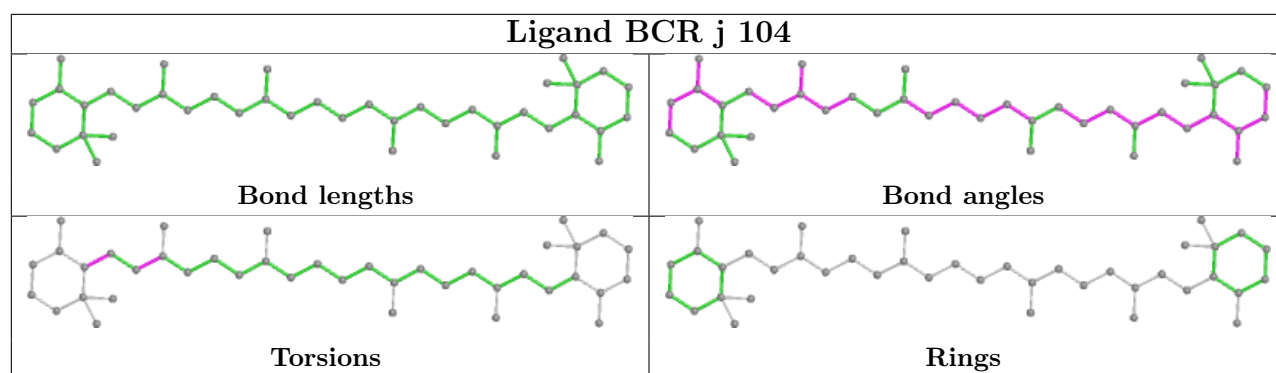


Torsions

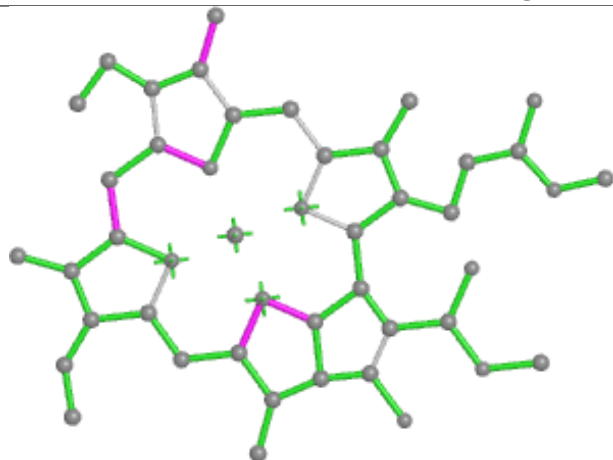


Rings

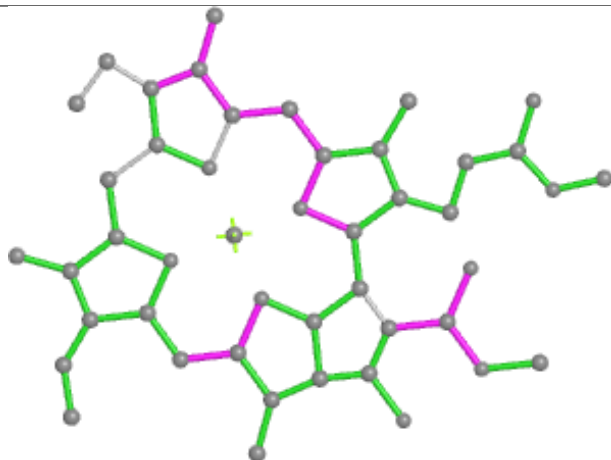




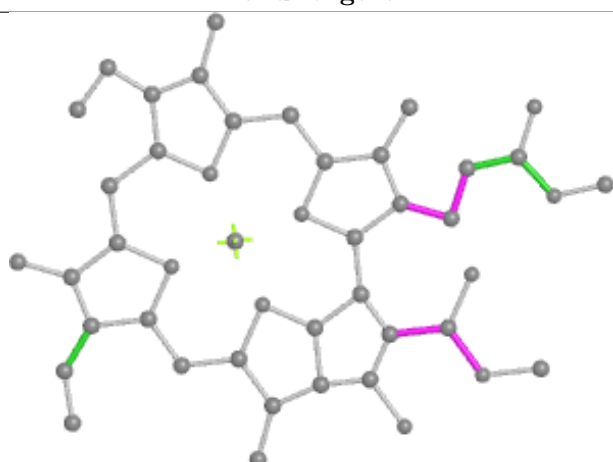
## Ligand CLA 9 311



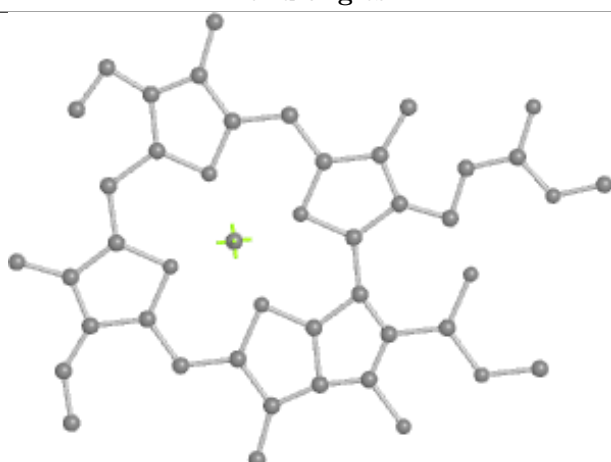
Bond lengths



Bond angles

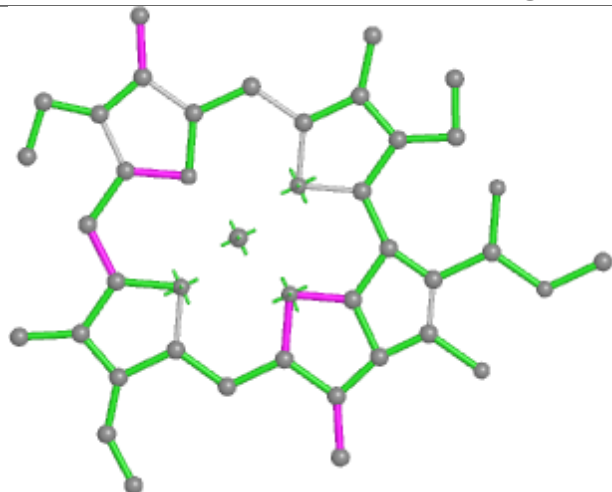


Torsions

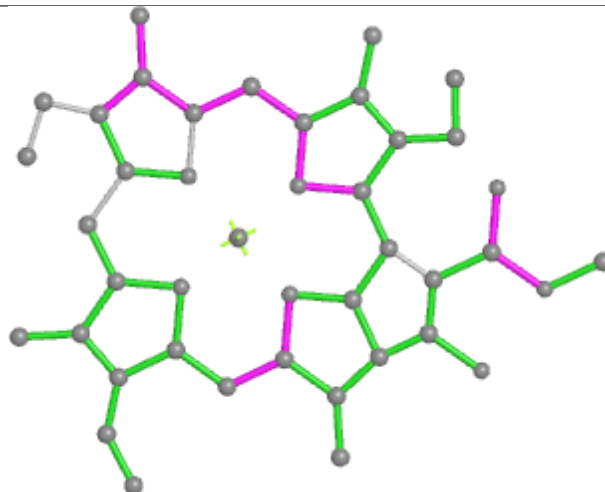


Rings

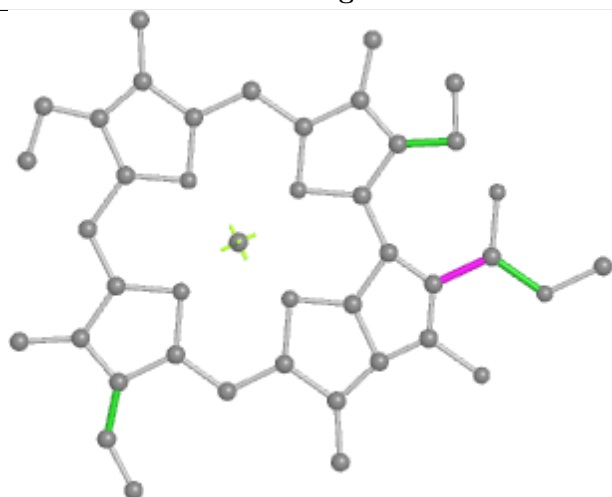
## Ligand CLA 1 202



Bond lengths



Bond angles

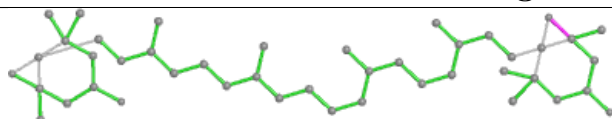


Torsions

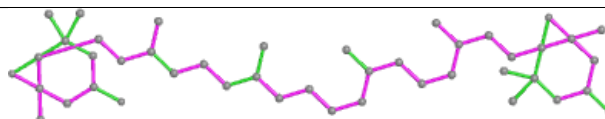


Rings

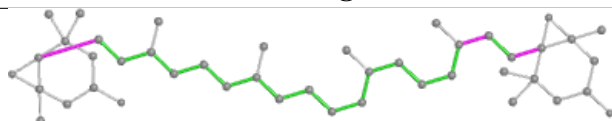
## Ligand XAT 9 303



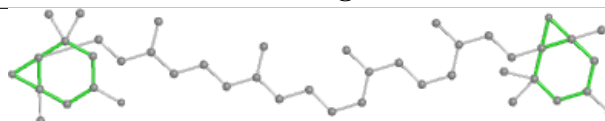
Bond lengths



Bond angles

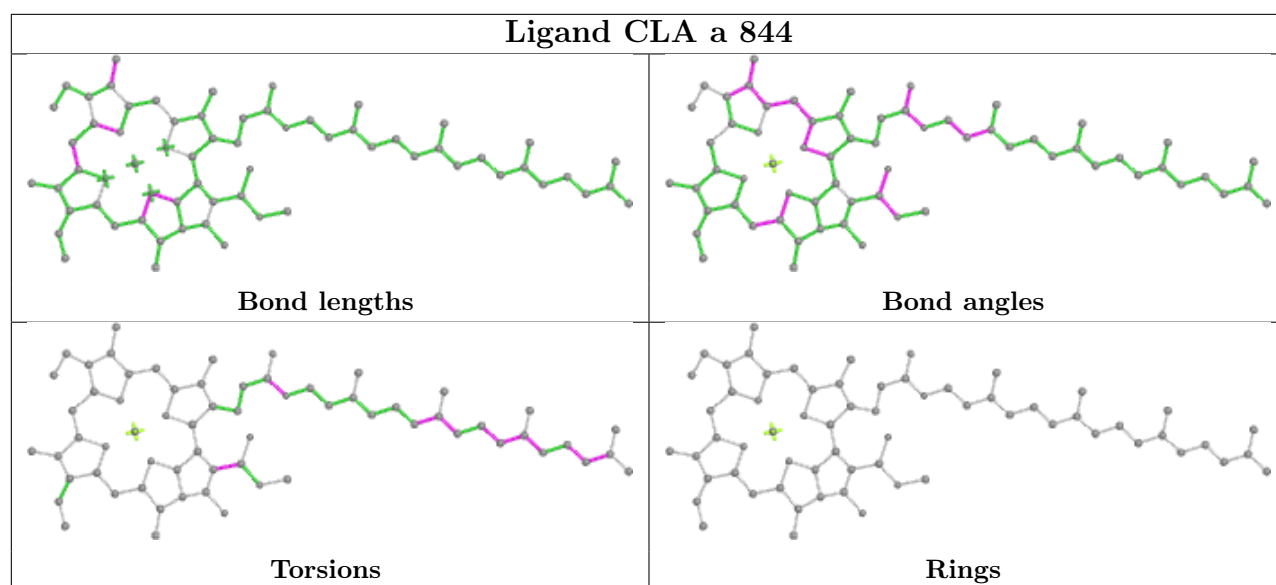


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

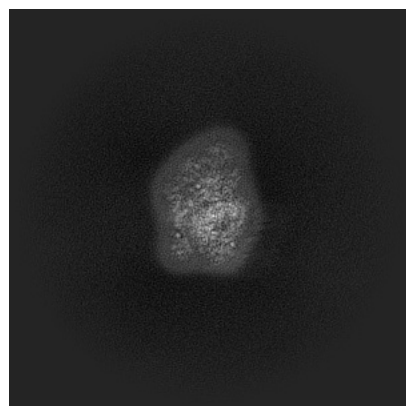
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60290. These allow visual inspection of the internal detail of the map and identification of artifacts.

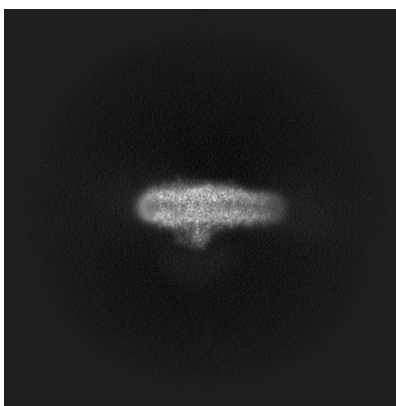
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

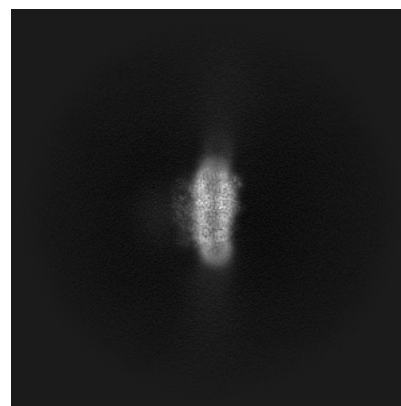
#### 6.1.1 Primary map



X

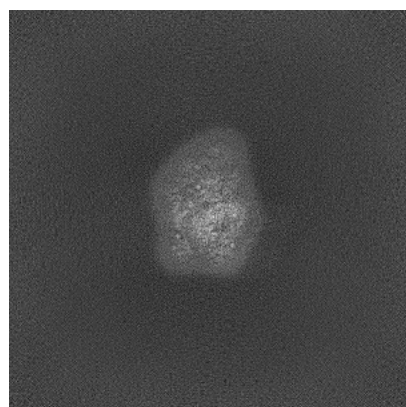


Y

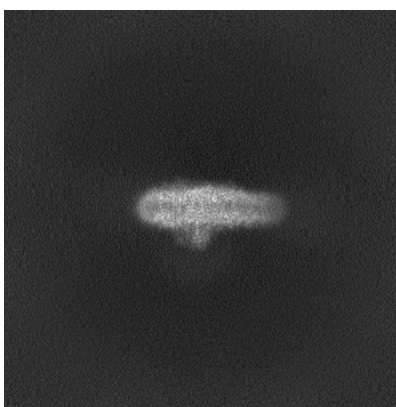


Z

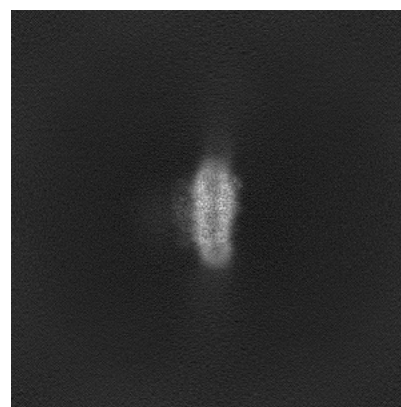
#### 6.1.2 Raw map



X



Y

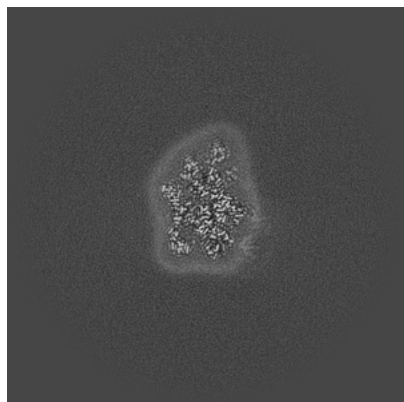


Z

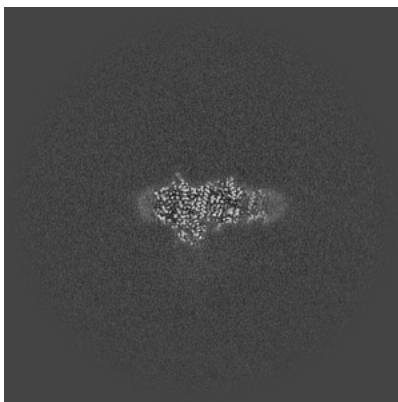
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

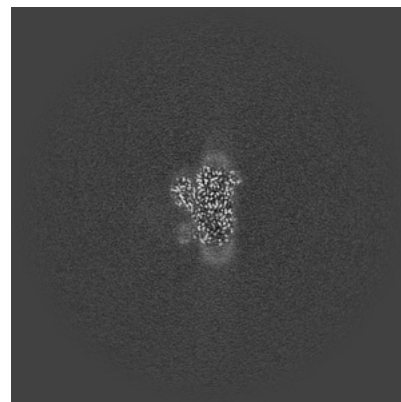
### 6.2.1 Primary map



X Index: 256

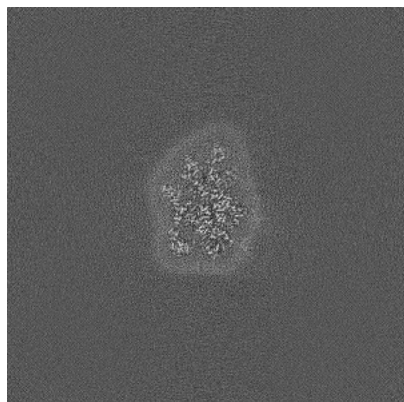


Y Index: 256

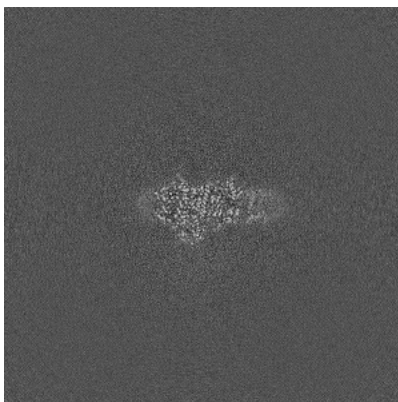


Z Index: 256

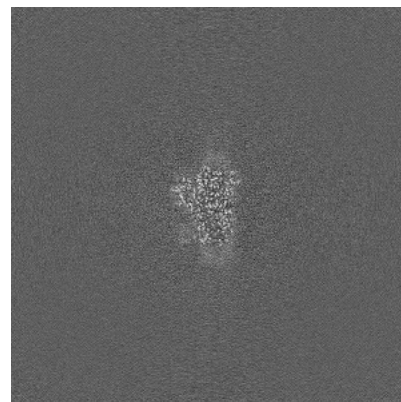
### 6.2.2 Raw map



X Index: 256



Y Index: 256

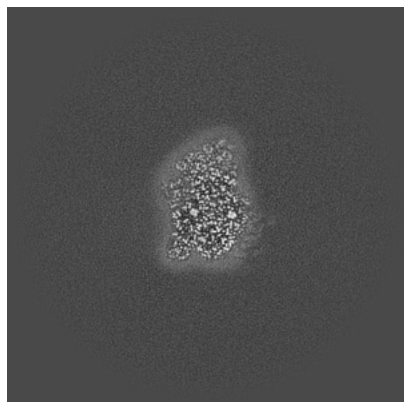


Z Index: 256

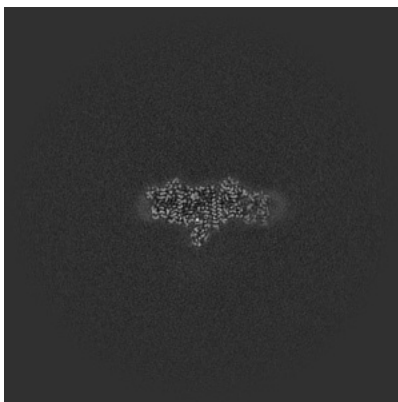
The images above show central slices of the map in three orthogonal directions.

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

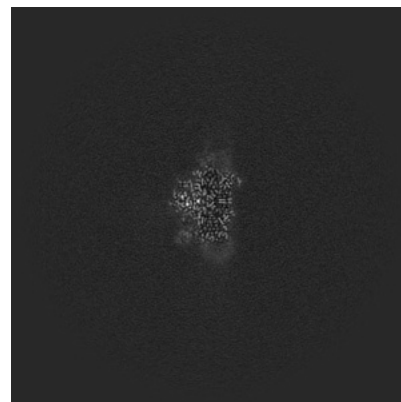
### 6.3.1 Primary map



X Index: 245

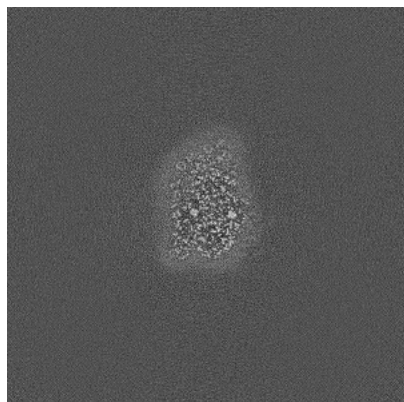


Y Index: 264

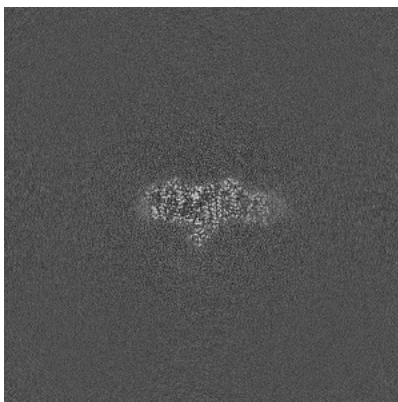


Z Index: 247

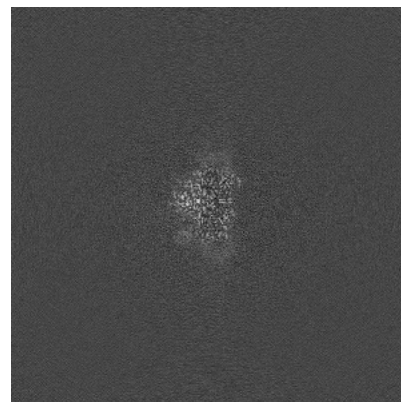
### 6.3.2 Raw map



X Index: 245



Y Index: 265



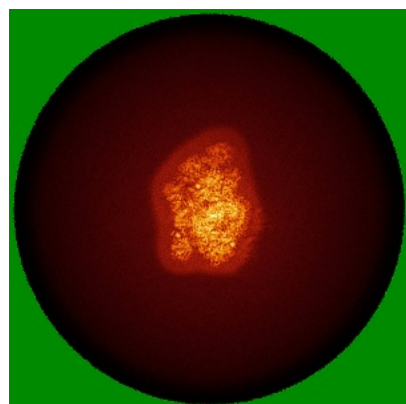
Z Index: 247

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

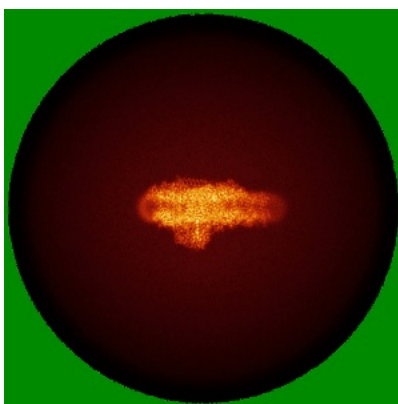


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

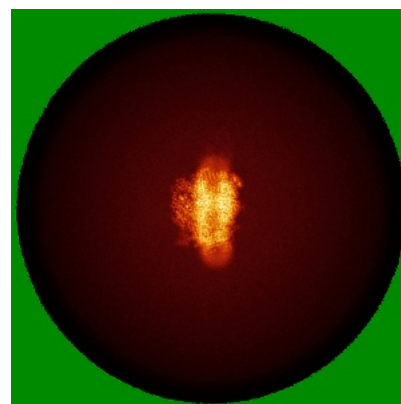
### 6.4.1 Primary map



X

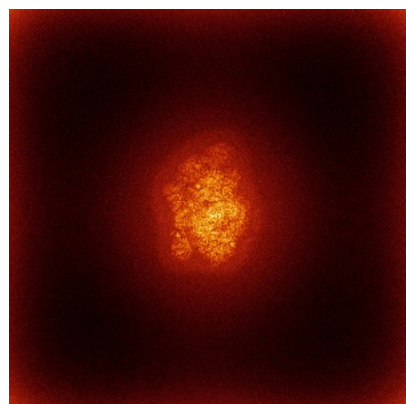


Y

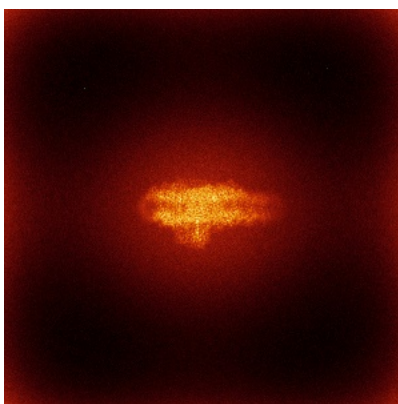


Z

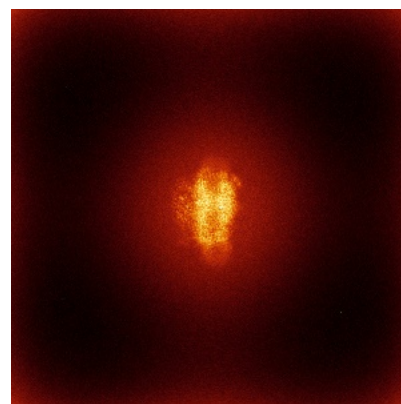
### 6.4.2 Raw map



X



Y

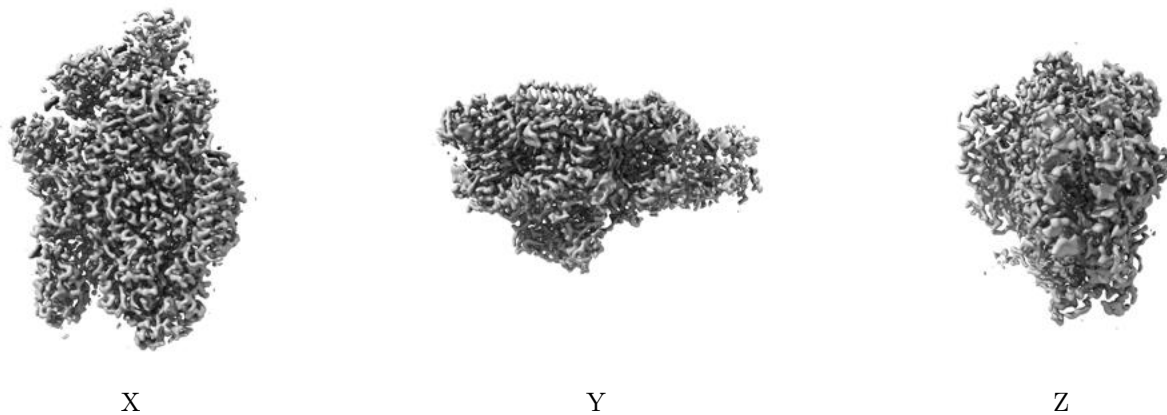


Z

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.

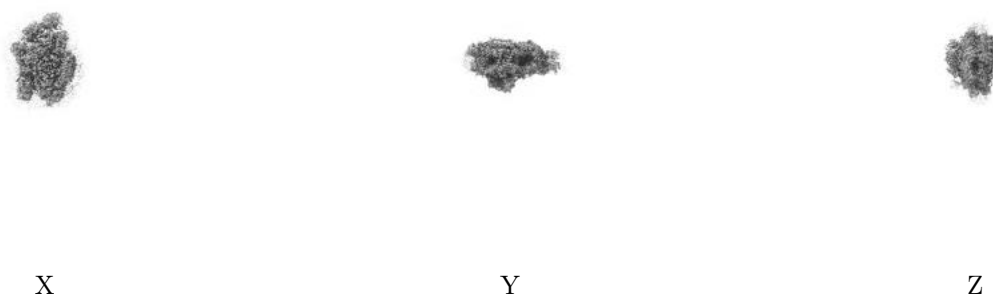
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.343. 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.

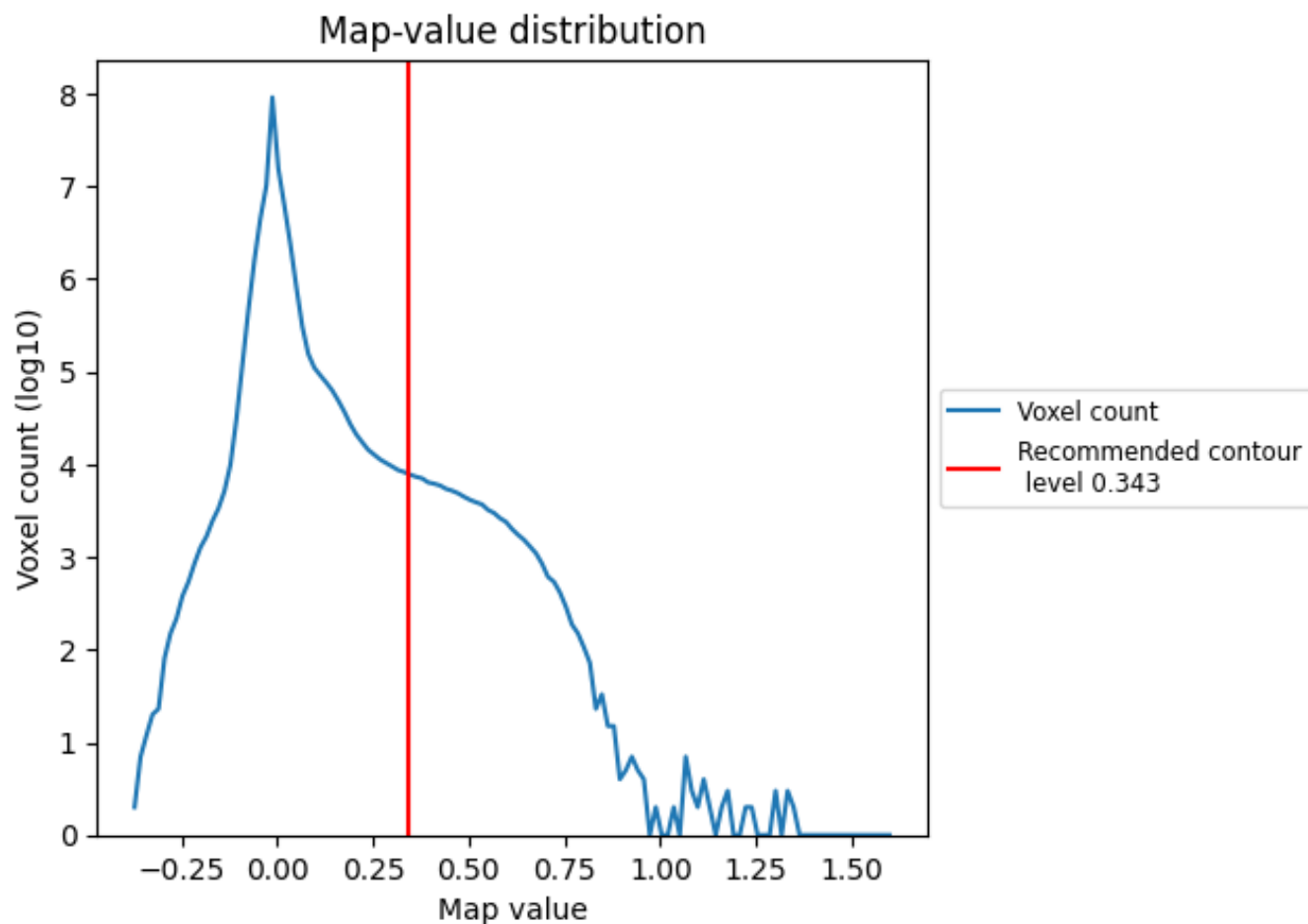
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

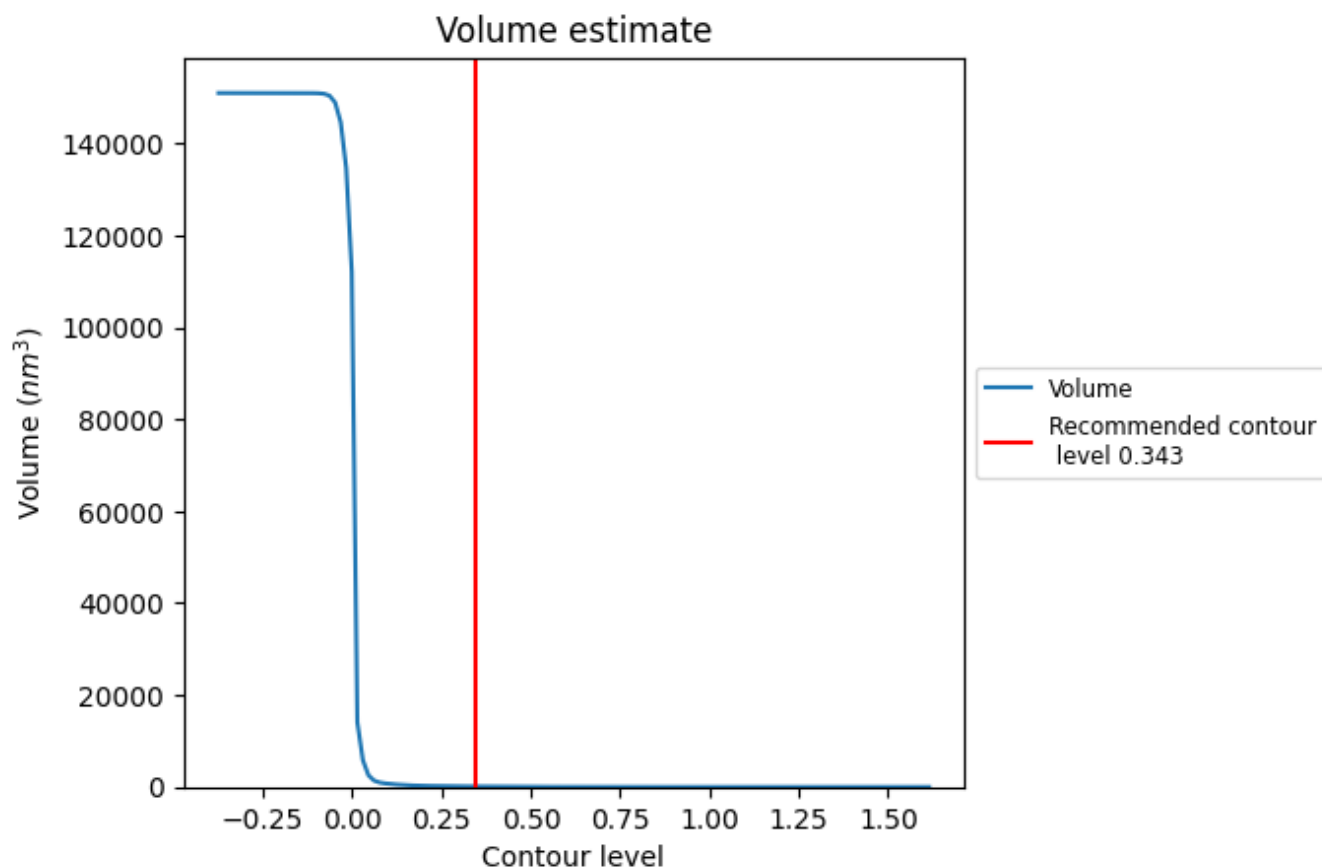
This section contains the results of statistical analysis of the map.

### 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](#)

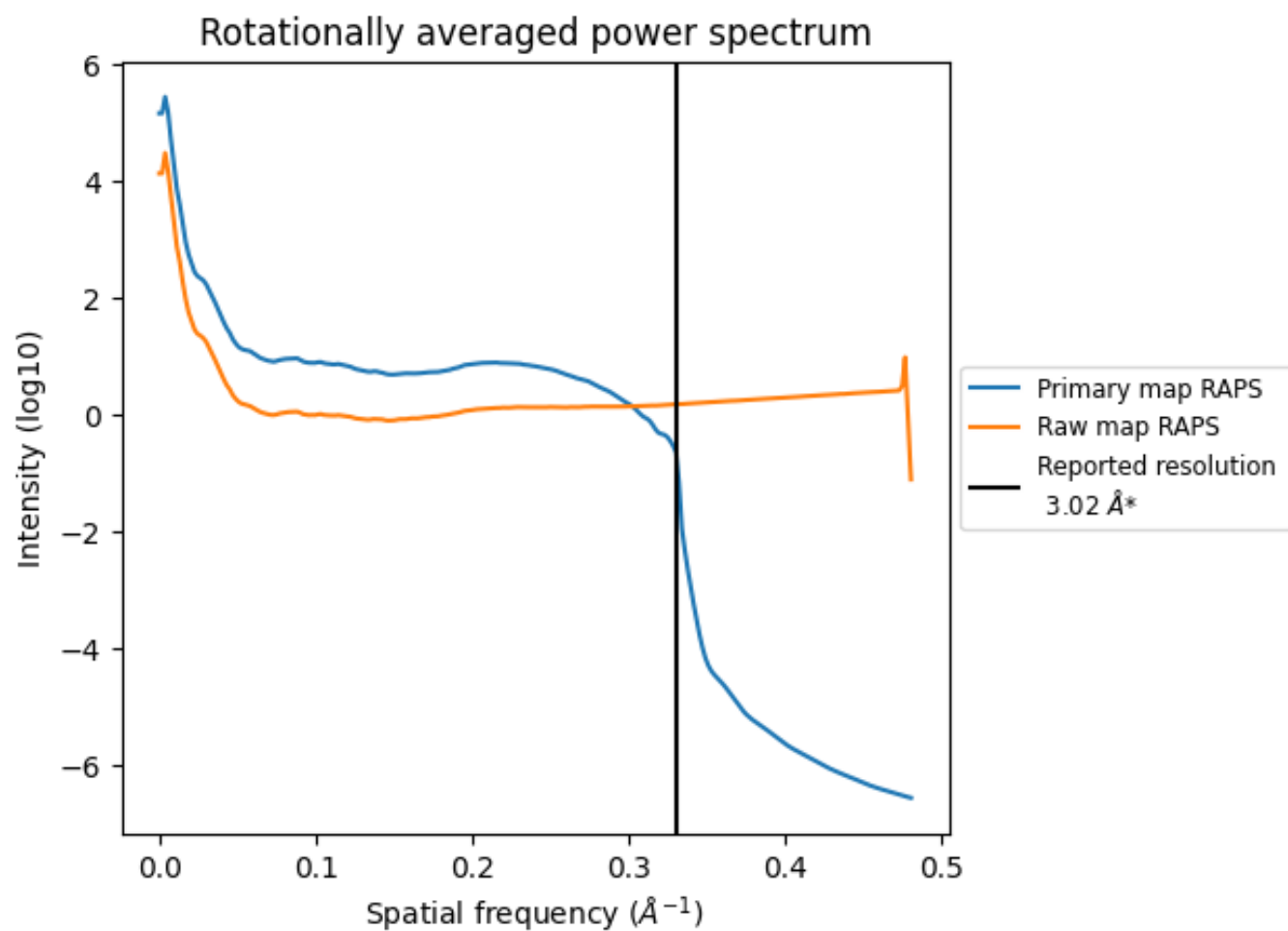


The volume at the recommended contour level is 109 nm<sup>3</sup>; this corresponds to an approximate mass of 98 kDa.

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 ⓘ

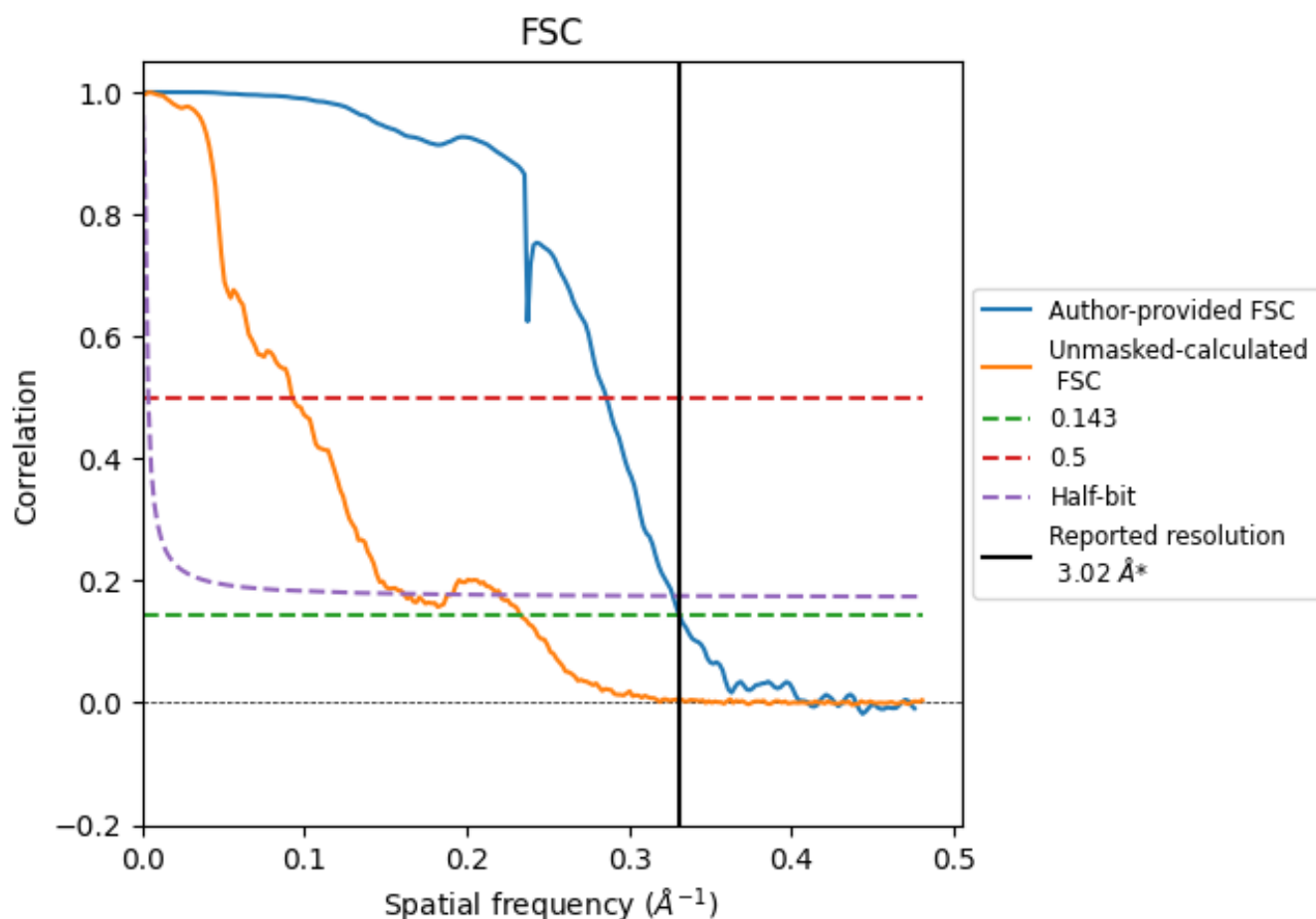


\*Reported resolution corresponds to spatial frequency of 0.331  $\text{\AA}^{-1}$

## 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 0.331  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

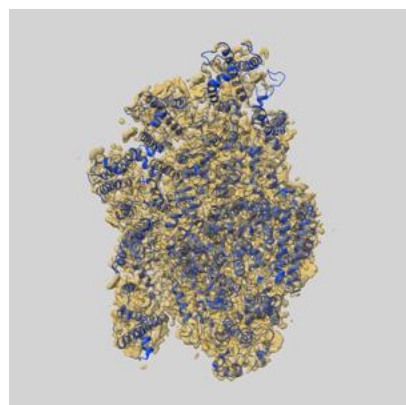
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.49	3.06
Unmasked-calculated*	4.29	10.78	6.20

\*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 4.29 differs from the reported value 3.02 by more than 10 %

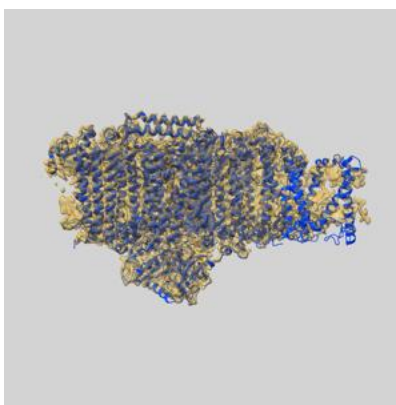
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60290 and PDB model 8ZOE. Per-residue inclusion information can be found in section 3 on page 25.

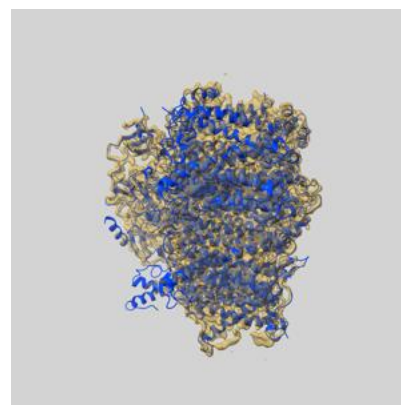
### 9.1 Map-model overlay [i](#)



X



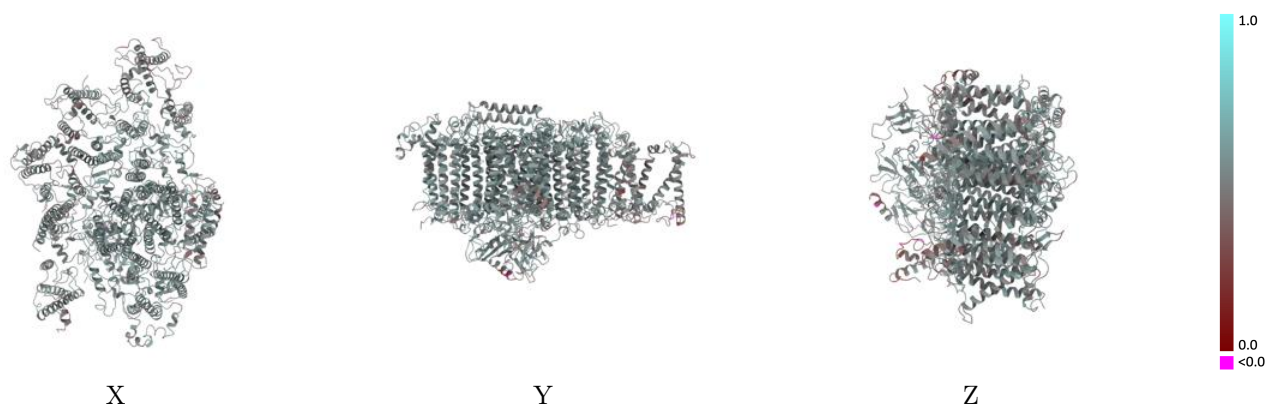
Y



Z

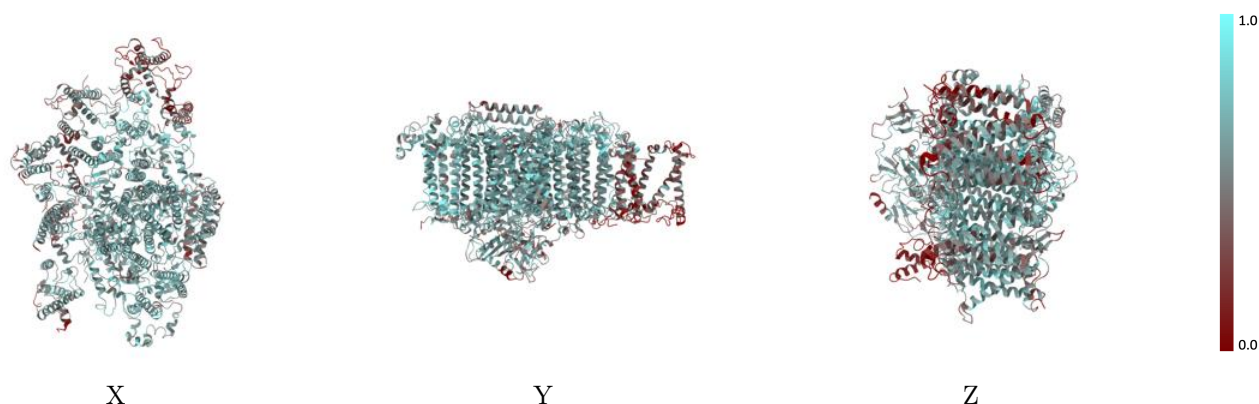
The images above show the 3D surface view of the map at the recommended contour level 0.343 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



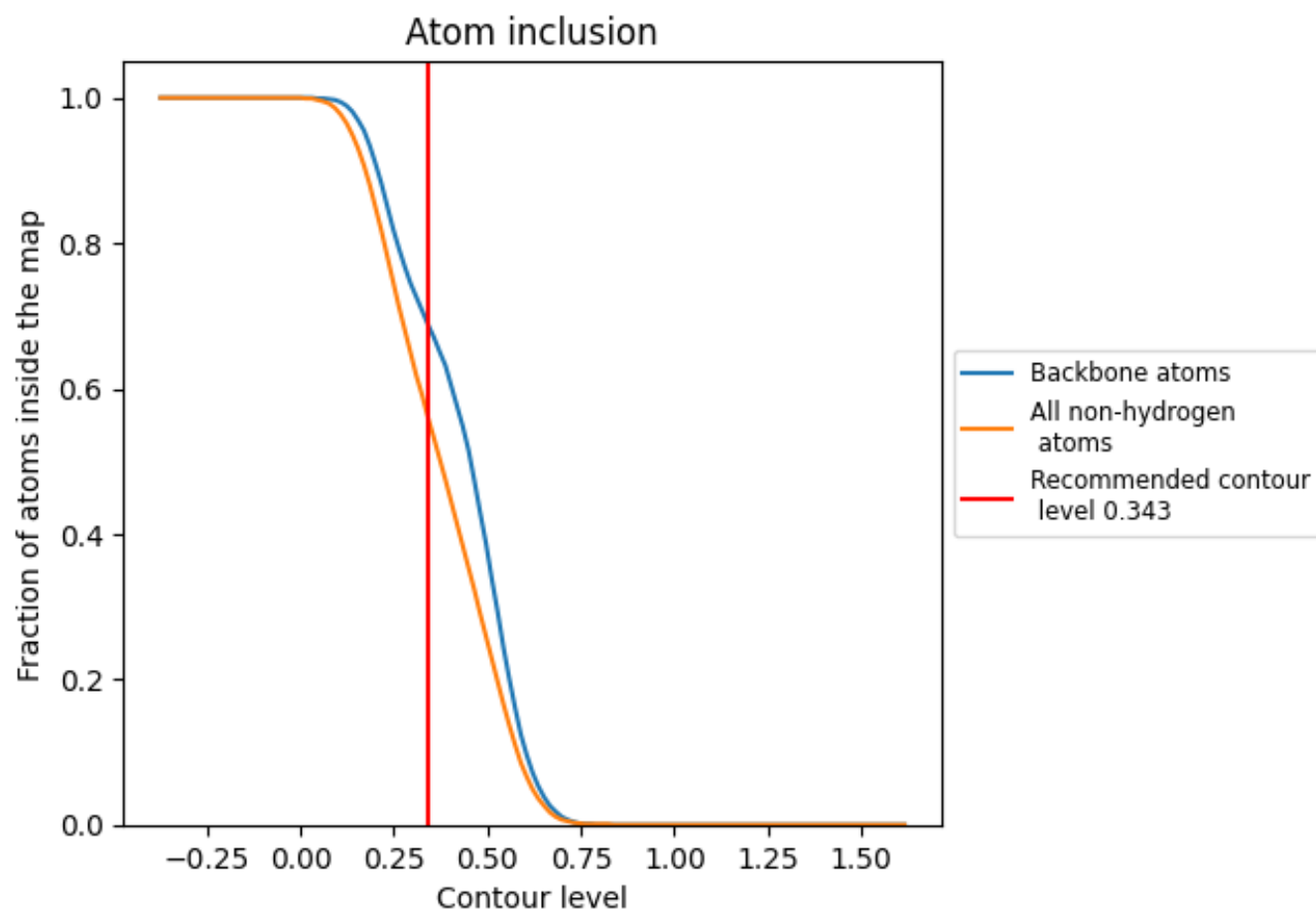
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.343).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 56% 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 (0.343) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5570	<div></div> 0.5290
1	<div></div> 0.5270	<div></div> 0.5130
7	<div></div> 0.2950	<div></div> 0.4690
8	<div></div> 0.4750	<div></div> 0.5070
9	<div></div> 0.4600	<div></div> 0.5090
a	<div></div> 0.6330	<div></div> 0.5490
b	<div></div> 0.6330	<div></div> 0.5530
c	<div></div> 0.6690	<div></div> 0.5330
d	<div></div> 0.5610	<div></div> 0.5350
e	<div></div> 0.5360	<div></div> 0.5270
f	<div></div> 0.5450	<div></div> 0.5040
g	<div></div> 0.3020	<div></div> 0.4240
h	<div></div> 0.2560	<div></div> 0.4810
i	<div></div> 0.5160	<div></div> 0.5240
j	<div></div> 0.5020	<div></div> 0.5350
l	<div></div> 0.5560	<div></div> 0.5060
m	<div></div> 0.5790	<div></div> 0.5080

