



wwPDB EM Validation Summary Report ⓘ

Dec 2, 2025 – 12:05 AM JST

PDB ID : 8ZOH / pdb_00008zoh
EMDB ID : EMD-60293
Title : Structure of the astaxanthin mutant PSI-7VCPI supercomplex in Nan-
nochloropsis oceanica
Authors : Shen, L.L.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

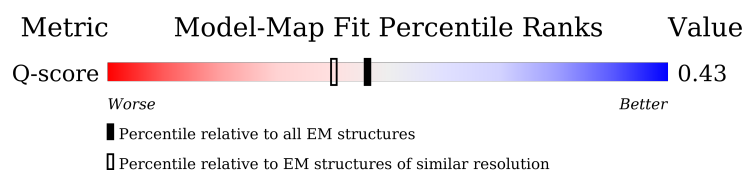
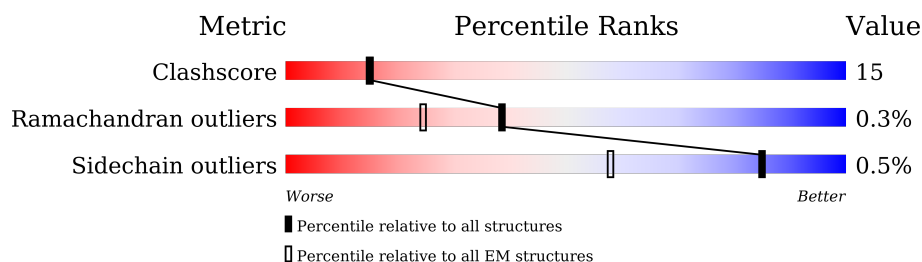
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	5	244	<div> <div>6%</div> <div>53%</div> <div>16%</div> <div>31%</div> </div>
2	9	232	<div> <div>7%</div> <div>64%</div> <div>22%</div> <div>13%</div> </div>
3	8	200	<div> <div>•</div> <div>62%</div> <div>18%</div> <div>18%</div> </div>
4	4	202	<div> <div>14%</div> <div>73%</div> <div>10%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
4	7	202	
5	6	259	
6	1	208	
7	a	745	
8	b	737	
9	d	136	
10	e	67	
11	f	185	
12	h	128	
13	i	45	
14	j	41	
15	l	172	
16	m	30	
17	g	55	
18	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
21	CLA	1	305	X	-	-	-
21	CLA	1	306	X	-	-	-
21	CLA	1	307	X	-	-	-
21	CLA	1	308	X	-	-	-
21	CLA	1	309	X	-	-	-
21	CLA	1	310	X	-	-	-
21	CLA	1	311	X	-	-	-
21	CLA	1	312	X	-	-	-
21	CLA	1	313	X	-	-	-
21	CLA	1	314	X	-	-	-
21	CLA	4	306	X	-	-	-
21	CLA	4	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	4	308	X	-	-	-
21	CLA	4	309	X	-	-	-
21	CLA	4	310	X	-	-	-
21	CLA	4	311	X	-	-	-
21	CLA	4	312	X	-	-	-
21	CLA	4	313	X	-	-	-
21	CLA	4	314	X	-	-	-
21	CLA	4	315	X	-	-	-
21	CLA	4	316	X	-	-	-
21	CLA	4	317	X	-	-	-
21	CLA	5	306	X	-	-	-
21	CLA	5	307	X	-	-	-
21	CLA	5	308	X	-	-	-
21	CLA	5	309	X	-	-	-
21	CLA	5	310	X	-	-	-
21	CLA	5	311	X	-	-	-
21	CLA	5	312	X	-	-	-
21	CLA	5	313	X	-	-	-
21	CLA	5	314	X	-	-	-
21	CLA	5	315	X	-	-	-
21	CLA	5	316	X	-	-	-
21	CLA	6	307	X	-	-	-
21	CLA	6	308	X	-	-	-
21	CLA	6	309	X	-	-	-
21	CLA	6	310	X	-	-	-
21	CLA	6	311	X	-	-	-
21	CLA	6	312	X	-	-	-
21	CLA	6	313	X	-	-	-
21	CLA	6	314	X	-	-	-
21	CLA	6	315	X	-	-	-
21	CLA	6	316	X	-	-	-
21	CLA	7	306	X	-	-	-
21	CLA	7	307	X	-	-	-
21	CLA	7	308	X	-	-	-
21	CLA	7	309	X	-	-	-
21	CLA	7	310	X	-	-	-
21	CLA	7	311	X	-	-	-
21	CLA	7	312	X	-	-	-
21	CLA	7	313	X	-	-	-
21	CLA	7	314	X	-	-	-
21	CLA	7	315	X	-	-	-
21	CLA	7	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	7	317	X	-	-	-
21	CLA	8	305	X	-	-	-
21	CLA	8	306	X	-	-	-
21	CLA	8	307	X	-	-	-
21	CLA	8	308	X	-	-	-
21	CLA	8	309	X	-	-	-
21	CLA	8	310	X	-	-	-
21	CLA	8	311	X	-	-	-
21	CLA	8	312	X	-	-	-
21	CLA	8	313	X	-	-	-
21	CLA	8	314	X	-	-	-
21	CLA	9	308	X	-	-	-
21	CLA	9	309	X	-	-	-
21	CLA	9	310	X	-	-	-
21	CLA	9	311	X	-	-	-
21	CLA	9	312	X	-	-	-
21	CLA	9	313	X	-	-	-
21	CLA	9	314	X	-	-	-
21	CLA	9	315	X	-	-	-
21	CLA	9	316	X	-	-	-
21	CLA	a	801	X	-	-	-
21	CLA	a	802	X	-	-	-
21	CLA	a	803	X	-	-	-
21	CLA	a	804	X	-	-	-
21	CLA	a	805	X	-	-	-
21	CLA	a	806	X	-	-	-
21	CLA	a	807	X	-	-	-
21	CLA	a	808	X	-	-	-
21	CLA	a	809	X	-	-	-
21	CLA	a	810	X	-	-	-
21	CLA	a	811	X	-	-	-
21	CLA	a	812	X	-	-	-
21	CLA	a	813	X	-	-	-
21	CLA	a	814	X	-	-	-
21	CLA	a	815	X	-	-	-
21	CLA	a	816	X	-	-	-
21	CLA	a	817	X	-	-	-
21	CLA	a	818	X	-	-	-
21	CLA	a	819	X	-	-	-
21	CLA	a	820	X	-	-	-
21	CLA	a	821	X	-	-	-
21	CLA	a	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	a	823	X	-	-	-
21	CLA	a	824	X	-	-	-
21	CLA	a	825	X	-	-	-
21	CLA	a	826	X	-	-	-
21	CLA	a	827	X	-	-	-
21	CLA	a	828	X	-	-	-
21	CLA	a	829	X	-	-	-
21	CLA	a	830	X	-	-	-
21	CLA	a	831	X	-	-	-
21	CLA	a	832	X	-	-	-
21	CLA	a	833	X	-	-	-
21	CLA	a	834	X	-	-	-
21	CLA	a	835	X	-	-	-
21	CLA	a	836	X	-	-	-
21	CLA	a	837	X	-	-	-
21	CLA	a	838	X	-	-	-
21	CLA	a	839	X	-	-	-
21	CLA	a	840	X	-	-	-
21	CLA	a	841	X	-	-	-
21	CLA	a	842	X	-	-	-
21	CLA	a	844	X	-	-	-
21	CLA	a	852	X	-	-	-
21	CLA	a	856	X	-	X	-
21	CLA	b	801	X	-	-	-
21	CLA	b	802	X	-	-	-
21	CLA	b	803	X	-	-	-
21	CLA	b	804	X	-	-	-
21	CLA	b	805	X	-	-	-
21	CLA	b	806	X	-	-	-
21	CLA	b	807	X	-	-	-
21	CLA	b	808	X	-	-	-
21	CLA	b	809	X	-	-	-
21	CLA	b	810	X	-	X	-
21	CLA	b	811	X	-	-	-
21	CLA	b	812	X	-	-	-
21	CLA	b	813	X	-	-	-
21	CLA	b	814	X	-	-	-
21	CLA	b	815	X	-	-	-
21	CLA	b	816	X	-	-	-
21	CLA	b	817	X	-	-	-
21	CLA	b	818	X	-	-	-
21	CLA	b	819	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	b	820	X	-	-	-
21	CLA	b	821	X	-	-	-
21	CLA	b	822	X	-	-	-
21	CLA	b	823	X	-	-	-
21	CLA	b	824	X	-	-	-
21	CLA	b	825	X	-	-	-
21	CLA	b	826	X	-	-	-
21	CLA	b	827	X	-	-	-
21	CLA	b	828	X	-	-	-
21	CLA	b	829	X	-	-	-
21	CLA	b	830	X	-	-	-
21	CLA	b	831	X	-	-	-
21	CLA	b	832	X	-	-	-
21	CLA	b	833	X	-	-	-
21	CLA	b	834	X	-	-	-
21	CLA	b	835	X	-	-	-
21	CLA	b	836	X	-	-	-
21	CLA	b	837	X	-	-	-
21	CLA	b	838	X	-	-	-
21	CLA	b	839	X	-	-	-
21	CLA	b	840	X	-	-	-
21	CLA	b	841	X	-	-	-
21	CLA	f	802	X	-	-	-
21	CLA	f	803	X	-	-	-
21	CLA	h	201	X	-	-	-
21	CLA	h	203	X	-	-	-
21	CLA	j	101	X	-	-	-
21	CLA	l	201	X	-	-	-
21	CLA	l	202	X	-	-	-
21	CLA	l	203	X	-	-	-
27	BCR	f	801	-	-	X	-
28	SF4	c	102	-	-	X	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 39574 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VCPI-5.

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

- Molecule 2 is a protein called VCPI-9.

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

- Molecule 3 is a protein called VCPI-8.

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

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

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

- Molecule 5 is a protein called VCPI-6.

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

- Molecule 6 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

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

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

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

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

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

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

- Molecule 10 is a protein called Photosystem I reaction center subunit IV.

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

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

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

- Molecule 12 is a protein called Psar.

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

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

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

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

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

- Molecule 15 is a protein called PSI subunit V.

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

- Molecule 16 is a protein called PsaM.

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

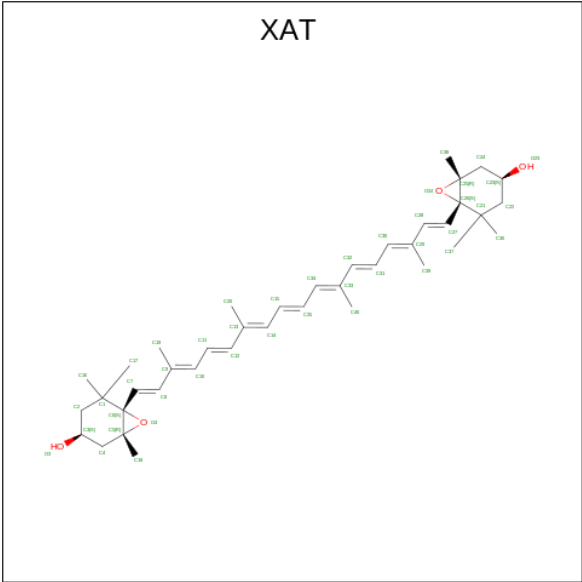
- Molecule 17 is a protein called PsaS.

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

- Molecule 18 is a protein called Photosystem I iron-sulfur center.

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

- 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: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



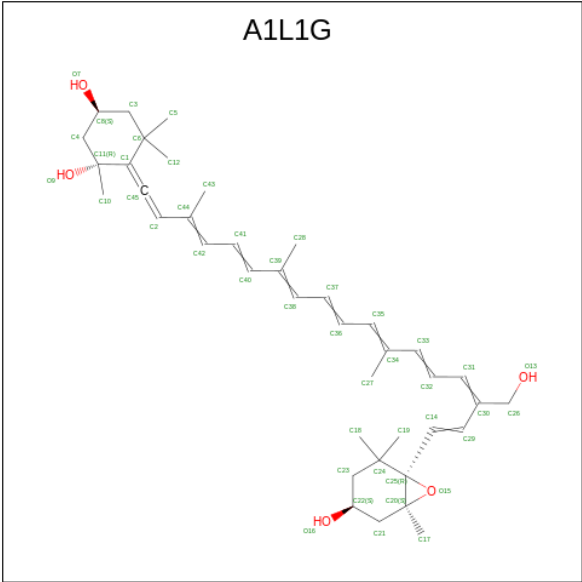
Mol	Chain	Residues	Atoms			AltConf
19	5	1	Total	C	O	0
			44	40	4	
19	5	1	Total	C	O	0
			44	40	4	
19	5	1	Total	C	O	0
			44	40	4	
19	5	1	Total	C	O	0
			44	40	4	
19	9	1	Total	C	O	0
			44	40	4	
19	9	1	Total	C	O	0
			44	40	4	
19	9	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	4	1	Total	C	O	0
			44	40	4	
19	4	1	Total	C	O	0
			44	40	4	
19	4	1	Total	C	O	0
			44	40	4	
19	4	1	Total	C	O	0
			44	40	4	

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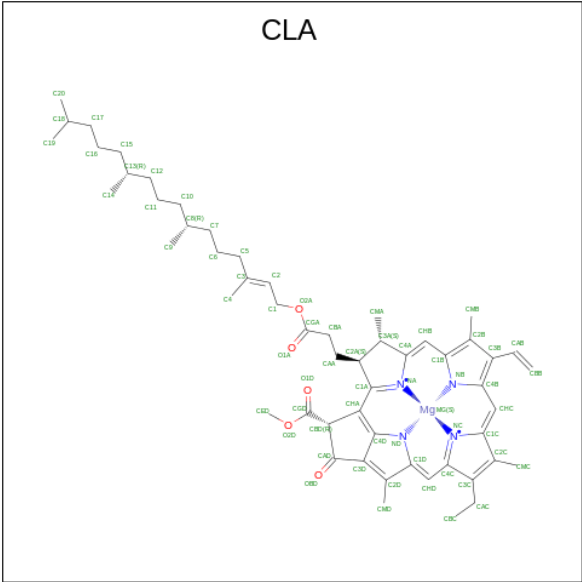
Mol	Chain	Residues	Atoms			AltConf
19	4	1	Total	C	O	0
			44	40	4	
19	6	1	Total	C	O	0
			44	40	4	
19	6	1	Total	C	O	0
			44	40	4	
19	6	1	Total	C	O	0
			44	40	4	
19	6	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			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	a	1	Total	C	O	0
			44	40	4	

- Molecule 20 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: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
20	5	1	Total	C	O	0
			45	40	5	
20	9	1	Total	C	O	0
			45	40	5	
20	9	1	Total	C	O	0
			45	40	5	
20	7	1	Total	C	O	0
			45	40	5	
20	1	1	Total	C	O	0
			45	40	5	

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	9	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	4	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	7	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
21	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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

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

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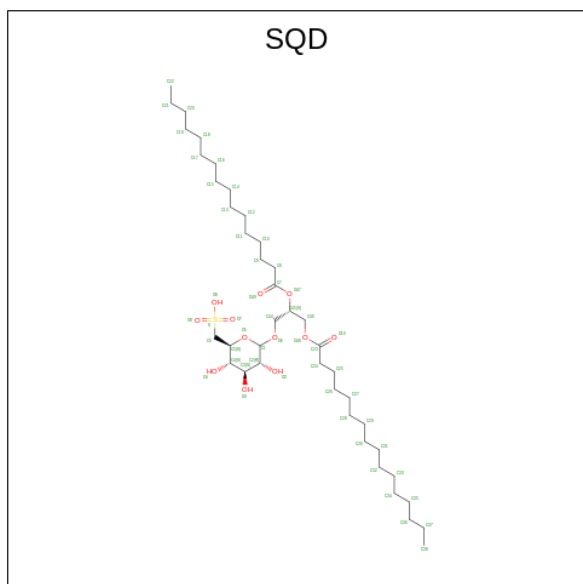
Mol	Chain	Residues	Atoms					AltConf
21	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total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

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

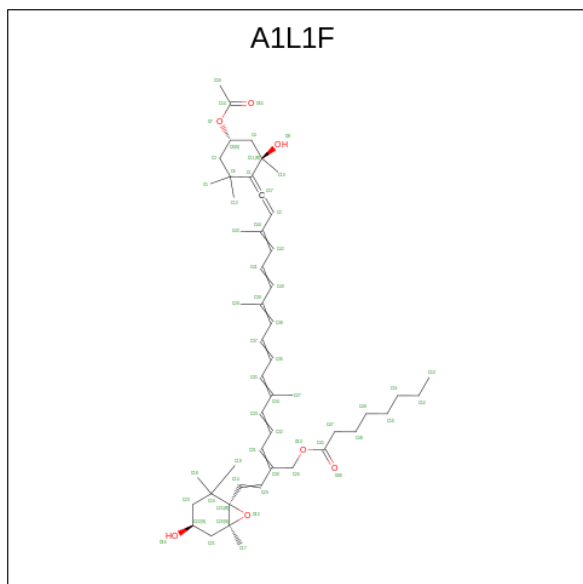
- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



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

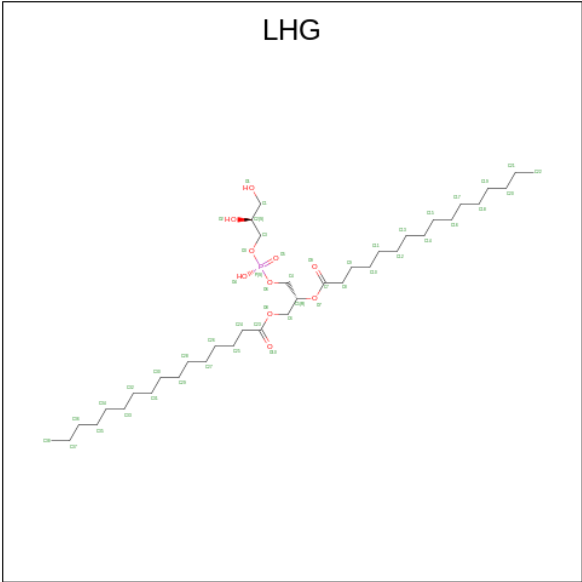
- Molecule 23 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyl oxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S},

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



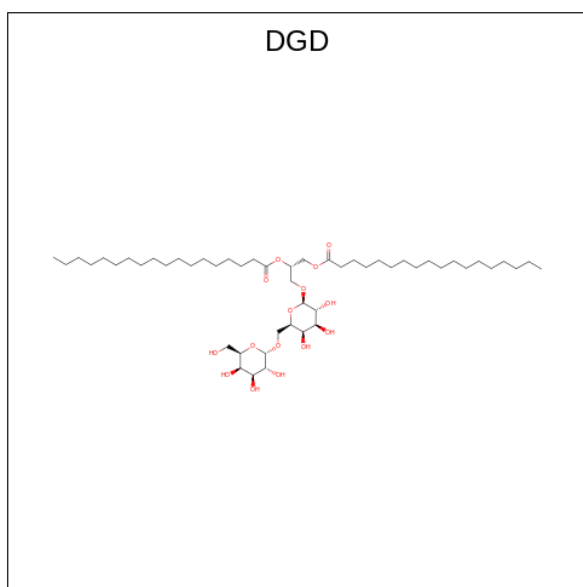
Mol	Chain	Residues	Atoms			AltConf
23	9	1	Total	C	O	0
			57	50	7	
23	8	1	Total	C	O	0
			57	50	7	
23	6	1	Total	C	O	0
			57	50	7	
23	6	1	Total	C	O	0
			53	46	7	
23	1	1	Total	C	O	0
			57	50	7	
23	h	1	Total	C	O	0
			57	50	7	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



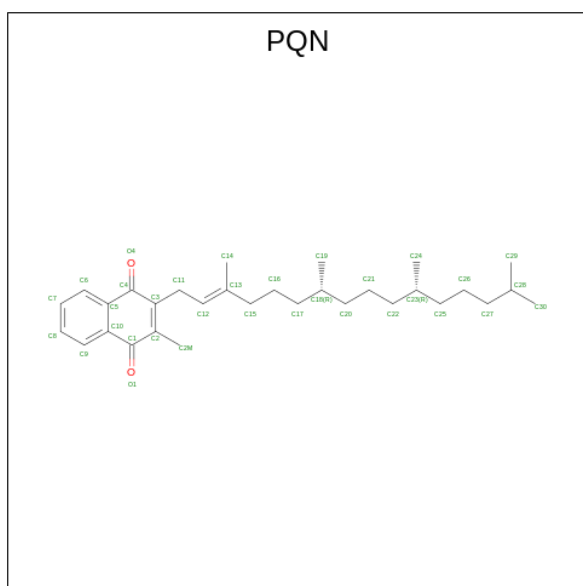
Mol	Chain	Residues	Atoms				AltConf
24	9	1	Total	C	O	P	0
			36	25	10	1	
24	a	1	Total	C	O	P	0
			48	37	10	1	
24	a	1	Total	C	O	P	0
			27	16	10	1	
24	b	1	Total	C	O	P	0
			31	20	10	1	
24	m	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



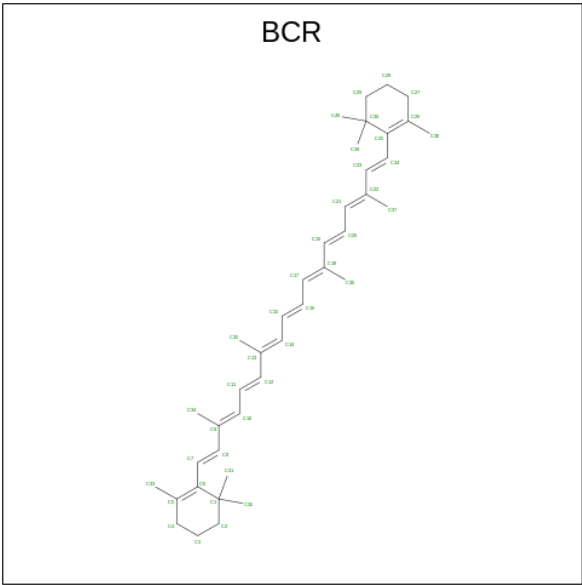
Mol	Chain	Residues	Atoms			AltConf
25	8	1	Total	C	O	0
			40	25	15	
25	4	1	Total	C	O	0
			40	25	15	
25	b	1	Total	C	O	0
			57	42	15	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



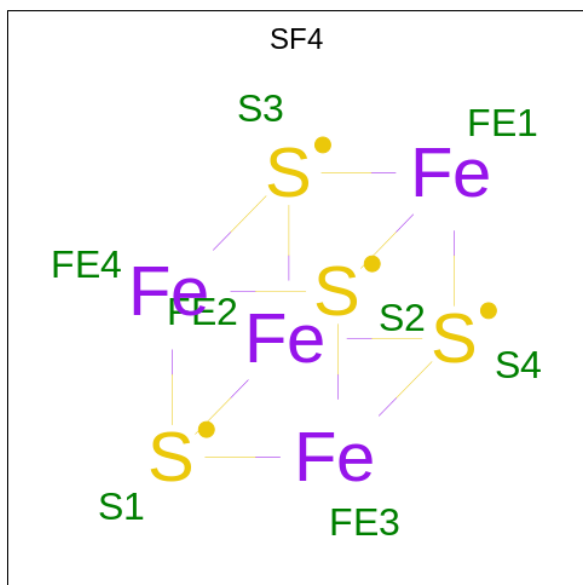
Mol	Chain	Residues	Atoms		AltConf
27	a	1	Total	C	0
			40	40	
27	a	1	Total	C	0
			40	40	
27	a	1	Total	C	0
			40	40	
27	a	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	

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

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



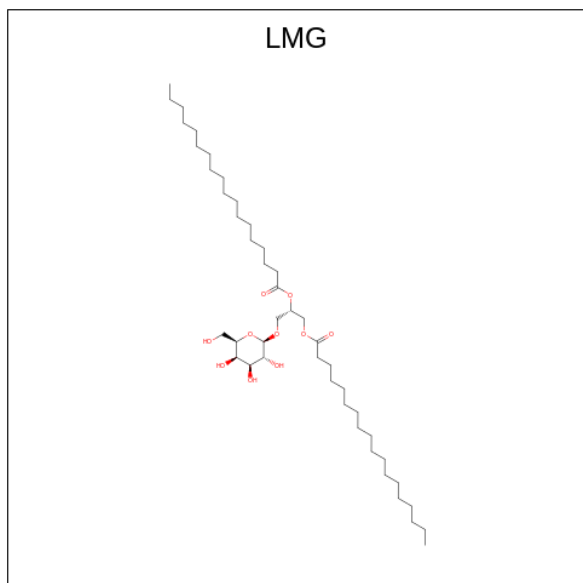
Mol	Chain	Residues	Atoms	AltConf
28	a	1	Total Fe S 8 4 4	0

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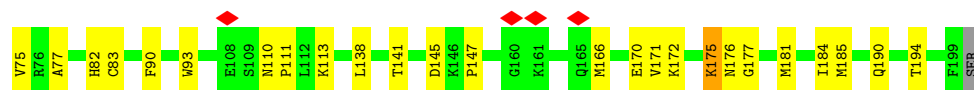
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Mol	Chain	Residues	Atoms			AltConf
28	c	1	Total	Fe	S	0
			8	4	4	
28	c	1	Total	Fe	S	0
			8	4	4	

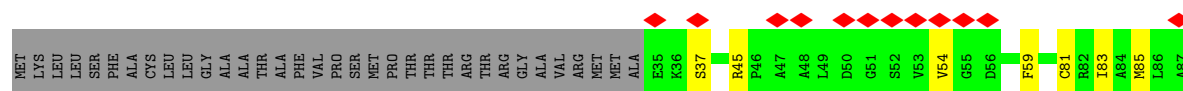
- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



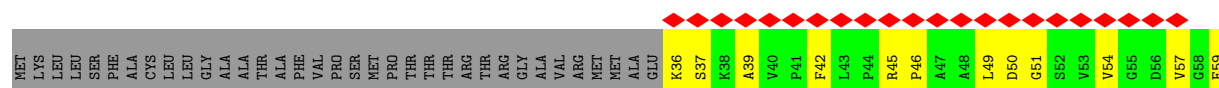
Mol	Chain	Residues	Atoms			AltConf
29	a	1	Total	C	O	0
			34	24	10	
29	j	1	Total	C	O	0
			32	22	10	



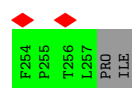
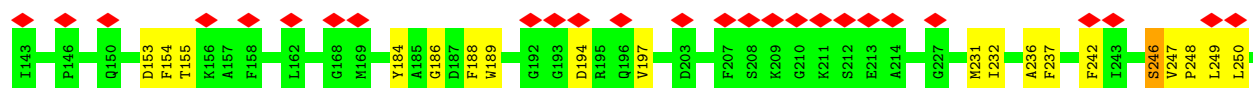
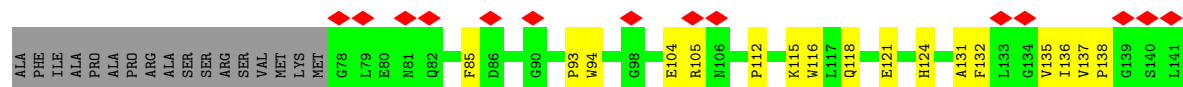
- Molecule 4: VCPI-4/7



- Molecule 4: VCPI-4/7

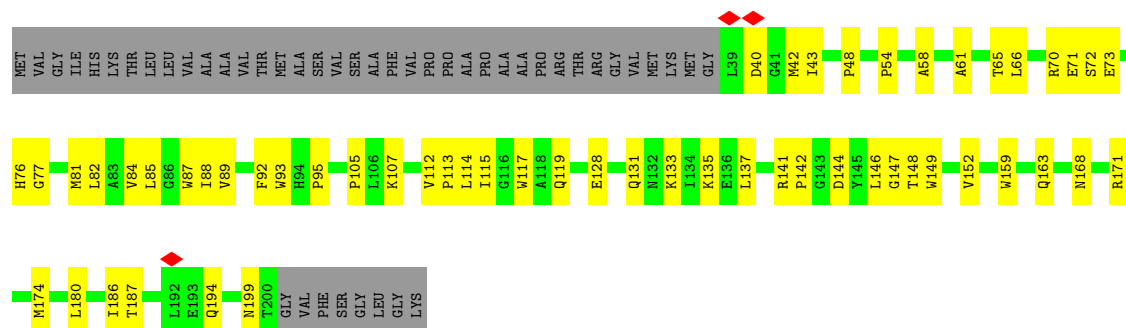


- Molecule 5: VCPI-6

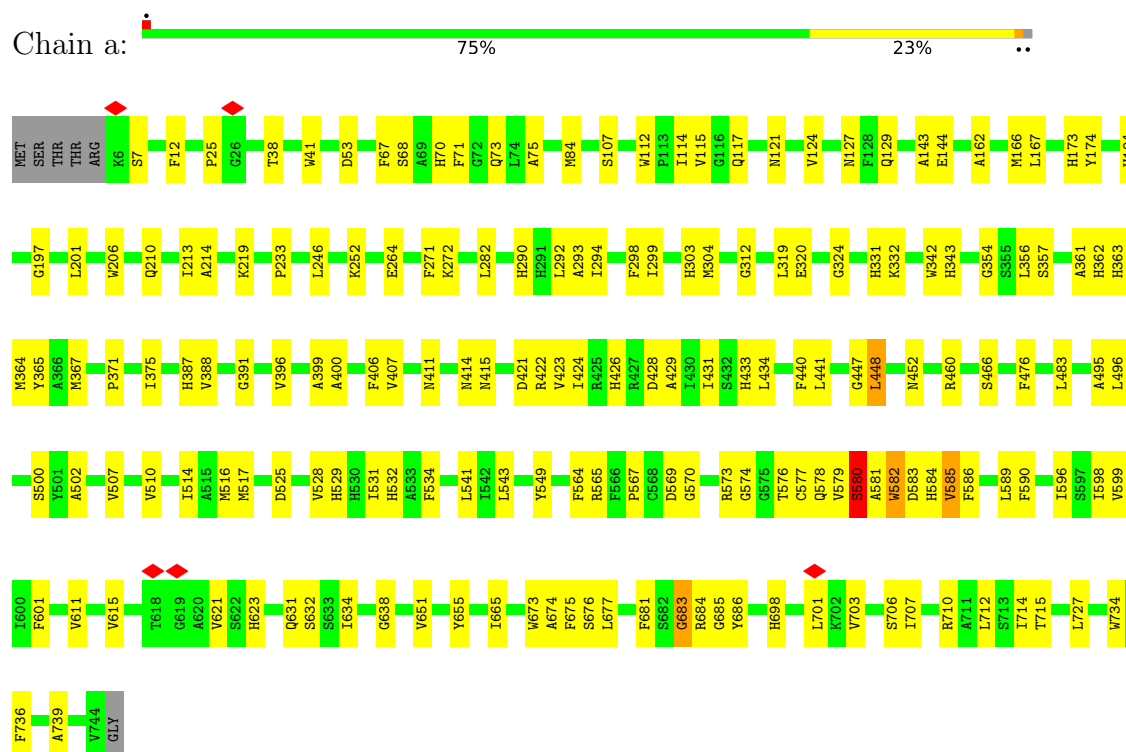


- Molecule 6: VCPI-1

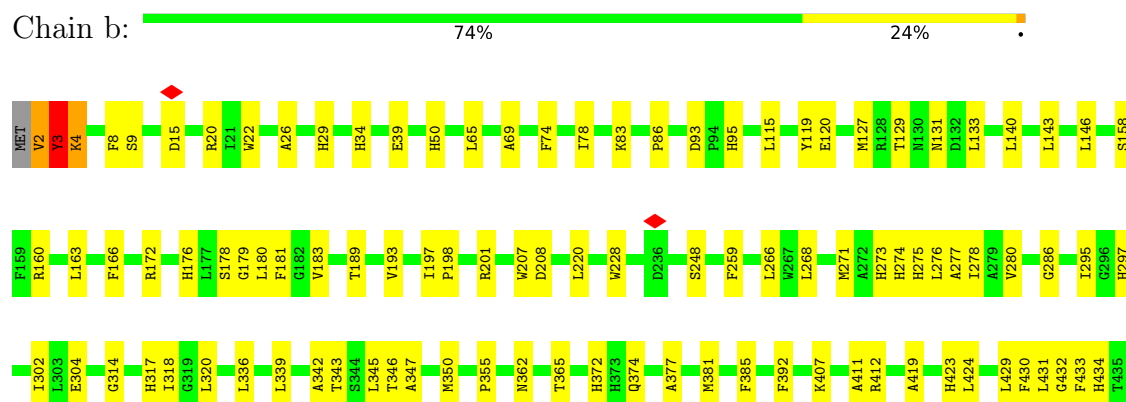


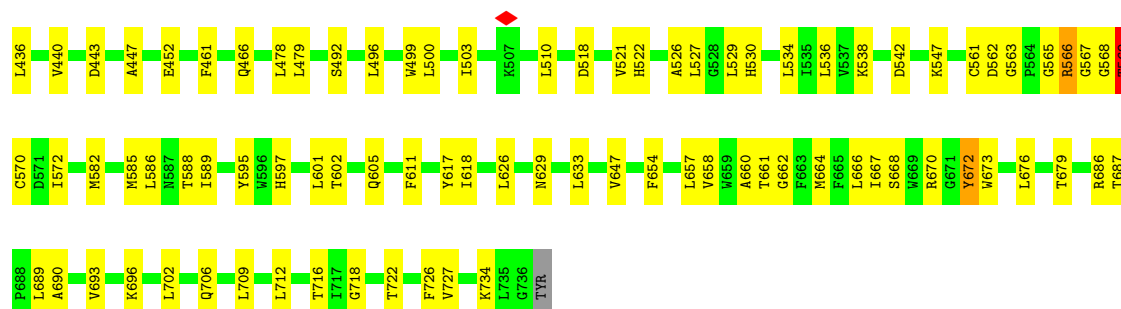


• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

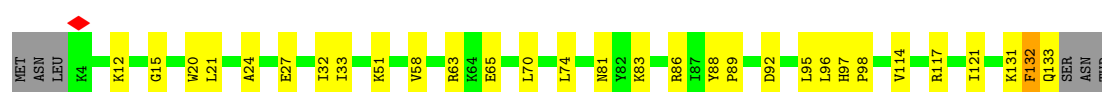
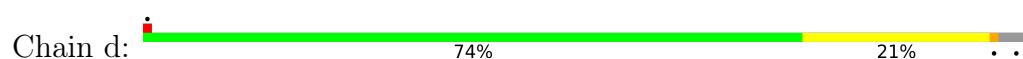


• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

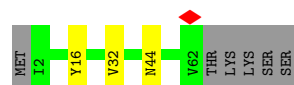
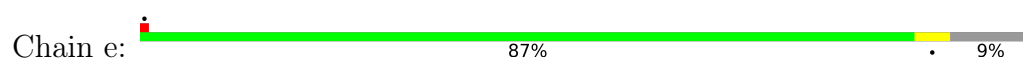




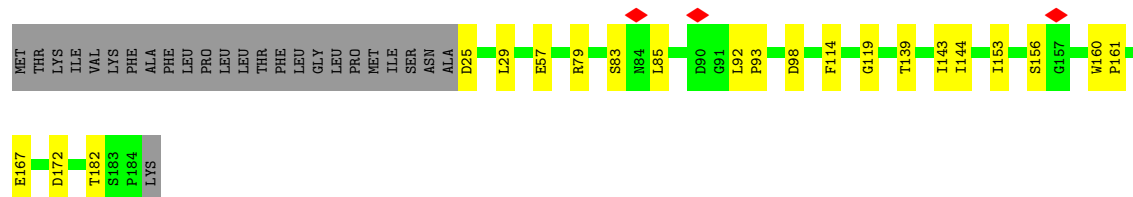
• Molecule 9: Photosystem I reaction center subunit II



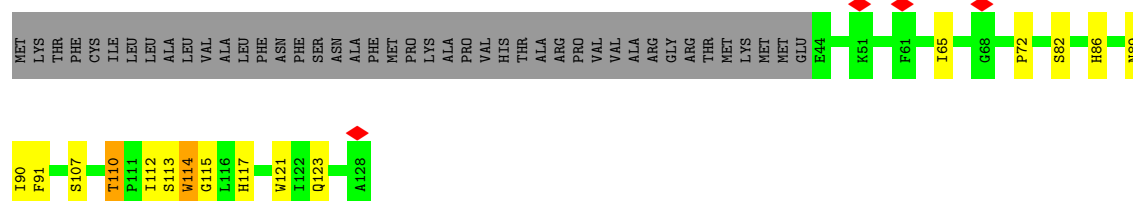
• Molecule 10: Photosystem I reaction center subunit IV



• Molecule 11: Photosystem I reaction center subunit III

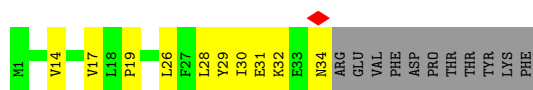


• Molecule 12: PsaR

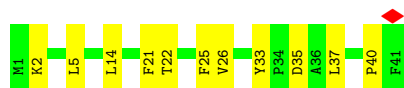


• Molecule 13: Photosystem I reaction center subunit VIII

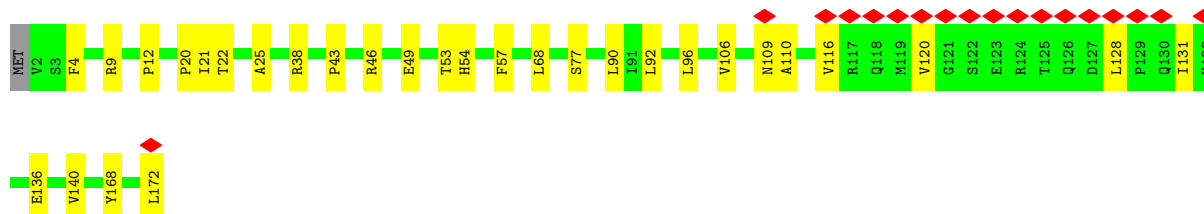
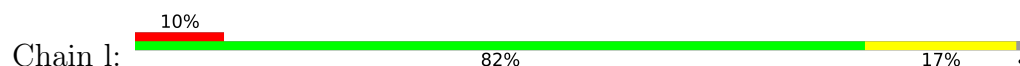




- Molecule 14: Photosystem I reaction center subunit IX



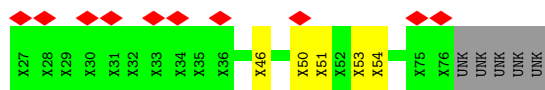
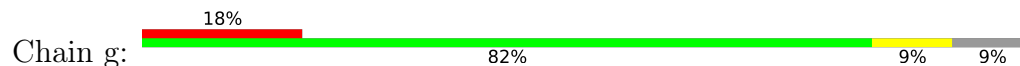
- Molecule 15: PSI subunit V



- Molecule 16: PsaM



- Molecule 17: PsaS



- Molecule 18: 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	19451	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.558	Depositor
Minimum map value	-0.396	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5	0.14	0/1353	0.29	0/1823
2	9	0.35	0/1496	0.34	0/2032
3	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
4	4	0.17	0/1298	0.32	0/1761
4	7	0.19	0/1248	0.37	0/1700
5	6	0.18	0/1390	0.32	0/1883
6	1	0.14	0/1293	0.33	0/1759
7	a	0.30	3/6024 (0.0%)	0.35	5/8219 (0.1%)
8	b	0.27	0/6080	0.35	2/8302 (0.0%)
9	d	0.19	0/1040	0.36	0/1402
10	e	0.09	0/502	0.20	0/681
11	f	0.14	0/1297	0.31	0/1762
12	h	0.52	1/667 (0.1%)	0.52	0/915
13	i	0.15	0/278	0.33	0/378
14	j	0.16	0/351	0.36	0/478
15	l	0.14	0/1315	0.31	0/1796
16	m	0.09	0/210	0.29	0/288
18	c	0.13	0/606	0.34	0/822
All	All	0.26	5/27734 (0.0%)	0.35	10/37744 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	580	SER	CA-C	-7.05	1.43	1.52
3	8	44	LEU	C-O	-6.18	1.15	1.23
12	h	114	TRP	C-O	-5.37	1.17	1.24
7	a	581	ALA	CA-C	-5.37	1.45	1.52
7	a	582	TRP	CA-C	-5.07	1.45	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	581	ALA	N-CA-C	-8.65	102.47	113.72
7	a	683	GLY	O-C-N	-8.45	116.29	123.73
8	b	568	GLY	N-CA-C	-7.49	100.73	110.69
3	8	39	LYS	N-CA-C	-6.09	105.68	113.23
7	a	448	LEU	N-CA-C	-6.05	104.24	111.69

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	5	1317	0	1318	34	0
2	9	1466	0	1470	57	0
3	8	1258	0	1280	31	0
4	4	1268	0	1288	21	0
4	7	1220	0	1209	39	0
5	6	1352	0	1334	29	0
6	1	1262	0	1237	40	0
7	a	5827	0	5697	156	0
8	b	5865	0	5711	200	0
9	d	1014	0	1015	28	0
10	e	494	0	495	3	0
11	f	1266	0	1262	32	0
12	h	646	0	649	11	0
13	i	271	0	292	17	0
14	j	339	0	342	15	0
15	l	1283	0	1278	28	0
16	m	210	0	226	2	0
17	g	250	0	57	4	0
18	c	596	0	583	23	0
19	1	88	0	112	4	0
19	4	220	0	280	25	0
19	5	176	0	224	21	0
19	6	176	0	224	20	0
19	7	176	0	224	29	0
19	8	132	0	168	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	9	132	0	168	16	0
19	a	88	0	112	7	0
20	1	45	0	0	1	0
20	5	45	0	0	1	0
20	7	45	0	0	2	0
20	9	90	0	0	3	0
21	1	547	0	508	17	0
21	4	613	0	522	30	0
21	5	563	0	472	23	0
21	6	499	0	413	12	0
21	7	576	0	444	24	0
21	8	507	0	429	22	0
21	9	454	0	380	39	0
21	a	2644	0	2634	207	0
21	b	2468	0	2519	166	0
21	f	117	0	115	2	0
21	h	120	0	121	7	0
21	j	42	0	31	2	0
21	l	148	0	123	10	0
22	1	45	0	54	3	0
22	5	35	0	34	1	0
23	1	57	0	0	11	0
23	6	110	0	0	6	0
23	8	57	0	0	2	0
23	9	57	0	0	2	0
23	h	57	0	0	4	0
24	9	36	0	45	1	0
24	a	75	0	93	5	0
24	b	31	0	32	2	0
24	m	46	0	65	2	0
25	4	40	0	38	11	0
25	8	40	0	38	2	0
25	b	57	0	72	6	0
26	a	33	0	46	4	0
26	b	33	0	46	6	0
27	a	160	0	224	14	0
27	b	360	0	504	55	0
27	f	80	0	112	31	0
27	i	80	0	112	18	0
27	j	40	0	56	14	0
27	m	40	0	56	1	0
28	a	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	c	16	0	0	3	0
29	a	34	0	38	11	0
29	j	32	0	34	6	0
All	All	39574	0	38665	1158	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 15.

The worst 5 of 1158 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)
7:a:698:HIS:NE2	21:a:856:CLA:HAC1	1.52	1.23
21:a:833:CLA:H61	21:l:202:CLA:H101	1.28	1.15
21:a:834:CLA:H151	26:b:842:PQN:H202	1.21	1.14
21:a:803:CLA:H151	21:b:810:CLA:HBC3	1.24	1.14
21:b:801:CLA:H142	21:b:839:CLA:H111	1.29	1.12

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	25	54
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	22	50
4	7	164/202 (81%)	144 (88%)	20 (12%)	0	100	100
5	6	178/259 (69%)	158 (89%)	20 (11%)	0	100	100
6	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	78
8	b	733/737 (100%)	697 (95%)	33 (4%)	3 (0%)	30	60
9	d	128/136 (94%)	112 (88%)	15 (12%)	1 (1%)	16	44
10	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
11	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
12	h	83/128 (65%)	76 (92%)	6 (7%)	1 (1%)	11	35
13	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
14	j	39/41 (95%)	39 (100%)	0	0	100	100
15	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	11	35
16	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3440/3914 (88%)	3224 (94%)	206 (6%)	10 (0%)	38	66

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	9	32	THR
15	l	120	VAL
8	b	566	ARG
7	a	580	SER
8	b	569	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	133/182 (73%)	133 (100%)	0	100	100
2	9	141/167 (84%)	139 (99%)	2 (1%)	62	77
3	8	132/160 (82%)	131 (99%)	1 (1%)	79	87
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	122/159 (77%)	121 (99%)	1 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	6	135/201 (67%)	134 (99%)	1 (1%)	81	88
6	1	128/165 (78%)	128 (100%)	0	100	100
7	a	607/613 (99%)	603 (99%)	4 (1%)	81	88
8	b	599/602 (100%)	595 (99%)	4 (1%)	81	88
9	d	107/113 (95%)	106 (99%)	1 (1%)	75	86
10	e	56/62 (90%)	56 (100%)	0	100	100
11	f	138/162 (85%)	138 (100%)	0	100	100
12	h	71/107 (66%)	70 (99%)	1 (1%)	62	77
13	i	32/43 (74%)	32 (100%)	0	100	100
14	j	36/36 (100%)	36 (100%)	0	100	100
15	l	130/141 (92%)	130 (100%)	0	100	100
16	m	21/24 (88%)	21 (100%)	0	100	100
18	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2788/3164 (88%)	2773 (100%)	15 (0%)	85	91

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

Mol	Chain	Res	Type
7	a	579	VAL
9	d	133	GLN
7	a	580	SER
12	h	110	THR
8	b	4	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
8	b	629	ASN
9	d	26	ASN
9	d	7	GLN
9	d	109	GLN
6	1	194	GLN

5.3.3 RNA ⓘ

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](#)

242 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
21	CLA	6	311	5	42,50,73	1.84	5 (11%)	48,85,113	1.58	7 (14%)
27	BCR	i	102	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
27	BCR	b	847	-	41,41,41	0.76	0	56,56,56	2.19	22 (39%)
21	CLA	7	306	4	48,56,73	1.73	6 (12%)	55,92,113	1.54	6 (10%)
24	LHG	m	101	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
21	CLA	a	825	-	55,63,73	1.62	5 (9%)	64,101,113	1.45	8 (12%)
21	CLA	b	819	-	55,63,73	1.62	6 (10%)	64,101,113	1.44	8 (12%)
21	CLA	a	838	-	51,59,73	1.66	5 (9%)	59,96,113	1.55	9 (15%)
27	BCR	b	845	-	41,41,41	0.68	0	56,56,56	2.10	15 (26%)
21	CLA	1	313	-	41,49,73	1.84	6 (14%)	47,84,113	1.64	7 (14%)
21	CLA	f	803	11	52,60,73	1.68	5 (9%)	60,97,113	1.49	8 (13%)
19	XAT	7	303	-	39,47,47	0.96	1 (2%)	54,74,74	2.60	17 (31%)
23	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
21	CLA	5	306	1	46,54,73	1.77	6 (13%)	53,90,113	1.55	8 (15%)
19	XAT	5	301	-	39,47,47	0.95	2 (5%)	54,74,74	2.62	19 (35%)
21	CLA	a	814	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
21	CLA	a	808	-	51,59,73	1.69	5 (9%)	59,96,113	1.50	8 (13%)
21	CLA	4	317	-	55,63,73	1.64	6 (10%)	64,101,113	1.46	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	b	802	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	8 (10%)
21	CLA	b	822	-	60,68,73	1.55	6 (10%)	70,107,113	1.37	7 (10%)
21	CLA	b	826	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	6 (7%)
21	CLA	6	307	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
21	CLA	7	317	-	45,53,73	1.80	5 (11%)	52,89,113	1.58	6 (11%)
21	CLA	b	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	9 (11%)
21	CLA	b	804	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
21	CLA	9	309	2	46,54,73	1.78	6 (13%)	53,90,113	1.55	7 (13%)
21	CLA	1	308	6	65,73,73	1.48	5 (7%)	76,113,113	1.43	8 (10%)
21	CLA	a	809	7	65,73,73	1.45	6 (9%)	76,113,113	1.44	9 (11%)
21	CLA	a	824	-	46,54,73	1.77	6 (13%)	53,90,113	1.49	7 (13%)
21	CLA	a	831	-	65,73,73	1.51	6 (9%)	76,113,113	1.48	8 (10%)
21	CLA	b	828	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
19	XAT	9	304	-	39,47,47	0.95	1 (2%)	54,74,74	2.42	19 (35%)
21	CLA	b	805	-	65,73,73	1.45	5 (7%)	76,113,113	1.42	7 (9%)
21	CLA	4	307	-	56,64,73	1.62	5 (8%)	65,102,113	1.44	7 (10%)
21	CLA	5	314	1	45,53,73	1.82	5 (11%)	52,89,113	1.58	6 (11%)
21	CLA	1	202	-	60,68,73	1.54	7 (11%)	70,107,113	1.47	7 (10%)
23	A1L1F	6	301	-	50,59,59	1.30	5 (10%)	62,85,85	2.49	20 (32%)
21	CLA	a	842	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	6 (7%)
21	CLA	1	305	-	61,69,73	1.55	6 (9%)	71,108,113	1.39	7 (9%)
19	XAT	8	303	-	39,47,47	0.87	1 (2%)	54,74,74	2.64	18 (33%)
21	CLA	a	806	-	65,73,73	1.50	11 (16%)	76,113,113	1.66	13 (17%)
21	CLA	b	824	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
21	CLA	1	312	6	52,60,73	1.72	5 (9%)	60,97,113	1.49	8 (13%)
21	CLA	8	310	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	7 (13%)
21	CLA	9	311	-	46,54,73	1.78	5 (10%)	53,90,113	1.61	8 (15%)
21	CLA	b	833	-	58,66,73	1.58	5 (8%)	67,104,113	1.42	8 (11%)
21	CLA	a	844	24	65,73,73	1.46	5 (7%)	76,113,113	1.40	9 (11%)
21	CLA	b	839	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
19	XAT	4	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.57	19 (35%)
21	CLA	4	309	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	8 (13%)
21	CLA	b	814	-	55,63,73	1.61	6 (10%)	64,101,113	1.56	8 (12%)
19	XAT	8	301	-	39,47,47	0.91	0	54,74,74	2.53	19 (35%)
21	CLA	b	837	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SF4	a	851	-	0,12,12	-	-	-		
21	CLA	6	314	-	46,54,73	1.72	6 (13%)	53,90,113	1.61	6 (11%)
21	CLA	8	312	3	52,60,73	1.65	5 (9%)	60,97,113	1.52	8 (13%)
21	CLA	a	841	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	9 (11%)
21	CLA	b	835	-	53,61,73	1.66	5 (9%)	61,98,113	1.51	8 (13%)
26	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.09	3 (7%)
21	CLA	5	307	22	45,53,73	1.79	5 (11%)	52,89,113	1.57	7 (13%)
21	CLA	a	821	-	45,53,73	1.77	6 (13%)	52,89,113	1.61	7 (13%)
21	CLA	5	315	-	52,60,73	1.65	5 (9%)	60,97,113	1.54	8 (13%)
21	CLA	b	811	-	54,62,73	1.67	7 (12%)	67,100,113	1.51	9 (13%)
21	CLA	l	203	-	46,54,73	1.75	6 (13%)	53,90,113	1.56	7 (13%)
21	CLA	9	313	2	46,54,73	1.77	6 (13%)	53,90,113	1.63	7 (13%)
19	XAT	a	853	-	39,47,47	0.88	1 (2%)	54,74,74	2.72	18 (33%)
24	LHG	a	846	21	26,26,48	1.27	4 (15%)	29,32,54	1.20	2 (6%)
21	CLA	a	852	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
21	CLA	a	803	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	6 (7%)
21	CLA	a	816	-	50,58,73	1.69	6 (12%)	58,95,113	1.56	9 (15%)
21	CLA	8	307	3	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
21	CLA	4	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	9 (11%)
21	CLA	8	308	-	55,63,73	1.61	5 (9%)	64,101,113	1.51	9 (14%)
21	CLA	4	316	-	46,54,73	1.77	5 (10%)	53,90,113	1.58	7 (13%)
21	CLA	a	823	-	49,57,73	1.68	6 (12%)	55,93,113	1.61	7 (12%)
21	CLA	a	834	-	65,73,73	1.49	5 (7%)	76,113,113	1.36	9 (11%)
21	CLA	b	829	-	65,73,73	1.52	6 (9%)	76,113,113	1.45	10 (13%)
29	LMG	j	103	-	32,32,55	1.13	2 (6%)	40,40,63	1.14	3 (7%)
24	LHG	b	849	21	30,30,48	1.34	6 (20%)	33,36,54	1.14	2 (6%)
21	CLA	6	315	5	41,49,73	1.87	6 (14%)	47,84,113	1.63	6 (12%)
27	BCR	b	844	-	41,41,41	0.72	0	56,56,56	1.93	16 (28%)
21	CLA	8	311	-	56,64,73	1.58	6 (10%)	65,102,113	1.49	8 (12%)
19	XAT	8	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.65	20 (37%)
21	CLA	a	818	-	56,64,73	1.61	6 (10%)	65,102,113	1.44	8 (12%)
21	CLA	a	827	-	65,73,73	1.49	6 (9%)	76,113,113	1.45	9 (11%)
21	CLA	b	841	24	65,73,73	1.53	6 (9%)	76,113,113	1.36	8 (10%)
25	DGD	8	315	21	41,41,67	1.04	2 (4%)	55,55,81	1.11	5 (9%)
21	CLA	a	820	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	a	810	7	65,73,73	1.50	6 (9%)	76,113,113	1.41	8 (10%)
21	CLA	b	821	-	51,59,73	1.65	6 (11%)	59,96,113	1.57	9 (15%)
19	XAT	6	306	-	39,47,47	0.93	1 (2%)	54,74,74	2.61	19 (35%)
21	CLA	4	313	-	53,61,73	1.65	5 (9%)	61,98,113	1.48	8 (13%)
21	CLA	8	314	-	41,49,73	1.85	5 (12%)	47,84,113	1.63	7 (14%)
21	CLA	l	201	-	42,50,73	1.82	6 (14%)	48,85,113	1.64	7 (14%)
27	BCR	b	852	-	41,41,41	0.73	0	56,56,56	2.05	15 (26%)
21	CLA	a	822	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
25	DGD	4	318	-	41,41,67	1.06	2 (4%)	55,55,81	1.82	5 (9%)
21	CLA	f	802	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	9 (11%)
21	CLA	9	314	-	55,63,73	1.62	6 (10%)	64,101,113	1.49	8 (12%)
19	XAT	4	303	-	39,47,47	0.89	2 (5%)	54,74,74	2.57	17 (31%)
19	XAT	4	304	-	39,47,47	0.88	1 (2%)	54,74,74	2.56	15 (27%)
19	XAT	9	305	-	39,47,47	0.97	1 (2%)	54,74,74	2.35	18 (33%)
20	A1L1G	9	301	-	38,47,47	1.46	6 (15%)	49,71,71	1.57	10 (20%)
20	A1L1G	1	301	-	38,47,47	1.44	6 (15%)	49,71,71	1.57	11 (22%)
21	CLA	1	307	-	54,62,73	1.63	5 (9%)	62,99,113	1.52	8 (12%)
21	CLA	b	817	-	59,67,73	1.56	5 (8%)	68,105,113	1.51	7 (10%)
21	CLA	7	309	-	46,55,73	1.75	5 (10%)	52,91,113	1.52	7 (13%)
21	CLA	1	311	-	53,61,73	1.64	5 (9%)	61,98,113	1.49	9 (14%)
21	CLA	6	312	5	51,59,73	1.67	6 (11%)	59,96,113	1.51	7 (11%)
21	CLA	7	316	-	51,59,73	1.63	6 (11%)	59,96,113	1.59	8 (13%)
21	CLA	6	308	-	58,66,73	1.61	5 (8%)	67,104,113	1.43	6 (8%)
21	CLA	a	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
21	CLA	1	310	6	65,73,73	1.50	5 (7%)	76,113,113	1.33	8 (10%)
21	CLA	b	832	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
21	CLA	b	840	-	65,73,73	1.51	5 (7%)	76,113,113	1.41	8 (10%)
21	CLA	a	805	21	55,63,73	1.61	6 (10%)	64,101,113	1.51	8 (12%)
21	CLA	8	313	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	7 (13%)
19	XAT	7	305	-	39,47,47	0.86	0	54,74,74	2.65	20 (37%)
21	CLA	5	309	-	55,63,73	1.63	5 (9%)	64,101,113	1.47	7 (10%)
21	CLA	4	312	-	46,54,73	1.79	6 (13%)	53,90,113	1.51	7 (13%)
21	CLA	a	856	-	65,73,73	1.48	5 (7%)	76,113,113	1.34	8 (10%)
27	BCR	b	843	-	41,41,41	0.69	0	56,56,56	2.29	21 (37%)
21	CLA	b	808	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	7	312	-	48,56,73	1.71	6 (12%)	55,92,113	1.56	8 (14%)
19	XAT	7	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.68	21 (38%)
21	CLA	b	810	-	65,73,73	1.47	6 (9%)	76,113,113	1.45	8 (10%)
22	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	4 (7%)
29	LMG	a	855	-	34,34,55	1.14	2 (5%)	42,42,63	1.15	3 (7%)
21	CLA	a	830	-	65,73,73	1.48	7 (10%)	76,113,113	1.40	8 (10%)
19	XAT	5	305	-	39,47,47	0.89	0	54,74,74	2.86	22 (40%)
21	CLA	b	831	-	49,57,73	1.69	5 (10%)	55,93,113	1.55	8 (14%)
27	BCR	a	850	-	41,41,41	0.74	0	56,56,56	2.16	15 (26%)
23	A1L1F	6	304	-	46,55,59	1.33	4 (8%)	58,81,85	2.55	20 (34%)
21	CLA	4	311	-	46,54,73	1.78	6 (13%)	53,90,113	1.56	7 (13%)
21	CLA	a	829	-	62,70,73	1.51	6 (9%)	72,109,113	1.39	8 (11%)
21	CLA	1	314	-	45,53,73	1.78	5 (11%)	52,89,113	1.56	6 (11%)
21	CLA	5	312	-	51,59,73	1.65	5 (9%)	59,96,113	1.53	9 (15%)
21	CLA	a	813	-	54,62,73	1.65	5 (9%)	62,99,113	1.45	7 (11%)
24	LHG	9	307	-	35,35,48	1.22	6 (17%)	38,41,54	0.97	2 (5%)
21	CLA	a	839	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
27	BCR	b	853	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
21	CLA	4	310	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
21	CLA	5	313	-	52,60,73	1.64	5 (9%)	60,97,113	1.53	9 (15%)
21	CLA	7	313	-	54,62,73	1.64	5 (9%)	62,99,113	1.49	9 (14%)
20	A1L1G	5	304	-	38,47,47	1.42	6 (15%)	49,71,71	1.44	7 (14%)
21	CLA	6	309	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	6 (7%)
21	CLA	7	310	-	46,54,73	1.78	6 (13%)	53,90,113	1.57	6 (11%)
21	CLA	h	203	-	55,63,73	1.62	6 (10%)	64,101,113	1.47	10 (15%)
27	BCR	m	102	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	6 (10%)
21	CLA	6	313	-	52,60,73	1.65	5 (9%)	60,97,113	1.52	7 (11%)
27	BCR	a	848	-	41,41,41	0.73	0	56,56,56	1.94	18 (32%)
20	A1L1G	9	306	-	38,47,47	1.41	6 (15%)	49,71,71	1.53	8 (16%)
21	CLA	1	306	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	9 (11%)
24	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
27	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.13	14 (25%)
19	XAT	6	305	-	39,47,47	0.89	1 (2%)	54,74,74	2.73	19 (35%)
21	CLA	j	101	14	42,50,73	1.83	5 (11%)	48,85,113	1.64	6 (12%)
21	CLA	4	315	4	41,49,73	1.87	6 (14%)	47,84,113	1.63	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	5	308	1	60,68,73	1.54	5 (8%)	70,107,113	1.42	8 (11%)
21	CLA	a	802	-	58,66,73	1.55	6 (10%)	67,104,113	1.49	8 (11%)
21	CLA	a	828	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
21	CLA	b	823	-	53,61,73	1.63	6 (11%)	61,98,113	1.46	8 (13%)
21	CLA	b	836	-	58,66,73	1.57	5 (8%)	67,104,113	1.52	8 (11%)
21	CLA	b	813	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	8 (10%)
21	CLA	b	830	-	41,49,73	1.83	6 (14%)	47,84,113	1.64	9 (19%)
21	CLA	9	316	-	62,70,73	1.55	6 (9%)	72,109,113	1.37	8 (11%)
27	BCR	b	850	-	41,41,41	0.73	0	56,56,56	1.89	17 (30%)
26	PQN	b	842	-	34,34,34	1.55	2 (5%)	42,45,45	1.20	4 (9%)
21	CLA	b	803	-	65,73,73	1.46	5 (7%)	76,113,113	1.54	13 (17%)
21	CLA	7	314	-	45,53,73	1.80	6 (13%)	52,89,113	1.64	7 (13%)
20	A1L1G	7	302	-	38,47,47	1.41	6 (15%)	49,71,71	1.51	9 (18%)
27	BCR	a	849	-	41,41,41	0.74	0	56,56,56	2.17	19 (33%)
19	XAT	1	303	-	39,47,47	0.90	1 (2%)	54,74,74	2.52	20 (37%)
21	CLA	a	801	-	65,73,73	1.51	8 (12%)	76,113,113	1.38	7 (9%)
21	CLA	4	306	4	45,53,73	1.79	6 (13%)	52,89,113	1.57	7 (13%)
21	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
25	DGD	b	851	-	58,58,67	1.15	7 (12%)	72,72,81	1.53	10 (13%)
21	CLA	b	838	-	65,73,73	1.52	6 (9%)	76,113,113	1.34	8 (10%)
27	BCR	b	848	-	41,41,41	0.76	0	56,56,56	1.79	16 (28%)
21	CLA	b	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
28	SF4	c	102	-	0,12,12	-	-	-		
19	XAT	7	301	-	39,47,47	0.93	1 (2%)	54,74,74	2.63	19 (35%)
21	CLA	a	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.59	8 (15%)
27	BCR	j	102	-	41,41,41	0.73	0	56,56,56	2.08	17 (30%)
19	XAT	4	301	-	39,47,47	0.92	2 (5%)	54,74,74	2.54	19 (35%)
22	SQD	5	317	21	34,35,54	1.47	4 (11%)	43,46,65	1.35	7 (16%)
21	CLA	b	809	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	8 (10%)
21	CLA	a	812	21	62,70,73	1.51	6 (9%)	72,109,113	1.45	8 (11%)
27	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
21	CLA	b	818	-	60,68,73	1.55	5 (8%)	70,107,113	1.40	7 (10%)
19	XAT	5	303	-	39,47,47	0.93	1 (2%)	54,74,74	2.59	20 (37%)
19	XAT	6	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.81	20 (37%)
21	CLA	5	310	1	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	XAT	4	305	-	39,47,47	0.89	1 (2%)	54,74,74	2.75	19 (35%)
21	CLA	5	316	-	46,54,73	1.75	5 (10%)	53,90,113	1.56	7 (13%)
21	CLA	b	820	-	50,58,73	1.69	6 (12%)	58,95,113	1.60	10 (17%)
21	CLA	b	827	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
21	CLA	9	310	-	46,54,73	1.75	5 (10%)	53,90,113	1.63	6 (11%)
21	CLA	8	309	-	57,65,73	1.60	5 (8%)	66,103,113	1.45	9 (13%)
27	BCR	f	801	-	41,41,41	0.68	0	56,56,56	2.14	15 (26%)
19	XAT	a	854	-	39,47,47	0.95	2 (5%)	54,74,74	2.70	20 (37%)
21	CLA	a	832	-	50,58,73	1.68	6 (12%)	58,95,113	1.55	9 (15%)
19	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.60	17 (31%)
21	CLA	8	306	25	46,54,73	1.75	6 (13%)	53,90,113	1.53	7 (13%)
21	CLA	1	309	6	46,54,73	1.79	6 (13%)	53,90,113	1.51	7 (13%)
19	XAT	6	303	-	39,47,47	0.90	2 (5%)	54,74,74	2.65	19 (35%)
21	CLA	a	817	-	45,53,73	1.80	5 (11%)	52,89,113	1.58	7 (13%)
21	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.54	8 (12%)
21	CLA	7	311	-	46,54,73	1.78	6 (13%)	53,90,113	1.58	7 (13%)
23	A1L1F	8	304	-	50,59,59	1.30	4 (8%)	62,85,85	2.79	23 (37%)
21	CLA	8	305	3	43,51,73	1.79	5 (11%)	49,86,113	1.65	7 (14%)
21	CLA	a	837	7	45,53,73	1.78	5 (11%)	52,89,113	1.59	7 (13%)
21	CLA	9	308	2	65,73,73	1.49	7 (10%)	76,113,113	1.42	8 (10%)
21	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	7 (9%)
21	CLA	b	815	-	45,53,73	1.76	6 (13%)	52,89,113	1.59	7 (13%)
21	CLA	6	316	5	46,54,73	1.75	5 (10%)	53,90,113	1.57	6 (11%)
21	CLA	a	819	-	54,62,73	1.62	7 (12%)	62,99,113	1.45	7 (11%)
23	A1L1F	h	202	-	50,59,59	1.39	5 (10%)	62,85,85	2.59	22 (35%)
21	CLA	h	201	-	65,73,73	1.51	6 (9%)	76,113,113	1.45	7 (9%)
21	CLA	5	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.53	7 (13%)
21	CLA	7	307	-	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
21	CLA	9	315	2	42,50,73	1.84	5 (11%)	48,85,113	1.61	7 (14%)
28	SF4	c	101	-	0,12,12	-	-	-	-	-
21	CLA	b	812	-	53,61,73	1.65	5 (9%)	61,98,113	1.50	8 (13%)
21	CLA	b	806	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
21	CLA	4	314	4	45,53,73	1.80	6 (13%)	52,89,113	1.56	7 (13%)
21	CLA	7	308	-	60,68,73	1.53	5 (8%)	70,107,113	1.44	7 (10%)
21	CLA	a	811	-	56,64,73	1.59	6 (10%)	65,102,113	1.48	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	a	840	-	65,73,73	1.52	5 (7%)	76,113,113	1.36	7 (9%)
21	CLA	a	826	-	65,73,73	1.45	6 (9%)	76,113,113	1.43	6 (7%)
23	A1L1F	9	302	-	50,59,59	1.37	5 (10%)	62,85,85	2.72	19 (30%)
27	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.04	17 (30%)
19	XAT	5	302	-	39,47,47	0.94	2 (5%)	54,74,74	2.58	19 (35%)
21	CLA	6	310	-	52,60,73	1.65	5 (9%)	60,97,113	1.53	8 (13%)
21	CLA	b	816	-	55,63,73	1.63	6 (10%)	64,101,113	1.48	9 (14%)
21	CLA	a	804	-	55,63,73	1.62	6 (10%)	64,101,113	1.55	10 (15%)
27	BCR	b	846	-	41,41,41	0.71	0	56,56,56	1.97	21 (37%)
21	CLA	7	315	4	41,49,73	1.85	5 (12%)	47,84,113	1.65	8 (17%)
21	CLA	a	836	-	50,58,73	1.70	6 (12%)	58,95,113	1.49	9 (15%)
21	CLA	9	312	-	46,54,73	1.75	6 (13%)	53,90,113	1.67	8 (15%)
21	CLA	b	825	-	64,72,73	1.48	5 (7%)	74,111,113	1.45	7 (9%)
19	XAT	9	303	-	39,47,47	0.95	1 (2%)	54,74,74	2.61	19 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	311	5	1/1/10/20	2/10/88/115	-
27	BCR	i	102	-	-	8/29/63/63	0/2/2/2
27	BCR	b	847	-	-	1/29/63/63	0/2/2/2
21	CLA	7	306	4	1/1/11/20	10/17/95/115	-
24	LHG	m	101	-	-	28/50/50/53	-
21	CLA	a	825	-	1/1/13/20	8/25/103/115	-
21	CLA	b	819	-	1/1/13/20	3/25/103/115	-
21	CLA	a	838	-	1/1/12/20	6/21/99/115	-
27	BCR	b	845	-	-	6/29/63/63	0/2/2/2
21	CLA	1	313	-	1/1/10/20	3/8/86/115	-
21	CLA	f	803	11	1/1/12/20	2/22/100/115	-
19	XAT	7	303	-	-	8/31/93/93	0/4/4/4
23	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
21	CLA	5	306	1	1/1/11/20	4/15/93/115	-
21	CLA	a	814	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	XAT	5	301	-	-	4/31/93/93	0/4/4/4
21	CLA	a	808	-	1/1/12/20	3/21/99/115	-
21	CLA	4	317	-	1/1/13/20	7/25/103/115	-
21	CLA	b	802	-	1/1/15/20	18/37/115/115	-
21	CLA	b	822	-	1/1/14/20	7/31/109/115	-
21	CLA	b	826	-	1/1/15/20	5/37/115/115	-
21	CLA	6	307	-	1/1/11/20	1/15/93/115	-
21	CLA	7	317	-	1/1/11/20	5/13/91/115	-
21	CLA	b	807	-	1/1/15/20	12/37/115/115	-
21	CLA	b	804	-	1/1/15/20	12/37/115/115	-
21	CLA	9	309	2	1/1/11/20	3/15/93/115	-
21	CLA	1	308	6	1/1/15/20	13/37/115/115	-
21	CLA	a	809	7	1/1/15/20	15/37/115/115	-
21	CLA	a	824	-	1/1/11/20	4/15/93/115	-
21	CLA	a	831	-	1/1/15/20	11/37/115/115	-
21	CLA	b	828	-	1/1/15/20	11/37/115/115	-
21	CLA	l	202	-	1/1/14/20	6/31/109/115	-
21	CLA	b	805	-	1/1/15/20	16/37/115/115	-
21	CLA	4	307	-	1/1/13/20	7/27/105/115	-
21	CLA	5	314	1	1/1/11/20	5/13/91/115	-
19	XAT	9	304	-	-	1/31/93/93	0/4/4/4
23	A1L1F	6	301	-	-	11/43/99/99	0/3/3/3
21	CLA	a	842	-	1/1/15/20	9/37/115/115	-
21	CLA	1	305	-	1/1/14/20	10/33/111/115	-
19	XAT	8	303	-	-	0/31/93/93	0/4/4/4
21	CLA	a	806	-	1/1/15/20	12/37/115/115	-
21	CLA	b	824	-	1/1/15/20	14/37/115/115	-
21	CLA	1	312	6	1/1/12/20	3/22/100/115	-
21	CLA	8	310	-	1/1/11/20	5/15/93/115	-
21	CLA	9	311	-	1/1/11/20	6/15/93/115	-
21	CLA	b	833	-	1/1/13/20	16/29/107/115	-
21	CLA	a	844	24	1/1/15/20	16/37/115/115	-
21	CLA	b	839	-	1/1/15/20	13/37/115/115	-
19	XAT	4	302	-	-	0/31/93/93	0/4/4/4
21	CLA	4	309	-	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	814	-	1/1/13/20	13/25/103/115	-
21	CLA	b	837	-	1/1/15/20	8/37/115/115	-
19	XAT	8	301	-	-	3/31/93/93	0/4/4/4
28	SF4	a	851	-	-	-	0/6/5/5
21	CLA	6	314	-	1/1/11/20	6/15/93/115	-
21	CLA	8	312	3	1/1/12/20	2/22/100/115	-
21	CLA	a	841	-	1/1/15/20	15/37/115/115	-
21	CLA	b	835	-	1/1/12/20	8/23/101/115	-
26	PQN	a	843	-	-	5/23/43/43	0/2/2/2
21	CLA	5	307	22	1/1/11/20	7/13/91/115	-
21	CLA	a	821	-	1/1/11/20	2/13/91/115	-
21	CLA	5	315	-	1/1/12/20	4/22/100/115	-
21	CLA	b	811	-	1/1/13/20	5/25/101/115	-
21	CLA	l	203	-	1/1/11/20	4/15/93/115	-
21	CLA	9	313	2	1/1/11/20	9/15/93/115	-
19	XAT	a	853	-	-	5/31/93/93	0/4/4/4
24	LHG	a	846	21	-	16/31/31/53	-
21	CLA	a	852	-	1/1/15/20	17/37/115/115	-
21	CLA	a	803	-	1/1/15/20	3/37/115/115	-
21	CLA	a	816	-	1/1/12/20	5/19/97/115	-
21	CLA	8	307	3	1/1/15/20	13/37/115/115	-
21	CLA	4	308	-	1/1/15/20	14/37/115/115	-
21	CLA	8	308	-	1/1/13/20	7/25/103/115	-
21	CLA	4	316	-	1/1/11/20	7/15/93/115	-
21	CLA	a	823	-	1/1/11/20	7/18/96/115	-
21	CLA	a	834	-	1/1/15/20	7/37/115/115	-
21	CLA	b	829	-	1/1/15/20	11/37/115/115	-
29	LMG	j	103	-	-	11/27/47/70	0/1/1/1
24	LHG	b	849	21	-	20/35/35/53	-
21	CLA	6	315	5	1/1/10/20	3/8/86/115	-
27	BCR	b	844	-	-	2/29/63/63	0/2/2/2
21	CLA	8	311	-	1/1/13/20	8/27/105/115	-
21	CLA	a	818	-	1/1/13/20	11/27/105/115	-
19	XAT	8	302	-	-	4/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	827	-	1/1/15/20	8/37/115/115	-
21	CLA	b	841	24	1/1/15/20	9/37/115/115	-
25	DGD	8	315	21	-	11/29/69/95	0/2/2/2
21	CLA	a	820	-	1/1/15/20	16/37/115/115	-
21	CLA	a	810	7	1/1/15/20	13/37/115/115	-
21	CLA	b	821	-	1/1/12/20	2/21/99/115	-
21	CLA	4	313	-	1/1/12/20	6/23/101/115	-
19	XAT	6	306	-	-	4/31/93/93	0/4/4/4
21	CLA	8	314	-	1/1/10/20	5/8/86/115	-
21	CLA	l	201	-	1/1/10/20	2/10/88/115	-
27	BCR	b	852	-	-	5/29/63/63	0/2/2/2
21	CLA	a	822	-	1/1/15/20	5/37/115/115	-
25	DGD	4	318	-	-	10/29/69/95	0/2/2/2
21	CLA	f	802	-	1/1/15/20	13/37/115/115	-
21	CLA	9	314	-	1/1/13/20	9/25/103/115	-
19	XAT	4	303	-	-	3/31/93/93	0/4/4/4
19	XAT	4	304	-	-	0/31/93/93	0/4/4/4
21	CLA	1	307	-	1/1/12/20	6/24/102/115	-
19	XAT	9	305	-	-	3/31/93/93	0/4/4/4
20	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
20	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
21	CLA	b	817	-	1/1/13/20	10/30/108/115	-
21	CLA	7	309	-	1/1/11/20	5/15/93/115	-
21	CLA	1	311	-	1/1/12/20	6/23/101/115	-
21	CLA	6	312	5	1/1/12/20	5/21/99/115	-
21	CLA	7	316	-	1/1/12/20	11/21/99/115	-
21	CLA	6	308	-	1/1/13/20	4/29/107/115	-
21	CLA	a	807	-	1/1/15/20	18/37/115/115	-
21	CLA	1	310	6	1/1/15/20	18/37/115/115	-
21	CLA	b	832	-	1/1/15/20	13/37/115/115	-
21	CLA	b	840	-	1/1/15/20	17/37/115/115	-
21	CLA	a	805	21	1/1/13/20	6/25/103/115	-
21	CLA	8	313	-	1/1/11/20	3/15/93/115	-
19	XAT	7	305	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	309	-	1/1/13/20	4/25/103/115	-
21	CLA	4	312	-	1/1/11/20	4/15/93/115	-
21	CLA	a	856	-	1/1/15/20	13/37/115/115	-
27	BCR	b	843	-	-	2/29/63/63	0/2/2/2
21	CLA	b	808	-	1/1/15/20	11/37/115/115	-
21	CLA	7	312	-	1/1/11/20	3/17/95/115	-
21	CLA	b	810	-	1/1/15/20	17/37/115/115	-
19	XAT	7	304	-	-	6/31/93/93	0/4/4/4
22	SQD	1	315	-	-	19/40/60/69	0/1/1/1
29	LMG	a	855	-	-	13/29/49/70	0/1/1/1
21	CLA	a	830	-	1/1/15/20	15/37/115/115	-
19	XAT	5	305	-	-	1/31/93/93	0/4/4/4
21	CLA	b	831	-	1/1/11/20	6/18/96/115	-
27	BCR	a	850	-	-	4/29/63/63	0/2/2/2
23	A1L1F	6	304	-	-	12/39/95/99	0/3/3/3
21	CLA	4	311	-	1/1/11/20	8/15/93/115	-
21	CLA	a	829	-	1/1/14/20	15/34/112/115	-
21	CLA	1	314	-	1/1/11/20	5/13/91/115	-
21	CLA	5	312	-	1/1/12/20	8/21/99/115	-
21	CLA	a	813	-	1/1/12/20	10/24/102/115	-
24	LHG	9	307	-	-	21/40/40/53	-
21	CLA	a	839	-	1/1/15/20	15/37/115/115	-
27	BCR	b	853	-	-	4/29/63/63	0/2/2/2
21	CLA	4	310	-	1/1/15/20	16/37/115/115	-
21	CLA	5	313	-	1/1/12/20	0/22/100/115	-
21	CLA	7	313	-	1/1/12/20	7/24/102/115	-
20	A1L1G	5	304	-	-	9/29/85/85	0/3/3/3
21	CLA	6	309	-	1/1/15/20	10/37/115/115	-
21	CLA	7	310	-	1/1/11/20	6/15/93/115	-
21	CLA	h	203	-	1/1/13/20	9/25/103/115	-
27	BCR	m	102	-	-	9/29/63/63	0/2/2/2
21	CLA	6	313	-	1/1/12/20	2/22/100/115	-
27	BCR	a	848	-	-	0/29/63/63	0/2/2/2
20	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
21	CLA	1	306	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	a	845	-	-	27/52/52/53	-
27	BCR	i	101	-	-	3/29/63/63	0/2/2/2
19	XAT	6	305	-	-	4/31/93/93	0/4/4/4
21	CLA	j	101	14	1/1/10/20	5/10/88/115	-
21	CLA	4	315	4	1/1/10/20	5/8/86/115	-
21	CLA	5	308	1	1/1/14/20	7/31/109/115	-
21	CLA	a	802	-	1/1/13/20	7/29/107/115	-
21	CLA	a	828	-	1/1/15/20	9/37/115/115	-
21	CLA	b	823	-	1/1/12/20	8/23/101/115	-
21	CLA	b	836	-	1/1/13/20	11/29/107/115	-
21	CLA	b	813	-	1/1/15/20	14/37/115/115	-
21	CLA	b	830	-	1/1/10/20	1/8/86/115	-
21	CLA	9	316	-	1/1/14/20	9/34/112/115	-
27	BCR	b	850	-	-	2/29/63/63	0/2/2/2
26	PQN	b	842	-	-	1/23/43/43	0/2/2/2
21	CLA	b	803	-	1/1/15/20	10/37/115/115	-
21	CLA	7	314	-	1/1/11/20	4/13/91/115	-
20	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
27	BCR	a	849	-	-	0/29/63/63	0/2/2/2
19	XAT	1	303	-	-	0/31/93/93	0/4/4/4
21	CLA	a	801	-	1/1/15/20	22/37/115/115	-
21	CLA	4	306	4	1/1/11/20	7/13/91/115	-
21	CLA	b	801	-	1/1/15/20	20/37/115/115	-
25	DGD	b	851	-	-	20/46/86/95	0/2/2/2
21	CLA	b	838	-	1/1/15/20	8/37/115/115	-
27	BCR	b	848	-	-	2/29/63/63	0/2/2/2
21	CLA	b	834	-	1/1/15/20	14/37/115/115	-
28	SF4	c	102	-	-	-	0/6/5/5
21	CLA	a	815	-	1/1/11/20	2/13/91/115	-
19	XAT	7	301	-	-	6/31/93/93	0/4/4/4
27	BCR	j	102	-	-	4/29/63/63	0/2/2/2
19	XAT	4	301	-	-	3/31/93/93	0/4/4/4
22	SQD	5	317	21	-	11/30/50/69	0/1/1/1
21	CLA	b	809	-	1/1/15/20	16/37/115/115	-
21	CLA	a	812	21	1/1/14/20	9/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	a	847	-	-	0/29/63/63	0/2/2/2
21	CLA	b	818	-	1/1/14/20	14/31/109/115	-
21	CLA	5	310	1	1/1/15/20	14/37/115/115	-
21	CLA	b	827	-	1/1/15/20	14/37/115/115	-
21	CLA	5	316	-	1/1/11/20	5/15/93/115	-
19	XAT	5	303	-	-	3/31/93/93	0/4/4/4
21	CLA	b	820	-	1/1/12/20	7/19/97/115	-
19	XAT	4	305	-	-	4/31/93/93	0/4/4/4
19	XAT	6	302	-	-	7/31/93/93	0/4/4/4
21	CLA	9	310	-	1/1/11/20	6/15/93/115	-
21	CLA	8	309	-	1/1/13/20	8/28/106/115	-
27	BCR	f	801	-	-	3/29/63/63	0/2/2/2
19	XAT	a	854	-	-	7/31/93/93	0/4/4/4
21	CLA	a	832	-	1/1/12/20	5/19/97/115	-
21	CLA	8	306	25	1/1/11/20	2/15/93/115	-
21	CLA	1	309	6	1/1/11/20	6/15/93/115	-
19	XAT	1	302	-	-	0/31/93/93	0/4/4/4
21	CLA	a	817	-	1/1/11/20	6/13/91/115	-
21	CLA	a	833	-	1/1/13/20	2/25/103/115	-
19	XAT	6	303	-	-	5/31/93/93	0/4/4/4
21	CLA	7	311	-	1/1/11/20	5/15/93/115	-
23	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
21	CLA	8	305	3	1/1/10/20	2/11/89/115	-
21	CLA	a	837	7	1/1/11/20	4/13/91/115	-
21	CLA	9	308	2	1/1/15/20	15/37/115/115	-
21	CLA	a	835	-	1/1/15/20	12/37/115/115	-
21	CLA	b	815	-	1/1/11/20	3/13/91/115	-
21	CLA	6	316	5	1/1/11/20	7/15/93/115	-
21	CLA	a	819	-	1/1/12/20	4/24/102/115	-
23	A1L1F	h	202	-	-	11/43/99/99	1/3/3/3
21	CLA	h	201	-	1/1/15/20	9/37/115/115	-
21	CLA	5	311	-	1/1/11/20	6/15/93/115	-
21	CLA	7	307	-	1/1/11/20	4/13/91/115	-
21	CLA	9	315	2	1/1/10/20	6/10/88/115	-
28	SF4	c	101	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	812	-	1/1/12/20	6/23/101/115	-
21	CLA	b	806	-	1/1/15/20	19/37/115/115	-
21	CLA	4	314	4	1/1/11/20	3/13/91/115	-
21	CLA	7	308	-	1/1/14/20	14/31/109/115	-
21	CLA	a	811	-	1/1/13/20	8/27/105/115	-
21	CLA	a	840	-	1/1/15/20	8/37/115/115	-
21	CLA	a	826	-	1/1/15/20	9/37/115/115	-
23	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
27	BCR	f	804	-	-	4/29/63/63	0/2/2/2
21	CLA	6	310	-	1/1/12/20	7/22/100/115	-
19	XAT	5	302	-	-	3/31/93/93	0/4/4/4
21	CLA	b	816	-	1/1/13/20	4/25/103/115	-
21	CLA	a	804	-	1/1/13/20	10/25/103/115	-
27	BCR	b	846	-	-	0/29/63/63	0/2/2/2
21	CLA	7	315	4	1/1/10/20	4/8/86/115	-
21	CLA	a	836	-	1/1/12/20	6/19/97/115	-
21	CLA	9	312	-	1/1/11/20	9/15/93/115	-
21	CLA	b	825	-	1/1/14/20	6/36/114/115	-
19	XAT	9	303	-	-	4/31/93/93	0/4/4/4

The worst 5 of 1091 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	312	CLA	C4B-NB	8.05	1.42	1.35
21	a	842	CLA	C4B-NB	7.78	1.42	1.35
21	4	312	CLA	C4B-NB	7.73	1.42	1.35
21	a	840	CLA	C4B-NB	7.73	1.42	1.35
21	5	314	CLA	C4B-NB	7.72	1.42	1.35

The worst 5 of 2339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	9	302	A1L1F	O15-C20-C21	13.19	123.29	113.38
25	4	318	DGD	C6E-C5E-C4E	-9.41	90.97	113.00
23	6	301	A1L1F	O15-C20-C21	8.71	119.93	113.38
23	6	304	A1L1F	O15-C20-C21	8.63	119.87	113.38
23	8	304	A1L1F	O15-C20-C21	8.54	119.80	113.38

5 of 168 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	5	306	CLA	ND
21	5	307	CLA	ND
21	5	308	CLA	ND
21	5	309	CLA	ND
21	5	310	CLA	ND

5 of 1904 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	5	301	XAT	C27-C28-C29-C30
19	5	301	XAT	C27-C28-C29-C39
19	5	303	XAT	O4-C6-C7-C8
19	5	303	XAT	C7-C8-C9-C10
19	5	303	XAT	C7-C8-C9-C19

All (1) ring outliers are listed below:

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

215 monomers are involved in 751 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	i	102	BCR	13	0
27	b	847	BCR	6	0
21	7	306	CLA	2	0
24	m	101	LHG	2	0
21	a	825	CLA	4	0
21	b	819	CLA	2	0
21	a	838	CLA	1	0
27	b	845	BCR	6	0
21	f	803	CLA	1	0
19	7	303	XAT	13	0
23	1	304	A1L1F	11	0
21	5	306	CLA	2	0
19	5	301	XAT	5	0
21	a	814	CLA	3	0
21	a	808	CLA	1	0
21	4	317	CLA	6	0
21	b	802	CLA	3	0
21	b	822	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	b	826	CLA	3	0
21	b	807	CLA	1	0
21	b	804	CLA	4	0
21	9	309	CLA	1	0
21	1	308	CLA	3	0
21	a	809	CLA	3	0
21	a	824	CLA	1	0
21	a	831	CLA	5	0
21	b	828	CLA	4	0
19	9	304	XAT	5	0
21	b	805	CLA	2	0
21	4	307	CLA	1	0
21	1	202	CLA	9	0
23	6	301	A1L1F	2	0
21	a	842	CLA	4	0
21	1	305	CLA	2	0
19	8	303	XAT	6	0
21	a	806	CLA	7	0
21	b	824	CLA	6	0
21	1	312	CLA	2	0
21	9	311	CLA	3	0
21	b	833	CLA	5	0
21	a	844	CLA	17	0
21	b	839	CLA	13	0
19	4	302	XAT	6	0
21	4	309	CLA	3	0
21	b	814	CLA	3	0
19	8	301	XAT	3	0
21	b	837	CLA	7	0
21	6	314	CLA	1	0
21	8	312	CLA	2	0
21	a	841	CLA	16	0
21	b	835	CLA	1	0
26	a	843	PQN	4	0
21	5	315	CLA	2	0
21	b	811	CLA	2	0
21	9	313	CLA	3	0
19	a	853	XAT	4	0
24	a	846	LHG	2	0
21	a	852	CLA	4	0
21	a	803	CLA	13	0
21	a	816	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	307	CLA	5	0
21	4	308	CLA	6	0
21	8	308	CLA	2	0
21	4	316	CLA	1	0
21	a	823	CLA	3	0
21	a	834	CLA	6	0
21	b	829	CLA	4	0
29	j	103	LMG	6	0
24	b	849	LHG	2	0
21	6	315	CLA	3	0
27	b	844	BCR	2	0
21	8	311	CLA	3	0
19	8	302	XAT	8	0
21	a	818	CLA	11	0
21	a	827	CLA	4	0
21	b	841	CLA	3	0
25	8	315	DGD	2	0
21	a	820	CLA	7	0
21	a	810	CLA	9	0
21	b	821	CLA	3	0
19	6	306	XAT	2	0
21	4	313	CLA	3	0
21	8	314	CLA	1	0
21	l	201	CLA	1	0
27	b	852	BCR	9	0
21	a	822	CLA	5	0
25	4	318	DGD	11	0
21	f	802	CLA	1	0
21	9	314	CLA	8	0
19	4	303	XAT	9	0
19	4	304	XAT	3	0
19	9	305	XAT	4	0
20	9	301	A1L1G	2	0
20	1	301	A1L1G	1	0
21	b	817	CLA	8	0
21	1	311	CLA	4	0
21	7	316	CLA	2	0
21	6	308	CLA	4	0
21	a	807	CLA	4	0
21	b	832	CLA	10	0
21	b	840	CLA	4	0
21	a	805	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	313	CLA	3	0
19	7	305	XAT	2	0
21	5	309	CLA	2	0
21	4	312	CLA	1	0
21	a	856	CLA	22	0
27	b	843	BCR	5	0
21	b	808	CLA	3	0
21	7	312	CLA	1	0
19	7	304	XAT	9	0
21	b	810	CLA	22	0
22	1	315	SQD	3	0
29	a	855	LMG	11	0
21	a	830	CLA	5	0
19	5	305	XAT	5	0
21	b	831	CLA	1	0
27	a	850	BCR	3	0
23	6	304	A1L1F	4	0
21	4	311	CLA	2	0
21	a	829	CLA	6	0
21	5	312	CLA	1	0
21	a	813	CLA	1	0
24	9	307	LHG	1	0
21	a	839	CLA	5	0
27	b	853	BCR	17	0
21	4	310	CLA	5	0
21	5	313	CLA	3	0
21	7	313	CLA	4	0
20	5	304	A1L1G	1	0
21	6	309	CLA	2	0
21	h	203	CLA	2	0
27	m	102	BCR	1	0
21	6	313	CLA	2	0
27	a	848	BCR	5	0
20	9	306	A1L1G	1	0
21	1	306	CLA	6	0
24	a	845	LHG	3	0
27	i	101	BCR	5	0
19	6	305	XAT	5	0
21	j	101	CLA	2	0
21	4	315	CLA	1	0
21	5	308	CLA	7	0
21	a	802	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	a	828	CLA	4	0
21	b	823	CLA	6	0
21	b	836	CLA	5	0
21	b	813	CLA	5	0
21	b	830	CLA	5	0
21	9	316	CLA	11	0
27	b	850	BCR	3	0
26	b	842	PQN	6	0
21	b	803	CLA	4	0
21	7	314	CLA	3	0
20	7	302	A1L1G	2	0
27	a	849	BCR	3	0
19	1	303	XAT	2	0
21	a	801	CLA	6	0
21	4	306	CLA	2	0
21	b	801	CLA	14	0
25	b	851	DGD	6	0
21	b	838	CLA	5	0
27	b	848	BCR	5	0
21	b	834	CLA	4	0
28	c	102	SF4	3	0
19	7	301	XAT	5	0
27	j	102	BCR	14	0
19	4	301	XAT	5	0
22	5	317	SQD	1	0
27	a	847	BCR	4	0
21	b	818	CLA	4	0
19	5	303	XAT	8	0
19	6	302	XAT	4	0
21	5	310	CLA	3	0
19	4	305	XAT	4	0
21	5	316	CLA	2	0
21	b	820	CLA	2	0
21	b	827	CLA	4	0
21	9	310	CLA	2	0
21	8	309	CLA	1	0
27	f	801	BCR	24	0
19	a	854	XAT	3	0
21	a	832	CLA	1	0
19	1	302	XAT	2	0
21	8	306	CLA	1	0
19	6	303	XAT	9	0

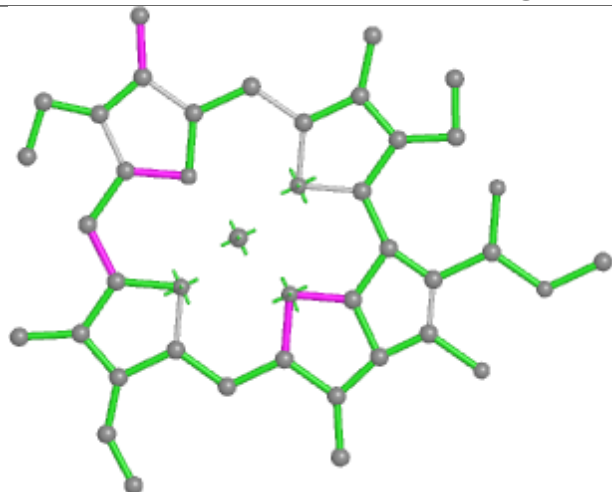
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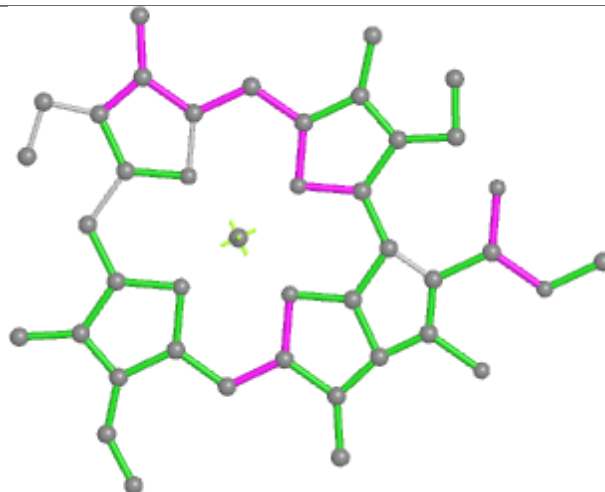
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	a	833	CLA	11	0
21	7	311	CLA	3	0
23	8	304	A1L1F	2	0
21	8	305	CLA	4	0
21	a	837	CLA	1	0
21	9	308	CLA	6	0
21	a	835	CLA	5	0
21	a	819	CLA	5	0
23	h	202	A1L1F	4	0
21	h	201	CLA	5	0
21	5	311	CLA	2	0
21	7	307	CLA	2	0
21	9	315	CLA	1	0
21	b	812	CLA	5	0
21	b	806	CLA	5	0
21	4	314	CLA	1	0
21	7	308	CLA	7	0
21	a	840	CLA	6	0
21	a	826	CLA	7	0
23	9	302	A1L1F	2	0
27	f	804	BCR	7	0
19	5	302	XAT	3	0
21	b	816	CLA	4	0
21	a	804	CLA	1	0
27	b	846	BCR	3	0
21	7	315	CLA	2	0
21	9	312	CLA	4	0
21	b	825	CLA	3	0
19	9	303	XAT	7	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.

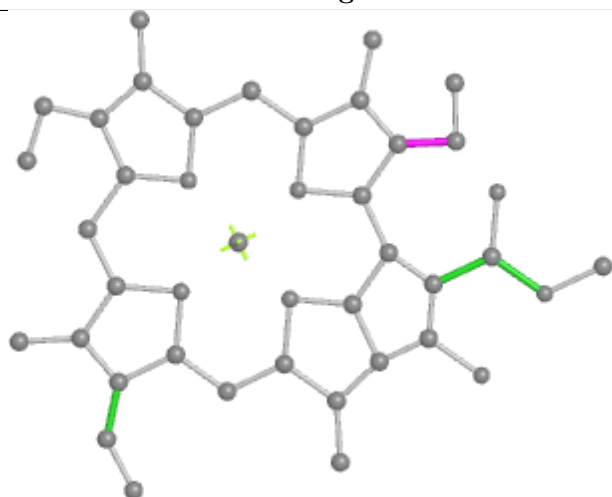
Ligand CLA 6 311



Bond lengths



Bond angles

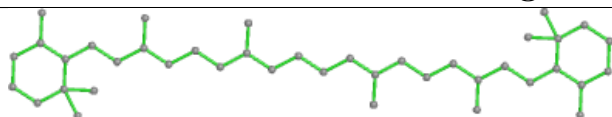


Torsions

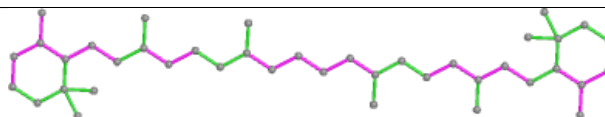


Rings

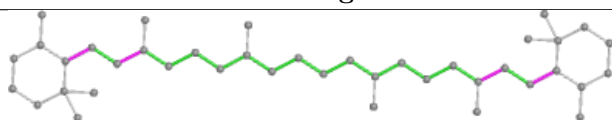
Ligand BCR i 102



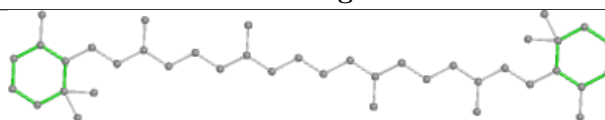
Bond lengths



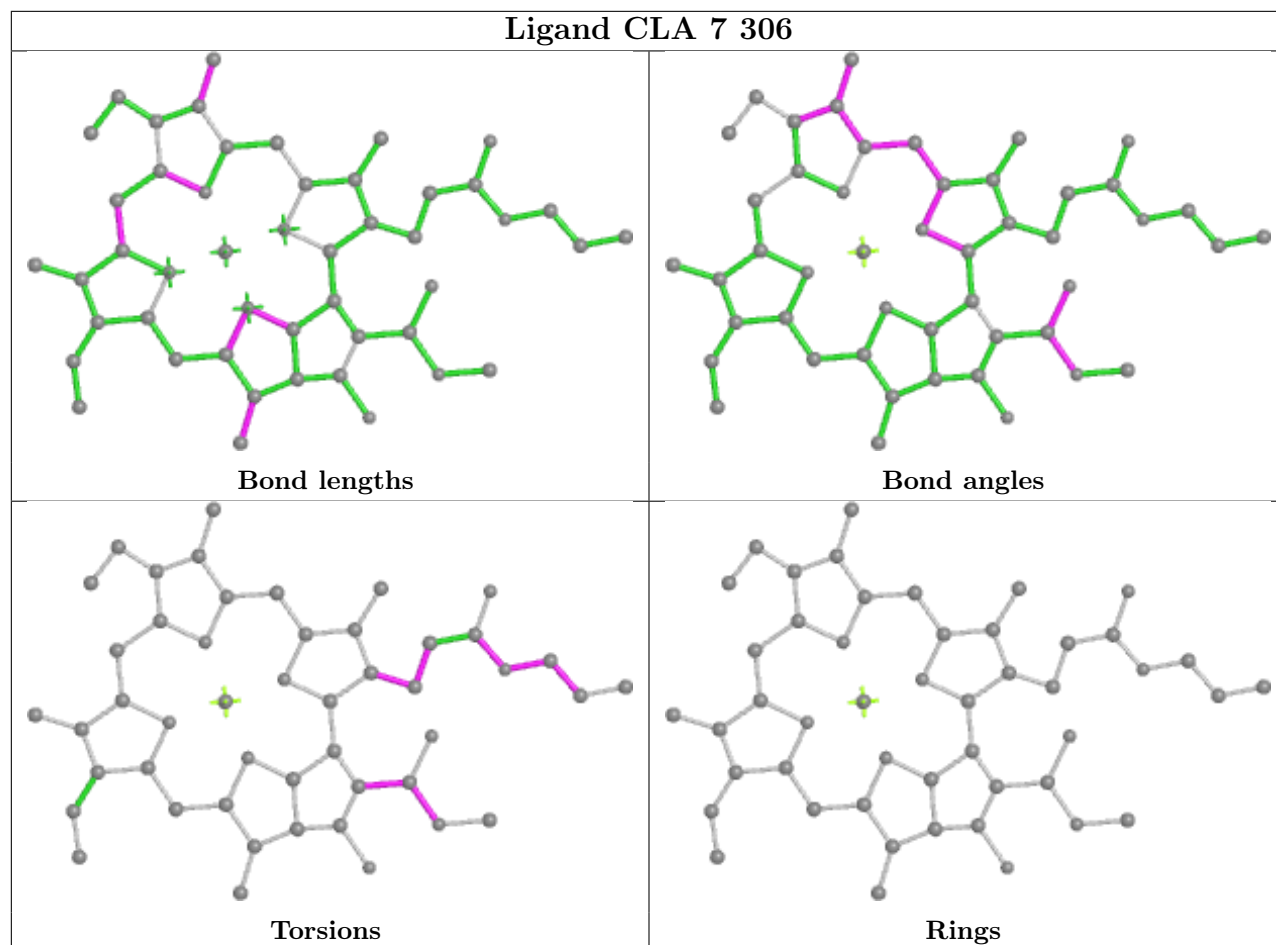
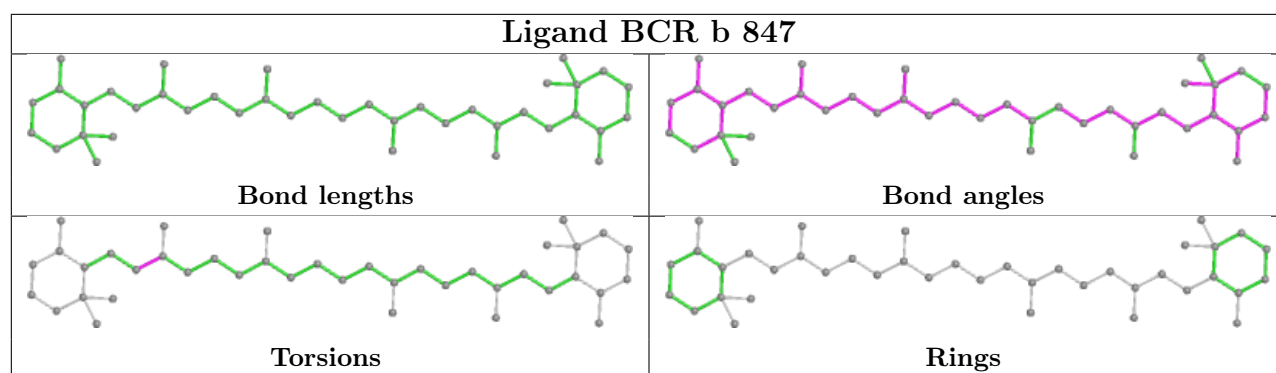
Bond angles

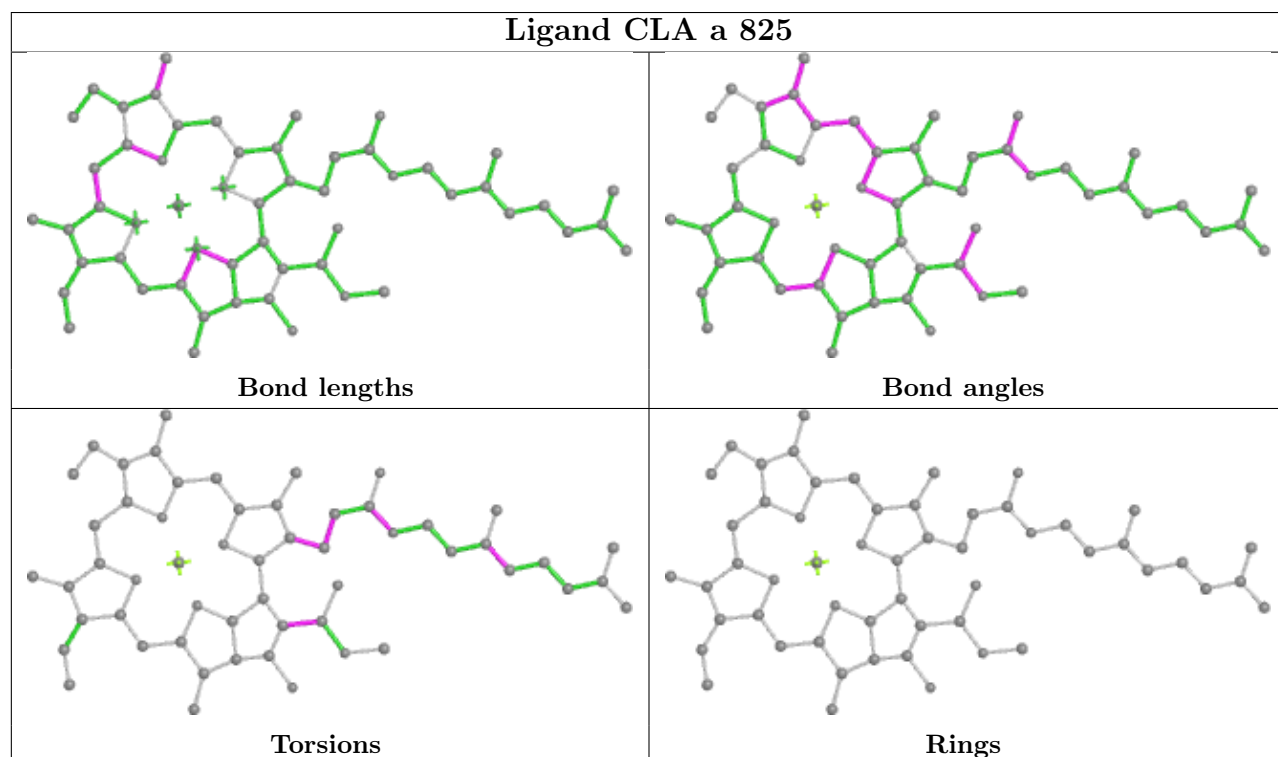
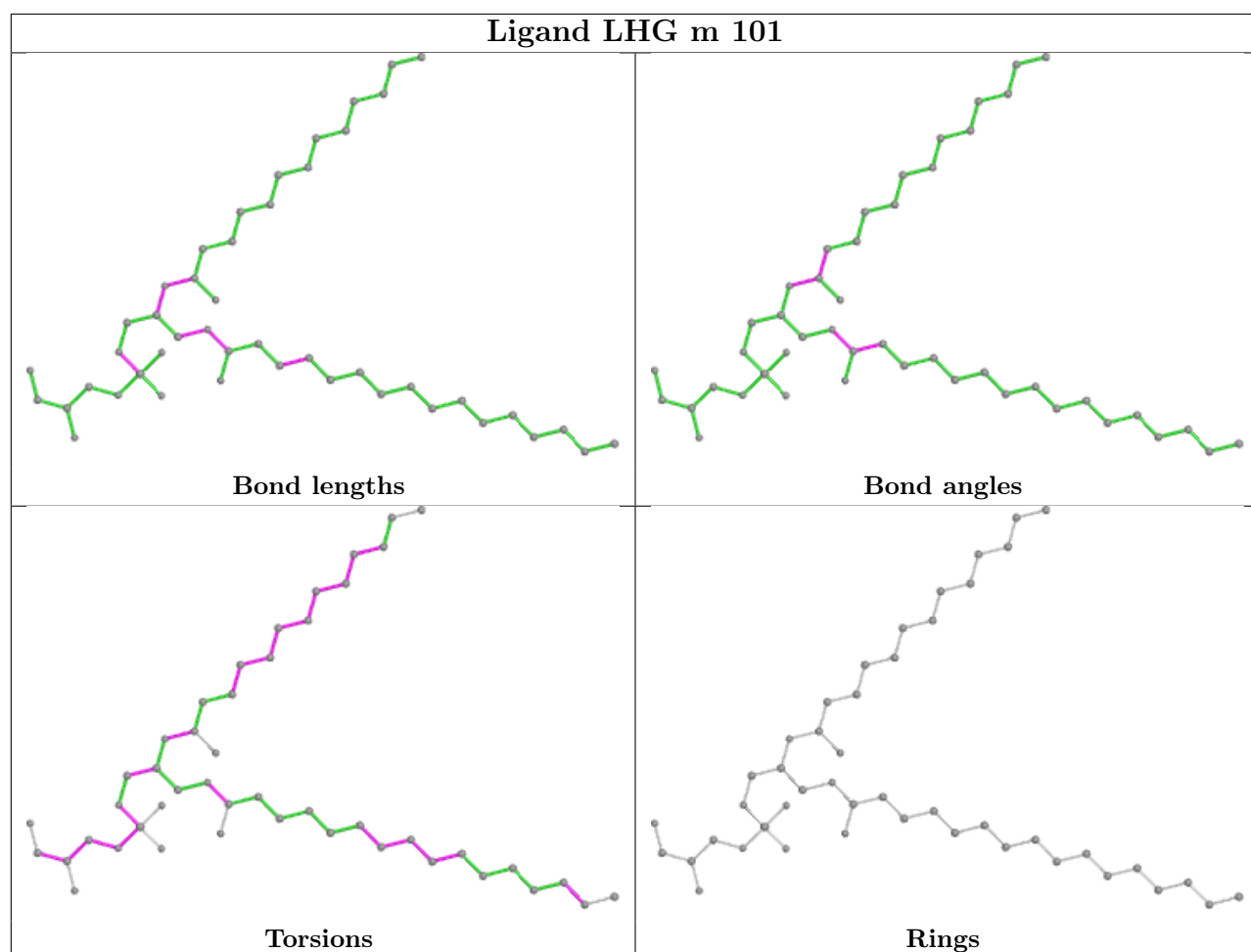


Torsions

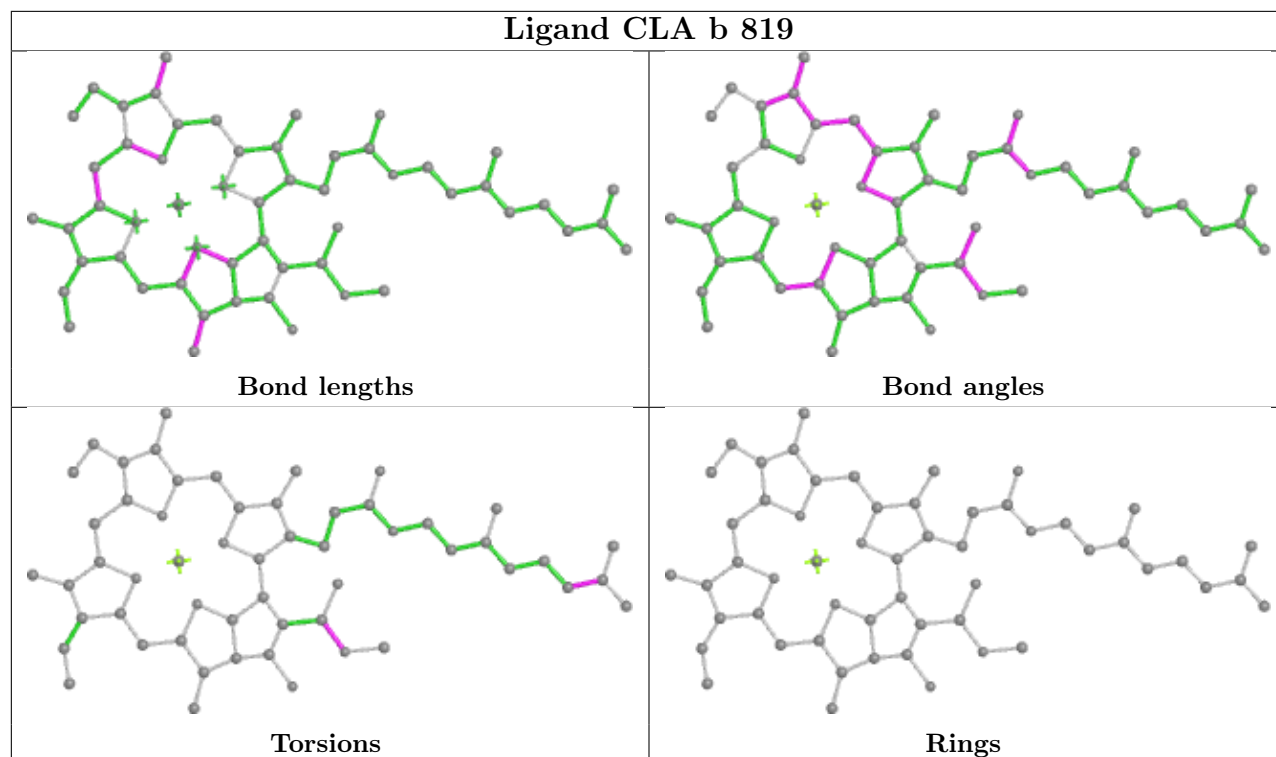


Rings

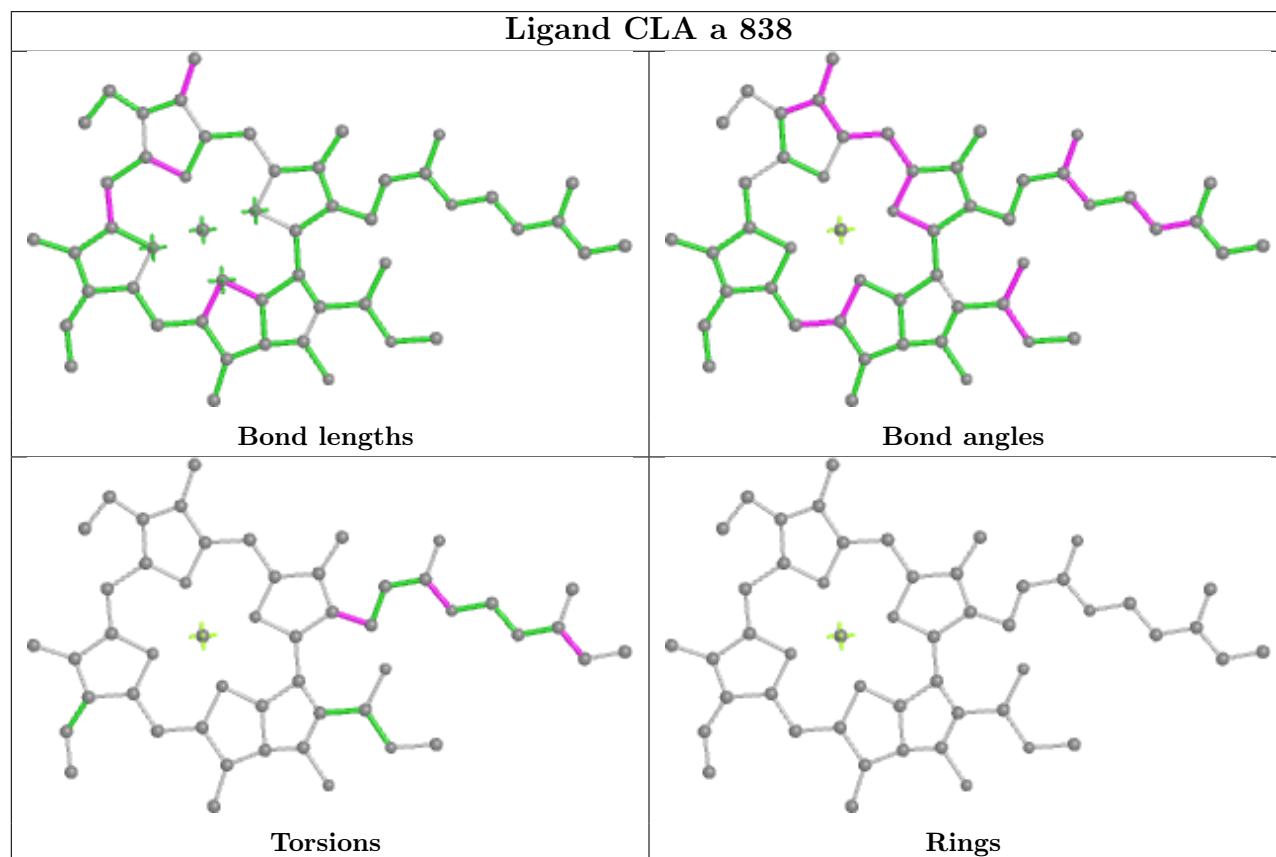


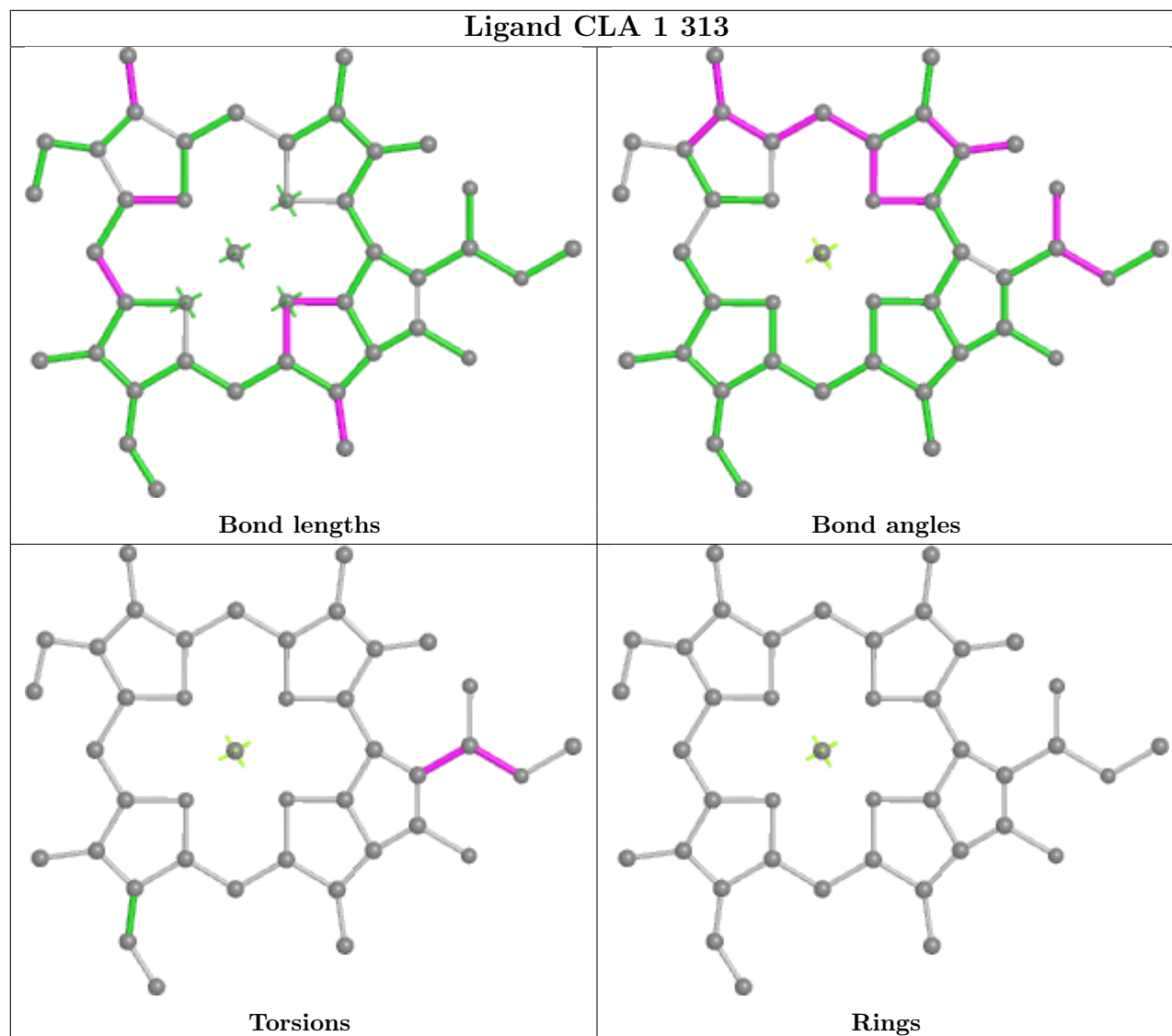
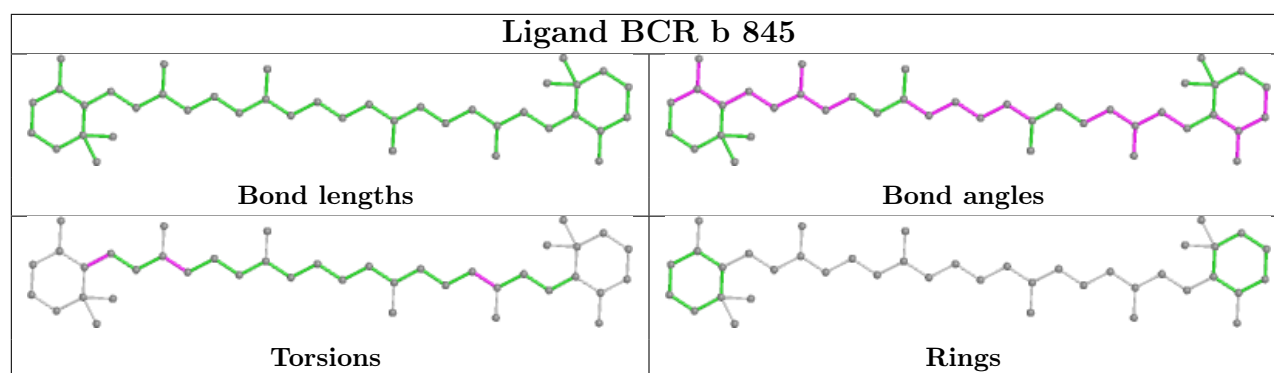


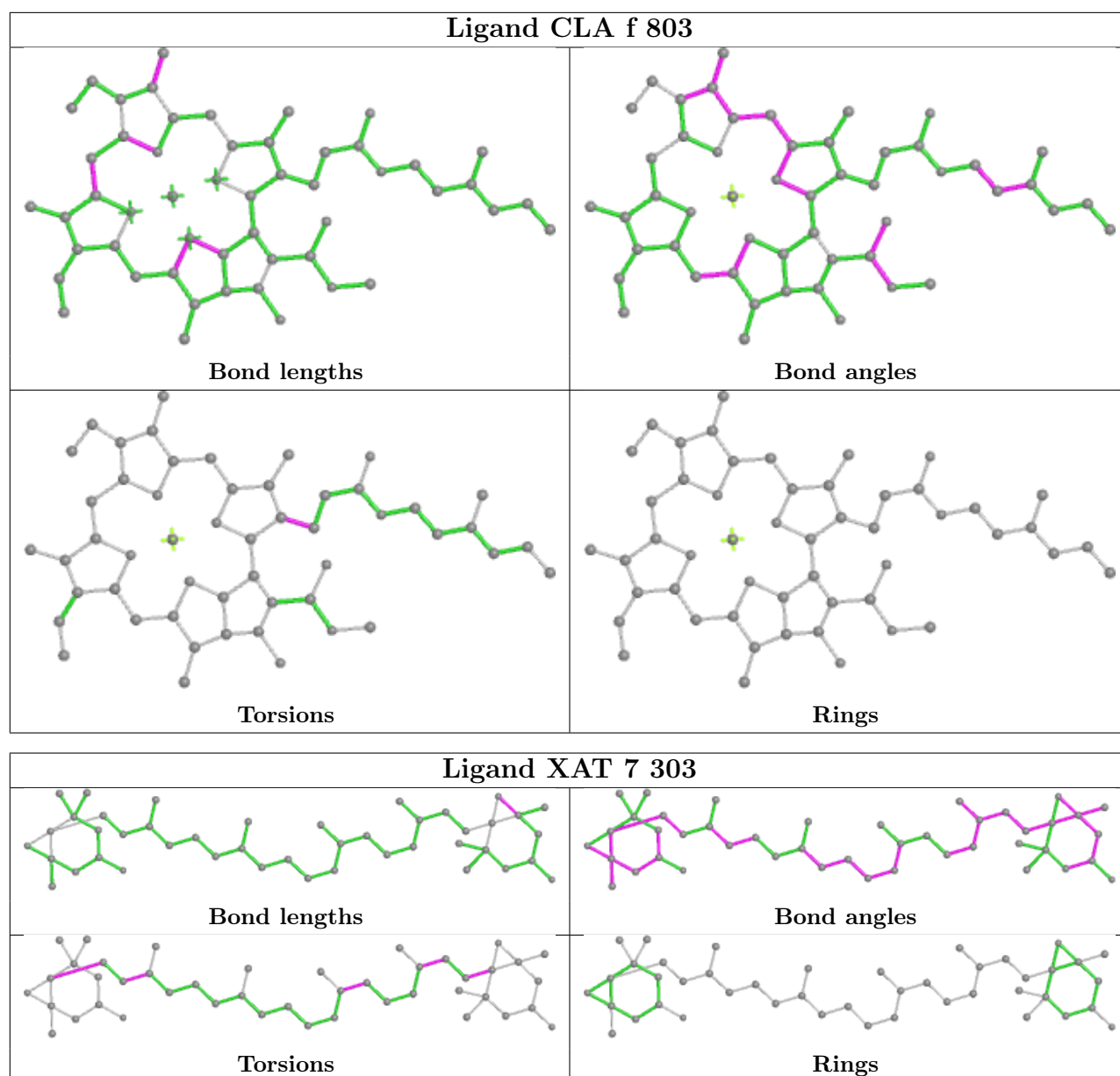
Ligand CLA b 819

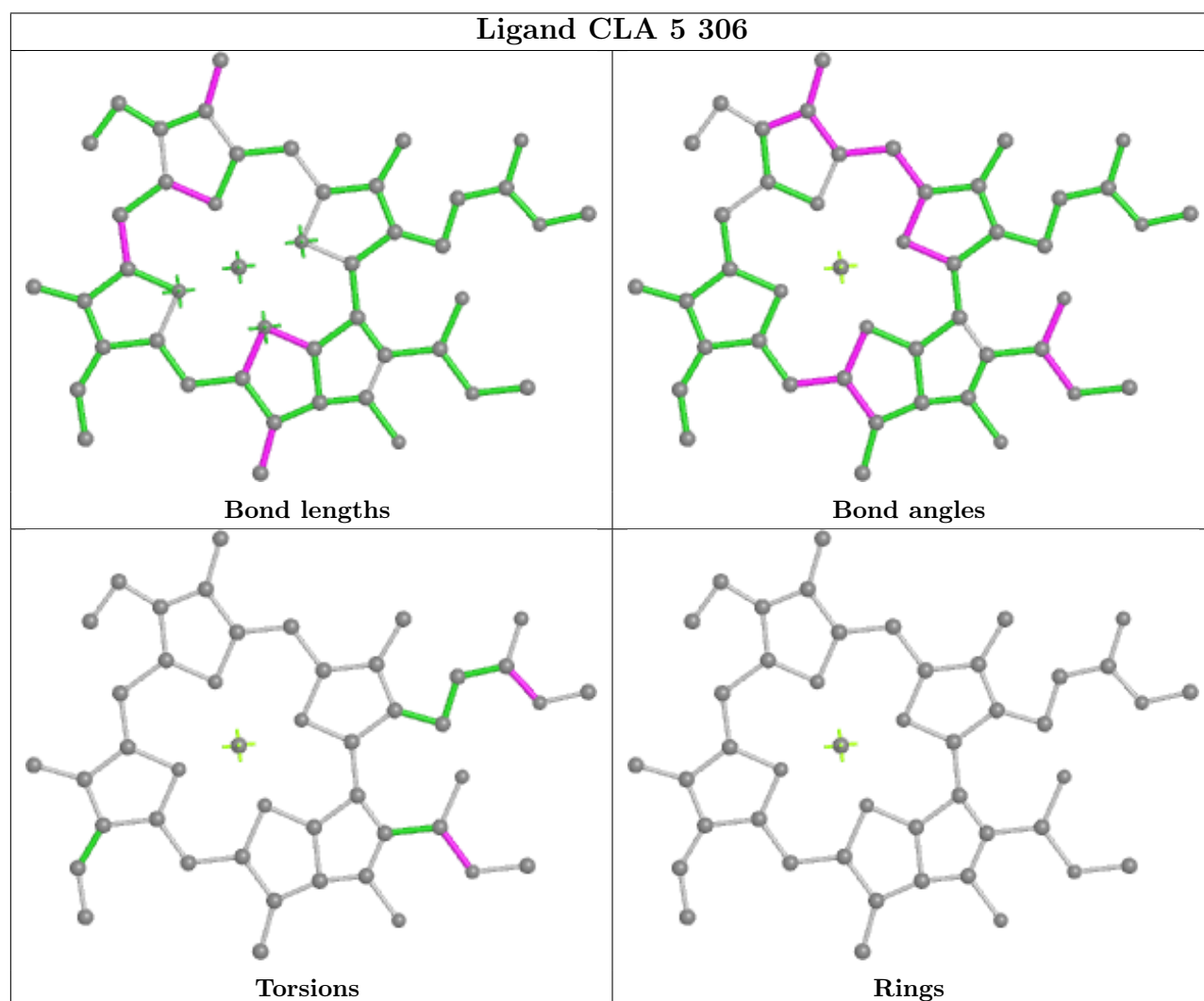
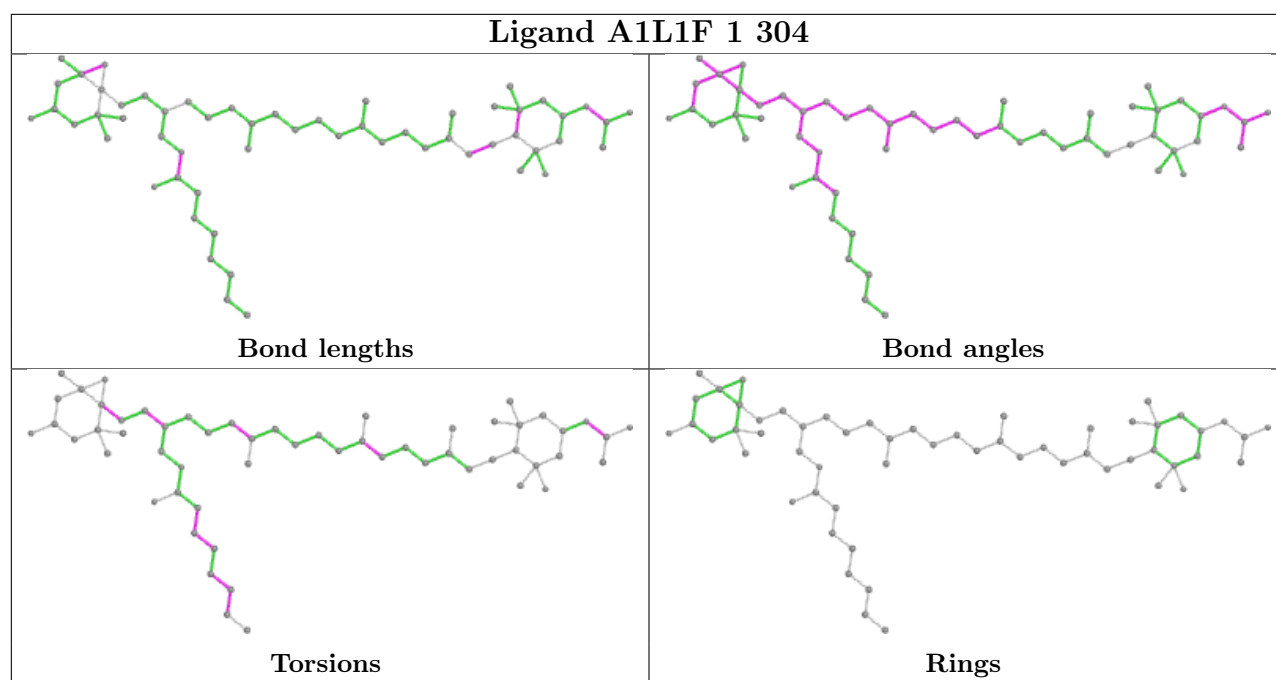


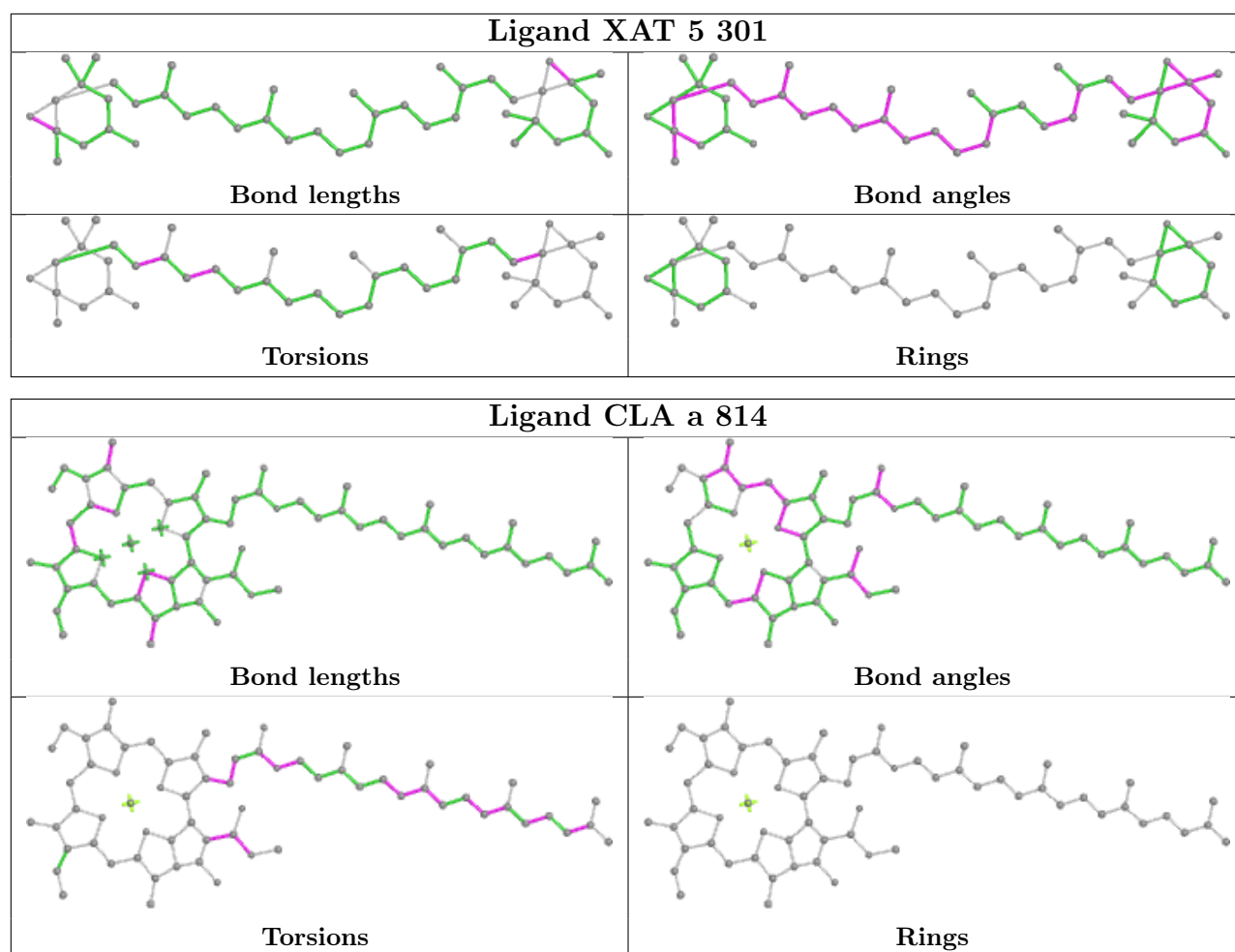
Ligand CLA a 838

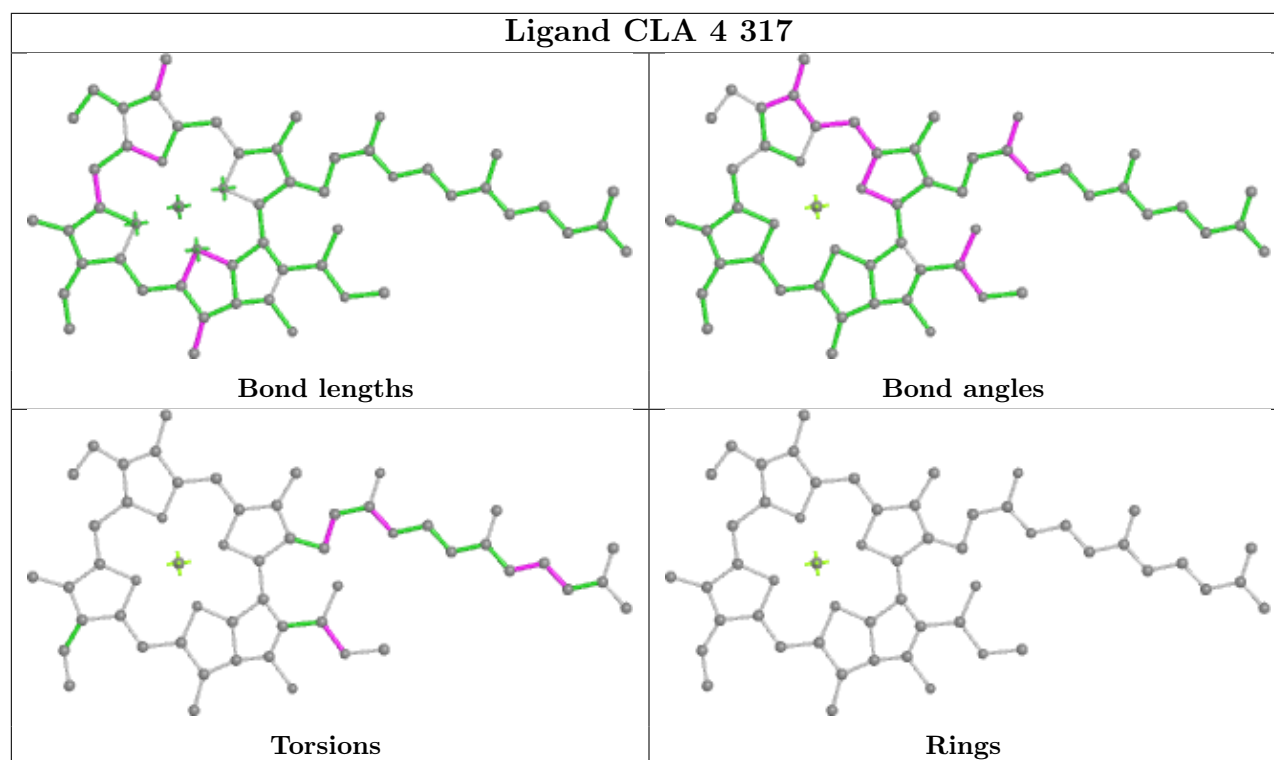
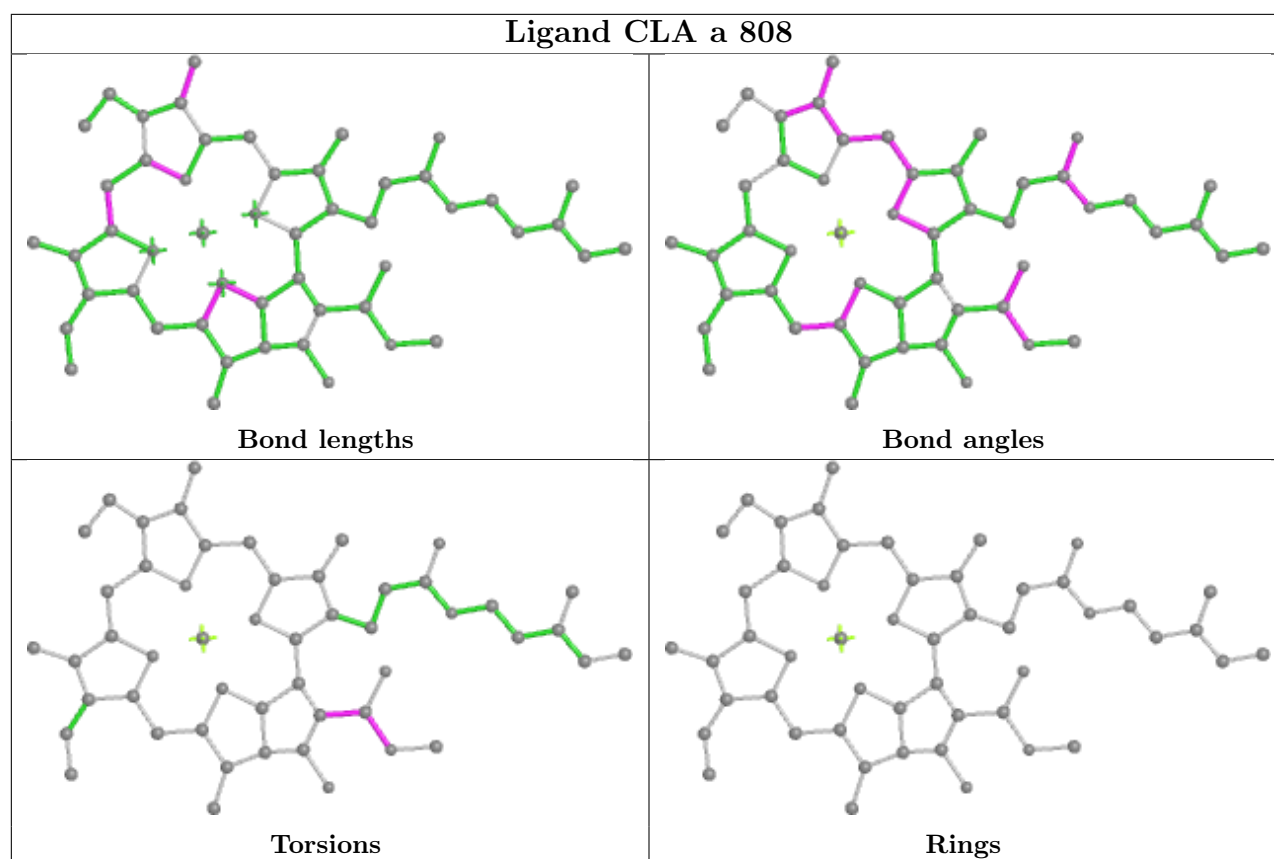


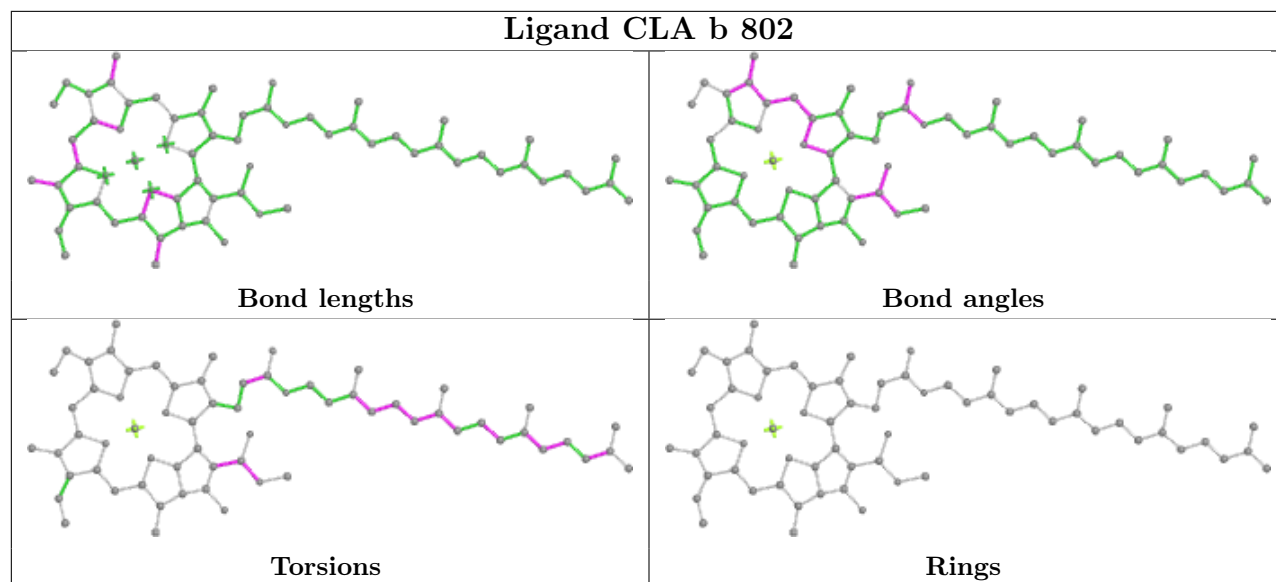
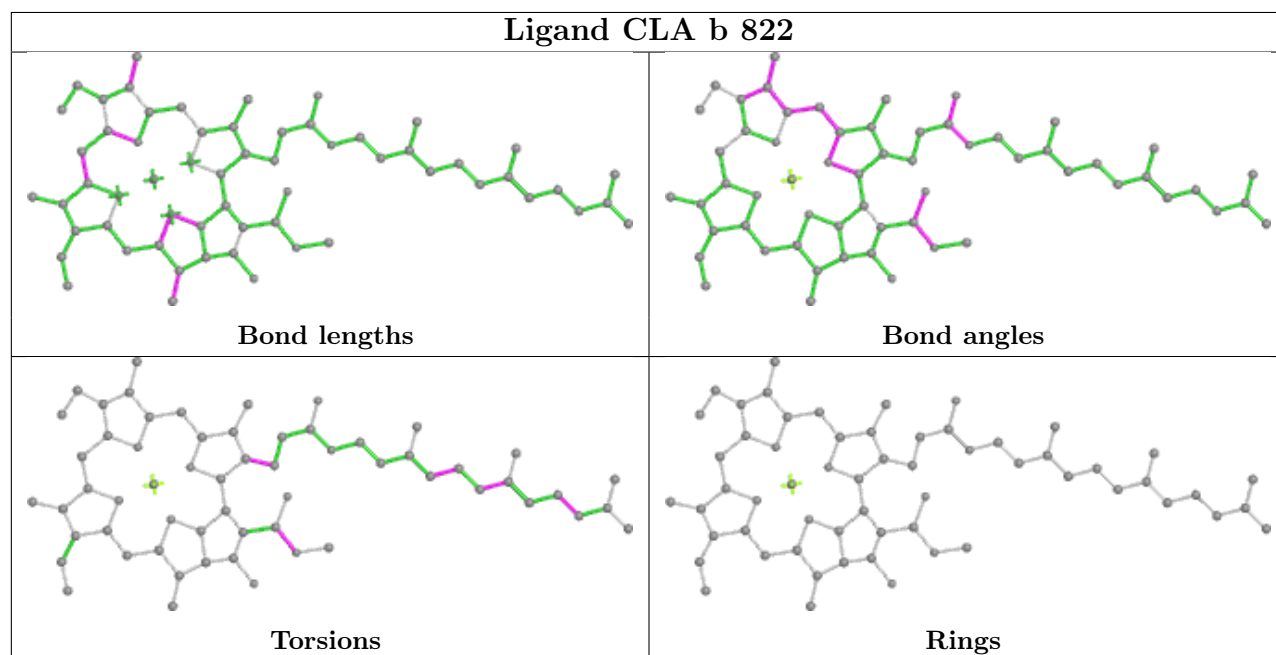




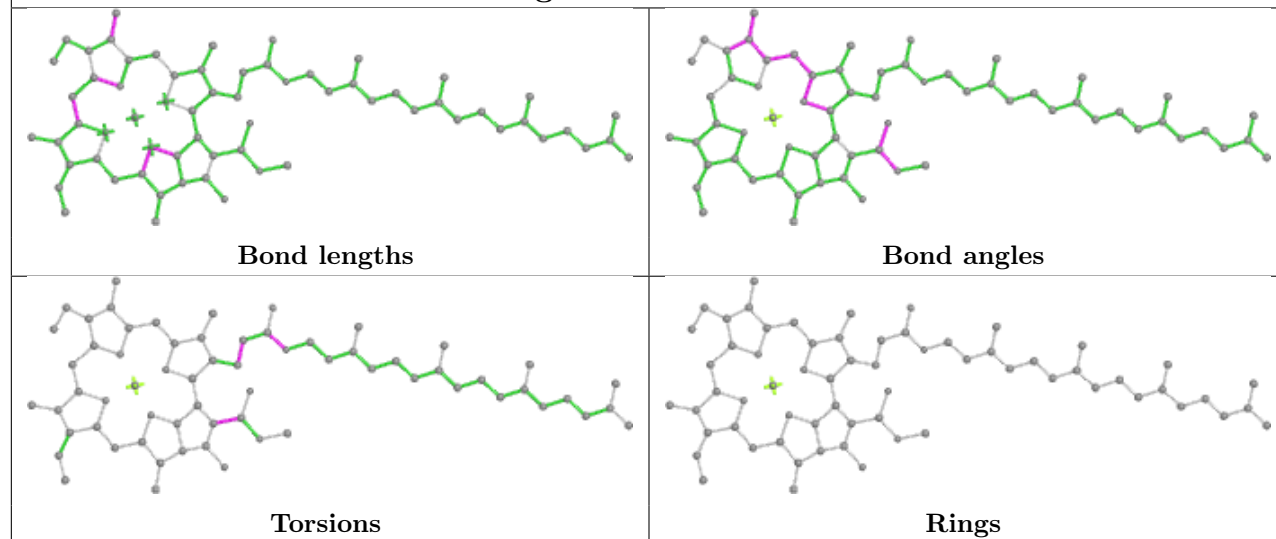




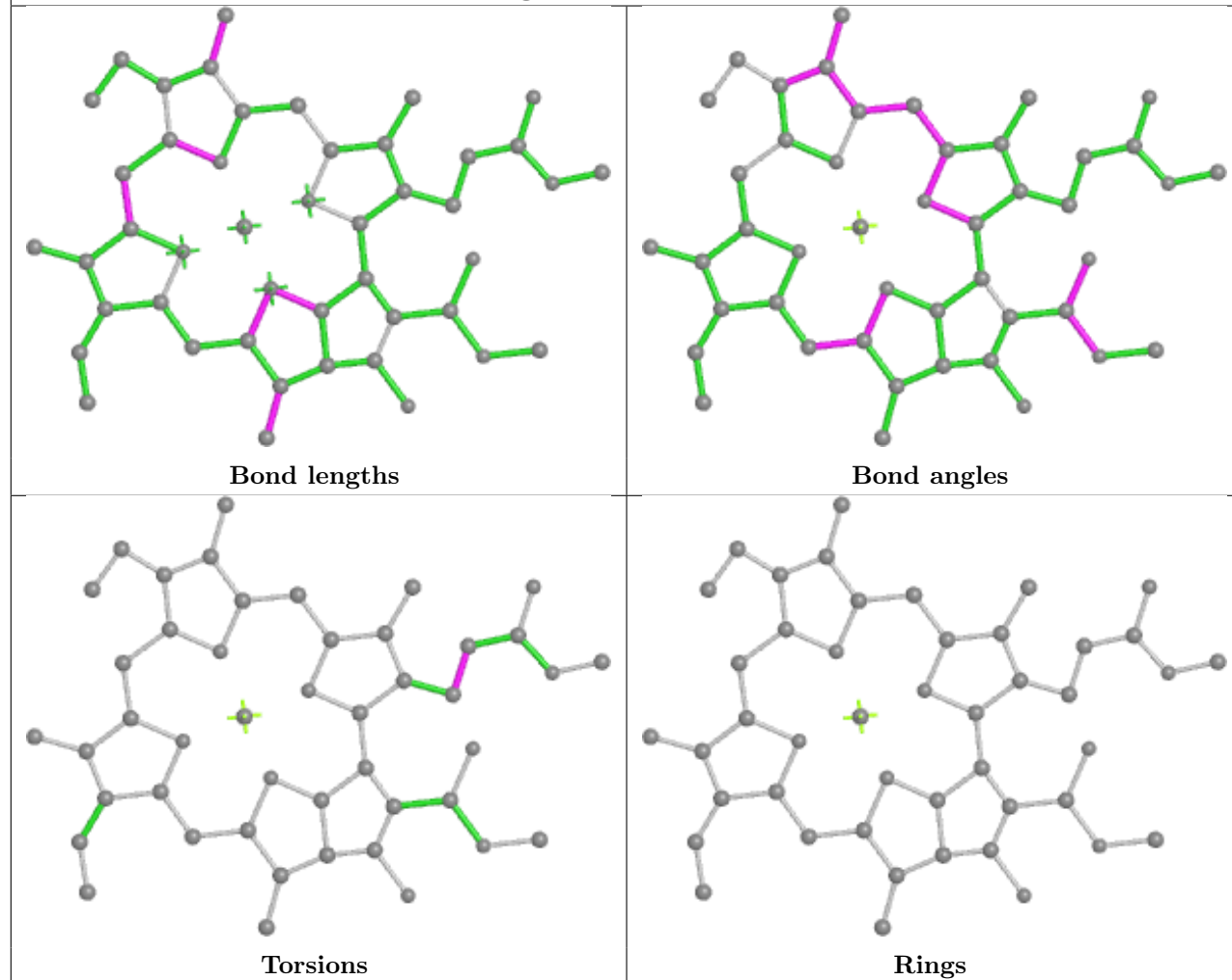


Ligand CLA b 802**Ligand CLA b 822**

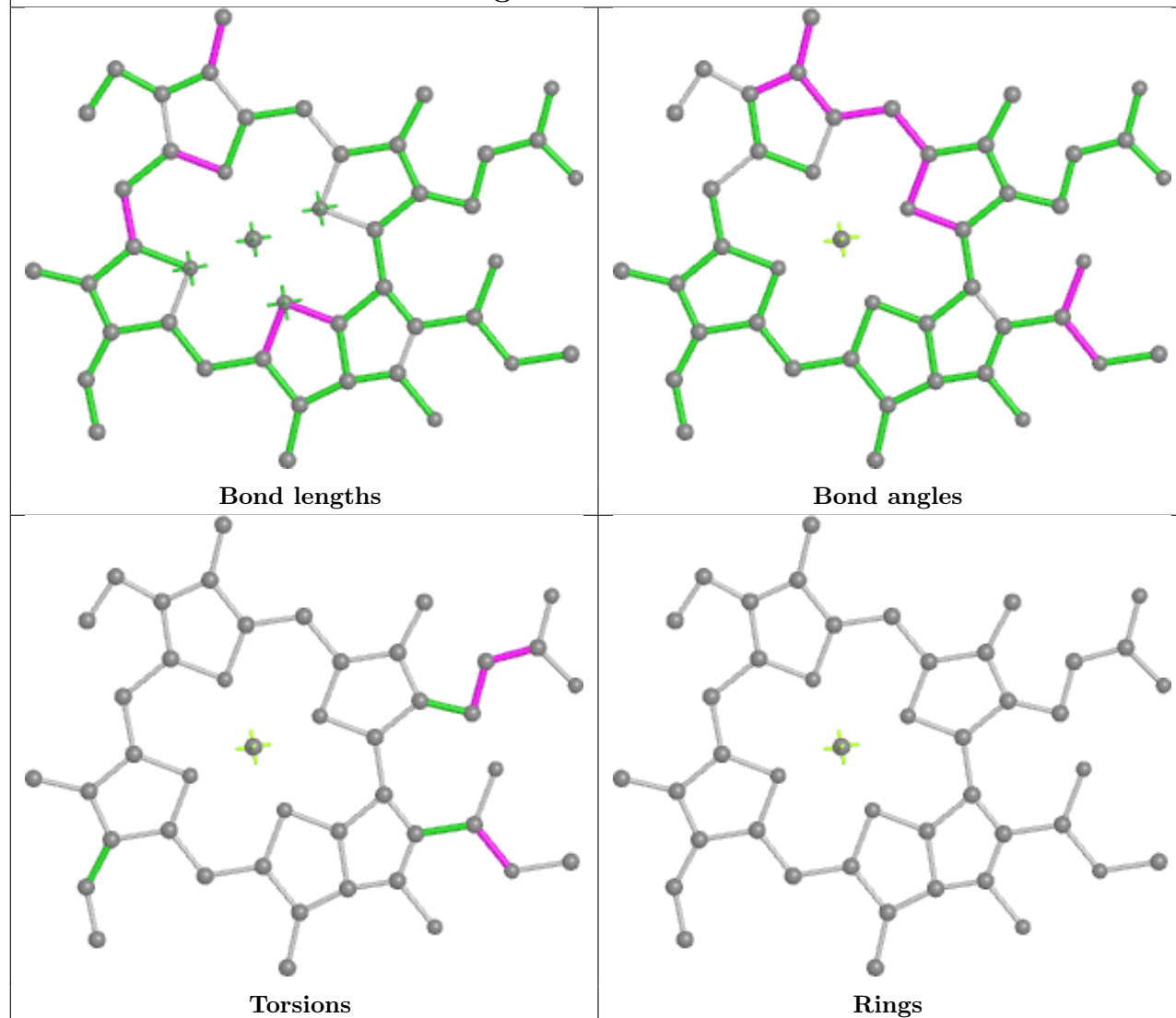
Ligand CLA b 826



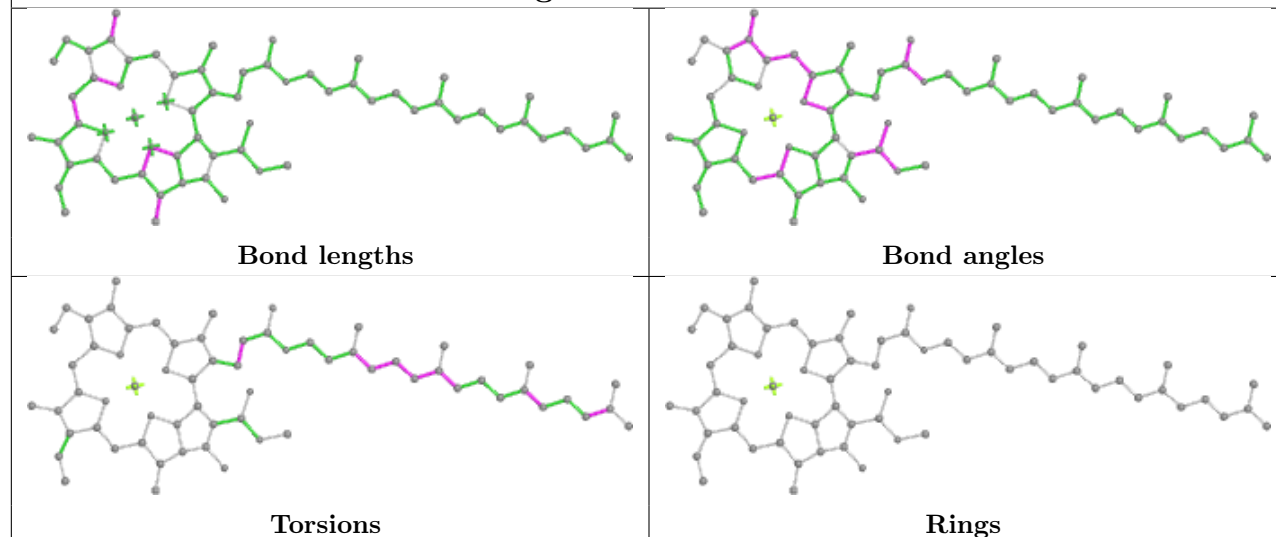
Ligand CLA 6 307



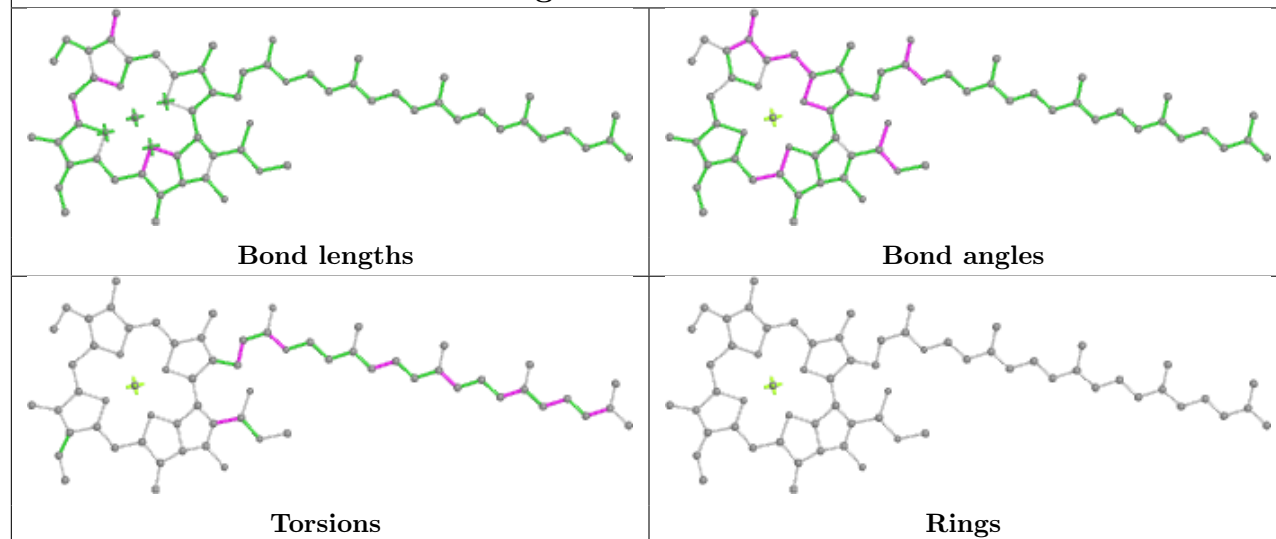
Ligand CLA 7 317



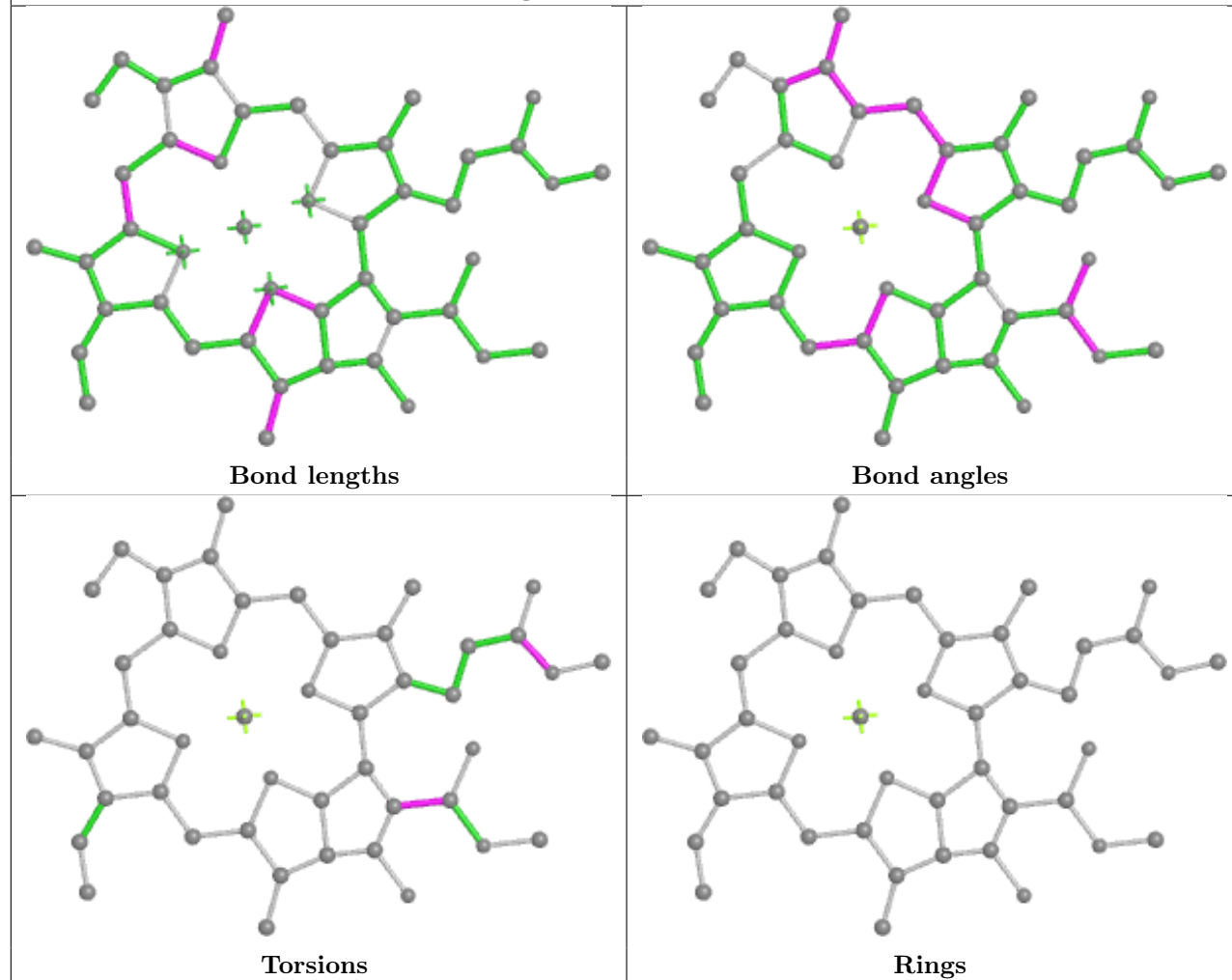
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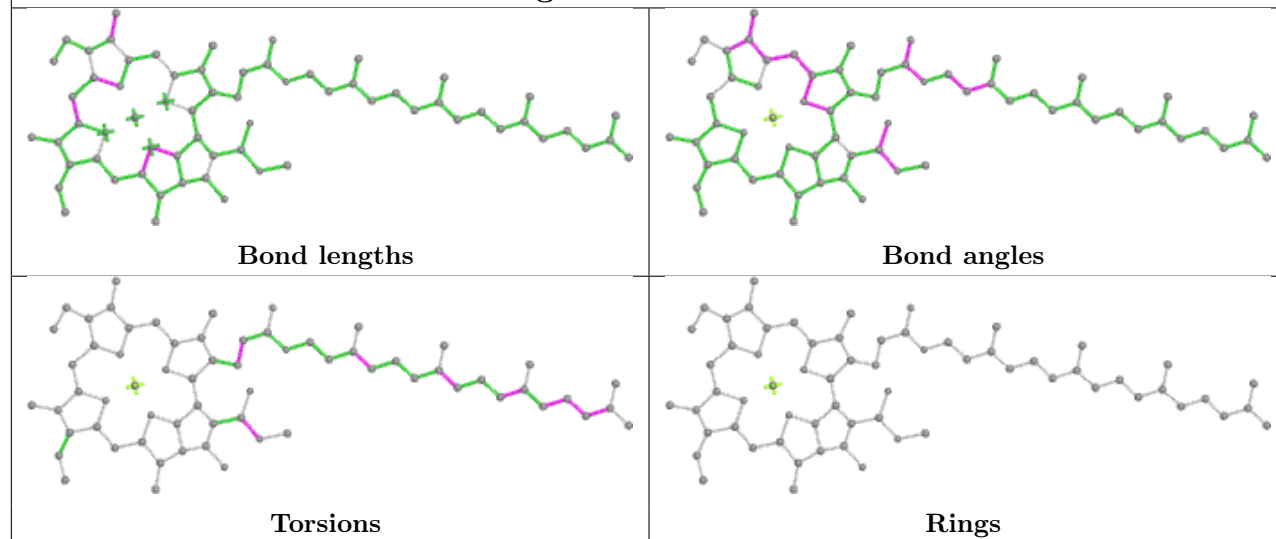
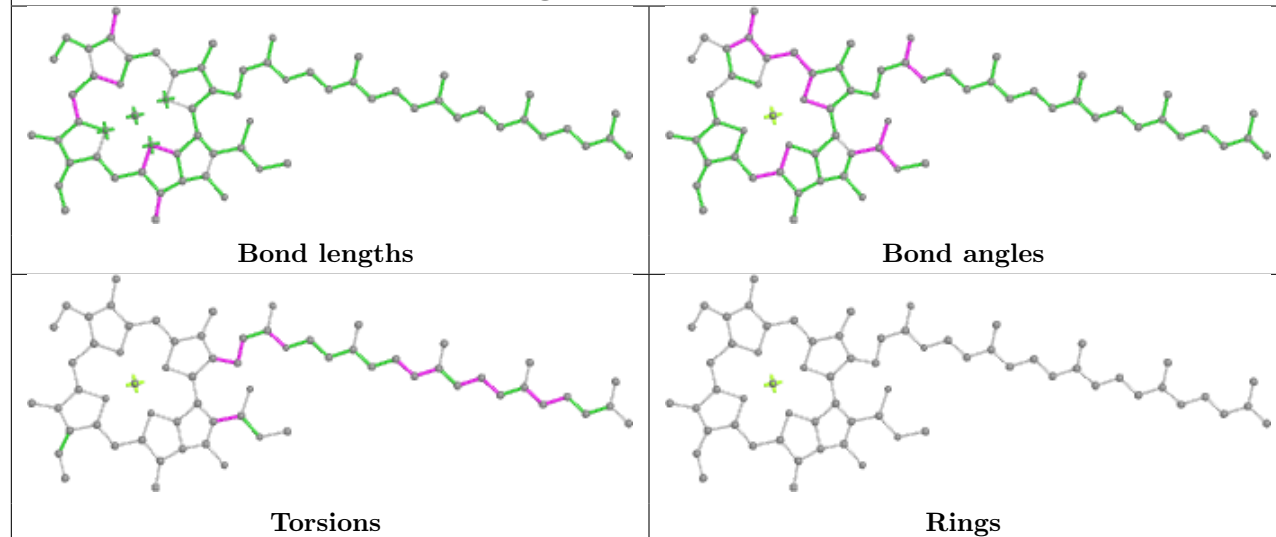


Ligand CLA b 804

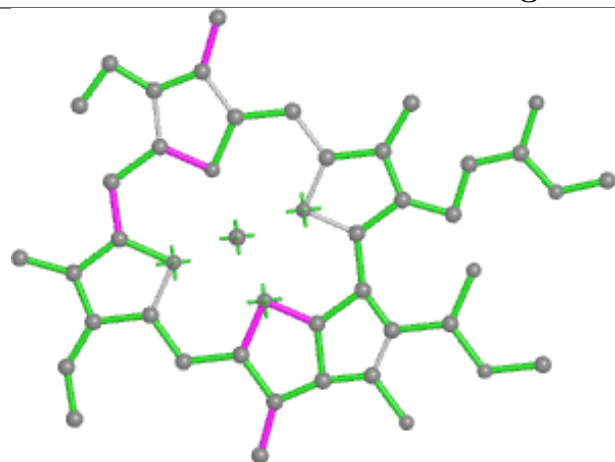


Ligand CLA 9 309

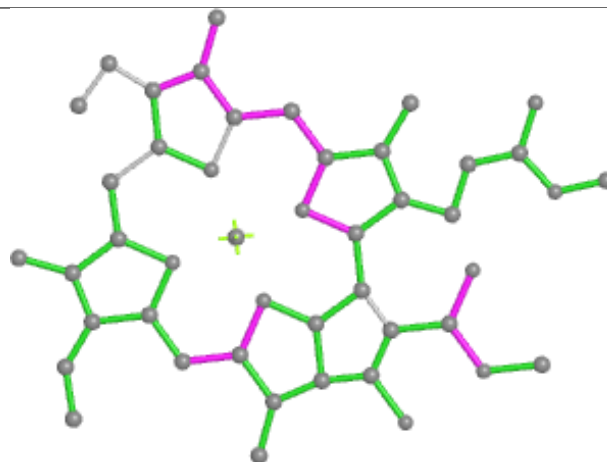


Ligand CLA 1 308**Ligand CLA a 809**

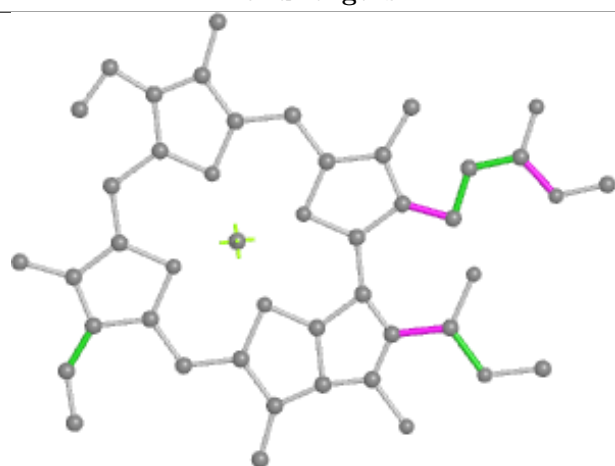
Ligand CLA a 824



Bond lengths



Bond angles

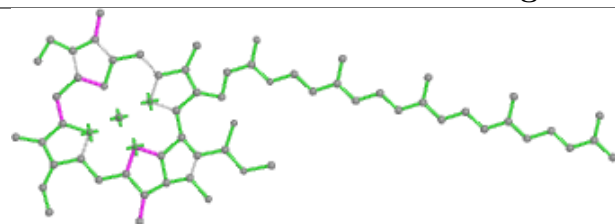


Torsions

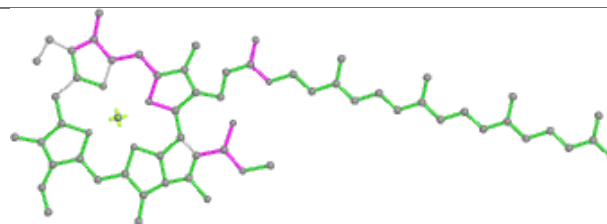


Rings

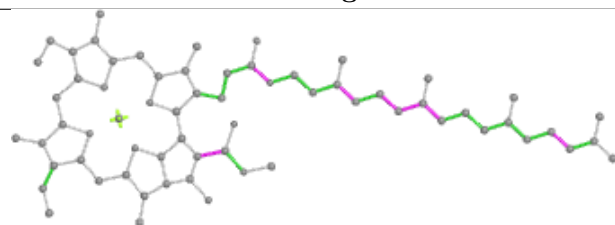
Ligand CLA a 831



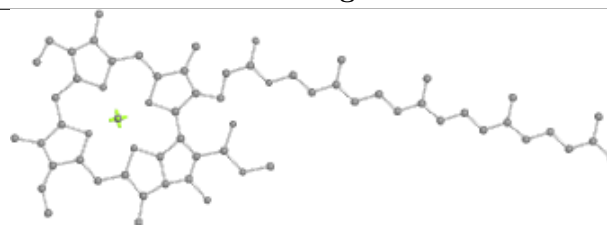
Bond lengths



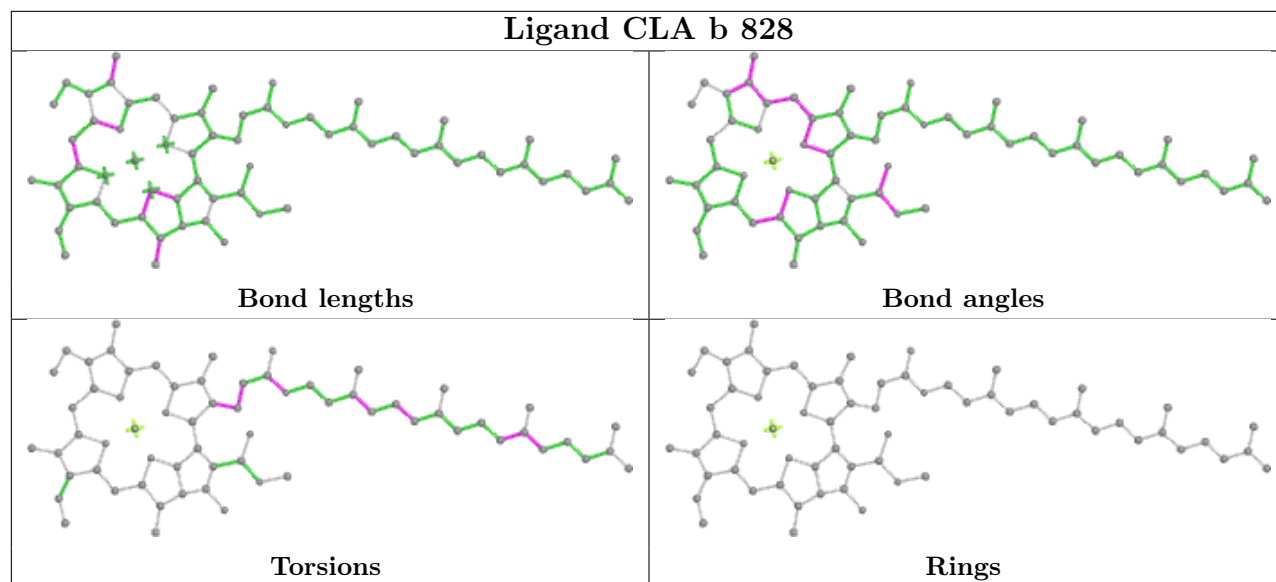
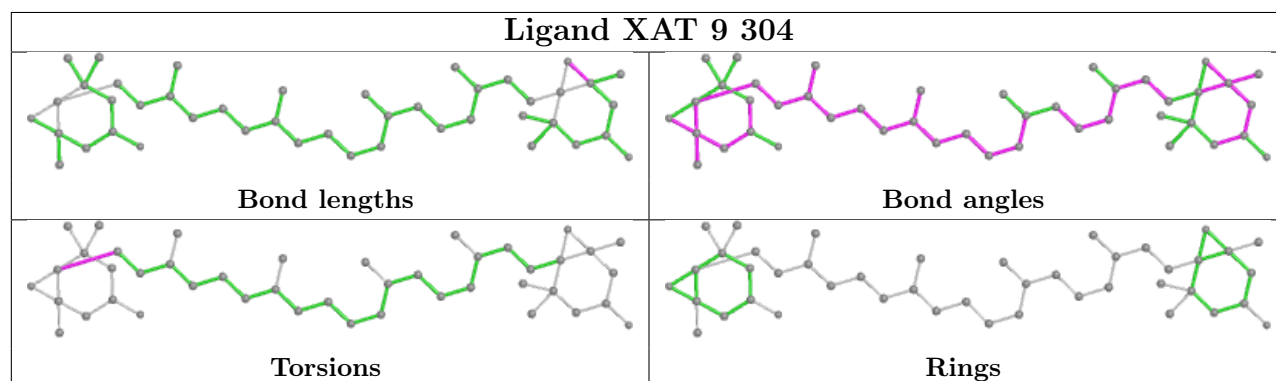
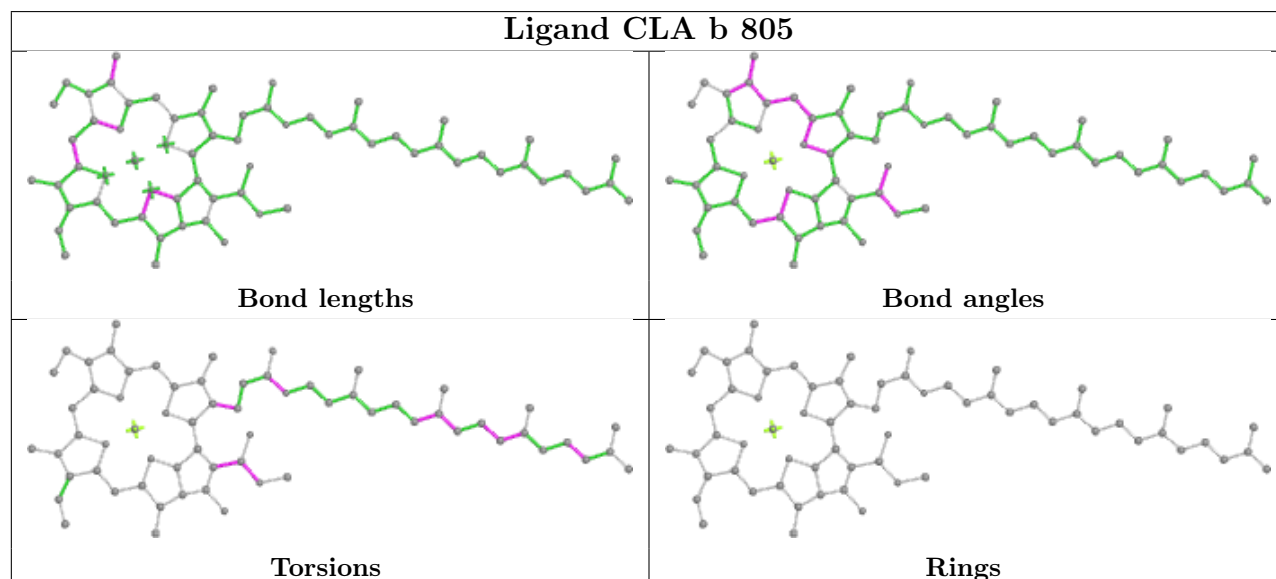
Bond angles

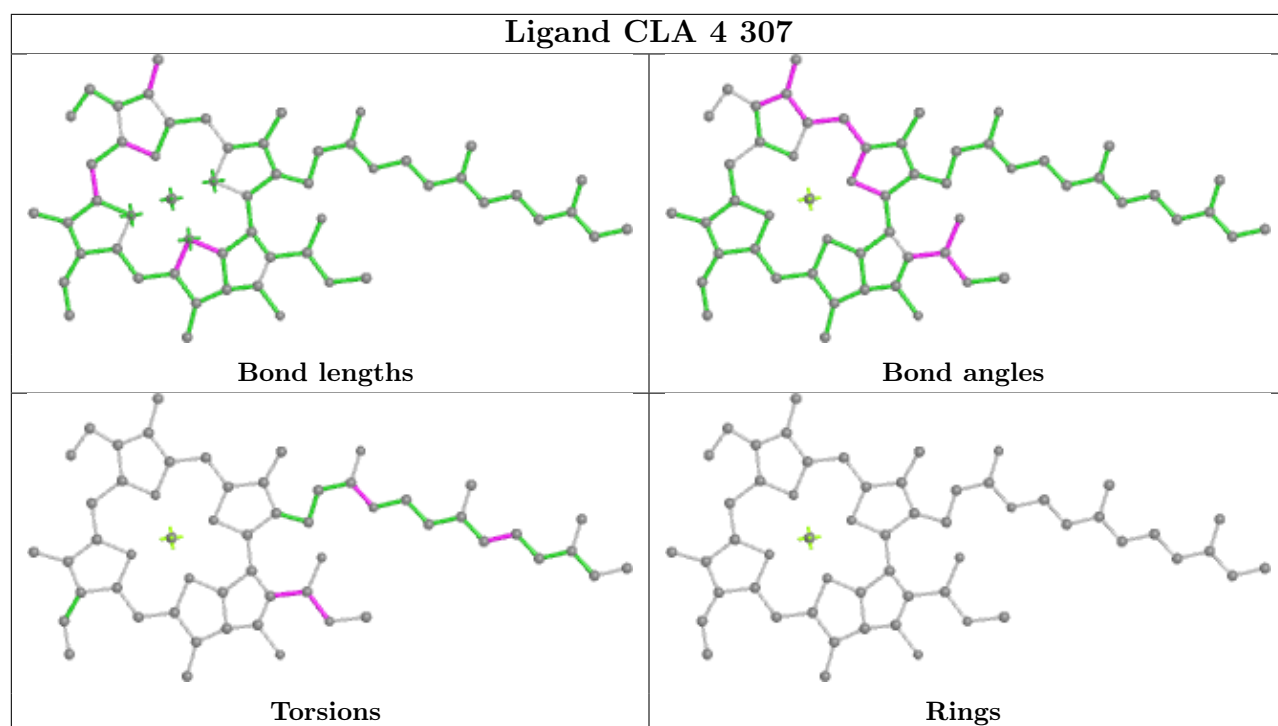


Torsions

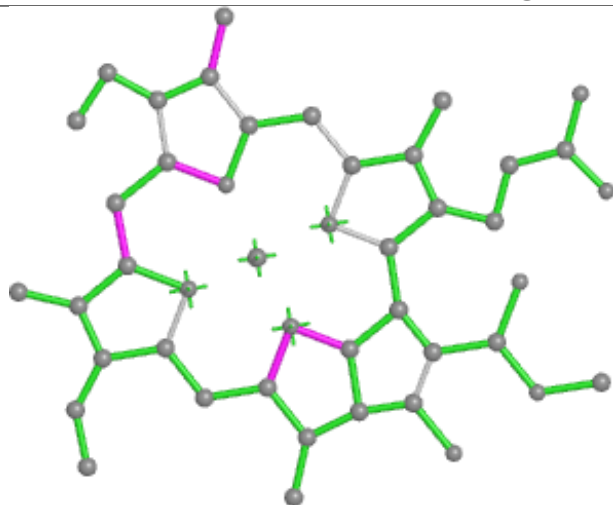


Rings

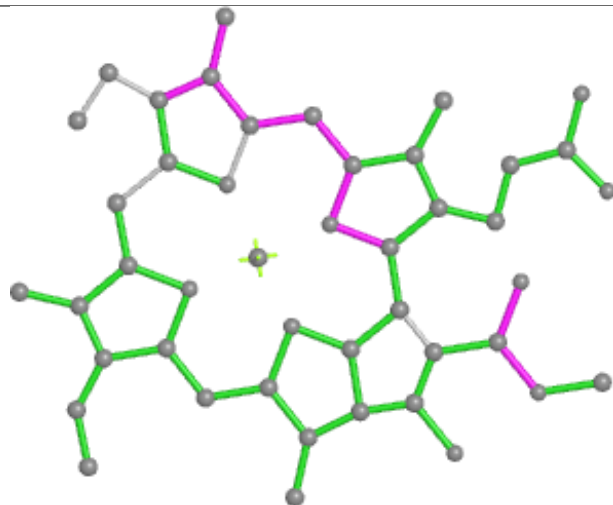
Ligand CLA b 828**Ligand XAT 9 304****Ligand CLA b 805**



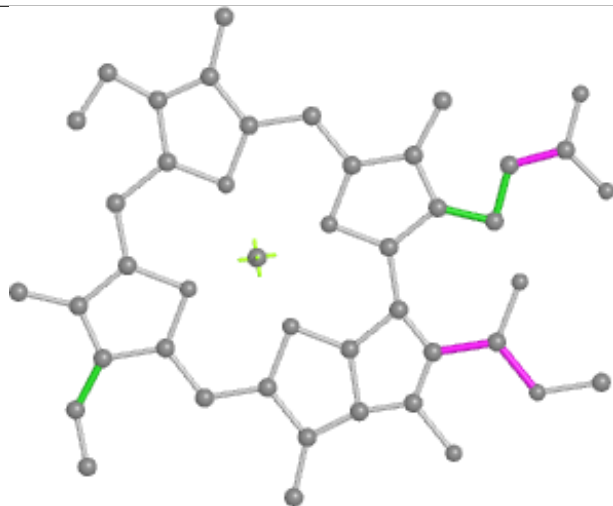
Ligand CLA 5 314



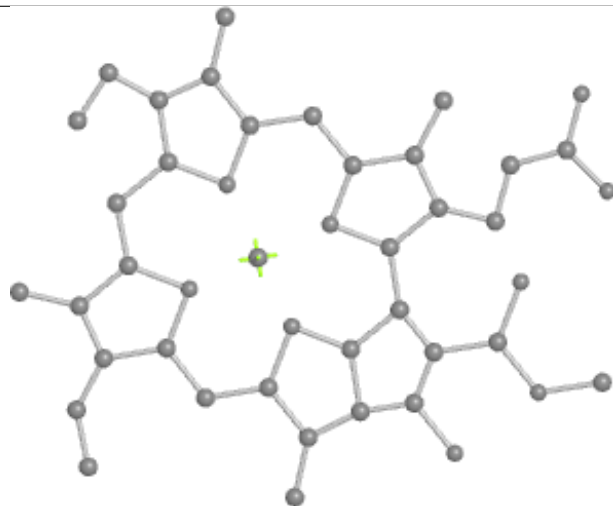
Bond lengths



Bond angles

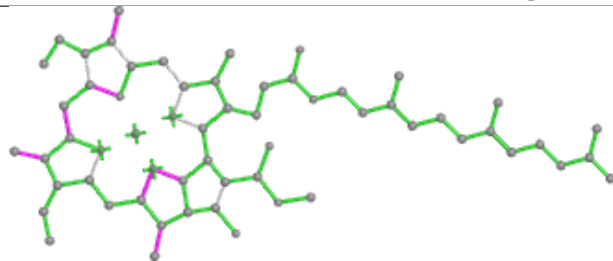


Torsions

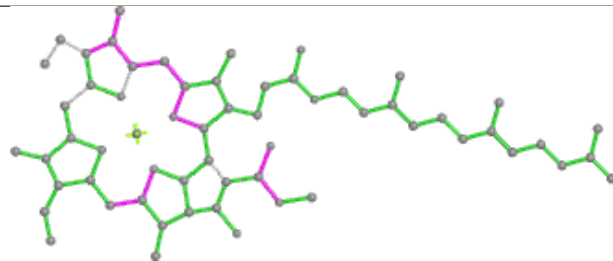


Rings

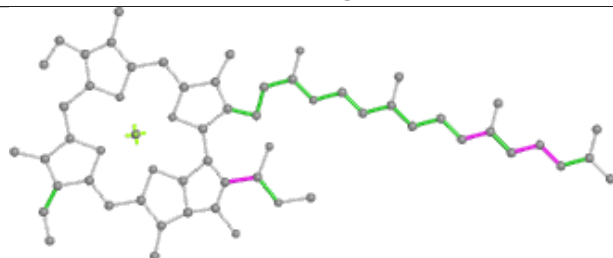
Ligand CLA 1 202



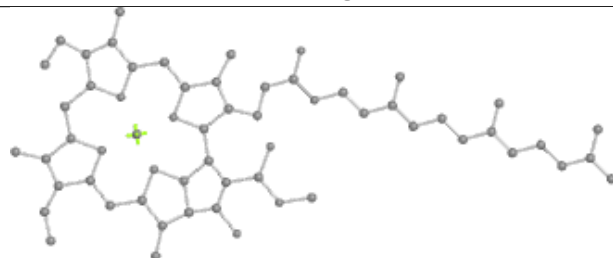
Bond lengths



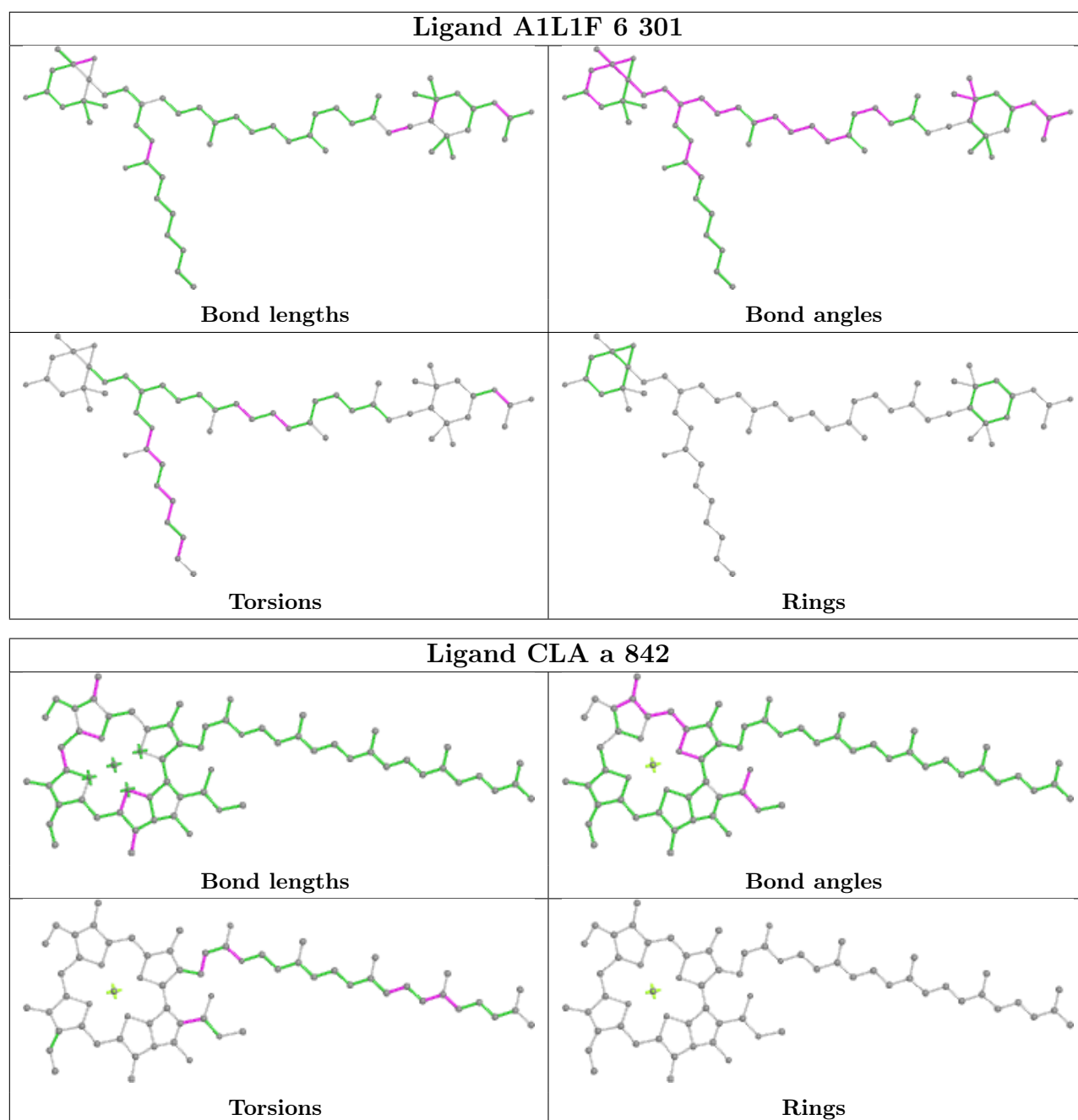
Bond angles

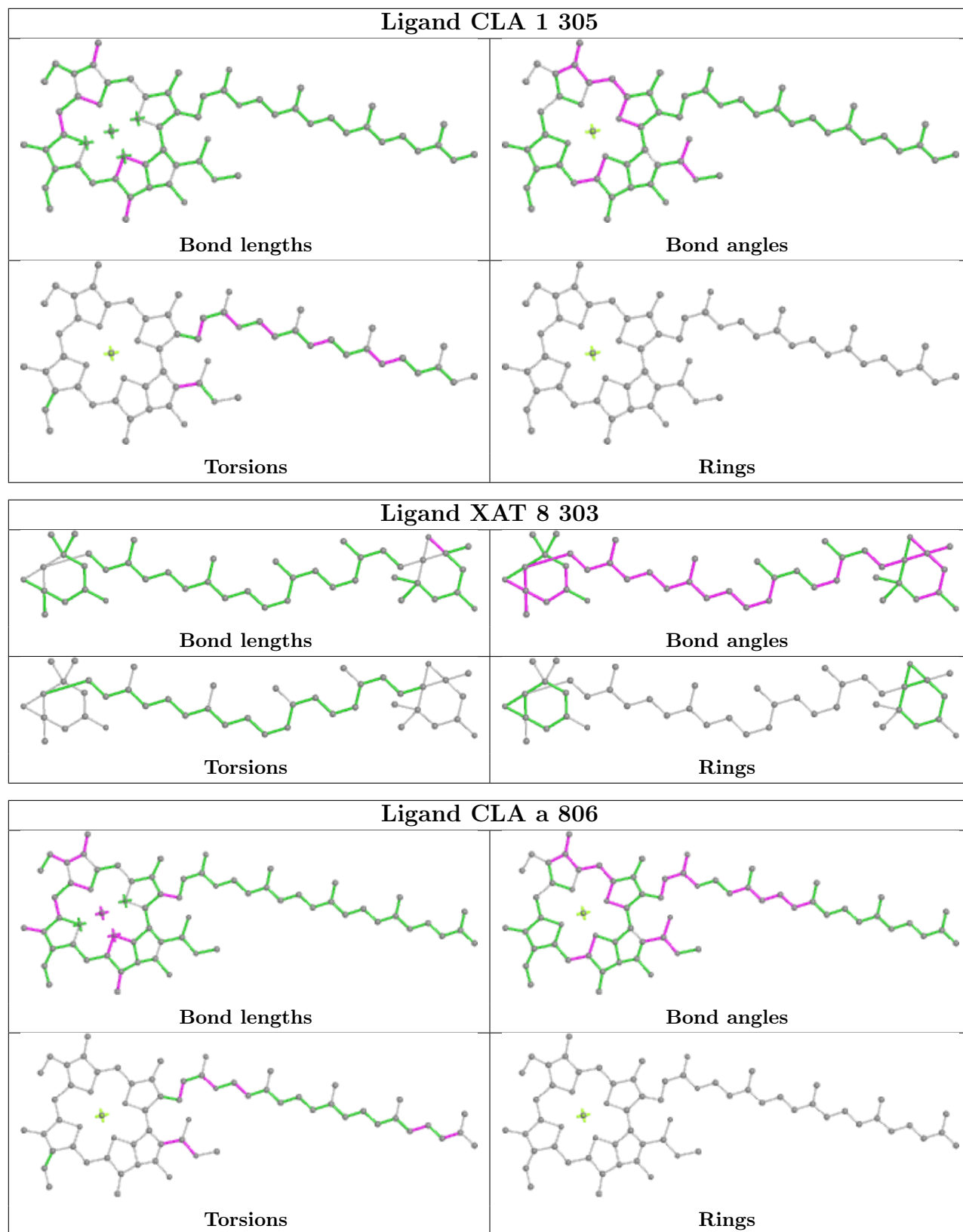


Torsions

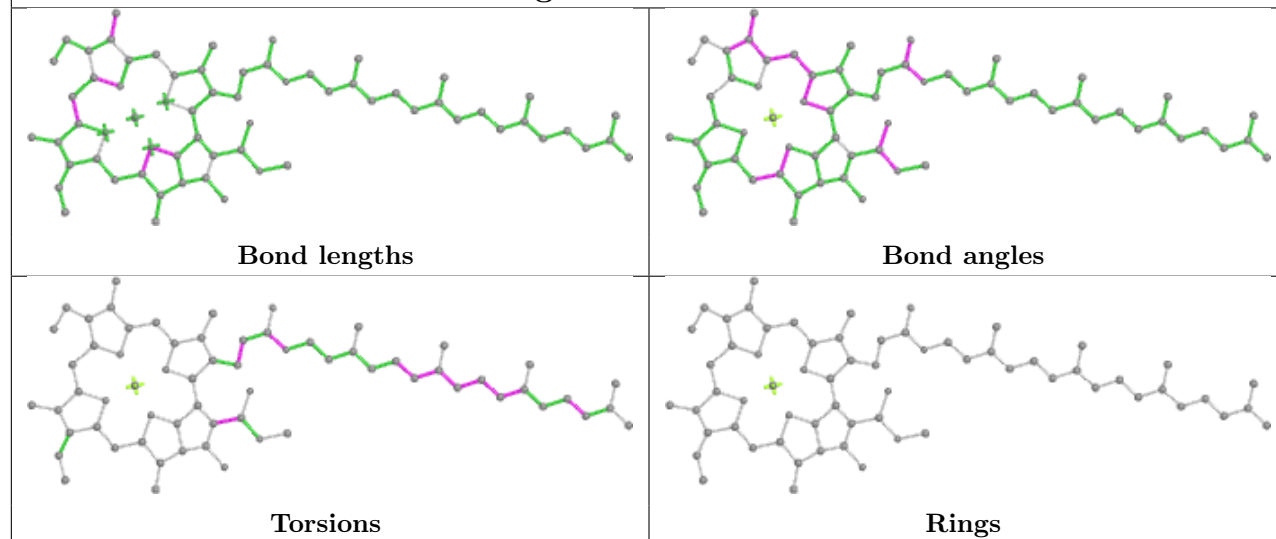


Rings

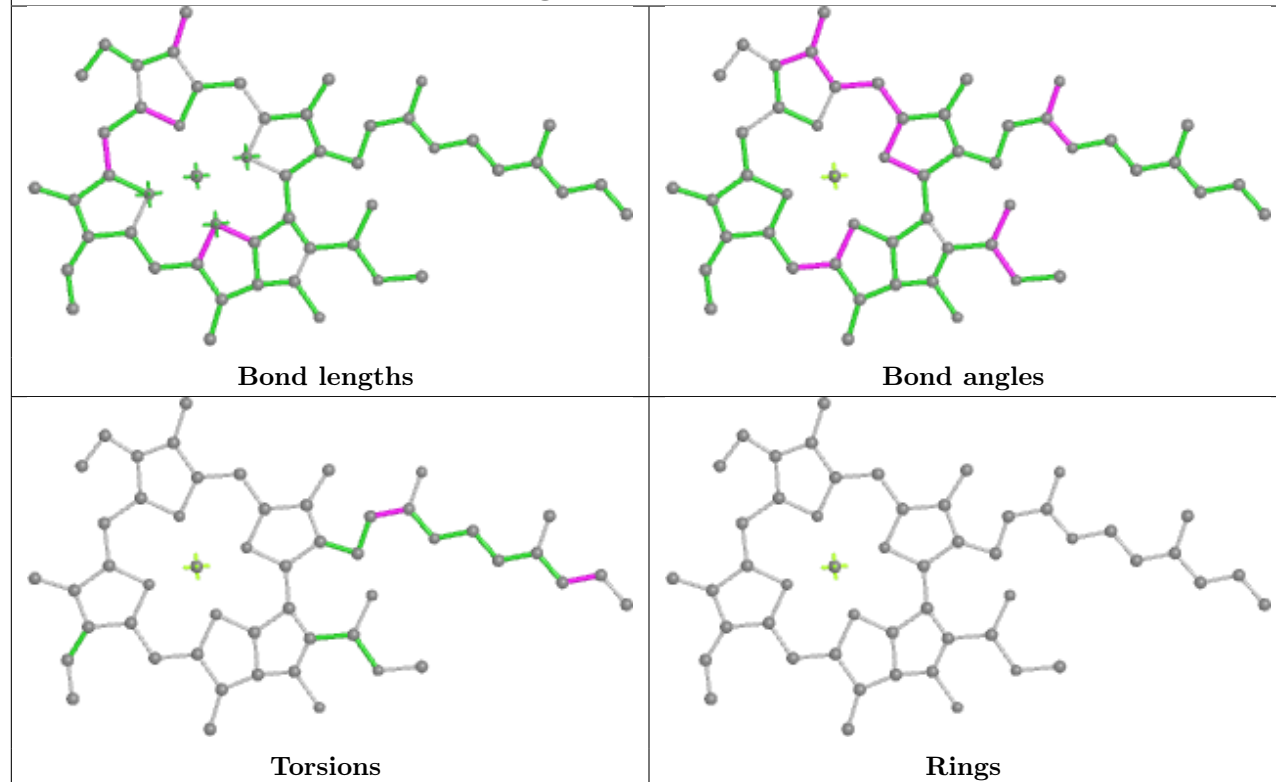




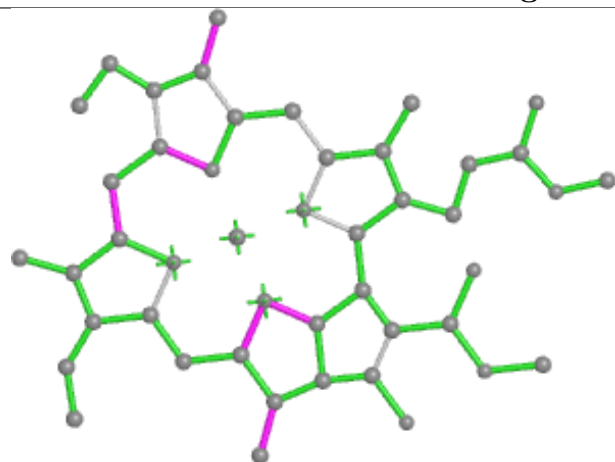
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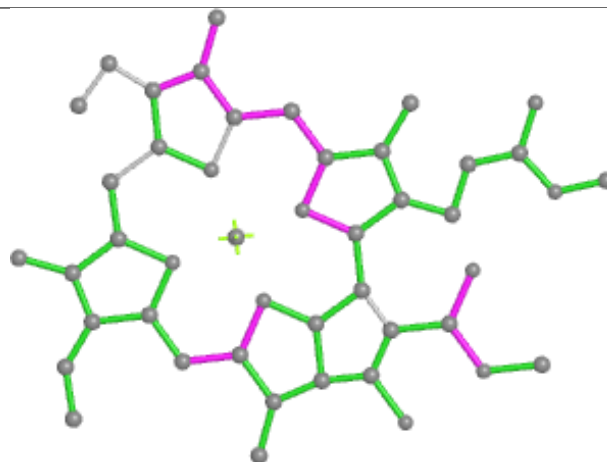
Ligand CLA 1 312



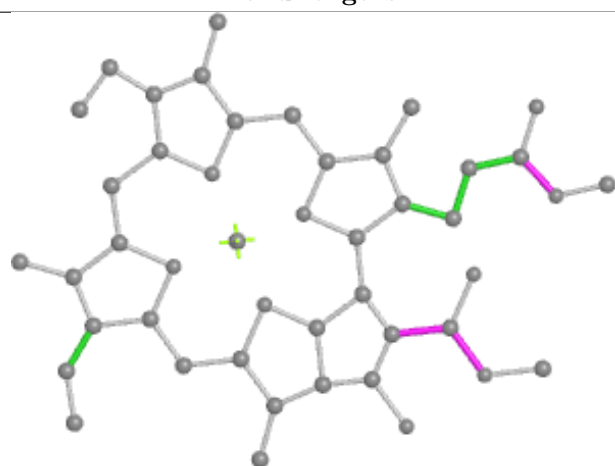
Ligand CLA 8 310



Bond lengths



Bond angles

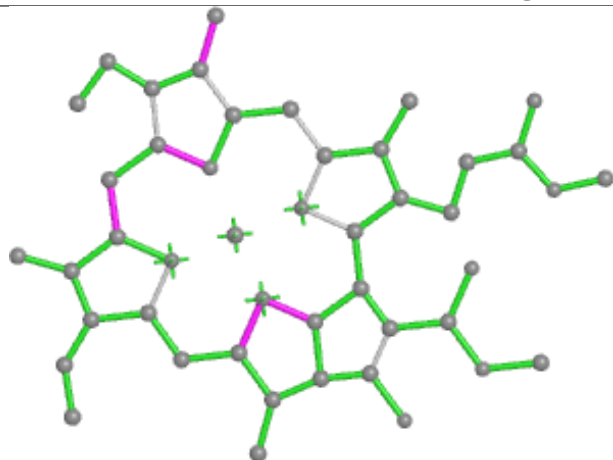


Torsions

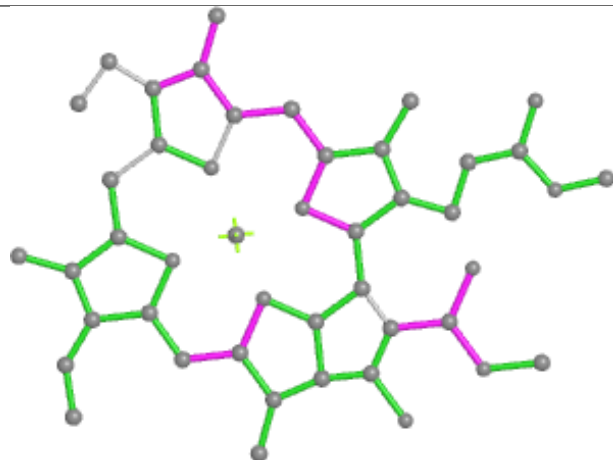


Rings

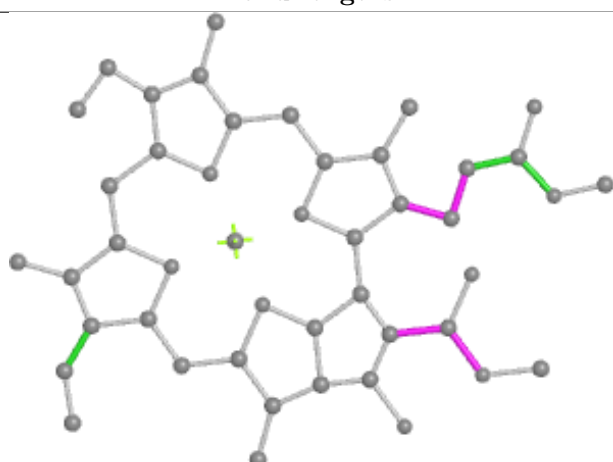
Ligand CLA 9 311



Bond lengths



Bond angles

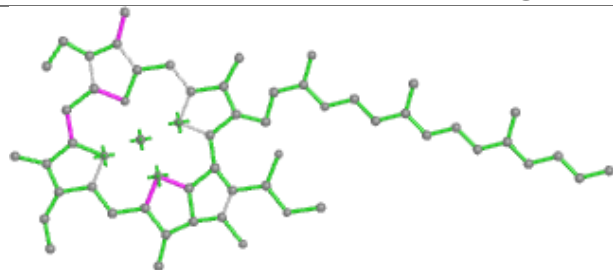


Torsions

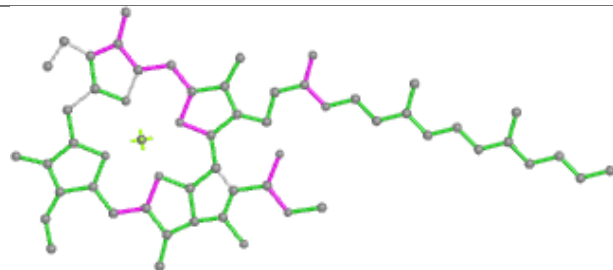


Rings

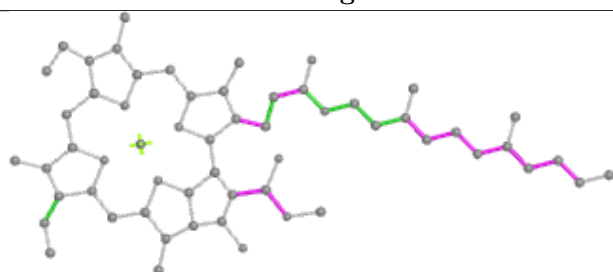
Ligand CLA b 833



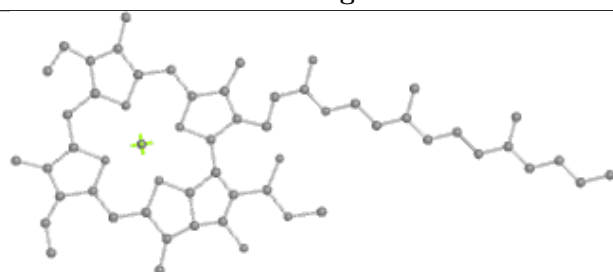
Bond lengths



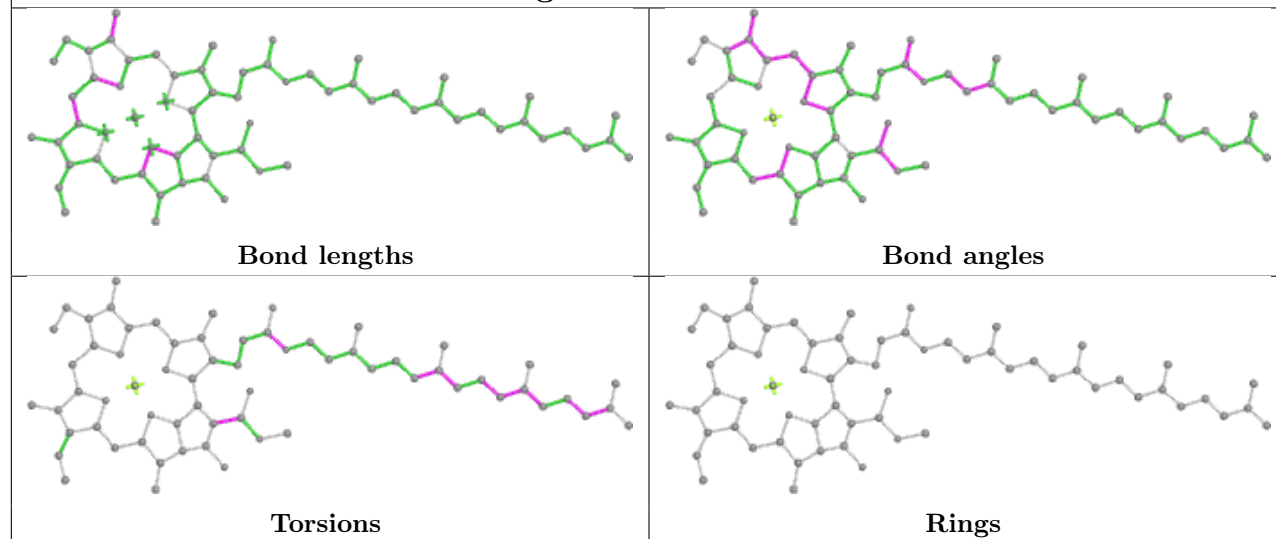
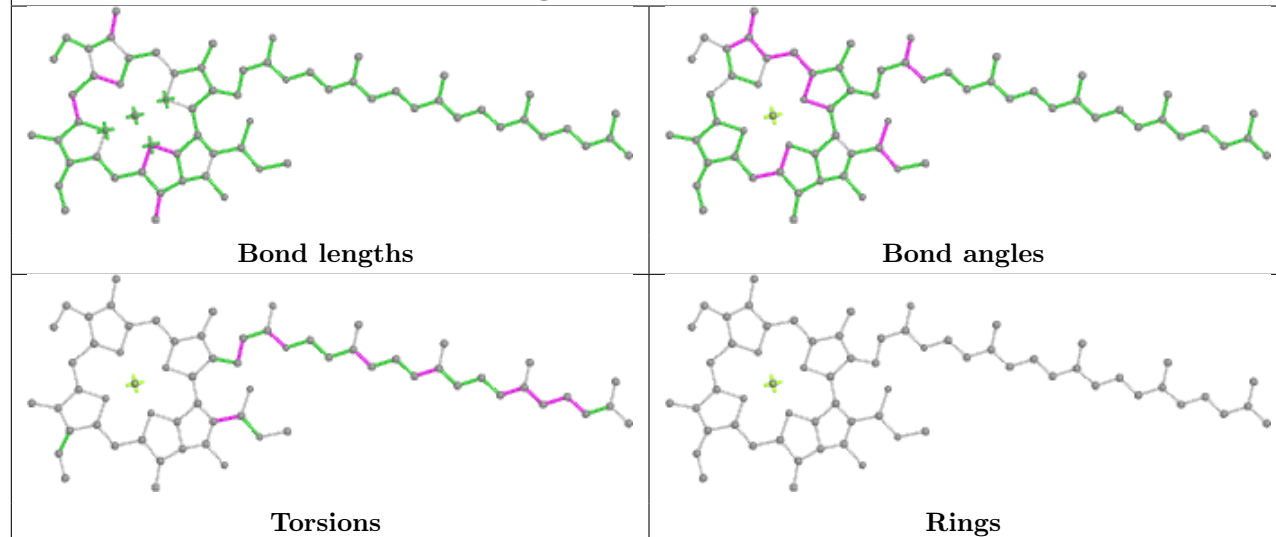
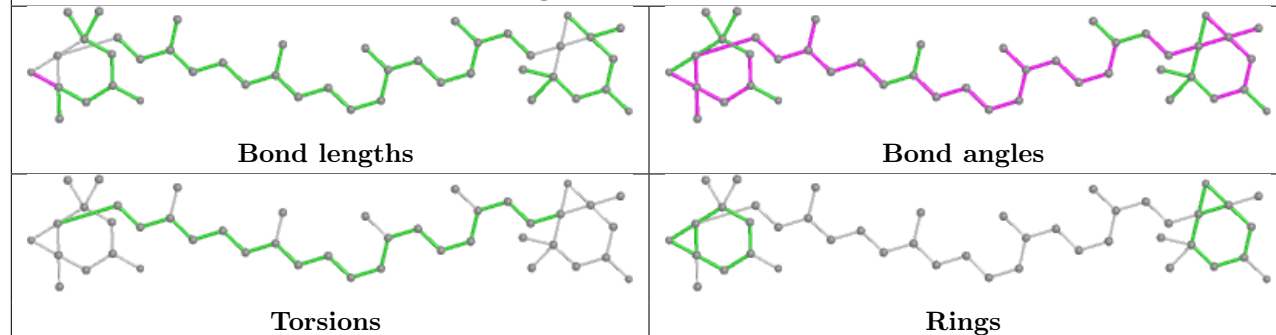
Bond angles



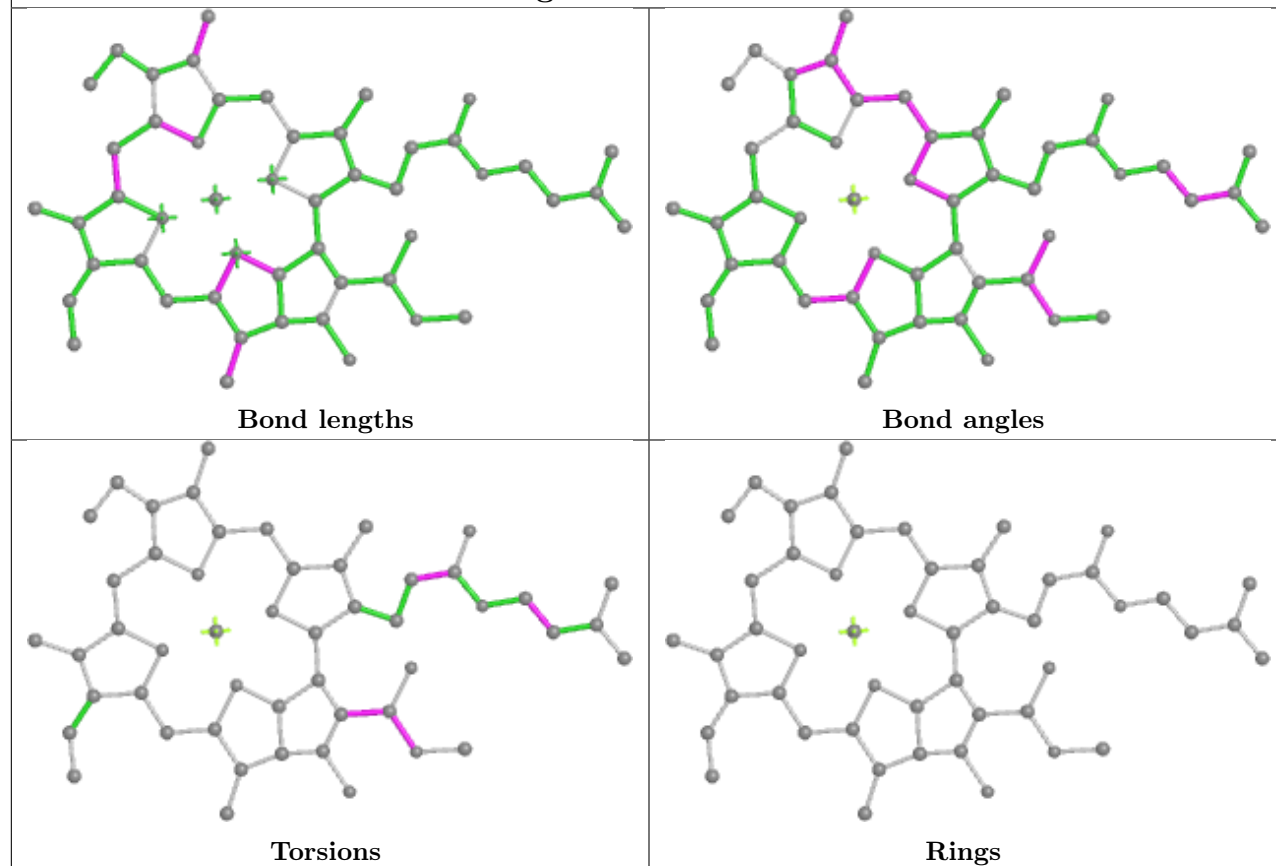
Torsions



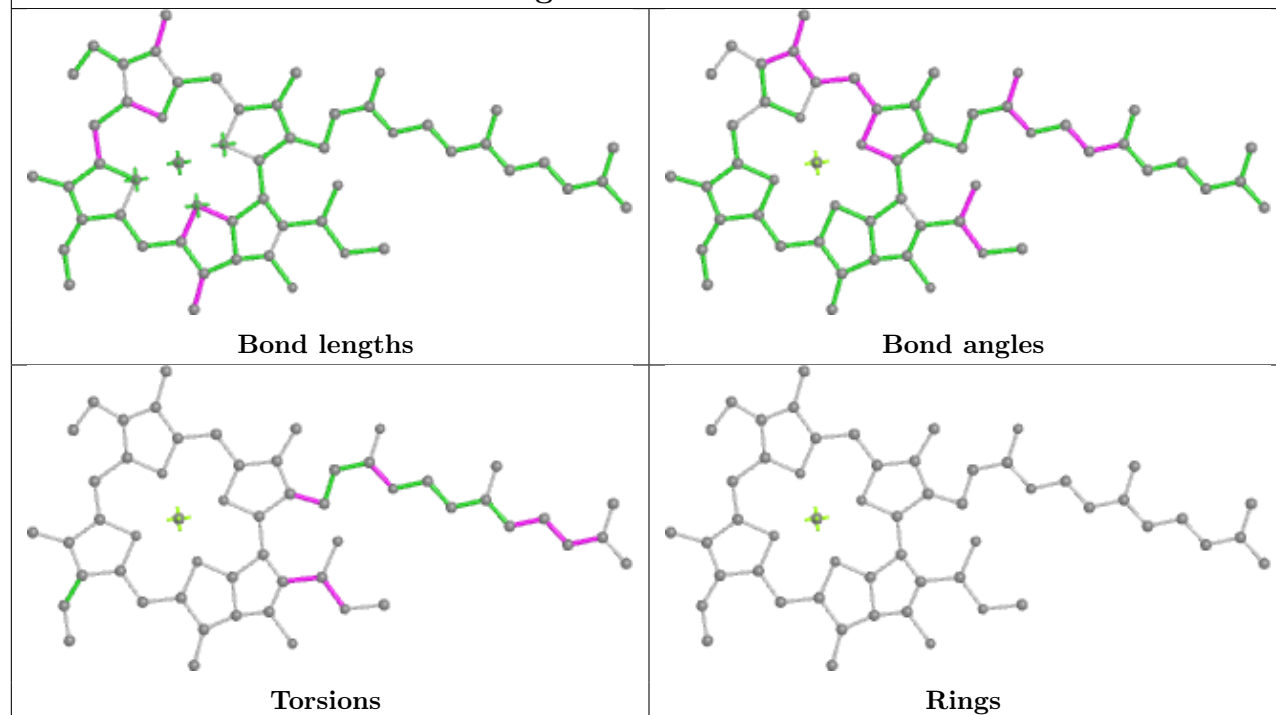
Rings

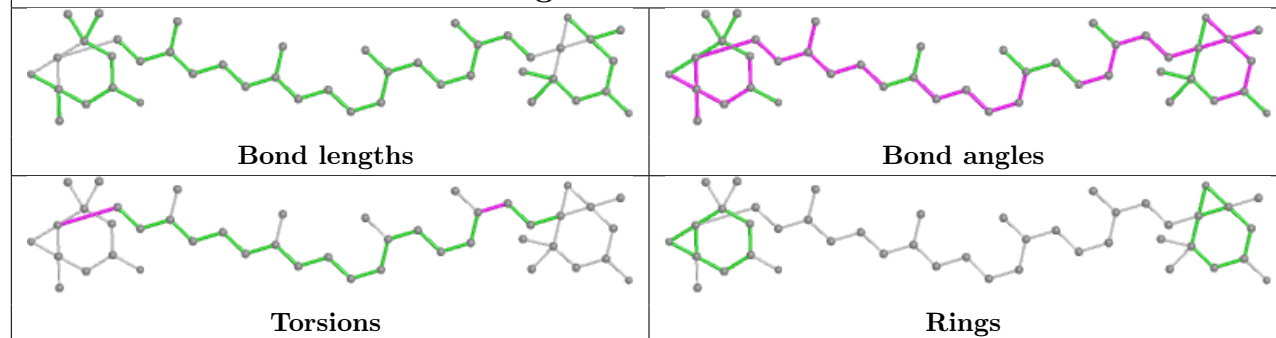
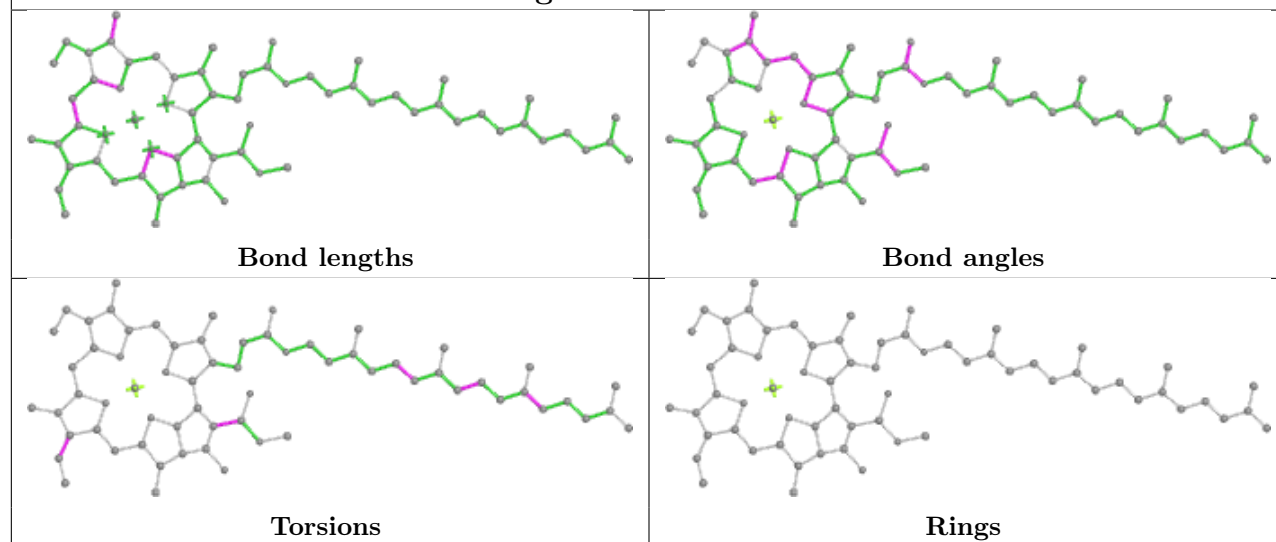
Ligand CLA a 844**Ligand CLA b 839****Ligand XAT 4 302**

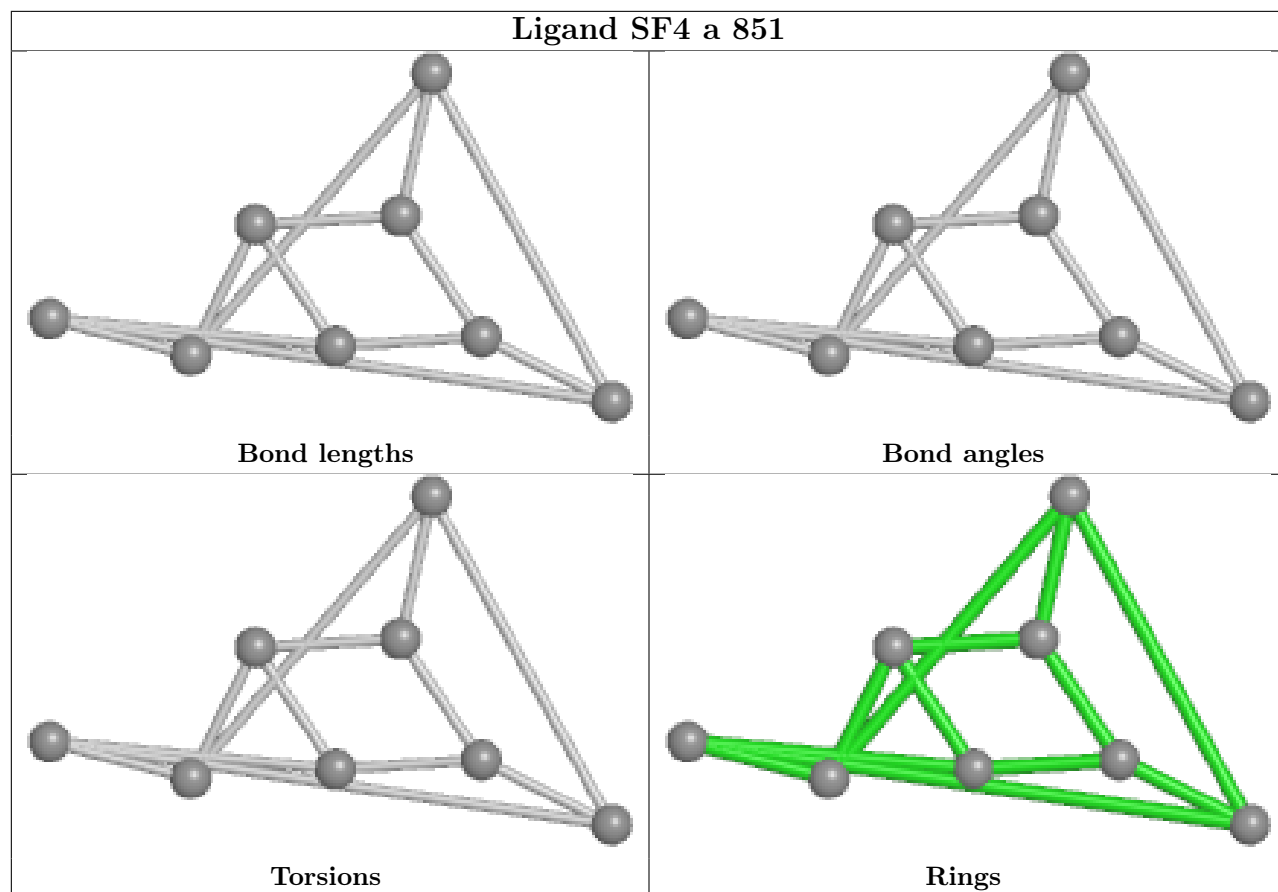
Ligand CLA 4 309



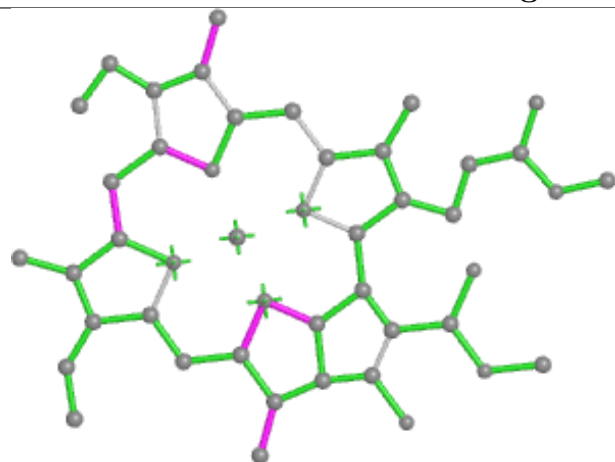
Ligand CLA b 814



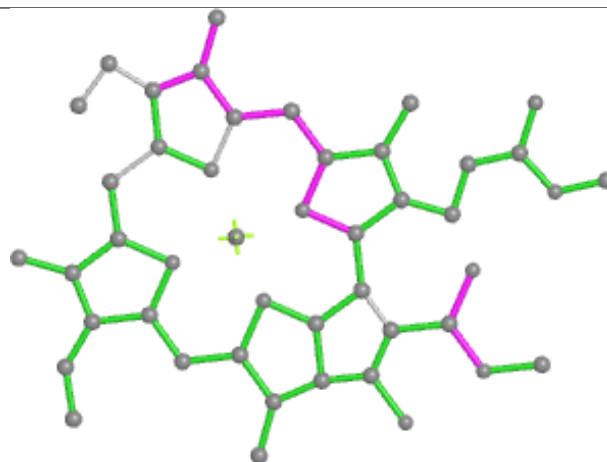
Ligand XAT 8 301**Ligand CLA b 837**



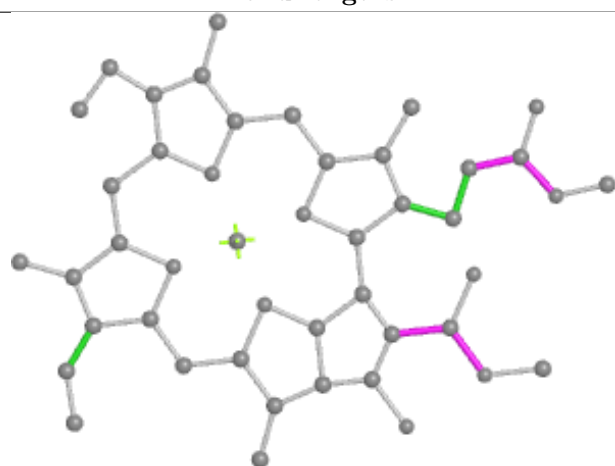
Ligand CLA 6 314



Bond lengths



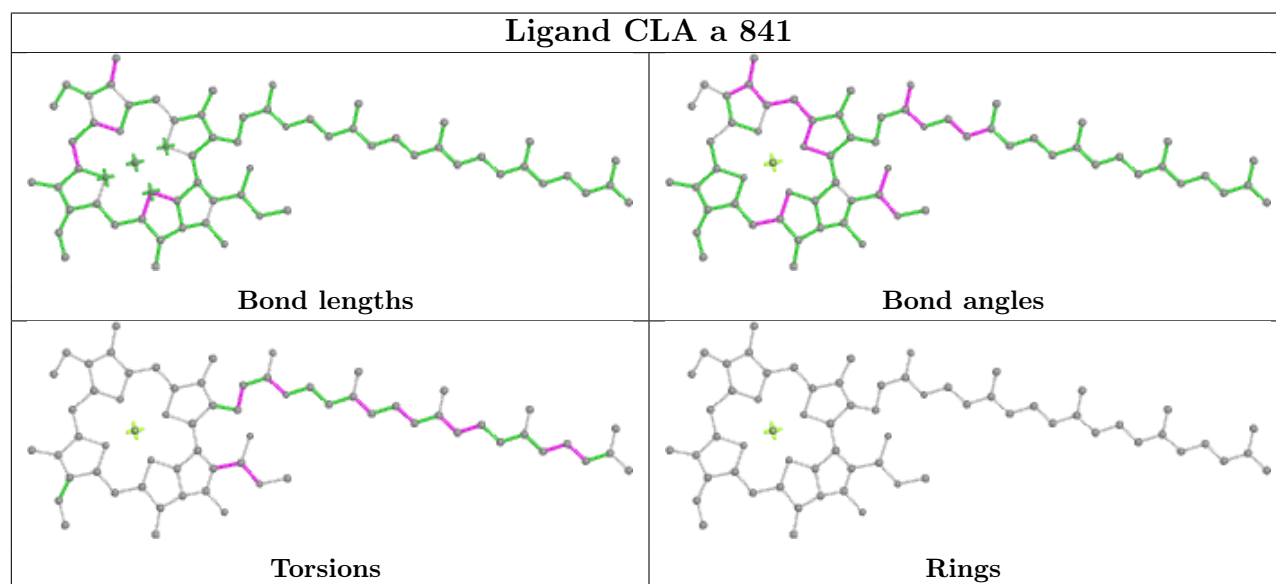
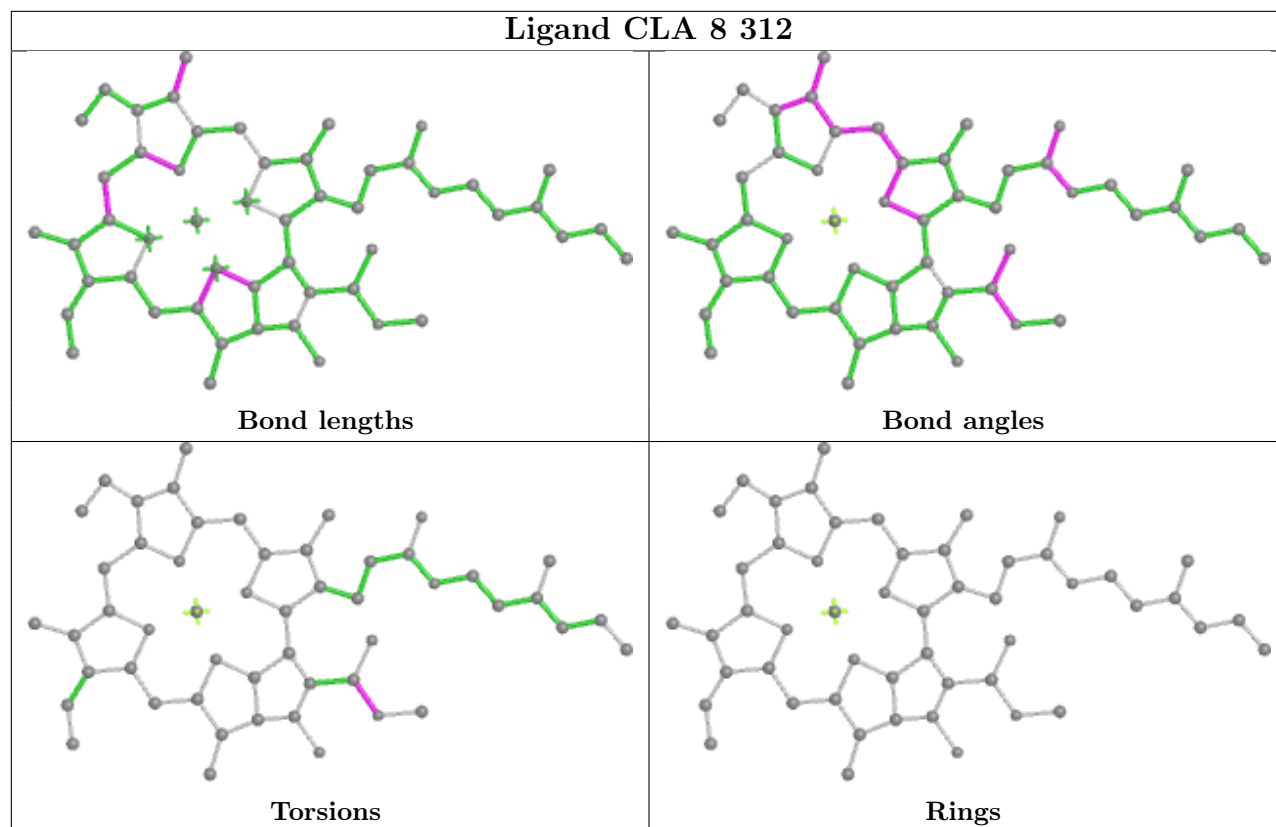
Bond angles

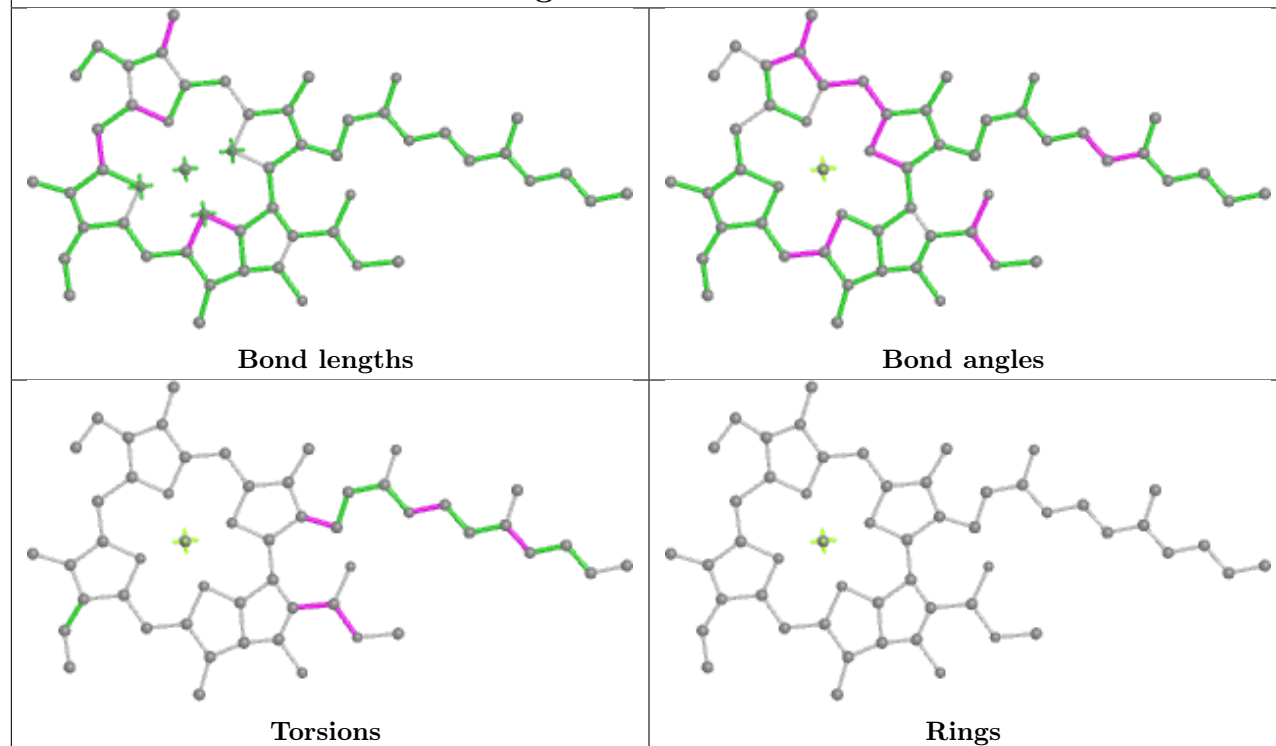
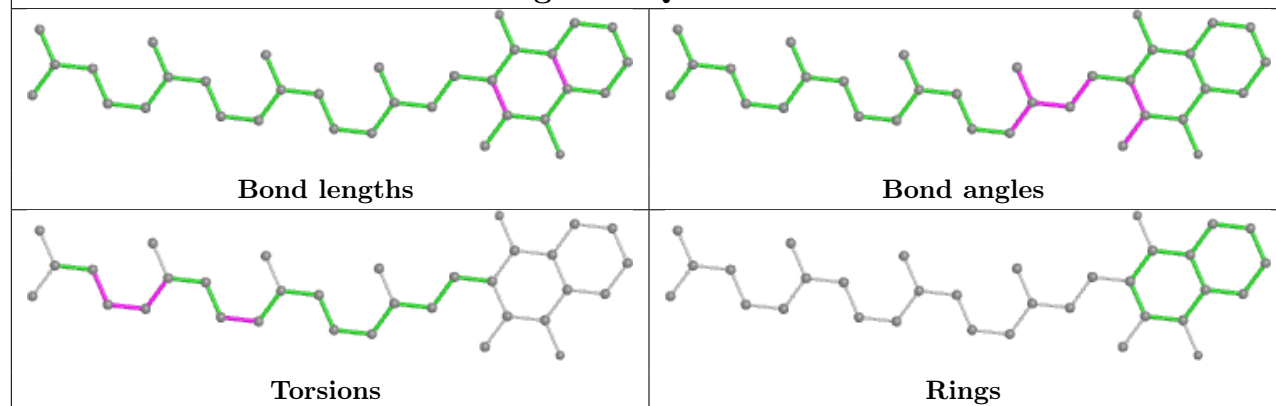


Torsions

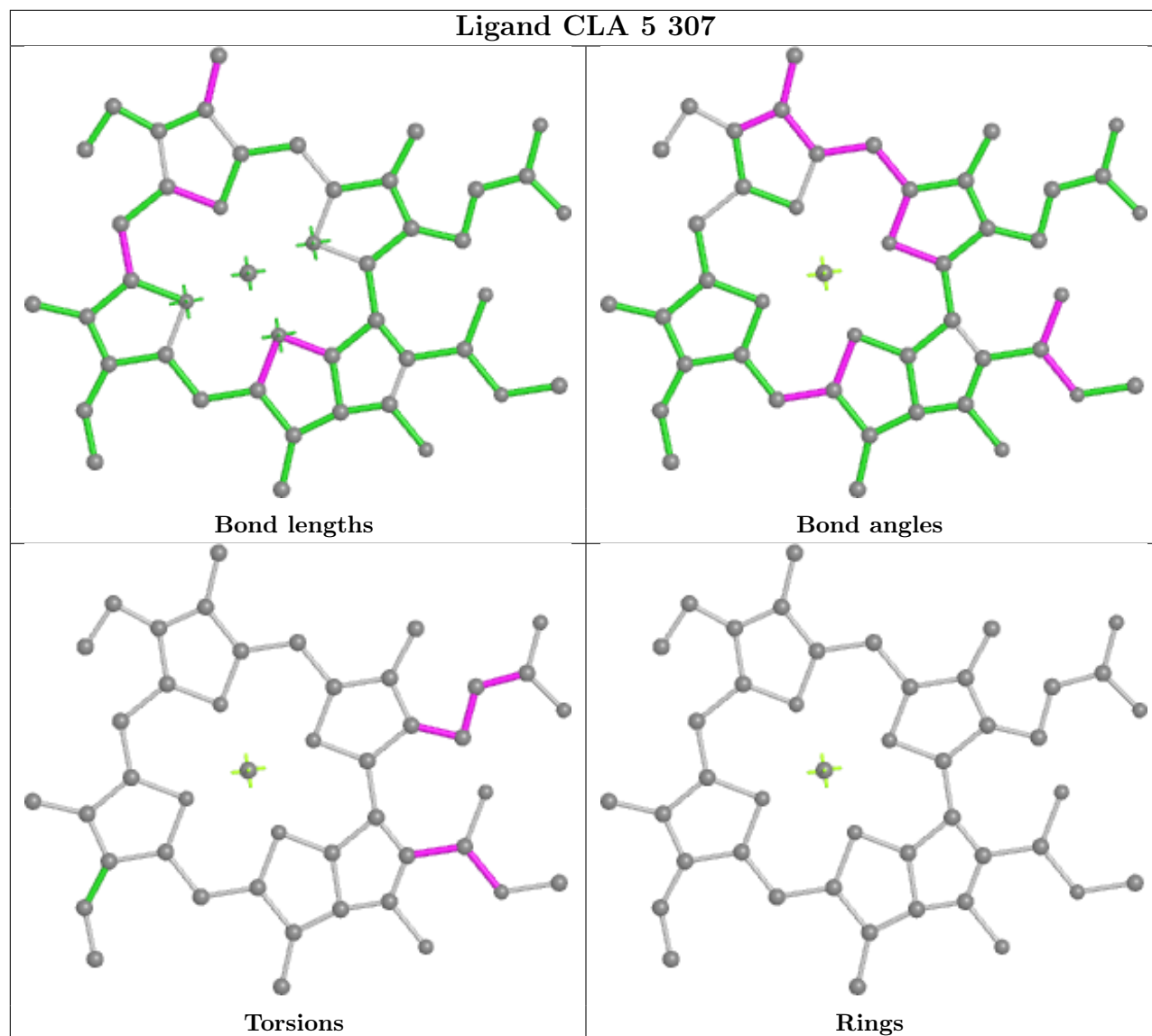


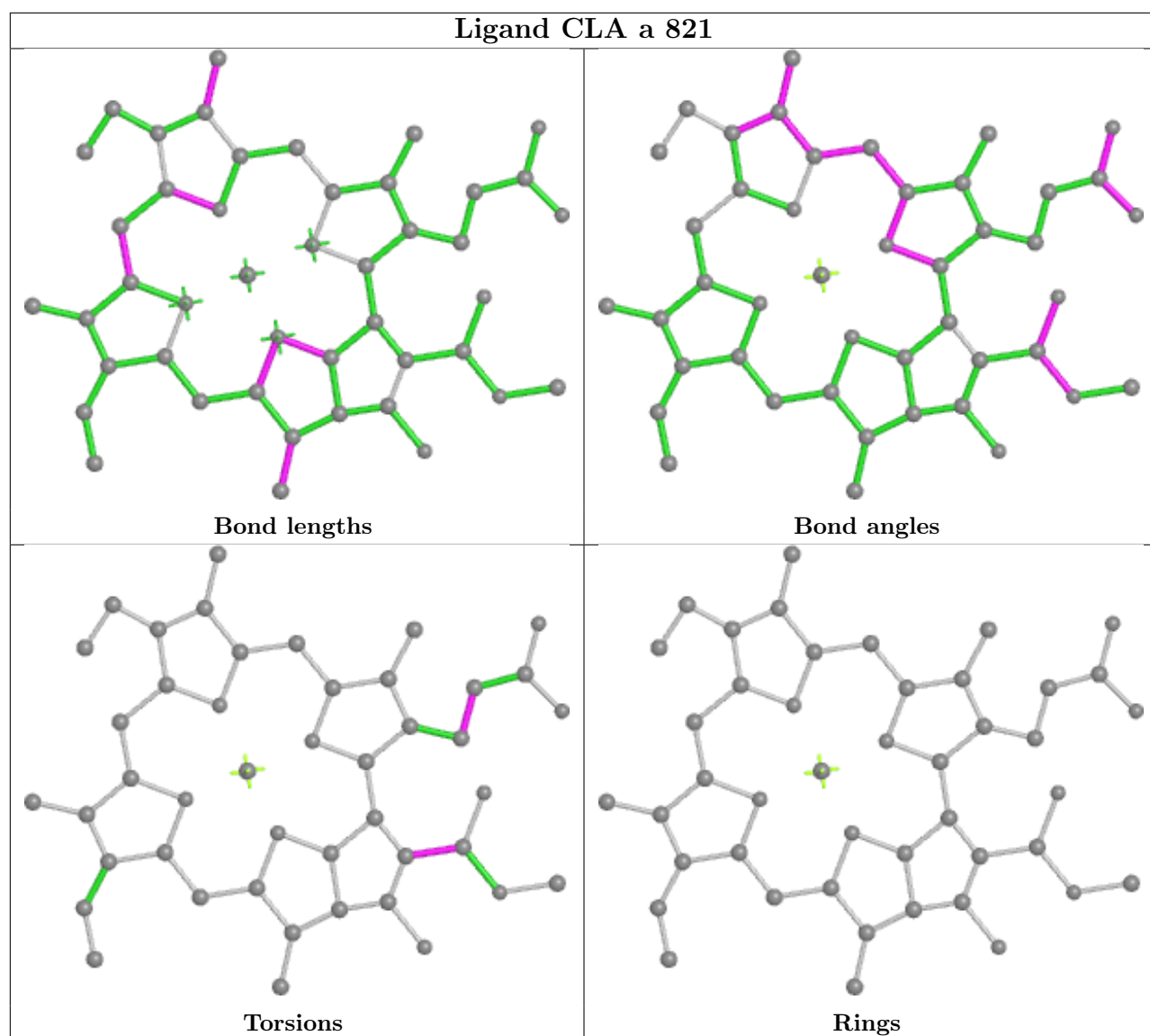
Rings

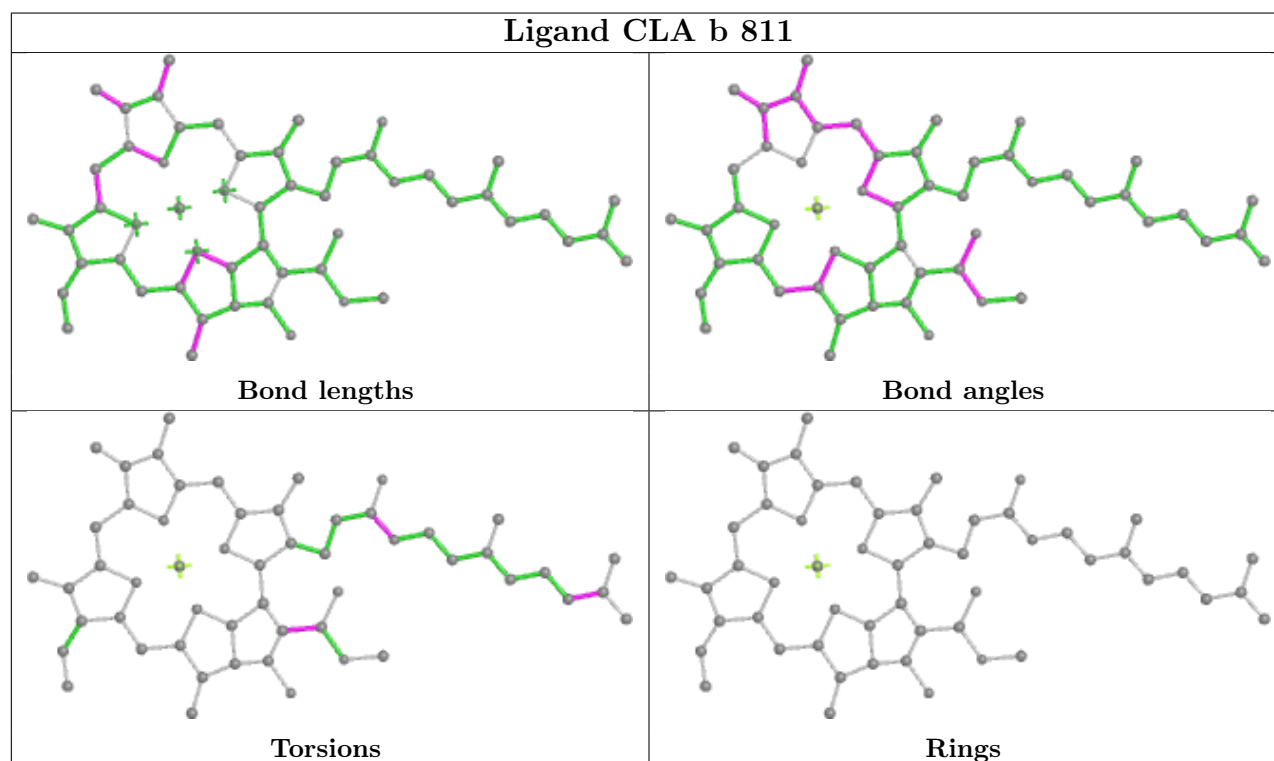
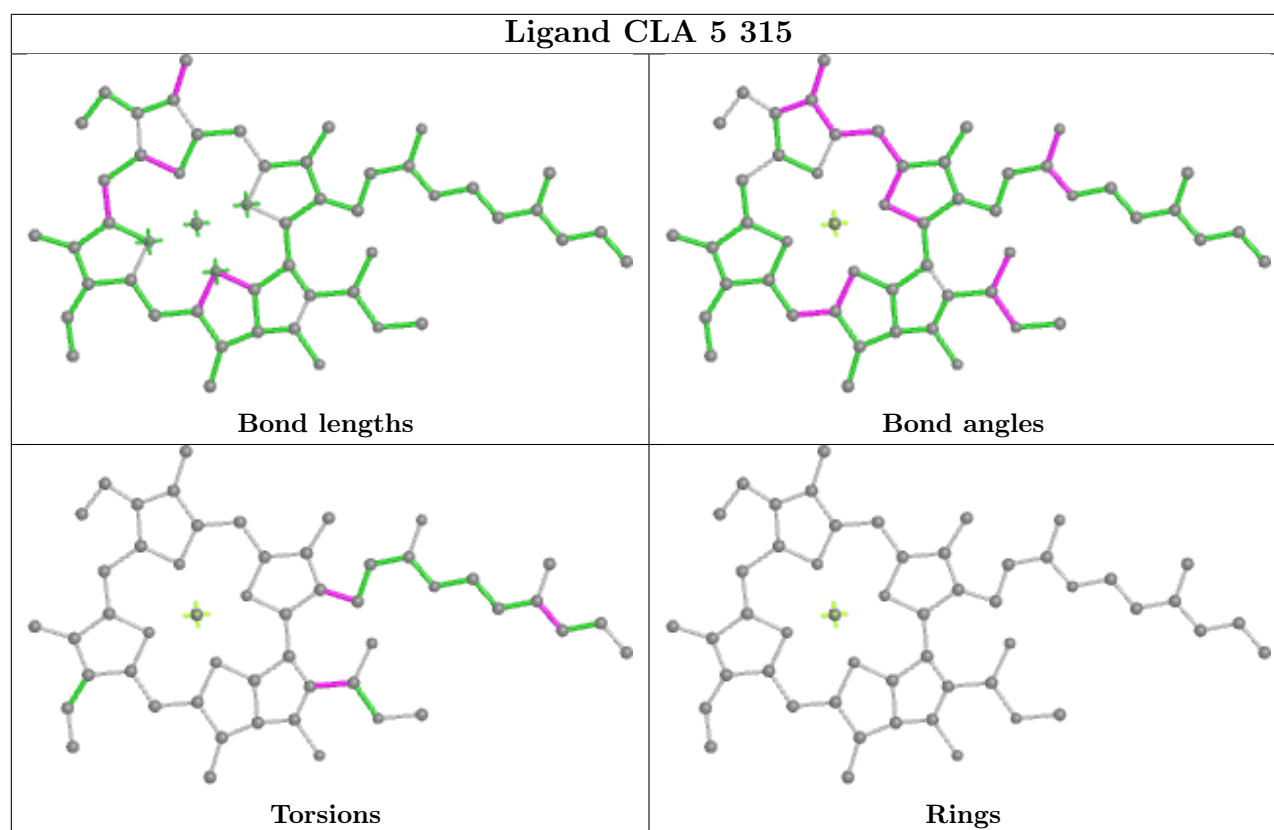


Ligand CLA b 835**Ligand PQN a 843**

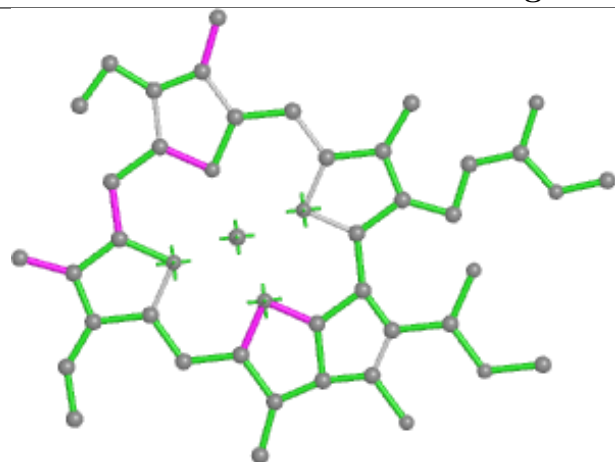
Ligand CLA 5 307



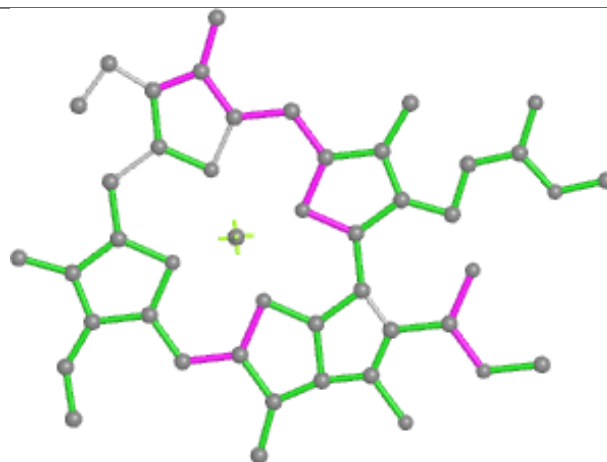




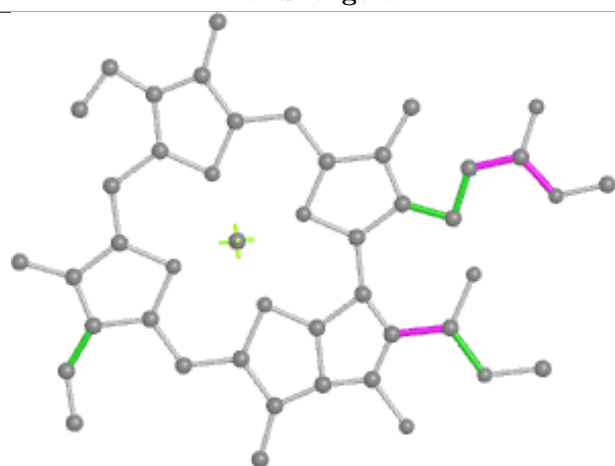
Ligand CLA 1 203



Bond lengths



Bond angles

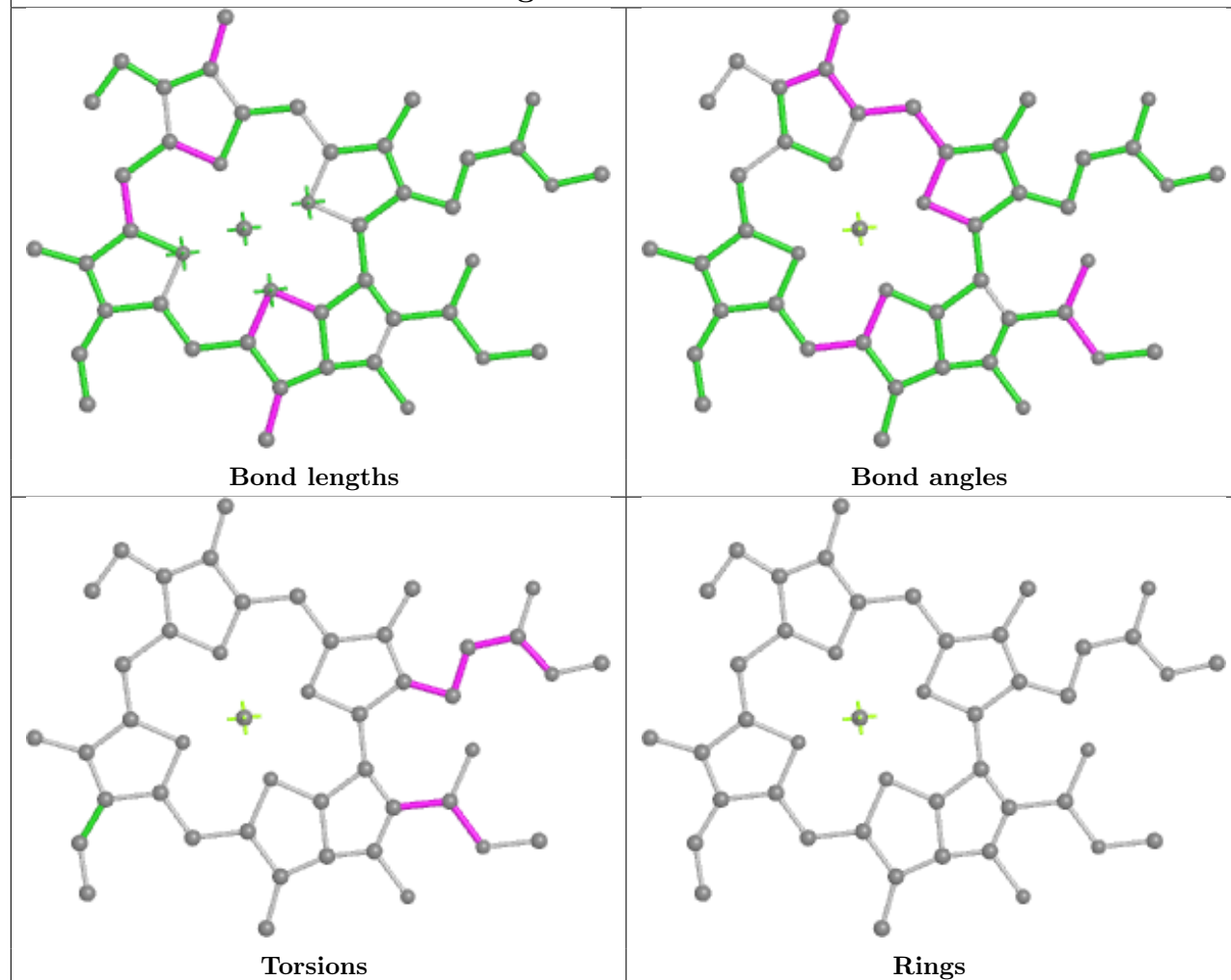


Torsions

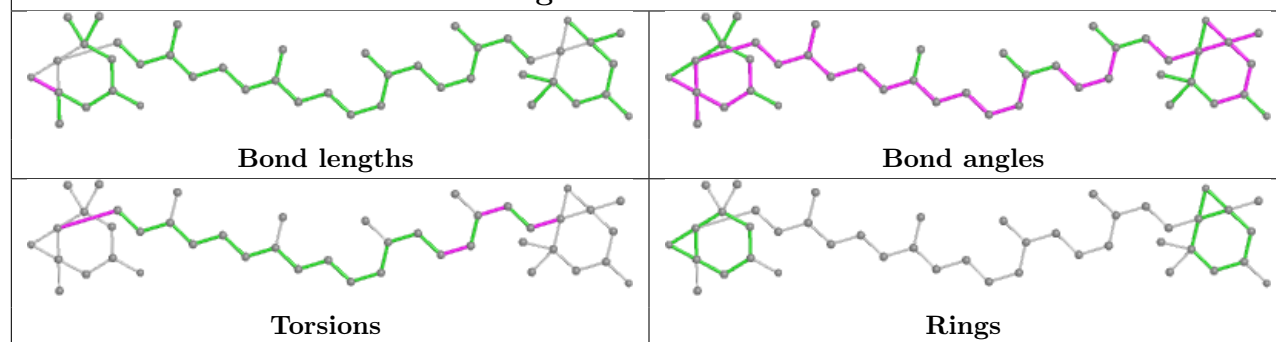


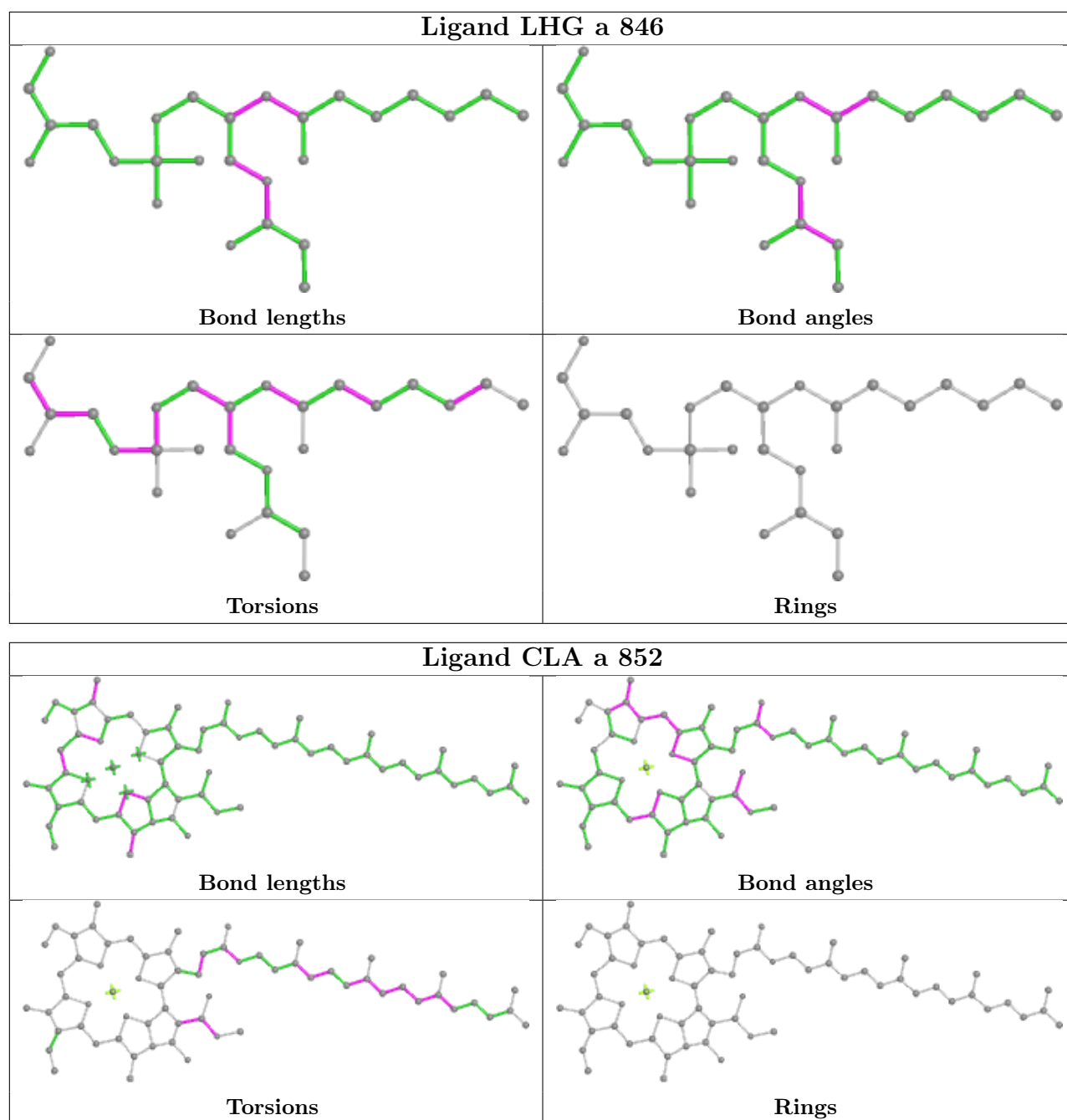
Rings

Ligand CLA 9 313

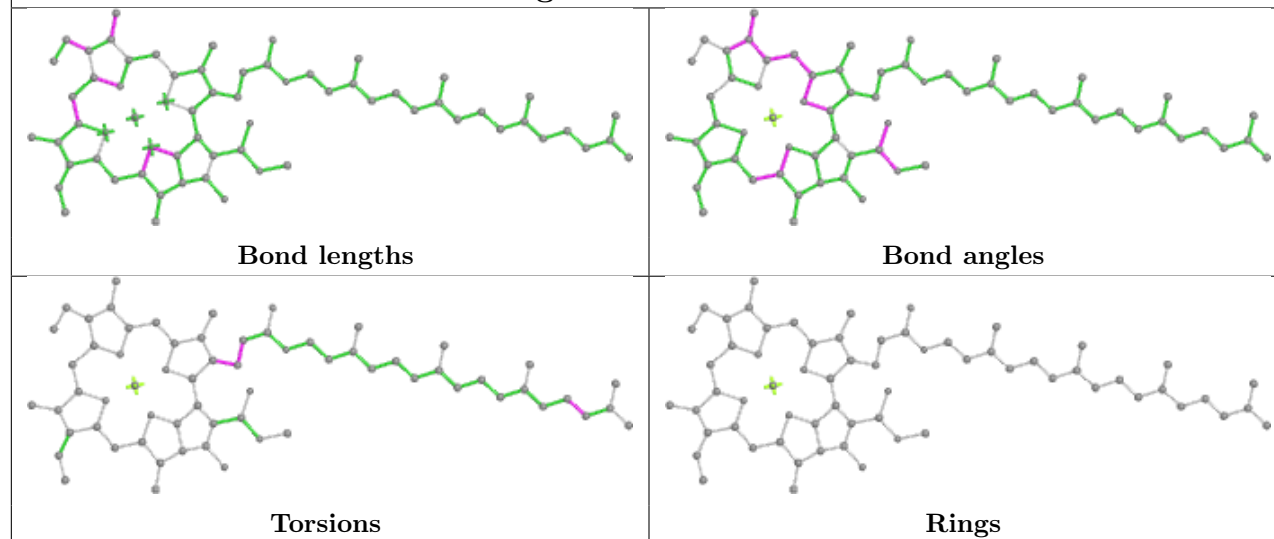


Ligand XAT a 853

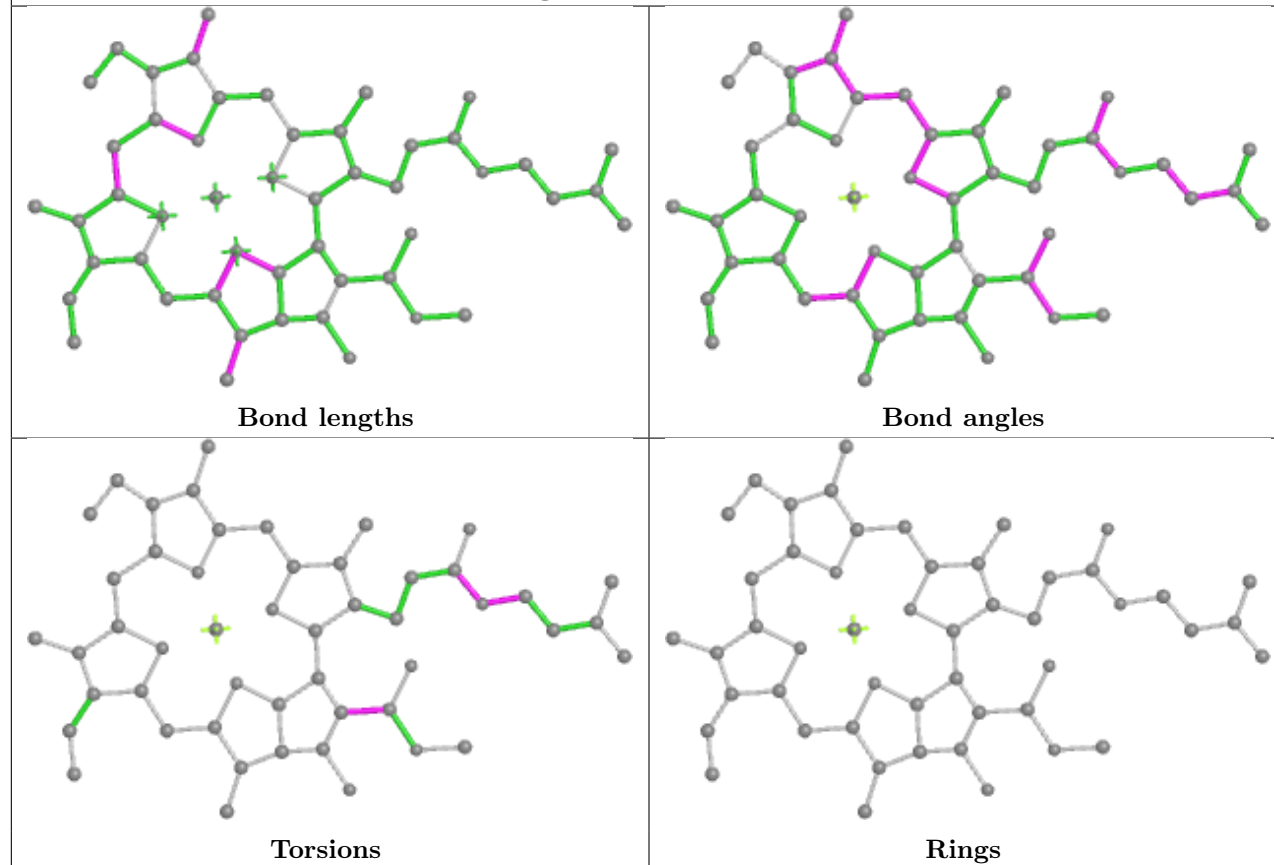


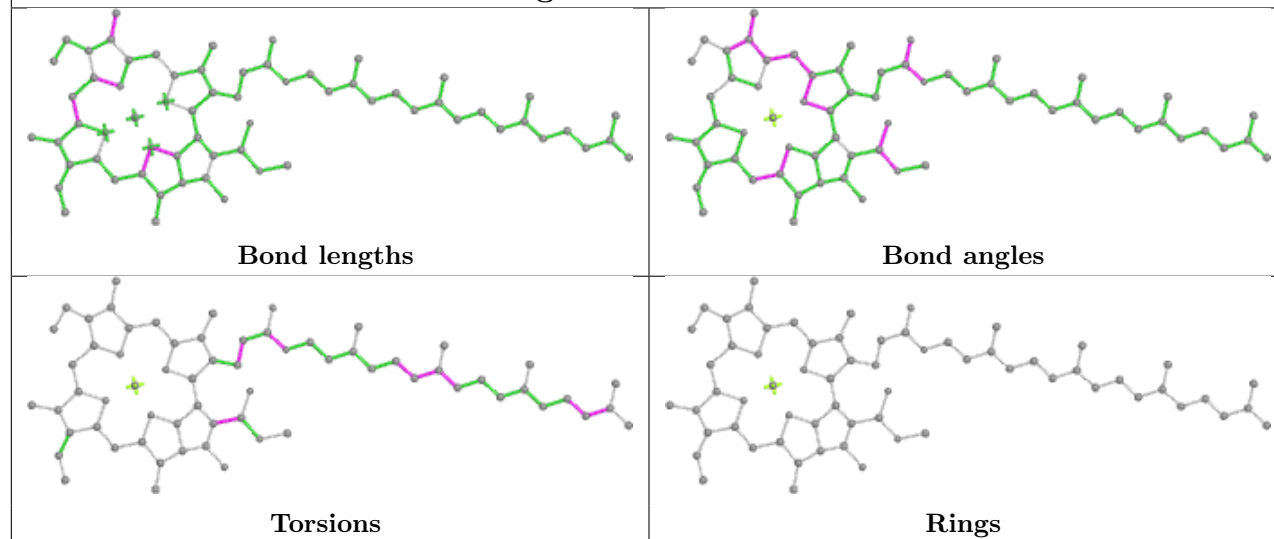
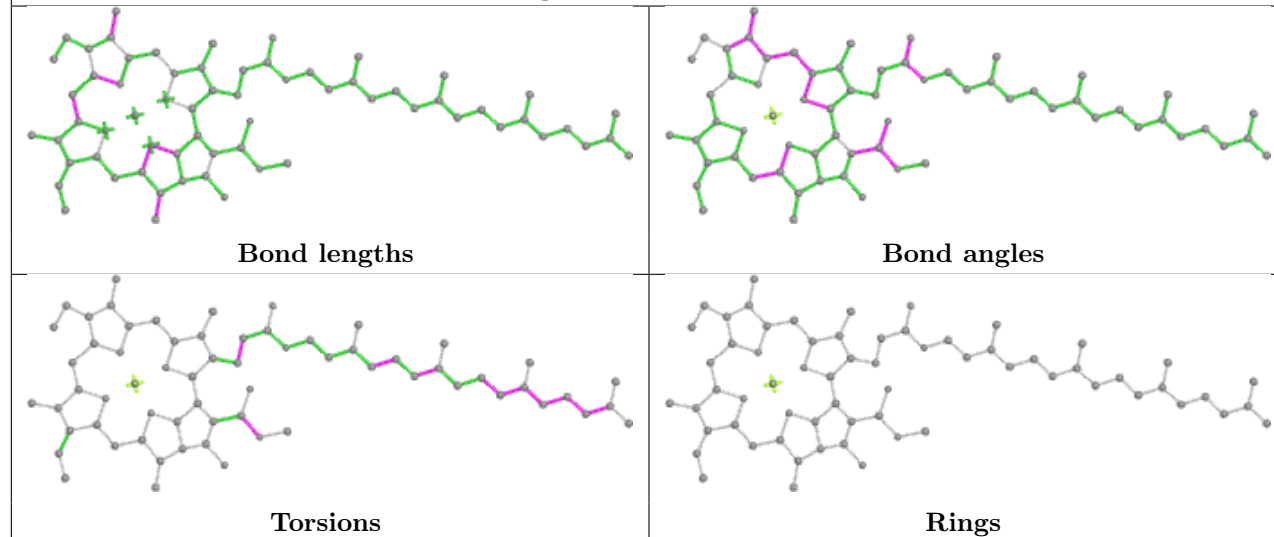


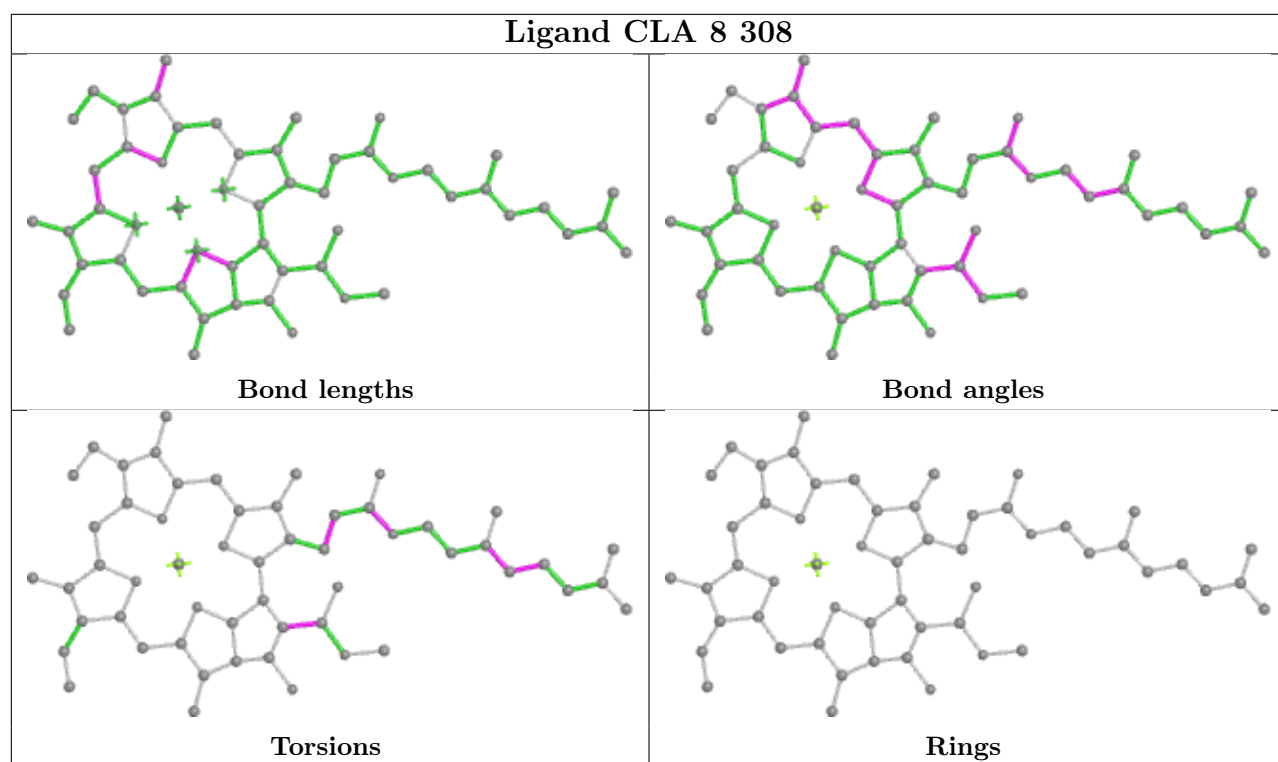
Ligand CLA a 803



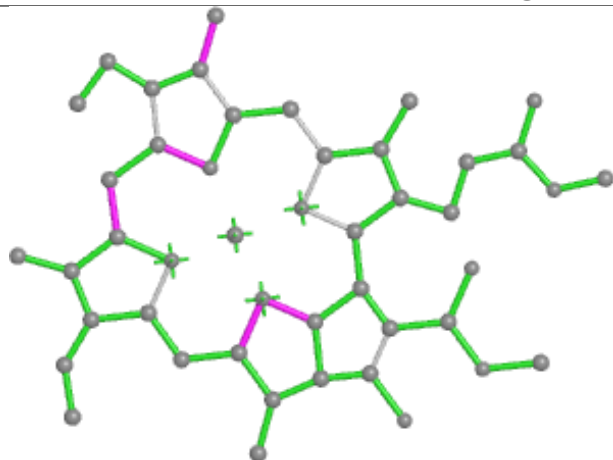
Ligand CLA a 816



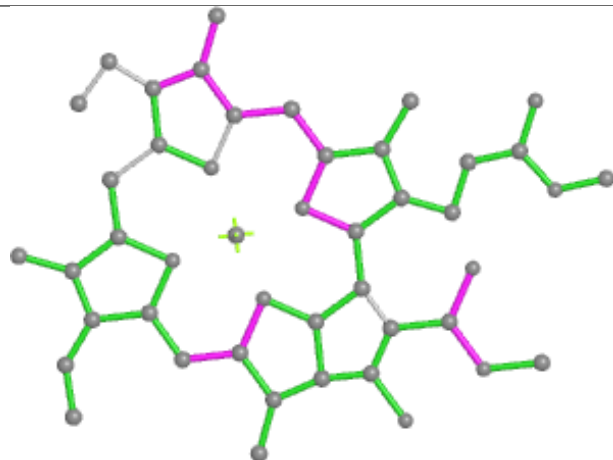
Ligand CLA 8 307**Ligand CLA 4 308**



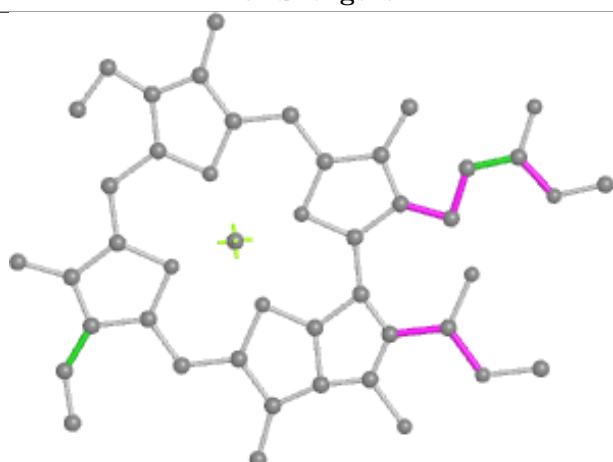
Ligand CLA 4 316



Bond lengths



Bond angles

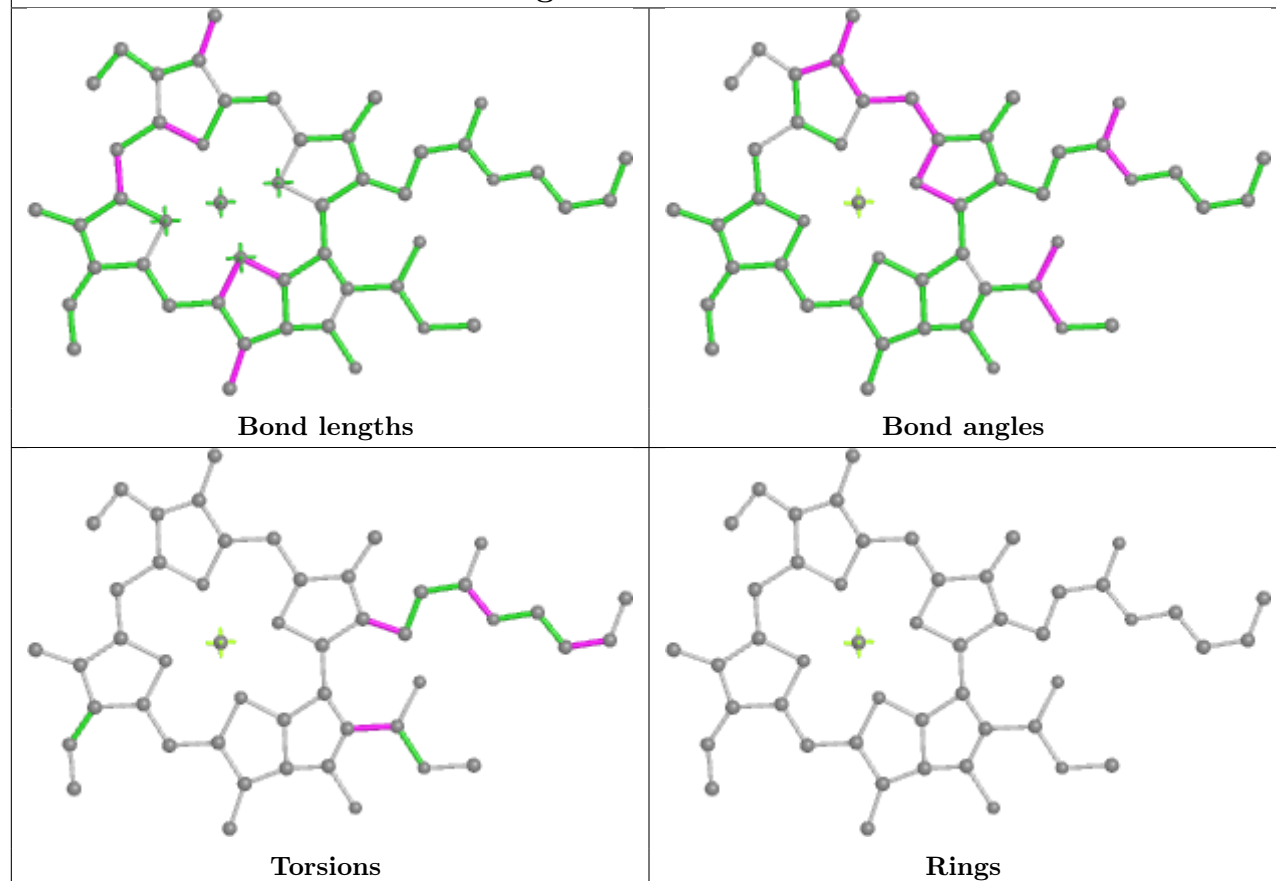


Torsions

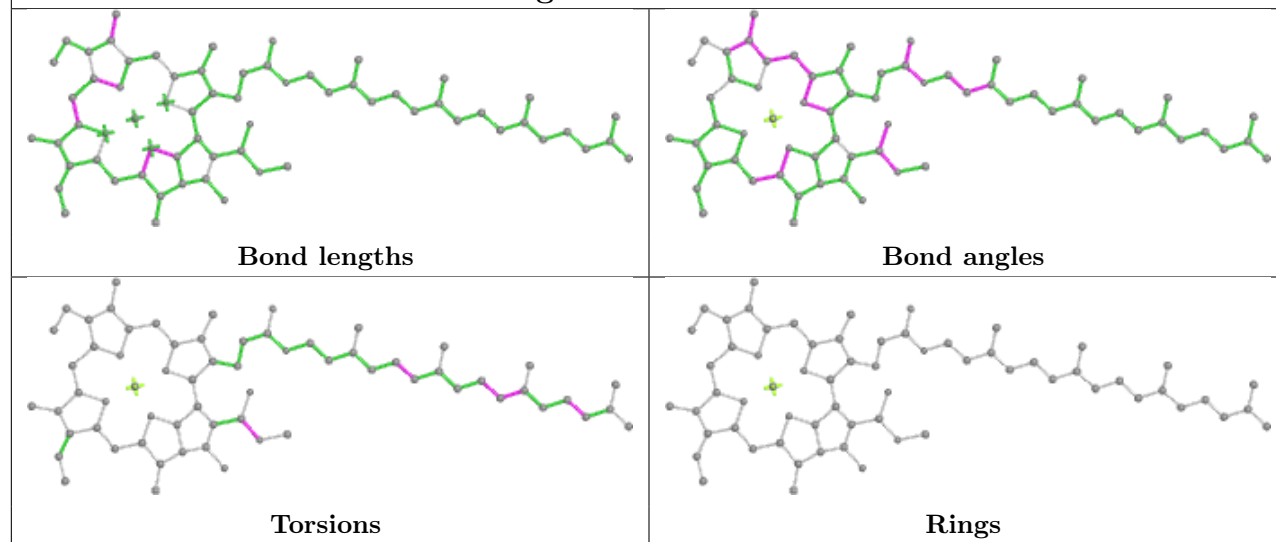


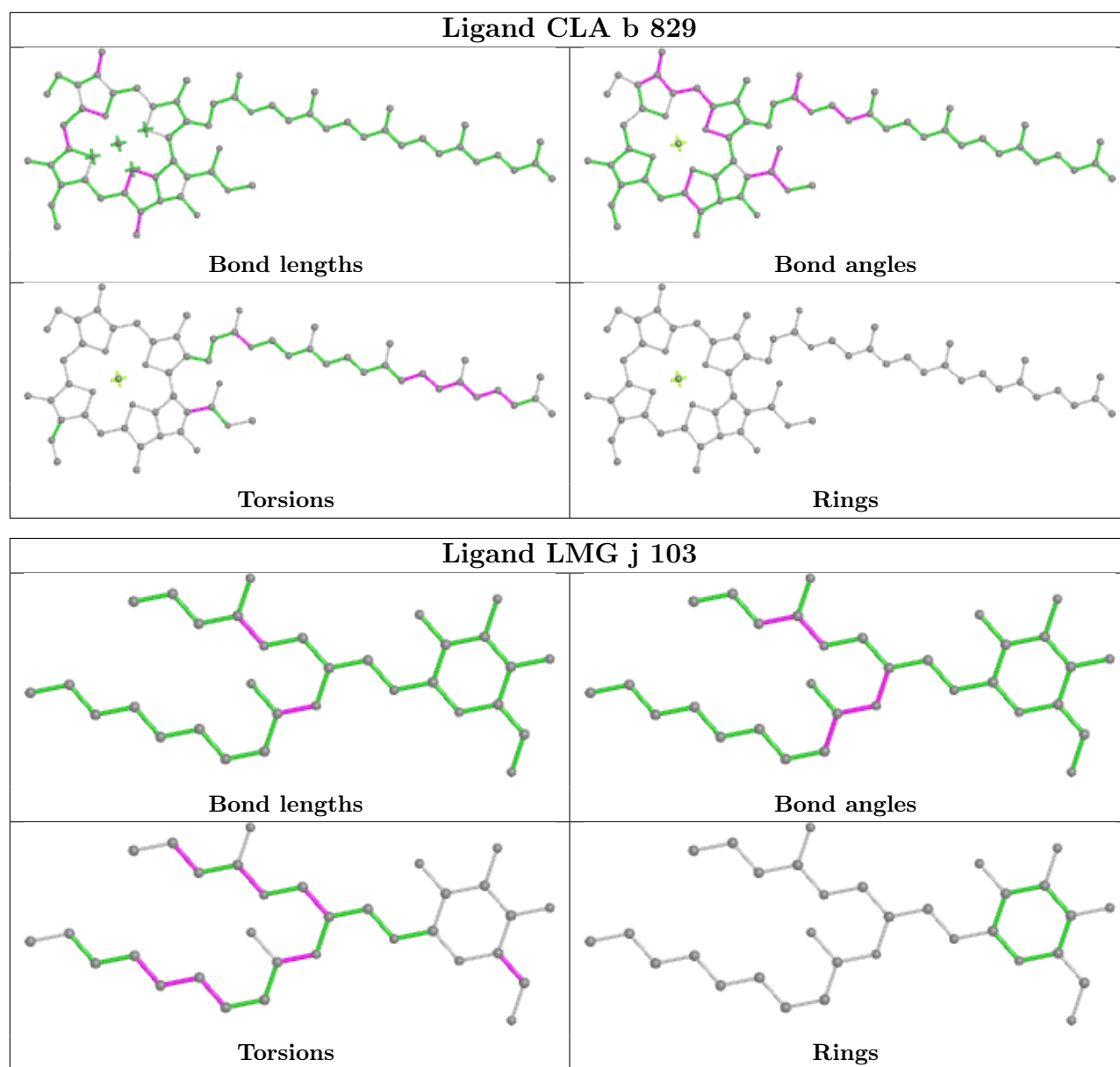
Rings

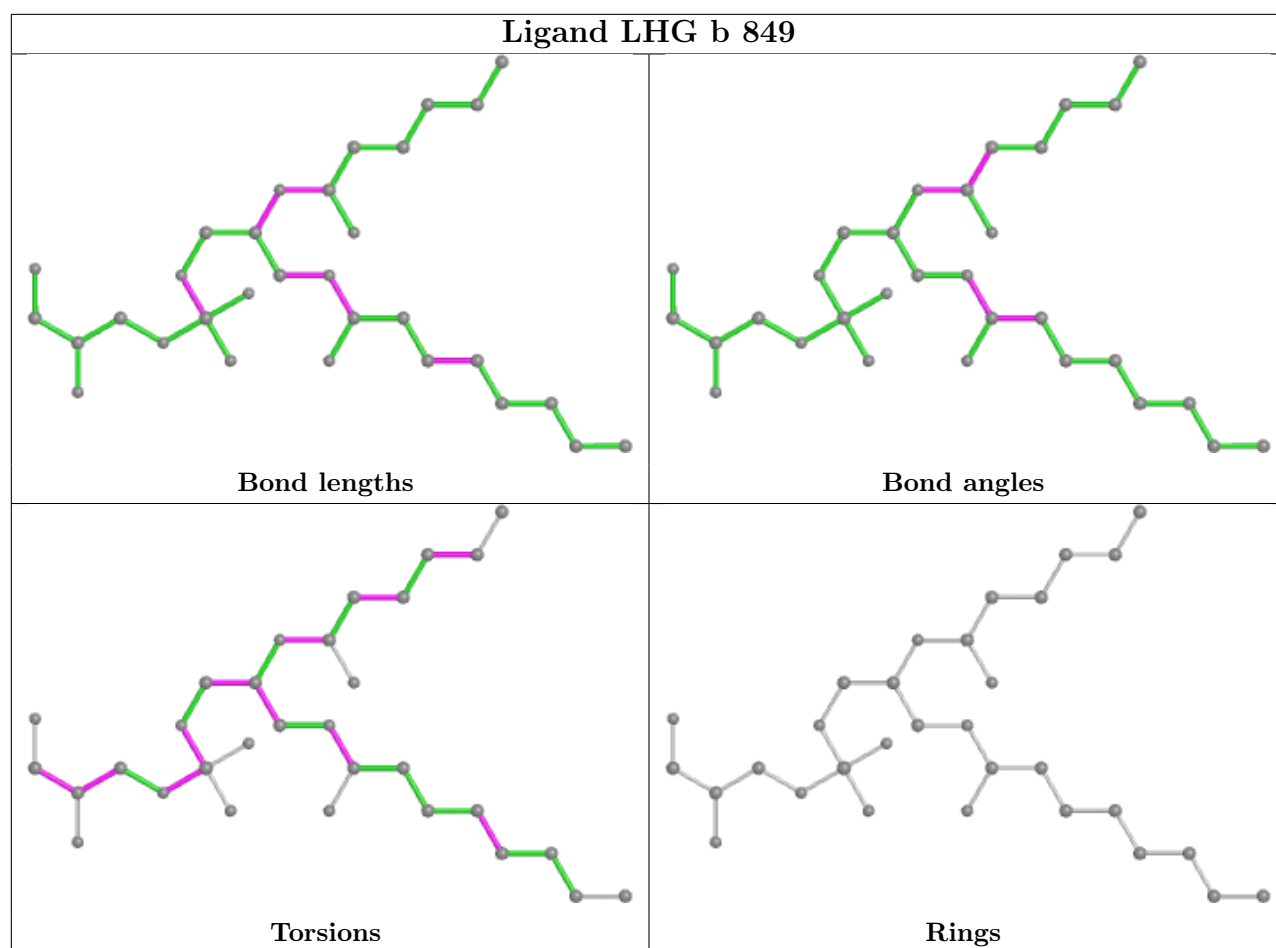
Ligand CLA a 823



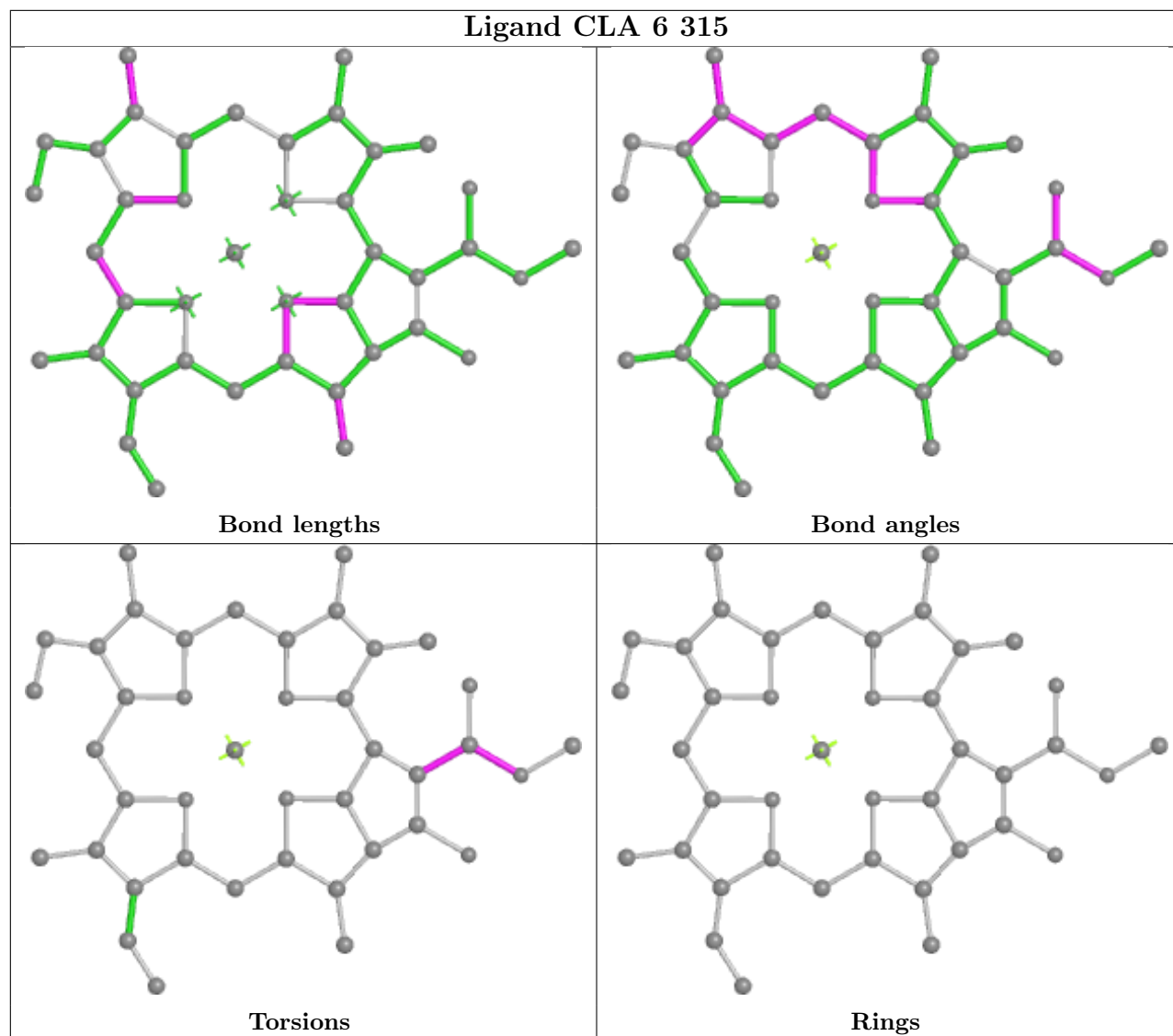
Ligand CLA a 834



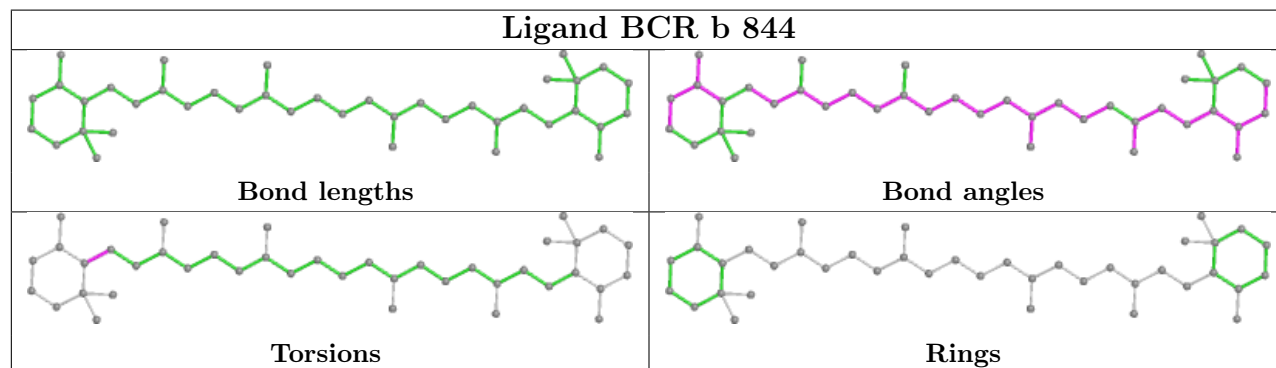


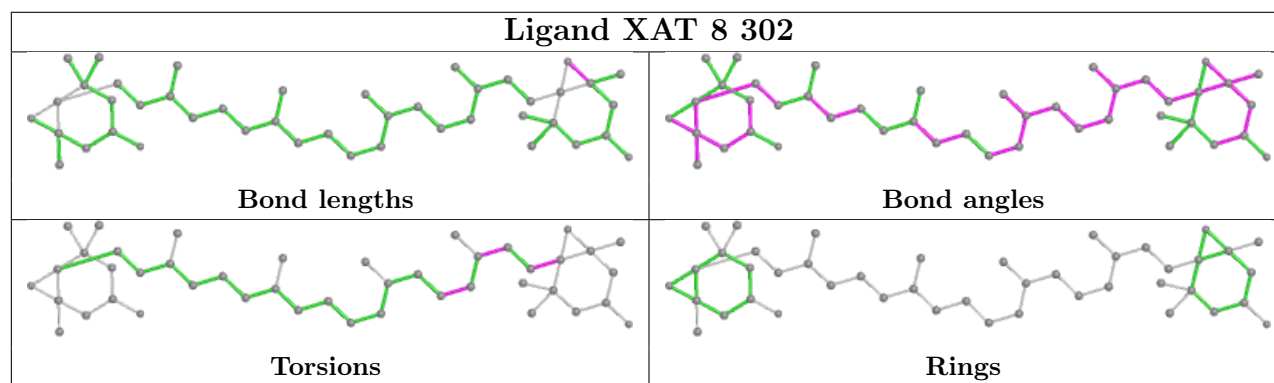
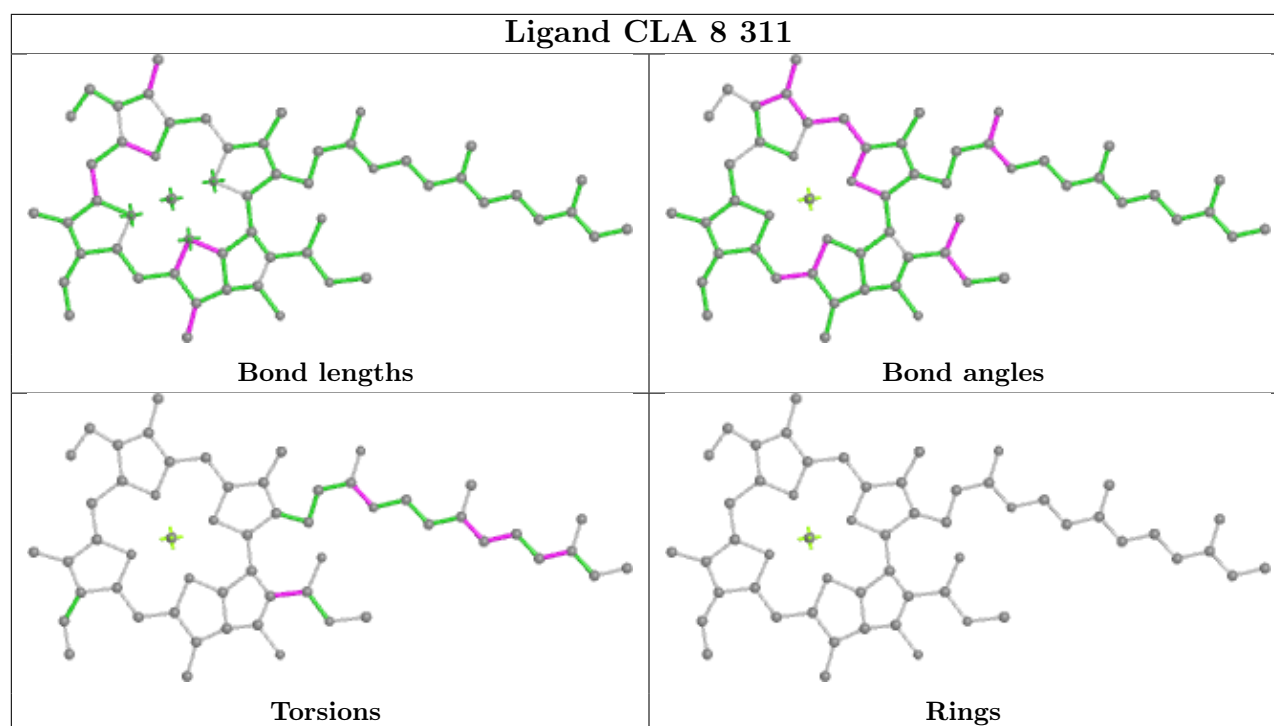


Ligand CLA 6 315

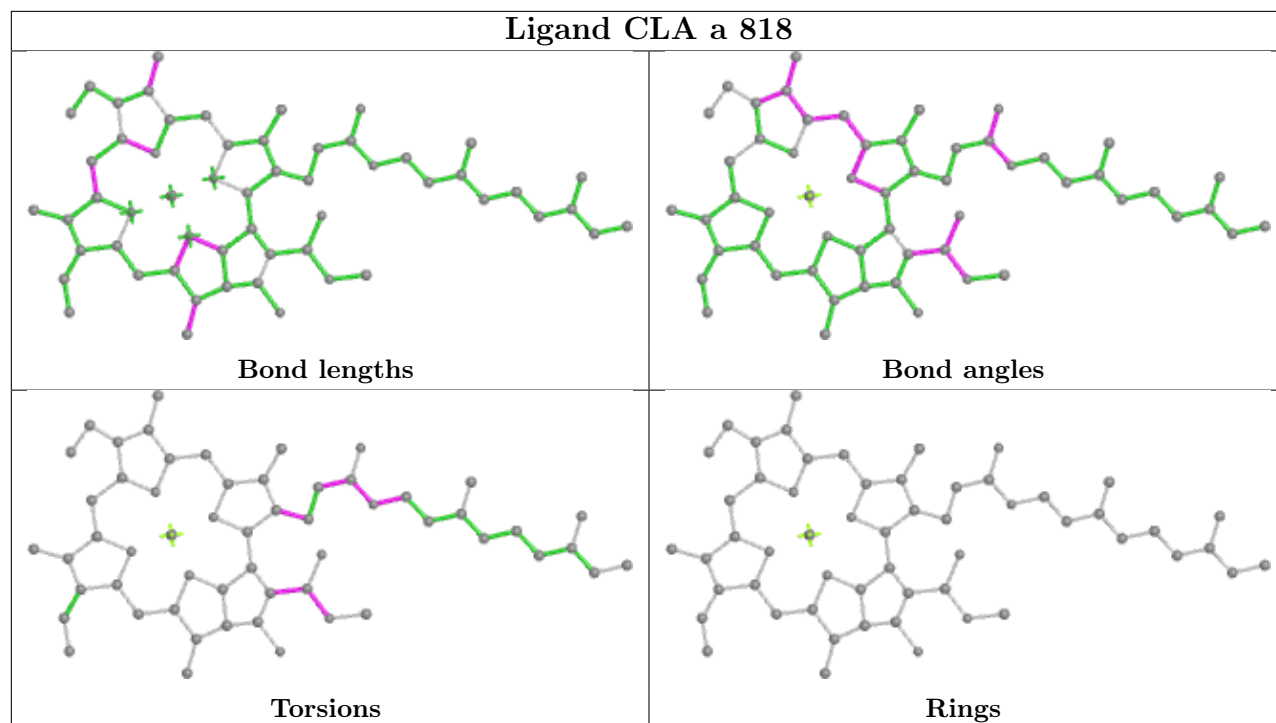


Ligand BCR b 844

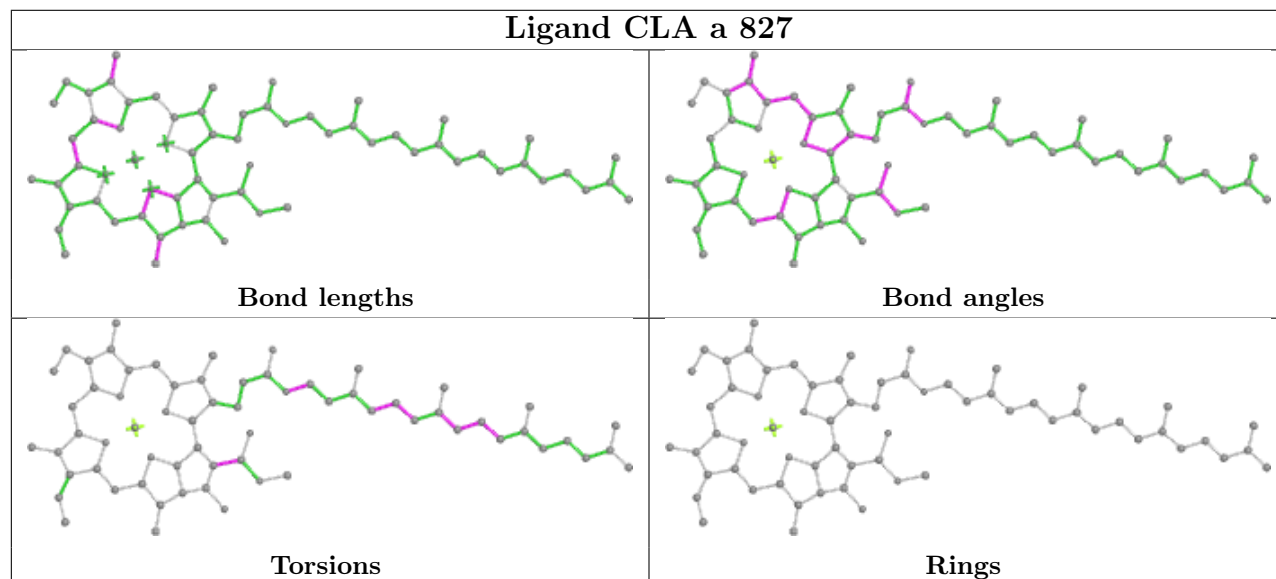


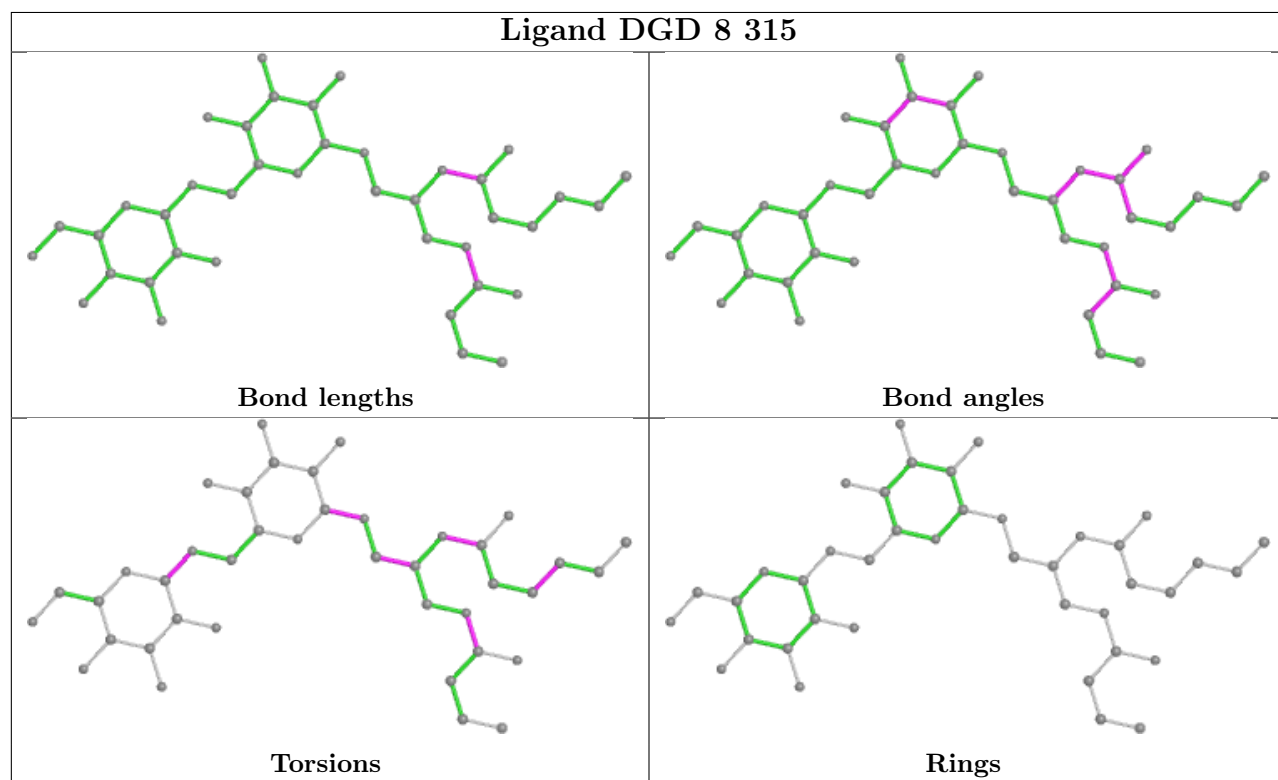
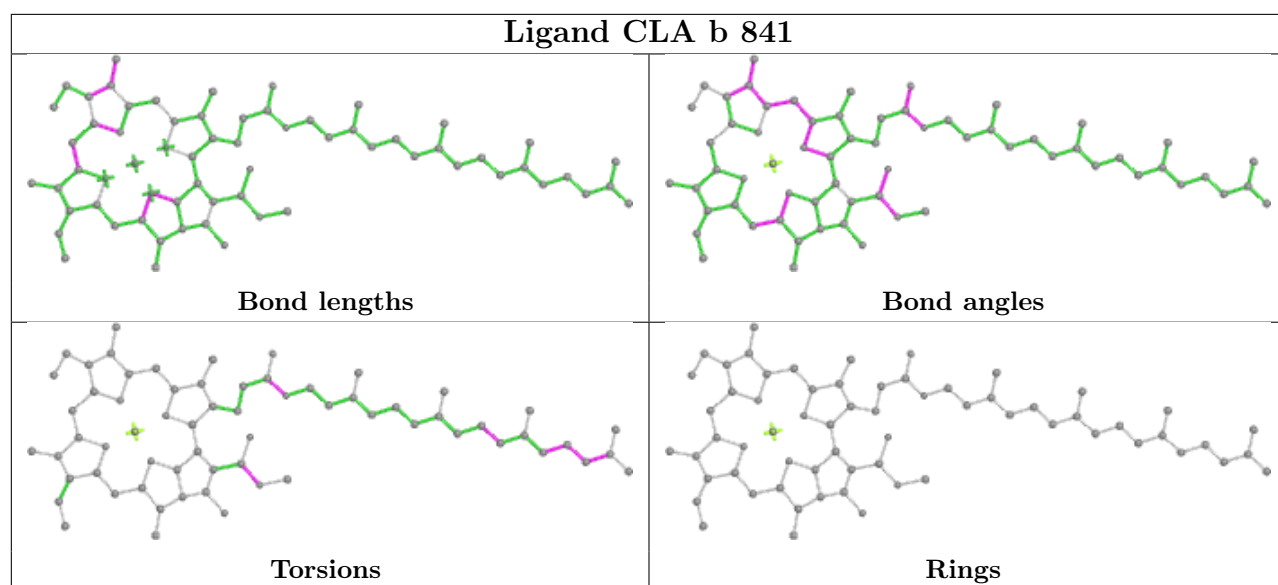


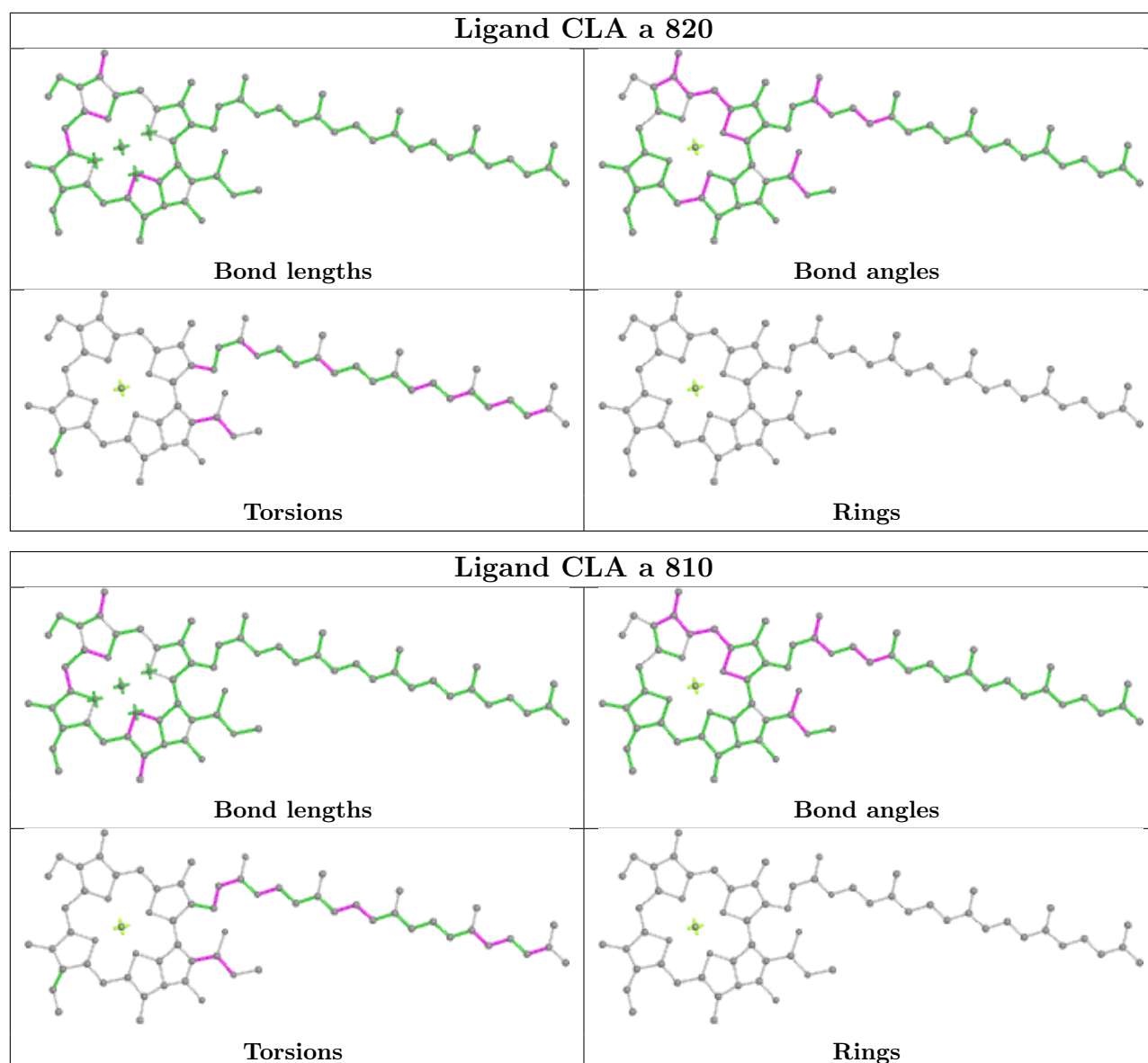
Ligand CLA a 818



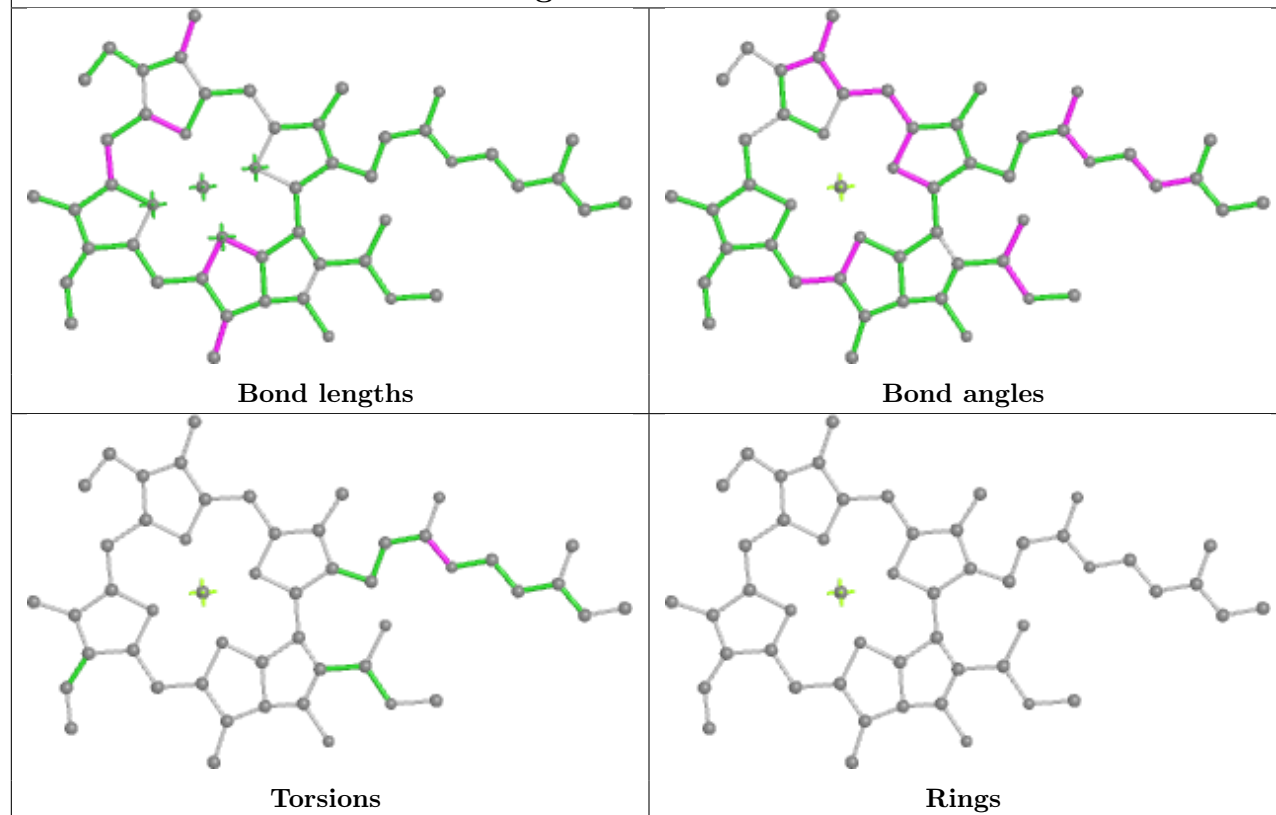
Ligand CLA a 827



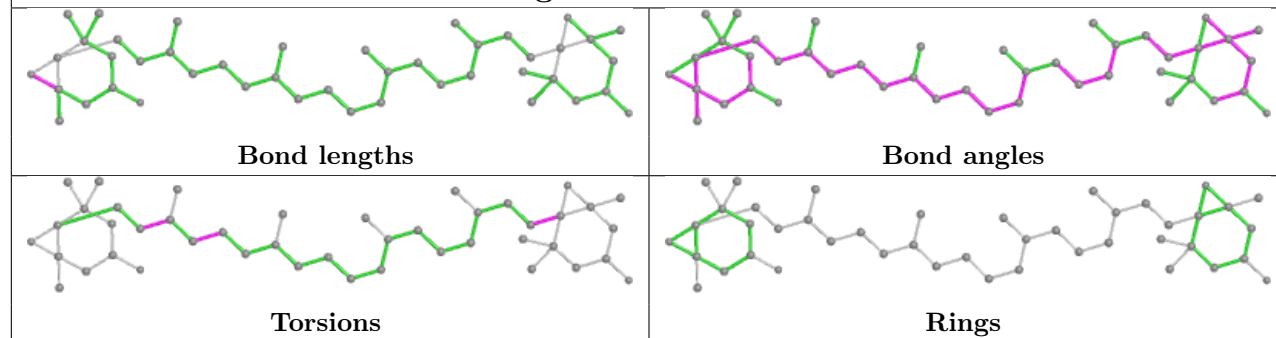


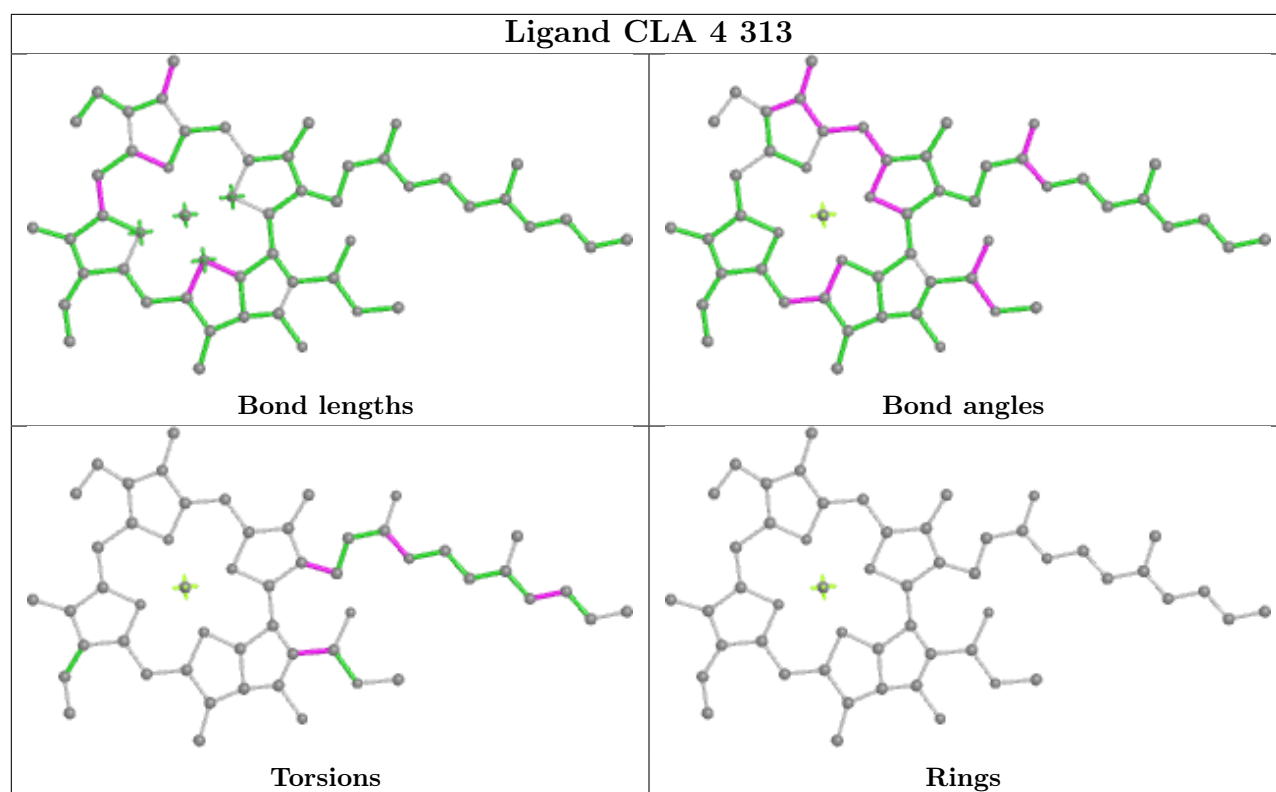


Ligand CLA b 821

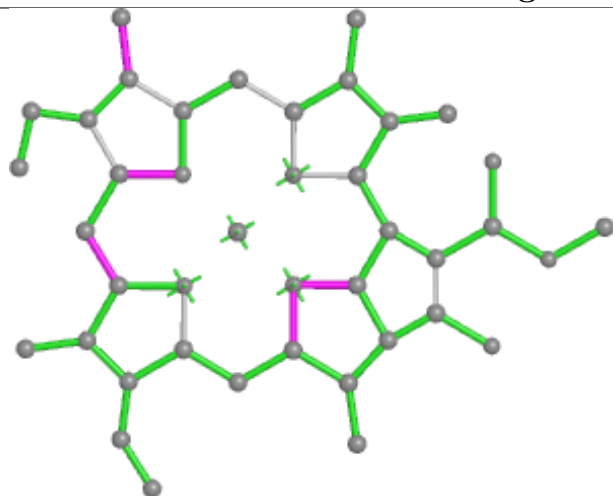


Ligand XAT 6 306

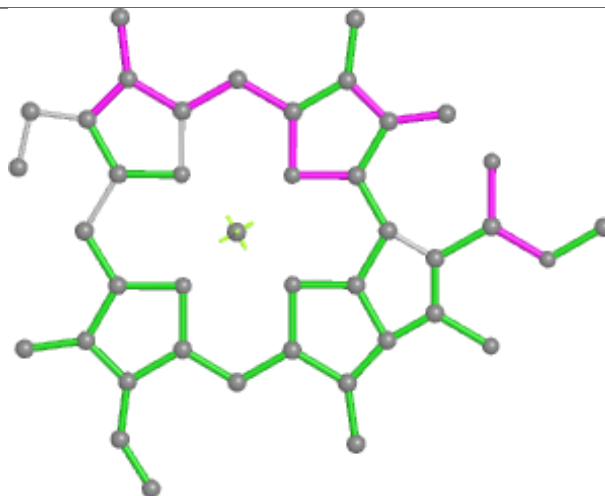




Ligand CLA 8 314



Bond lengths



Bond angles

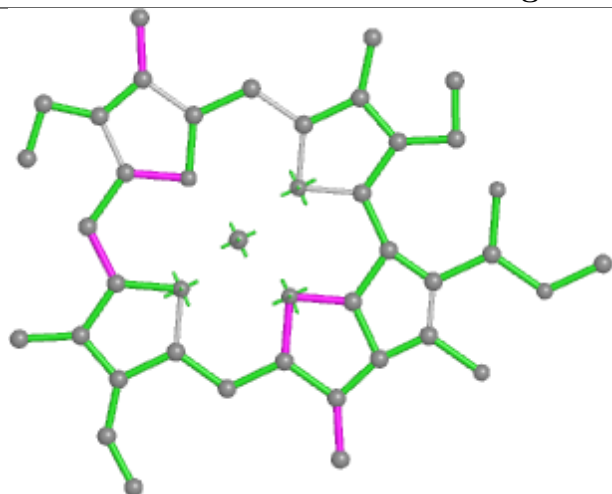


Torsions

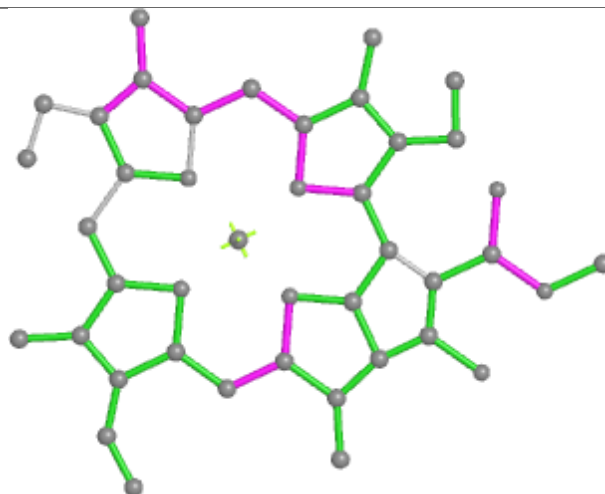


Rings

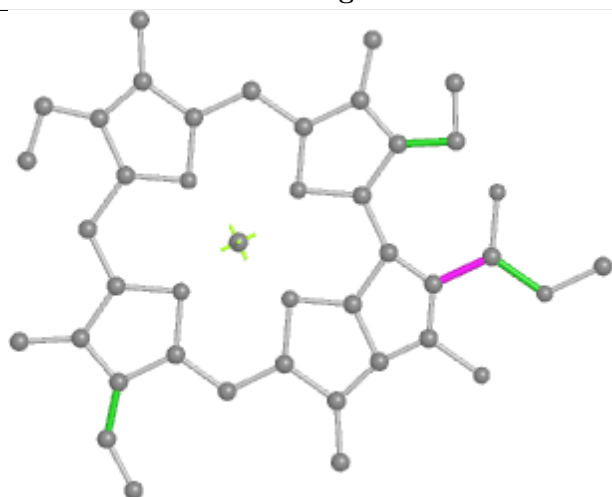
Ligand CLA 1 201



Bond lengths



Bond angles

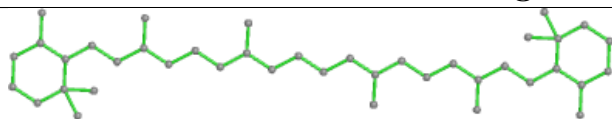


Torsions

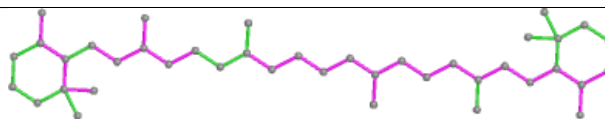


Rings

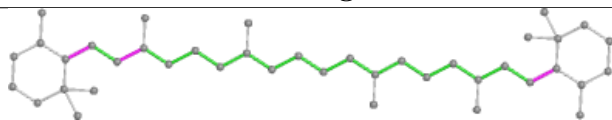
Ligand BCR b 852



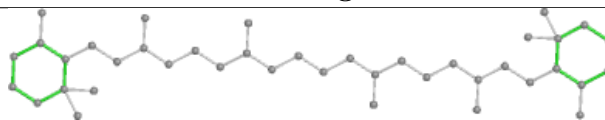
Bond lengths



Bond angles

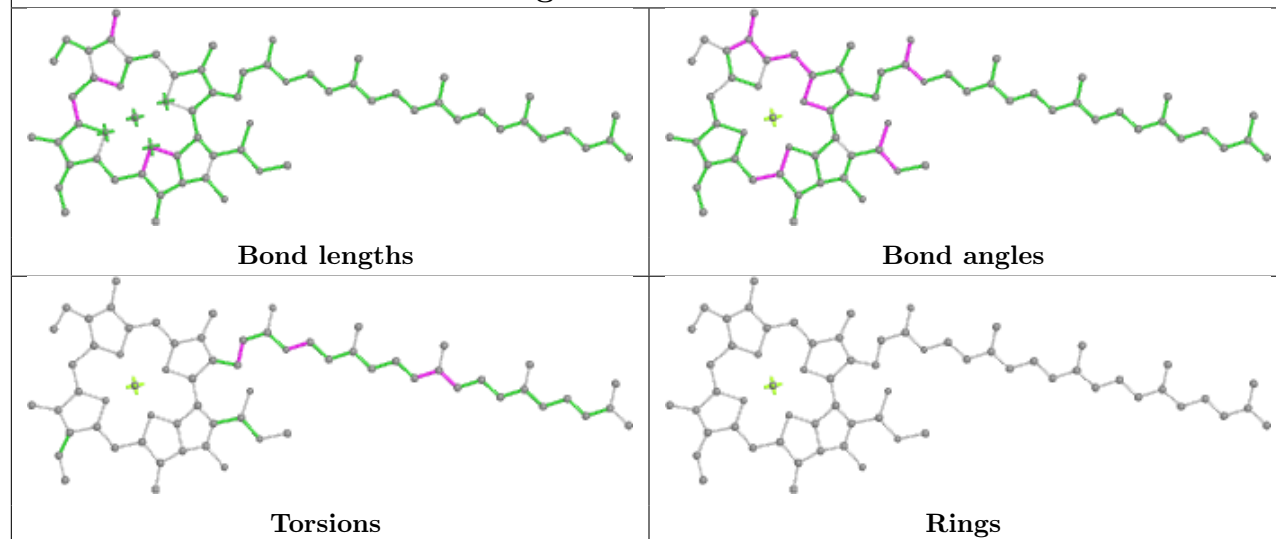


Torsions

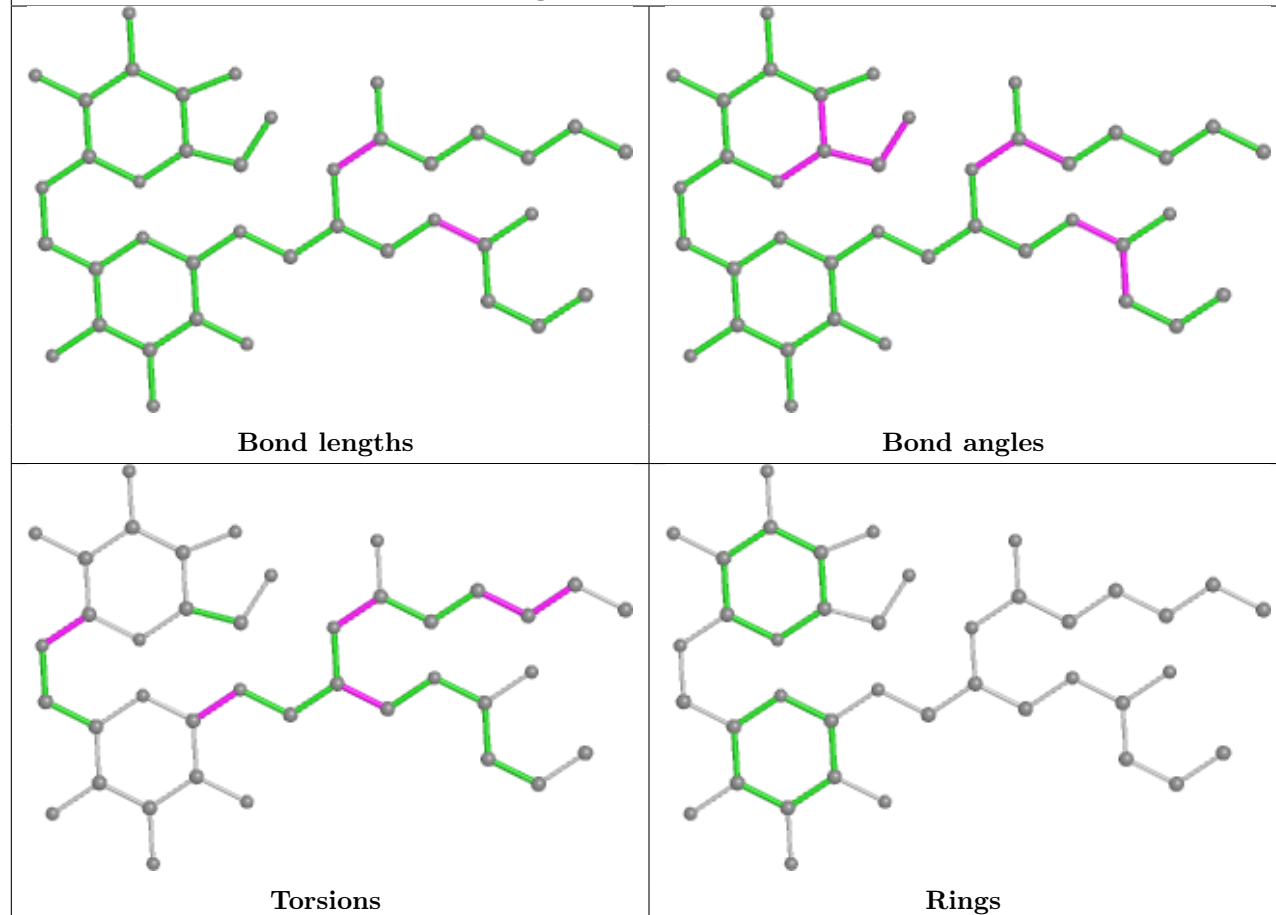


Rings

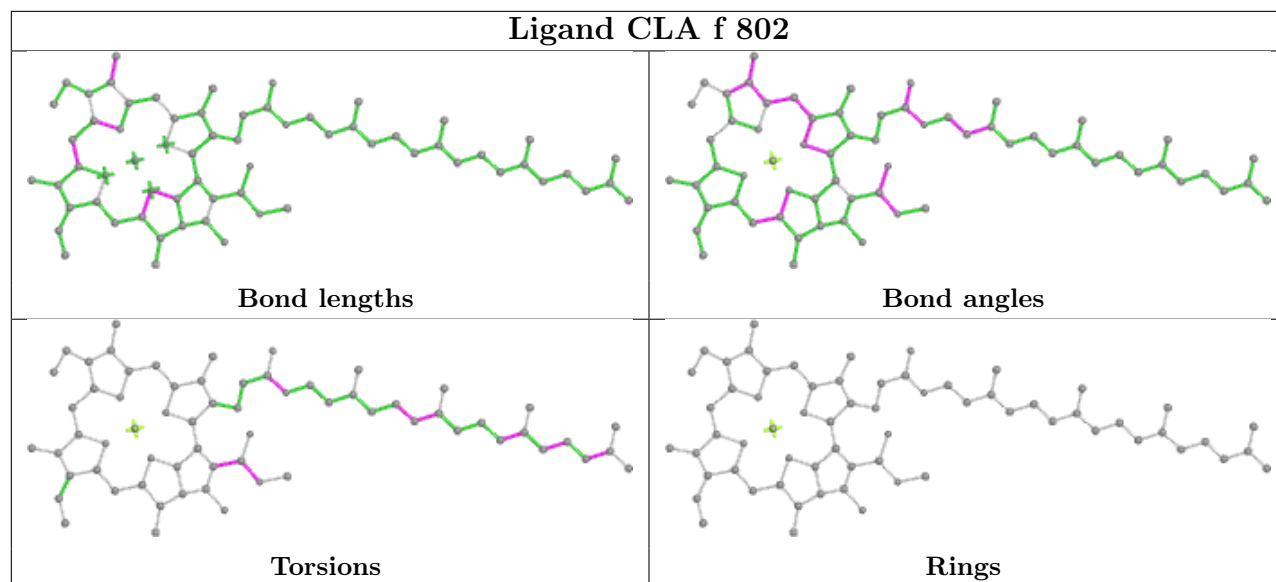
Ligand CLA a 822



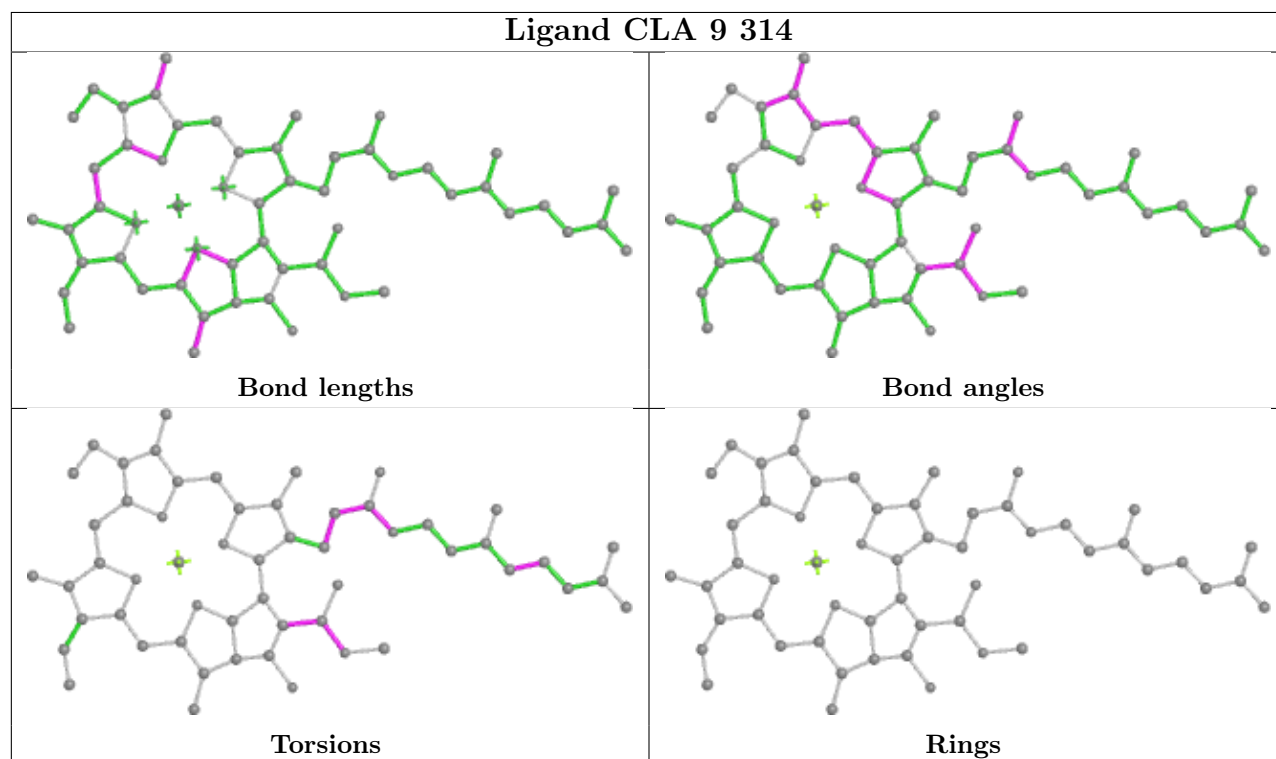
Ligand DGD 4 318



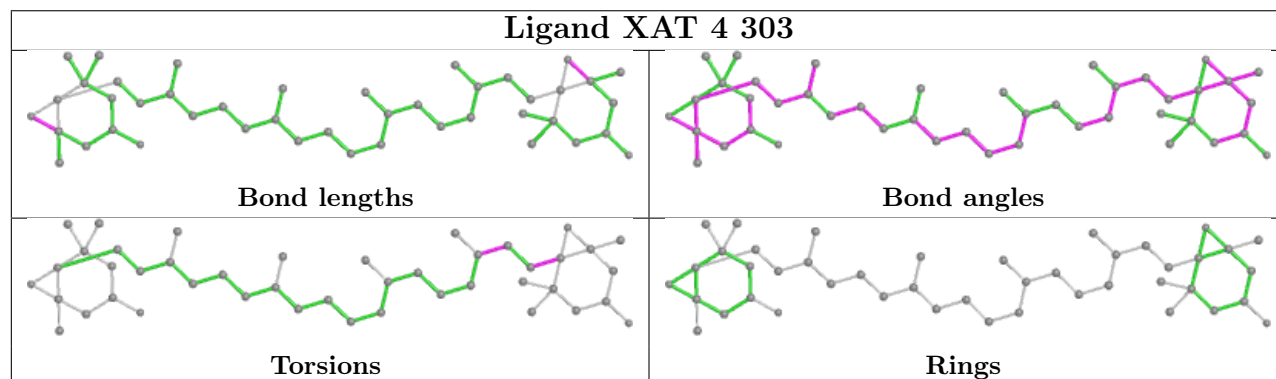
Ligand CLA f 802

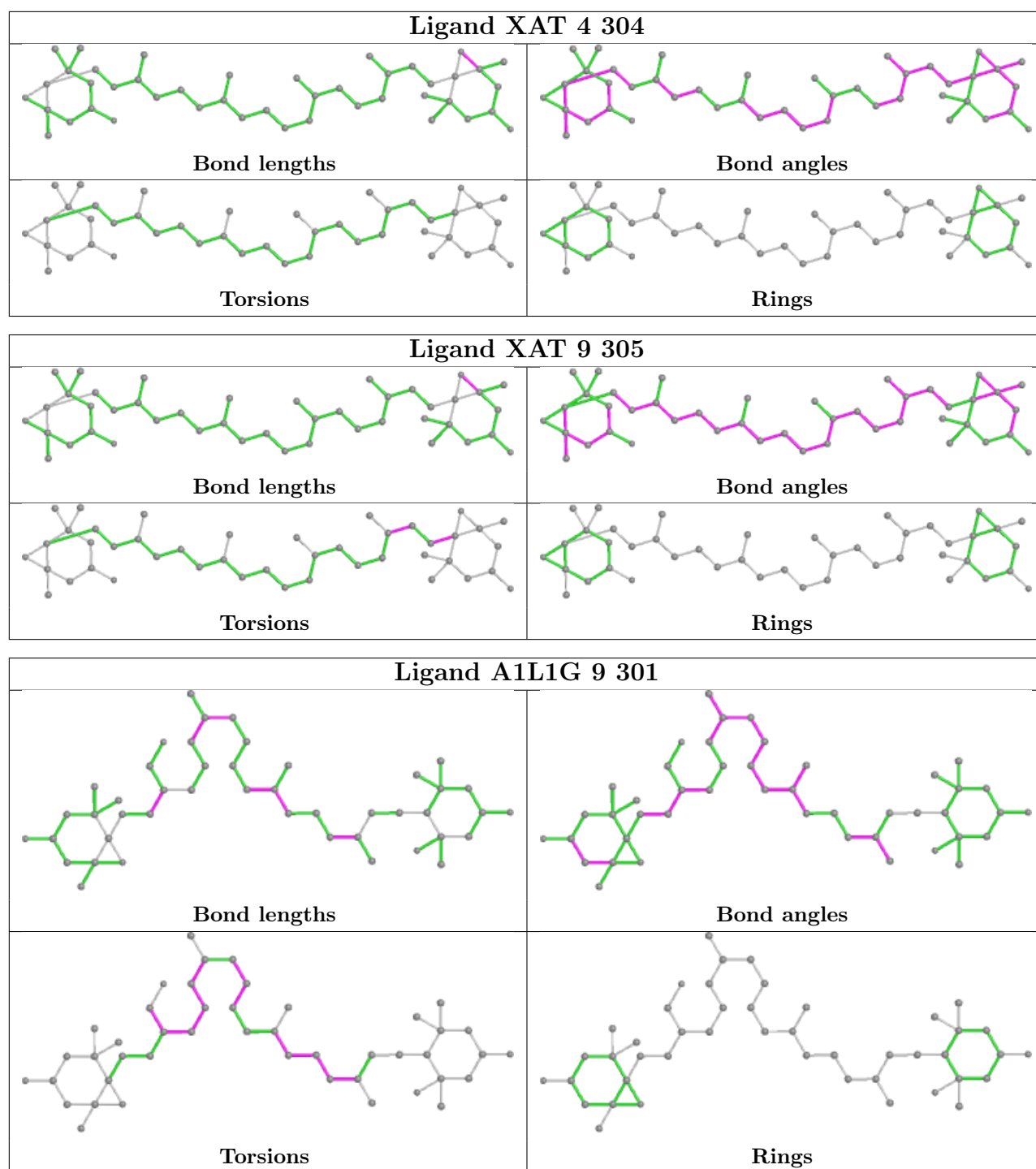


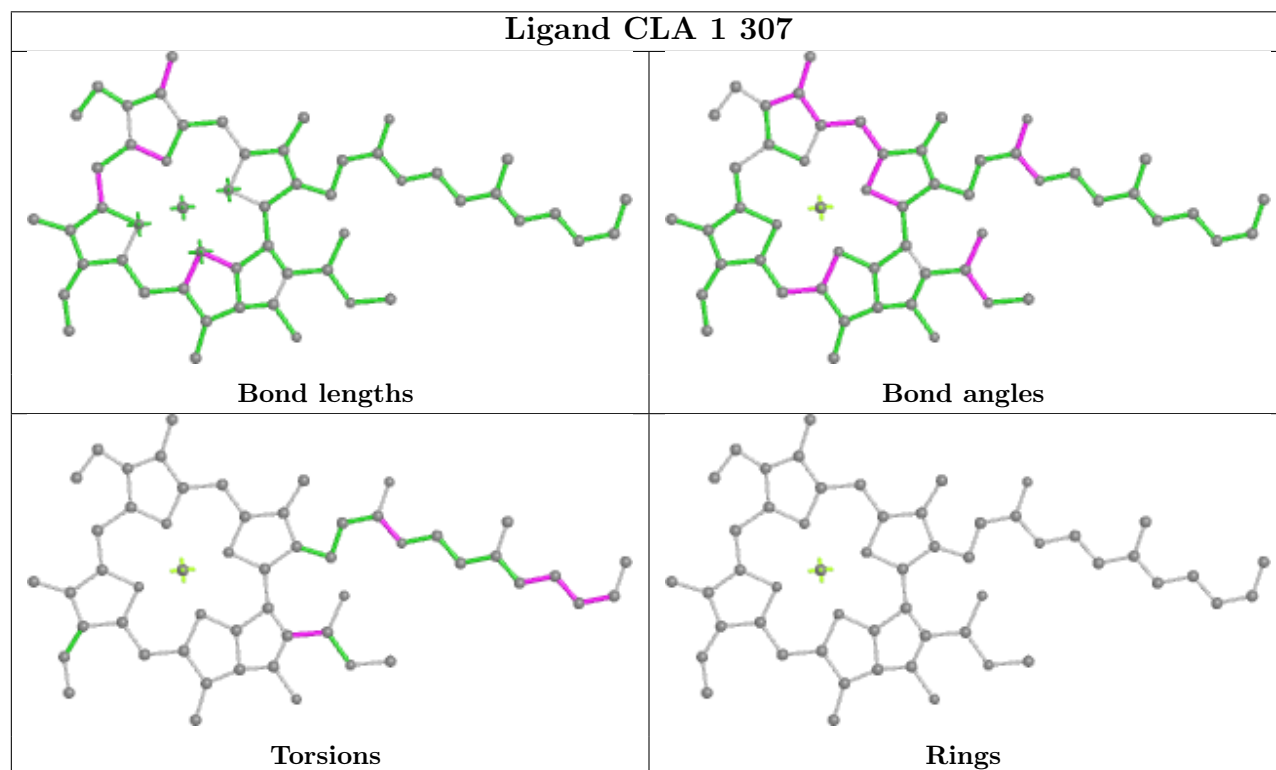
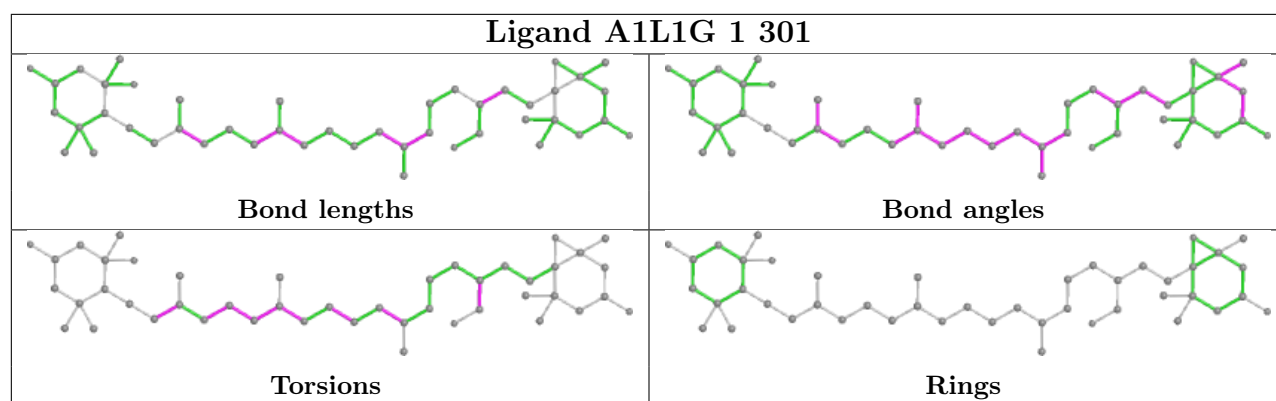
Ligand CLA 9 314



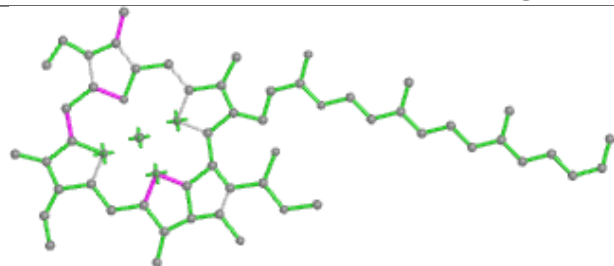
Ligand XAT 4 303



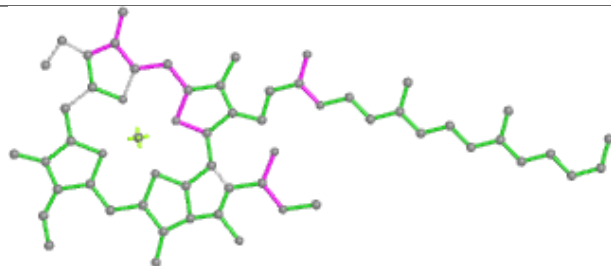




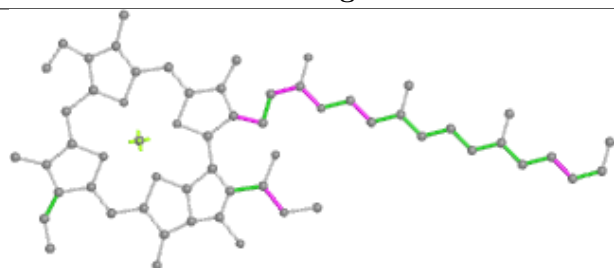
Ligand CLA b 817



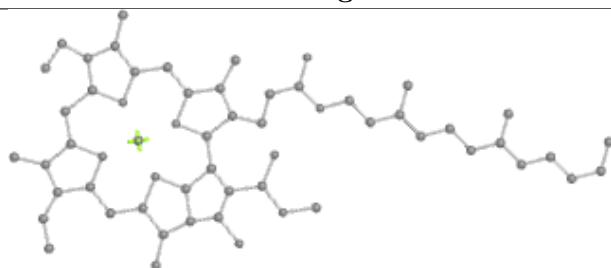
Bond lengths



Bond angles

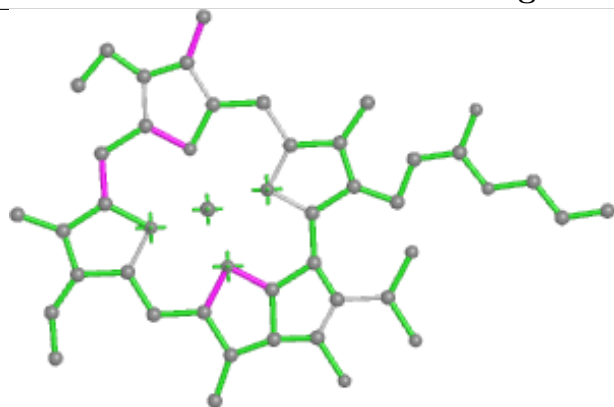


Torsions

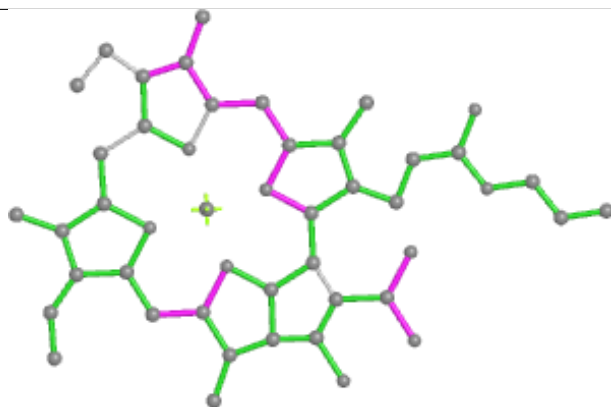


Rings

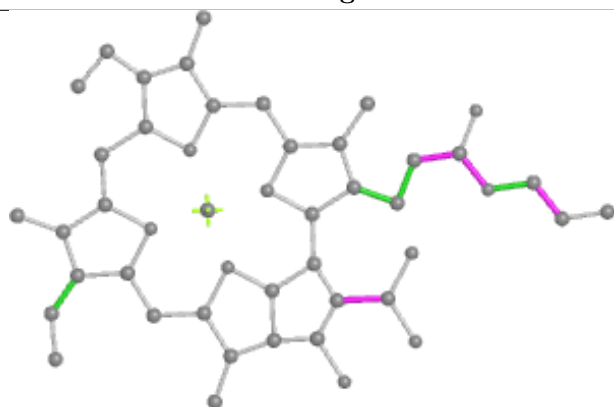
Ligand CLA 7 309



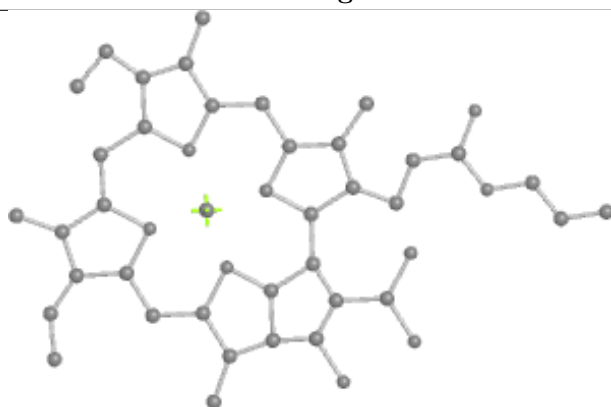
Bond lengths



Bond angles

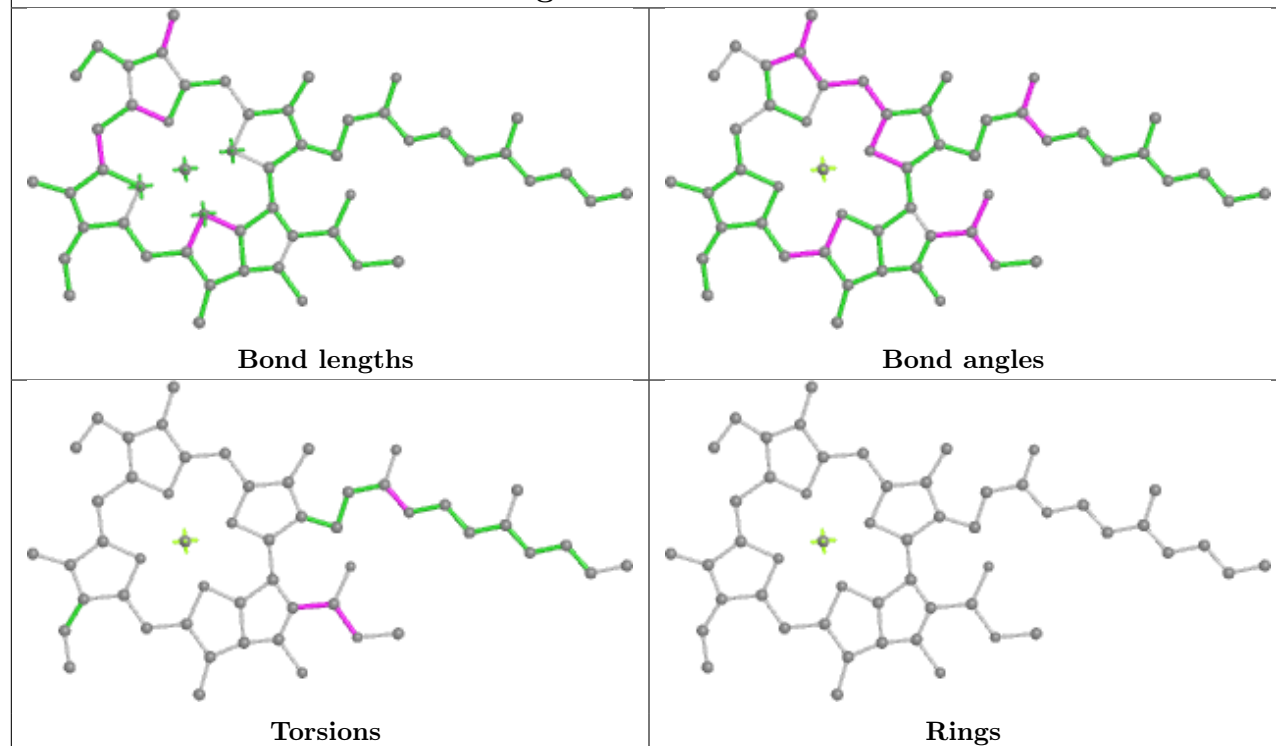


Torsions

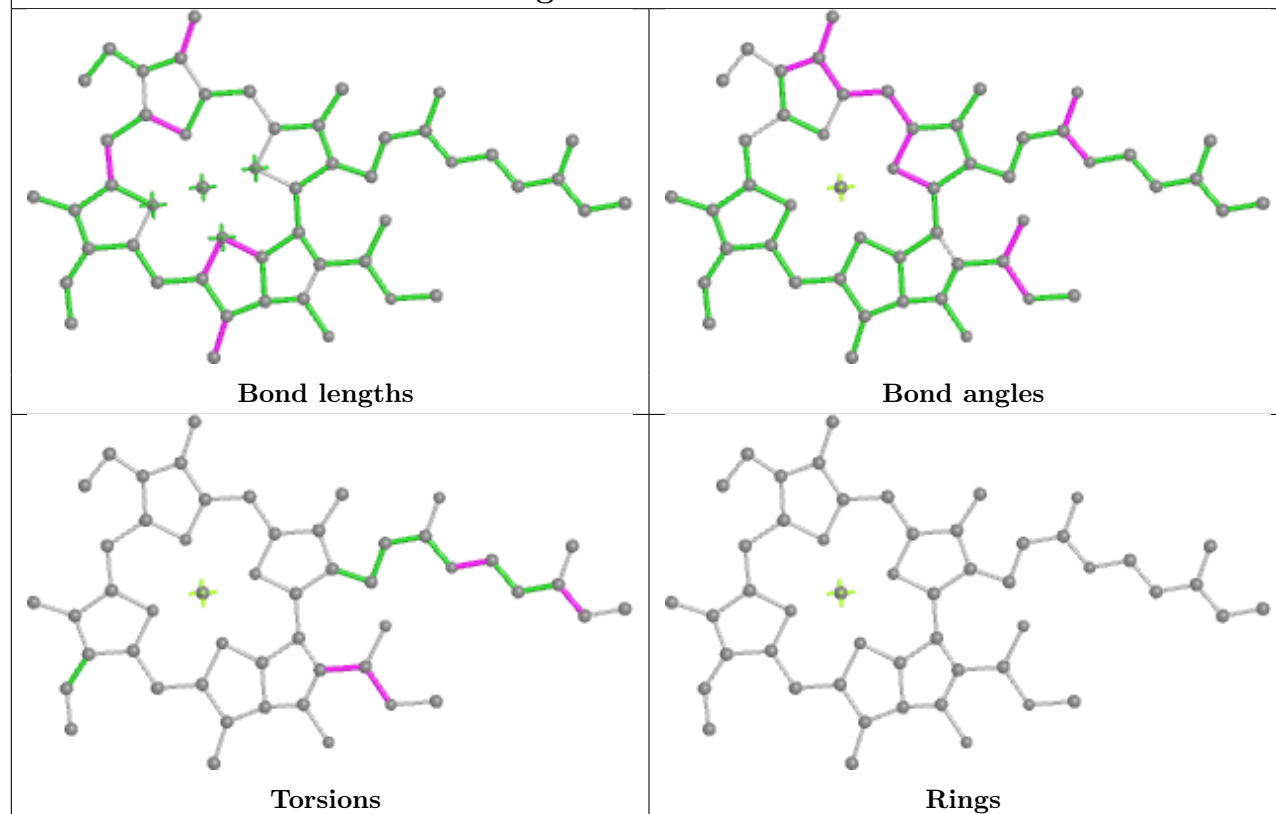


Rings

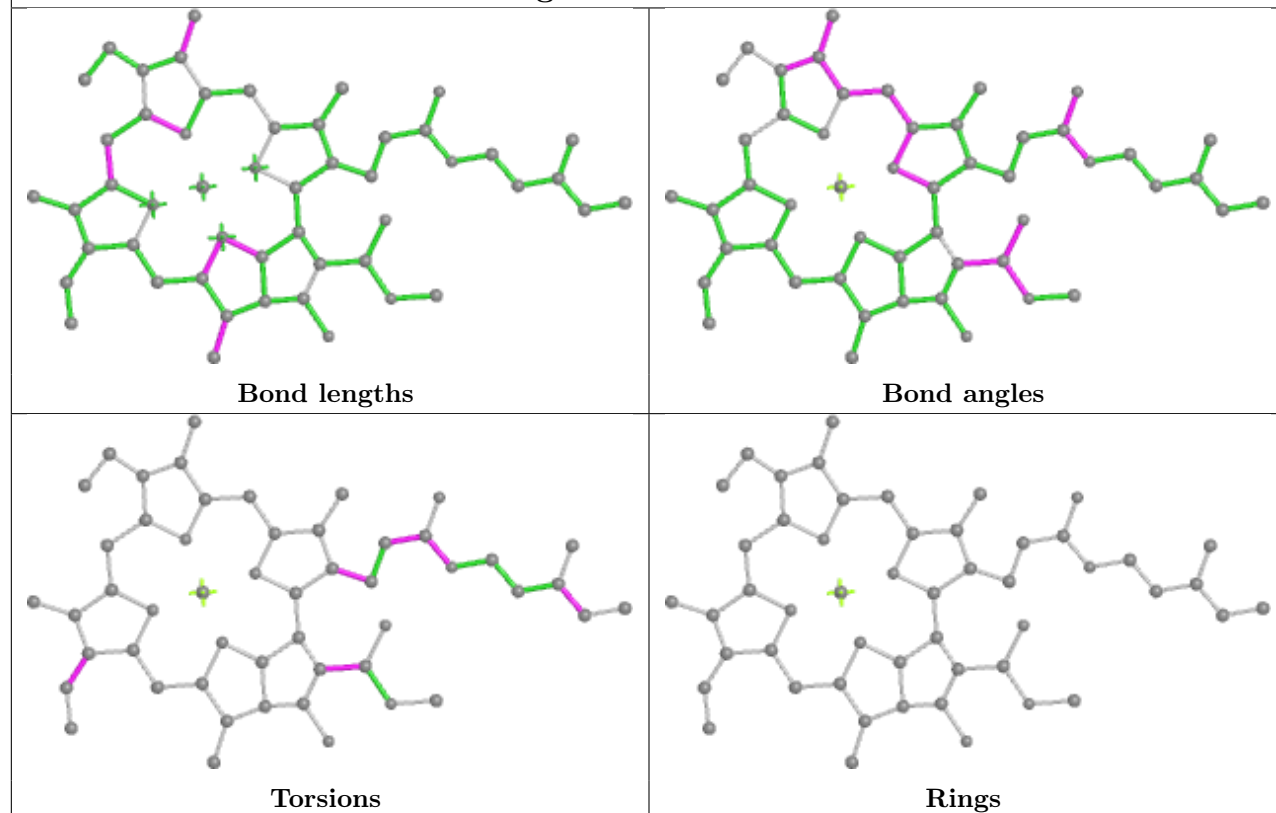
Ligand CLA 1 311



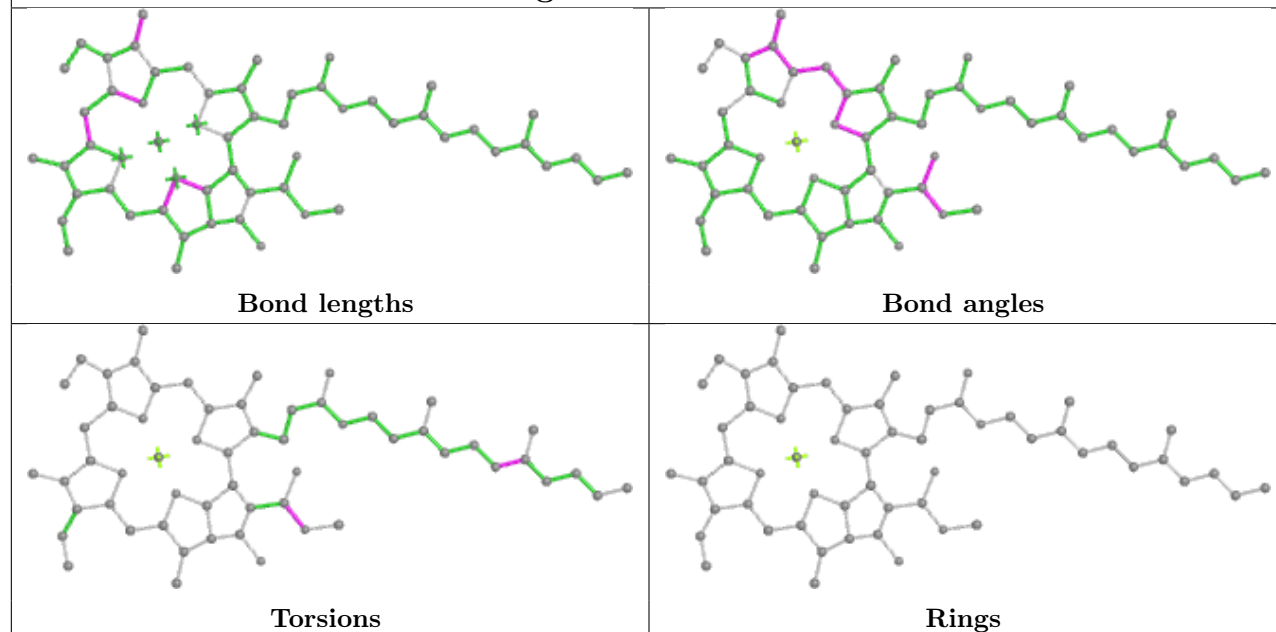
Ligand CLA 6 312



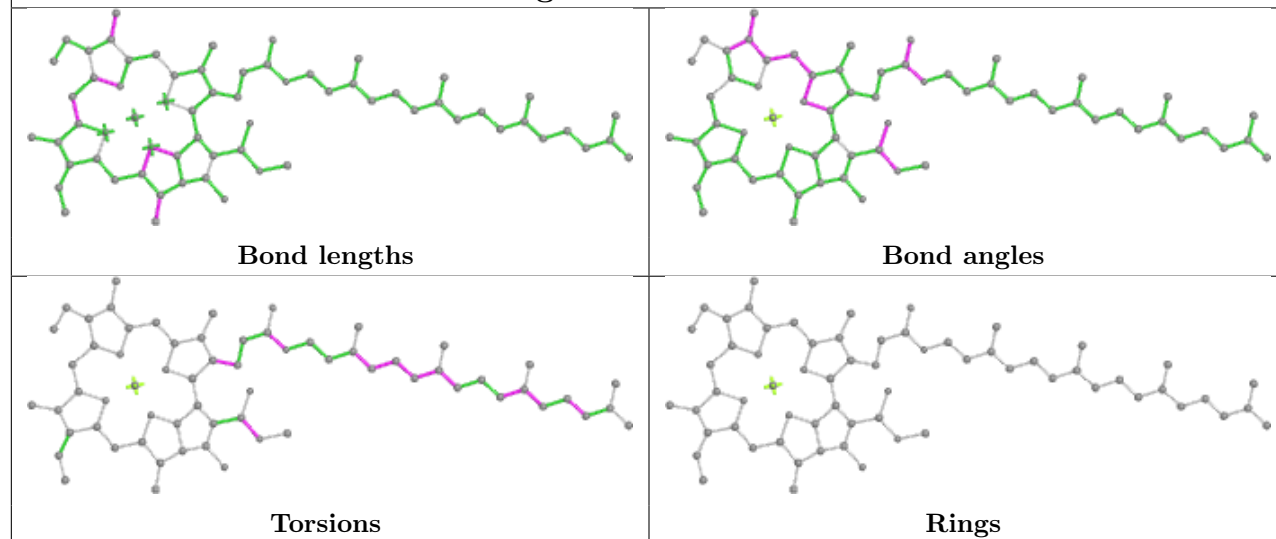
Ligand CLA 7 316



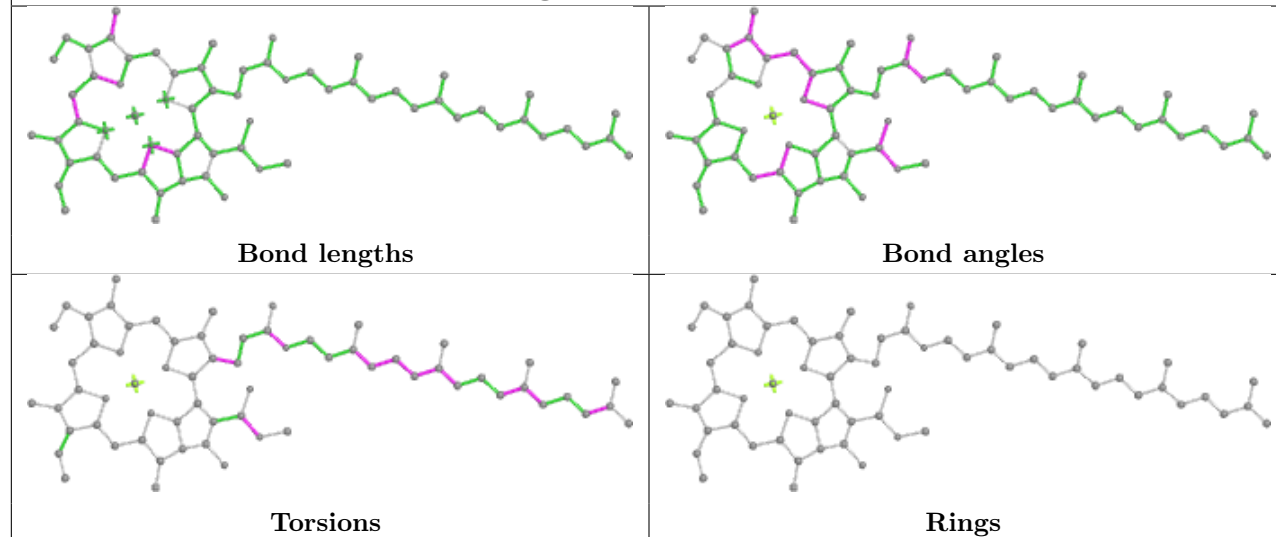
Ligand CLA 6 308



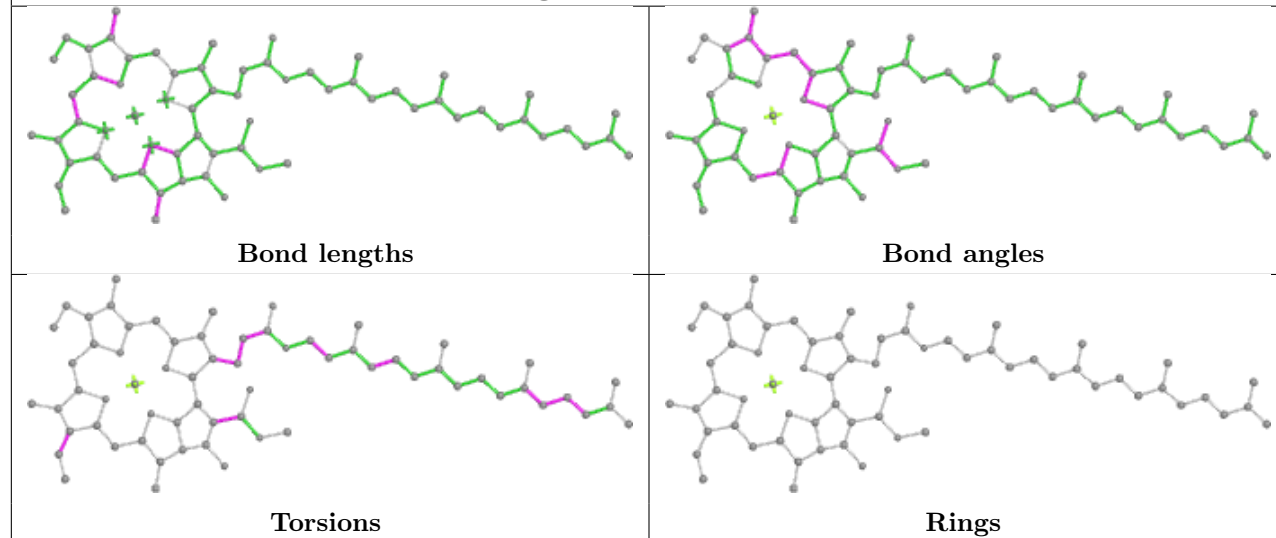
Ligand CLA a 807



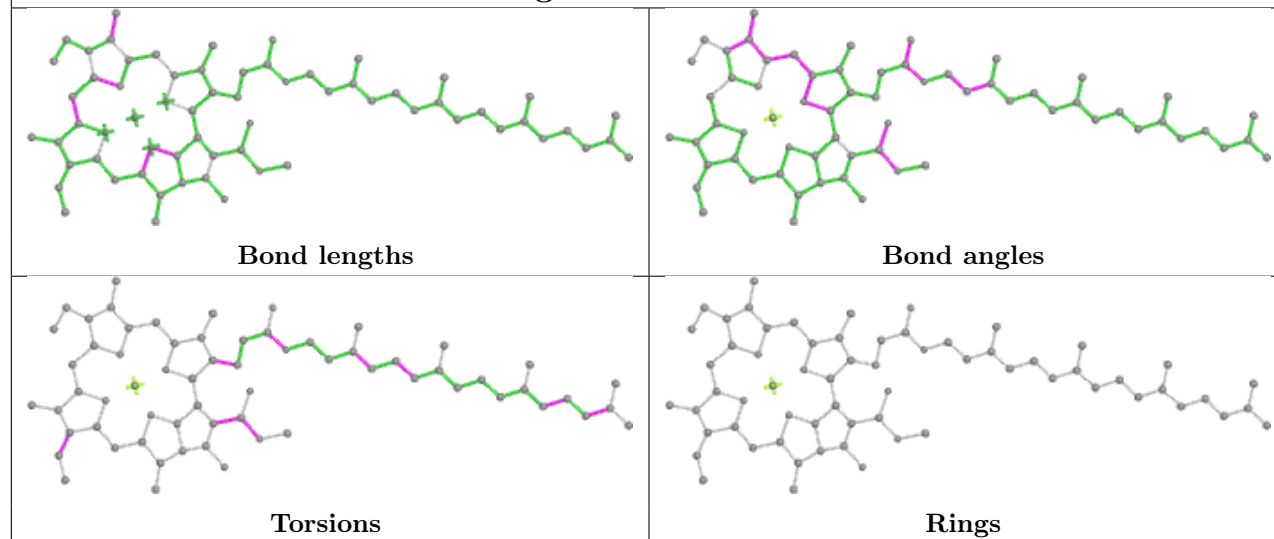
Ligand CLA 1 310



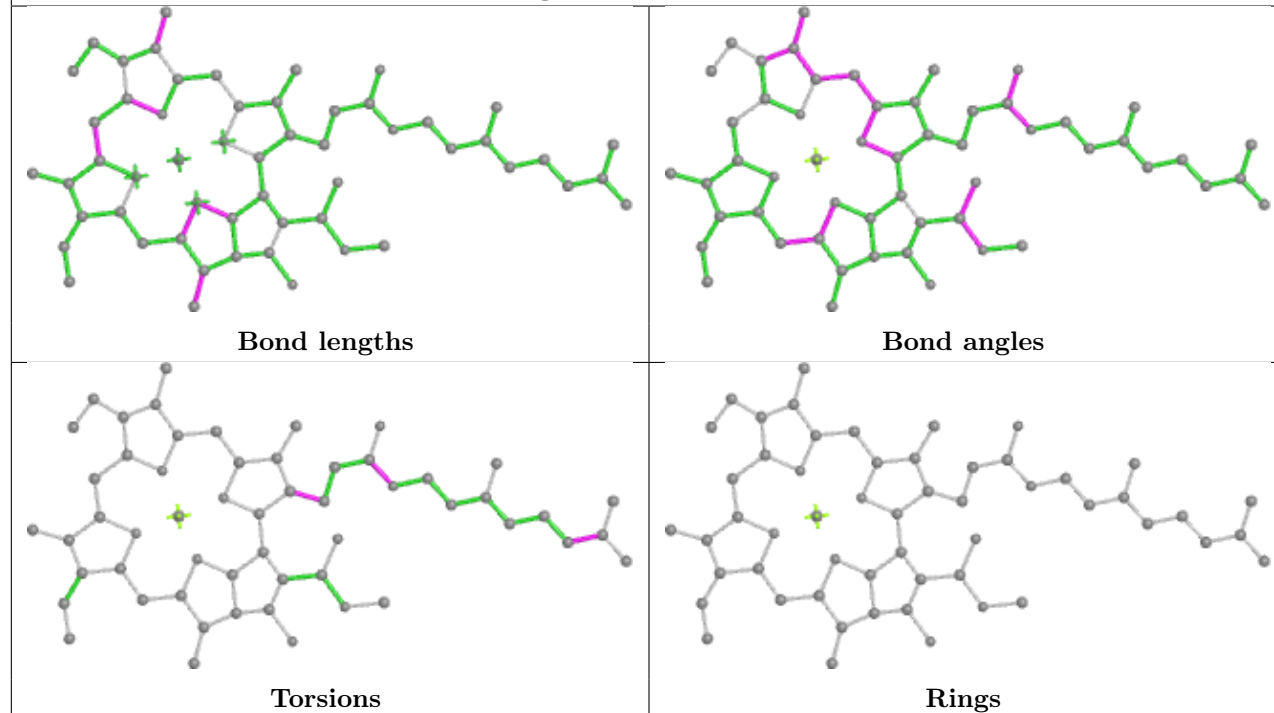
Ligand CLA b 832



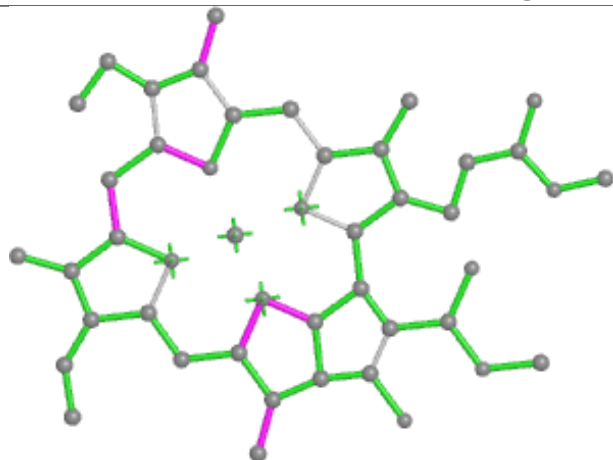
Ligand CLA b 840



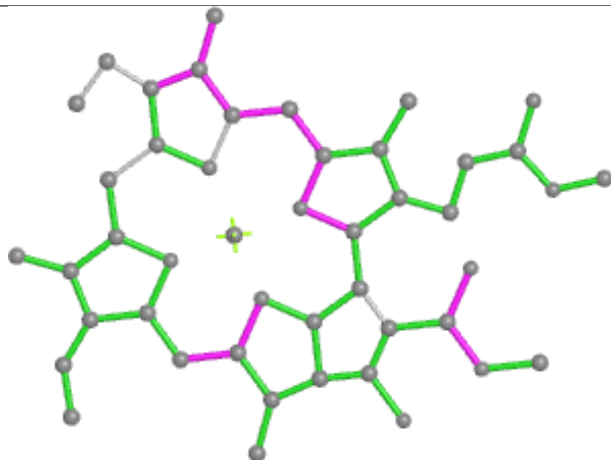
Ligand CLA a 805



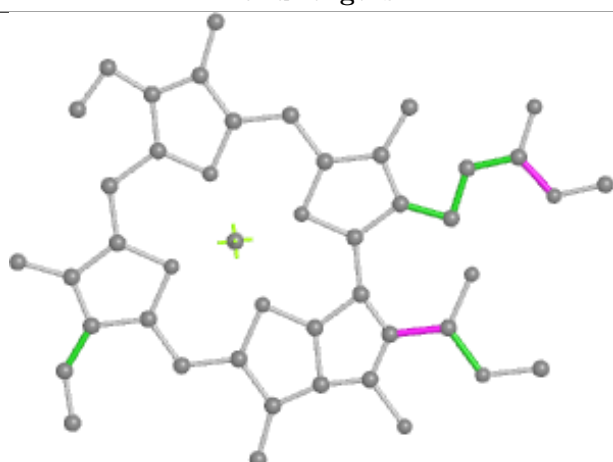
Ligand CLA 8 313



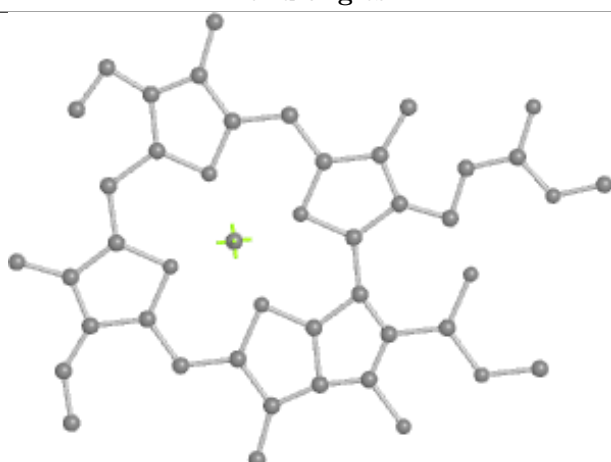
Bond lengths



Bond angles

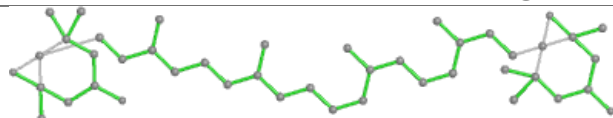


Torsions

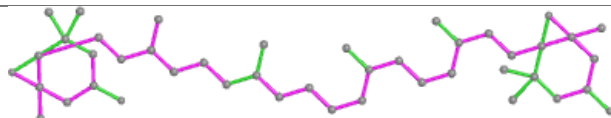


Rings

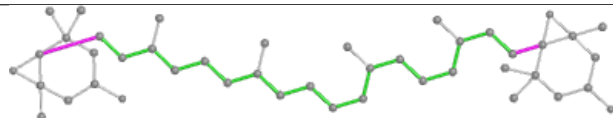
Ligand XAT 7 305



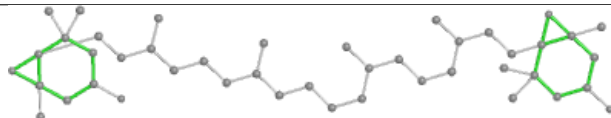
Bond lengths



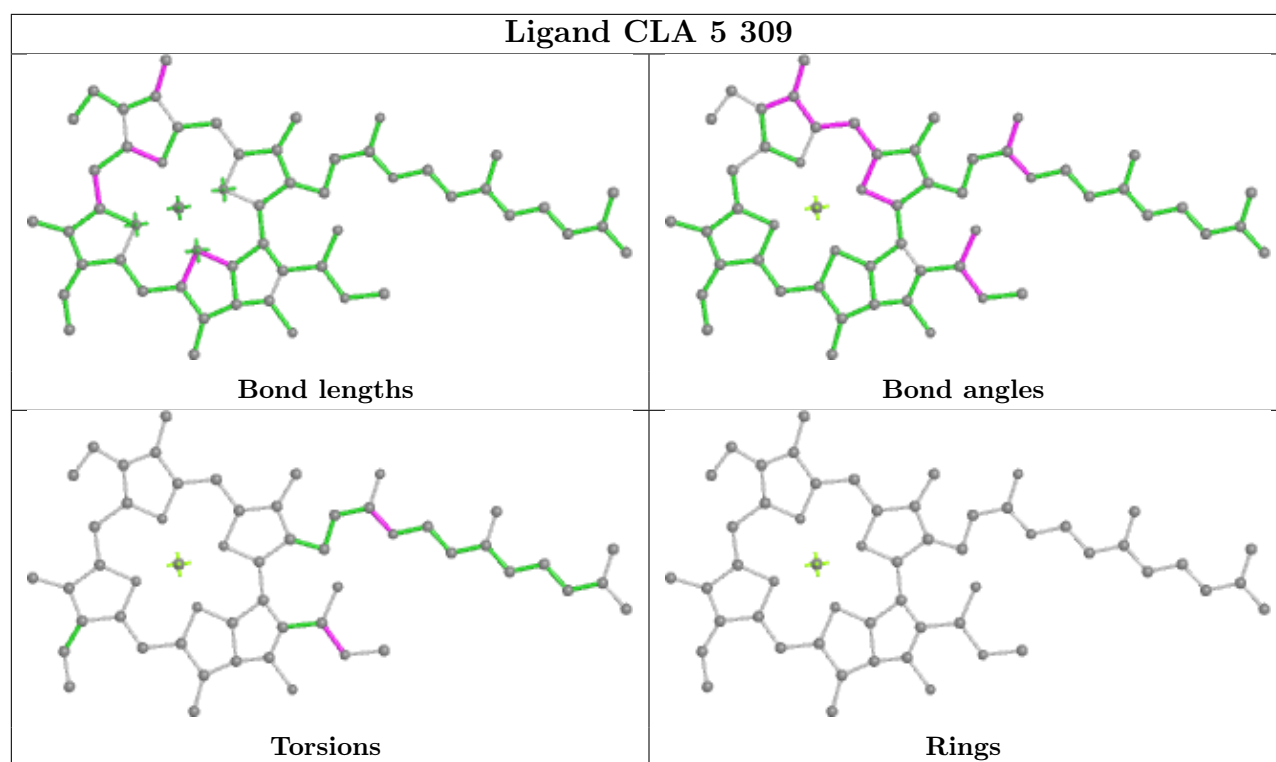
Bond angles



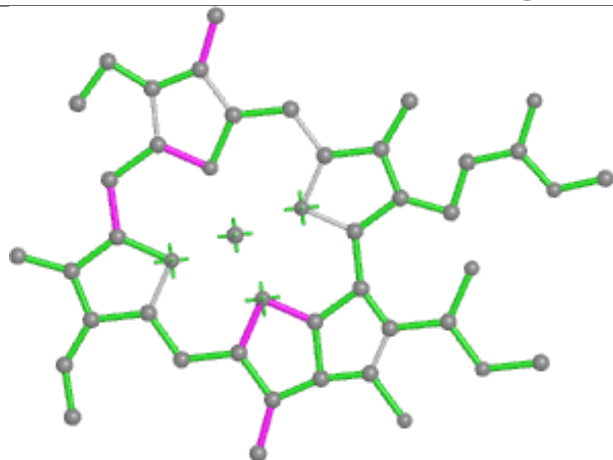
Torsions



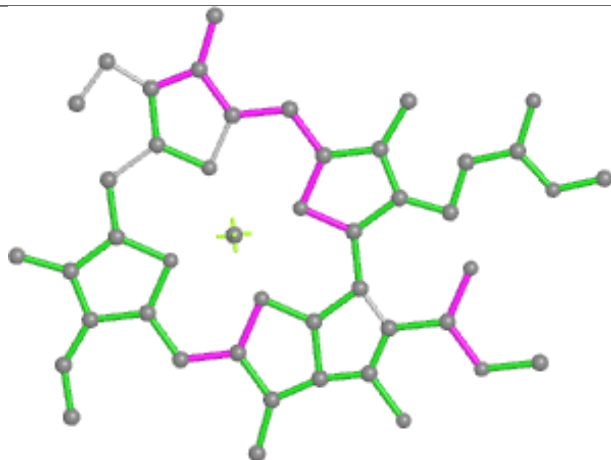
Rings



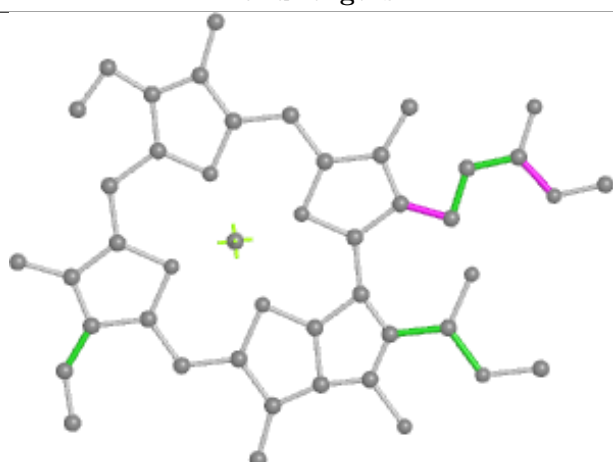
Ligand CLA 4 312



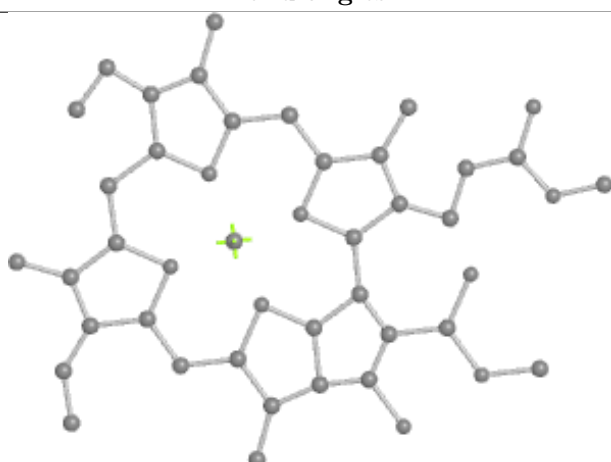
Bond lengths



Bond angles

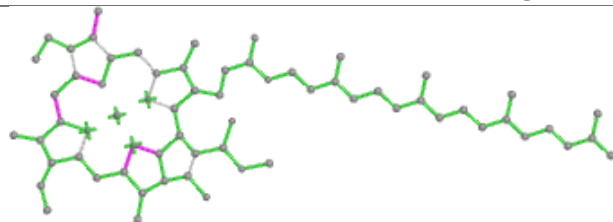


Torsions

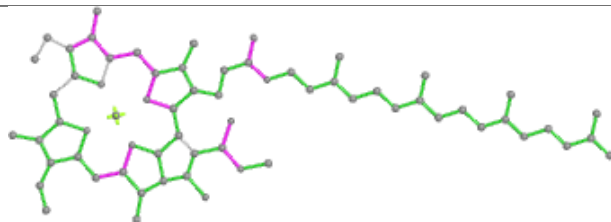


Rings

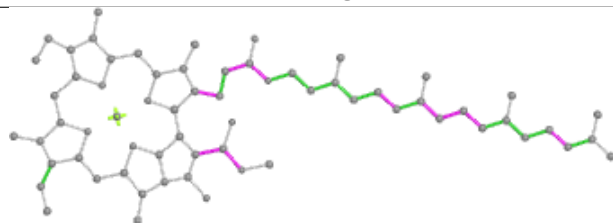
Ligand CLA a 856



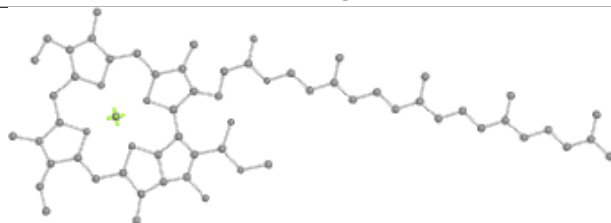
Bond lengths



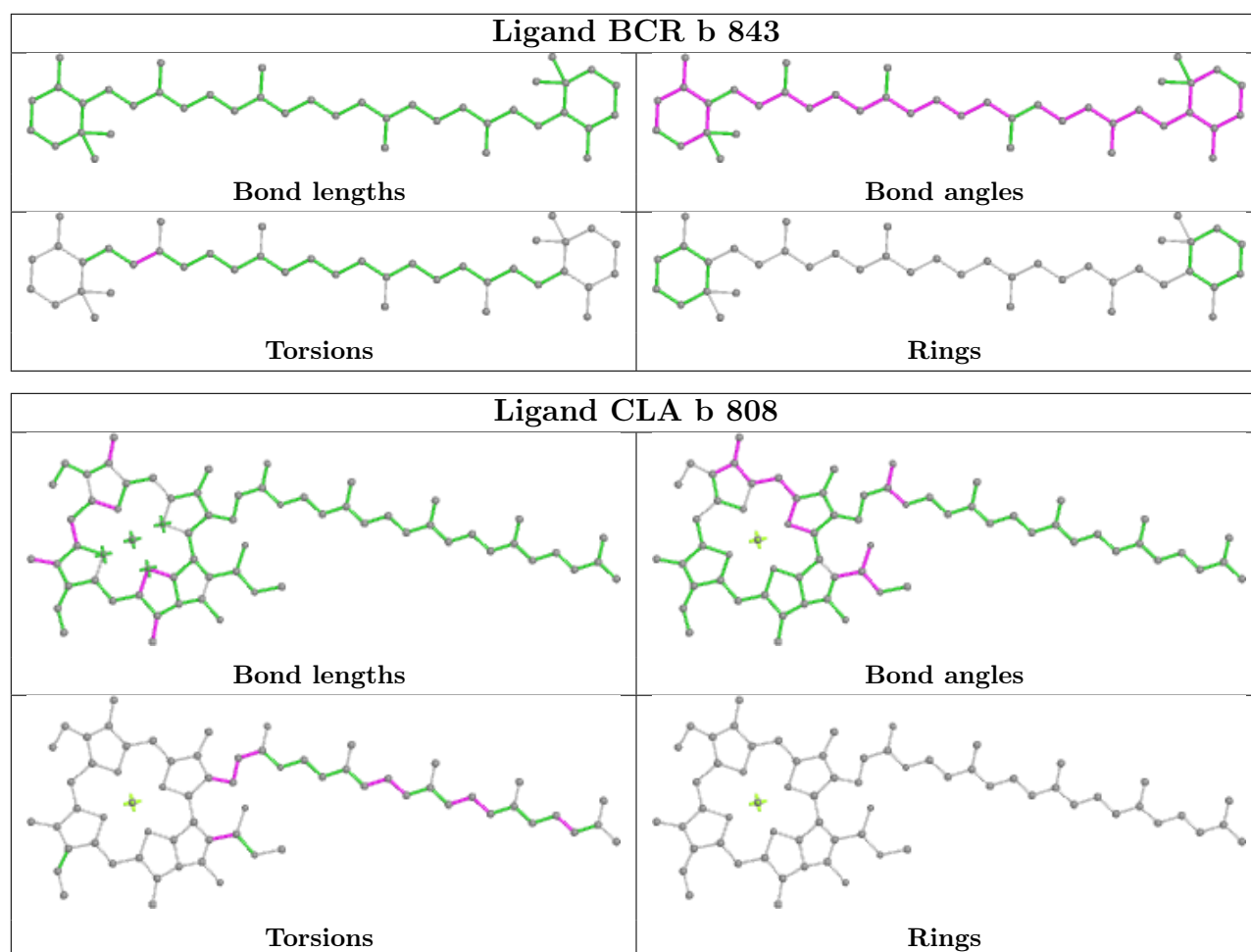
Bond angles



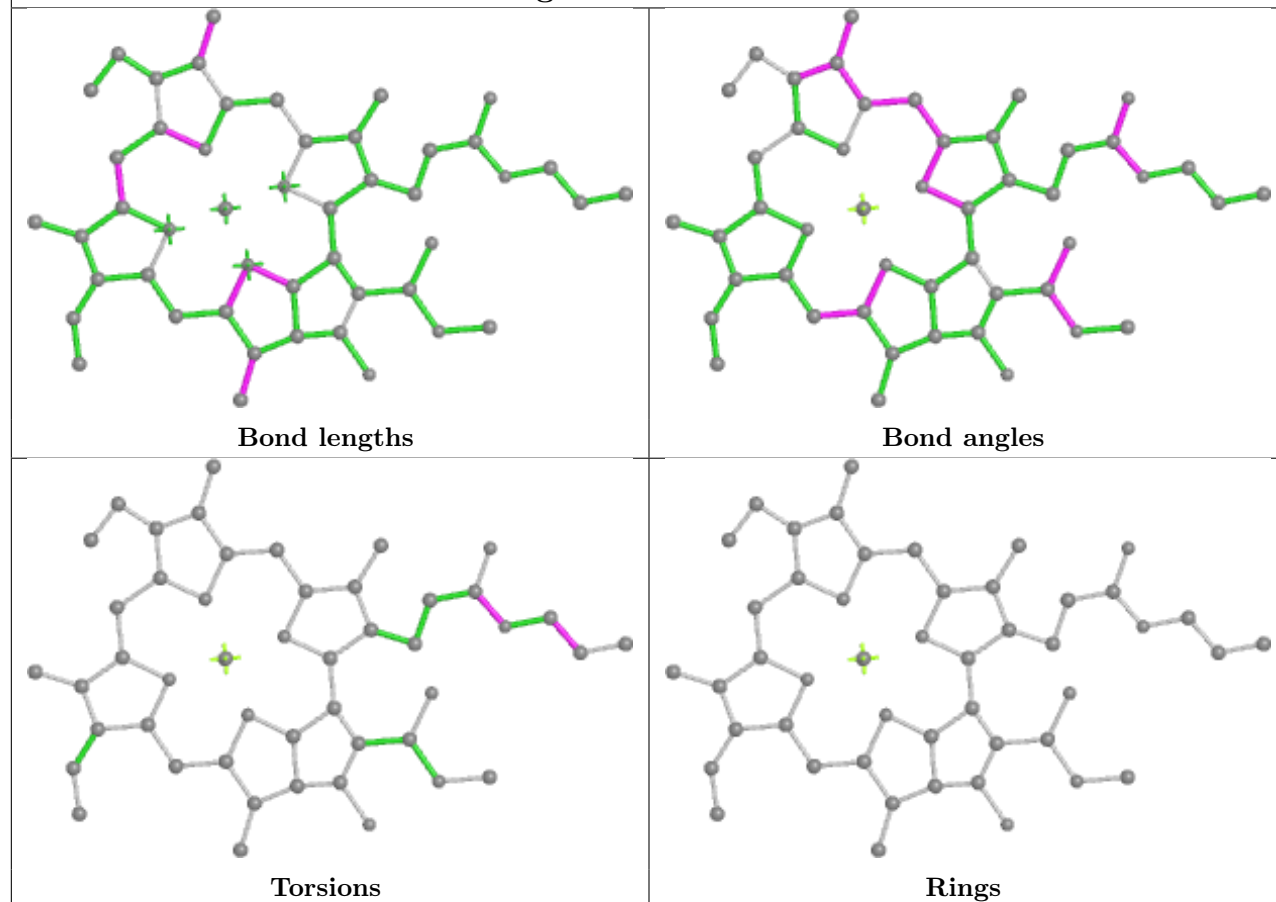
Torsions



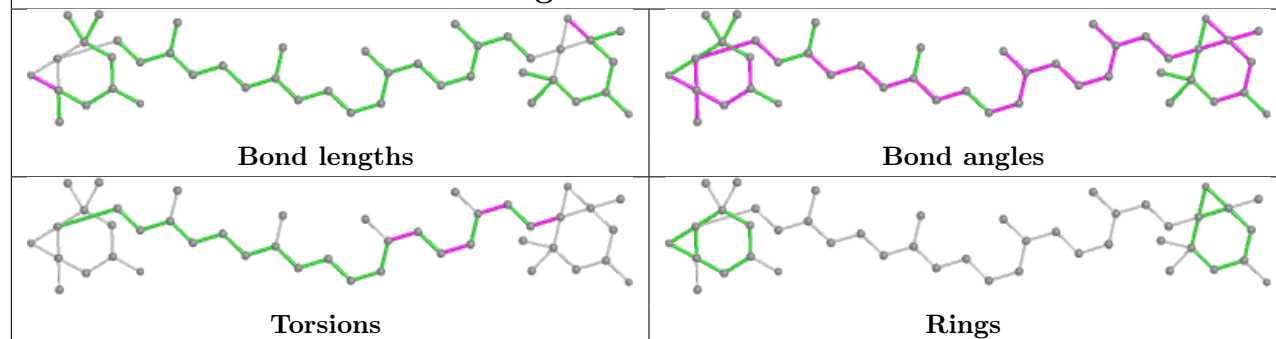
Rings



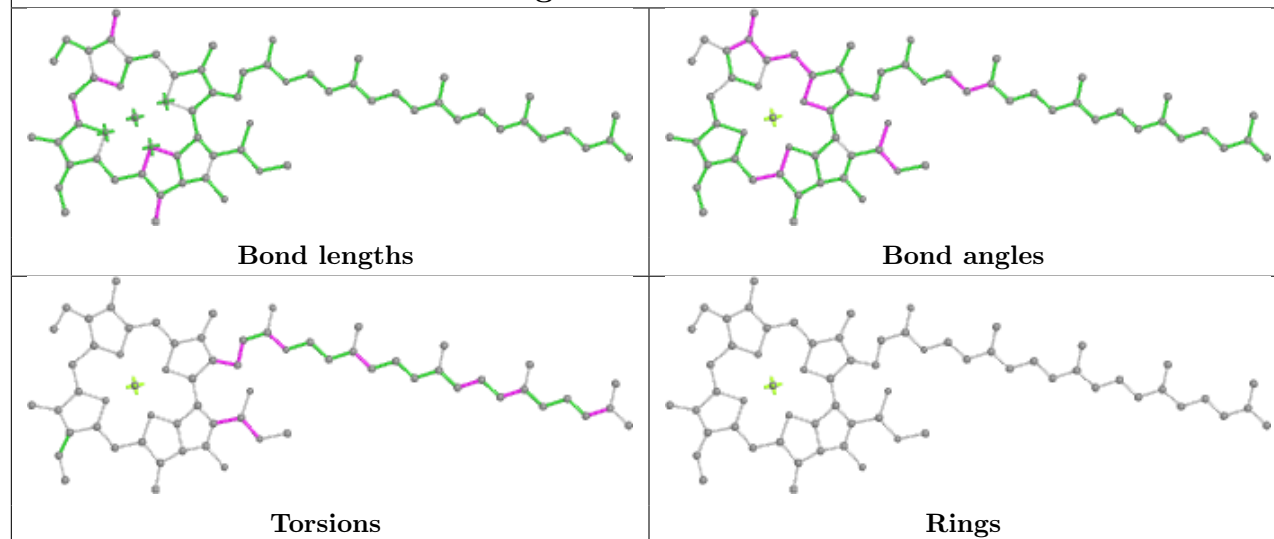
Ligand CLA 7 312



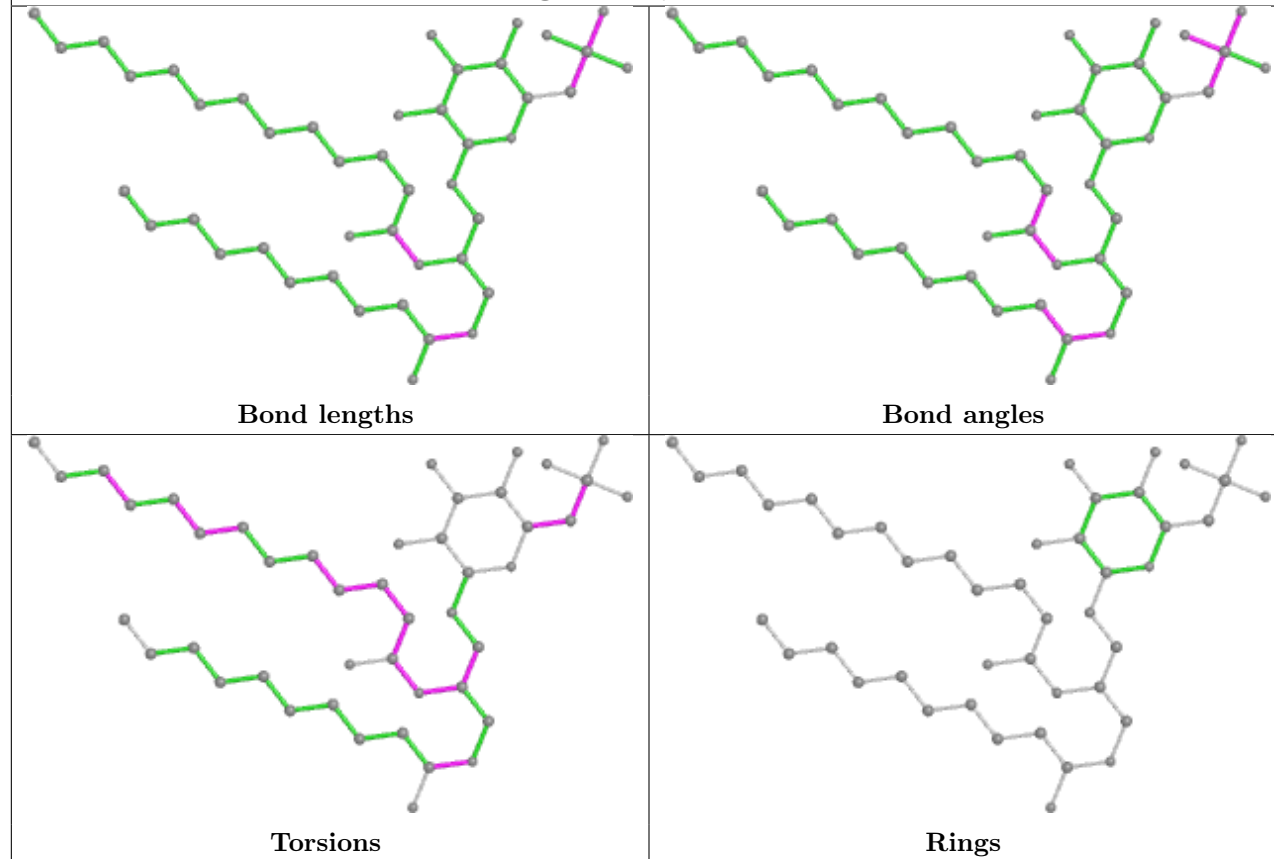
Ligand XAT 7 304

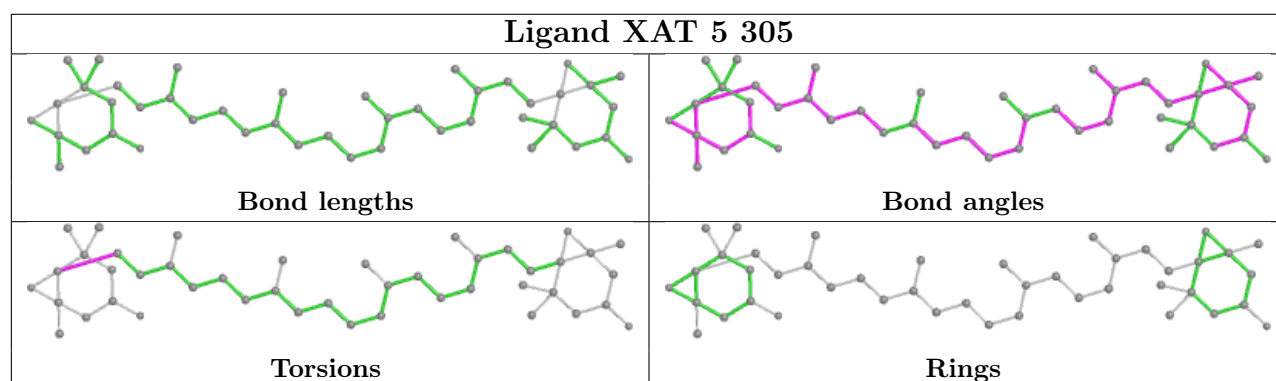
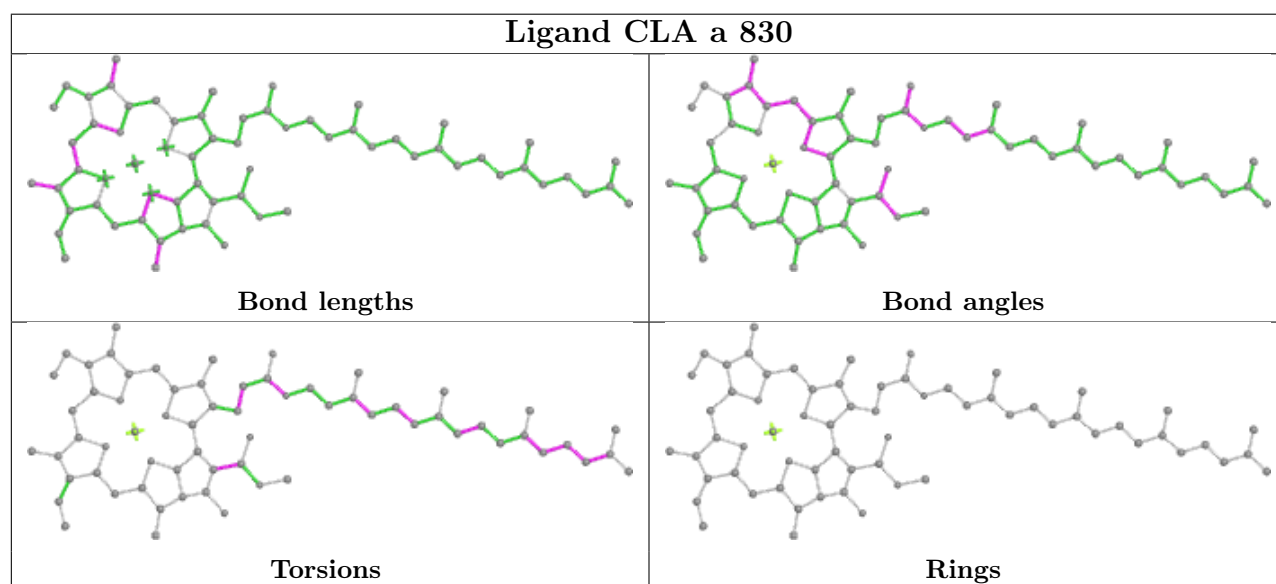
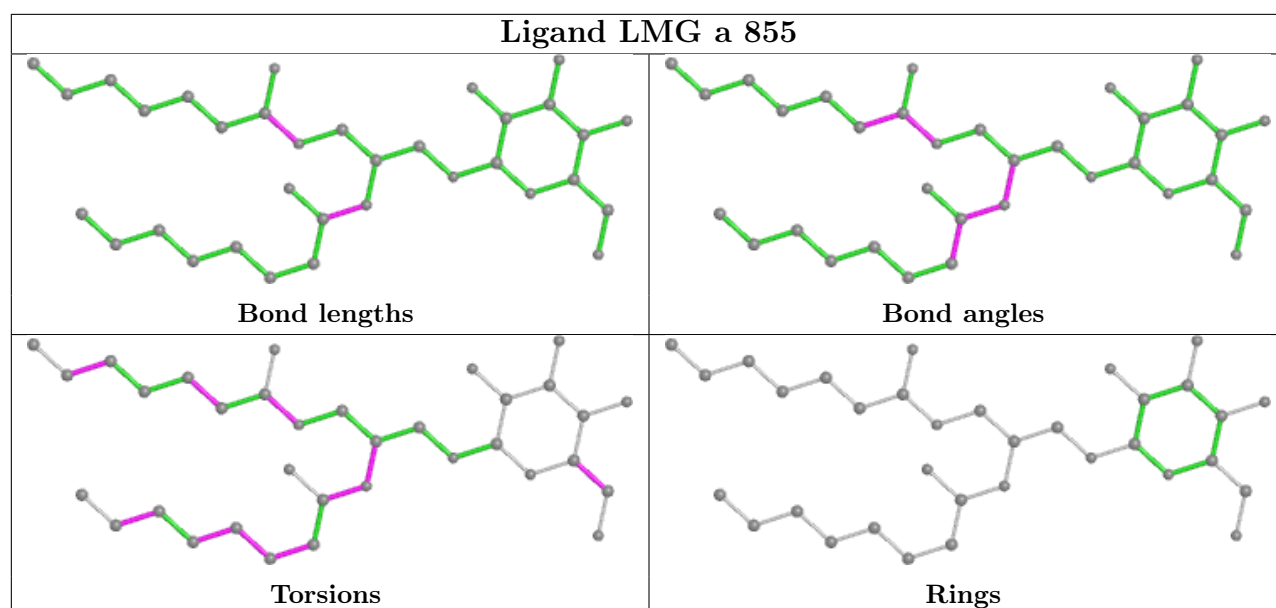


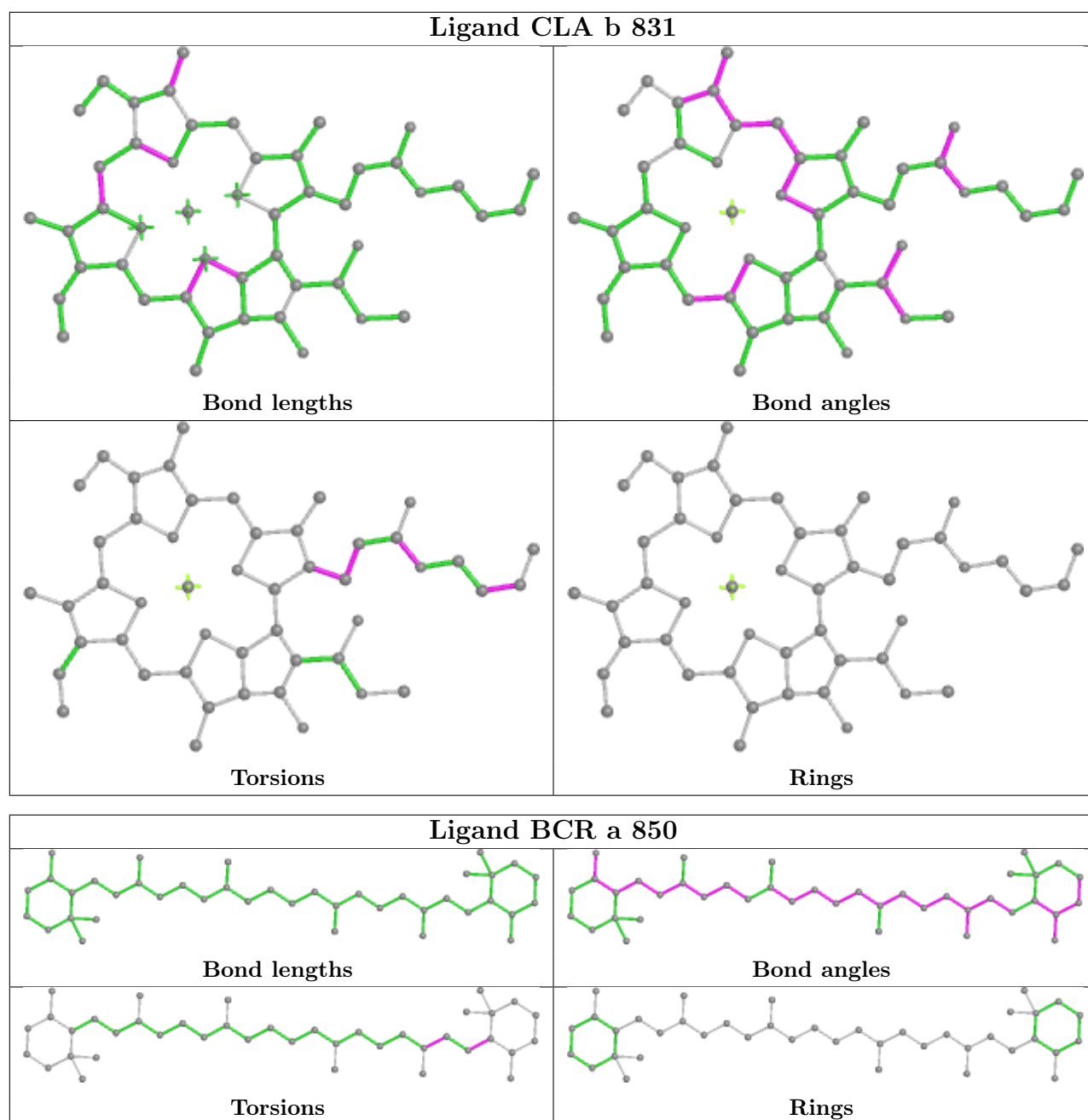
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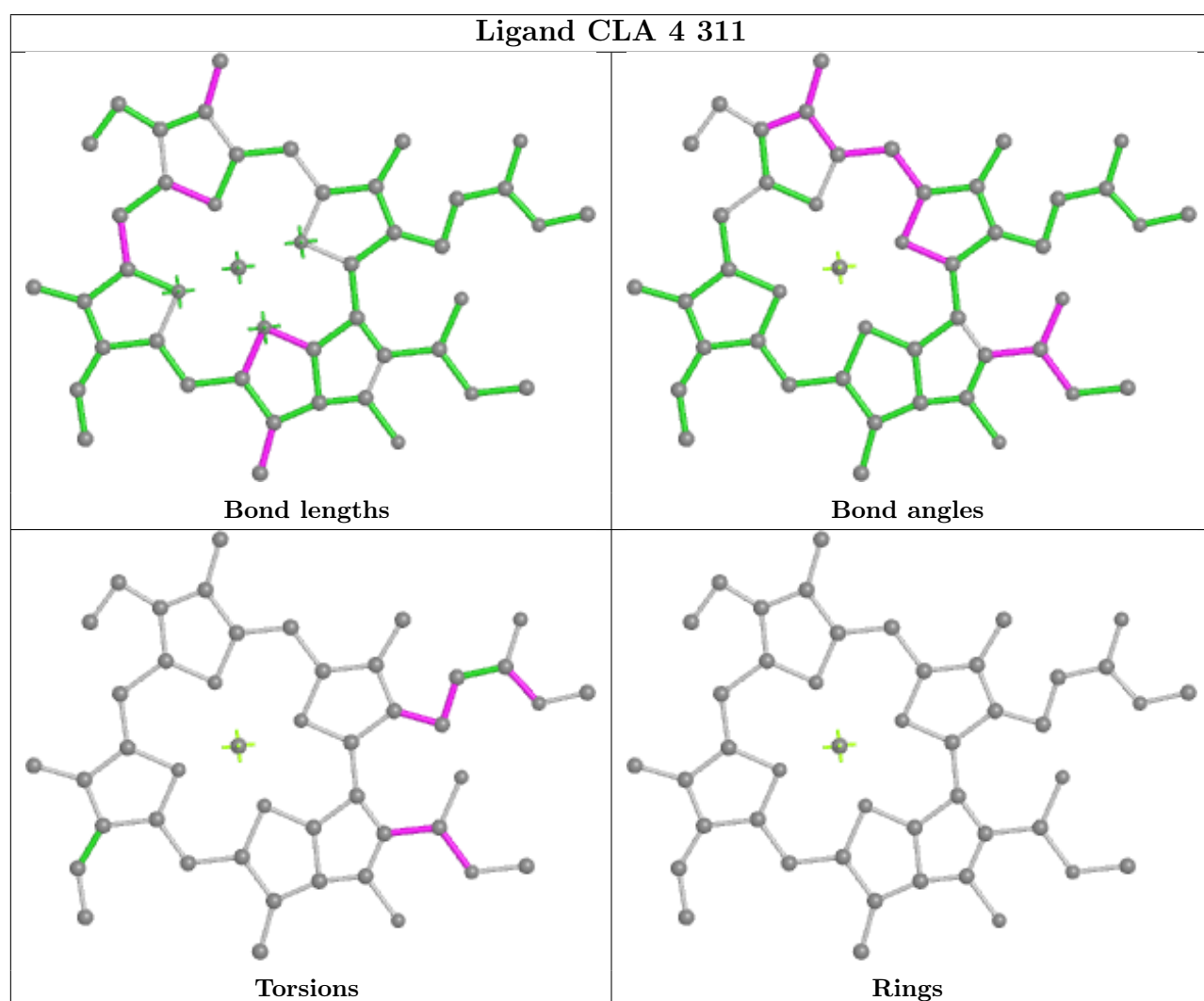
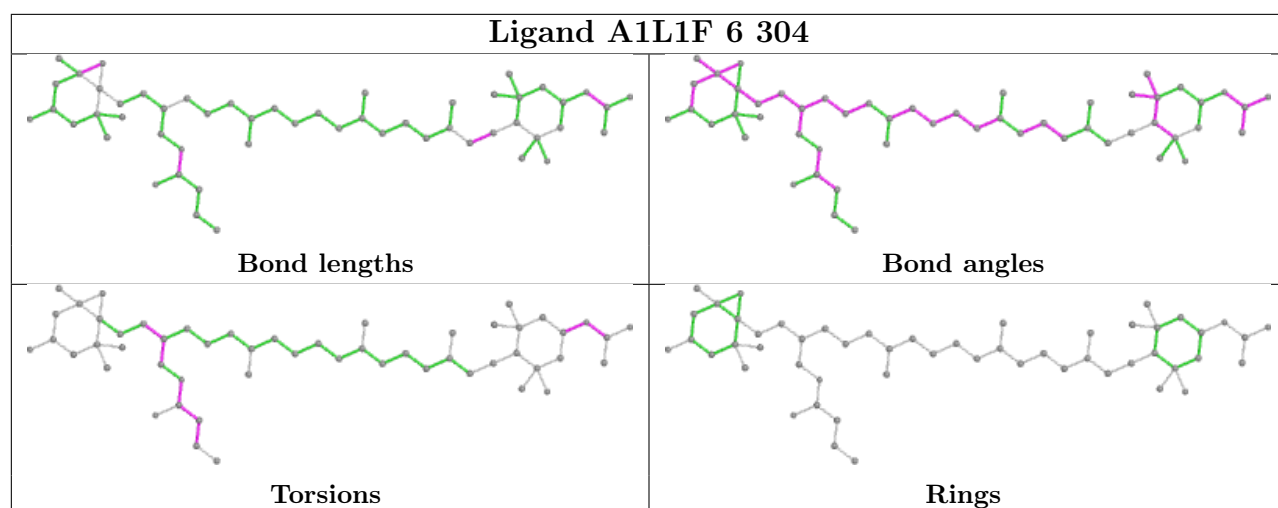


Ligand SQD 1 315

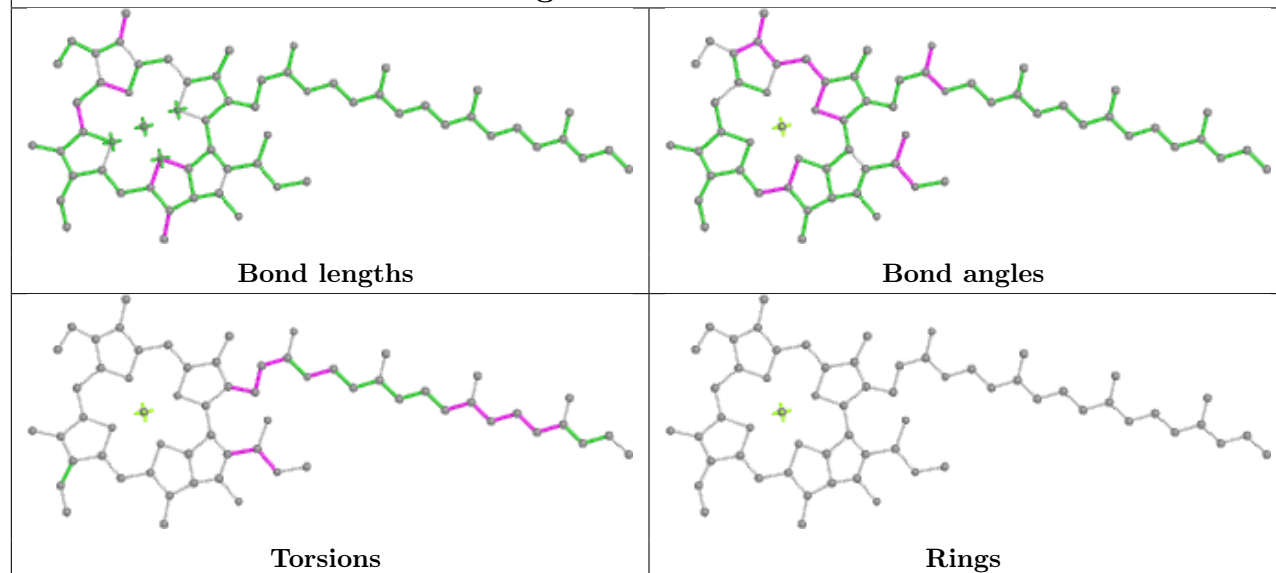




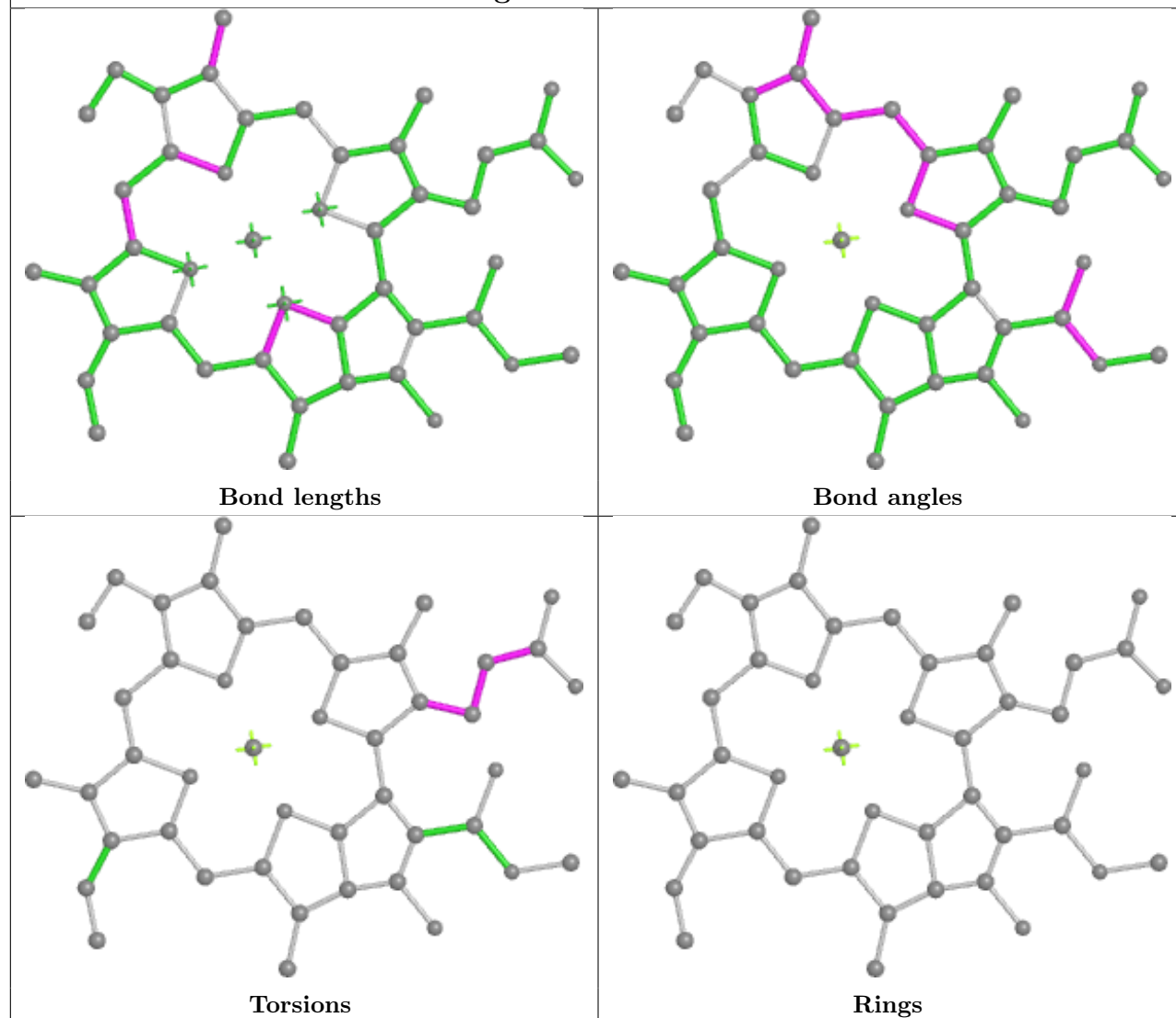




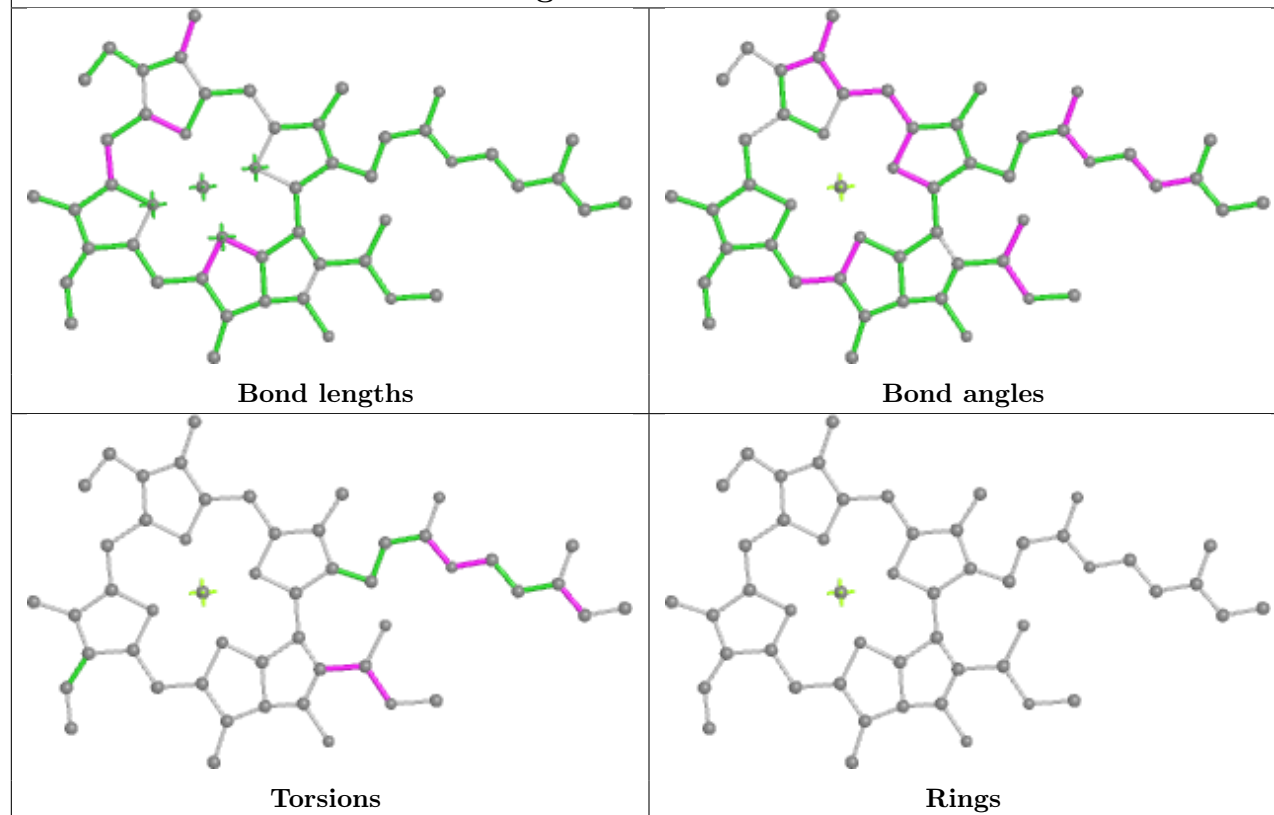
Ligand CLA a 829



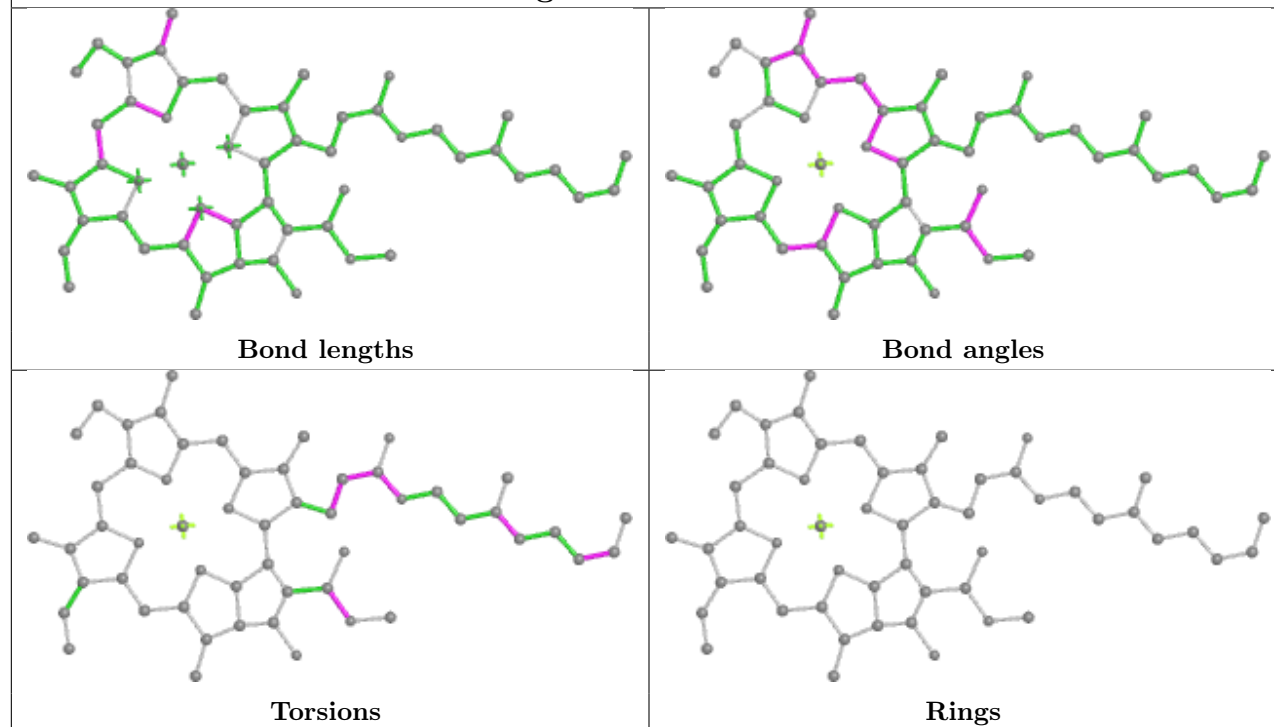
Ligand CLA 1 314

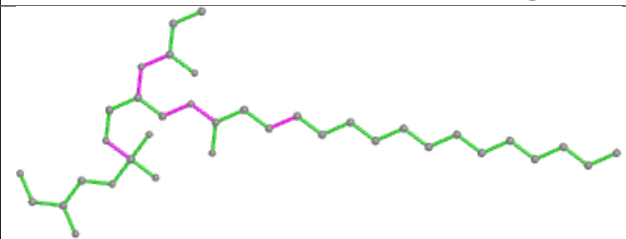
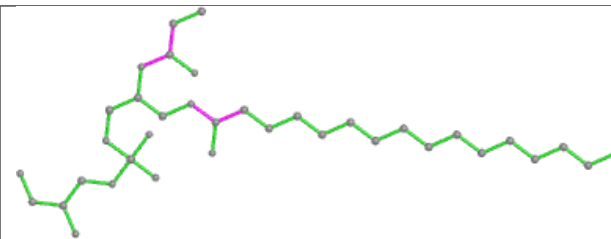
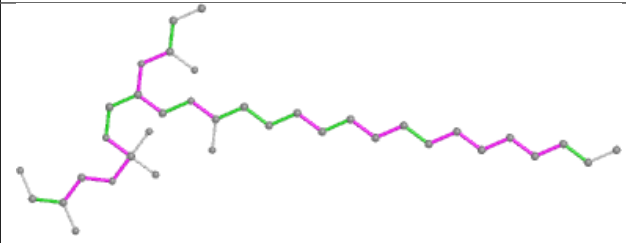
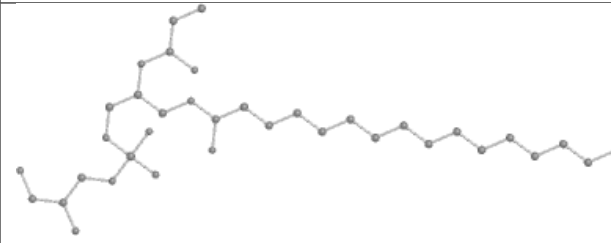


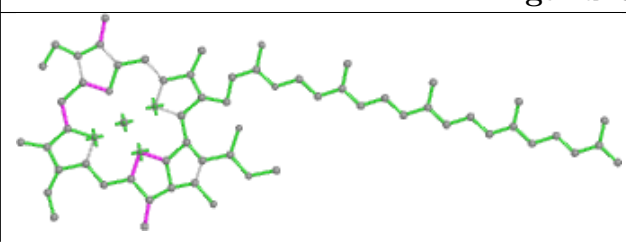
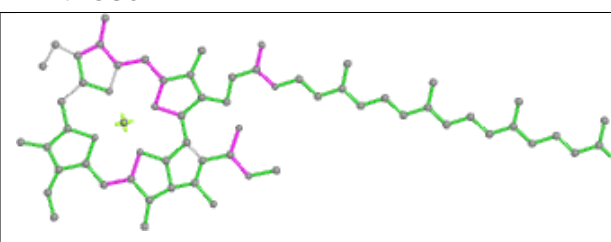
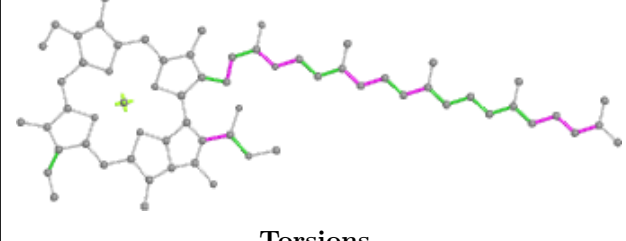
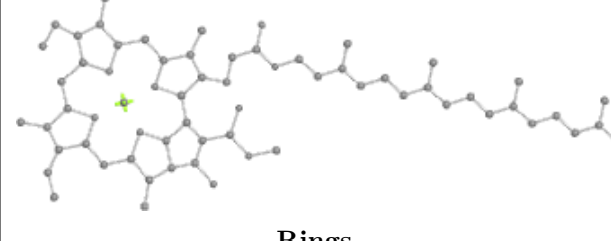
Ligand CLA 5 312

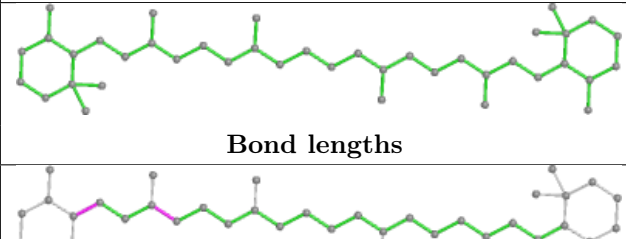
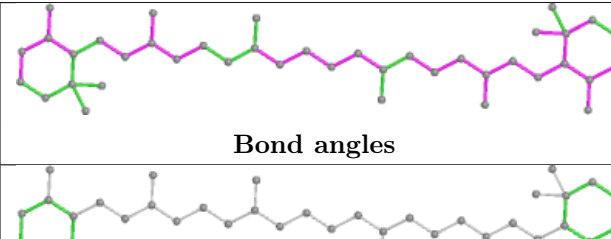
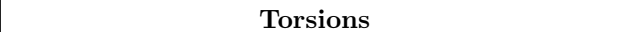



Ligand CLA a 813

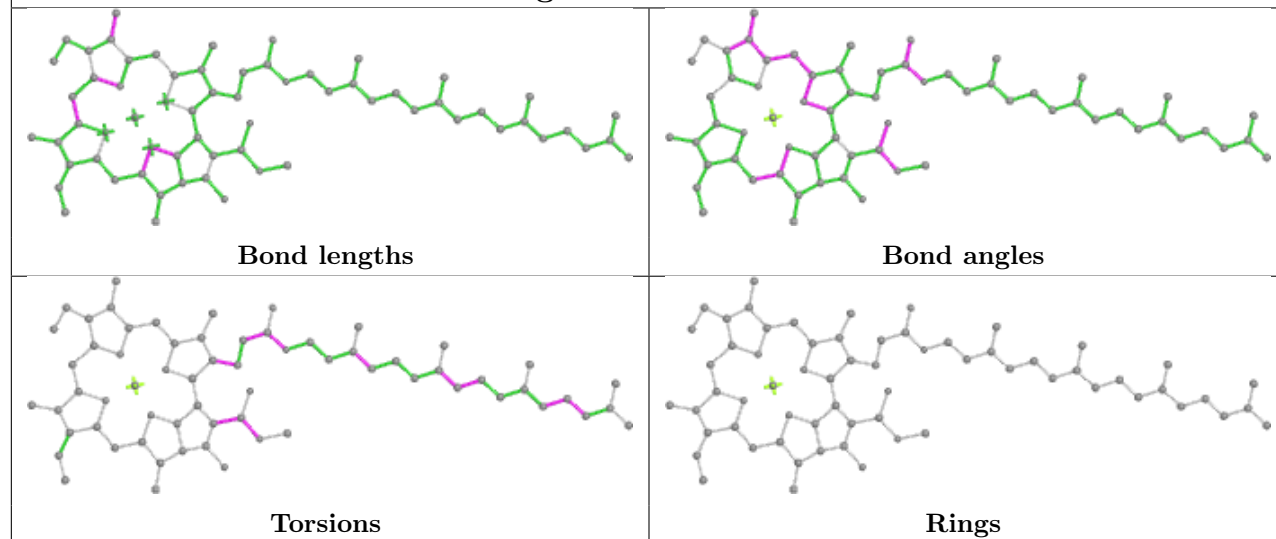


Ligand LHG 9 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

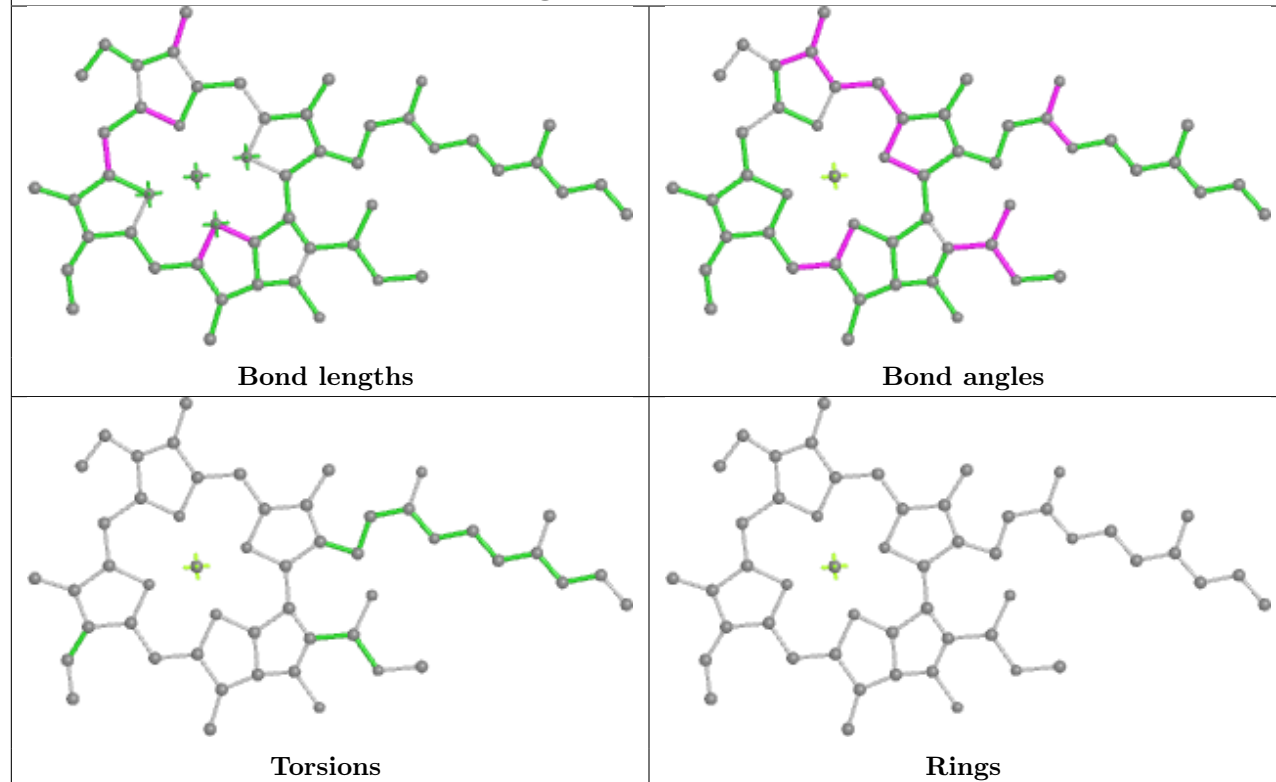
Ligand CLA a 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 853	
	
Bond lengths	Bond angles
	
Torsions	Rings

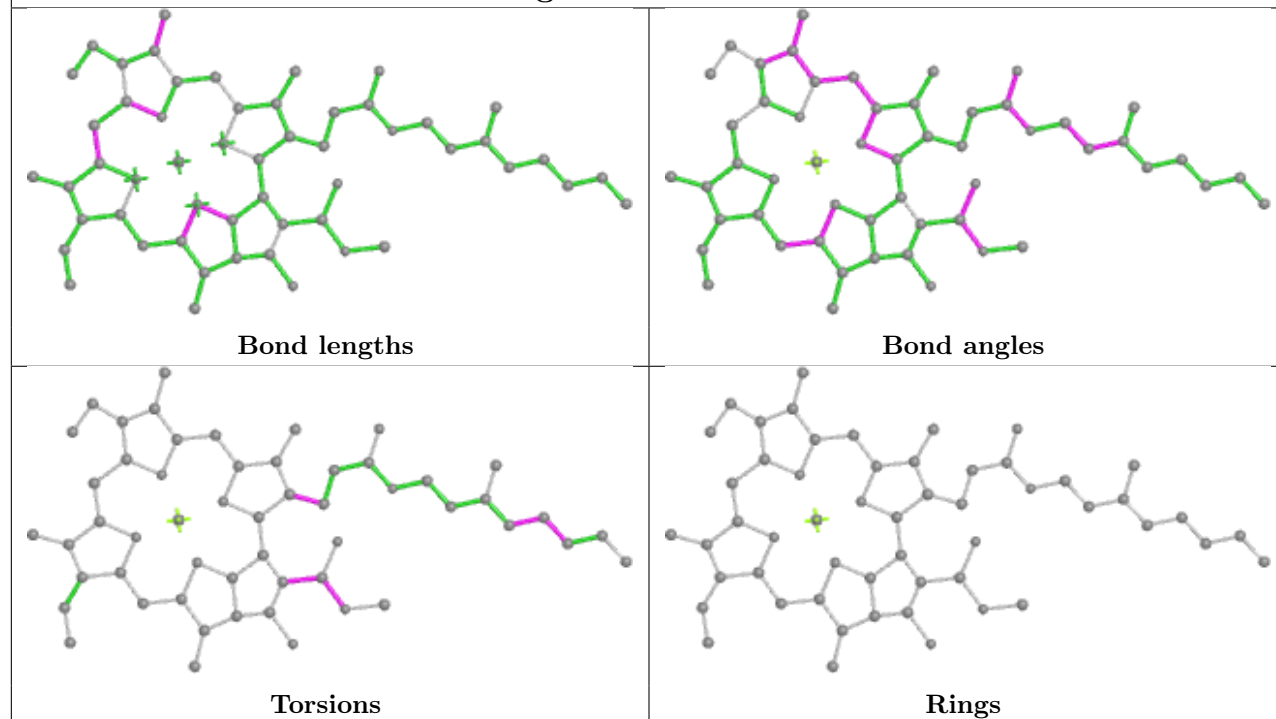
Ligand CLA 4 310



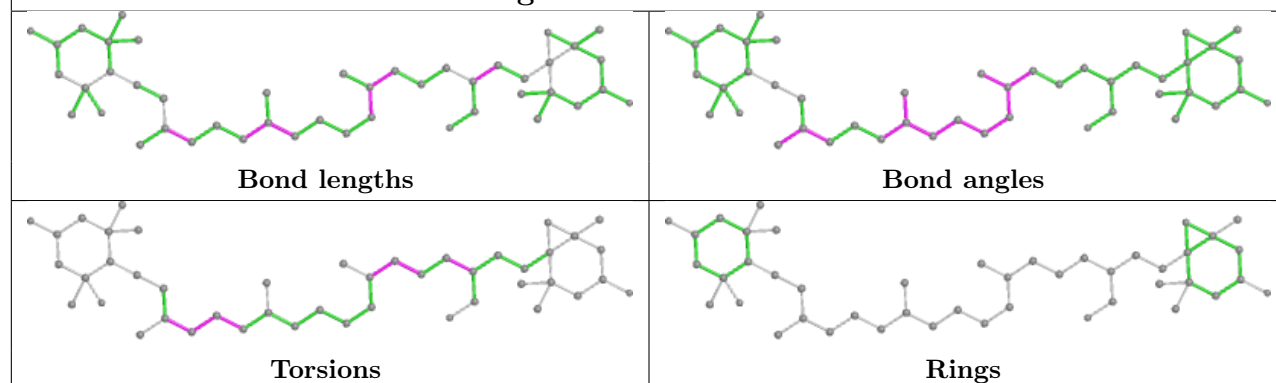
Ligand CLA 5 313



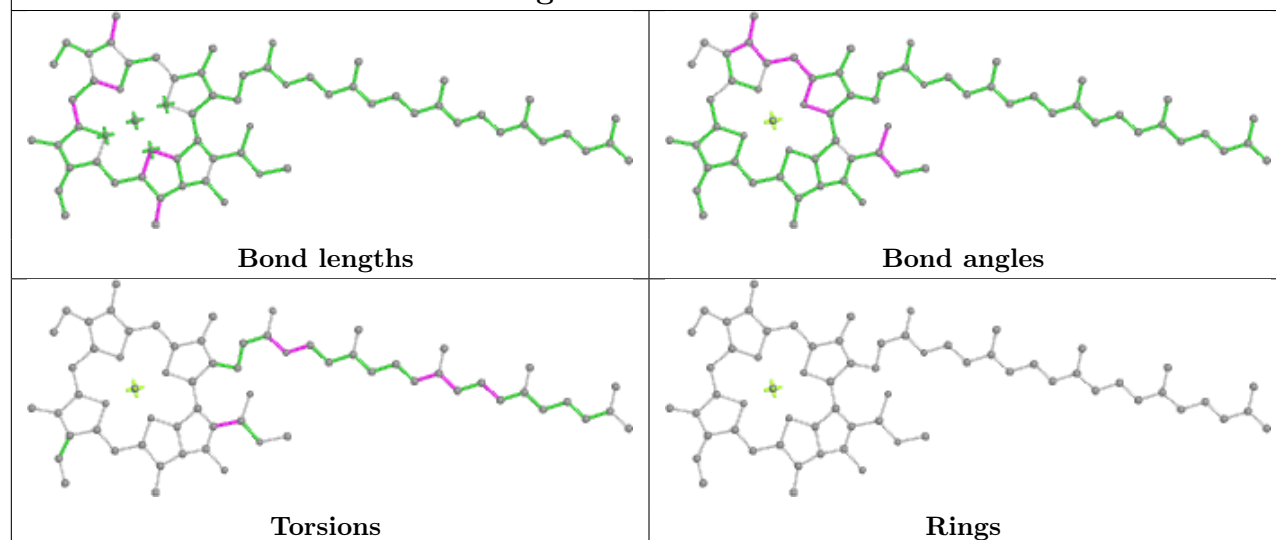
Ligand CLA 7 313



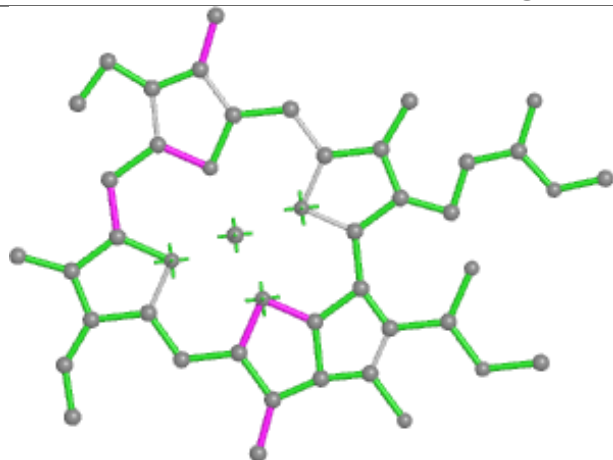
Ligand A1L1G 5 304



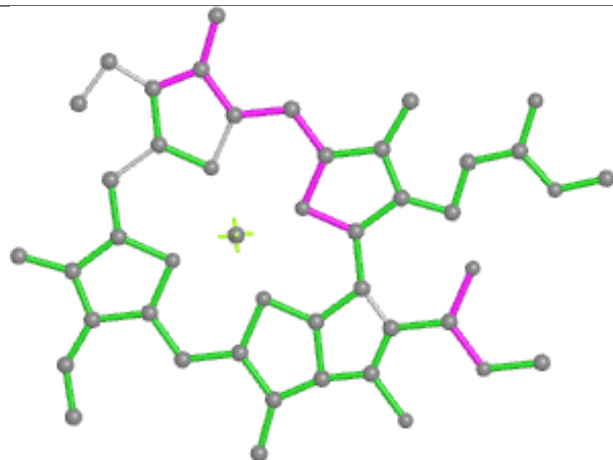
Ligand CLA 6 309



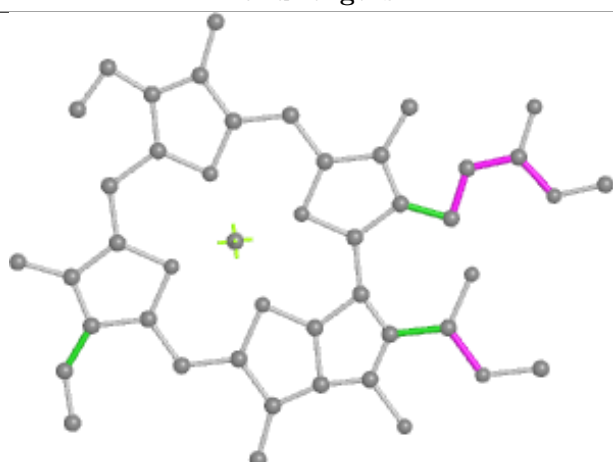
Ligand CLA 7 310



Bond lengths



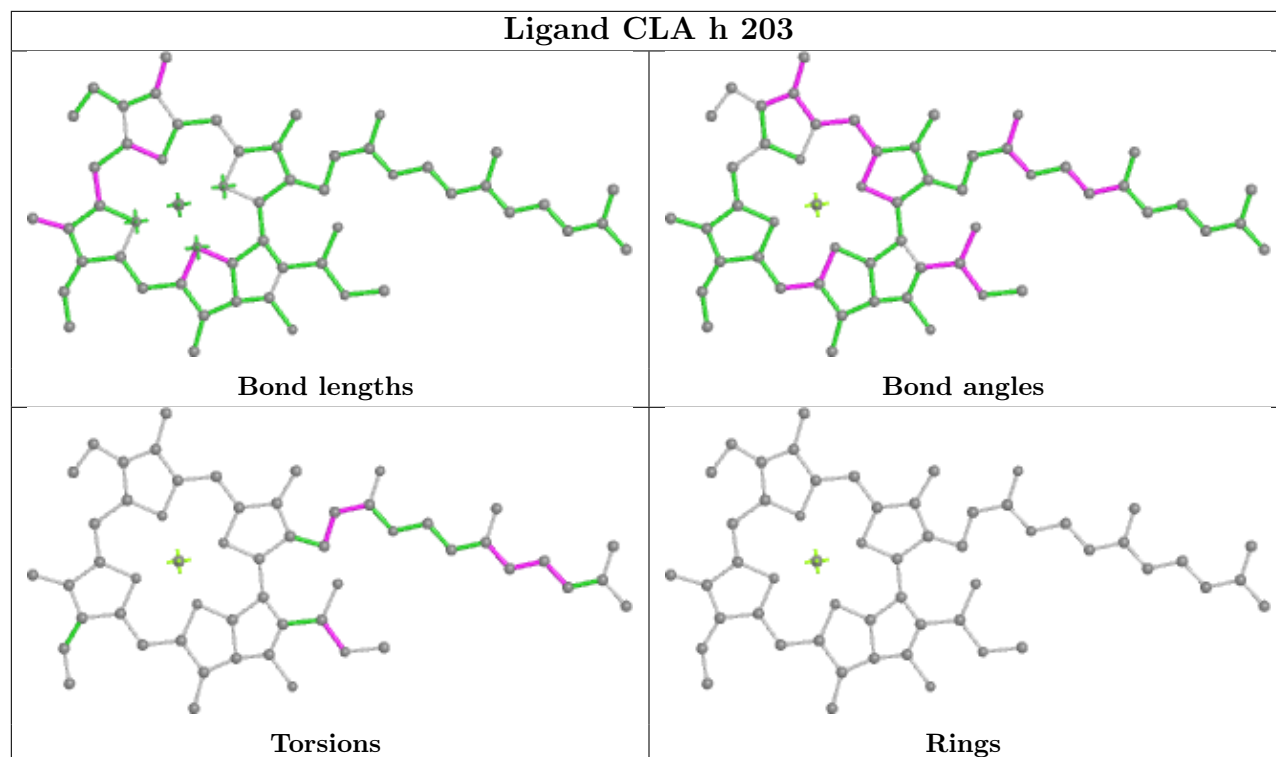
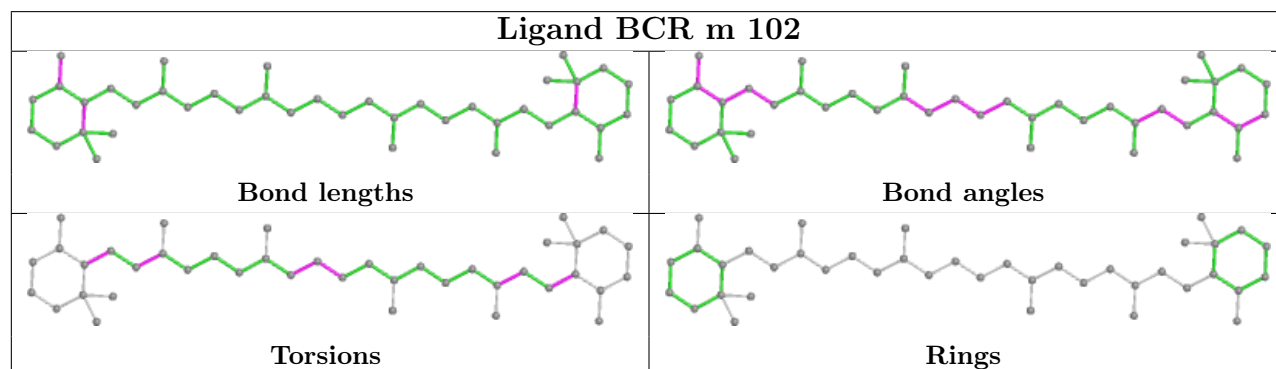
Bond angles

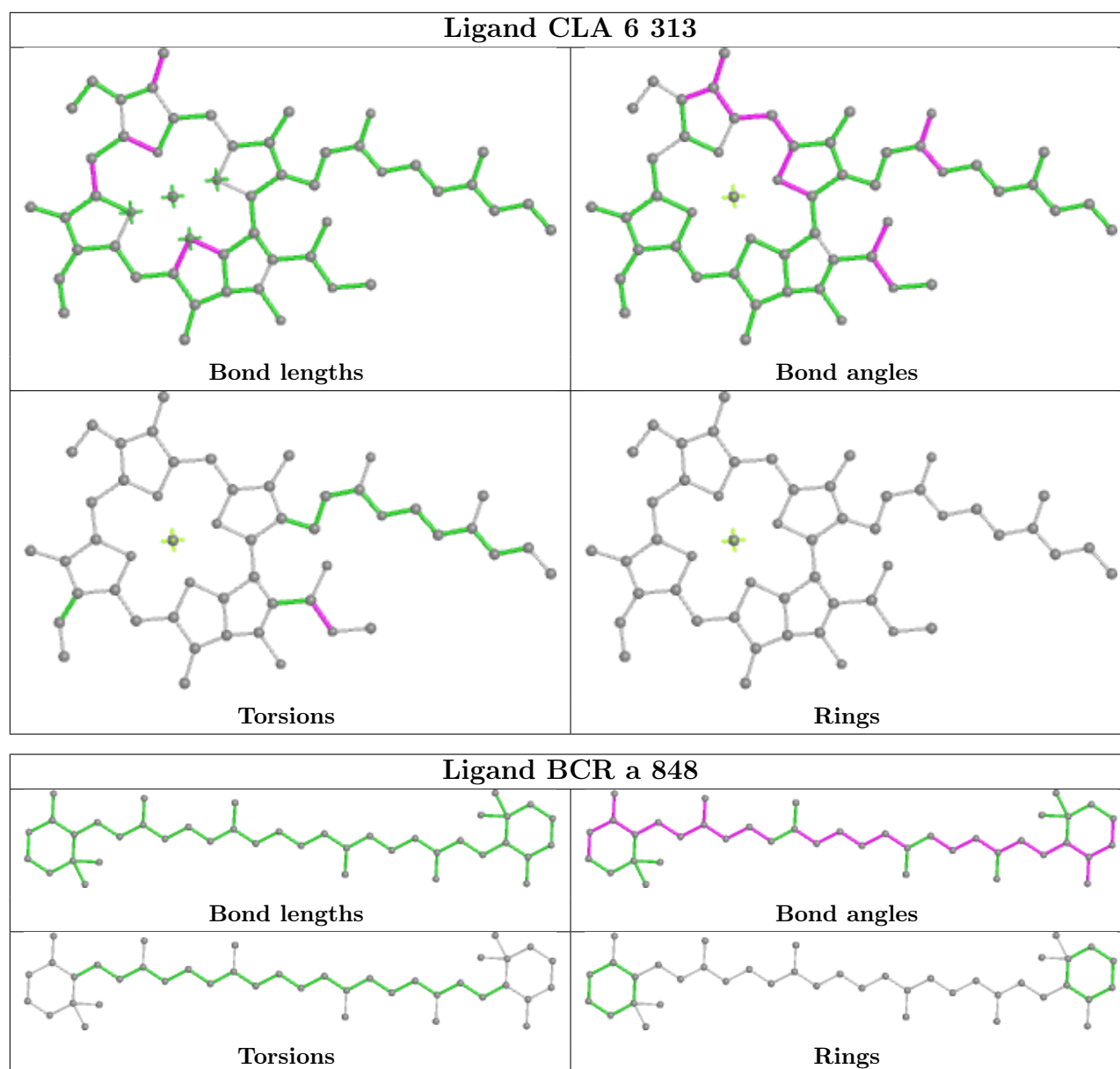


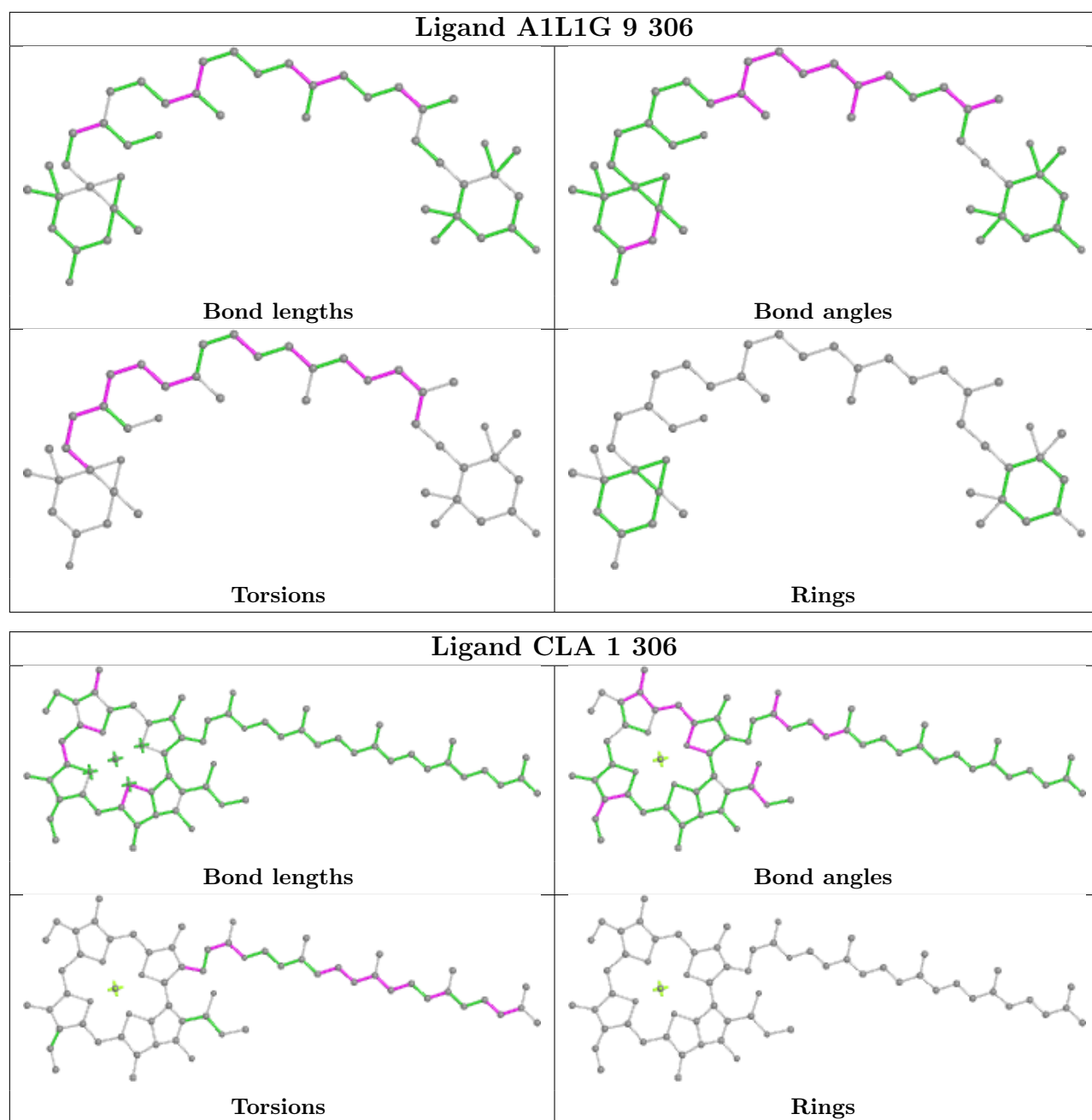
Torsions

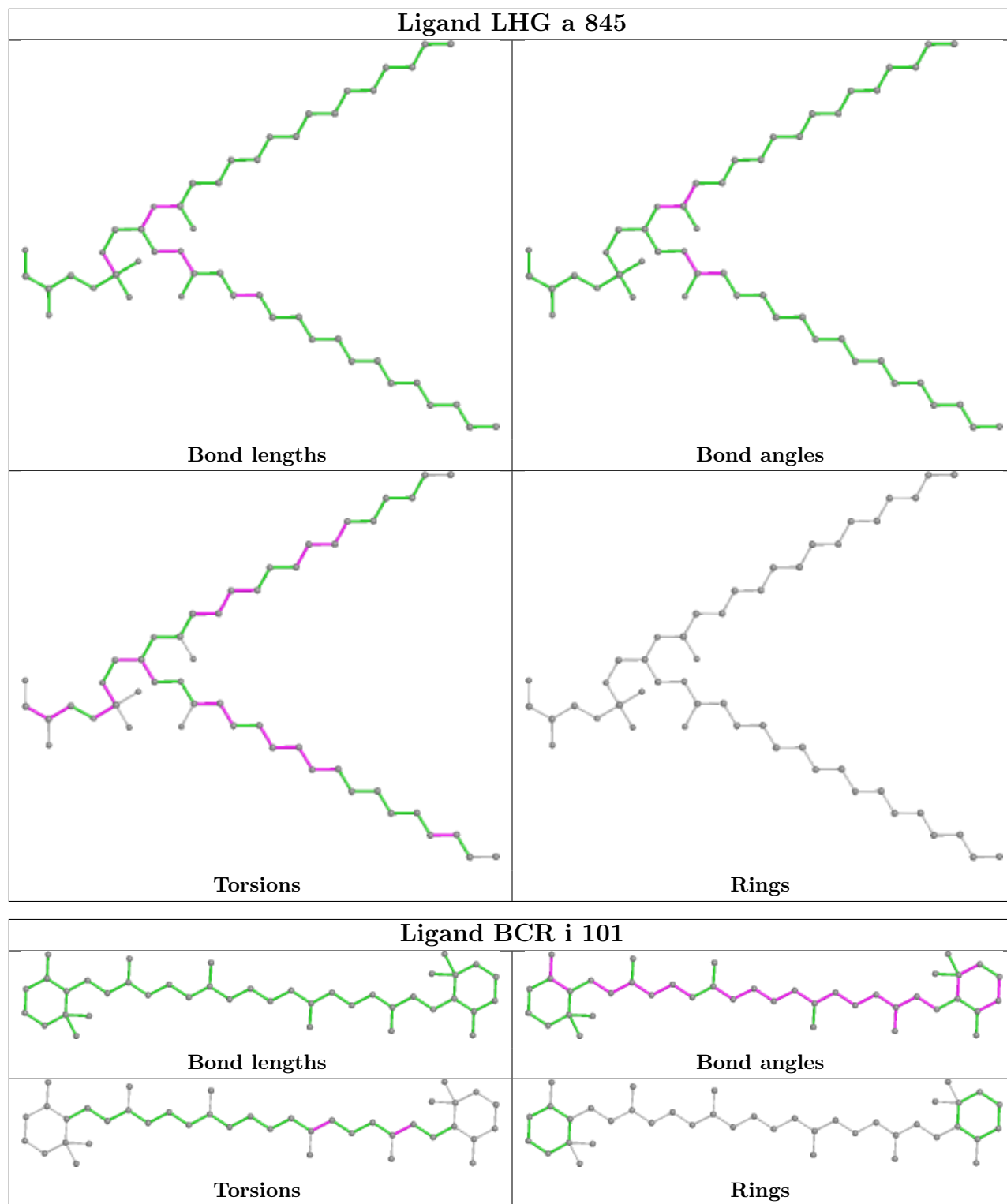


Rings

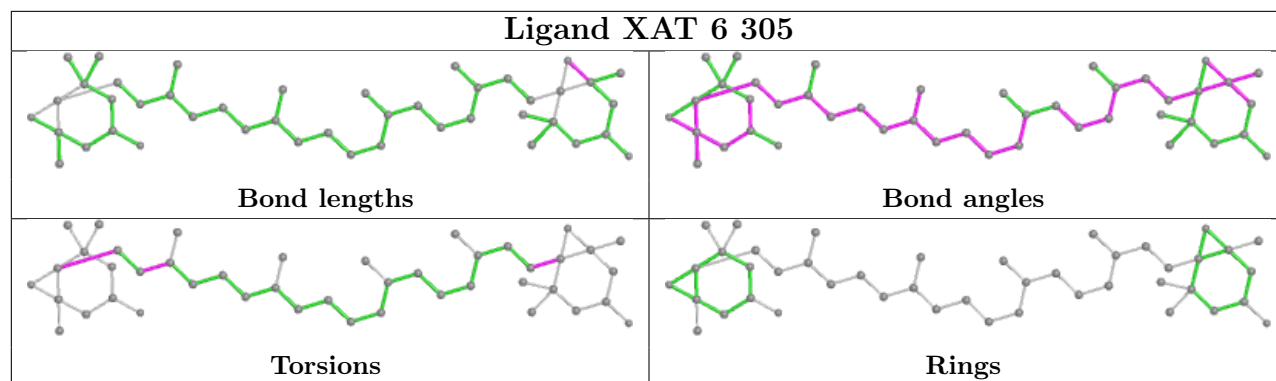
Ligand CLA h 203**Ligand BCR m 102**



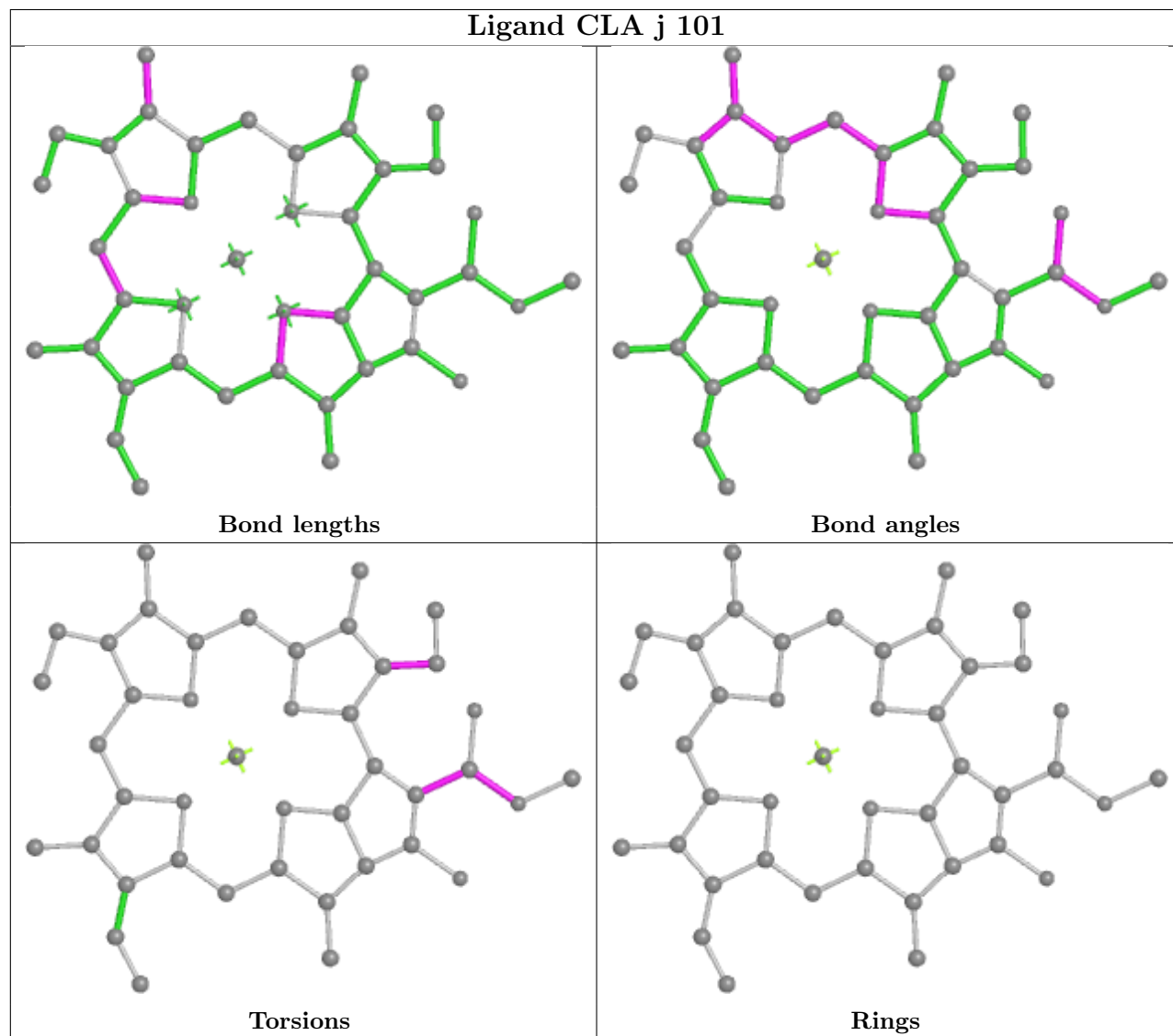




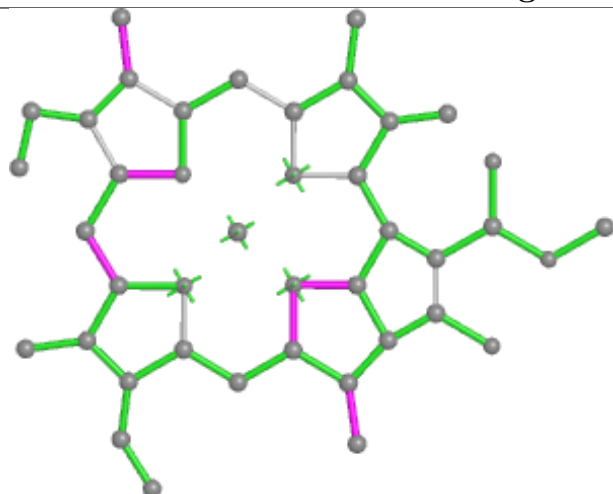
Ligand XAT 6 305



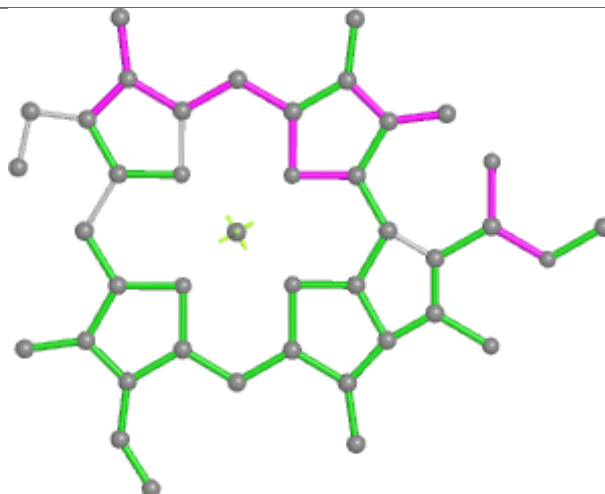
Ligand CLA j 101



Ligand CLA 4 315



Bond lengths



Bond angles

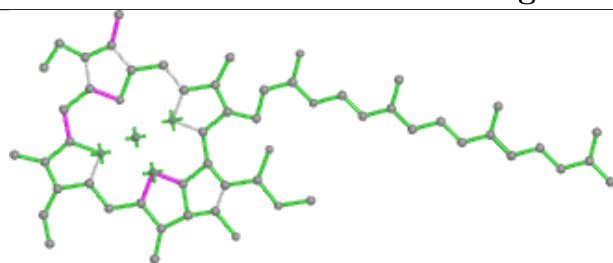


Torsions

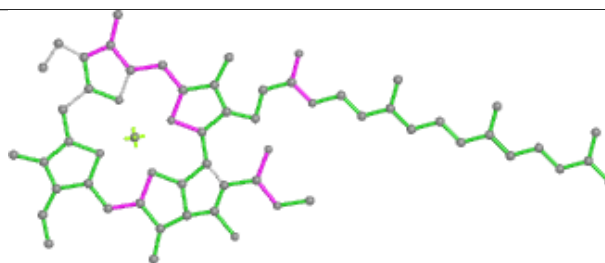


Rings

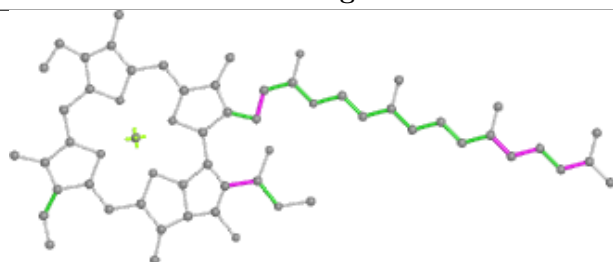
Ligand CLA 5 308



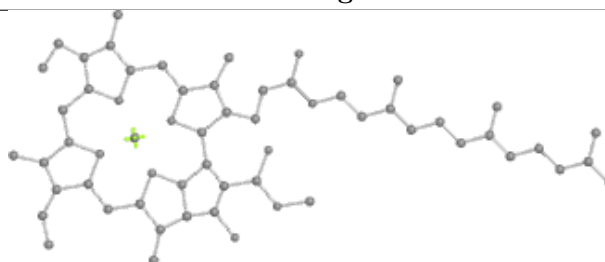
Bond lengths



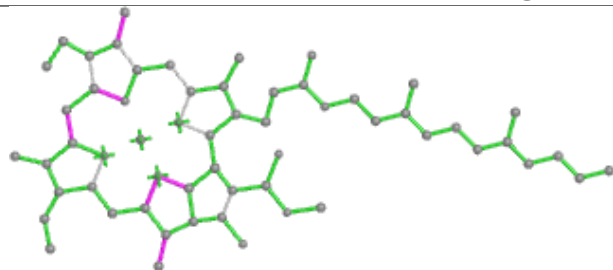
Bond angles



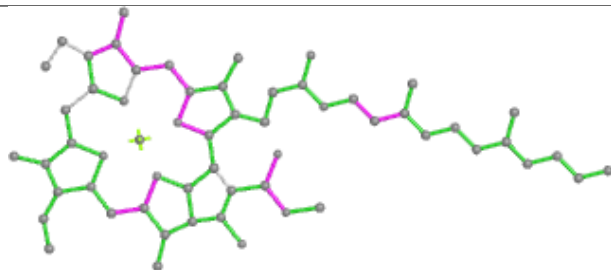
Torsions



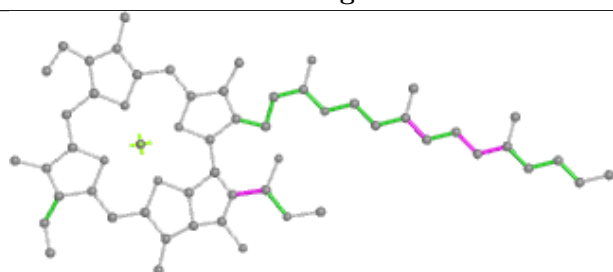
Rings

Ligand CLA a 802

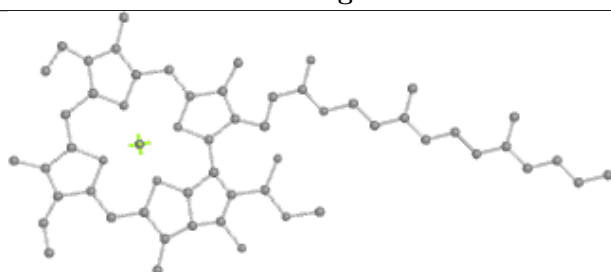
Bond lengths



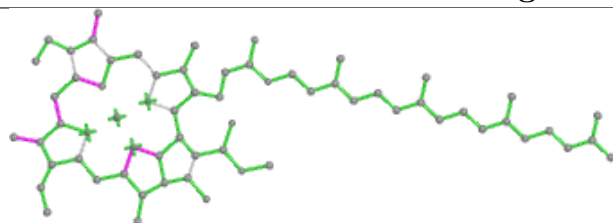
Bond angles



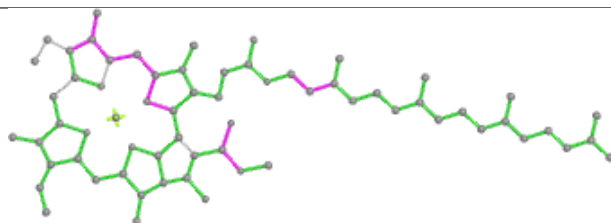
Torsions



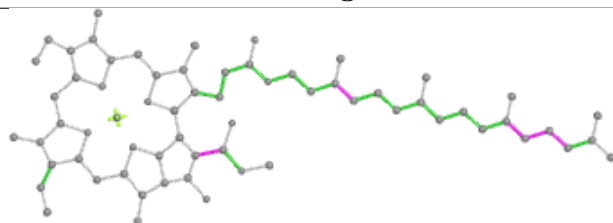
Rings

Ligand CLA a 828

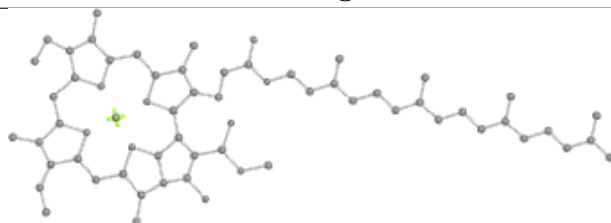
Bond lengths



Bond angles

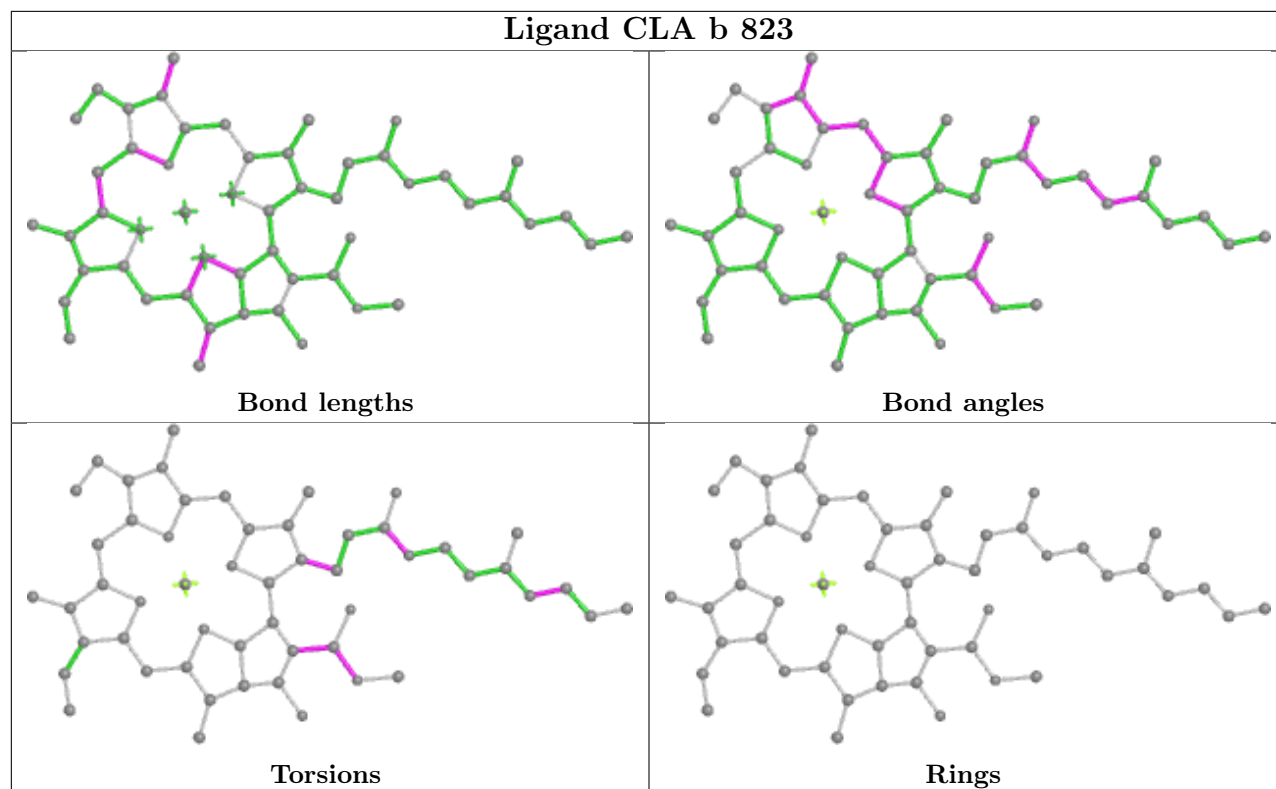


Torsions

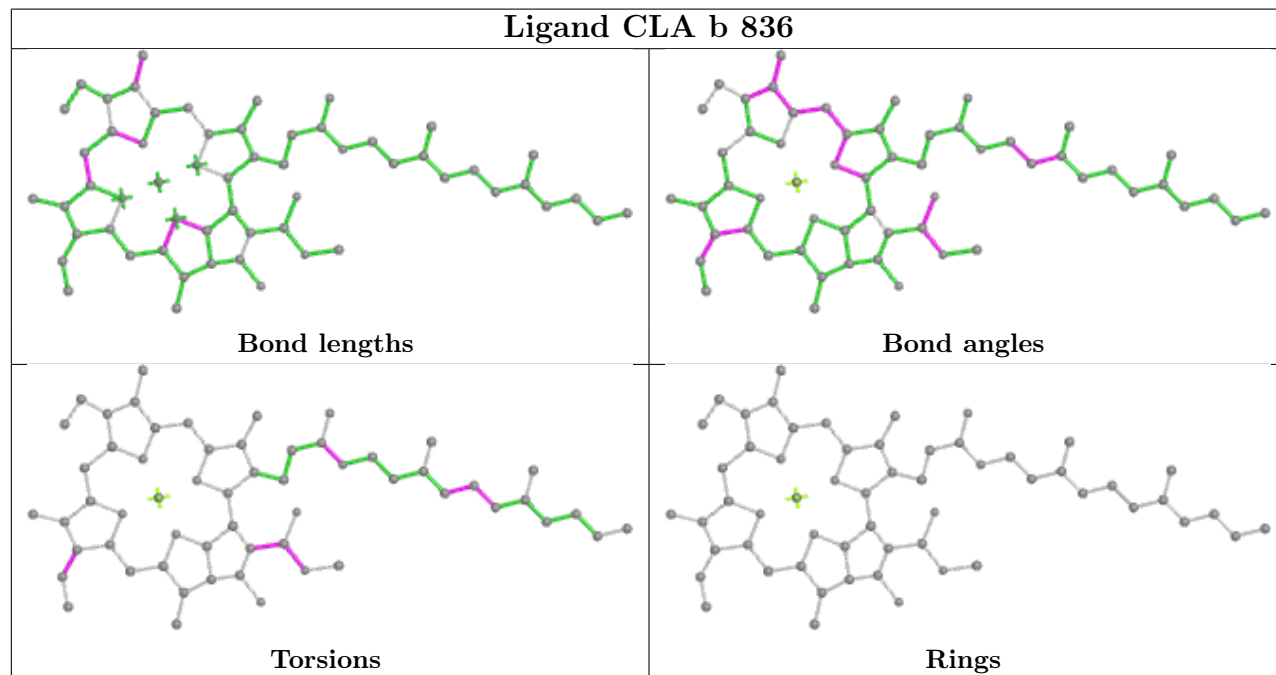


Rings

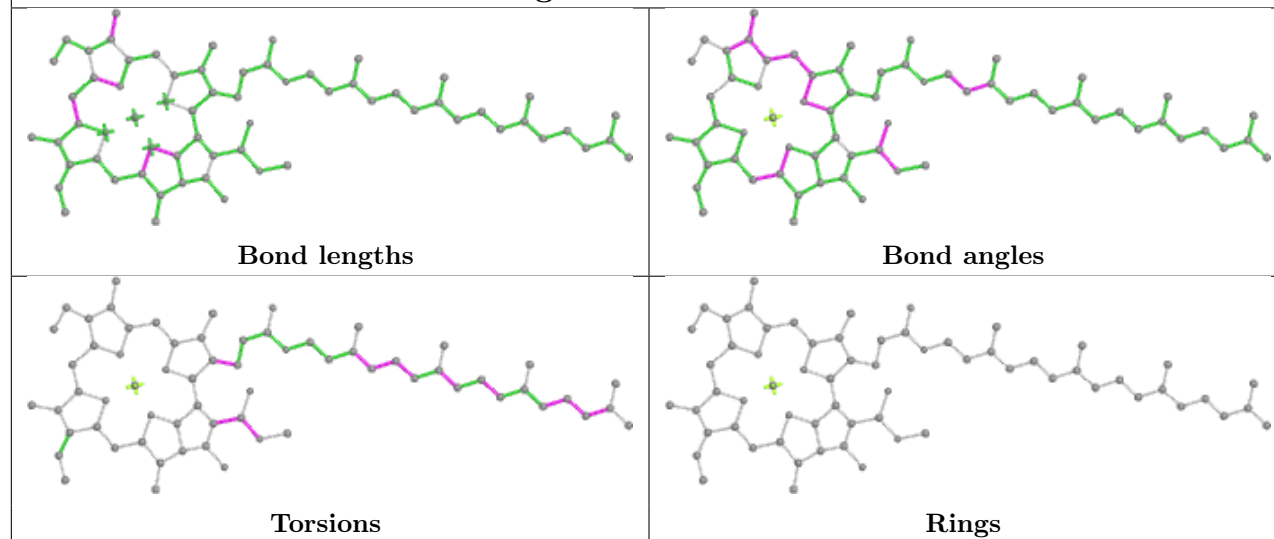
Ligand CLA b 823



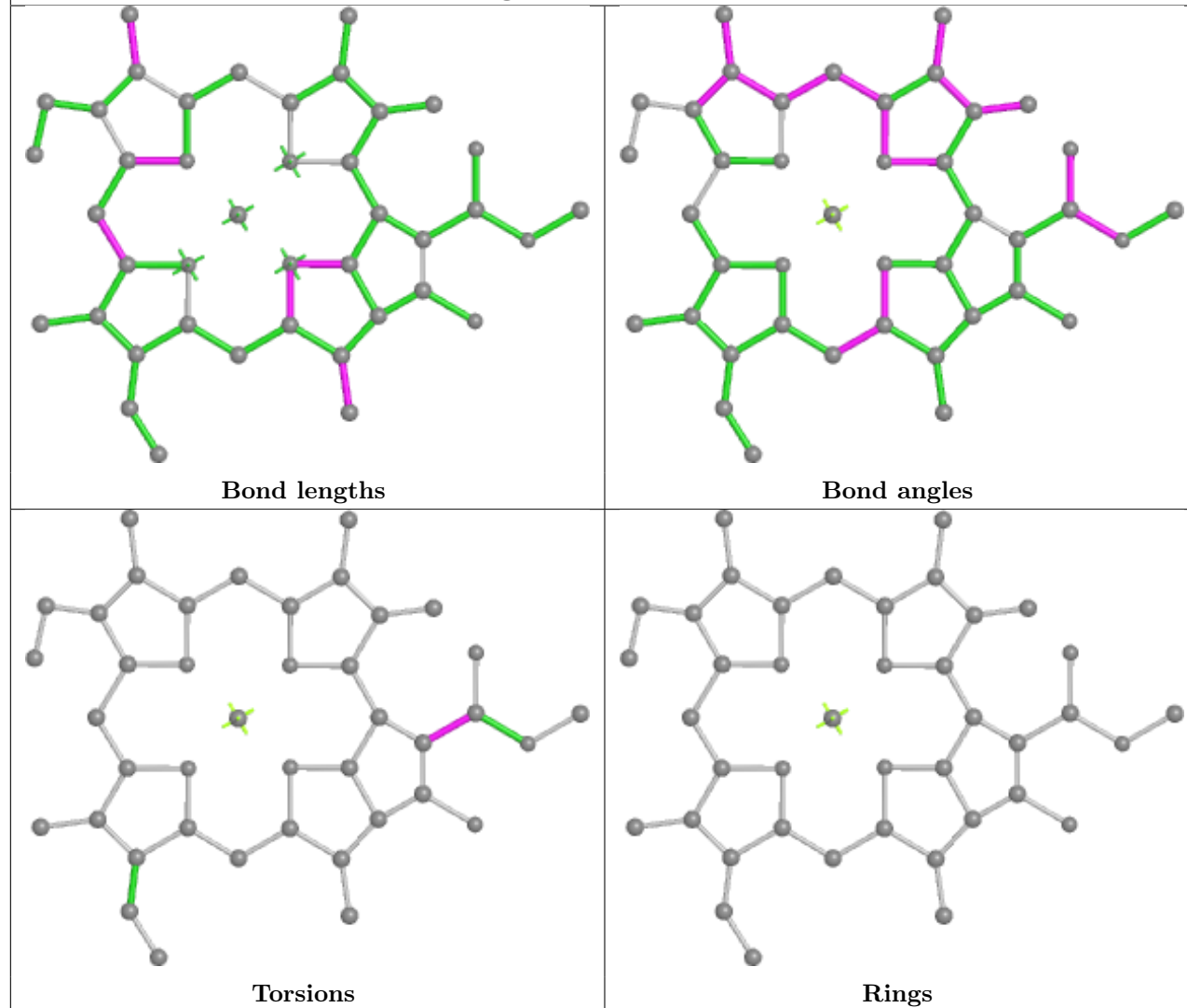
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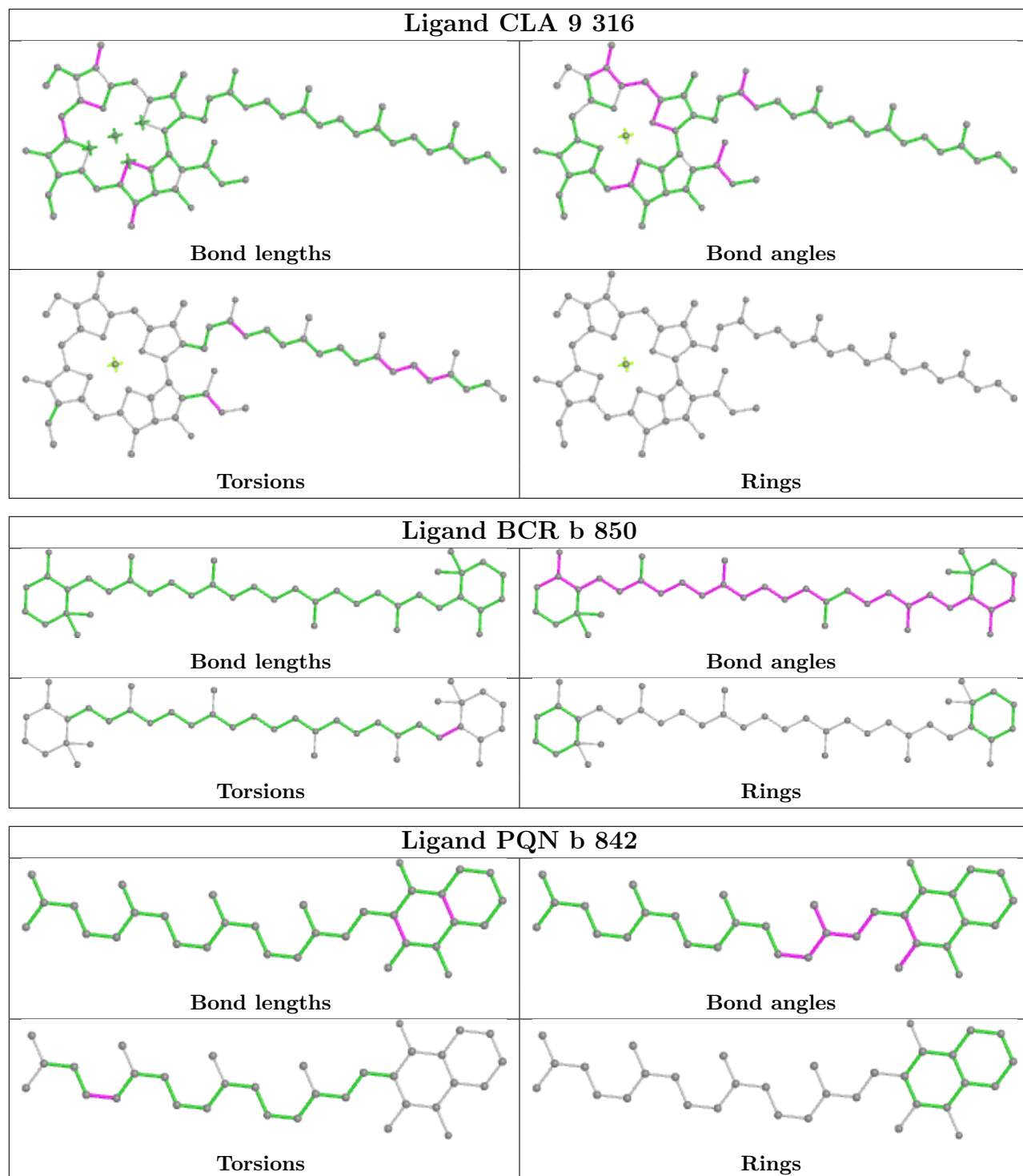


Ligand CLA b 813

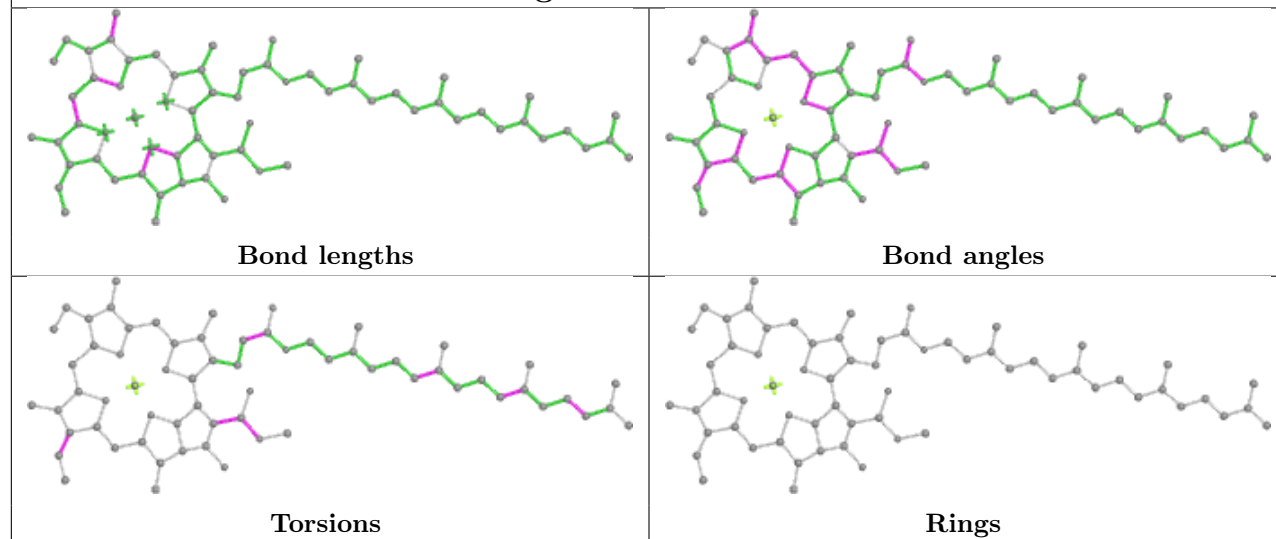


Ligand CLA b 830

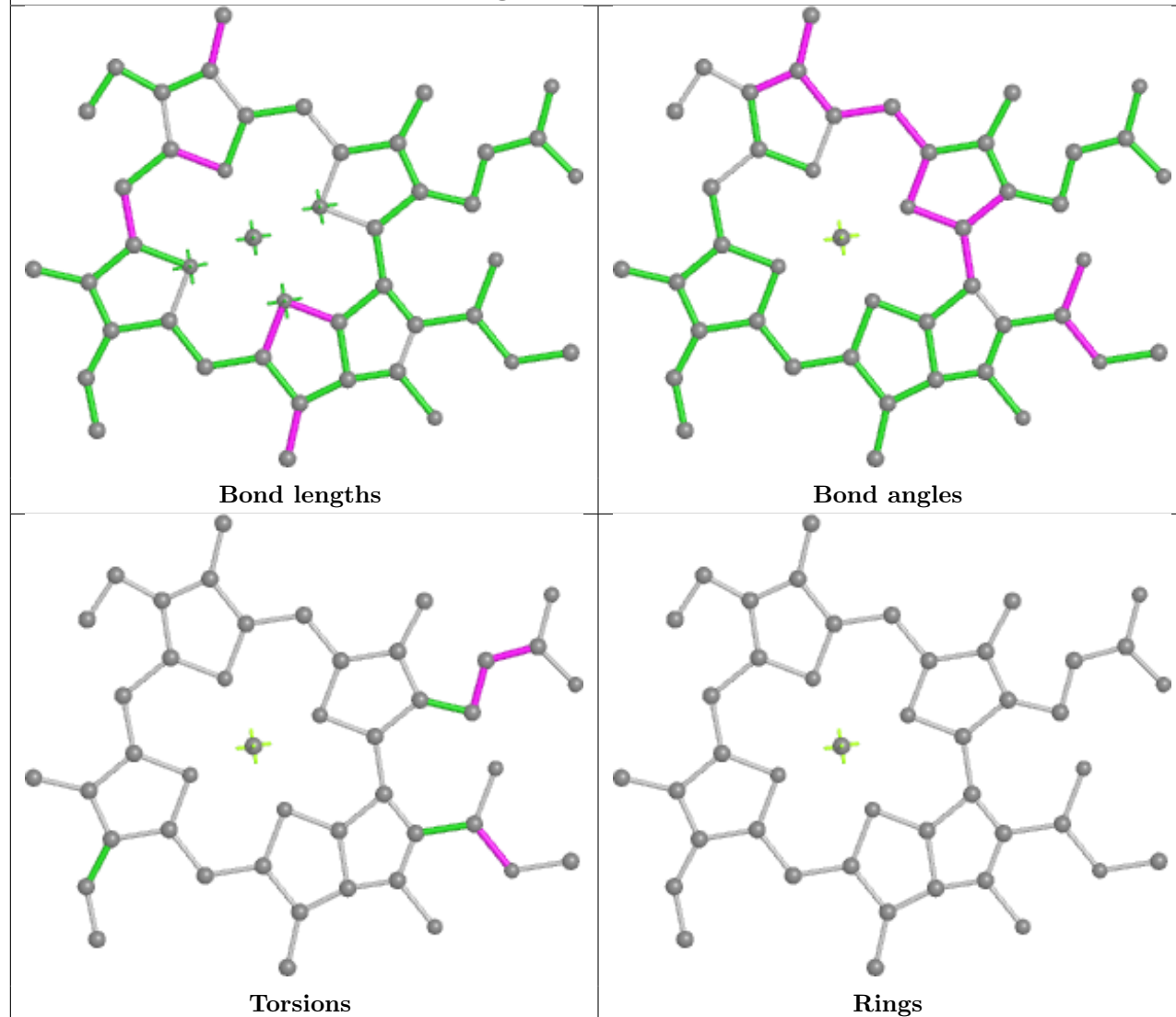


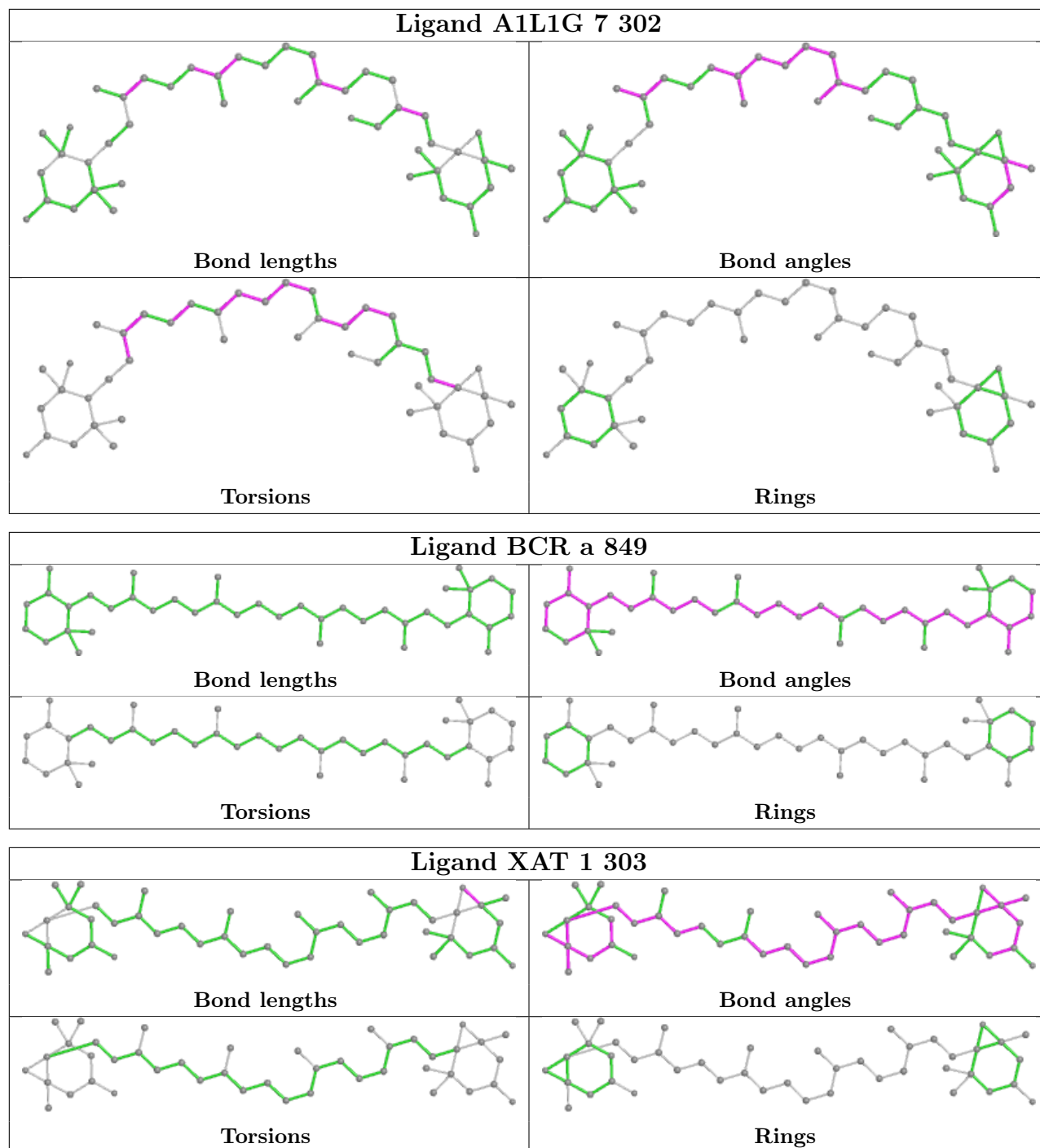


Ligand CLA b 803

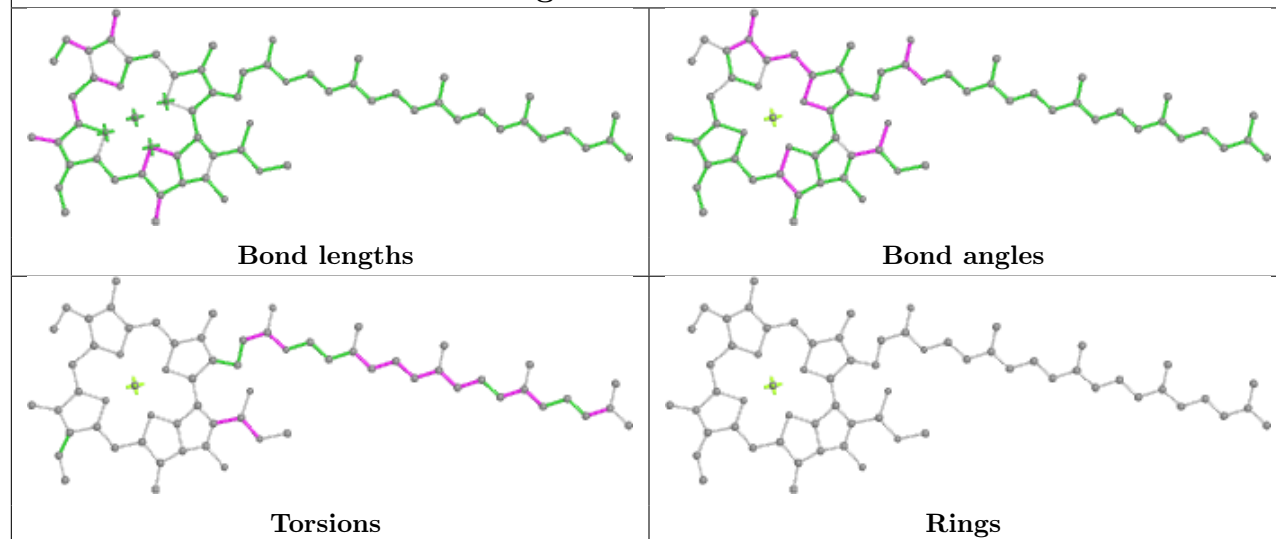


Ligand CLA 7 314

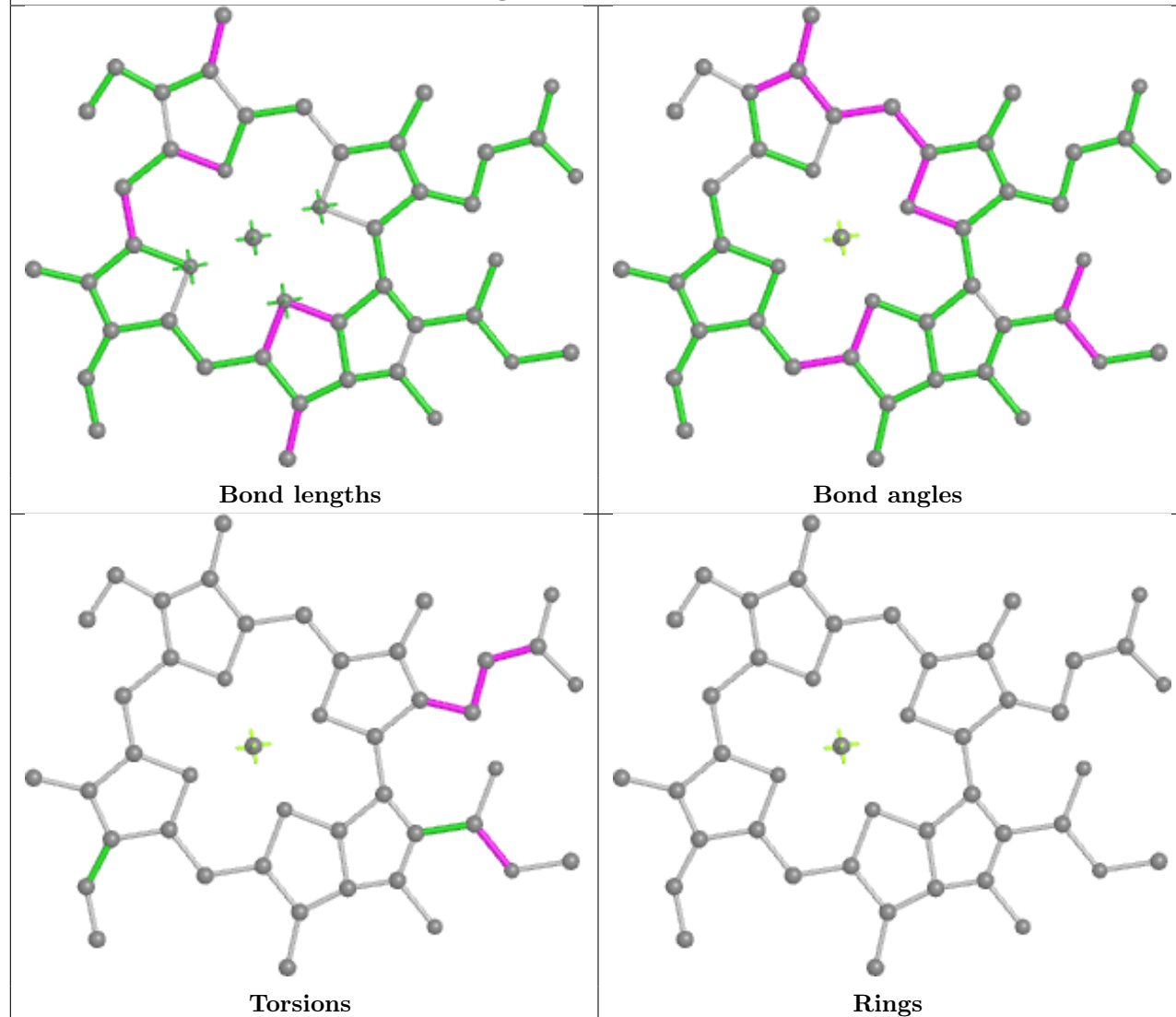




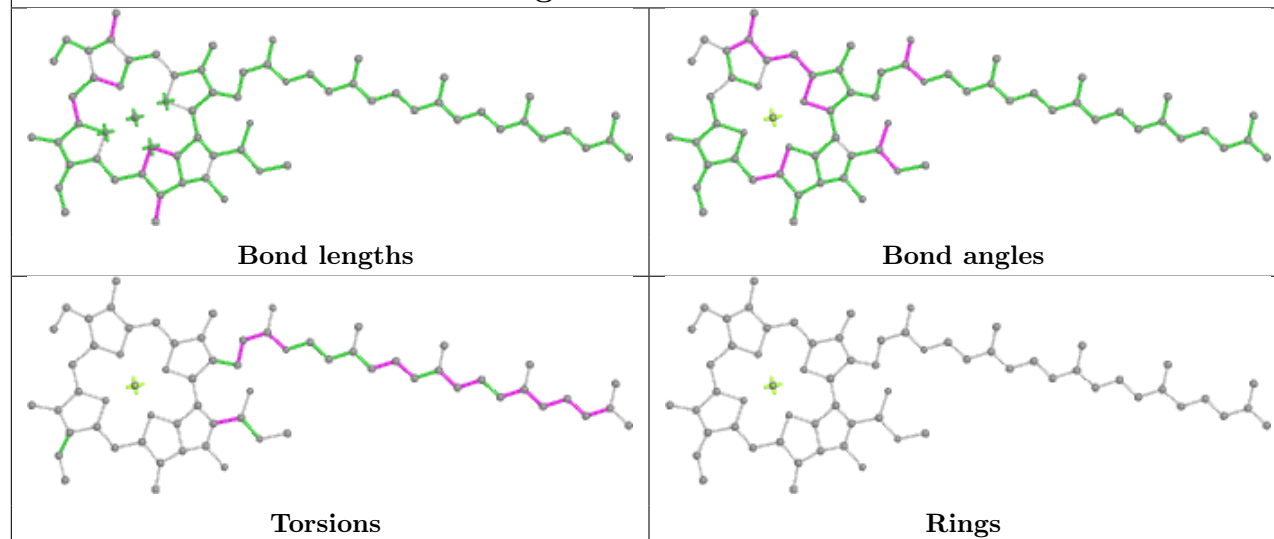
Ligand CLA a 801



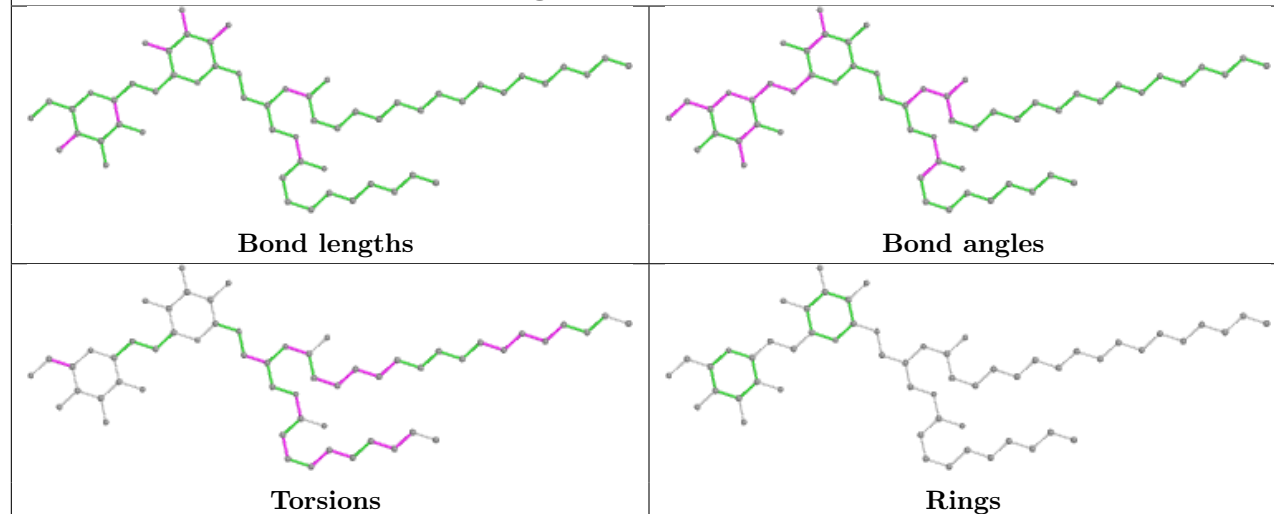
Ligand CLA 4 306



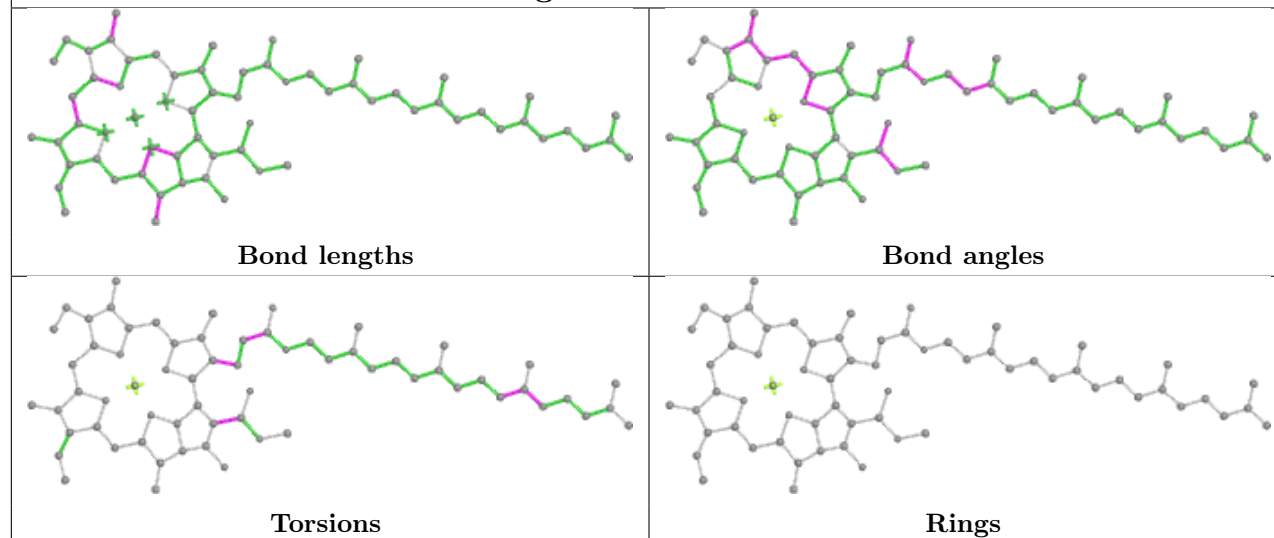
Ligand CLA b 801

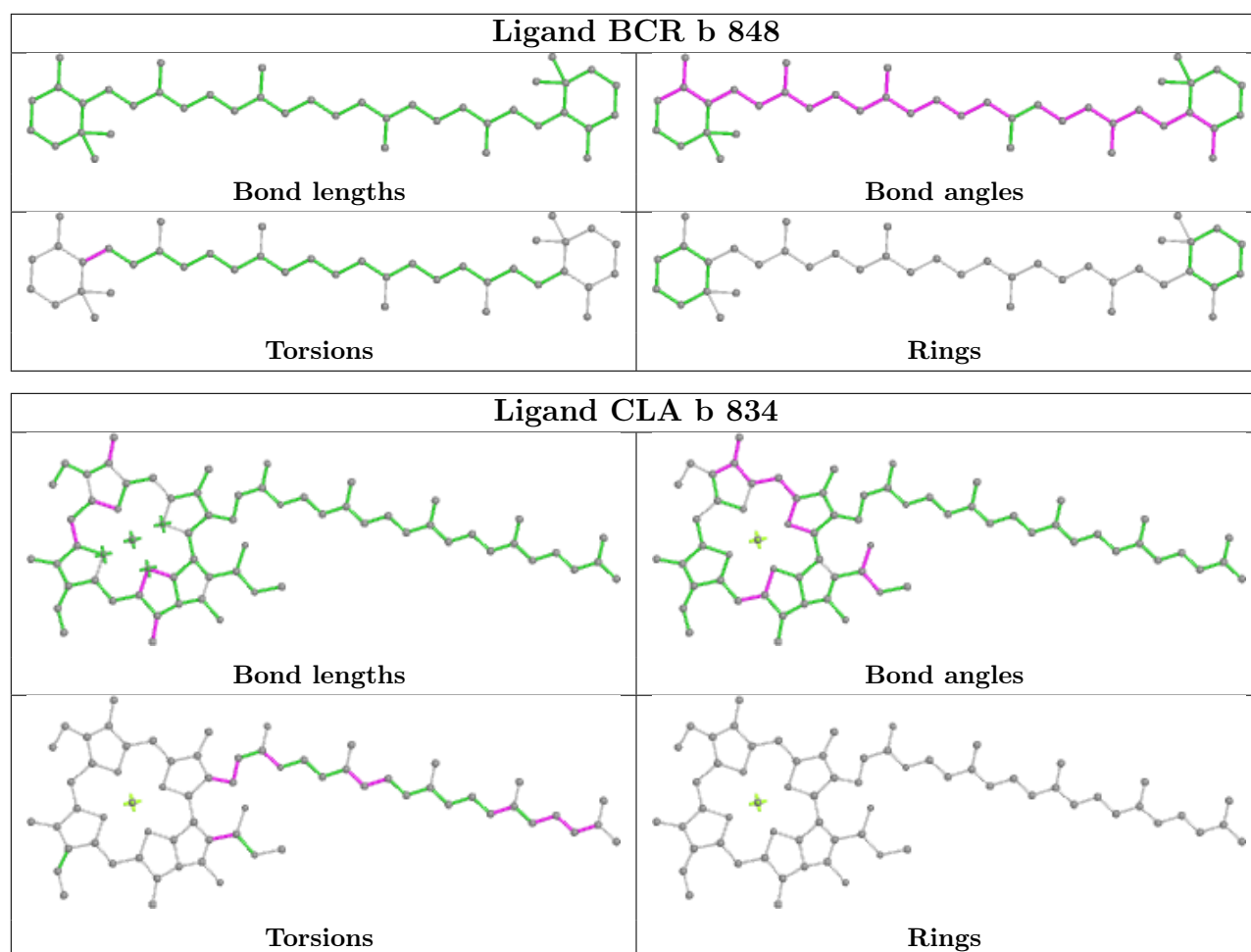


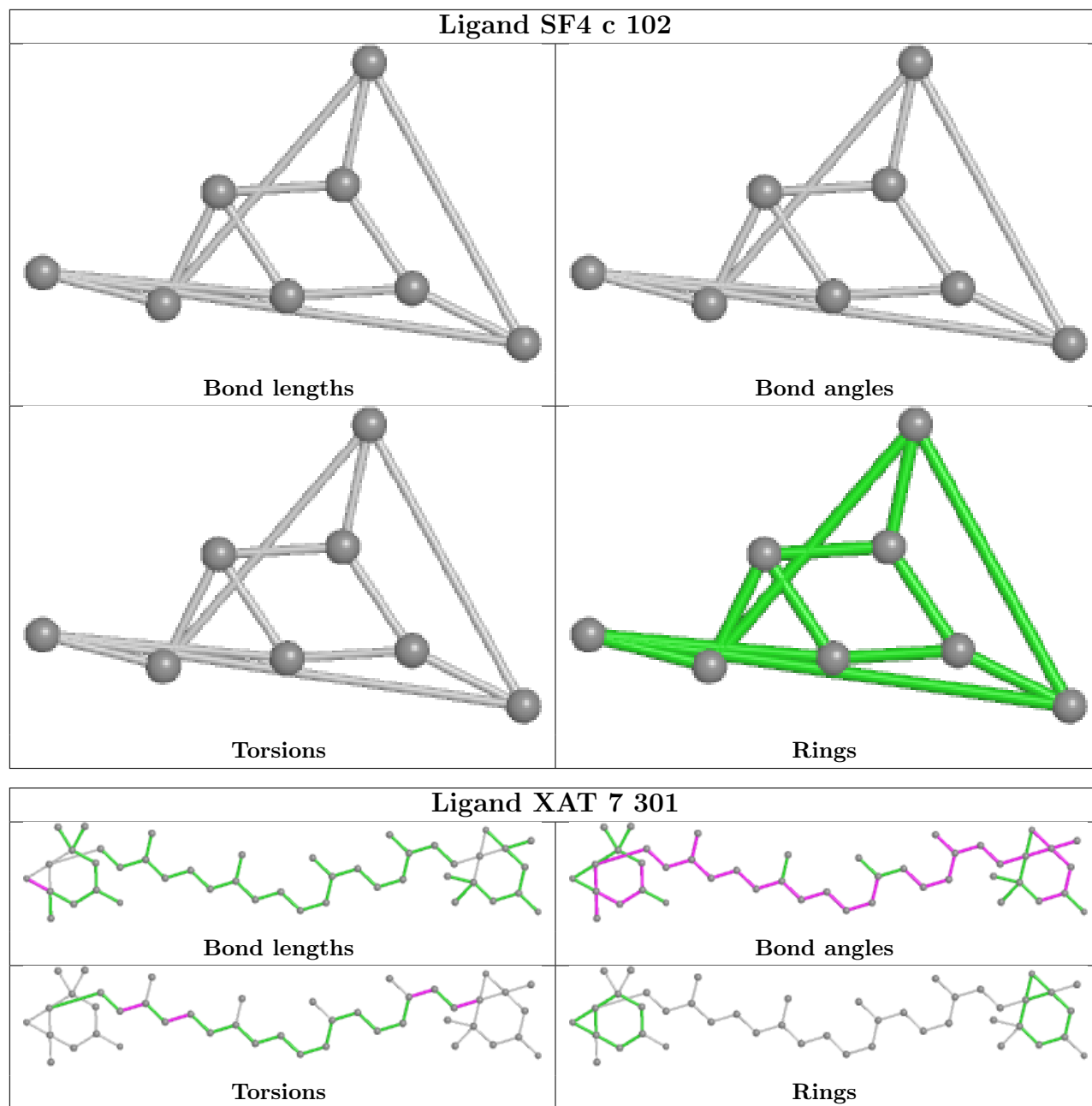
Ligand DGD b 851



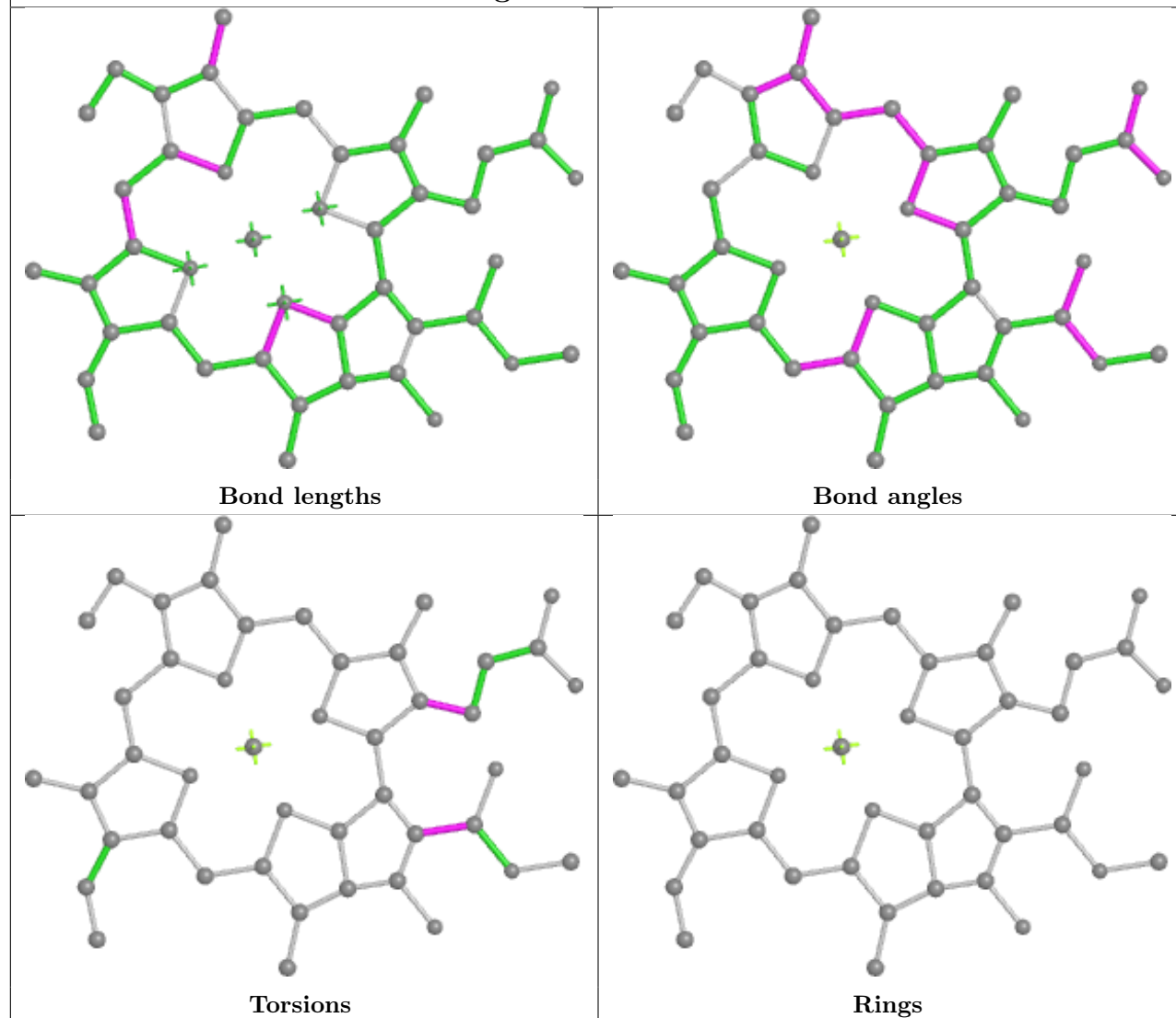
Ligand CLA b 838



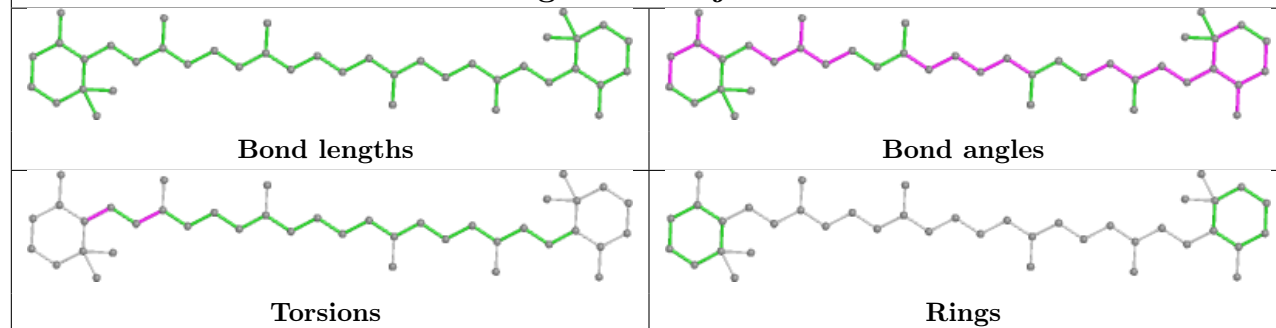


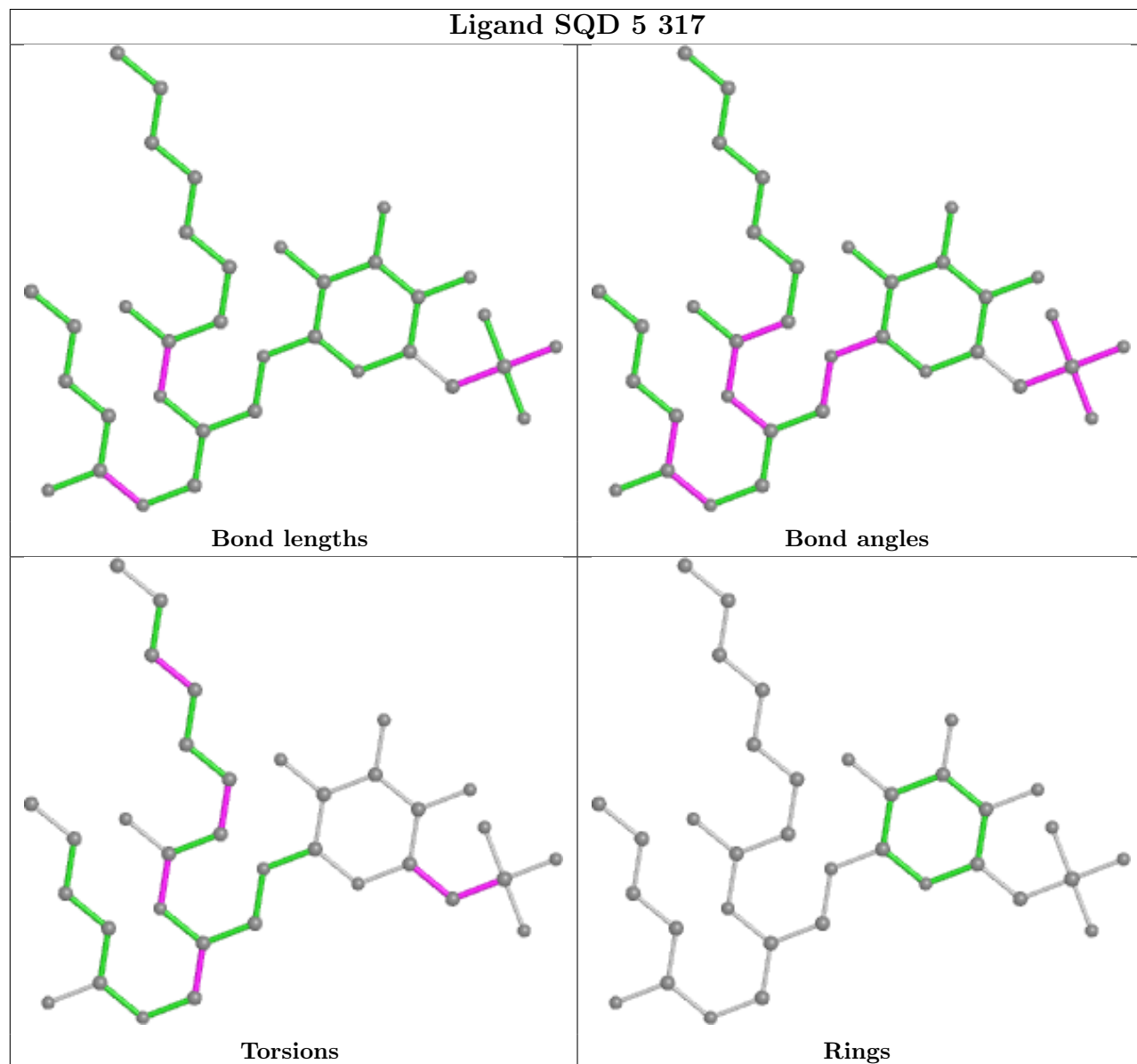
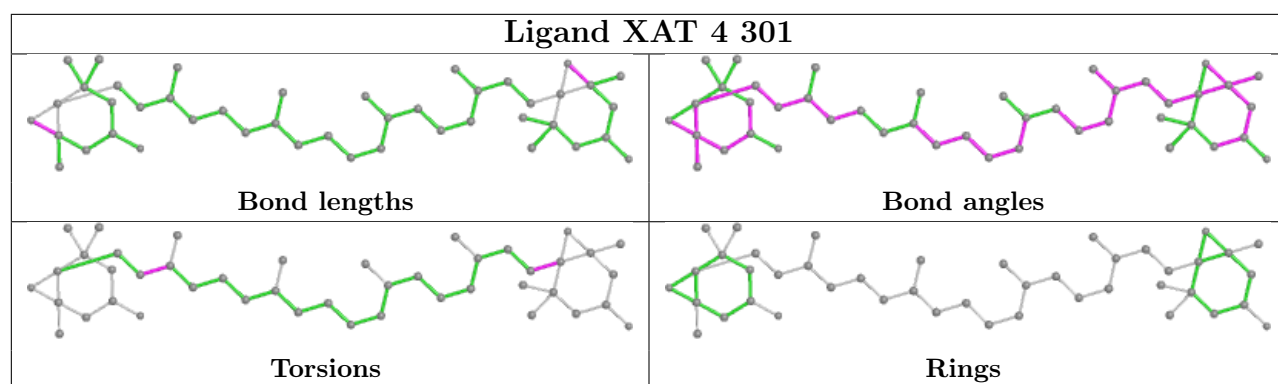


Ligand CLA a 815

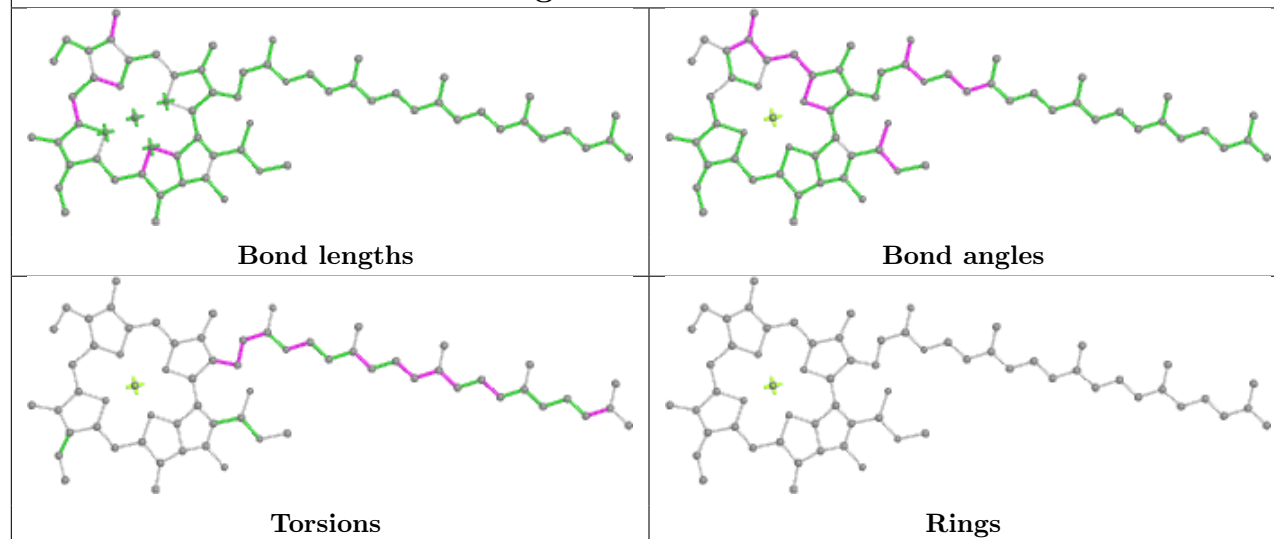


Ligand BCR j 102

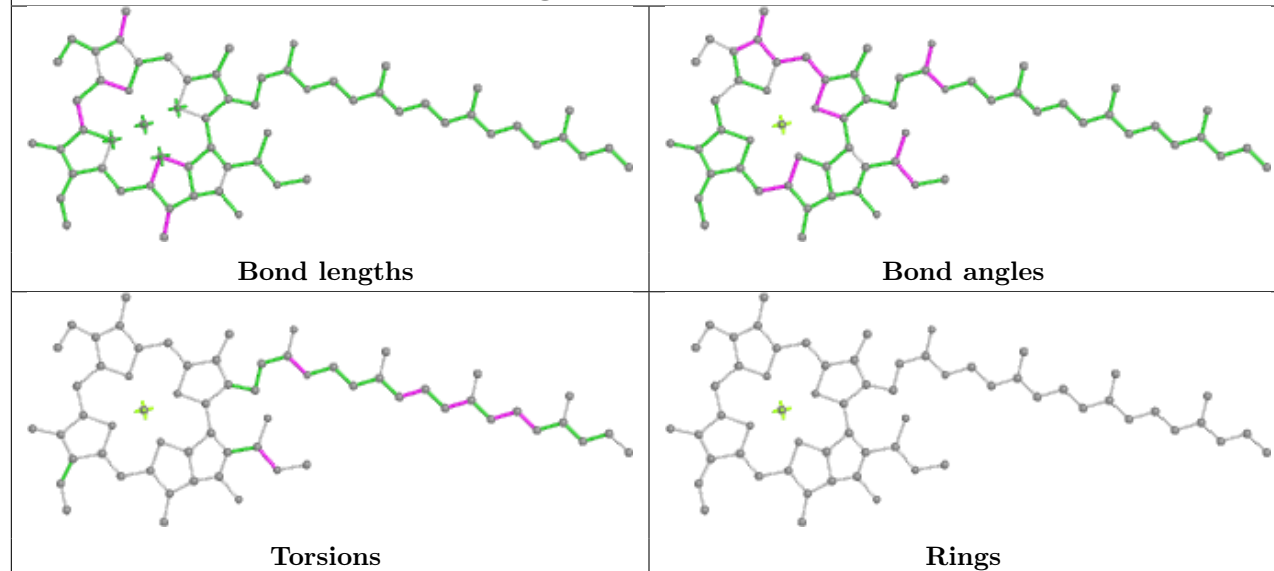




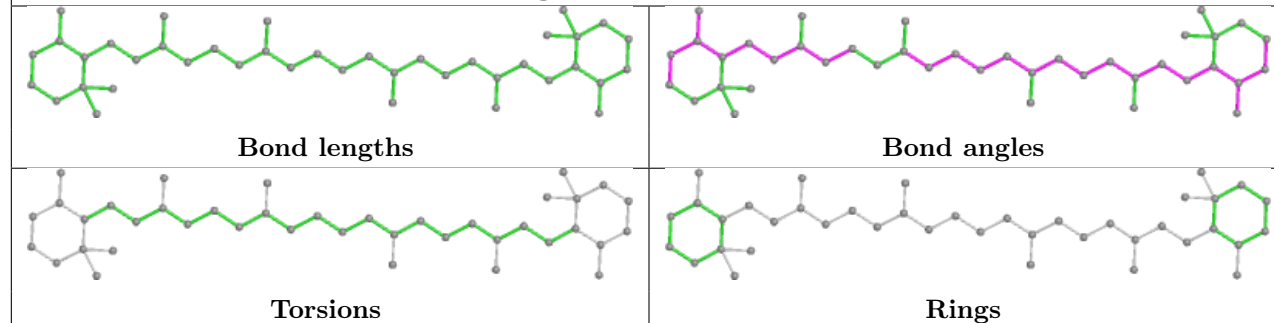
Ligand CLA b 809

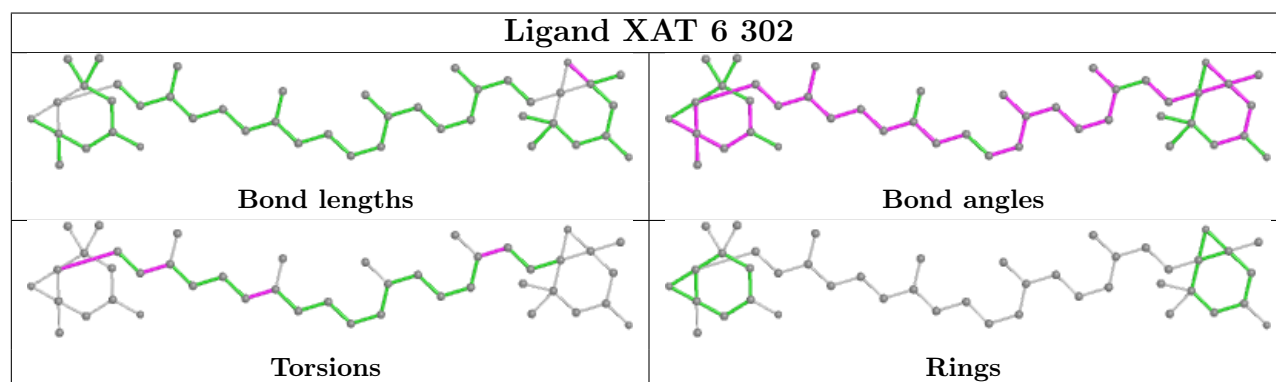
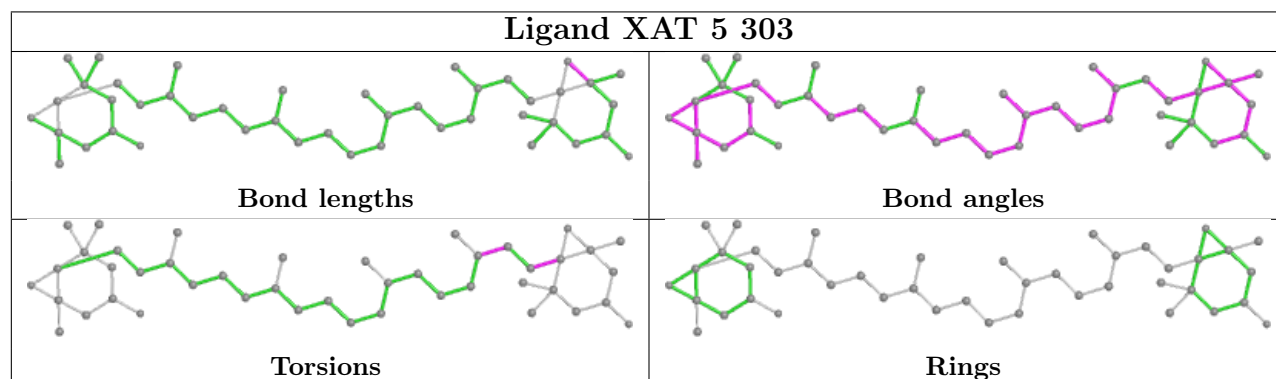
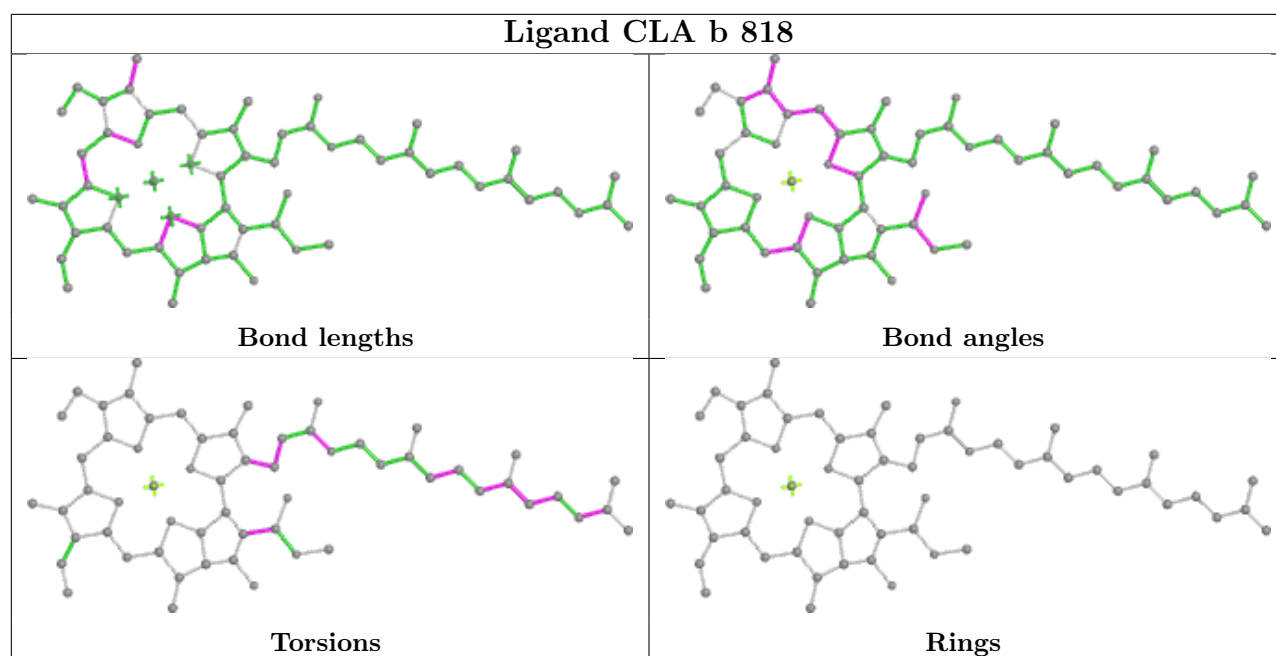


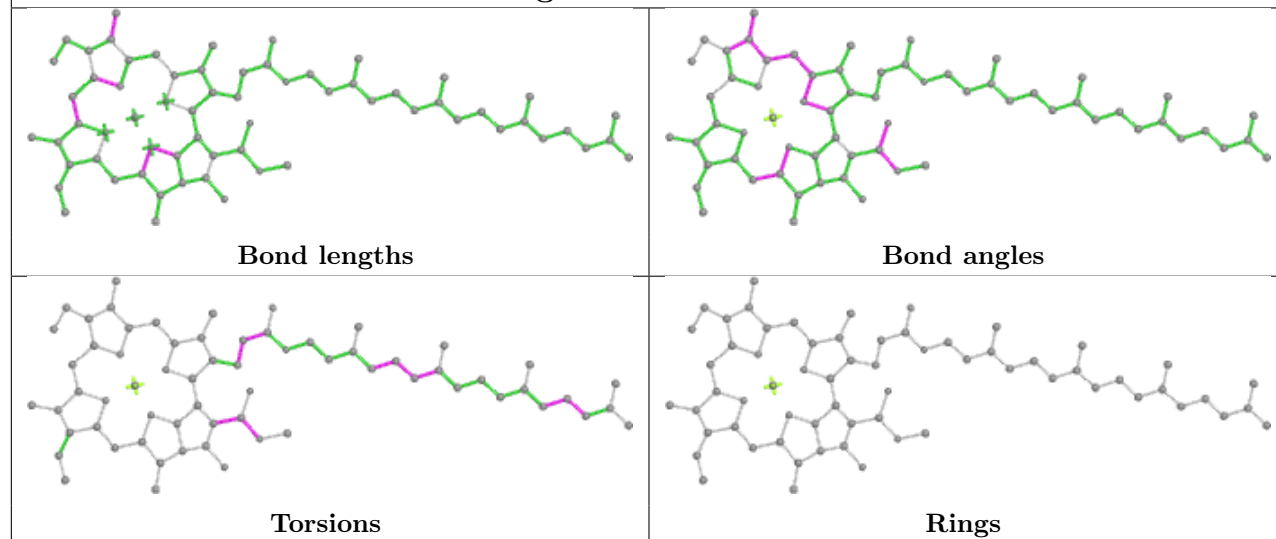
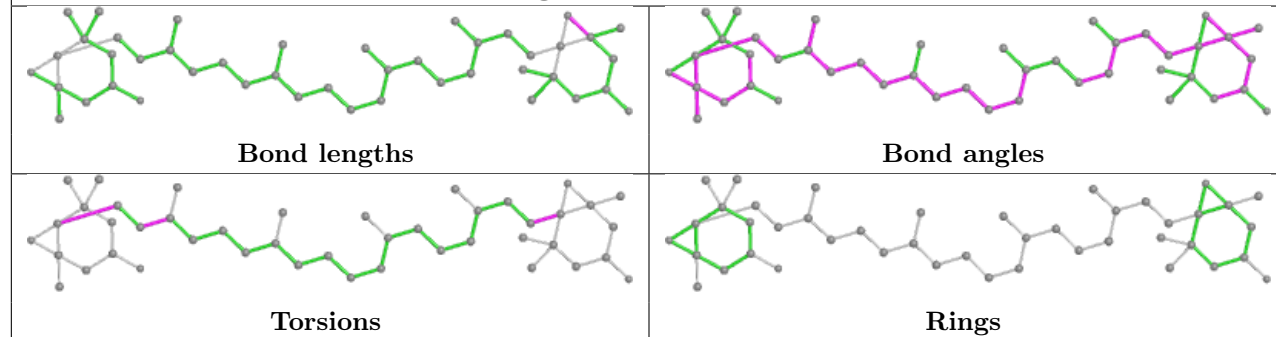
Ligand CLA a 812



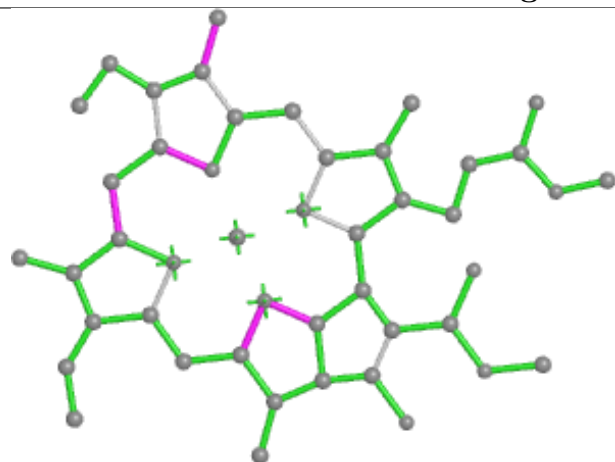
Ligand BCR a 847



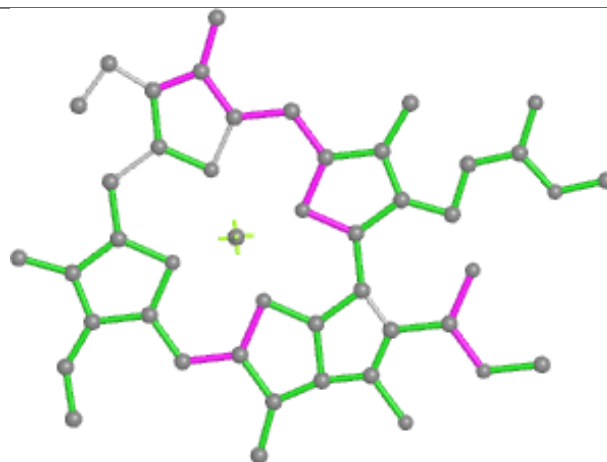


Ligand CLA 5 310**Ligand XAT 4 305**

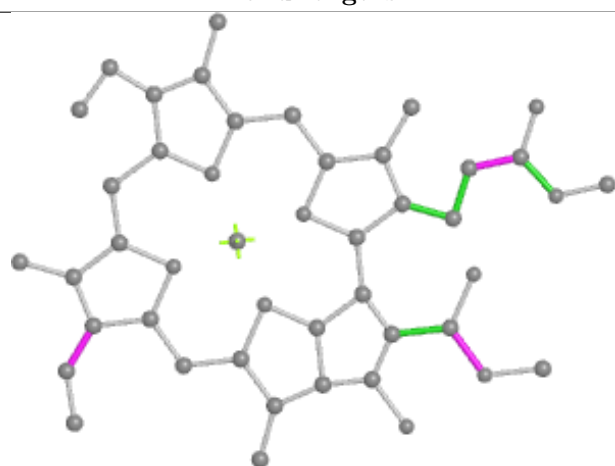
Ligand CLA 5 316



Bond lengths



Bond angles

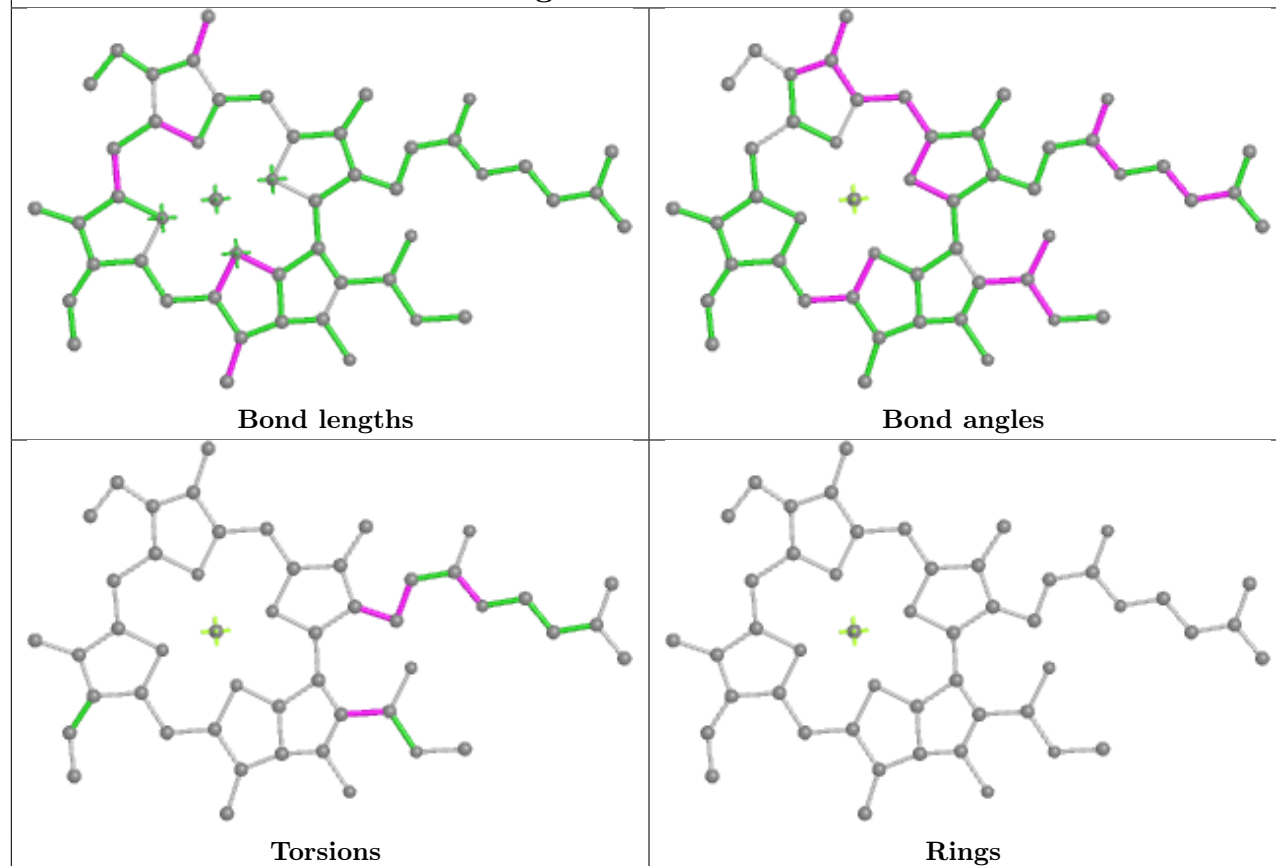


Torsions

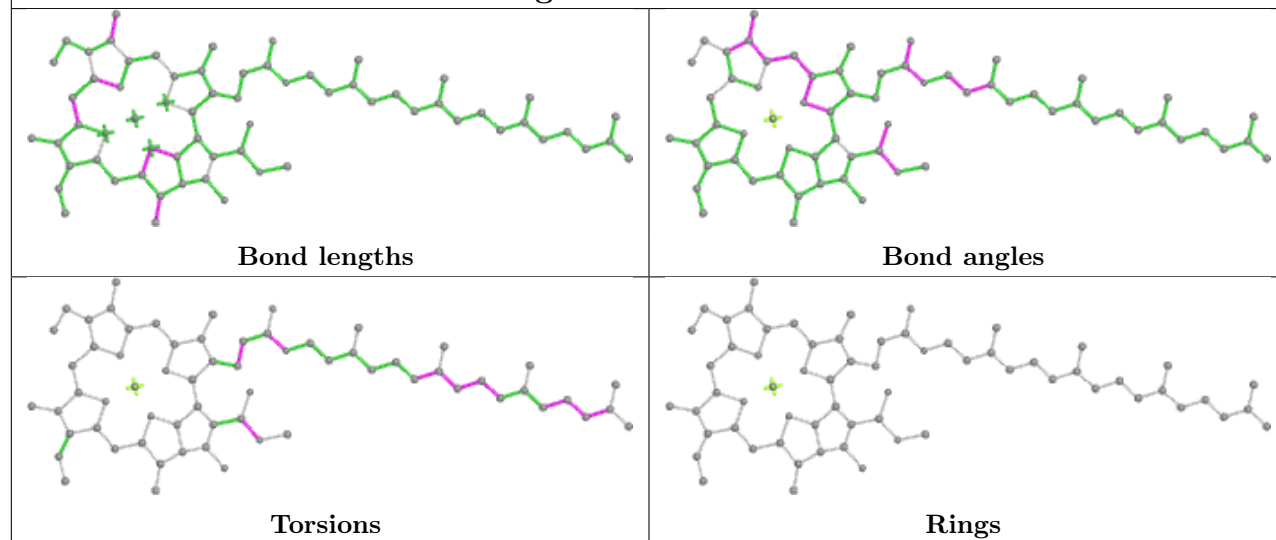


Rings

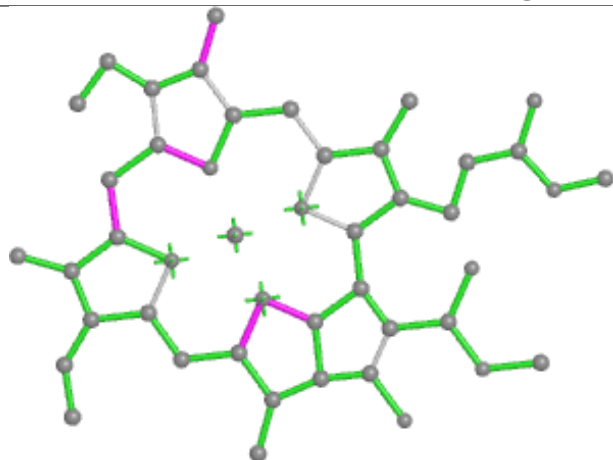
Ligand CLA b 820



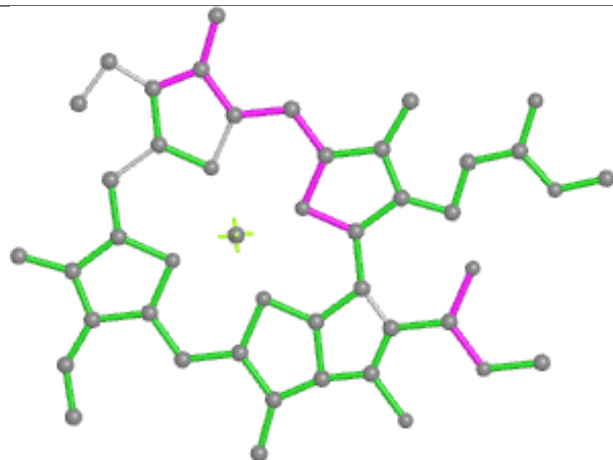
Ligand CLA b 827



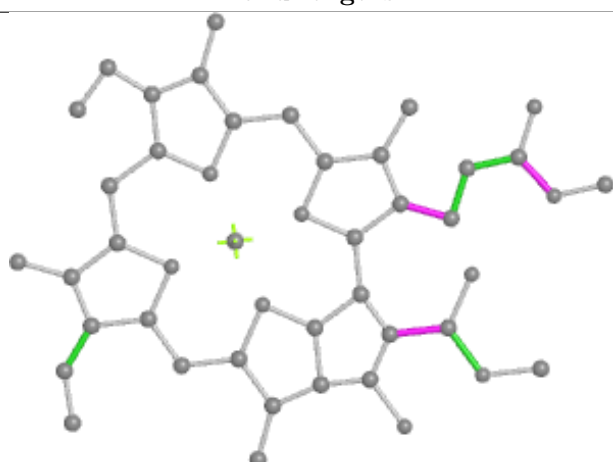
Ligand CLA 9 310



Bond lengths



Bond angles

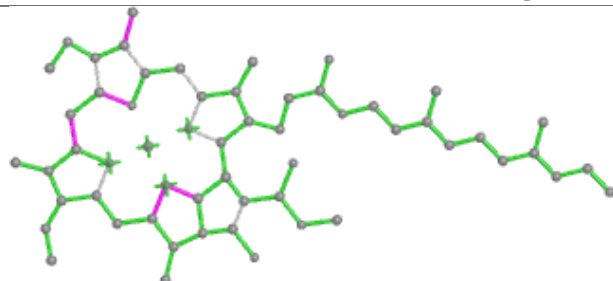


Torsions

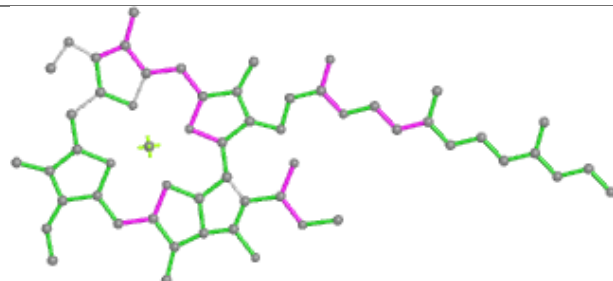


Rings

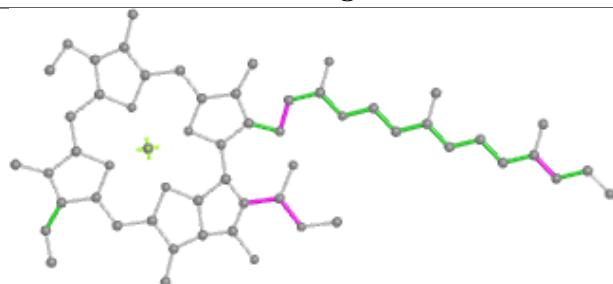
Ligand CLA 8 309



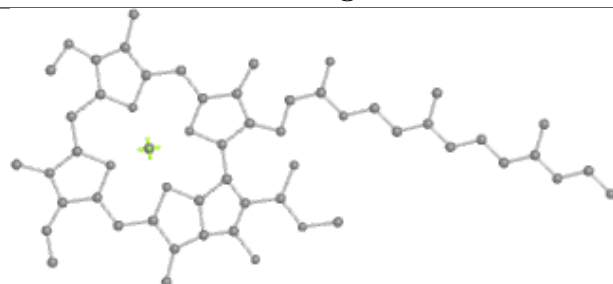
Bond lengths



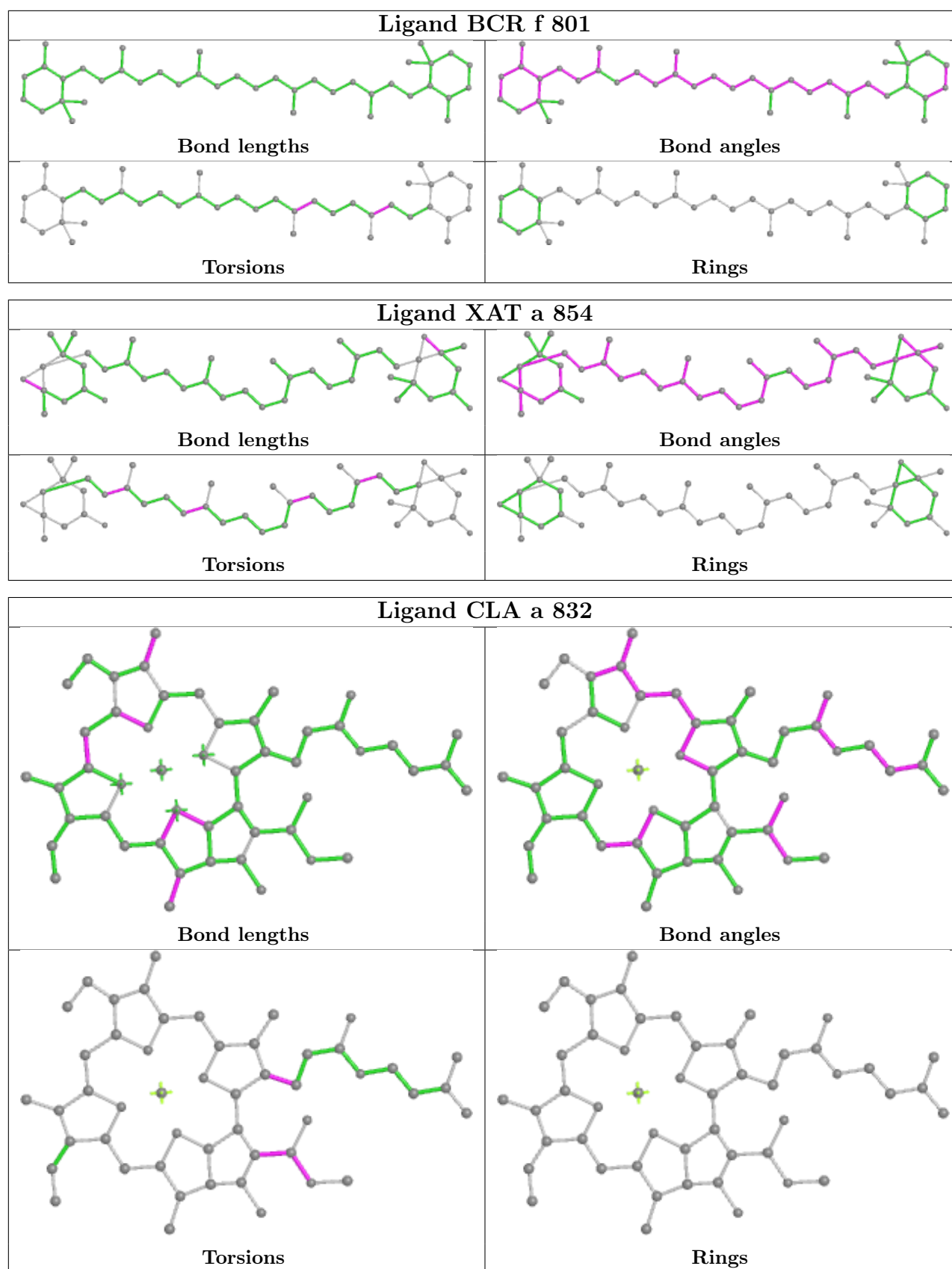
Bond angles

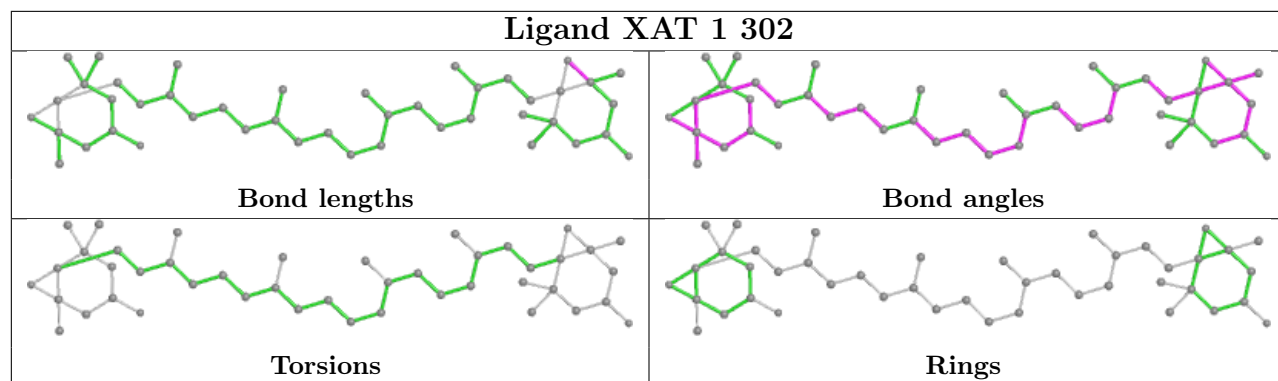
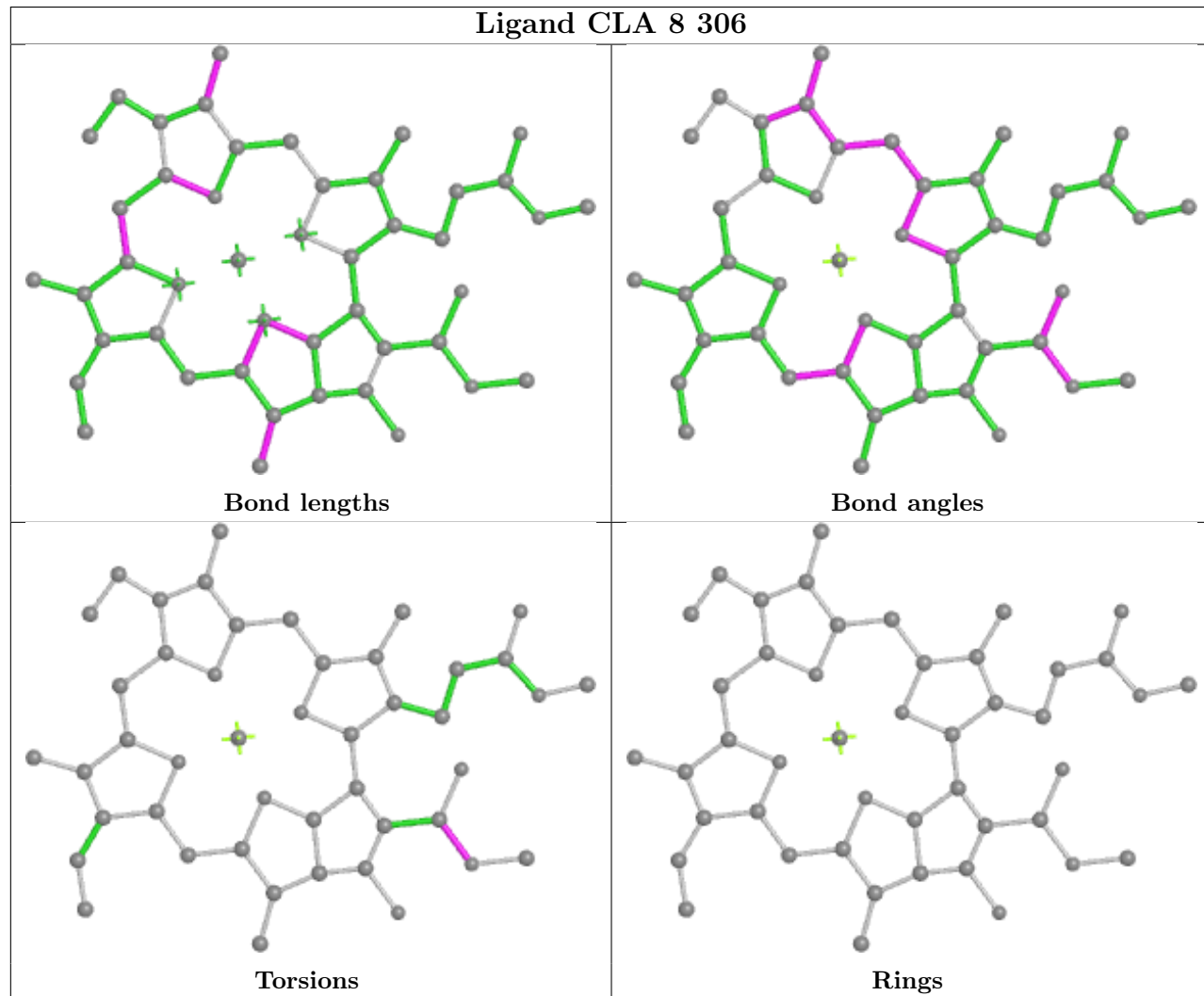


Torsions

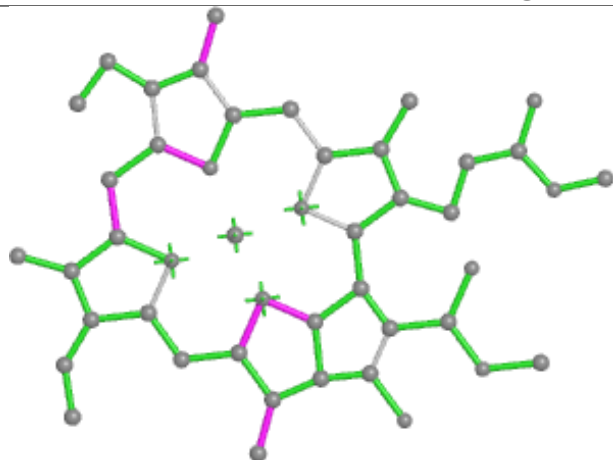


Rings

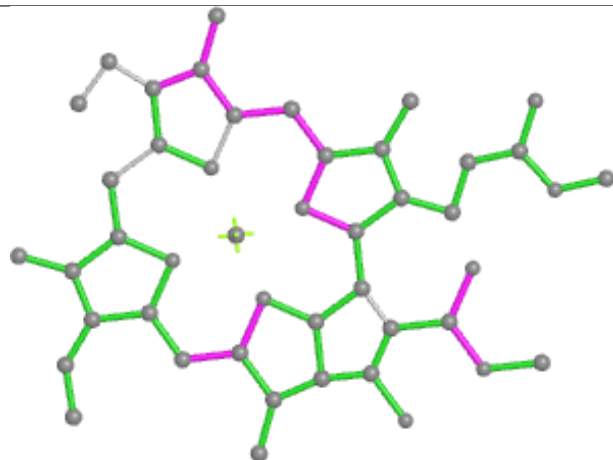


Ligand XAT 1 302**Ligand CLA 8 306**

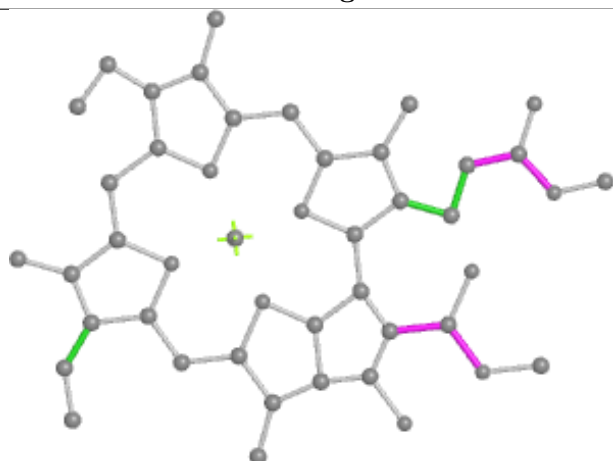
Ligand CLA 1 309



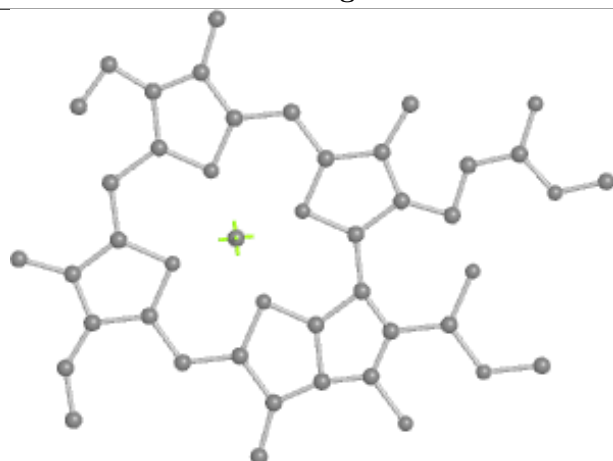
Bond lengths



Bond angles

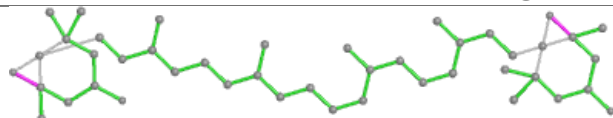


Torsions

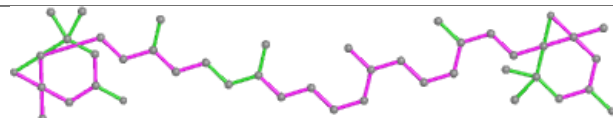


Rings

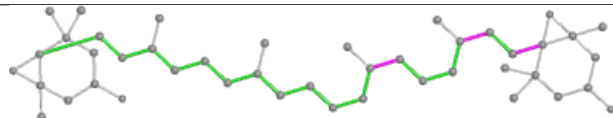
Ligand XAT 6 303



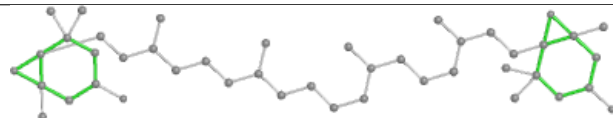
Bond lengths



Bond angles

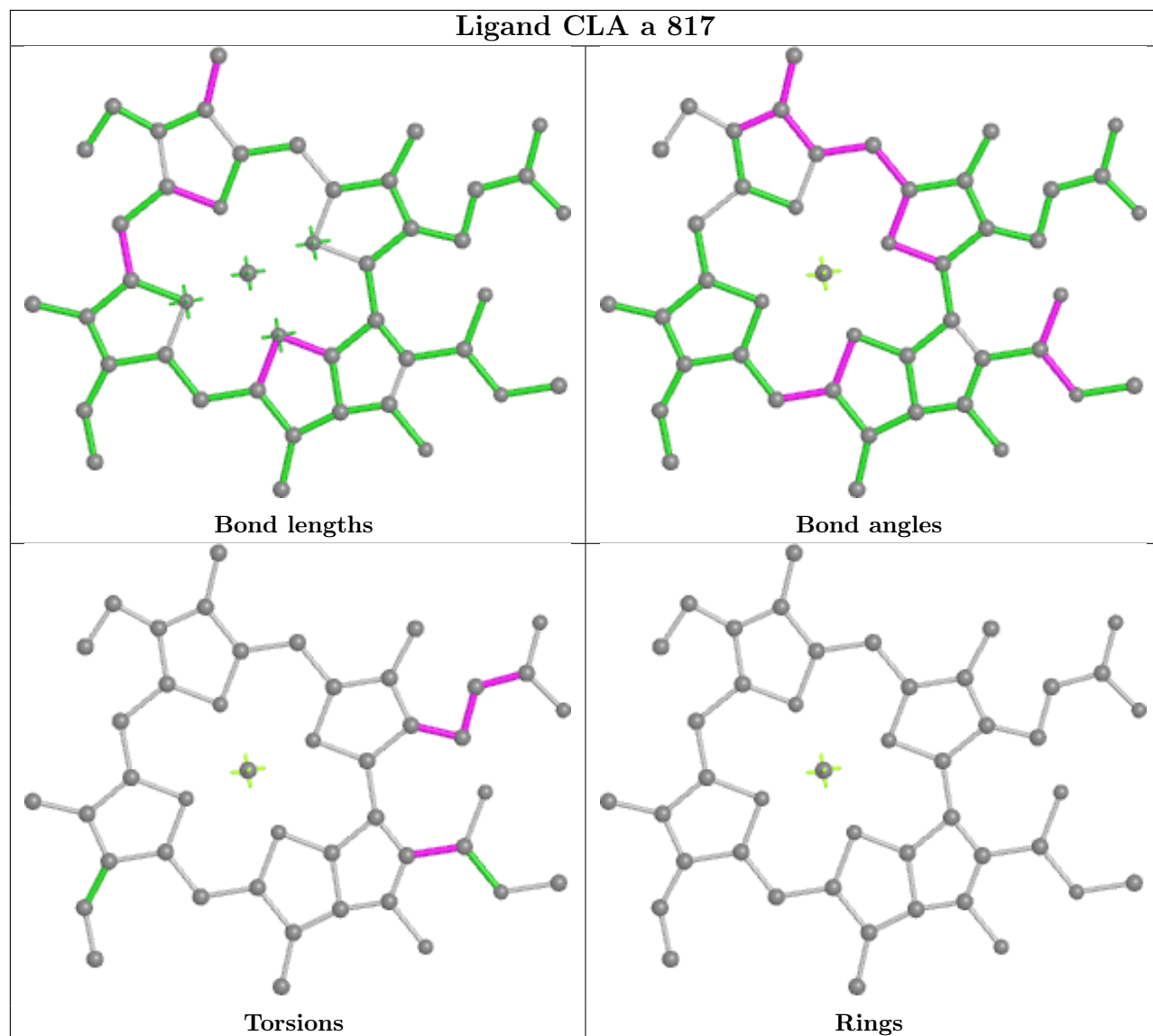


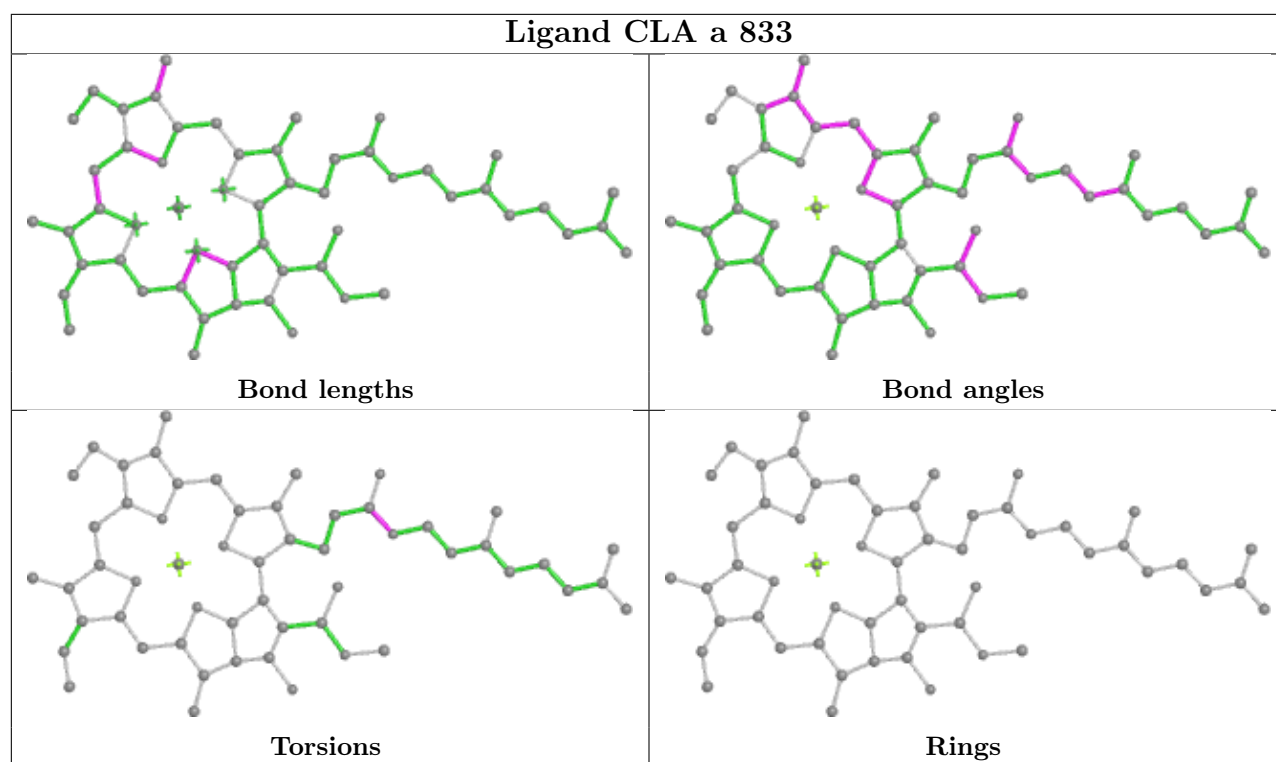
Torsions



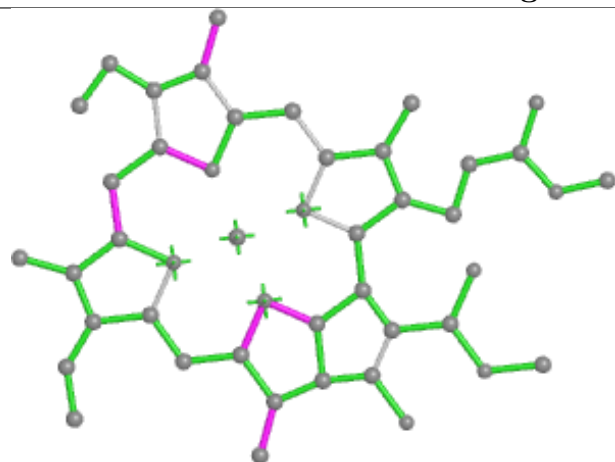
Rings

Ligand CLA a 817

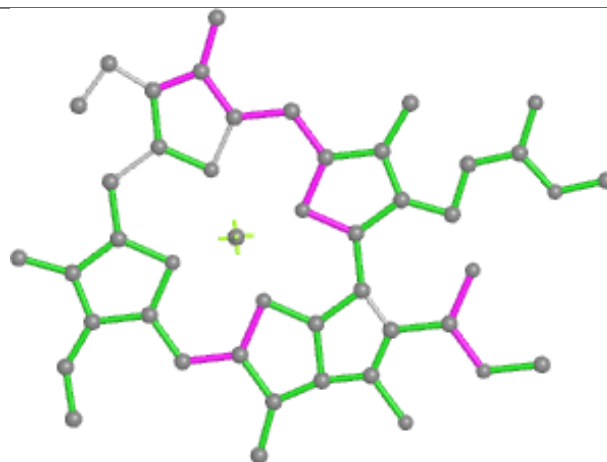




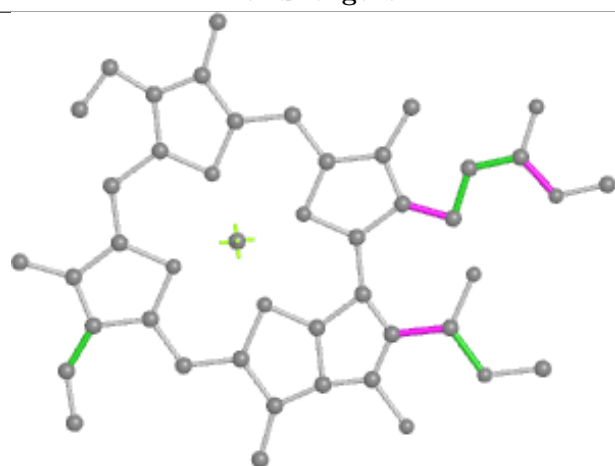
Ligand CLA 7 311



Bond lengths



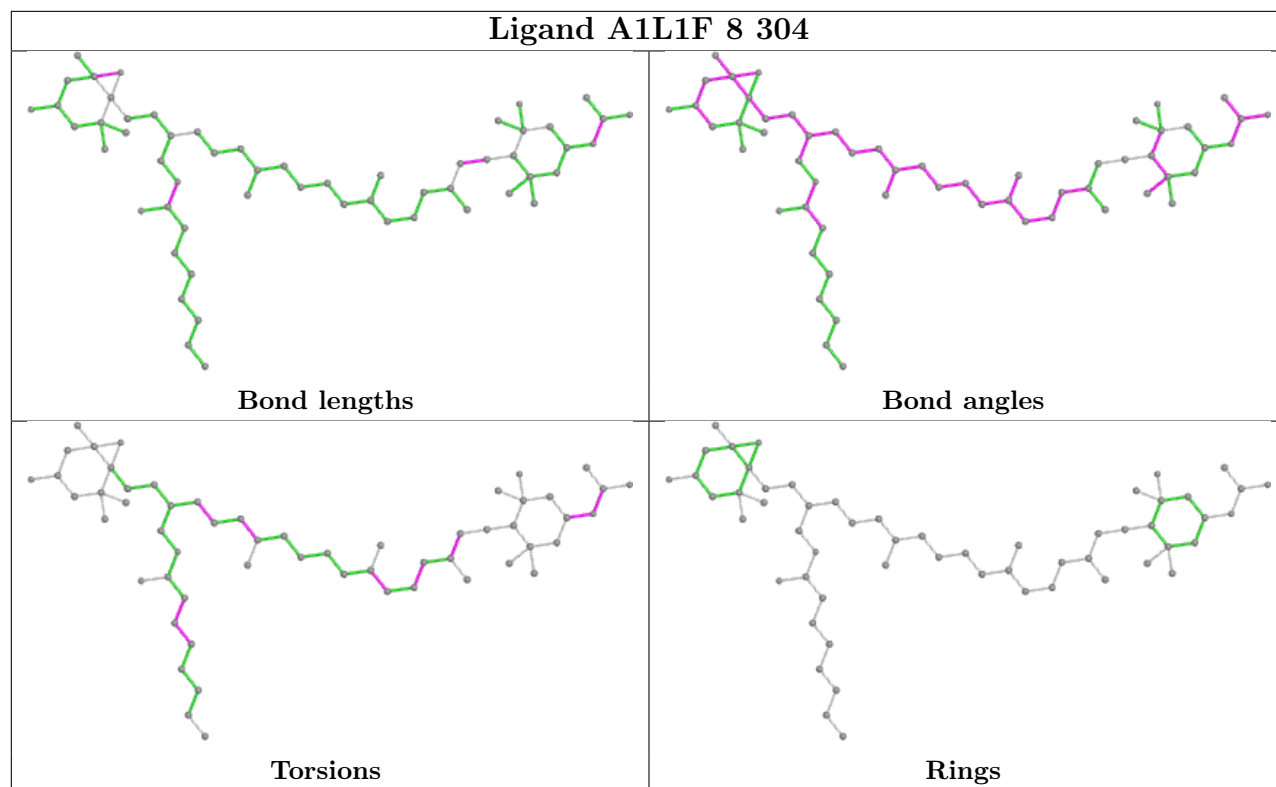
Bond angles



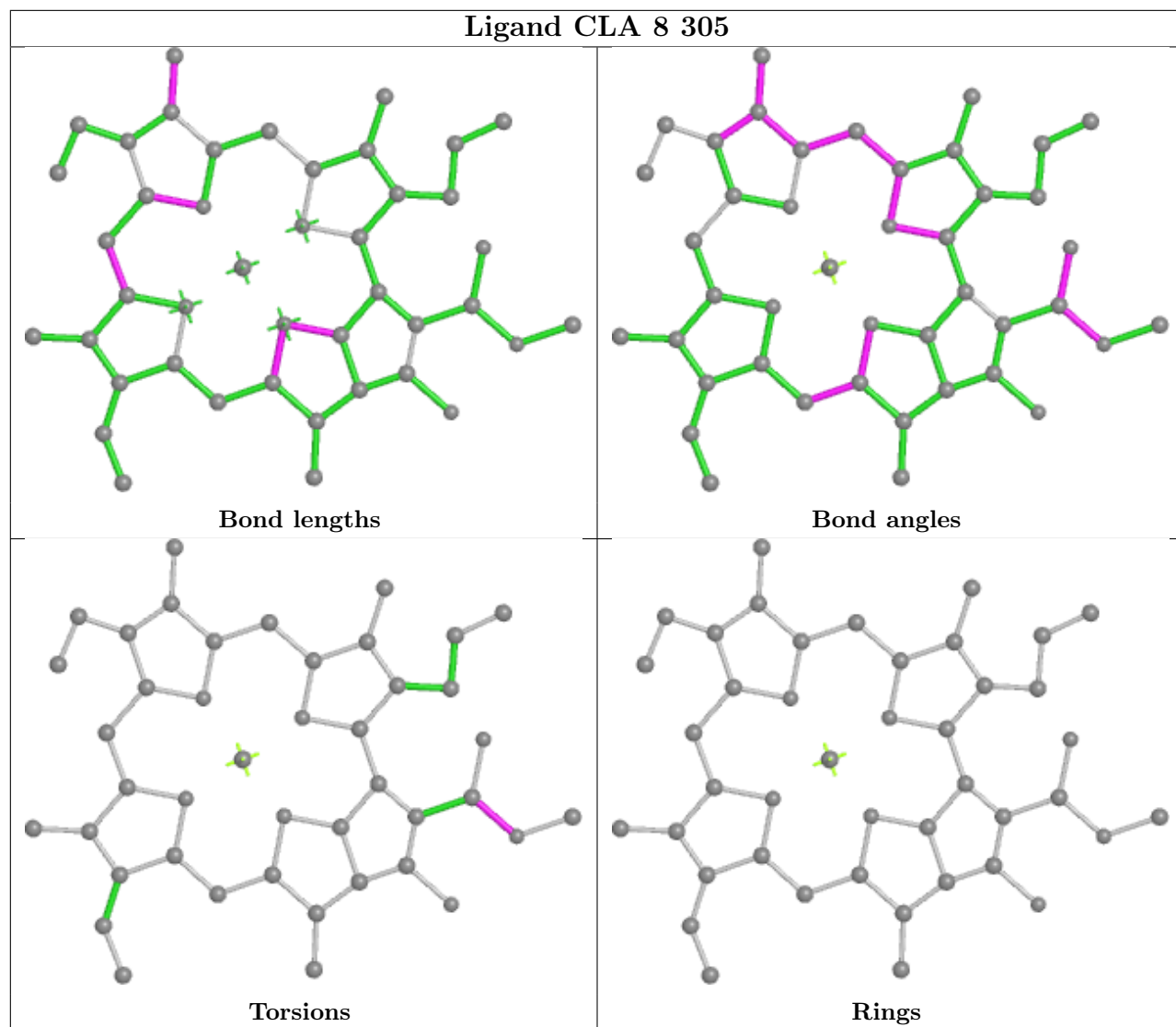
Torsions



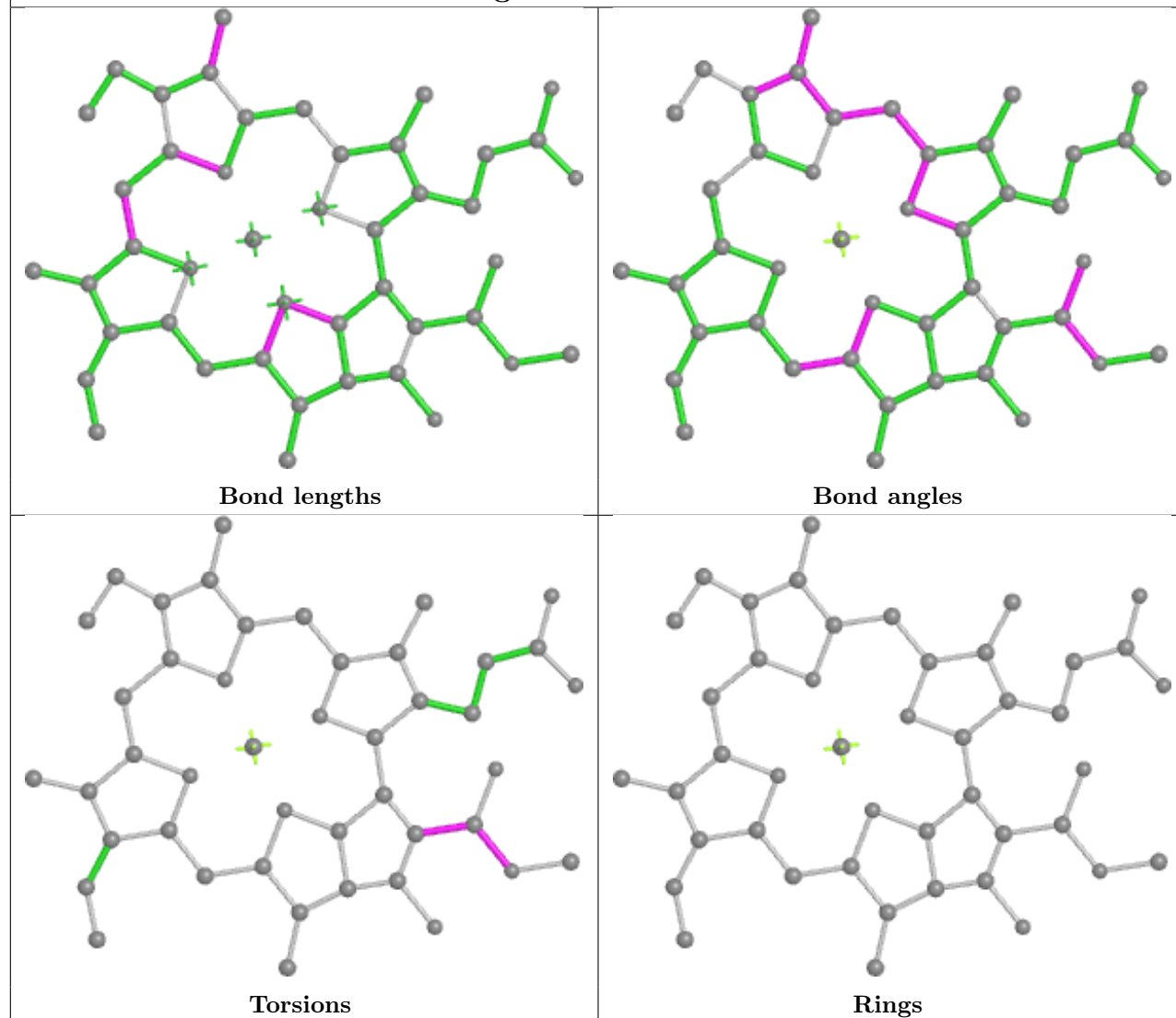
Rings



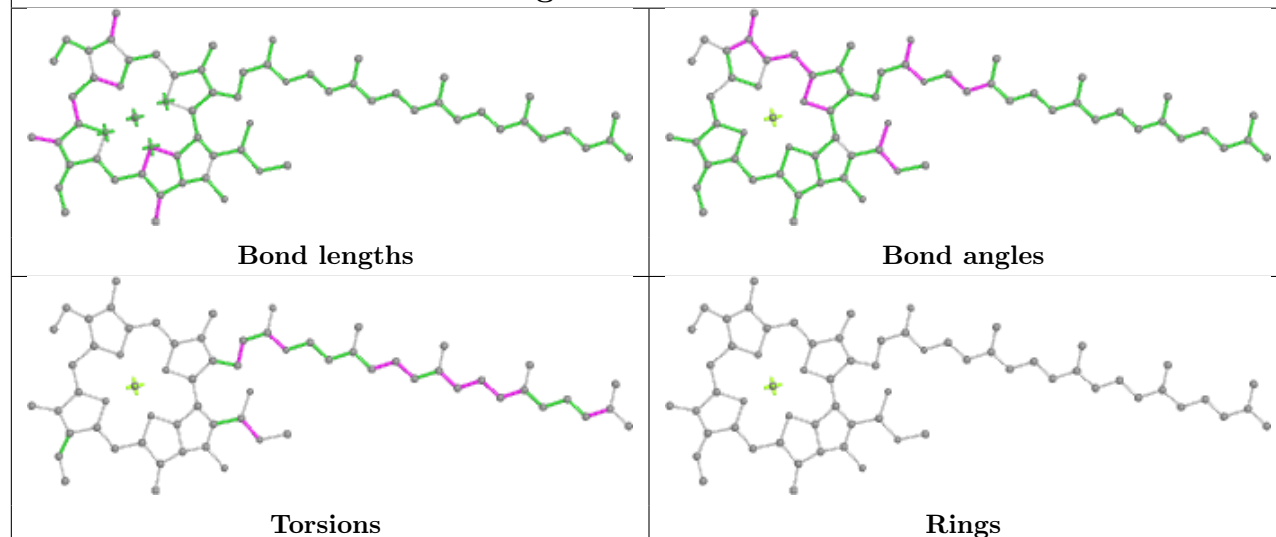
Ligand CLA 8 305



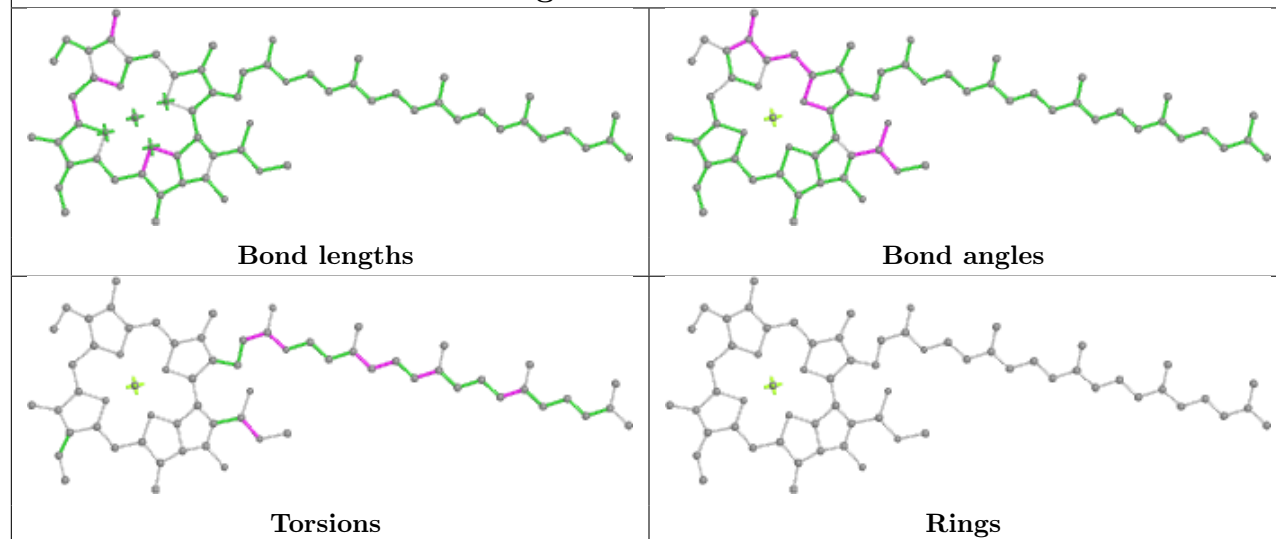
Ligand CLA a 837



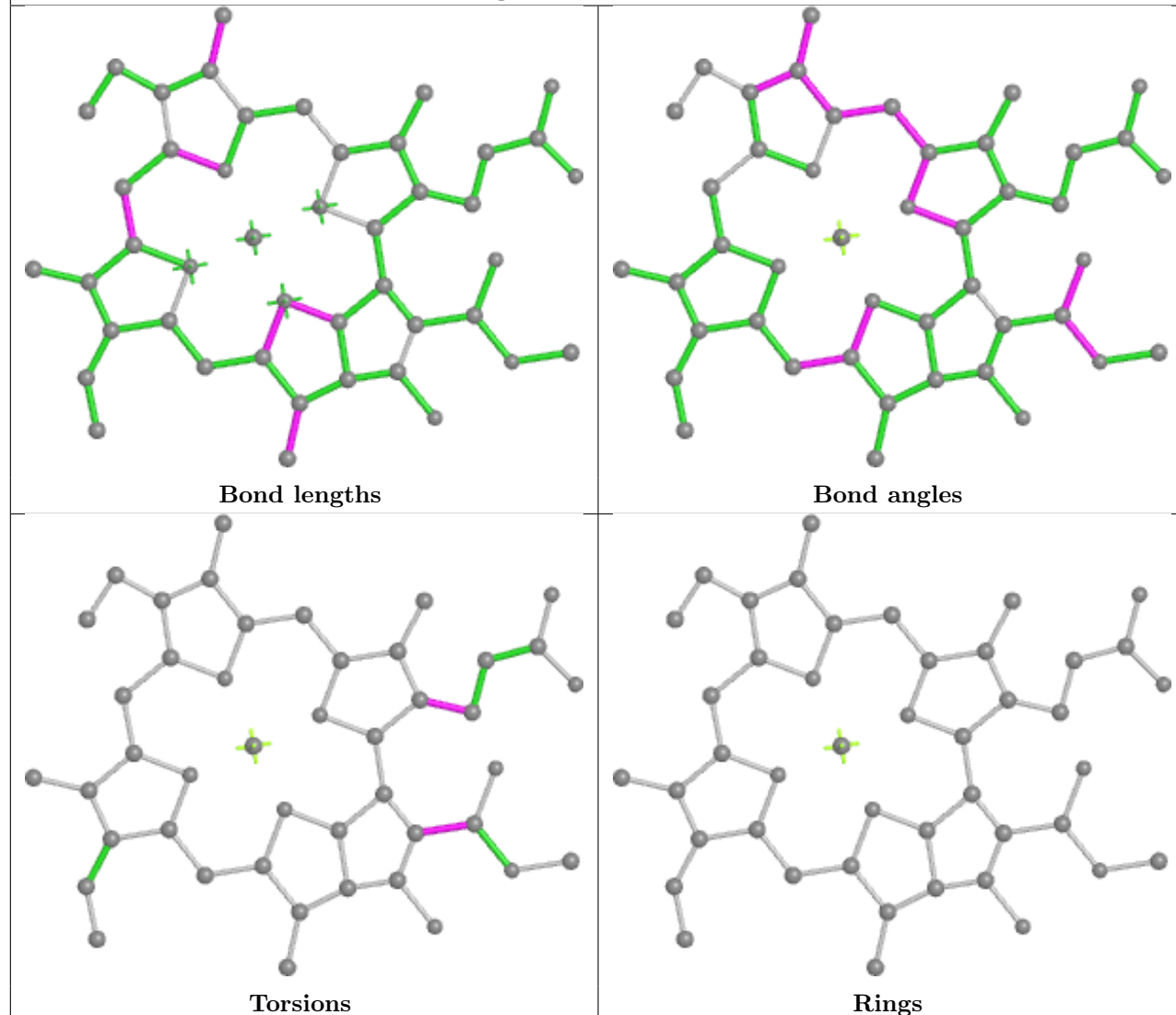
Ligand CLA 9 308



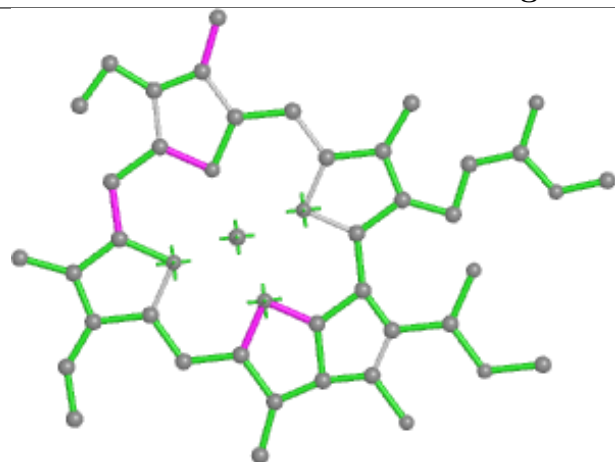
Ligand CLA a 835



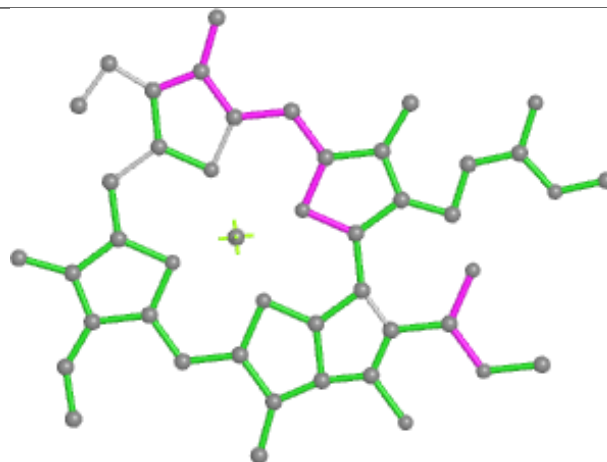
Ligand CLA b 815



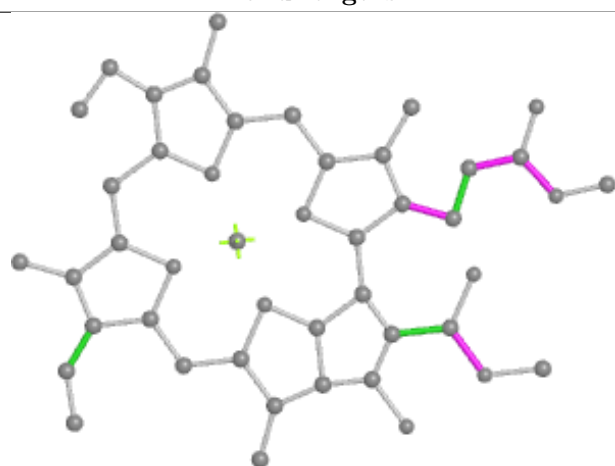
Ligand CLA 6 316



Bond lengths



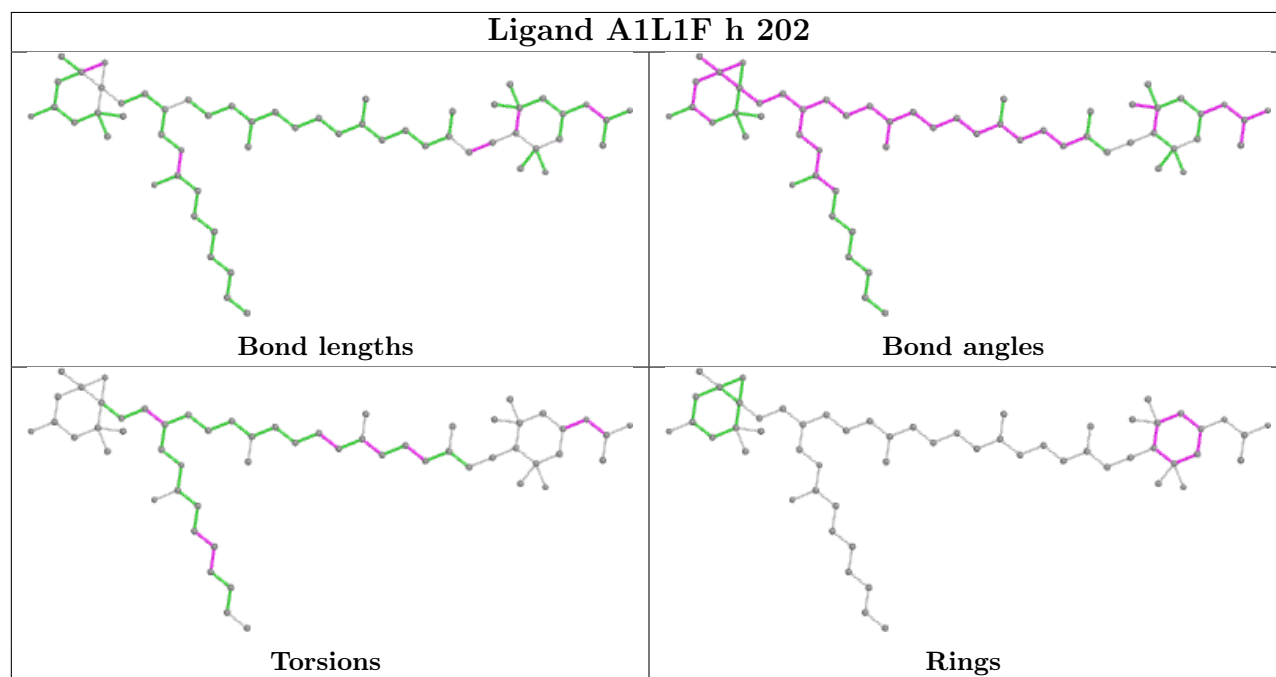
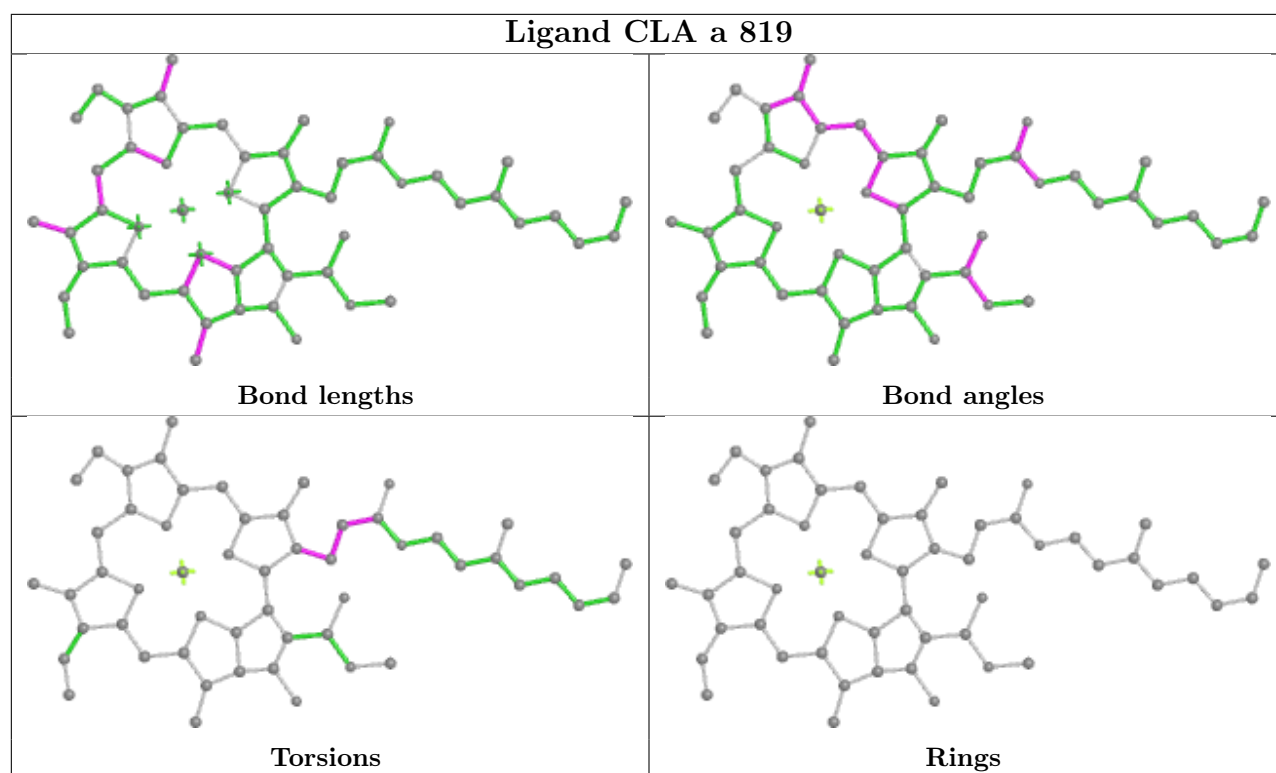
Bond angles



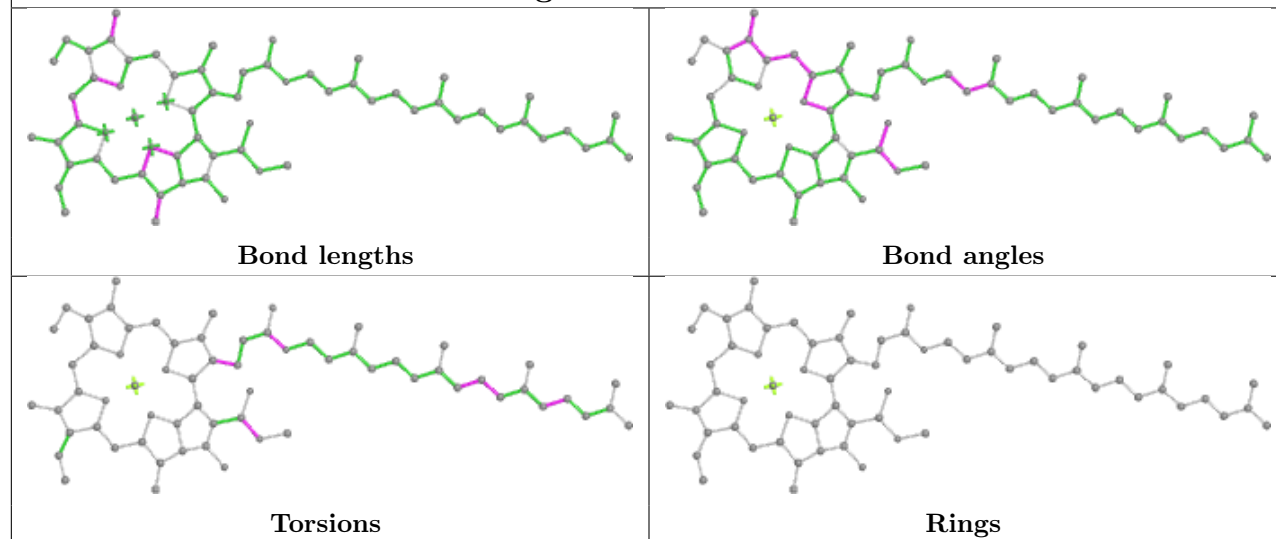
Torsions



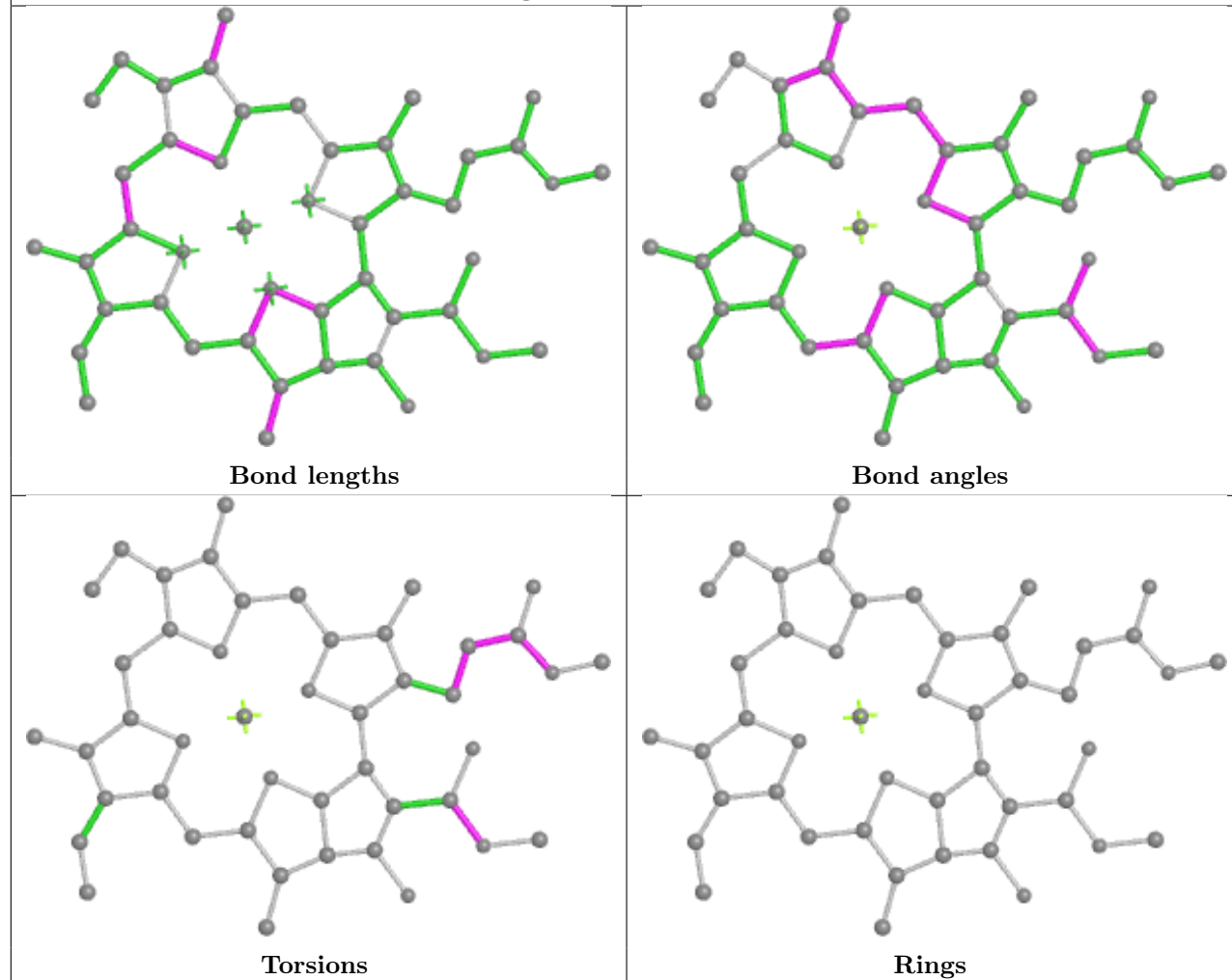
Rings



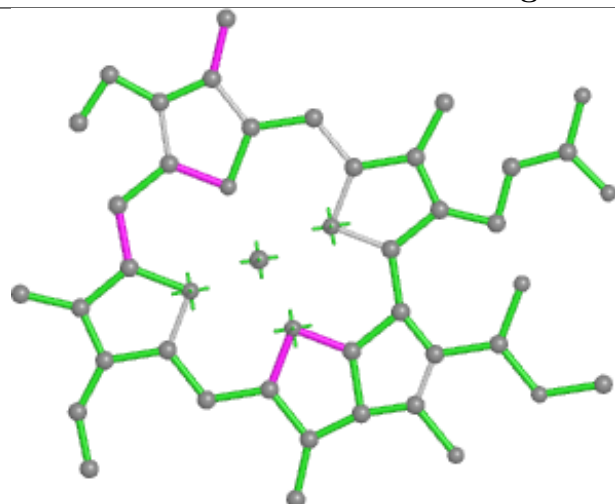
Ligand CLA h 201



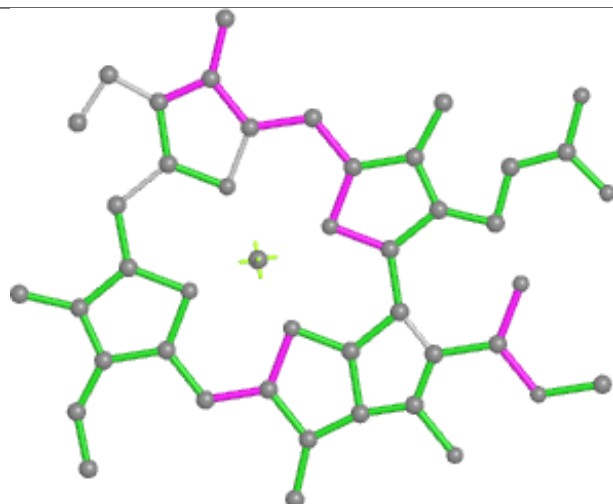
Ligand CLA 5 311



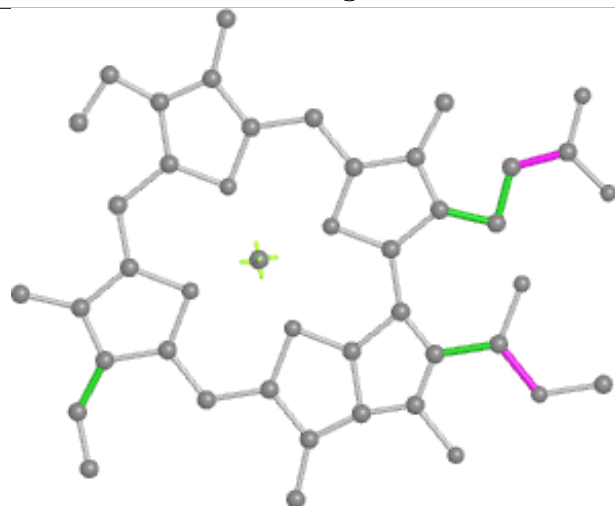
Ligand CLA 7 307



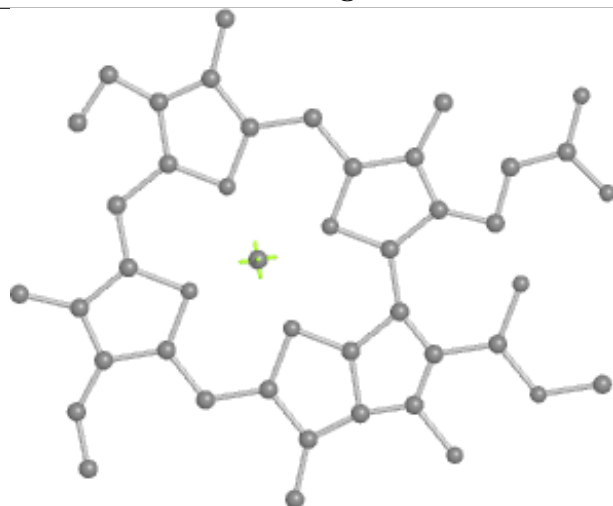
Bond lengths



Bond angles

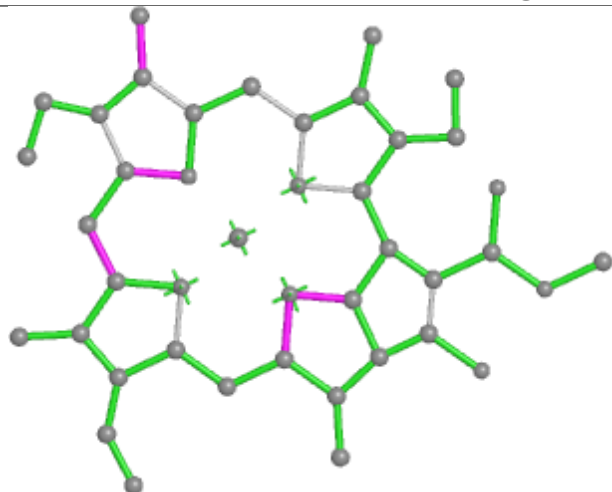


Torsions

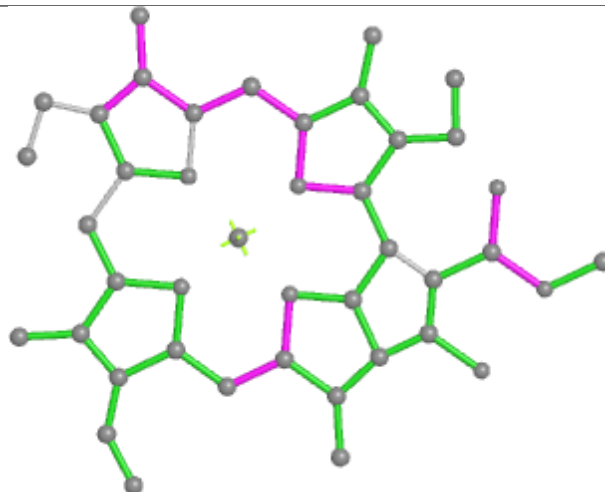


Rings

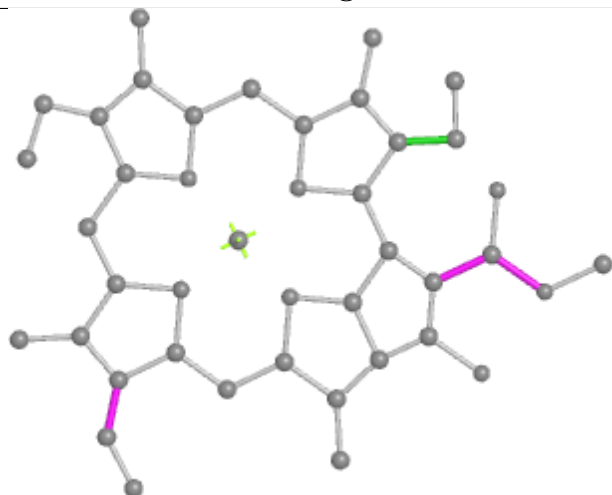
Ligand CLA 9 315



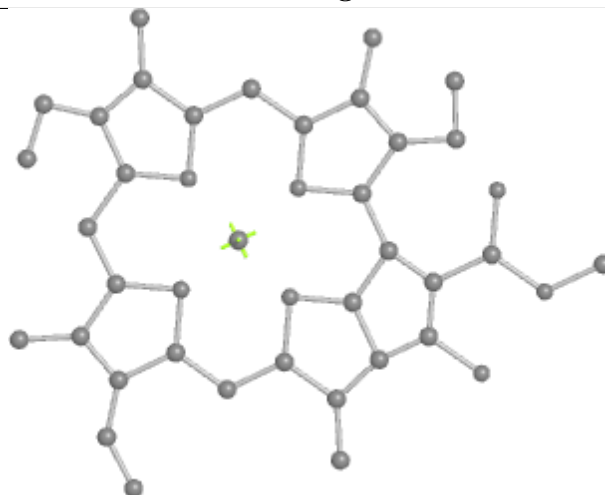
Bond lengths



Bond angles

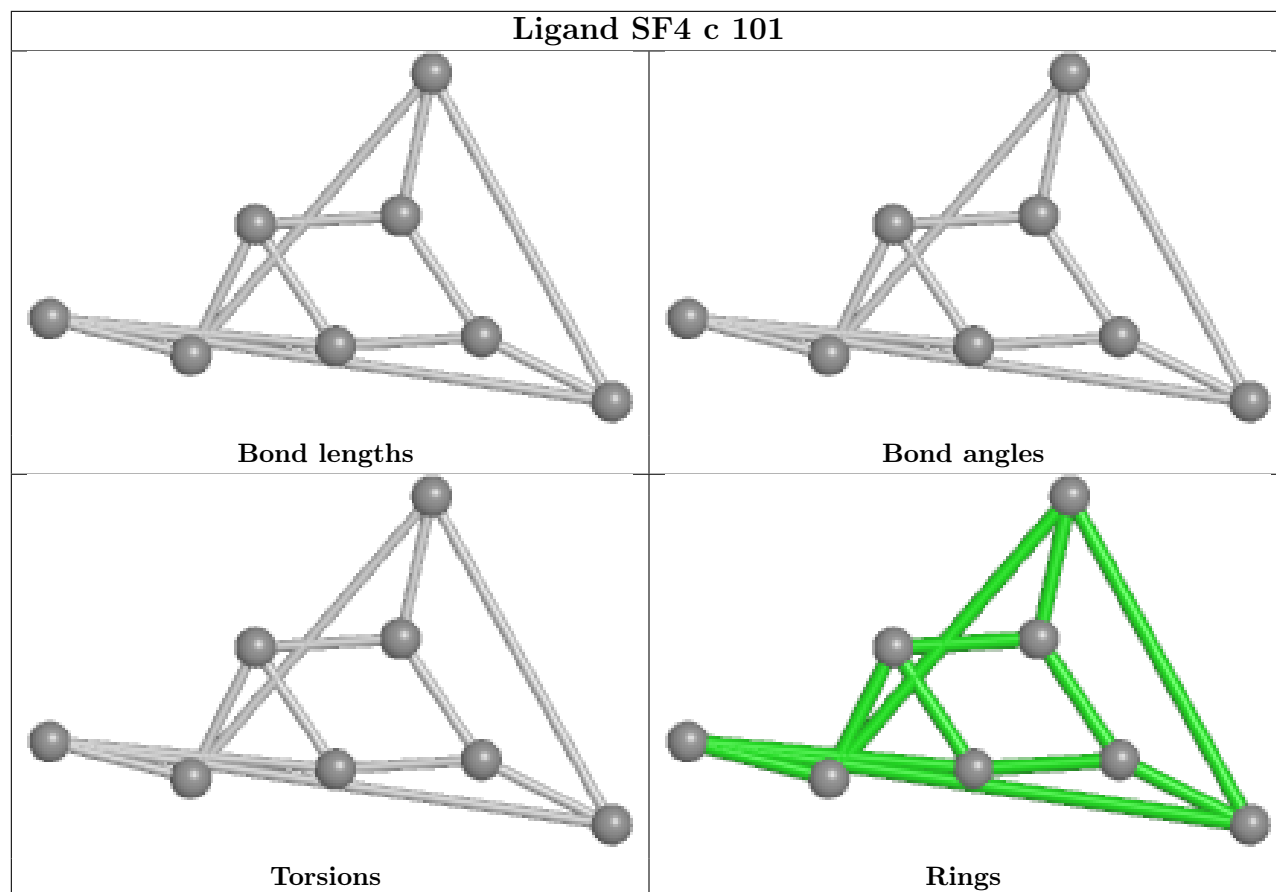


Torsions

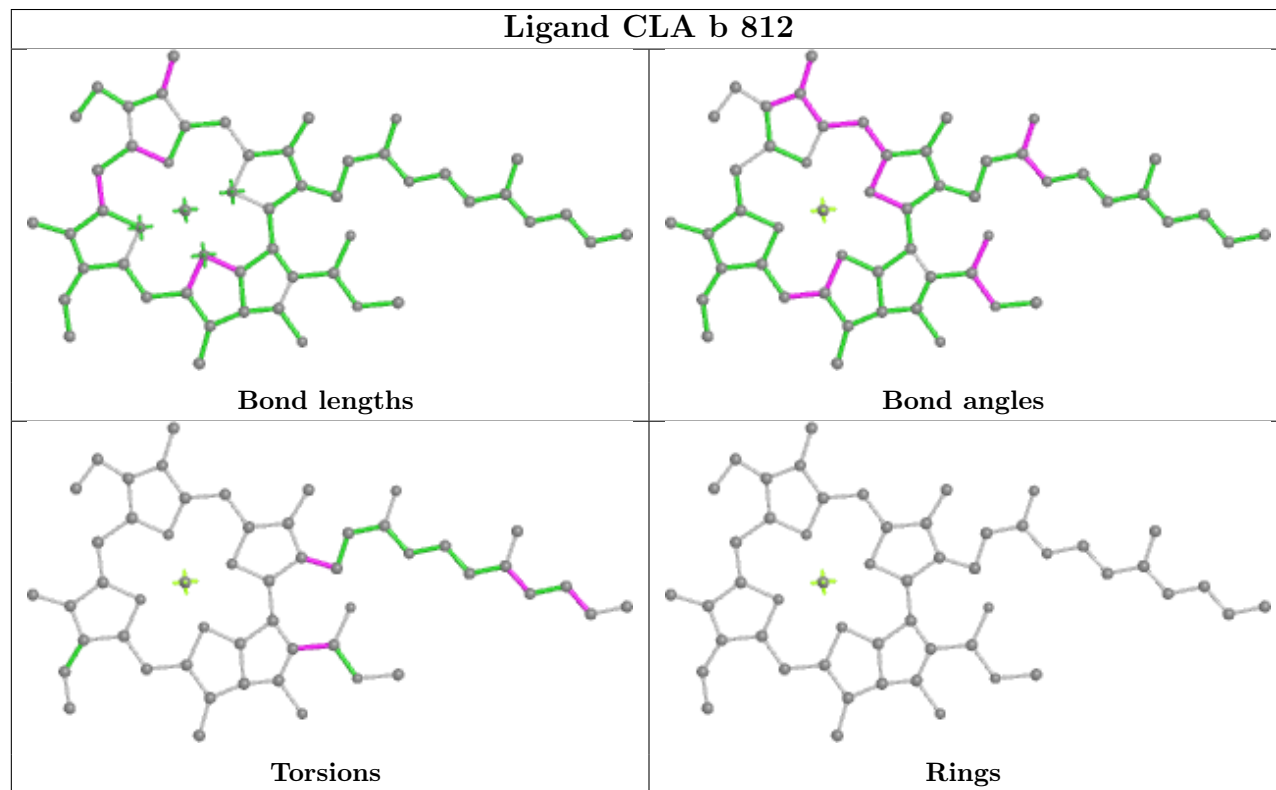


Rings

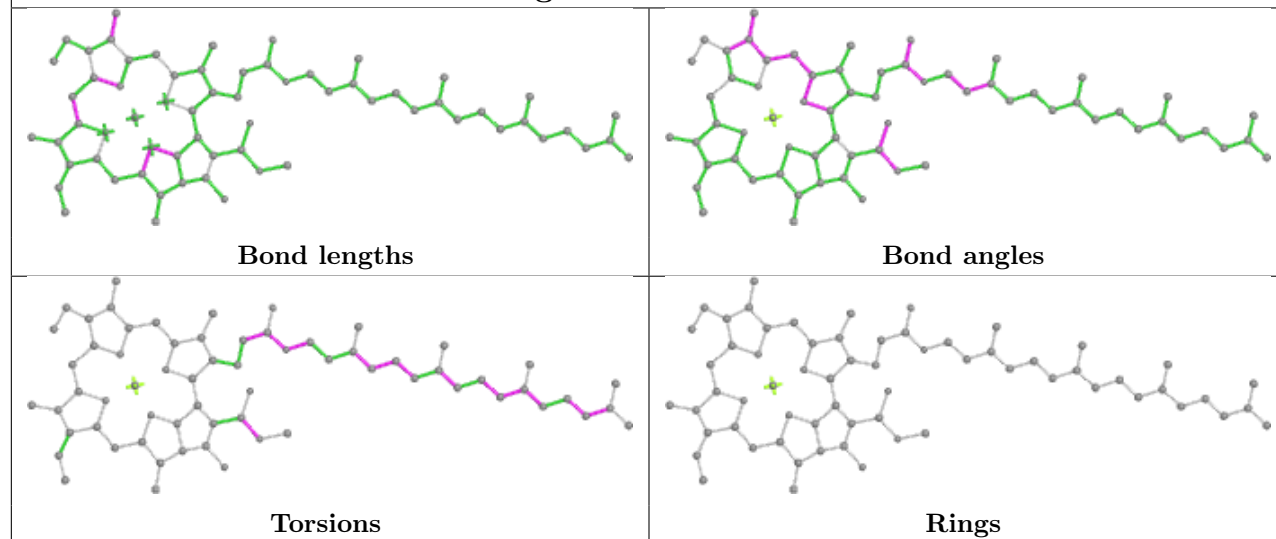
Ligand SF4 c 101



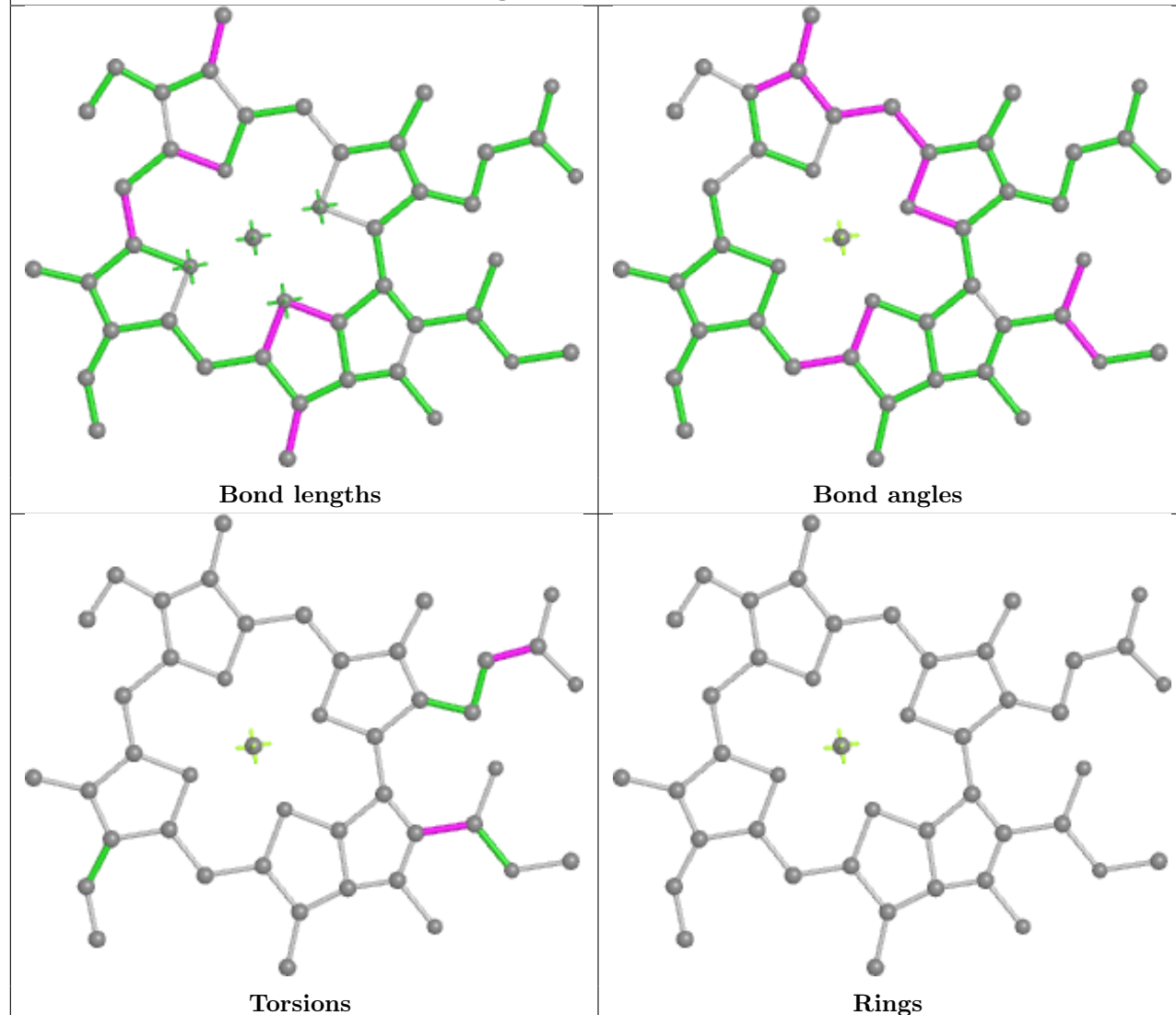
Ligand CLA b 812

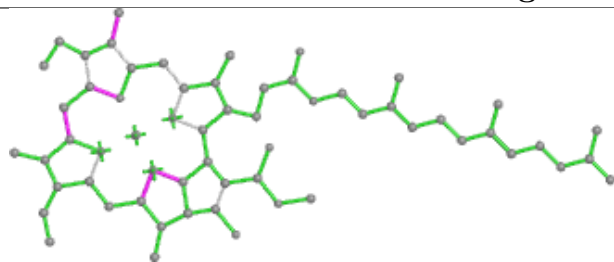


Ligand CLA b 806

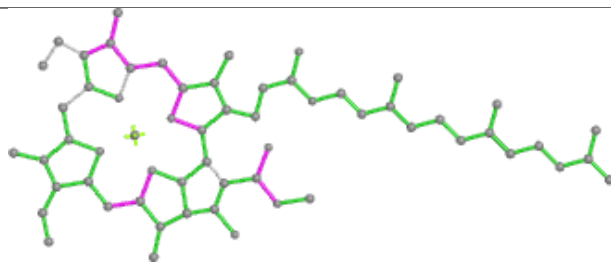


Ligand CLA 4 314

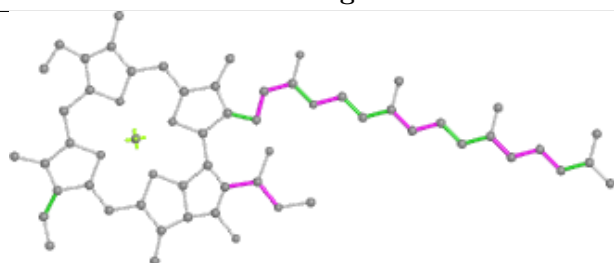


Ligand CLA 7 308

Bond lengths



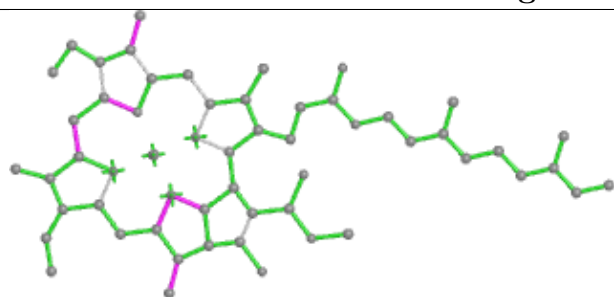
Bond angles



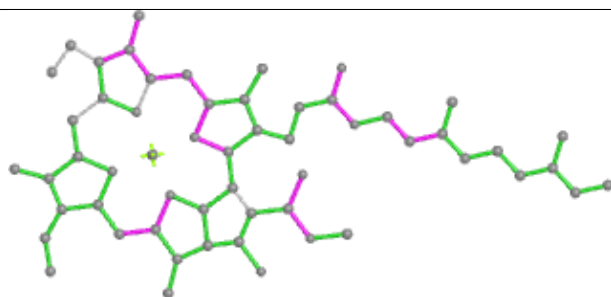
Torsions



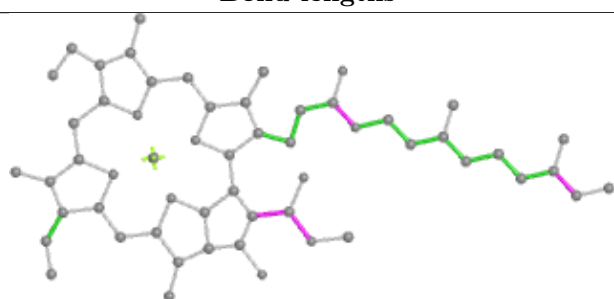
Rings

Ligand CLA a 811

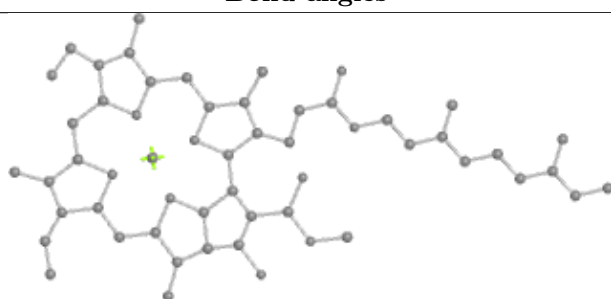
Bond lengths



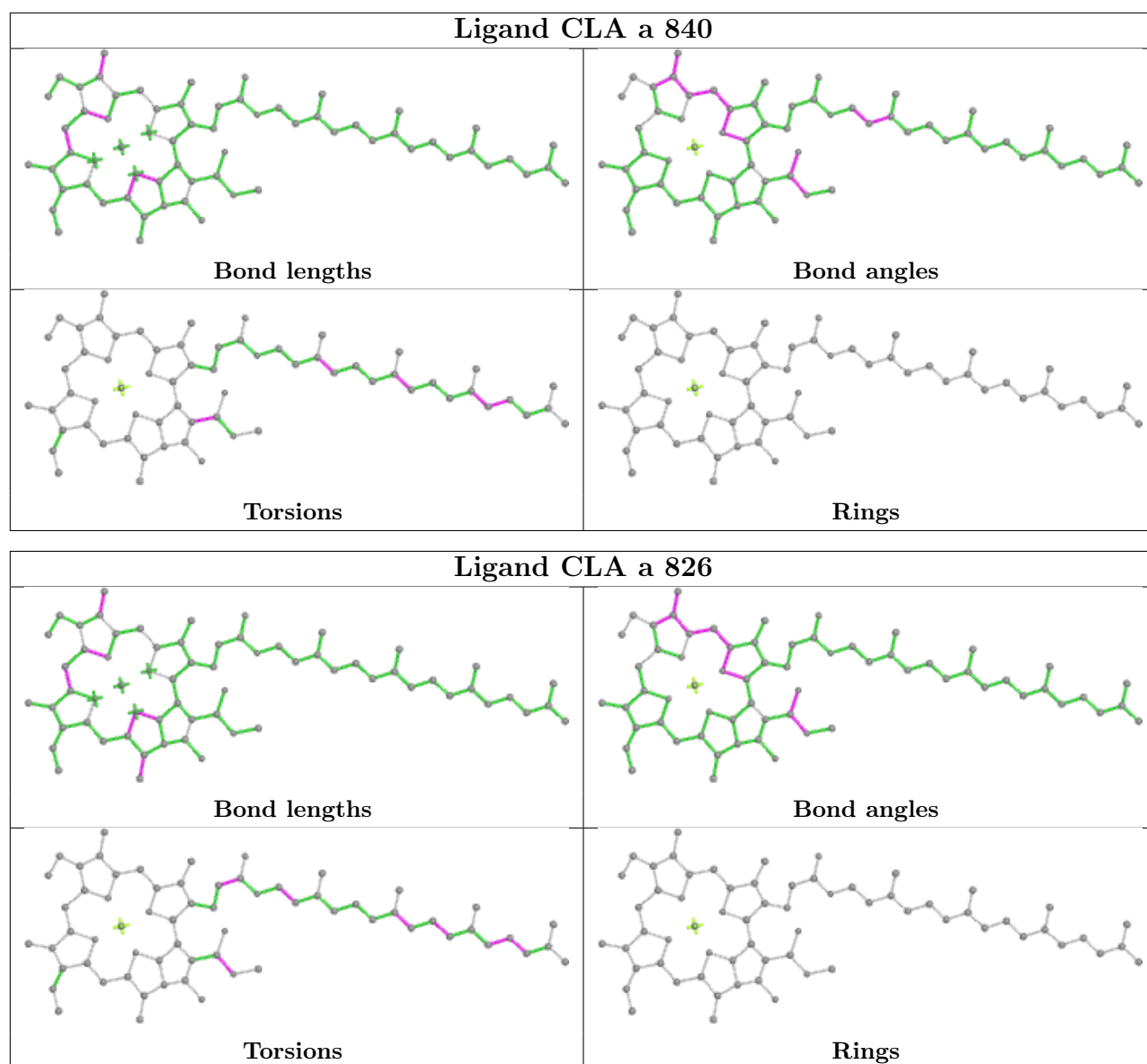
Bond angles

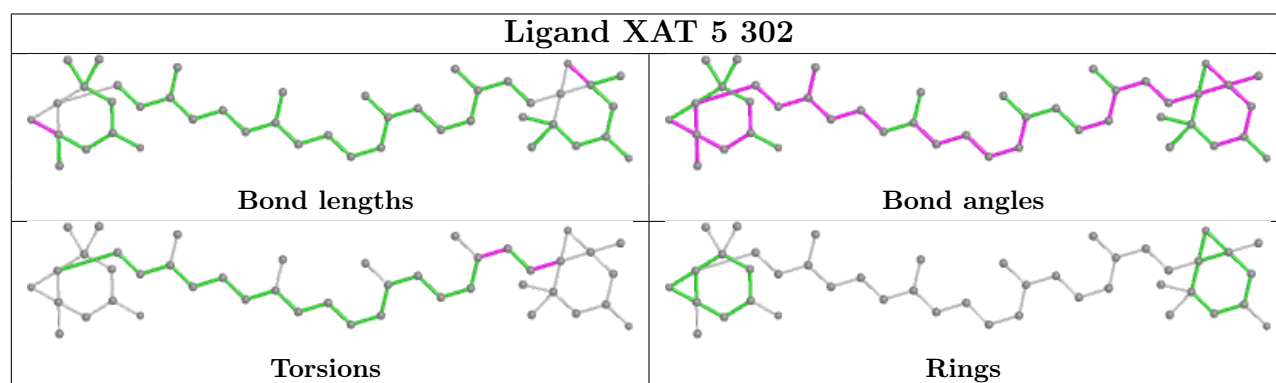
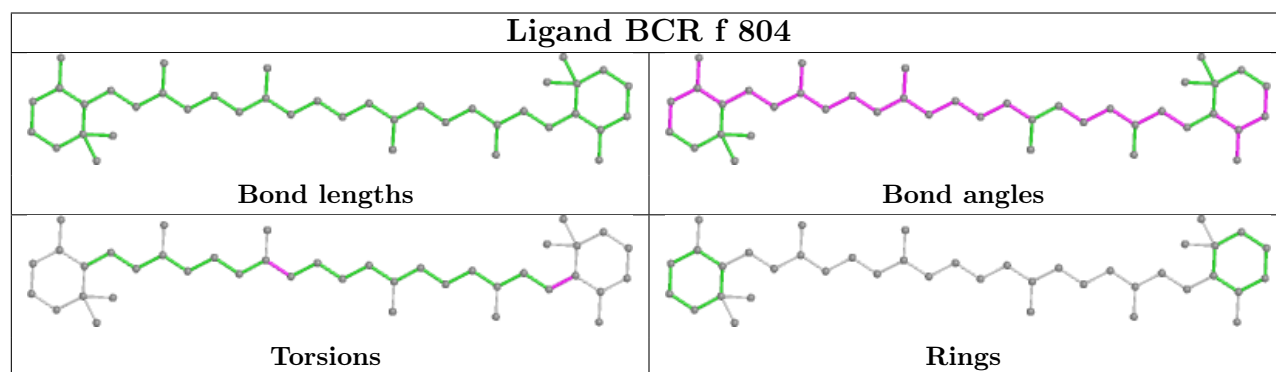
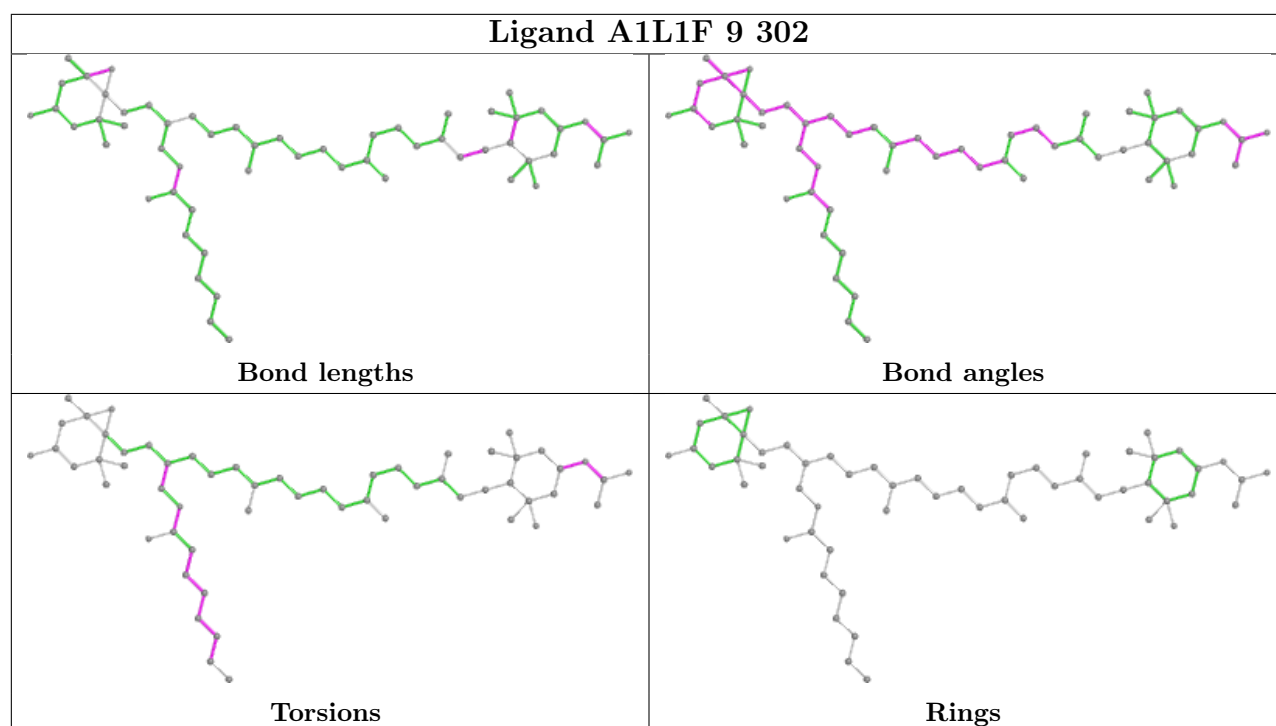


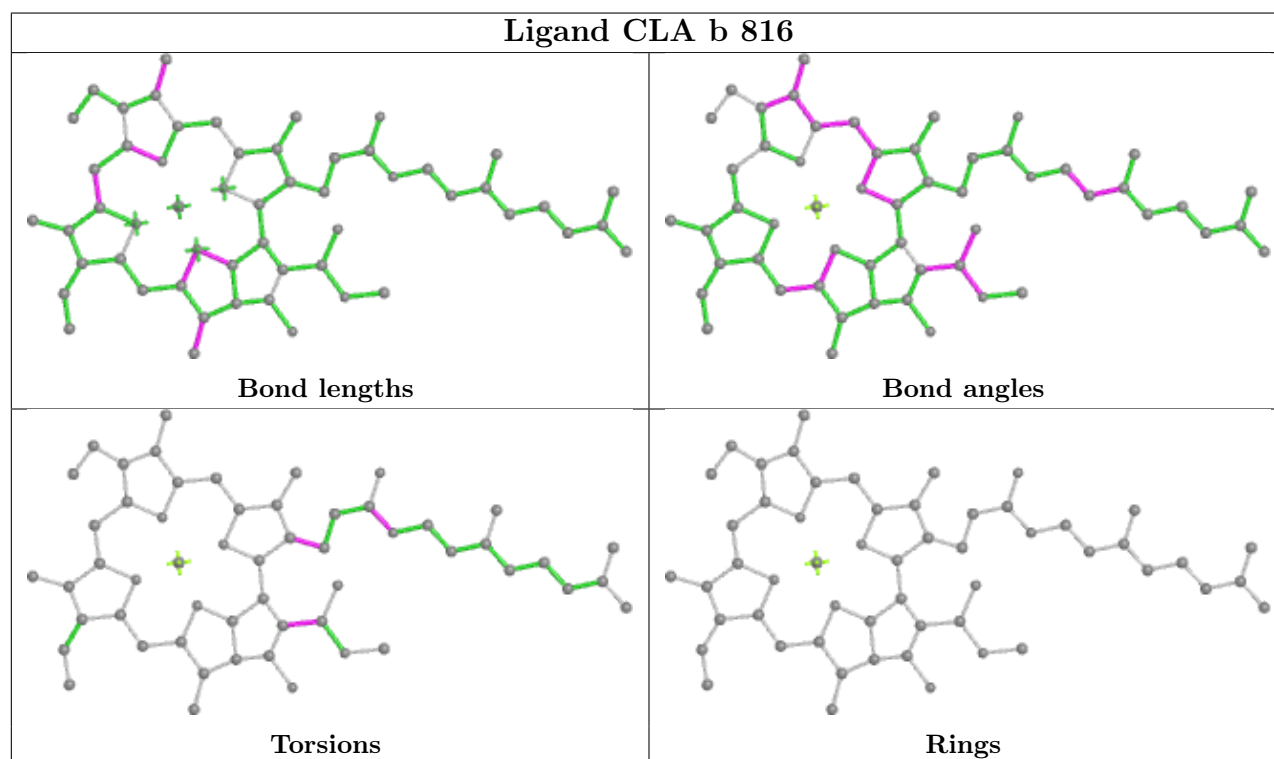
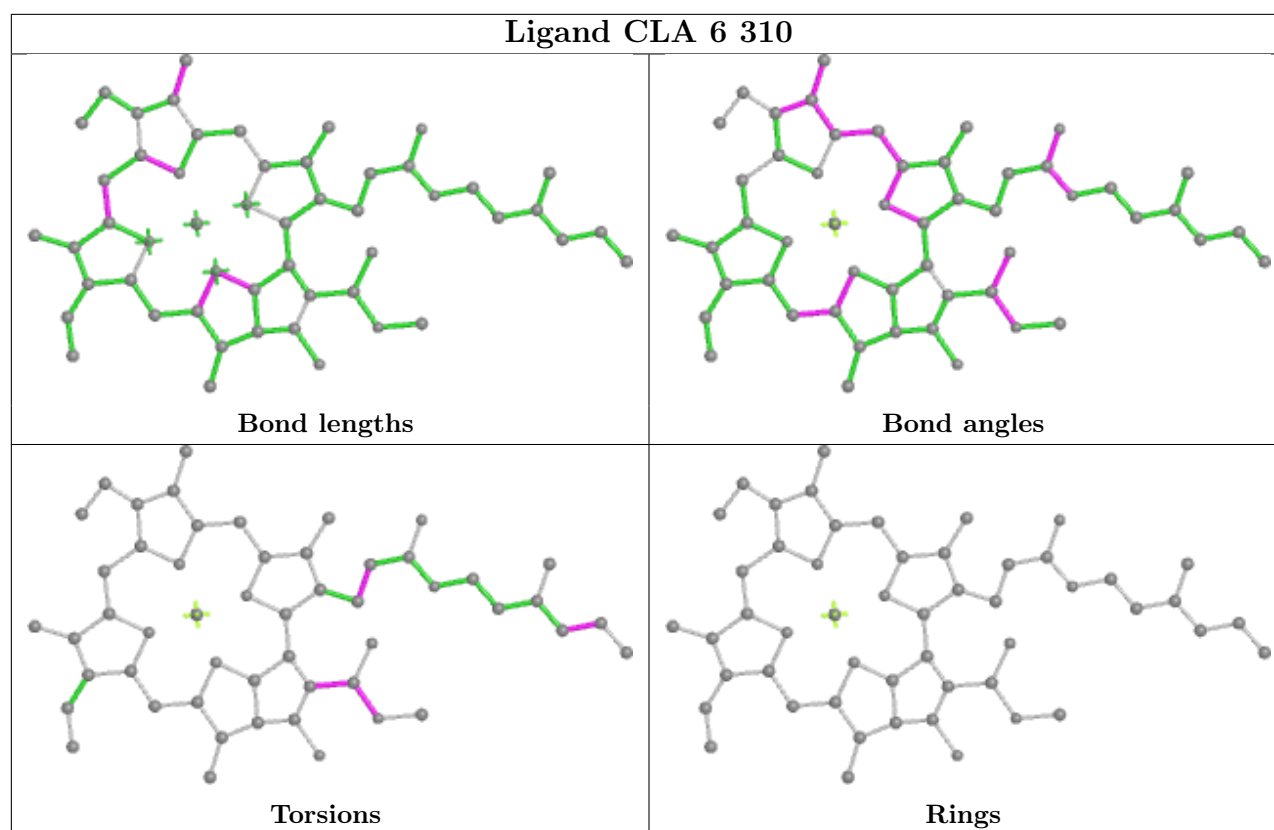
Torsions

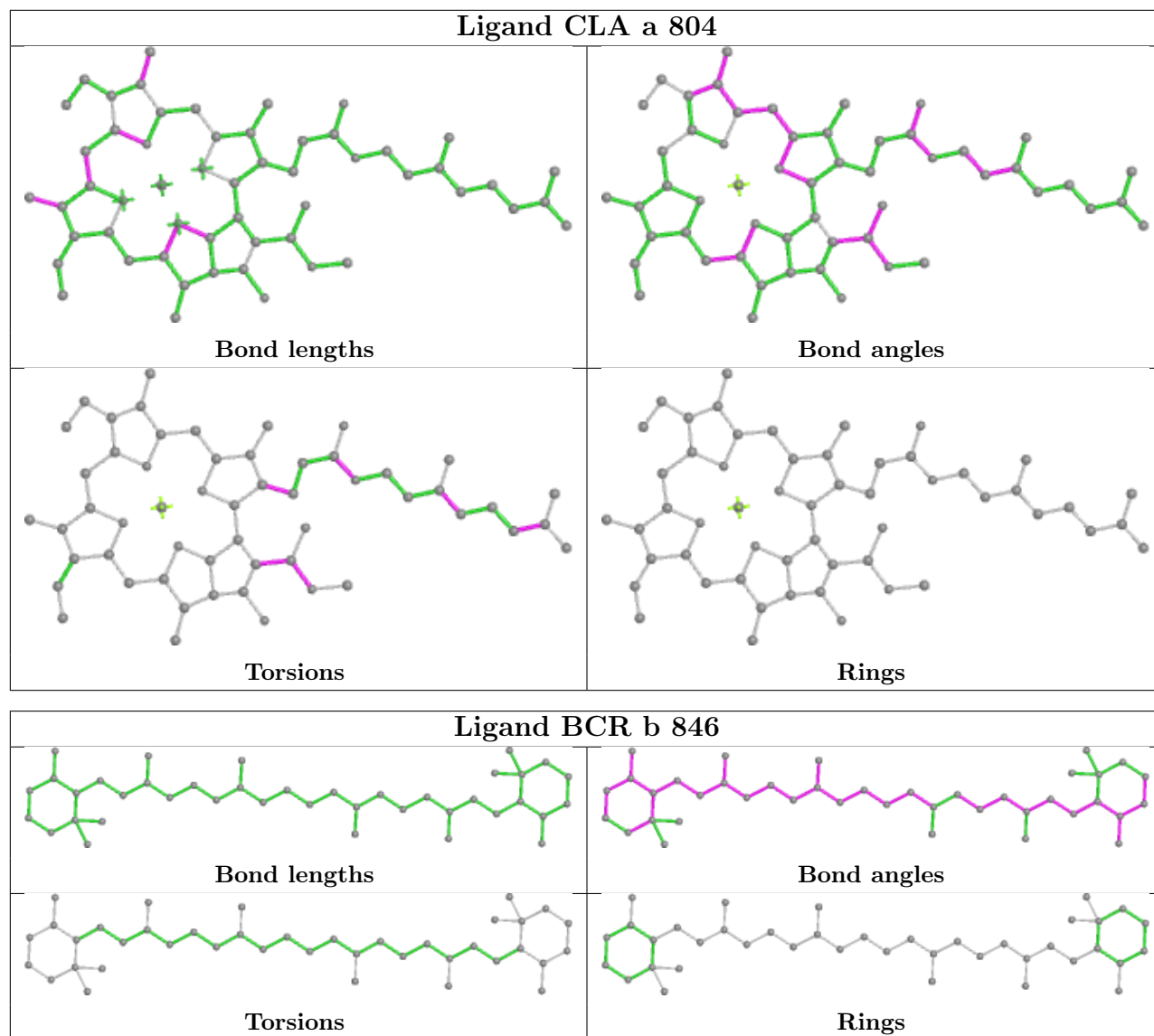


Rings

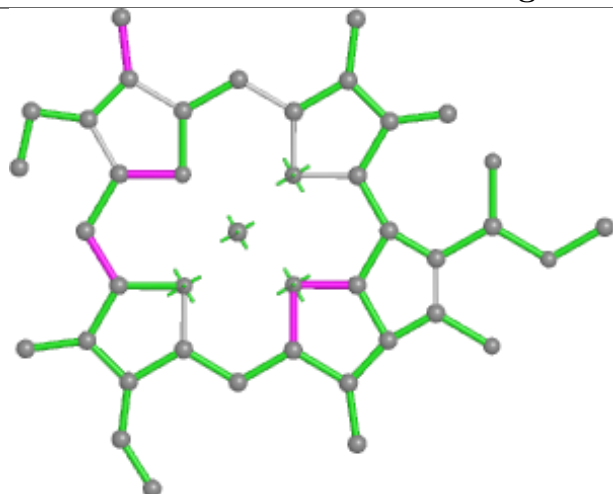




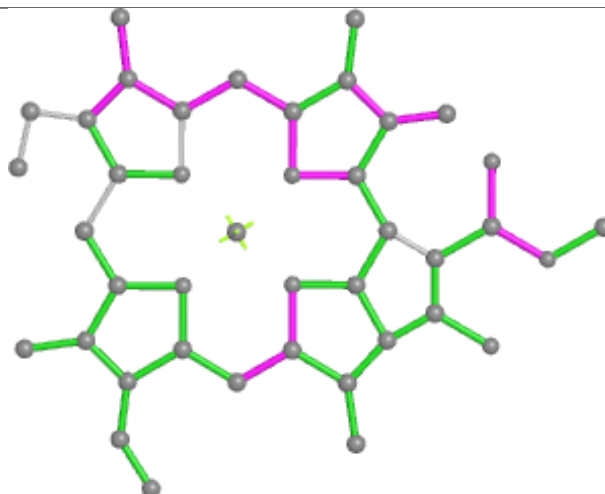




Ligand CLA 7 315



Bond lengths



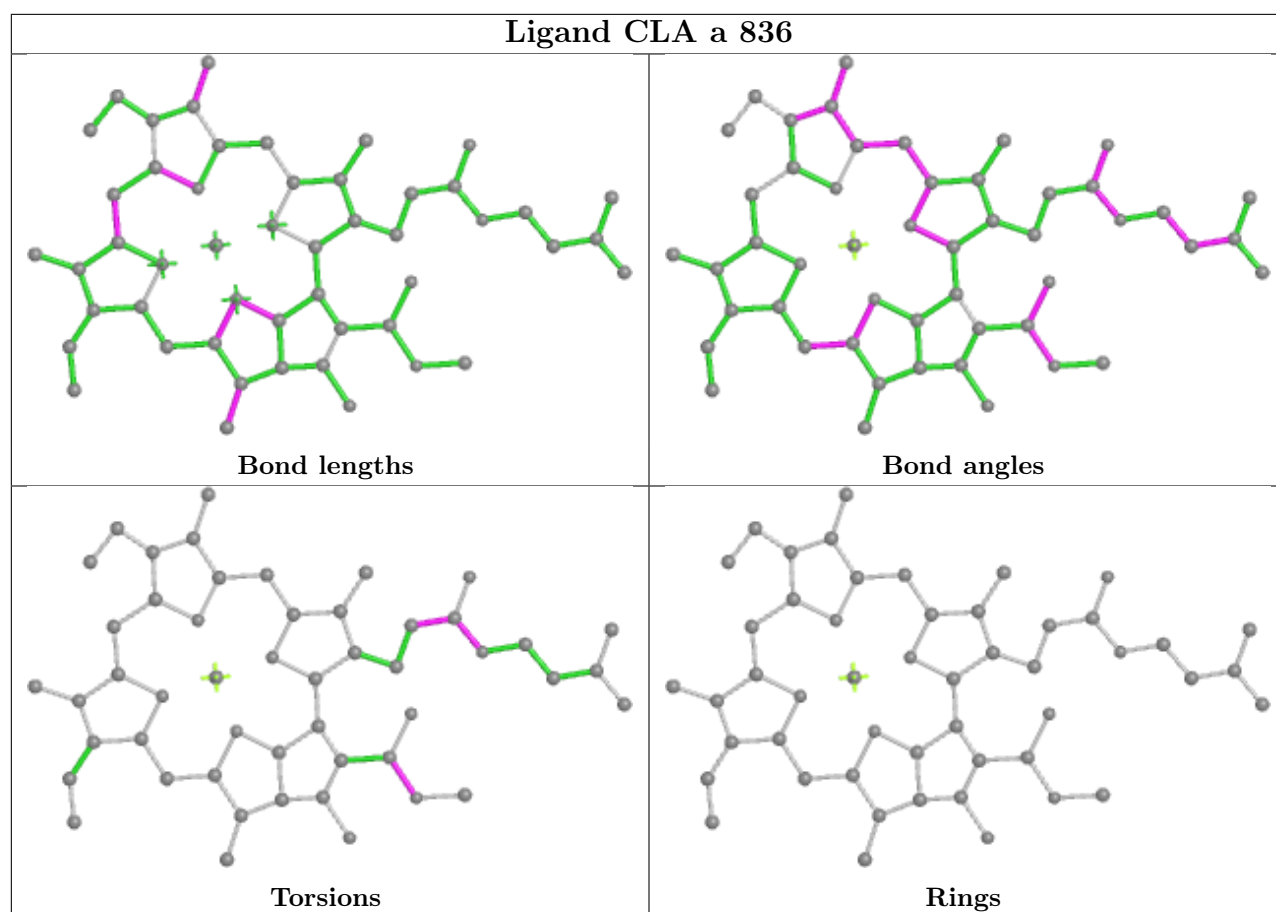
Bond angles



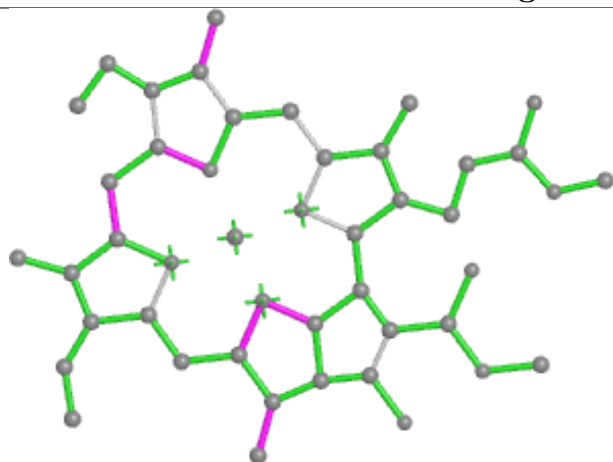
Torsions



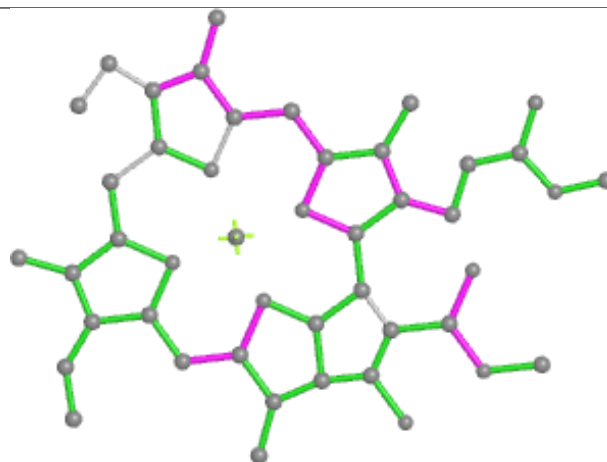
Rings



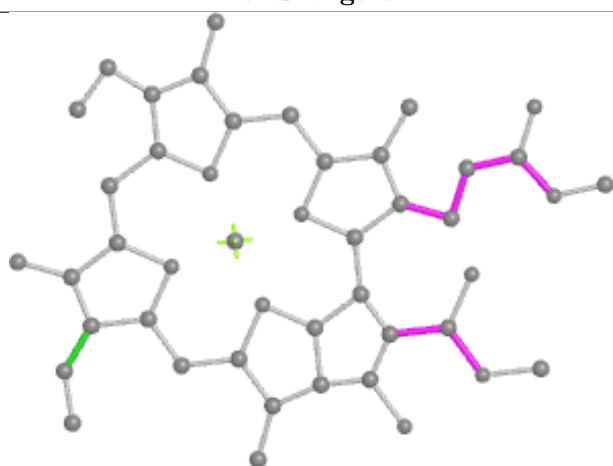
Ligand CLA 9 312



Bond lengths



Bond angles

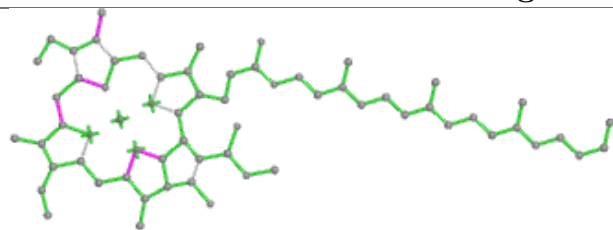


Torsions

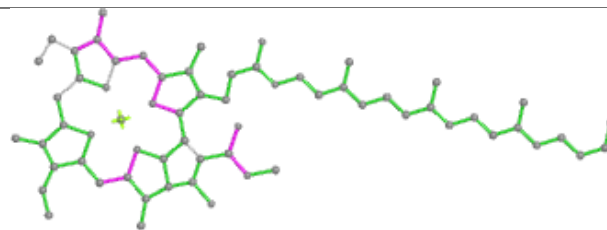


Rings

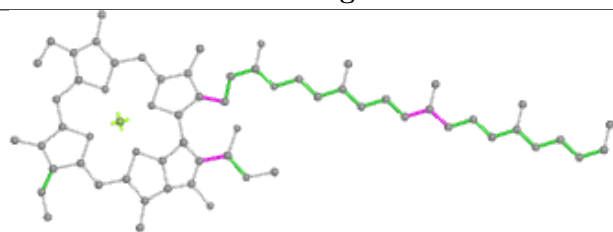
Ligand CLA b 825



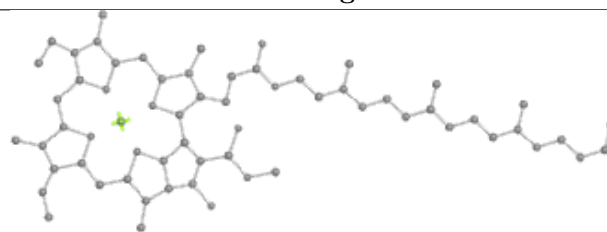
Bond lengths



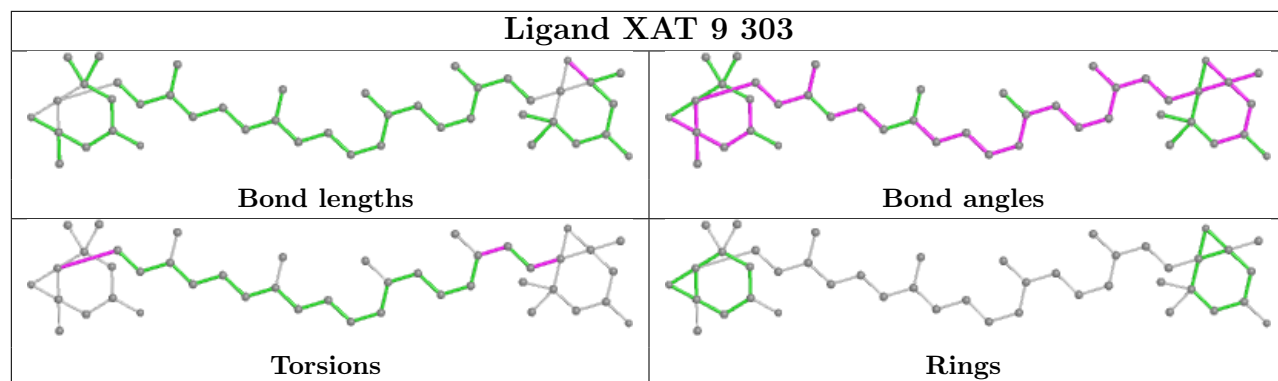
Bond angles



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.

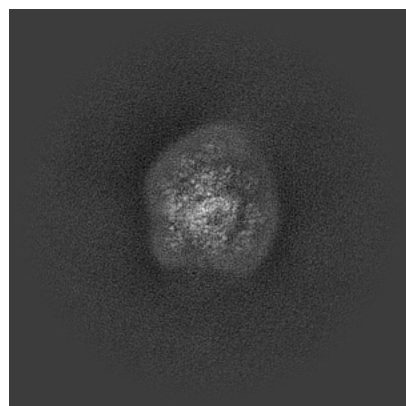
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60293. These allow visual inspection of the internal detail of the map and identification of artifacts.

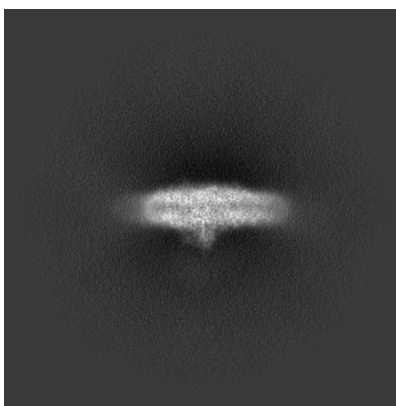
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

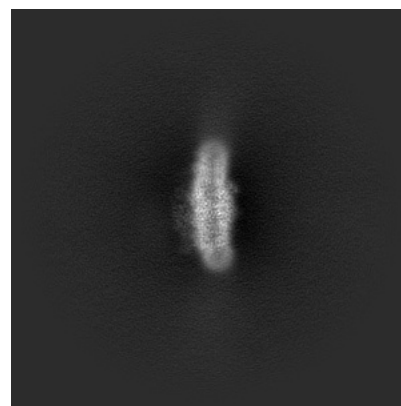
6.1.1 Primary map



X

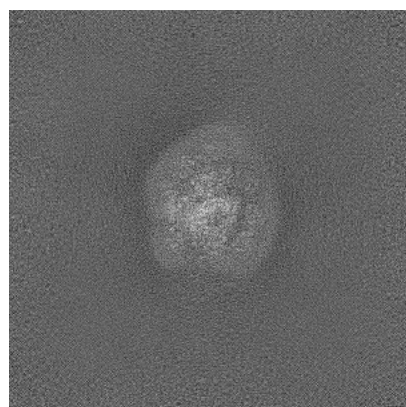


Y

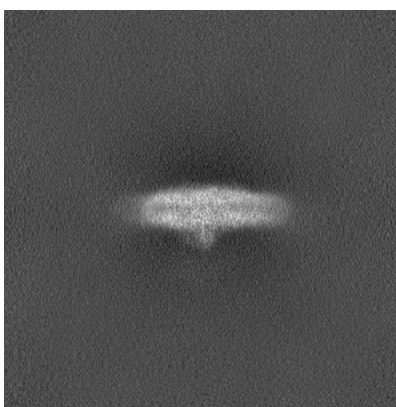


Z

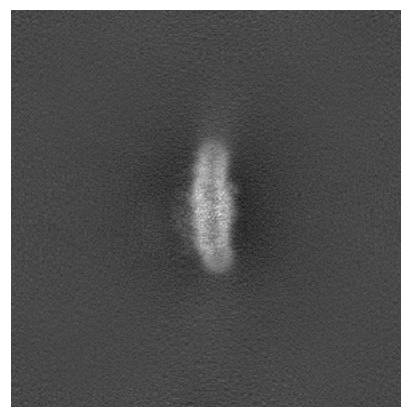
6.1.2 Raw map



X



Y

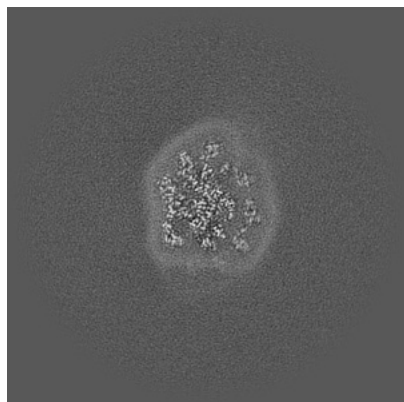


Z

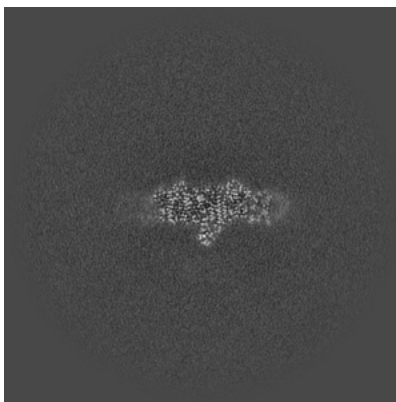
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

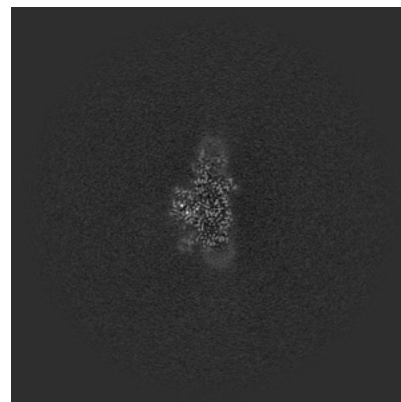
6.2.1 Primary map



X Index: 256

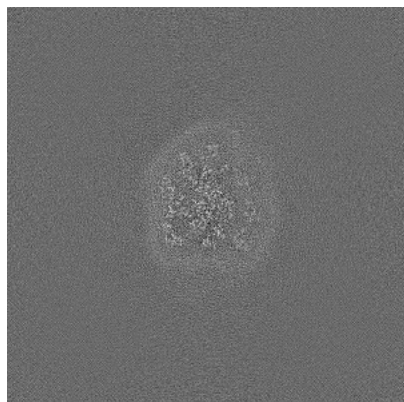


Y Index: 256

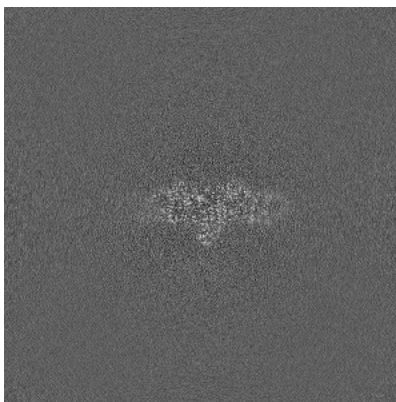


Z Index: 256

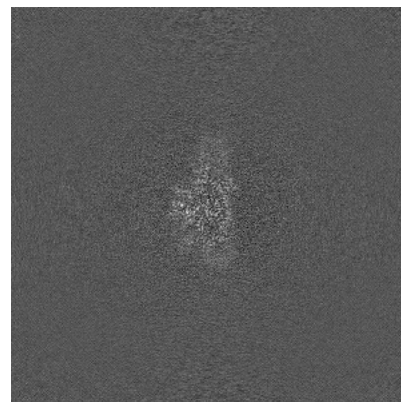
6.2.2 Raw map



X Index: 256



Y Index: 256

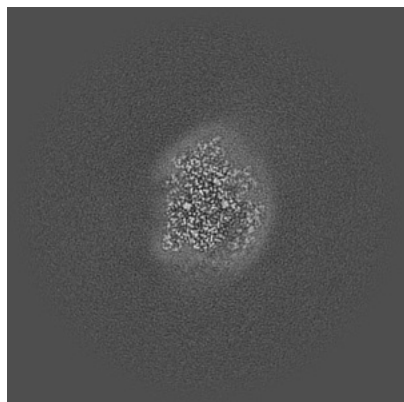


Z Index: 256

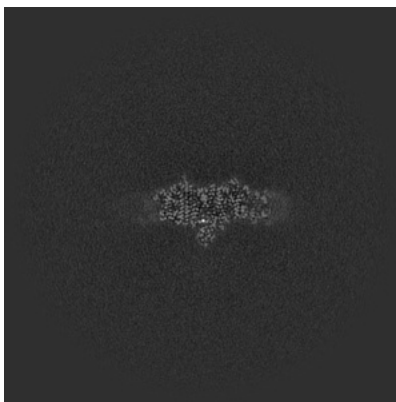
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

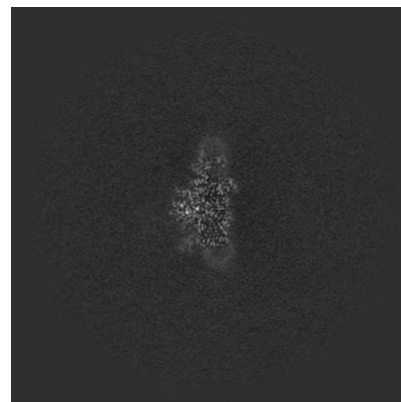
6.3.1 Primary map



X Index: 245

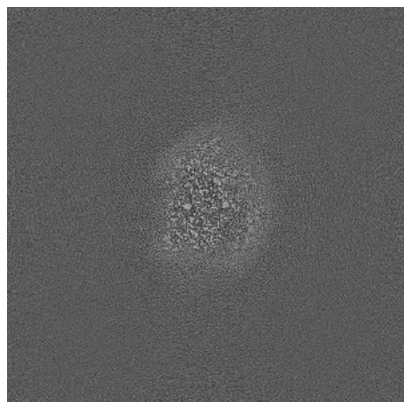


Y Index: 253

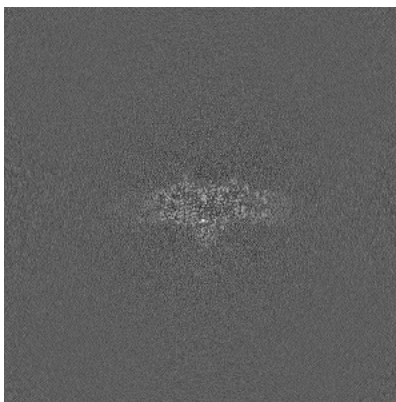


Z Index: 255

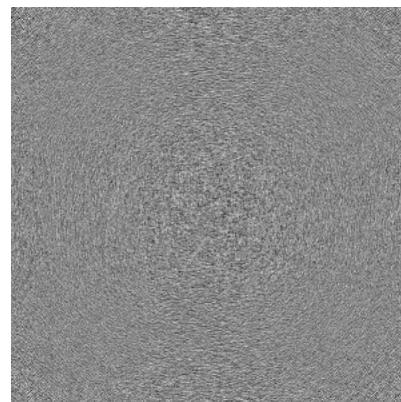
6.3.2 Raw map



X Index: 245



Y Index: 253

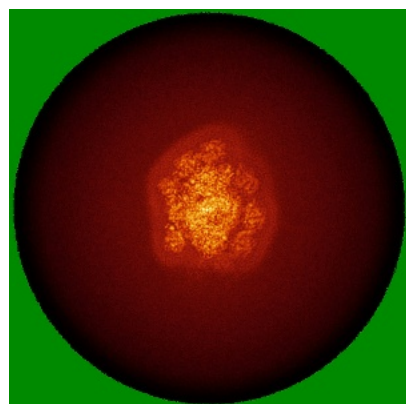


Z Index: 0

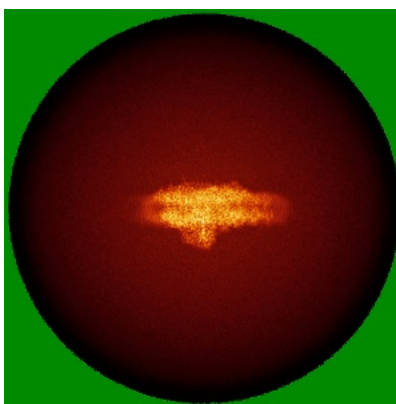
The images above show the largest variance slices of the map in three orthogonal directions.

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

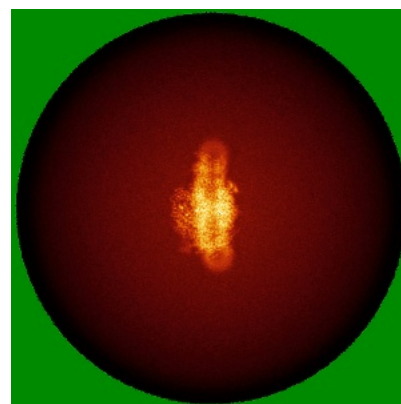
6.4.1 Primary map



X

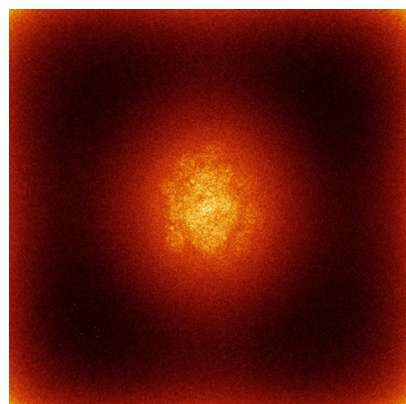


Y

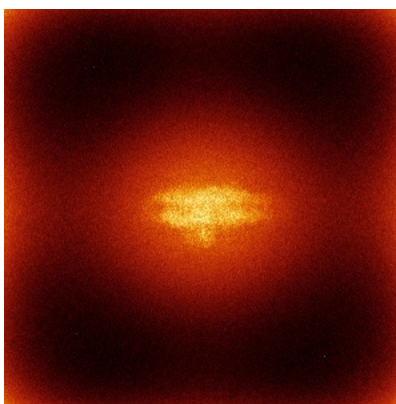


Z

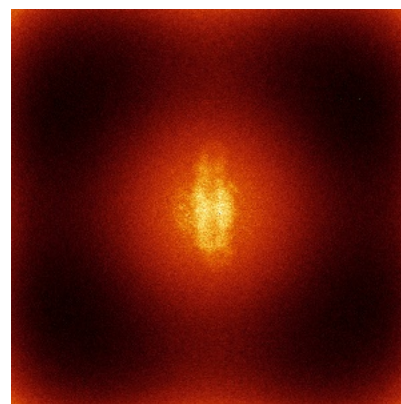
6.4.2 Raw map



X



Y

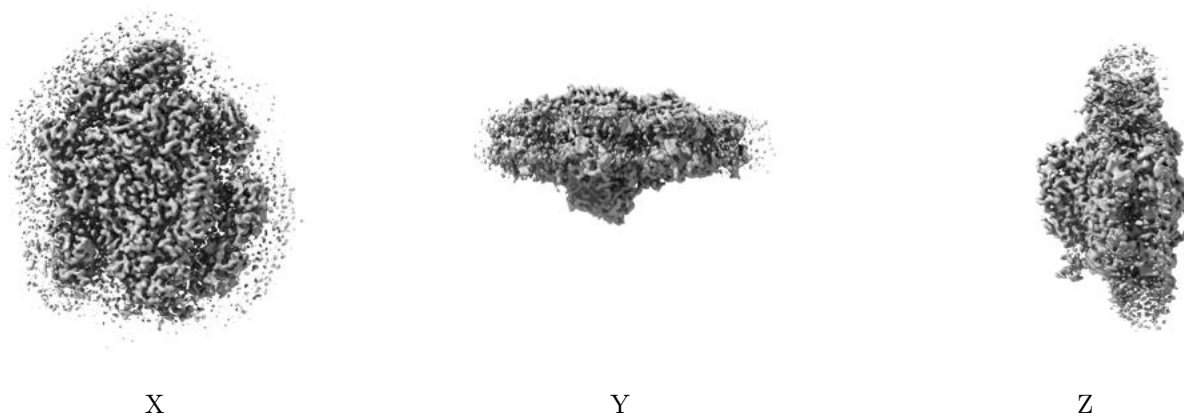


Z

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.

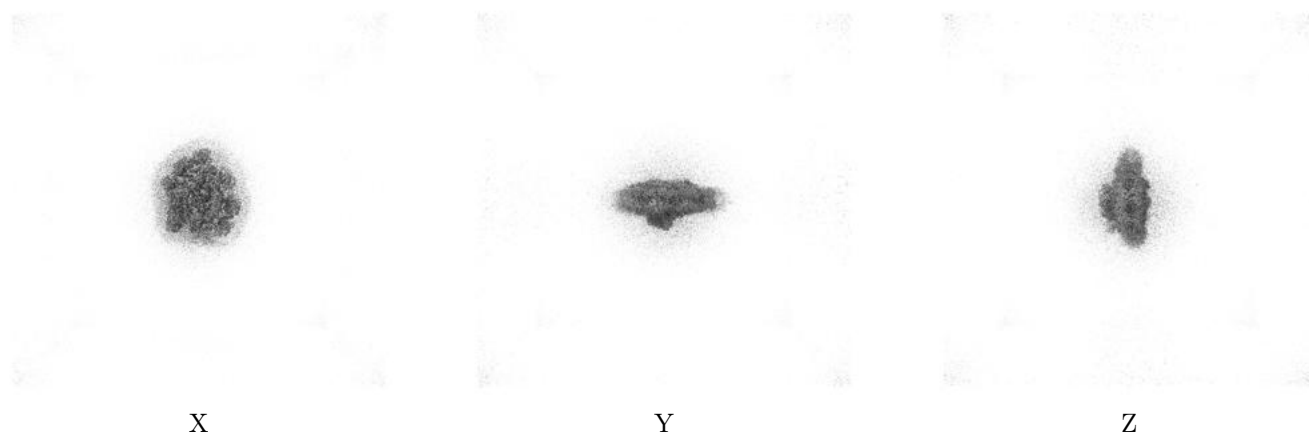
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

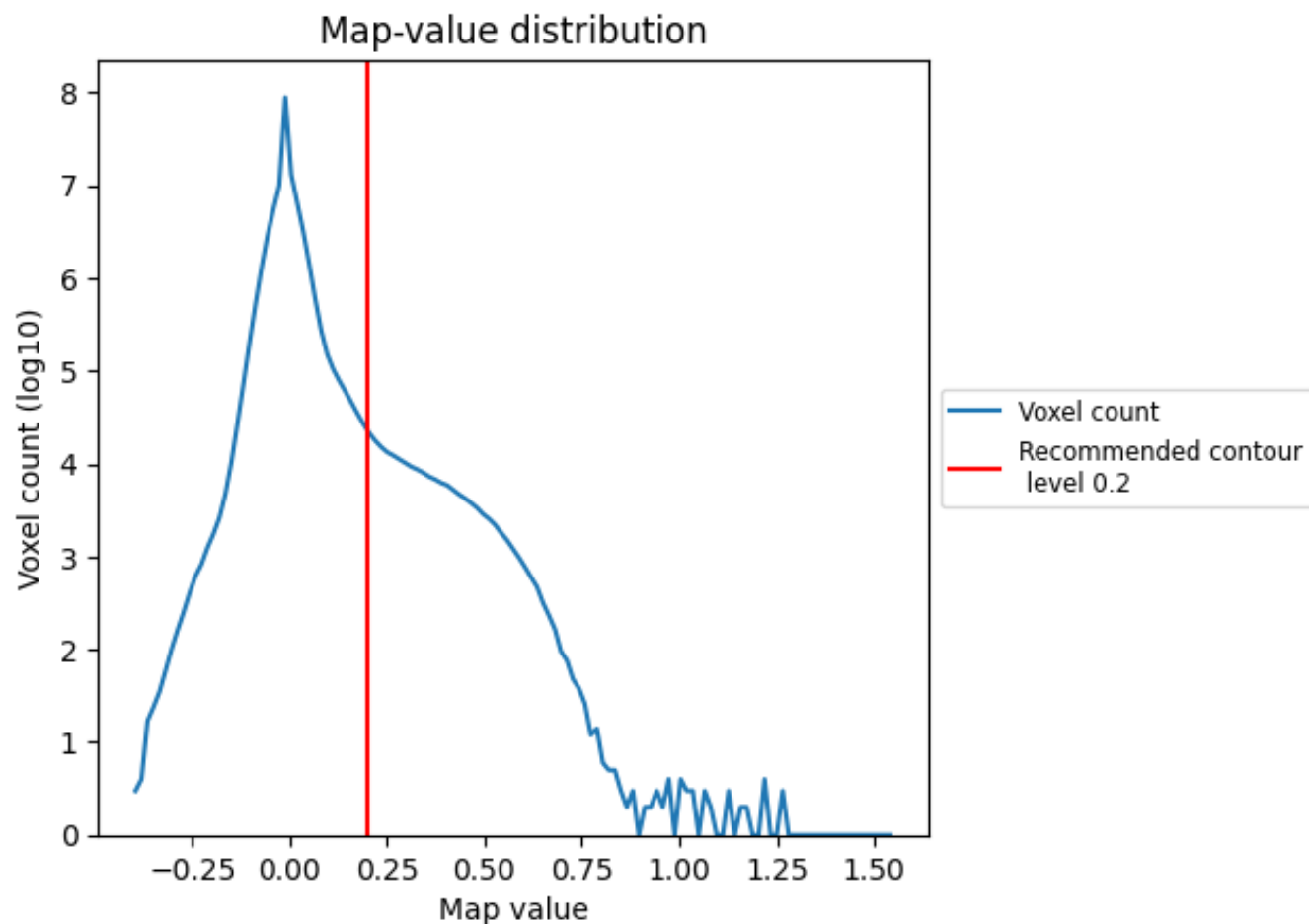
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

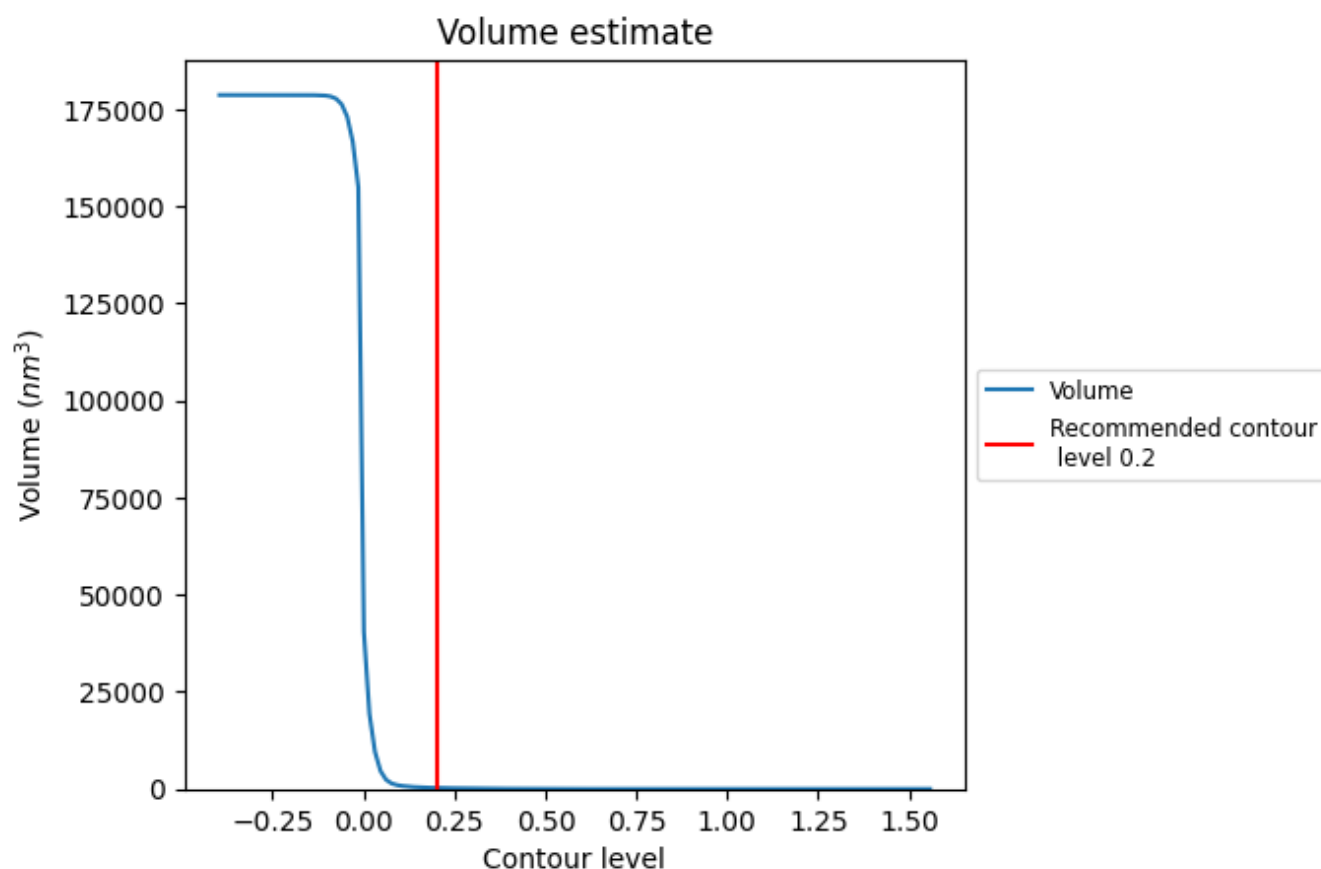
This section contains the results of statistical analysis of the map.

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.

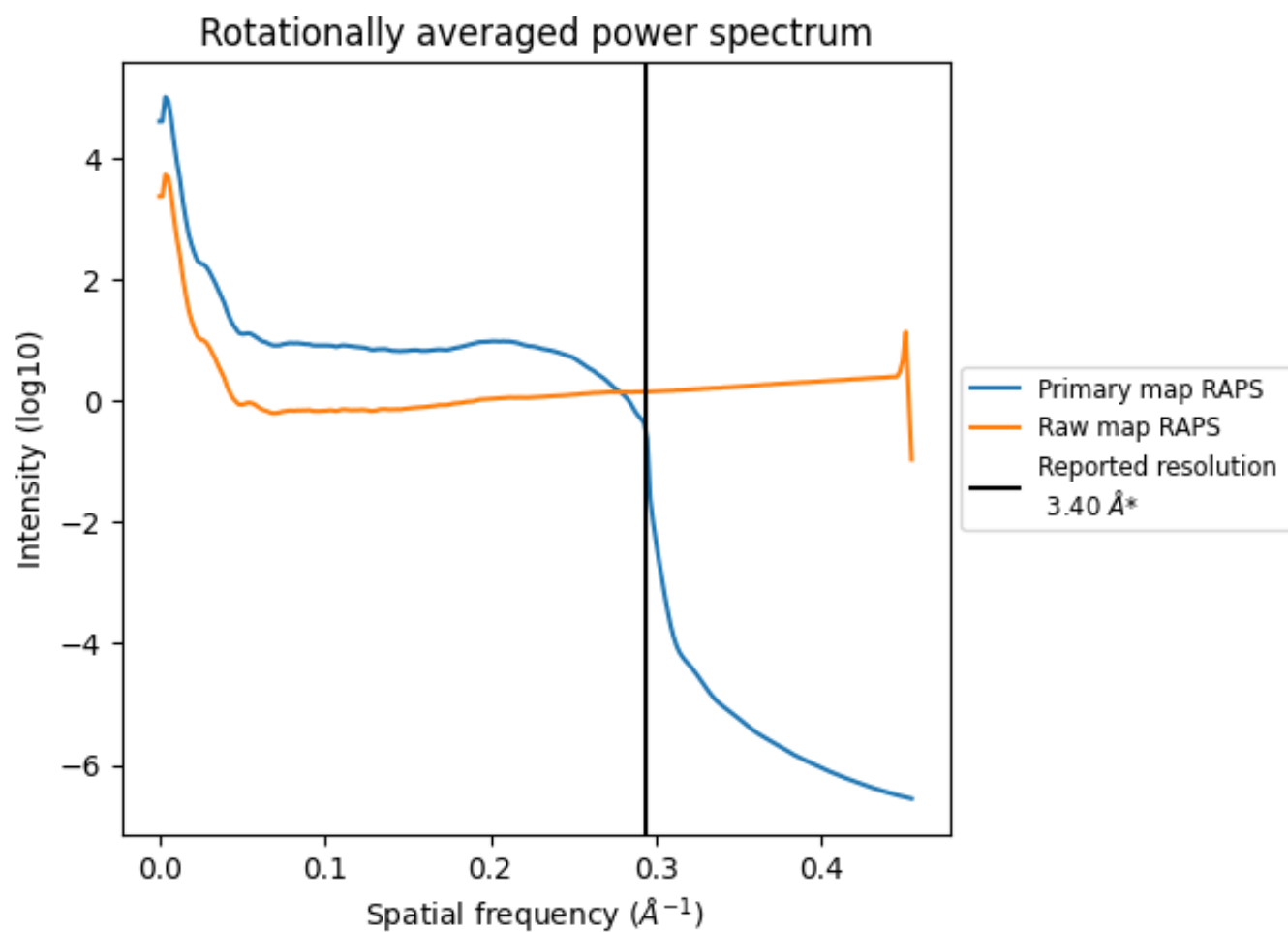
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm^3 ; this corresponds to an approximate mass of 237 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 [i](#)

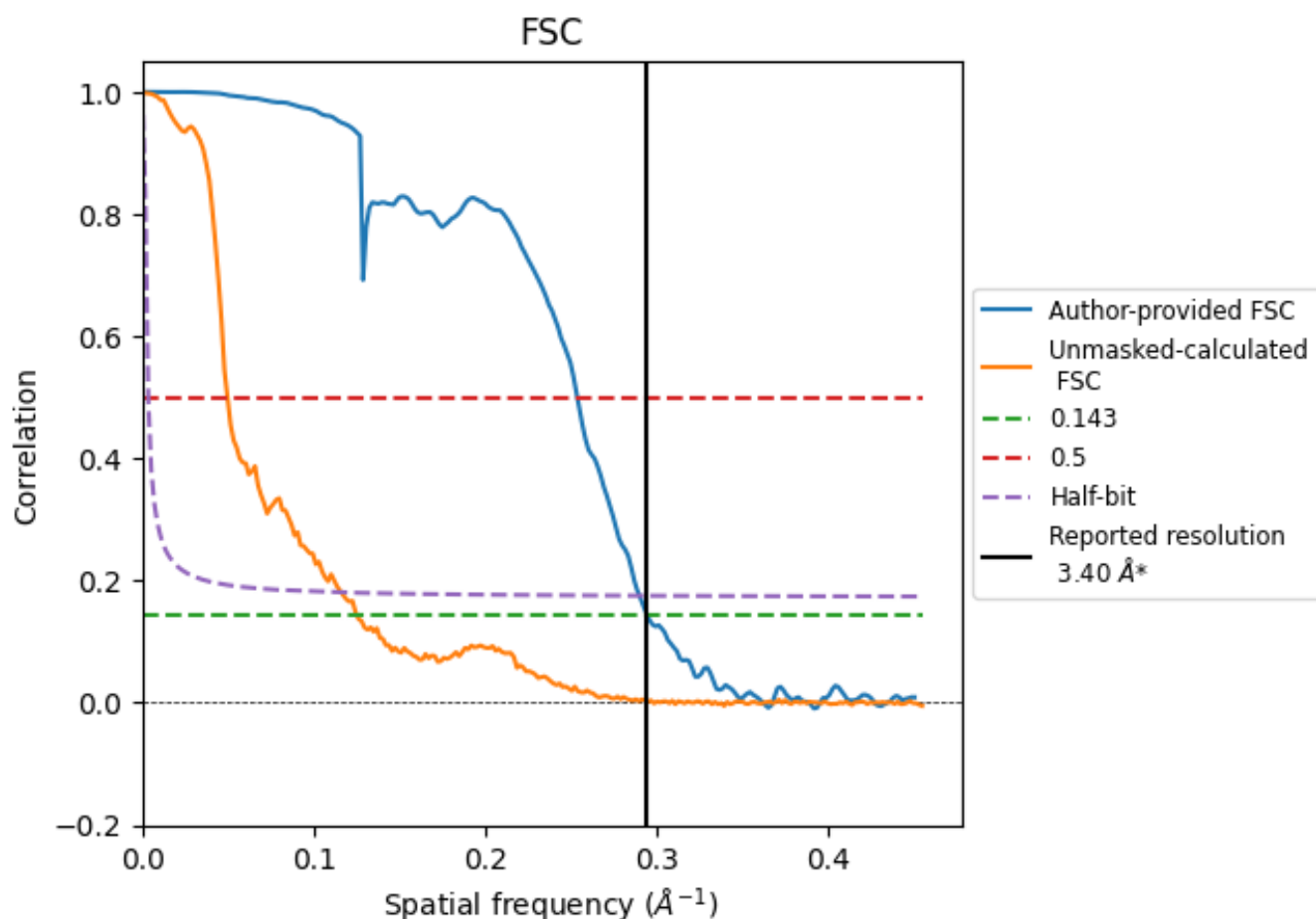


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

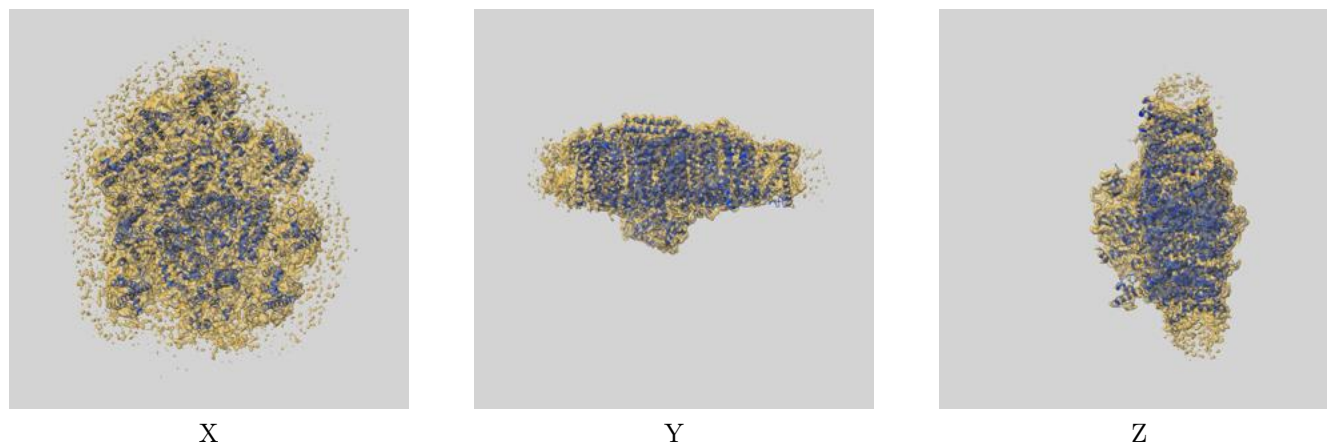
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.94	3.45
Unmasked-calculated*	7.99	20.12	8.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.99 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

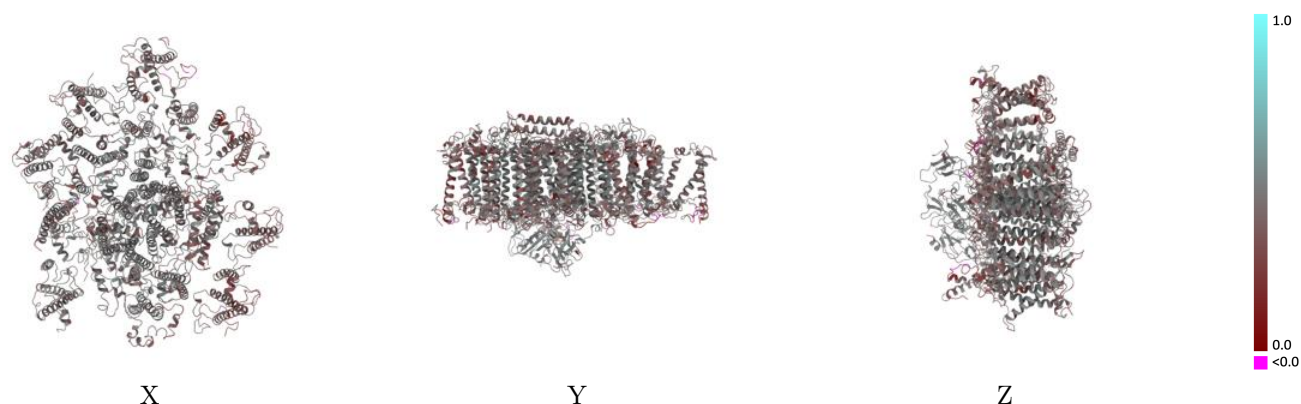
This section contains information regarding the fit between EMDB map EMD-60293 and PDB model 8ZOH. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



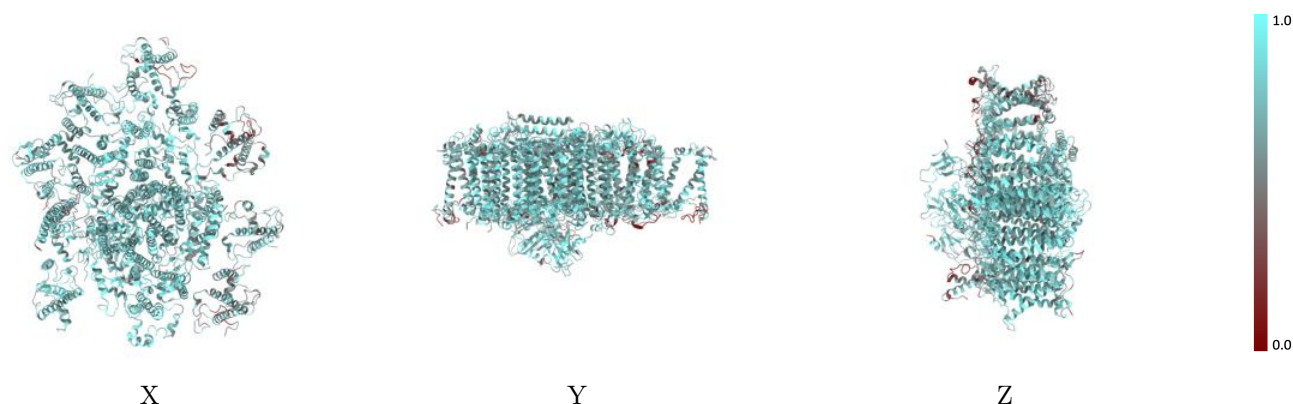
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



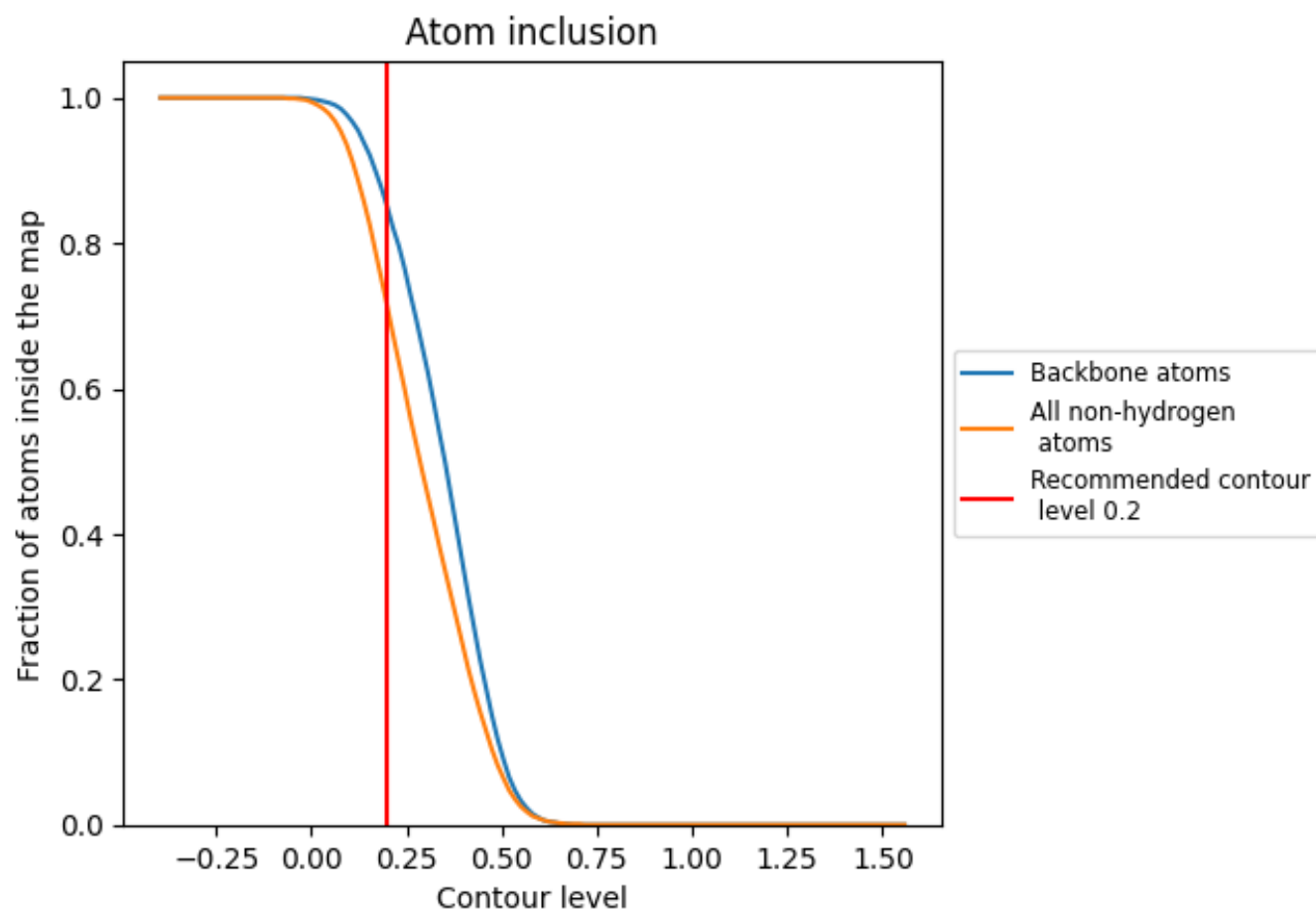
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.4300
1	 0.7230	 0.4360
4	 0.5480	 0.3590
5	 0.6560	 0.3970
6	 0.5340	 0.3670
7	 0.6100	 0.3860
8	 0.7240	 0.4350
9	 0.6920	 0.4250
a	 0.7560	 0.4490
b	 0.7590	 0.4500
c	 0.8610	 0.4780
d	 0.7960	 0.4630
e	 0.7800	 0.4640
f	 0.7280	 0.4210
g	 0.6640	 0.3950
h	 0.7020	 0.4340
i	 0.7370	 0.4740
j	 0.7050	 0.4500
l	 0.7330	 0.4220
m	 0.7130	 0.4580

