



## wwPDB EM Validation Summary Report ⓘ

Dec 1, 2025 – 09:42 PM JST

PDB ID : 8ZOI / pdb\_00008zoi  
EMDB ID : EMD-60294  
Title : Structure of the astaxanthin mutant PSI-5VCPI supercomplex in Nan-  
nochloropsis oceanica  
Authors : Shen, L.L.; Shen, J.R.; Wang, W.D.  
Deposited on : 2024-05-28  
Resolution : 3.31 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

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

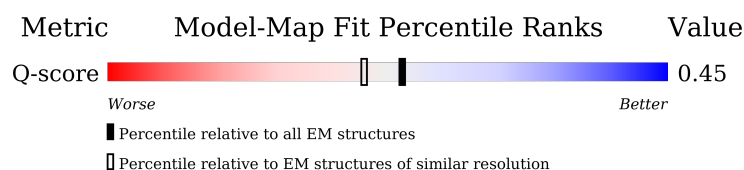
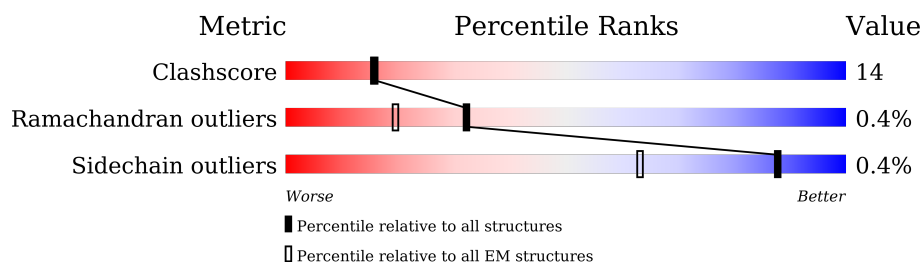
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.31 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.




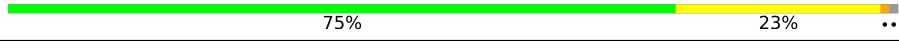
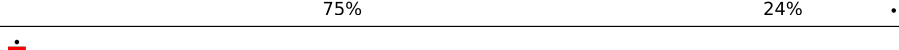
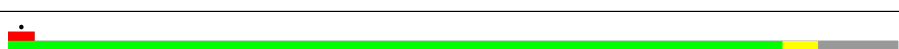



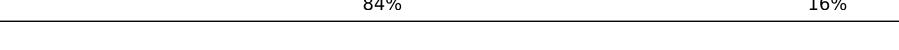


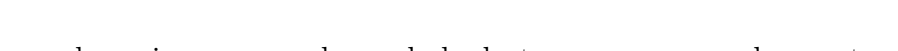

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14550 ( 2.81 - 3.81 )

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

Mol	Chain	Length	Quality of chain
1	5	244	<div> <div>52%</div> <div>17%</div> <div>31%</div> </div>
2	4	202	<div> <div>72%</div> <div>11%</div> <div>17%</div> </div>
3	3	220	<div> <div>67%</div> <div>14%</div> <div>20%</div> </div>
4	2	223	<div> <div>10%</div> <div>68%</div> <div>14%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
5	1	208	
6	a	745	
7	b	737	
8	d	136	
9	e	67	
10	f	185	
11	i	45	
12	j	41	
13	l	172	
14	m	30	
15	g	55	
16	c	81	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	305	X	-	-	-
19	CLA	1	306	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	1	311	X	-	-	-
19	CLA	1	312	X	-	-	-
19	CLA	1	313	X	-	-	-
19	CLA	1	314	X	-	-	-
19	CLA	2	306	X	-	-	-
19	CLA	2	307	X	-	-	-
19	CLA	2	308	X	-	-	-
19	CLA	2	309	X	-	-	-
19	CLA	2	310	X	-	-	-
19	CLA	2	311	X	-	-	-
19	CLA	2	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	313	X	-	-	-
19	CLA	2	314	X	-	-	-
19	CLA	2	315	X	-	-	-
19	CLA	2	316	X	-	-	-
19	CLA	3	307	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	309	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	311	X	-	-	-
19	CLA	3	312	X	-	-	-
19	CLA	3	313	X	-	-	-
19	CLA	3	314	X	-	-	-
19	CLA	3	315	X	-	-	-
19	CLA	4	305	X	-	-	-
19	CLA	4	306	X	-	-	-
19	CLA	4	307	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	4	314	X	-	-	-
19	CLA	4	315	X	-	-	-
19	CLA	4	316	X	-	-	-
19	CLA	5	306	X	-	-	-
19	CLA	5	307	X	-	-	-
19	CLA	5	308	X	-	-	-
19	CLA	5	309	X	-	-	-
19	CLA	5	310	X	-	-	-
19	CLA	5	311	X	-	-	-
19	CLA	5	312	X	-	-	-
19	CLA	5	313	X	-	-	-
19	CLA	5	314	X	-	-	-
19	CLA	5	315	X	-	-	-
19	CLA	5	316	X	-	-	-
19	CLA	a	801	X	-	-	-
19	CLA	a	802	X	-	-	-
19	CLA	a	803	X	-	-	-
19	CLA	a	804	X	-	-	-
19	CLA	a	805	X	-	-	-
19	CLA	a	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	807	X	-	-	-
19	CLA	a	808	X	-	-	-
19	CLA	a	809	X	-	-	-
19	CLA	a	810	X	-	-	-
19	CLA	a	811	X	-	-	-
19	CLA	a	812	X	-	-	-
19	CLA	a	813	X	-	-	-
19	CLA	a	814	X	-	-	-
19	CLA	a	815	X	-	-	-
19	CLA	a	816	X	-	-	-
19	CLA	a	817	X	-	-	-
19	CLA	a	818	X	-	-	-
19	CLA	a	819	X	-	-	-
19	CLA	a	820	X	-	-	-
19	CLA	a	821	X	-	-	-
19	CLA	a	822	X	-	-	-
19	CLA	a	823	X	-	-	-
19	CLA	a	824	X	-	-	-
19	CLA	a	825	X	-	-	-
19	CLA	a	826	X	-	-	-
19	CLA	a	827	X	-	-	-
19	CLA	a	828	X	-	-	-
19	CLA	a	829	X	-	-	-
19	CLA	a	830	X	-	-	-
19	CLA	a	831	X	-	-	-
19	CLA	a	832	X	-	-	-
19	CLA	a	833	X	-	-	-
19	CLA	a	834	X	-	-	-
19	CLA	a	835	X	-	-	-
19	CLA	a	836	X	-	-	-
19	CLA	a	837	X	-	-	-
19	CLA	a	838	X	-	-	-
19	CLA	a	839	X	-	-	-
19	CLA	a	840	X	-	-	-
19	CLA	a	841	X	-	-	-
19	CLA	a	842	X	-	-	-
19	CLA	a	844	X	-	-	-
19	CLA	a	852	X	-	-	-
19	CLA	a	856	X	-	X	-
19	CLA	b	801	X	-	-	-
19	CLA	b	802	X	-	-	-
19	CLA	b	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	804	X	-	-	-
19	CLA	b	805	X	-	-	-
19	CLA	b	806	X	-	-	-
19	CLA	b	807	X	-	-	-
19	CLA	b	808	X	-	-	-
19	CLA	b	809	X	-	-	-
19	CLA	b	810	X	-	-	-
19	CLA	b	811	X	-	-	-
19	CLA	b	812	X	-	-	-
19	CLA	b	813	X	-	-	-
19	CLA	b	814	X	-	-	-
19	CLA	b	815	X	-	-	-
19	CLA	b	816	X	-	-	-
19	CLA	b	817	X	-	-	-
19	CLA	b	818	X	-	-	-
19	CLA	b	819	X	-	-	-
19	CLA	b	820	X	-	-	-
19	CLA	b	821	X	-	-	-
19	CLA	b	822	X	-	-	-
19	CLA	b	823	X	-	-	-
19	CLA	b	824	X	-	-	-
19	CLA	b	825	X	-	-	-
19	CLA	b	826	X	-	-	-
19	CLA	b	827	X	-	-	-
19	CLA	b	828	X	-	-	-
19	CLA	b	829	X	-	-	-
19	CLA	b	830	X	-	-	-
19	CLA	b	831	X	-	-	-
19	CLA	b	832	X	-	-	-
19	CLA	b	833	X	-	-	-
19	CLA	b	834	X	-	-	-
19	CLA	b	835	X	-	-	-
19	CLA	b	836	X	-	-	-
19	CLA	b	837	X	-	-	-
19	CLA	b	838	X	-	-	-
19	CLA	b	839	X	-	-	-
19	CLA	b	840	X	-	-	-
19	CLA	b	841	X	-	-	-
19	CLA	f	802	X	-	-	-
19	CLA	f	803	X	-	-	-
19	CLA	i	102	X	-	-	-
19	CLA	j	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	l	201	X	-	-	-
19	CLA	l	202	X	-	-	-
19	CLA	l	203	X	-	-	-
26	BCR	f	801	-	-	X	-
27	SF4	c	102	-	-	X	-

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 34605 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-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	168	Total	C	N	O	S	0	0
			1268	822	211	229	6		

- Molecule 3 is a protein called VCPI-3.

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

- Molecule 4 is a protein called VCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	185	Total	C	N	O	S	0	0
			1372	892	224	249	7		

- Molecule 5 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called PSI subunit V.

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

- Molecule 14 is a protein called PsaM.

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

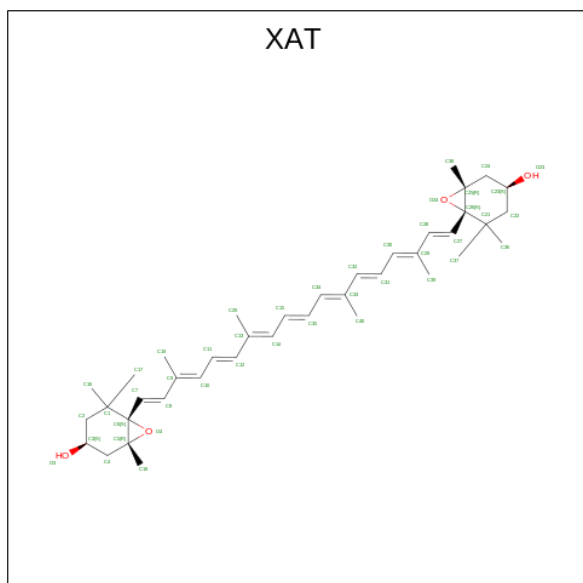
- Molecule 15 is a protein called PsaS.

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

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

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

- Molecule 17 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).



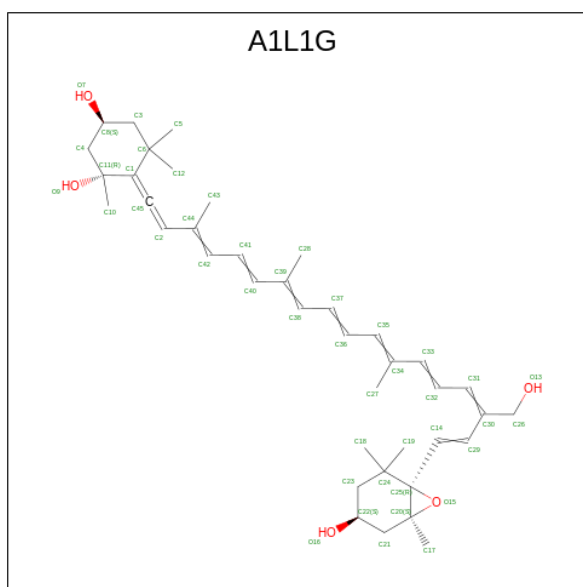
Mol	Chain	Residues	Atoms			AltConf
17	5	1	Total	C	O	0
			44	40	4	
17	5	1	Total	C	O	0
			44	40	4	
17	5	1	Total	C	O	0
			44	40	4	

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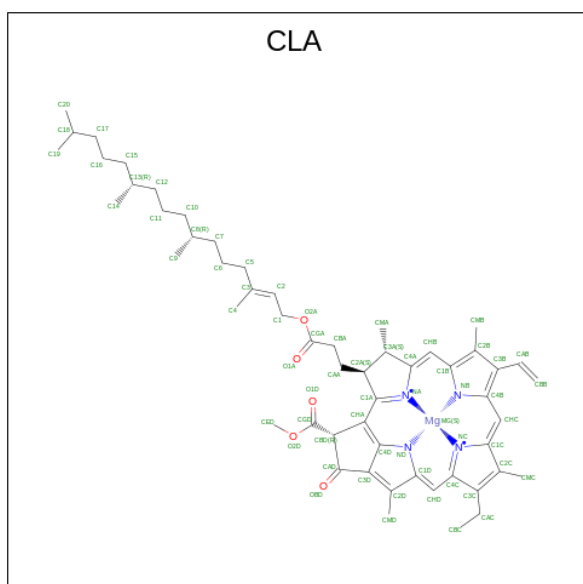
Mol	Chain	Residues	Atoms			AltConf
17	5	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	1	1	Total	C	O	0
			44	40	4	
17	1	1	Total	C	O	0
			44	40	4	
17	a	1	Total	C	O	0
			44	40	4	
17	a	1	Total	C	O	0
			44	40	4	

- Molecule 18 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	5	1	Total	C	O	0
			45	40	5	
18	3	1	Total	C	O	0
			45	40	5	
18	3	1	Total	C	O	0
			45	40	5	
18	1	1	Total	C	O	0
			45	40	5	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 53	C 43	Mg 1	N 4	O 5	0
19	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
19	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 56	C 46	Mg 1	N 4	O 5	0

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

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

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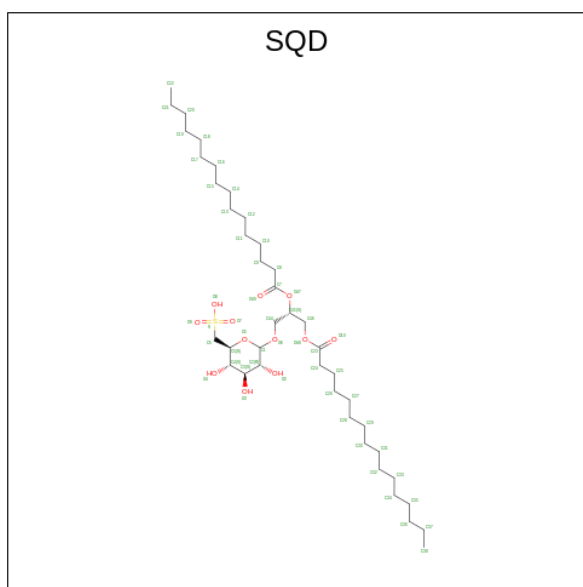
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	b	1	Total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

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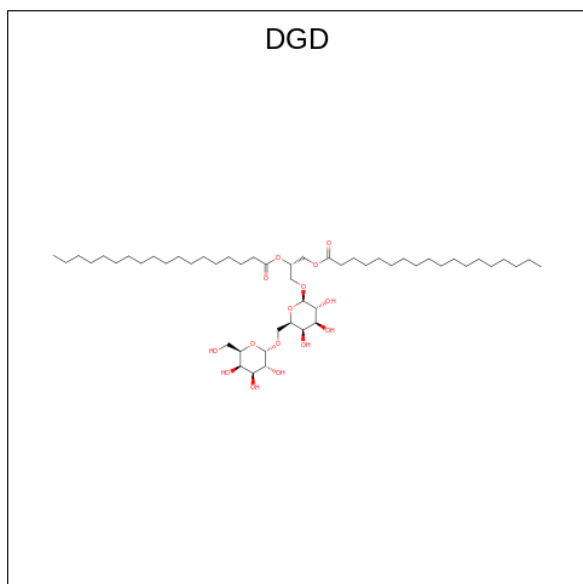
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
20	5	1	Total	C	O	S	0
			35	22	12	1	
20	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	4	1	Total	C	O	0
			40	25	15	

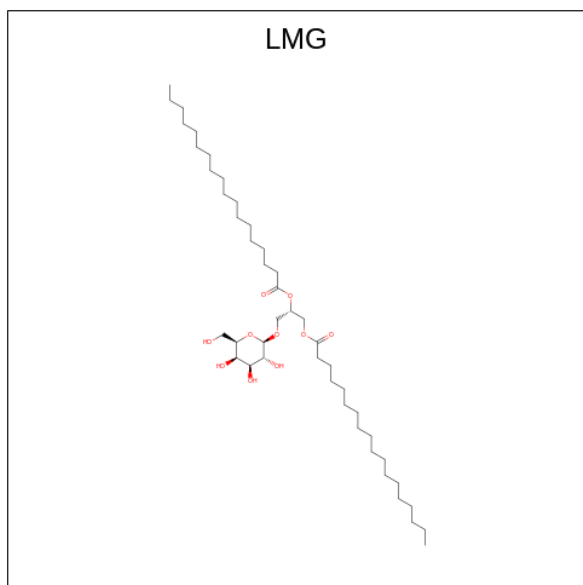
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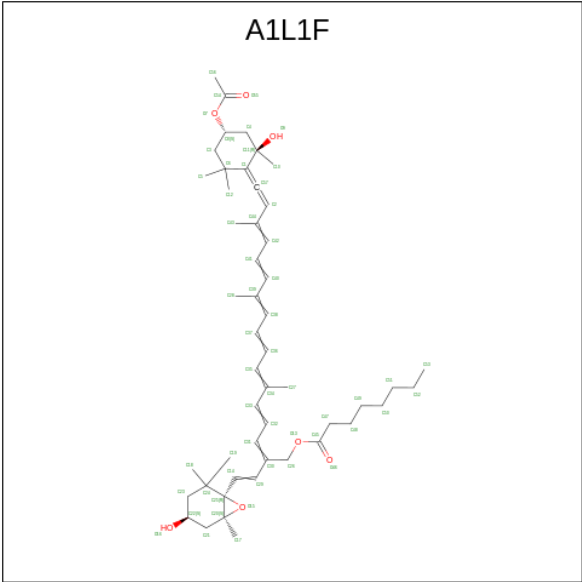
Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			57	42	15	

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



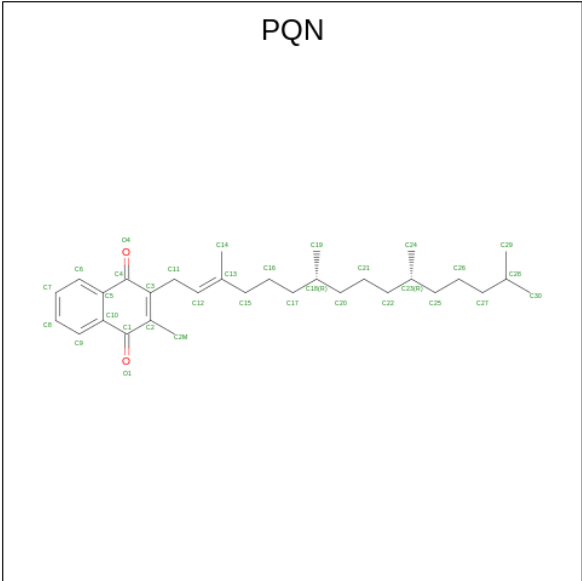
Mol	Chain	Residues	Atoms			AltConf
22	2	1	Total	C	O	0
			35	25	10	
22	a	1	Total	C	O	0
			34	24	10	
22	j	1	Total	C	O	0
			32	22	10	

- Molecule 23 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[( {E})-2-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula:  $C_{50}H_{72}O_7$ ) (labeled as "Ligand of Interest" by depositor).



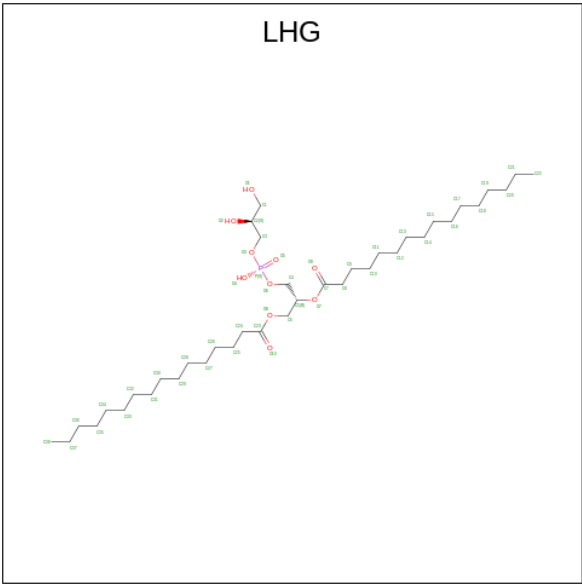
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			57	50	7	

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



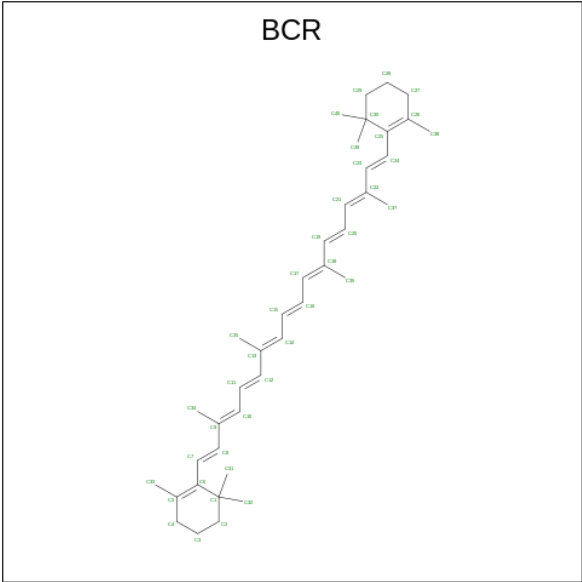
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			33	31	2	
24	b	1	Total	C	O	0
			33	31	2	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



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

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



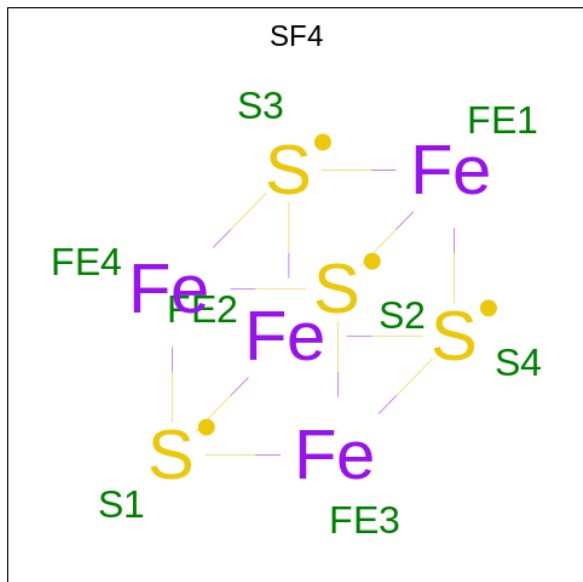
Mol	Chain	Residues	Atoms	AltConf
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C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

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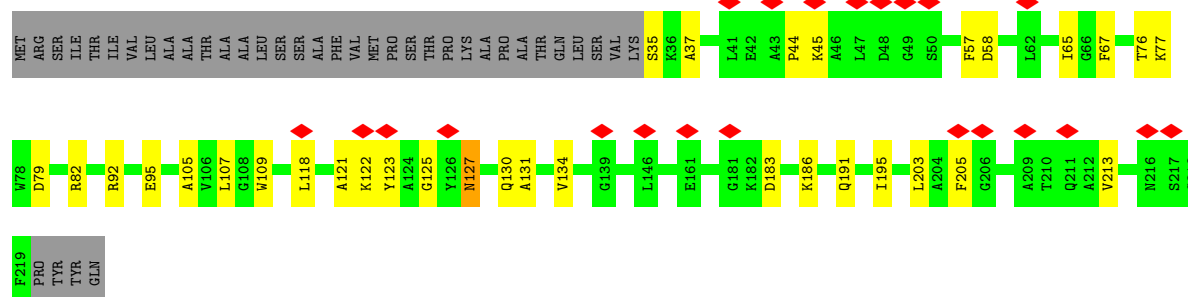
Mol	Chain	Residues	Atoms	AltConf
26	f	1	Total C 40 40	0
26	i	1	Total C 40 40	0
26	i	1	Total C 40 40	0
26	j	1	Total C 40 40	0
26	m	1	Total C 40 40	0

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

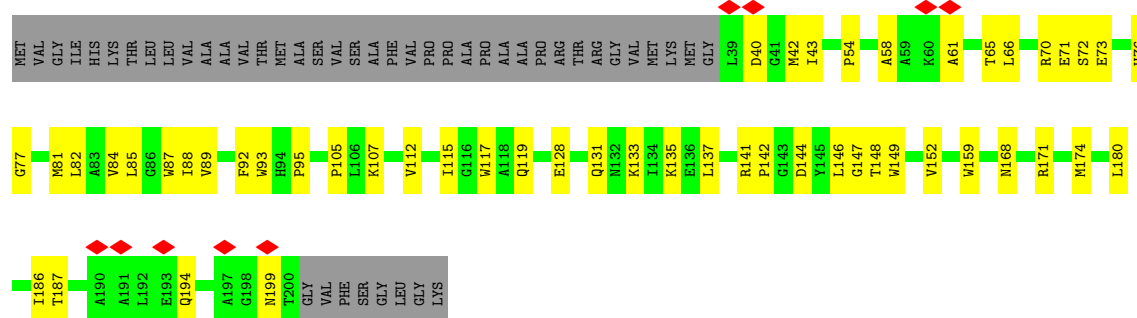


Mol	Chain	Residues	Atoms	AltConf
27	a	1	Total Fe S 8 4 4	0
27	c	1	Total Fe S 8 4 4	0
27	c	1	Total Fe S 8 4 4	0

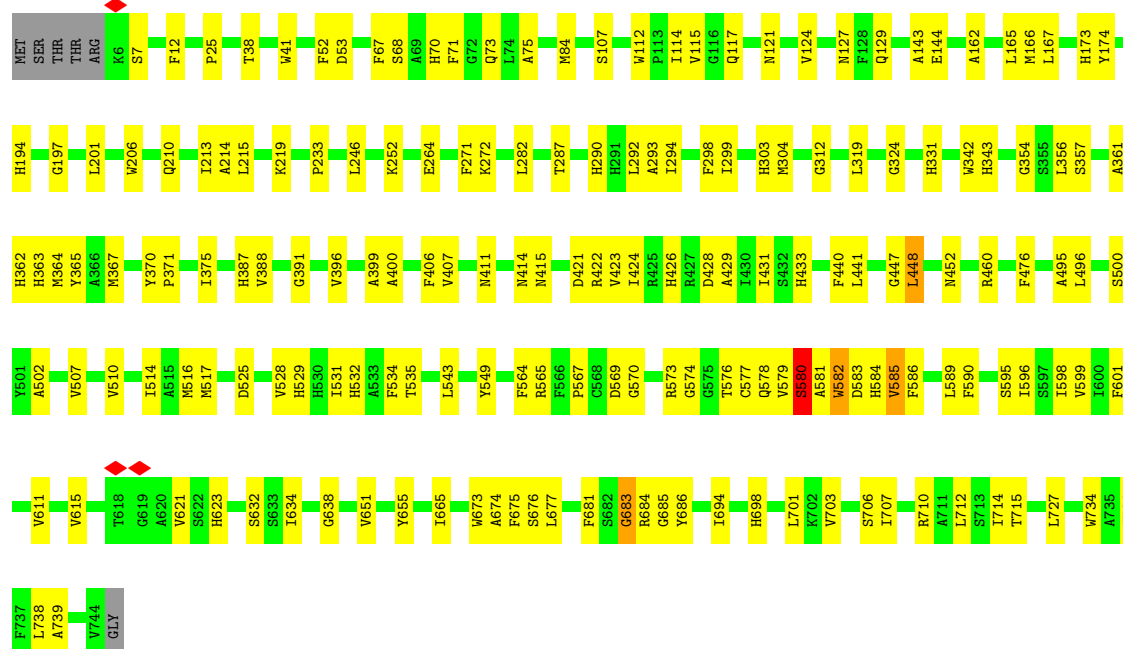




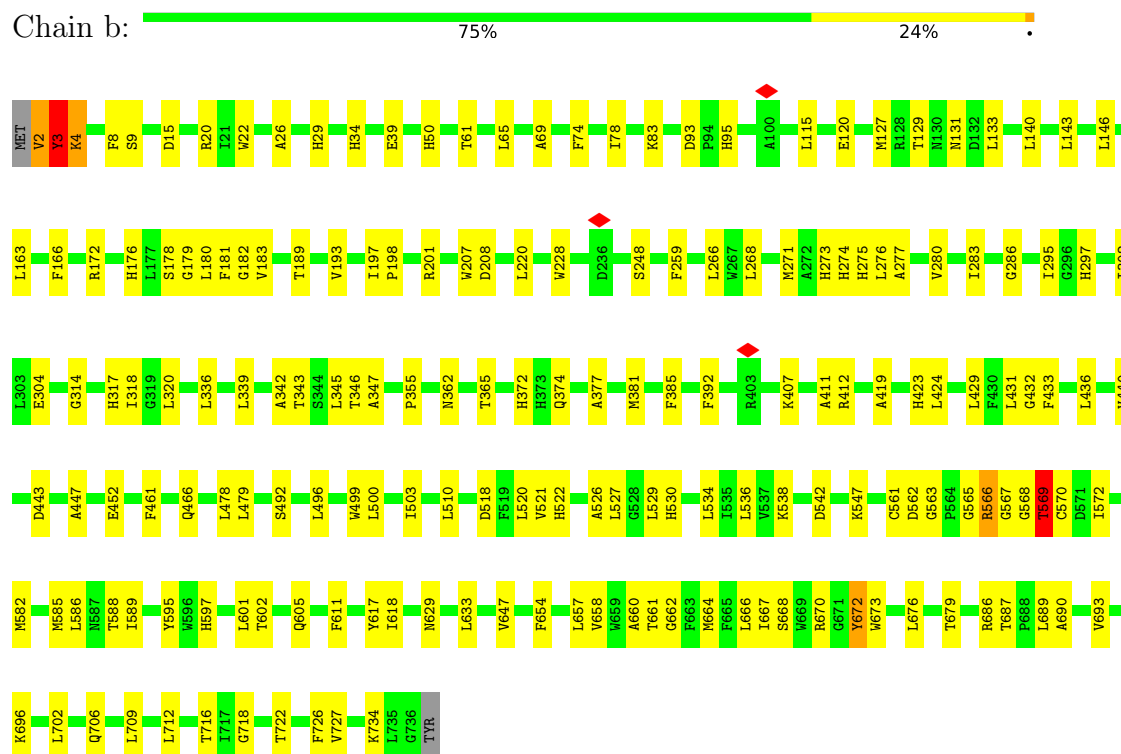
• Molecule 5: VCPI-1



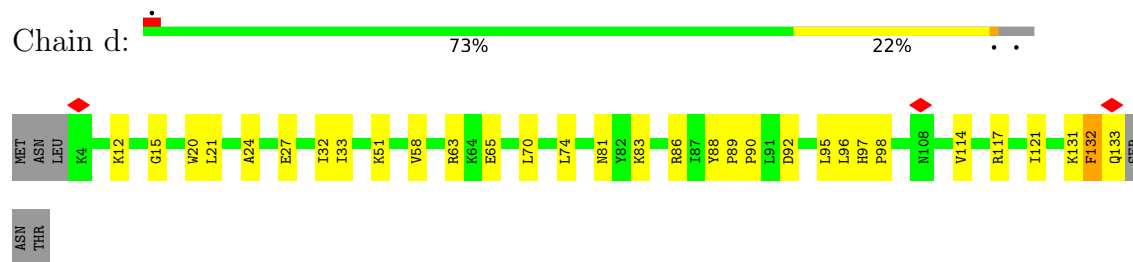
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1



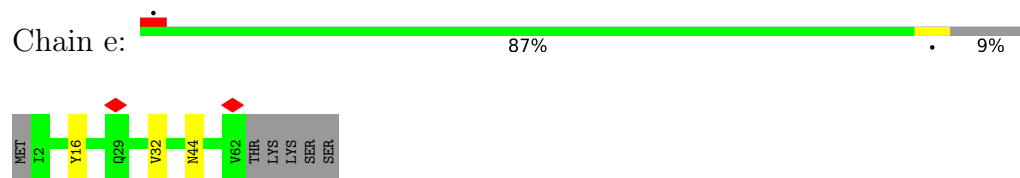
- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2



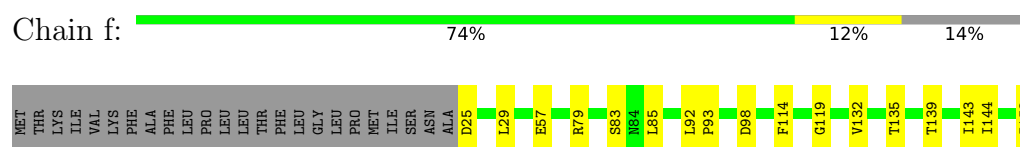
- Molecule 8: Photosystem I reaction center subunit II



- Molecule 9: Photosystem I reaction center subunit IV



- Molecule 10: Photosystem I reaction center subunit III







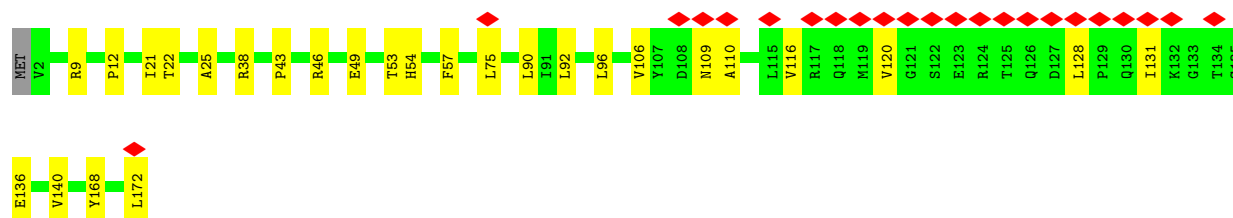
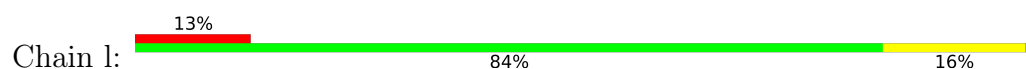
• Molecule 11: Photosystem I reaction center subunit VIII



• Molecule 12: Photosystem I reaction center subunit IX



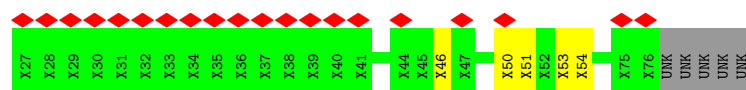
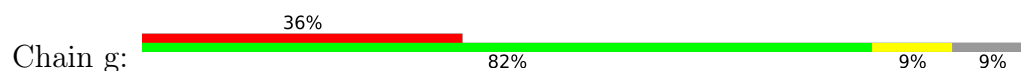
• Molecule 13: PSI subunit V



• Molecule 14: PsaM



• Molecule 15: PsaS



• Molecule 16: Photosystem I iron-sulfur center



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35738	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	1.455	Depositor
Minimum map value	-0.346	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	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 [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	5	0.14	0/1353	0.29	0/1823
2	4	0.17	0/1298	0.32	0/1761
3	3	0.13	0/1350	0.28	0/1821
4	2	0.14	0/1405	0.36	0/1904
5	1	0.14	0/1293	0.33	0/1759
6	a	0.30	3/6024 (0.0%)	0.35	5/8219 (0.1%)
7	b	0.27	0/6080	0.35	2/8302 (0.0%)
8	d	0.19	0/1040	0.36	0/1402
9	e	0.09	0/502	0.20	0/681
10	f	0.14	0/1297	0.31	0/1762
11	i	0.15	0/278	0.33	0/378
12	j	0.16	0/351	0.35	0/478
13	l	0.14	0/1315	0.31	0/1796
14	m	0.10	0/210	0.28	0/288
16	c	0.13	0/606	0.34	0/822
All	All	0.23	3/24402 (0.0%)	0.34	7/33196 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	580	SER	CA-C	-7.01	1.43	1.52
6	a	581	ALA	CA-C	-5.37	1.45	1.52
6	a	582	TRP	CA-C	-5.10	1.45	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	581	ALA	N-CA-C	-8.64	102.49	113.72
6	a	683	GLY	O-C-N	-8.44	116.31	123.73
7	b	568	GLY	N-CA-C	-7.48	100.74	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	448	LEU	N-CA-C	-6.04	104.27	111.69
6	a	584	HIS	N-CA-C	-5.87	106.46	113.97

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	4	1268	0	1288	24	0
3	3	1324	0	1340	21	0
4	2	1372	0	1347	21	0
5	1	1262	0	1237	37	0
6	a	5827	0	5697	158	0
7	b	5865	0	5711	188	0
8	d	1014	0	1015	29	0
9	e	494	0	495	3	0
10	f	1266	0	1262	32	0
11	i	271	0	292	17	0
12	j	339	0	342	14	0
13	l	1283	0	1278	27	0
14	m	210	0	226	1	0
15	g	250	0	57	4	0
16	c	596	0	583	23	0
17	1	88	0	112	6	0
17	2	220	0	280	22	0
17	3	176	0	224	18	0
17	4	176	0	224	21	0
17	5	176	0	224	25	0
17	a	88	0	112	7	0
18	1	45	0	0	1	0
18	3	90	0	0	0	0
18	5	45	0	0	1	0
19	1	547	0	508	16	0
19	2	544	0	452	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	3	458	0	378	9	0
19	4	613	0	522	35	0
19	5	563	0	472	22	0
19	a	2644	0	2634	213	0
19	b	2468	0	2519	167	0
19	f	117	0	115	2	0
19	i	62	0	63	7	0
19	j	42	0	31	2	0
19	l	148	0	123	10	0
20	1	45	0	54	3	0
20	5	35	0	34	1	0
21	4	40	0	38	11	0
21	b	57	0	72	5	0
22	2	35	0	40	3	0
22	a	34	0	38	10	0
22	j	32	0	34	5	0
23	1	57	0	0	10	0
24	a	33	0	46	4	0
24	b	33	0	46	7	0
25	a	75	0	93	5	0
25	b	31	0	32	0	0
25	m	46	0	65	2	0
26	a	160	0	224	15	0
26	b	360	0	504	54	0
26	f	80	0	112	31	0
26	i	80	0	112	16	0
26	j	40	0	56	14	0
26	m	40	0	56	0	0
27	a	8	0	0	0	0
27	c	16	0	0	3	0
All	All	34605	0	34137	983	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 983 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)
6:a:698:HIS:NE2	19:a:856:CLA:HAC1	1.52	1.24
19:a:834:CLA:H151	24:b:842:PQN:H202	1.21	1.20
19:a:802:CLA:HED3	26:f:801:BCR:H401	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:802:CLA:HED3	26:f:801:BCR:C40	1.80	1.11
19:a:833:CLA:H61	19:l:202:CLA:H101	1.28	1.11

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	22	53
3	3	175/220 (80%)	166 (95%)	9 (5%)	0	100	100
4	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	8	33
5	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
6	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	77
7	b	733/737 (100%)	697 (95%)	33 (4%)	3 (0%)	30	61
8	d	128/136 (94%)	112 (88%)	15 (12%)	1 (1%)	16	47
9	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
10	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
11	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
12	j	39/41 (95%)	39 (100%)	0	0	100	100
13	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	11	39
14	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3012/3336 (90%)	2828 (94%)	173 (6%)	11 (0%)	32	61

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	45	LYS
13	l	120	VAL
4	2	127	ASN
4	2	213	VAL
7	b	566	ARG

### 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	4	133/159 (84%)	133 (100%)	0	100	100
3	3	136/164 (83%)	136 (100%)	0	100	100
4	2	134/172 (78%)	134 (100%)	0	100	100
5	1	128/165 (78%)	128 (100%)	0	100	100
6	a	607/613 (99%)	603 (99%)	4 (1%)	81	88
7	b	599/602 (100%)	595 (99%)	4 (1%)	81	88
8	d	107/113 (95%)	106 (99%)	1 (1%)	75	85
9	e	56/62 (90%)	56 (100%)	0	100	100
10	f	138/162 (85%)	138 (100%)	0	100	100
11	i	32/43 (74%)	32 (100%)	0	100	100
12	j	36/36 (100%)	36 (100%)	0	100	100
13	l	130/141 (92%)	130 (100%)	0	100	100
14	m	21/24 (88%)	21 (100%)	0	100	100
16	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2457/2706 (91%)	2448 (100%)	9 (0%)	88	93

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

Mol	Chain	Res	Type
7	b	569	THR
8	d	133	GLN

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Mol	Chain	Res	Type
6	a	580	SER
7	b	2	VAL
7	b	3	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
7	b	605	GLN
8	d	26	ASN
8	d	7	GLN
8	d	109	GLN
6	a	186	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

207 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	$\# Z  > 2$
19	CLA	2	316	4	46,54,73	1.76	6 (13%)	53,90,113	1.54	6 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
19	CLA	b	818	-	60,68,73	1.56	5 (8%)	70,107,113	1.41	7 (10%)
20	SQD	1	315	-	44,45,54	1.30	4 (9%)	53,56,65	1.16	5 (9%)
19	CLA	b	829	-	65,73,73	1.52	6 (9%)	76,113,113	1.44	10 (13%)
19	CLA	3	311	-	50,58,73	1.71	5 (10%)	58,95,113	1.54	9 (15%)
17	XAT	a	854	-	39,47,47	0.95	2 (5%)	54,74,74	2.70	20 (37%)
19	CLA	b	827	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	8 (10%)
19	CLA	a	842	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
17	XAT	2	301	-	39,47,47	0.91	0	54,74,74	2.71	19 (35%)
19	CLA	4	312	-	53,61,73	1.65	5 (9%)	61,98,113	1.48	8 (13%)
19	CLA	5	309	-	55,63,73	1.64	6 (10%)	64,101,113	1.48	8 (12%)
19	CLA	b	832	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
19	CLA	3	314	3	47,55,73	1.75	6 (12%)	54,91,113	1.55	7 (12%)
19	CLA	5	315	-	52,60,73	1.66	5 (9%)	60,97,113	1.54	8 (13%)
19	CLA	l	201	-	42,50,73	1.82	6 (14%)	48,85,113	1.64	7 (14%)
23	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
19	CLA	a	810	6	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)
19	CLA	a	825	-	55,63,73	1.62	5 (9%)	64,101,113	1.45	8 (12%)
19	CLA	1	312	5	52,60,73	1.71	5 (9%)	60,97,113	1.49	8 (13%)
19	CLA	a	834	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	9 (11%)
19	CLA	b	809	-	65,73,73	1.45	5 (7%)	76,113,113	1.42	9 (11%)
19	CLA	b	822	-	60,68,73	1.55	6 (10%)	70,107,113	1.36	7 (10%)
26	BCR	a	850	-	41,41,41	0.75	0	56,56,56	2.16	14 (25%)
25	LHG	m	101	-	45,45,48	1.15	6 (13%)	48,51,54	0.95	2 (4%)
19	CLA	b	833	-	58,66,73	1.58	5 (8%)	67,104,113	1.43	8 (11%)
19	CLA	a	830	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	8 (10%)
19	CLA	b	826	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	6 (7%)
19	CLA	a	840	-	65,73,73	1.52	6 (9%)	76,113,113	1.37	7 (9%)
19	CLA	b	805	-	65,73,73	1.45	5 (7%)	76,113,113	1.42	7 (9%)
19	CLA	2	307	-	47,55,73	1.75	5 (10%)	54,91,113	1.64	8 (14%)
19	CLA	a	832	-	50,58,73	1.68	6 (12%)	58,95,113	1.55	9 (15%)
19	CLA	f	803	10	52,60,73	1.66	5 (9%)	60,97,113	1.48	8 (13%)
19	CLA	a	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
26	BCR	b	853	-	41,41,41	0.72	0	56,56,56	1.97	18 (32%)
21	DGD	b	851	-	58,58,67	1.15	7 (12%)	72,72,81	1.53	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	a	821	-	45,53,73	1.77	6 (13%)	52,89,113	1.61	7 (13%)
19	CLA	4	306	-	56,64,73	1.62	5 (8%)	65,102,113	1.44	9 (13%)
18	A1L1G	3	302	-	38,47,47	1.46	6 (15%)	49,71,71	1.38	7 (14%)
17	XAT	3	304	-	39,47,47	0.91	2 (5%)	54,74,74	2.62	19 (35%)
19	CLA	1	313	-	41,49,73	1.85	6 (14%)	47,84,113	1.65	7 (14%)
19	CLA	b	819	-	55,63,73	1.62	5 (9%)	64,101,113	1.43	8 (12%)
19	CLA	a	835	-	65,73,73	1.46	5 (7%)	76,113,113	1.44	7 (9%)
19	CLA	a	831	-	65,73,73	1.51	5 (7%)	76,113,113	1.48	8 (10%)
19	CLA	a	841	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	9 (11%)
24	PQN	b	842	-	34,34,34	1.55	2 (5%)	42,45,45	1.21	4 (9%)
17	XAT	5	305	-	39,47,47	0.91	1 (2%)	54,74,74	2.86	22 (40%)
19	CLA	3	309	3	56,64,73	1.59	6 (10%)	65,102,113	1.46	7 (10%)
19	CLA	a	823	-	49,57,73	1.69	5 (10%)	55,93,113	1.61	7 (12%)
19	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.39	8 (10%)
18	A1L1G	3	306	-	38,47,47	1.44	6 (15%)	49,71,71	1.49	9 (18%)
19	CLA	b	806	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
26	BCR	f	804	-	41,41,41	0.71	0	56,56,56	2.04	17 (30%)
19	CLA	2	306	-	41,50,73	1.85	5 (12%)	46,85,113	1.57	6 (13%)
19	CLA	1	308	5	65,73,73	1.48	5 (7%)	76,113,113	1.43	9 (11%)
17	XAT	3	305	-	39,47,47	0.87	1 (2%)	54,74,74	2.57	17 (31%)
19	CLA	b	802	-	65,73,73	1.48	7 (10%)	76,113,113	1.35	8 (10%)
19	CLA	a	809	6	65,73,73	1.45	5 (7%)	76,113,113	1.44	9 (11%)
26	BCR	b	847	-	41,41,41	0.77	0	56,56,56	2.19	21 (37%)
19	CLA	3	312	3	59,67,73	1.57	6 (10%)	68,105,113	1.43	7 (10%)
26	BCR	b	846	-	41,41,41	0.70	0	56,56,56	1.97	21 (37%)
26	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.95	16 (28%)
19	CLA	b	830	-	41,49,73	1.82	6 (14%)	47,84,113	1.66	8 (17%)
19	CLA	4	313	2	45,53,73	1.80	6 (13%)	52,89,113	1.56	7 (13%)
19	CLA	b	823	-	53,61,73	1.63	6 (11%)	61,98,113	1.46	8 (13%)
19	CLA	4	316	-	55,63,73	1.63	6 (10%)	64,101,113	1.45	7 (10%)
19	CLA	2	313	4	41,49,73	1.84	5 (12%)	47,84,113	1.68	8 (17%)
19	CLA	a	806	-	65,73,73	1.50	11 (16%)	76,113,113	1.67	13 (17%)
19	CLA	a	816	-	50,58,73	1.69	6 (12%)	58,95,113	1.56	9 (15%)
26	BCR	b	844	-	41,41,41	0.71	0	56,56,56	1.92	16 (28%)
19	CLA	a	803	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	XAT	1	303	-	39,47,47	0.90	1 (2%)	54,74,74	2.52	19 (35%)
19	CLA	a	827	-	65,73,73	1.49	6 (9%)	76,113,113	1.45	9 (11%)
26	BCR	m	102	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	6 (10%)
17	XAT	2	304	-	39,47,47	0.88	0	54,74,74	2.55	20 (37%)
19	CLA	2	315	-	42,50,73	1.85	6 (14%)	48,85,113	1.55	7 (14%)
19	CLA	1	311	-	53,61,73	1.63	5 (9%)	61,98,113	1.50	9 (14%)
19	CLA	4	311	-	46,54,73	1.78	6 (13%)	53,90,113	1.51	7 (13%)
19	CLA	a	818	-	56,64,73	1.62	5 (8%)	65,102,113	1.44	8 (12%)
19	CLA	b	808	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	8 (10%)
19	CLA	2	310	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
19	CLA	2	311	-	58,66,73	1.58	5 (8%)	67,104,113	1.41	7 (10%)
19	CLA	4	310	-	46,54,73	1.78	6 (13%)	53,90,113	1.56	7 (13%)
19	CLA	b	815	-	45,53,73	1.76	6 (13%)	52,89,113	1.58	7 (13%)
19	CLA	b	825	-	64,72,73	1.49	5 (7%)	74,111,113	1.44	7 (9%)
21	DGD	4	317	-	41,41,67	1.06	2 (4%)	55,55,81	1.82	5 (9%)
26	BCR	b	843	-	41,41,41	0.70	0	56,56,56	2.29	21 (37%)
19	CLA	b	814	-	55,63,73	1.60	6 (10%)	64,101,113	1.56	8 (12%)
19	CLA	5	312	-	51,59,73	1.64	5 (9%)	59,96,113	1.52	9 (15%)
19	CLA	a	811	-	56,64,73	1.58	6 (10%)	65,102,113	1.47	9 (13%)
19	CLA	2	314	-	56,64,73	1.63	6 (10%)	65,102,113	1.45	7 (10%)
26	BCR	a	849	-	41,41,41	0.74	0	56,56,56	2.17	19 (33%)
17	XAT	5	302	-	39,47,47	0.94	1 (2%)	54,74,74	2.57	19 (35%)
17	XAT	2	305	-	39,47,47	0.91	1 (2%)	54,74,74	2.43	18 (33%)
19	CLA	3	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.56	8 (14%)
22	LMG	a	855	-	34,34,55	1.14	2 (5%)	42,42,63	1.16	3 (7%)
19	CLA	3	307	3	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
19	CLA	1	306	-	65,73,73	1.46	5 (7%)	76,113,113	1.41	9 (11%)
17	XAT	2	303	-	39,47,47	0.98	1 (2%)	54,74,74	2.63	20 (37%)
19	CLA	a	817	-	45,53,73	1.79	5 (11%)	52,89,113	1.58	6 (11%)
19	CLA	b	841	25	65,73,73	1.52	5 (7%)	76,113,113	1.36	8 (10%)
22	LMG	j	103	-	32,32,55	1.13	2 (6%)	40,40,63	1.14	3 (7%)
19	CLA	b	838	-	65,73,73	1.52	6 (9%)	76,113,113	1.34	9 (11%)
19	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.53	8 (12%)
19	CLA	4	315	-	46,54,73	1.76	5 (10%)	53,90,113	1.56	7 (13%)
22	LMG	2	317	-	35,35,55	1.11	2 (5%)	43,43,63	1.31	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	b	813	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	8 (10%)
19	CLA	3	315	3	46,54,73	1.79	6 (13%)	53,90,113	1.54	7 (13%)
19	CLA	4	308	-	50,58,73	1.68	6 (12%)	58,95,113	1.55	8 (13%)
26	BCR	i	101	-	41,41,41	0.74	0	56,56,56	2.13	14 (25%)
26	BCR	j	102	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
26	BCR	f	801	-	41,41,41	0.68	0	56,56,56	2.14	15 (26%)
19	CLA	b	836	-	58,66,73	1.57	5 (8%)	67,104,113	1.53	8 (11%)
19	CLA	b	837	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	9 (11%)
17	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.60	17 (31%)
19	CLA	5	316	-	46,54,73	1.74	5 (10%)	53,90,113	1.57	7 (13%)
17	XAT	4	301	-	39,47,47	0.91	1 (2%)	54,74,74	2.57	19 (35%)
19	CLA	a	822	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	8 (10%)
20	SQD	5	317	19	34,35,54	1.47	4 (11%)	43,46,65	1.34	7 (16%)
19	CLA	1	309	5	46,54,73	1.79	5 (10%)	53,90,113	1.51	7 (13%)
19	CLA	a	826	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	6 (7%)
26	BCR	b	850	-	41,41,41	0.72	0	56,56,56	1.88	17 (30%)
19	CLA	2	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.54	7 (13%)
19	CLA	b	828	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
24	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.10	3 (7%)
19	CLA	b	807	-	65,73,73	1.47	5 (7%)	76,113,113	1.37	9 (11%)
19	CLA	j	101	12	42,50,73	1.82	5 (11%)	48,85,113	1.64	6 (12%)
27	SF4	c	101	-	0,12,12	-	-	-	-	-
19	CLA	a	804	-	55,63,73	1.62	6 (10%)	64,101,113	1.55	10 (15%)
19	CLA	4	307	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	9 (11%)
19	CLA	b	816	-	55,63,73	1.62	5 (9%)	64,101,113	1.48	8 (12%)
19	CLA	b	834	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
19	CLA	1	314	-	45,53,73	1.79	5 (11%)	52,89,113	1.55	6 (11%)
19	CLA	b	810	-	65,73,73	1.47	5 (7%)	76,113,113	1.46	8 (10%)
19	CLA	a	805	19	55,63,73	1.62	6 (10%)	64,101,113	1.51	8 (12%)
19	CLA	a	801	-	65,73,73	1.51	9 (13%)	76,113,113	1.37	7 (9%)
19	CLA	4	314	2	41,49,73	1.86	5 (12%)	47,84,113	1.64	7 (14%)
19	CLA	a	819	-	54,62,73	1.63	7 (12%)	62,99,113	1.46	7 (11%)
19	CLA	a	814	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	8 (10%)
19	CLA	l	202	-	60,68,73	1.54	6 (10%)	70,107,113	1.46	7 (10%)
25	LHG	b	849	19	30,30,48	1.34	6 (20%)	33,36,54	1.15	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	a	802	-	58,66,73	1.55	6 (10%)	67,104,113	1.49	8 (11%)
19	CLA	a	838	-	51,59,73	1.65	5 (9%)	59,96,113	1.55	8 (13%)
19	CLA	a	856	-	65,73,73	1.48	6 (9%)	76,113,113	1.34	8 (10%)
17	XAT	3	303	-	39,47,47	0.90	0	54,74,74	2.59	20 (37%)
25	LHG	a	846	19	26,26,48	1.27	4 (15%)	29,32,54	1.20	2 (6%)
19	CLA	5	308	1	60,68,73	1.55	5 (8%)	70,107,113	1.43	8 (11%)
19	CLA	b	821	-	51,59,73	1.66	6 (11%)	59,96,113	1.57	9 (15%)
19	CLA	b	831	-	49,57,73	1.69	5 (10%)	55,93,113	1.55	8 (14%)
19	CLA	1	310	5	65,73,73	1.50	5 (7%)	76,113,113	1.33	8 (10%)
19	CLA	a	829	-	62,70,73	1.51	5 (8%)	72,109,113	1.40	8 (11%)
17	XAT	4	302	-	39,47,47	0.90	1 (2%)	54,74,74	2.58	17 (31%)
27	SF4	c	102	-	0,12,12	-	-	-	-	-
19	CLA	5	306	1	46,54,73	1.78	6 (13%)	53,90,113	1.55	8 (15%)
19	CLA	i	102	-	62,70,73	1.55	6 (9%)	72,109,113	1.37	8 (11%)
19	CLA	a	824	-	46,54,73	1.78	6 (13%)	53,90,113	1.50	7 (13%)
19	CLA	a	852	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
19	CLA	b	840	-	65,73,73	1.50	6 (9%)	76,113,113	1.40	8 (10%)
19	CLA	a	808	-	51,59,73	1.70	5 (9%)	59,96,113	1.50	8 (13%)
17	XAT	5	301	-	39,47,47	0.95	2 (5%)	54,74,74	2.62	19 (35%)
19	CLA	4	309	-	65,73,73	1.51	5 (7%)	76,113,113	1.41	8 (10%)
19	CLA	a	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
19	CLA	1	307	-	54,62,73	1.63	5 (9%)	62,99,113	1.51	7 (11%)
19	CLA	a	815	-	45,53,73	1.78	5 (11%)	52,89,113	1.59	8 (15%)
19	CLA	b	820	-	50,58,73	1.69	6 (12%)	58,95,113	1.60	10 (17%)
18	A1L1G	5	304	-	38,47,47	1.41	6 (15%)	49,71,71	1.45	7 (14%)
19	CLA	1	305	-	61,69,73	1.55	6 (9%)	71,108,113	1.41	7 (9%)
25	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
19	CLA	5	313	-	52,60,73	1.65	5 (9%)	60,97,113	1.54	9 (15%)
19	CLA	5	310	1	65,73,73	1.48	5 (7%)	76,113,113	1.36	7 (9%)
17	XAT	4	303	-	39,47,47	0.88	2 (5%)	54,74,74	2.56	15 (27%)
19	CLA	2	312	-	47,55,73	1.75	6 (12%)	54,91,113	1.57	7 (12%)
19	CLA	b	803	-	65,73,73	1.45	5 (7%)	76,113,113	1.53	13 (17%)
19	CLA	5	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
26	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
19	CLA	5	307	20	45,53,73	1.79	5 (11%)	52,89,113	1.56	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	XAT	2	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.51	18 (33%)
19	CLA	a	812	19	62,70,73	1.51	6 (9%)	72,109,113	1.46	8 (11%)
17	XAT	3	301	-	39,47,47	0.92	2 (5%)	54,74,74	2.54	18 (33%)
19	CLA	3	313	-	52,60,73	1.65	6 (11%)	60,97,113	1.53	9 (15%)
19	CLA	4	305	2	45,53,73	1.80	6 (13%)	52,89,113	1.56	7 (13%)
19	CLA	3	310	-	56,64,73	1.60	6 (10%)	65,102,113	1.46	7 (10%)
17	XAT	a	853	-	39,47,47	0.87	1 (2%)	54,74,74	2.72	18 (33%)
19	CLA	b	835	-	53,61,73	1.68	5 (9%)	61,98,113	1.50	8 (13%)
19	CLA	a	844	25	65,73,73	1.47	5 (7%)	76,113,113	1.39	9 (11%)
19	CLA	b	817	-	59,67,73	1.55	5 (8%)	68,105,113	1.51	9 (13%)
19	CLA	5	314	1	45,53,73	1.81	5 (11%)	52,89,113	1.59	6 (11%)
19	CLA	a	837	6	45,53,73	1.78	5 (11%)	52,89,113	1.58	7 (13%)
27	SF4	a	851	-	0,12,12	-	-	-	-	-
19	CLA	b	811	-	54,62,73	1.67	7 (12%)	67,100,113	1.50	9 (13%)
26	BCR	i	103	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
17	XAT	4	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.75	19 (35%)
18	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.57	11 (22%)
19	CLA	b	804	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
19	CLA	b	824	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
19	CLA	l	203	-	46,54,73	1.75	7 (15%)	53,90,113	1.57	6 (11%)
19	CLA	a	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
26	BCR	b	848	-	41,41,41	0.76	0	56,56,56	1.79	16 (28%)
26	BCR	b	852	-	41,41,41	0.72	0	56,56,56	2.06	15 (26%)
19	CLA	b	812	-	53,61,73	1.64	5 (9%)	61,98,113	1.49	8 (13%)
17	XAT	5	303	-	39,47,47	0.93	1 (2%)	54,74,74	2.59	20 (37%)
19	CLA	a	813	-	54,62,73	1.65	6 (11%)	62,99,113	1.45	7 (11%)
19	CLA	a	836	-	50,58,73	1.70	6 (12%)	58,95,113	1.50	9 (15%)
19	CLA	b	839	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
26	BCR	b	845	-	41,41,41	0.69	0	56,56,56	2.10	16 (28%)
19	CLA	a	820	-	65,73,73	1.49	5 (7%)	76,113,113	1.44	9 (11%)
19	CLA	2	308	4	54,62,73	1.64	6 (11%)	62,99,113	1.46	8 (12%)

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
19	CLA	2	316	4	1/1/11/20	5/15/93/115	-
19	CLA	f	802	-	1/1/15/20	13/37/115/115	-
19	CLA	b	818	-	1/1/14/20	14/31/109/115	-
20	SQD	1	315	-	-	19/40/60/69	0/1/1/1
19	CLA	b	829	-	1/1/15/20	11/37/115/115	-
19	CLA	3	311	-	1/1/12/20	4/19/97/115	-
17	XAT	a	854	-	-	7/31/93/93	0/4/4/4
19	CLA	b	827	-	1/1/15/20	14/37/115/115	-
19	CLA	a	842	-	1/1/15/20	9/37/115/115	-
17	XAT	2	301	-	-	3/31/93/93	0/4/4/4
19	CLA	4	312	-	1/1/12/20	6/23/101/115	-
19	CLA	5	309	-	1/1/13/20	4/25/103/115	-
19	CLA	b	832	-	1/1/15/20	13/37/115/115	-
19	CLA	3	314	3	1/1/11/20	7/16/94/115	-
19	CLA	5	315	-	1/1/12/20	4/22/100/115	-
19	CLA	l	201	-	1/1/10/20	2/10/88/115	-
23	A1L1F	1	304	-	-	11/43/99/99	0/3/3/3
19	CLA	a	810	6	1/1/15/20	13/37/115/115	-
19	CLA	a	825	-	1/1/13/20	8/25/103/115	-
19	CLA	1	312	5	1/1/12/20	3/22/100/115	-
19	CLA	a	834	-	1/1/15/20	7/37/115/115	-
19	CLA	b	809	-	1/1/15/20	16/37/115/115	-
19	CLA	b	822	-	1/1/14/20	7/31/109/115	-
26	BCR	a	850	-	-	4/29/63/63	0/2/2/2
25	LHG	m	101	-	-	28/50/50/53	-
19	CLA	b	833	-	1/1/13/20	16/29/107/115	-
19	CLA	a	830	-	1/1/15/20	15/37/115/115	-
19	CLA	b	826	-	1/1/15/20	5/37/115/115	-
19	CLA	a	840	-	1/1/15/20	8/37/115/115	-
19	CLA	b	805	-	1/1/15/20	16/37/115/115	-
19	CLA	2	307	-	1/1/11/20	6/16/94/115	-
19	CLA	a	832	-	1/1/12/20	5/19/97/115	-
19	CLA	f	803	10	1/1/12/20	2/22/100/115	-
19	CLA	a	839	-	1/1/15/20	15/37/115/115	-
26	BCR	b	853	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DGD	b	851	-	-	20/46/86/95	0/2/2/2
19	CLA	a	821	-	1/1/11/20	2/13/91/115	-
19	CLA	4	306	-	1/1/13/20	7/27/105/115	-
18	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
17	XAT	3	304	-	-	3/31/93/93	0/4/4/4
19	CLA	1	313	-	1/1/10/20	3/8/86/115	-
19	CLA	b	819	-	1/1/13/20	3/25/103/115	-
19	CLA	a	835	-	1/1/15/20	12/37/115/115	-
19	CLA	a	831	-	1/1/15/20	11/37/115/115	-
19	CLA	a	841	-	1/1/15/20	15/37/115/115	-
24	PQN	b	842	-	-	1/23/43/43	0/2/2/2
19	CLA	3	309	3	1/1/13/20	5/27/105/115	-
17	XAT	5	305	-	-	1/31/93/93	0/4/4/4
19	CLA	a	823	-	1/1/11/20	7/18/96/115	-
19	CLA	b	801	-	1/1/15/20	20/37/115/115	-
18	A1L1G	3	306	-	-	18/29/85/85	0/3/3/3
19	CLA	b	806	-	1/1/15/20	19/37/115/115	-
26	BCR	f	804	-	-	4/29/63/63	0/2/2/2
19	CLA	2	306	-	1/1/10/20	2/9/87/115	-
19	CLA	1	308	5	1/1/15/20	13/37/115/115	-
17	XAT	3	305	-	-	0/31/93/93	0/4/4/4
19	CLA	b	802	-	1/1/15/20	18/37/115/115	-
19	CLA	a	809	6	1/1/15/20	15/37/115/115	-
26	BCR	b	847	-	-	1/29/63/63	0/2/2/2
19	CLA	3	312	3	1/1/13/20	9/30/108/115	-
26	BCR	b	846	-	-	0/29/63/63	0/2/2/2
26	BCR	a	847	-	-	0/29/63/63	0/2/2/2
19	CLA	b	830	-	1/1/10/20	1/8/86/115	-
19	CLA	4	313	2	1/1/11/20	3/13/91/115	-
19	CLA	b	823	-	1/1/12/20	8/23/101/115	-
19	CLA	4	316	-	1/1/13/20	7/25/103/115	-
19	CLA	2	313	4	1/1/10/20	4/8/86/115	-
19	CLA	a	806	-	1/1/15/20	12/37/115/115	-
19	CLA	a	816	-	1/1/12/20	5/19/97/115	-
26	BCR	b	844	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	803	-	1/1/15/20	3/37/115/115	-
17	XAT	1	303	-	-	0/31/93/93	0/4/4/4
19	CLA	a	827	-	1/1/15/20	8/37/115/115	-
26	BCR	m	102	-	-	9/29/63/63	0/2/2/2
17	XAT	2	304	-	-	3/31/93/93	0/4/4/4
19	CLA	2	315	-	1/1/10/20	1/10/88/115	-
19	CLA	1	311	-	1/1/12/20	6/23/101/115	-
19	CLA	4	311	-	1/1/11/20	4/15/93/115	-
19	CLA	a	818	-	1/1/13/20	11/27/105/115	-
19	CLA	b	808	-	1/1/15/20	11/37/115/115	-
19	CLA	2	310	-	1/1/15/20	14/37/115/115	-
19	CLA	2	311	-	1/1/13/20	5/29/107/115	-
19	CLA	4	310	-	1/1/11/20	8/15/93/115	-
19	CLA	b	815	-	1/1/11/20	3/13/91/115	-
19	CLA	b	825	-	1/1/14/20	6/36/114/115	-
21	DGD	4	317	-	-	10/29/69/95	0/2/2/2
26	BCR	b	843	-	-	2/29/63/63	0/2/2/2
19	CLA	b	814	-	1/1/13/20	13/25/103/115	-
19	CLA	5	312	-	1/1/12/20	8/21/99/115	-
19	CLA	a	811	-	1/1/13/20	8/27/105/115	-
19	CLA	2	314	-	1/1/13/20	13/27/105/115	-
26	BCR	a	849	-	-	0/29/63/63	0/2/2/2
17	XAT	5	302	-	-	3/31/93/93	0/4/4/4
17	XAT	2	305	-	-	2/31/93/93	0/4/4/4
19	CLA	3	308	-	1/1/11/20	5/16/94/115	-
22	LMG	a	855	-	-	13/29/49/70	0/1/1/1
19	CLA	3	307	3	1/1/11/20	1/13/91/115	-
19	CLA	1	306	-	1/1/15/20	15/37/115/115	-
17	XAT	2	303	-	-	6/31/93/93	0/4/4/4
19	CLA	a	817	-	1/1/11/20	6/13/91/115	-
19	CLA	b	841	25	1/1/15/20	9/37/115/115	-
22	LMG	j	103	-	-	11/27/47/70	0/1/1/1
19	CLA	b	838	-	1/1/15/20	8/37/115/115	-
19	CLA	a	833	-	1/1/13/20	2/25/103/115	-
19	CLA	4	315	-	1/1/11/20	7/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMG	2	317	-	-	11/30/50/70	0/1/1/1
19	CLA	b	813	-	1/1/15/20	14/37/115/115	-
19	CLA	3	315	3	1/1/11/20	8/15/93/115	-
19	CLA	4	308	-	1/1/12/20	7/19/97/115	-
26	BCR	i	101	-	-	3/29/63/63	0/2/2/2
26	BCR	j	102	-	-	4/29/63/63	0/2/2/2
26	BCR	f	801	-	-	3/29/63/63	0/2/2/2
19	CLA	b	836	-	1/1/13/20	11/29/107/115	-
19	CLA	b	837	-	1/1/15/20	8/37/115/115	-
17	XAT	1	302	-	-	0/31/93/93	0/4/4/4
19	CLA	5	316	-	1/1/11/20	5/15/93/115	-
17	XAT	4	301	-	-	0/31/93/93	0/4/4/4
19	CLA	a	822	-	1/1/15/20	5/37/115/115	-
20	SQD	5	317	19	-	11/30/50/69	0/1/1/1
19	CLA	1	309	5	1/1/11/20	6/15/93/115	-
19	CLA	a	826	-	1/1/15/20	10/37/115/115	-
26	BCR	b	850	-	-	2/29/63/63	0/2/2/2
19	CLA	2	309	-	1/1/11/20	4/15/93/115	-
19	CLA	b	828	-	1/1/15/20	11/37/115/115	-
24	PQN	a	843	-	-	5/23/43/43	0/2/2/2
19	CLA	b	807	-	1/1/15/20	12/37/115/115	-
19	CLA	j	101	12	1/1/10/20	5/10/88/115	-
27	SF4	c	101	-	-	-	0/6/5/5
19	CLA	a	804	-	1/1/13/20	10/25/103/115	-
19	CLA	4	307	-	1/1/15/20	14/37/115/115	-
19	CLA	b	816	-	1/1/13/20	4/25/103/115	-
19	CLA	b	834	-	1/1/15/20	14/37/115/115	-
19	CLA	1	314	-	1/1/11/20	5/13/91/115	-
19	CLA	b	810	-	1/1/15/20	17/37/115/115	-
19	CLA	a	805	19	1/1/13/20	6/25/103/115	-
19	CLA	a	801	-	1/1/15/20	22/37/115/115	-
19	CLA	4	314	2	1/1/10/20	5/8/86/115	-
19	CLA	a	819	-	1/1/12/20	4/24/102/115	-
19	CLA	a	814	-	1/1/15/20	20/37/115/115	-
19	CLA	l	202	-	1/1/14/20	6/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	b	849	19	-	20/35/35/53	-
19	CLA	a	802	-	1/1/13/20	7/29/107/115	-
19	CLA	a	838	-	1/1/12/20	6/21/99/115	-
19	CLA	a	856	-	1/1/15/20	13/37/115/115	-
17	XAT	3	303	-	-	3/31/93/93	0/4/4/4
25	LHG	a	846	19	-	16/31/31/53	-
19	CLA	5	308	1	1/1/14/20	7/31/109/115	-
19	CLA	b	821	-	1/1/12/20	2/21/99/115	-
19	CLA	b	831	-	1/1/11/20	6/18/96/115	-
19	CLA	1	310	5	1/1/15/20	18/37/115/115	-
19	CLA	a	829	-	1/1/14/20	14/34/112/115	-
17	XAT	4	302	-	-	3/31/93/93	0/4/4/4
27	SF4	c	102	-	-	-	0/6/5/5
19	CLA	5	306	1	1/1/11/20	4/15/93/115	-
19	CLA	i	102	-	1/1/14/20	9/34/112/115	-
19	CLA	a	824	-	1/1/11/20	4/15/93/115	-
19	CLA	a	852	-	1/1/15/20	17/37/115/115	-
19	CLA	b	840	-	1/1/15/20	17/37/115/115	-
19	CLA	a	808	-	1/1/12/20	3/21/99/115	-
17	XAT	5	301	-	-	4/31/93/93	0/4/4/4
19	CLA	4	309	-	1/1/15/20	16/37/115/115	-
19	CLA	a	807	-	1/1/15/20	18/37/115/115	-
19	CLA	1	307	-	1/1/12/20	6/24/102/115	-
19	CLA	a	815	-	1/1/11/20	2/13/91/115	-
19	CLA	b	820	-	1/1/12/20	7/19/97/115	-
18	A1L1G	5	304	-	-	9/29/85/85	0/3/3/3
19	CLA	1	305	-	1/1/14/20	10/33/111/115	-
25	LHG	a	845	-	-	27/52/52/53	-
19	CLA	5	313	-	1/1/12/20	0/22/100/115	-
19	CLA	5	310	1	1/1/15/20	14/37/115/115	-
17	XAT	4	303	-	-	0/31/93/93	0/4/4/4
19	CLA	2	312	-	1/1/11/20	4/16/94/115	-
19	CLA	b	803	-	1/1/15/20	10/37/115/115	-
19	CLA	5	311	-	1/1/11/20	6/15/93/115	-
26	BCR	a	848	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	5	307	20	1/1/11/20	7/13/91/115	-
17	XAT	2	302	-	-	0/31/93/93	0/4/4/4
19	CLA	a	812	19	1/1/14/20	9/34/112/115	-
19	CLA	3	313	-	1/1/12/20	1/22/100/115	-
17	XAT	3	301	-	-	3/31/93/93	0/4/4/4
19	CLA	4	305	2	1/1/11/20	7/13/91/115	-
19	CLA	3	310	-	1/1/13/20	4/27/105/115	-
17	XAT	a	853	-	-	5/31/93/93	0/4/4/4
19	CLA	b	835	-	1/1/12/20	8/23/101/115	-
19	CLA	a	844	25	1/1/15/20	16/37/115/115	-
19	CLA	b	817	-	1/1/13/20	10/30/108/115	-
19	CLA	5	314	1	1/1/11/20	5/13/91/115	-
19	CLA	a	837	6	1/1/11/20	4/13/91/115	-
27	SF4	a	851	-	-	-	0/6/5/5
19	CLA	b	811	-	1/1/13/20	5/25/101/115	-
26	BCR	i	103	-	-	8/29/63/63	0/2/2/2
17	XAT	4	304	-	-	4/31/93/93	0/4/4/4
18	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
19	CLA	b	804	-	1/1/15/20	12/37/115/115	-
19	CLA	b	824	-	1/1/15/20	14/37/115/115	-
19	CLA	l	203	-	1/1/11/20	4/15/93/115	-
19	CLA	a	828	-	1/1/15/20	9/37/115/115	-
26	BCR	b	848	-	-	2/29/63/63	0/2/2/2
26	BCR	b	852	-	-	4/29/63/63	0/2/2/2
19	CLA	b	812	-	1/1/12/20	6/23/101/115	-
19	CLA	a	813	-	1/1/12/20	10/24/102/115	-
17	XAT	5	303	-	-	3/31/93/93	0/4/4/4
19	CLA	a	836	-	1/1/12/20	6/19/97/115	-
19	CLA	b	839	-	1/1/15/20	13/37/115/115	-
26	BCR	b	845	-	-	6/29/63/63	0/2/2/2
19	CLA	a	820	-	1/1/15/20	16/37/115/115	-
19	CLA	2	308	4	1/1/12/20	5/24/102/115	-

The worst 5 of 926 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	312	CLA	C4B-NB	7.99	1.42	1.35
19	3	315	CLA	C4B-NB	7.78	1.42	1.35
19	a	818	CLA	C4B-NB	7.77	1.42	1.35
19	a	840	CLA	C4B-NB	7.74	1.42	1.35
19	1	309	CLA	C4B-NB	7.74	1.42	1.35

The worst 5 of 1946 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	317	DGD	C6E-C5E-C4E	-9.39	91.01	113.00
23	1	304	A1L1F	C17-C20-C25	-8.11	108.67	122.26
19	b	802	CLA	C4A-NA-C1A	7.26	109.97	106.71
23	1	304	A1L1F	O15-C20-C21	7.25	118.83	113.38
19	a	835	CLA	C4A-NA-C1A	7.24	109.96	106.71

5 of 146 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	5	306	CLA	ND
19	5	307	CLA	ND
19	5	308	CLA	ND
19	5	309	CLA	ND
19	5	310	CLA	ND

5 of 1617 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	5	301	XAT	C27-C28-C29-C30
17	5	301	XAT	C27-C28-C29-C39
17	5	303	XAT	O4-C6-C7-C8
17	5	303	XAT	C7-C8-C9-C10
17	5	303	XAT	C7-C8-C9-C19

There are no ring outliers.

177 monomers are involved in 640 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	316	CLA	2	0
19	f	802	CLA	1	0
19	b	818	CLA	3	0
20	1	315	SQD	3	0
19	b	829	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	311	CLA	1	0
17	a	854	XAT	3	0
19	b	827	CLA	5	0
19	a	842	CLA	4	0
17	2	301	XAT	4	0
19	4	312	CLA	4	0
19	5	309	CLA	1	0
19	b	832	CLA	11	0
19	5	315	CLA	2	0
19	l	201	CLA	1	0
23	1	304	A1L1F	10	0
19	a	810	CLA	9	0
19	a	825	CLA	5	0
19	1	312	CLA	2	0
19	a	834	CLA	7	0
19	b	822	CLA	5	0
26	a	850	BCR	3	0
25	m	101	LHG	2	0
19	b	833	CLA	5	0
19	a	830	CLA	8	0
19	b	826	CLA	4	0
19	a	840	CLA	7	0
19	b	805	CLA	2	0
19	2	307	CLA	1	0
19	a	832	CLA	1	0
19	f	803	CLA	1	0
19	a	839	CLA	4	0
26	b	853	BCR	16	0
21	b	851	DGD	5	0
19	4	306	CLA	1	0
17	3	304	XAT	5	0
19	b	819	CLA	1	0
19	a	835	CLA	4	0
19	a	831	CLA	4	0
19	a	841	CLA	16	0
24	b	842	PQN	7	0
17	5	305	XAT	5	0
19	3	309	CLA	1	0
19	a	823	CLA	3	0
19	b	801	CLA	15	0
19	b	806	CLA	7	0
26	f	804	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	308	CLA	3	0
17	3	305	XAT	6	0
19	b	802	CLA	2	0
19	a	809	CLA	2	0
26	b	847	BCR	5	0
19	3	312	CLA	1	0
26	b	846	BCR	3	0
26	a	847	BCR	4	0
19	b	830	CLA	5	0
19	4	313	CLA	1	0
19	b	823	CLA	6	0
19	4	316	CLA	7	0
19	a	806	CLA	8	0
19	a	816	CLA	2	0
26	b	844	BCR	2	0
19	a	803	CLA	13	0
17	1	303	XAT	4	0
19	a	827	CLA	4	0
17	2	304	XAT	2	0
19	1	311	CLA	4	0
19	4	311	CLA	1	0
19	a	818	CLA	11	0
19	b	808	CLA	2	0
19	2	310	CLA	3	0
19	4	310	CLA	2	0
19	b	825	CLA	2	0
21	4	317	DGD	11	0
26	b	843	BCR	4	0
19	b	814	CLA	2	0
19	5	312	CLA	1	0
19	a	811	CLA	1	0
19	2	314	CLA	2	0
26	a	849	BCR	2	0
17	5	302	XAT	6	0
17	2	305	XAT	4	0
19	3	308	CLA	2	0
22	a	855	LMG	10	0
19	1	306	CLA	6	0
17	2	303	XAT	10	0
19	b	841	CLA	5	0
22	j	103	LMG	5	0
19	b	838	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	833	CLA	12	0
19	4	315	CLA	1	0
22	2	317	LMG	3	0
19	b	813	CLA	7	0
19	4	308	CLA	3	0
26	i	101	BCR	5	0
26	j	102	BCR	14	0
26	f	801	BCR	24	0
19	b	836	CLA	5	0
19	b	837	CLA	7	0
17	1	302	XAT	2	0
19	5	316	CLA	1	0
17	4	301	XAT	4	0
19	a	822	CLA	5	0
20	5	317	SQD	1	0
19	a	826	CLA	6	0
26	b	850	BCR	3	0
19	2	309	CLA	1	0
19	b	828	CLA	2	0
24	a	843	PQN	4	0
19	b	807	CLA	1	0
19	j	101	CLA	2	0
19	a	804	CLA	2	0
19	4	307	CLA	7	0
19	b	816	CLA	4	0
19	b	834	CLA	7	0
19	b	810	CLA	20	0
19	a	805	CLA	2	0
19	a	801	CLA	5	0
19	4	314	CLA	1	0
19	a	819	CLA	5	0
19	a	814	CLA	3	0
19	l	202	CLA	9	0
19	a	802	CLA	15	0
19	a	838	CLA	1	0
19	a	856	CLA	24	0
17	3	303	XAT	2	0
25	a	846	LHG	2	0
19	5	308	CLA	7	0
19	b	821	CLA	3	0
19	b	831	CLA	1	0
19	1	310	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	829	CLA	8	0
17	4	302	XAT	9	0
27	c	102	SF4	3	0
19	5	306	CLA	2	0
19	i	102	CLA	7	0
19	a	824	CLA	1	0
19	a	852	CLA	4	0
19	b	840	CLA	5	0
19	a	808	CLA	1	0
17	5	301	XAT	4	0
19	4	309	CLA	7	0
19	a	807	CLA	5	0
19	b	820	CLA	1	0
18	5	304	A1L1G	1	0
25	a	845	LHG	3	0
19	5	313	CLA	3	0
19	5	310	CLA	4	0
17	4	303	XAT	4	0
19	b	803	CLA	3	0
19	5	311	CLA	1	0
26	a	848	BCR	7	0
17	2	302	XAT	2	0
17	3	301	XAT	5	0
19	3	313	CLA	3	0
19	4	305	CLA	2	0
19	3	310	CLA	1	0
17	a	853	XAT	4	0
19	a	844	CLA	16	0
19	b	817	CLA	9	0
19	a	837	CLA	1	0
19	b	811	CLA	2	0
26	i	103	BCR	11	0
17	4	304	XAT	4	0
18	1	301	A1L1G	1	0
19	b	804	CLA	3	0
19	b	824	CLA	5	0
19	a	828	CLA	5	0
26	b	848	BCR	5	0
26	b	852	BCR	11	0
19	b	812	CLA	4	0
17	5	303	XAT	10	0
19	a	813	CLA	2	0

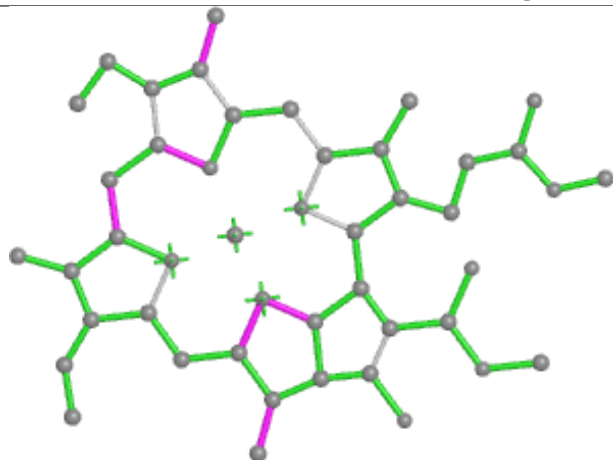
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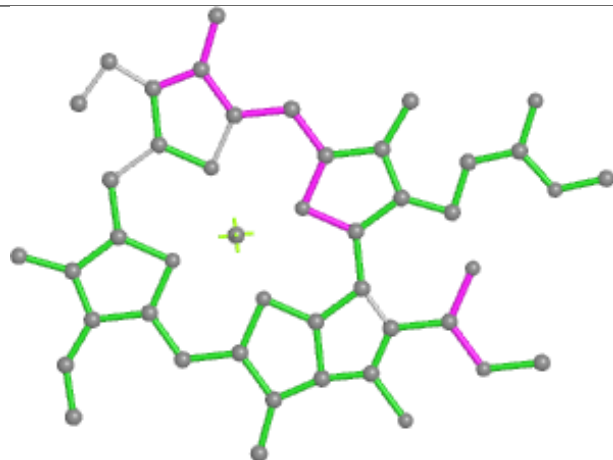
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	839	CLA	15	0
26	b	845	BCR	6	0
19	a	820	CLA	7	0
19	2	308	CLA	3	0

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.

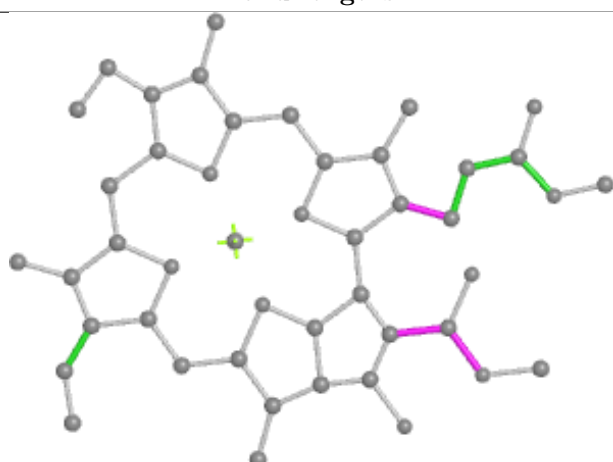
## Ligand CLA 2 316



Bond lengths



Bond angles

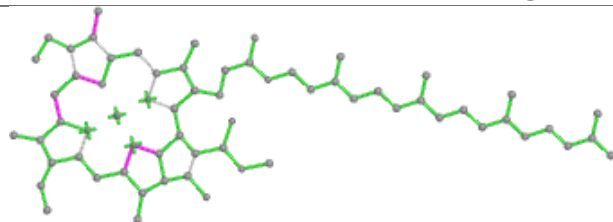


Torsions

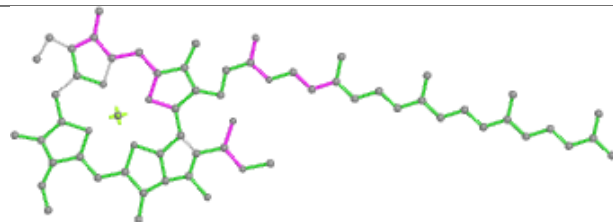


Rings

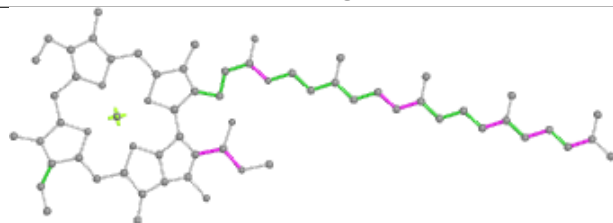
## Ligand CLA f 802



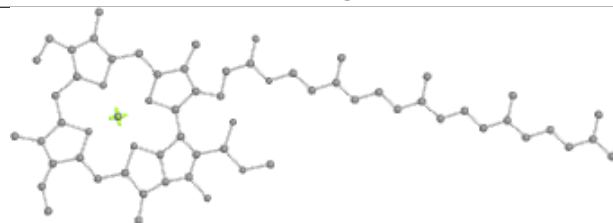
Bond lengths



Bond angles

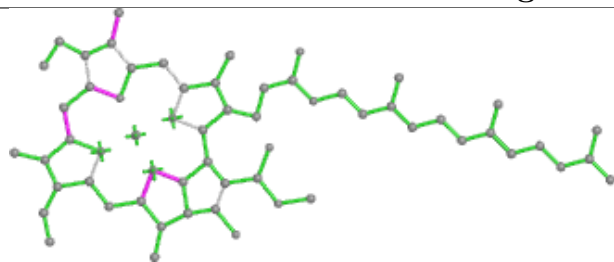


Torsions

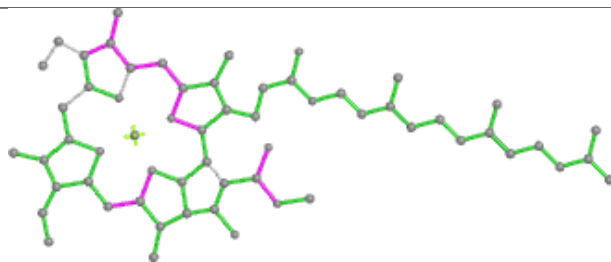


Rings

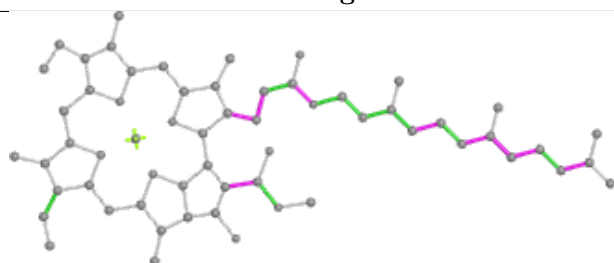
## Ligand CLA b 818



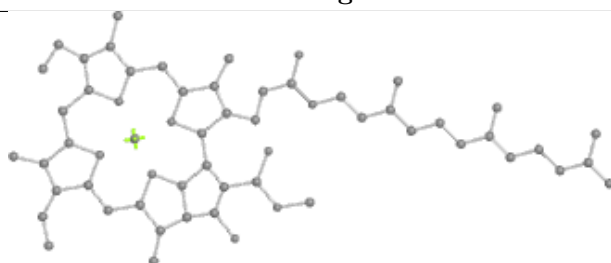
Bond lengths



Bond angles

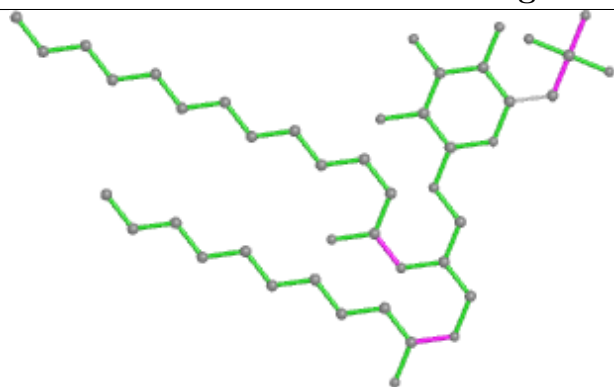


Torsions

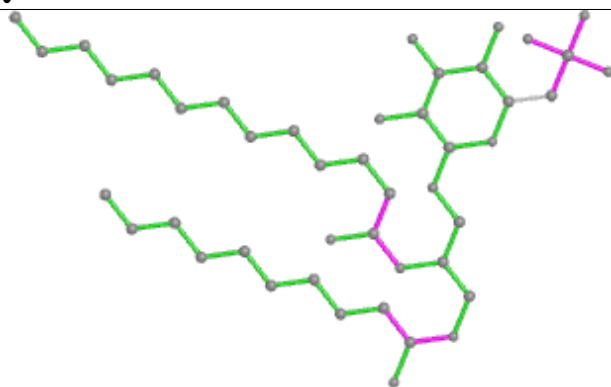


Rings

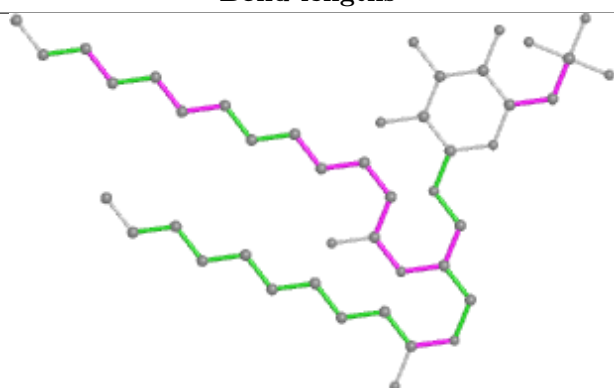
## Ligand SQD 1 315



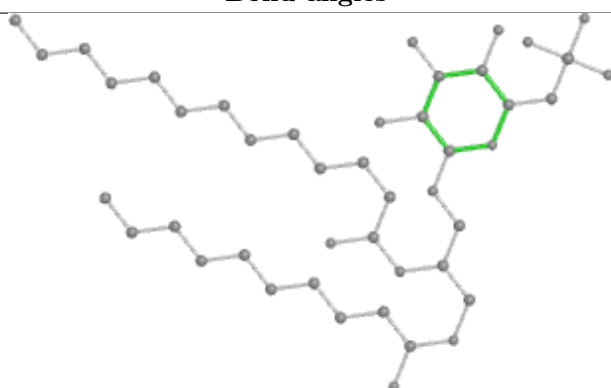
Bond lengths



Bond angles

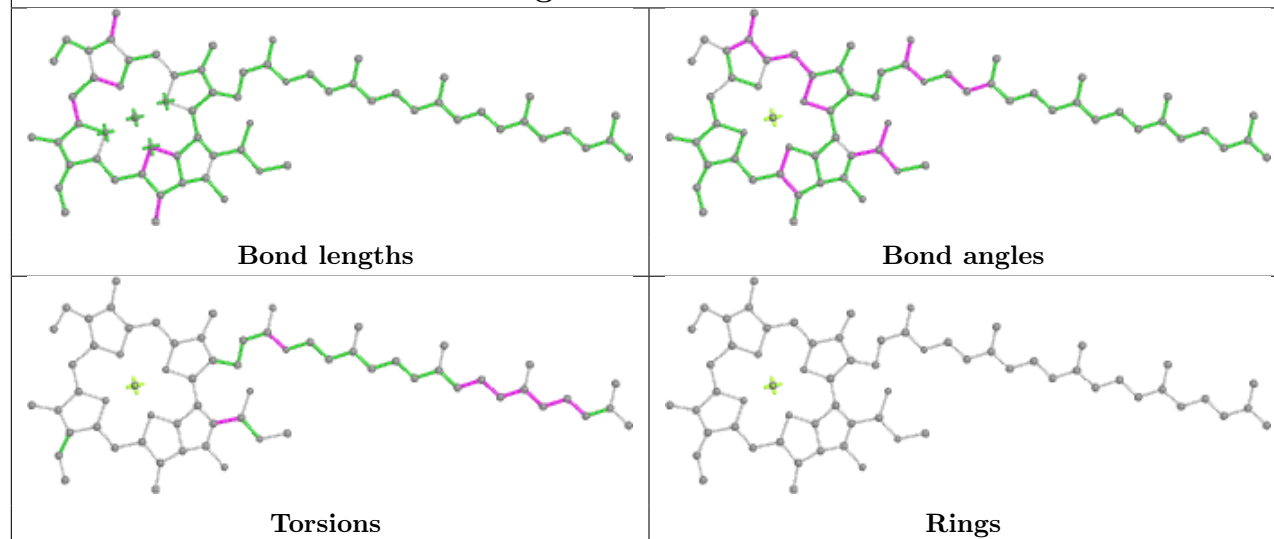


Torsions

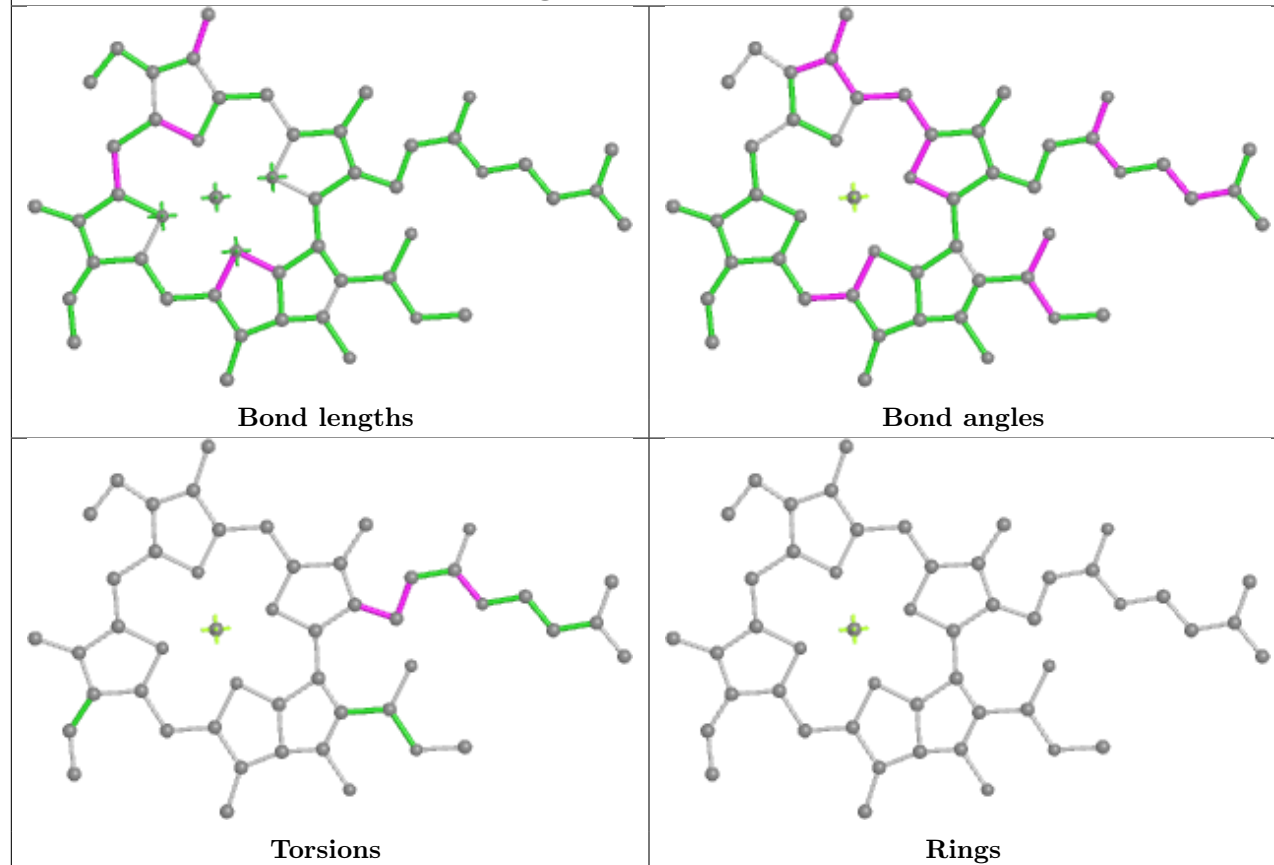


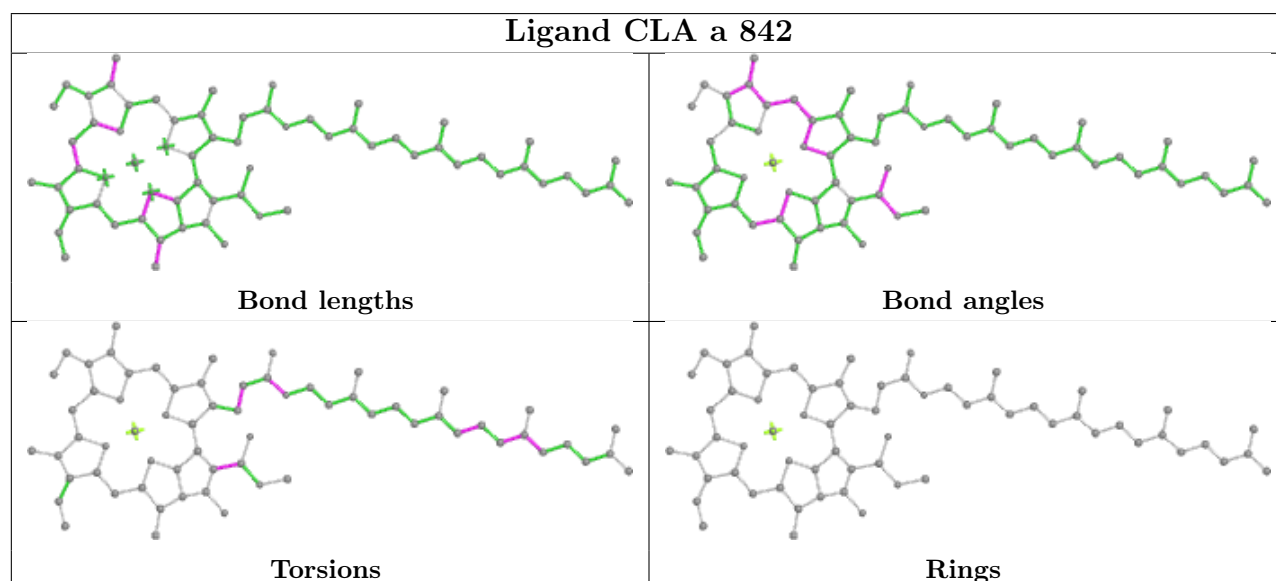
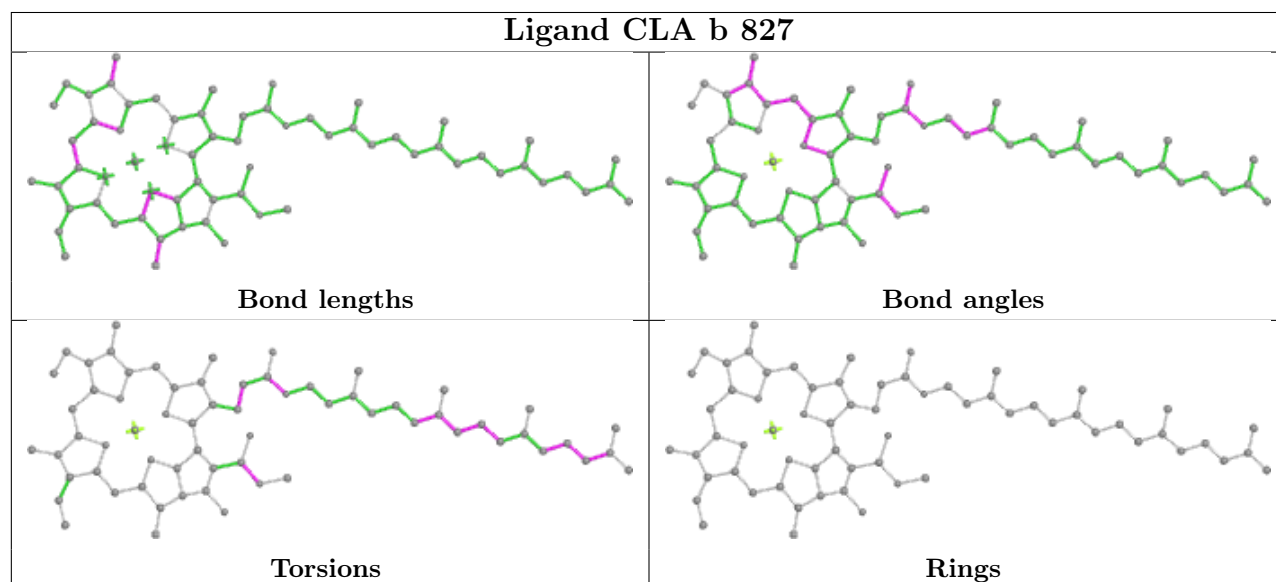
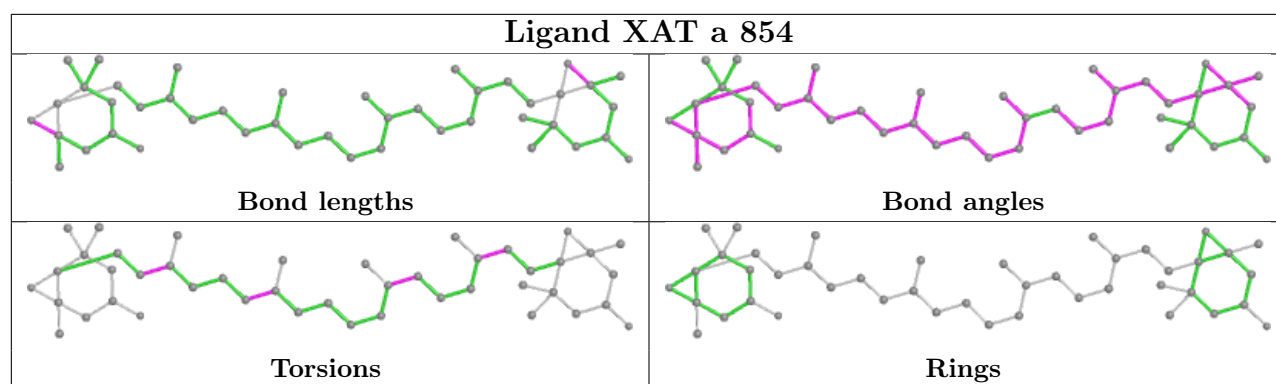
Rings

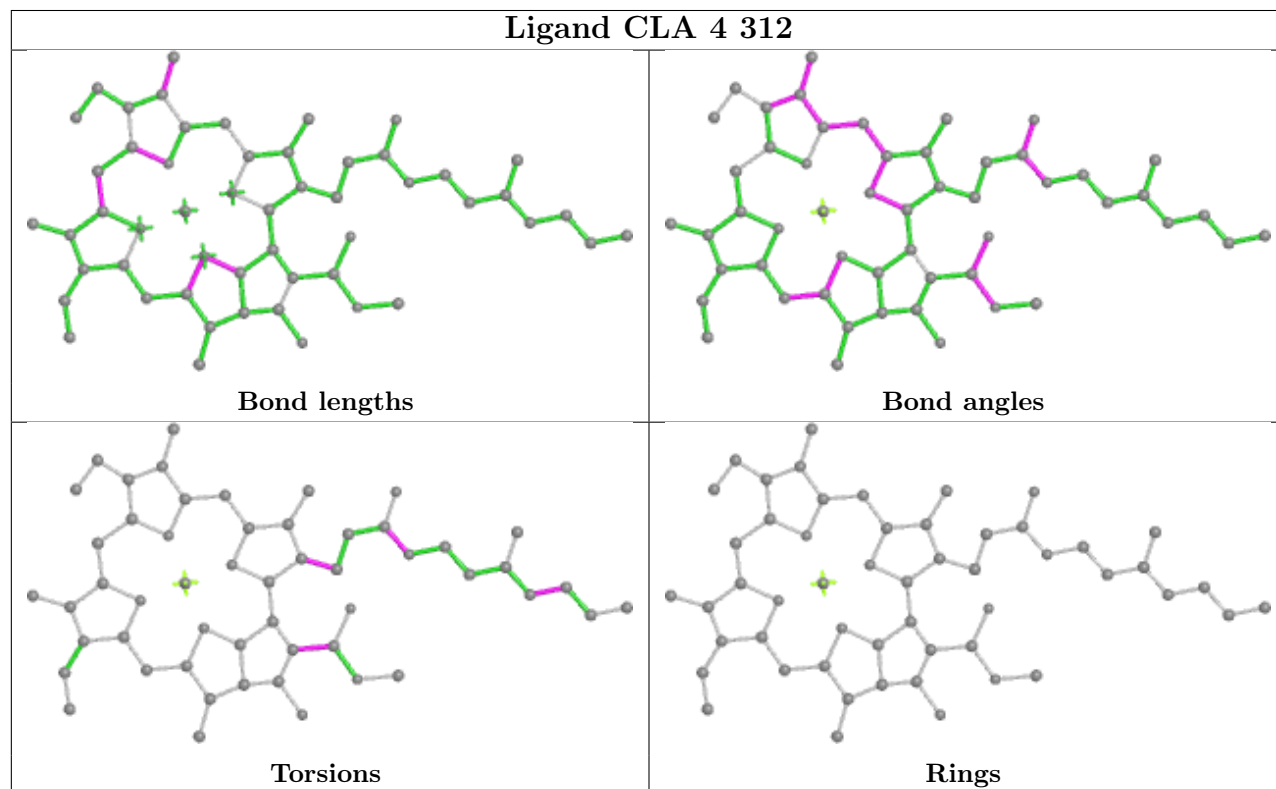
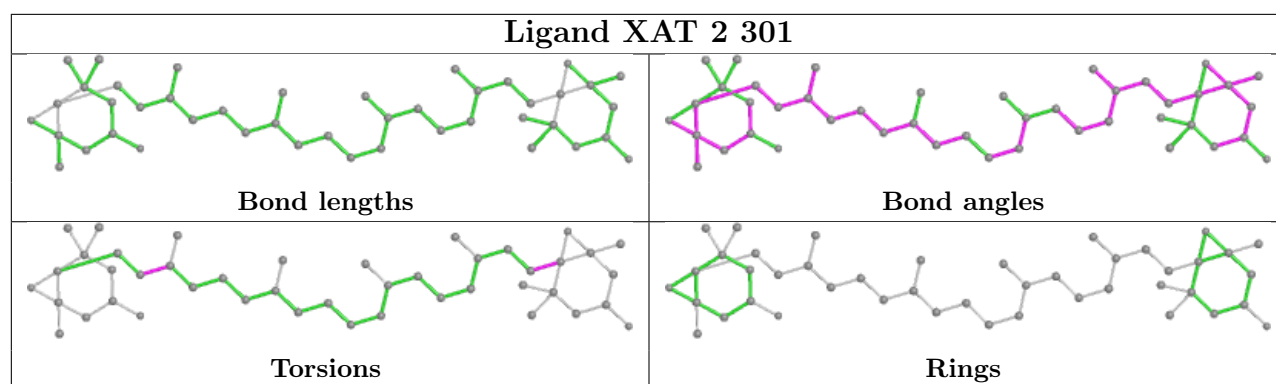
## Ligand CLA b 829

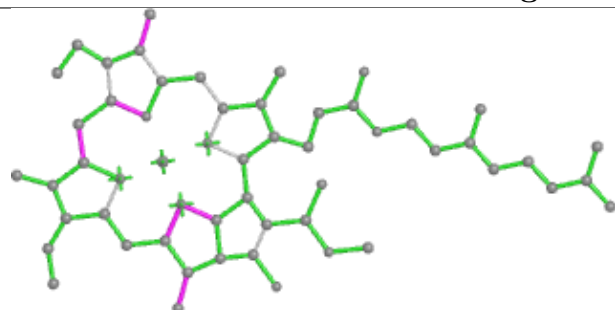
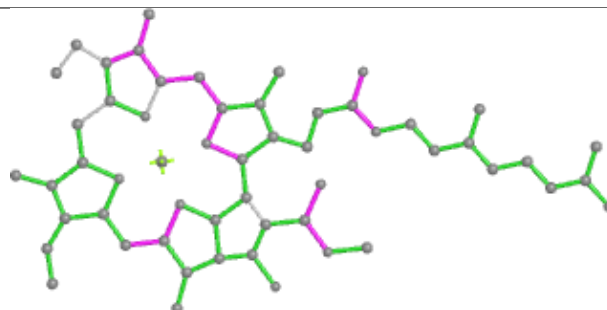
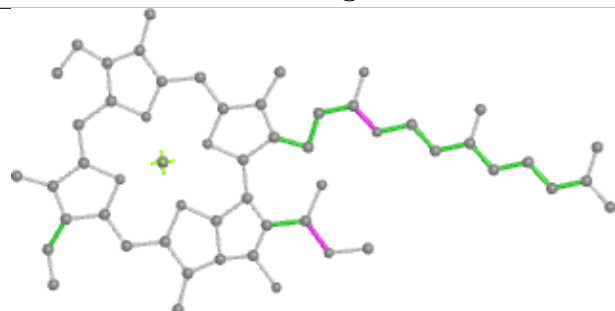
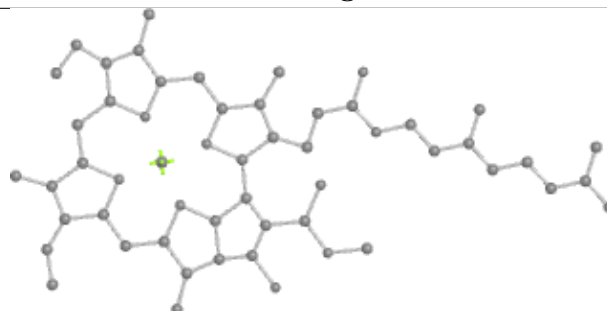
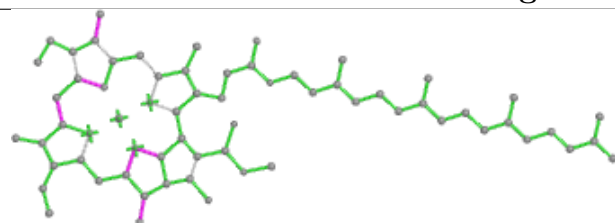
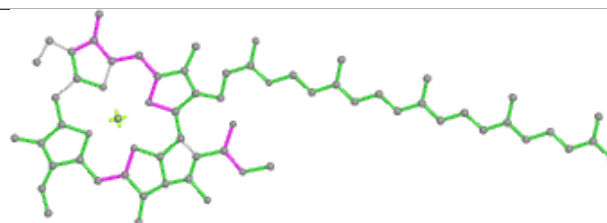
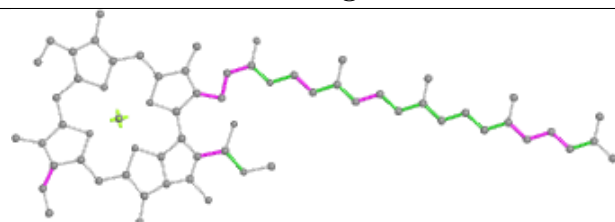
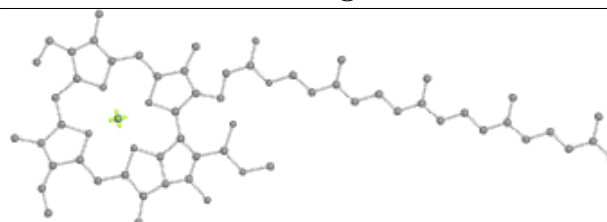


## Ligand CLA 3 311



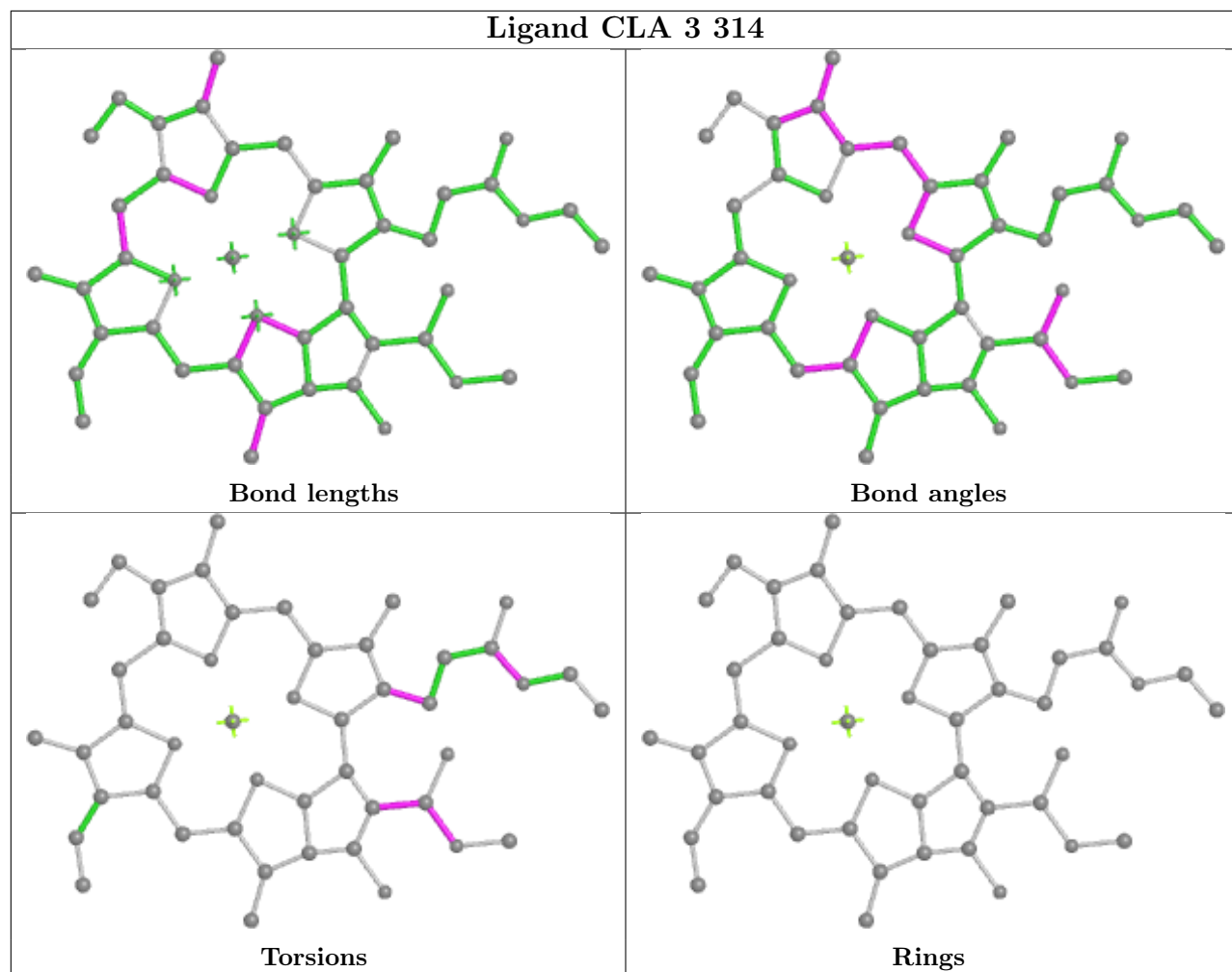


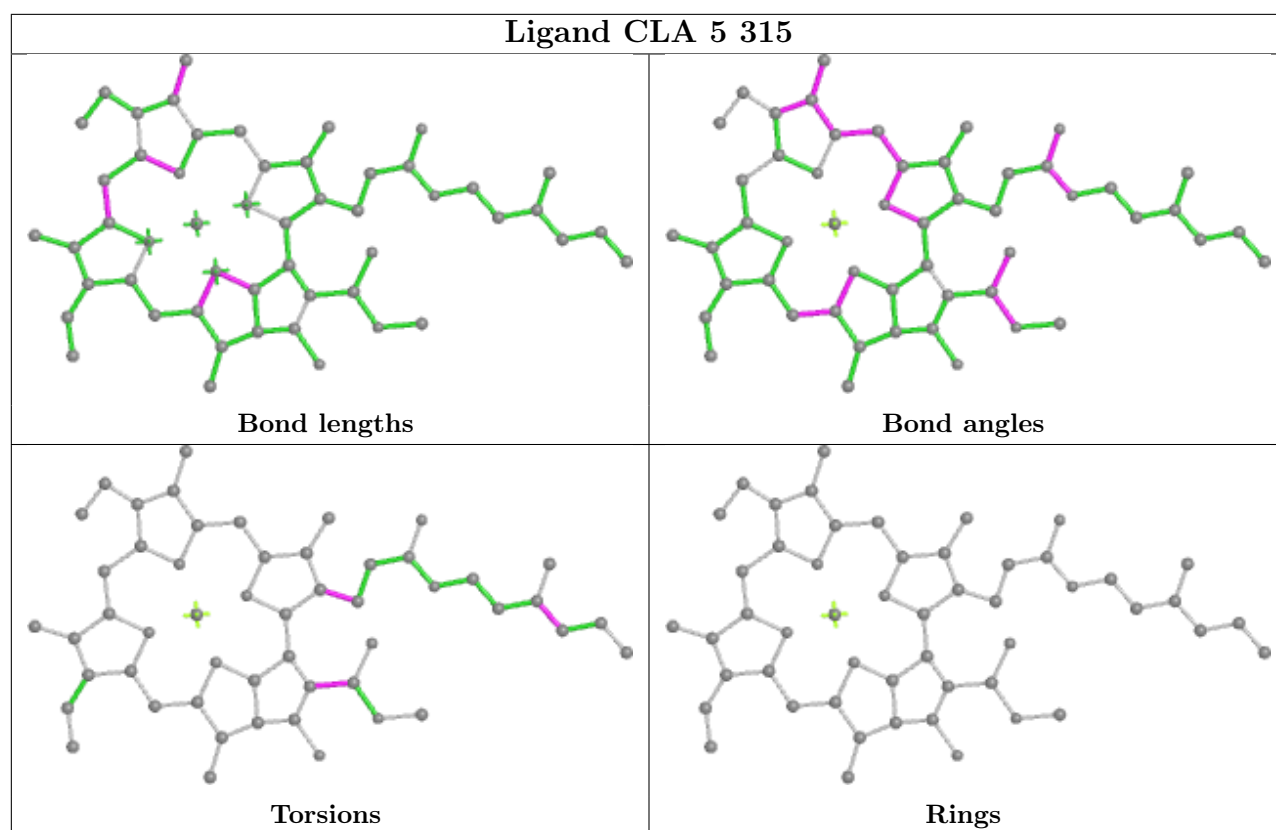


**Ligand CLA 5 309****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA b 832****Bond lengths****Bond angles****Torsions****Rings**

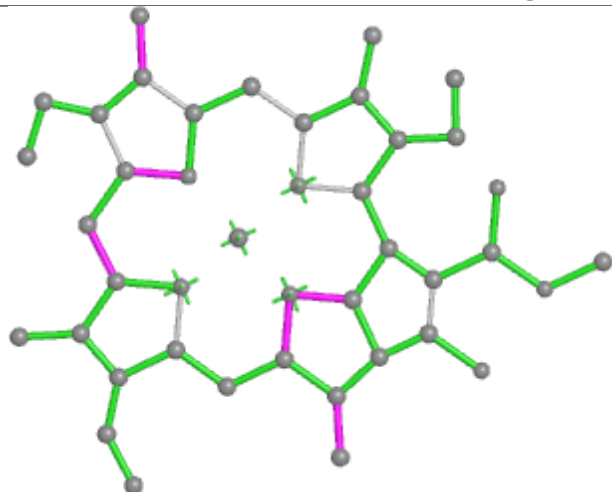


## Ligand CLA 3 314

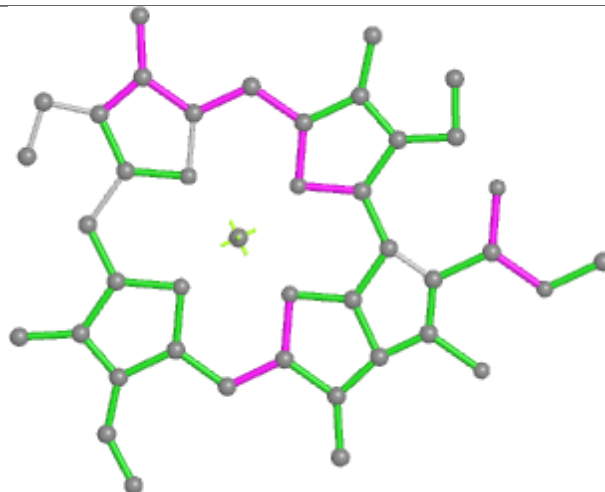




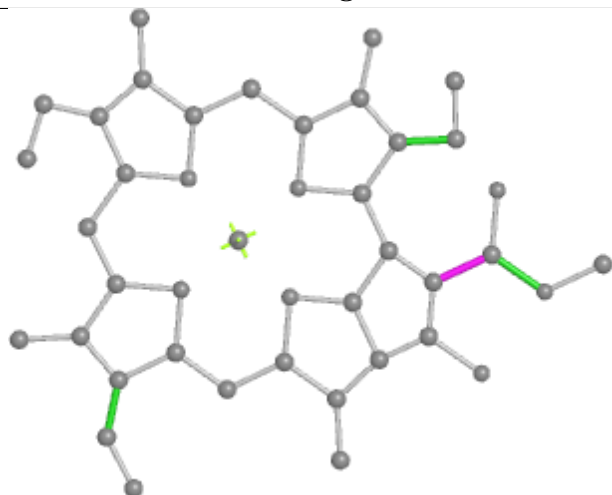
## Ligand CLA 1 201



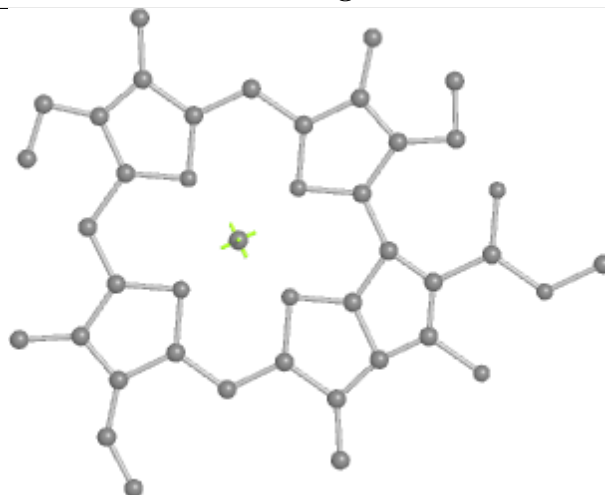
Bond lengths



Bond angles

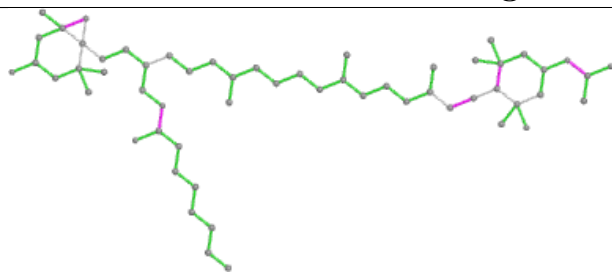


Torsions

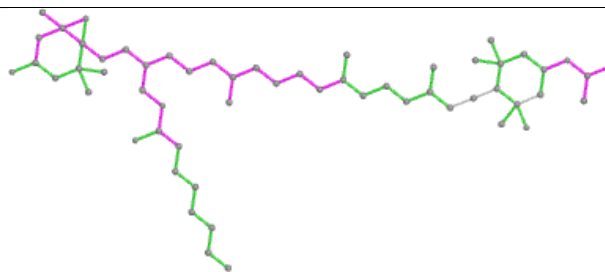


Rings

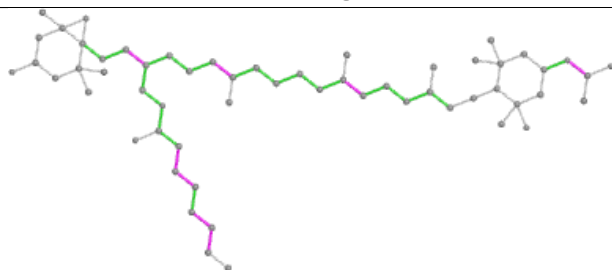
## Ligand A1L1F 1 304



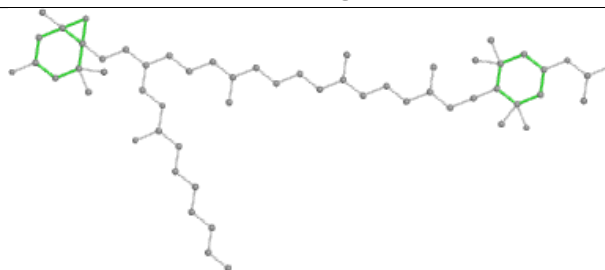
Bond lengths



Bond angles

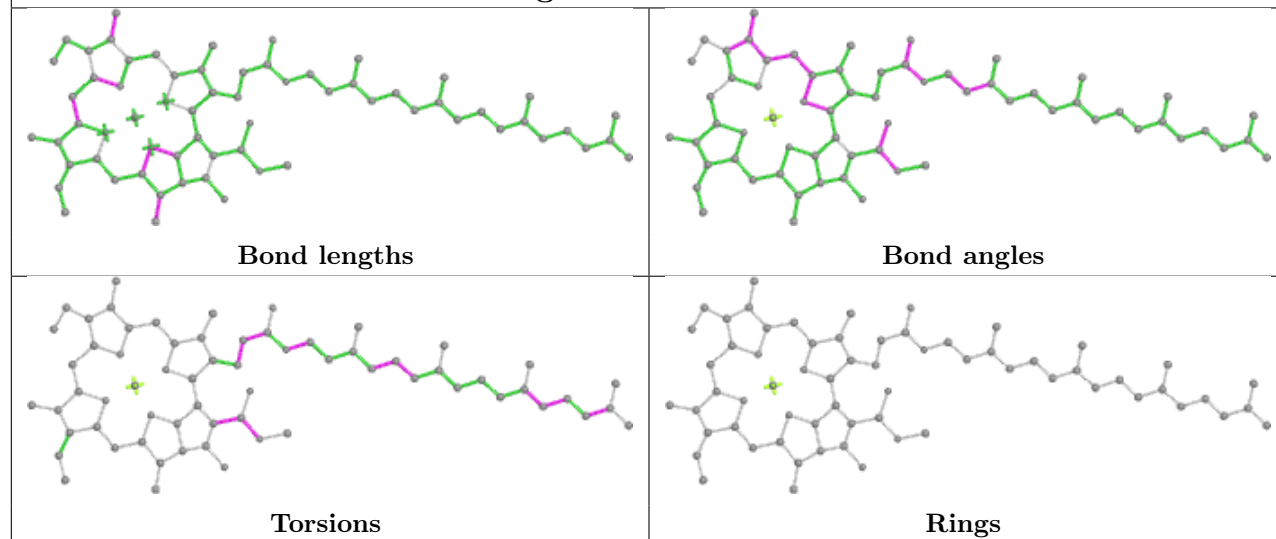


Torsions

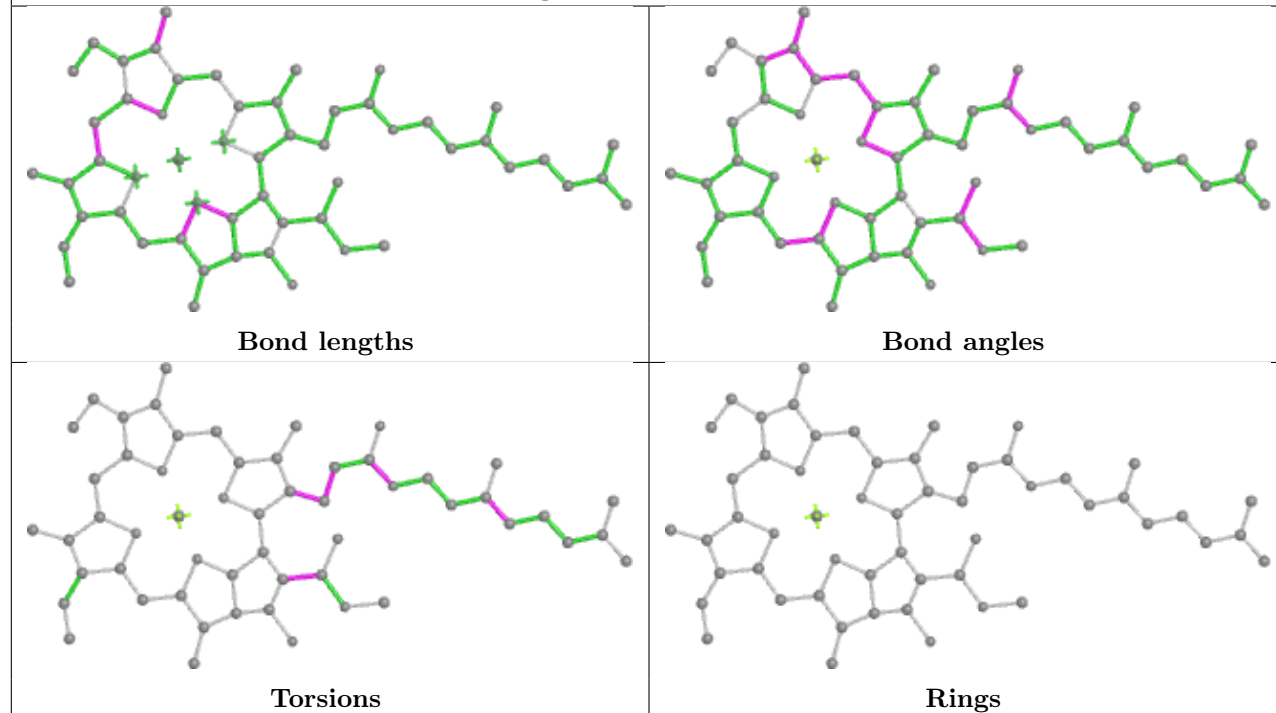


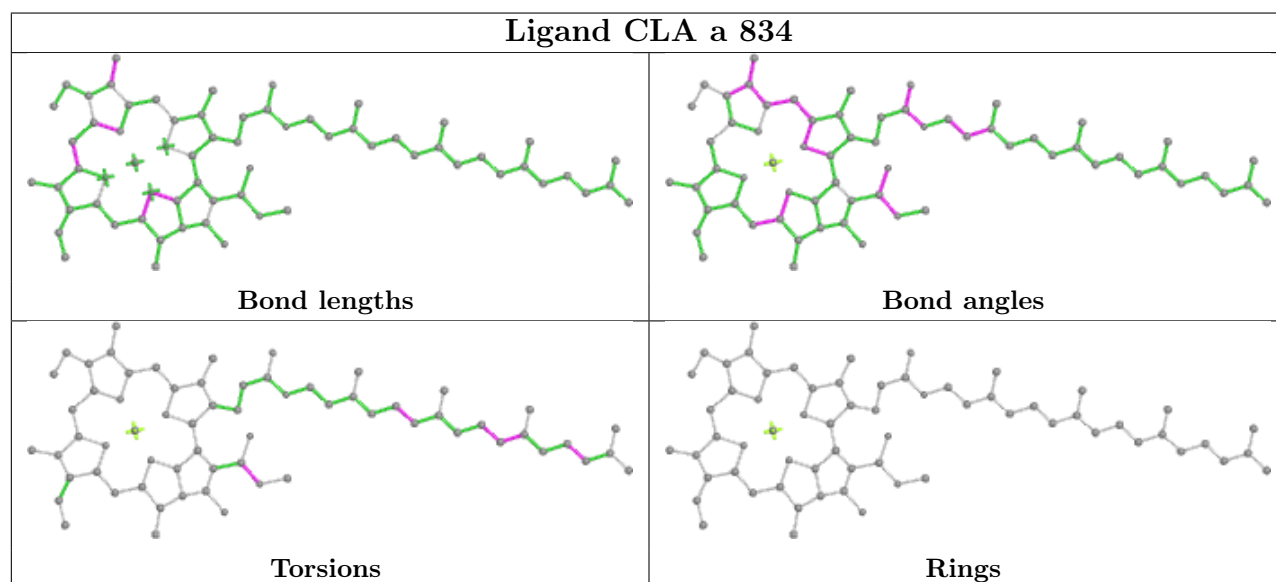
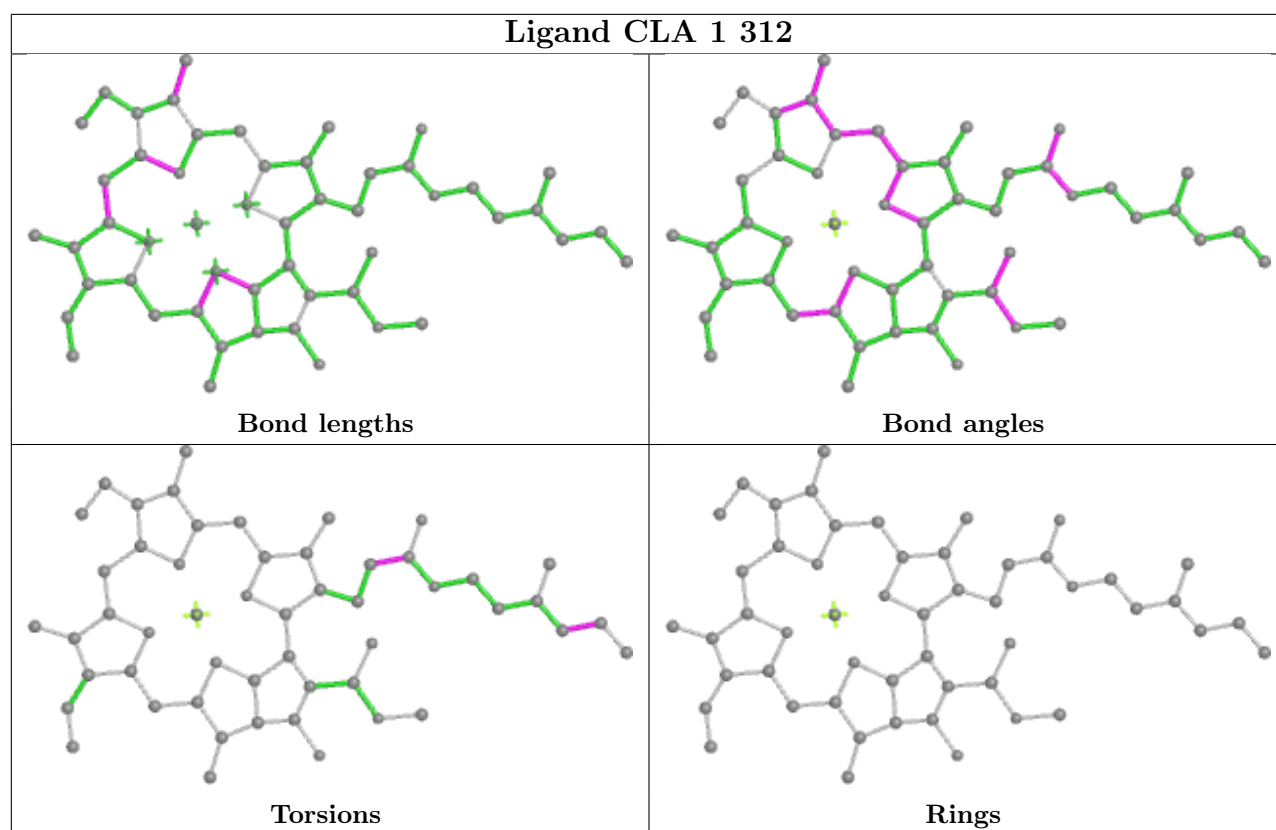
Rings

## Ligand CLA a 810

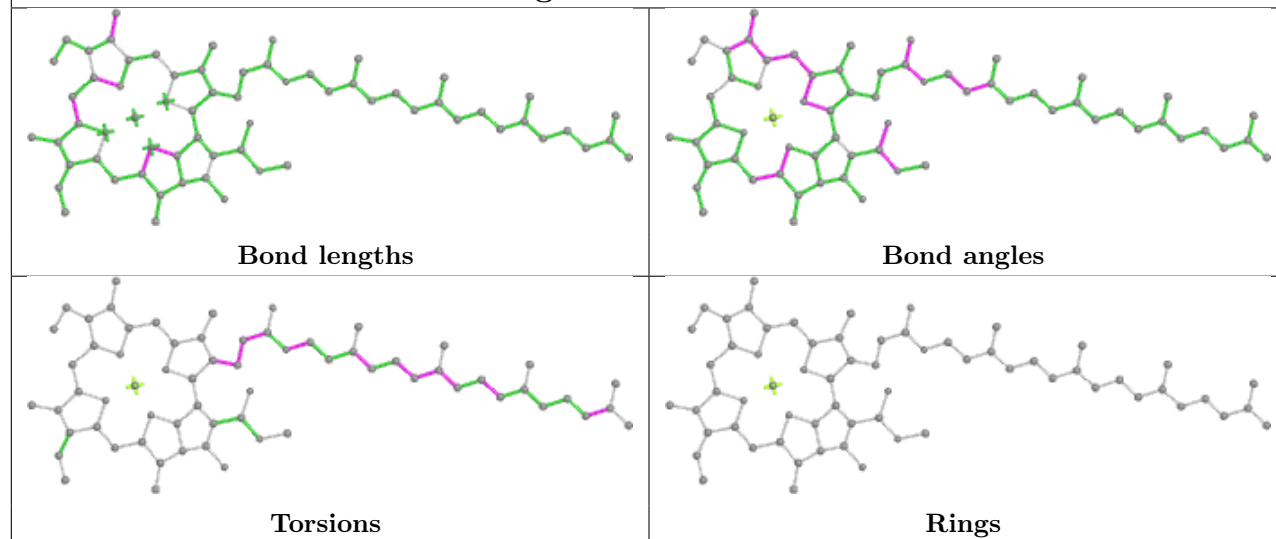


## Ligand CLA a 825

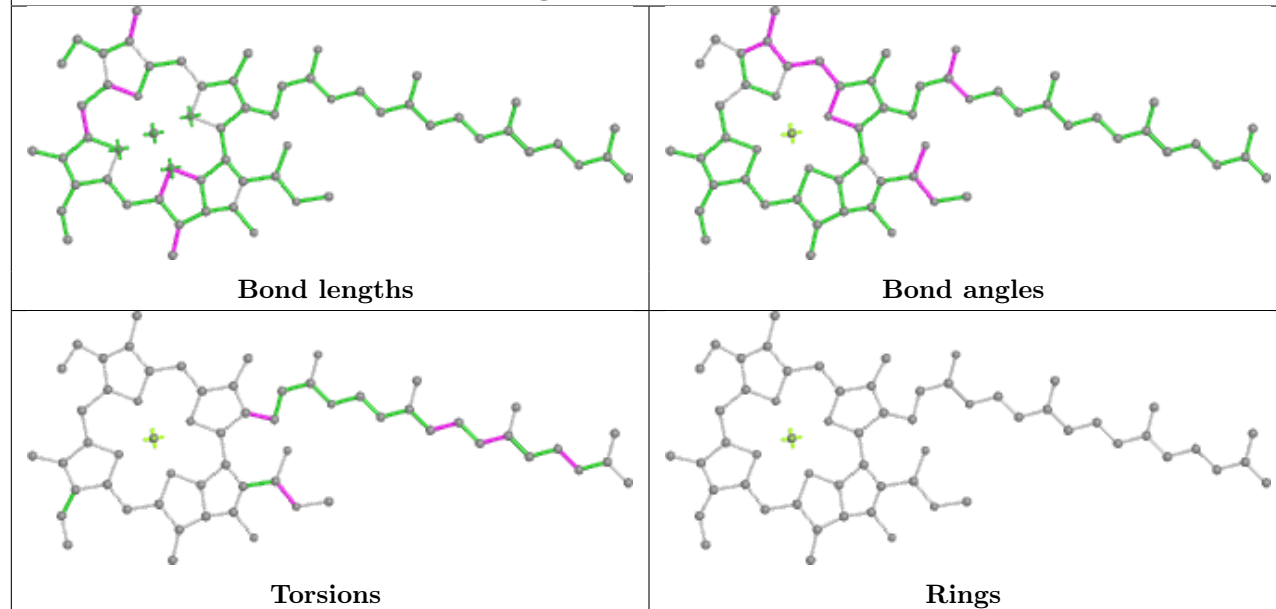




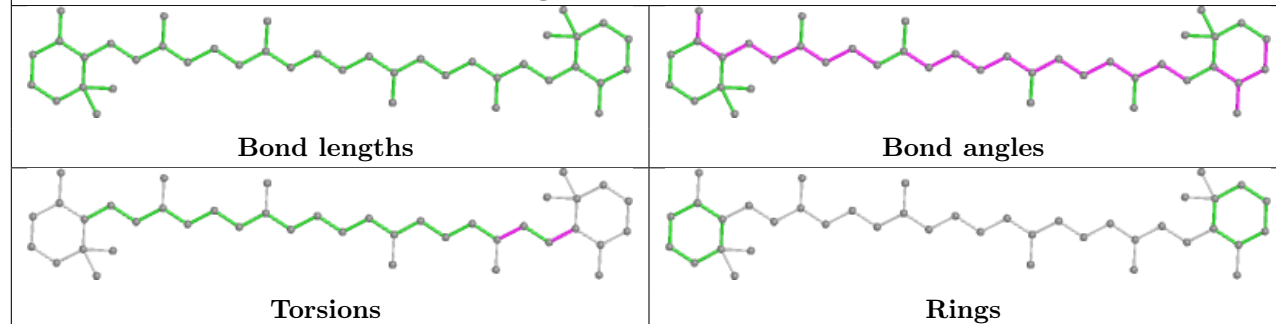
## Ligand CLA b 809

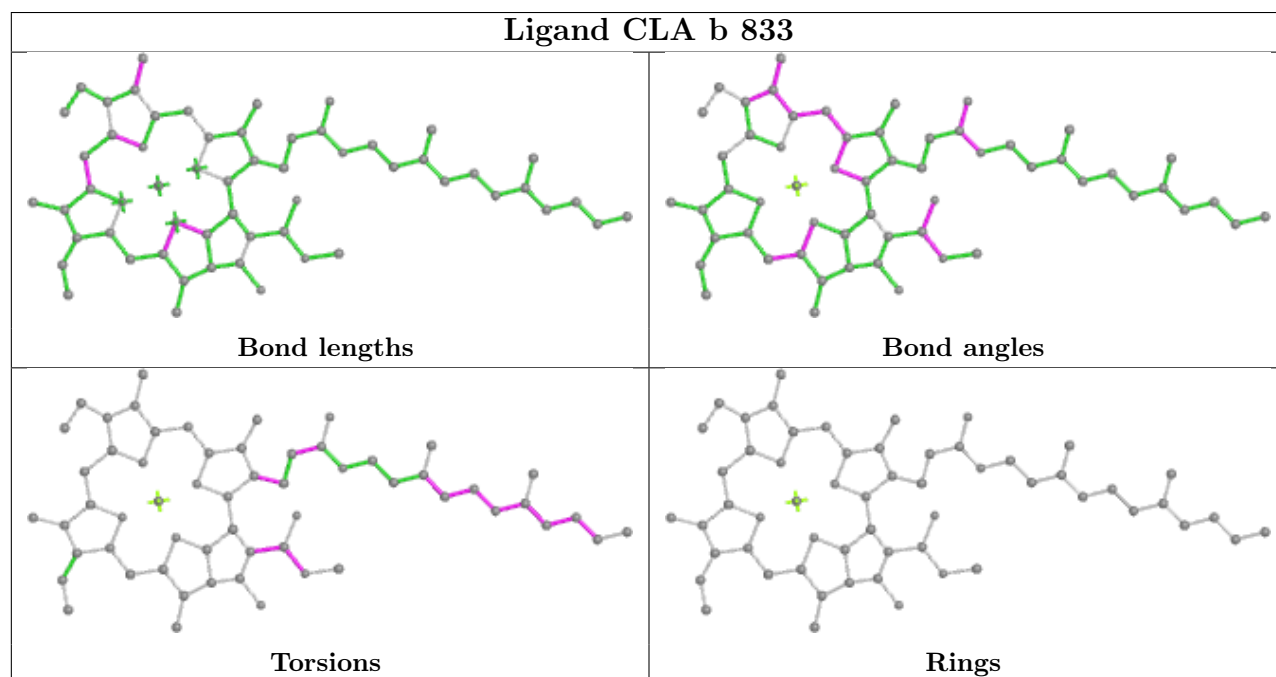
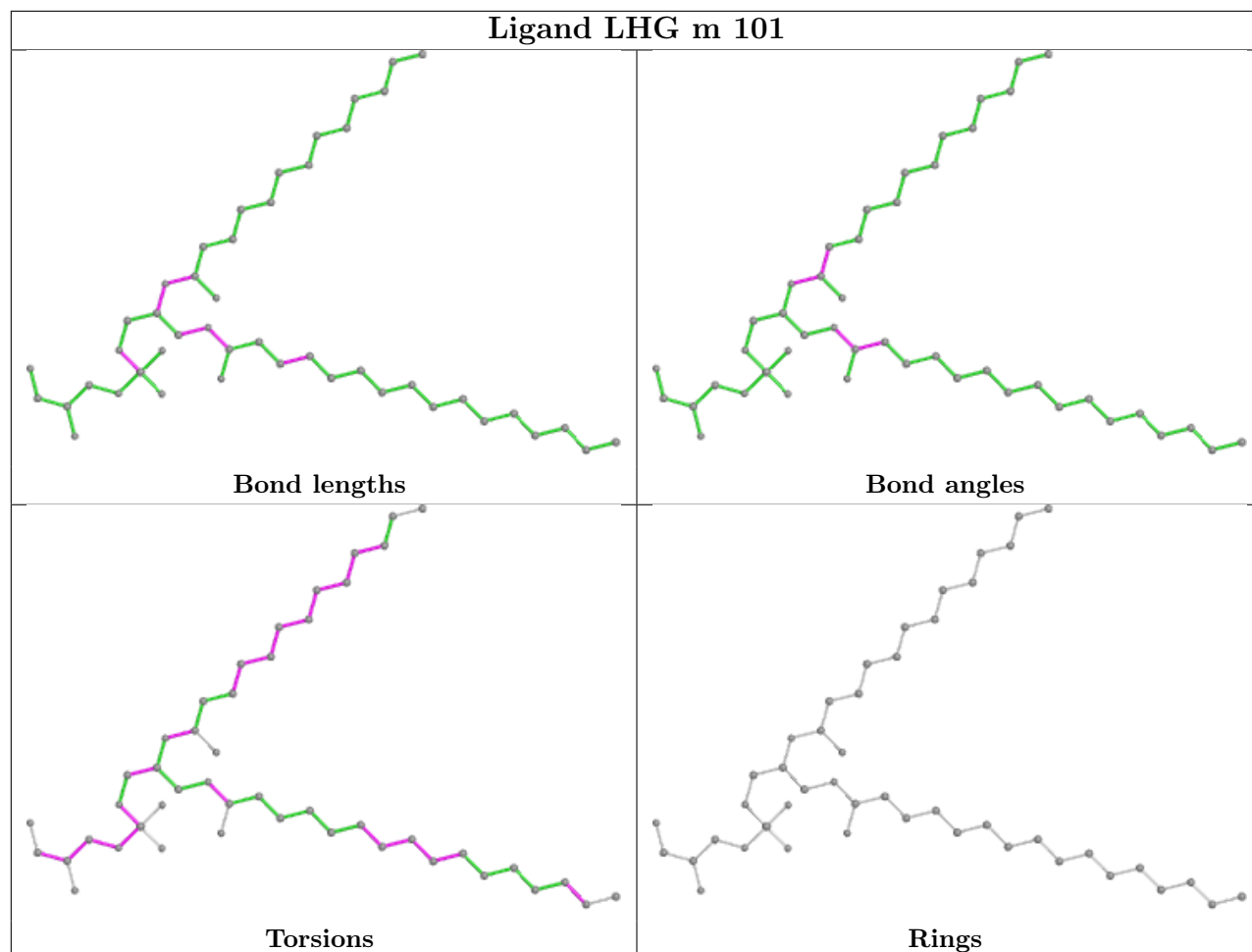


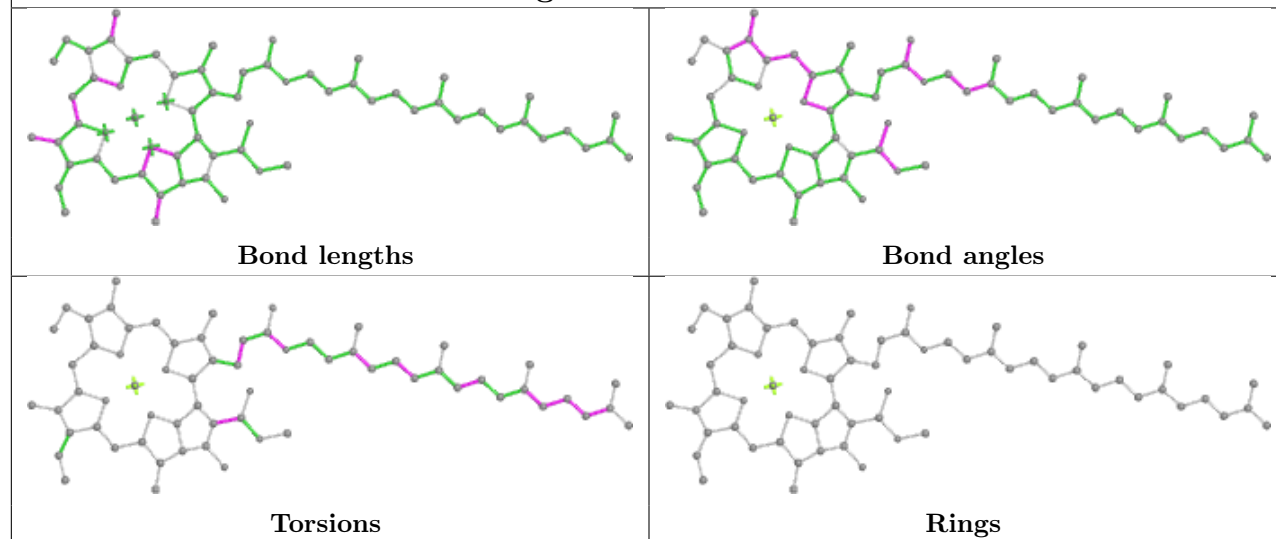
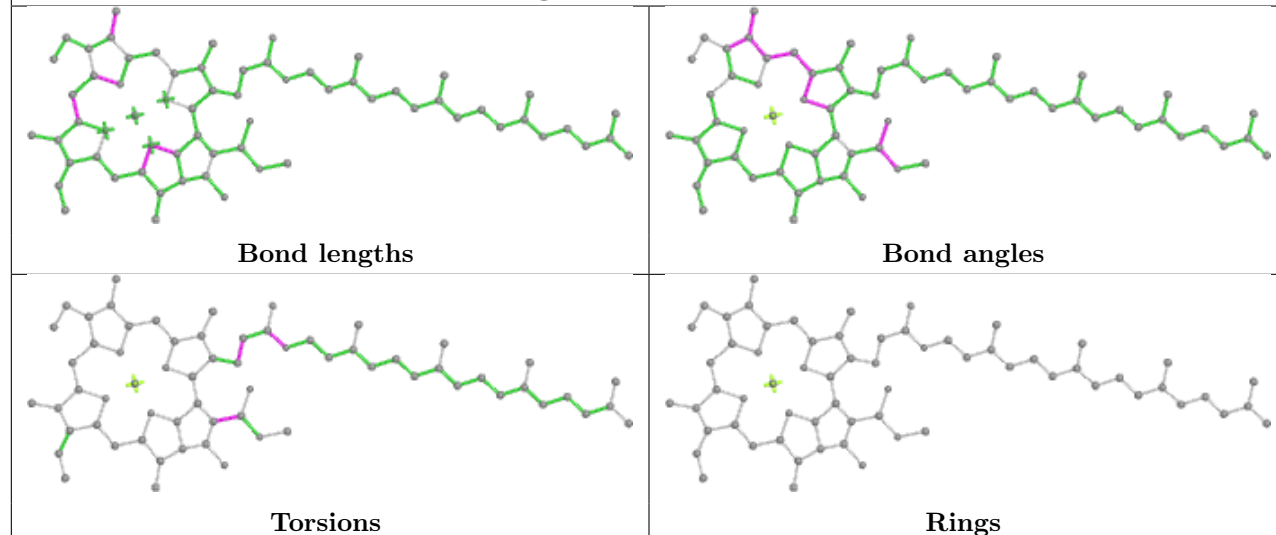
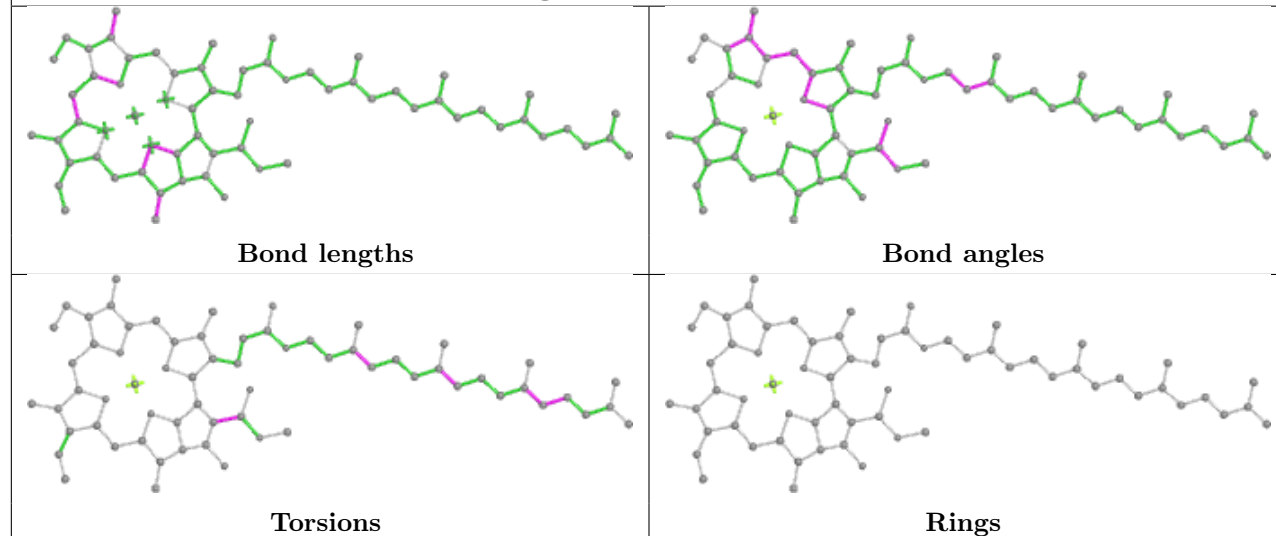
## Ligand CLA b 822



## Ligand BCR a 850

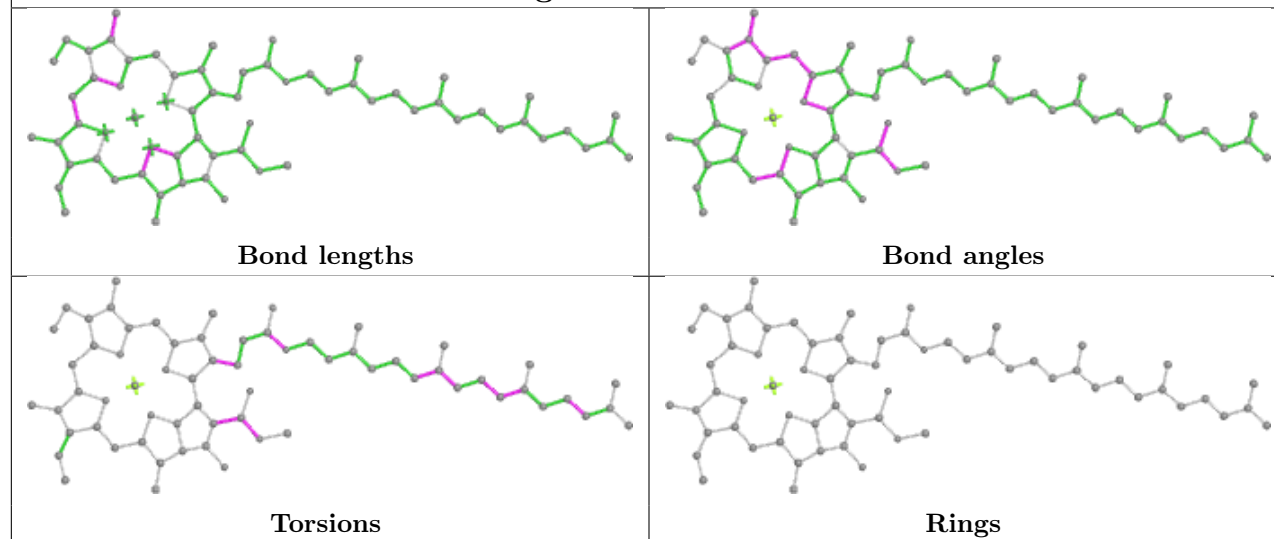




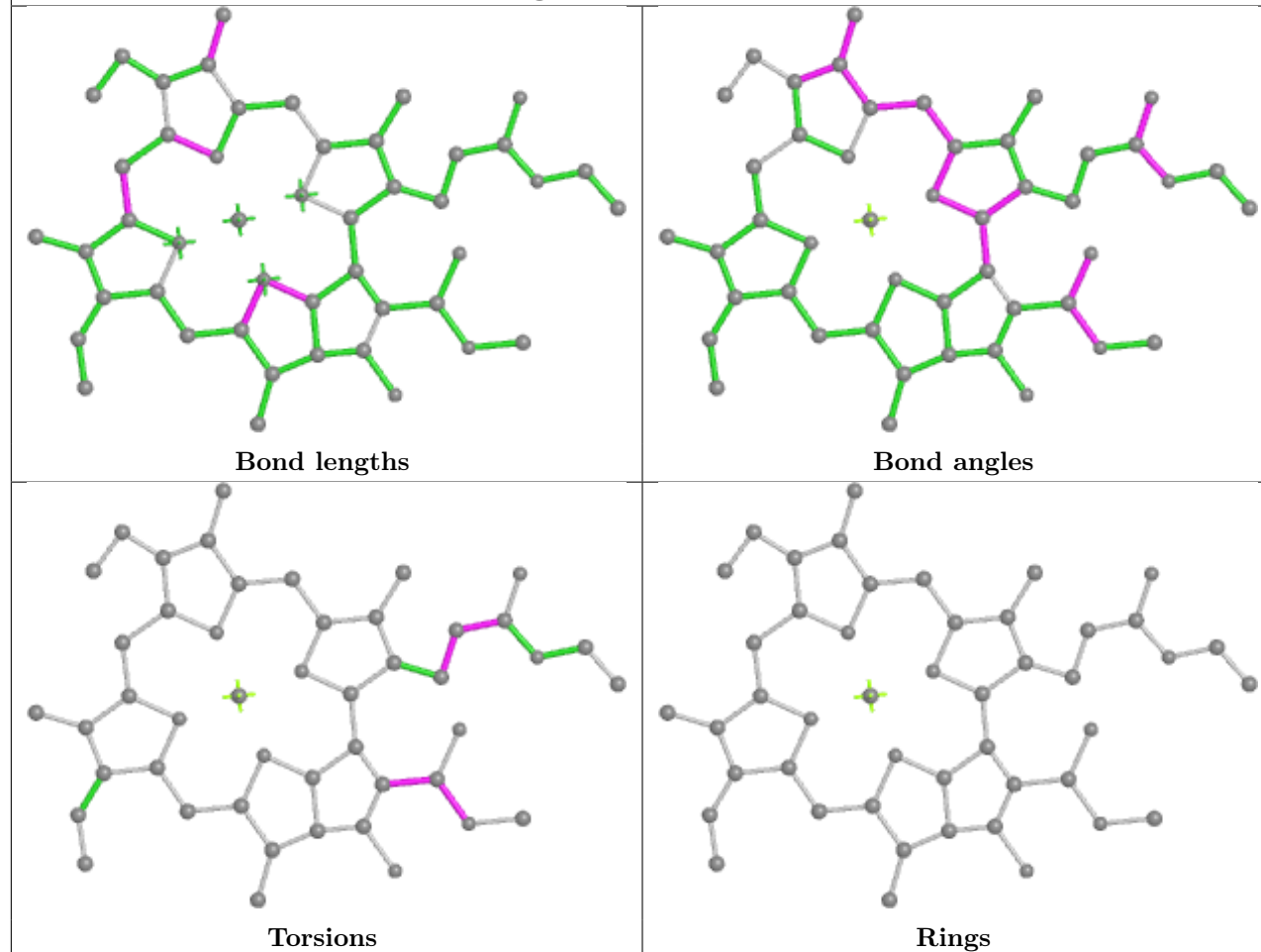
**Ligand CLA a 830****Ligand CLA b 826****Ligand CLA a 840**



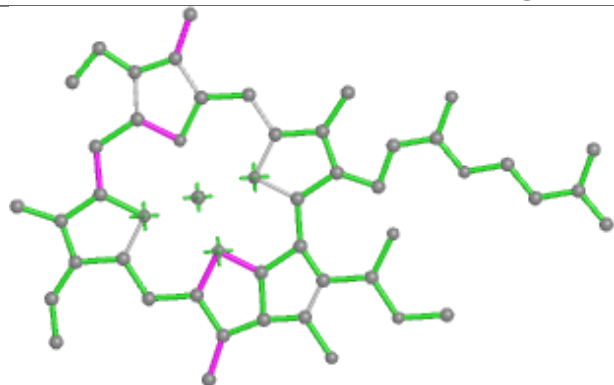
## Ligand CLA b 805



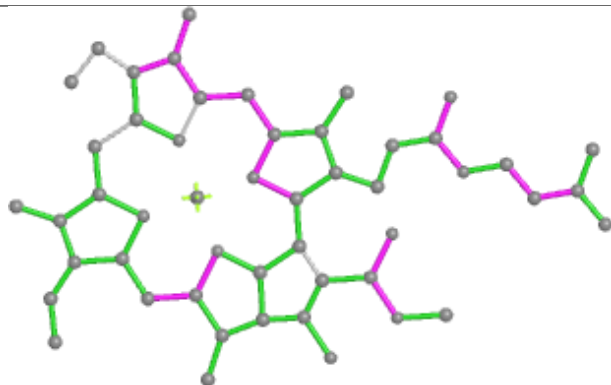
## Ligand CLA 2 307



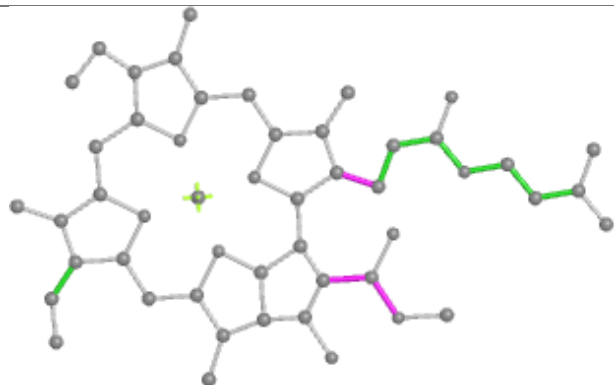
## Ligand CLA a 832



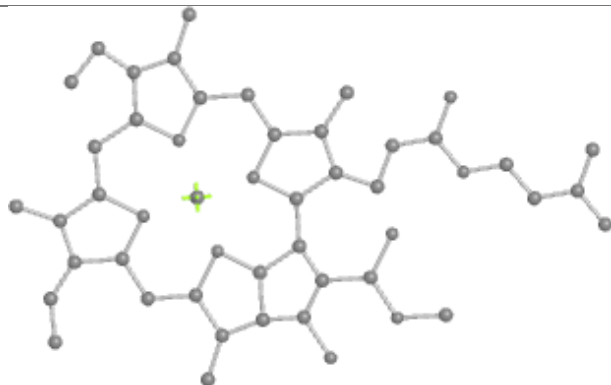
Bond lengths



Bond angles

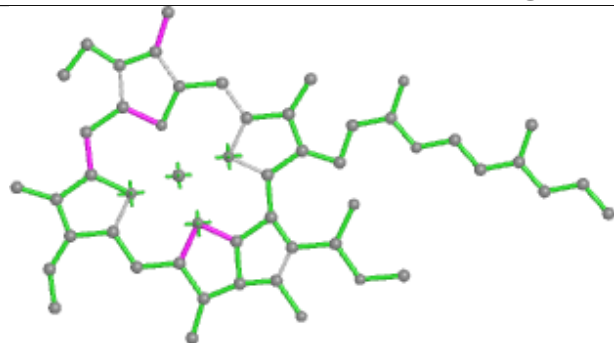


Torsions

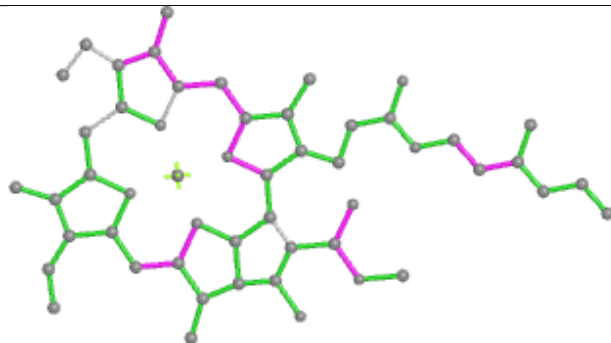


Rings

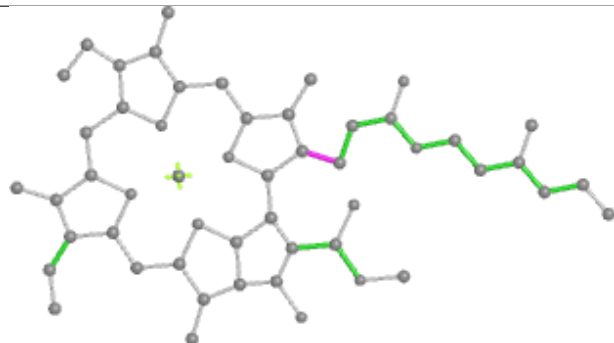
## Ligand CLA f 803



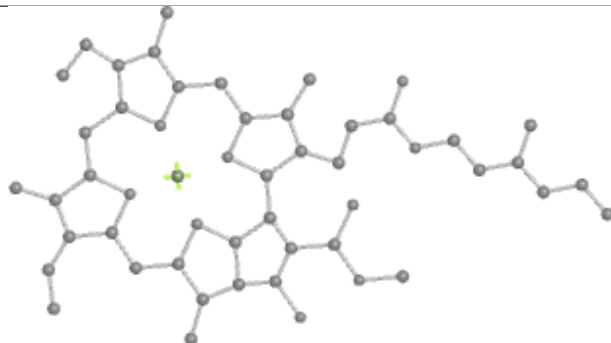
Bond lengths



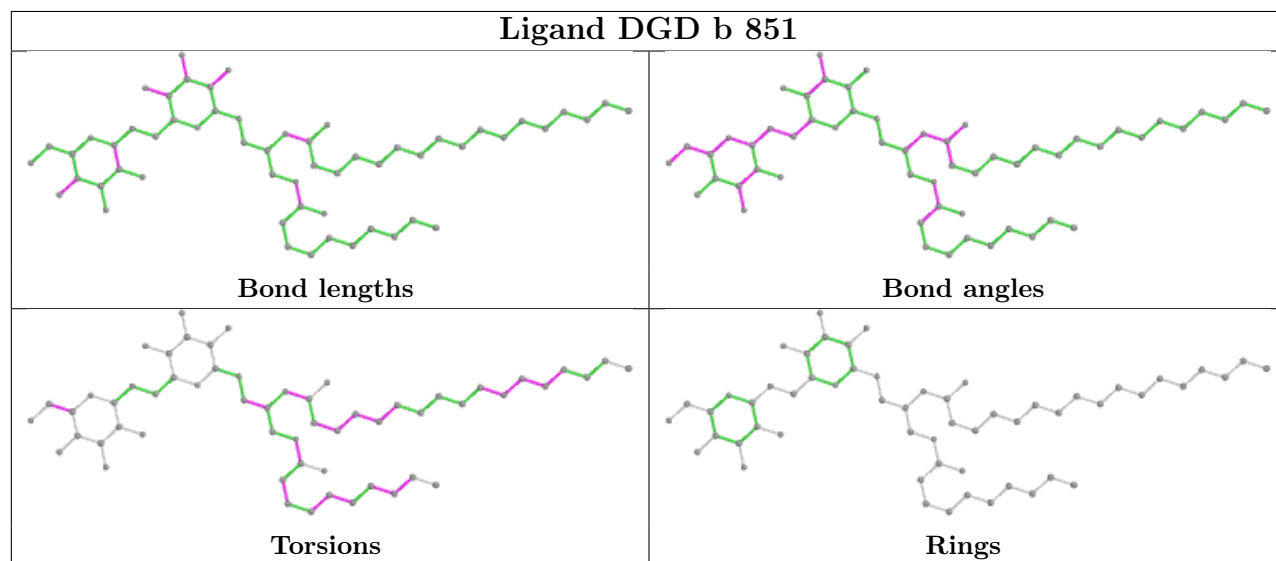
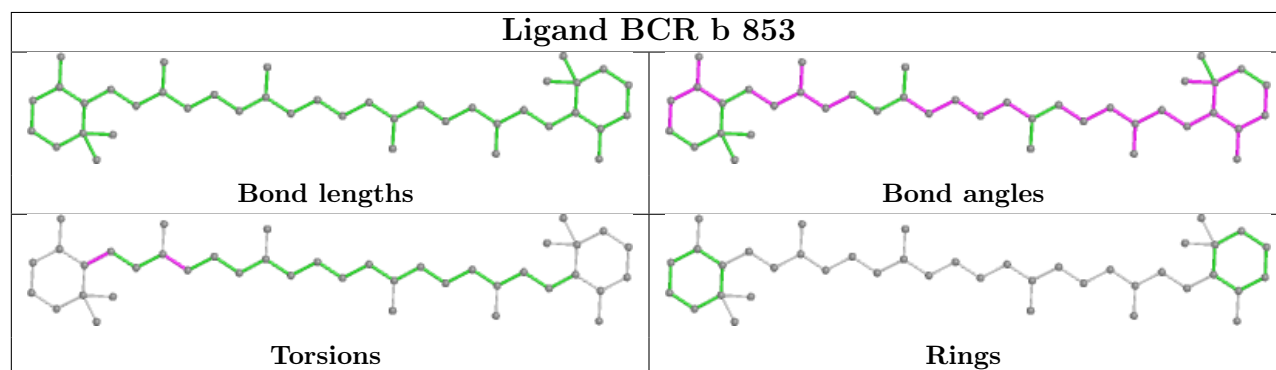
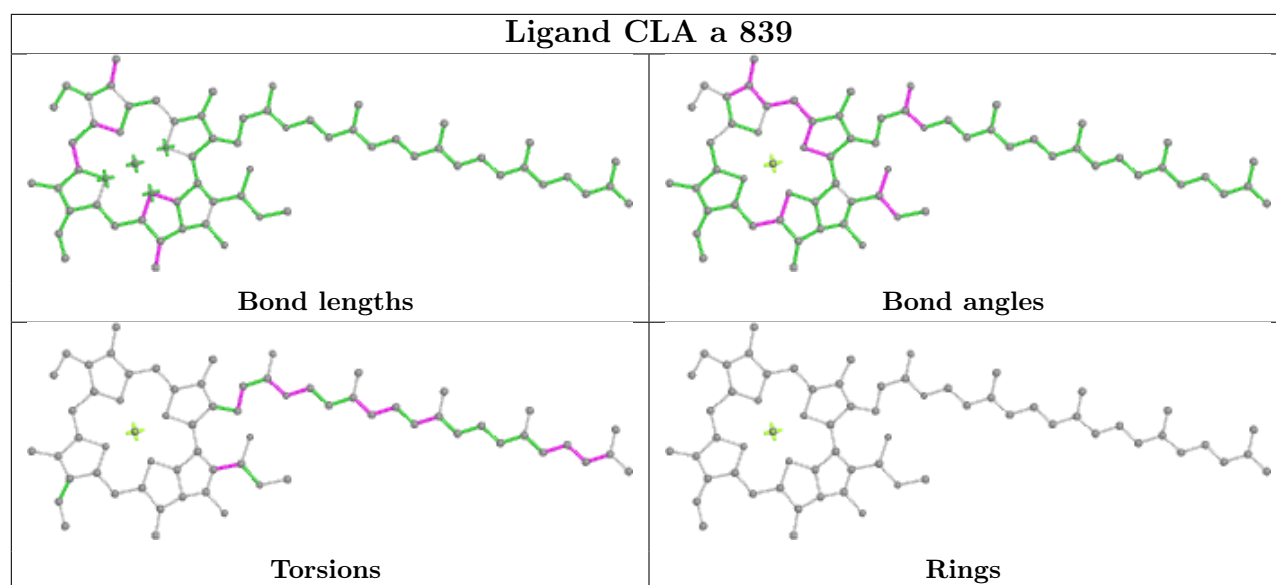
Bond angles



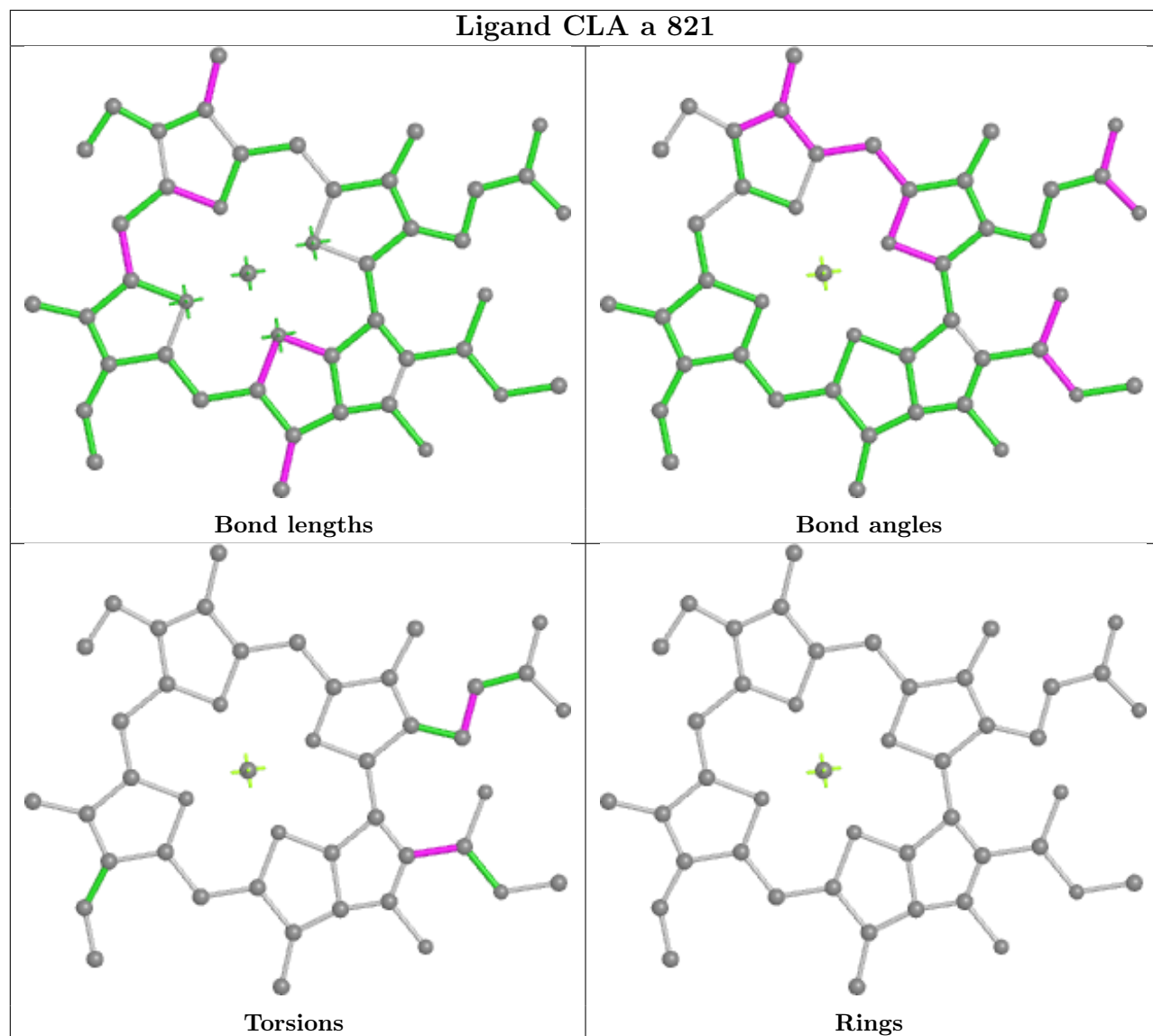
Torsions

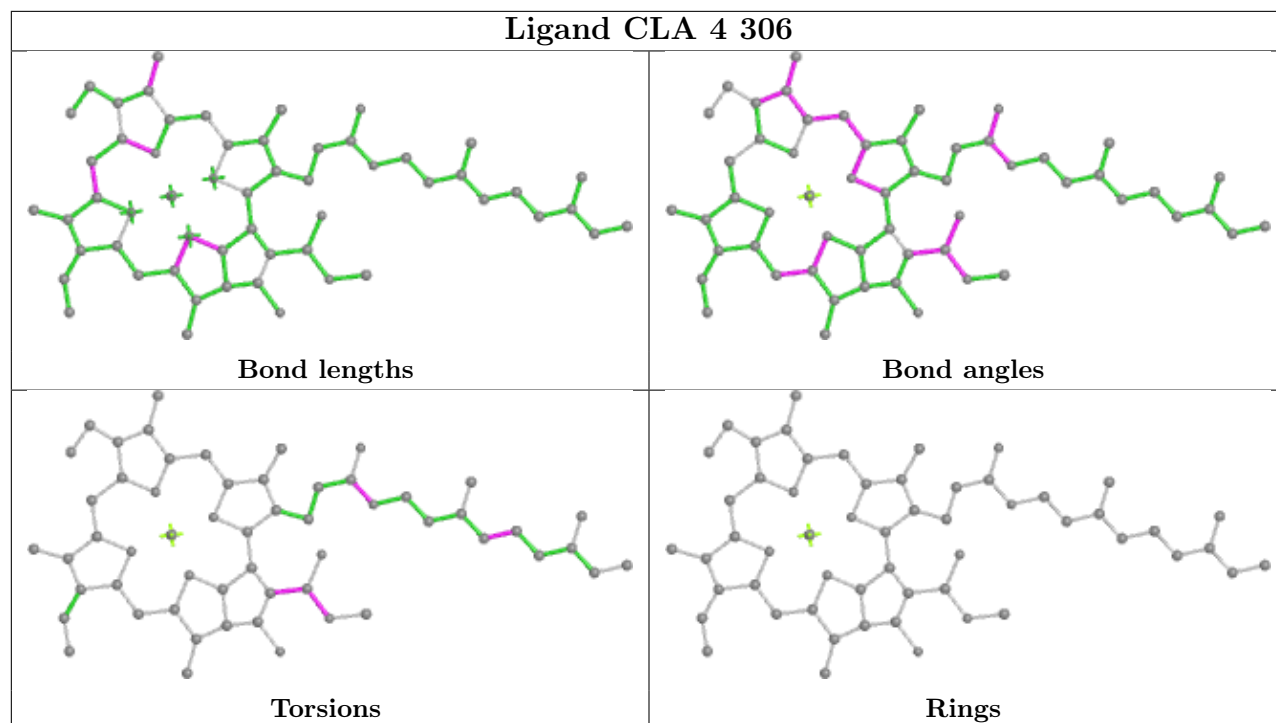
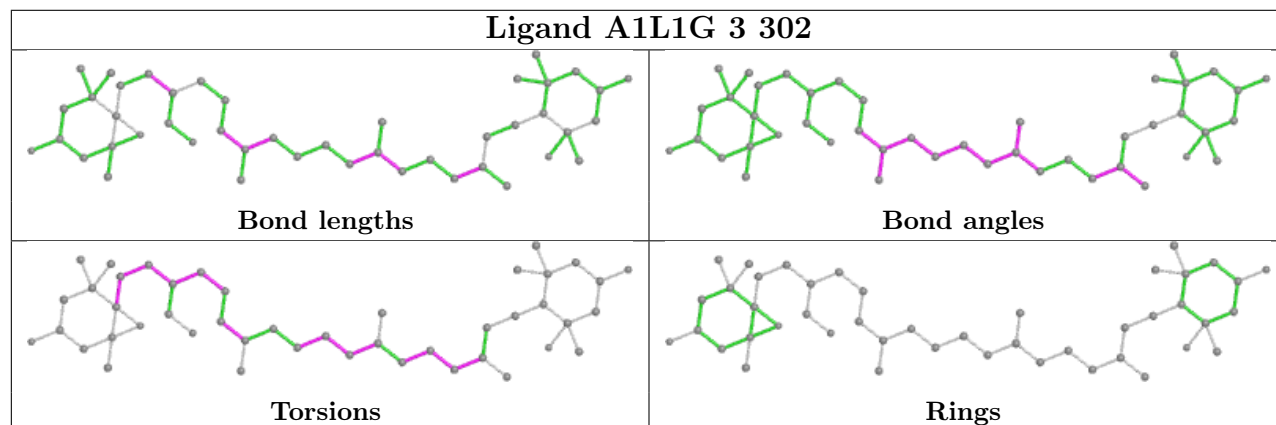
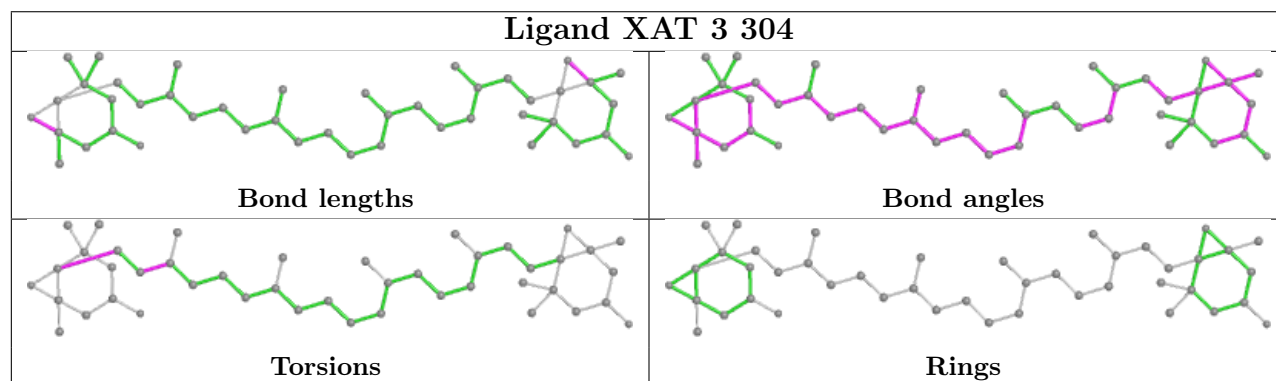


Rings

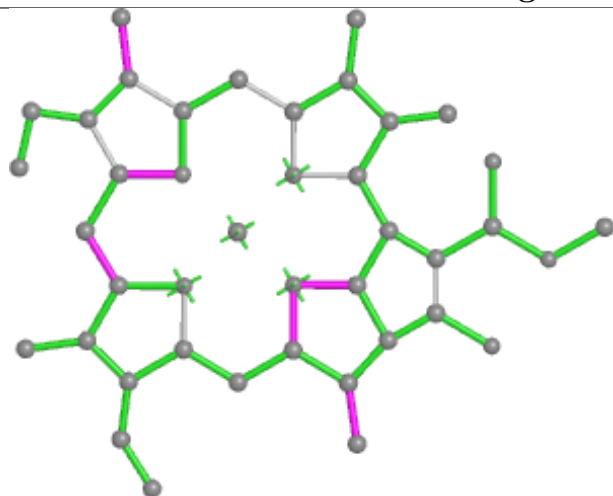


## Ligand CLA a 821

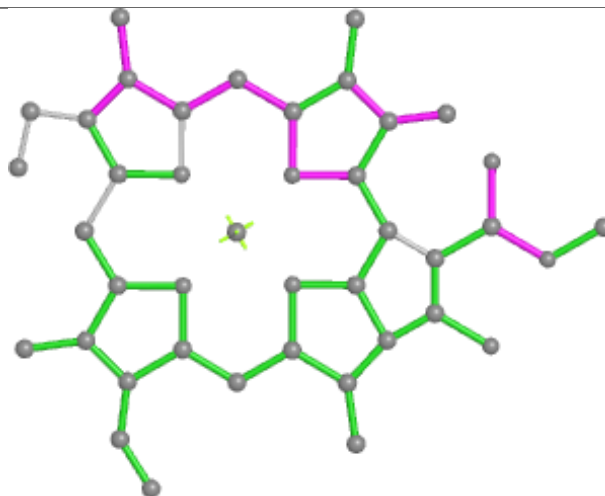


**Ligand CLA 4 306****Ligand A1L1G 3 302****Ligand XAT 3 304**

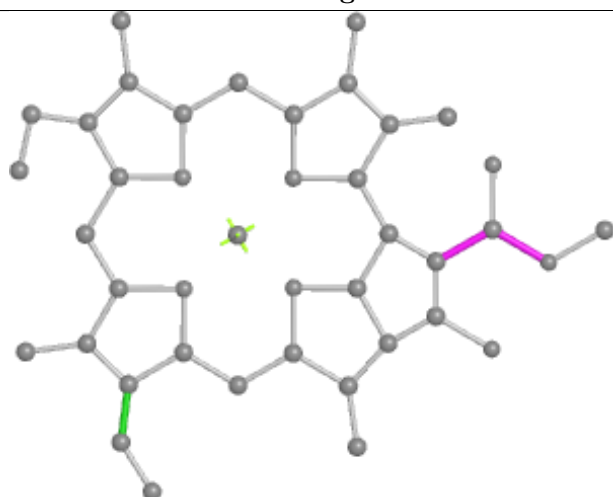
## Ligand CLA 1 313



Bond lengths



Bond angles

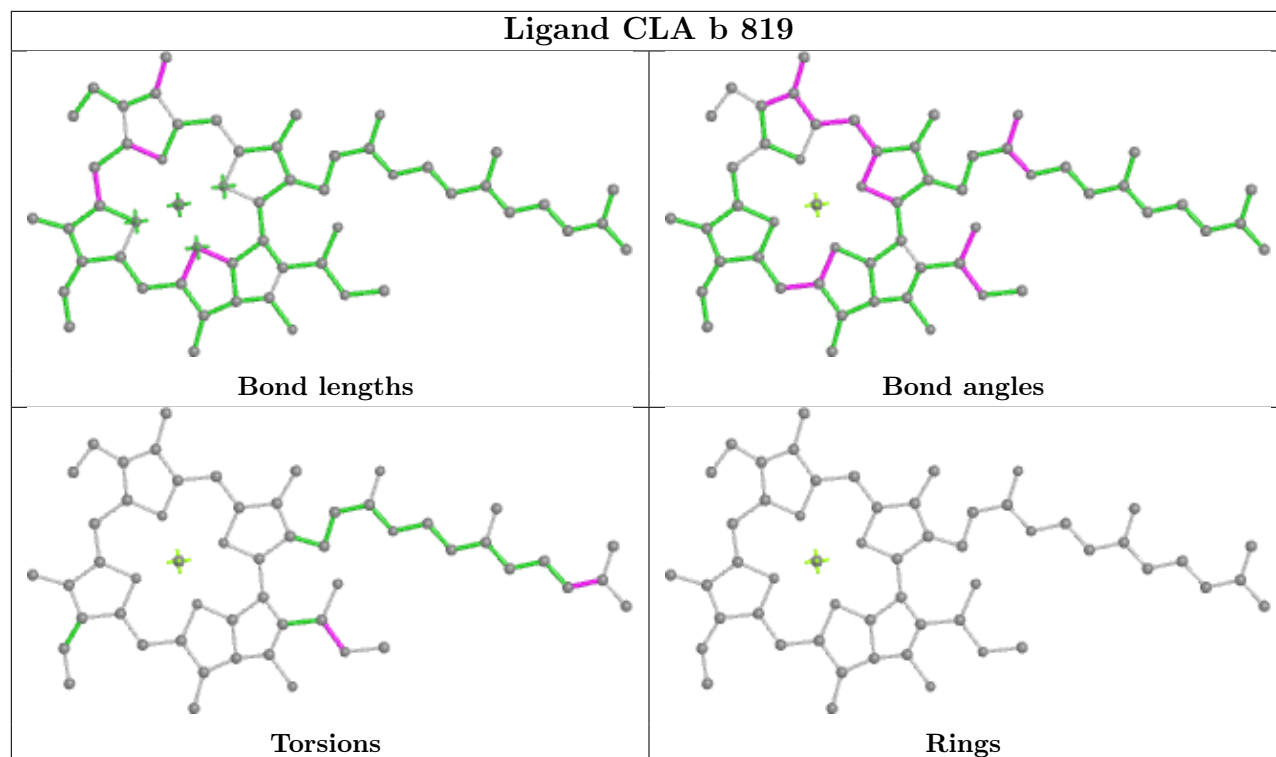


Torsions

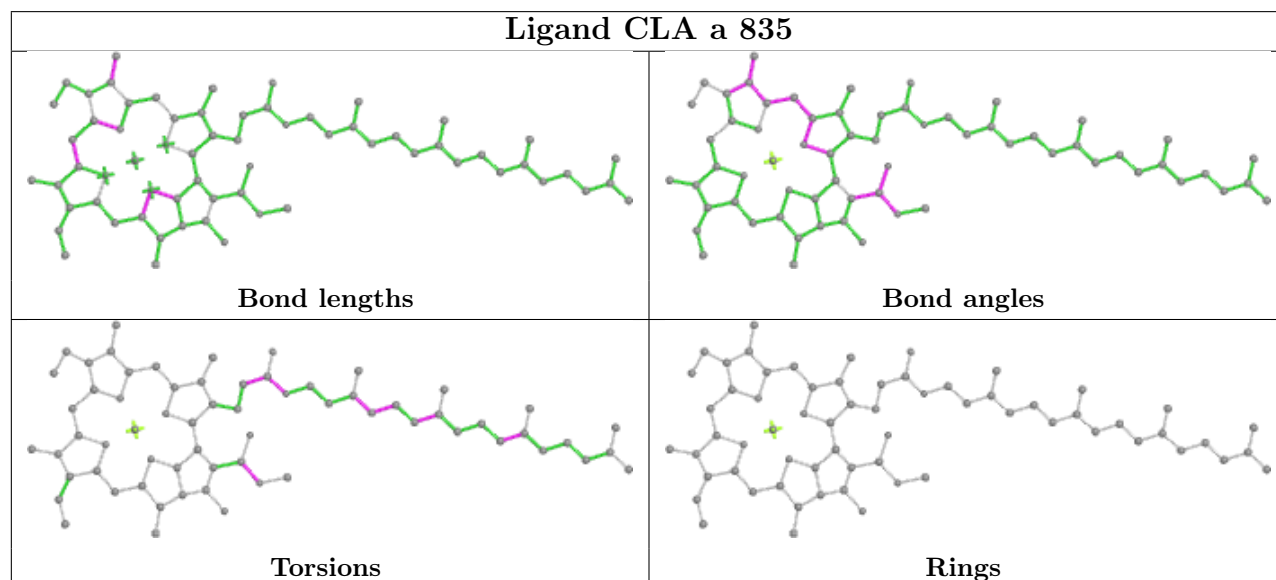


Rings

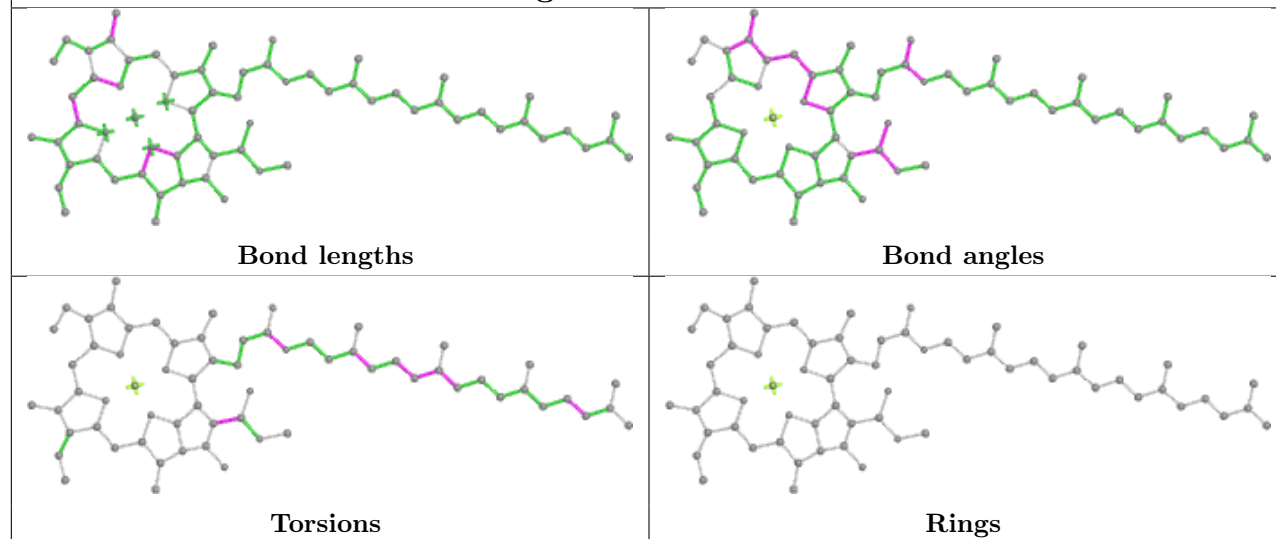
## Ligand CLA b 819



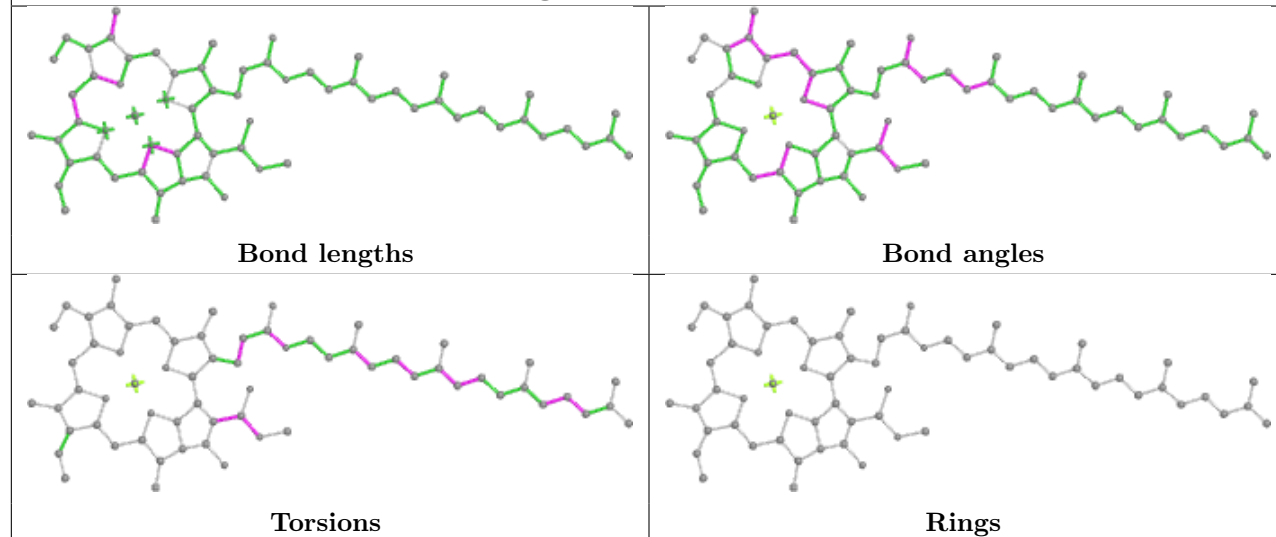
## Ligand CLA a 835



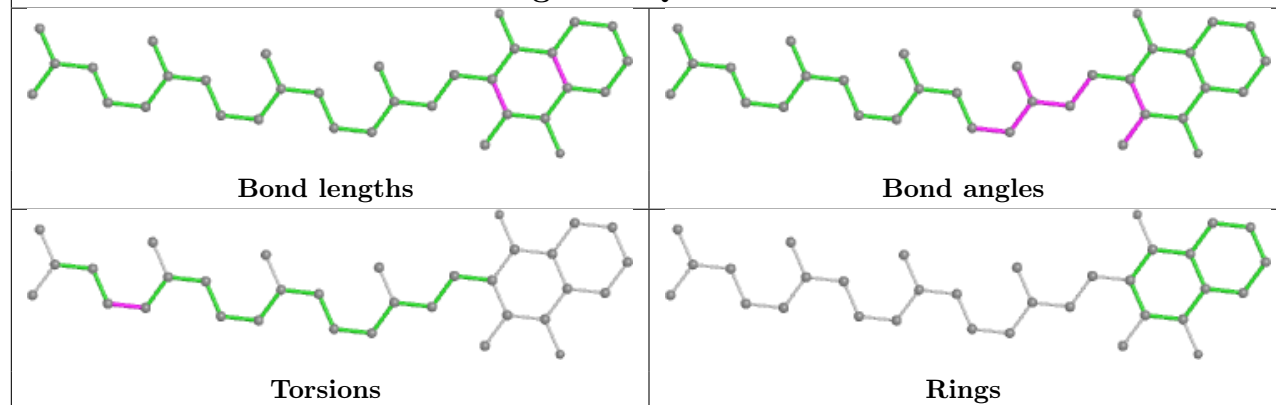
## Ligand CLA a 831



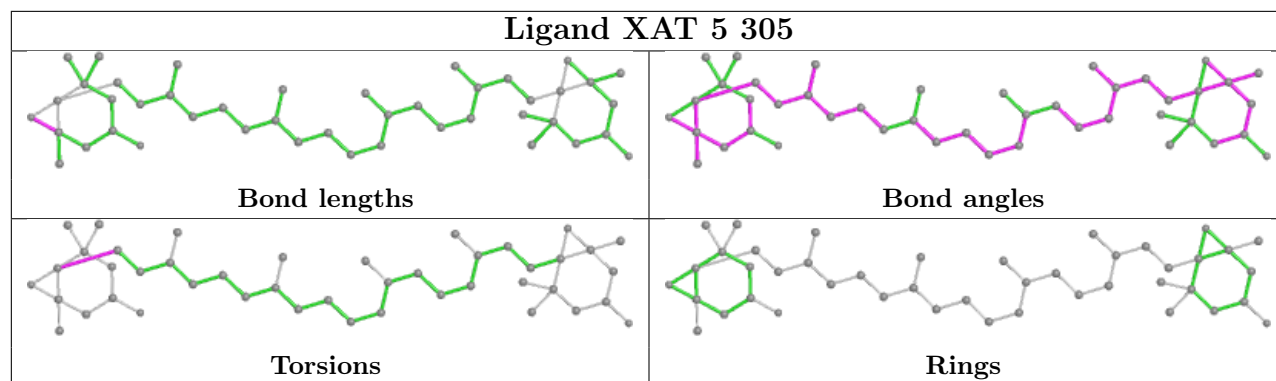
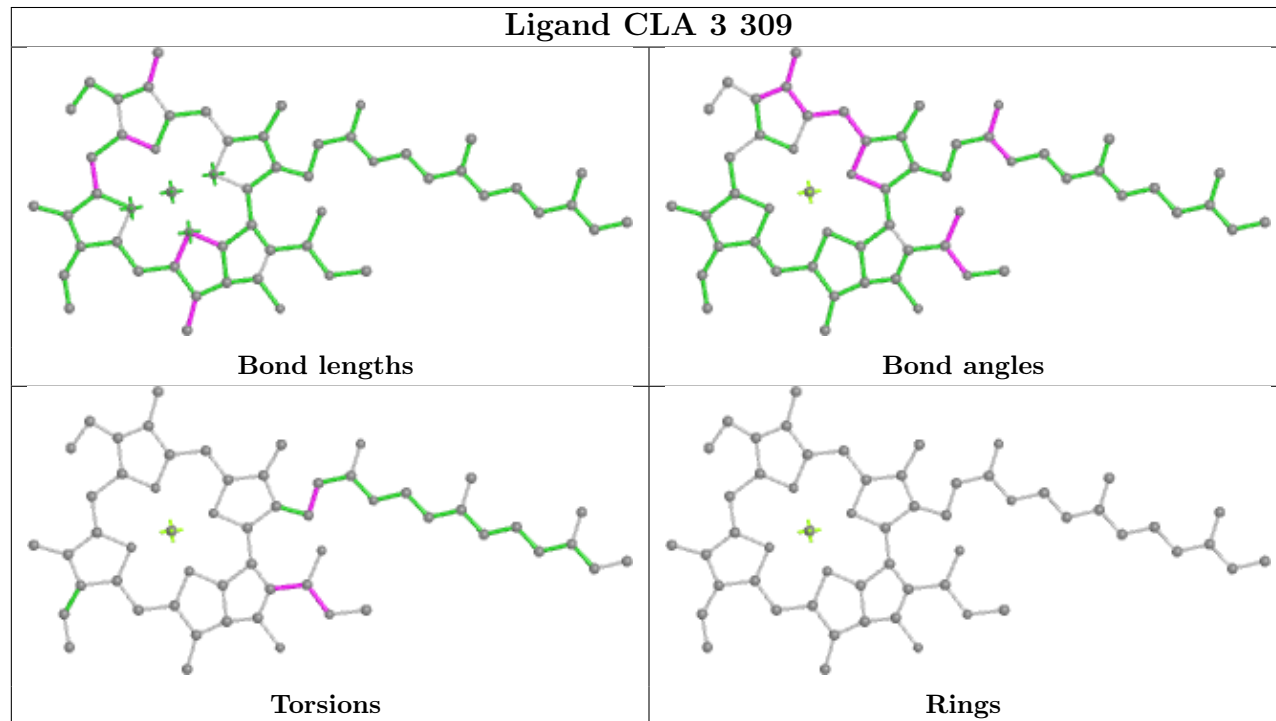
## Ligand CLA a 841



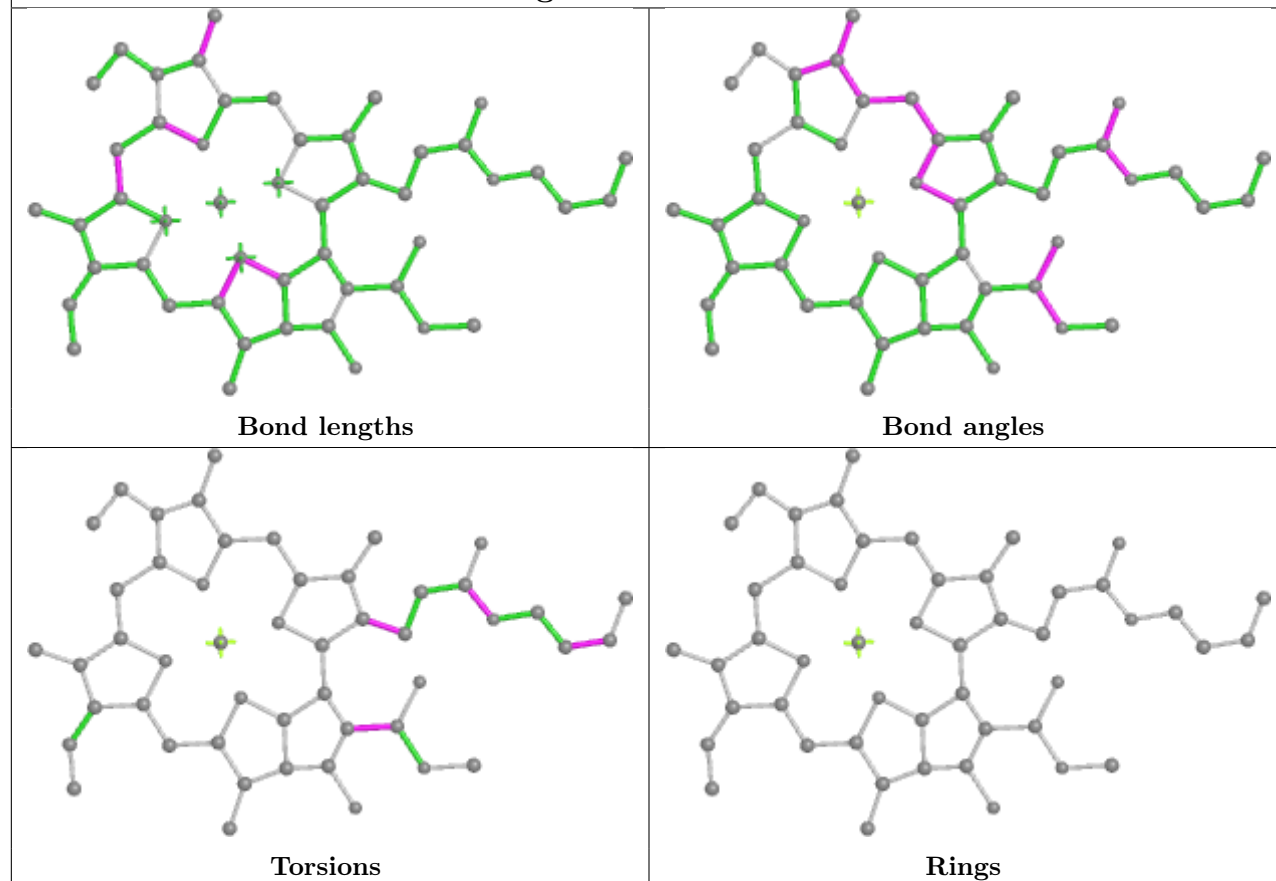
## Ligand PQN b 842



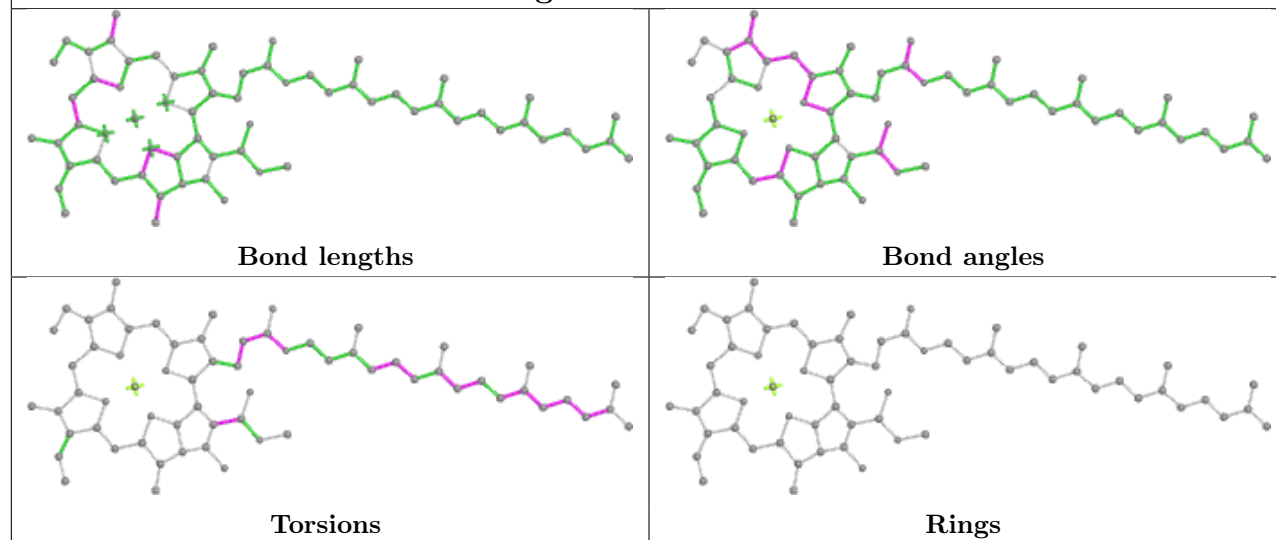


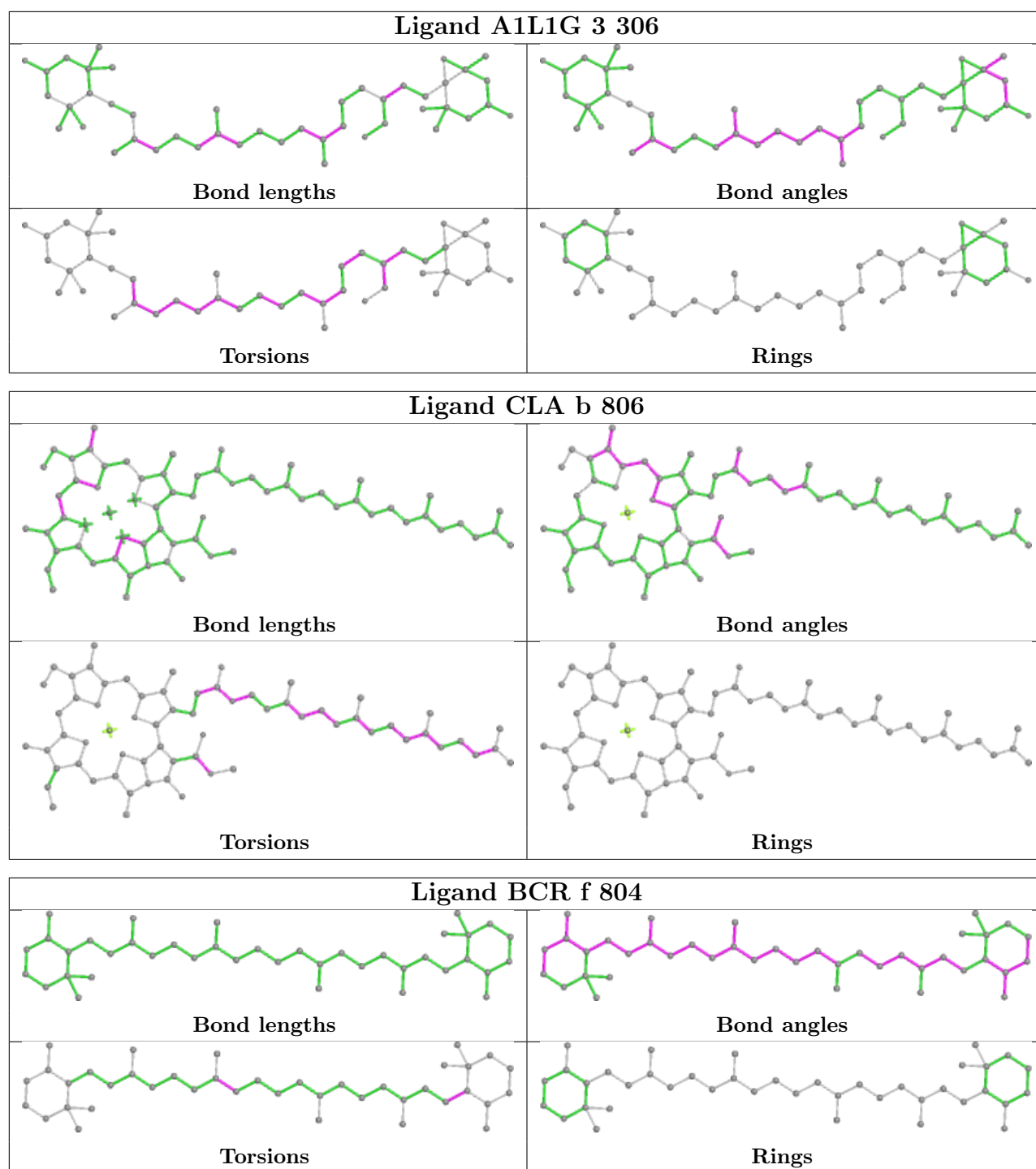
**Ligand XAT 5 305****Ligand CLA 3 309**

## Ligand CLA a 823

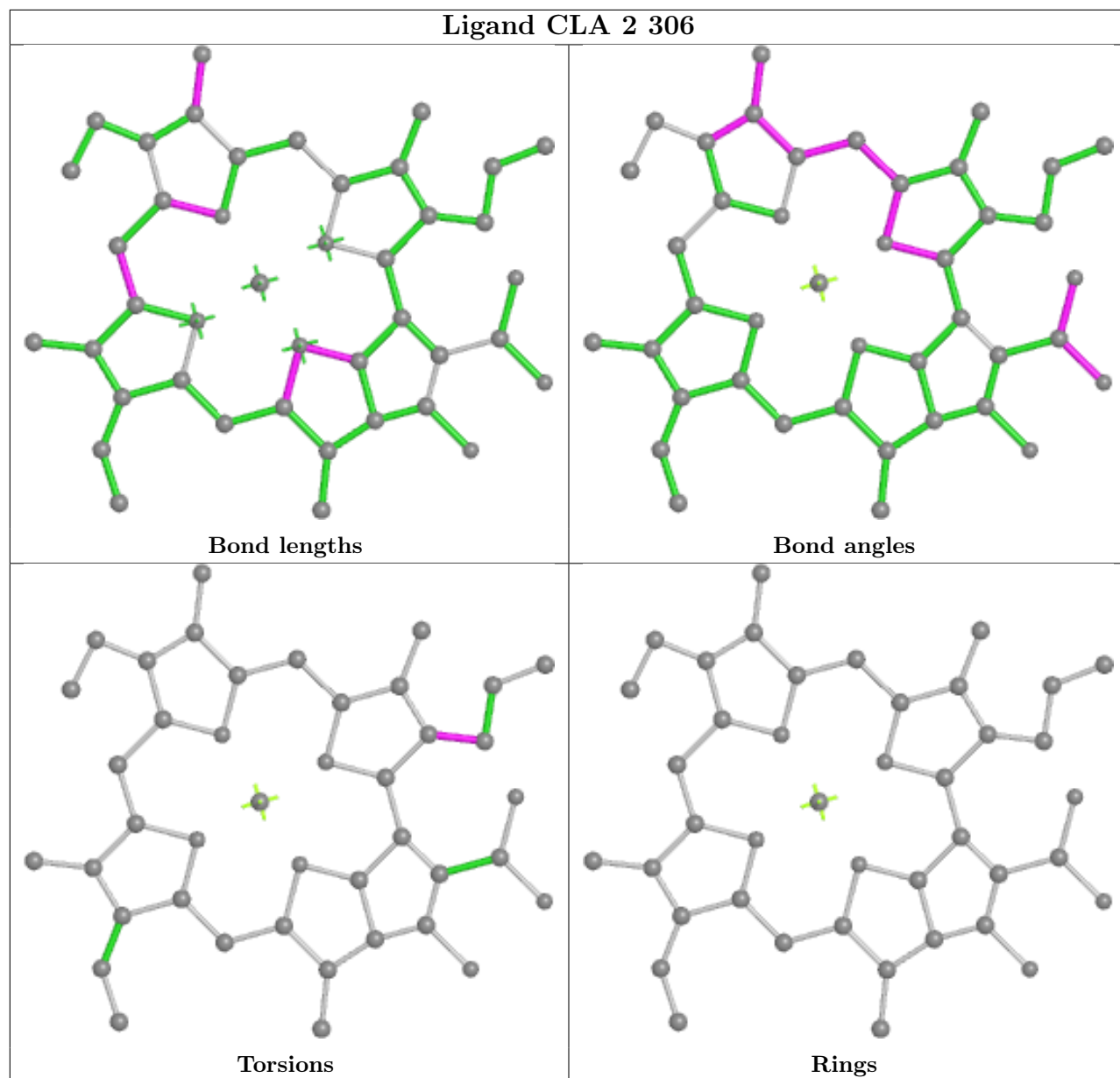


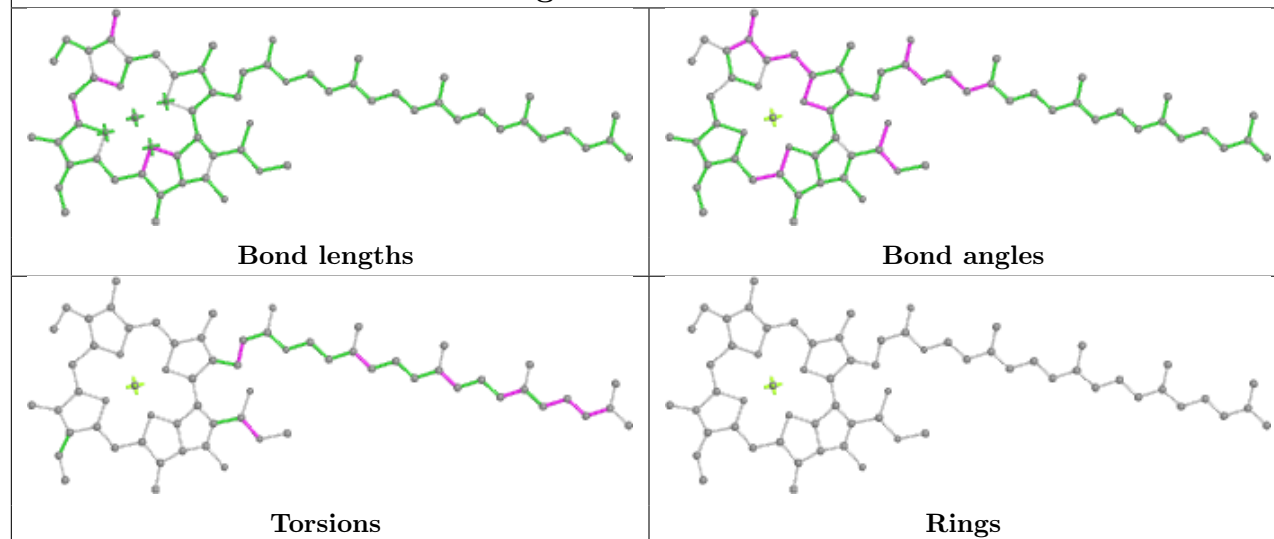
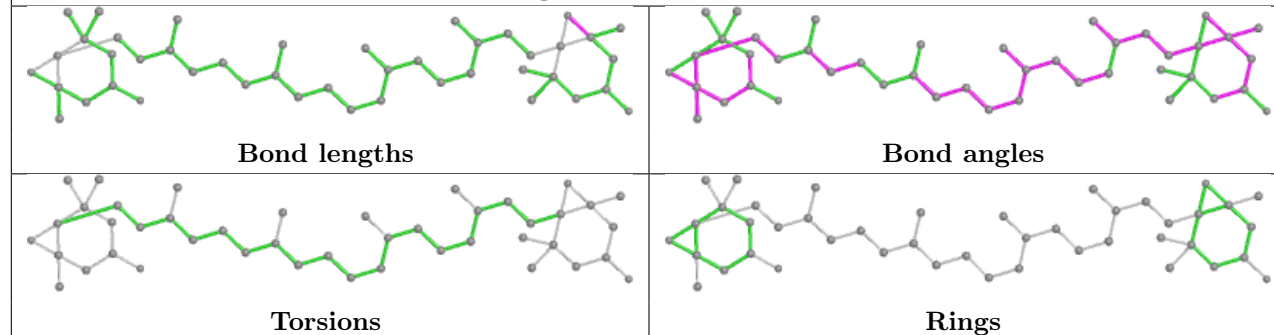
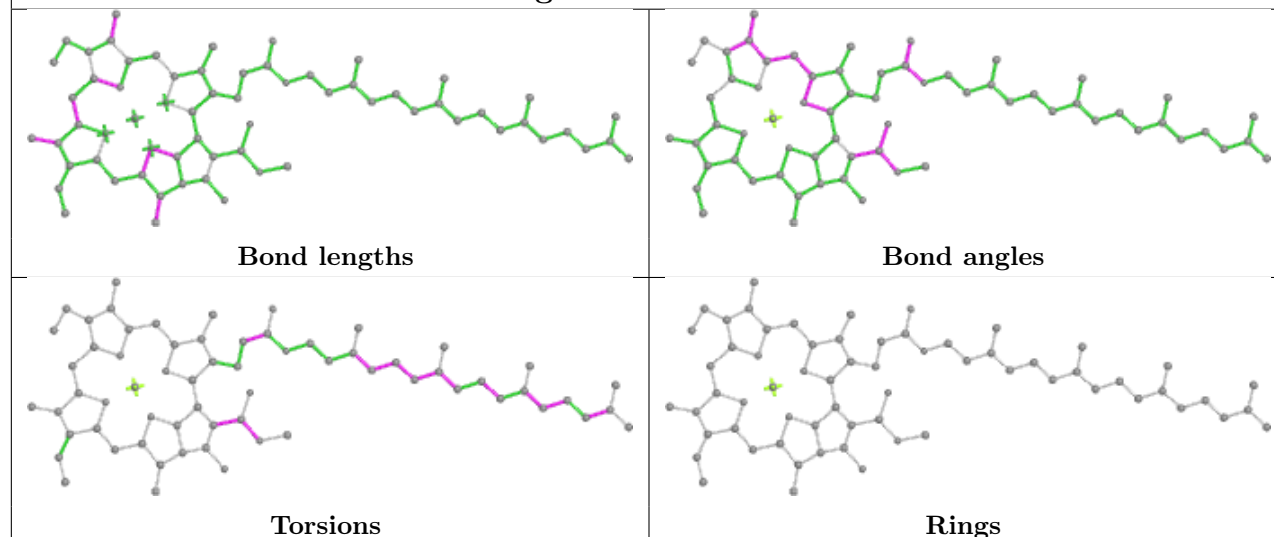
## Ligand CLA b 801

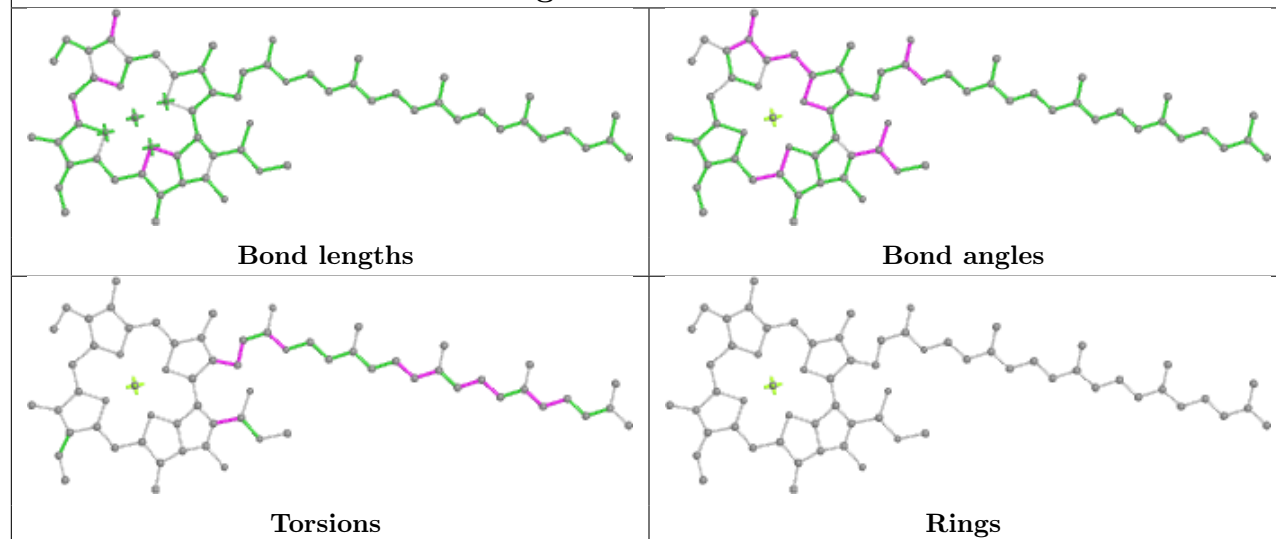
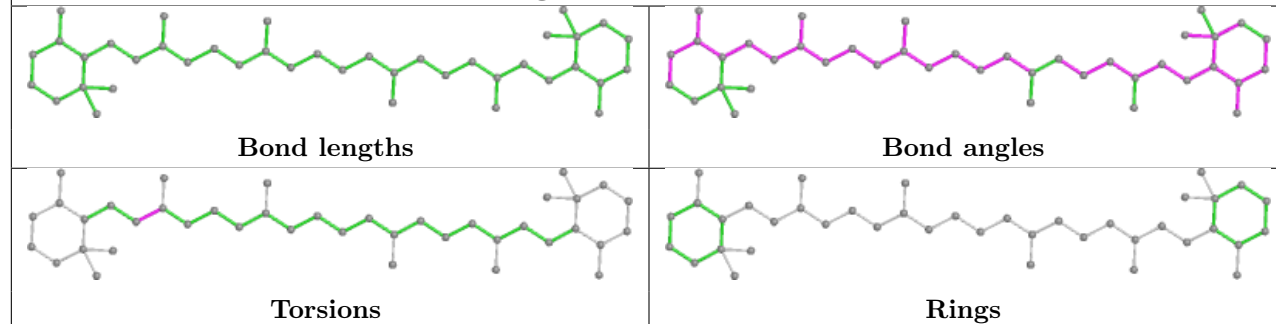
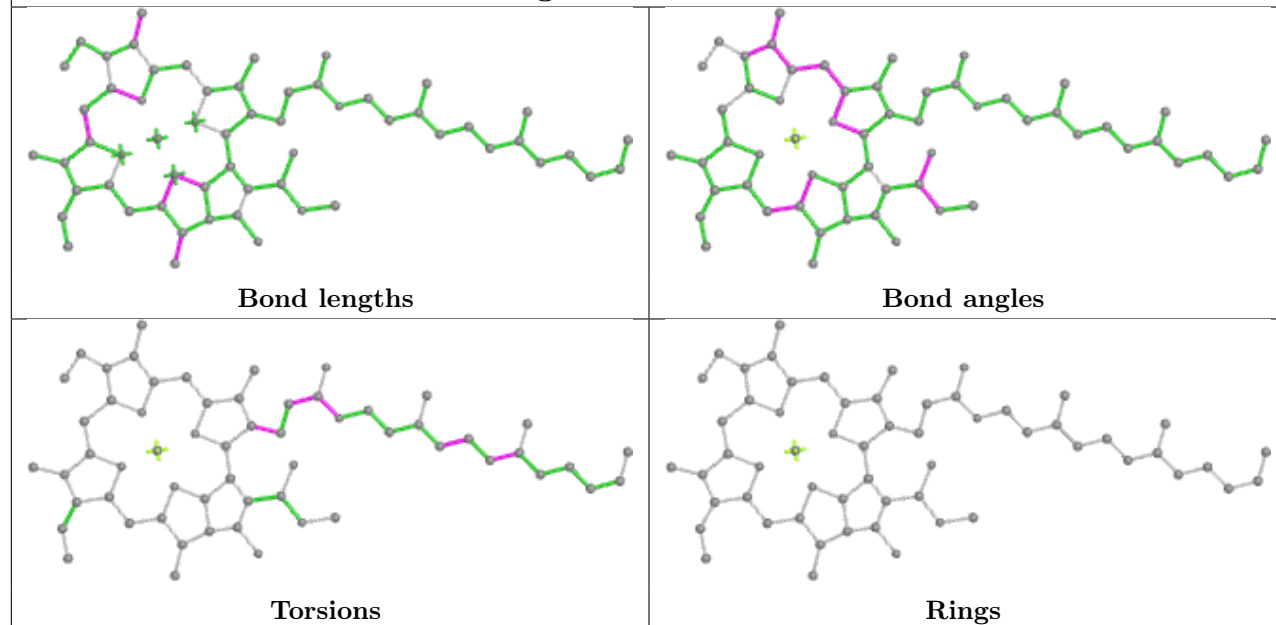


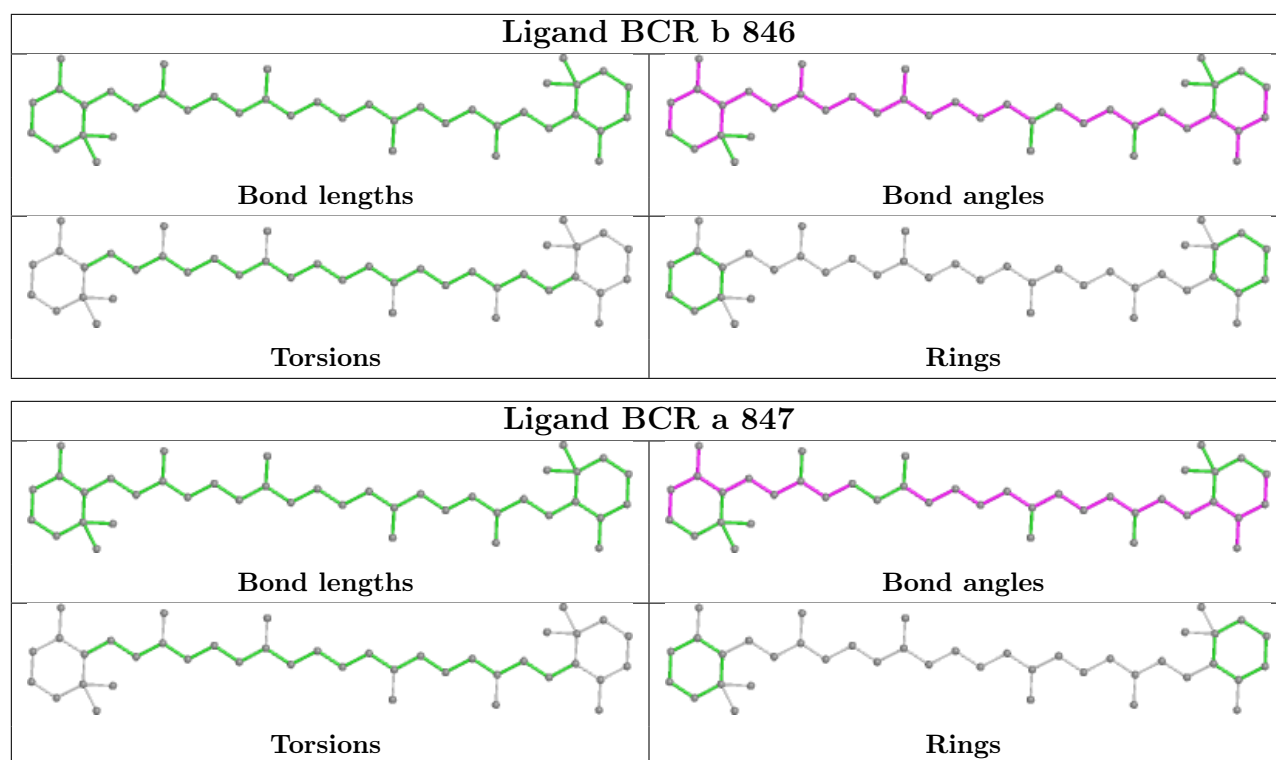


## Ligand CLA 2 306

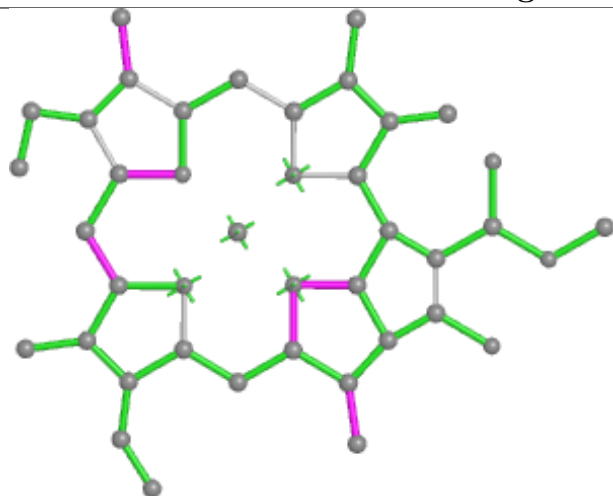


**Ligand CLA 1 308****Ligand XAT 3 305****Ligand CLA b 802**

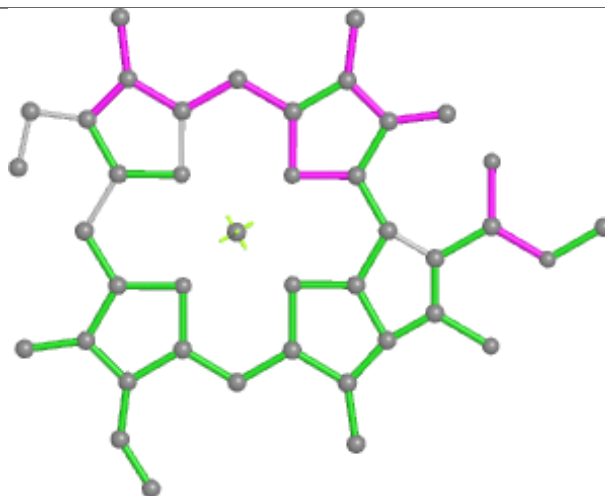
**Ligand CLA a 809****Ligand BCR b 847****Ligand CLA 3 312**



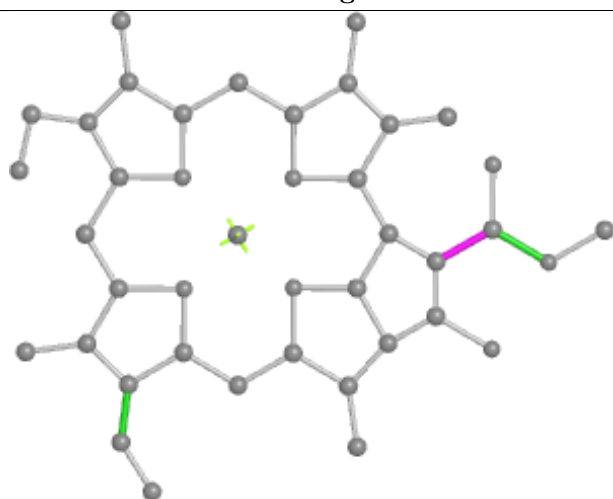
## Ligand CLA b 830



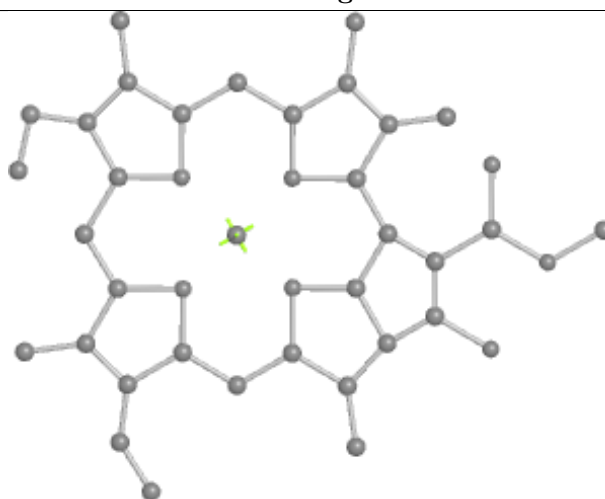
Bond lengths



Bond angles



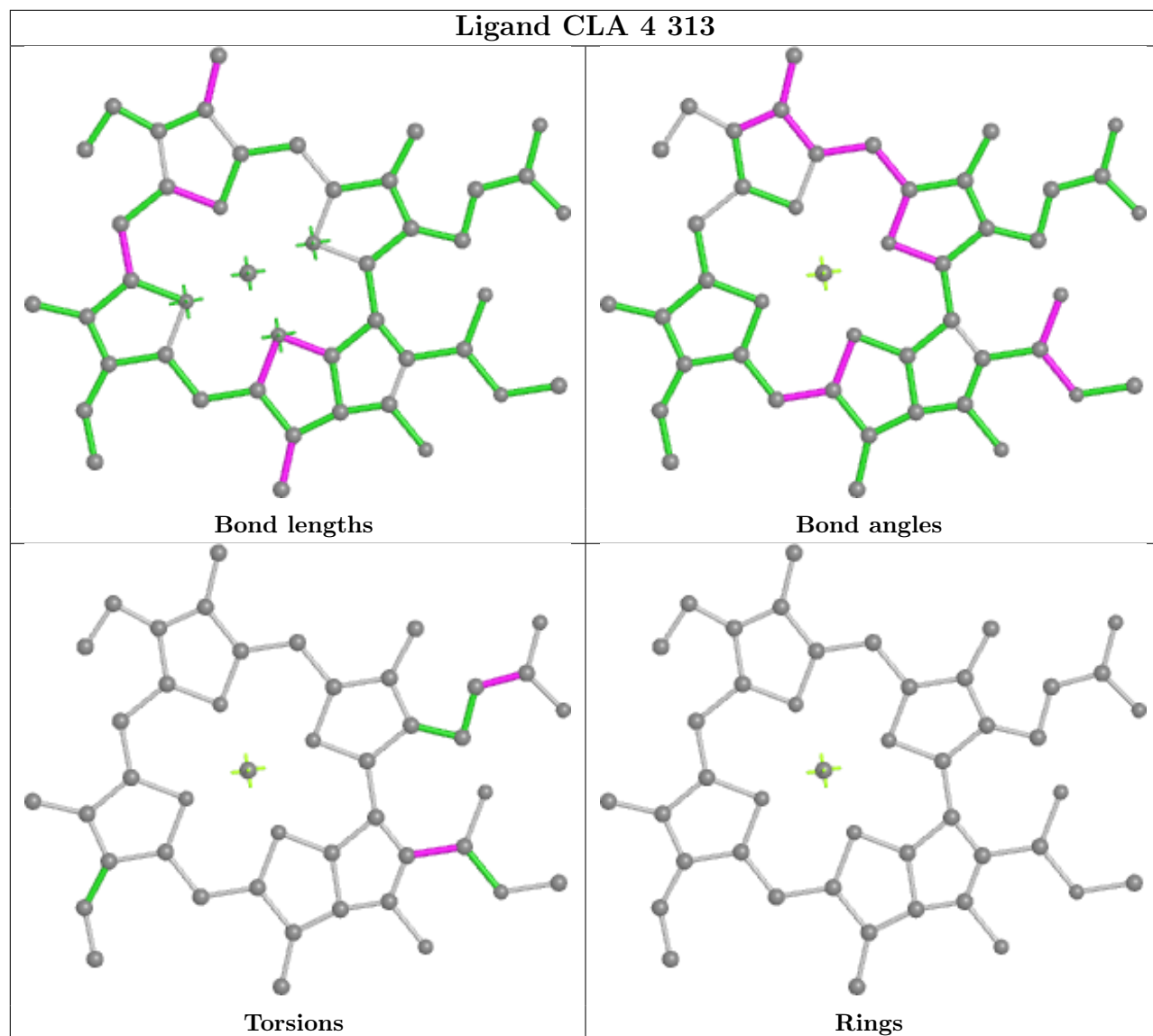
Torsions



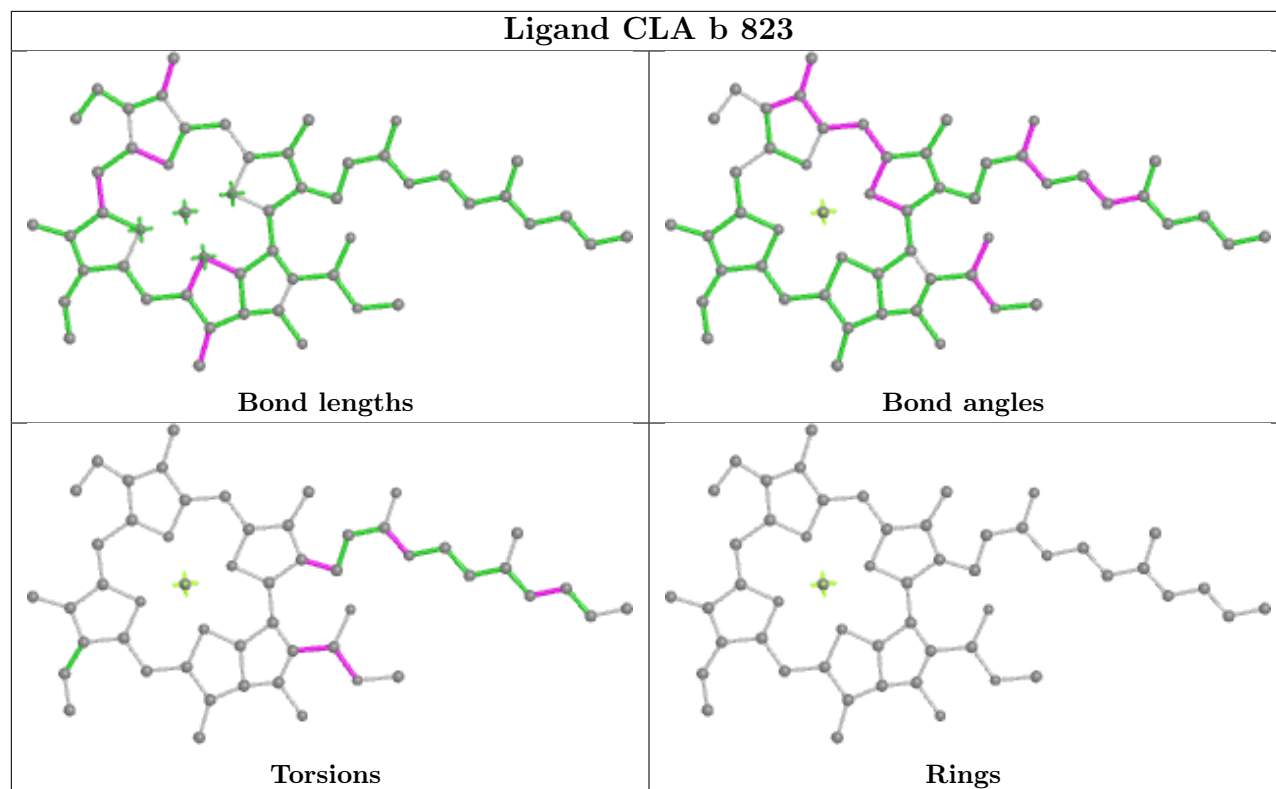
Rings



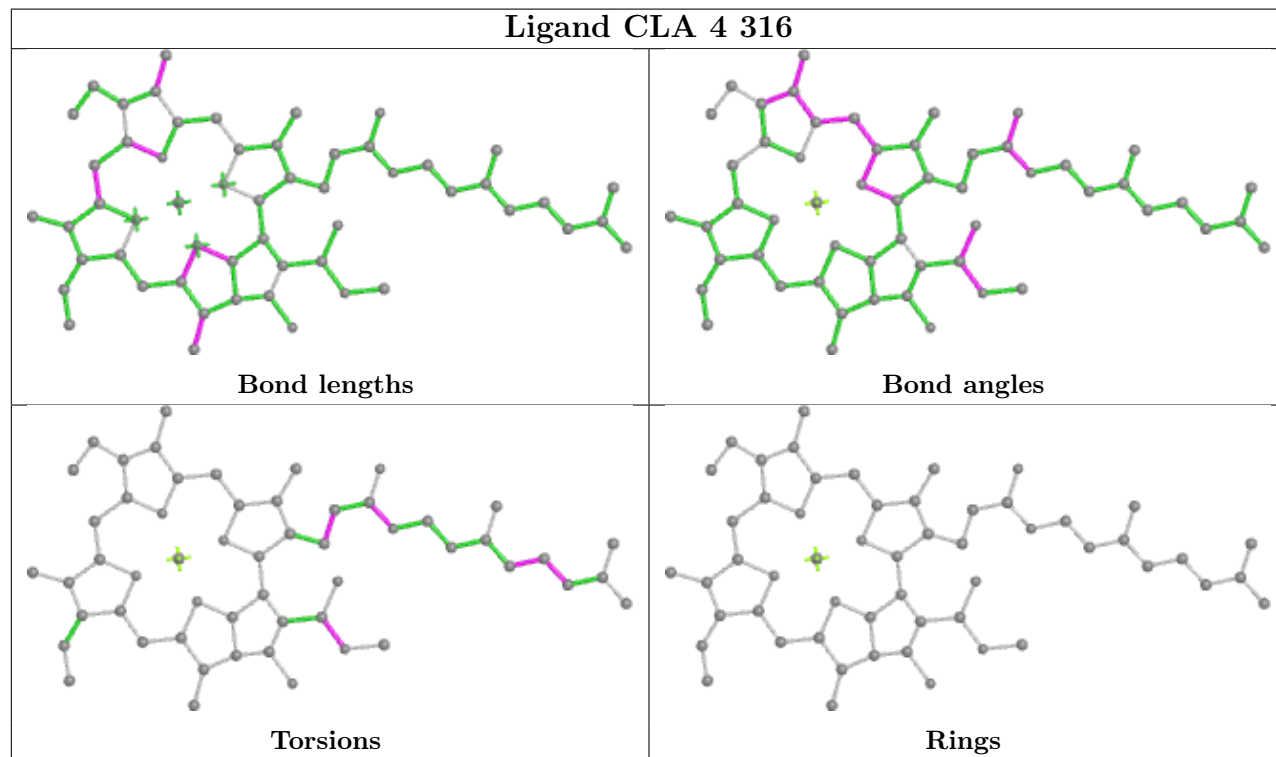
## Ligand CLA 4 313



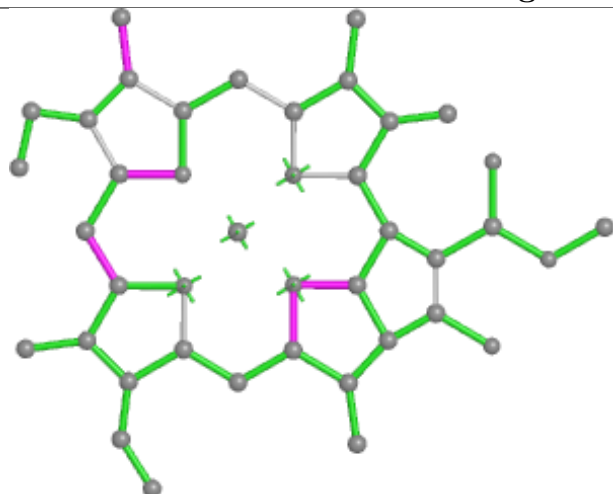
## Ligand CLA b 823



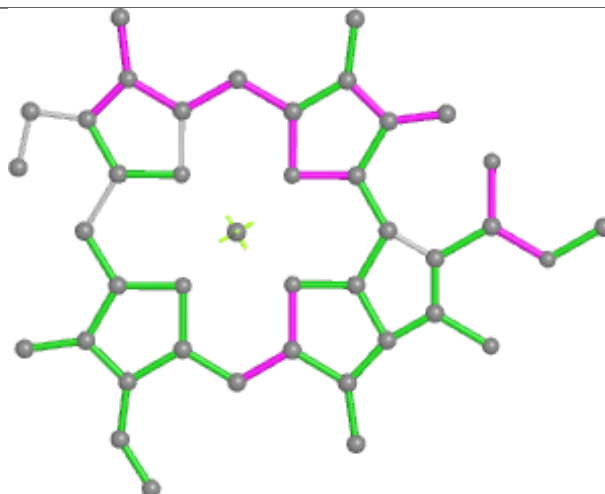
## Ligand CLA 4 316



## Ligand CLA 2 313



Bond lengths



Bond angles

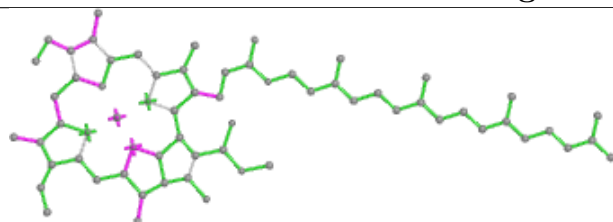


Torsions

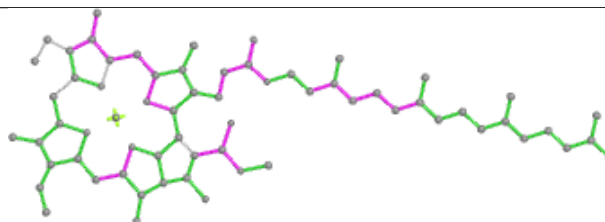


Rings

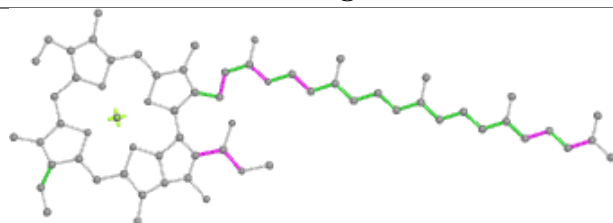
## Ligand CLA a 806



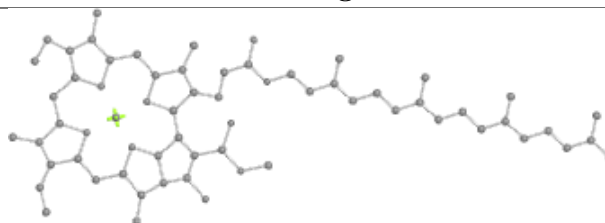
Bond lengths



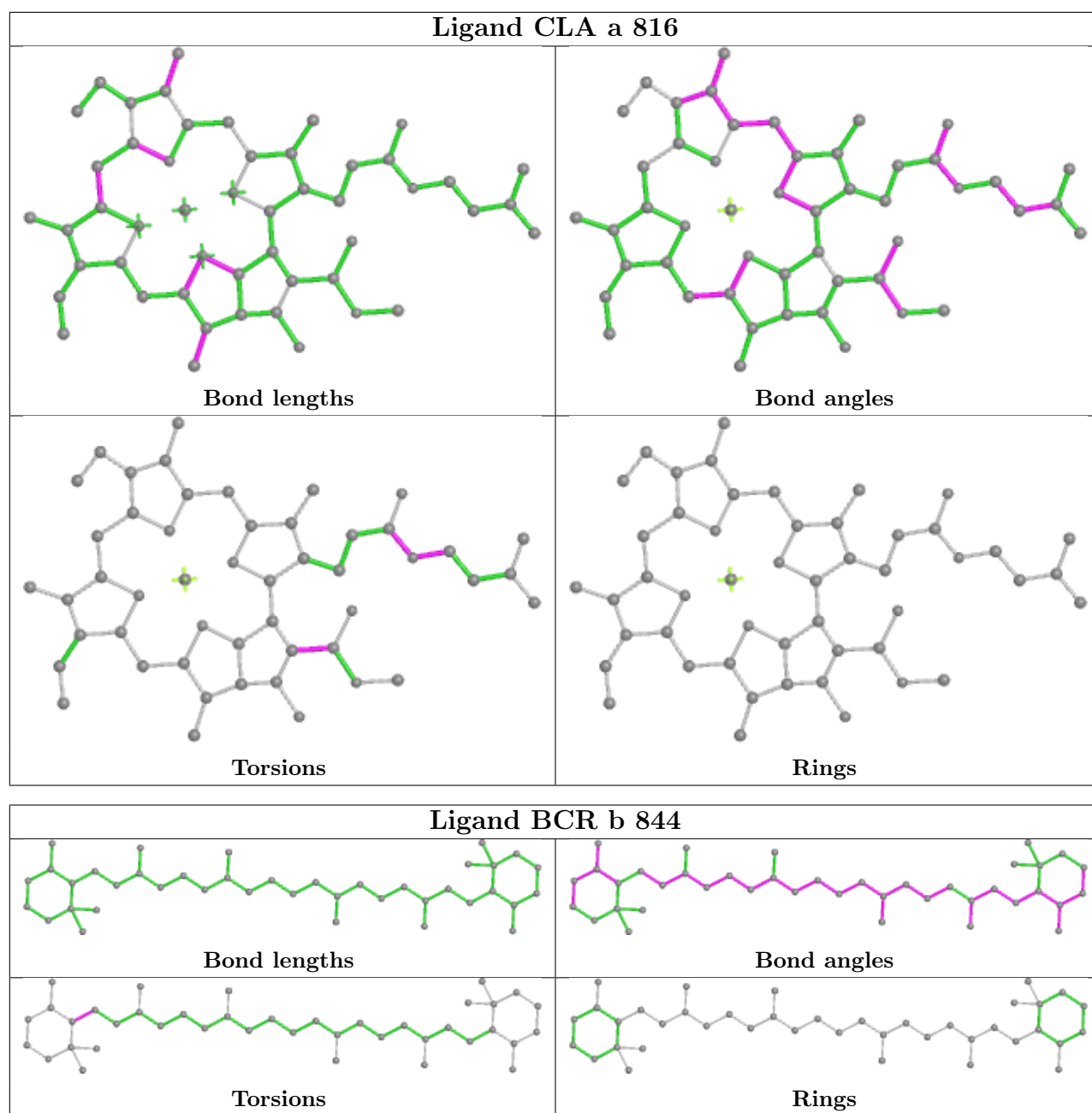
Bond angles

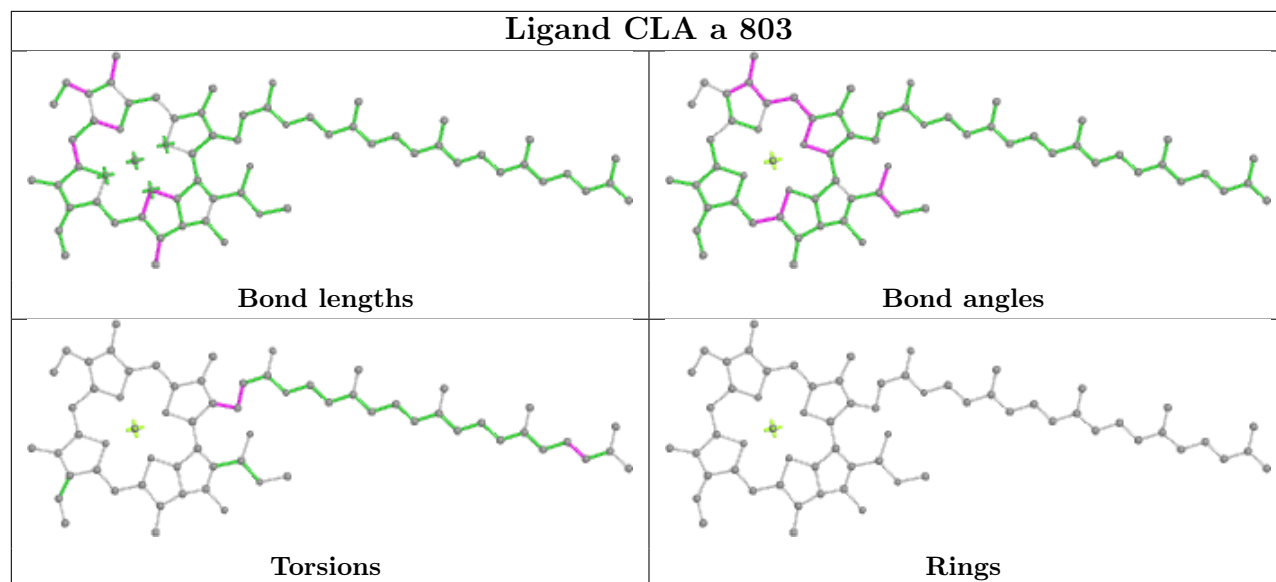
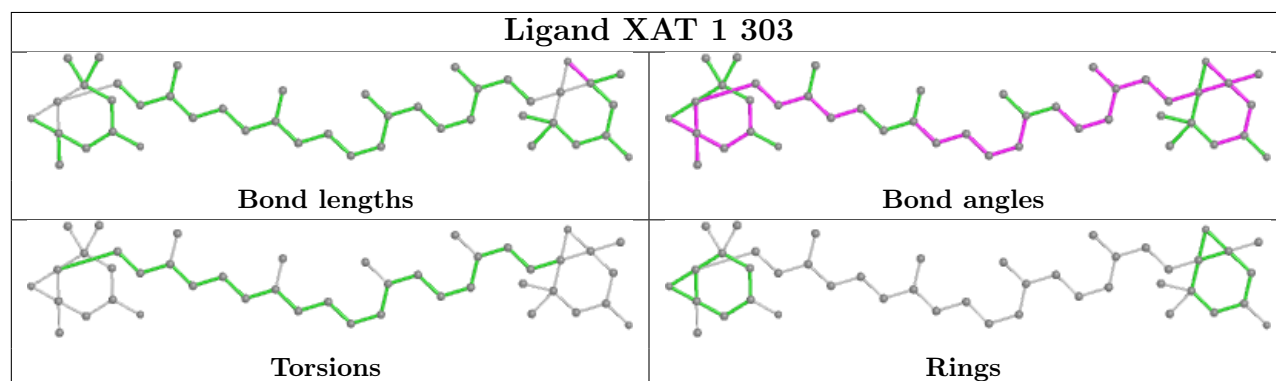
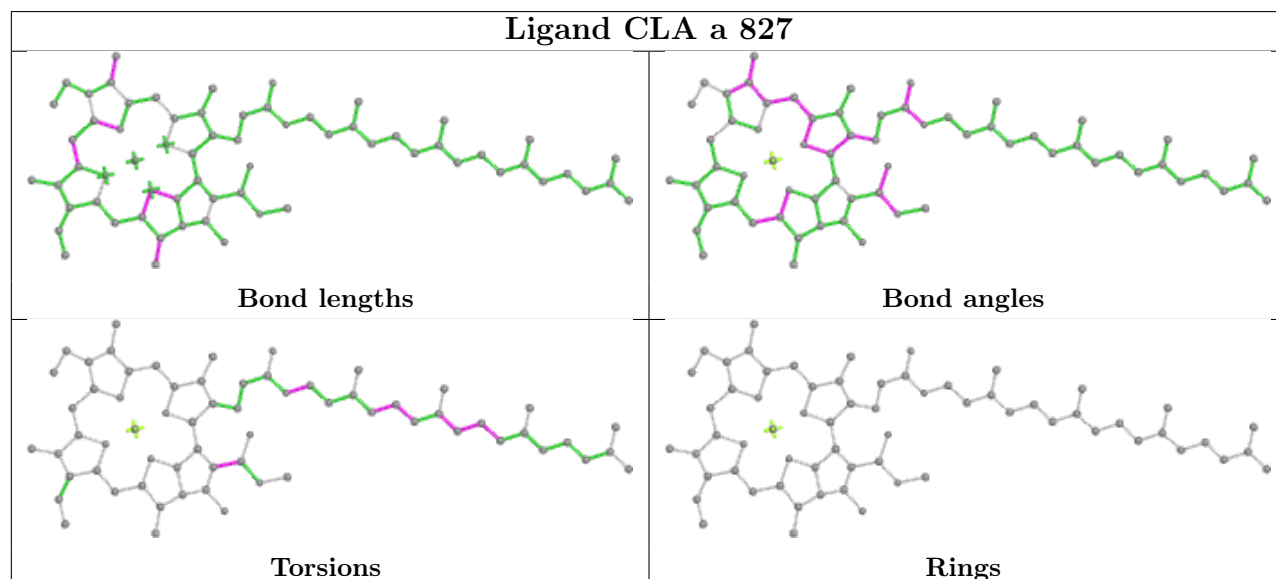


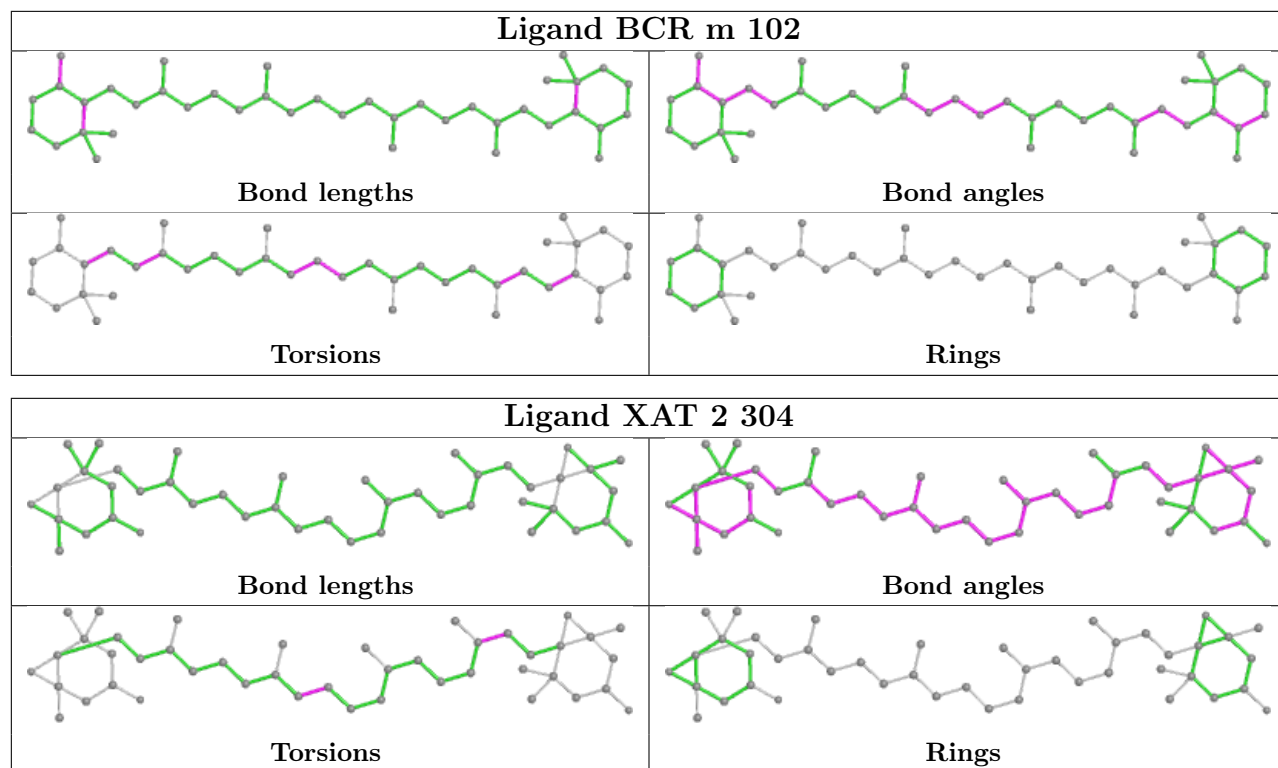
Torsions



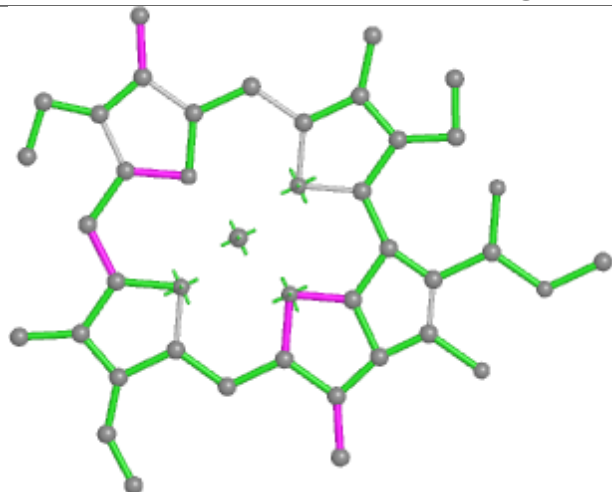
Rings



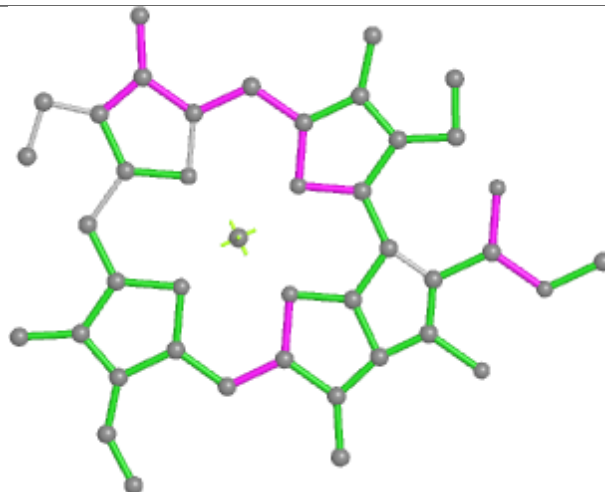
**Ligand CLA a 803****Ligand XAT 1 303****Ligand CLA a 827**



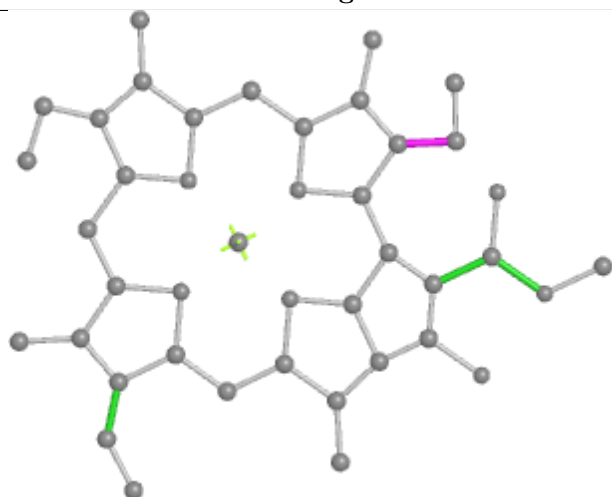
## Ligand CLA 2 315



Bond lengths



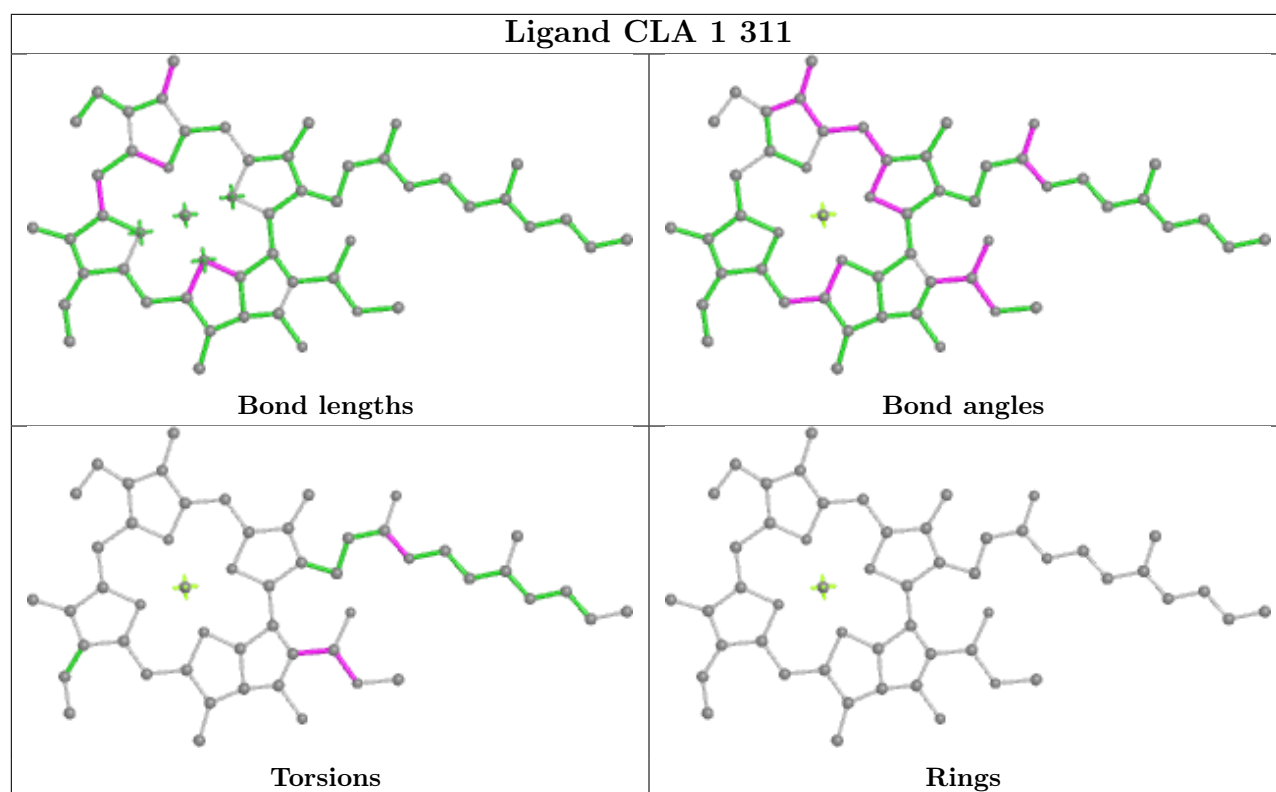
Bond angles



Torsions

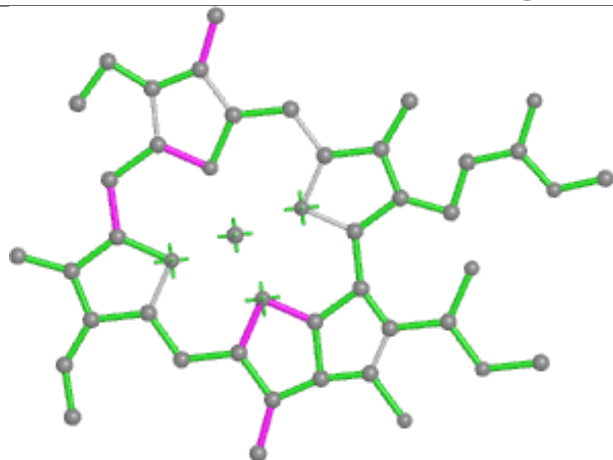


Rings

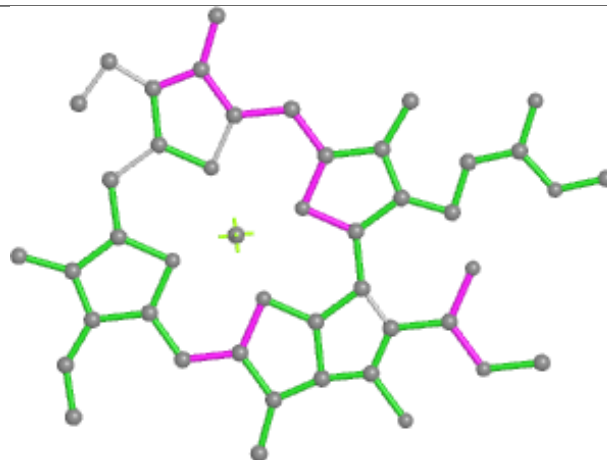




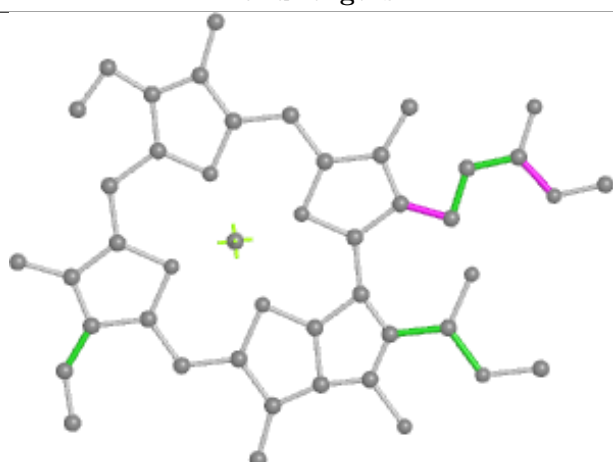
## Ligand CLA 4 311



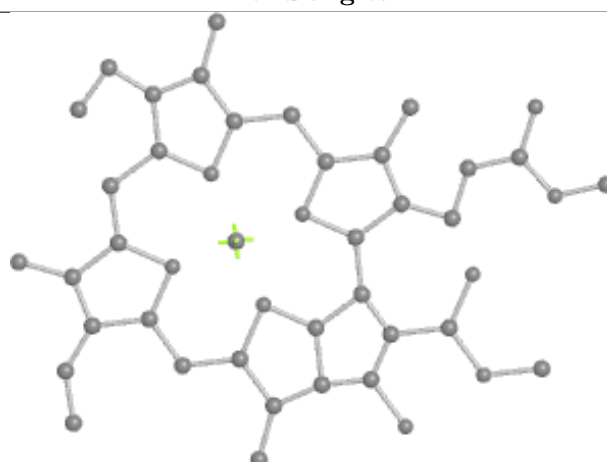
Bond lengths



Bond angles

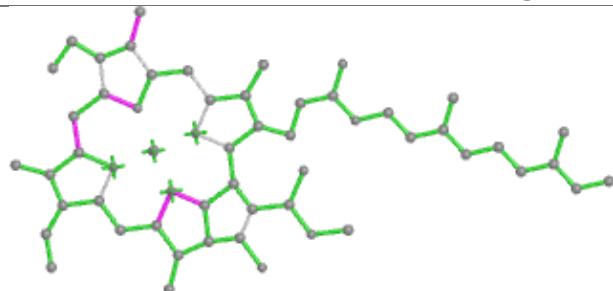


Torsions

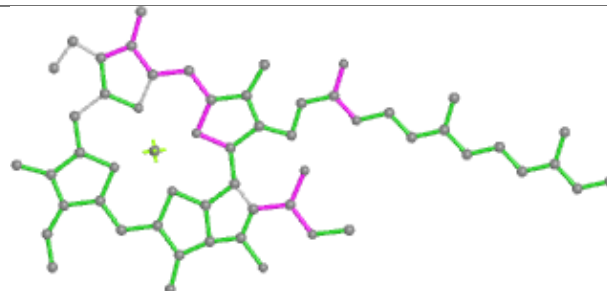


Rings

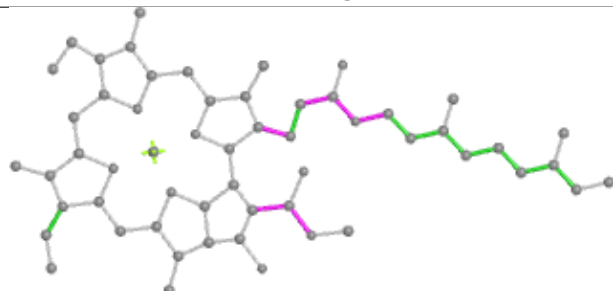
## Ligand CLA a 818



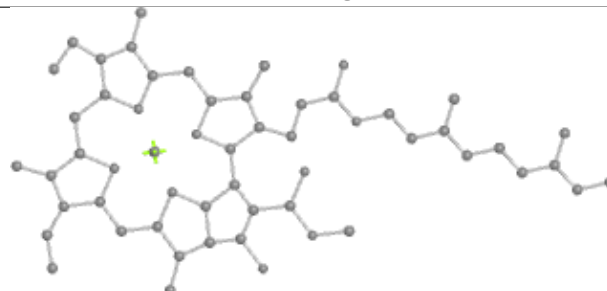
Bond lengths



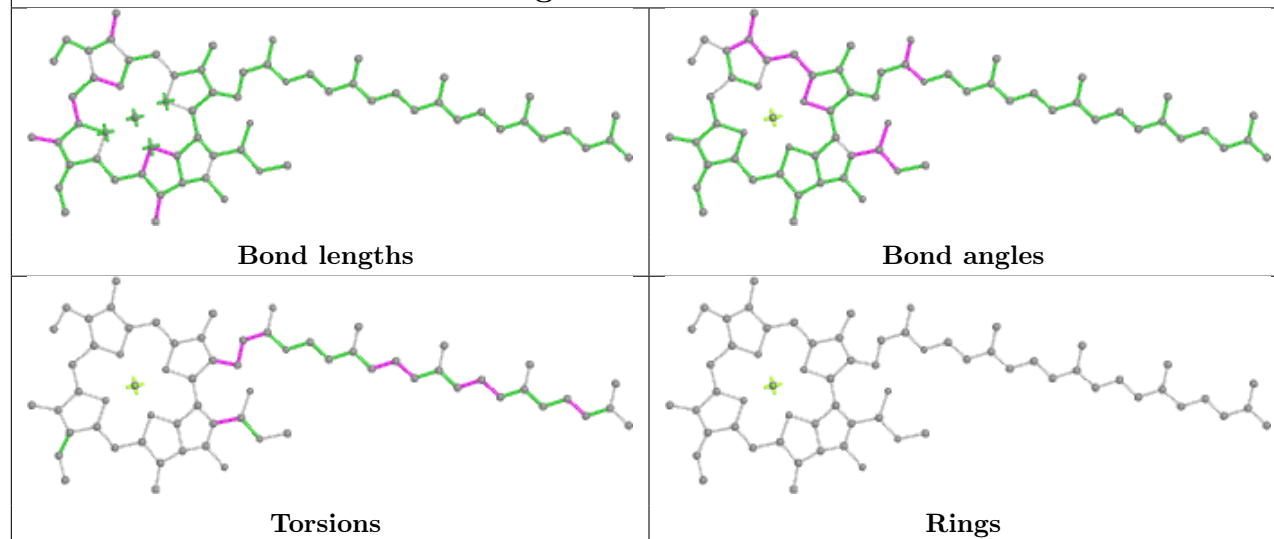
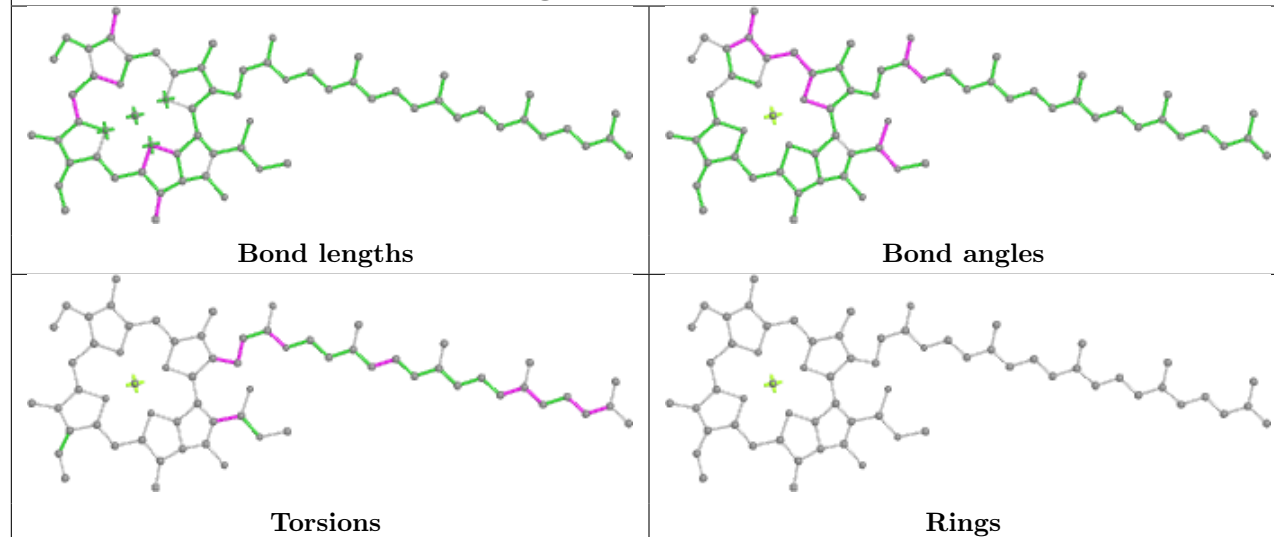
Bond angles



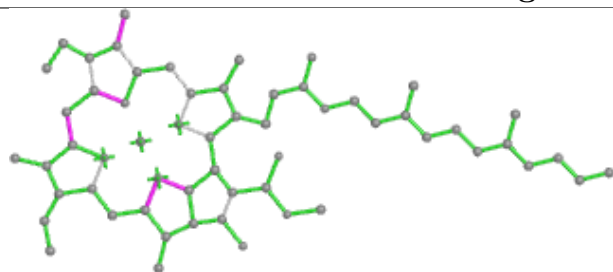
Torsions



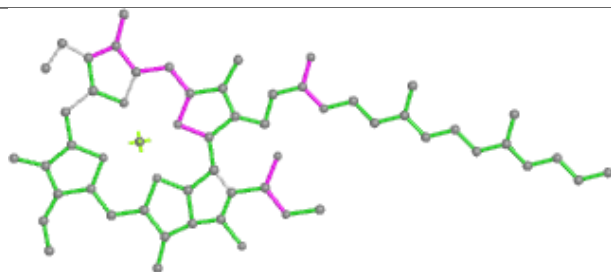
Rings

**Ligand CLA b 808****Ligand CLA 2 310**

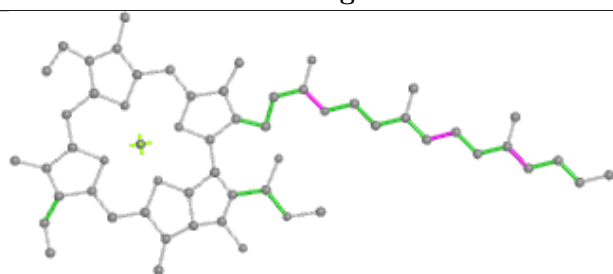
## Ligand CLA 2 311



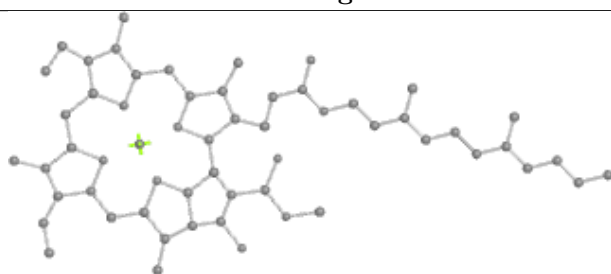
Bond lengths



Bond angles

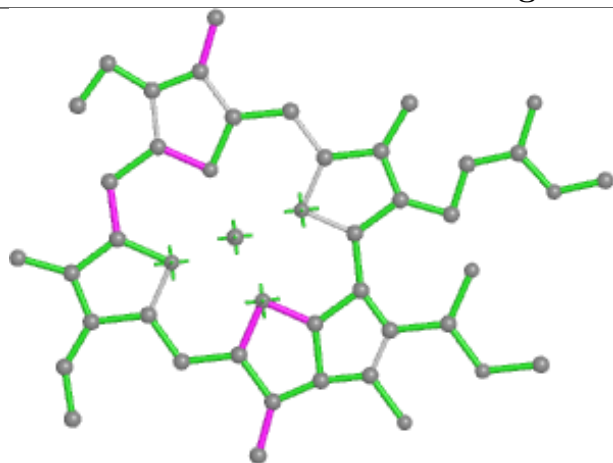


Torsions

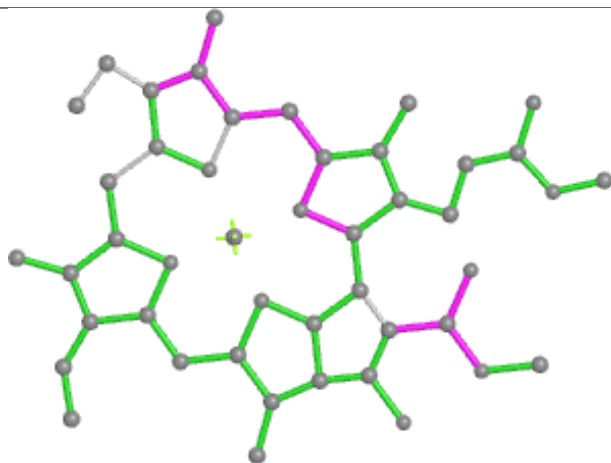


Rings

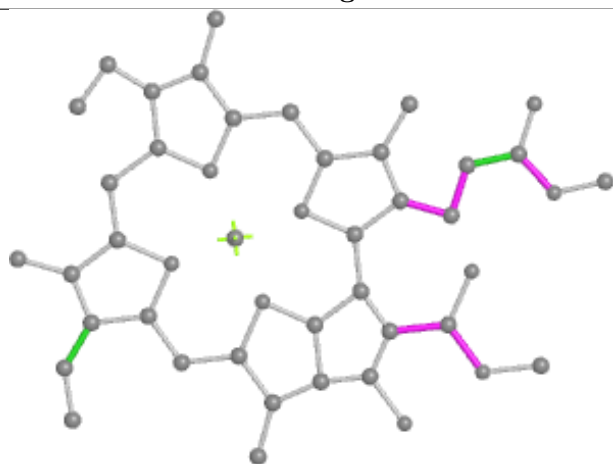
## Ligand CLA 4 310



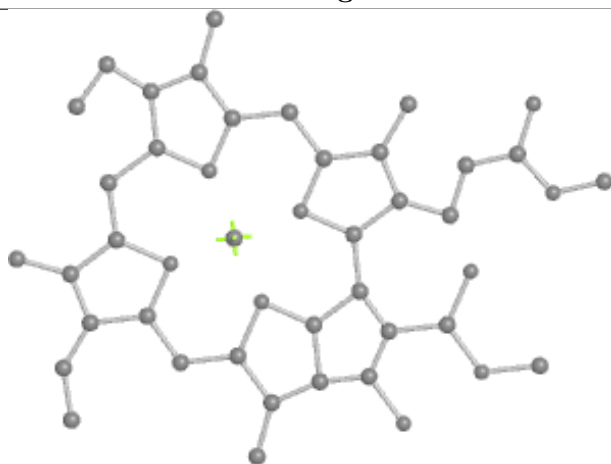
Bond lengths



Bond angles

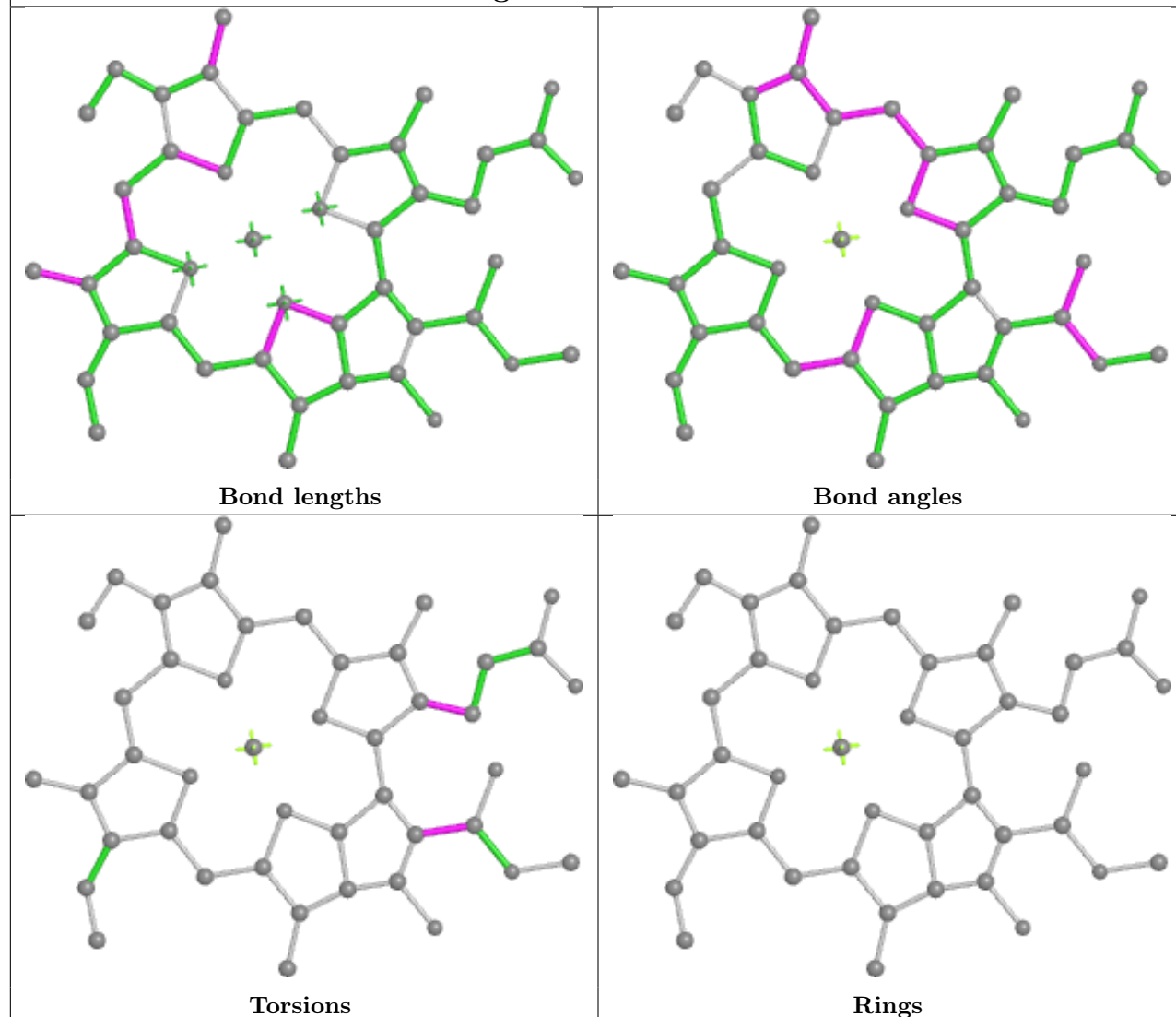


Torsions

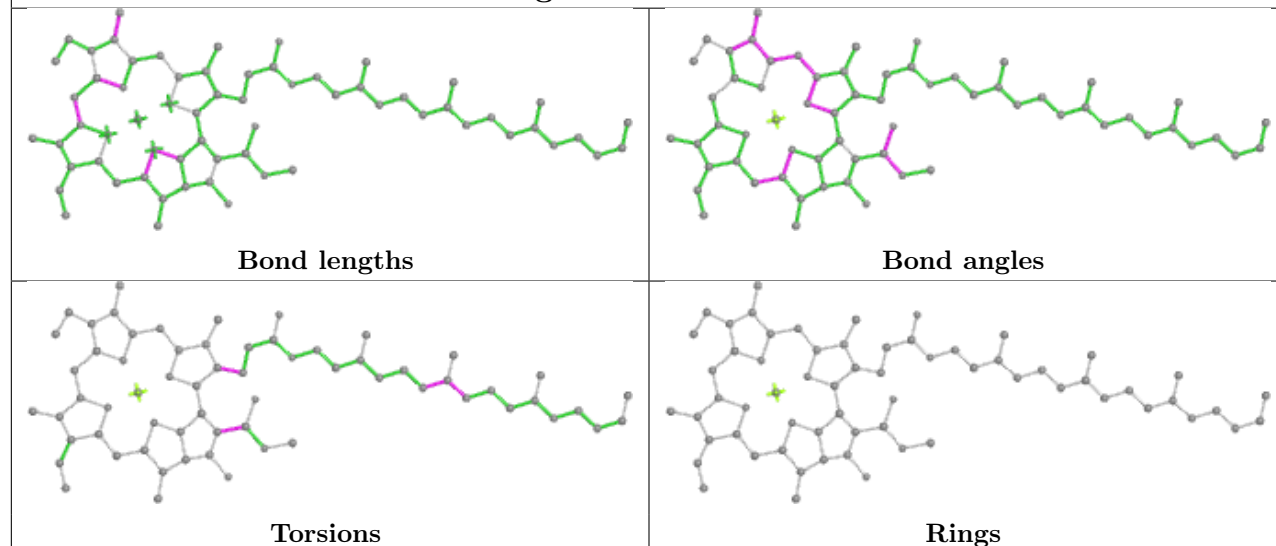


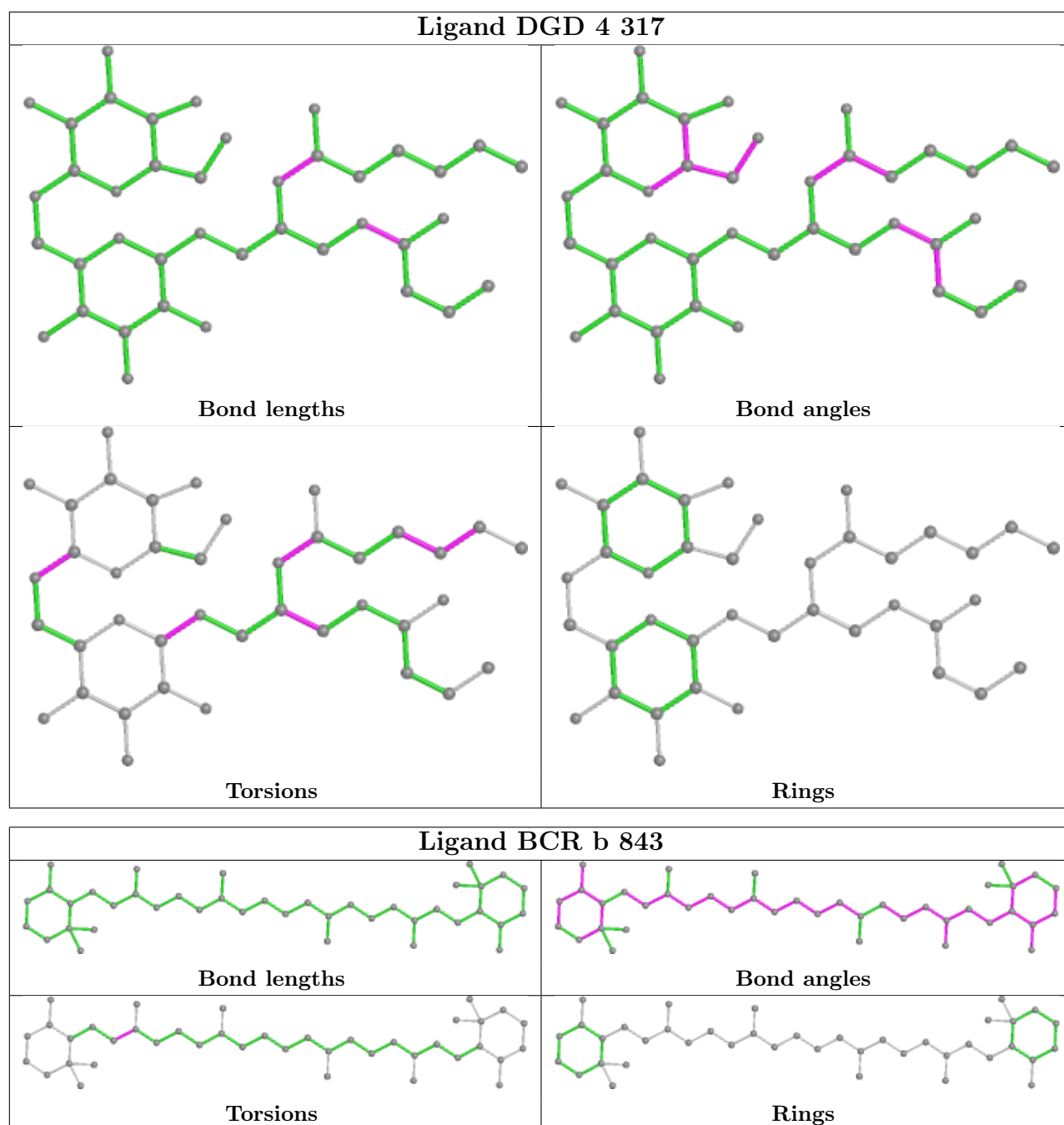
Rings

## Ligand CLA b 815

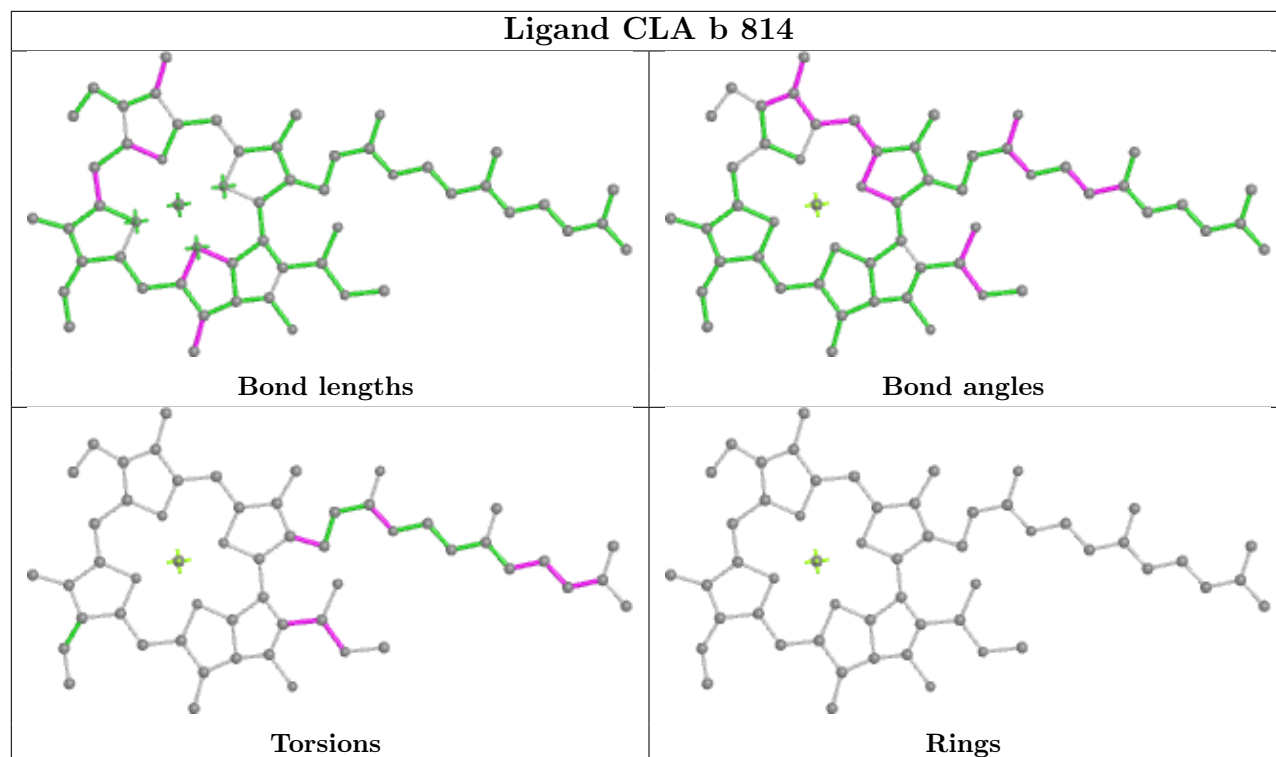


## Ligand CLA b 825

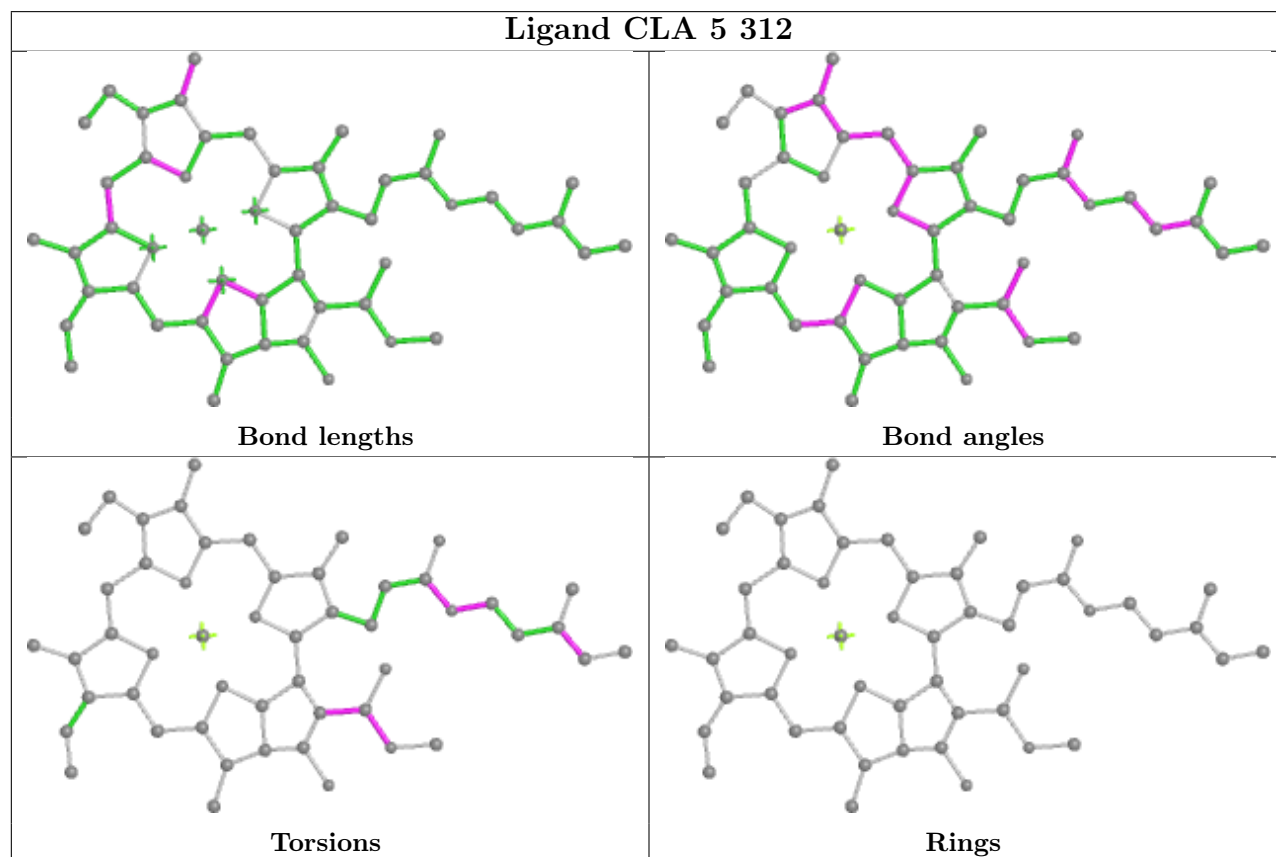




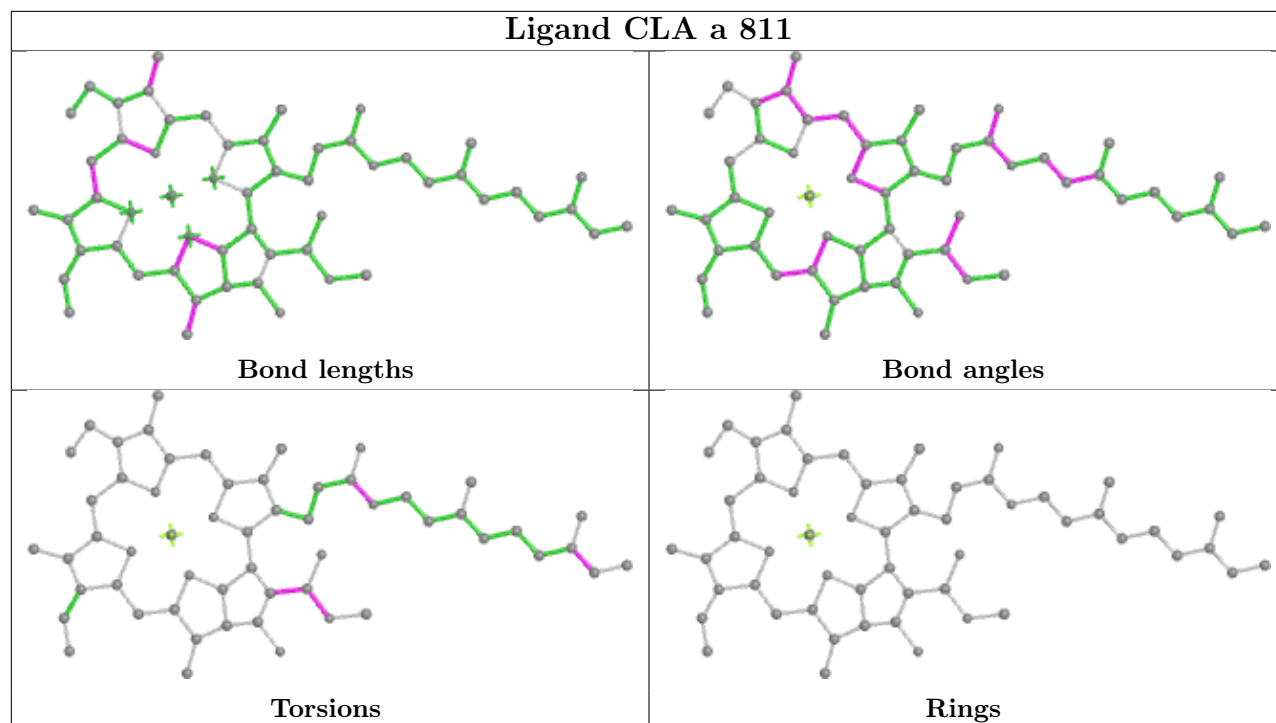
## Ligand CLA b 814



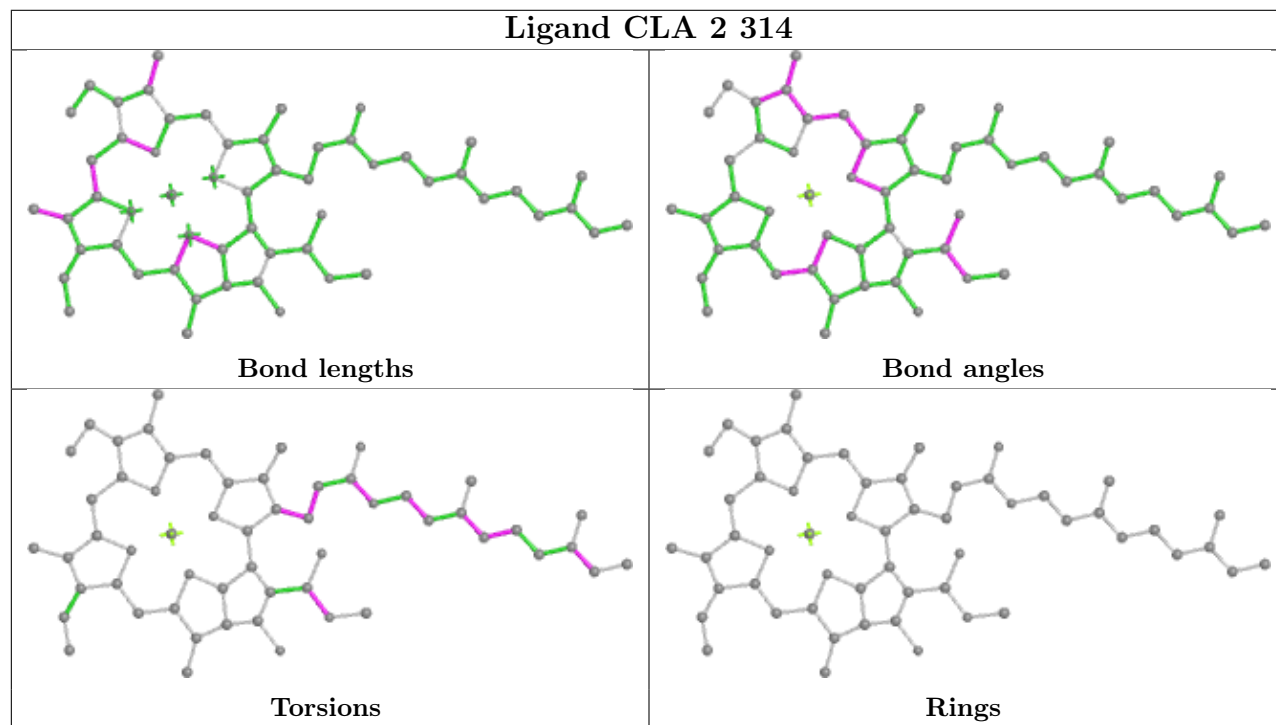
## Ligand CLA 5 312

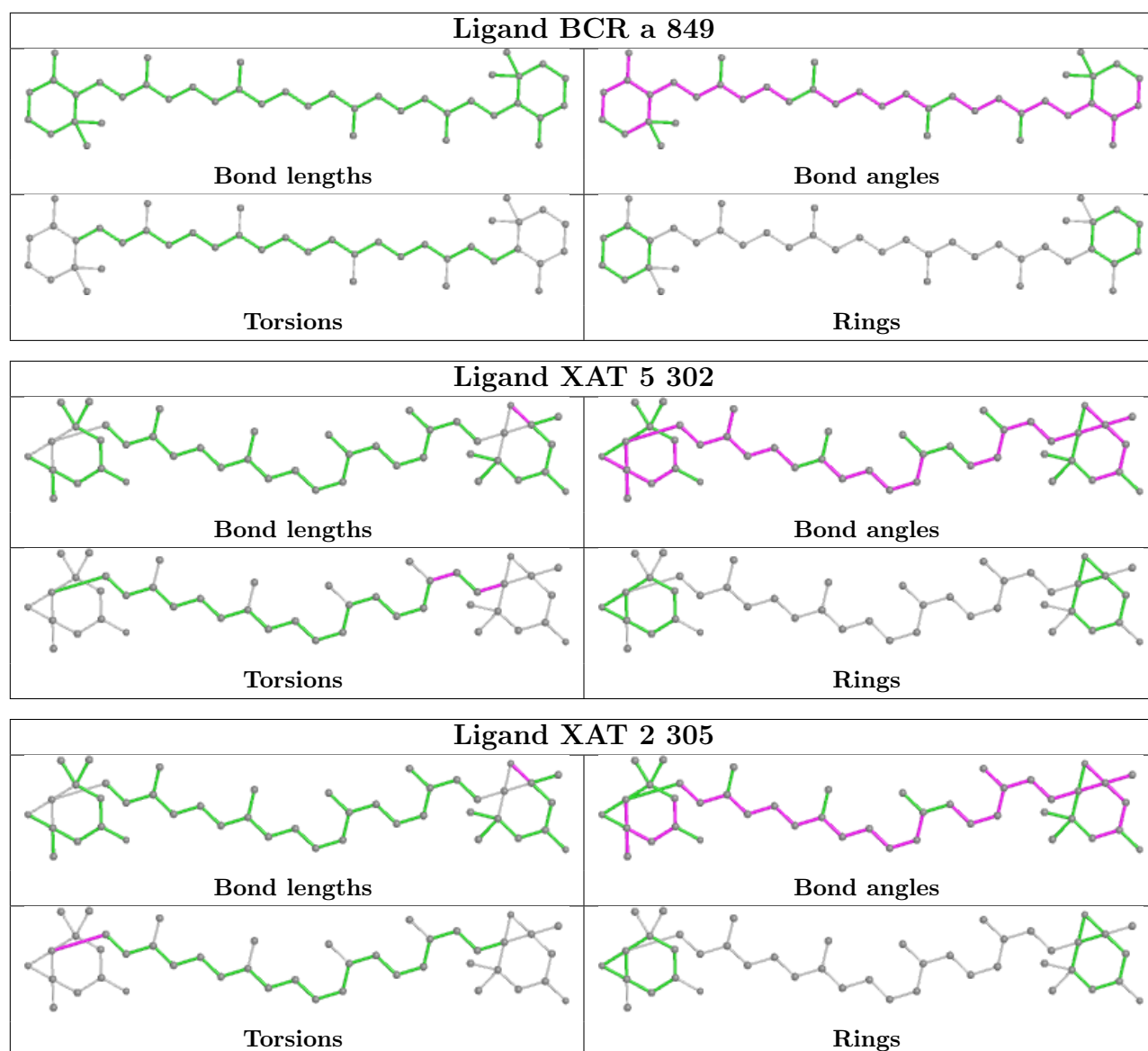


## Ligand CLA a 811



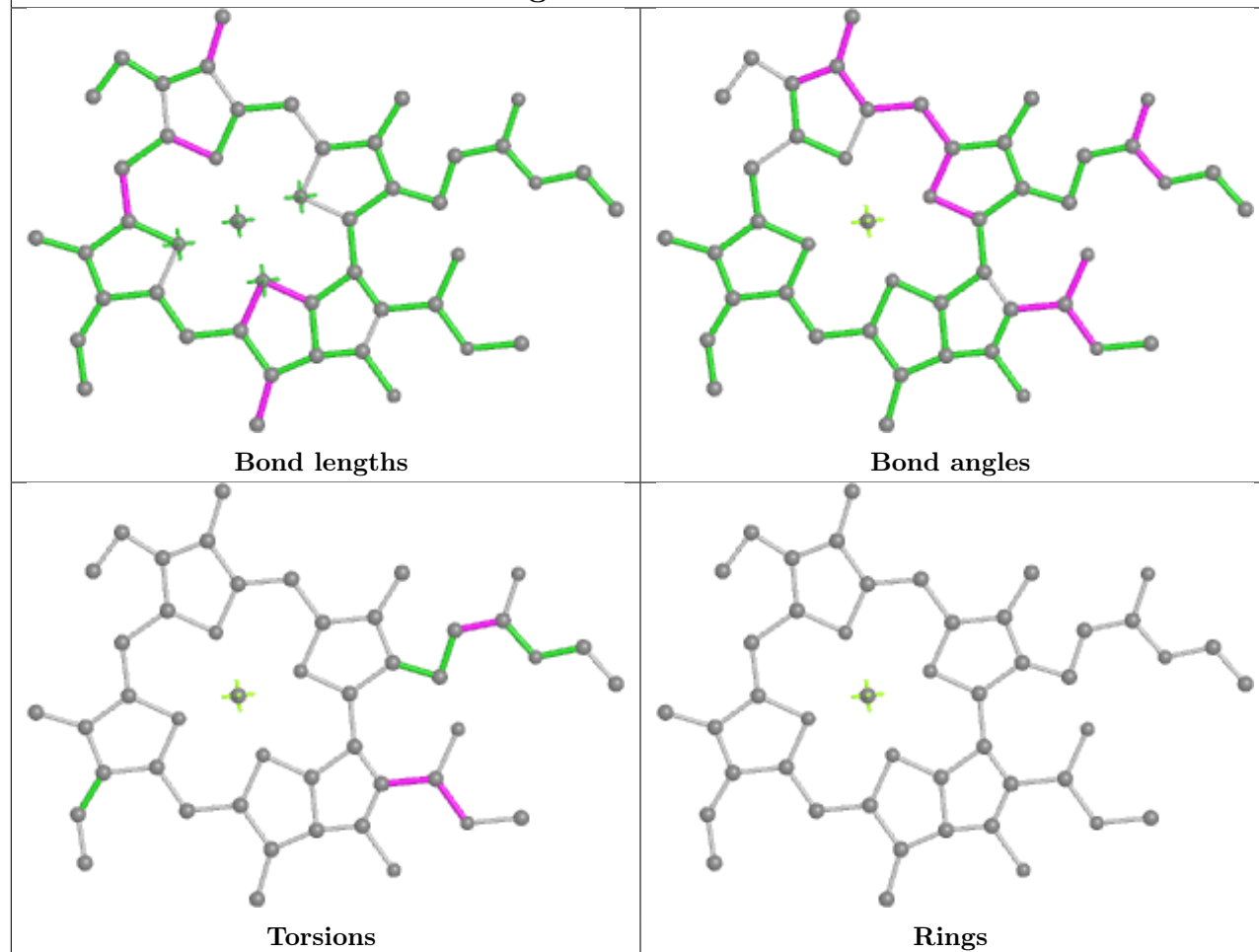
## Ligand CLA 2 314



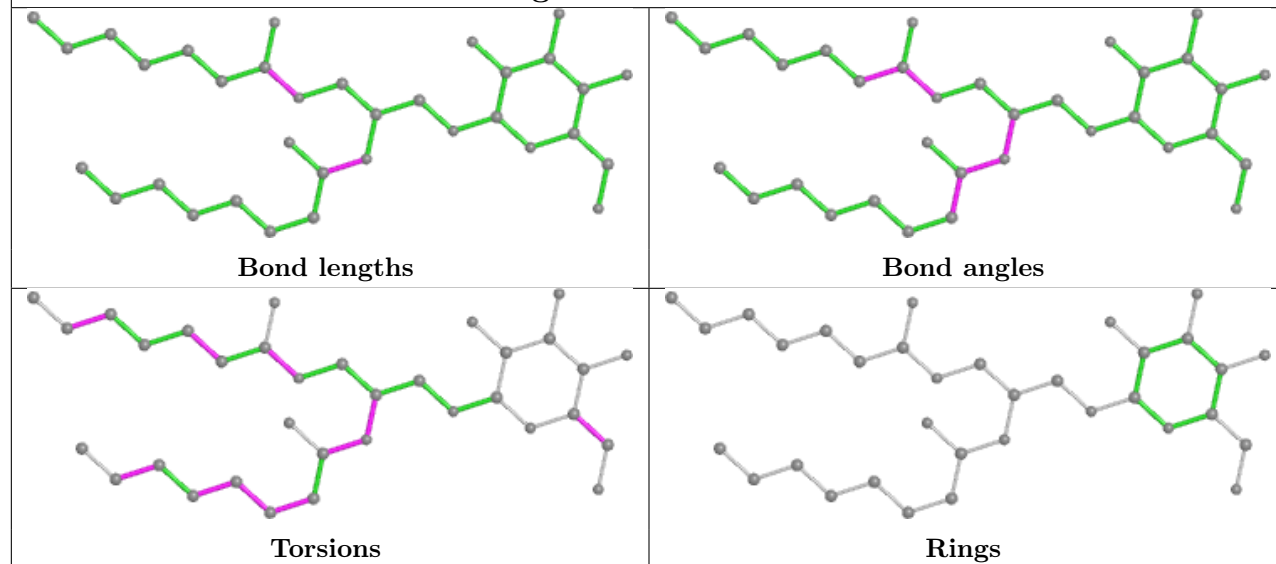




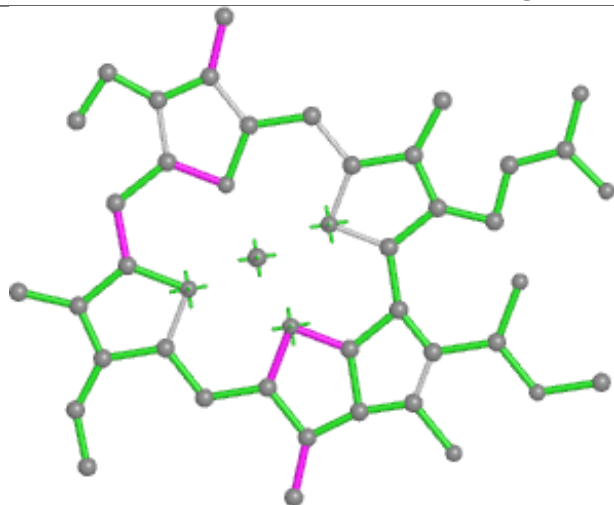
## Ligand CLA 3 308



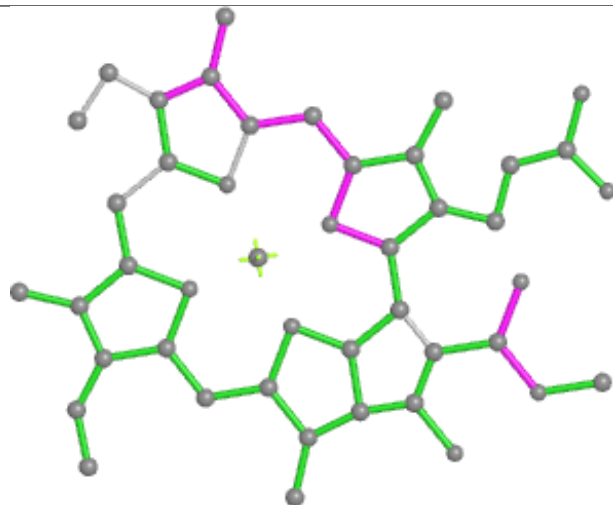
## Ligand LMG a 855



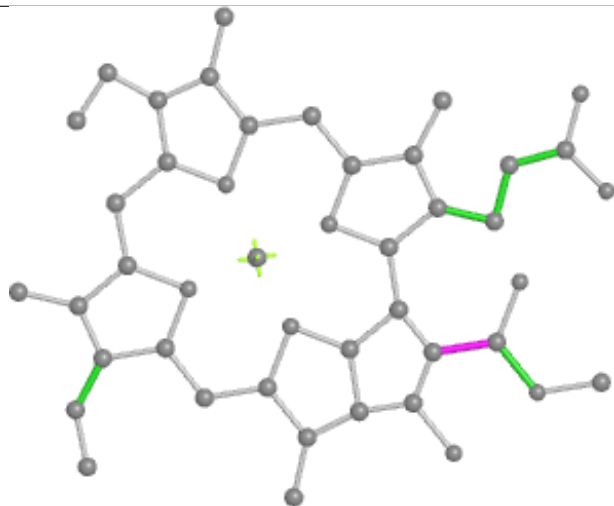
## Ligand CLA 3 307



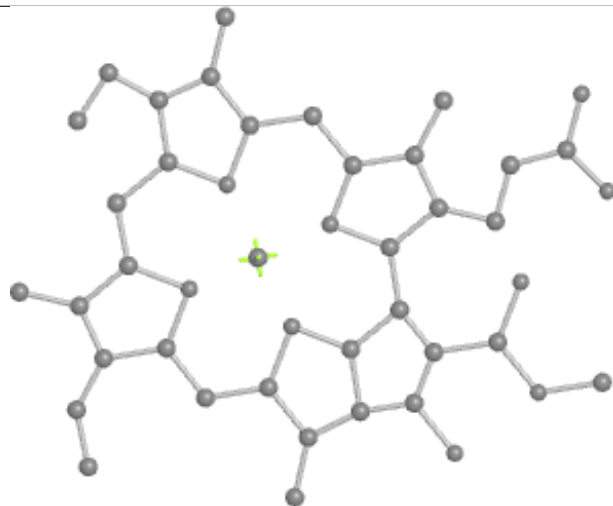
Bond lengths



Bond angles

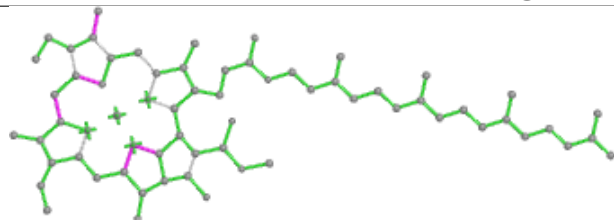


Torsions

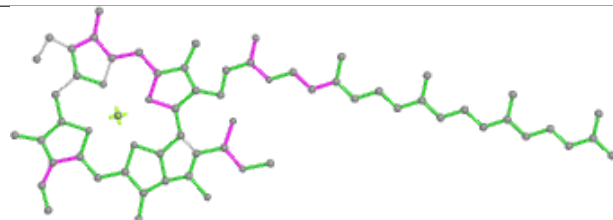


Rings

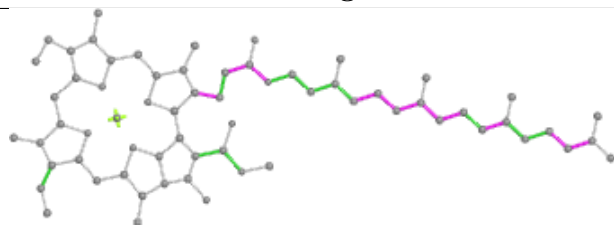
## Ligand CLA 1 306



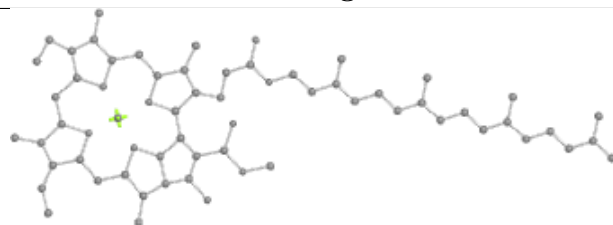
Bond lengths



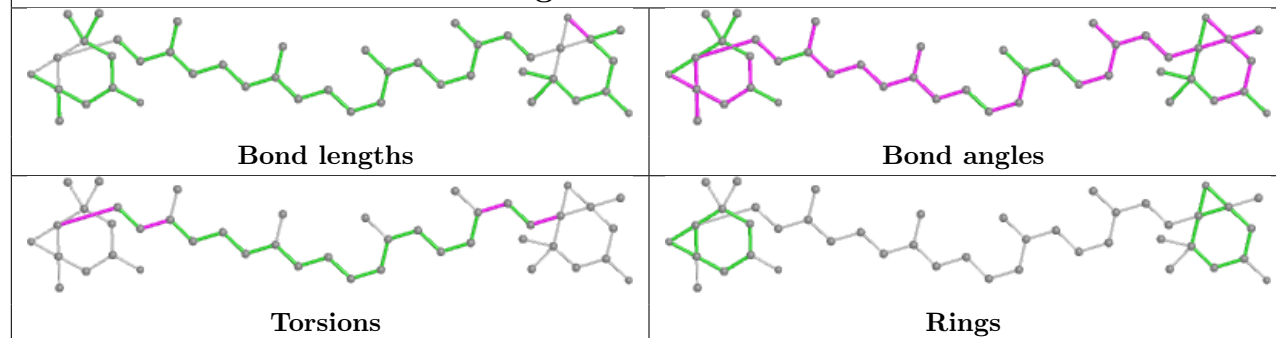
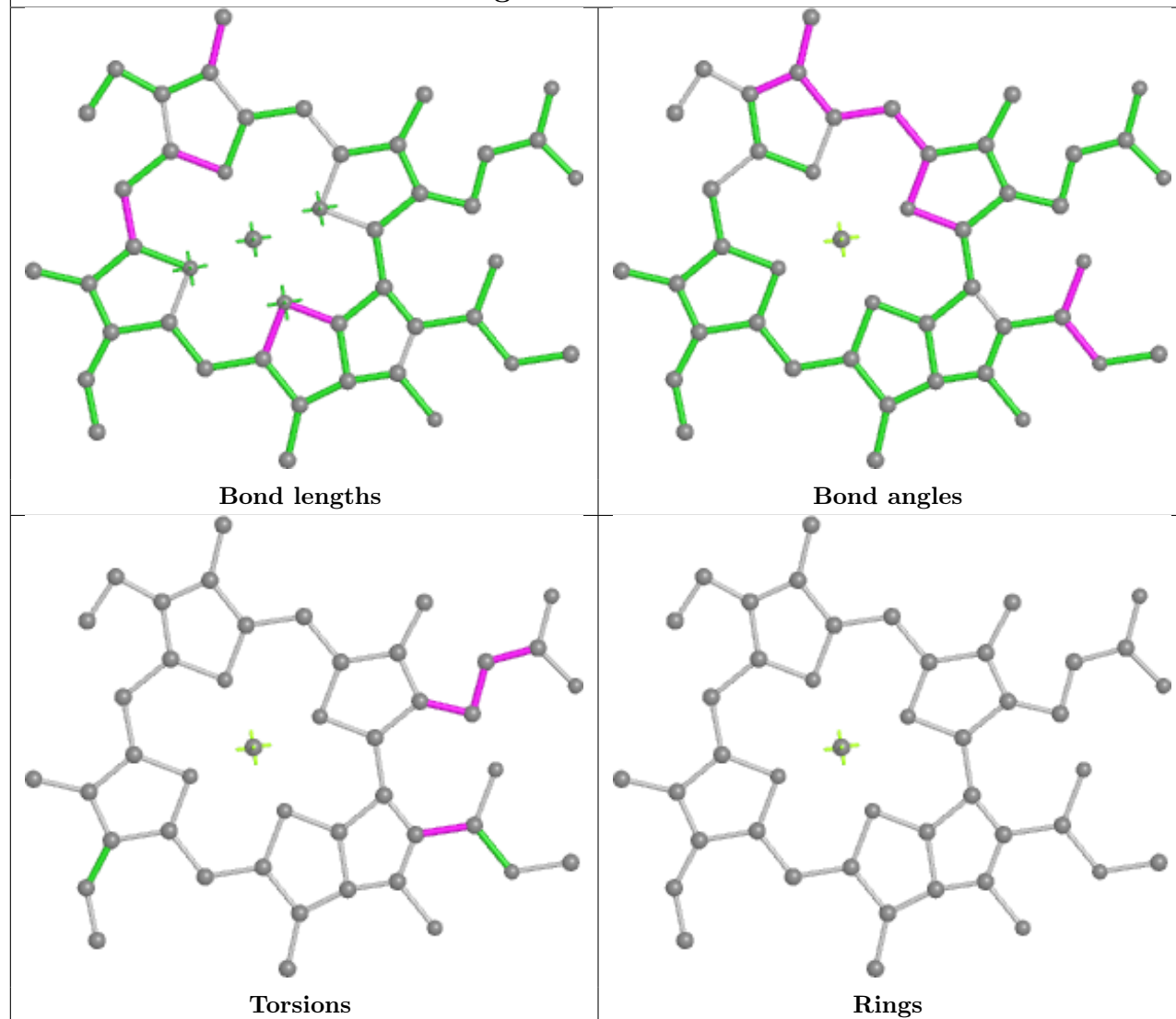
Bond angles



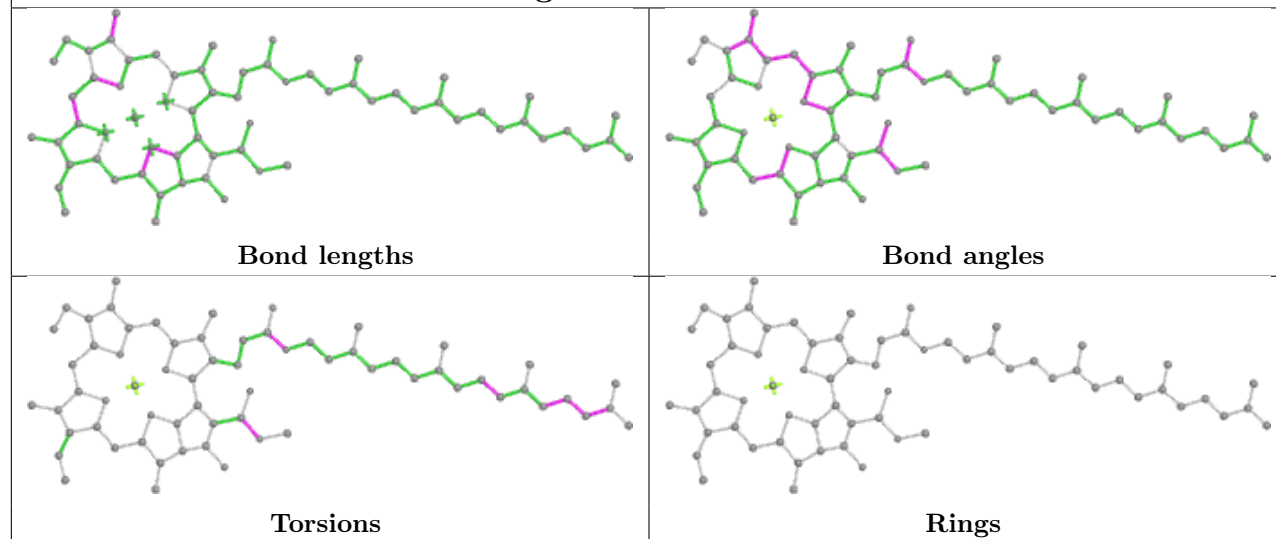
Torsions



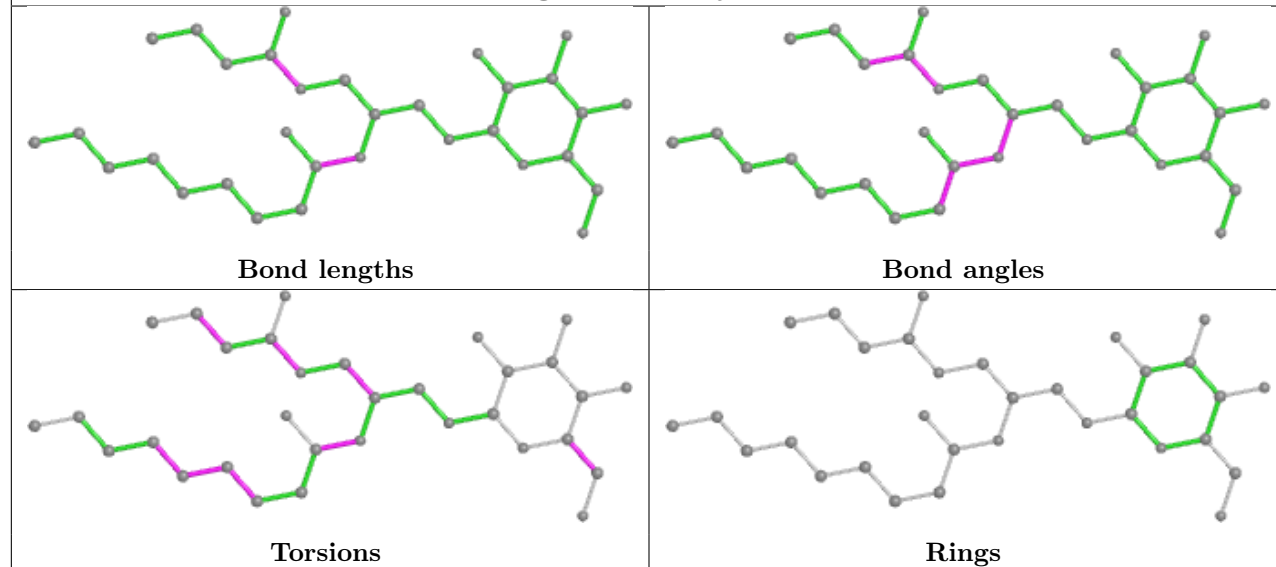
Rings

**Ligand XAT 2 303****Ligand CLA a 817**

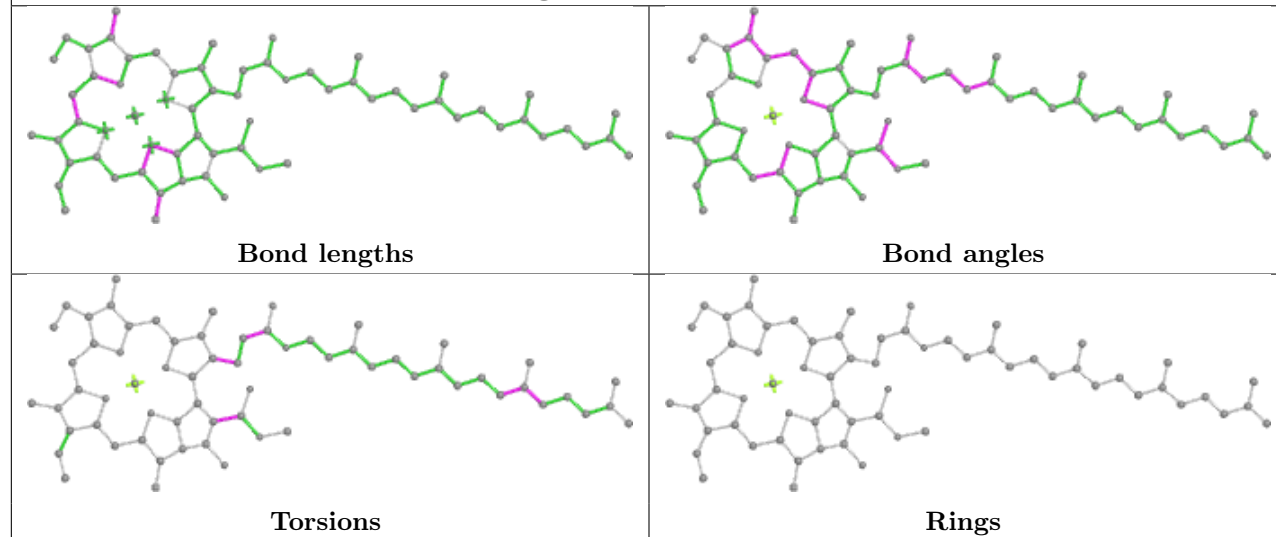
## Ligand CLA b 841

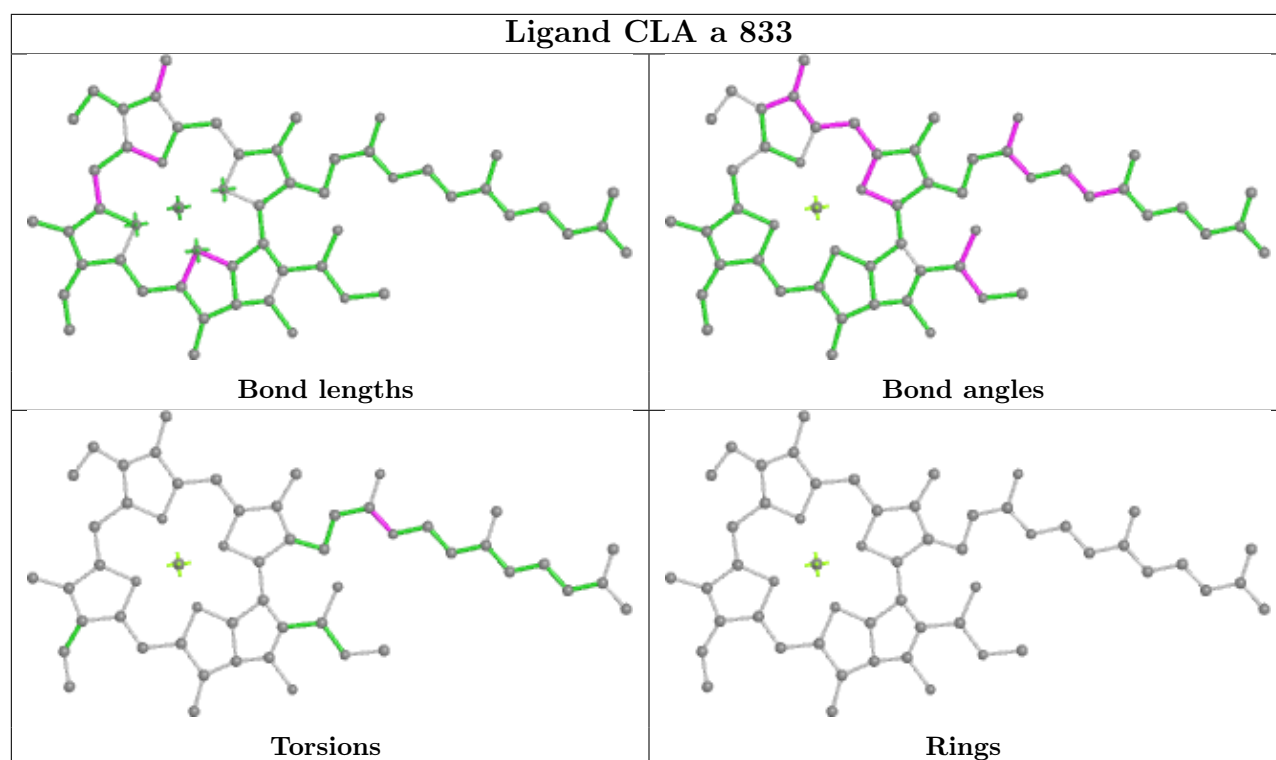


## Ligand LMG j 103

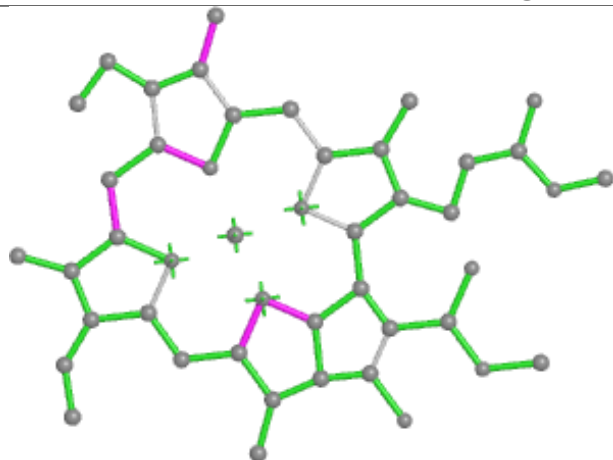


## Ligand CLA b 838

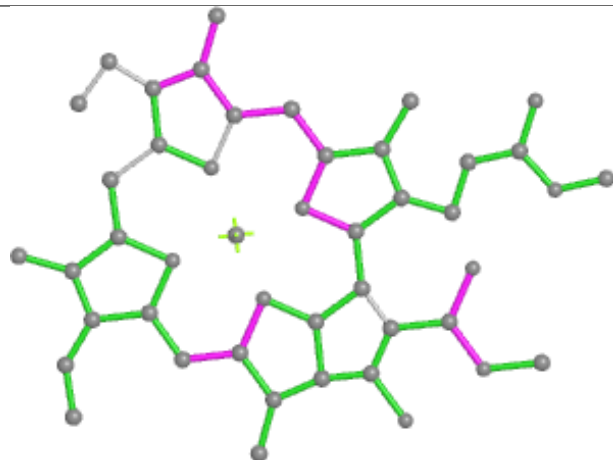




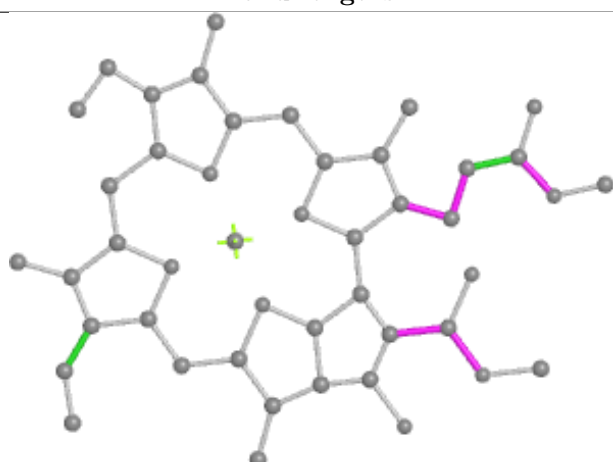
## Ligand CLA 4 315



Bond lengths



Bond angles

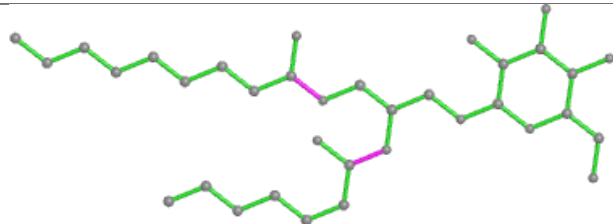


Torsions

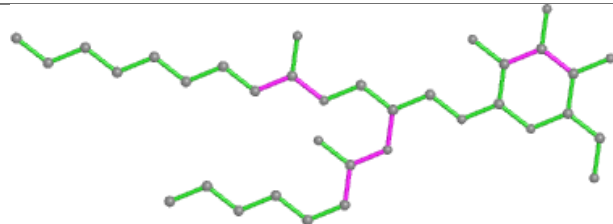


Rings

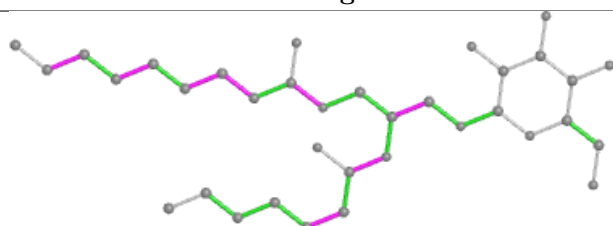
## Ligand LMG 2 317



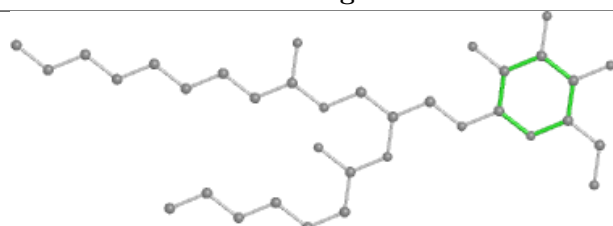
Bond lengths



Bond angles

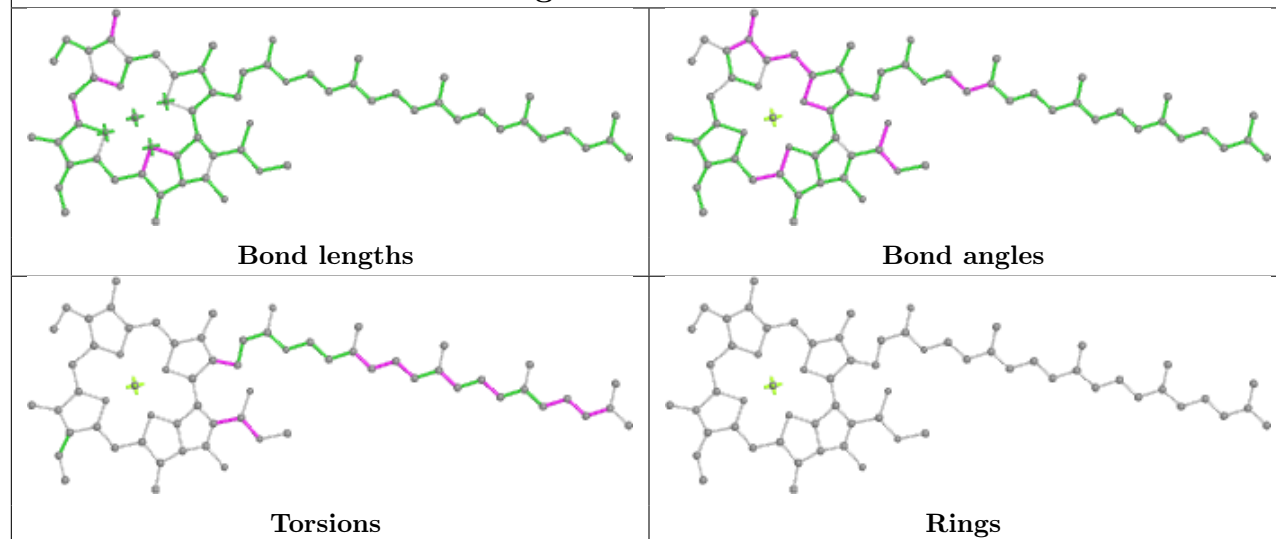


Torsions

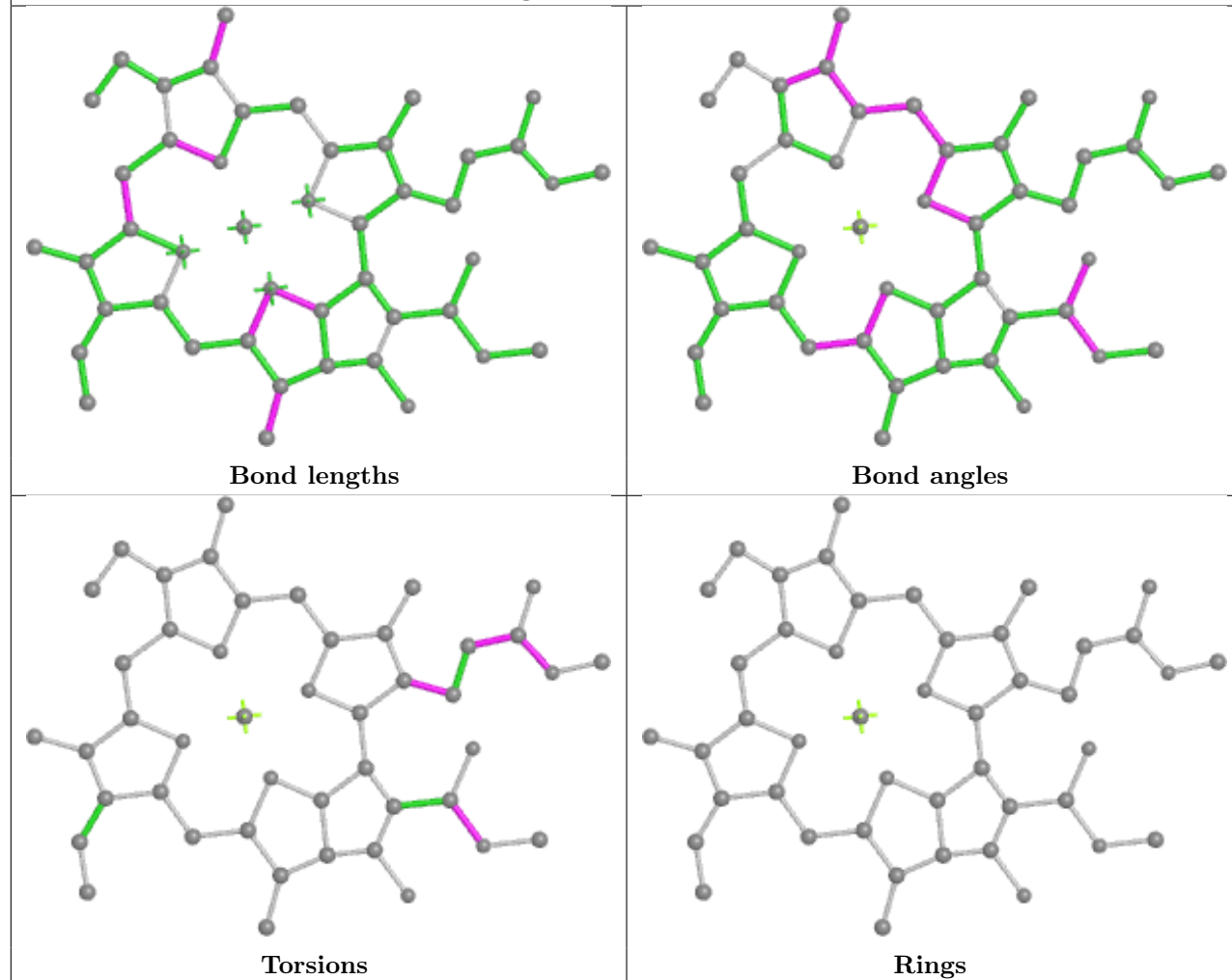


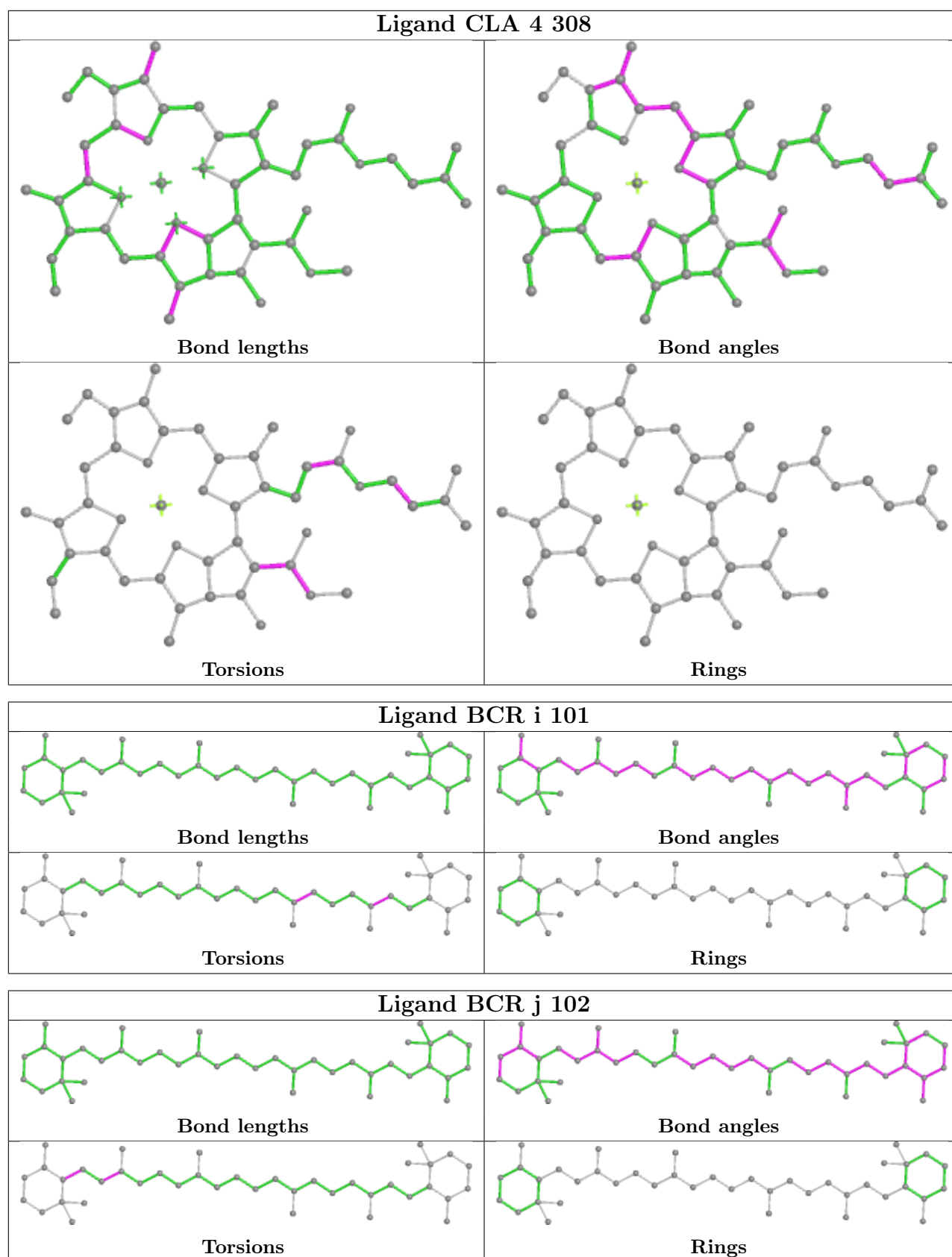
Rings

## Ligand CLA b 813

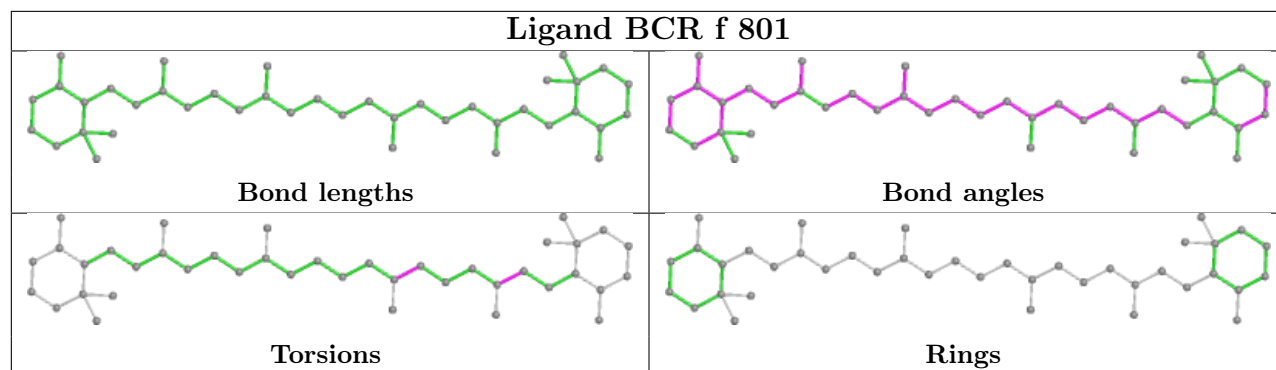
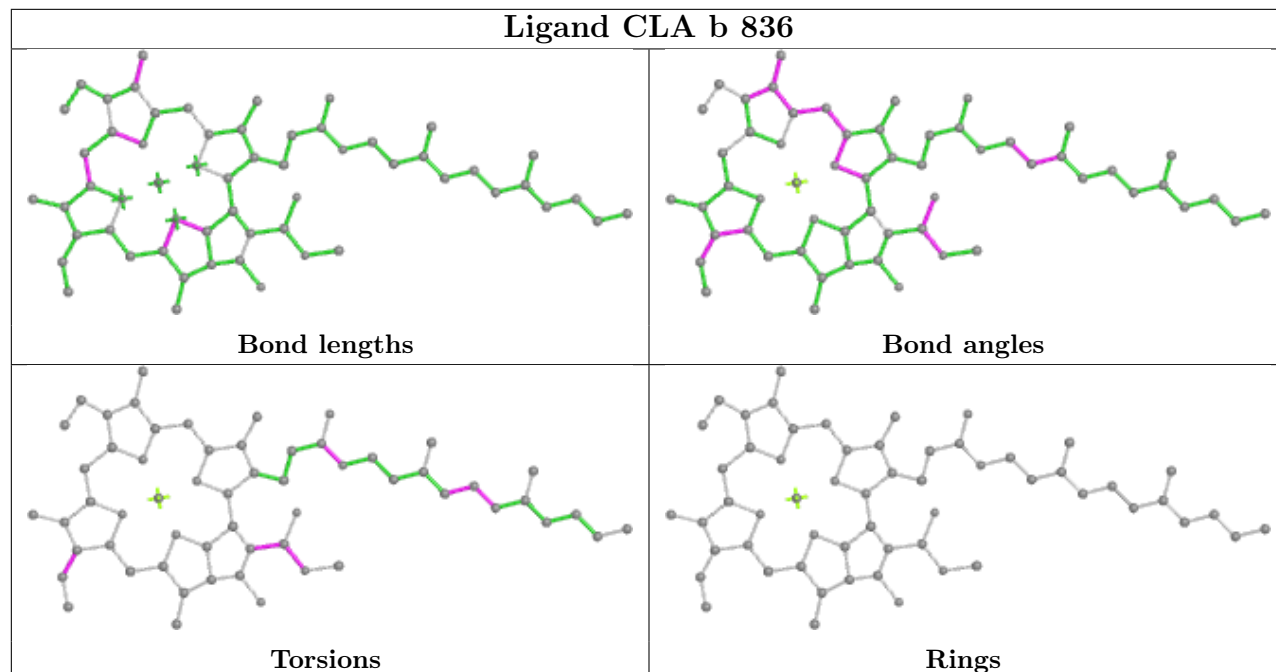
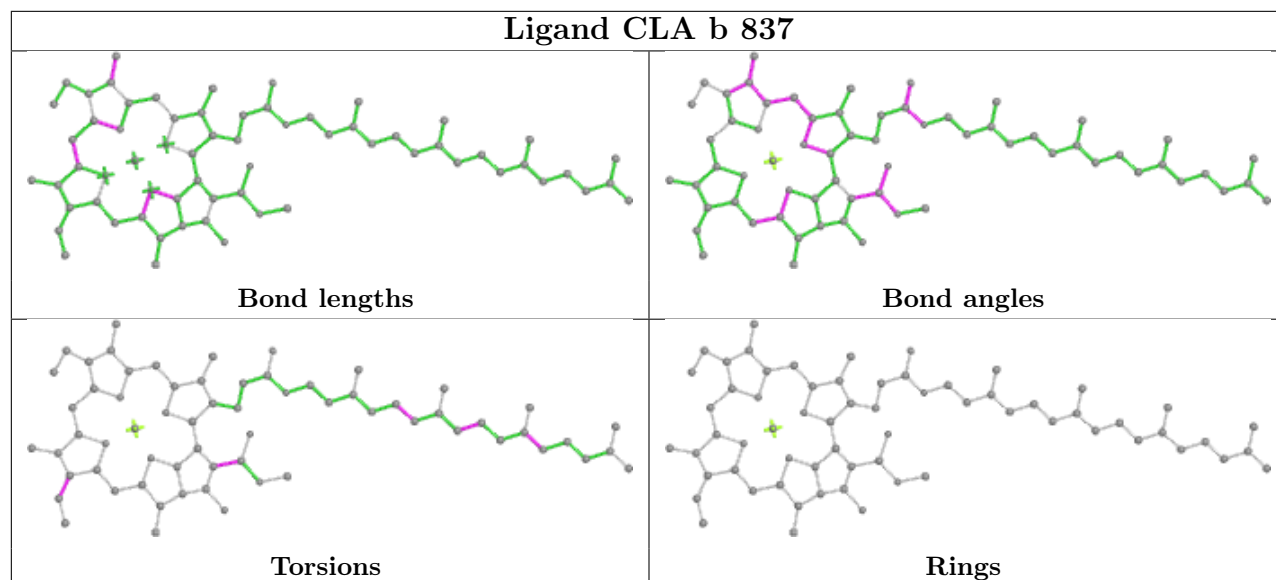


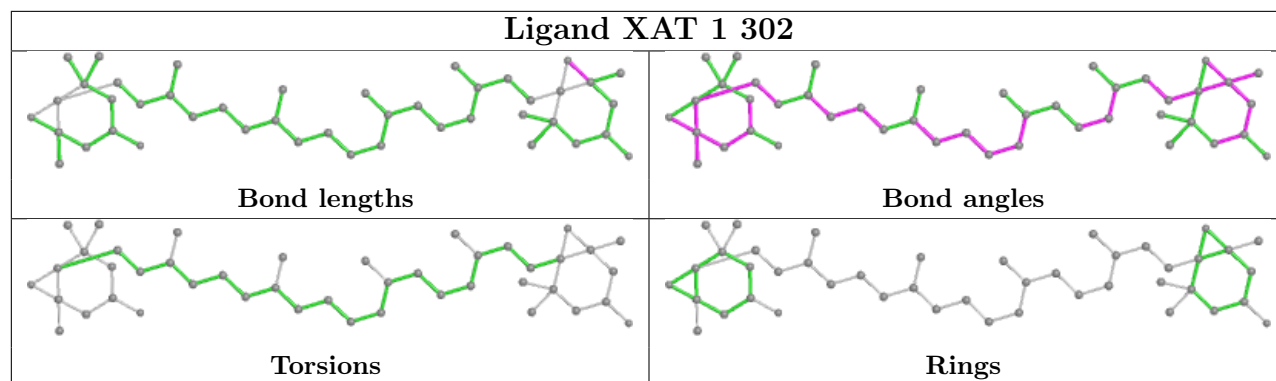
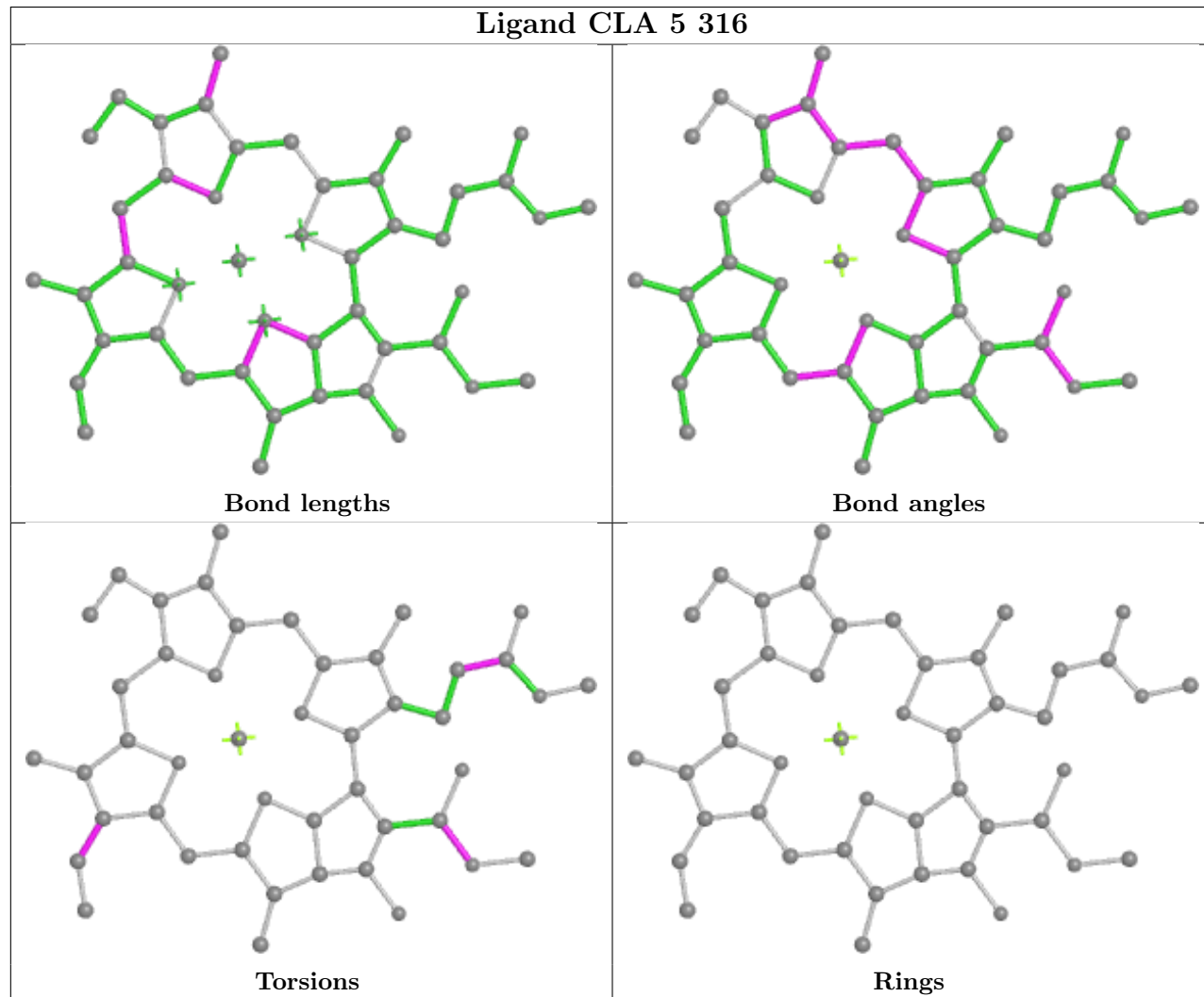
## Ligand CLA 3 315

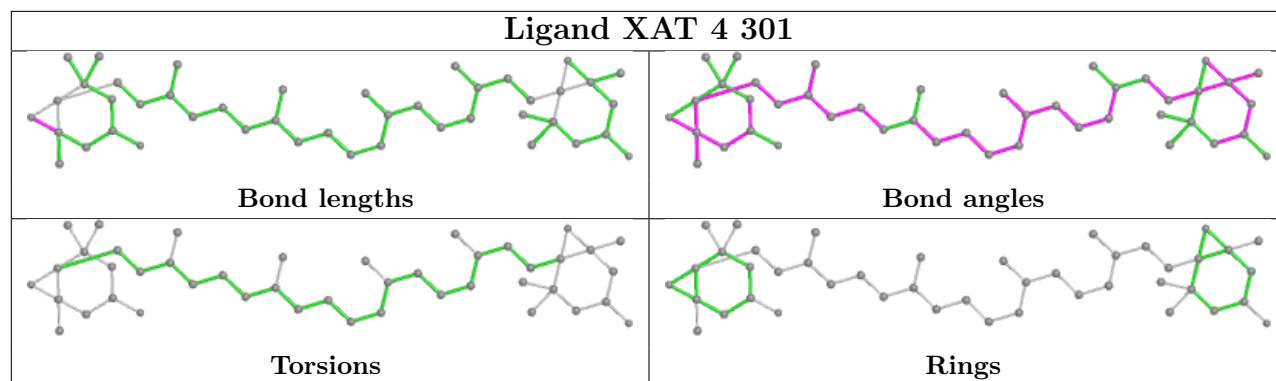
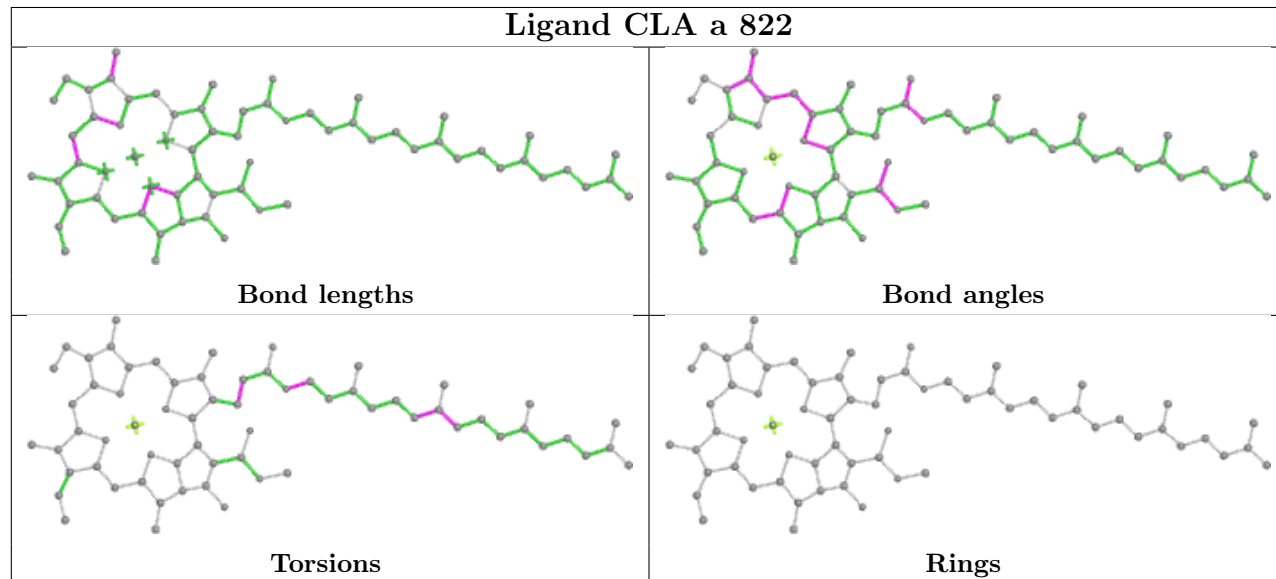




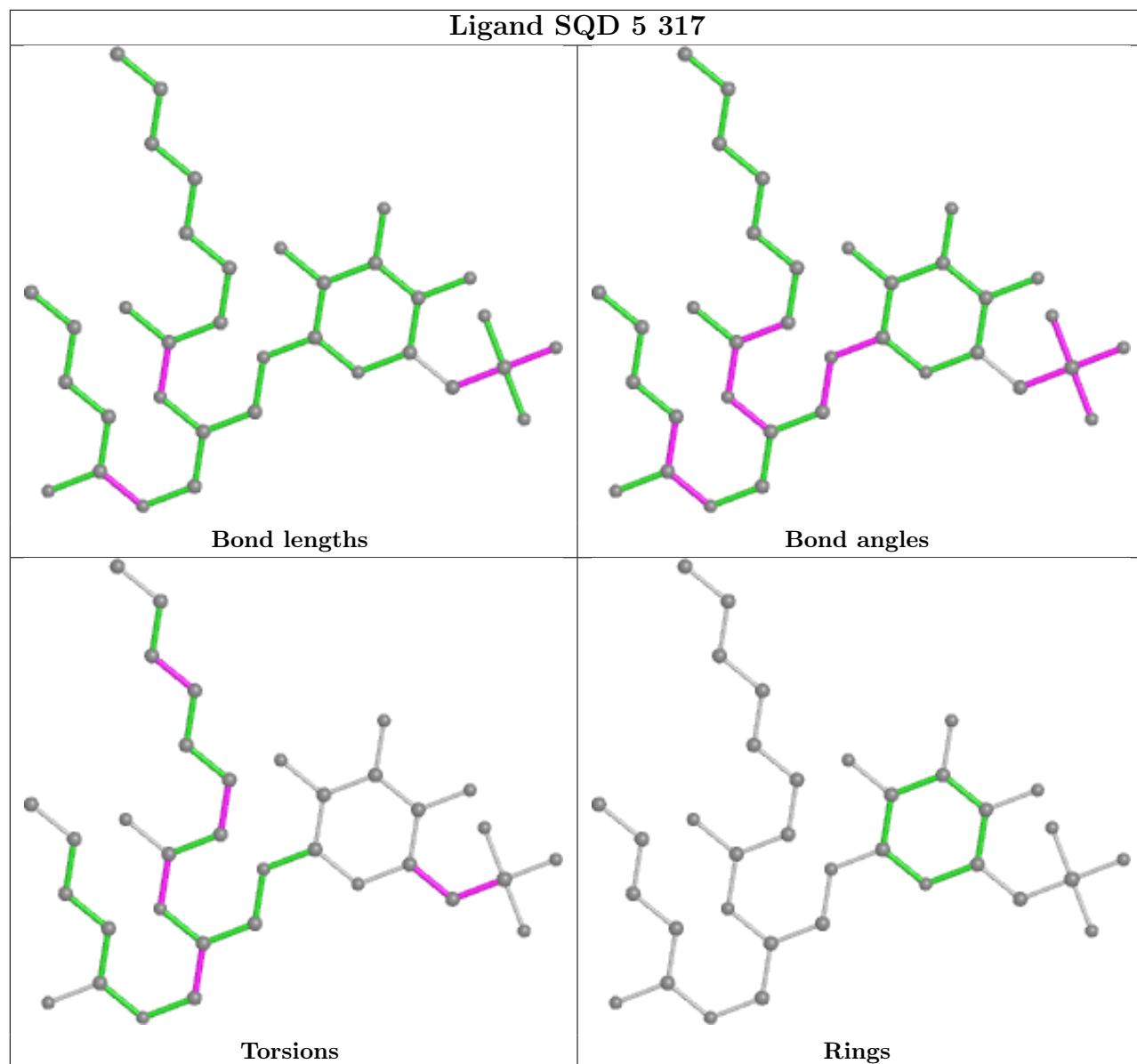


**Ligand BCR f 801****Ligand CLA b 836****Ligand CLA b 837**

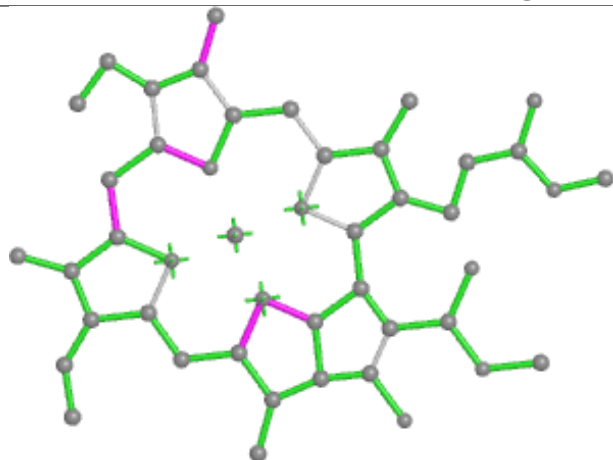
**Ligand XAT 1 302****Ligand CLA 5 316**

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

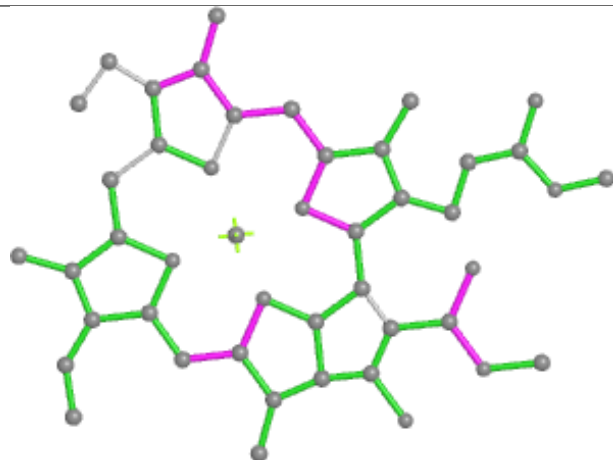
## Ligand SQD 5 317



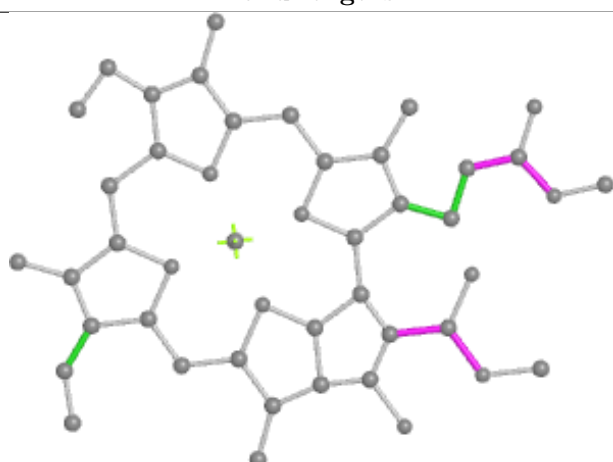
## Ligand CLA 1 309



Bond lengths



Bond angles

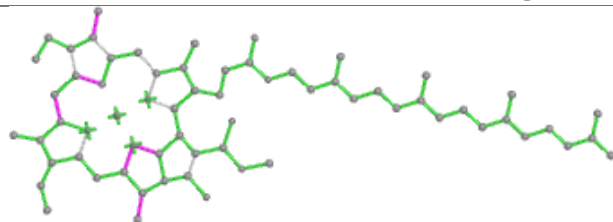


Torsions

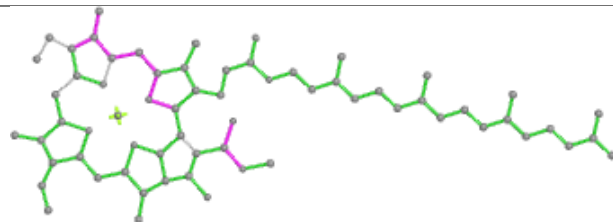


Rings

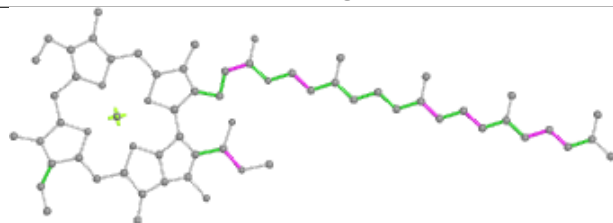
## Ligand CLA a 826



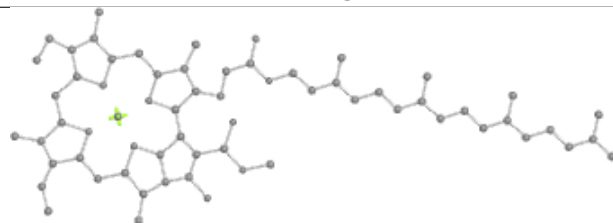
Bond lengths



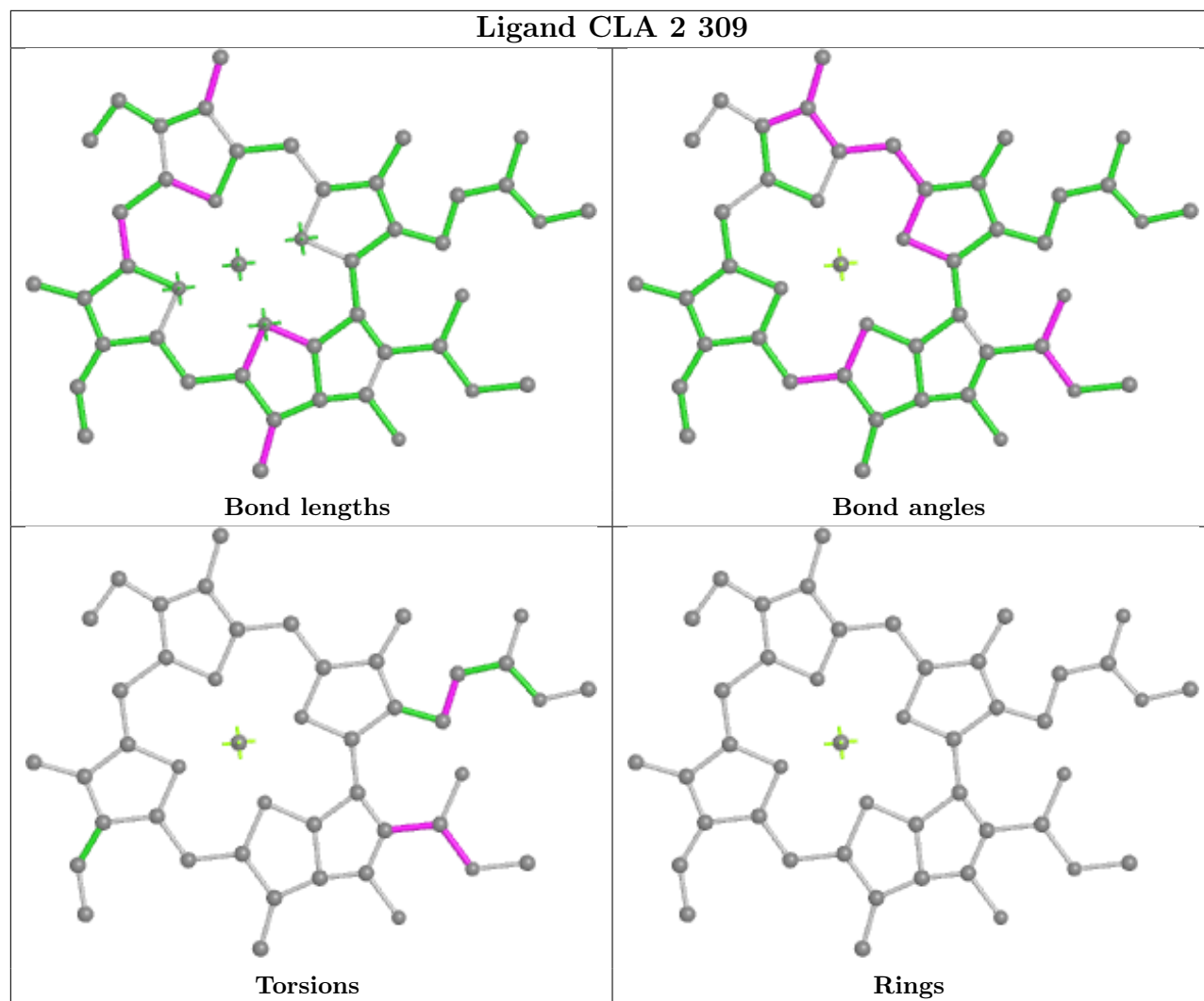
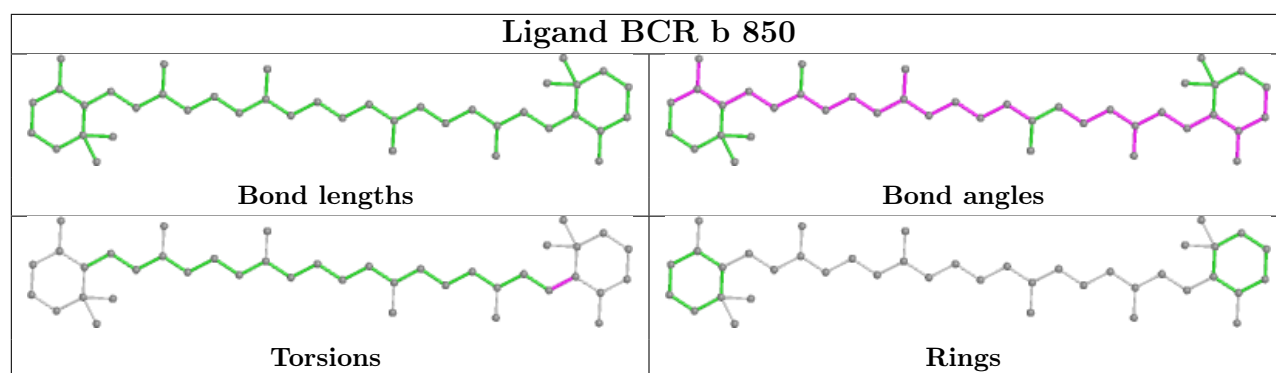
Bond angles



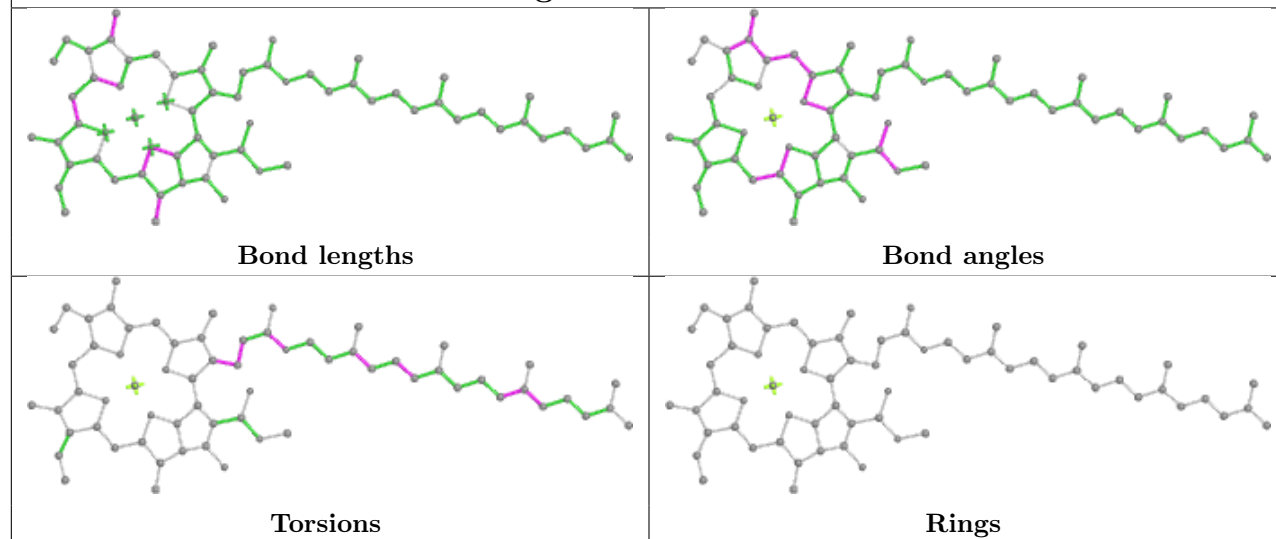
Torsions



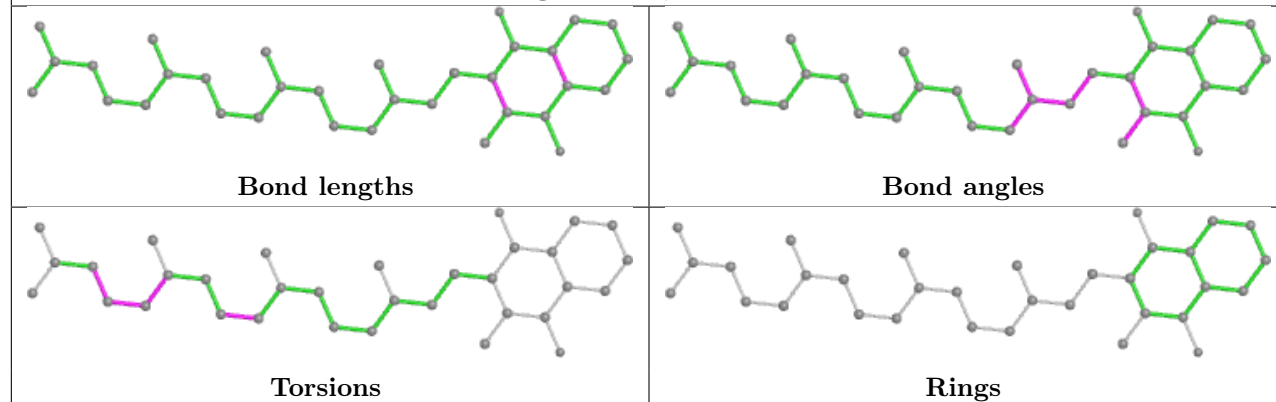
Rings



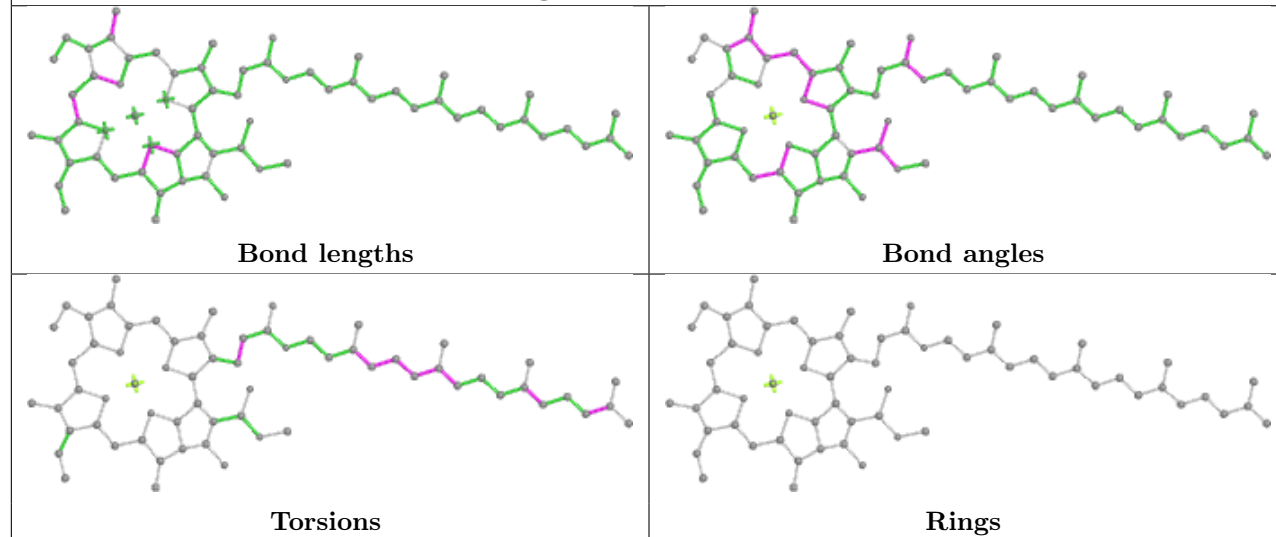
## Ligand CLA b 828



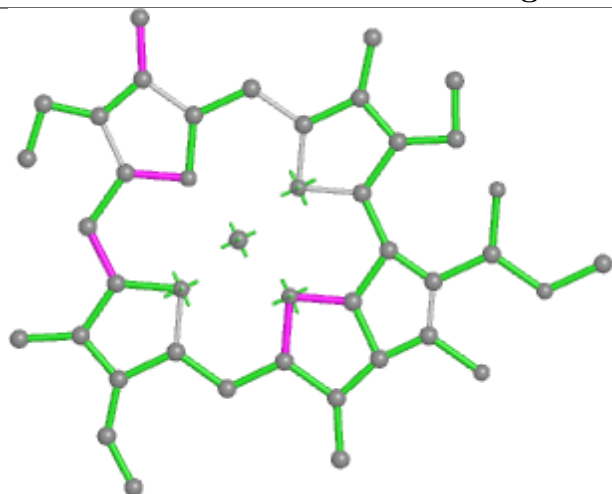
## Ligand PQN a 843



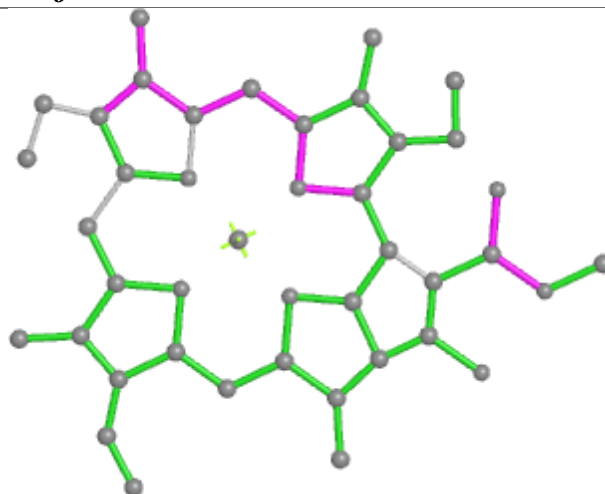
## Ligand CLA b 807



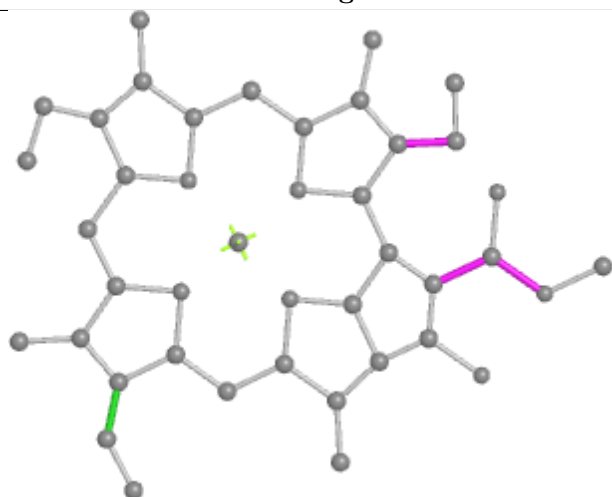
## Ligand CLA j 101



Bond lengths



Bond angles

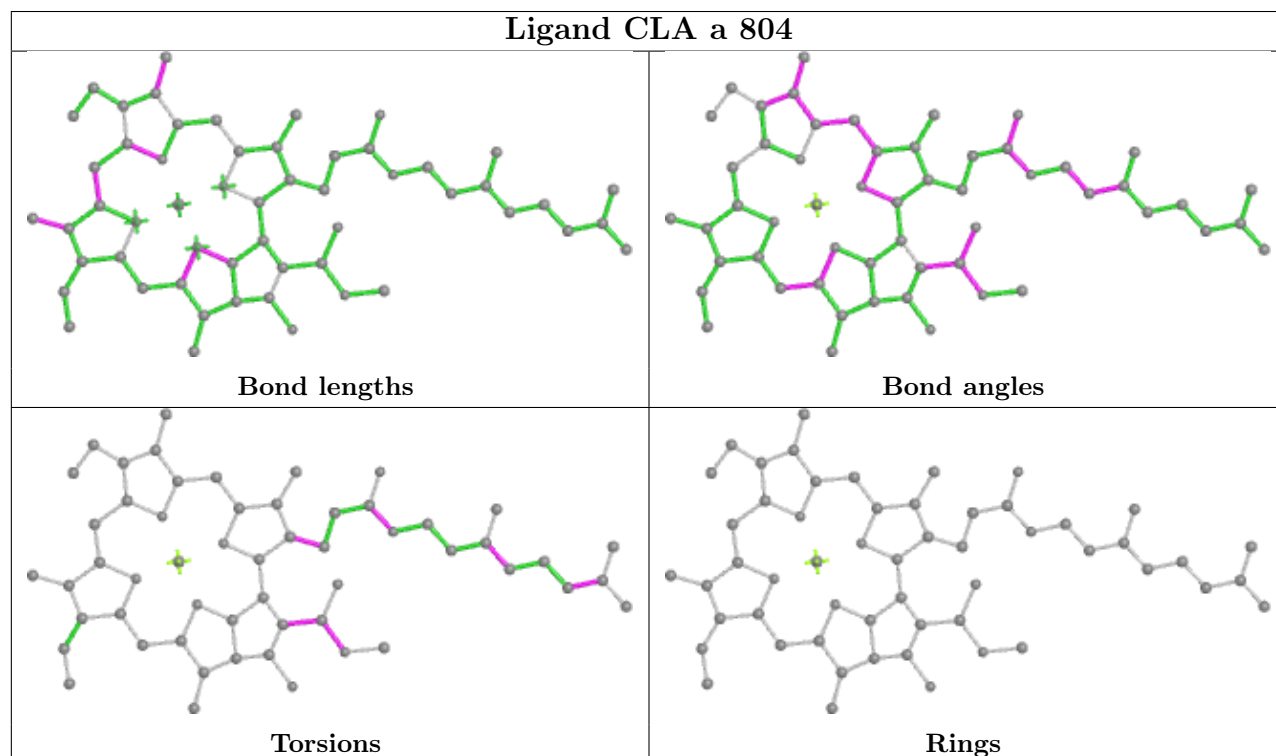
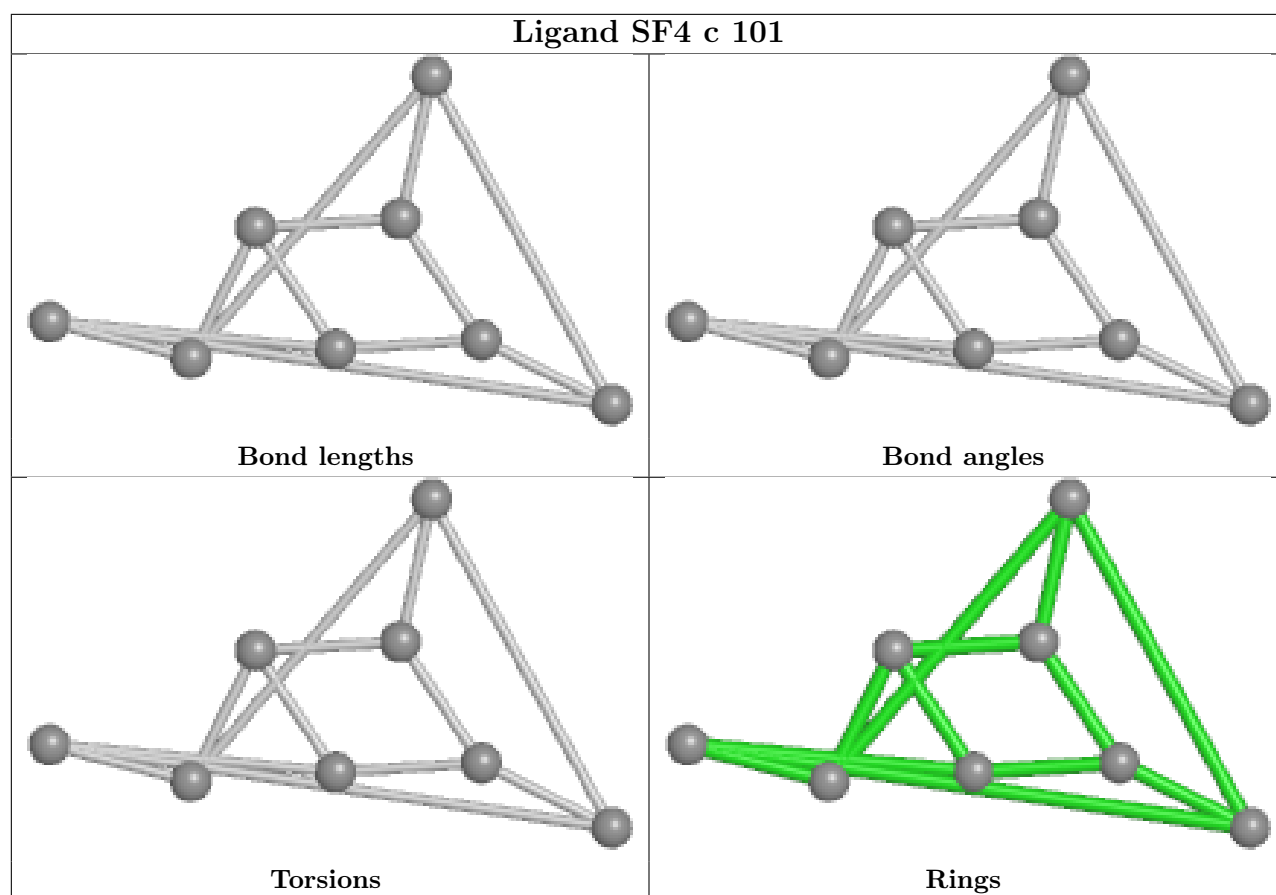


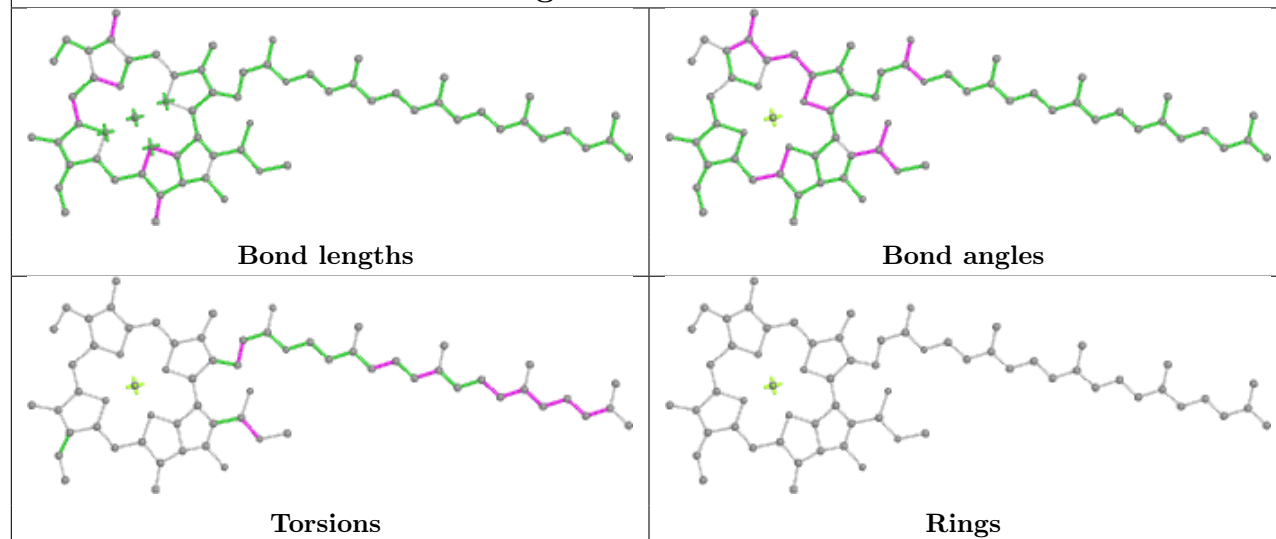
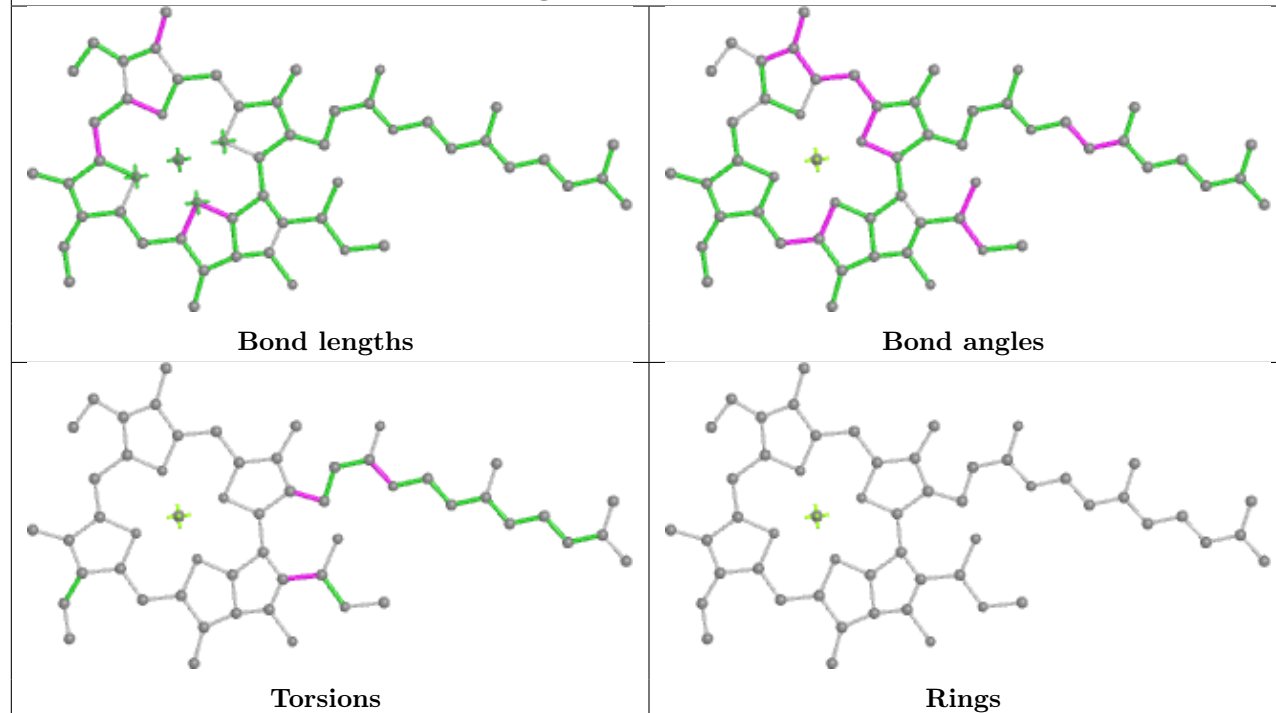
Torsions



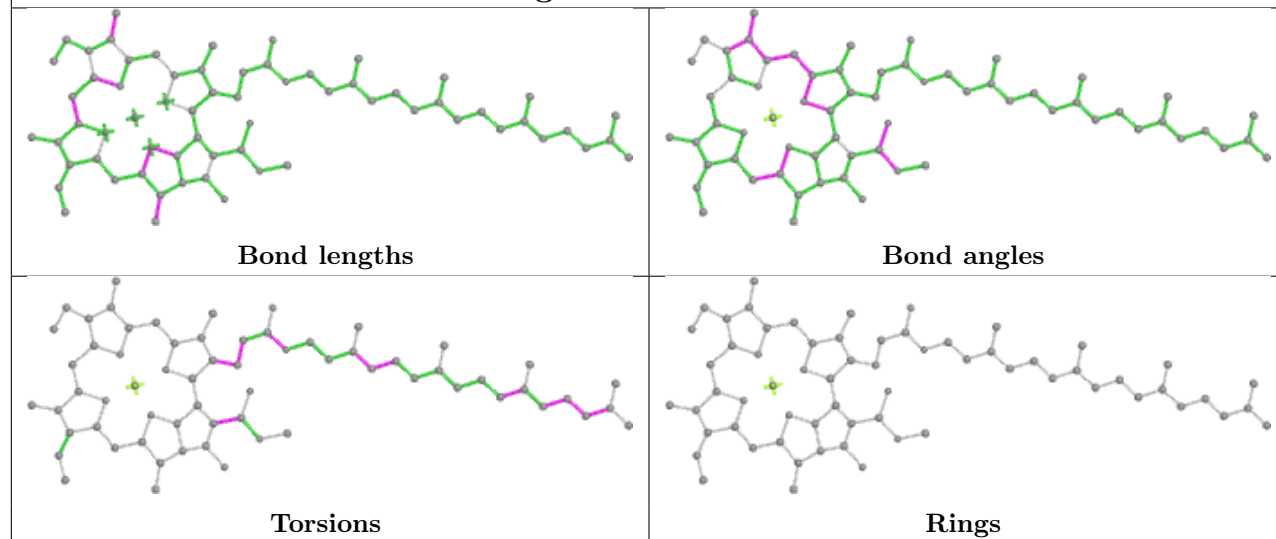
Rings



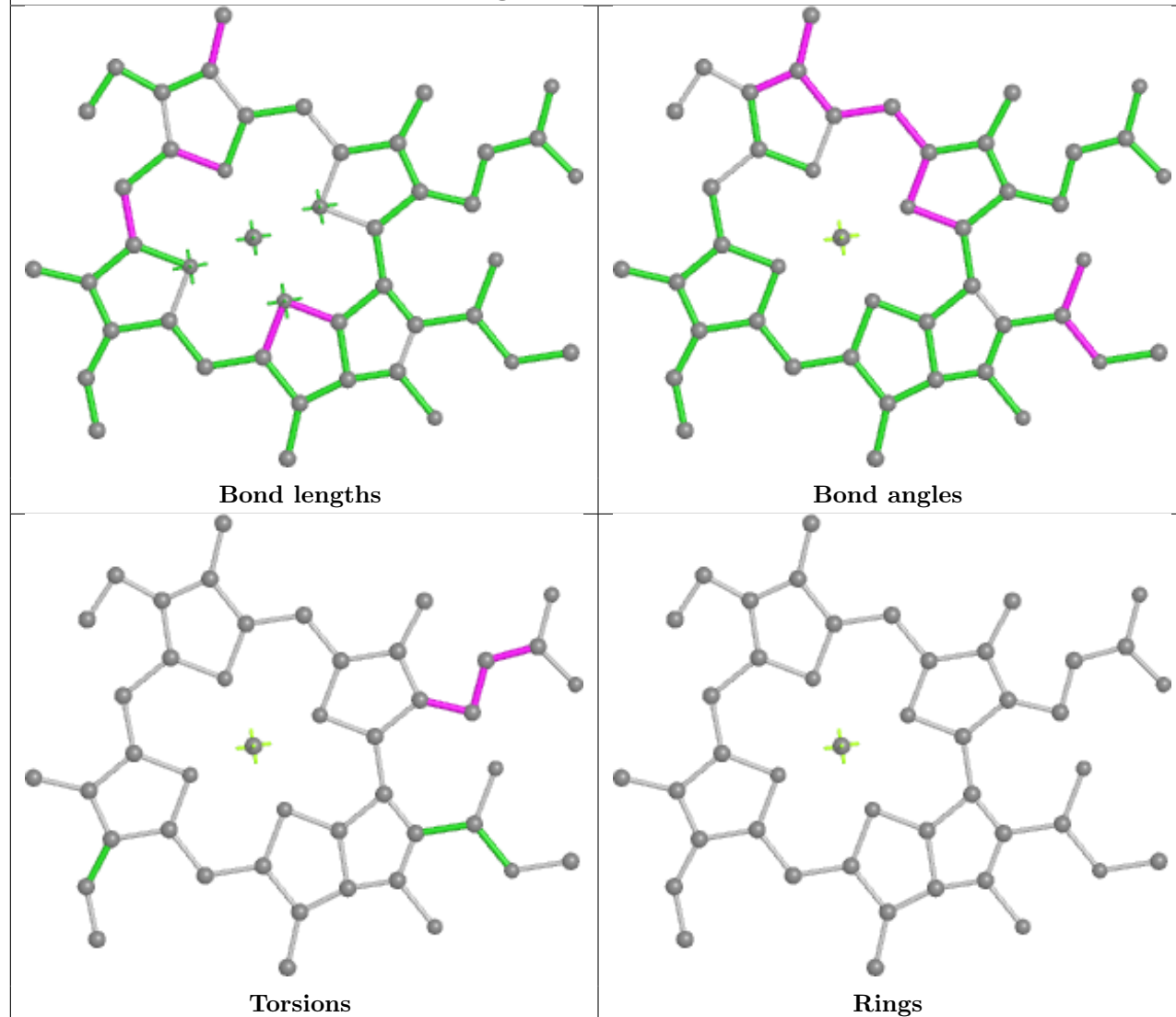


**Ligand CLA 4 307****Ligand CLA b 816**

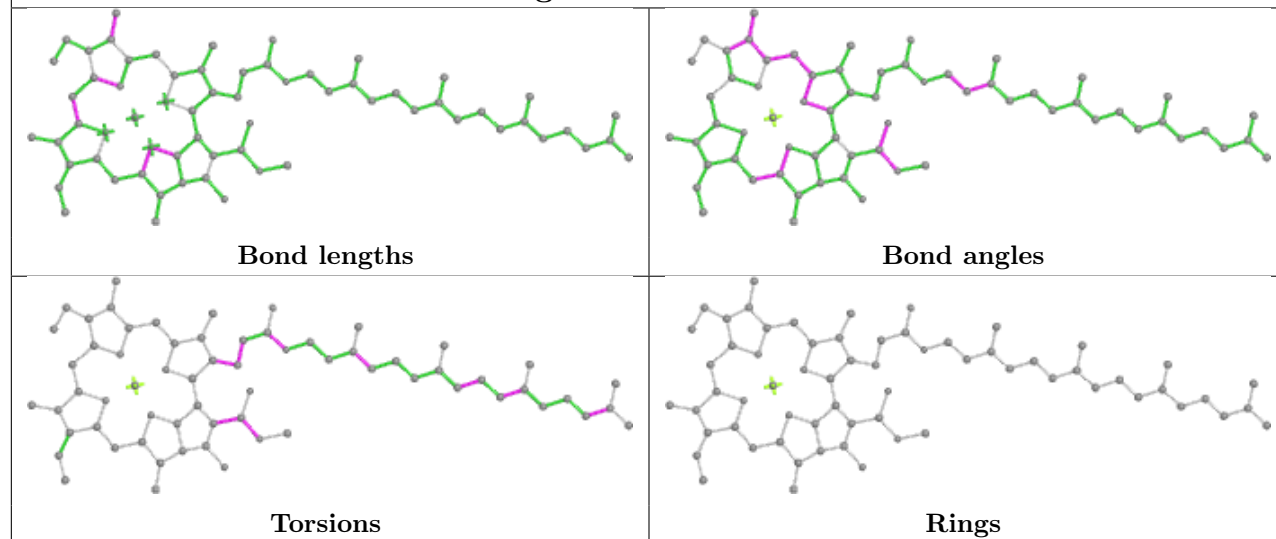
## Ligand CLA b 834



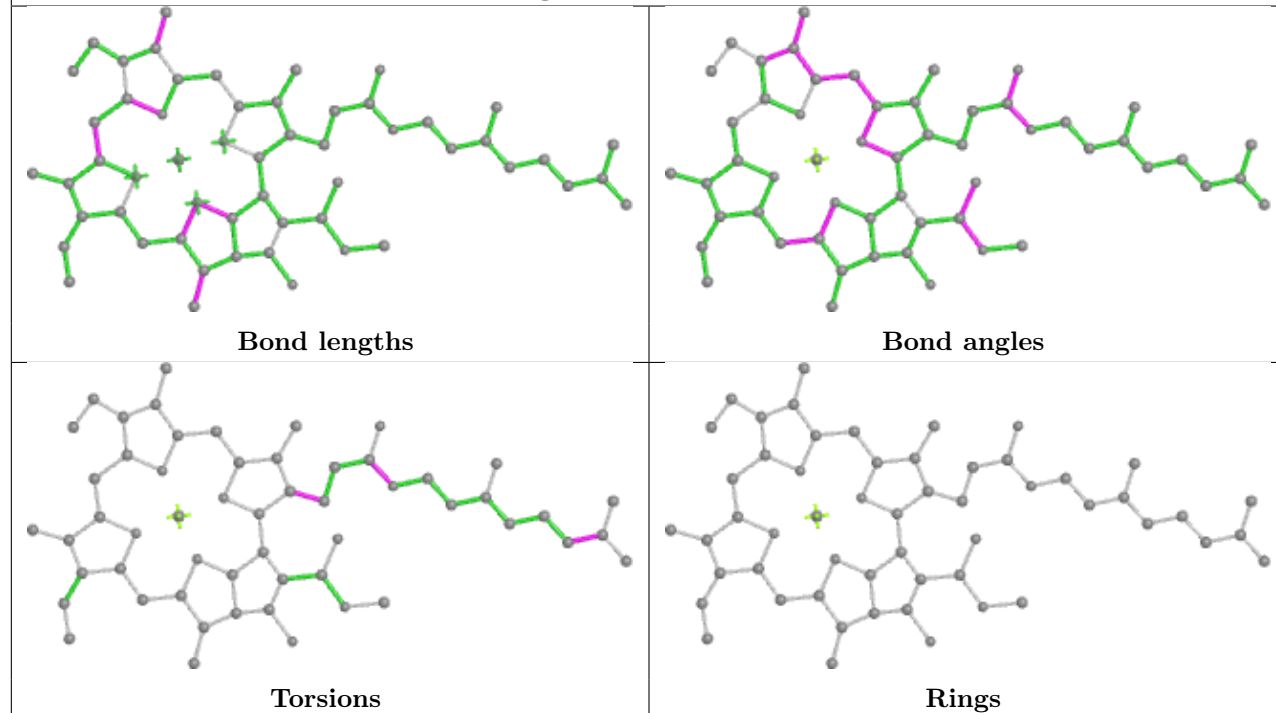
## Ligand CLA 1 314



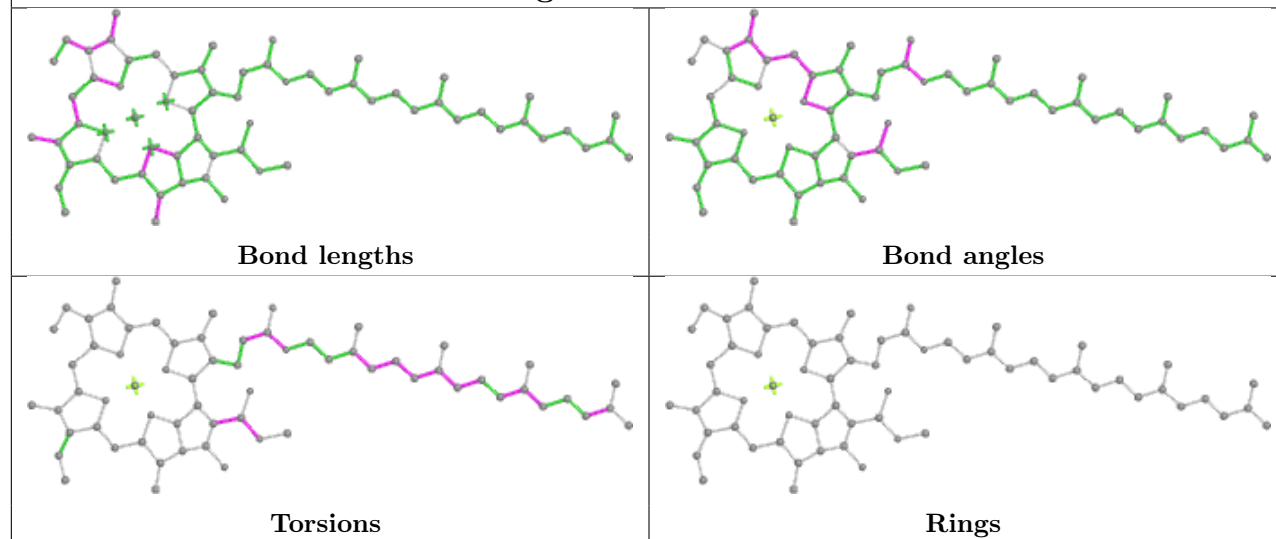
## Ligand CLA b 810



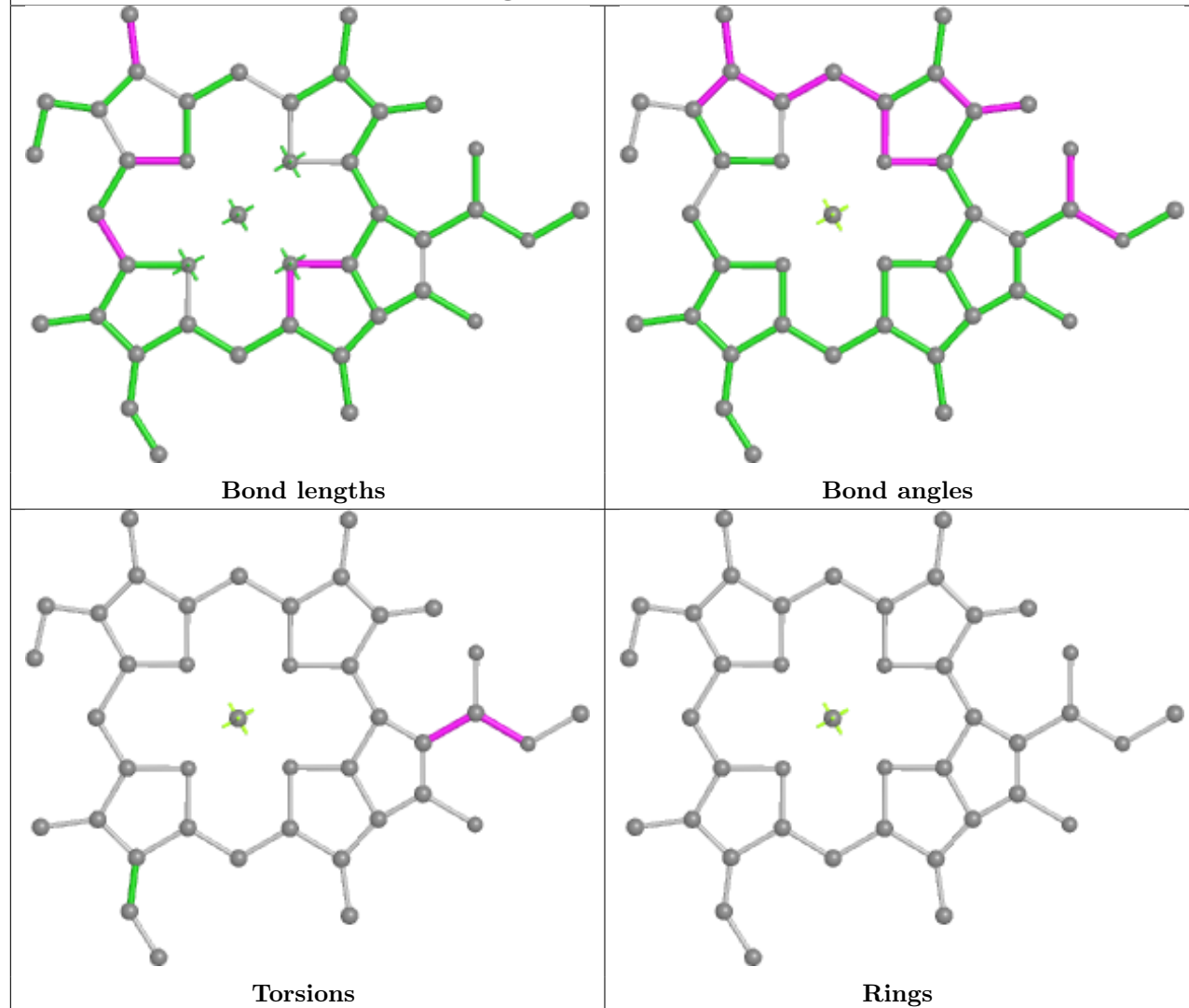
## Ligand CLA a 805

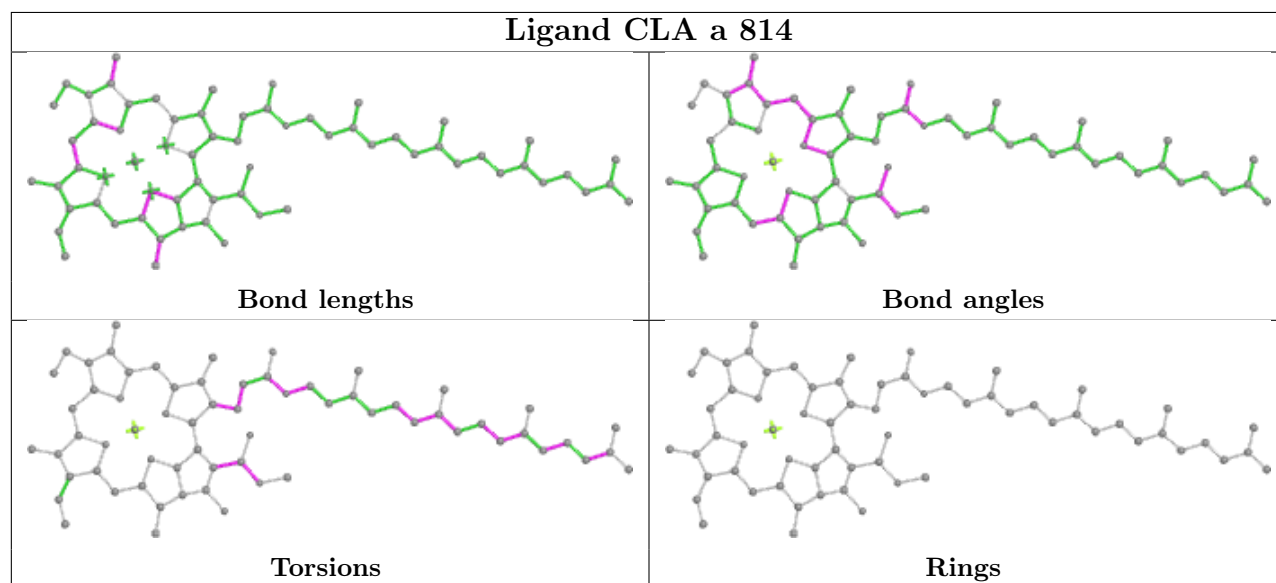
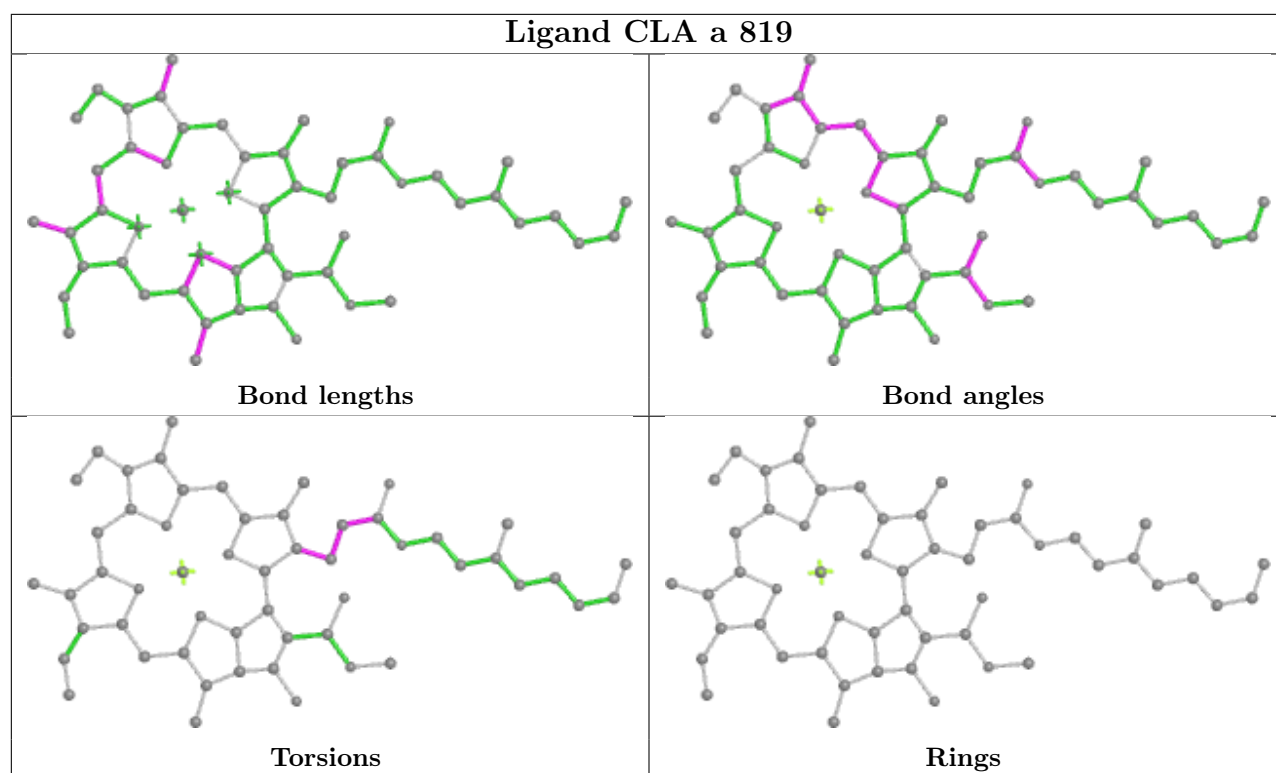


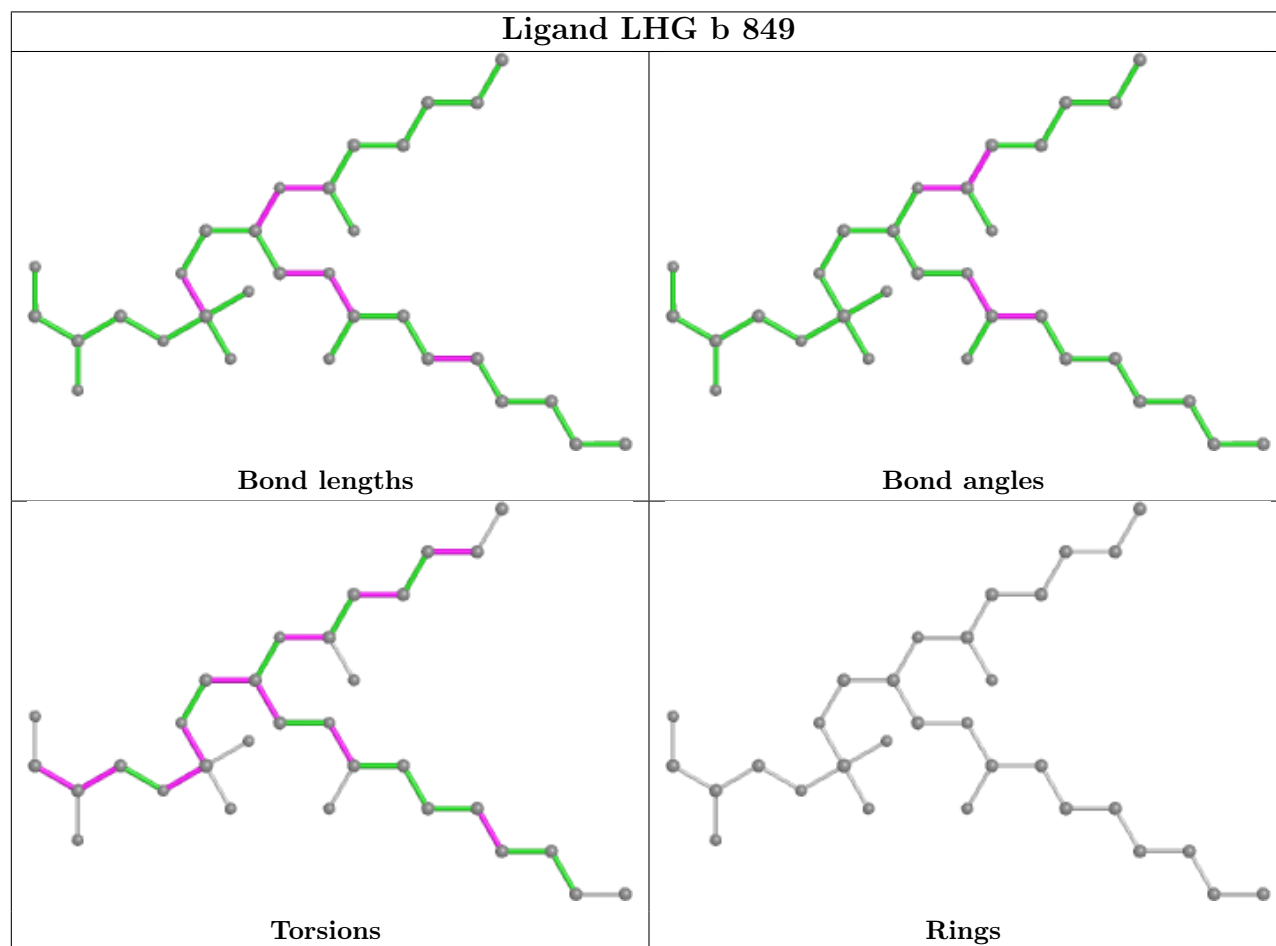
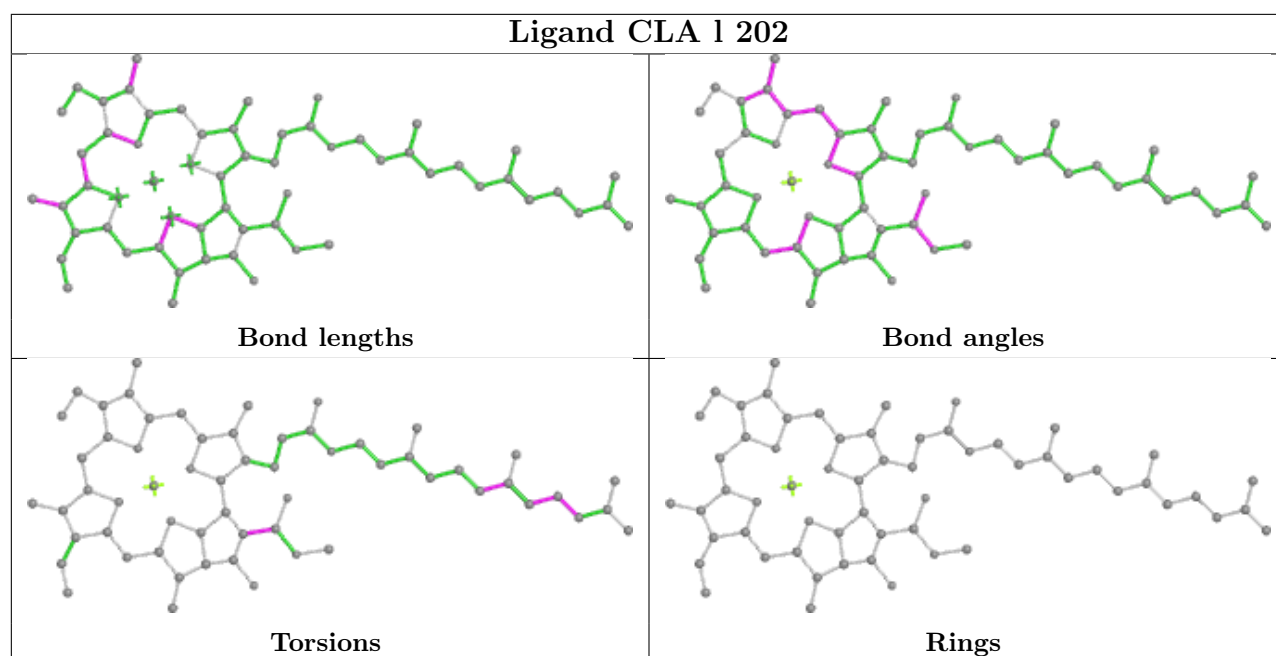
## Ligand CLA a 801



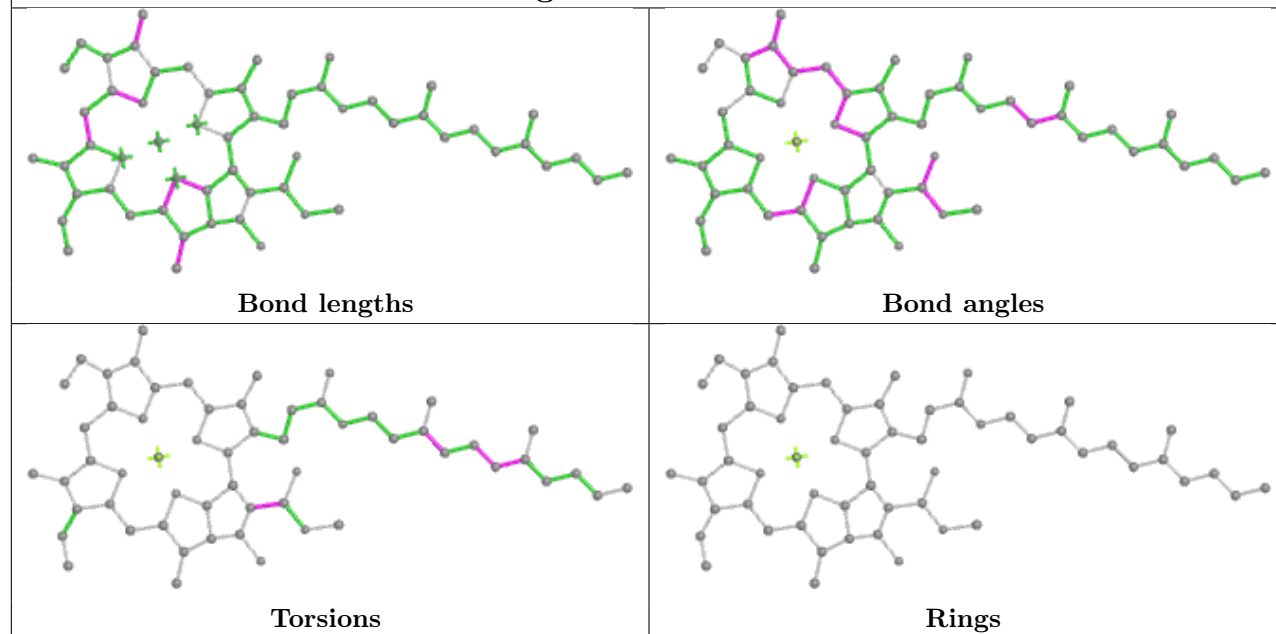
## Ligand CLA 4 314



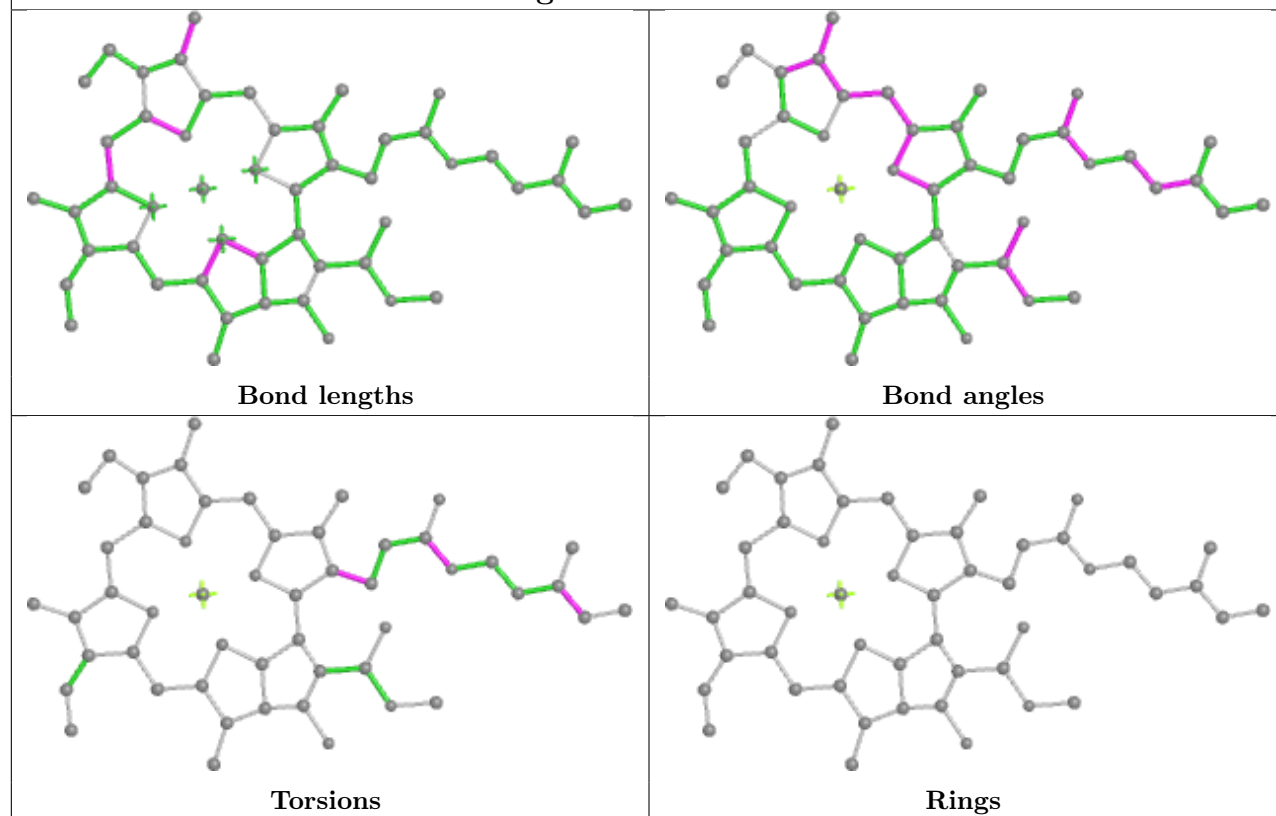




## Ligand CLA a 802

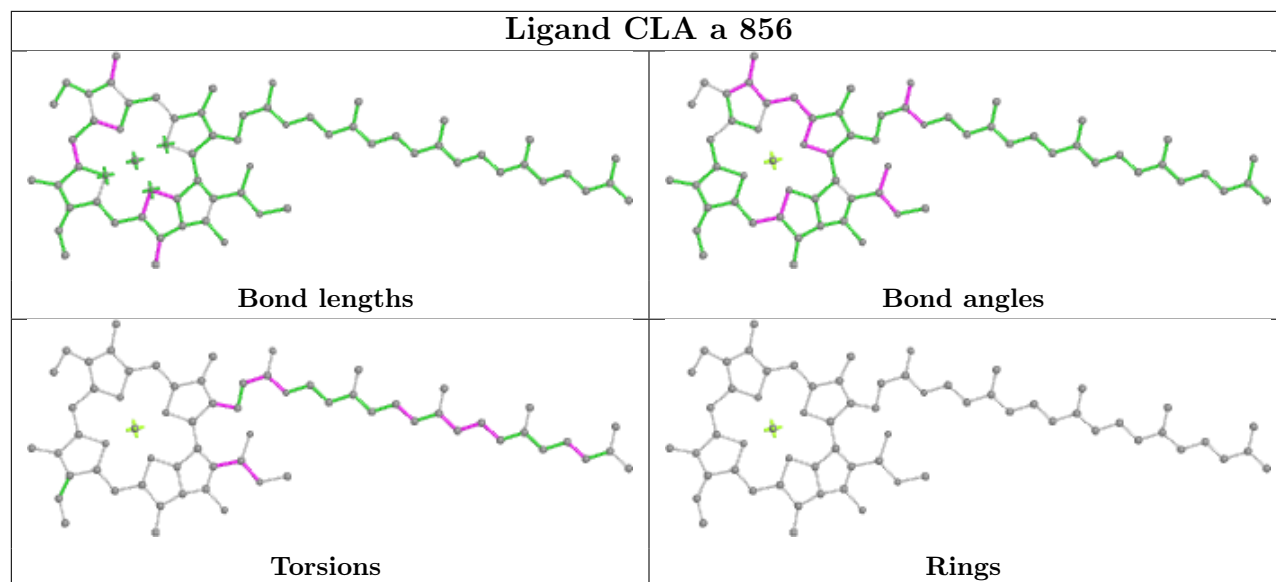


## Ligand CLA a 838

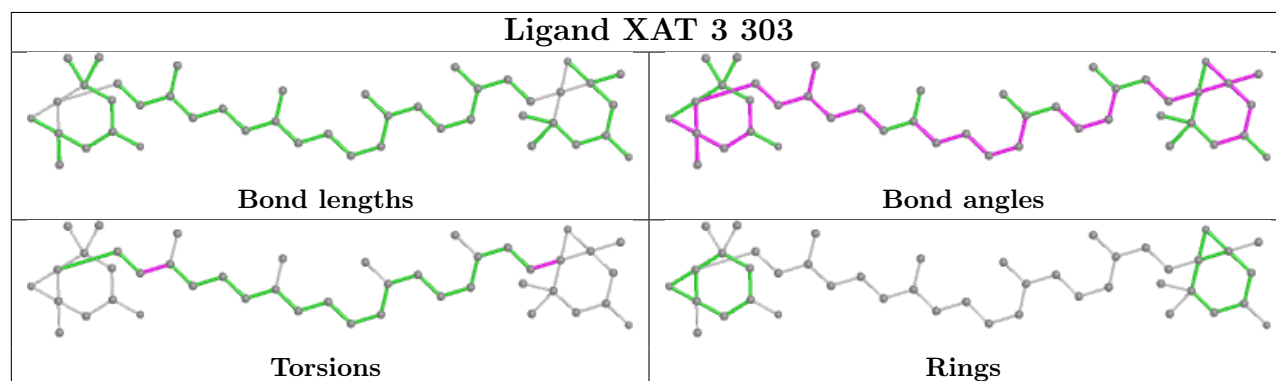




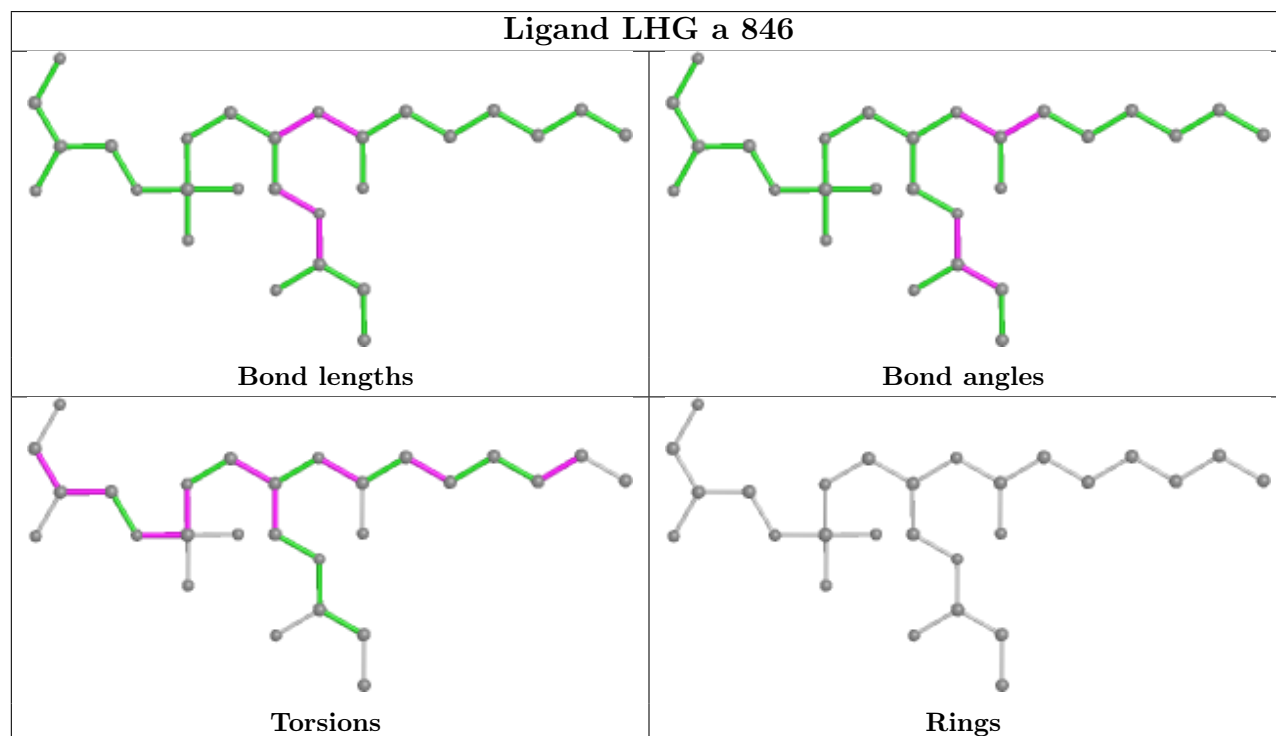
## Ligand CLA a 856



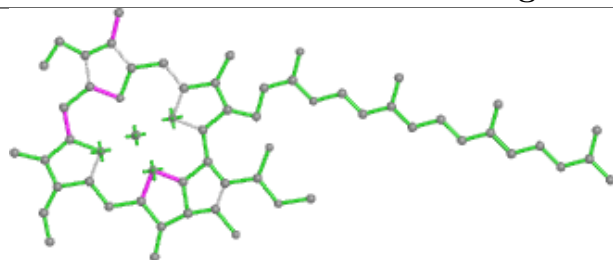
## Ligand XAT 3 303



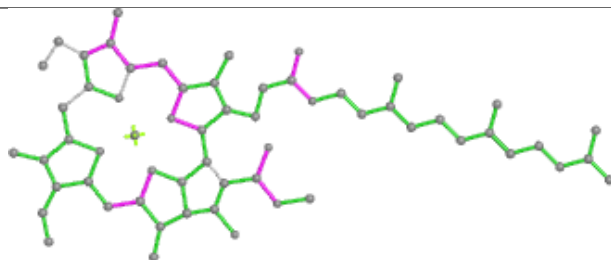
## Ligand LHG a 846



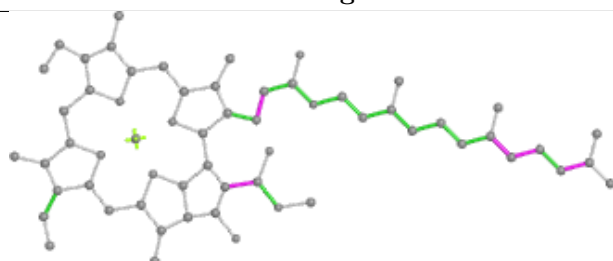
## Ligand CLA 5 308



Bond lengths



Bond angles

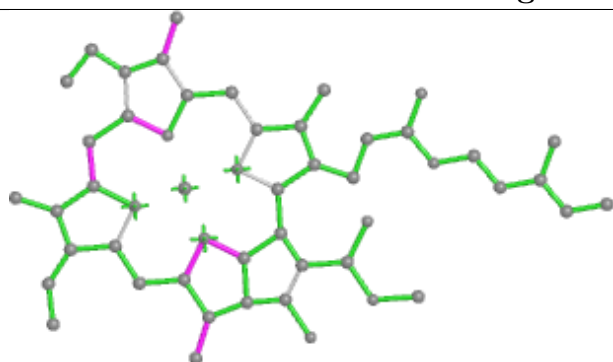


Torsions

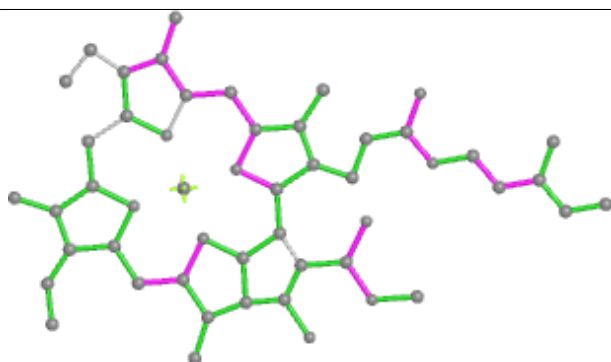


Rings

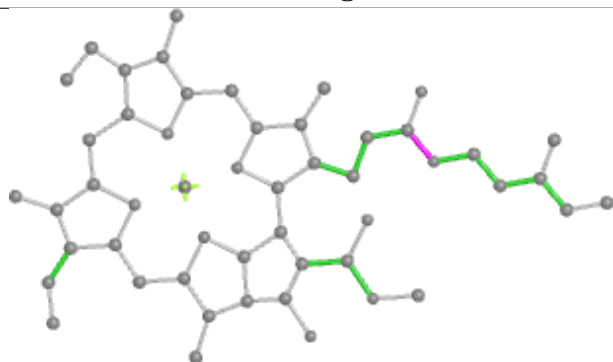
## Ligand CLA b 821



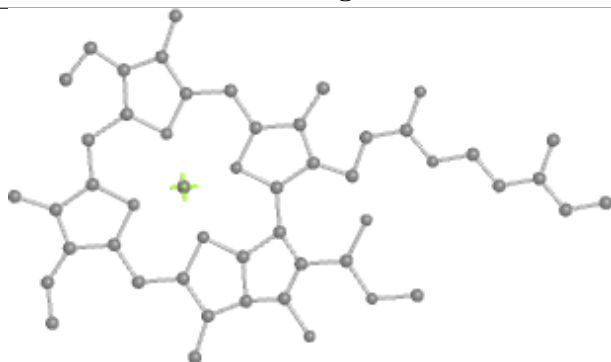
Bond lengths



Bond angles

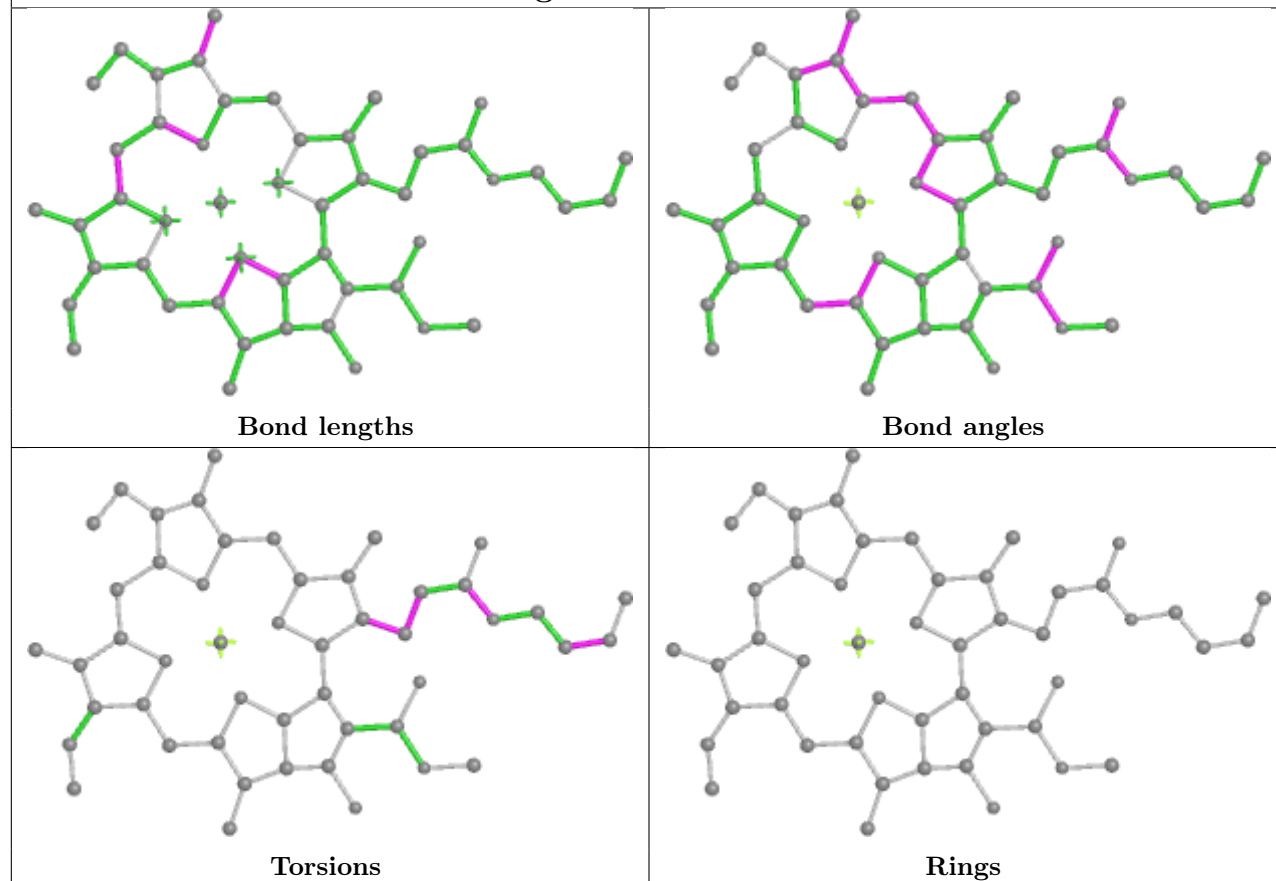


Torsions

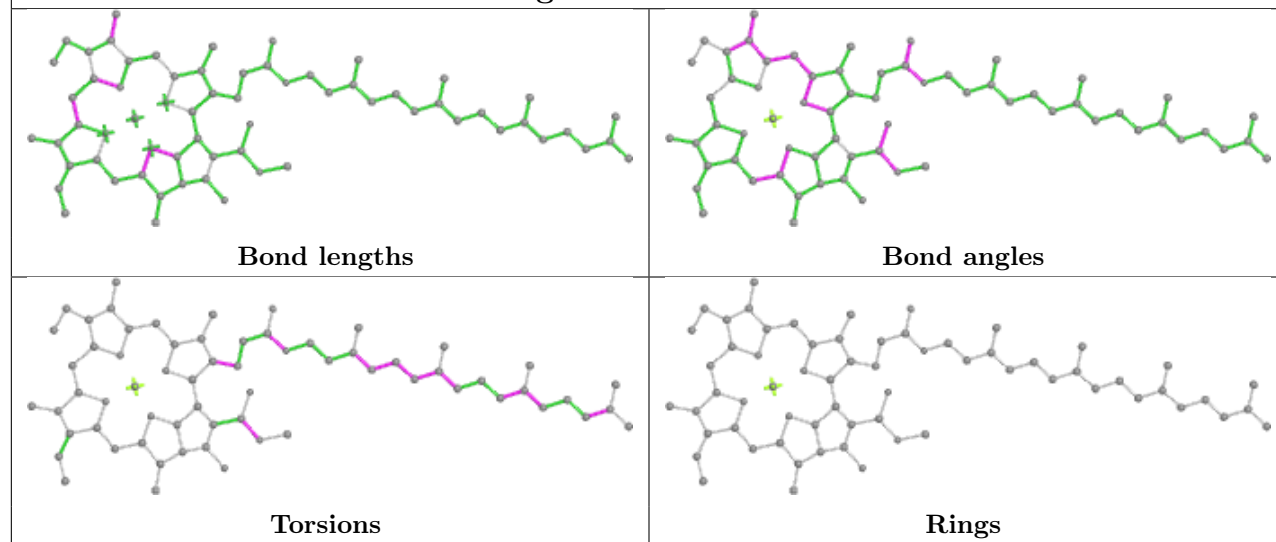


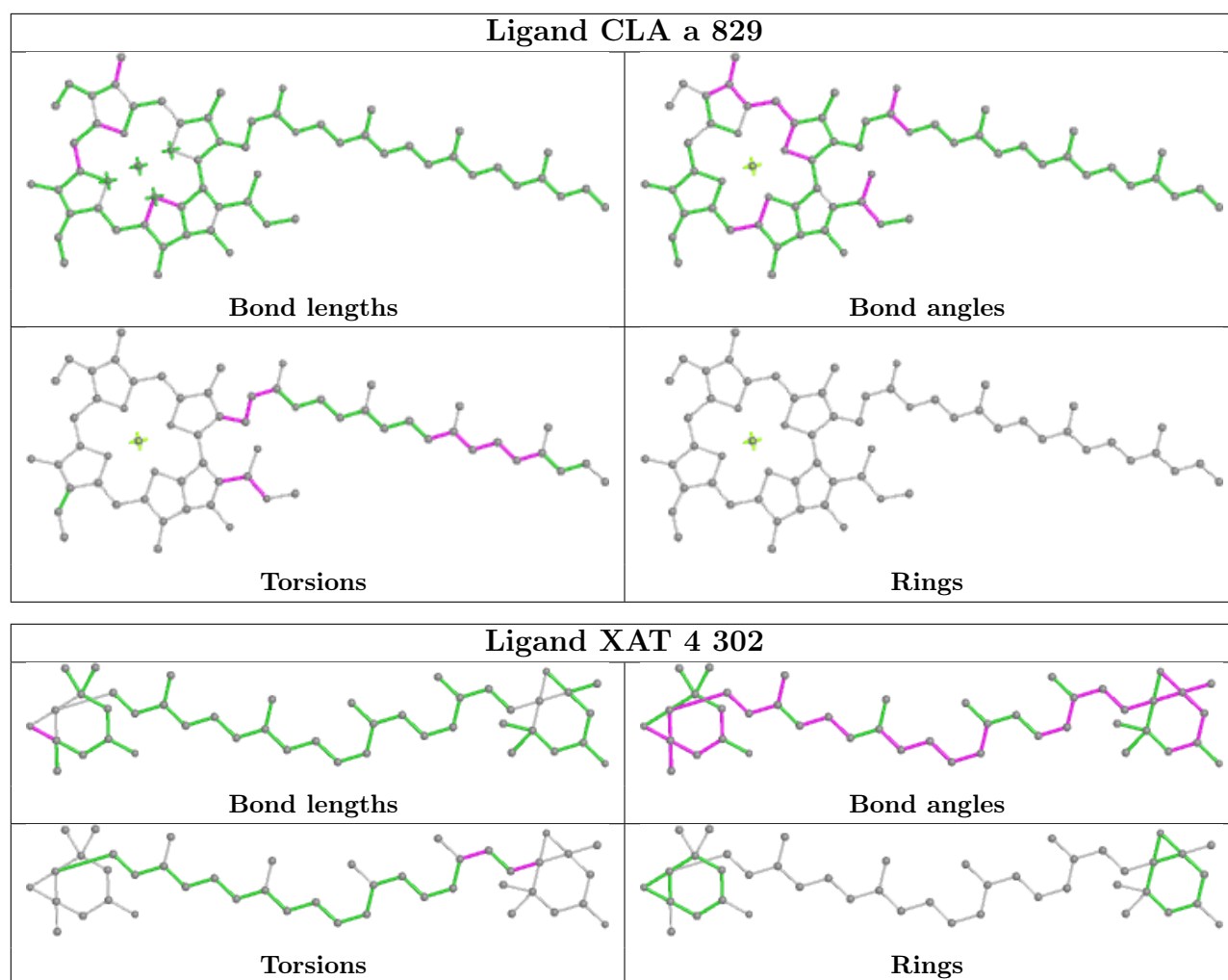
Rings

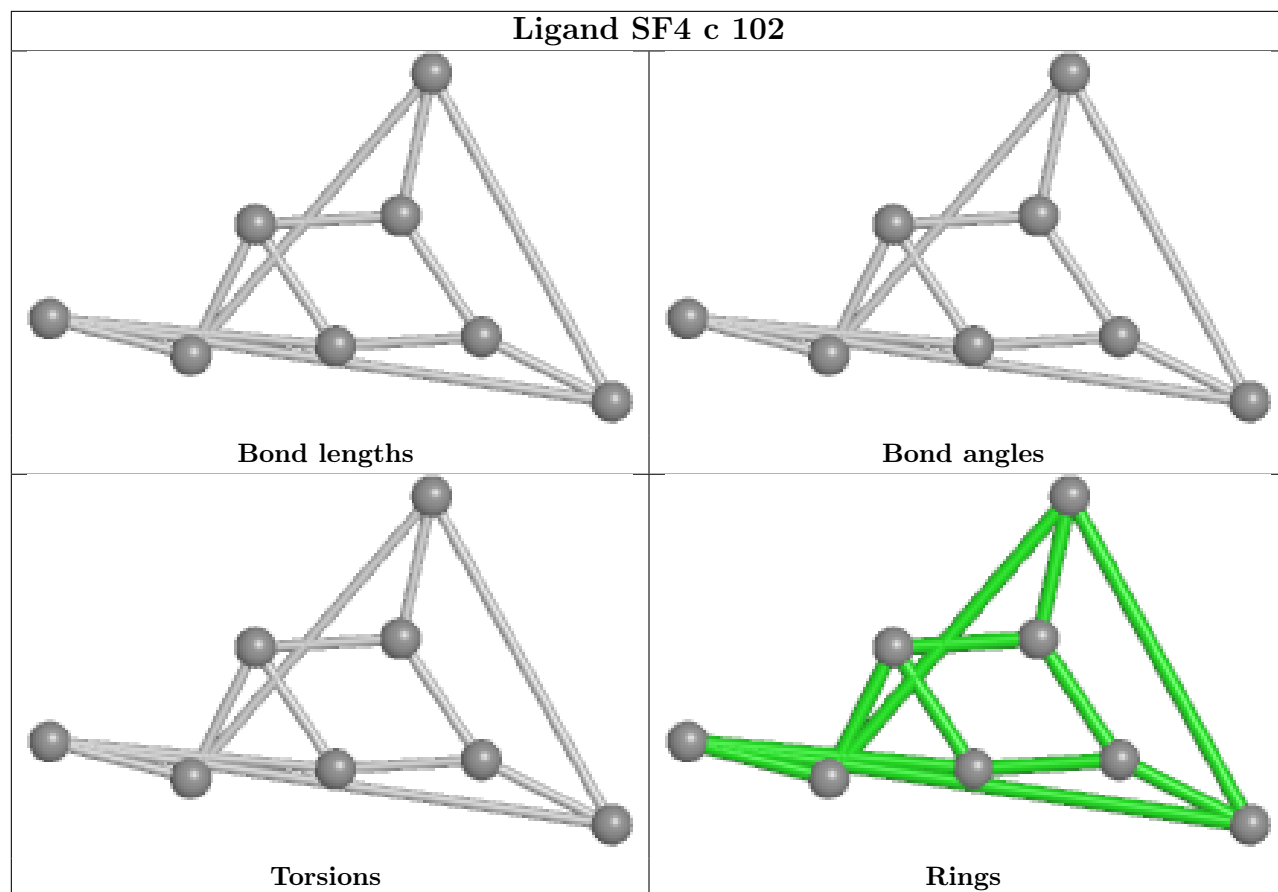
## Ligand CLA b 831



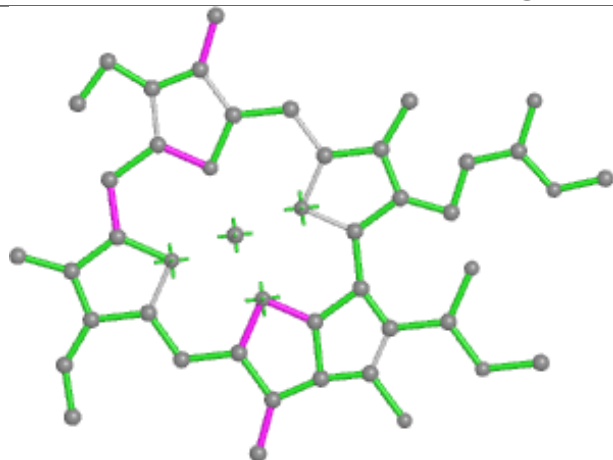
## Ligand CLA 1 310



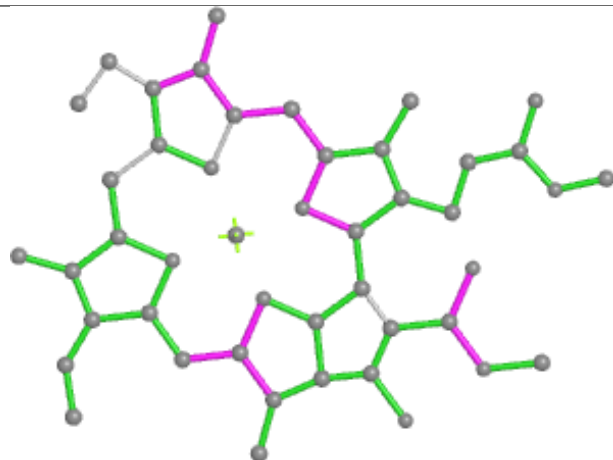




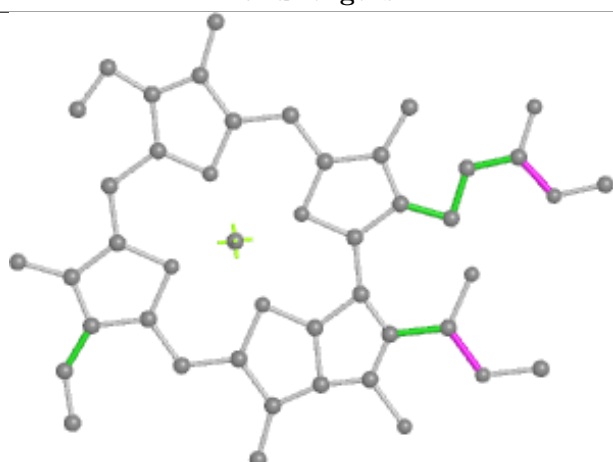
## Ligand CLA 5 306



Bond lengths



Bond angles

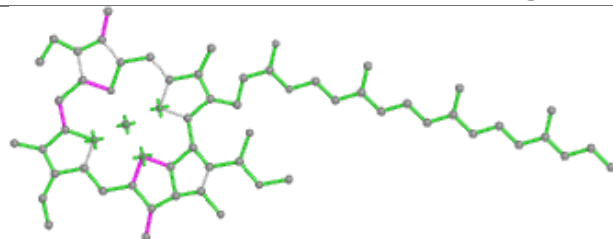


Torsions

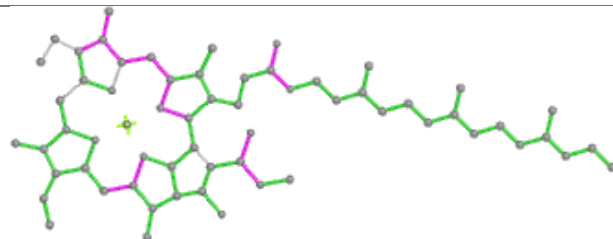


Rings

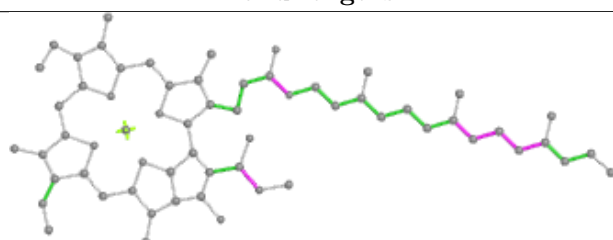
## Ligand CLA i 102



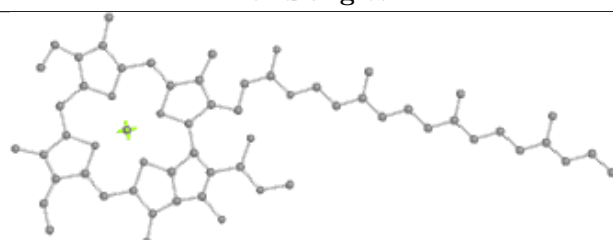
Bond lengths



Bond angles

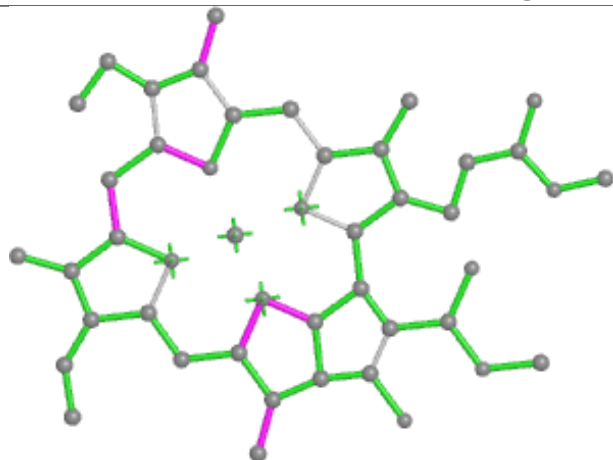


Torsions

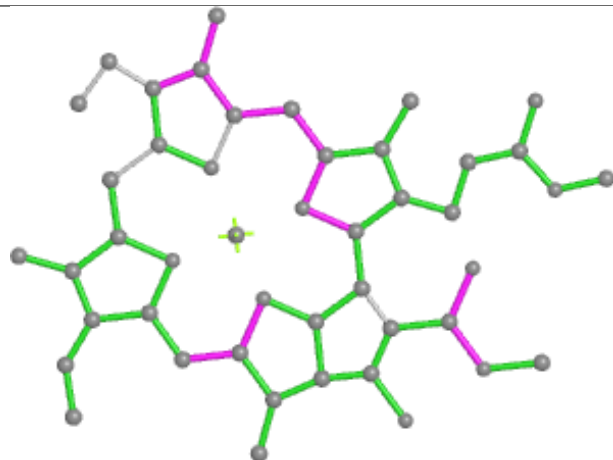


Rings

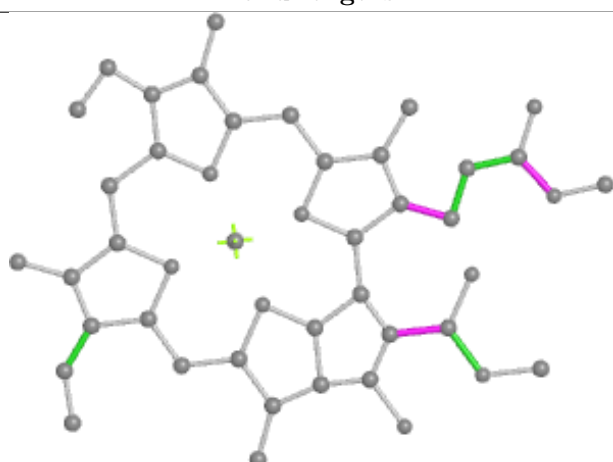
## Ligand CLA a 824



Bond lengths



Bond angles

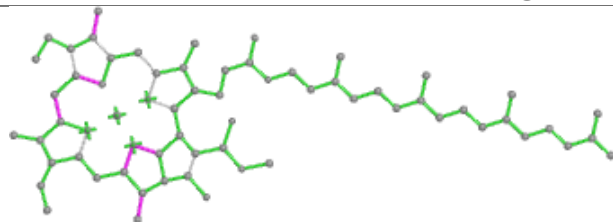


Torsions

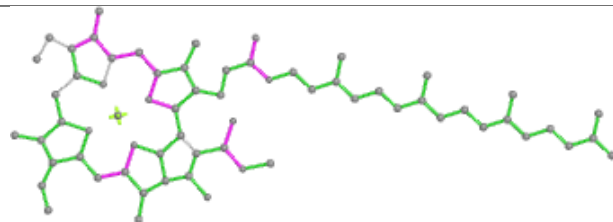


Rings

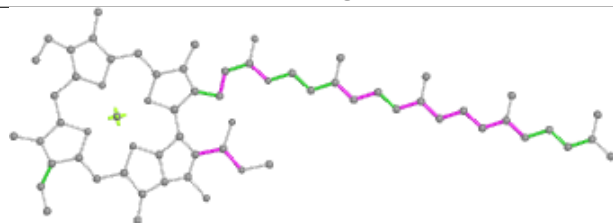
## Ligand CLA a 852



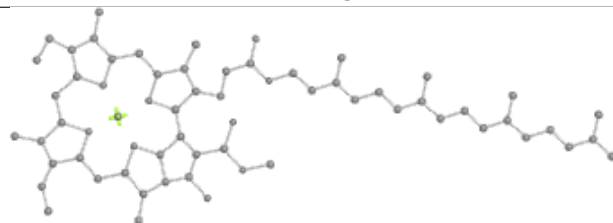
Bond lengths



Bond angles

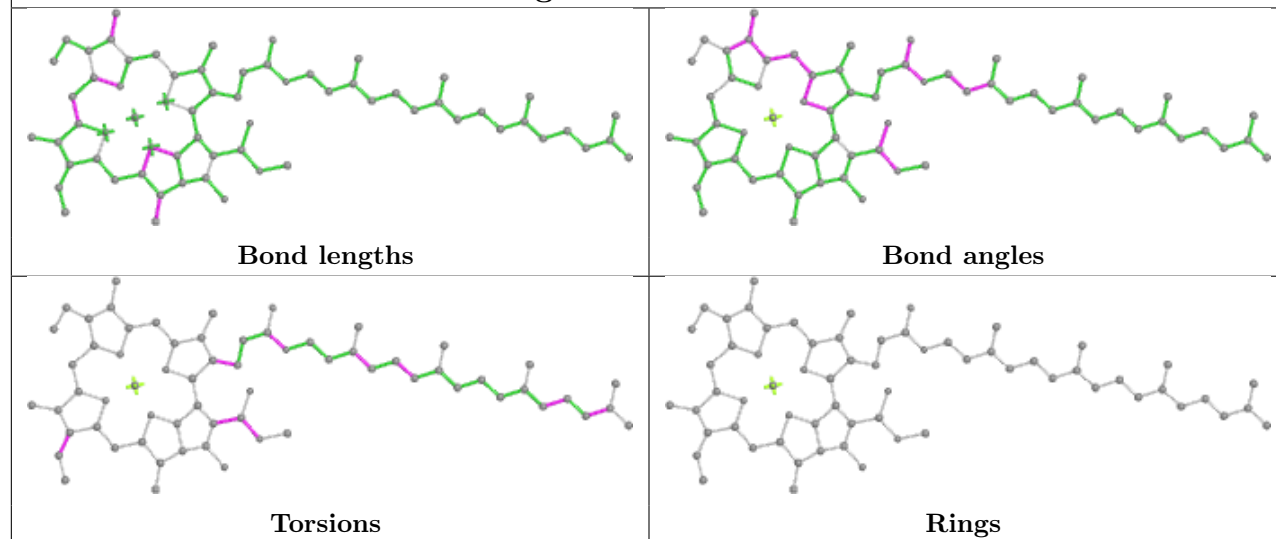


Torsions

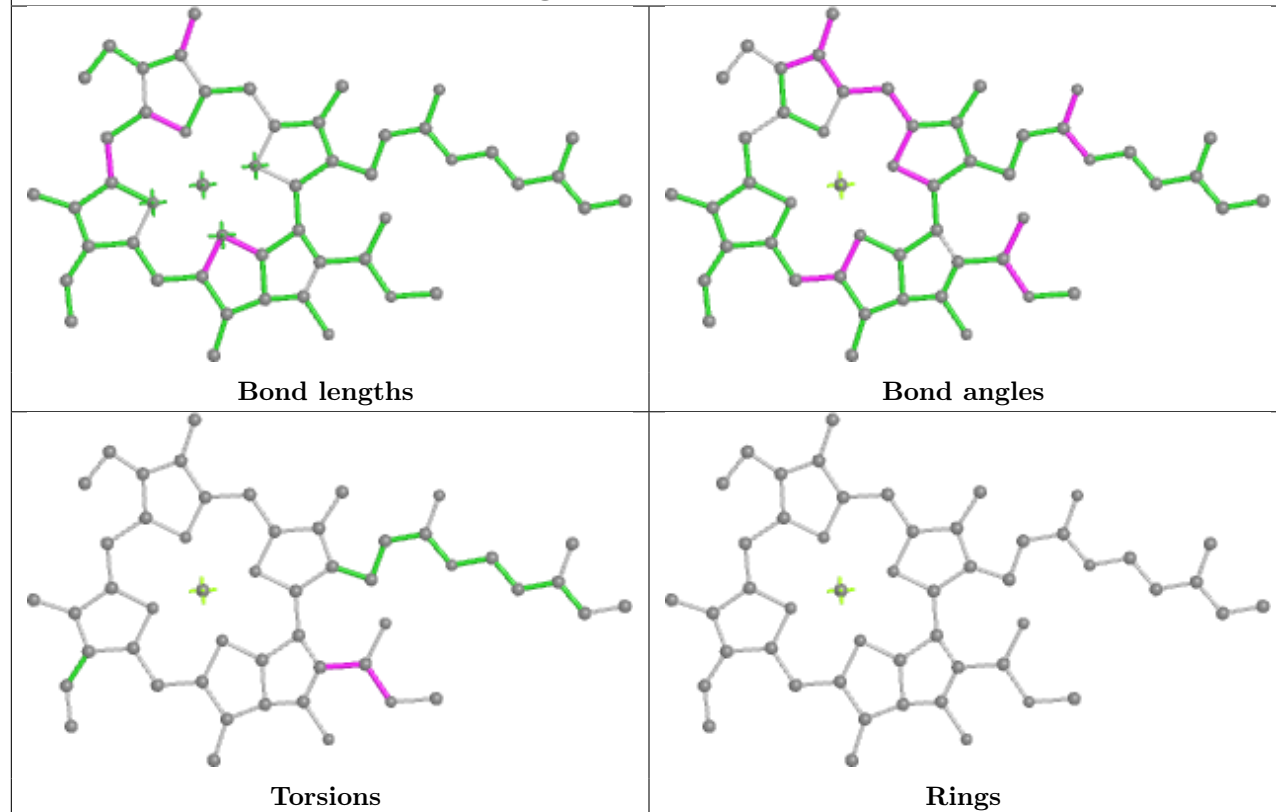


Rings

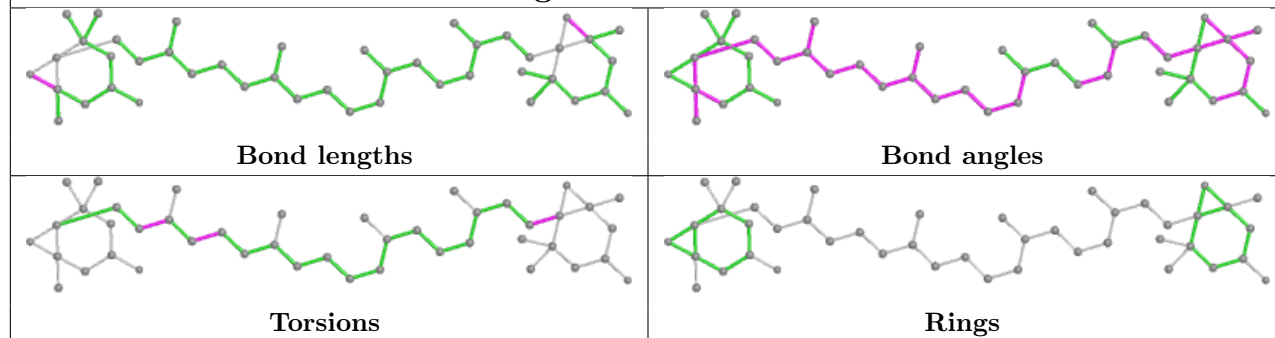
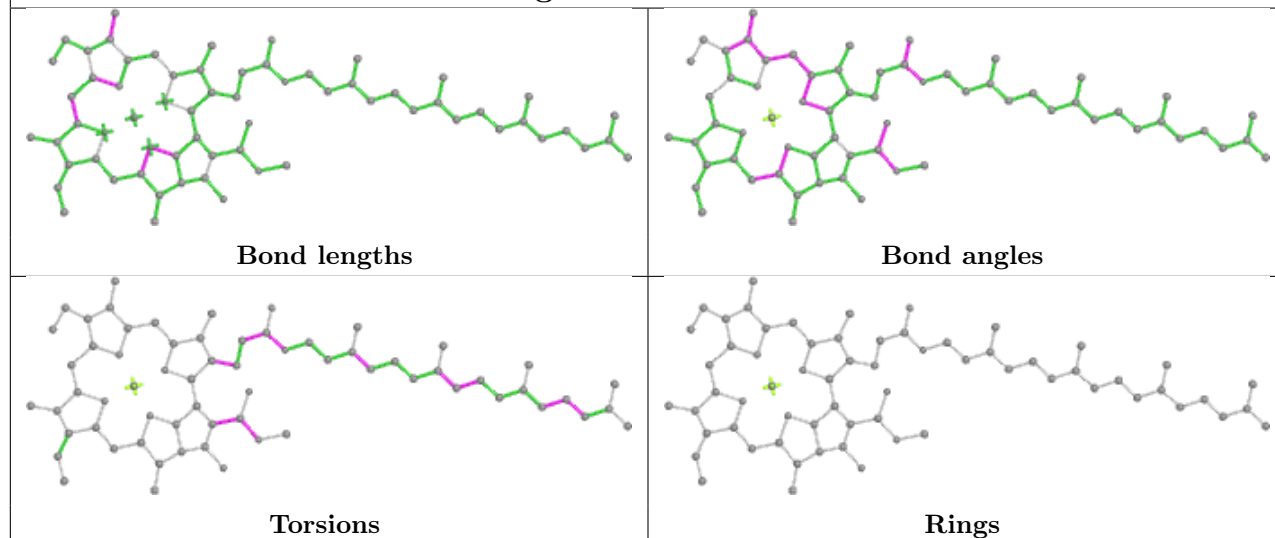
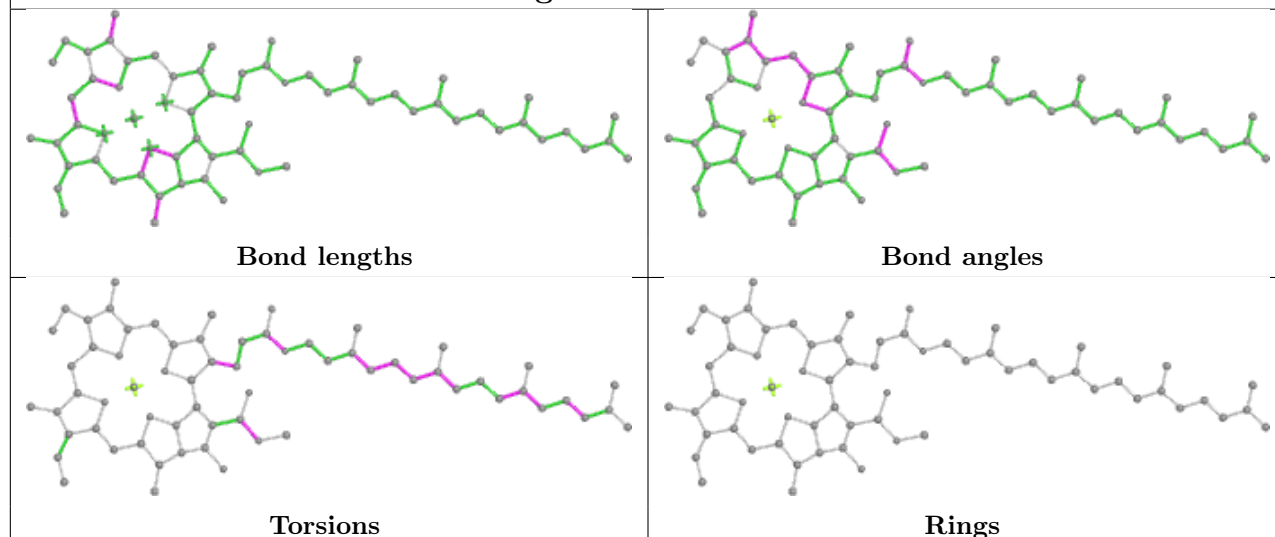
## Ligand CLA b 840

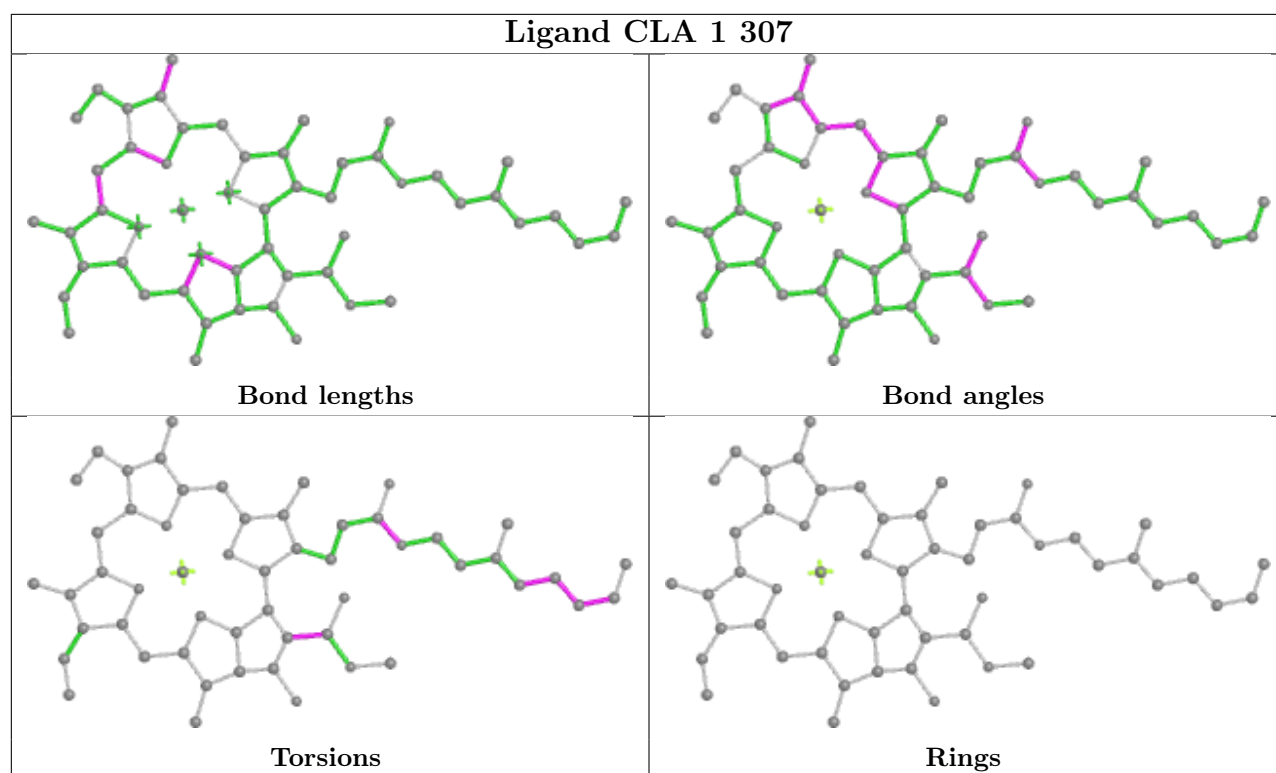


## Ligand CLA a 808

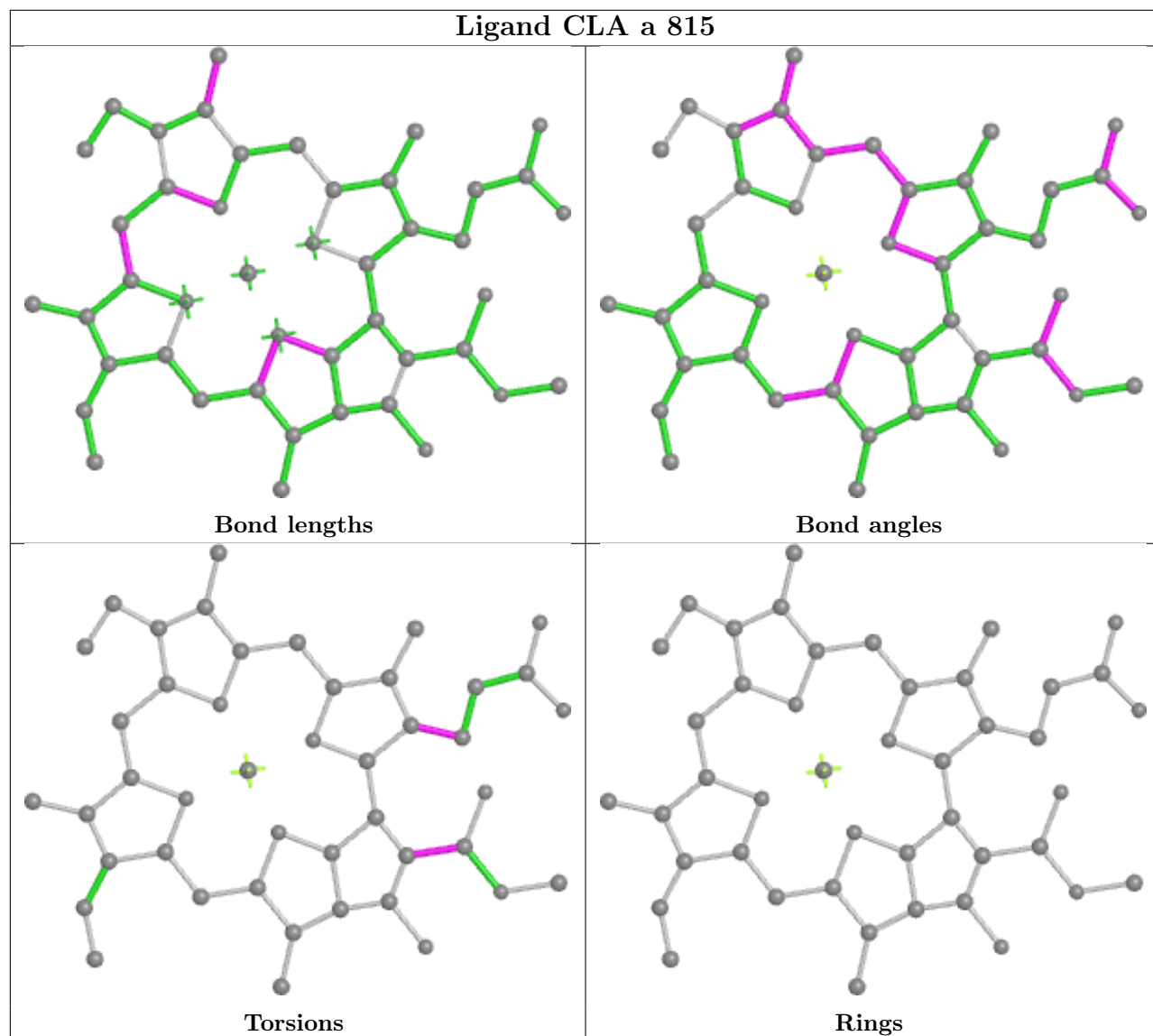




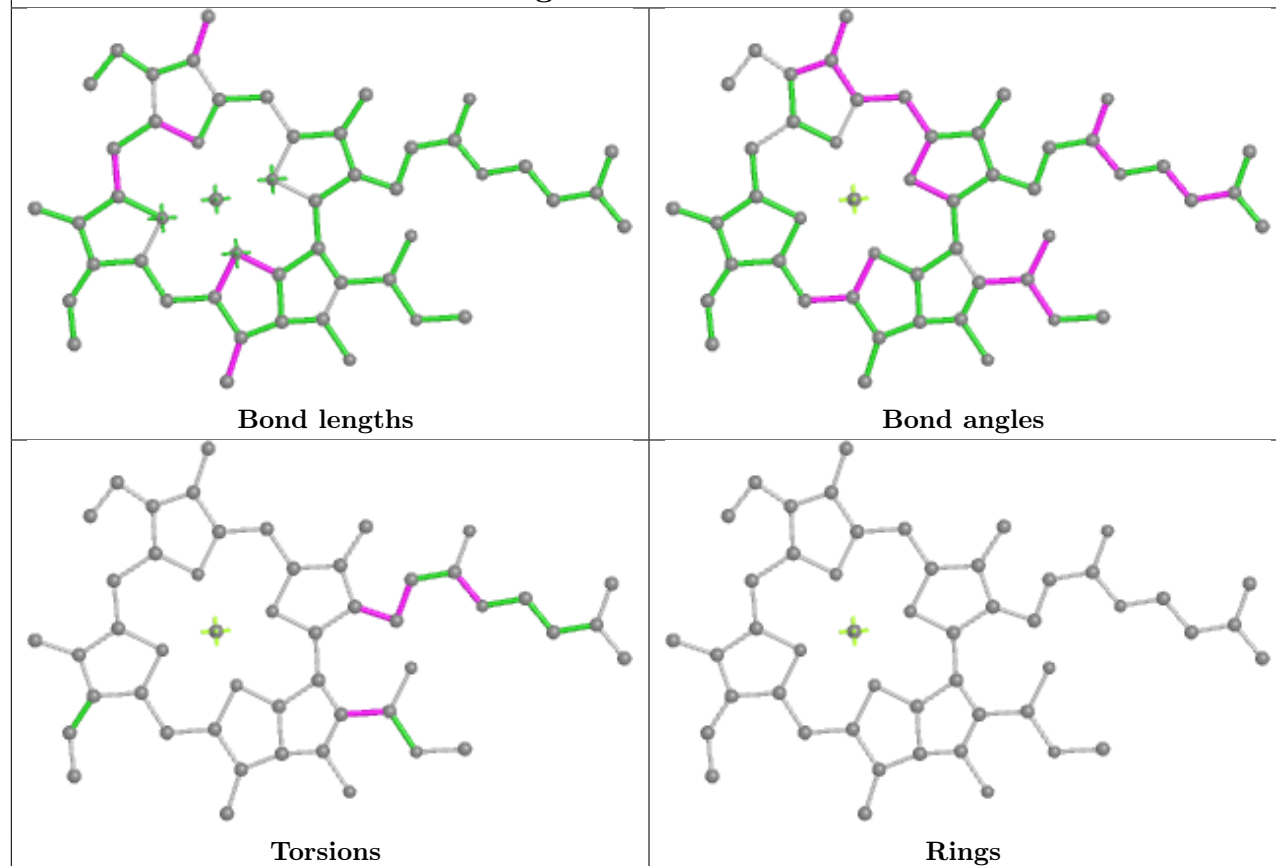
**Ligand XAT 5 301****Ligand CLA 4 309****Ligand CLA a 807**



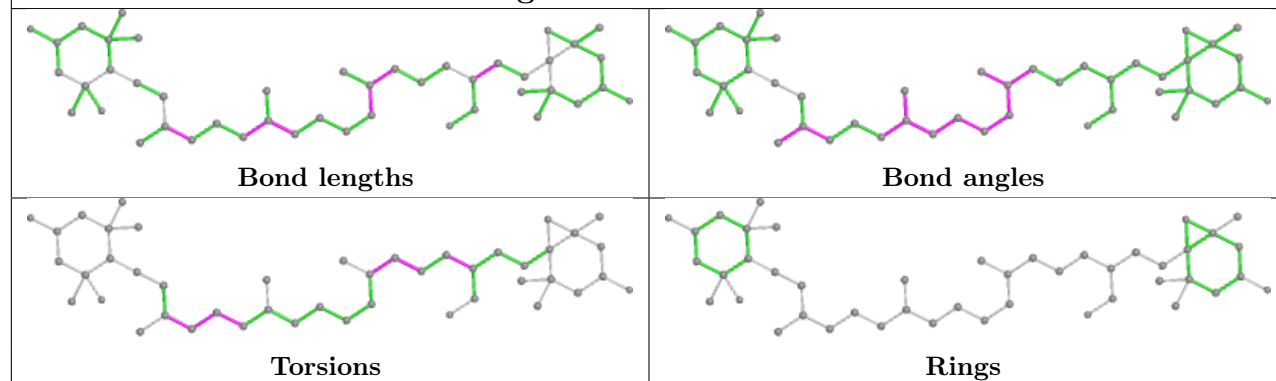
## Ligand CLA a 815

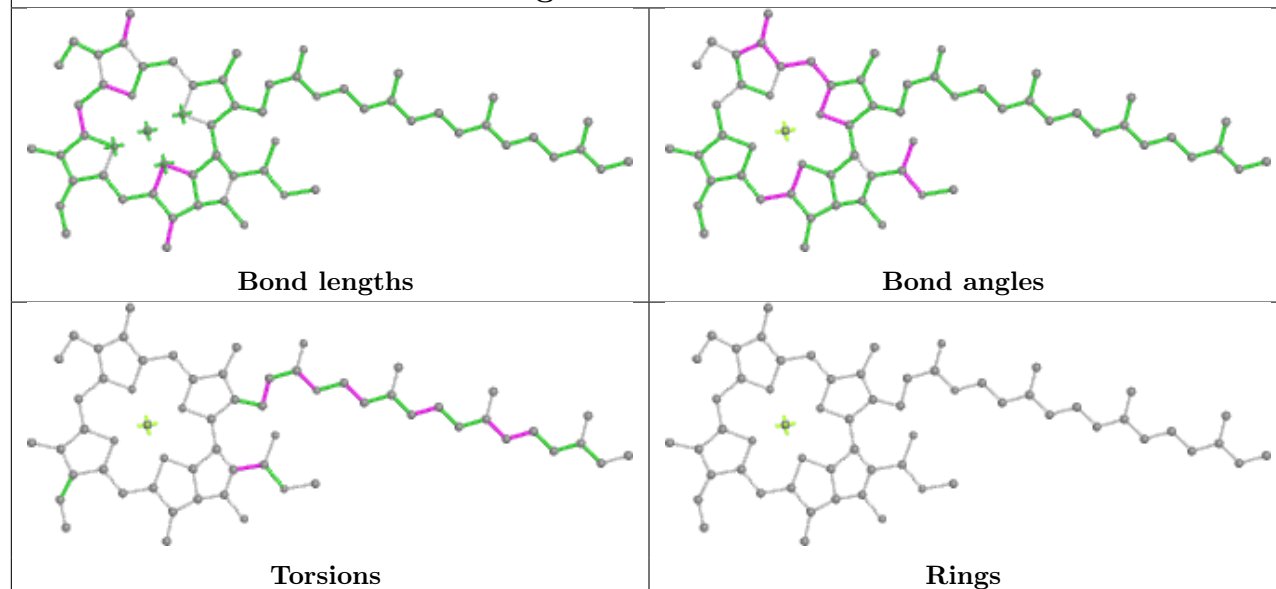
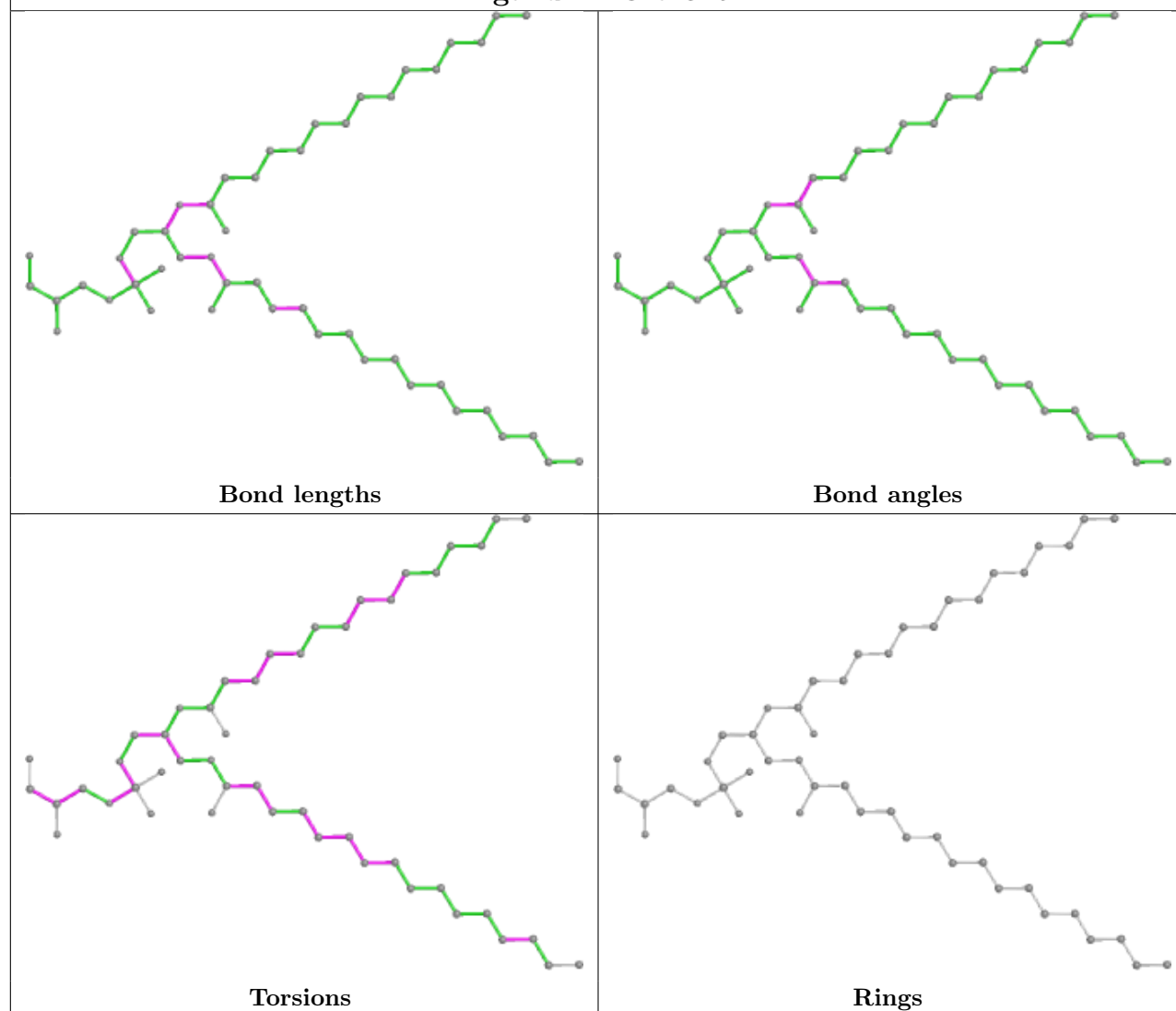


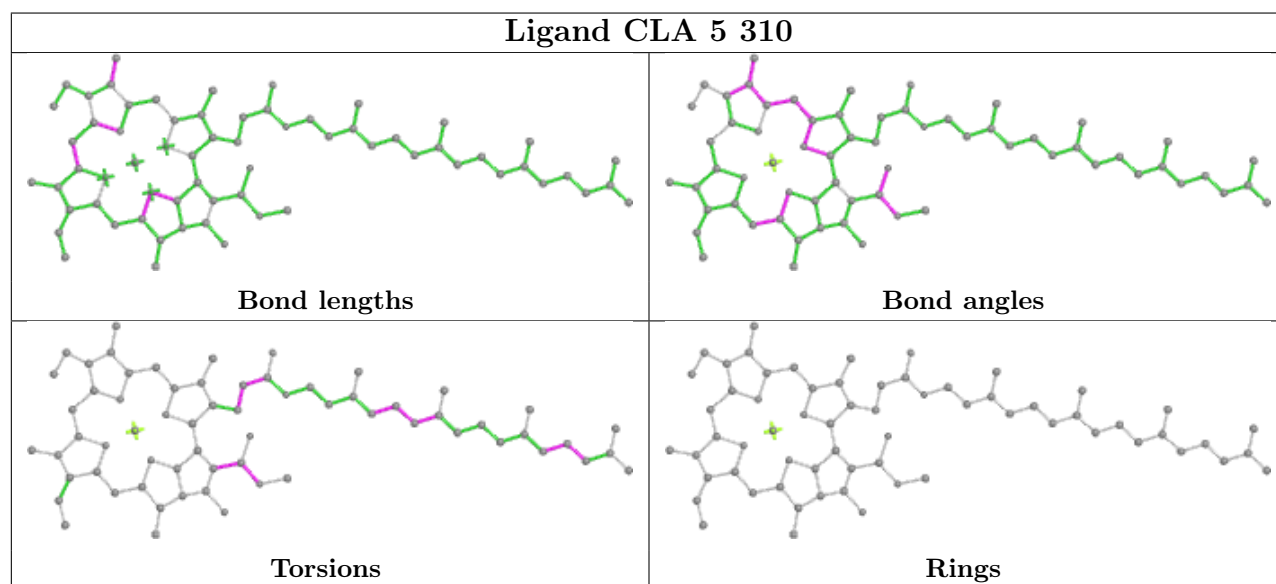
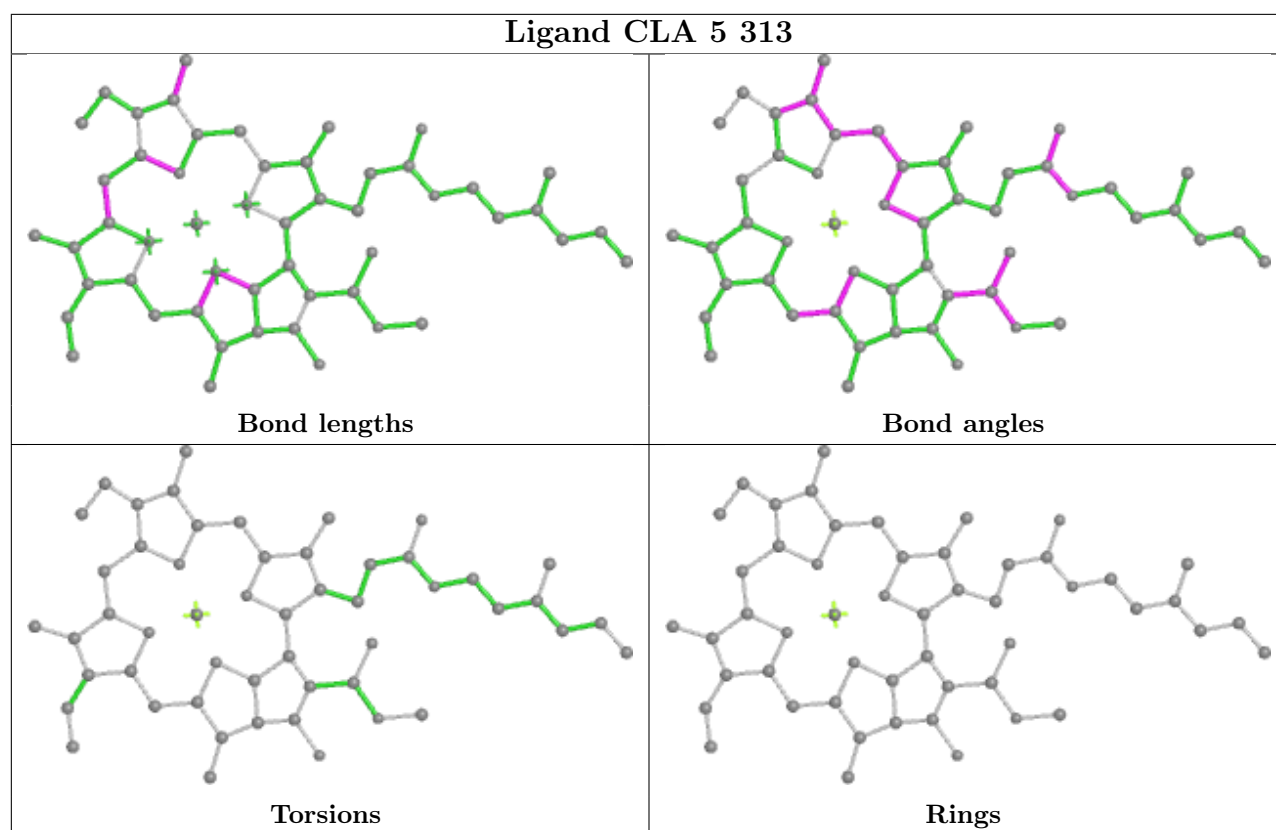
## Ligand CLA b 820

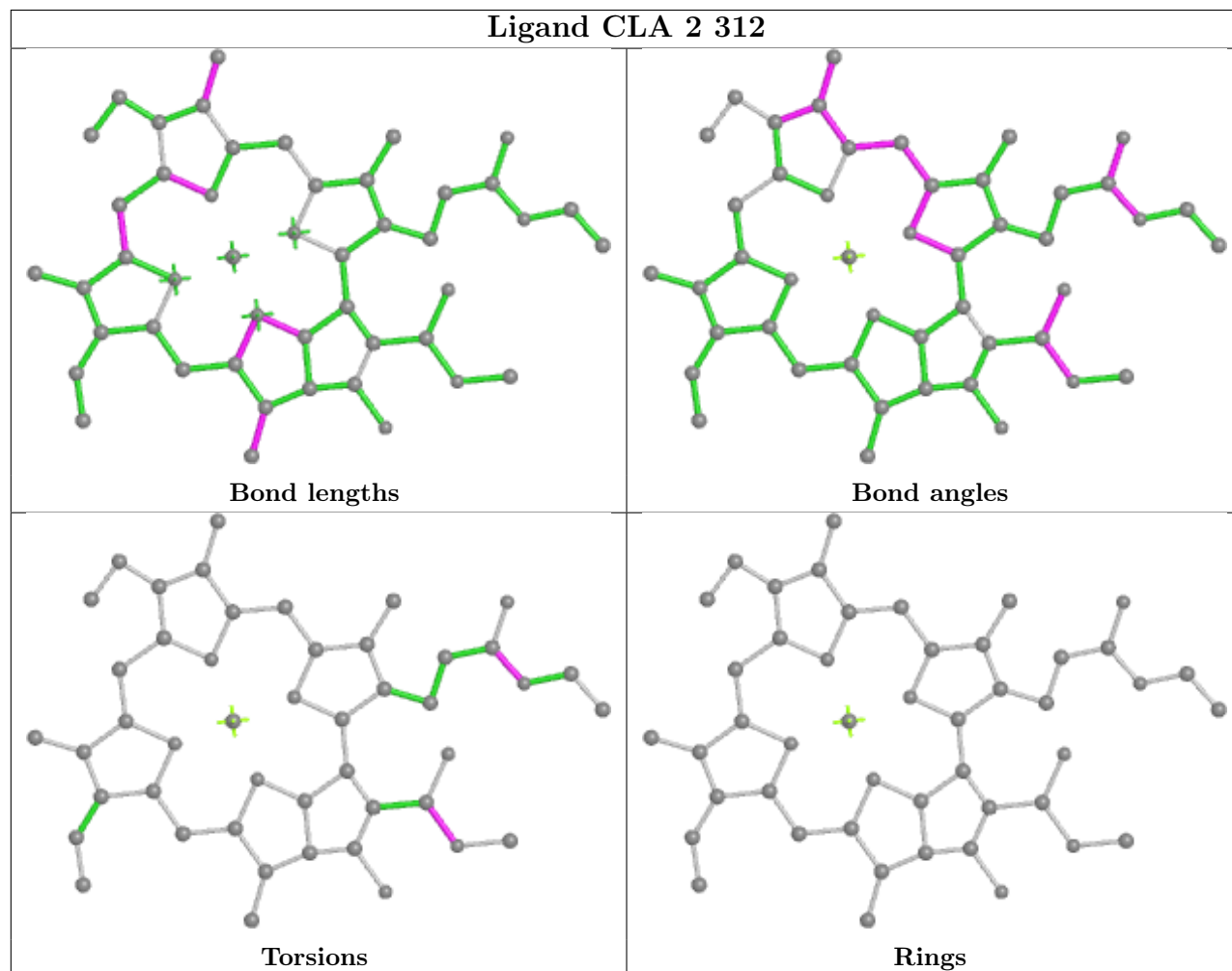
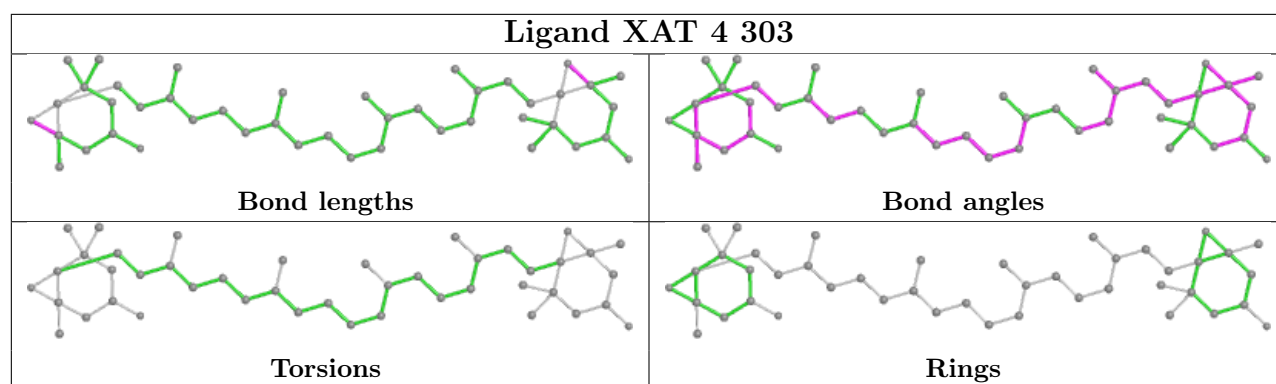


## Ligand A1L1G 5 304

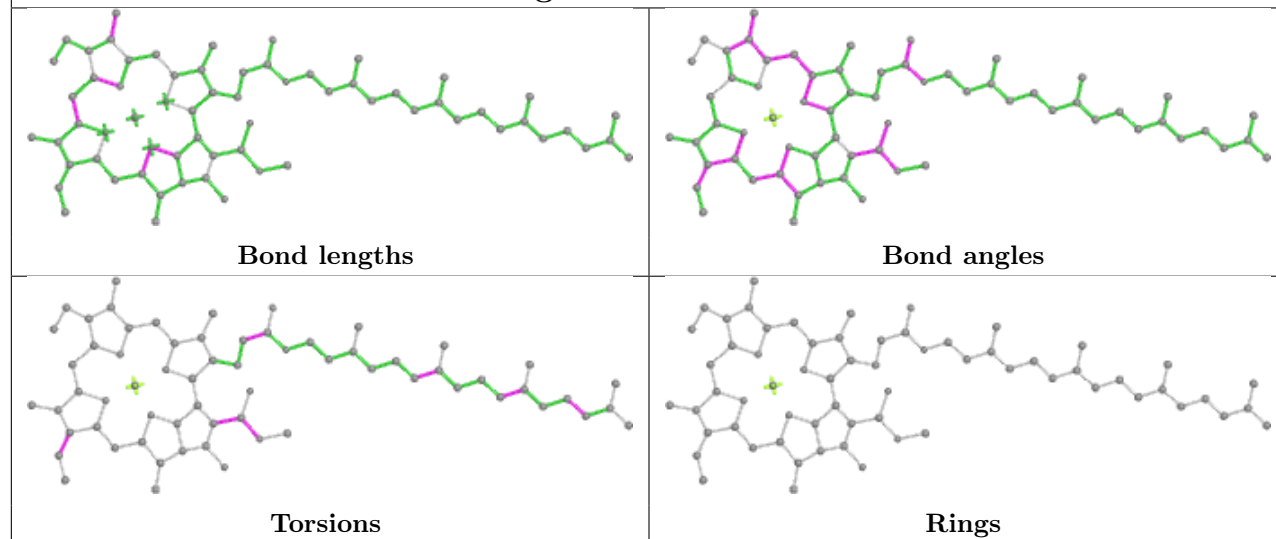


**Ligand CLA 1 305****Ligand LHG a 845**

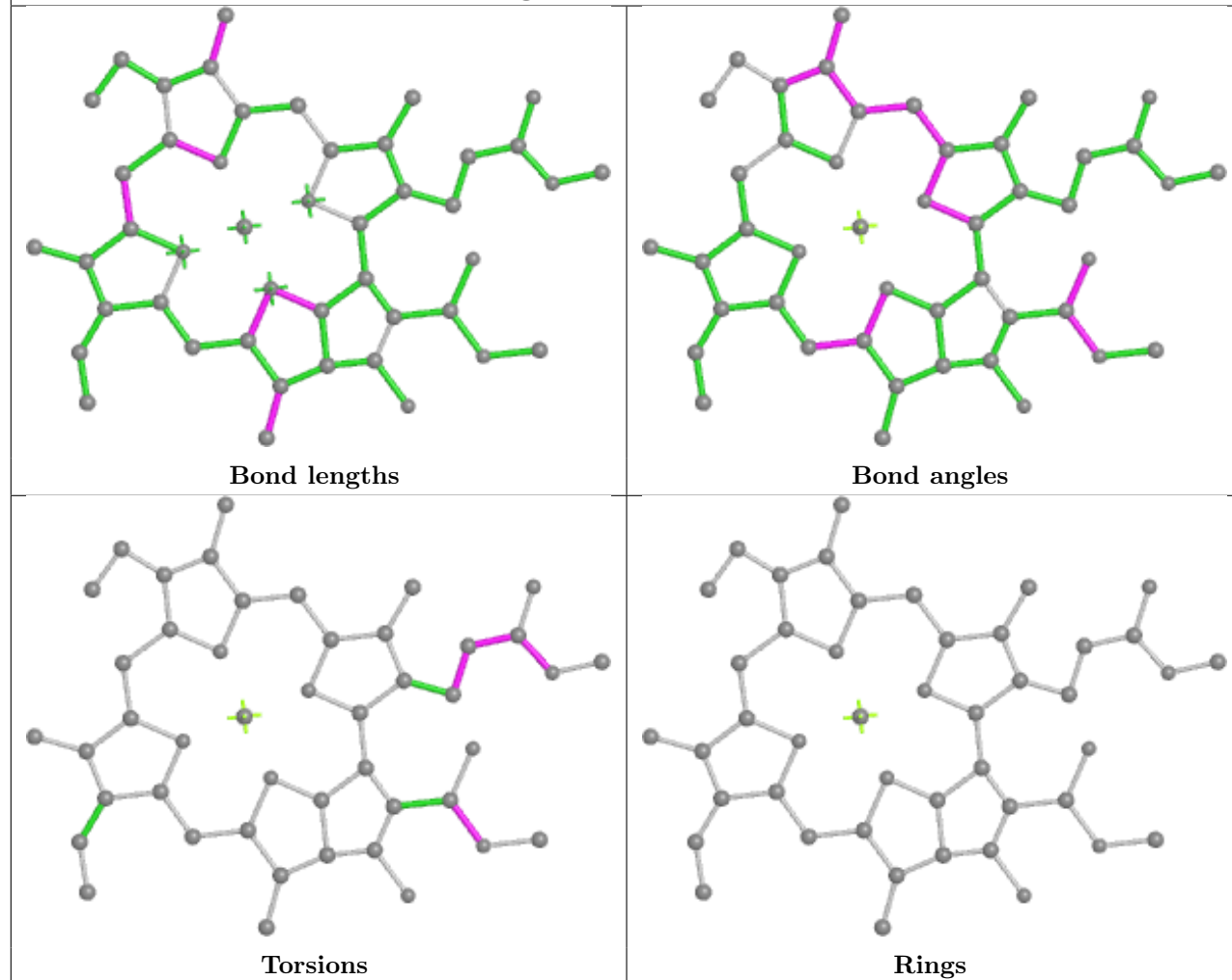




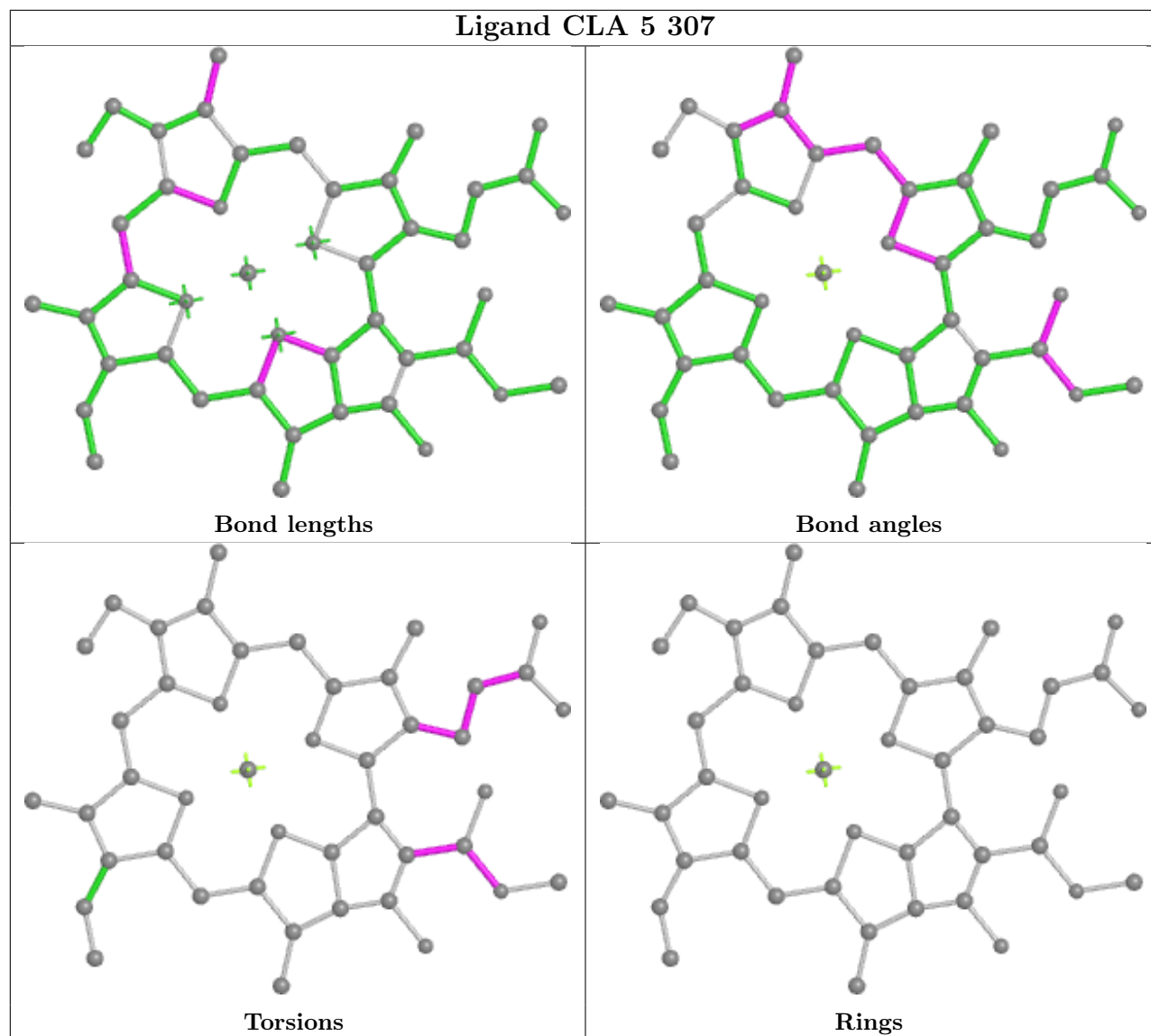
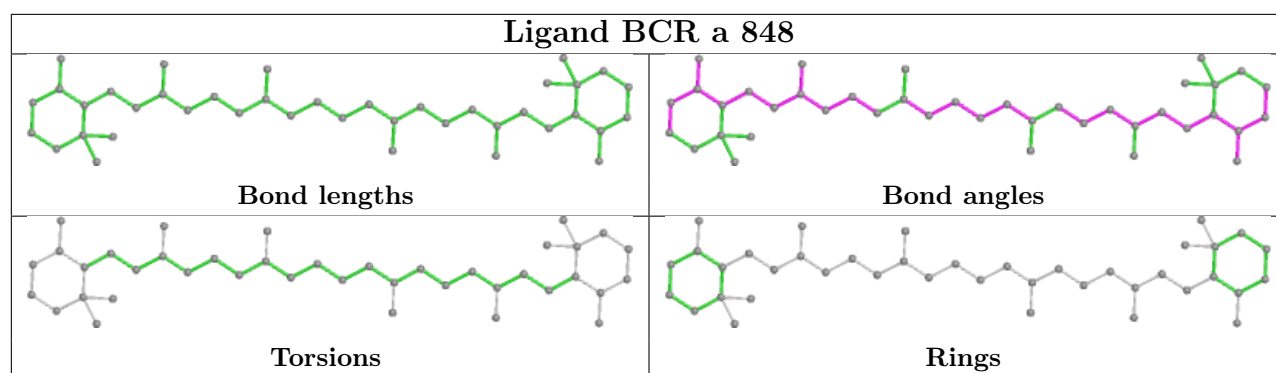
## Ligand CLA b 803

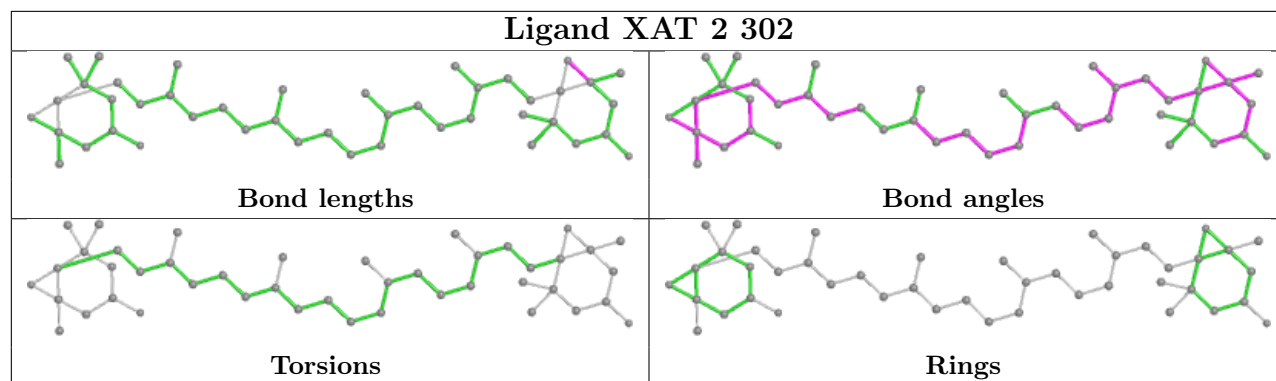
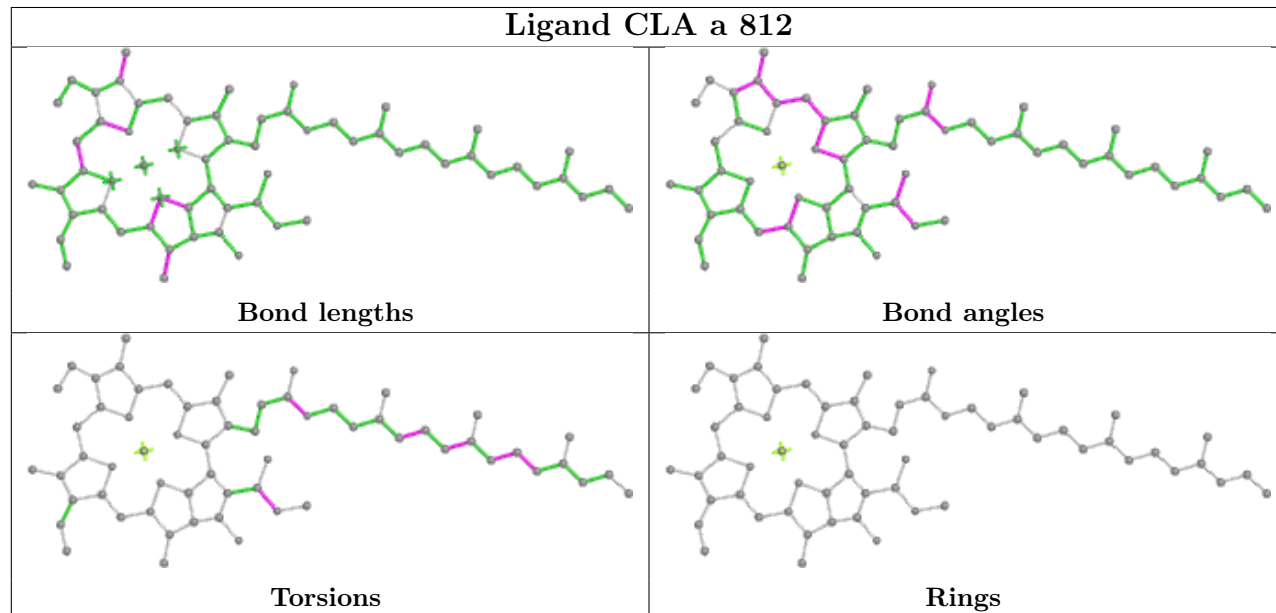
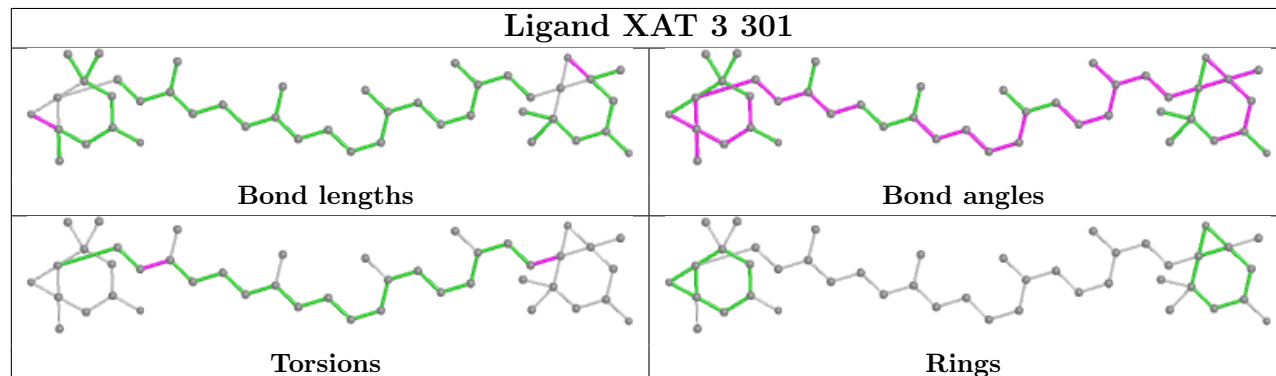


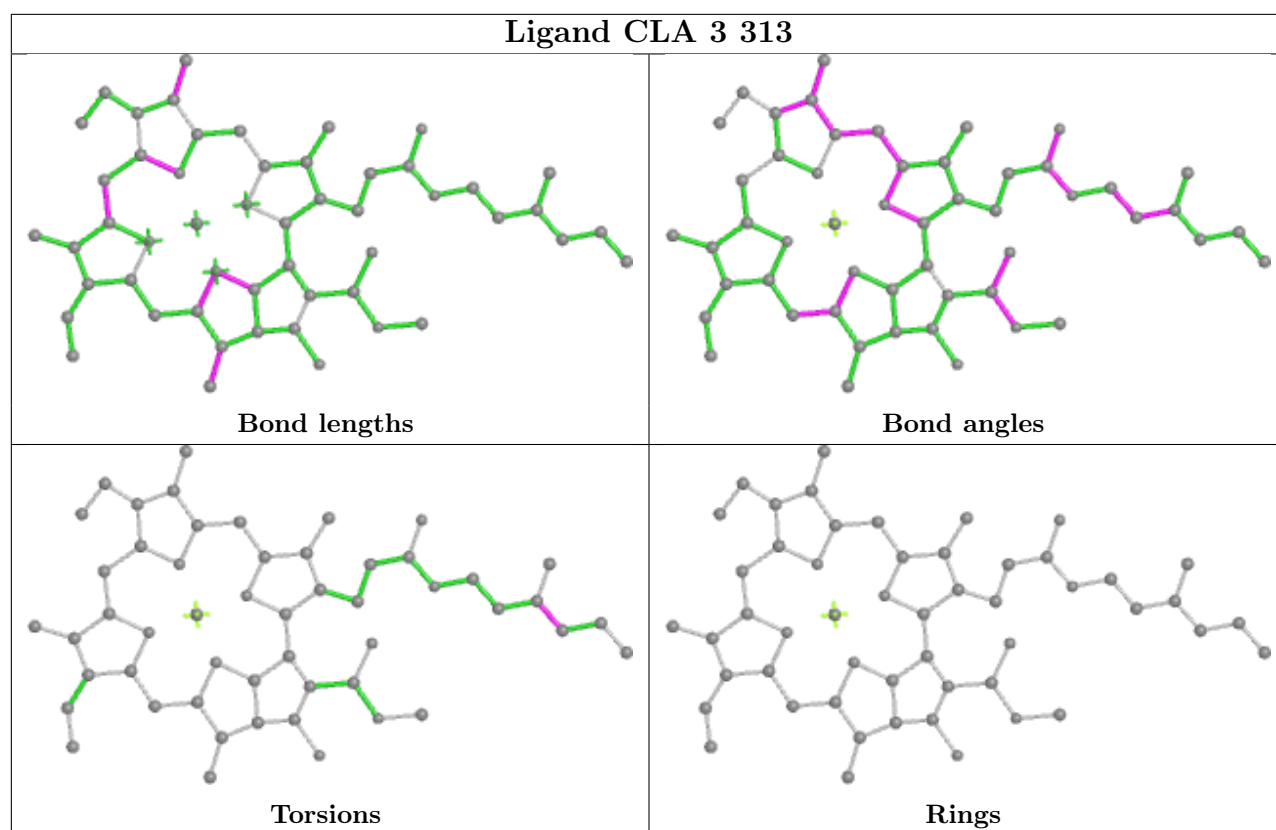
## Ligand CLA 5 311



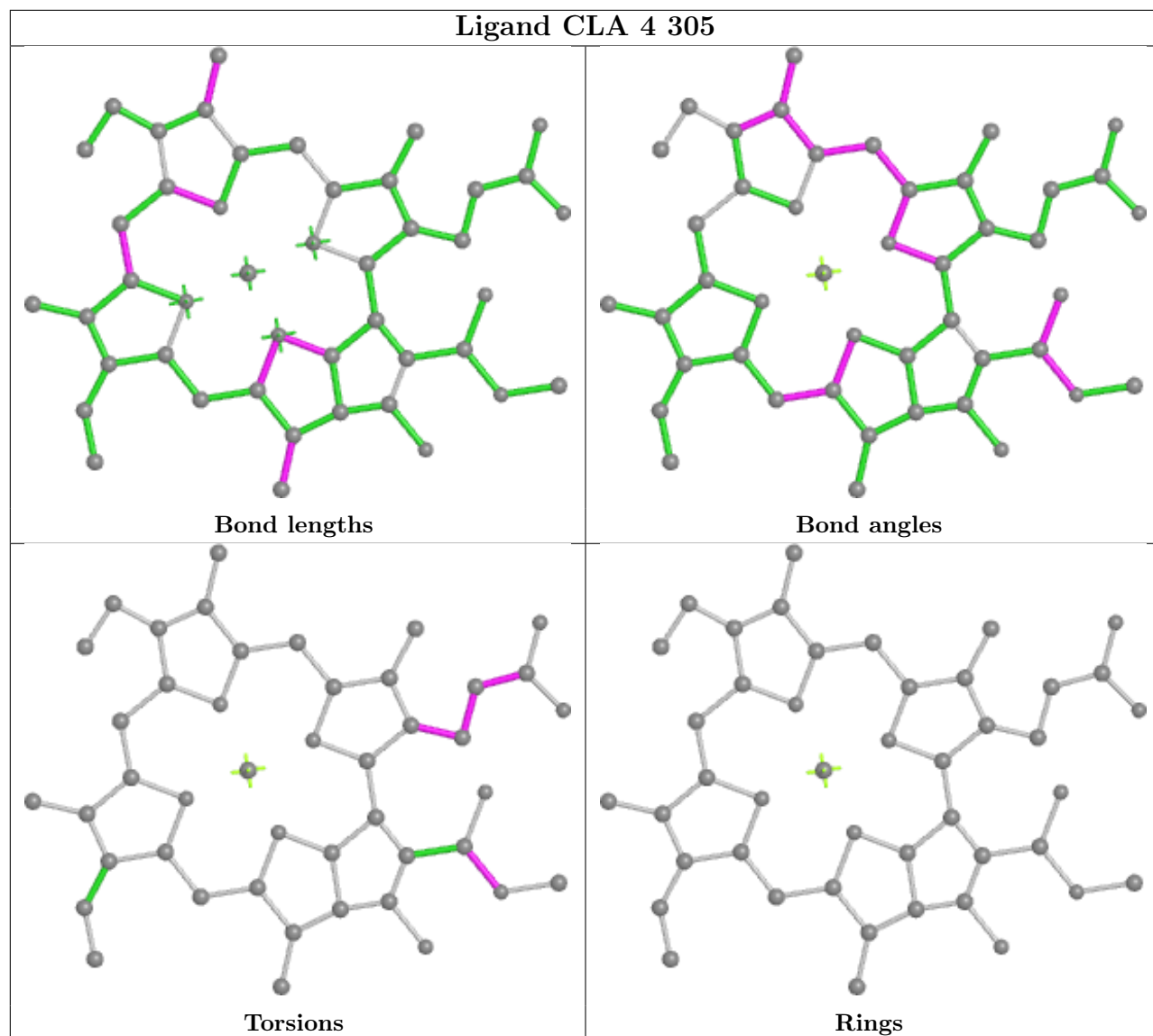


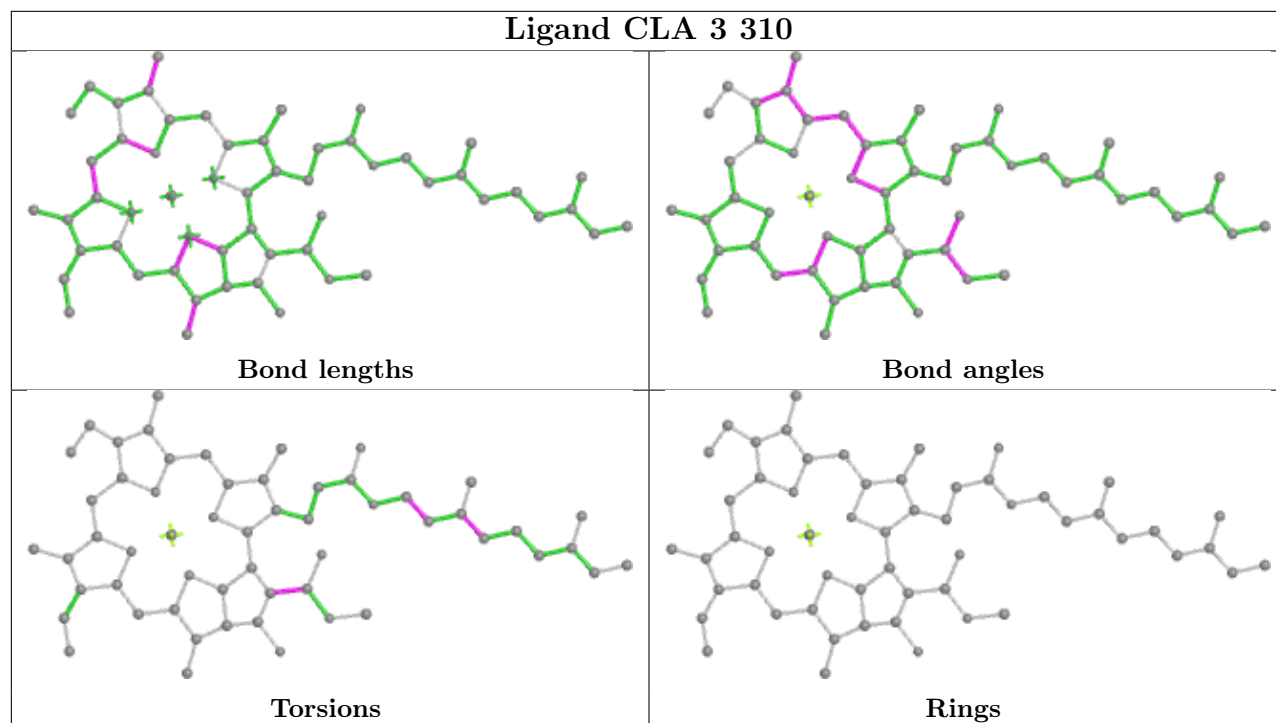
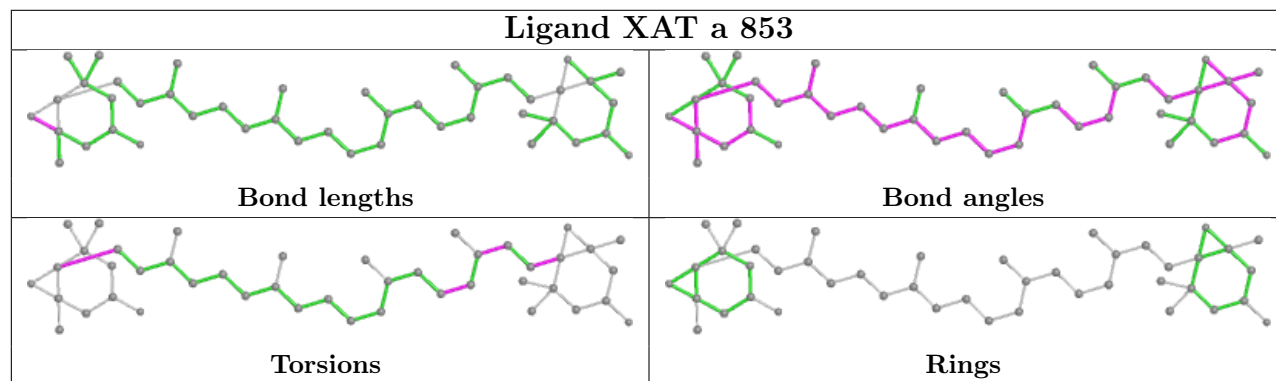


**Ligand XAT 2 302****Ligand CLA a 812****Ligand XAT 3 301**

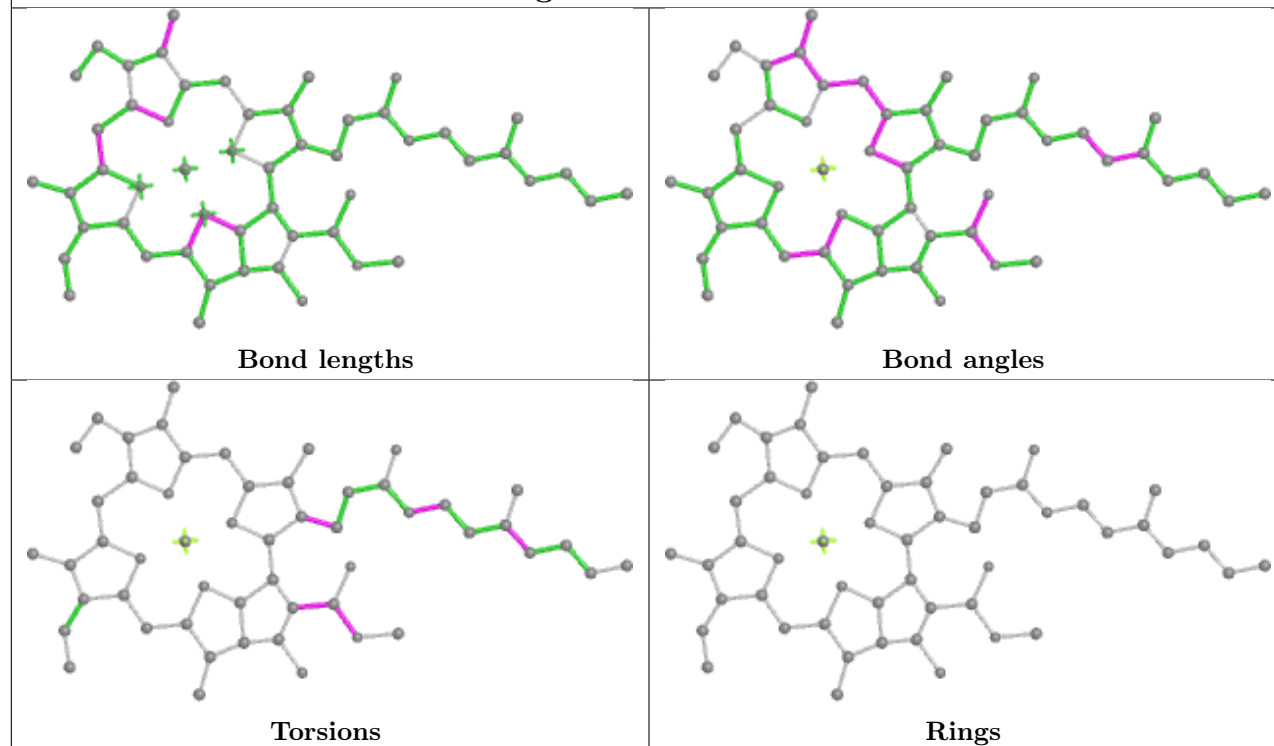


## Ligand CLA 4 305

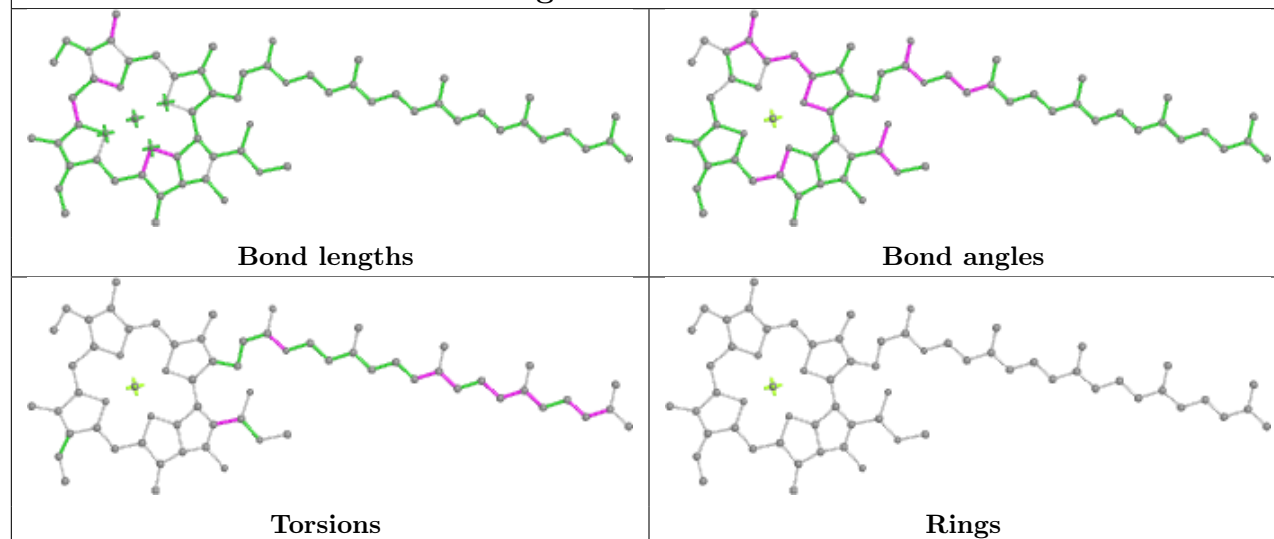


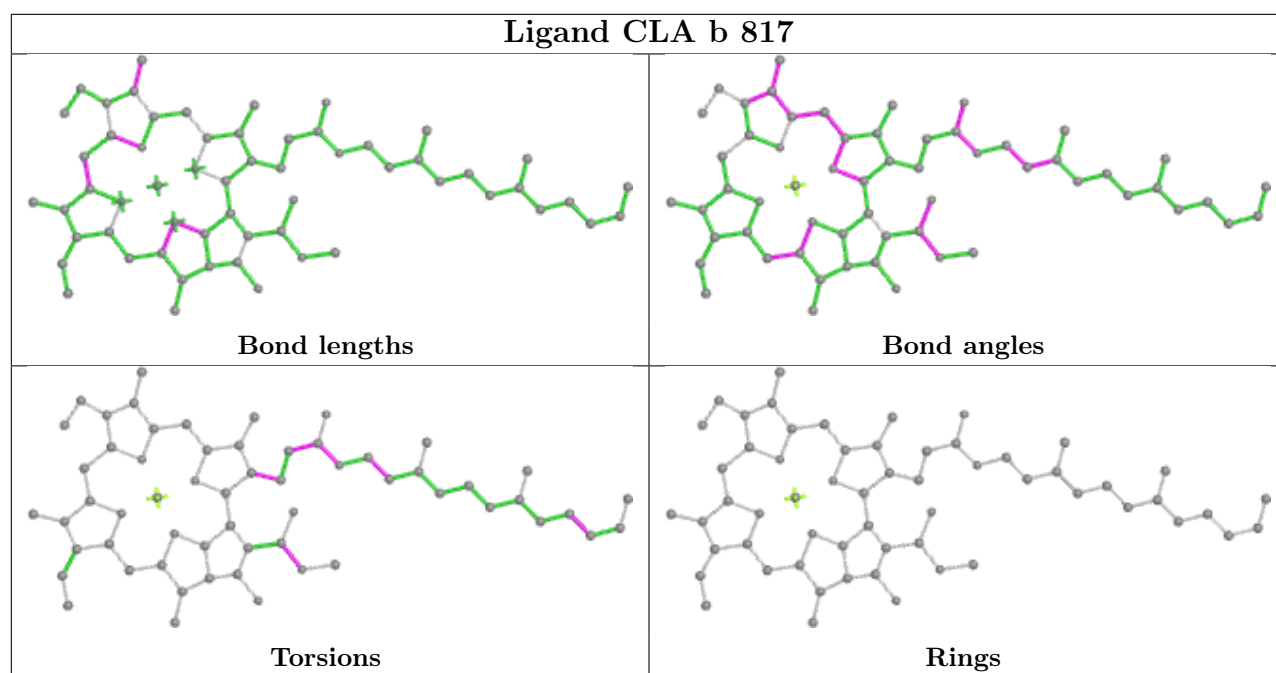
**Ligand CLA 3 310****Ligand XAT a 853**

## Ligand CLA b 835

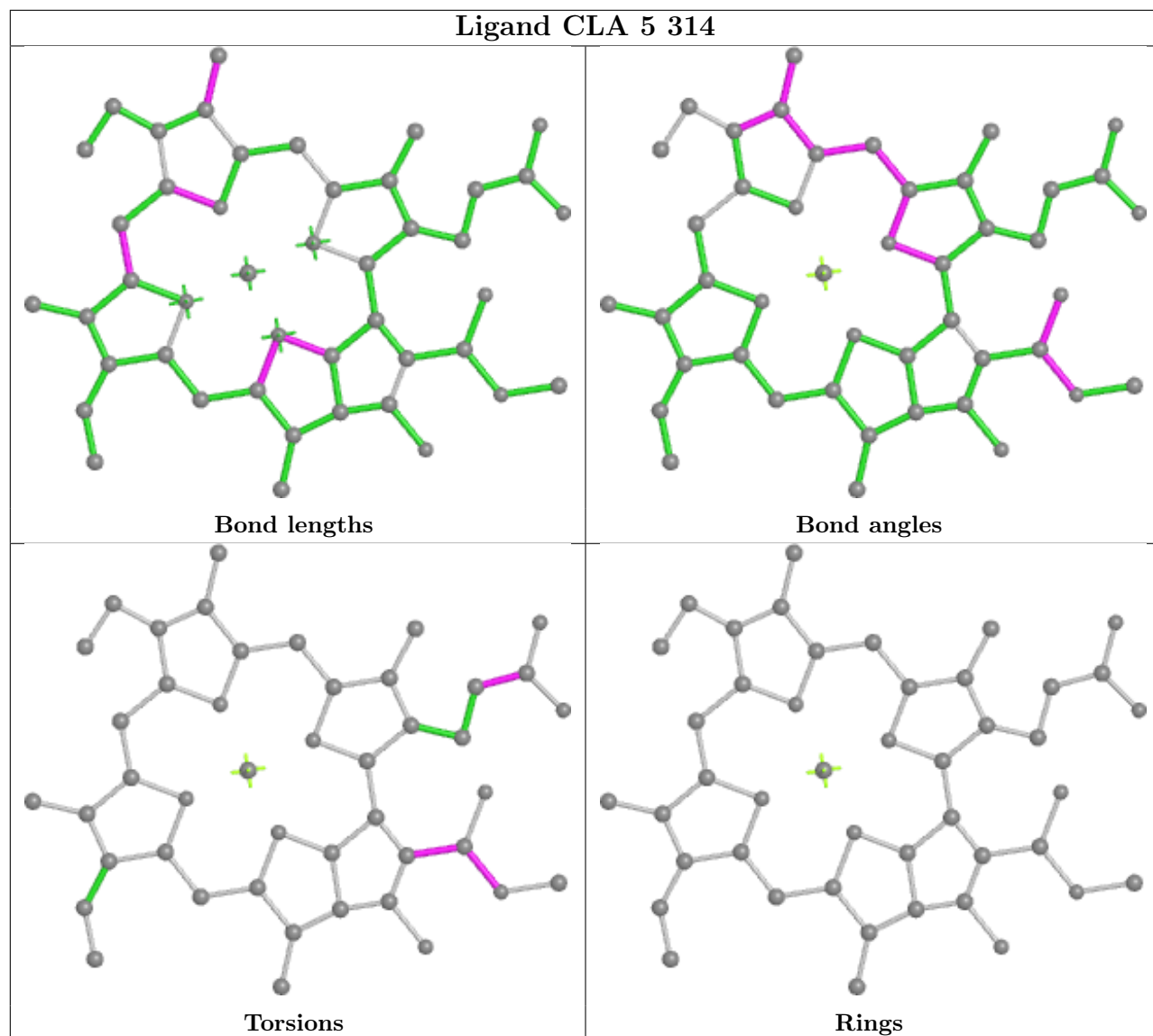


## Ligand CLA a 844



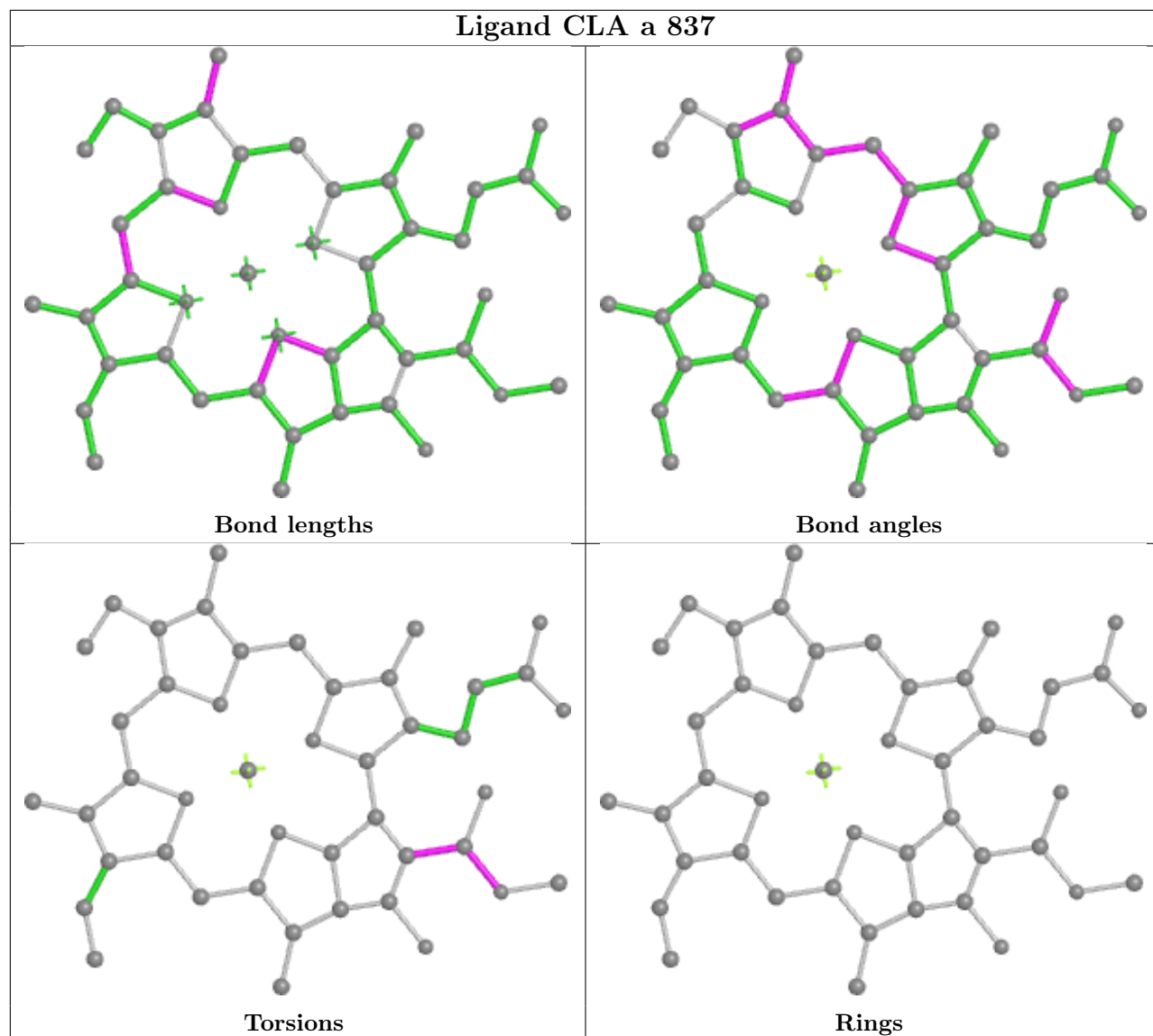


## Ligand CLA 5 314

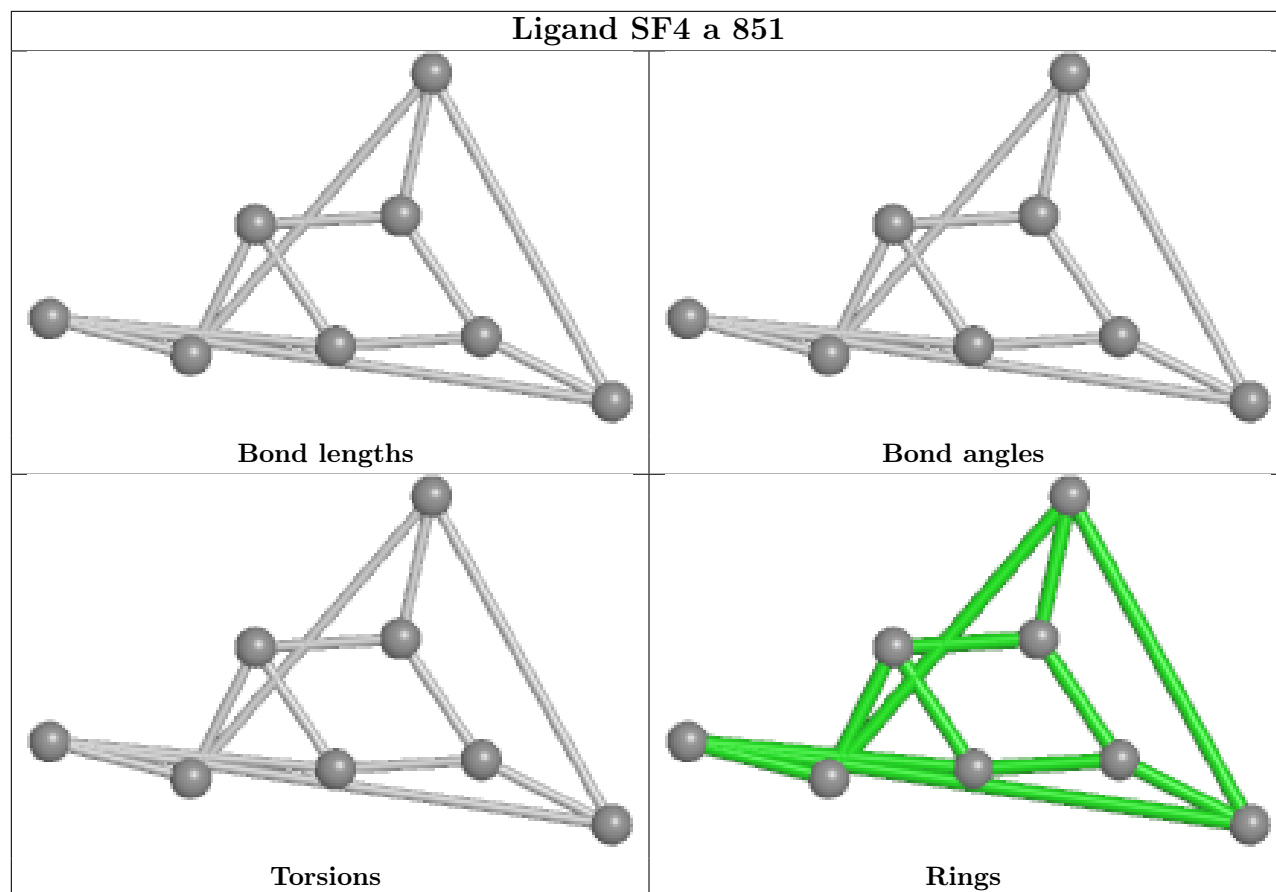




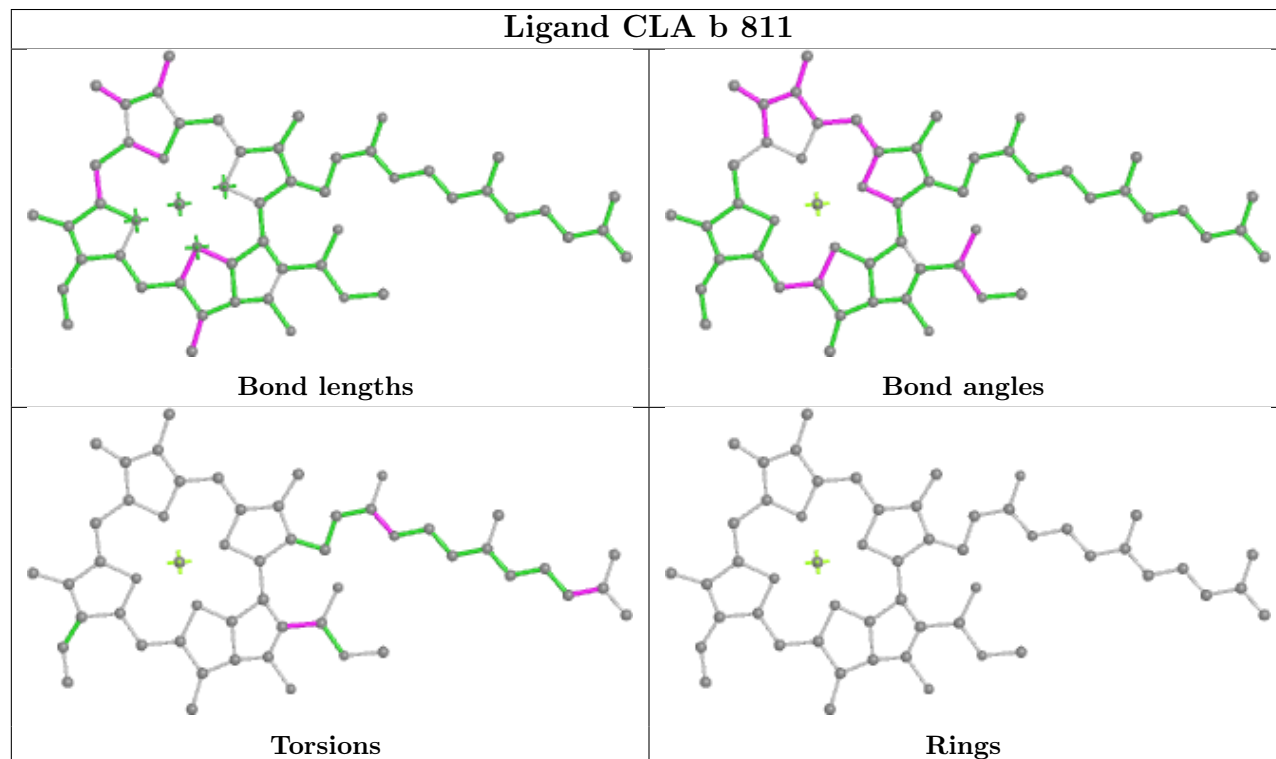
## Ligand CLA a 837

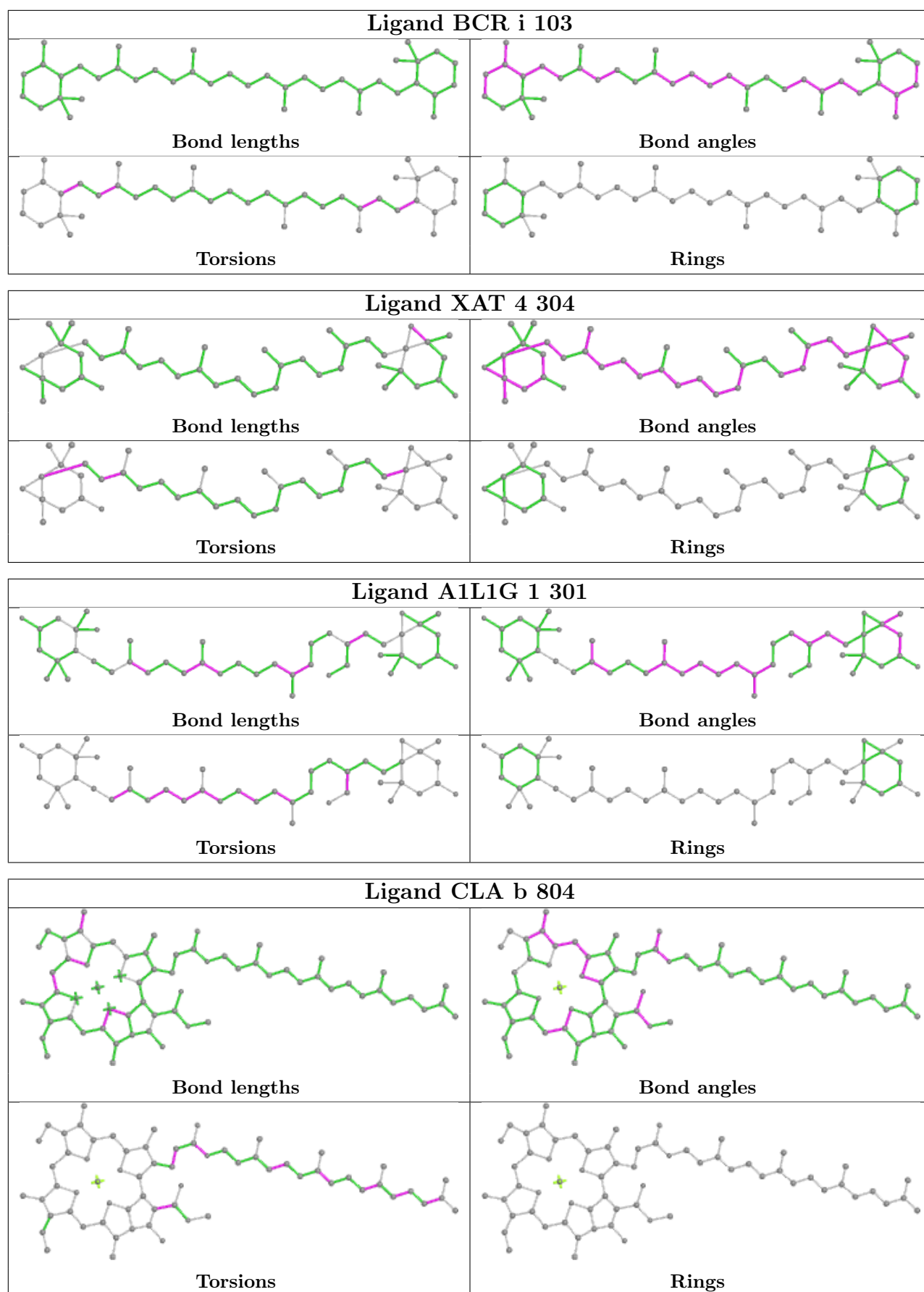


## Ligand SF4 a 851

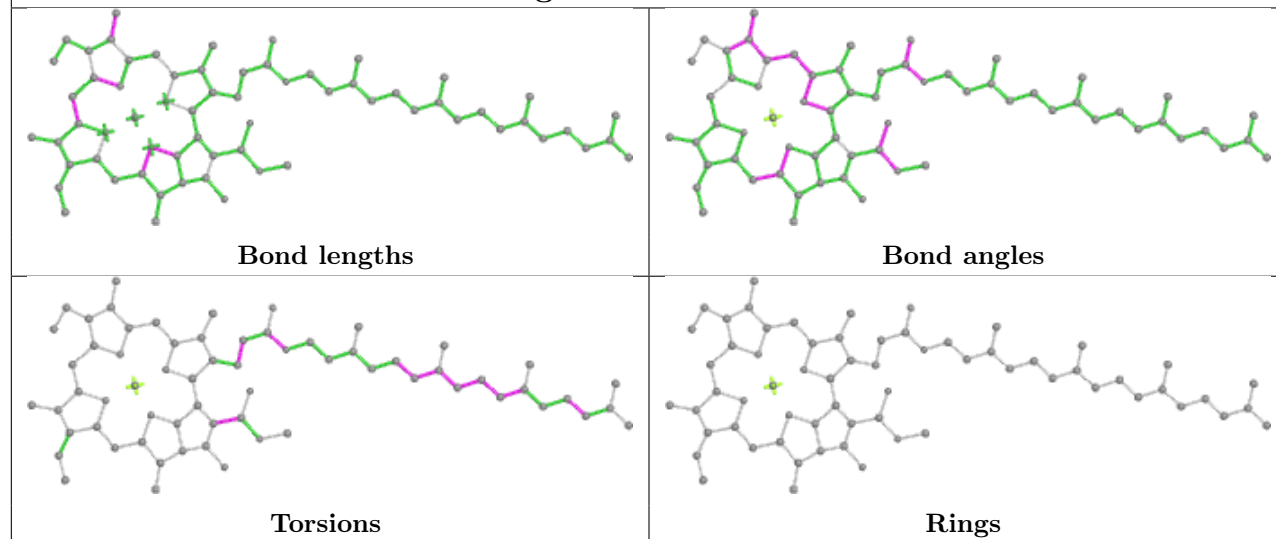


## Ligand CLA b 811

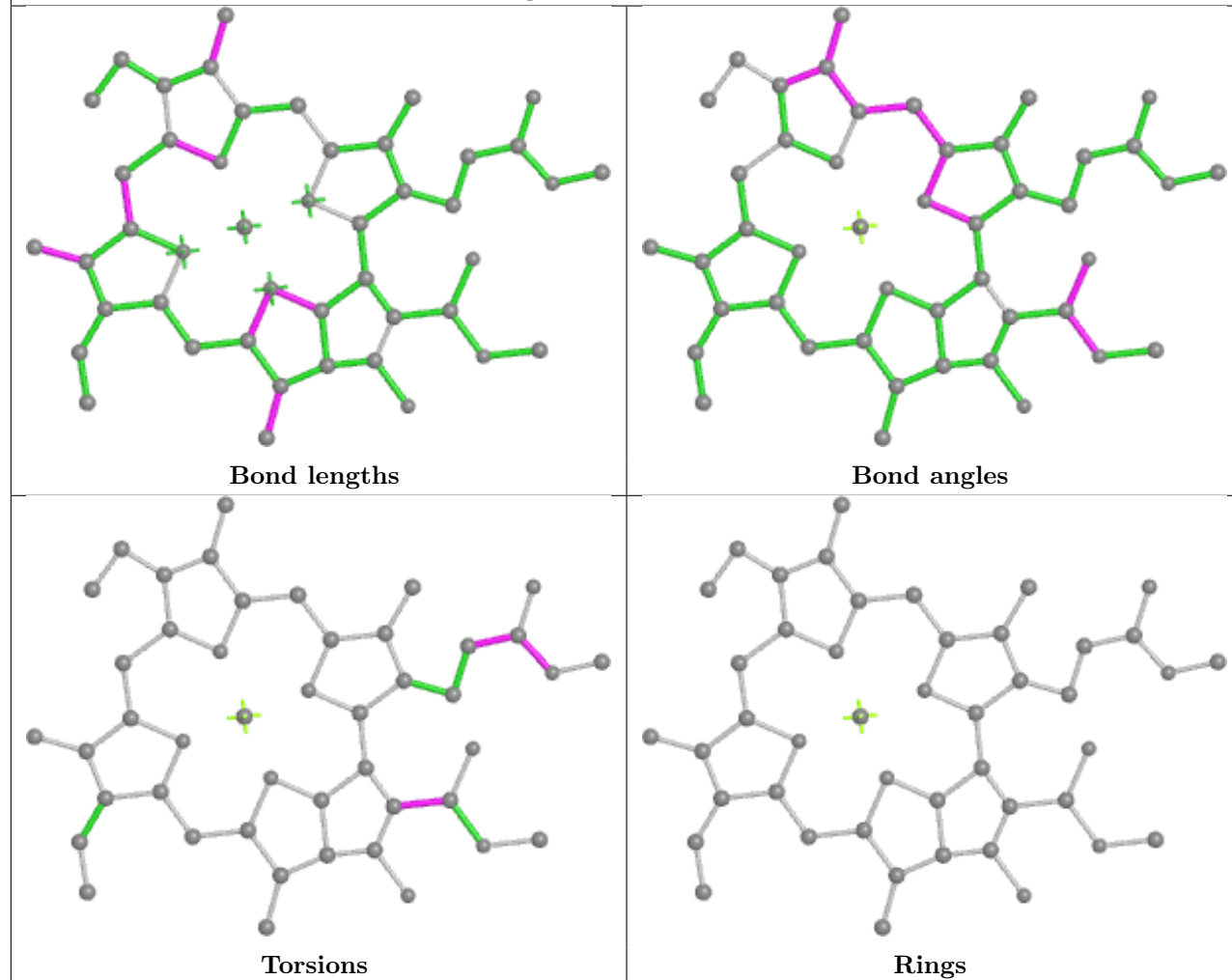


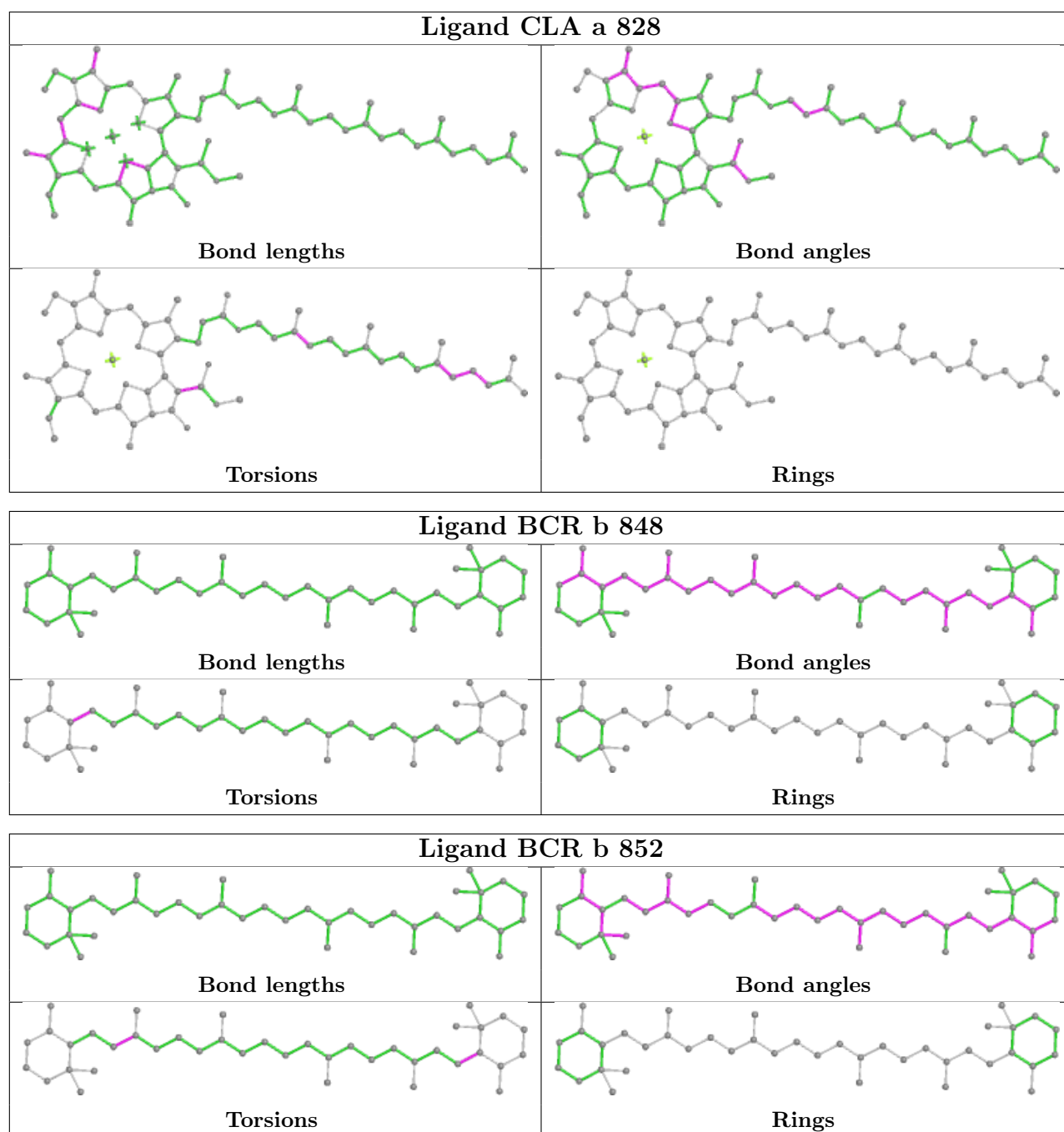


## Ligand CLA b 824

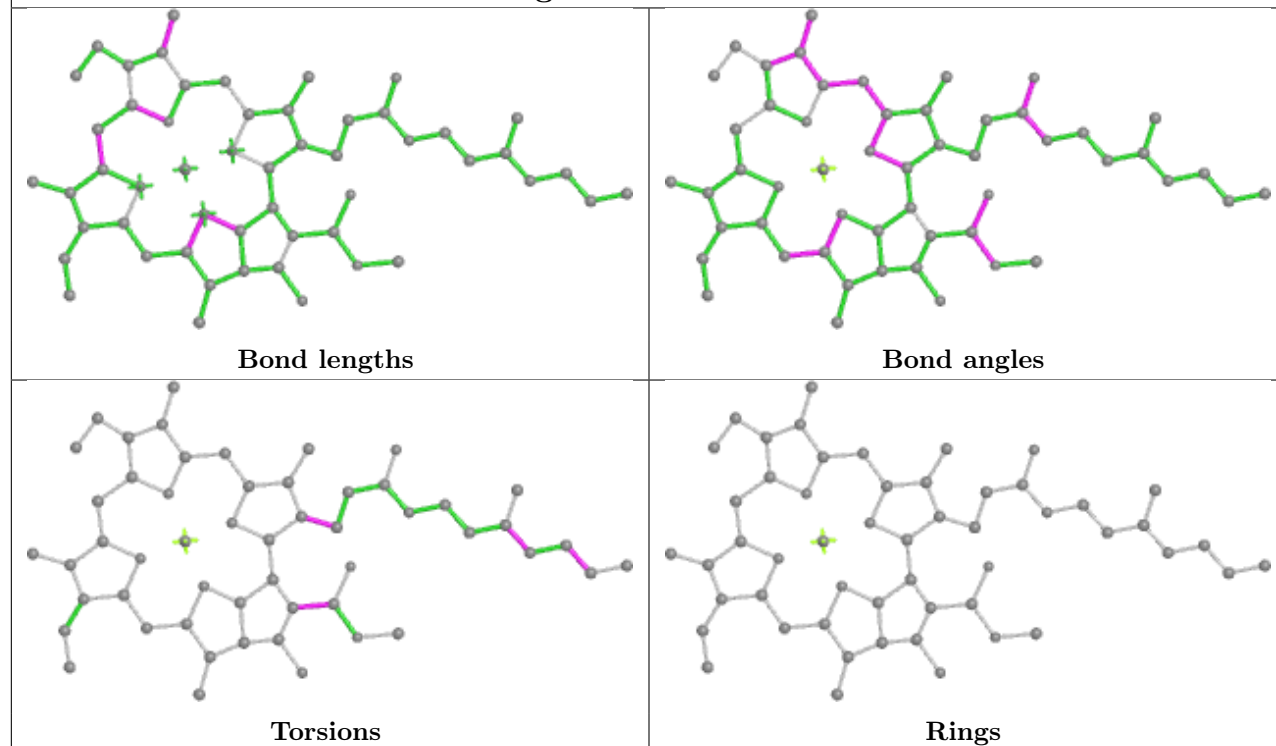


## Ligand CLA l 203

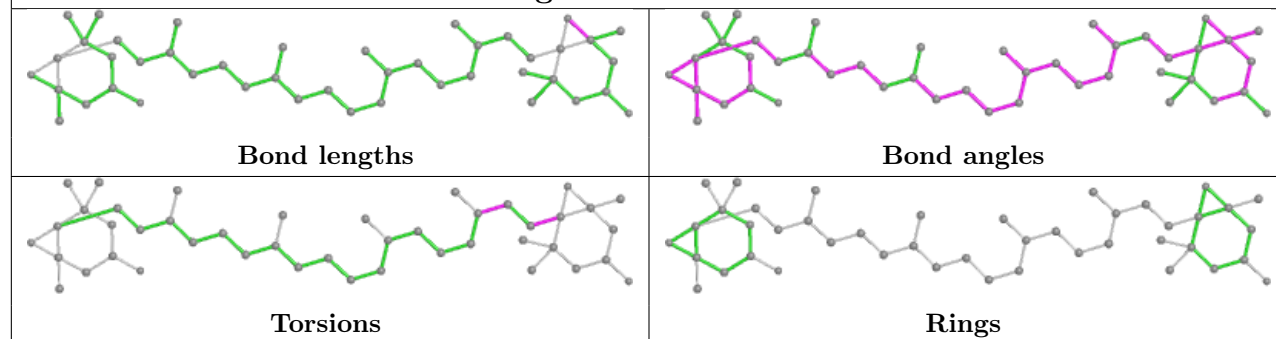




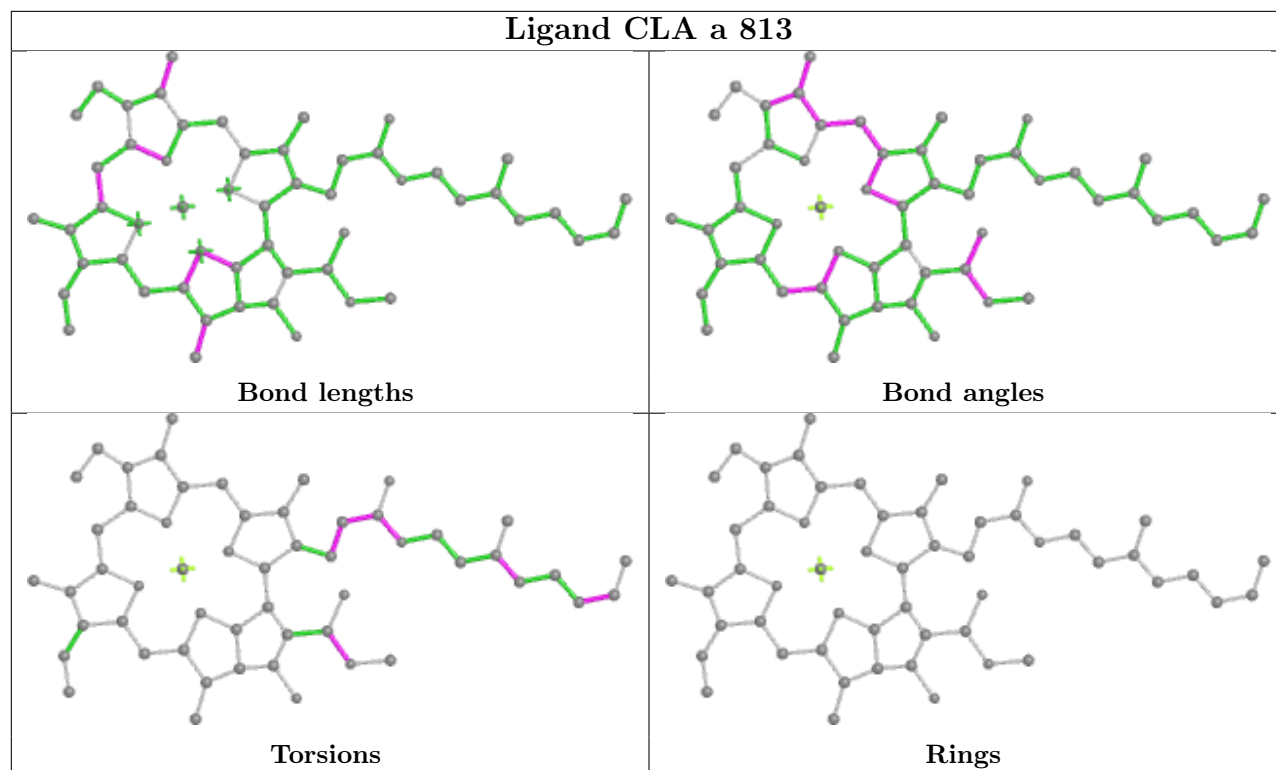
## Ligand CLA b 812



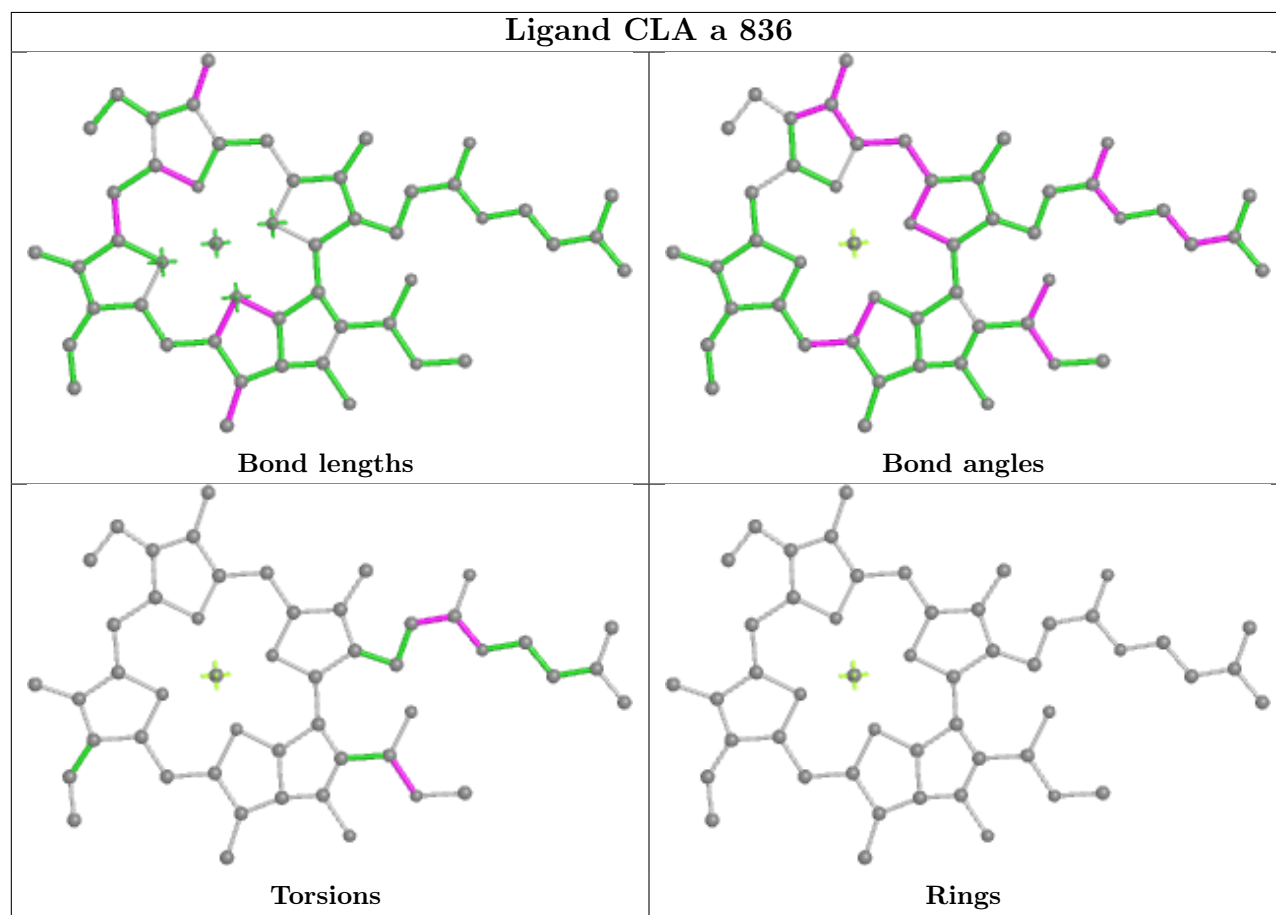
## Ligand XAT 5 303

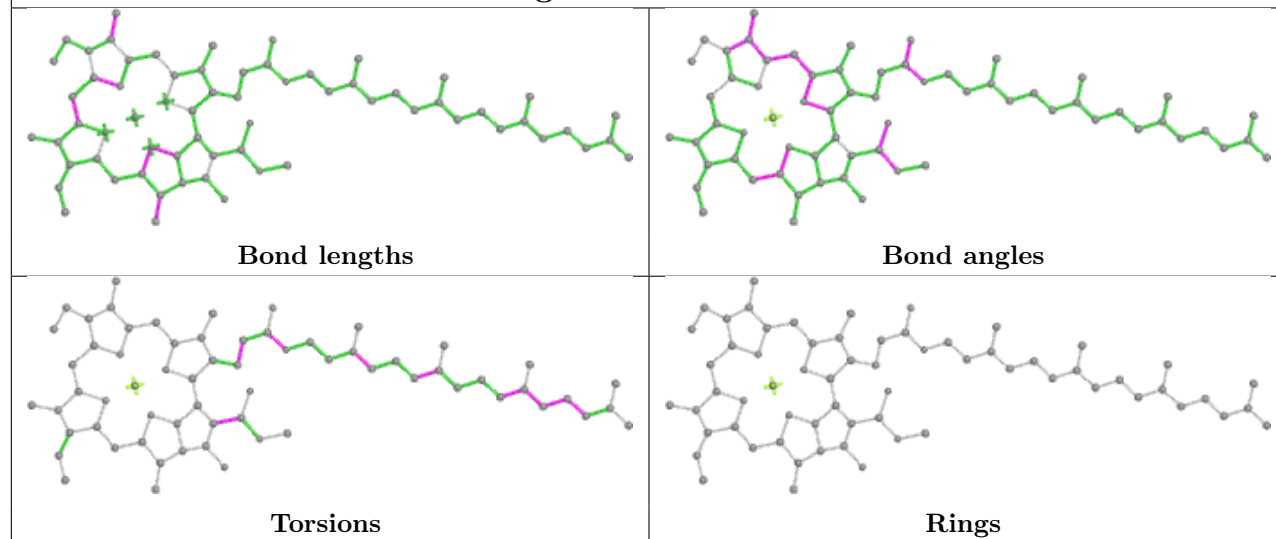
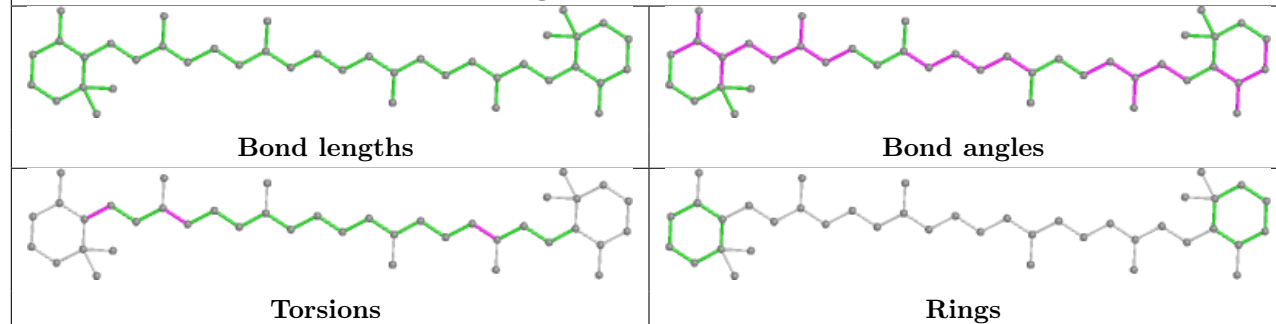
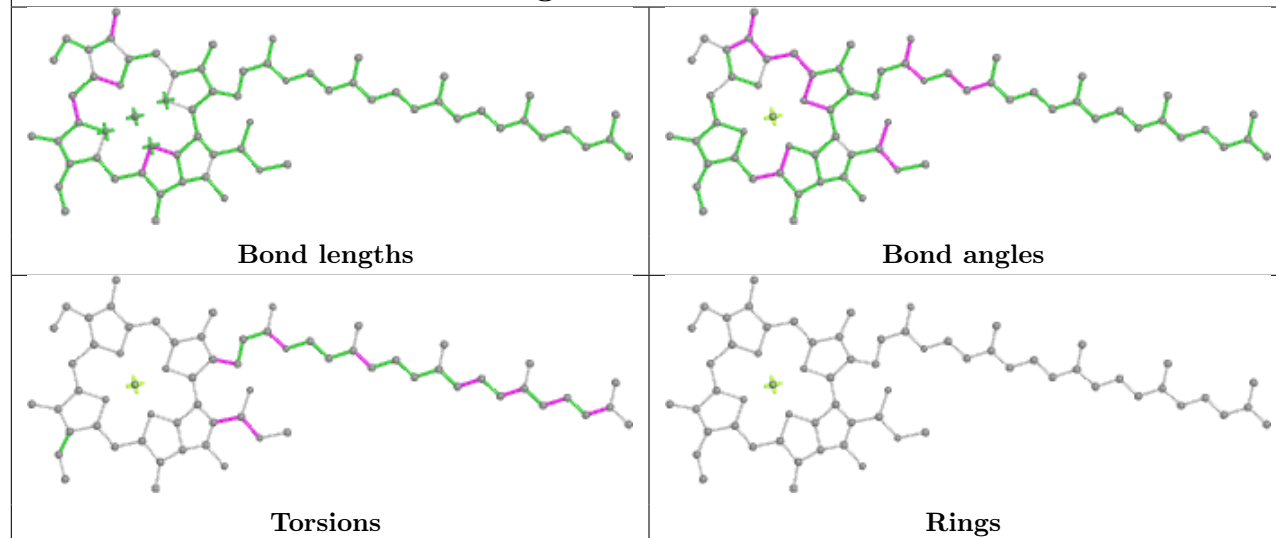


## Ligand CLA a 813

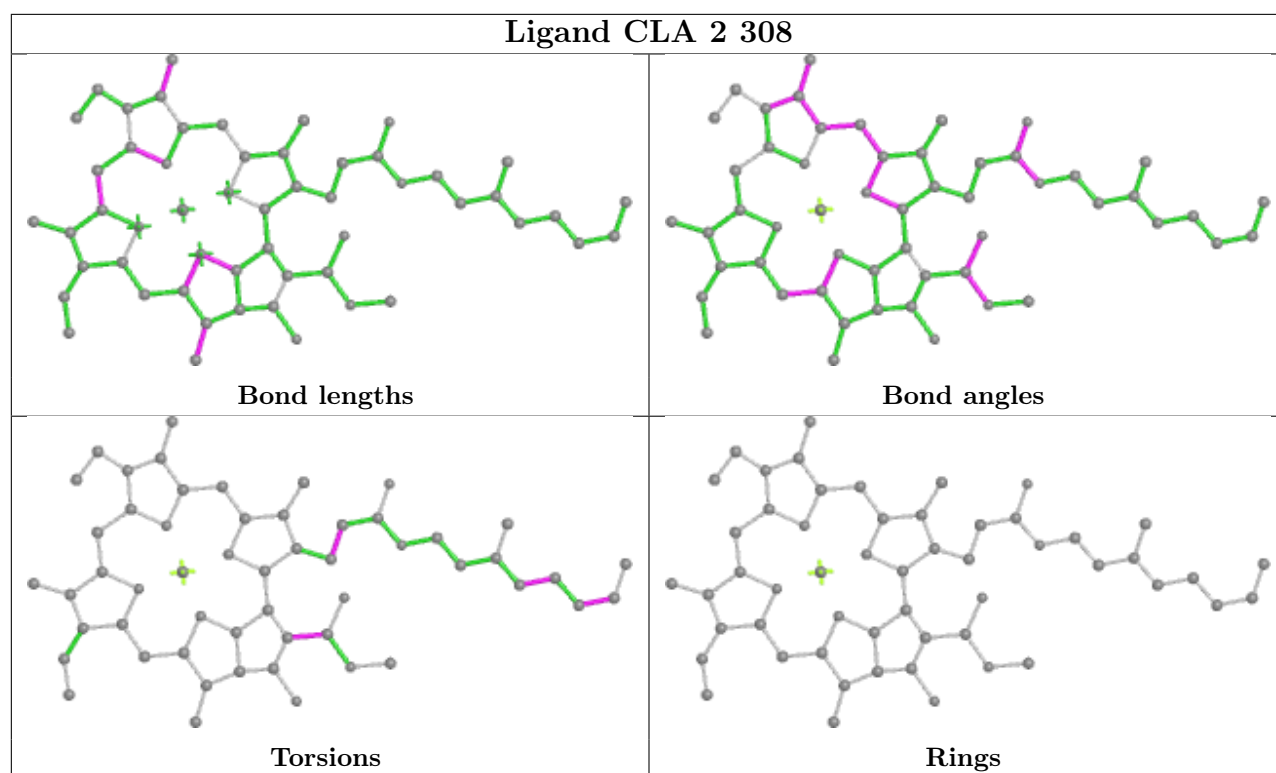


## Ligand CLA a 836



**Ligand CLA b 839****Ligand BCR b 845****Ligand CLA a 820**





## 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.

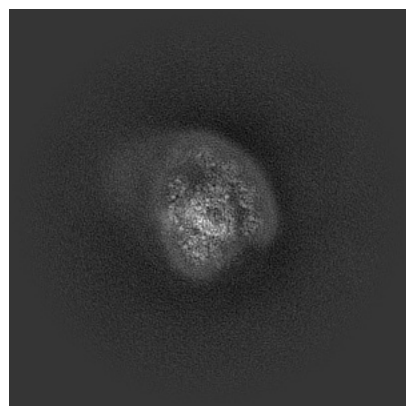
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60294. These allow visual inspection of the internal detail of the map and identification of artifacts.

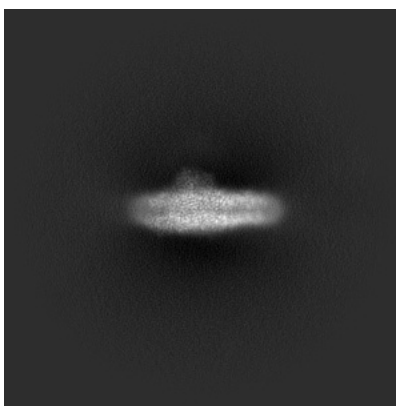
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

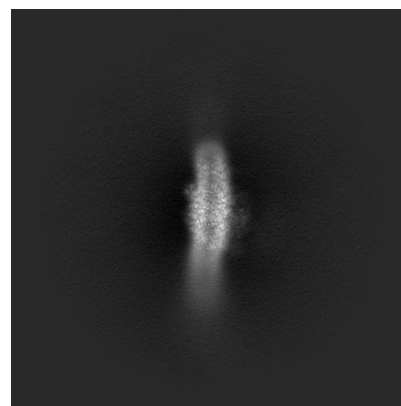
#### 6.1.1 Primary map



X

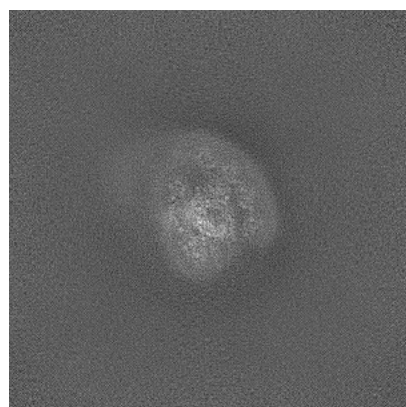


Y

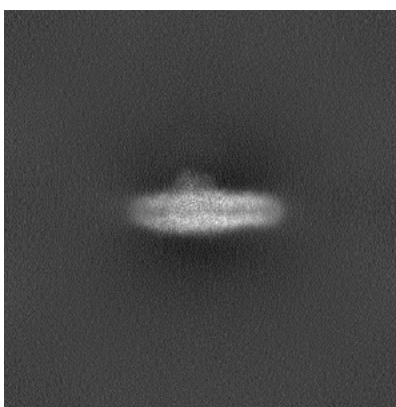


Z

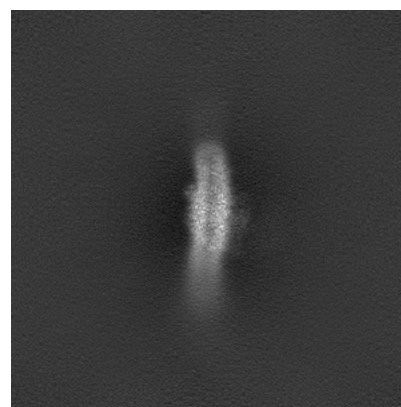
#### 6.1.2 Raw map



X



Y

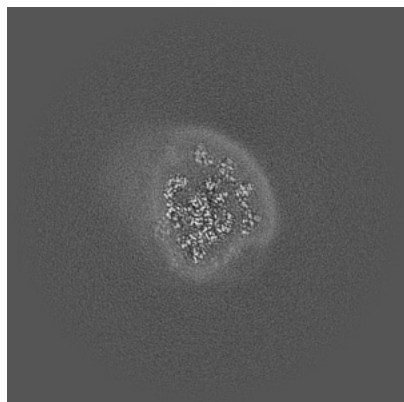


Z

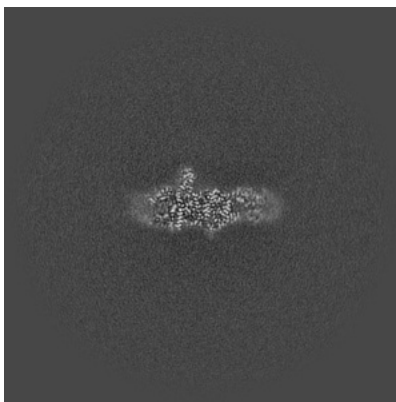
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

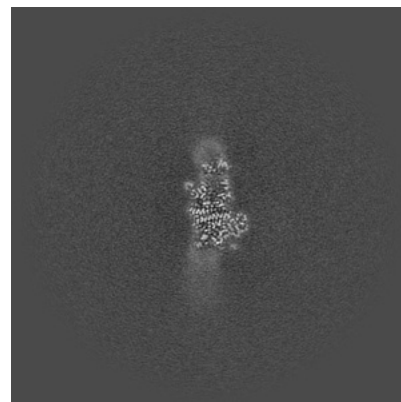
### 6.2.1 Primary map



X Index: 256

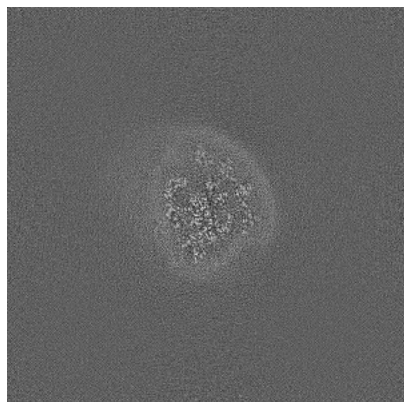


Y Index: 256

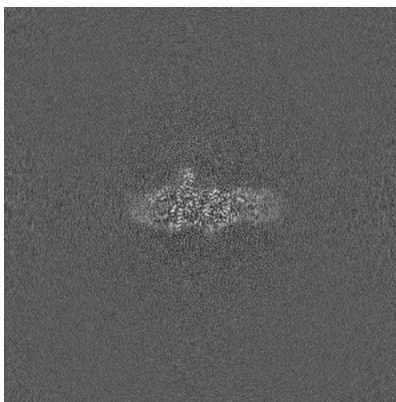


Z Index: 256

### 6.2.2 Raw map



X Index: 256



Y Index: 256

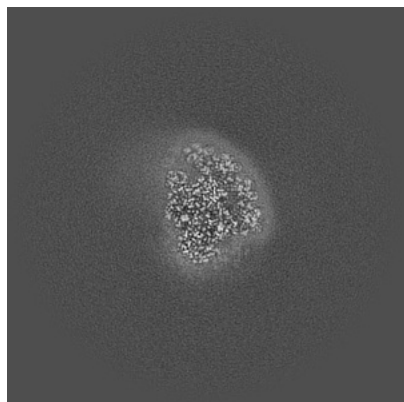


Z Index: 256

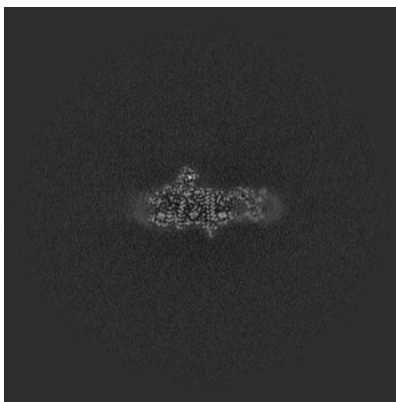
The images above show central slices of the map in three orthogonal directions.

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

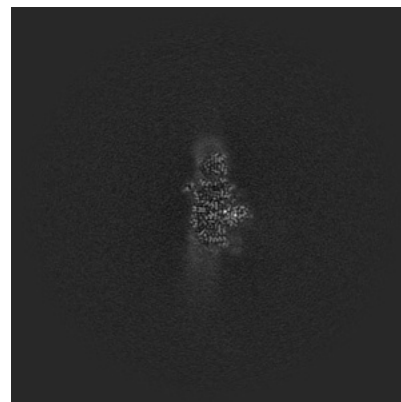
### 6.3.1 Primary map



X Index: 266

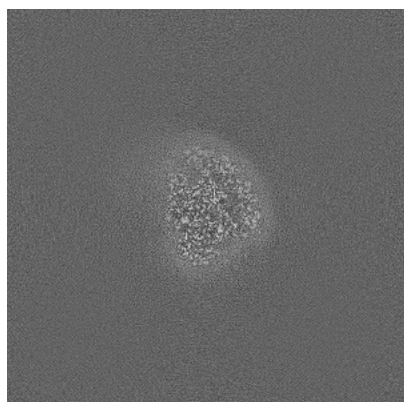


Y Index: 253

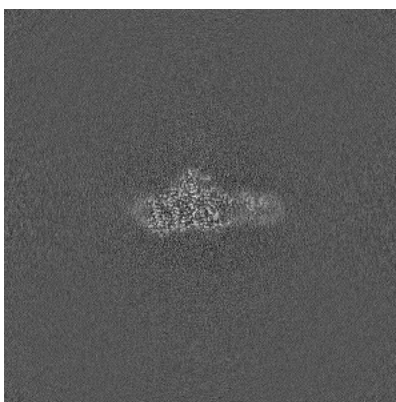


Z Index: 240

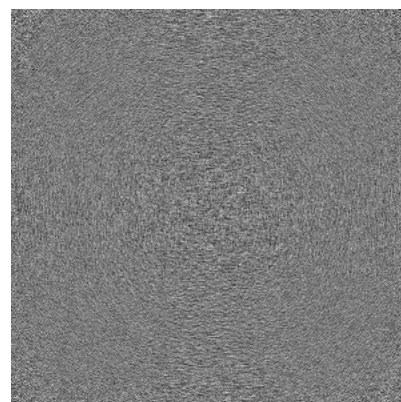
### 6.3.2 Raw map



X Index: 266



Y Index: 247



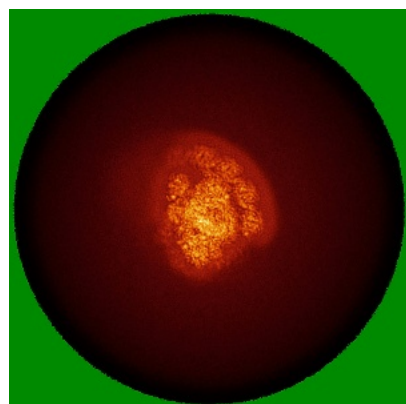
Z Index: 511

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

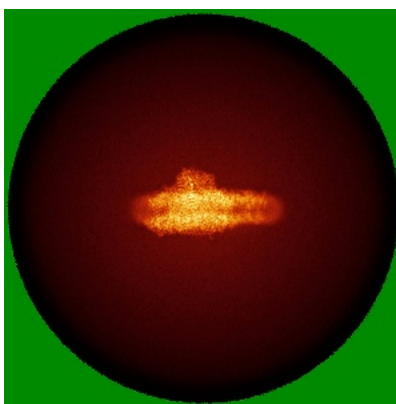


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

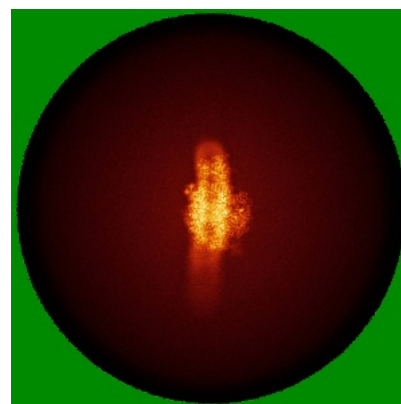
### 6.4.1 Primary map



X

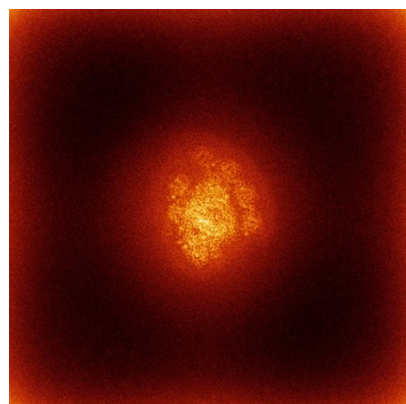


Y

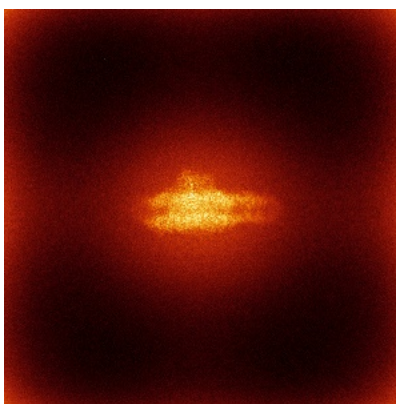


Z

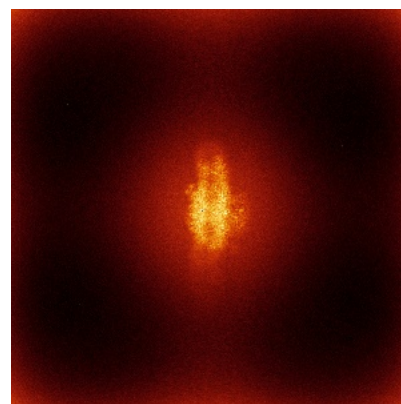
### 6.4.2 Raw map



X



Y

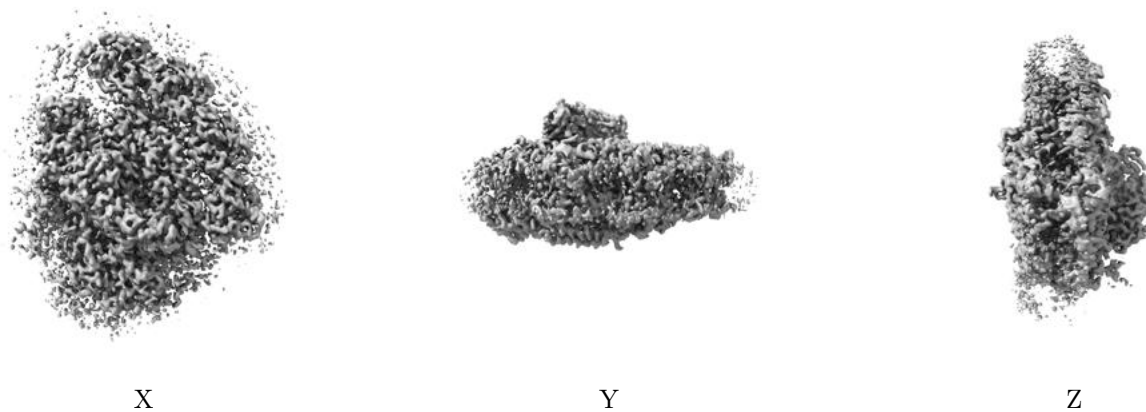


Z

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.

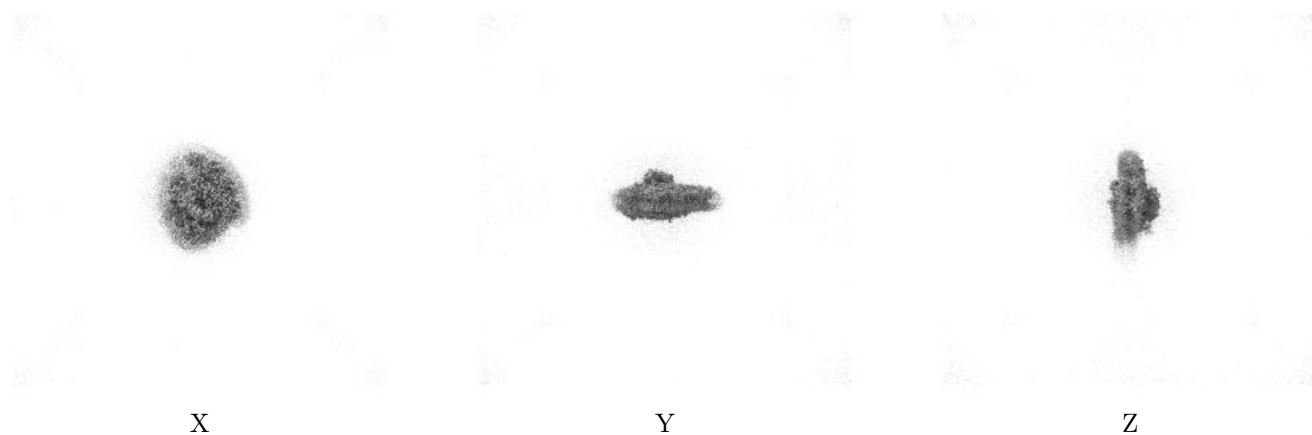
## 6.5 Orthogonal surface views [i](#)

### 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.

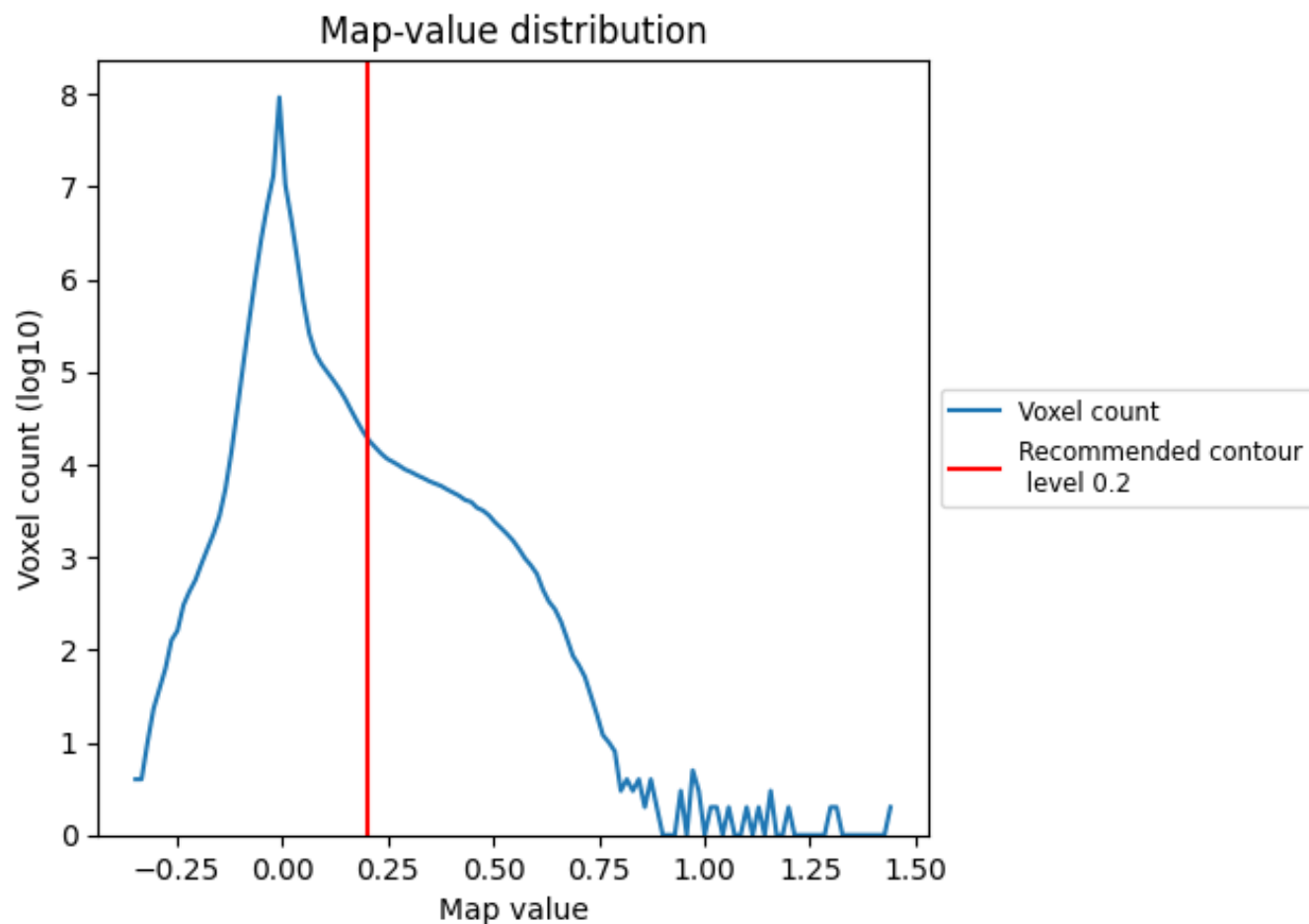
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

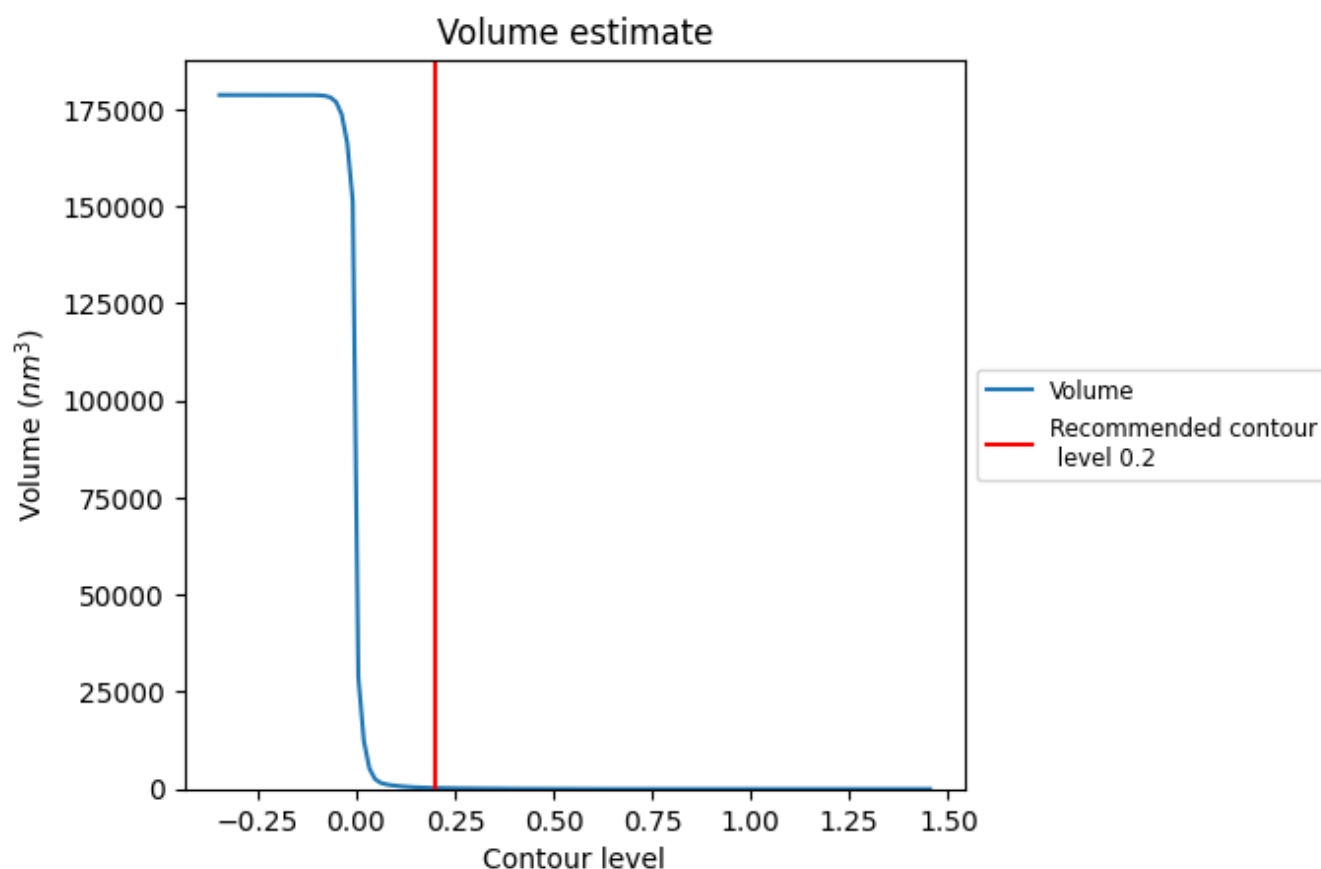
This section contains the results of statistical analysis of the map.

### 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](#)

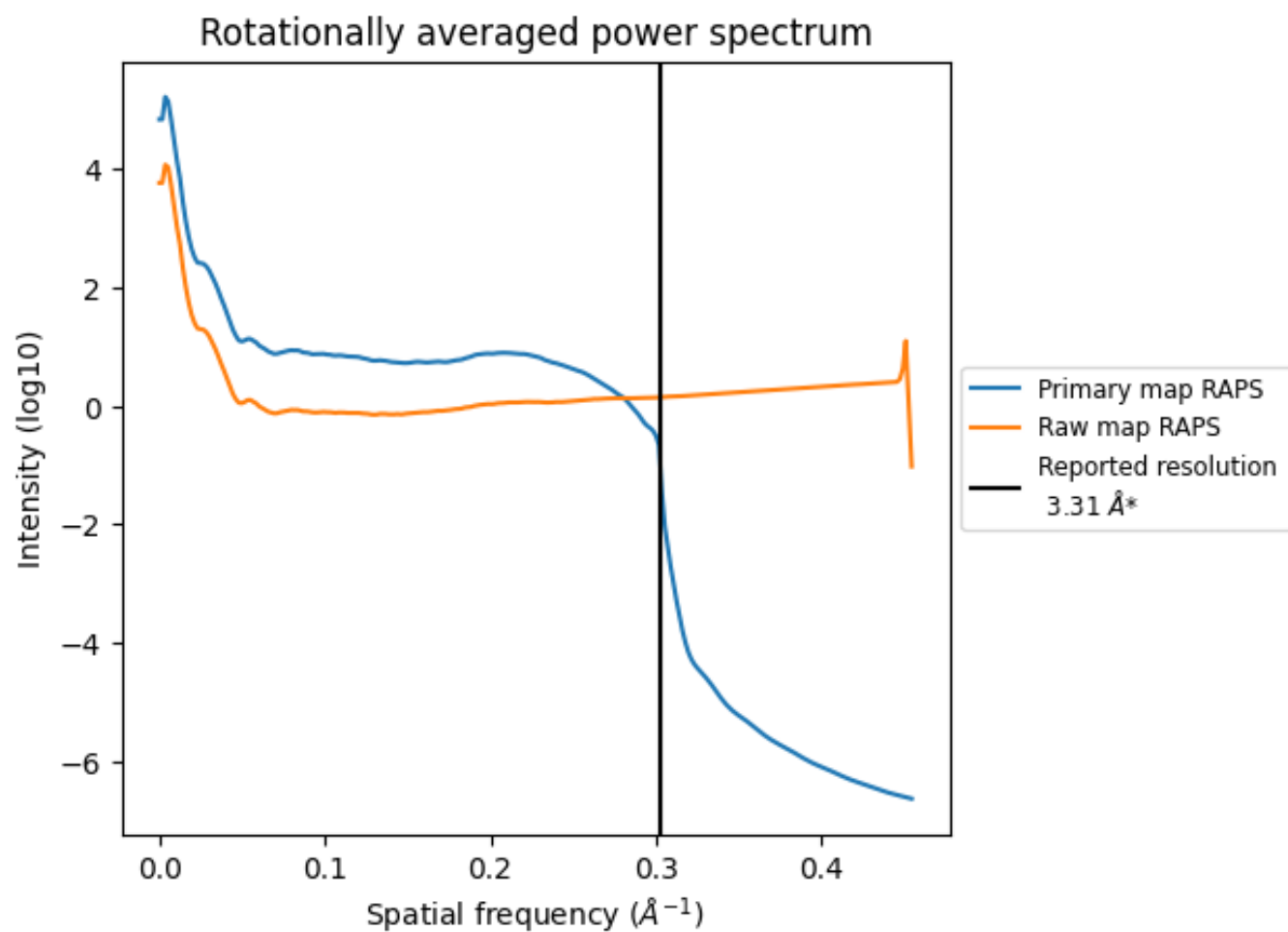


The volume at the recommended contour level is 246  $\text{nm}^3$ ; this corresponds to an approximate mass of 222 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

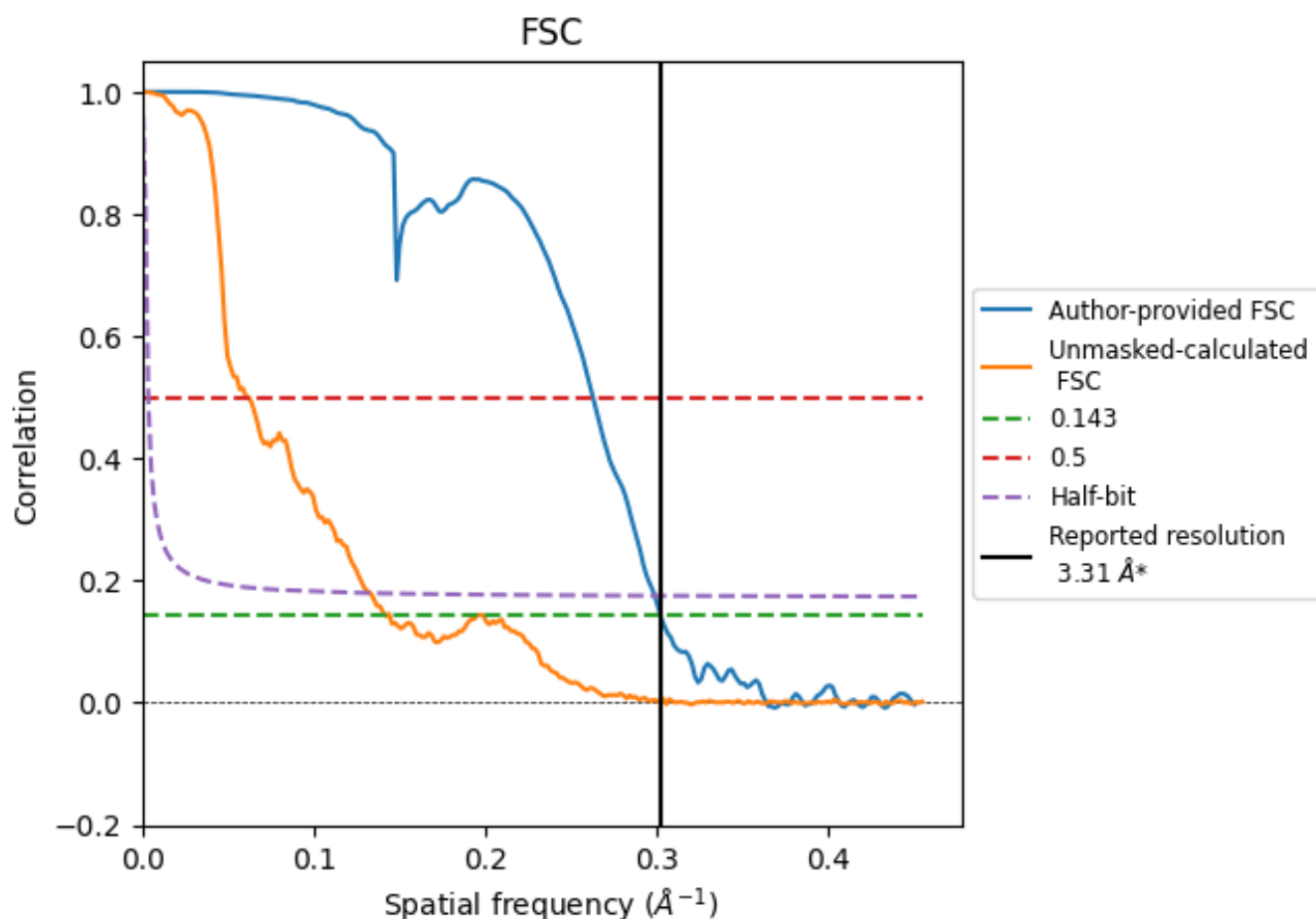


\*Reported resolution corresponds to spatial frequency of 0.302  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.302  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

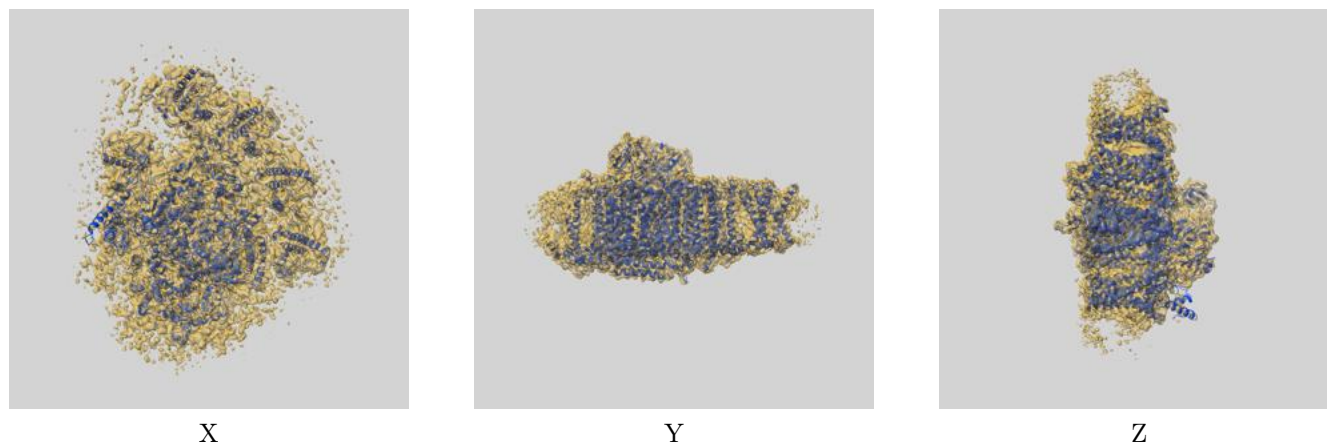
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.31	3.81	3.35
Unmasked-calculated*	7.06	16.08	7.53

\*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 7.06 differs from the reported value 3.31 by more than 10 %

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

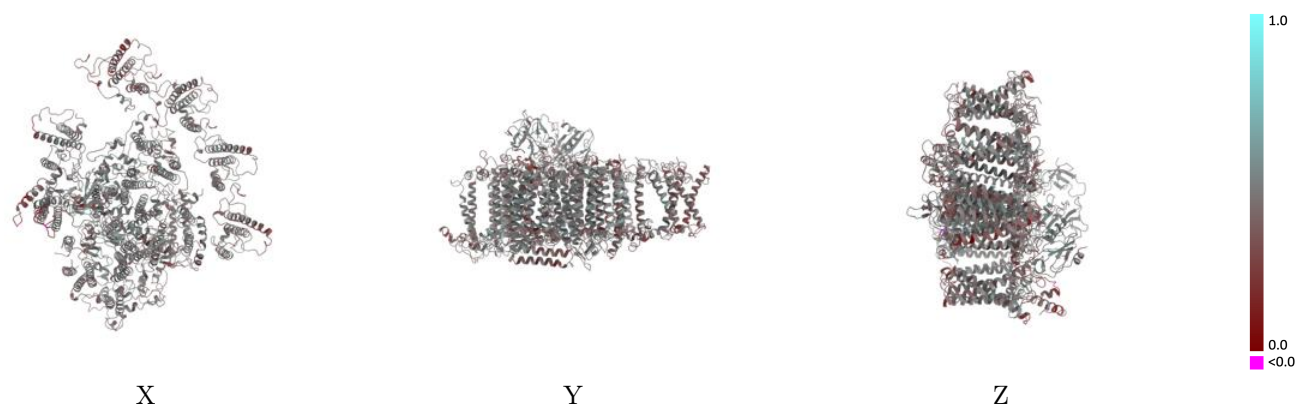
This section contains information regarding the fit between EMDB map EMD-60294 and PDB model 8ZOI. Per-residue inclusion information can be found in section [3](#) on page [26](#).

### 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](#)



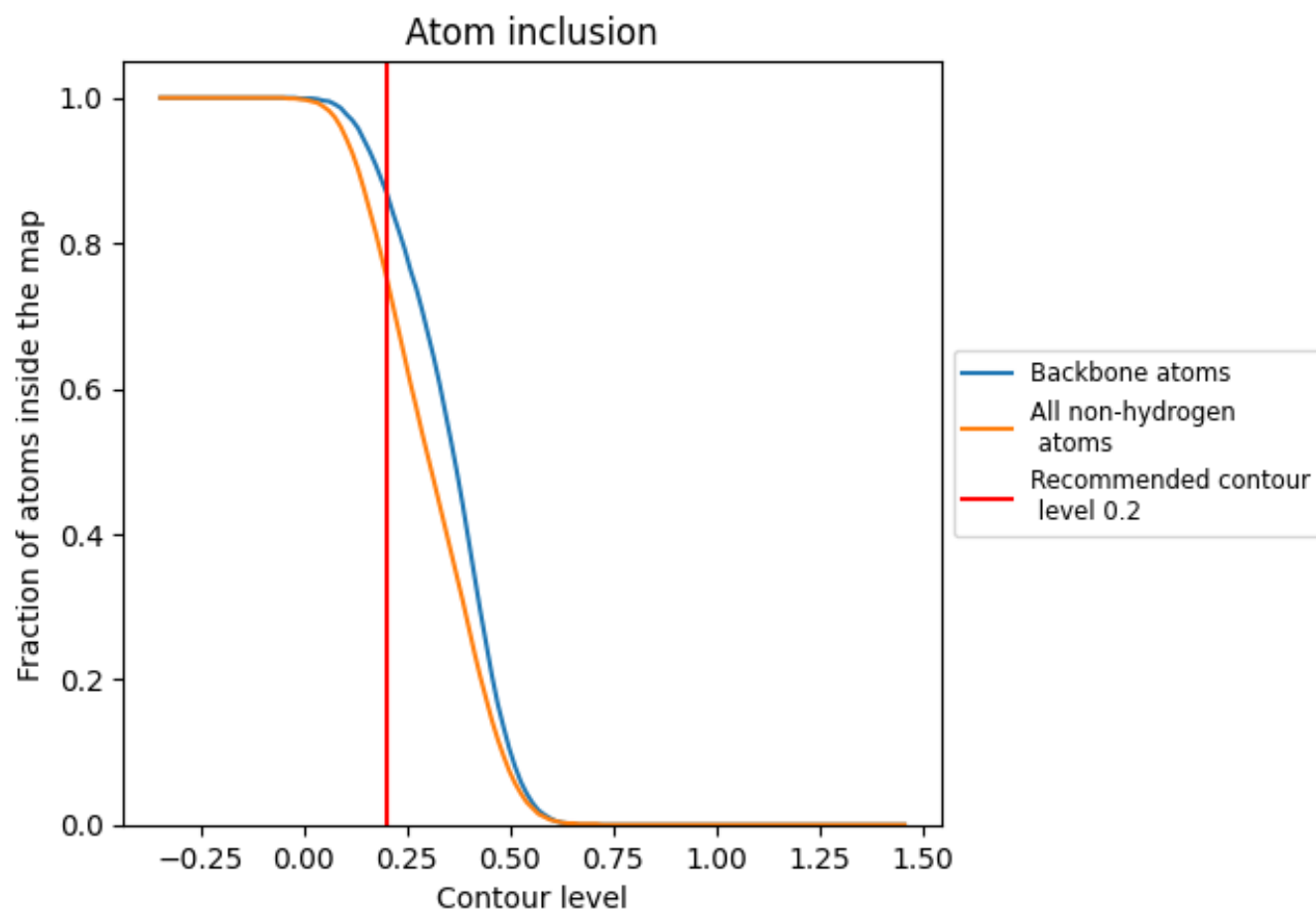
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 76% 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	<div><div></div>0.7550</div>	<div><div></div>0.4500</div>
1	<div><div></div>0.7210</div>	<div><div></div>0.4450</div>
2	<div><div></div>0.6270</div>	<div><div></div>0.3770</div>
3	<div><div></div>0.7350</div>	<div><div></div>0.4430</div>
4	<div><div></div>0.7630</div>	<div><div></div>0.4500</div>
5	<div><div></div>0.7380</div>	<div><div></div>0.4260</div>
a	<div><div></div>0.7820</div>	<div><div></div>0.4670</div>
b	<div><div></div>0.7790</div>	<div><div></div>0.4580</div>
c	<div><div></div>0.8750</div>	<div><div></div>0.4900</div>
d	<div><div></div>0.7760</div>	<div><div></div>0.4790</div>
e	<div><div></div>0.7550</div>	<div><div></div>0.4650</div>
f	<div><div></div>0.7530</div>	<div><div></div>0.4360</div>
g	<div><div></div>0.5400</div>	<div><div></div>0.3760</div>
i	<div><div></div>0.7130</div>	<div><div></div>0.4630</div>
j	<div><div></div>0.7540</div>	<div><div></div>0.4800</div>
l	<div><div></div>0.7150</div>	<div><div></div>0.4330</div>
m	<div><div></div>0.7070</div>	<div><div></div>0.4470</div>

1.0

0.0

<0.0