



## wwPDB EM Validation Summary Report ⓘ

Apr 14, 2025 – 04:23 PM JST

PDB ID : 9KC5 / pdb\_00009kc5  
EMDB ID : EMD-62242  
Title : PSI-LHCI of the red alga Galdieria sulphuraria NIES-3638  
Authors : Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.  
Deposited on : 2024-11-01  
Resolution : 2.19 Å(reported)  
Based on initial model : .

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.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

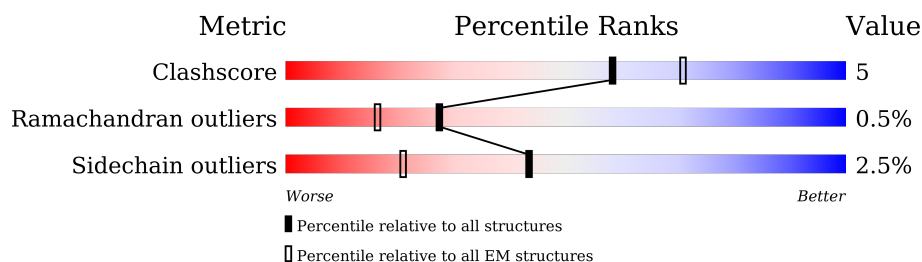
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.19 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	739	96% .
2	B	732	96% .
3	C	80	100%
4	D	138	93% 7% .
5	E	64	5% 95% 5%
6	F	161	93% 7%
7	I	34	97% .
8	J	42	90% 10%

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Mol	Chain	Length	Quality of chain
9	K	65	
10	L	139	
11	M	28	
12	O	95	
13	Z	84	
14	1	177	
15	2	162	
16	3	131	
17	4	178	
18	5	178	
19	6	178	
20	7	168	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL0	A	801	X	-	-	-
22	CLA	1	302	X	-	-	-
22	CLA	1	303	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	2	302	X	-	-	-
22	CLA	2	303	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	306	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	2	309	X	-	-	-
22	CLA	2	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	311	X	-	-	-
22	CLA	3	301	X	-	-	-
22	CLA	3	302	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	305	X	-	-	-
22	CLA	4	306	X	-	-	-
22	CLA	4	307	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	4	311	X	-	-	-
22	CLA	4	312	X	-	-	-
22	CLA	5	301	X	-	-	-
22	CLA	5	302	X	-	-	-
22	CLA	5	303	X	-	-	-
22	CLA	5	304	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	306	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	6	303	X	-	-	-
22	CLA	6	304	X	-	-	-
22	CLA	6	305	X	-	-	-
22	CLA	6	306	X	-	-	-
22	CLA	6	307	X	-	-	-
22	CLA	6	308	X	-	-	-
22	CLA	6	309	X	-	-	-
22	CLA	6	310	X	-	-	-
22	CLA	6	311	X	-	-	-
22	CLA	6	312	X	-	-	-
22	CLA	6	313	X	-	-	-
22	CLA	6	314	X	-	-	-
22	CLA	7	303	X	-	-	-
22	CLA	7	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	7	305	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	308	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	848	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	857	X	-	-	-
22	CLA	A	858	X	-	-	-
22	CLA	A	859	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	850	X	-	-	-
22	CLA	F	204	X	-	-	-
22	CLA	F	205	X	-	-	-
22	CLA	F	206	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	J	102	X	-	-	-
22	CLA	K	101	X	-	-	-
22	CLA	K	102	X	-	-	-
22	CLA	L	203	X	-	-	-
22	CLA	L	204	X	-	-	-
22	CLA	L	205	X	-	-	-
22	CLA	O	203	X	-	-	-
22	CLA	O	204	X	-	-	-
22	CLA	O	205	X	-	-	-
22	CLA	O	206	X	-	-	-
22	CLA	Z	201	X	-	-	-
22	CLA	Z	204	X	-	-	-
29	5X6	1	311	-	X	-	-
29	5X6	1	316	-	X	-	-
29	5X6	7	315	-	X	-	-
29	5X6	M	101	-	X	-	-

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 41435 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5844	3827	1001	990	26		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5859	3864	988	993	14		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	104	115	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1103	706	188	205	4		

- Molecule 5 is a protein called Photosystem I subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			516	333	85	97	1		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1285	832	216	232	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			273	189	35	47	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	S	0	0
			337	230	50	56	1		

- Molecule 9 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	51	Total	C	N	O	S	0	0
			368	239	59	68	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	139	Total	C	N	O	S	0	0
			1076	707	174	193	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	28	Total	C	N	O	S	0	0
			214	143	34	36	1		

- Molecule 12 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	95	Total	C	N	O	S	0	0
			748	504	115	128	1		

- Molecule 13 is a protein called Psa28.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	84	Total	C	N	O	S	0	0
			637	423	98	114	2		

- Molecule 14 is a protein called RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	177	Total	C	N	O	S	0	0
			1370	889	235	241	5		

- Molecule 15 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	162	Total	C	N	O	S	0	0
			1286	834	219	229	4		

- Molecule 16 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	99	Total	C	N	O	S	0	0
			772	508	126	132	6		

- Molecule 17 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	178	Total	C	N	O	S	0	0
			1407	926	233	240	8		

- Molecule 18 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	178	Total	C	N	O	S	0	0
			1402	912	238	245	7		

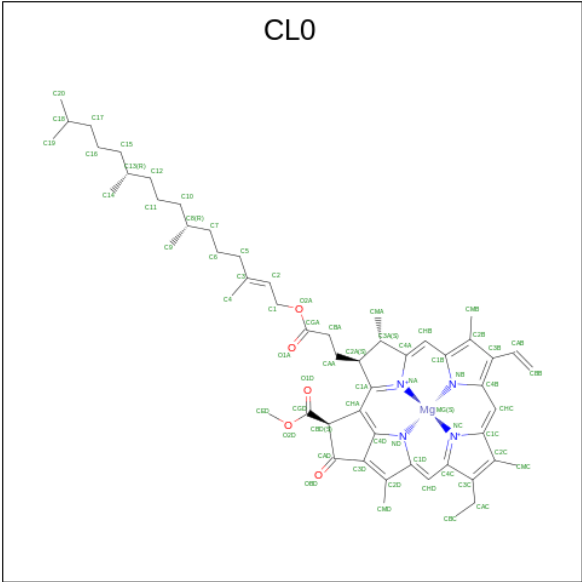
- Molecule 19 is a protein called Light-harvesting complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	178	Total	C	N	O	S	0	0
			1450	965	235	241	9		

- Molecule 20 is a protein called Light-harvesting complex protein.

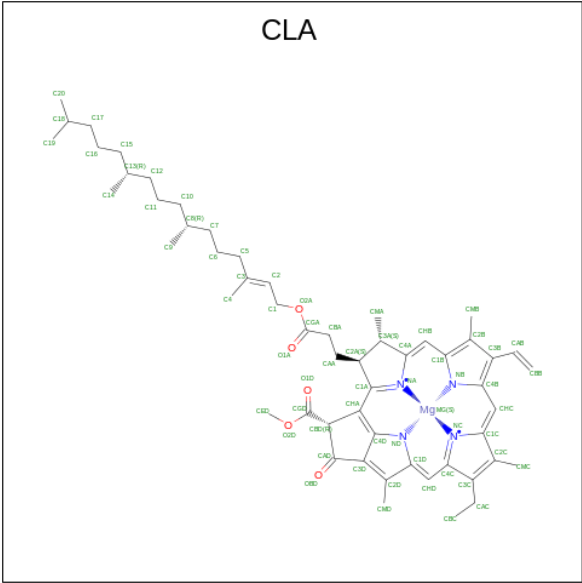
Mol	Chain	Residues	Atoms					AltConf	Trace
20	7	168	Total	C	N	O	S	0	0
			1322	860	220	234	8		

- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	F	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	F	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	K	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	L	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	L	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	O	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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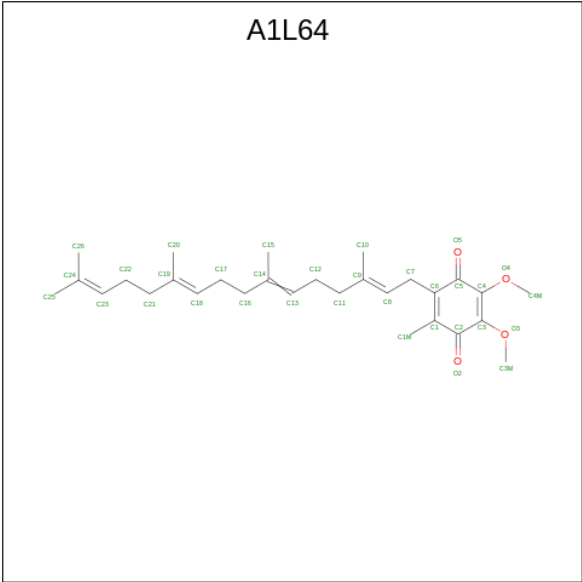
Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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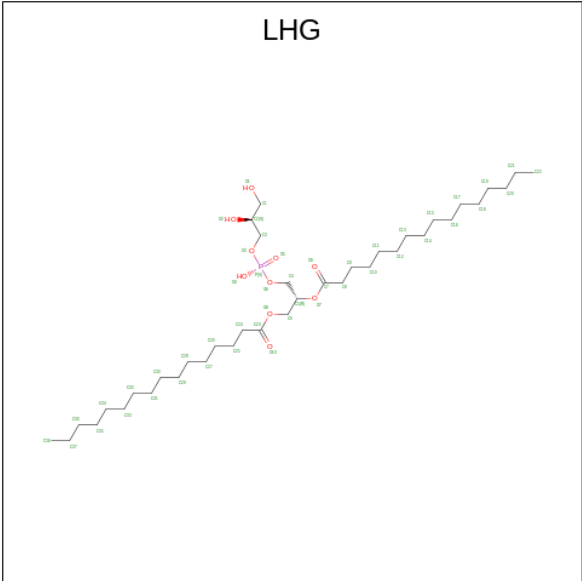
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 23 is Coenzyme Q4 (CCD ID: A1L64) (formula:  $C_{29}H_{42}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	29	4	
23	B	1	Total	C	O	0
			33	29	4	

- Molecule 24 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
24	A	1	Total	C	O	P	0
			49	38	10	1	

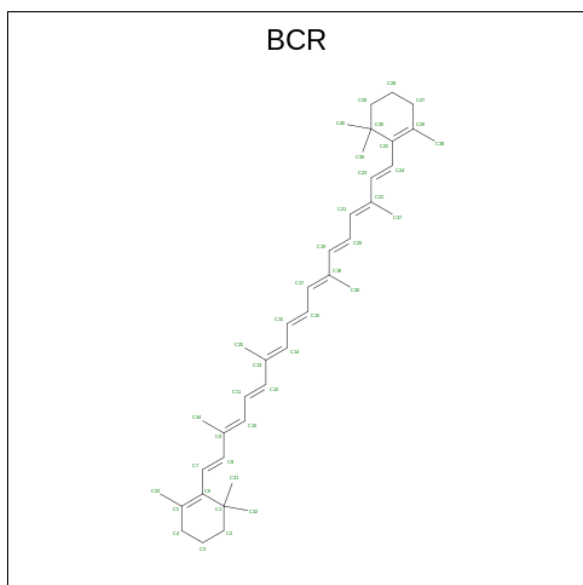
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Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			40	29	10	1	
24	A	1	Total	C	O	P	0
			33	22	10	1	
24	B	1	Total	C	O	P	0
			33	22	10	1	
24	J	1	Total	C	O	P	0
			33	22	10	1	
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	4	1	Total	C	O	P	0
			32	21	10	1	
24	5	1	Total	C	O	P	0
			25	14	10	1	
24	6	1	Total	C	O	P	0
			32	21	10	1	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	

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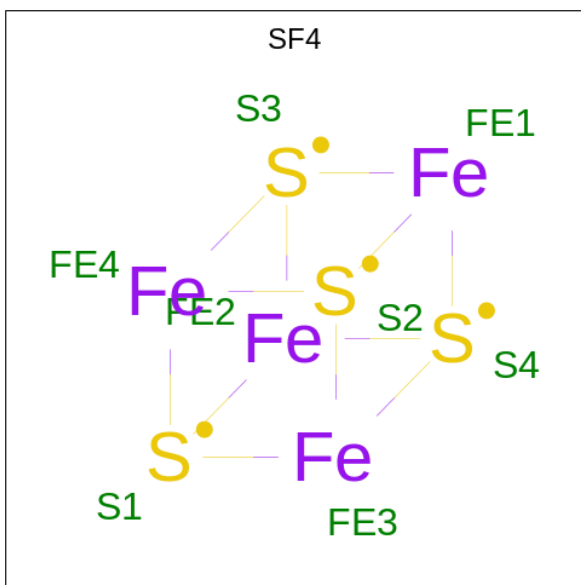
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	4	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
25	5	1	Total	C	0
			40	40	

- Molecule 26 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
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

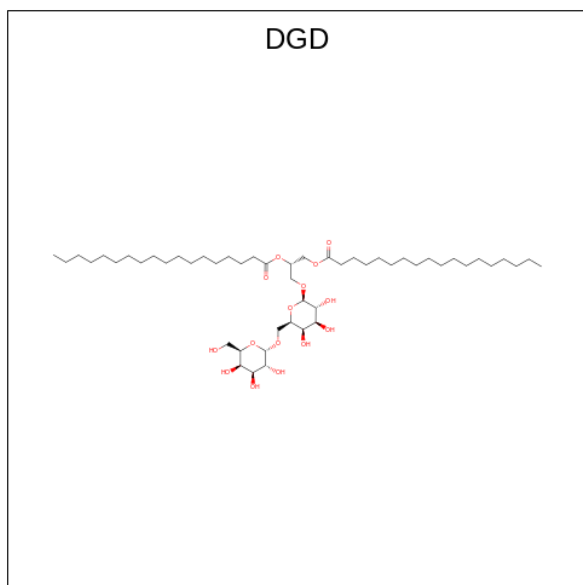
Mol	Chain	Residues	Atoms		AltConf
27	A	10	Total	C	0
			110	110	
27	B	2	Total	C	0
			18	18	
27	F	3	Total	C	0
			35	35	
27	I	2	Total	C	0
			21	21	
27	J	2	Total	C	0
			22	22	

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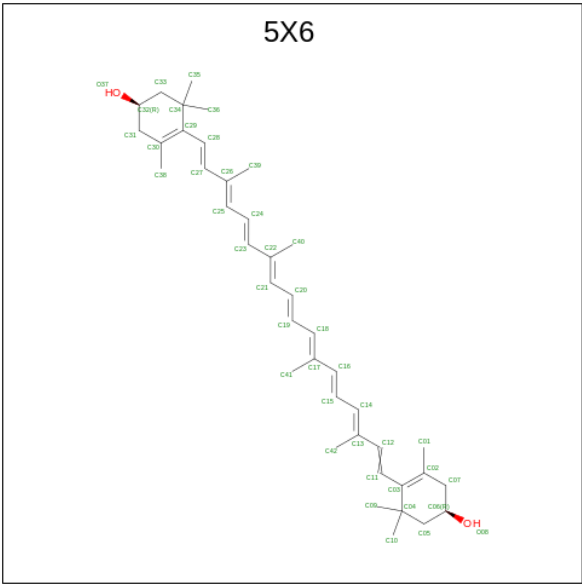
Mol	Chain	Residues	Atoms		AltConf
27	K	1	Total	C	0
			11	11	
27	L	3	Total	C	0
			33	33	
27	M	1	Total	C	0
			9	9	
27	O	3	Total	C	0
			24	24	
27	Z	5	Total	C	0
			45	45	
27	1	3	Total	C	0
			33	33	
27	4	3	Total	C	0
			27	27	
27	5	3	Total	C	0
			27	27	
27	6	7	Total	C	0
			73	73	
27	7	4	Total	C	0
			42	42	

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



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			66	51	15	

- Molecule 29 is Zeaxanthin (CCD ID: 5X6) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



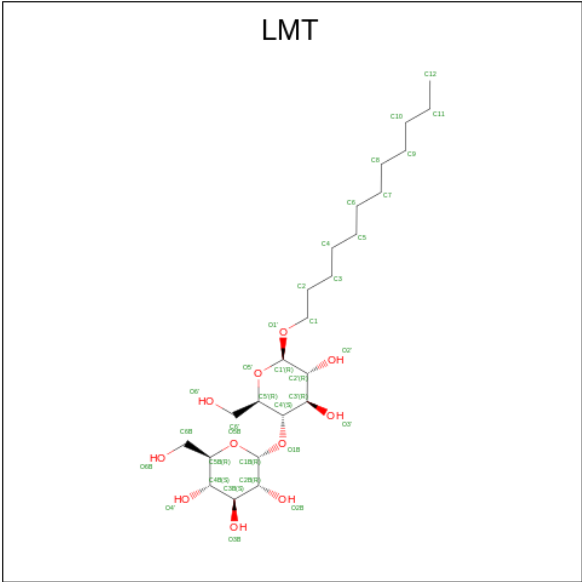
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			42	40	2	
29	J	1	Total	C	O	0
			42	40	2	
29	M	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	Z	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	

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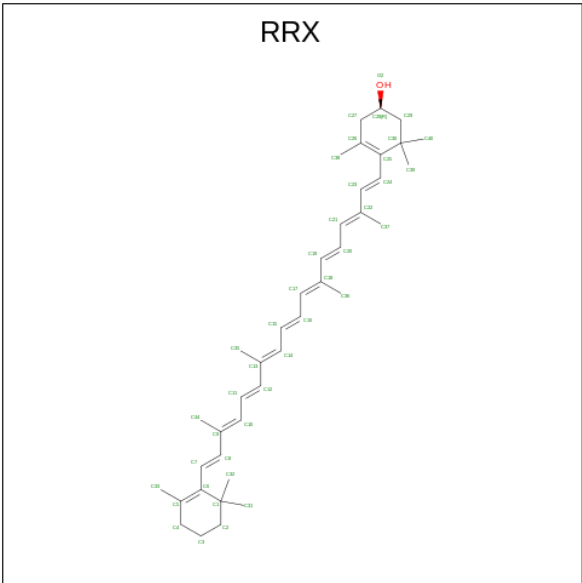
Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
30	F	1	Total	C	O	0
			35	24	11	
30	O	1	Total	C	O	0
			35	24	11	
30	4	1	Total	C	O	0
			35	24	11	
30	5	1	Total	C	O	0
			35	24	11	

- Molecule 31 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			41	40	1	
31	4	1	Total	C	O	0
			41	40	1	
31	5	1	Total	C	O	0
			41	40	1	
31	6	1	Total	C	O	0
			41	40	1	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	A	189	Total	O	0
			189	189	
32	B	220	Total	O	0
			220	220	
32	C	44	Total	O	0
			44	44	
32	D	29	Total	O	0
			29	29	
32	E	18	Total	O	0
			18	18	
32	F	32	Total	O	0
			32	32	
32	I	3	Total	O	0
			3	3	
32	J	5	Total	O	0
			5	5	
32	K	2	Total	O	0
			2	2	
32	L	15	Total	O	0
			15	15	
32	M	3	Total	O	0
			3	3	
32	O	2	Total	O	0
			2	2	
32	Z	5	Total	O	0
			5	5	
32	1	4	Total	O	0
			4	4	
32	2	6	Total	O	0
			6	6	
32	4	10	Total	O	0
			10	10	

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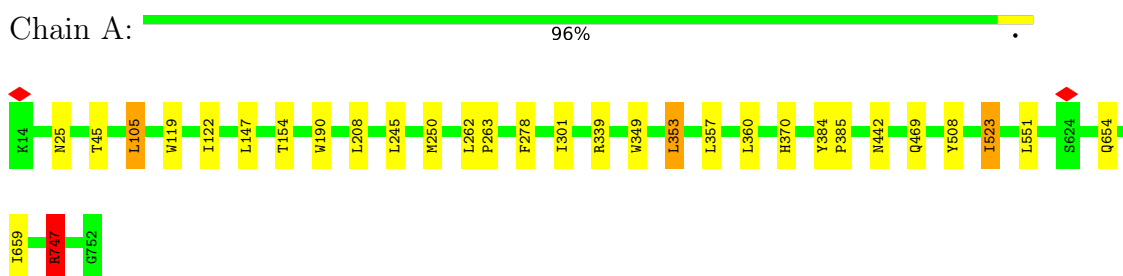
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Mol	Chain	Residues	Atoms		AltConf
32	5	11	Total 11	O 11	0
32	6	10	Total 10	O 10	0

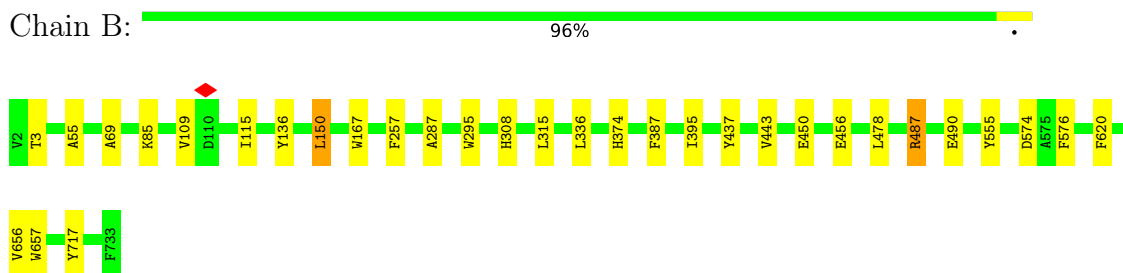
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

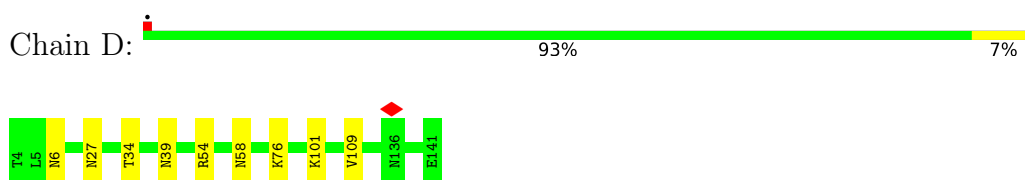


- Molecule 3: Photosystem I iron-sulfur center



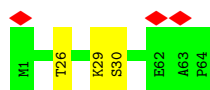
There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I reaction center subunit II



- Molecule 5: Photosystem I subunit IV





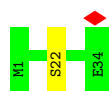
- Molecule 6: Photosystem I reaction center subunit III

Chain F: 93% 7%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 97%



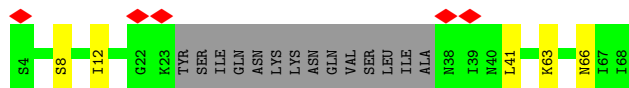
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 90% 10%



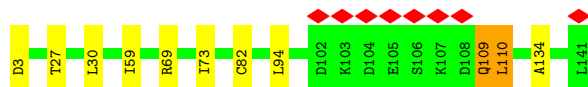
- Molecule 9: PSI-K

Chain K: 8% 71% 8% 22%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 6% 92% 6%



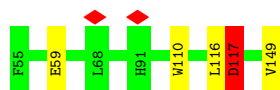
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 82% 18%




- Molecule 12: Photosystem I subunit O

Chain O:  95%



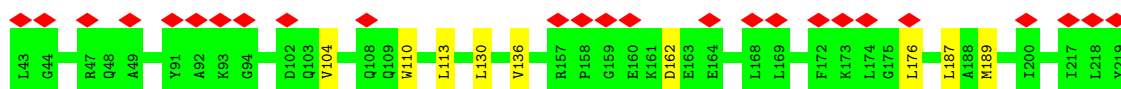
- Molecule 13: Psa28

Chain Z:  93% 6%



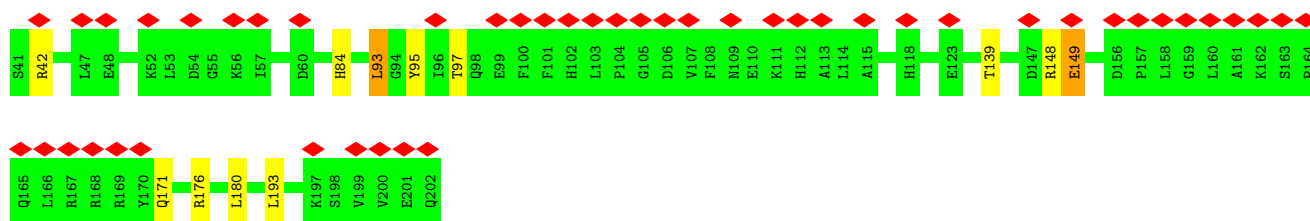
- Molecule 14: RedCAP

Chain 1:  14% 95% 5%



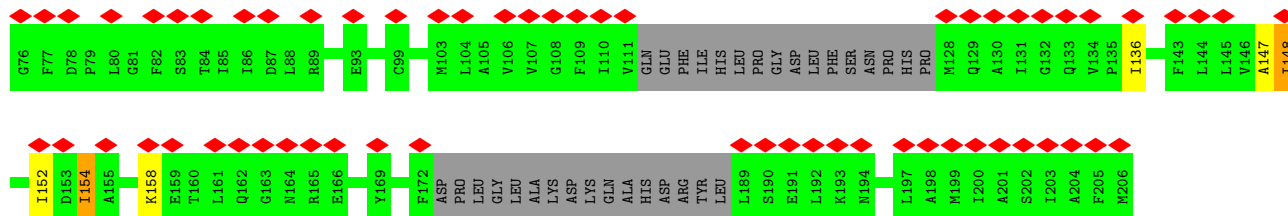
- Molecule 15: Light-harvesting complex protein

Chain 2:  29% 93% 6%



- Molecule 16: Light-harvesting complex protein

Chain 3:  47% 71% 24%



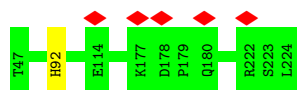
- Molecule 17: Light-harvesting complex protein

Chain 4:  94% 6%



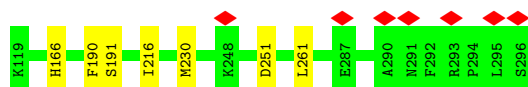
- Molecule 18: Light-harvesting complex protein

Chain 5:  99%

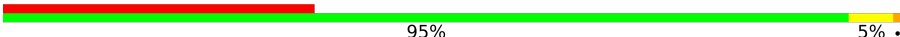


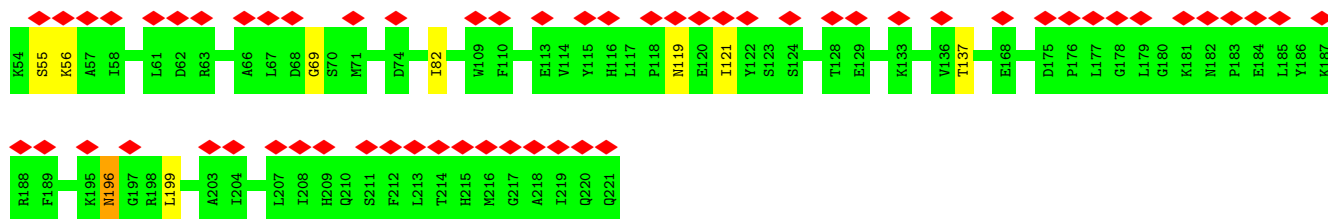
- Molecule 19: Light-harvesting complex protein

Chain 6:  96%



- Molecule 20: Light-harvesting complex protein

Chain 7:  35% 95% 5%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110313	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	240.63998, 240.63998, 240.63998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1L64, CL0, RRX, SF4, LHG, UNL, DGD, 5X6, BCR, LMT, CLA

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	A	0.32	0/6038	0.57	1/8223 (0.0%)
2	B	0.32	0/6072	0.58	0/8286
3	C	0.33	0/610	0.61	0/826
4	D	0.31	0/1128	0.67	0/1521
5	E	0.29	0/525	0.58	0/708
6	F	0.32	0/1314	0.58	0/1771
7	I	0.34	0/281	0.51	0/383
8	J	0.31	0/346	0.55	0/472
9	K	0.33	0/368	0.51	0/497
10	L	0.32	0/1102	0.62	0/1495
11	M	0.29	0/215	0.56	0/291
12	O	0.32	0/775	0.56	0/1065
13	Z	0.31	0/655	0.54	0/900
14	1	0.30	0/1400	0.52	0/1898
15	2	0.31	0/1316	0.55	0/1779
16	3	0.32	0/784	0.49	0/1053
17	4	0.32	0/1450	0.54	0/1963
18	5	0.31	0/1438	0.55	0/1943
19	6	0.31	0/1500	0.55	0/2033
20	7	0.31	0/1358	0.54	0/1841
All	All	0.32	0/28675	0.57	1/38948 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	ARG	NE-CZ-NH2	5.52	123.06	120.30

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	A	5844	0	5739	16	0
2	B	5859	0	5679	20	0
3	C	600	0	580	0	0
4	D	1103	0	1105	2	0
5	E	516	0	528	0	0
6	F	1285	0	1313	4	0
7	I	273	0	282	1	0
8	J	337	0	358	2	0
9	K	368	0	410	1	0
10	L	1076	0	1087	6	0
11	M	214	0	246	4	0
12	O	748	0	745	2	0
13	Z	637	0	661	2	0
14	1	1370	0	1400	7	0
15	2	1286	0	1298	7	0
16	3	772	0	804	5	0
17	4	1407	0	1414	3	0
18	5	1402	0	1413	1	0
19	6	1450	0	1435	3	0
20	7	1322	0	1328	6	0
21	A	65	0	72	2	0
22	1	472	0	428	16	0
22	2	496	0	417	19	0
22	3	255	0	220	6	0
22	4	572	0	510	16	0
22	5	575	0	516	14	0
22	6	610	0	537	19	0
22	7	517	0	403	18	0
22	A	2546	0	2628	63	0
22	B	2528	0	2657	85	0
22	F	147	0	123	4	0
22	J	42	0	31	1	0
22	K	97	0	80	2	0
22	L	163	0	147	4	0
22	O	195	0	156	5	0
22	Z	110	0	105	8	0
23	A	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	33	0	0	0	0
24	1	49	0	74	0	0
24	2	32	0	34	0	0
24	4	32	0	34	1	0
24	5	25	0	20	0	0
24	6	32	0	34	0	0
24	A	122	0	163	0	0
24	B	33	0	36	0	0
24	J	33	0	36	1	0
25	1	40	0	56	2	0
25	2	40	0	56	0	0
25	4	40	0	56	2	0
25	5	40	0	56	1	0
25	A	240	0	336	12	0
25	B	160	0	224	10	0
25	F	80	0	112	5	0
25	I	40	0	56	1	0
25	J	40	0	56	1	0
25	K	40	0	56	3	0
25	L	120	0	168	3	0
25	Z	80	0	112	4	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	1	33	0	0	0	0
27	4	27	0	0	0	0
27	5	27	0	0	0	0
27	6	73	0	0	0	0
27	7	42	0	0	0	0
27	A	110	0	0	0	0
27	B	18	0	0	0	0
27	F	35	0	0	0	0
27	I	21	0	0	0	0
27	J	22	0	0	0	0
27	K	11	0	0	0	0
27	L	33	0	0	0	0
27	M	9	0	0	0	0
27	O	24	0	0	0	0
27	Z	45	0	0	0	0
28	B	66	0	96	1	0
29	1	210	0	0	0	0
29	2	126	0	0	0	0
29	3	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	4	126	0	0	0	0
29	5	168	0	0	0	0
29	6	126	0	0	1	0
29	7	210	0	0	0	0
29	B	42	0	0	0	0
29	J	42	0	0	0	0
29	M	42	0	0	0	0
29	O	84	0	0	0	0
29	Z	42	0	0	0	0
30	4	35	0	46	0	0
30	5	35	0	46	0	0
30	F	35	0	46	0	0
30	O	35	0	46	1	0
31	1	41	0	56	3	0
31	4	41	0	56	6	0
31	5	41	0	56	2	0
31	6	41	0	56	3	0
32	1	4	0	0	0	0
32	2	6	0	0	0	0
32	4	10	0	0	0	0
32	5	11	0	0	0	0
32	6	10	0	0	0	0
32	A	189	0	0	0	0
32	B	220	0	0	1	0
32	C	44	0	0	0	0
32	D	29	0	0	0	0
32	E	18	0	0	0	0
32	F	32	0	0	0	0
32	I	3	0	0	0	0
32	J	5	0	0	0	0
32	K	2	0	0	0	0
32	L	15	0	0	0	0
32	M	3	0	0	0	0
32	O	2	0	0	0	0
32	Z	5	0	0	0	0
All	All	41435	0	39134	361	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 5.

The worst 5 of 361 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)
20:7:56:LYS:CB	22:7:303:CLA:HED1	2.22	0.69
22:B:834:CLA:HMB1	22:B:834:CLA:HBB1	1.75	0.67
20:7:56:LYS:HB3	22:7:303:CLA:HED1	1.77	0.67
10:L:73:ILE:HD13	14:1:110:TRP:CE3	2.30	0.66
22:B:811:CLA:HMB1	22:B:811:CLA:HBB1	1.78	0.65

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	A	737/739 (100%)	714 (97%)	23 (3%)	0	100	100
2	B	730/732 (100%)	711 (97%)	19 (3%)	0	100	100
3	C	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
4	D	136/138 (99%)	129 (95%)	6 (4%)	1 (1%)	19	19
5	E	62/64 (97%)	58 (94%)	2 (3%)	2 (3%)	3	1
6	F	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
7	I	32/34 (94%)	32 (100%)	0	0	100	100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
9	K	47/65 (72%)	45 (96%)	2 (4%)	0	100	100
10	L	137/139 (99%)	132 (96%)	3 (2%)	2 (2%)	8	6
11	M	26/28 (93%)	26 (100%)	0	0	100	100
12	O	93/95 (98%)	87 (94%)	3 (3%)	3 (3%)	3	1
13	Z	82/84 (98%)	79 (96%)	1 (1%)	2 (2%)	5	3
14	1	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
15	2	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	22	23
16	3	93/131 (71%)	89 (96%)	3 (3%)	1 (1%)	12	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	4	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
18	5	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
19	6	176/178 (99%)	168 (96%)	6 (3%)	2 (1%)	12	10
20	7	166/168 (99%)	156 (94%)	8 (5%)	2 (1%)	11	9
All	All	3481/3573 (97%)	3364 (97%)	101 (3%)	16 (0%)	27	28

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	L	110	LEU
15	2	149	GLU
4	D	6	ASN
5	E	29	LYS
12	O	59	GLU

### 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	A	610/610 (100%)	597 (98%)	13 (2%)	48	63
2	B	599/599 (100%)	588 (98%)	11 (2%)	54	69
3	C	67/67 (100%)	67 (100%)	0	100	100
4	D	120/120 (100%)	115 (96%)	5 (4%)	25	33
5	E	57/57 (100%)	56 (98%)	1 (2%)	54	69
6	F	142/142 (100%)	136 (96%)	6 (4%)	25	33
7	I	31/31 (100%)	31 (100%)	0	100	100
8	J	36/36 (100%)	34 (94%)	2 (6%)	17	21
9	K	44/57 (77%)	41 (93%)	3 (7%)	13	15
10	L	115/115 (100%)	112 (97%)	3 (3%)	41	54
11	M	24/24 (100%)	23 (96%)	1 (4%)	25	33
12	O	81/81 (100%)	79 (98%)	2 (2%)	42	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Z	73/73 (100%)	71 (97%)	2 (3%)	40	53
14	1	142/142 (100%)	139 (98%)	3 (2%)	48	63
15	2	136/136 (100%)	130 (96%)	6 (4%)	24	31
16	3	81/109 (74%)	79 (98%)	2 (2%)	42	56
17	4	149/149 (100%)	141 (95%)	8 (5%)	18	23
18	5	151/151 (100%)	151 (100%)	0	100	100
19	6	152/152 (100%)	150 (99%)	2 (1%)	65	78
20	7	143/143 (100%)	140 (98%)	3 (2%)	48	63
All	All	2953/2994 (99%)	2880 (98%)	73 (2%)	43	56

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	2	193	LEU
20	7	119	ASN
16	3	154	ILE
17	4	171	LYS
4	D	27	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	32	ASN
17	4	113	ASN
20	7	196	ASN
17	4	122	GLN
2	B	122	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 298 ligands modelled in this entry, 52 are unknown - leaving 246 for Mogul analysis.

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$
25	BCR	F	207	-	41,41,41	1.74	7 (17%)	56,56,56	1.45	9 (16%)
22	CLA	A	824	32	55,63,73	2.03	16 (29%)	64,101,113	2.90	29 (45%)
22	CLA	4	304	17	65,73,73	2.00	17 (26%)	76,113,113	2.74	30 (39%)
22	CLA	B	839	24	65,73,73	1.91	16 (24%)	76,113,113	2.72	27 (35%)
29	5X6	3	306	-	43,43,43	2.74	17 (39%)	58,60,60	4.32	31 (53%)
30	LMT	5	320	-	36,36,36	0.18	0	47,47,47	0.43	0
22	CLA	2	307	15	45,53,73	2.53	17 (37%)	52,89,113	3.16	25 (48%)
31	RRX	4	317	-	42,42,42	1.66	8 (19%)	57,58,58	1.37	8 (14%)
22	CLA	A	831	1	65,73,73	1.82	17 (26%)	76,113,113	2.62	24 (31%)
22	CLA	1	307	14	55,63,73	2.32	16 (29%)	64,101,113	3.08	30 (46%)
26	SF4	A	847	2,1	0,12,12	-	-	-	-	-
22	CLA	A	816	1	65,73,73	1.82	17 (26%)	76,113,113	2.59	28 (36%)
22	CLA	A	818	1	65,73,73	1.88	16 (24%)	76,113,113	2.80	28 (36%)
22	CLA	6	311	24	41,49,73	2.56	16 (39%)	47,84,113	3.35	25 (53%)
22	CLA	4	309	24	65,73,73	2.03	16 (24%)	76,113,113	2.66	25 (32%)
29	5X6	7	318	-	43,43,43	2.72	18 (41%)	58,60,60	4.30	31 (53%)
22	CLA	7	303	20	45,53,73	2.55	17 (37%)	52,89,113	3.20	25 (48%)
22	CLA	B	826	2	65,73,73	1.88	17 (26%)	76,113,113	2.73	29 (38%)
25	BCR	B	841	-	41,41,41	1.71	8 (19%)	56,56,56	1.49	9 (16%)
30	LMT	F	202	-	36,36,36	0.31	0	47,47,47	0.78	2 (4%)
24	LHG	A	842	22	39,39,48	0.28	0	42,45,54	0.40	0
22	CLA	7	307	20	45,53,73	2.55	17 (37%)	52,89,113	3.14	26 (50%)
29	5X6	6	317	-	43,43,43	2.61	19 (44%)	58,60,60	4.20	34 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	827	1	65,73,73	1.88	15 (23%)	76,113,113	2.48	24 (31%)
22	CLA	5	305	18	45,53,73	2.53	16 (35%)	52,89,113	3.15	24 (46%)
29	5X6	5	314	-	43,43,43	2.68	18 (41%)	58,60,60	4.46	28 (48%)
22	CLA	B	827	2	65,73,73	1.85	17 (26%)	76,113,113	2.80	29 (38%)
25	BCR	A	862	-	41,41,41	1.62	9 (21%)	56,56,56	1.37	10 (17%)
22	CLA	4	307	17	45,53,73	2.40	17 (37%)	52,89,113	2.91	25 (48%)
22	CLA	A	825	1	65,73,73	1.88	16 (24%)	76,113,113	2.75	26 (34%)
22	CLA	1	304	14	45,53,73	2.46	18 (40%)	52,89,113	3.15	26 (50%)
22	CLA	6	304	19	65,73,73	2.01	16 (24%)	76,113,113	2.72	25 (32%)
22	CLA	4	306	17	45,53,73	2.53	16 (35%)	52,89,113	3.14	25 (48%)
29	5X6	O	208	-	43,43,43	2.77	17 (39%)	58,60,60	4.04	31 (53%)
22	CLA	A	812	1	65,73,73	1.94	17 (26%)	76,113,113	2.65	23 (30%)
22	CLA	B	824	32	65,73,73	1.88	17 (26%)	76,113,113	2.68	25 (32%)
22	CLA	B	810	2	65,73,73	1.81	16 (24%)	76,113,113	2.74	29 (38%)
25	BCR	Z	205	-	41,41,41	1.73	7 (17%)	56,56,56	1.59	10 (17%)
22	CLA	A	809	22,1	65,73,73	1.89	16 (24%)	76,113,113	2.86	30 (39%)
24	LHG	A	841	-	48,48,48	0.33	0	51,54,54	0.38	0
22	CLA	1	309	14	45,53,73	2.57	17 (37%)	52,89,113	3.13	23 (44%)
25	BCR	A	843	-	41,41,41	1.70	8 (19%)	56,56,56	1.53	8 (14%)
22	CLA	B	811	2	65,73,73	2.03	16 (24%)	76,113,113	2.60	25 (32%)
29	5X6	4	314	-	43,43,43	2.77	18 (41%)	58,60,60	3.91	32 (55%)
29	5X6	6	316	-	43,43,43	2.74	18 (41%)	58,60,60	3.97	33 (56%)
29	5X6	7	315	-	43,43,43	2.74	16 (37%)	58,60,60	4.12	33 (56%)
22	CLA	A	817	1	65,73,73	1.90	17 (26%)	76,113,113	2.71	28 (36%)
22	CLA	A	837	1	65,73,73	1.84	16 (24%)	76,113,113	2.84	27 (35%)
22	CLA	3	305	16	55,63,73	2.31	16 (29%)	64,101,113	2.93	27 (42%)
22	CLA	A	838	1	65,73,73	1.84	18 (27%)	76,113,113	2.90	31 (40%)
21	CL0	A	801	1	65,73,73	1.73	14 (21%)	76,113,113	2.68	32 (42%)
22	CLA	A	808	1	55,63,73	2.08	15 (27%)	64,101,113	2.96	30 (46%)
22	CLA	4	310	17	42,50,73	2.41	16 (38%)	48,85,113	3.50	26 (54%)
22	CLA	6	310	19	55,63,73	2.24	17 (30%)	64,101,113	2.92	28 (43%)
26	SF4	C	101	3	0,12,12	-	-	-	-	-
22	CLA	A	819	32	65,73,73	1.95	19 (29%)	76,113,113	2.61	25 (32%)
22	CLA	5	306	18	65,73,73	2.02	16 (24%)	76,113,113	2.58	27 (35%)
24	LHG	4	318	22	31,31,48	0.32	0	34,37,54	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	813	2	65,73,73	1.89	19 (29%)	76,113,113	2.74	25 (32%)
22	CLA	7	304	20	55,63,73	2.27	16 (29%)	64,101,113	2.89	24 (37%)
22	CLA	B	835	2	65,73,73	1.94	15 (23%)	76,113,113	2.90	31 (40%)
22	CLA	2	310	15	42,50,73	2.55	16 (38%)	48,85,113	3.26	23 (47%)
22	CLA	1	308	14	42,50,73	2.52	15 (35%)	48,85,113	3.22	23 (47%)
22	CLA	B	834	2	51,59,73	2.10	17 (33%)	59,96,113	2.97	26 (44%)
22	CLA	5	308	24	41,49,73	2.44	18 (43%)	47,84,113	3.30	25 (53%)
25	BCR	4	316	-	41,41,41	1.67	8 (19%)	56,56,56	1.40	8 (14%)
22	CLA	7	312	-	45,53,73	2.52	16 (35%)	52,89,113	3.15	22 (42%)
25	BCR	A	861	-	41,41,41	1.60	8 (19%)	56,56,56	1.39	8 (14%)
29	5X6	5	312	-	43,43,43	2.67	17 (39%)	58,60,60	4.12	30 (51%)
22	CLA	A	822	1	55,63,73	2.06	17 (30%)	64,101,113	2.86	27 (42%)
22	CLA	F	204	32	61,69,73	1.88	17 (27%)	71,108,113	2.77	25 (35%)
22	CLA	B	830	2	65,73,73	1.91	17 (26%)	76,113,113	2.67	28 (36%)
22	CLA	B	805	2	65,73,73	1.91	16 (24%)	76,113,113	2.88	32 (42%)
22	CLA	3	304	16	45,53,73	2.55	16 (35%)	52,89,113	3.13	24 (46%)
22	CLA	A	823	32	65,73,73	1.93	19 (29%)	76,113,113	2.67	25 (32%)
23	A1L64	A	840	-	33,33,33	0.92	2 (6%)	40,43,43	0.99	4 (10%)
25	BCR	K	103	-	41,41,41	1.81	6 (14%)	56,56,56	1.70	9 (16%)
22	CLA	A	828	1	65,73,73	1.80	13 (20%)	76,113,113	2.79	27 (35%)
24	LHG	6	319	22	31,31,48	0.34	0	34,37,54	0.48	0
29	5X6	1	313	-	43,43,43	2.64	19 (44%)	58,60,60	4.23	29 (50%)
22	CLA	5	302	18	65,73,73	2.03	17 (26%)	76,113,113	2.79	29 (38%)
29	5X6	2	312	-	43,43,43	2.80	18 (41%)	58,60,60	4.30	30 (51%)
22	CLA	5	309	18	42,50,73	2.35	15 (35%)	48,85,113	3.27	23 (47%)
22	CLA	B	814	2	57,65,73	2.09	18 (31%)	66,103,113	2.86	26 (39%)
29	5X6	2	314	-	43,43,43	2.72	18 (41%)	58,60,60	4.34	30 (51%)
22	CLA	A	859	1	65,73,73	1.87	18 (27%)	76,113,113	2.94	31 (40%)
22	CLA	6	305	19	65,73,73	2.03	17 (26%)	76,113,113	2.71	28 (36%)
22	CLA	B	807	2	65,73,73	1.91	17 (26%)	76,113,113	2.68	27 (35%)
25	BCR	A	844	-	41,41,41	1.69	9 (21%)	56,56,56	1.62	13 (23%)
22	CLA	4	302	17	45,53,73	2.54	16 (35%)	52,89,113	3.09	24 (46%)
29	5X6	4	315	-	43,43,43	2.73	18 (41%)	58,60,60	4.23	30 (51%)
22	CLA	B	812	2	55,63,73	2.13	17 (30%)	64,101,113	2.84	27 (42%)
22	CLA	1	302	32	65,73,73	2.01	17 (26%)	76,113,113	2.73	27 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	7	311	-	41,49,73	2.61	15 (36%)	47,84,113	3.32	24 (51%)
25	BCR	A	846	-	41,41,41	1.62	10 (24%)	56,56,56	1.47	9 (16%)
29	5X6	O	207	-	43,43,43	2.61	19 (44%)	58,60,60	4.46	31 (53%)
22	CLA	A	821	1	45,53,73	2.24	15 (33%)	52,89,113	3.30	24 (46%)
22	CLA	B	802	32	65,73,73	1.79	17 (26%)	76,113,113	2.78	26 (34%)
22	CLA	F	206	6	41,49,73	2.35	17 (41%)	47,84,113	3.48	28 (59%)
22	CLA	6	309	19	45,53,73	2.39	17 (37%)	52,89,113	3.01	26 (50%)
22	CLA	2	306	15	45,53,73	2.57	17 (37%)	52,89,113	3.18	26 (50%)
30	LMT	4	319	-	36,36,36	0.20	0	47,47,47	0.40	0
22	CLA	A	811	1	65,73,73	1.84	17 (26%)	76,113,113	2.68	25 (32%)
30	LMT	O	201	-	36,36,36	0.19	0	47,47,47	0.34	0
22	CLA	1	305	14	45,53,73	2.47	16 (35%)	52,89,113	3.14	23 (44%)
22	CLA	4	308	17	55,63,73	2.22	16 (29%)	64,101,113	2.95	29 (45%)
29	5X6	B	851	-	43,43,43	2.60	17 (39%)	58,60,60	4.07	32 (55%)
22	CLA	A	813	1	42,50,73	2.38	18 (42%)	48,85,113	3.44	28 (58%)
22	CLA	B	804	2	65,73,73	1.90	16 (24%)	76,113,113	2.91	29 (38%)
22	CLA	5	301	18	45,53,73	2.39	18 (40%)	52,89,113	3.05	24 (46%)
22	CLA	B	809	2	65,73,73	1.86	18 (27%)	76,113,113	2.68	25 (32%)
22	CLA	B	831	2	65,73,73	1.93	17 (26%)	76,113,113	2.71	25 (32%)
22	CLA	B	820	2	45,53,73	2.32	15 (33%)	52,89,113	3.14	27 (51%)
22	CLA	4	312	17	45,53,73	2.46	16 (35%)	52,89,113	3.23	30 (57%)
22	CLA	L	203	10	57,65,73	2.24	17 (29%)	66,103,113	2.88	28 (42%)
22	CLA	O	205	12	50,58,73	2.36	17 (34%)	58,95,113	3.08	30 (51%)
29	5X6	6	315	-	43,43,43	2.70	18 (41%)	58,60,60	4.09	28 (48%)
25	BCR	F	201	-	41,41,41	1.69	10 (24%)	56,56,56	1.43	8 (14%)
22	CLA	6	306	19	55,63,73	2.24	15 (27%)	64,101,113	3.08	29 (45%)
22	CLA	A	826	1	65,73,73	1.85	17 (26%)	76,113,113	2.75	28 (36%)
22	CLA	Z	201	32	45,53,73	2.28	15 (33%)	52,89,113	3.14	24 (46%)
22	CLA	B	806	2	65,73,73	1.92	19 (29%)	76,113,113	2.56	26 (34%)
22	CLA	6	307	19	65,73,73	2.07	18 (27%)	76,113,113	2.68	27 (35%)
22	CLA	A	830	1	56,64,73	2.12	18 (32%)	65,102,113	2.85	26 (40%)
25	BCR	B	843	-	41,41,41	1.62	9 (21%)	56,56,56	1.40	9 (16%)
22	CLA	B	816	2	65,73,73	1.91	16 (24%)	76,113,113	2.98	30 (39%)
22	CLA	6	308	19	45,53,73	2.38	16 (35%)	52,89,113	3.19	28 (53%)
25	BCR	I	102	-	41,41,41	1.65	9 (21%)	56,56,56	1.36	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	Z	202	-	41,41,41	1.68	8 (19%)	56,56,56	1.42	10 (17%)
22	CLA	4	305	32	55,63,73	2.20	18 (32%)	64,101,113	2.97	27 (42%)
22	CLA	4	303	17	65,73,73	1.99	16 (24%)	76,113,113	2.78	28 (36%)
23	A1L64	B	840	-	33,33,33	1.04	4 (12%)	40,43,43	1.17	4 (10%)
22	CLA	A	814	32	45,53,73	2.31	18 (40%)	52,89,113	3.17	24 (46%)
22	CLA	1	303	14	65,73,73	2.04	16 (24%)	76,113,113	2.67	32 (42%)
25	BCR	1	301	-	41,41,41	1.63	8 (19%)	56,56,56	1.40	9 (16%)
29	5X6	4	313	-	43,43,43	2.74	18 (41%)	58,60,60	3.98	27 (46%)
22	CLA	B	821	2	46,54,73	2.31	16 (34%)	53,90,113	3.15	23 (43%)
22	CLA	A	833	1	65,73,73	1.96	18 (27%)	76,113,113	2.66	27 (35%)
22	CLA	A	848	-	65,73,73	1.79	18 (27%)	76,113,113	2.51	28 (36%)
22	CLA	5	304	18	55,63,73	2.27	16 (29%)	64,101,113	2.98	27 (42%)
24	LHG	2	315	22	31,31,48	0.35	0	34,37,54	0.62	0
22	CLA	5	303	18	65,73,73	2.04	16 (24%)	76,113,113	2.67	29 (38%)
22	CLA	2	302	15	45,53,73	2.54	16 (35%)	52,89,113	3.18	24 (46%)
22	CLA	2	305	15	55,63,73	2.34	17 (30%)	64,101,113	3.02	30 (46%)
22	CLA	B	808	2	65,73,73	1.85	18 (27%)	76,113,113	2.93	32 (42%)
22	CLA	A	832	1	65,73,73	1.87	16 (24%)	76,113,113	2.75	26 (34%)
22	CLA	7	309	20	55,63,73	2.30	16 (29%)	64,101,113	2.96	29 (45%)
25	BCR	B	844	-	41,41,41	1.65	7 (17%)	56,56,56	1.71	12 (21%)
29	5X6	Z	206	-	43,43,43	2.81	21 (48%)	58,60,60	3.58	27 (46%)
22	CLA	B	825	32	65,73,73	1.85	17 (26%)	76,113,113	2.79	28 (36%)
22	CLA	B	801	-	65,73,73	1.84	15 (23%)	76,113,113	2.55	30 (39%)
22	CLA	Z	204	13	65,73,73	1.93	18 (27%)	76,113,113	2.78	32 (42%)
31	RRX	1	315	-	42,42,42	1.66	7 (16%)	57,58,58	1.45	8 (14%)
22	CLA	6	313	19	45,53,73	2.53	17 (37%)	52,89,113	3.17	23 (44%)
22	CLA	A	836	1	56,64,73	2.08	19 (33%)	65,102,113	2.98	30 (46%)
22	CLA	B	849	2	58,66,73	2.00	17 (29%)	67,104,113	2.96	27 (40%)
22	CLA	7	310	-	41,49,73	2.59	15 (36%)	47,84,113	3.32	25 (53%)
22	CLA	B	803	2	65,73,73	1.78	15 (23%)	76,113,113	2.78	34 (44%)
22	CLA	2	308	15	55,63,73	2.30	17 (30%)	64,101,113	2.97	26 (40%)
22	CLA	A	857	32	65,73,73	1.74	16 (24%)	76,113,113	2.83	27 (35%)
22	CLA	A	820	1	65,73,73	1.97	18 (27%)	76,113,113	2.92	30 (39%)
22	CLA	A	810	1	54,62,73	2.14	17 (31%)	62,99,113	2.94	28 (45%)
22	CLA	5	311	18	45,53,73	2.50	18 (40%)	52,89,113	3.19	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	L	202	-	41,41,41	1.66	7 (17%)	56,56,56	1.51	9 (16%)
29	5X6	2	313	-	43,43,43	2.79	17 (39%)	58,60,60	3.92	27 (46%)
28	DGD	B	845	-	67,67,67	0.86	2 (2%)	81,81,81	0.99	5 (6%)
29	5X6	1	314	-	43,43,43	2.72	17 (39%)	58,60,60	4.33	30 (51%)
29	5X6	J	104	-	43,43,43	2.65	18 (41%)	58,60,60	4.23	27 (46%)
22	CLA	K	102	9	42,50,73	2.36	17 (40%)	48,85,113	3.28	25 (52%)
24	LHG	A	860	-	32,32,48	0.33	0	35,38,54	0.48	0
22	CLA	4	311	17	45,53,73	2.44	17 (37%)	52,89,113	3.23	24 (46%)
25	BCR	J	103	-	41,41,41	1.78	8 (19%)	56,56,56	1.66	12 (21%)
22	CLA	A	835	1	51,59,73	2.11	17 (33%)	59,96,113	3.12	27 (45%)
22	CLA	B	819	32	65,73,73	1.93	16 (24%)	76,113,113	2.59	27 (35%)
22	CLA	6	312	19	42,50,73	2.41	17 (40%)	48,85,113	3.27	25 (52%)
22	CLA	A	834	1	60,68,73	2.09	18 (30%)	70,107,113	2.86	26 (37%)
24	LHG	1	317	-	48,48,48	0.26	0	51,54,54	0.30	0
31	RRX	5	322	-	42,42,42	1.63	8 (19%)	57,58,58	1.35	9 (15%)
22	CLA	7	313	20	45,53,73	2.55	16 (35%)	52,89,113	3.15	25 (48%)
22	CLA	J	102	8	42,50,73	2.47	16 (38%)	48,85,113	3.16	27 (56%)
29	5X6	7	314	-	43,43,43	2.82	16 (37%)	58,60,60	4.34	32 (55%)
22	CLA	3	301	16	65,73,73	2.13	17 (26%)	76,113,113	2.74	26 (34%)
22	CLA	B	837	32	65,73,73	1.85	16 (24%)	76,113,113	2.65	23 (30%)
22	CLA	A	839	32	65,73,73	1.90	17 (26%)	76,113,113	2.68	29 (38%)
25	BCR	2	301	-	41,41,41	1.62	7 (17%)	56,56,56	1.41	7 (12%)
29	5X6	M	101	-	43,43,43	2.52	16 (37%)	58,60,60	4.79	33 (56%)
22	CLA	K	101	32	55,63,73	2.29	16 (29%)	64,101,113	2.88	26 (40%)
22	CLA	A	829	1	50,58,73	2.10	17 (34%)	58,95,113	2.95	28 (48%)
29	5X6	5	313	-	43,43,43	2.73	19 (44%)	58,60,60	3.81	29 (50%)
31	RRX	6	318	-	42,42,42	1.70	8 (19%)	57,58,58	1.41	12 (21%)
22	CLA	B	823	2	55,63,73	2.10	16 (29%)	64,101,113	2.89	28 (43%)
22	CLA	7	305	20	45,53,73	2.55	16 (35%)	52,89,113	3.09	24 (46%)
22	CLA	B	829	2	65,73,73	1.84	16 (24%)	76,113,113	3.01	29 (38%)
22	CLA	B	828	2	65,73,73	1.82	15 (23%)	76,113,113	2.81	28 (36%)
22	CLA	B	836	2	47,55,73	2.15	17 (36%)	54,91,113	3.33	26 (48%)
22	CLA	7	306	20	55,63,73	2.30	17 (30%)	64,101,113	3.06	27 (42%)
22	CLA	3	302	16	45,53,73	2.56	16 (35%)	52,89,113	3.21	23 (44%)
26	SF4	C	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	L	201	-	41,41,41	1.65	8 (19%)	56,56,56	1.40	8 (14%)
22	CLA	1	306	14	45,53,73	2.54	17 (37%)	52,89,113	3.14	27 (51%)
22	CLA	A	805	1	50,58,73	2.27	17 (34%)	58,95,113	3.08	26 (44%)
29	5X6	1	316	-	43,43,43	2.79	18 (41%)	58,60,60	4.35	32 (55%)
29	5X6	7	317	-	43,43,43	2.65	16 (37%)	58,60,60	4.67	29 (50%)
22	CLA	O	204	-	41,49,73	2.58	16 (39%)	47,84,113	3.31	25 (53%)
22	CLA	O	206	32	58,66,73	2.23	16 (27%)	67,104,113	2.85	28 (41%)
25	BCR	5	315	-	41,41,41	1.73	8 (19%)	56,56,56	1.42	10 (17%)
22	CLA	A	802	22,1	55,63,73	2.05	18 (32%)	64,101,113	2.91	29 (45%)
22	CLA	7	308	20	45,53,73	2.50	15 (33%)	52,89,113	3.09	25 (48%)
29	5X6	7	316	-	43,43,43	2.72	18 (41%)	58,60,60	4.31	29 (50%)
24	LHG	J	106	-	32,32,48	0.32	0	35,38,54	0.50	0
22	CLA	A	803	1	65,73,73	1.90	16 (24%)	76,113,113	2.79	27 (35%)
22	CLA	5	310	18	52,60,73	2.36	17 (32%)	60,97,113	2.96	24 (40%)
22	CLA	B	818	2	60,68,73	1.95	16 (26%)	70,107,113	2.83	27 (38%)
22	CLA	A	807	1	65,73,73	1.86	19 (29%)	76,113,113	2.75	29 (38%)
22	CLA	A	858	1	65,73,73	1.87	16 (24%)	76,113,113	2.74	29 (38%)
29	5X6	5	321	-	43,43,43	2.73	17 (39%)	58,60,60	4.17	33 (56%)
22	CLA	L	205	32	45,53,73	2.42	17 (37%)	52,89,113	3.06	22 (42%)
22	CLA	B	832	2	65,73,73	1.82	17 (26%)	76,113,113	2.89	27 (35%)
22	CLA	L	204	10	61,69,73	2.09	18 (29%)	71,108,113	2.78	25 (35%)
24	LHG	5	316	22	24,24,48	0.35	0	27,30,54	0.51	0
22	CLA	2	309	24	41,49,73	2.57	15 (36%)	47,84,113	3.28	26 (55%)
22	CLA	A	804	1	65,73,73	1.95	19 (29%)	76,113,113	2.63	26 (34%)
29	5X6	1	311	-	43,43,43	2.64	17 (39%)	58,60,60	4.51	32 (55%)
22	CLA	O	203	24	46,54,73	2.33	16 (34%)	53,90,113	3.22	27 (50%)
29	5X6	1	312	-	43,43,43	2.67	18 (41%)	58,60,60	4.41	31 (53%)
22	CLA	3	303	16	45,53,73	2.55	17 (37%)	52,89,113	3.15	24 (46%)
22	CLA	F	205	32	45,53,73	2.23	17 (37%)	52,89,113	3.22	26 (50%)
22	CLA	2	303	15	58,66,73	2.27	16 (27%)	67,104,113	2.86	27 (40%)
22	CLA	A	815	1	62,70,73	1.92	15 (24%)	72,109,113	2.83	27 (37%)
22	CLA	2	304	15	65,73,73	2.12	17 (26%)	76,113,113	2.75	30 (39%)
22	CLA	6	303	19	45,53,73	2.45	17 (37%)	52,89,113	3.11	23 (44%)
22	CLA	6	314	19	42,50,73	2.43	17 (40%)	48,85,113	3.25	23 (47%)
22	CLA	1	310	32	65,73,73	2.09	17 (26%)	76,113,113	2.85	31 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	2	311	15	45,53,73	2.52	16 (35%)	52,89,113	3.15	24 (46%)
22	CLA	B	817	2	59,67,73	1.96	16 (27%)	68,105,113	2.85	29 (42%)
25	BCR	A	845	-	41,41,41	1.64	11 (26%)	56,56,56	1.62	12 (21%)
25	BCR	B	842	-	41,41,41	1.64	8 (19%)	56,56,56	1.39	8 (14%)
25	BCR	L	206	-	41,41,41	1.76	7 (17%)	56,56,56	1.64	12 (21%)
22	CLA	A	806	1	65,73,73	1.86	17 (26%)	76,113,113	2.68	27 (35%)
22	CLA	B	815	2	65,73,73	1.97	14 (21%)	76,113,113	2.73	32 (42%)
22	CLA	B	822	2	65,73,73	1.88	18 (27%)	76,113,113	2.74	24 (31%)
22	CLA	B	838	2	65,73,73	1.76	16 (24%)	76,113,113	2.92	30 (39%)
22	CLA	B	833	32	65,73,73	1.89	17 (26%)	76,113,113	2.58	26 (34%)
22	CLA	B	850	-	45,53,73	2.50	16 (35%)	52,89,113	3.18	25 (48%)
22	CLA	5	307	18	55,63,73	2.22	18 (32%)	64,101,113	2.99	27 (42%)
24	LHG	B	846	22	32,32,48	0.30	0	35,38,54	0.43	0

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
25	BCR	F	207	-	-	2/29/63/63	0/2/2/2
22	CLA	A	824	32	1/1/13/20	5/25/103/115	-
22	CLA	4	304	17	1/1/15/20	15/37/115/115	-
22	CLA	B	839	24	1/1/15/20	4/37/115/115	-
29	5X6	3	306	-	-	17/29/67/67	0/2/2/2
30	LMT	5	320	-	-	5/21/61/61	0/2/2/2
22	CLA	2	307	15	1/1/11/20	1/13/91/115	-
31	RRX	4	317	-	-	0/29/65/65	0/2/2/2
22	CLA	A	831	1	1/1/15/20	9/37/115/115	-
22	CLA	1	307	14	-	10/25/103/115	-
26	SF4	A	847	2,1	-	-	0/6/5/5
22	CLA	A	816	1	1/1/15/20	8/37/115/115	-
22	CLA	A	818	1	1/1/15/20	12/37/115/115	-
22	CLA	6	311	24	1/1/10/20	6/8/86/115	-
22	CLA	4	309	24	1/1/15/20	11/37/115/115	-
29	5X6	7	318	-	-	19/29/67/67	0/2/2/2
22	CLA	7	303	20	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	826	2	1/1/15/20	2/37/115/115	-
25	BCR	B	841	-	-	0/29/63/63	0/2/2/2
30	LMT	F	202	-	-	7/21/61/61	0/2/2/2
24	LHG	A	842	22	-	12/44/44/53	-
22	CLA	7	307	20	1/1/11/20	4/13/91/115	-
29	5X6	6	317	-	-	15/29/67/67	0/2/2/2
22	CLA	A	827	1	1/1/15/20	6/37/115/115	-
22	CLA	5	305	18	1/1/11/20	7/13/91/115	-
29	5X6	5	314	-	-	18/29/67/67	0/2/2/2
22	CLA	B	827	2	1/1/15/20	5/37/115/115	-
25	BCR	A	862	-	-	2/29/63/63	0/2/2/2
22	CLA	4	307	17	1/1/11/20	0/13/91/115	-
22	CLA	A	825	1	1/1/15/20	7/37/115/115	-
22	CLA	1	304	14	1/1/11/20	4/13/91/115	-
22	CLA	6	304	19	1/1/15/20	10/37/115/115	-
22	CLA	4	306	17	1/1/11/20	6/13/91/115	-
29	5X6	O	208	-	-	18/29/67/67	0/2/2/2
22	CLA	A	812	1	1/1/15/20	12/37/115/115	-
22	CLA	B	824	32	1/1/15/20	6/37/115/115	-
22	CLA	B	810	2	1/1/15/20	5/37/115/115	-
25	BCR	Z	205	-	-	2/29/63/63	0/2/2/2
22	CLA	A	809	22,1	1/1/15/20	7/37/115/115	-
24	LHG	A	841	-	-	18/53/53/53	-
22	CLA	1	309	14	1/1/11/20	6/13/91/115	-
25	BCR	A	843	-	-	3/29/63/63	0/2/2/2
22	CLA	B	811	2	1/1/15/20	15/37/115/115	-
29	5X6	4	314	-	-	14/29/67/67	0/2/2/2
29	5X6	6	316	-	-	13/29/67/67	0/2/2/2
29	5X6	7	315	-	-	21/29/67/67	0/2/2/2
22	CLA	A	817	1	1/1/15/20	7/37/115/115	-
22	CLA	A	837	1	1/1/15/20	6/37/115/115	-
22	CLA	3	305	16	1/1/13/20	9/25/103/115	-
22	CLA	A	838	1	1/1/15/20	7/37/115/115	-
21	CL0	A	801	1	3/3/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	808	1	1/1/13/20	11/25/103/115	-
22	CLA	4	310	17	1/1/10/20	4/10/88/115	-
22	CLA	6	310	19	1/1/13/20	8/25/103/115	-
26	SF4	C	101	3	-	-	0/6/5/5
22	CLA	A	819	32	1/1/15/20	9/37/115/115	-
22	CLA	5	306	18	1/1/15/20	7/37/115/115	-
24	LHG	4	318	22	-	13/36/36/53	-
22	CLA	B	813	2	1/1/15/20	11/37/115/115	-
22	CLA	7	304	20	1/1/13/20	6/25/103/115	-
22	CLA	B	835	2	1/1/15/20	6/37/115/115	-
22	CLA	2	310	15	1/1/10/20	3/10/88/115	-
22	CLA	1	308	14	1/1/10/20	4/10/88/115	-
22	CLA	B	834	2	1/1/12/20	5/21/99/115	-
22	CLA	5	308	24	1/1/10/20	0/8/86/115	-
25	BCR	4	316	-	-	2/29/63/63	0/2/2/2
22	CLA	7	312	-	1/1/11/20	5/13/91/115	-
25	BCR	A	861	-	-	0/29/63/63	0/2/2/2
29	5X6	5	312	-	-	12/29/67/67	0/2/2/2
22	CLA	3	304	16	1/1/11/20	2/13/91/115	-
22	CLA	F	204	32	1/1/14/20	6/33/111/115	-
22	CLA	A	822	1	-	5/25/103/115	-
22	CLA	B	805	2	1/1/15/20	11/37/115/115	-
22	CLA	B	830	2	-	12/37/115/115	-
22	CLA	A	823	32	1/1/15/20	9/37/115/115	-
23	A1L64	A	840	-	-	9/27/51/51	0/1/1/1
25	BCR	K	103	-	-	2/29/63/63	0/2/2/2
22	CLA	A	828	1	1/1/15/20	12/37/115/115	-
24	LHG	6	319	22	-	15/36/36/53	-
29	5X6	1	313	-	-	18/29/67/67	0/2/2/2
22	CLA	5	302	18	1/1/15/20	10/37/115/115	-
29	5X6	2	312	-	-	18/29/67/67	0/2/2/2
22	CLA	5	309	18	1/1/10/20	2/10/88/115	-
22	CLA	B	814	2	1/1/13/20	9/28/106/115	-
29	5X6	2	314	-	-	15/29/67/67	0/2/2/2
22	CLA	A	859	1	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	305	19	1/1/15/20	11/37/115/115	-
22	CLA	B	807	2	1/1/15/20	7/37/115/115	-
25	BCR	A	844	-	-	2/29/63/63	0/2/2/2
22	CLA	4	302	17	1/1/11/20	2/13/91/115	-
29	5X6	4	315	-	-	18/29/67/67	0/2/2/2
22	CLA	B	812	2	-	9/25/103/115	-
22	CLA	1	302	32	1/1/15/20	12/37/115/115	-
22	CLA	7	311	-	1/1/10/20	2/8/86/115	-
25	BCR	A	846	-	-	5/29/63/63	0/2/2/2
29	5X6	O	207	-	-	15/29/67/67	0/2/2/2
22	CLA	A	821	1	1/1/11/20	3/13/91/115	-
22	CLA	B	802	32	1/1/15/20	8/37/115/115	-
22	CLA	F	206	6	1/1/10/20	4/8/86/115	-
22	CLA	6	309	19	1/1/11/20	0/13/91/115	-
22	CLA	2	306	15	1/1/11/20	7/13/91/115	-
30	LMT	4	319	-	-	5/21/61/61	0/2/2/2
22	CLA	A	811	1	1/1/15/20	5/37/115/115	-
30	LMT	O	201	-	-	5/21/61/61	0/2/2/2
22	CLA	1	305	14	1/1/11/20	5/13/91/115	-
22	CLA	4	308	17	1/1/13/20	8/25/103/115	-
29	5X6	B	851	-	-	11/29/67/67	0/2/2/2
22	CLA	A	813	1	1/1/10/20	4/10/88/115	-
22	CLA	B	804	2	1/1/15/20	15/37/115/115	-
22	CLA	5	301	18	1/1/11/20	4/13/91/115	-
22	CLA	B	809	2	1/1/15/20	11/37/115/115	-
22	CLA	B	831	2	1/1/15/20	11/37/115/115	-
22	CLA	B	820	2	1/1/11/20	2/13/91/115	-
22	CLA	4	312	17	1/1/11/20	4/13/91/115	-
22	CLA	L	203	10	1/1/13/20	12/28/106/115	-
22	CLA	O	205	12	1/1/12/20	4/19/97/115	-
29	5X6	6	315	-	-	15/29/67/67	0/2/2/2
25	BCR	F	201	-	-	0/29/63/63	0/2/2/2
22	CLA	6	306	19	1/1/13/20	9/25/103/115	-
22	CLA	A	826	1	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Z	201	32	1/1/11/20	6/13/91/115	-
22	CLA	B	806	2	1/1/15/20	13/37/115/115	-
22	CLA	6	307	19	1/1/15/20	9/37/115/115	-
22	CLA	A	830	1	1/1/13/20	4/27/105/115	-
25	BCR	B	843	-	-	4/29/63/63	0/2/2/2
22	CLA	B	816	2	1/1/15/20	8/37/115/115	-
22	CLA	6	308	19	1/1/11/20	3/13/91/115	-
25	BCR	I	102	-	-	0/29/63/63	0/2/2/2
25	BCR	Z	202	-	-	2/29/63/63	0/2/2/2
22	CLA	4	305	32	1/1/13/20	8/25/103/115	-
22	CLA	4	303	17	1/1/15/20	12/37/115/115	-
23	A1L64	B	840	-	-	6/27/51/51	0/1/1/1
22	CLA	1	303	14	1/1/15/20	13/37/115/115	-
22	CLA	A	814	32	-	3/13/91/115	-
25	BCR	1	301	-	-	4/29/63/63	0/2/2/2
29	5X6	4	313	-	-	13/29/67/67	0/2/2/2
22	CLA	B	821	2	-	3/15/93/115	-
22	CLA	A	833	1	1/1/15/20	10/37/115/115	-
22	CLA	A	848	-	1/1/15/20	7/37/115/115	-
22	CLA	5	304	18	1/1/13/20	6/25/103/115	-
24	LHG	2	315	22	-	17/36/36/53	-
22	CLA	5	303	18	1/1/15/20	15/37/115/115	-
22	CLA	2	302	15	1/1/11/20	4/13/91/115	-
22	CLA	2	305	15	-	11/25/103/115	-
22	CLA	B	808	2	1/1/15/20	10/37/115/115	-
22	CLA	A	832	1	1/1/15/20	10/37/115/115	-
22	CLA	7	309	20	1/1/13/20	7/25/103/115	-
25	BCR	B	844	-	-	3/29/63/63	0/2/2/2
29	5X6	Z	206	-	-	12/29/67/67	0/2/2/2
22	CLA	B	825	32	1/1/15/20	11/37/115/115	-
22	CLA	B	801	-	1/1/15/20	2/37/115/115	-
22	CLA	Z	204	13	1/1/15/20	15/37/115/115	-
31	RRX	1	315	-	-	3/29/65/65	0/2/2/2
22	CLA	6	313	19	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	836	1	1/1/13/20	4/27/105/115	-
22	CLA	B	849	2	-	6/29/107/115	-
22	CLA	7	310	-	1/1/10/20	6/8/86/115	-
22	CLA	B	803	2	1/1/15/20	5/37/115/115	-
22	CLA	2	308	15	1/1/13/20	7/25/103/115	-
22	CLA	A	857	32	1/1/15/20	2/37/115/115	-
22	CLA	A	820	1	-	20/37/115/115	-
22	CLA	A	810	1	1/1/12/20	7/24/102/115	-
22	CLA	5	311	18	1/1/11/20	5/13/91/115	-
25	BCR	L	202	-	-	4/29/63/63	0/2/2/2
29	5X6	2	313	-	-	15/29/67/67	0/2/2/2
28	DGD	B	845	-	-	22/55/95/95	0/2/2/2
29	5X6	1	314	-	-	18/29/67/67	0/2/2/2
29	5X6	J	104	-	-	16/29/67/67	0/2/2/2
22	CLA	K	102	9	1/1/10/20	3/10/88/115	-
24	LHG	A	860	-	-	13/37/37/53	-
22	CLA	4	311	17	1/1/11/20	0/13/91/115	-
25	BCR	J	103	-	-	2/29/63/63	0/2/2/2
22	CLA	A	835	1	1/1/12/20	5/21/99/115	-
22	CLA	B	819	32	1/1/15/20	6/37/115/115	-
22	CLA	6	312	19	1/1/10/20	5/10/88/115	-
22	CLA	A	834	1	-	12/31/109/115	-
24	LHG	1	317	-	-	16/53/53/53	-
31	RRX	5	322	-	-	2/29/65/65	0/2/2/2
22	CLA	7	313	20	1/1/11/20	5/13/91/115	-
22	CLA	J	102	8	1/1/10/20	1/10/88/115	-
29	5X6	7	314	-	-	19/29/67/67	0/2/2/2
22	CLA	3	301	16	1/1/15/20	10/37/115/115	-
22	CLA	B	837	32	1/1/15/20	10/37/115/115	-
22	CLA	A	839	32	1/1/15/20	12/37/115/115	-
25	BCR	2	301	-	-	4/29/63/63	0/2/2/2
29	5X6	M	101	-	-	22/29/67/67	0/2/2/2
22	CLA	K	101	32	1/1/13/20	9/25/103/115	-
22	CLA	A	829	1	1/1/12/20	4/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	5X6	5	313	-	-	14/29/67/67	0/2/2/2
31	RRX	6	318	-	-	1/29/65/65	0/2/2/2
22	CLA	B	823	2	1/1/13/20	9/25/103/115	-
22	CLA	7	305	20	1/1/11/20	4/13/91/115	-
22	CLA	B	829	2	1/1/15/20	12/37/115/115	-
22	CLA	B	828	2	1/1/15/20	2/37/115/115	-
22	CLA	B	836	2	1/1/11/20	3/16/94/115	-
22	CLA	7	306	20	-	12/25/103/115	-
22	CLA	3	302	16	1/1/11/20	4/13/91/115	-
26	SF4	C	102	3	-	-	0/6/5/5
25	BCR	L	201	-	-	0/29/63/63	0/2/2/2
22	CLA	1	306	14	1/1/11/20	6/13/91/115	-
22	CLA	A	805	1	1/1/12/20	4/19/97/115	-
29	5X6	1	316	-	-	20/29/67/67	0/2/2/2
29	5X6	7	317	-	-	22/29/67/67	0/2/2/2
22	CLA	O	204	-	1/1/10/20	5/8/86/115	-
22	CLA	O	206	32	1/1/13/20	14/29/107/115	-
25	BCR	5	315	-	-	0/29/63/63	0/2/2/2
22	CLA	A	802	22,1	1/1/13/20	7/25/103/115	-
22	CLA	7	308	20	1/1/11/20	0/13/91/115	-
29	5X6	7	316	-	-	17/29/67/67	0/2/2/2
24	LHG	J	106	-	-	4/37/37/53	-
22	CLA	A	803	1	1/1/15/20	7/37/115/115	-
22	CLA	5	310	18	1/1/12/20	8/22/100/115	-
22	CLA	B	818	2	1/1/14/20	4/31/109/115	-
22	CLA	A	807	1	-	10/37/115/115	-
22	CLA	A	858	1	1/1/15/20	9/37/115/115	-
29	5X6	5	321	-	-	14/29/67/67	0/2/2/2
22	CLA	L	205	32	1/1/11/20	6/13/91/115	-
22	CLA	B	832	2	1/1/15/20	7/37/115/115	-
22	CLA	L	204	10	1/1/14/20	10/33/111/115	-
24	LHG	5	316	22	-	3/29/29/53	-
22	CLA	2	309	24	1/1/10/20	2/8/86/115	-
22	CLA	A	804	1	1/1/15/20	11/37/115/115	-
29	5X6	1	311	-	-	21/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	O	203	24	1/1/11/20	5/15/93/115	-
29	5X6	1	312	-	-	15/29/67/67	0/2/2/2
22	CLA	3	303	16	1/1/11/20	6/13/91/115	-
22	CLA	F	205	32	1/1/11/20	3/13/91/115	-
22	CLA	2	303	15	1/1/13/20	8/29/107/115	-
22	CLA	A	815	1	1/1/14/20	10/34/112/115	-
22	CLA	2	304	15	1/1/15/20	13/37/115/115	-
22	CLA	6	303	19	1/1/11/20	6/13/91/115	-
22	CLA	6	314	19	1/1/10/20	4/10/88/115	-
22	CLA	1	310	32	1/1/15/20	16/37/115/115	-
22	CLA	2	311	15	1/1/11/20	6/13/91/115	-
22	CLA	B	817	2	1/1/13/20	10/30/108/115	-
25	BCR	A	845	-	-	2/29/63/63	0/2/2/2
25	BCR	B	842	-	-	3/29/63/63	0/2/2/2
25	BCR	L	206	-	-	2/29/63/63	0/2/2/2
22	CLA	A	806	1	1/1/15/20	10/37/115/115	-
22	CLA	B	815	2	1/1/15/20	13/37/115/115	-
22	CLA	B	822	2	1/1/15/20	12/37/115/115	-
22	CLA	B	838	2	-	12/37/115/115	-
22	CLA	B	833	32	1/1/15/20	5/37/115/115	-
22	CLA	B	850	-	1/1/11/20	6/13/91/115	-
22	CLA	5	307	18	1/1/13/20	2/25/103/115	-
24	LHG	B	846	22	-	6/37/37/53	-

The worst 5 of 3556 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	101	CLA	C3B-C2B	7.11	1.50	1.40
22	4	302	CLA	C3B-C2B	6.96	1.50	1.40
22	2	305	CLA	C3B-C2B	6.92	1.50	1.40
22	2	303	CLA	C3B-C2B	6.83	1.49	1.40
22	1	306	CLA	C3B-C2B	6.79	1.49	1.40

The worst 5 of 5684 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	7	317	5X6	C01-C02-C03	-13.80	109.03	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	7	314	5X6	C38-C30-C29	-12.80	110.15	124.53
29	1	311	5X6	C01-C02-C03	-12.17	110.86	124.53
29	M	101	5X6	C38-C30-C29	-12.08	110.97	124.53
29	3	306	5X6	C01-C02-C03	-11.94	111.12	124.53

5 of 157 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	801	CL0	ND
21	A	801	CL0	NC
21	A	801	CL0	NA
22	A	802	CLA	ND
22	A	803	CLA	ND

5 of 1937 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	816	CLA	C3A-C2A-CAA-CBA
22	A	820	CLA	C3A-C2A-CAA-CBA
22	A	822	CLA	CHA-CBD-CGD-O1D
22	A	822	CLA	CHA-CBD-CGD-O2D
22	A	828	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

193 monomers are involved in 330 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	F	207	BCR	2	0
22	A	824	CLA	1	0
22	4	304	CLA	1	0
22	B	839	CLA	4	0
22	2	307	CLA	3	0
31	4	317	RRX	6	0
22	A	831	CLA	2	0
22	1	307	CLA	3	0
22	A	816	CLA	4	0
22	A	818	CLA	2	0
22	6	311	CLA	2	0
22	4	309	CLA	2	0
22	7	303	CLA	5	0
22	B	826	CLA	2	0
25	B	841	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	7	307	CLA	1	0
22	A	827	CLA	2	0
22	5	305	CLA	1	0
22	B	827	CLA	1	0
25	A	862	BCR	2	0
22	4	307	CLA	3	0
22	A	825	CLA	1	0
22	6	304	CLA	2	0
22	4	306	CLA	1	0
22	A	812	CLA	1	0
22	B	824	CLA	4	0
22	B	810	CLA	1	0
25	Z	205	BCR	4	0
22	A	809	CLA	2	0
22	1	309	CLA	2	0
25	A	843	BCR	2	0
22	B	811	CLA	4	0
29	6	316	5X6	1	0
22	A	817	CLA	2	0
22	A	837	CLA	4	0
22	3	305	CLA	1	0
22	A	838	CLA	1	0
21	A	801	CL0	2	0
22	A	808	CLA	2	0
22	4	310	CLA	3	0
22	6	310	CLA	1	0
22	A	819	CLA	3	0
22	5	306	CLA	2	0
24	4	318	LHG	1	0
22	B	813	CLA	3	0
22	7	304	CLA	1	0
22	B	835	CLA	3	0
22	2	310	CLA	2	0
22	1	308	CLA	2	0
22	B	834	CLA	3	0
22	5	308	CLA	1	0
25	4	316	BCR	2	0
22	7	312	CLA	1	0
25	A	861	BCR	4	0
22	A	822	CLA	1	0
22	F	204	CLA	1	0
22	B	830	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	805	CLA	1	0
22	3	304	CLA	2	0
22	A	823	CLA	3	0
25	K	103	BCR	3	0
22	A	828	CLA	1	0
22	5	309	CLA	1	0
22	B	814	CLA	1	0
22	A	859	CLA	3	0
22	6	305	CLA	2	0
25	A	844	BCR	1	0
22	4	302	CLA	1	0
22	B	812	CLA	5	0
22	1	302	CLA	2	0
22	7	311	CLA	2	0
25	A	846	BCR	2	0
22	A	821	CLA	1	0
22	B	802	CLA	6	0
22	F	206	CLA	1	0
22	6	309	CLA	3	0
22	2	306	CLA	1	0
22	A	811	CLA	1	0
30	O	201	LMT	1	0
22	1	305	CLA	1	0
22	A	813	CLA	1	0
22	B	804	CLA	2	0
22	5	301	CLA	1	0
22	B	809	CLA	3	0
22	B	831	CLA	2	0
22	B	820	CLA	1	0
22	4	312	CLA	1	0
22	L	203	CLA	1	0
22	O	205	CLA	1	0
25	F	201	BCR	3	0
22	6	306	CLA	2	0
22	A	826	CLA	1	0
22	Z	201	CLA	3	0
22	B	806	CLA	4	0
22	6	307	CLA	2	0
22	A	830	CLA	3	0
25	B	843	BCR	2	0
22	B	816	CLA	1	0
22	6	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	I	102	BCR	1	0
22	4	305	CLA	3	0
22	A	814	CLA	2	0
22	1	303	CLA	3	0
25	1	301	BCR	2	0
22	B	821	CLA	1	0
22	A	833	CLA	1	0
22	A	848	CLA	1	0
22	5	304	CLA	2	0
22	5	303	CLA	1	0
22	2	302	CLA	5	0
22	2	305	CLA	3	0
22	B	808	CLA	3	0
22	A	832	CLA	1	0
25	B	844	BCR	2	0
22	B	825	CLA	3	0
22	B	801	CLA	3	0
22	Z	204	CLA	5	0
31	1	315	RRX	3	0
22	6	313	CLA	2	0
22	A	836	CLA	2	0
22	B	849	CLA	2	0
22	7	310	CLA	2	0
22	B	803	CLA	7	0
22	2	308	CLA	1	0
22	A	857	CLA	3	0
22	A	820	CLA	1	0
22	A	810	CLA	1	0
22	5	311	CLA	1	0
25	L	202	BCR	1	0
28	B	845	DGD	1	0
22	K	102	CLA	1	0
22	4	311	CLA	2	0
25	J	103	BCR	1	0
22	A	835	CLA	1	0
22	B	819	CLA	3	0
22	6	312	CLA	1	0
22	A	834	CLA	1	0
31	5	322	RRX	2	0
22	7	313	CLA	1	0
22	J	102	CLA	1	0
22	3	301	CLA	1	0

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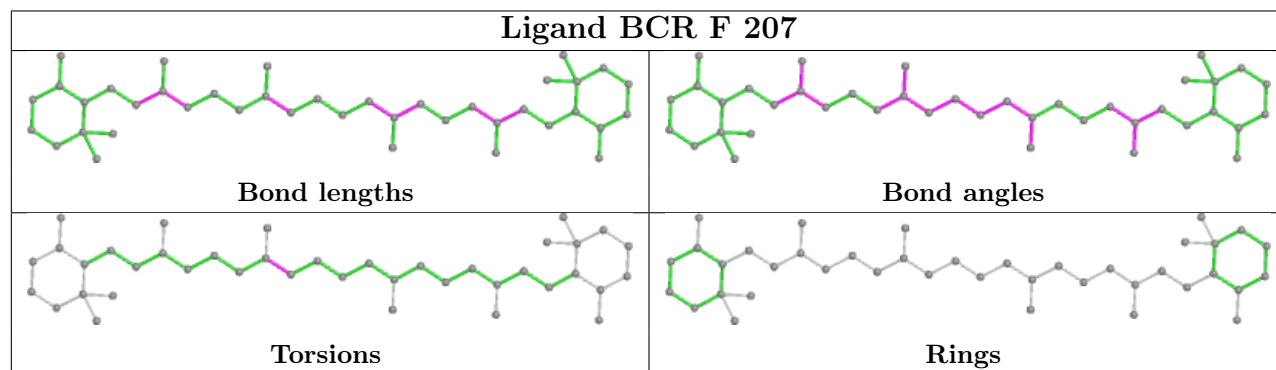
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	837	CLA	2	0
22	A	839	CLA	2	0
22	K	101	CLA	1	0
22	A	829	CLA	1	0
31	6	318	RRX	3	0
22	B	823	CLA	1	0
22	7	305	CLA	2	0
22	B	829	CLA	1	0
22	B	828	CLA	3	0
22	B	836	CLA	3	0
22	7	306	CLA	2	0
22	3	302	CLA	1	0
25	L	201	BCR	1	0
22	1	306	CLA	2	0
22	A	805	CLA	1	0
22	O	204	CLA	1	0
22	O	206	CLA	1	0
25	5	315	BCR	1	0
22	A	802	CLA	2	0
22	7	308	CLA	2	0
24	J	106	LHG	1	0
22	A	803	CLA	2	0
22	5	310	CLA	2	0
22	B	818	CLA	2	0
22	A	807	CLA	2	0
22	A	858	CLA	1	0
22	L	205	CLA	2	0
22	B	832	CLA	1	0
22	L	204	CLA	1	0
22	2	309	CLA	1	0
22	A	804	CLA	2	0
22	O	203	CLA	2	0
22	3	303	CLA	1	0
22	F	205	CLA	2	0
22	2	303	CLA	1	0
22	A	815	CLA	1	0
22	2	304	CLA	2	0
22	6	303	CLA	1	0
22	6	314	CLA	1	0
22	1	310	CLA	1	0
22	2	311	CLA	1	0
22	B	817	CLA	1	0

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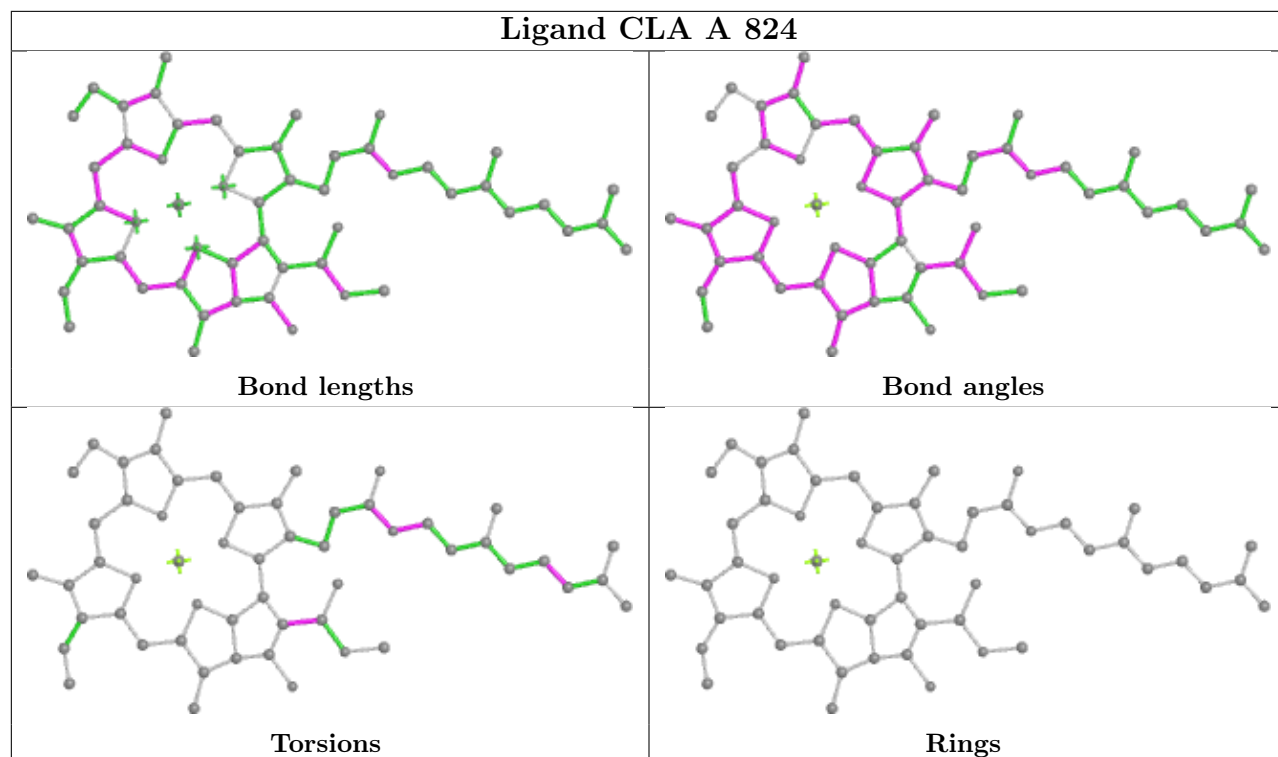
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	845	BCR	1	0
25	B	842	BCR	2	0
25	L	206	BCR	1	0
22	A	806	CLA	1	0
22	B	815	CLA	1	0
22	B	822	CLA	3	0
22	B	838	CLA	3	0
22	B	833	CLA	4	0
22	B	850	CLA	1	0
22	5	307	CLA	2	0

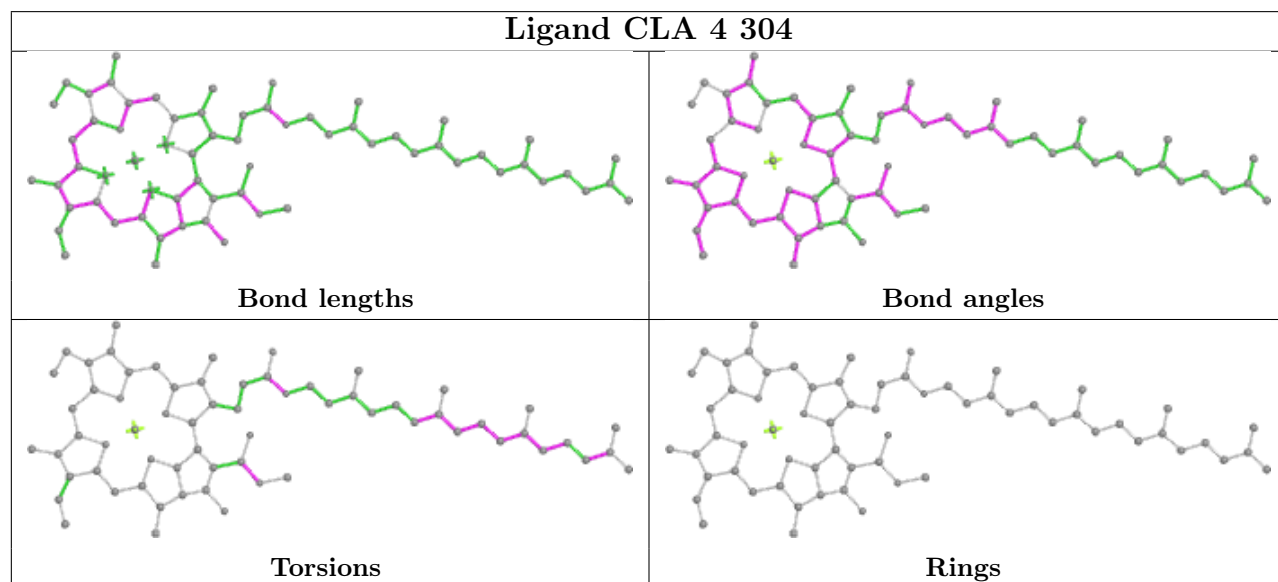
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

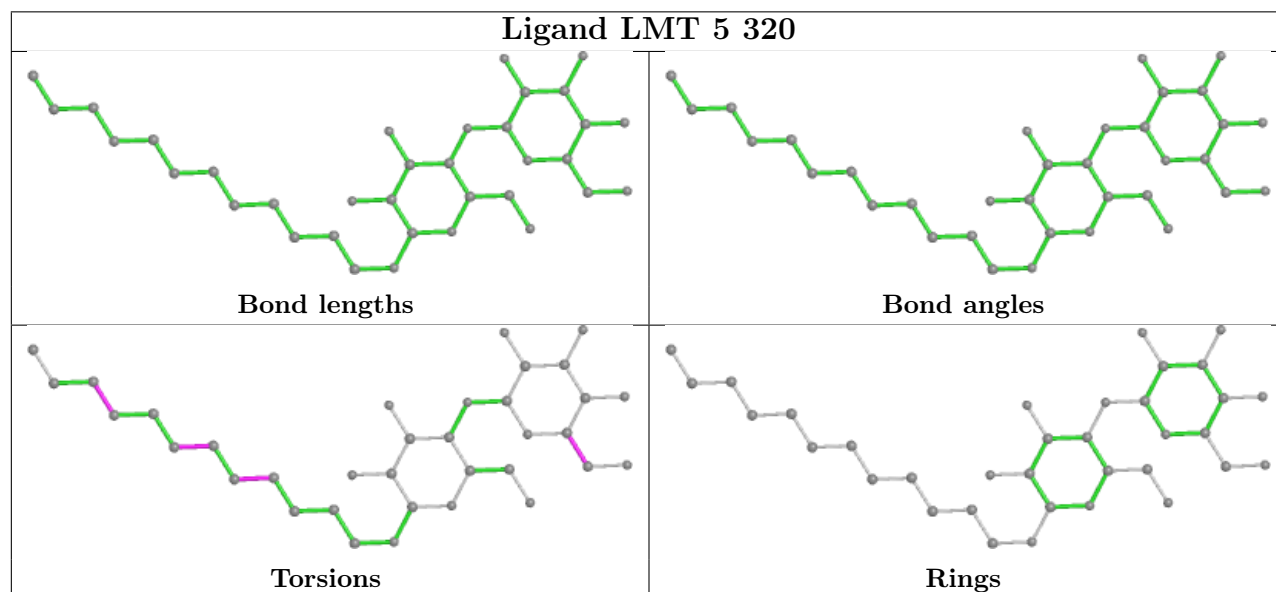
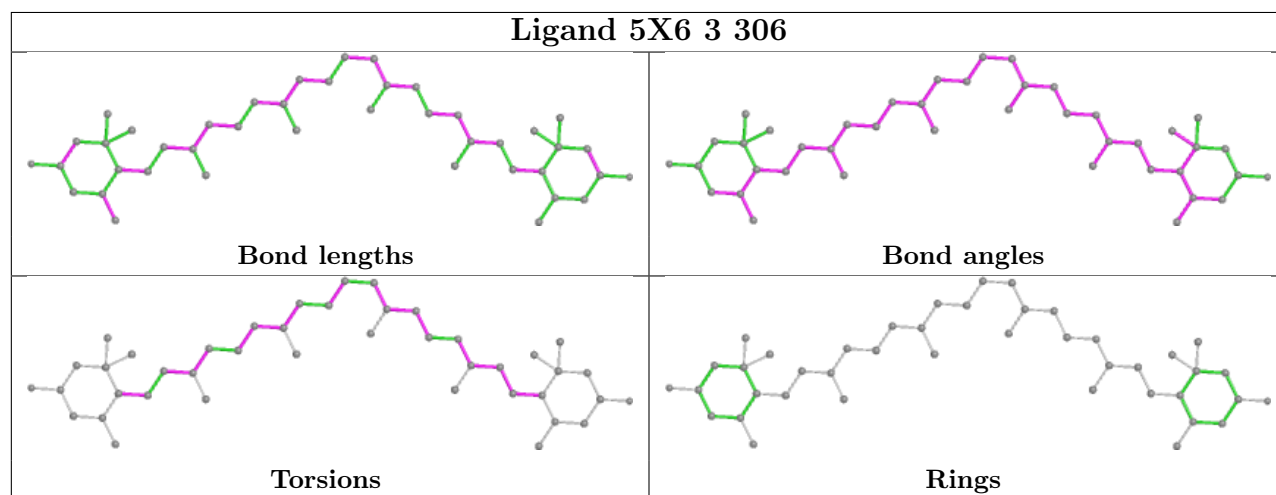
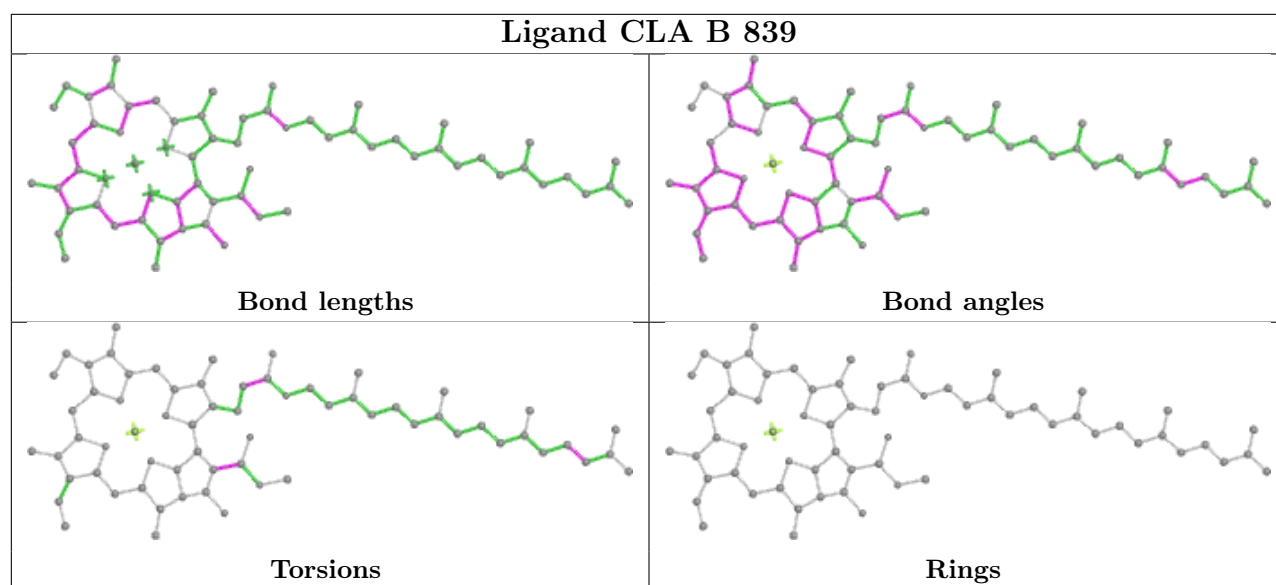


## Ligand CLA A 824

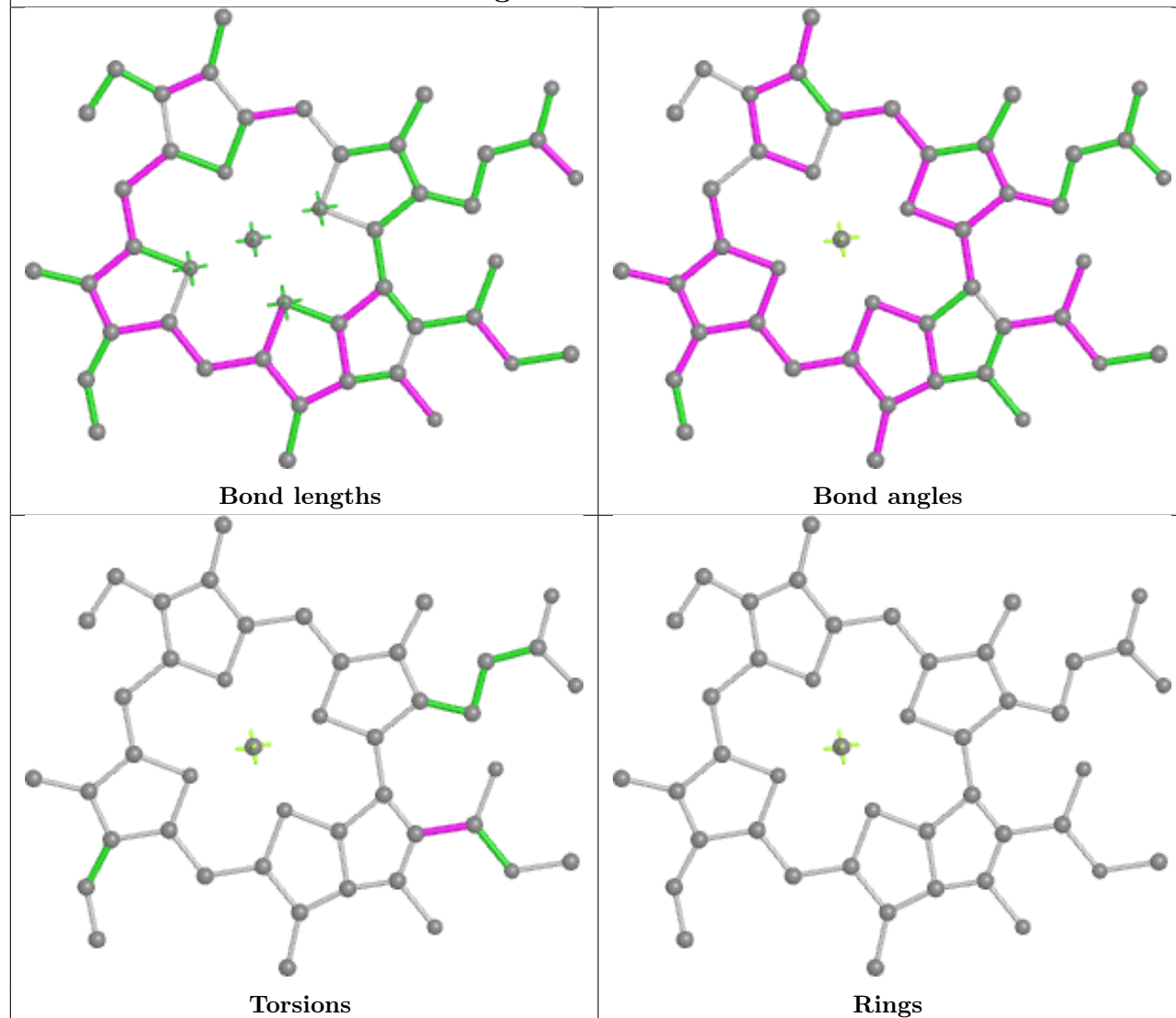


## Ligand CLA 4 304

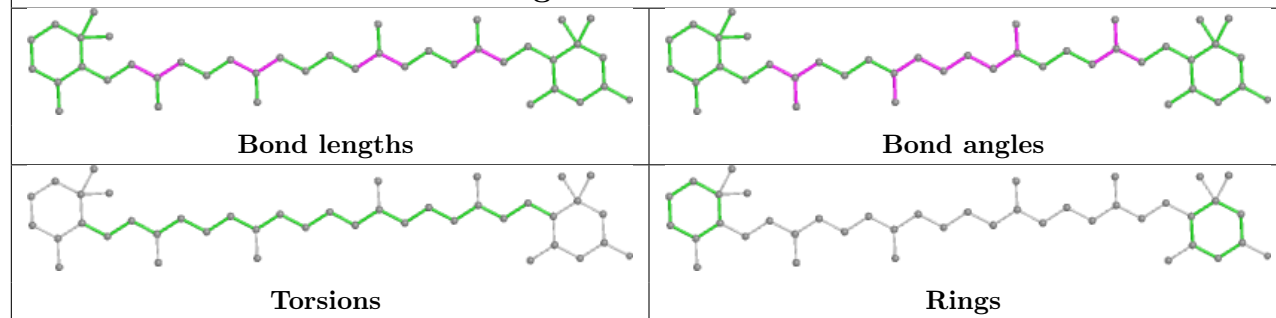




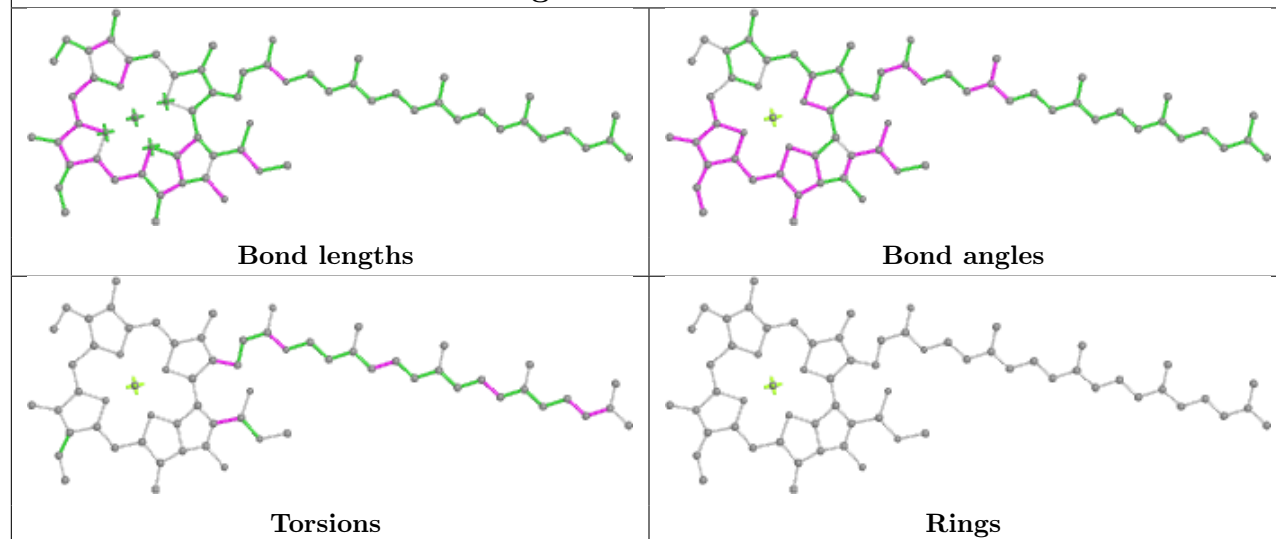
## Ligand CLA 2 307



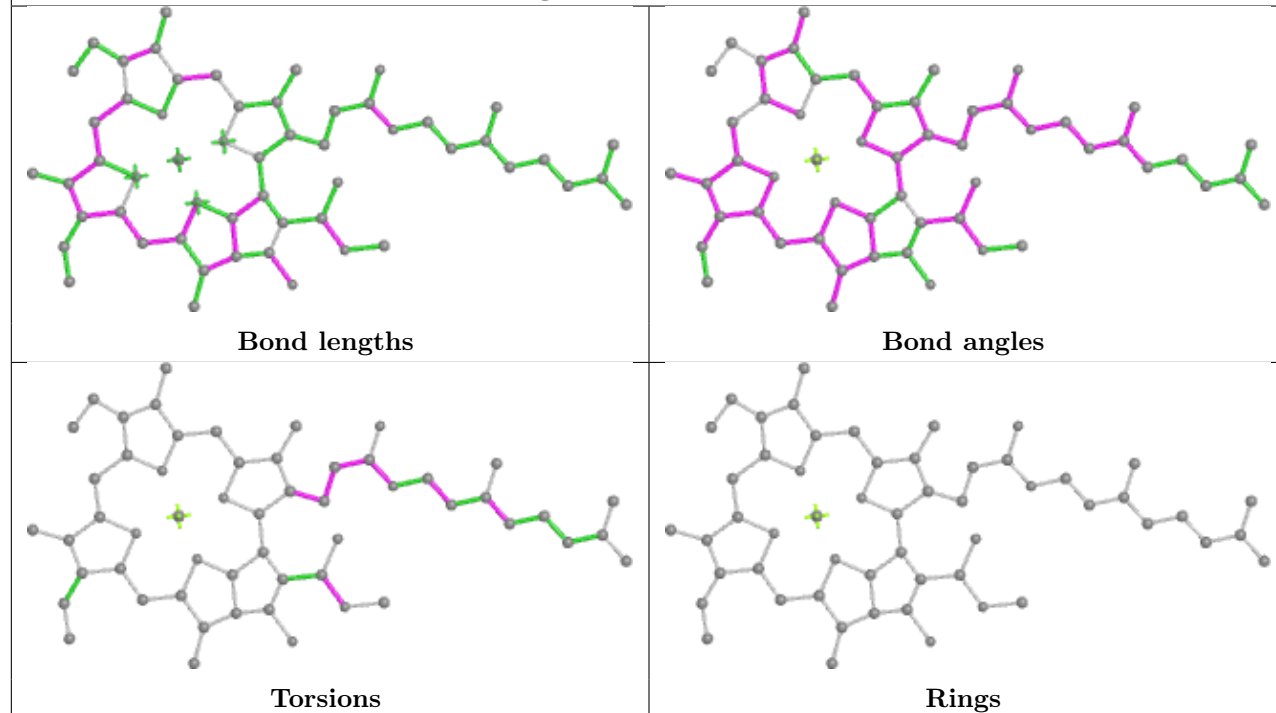
## Ligand RRX 4 317



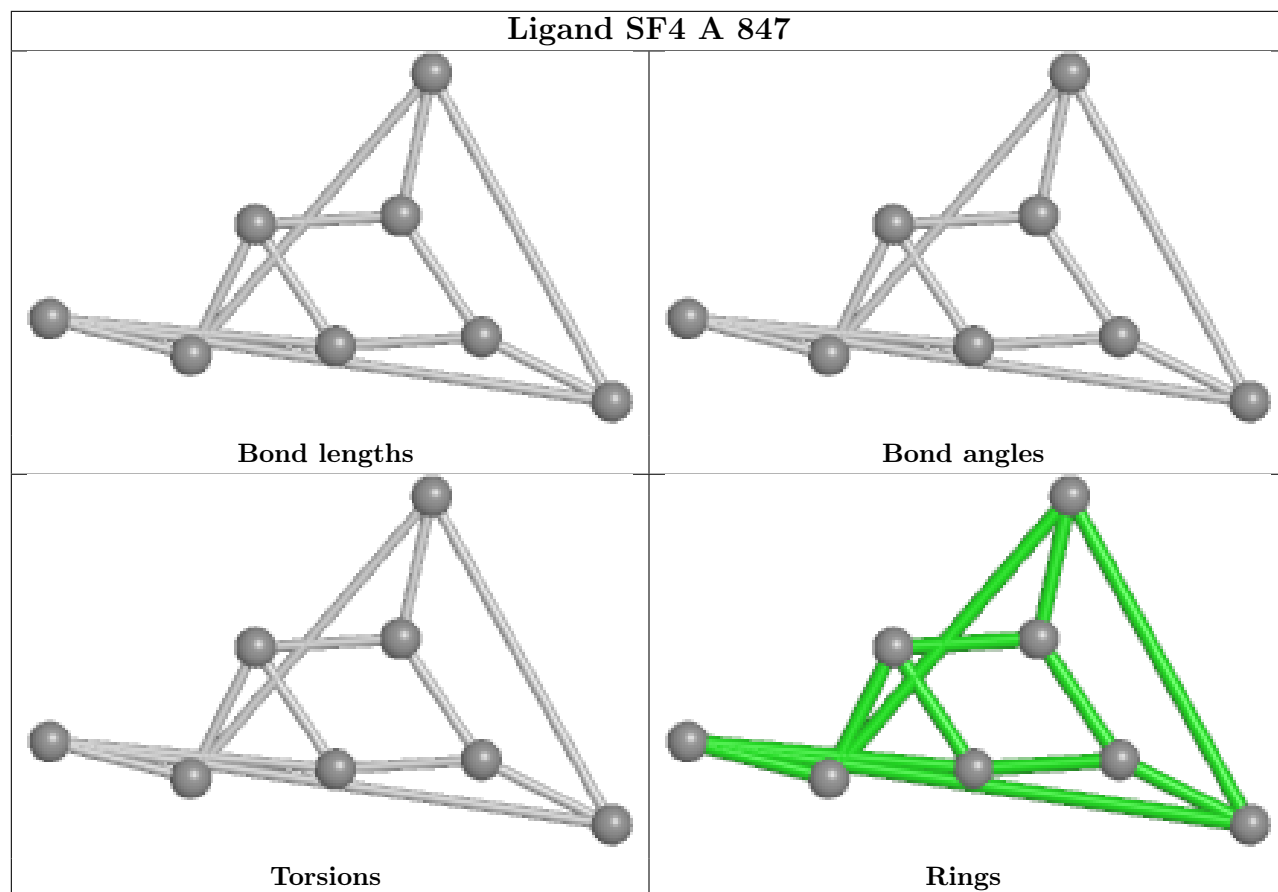
## Ligand CLA A 831



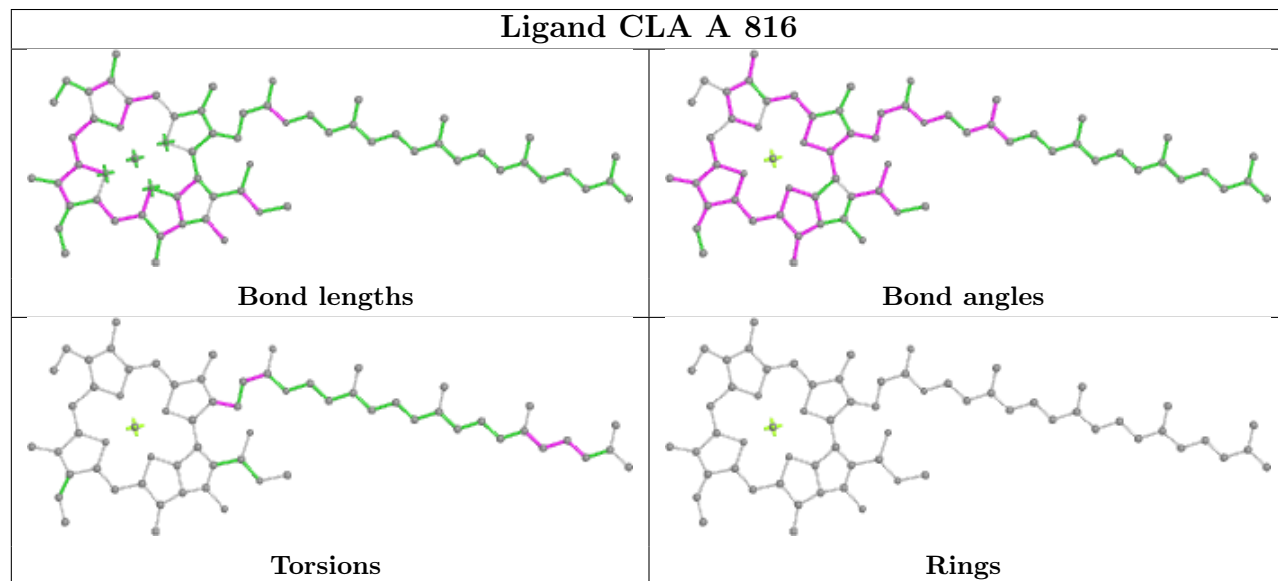
## Ligand CLA 1 307



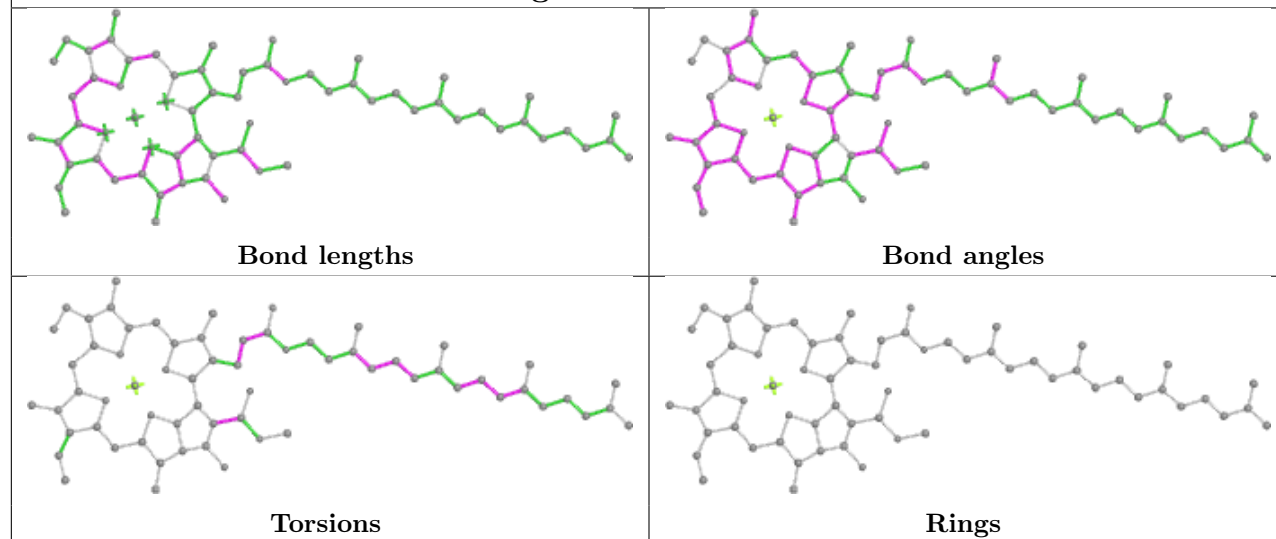
## Ligand SF4 A 847



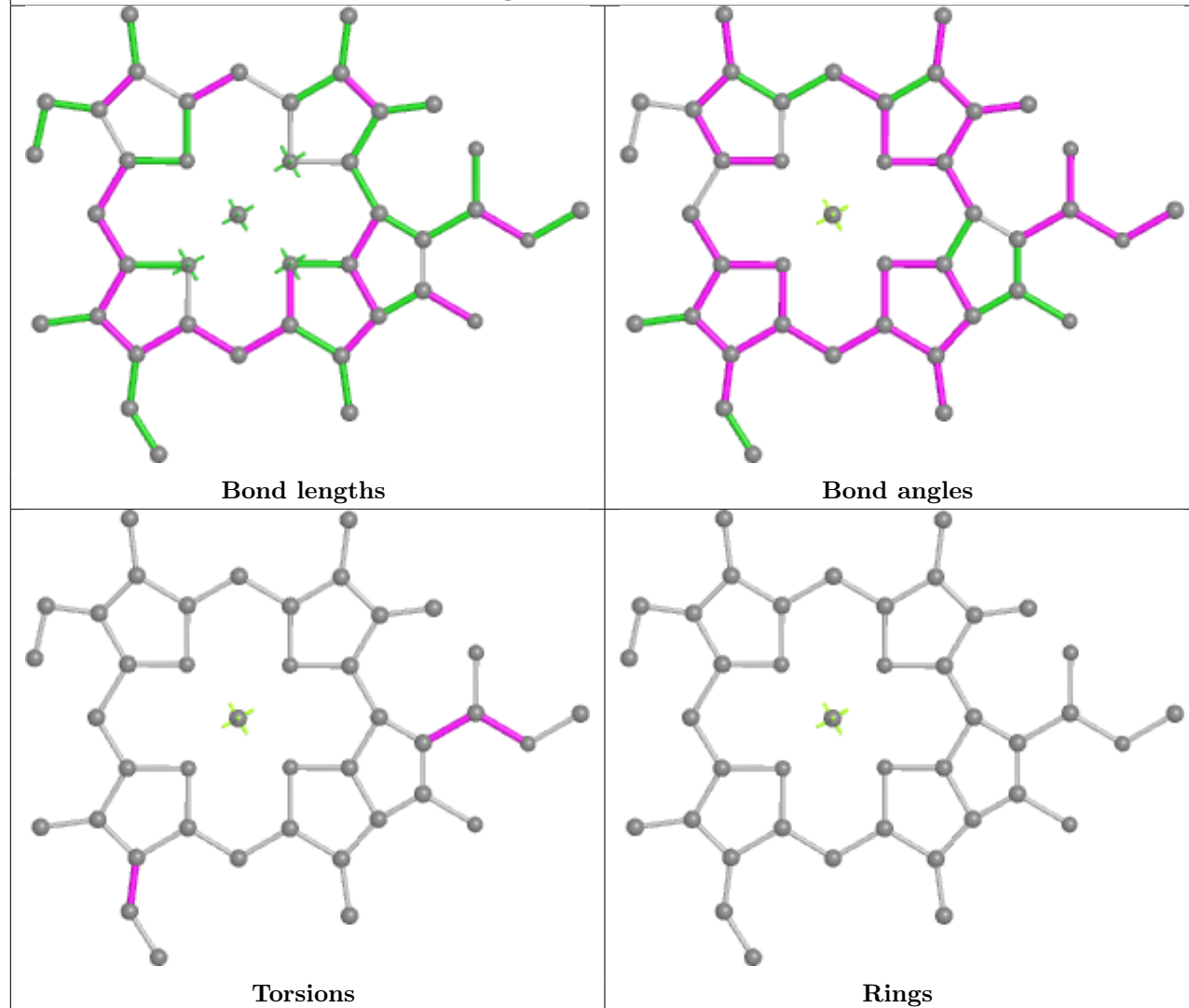
## Ligand CLA A 816



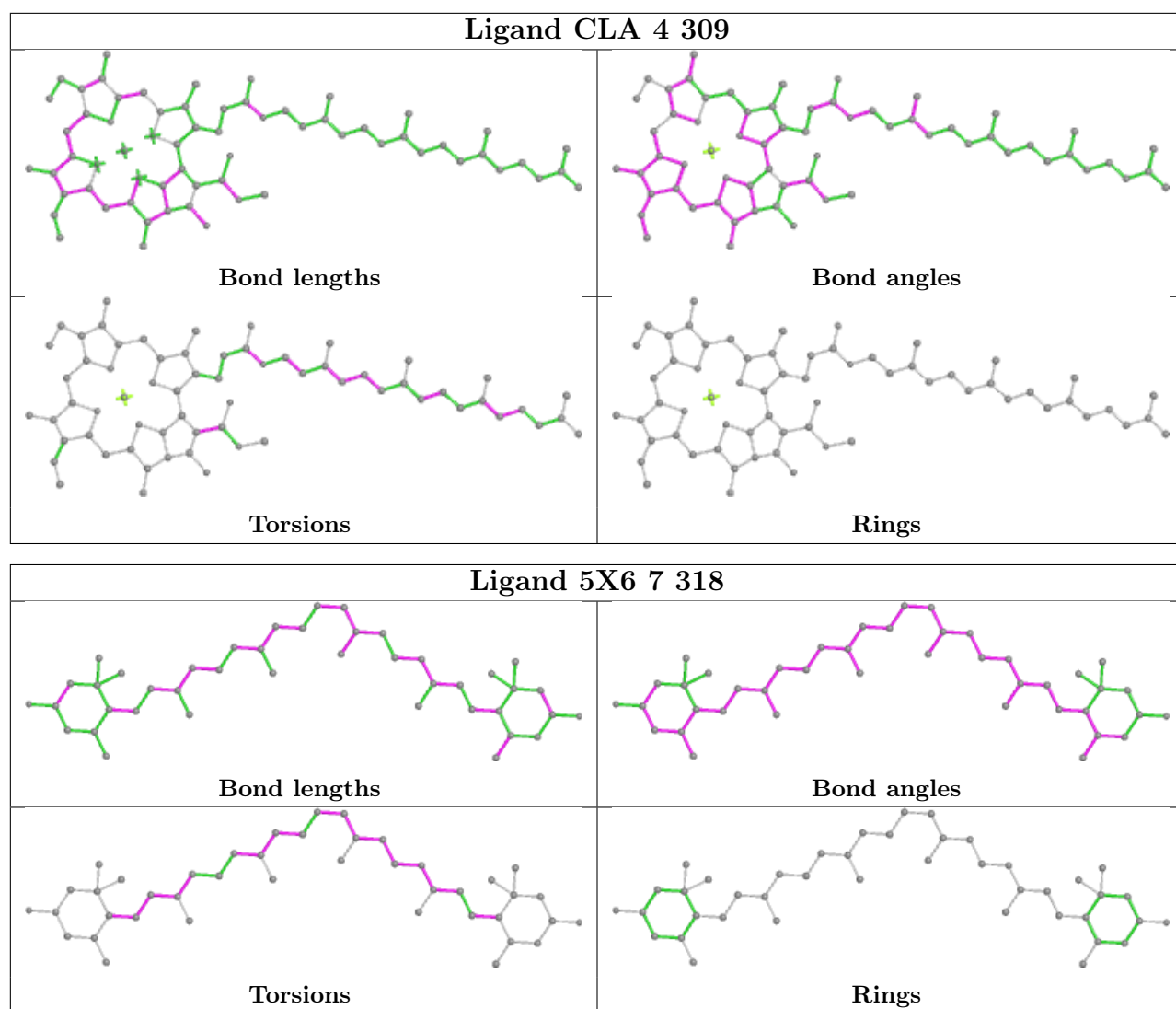
## Ligand CLA A 818



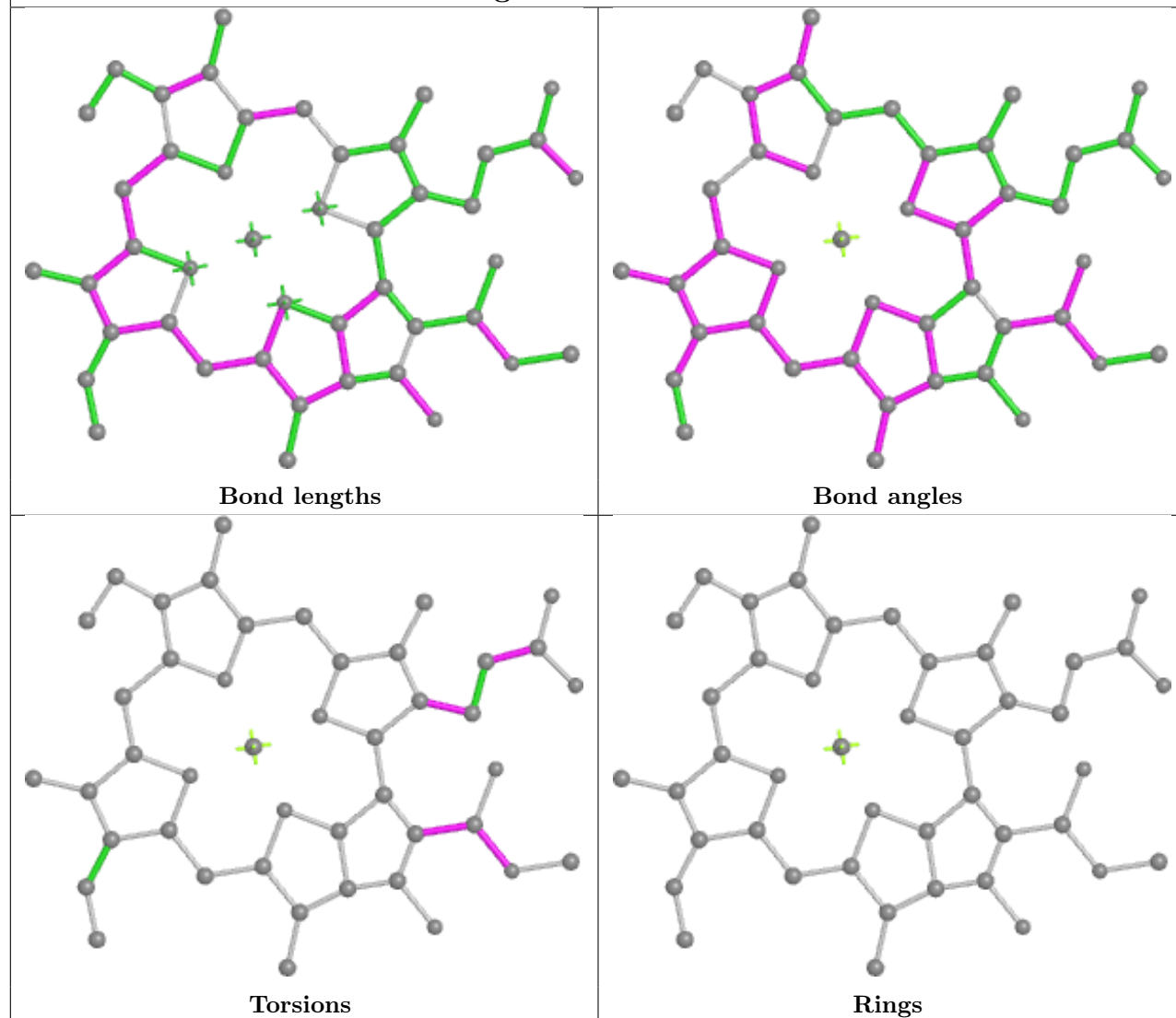
## Ligand CLA 6 311



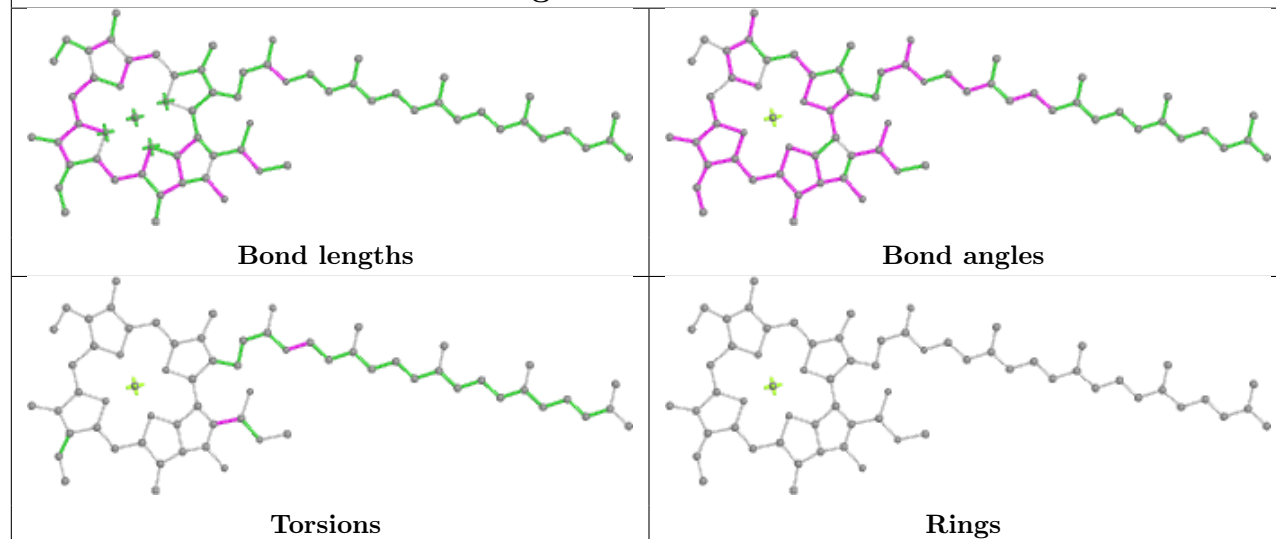


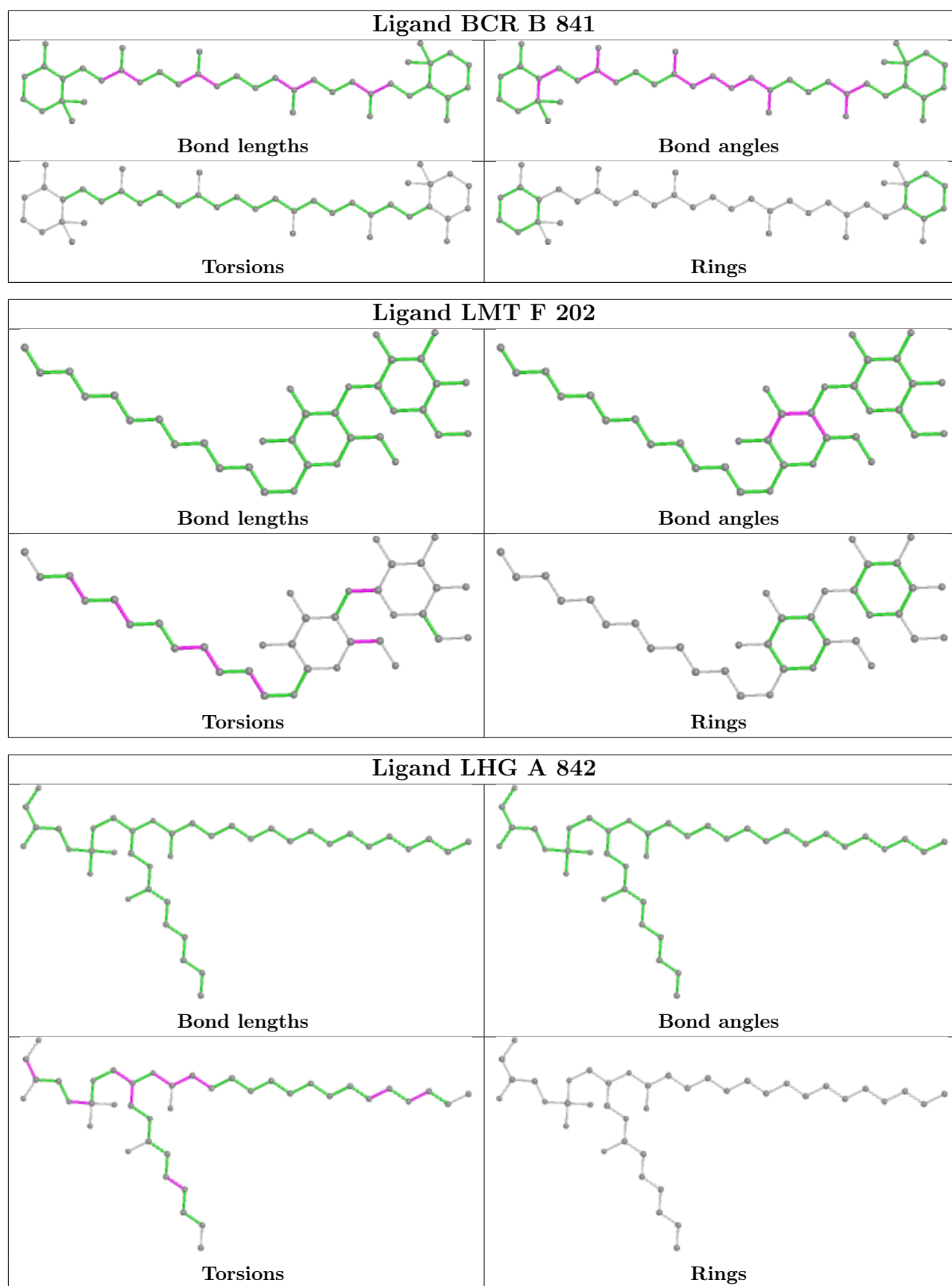


## Ligand CLA 7 303

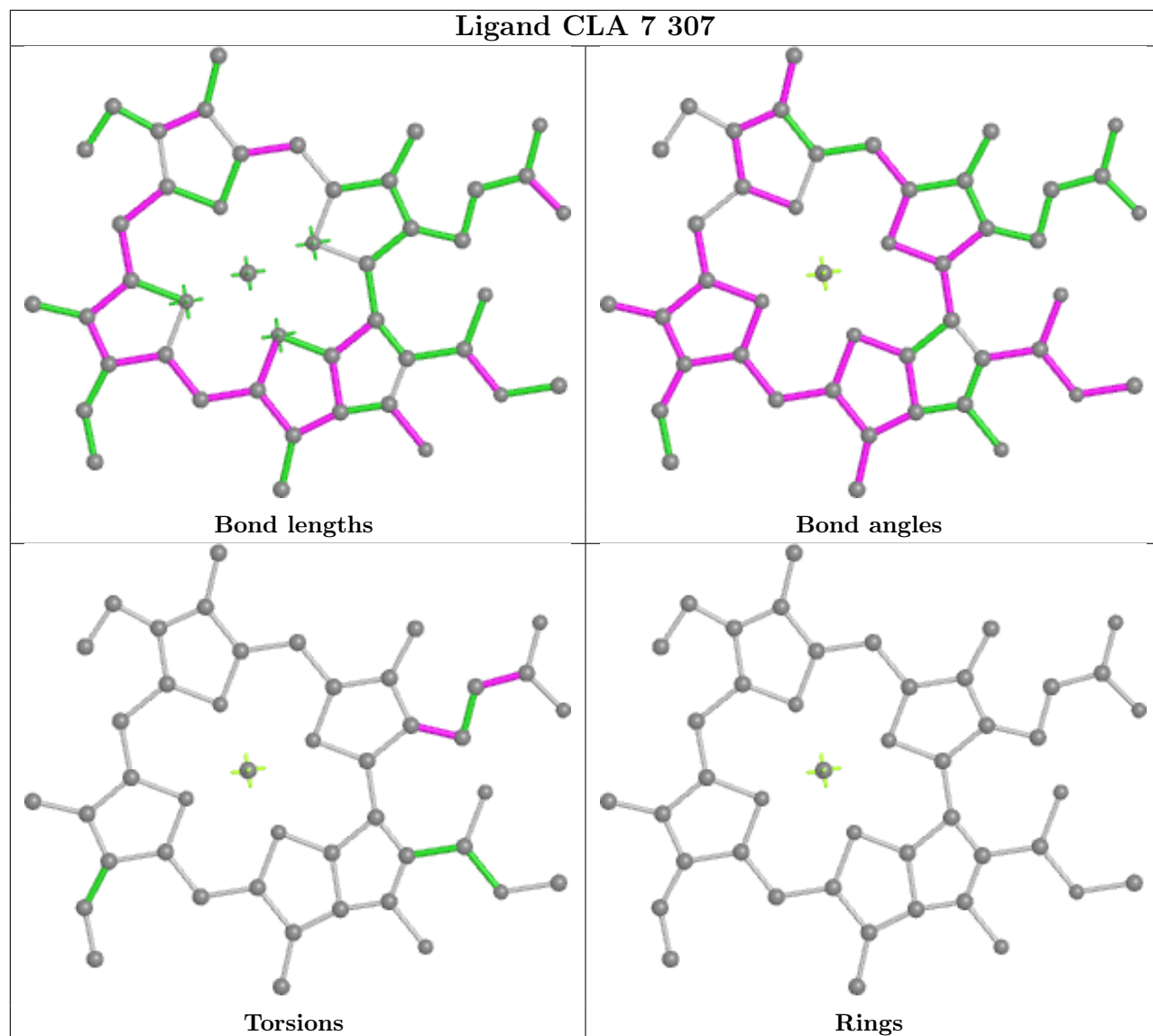


## Ligand CLA B 826

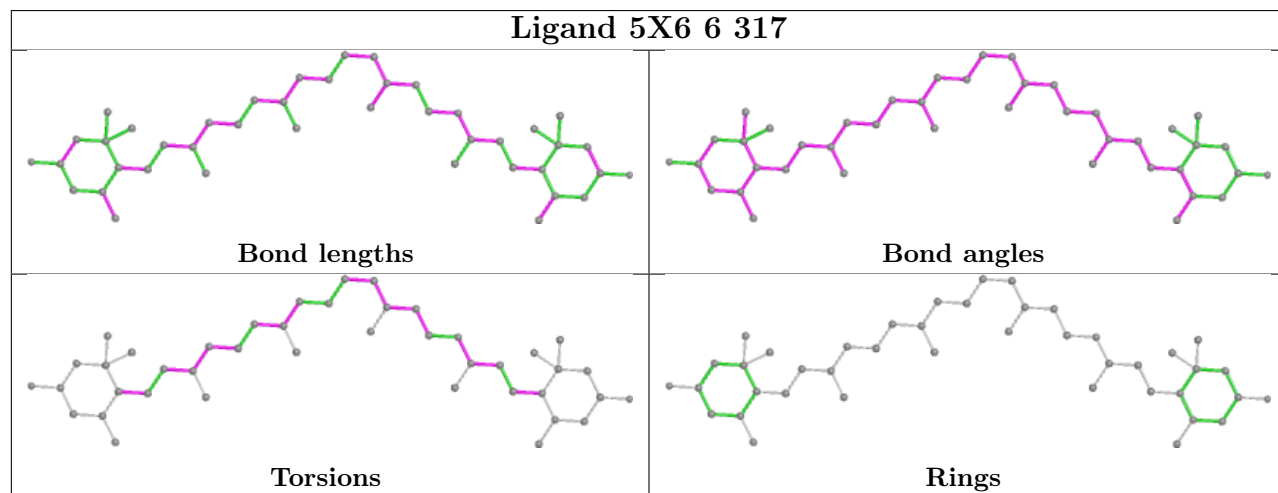




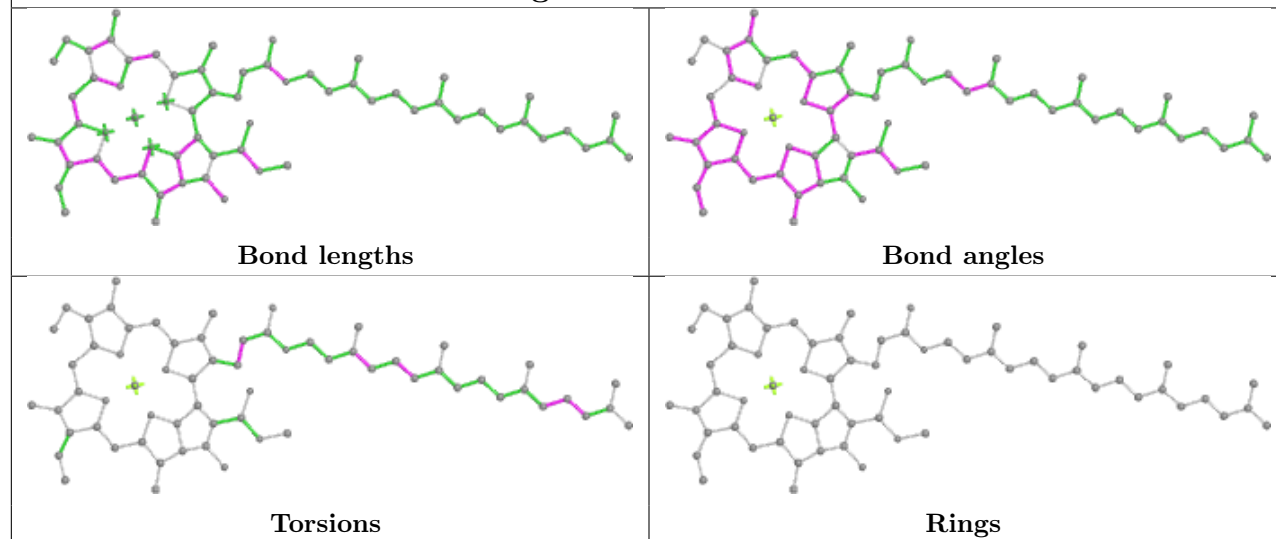
## Ligand CLA 7 307



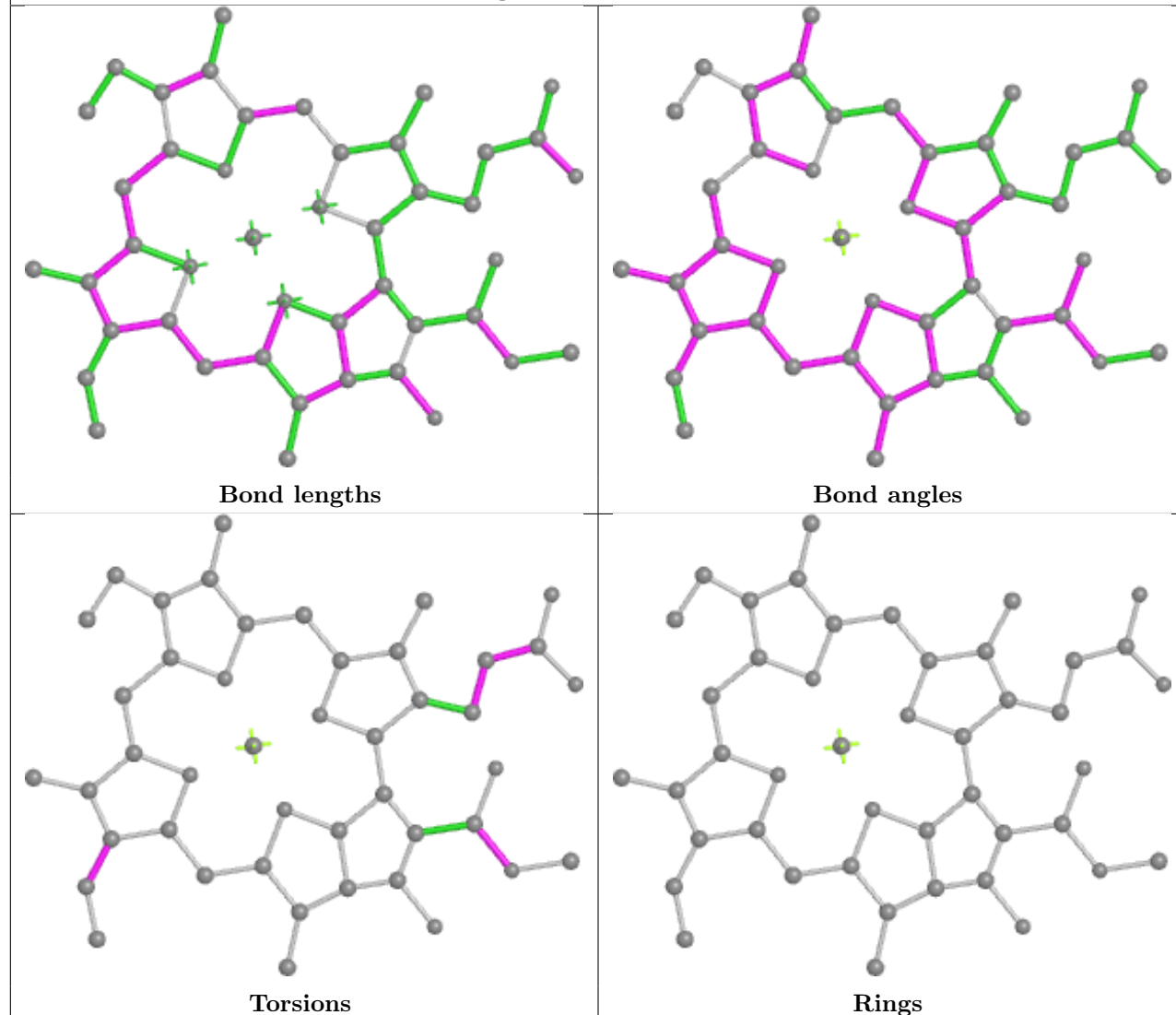
## Ligand 5X6 6 317

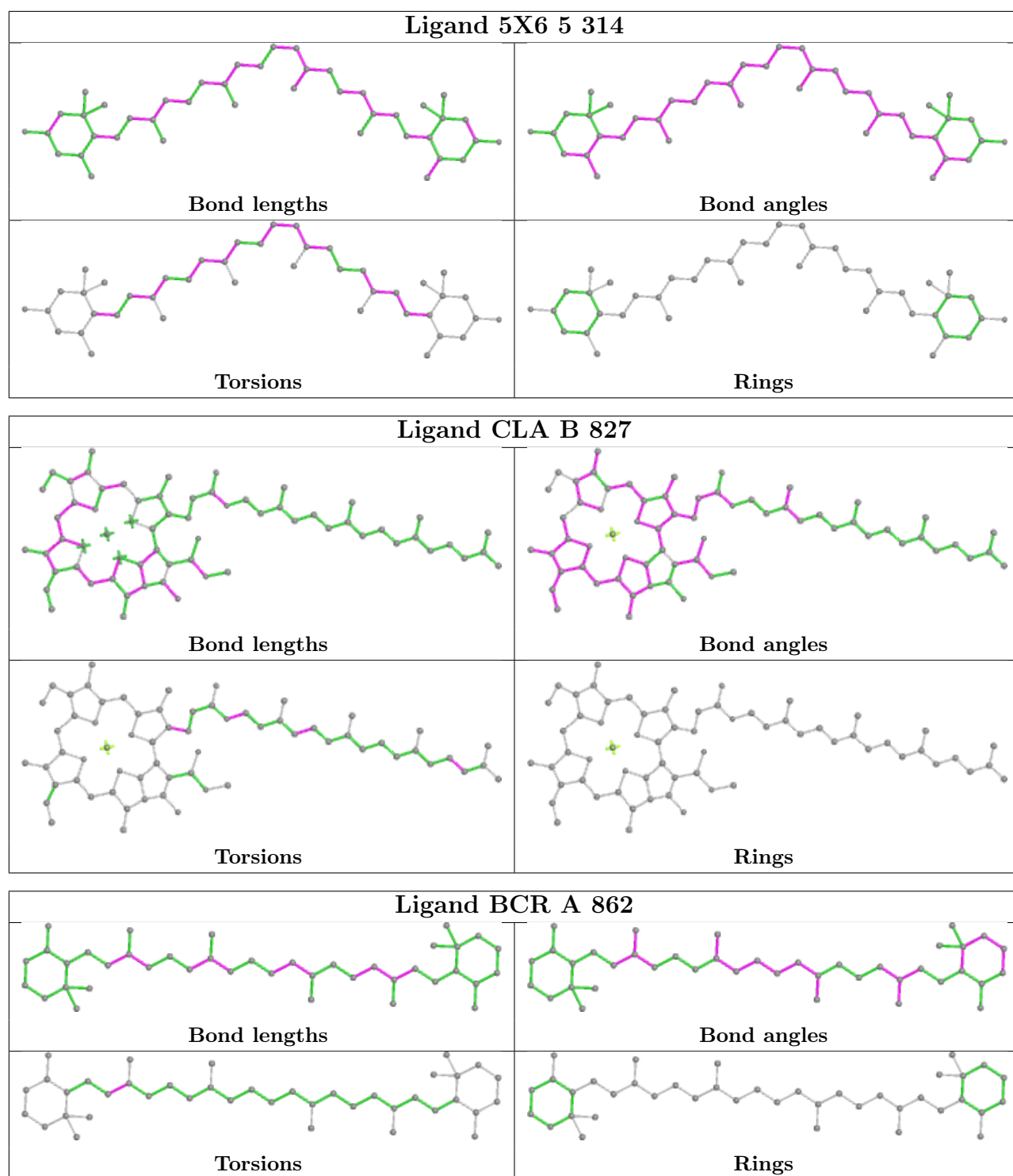


## Ligand CLA A 827

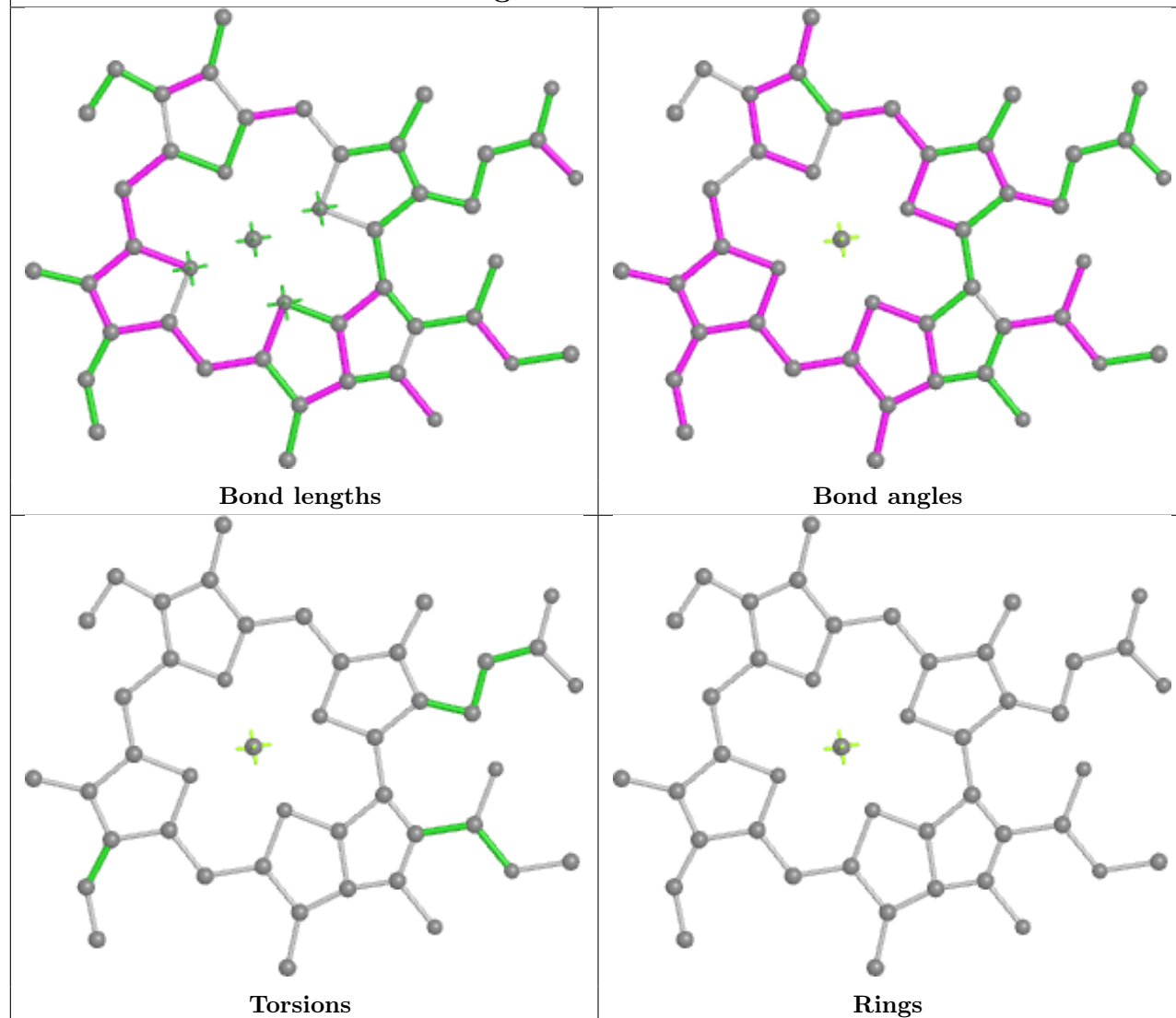


## Ligand CLA 5 305

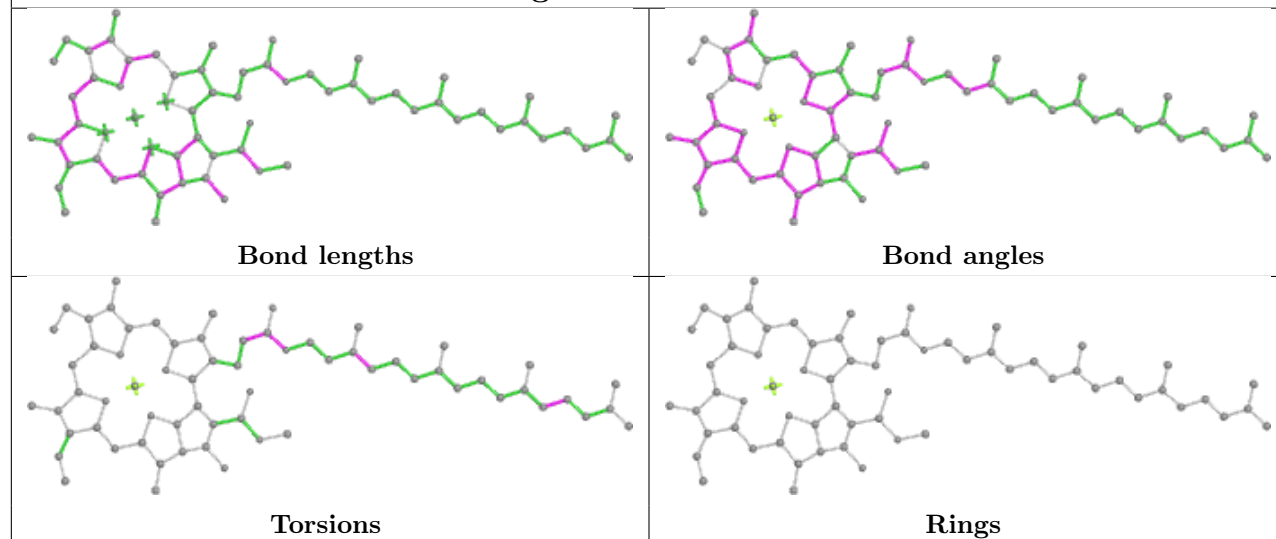




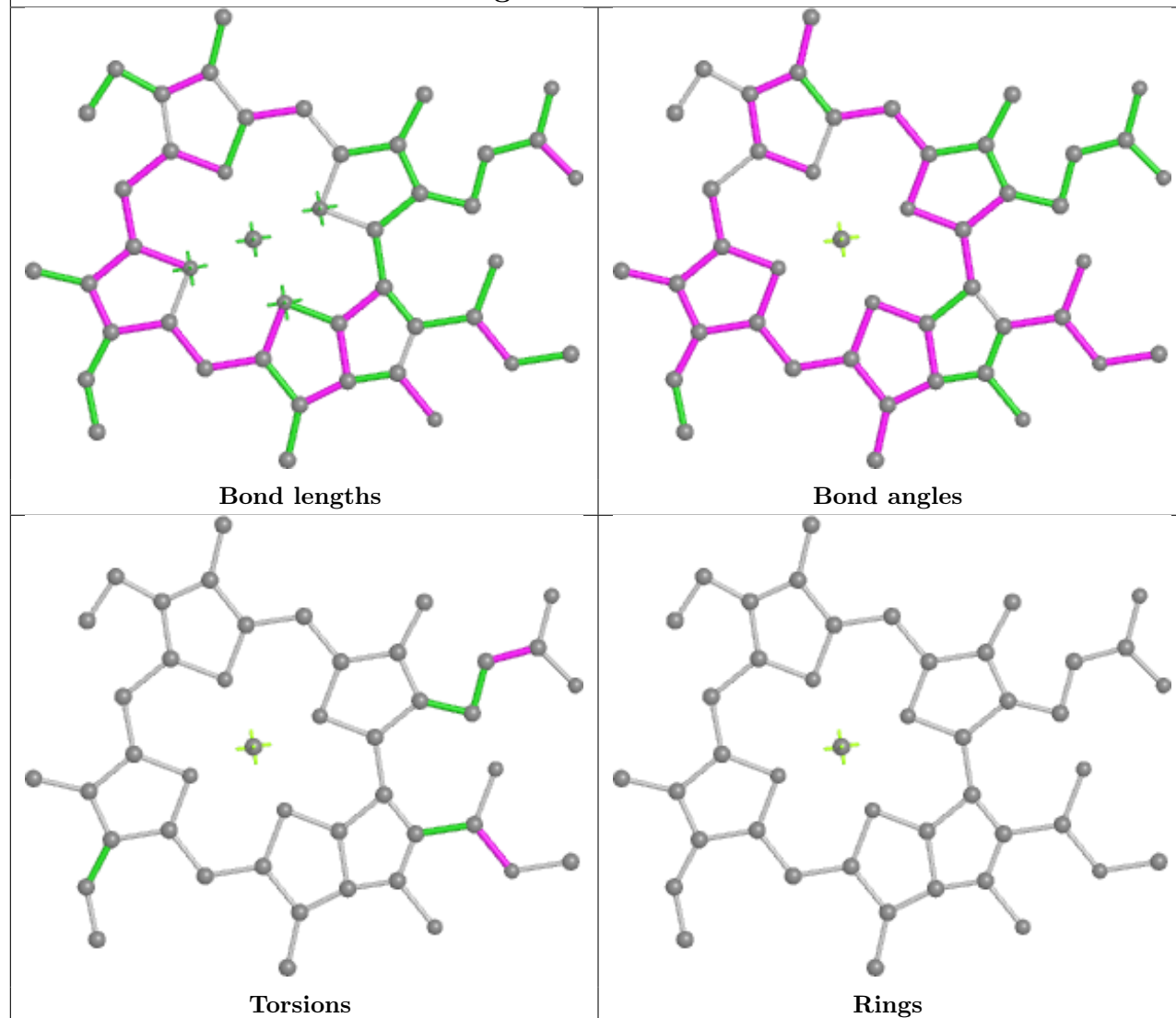
## Ligand CLA 4 307



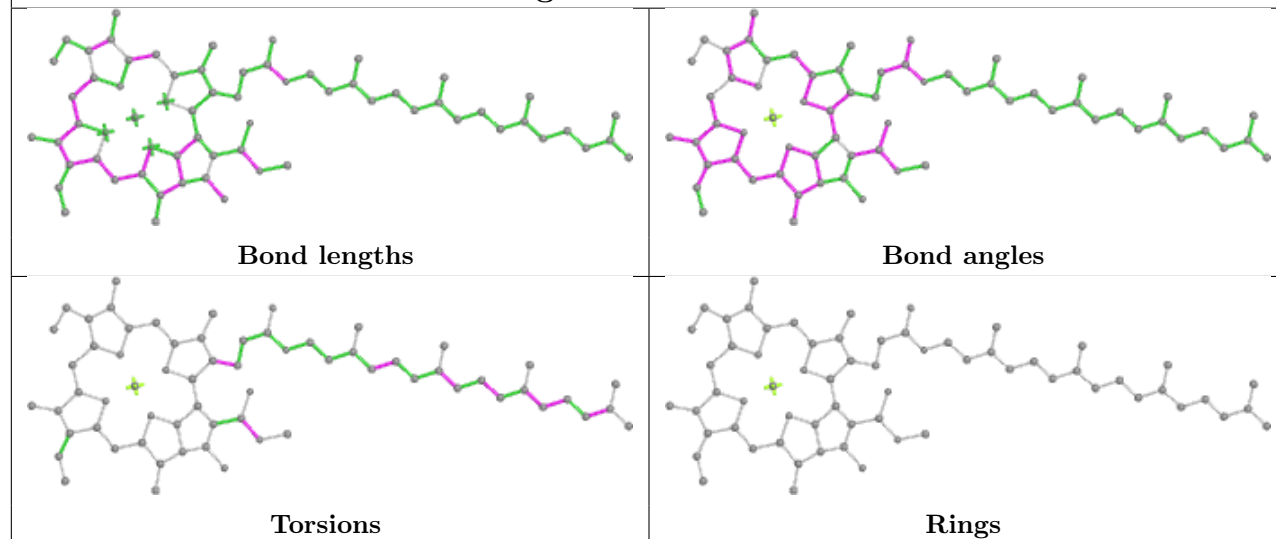
## Ligand CLA A 825



## Ligand CLA 1 304

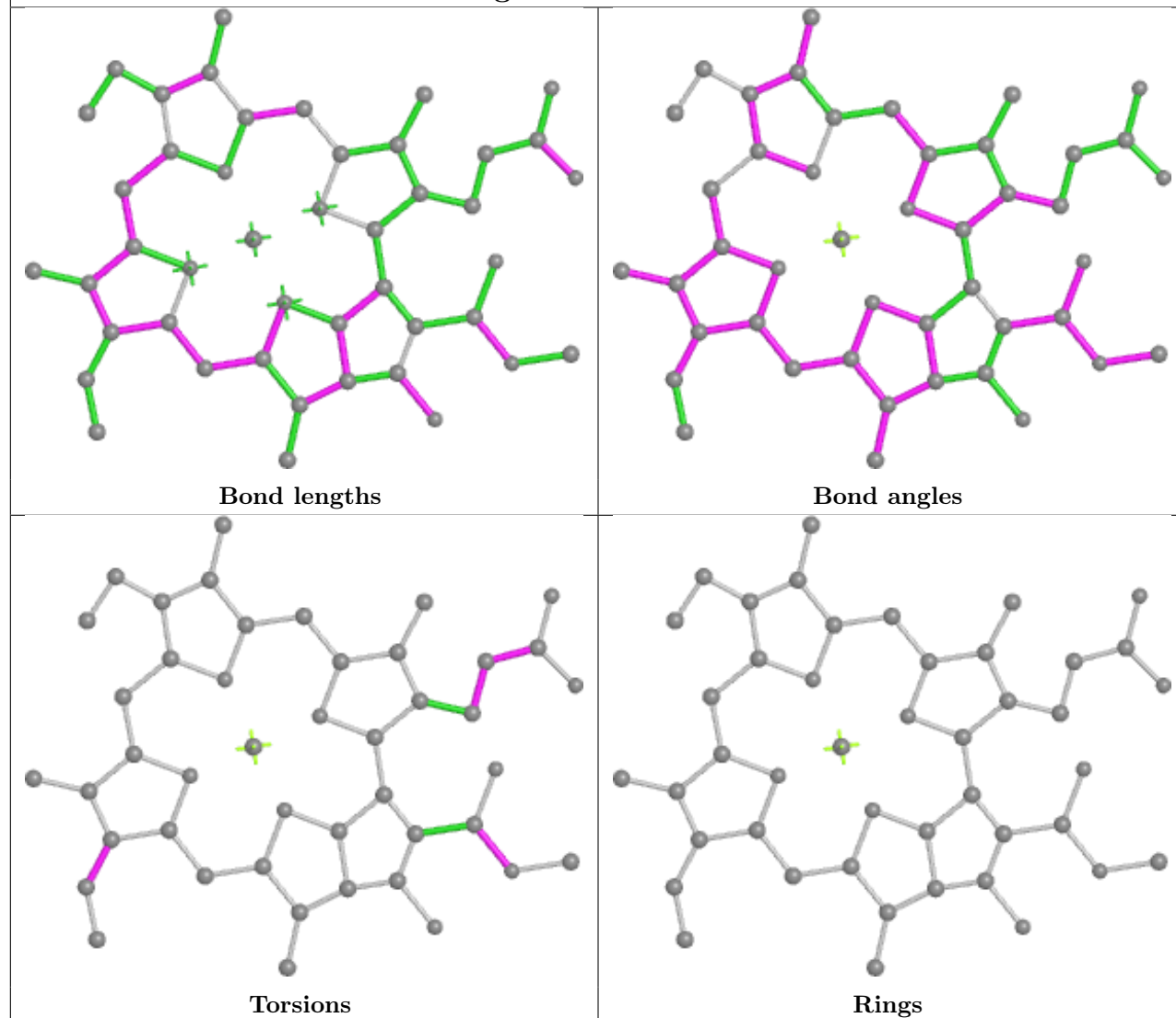


## Ligand CLA 6 304

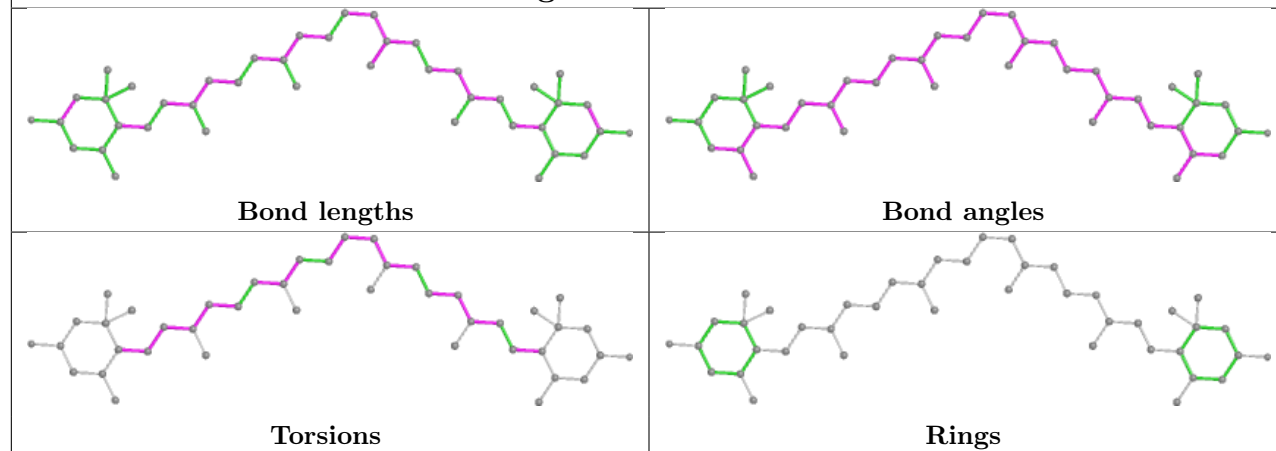


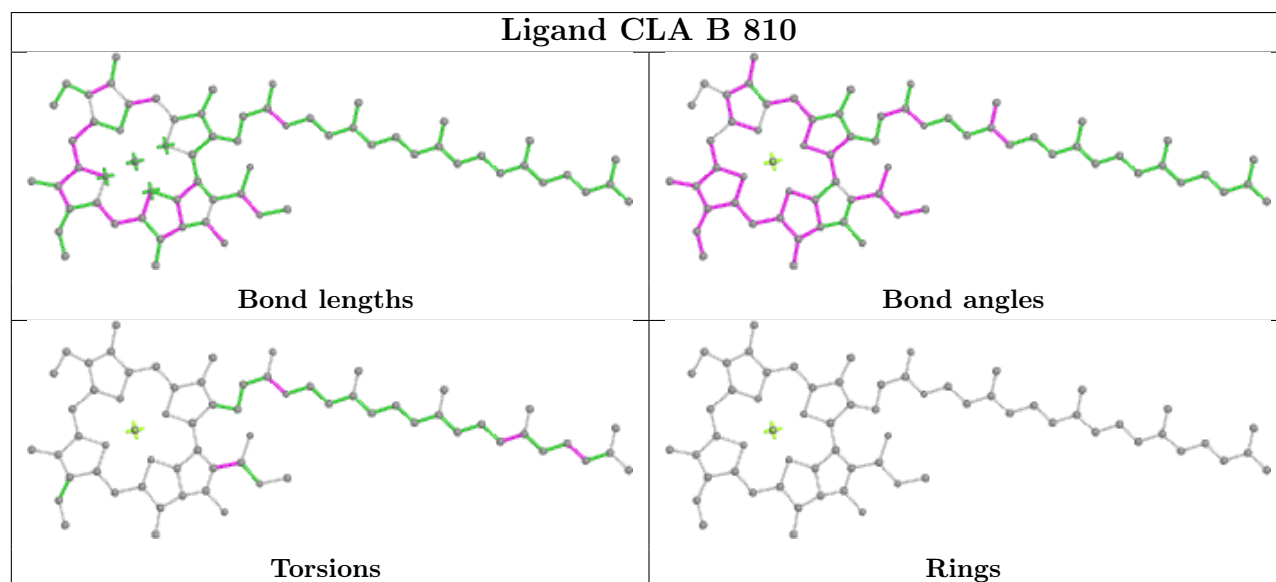
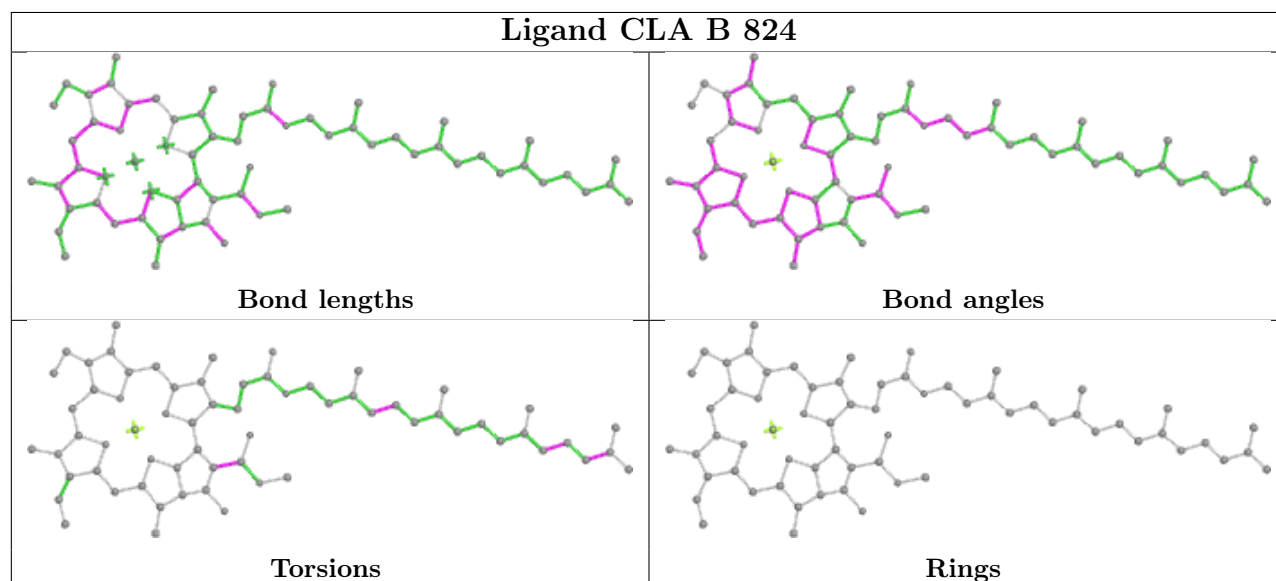
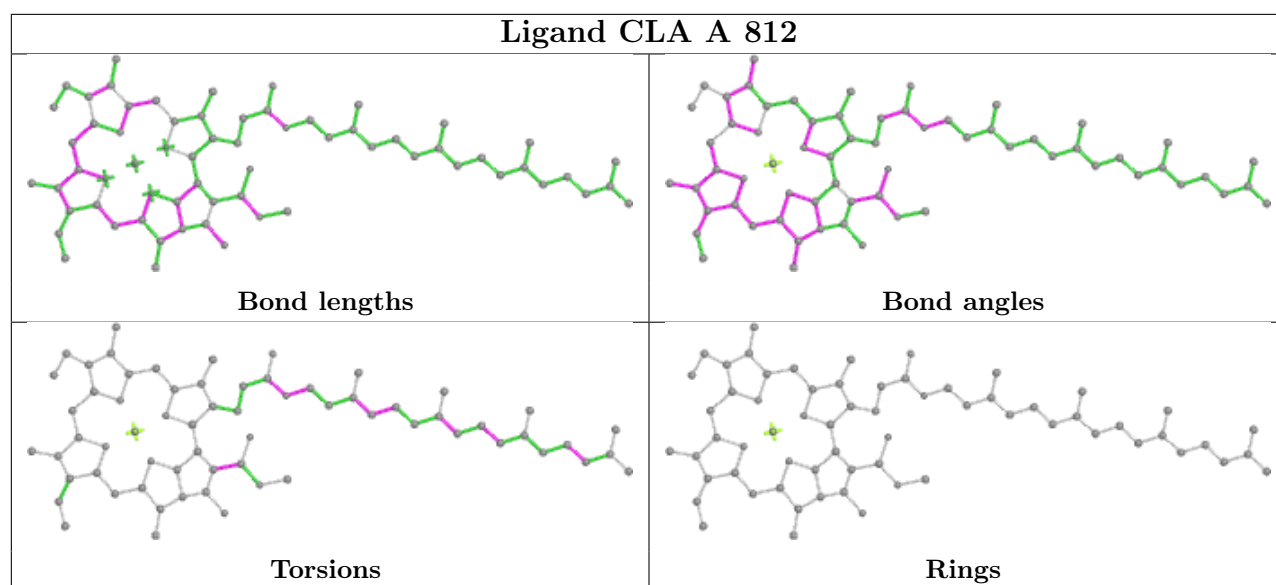


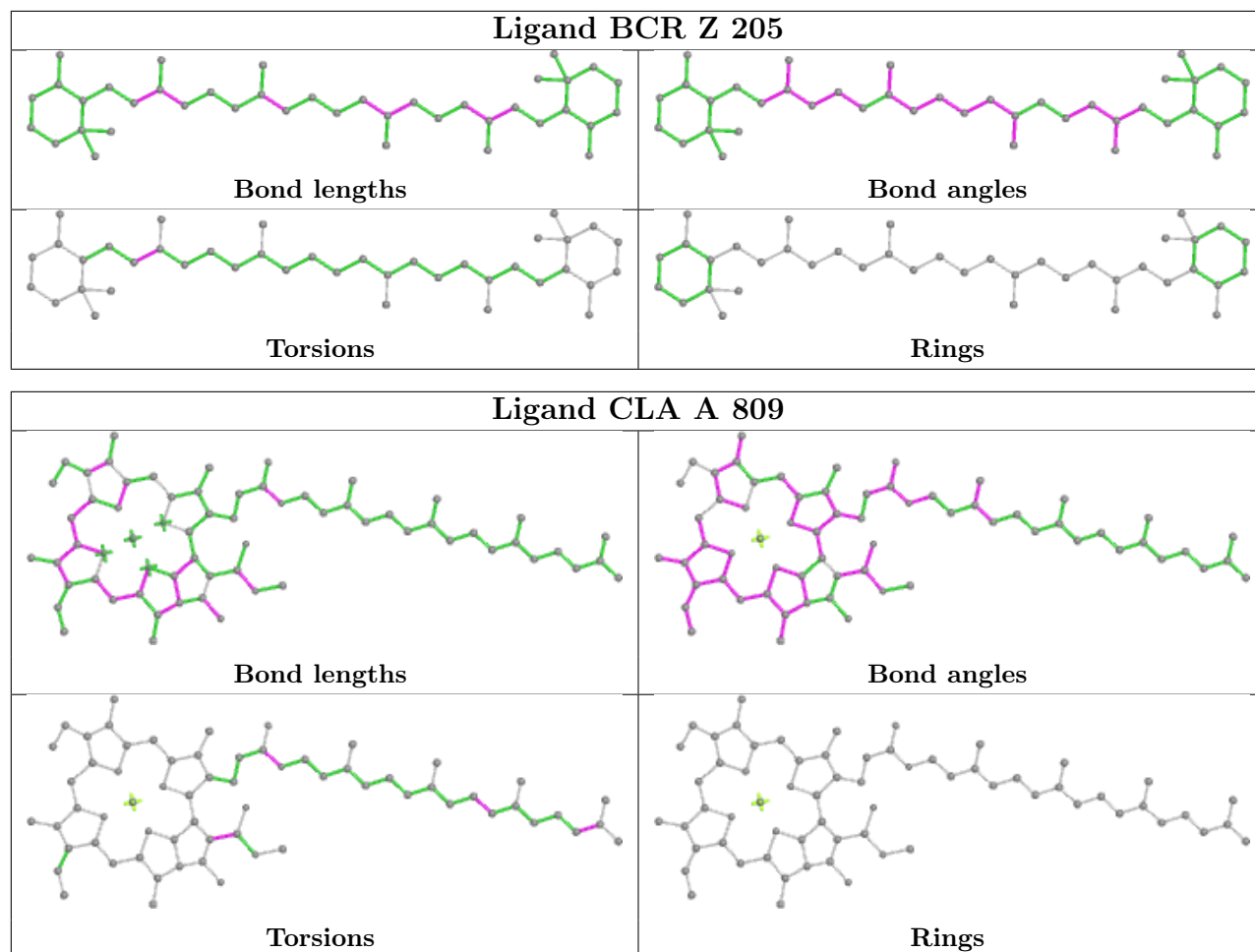
## Ligand CLA 4 306

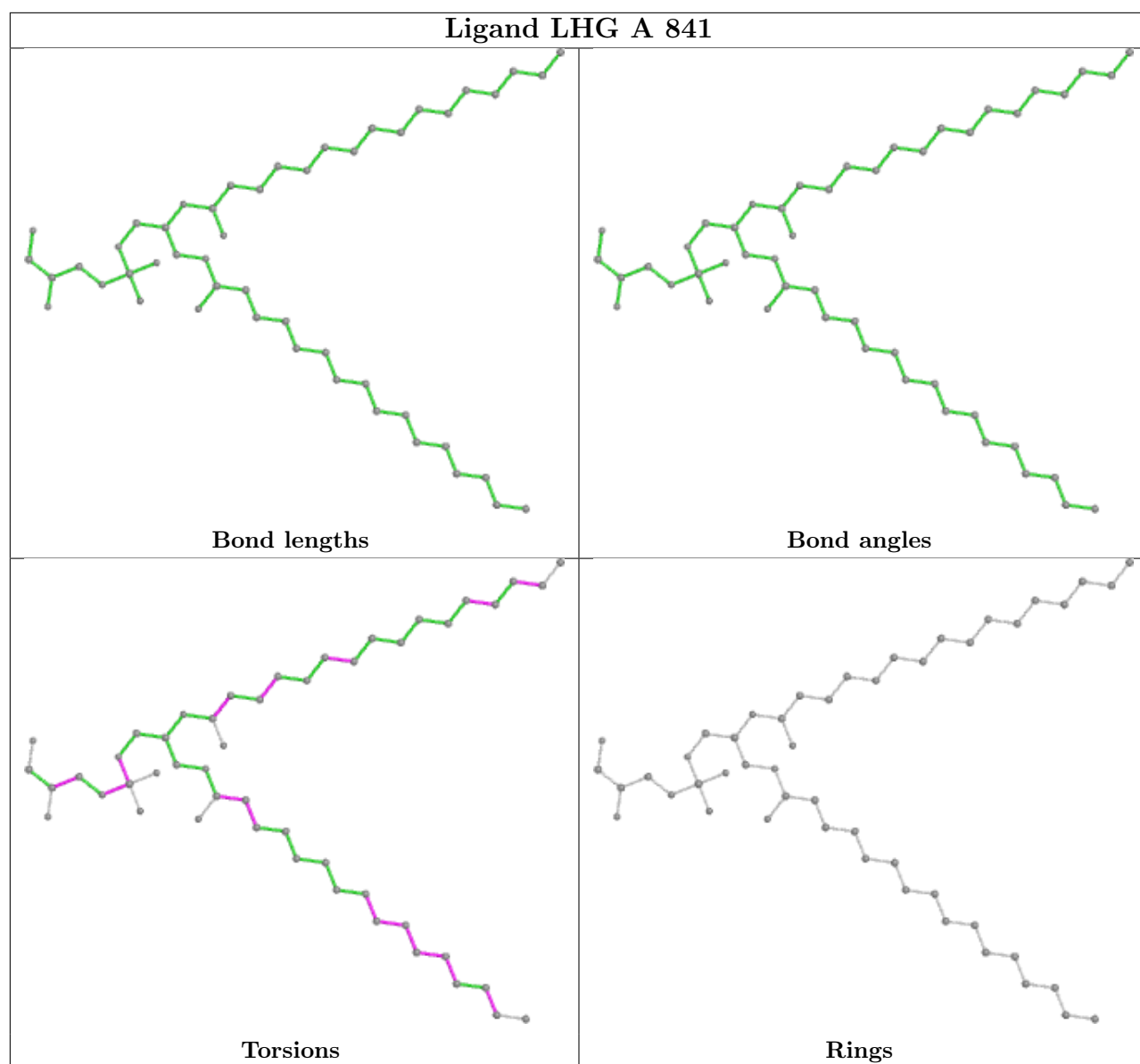


## Ligand 5X6 O 208

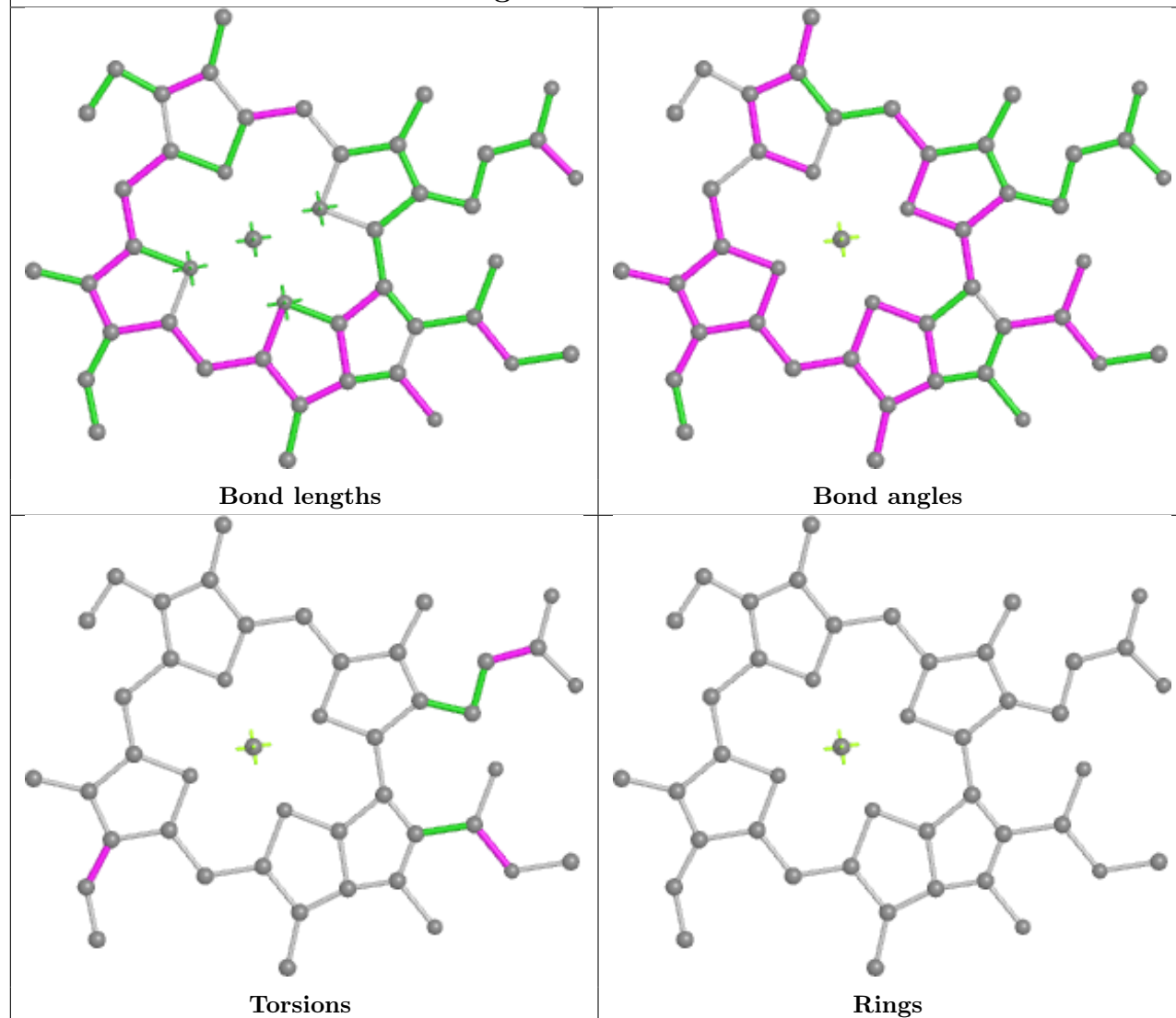




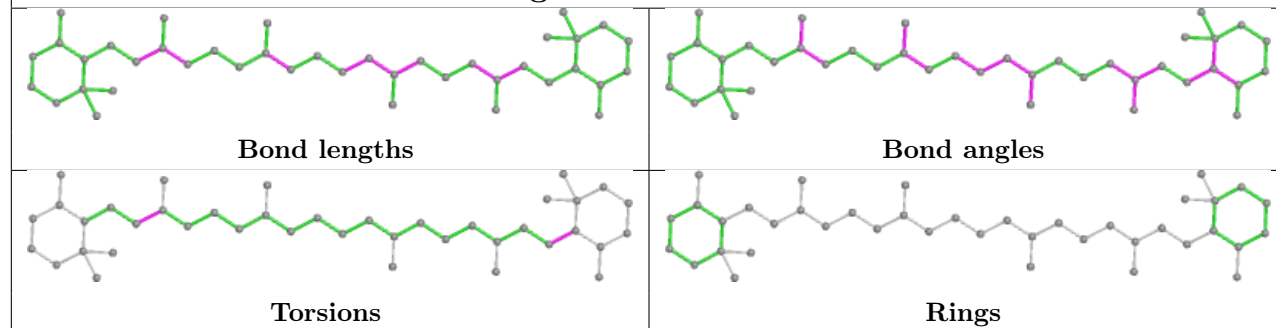


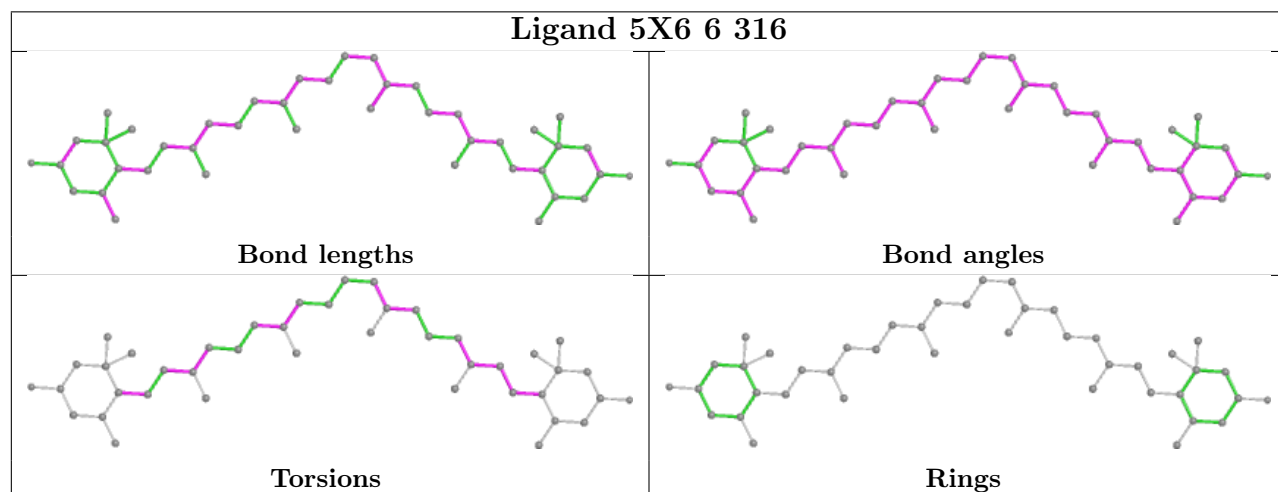
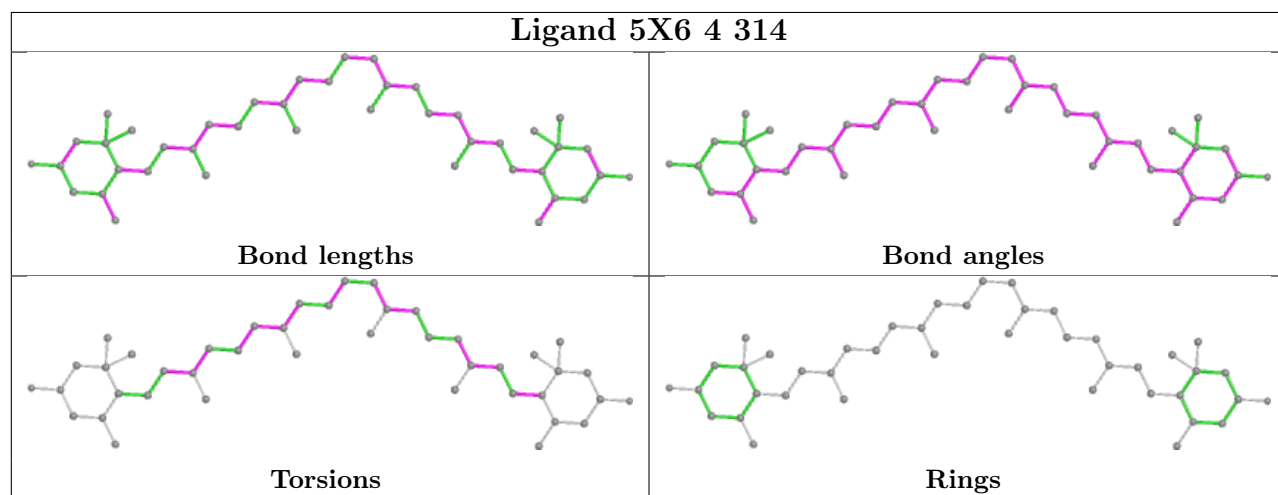
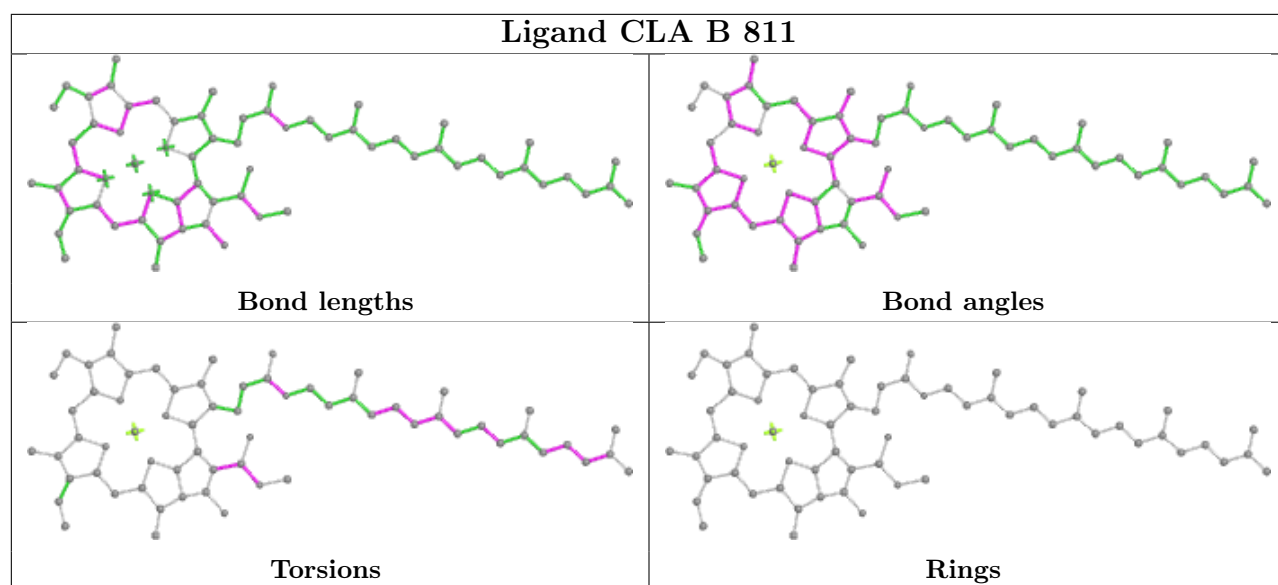


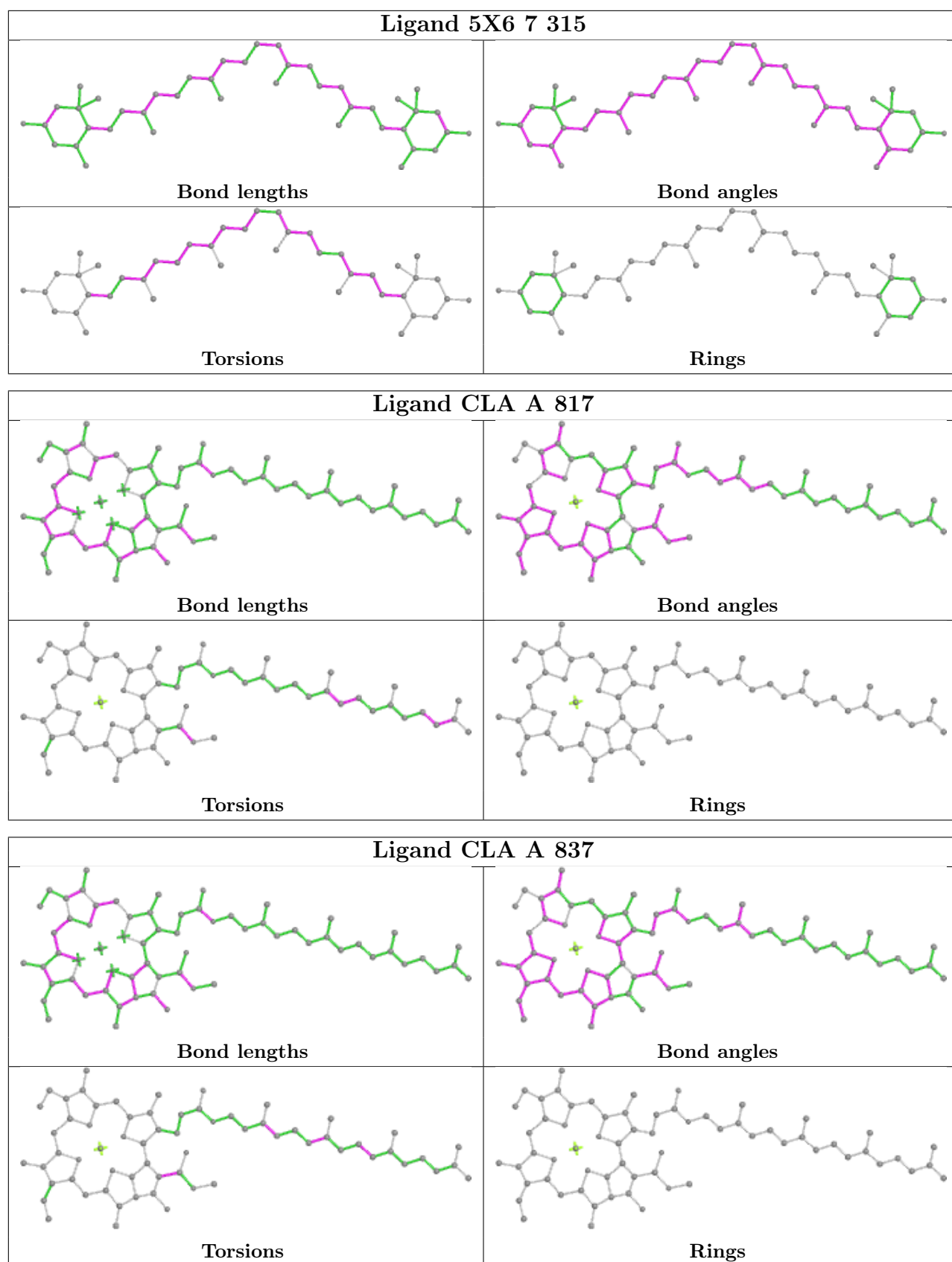
## Ligand CLA 1 309

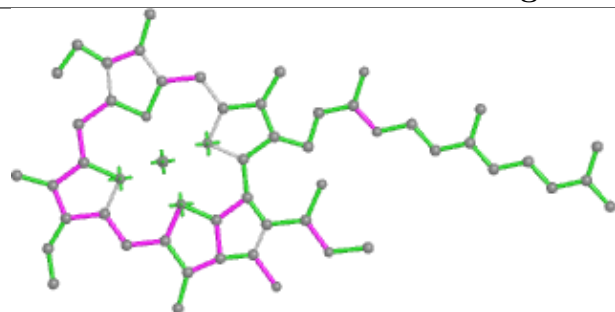


## Ligand BCR A 843

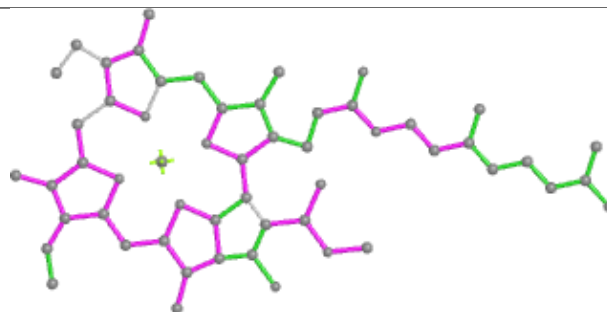




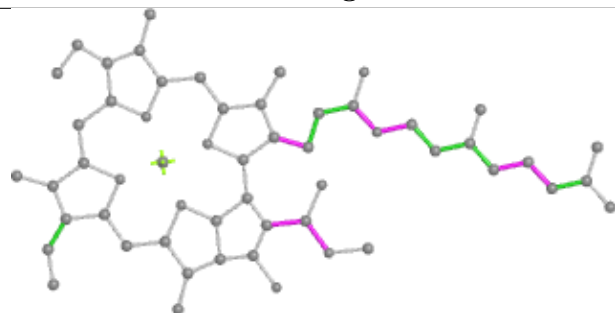


**Ligand CLA 3 305**

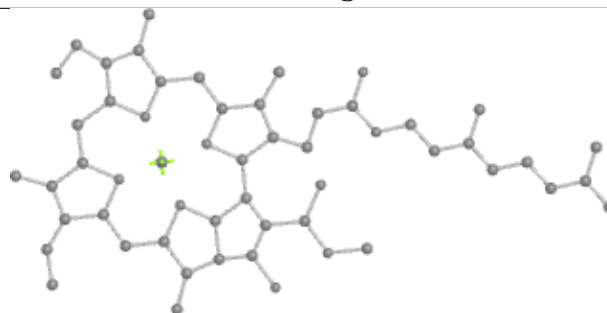
Bond lengths



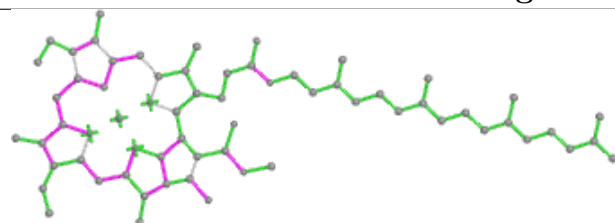
Bond angles



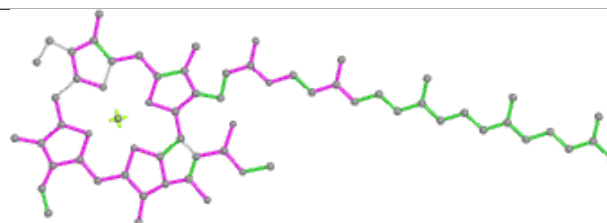
Torsions



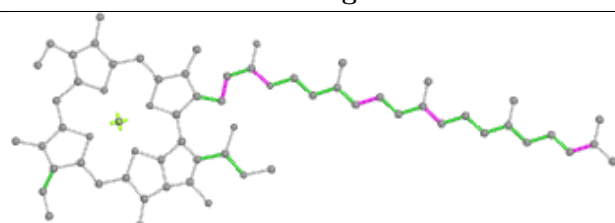
Rings

**Ligand CLA A 838**

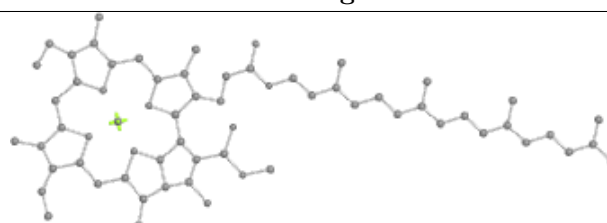
Bond lengths



Bond angles



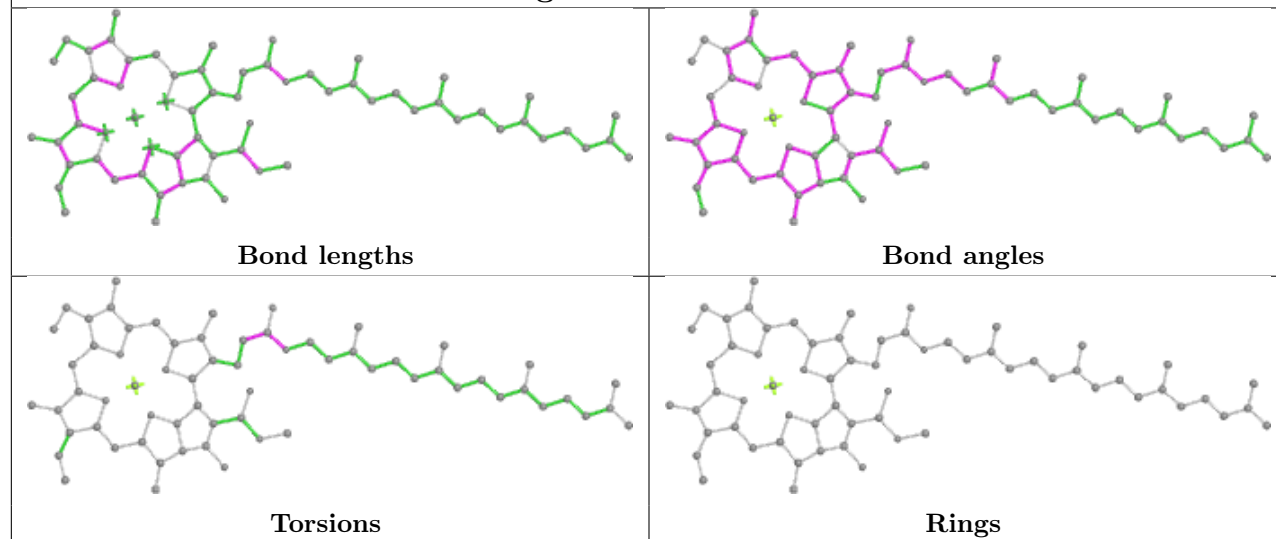
Torsions



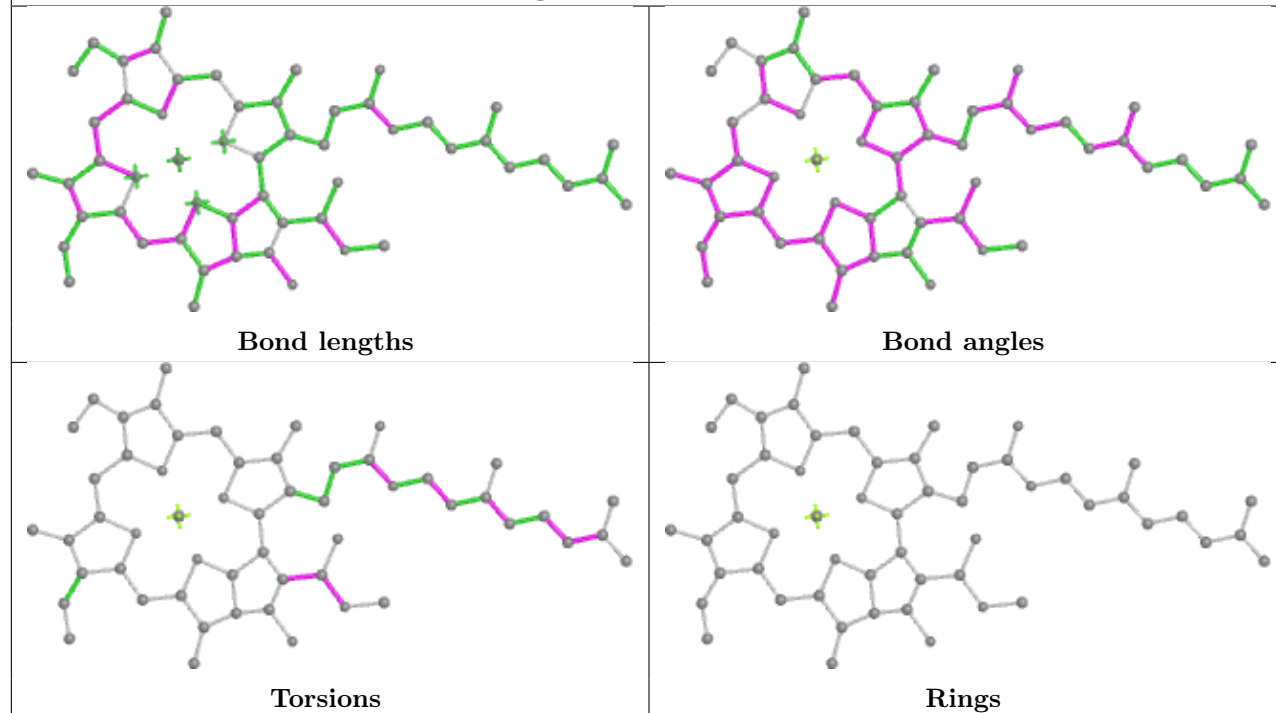
Rings



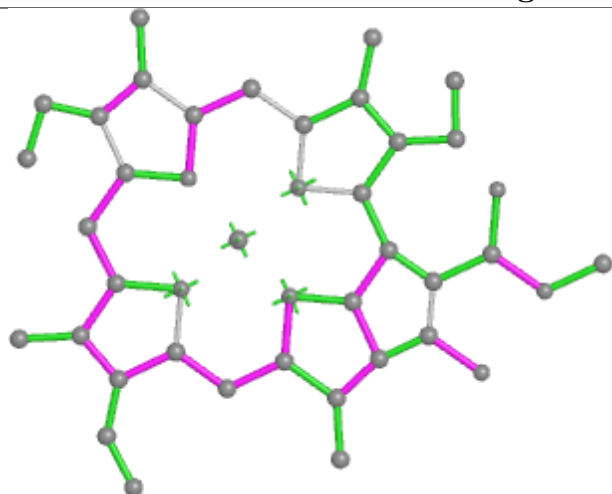
## Ligand CL0 A 801



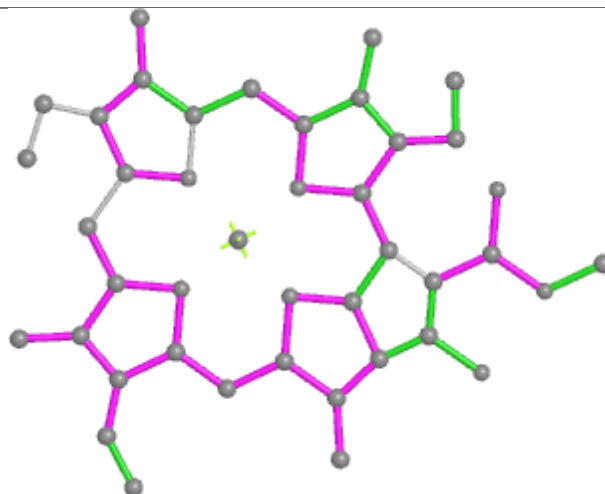
## Ligand CLA A 808



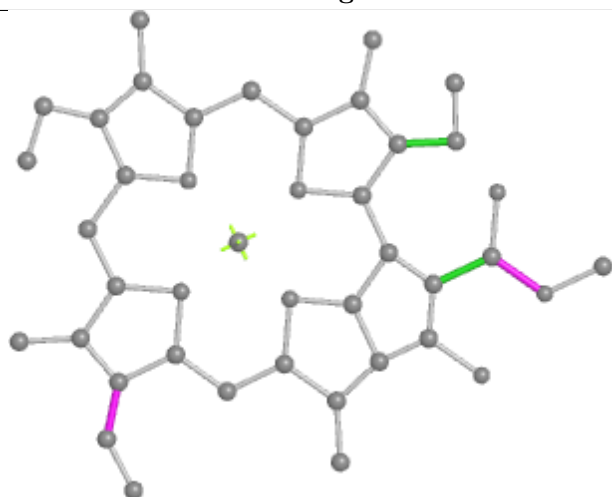
## Ligand CLA 4 310



Bond lengths



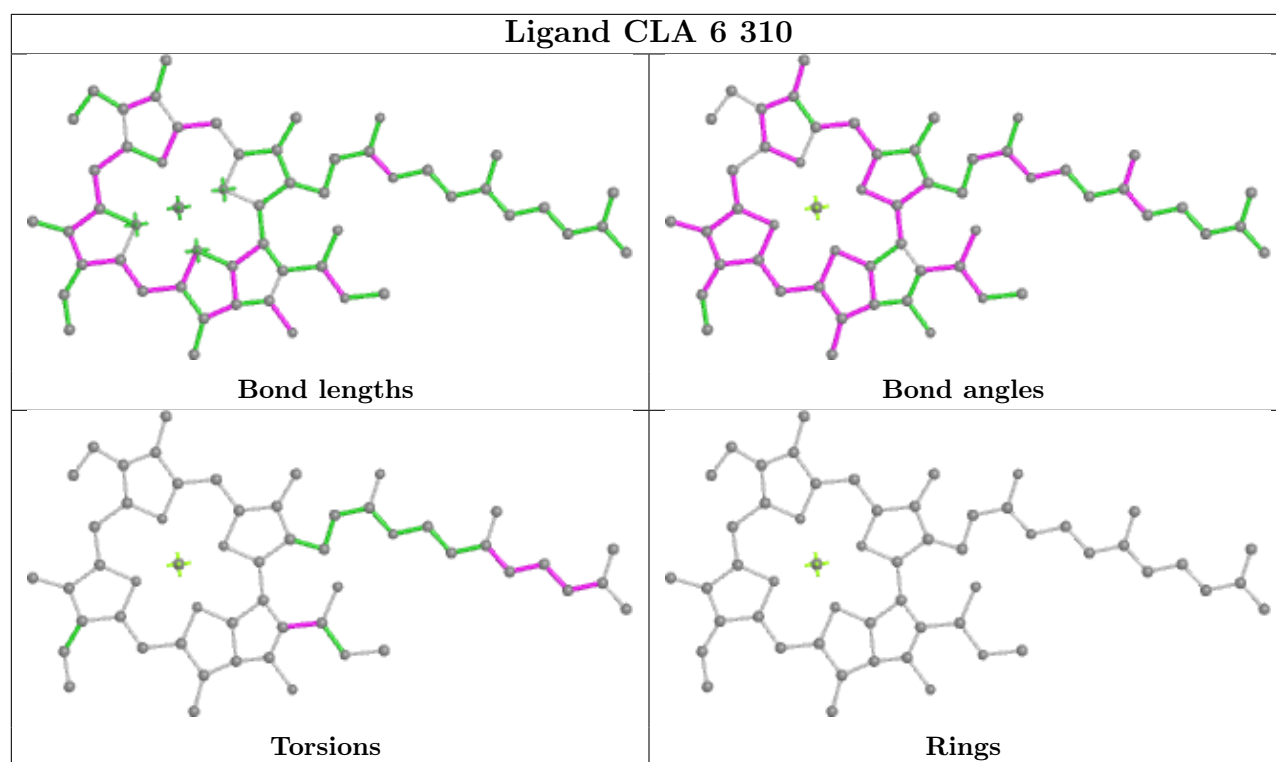
Bond angles

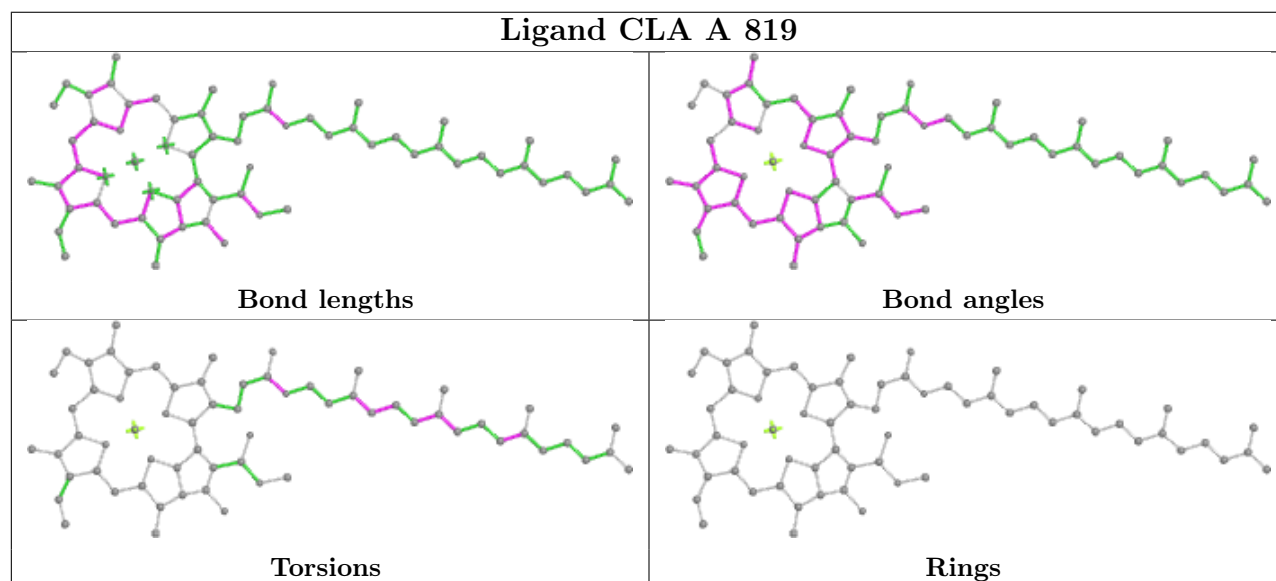
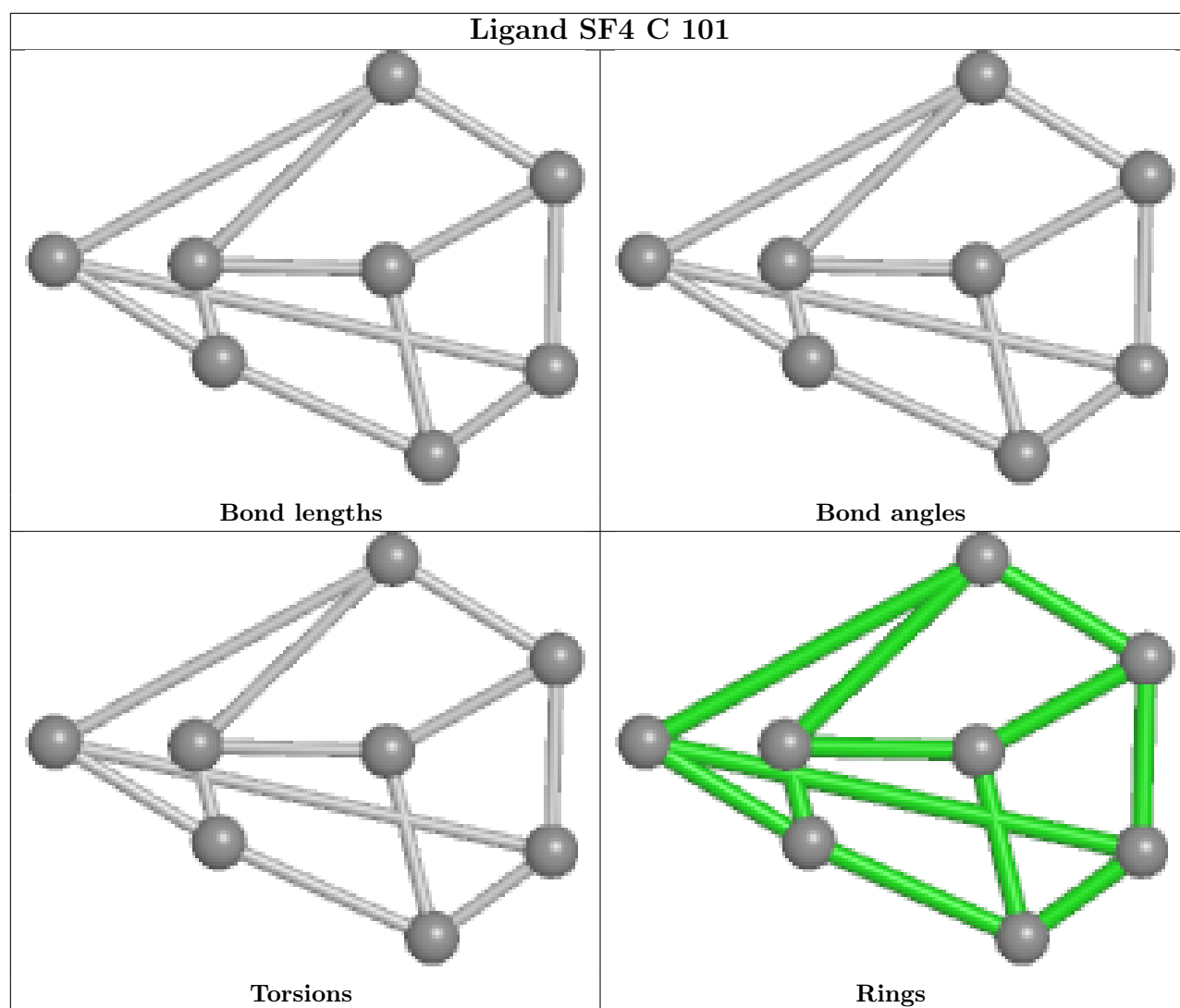


Torsions

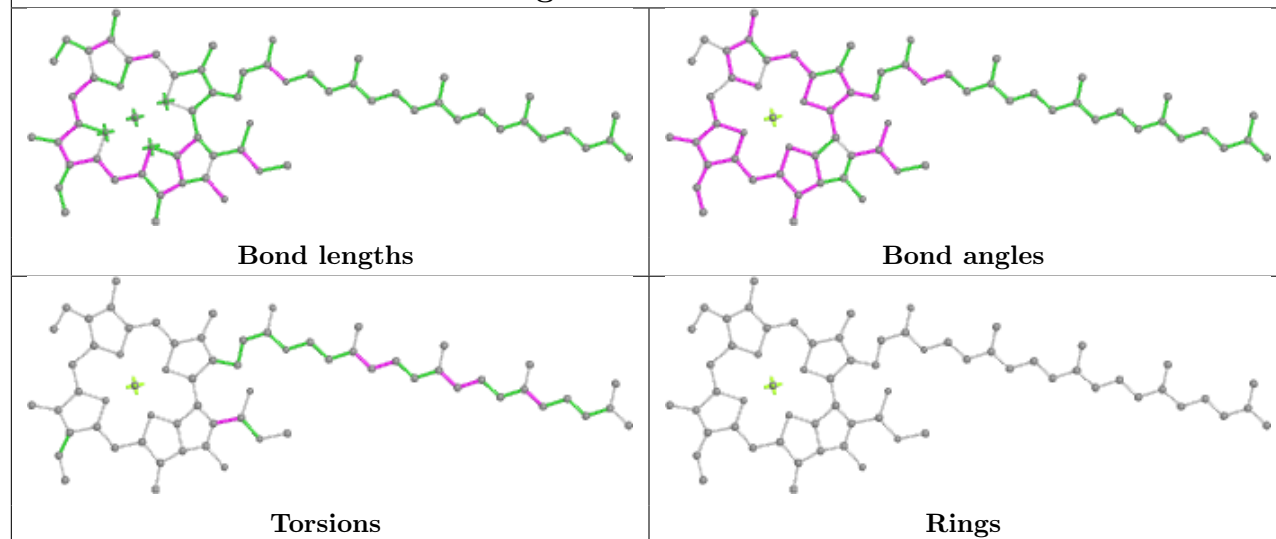


Rings

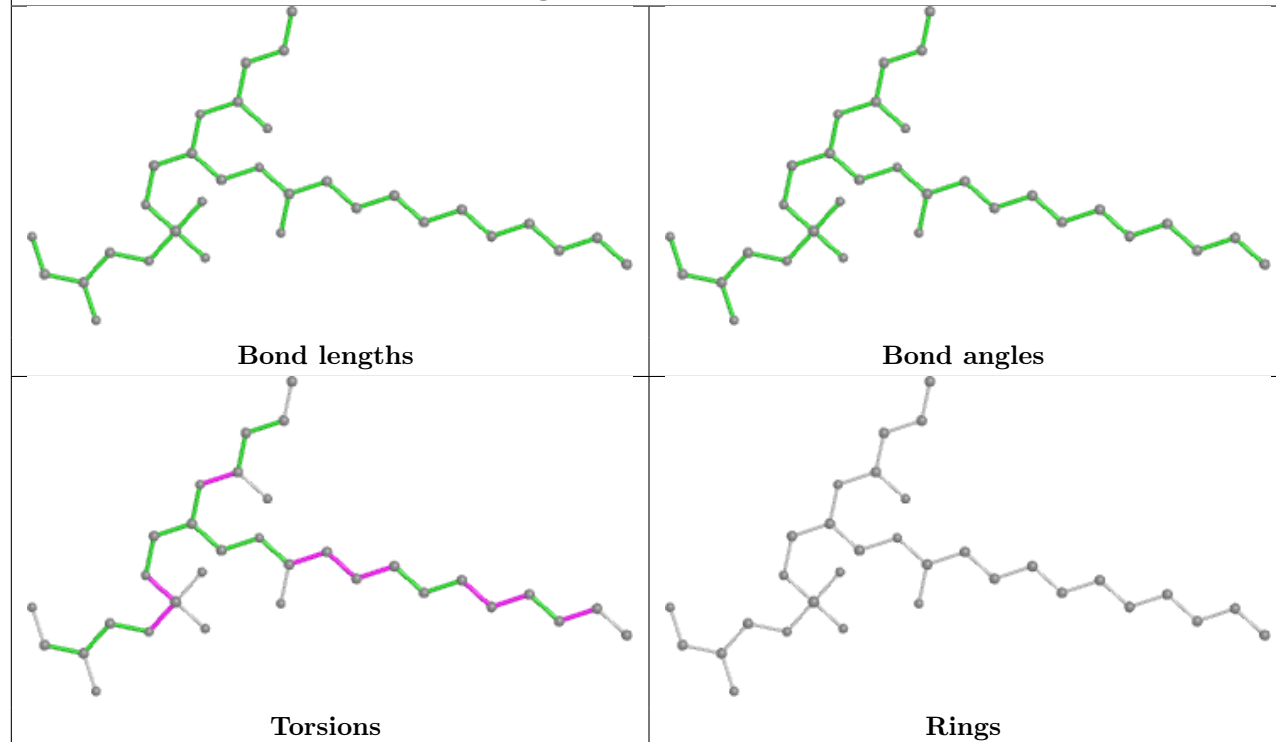


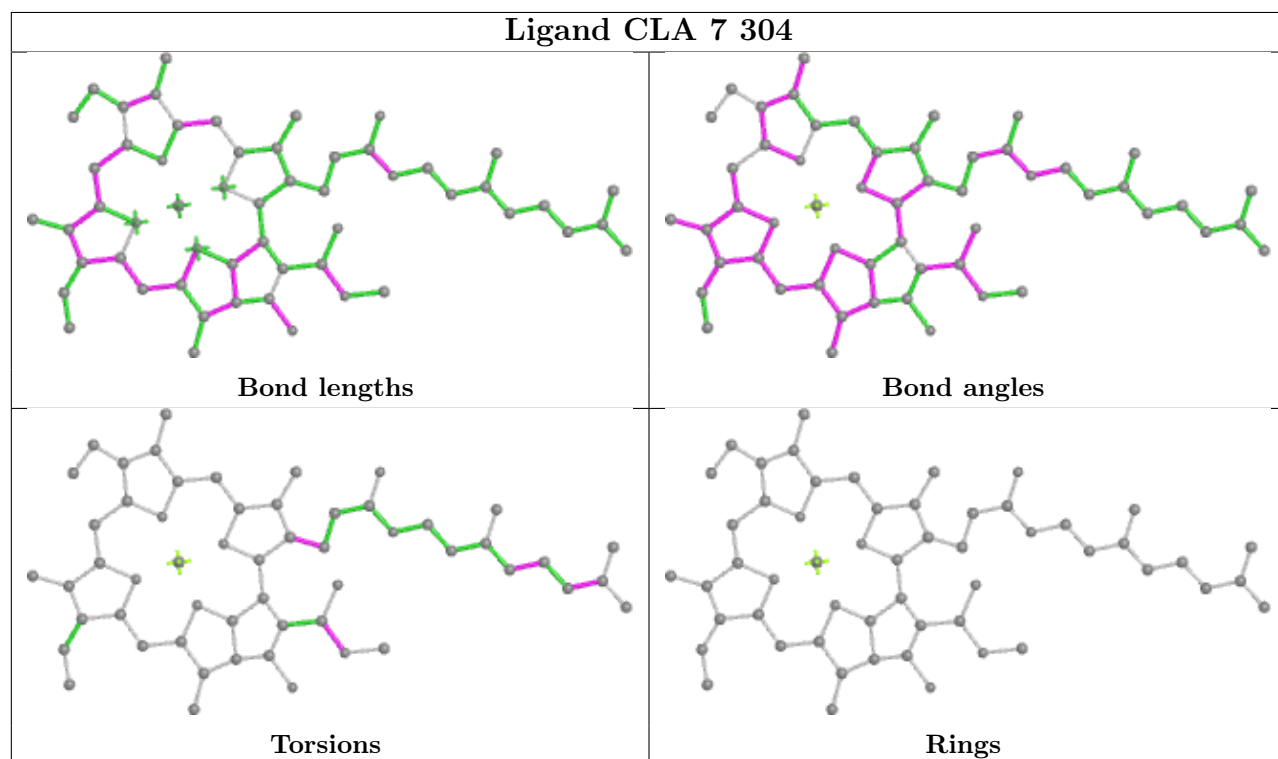
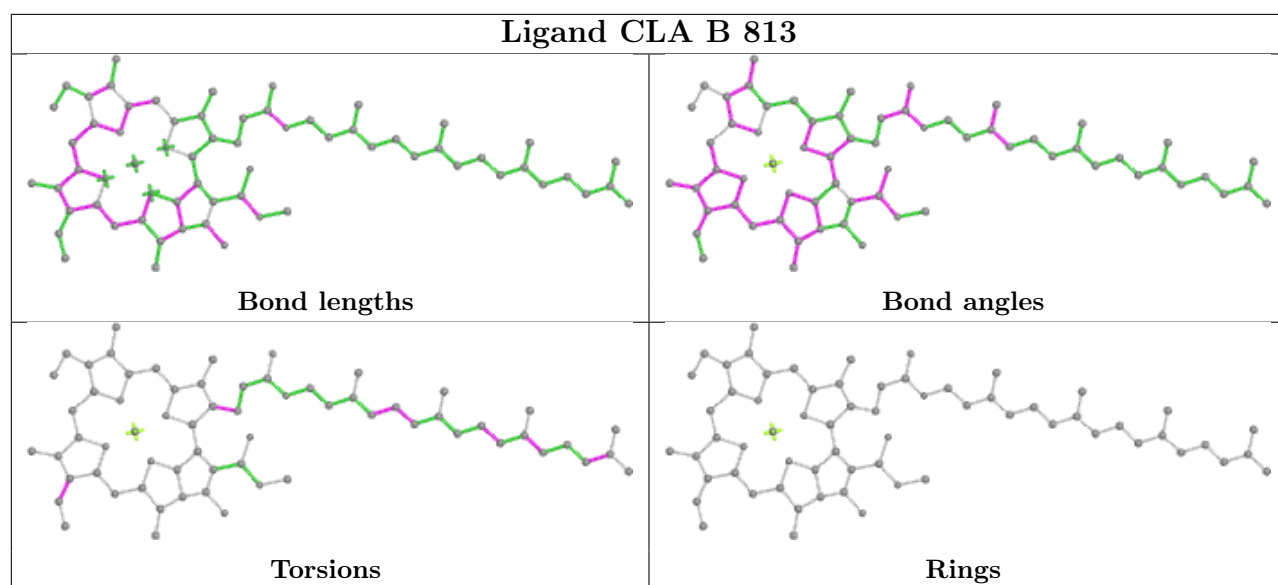


## Ligand CLA 5 306

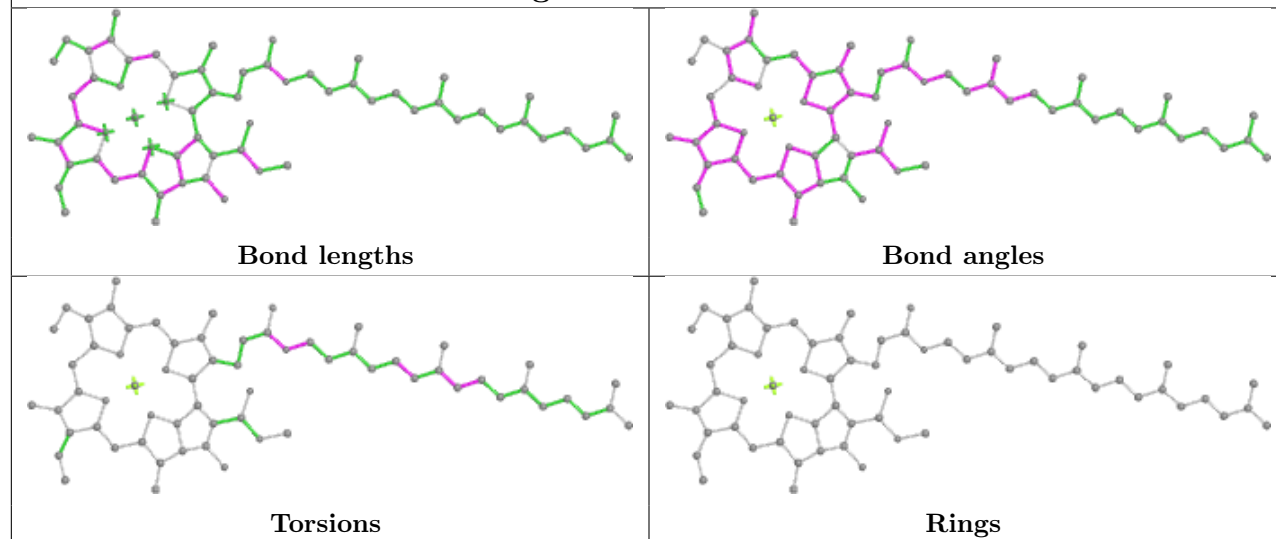


## Ligand LHG 4 318

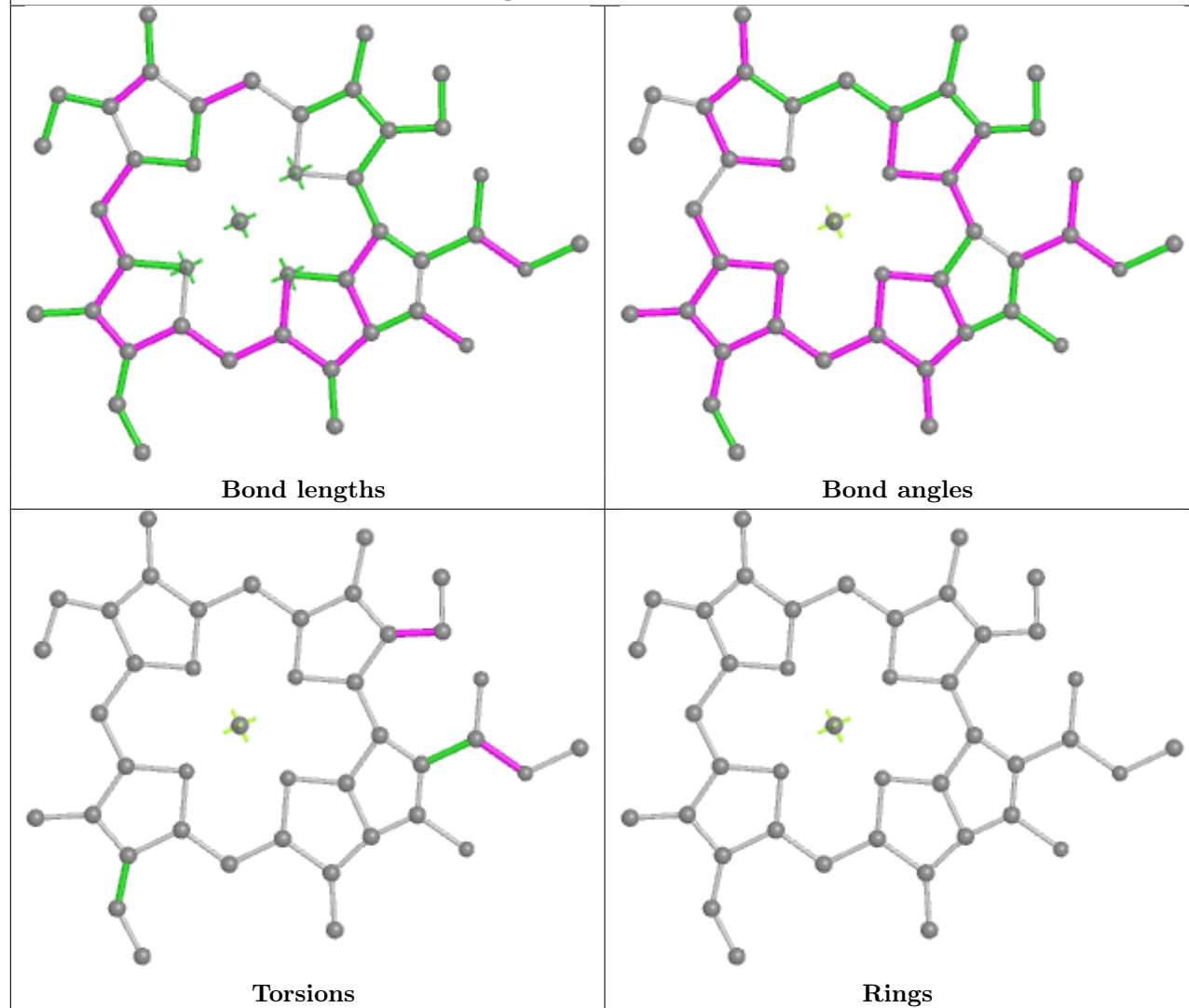




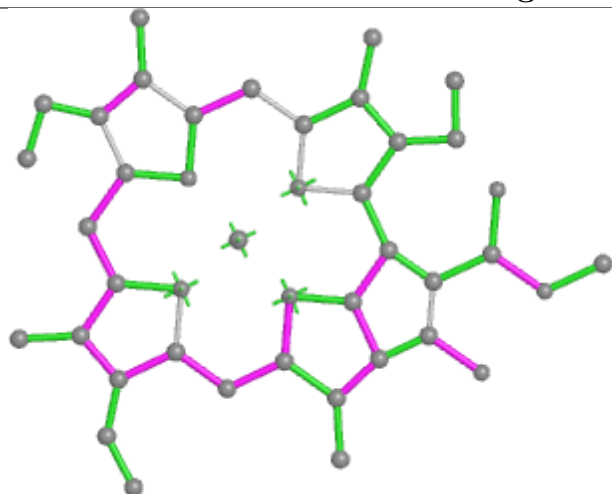
## Ligand CLA B 835



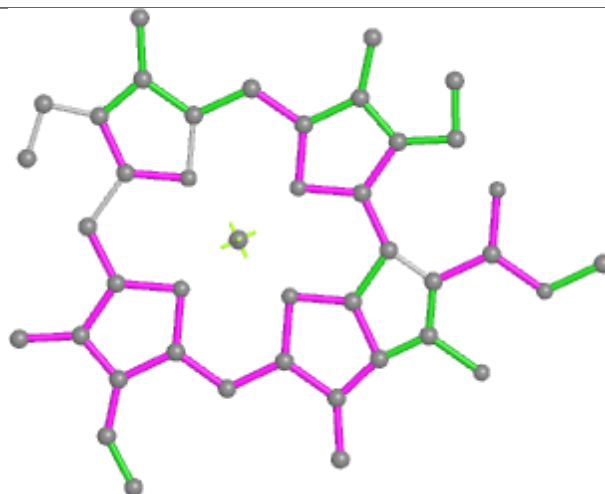
## Ligand CLA 2 310



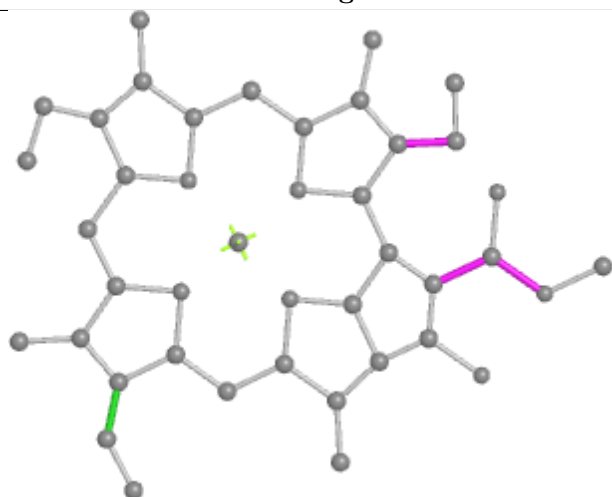
## Ligand CLA 1 308



Bond lengths



Bond angles

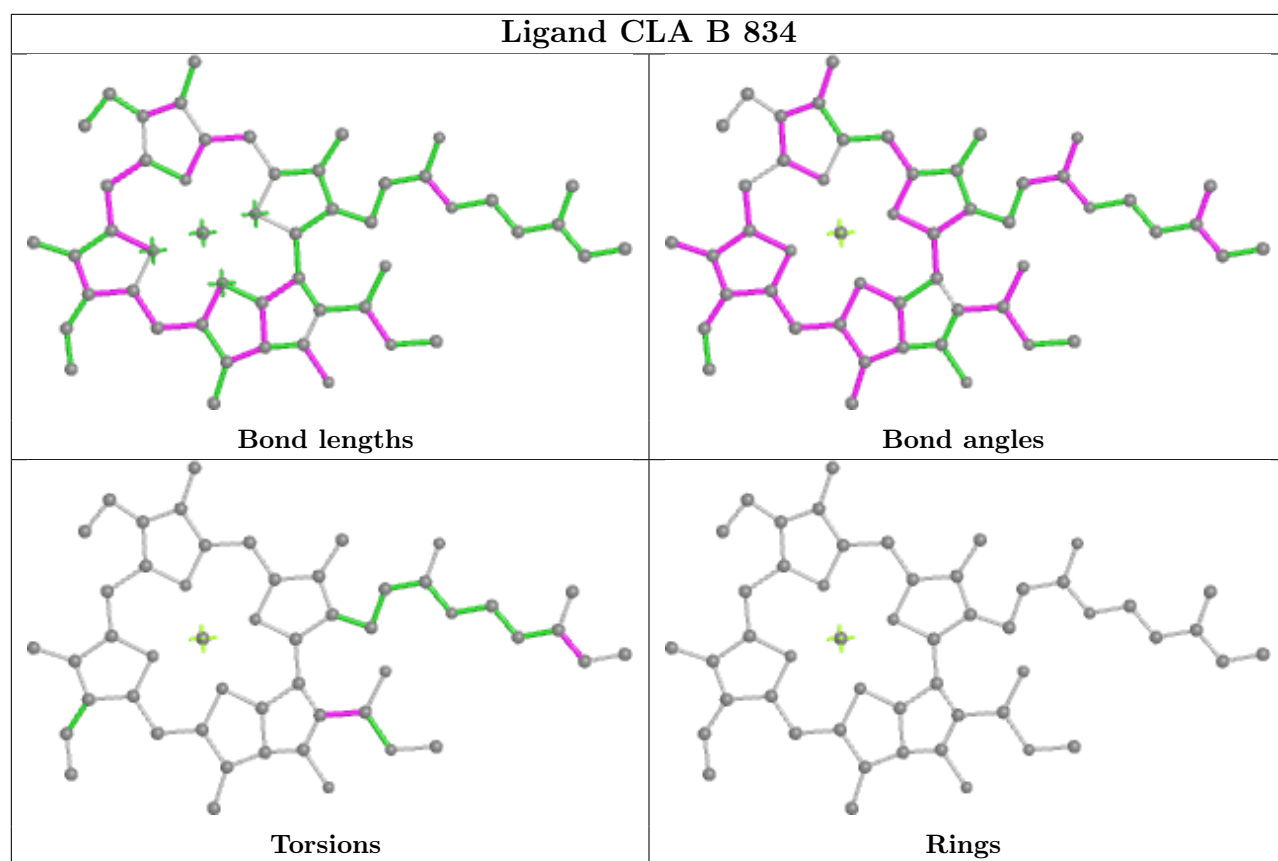


Torsions

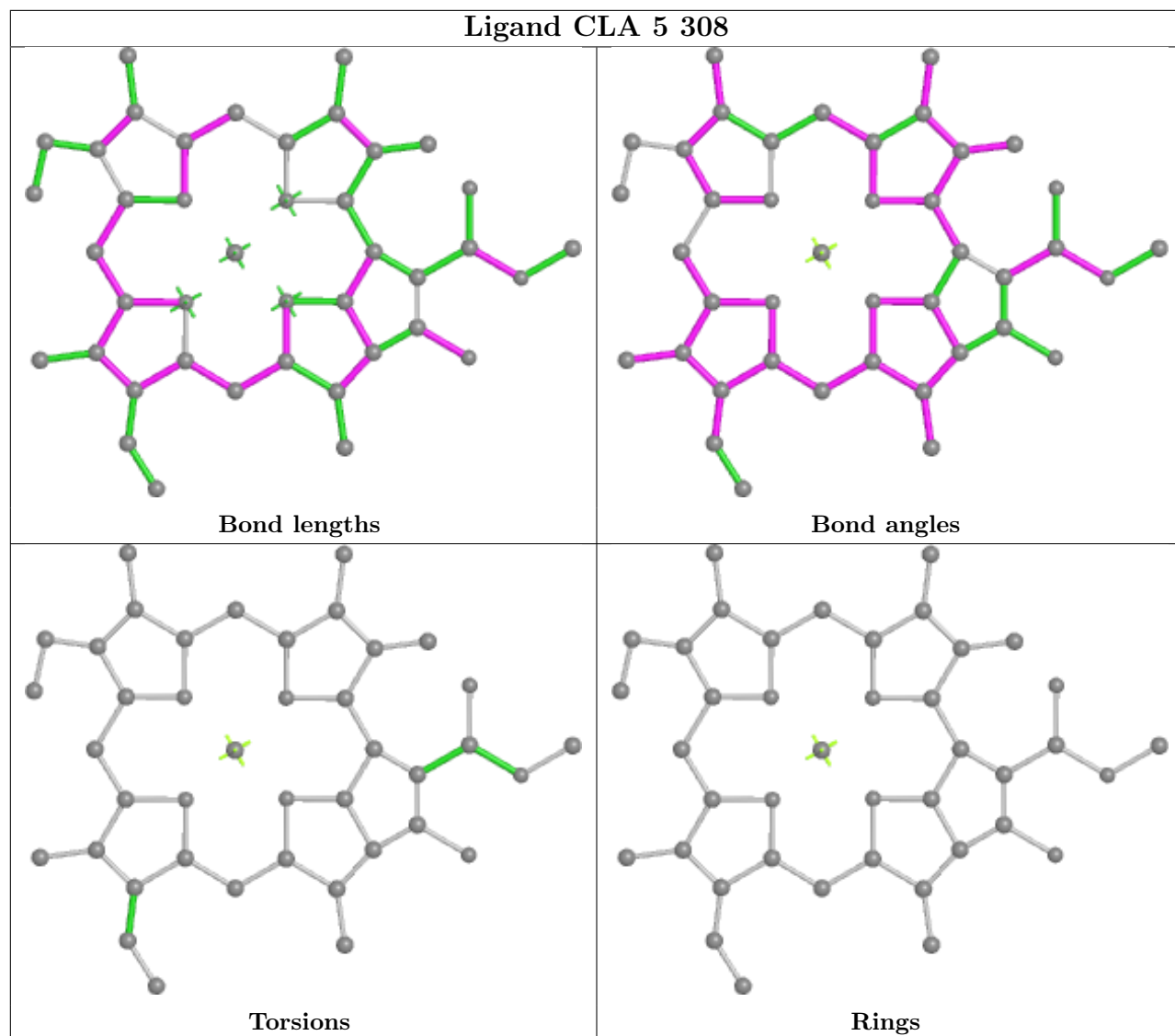


Rings

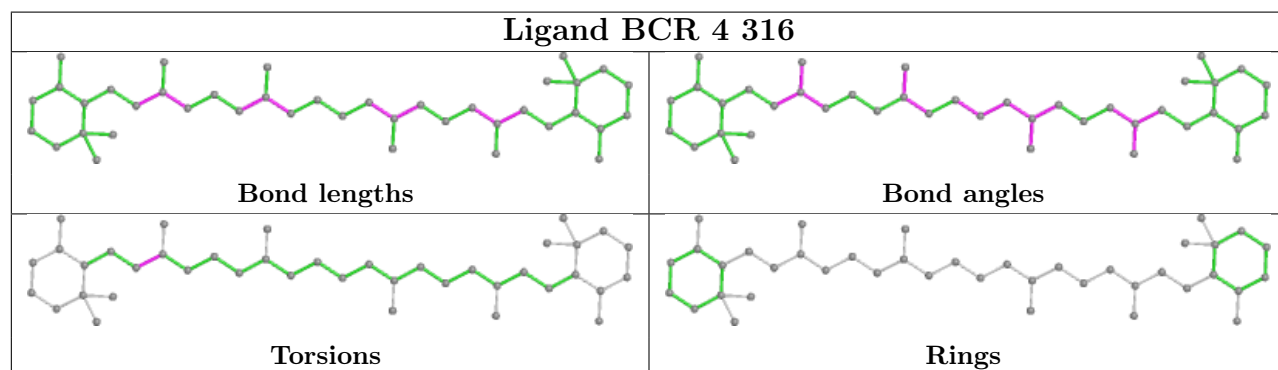




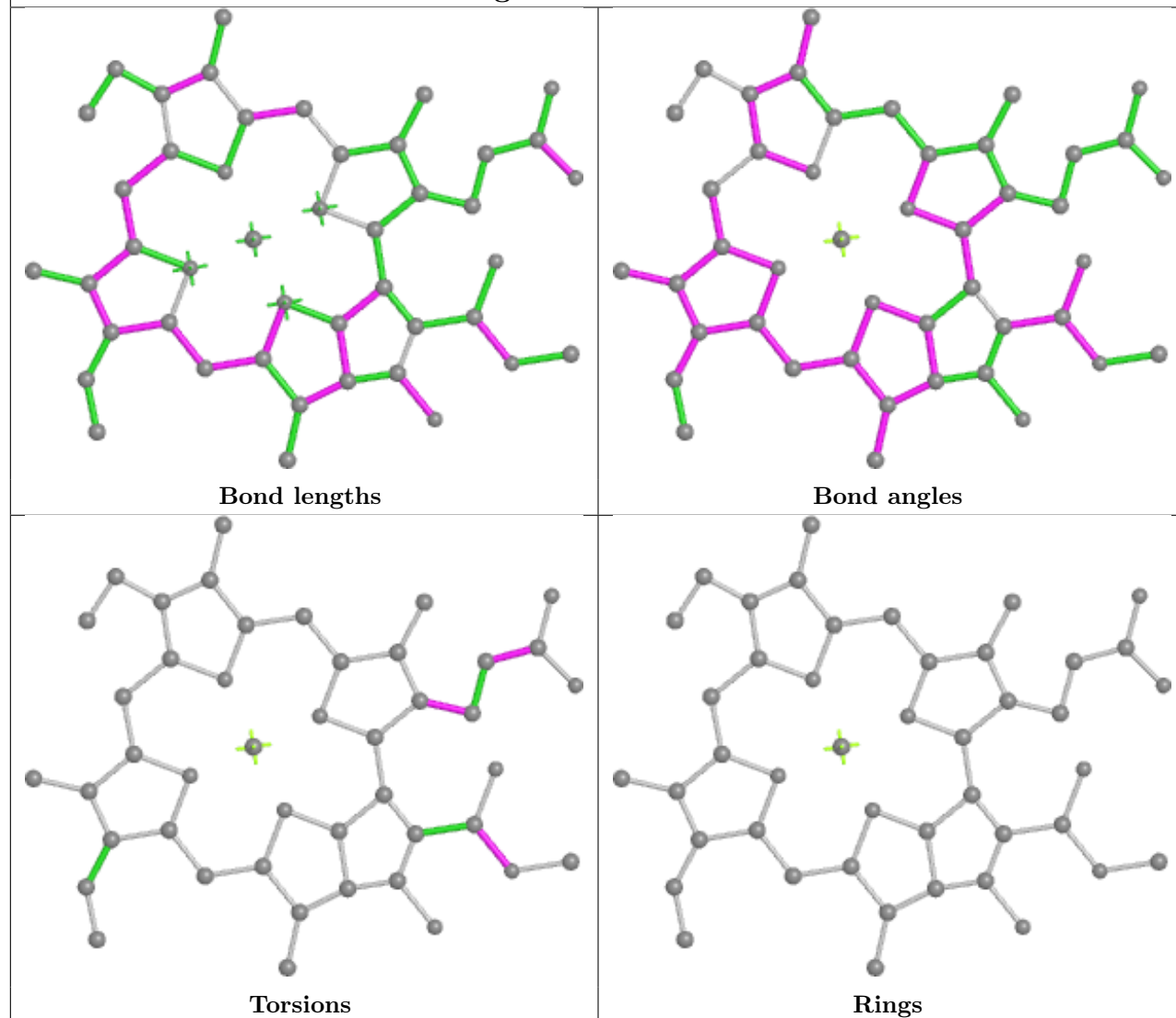
## Ligand CLA 5 308



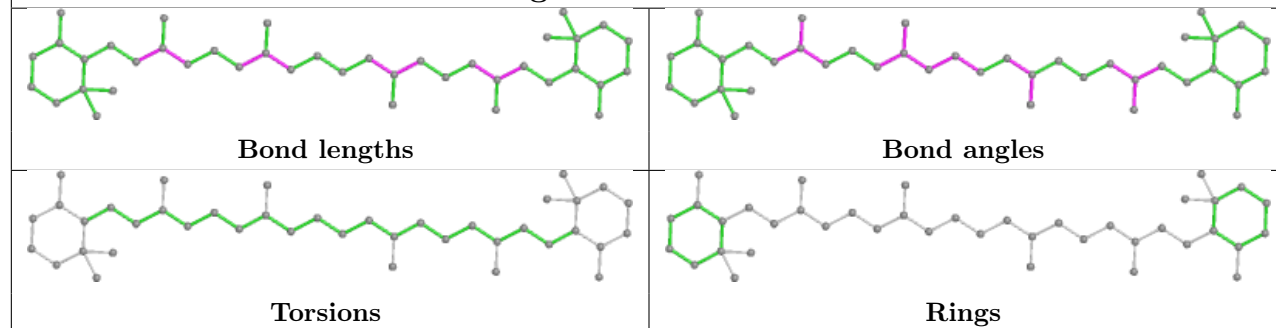
## Ligand BCR 4 316

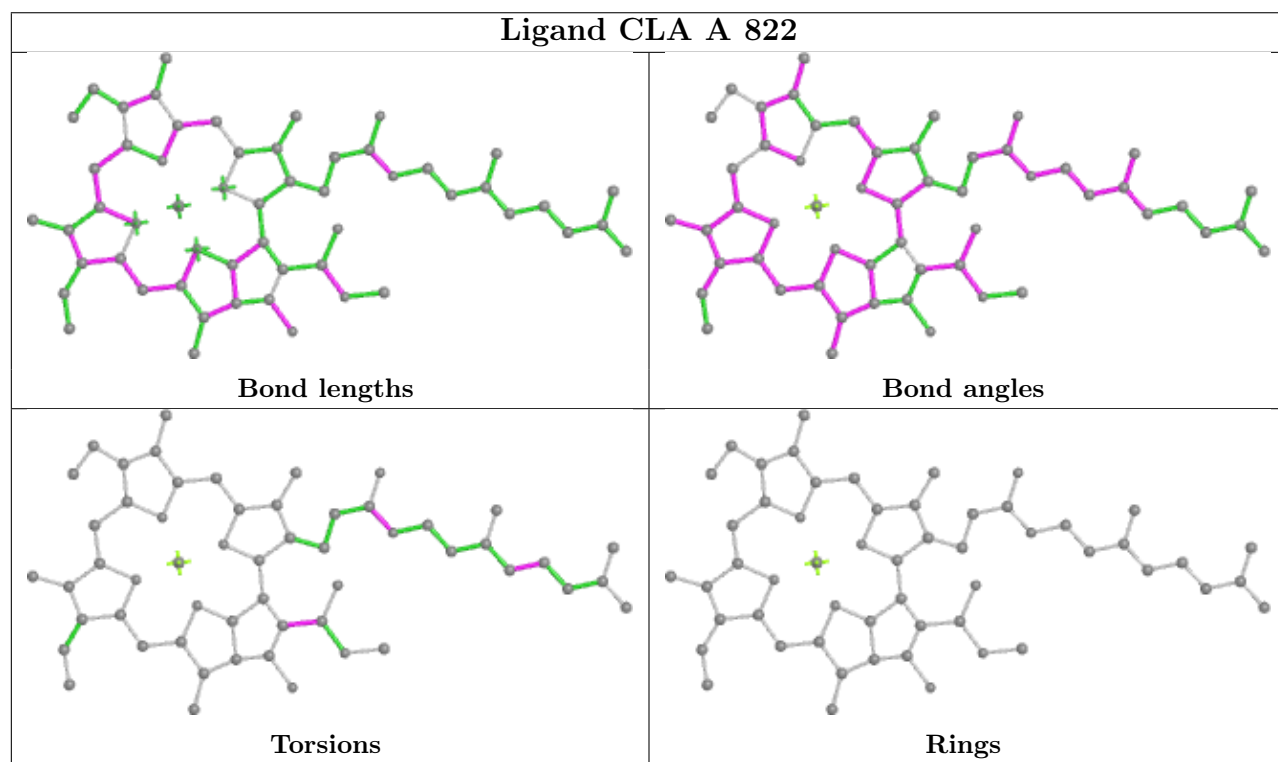
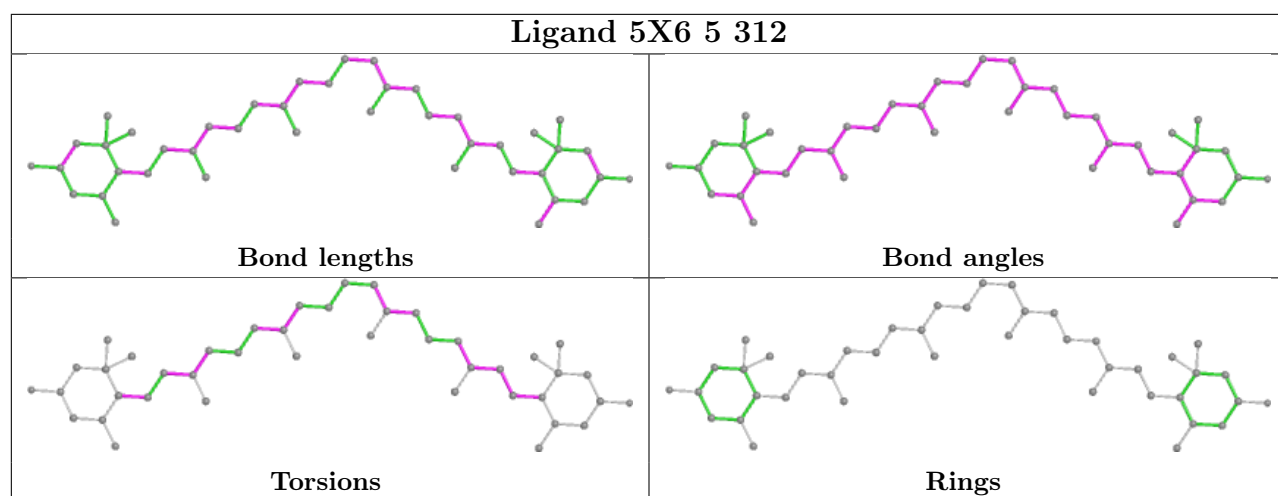


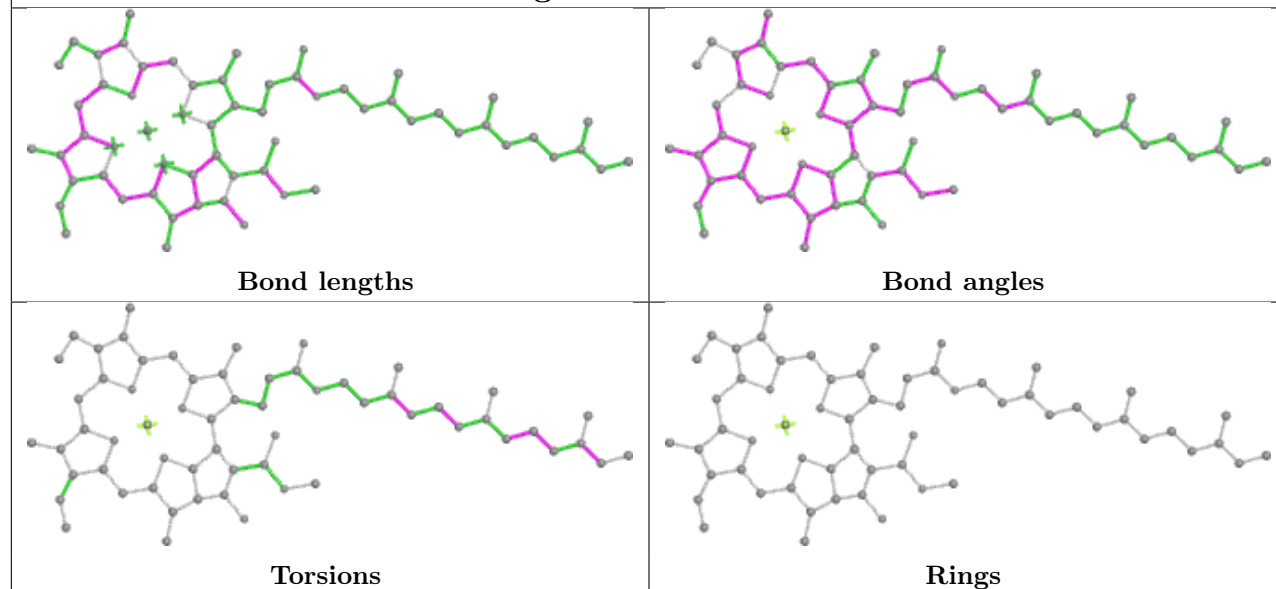
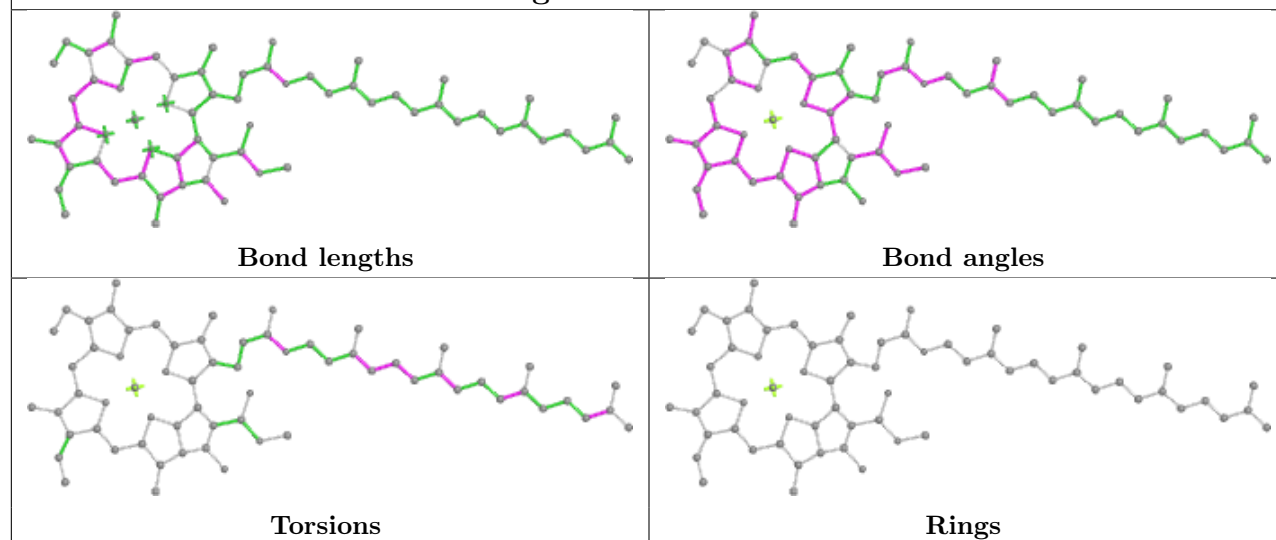
## Ligand CLA 7 312



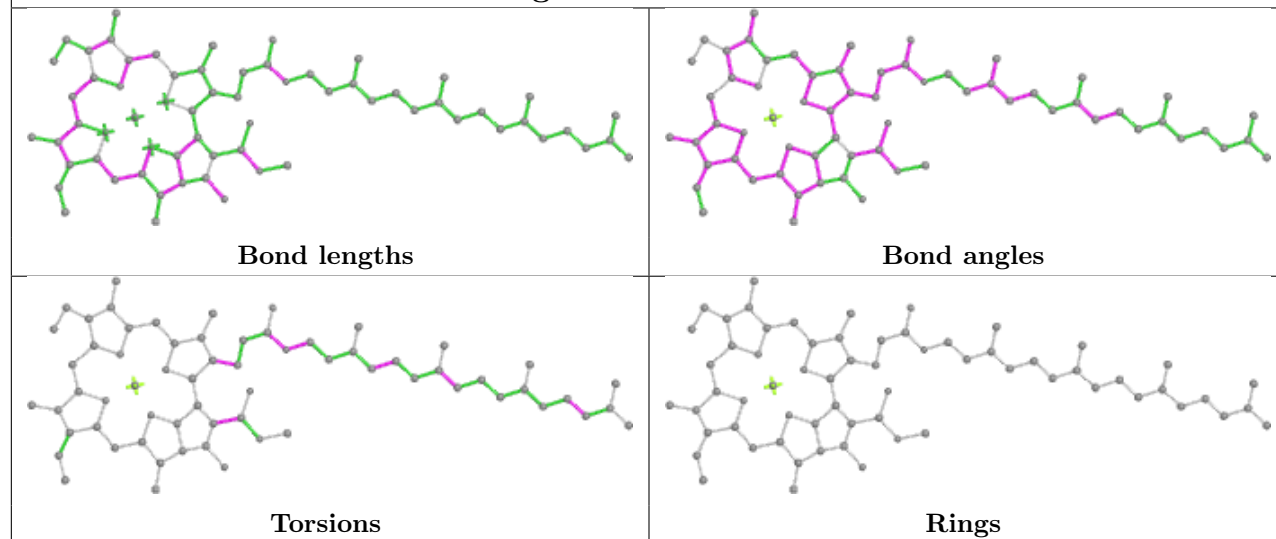
## Ligand BCR A 861



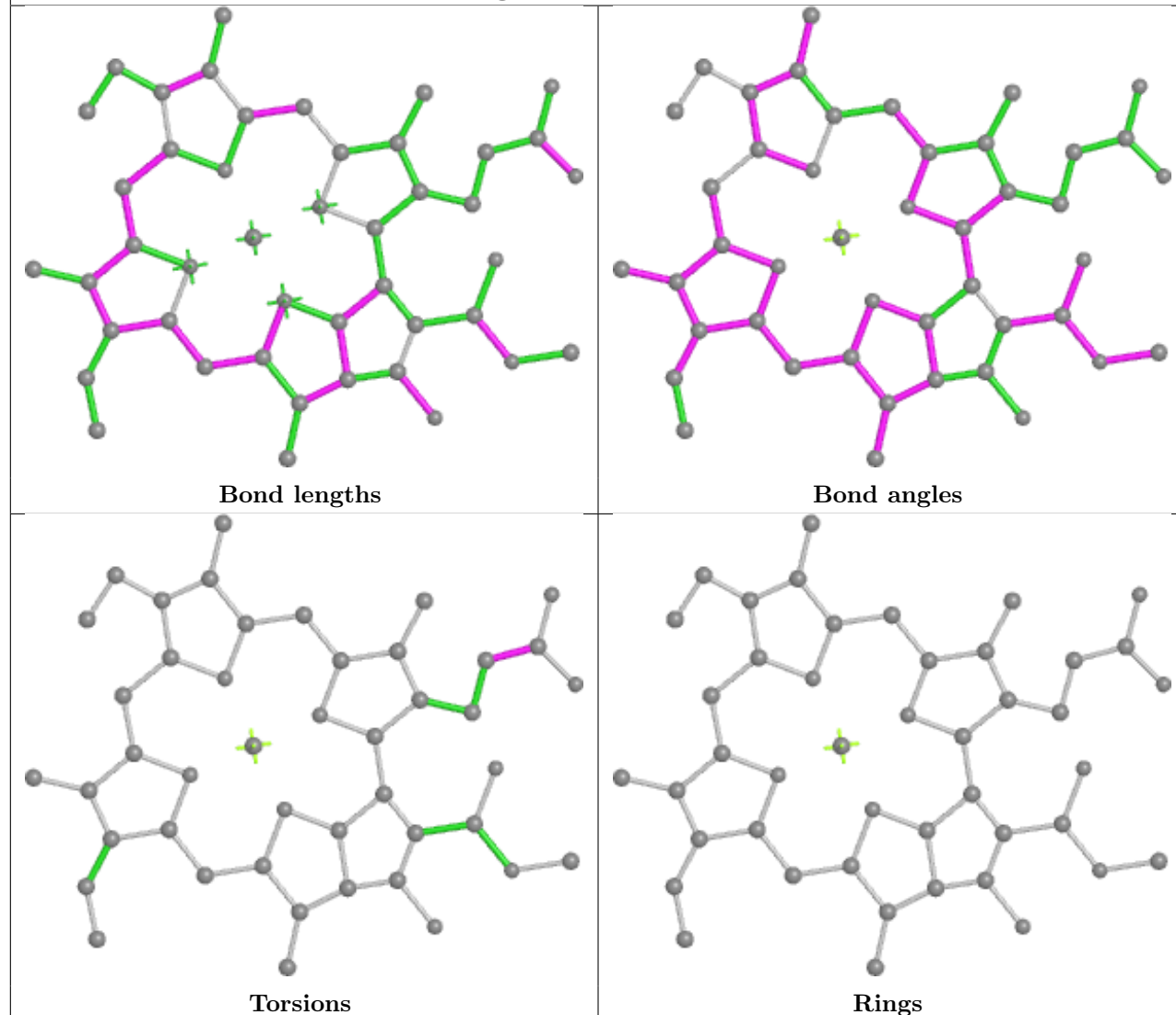


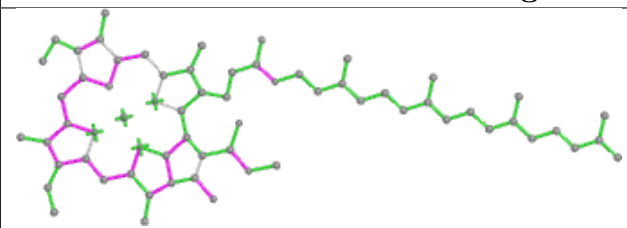
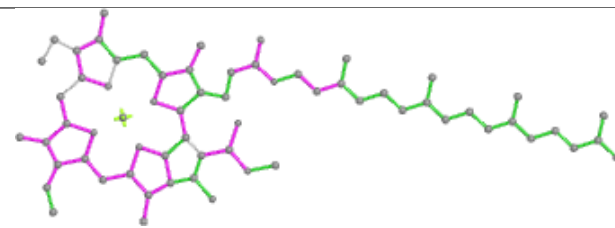
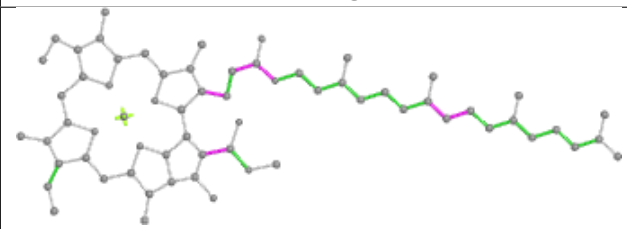
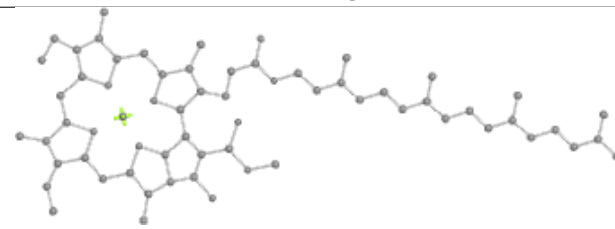
**Ligand CLA F 204****Ligand CLA B 830**

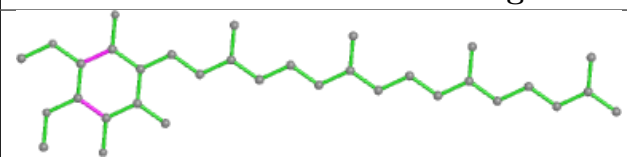
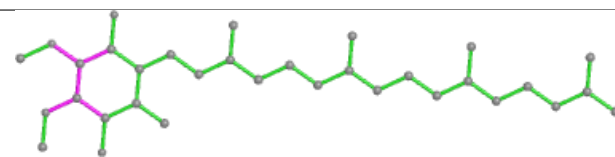
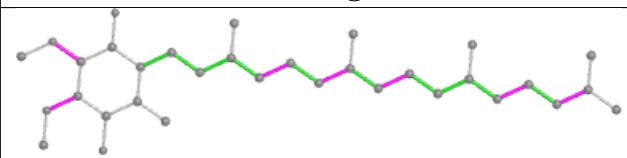
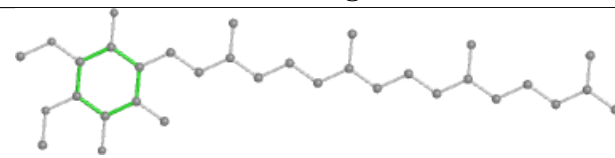
## Ligand CLA B 805

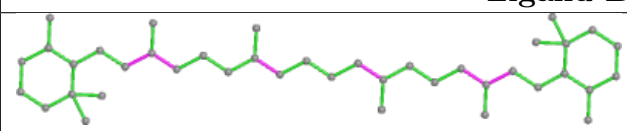
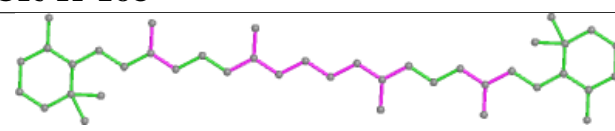
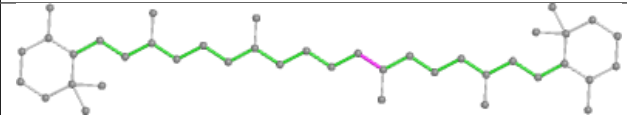
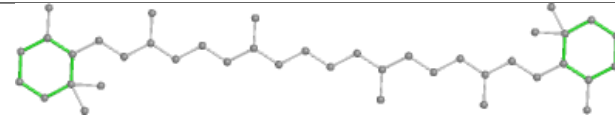


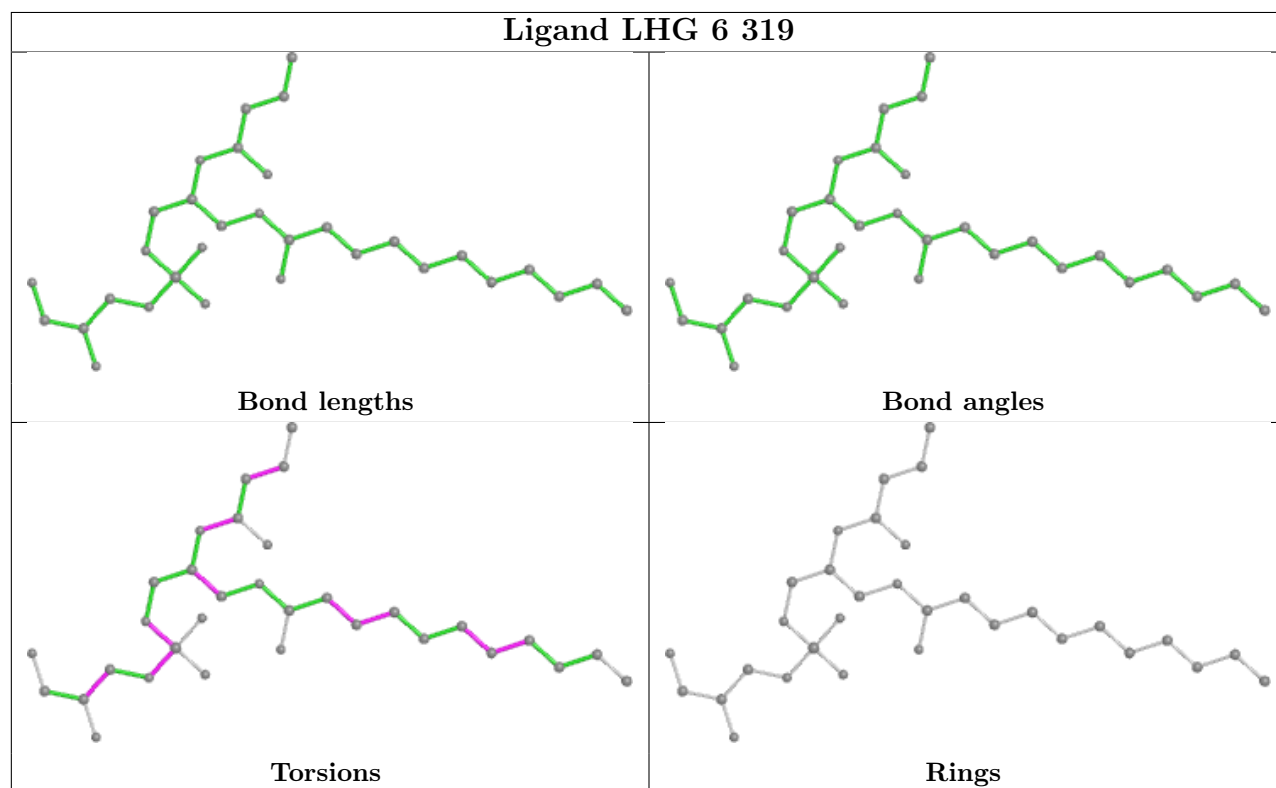
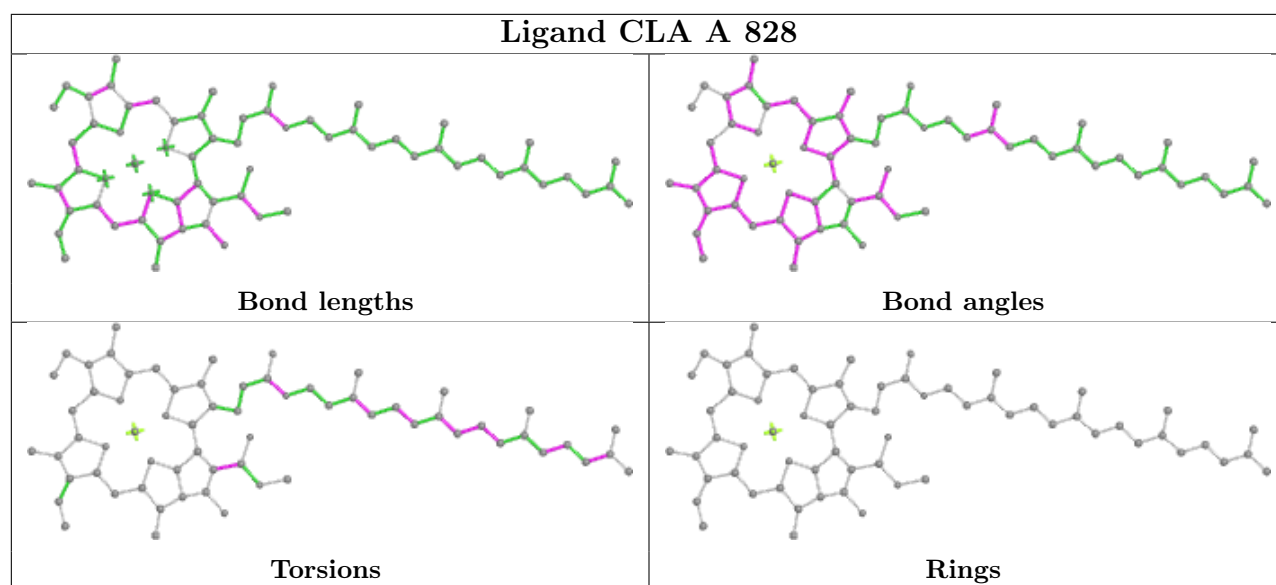
## Ligand CLA 3 304



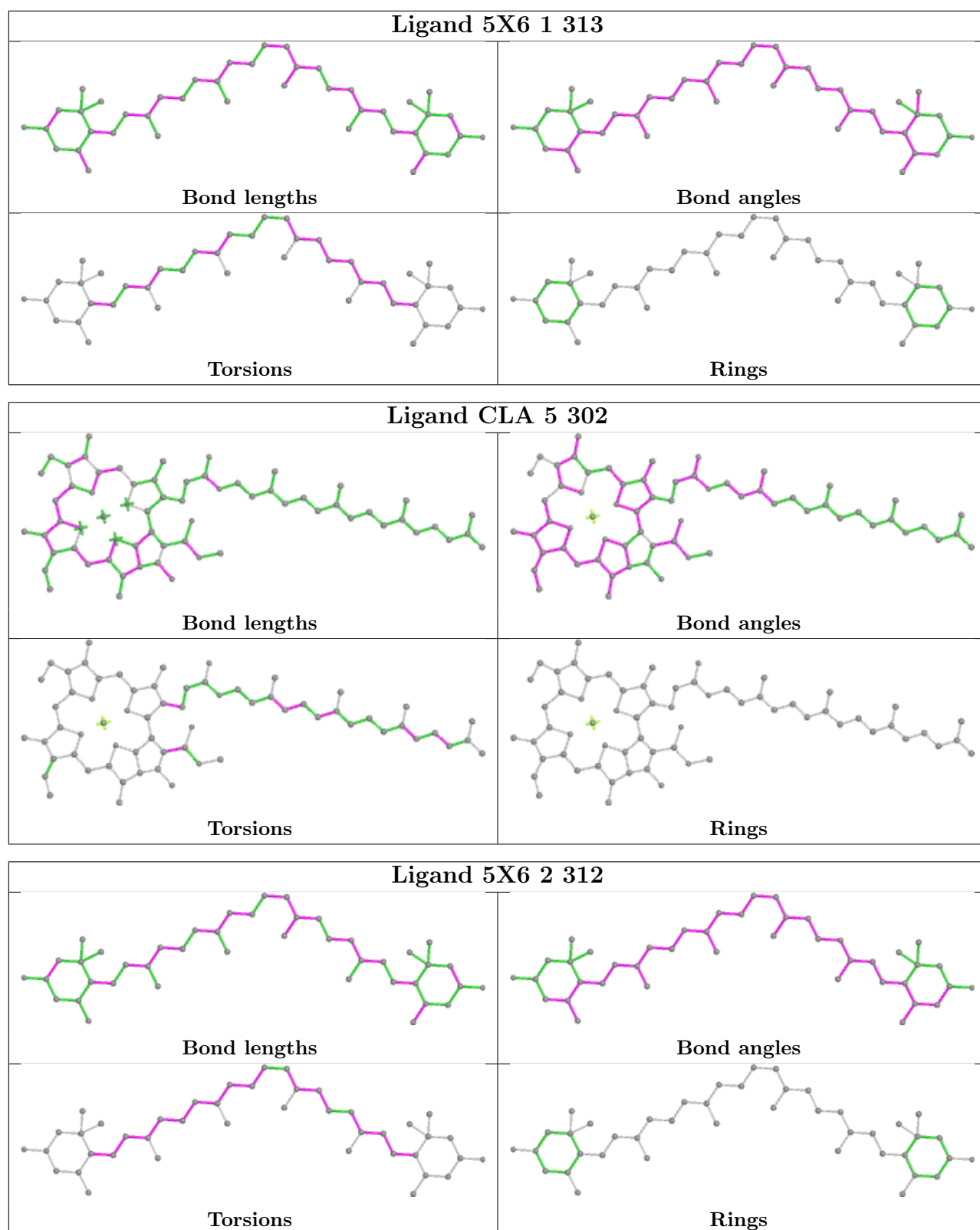
Ligand CLA A 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1L64 A 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

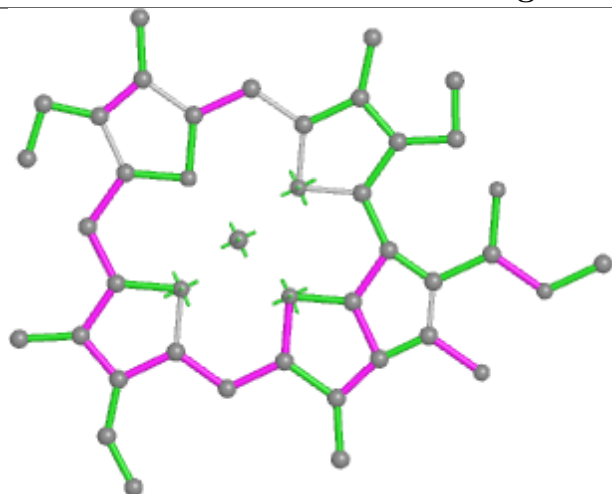
Ligand BCR K 103	
	
Bond lengths	Bond angles
	
Torsions	Rings



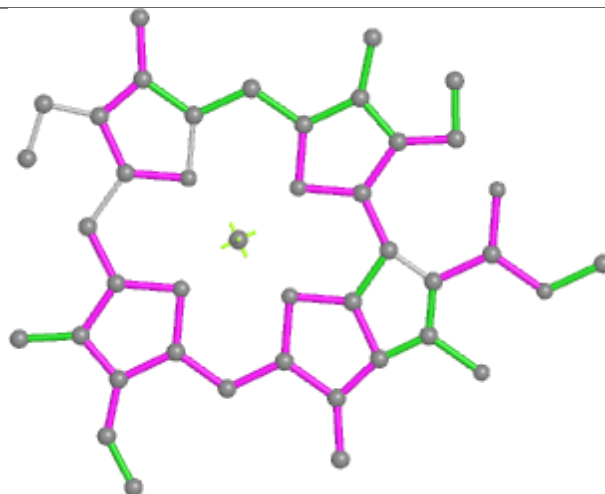




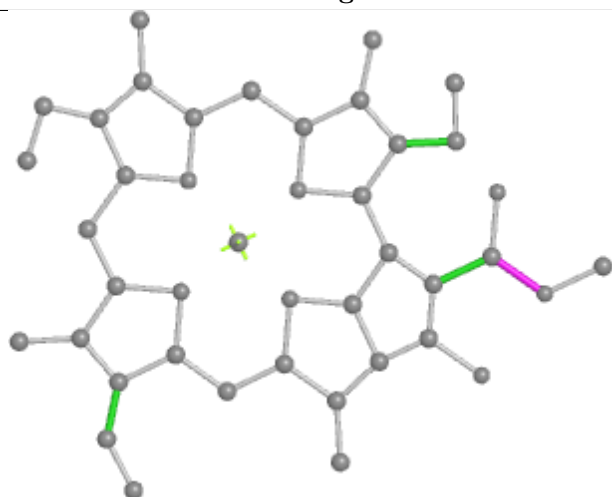
## Ligand CLA 5 309



Bond lengths



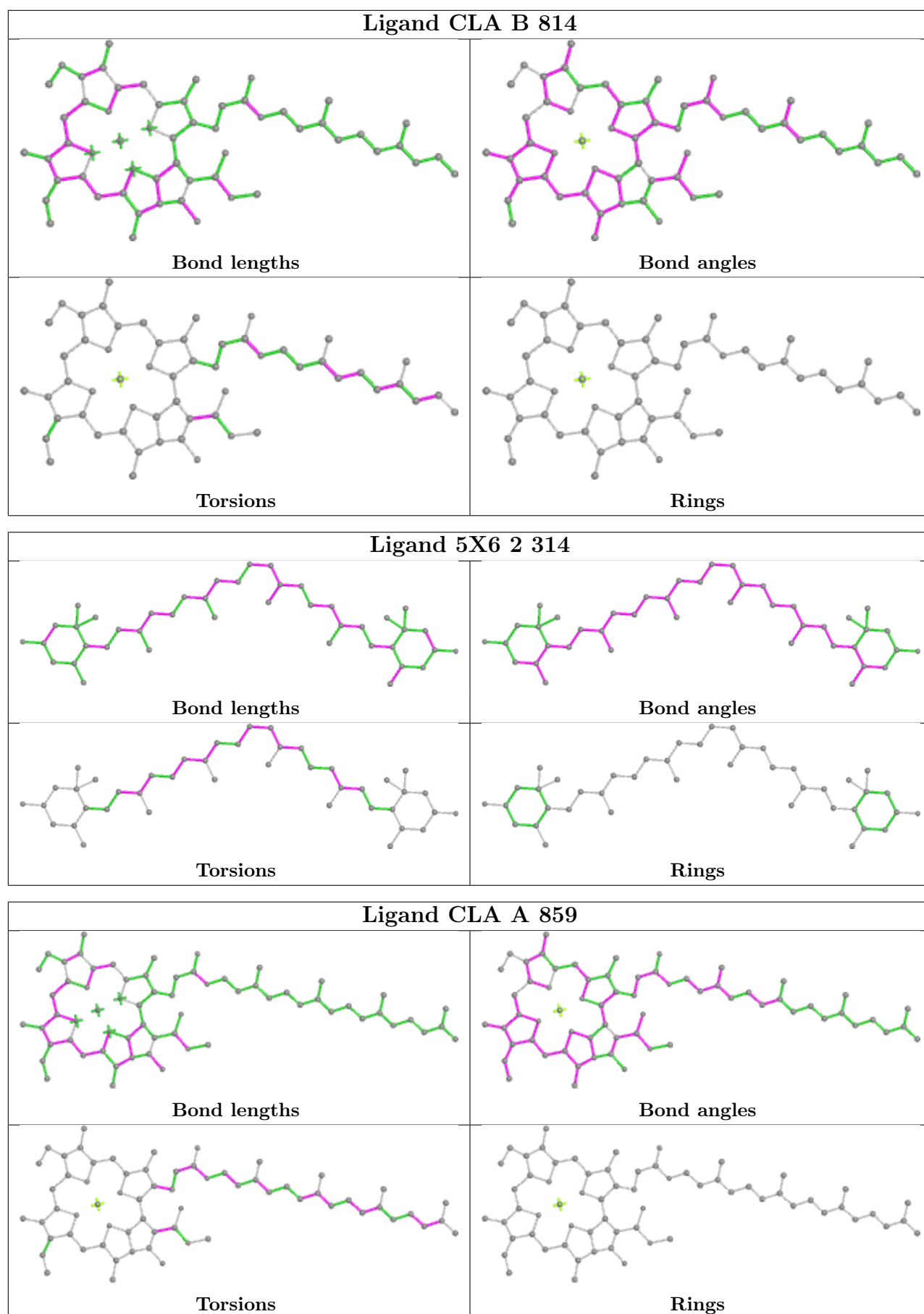
Bond angles

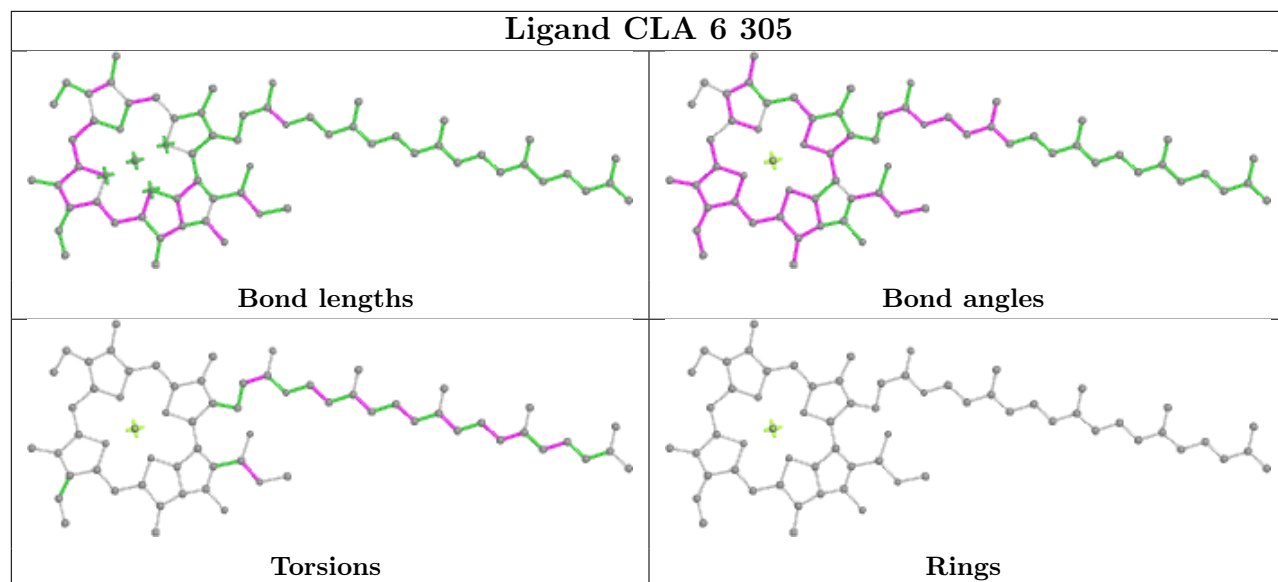
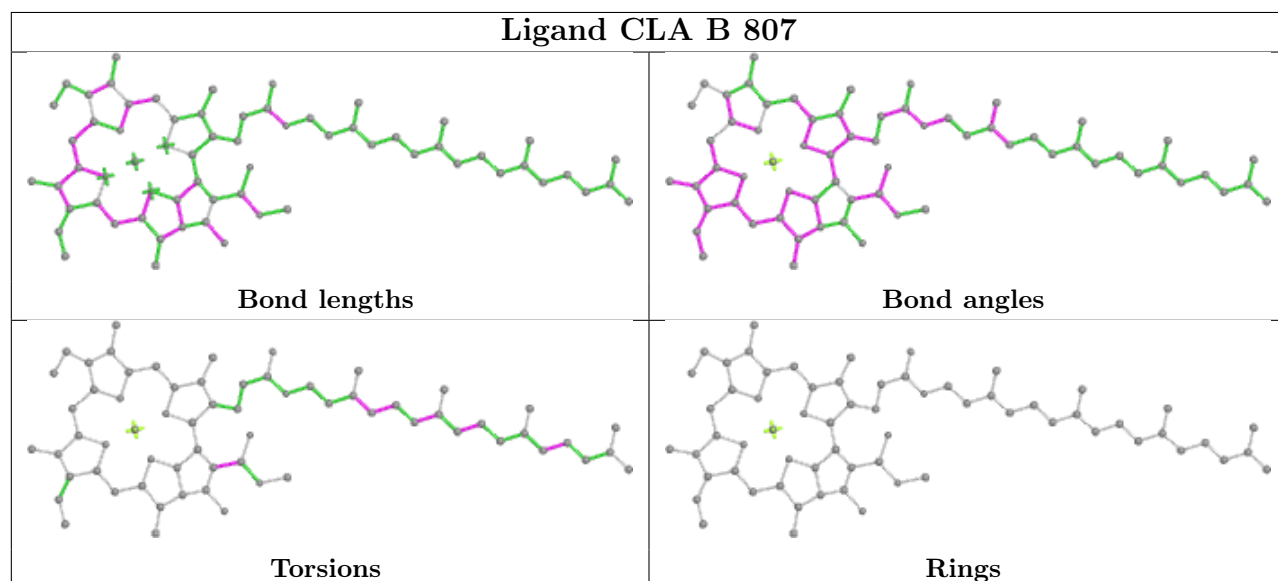
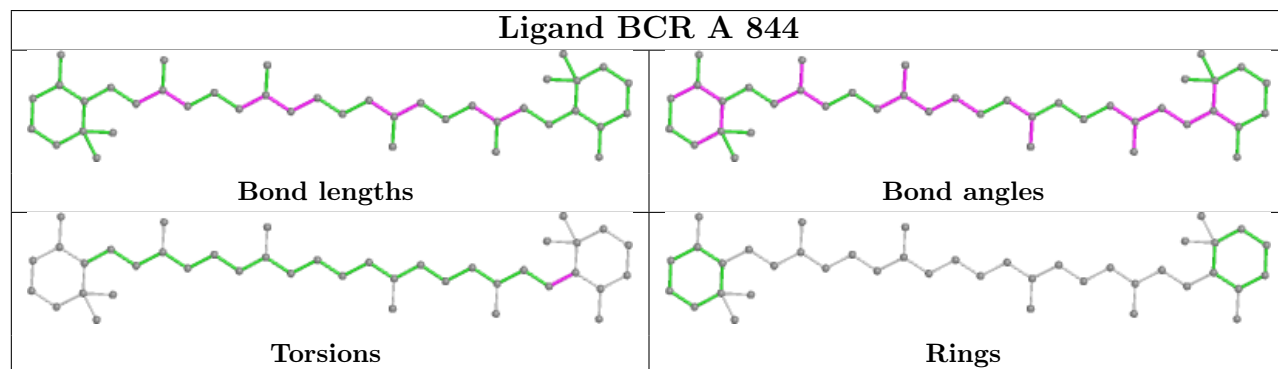


Torsions

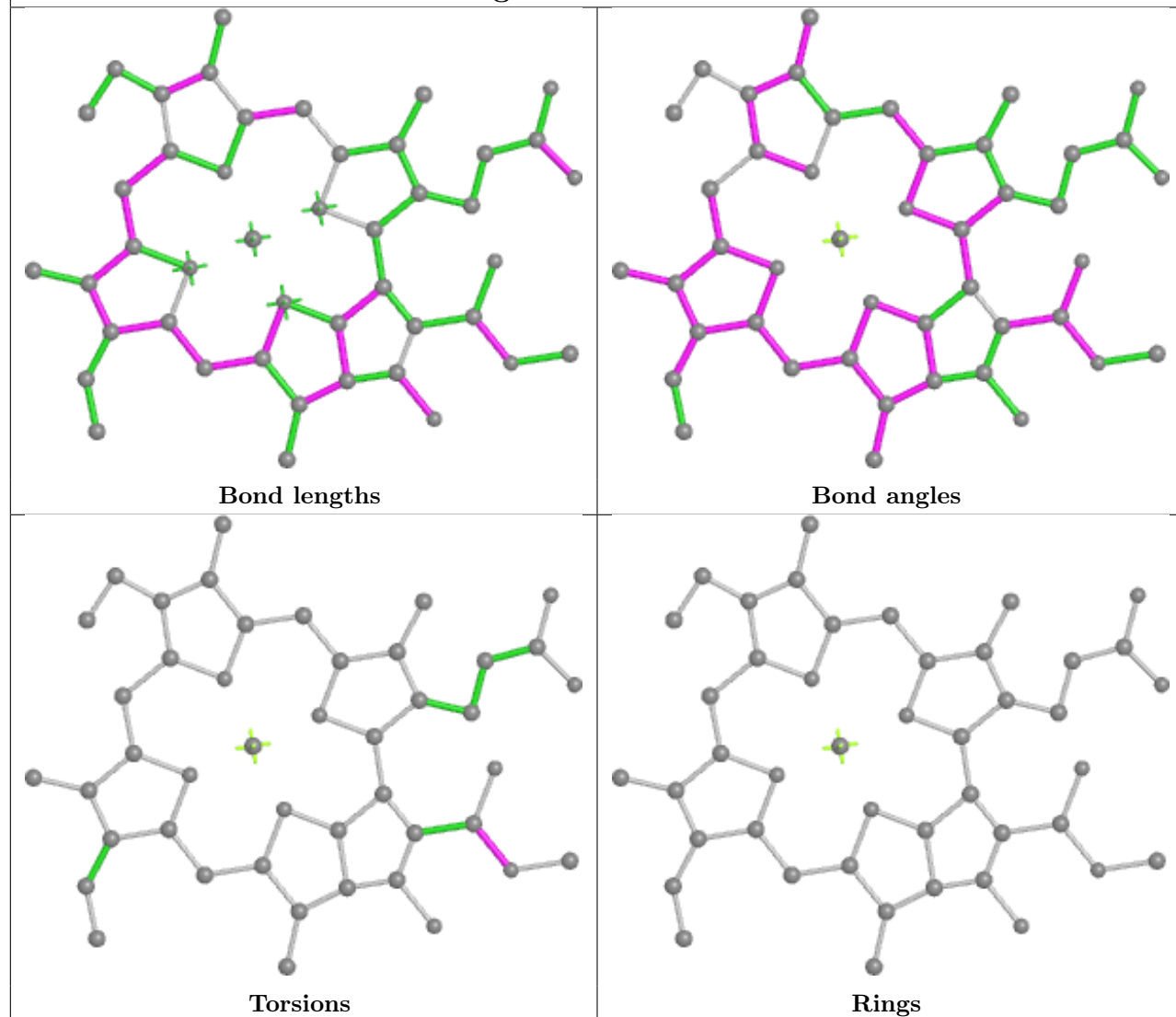


Rings

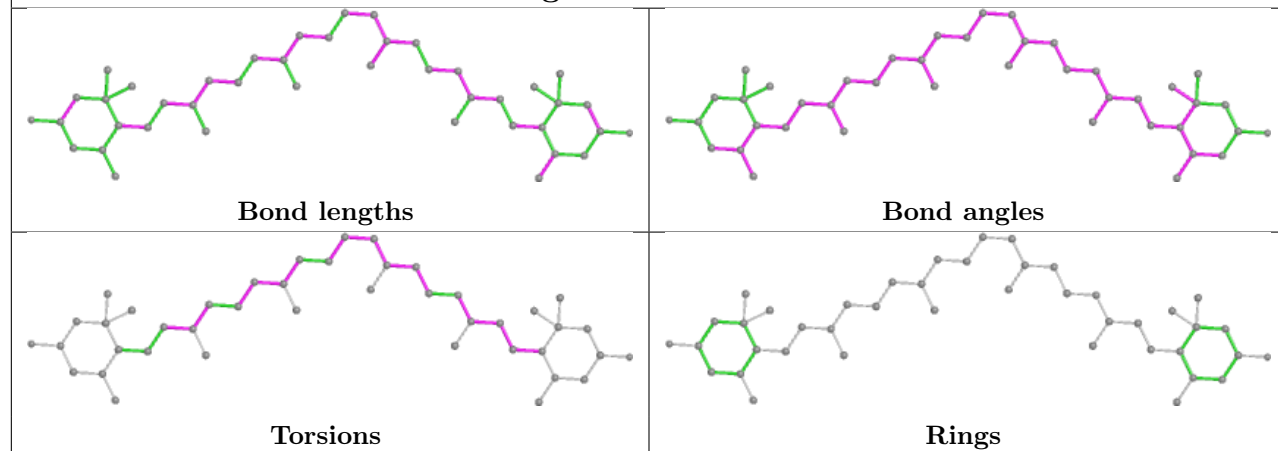


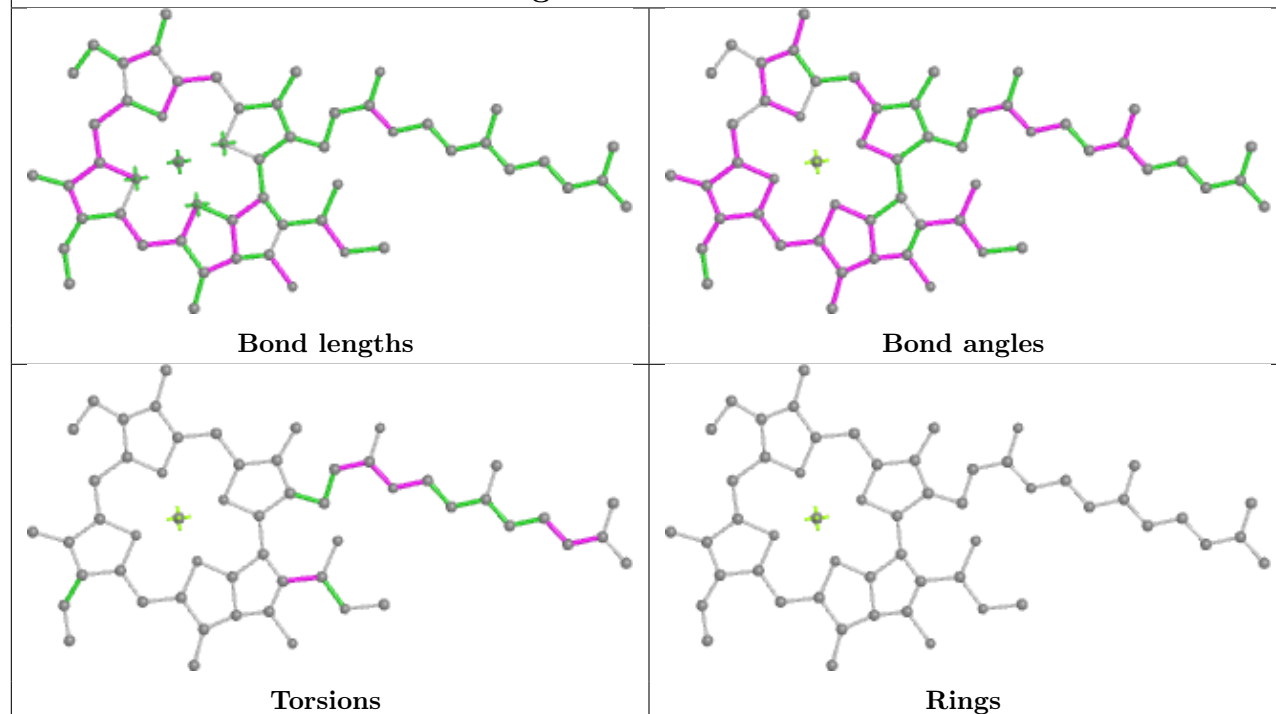
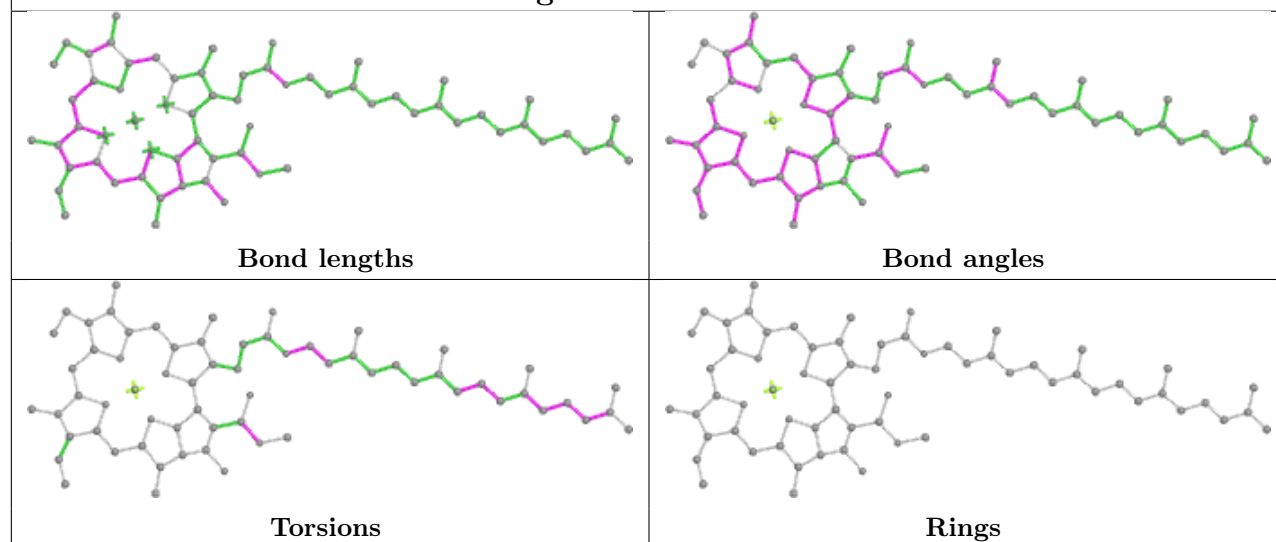
**Ligand CLA 6 305****Ligand CLA B 807****Ligand BCR A 844**

## Ligand CLA 4 302

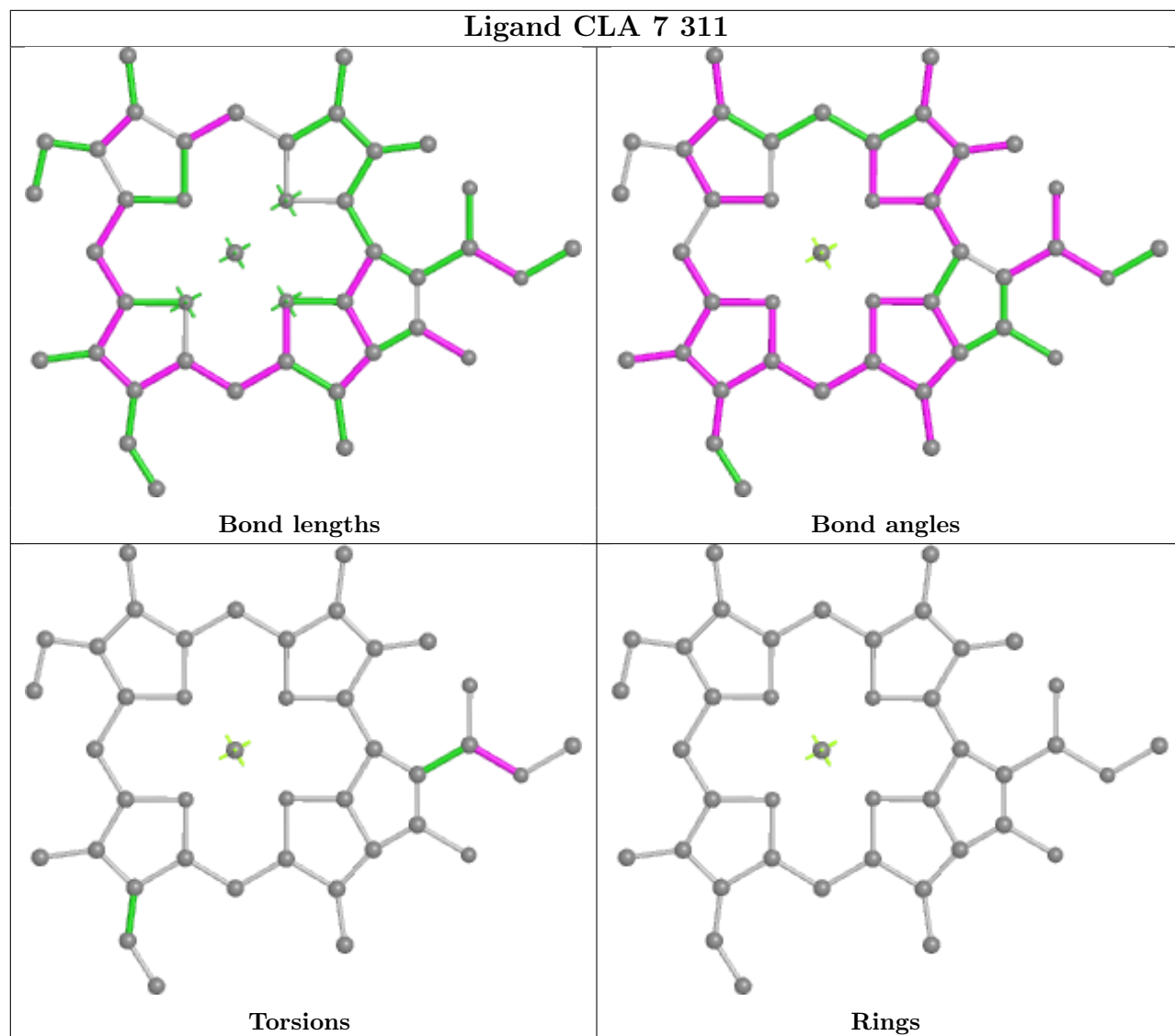


## Ligand 5X6 4 315

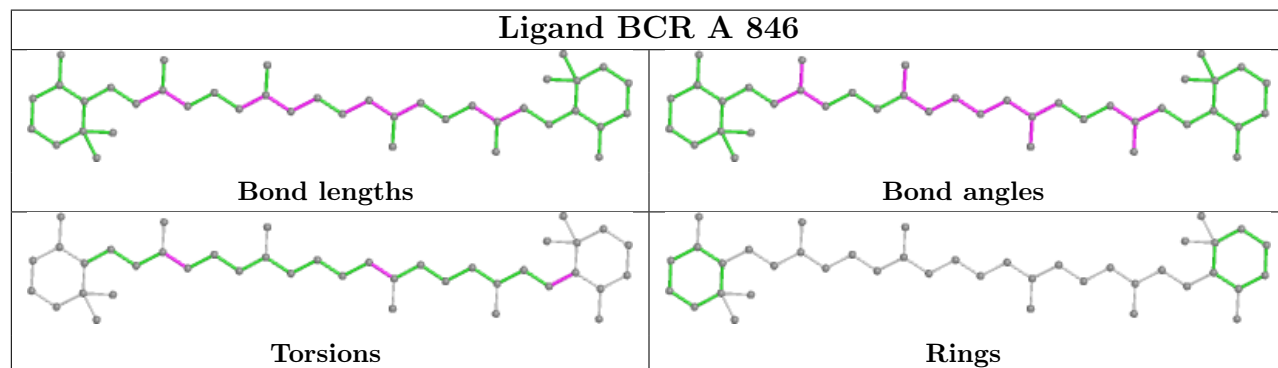


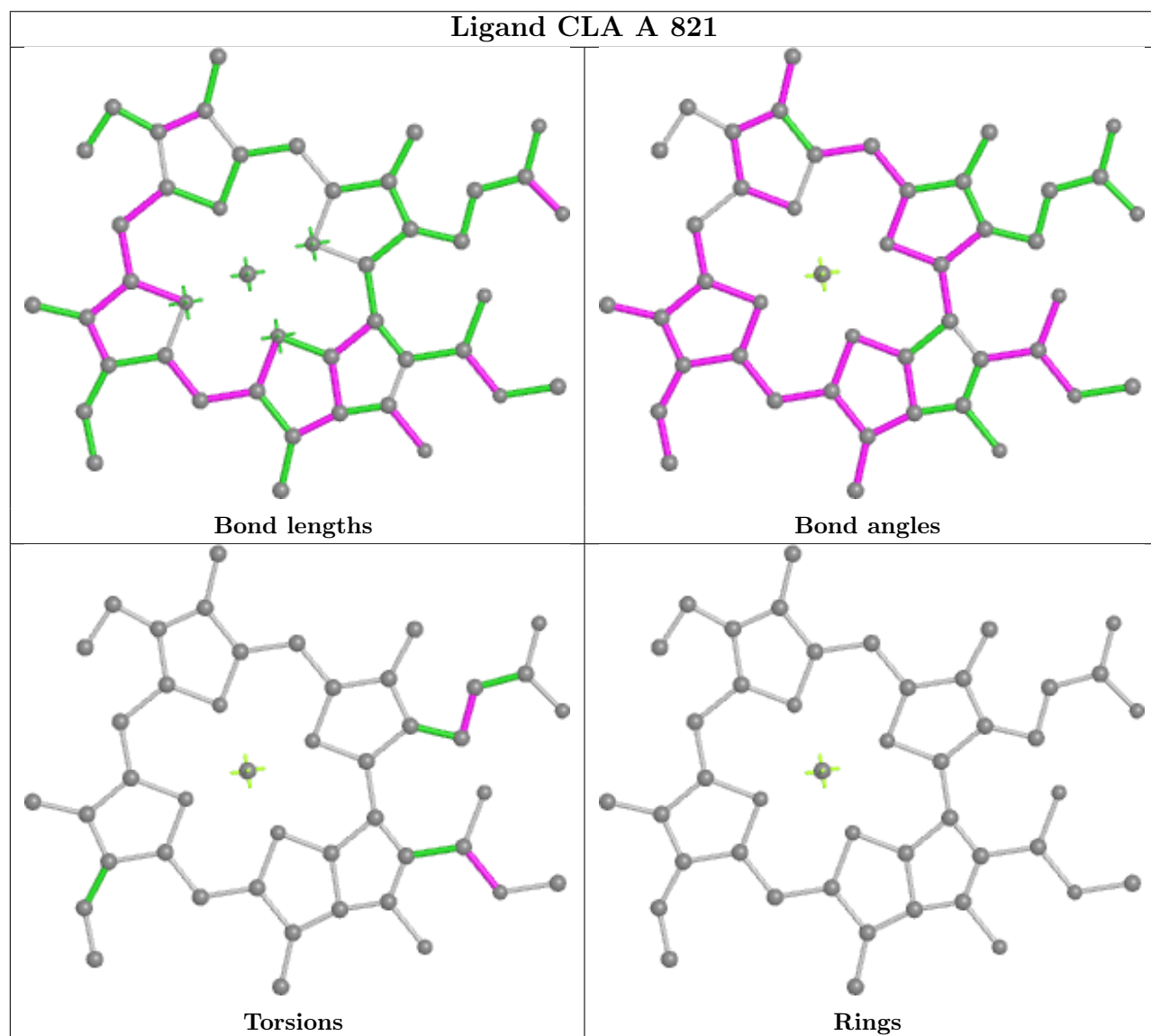
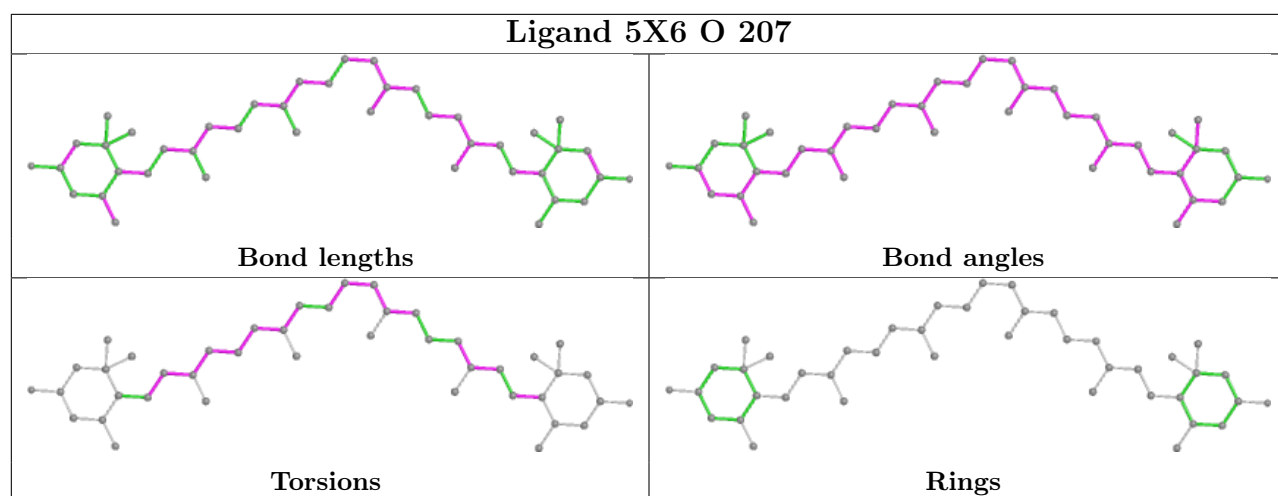
**Ligand CLA B 812****Ligand CLA 1 302**

## Ligand CLA 7 311



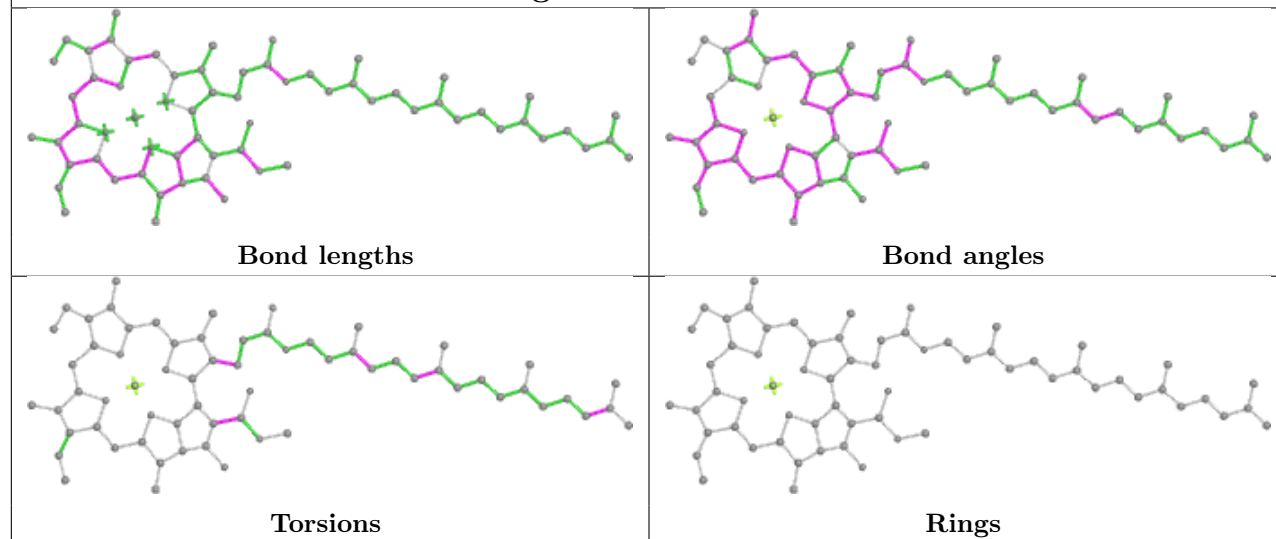
## Ligand BCR A 846



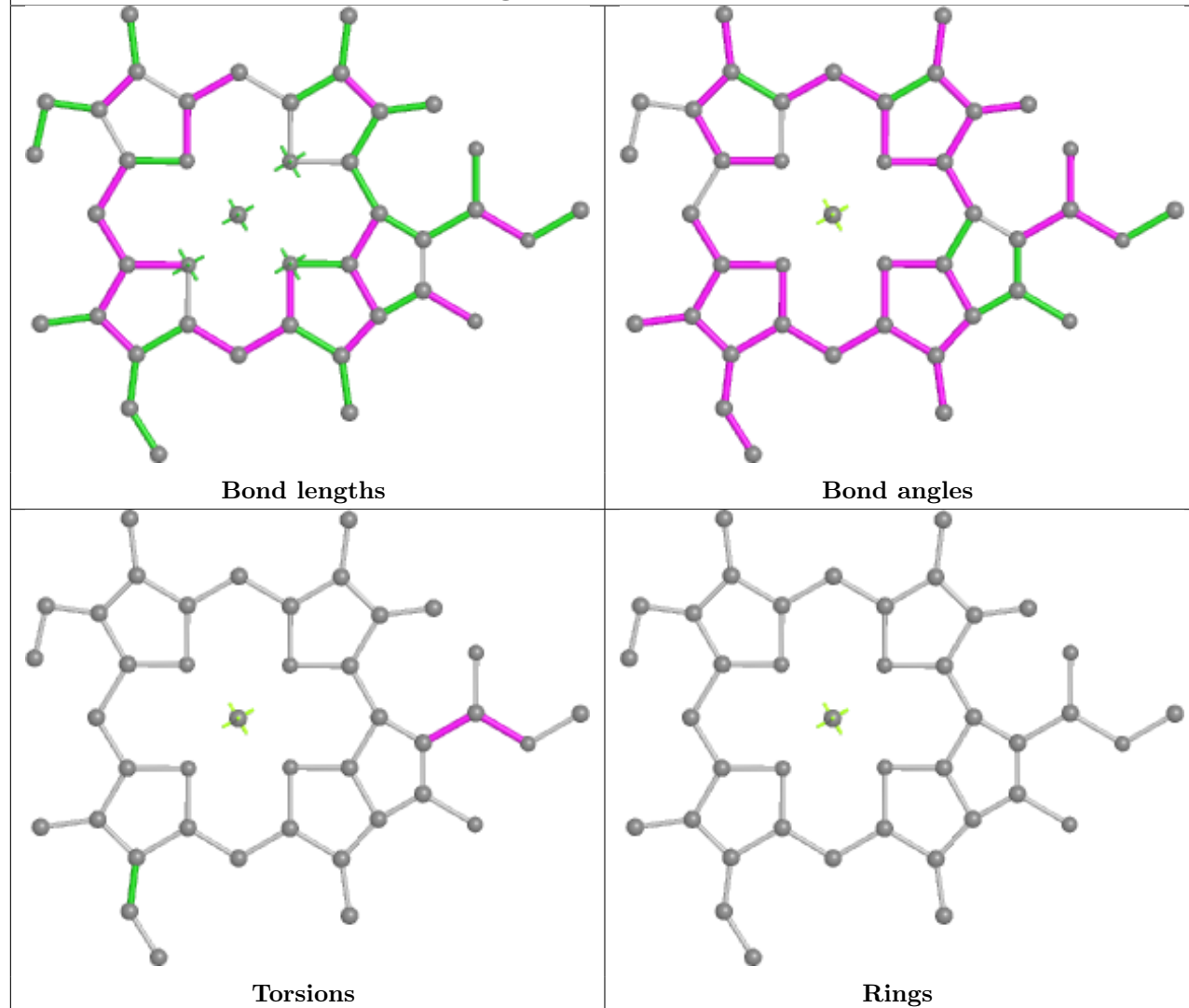




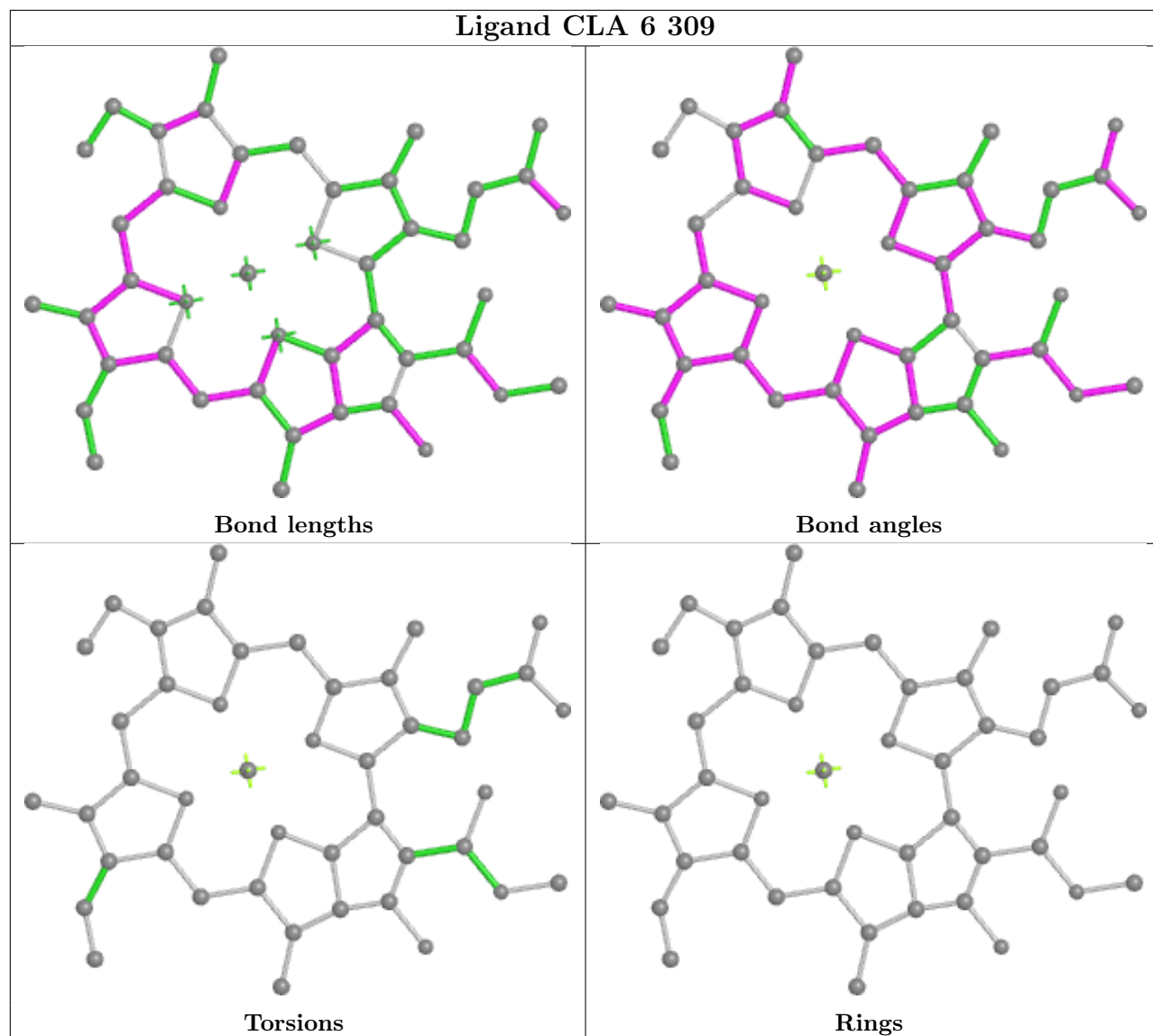
## Ligand CLA B 802



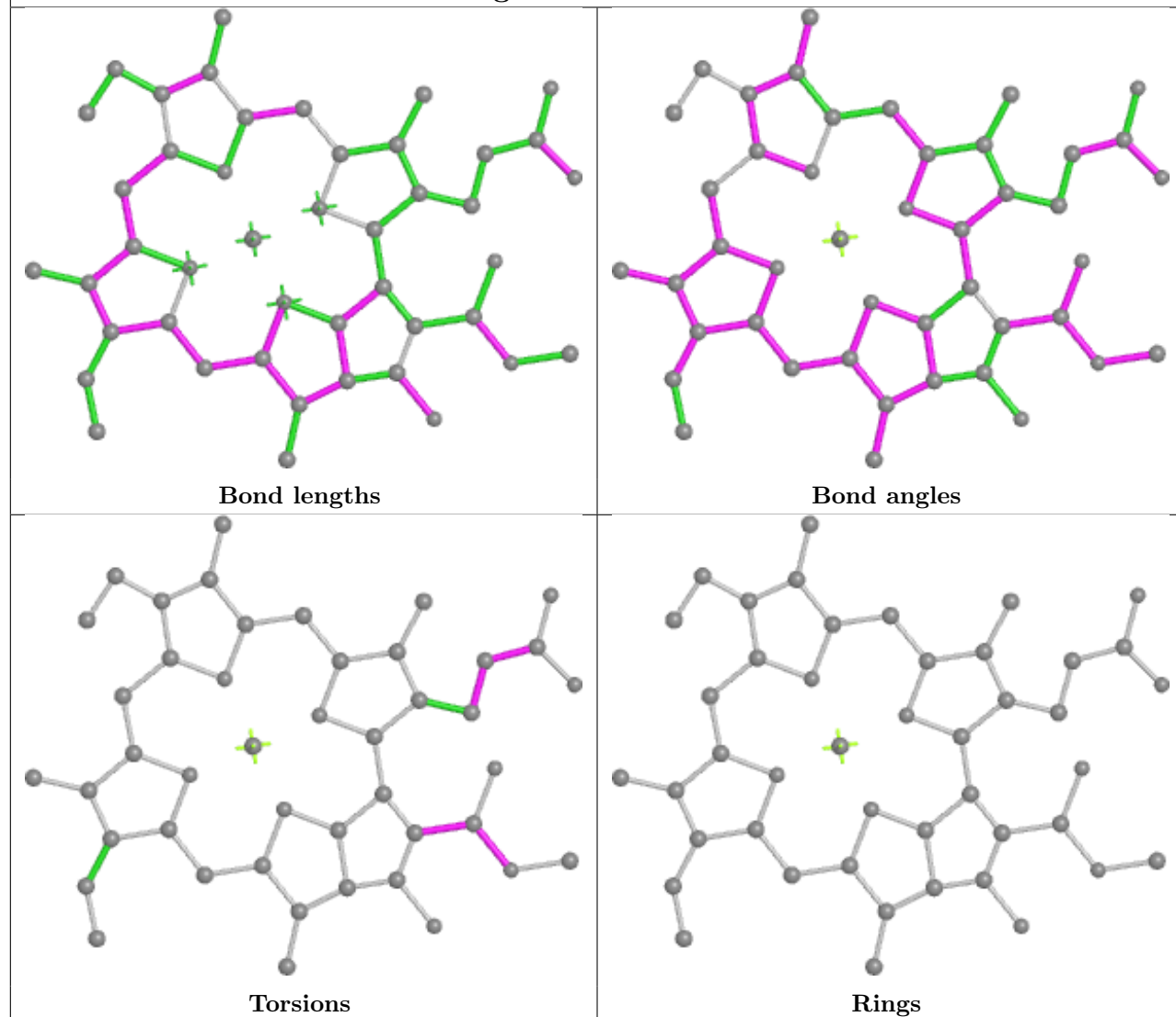
## Ligand CLA F 206



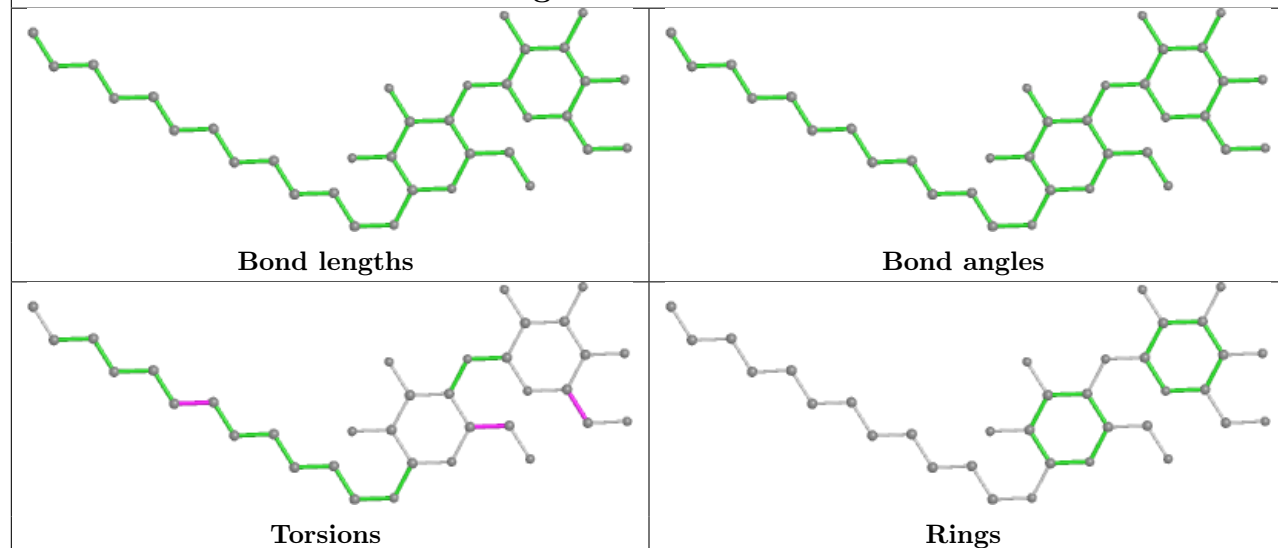
## Ligand CLA 6 309

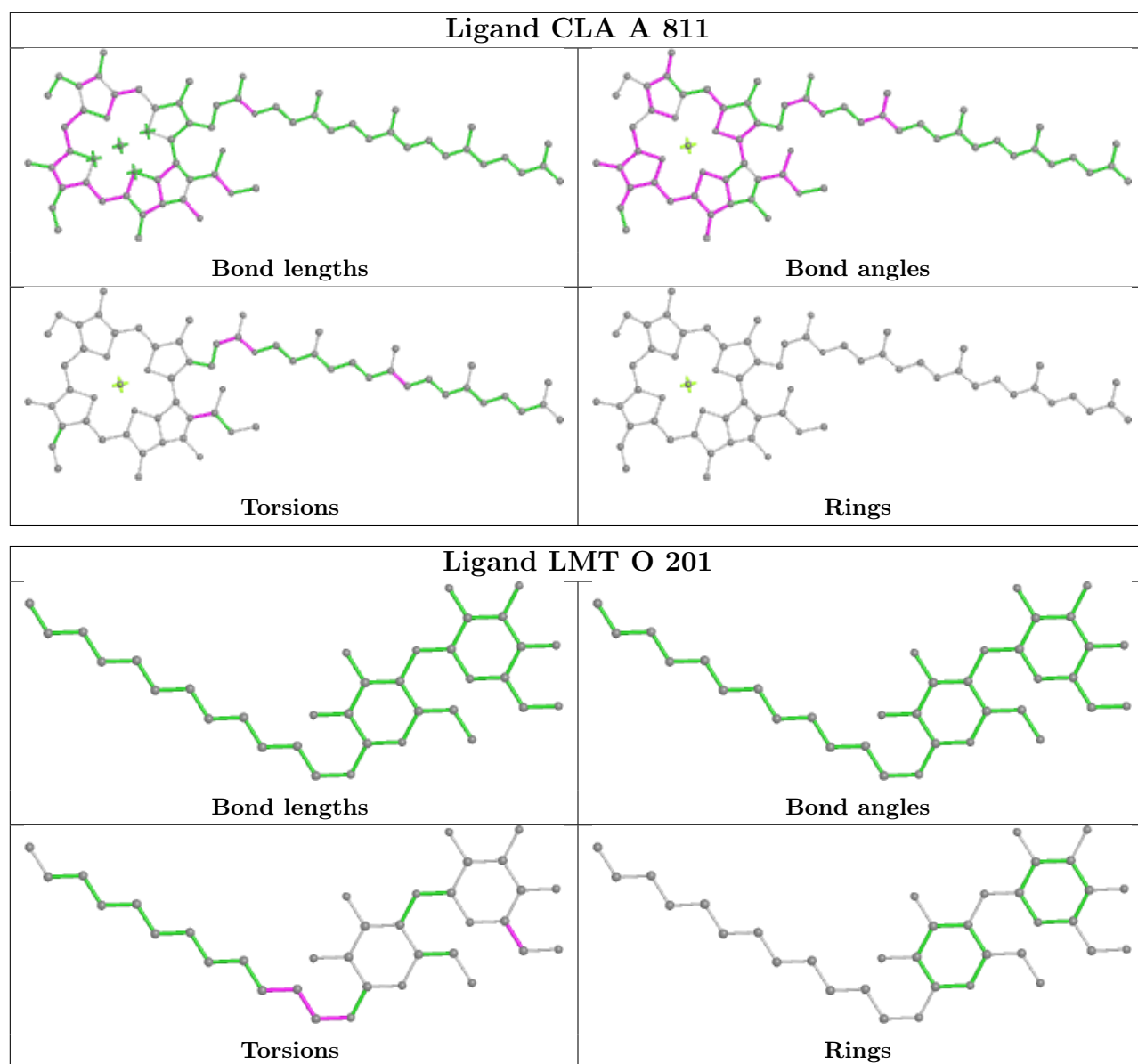


## Ligand CLA 2 306

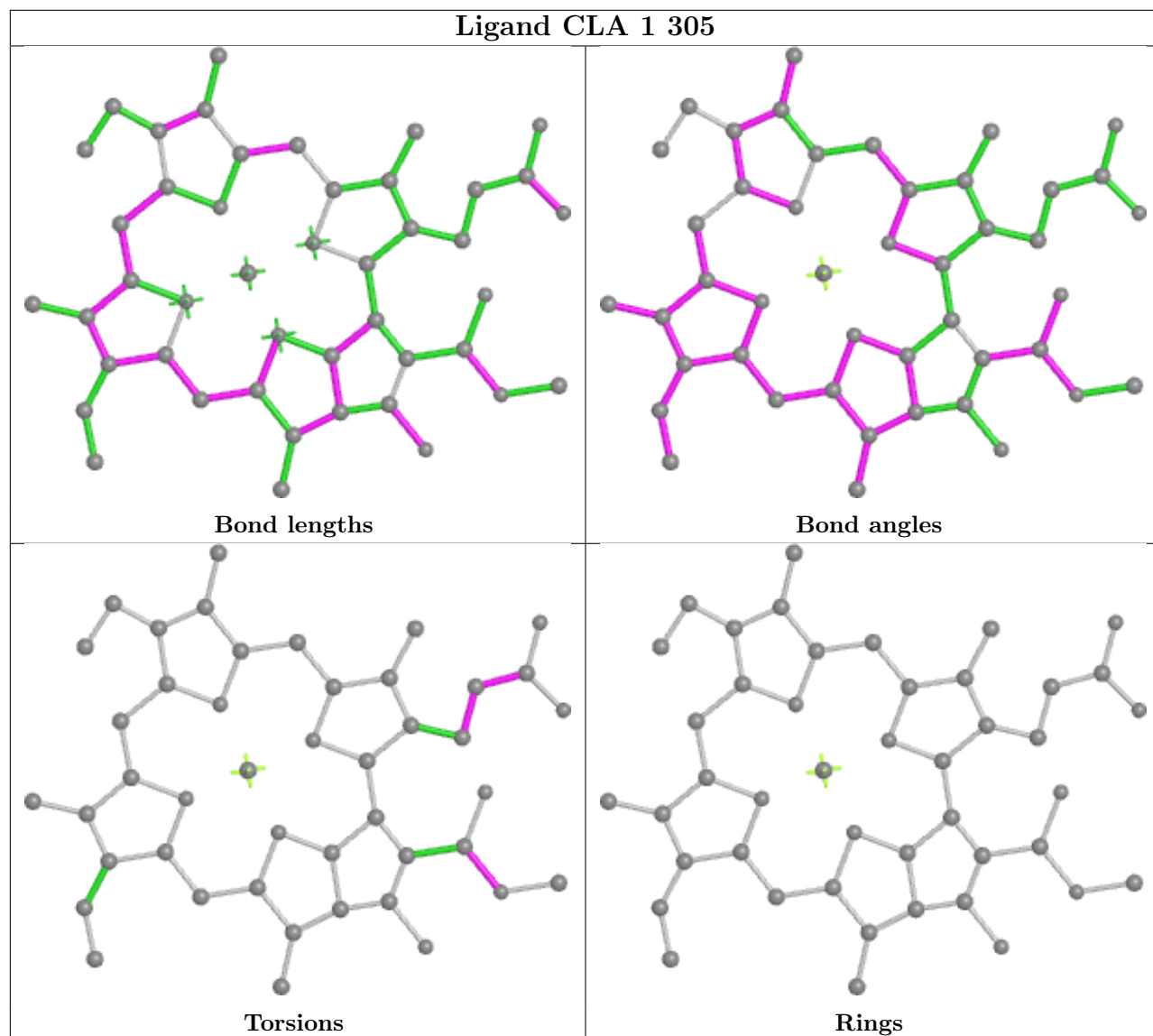


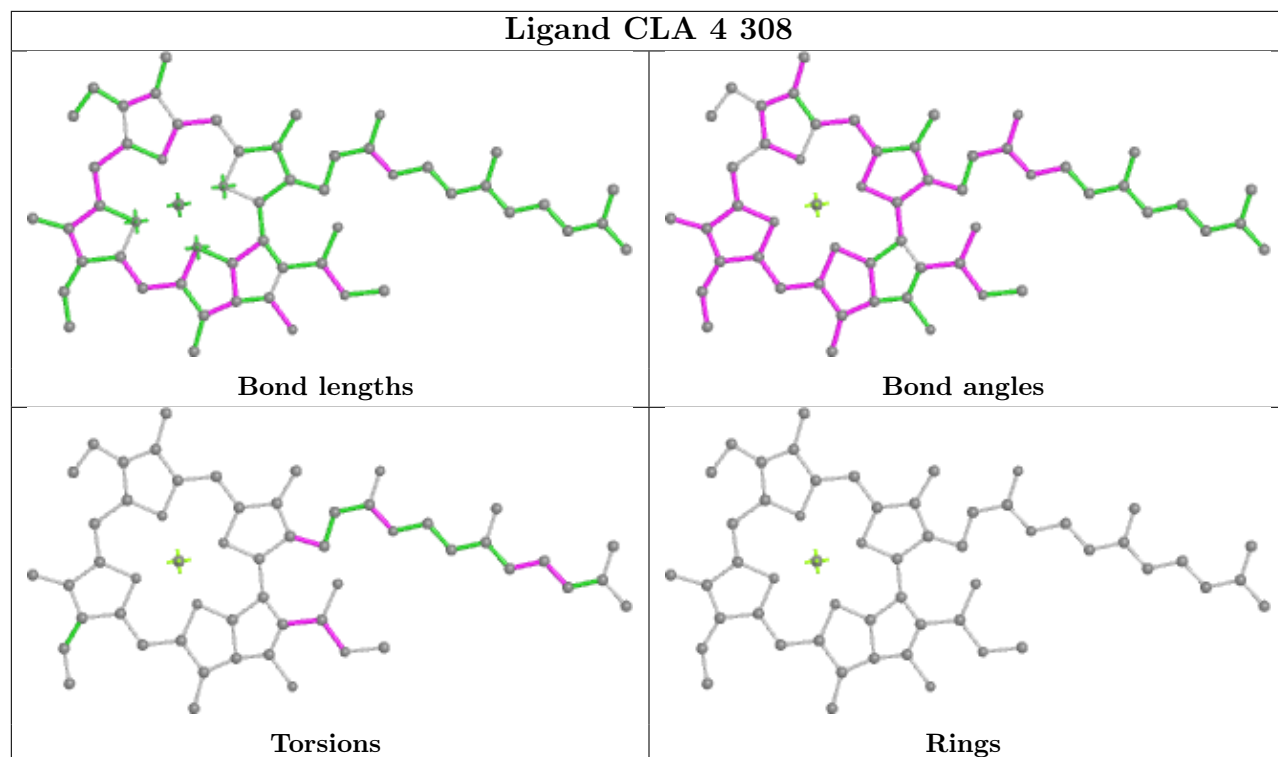
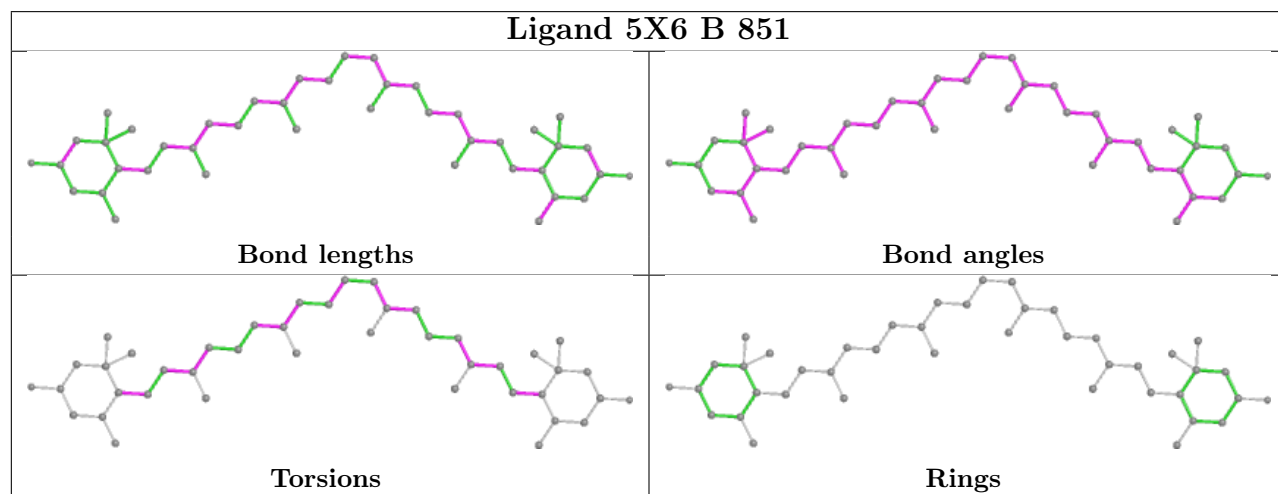
## Ligand LMT 4 319



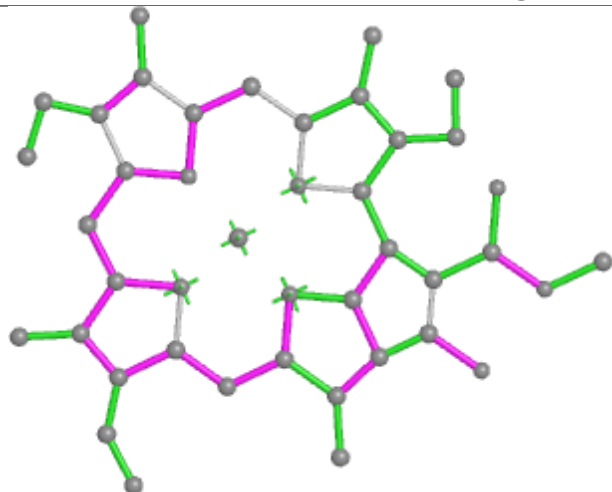


## Ligand CLA 1 305

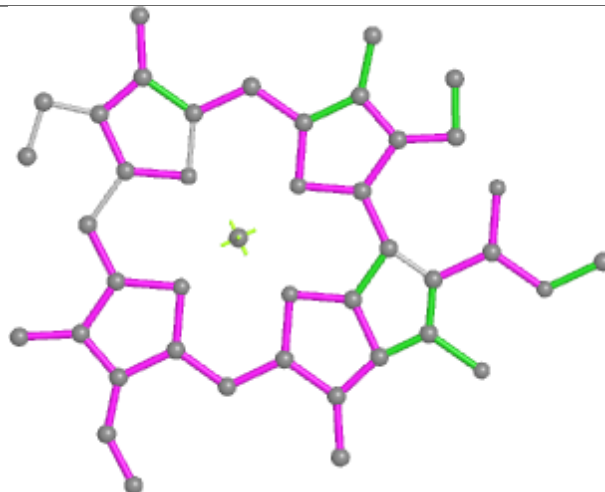


**Ligand CLA 4 308****Ligand 5X6 B 851**

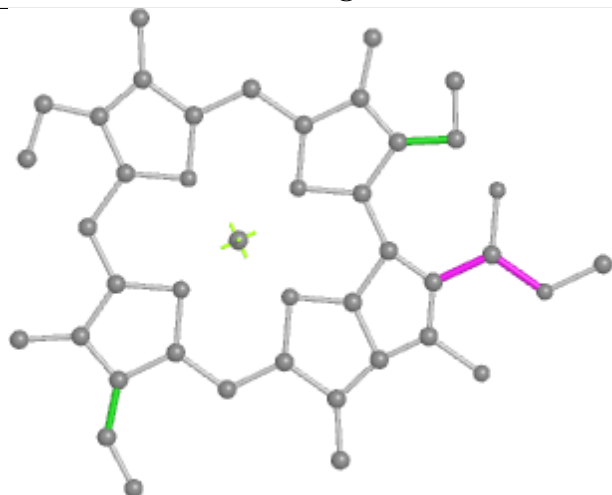
## Ligand CLA A 813



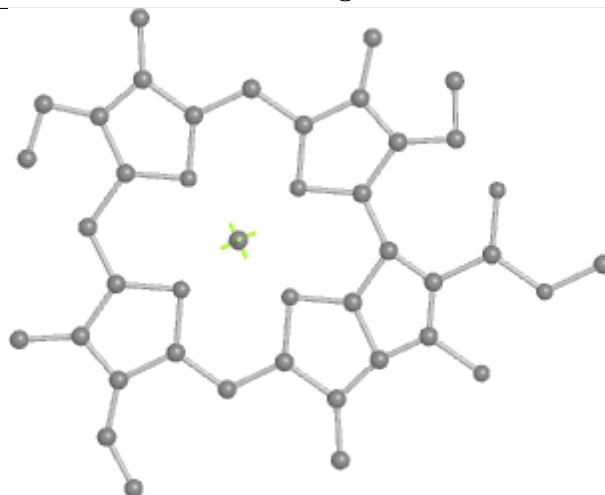
Bond lengths



Bond angles

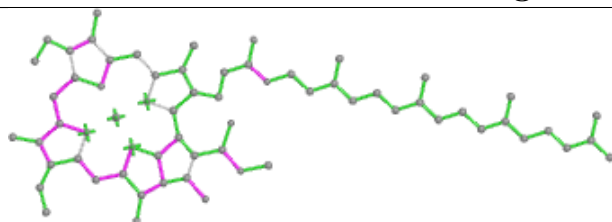


Torsions

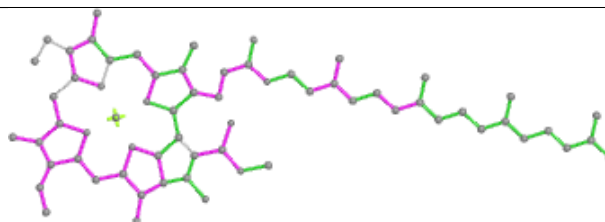


Rings

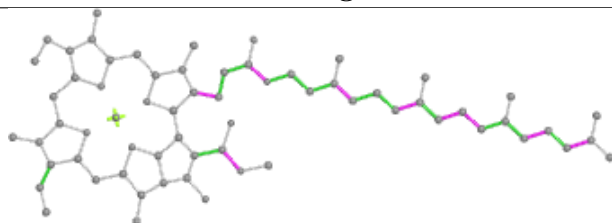
## Ligand CLA B 804



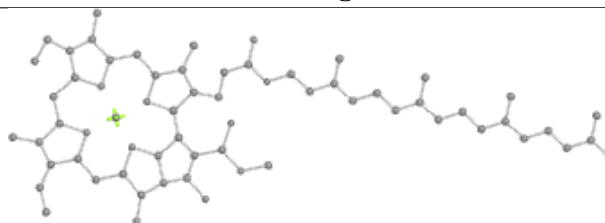
Bond lengths



Bond angles

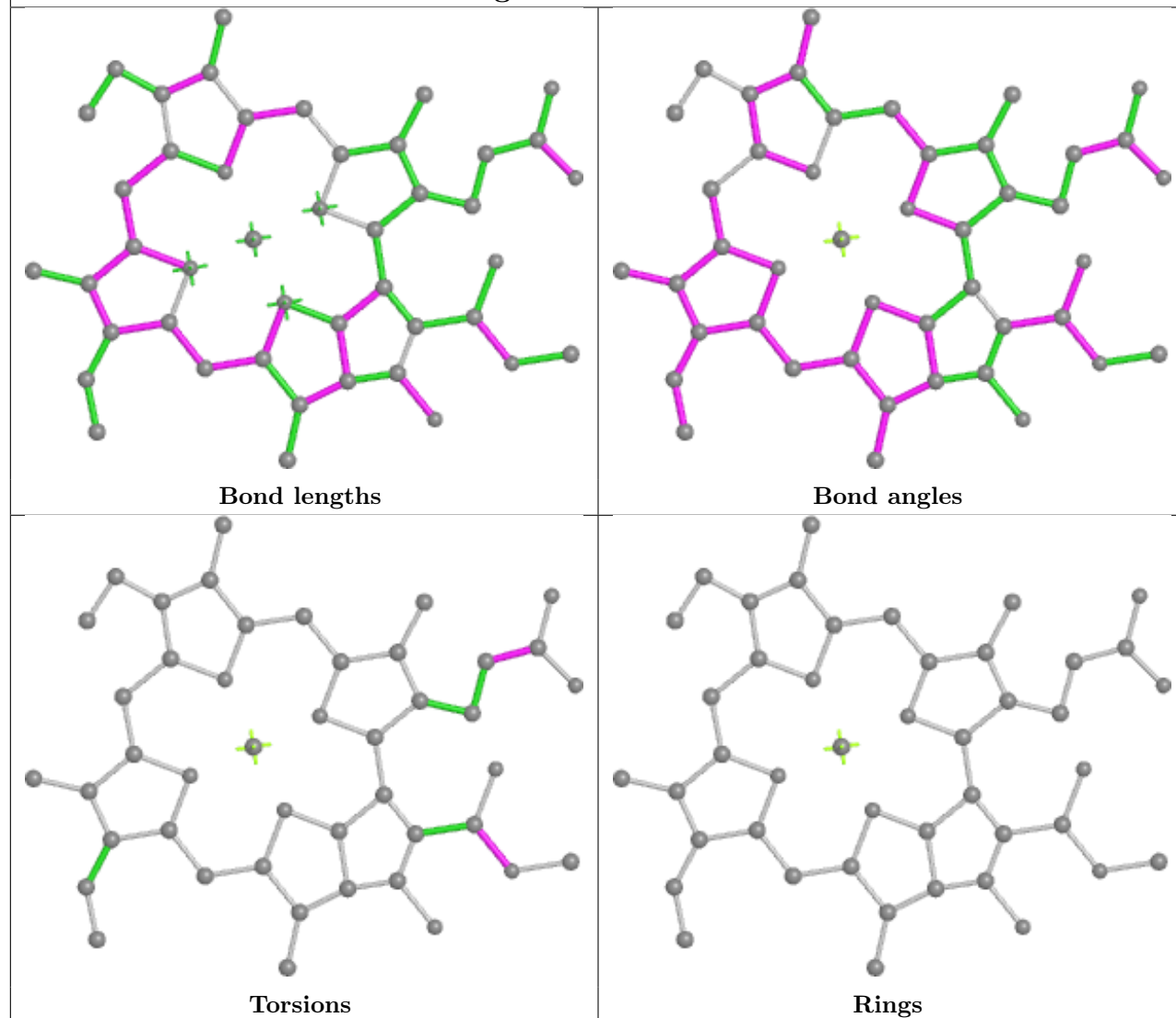


Torsions

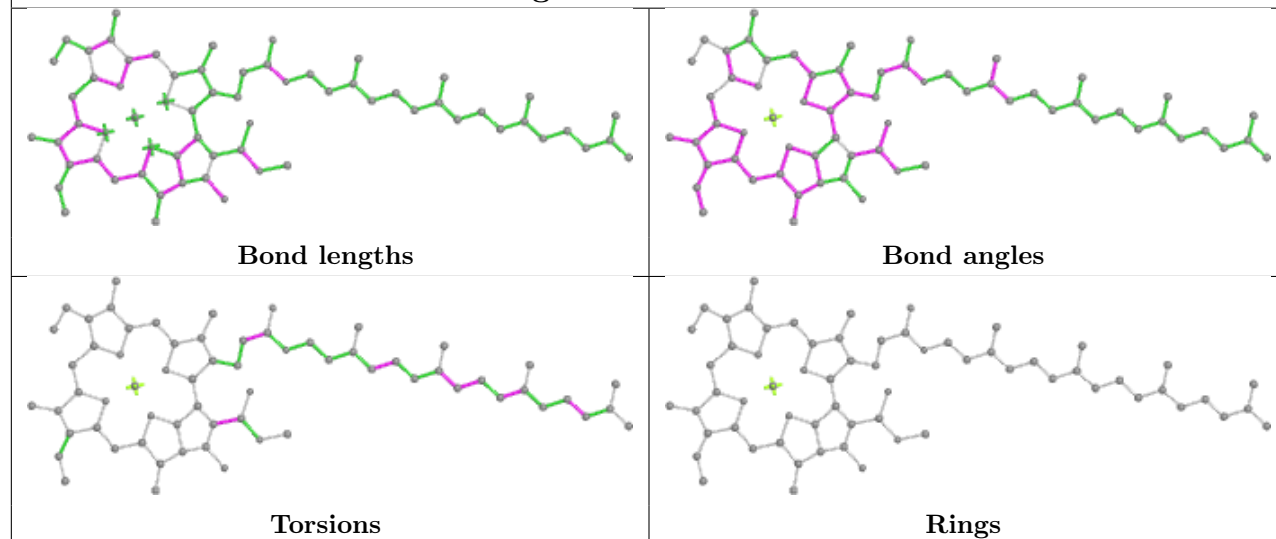


Rings

## Ligand CLA 5 301

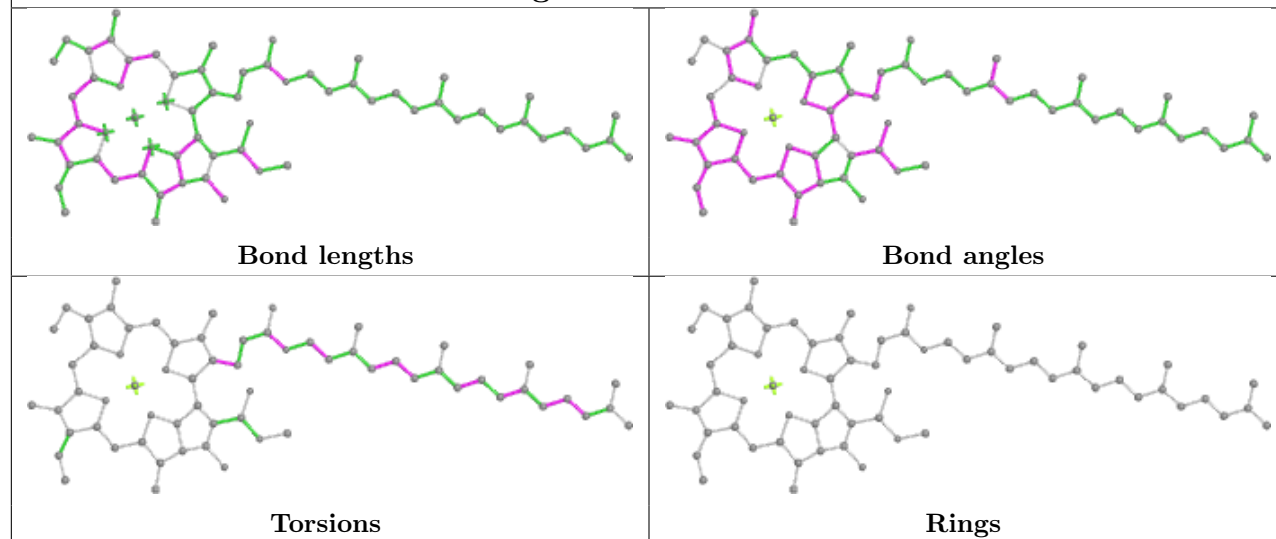


## Ligand CLA B 809

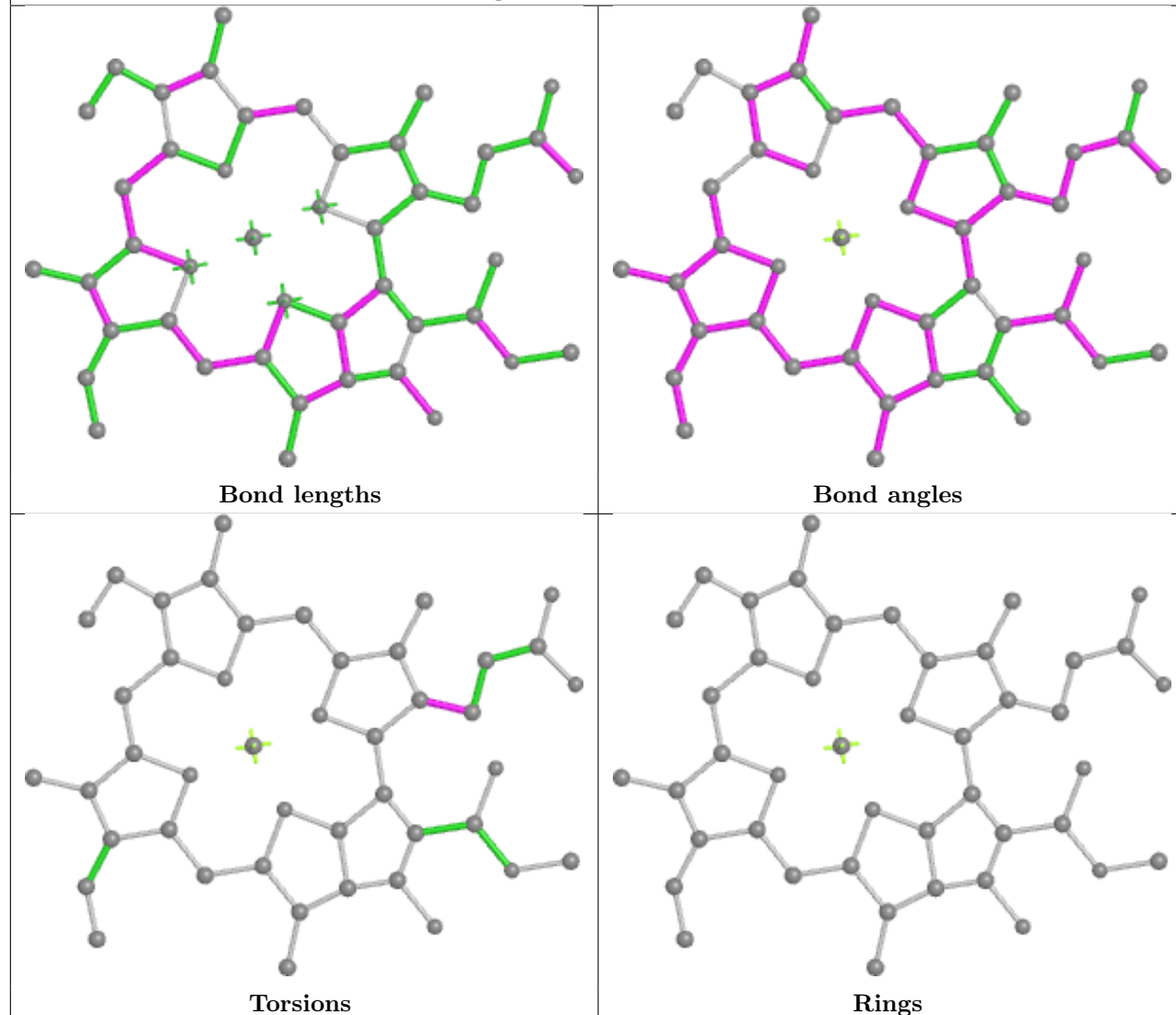




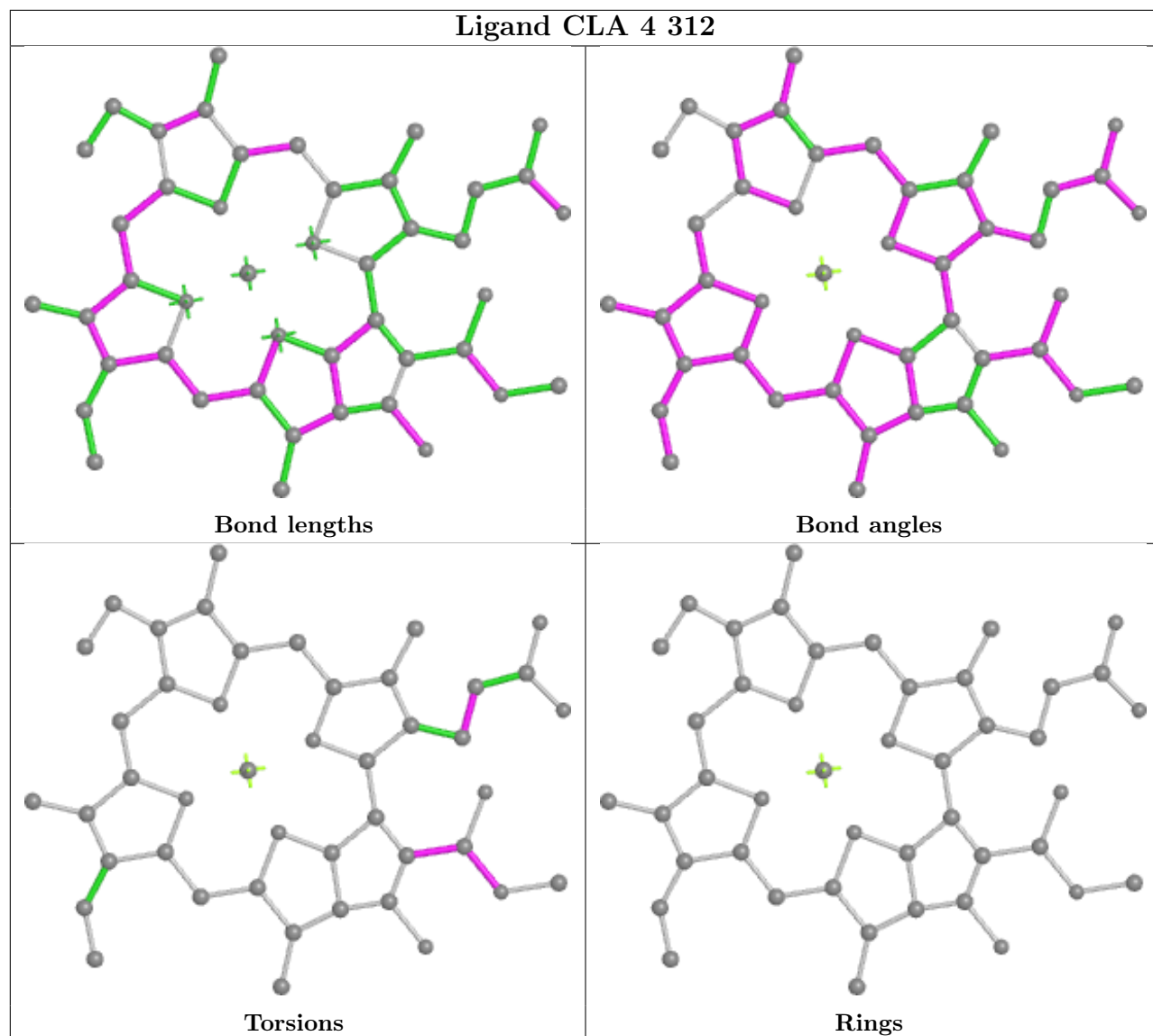
## Ligand CLA B 831



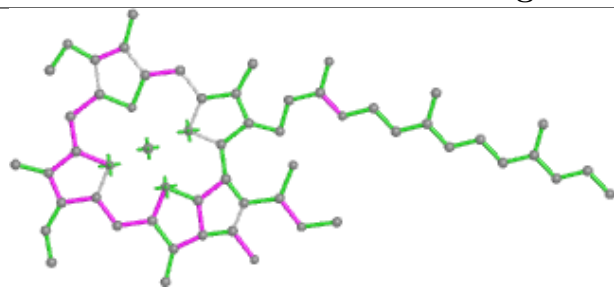
## Ligand CLA B 820



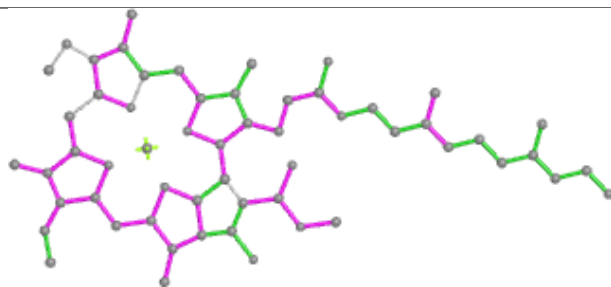
## Ligand CLA 4 312



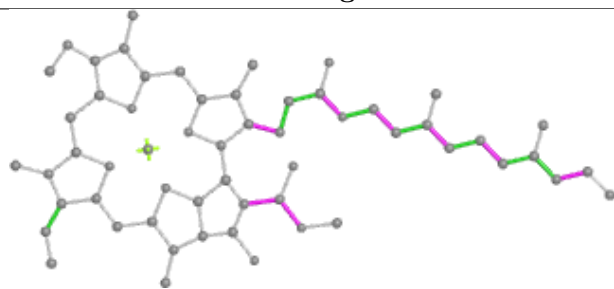
## Ligand CLA L 203



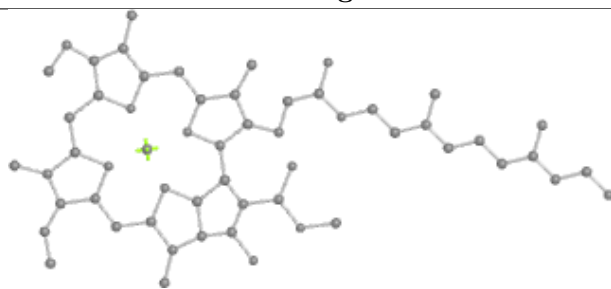
Bond lengths



Bond angles

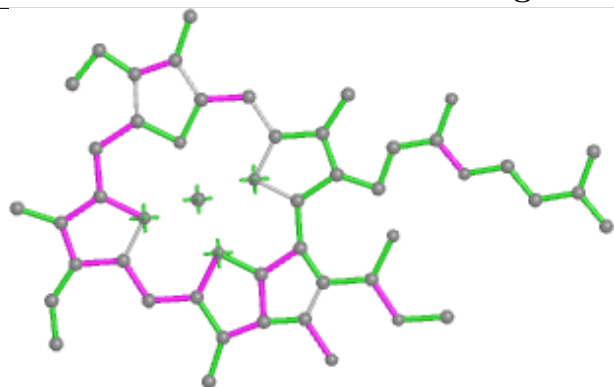


Torsions

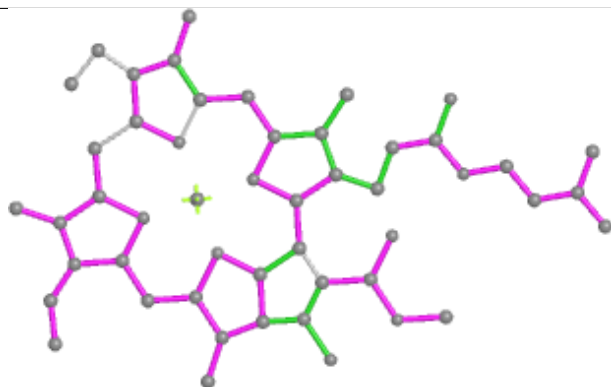


Rings

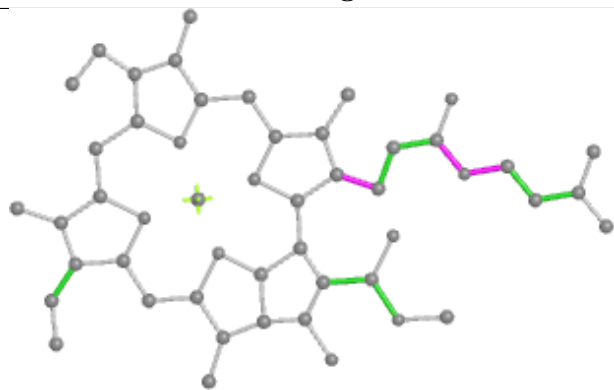
## Ligand CLA O 205



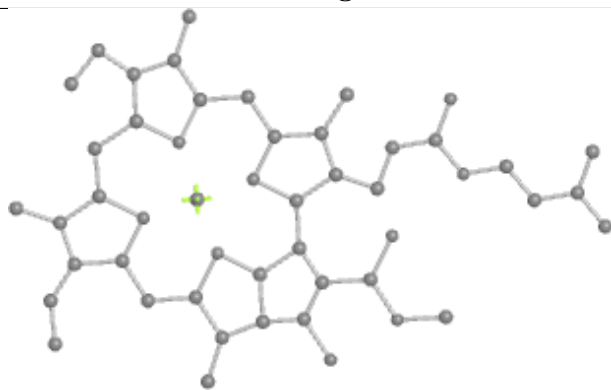
Bond lengths



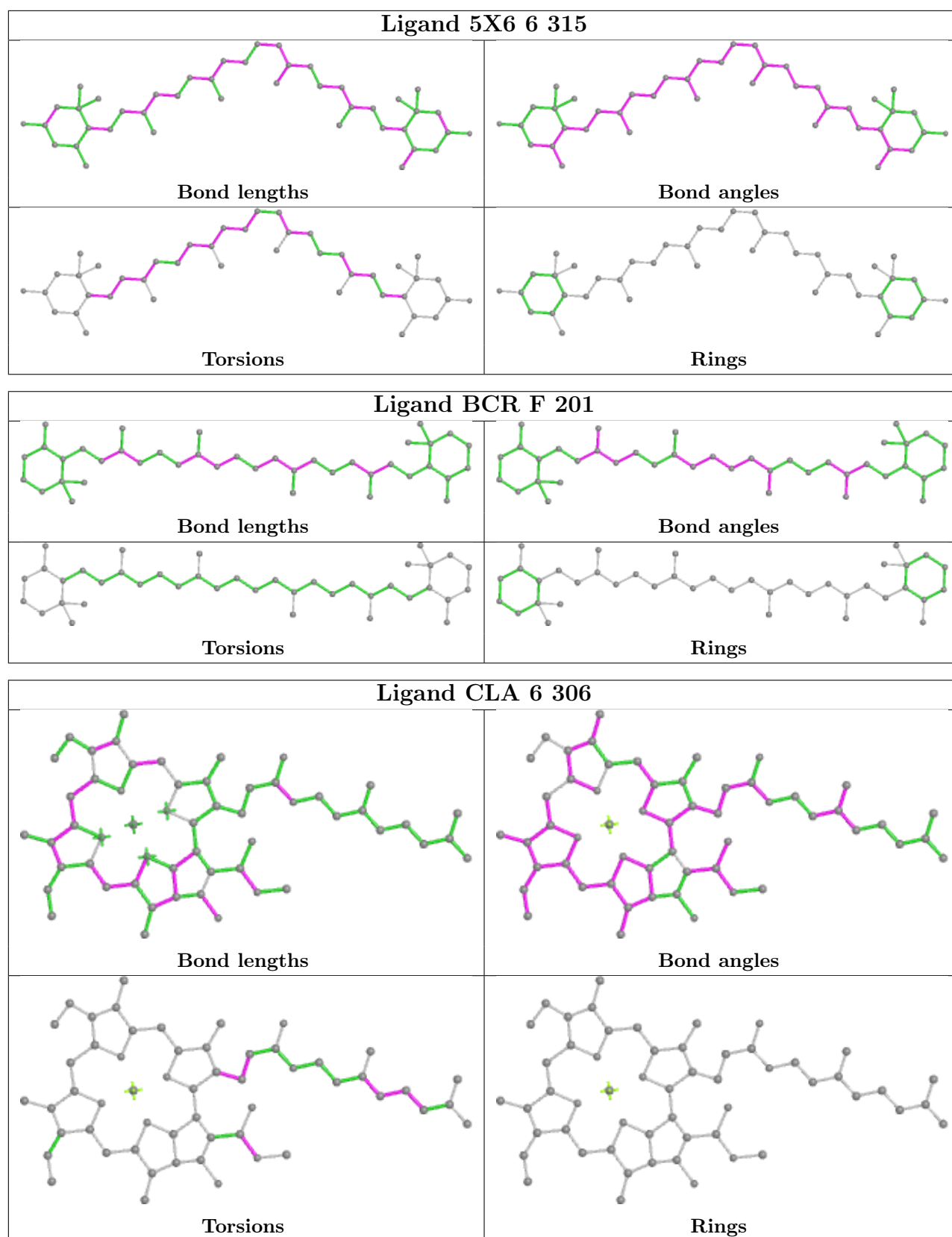
Bond angles



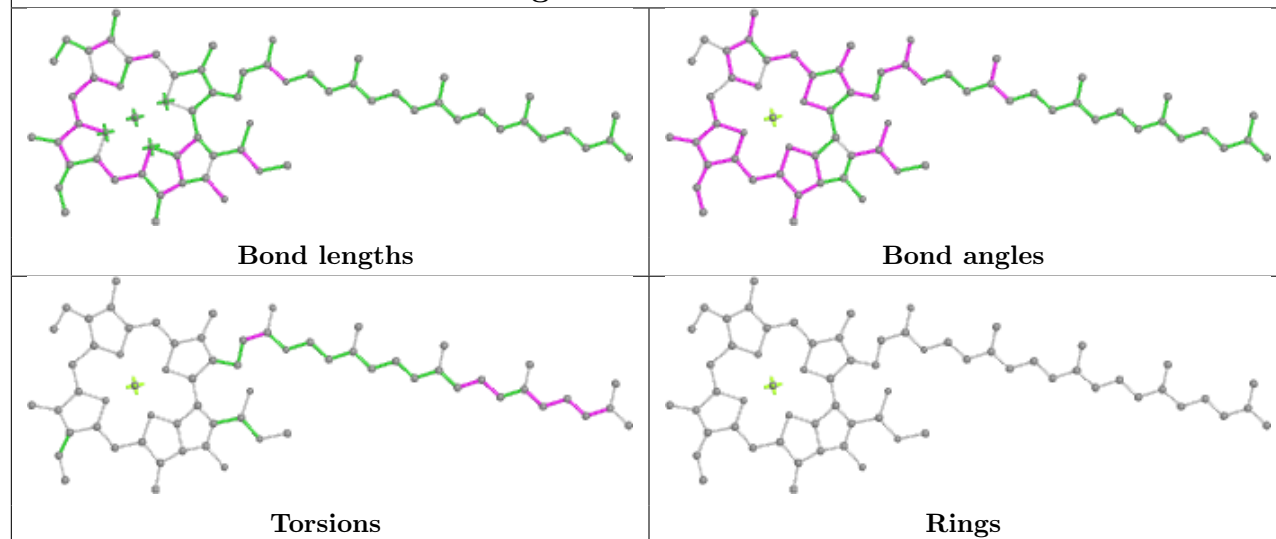
Torsions



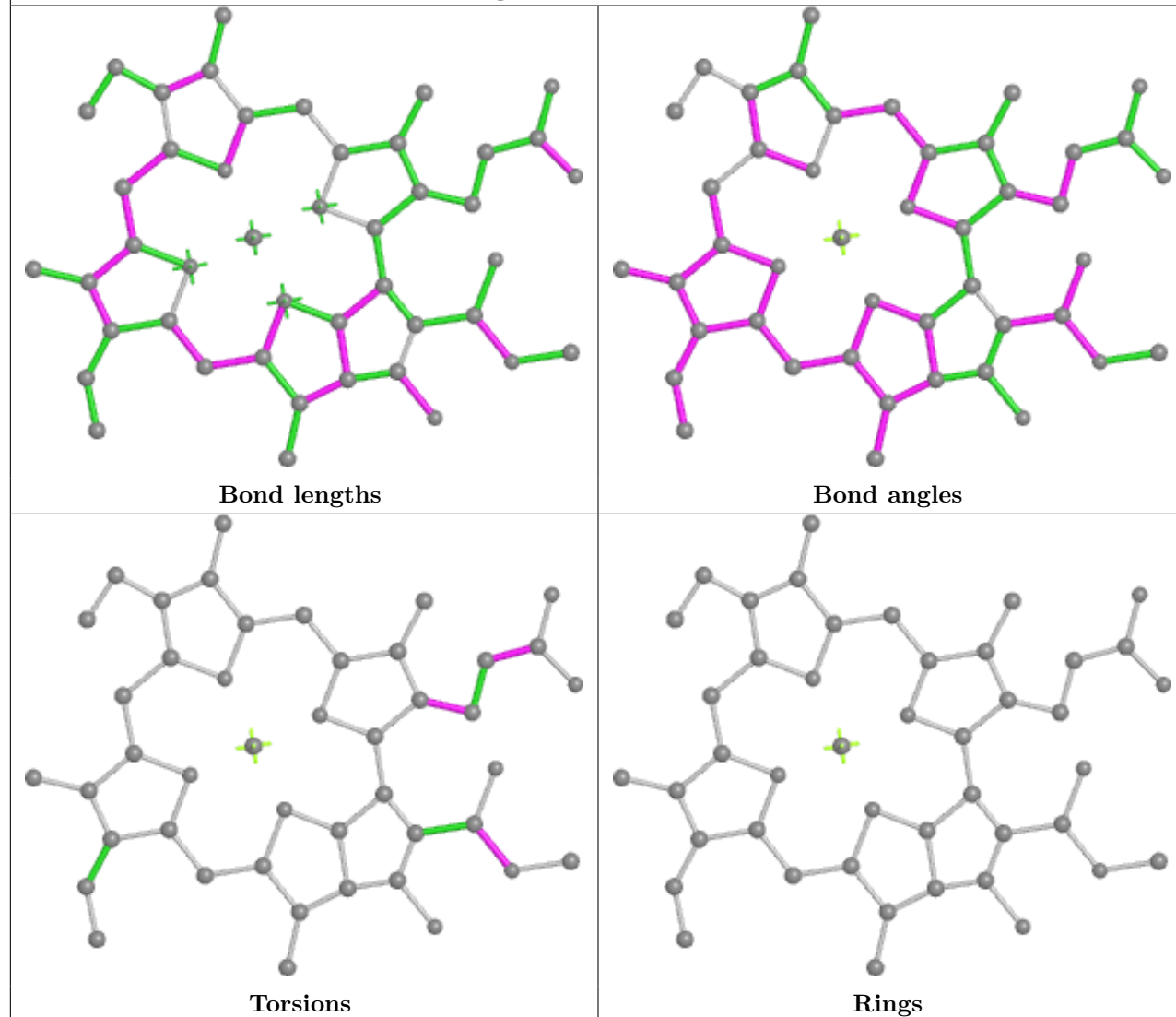
Rings

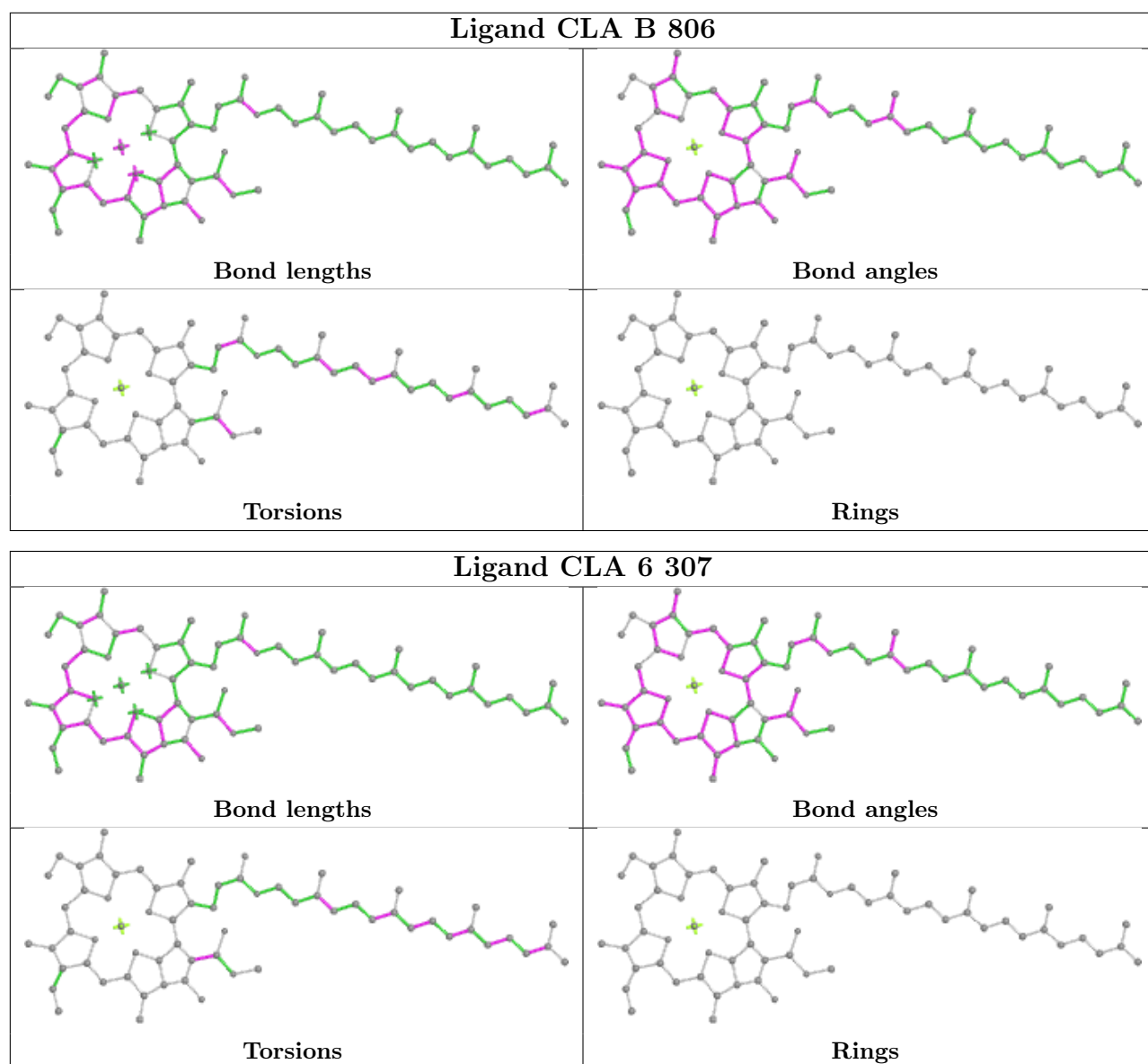


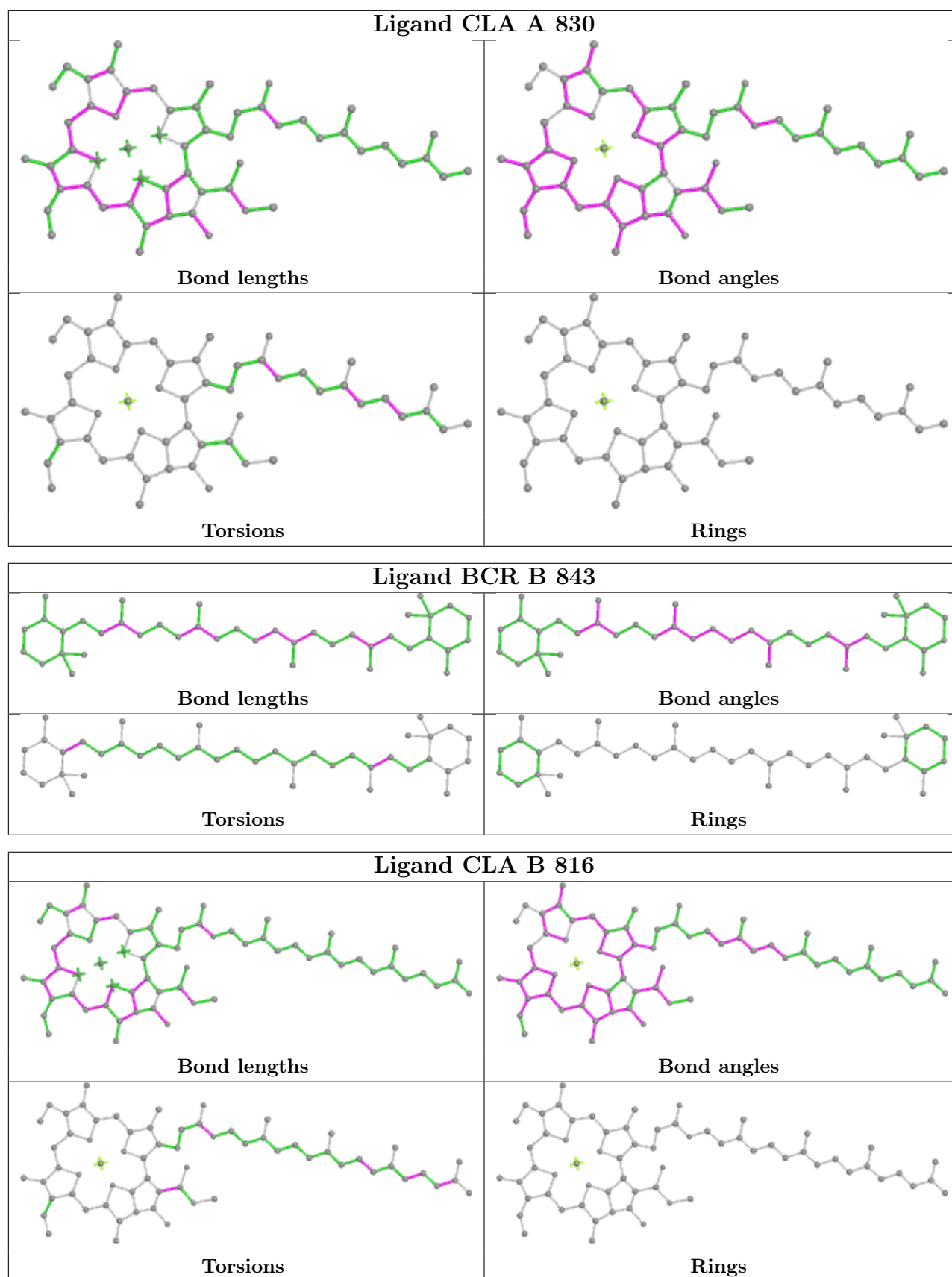
## Ligand CLA A 826



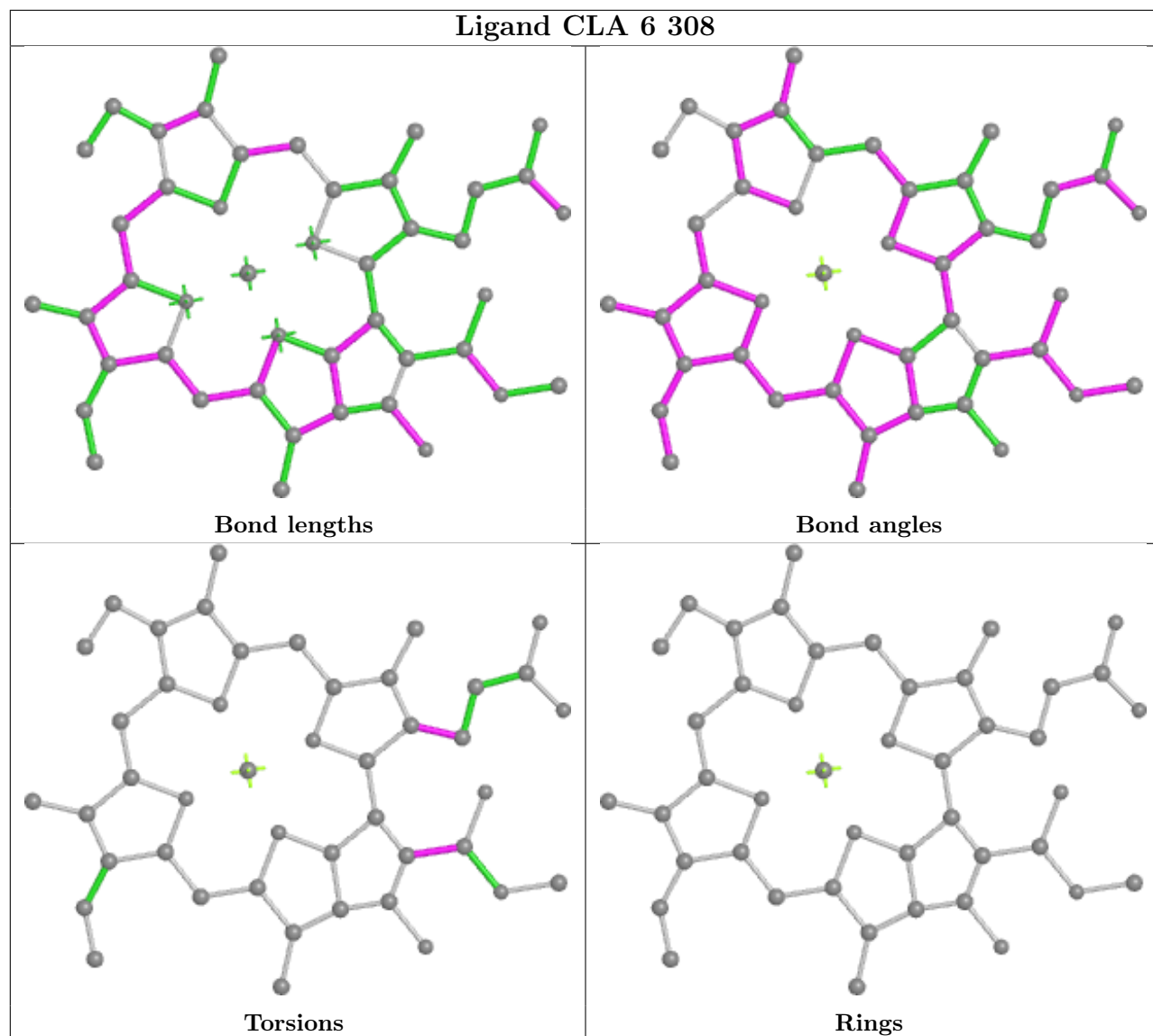
## Ligand CLA Z 201



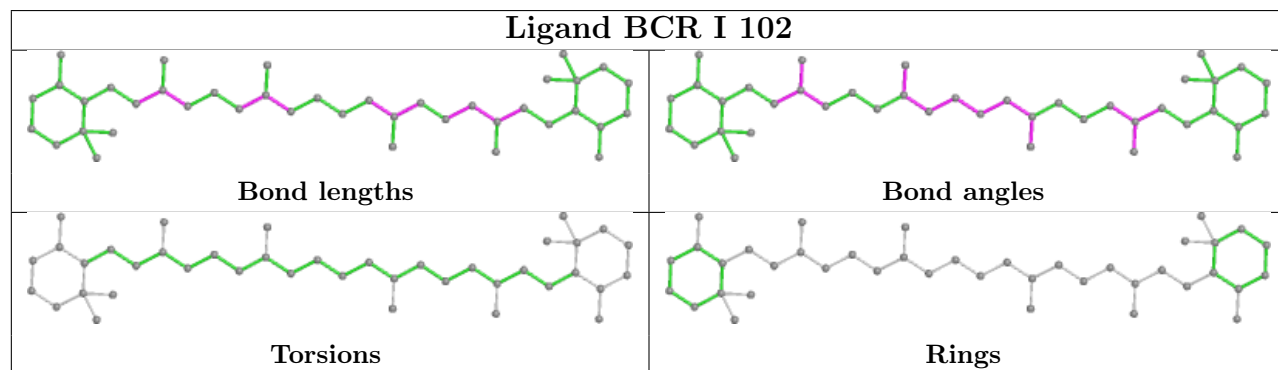




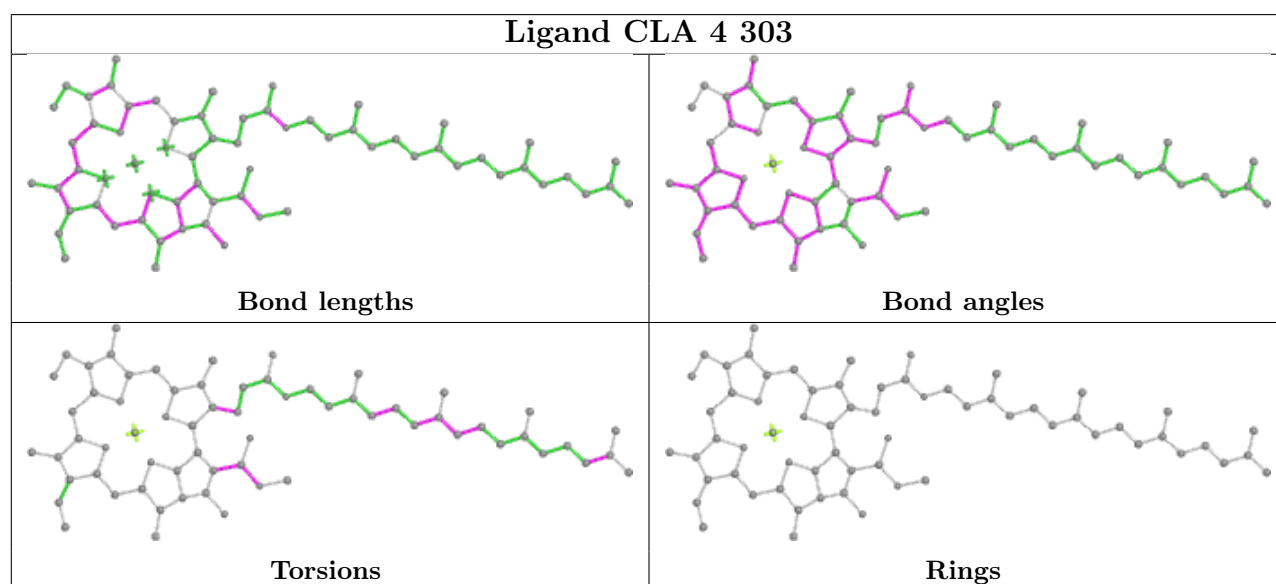
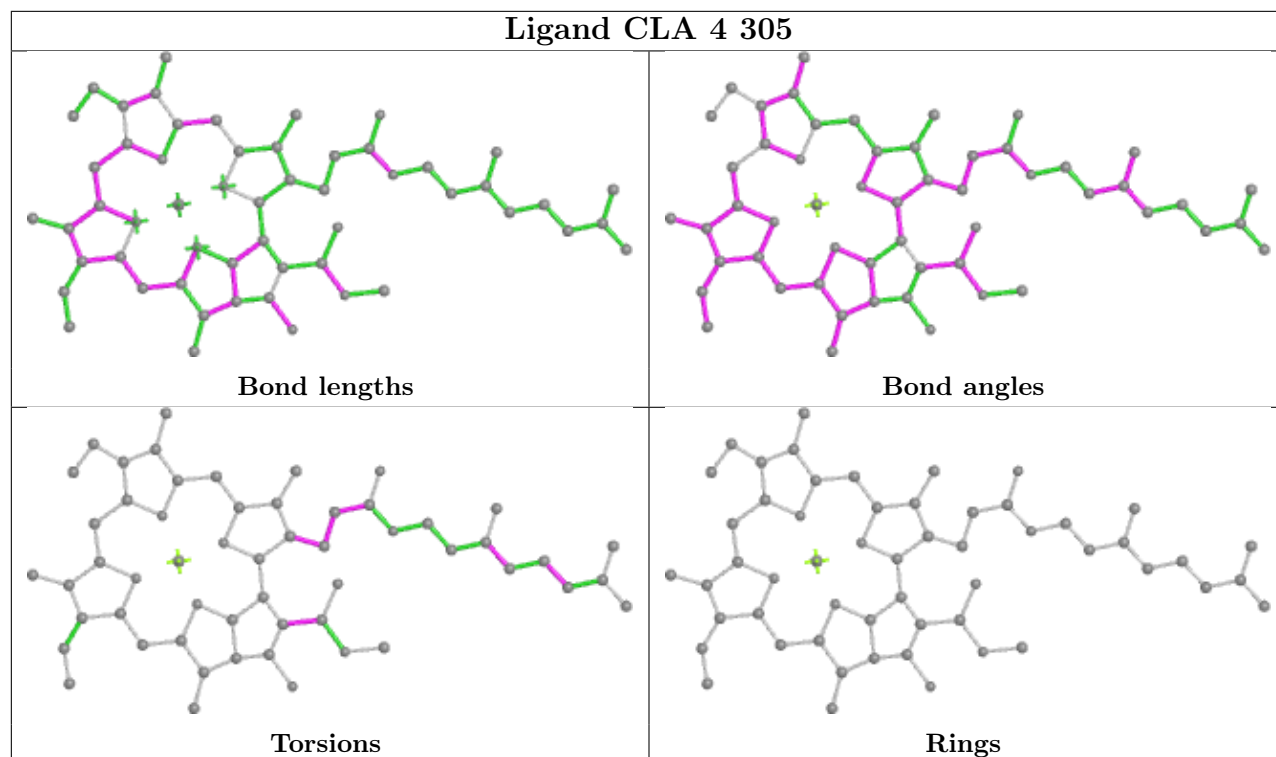
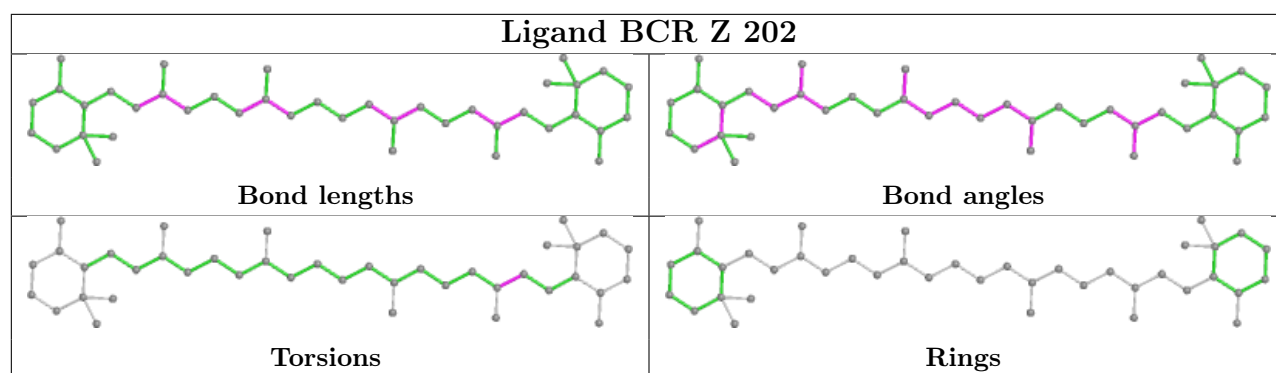
## Ligand CLA 6 308

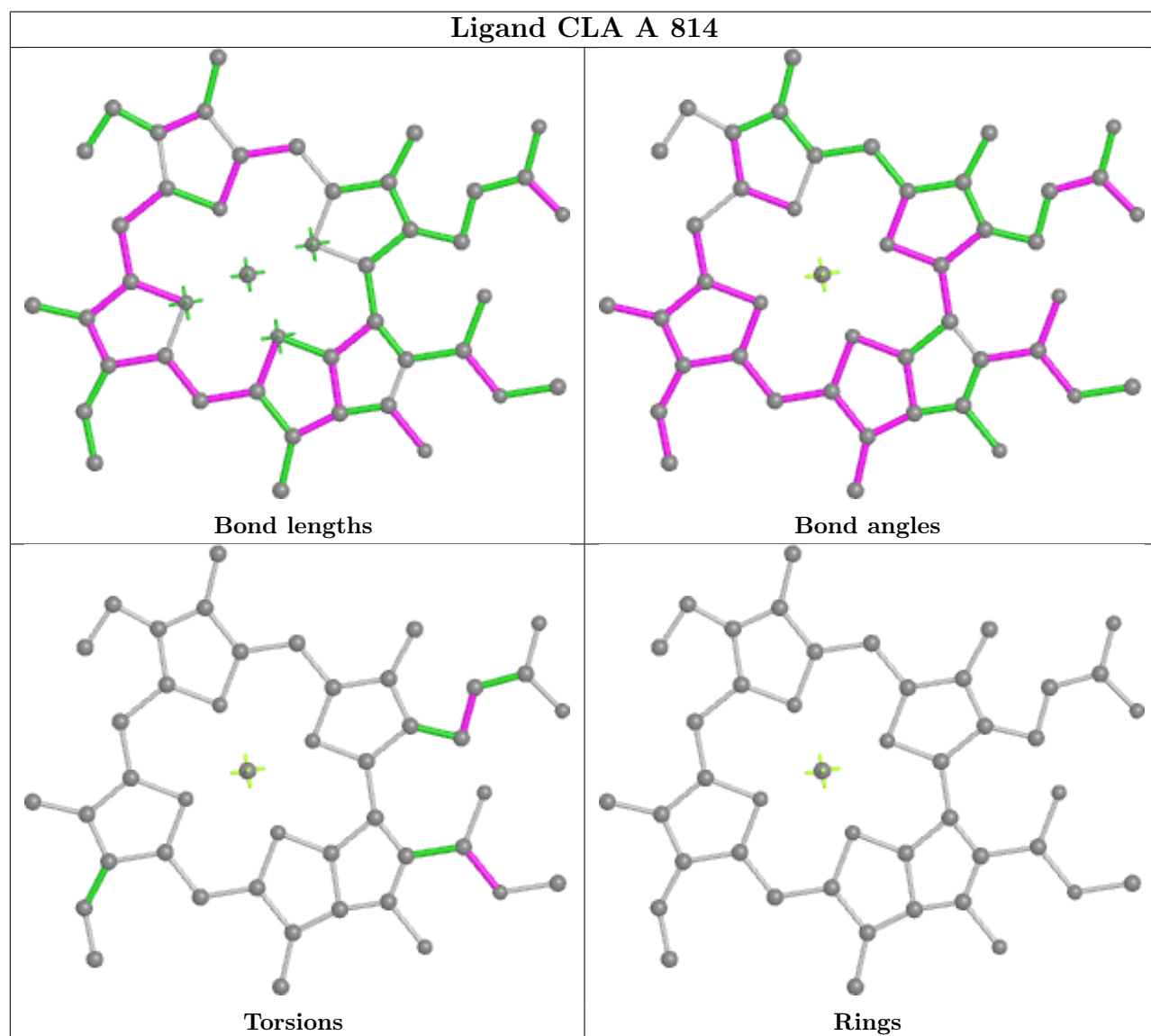
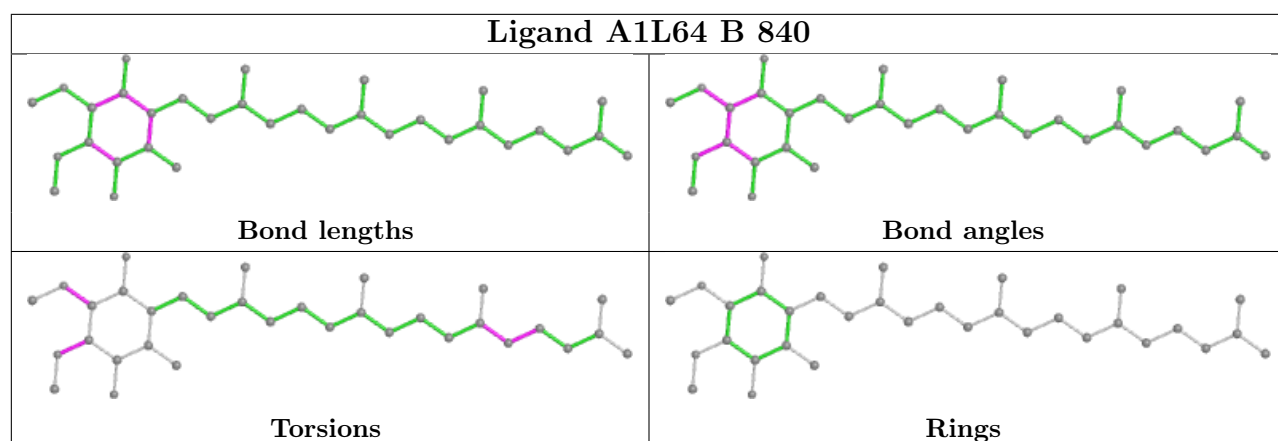


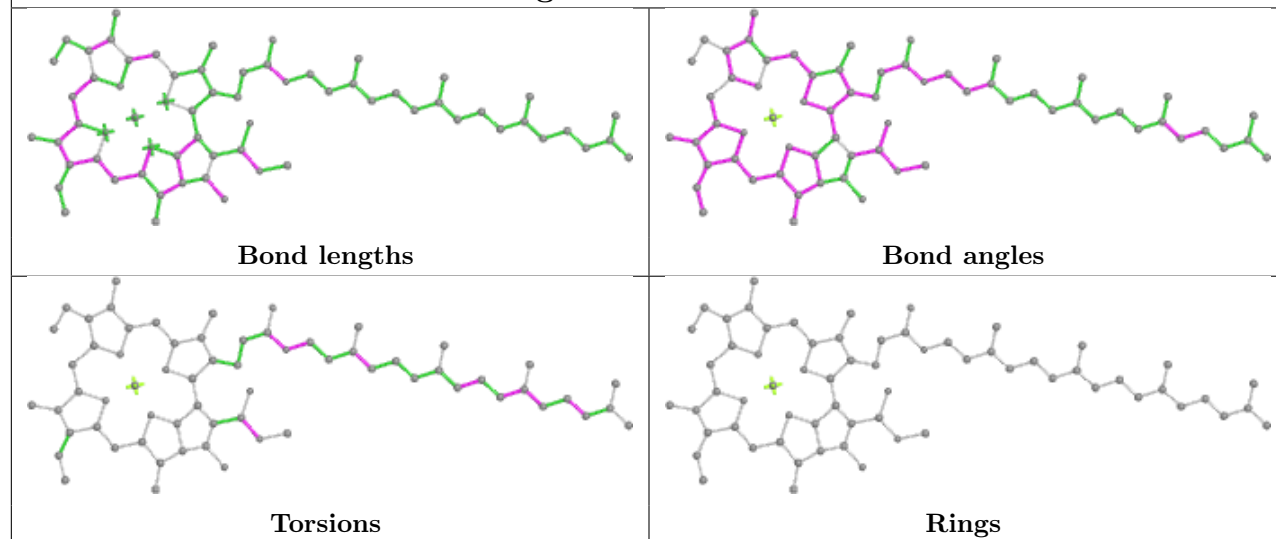
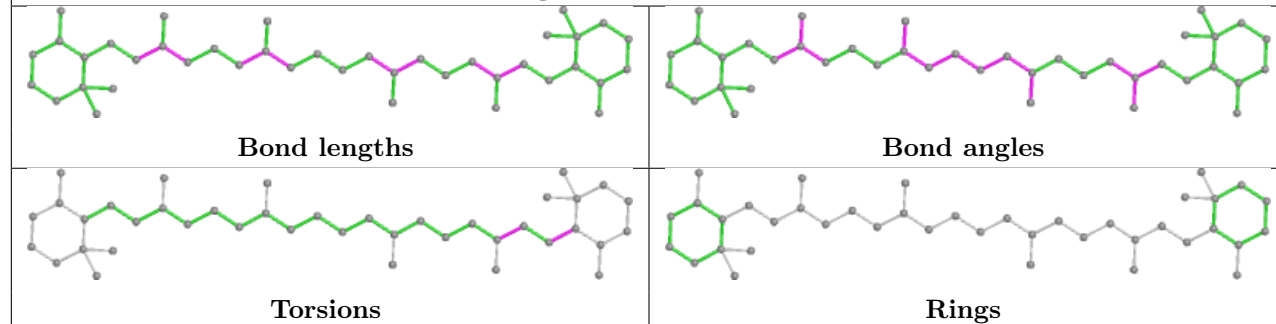
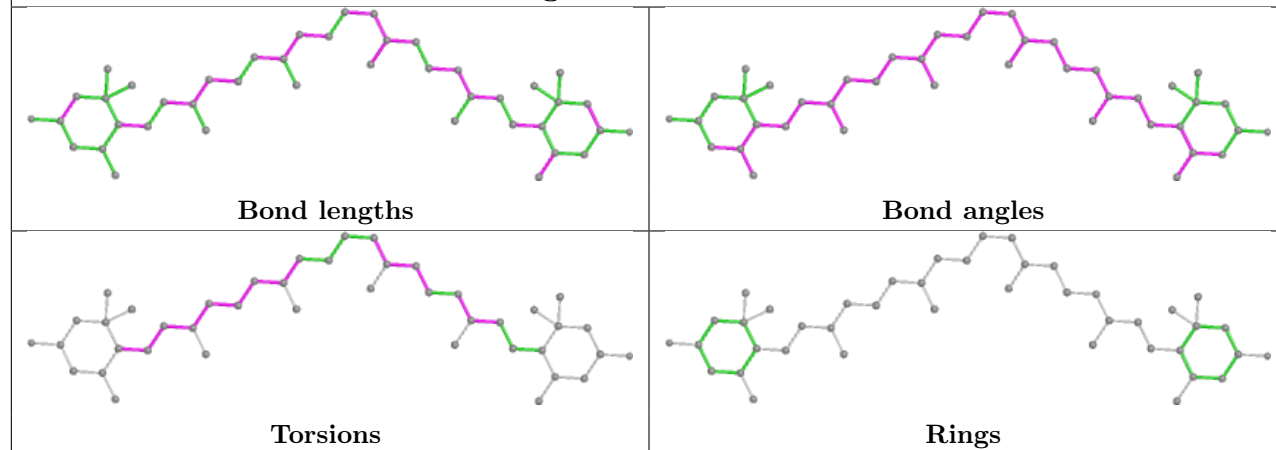
## Ligand BCR I 102



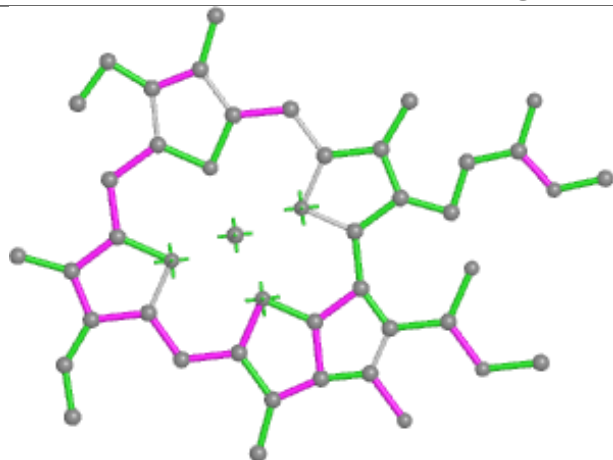




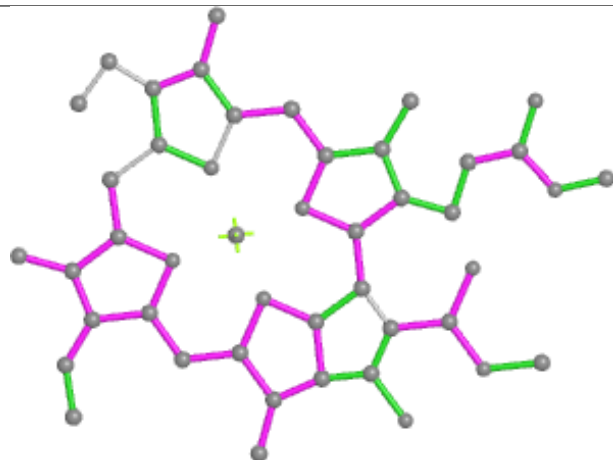


**Ligand CLA 1 303****Ligand BCR 1 301****Ligand 5X6 4 313**

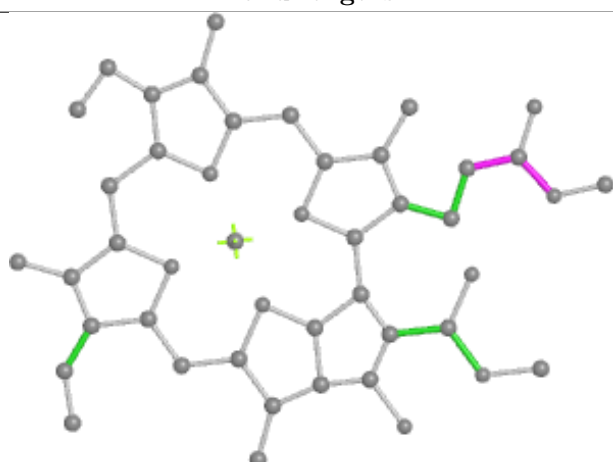
## Ligand CLA B 821



Bond lengths



Bond angles

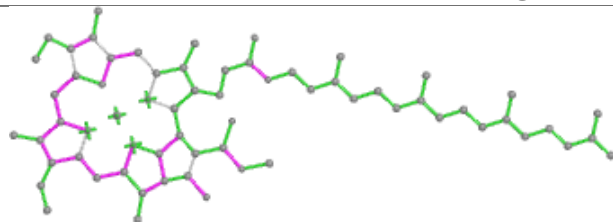


Torsions

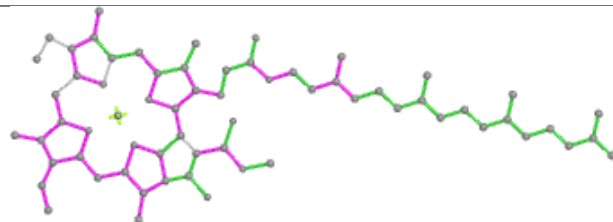


Rings

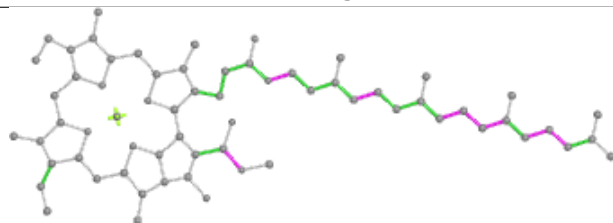
## Ligand CLA A 833



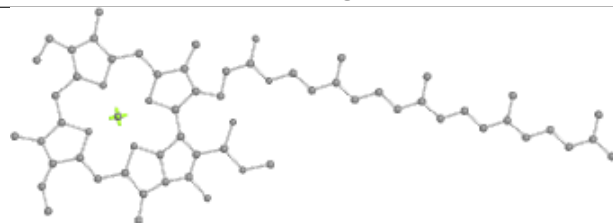
Bond lengths



Bond angles

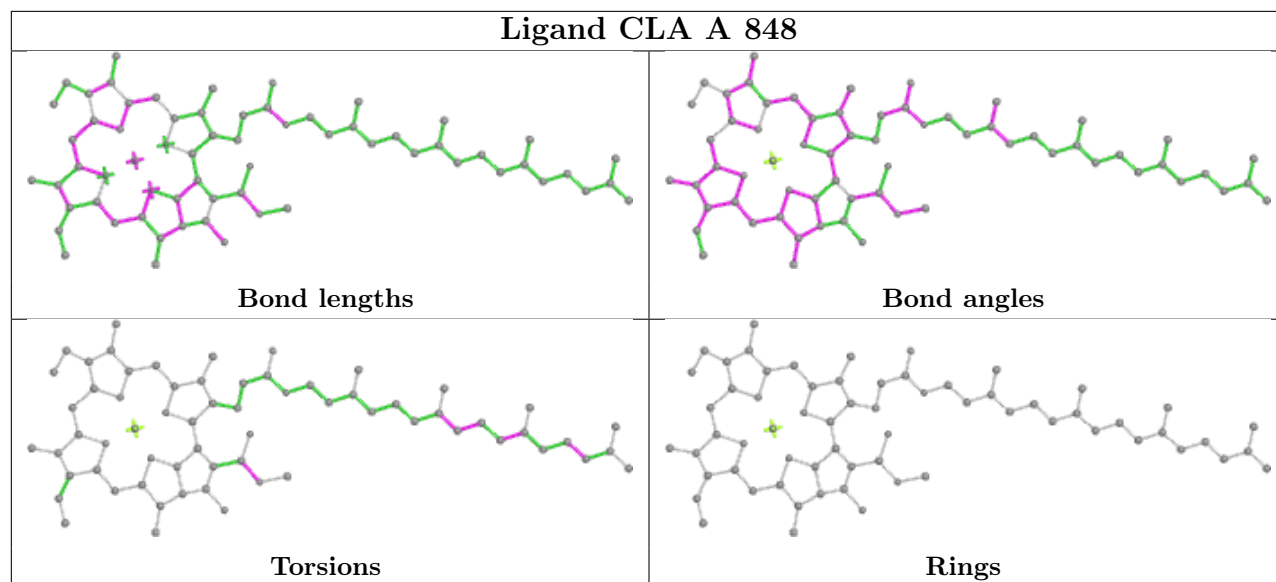


Torsions

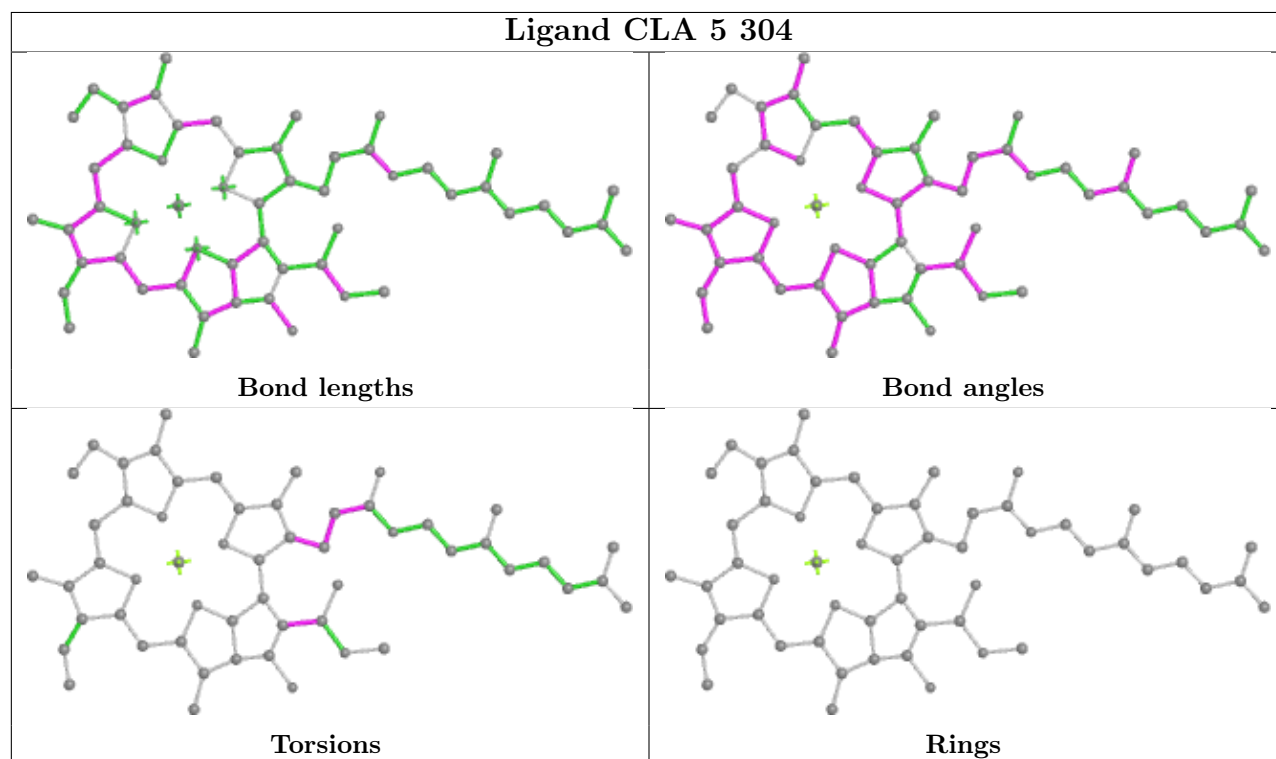


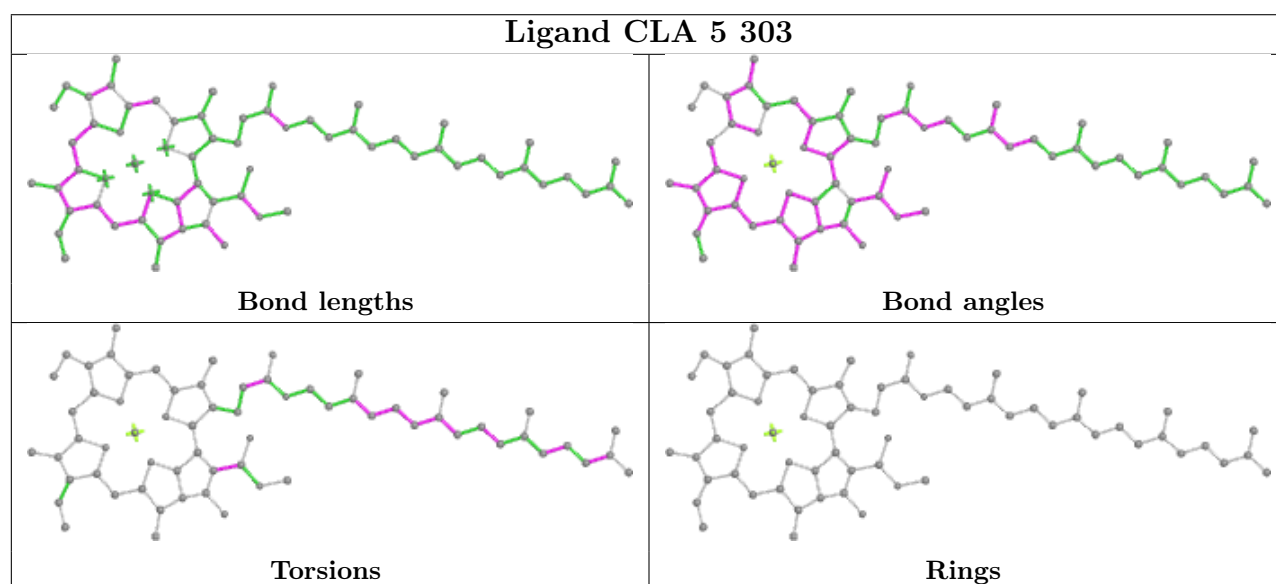
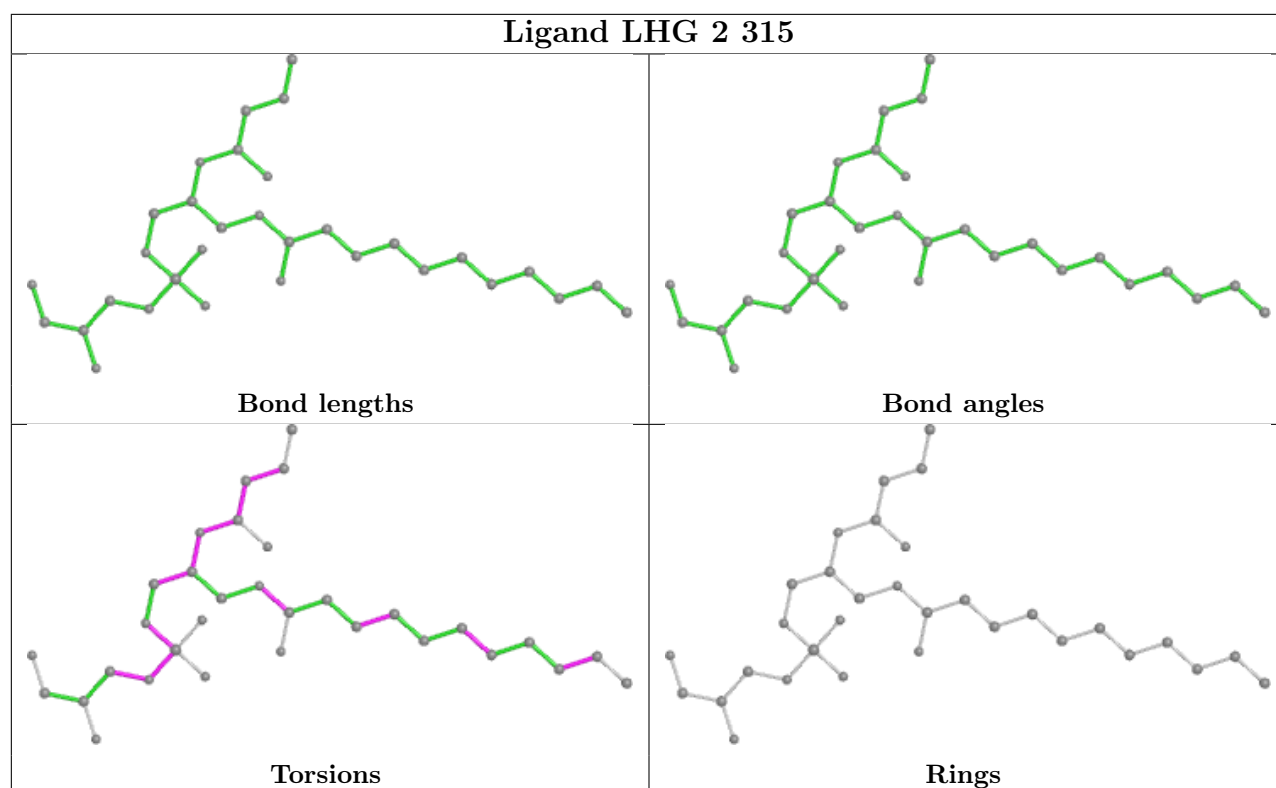
Rings

## Ligand CLA A 848

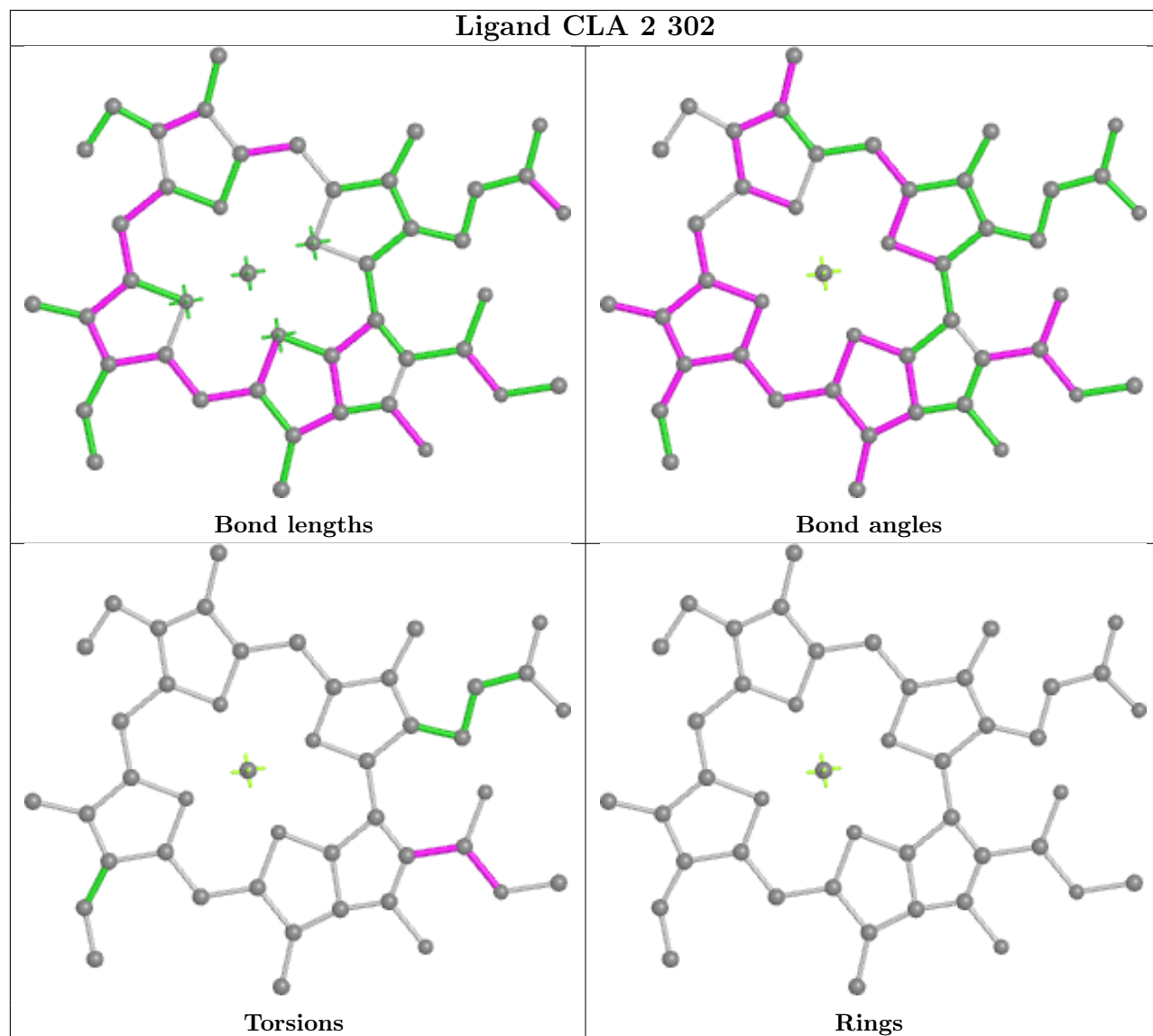


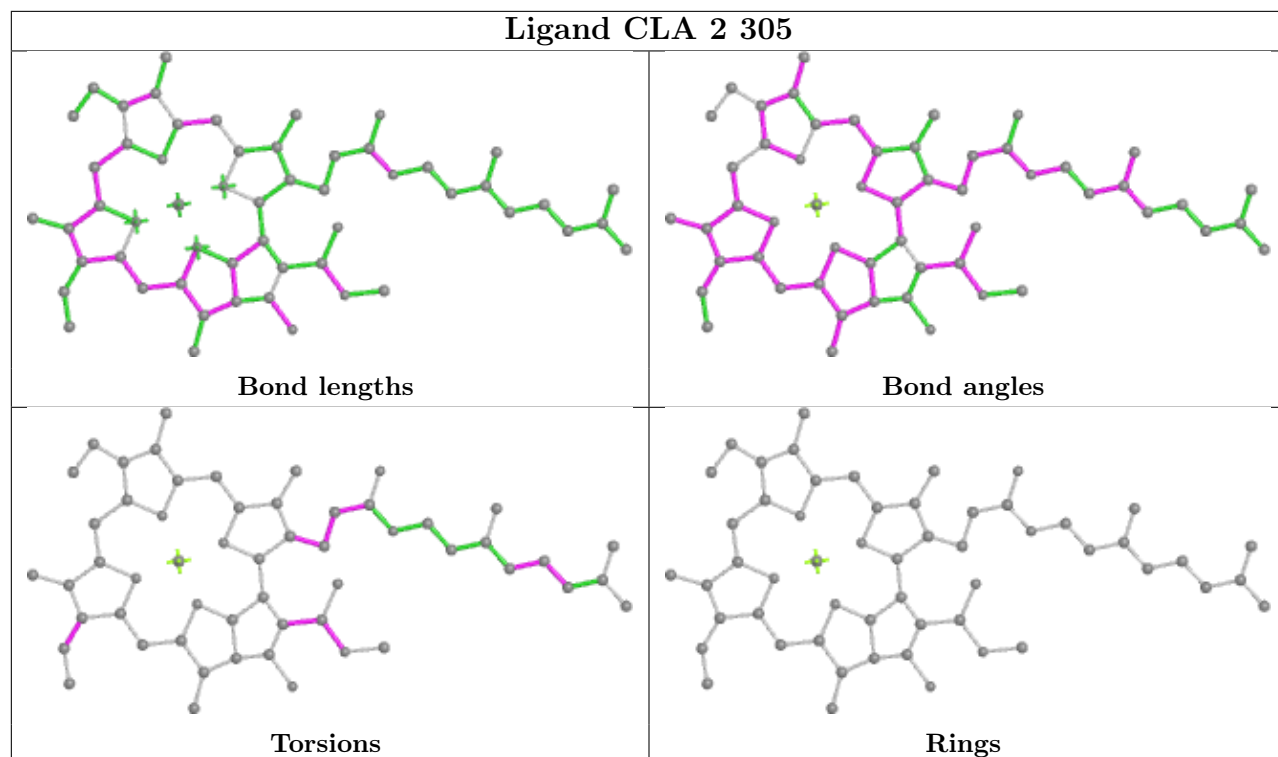
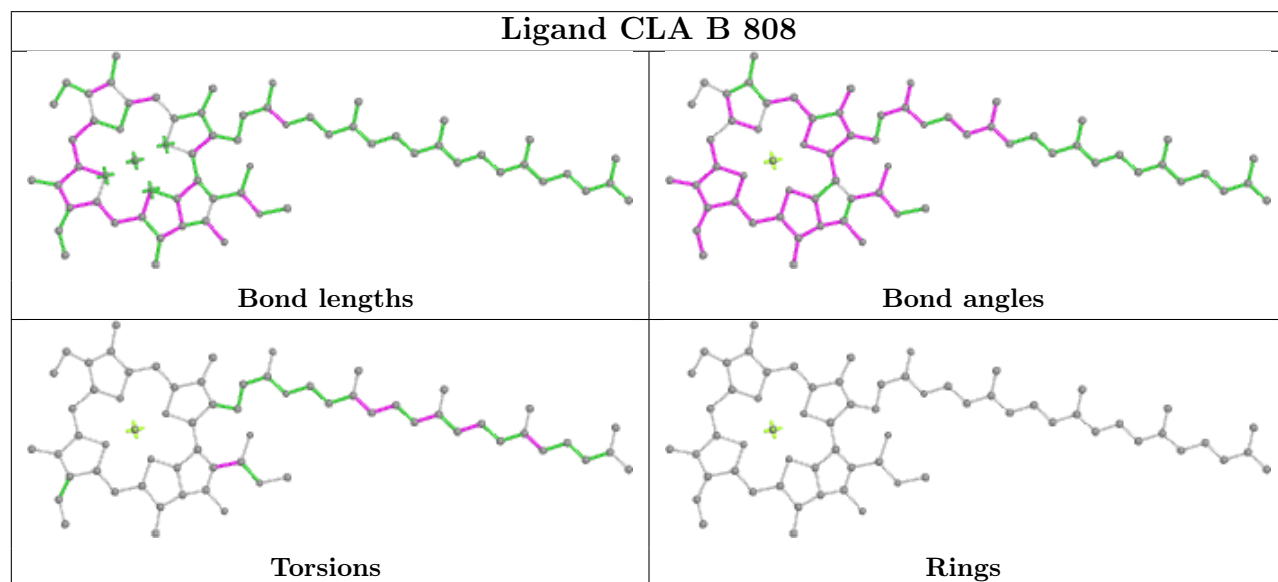
## Ligand CLA 5 304



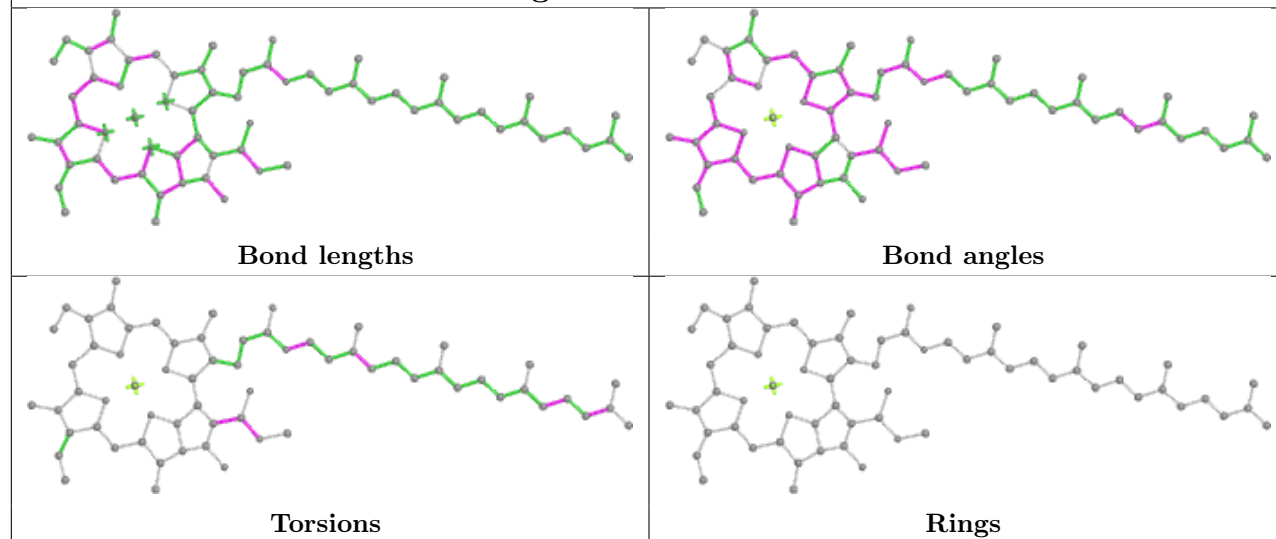
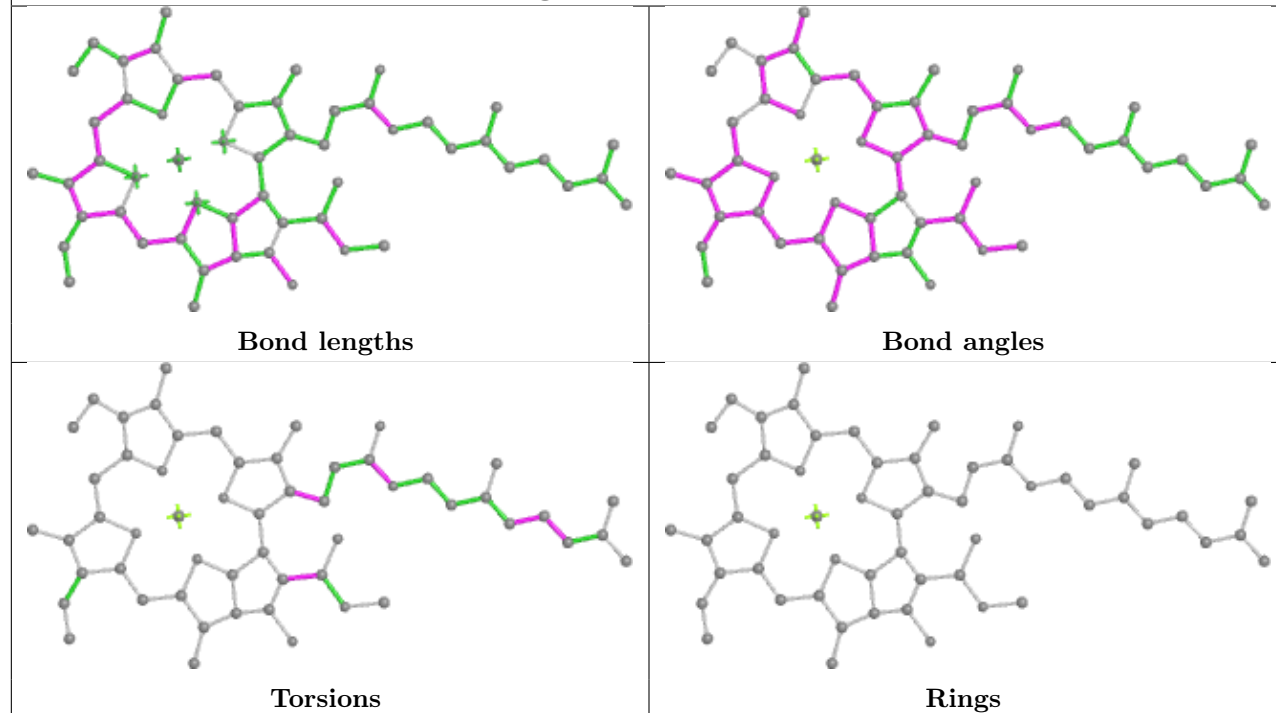
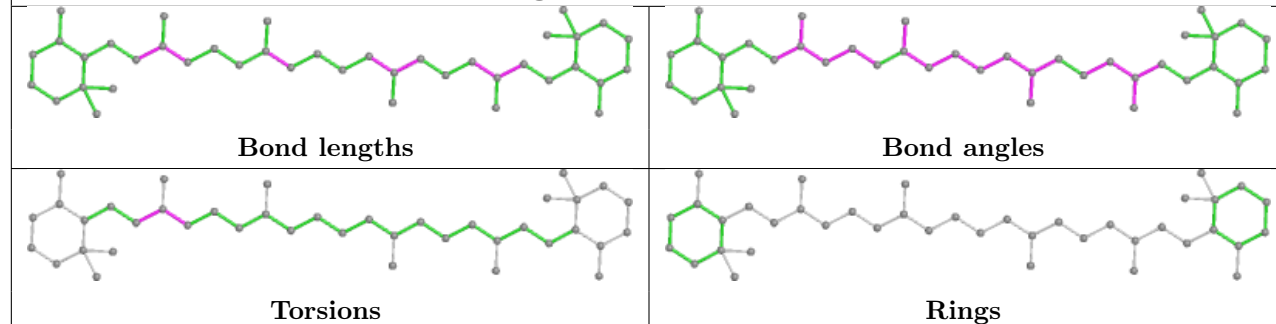


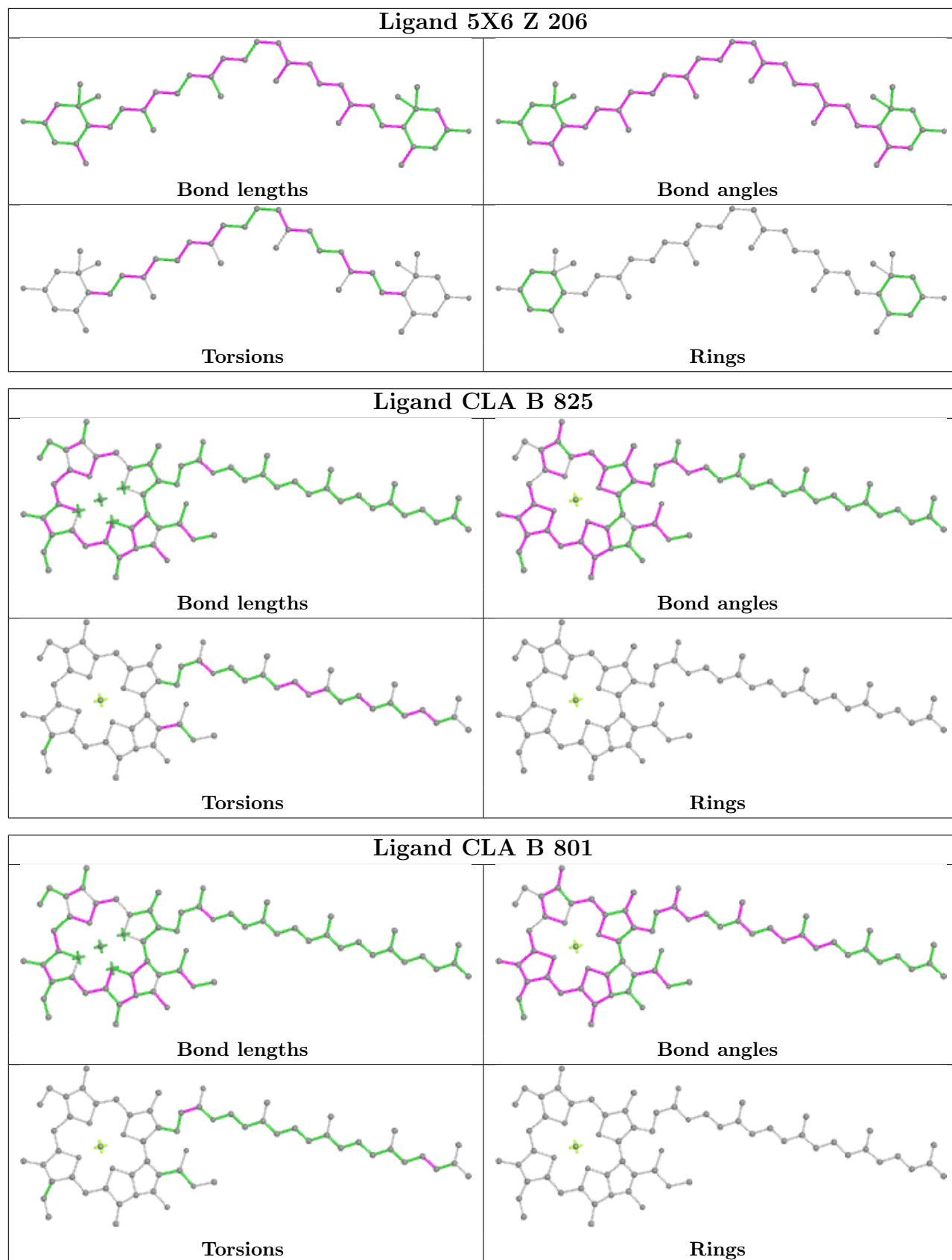
## Ligand CLA 2 302

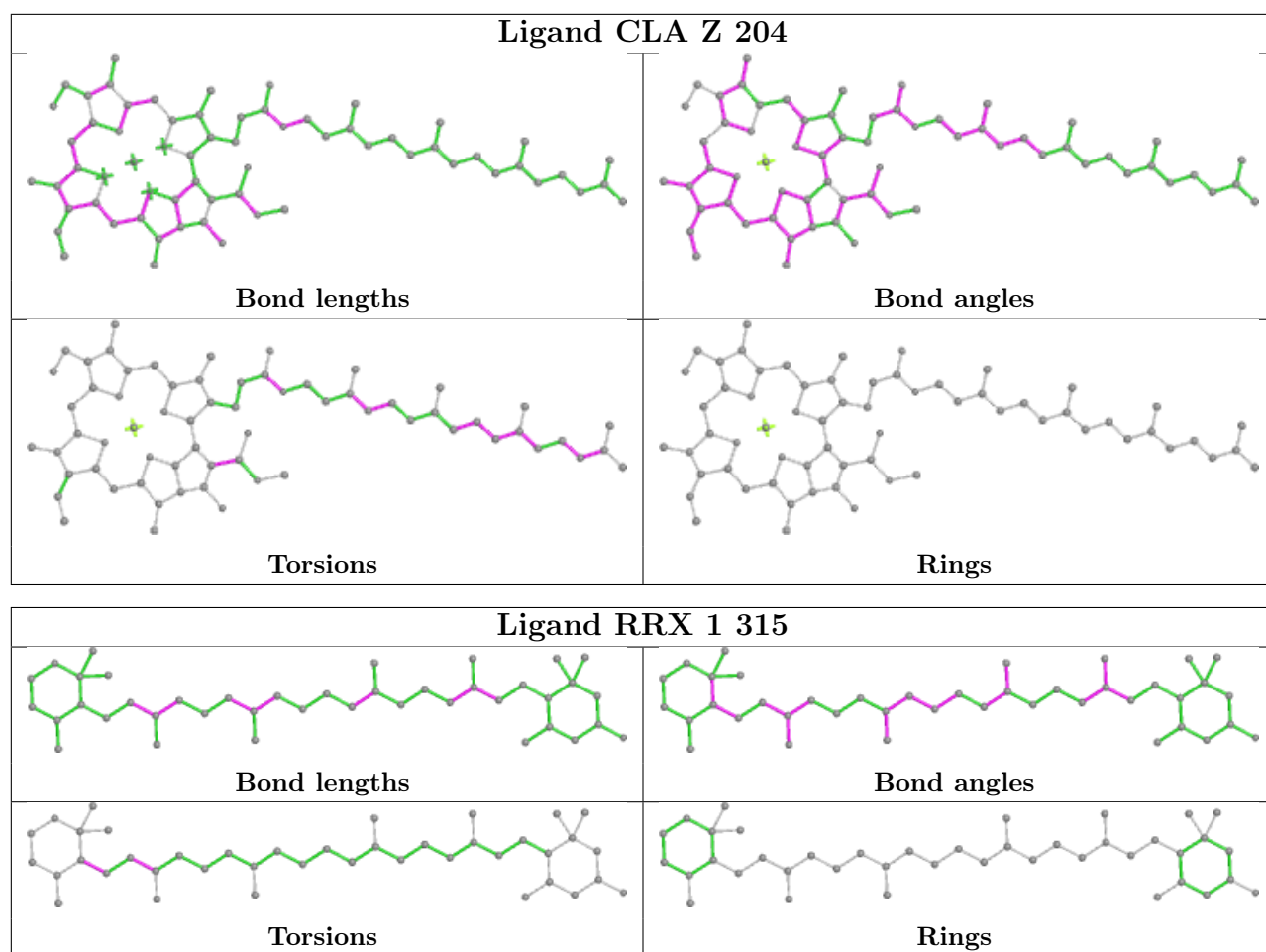


**Ligand CLA 2 305****Ligand CLA B 808**

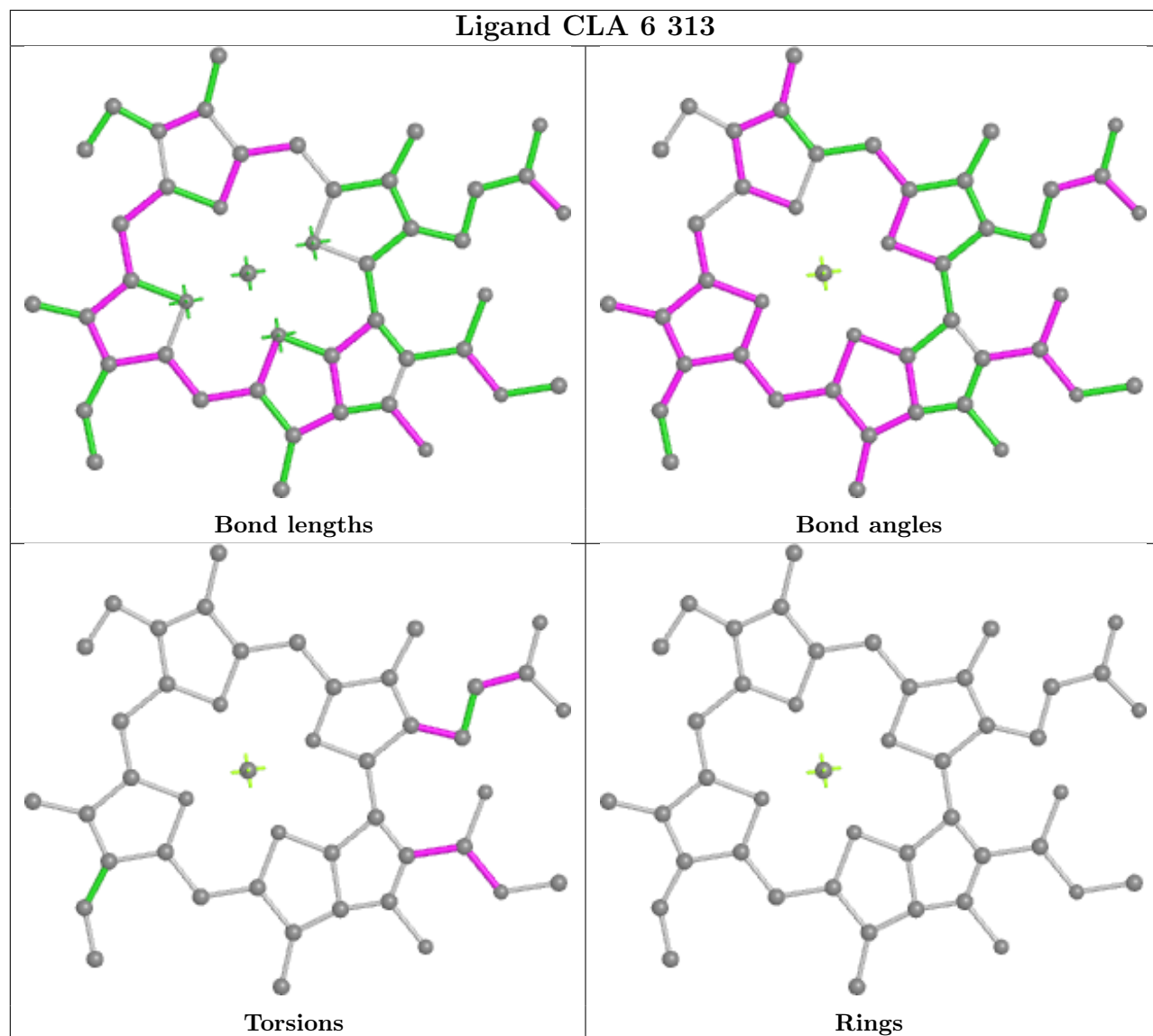


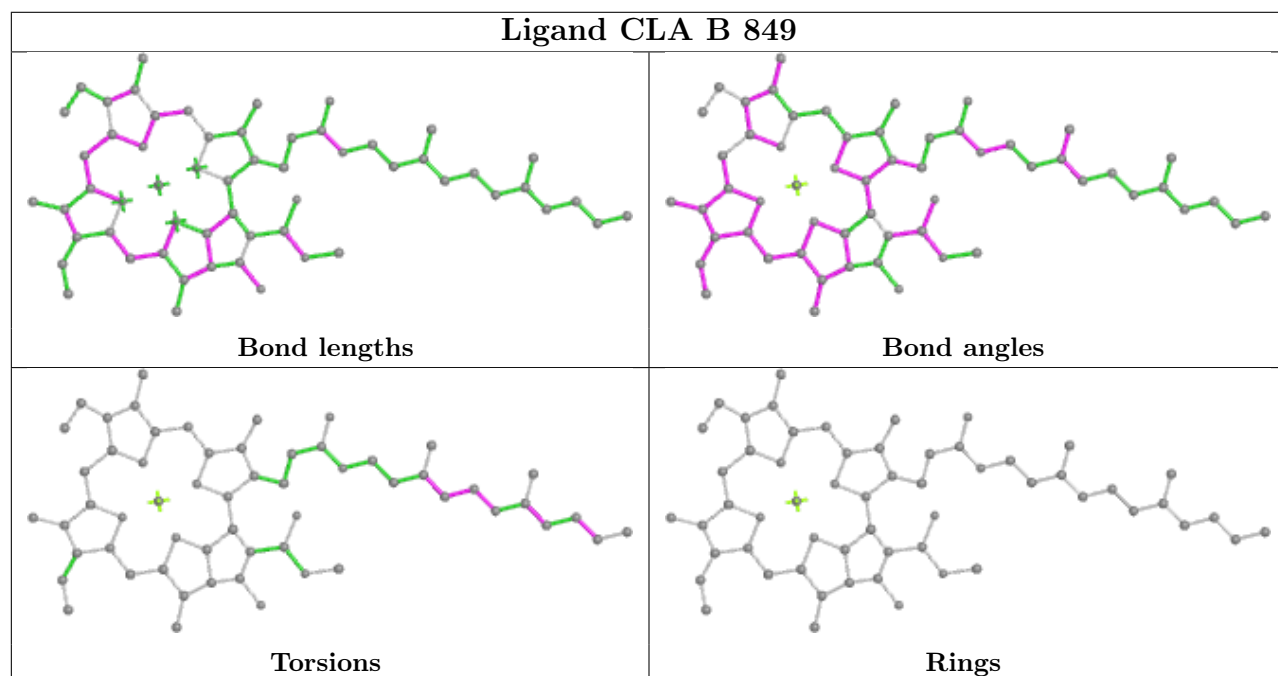
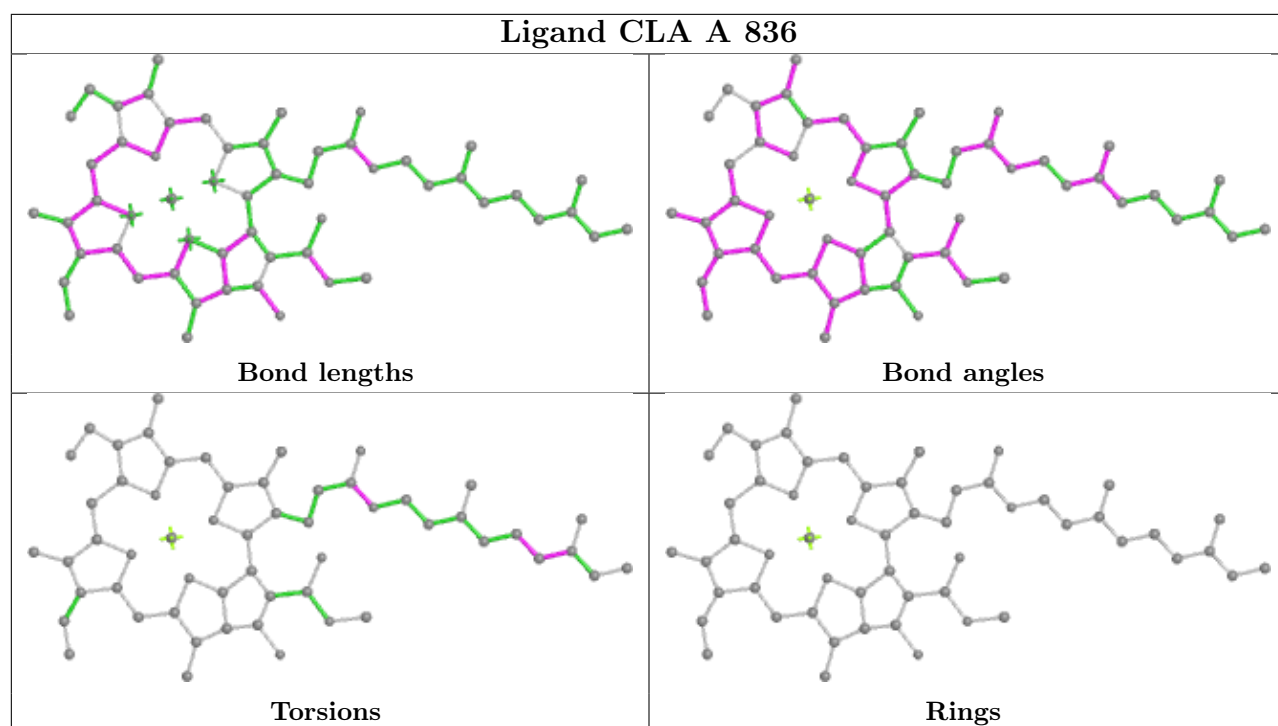
**Ligand CLA A 832****Ligand CLA 7 309****Ligand BCR B 844**



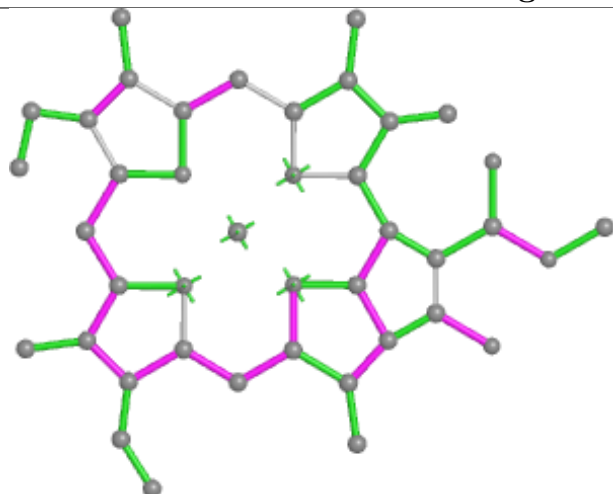


## Ligand CLA 6 313

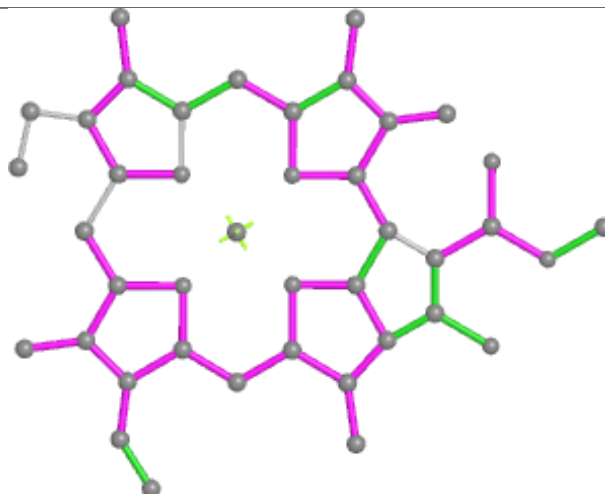




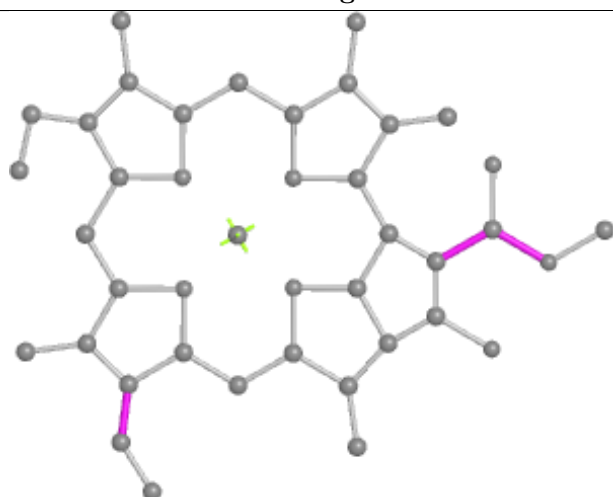
## Ligand CLA 7 310



Bond lengths



Bond angles

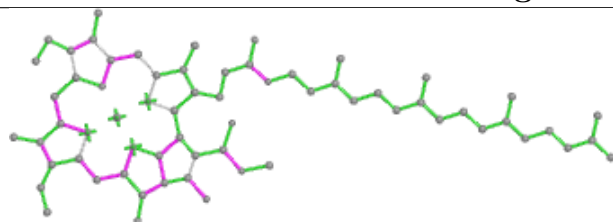


Torsions

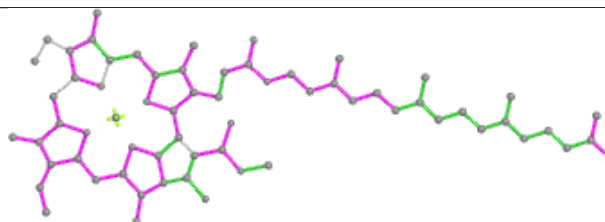


Rings

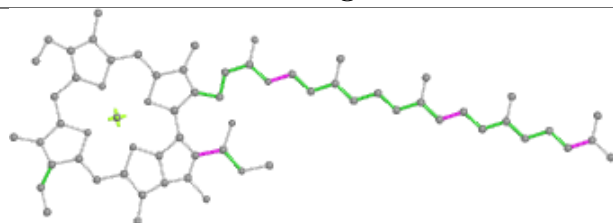
## Ligand CLA B 803



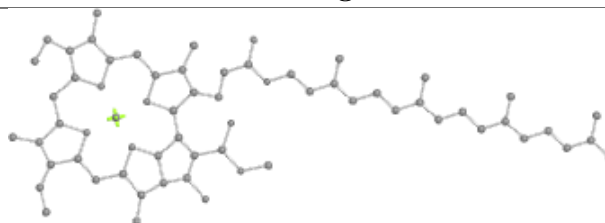
Bond lengths



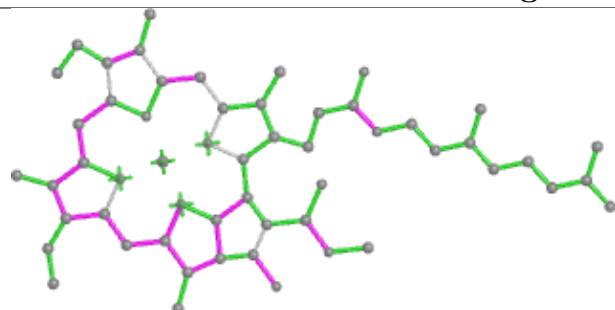
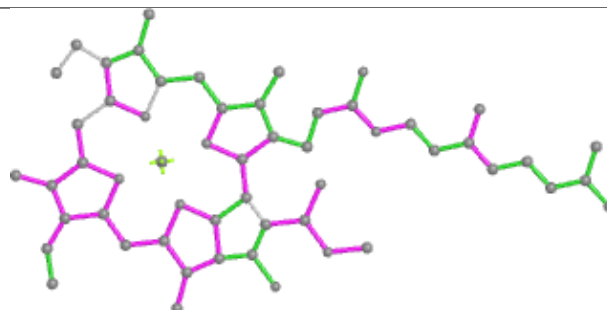
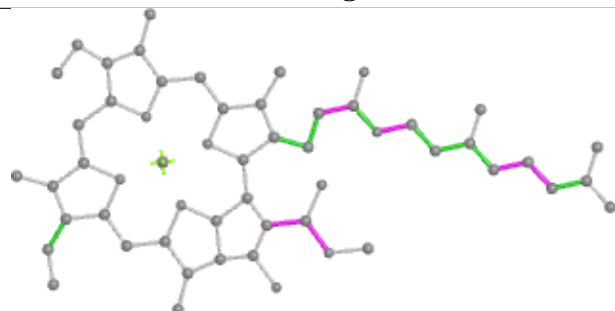
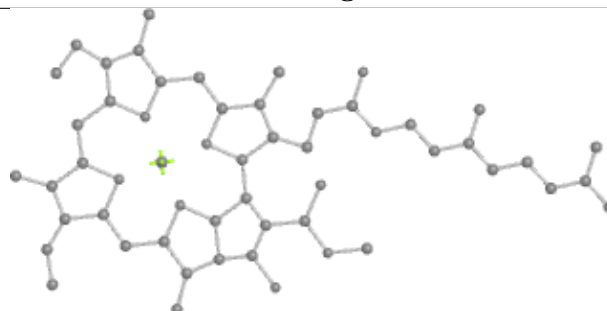
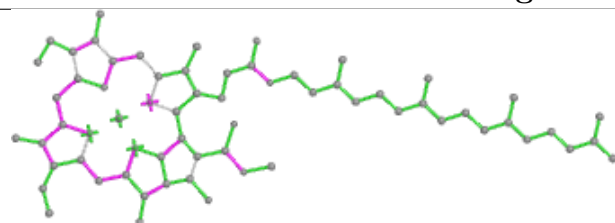
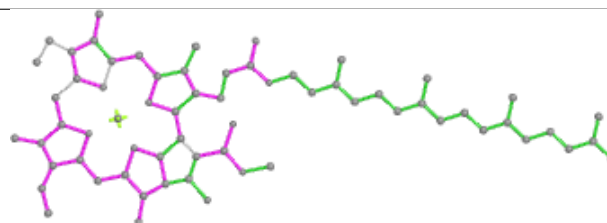
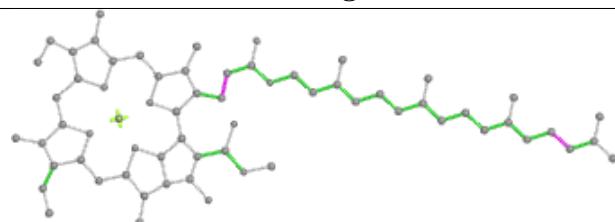
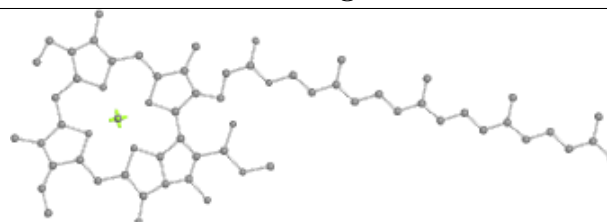
Bond angles

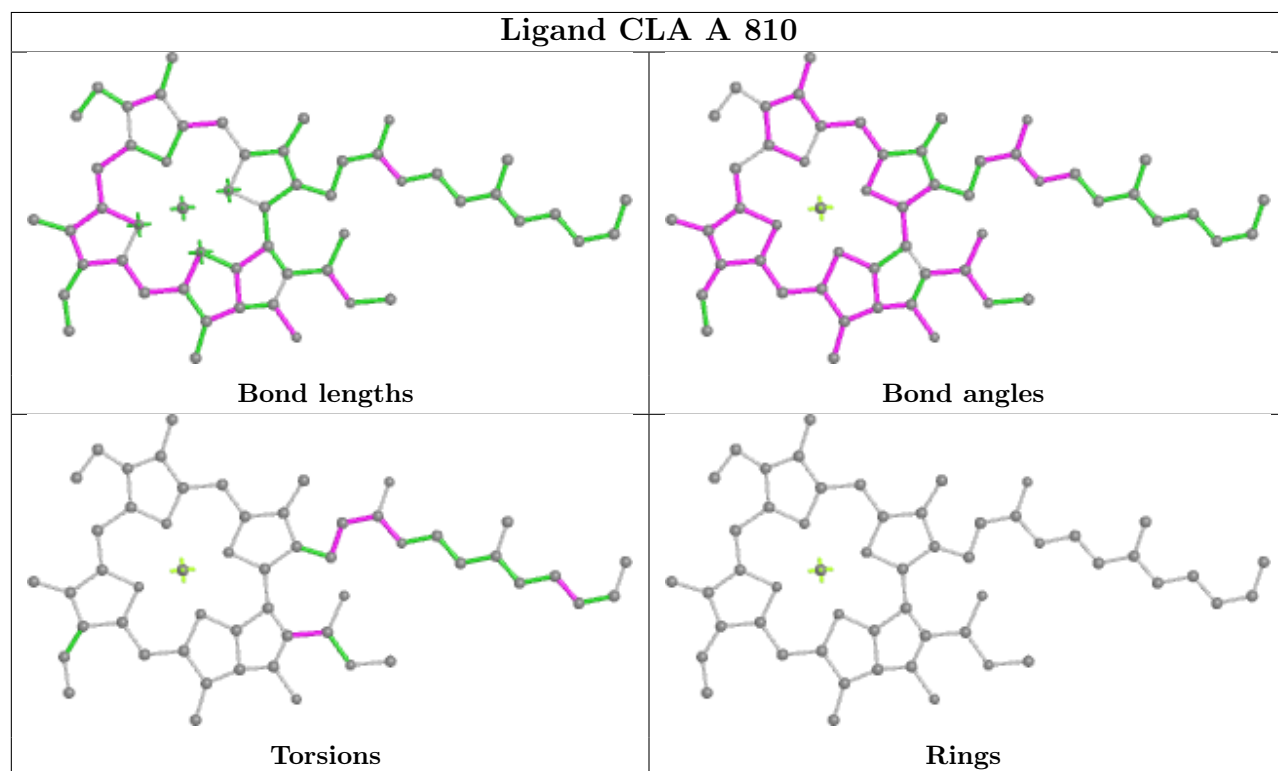
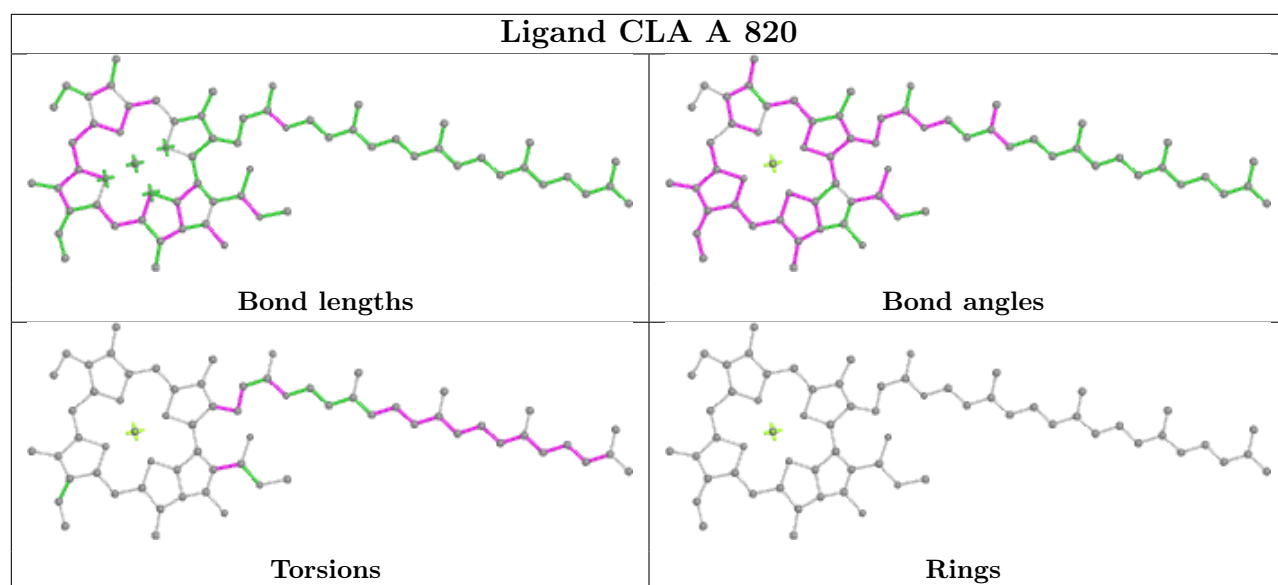


Torsions



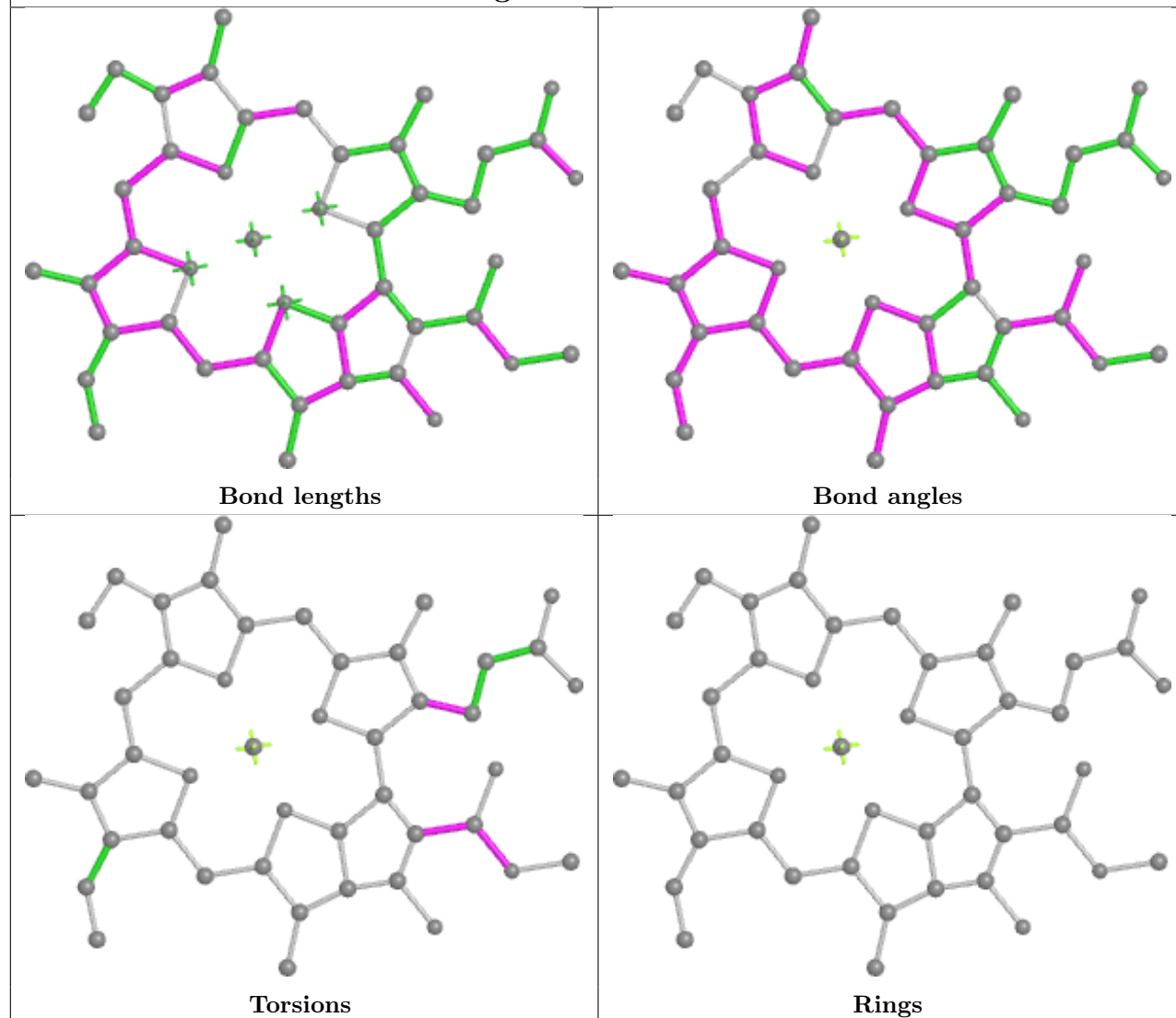
Rings

**Ligand CLA 2 308****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 857****Bond lengths****Bond angles****Torsions****Rings**

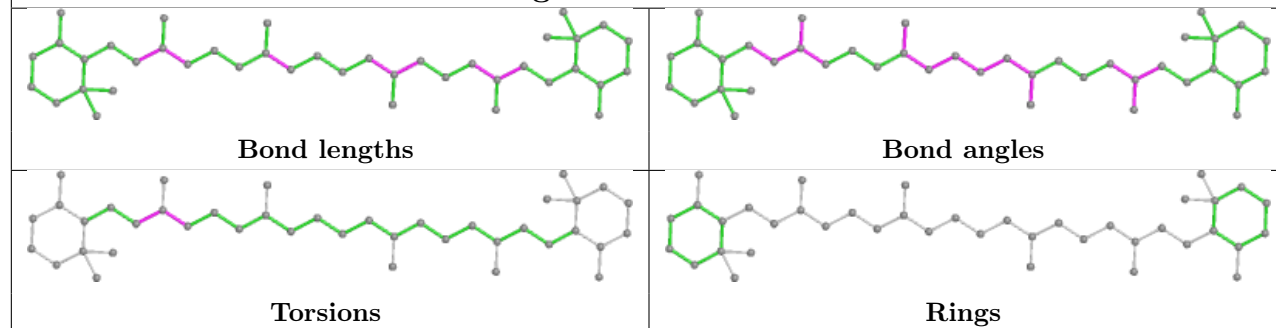


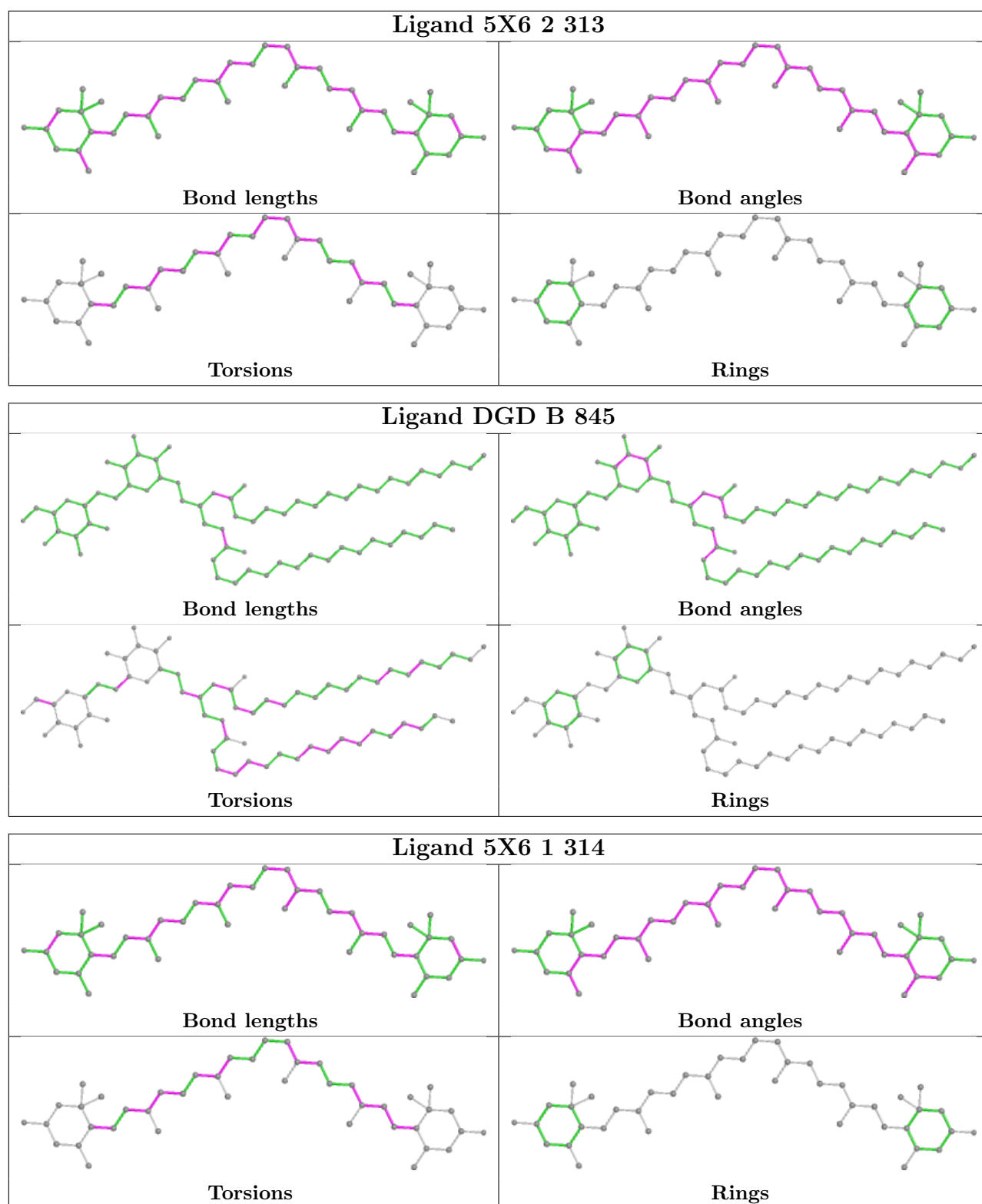


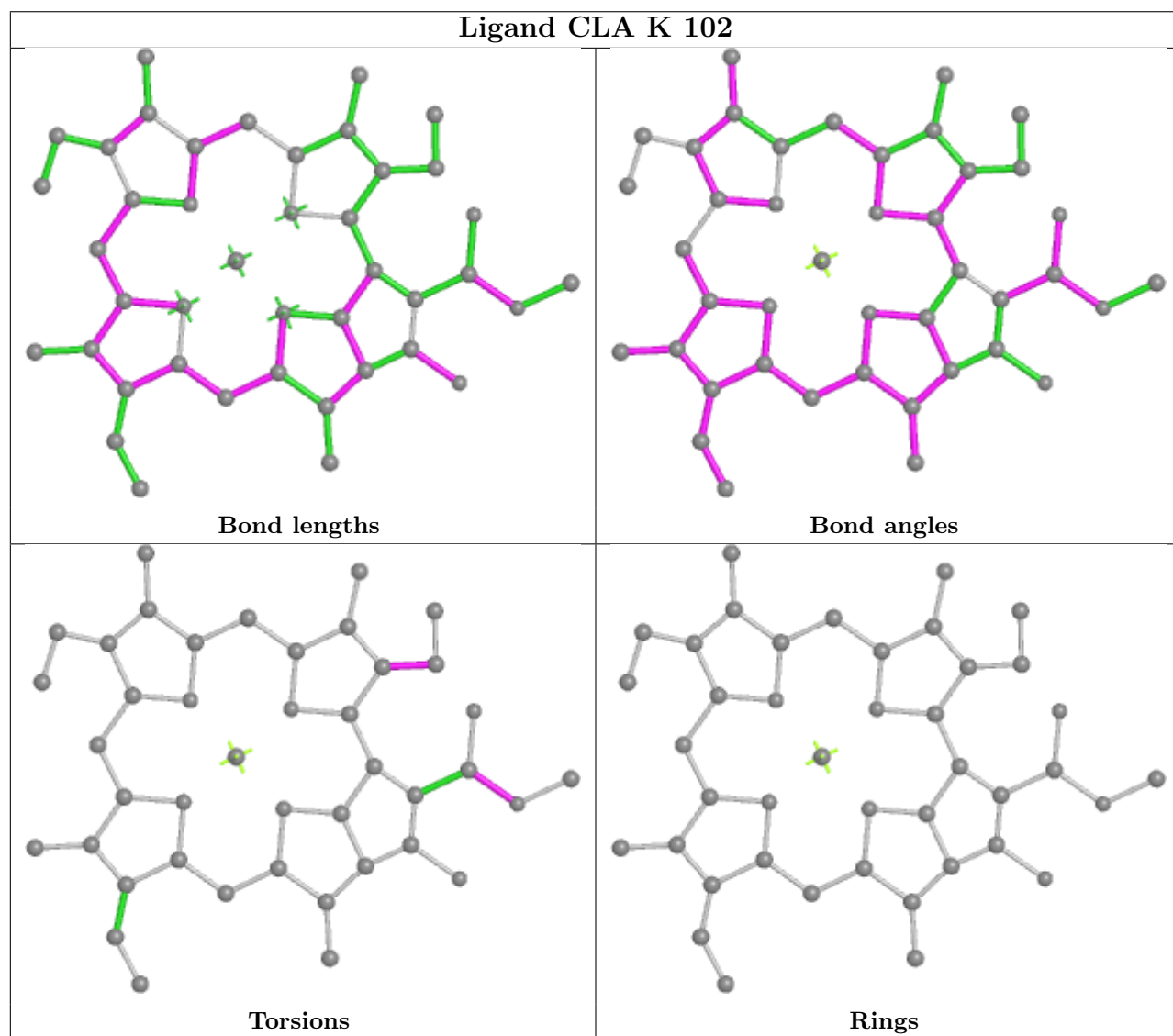
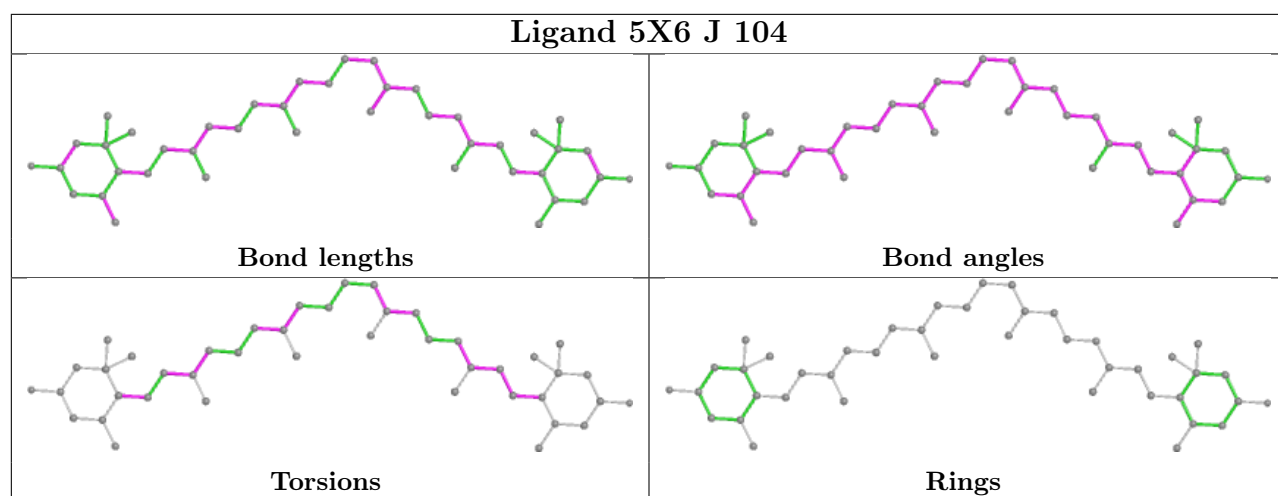
## Ligand CLA 5 311

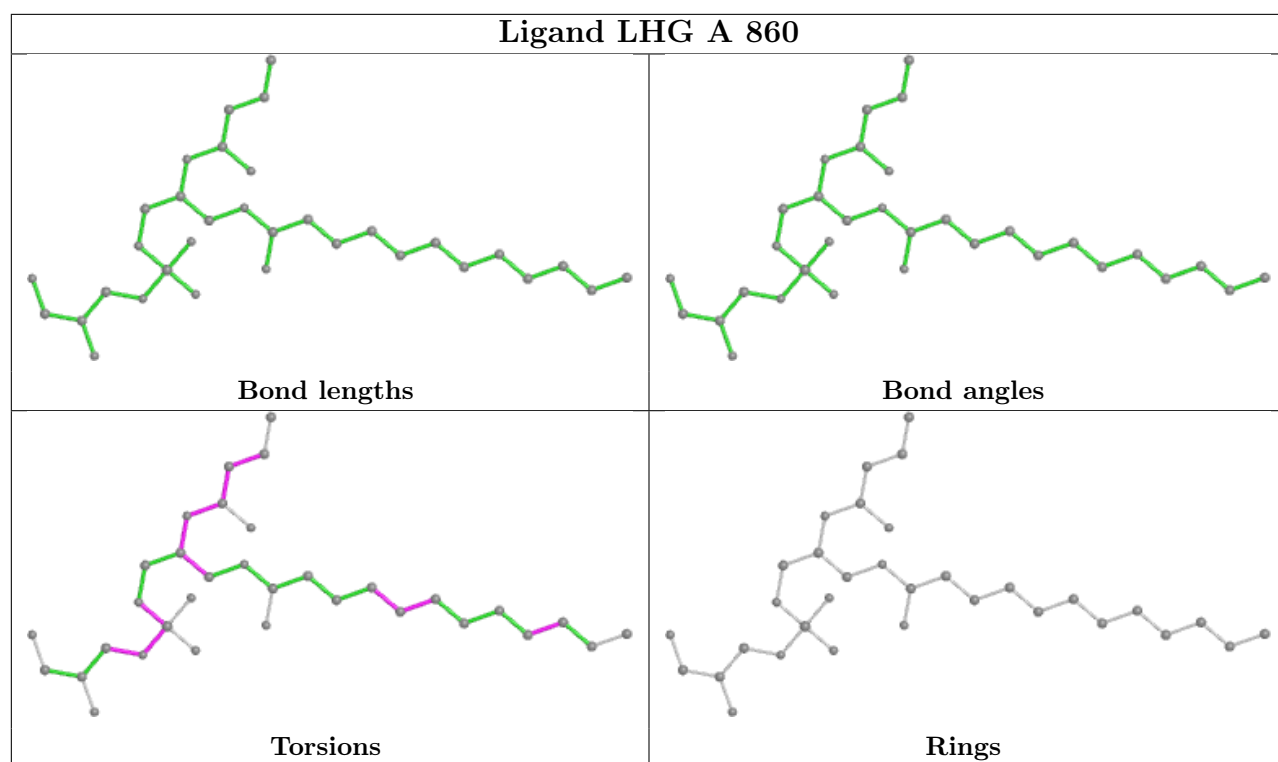


## Ligand BCR L 202

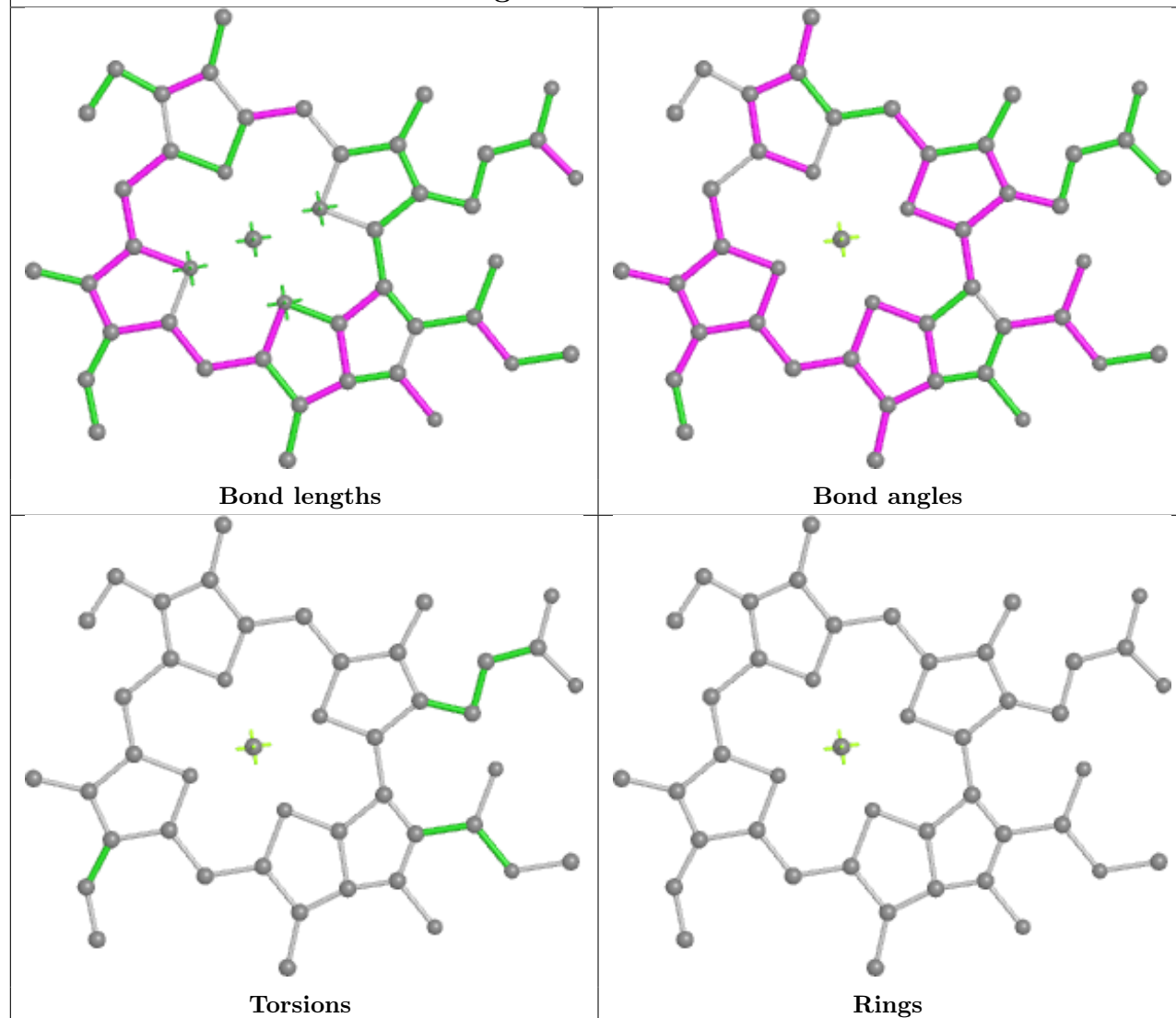




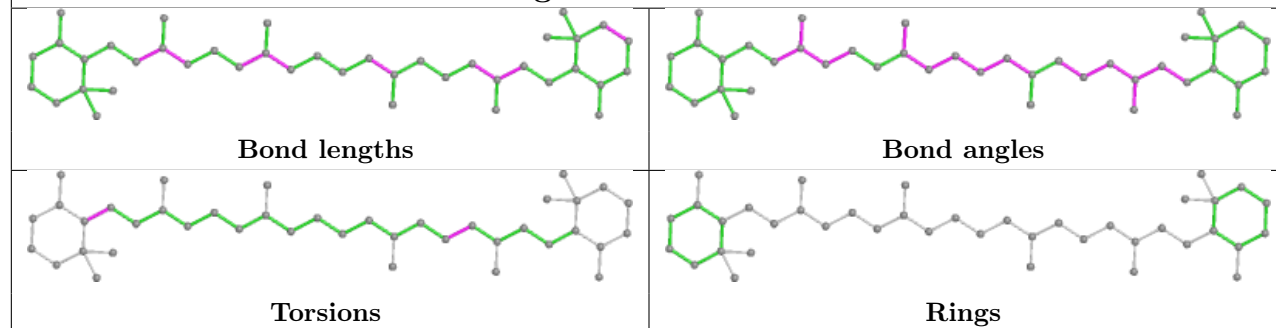




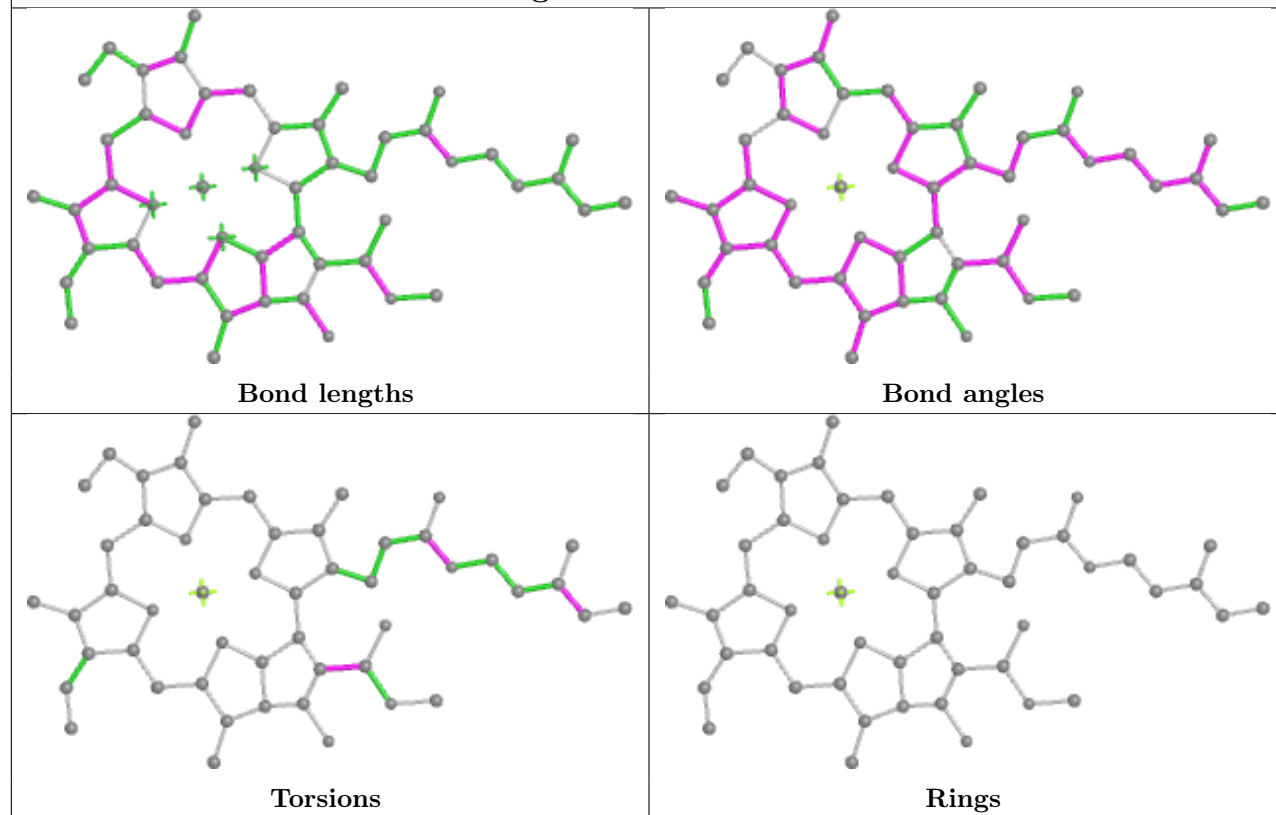
## Ligand CLA 4 311



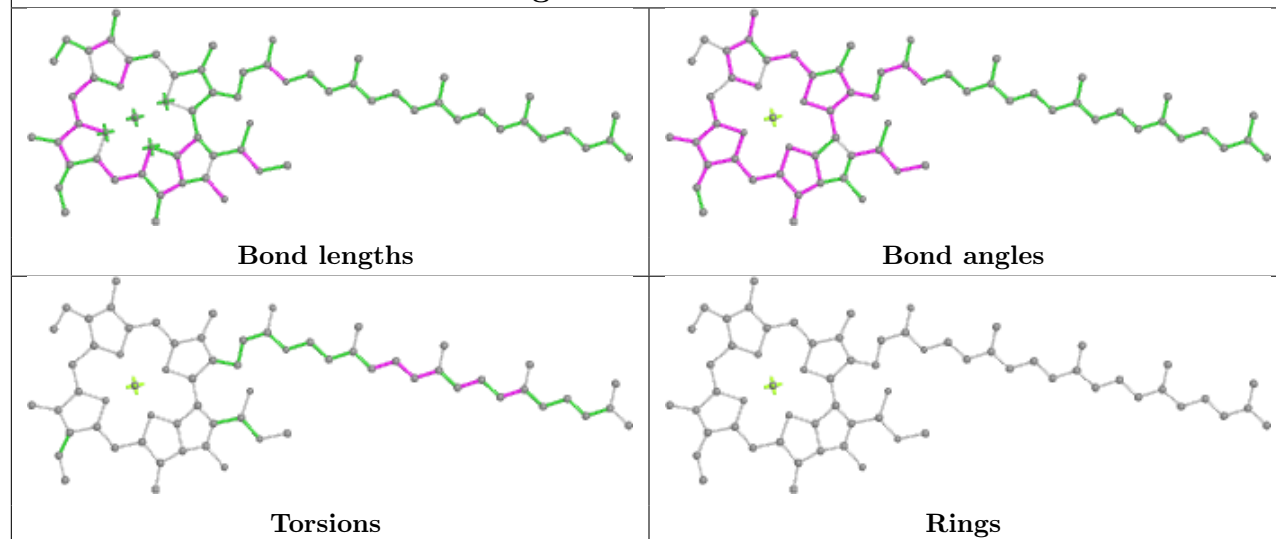
## Ligand BCR J 103



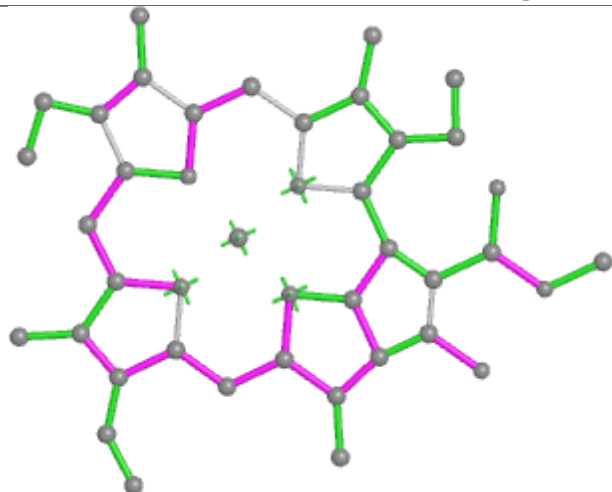
## Ligand CLA A 835



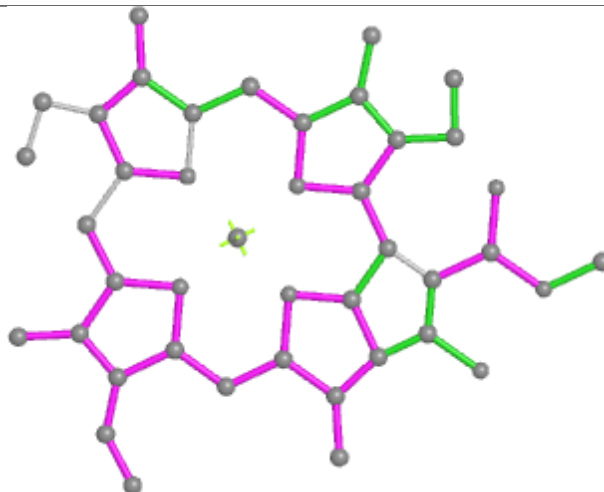
## Ligand CLA B 819



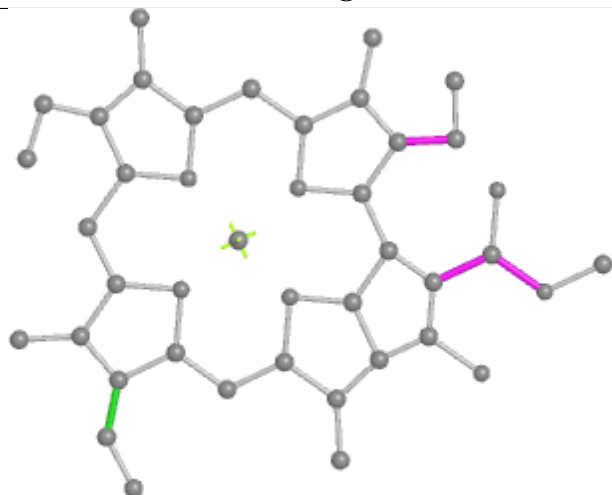
## Ligand CLA 6 312



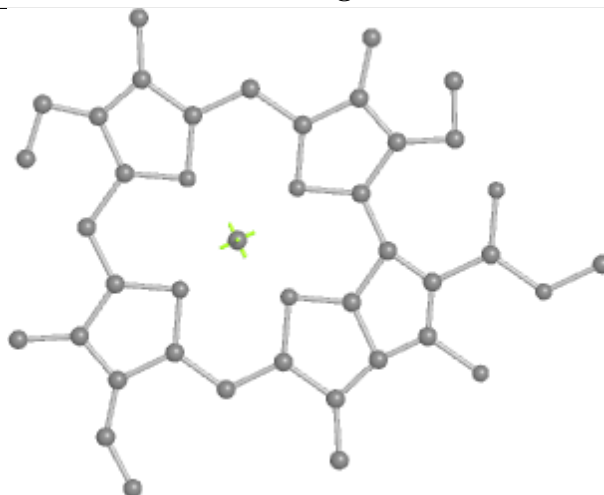
Bond lengths



Bond angles

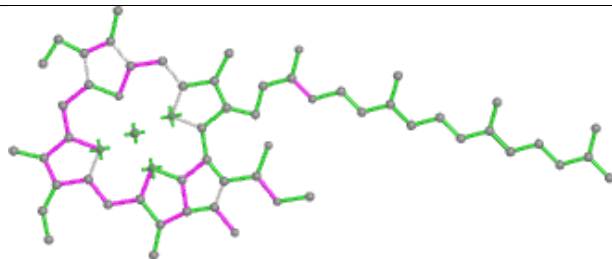


Torsions

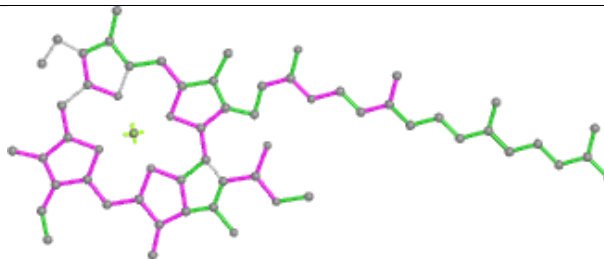


Rings

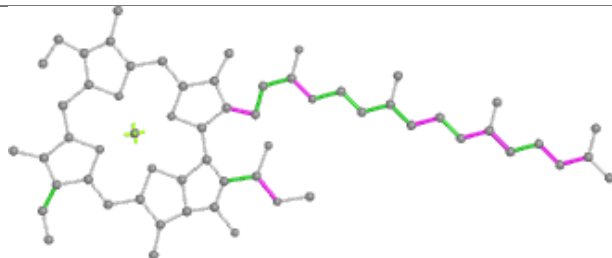
## Ligand CLA A 834



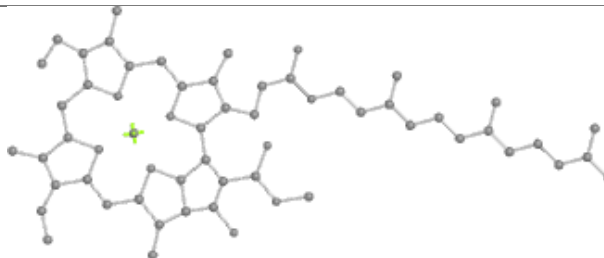
Bond lengths



Bond angles

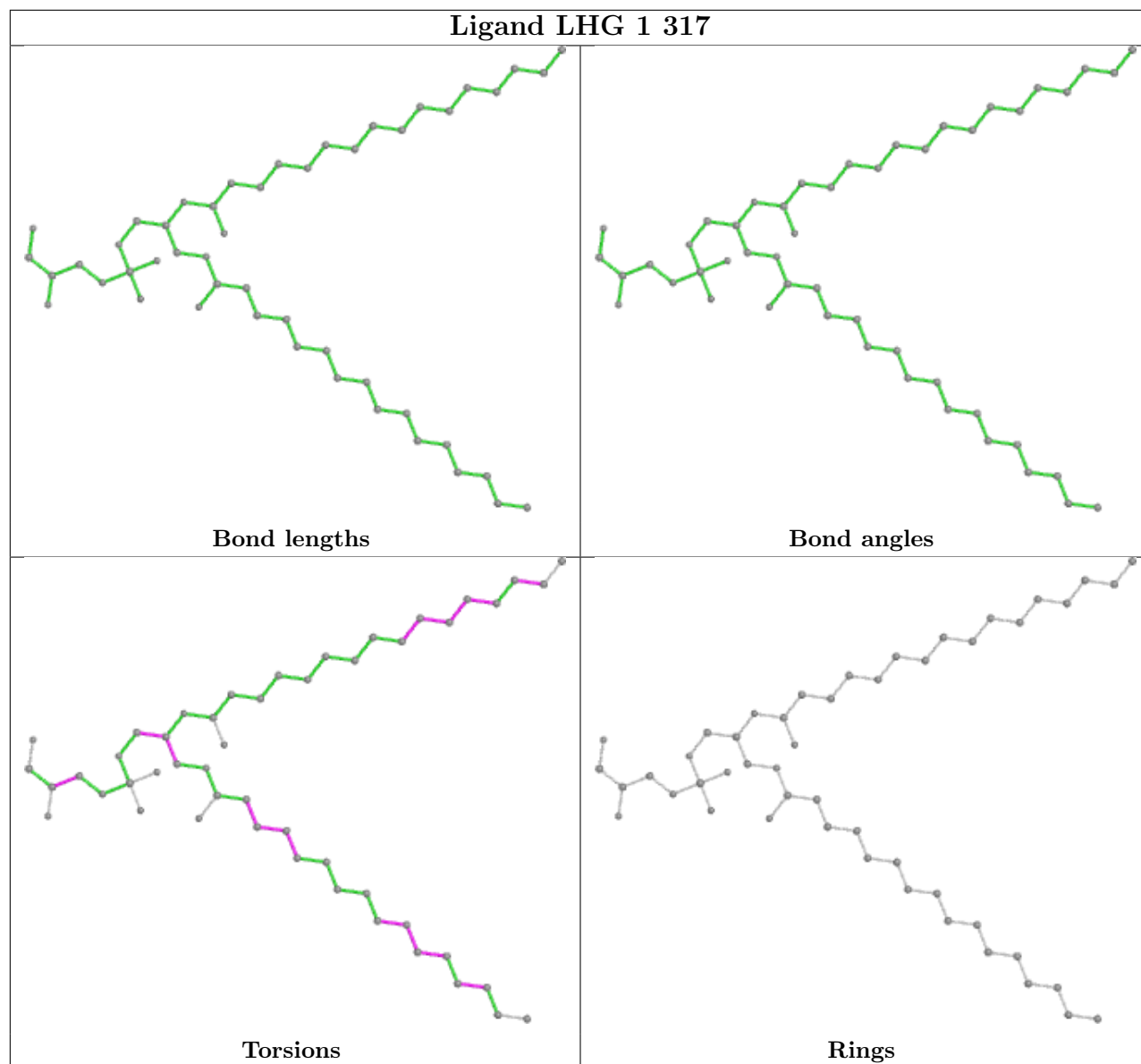


Torsions

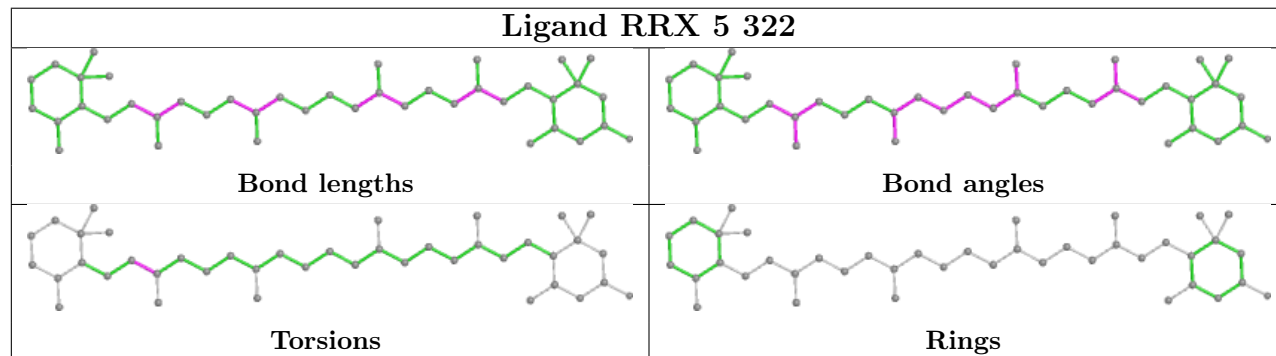


Rings

## Ligand LHG 1 317

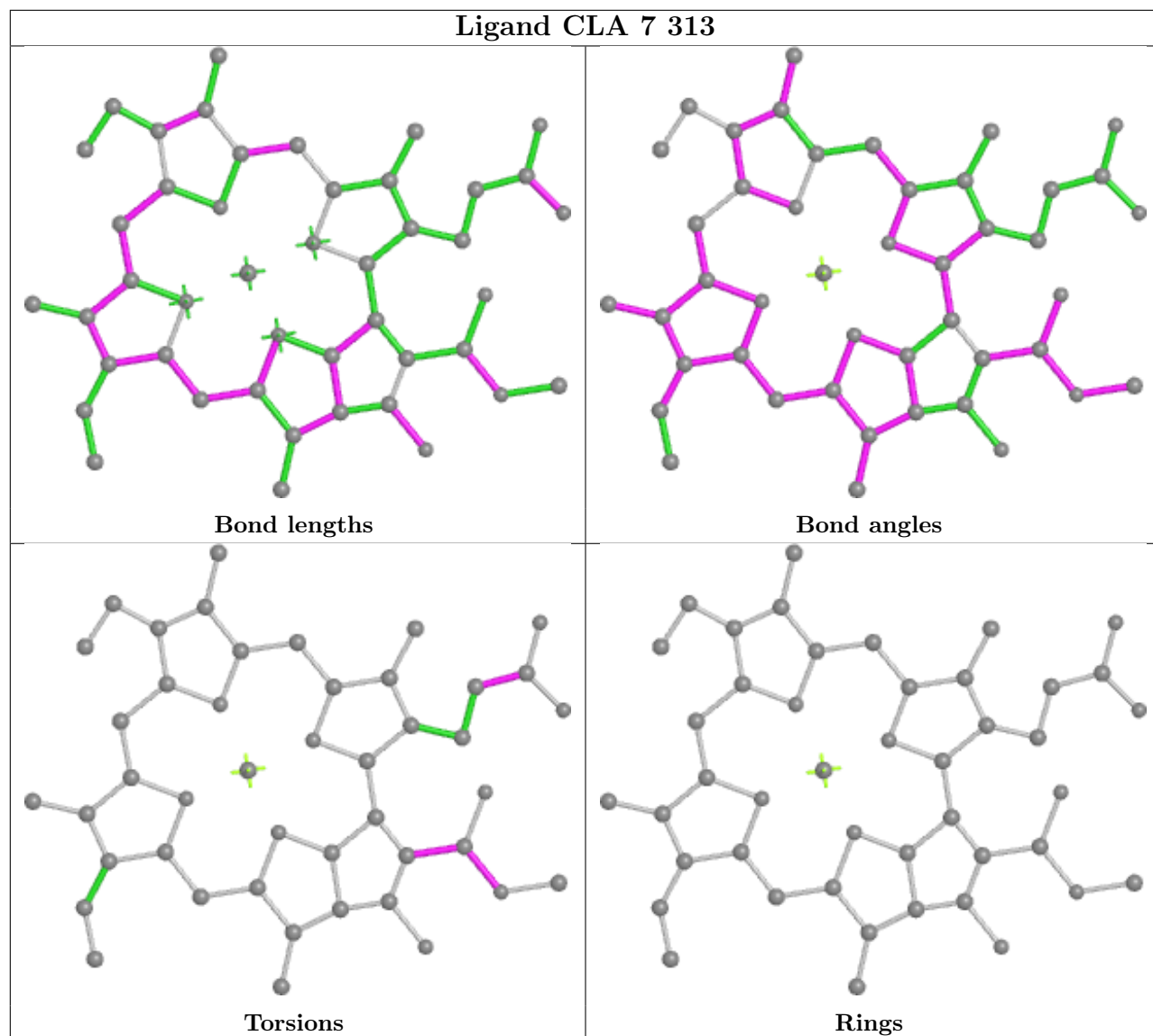


## Ligand RRX 5 322

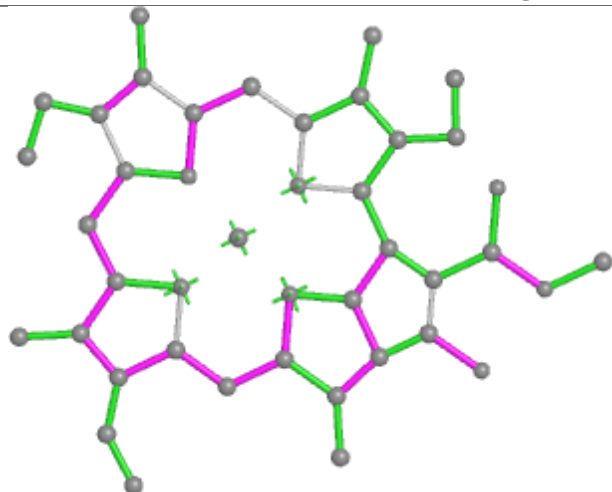




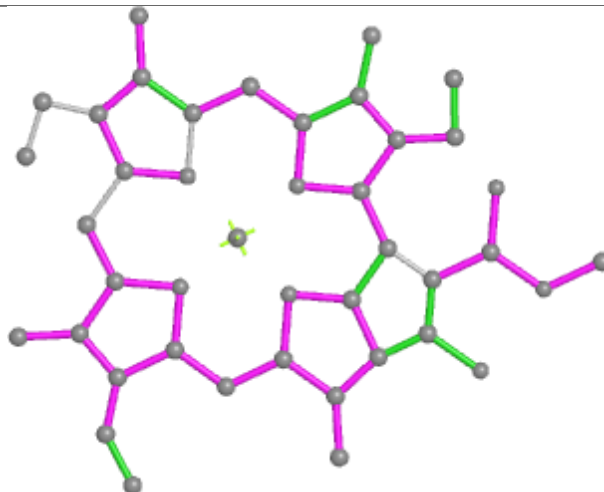
## Ligand CLA 7 313



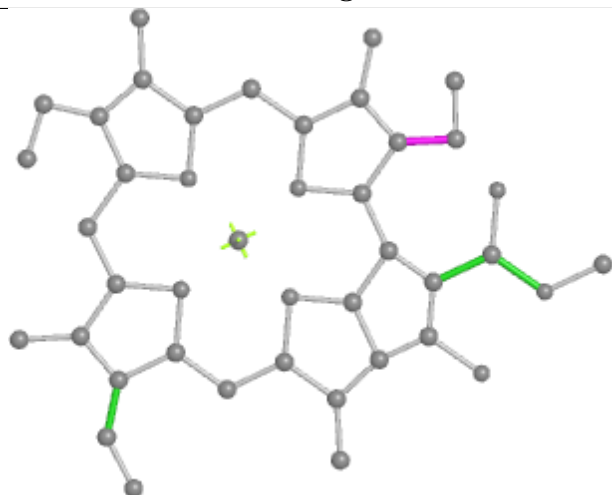
## Ligand CLA J 102



Bond lengths



Bond angles

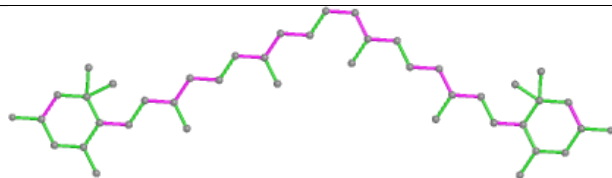


Torsions

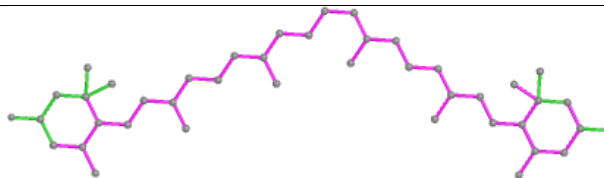


Rings

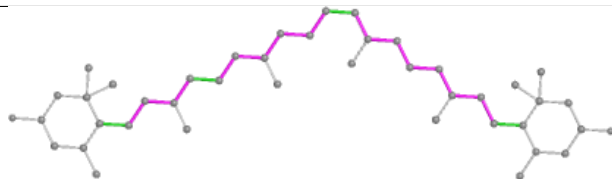
## Ligand 5X6 7 314



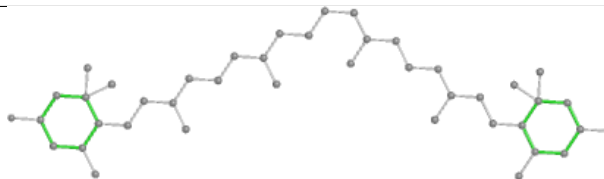
Bond lengths



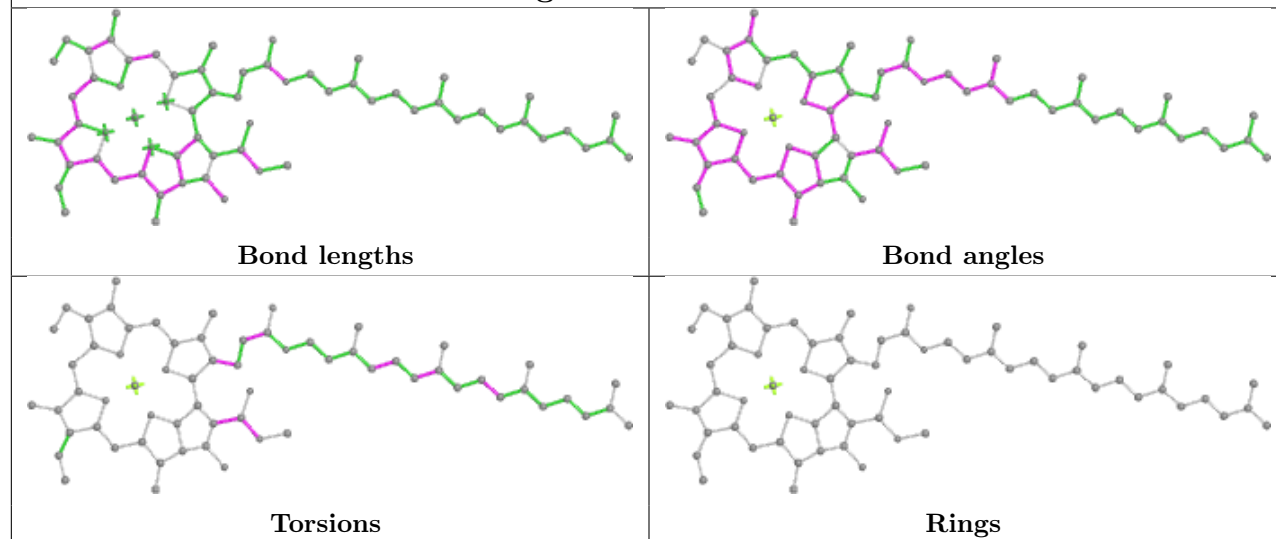
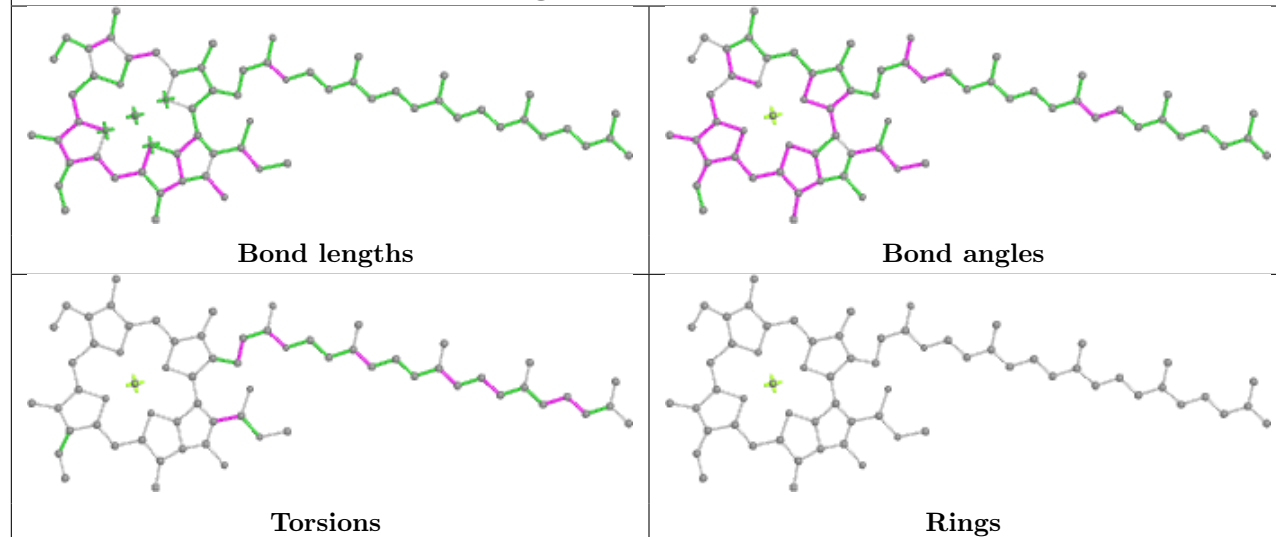
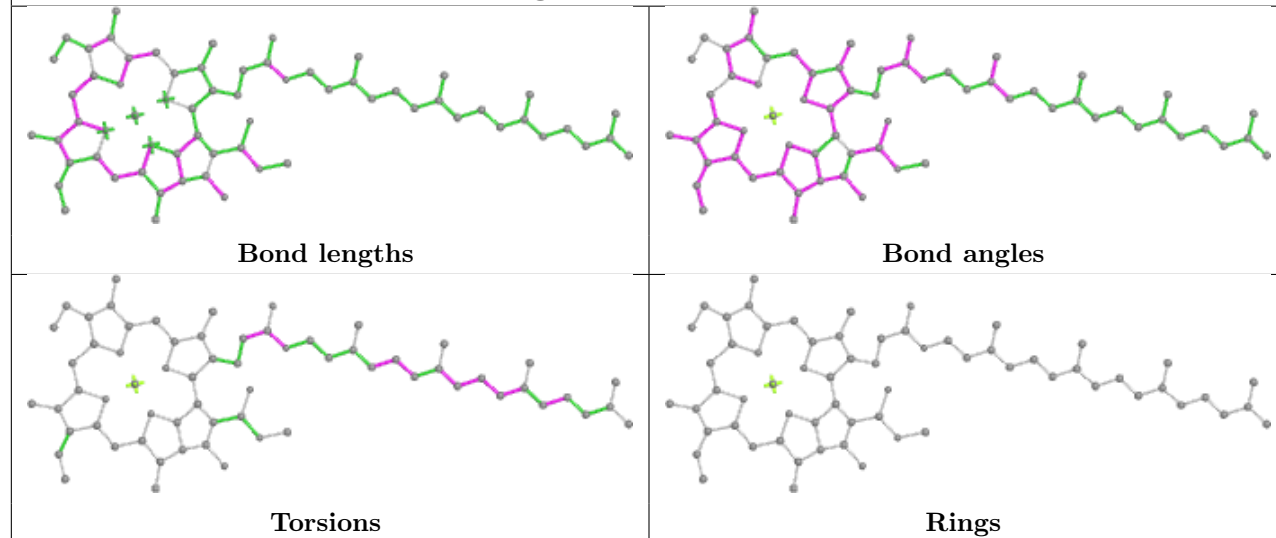
Bond angles

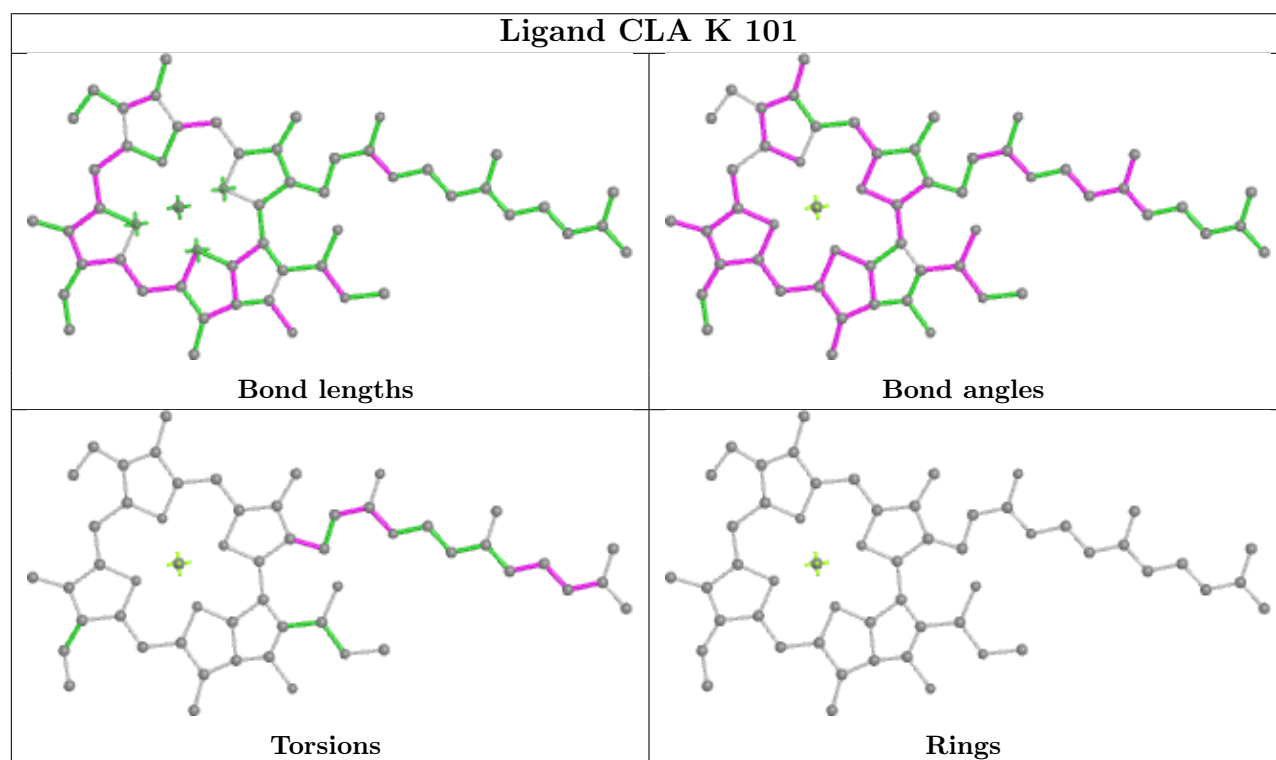
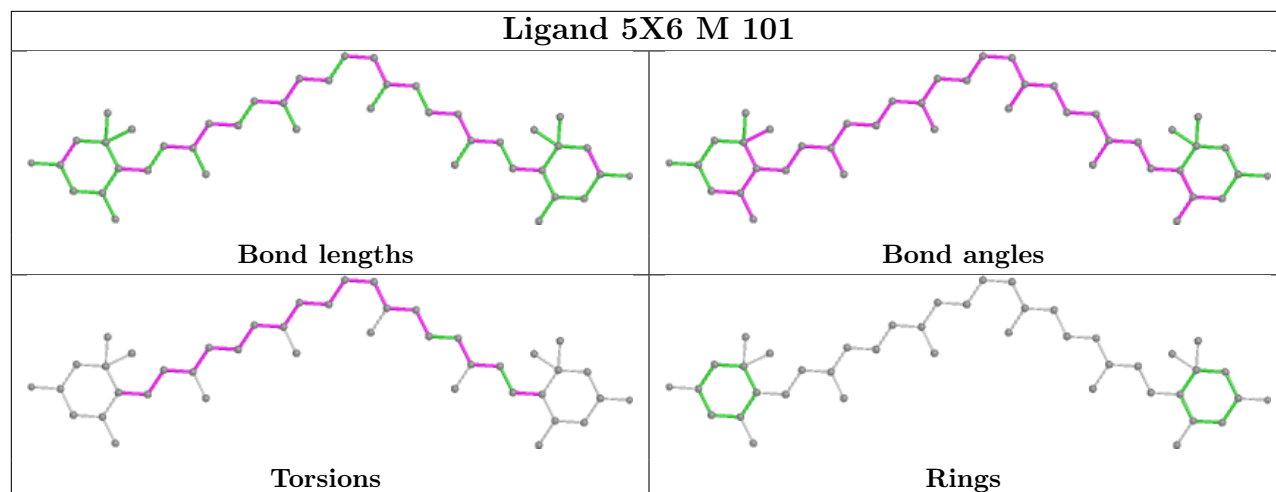
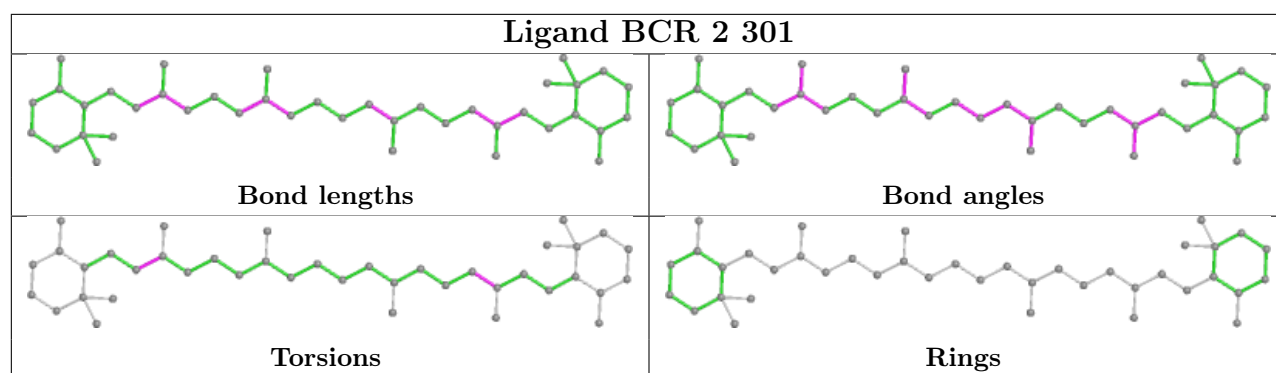


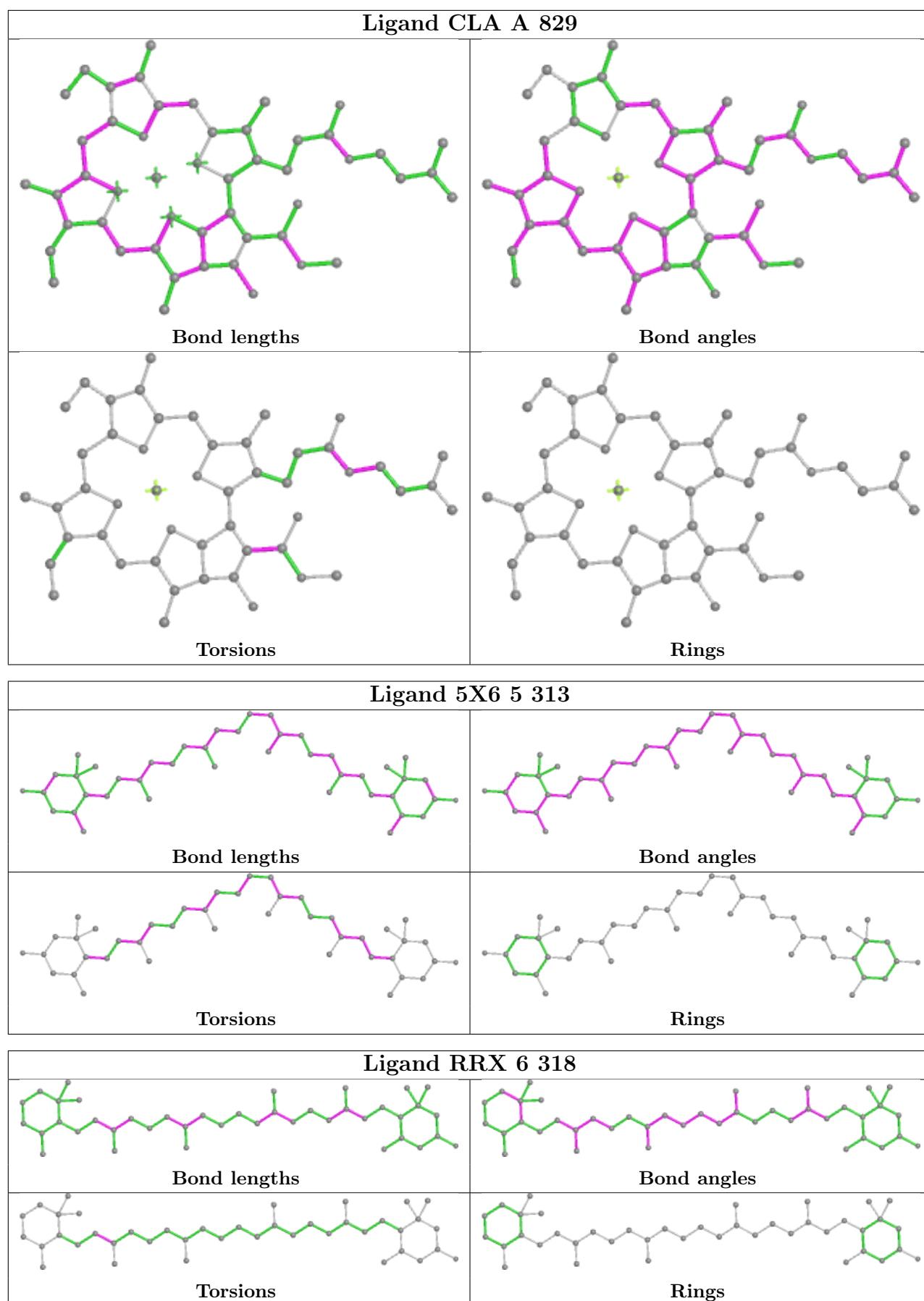
Torsions

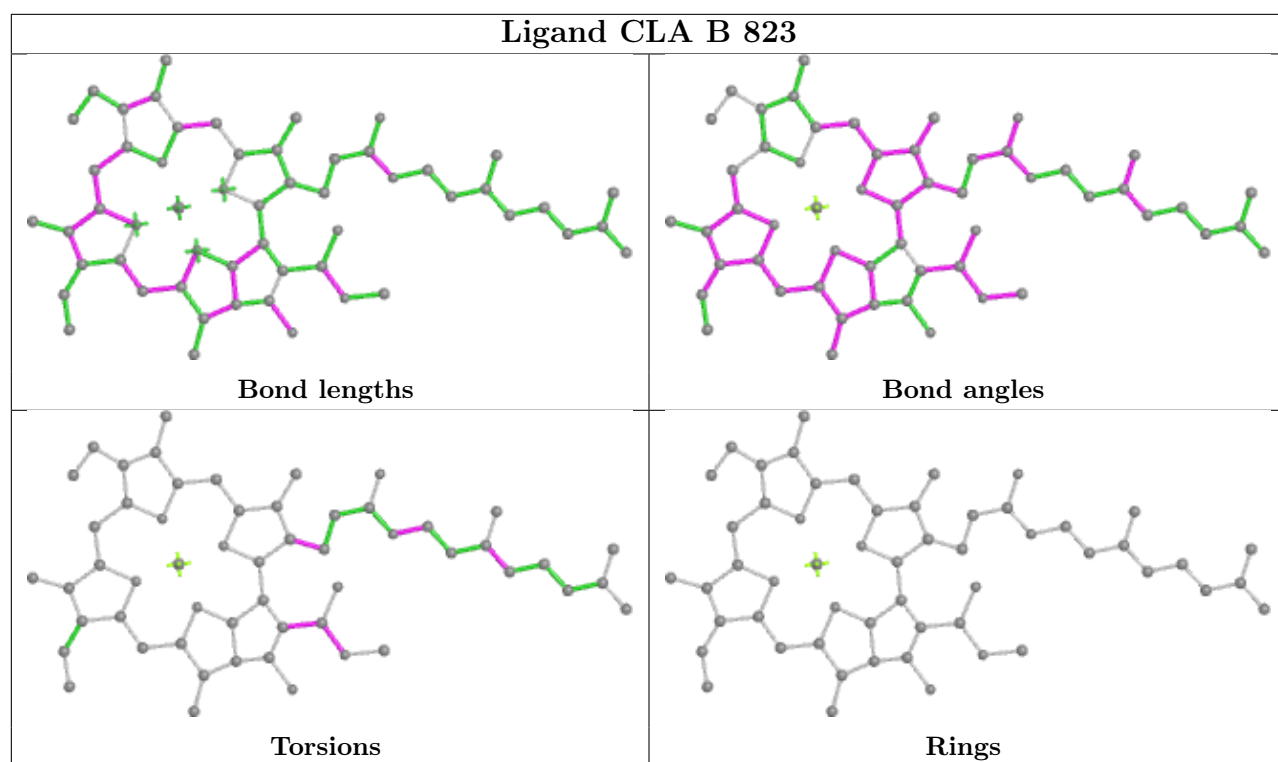


Rings

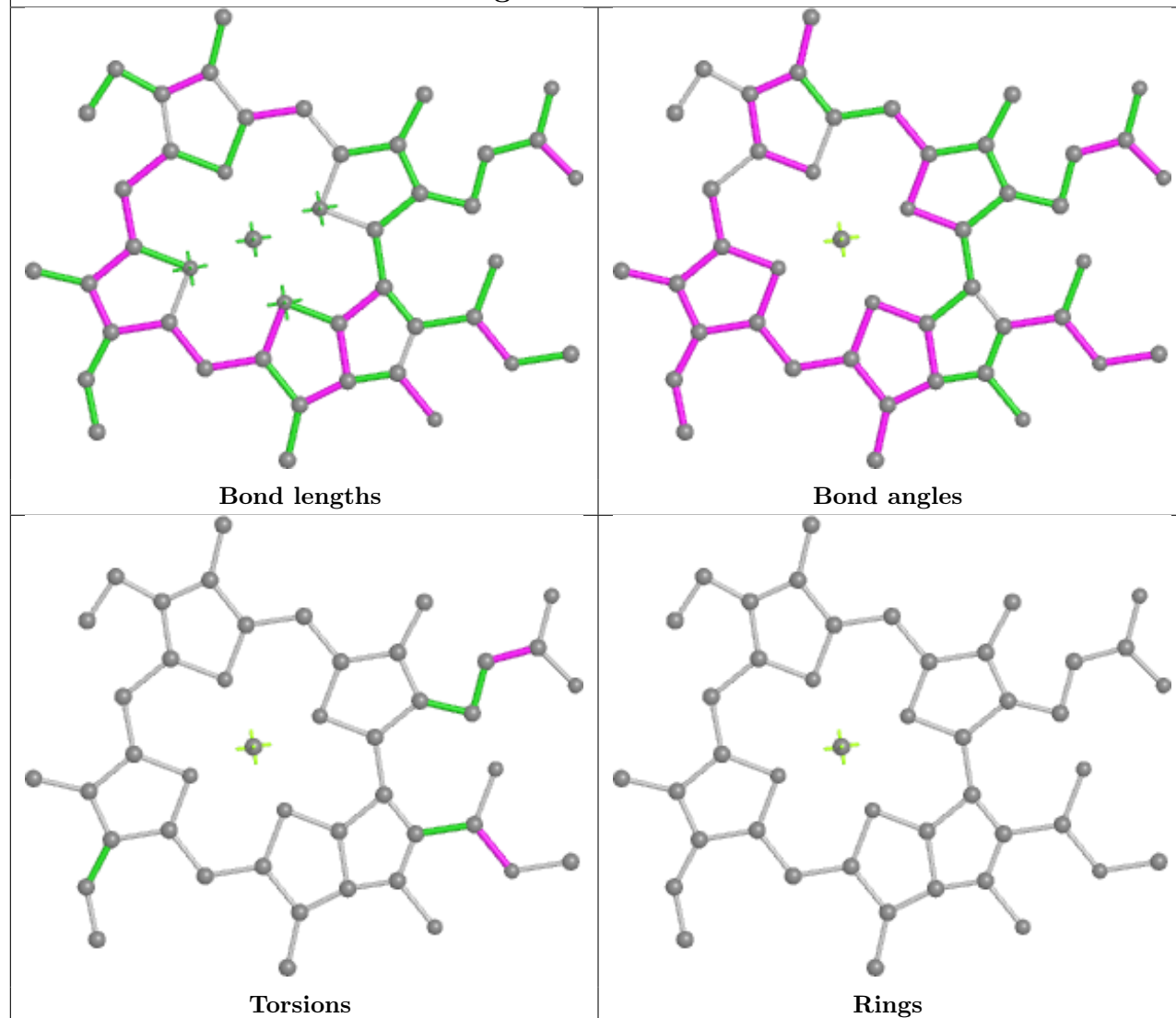
**Ligand CLA 3 301****Ligand CLA B 837****Ligand CLA A 839**



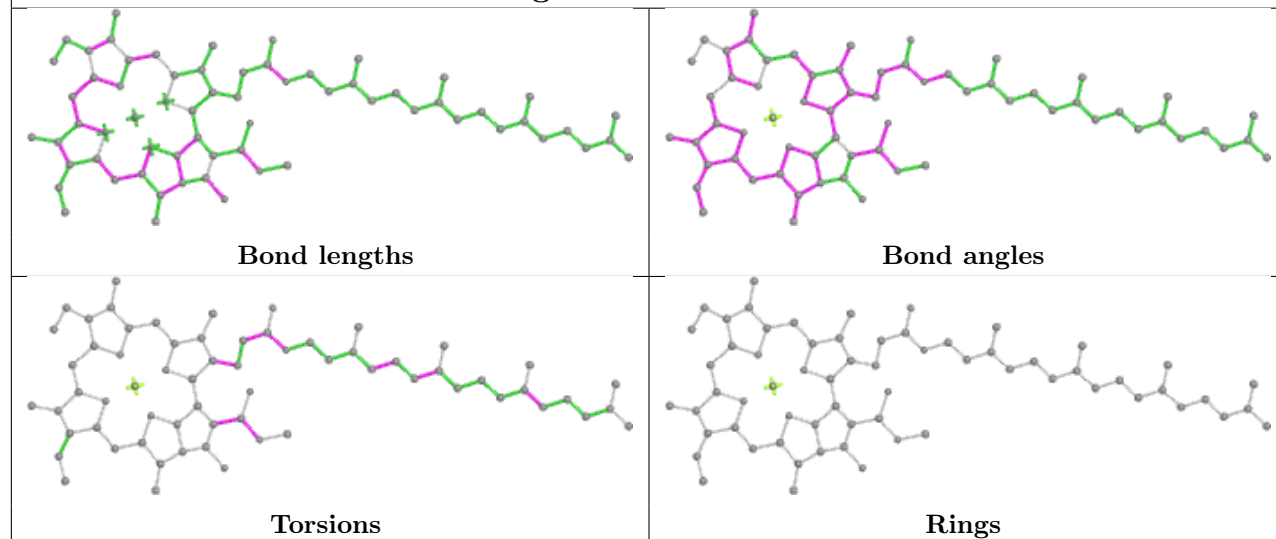




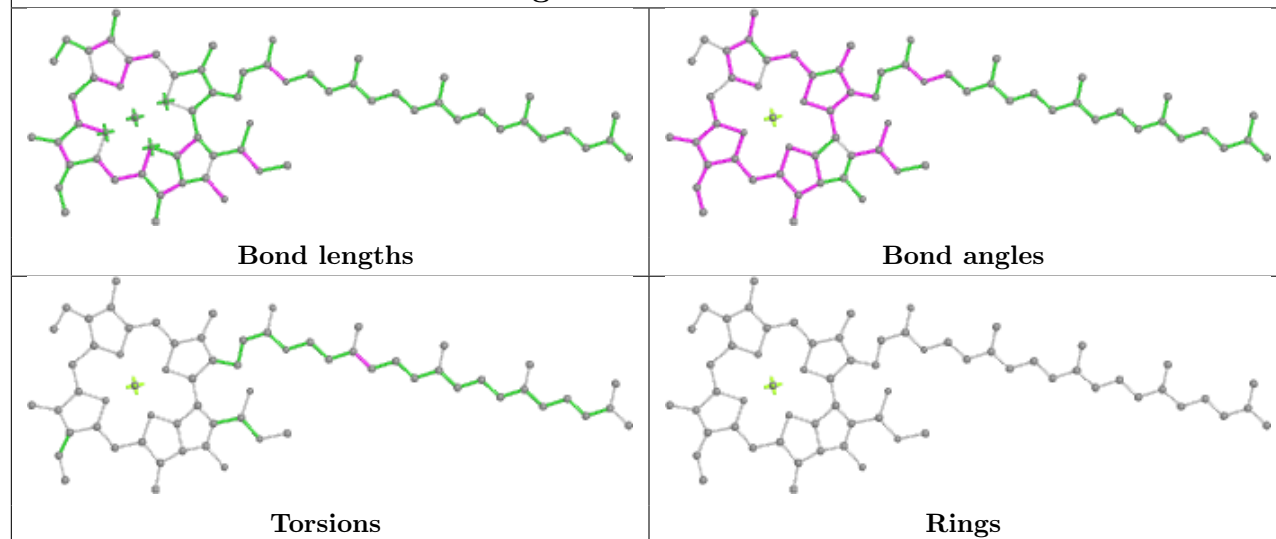
## Ligand CLA 7 305



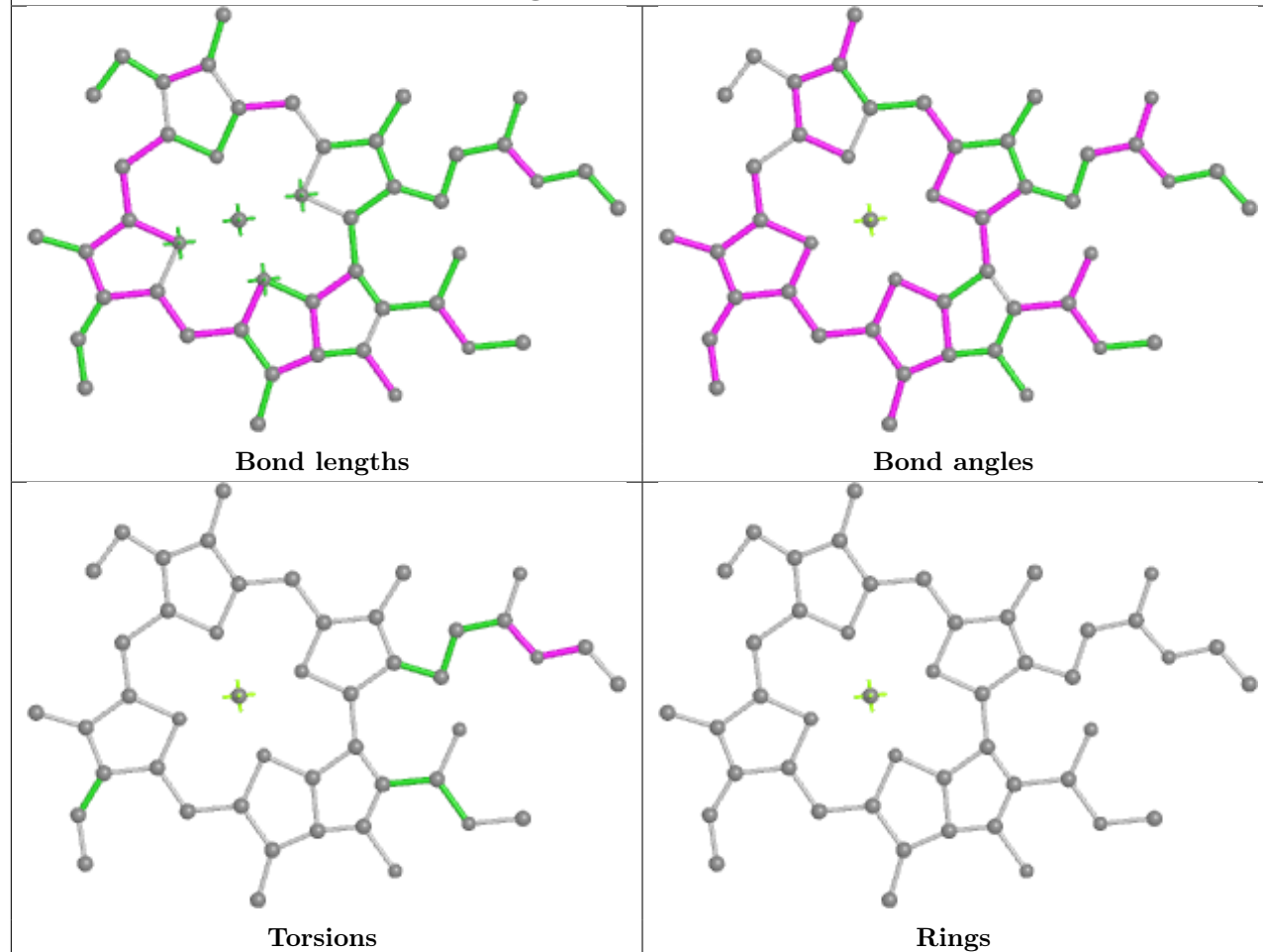
## Ligand CLA B 829



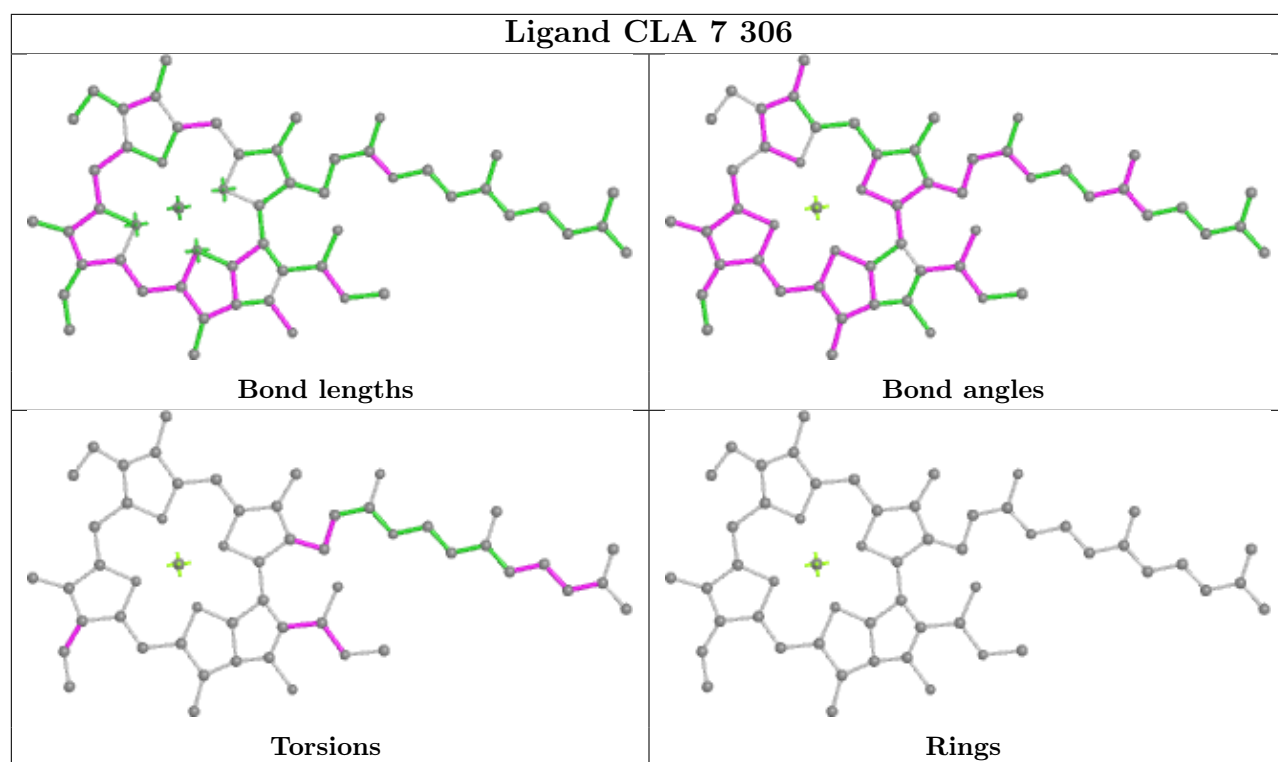
## Ligand CLA B 828



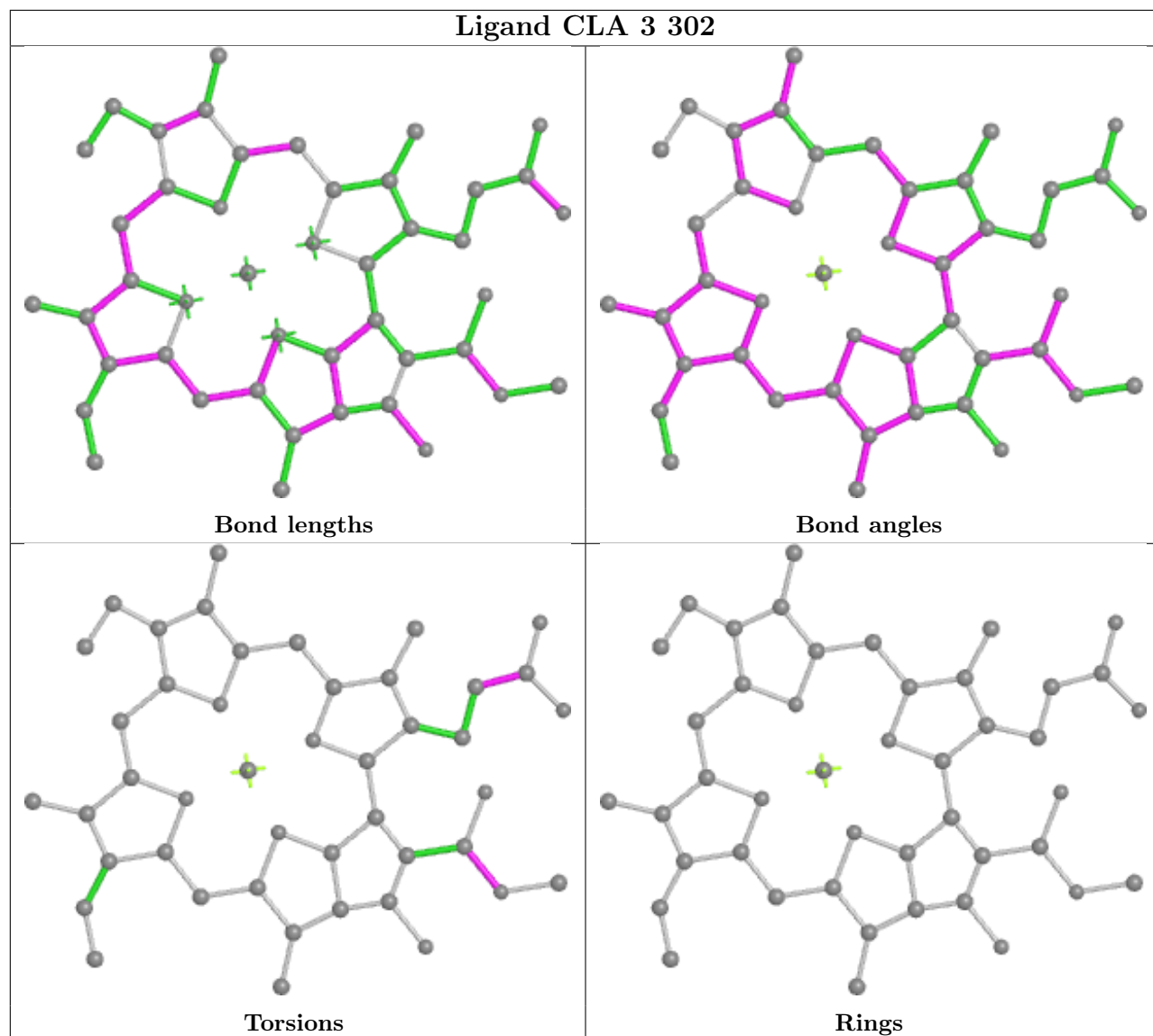
## Ligand CLA B 836

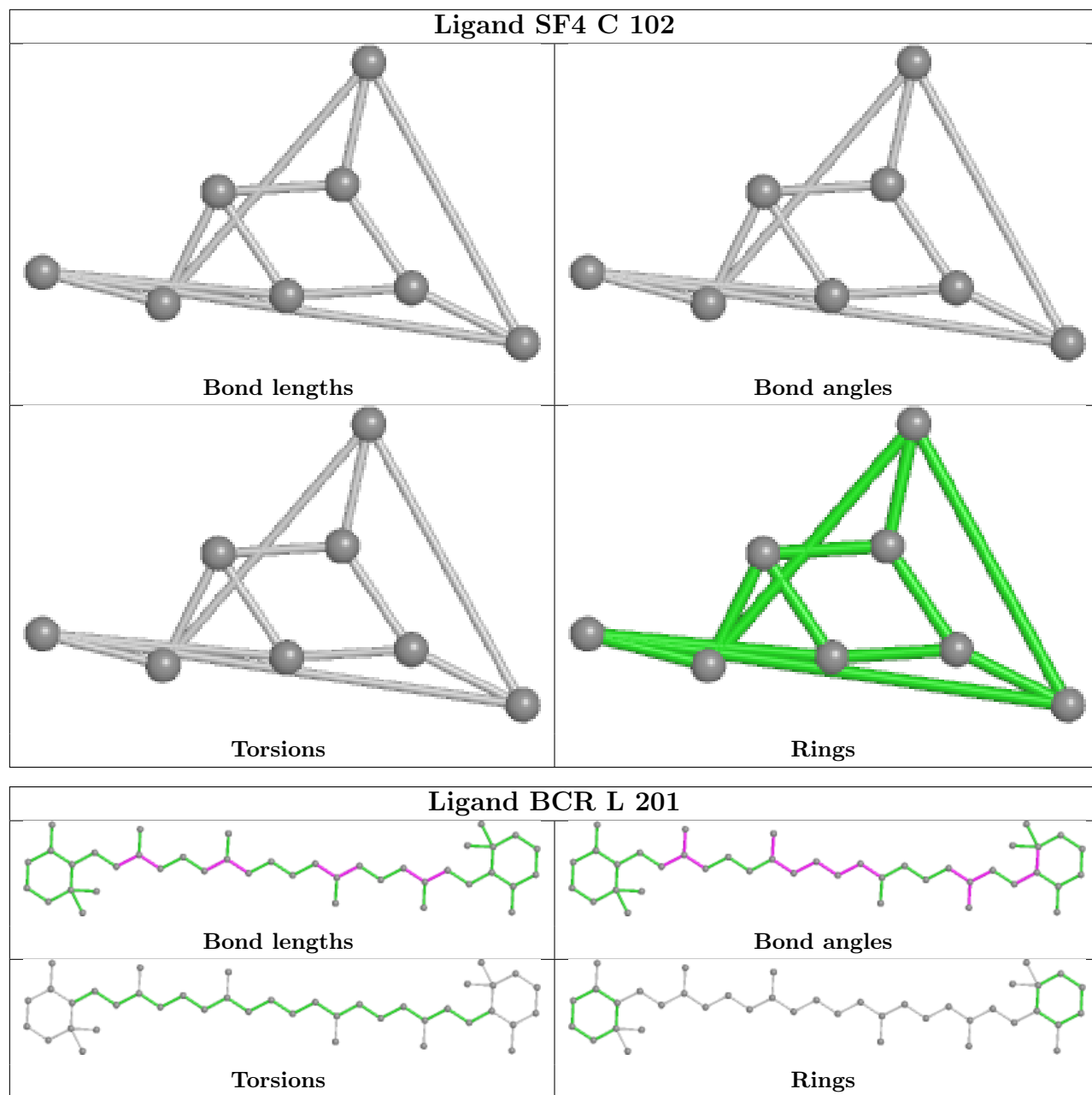




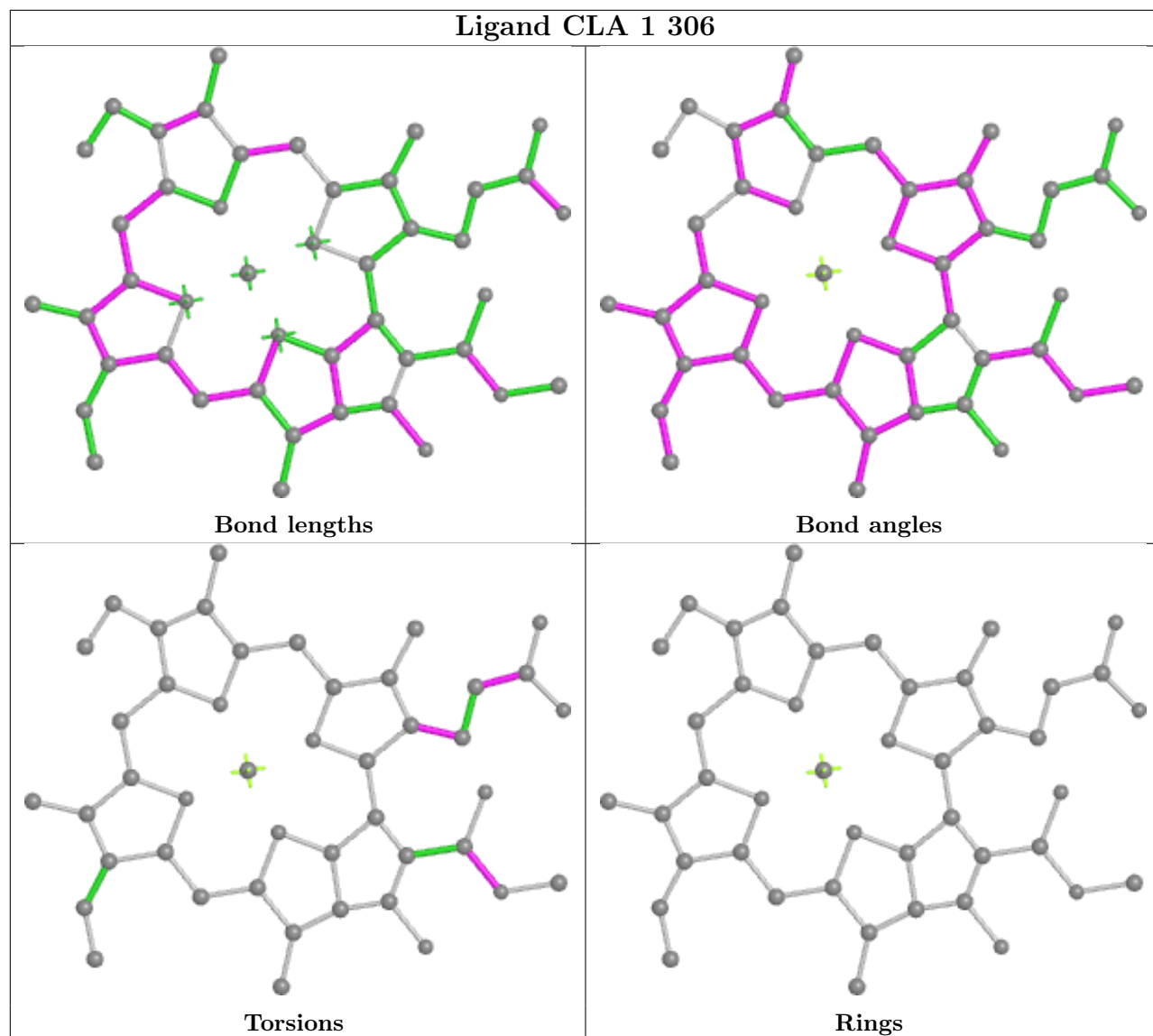


## Ligand CLA 3 302

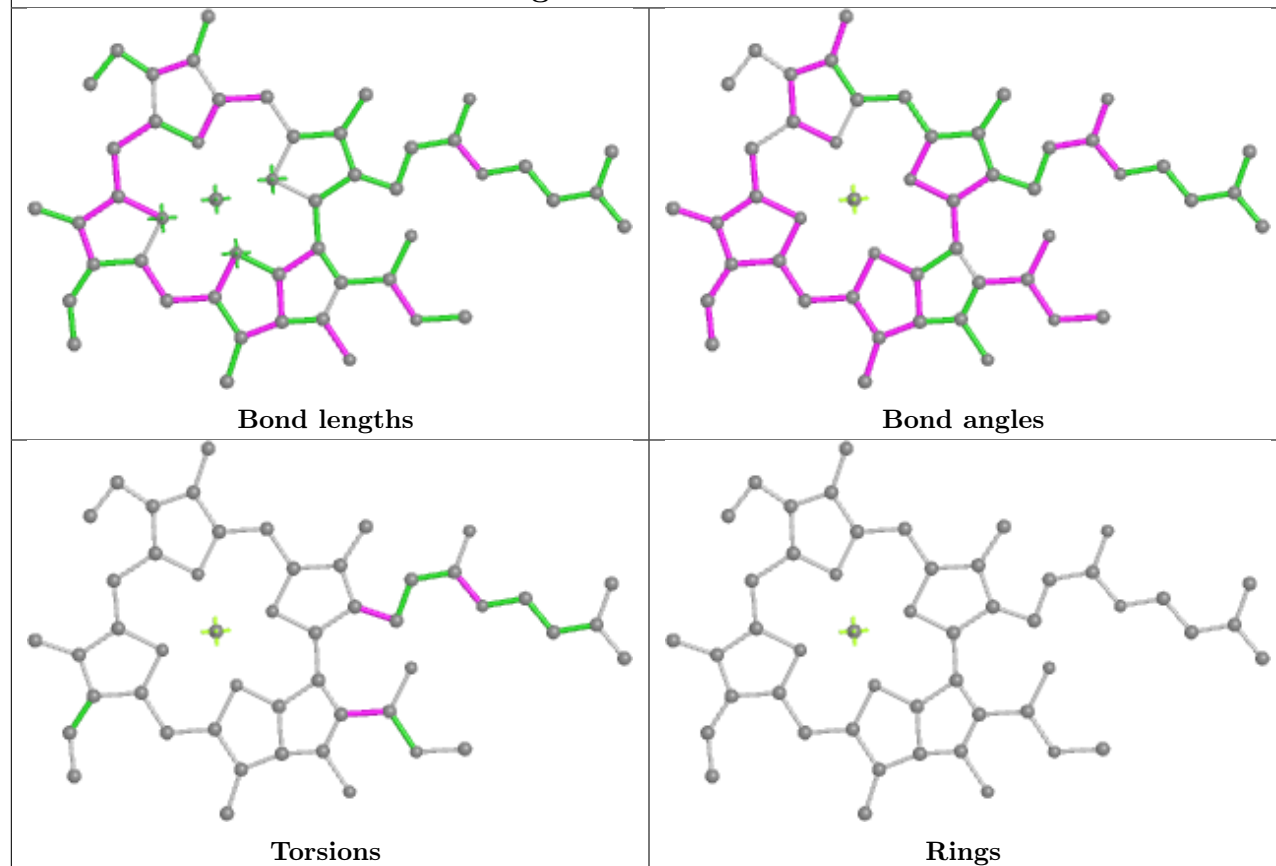




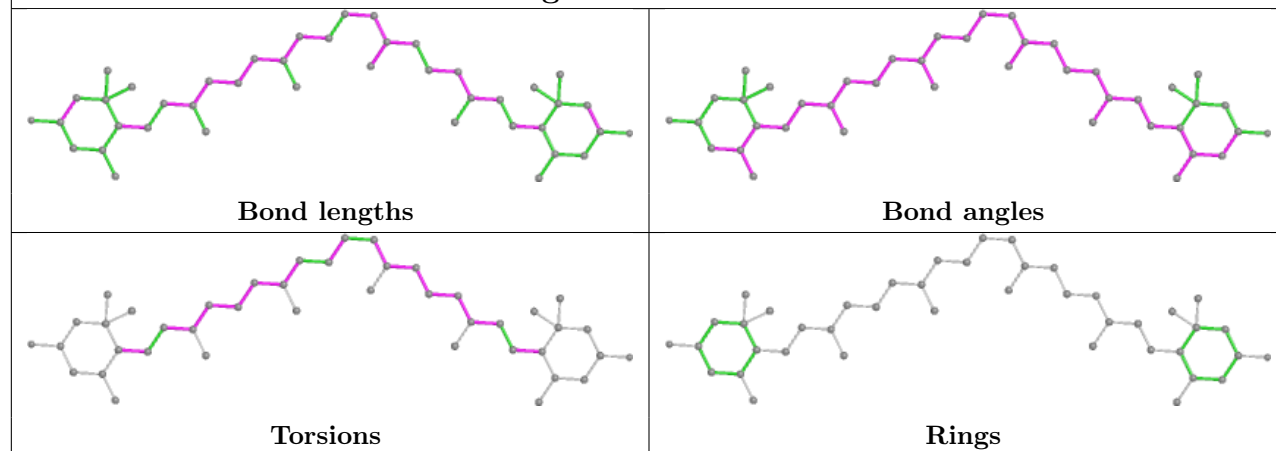
## Ligand CLA 1 306



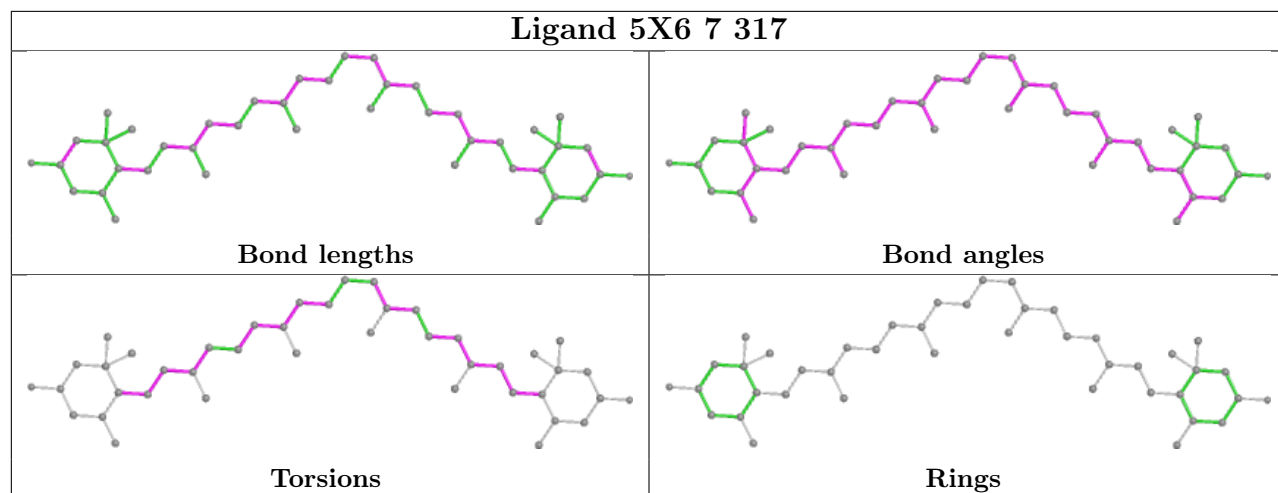
## Ligand CLA A 805



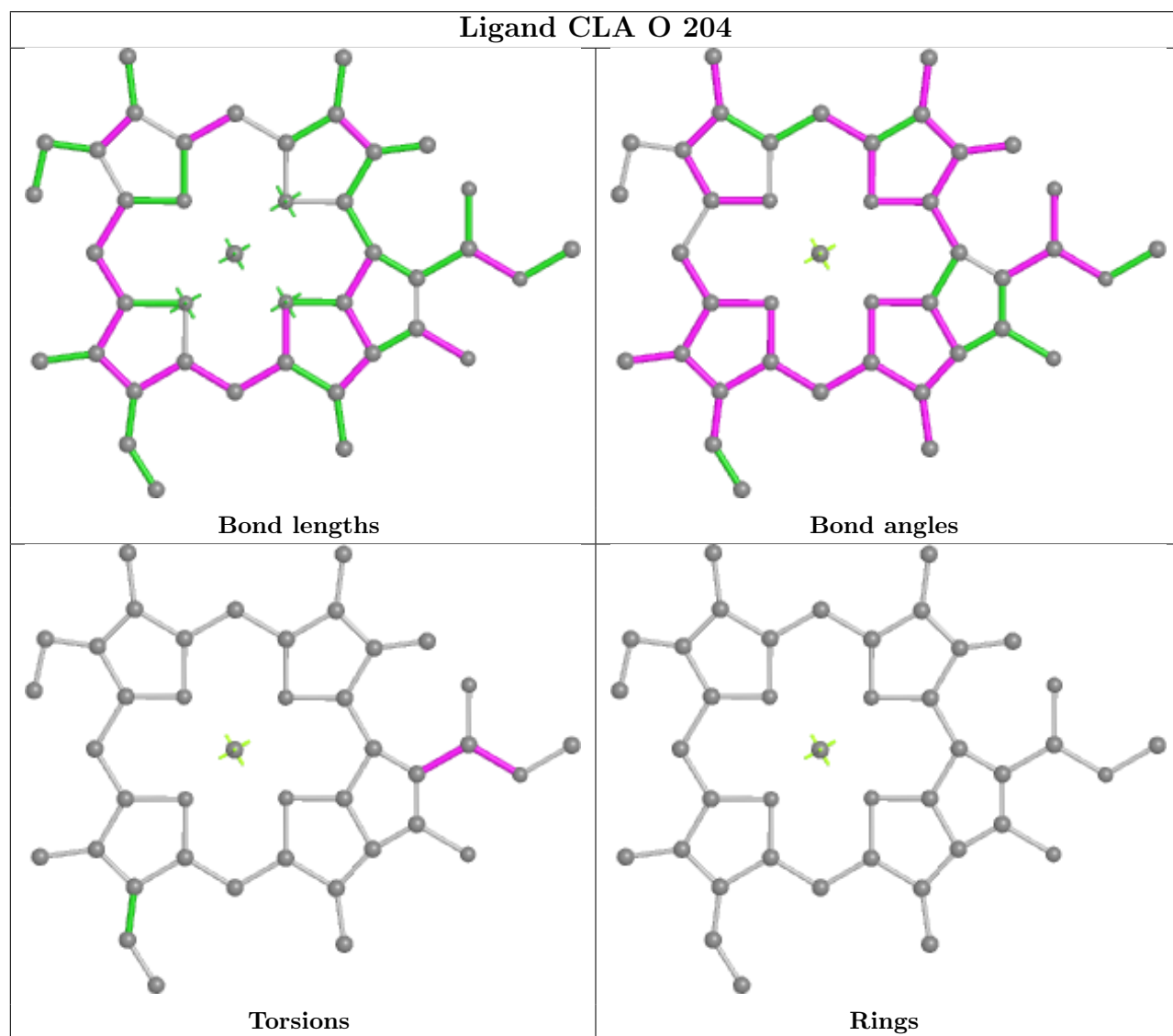
## Ligand 5X6 1 316

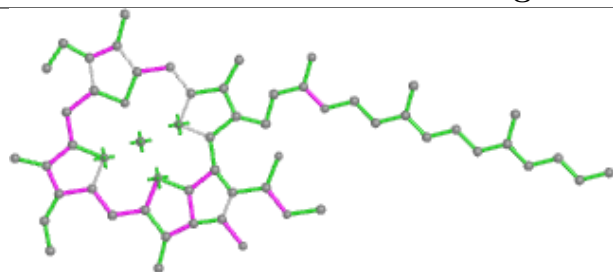


## Ligand 5X6 7 317

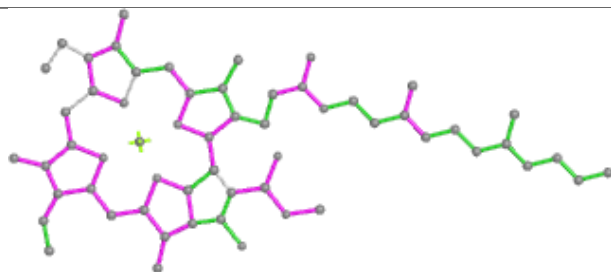


## Ligand CLA O 204

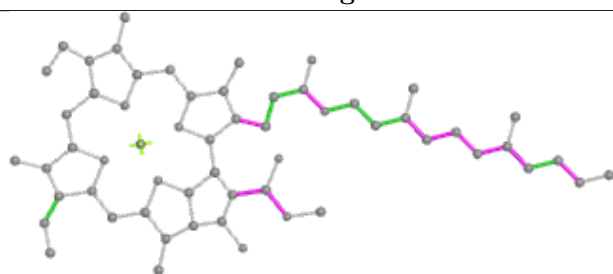


**Ligand CLA O 206**

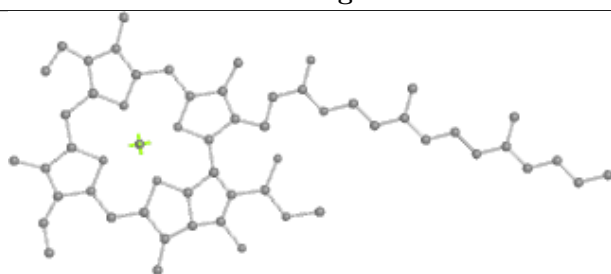
Bond lengths



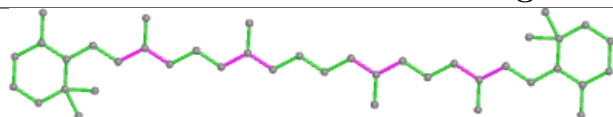
Bond angles



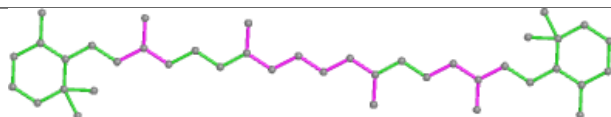
Torsions



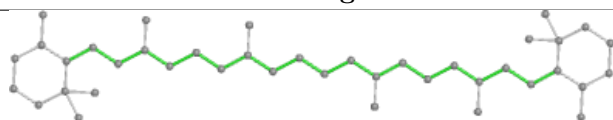
Rings

**Ligand BCR 5 315**

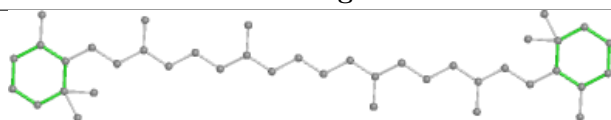
Bond lengths



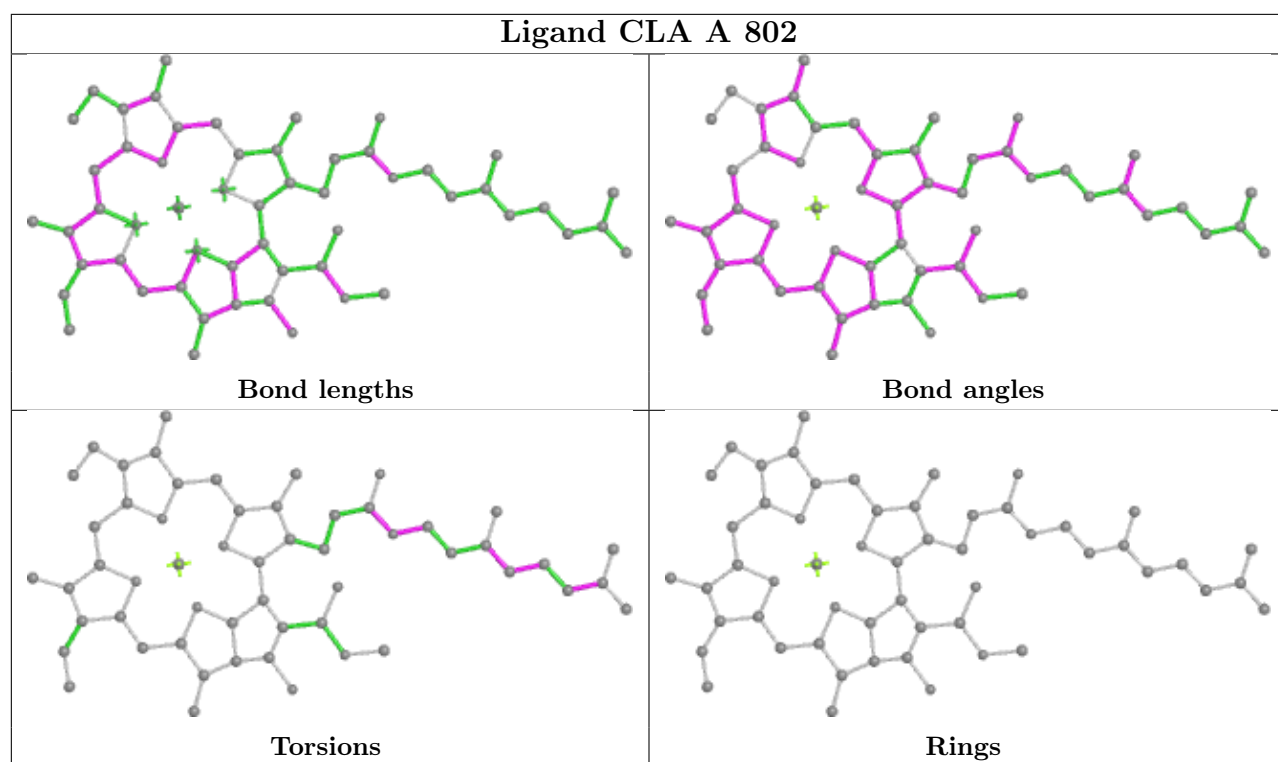
Bond angles



Torsions

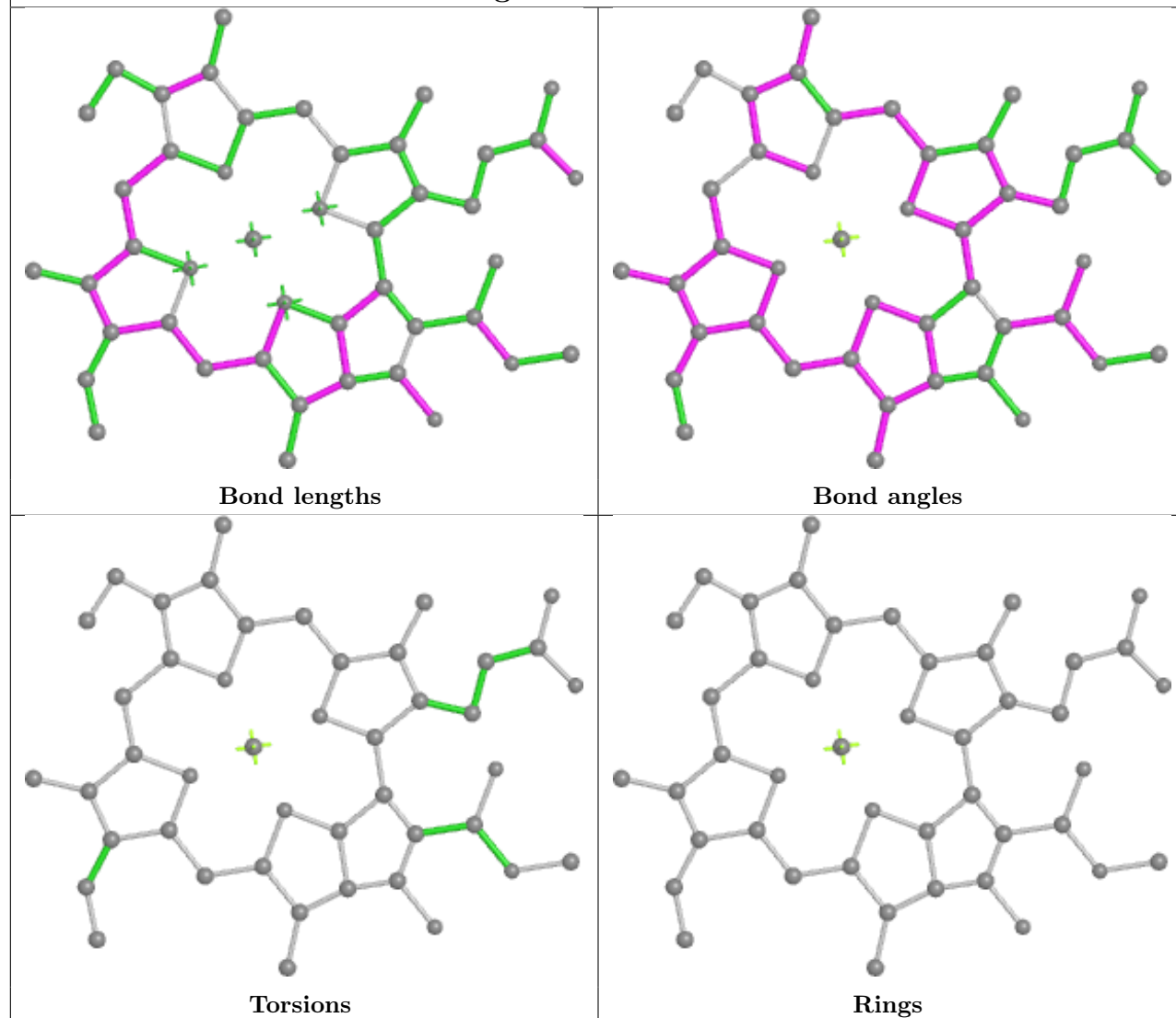


Rings

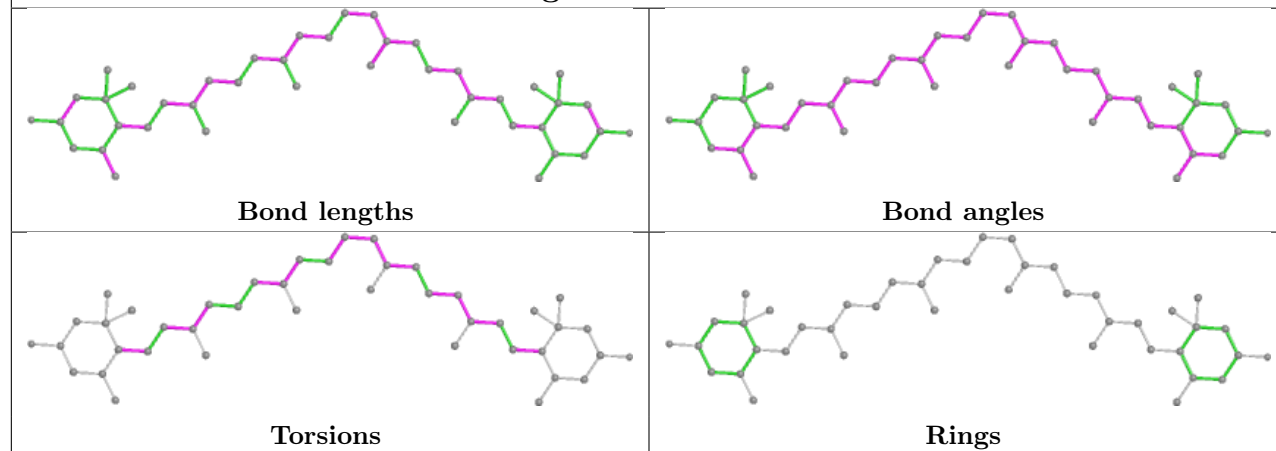


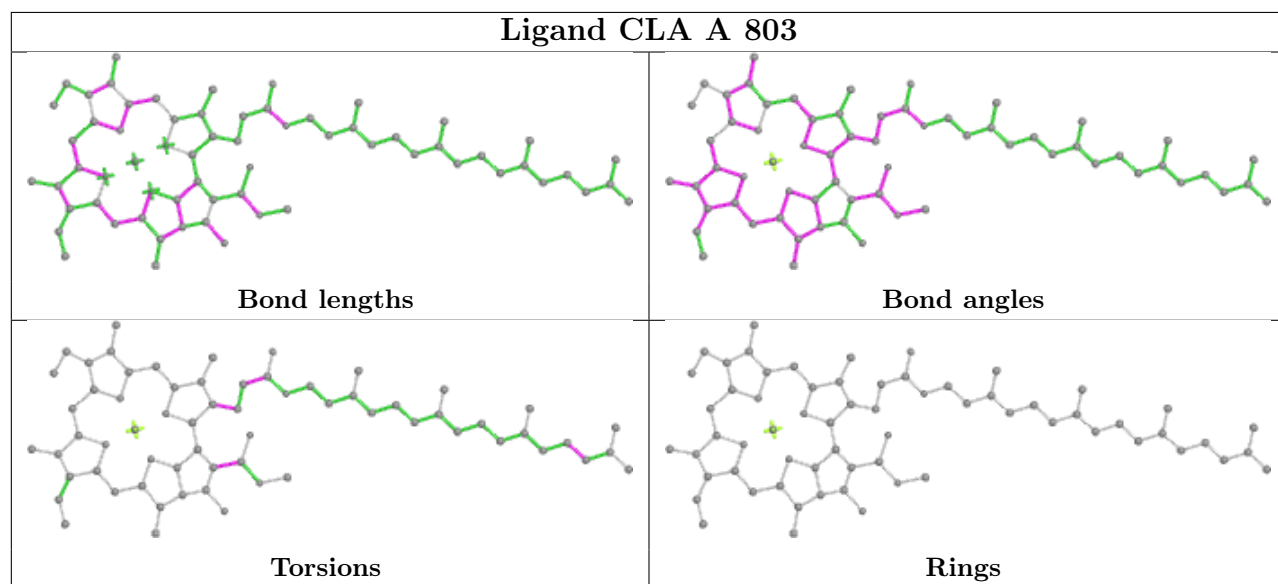
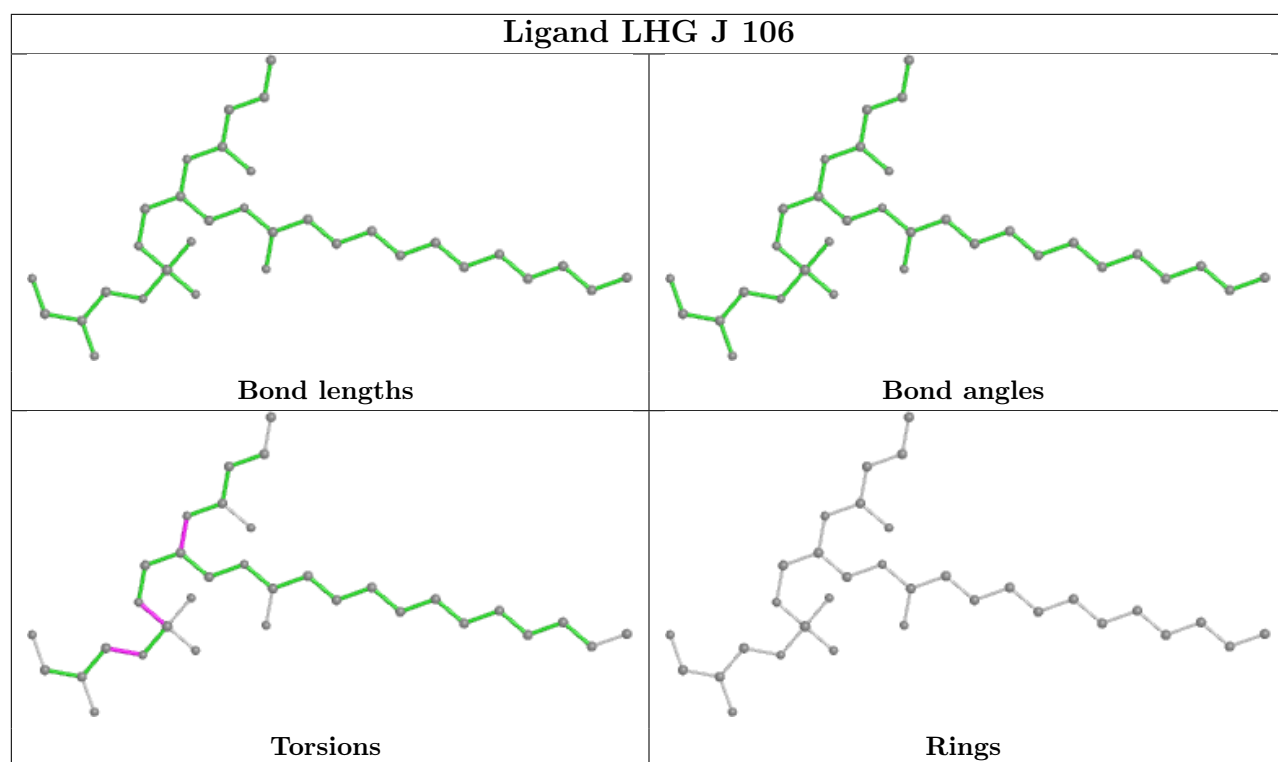


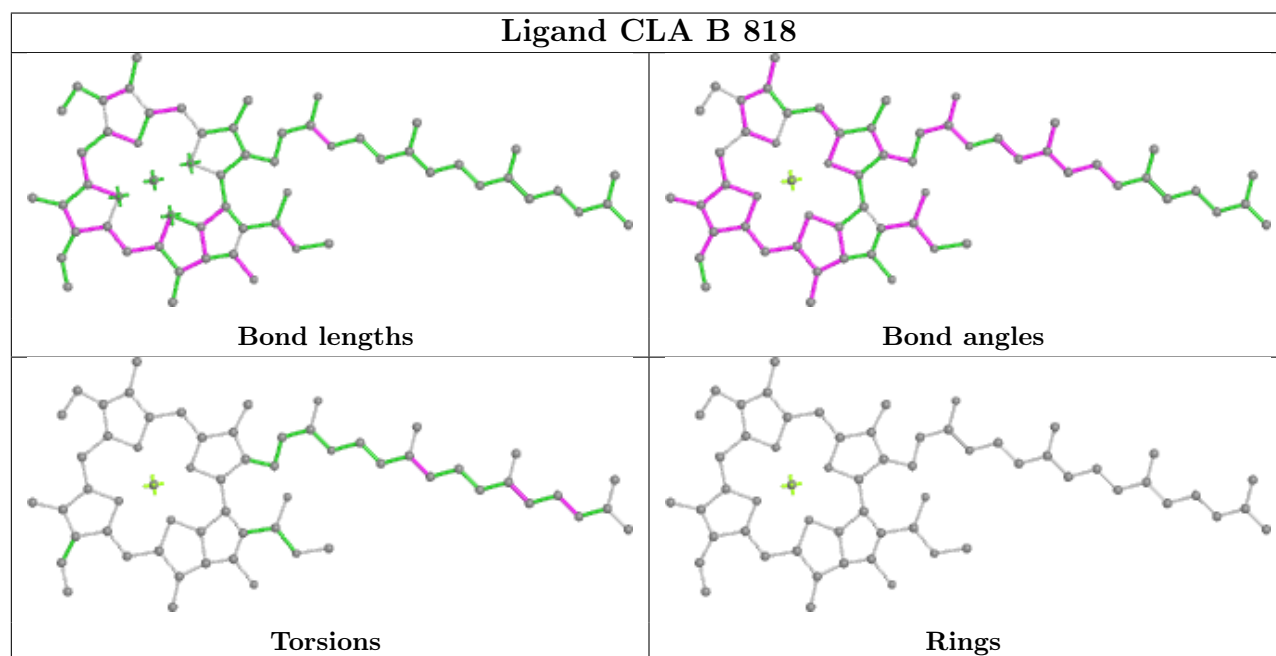
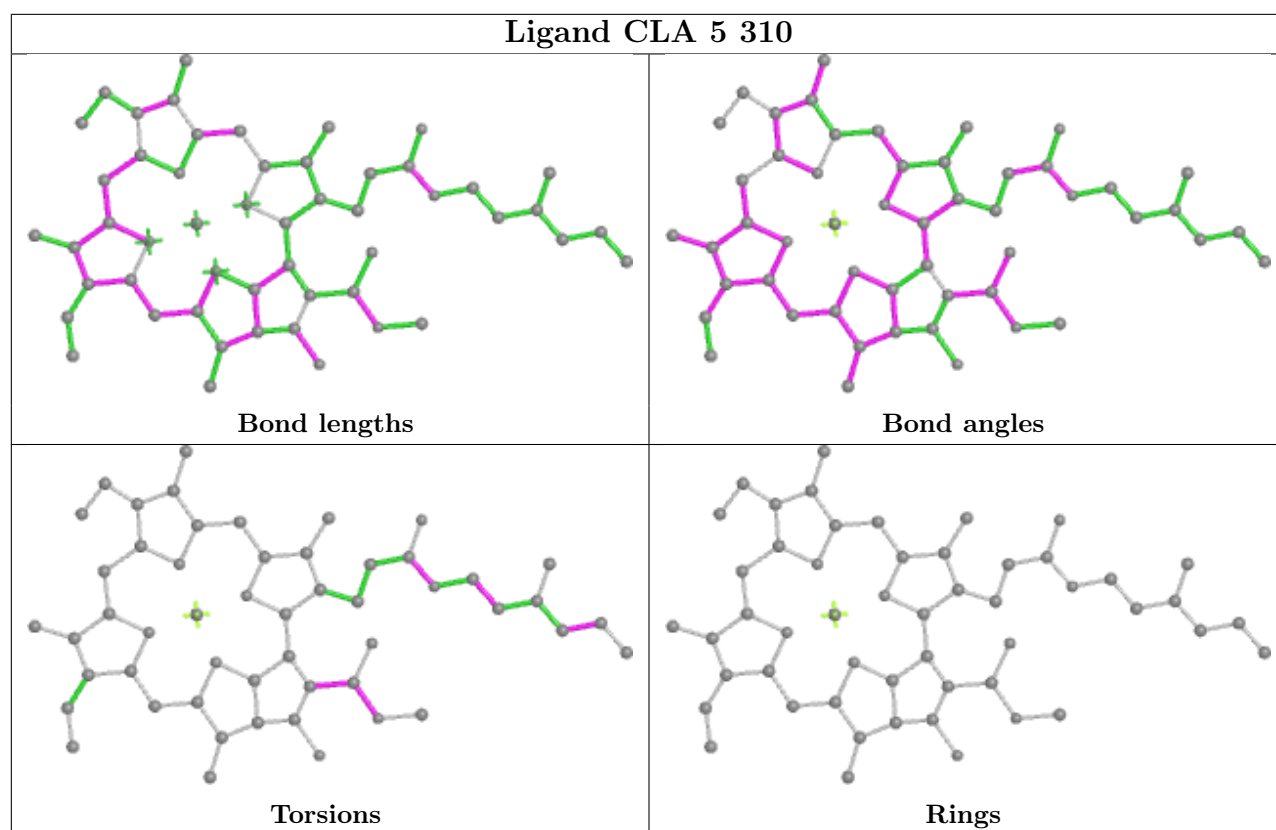
## Ligand CLA 7 308

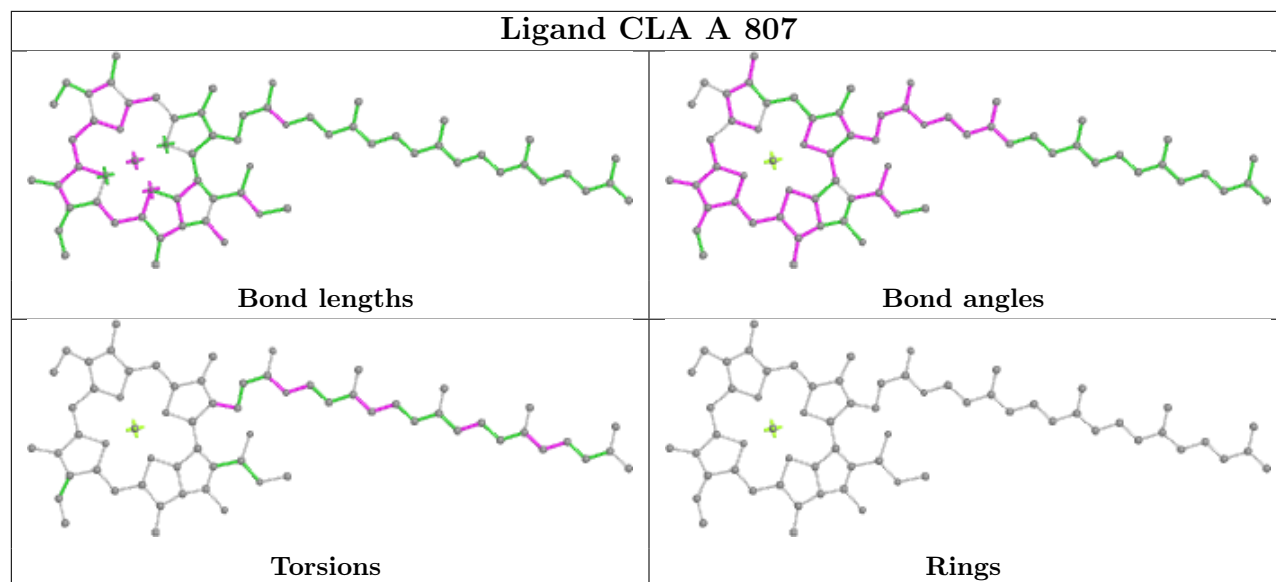
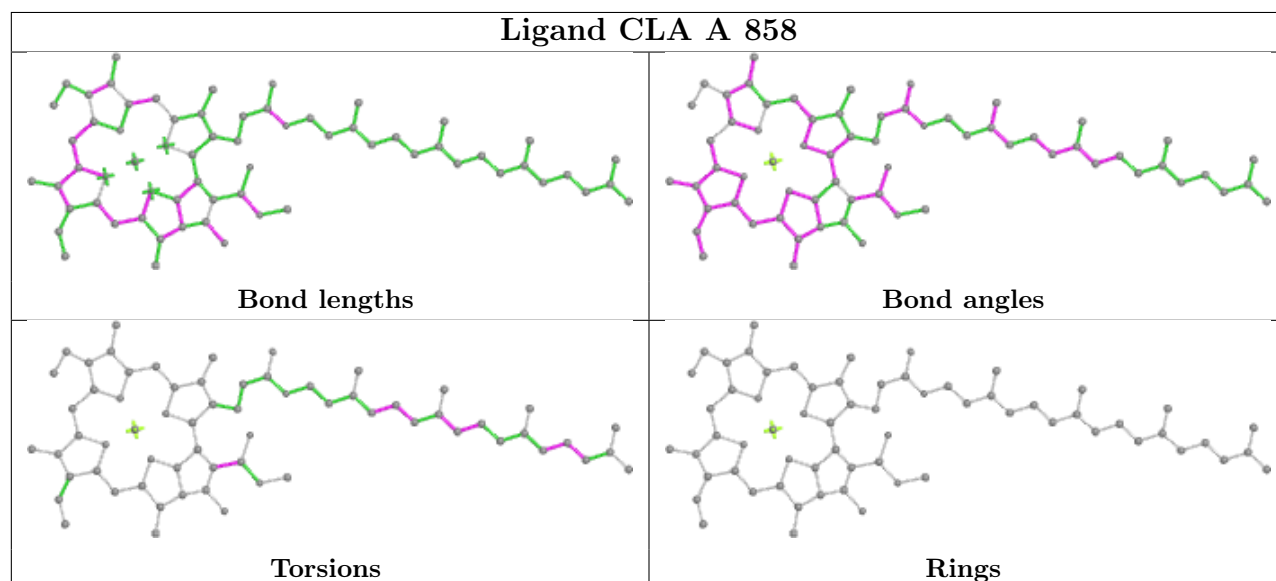
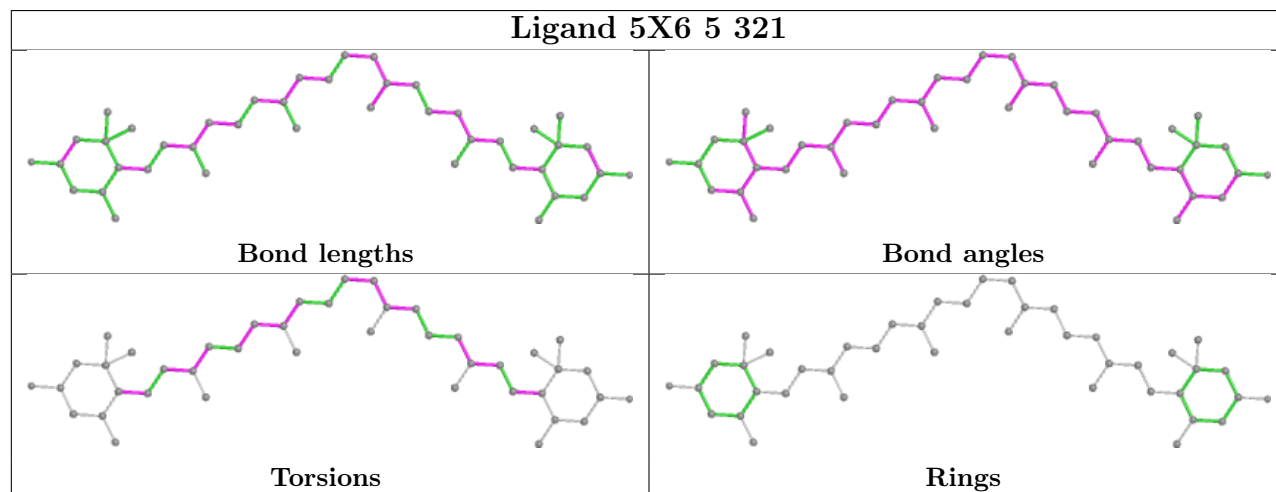


## Ligand 5X6 7 316

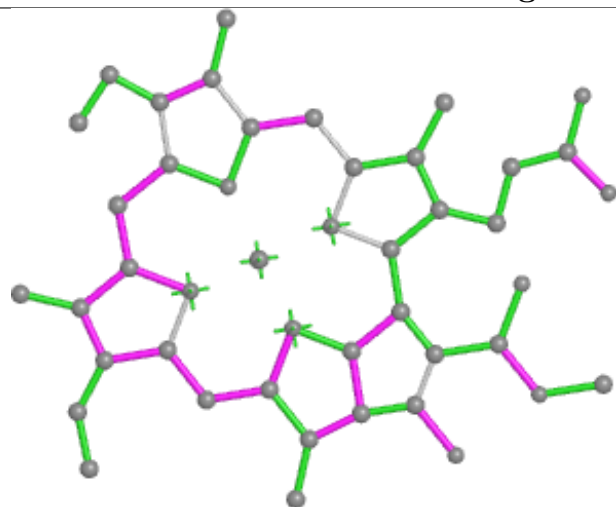




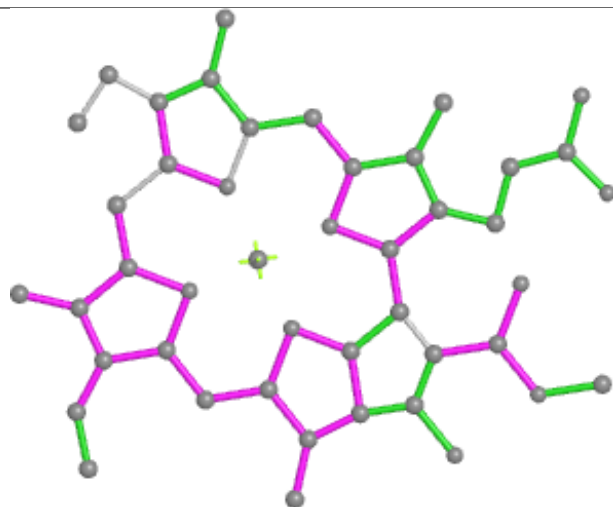


**Ligand CLA A 807****Ligand CLA A 858****Ligand 5X6 5 321**

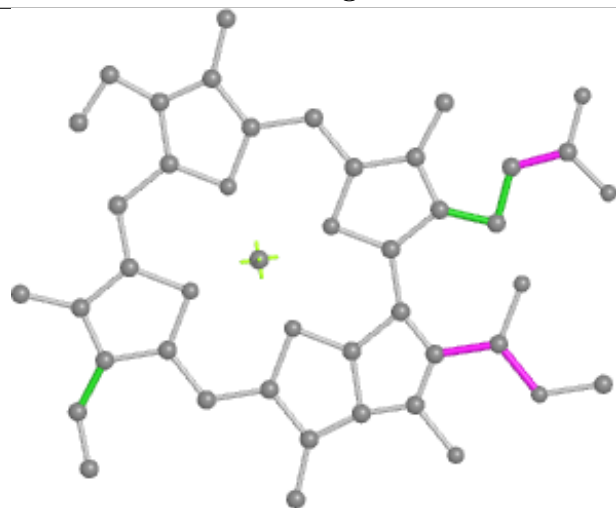
## Ligand CLA L 205



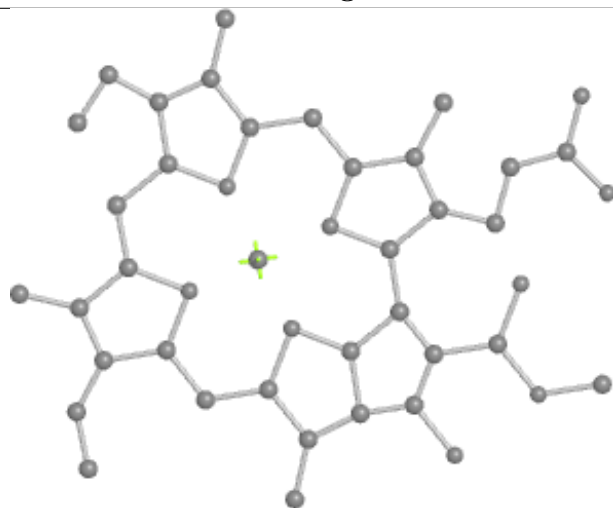
Bond lengths



Bond angles

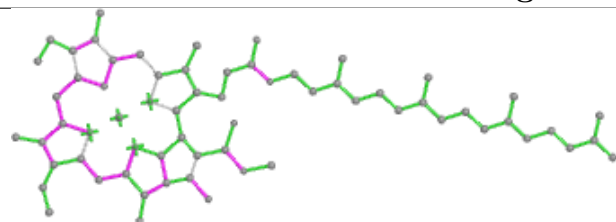


Torsions

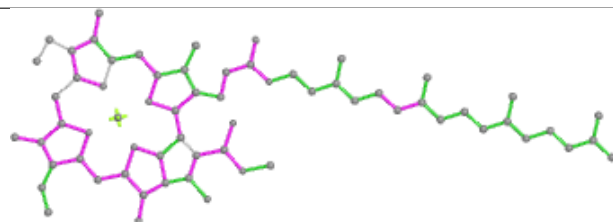


Rings

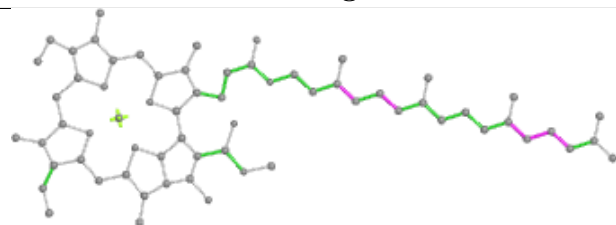
## Ligand CLA B 832



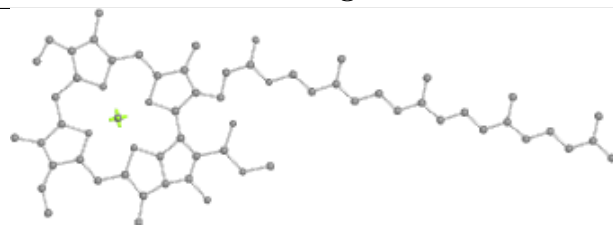
Bond lengths



Bond angles

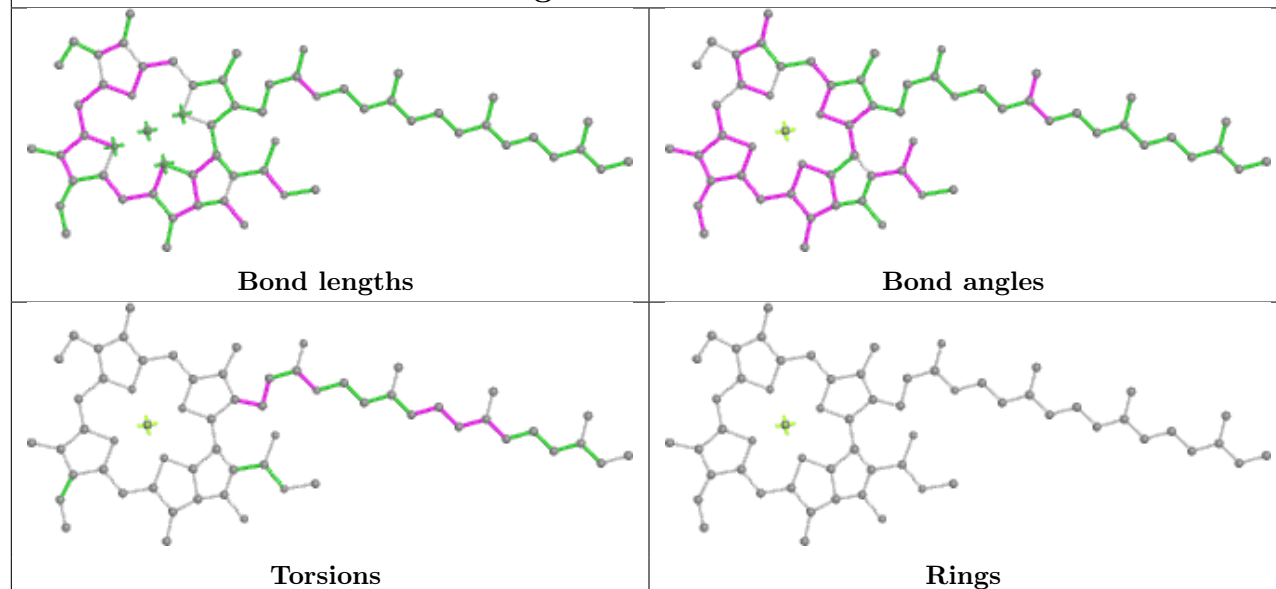


Torsions

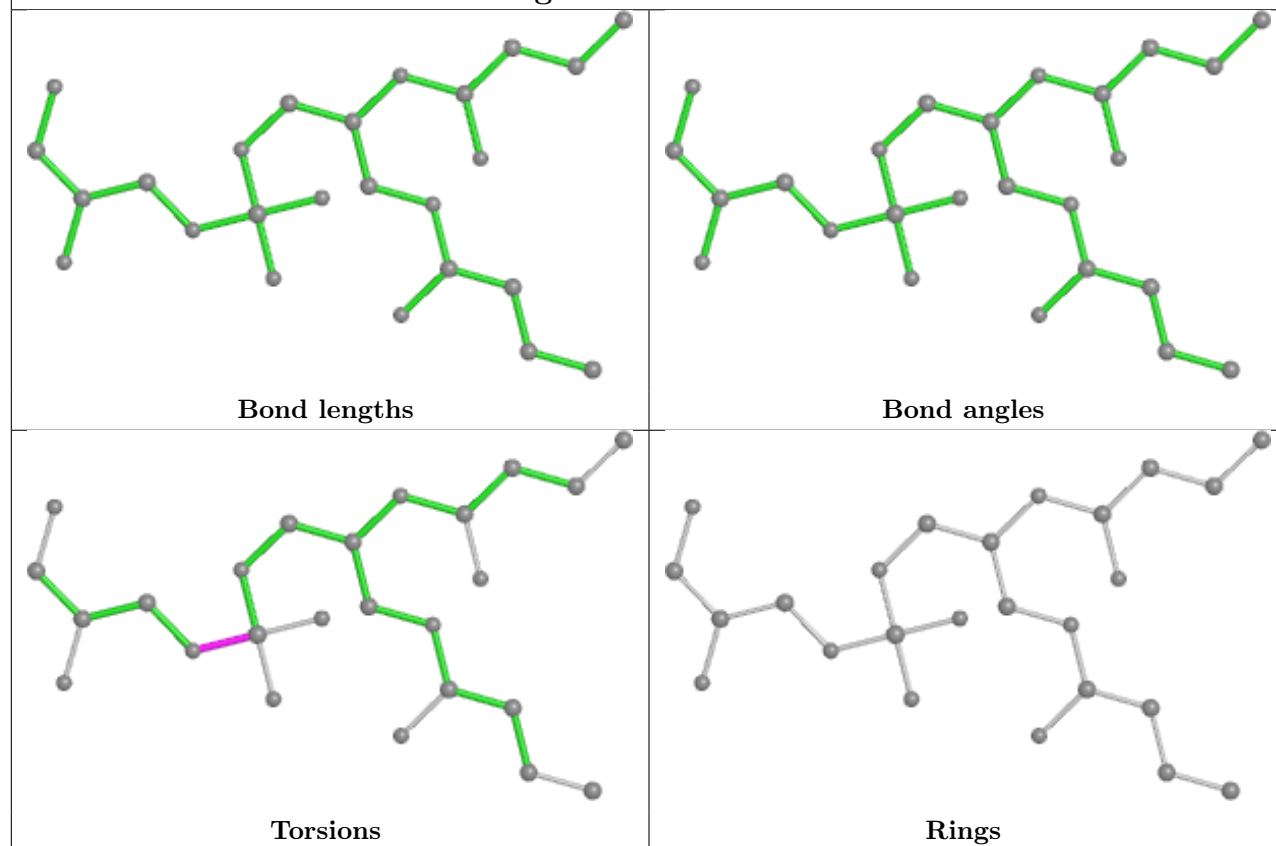


Rings

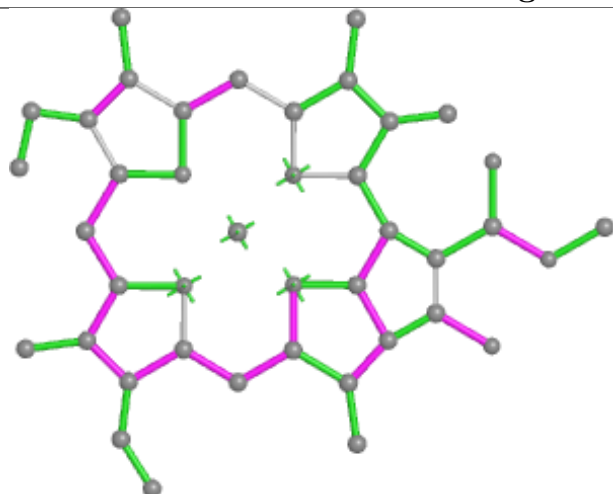
## Ligand CLA L 204



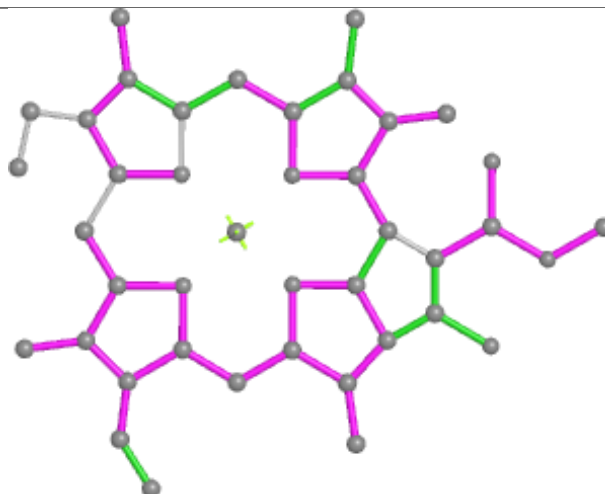
## Ligand LHG 5 316



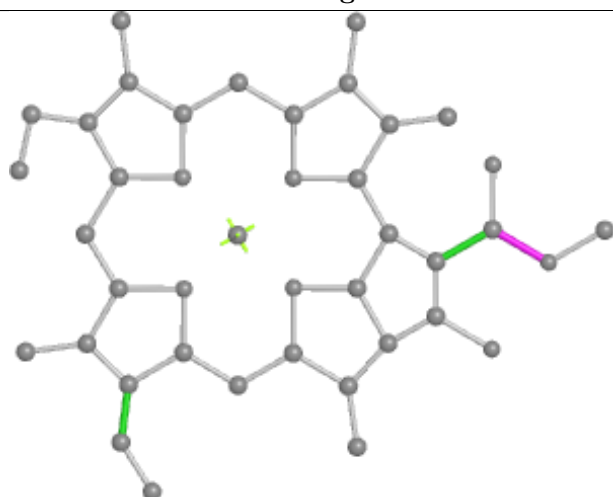
## Ligand CLA 2 309



Bond lengths



Bond angles

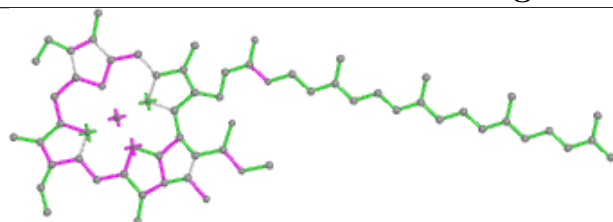


Torsions

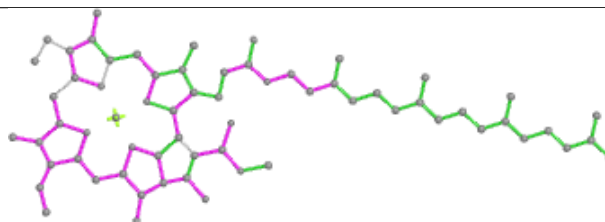


Rings

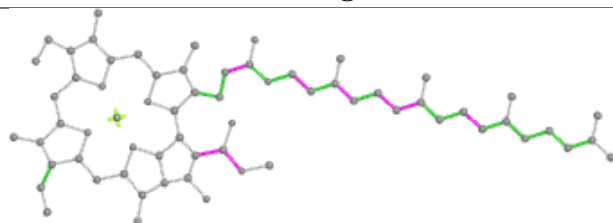
## Ligand CLA A 804



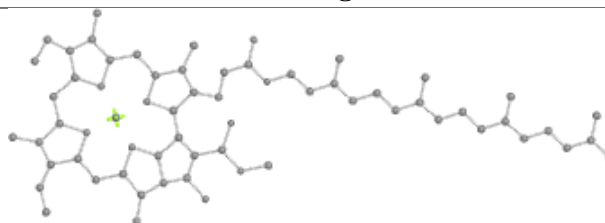
Bond lengths



Bond angles

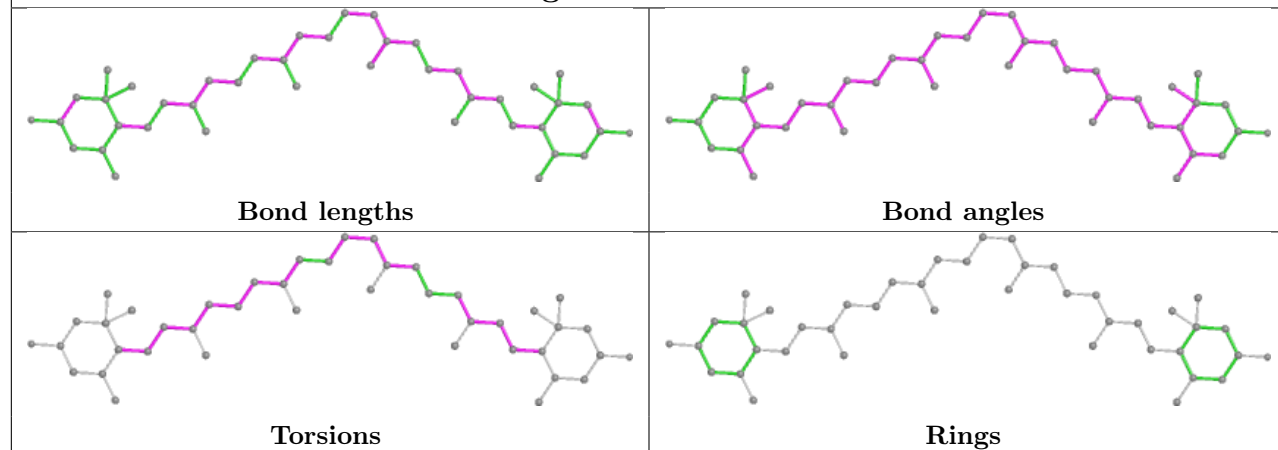


Torsions

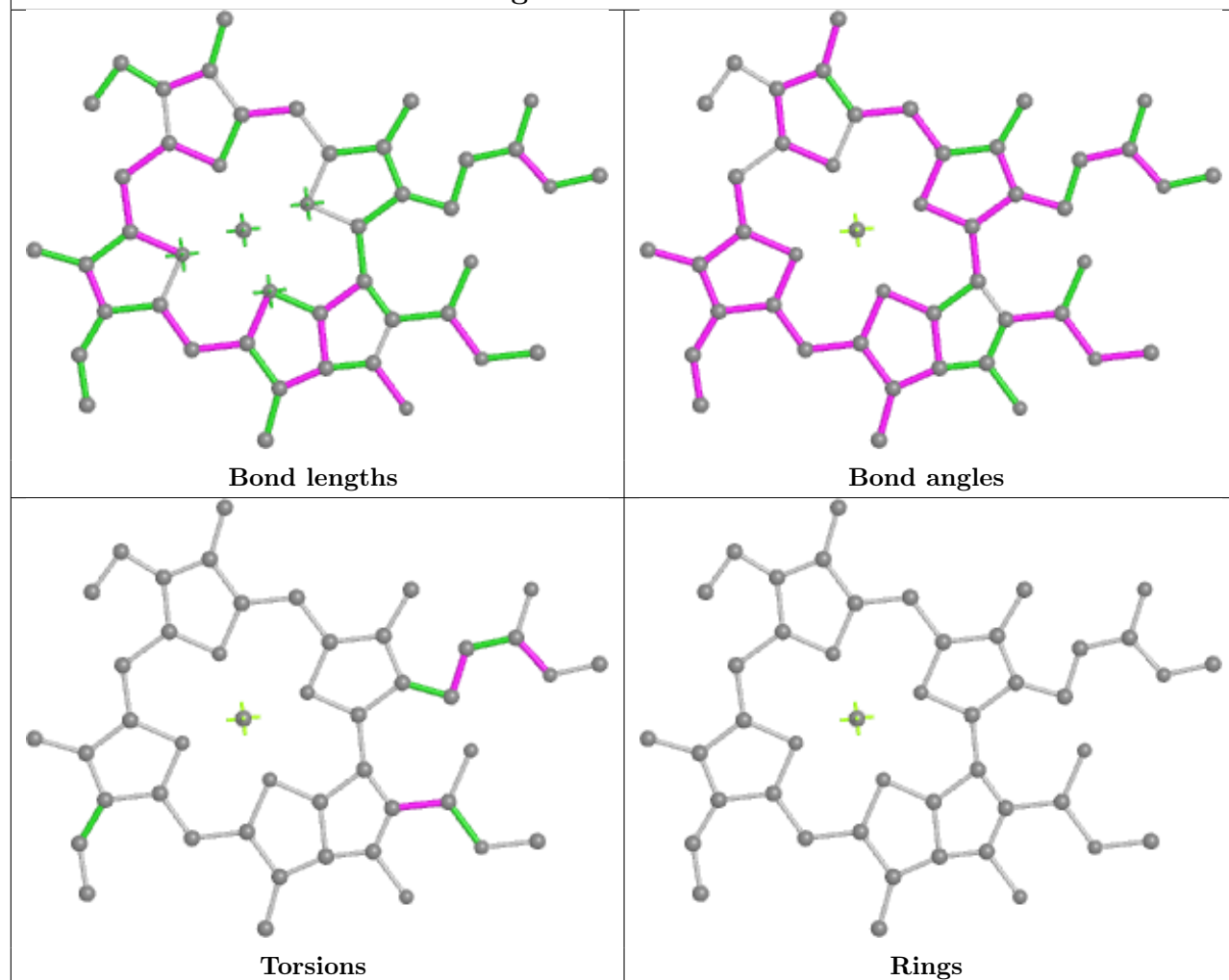


Rings

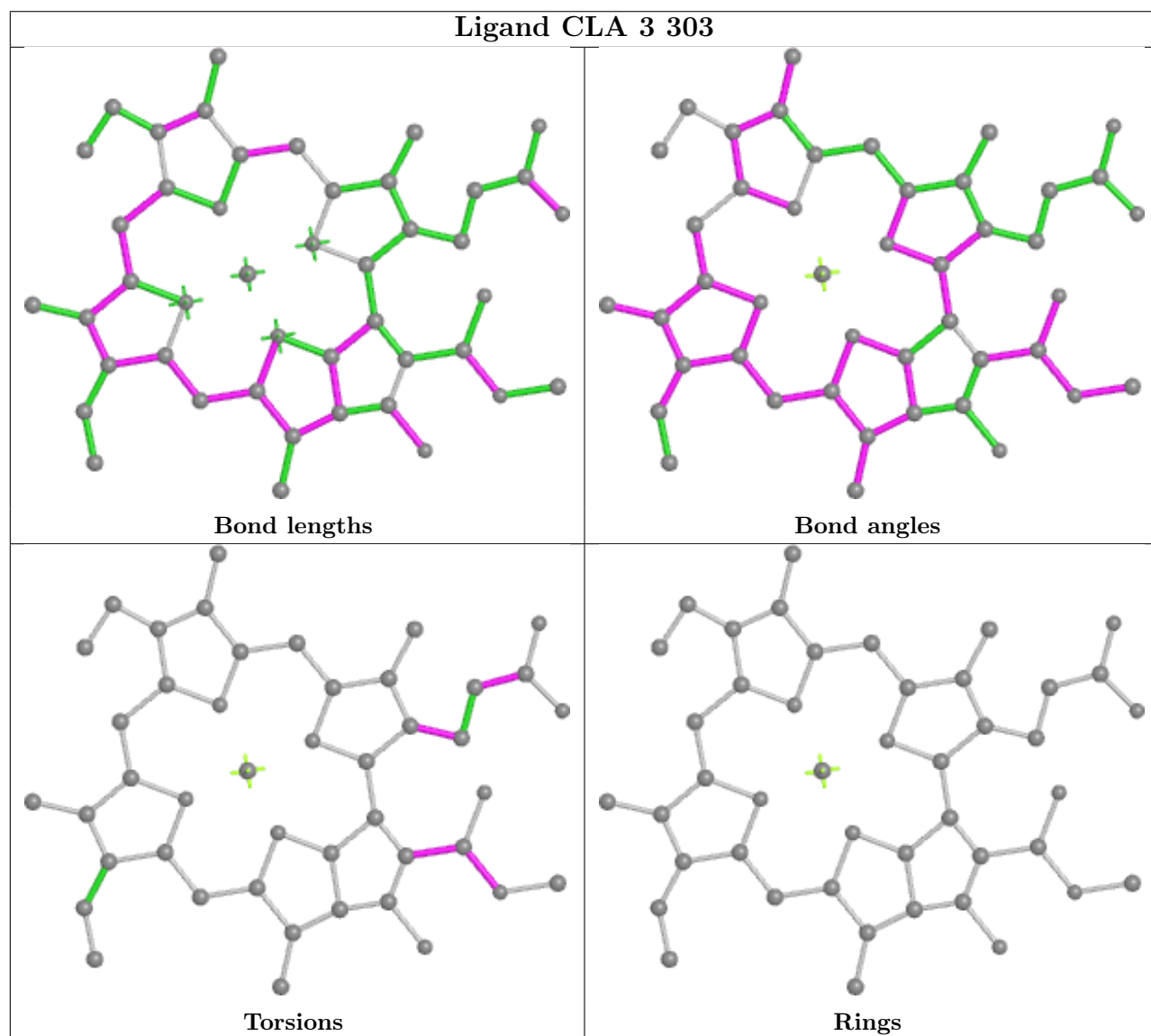
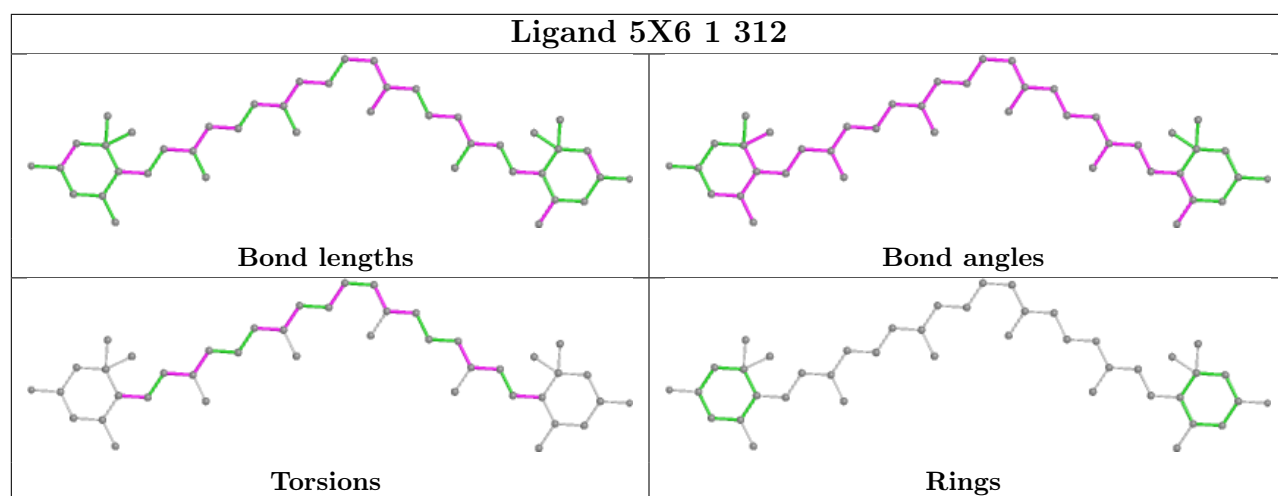
## Ligand 5X6 1 311



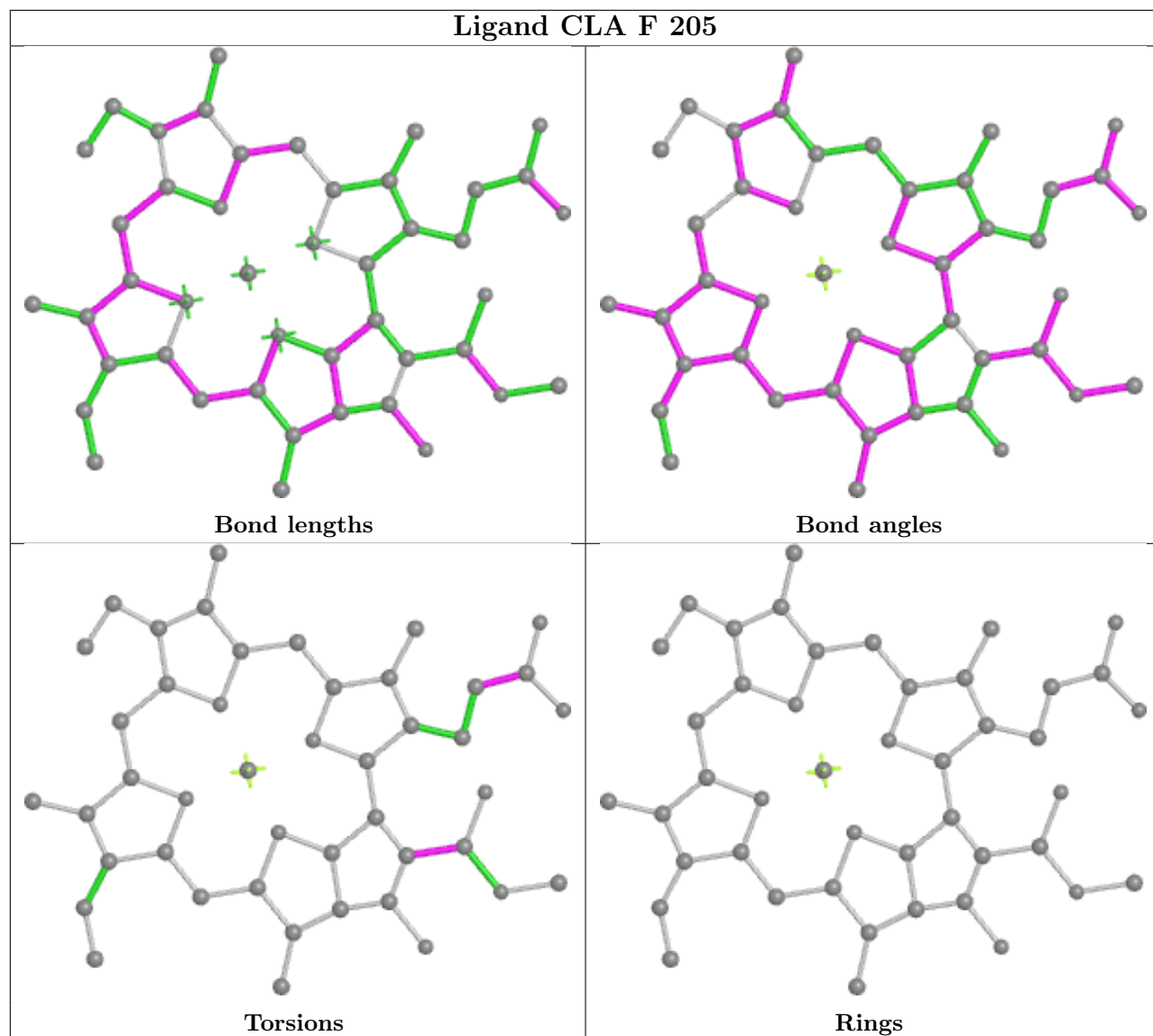
## Ligand CLA O 203

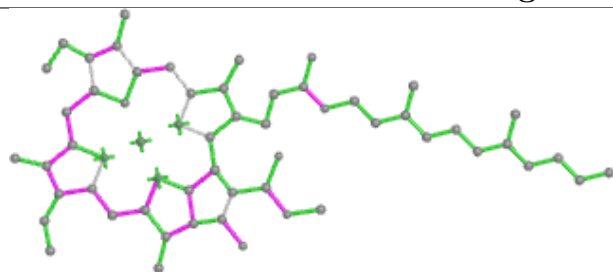




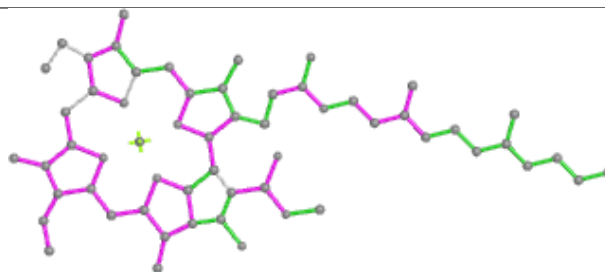


## Ligand CLA F 205

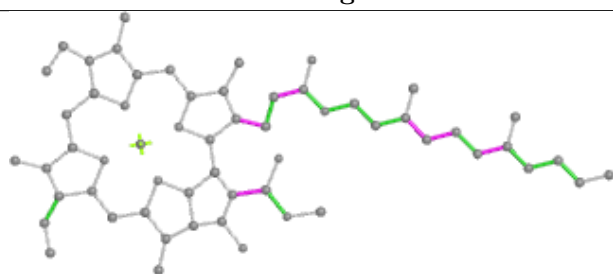


**Ligand CLA 2 303**

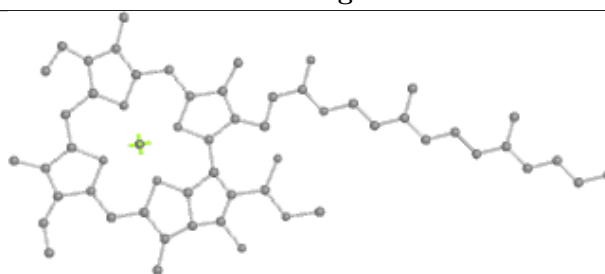
Bond lengths



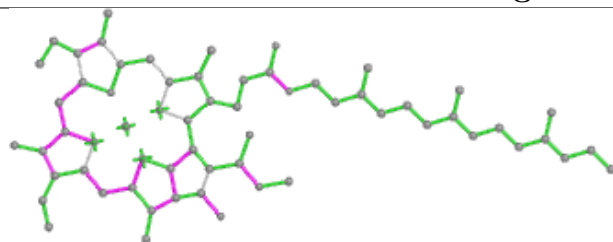
Bond angles



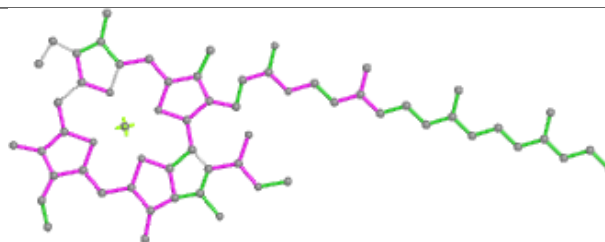
Torsions



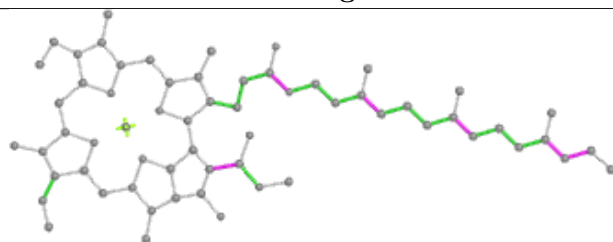
Rings

**Ligand CLA A 815**

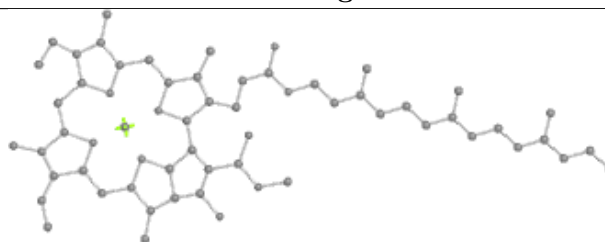
Bond lengths



Bond angles

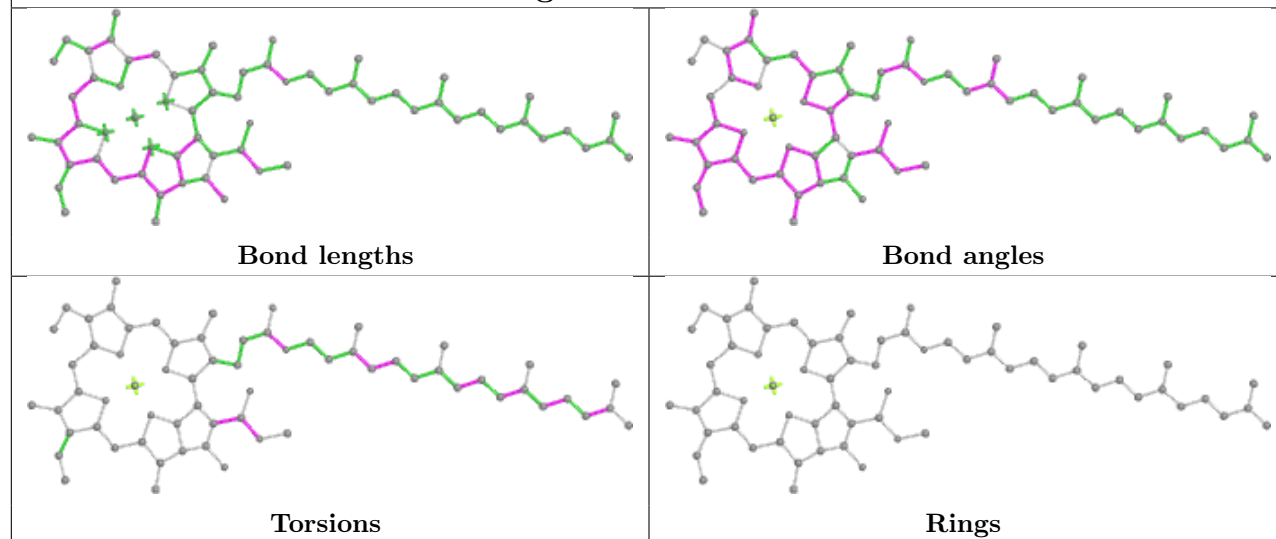


Torsions

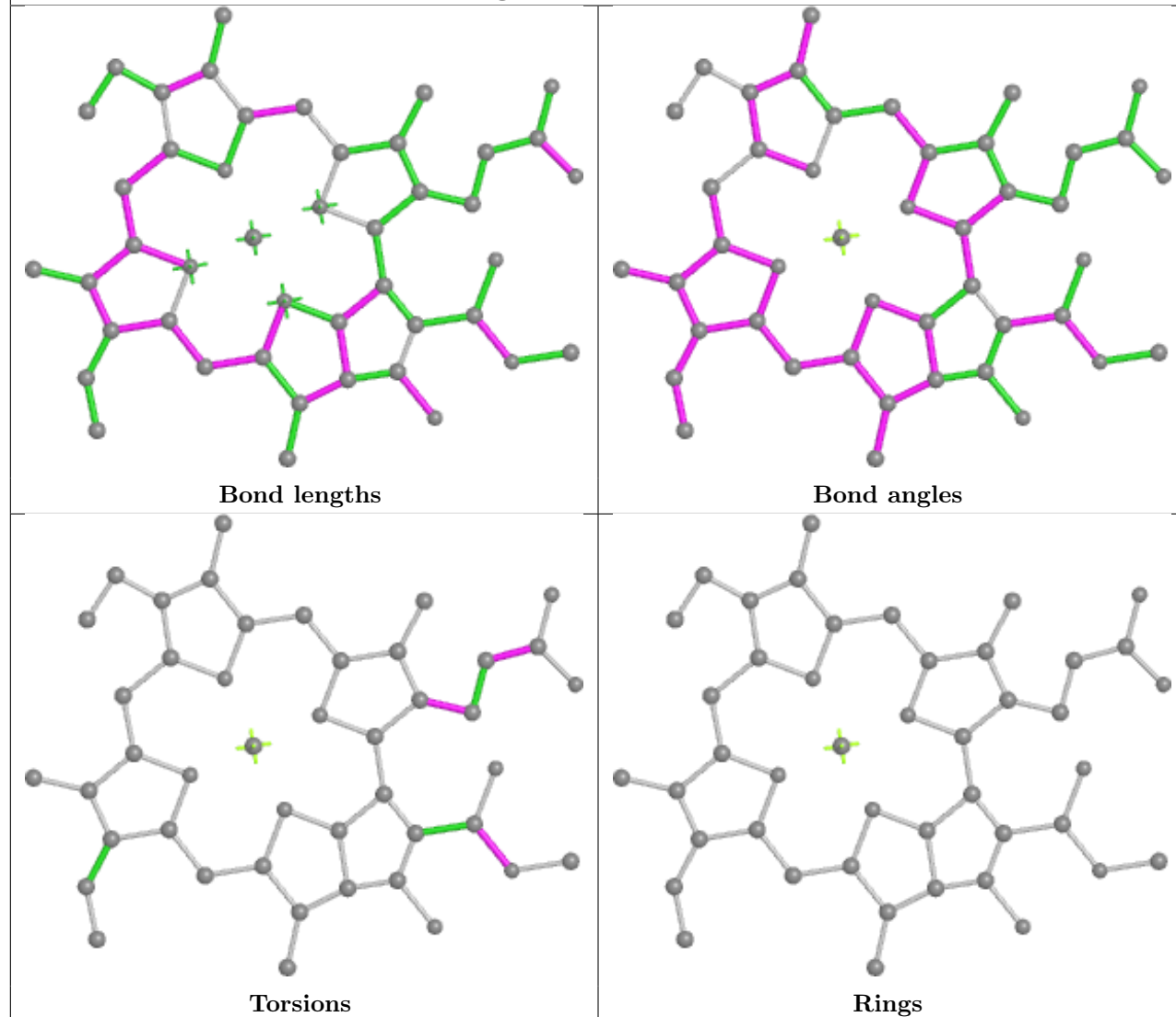


Rings

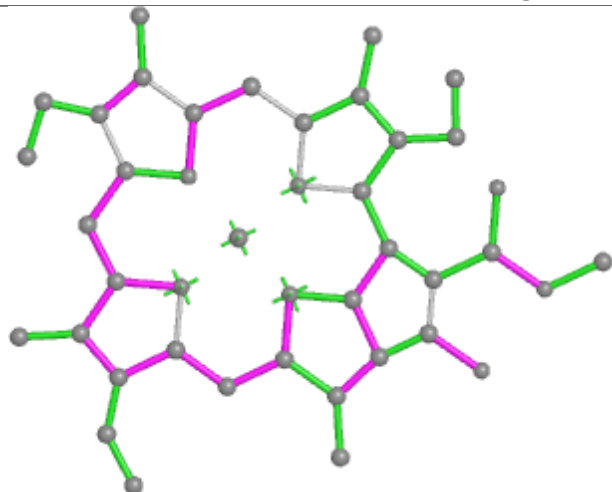
## Ligand CLA 2 304



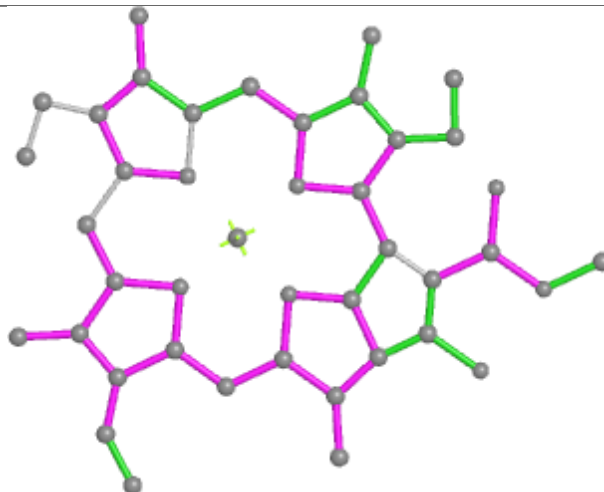
## Ligand CLA 6 303



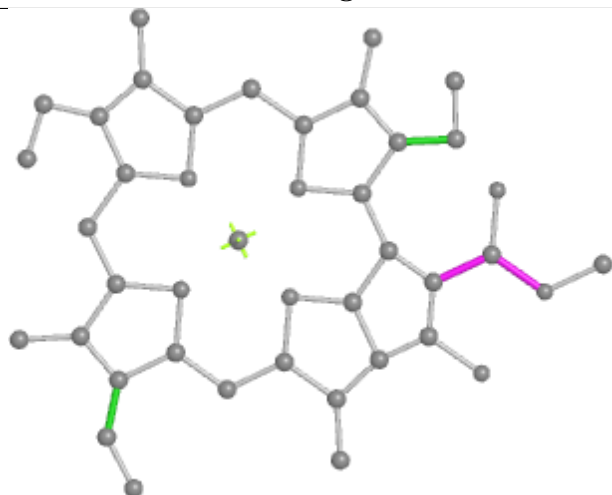
## Ligand CLA 6 314



Bond lengths



Bond angles

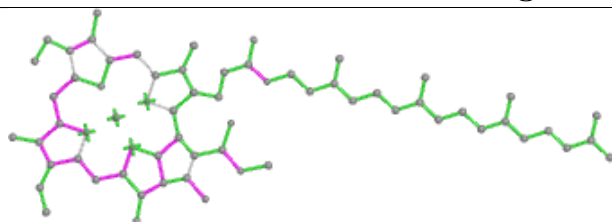


Torsions

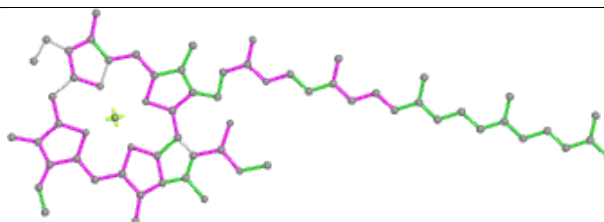


Rings

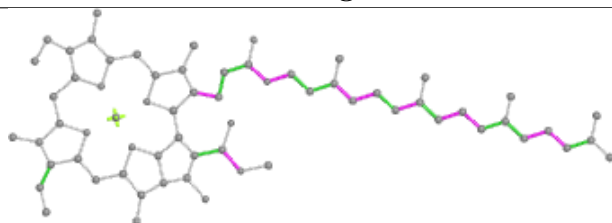
## Ligand CLA 1 310



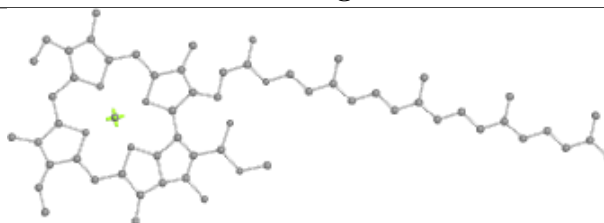
Bond lengths



Bond angles

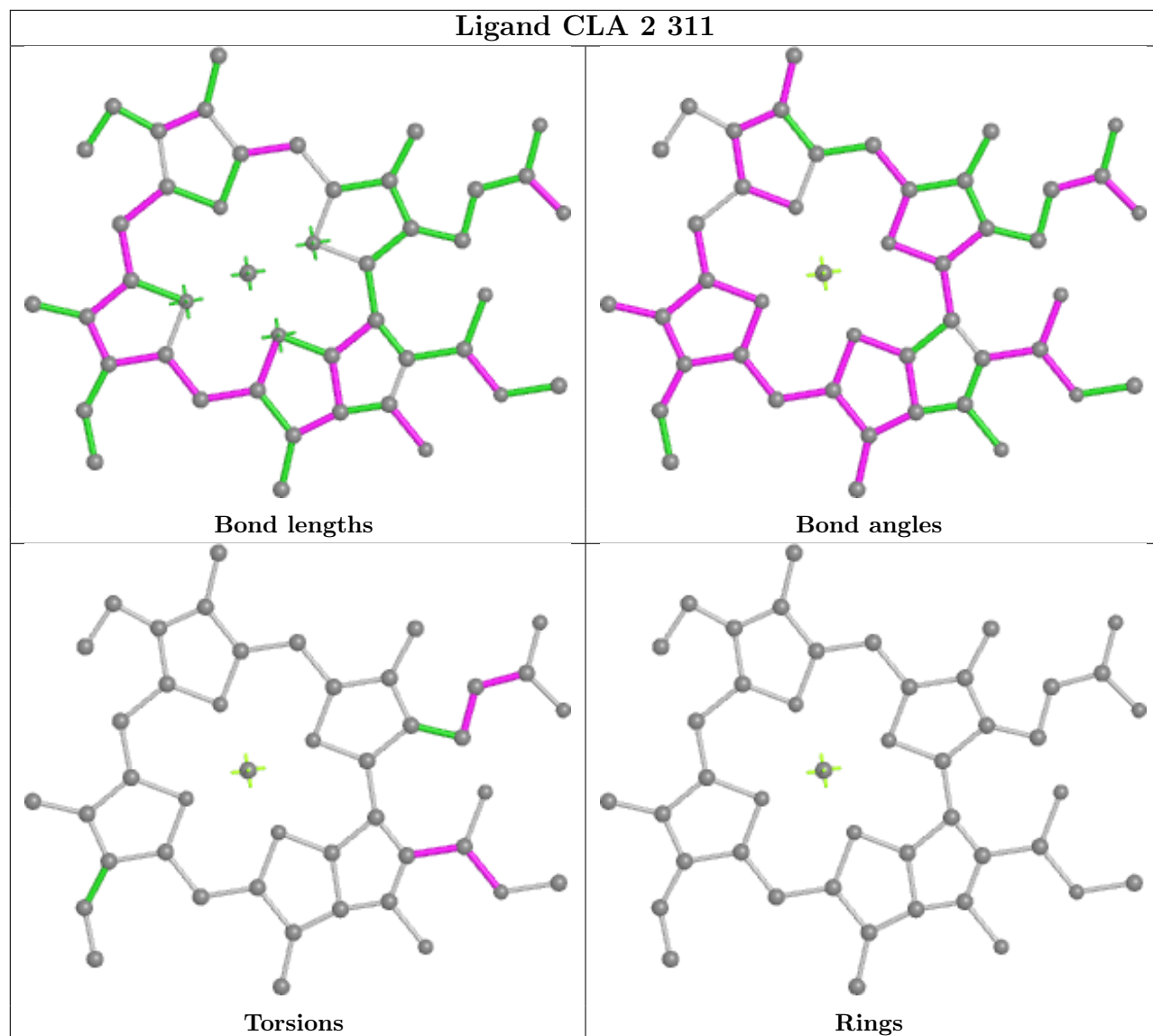


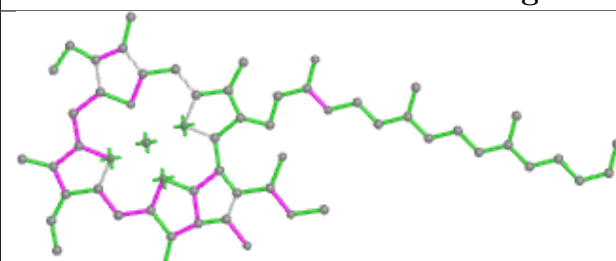
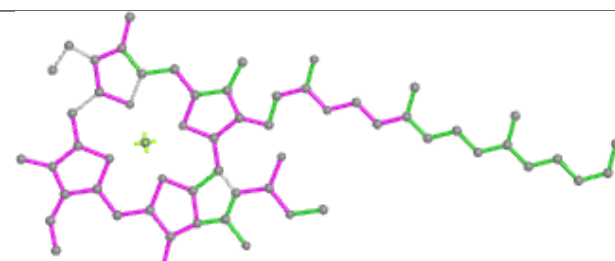
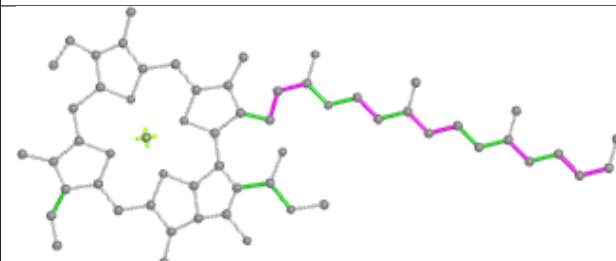
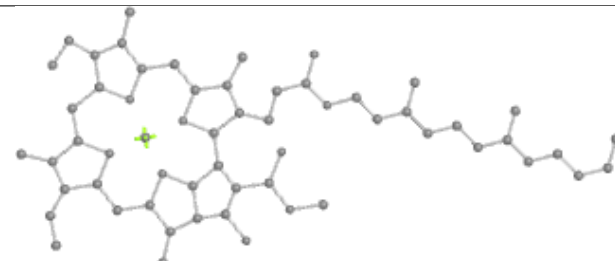
Torsions

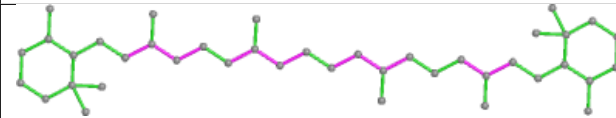
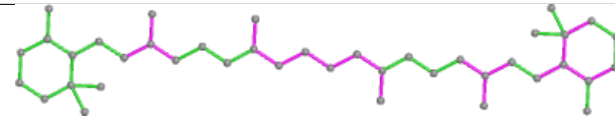
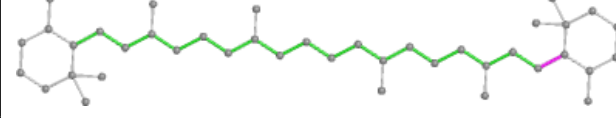
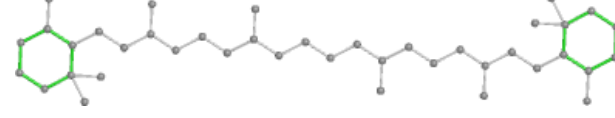


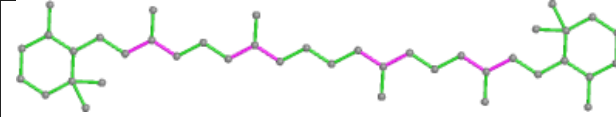
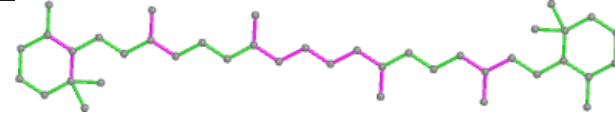
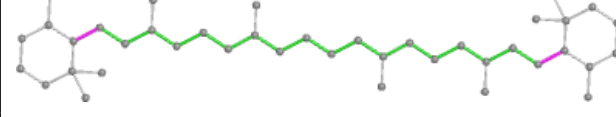
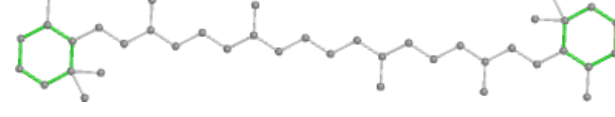
Rings

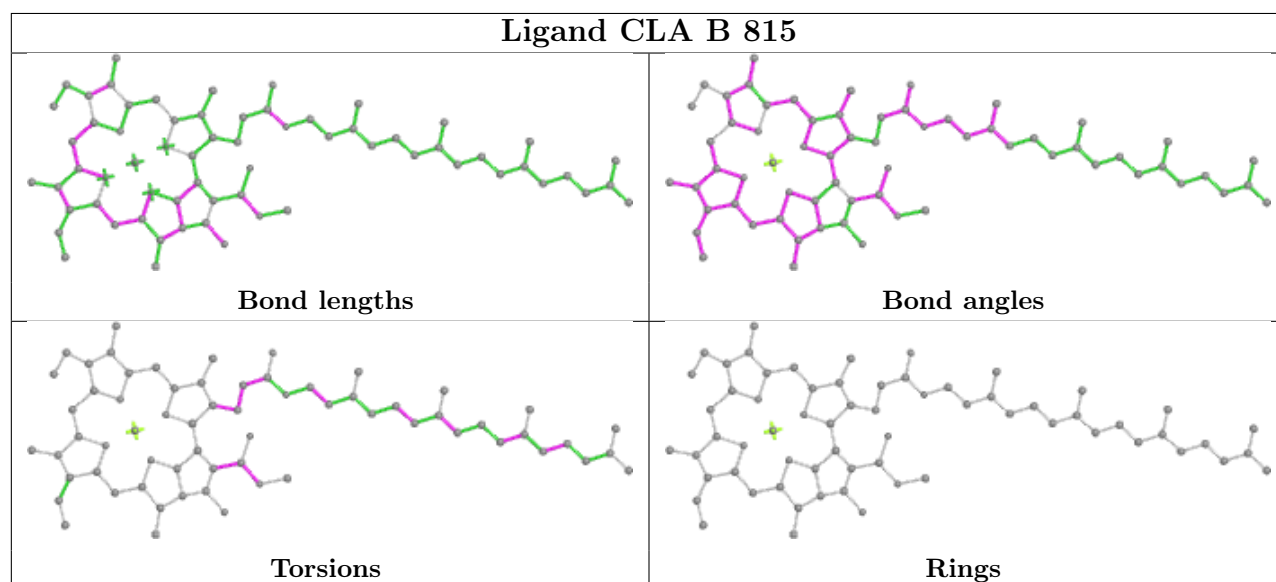
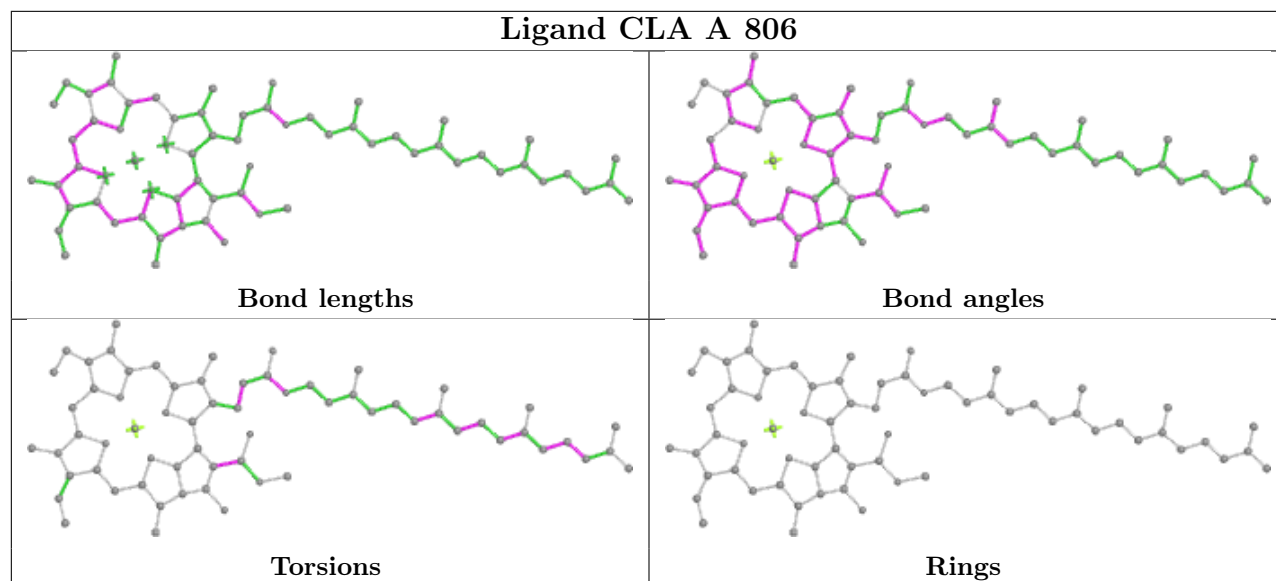
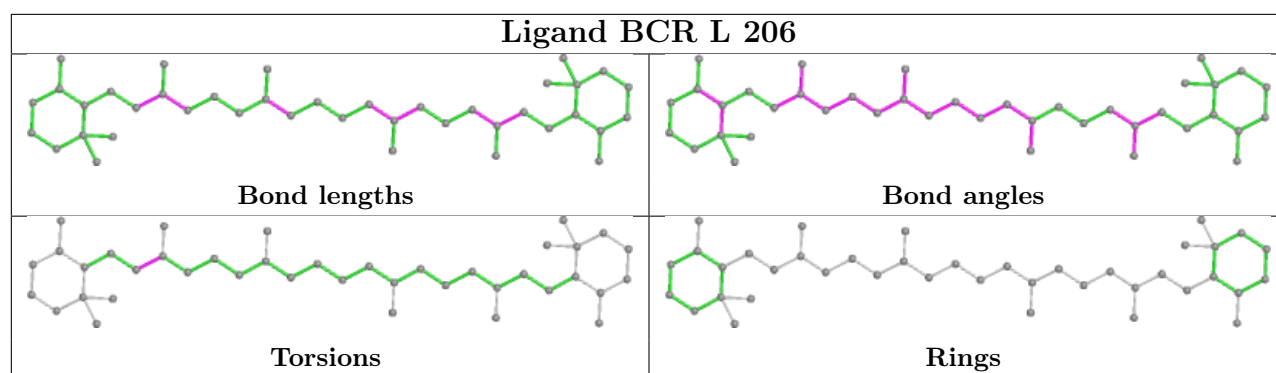
## Ligand CLA 2 311



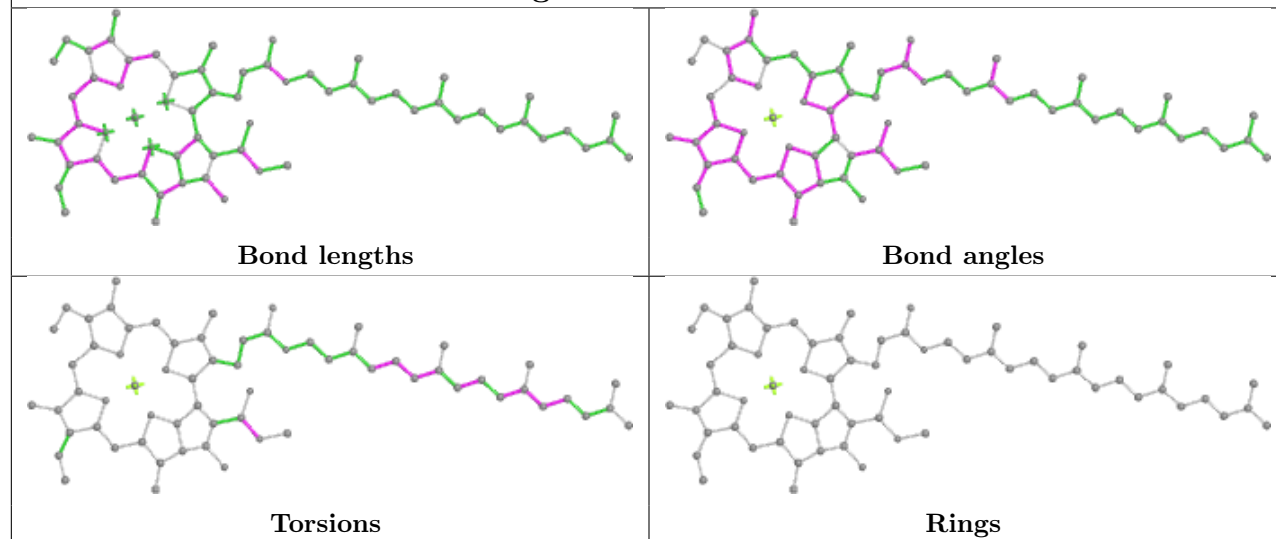
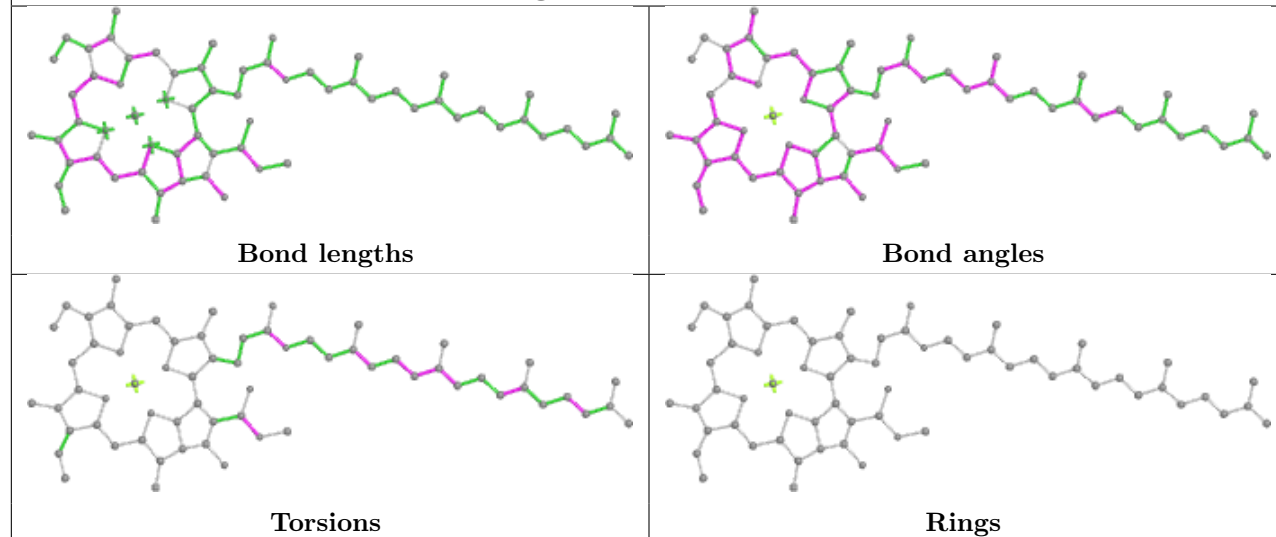
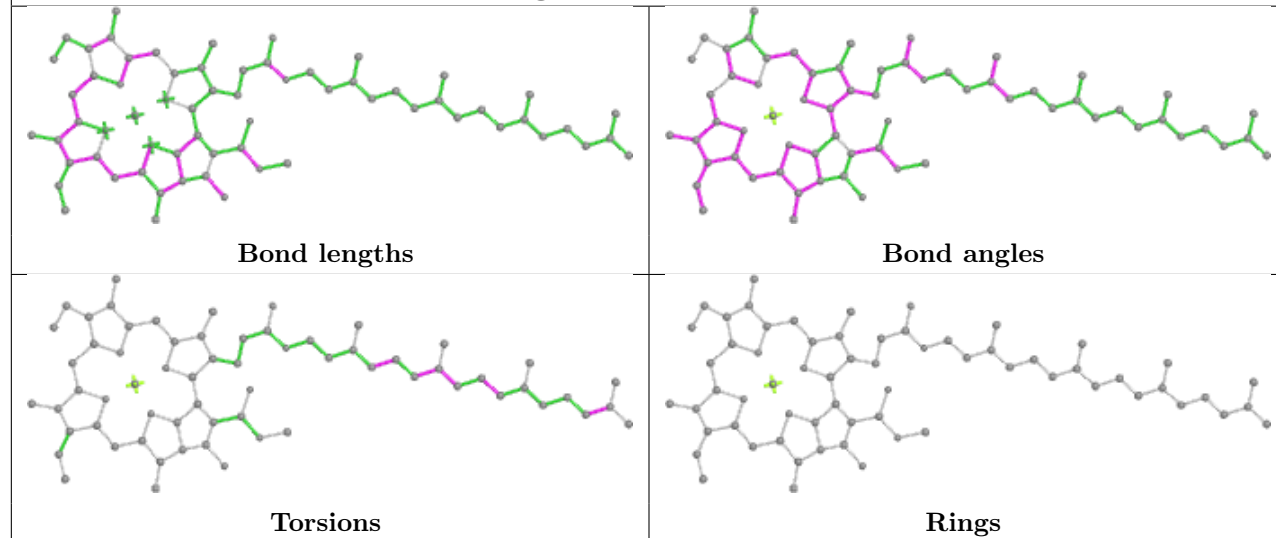
Ligand CLA B 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

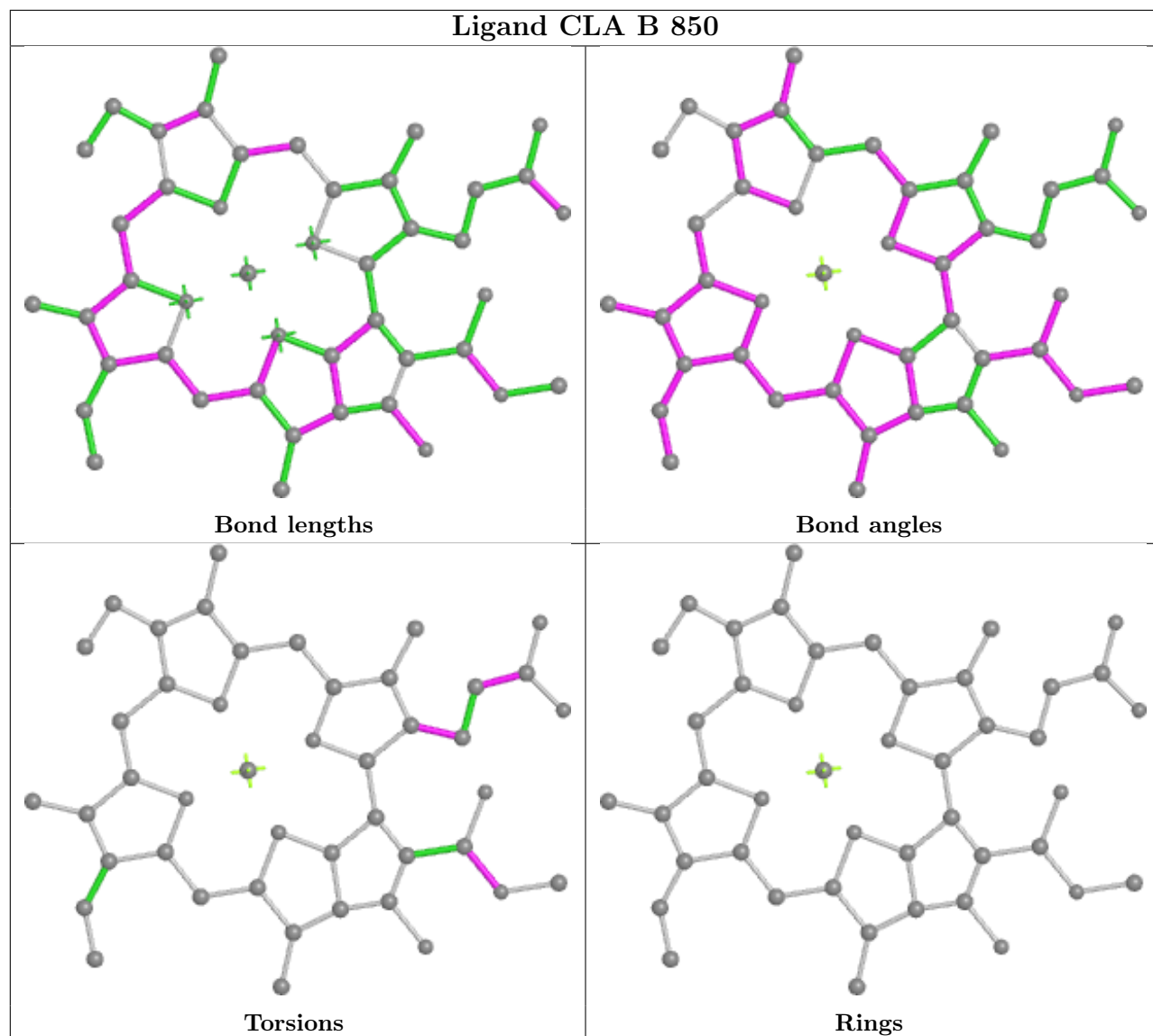
Ligand BCR B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

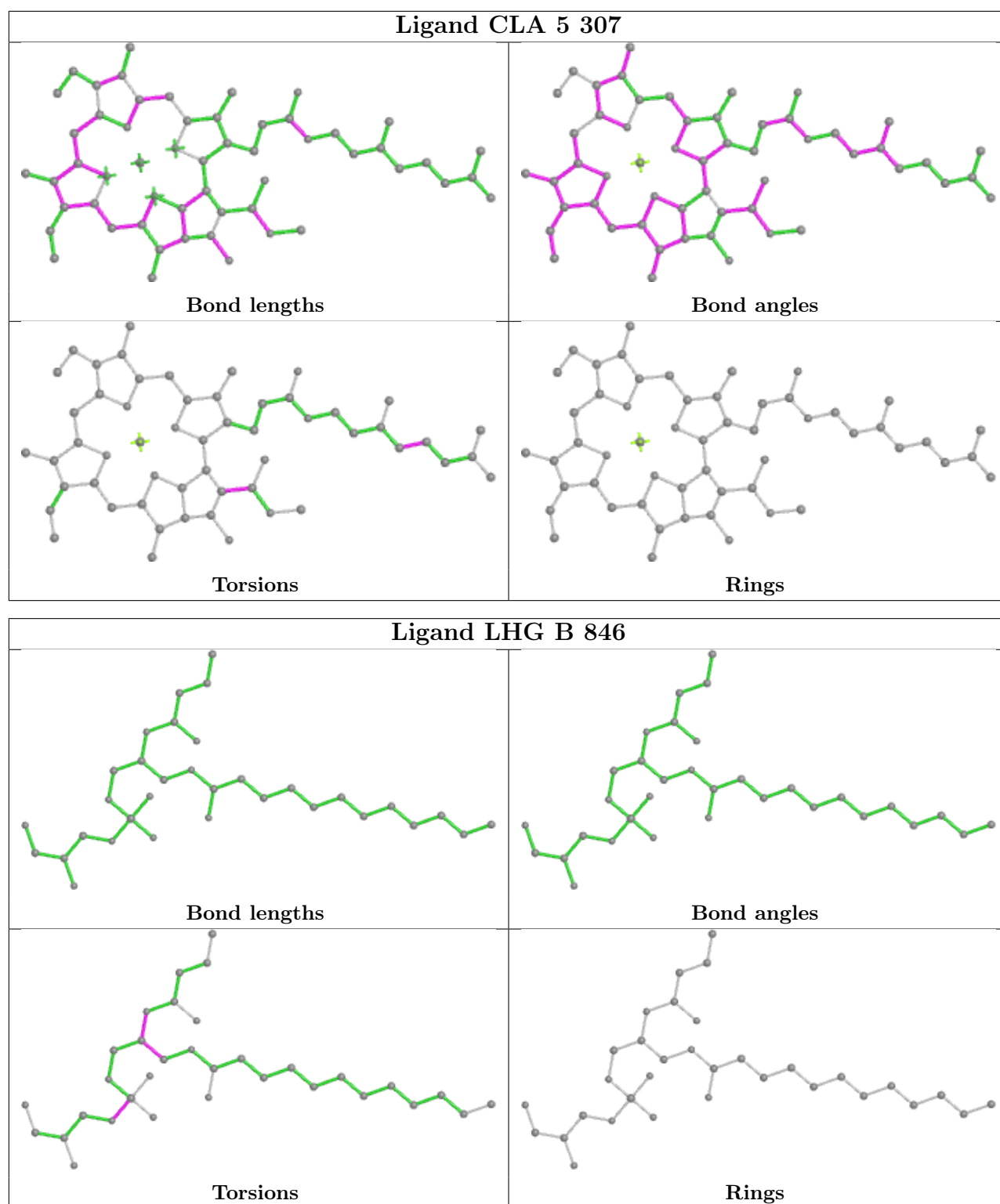




**Ligand CLA B 822****Ligand CLA B 838****Ligand CLA B 833**

## Ligand CLA B 850





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

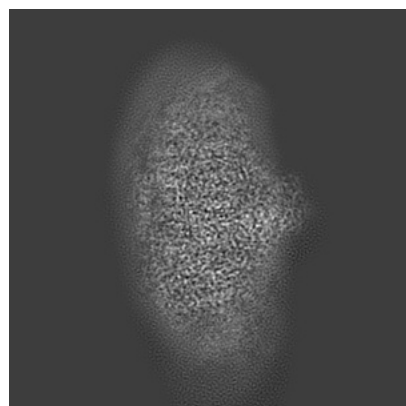
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62242. These allow visual inspection of the internal detail of the map and identification of artifacts.

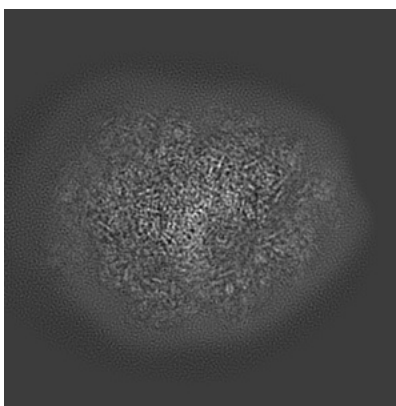
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

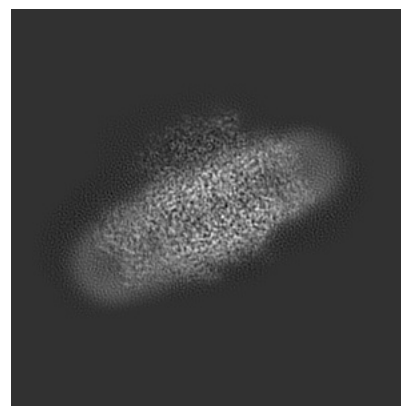
#### 6.1.1 Primary map



X

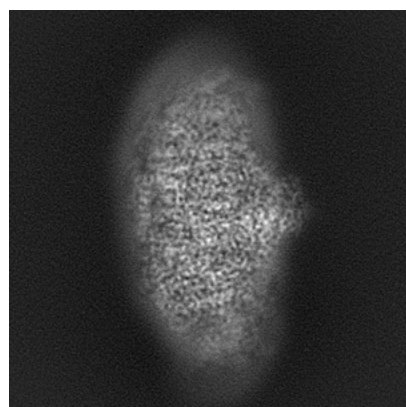


Y

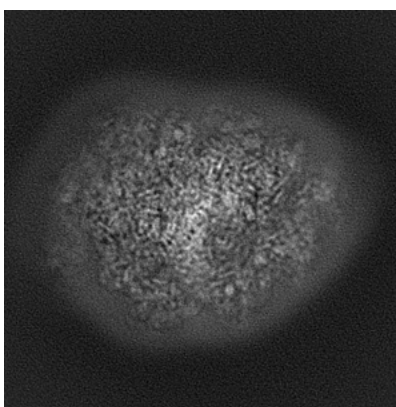


Z

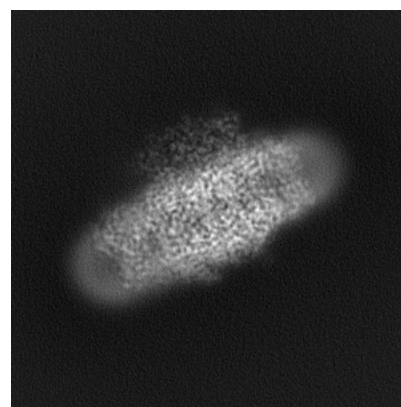
#### 6.1.2 Raw map



X



Y

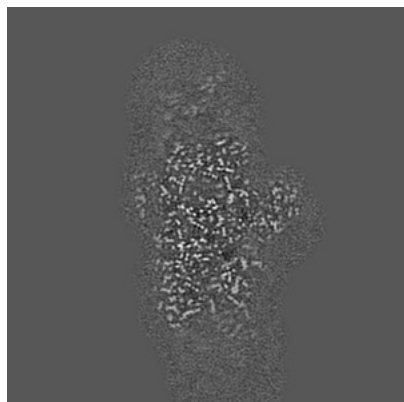


Z

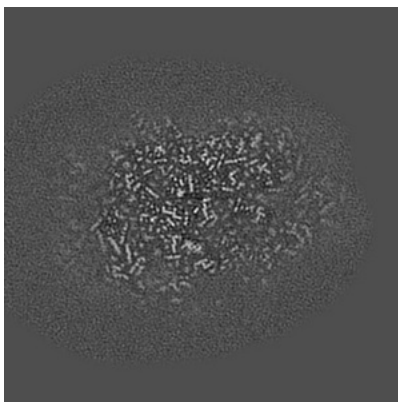
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

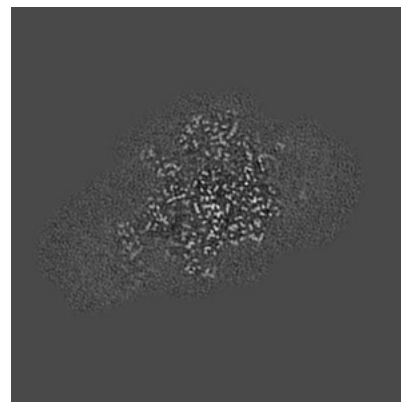
### 6.2.1 Primary map



X Index: 160

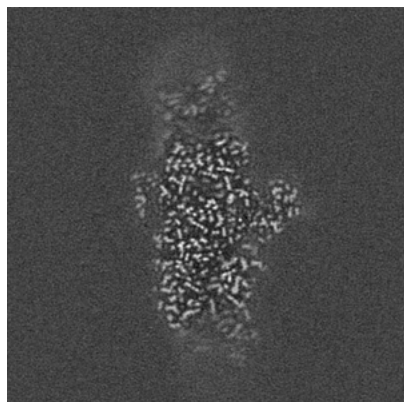


Y Index: 160

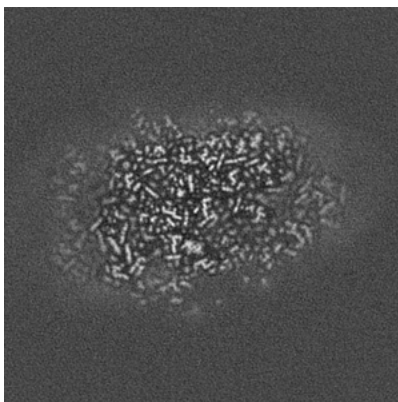


Z Index: 160

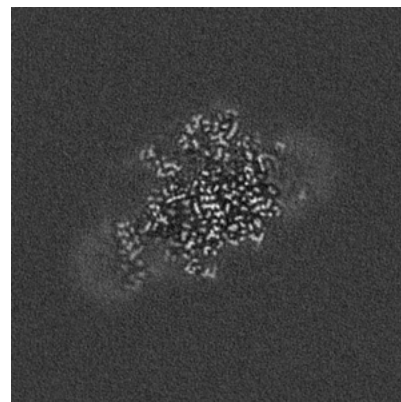
### 6.2.2 Raw map



X Index: 160



Y Index: 160

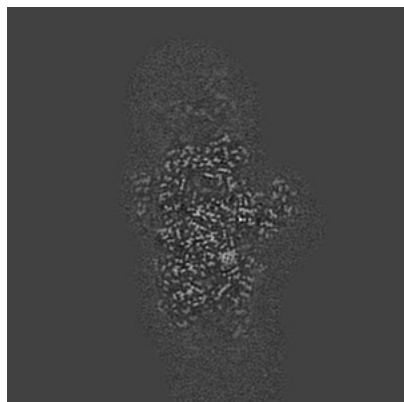


Z Index: 160

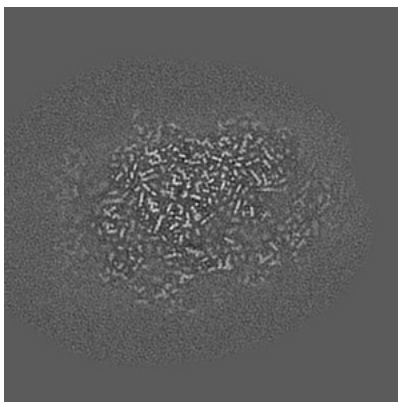
The images above show central slices of the map in three orthogonal directions.

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

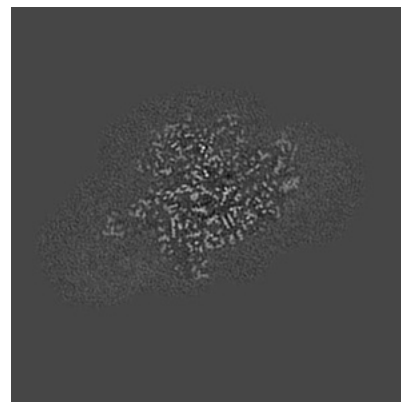
### 6.3.1 Primary map



X Index: 158

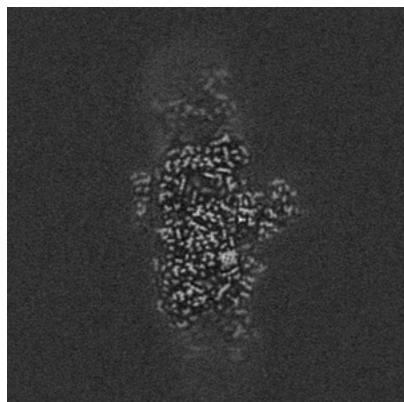


Y Index: 158

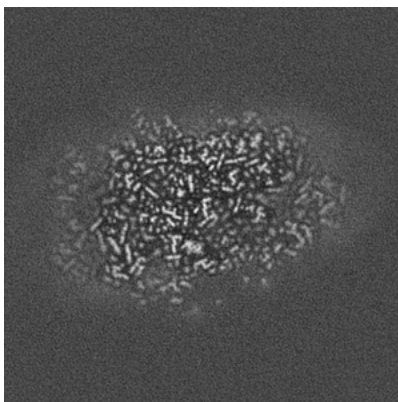


Z Index: 147

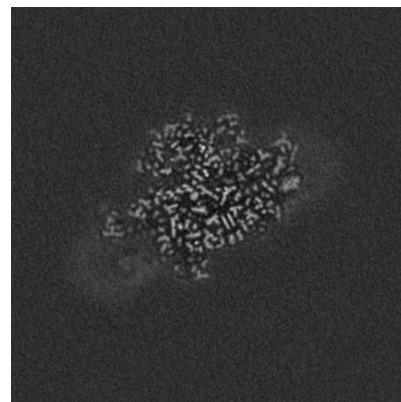
### 6.3.2 Raw map



X Index: 158



Y Index: 160



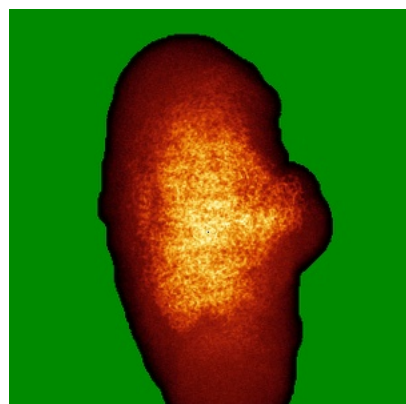
Z Index: 147

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

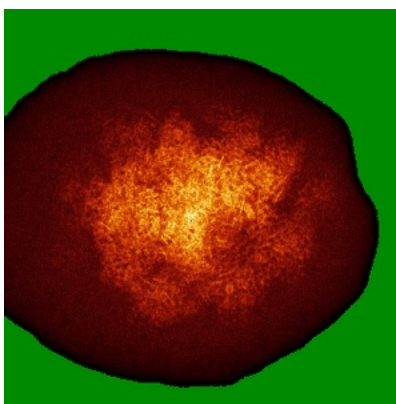


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

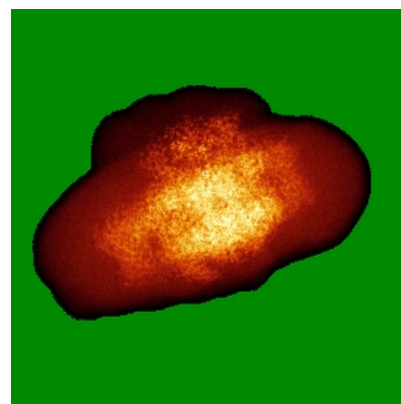
### 6.4.1 Primary map



X

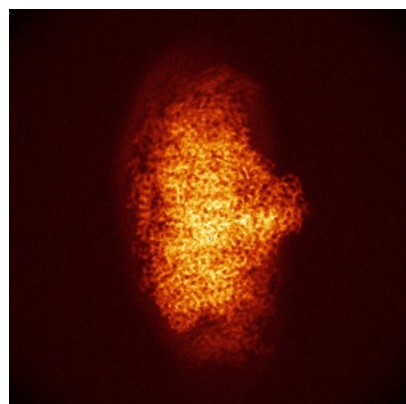


Y

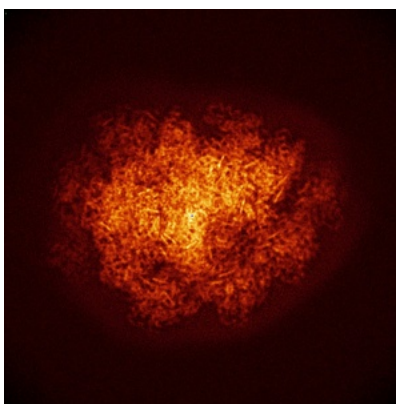


Z

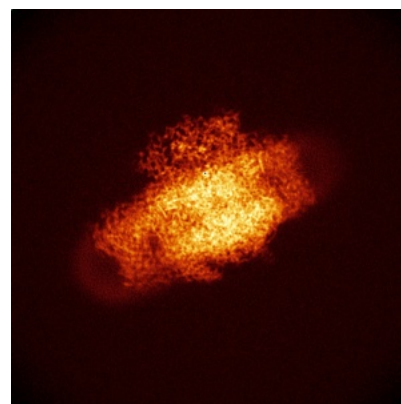
### 6.4.2 Raw map



X



Y



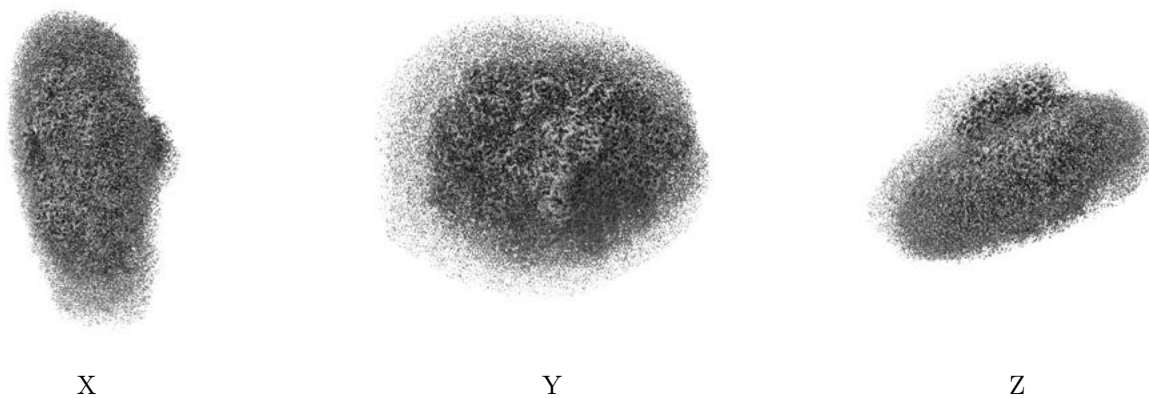
Z

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.



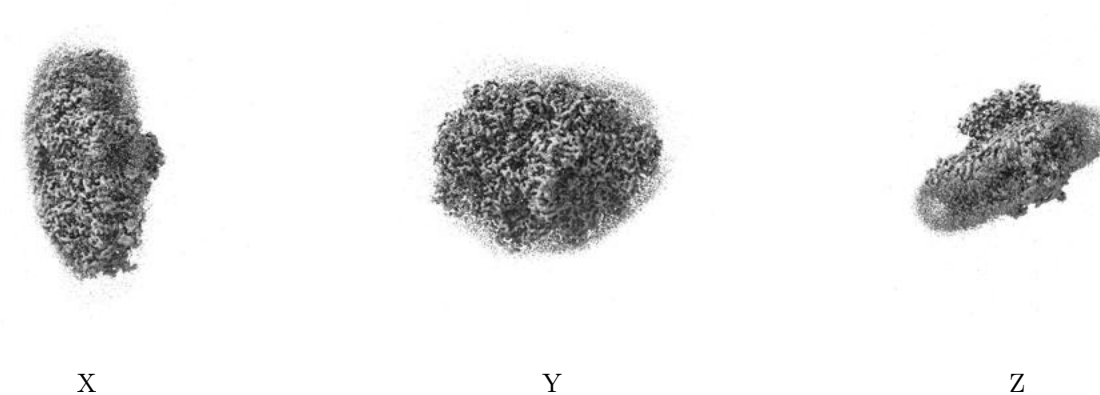
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

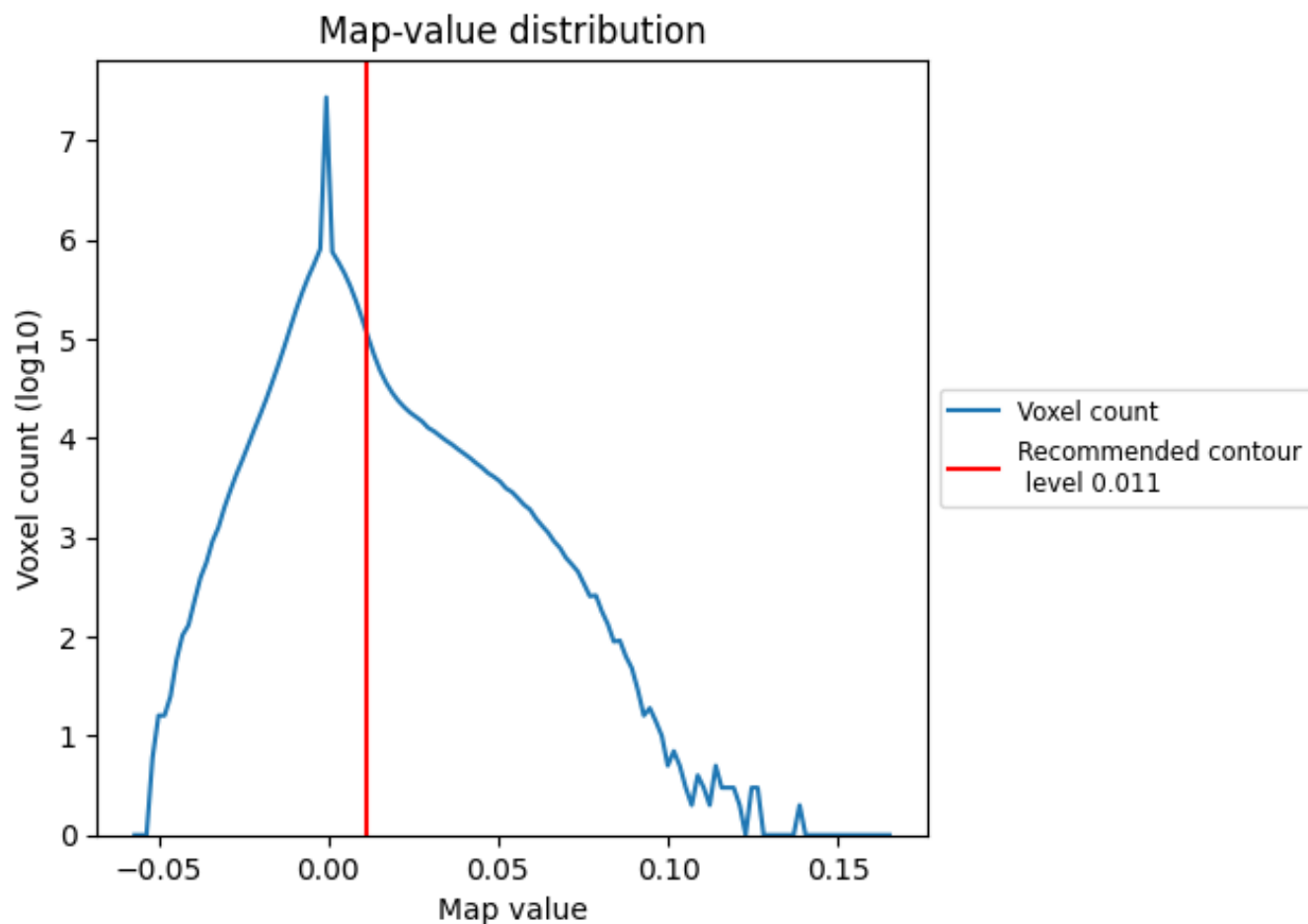
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

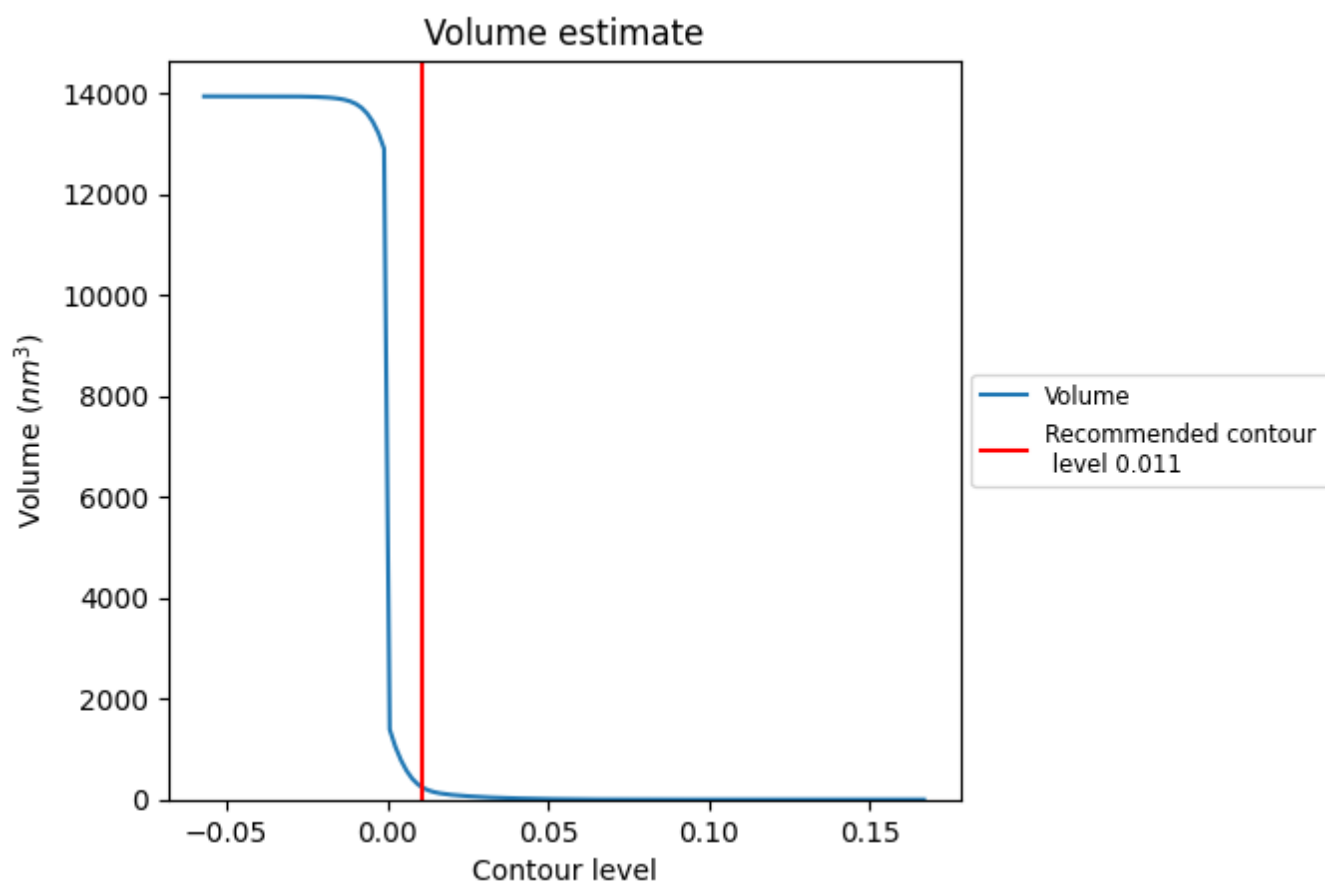
This section contains the results of statistical analysis of the map.

### 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.

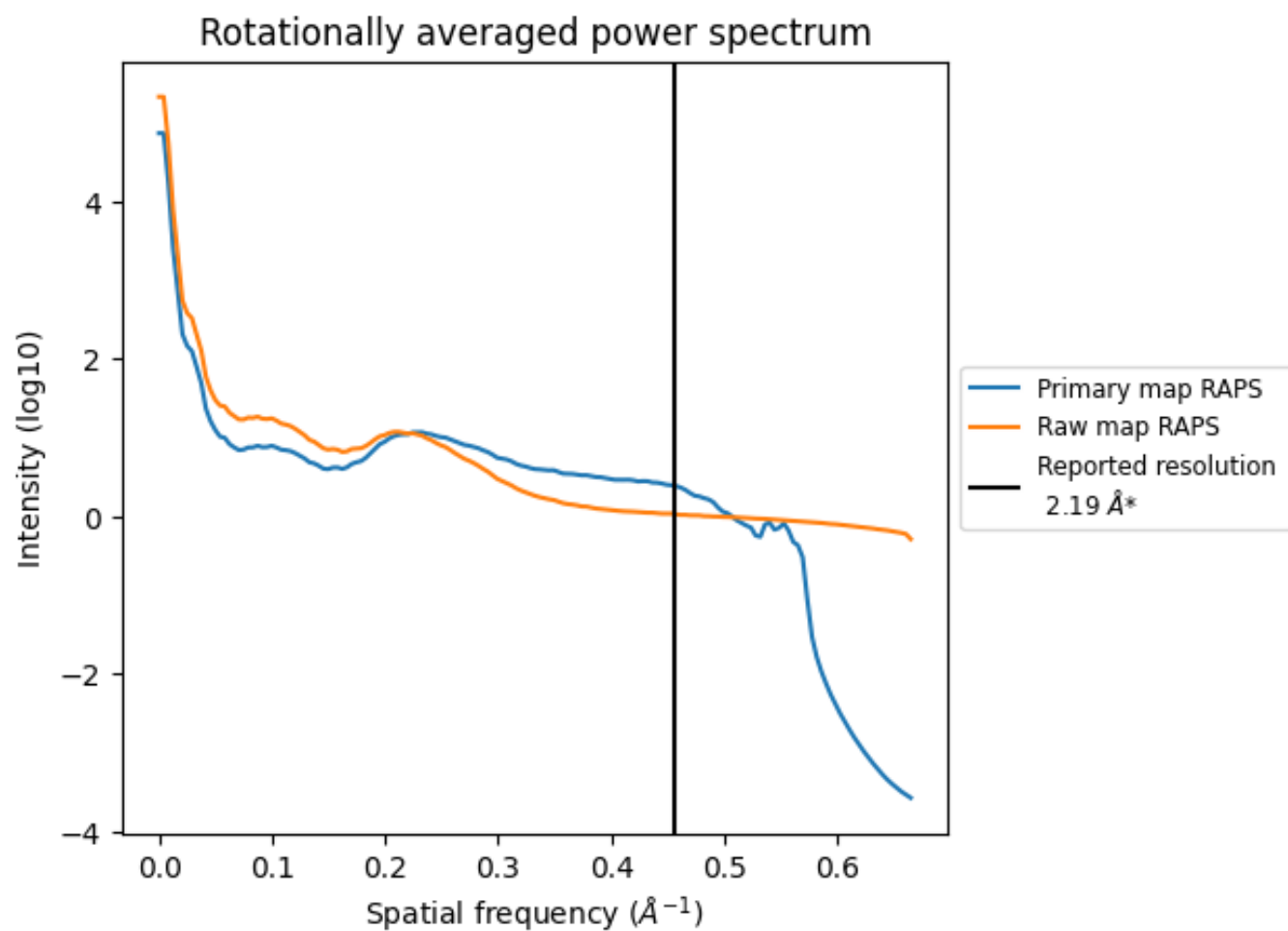
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238  $\text{nm}^3$ ; this corresponds to an approximate mass of 215 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 ⓘ

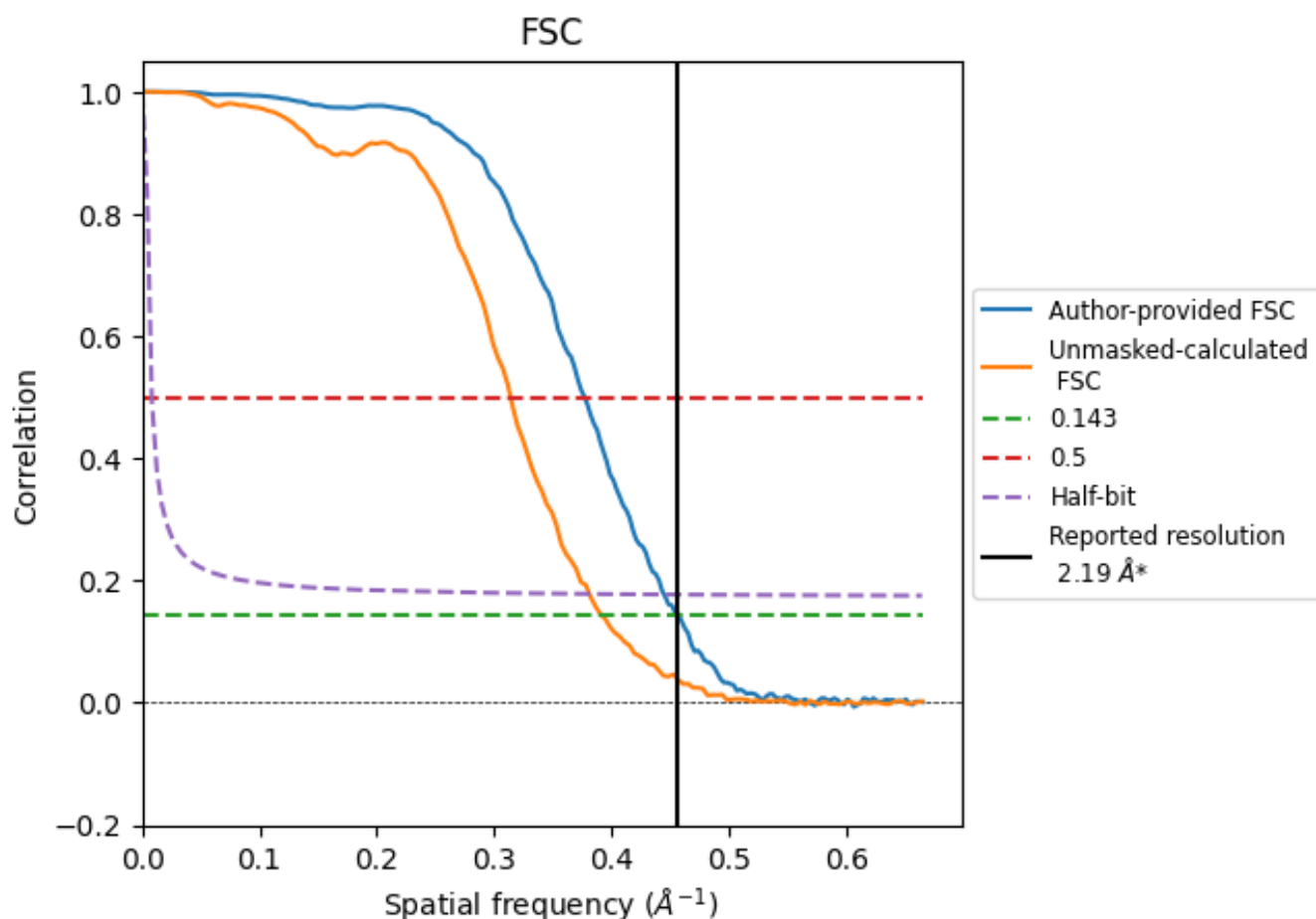


\*Reported resolution corresponds to spatial frequency of 0.457 Å<sup>-1</sup>

## 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 0.457 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

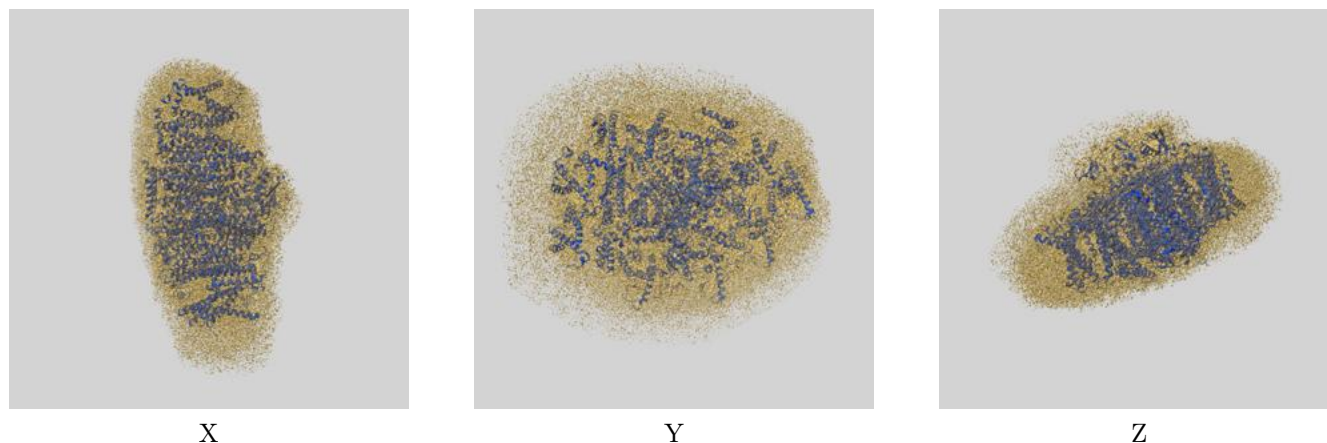
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.19	2.65	2.24
Unmasked-calculated*	2.55	3.18	2.62

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.55 differs from the reported value 2.19 by more than 10 %

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

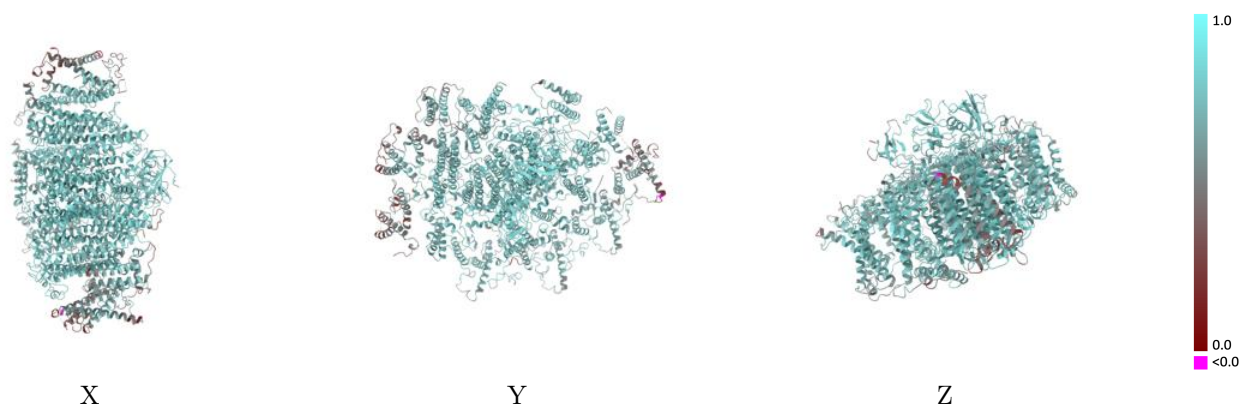
This section contains information regarding the fit between EMDB map EMD-62242 and PDB model 9KC5. Per-residue inclusion information can be found in section [3](#) on page [30](#).

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



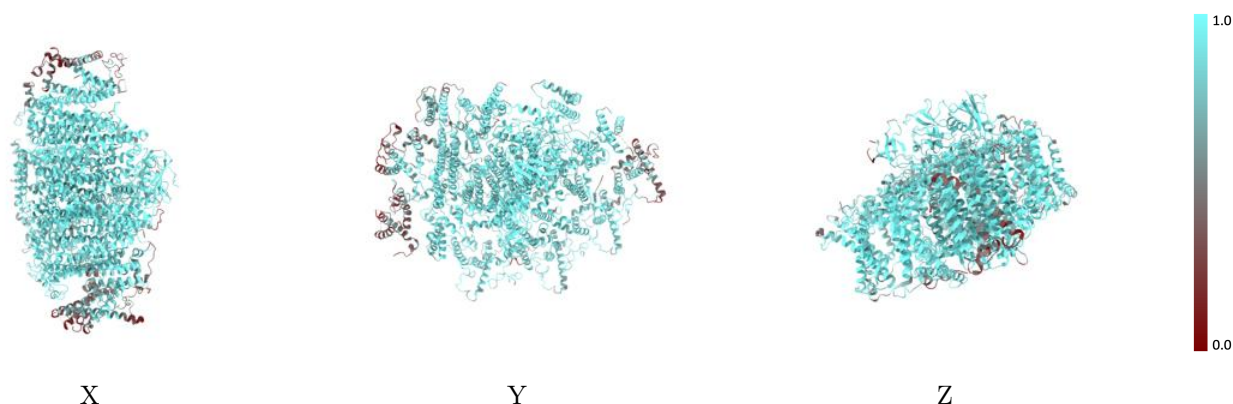
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

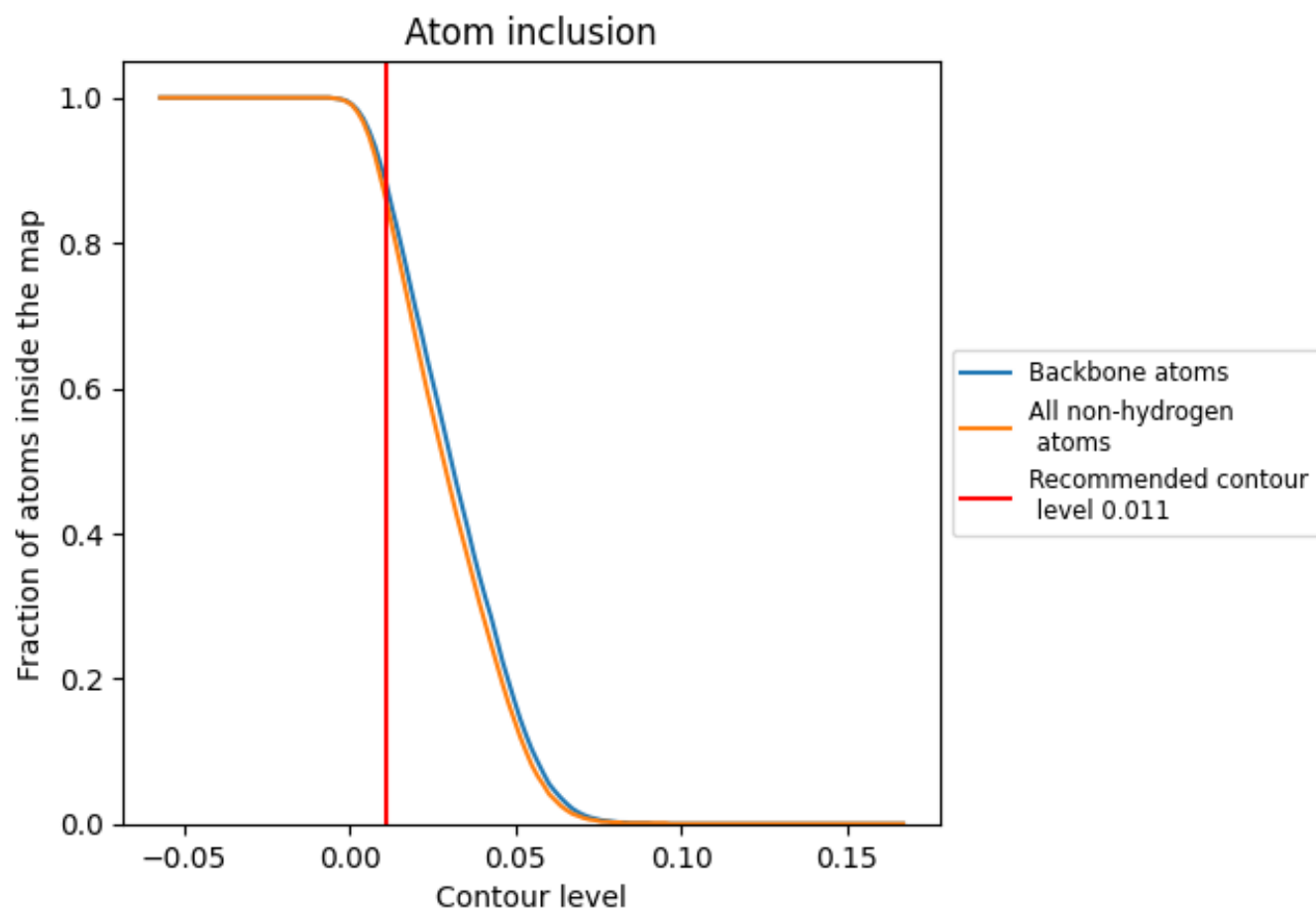
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8610	<div><div></div></div> 0.6870
1	<div><div></div></div> 0.7200	<div><div></div></div> 0.6010
2	<div><div></div></div> 0.5950	<div><div></div></div> 0.5410
3	<div><div></div></div> 0.3740	<div><div></div></div> 0.4350
4	<div><div></div></div> 0.8710	<div><div></div></div> 0.6700
5	<div><div></div></div> 0.8700	<div><div></div></div> 0.6590
6	<div><div></div></div> 0.8630	<div><div></div></div> 0.6520
7	<div><div></div></div> 0.5370	<div><div></div></div> 0.4840
A	<div><div></div></div> 0.9510	<div><div></div></div> 0.7560
B	<div><div></div></div> 0.9530	<div><div></div></div> 0.7560
C	<div><div></div></div> 0.9900	<div><div></div></div> 0.7830
D	<div><div></div></div> 0.9280	<div><div></div></div> 0.7280
E	<div><div></div></div> 0.8640	<div><div></div></div> 0.6980
F	<div><div></div></div> 0.9240	<div><div></div></div> 0.7260
I	<div><div></div></div> 0.8890	<div><div></div></div> 0.6970
J	<div><div></div></div> 0.9190	<div><div></div></div> 0.7140
K	<div><div></div></div> 0.8370	<div><div></div></div> 0.6510
L	<div><div></div></div> 0.8750	<div><div></div></div> 0.6870
M	<div><div></div></div> 0.7980	<div><div></div></div> 0.6310
O	<div><div></div></div> 0.8420	<div><div></div></div> 0.6600
Z	<div><div></div></div> 0.9320	<div><div></div></div> 0.7120

