



## wwPDB EM Validation Summary Report ⓘ

Sep 17, 2025 – 01:39 pm BST

PDB ID : 9GC2 / pdb\_00009gc2  
EMDB ID : EMD-51227  
Title : Cryo-EM structure of Arabidopsis thaliana PSI-LHCI- a603-NH mutant  
Authors : Capaldi, S.; Chaves-Sanjuan, A.; Bonnet, D.M.V.; Bassi, R.  
Deposited on : 2024-08-01  
Resolution : 3.29 Å(reported)  
Based on initial model : 9GBI

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>.

---

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

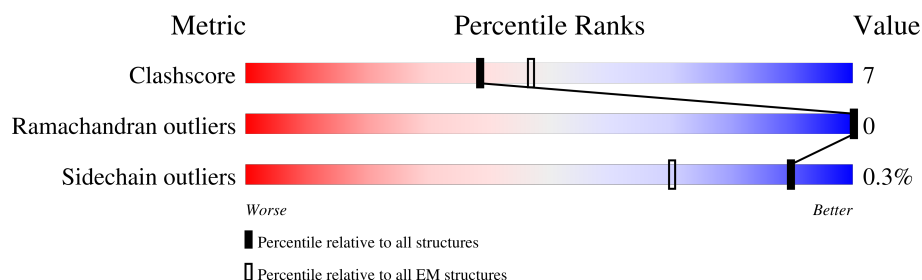
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.29 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.





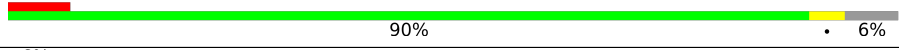



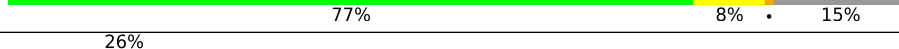
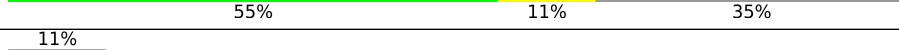
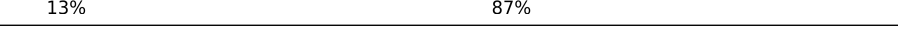
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	206	<div> <div>13%</div> <div>78%</div> <div>17%</div> <div>6%</div> </div>
2	2	214	<div> <div>5%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
3	3	234	<div> <div>6%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
4	4	199	<div> <div>6%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
5	A	750	<div> <div>.</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
6	B	734	<div> <div>89%</div> <div>11%</div> </div>
7	C	81	<div> <div>79%</div> <div>20%</div> <div>.</div> </div>
8	D	160	<div> <div>72%</div> <div>15%</div> <div>.</div> <div>12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	E	99	
10	F	154	
11	G	100	
12	H	95	
13	I	37	
14	J	44	
15	L	169	
16	K	84	
17	N	85	

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
18	CHL	1	301	X	-	-	-
18	CHL	1	306	X	-	-	-
18	CHL	2	301	X	-	-	-
18	CHL	2	305	X	-	-	-
18	CHL	2	306	X	-	-	-
18	CHL	2	307	X	-	-	-
18	CHL	2	314	X	-	-	-
18	CHL	3	307	X	-	-	-
18	CHL	4	305	X	-	-	-
18	CHL	4	306	X	-	-	-
18	CHL	4	307	X	-	-	-
18	CHL	4	314	X	-	-	-
19	CLA	1	302	X	-	-	-
19	CLA	1	303	X	-	-	-
19	CLA	1	304	X	-	-	-
19	CLA	1	305	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	1	311	X	-	-	-
19	CLA	1	312	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	313	X	-	-	-
19	CLA	1	314	X	-	-	-
19	CLA	1	318	X	-	-	-
19	CLA	2	302	X	-	-	-
19	CLA	2	303	X	-	-	-
19	CLA	2	304	X	-	-	-
19	CLA	2	308	X	-	-	-
19	CLA	2	309	X	-	-	-
19	CLA	2	310	X	-	-	-
19	CLA	2	311	X	-	-	-
19	CLA	2	312	X	-	-	-
19	CLA	2	313	X	-	-	-
19	CLA	3	301	X	-	-	-
19	CLA	3	302	X	-	-	-
19	CLA	3	303	X	-	-	-
19	CLA	3	304	X	-	-	-
19	CLA	3	305	X	-	-	-
19	CLA	3	306	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	309	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	311	X	-	-	-
19	CLA	3	312	X	-	-	-
19	CLA	3	313	X	-	-	-
19	CLA	3	314	X	-	-	-
19	CLA	4	301	X	-	-	-
19	CLA	4	302	X	-	-	-
19	CLA	4	303	X	-	-	-
19	CLA	4	304	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	A	801	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	852	X	-	-	-
19	CLA	A	853	X	-	-	-
19	CLA	A	854	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	839	X	-	-	-
19	CLA	B	840	X	-	-	-
19	CLA	B	851	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	G	202	X	-	-	-
19	CLA	G	203	X	-	-	-
19	CLA	G	204	X	-	-	-
19	CLA	H	201	X	-	-	-
19	CLA	H	202	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	J	102	X	-	-	-
19	CLA	K	201	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	L	301	X	-	-	-
19	CLA	L	302	X	-	-	-

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 35543 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 Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	194	Total	C	N	O	S	0	0
			1501	978	249	269	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	203	Total	C	N	O	S	0	0
			1582	1036	258	284	4		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	219	Total	C	N	O	S	0	0
			1680	1102	270	303	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	103	HIS	ASN	engineered mutation	UNP Q9SY97

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	197	Total	C	N	O	S	0	0
			1564	1024	255	282	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	99	HIS	ASN	engineered mutation	UNP P27521

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5834	3821	991	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5852	3840	1000	999	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	141	Total	C	N	O	S	0	0
			1112	712	193	203	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			509	326	89	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	152	Total	C	N	O	S	0	0
			1208	789	207	209	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	94	Total	C	N	O	0	0
			731	472	121	138		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	90	Total	C	N	O	0	0
			692	452	111	129		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	30	Total	C	N	O	S	0	0
			230	156	37	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	42	Total	C	N	O	S	0	0
			339	233	51	54	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	144	Total	C	N	O	S	0	0
			1076	710	172	192	2		

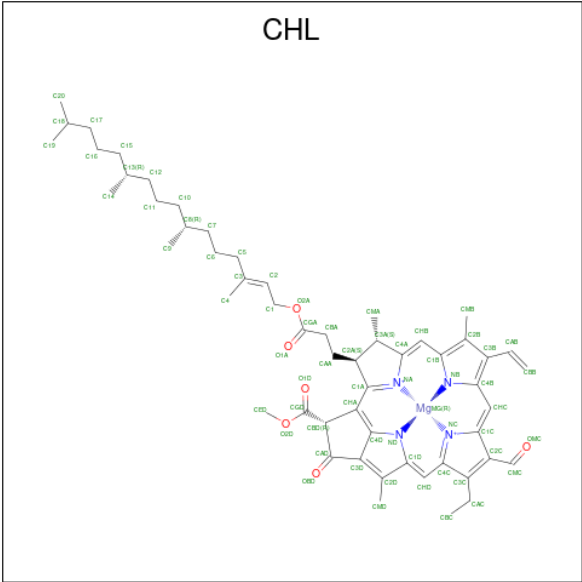
- Molecule 16 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	55	Total	C	N	O	S	0	0
			382	245	63	71	3		

- Molecule 17 is a protein called Photosystem I reaction center subunit N, chloroplastic.

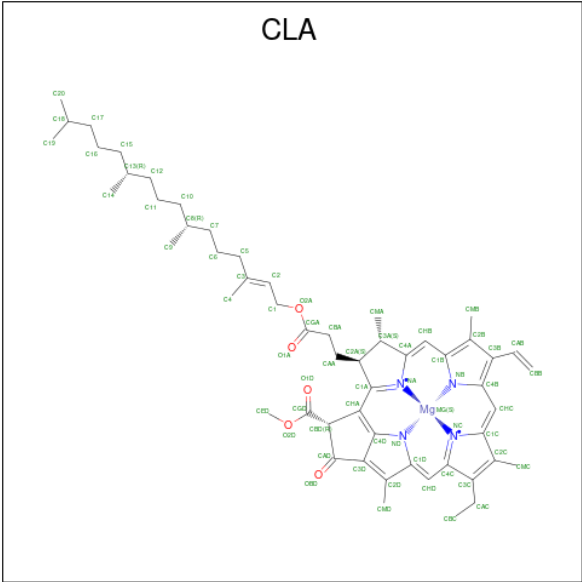
Mol	Chain	Residues	Atoms				AltConf	Trace
17	N	11	Total	C	N	O	0	0
			80	51	15	14		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
18	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 19 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
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 63	C 53	Mg 1	N 4	O 5	0
19	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

*Continued on next page...*

*Continued from previous page...*

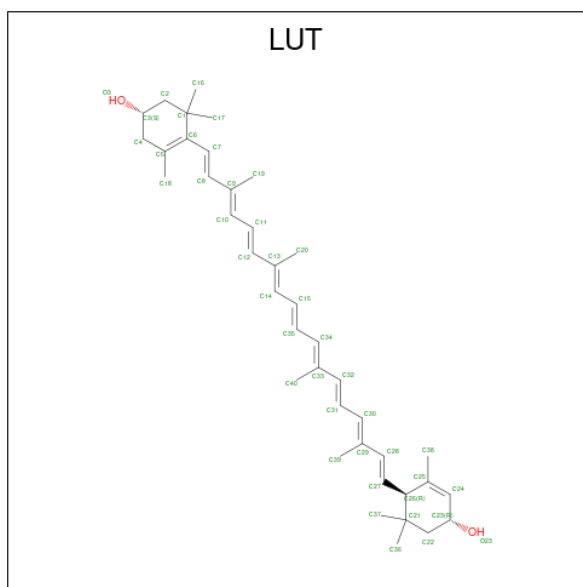
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
19	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

*Continued on next page...*

Continued from previous page...

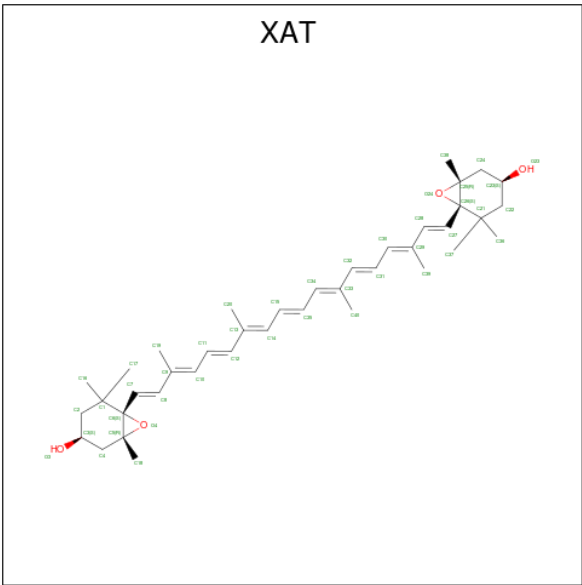
Mol	Chain	Residues	Atoms					AltConf
19	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	

- Molecule 20 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula:  $C_{40}H_{56}O_2$ ) (labeled as "Ligand of Interest" by depositor).



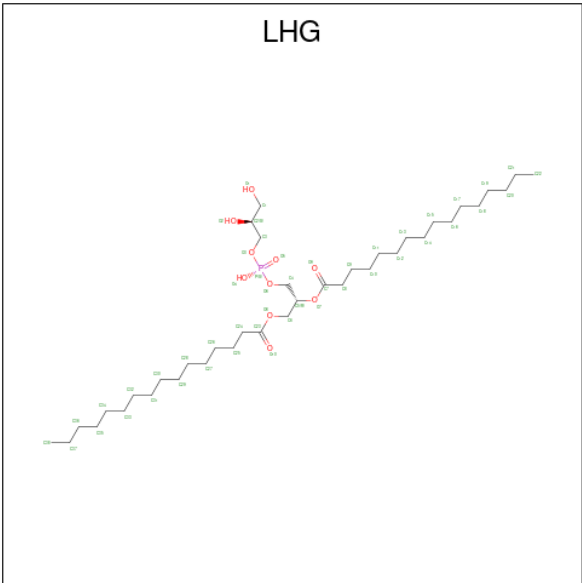
Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			42	40	2	
20	1	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	3	1	Total	C	O	0
			42	40	2	
20	4	1	Total	C	O	0
			42	40	2	

- Molecule 21 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).



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

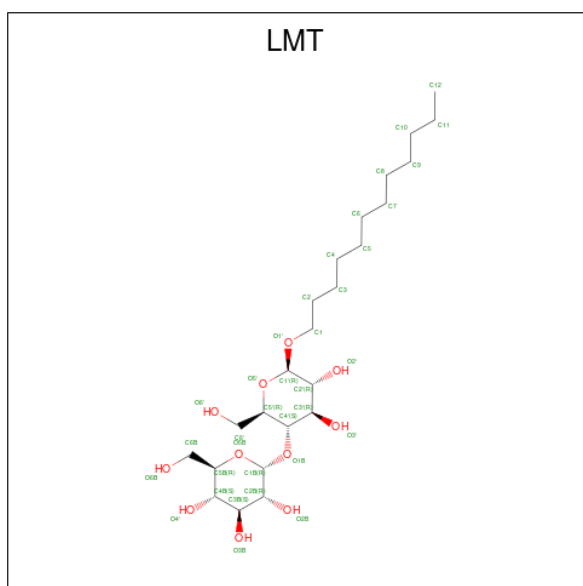
- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).





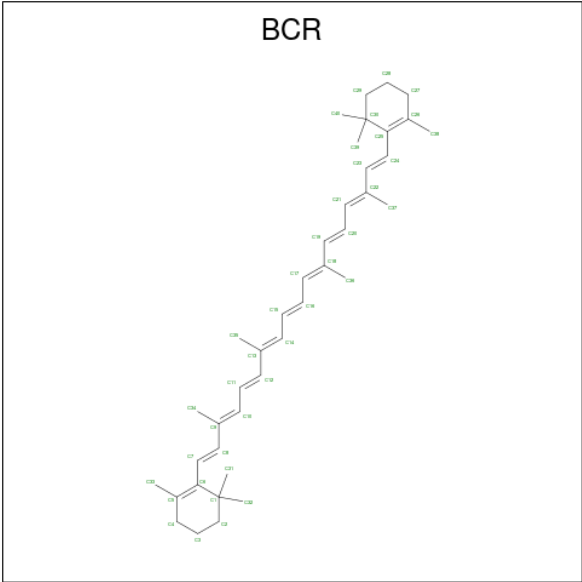
Mol	Chain	Residues	Atoms				AltConf
22	1	1	Total	C	O	P	0
			49	38	10	1	
22	1	1	Total	C	O	P	0
			49	38	10	1	
22	2	1	Total	C	O	P	0
			37	26	10	1	
22	A	1	Total	C	O	P	0
			49	38	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
23	2	1	Total	C	O	0
			35	24	11	
23	A	1	Total	C	O	0
			35	24	11	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



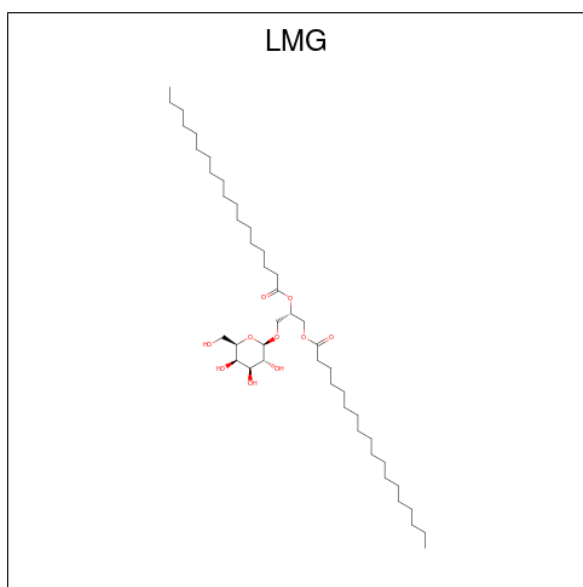
Mol	Chain	Residues	Atoms		AltConf
24	2	1	Total	C	0
			40	40	
24	3	1	Total	C	0
			40	40	
24	4	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	

Continued on next page...

*Continued from previous page...*

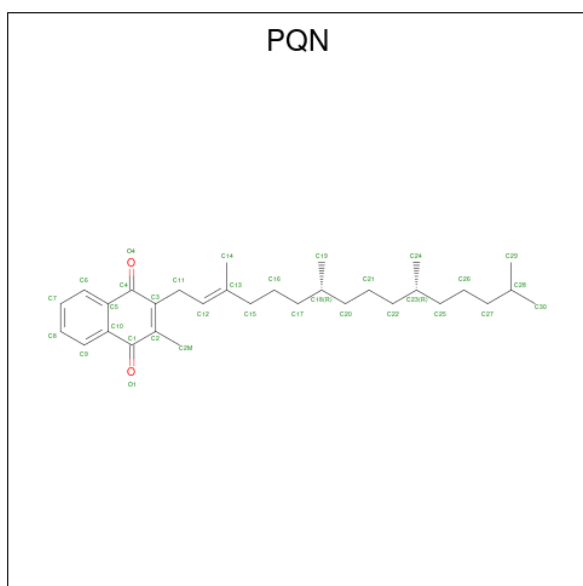
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



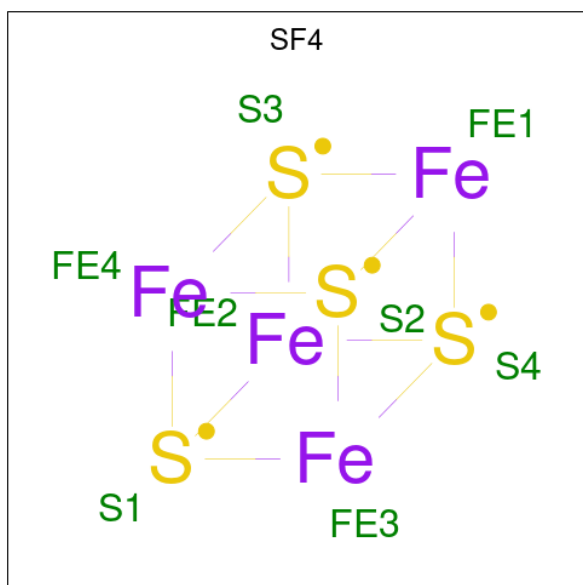
Mol	Chain	Residues	Atoms			AltConf
25	4	1	Total	C	O	0
			36	26	10	
25	B	1	Total	C	O	0
			52	42	10	
25	F	1	Total	C	O	0
			30	20	10	

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



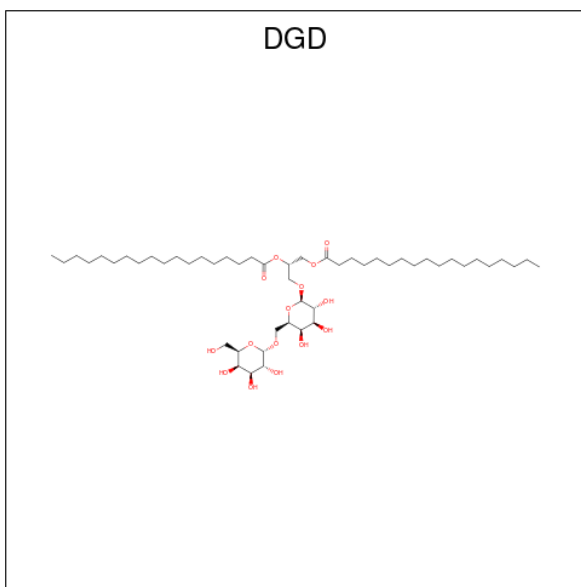
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	
26	B	1	Total	C	O	0
			33	31	2	

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



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $\text{C}_{51}\text{H}_{96}\text{O}_{15}$ ) (labeled as "Ligand of Interest" by depositor).

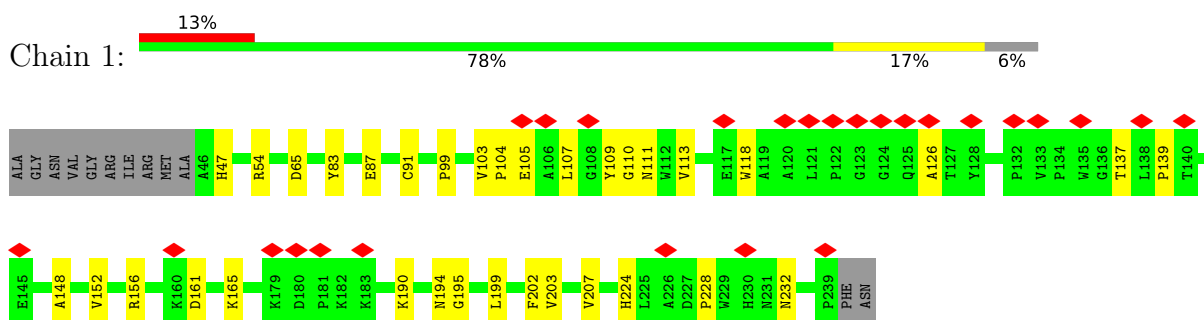


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	B	1	66	51	15	0

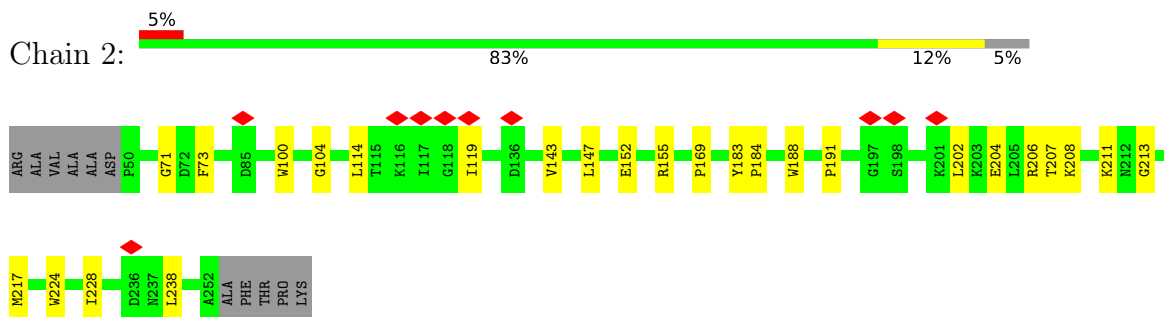
### 3 Residue-property plots [i](#)

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.

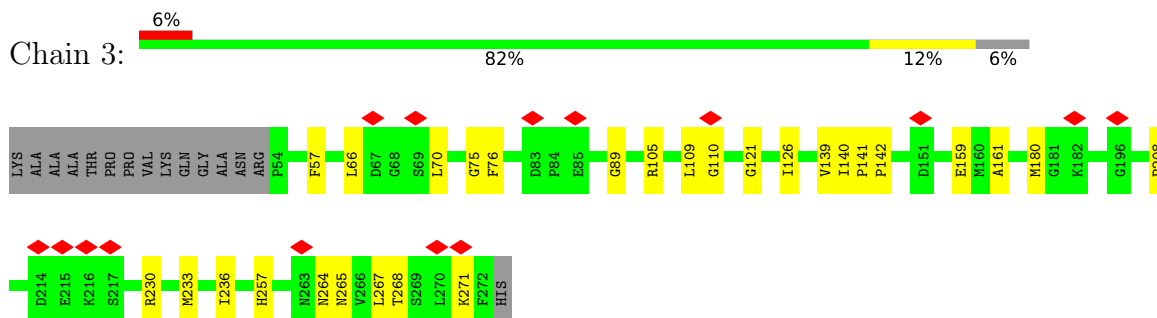
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



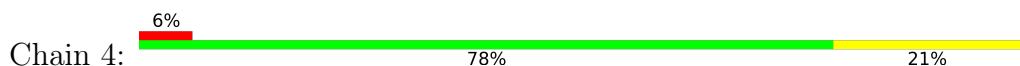
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

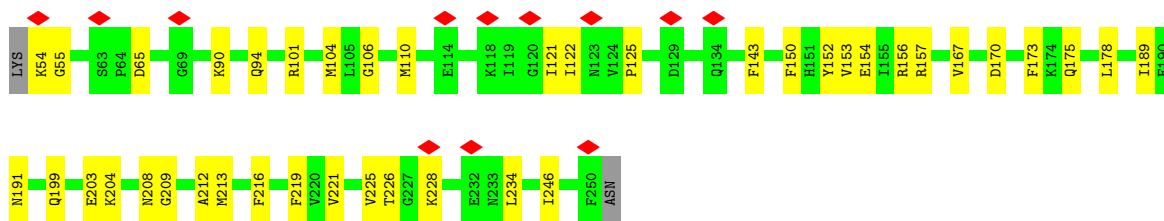


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic



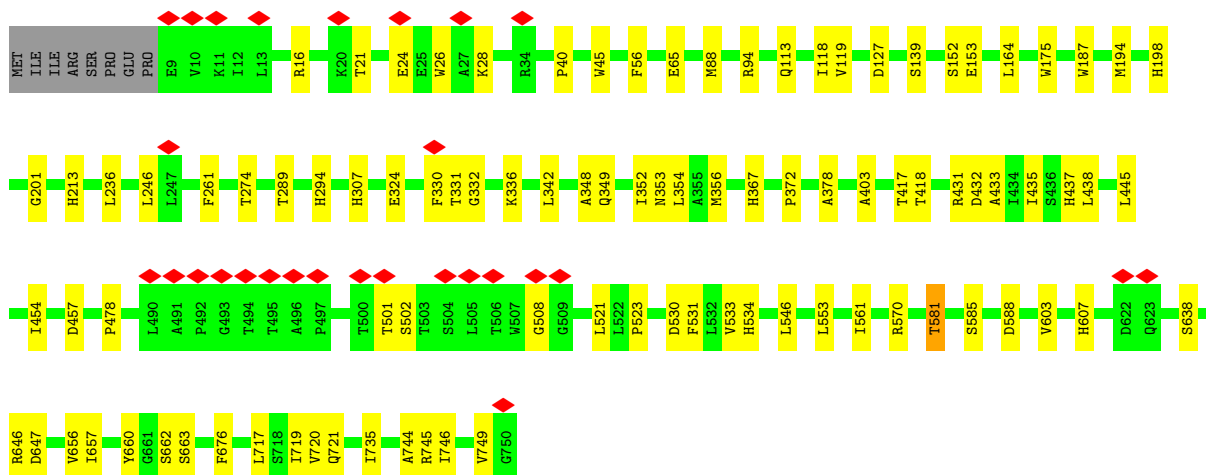
- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic





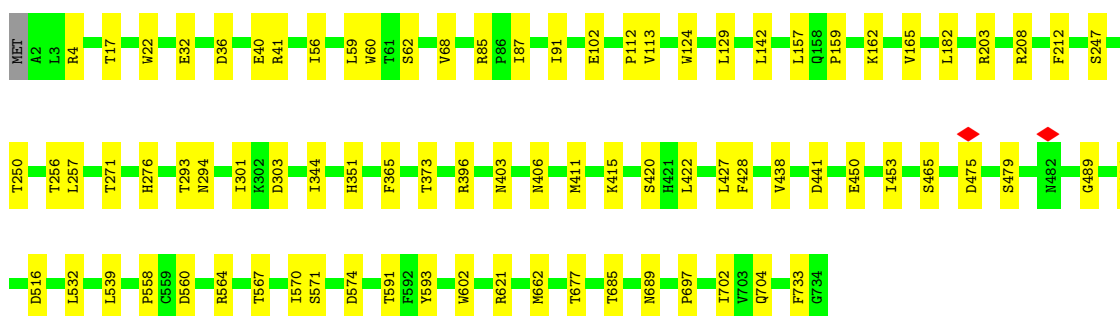
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 86% 13%



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 89% 11%



- Molecule 7: Photosystem I iron-sulfur center

Chain C: 79% 20%



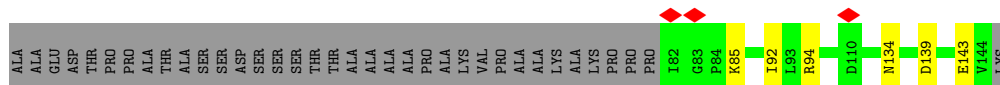
- Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

Chain D: 72% 15% 12%

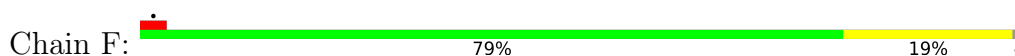




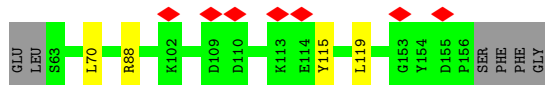
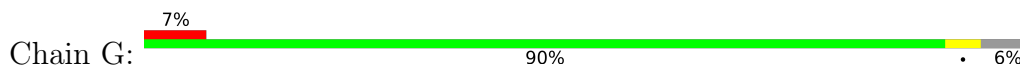
- Molecule 9: Photosystem I reaction center subunit IV B, chloroplastic



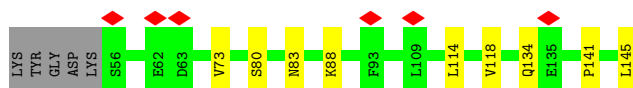
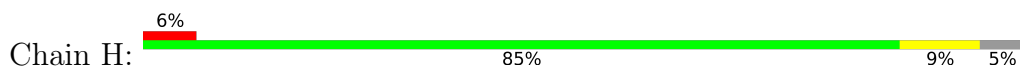
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic



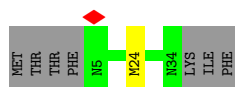
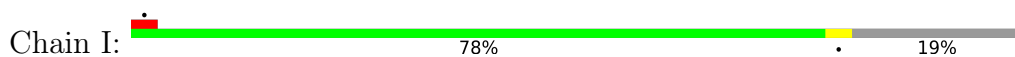
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic



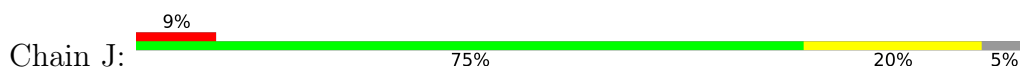
- Molecule 12: Photosystem I reaction center subunit VI-1, chloroplastic



- Molecule 13: Photosystem I reaction center subunit VIII



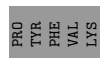
- Molecule 14: Photosystem I reaction center subunit IX





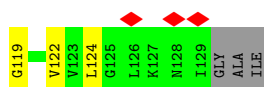
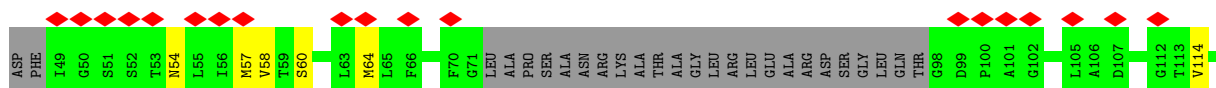
- Molecule 15: Photosystem I reaction center subunit XI, chloroplastic

Chain L: 77% 8% 15%



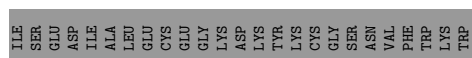
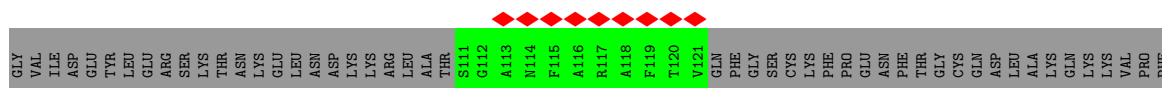
- Molecule 16: Photosystem I reaction center subunit psaK, chloroplastic

Chain K: 26% 55% 11% 35%



- Molecule 17: Photosystem I reaction center subunit N, chloroplastic

Chain N: 11% 13% 87%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.611	Depositor
Minimum map value	-1.558	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	398.272, 398.272, 398.272	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.889, 0.889, 0.889	Depositor

## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.12	0/1551	0.27	0/2117
2	2	0.12	0/1639	0.26	0/2242
3	3	0.14	0/1733	0.29	0/2356
4	4	0.13	0/1614	0.28	0/2198
5	A	0.14	0/6031	0.27	0/8226
6	B	0.14	0/6063	0.27	0/8281
7	C	0.16	0/628	0.35	0/852
8	D	0.12	0/1140	0.28	0/1542
9	E	0.11	0/519	0.28	0/703
10	F	0.14	0/1238	0.31	0/1670
11	G	0.10	0/749	0.21	0/1016
12	H	0.11	0/712	0.28	0/968
13	I	0.15	0/236	0.37	0/322
14	J	0.12	0/349	0.25	0/476
15	L	0.12	0/1108	0.25	0/1512
16	K	0.10	0/385	0.30	0/520
17	N	0.07	0/81	0.14	0/108
All	All	0.13	0/25776	0.28	0/35109

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	161	HIS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1501	0	1476	23	0
2	2	1582	0	1533	21	0
3	3	1680	0	1647	23	0
4	4	1564	0	1518	31	0
5	A	5834	0	5683	76	0
6	B	5852	0	5639	58	0
7	C	615	0	592	15	0
8	D	1112	0	1122	19	0
9	E	509	0	518	5	0
10	F	1208	0	1241	21	0
11	G	731	0	712	3	0
12	H	692	0	693	8	0
13	I	230	0	245	0	0
14	J	339	0	357	8	0
15	L	1076	0	1081	11	0
16	K	382	0	399	8	0
17	N	80	0	75	0	0
18	1	102	0	78	3	0
18	2	229	0	157	8	0
18	3	47	0	31	0	0
18	4	195	0	141	4	0
19	1	693	0	616	16	0
19	2	459	0	403	5	0
19	3	646	0	538	14	0
19	4	527	0	458	14	0
19	A	2569	0	2615	74	0
19	B	2434	0	2441	56	0
19	F	90	0	66	1	0
19	G	137	0	101	1	0
19	H	100	0	74	4	0
19	J	42	0	31	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	128	0	91	4	0
19	L	115	0	111	2	0
20	1	84	0	112	7	0
20	2	42	0	56	4	0
20	3	42	0	56	6	0
20	4	42	0	56	7	0
21	1	44	0	56	3	0
21	2	44	0	56	1	0
21	3	44	0	56	2	0
21	4	44	0	56	1	0
22	1	98	0	148	5	0
22	2	37	0	44	2	0
22	A	49	0	74	0	0
22	B	49	0	74	5	0
23	2	35	0	46	1	0
23	A	35	0	46	1	0
24	2	40	0	56	6	0
24	3	40	0	56	4	0
24	4	40	0	56	0	0
24	A	280	0	392	20	0
24	B	240	0	336	9	0
24	F	80	0	112	4	0
24	G	80	0	112	5	0
24	I	40	0	56	4	0
24	J	120	0	168	10	0
24	L	120	0	168	10	0
25	4	36	0	42	0	0
25	B	52	0	77	1	0
25	F	30	0	30	2	0
26	A	33	0	46	0	0
26	B	33	0	46	2	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	B	66	0	96	2	0
All	All	35543	0	35268	504	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 7.

The worst 5 of 504 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)
20:3:315:LUT:H171	20:3:315:LUT:H8	1.58	0.85
20:4:315:LUT:H171	20:4:315:LUT:H8	1.60	0.84
19:B:851:CLA:HBA1	19:B:851:CLA:HBD	1.64	0.80
20:1:315:LUT:H8	20:1:315:LUT:H171	1.62	0.79
19:A:808:CLA:HBB2	19:A:811:CLA:HMA3	1.67	0.77

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	192/206 (93%)	187 (97%)	5 (3%)	0	100	100
2	2	201/214 (94%)	196 (98%)	5 (2%)	0	100	100
3	3	217/234 (93%)	213 (98%)	4 (2%)	0	100	100
4	4	195/199 (98%)	191 (98%)	4 (2%)	0	100	100
5	A	740/750 (99%)	727 (98%)	13 (2%)	0	100	100
6	B	731/734 (100%)	718 (98%)	13 (2%)	0	100	100
7	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
8	D	139/160 (87%)	131 (94%)	8 (6%)	0	100	100
9	E	61/99 (62%)	56 (92%)	5 (8%)	0	100	100
10	F	150/154 (97%)	147 (98%)	3 (2%)	0	100	100
11	G	92/100 (92%)	91 (99%)	1 (1%)	0	100	100
12	H	88/95 (93%)	87 (99%)	1 (1%)	0	100	100
13	I	28/37 (76%)	27 (96%)	1 (4%)	0	100	100
14	J	40/44 (91%)	39 (98%)	1 (2%)	0	100	100
15	L	142/169 (84%)	140 (99%)	2 (1%)	0	100	100
16	K	51/84 (61%)	49 (96%)	2 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	N	9/85 (11%)	9 (100%)	0	0	100	100
All	All	3154/3445 (92%)	3081 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1	153/161 (95%)	153 (100%)	0	100	100
2	2	164/171 (96%)	164 (100%)	0	100	100
3	3	169/179 (94%)	168 (99%)	1 (1%)	84	90
4	4	164/166 (99%)	164 (100%)	0	100	100
5	A	601/609 (99%)	598 (100%)	3 (0%)	86	91
6	B	597/598 (100%)	596 (100%)	1 (0%)	92	95
7	C	70/71 (99%)	70 (100%)	0	100	100
8	D	120/134 (90%)	119 (99%)	1 (1%)	79	87
9	E	56/80 (70%)	55 (98%)	1 (2%)	54	74
10	F	125/127 (98%)	125 (100%)	0	100	100
11	G	79/84 (94%)	79 (100%)	0	100	100
12	H	75/79 (95%)	75 (100%)	0	100	100
13	I	26/33 (79%)	25 (96%)	1 (4%)	28	56
14	J	36/38 (95%)	36 (100%)	0	100	100
15	L	111/134 (83%)	110 (99%)	1 (1%)	75	85
16	K	41/61 (67%)	41 (100%)	0	100	100
17	N	7/73 (10%)	7 (100%)	0	100	100
All	All	2594/2798 (93%)	2585 (100%)	9 (0%)	90	94

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



Mol	Chain	Res	Type
13	I	24	MET
15	L	178	VAL
5	A	581	THR
6	B	303	ASP
8	D	161	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
7	C	16	GLN
11	G	87	GLN
8	D	71	ASN
9	E	134	ASN
11	G	99	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

206 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LUT	4	315	-	42,43,43	1.61	8 (19%)	51,60,60	1.59	11 (21%)
24	BCR	B	844	-	41,41,41	0.16	0	56,56,56	0.65	2 (3%)
19	CLA	B	840	22	65,73,73	1.35	7 (10%)	76,113,113	1.77	11 (14%)
19	CLA	B	833	-	56,64,73	1.45	7 (12%)	65,102,113	1.89	9 (13%)
19	CLA	B	820	-	45,53,73	1.57	7 (15%)	52,89,113	1.89	6 (11%)
19	CLA	A	826	-	65,73,73	1.33	7 (10%)	76,113,113	1.74	8 (10%)
25	LMG	B	849	-	52,52,55	0.19	0	60,60,63	0.15	0
19	CLA	A	829	-	65,73,73	1.36	7 (10%)	76,113,113	1.74	9 (11%)
18	CHL	4	307	-	51,59,74	1.66	10 (19%)	55,96,114	2.06	12 (21%)
19	CLA	B	806	-	65,73,73	1.34	7 (10%)	76,113,113	1.79	13 (17%)
22	LHG	1	320	-	48,48,48	0.30	0	51,54,54	0.28	0
19	CLA	B	839	-	65,73,73	1.34	7 (10%)	76,113,113	1.67	10 (13%)
19	CLA	B	816	-	55,63,73	1.45	7 (12%)	64,101,113	1.80	10 (15%)
19	CLA	B	811	-	54,62,73	1.42	7 (12%)	67,100,113	1.91	14 (20%)
19	CLA	2	302	2	65,73,73	1.35	7 (10%)	76,113,113	1.67	10 (13%)
19	CLA	3	314	-	46,54,73	1.56	7 (15%)	53,90,113	1.90	8 (15%)
22	LHG	2	317	19	36,36,48	0.34	0	39,42,54	0.31	0
19	CLA	A	807	5	62,70,73	1.37	7 (11%)	72,109,113	1.79	9 (12%)
19	CLA	A	832	-	45,53,73	1.58	7 (15%)	52,89,113	1.92	7 (13%)
19	CLA	A	825	-	65,73,73	1.33	7 (10%)	76,113,113	1.79	11 (14%)
19	CLA	A	827	-	65,73,73	1.35	7 (10%)	76,113,113	1.70	10 (13%)
19	CLA	B	819	-	60,68,73	1.40	7 (11%)	70,107,113	1.74	9 (12%)
19	CLA	3	312	-	55,63,73	1.45	7 (12%)	64,101,113	1.82	7 (10%)
19	CLA	A	814	-	45,53,73	1.57	7 (15%)	52,89,113	1.98	7 (13%)
19	CLA	A	822	-	55,63,73	1.46	7 (12%)	64,101,113	1.75	9 (14%)
24	BCR	J	101	-	41,41,41	0.18	0	56,56,56	0.93	4 (7%)
19	CLA	F	301	-	45,53,73	1.57	7 (15%)	52,89,113	1.95	7 (13%)
22	LHG	1	317	19	48,48,48	0.30	0	51,54,54	0.31	0
24	BCR	B	845	-	41,41,41	0.11	0	56,56,56	0.30	0
19	CLA	G	204	11	46,54,73	1.55	7 (15%)	53,90,113	1.93	8 (15%)
19	CLA	3	313	-	45,53,73	1.57	7 (15%)	52,89,113	1.89	7 (13%)
19	CLA	1	307	-	45,53,73	1.57	7 (15%)	52,89,113	1.89	8 (15%)
21	XAT	4	316	-	39,47,47	0.09	0	54,74,74	0.80	3 (5%)
18	CHL	1	306	1	46,54,74	1.73	11 (23%)	49,90,114	2.11	10 (20%)
19	CLA	A	812	-	45,53,73	1.56	7 (15%)	52,89,113	1.99	9 (17%)
19	CLA	A	808	-	59,67,73	1.41	7 (11%)	68,105,113	1.80	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	G	205	-	41,41,41	0.11	0	56,56,56	0.31	0
24	BCR	L	304	-	41,41,41	0.22	0	56,56,56	0.87	2 (3%)
18	CHL	3	307	-	47,55,74	1.67	9 (19%)	50,91,114	2.23	10 (20%)
19	CLA	A	811	-	65,73,73	1.33	7 (10%)	76,113,113	1.79	12 (15%)
19	CLA	A	824	-	65,73,73	1.35	6 (9%)	76,113,113	1.71	11 (14%)
19	CLA	B	818	-	60,68,73	1.40	7 (11%)	70,107,113	1.83	12 (17%)
24	BCR	4	317	-	41,41,41	0.13	0	56,56,56	0.32	0
20	LUT	2	315	-	42,43,43	1.65	8 (19%)	51,60,60	1.52	11 (21%)
19	CLA	A	840	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	9 (11%)
23	LMT	2	318	-	36,36,36	0.11	0	47,47,47	0.13	0
19	CLA	A	820	-	45,53,73	1.58	7 (15%)	52,89,113	1.92	7 (13%)
19	CLA	A	817	-	65,73,73	1.35	7 (10%)	76,113,113	1.65	11 (14%)
19	CLA	1	314	1	45,53,73	1.56	7 (15%)	52,89,113	1.93	8 (15%)
20	LUT	1	319	-	42,43,43	1.65	8 (19%)	51,60,60	1.63	10 (19%)
19	CLA	A	806	5	65,73,73	1.34	7 (10%)	76,113,113	1.64	12 (15%)
19	CLA	B	807	-	65,73,73	1.34	7 (10%)	76,113,113	1.72	10 (13%)
19	CLA	B	815	-	55,63,73	1.46	7 (12%)	64,101,113	1.86	9 (14%)
24	BCR	B	847	-	41,41,41	0.12	0	56,56,56	0.30	0
19	CLA	A	839	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	11 (14%)
18	CHL	2	314	2	43,51,74	1.66	9 (20%)	45,86,114	1.94	9 (20%)
19	CLA	4	313	-	45,53,73	1.57	7 (15%)	52,89,113	1.84	8 (15%)
19	CLA	B	824	-	65,73,73	1.34	7 (10%)	76,113,113	1.68	10 (13%)
24	BCR	L	303	-	41,41,41	0.16	0	56,56,56	0.31	0
24	BCR	B	843	-	41,41,41	0.14	0	56,56,56	0.29	0
19	CLA	A	838	-	65,73,73	1.34	7 (10%)	76,113,113	1.79	13 (17%)
19	CLA	1	308	1	57,65,73	1.42	7 (12%)	66,103,113	2.01	11 (16%)
18	CHL	2	306	-	46,54,74	1.74	9 (19%)	49,90,114	2.20	11 (22%)
19	CLA	4	301	4	46,54,73	1.54	7 (15%)	53,90,113	1.96	9 (16%)
19	CLA	K	201	-	45,53,73	1.57	7 (15%)	52,89,113	1.90	8 (15%)
19	CLA	B	836	-	65,73,73	1.33	7 (10%)	76,113,113	1.72	9 (11%)
21	XAT	2	316	-	39,47,47	0.14	0	54,74,74	0.75	2 (3%)
19	CLA	1	311	1	50,58,73	1.53	7 (14%)	58,95,113	1.91	10 (17%)
19	CLA	3	311	-	45,53,73	1.59	7 (15%)	52,89,113	1.99	8 (15%)
19	CLA	B	809	6	65,73,73	1.36	7 (10%)	76,113,113	1.72	11 (14%)
19	CLA	3	304	-	47,55,73	1.52	7 (14%)	54,91,113	1.95	10 (18%)
19	CLA	1	305	-	42,50,73	1.58	7 (16%)	48,85,113	1.92	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	A	837	-	65,73,73	1.32	7 (10%)	76,113,113	1.72	13 (17%)
19	CLA	B	821	-	50,58,73	1.52	7 (14%)	58,95,113	1.88	9 (15%)
20	LUT	1	315	-	42,43,43	1.64	8 (19%)	51,60,60	1.59	11 (21%)
22	LHG	B	850	19	48,48,48	0.30	0	51,54,54	0.28	0
24	BCR	A	848	-	41,41,41	0.13	0	56,56,56	0.20	0
24	BCR	3	317	-	41,41,41	0.11	0	56,56,56	0.28	0
19	CLA	B	802	-	65,73,73	1.33	7 (10%)	76,113,113	1.68	11 (14%)
19	CLA	1	313	-	45,53,73	1.56	7 (15%)	52,89,113	1.88	7 (13%)
19	CLA	1	312	-	60,68,73	1.40	7 (11%)	70,107,113	1.81	12 (17%)
19	CLA	B	831	-	60,68,73	1.40	7 (11%)	70,107,113	1.74	11 (15%)
19	CLA	F	302	-	45,53,73	1.57	7 (15%)	52,89,113	1.97	8 (15%)
19	CLA	B	828	-	65,73,73	1.35	7 (10%)	76,113,113	1.71	11 (14%)
19	CLA	A	818	-	45,53,73	1.55	7 (15%)	52,89,113	1.91	6 (11%)
19	CLA	A	853	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	8 (10%)
19	CLA	2	310	22	41,49,73	1.61	7 (17%)	47,84,113	2.01	9 (19%)
19	CLA	3	308	3	65,73,73	1.35	7 (10%)	76,113,113	1.71	10 (13%)
19	CLA	A	833	-	65,73,73	1.34	7 (10%)	76,113,113	1.61	11 (14%)
19	CLA	2	309	2	60,68,73	1.40	7 (11%)	70,107,113	1.76	10 (14%)
19	CLA	4	302	4	60,68,73	1.41	7 (11%)	70,107,113	1.81	10 (14%)
19	CLA	4	303	-	60,68,73	1.40	7 (11%)	70,107,113	1.84	12 (17%)
19	CLA	K	202	-	46,54,73	1.57	7 (15%)	53,90,113	1.94	7 (13%)
19	CLA	B	827	-	60,68,73	1.39	7 (11%)	70,107,113	1.70	11 (15%)
19	CLA	4	304	-	45,53,73	1.58	7 (15%)	52,89,113	1.95	6 (11%)
19	CLA	3	301	3	60,68,73	1.41	7 (11%)	70,107,113	1.75	13 (18%)
19	CLA	B	810	-	65,73,73	1.34	7 (10%)	76,113,113	1.72	9 (11%)
19	CLA	B	835	-	55,63,73	1.47	7 (12%)	64,101,113	1.84	7 (10%)
20	LUT	3	315	-	42,43,43	1.64	8 (19%)	51,60,60	1.63	12 (23%)
24	BCR	I	101	-	41,41,41	0.13	0	56,56,56	0.22	0
24	BCR	A	843	-	41,41,41	0.14	0	56,56,56	0.43	0
19	CLA	B	803	-	65,73,73	1.34	6 (9%)	76,113,113	1.74	11 (14%)
18	CHL	2	307	-	46,54,74	1.74	10 (21%)	49,90,114	2.17	9 (18%)
19	CLA	A	819	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	12 (15%)
19	CLA	B	805	-	65,73,73	1.35	7 (10%)	76,113,113	1.79	10 (13%)
19	CLA	A	816	-	55,63,73	1.45	7 (12%)	64,101,113	1.82	8 (12%)
19	CLA	B	832	-	58,66,73	1.40	7 (12%)	67,104,113	1.80	7 (10%)
19	CLA	L	302	-	50,58,73	1.53	7 (14%)	58,95,113	1.79	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	B	825	-	55,63,73	1.47	7 (12%)	64,101,113	1.84	11 (17%)
19	CLA	2	312	-	65,73,73	1.34	7 (10%)	76,113,113	1.74	8 (10%)
25	LMG	4	318	-	36,36,55	0.20	0	44,44,63	0.19	0
19	CLA	B	851	-	65,73,73	1.33	7 (10%)	76,113,113	1.77	12 (15%)
26	PQN	A	841	-	34,34,34	0.26	0	42,45,45	0.50	1 (2%)
19	CLA	B	822	-	55,63,73	1.45	7 (12%)	64,101,113	1.77	10 (15%)
19	CLA	1	310	22	55,63,73	1.47	7 (12%)	64,101,113	1.91	10 (15%)
19	CLA	2	304	-	45,53,73	1.58	7 (15%)	52,89,113	2.03	10 (19%)
24	BCR	A	846	-	41,41,41	0.11	0	56,56,56	0.19	0
19	CLA	A	821	-	51,59,73	1.50	7 (13%)	59,96,113	1.91	9 (15%)
19	CLA	A	831	-	65,73,73	1.35	7 (10%)	76,113,113	1.64	11 (14%)
19	CLA	B	826	-	65,73,73	1.35	7 (10%)	76,113,113	1.81	11 (14%)
19	CLA	B	823	-	55,63,73	1.46	7 (12%)	64,101,113	1.71	10 (15%)
19	CLA	G	203	-	50,58,73	1.54	7 (14%)	58,95,113	1.93	9 (15%)
19	CLA	A	854	-	65,73,73	1.33	7 (10%)	76,113,113	1.78	13 (17%)
19	CLA	4	310	-	60,68,73	1.40	7 (11%)	70,107,113	1.69	11 (15%)
19	CLA	H	201	12	45,53,73	1.56	7 (15%)	52,89,113	1.84	9 (17%)
19	CLA	3	302	-	60,68,73	1.40	7 (11%)	70,107,113	1.78	10 (14%)
19	CLA	1	304	-	51,59,73	1.51	7 (13%)	59,96,113	1.96	11 (18%)
19	CLA	3	303	-	45,53,73	1.57	7 (15%)	52,89,113	1.91	10 (19%)
19	CLA	L	301	-	65,73,73	1.35	7 (10%)	76,113,113	1.66	10 (13%)
26	PQN	B	841	-	34,34,34	0.26	0	42,45,45	0.51	1 (2%)
24	BCR	F	304	-	41,41,41	0.14	0	56,56,56	0.34	0
23	LMT	A	851	-	36,36,36	0.10	0	47,47,47	0.26	0
19	CLA	B	829	-	65,73,73	1.36	7 (10%)	76,113,113	1.77	11 (14%)
18	CHL	4	314	4	41,50,74	1.69	8 (19%)	42,85,114	2.14	8 (19%)
25	LMG	F	305	-	30,30,55	0.21	0	38,38,63	0.15	0
19	CLA	B	804	-	45,53,73	1.58	7 (15%)	52,89,113	1.93	8 (15%)
19	CLA	A	810	-	54,62,73	1.46	7 (12%)	62,99,113	1.84	10 (16%)
19	CLA	A	835	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	10 (13%)
19	CLA	3	310	-	41,49,73	1.60	7 (17%)	47,84,113	2.03	9 (19%)
24	BCR	G	201	-	41,41,41	0.13	0	56,56,56	0.58	0
19	CLA	1	303	-	58,66,73	1.42	7 (12%)	67,104,113	1.82	11 (16%)
19	CLA	3	309	3	50,58,73	1.52	7 (14%)	58,95,113	1.86	11 (18%)
19	CLA	A	813	-	50,58,73	1.53	7 (14%)	58,95,113	1.87	7 (12%)
24	BCR	F	303	-	41,41,41	0.11	0	56,56,56	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	XAT	1	316	-	39,47,47	0.11	0	54,74,74	0.87	3 (5%)
19	CLA	A	805	-	50,58,73	1.53	7 (14%)	58,95,113	1.89	10 (17%)
18	CHL	4	306	-	46,54,74	1.74	10 (21%)	49,90,114	2.09	11 (22%)
19	CLA	A	834	-	51,59,73	1.51	7 (13%)	59,96,113	1.99	8 (13%)
18	CHL	4	305	-	56,64,74	1.61	9 (16%)	61,102,114	2.00	11 (18%)
18	CHL	2	301	2	51,59,74	1.67	10 (19%)	55,96,114	2.11	13 (23%)
19	CLA	2	308	2	45,53,73	1.57	7 (15%)	52,89,113	1.90	7 (13%)
19	CLA	3	306	3	45,53,73	1.57	7 (15%)	52,89,113	1.88	8 (15%)
19	CLA	B	838	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	11 (14%)
24	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.33	0
24	BCR	L	305	-	41,41,41	0.15	0	56,56,56	0.43	0
19	CLA	A	836	-	52,60,73	1.51	7 (13%)	60,97,113	1.84	8 (13%)
19	CLA	K	203	16	38,45,73	1.69	7 (18%)	43,78,113	2.07	8 (18%)
19	CLA	A	809	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	10 (13%)
19	CLA	A	830	-	65,73,73	1.35	7 (10%)	76,113,113	1.74	12 (15%)
19	CLA	2	311	2	45,53,73	1.57	7 (15%)	52,89,113	1.98	8 (15%)
19	CLA	J	102	14	42,50,73	1.58	7 (16%)	48,85,113	1.83	8 (16%)
27	SF4	C	102	7	0,12,12	-	-	-	-	-
19	CLA	A	815	-	63,72,73	1.36	7 (11%)	73,112,113	1.63	9 (12%)
19	CLA	B	801	-	65,73,73	1.33	7 (10%)	76,113,113	1.65	9 (11%)
19	CLA	B	817	-	59,67,73	1.40	7 (11%)	68,105,113	1.69	10 (14%)
24	BCR	2	319	-	41,41,41	0.19	0	56,56,56	0.77	3 (5%)
19	CLA	A	804	5	65,73,73	1.33	7 (10%)	76,113,113	1.70	14 (18%)
19	CLA	G	202	-	41,49,73	1.63	7 (17%)	47,84,113	1.93	9 (19%)
19	CLA	A	828	-	65,73,73	1.35	7 (10%)	76,113,113	1.73	10 (13%)
24	BCR	A	845	-	41,41,41	0.12	0	56,56,56	0.22	0
19	CLA	A	802	-	50,58,73	1.53	7 (14%)	58,95,113	1.89	8 (13%)
19	CLA	4	311	4	45,53,73	1.58	7 (15%)	52,89,113	1.97	7 (13%)
19	CLA	1	302	1	60,68,73	1.39	7 (11%)	70,107,113	1.77	11 (15%)
19	CLA	3	305	-	42,50,73	1.59	7 (16%)	48,85,113	1.90	7 (14%)
18	CHL	1	301	1	56,64,74	1.59	10 (17%)	61,102,114	2.05	15 (24%)
24	BCR	B	842	-	41,41,41	0.13	0	56,56,56	0.28	0
19	CLA	2	313	-	43,51,73	1.56	7 (16%)	49,86,113	1.96	6 (12%)
19	CLA	A	823	-	65,73,73	1.34	7 (10%)	76,113,113	1.63	11 (14%)
27	SF4	A	850	6,5	0,12,12	-	-	-	-	-
19	CLA	1	318	-	65,73,73	1.34	7 (10%)	76,113,113	1.72	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	B	813	-	65,73,73	1.33	7 (10%)	76,113,113	1.75	12 (15%)
19	CLA	B	814	-	65,73,73	1.34	7 (10%)	76,113,113	1.74	11 (14%)
21	XAT	3	316	-	39,47,47	0.11	0	54,74,74	0.93	4 (7%)
19	CLA	B	834	-	45,53,73	1.58	7 (15%)	52,89,113	1.95	5 (9%)
19	CLA	B	830	-	50,58,73	1.55	7 (14%)	58,95,113	1.78	9 (15%)
28	DGD	B	848	-	67,67,67	0.16	0	81,81,81	0.15	0
24	BCR	A	844	-	41,41,41	0.24	0	56,56,56	0.76	2 (3%)
18	CHL	2	305	-	43,51,74	1.66	8 (18%)	45,86,114	2.13	10 (22%)
19	CLA	A	803	-	65,73,73	1.34	7 (10%)	76,113,113	1.82	11 (14%)
19	CLA	H	202	15	55,63,73	1.46	7 (12%)	64,101,113	1.73	10 (15%)
19	CLA	4	308	4	50,58,73	1.53	7 (14%)	58,95,113	1.91	7 (12%)
19	CLA	B	837	-	47,55,73	1.53	7 (14%)	54,91,113	1.91	8 (14%)
24	BCR	J	104	-	41,41,41	0.13	0	56,56,56	0.27	0
24	BCR	J	103	-	41,41,41	0.13	0	56,56,56	0.23	0
27	SF4	C	101	7	0,12,12	-	-	-	-	-
24	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.33	0
19	CLA	2	303	-	50,58,73	1.53	7 (14%)	58,95,113	1.85	9 (15%)
19	CLA	1	309	1	60,68,73	1.39	7 (11%)	70,107,113	1.78	11 (15%)
19	CLA	4	312	-	56,64,73	1.45	7 (12%)	65,102,113	1.77	9 (13%)
19	CLA	A	801	-	65,73,73	1.33	7 (10%)	76,113,113	1.74	13 (17%)
22	LHG	A	842	-	48,48,48	0.29	0	51,54,54	0.28	0
19	CLA	B	812	-	55,63,73	1.46	7 (12%)	64,101,113	1.85	9 (14%)
24	BCR	A	847	-	41,41,41	0.13	0	56,56,56	0.56	1 (1%)
19	CLA	4	309	4	60,68,73	1.38	7 (11%)	70,107,113	1.80	12 (17%)
19	CLA	A	852	-	65,73,73	1.33	7 (10%)	76,113,113	1.68	11 (14%)
19	CLA	B	808	-	65,73,73	1.33	7 (10%)	76,113,113	1.72	11 (14%)

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
20	LUT	4	315	-	-	0/29/67/67	0/2/2/2
24	BCR	B	844	-	-	6/29/63/63	0/2/2/2
19	CLA	B	840	22	1/1/15/20	16/37/115/115	-
19	CLA	B	833	-	1/1/13/20	12/27/105/115	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	820	-	1/1/11/20	2/13/91/115	-
19	CLA	A	826	-	1/1/15/20	22/37/115/115	-
25	LMG	B	849	-	-	11/47/67/70	0/1/1/1
19	CLA	A	829	-	1/1/15/20	18/37/115/115	-
18	CHL	4	307	-	3/3/17/26	9/21/119/137	-
19	CLA	B	806	-	1/1/15/20	16/37/115/115	-
22	LHG	1	320	-	-	17/53/53/53	-
19	CLA	B	839	-	1/1/15/20	12/37/115/115	-
19	CLA	B	816	-	1/1/13/20	9/25/103/115	-
19	CLA	B	811	-	1/1/13/20	10/25/101/115	-
19	CLA	2	302	2	1/1/15/20	14/37/115/115	-
19	CLA	3	314	-	1/1/11/20	8/15/93/115	-
22	LHG	2	317	19	-	11/41/41/53	-
19	CLA	A	807	5	1/1/14/20	16/34/112/115	-
19	CLA	A	832	-	1/1/11/20	3/13/91/115	-
19	CLA	A	825	-	1/1/15/20	10/37/115/115	-
19	CLA	A	827	-	1/1/15/20	15/37/115/115	-
19	CLA	B	819	-	1/1/14/20	16/31/109/115	-
19	CLA	3	312	-	1/1/13/20	7/25/103/115	-
19	CLA	A	814	-	1/1/11/20	4/13/91/115	-
19	CLA	A	822	-	1/1/13/20	9/25/103/115	-
24	BCR	J	101	-	-	13/29/63/63	0/2/2/2
19	CLA	F	301	-	1/1/11/20	6/13/91/115	-
22	LHG	1	317	19	-	9/53/53/53	-
24	BCR	B	845	-	-	0/29/63/63	0/2/2/2
19	CLA	G	204	11	1/1/11/20	7/15/93/115	-
19	CLA	3	313	-	1/1/11/20	5/13/91/115	-
19	CLA	1	307	-	1/1/11/20	2/13/91/115	-
21	XAT	4	316	-	-	0/31/93/93	0/4/4/4
18	CHL	1	306	1	2/2/16/26	4/15/113/137	-
19	CLA	A	812	-	1/1/11/20	4/13/91/115	-
19	CLA	A	808	-	1/1/13/20	14/30/108/115	-
24	BCR	G	205	-	-	1/29/63/63	0/2/2/2
24	BCR	L	304	-	-	1/29/63/63	0/2/2/2
18	CHL	3	307	-	3/3/16/26	4/17/115/137	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	811	-	1/1/15/20	23/37/115/115	-
19	CLA	A	824	-	1/1/15/20	8/37/115/115	-
19	CLA	B	818	-	1/1/14/20	16/31/109/115	-
24	BCR	4	317	-	-	2/29/63/63	0/2/2/2
20	LUT	2	315	-	-	1/29/67/67	0/2/2/2
19	CLA	A	840	-	1/1/15/20	17/37/115/115	-
23	LMT	2	318	-	-	4/21/61/61	0/2/2/2
19	CLA	A	820	-	1/1/11/20	6/13/91/115	-
19	CLA	A	817	-	1/1/15/20	11/37/115/115	-
19	CLA	1	314	1	1/1/11/20	8/13/91/115	-
20	LUT	1	319	-	-	2/29/67/67	0/2/2/2
19	CLA	A	806	5	1/1/15/20	18/37/115/115	-
19	CLA	B	807	-	1/1/15/20	14/37/115/115	-
19	CLA	B	815	-	1/1/13/20	10/25/103/115	-
24	BCR	B	847	-	-	2/29/63/63	0/2/2/2
19	CLA	A	839	-	1/1/15/20	20/37/115/115	-
18	CHL	2	314	2	2/2/15/26	2/12/110/137	-
19	CLA	4	313	-	1/1/11/20	4/13/91/115	-
19	CLA	B	824	-	1/1/15/20	15/37/115/115	-
24	BCR	L	303	-	-	4/29/63/63	0/2/2/2
24	BCR	B	843	-	-	4/29/63/63	0/2/2/2
19	CLA	A	838	-	1/1/15/20	18/37/115/115	-
19	CLA	1	308	1	1/1/13/20	12/28/106/115	-
18	CHL	2	306	-	3/3/16/26	6/15/113/137	-
19	CLA	4	301	4	1/1/11/20	6/15/93/115	-
19	CLA	K	201	-	1/1/11/20	5/13/91/115	-
19	CLA	B	836	-	1/1/15/20	16/37/115/115	-
21	XAT	2	316	-	-	3/31/93/93	0/4/4/4
19	CLA	1	311	1	1/1/12/20	8/19/97/115	-
19	CLA	3	311	-	1/1/11/20	7/13/91/115	-
19	CLA	B	809	6	1/1/15/20	13/37/115/115	-
19	CLA	3	304	-	1/1/11/20	6/16/94/115	-
19	CLA	1	305	-	1/1/10/20	4/10/88/115	-
19	CLA	A	837	-	1/1/15/20	16/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	821	-	1/1/12/20	11/19/97/115	-
20	LUT	1	315	-	-	0/29/67/67	0/2/2/2
22	LHG	B	850	19	-	8/53/53/53	-
24	BCR	A	848	-	-	0/29/63/63	0/2/2/2
24	BCR	3	317	-	-	0/29/63/63	0/2/2/2
19	CLA	B	802	-	1/1/15/20	17/37/115/115	-
19	CLA	1	313	-	1/1/11/20	5/13/91/115	-
19	CLA	1	312	-	1/1/14/20	12/31/109/115	-
19	CLA	B	831	-	1/1/14/20	16/31/109/115	-
19	CLA	F	302	-	1/1/11/20	6/13/91/115	-
19	CLA	B	828	-	1/1/15/20	17/37/115/115	-
19	CLA	A	818	-	1/1/11/20	0/13/91/115	-
19	CLA	A	853	-	1/1/15/20	23/37/115/115	-
19	CLA	2	310	22	1/1/10/20	3/8/86/115	-
19	CLA	3	308	3	1/1/15/20	14/37/115/115	-
19	CLA	A	833	-	1/1/15/20	20/37/115/115	-
19	CLA	2	309	2	1/1/14/20	11/31/109/115	-
19	CLA	4	302	4	1/1/14/20	6/31/109/115	-
19	CLA	4	303	-	1/1/14/20	17/31/109/115	-
19	CLA	K	202	-	1/1/11/20	7/15/93/115	-
19	CLA	B	827	-	1/1/14/20	12/31/109/115	-
19	CLA	4	304	-	1/1/11/20	4/13/91/115	-
19	CLA	3	301	3	1/1/14/20	12/31/109/115	-
19	CLA	B	810	-	1/1/15/20	22/37/115/115	-
19	CLA	B	835	-	1/1/13/20	7/25/103/115	-
20	LUT	3	315	-	-	0/29/67/67	0/2/2/2
24	BCR	I	101	-	-	0/29/63/63	0/2/2/2
24	BCR	A	843	-	-	8/29/63/63	0/2/2/2
19	CLA	B	803	-	1/1/15/20	14/37/115/115	-
18	CHL	2	307	-	3/3/16/26	6/15/113/137	-
19	CLA	A	819	-	1/1/15/20	10/37/115/115	-
19	CLA	B	805	-	1/1/15/20	15/37/115/115	-
19	CLA	A	816	-	1/1/13/20	9/25/103/115	-
19	CLA	B	832	-	1/1/13/20	14/29/107/115	-
19	CLA	L	302	-	1/1/12/20	11/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	825	-	1/1/13/20	7/25/103/115	-
19	CLA	2	312	-	1/1/15/20	19/37/115/115	-
25	LMG	4	318	-	-	5/31/51/70	0/1/1/1
19	CLA	B	851	-	1/1/15/20	18/37/115/115	-
26	PQN	A	841	-	-	5/23/43/43	0/2/2/2
19	CLA	B	822	-	1/1/13/20	9/25/103/115	-
19	CLA	1	310	22	1/1/13/20	9/25/103/115	-
19	CLA	2	304	-	1/1/11/20	4/13/91/115	-
24	BCR	A	846	-	-	0/29/63/63	0/2/2/2
19	CLA	A	821	-	1/1/12/20	9/21/99/115	-
19	CLA	A	831	-	1/1/15/20	21/37/115/115	-
19	CLA	B	826	-	1/1/15/20	13/37/115/115	-
19	CLA	B	823	-	1/1/13/20	8/25/103/115	-
19	CLA	G	203	-	1/1/12/20	8/19/97/115	-
19	CLA	A	854	-	1/1/15/20	15/37/115/115	-
19	CLA	4	310	-	1/1/14/20	15/31/109/115	-
19	CLA	H	201	12	1/1/11/20	7/13/91/115	-
19	CLA	3	302	-	1/1/14/20	14/31/109/115	-
19	CLA	1	304	-	1/1/12/20	11/21/99/115	-
19	CLA	3	303	-	1/1/11/20	6/13/91/115	-
19	CLA	L	301	-	1/1/15/20	14/37/115/115	-
26	PQN	B	841	-	-	6/23/43/43	0/2/2/2
24	BCR	F	304	-	-	0/29/63/63	0/2/2/2
23	LMT	A	851	-	-	4/21/61/61	0/2/2/2
19	CLA	B	829	-	1/1/15/20	11/37/115/115	-
18	CHL	4	314	4	3/3/15/26	0/10/108/137	-
25	LMG	F	305	-	-	1/25/45/70	0/1/1/1
19	CLA	B	804	-	1/1/11/20	7/13/91/115	-
19	CLA	A	810	-	1/1/12/20	9/24/102/115	-
19	CLA	A	835	-	1/1/15/20	21/37/115/115	-
19	CLA	3	310	-	1/1/10/20	3/8/86/115	-
24	BCR	G	201	-	-	8/29/63/63	0/2/2/2
19	CLA	1	303	-	1/1/13/20	9/29/107/115	-
19	CLA	3	309	3	1/1/12/20	6/19/97/115	-
19	CLA	A	813	-	1/1/12/20	8/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	F	303	-	-	2/29/63/63	0/2/2/2
21	XAT	1	316	-	-	0/31/93/93	0/4/4/4
19	CLA	A	805	-	1/1/12/20	3/19/97/115	-
18	CHL	4	306	-	3/3/16/26	6/15/113/137	-
19	CLA	A	834	-	1/1/12/20	10/21/99/115	-
18	CHL	4	305	-	3/3/18/26	11/27/125/137	-
18	CHL	2	301	2	3/3/17/26	9/21/119/137	-
19	CLA	2	308	2	1/1/11/20	3/13/91/115	-
19	CLA	3	306	3	1/1/11/20	5/13/91/115	-
19	CLA	B	838	-	1/1/15/20	18/37/115/115	-
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2
24	BCR	L	305	-	-	3/29/63/63	0/2/2/2
19	CLA	A	836	-	1/1/12/20	7/22/100/115	-
19	CLA	K	203	16	1/1/8/20	0/2/76/115	-
19	CLA	A	809	-	1/1/15/20	9/37/115/115	-
19	CLA	A	830	-	1/1/15/20	19/37/115/115	-
19	CLA	2	311	2	1/1/11/20	5/13/91/115	-
19	CLA	J	102	14	1/1/10/20	5/10/88/115	-
27	SF4	C	102	7	-	-	0/6/5/5
19	CLA	A	815	-	1/1/15/20	22/35/113/115	-
19	CLA	B	801	-	1/1/15/20	12/37/115/115	-
19	CLA	B	817	-	1/1/13/20	13/30/108/115	-
24	BCR	2	319	-	-	15/29/63/63	0/2/2/2
19	CLA	A	804	5	1/1/15/20	14/37/115/115	-
19	CLA	G	202	-	1/1/10/20	4/8/86/115	-
19	CLA	A	828	-	1/1/15/20	16/37/115/115	-
24	BCR	A	845	-	-	2/29/63/63	0/2/2/2
19	CLA	A	802	-	1/1/12/20	9/19/97/115	-
19	CLA	4	311	4	1/1/11/20	3/13/91/115	-
19	CLA	1	302	1	1/1/14/20	9/31/109/115	-
19	CLA	3	305	-	1/1/10/20	2/10/88/115	-
18	CHL	1	301	1	3/3/18/26	11/27/125/137	-
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
19	CLA	2	313	-	1/1/10/20	0/11/89/115	-
19	CLA	A	823	-	1/1/15/20	19/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SF4	A	850	6,5	-	-	0/6/5/5
19	CLA	1	318	-	1/1/15/20	19/37/115/115	-
19	CLA	B	813	-	1/1/15/20	20/37/115/115	-
19	CLA	B	814	-	1/1/15/20	20/37/115/115	-
21	XAT	3	316	-	-	1/31/93/93	0/4/4/4
19	CLA	B	834	-	1/1/11/20	9/13/91/115	-
19	CLA	B	830	-	1/1/12/20	7/19/97/115	-
28	DGD	B	848	-	-	12/55/95/95	0/2/2/2
24	BCR	A	844	-	-	1/29/63/63	0/2/2/2
18	CHL	2	305	-	3/3/15/26	5/12/110/137	-
19	CLA	A	803	-	1/1/15/20	14/37/115/115	-
19	CLA	H	202	15	1/1/13/20	11/25/103/115	-
19	CLA	4	308	4	1/1/12/20	8/19/97/115	-
19	CLA	B	837	-	1/1/11/20	2/16/94/115	-
24	BCR	J	104	-	-	4/29/63/63	0/2/2/2
24	BCR	J	103	-	-	2/29/63/63	0/2/2/2
27	SF4	C	101	7	-	-	0/6/5/5
24	BCR	A	849	-	-	4/29/63/63	0/2/2/2
19	CLA	2	303	-	1/1/12/20	7/19/97/115	-
19	CLA	1	309	1	1/1/14/20	9/31/109/115	-
19	CLA	4	312	-	1/1/13/20	8/27/105/115	-
19	CLA	A	801	-	1/1/15/20	18/37/115/115	-
22	LHG	A	842	-	-	5/53/53/53	-
19	CLA	B	812	-	1/1/13/20	11/25/103/115	-
24	BCR	A	847	-	-	4/29/63/63	0/2/2/2
19	CLA	4	309	4	1/1/14/20	6/31/109/115	-
19	CLA	A	852	-	1/1/15/20	11/37/115/115	-
19	CLA	B	808	-	1/1/15/20	12/37/115/115	-

The worst 5 of 1145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	305	CHL	CMC-C2C	5.43	1.56	1.45
18	4	305	CHL	CMC-C2C	5.41	1.56	1.45
18	4	306	CHL	CMC-C2C	5.41	1.56	1.45
18	1	306	CHL	CMC-C2C	5.41	1.56	1.45
18	2	301	CHL	CMC-C2C	5.39	1.56	1.45

The worst 5 of 1570 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	308	CLA	C4A-NA-C1A	11.53	111.89	106.71
19	A	803	CLA	C4A-NA-C1A	11.17	111.73	106.71
18	3	307	CHL	C4A-NA-C1A	10.94	111.62	106.71
19	B	826	CLA	C4A-NA-C1A	10.81	111.57	106.71
18	1	301	CHL	C4A-NA-C1A	10.76	111.54	106.71

5 of 176 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	1	301	CHL	ND
18	1	301	CHL	NA
18	1	301	CHL	NC
18	1	306	CHL	ND
18	1	306	CHL	NC

5 of 1799 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	301	CHL	CBD-CGD-O2D-CED
18	1	301	CHL	C1-C2-C3-C5
18	1	306	CHL	C3C-C2C-CMC-OMC
18	1	306	CHL	CHA-CBD-CGD-O2D
18	2	301	CHL	O2A-C1-C2-C3

There are no ring outliers.

156 monomers are involved in 293 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	315	LUT	7	0
24	B	844	BCR	2	0
19	B	840	CLA	2	0
19	B	833	CLA	1	0
19	B	820	CLA	1	0
19	A	826	CLA	2	0
25	B	849	LMG	1	0
18	4	307	CHL	1	0
19	B	806	CLA	4	0
22	1	320	LHG	2	0
19	B	839	CLA	2	0
19	B	816	CLA	1	0
19	2	302	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	314	CLA	1	0
22	2	317	LHG	2	0
19	A	807	CLA	5	0
19	A	825	CLA	1	0
19	A	827	CLA	1	0
19	3	312	CLA	2	0
19	A	814	CLA	1	0
19	A	822	CLA	2	0
24	J	101	BCR	7	0
19	F	301	CLA	1	0
22	1	317	LHG	3	0
24	B	845	BCR	2	0
21	4	316	XAT	1	0
18	1	306	CHL	1	0
19	A	812	CLA	1	0
19	A	808	CLA	2	0
24	G	205	BCR	1	0
24	L	304	BCR	6	0
19	A	811	CLA	7	0
19	A	824	CLA	1	0
19	B	818	CLA	3	0
20	2	315	LUT	4	0
19	A	840	CLA	3	0
23	2	318	LMT	1	0
20	1	319	LUT	3	0
19	A	806	CLA	4	0
19	B	807	CLA	4	0
19	A	839	CLA	1	0
19	B	824	CLA	2	0
24	B	843	BCR	1	0
19	A	838	CLA	1	0
19	1	308	CLA	3	0
18	2	306	CHL	1	0
19	4	301	CLA	1	0
19	K	201	CLA	3	0
19	B	836	CLA	1	0
21	2	316	XAT	1	0
19	1	311	CLA	1	0
19	3	311	CLA	1	0
19	3	304	CLA	2	0
19	A	837	CLA	1	0
19	B	821	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	315	LUT	4	0
22	B	850	LHG	5	0
24	A	848	BCR	2	0
24	3	317	BCR	4	0
19	1	313	CLA	1	0
19	1	312	CLA	3	0
19	B	831	CLA	1	0
19	B	828	CLA	1	0
19	A	818	CLA	1	0
19	A	853	CLA	4	0
19	2	310	CLA	1	0
19	3	308	CLA	3	0
19	A	833	CLA	7	0
19	2	309	CLA	2	0
19	4	302	CLA	2	0
19	4	303	CLA	3	0
19	K	202	CLA	1	0
19	B	827	CLA	1	0
19	4	304	CLA	1	0
19	3	301	CLA	1	0
19	B	810	CLA	1	0
19	B	835	CLA	1	0
20	3	315	LUT	6	0
24	I	101	BCR	4	0
24	A	843	BCR	4	0
19	B	803	CLA	1	0
18	2	307	CHL	3	0
19	A	819	CLA	2	0
19	B	805	CLA	1	0
19	A	816	CLA	4	0
19	B	832	CLA	3	0
19	B	825	CLA	1	0
19	B	851	CLA	2	0
19	B	822	CLA	1	0
24	A	846	BCR	2	0
19	A	831	CLA	1	0
19	B	826	CLA	4	0
19	B	823	CLA	3	0
19	G	203	CLA	1	0
19	A	854	CLA	1	0
19	H	201	CLA	2	0
19	3	302	CLA	2	0

*Continued on next page...*



*Continued from previous page...*

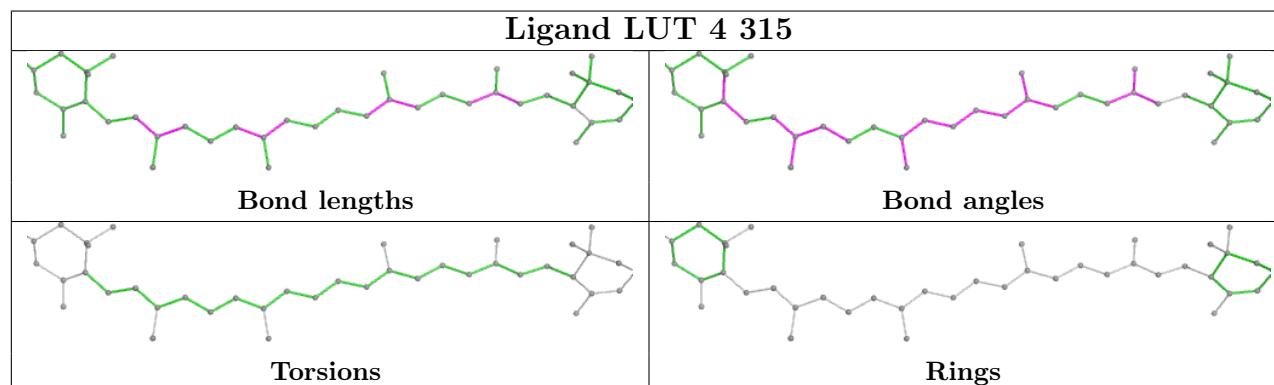
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	303	CLA	1	0
19	L	301	CLA	2	0
26	B	841	PQN	2	0
24	F	304	BCR	1	0
23	A	851	LMT	1	0
19	B	829	CLA	2	0
25	F	305	LMG	2	0
19	B	804	CLA	1	0
19	A	810	CLA	1	0
19	A	835	CLA	3	0
19	3	310	CLA	1	0
24	G	201	BCR	4	0
19	3	309	CLA	2	0
19	A	813	CLA	1	0
24	F	303	BCR	3	0
21	1	316	XAT	3	0
19	A	805	CLA	1	0
18	4	306	CHL	2	0
18	4	305	CHL	1	0
18	2	301	CHL	4	0
19	2	308	CLA	1	0
19	3	306	CLA	1	0
19	B	838	CLA	4	0
24	B	846	BCR	2	0
24	L	305	BCR	4	0
19	A	809	CLA	2	0
19	A	830	CLA	2	0
19	J	102	CLA	1	0
19	A	815	CLA	2	0
19	B	817	CLA	3	0
24	2	319	BCR	6	0
19	A	804	CLA	1	0
19	A	828	CLA	4	0
24	A	845	BCR	1	0
19	1	302	CLA	4	0
18	1	301	CHL	2	0
24	B	842	BCR	2	0
19	A	823	CLA	5	0
19	1	318	CLA	2	0
19	B	813	CLA	5	0
19	B	814	CLA	1	0
21	3	316	XAT	2	0

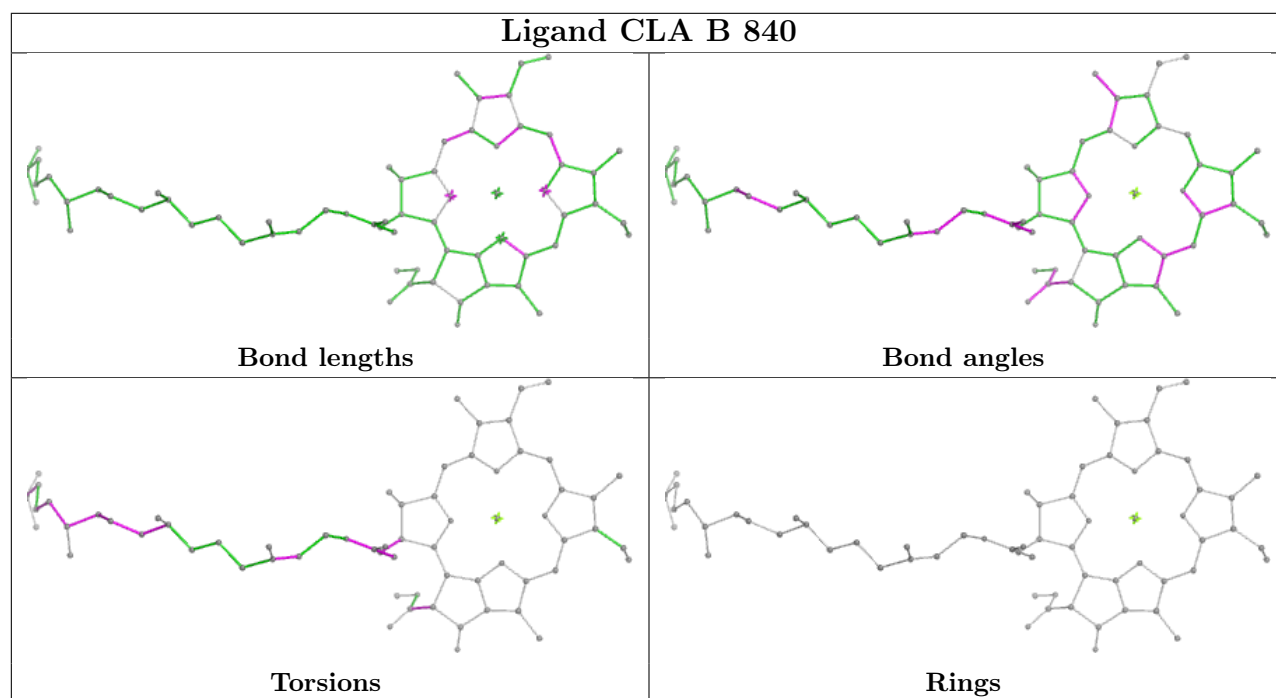
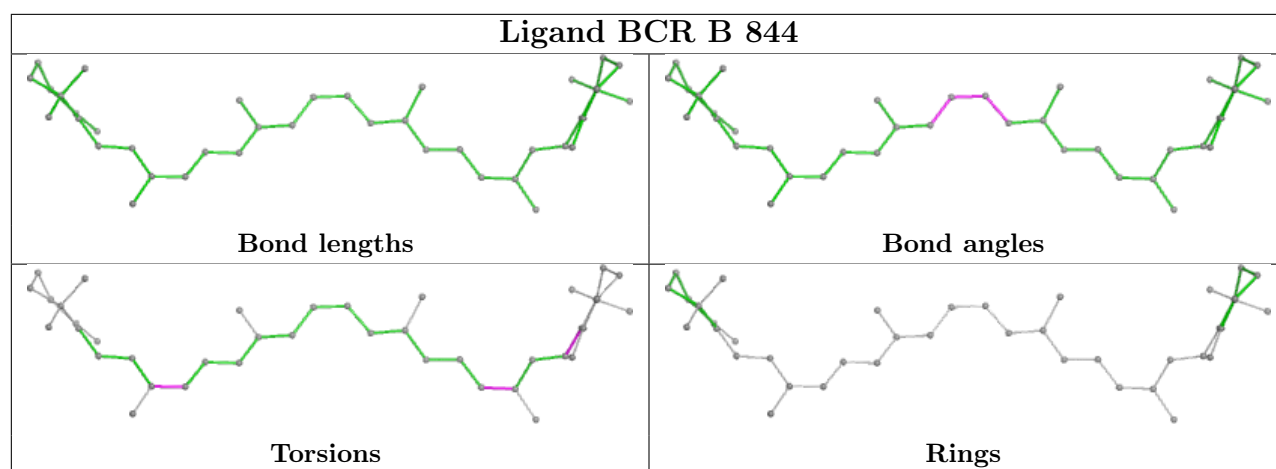
*Continued on next page...*

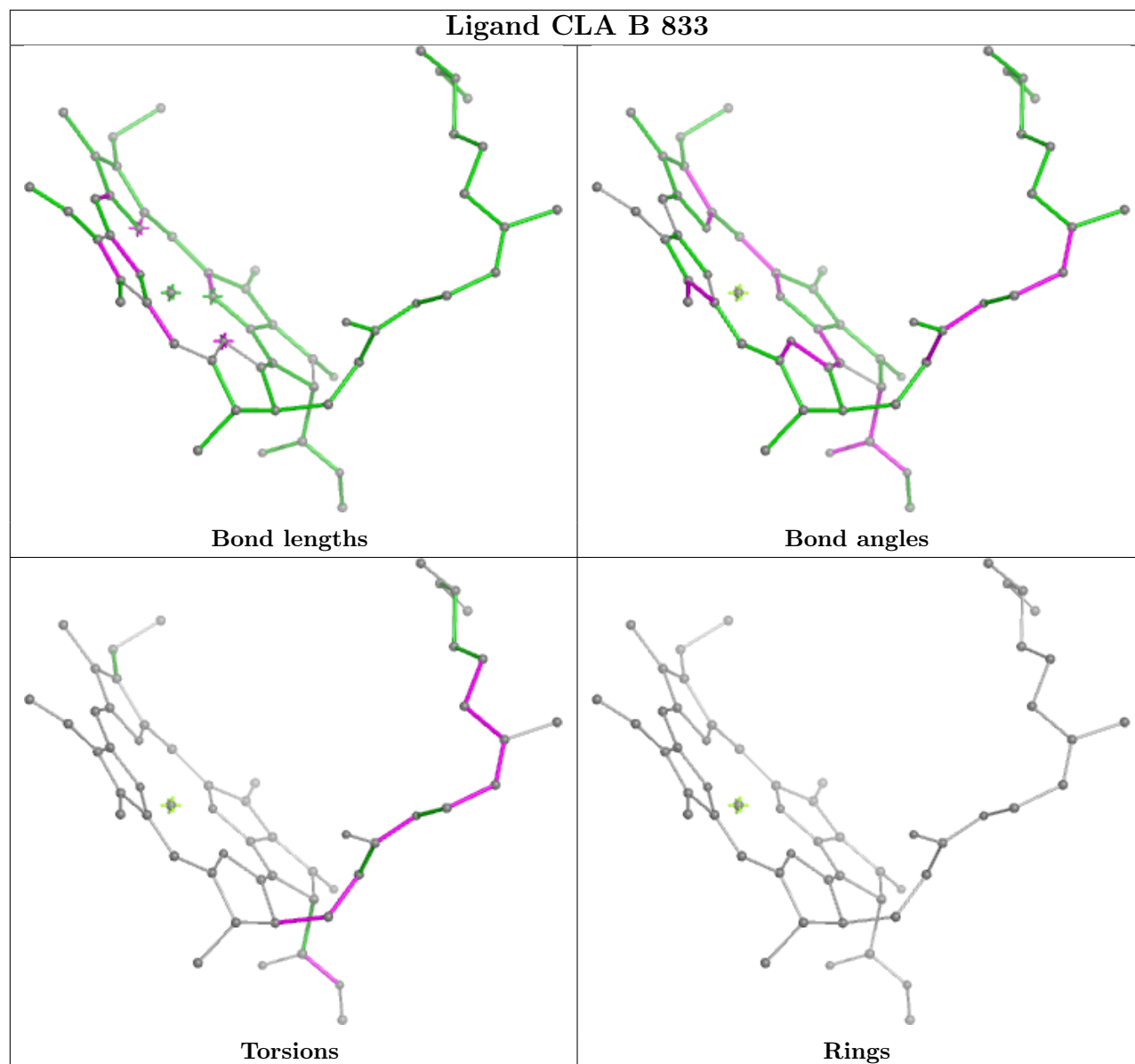
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	834	CLA	1	0
19	B	830	CLA	1	0
28	B	848	DGD	2	0
24	A	844	BCR	7	0
19	A	803	CLA	3	0
19	H	202	CLA	2	0
24	J	104	BCR	1	0
24	J	103	BCR	2	0
24	A	849	BCR	2	0
19	1	309	CLA	2	0
19	4	312	CLA	6	0
19	A	801	CLA	2	0
19	B	812	CLA	4	0
24	A	847	BCR	2	0
19	4	309	CLA	3	0
19	A	852	CLA	3	0
19	B	808	CLA	1	0

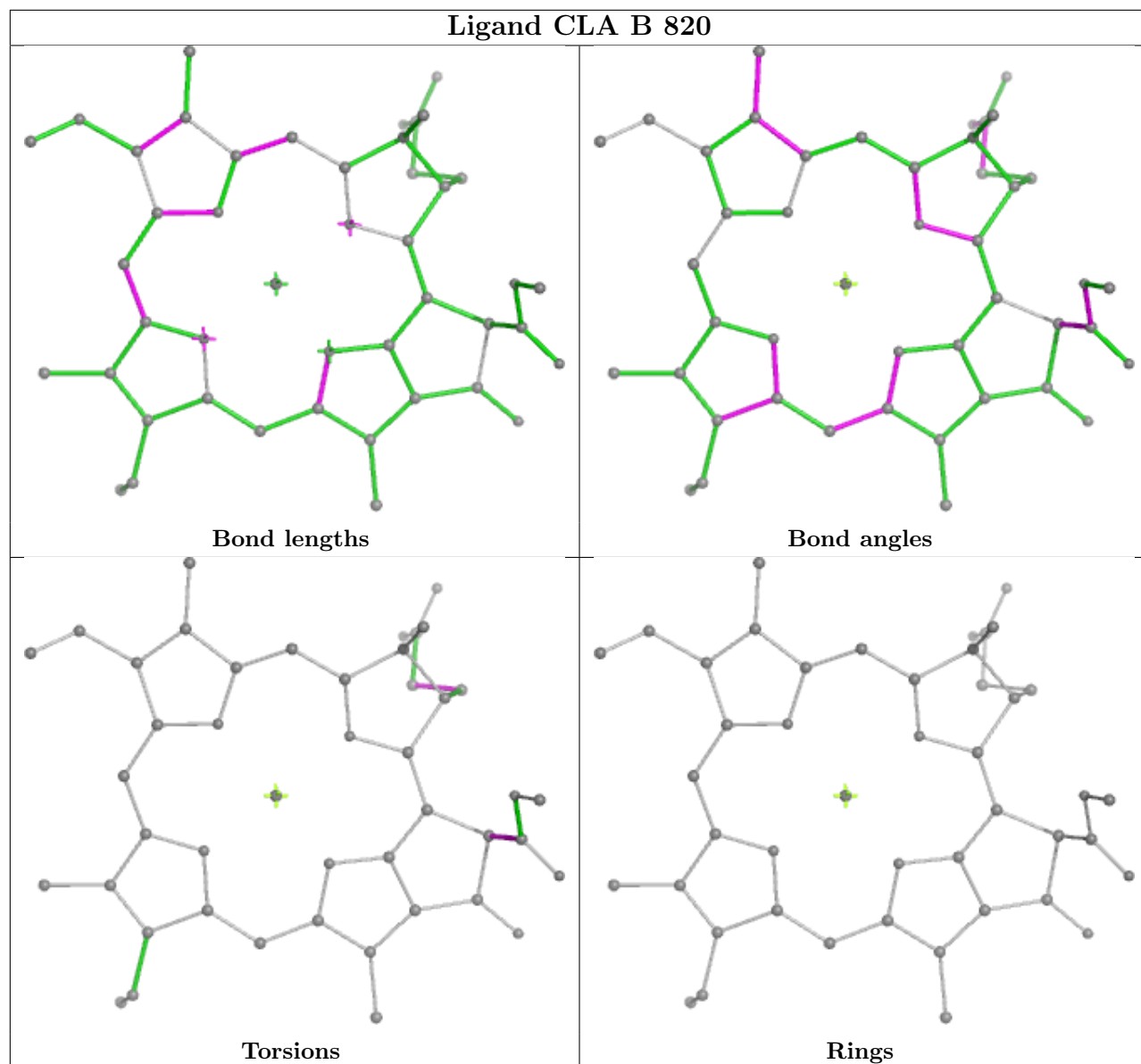
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

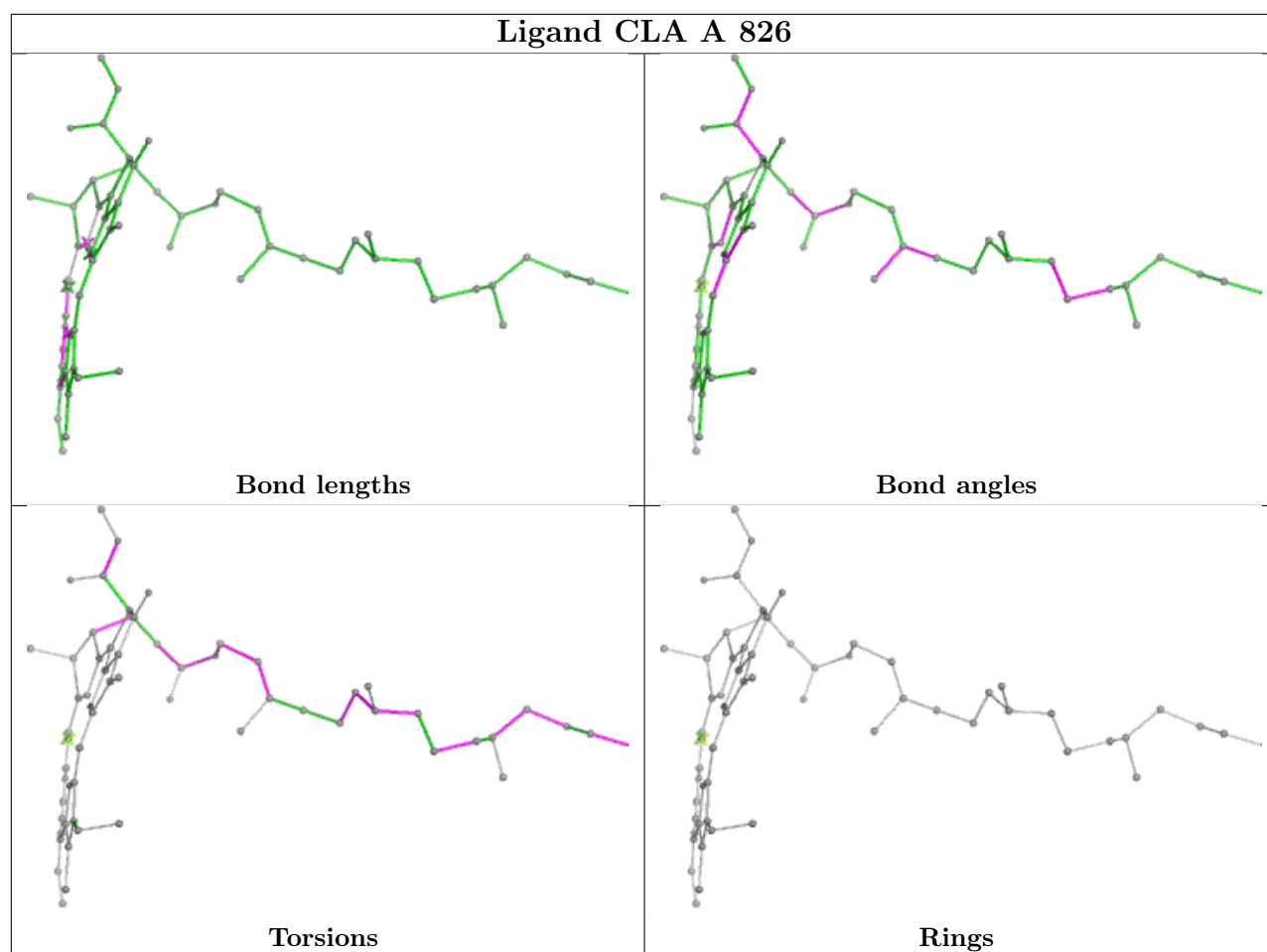


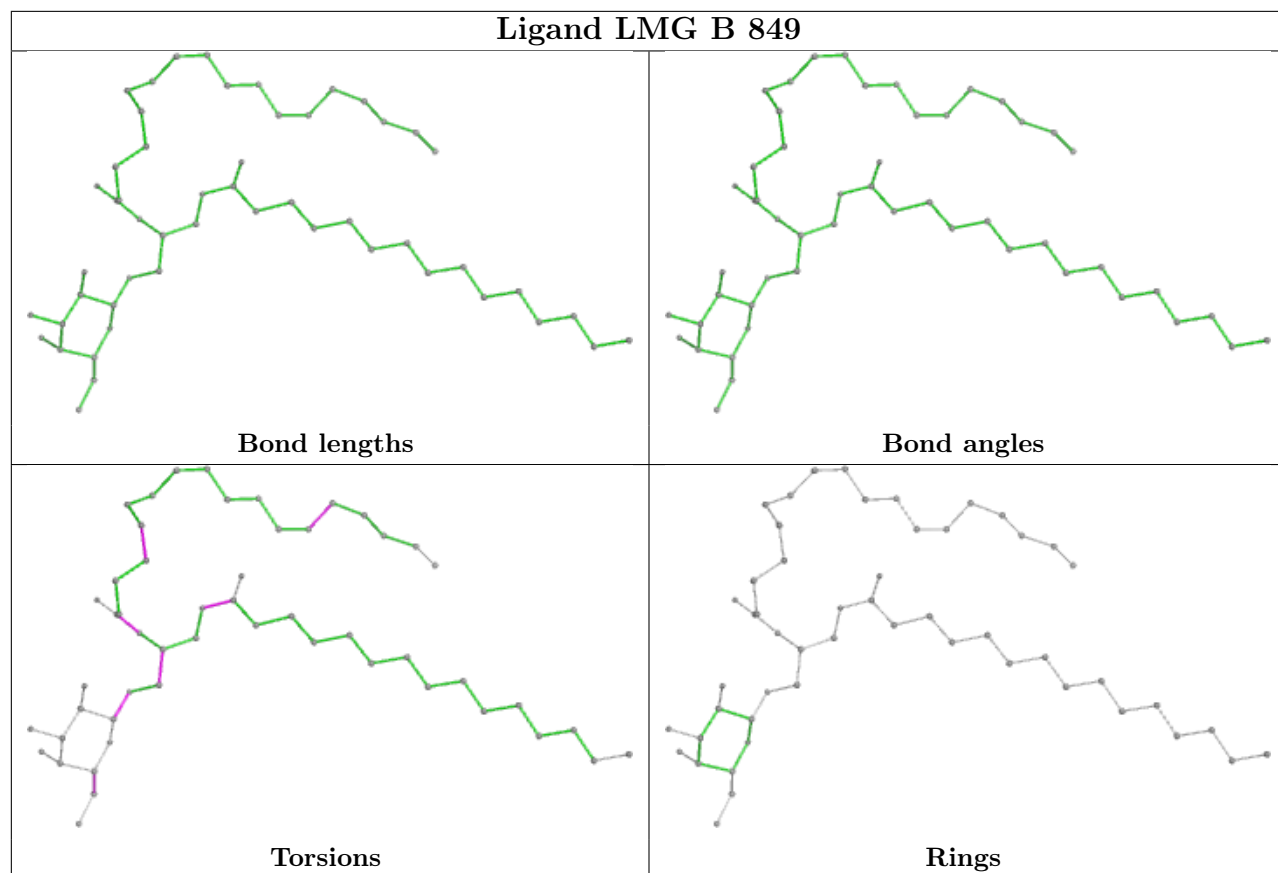


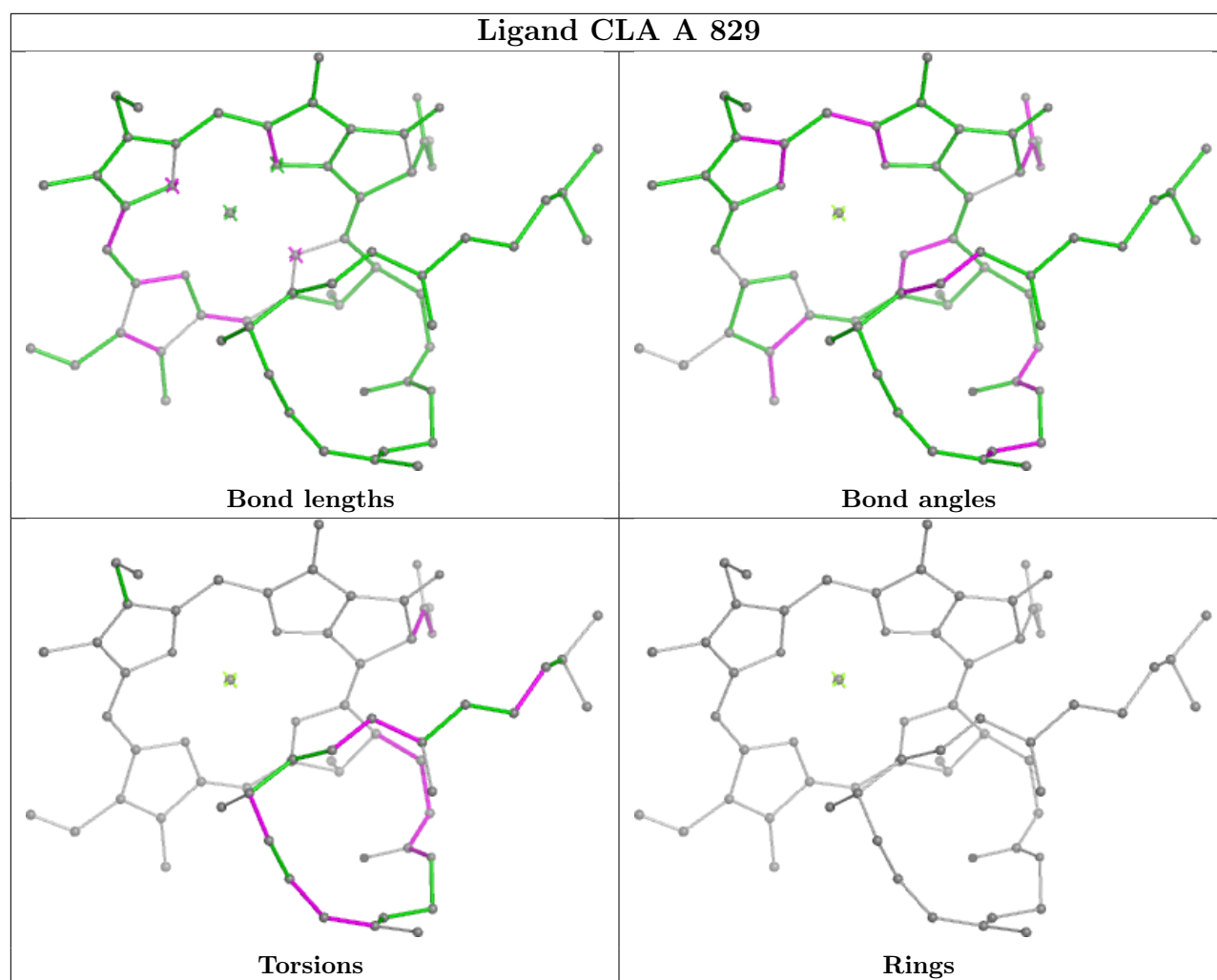


## Ligand CLA B 820



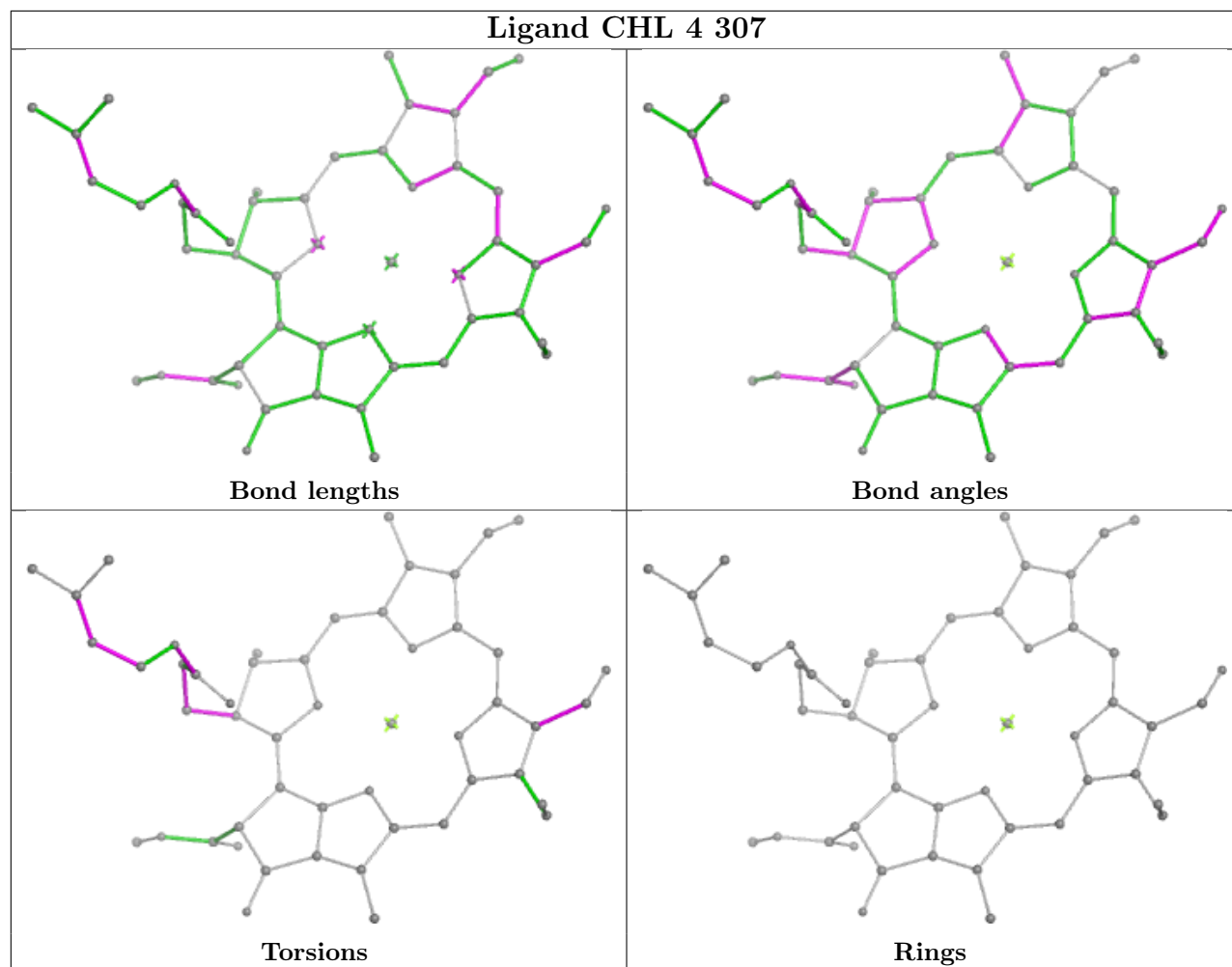




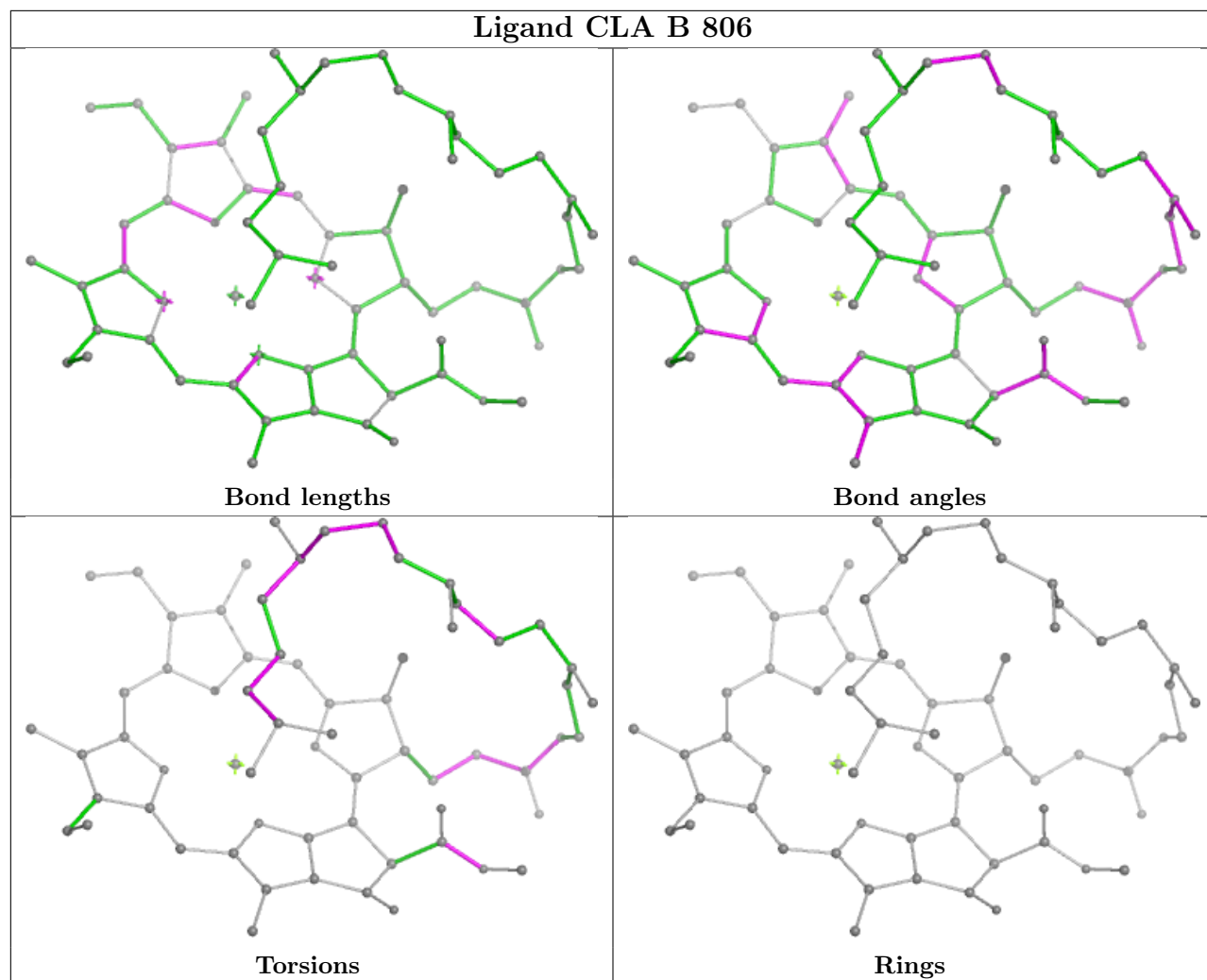


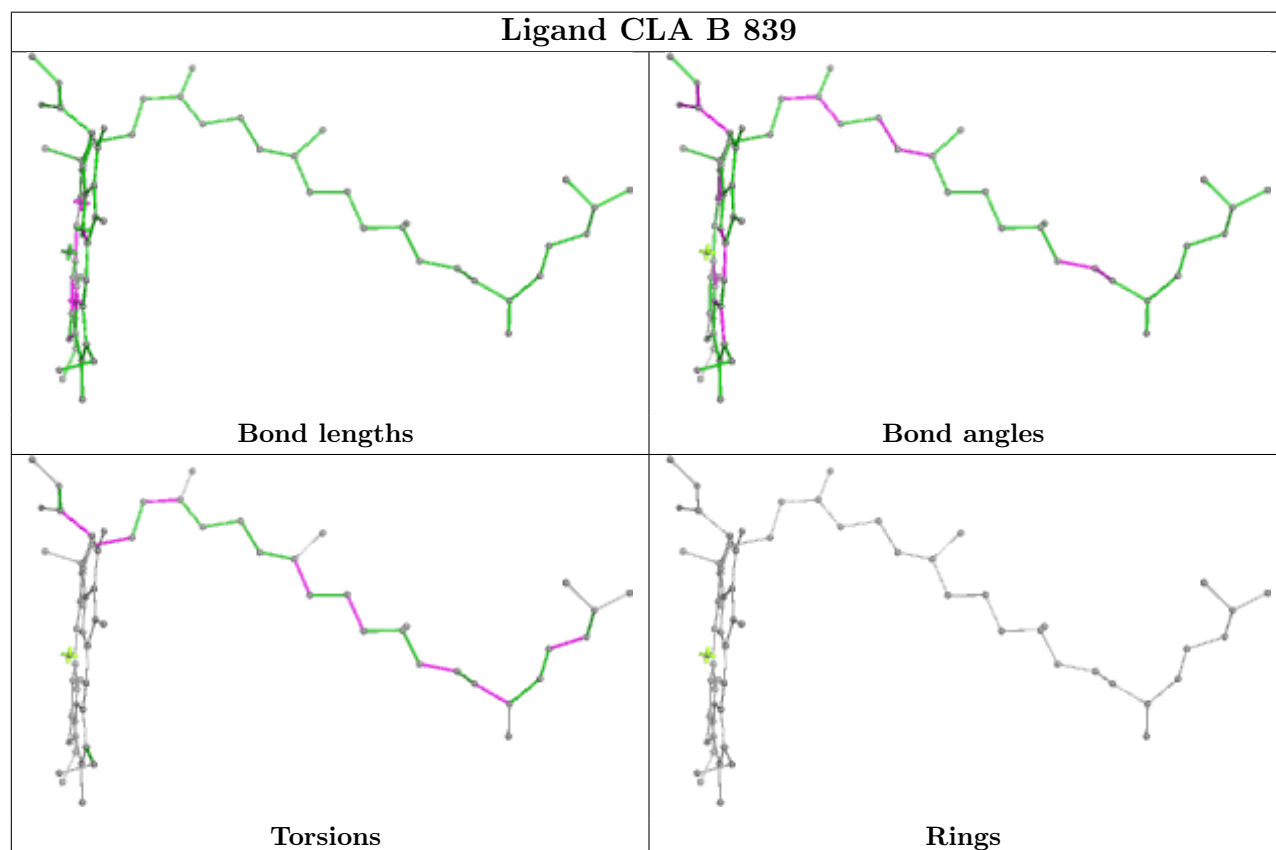
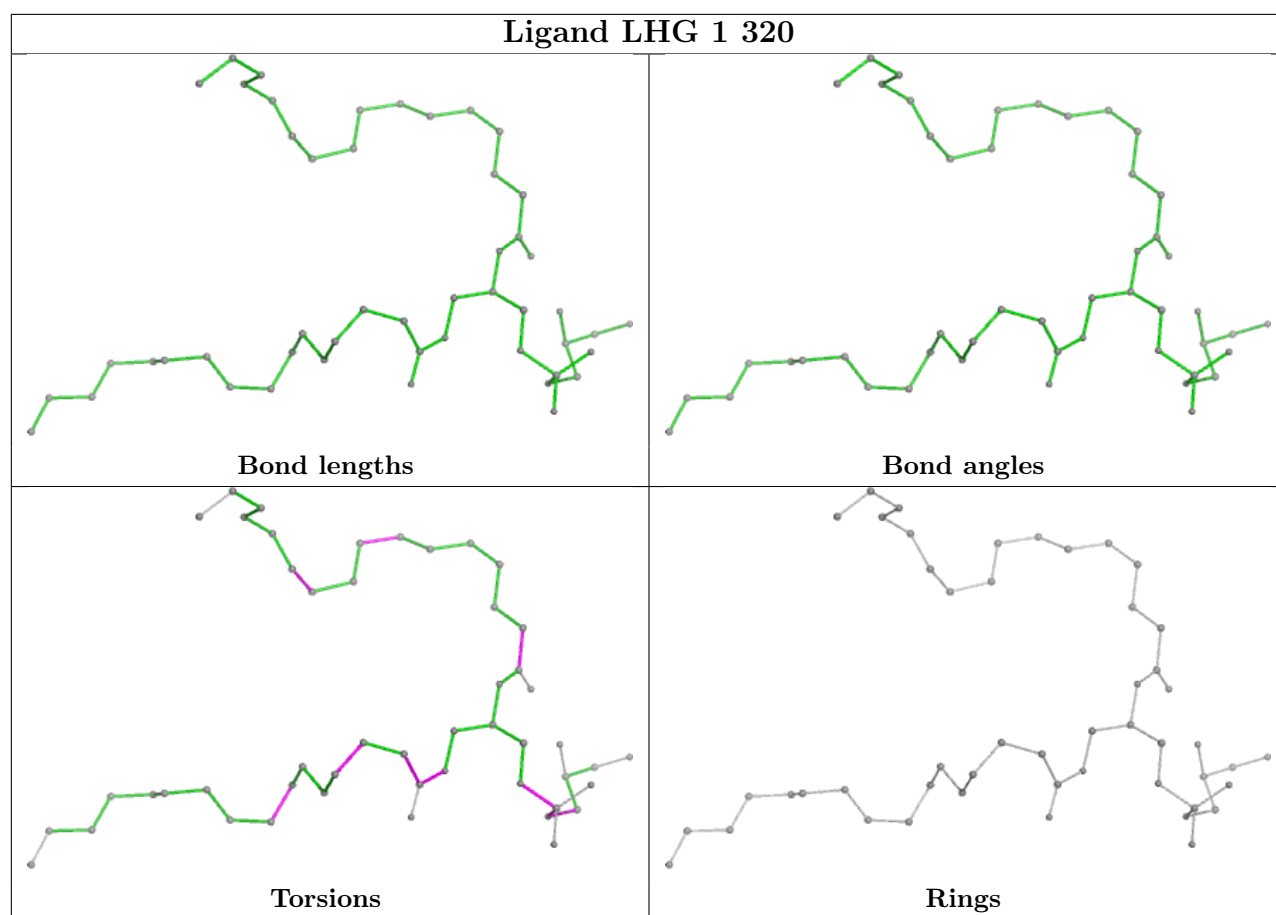


## Ligand CHL 4 307

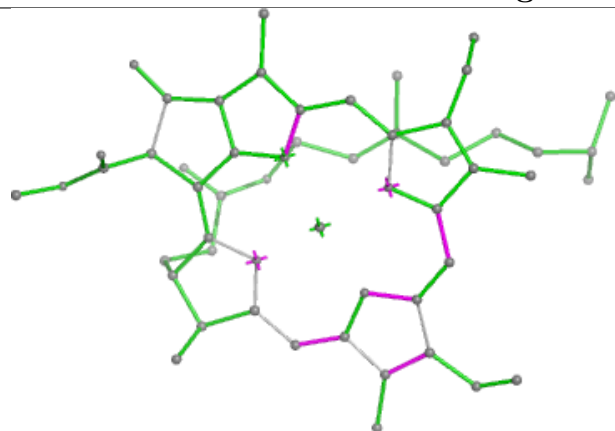


## Ligand CLA B 806

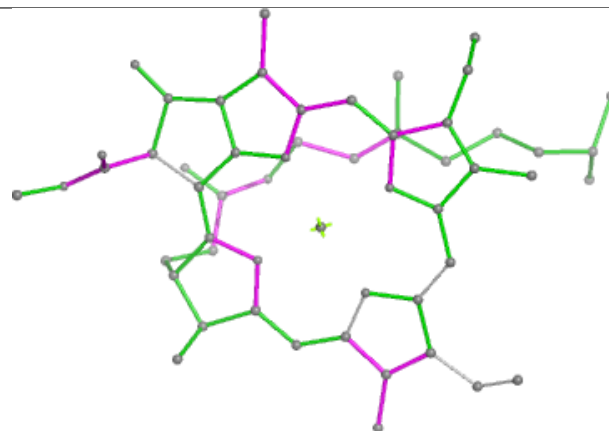




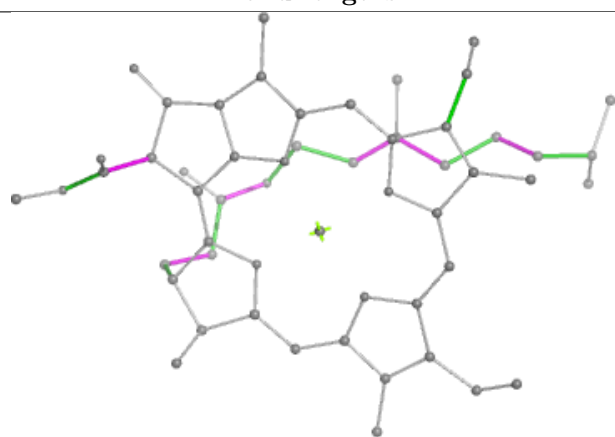
## Ligand CLA B 816



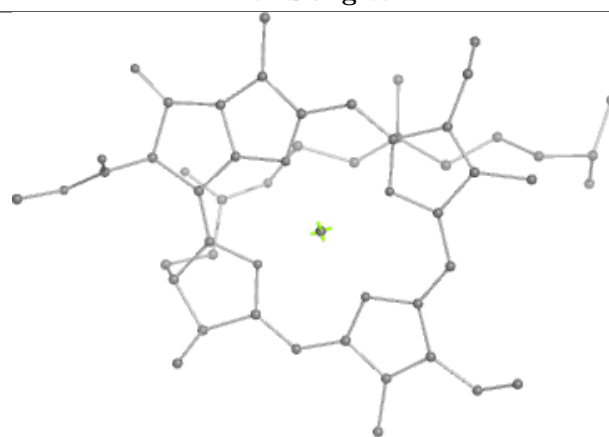
Bond lengths



Bond angles

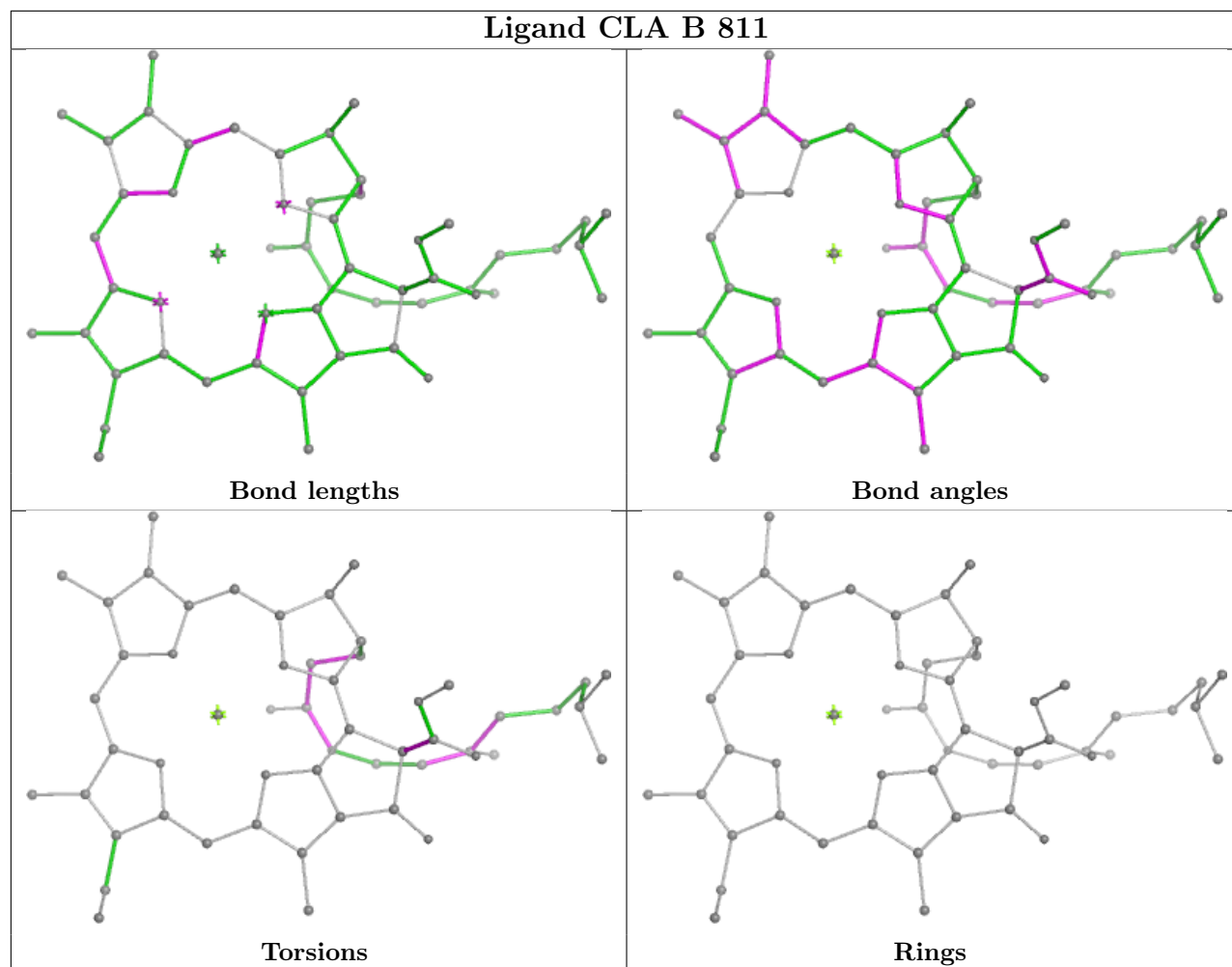


Torsions

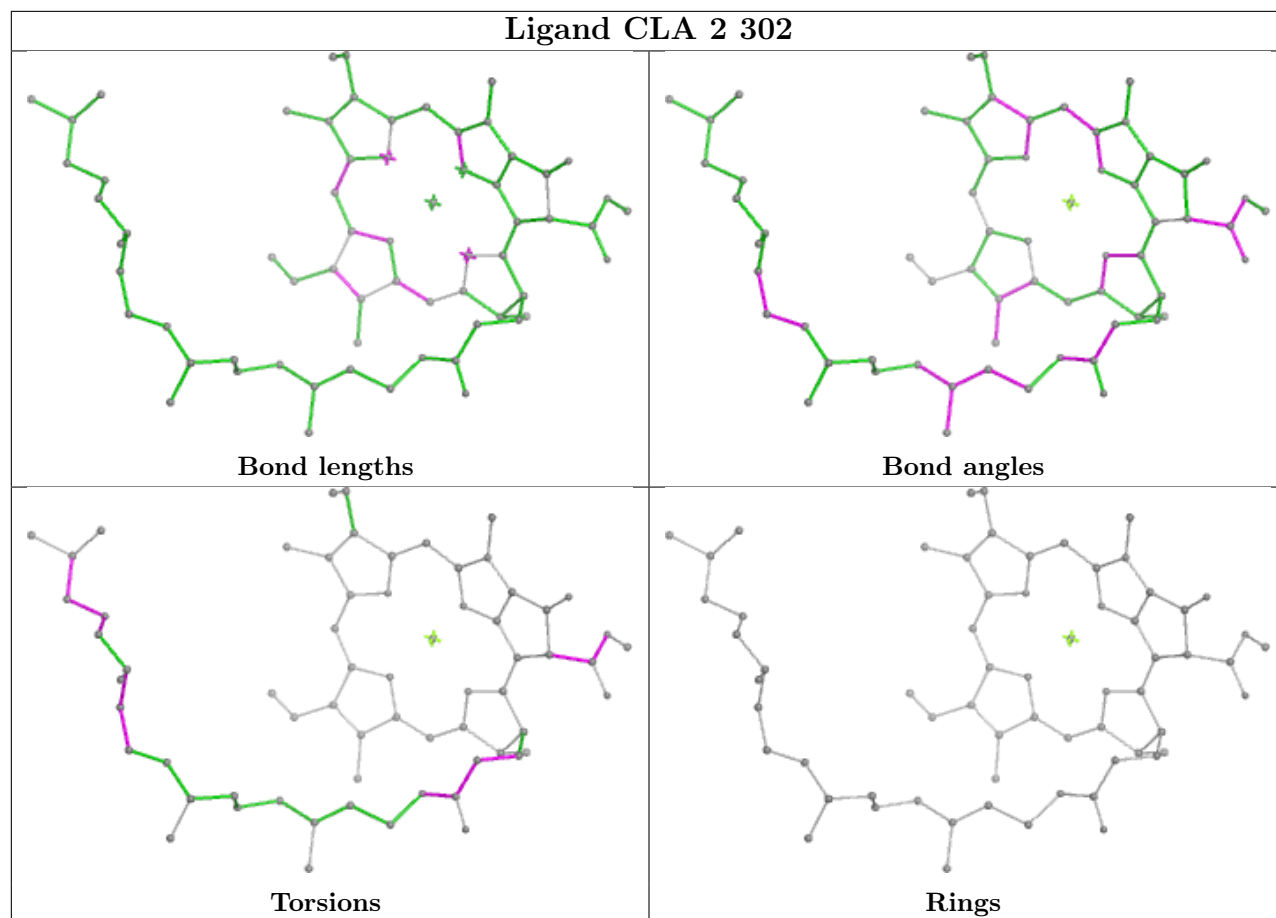


Rings

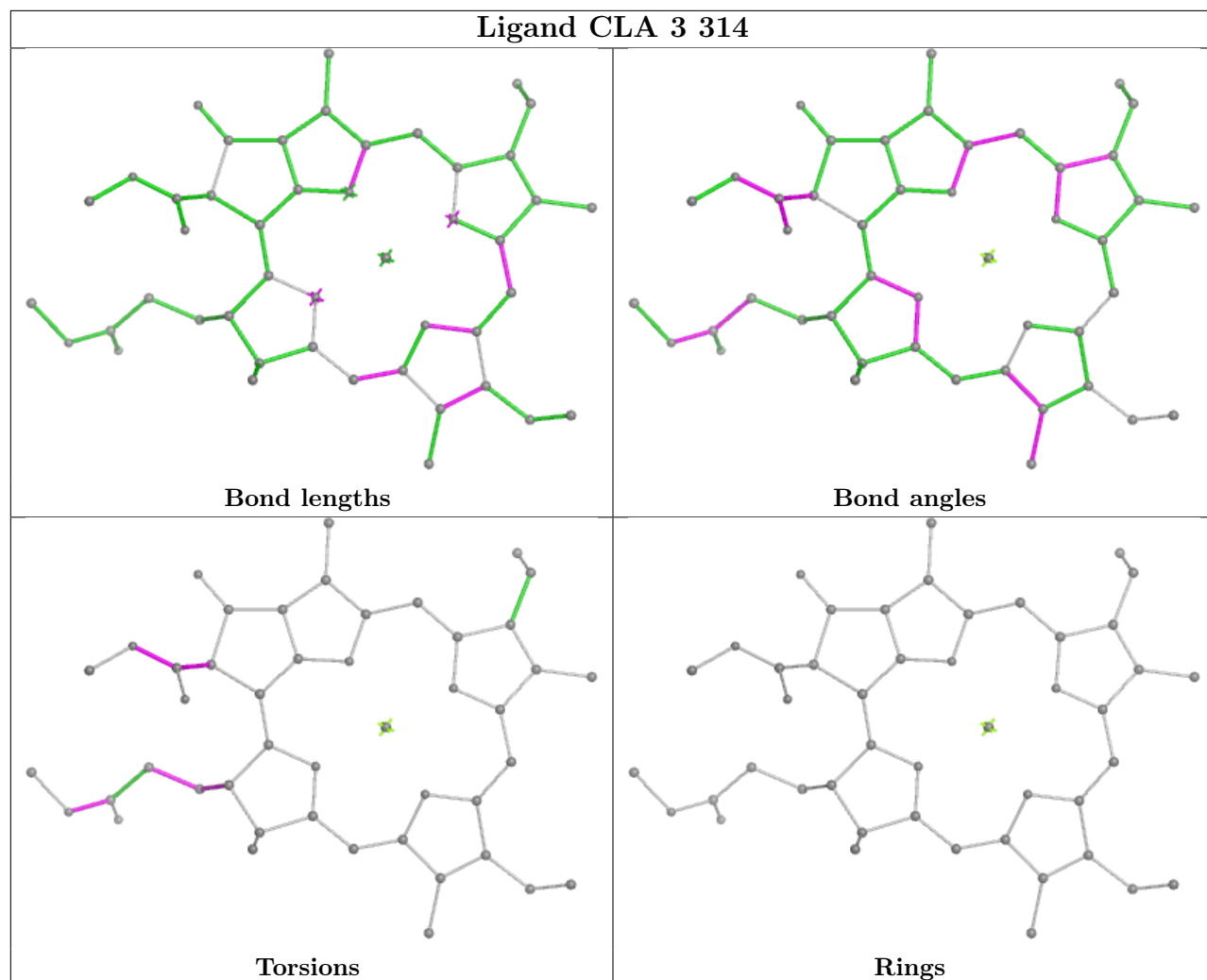
## Ligand CLA B 811

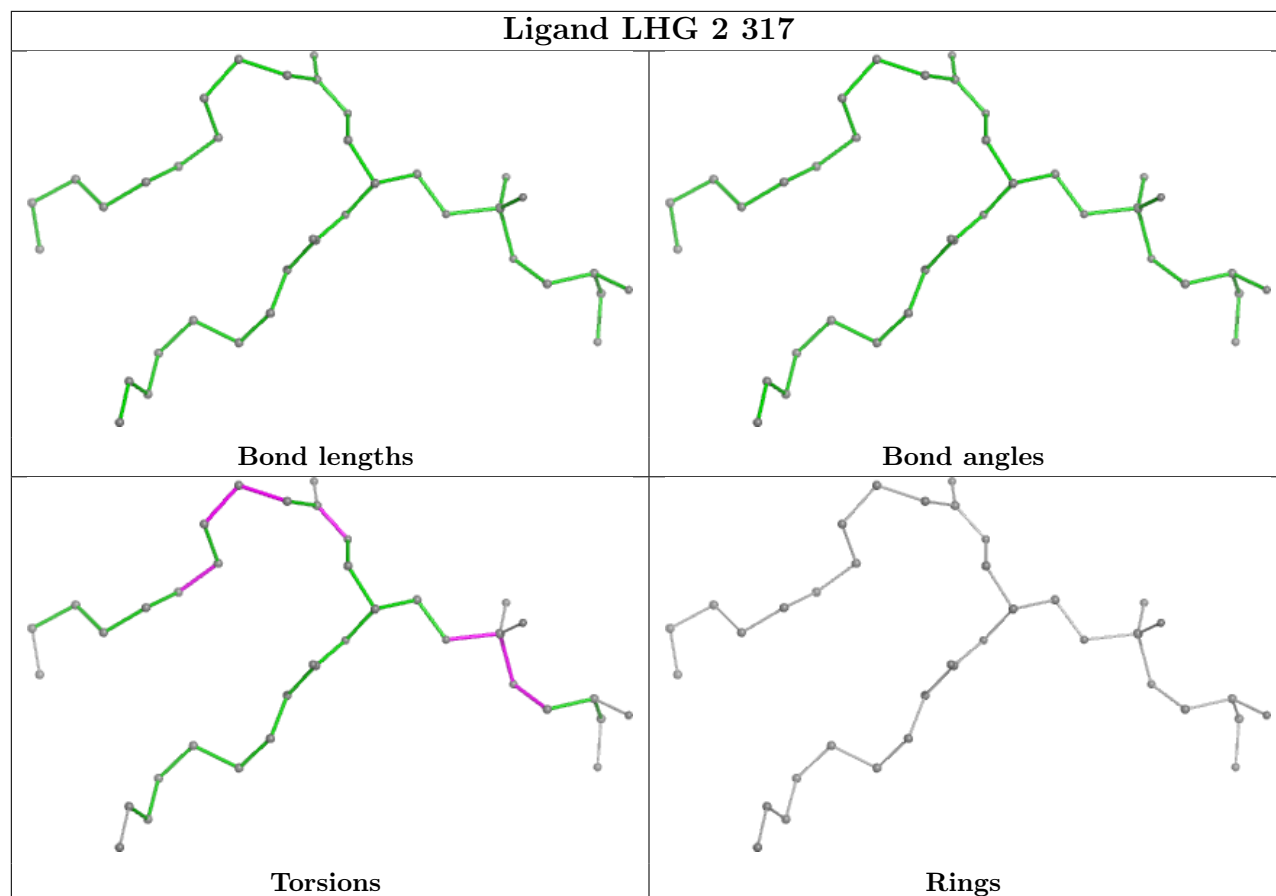
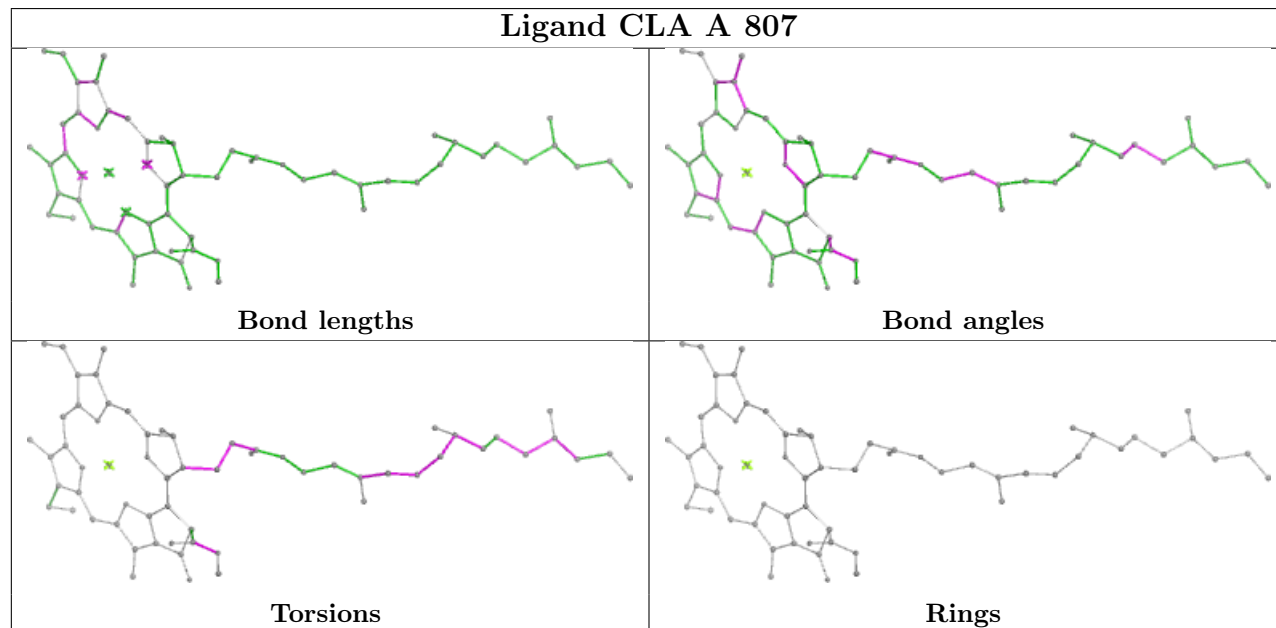


## Ligand CLA 2 302



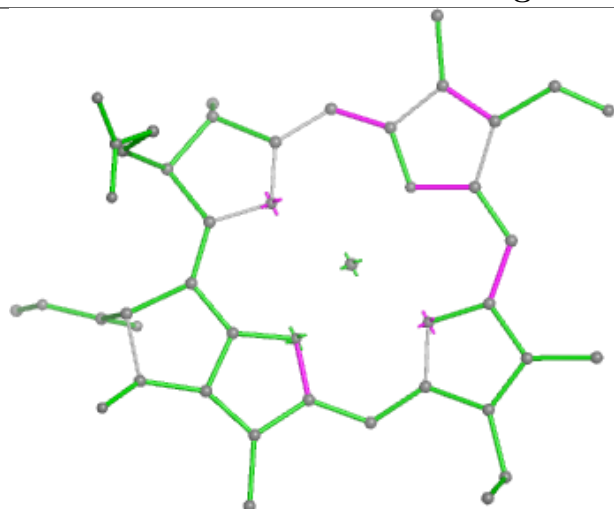
## Ligand CLA 3 314



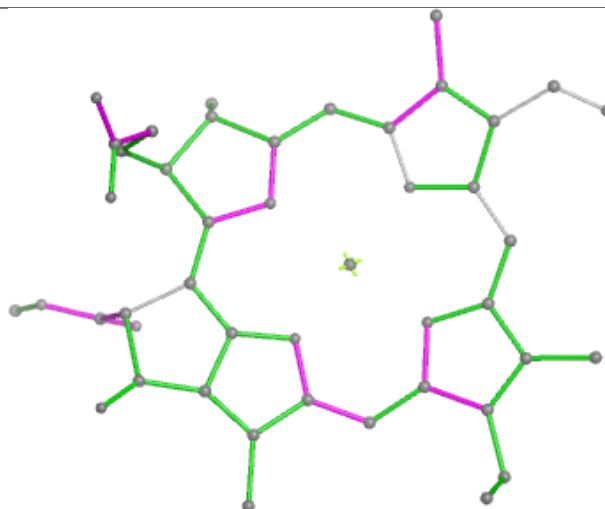
**Ligand LHG 2 317****Ligand CLA A 807**



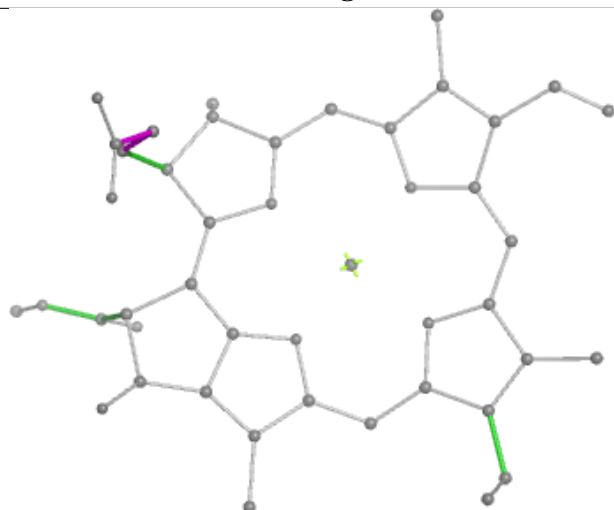
## Ligand CLA A 832



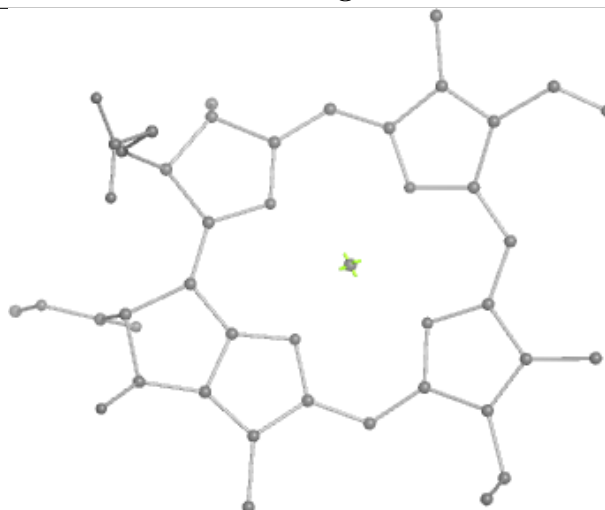
Bond lengths



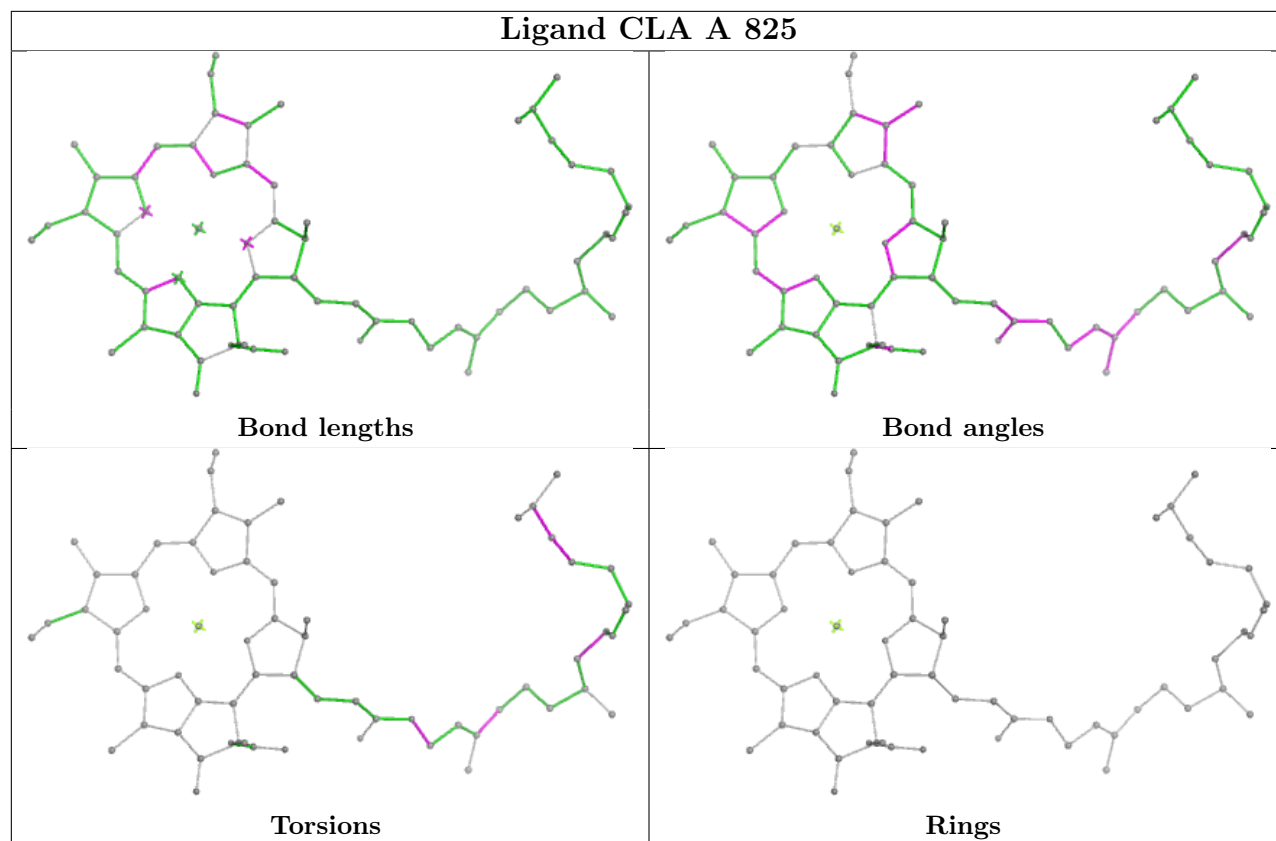
Bond angles

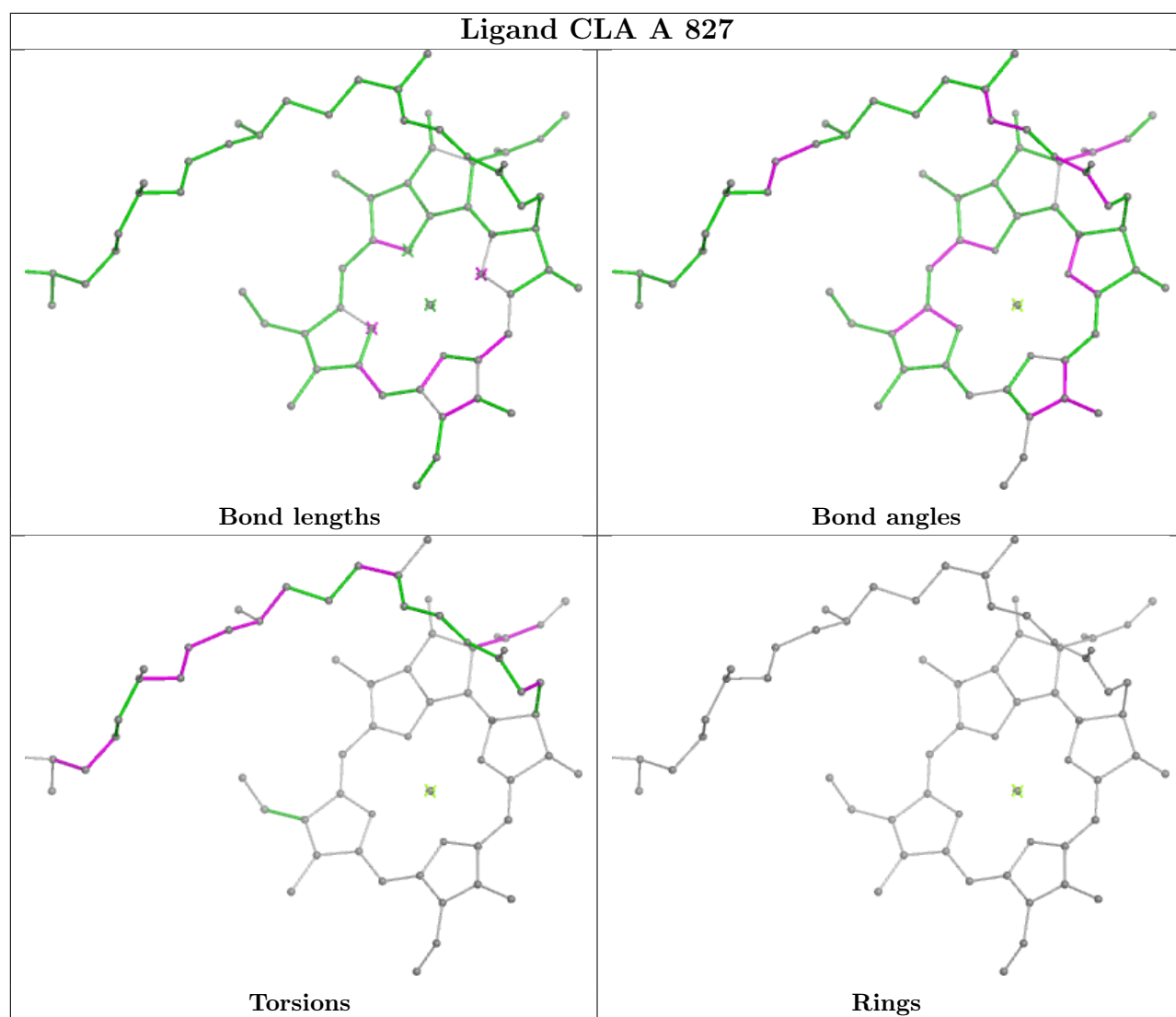


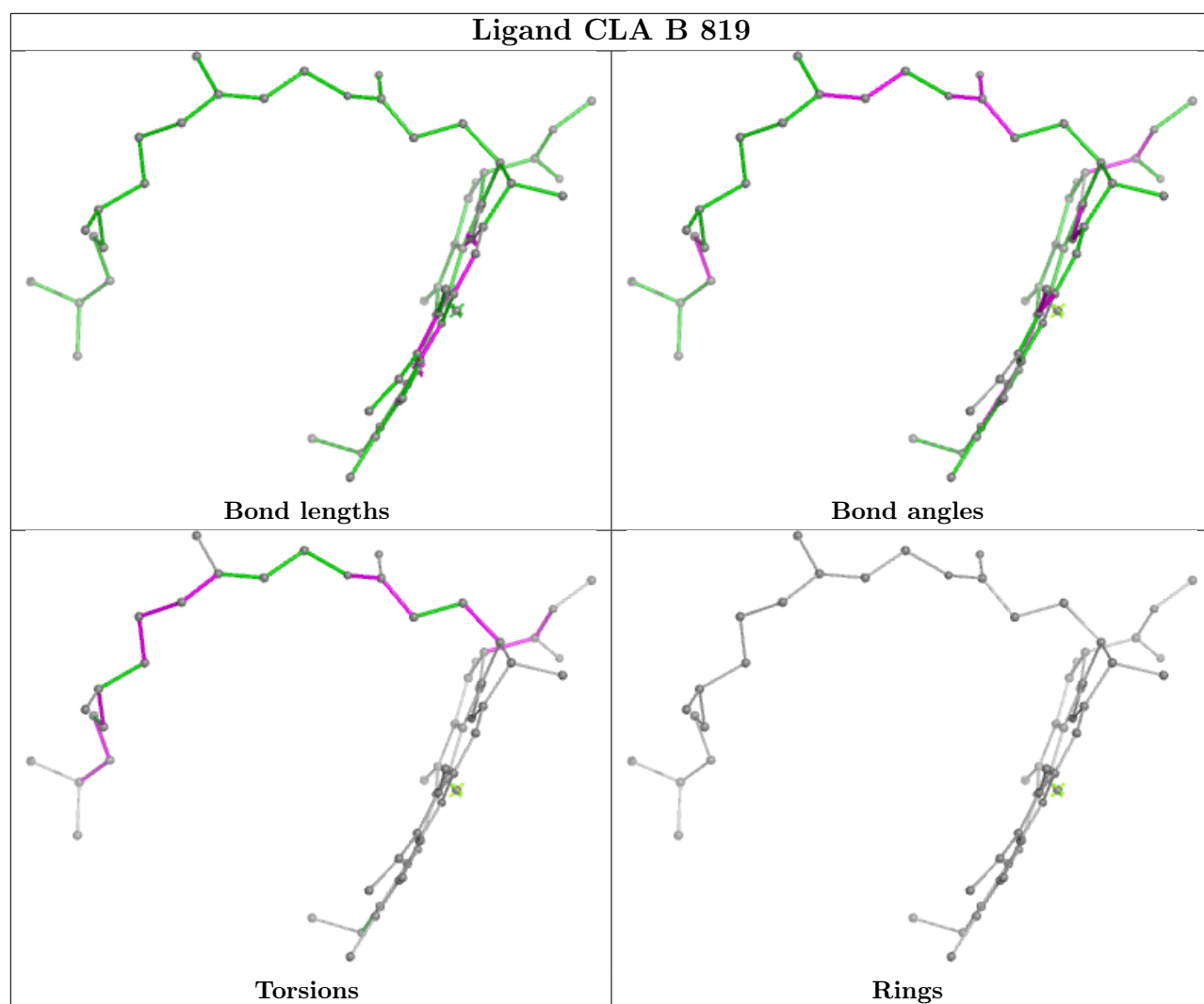
Torsions



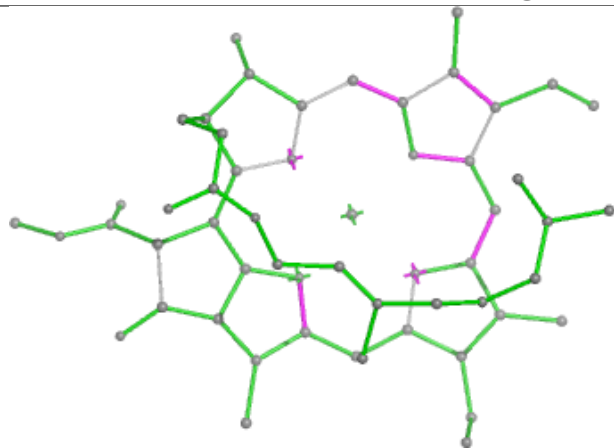
Rings



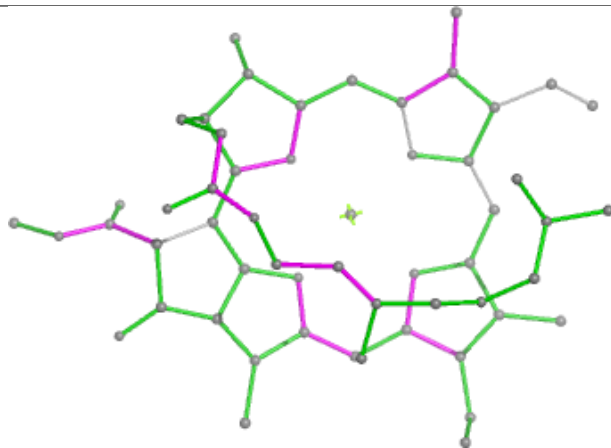




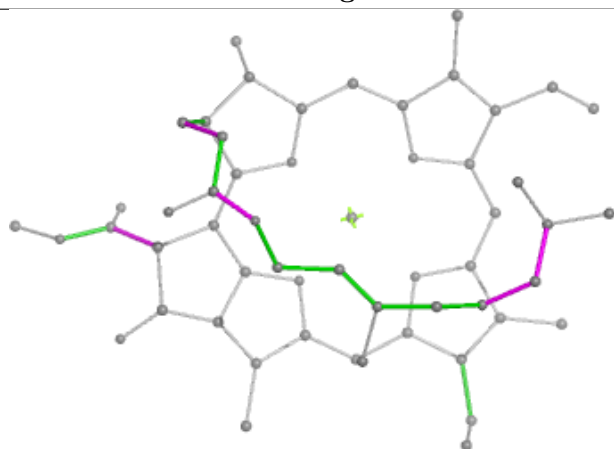
## Ligand CLA 3 312



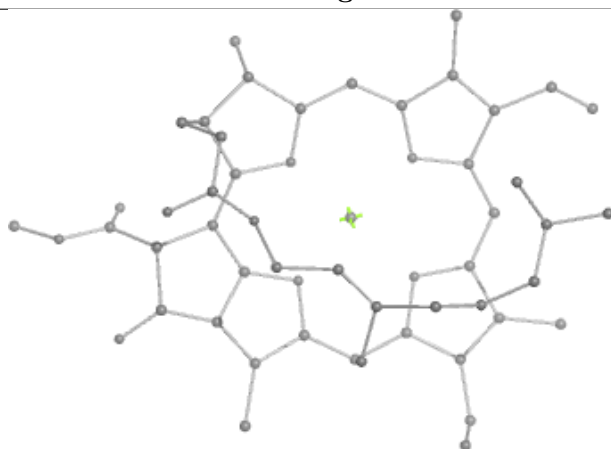
Bond lengths



Bond angles

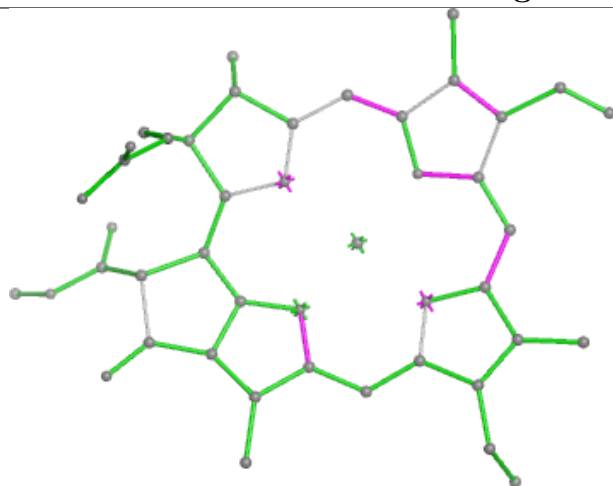


Torsions

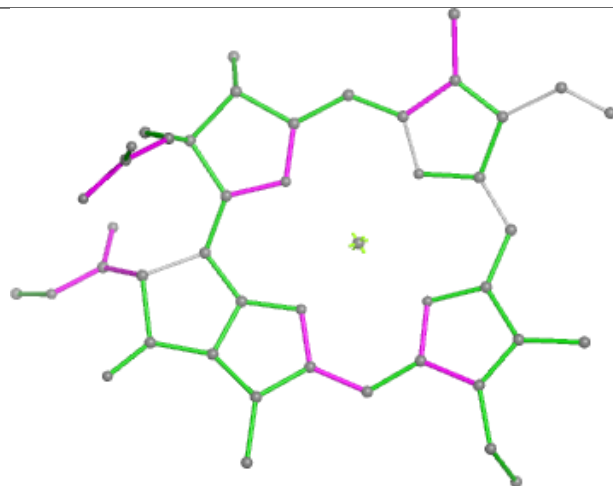


Rings

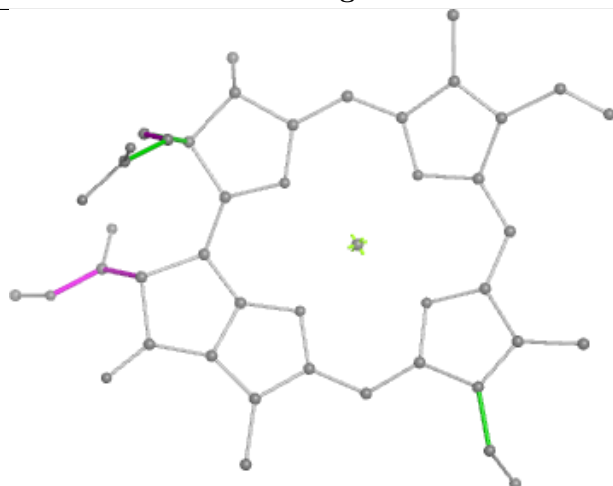
## Ligand CLA A 814



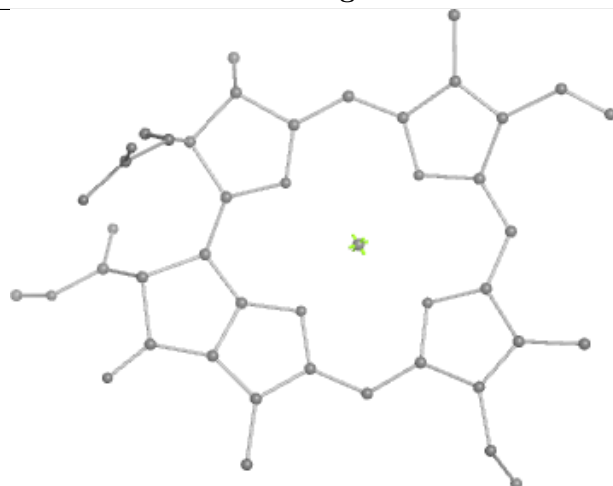
Bond lengths



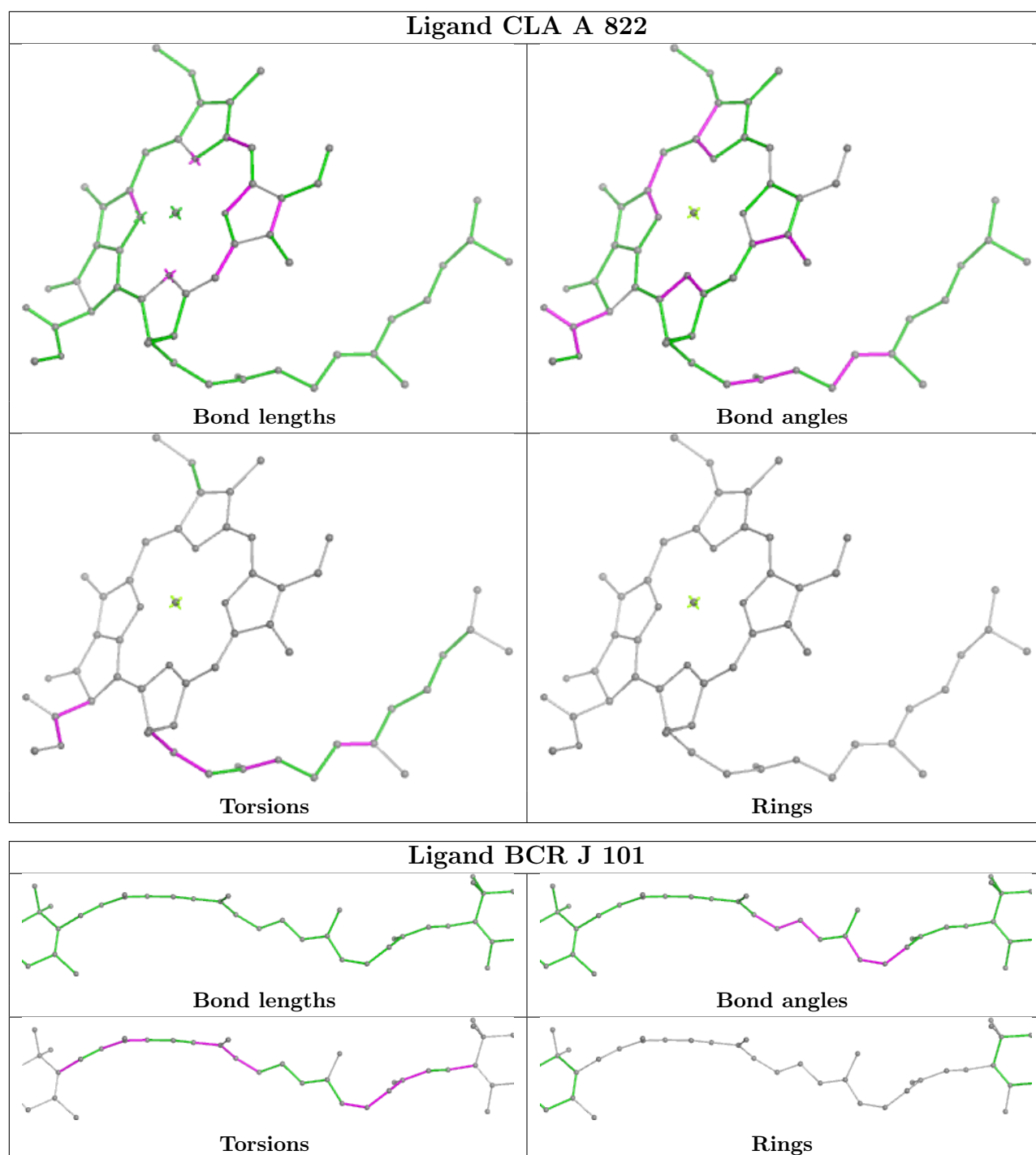
Bond angles



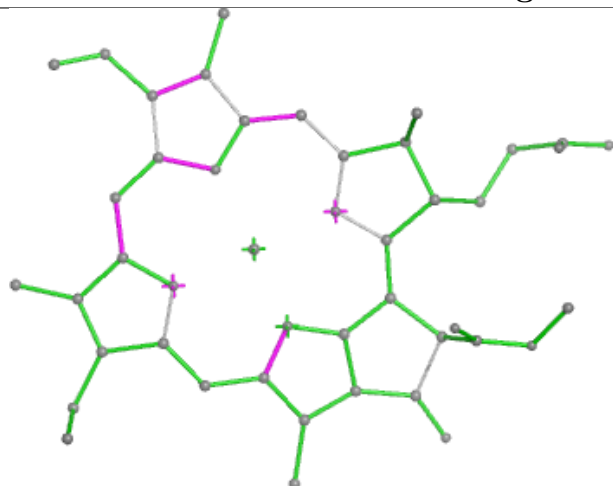
Torsions



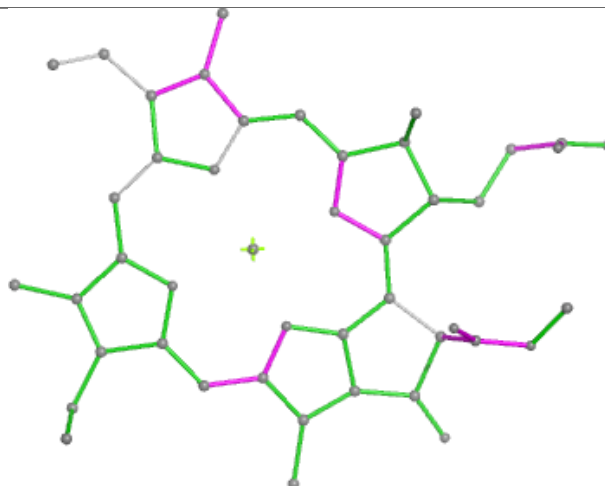
Rings



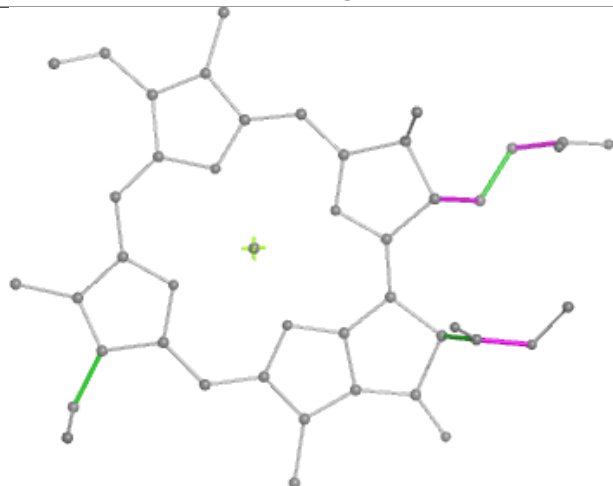
## Ligand CLA F 301



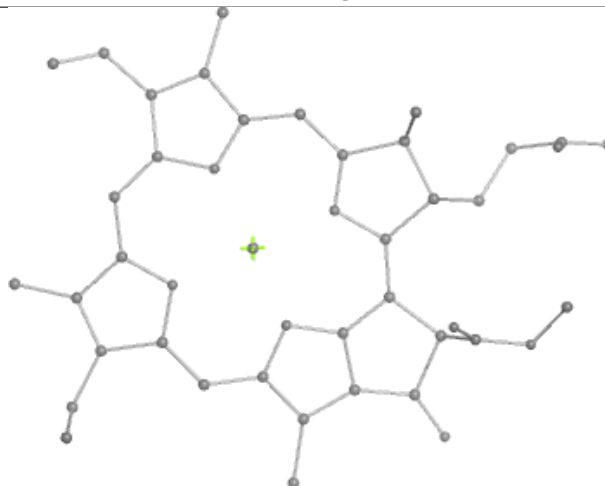
Bond lengths



Bond angles

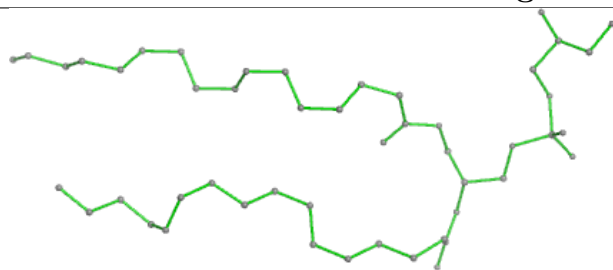


Torsions

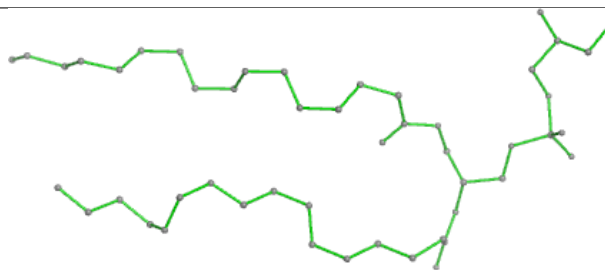


Rings

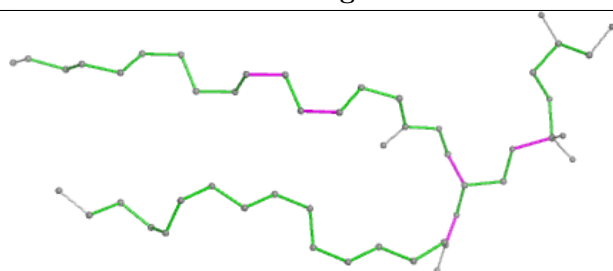
## Ligand LHG 1 317



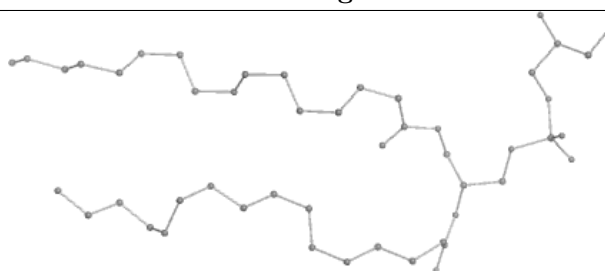
Bond lengths



Bond angles

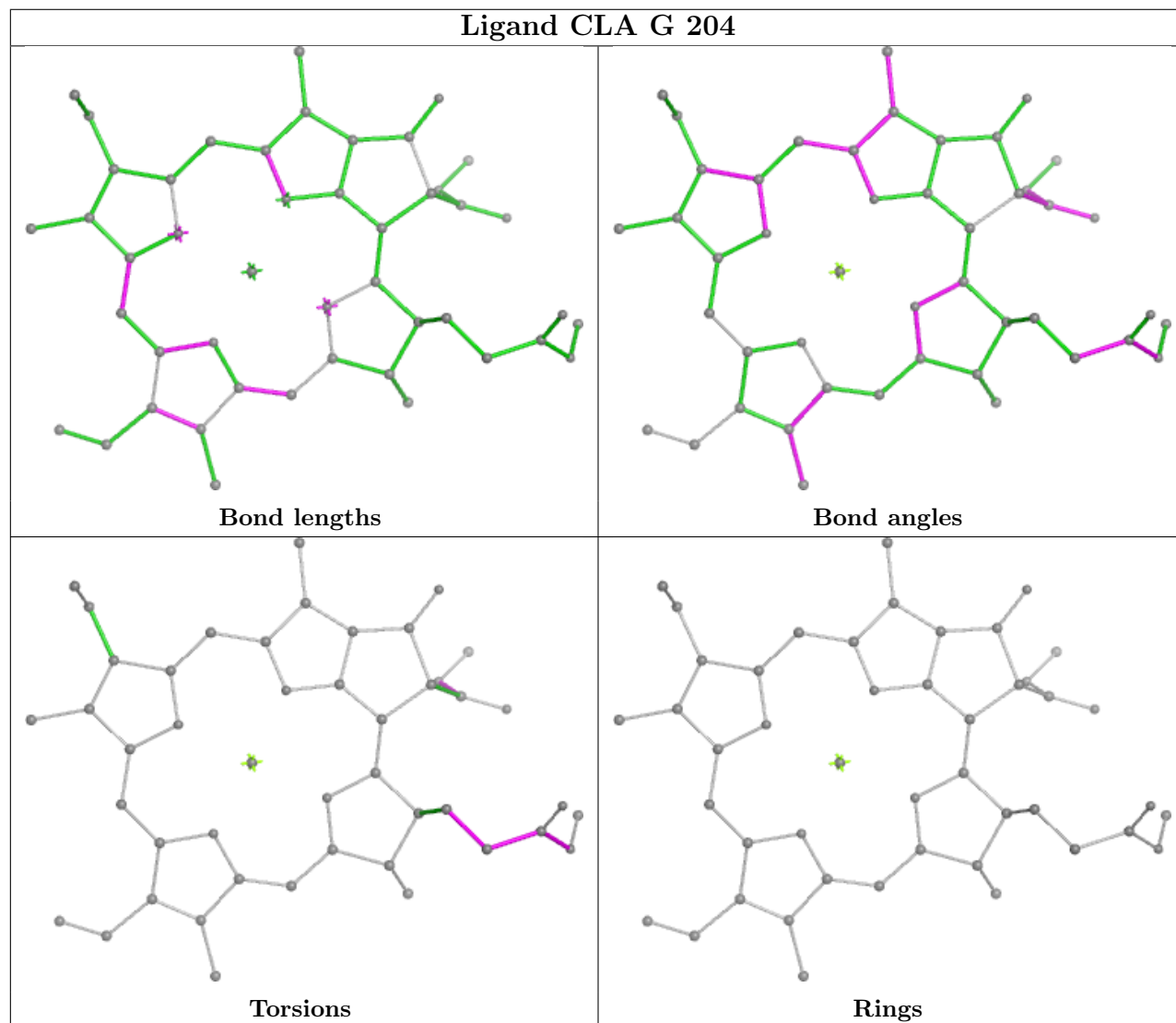
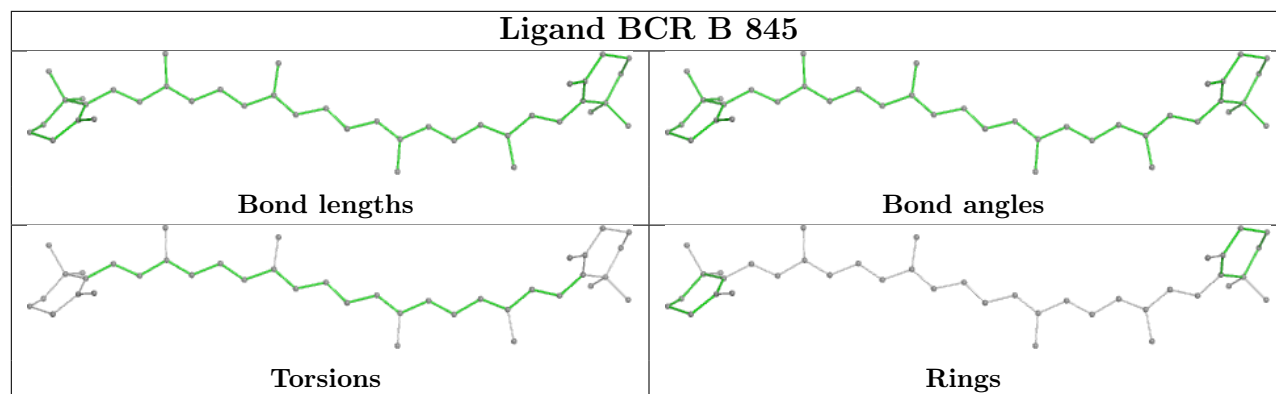


Torsions

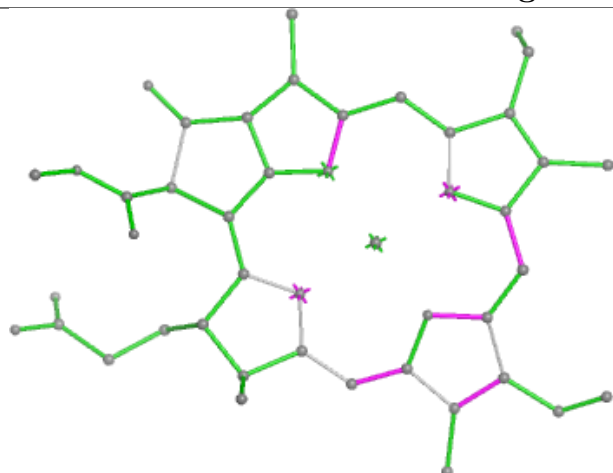


Rings

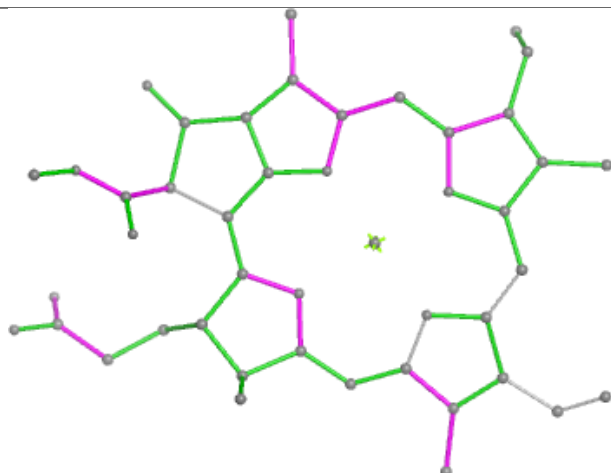




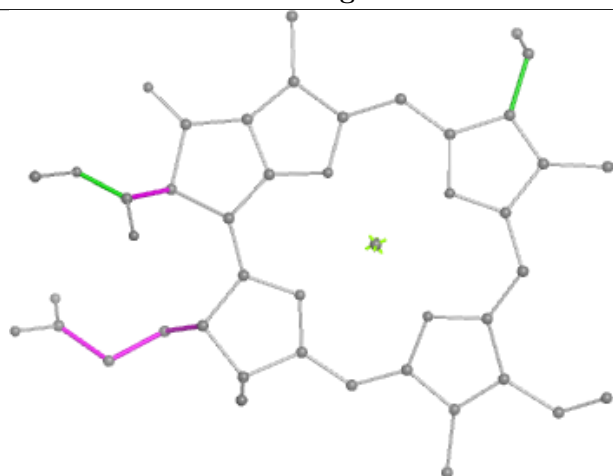
## Ligand CLA 3 313



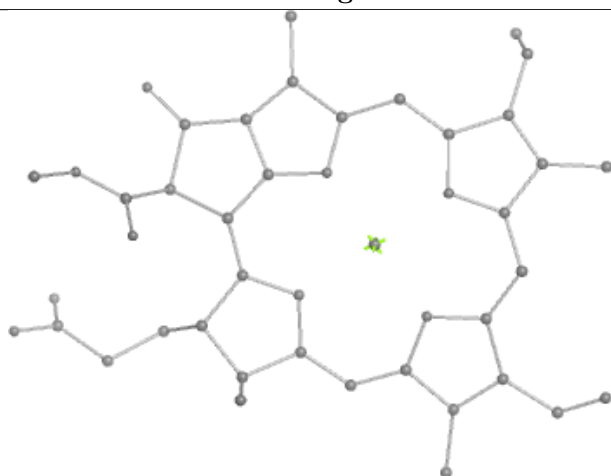
Bond lengths



Bond angles

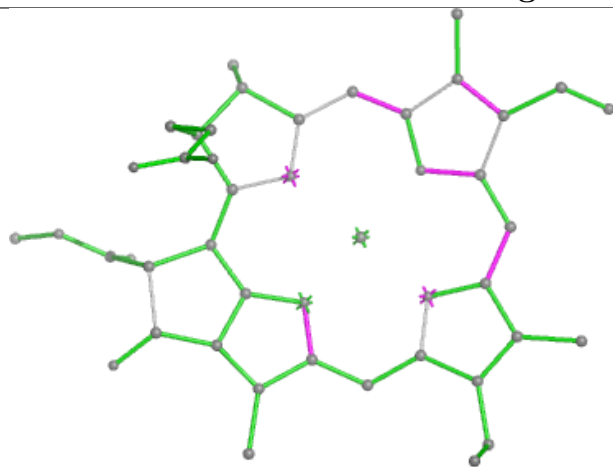


Torsions

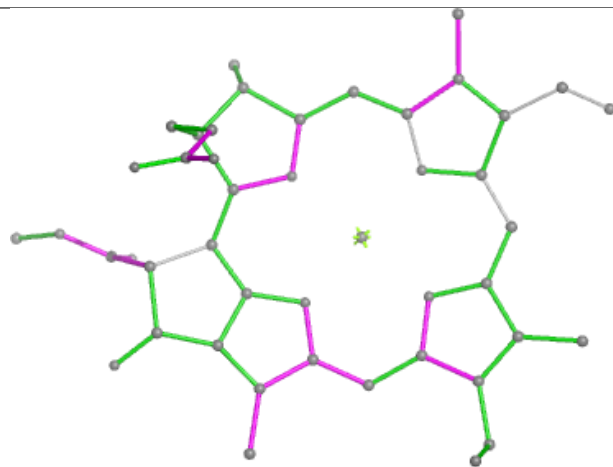


Rings

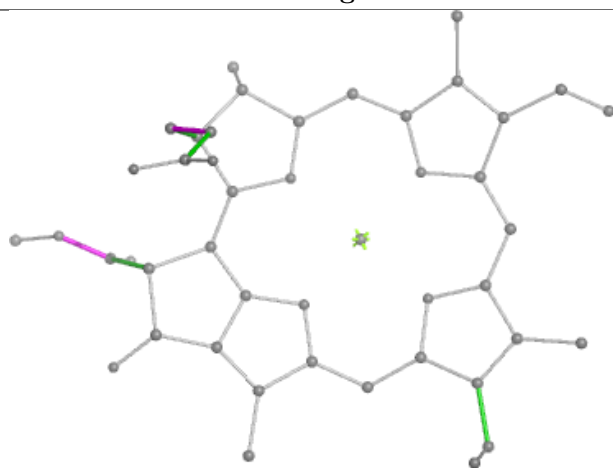
## Ligand CLA 1 307



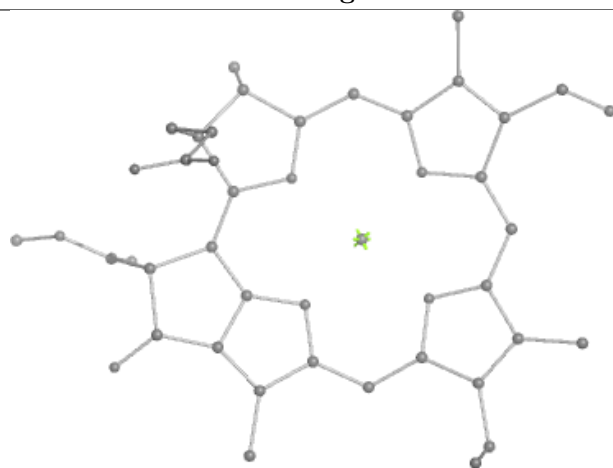
Bond lengths



Bond angles

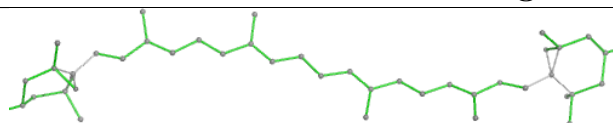


Torsions

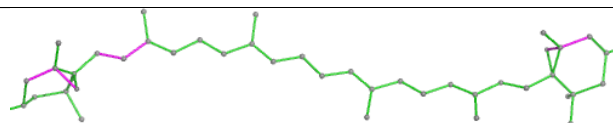


Rings

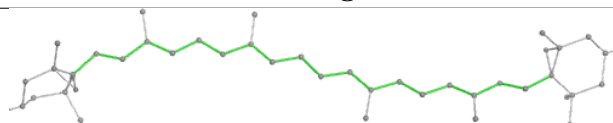
## Ligand XAT 4 316



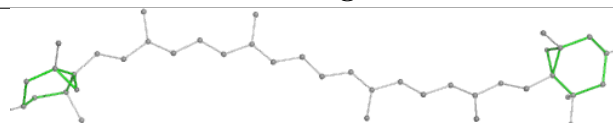
Bond lengths



Bond angles

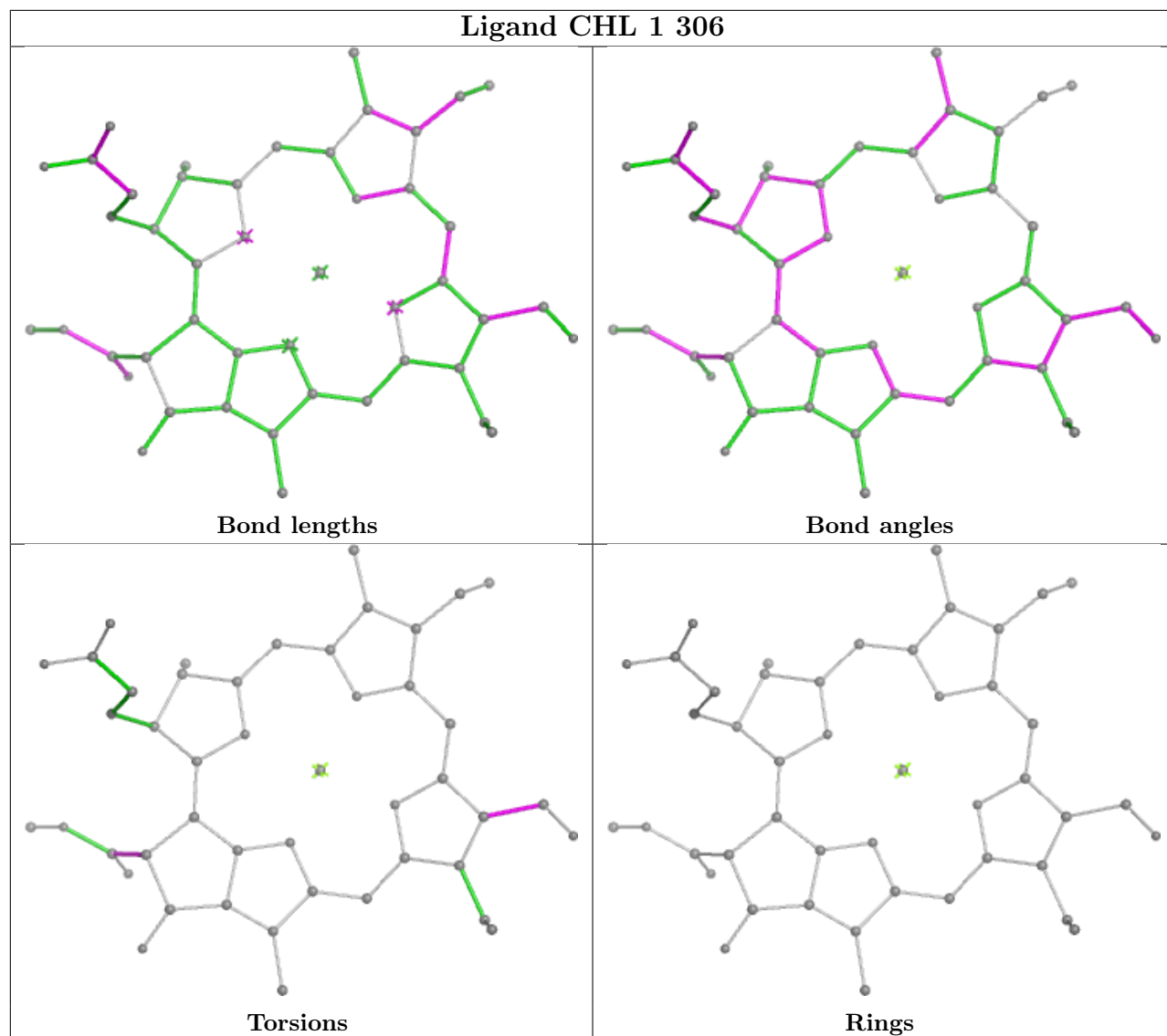


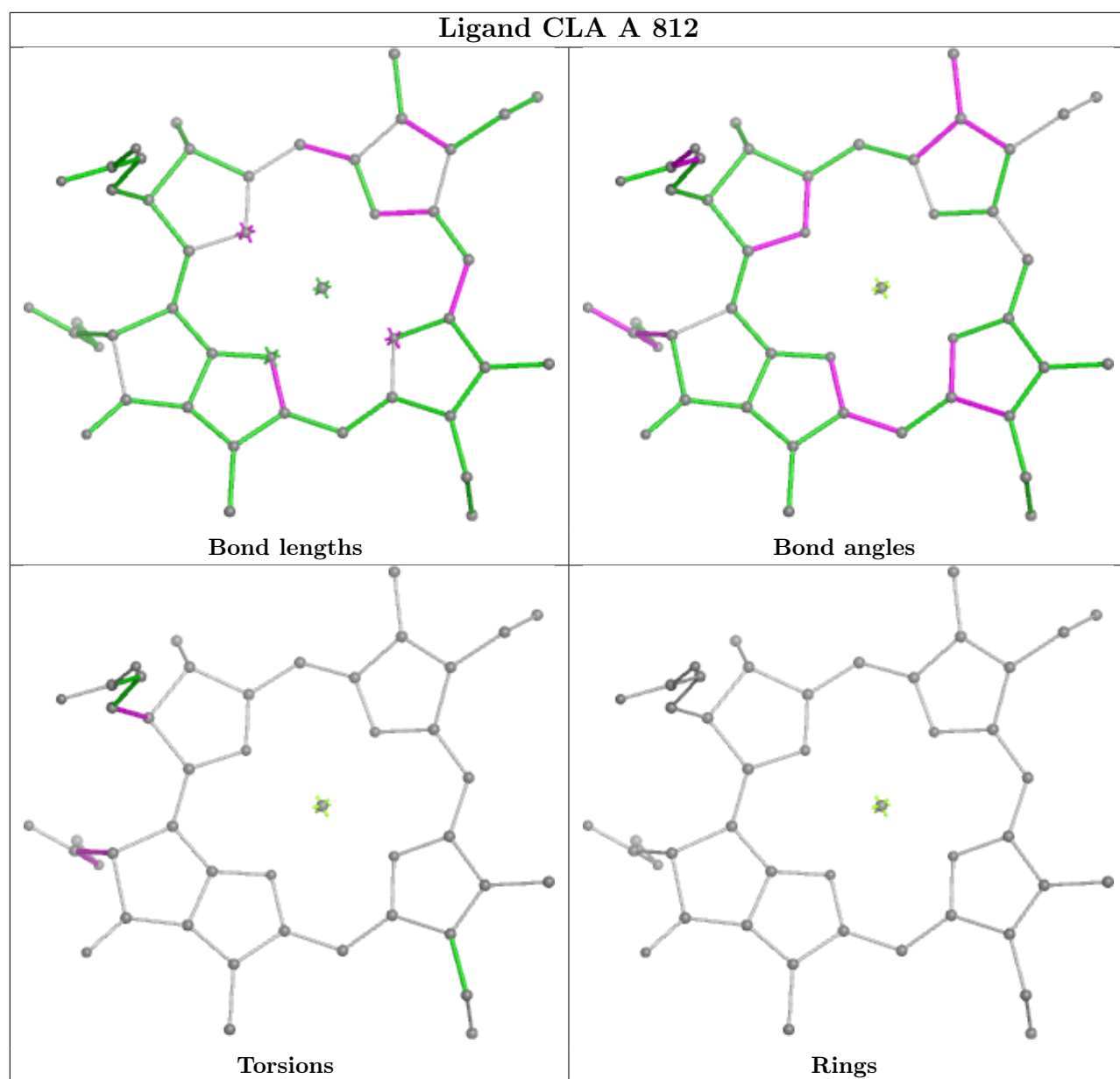
Torsions

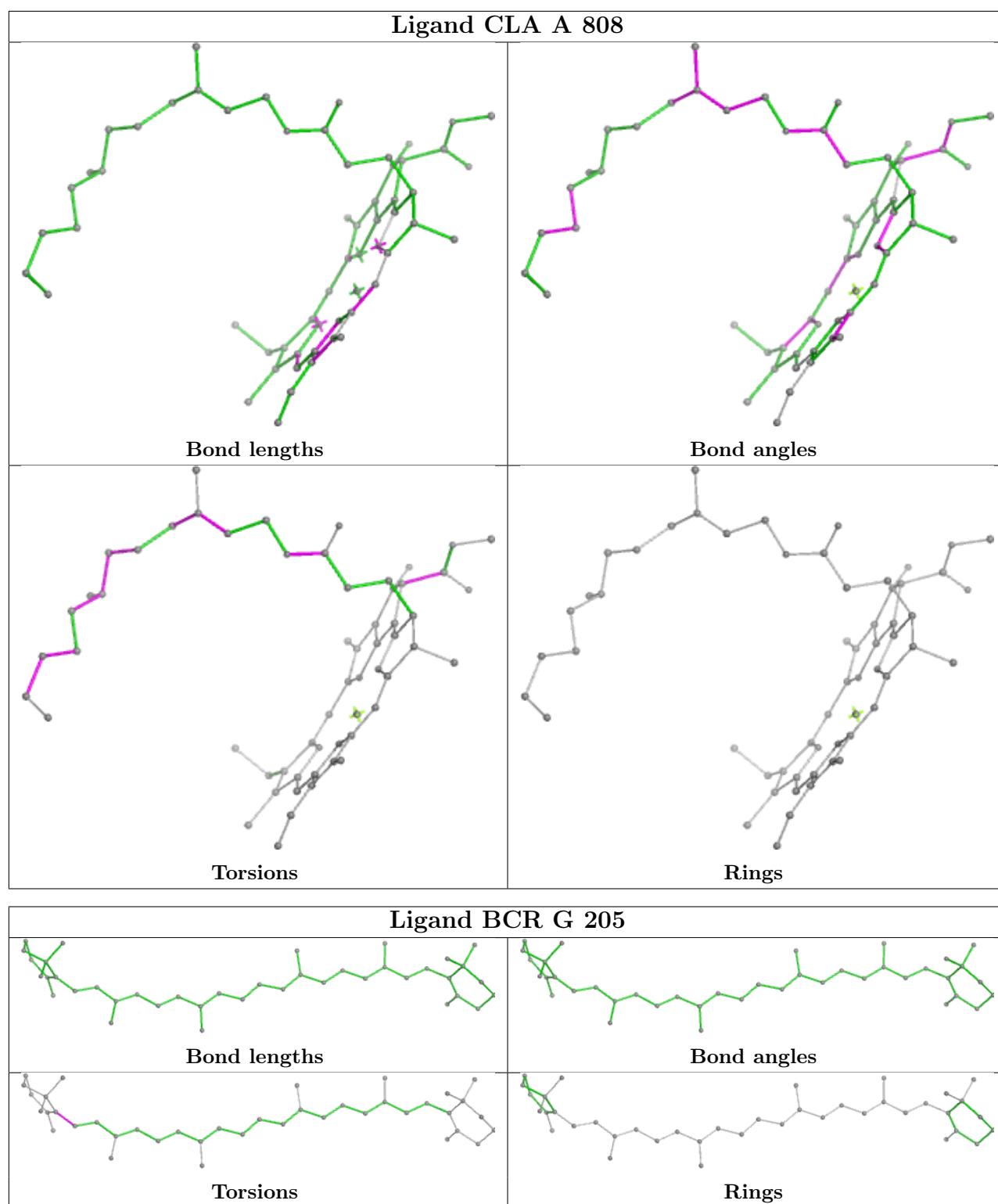


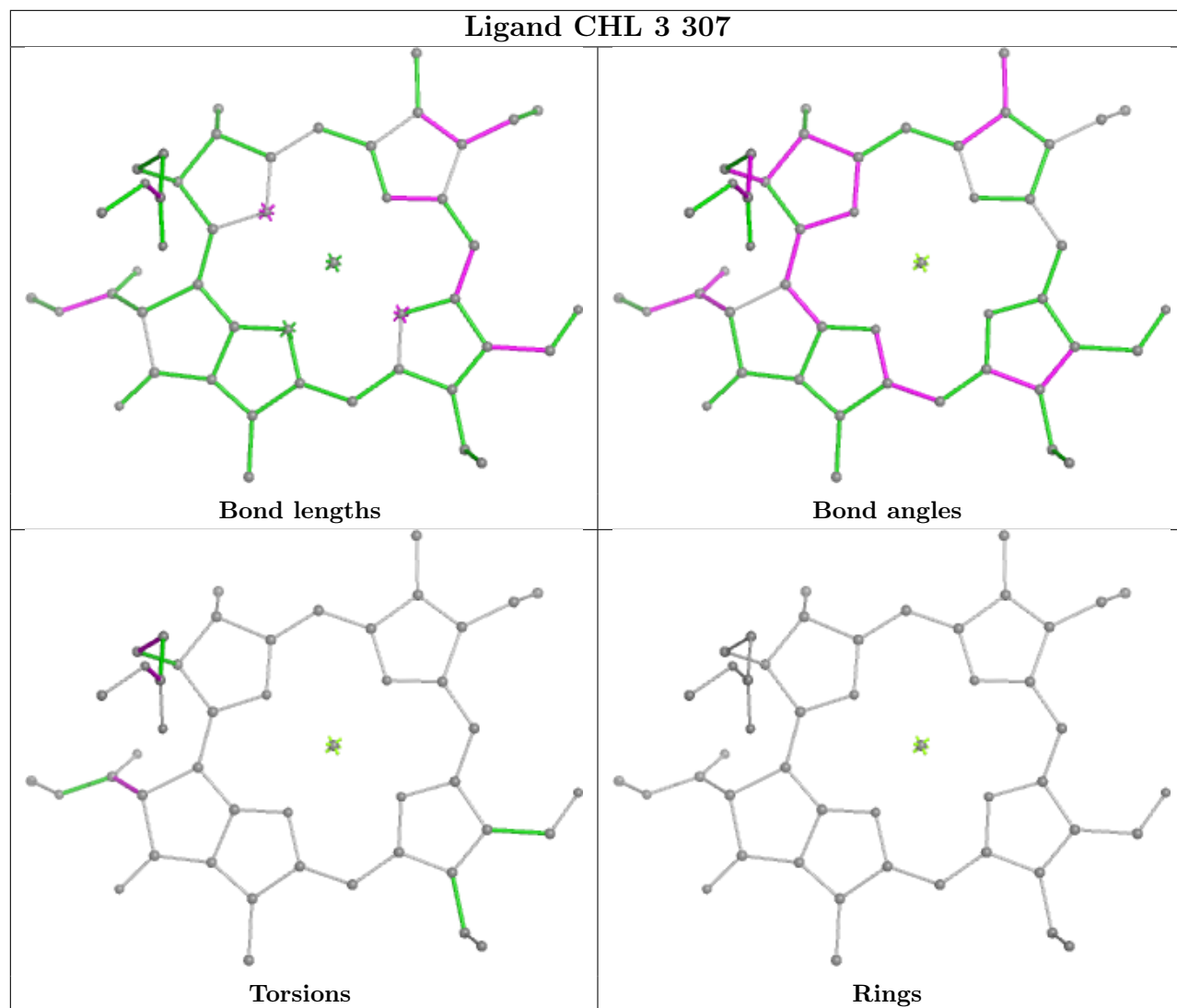
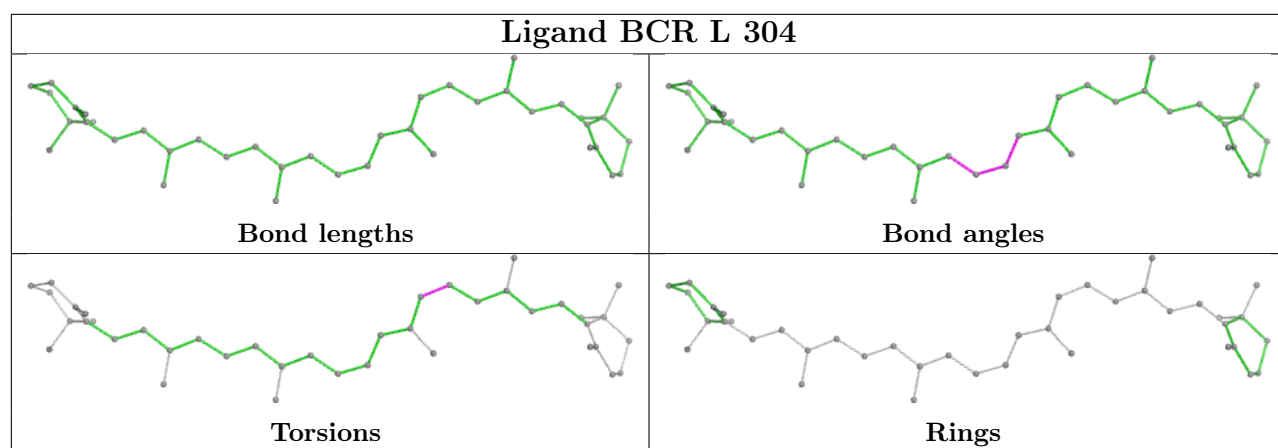
Rings

## Ligand CHL 1 306

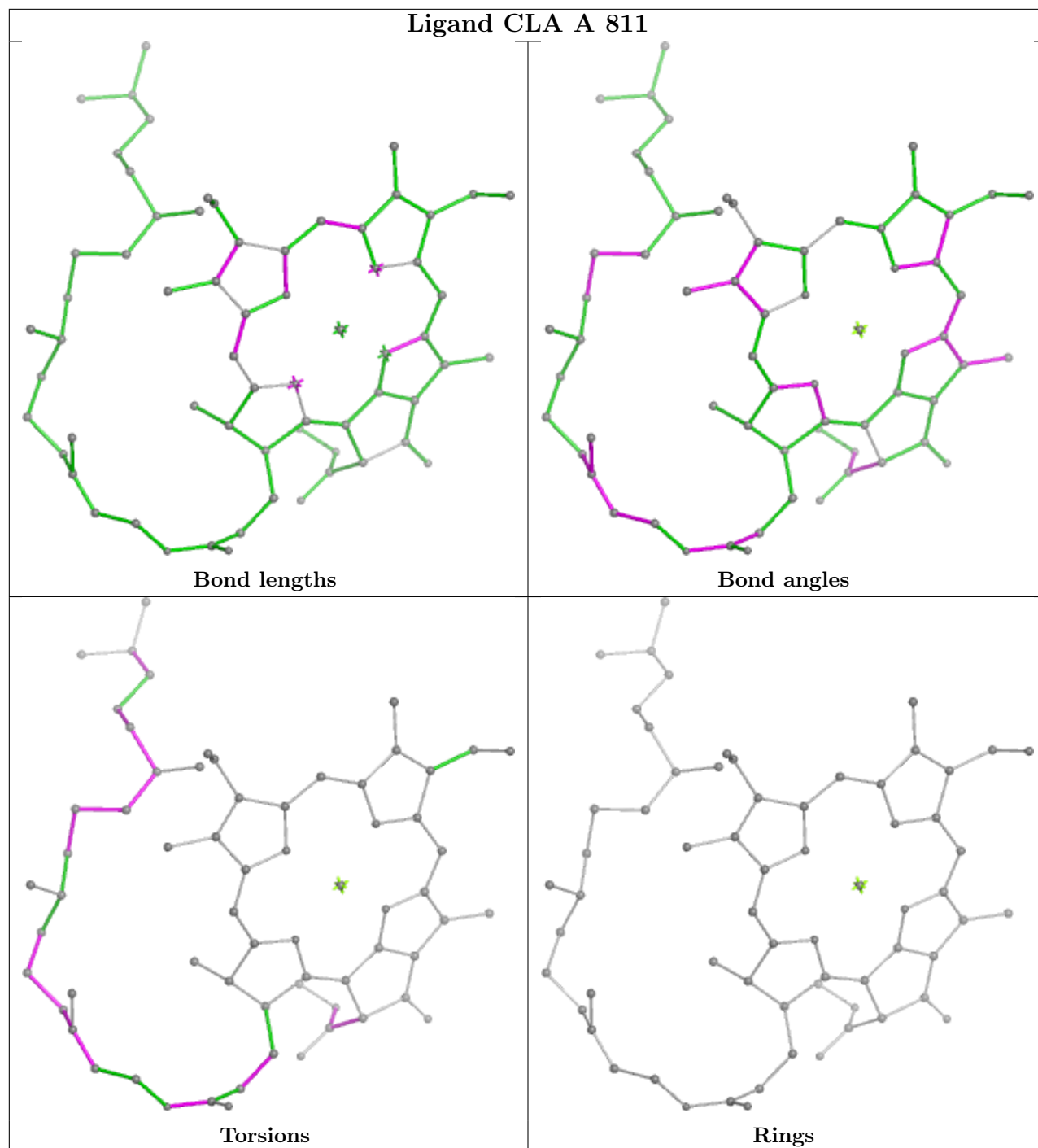




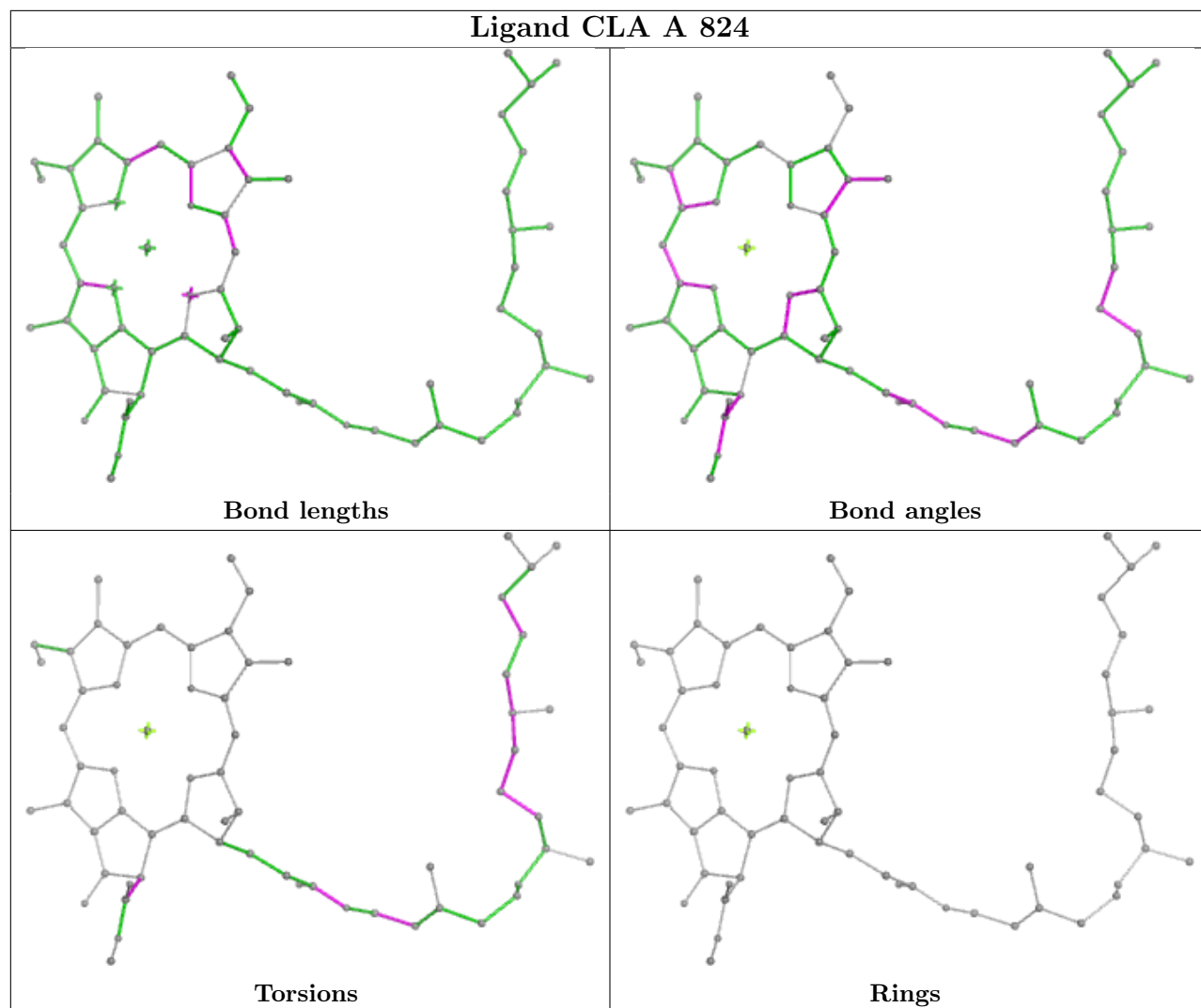




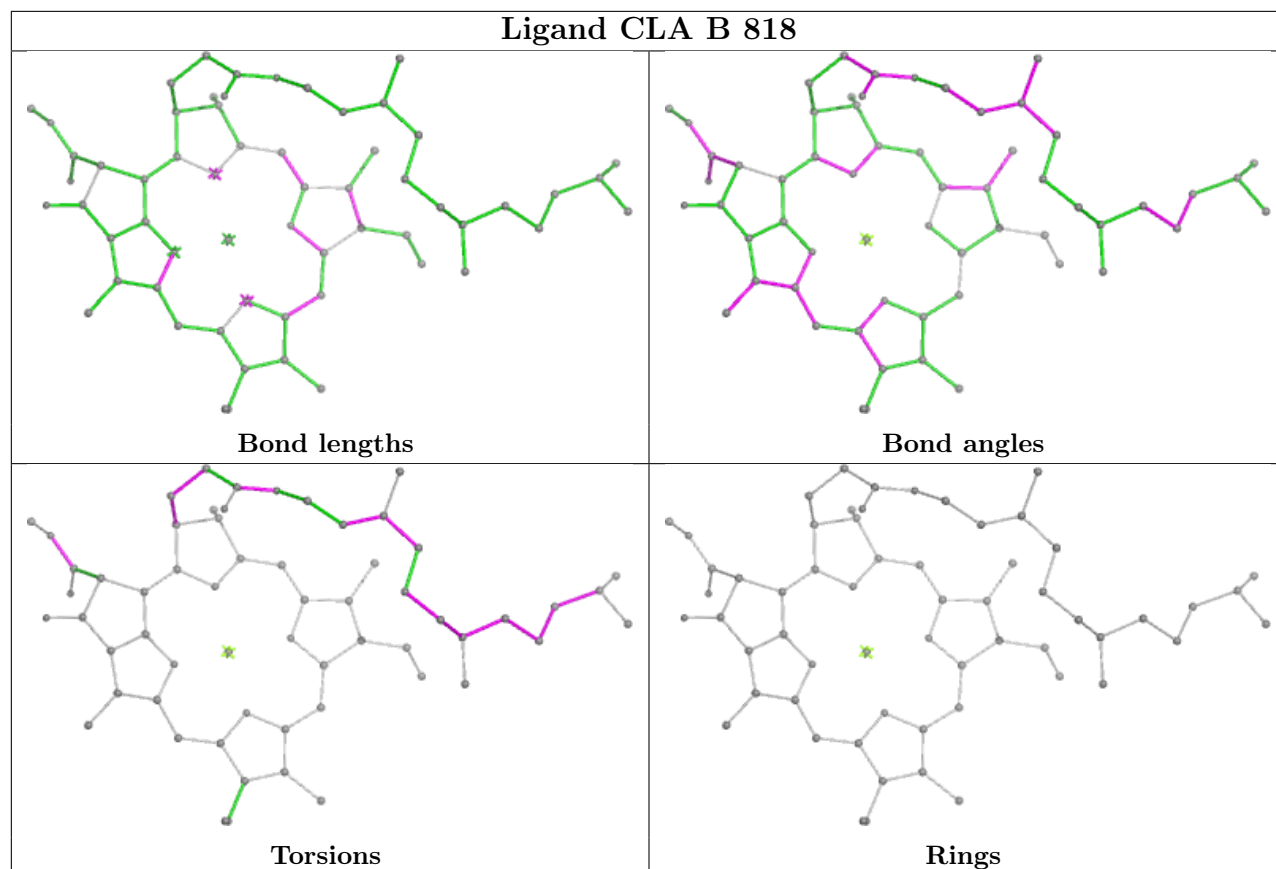
## Ligand CLA A 811



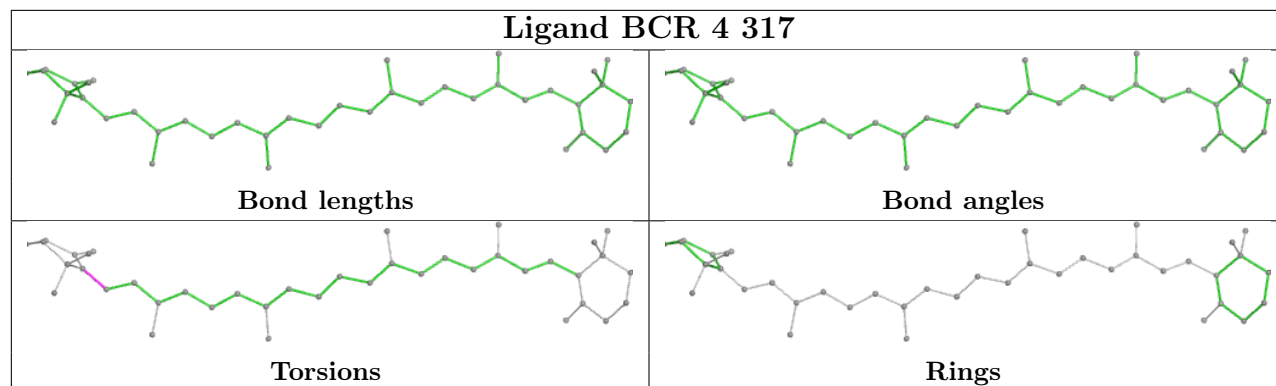




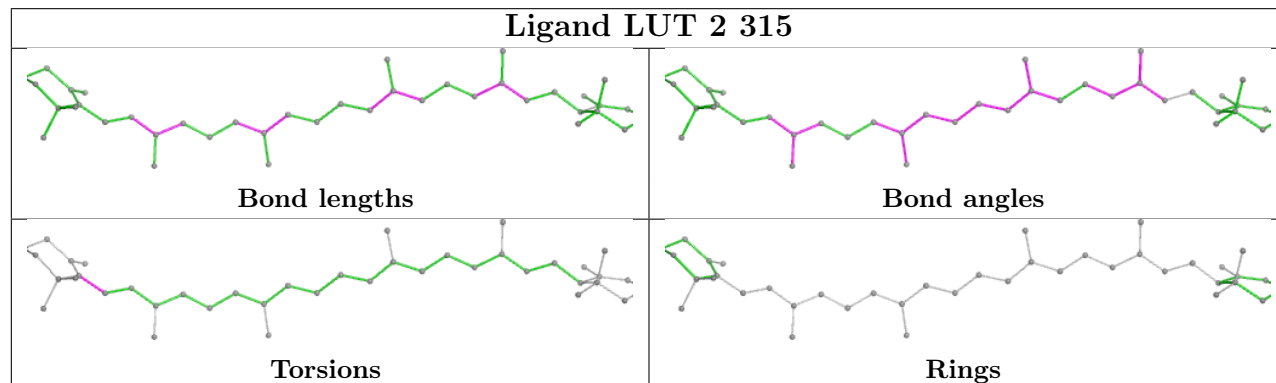
## Ligand CLA B 818

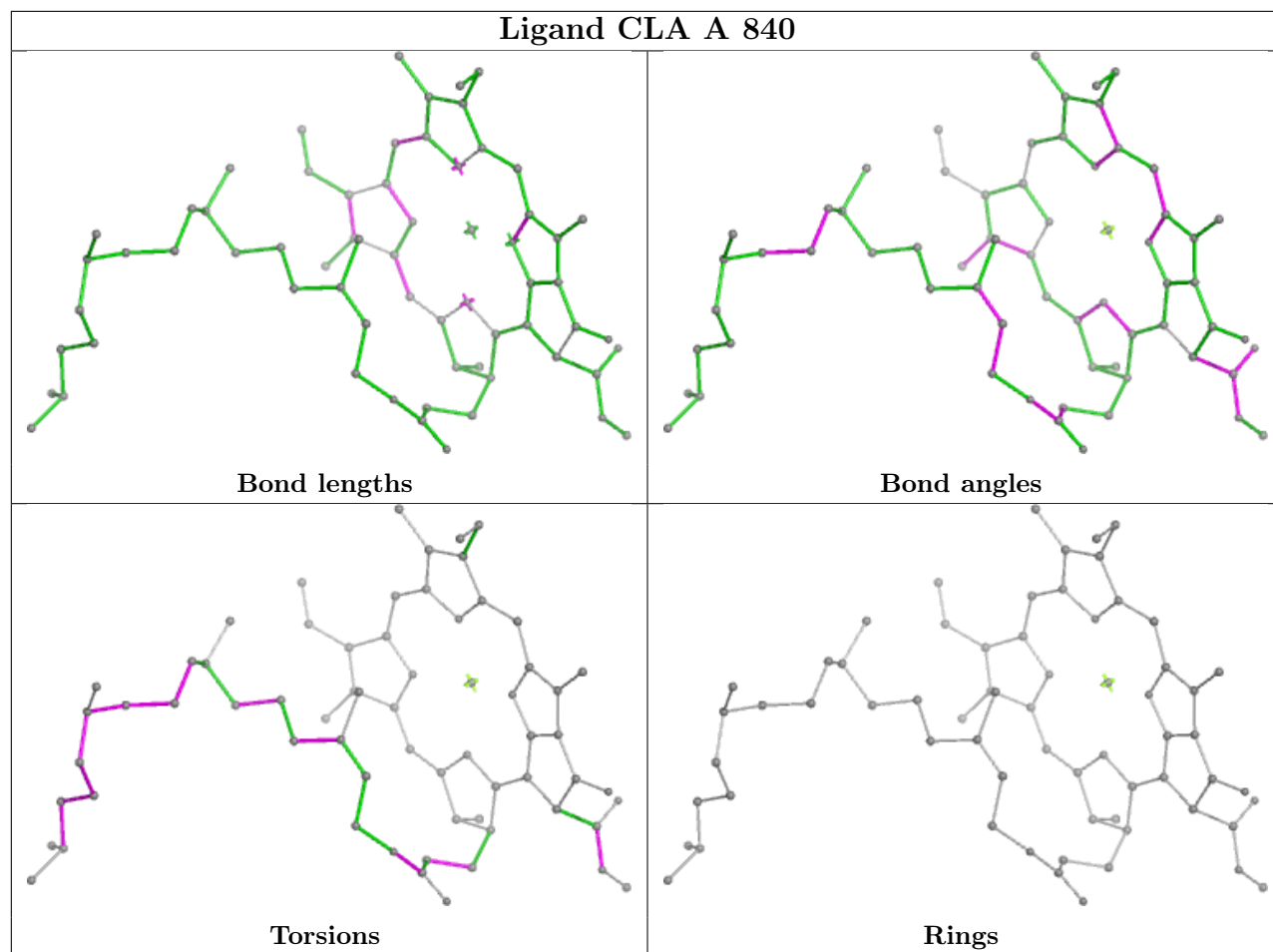


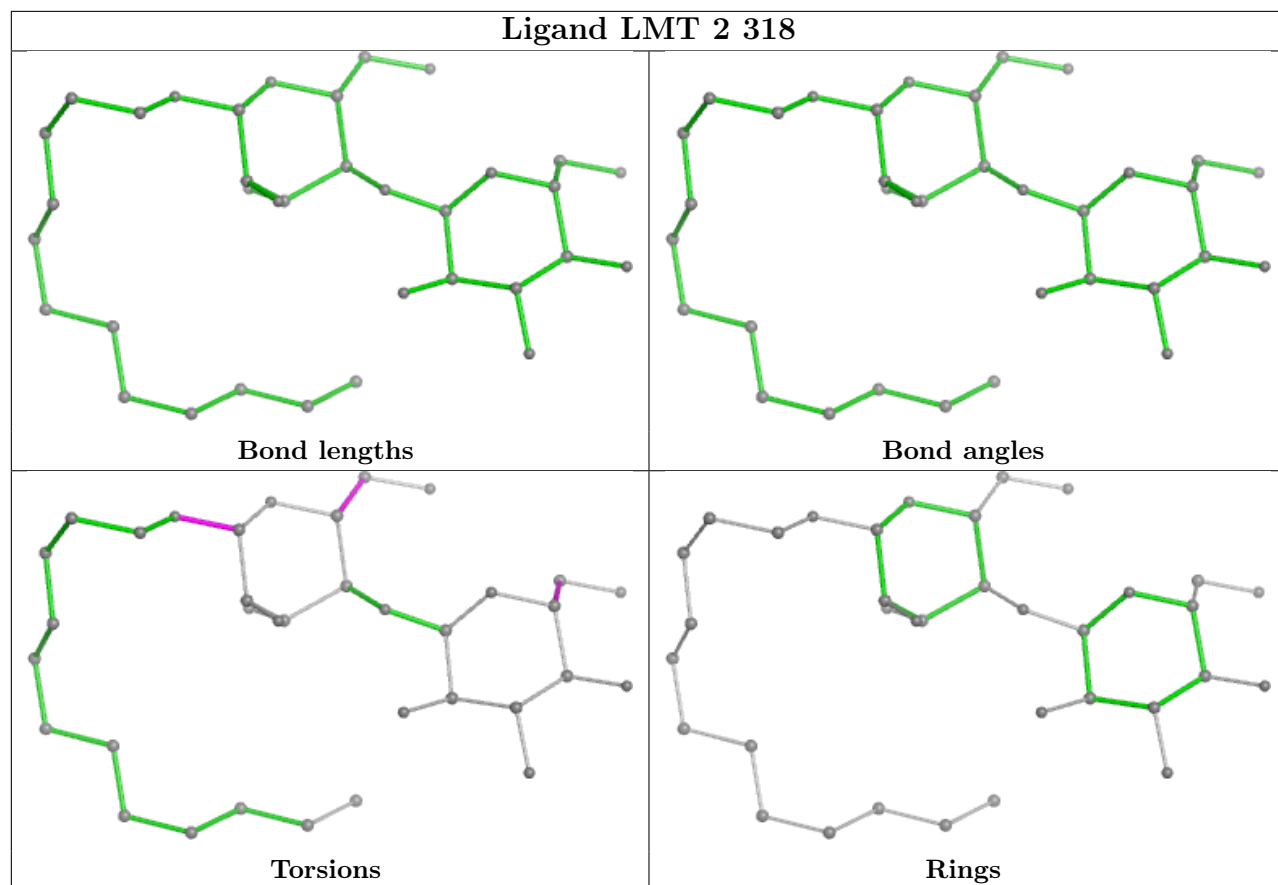
## Ligand BCR 4 317



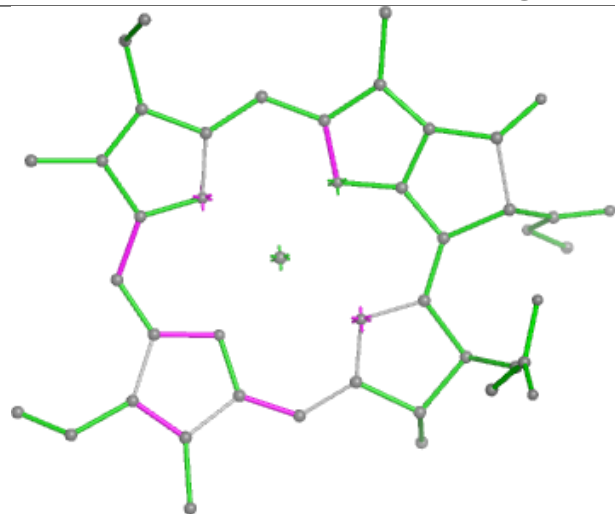
## Ligand LUT 2 315



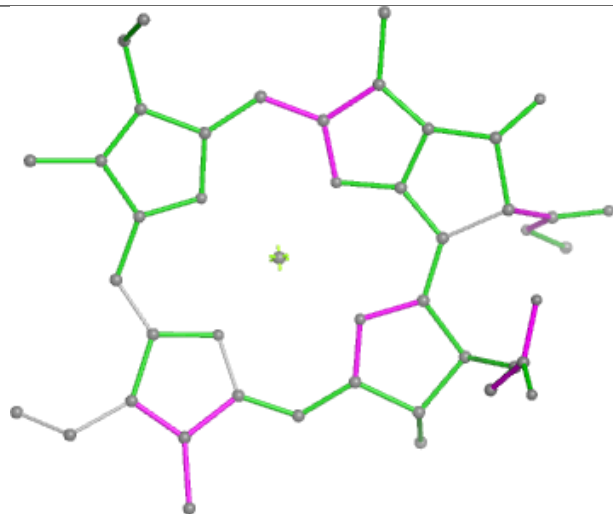




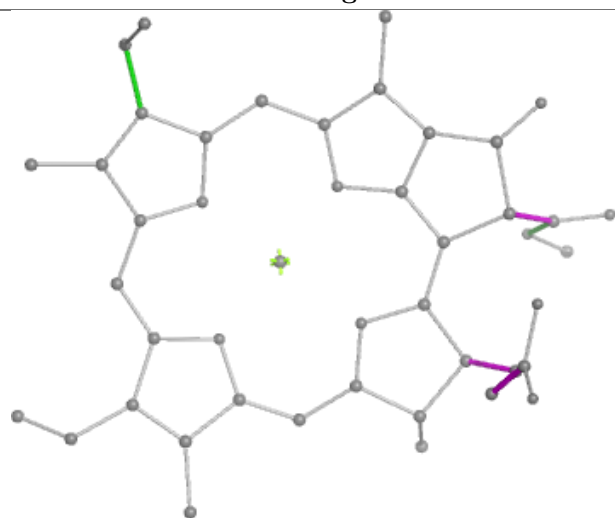
## Ligand CLA A 820



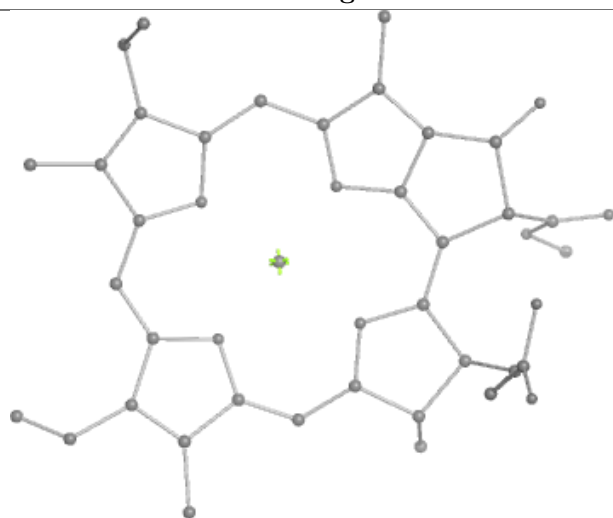
Bond lengths



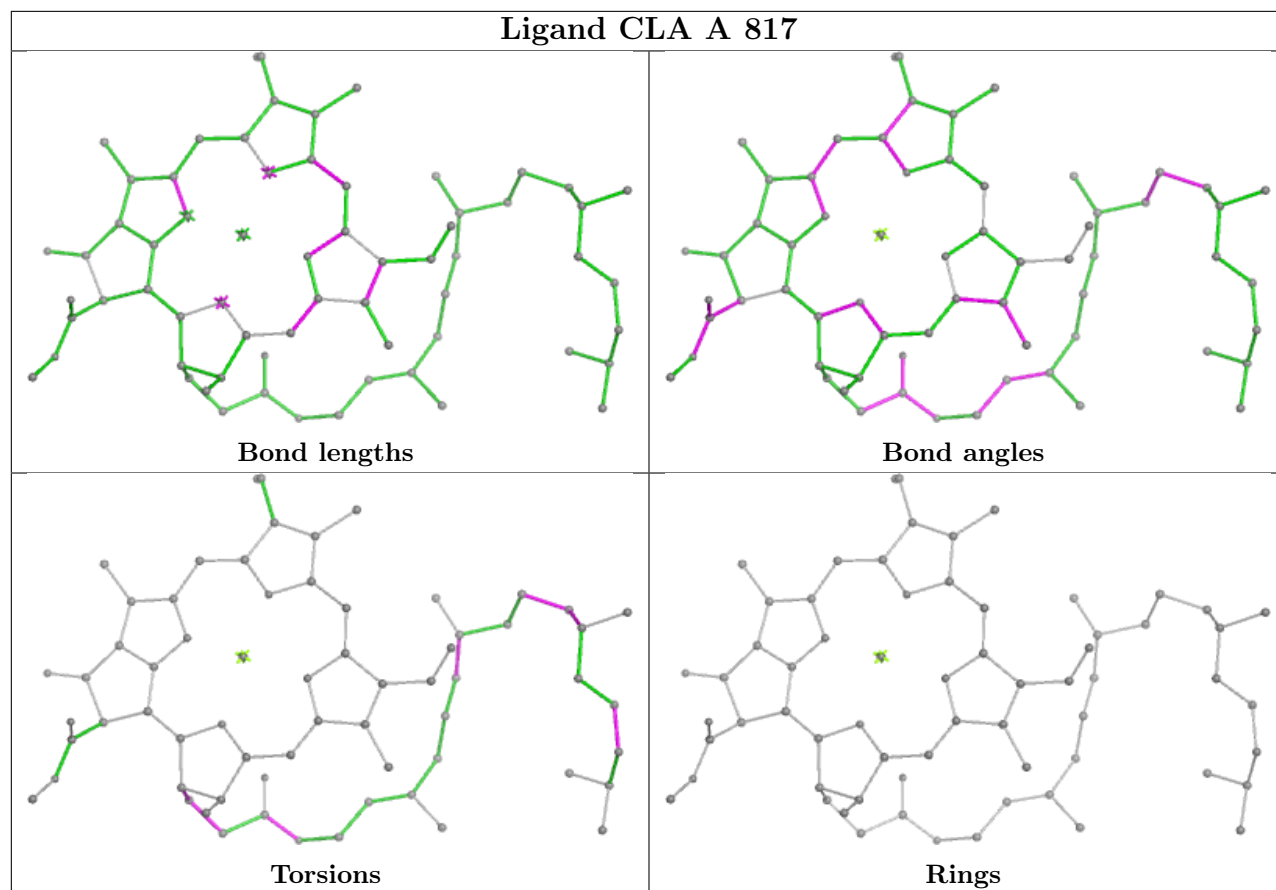
Bond angles



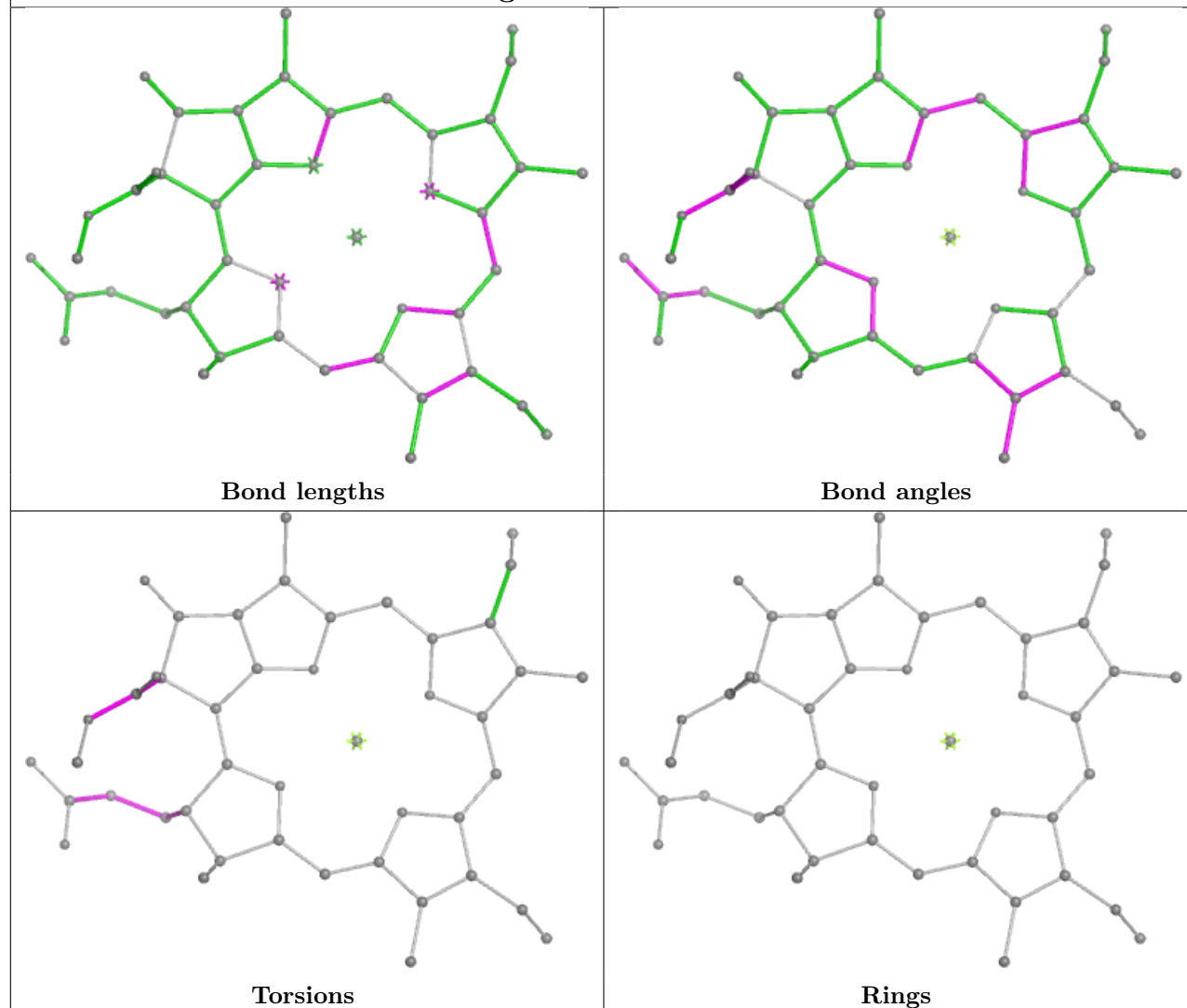
Torsions



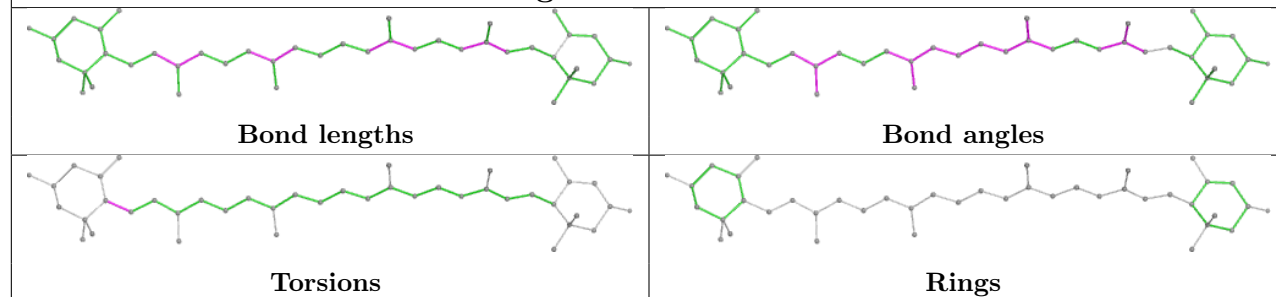
Rings

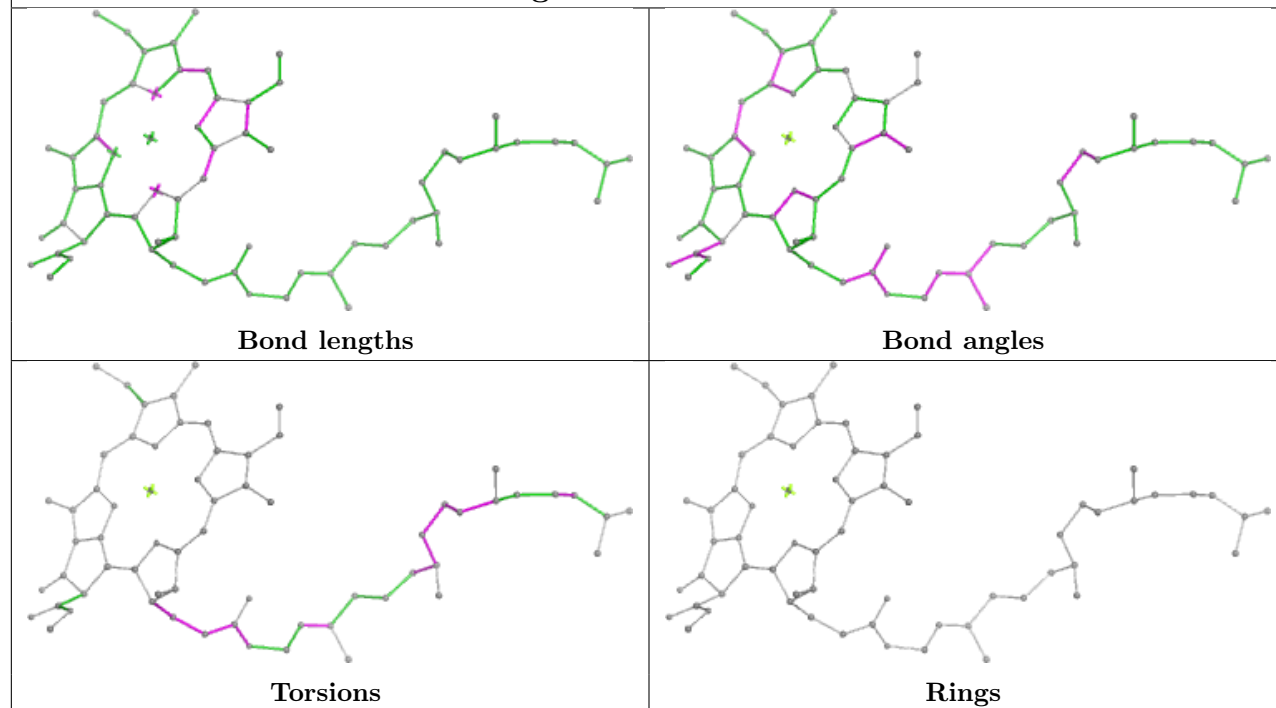
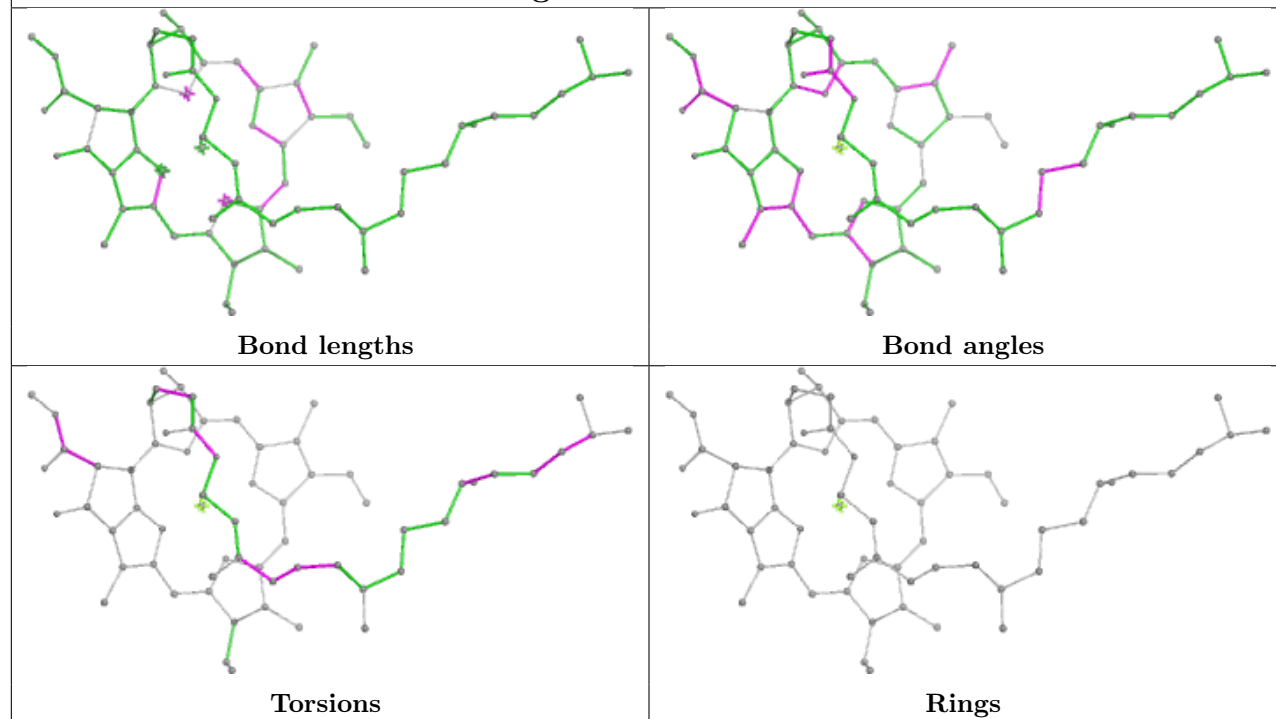


## Ligand CLA 1 314



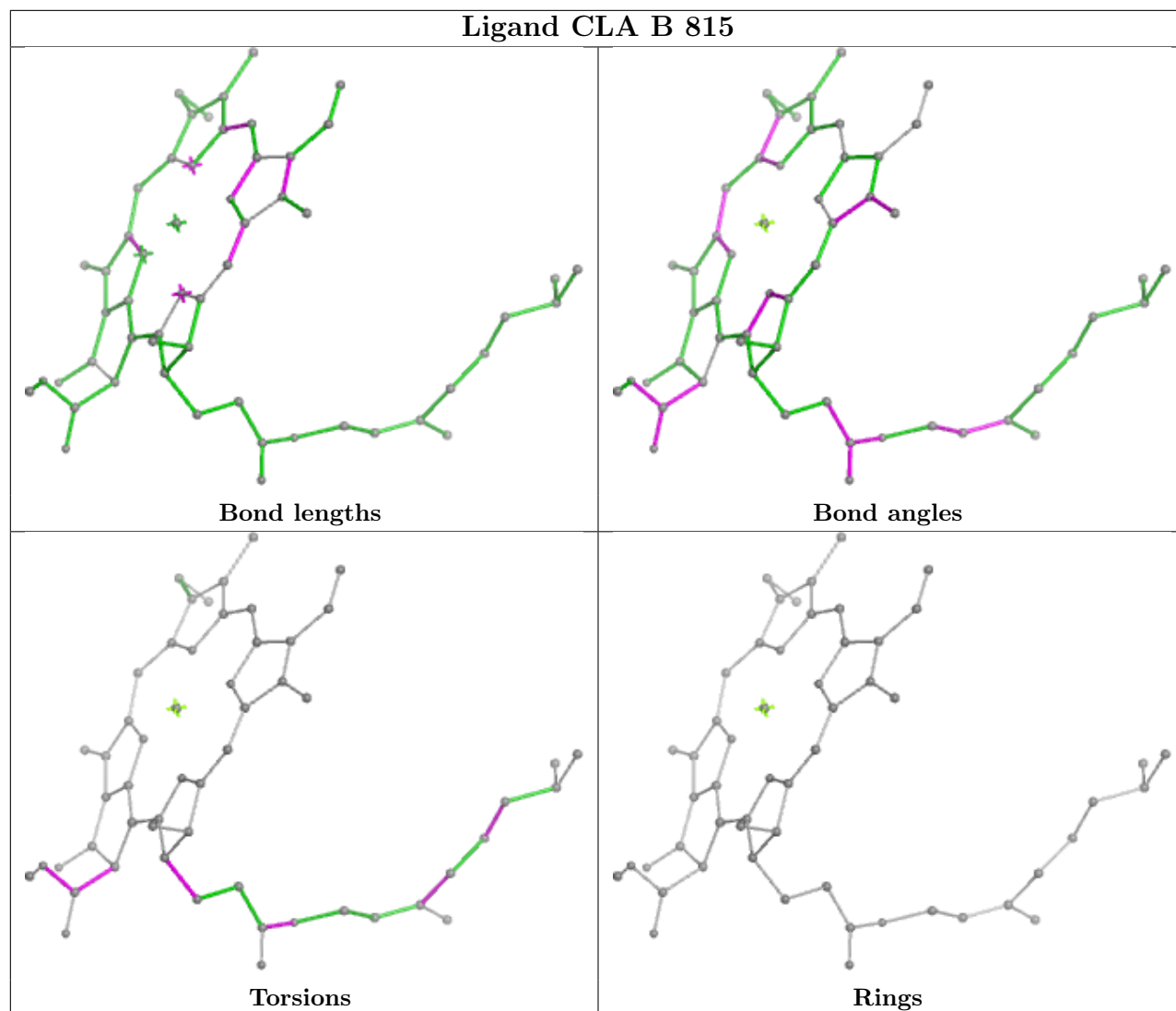
## Ligand LUT 1 319



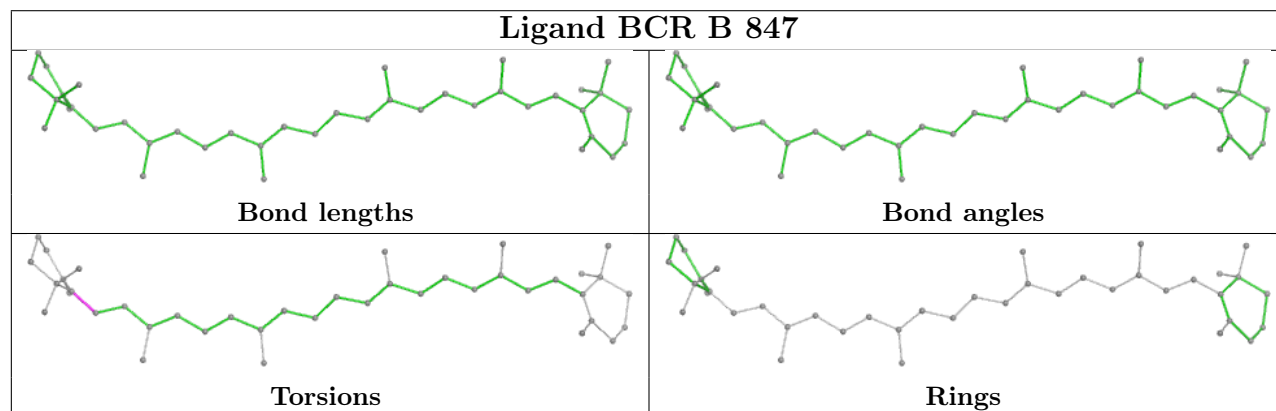
**Ligand CLA A 806****Ligand CLA B 807**

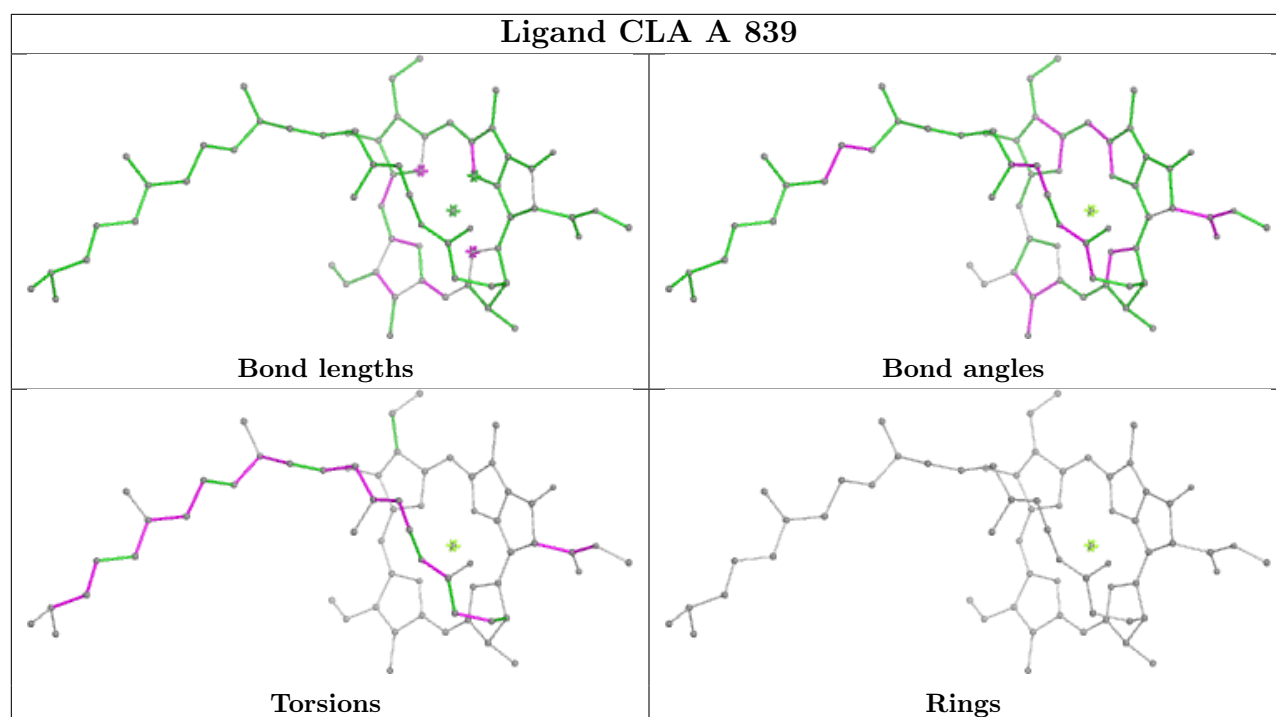


## Ligand CLA B 815

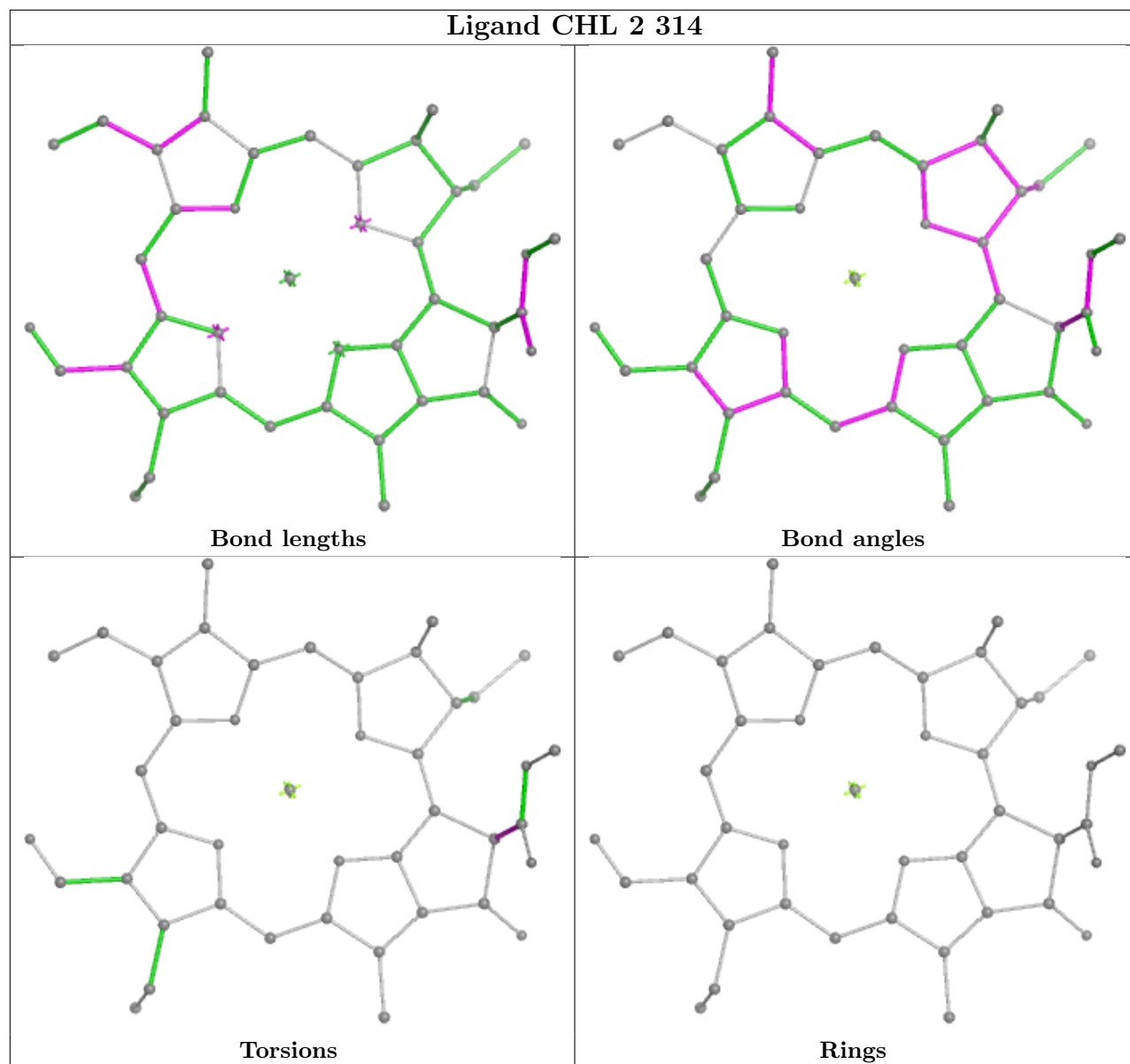


## Ligand BCR B 847

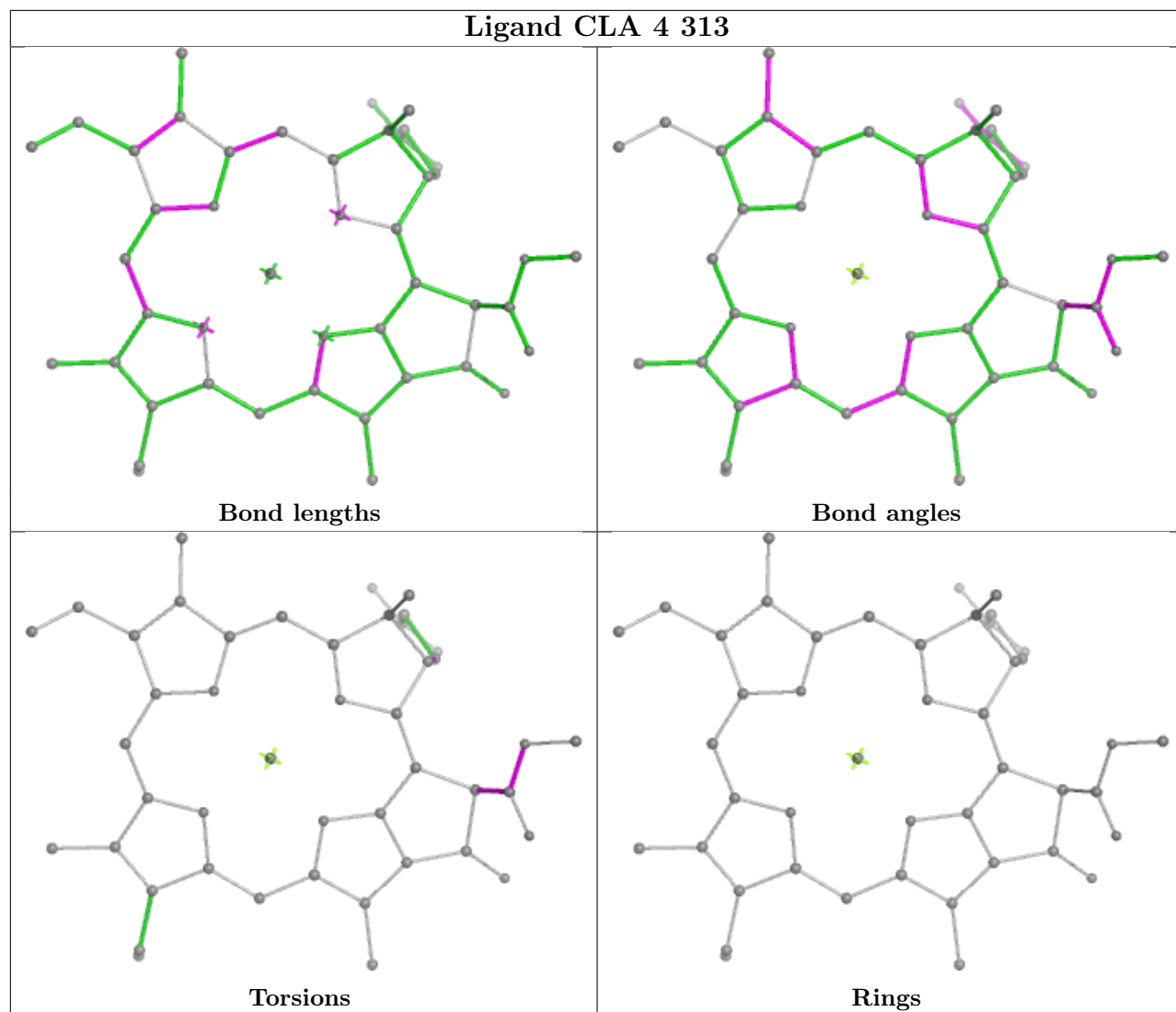


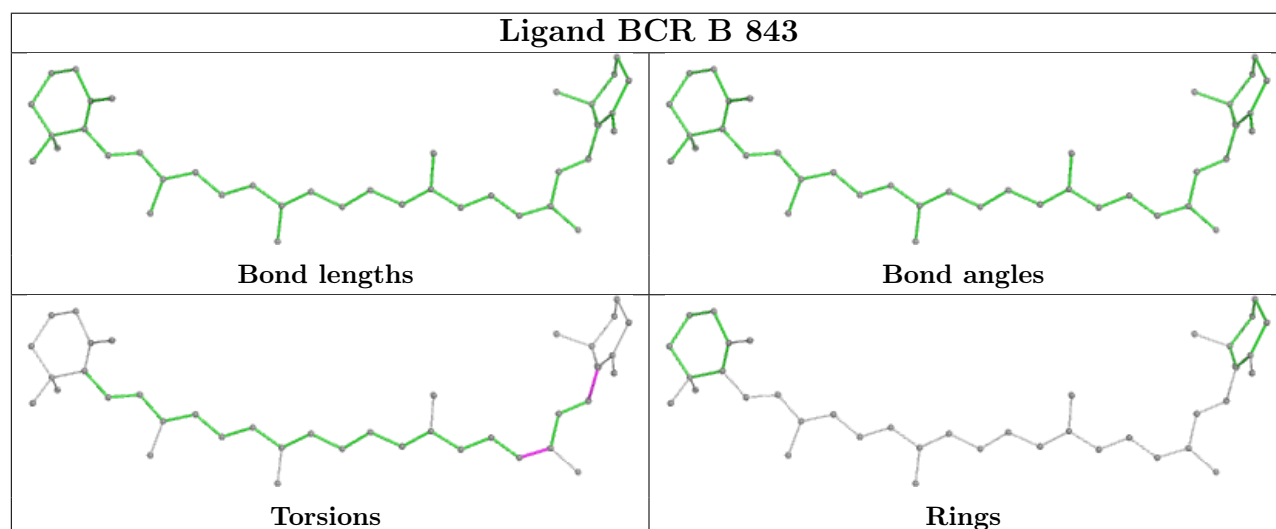
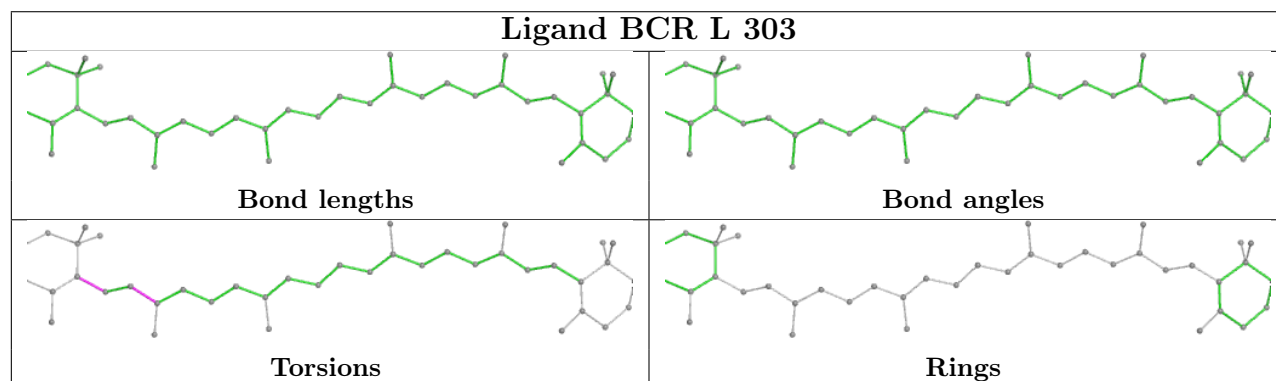
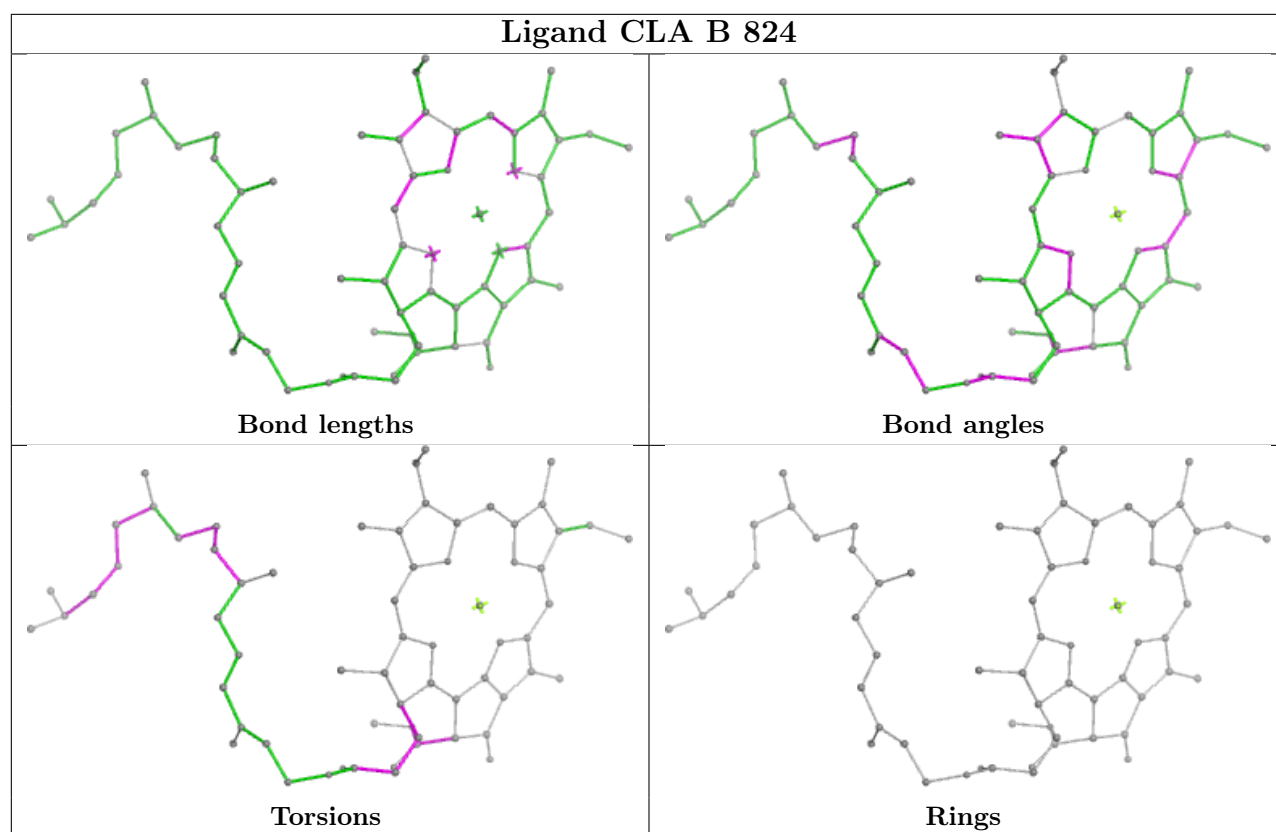


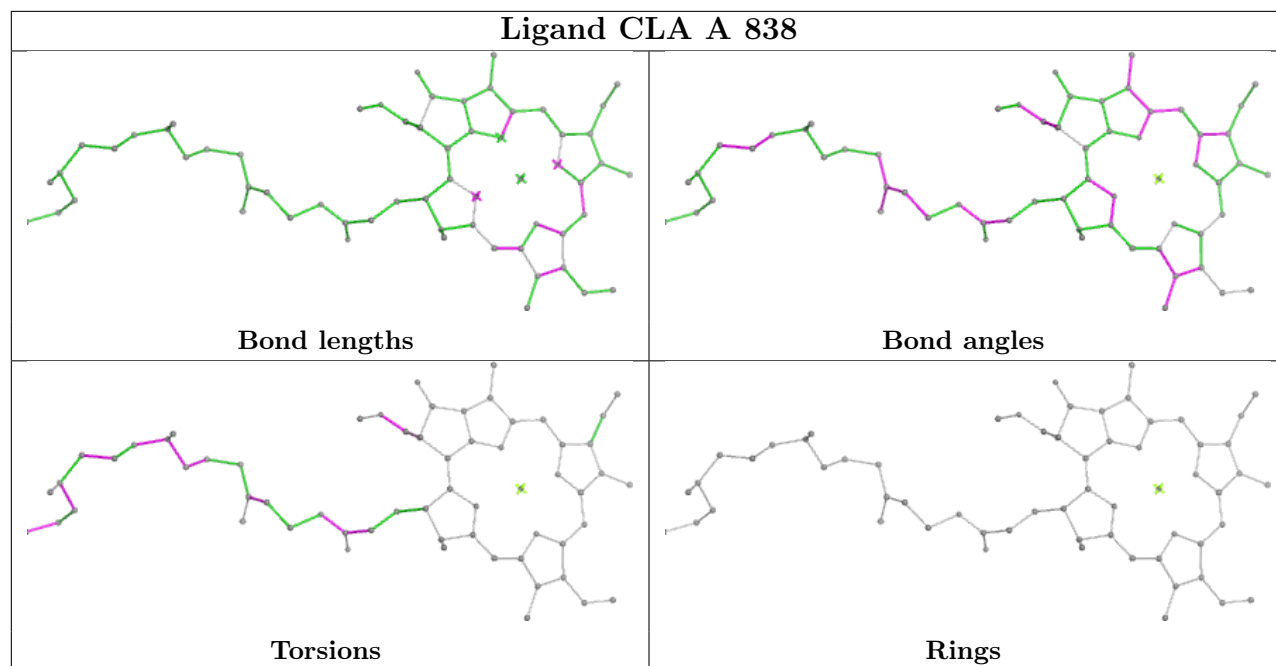
## Ligand CHL 2 314



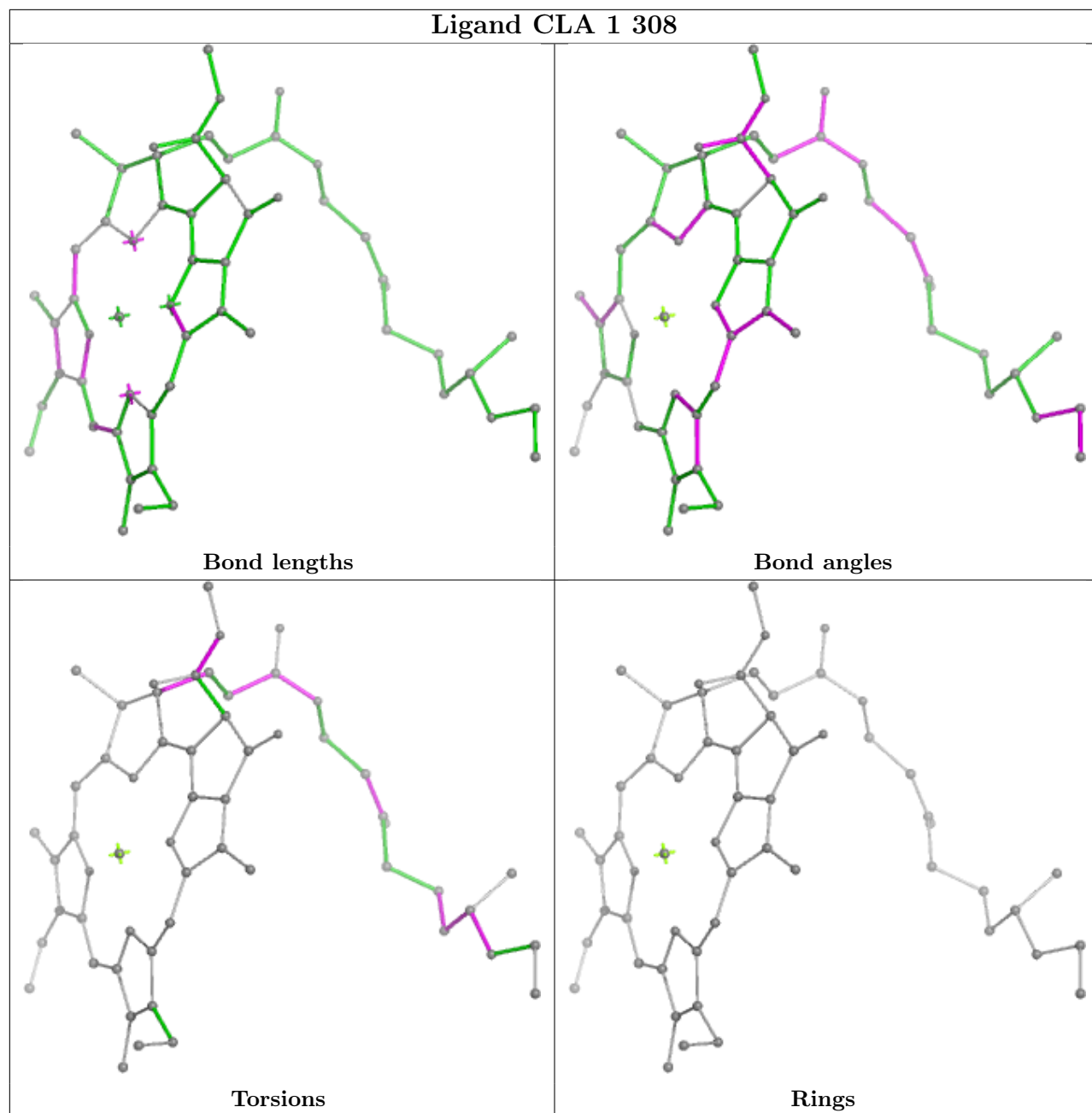
## Ligand CLA 4 313



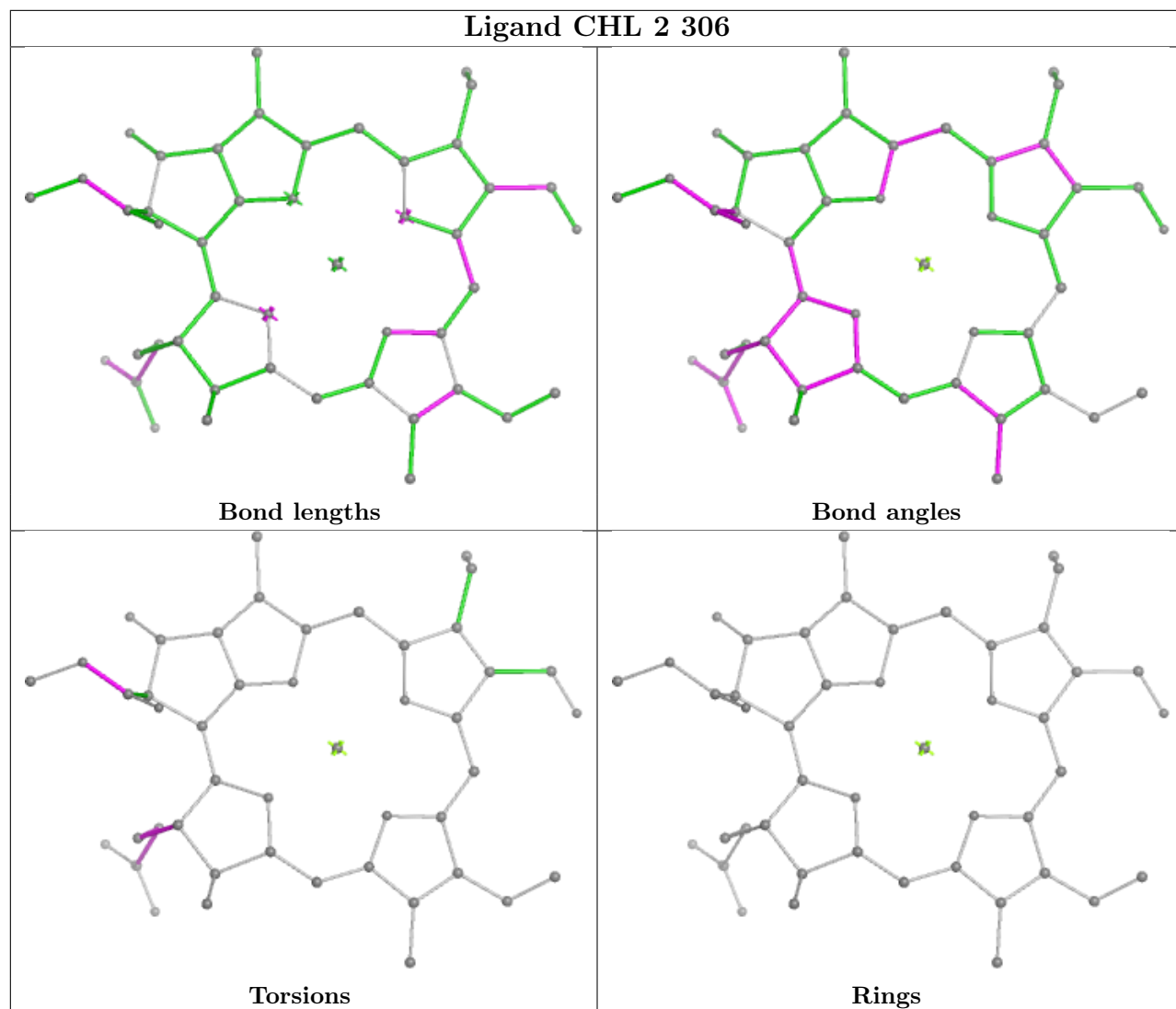




## Ligand CLA 1 308

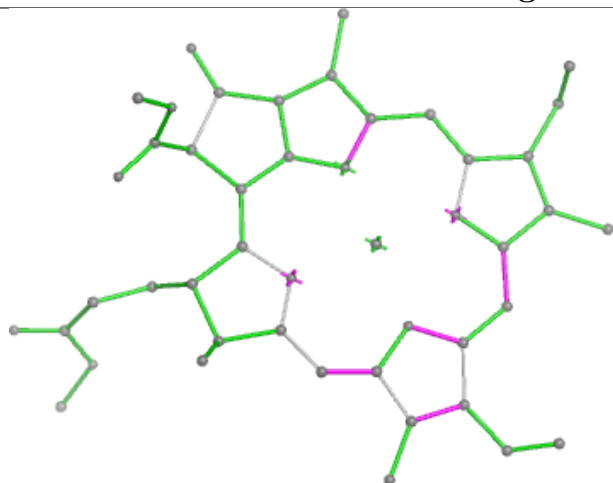


## Ligand CHL 2 306

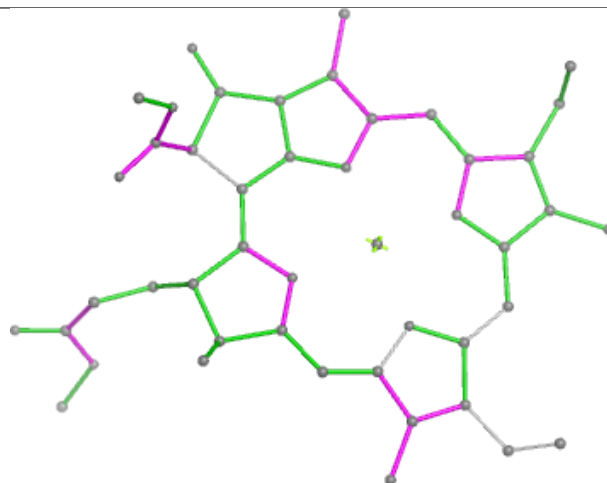




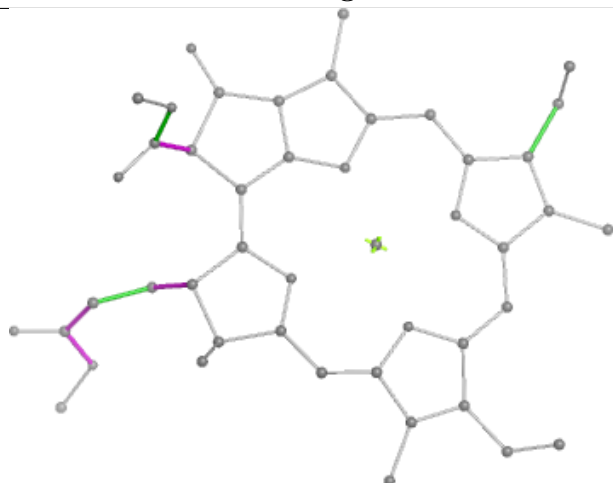
## Ligand CLA 4 301



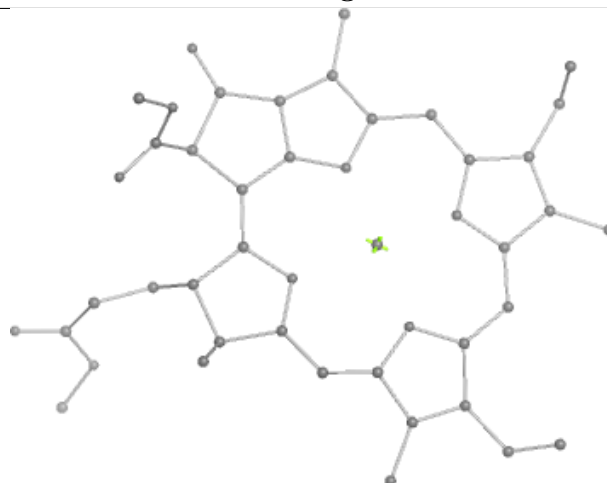
Bond lengths



Bond angles

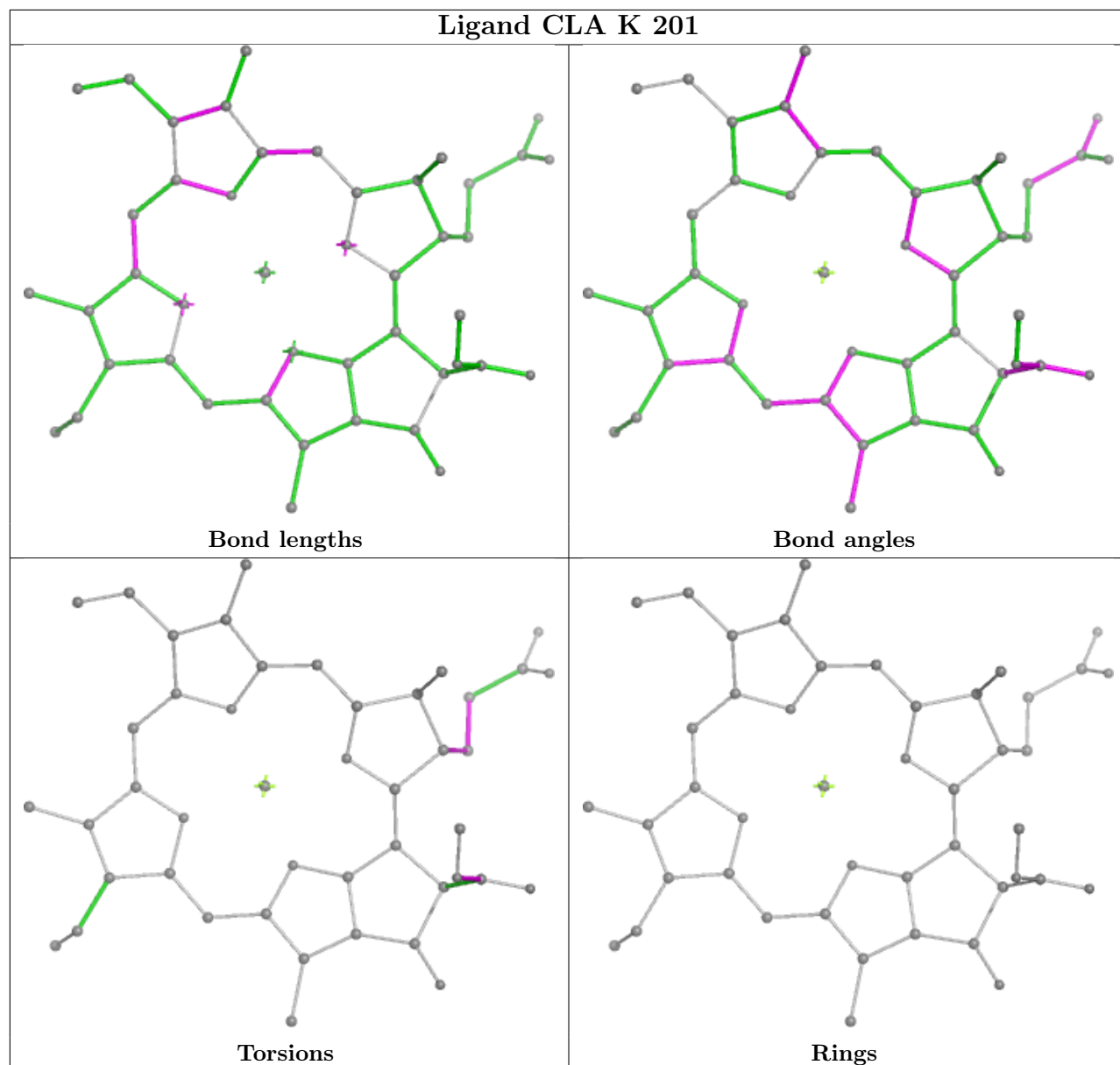


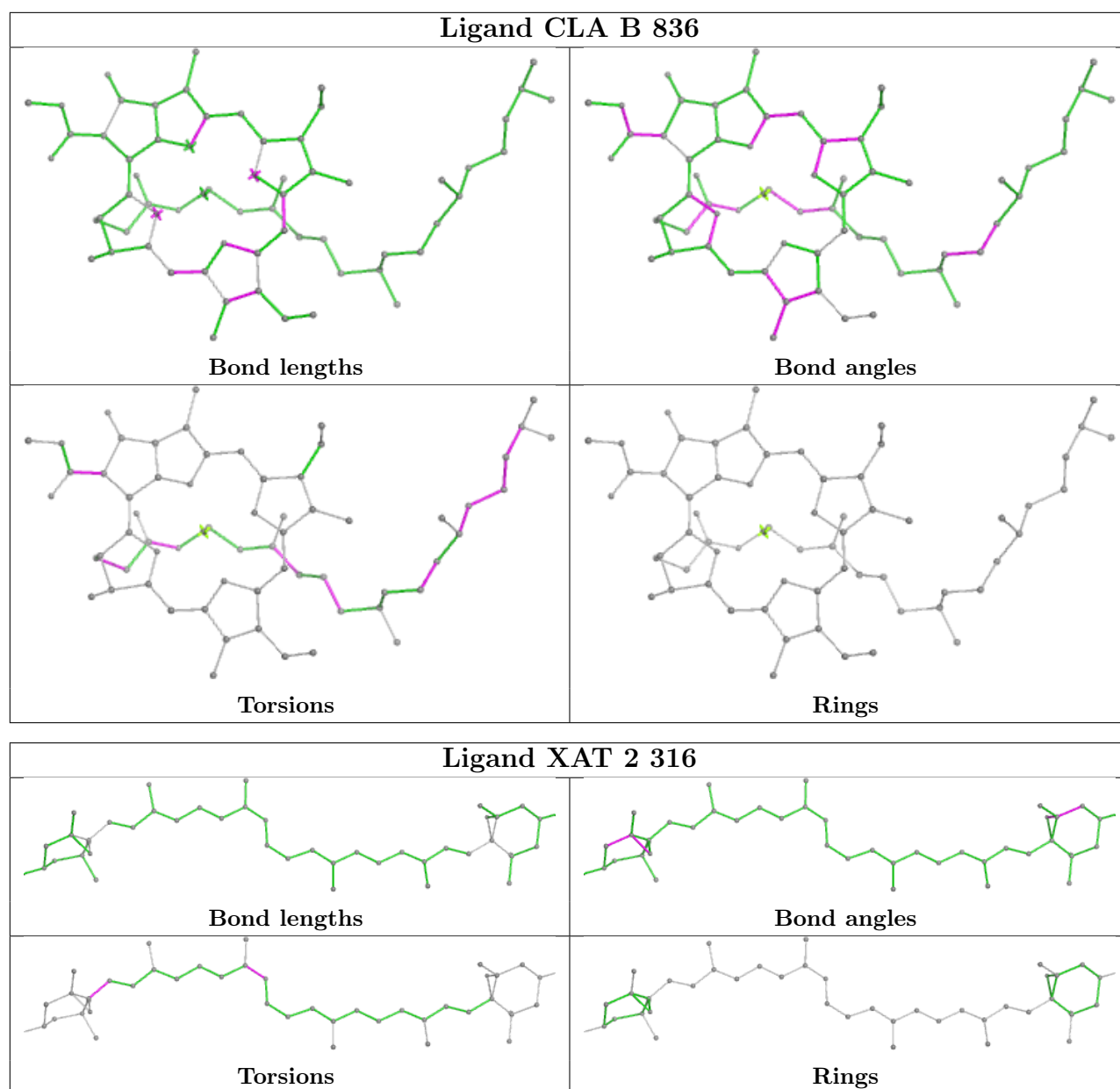
Torsions



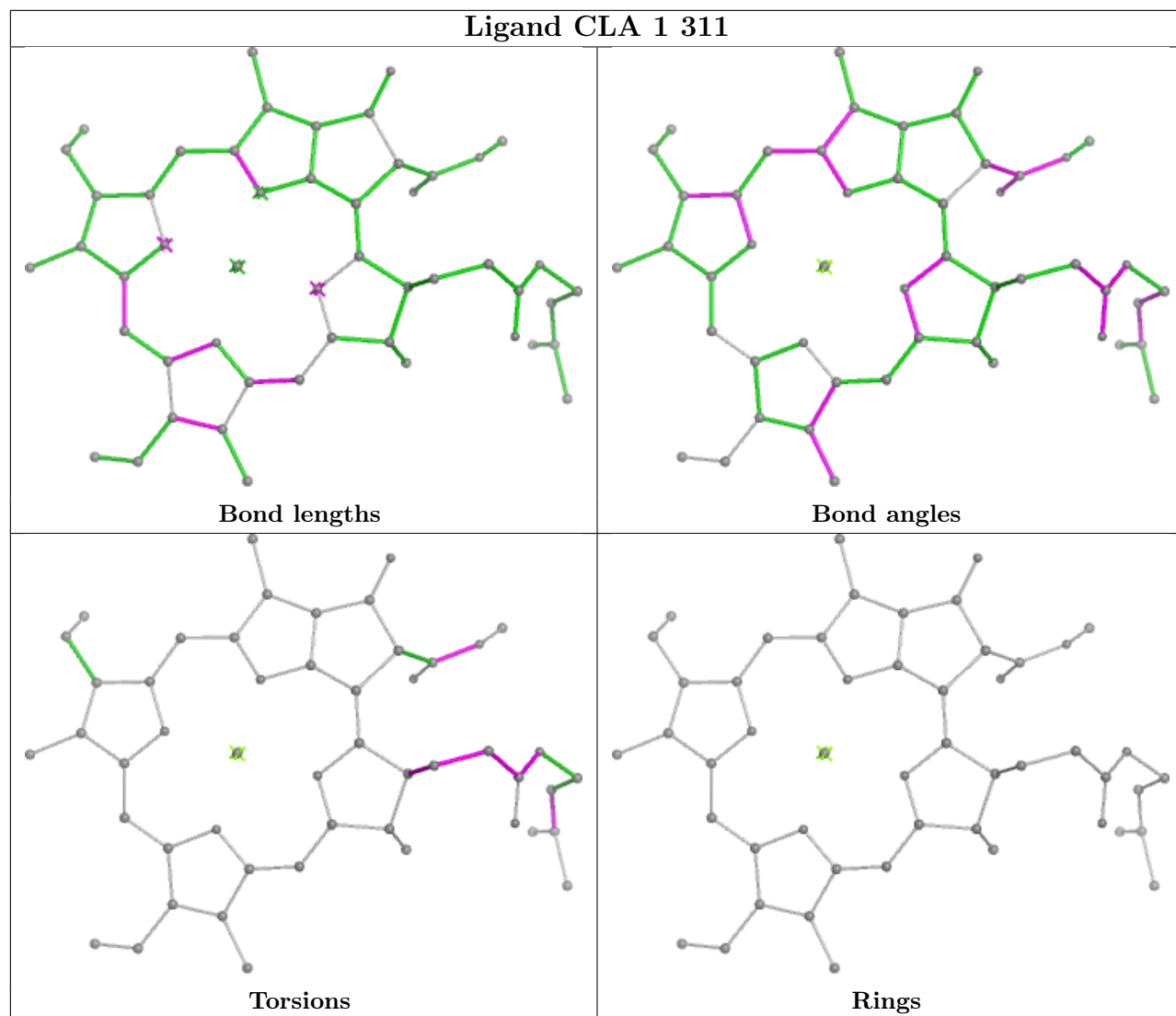
Rings

## Ligand CLA K 201

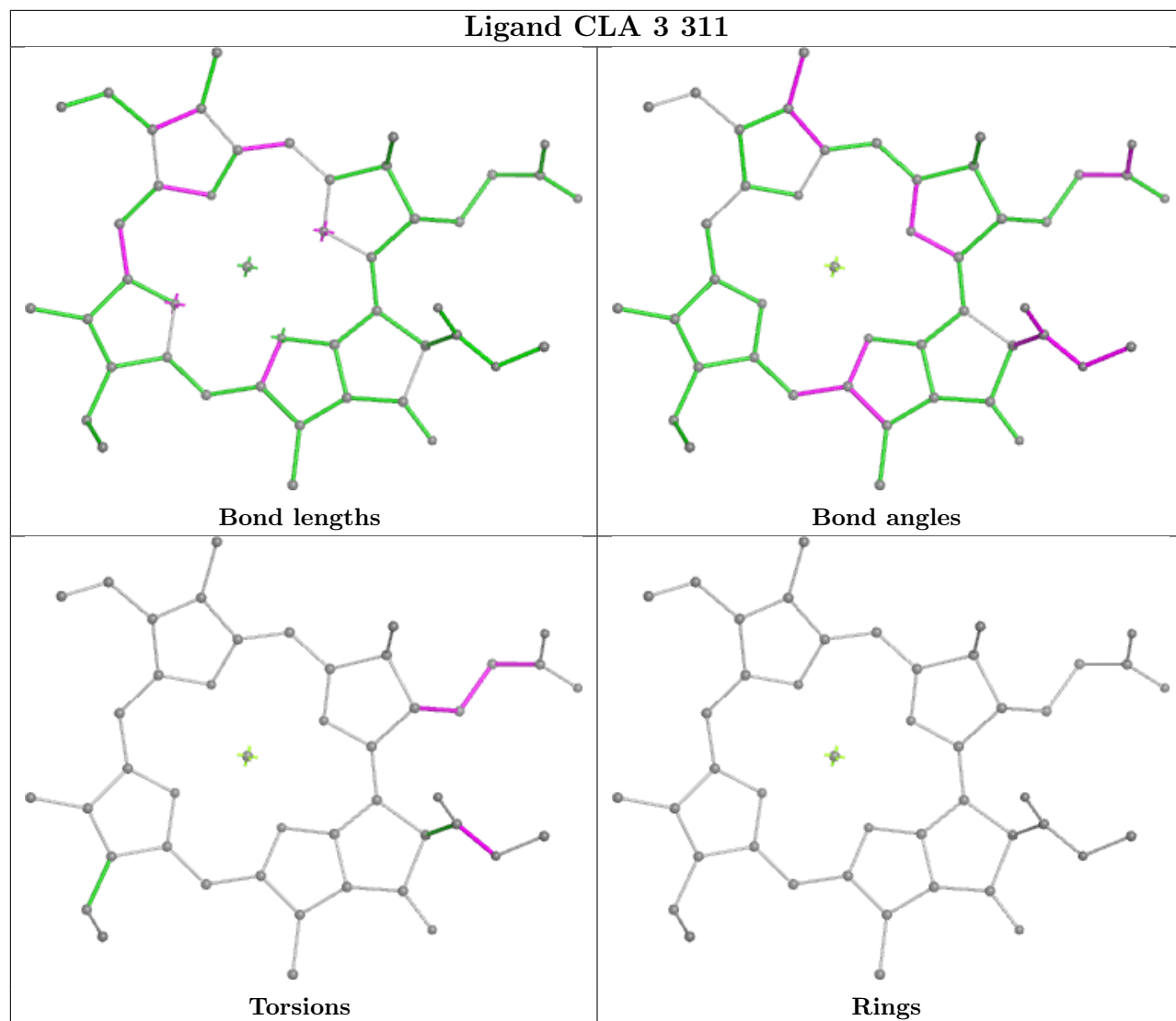


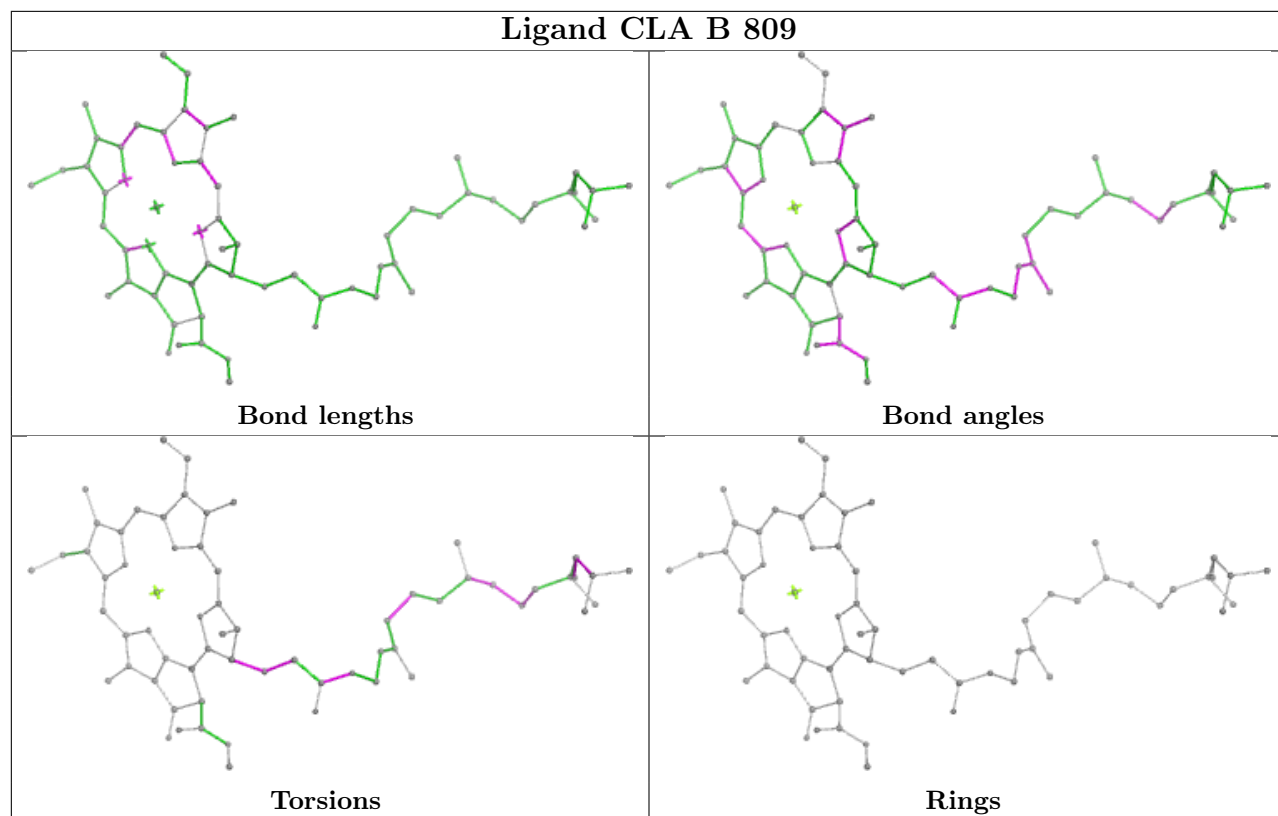


## Ligand CLA 1 311

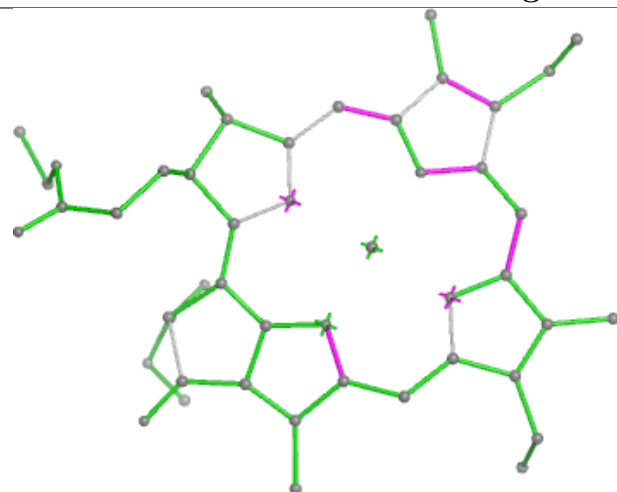


## Ligand CLA 3 311

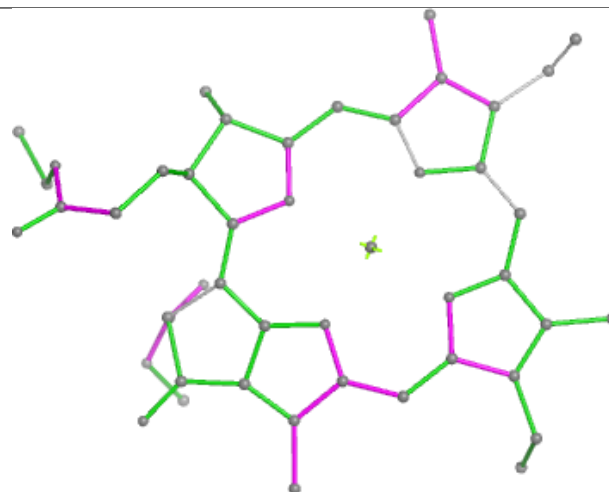




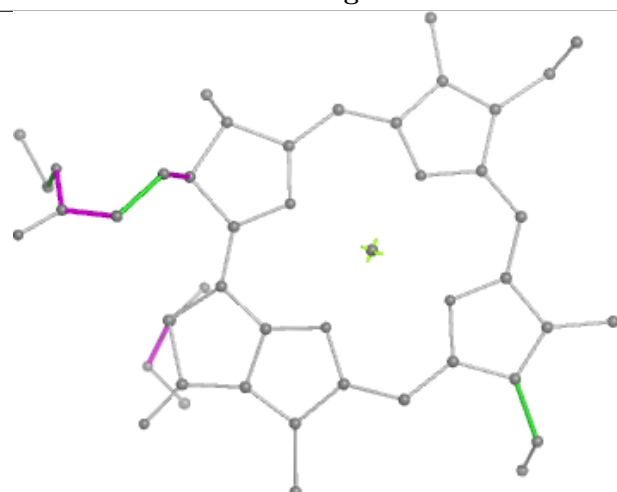
## Ligand CLA 3 304



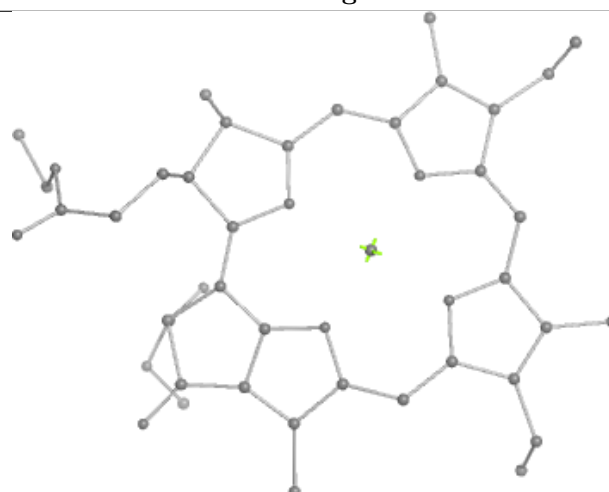
Bond lengths



Bond angles

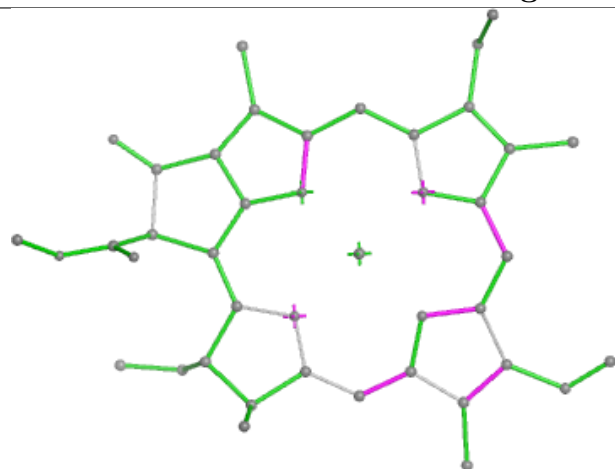


Torsions

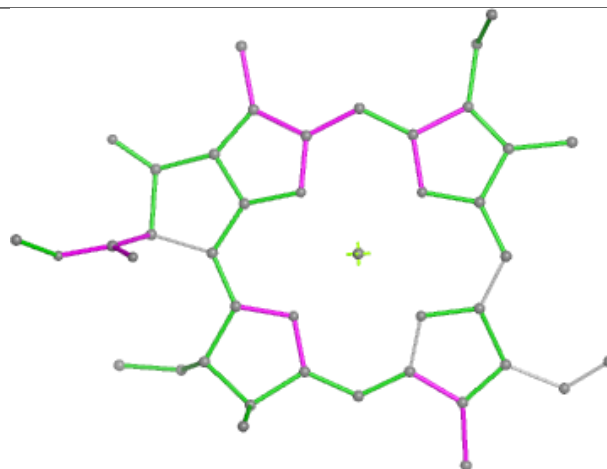


Rings

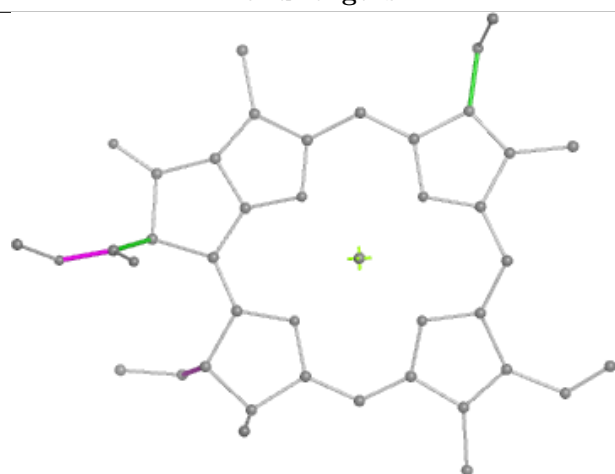
## Ligand CLA 1 305



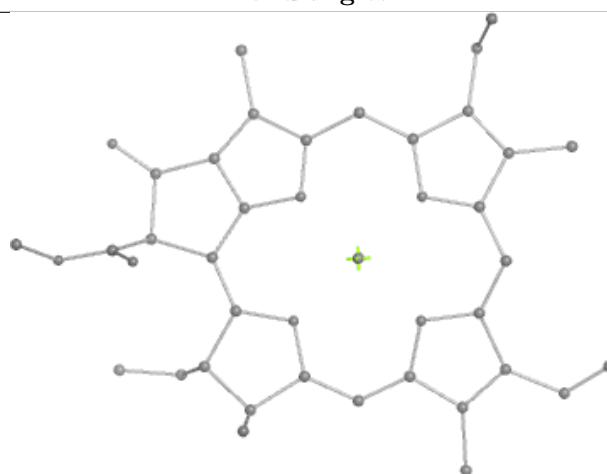
Bond lengths



Bond angles

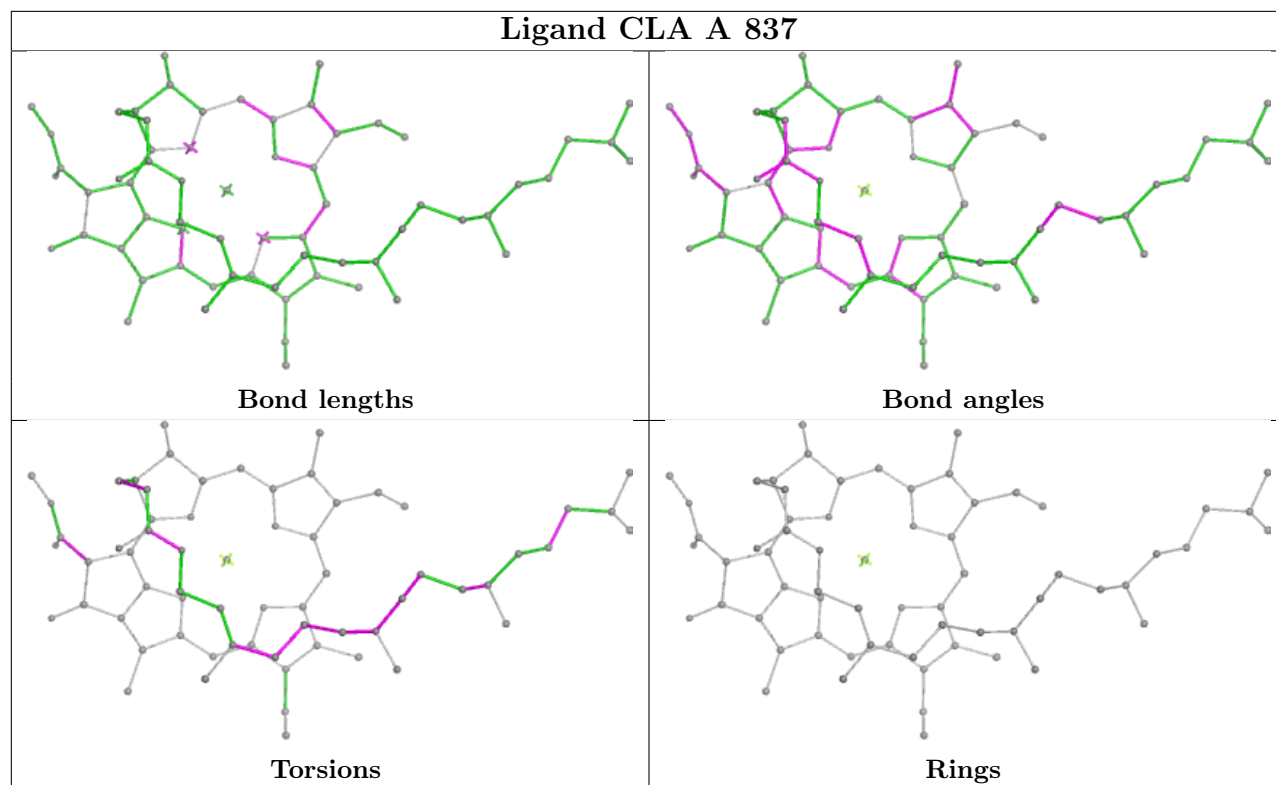


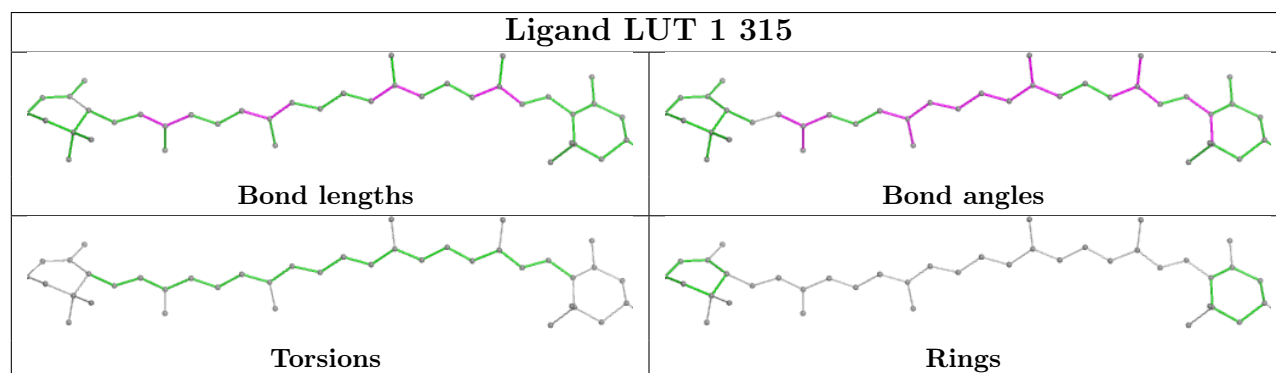
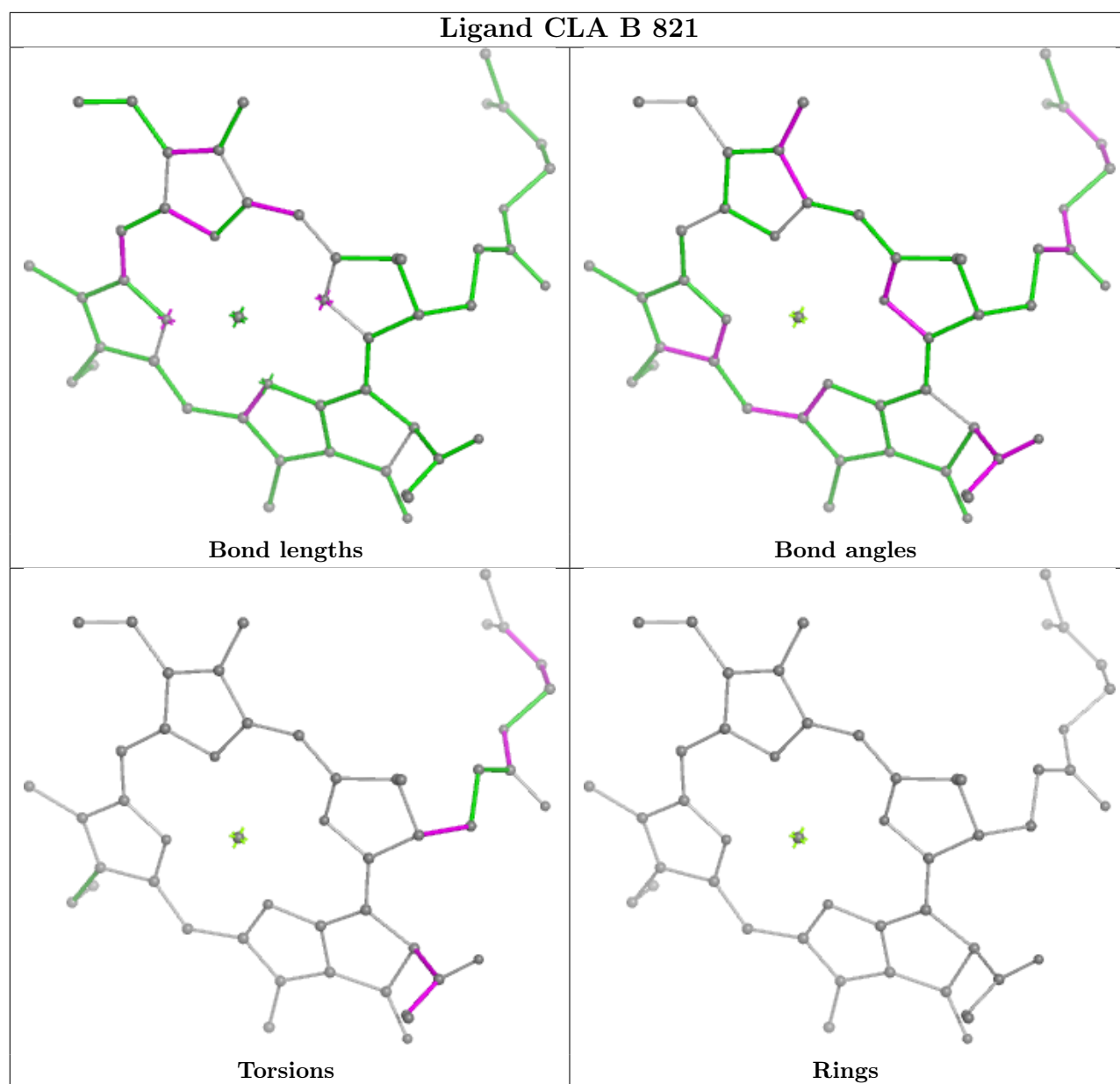
Torsions

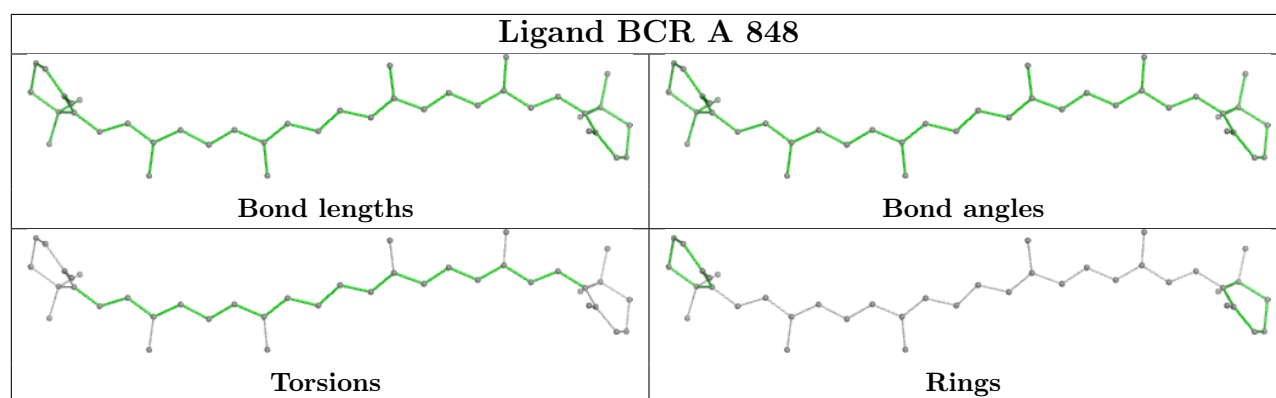
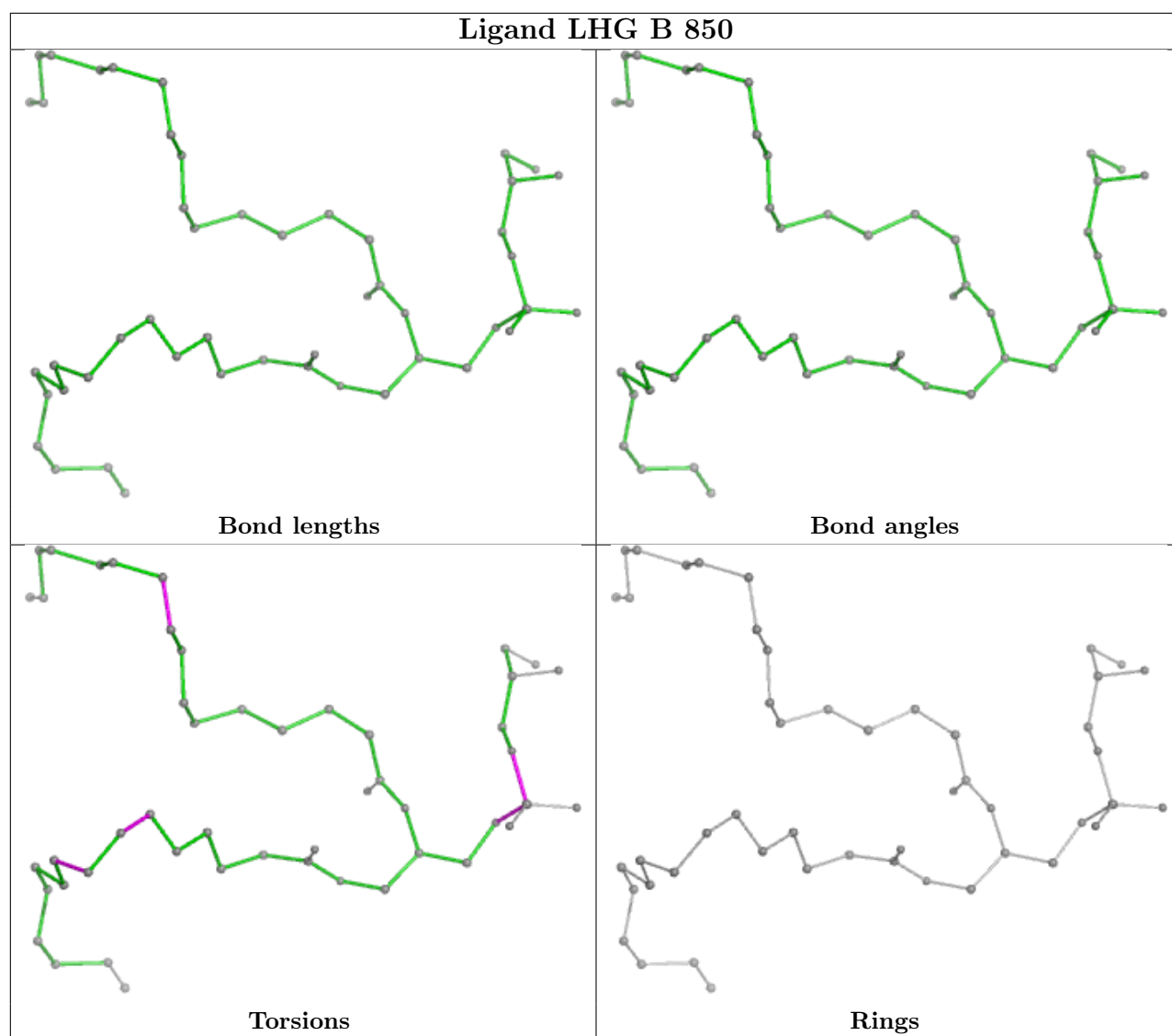


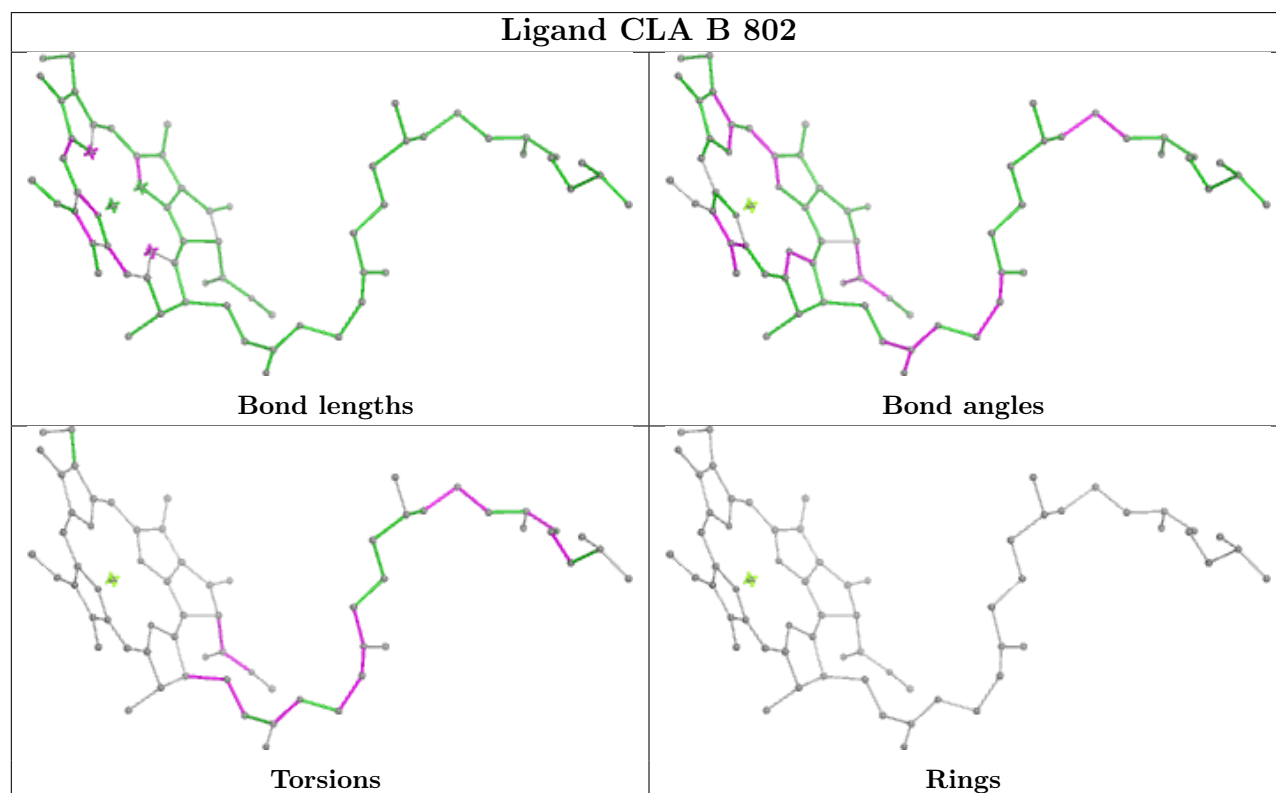
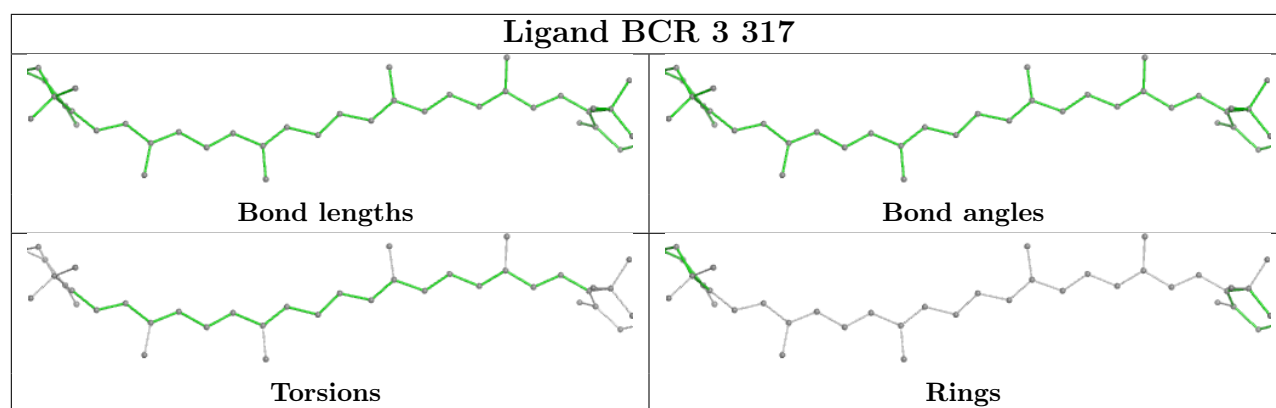
Rings



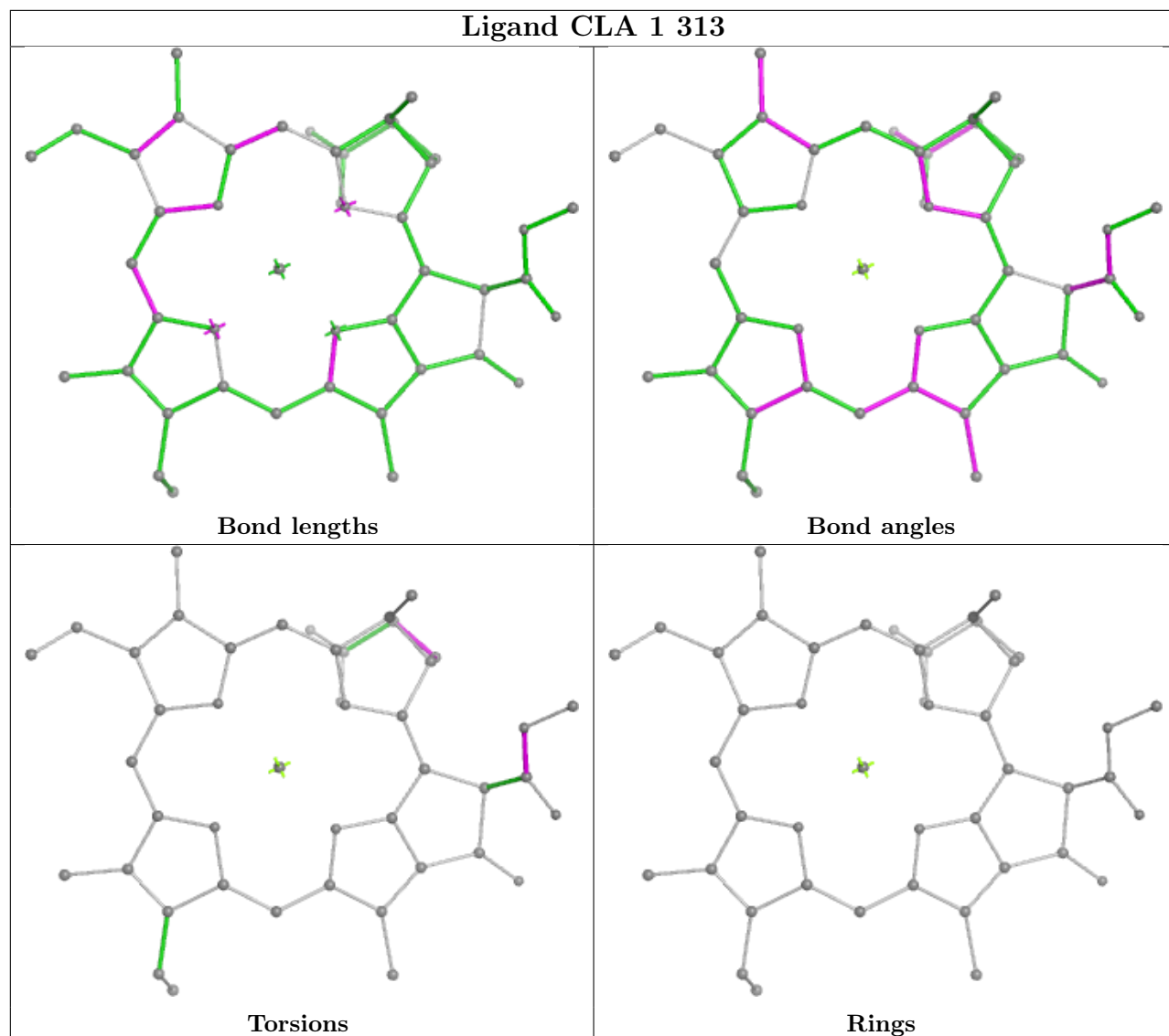




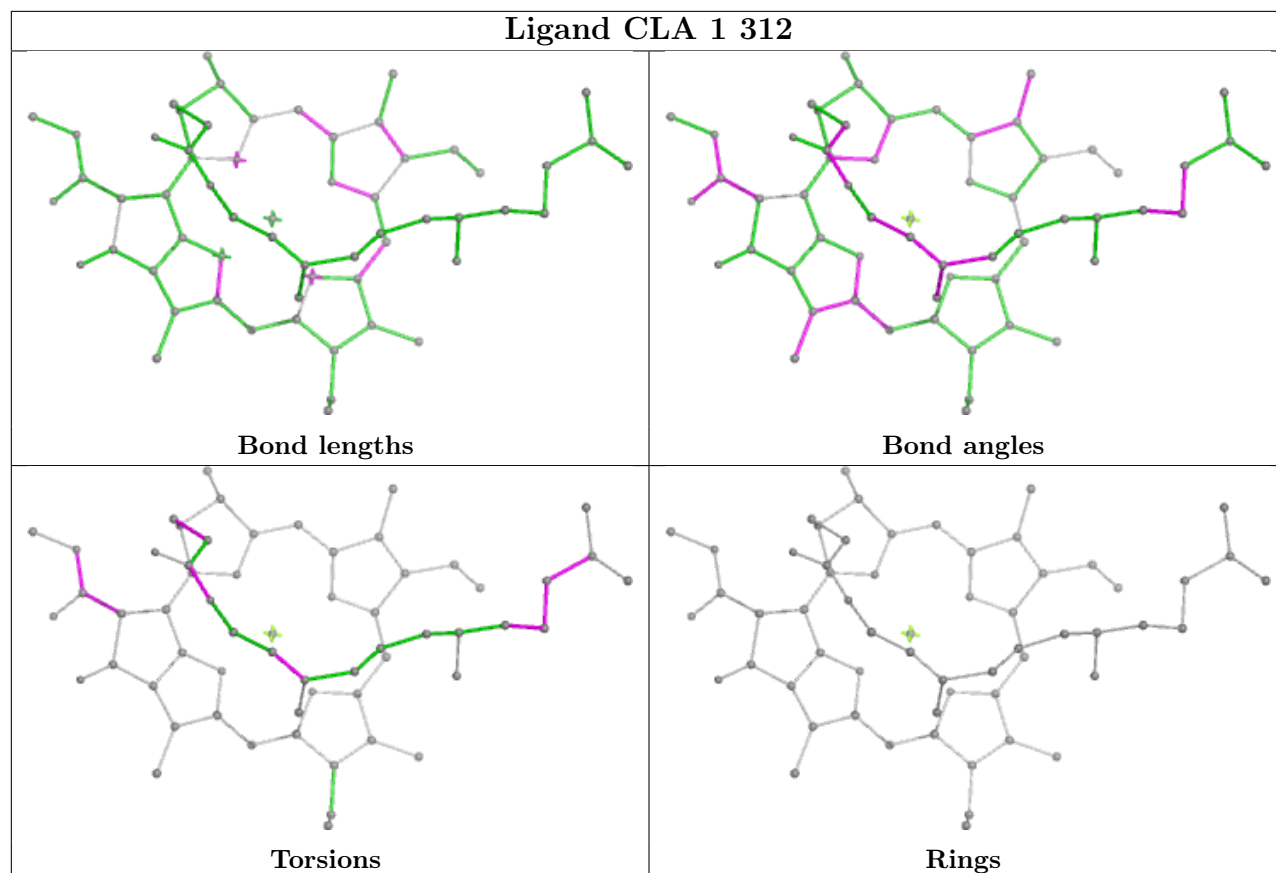




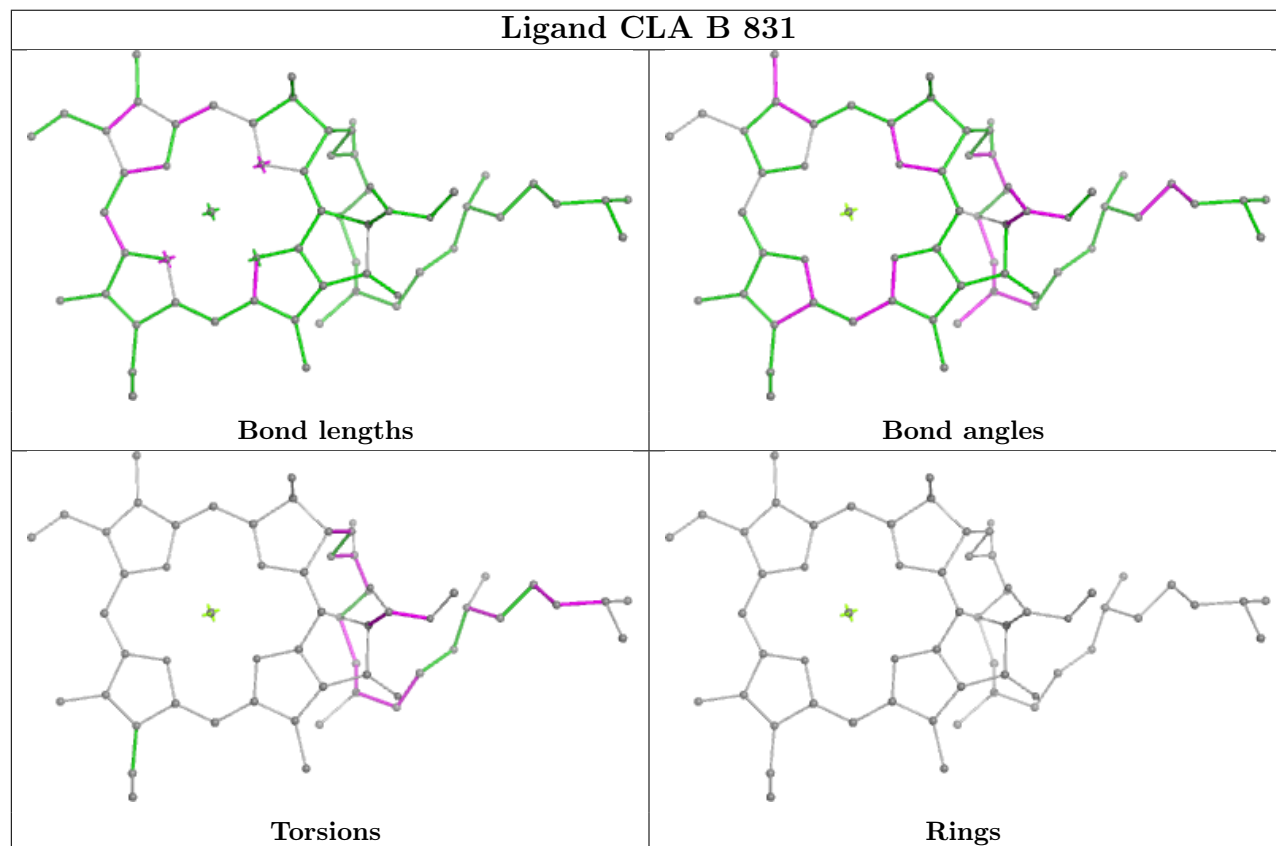
## Ligand CLA 1 313



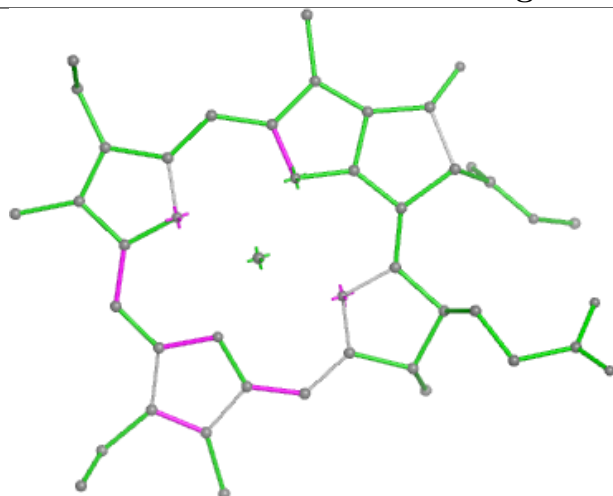
## Ligand CLA 1 312



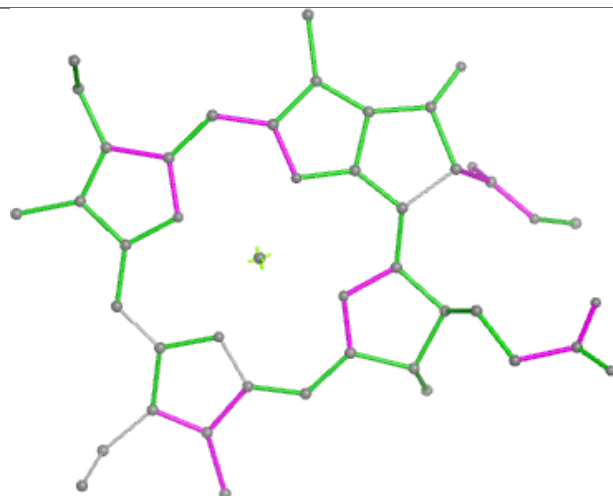
## Ligand CLA B 831



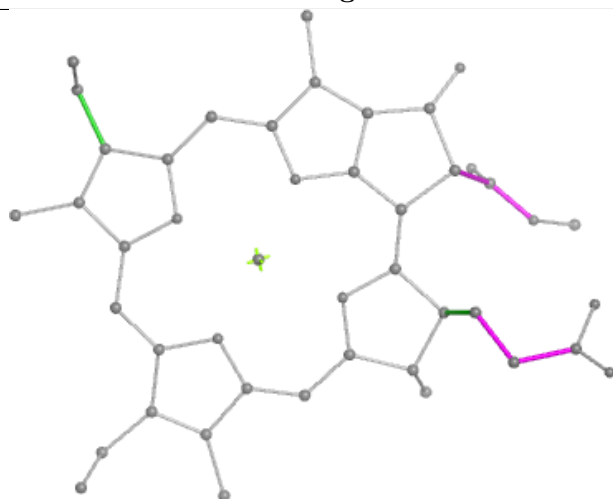
## Ligand CLA F 302



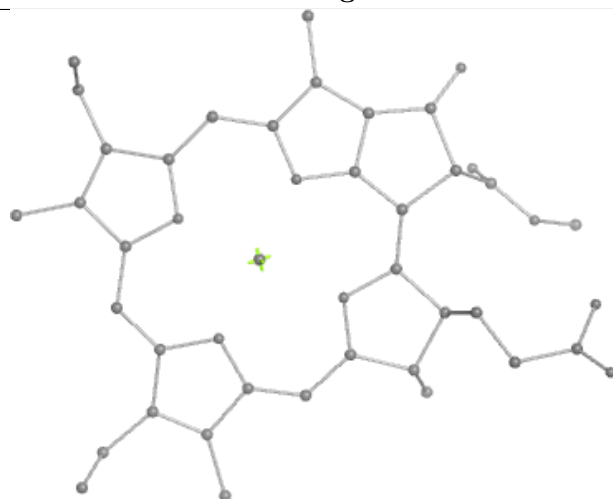
Bond lengths



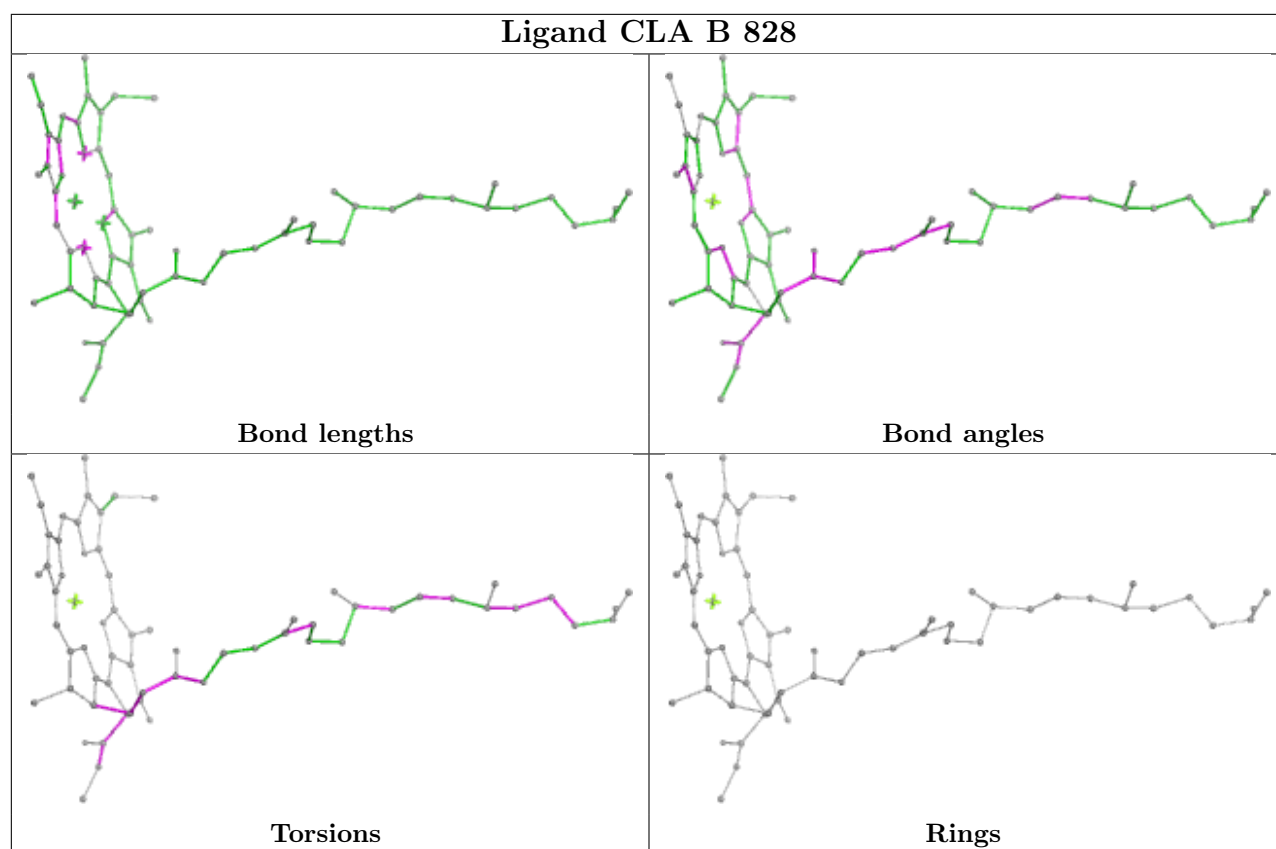
Bond angles



Torsions

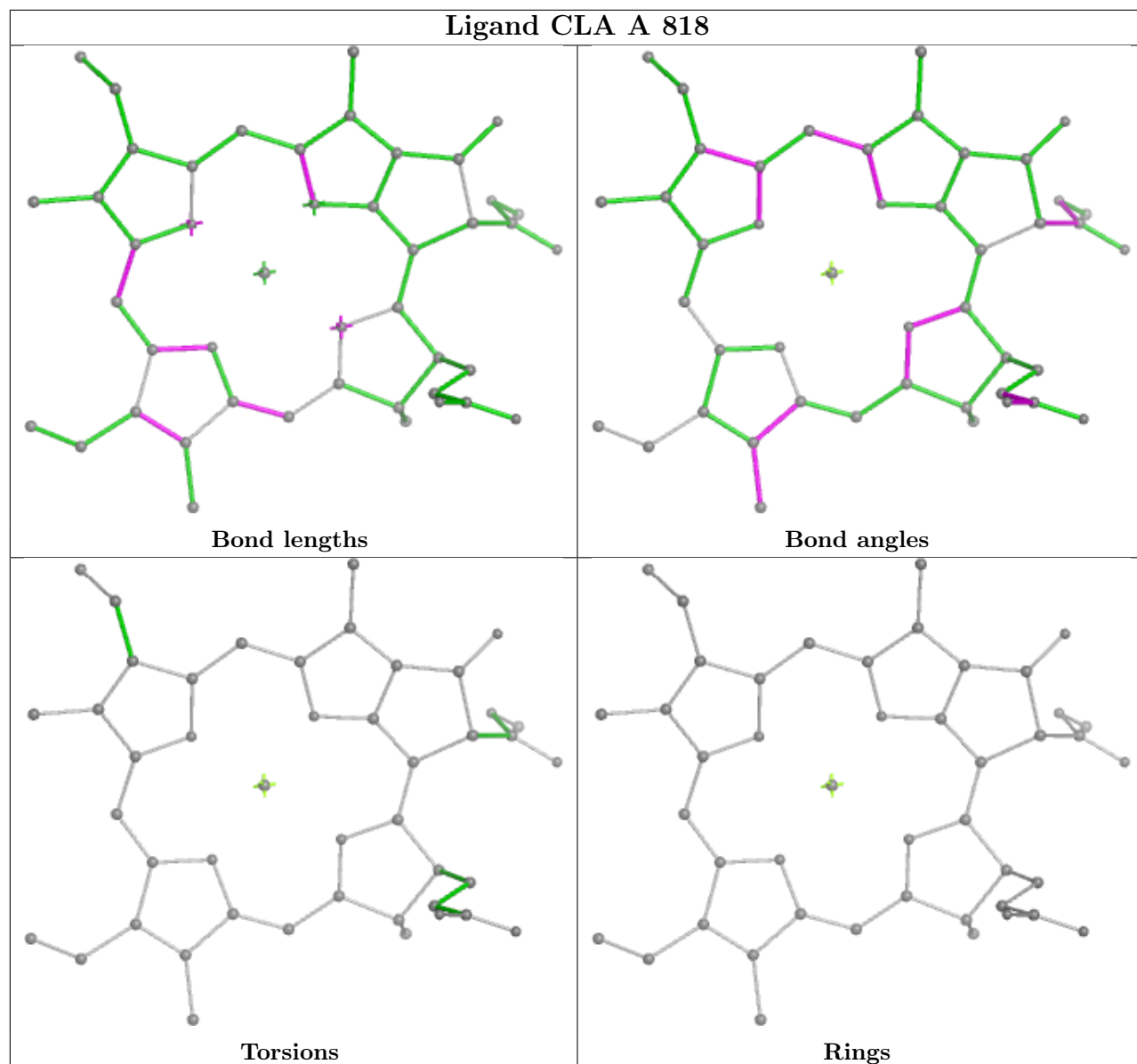


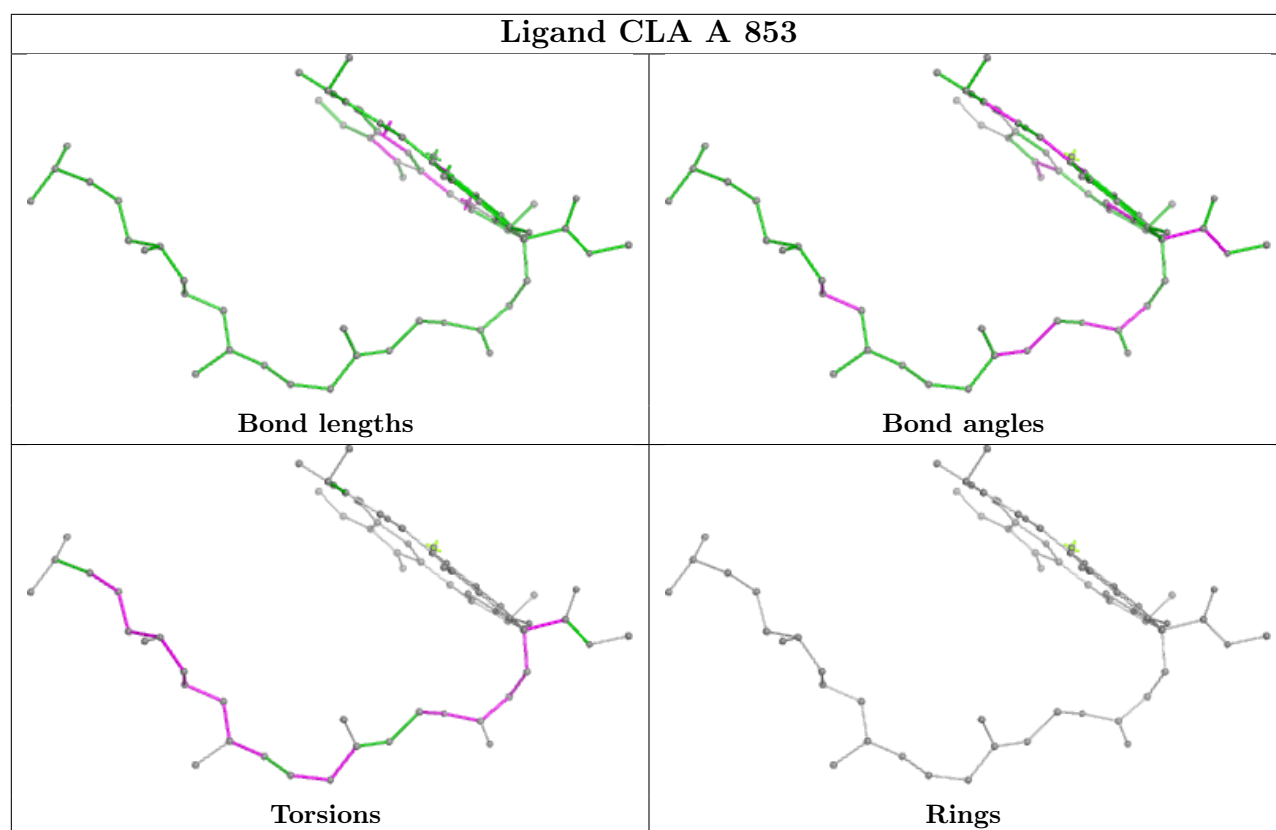
Rings



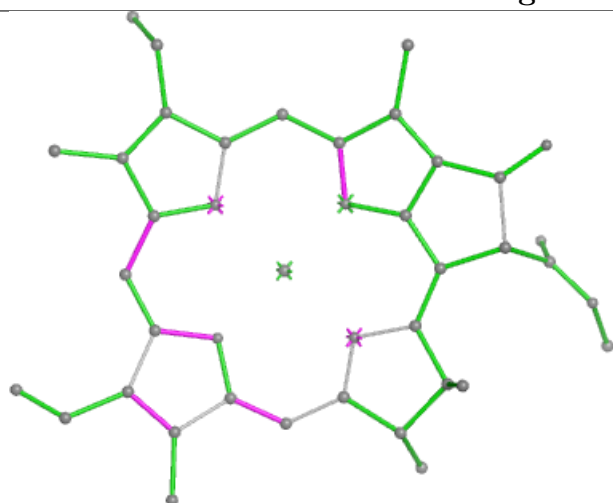


## Ligand CLA A 818

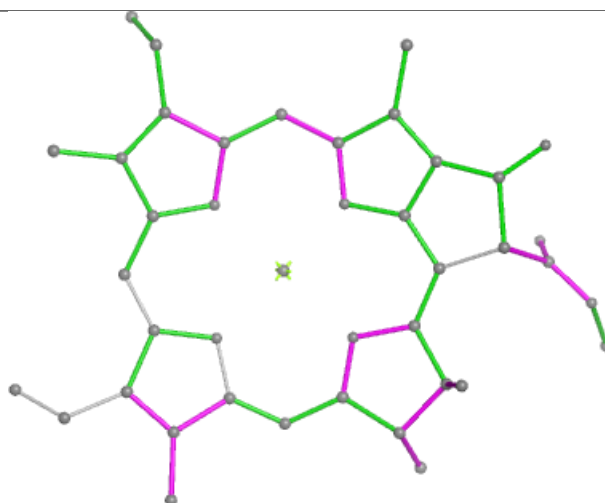




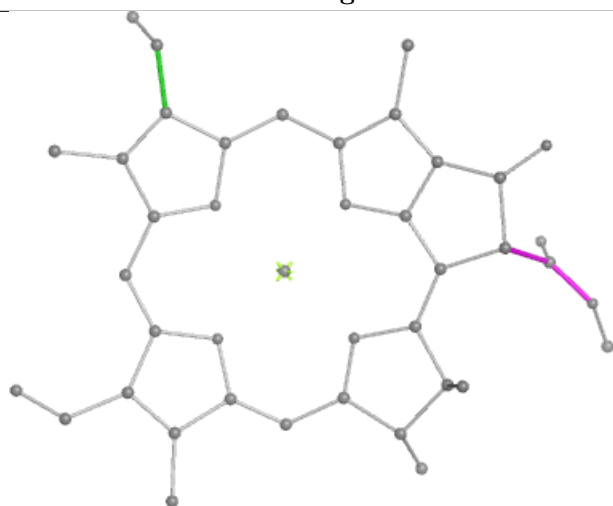
## Ligand CLA 2 310



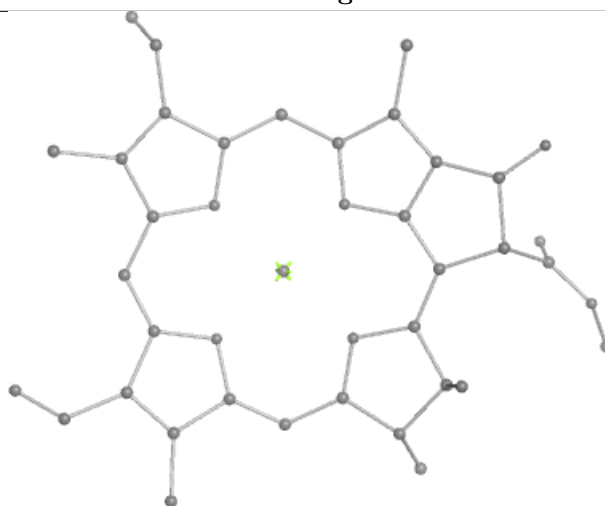
Bond lengths



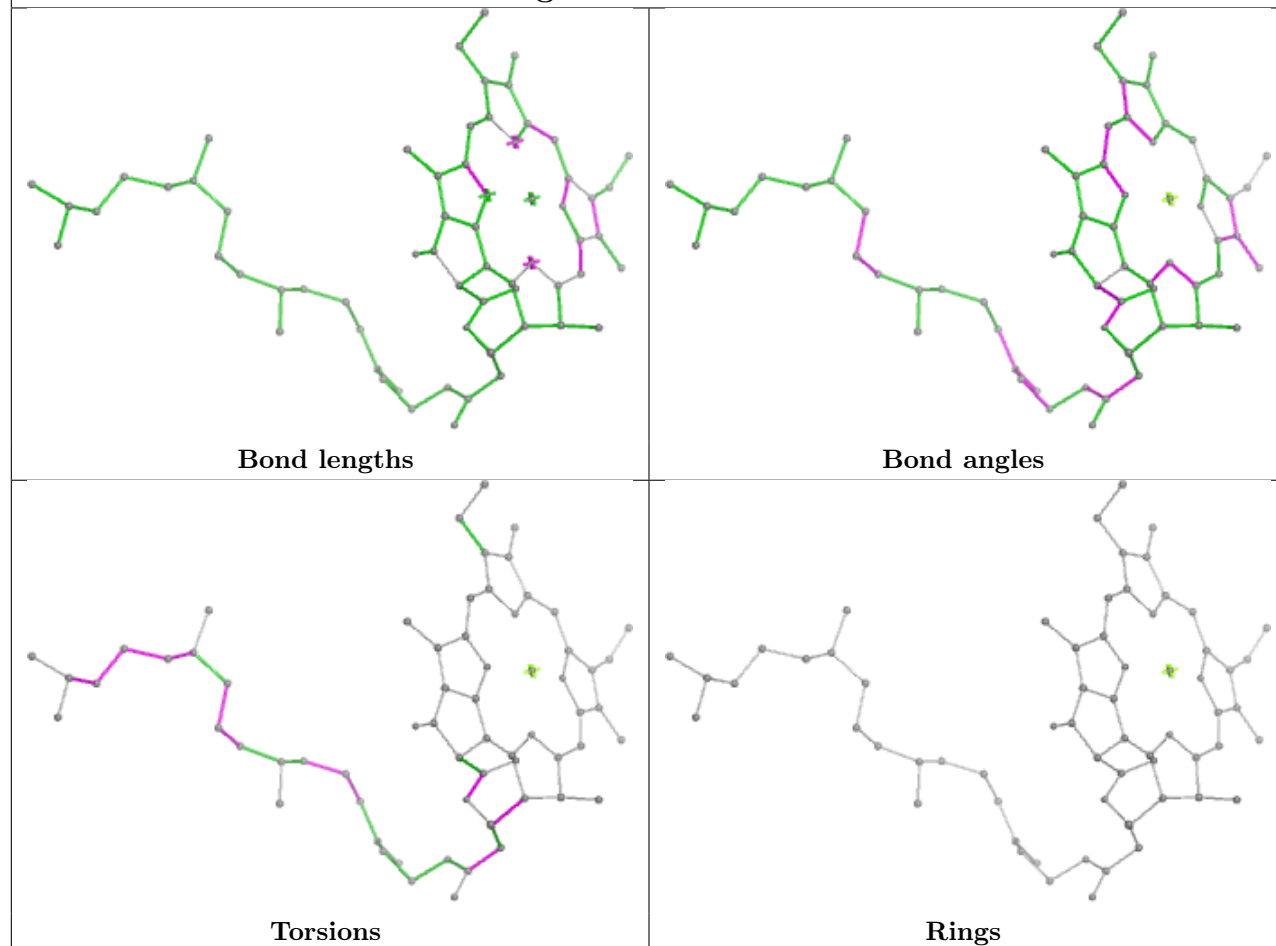
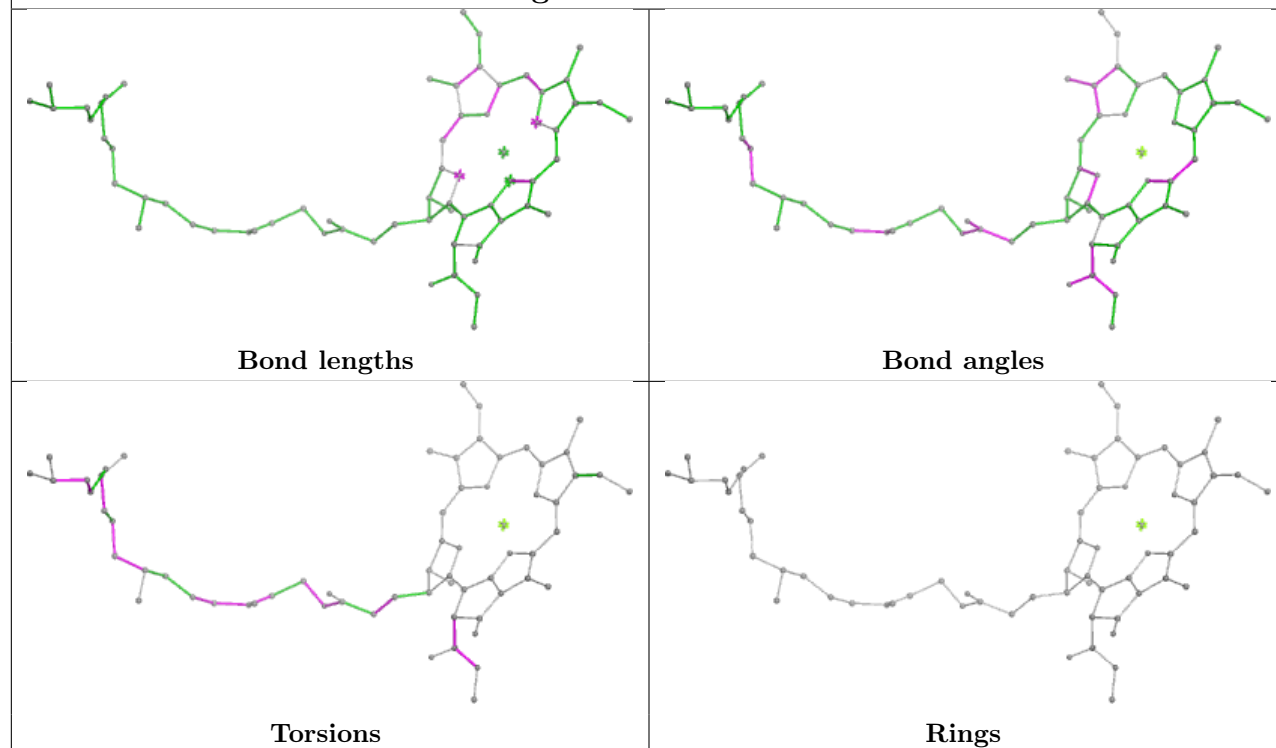
Bond angles

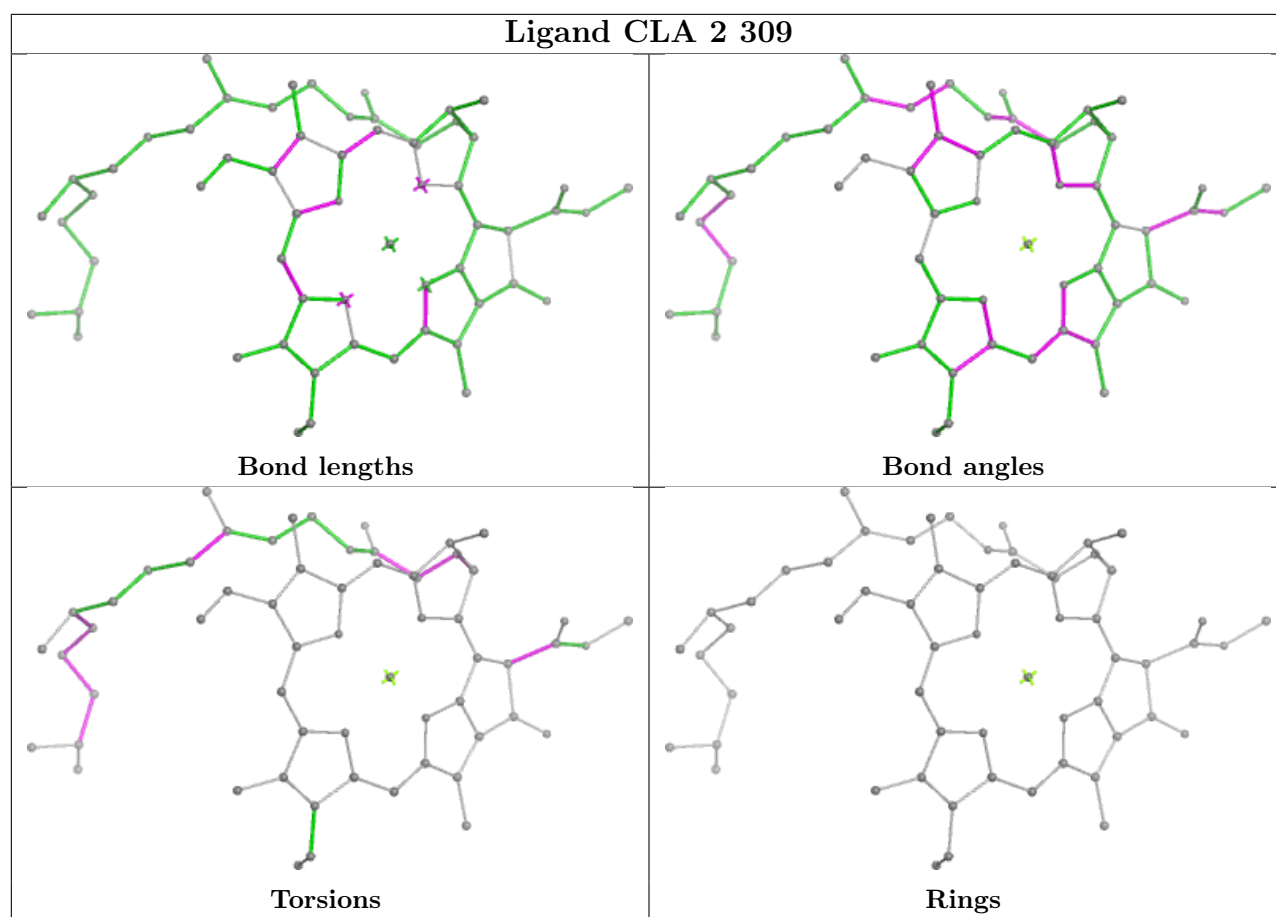


Torsions

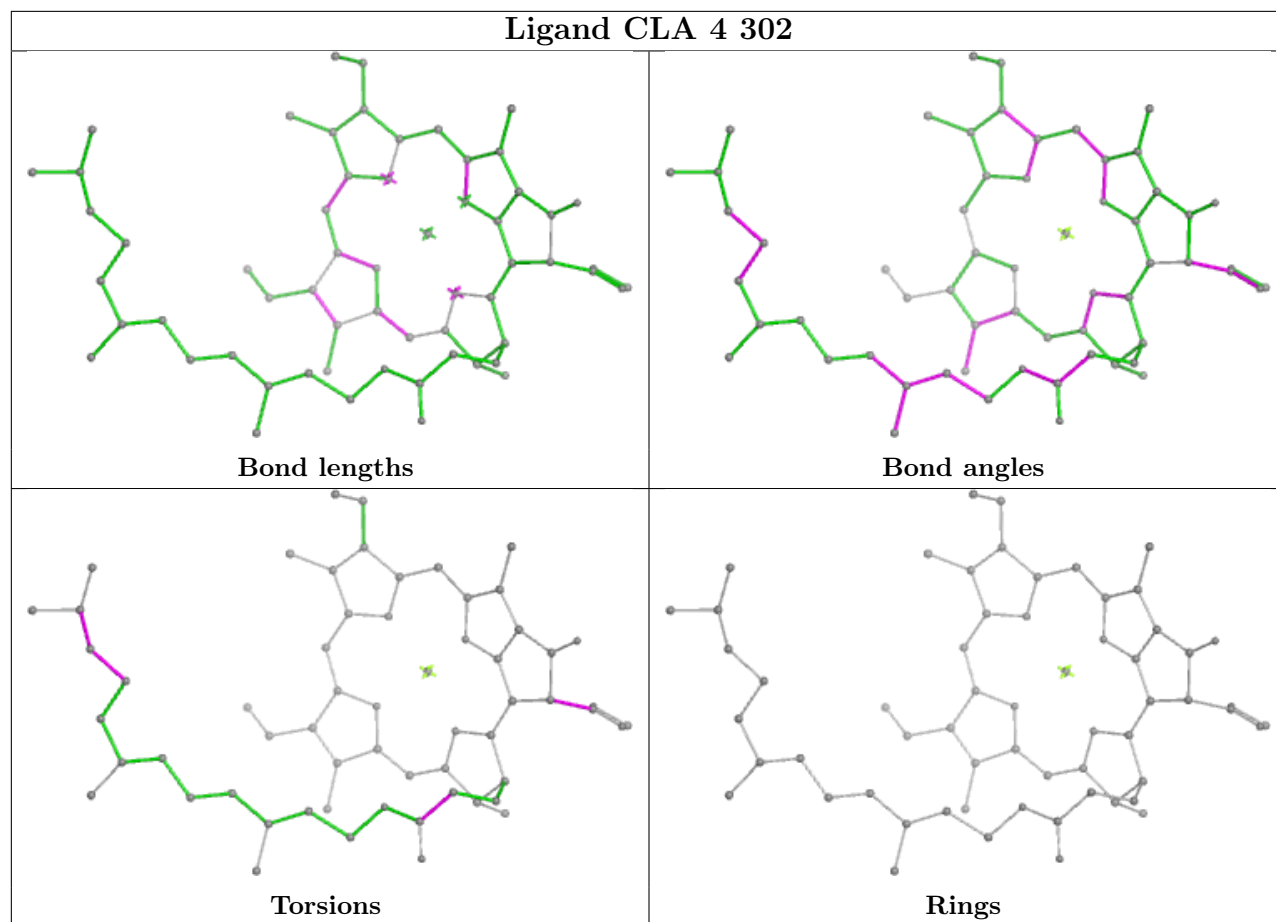


Rings

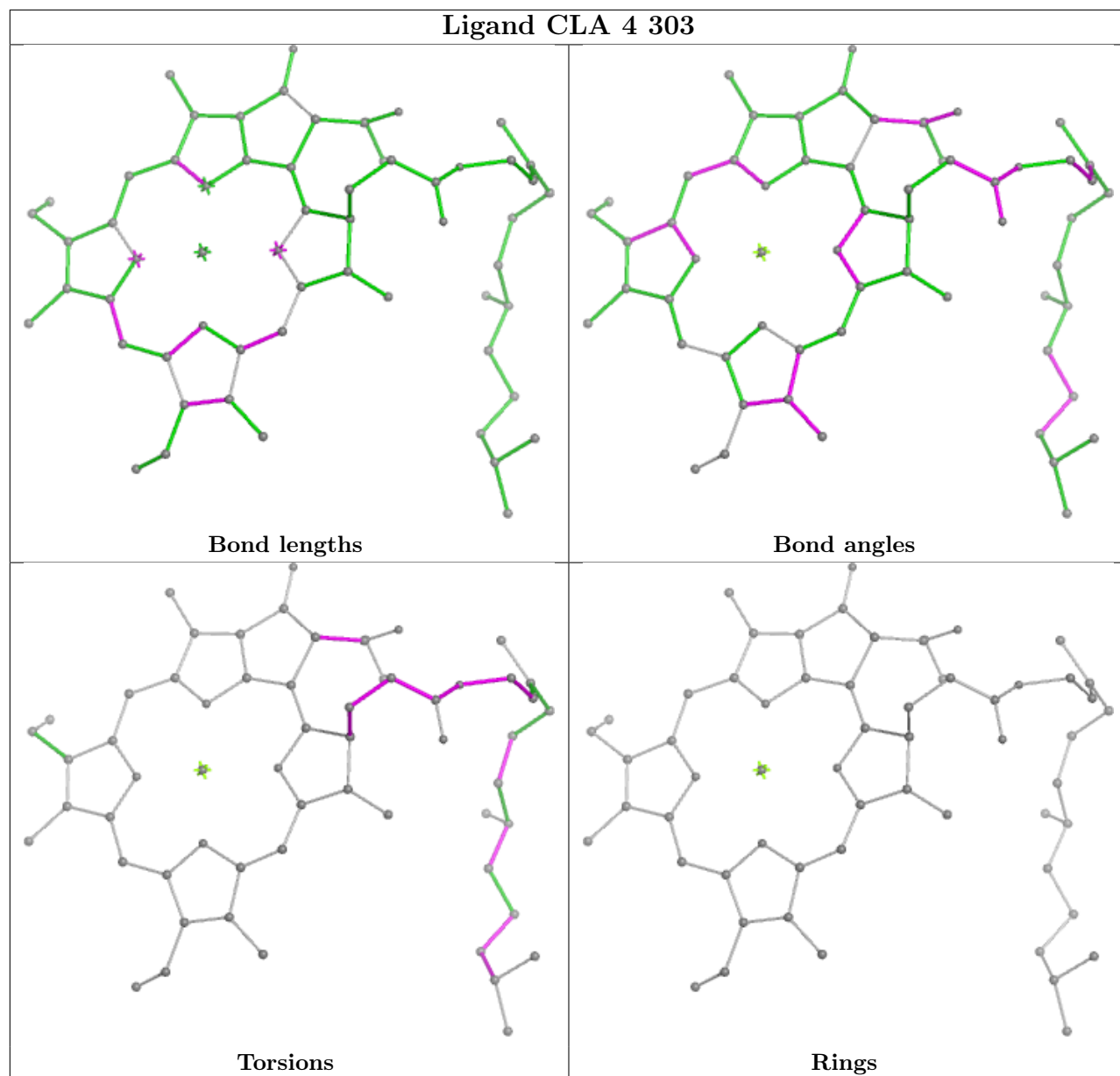
**Ligand CLA 3 308****Ligand CLA A 833**



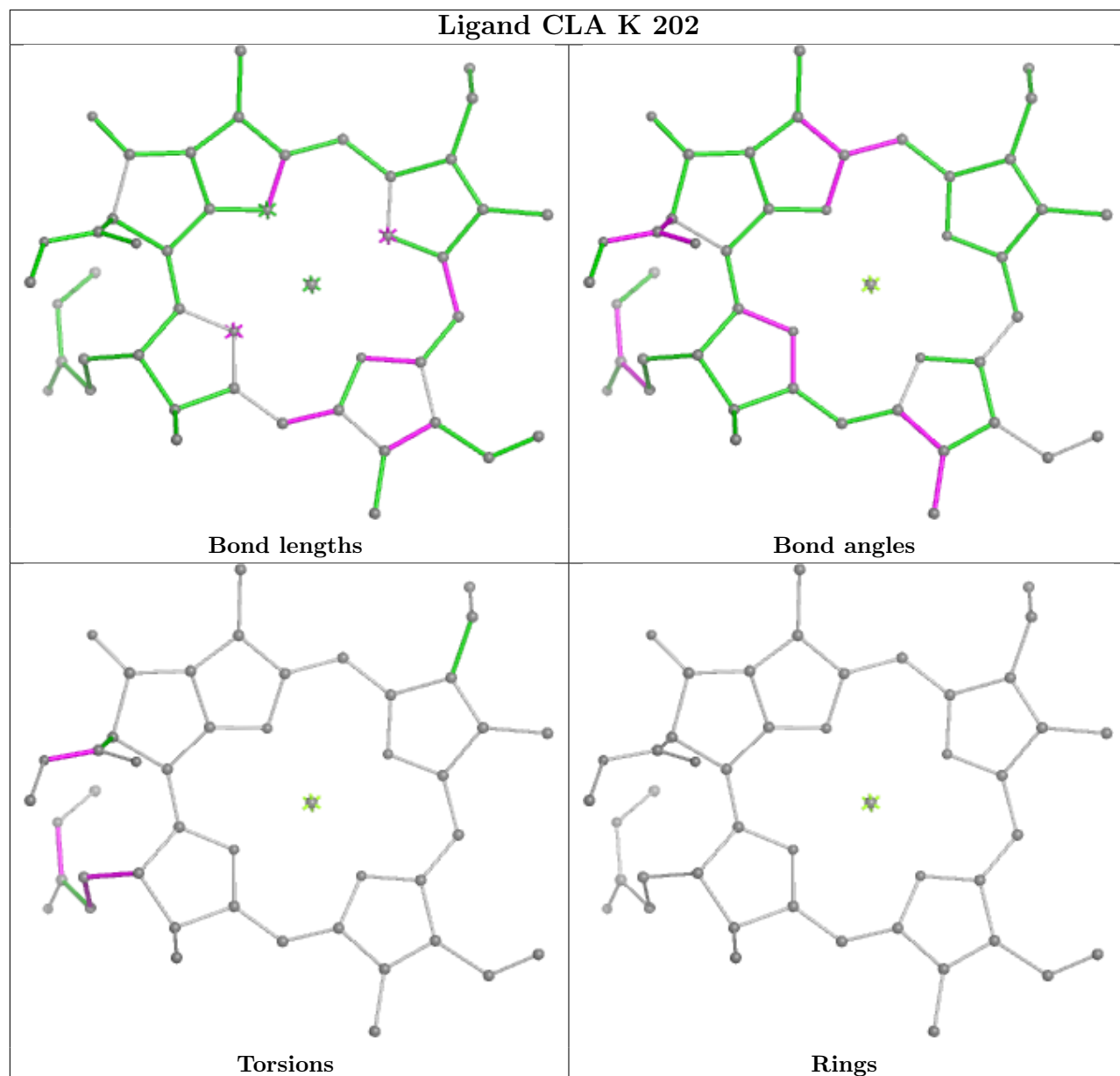
## Ligand CLA 4 302



## Ligand CLA 4 303

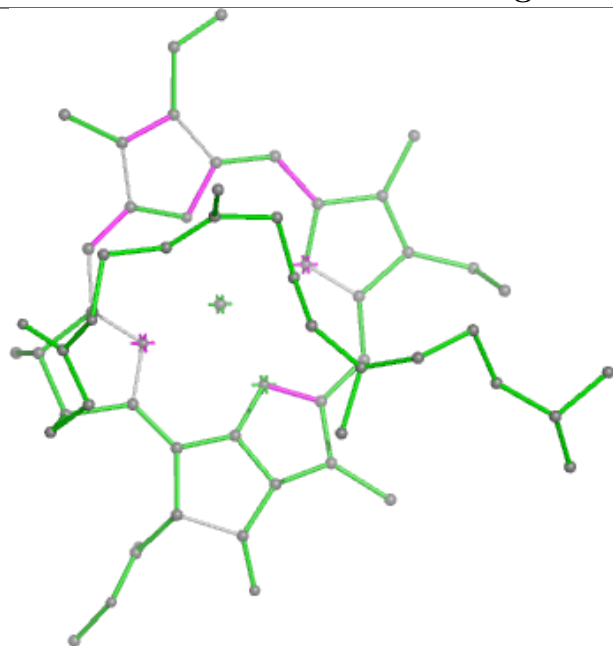


## Ligand CLA K 202

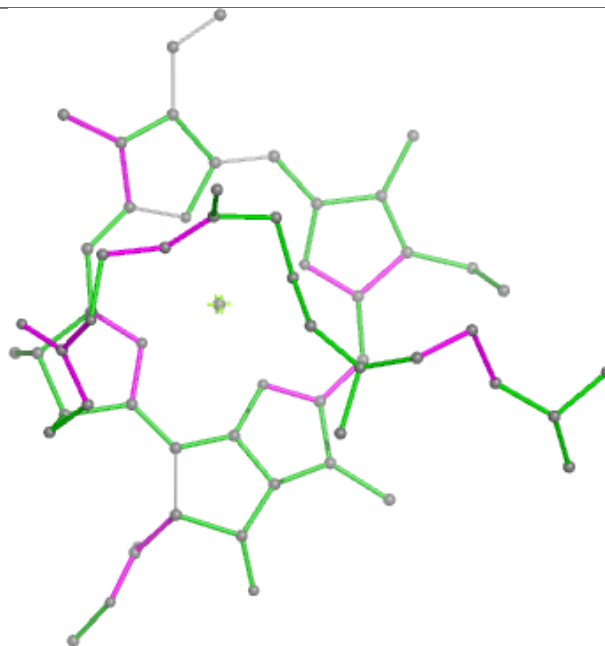




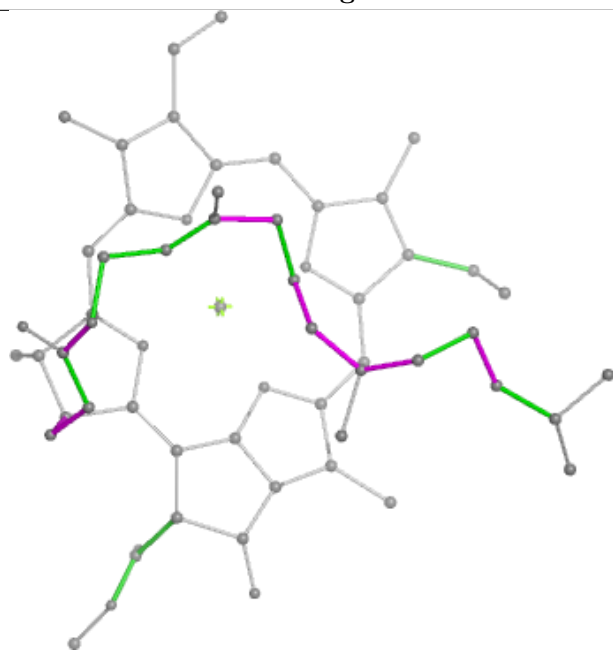
## Ligand CLA B 827



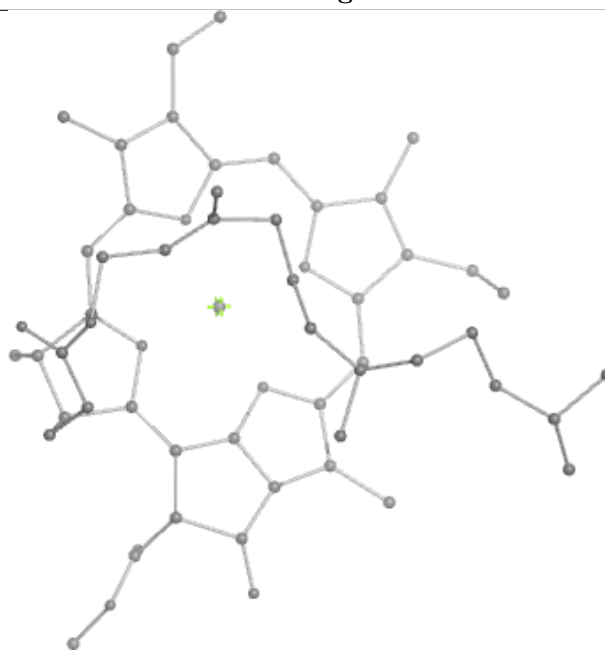
Bond lengths



Bond angles

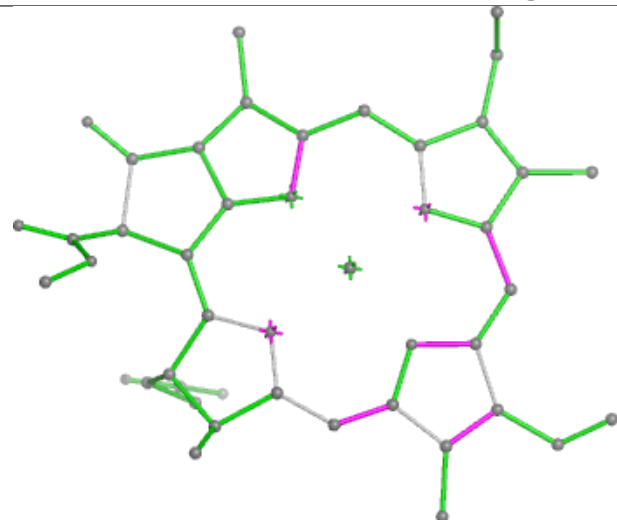


Torsions

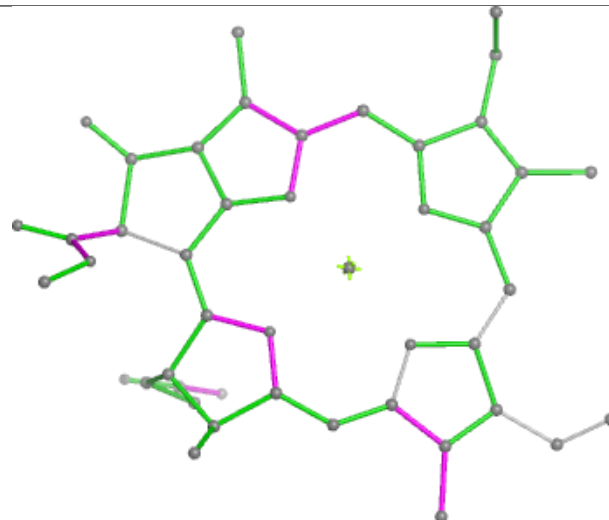


Rings

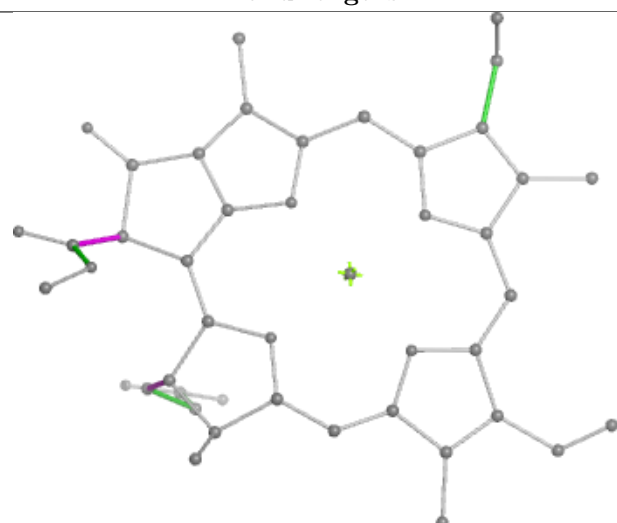
## Ligand CLA 4 304



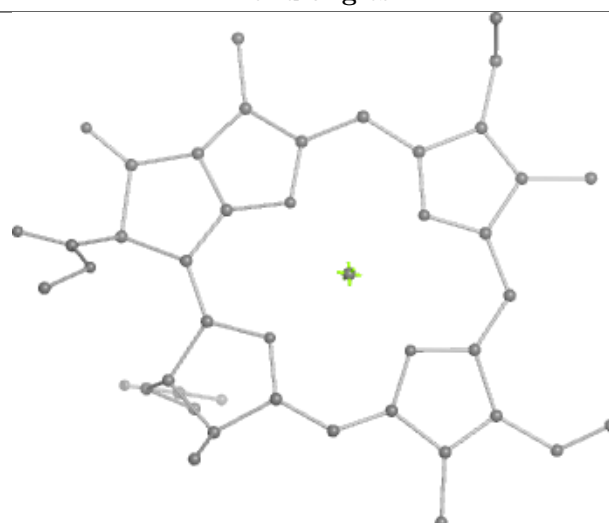
Bond lengths



Bond angles

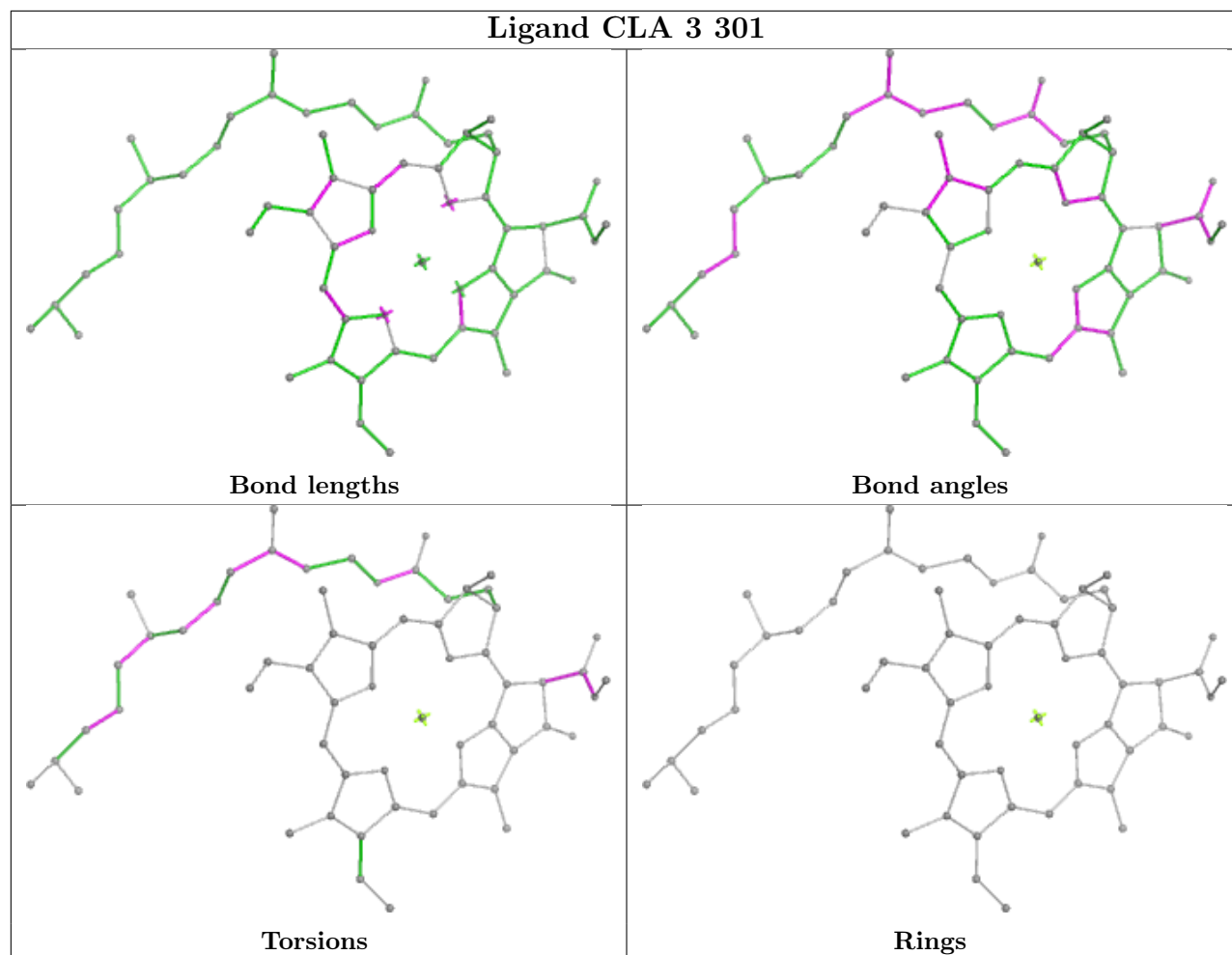


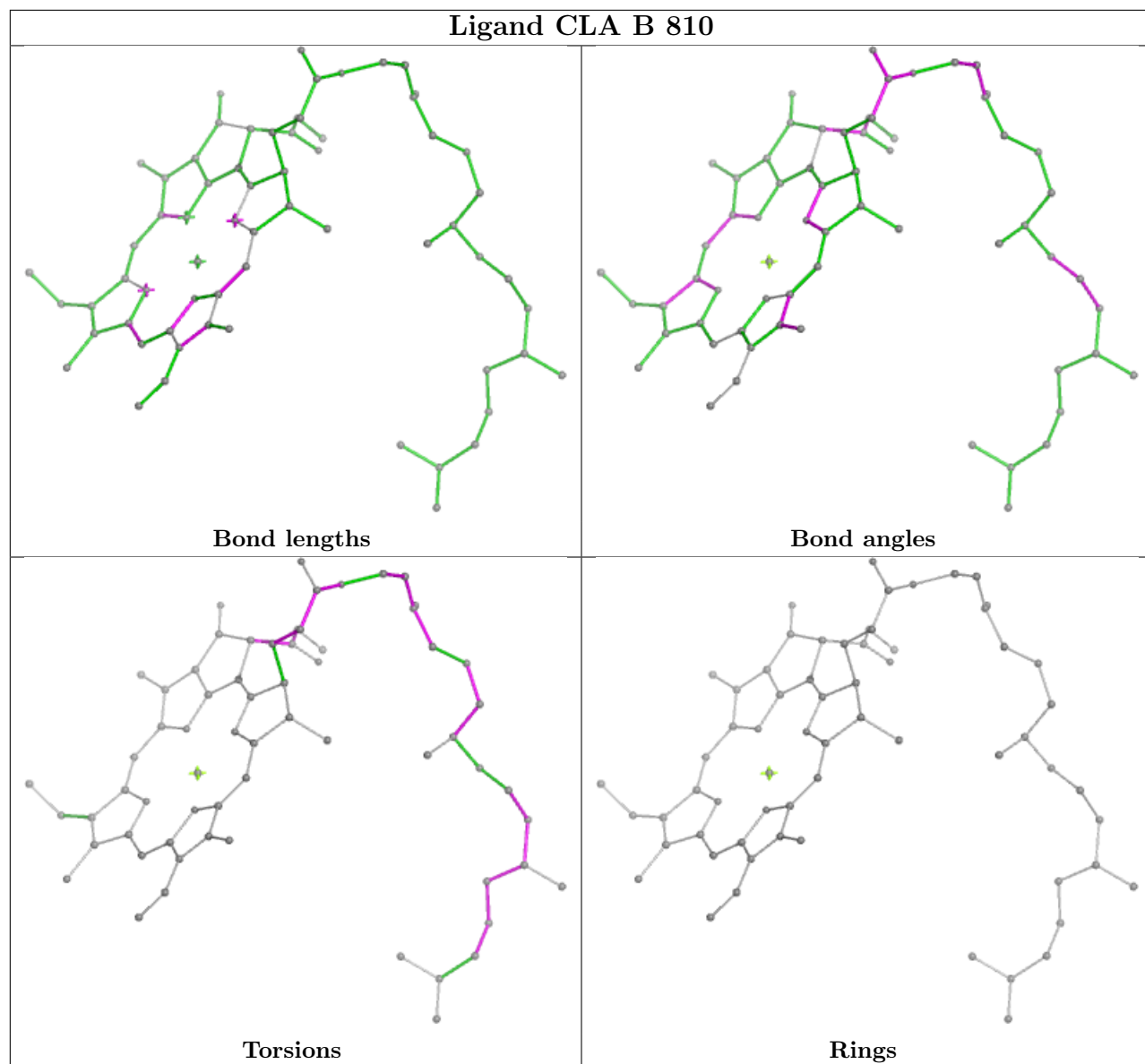
Torsions

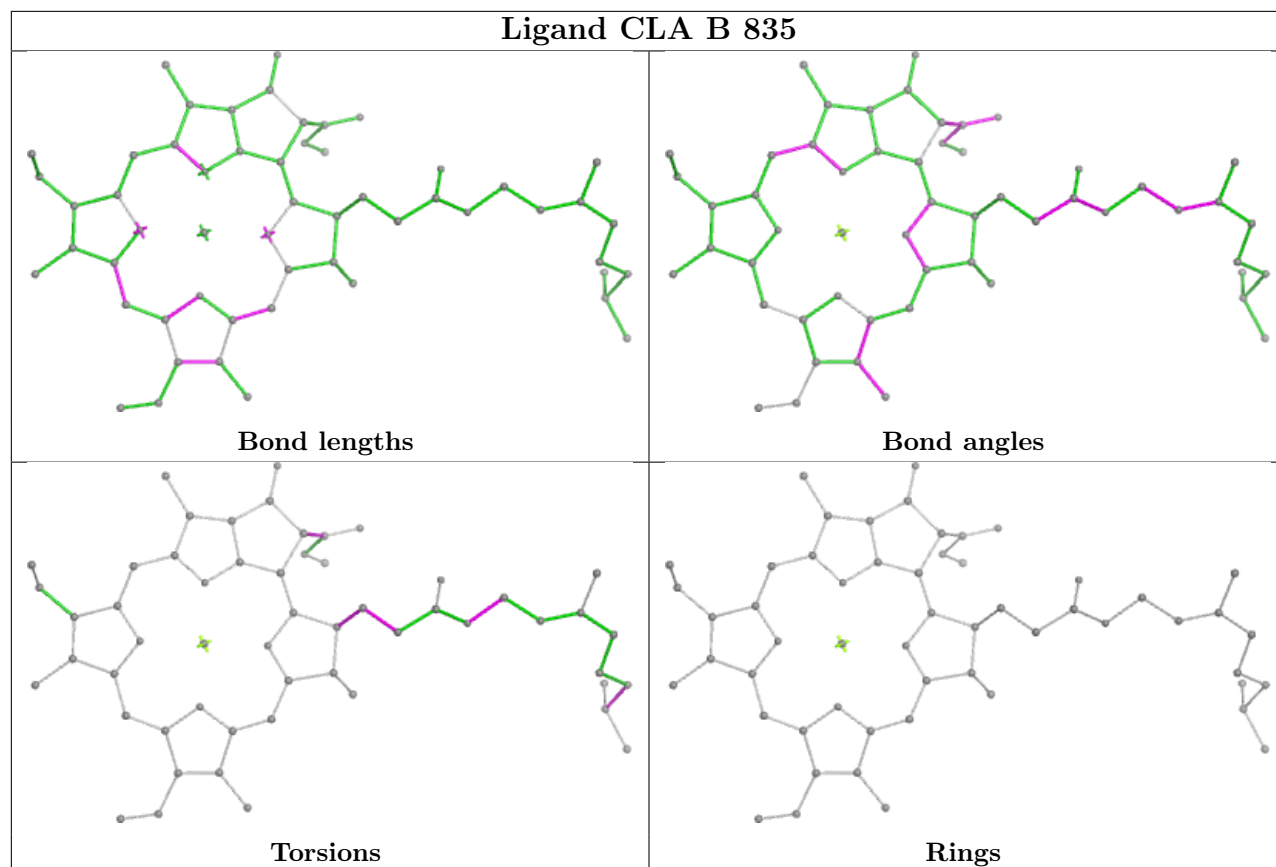
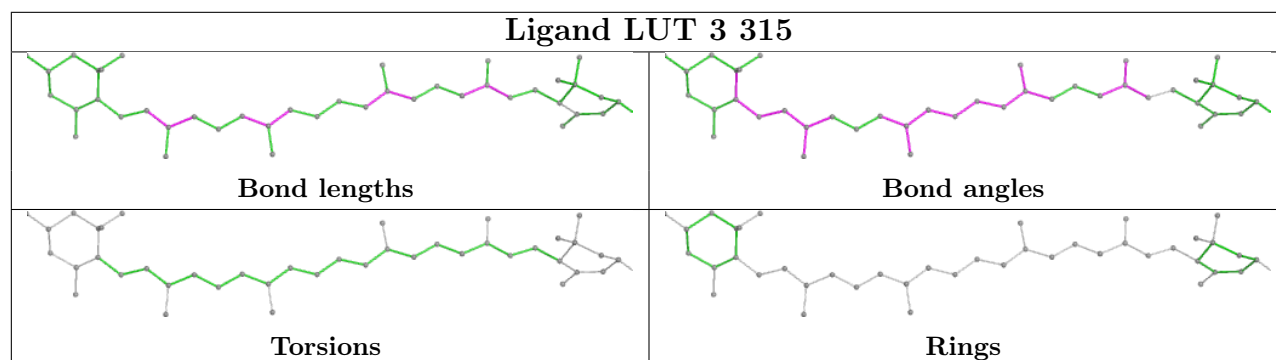
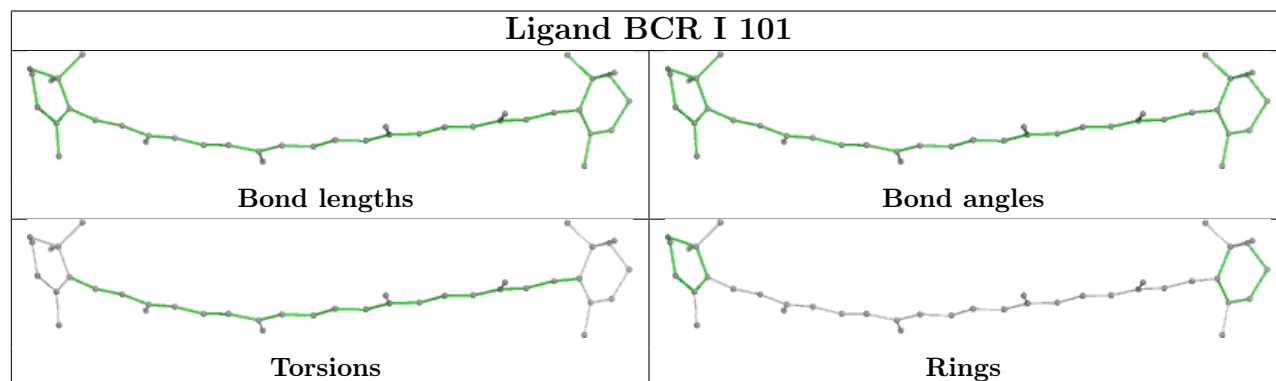


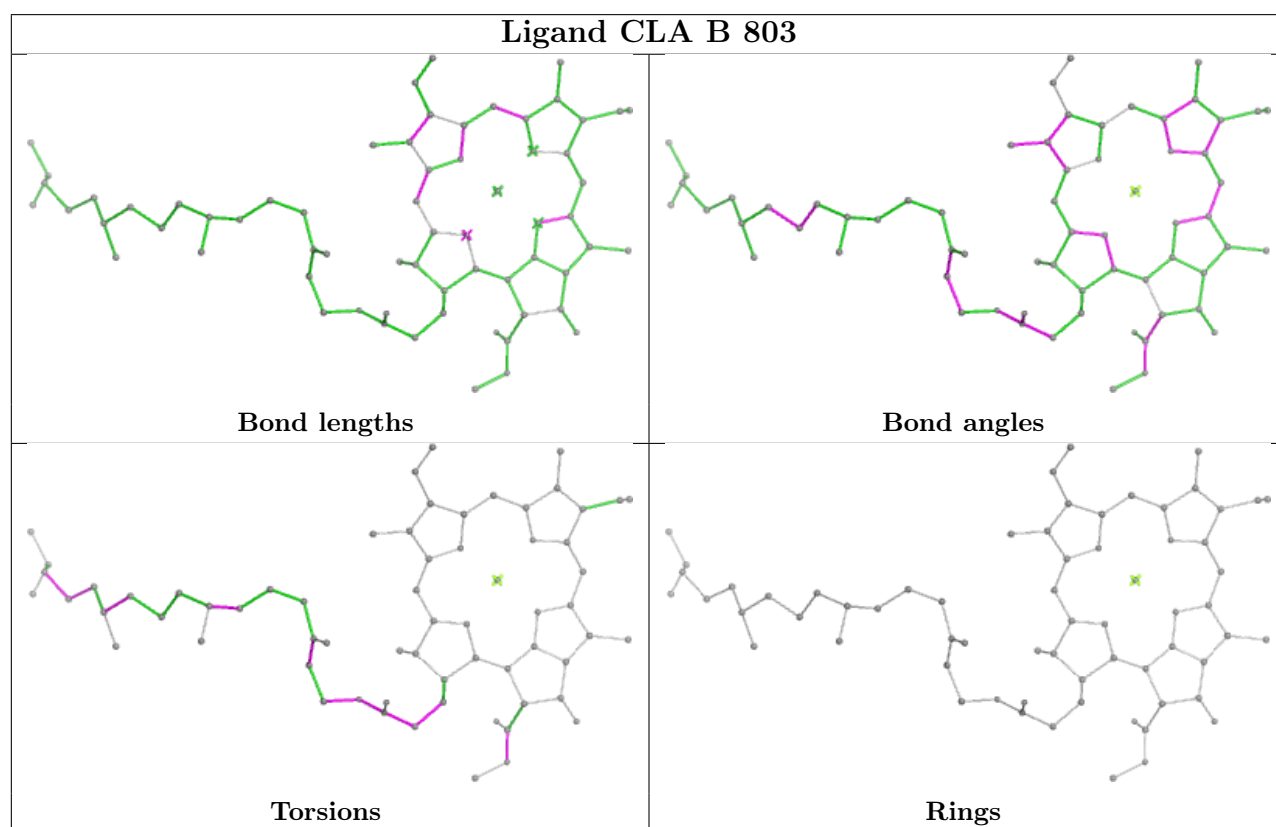
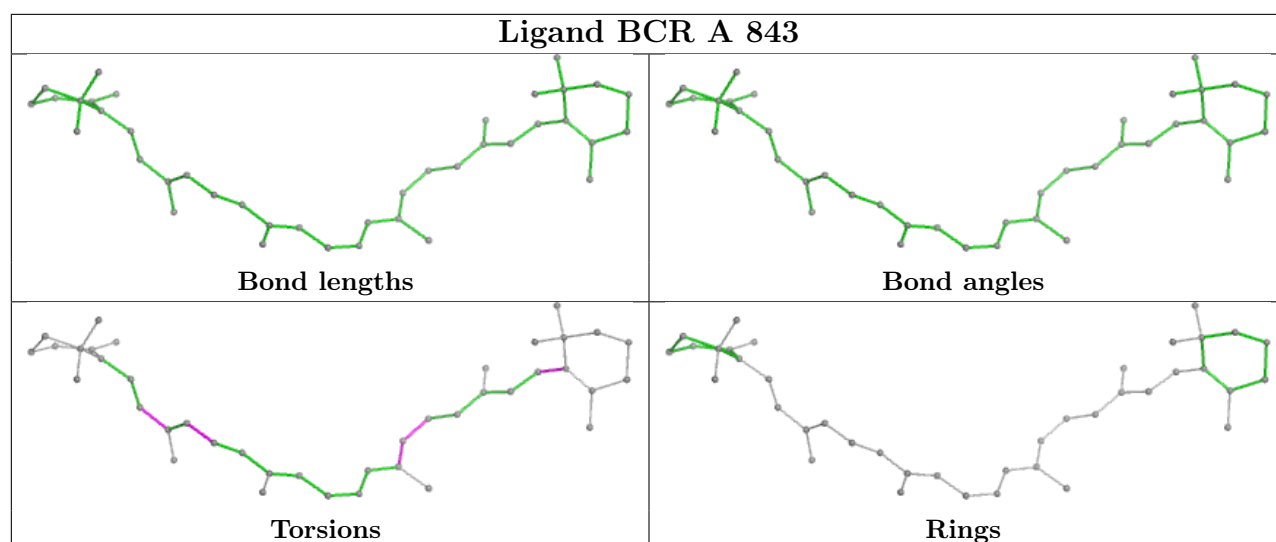
Rings

## Ligand CLA 3 301

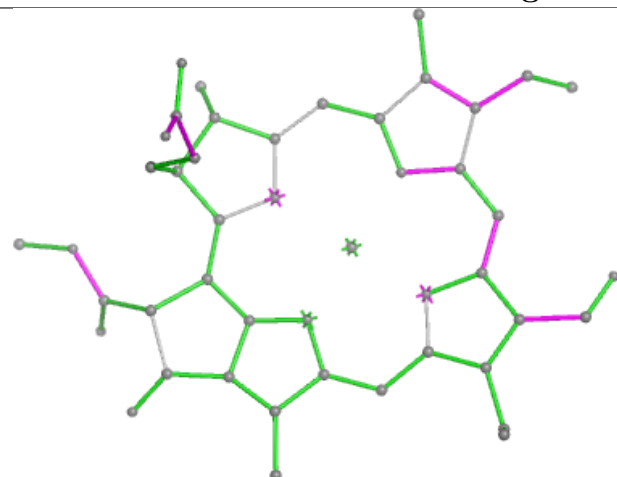




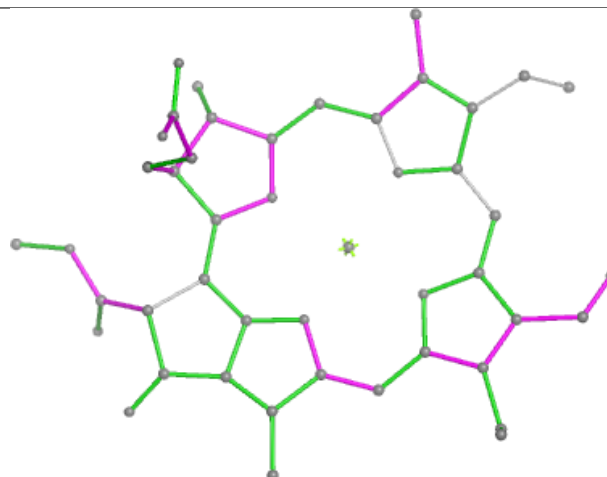
**Ligand CLA B 835****Ligand LUT 3 315****Ligand BCR I 101**



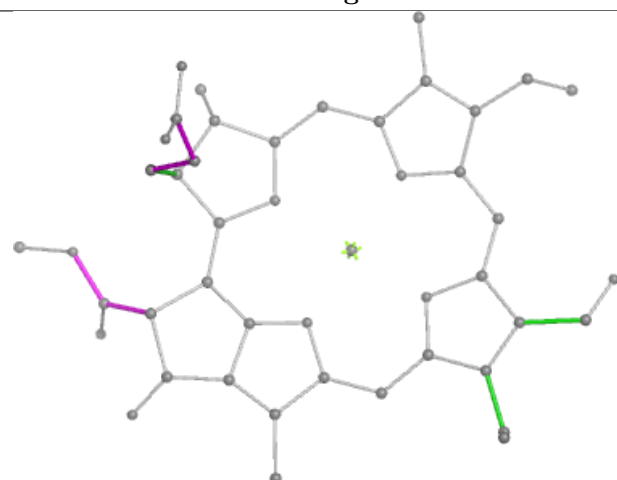
## Ligand CHL 2 307



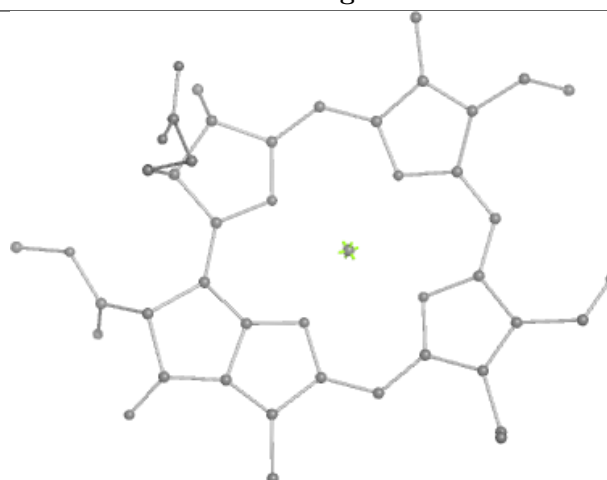
Bond lengths



Bond angles

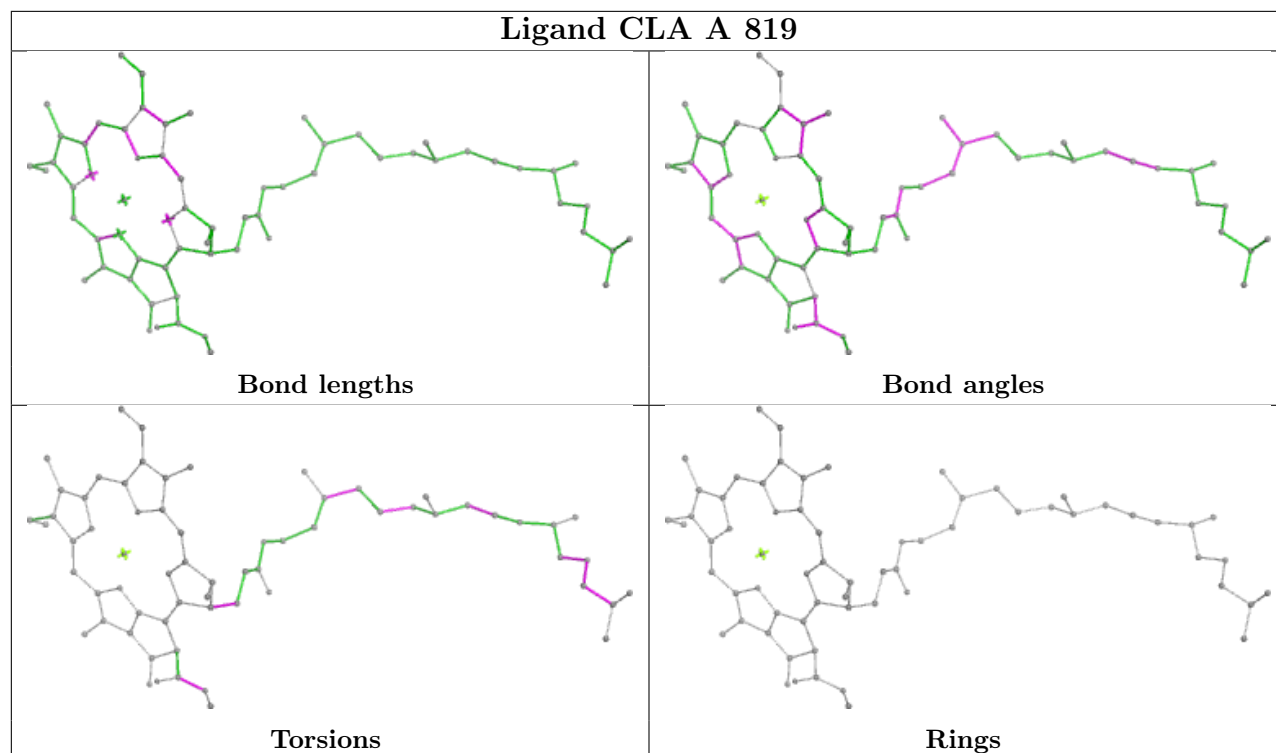


Torsions

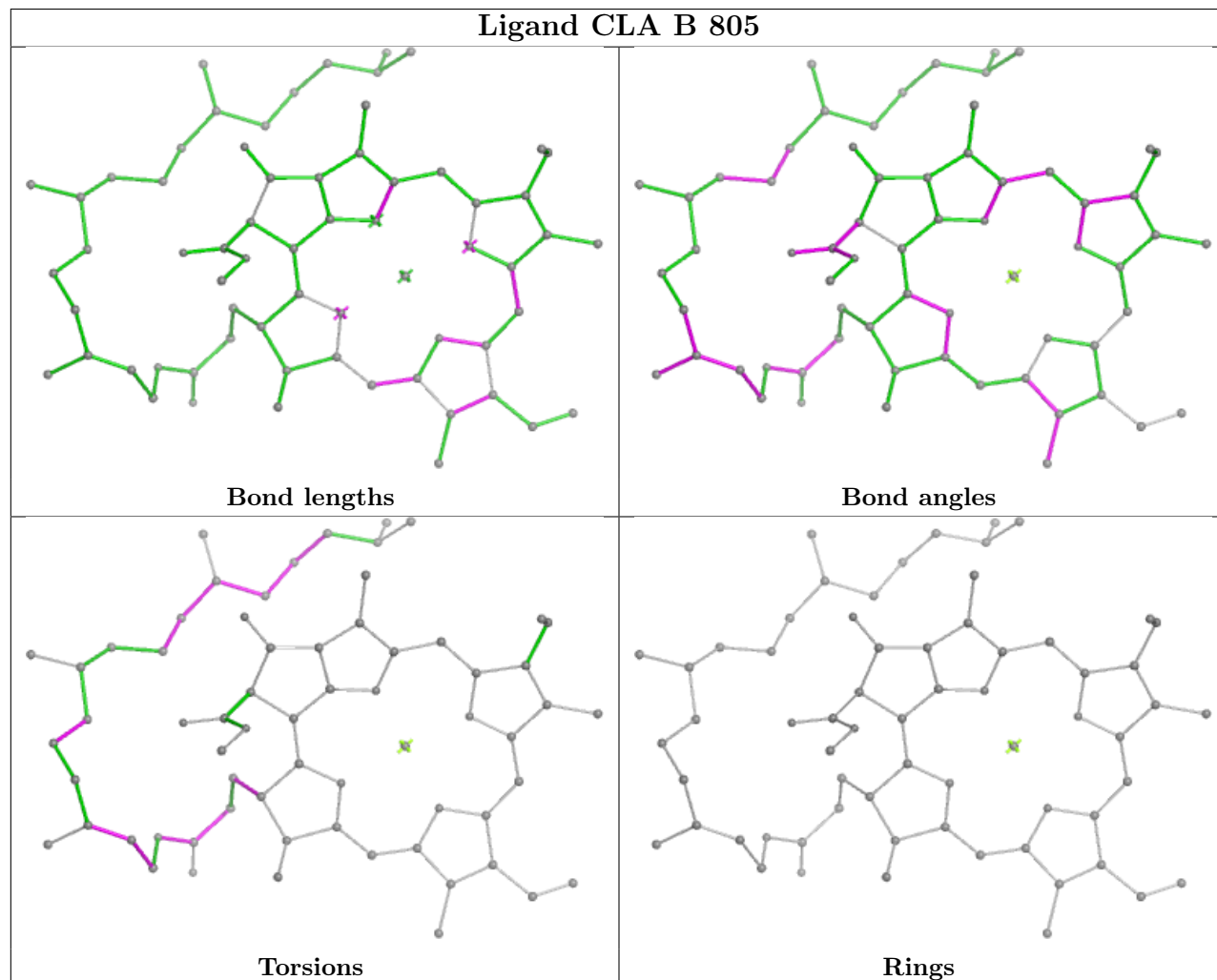


Rings

## Ligand CLA A 819

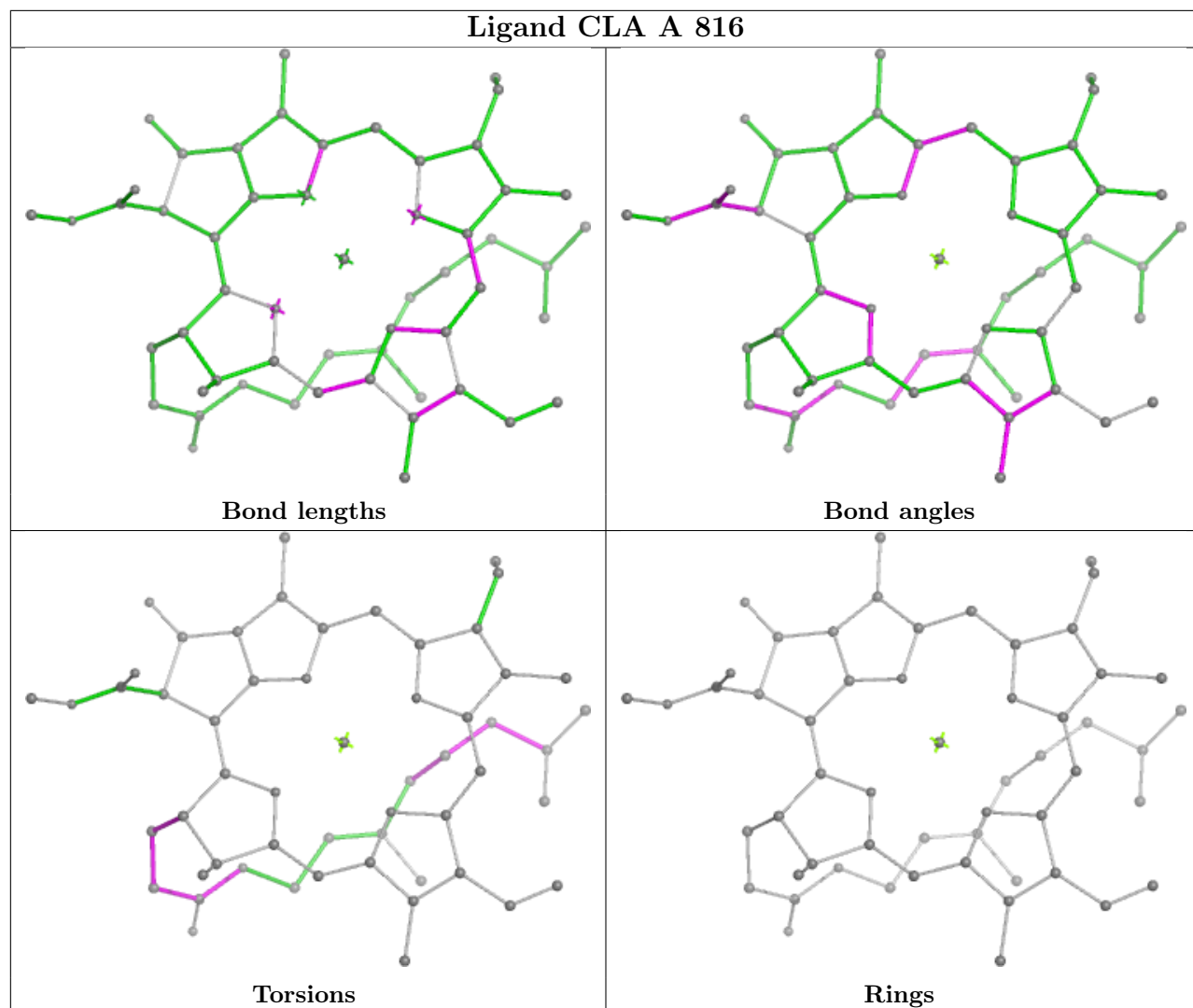


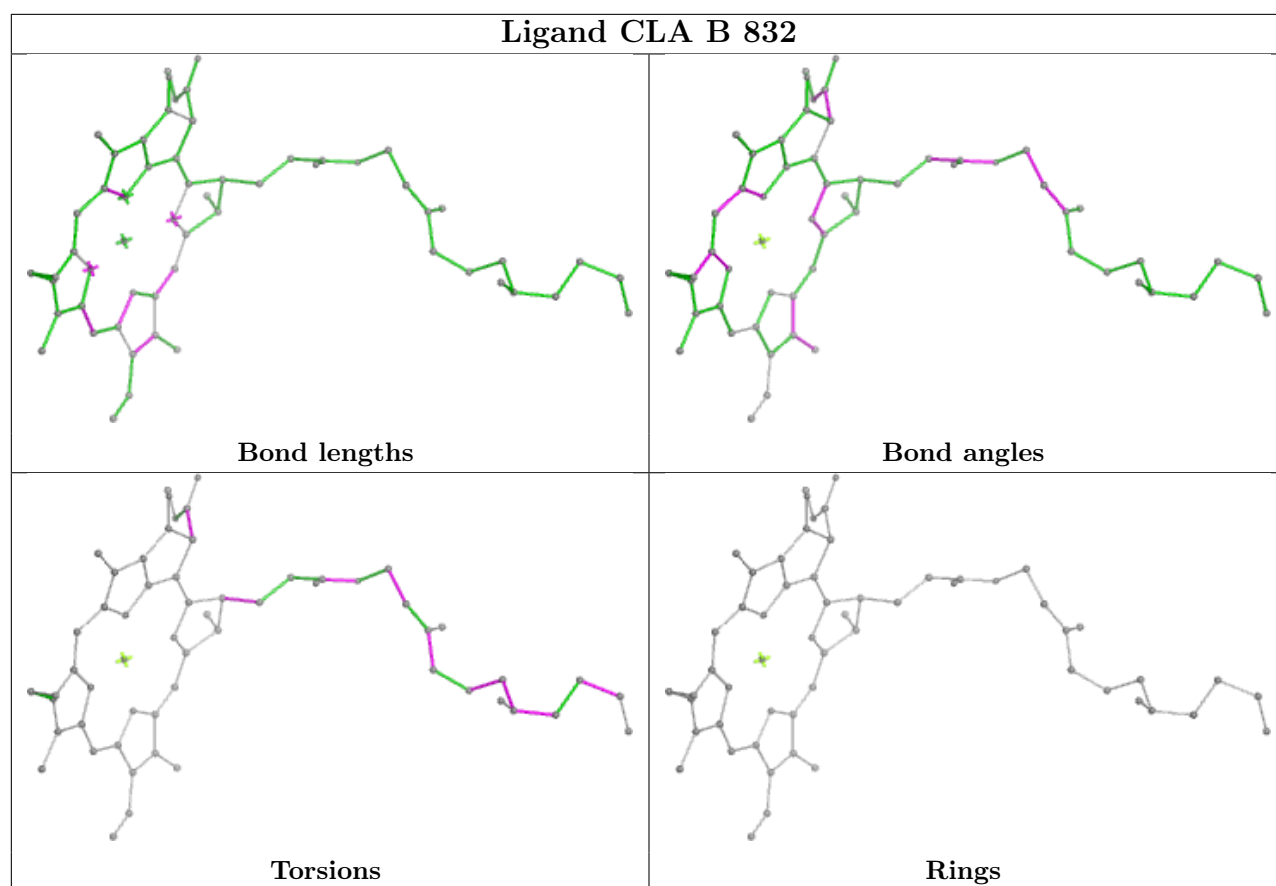
## Ligand CLA B 805



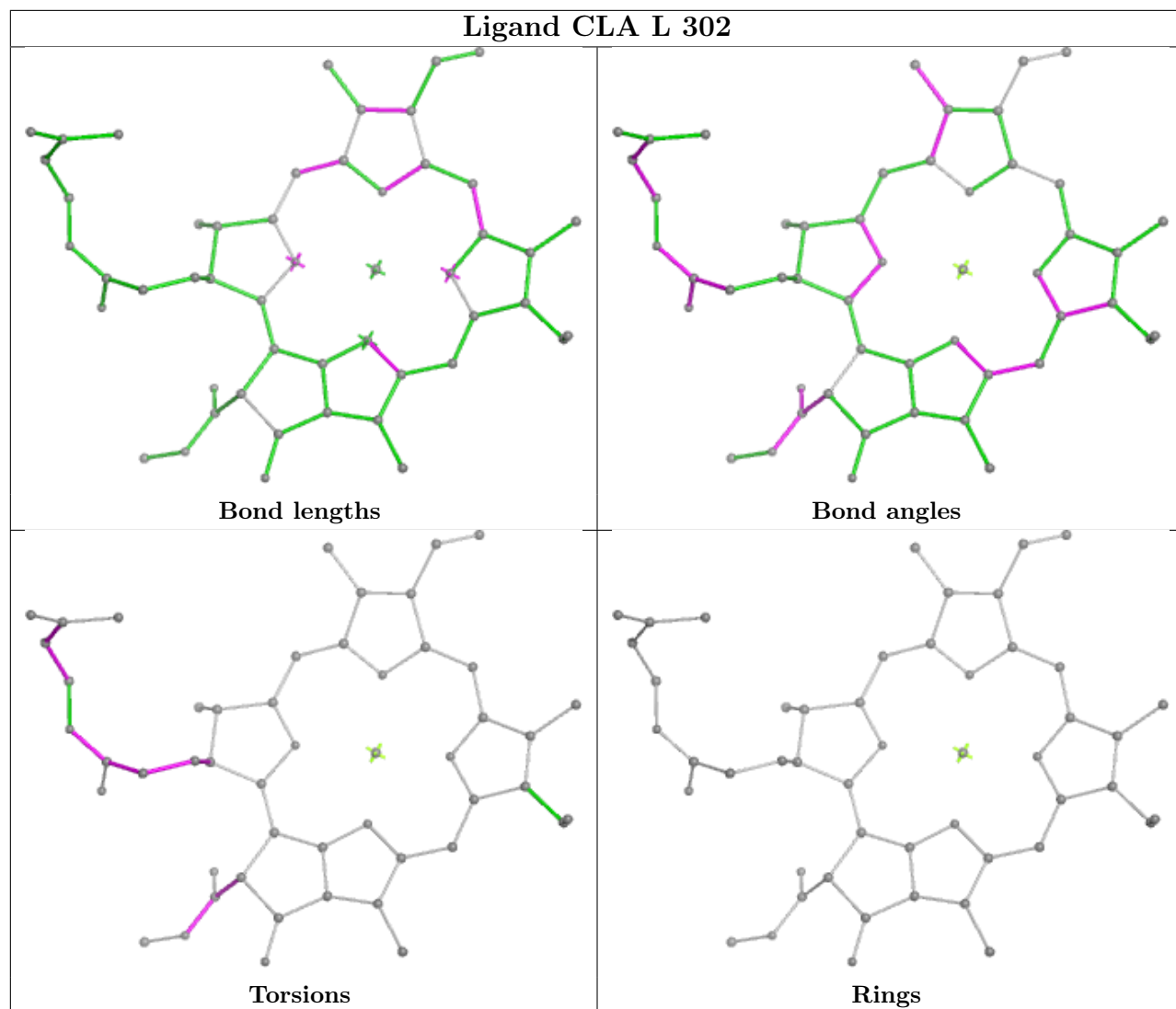


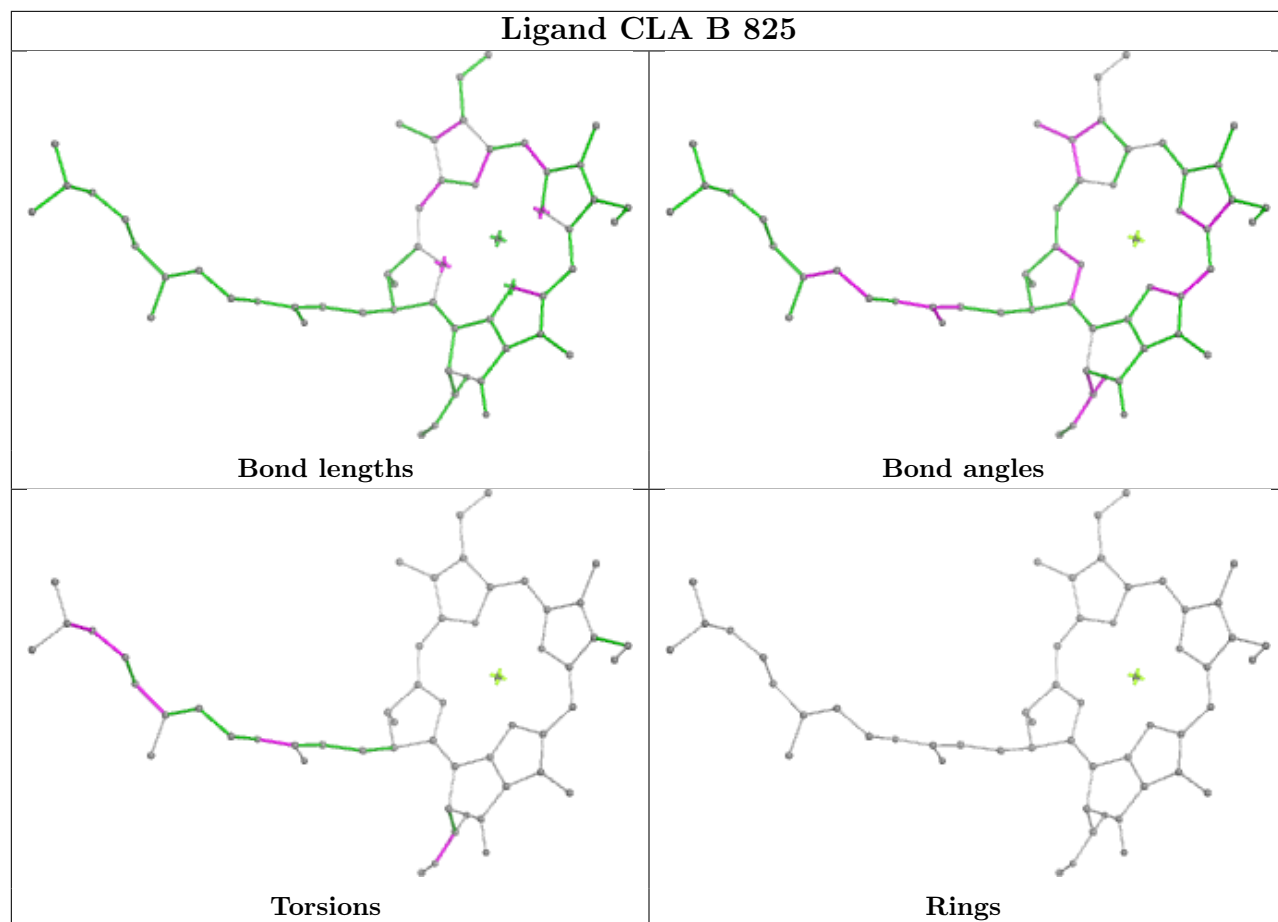
## Ligand CLA A 816



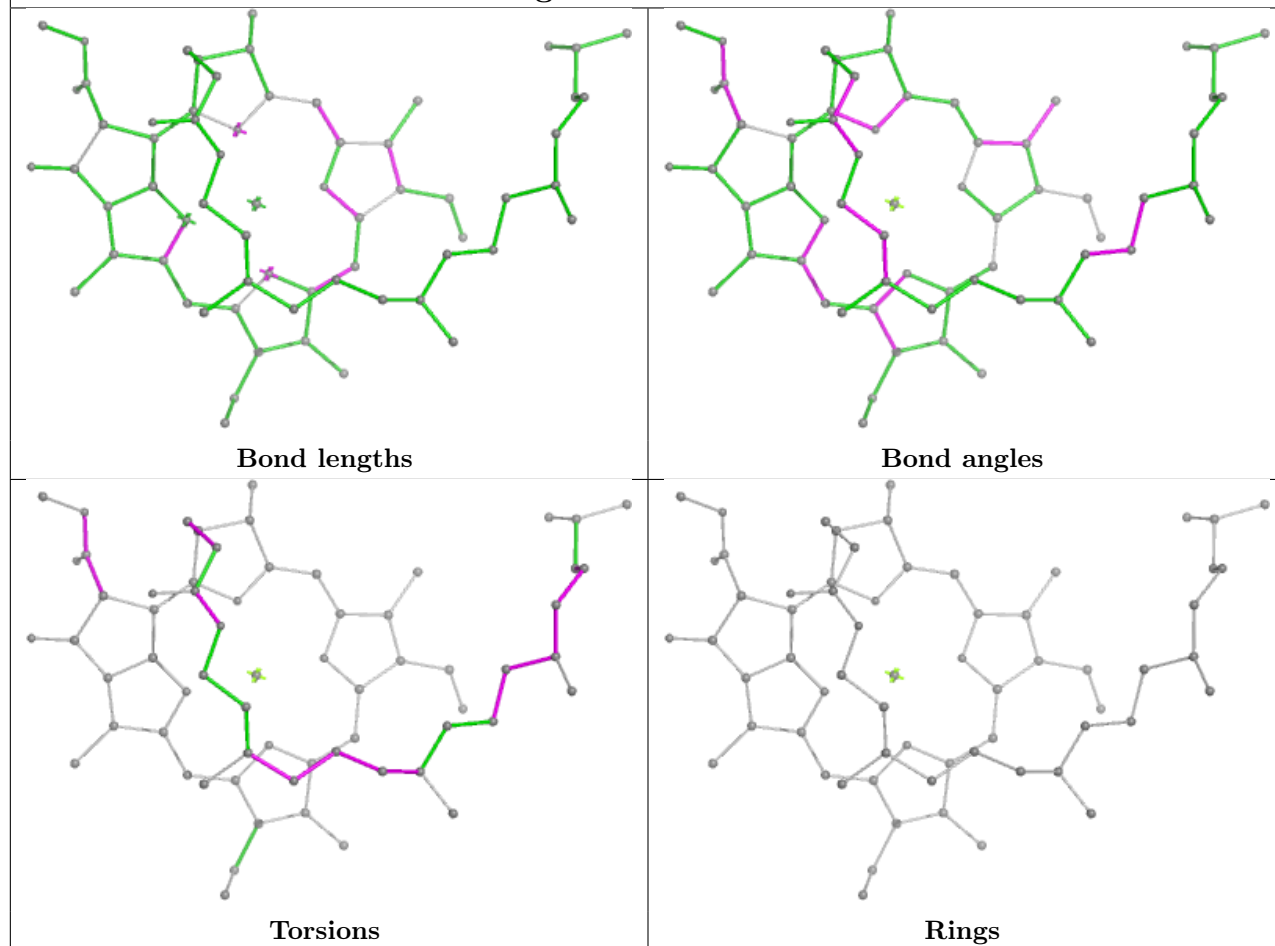


## Ligand CLA L 302

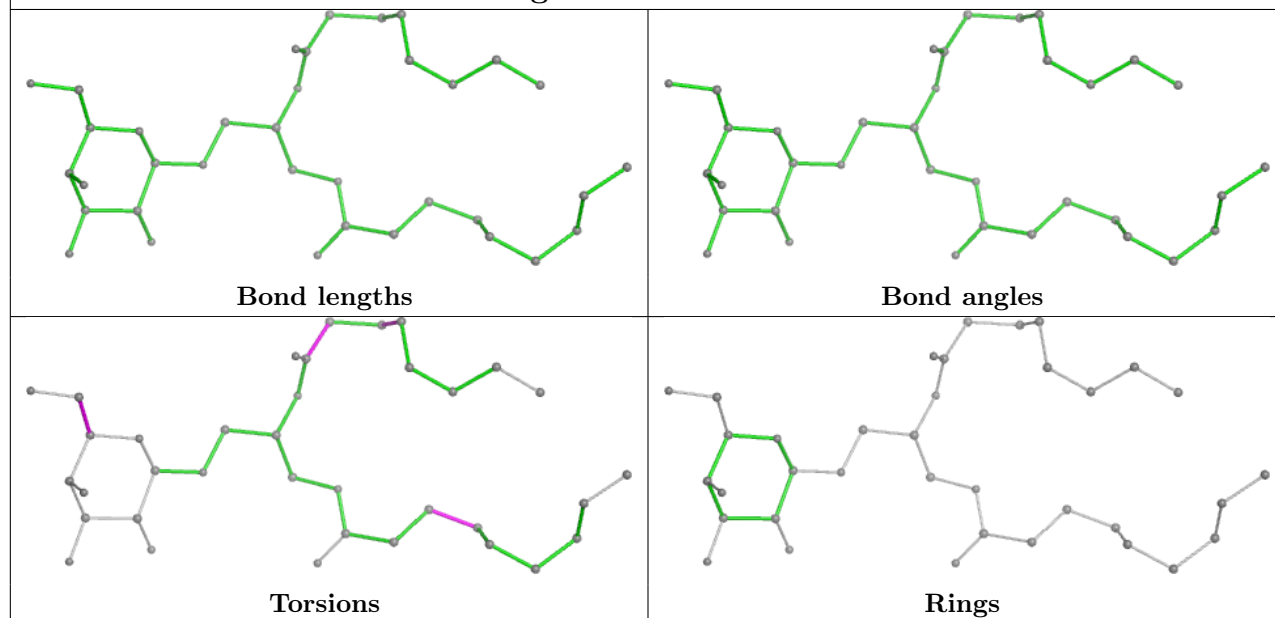


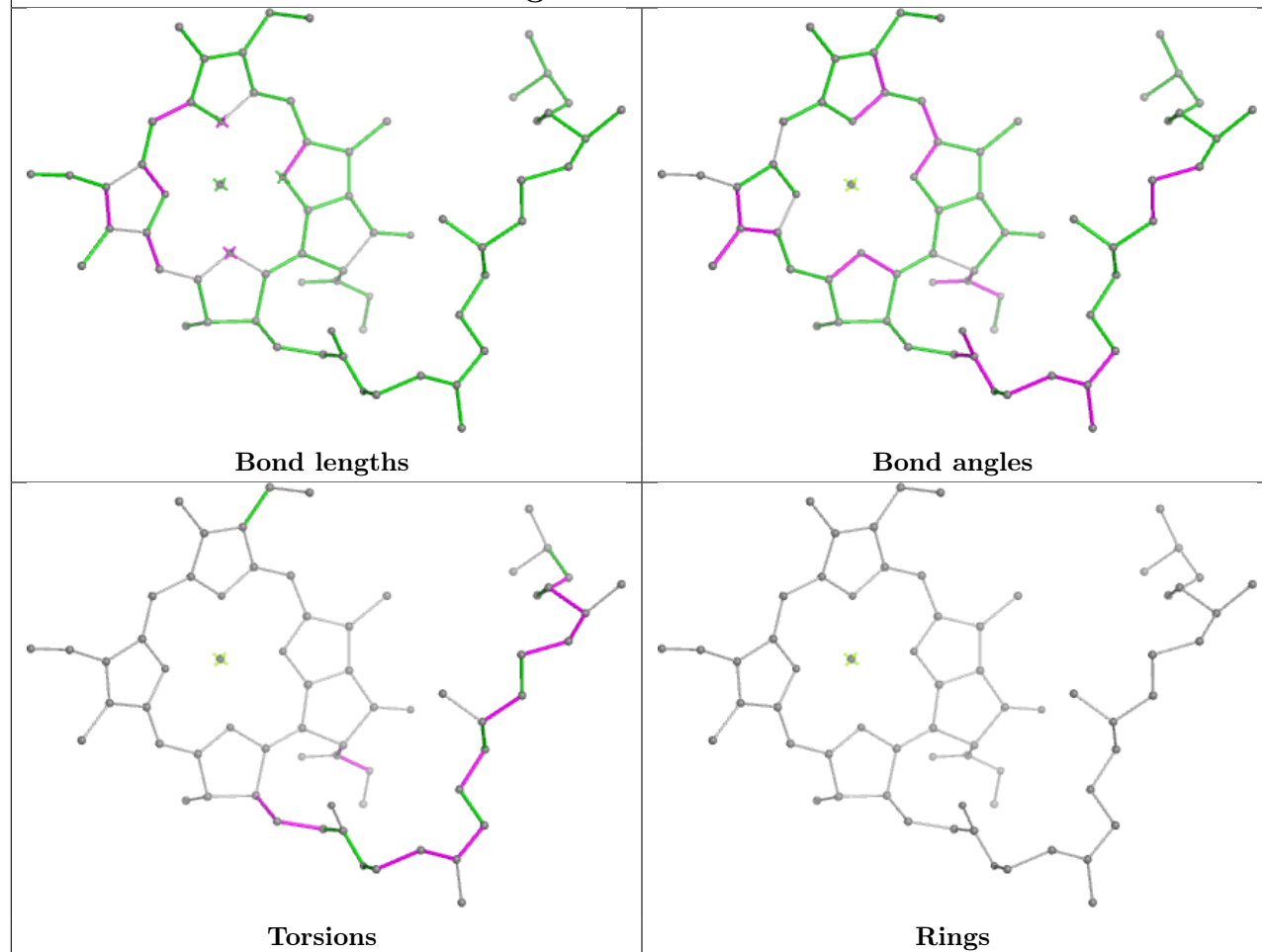
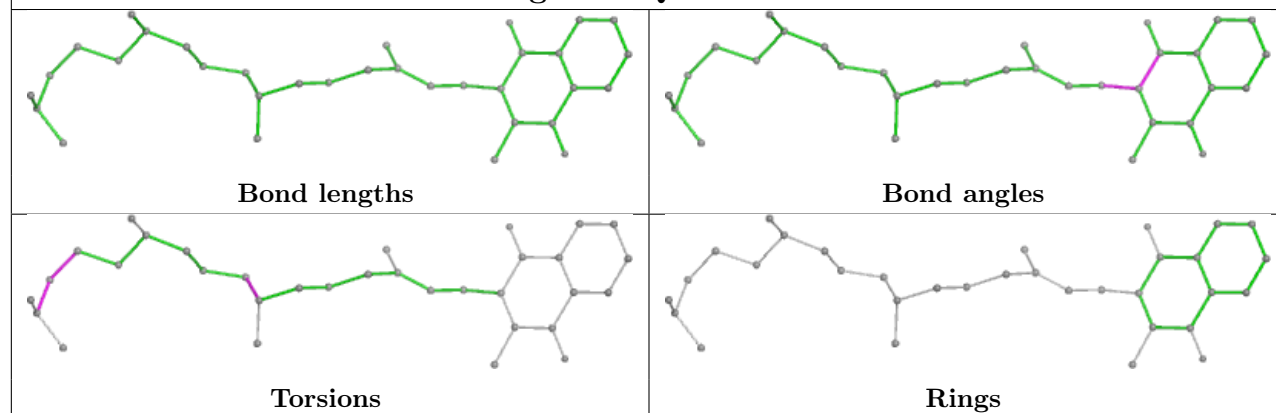


## Ligand CLA 2 312

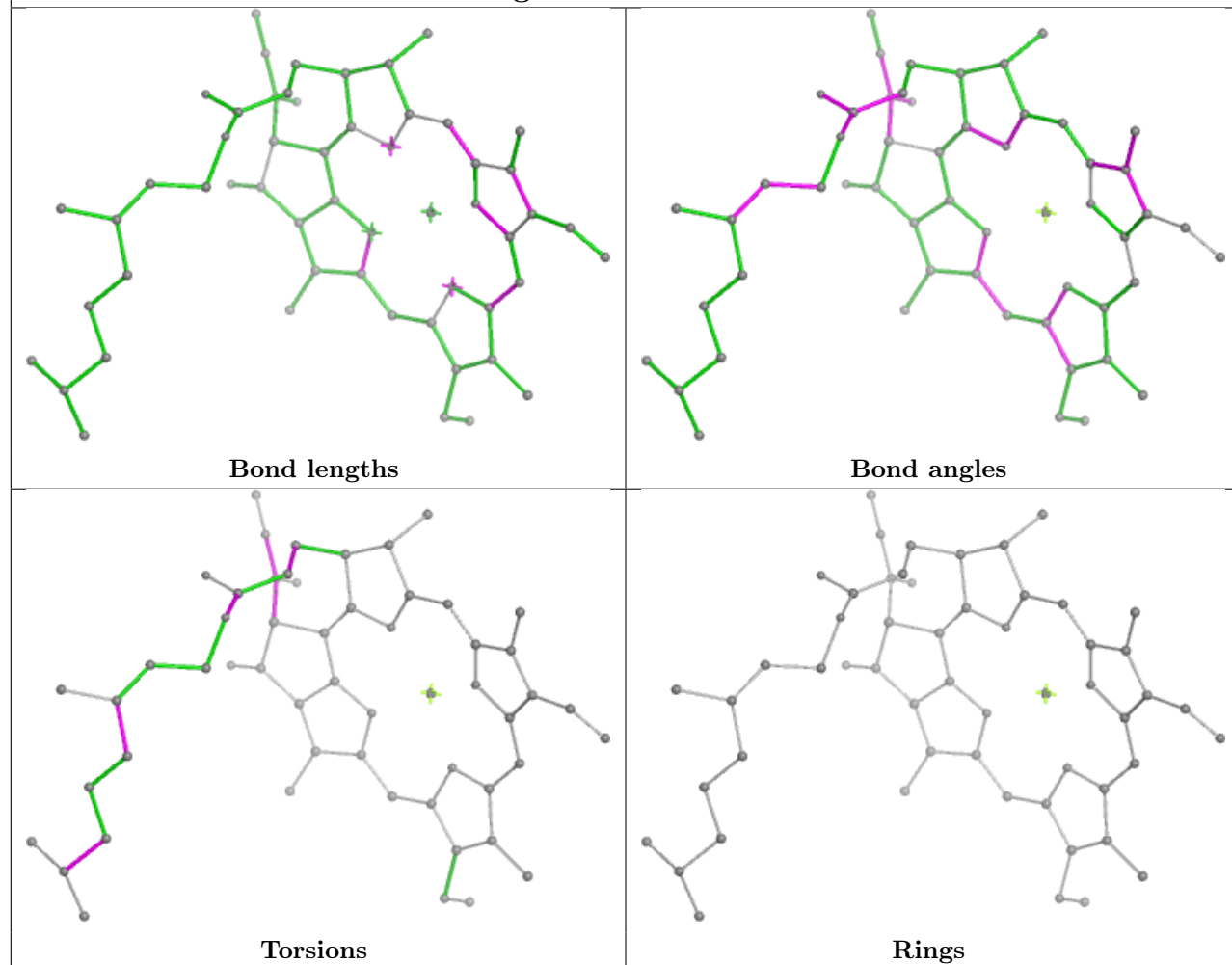


## Ligand LMG 4 318

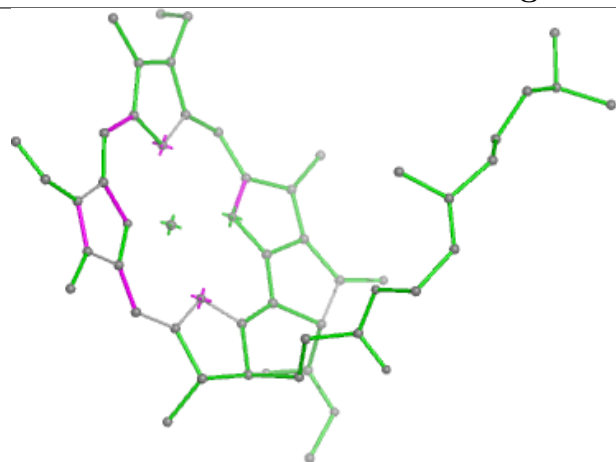


**Ligand CLA B 851****Ligand PQN A 841**

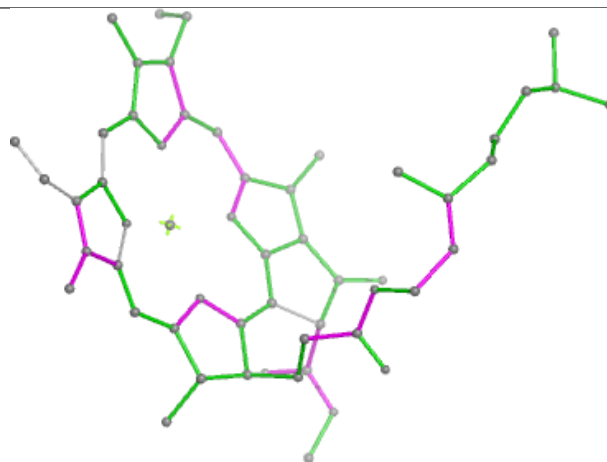
## Ligand CLA B 822



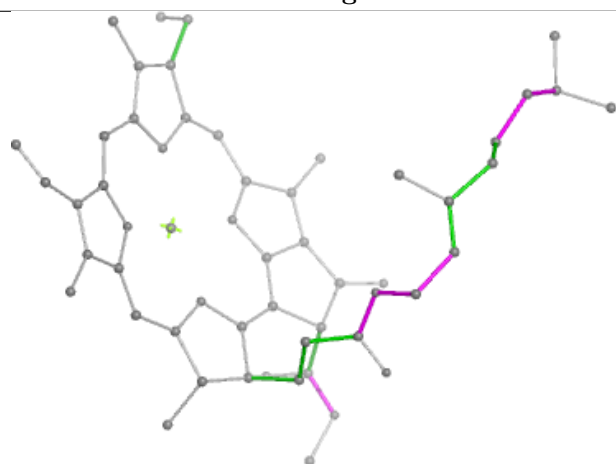
## Ligand CLA 1 310



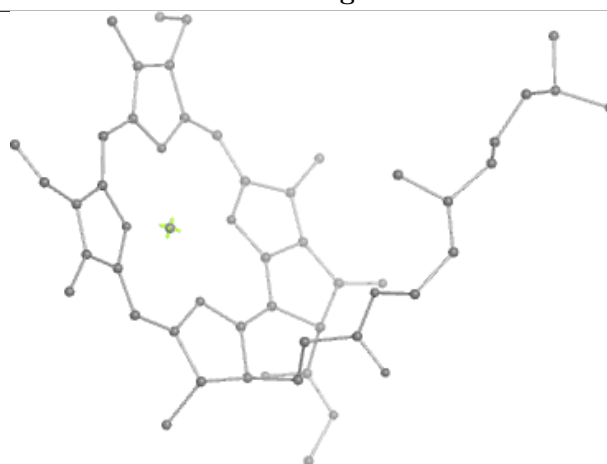
Bond lengths



Bond angles



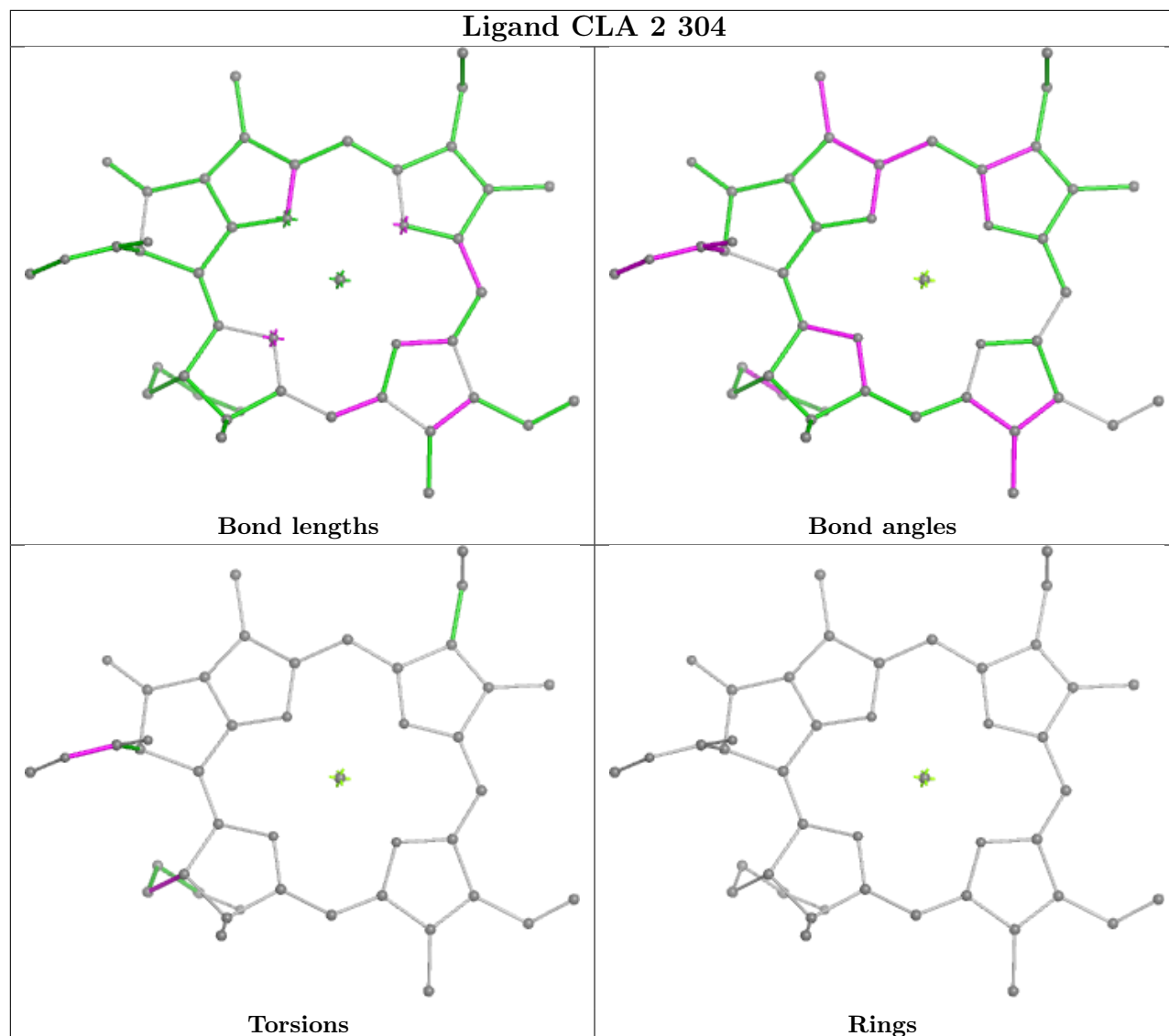
Torsions



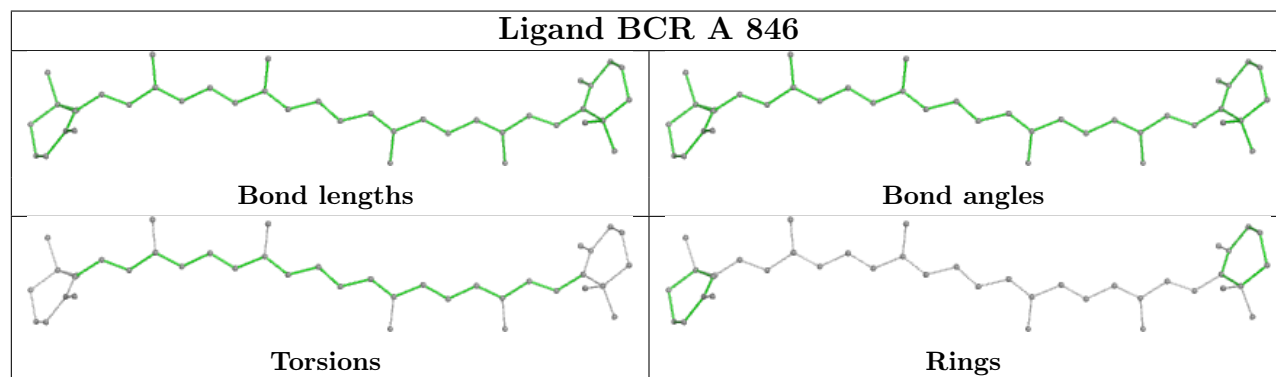
Rings



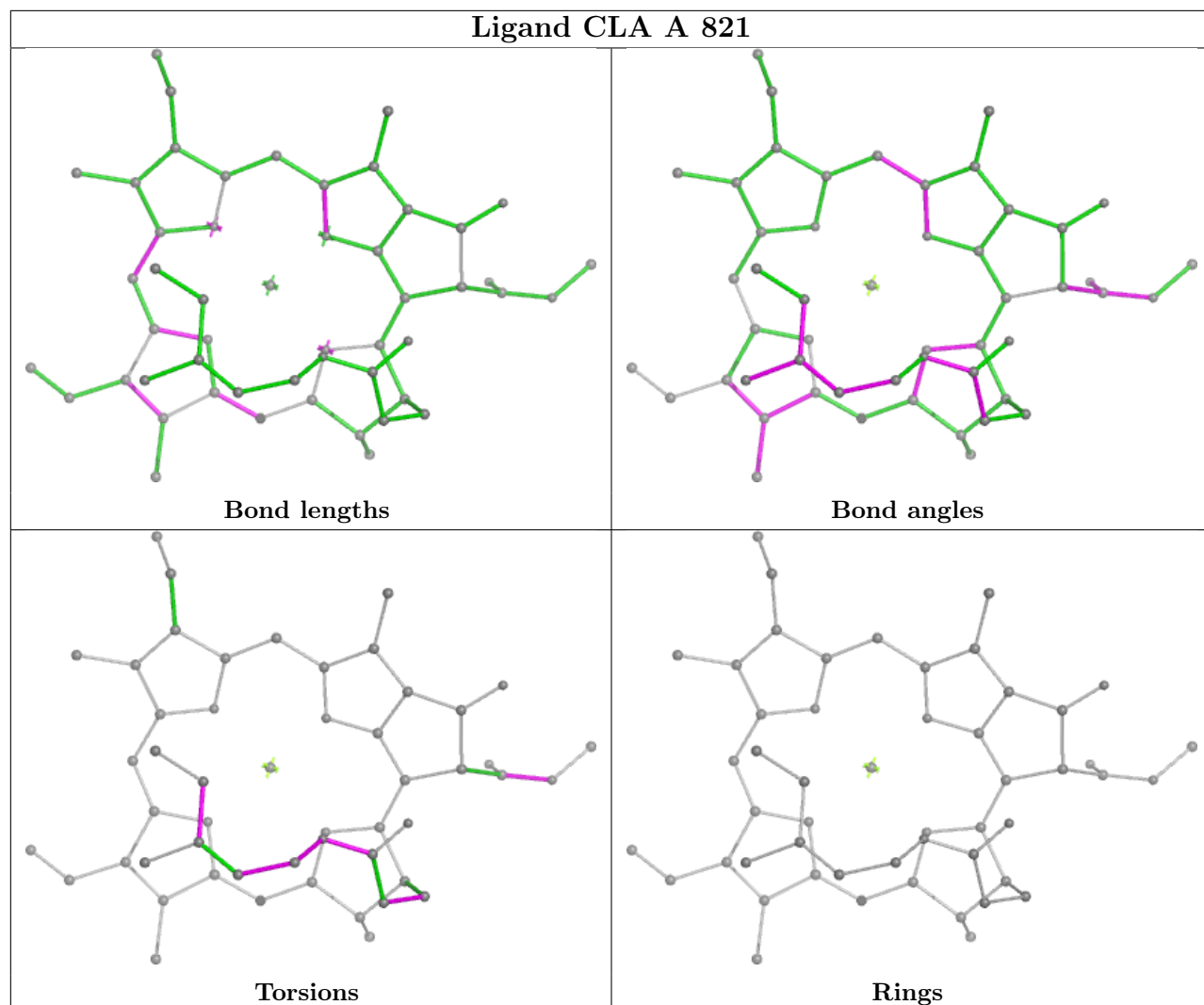
## Ligand CLA 2 304

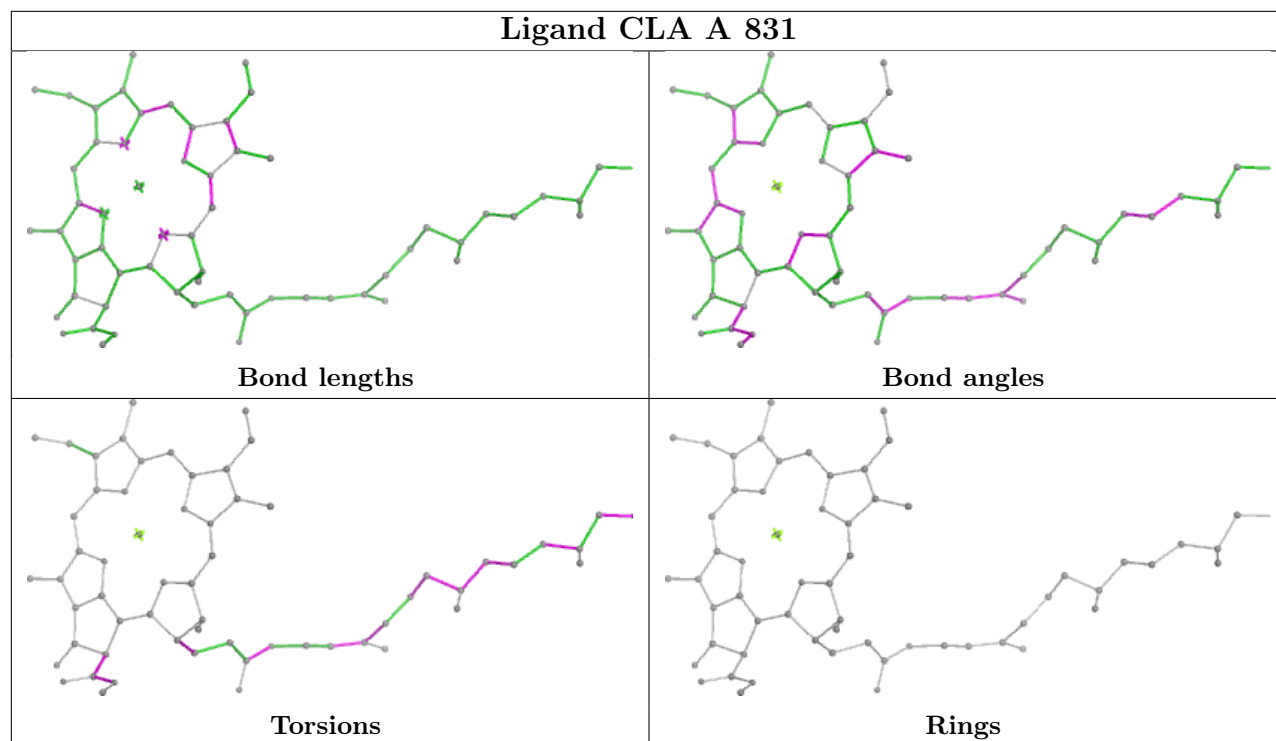
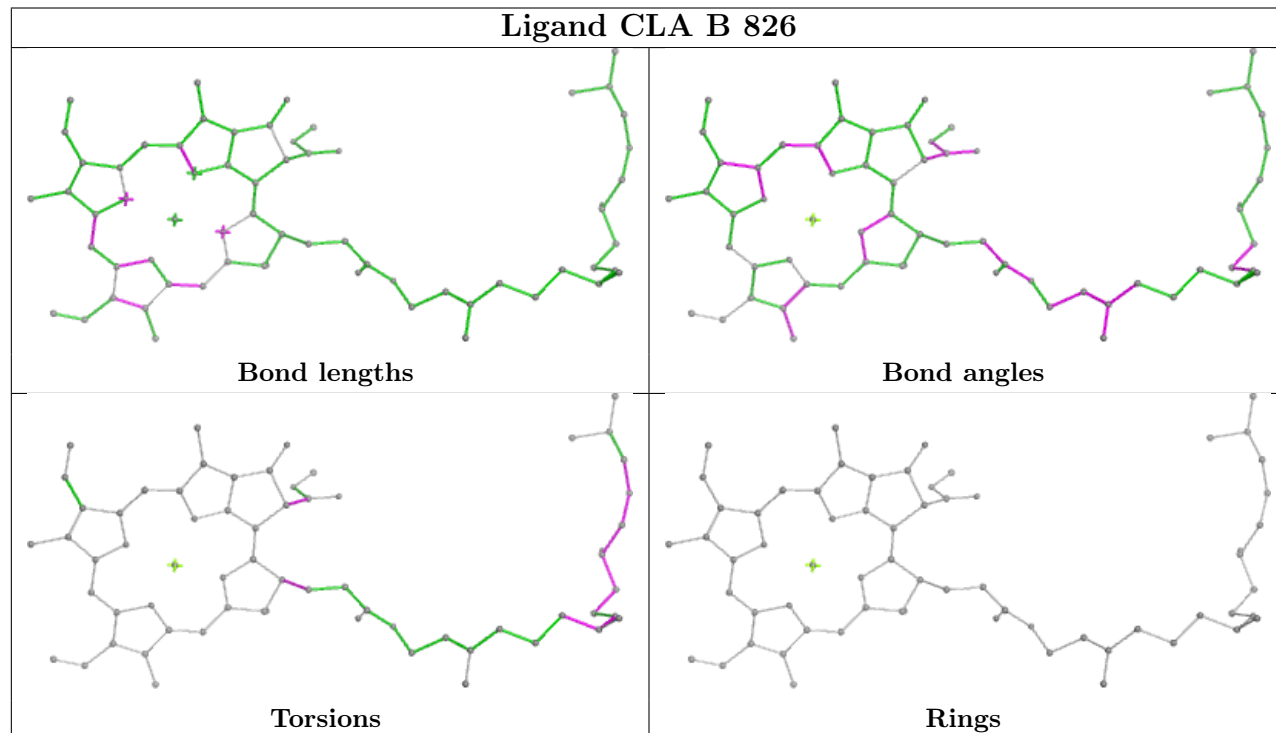


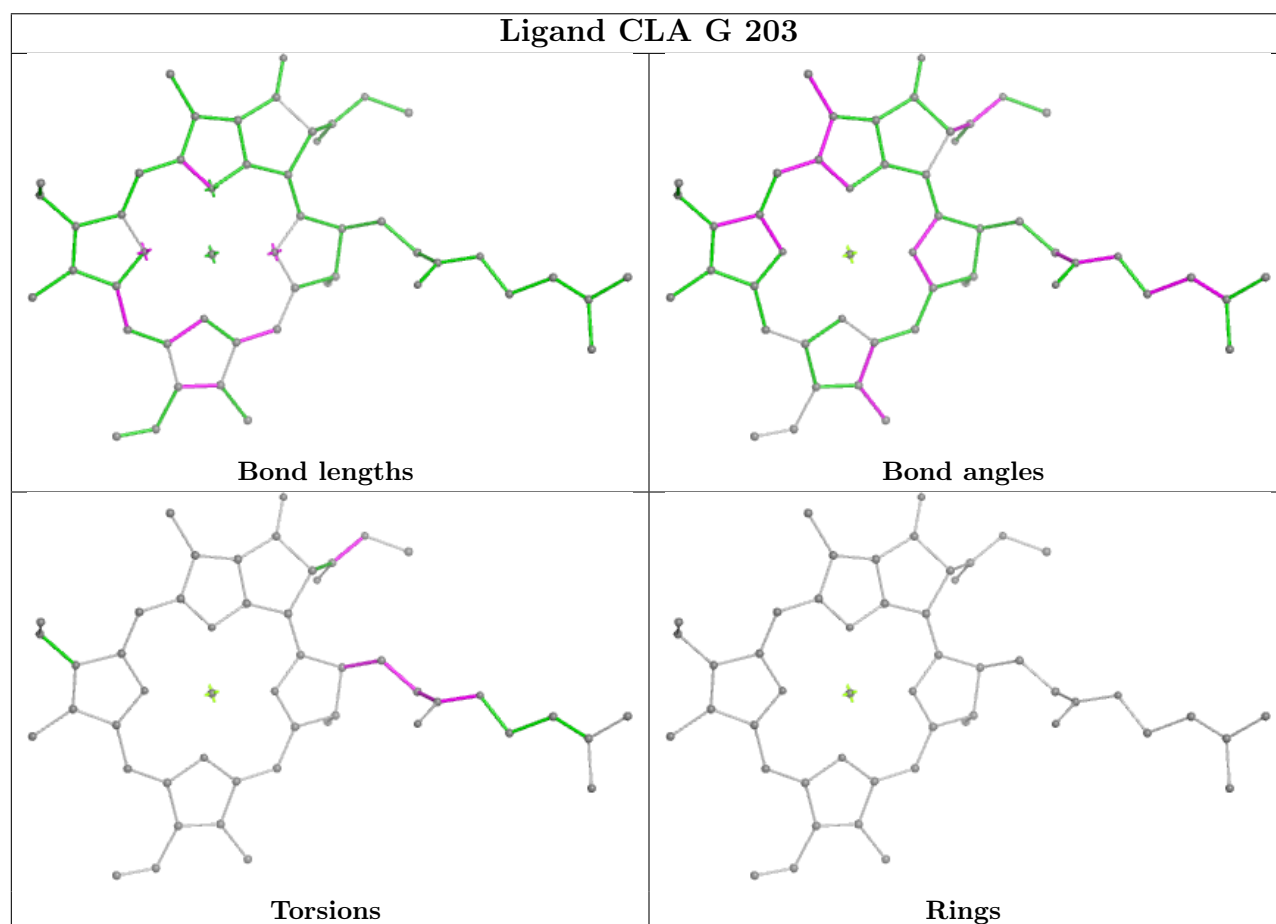
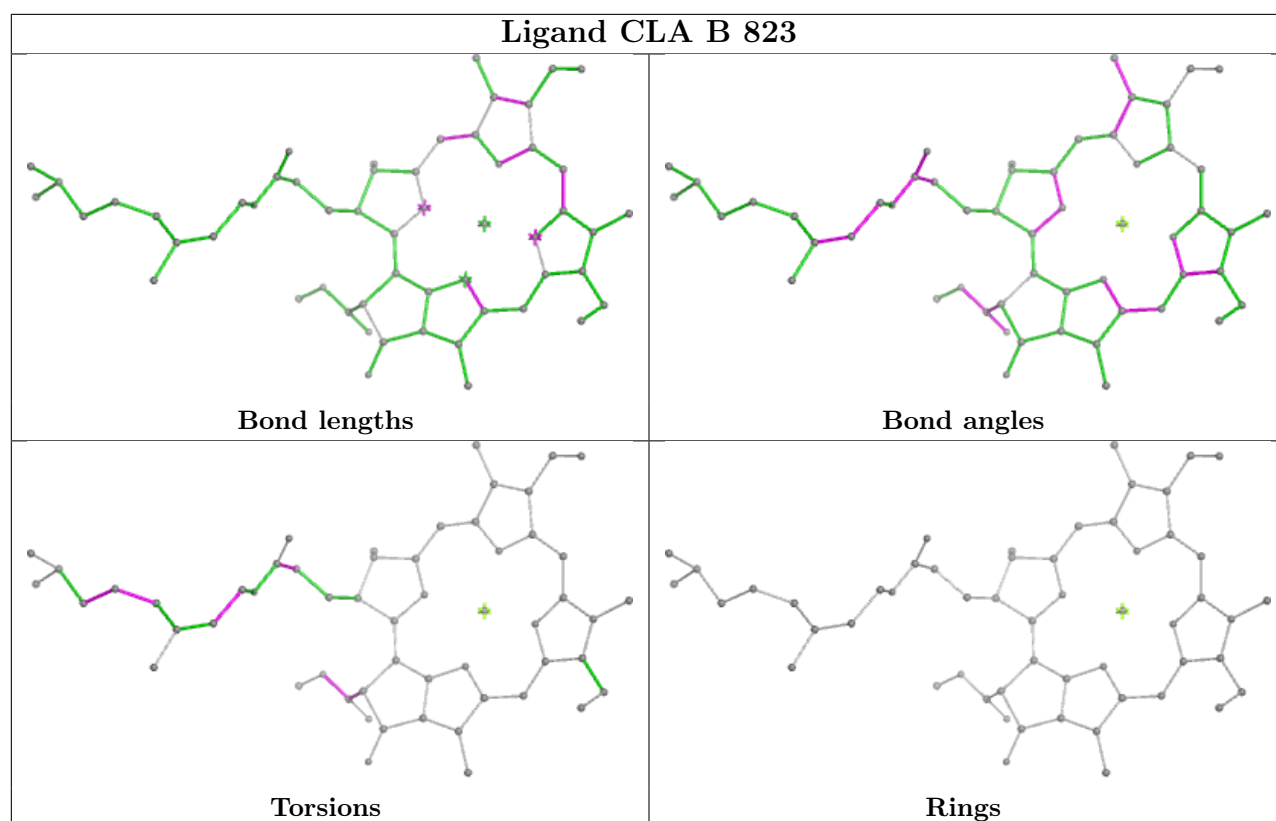
## Ligand BCR A 846

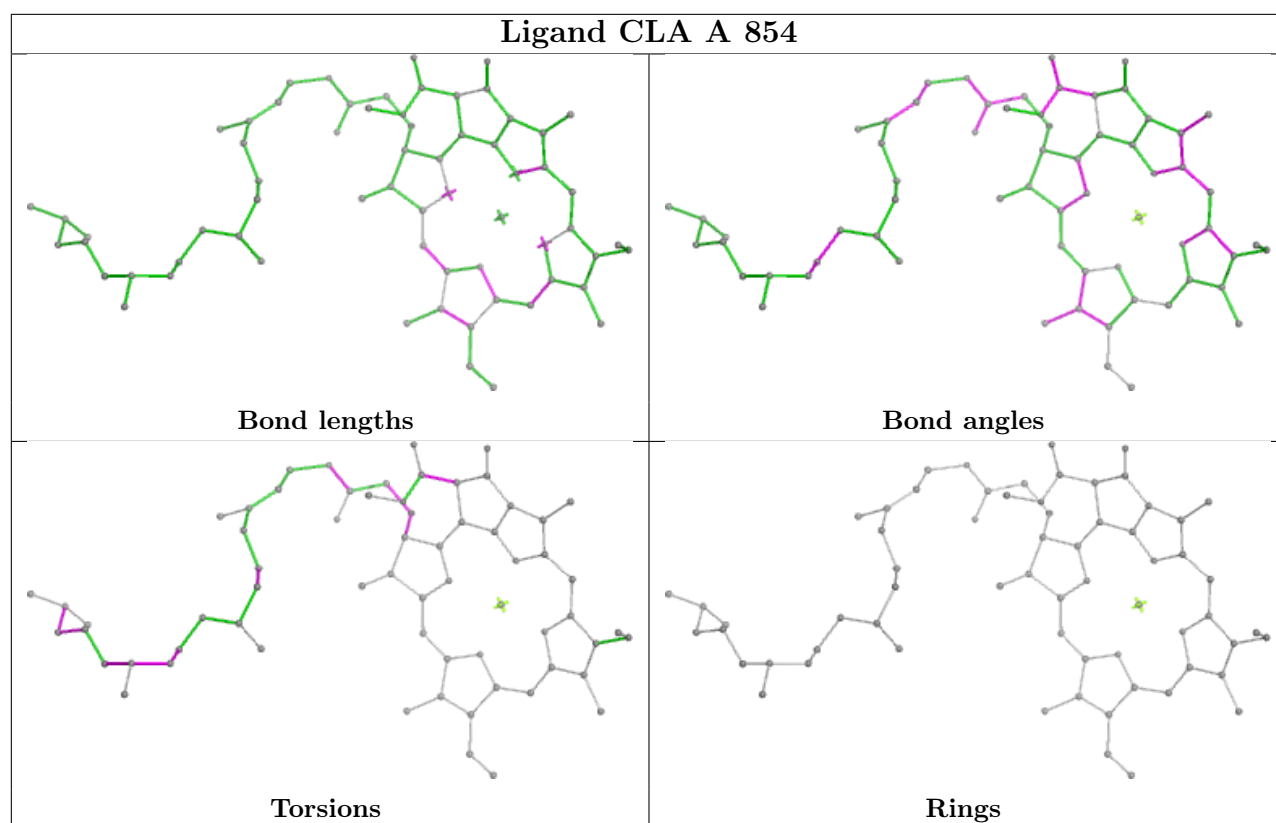


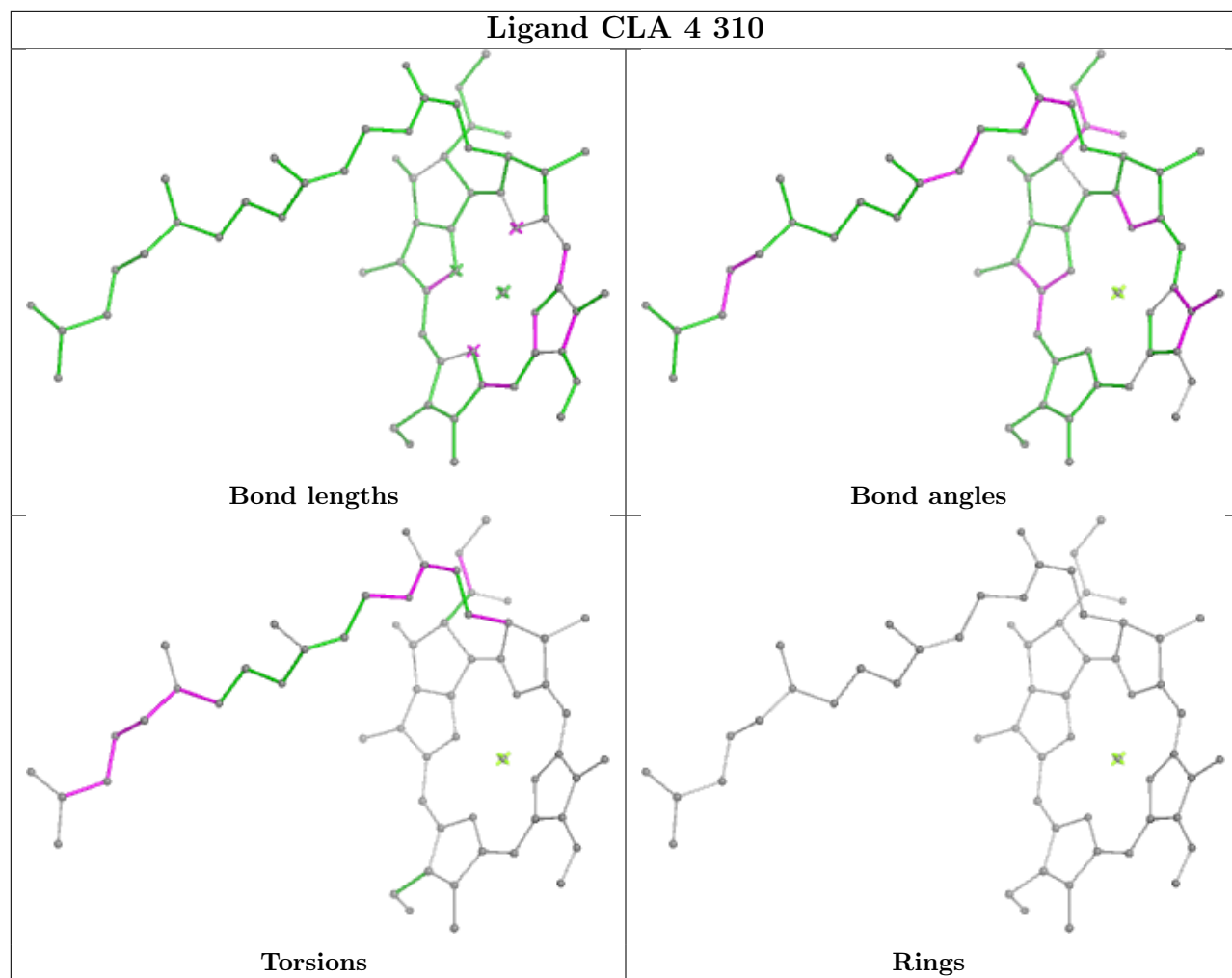
## Ligand CLA A 821



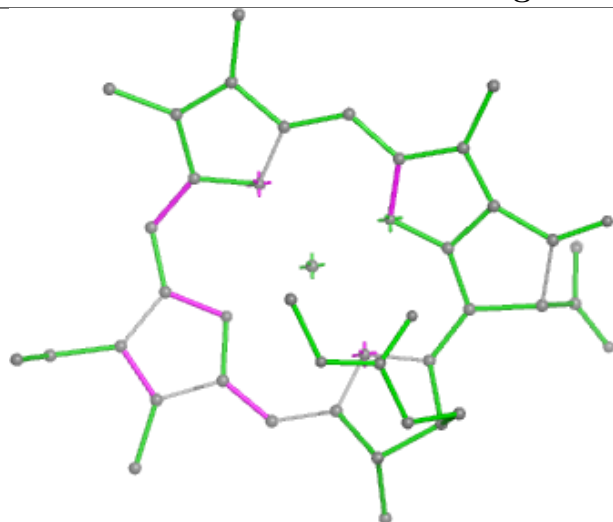
**Ligand CLA A 831****Ligand CLA B 826**



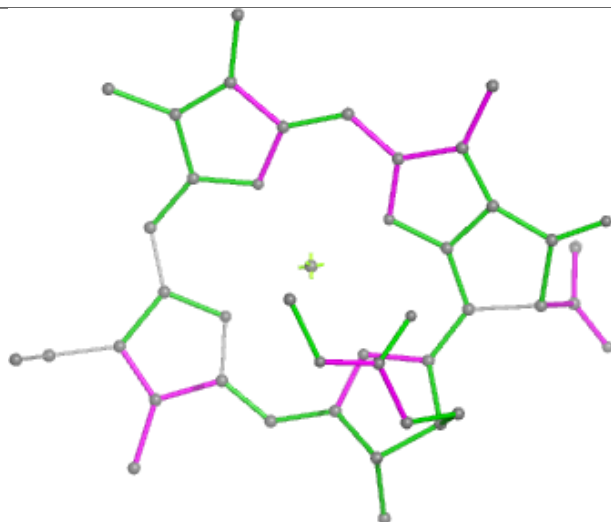




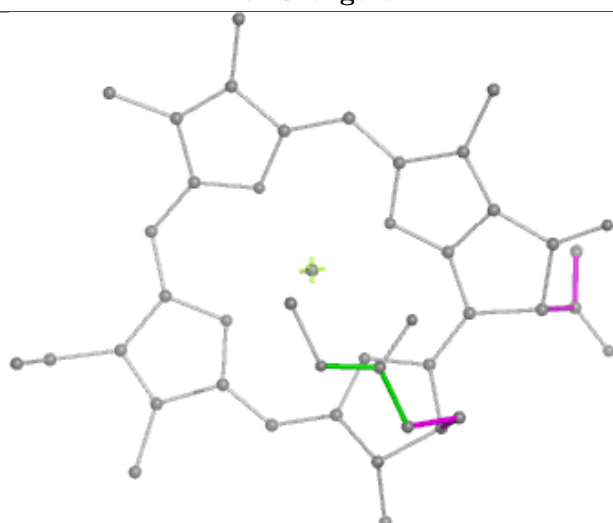
## Ligand CLA H 201



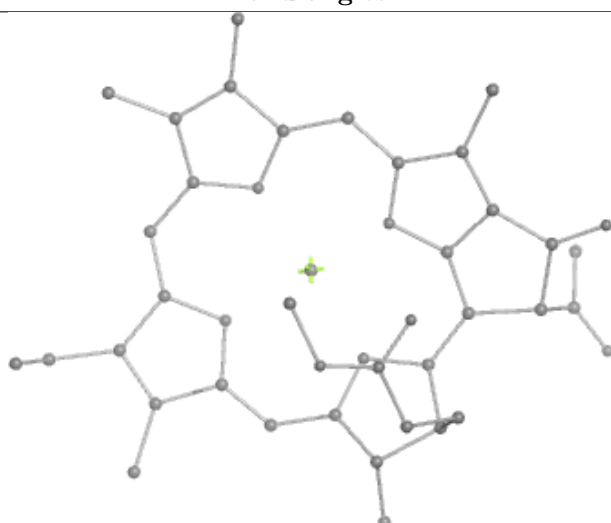
Bond lengths



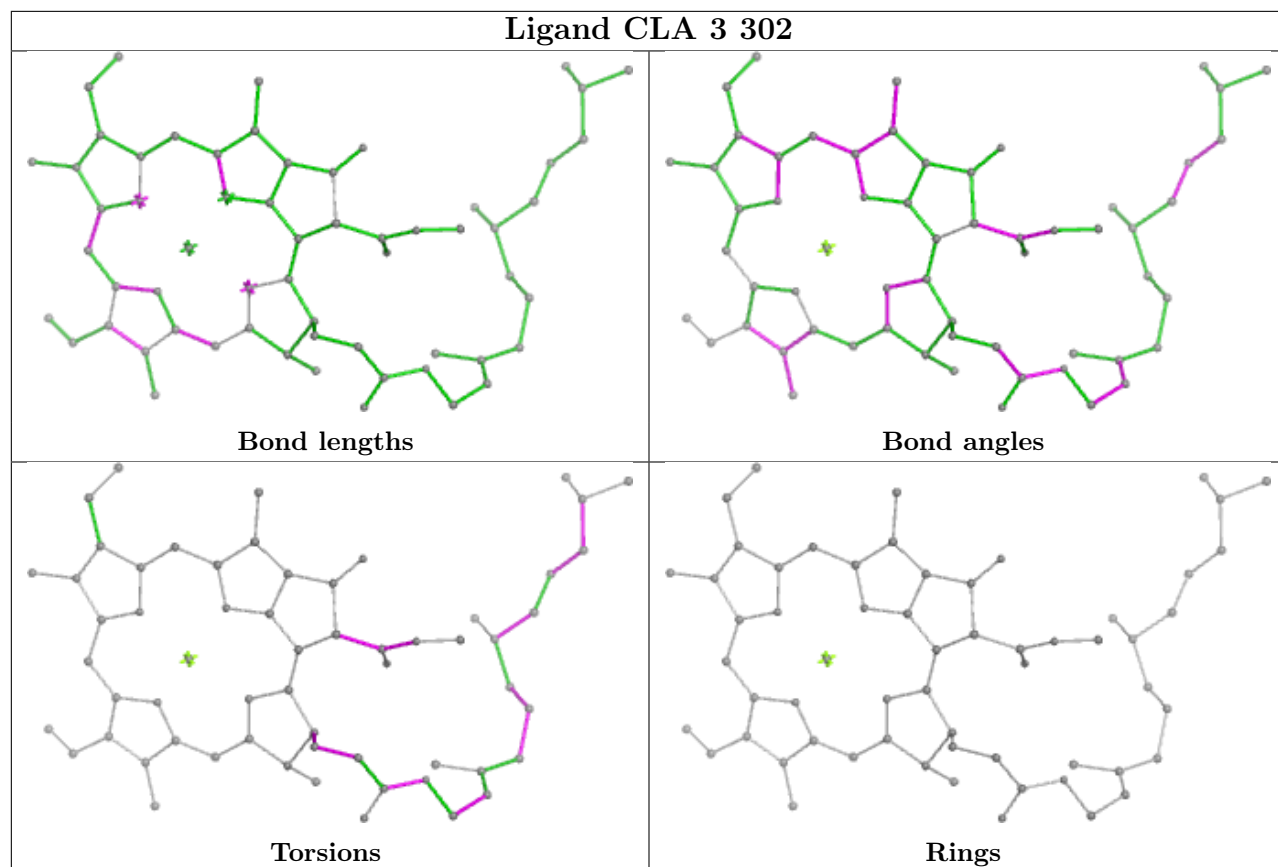
Bond angles



Torsions

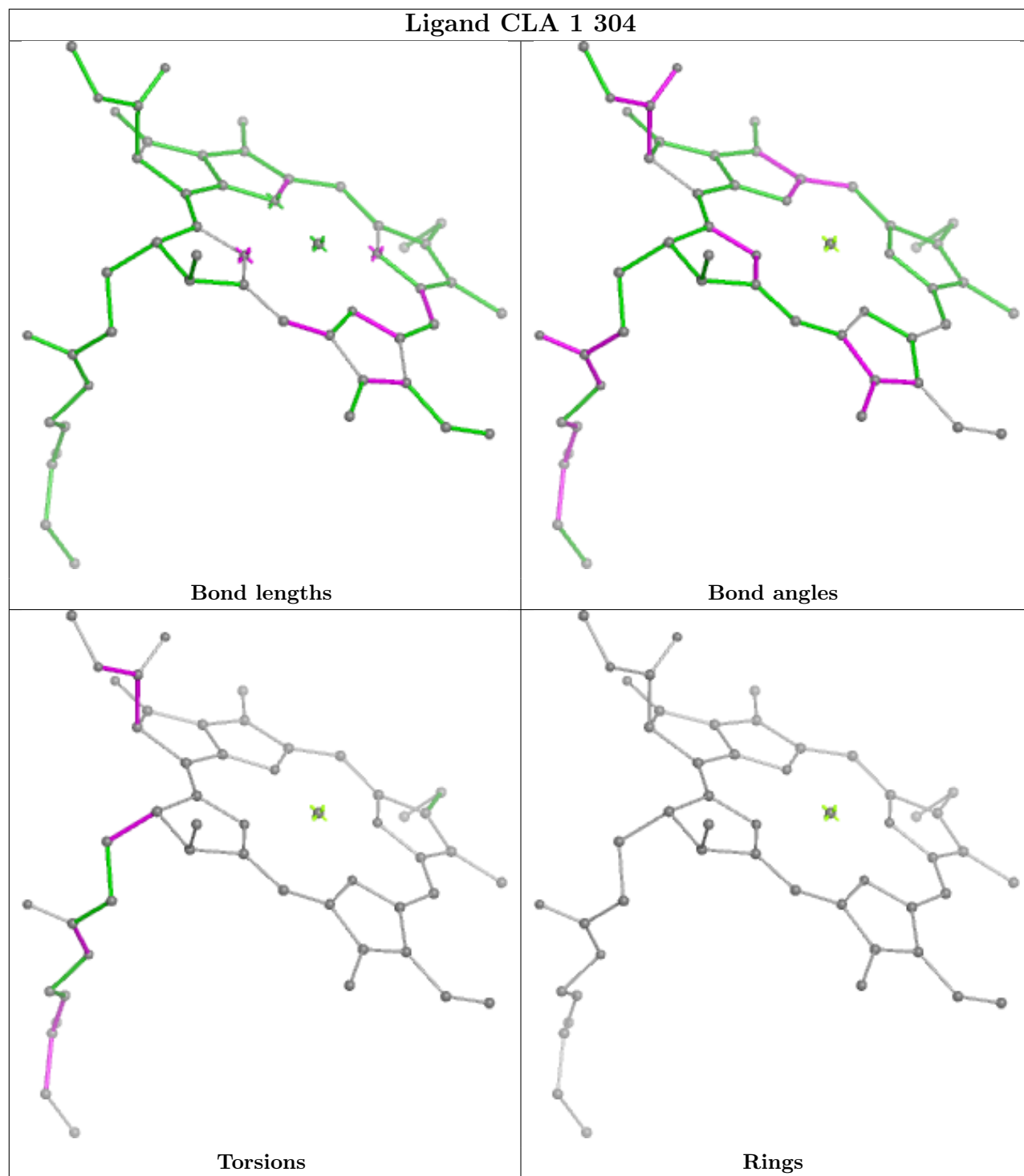


Rings

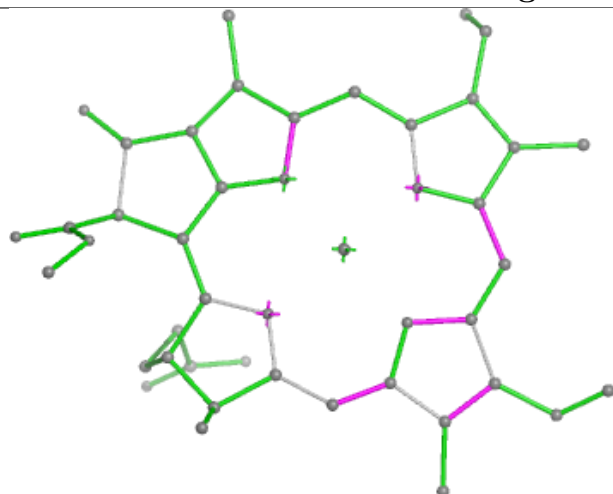




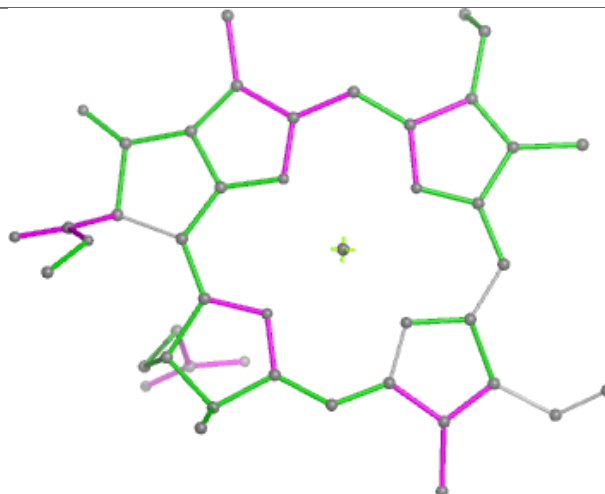
## Ligand CLA 1 304



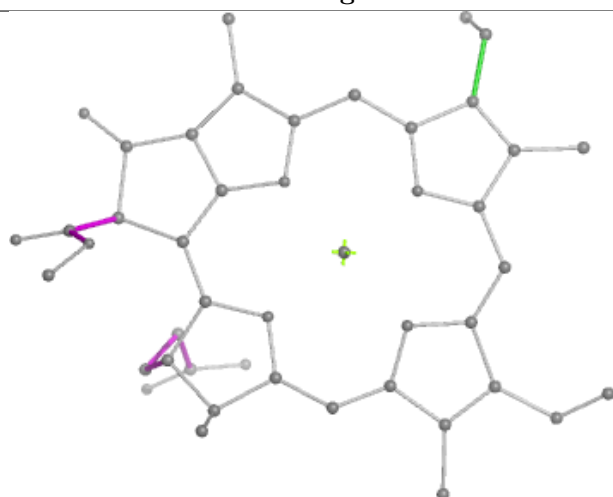
## Ligand CLA 3 303



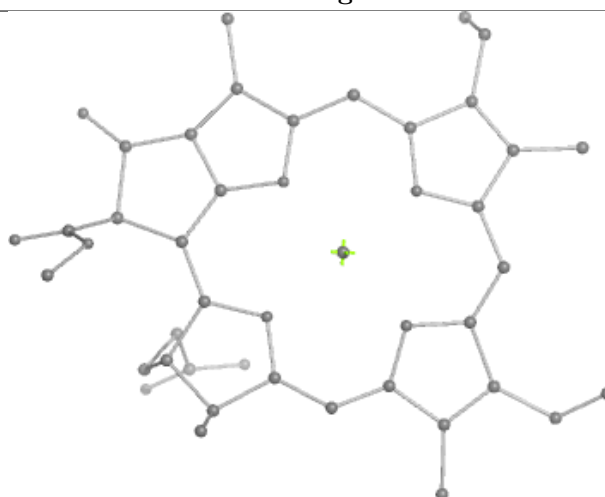
Bond lengths



Bond angles

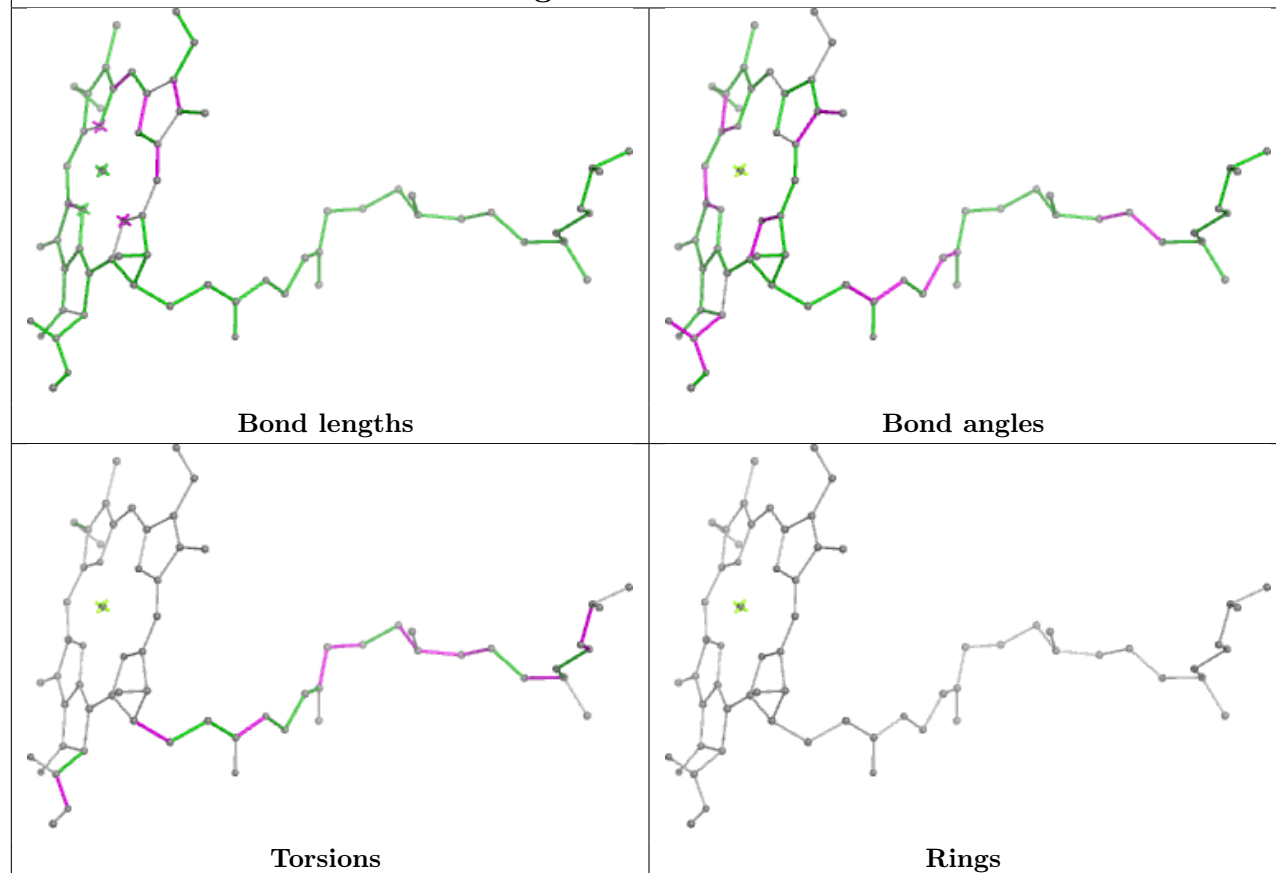


Torsions

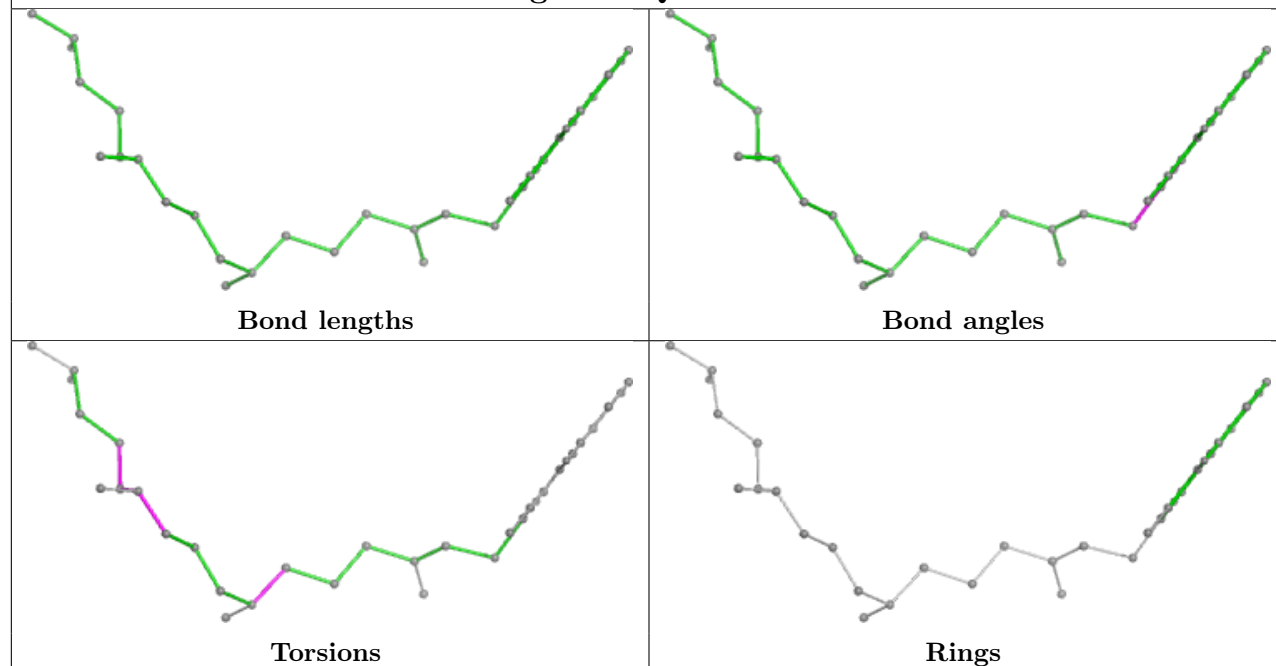


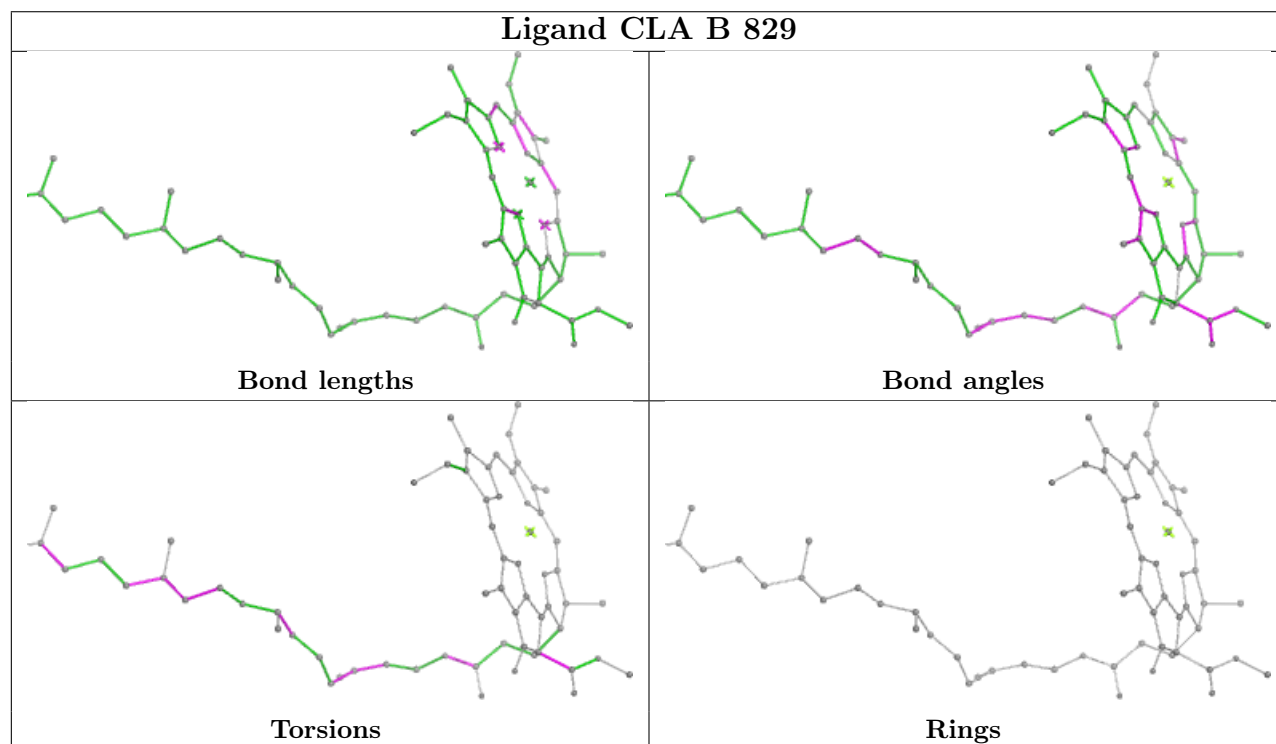
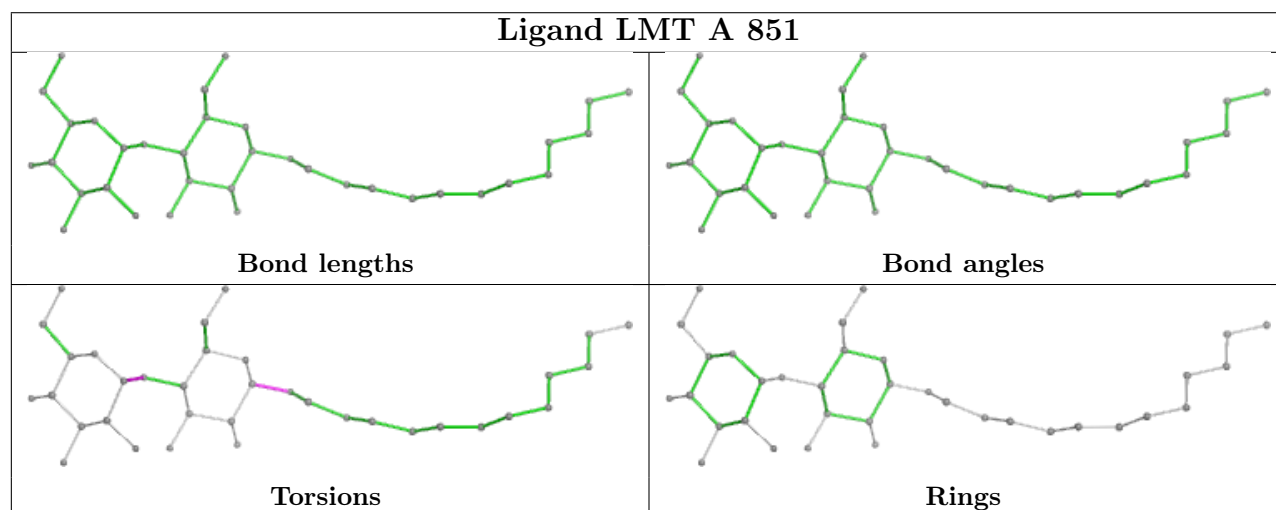
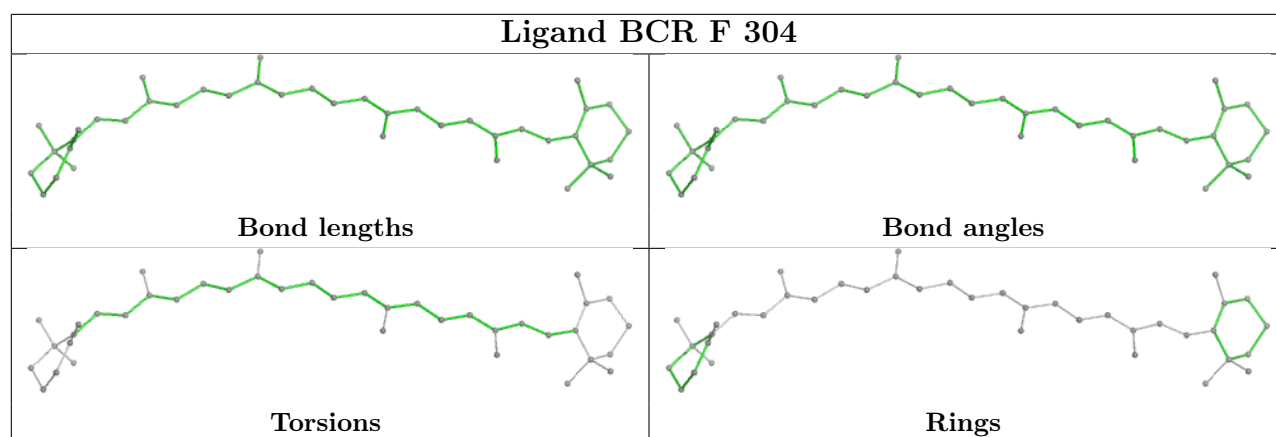
Rings

## Ligand CLA L 301

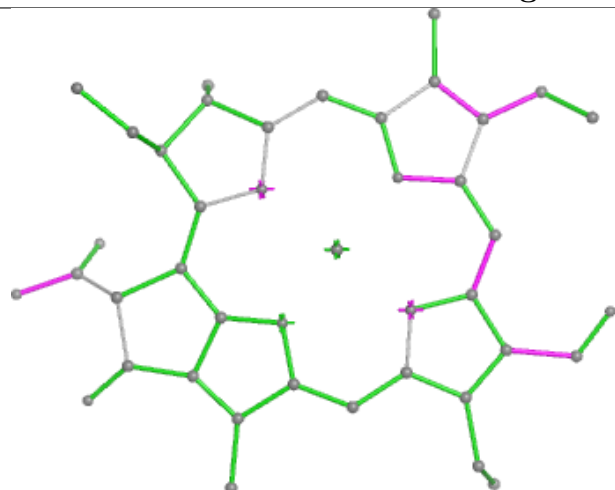


## Ligand PQN B 841

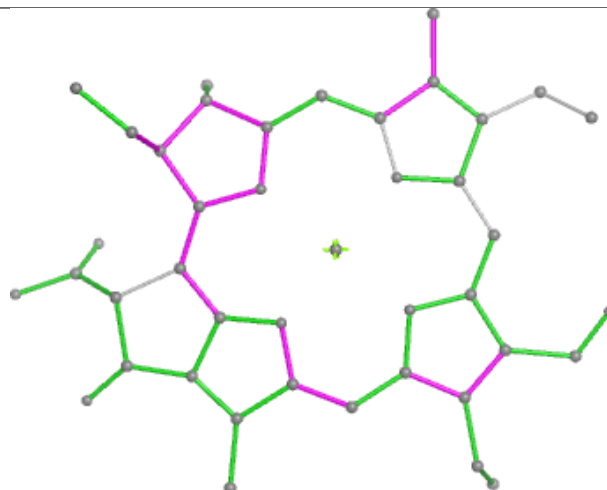




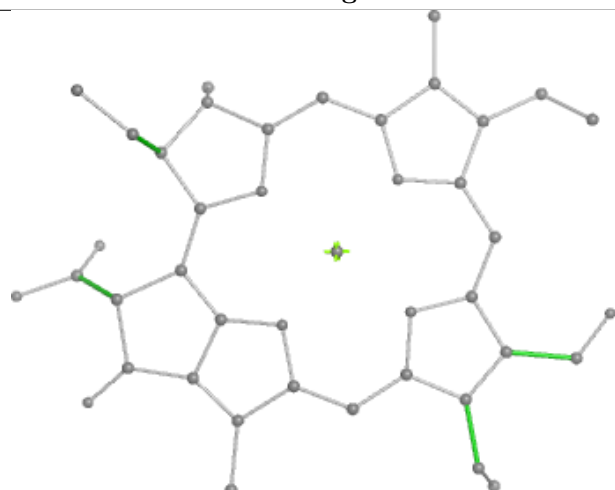
## Ligand CHL 4 314



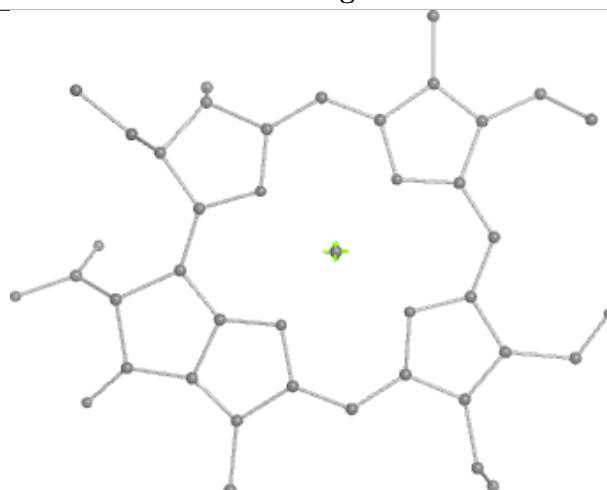
Bond lengths



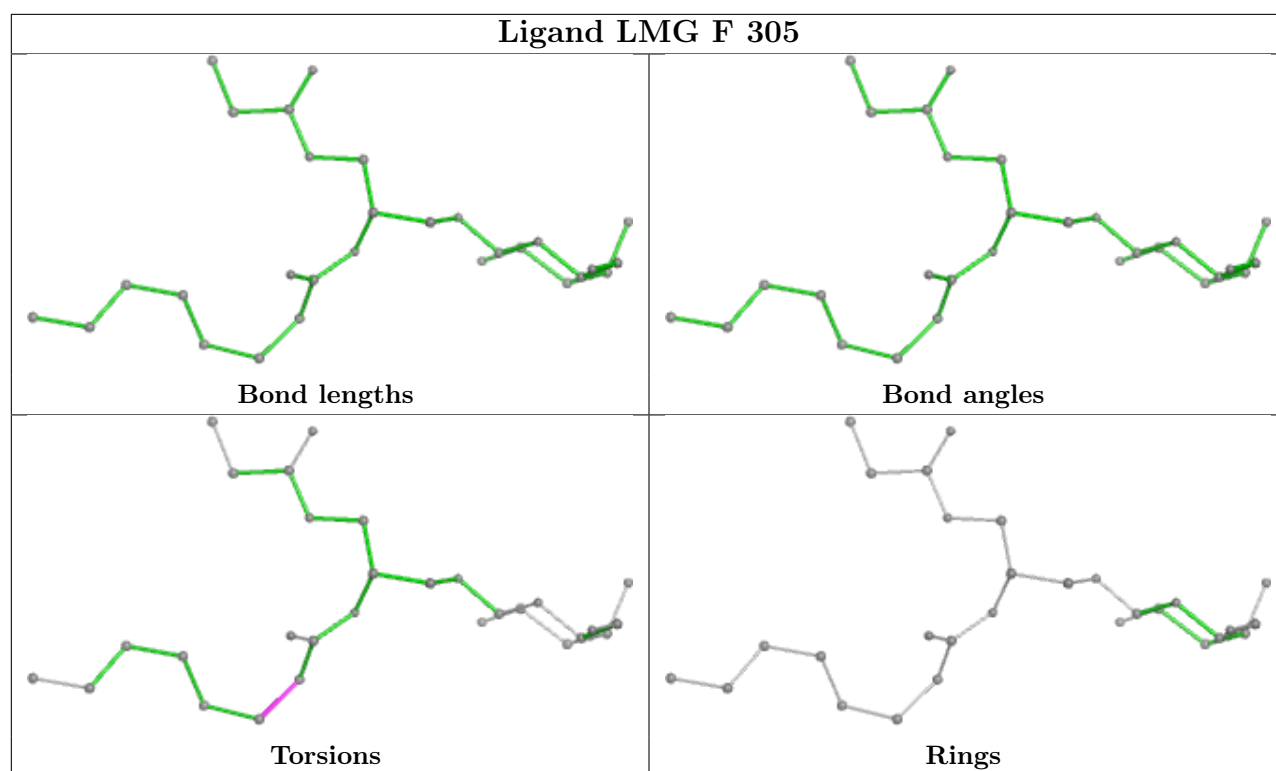
Bond angles



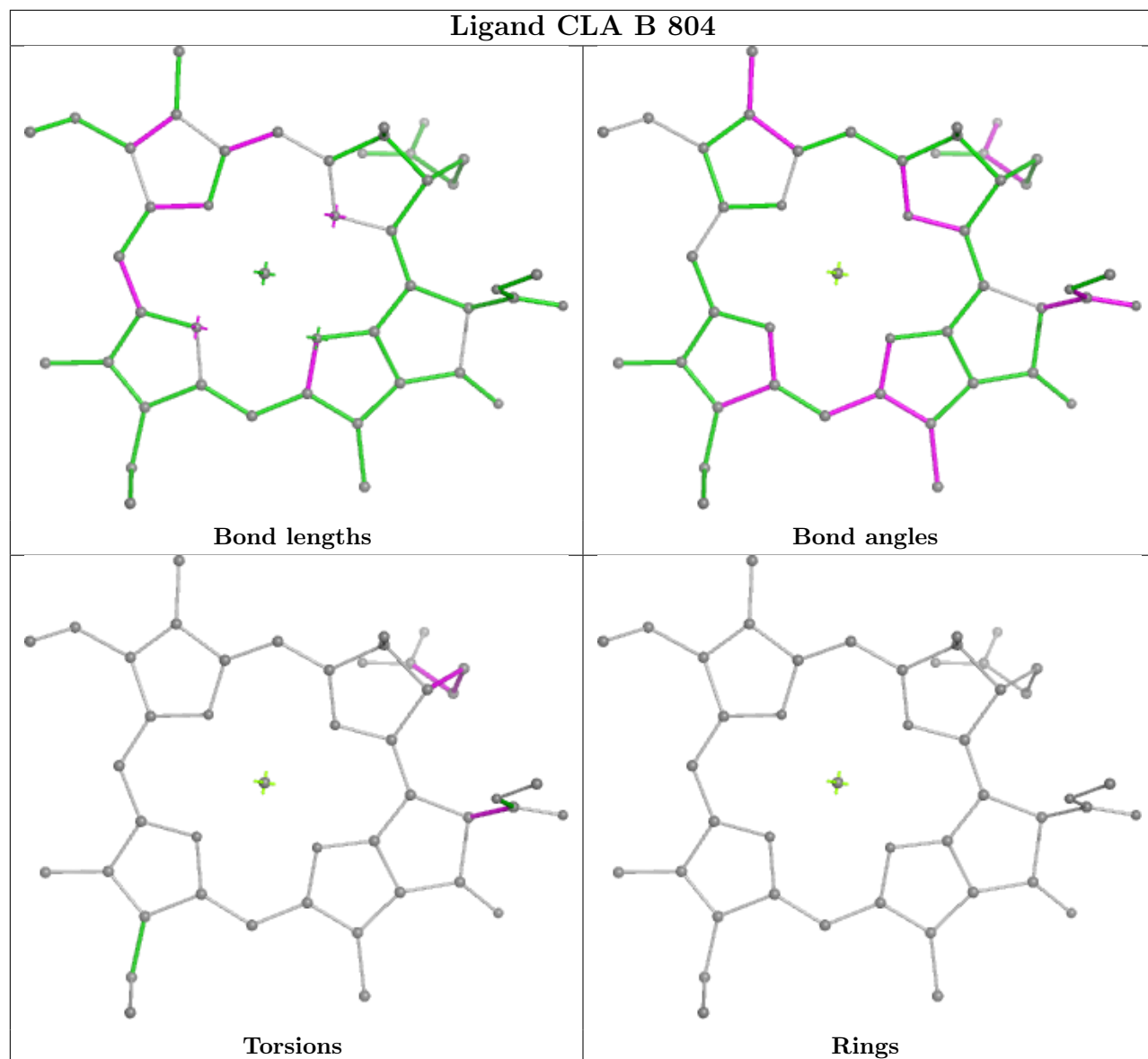
Torsions



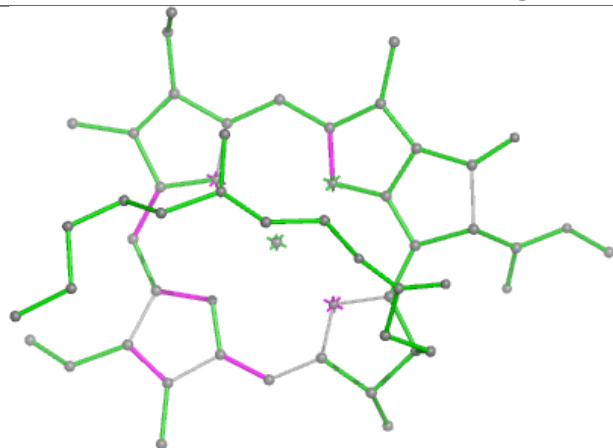
Rings



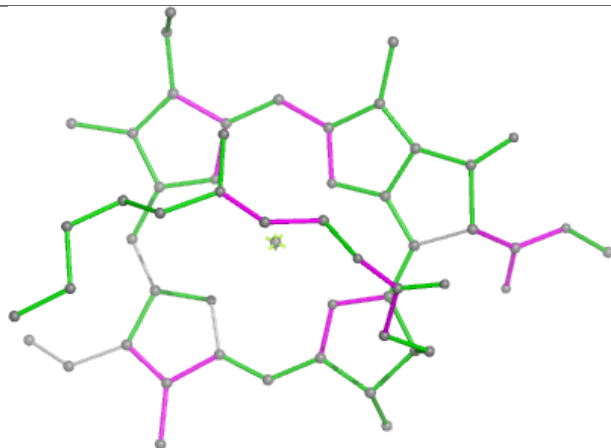
## Ligand CLA B 804



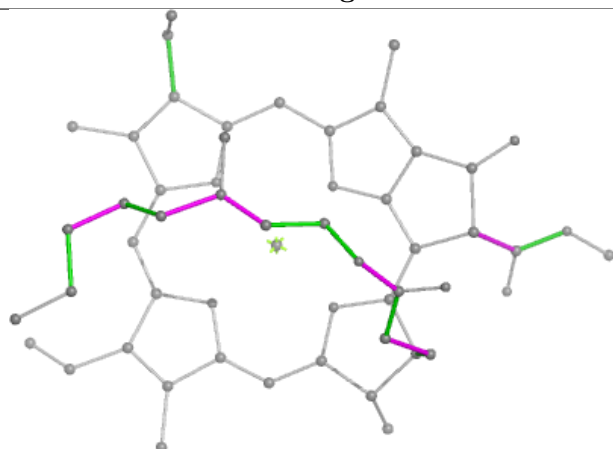
## Ligand CLA A 810



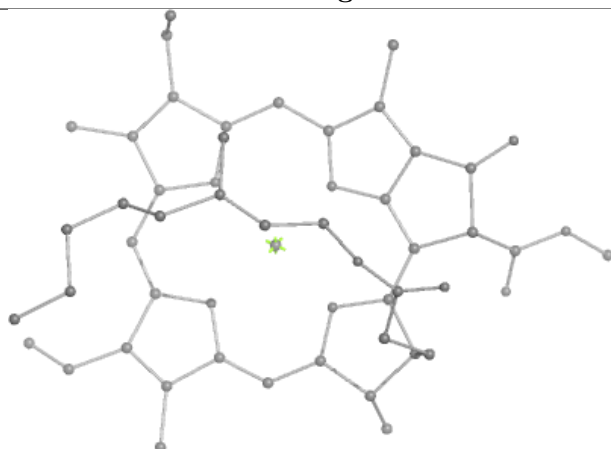
Bond lengths



Bond angles

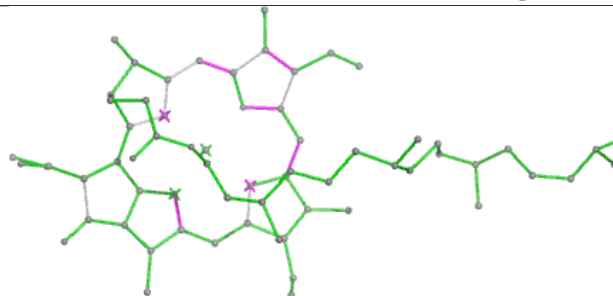


Torsions

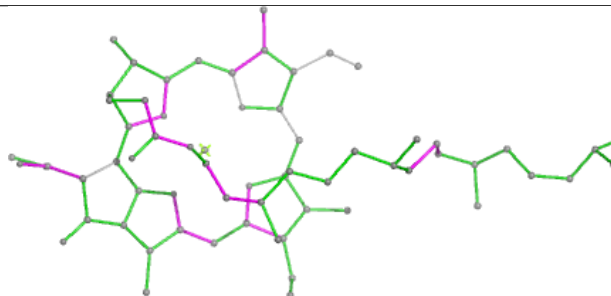


Rings

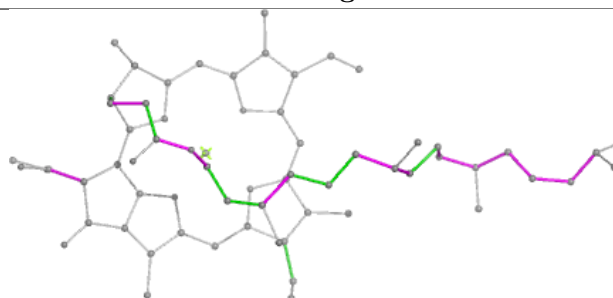
## Ligand CLA A 835



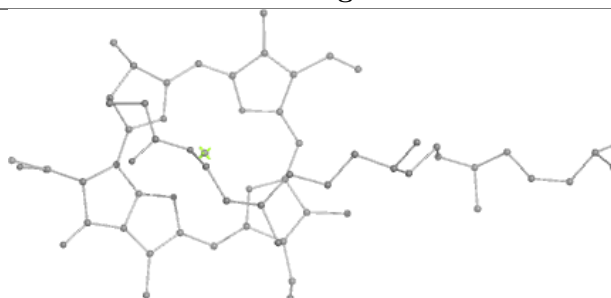
Bond lengths



Bond angles



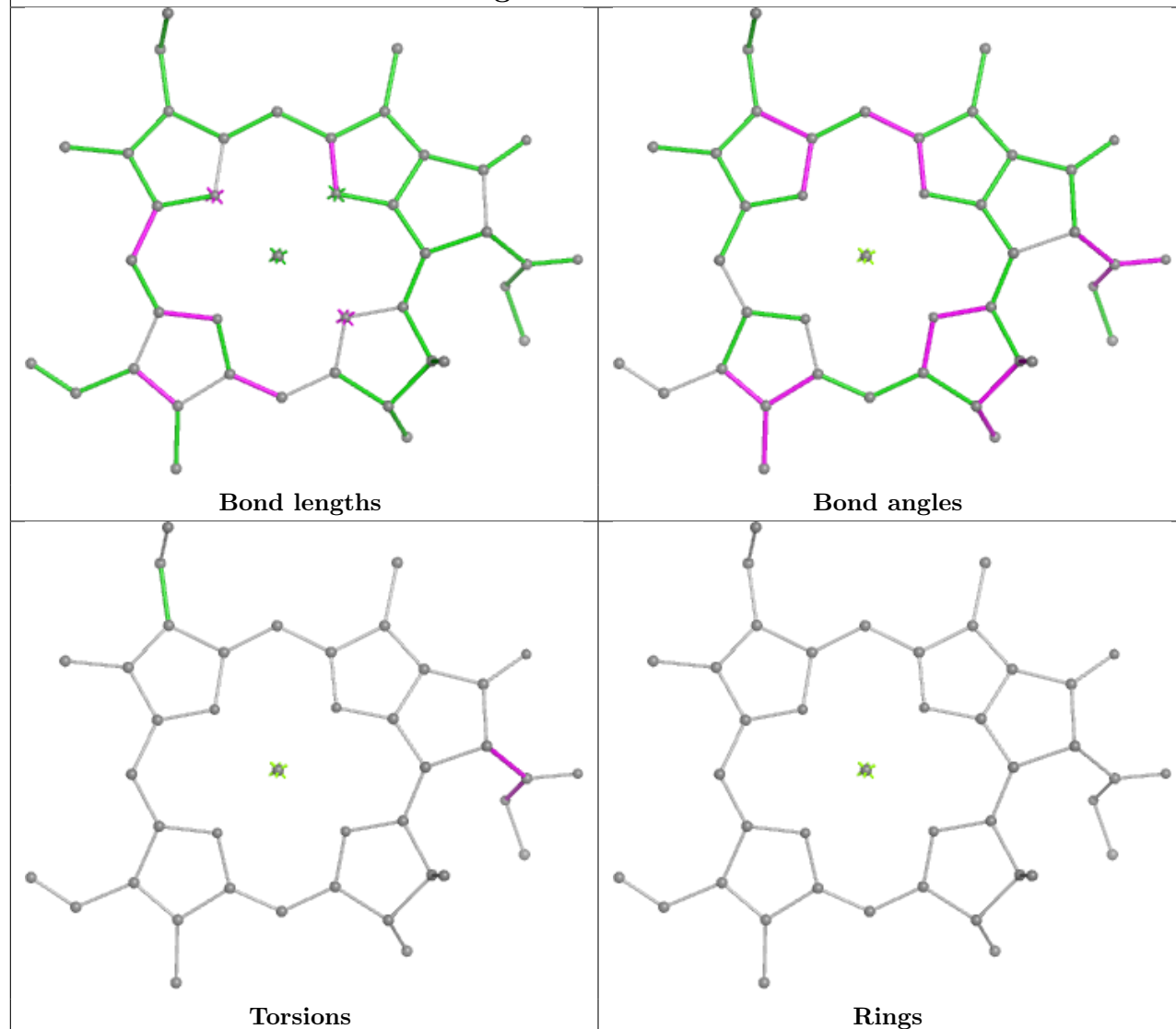
Torsions



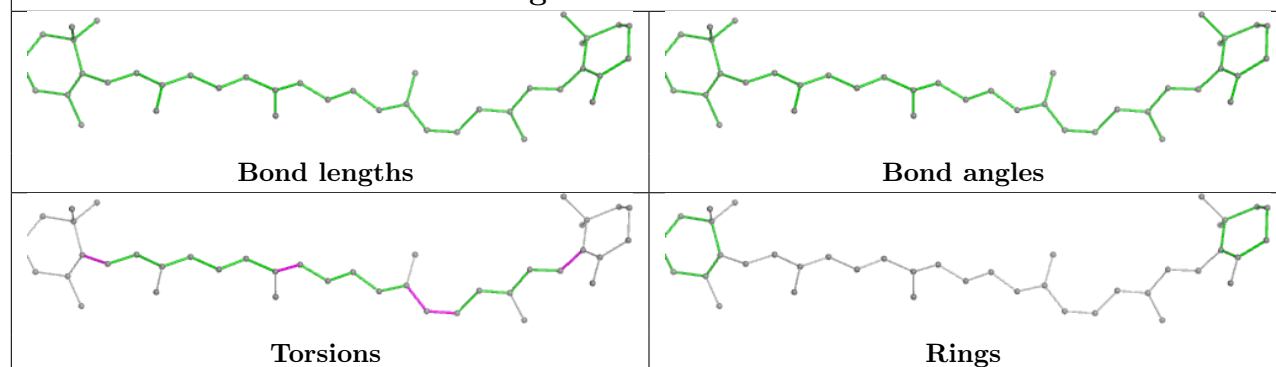
Rings

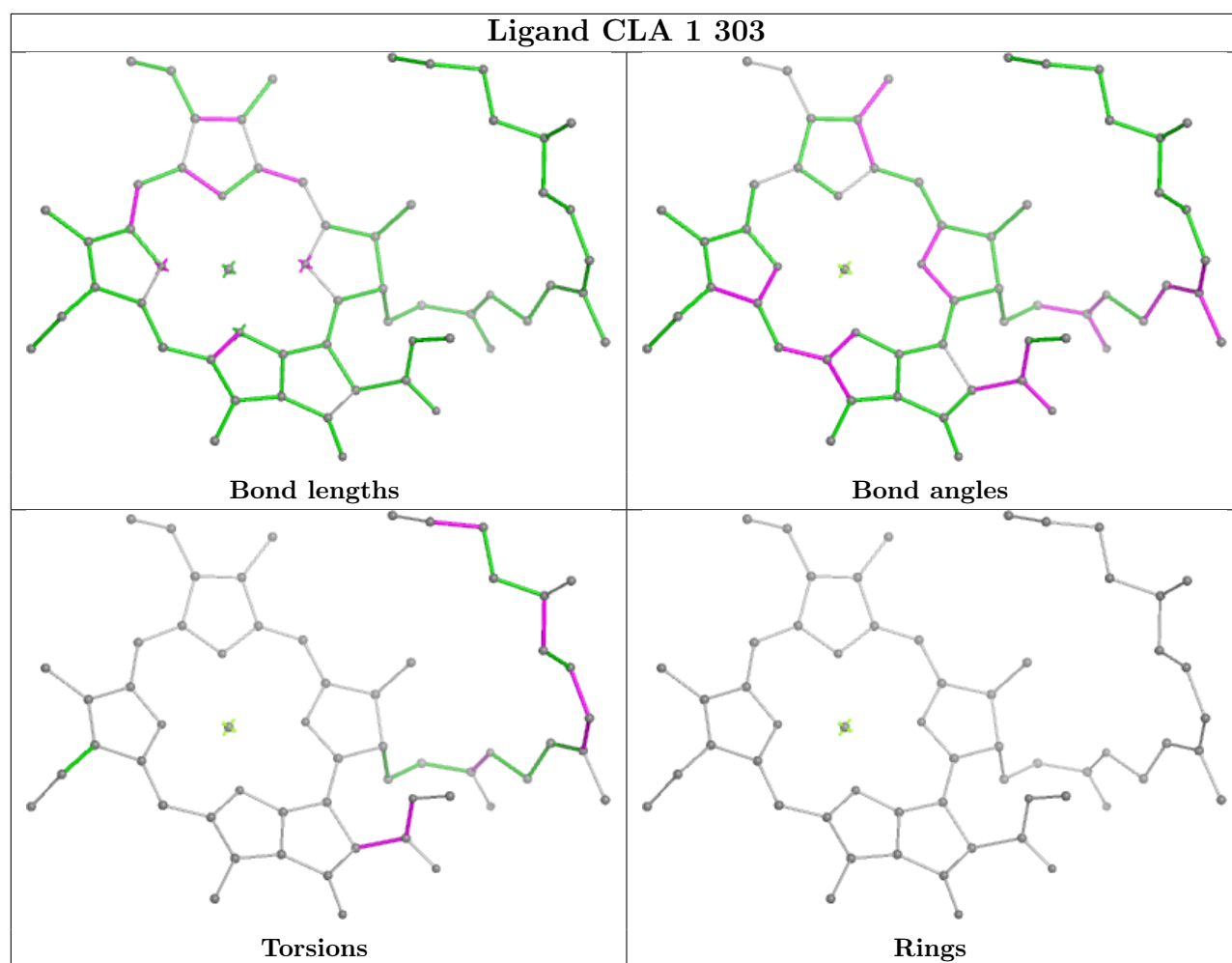


## Ligand CLA 3 310

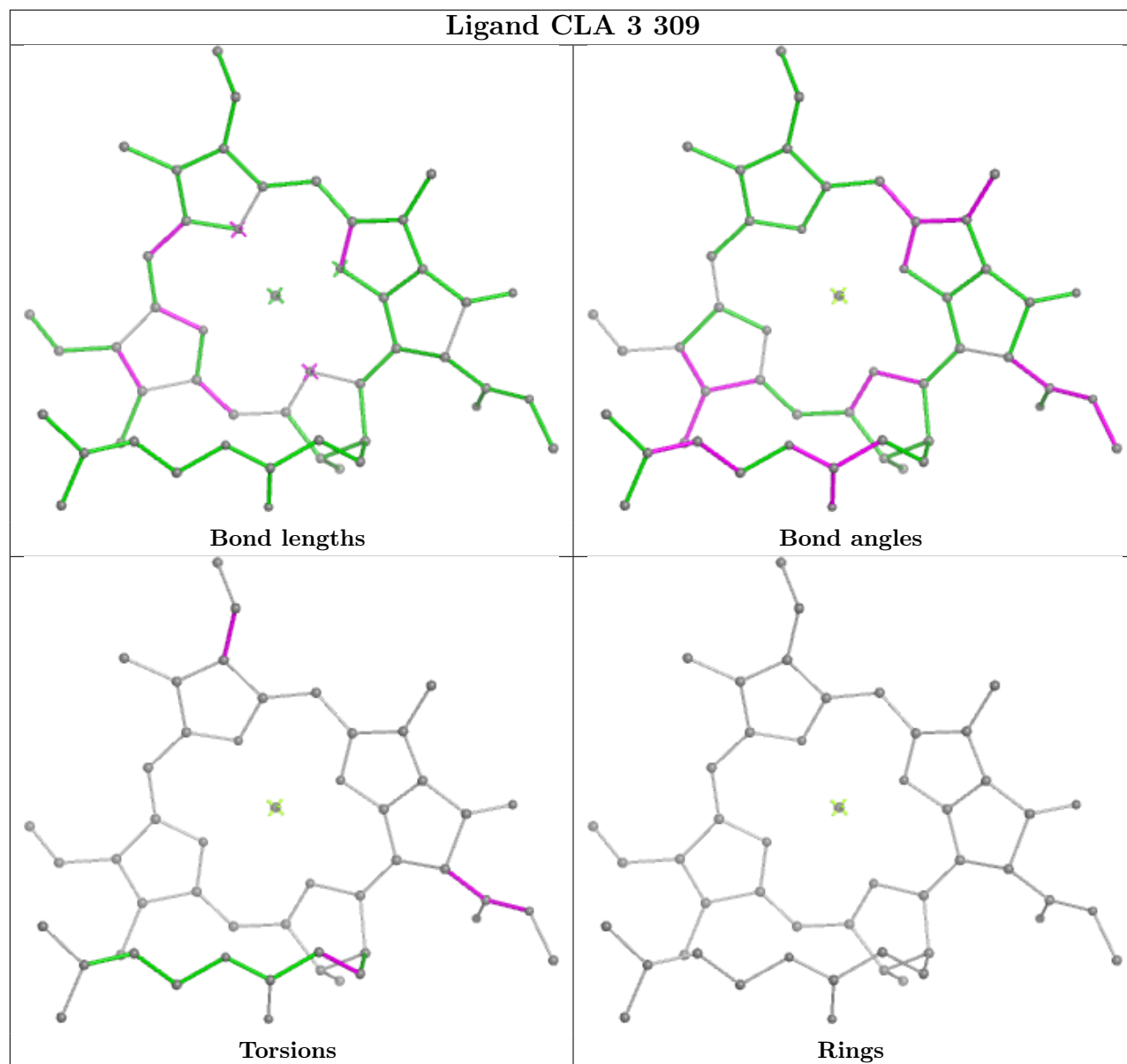


## Ligand BCR G 201

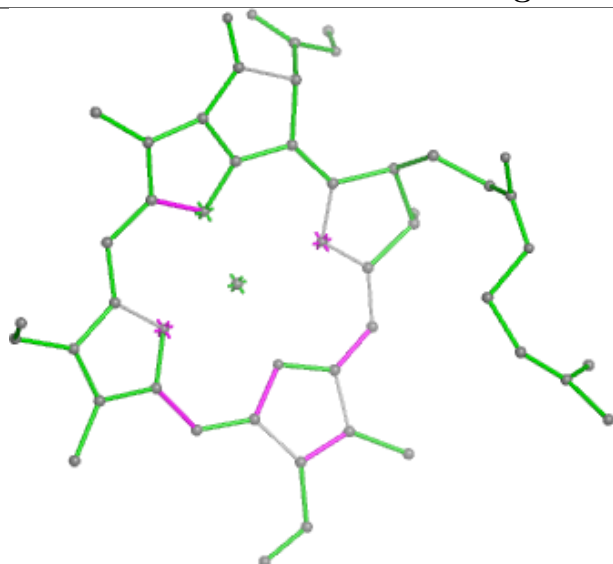




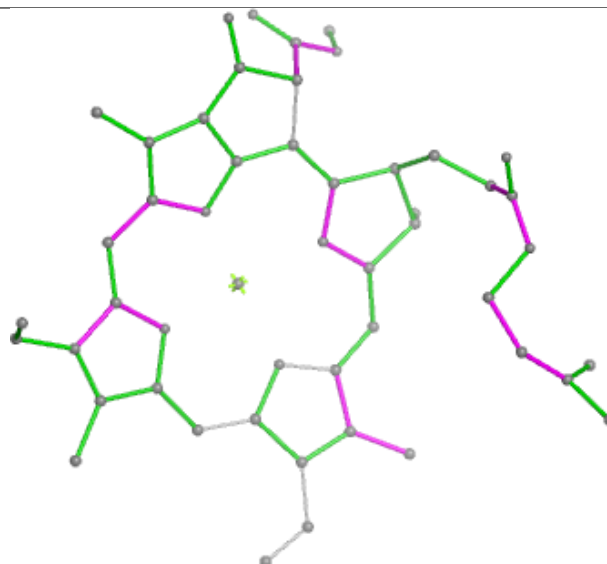
## Ligand CLA 3 309



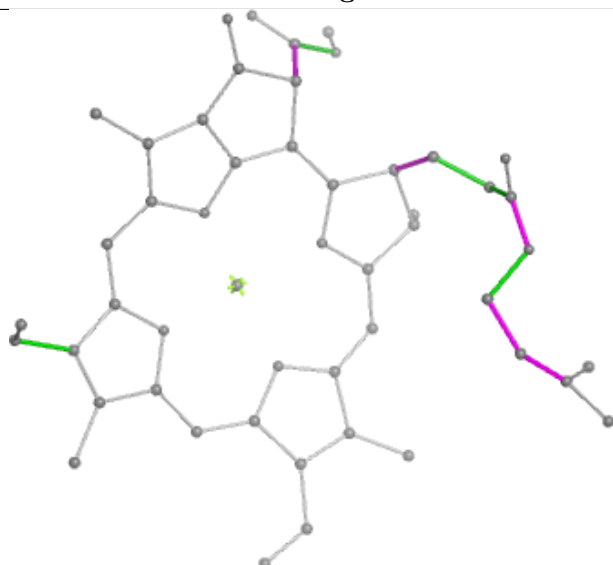
## Ligand CLA A 813



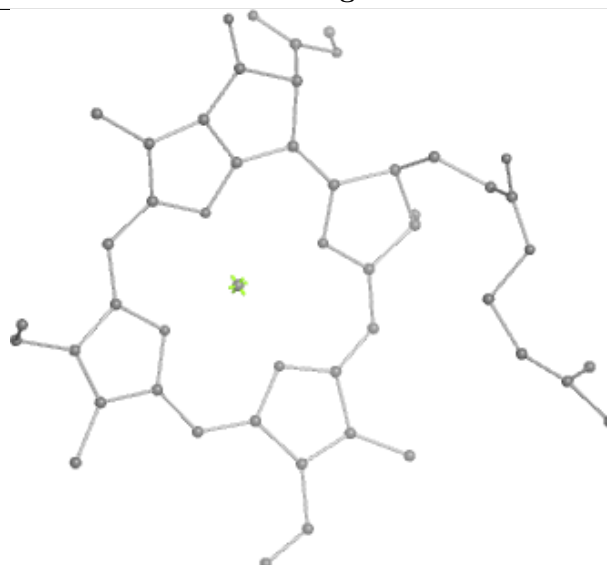
Bond lengths



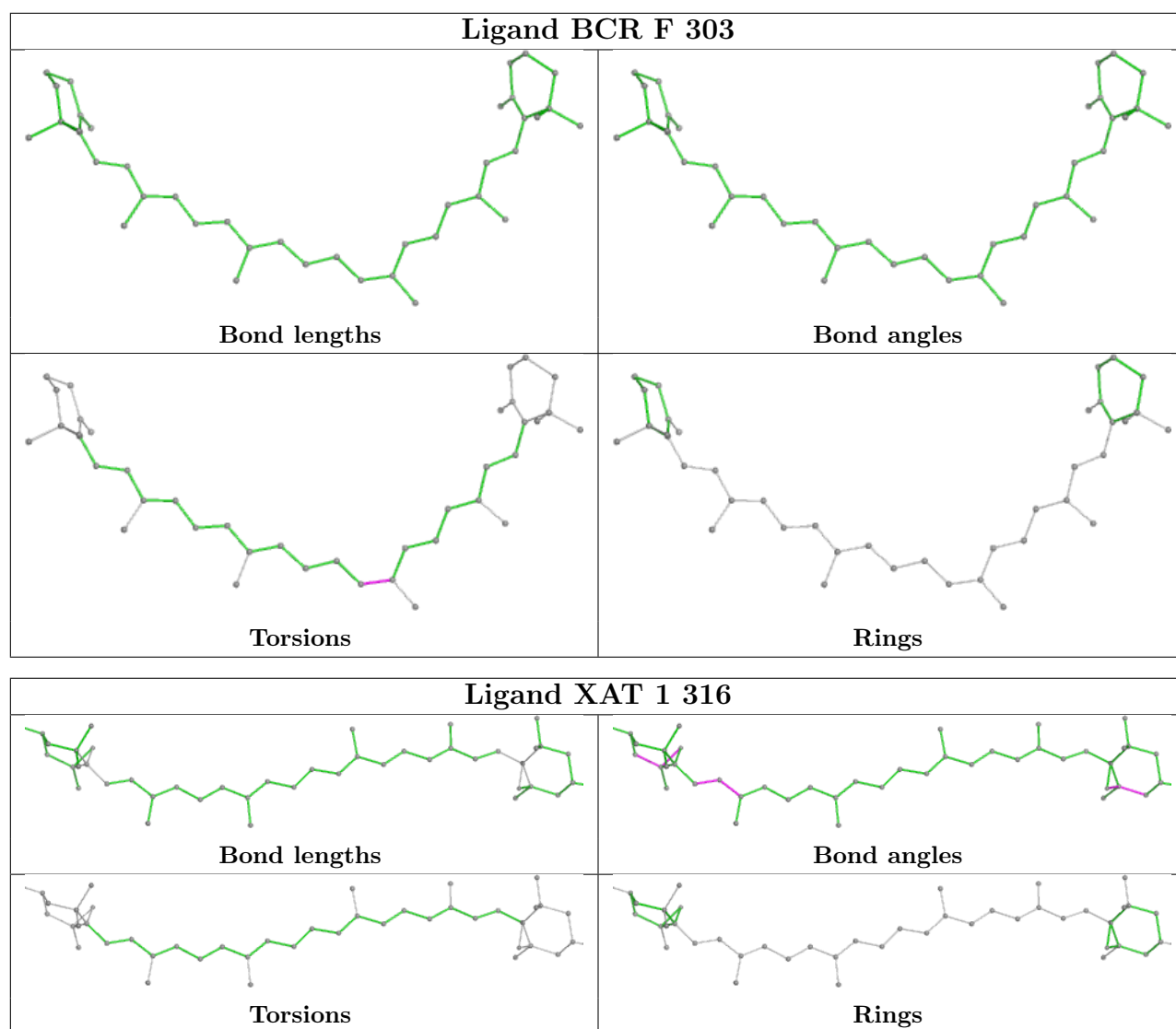
Bond angles



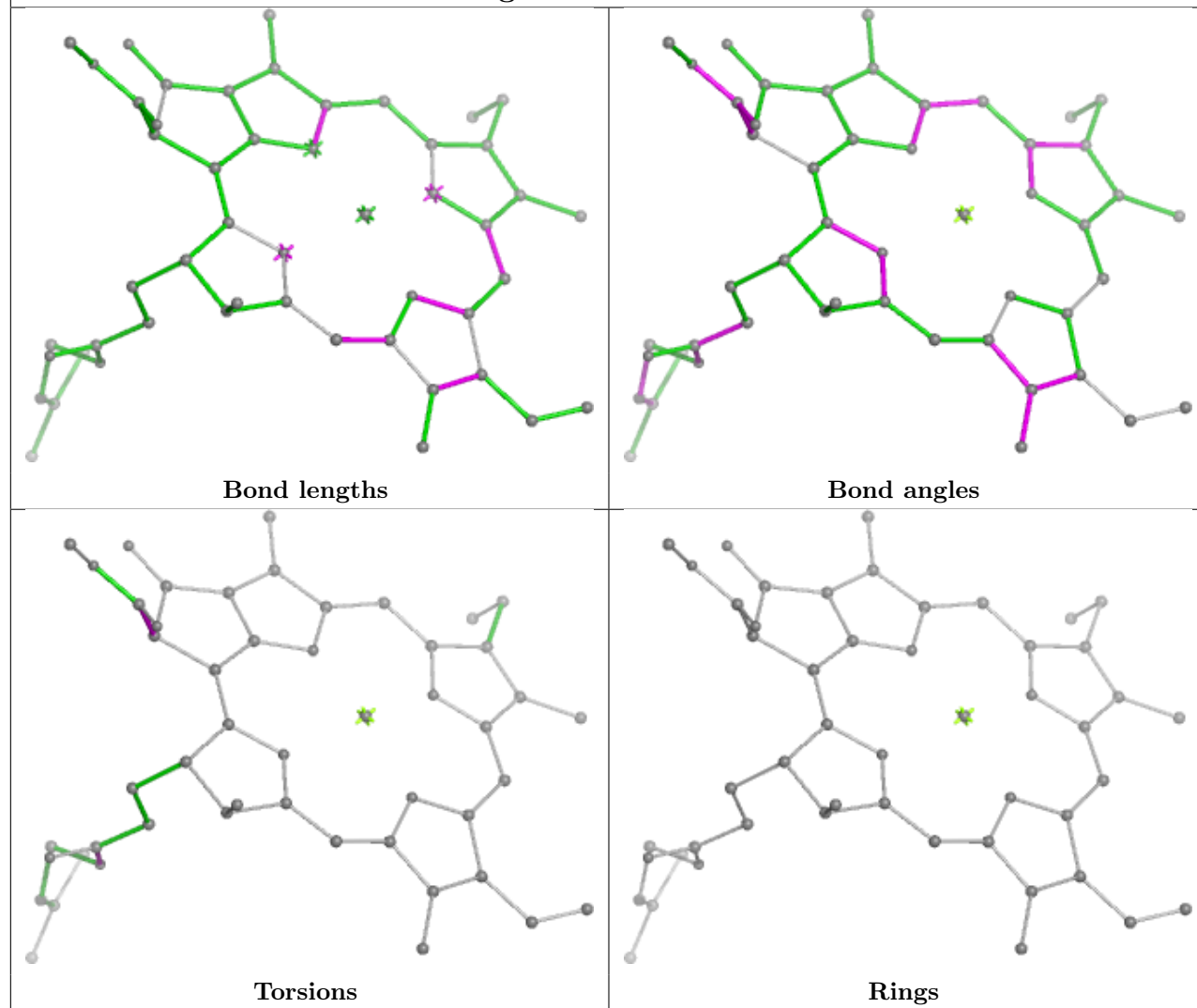
Torsions



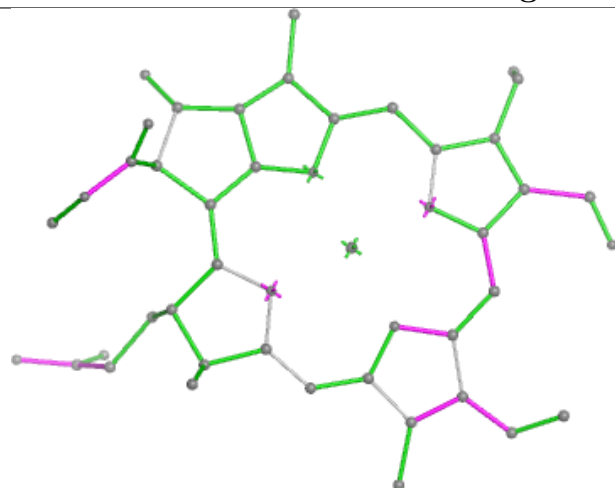
Rings



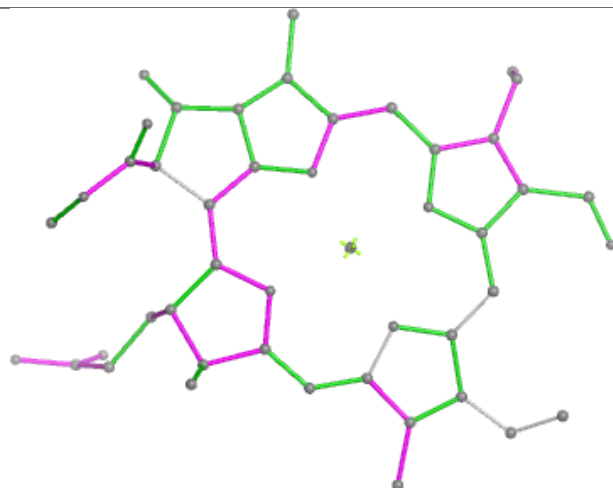
## Ligand CLA A 805



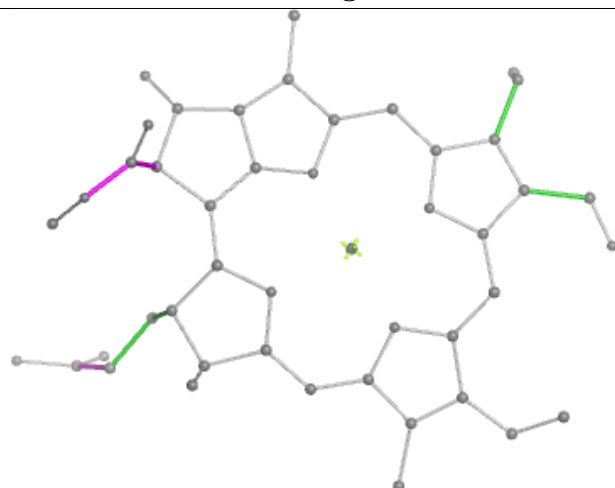
## Ligand CHL 4 306



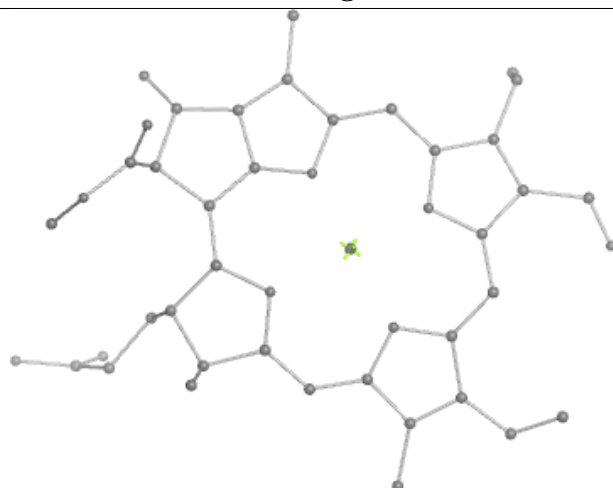
Bond lengths



Bond angles

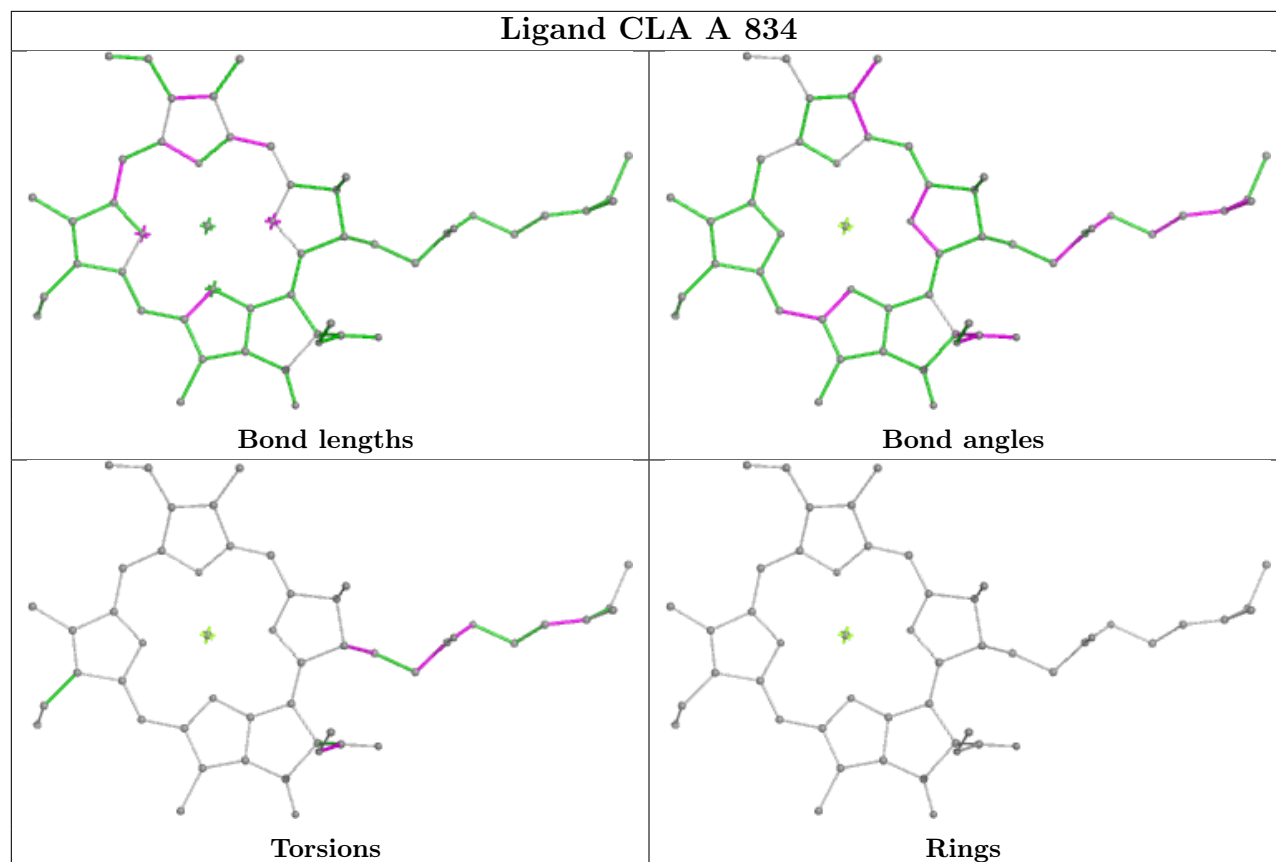


Torsions

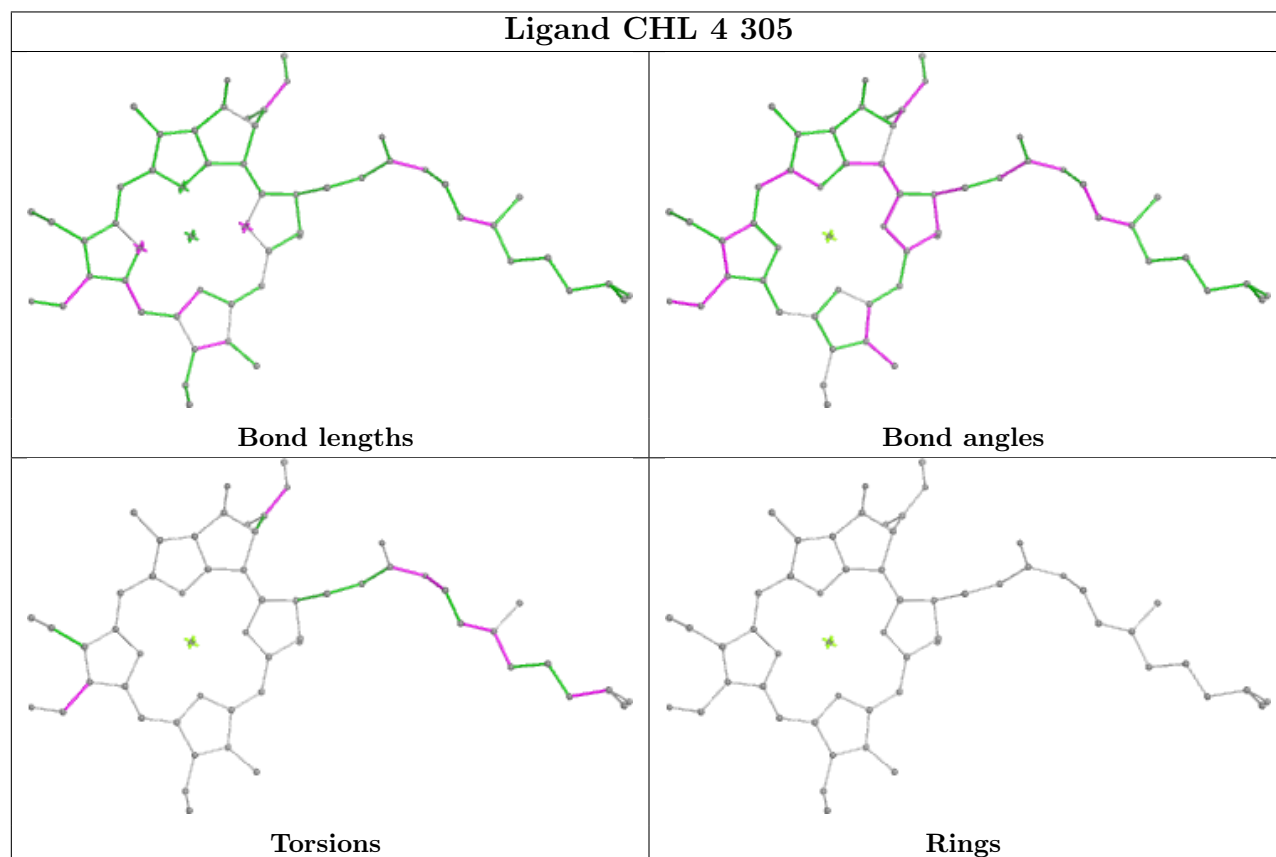


Rings

## Ligand CLA A 834

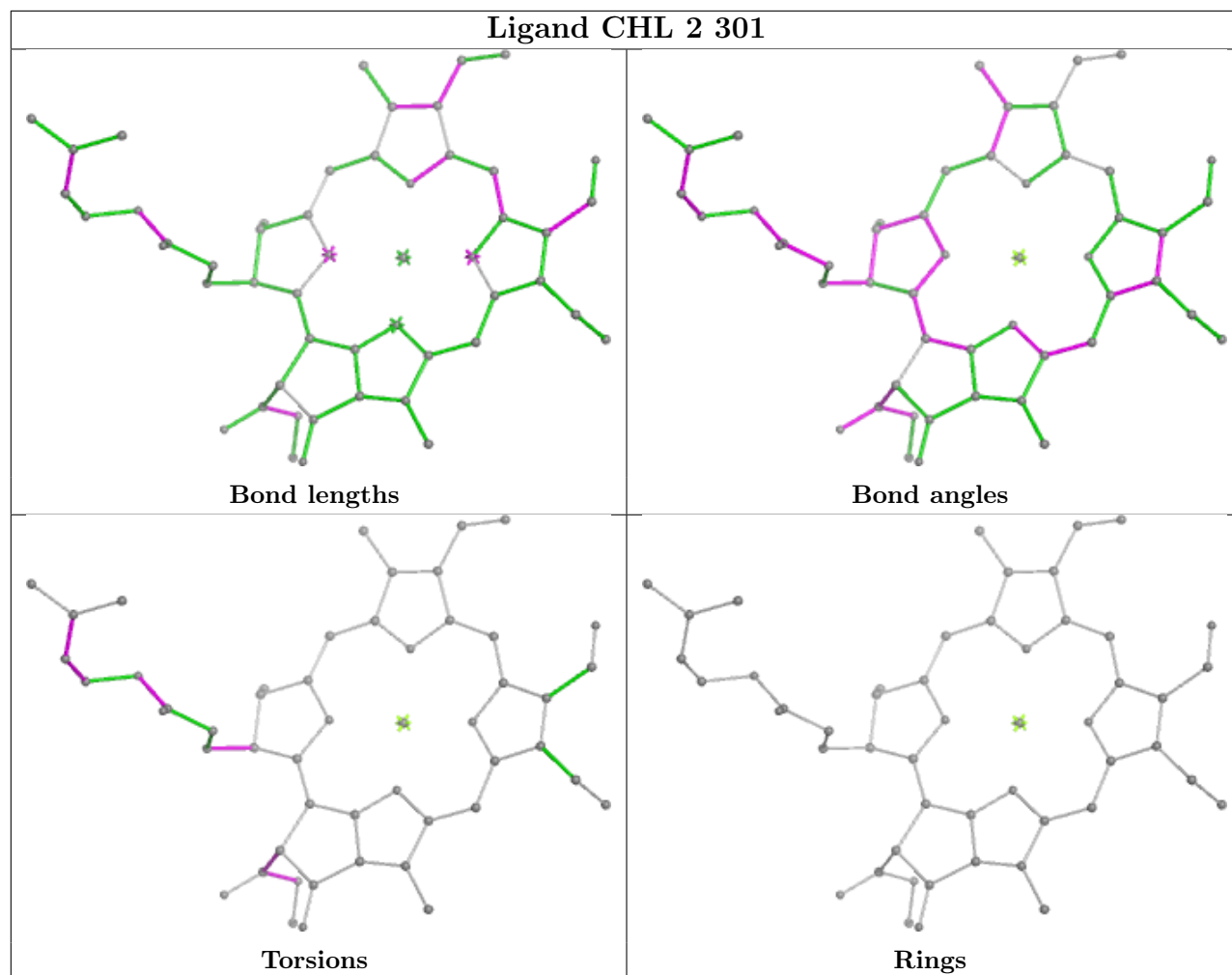


## Ligand CHL 4 305

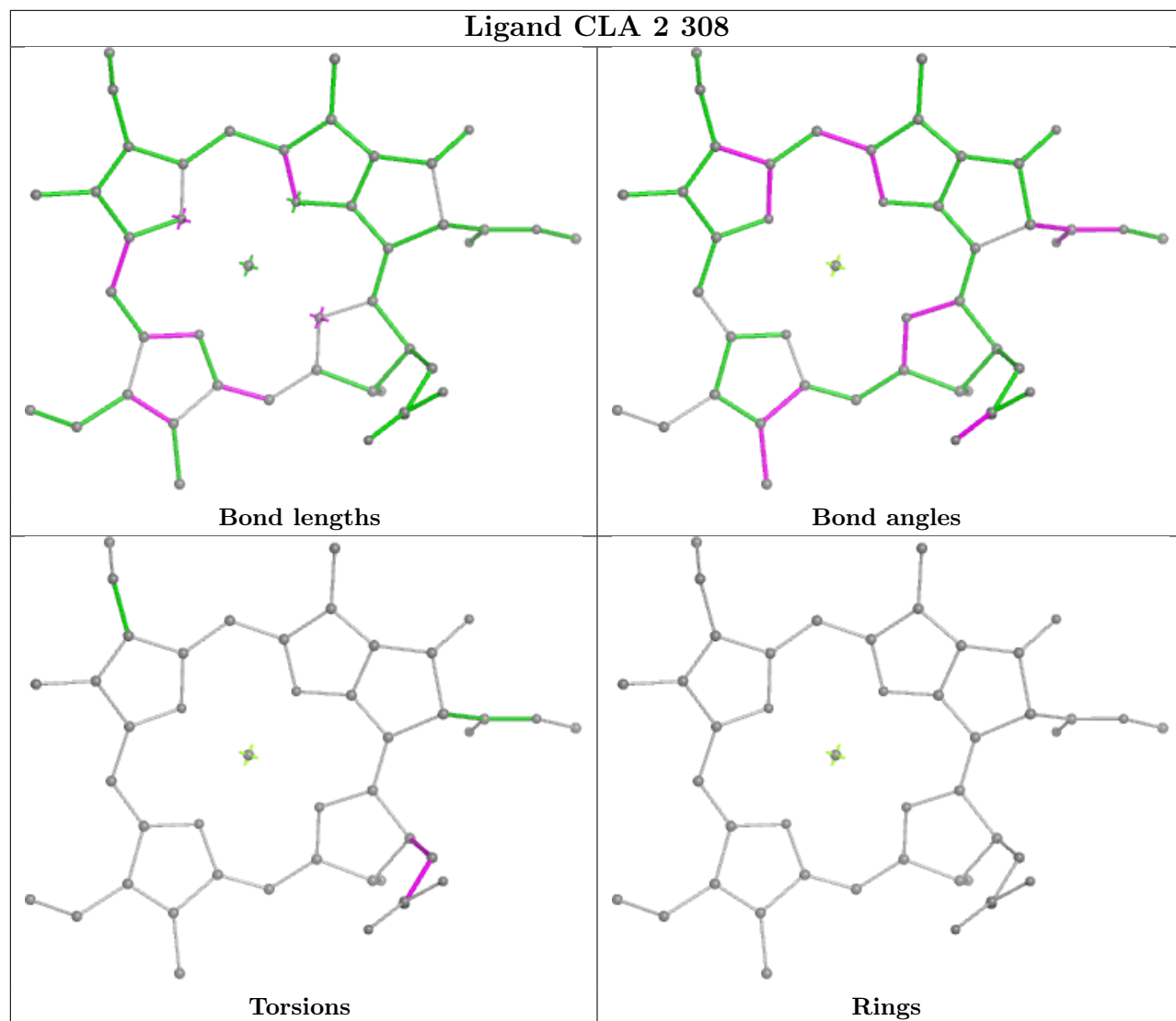




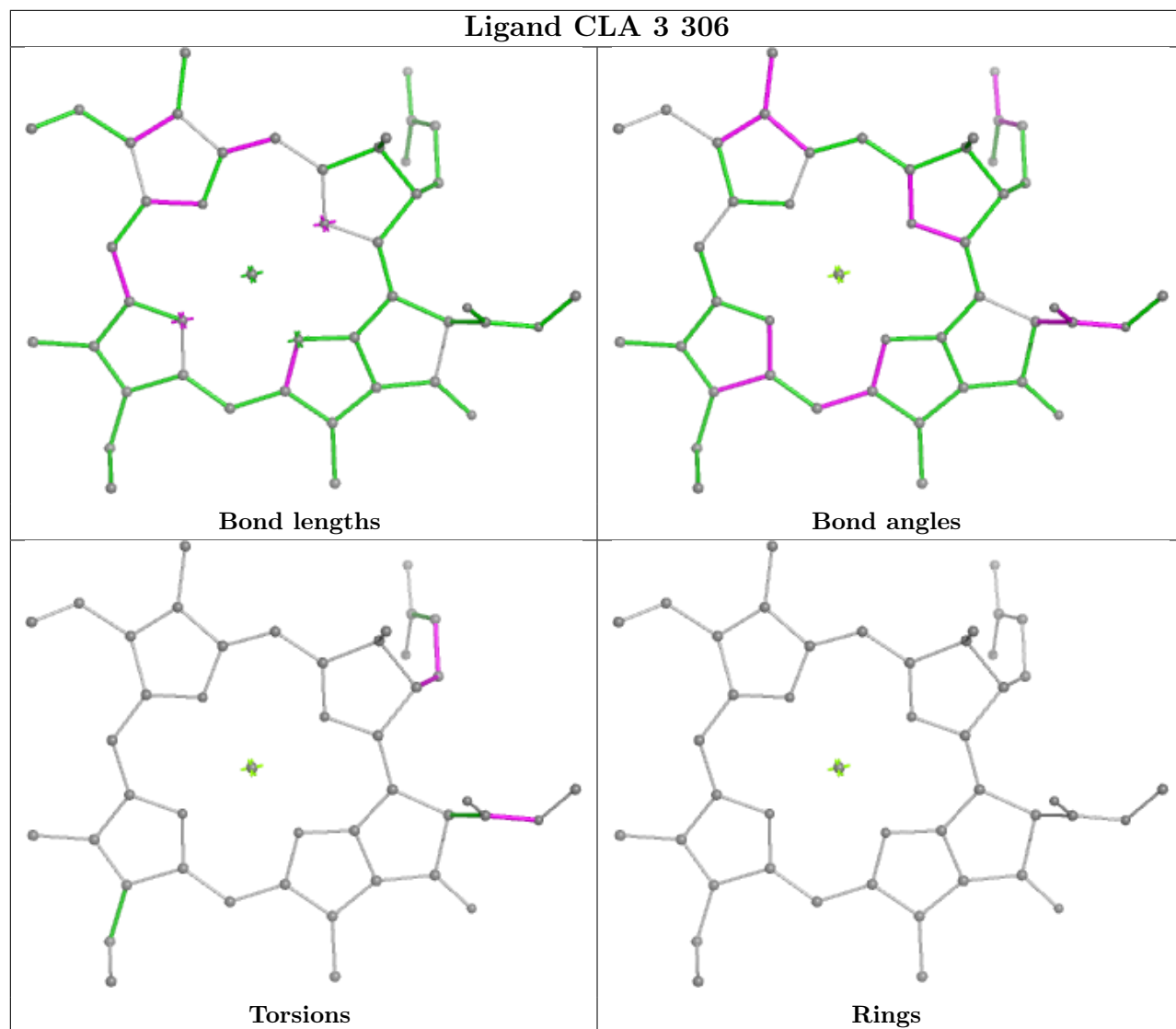
## Ligand CHL 2 301

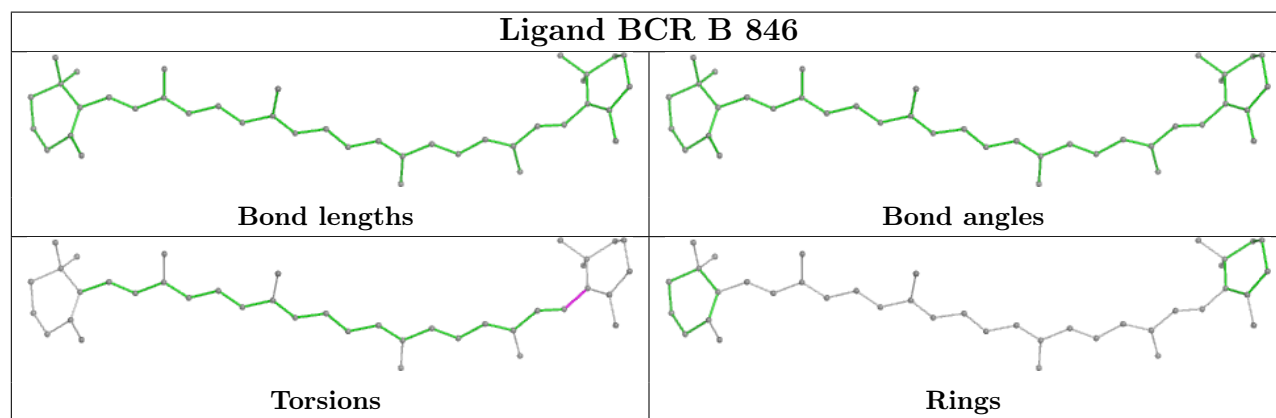
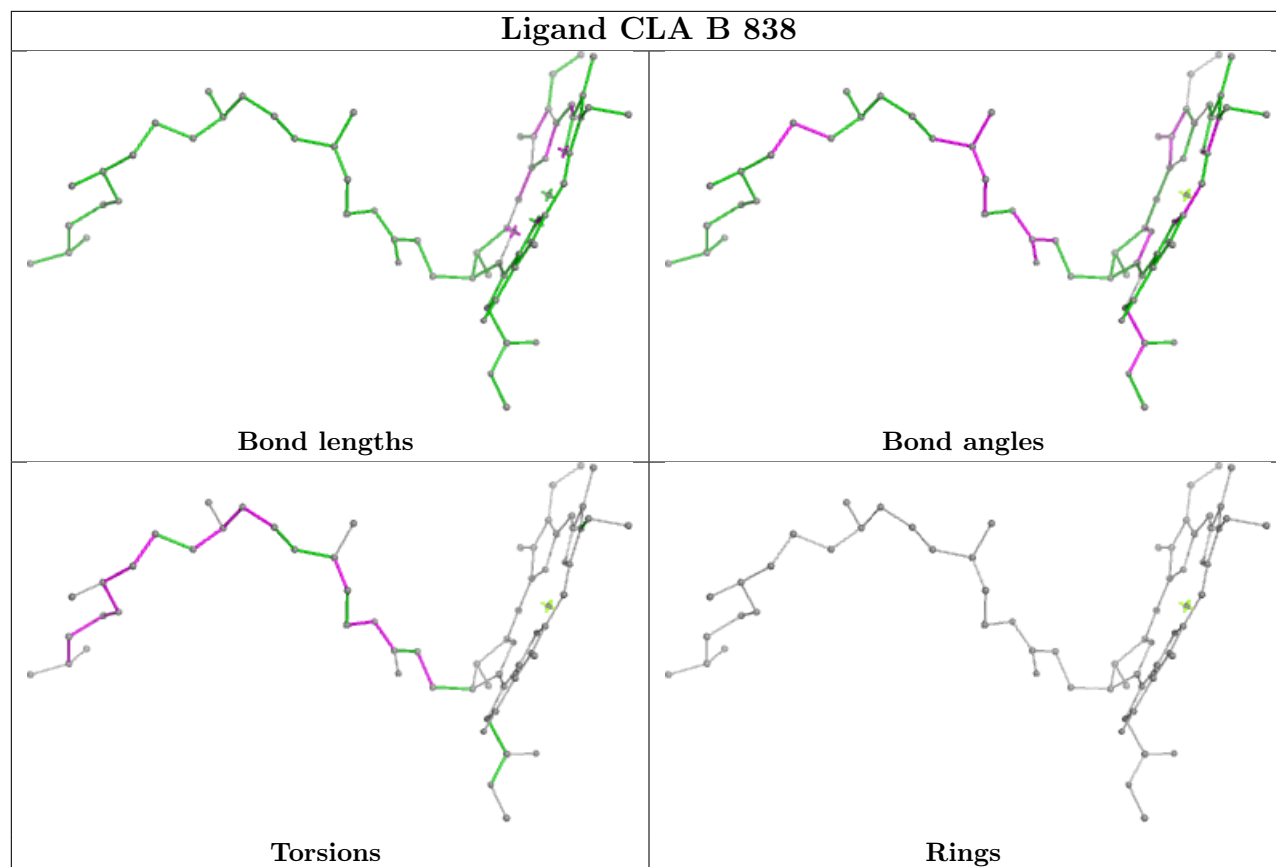


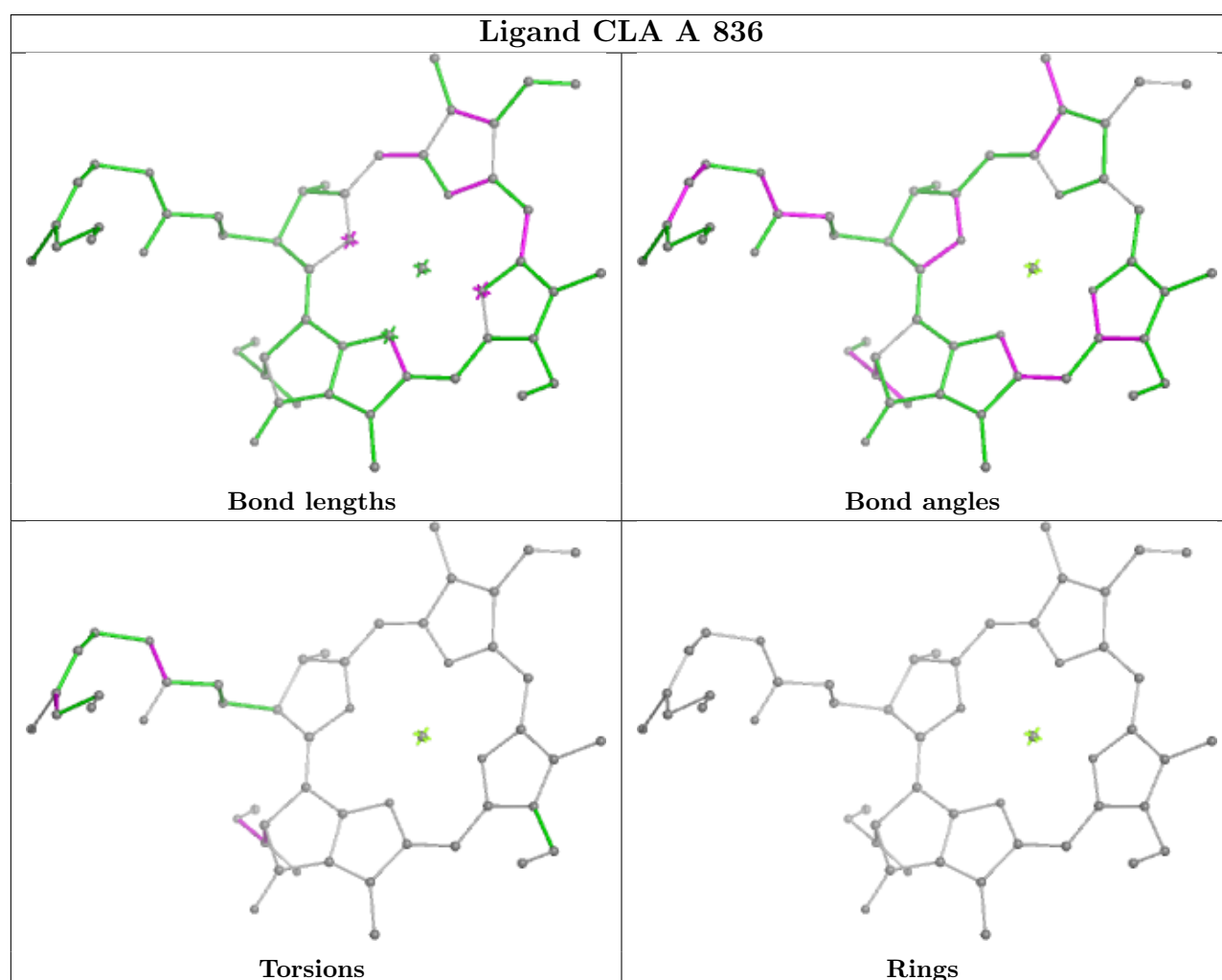
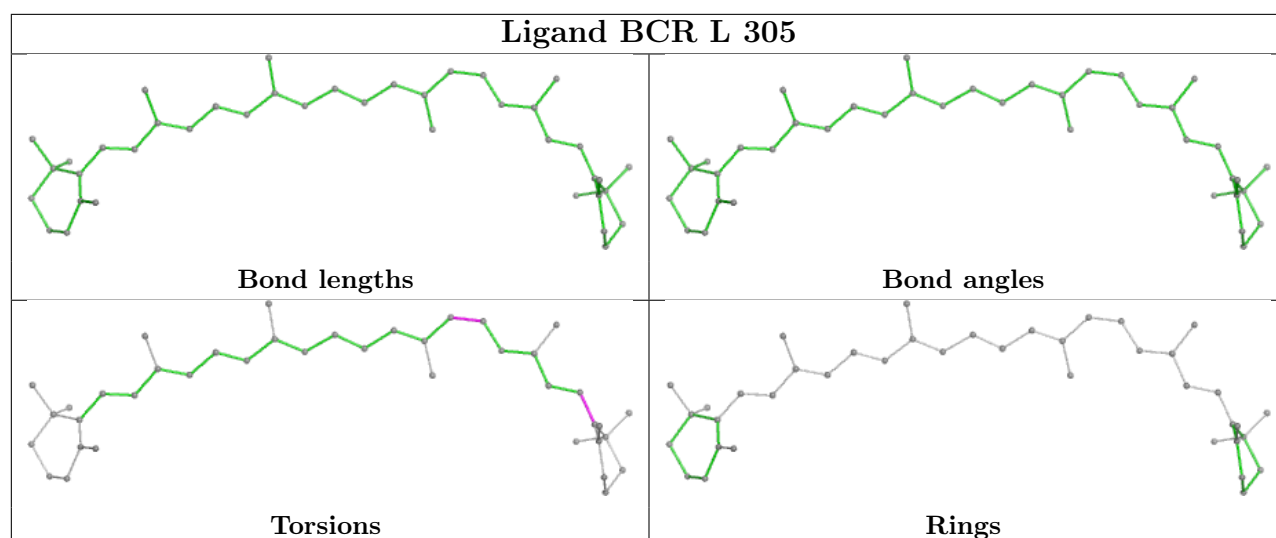
## Ligand CLA 2 308

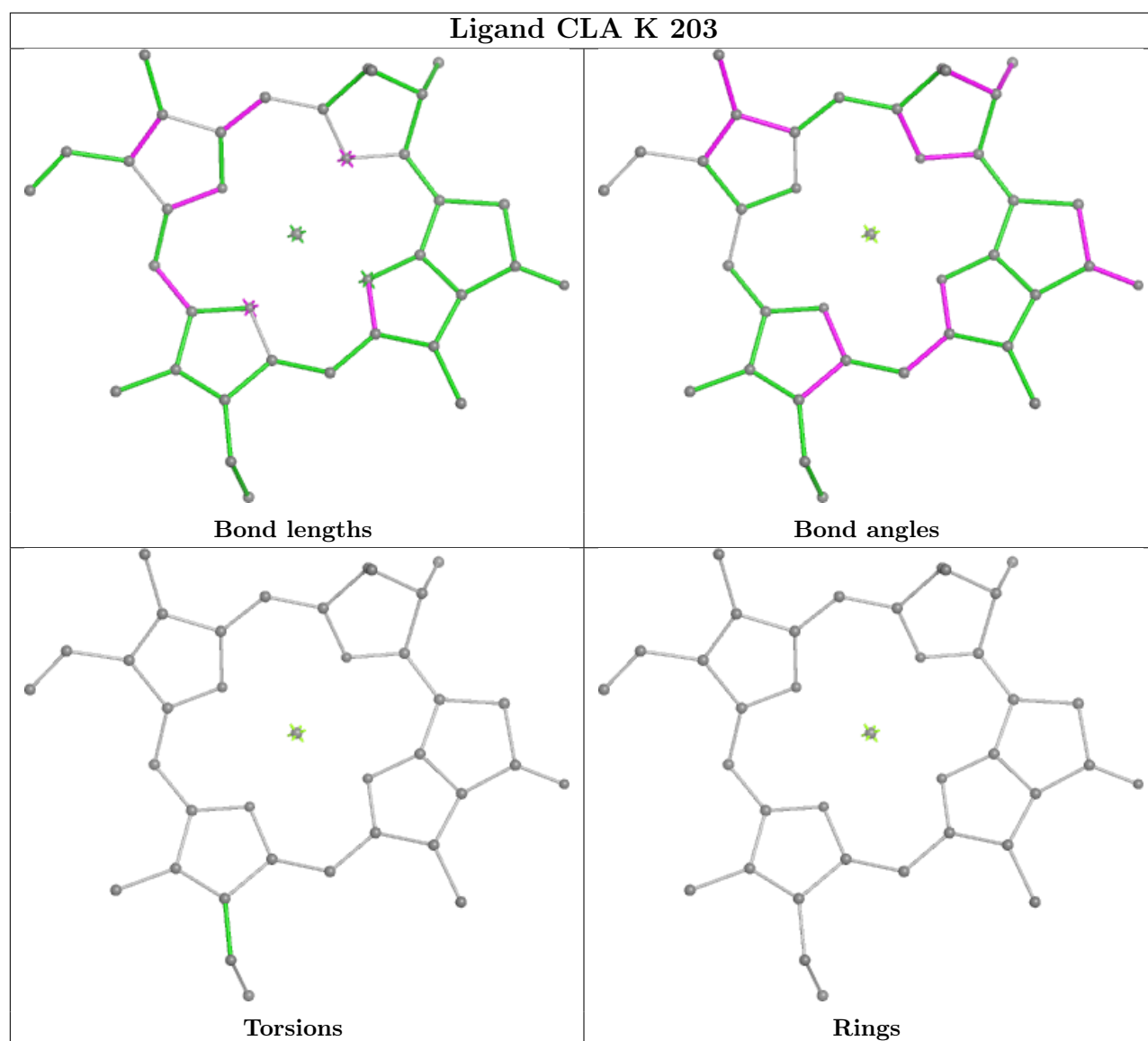


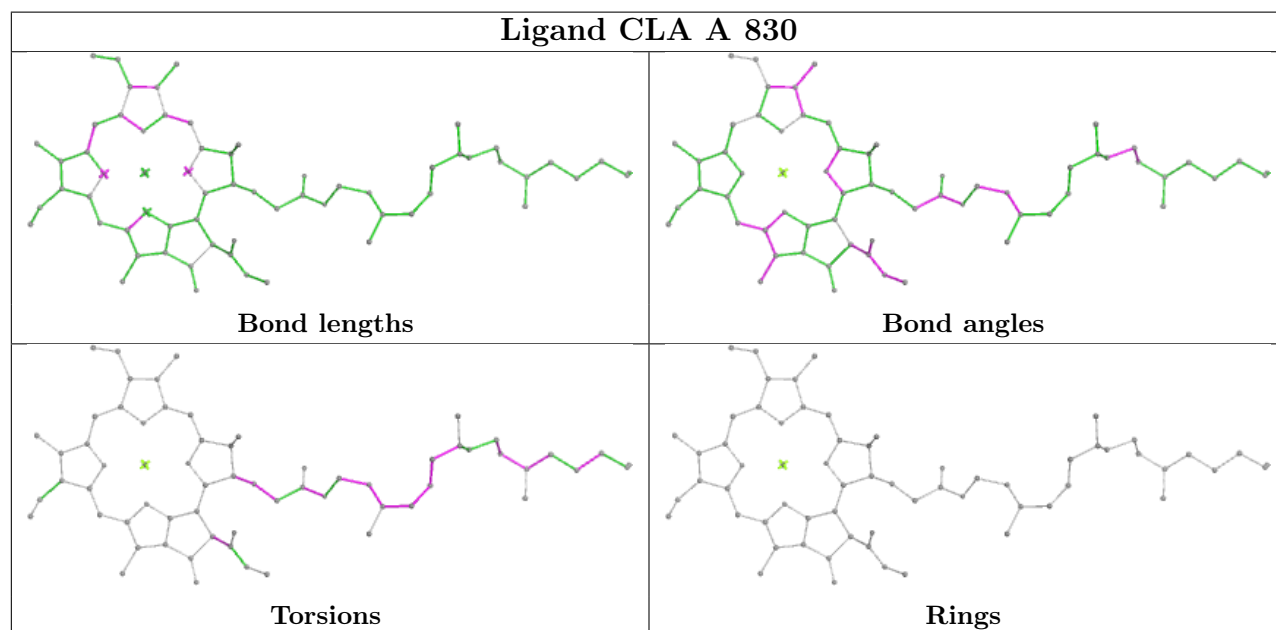
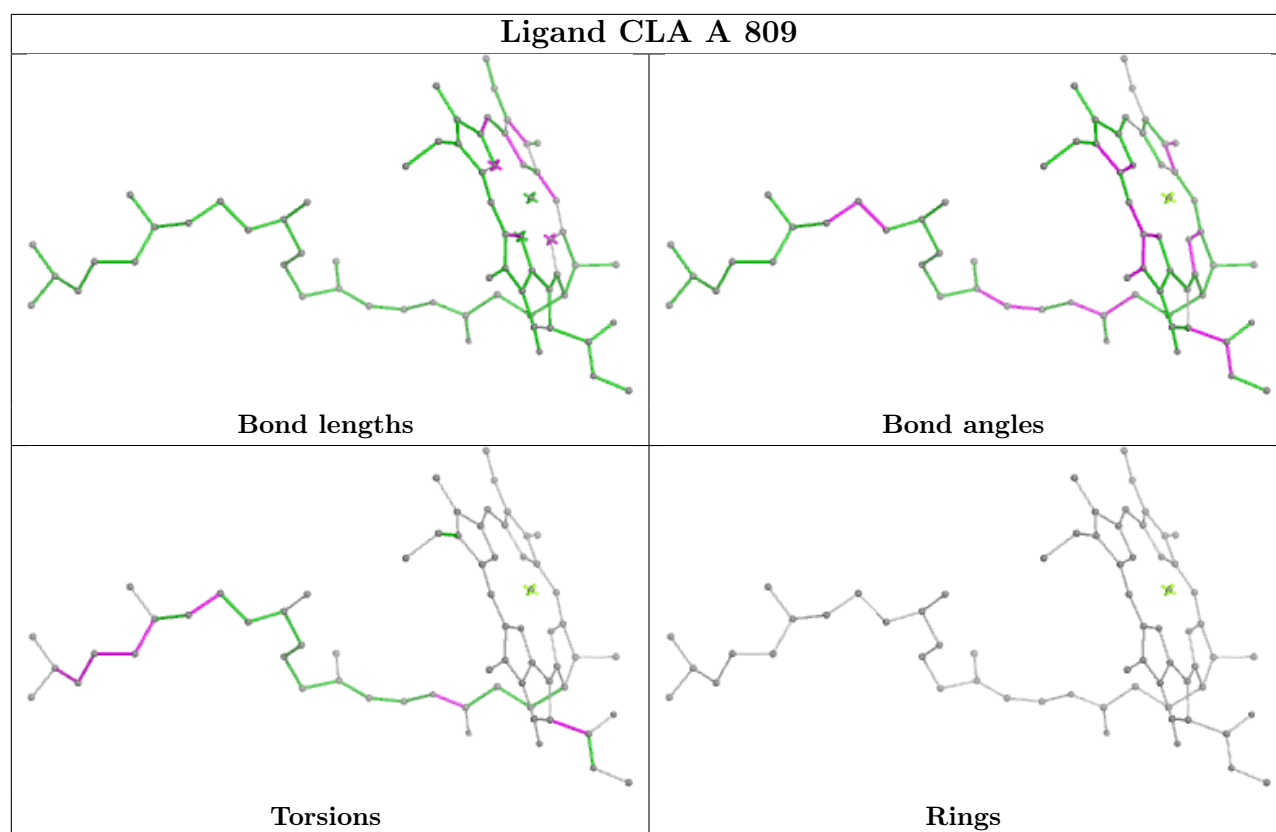
## Ligand CLA 3 306



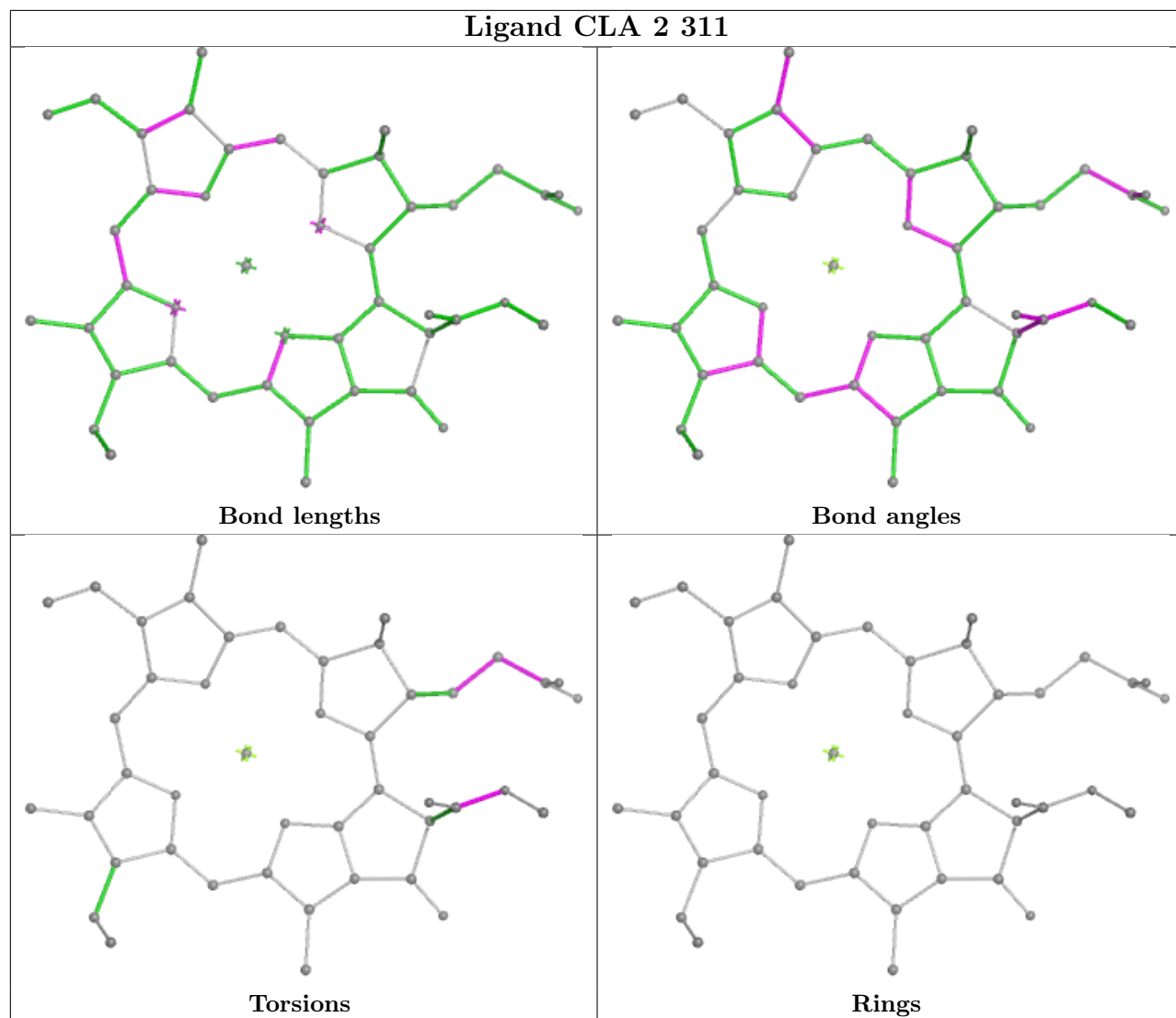






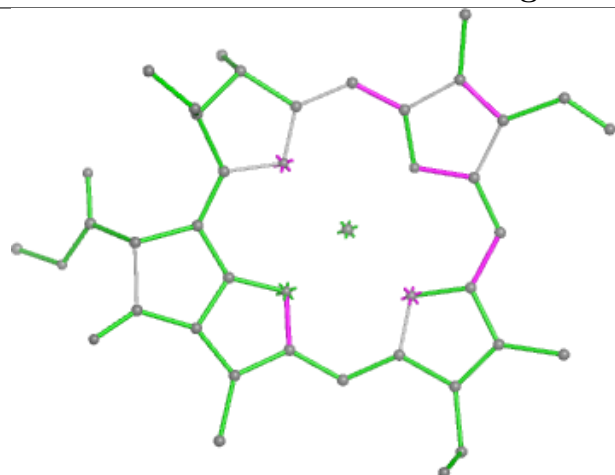


## Ligand CLA 2 311

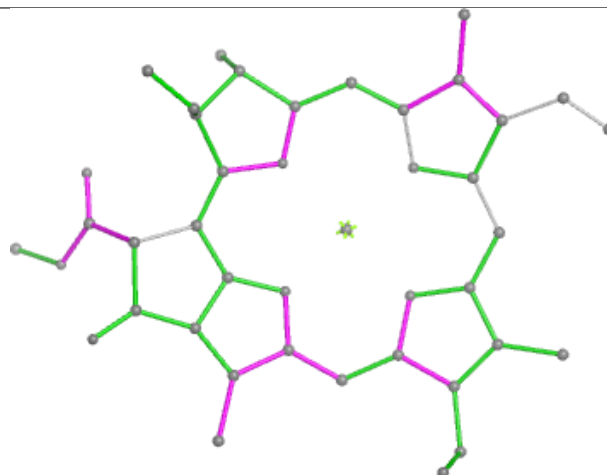




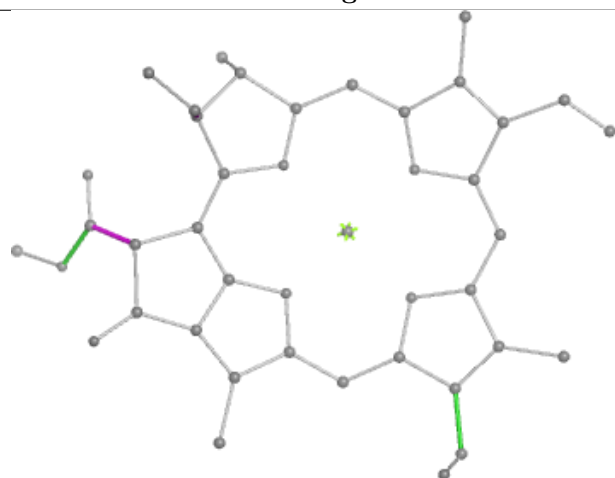
## Ligand CLA J 102



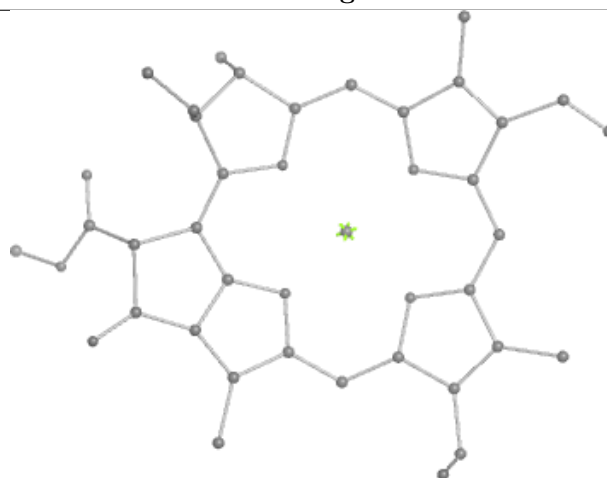
Bond lengths



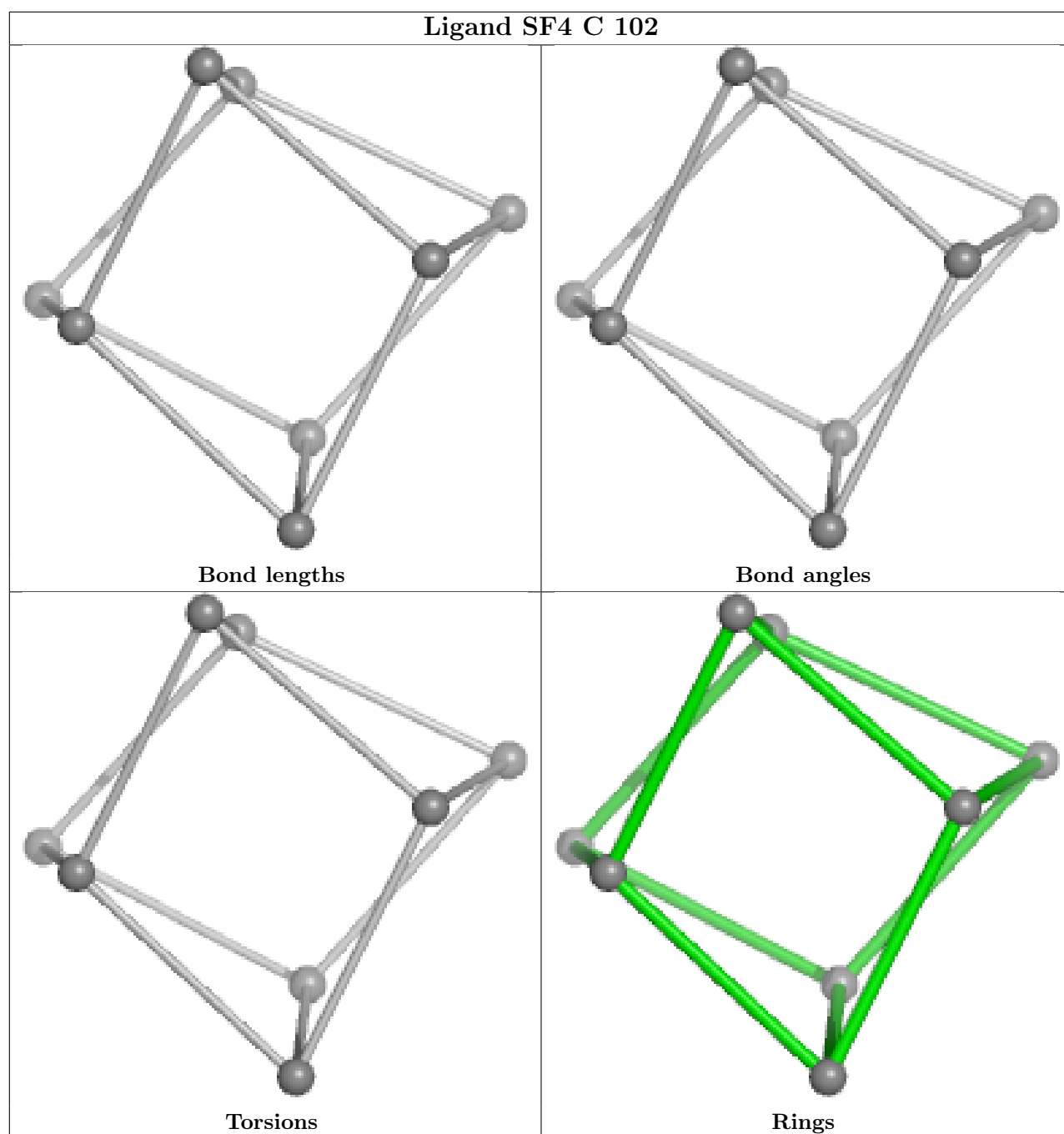
Bond angles

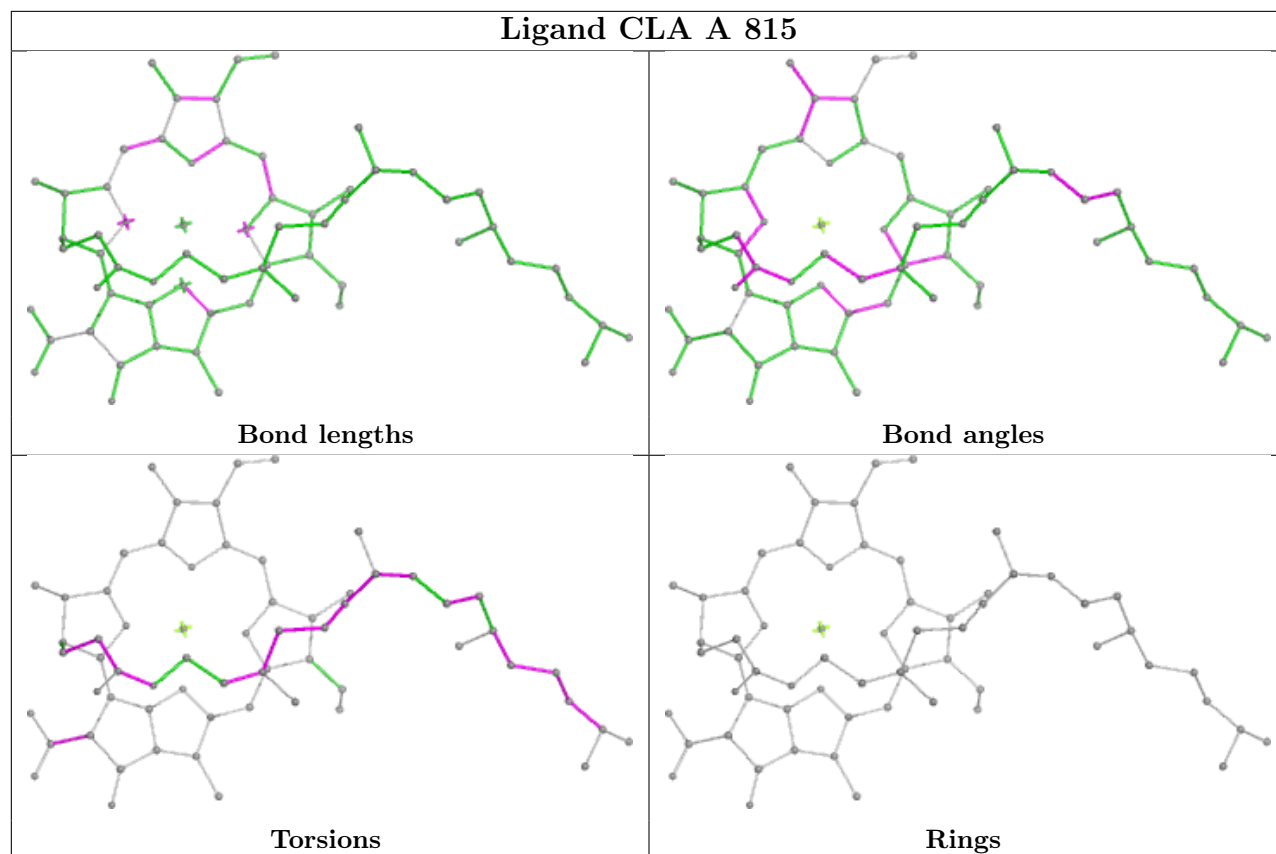
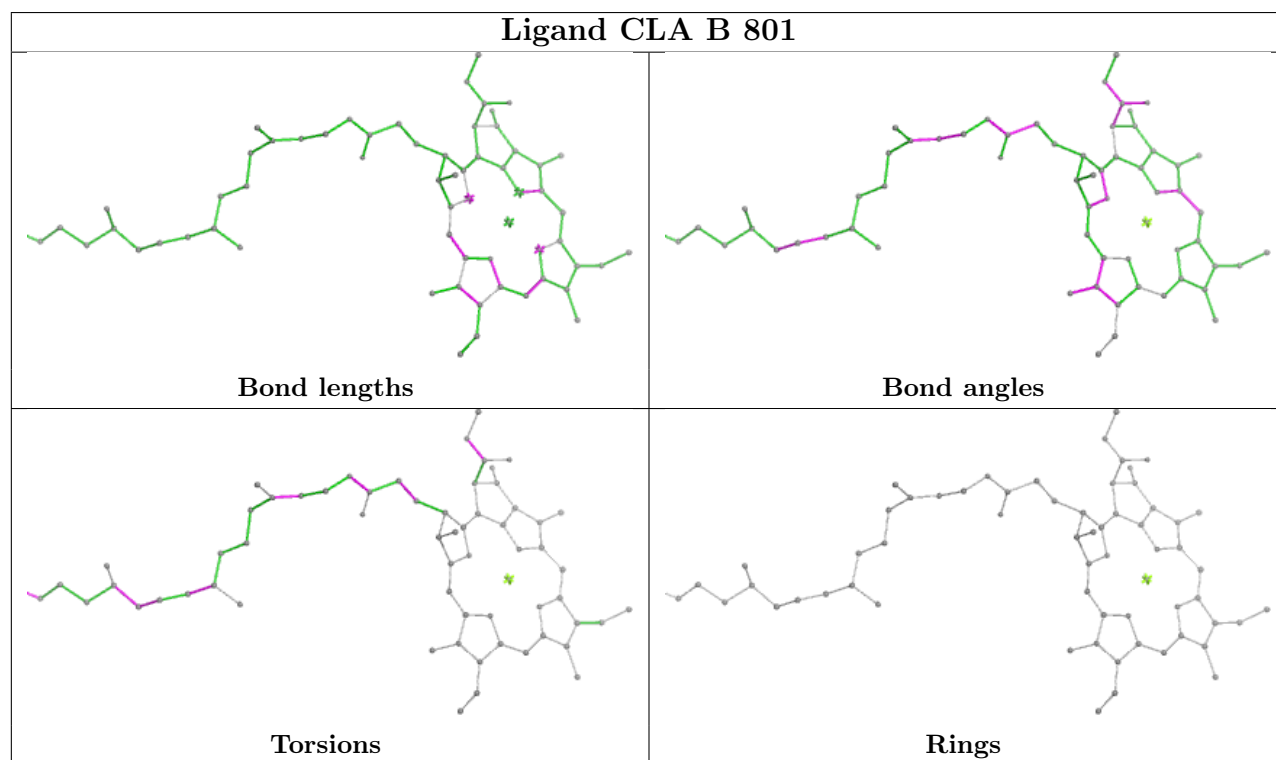


Torsions

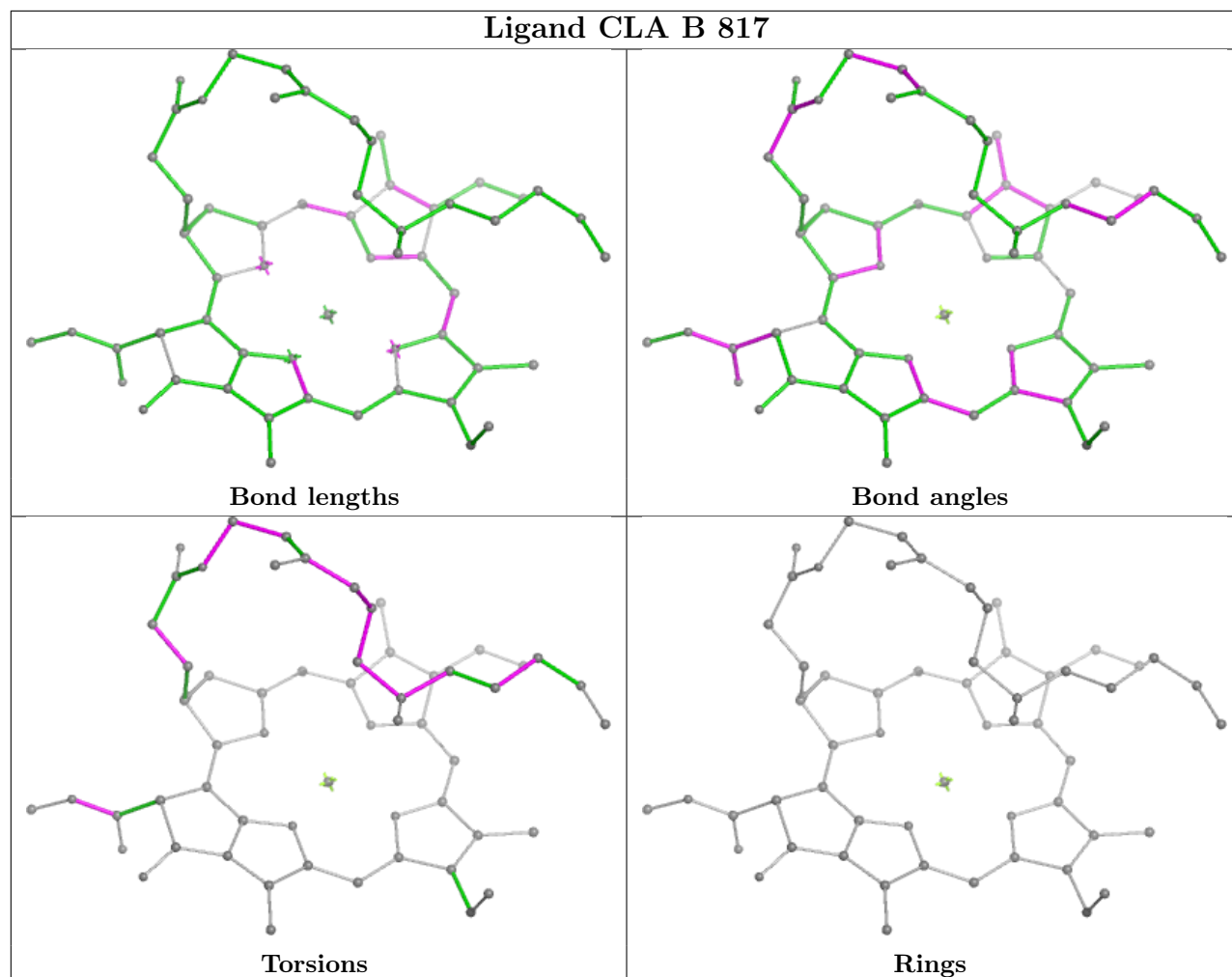


Rings

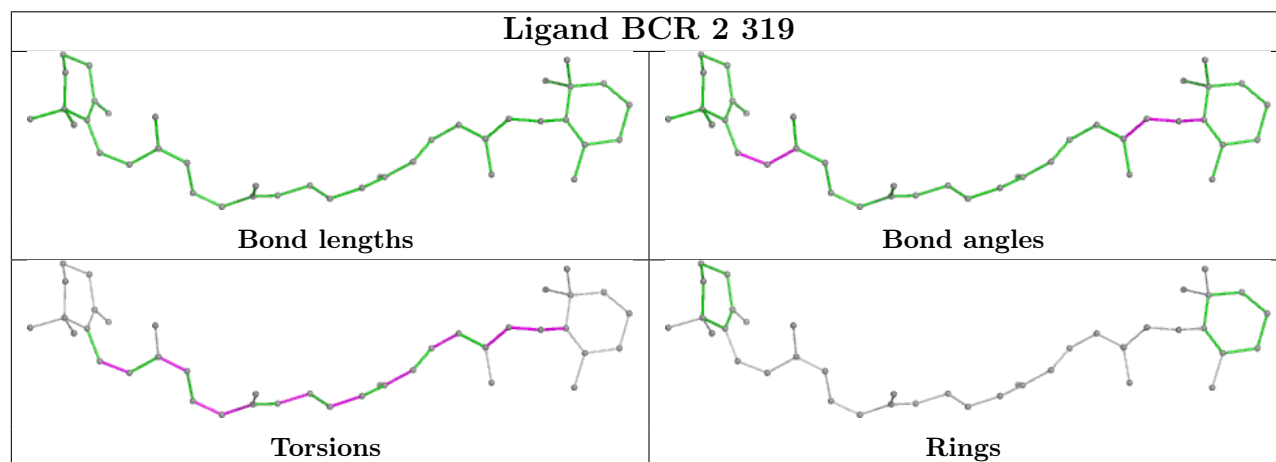


**Ligand CLA A 815****Ligand CLA B 801**

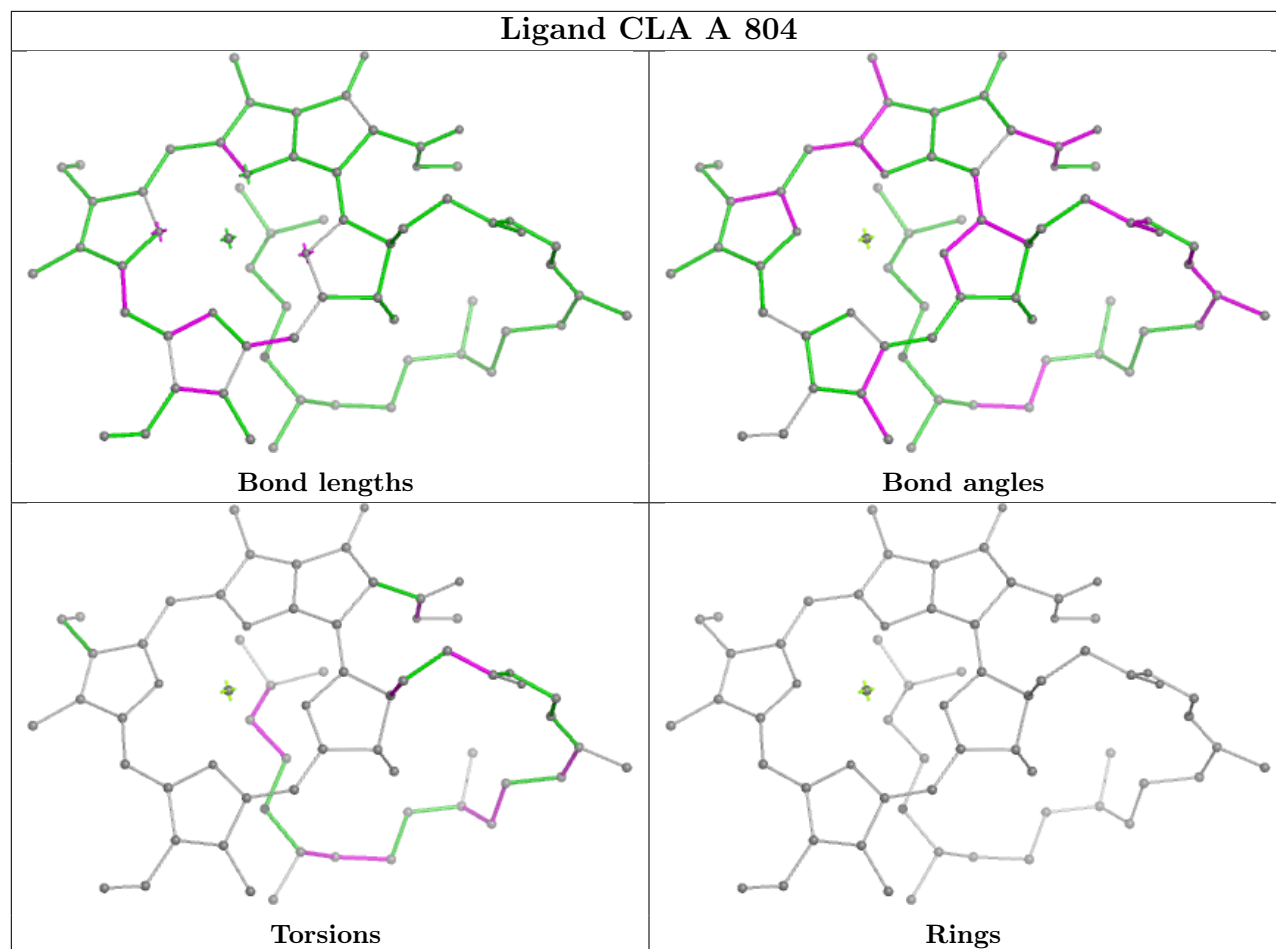
## Ligand CLA B 817



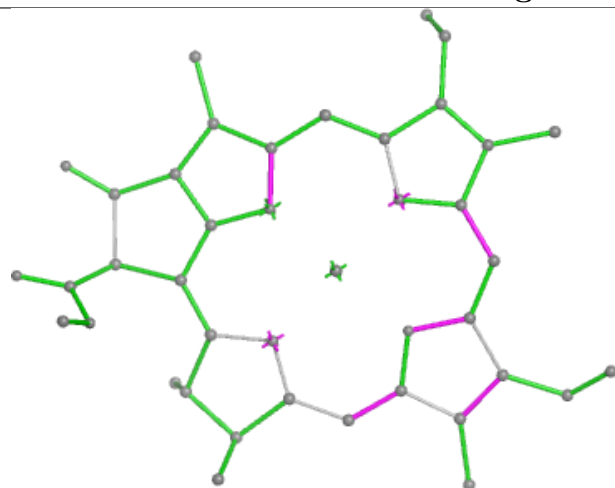
## Ligand BCR 2 319



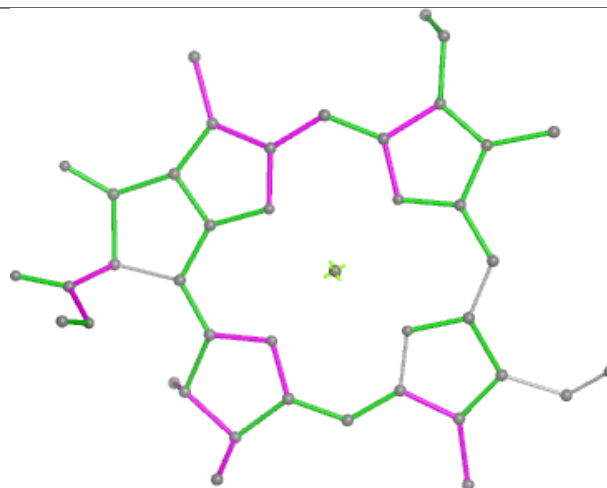
## Ligand CLA A 804



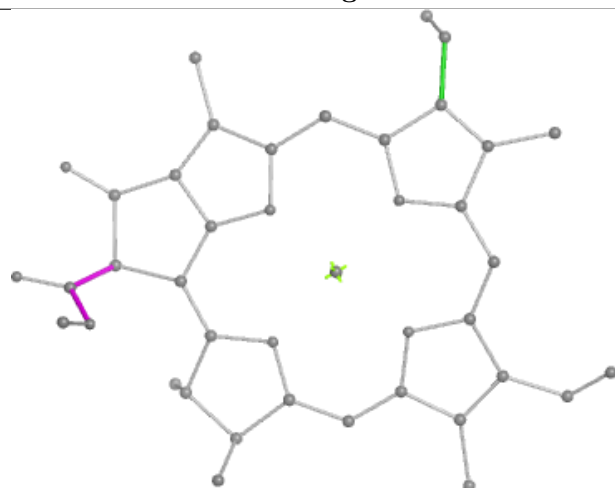
## Ligand CLA G 202



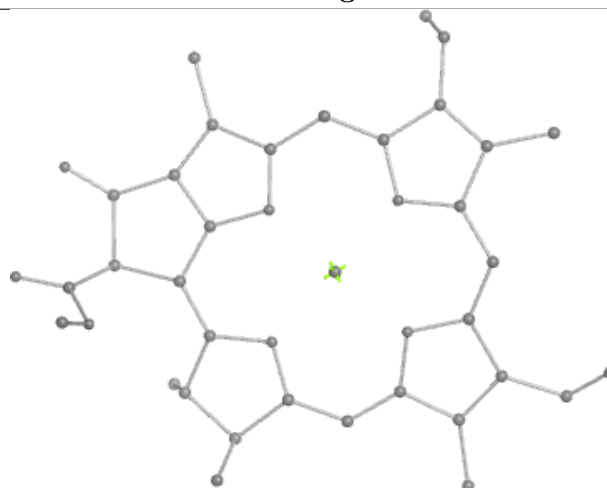
Bond lengths



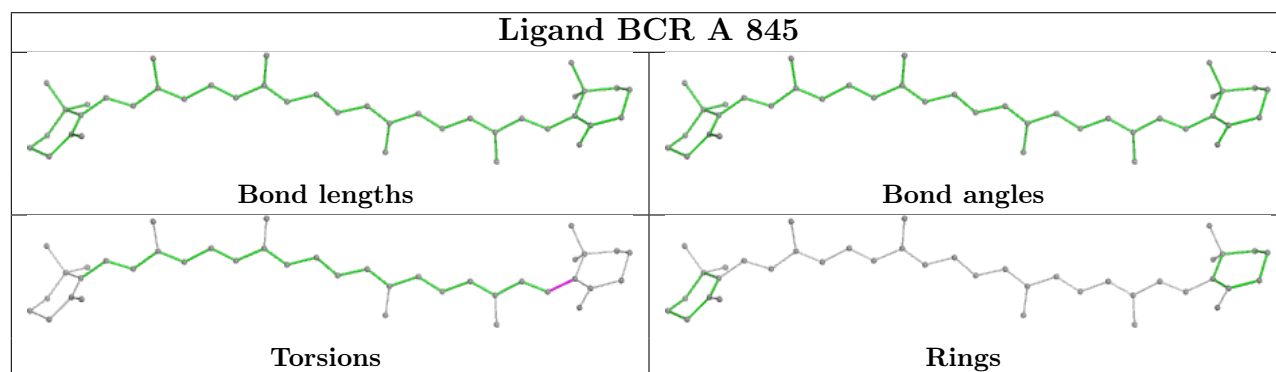
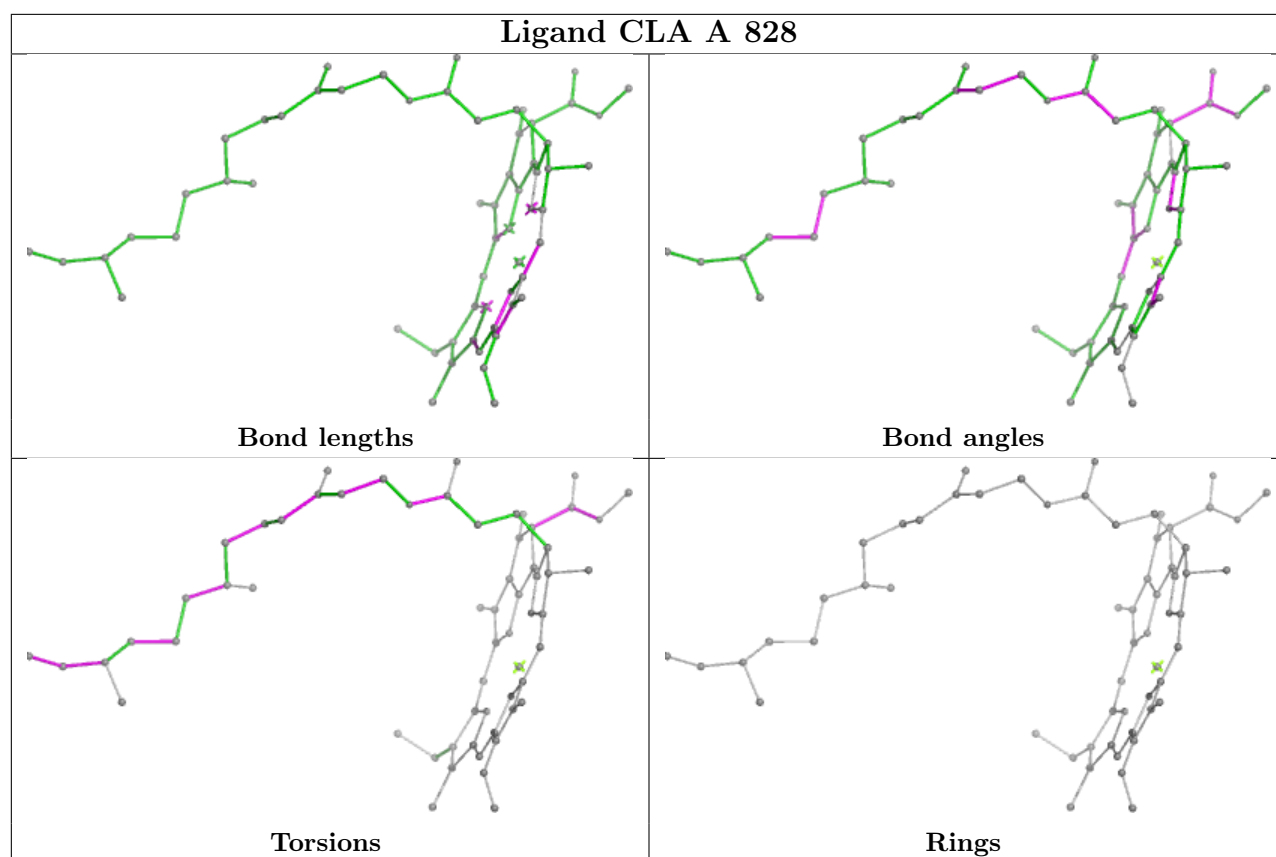
Bond angles



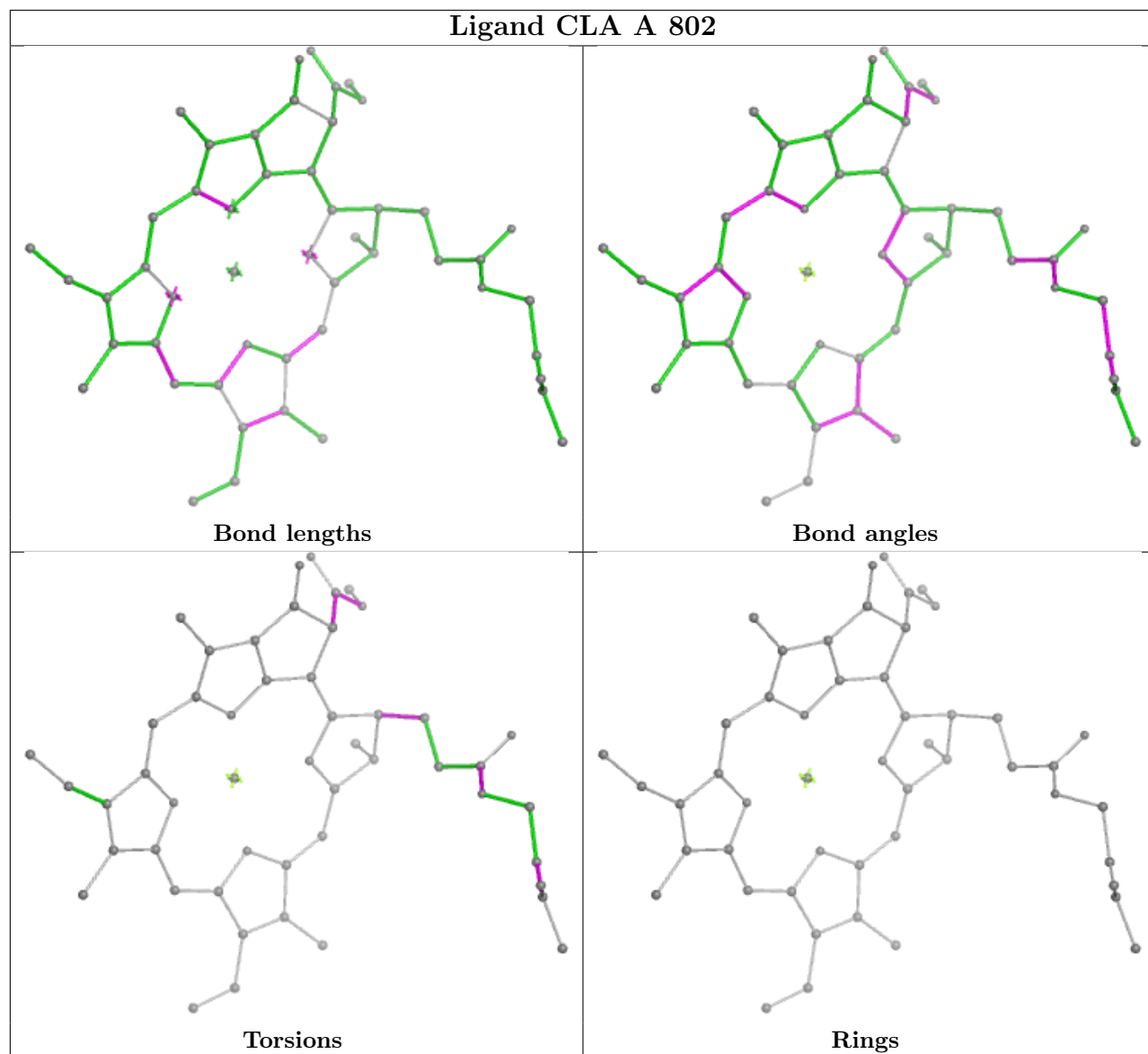
Torsions



Rings

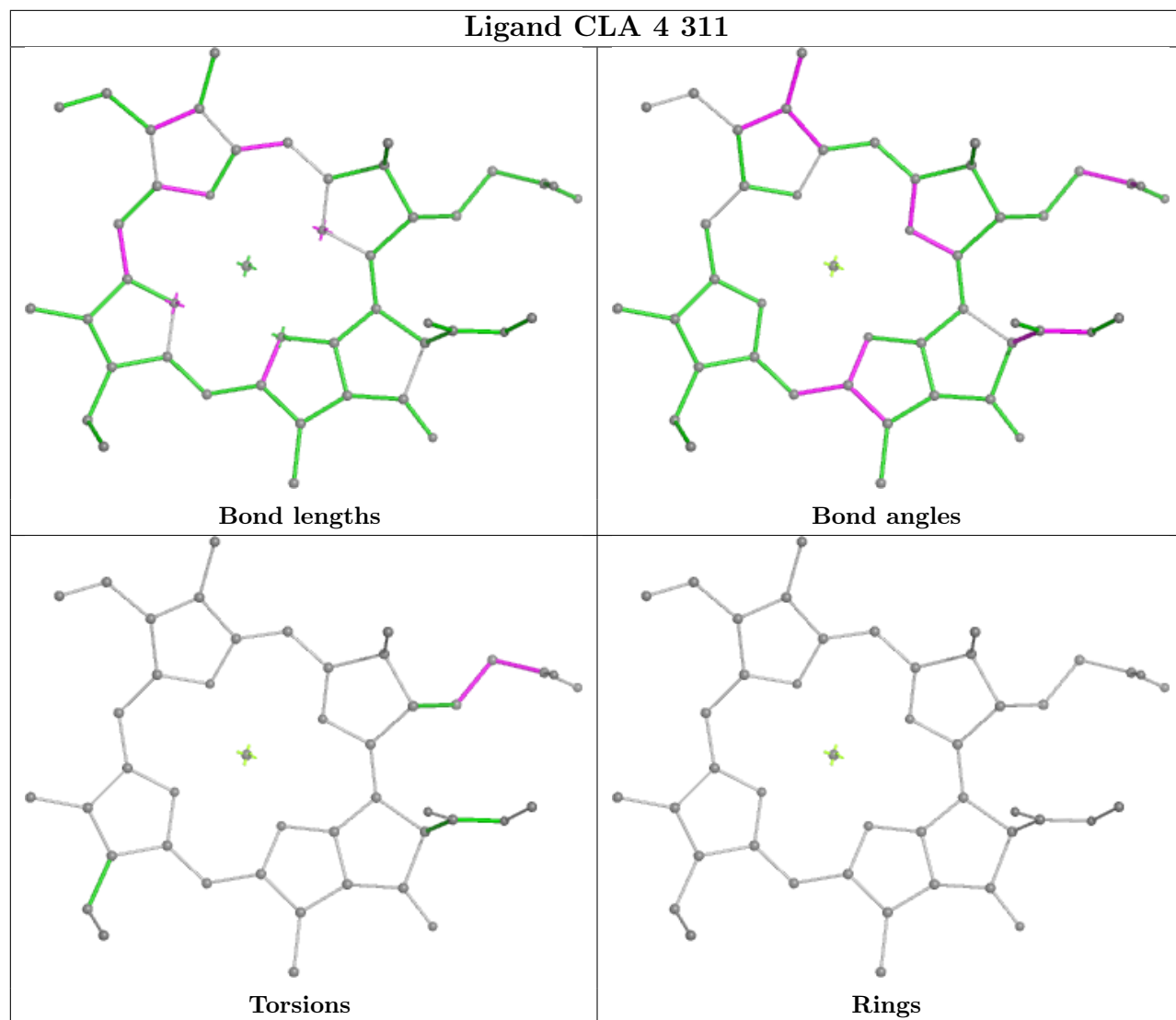


## Ligand CLA A 802

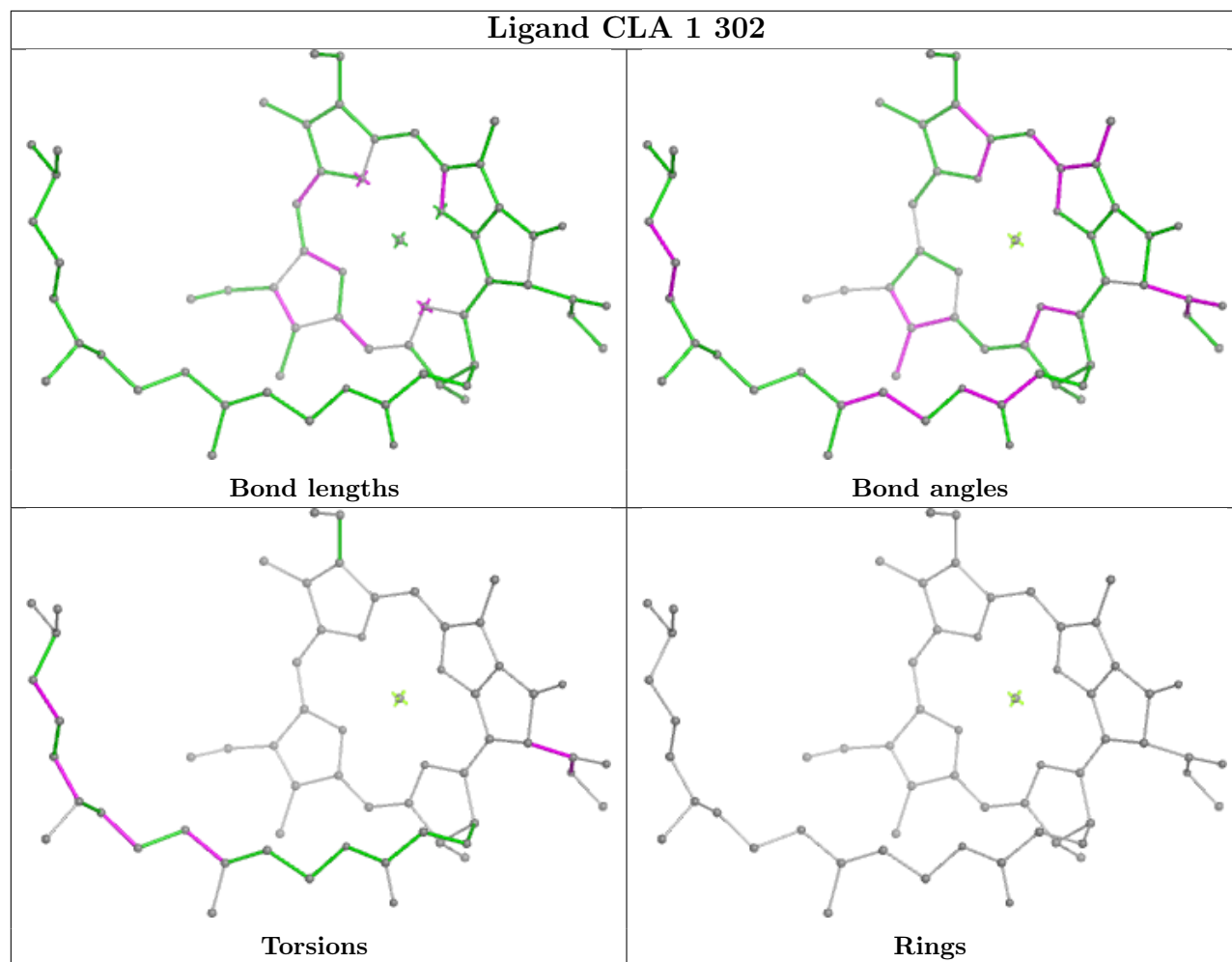




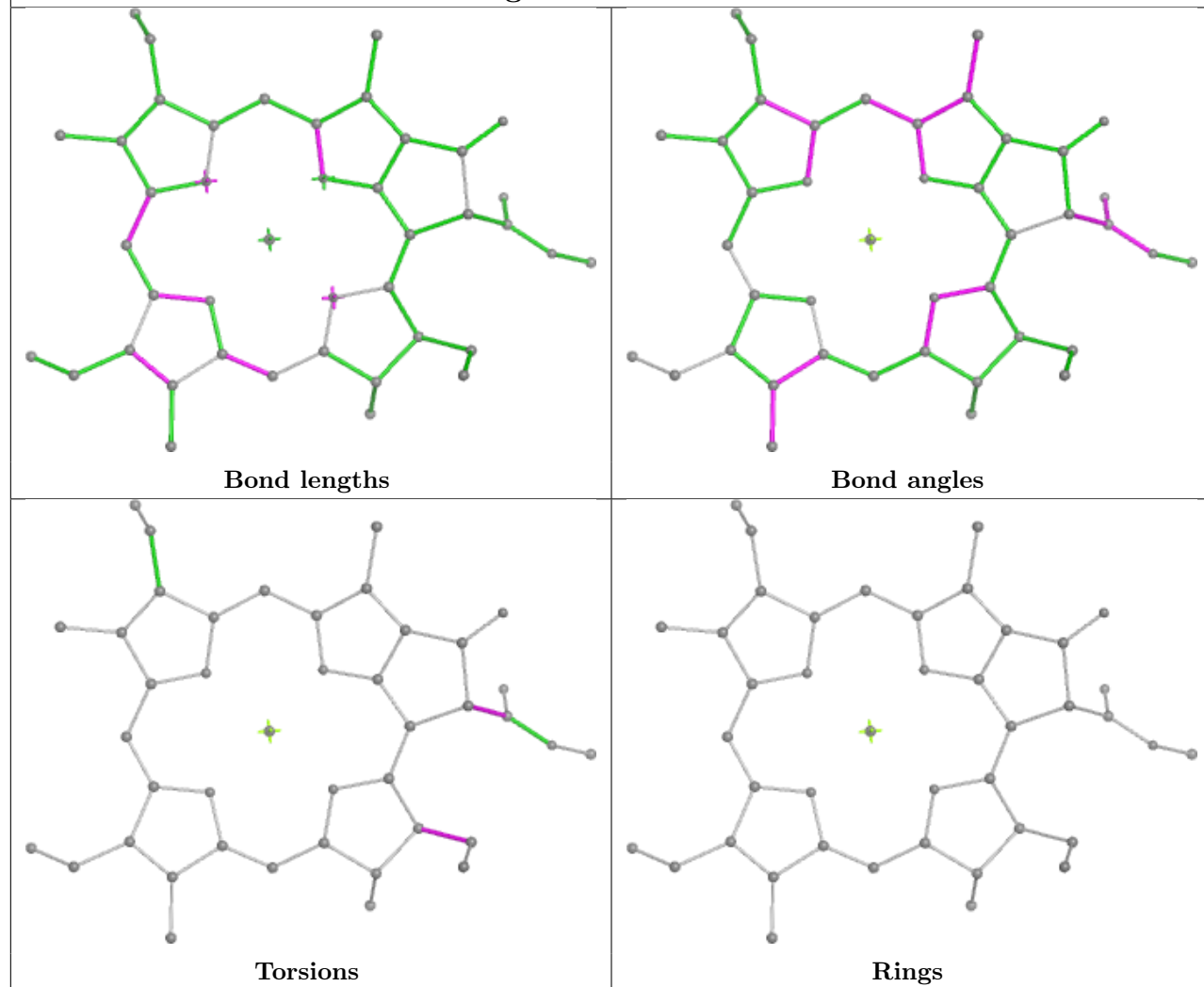
## Ligand CLA 4 311



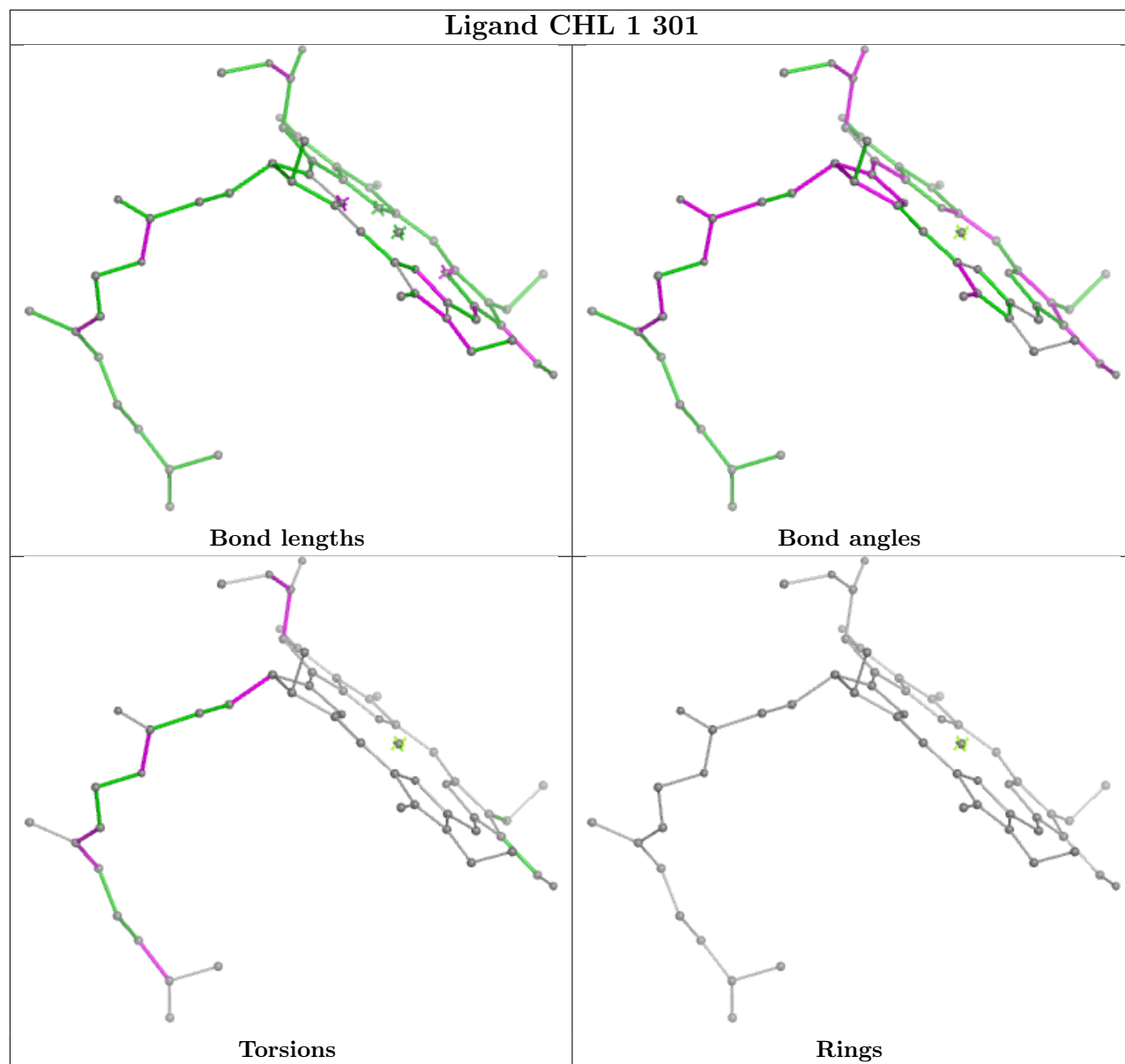
## Ligand CLA 1 302



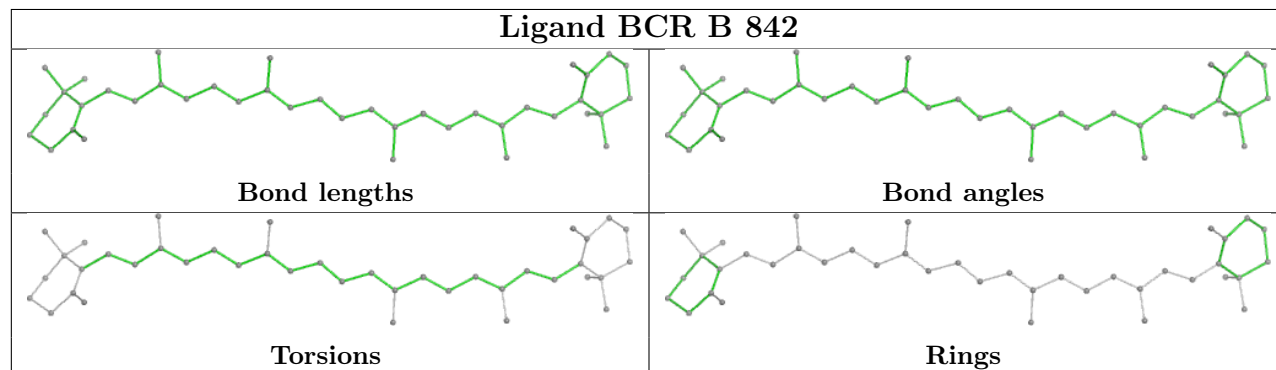
## Ligand CLA 3 305



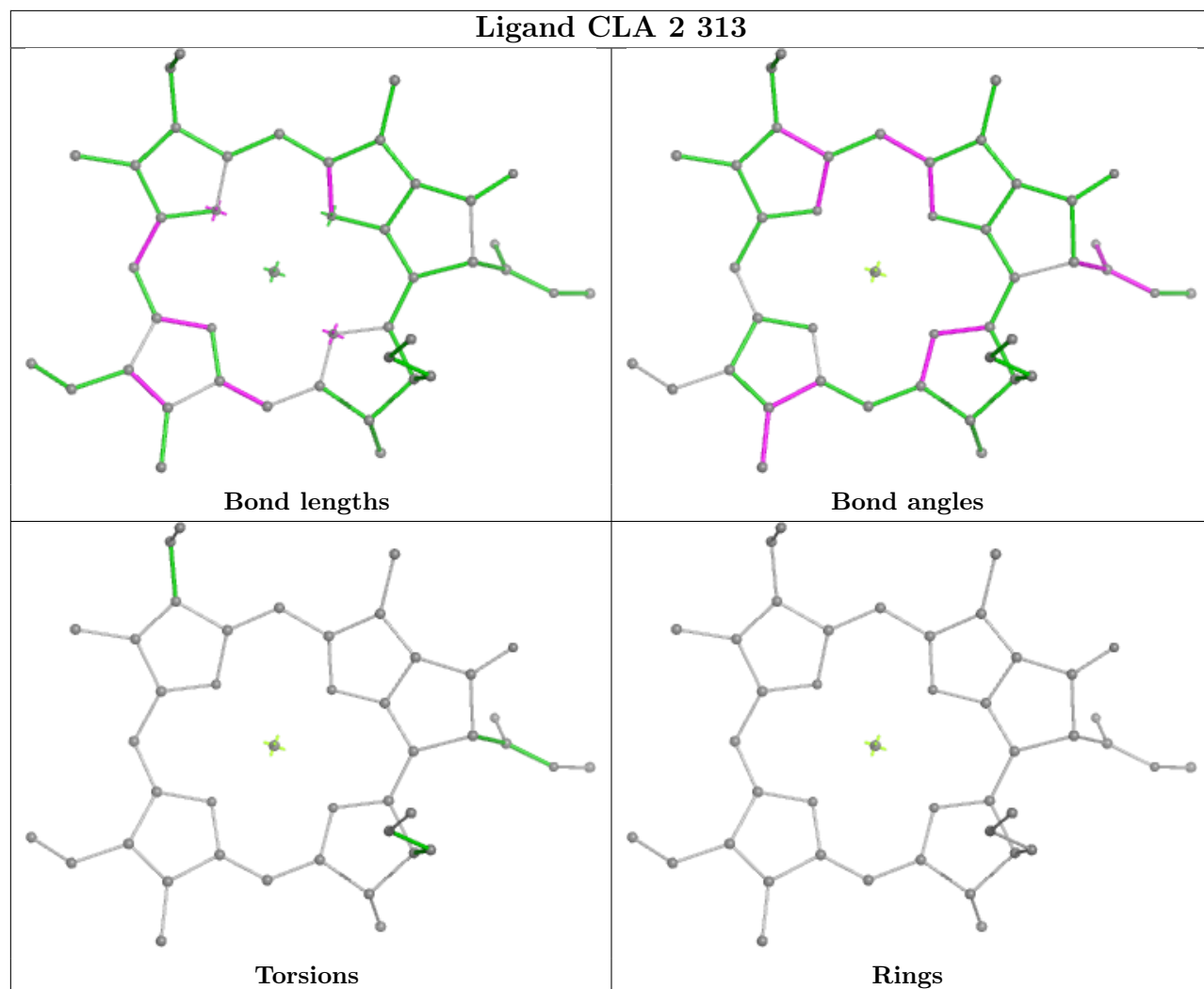
## Ligand CHL 1 301



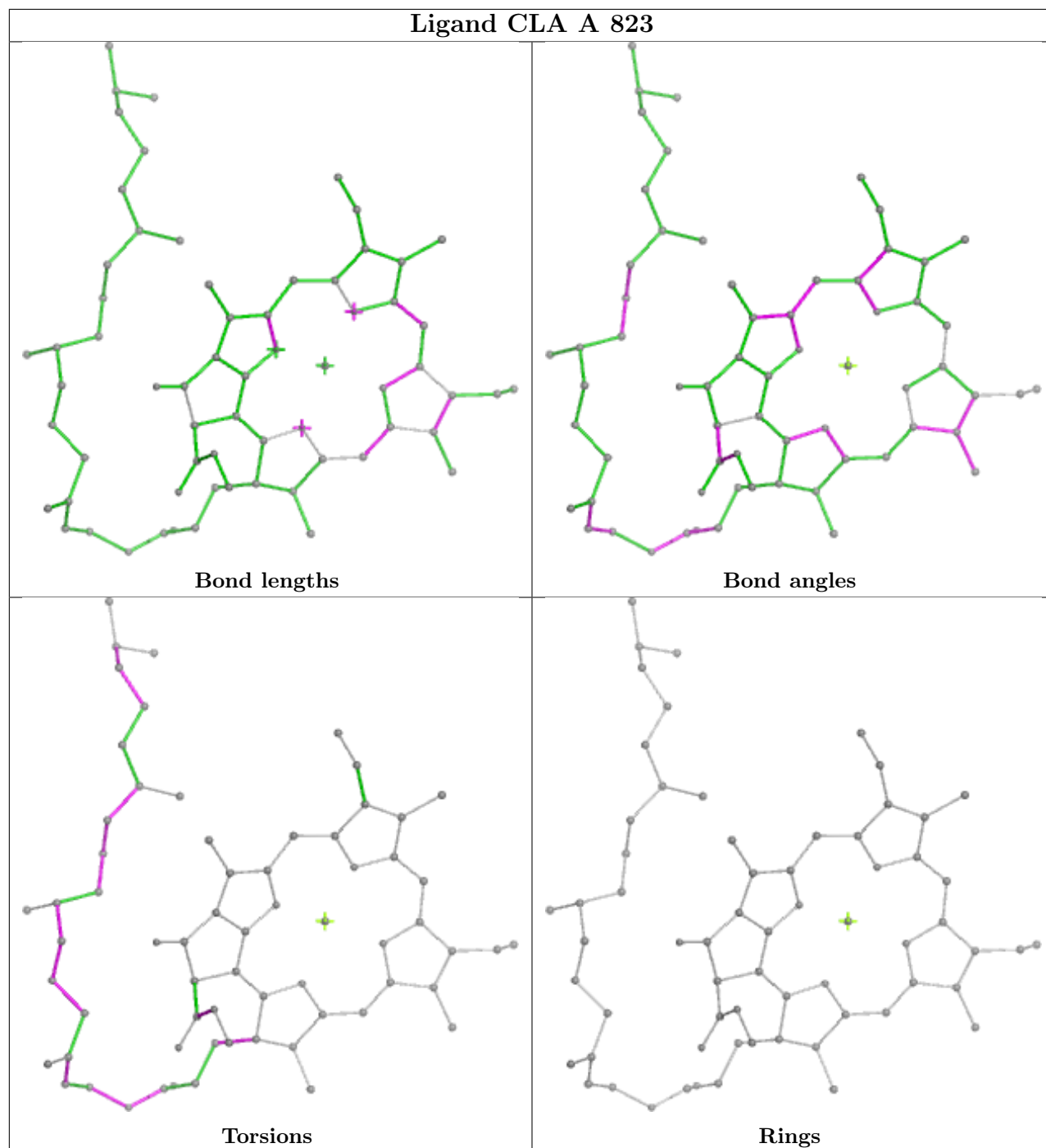
## Ligand BCR B 842



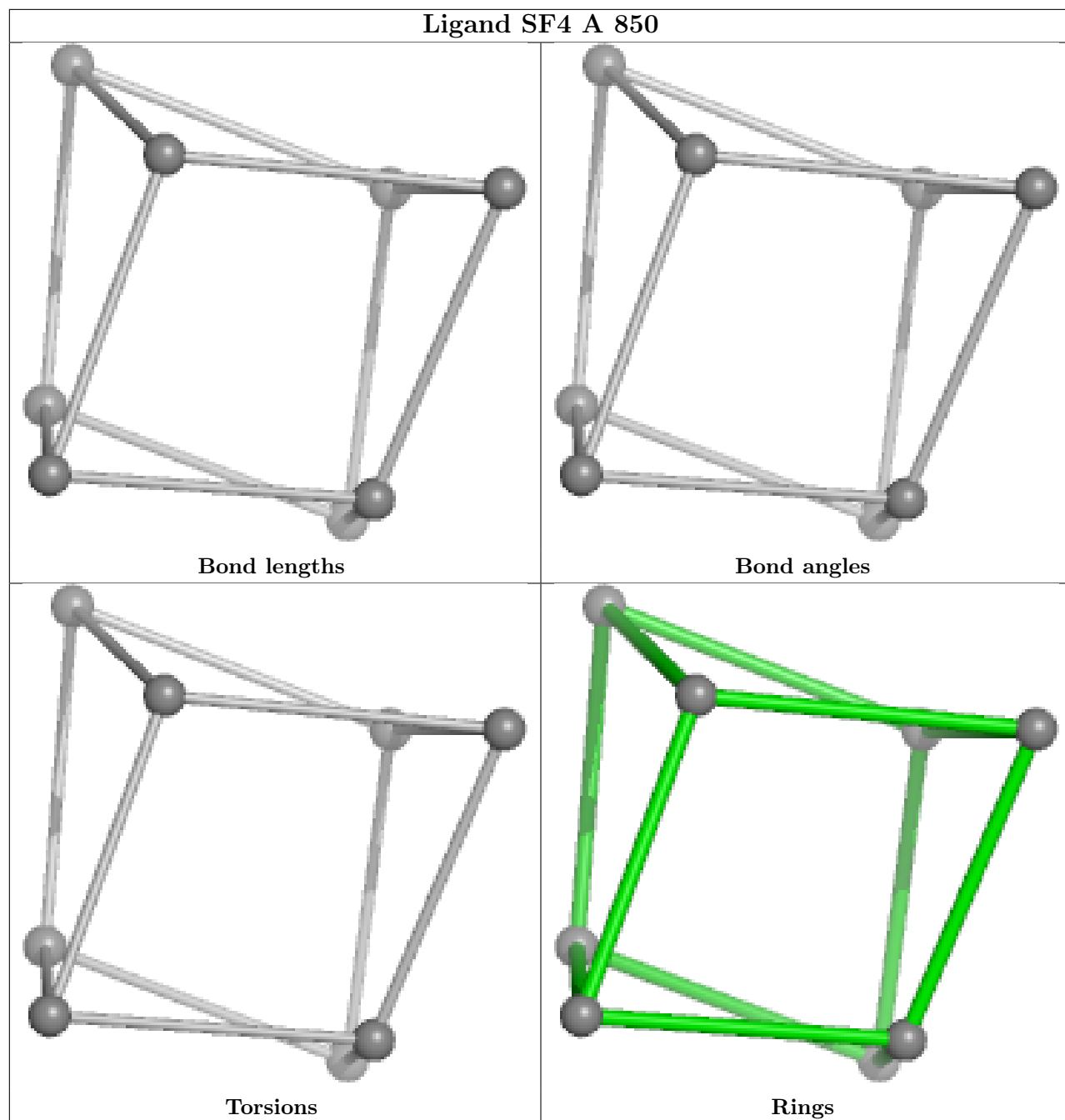
## Ligand CLA 2 313



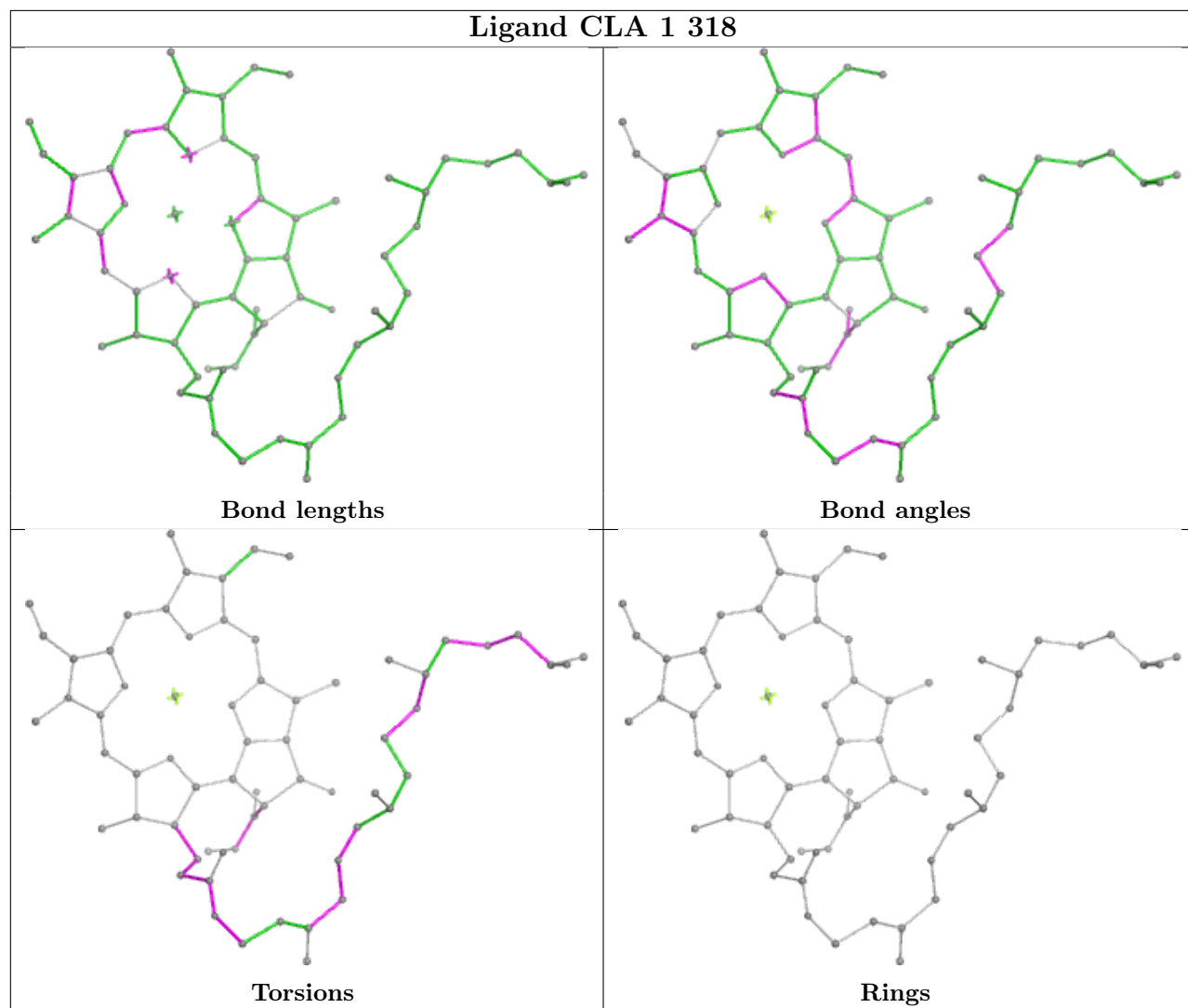
## Ligand CLA A 823



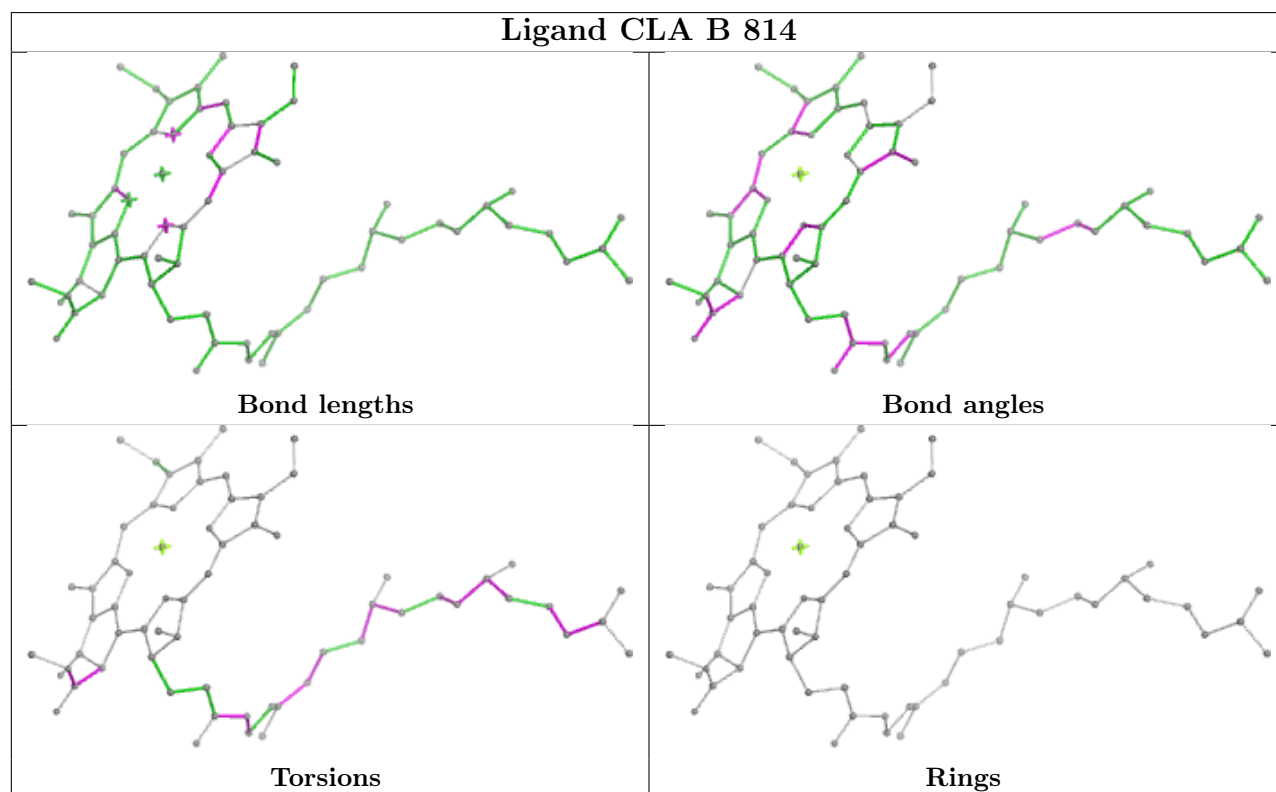
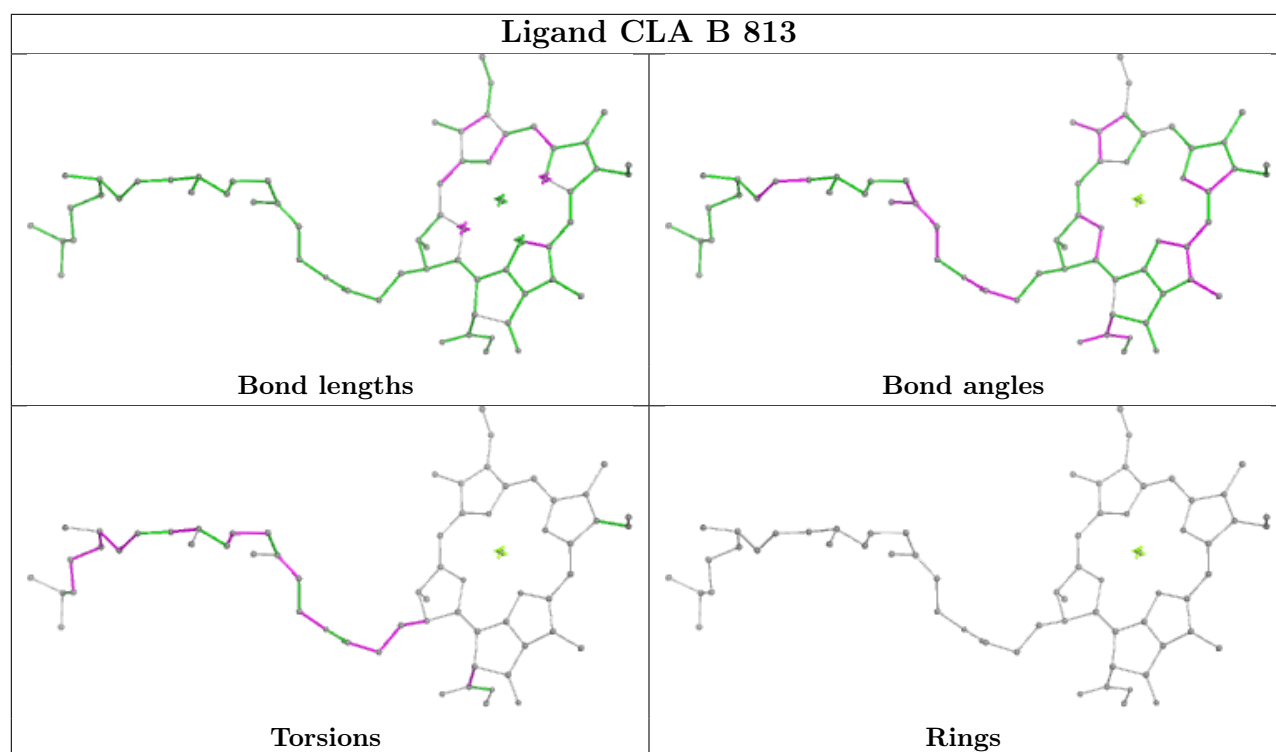
## Ligand SF4 A 850

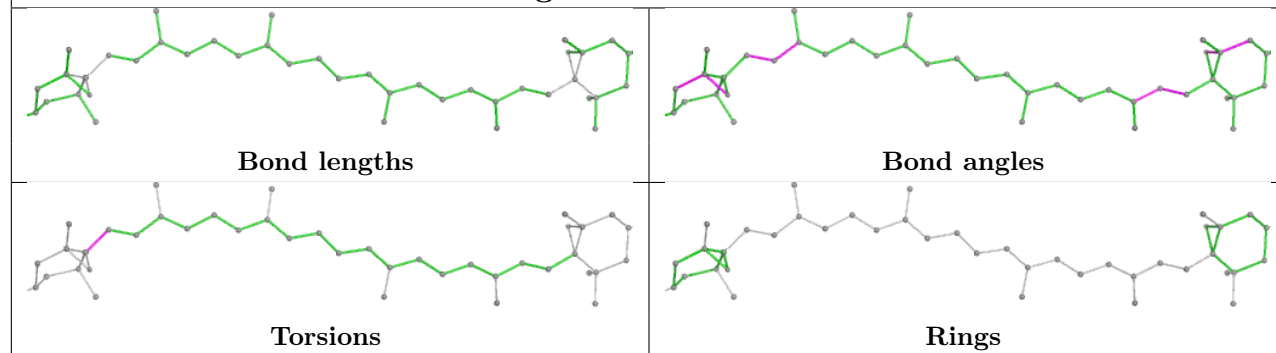
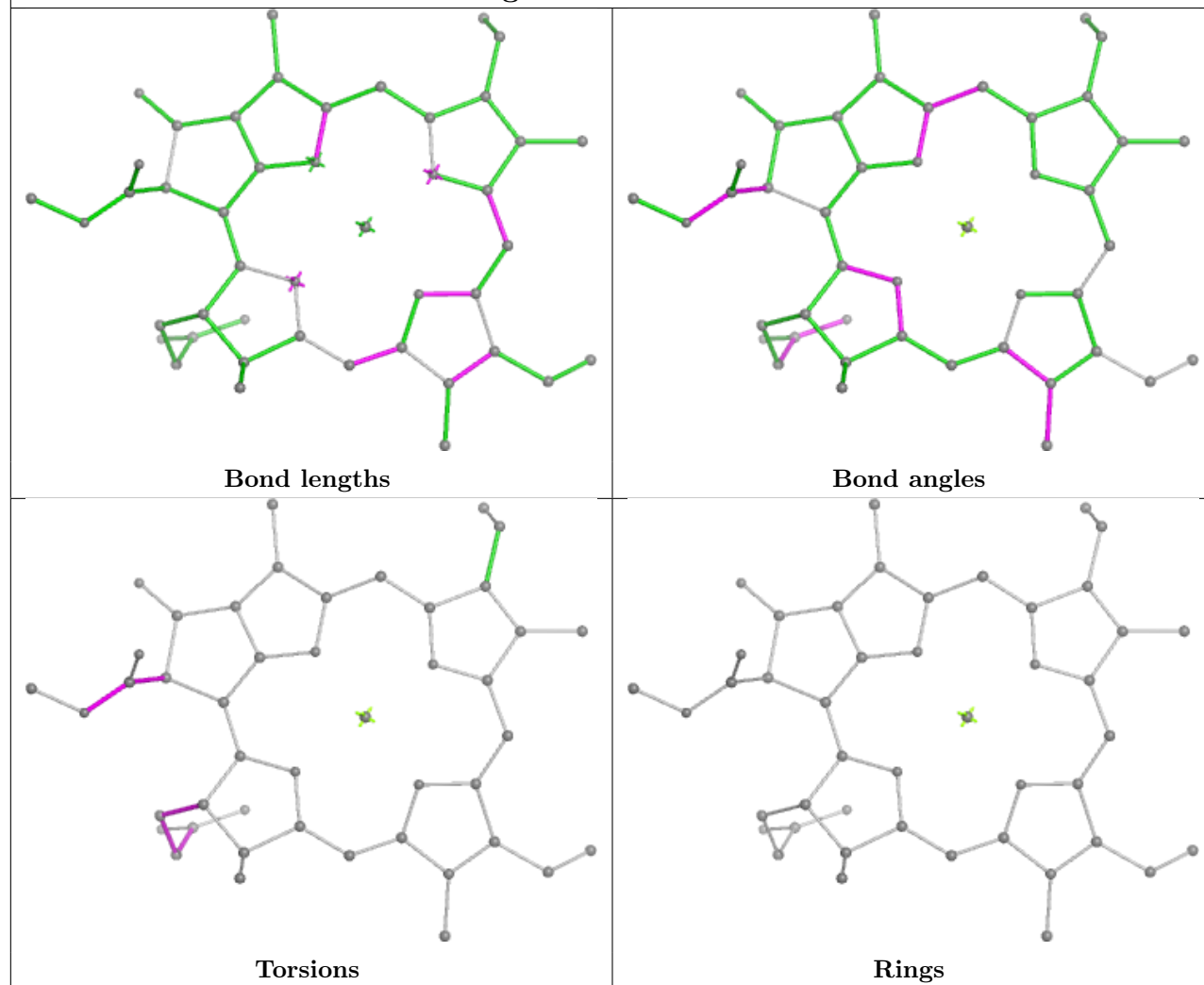


## Ligand CLA 1 318

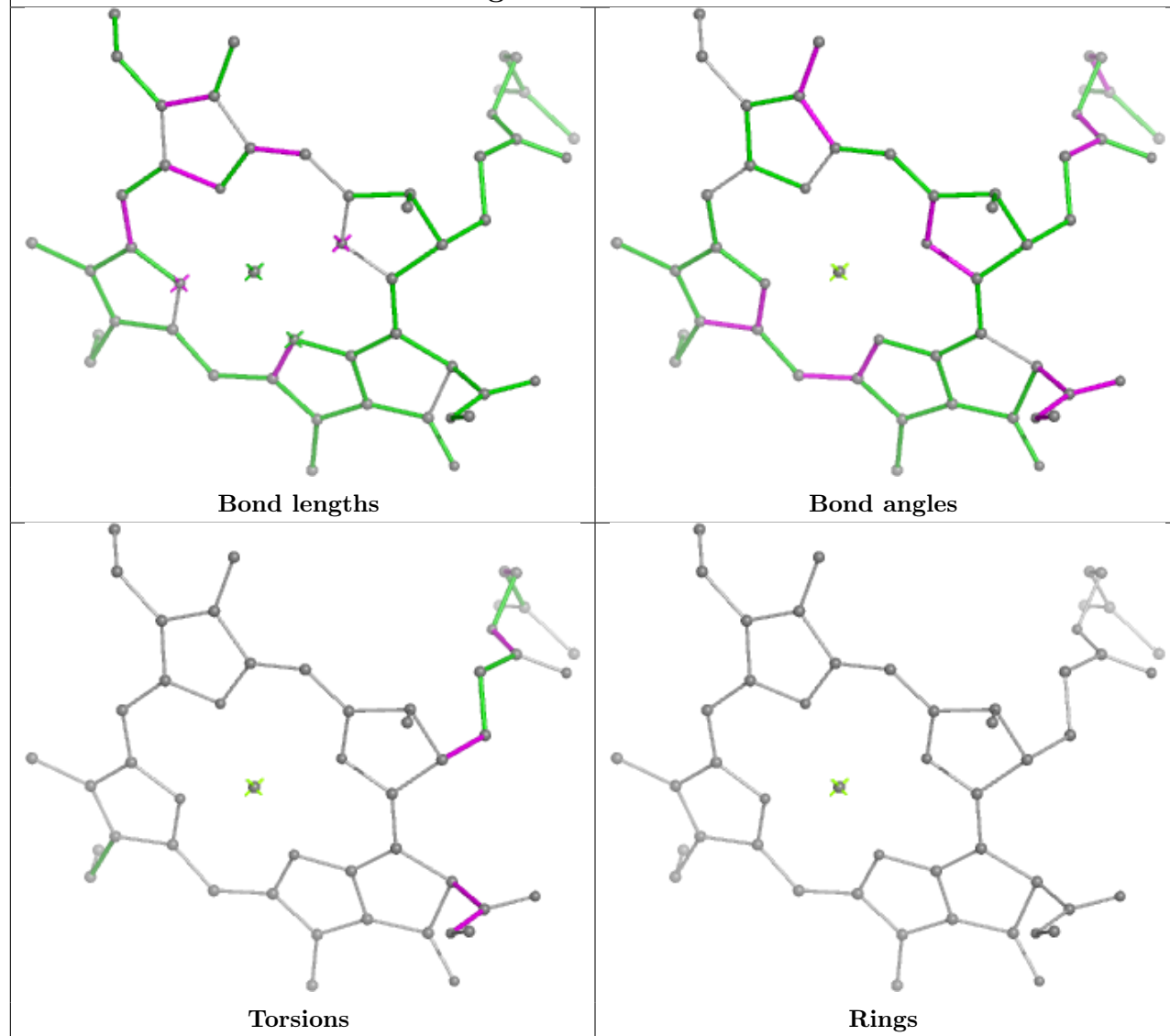




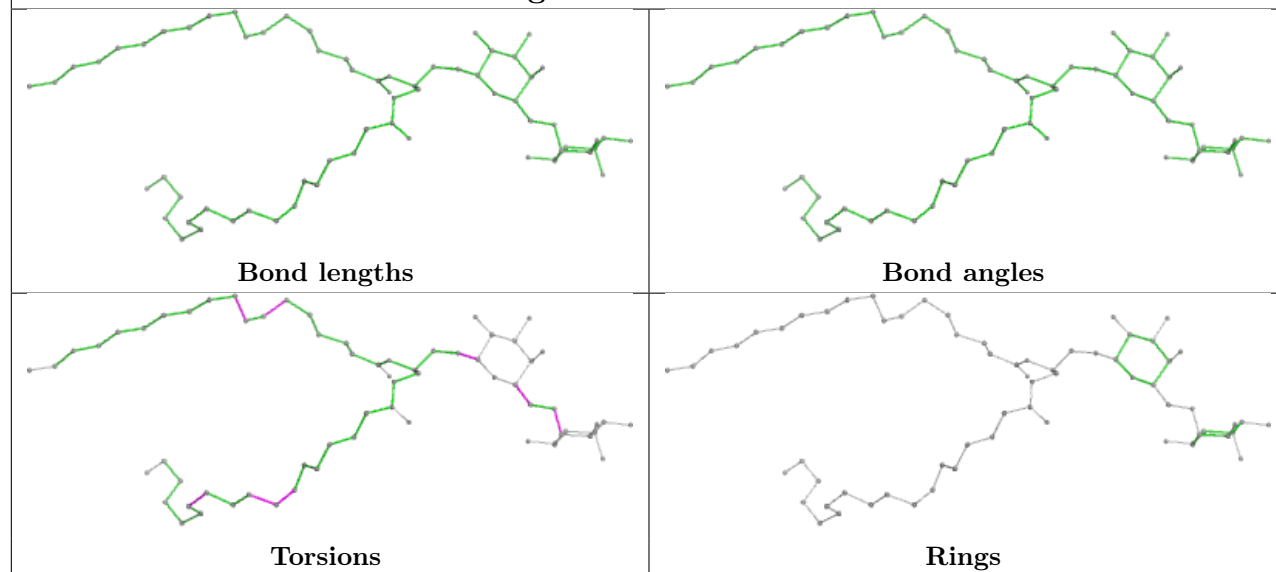


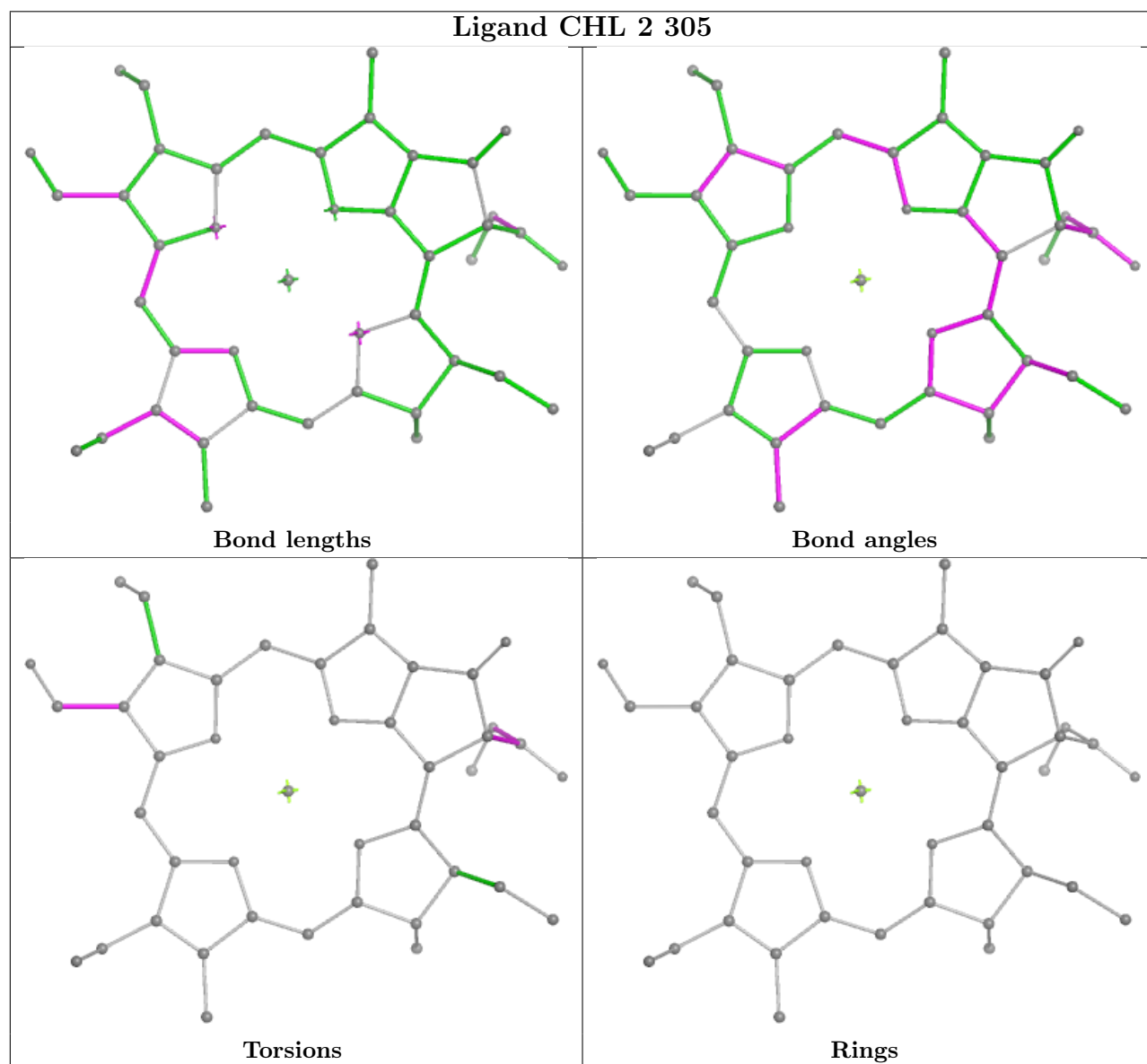
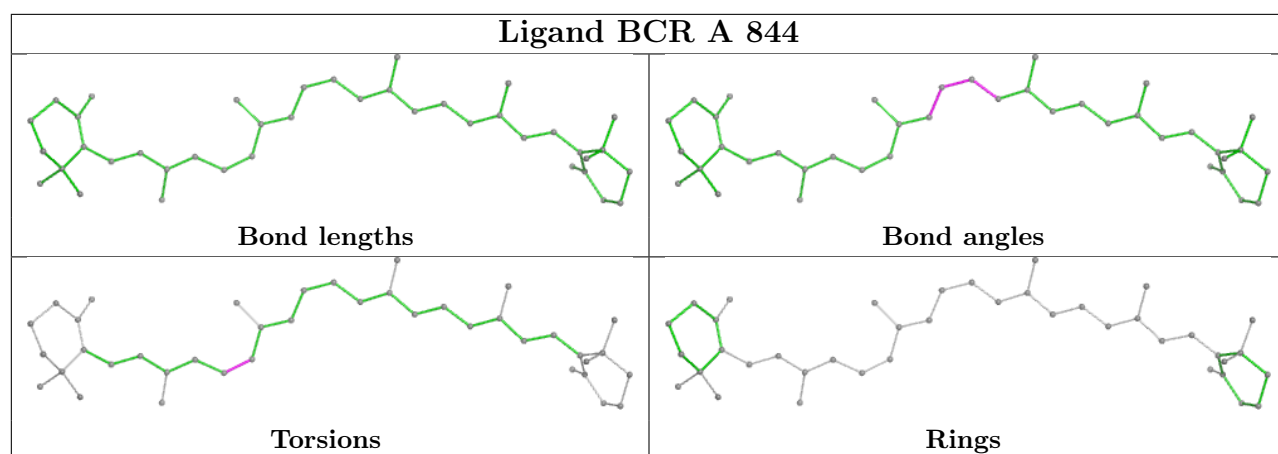
**Ligand XAT 3 316****Ligand CLA B 834**

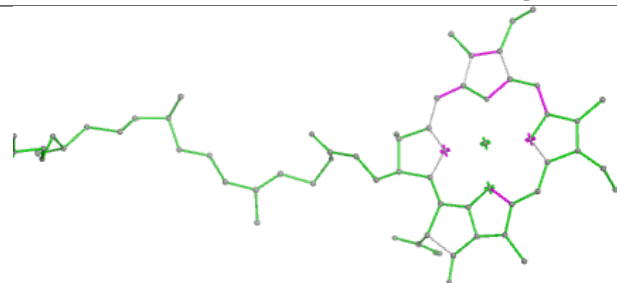
## Ligand CLA B 830



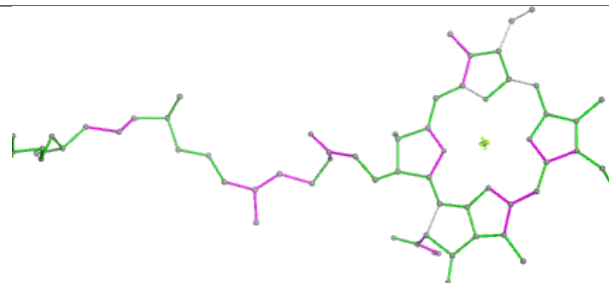
## Ligand DGD B 848



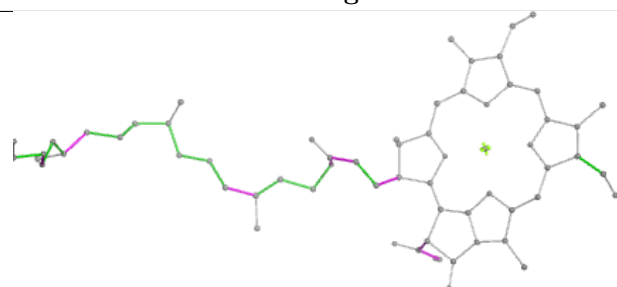


**Ligand CLA A 803**

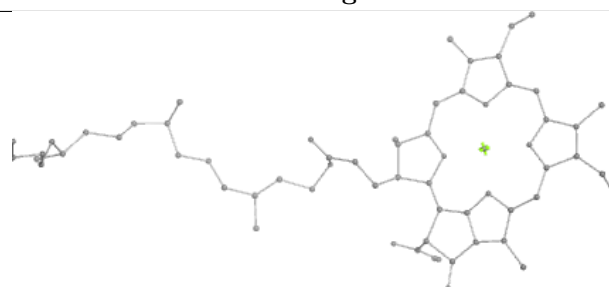
Bond lengths



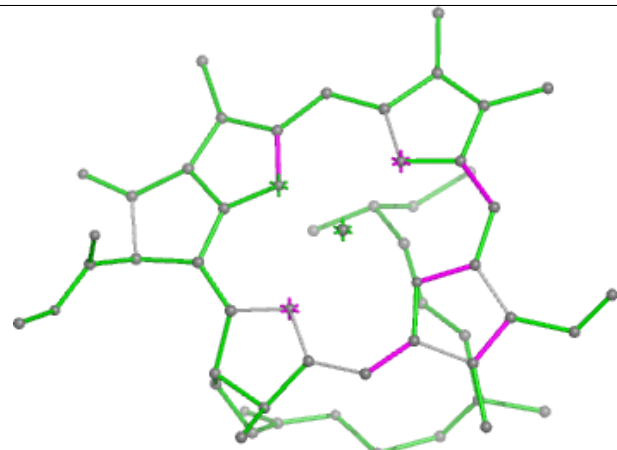
Bond angles



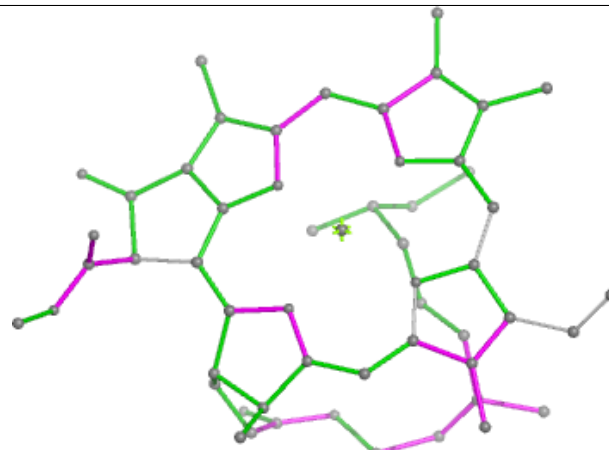
Torsions



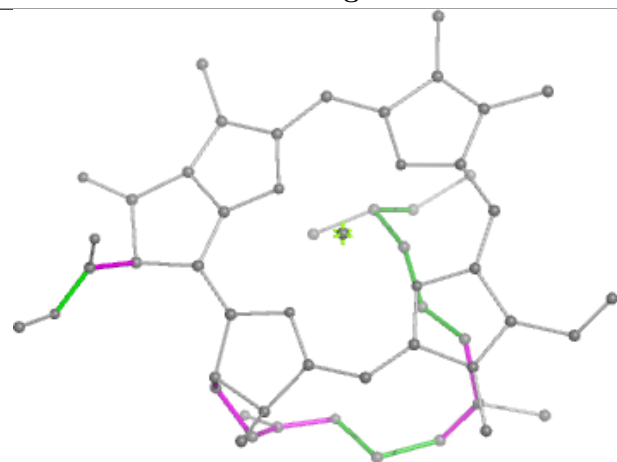
Rings

**Ligand CLA H 202**

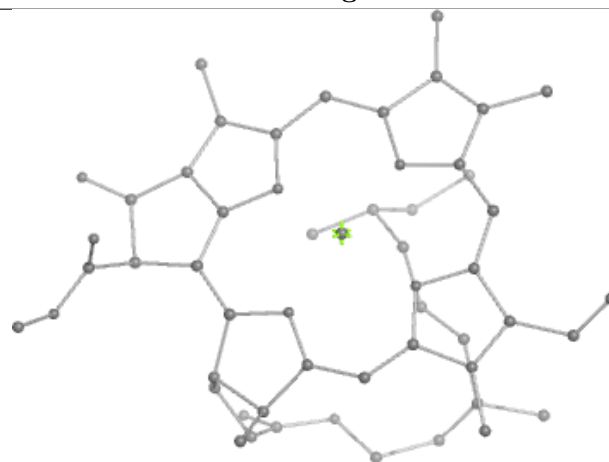
Bond lengths



Bond angles

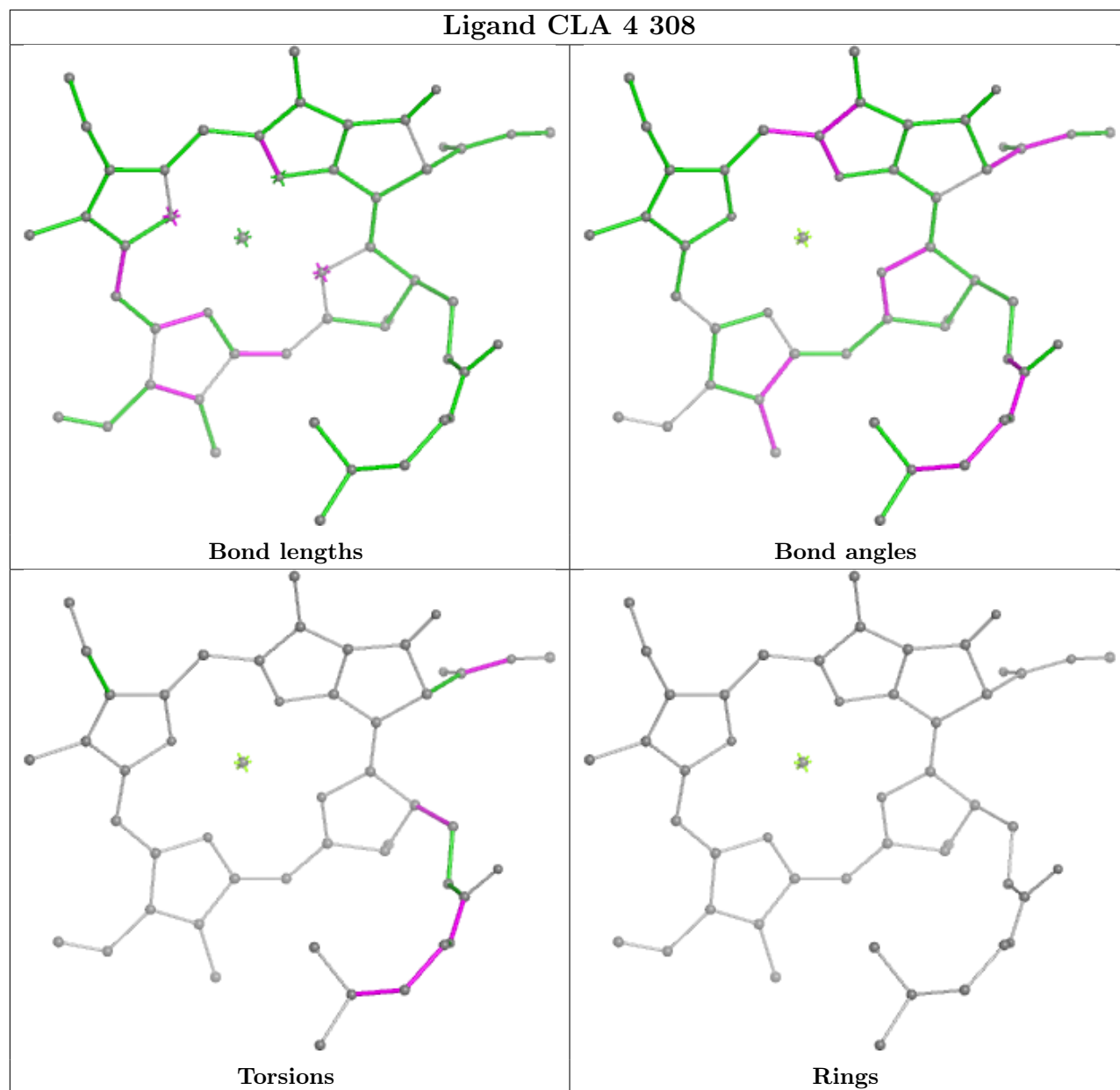


Torsions

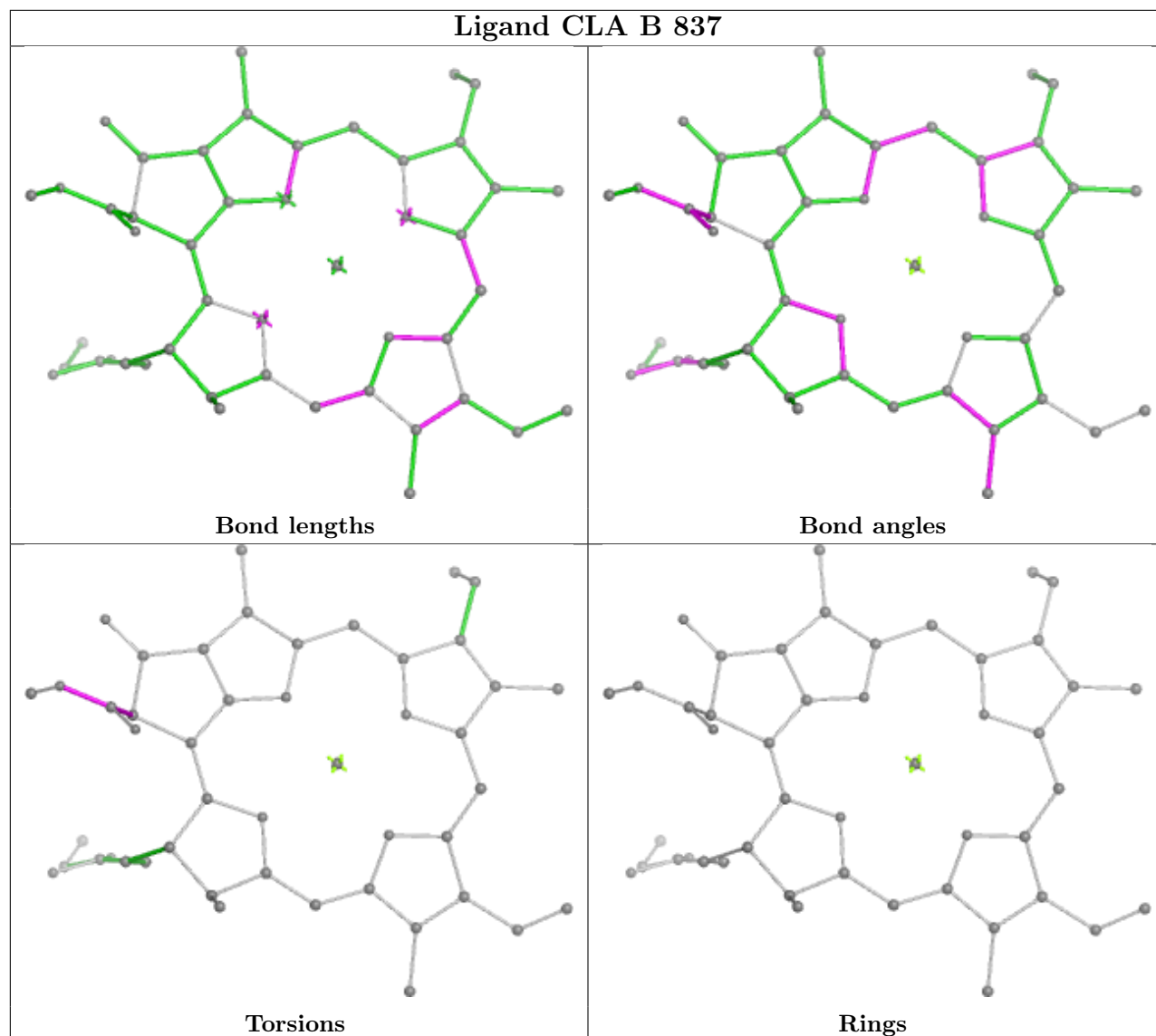


Rings

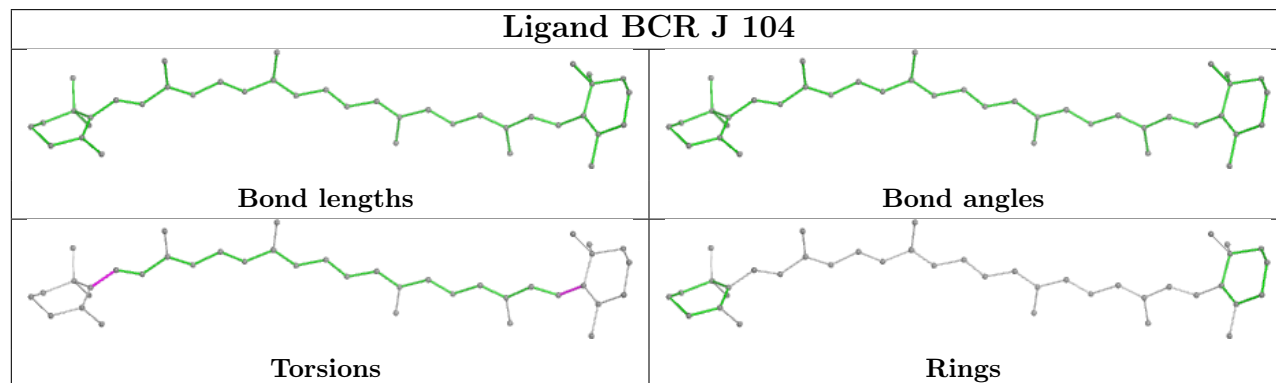
## Ligand CLA 4 308

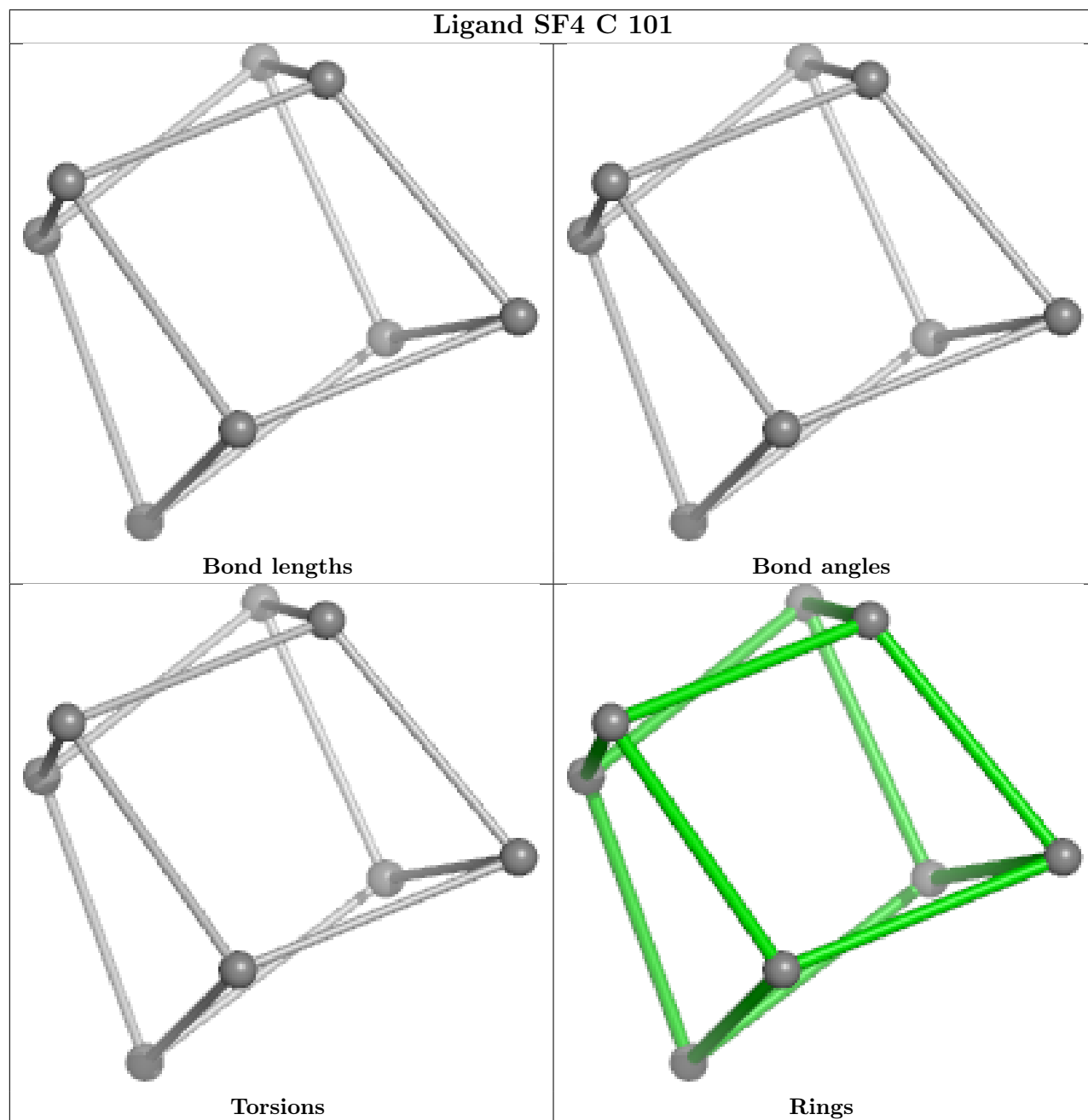
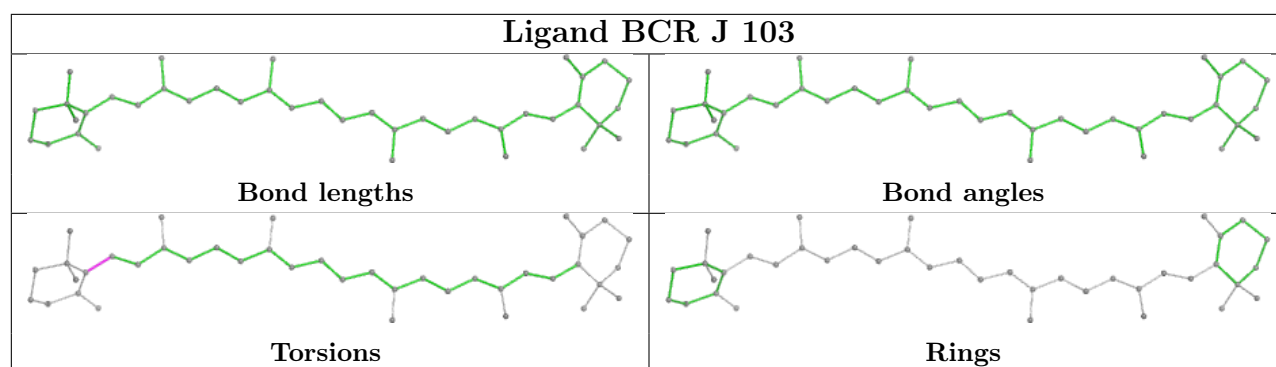


## Ligand CLA B 837

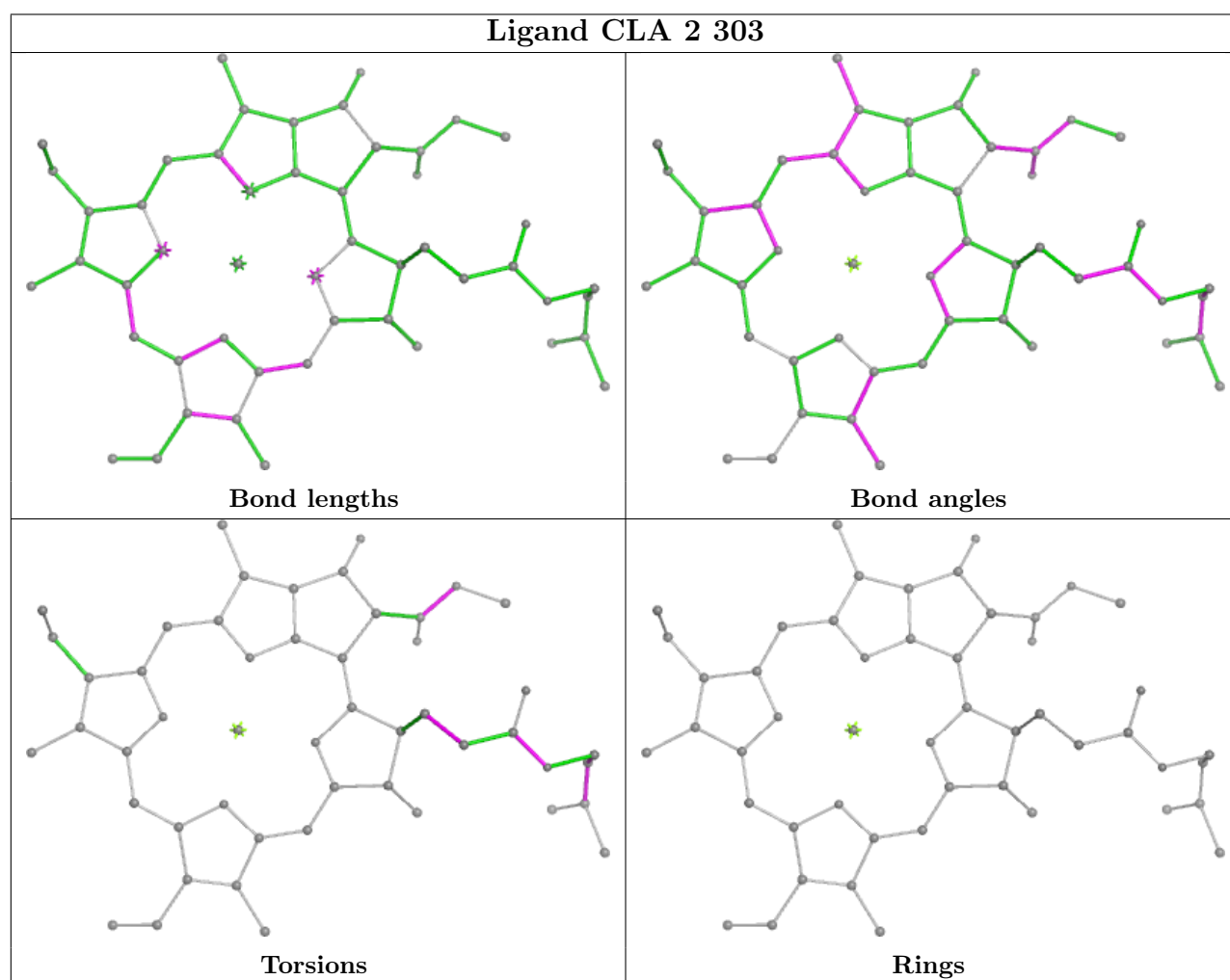
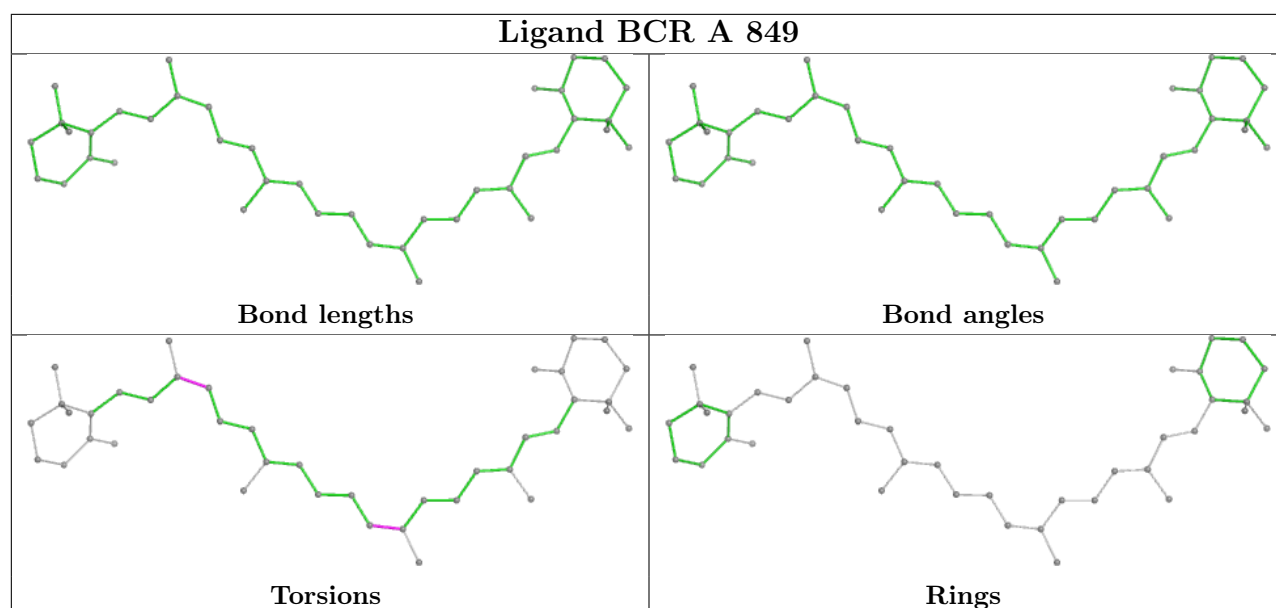


## Ligand BCR J 104

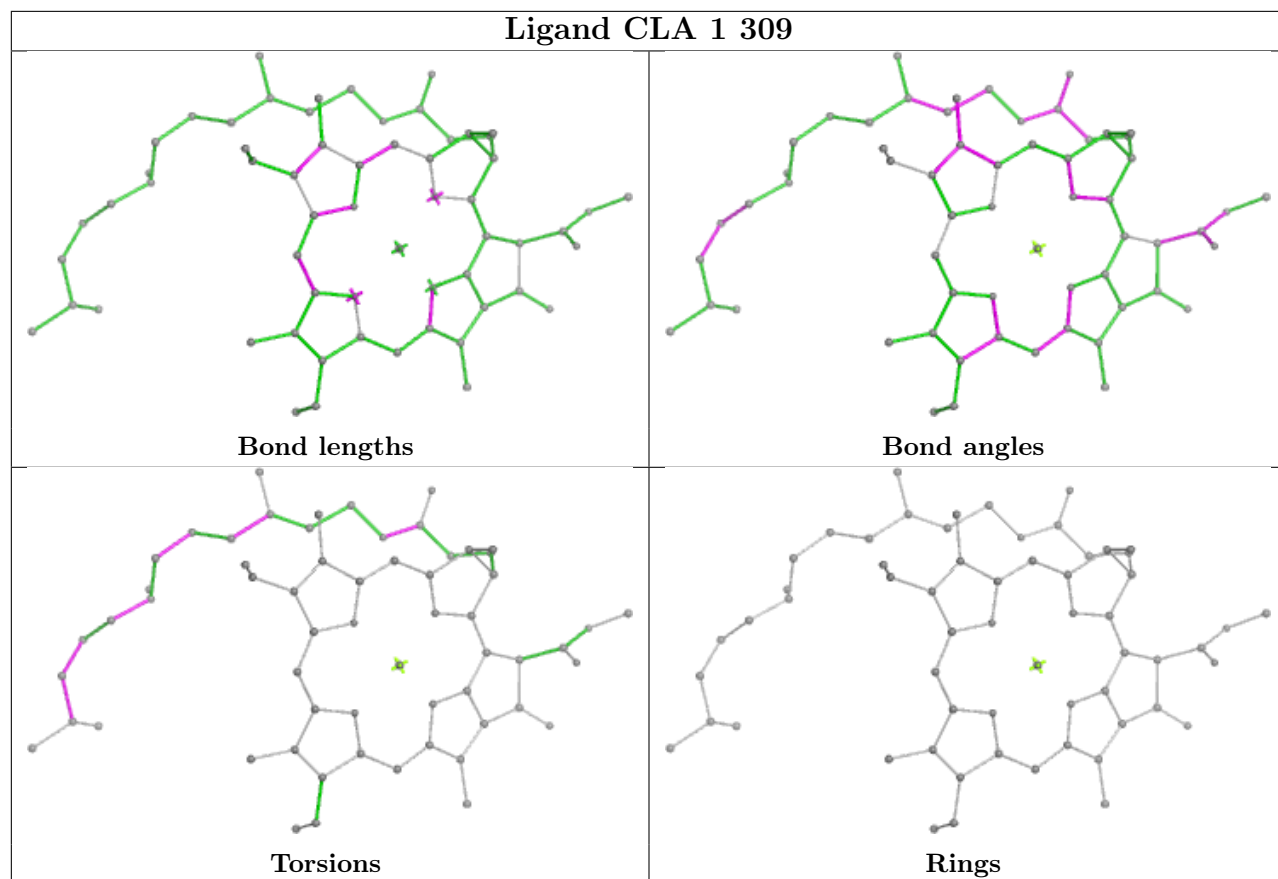




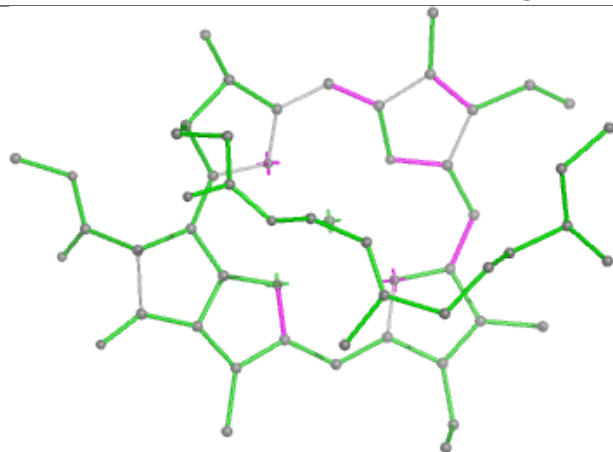




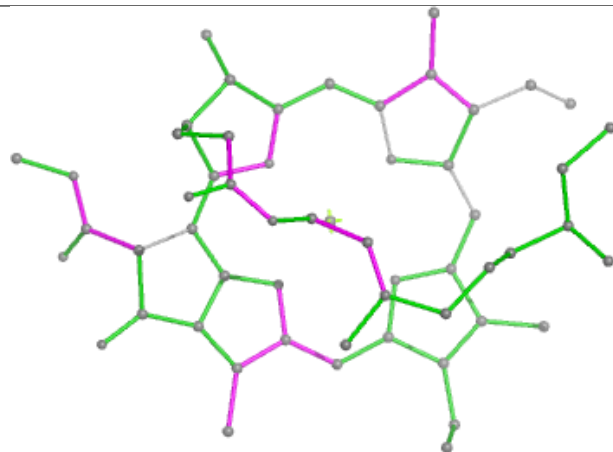
## Ligand CLA 1 309



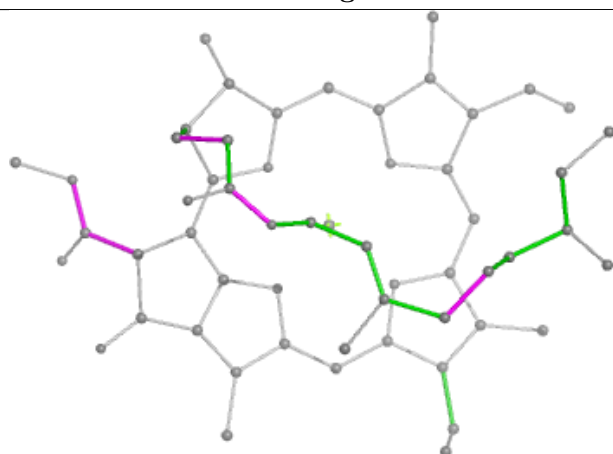
## Ligand CLA 4 312



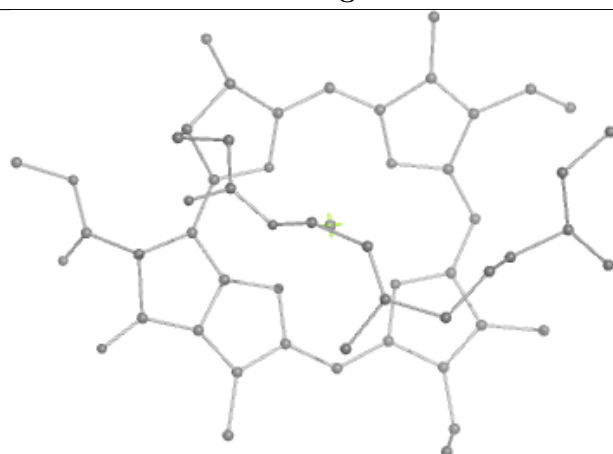
Bond lengths



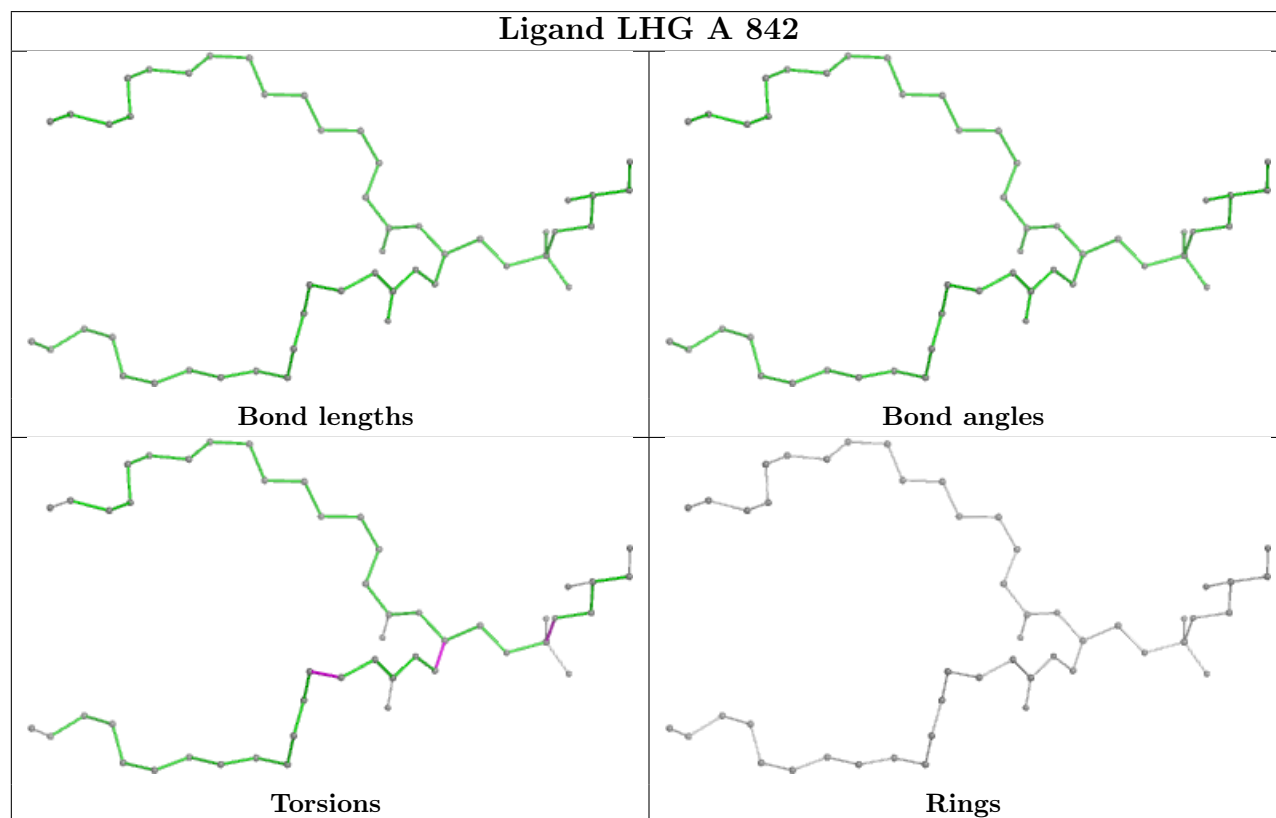
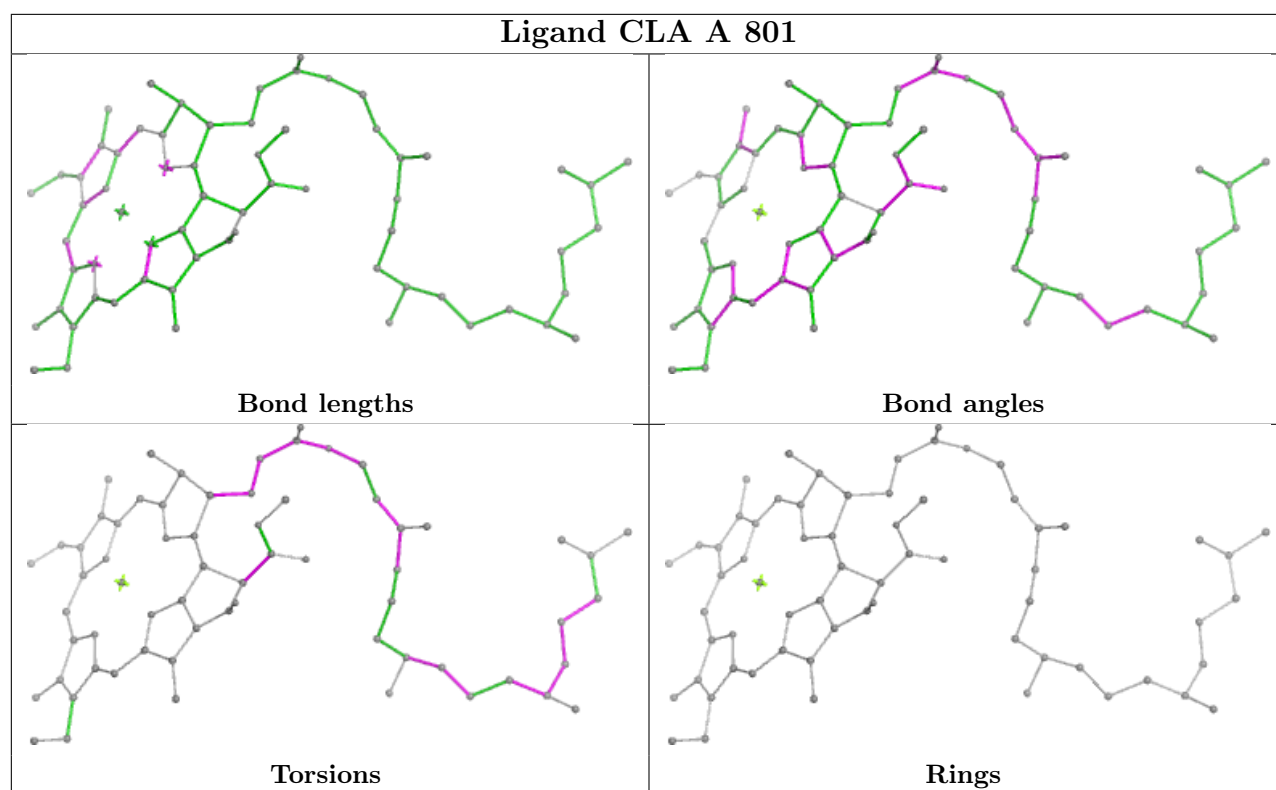
Bond angles



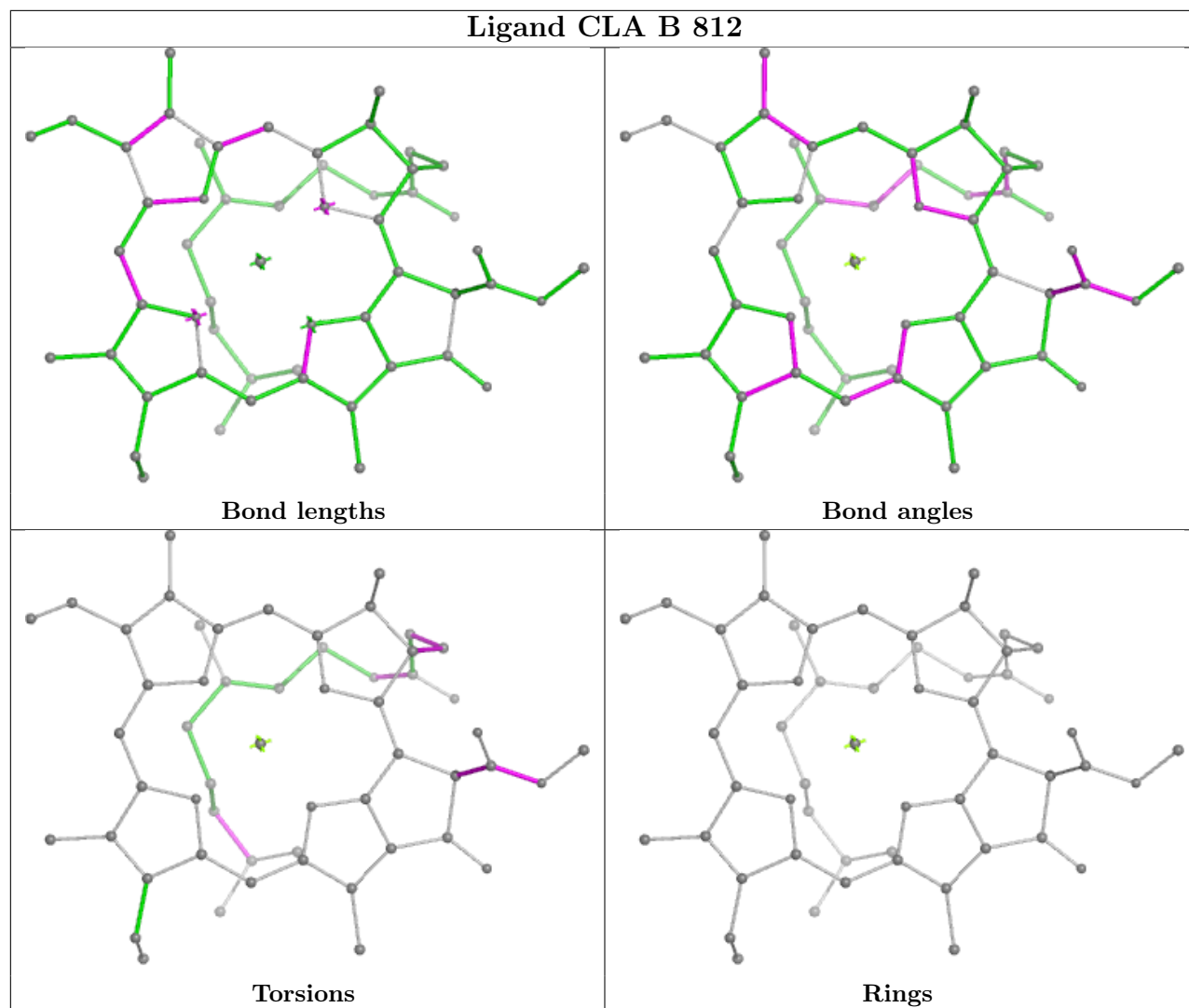
Torsions



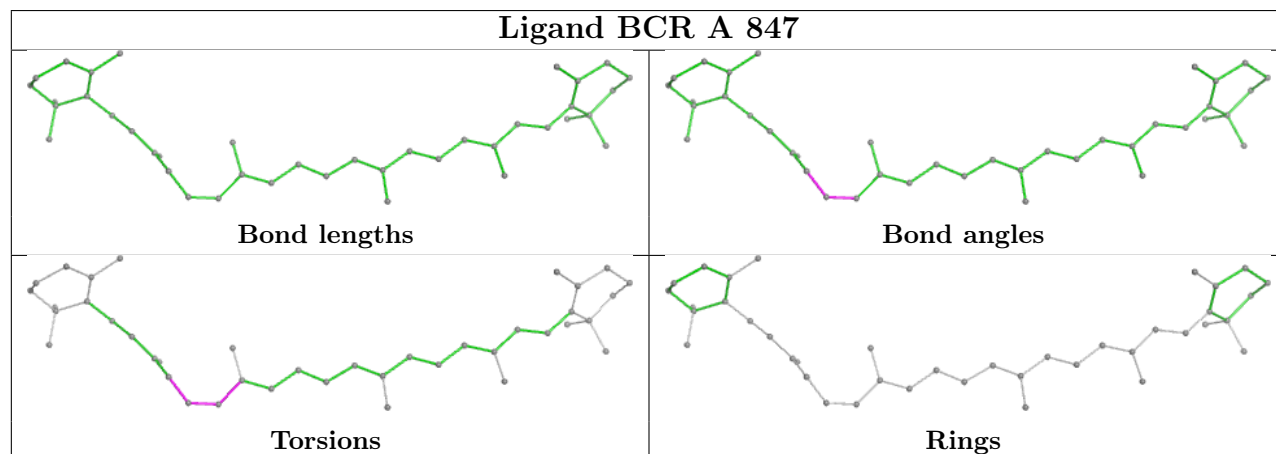
Rings

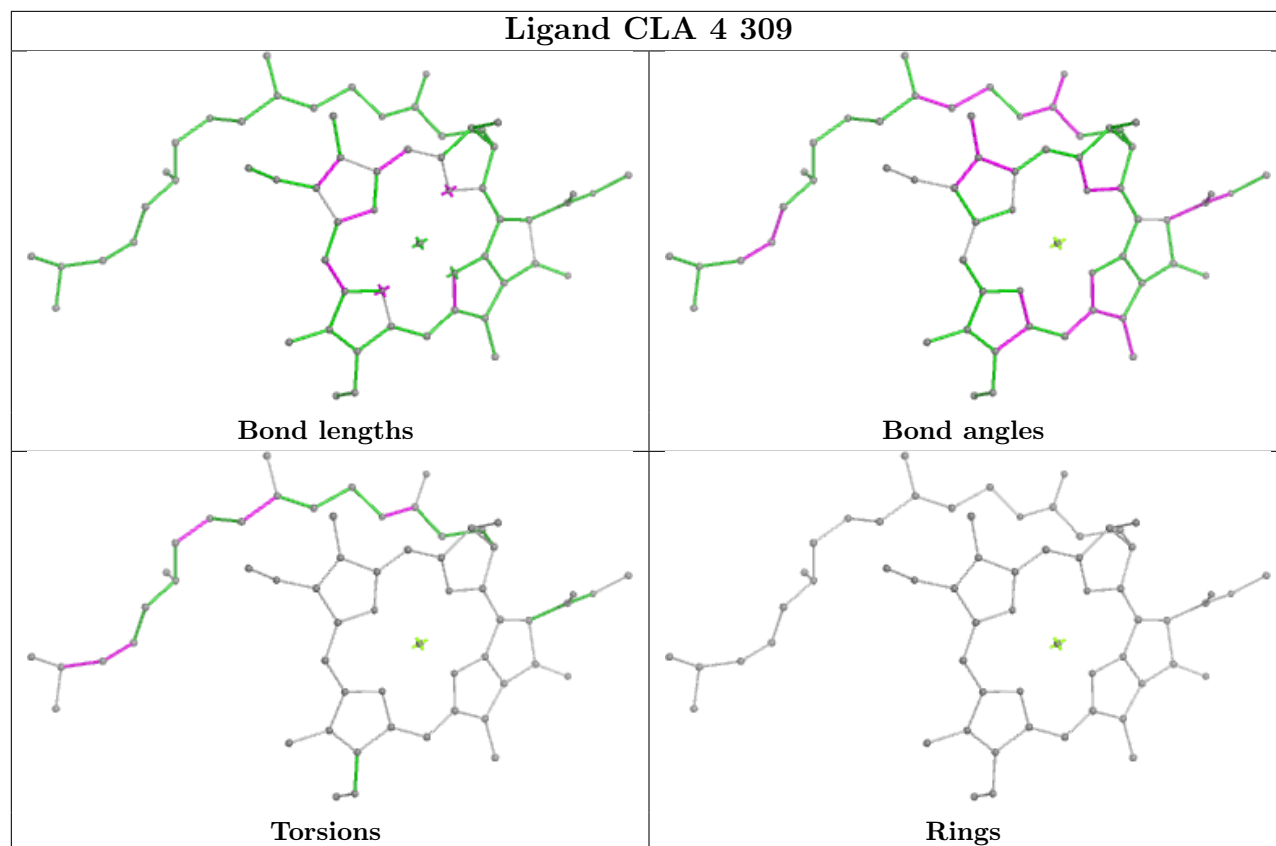
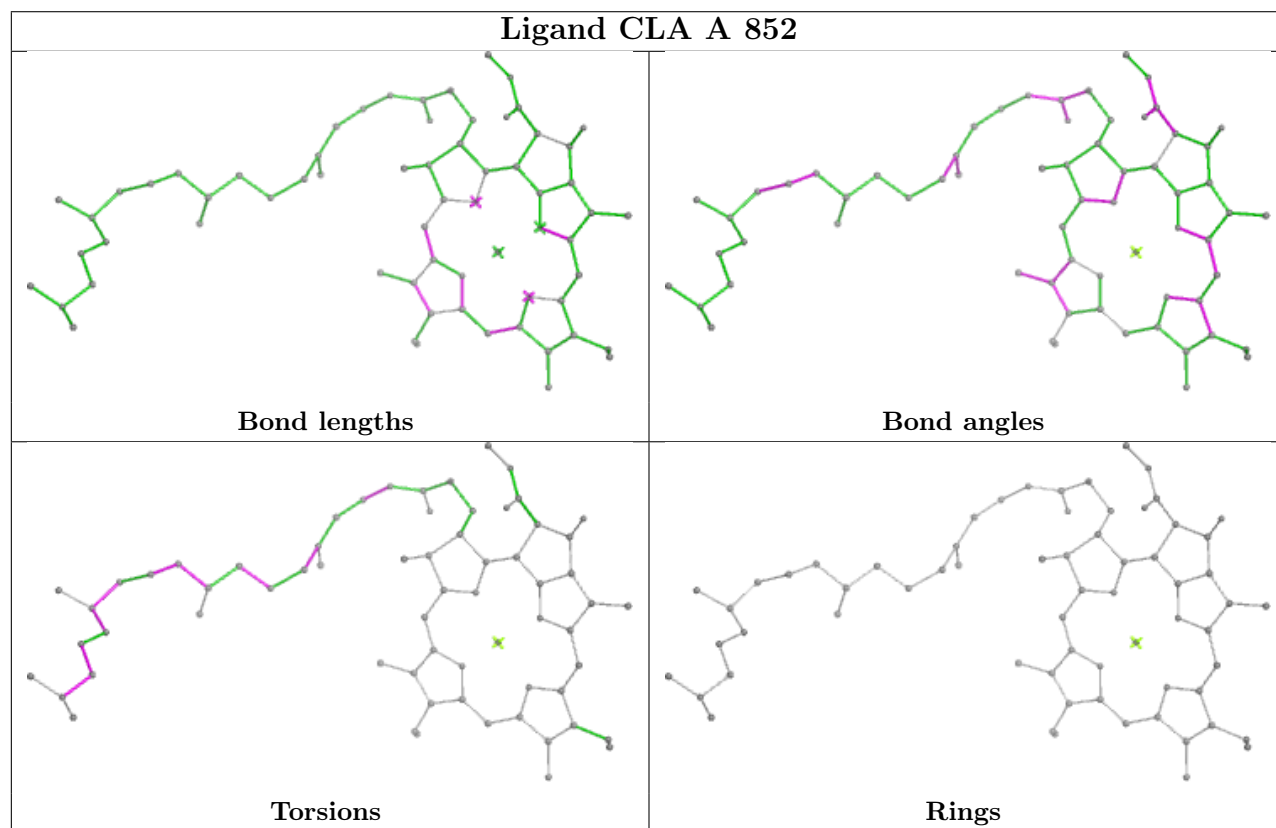


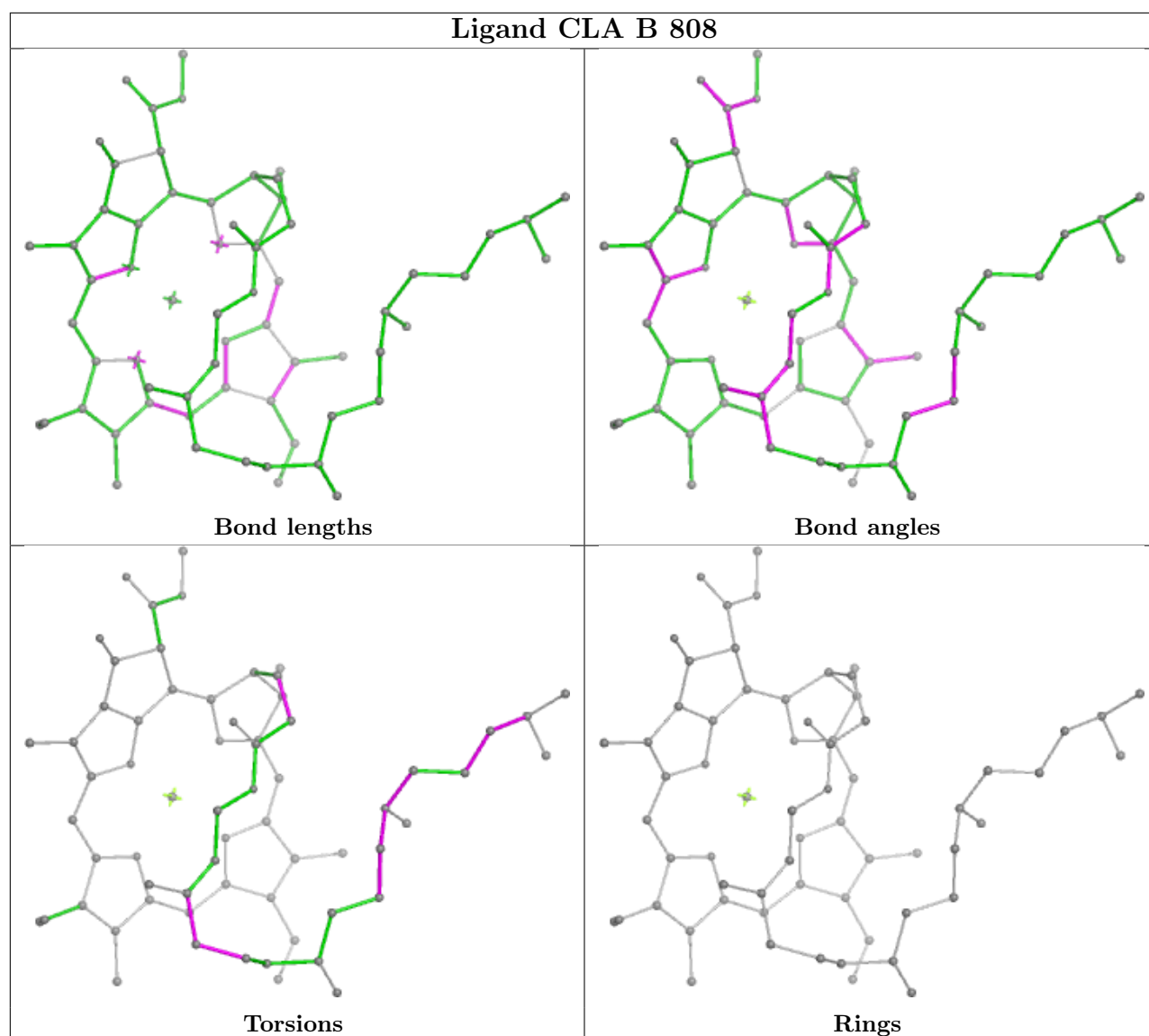
## Ligand CLA B 812



## Ligand BCR A 847



**Ligand CLA 4 309****Ligand CLA A 852**



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

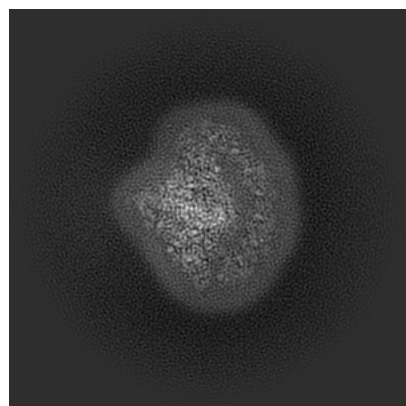
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51227. These allow visual inspection of the internal detail of the map and identification of artifacts.

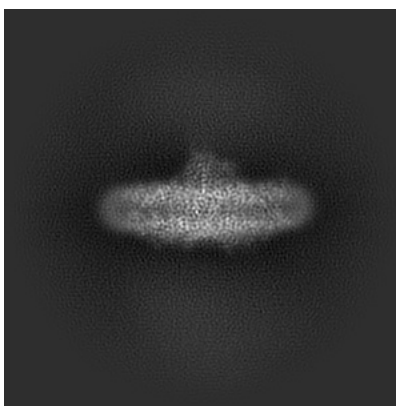
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

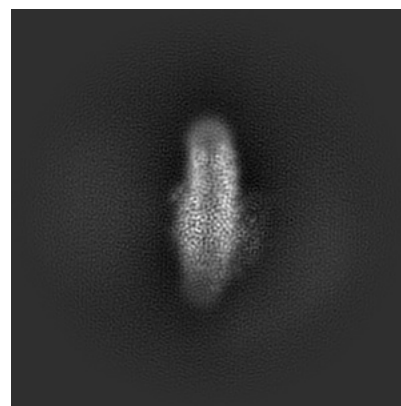
#### 6.1.1 Primary map



X

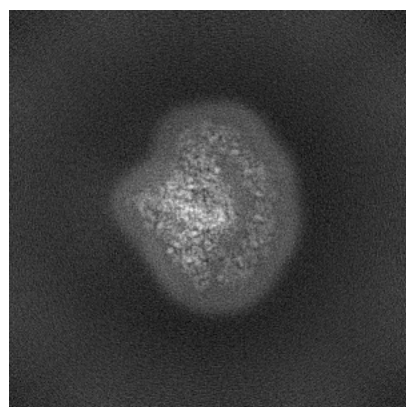


Y

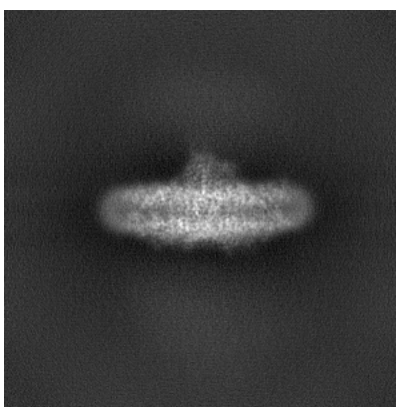


Z

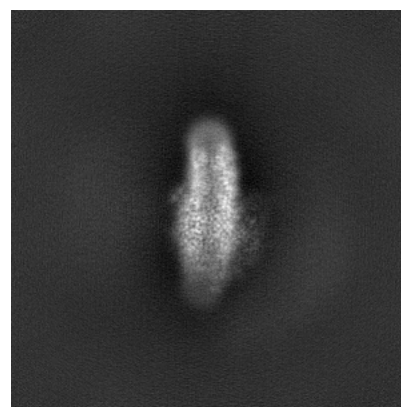
#### 6.1.2 Raw map



X



Y



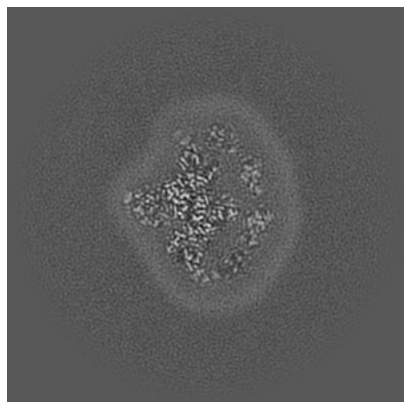
Z

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

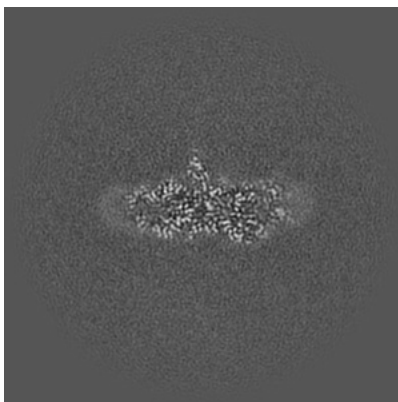


## 6.2 Central slices [i](#)

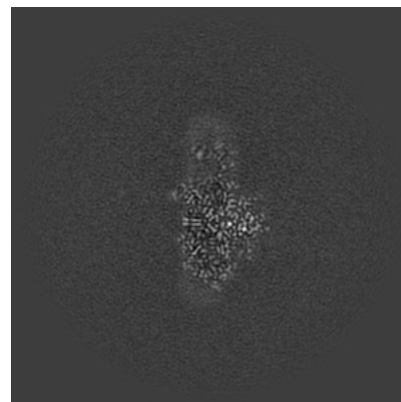
### 6.2.1 Primary map



X Index: 224

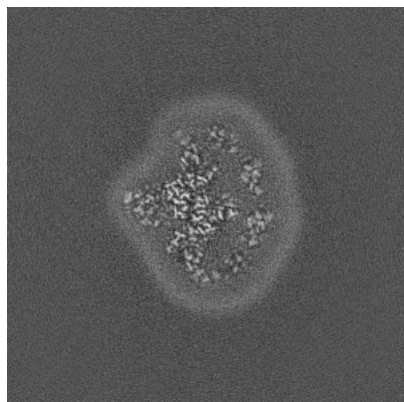


Y Index: 224

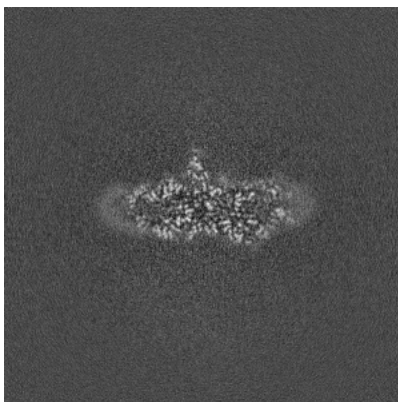


Z Index: 224

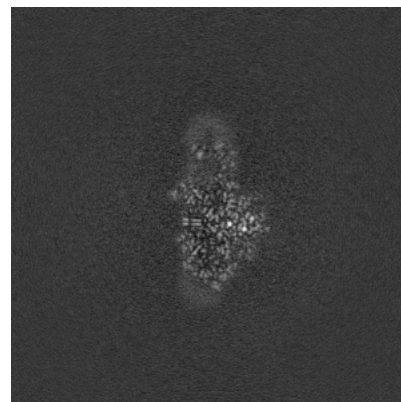
### 6.2.2 Raw map



X Index: 224



Y Index: 224

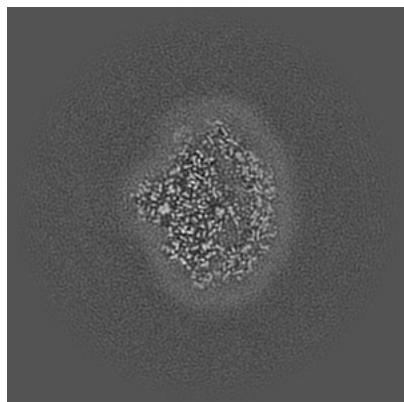


Z Index: 224

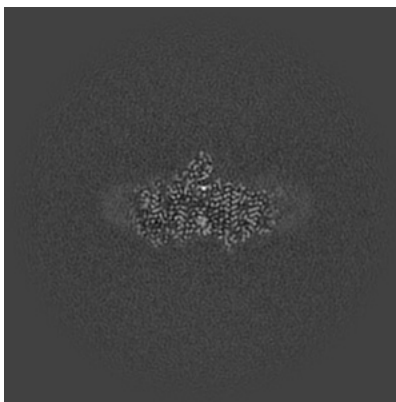
The images above show central slices of the map in three orthogonal directions.

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

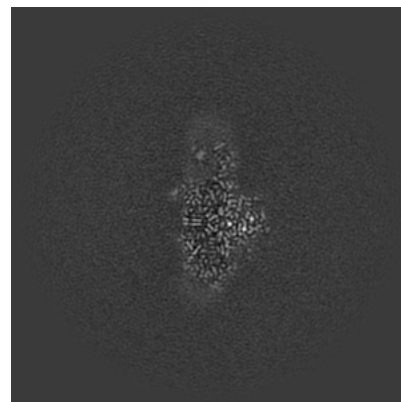
### 6.3.1 Primary map



X Index: 236

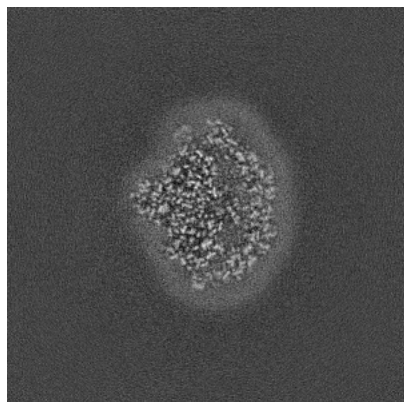


Y Index: 204

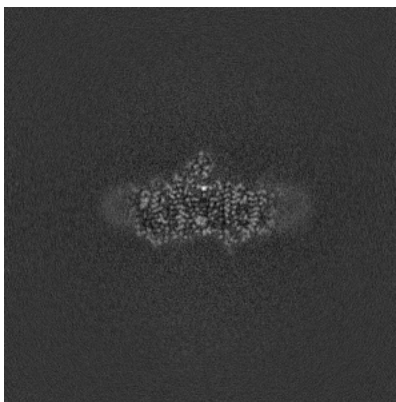


Z Index: 223

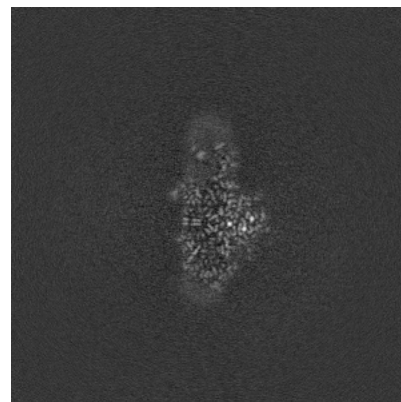
### 6.3.2 Raw map



X Index: 237



Y Index: 205

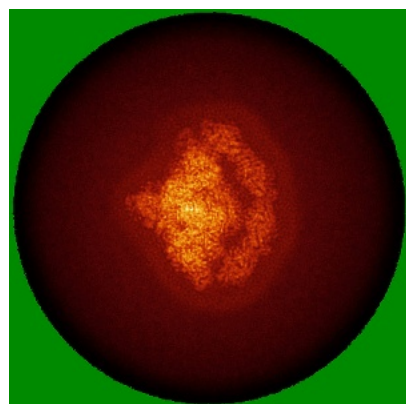


Z Index: 223

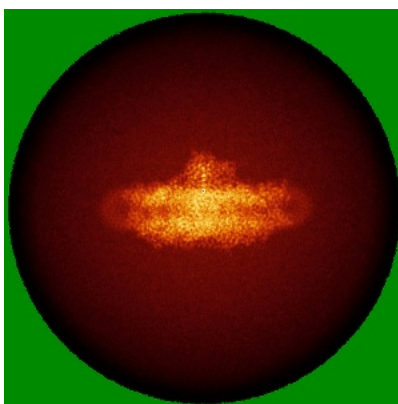
The images above show the largest variance slices of the map in three orthogonal directions.

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

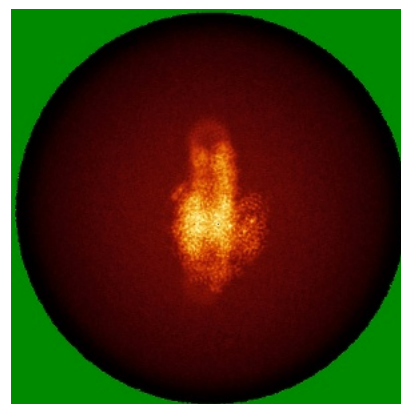
### 6.4.1 Primary map



X

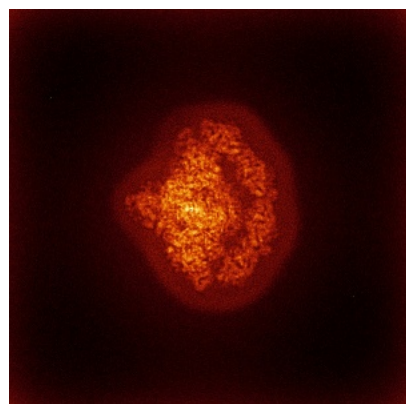


Y

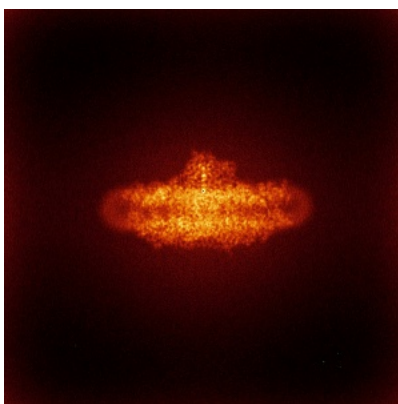


Z

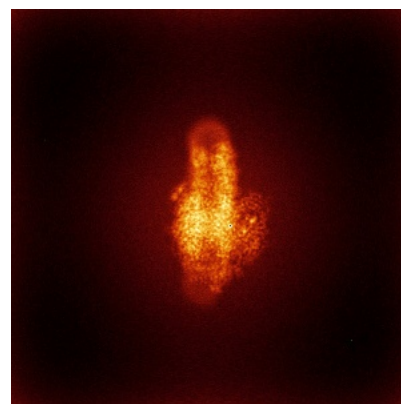
### 6.4.2 Raw map



X



Y

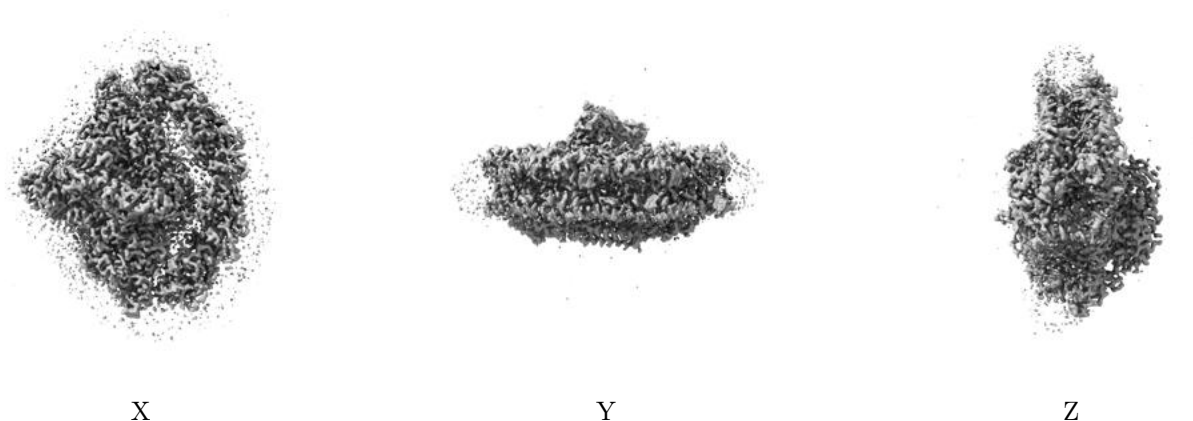


Z

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.

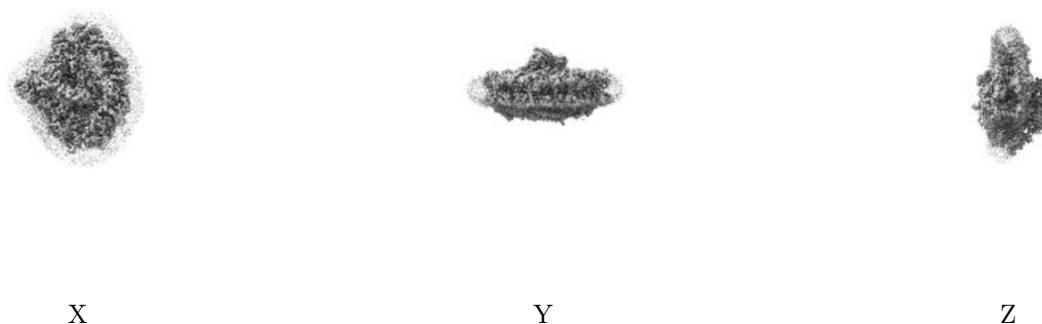
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

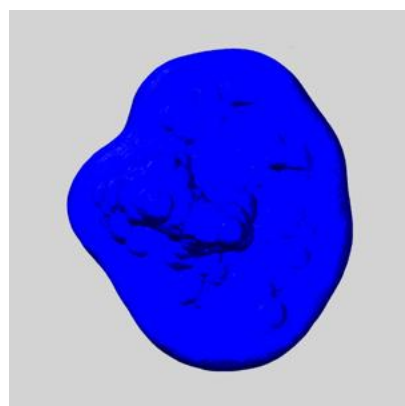
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

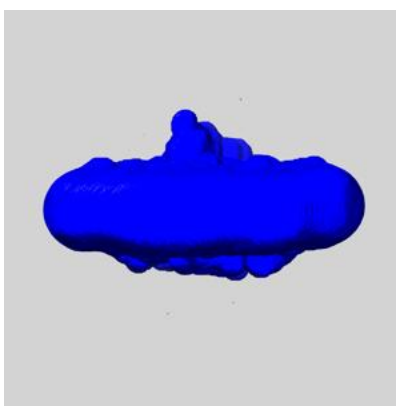
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

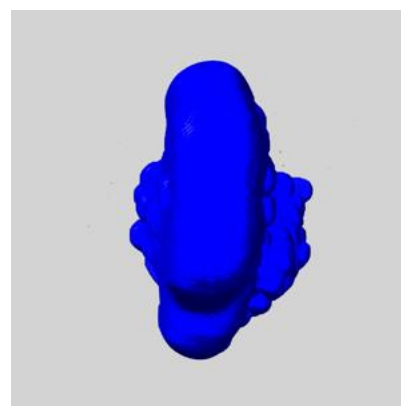
### 6.6.1 emd\_51227\_msk\_1.map [i](#)



X



Y

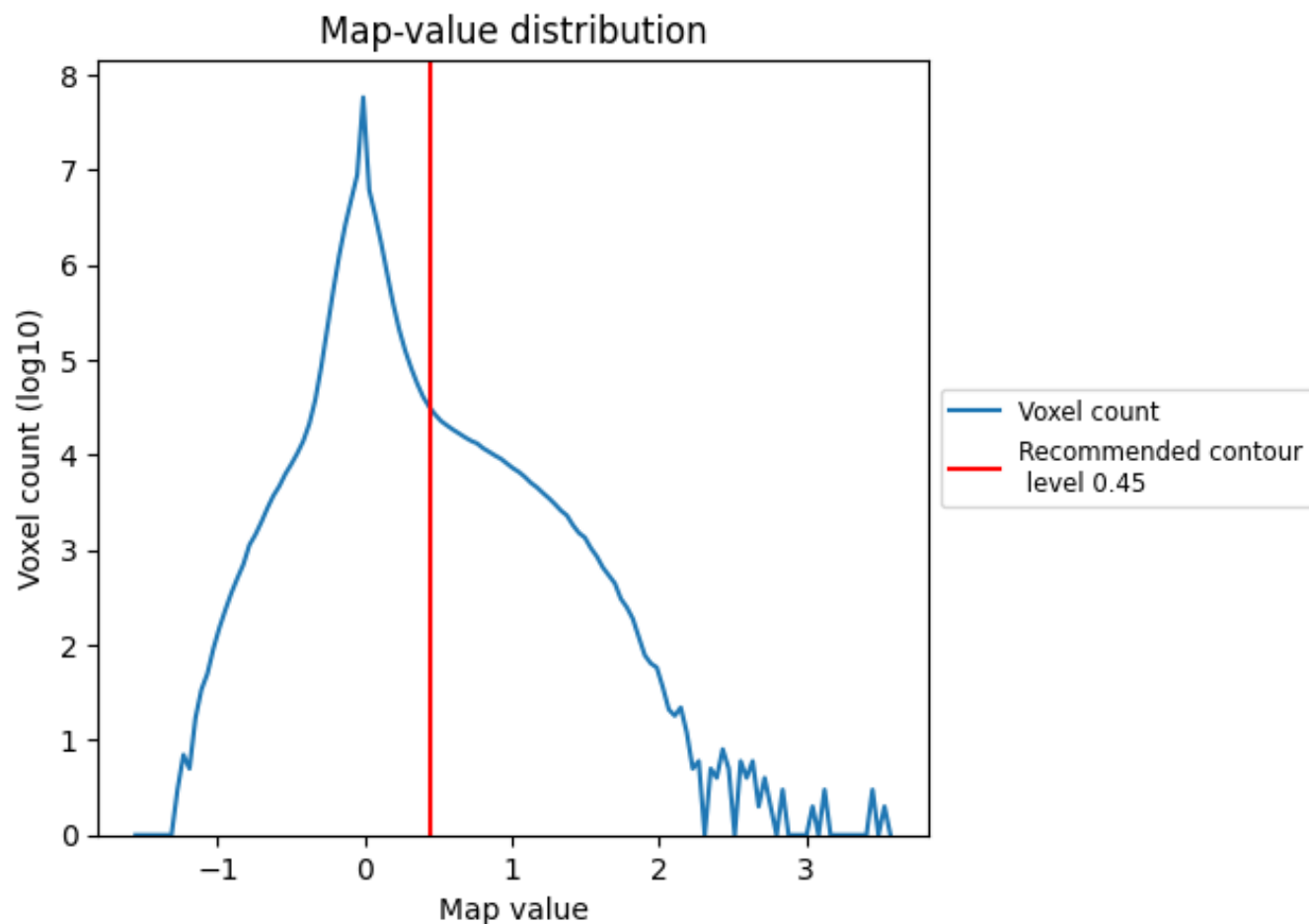


Z

## 7 Map analysis [i](#)

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

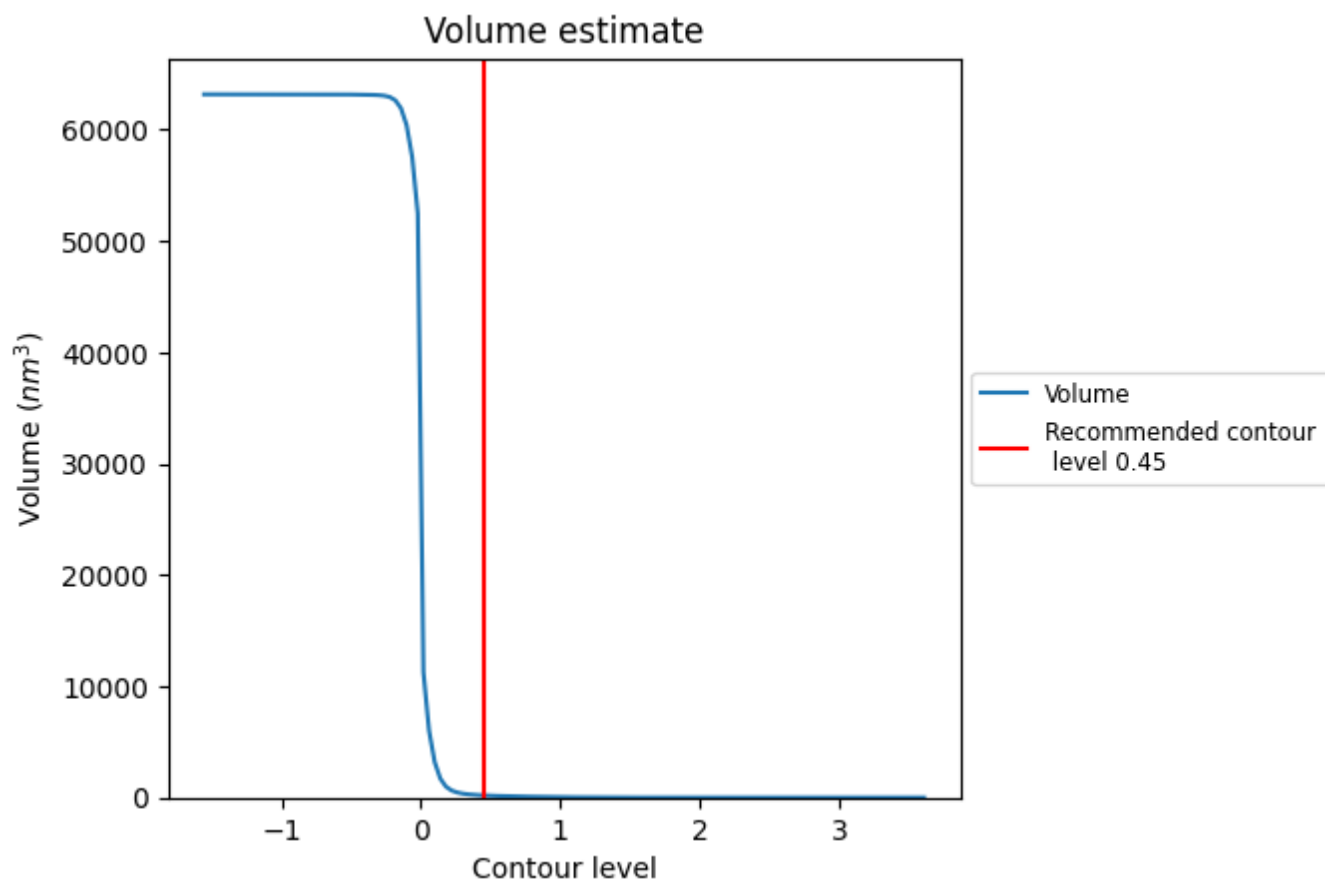
### 7.1 Map-value distribution [i](#)



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.



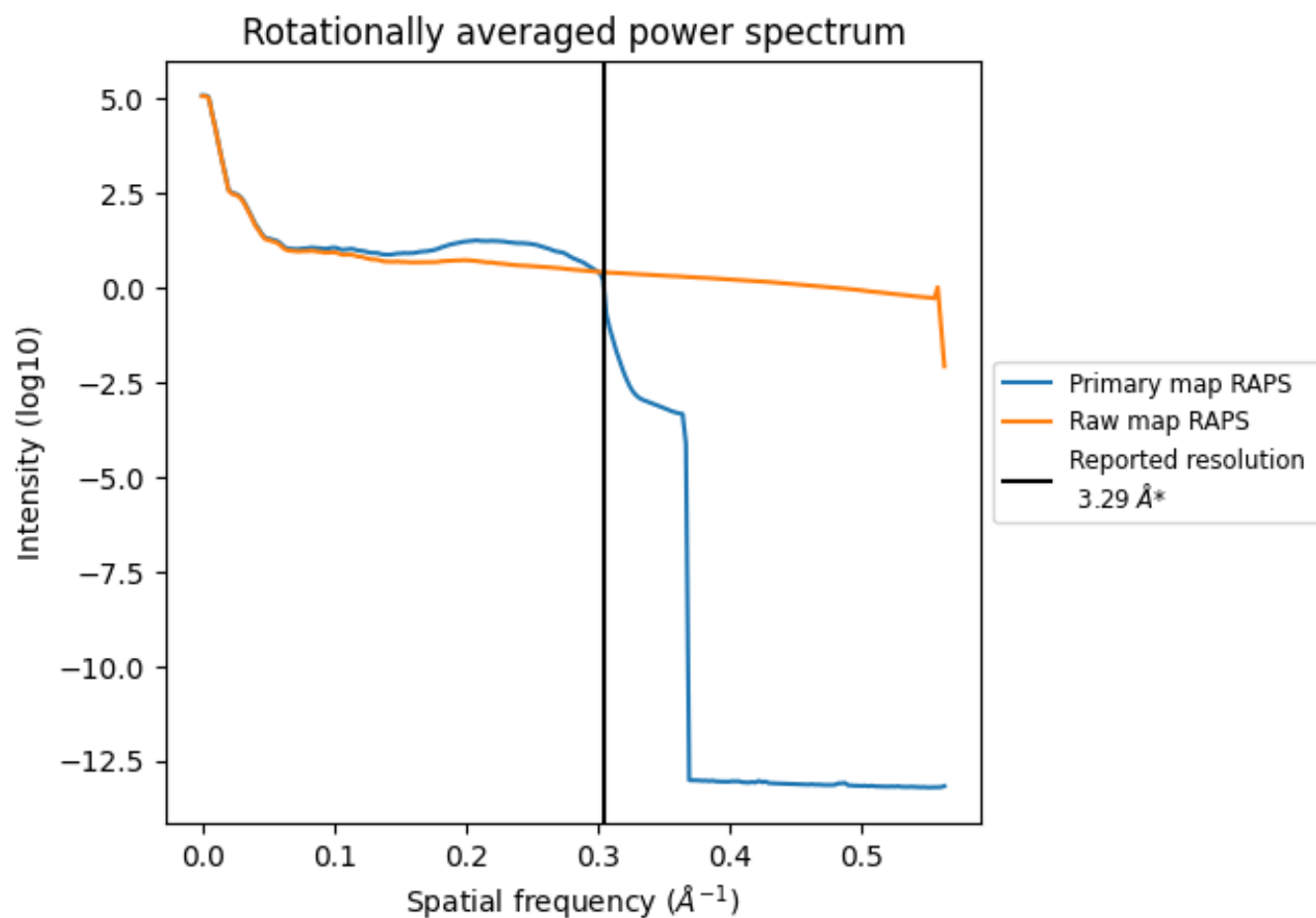
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192  $\text{nm}^3$ ; this corresponds to an approximate mass of 174 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 ⓘ



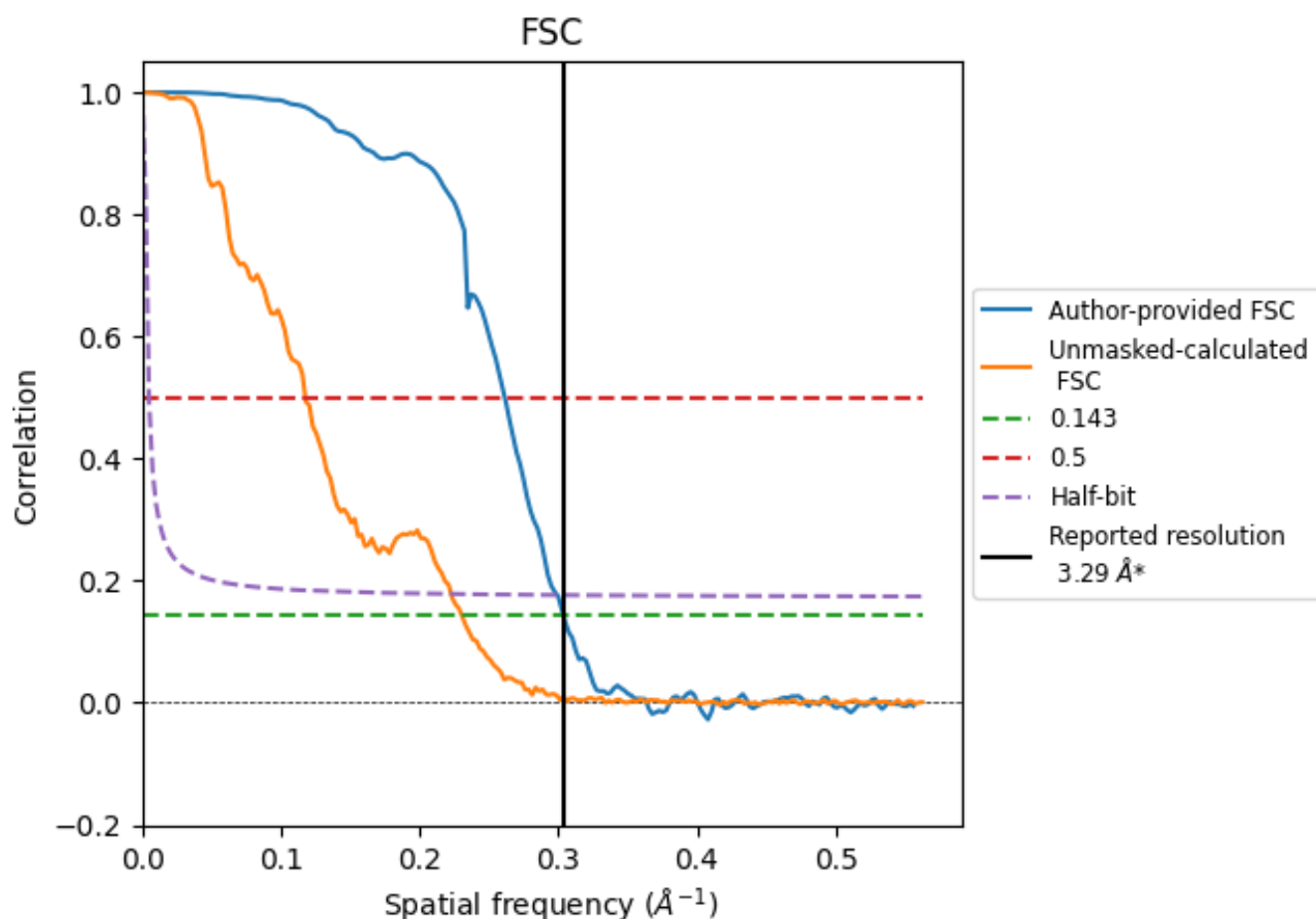
\*Reported resolution corresponds to spatial frequency of 0.304 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

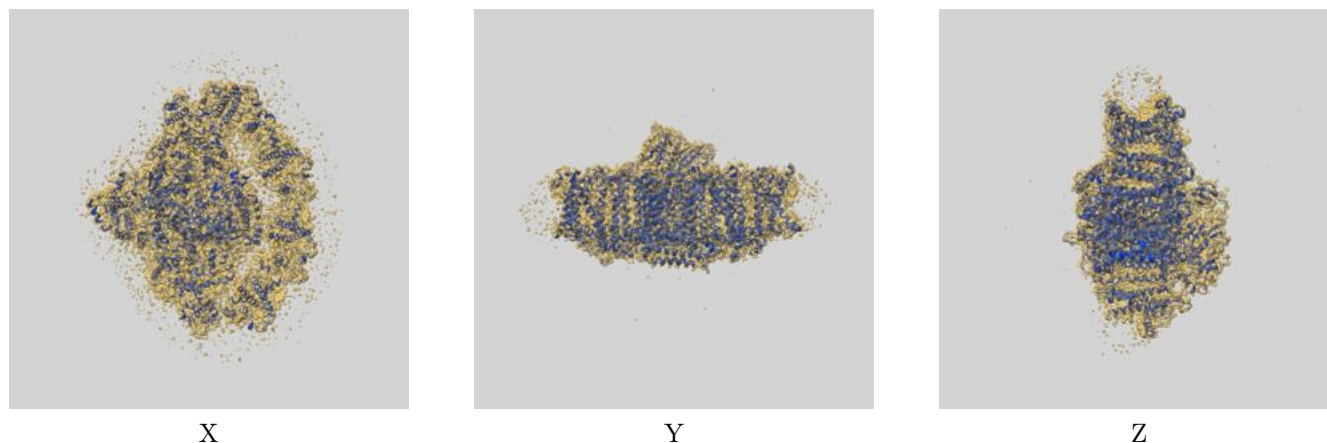
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.29	3.82	3.34
Unmasked-calculated*	4.34	8.50	4.49

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.29 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-51227 and PDB model 9GC2. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

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



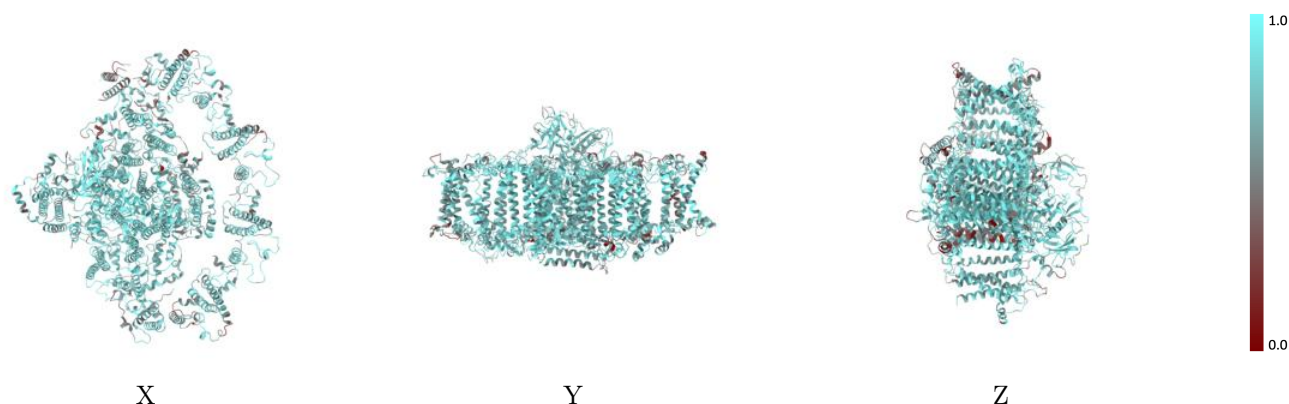
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



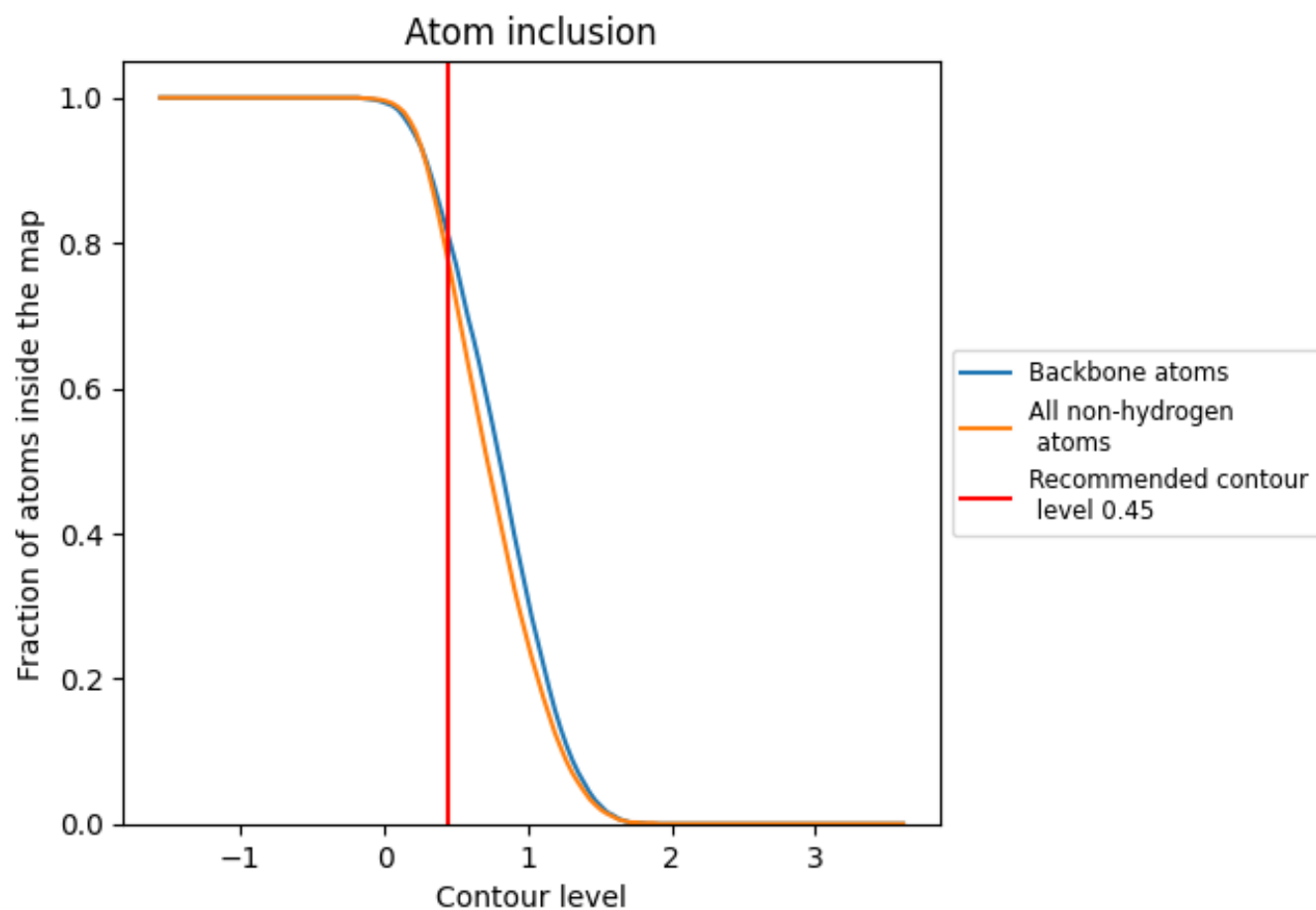
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7710	<div></div> 0.5350
1	<div></div> 0.6620	<div></div> 0.4900
2	<div></div> 0.7100	<div></div> 0.4990
3	<div></div> 0.7130	<div></div> 0.5060
4	<div></div> 0.7340	<div></div> 0.5160
A	<div></div> 0.8080	<div></div> 0.5540
B	<div></div> 0.8480	<div></div> 0.5650
C	<div></div> 0.8690	<div></div> 0.5520
D	<div></div> 0.7950	<div></div> 0.5440
E	<div></div> 0.7620	<div></div> 0.5410
F	<div></div> 0.7530	<div></div> 0.5280
G	<div></div> 0.6710	<div></div> 0.5110
H	<div></div> 0.7100	<div></div> 0.5250
I	<div></div> 0.7850	<div></div> 0.5400
J	<div></div> 0.6410	<div></div> 0.5130
K	<div></div> 0.4700	<div></div> 0.4390
L	<div></div> 0.7670	<div></div> 0.5330
N	<div></div> 0.2310	<div></div> 0.4100

