



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2025 – 01:38 pm BST

PDB ID : 9GBI / pdb_00009gbi
EMDB ID : EMD-51219
Title : Cryo-EM structure of Arabidopsis thaliana PSI-LHCI wild-type
Authors : Capaldi, S.; Chaves-Sanjuan, A.; Bonnet, D.M.V.; Bassi, R.
Deposited on : 2024-07-31
Resolution : 3.13 Å(reported)
Based on initial model : 7DKZ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

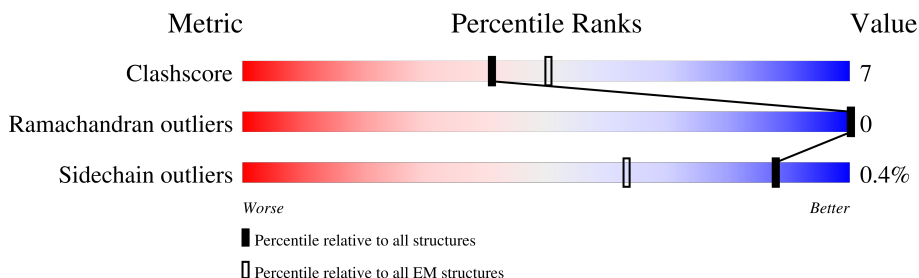
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY








The reported resolution of this entry is 3.13 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.





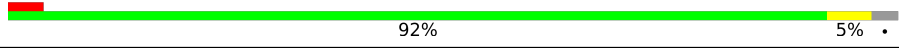



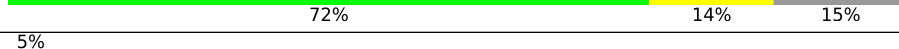
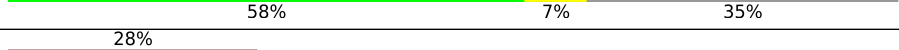
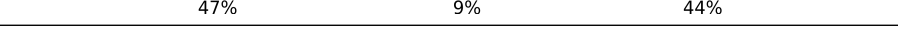
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	 83% 11% 6%
2	2	214	 7% 82% 13% 5%
3	3	234	 5% 81% 12% 6%
4	4	199	 82% 17% .
5	A	750	 87% 12% .
6	B	734	 89% 10%
7	C	81	 80% 19% .
8	D	160	 80% 8% . 12%

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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	304	X	-	-	-
18	CHL	4	305	X	-	-	-
18	CHL	4	306	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	313	X	-	-	-
19	CLA	1	314	X	-	-	-
19	CLA	1	321	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	2	320	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	307	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	A	801	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	F	303	X	-	-	-
19	CLA	F	304	X	-	-	-
19	CLA	G	202	X	-	-	-
19	CLA	G	203	X	-	-	-
19	CLA	G	204	X	-	-	-
19	CLA	H	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	J	102	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	K	204	X	-	-	-
19	CLA	L	301	X	-	-	-
19	CLA	L	302	X	-	-	-
19	CLA	L	303	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 36064 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
			1678	1100	269	304	5		

- 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
			1562	1022	254	283	3		

- 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	97	Total	C	N	O	0	0
			759	493	124	142		

- 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		

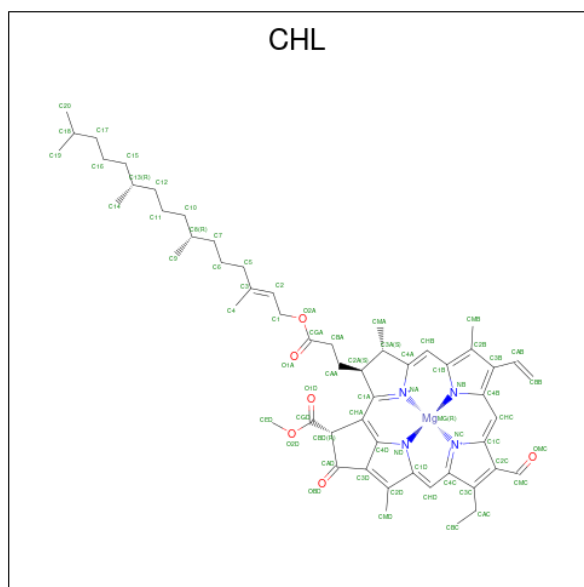
- Molecule 16 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

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	48	Total	C	N	O	S	0	0
			381	239	67	73	2		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



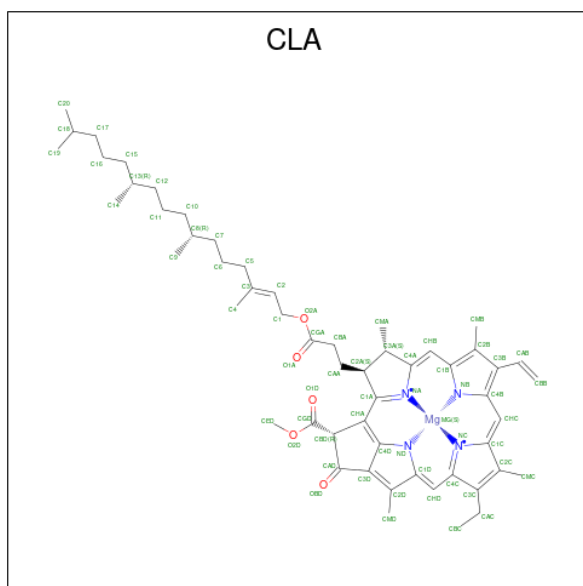
Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
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: $C_{55}H_{72}MgN_4O_5$) (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
			56	46	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
			45	35	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	
19	2	1	Total	C	Mg	N	O	0
			50	40	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
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			57	47	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
			58	48	1	4	5	

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

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

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

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

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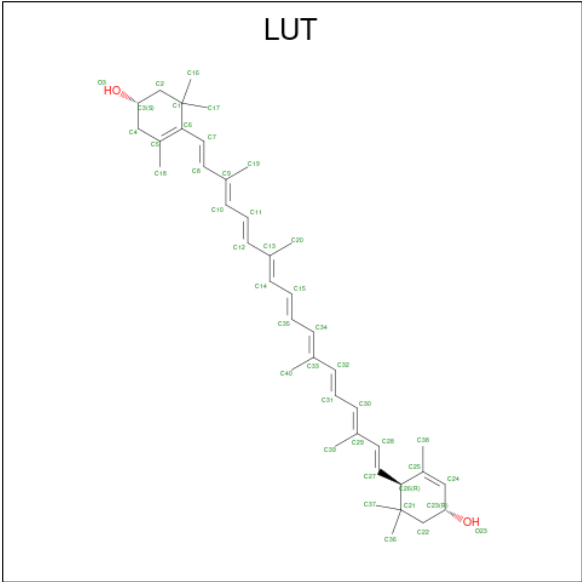
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 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 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 58	C 48	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 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

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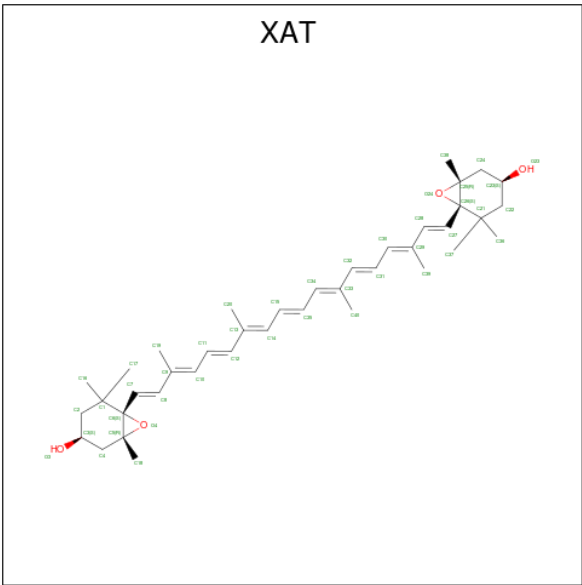
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
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: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



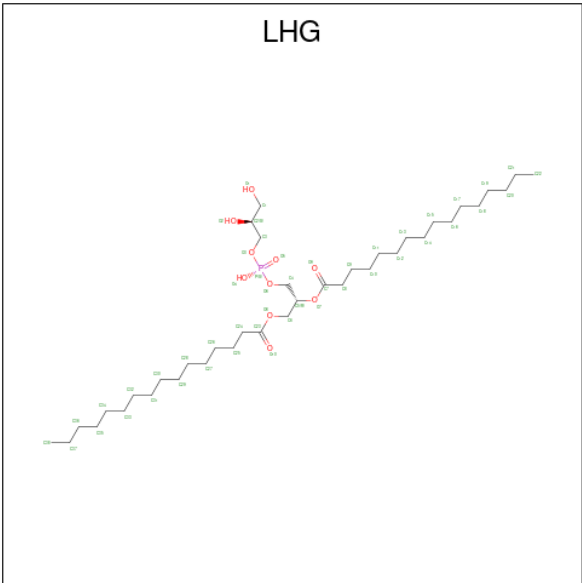
Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			42	40	2	
20	1	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	3	1	Total	C	O	0
			42	40	2	
20	4	1	Total	C	O	0
			42	40	2	

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



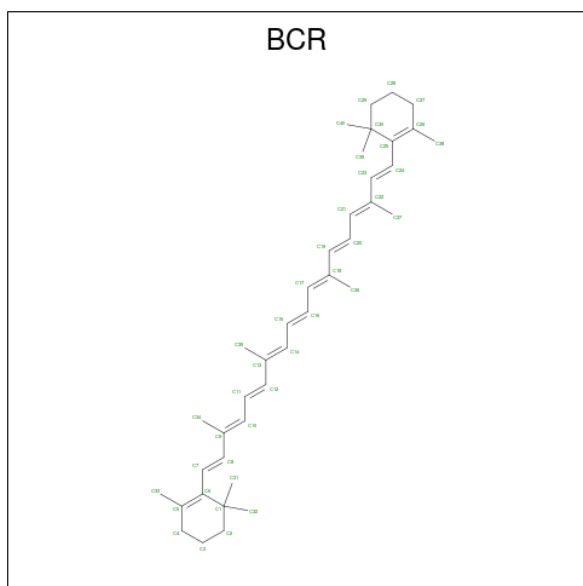
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (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
			45	34	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
23	1	1	Total	C	0
			40	40	
23	2	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	4	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	

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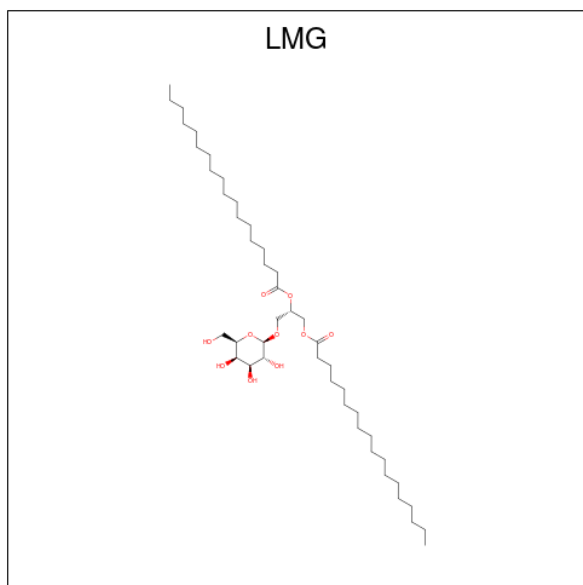
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C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

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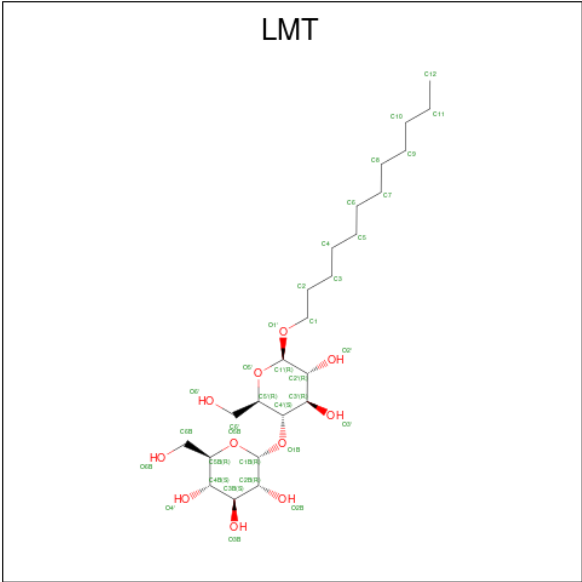
Mol	Chain	Residues	Atoms		AltConf
23	K	1	Total	C	0
			40	40	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



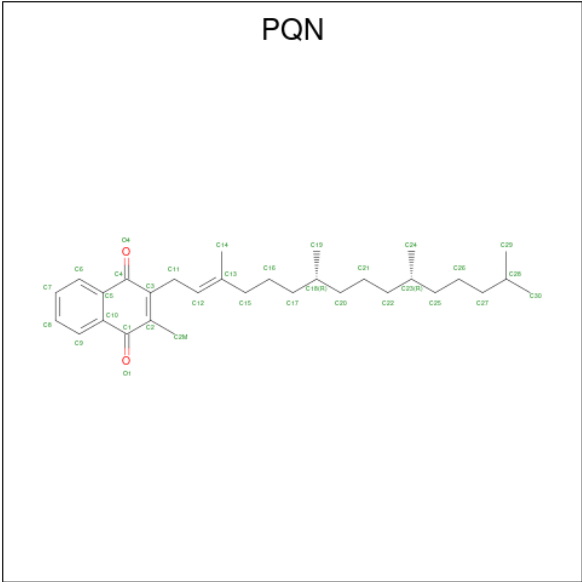
Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			50	40	10	
24	4	1	Total	C	O	0
			36	26	10	
24	B	1	Total	C	O	0
			52	42	10	
24	F	1	Total	C	O	0
			30	20	10	

- Molecule 25 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



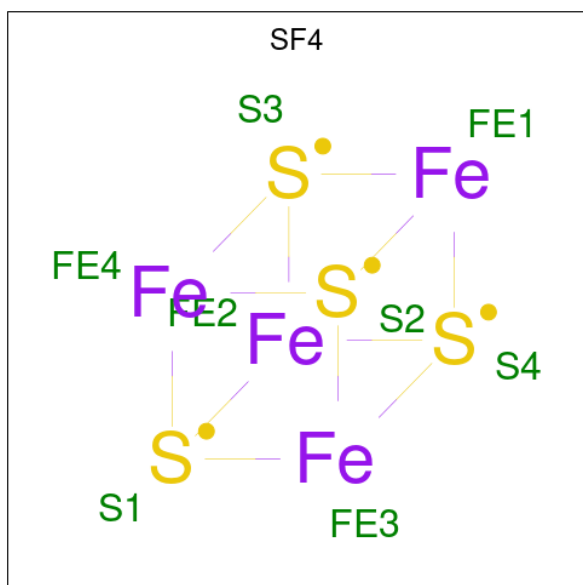
Mol	Chain	Residues	Atoms			AltConf
25	2	1	Total	C	O	0
			35	24	11	
25	G	1	Total	C	O	0
			35	24	11	
25	N	1	Total	C	O	0
			35	24	11	

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



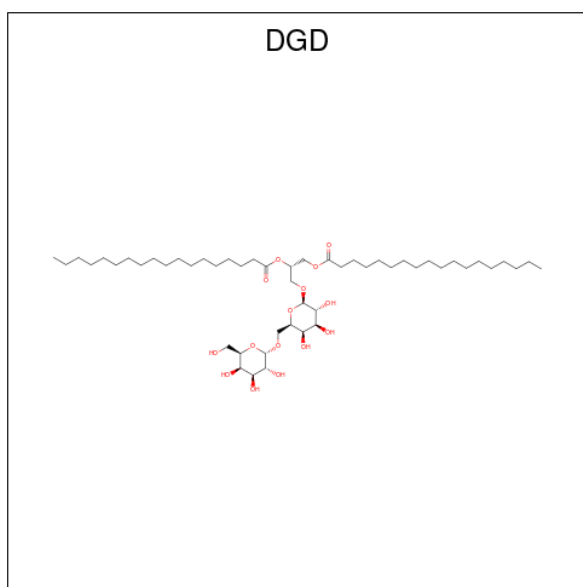
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	
26	B	1	Total	C	O	0
			33	31	2	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_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).

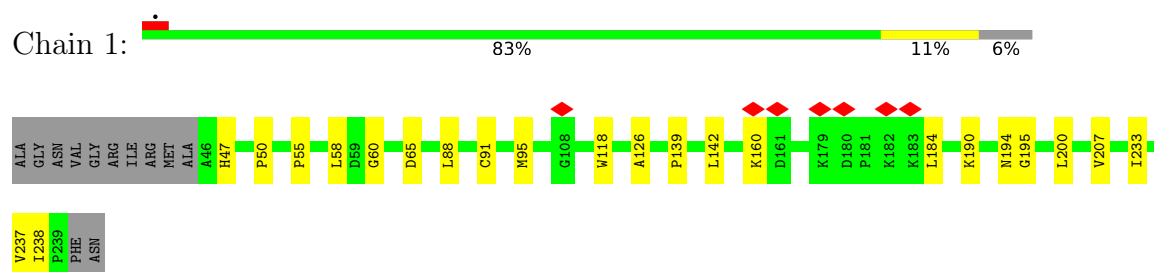


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	B	1	66	51	15	0

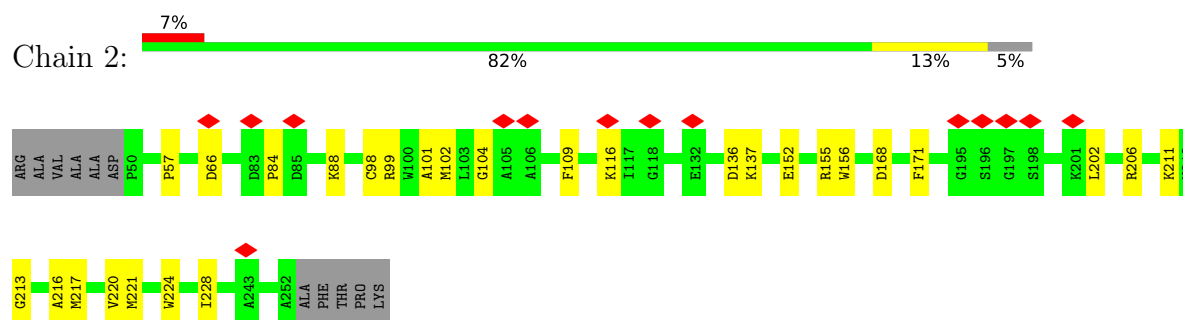
3 Residue-property plots [i](#)

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.

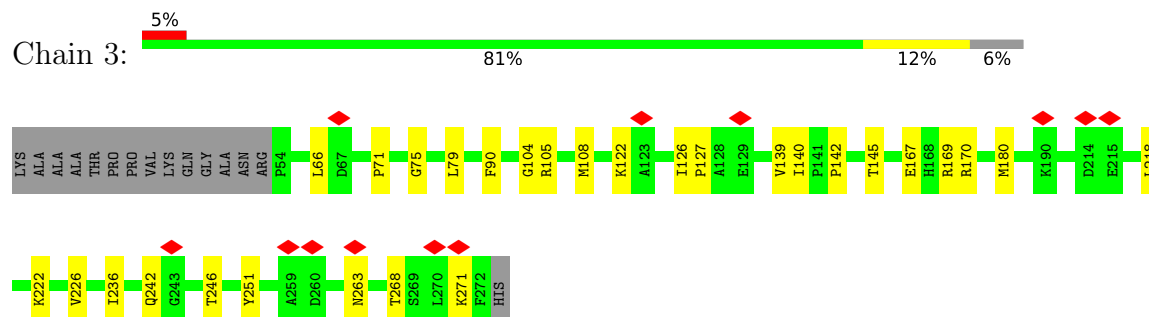
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



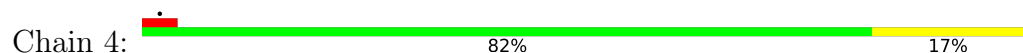
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

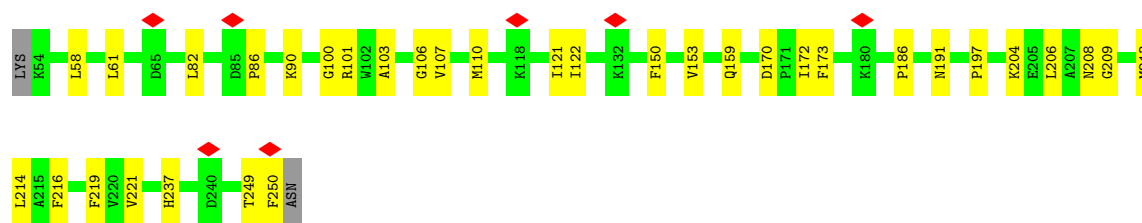


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic



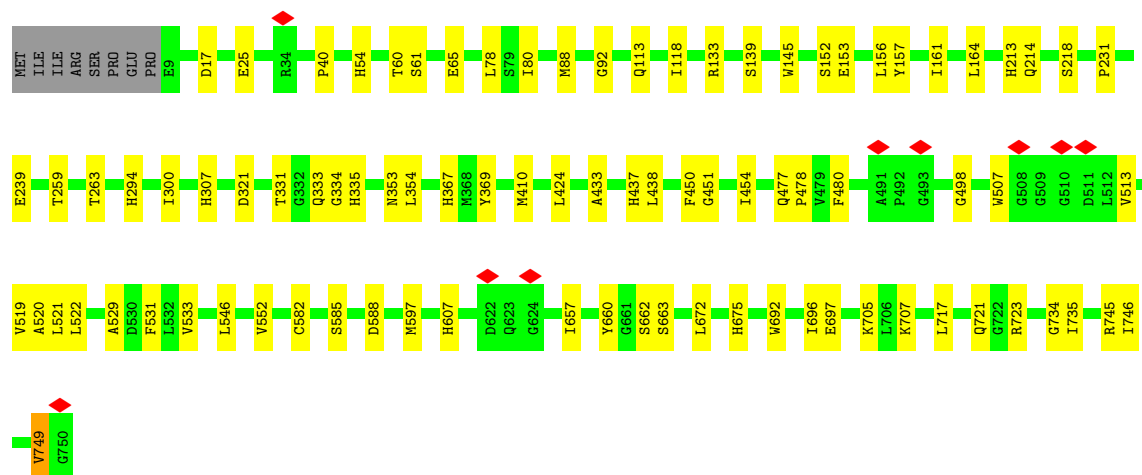
- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic





- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 87% 12%



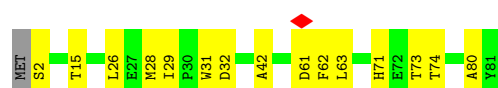
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 89% 10%



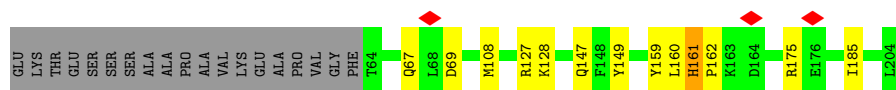
- Molecule 7: Photosystem I iron-sulfur center

Chain C: 80% 19%

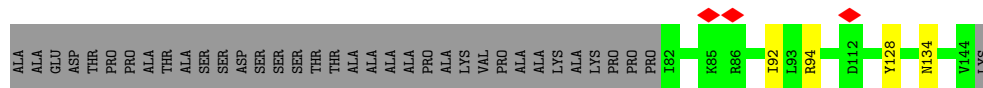


- Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

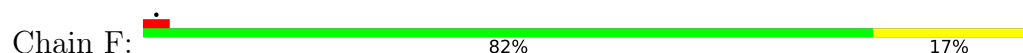
Chain D: 80% 8% 12%



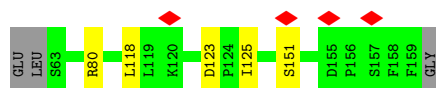
- Molecule 9: Photosystem I reaction center subunit IV B, chloroplastic



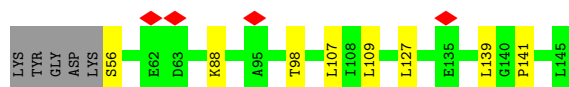
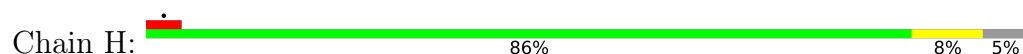
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic



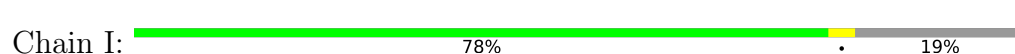
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic



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



- Molecule 13: Photosystem I reaction center subunit VIII

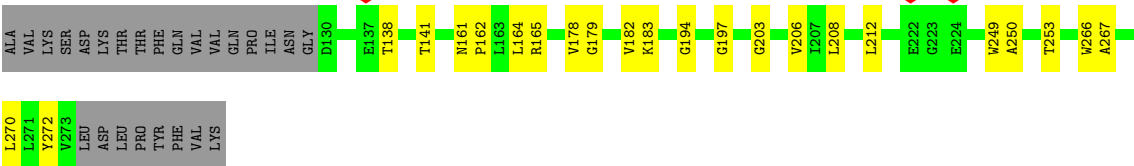


- Molecule 14: Photosystem I reaction center subunit IX



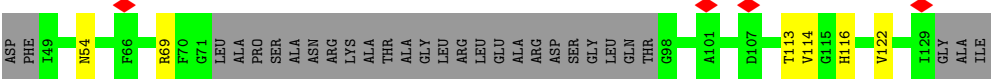
- Molecule 15: Photosystem I reaction center subunit XI, chloroplastic

Chain L: 



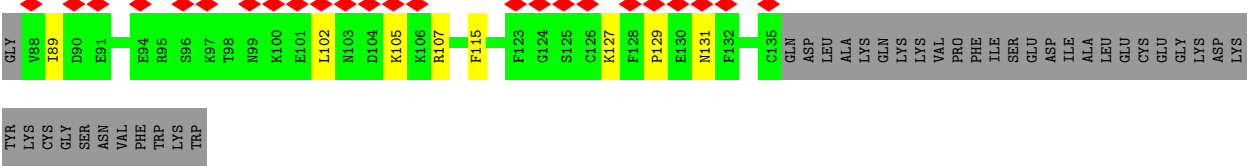
• Molecule 16: Photosystem I reaction center subunit psaK, chloroplastic

Chain K: 



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

Chain N: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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	3.854	Depositor
Minimum map value	-1.833	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	398.272, 398.272, 398.272	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.889, 0.889, 0.889	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.11	0/1551	0.28	0/2117
2	2	0.11	0/1639	0.25	0/2242
3	3	0.12	0/1730	0.26	0/2352
4	4	0.10	0/1611	0.31	0/2194
5	A	0.11	0/6031	0.24	0/8226
6	B	0.12	0/6063	0.27	0/8281
7	C	0.10	0/628	0.29	0/852
8	D	0.11	0/1140	0.28	0/1542
9	E	0.08	0/519	0.24	0/703
10	F	0.11	0/1238	0.26	0/1670
11	G	0.09	0/779	0.25	0/1056
12	H	0.10	0/712	0.27	0/968
13	I	0.11	0/236	0.26	0/322
14	J	0.10	0/349	0.24	0/476
15	L	0.12	0/1108	0.26	0/1512
16	K	0.08	0/385	0.19	0/520
17	N	0.10	0/387	0.31	0/517
All	All	0.11	0/26106	0.26	0/35550

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	18	0
2	2	1582	0	1533	21	0
3	3	1678	0	1646	19	0
4	4	1562	0	1517	26	0
5	A	5834	0	5683	67	0
6	B	5852	0	5639	60	0
7	C	615	0	592	10	0
8	D	1112	0	1122	10	0
9	E	509	0	518	4	0
10	F	1208	0	1241	23	0
11	G	759	0	735	4	0
12	H	692	0	693	7	0
13	I	230	0	245	1	0
14	J	339	0	357	9	0
15	L	1076	0	1081	16	0
16	K	382	0	399	6	0
17	N	381	0	370	5	0
18	1	102	0	78	3	0
18	2	229	0	157	3	0
18	3	47	0	31	2	0
18	4	195	0	141	4	0
19	1	684	0	602	17	0
19	2	537	0	491	12	0
19	3	646	0	538	9	0
19	4	546	0	497	12	0
19	A	2599	0	2608	73	0
19	B	2262	0	2271	50	0
19	F	219	0	206	4	0
19	G	137	0	101	1	0
19	H	45	0	28	2	0
19	J	42	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	128	0	91	4	0
19	L	170	0	157	7	0
20	1	84	0	112	8	0
20	2	42	0	56	3	0
20	3	42	0	56	2	0
20	4	42	0	56	5	0
21	1	44	0	56	1	0
21	2	44	0	56	2	0
21	3	44	0	56	1	0
21	4	44	0	56	2	0
22	1	98	0	148	6	0
22	2	37	0	44	1	0
22	A	49	0	74	0	0
22	B	45	0	63	3	0
23	1	40	0	56	2	0
23	2	40	0	56	3	0
23	3	40	0	56	1	0
23	4	40	0	56	2	0
23	A	280	0	392	27	0
23	B	240	0	336	11	0
23	F	80	0	112	6	0
23	G	40	0	56	2	0
23	I	40	0	56	1	0
23	J	120	0	168	12	0
23	K	40	0	56	2	0
23	L	120	0	168	10	0
24	1	50	0	70	3	0
24	4	36	0	42	0	0
24	B	52	0	77	1	0
24	F	30	0	30	1	0
25	2	35	0	46	5	0
25	G	35	0	46	0	0
25	N	35	0	46	2	0
26	A	33	0	46	0	0
26	B	33	0	46	1	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	B	66	0	96	4	0
All	All	36064	0	35821	479	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 479 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)
19:1:305:CLA:HBB1	18:1:306:CHL:HMC	1.60	0.84
7:C:61:ASP:HB3	9:E:134:ASN:HD21	1.44	0.82
4:4:121:ILE:HG22	4:4:122:ILE:HG12	1.62	0.81
20:1:315:LUT:H8	20:1:315:LUT:H171	1.64	0.80
20:2:315:LUT:H171	20:2:315:LUT:H8	1.64	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	192/206 (93%)	186 (97%)	6 (3%)	0	100	100
2	2	201/214 (94%)	195 (97%)	6 (3%)	0	100	100
3	3	217/234 (93%)	210 (97%)	7 (3%)	0	100	100
4	4	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
5	A	740/750 (99%)	724 (98%)	16 (2%)	0	100	100
6	B	731/734 (100%)	717 (98%)	14 (2%)	0	100	100
7	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
8	D	139/160 (87%)	132 (95%)	7 (5%)	0	100	100
9	E	61/99 (62%)	56 (92%)	5 (8%)	0	100	100
10	F	150/154 (97%)	149 (99%)	1 (1%)	0	100	100
11	G	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
12	H	88/95 (93%)	88 (100%)	0	0	100	100
13	I	28/37 (76%)	28 (100%)	0	0	100	100
14	J	40/44 (91%)	39 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	L	142/169 (84%)	139 (98%)	3 (2%)	0	100	100
16	K	51/84 (61%)	50 (98%)	1 (2%)	0	100	100
17	N	46/85 (54%)	42 (91%)	4 (9%)	0	100	100
All	All	3194/3445 (93%)	3112 (97%)	82 (3%)	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%)	152 (99%)	1 (1%)	81	89
2	2	164/171 (96%)	164 (100%)	0	100	100
3	3	169/179 (94%)	168 (99%)	1 (1%)	84	91
4	4	164/166 (99%)	164 (100%)	0	100	100
5	A	601/609 (99%)	597 (99%)	4 (1%)	81	89
6	B	597/598 (100%)	596 (100%)	1 (0%)	92	96
7	C	70/71 (99%)	69 (99%)	1 (1%)	62	79
8	D	120/134 (90%)	120 (100%)	0	100	100
9	E	56/80 (70%)	56 (100%)	0	100	100
10	F	125/127 (98%)	125 (100%)	0	100	100
11	G	82/84 (98%)	82 (100%)	0	100	100
12	H	75/79 (95%)	74 (99%)	1 (1%)	65	80
13	I	26/33 (79%)	26 (100%)	0	100	100
14	J	36/38 (95%)	36 (100%)	0	100	100
15	L	111/134 (83%)	111 (100%)	0	100	100
16	K	41/61 (67%)	41 (100%)	0	100	100
17	N	41/73 (56%)	40 (98%)	1 (2%)	44	67
All	All	2631/2798 (94%)	2621 (100%)	10 (0%)	88	94

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	63	LEU
12	H	109	LEU
17	N	89	ILE
5	A	118	ILE
5	A	369	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	236	ASN
16	K	128	ASN
6	B	402	GLN
15	L	161	ASN
11	G	90	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

210 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	815	-	45,53,73	1.57	7 (15%)	52,89,113	1.93	8 (15%)
19	CLA	B	825	-	65,73,73	1.35	7 (10%)	76,113,113	1.80	10 (13%)
19	CLA	A	836	-	65,73,73	1.36	7 (10%)	76,113,113	1.68	10 (13%)
20	LUT	1	315	-	42,43,43	1.63	8 (19%)	51,60,60	1.62	12 (23%)
20	LUT	2	315	-	42,43,43	1.64	8 (19%)	51,60,60	1.61	11 (21%)
19	CLA	A	819	-	45,53,73	1.56	7 (15%)	52,89,113	1.93	6 (11%)
19	CLA	4	311	-	56,64,73	1.45	7 (12%)	65,102,113	1.79	7 (10%)
19	CLA	A	830	-	50,58,73	1.54	7 (14%)	58,95,113	1.83	10 (17%)
19	CLA	G	203	-	50,58,73	1.53	7 (14%)	58,95,113	1.97	7 (12%)
23	BCR	2	319	-	41,41,41	0.23	0	56,56,56	0.74	2 (3%)
18	CHL	4	314	4	41,50,74	1.69	8 (19%)	42,85,114	2.23	9 (21%)
19	CLA	2	308	2	45,53,73	1.58	7 (15%)	52,89,113	1.89	7 (13%)
19	CLA	3	301	3	60,68,73	1.41	7 (11%)	70,107,113	1.74	11 (15%)
19	CLA	A	818	-	65,73,73	1.36	7 (10%)	76,113,113	1.67	11 (14%)
19	CLA	A	840	-	65,73,73	1.35	7 (10%)	76,113,113	1.66	9 (11%)
19	CLA	A	811	-	54,62,73	1.48	7 (12%)	62,99,113	1.84	8 (12%)
21	XAT	4	316	-	39,47,47	0.09	0	54,74,74	0.70	1 (1%)
19	CLA	B	805	6	65,73,73	1.35	7 (10%)	76,113,113	1.74	10 (13%)
19	CLA	B	810	-	54,62,73	1.43	6 (11%)	67,100,113	1.99	11 (16%)
19	CLA	K	204	16	38,45,73	1.71	8 (21%)	43,78,113	2.05	8 (18%)
23	BCR	B	842	-	41,41,41	0.16	0	56,56,56	0.78	2 (3%)
19	CLA	B	812	-	65,73,73	1.33	7 (10%)	76,113,113	1.79	10 (13%)
19	CLA	4	312	-	45,53,73	1.57	7 (15%)	52,89,113	1.89	8 (15%)
19	CLA	1	313	-	45,53,73	1.57	7 (15%)	52,89,113	1.84	8 (15%)
19	CLA	B	831	-	58,66,73	1.43	7 (12%)	67,104,113	1.76	8 (11%)
19	CLA	3	314	-	46,54,73	1.57	7 (15%)	53,90,113	1.89	6 (11%)
19	CLA	B	838	-	65,73,73	1.35	7 (10%)	76,113,113	1.66	11 (14%)
22	LHG	A	842	-	48,48,48	0.30	0	51,54,54	0.28	0
19	CLA	B	824	-	60,68,73	1.42	7 (11%)	70,107,113	1.79	10 (14%)
19	CLA	1	302	1	60,68,73	1.40	7 (11%)	70,107,113	1.78	11 (15%)
19	CLA	B	820	-	55,63,73	1.46	7 (12%)	64,101,113	1.80	9 (14%)
22	LHG	B	848	19	44,44,48	0.32	0	47,50,54	0.29	0
23	BCR	1	318	-	41,41,41	0.16	0	56,56,56	0.80	2 (3%)
19	CLA	2	311	2	45,53,73	1.58	7 (15%)	52,89,113	1.98	7 (13%)
23	BCR	A	846	-	41,41,41	0.11	0	56,56,56	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	807	5	65,73,73	1.34	7 (10%)	76,113,113	1.65	11 (14%)
19	CLA	1	305	-	42,50,73	1.59	7 (16%)	48,85,113	1.95	7 (14%)
19	CLA	1	310	22	55,63,73	1.48	7 (12%)	64,101,113	1.82	11 (17%)
19	CLA	3	304	-	47,55,73	1.54	7 (14%)	54,91,113	1.94	10 (18%)
19	CLA	A	803	19	50,58,73	1.54	7 (14%)	58,95,113	1.85	8 (13%)
23	BCR	A	849	-	41,41,41	0.15	0	56,56,56	0.31	0
19	CLA	B	832	-	65,73,73	1.36	7 (10%)	76,113,113	1.69	9 (11%)
19	CLA	B	827	-	65,73,73	1.35	7 (10%)	76,113,113	1.67	9 (11%)
23	BCR	I	101	-	41,41,41	0.11	0	56,56,56	0.21	0
19	CLA	1	308	1	57,65,73	1.44	7 (12%)	66,103,113	1.84	9 (13%)
24	LMG	F	307	-	30,30,55	0.21	0	38,38,63	0.14	0
24	LMG	4	318	-	36,36,55	0.20	0	44,44,63	0.13	0
25	LMT	N	201	-	36,36,36	0.10	0	47,47,47	0.25	0
23	BCR	K	201	-	41,41,41	0.18	0	56,56,56	0.50	0
23	BCR	B	841	-	41,41,41	0.14	0	56,56,56	0.25	0
18	CHL	2	301	2	51,59,74	1.69	10 (19%)	55,96,114	2.09	11 (20%)
25	LMT	2	318	-	36,36,36	0.15	0	47,47,47	0.16	0
18	CHL	2	305	-	43,51,74	1.68	8 (18%)	45,86,114	2.24	7 (15%)
27	SF4	C	102	7	0,12,12	-	-	-	-	-
18	CHL	2	307	-	46,54,74	1.74	11 (23%)	49,90,114	2.12	7 (14%)
19	CLA	2	313	-	58,66,73	1.44	8 (13%)	67,104,113	1.88	10 (14%)
19	CLA	B	806	-	54,62,73	1.47	7 (12%)	62,99,113	1.84	8 (12%)
21	XAT	3	316	-	39,47,47	0.10	0	54,74,74	0.77	2 (3%)
19	CLA	B	823	-	65,73,73	1.35	7 (10%)	76,113,113	1.70	11 (14%)
19	CLA	A	817	-	55,63,73	1.46	7 (12%)	64,101,113	1.79	9 (14%)
19	CLA	B	817	-	60,68,73	1.40	7 (11%)	70,107,113	1.76	12 (17%)
23	BCR	J	101	-	41,41,41	0.17	0	56,56,56	0.96	4 (7%)
20	LUT	3	315	-	42,43,43	1.65	8 (19%)	51,60,60	1.54	9 (17%)
19	CLA	A	814	-	50,58,73	1.53	7 (14%)	58,95,113	1.90	9 (15%)
19	CLA	4	303	-	45,53,73	1.58	7 (15%)	52,89,113	1.93	8 (15%)
19	CLA	A	802	-	65,73,73	1.35	7 (10%)	76,113,113	1.62	10 (13%)
19	CLA	2	309	2	57,65,73	1.44	7 (12%)	66,103,113	1.80	11 (16%)
19	CLA	B	835	-	65,73,73	1.35	7 (10%)	76,113,113	1.73	9 (11%)
18	CHL	3	307	-	47,55,74	1.69	10 (21%)	50,91,114	2.20	12 (24%)
19	CLA	B	822	-	60,68,73	1.41	7 (11%)	70,107,113	1.70	10 (14%)
18	CHL	4	304	-	56,64,74	1.63	11 (19%)	61,102,114	1.95	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	809	-	59,67,73	1.42	7 (11%)	68,105,113	1.82	11 (16%)
19	CLA	B	816	-	59,67,73	1.41	7 (11%)	68,105,113	1.72	11 (16%)
23	BCR	A	848	-	41,41,41	0.12	0	56,56,56	0.19	0
19	CLA	A	833	-	50,58,73	1.54	7 (14%)	58,95,113	1.81	9 (15%)
19	CLA	B	815	-	55,63,73	1.47	7 (12%)	64,101,113	1.81	8 (12%)
19	CLA	3	312	-	55,63,73	1.46	7 (12%)	64,101,113	1.81	7 (10%)
19	CLA	B	819	-	50,58,73	1.53	7 (14%)	58,95,113	1.88	8 (13%)
23	BCR	A	844	-	41,41,41	0.25	0	56,56,56	0.86	2 (3%)
19	CLA	A	828	-	65,73,73	1.36	7 (10%)	76,113,113	1.69	12 (15%)
23	BCR	J	103	-	41,41,41	0.12	0	56,56,56	0.22	0
19	CLA	F	304	10	45,53,73	1.57	7 (15%)	52,89,113	1.98	7 (13%)
19	CLA	3	302	3	60,68,73	1.41	7 (11%)	70,107,113	1.77	13 (18%)
19	CLA	B	828	-	65,73,73	1.36	7 (10%)	76,113,113	1.65	11 (14%)
19	CLA	A	825	-	65,73,73	1.36	7 (10%)	76,113,113	1.74	10 (13%)
18	CHL	2	306	-	46,54,74	1.74	10 (21%)	49,90,114	2.14	10 (20%)
19	CLA	4	309	-	60,68,73	1.41	7 (11%)	70,107,113	1.70	9 (12%)
19	CLA	A	805	5	65,73,73	1.34	7 (10%)	76,113,113	1.74	12 (15%)
23	BCR	L	306	-	41,41,41	0.14	0	56,56,56	0.42	0
19	CLA	A	826	-	65,73,73	1.35	7 (10%)	76,113,113	1.79	10 (13%)
19	CLA	B	801	-	65,73,73	1.35	7 (10%)	76,113,113	1.67	11 (14%)
19	CLA	J	102	-	42,50,73	1.58	7 (16%)	48,85,113	1.92	7 (14%)
20	LUT	4	315	-	42,43,43	1.67	8 (19%)	51,60,60	1.52	9 (17%)
19	CLA	A	831	-	65,73,73	1.36	7 (10%)	76,113,113	1.71	9 (11%)
19	CLA	B	811	-	55,63,73	1.47	7 (12%)	64,101,113	1.85	10 (15%)
19	CLA	K	203	-	46,54,73	1.56	7 (15%)	53,90,113	1.92	7 (13%)
19	CLA	3	303	-	45,53,73	1.58	7 (15%)	52,89,113	1.88	8 (15%)
19	CLA	A	832	-	65,73,73	1.36	7 (10%)	76,113,113	1.67	8 (10%)
19	CLA	A	823	-	55,63,73	1.46	7 (12%)	64,101,113	1.78	9 (14%)
19	CLA	2	320	4	46,54,73	1.54	7 (15%)	53,90,113	1.96	8 (15%)
19	CLA	3	311	-	45,53,73	1.59	7 (15%)	52,89,113	2.01	8 (15%)
19	CLA	A	821	-	45,53,73	1.58	7 (15%)	52,89,113	1.94	8 (15%)
19	CLA	B	836	-	47,55,73	1.54	7 (14%)	54,91,113	1.88	7 (12%)
19	CLA	B	803	-	45,53,73	1.58	7 (15%)	52,89,113	1.91	6 (11%)
19	CLA	1	314	1	45,53,73	1.56	7 (15%)	52,89,113	1.89	7 (13%)
19	CLA	G	204	11	46,54,73	1.55	7 (15%)	53,90,113	1.96	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	838	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	10 (13%)
19	CLA	A	824	-	65,73,73	1.34	7 (10%)	76,113,113	1.69	13 (17%)
19	CLA	B	826	-	65,73,73	1.34	7 (10%)	76,113,113	1.67	11 (14%)
19	CLA	1	311	1	45,53,73	1.58	7 (15%)	52,89,113	1.94	6 (11%)
19	CLA	A	820	-	65,73,73	1.36	7 (10%)	76,113,113	1.68	10 (13%)
19	CLA	B	807	-	65,73,73	1.35	7 (10%)	76,113,113	1.73	9 (11%)
19	CLA	1	303	-	58,66,73	1.42	7 (12%)	67,104,113	1.78	9 (13%)
19	CLA	A	854	-	65,73,73	1.35	7 (10%)	76,113,113	1.73	11 (14%)
19	CLA	H	201	12	45,53,73	1.57	7 (15%)	52,89,113	1.90	10 (19%)
19	CLA	3	305	-	42,50,73	1.59	7 (16%)	48,85,113	1.94	8 (16%)
19	CLA	3	310	-	41,49,73	1.62	8 (19%)	47,84,113	1.97	9 (19%)
19	CLA	4	302	-	60,68,73	1.42	7 (11%)	70,107,113	1.76	11 (15%)
18	CHL	2	314	2	43,51,74	1.66	8 (18%)	45,86,114	2.08	8 (17%)
23	BCR	B	843	-	41,41,41	0.12	0	56,56,56	0.31	0
19	CLA	B	818	-	60,68,73	1.42	7 (11%)	70,107,113	1.76	10 (14%)
19	CLA	2	312	-	65,73,73	1.35	7 (10%)	76,113,113	1.71	9 (11%)
19	CLA	A	808	5	62,70,73	1.38	7 (11%)	72,109,113	1.80	10 (13%)
19	CLA	B	808	6	65,73,73	1.36	7 (10%)	76,113,113	1.71	11 (14%)
19	CLA	B	837	-	65,73,73	1.36	7 (10%)	76,113,113	1.70	11 (14%)
19	CLA	3	313	-	45,53,73	1.58	7 (15%)	52,89,113	1.89	8 (15%)
27	SF4	C	101	7	0,12,12	-	-	-	-	-
19	CLA	A	834	-	65,73,73	1.35	7 (10%)	76,113,113	1.62	10 (13%)
18	CHL	4	305	-	46,54,74	1.74	12 (26%)	49,90,114	2.04	8 (16%)
19	CLA	A	804	-	65,73,73	1.35	7 (10%)	76,113,113	1.81	12 (15%)
19	CLA	B	804	-	65,73,73	1.35	7 (10%)	76,113,113	1.76	9 (11%)
19	CLA	4	310	4	45,53,73	1.58	7 (15%)	52,89,113	1.97	7 (13%)
19	CLA	K	202	-	45,53,73	1.58	7 (15%)	52,89,113	1.92	9 (17%)
19	CLA	A	806	-	50,58,73	1.54	7 (14%)	58,95,113	1.85	9 (15%)
19	CLA	F	302	-	65,73,73	1.34	7 (10%)	76,113,113	1.74	14 (18%)
19	CLA	3	309	3	50,58,73	1.53	7 (14%)	58,95,113	1.84	11 (18%)
19	CLA	B	809	-	65,73,73	1.35	7 (10%)	76,113,113	1.65	10 (13%)
19	CLA	B	830	-	60,68,73	1.42	7 (11%)	70,107,113	1.78	10 (14%)
19	CLA	L	302	-	65,73,73	1.36	7 (10%)	76,113,113	1.69	11 (14%)
19	CLA	1	312	-	60,68,73	1.40	7 (11%)	70,107,113	1.75	9 (12%)
21	XAT	1	316	-	39,47,47	0.10	0	54,74,74	0.68	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	A	843	-	41,41,41	0.19	0	56,56,56	0.67	2 (3%)
23	BCR	4	317	-	41,41,41	0.14	0	56,56,56	0.32	0
24	LMG	B	847	-	52,52,55	0.19	0	60,60,63	0.16	0
27	SF4	A	850	5,6	0,12,12	-	-	-	-	-
19	CLA	L	301	15	55,63,73	1.46	7 (12%)	64,101,113	1.80	9 (14%)
19	CLA	B	813	-	65,73,73	1.36	7 (10%)	76,113,113	1.71	8 (10%)
19	CLA	A	827	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	9 (11%)
22	LHG	1	322	-	48,48,48	0.31	0	51,54,54	0.27	0
19	CLA	3	306	3	45,53,73	1.57	7 (15%)	52,89,113	1.87	8 (15%)
19	CLA	A	853	-	60,68,73	1.41	7 (11%)	70,107,113	1.71	8 (11%)
19	CLA	A	835	-	51,59,73	1.51	7 (13%)	59,96,113	1.95	8 (13%)
19	CLA	4	307	4	50,58,73	1.54	7 (14%)	58,95,113	1.90	8 (13%)
19	CLA	A	816	-	63,72,73	1.37	7 (11%)	73,112,113	1.63	10 (13%)
19	CLA	A	822	-	51,59,73	1.51	7 (13%)	59,96,113	1.93	11 (18%)
28	DGD	B	846	-	67,67,67	0.16	0	81,81,81	0.15	0
20	LUT	1	320	-	42,43,43	1.63	8 (19%)	51,60,60	1.65	11 (21%)
19	CLA	4	308	4	60,68,73	1.40	7 (11%)	70,107,113	1.78	11 (15%)
19	CLA	4	313	-	65,73,73	1.36	7 (10%)	76,113,113	1.72	11 (14%)
22	LHG	1	317	19	48,48,48	0.30	0	51,54,54	0.29	0
25	LMT	G	201	-	36,36,36	0.10	0	47,47,47	0.20	0
19	CLA	B	829	-	50,58,73	1.53	7 (14%)	58,95,113	1.82	10 (17%)
19	CLA	A	801	-	65,73,73	1.35	7 (10%)	76,113,113	1.70	11 (14%)
19	CLA	F	303	-	45,53,73	1.58	7 (15%)	52,89,113	1.96	10 (19%)
19	CLA	1	307	-	45,53,73	1.57	7 (15%)	52,89,113	1.89	8 (15%)
18	CHL	1	301	1	56,64,74	1.61	10 (17%)	61,102,114	1.98	11 (18%)
19	CLA	A	810	19	65,73,73	1.35	7 (10%)	76,113,113	1.70	11 (14%)
19	CLA	A	813	-	45,53,73	1.57	7 (15%)	52,89,113	2.00	7 (13%)
23	BCR	A	847	-	41,41,41	0.14	0	56,56,56	0.71	0
23	BCR	F	305	-	41,41,41	0.11	0	56,56,56	0.24	0
19	CLA	A	851	5	45,53,73	1.58	7 (15%)	52,89,113	1.93	7 (13%)
18	CHL	1	306	-	46,54,74	1.75	11 (23%)	49,90,114	2.14	10 (20%)
23	BCR	B	840	-	41,41,41	0.13	0	56,56,56	0.28	0
23	BCR	J	104	-	41,41,41	0.11	0	56,56,56	0.20	0
19	CLA	A	852	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	13 (17%)
19	CLA	B	814	-	55,63,73	1.47	7 (12%)	64,101,113	1.87	10 (15%)
21	XAT	2	316	-	39,47,47	0.13	0	54,74,74	0.72	1 (1%)
19	CLA	G	202	-	41,49,73	1.63	7 (17%)	47,84,113	1.99	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	821	-	55,63,73	1.46	7 (12%)	64,101,113	1.82	8 (12%)
26	PQN	B	839	-	34,34,34	0.27	0	42,45,45	0.50	1 (2%)
24	LMG	1	319	-	50,50,55	0.20	0	58,58,63	0.14	0
19	CLA	A	829	-	65,73,73	1.36	7 (10%)	76,113,113	1.74	9 (11%)
19	CLA	2	304	-	65,73,73	1.37	8 (12%)	76,113,113	1.70	11 (14%)
19	CLA	A	839	-	65,73,73	1.36	7 (10%)	76,113,113	1.72	11 (14%)
19	CLA	1	304	-	51,59,73	1.51	7 (13%)	59,96,113	1.90	8 (13%)
19	CLA	B	802	-	65,73,73	1.34	7 (10%)	76,113,113	1.75	11 (14%)
19	CLA	2	310	22	41,49,73	1.62	7 (17%)	47,84,113	1.99	8 (17%)
19	CLA	4	301	4	60,68,73	1.41	7 (11%)	70,107,113	1.79	9 (12%)
23	BCR	G	205	-	41,41,41	0.10	0	56,56,56	0.33	0
19	CLA	F	301	-	64,72,73	1.37	7 (10%)	74,111,113	1.81	11 (14%)
19	CLA	B	834	-	55,63,73	1.47	7 (12%)	64,101,113	1.88	8 (12%)
19	CLA	2	302	2	65,73,73	1.35	7 (10%)	76,113,113	1.69	11 (14%)
26	PQN	A	841	-	34,34,34	0.28	0	42,45,45	0.50	1 (2%)
19	CLA	L	303	-	50,58,73	1.54	7 (14%)	58,95,113	1.82	11 (18%)
22	LHG	2	317	19	36,36,48	0.34	0	39,42,54	0.30	0
19	CLA	1	321	22	65,73,73	1.34	7 (10%)	76,113,113	1.80	8 (10%)
19	CLA	3	308	3	65,73,73	1.36	7 (10%)	76,113,113	1.70	8 (10%)
19	CLA	A	837	-	52,60,73	1.51	7 (13%)	60,97,113	1.84	10 (16%)
23	BCR	L	304	-	41,41,41	0.15	0	56,56,56	0.29	0
19	CLA	2	303	-	50,58,73	1.54	7 (14%)	58,95,113	1.88	8 (13%)
23	BCR	L	305	-	41,41,41	0.22	0	56,56,56	0.86	2 (3%)
19	CLA	B	833	-	45,53,73	1.58	7 (15%)	52,89,113	1.97	7 (13%)
19	CLA	A	812	-	65,73,73	1.34	7 (10%)	76,113,113	1.78	10 (13%)
23	BCR	3	317	-	41,41,41	0.12	0	56,56,56	0.32	0
19	CLA	1	309	1	56,64,73	1.46	7 (12%)	65,102,113	1.82	9 (13%)
23	BCR	F	306	-	41,41,41	0.13	0	56,56,56	0.28	0
23	BCR	B	844	-	41,41,41	0.11	0	56,56,56	0.33	0
23	BCR	A	845	-	41,41,41	0.14	0	56,56,56	0.22	0
23	BCR	B	845	-	41,41,41	0.11	0	56,56,56	0.24	0
18	CHL	4	306	-	51,59,74	1.68	11 (21%)	55,96,114	2.04	11 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	815	-	1/1/11/20	4/13/91/115	-
19	CLA	B	825	-	1/1/15/20	14/37/115/115	-
19	CLA	A	836	-	1/1/15/20	14/37/115/115	-
20	LUT	1	315	-	-	0/29/67/67	0/2/2/2
20	LUT	2	315	-	-	0/29/67/67	0/2/2/2
19	CLA	A	819	-	1/1/11/20	0/13/91/115	-
19	CLA	4	311	-	1/1/13/20	10/27/105/115	-
19	CLA	A	830	-	1/1/12/20	9/19/97/115	-
19	CLA	G	203	-	1/1/12/20	8/19/97/115	-
23	BCR	2	319	-	-	9/29/63/63	0/2/2/2
18	CHL	4	314	4	3/3/15/26	1/10/108/137	-
19	CLA	2	308	2	1/1/11/20	5/13/91/115	-
19	CLA	3	301	3	1/1/14/20	13/31/109/115	-
19	CLA	A	818	-	1/1/15/20	17/37/115/115	-
19	CLA	A	840	-	1/1/15/20	20/37/115/115	-
19	CLA	A	811	-	1/1/12/20	6/24/102/115	-
21	XAT	4	316	-	-	0/31/93/93	0/4/4/4
19	CLA	B	805	6	1/1/15/20	13/37/115/115	-
19	CLA	B	810	-	1/1/13/20	11/25/101/115	-
19	CLA	K	204	16	1/1/8/20	0/2/76/115	-
23	BCR	B	842	-	-	9/29/63/63	0/2/2/2
19	CLA	B	812	-	1/1/15/20	16/37/115/115	-
19	CLA	4	312	-	1/1/11/20	6/13/91/115	-
19	CLA	1	313	-	1/1/11/20	8/13/91/115	-
19	CLA	B	831	-	1/1/13/20	17/29/107/115	-
19	CLA	3	314	-	1/1/11/20	7/15/93/115	-
19	CLA	B	838	-	1/1/15/20	14/37/115/115	-
22	LHG	A	842	-	-	8/53/53/53	-
19	CLA	B	824	-	1/1/14/20	9/31/109/115	-
19	CLA	1	302	1	1/1/14/20	9/31/109/115	-
19	CLA	B	820	-	1/1/13/20	12/25/103/115	-
22	LHG	B	848	19	-	9/49/49/53	-
23	BCR	1	318	-	-	8/29/63/63	0/2/2/2
19	CLA	2	311	2	1/1/11/20	6/13/91/115	-
23	BCR	A	846	-	-	0/29/63/63	0/2/2/2
19	CLA	A	807	5	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	305	-	1/1/10/20	3/10/88/115	-
19	CLA	1	310	22	1/1/13/20	5/25/103/115	-
19	CLA	3	304	-	1/1/11/20	7/16/94/115	-
19	CLA	A	803	19	1/1/12/20	10/19/97/115	-
23	BCR	A	849	-	-	4/29/63/63	0/2/2/2
19	CLA	B	832	-	1/1/15/20	19/37/115/115	-
19	CLA	B	827	-	1/1/15/20	19/37/115/115	-
23	BCR	I	101	-	-	0/29/63/63	0/2/2/2
19	CLA	1	308	1	1/1/13/20	10/28/106/115	-
24	LMG	F	307	-	-	2/25/45/70	0/1/1/1
24	LMG	4	318	-	-	5/31/51/70	0/1/1/1
25	LMT	N	201	-	-	5/21/61/61	0/2/2/2
23	BCR	K	201	-	-	9/29/63/63	0/2/2/2
23	BCR	B	841	-	-	4/29/63/63	0/2/2/2
18	CHL	2	301	2	3/3/17/26	12/21/119/137	-
25	LMT	2	318	-	-	7/21/61/61	0/2/2/2
18	CHL	2	305	-	3/3/15/26	4/12/110/137	-
27	SF4	C	102	7	-	-	0/6/5/5
18	CHL	2	307	-	3/3/16/26	6/15/113/137	-
19	CLA	2	313	-	1/1/13/20	8/29/107/115	-
19	CLA	B	806	-	1/1/12/20	7/24/102/115	-
21	XAT	3	316	-	-	0/31/93/93	0/4/4/4
19	CLA	B	823	-	1/1/15/20	14/37/115/115	-
19	CLA	A	817	-	1/1/13/20	8/25/103/115	-
19	CLA	B	817	-	1/1/14/20	17/31/109/115	-
23	BCR	J	101	-	-	11/29/63/63	0/2/2/2
20	LUT	3	315	-	-	1/29/67/67	0/2/2/2
19	CLA	A	814	-	1/1/12/20	11/19/97/115	-
19	CLA	4	303	-	1/1/11/20	6/13/91/115	-
19	CLA	A	802	-	1/1/15/20	10/37/115/115	-
19	CLA	2	309	2	1/1/13/20	12/28/106/115	-
19	CLA	B	835	-	1/1/15/20	15/37/115/115	-
18	CHL	3	307	-	3/3/16/26	5/17/115/137	-
19	CLA	B	822	-	1/1/14/20	19/31/109/115	-
18	CHL	4	304	-	3/3/18/26	7/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	809	-	1/1/13/20	11/30/108/115	-
19	CLA	B	816	-	1/1/13/20	12/30/108/115	-
23	BCR	A	848	-	-	0/29/63/63	0/2/2/2
19	CLA	A	833	-	1/1/12/20	5/19/97/115	-
19	CLA	B	815	-	1/1/13/20	7/25/103/115	-
19	CLA	3	312	-	1/1/13/20	8/25/103/115	-
19	CLA	B	819	-	1/1/12/20	10/19/97/115	-
23	BCR	A	844	-	-	1/29/63/63	0/2/2/2
19	CLA	A	828	-	1/1/15/20	12/37/115/115	-
23	BCR	J	103	-	-	2/29/63/63	0/2/2/2
19	CLA	F	304	10	1/1/11/20	6/13/91/115	-
19	CLA	3	302	3	1/1/14/20	10/31/109/115	-
19	CLA	B	828	-	1/1/15/20	15/37/115/115	-
19	CLA	A	825	-	1/1/15/20	6/37/115/115	-
18	CHL	2	306	-	3/3/16/26	9/15/113/137	-
19	CLA	4	309	-	1/1/14/20	11/31/109/115	-
19	CLA	A	805	5	1/1/15/20	18/37/115/115	-
23	BCR	L	306	-	-	3/29/63/63	0/2/2/2
19	CLA	A	826	-	1/1/15/20	14/37/115/115	-
19	CLA	B	801	-	1/1/15/20	14/37/115/115	-
19	CLA	J	102	-	1/1/10/20	5/10/88/115	-
20	LUT	4	315	-	-	1/29/67/67	0/2/2/2
19	CLA	A	831	-	1/1/15/20	14/37/115/115	-
19	CLA	B	811	-	1/1/13/20	11/25/103/115	-
19	CLA	K	203	-	1/1/11/20	4/15/93/115	-
19	CLA	3	303	-	1/1/11/20	5/13/91/115	-
19	CLA	A	832	-	1/1/15/20	15/37/115/115	-
19	CLA	A	823	-	1/1/13/20	8/25/103/115	-
19	CLA	2	320	4	1/1/11/20	2/15/93/115	-
19	CLA	3	311	-	1/1/11/20	4/13/91/115	-
19	CLA	A	821	-	1/1/11/20	5/13/91/115	-
19	CLA	B	836	-	1/1/11/20	0/16/94/115	-
19	CLA	B	803	-	1/1/11/20	6/13/91/115	-
19	CLA	1	314	1	1/1/11/20	6/13/91/115	-
19	CLA	G	204	11	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	838	-	1/1/15/20	14/37/115/115	-
19	CLA	A	824	-	1/1/15/20	13/37/115/115	-
19	CLA	B	826	-	1/1/15/20	15/37/115/115	-
19	CLA	1	311	1	1/1/11/20	7/13/91/115	-
19	CLA	A	820	-	1/1/15/20	14/37/115/115	-
19	CLA	B	807	-	1/1/15/20	12/37/115/115	-
19	CLA	1	303	-	1/1/13/20	9/29/107/115	-
19	CLA	A	854	-	1/1/15/20	14/37/115/115	-
19	CLA	H	201	12	1/1/11/20	9/13/91/115	-
19	CLA	3	305	-	1/1/10/20	2/10/88/115	-
19	CLA	3	310	-	1/1/10/20	4/8/86/115	-
19	CLA	4	302	-	1/1/14/20	14/31/109/115	-
18	CHL	2	314	2	2/2/15/26	6/12/110/137	-
23	BCR	B	843	-	-	0/29/63/63	0/2/2/2
19	CLA	B	818	-	1/1/14/20	10/31/109/115	-
19	CLA	2	312	-	1/1/15/20	21/37/115/115	-
19	CLA	A	808	5	1/1/14/20	15/34/112/115	-
19	CLA	B	808	6	1/1/15/20	12/37/115/115	-
19	CLA	B	837	-	1/1/15/20	17/37/115/115	-
19	CLA	3	313	-	1/1/11/20	5/13/91/115	-
27	SF4	C	101	7	-	-	0/6/5/5
19	CLA	A	834	-	1/1/15/20	17/37/115/115	-
18	CHL	4	305	-	3/3/16/26	7/15/113/137	-
19	CLA	A	804	-	1/1/15/20	20/37/115/115	-
19	CLA	B	804	-	1/1/15/20	12/37/115/115	-
19	CLA	4	310	4	1/1/11/20	6/13/91/115	-
19	CLA	K	202	-	1/1/11/20	7/13/91/115	-
19	CLA	A	806	-	1/1/12/20	3/19/97/115	-
19	CLA	F	302	-	1/1/15/20	20/37/115/115	-
19	CLA	3	309	3	1/1/12/20	6/19/97/115	-
19	CLA	B	809	-	1/1/15/20	18/37/115/115	-
19	CLA	B	830	-	1/1/14/20	15/31/109/115	-
19	CLA	L	302	-	1/1/15/20	19/37/115/115	-
19	CLA	1	312	-	1/1/14/20	12/31/109/115	-
21	XAT	1	316	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A	843	-	-	11/29/63/63	0/2/2/2
23	BCR	4	317	-	-	2/29/63/63	0/2/2/2
24	LMG	B	847	-	-	11/47/67/70	0/1/1/1
27	SF4	A	850	5,6	-	-	0/6/5/5
19	CLA	L	301	15	1/1/13/20	17/25/103/115	-
19	CLA	B	813	-	1/1/15/20	16/37/115/115	-
19	CLA	A	827	-	1/1/15/20	13/37/115/115	-
22	LHG	1	322	-	-	9/53/53/53	-
19	CLA	3	306	3	1/1/11/20	5/13/91/115	-
19	CLA	A	853	-	1/1/14/20	15/31/109/115	-
19	CLA	A	835	-	1/1/12/20	9/21/99/115	-
19	CLA	4	307	4	1/1/12/20	7/19/97/115	-
19	CLA	A	816	-	1/1/15/20	13/35/113/115	-
19	CLA	A	822	-	1/1/12/20	13/21/99/115	-
28	DGD	B	846	-	-	7/55/95/95	0/2/2/2
20	LUT	1	320	-	-	0/29/67/67	0/2/2/2
19	CLA	4	308	4	1/1/14/20	6/31/109/115	-
19	CLA	4	313	-	1/1/15/20	20/37/115/115	-
22	LHG	1	317	19	-	8/53/53/53	-
25	LMT	G	201	-	-	4/21/61/61	0/2/2/2
19	CLA	B	829	-	1/1/12/20	6/19/97/115	-
19	CLA	A	801	-	1/1/15/20	12/37/115/115	-
19	CLA	F	303	-	1/1/11/20	4/13/91/115	-
19	CLA	1	307	-	1/1/11/20	5/13/91/115	-
18	CHL	1	301	1	3/3/18/26	10/27/125/137	-
19	CLA	A	810	19	1/1/15/20	16/37/115/115	-
19	CLA	A	813	-	1/1/11/20	4/13/91/115	-
23	BCR	A	847	-	-	3/29/63/63	0/2/2/2
23	BCR	F	305	-	-	2/29/63/63	0/2/2/2
19	CLA	A	851	5	1/1/11/20	4/13/91/115	-
18	CHL	1	306	-	3/3/16/26	7/15/113/137	-
23	BCR	B	840	-	-	0/29/63/63	0/2/2/2
23	BCR	J	104	-	-	4/29/63/63	0/2/2/2
19	CLA	A	852	-	1/1/15/20	14/37/115/115	-
19	CLA	B	814	-	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	XAT	2	316	-	-	2/31/93/93	0/4/4/4
19	CLA	G	202	-	1/1/10/20	4/8/86/115	-
19	CLA	B	821	-	1/1/13/20	6/25/103/115	-
26	PQN	B	839	-	-	5/23/43/43	0/2/2/2
24	LMG	1	319	-	-	11/45/65/70	0/1/1/1
19	CLA	A	829	-	1/1/15/20	18/37/115/115	-
19	CLA	2	304	-	1/1/15/20	20/37/115/115	-
19	CLA	A	839	-	1/1/15/20	15/37/115/115	-
19	CLA	1	304	-	1/1/12/20	12/21/99/115	-
19	CLA	B	802	-	1/1/15/20	13/37/115/115	-
19	CLA	2	310	22	1/1/10/20	2/8/86/115	-
19	CLA	4	301	4	1/1/14/20	8/31/109/115	-
23	BCR	G	205	-	-	2/29/63/63	0/2/2/2
19	CLA	F	301	-	1/1/14/20	20/36/114/115	-
19	CLA	B	834	-	1/1/13/20	7/25/103/115	-
19	CLA	2	302	2	1/1/15/20	16/37/115/115	-
26	PQN	A	841	-	-	2/23/43/43	0/2/2/2
19	CLA	L	303	-	1/1/12/20	11/19/97/115	-
22	LHG	2	317	19	-	9/41/41/53	-
19	CLA	1	321	22	1/1/15/20	14/37/115/115	-
19	CLA	3	308	3	1/1/15/20	21/37/115/115	-
19	CLA	A	837	-	1/1/12/20	10/22/100/115	-
23	BCR	L	304	-	-	4/29/63/63	0/2/2/2
19	CLA	2	303	-	1/1/12/20	6/19/97/115	-
23	BCR	L	305	-	-	2/29/63/63	0/2/2/2
19	CLA	B	833	-	1/1/11/20	5/13/91/115	-
19	CLA	A	812	-	1/1/15/20	24/37/115/115	-
23	BCR	3	317	-	-	3/29/63/63	0/2/2/2
19	CLA	1	309	1	1/1/13/20	5/27/105/115	-
23	BCR	F	306	-	-	0/29/63/63	0/2/2/2
23	BCR	B	844	-	-	2/29/63/63	0/2/2/2
23	BCR	A	845	-	-	3/29/63/63	0/2/2/2
23	BCR	B	845	-	-	2/29/63/63	0/2/2/2
18	CHL	4	306	-	3/3/17/26	7/21/119/137	-

The worst 5 of 1164 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	305	CHL	CMC-C2C	5.46	1.56	1.45
18	4	304	CHL	CMC-C2C	5.45	1.56	1.45
18	2	301	CHL	CMC-C2C	5.45	1.56	1.45
18	2	307	CHL	CMC-C2C	5.42	1.56	1.45
18	1	306	CHL	CMC-C2C	5.42	1.56	1.45

The worst 5 of 1522 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	321	CLA	C4A-NA-C1A	10.93	111.62	106.71
19	A	804	CLA	C4A-NA-C1A	10.89	111.60	106.71
19	G	203	CLA	C4A-NA-C1A	10.87	111.59	106.71
19	B	825	CLA	C4A-NA-C1A	10.83	111.57	106.71
18	3	307	CHL	C4A-NA-C1A	10.81	111.57	106.71

5 of 178 chirality outliers are listed below:

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

5 of 1811 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	301	CHL	CHA-CBD-CGD-O1D
18	1	301	CHL	CHA-CBD-CGD-O2D
18	1	301	CHL	CBD-CGD-O2D-CED
18	1	301	CHL	O1D-CGD-O2D-CED
18	1	306	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

156 monomers are involved in 290 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	825	CLA	2	0
19	A	836	CLA	3	0
20	1	315	LUT	3	0
20	2	315	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	311	CLA	3	0
19	G	203	CLA	1	0
23	2	319	BCR	3	0
19	A	818	CLA	2	0
19	A	840	CLA	1	0
19	A	811	CLA	1	0
21	4	316	XAT	2	0
19	B	805	CLA	4	0
19	B	810	CLA	1	0
19	K	204	CLA	1	0
23	B	842	BCR	4	0
19	B	812	CLA	1	0
19	1	313	CLA	1	0
19	B	831	CLA	3	0
19	B	838	CLA	1	0
19	1	302	CLA	1	0
22	B	848	LHG	3	0
23	1	318	BCR	2	0
23	A	846	BCR	3	0
19	A	807	CLA	5	0
19	1	305	CLA	2	0
19	3	304	CLA	1	0
23	A	849	BCR	1	0
19	B	832	CLA	1	0
19	B	827	CLA	2	0
23	I	101	BCR	1	0
19	1	308	CLA	3	0
24	F	307	LMG	1	0
25	N	201	LMT	2	0
23	K	201	BCR	2	0
23	B	841	BCR	1	0
18	2	301	CHL	2	0
25	2	318	LMT	5	0
18	2	307	CHL	1	0
19	2	313	CLA	1	0
19	B	806	CLA	2	0
21	3	316	XAT	1	0
19	B	823	CLA	2	0
19	A	817	CLA	3	0
23	J	101	BCR	6	0
20	3	315	LUT	2	0
19	A	814	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	309	CLA	3	0
19	B	835	CLA	1	0
18	3	307	CHL	2	0
19	B	822	CLA	4	0
18	4	304	CHL	1	0
19	A	809	CLA	2	0
19	B	816	CLA	3	0
23	A	848	BCR	3	0
19	A	833	CLA	2	0
19	B	815	CLA	1	0
19	B	819	CLA	1	0
23	A	844	BCR	9	0
19	A	828	CLA	1	0
23	J	103	BCR	3	0
19	F	304	CLA	1	0
19	3	302	CLA	2	0
19	B	828	CLA	2	0
19	A	825	CLA	2	0
19	A	805	CLA	1	0
23	L	306	BCR	2	0
19	A	826	CLA	4	0
19	B	801	CLA	1	0
19	J	102	CLA	1	0
20	4	315	LUT	5	0
19	A	831	CLA	1	0
19	B	811	CLA	5	0
19	K	203	CLA	1	0
19	A	832	CLA	4	0
19	A	823	CLA	3	0
19	2	320	CLA	2	0
19	A	821	CLA	1	0
19	A	824	CLA	3	0
19	B	826	CLA	2	0
19	1	311	CLA	1	0
19	B	807	CLA	1	0
19	A	854	CLA	2	0
19	H	201	CLA	2	0
19	4	302	CLA	2	0
23	B	843	BCR	1	0
19	B	818	CLA	3	0
19	2	312	CLA	1	0
19	A	808	CLA	3	0

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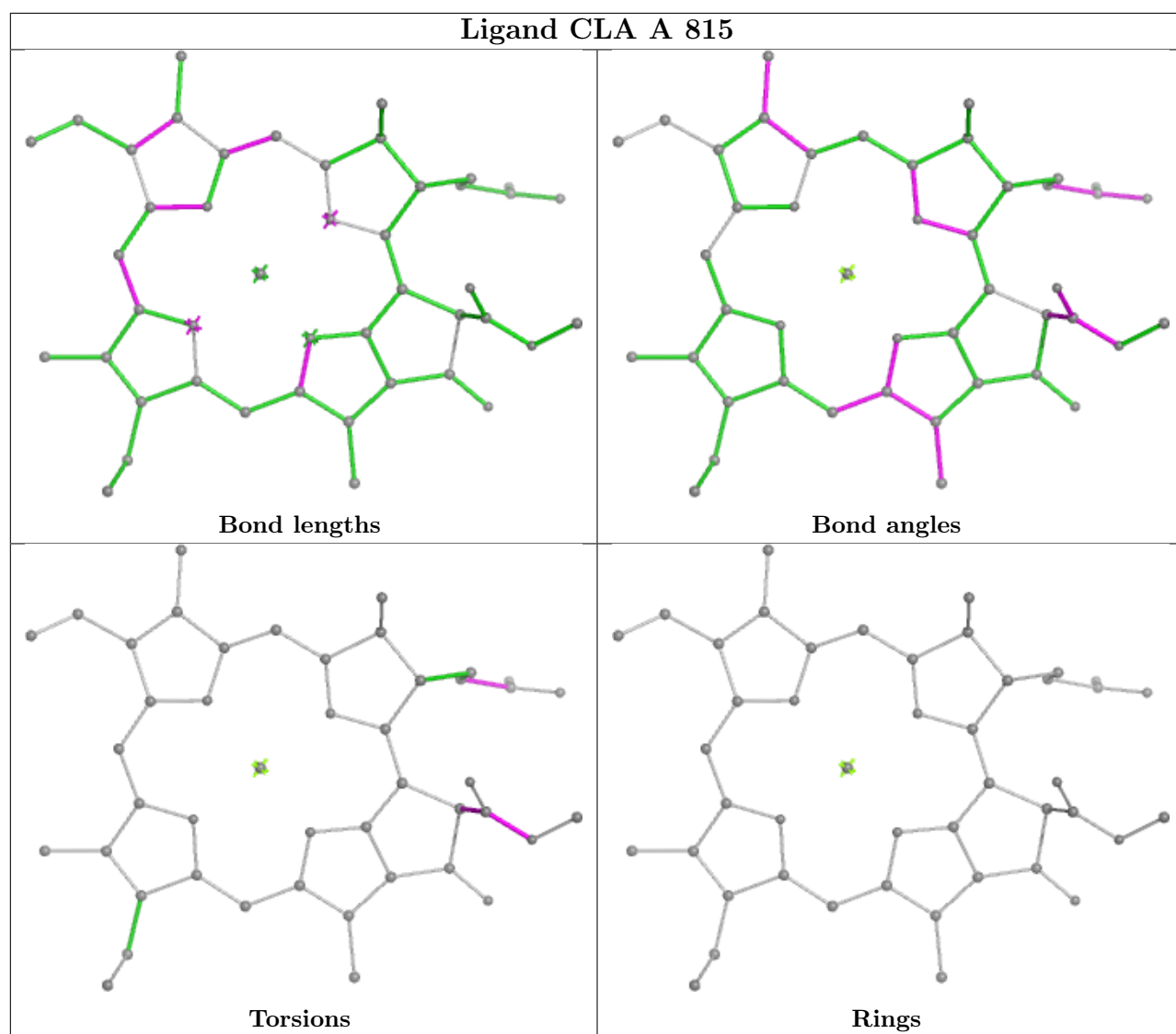
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	808	CLA	1	0
19	B	837	CLA	2	0
19	A	834	CLA	4	0
18	4	305	CHL	1	0
19	A	804	CLA	5	0
19	B	804	CLA	1	0
19	K	202	CLA	2	0
19	A	806	CLA	1	0
19	F	302	CLA	2	0
19	3	309	CLA	2	0
19	B	809	CLA	1	0
19	B	830	CLA	2	0
19	L	302	CLA	5	0
19	1	312	CLA	5	0
21	1	316	XAT	1	0
23	A	843	BCR	5	0
23	4	317	BCR	2	0
24	B	847	LMG	1	0
19	L	301	CLA	1	0
19	B	813	CLA	7	0
19	A	827	CLA	2	0
22	1	322	LHG	4	0
19	3	306	CLA	1	0
19	A	853	CLA	3	0
19	A	822	CLA	1	0
28	B	846	DGD	4	0
20	1	320	LUT	5	0
19	4	308	CLA	1	0
19	4	313	CLA	4	0
22	1	317	LHG	2	0
19	A	801	CLA	4	0
19	F	303	CLA	1	0
18	1	301	CHL	1	0
19	A	810	CLA	3	0
19	A	813	CLA	1	0
23	A	847	BCR	4	0
23	F	305	BCR	3	0
19	A	851	CLA	1	0
18	1	306	CHL	2	0
23	B	840	BCR	3	0
23	J	104	BCR	3	0
19	A	852	CLA	2	0

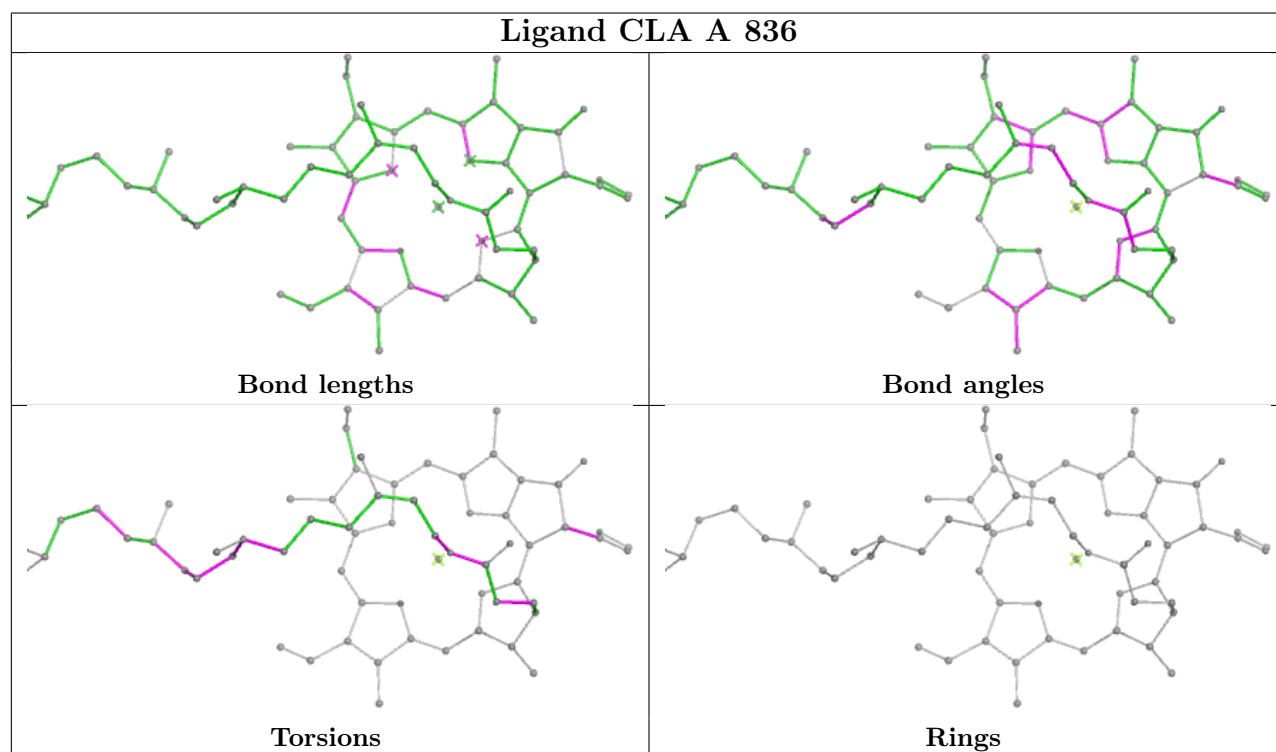
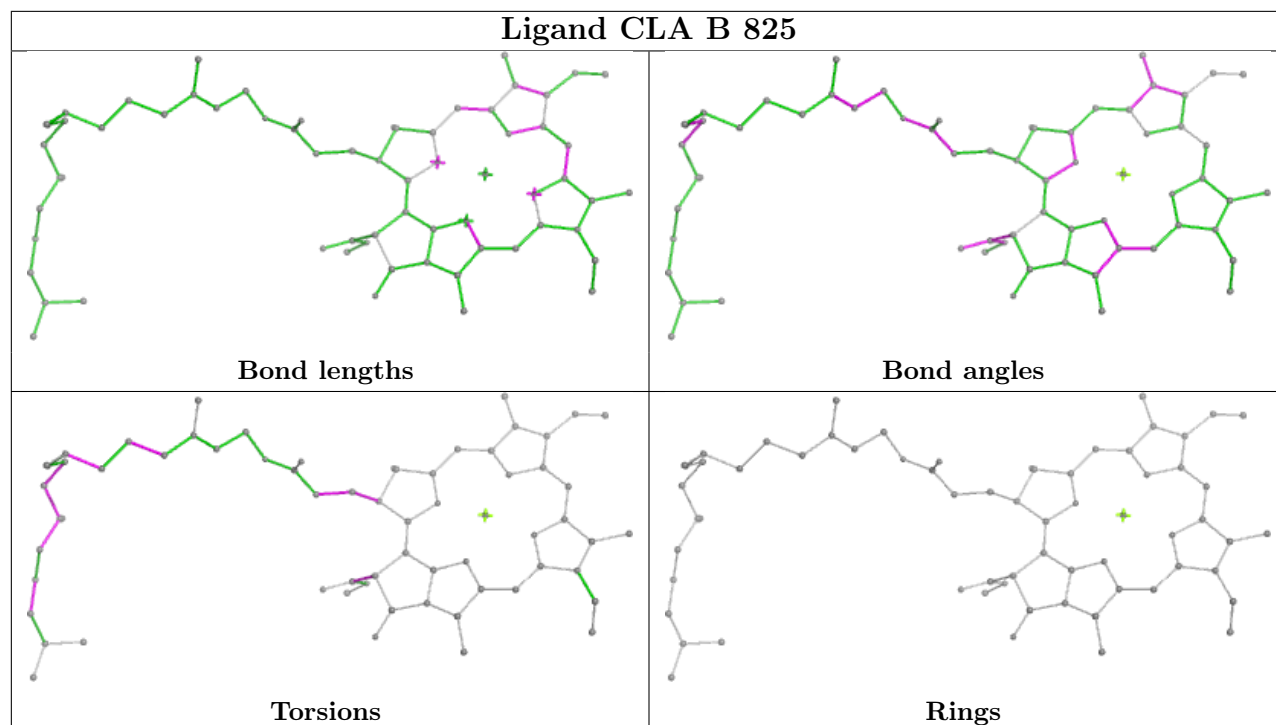
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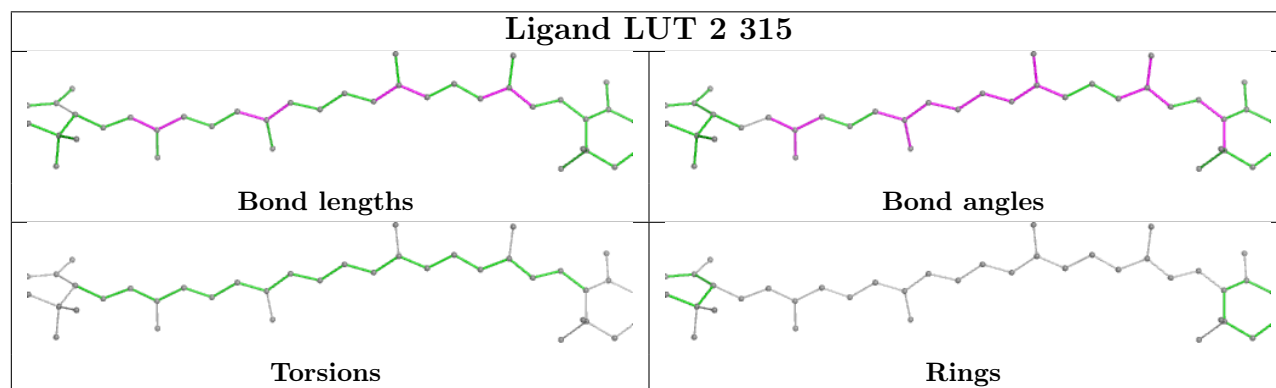
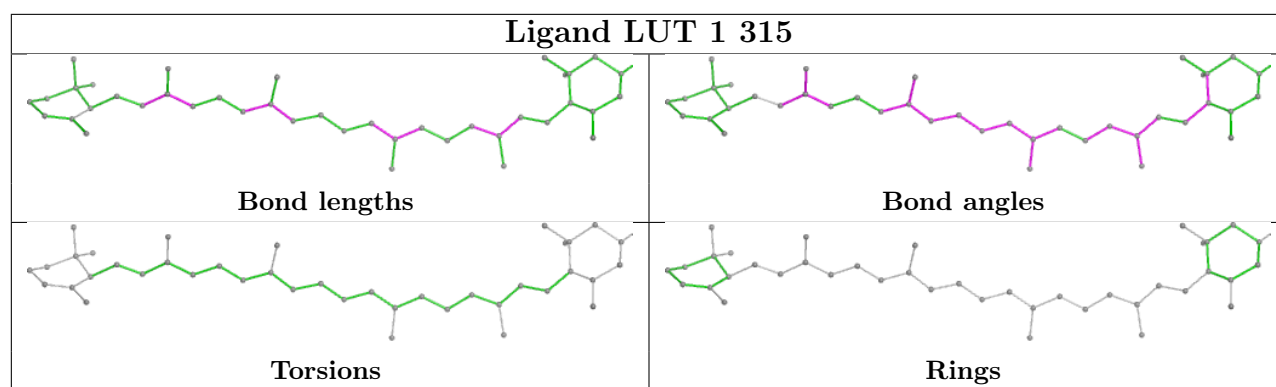
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	316	XAT	2	0
19	B	821	CLA	1	0
26	B	839	PQN	1	0
24	1	319	LMG	3	0
19	A	829	CLA	2	0
19	2	304	CLA	2	0
19	A	839	CLA	1	0
19	2	310	CLA	1	0
19	4	301	CLA	3	0
23	G	205	BCR	2	0
19	L	303	CLA	1	0
22	2	317	LHG	1	0
19	1	321	CLA	2	0
19	3	308	CLA	4	0
19	A	837	CLA	1	0
23	L	304	BCR	2	0
19	2	303	CLA	2	0
23	L	305	BCR	6	0
19	B	833	CLA	1	0
19	A	812	CLA	4	0
23	3	317	BCR	1	0
19	1	309	CLA	2	0
23	F	306	BCR	3	0
23	B	844	BCR	2	0
23	A	845	BCR	2	0
18	4	306	CHL	2	0

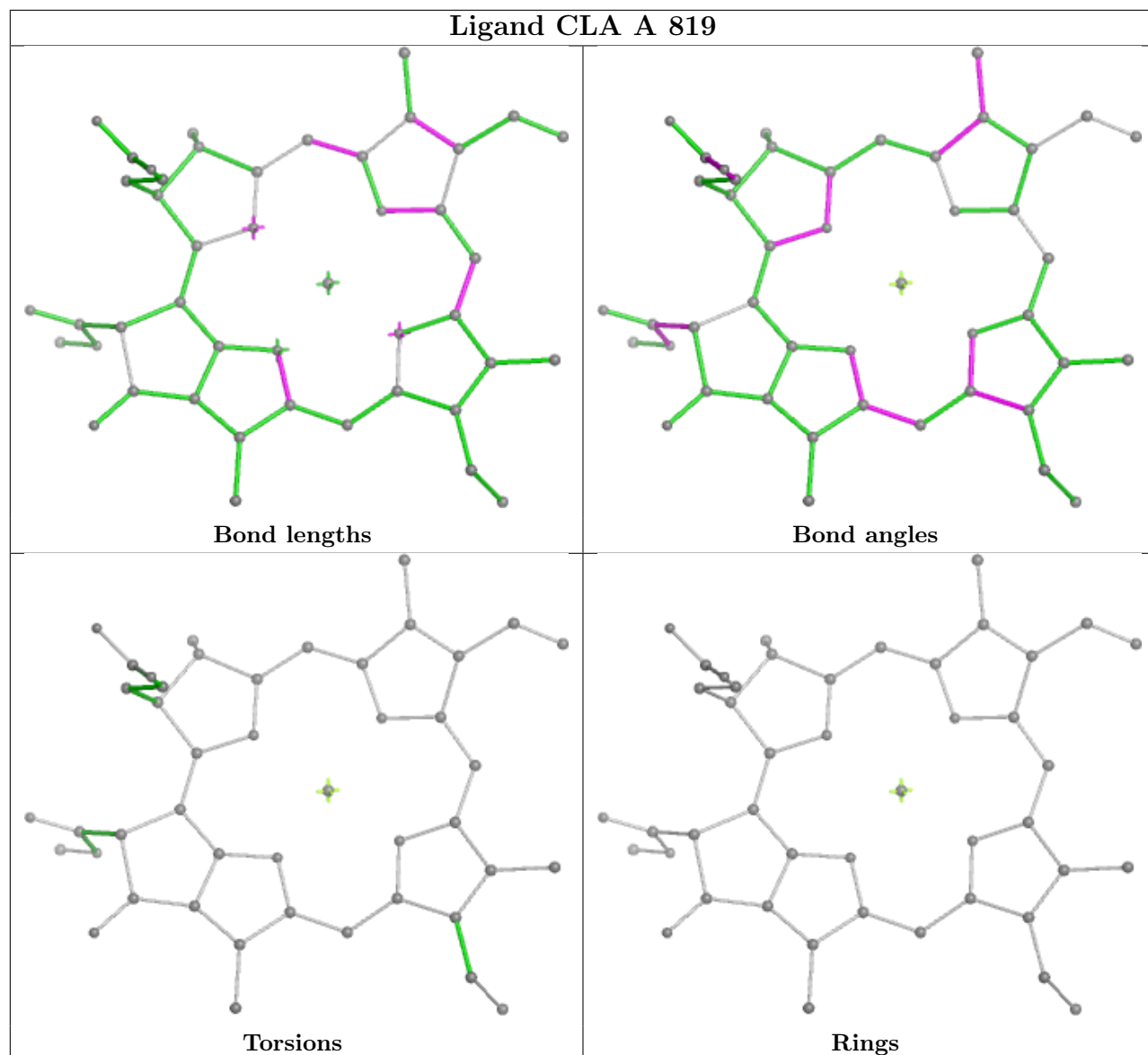
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



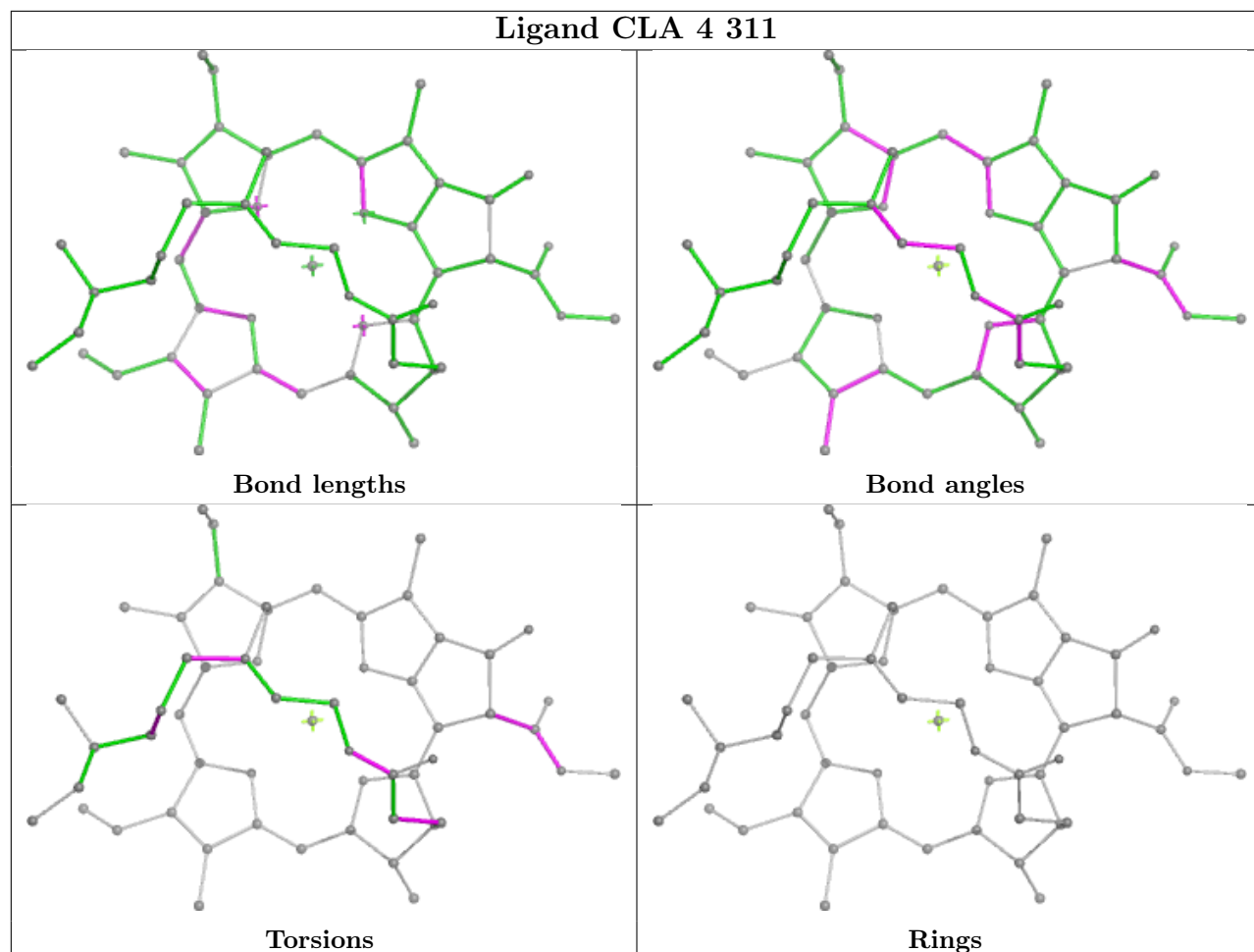


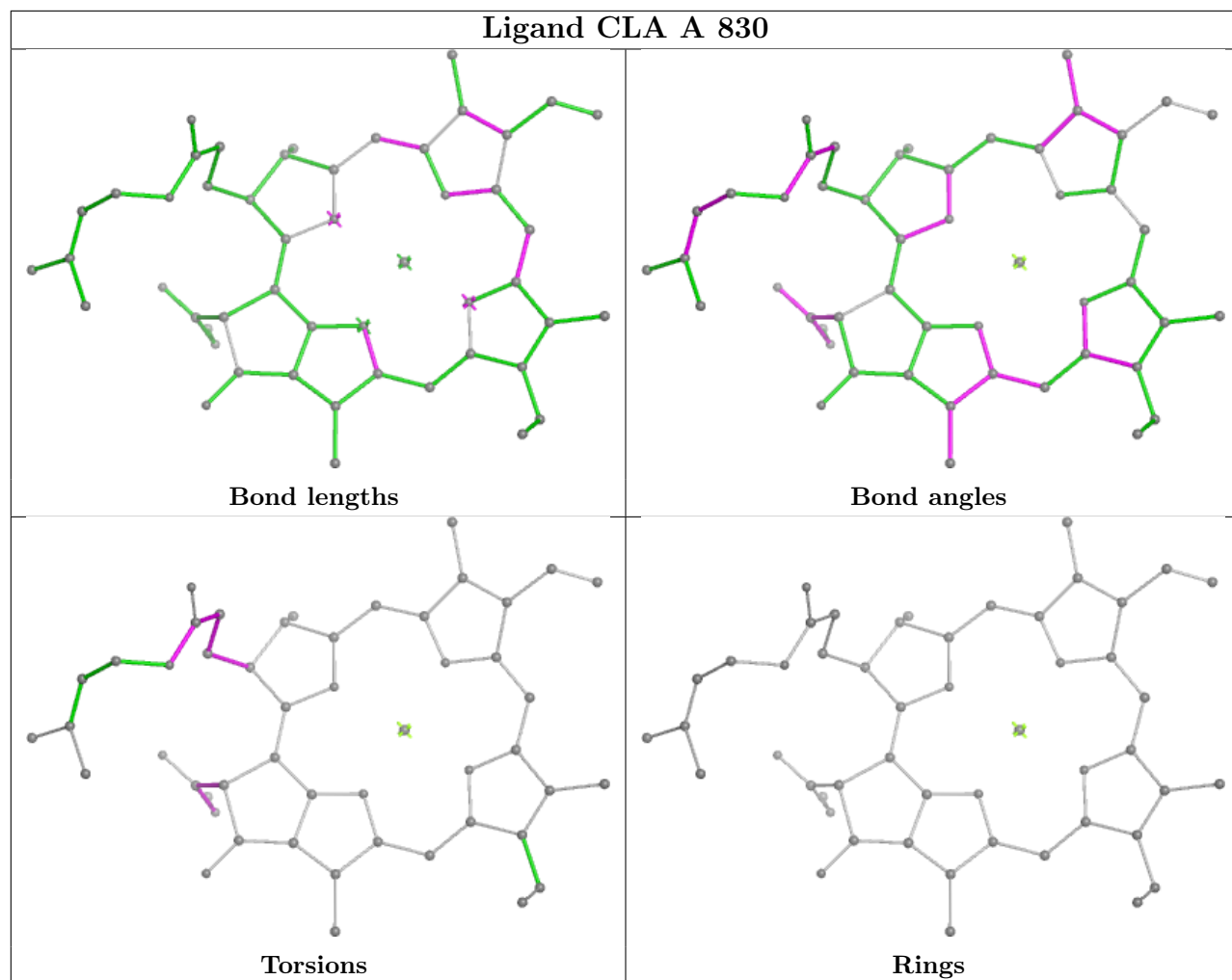


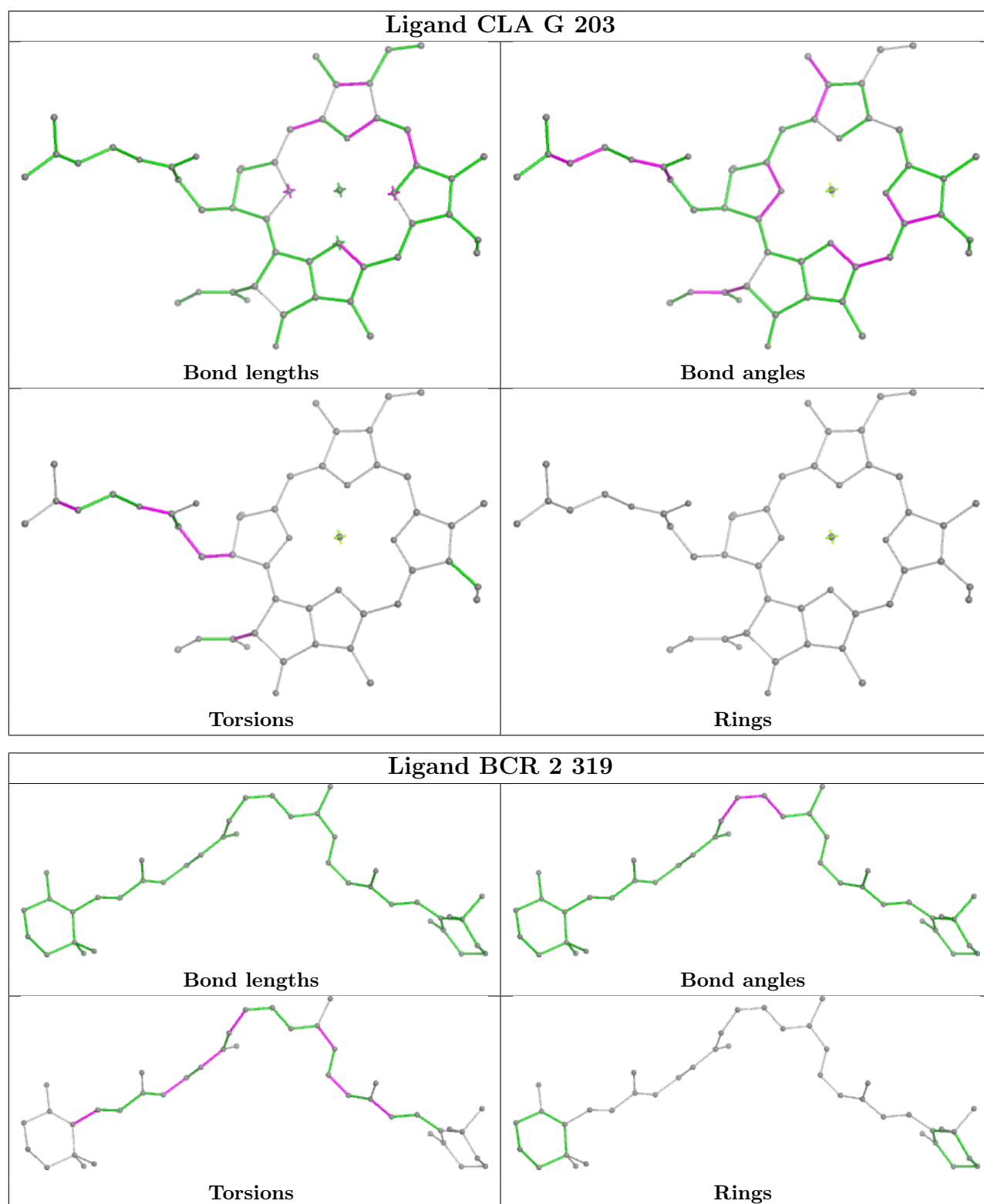
Ligand CLA A 819



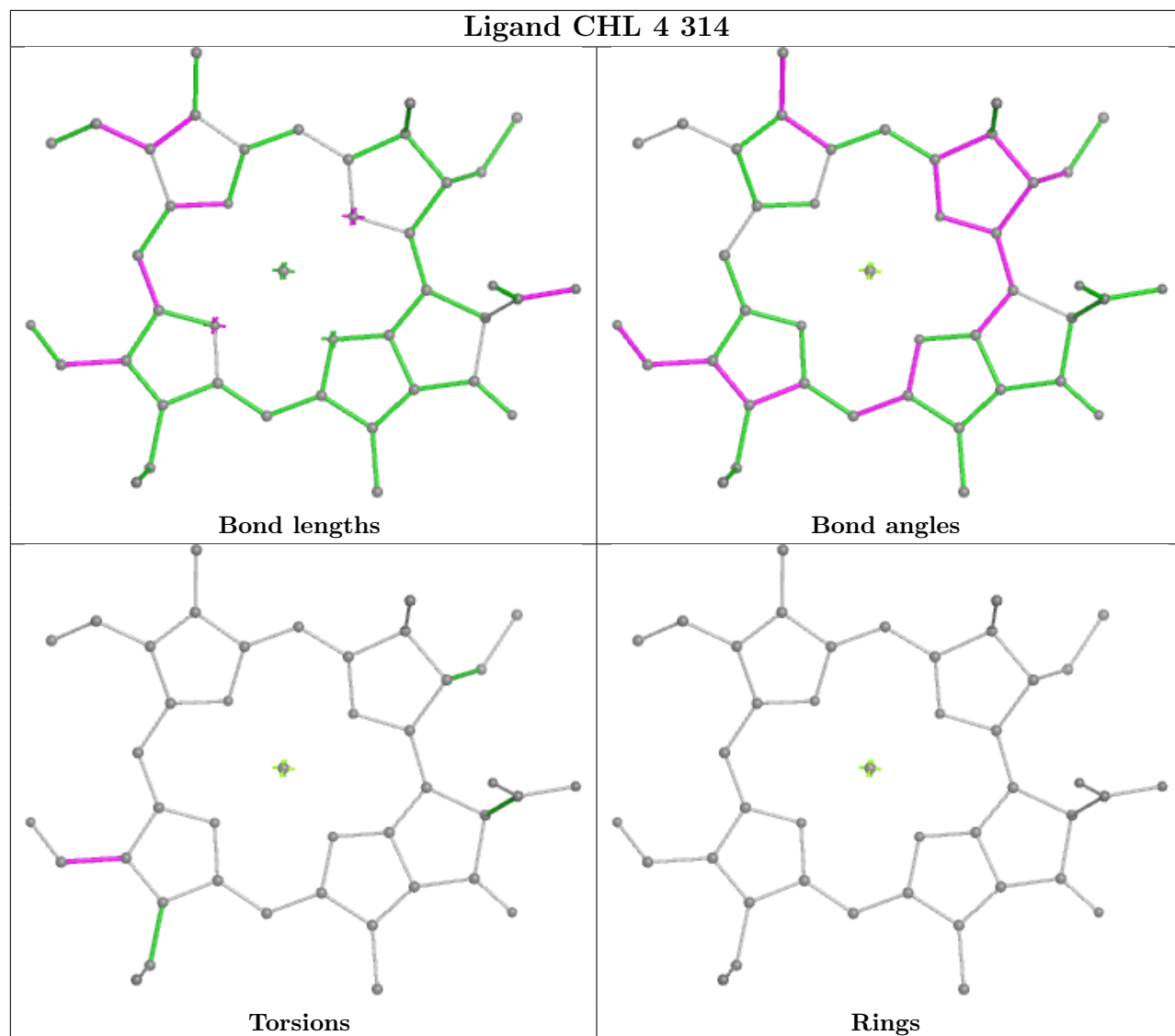
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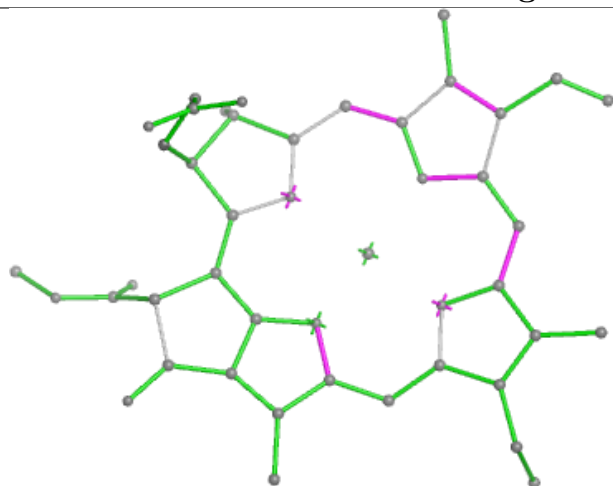




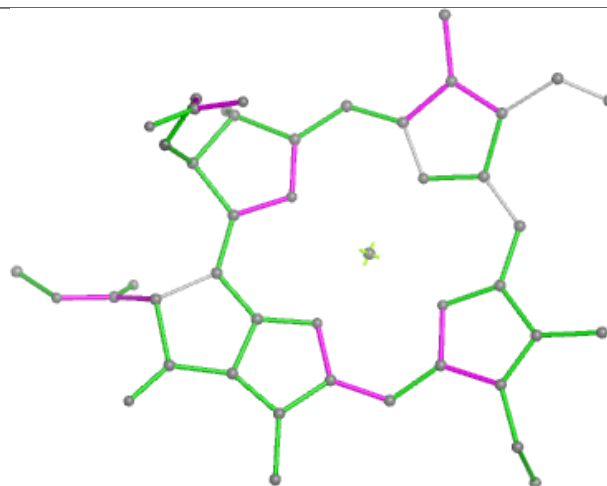
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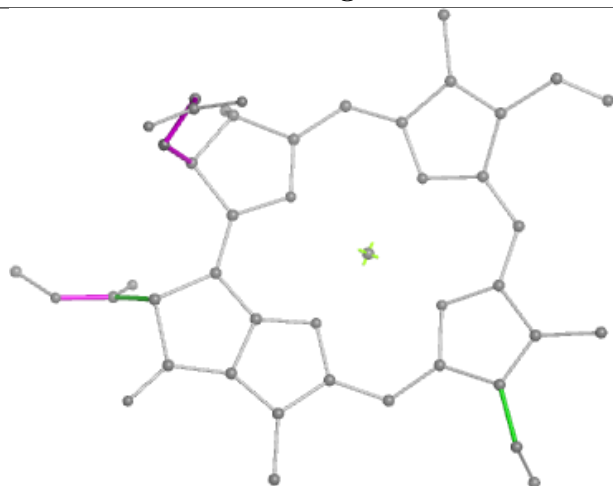
Ligand CLA 2 308



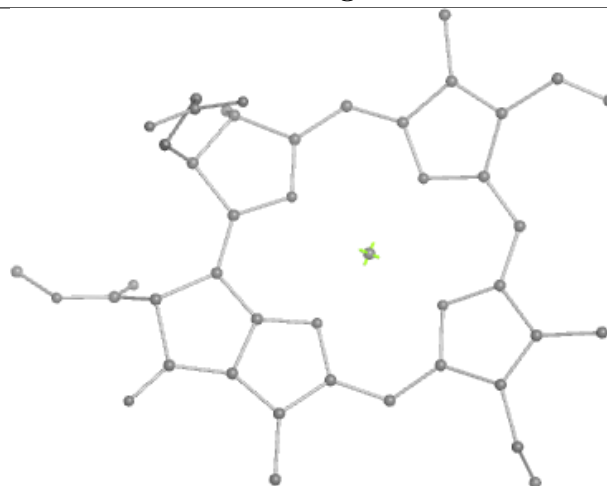
Bond lengths



Bond angles

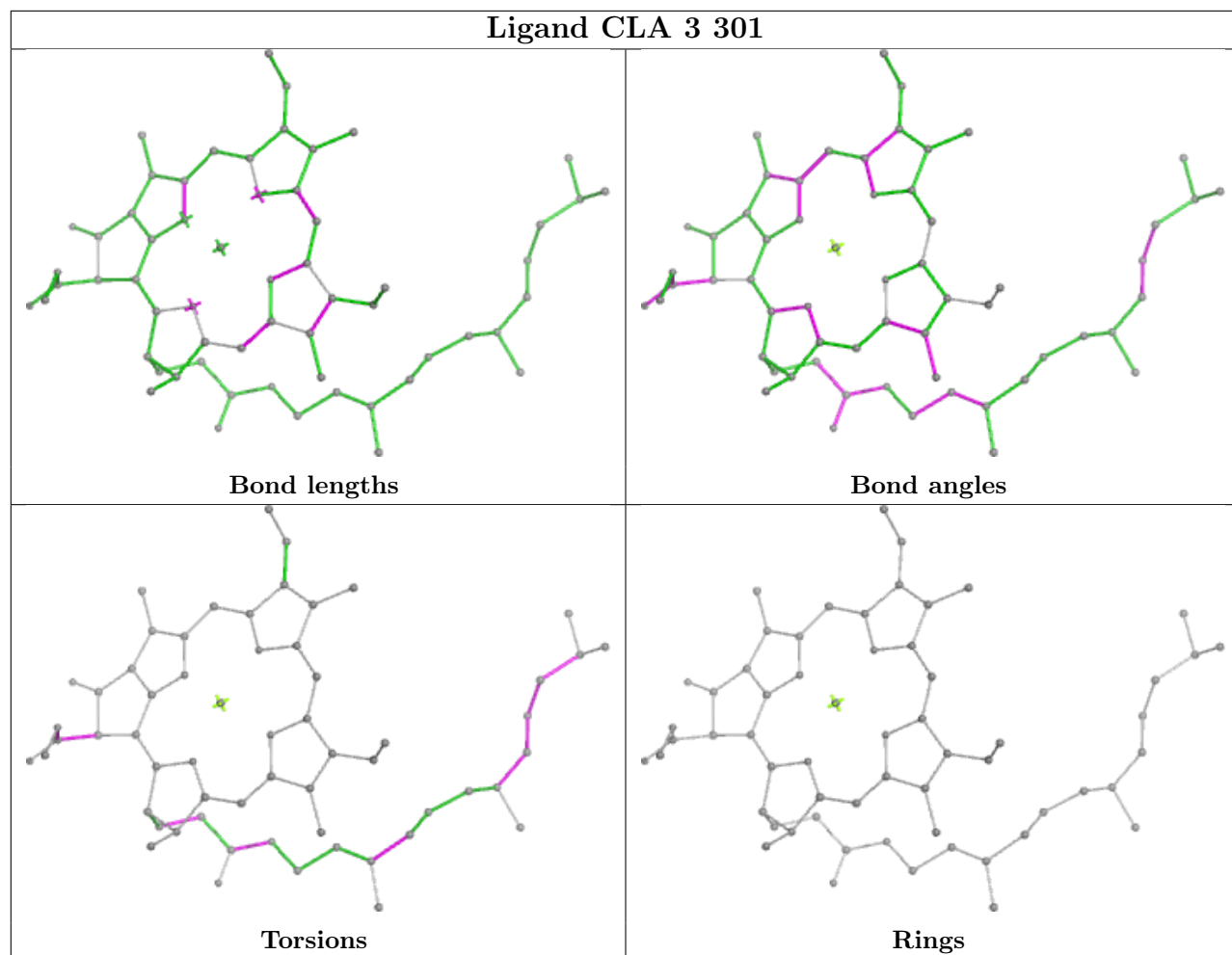


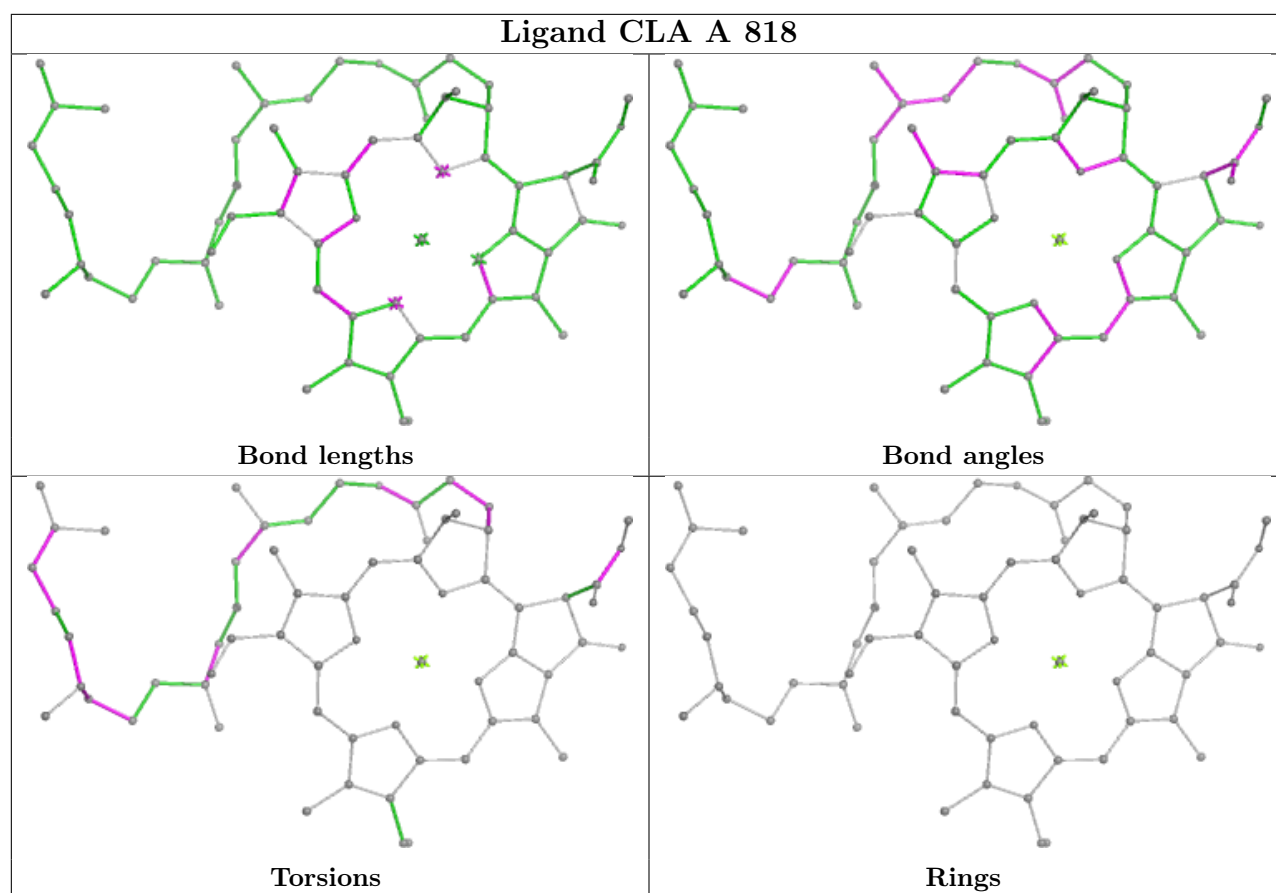
Torsions

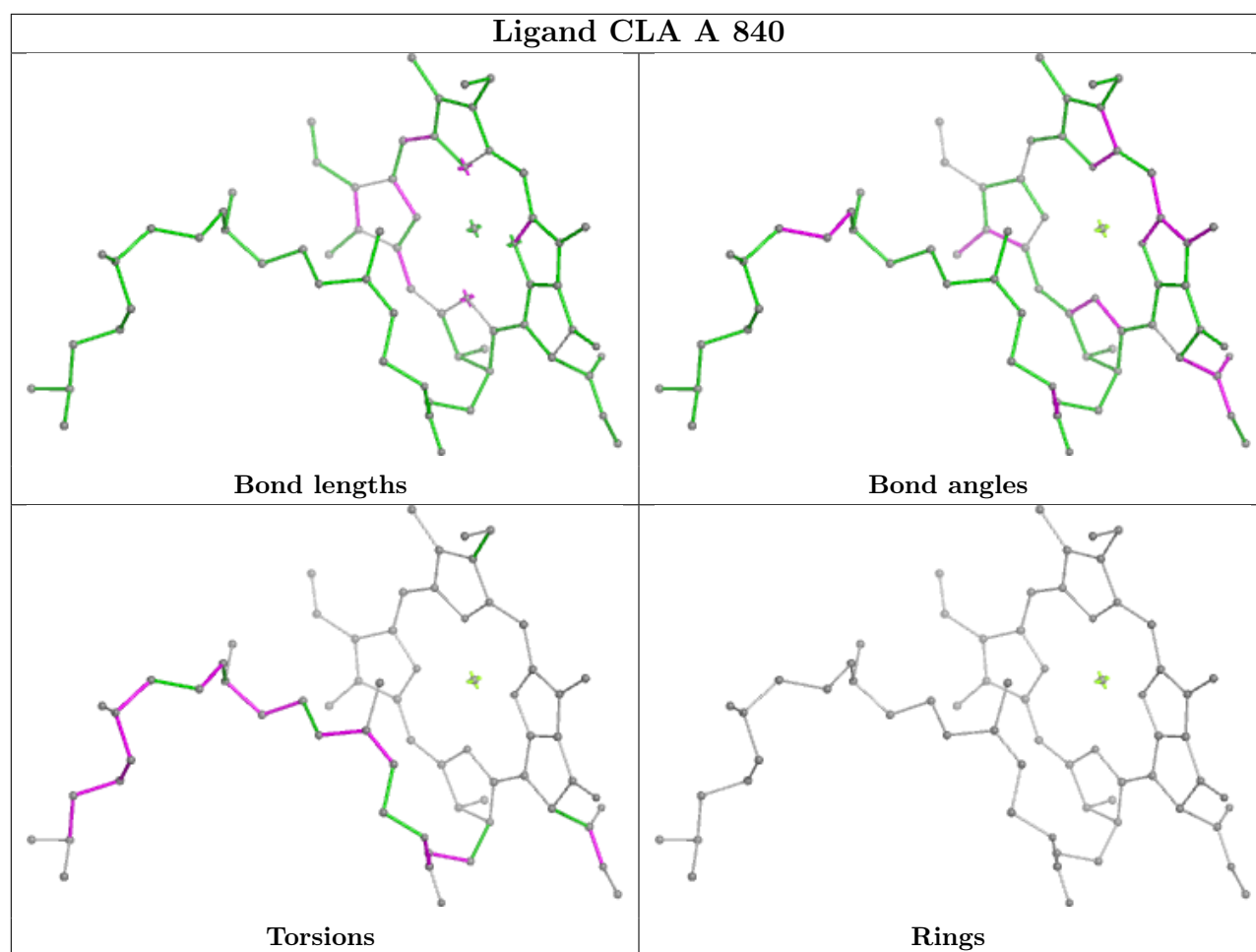


Rings

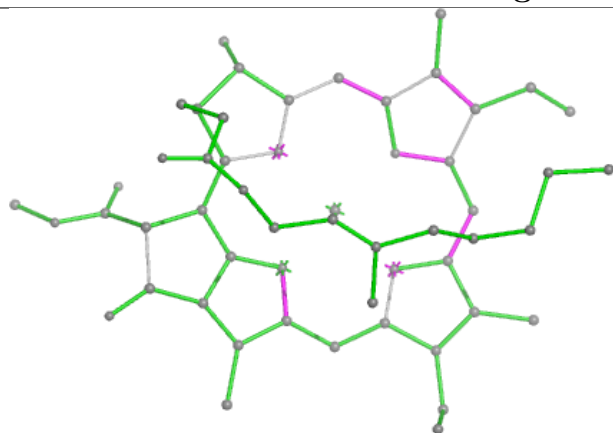
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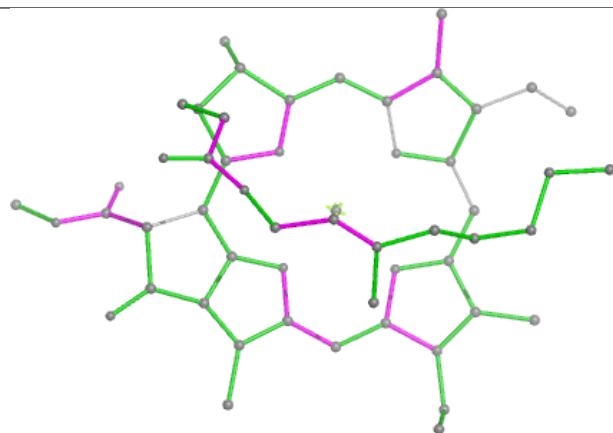




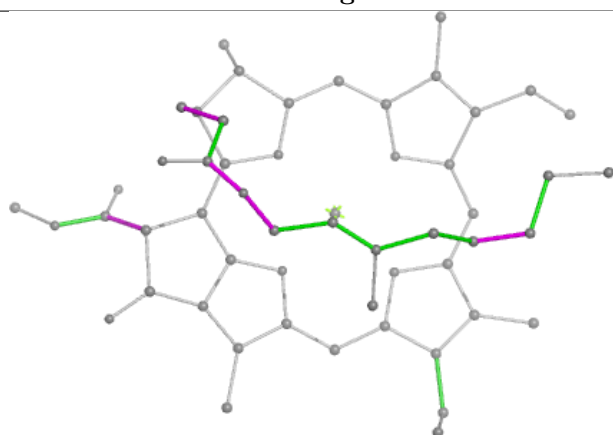
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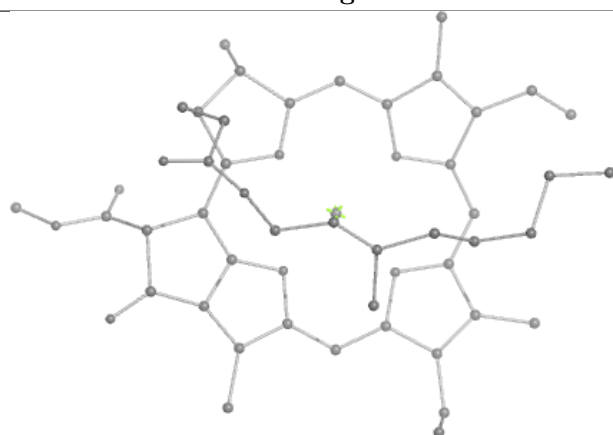
Bond lengths



Bond angles

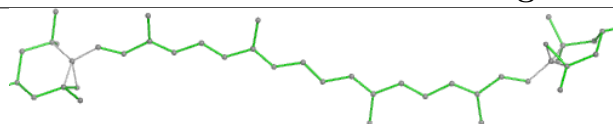


Torsions

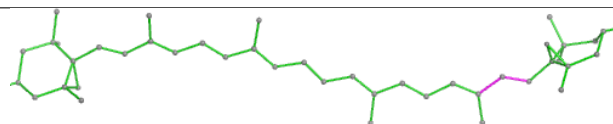


Rings

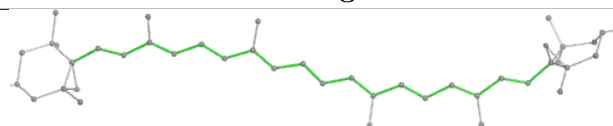
Ligand XAT 4 316



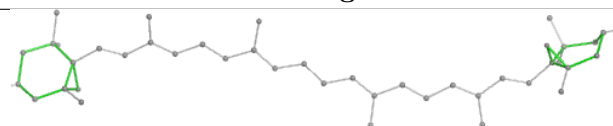
Bond lengths



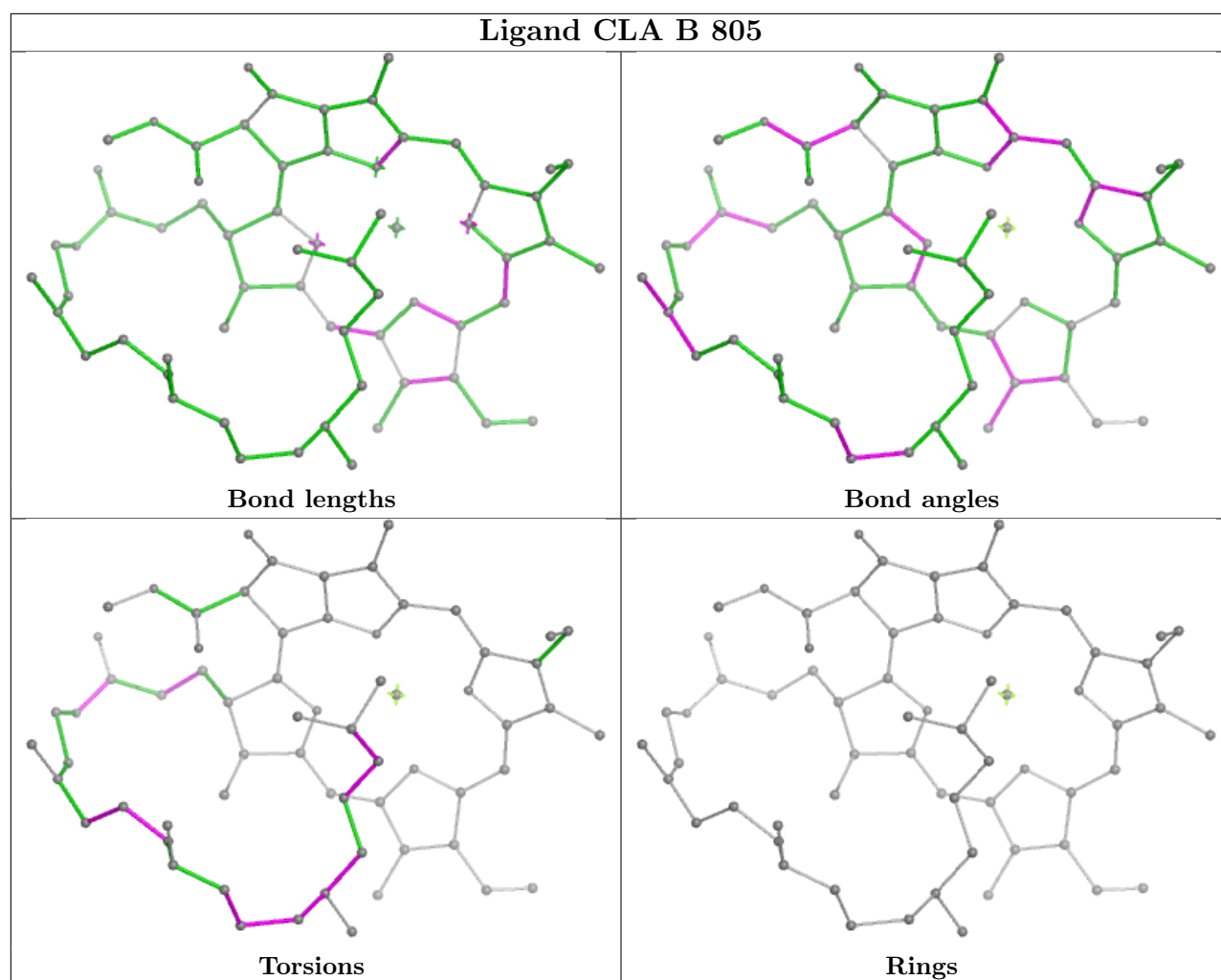
Bond angles

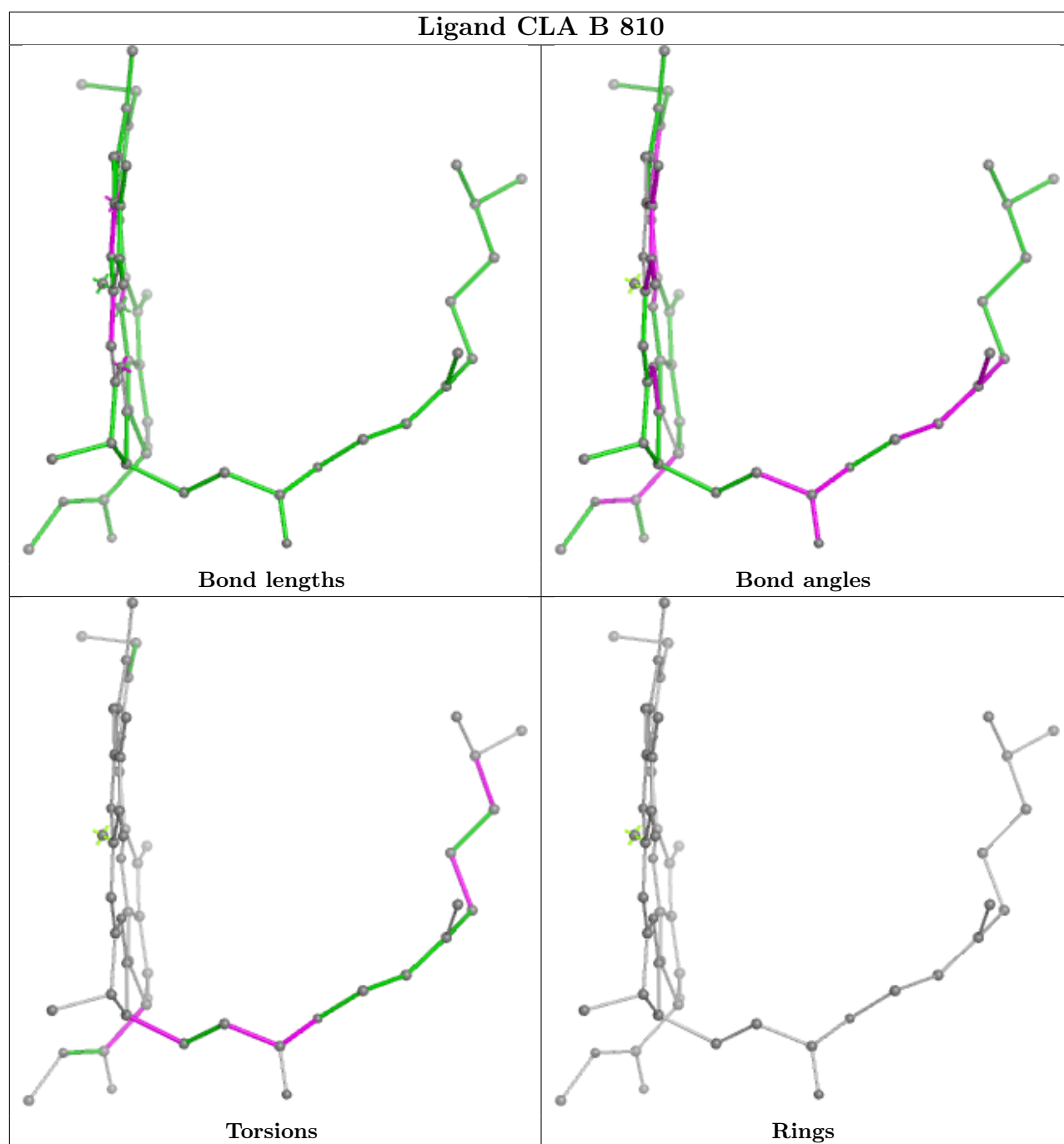


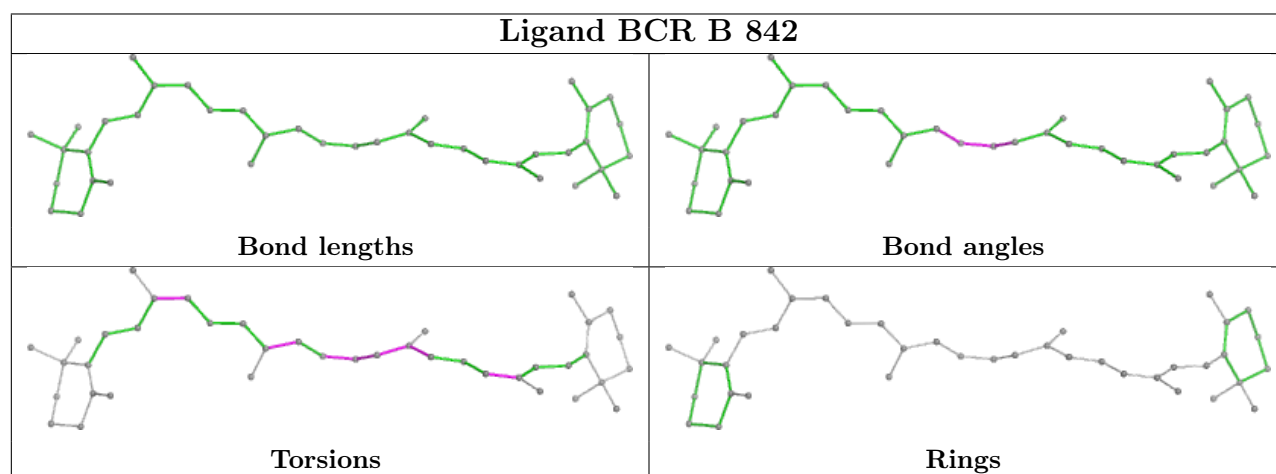
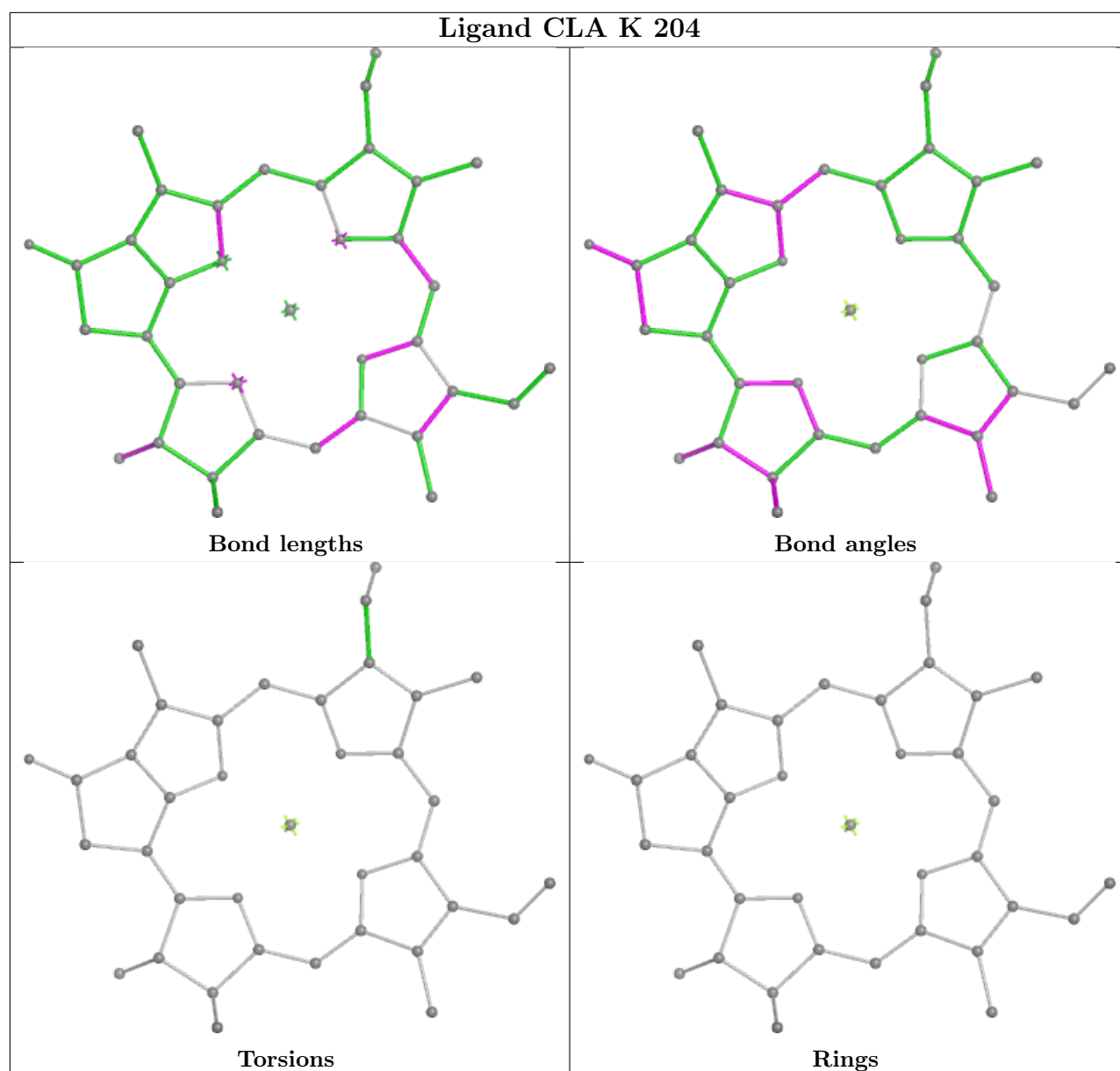
Torsions

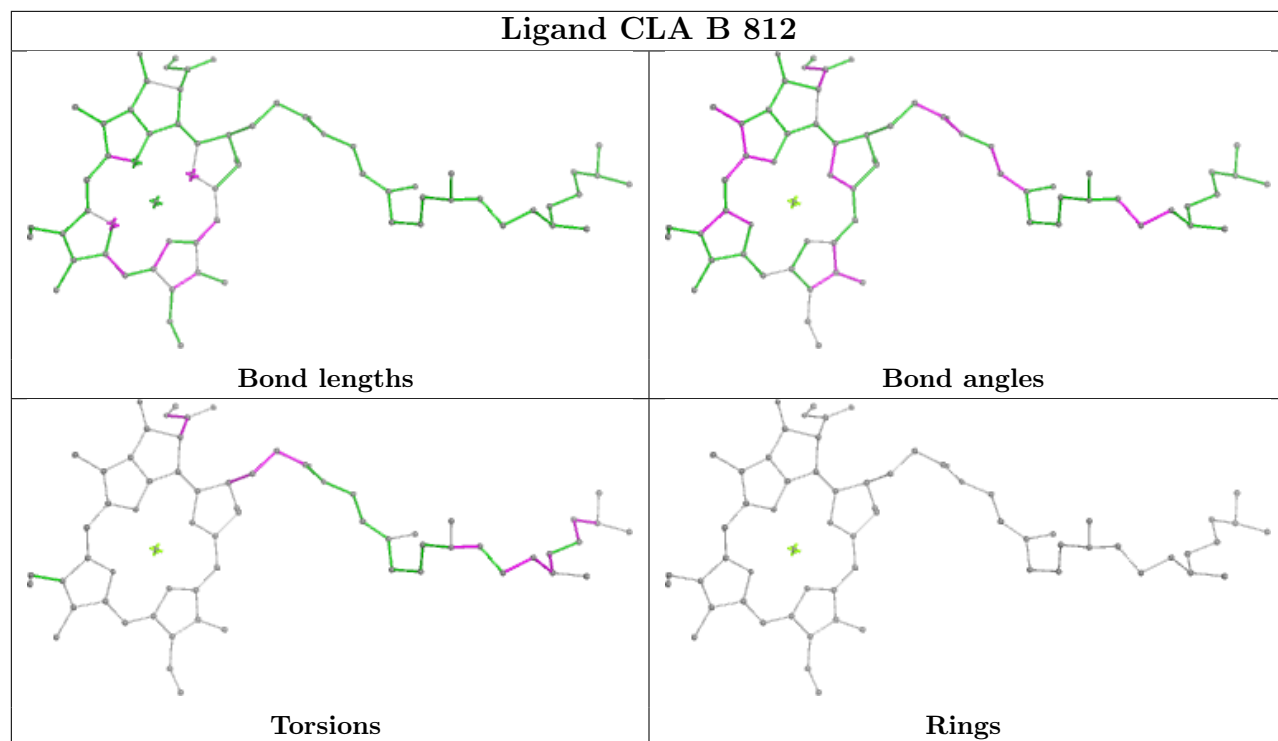


Rings

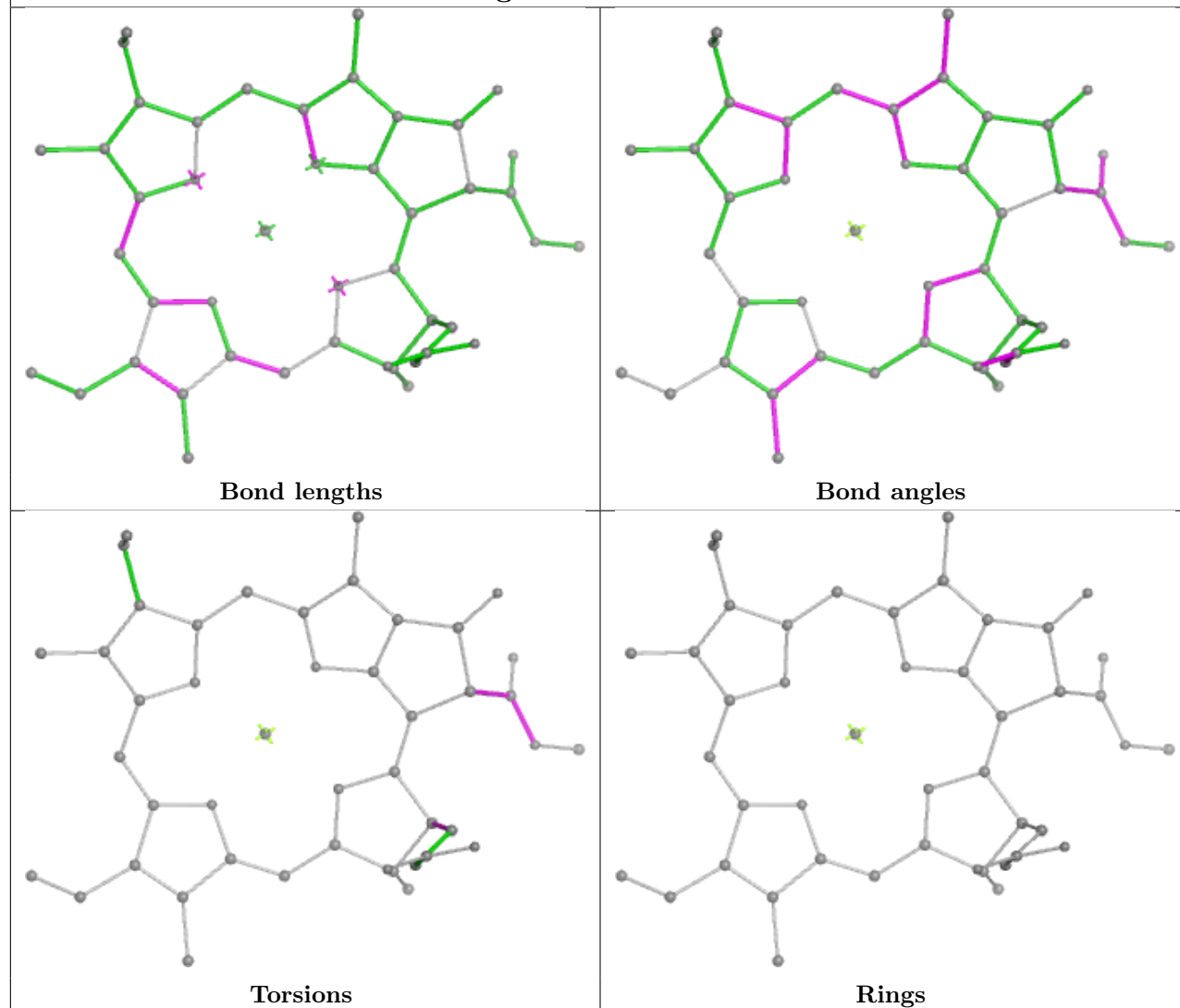




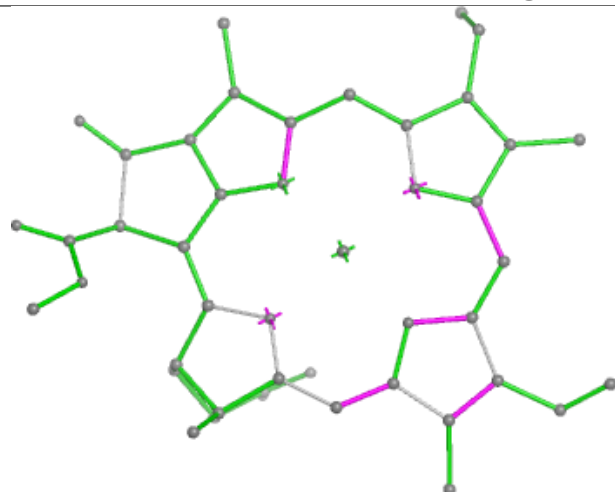




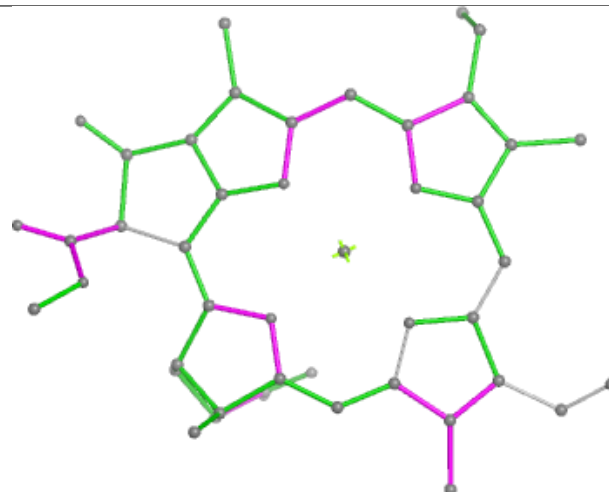
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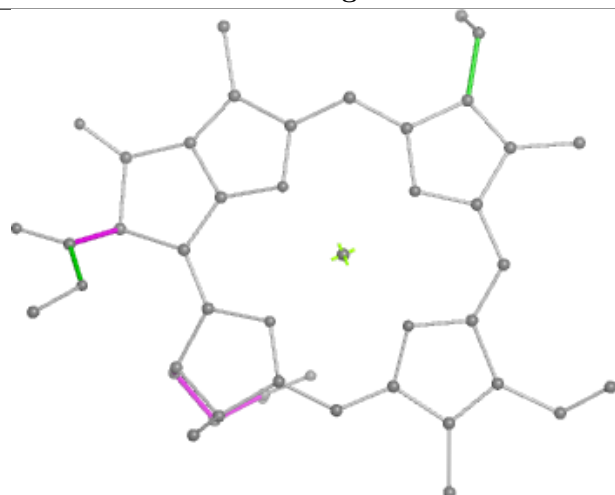
Ligand CLA 1 313



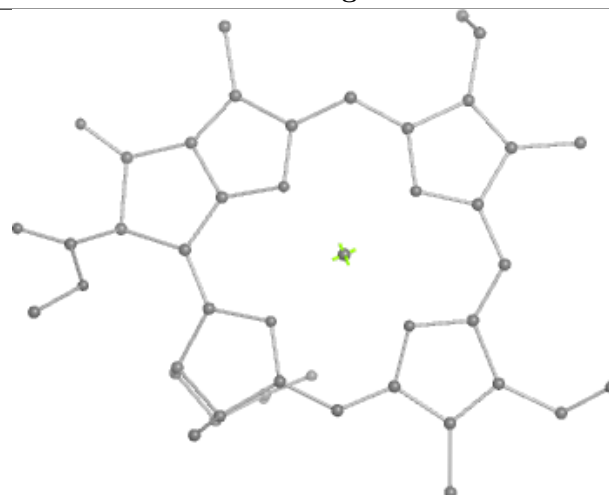
Bond lengths



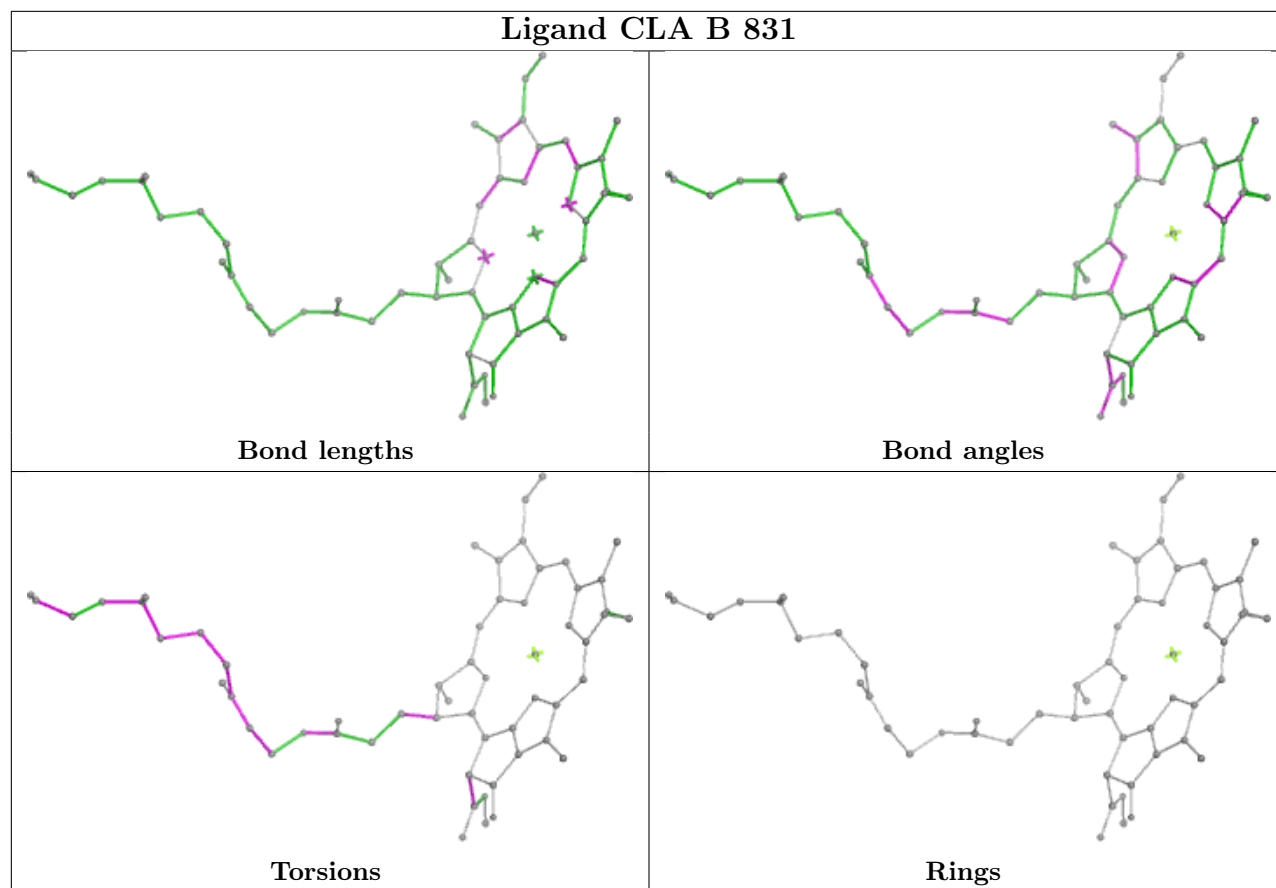
Bond angles



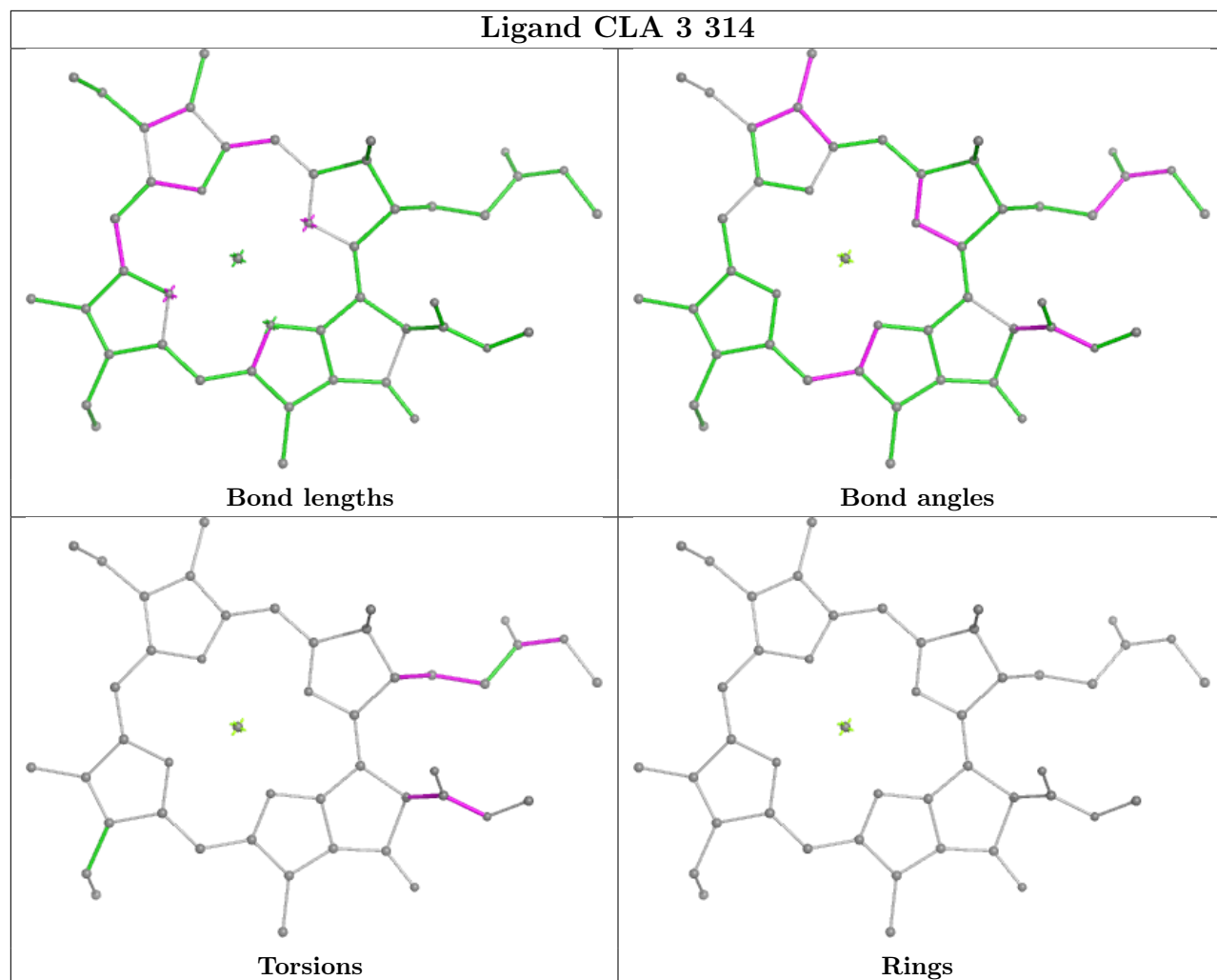
Torsions

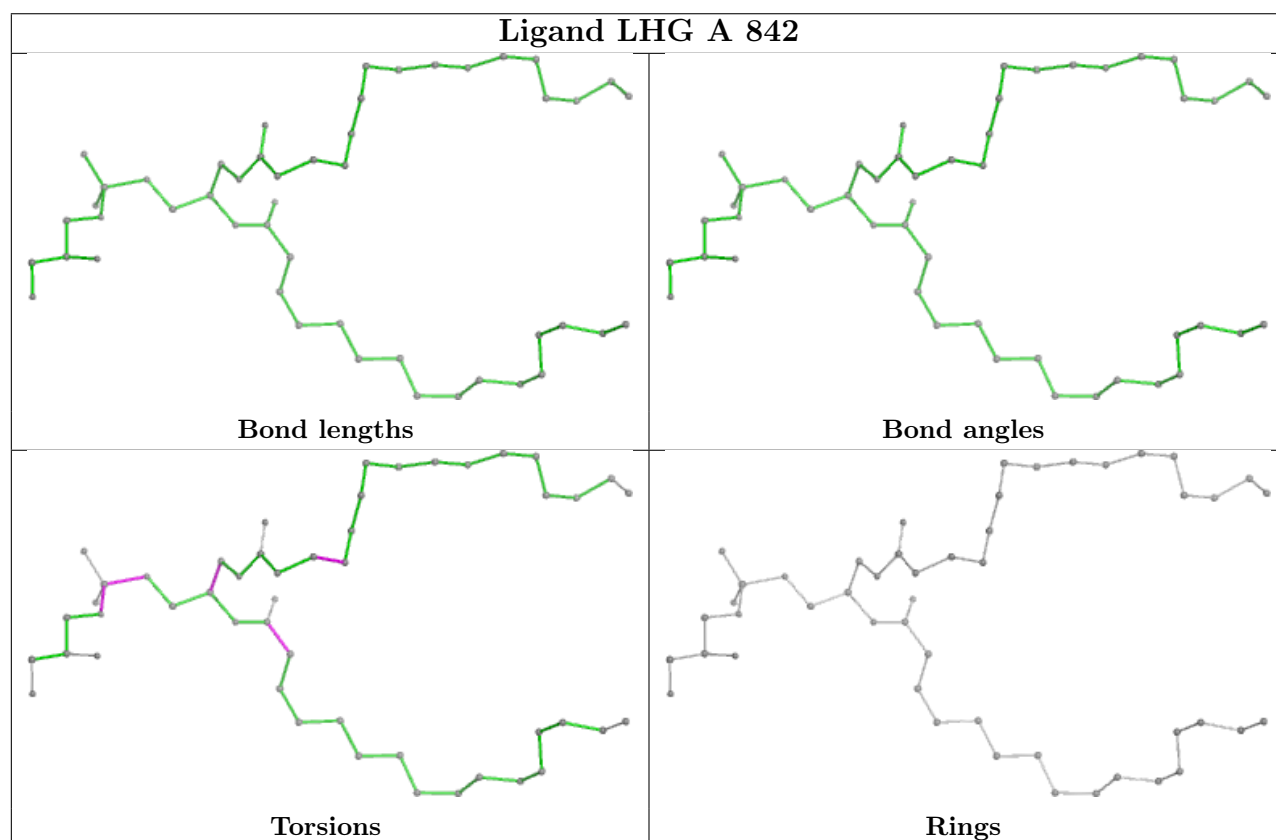
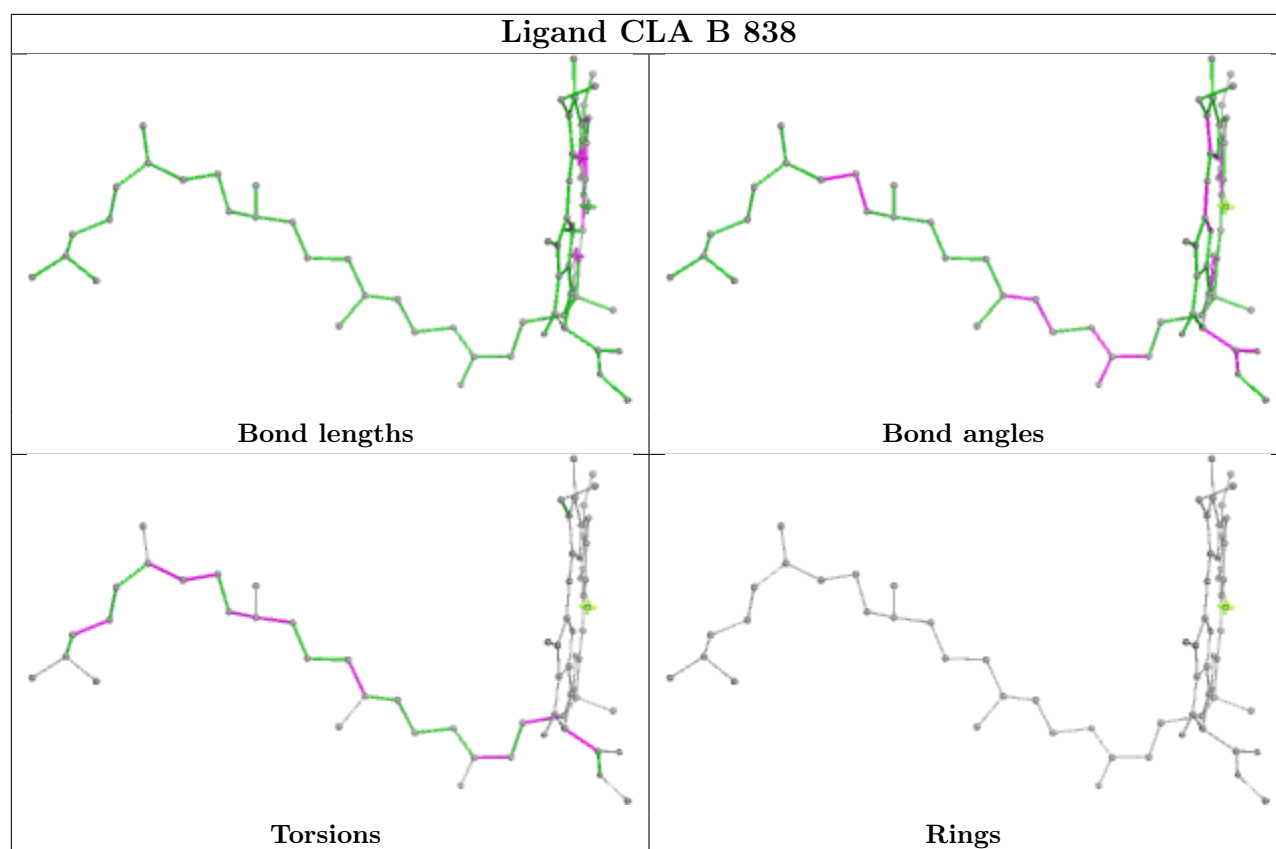


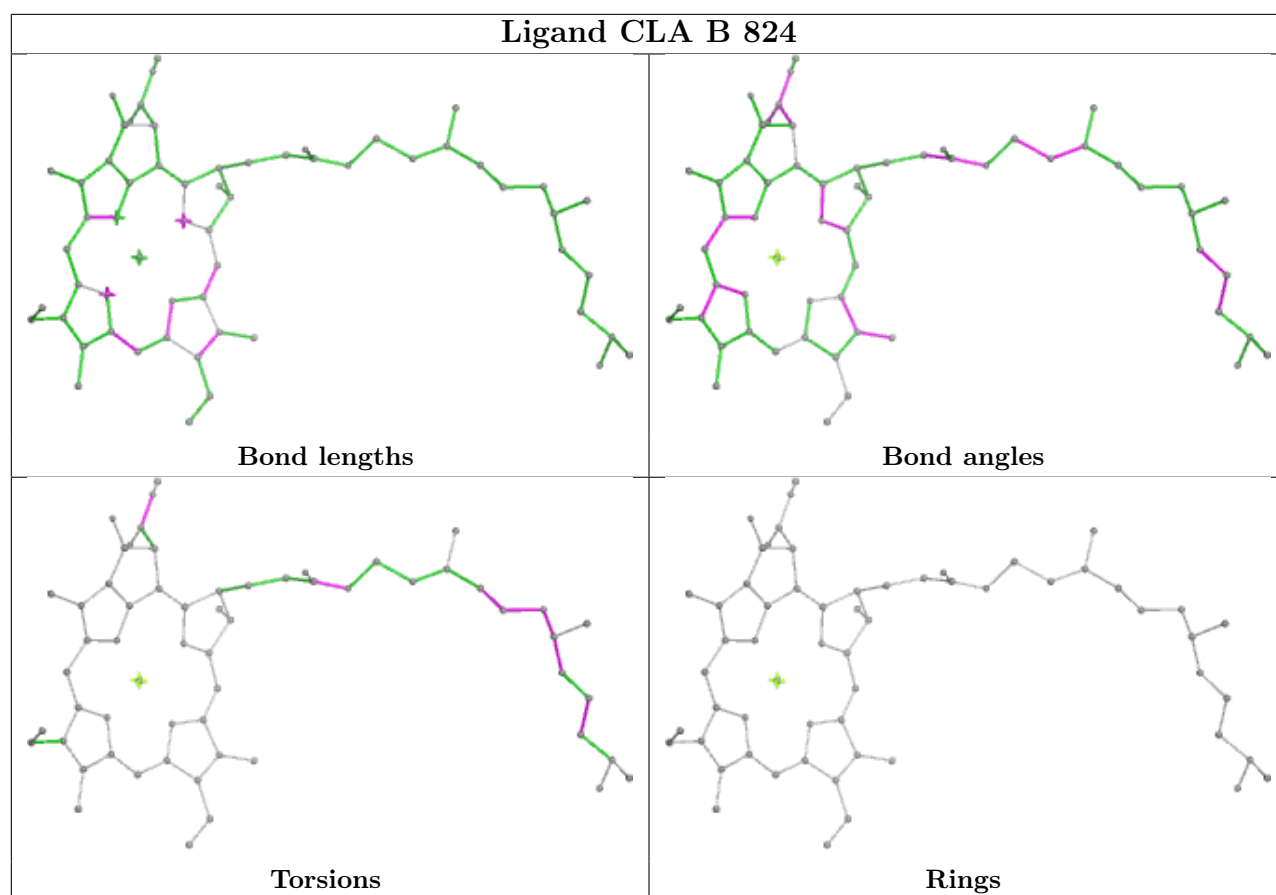
Rings



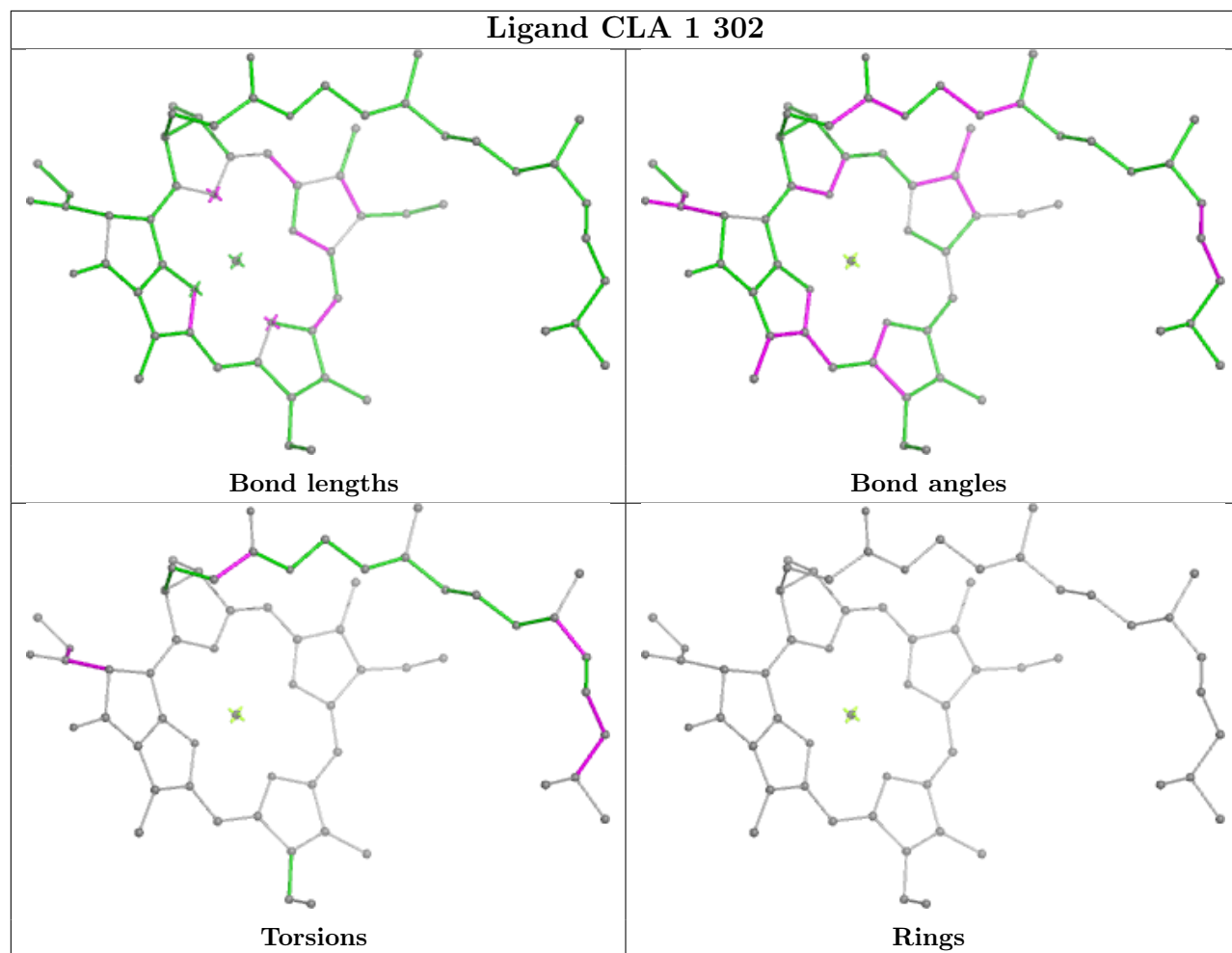
Ligand CLA 3 314

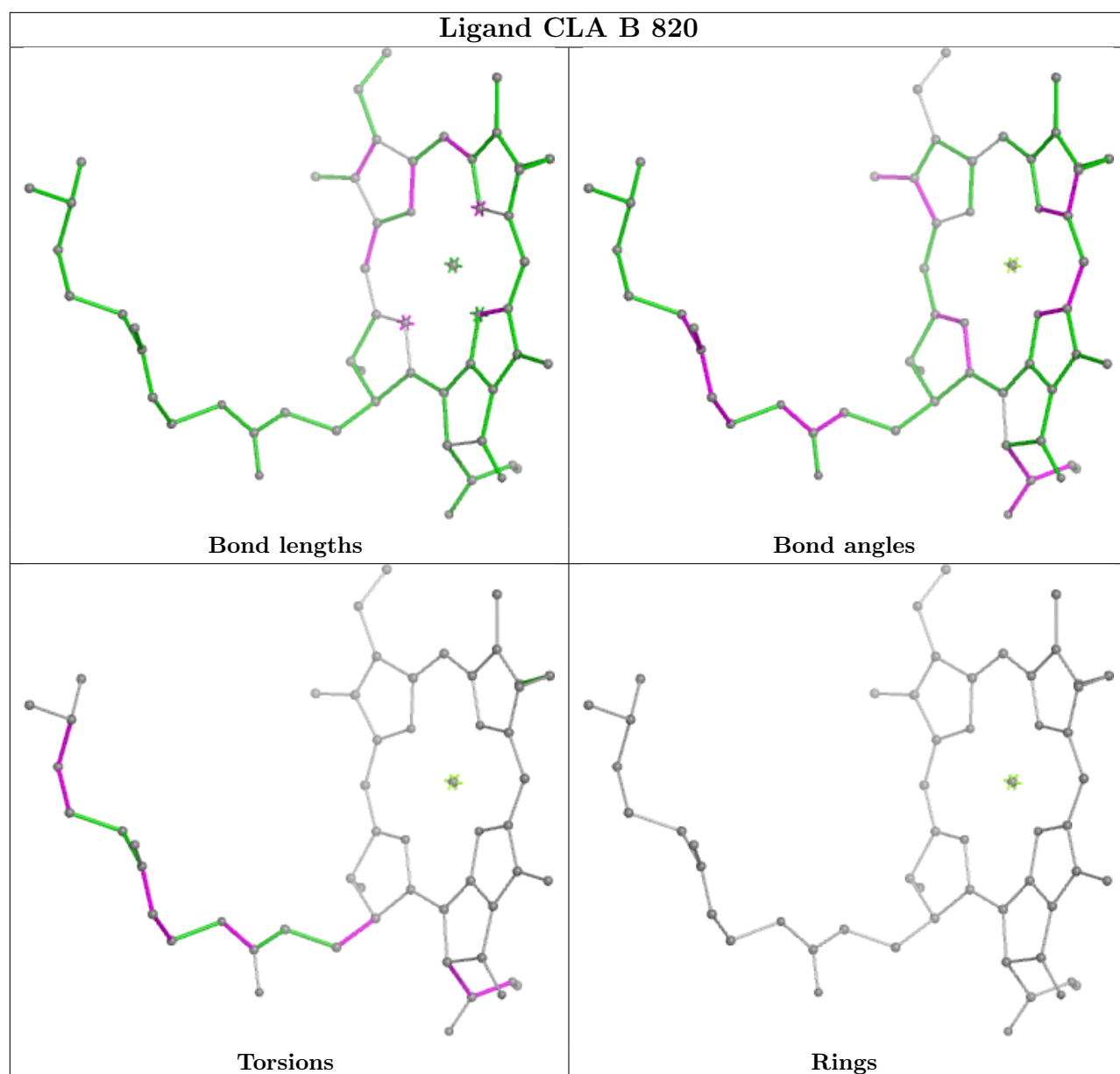


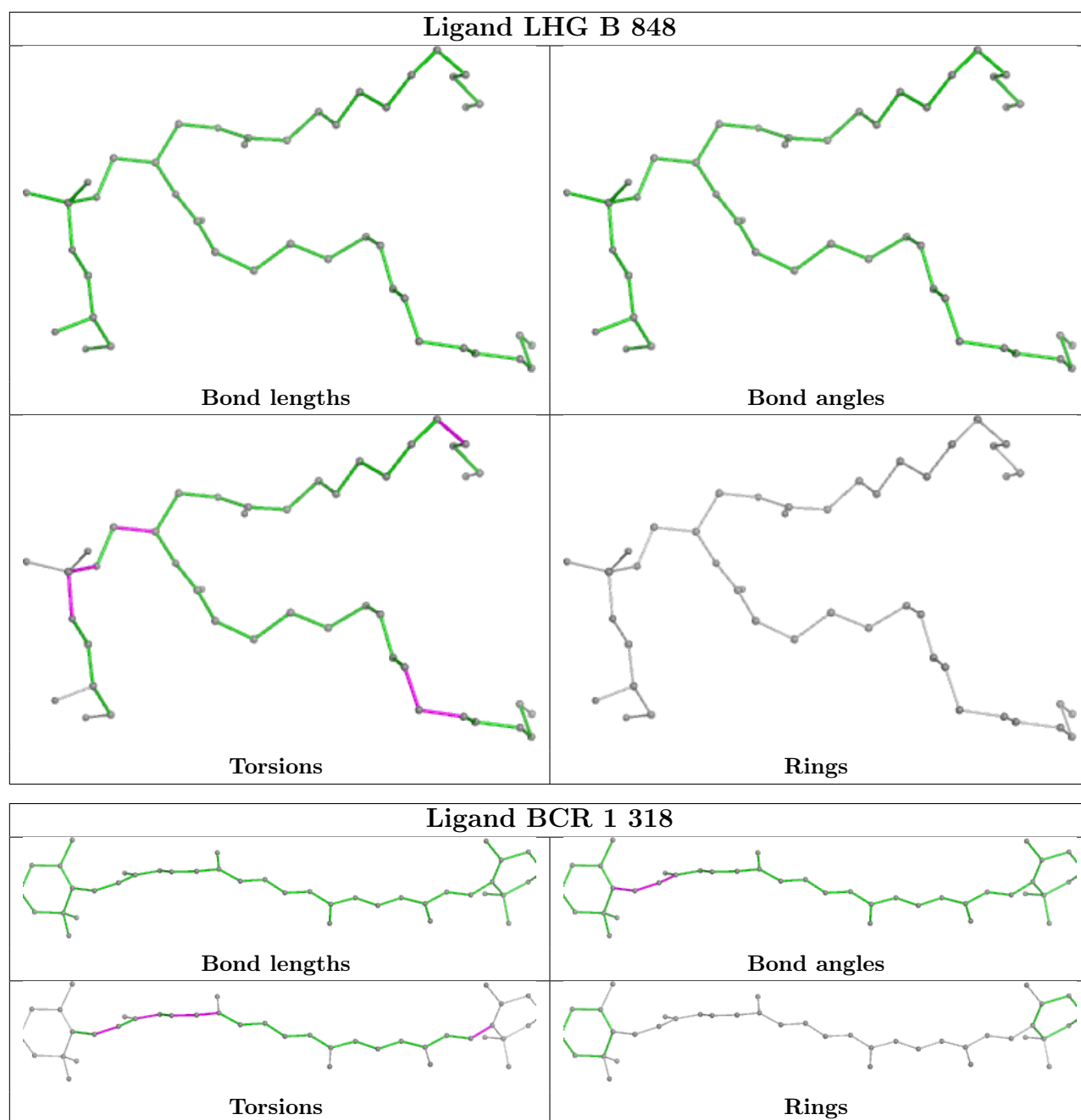




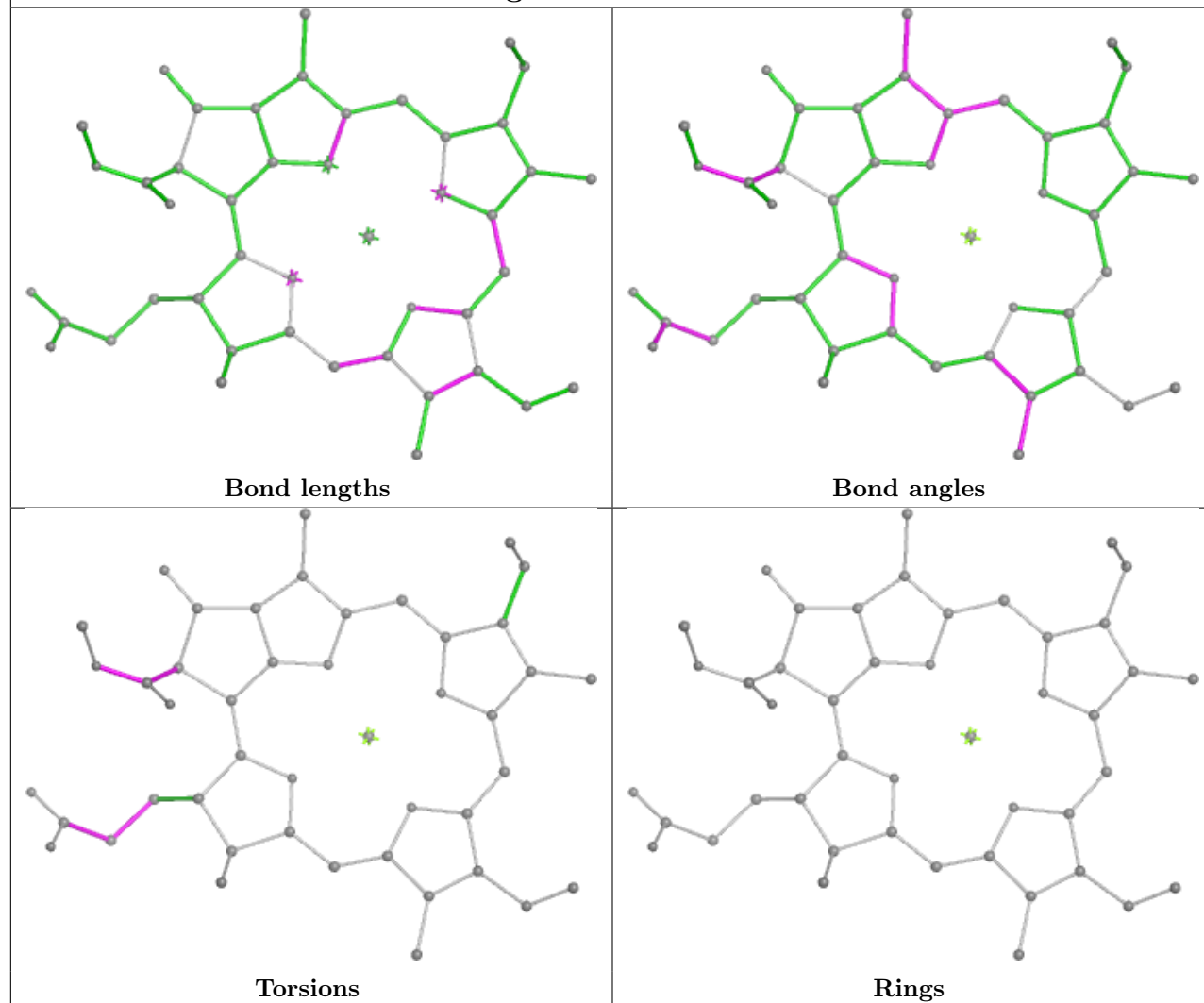
Ligand CLA 1 302



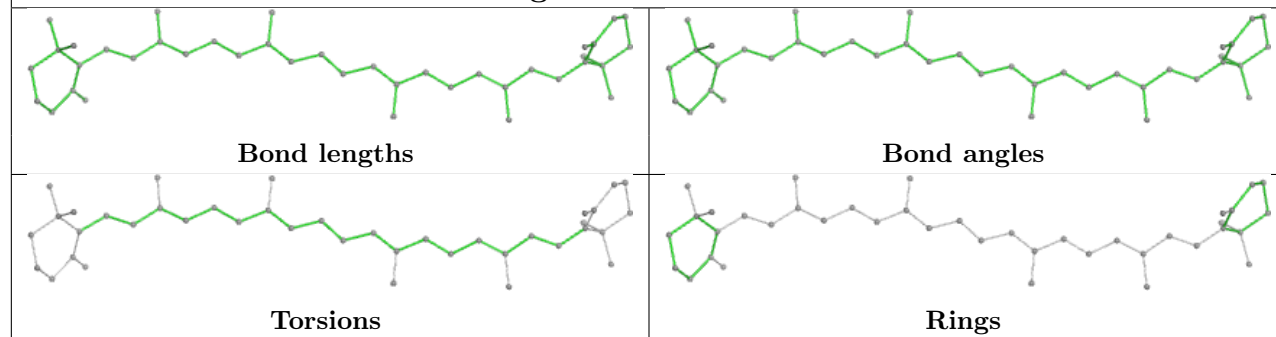


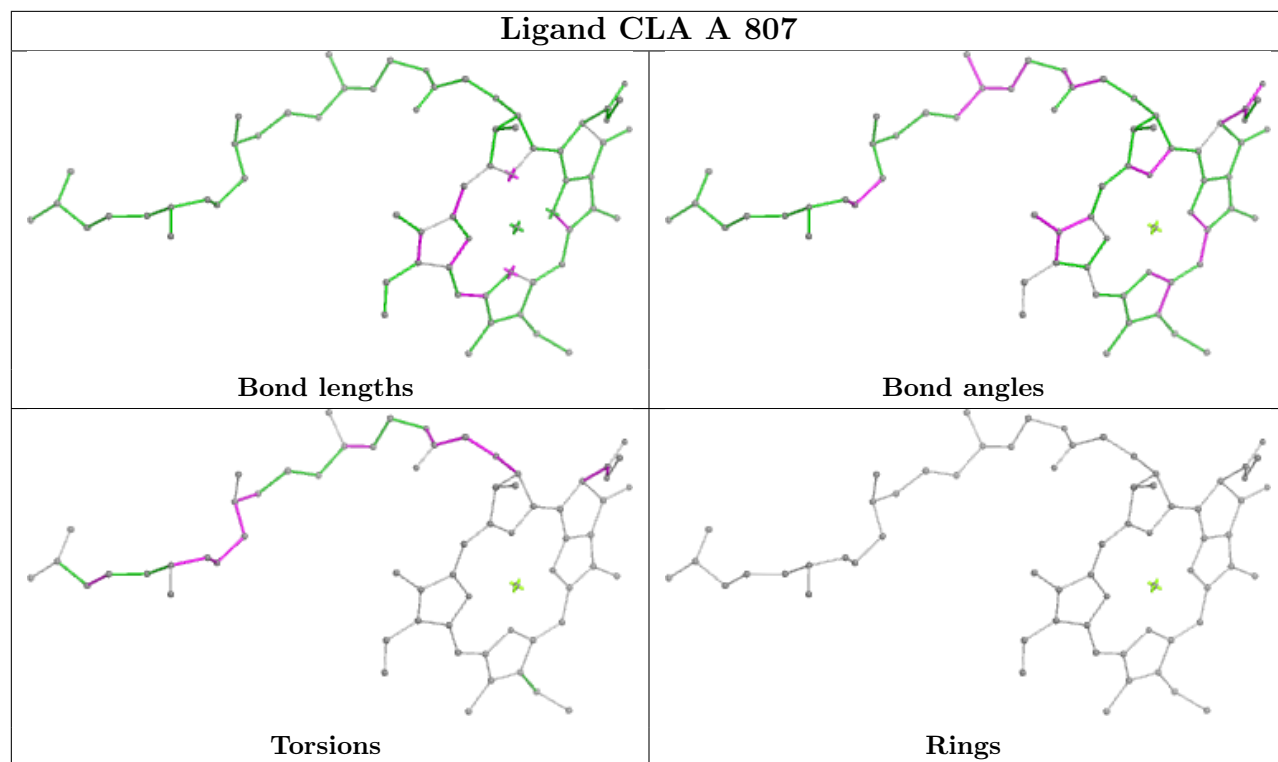


Ligand CLA 2 311

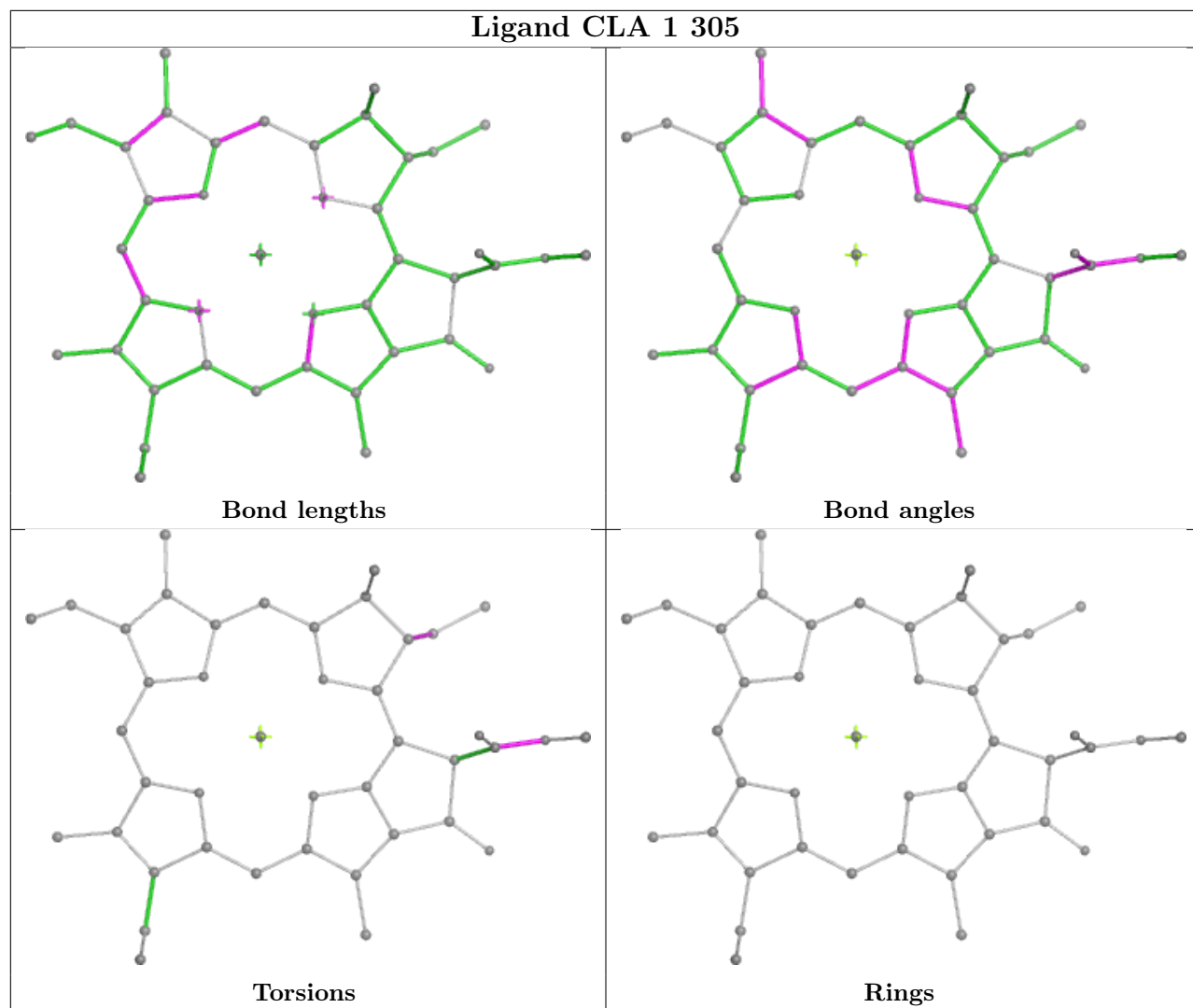


Ligand BCR A 846

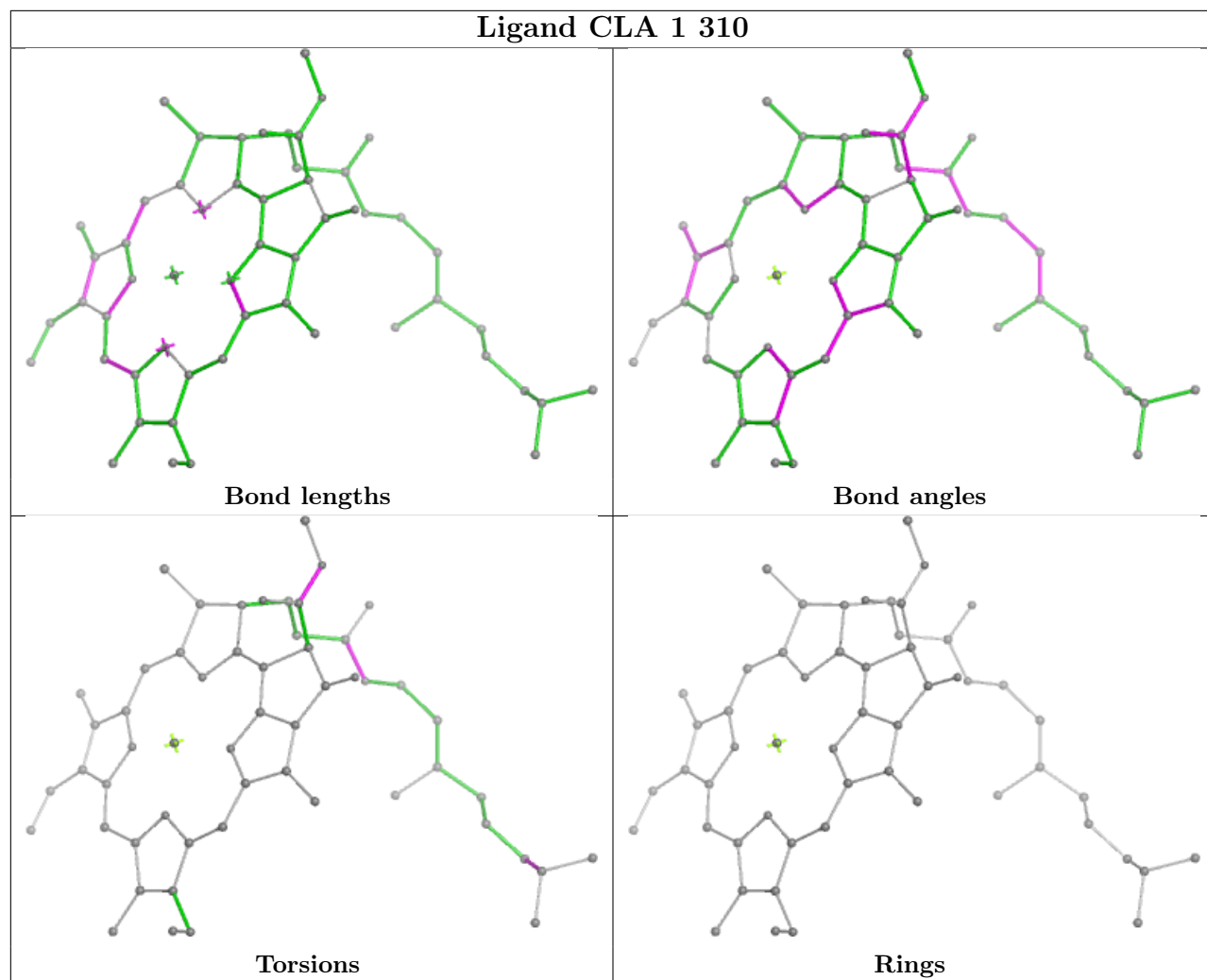




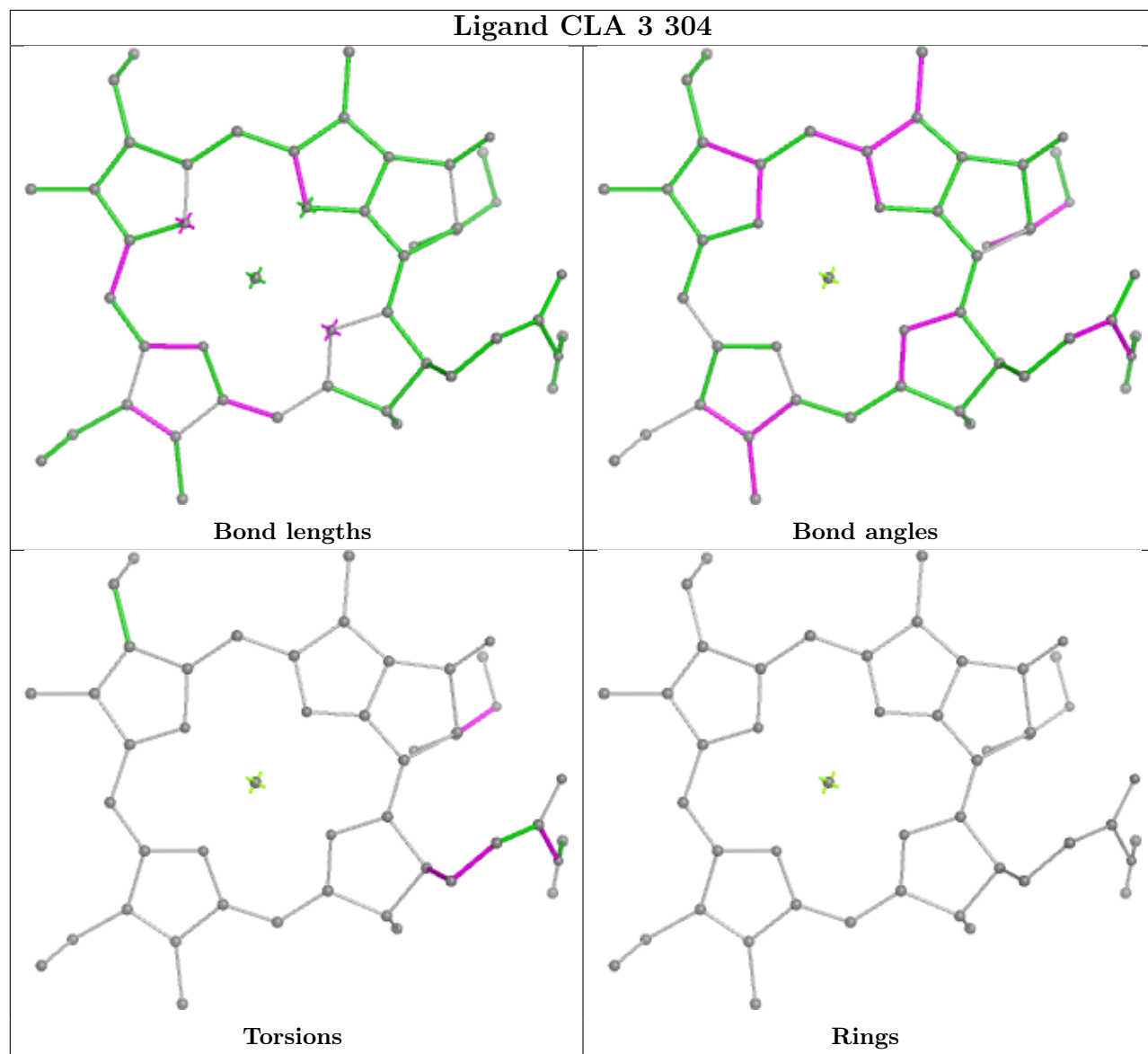
Ligand CLA 1 305



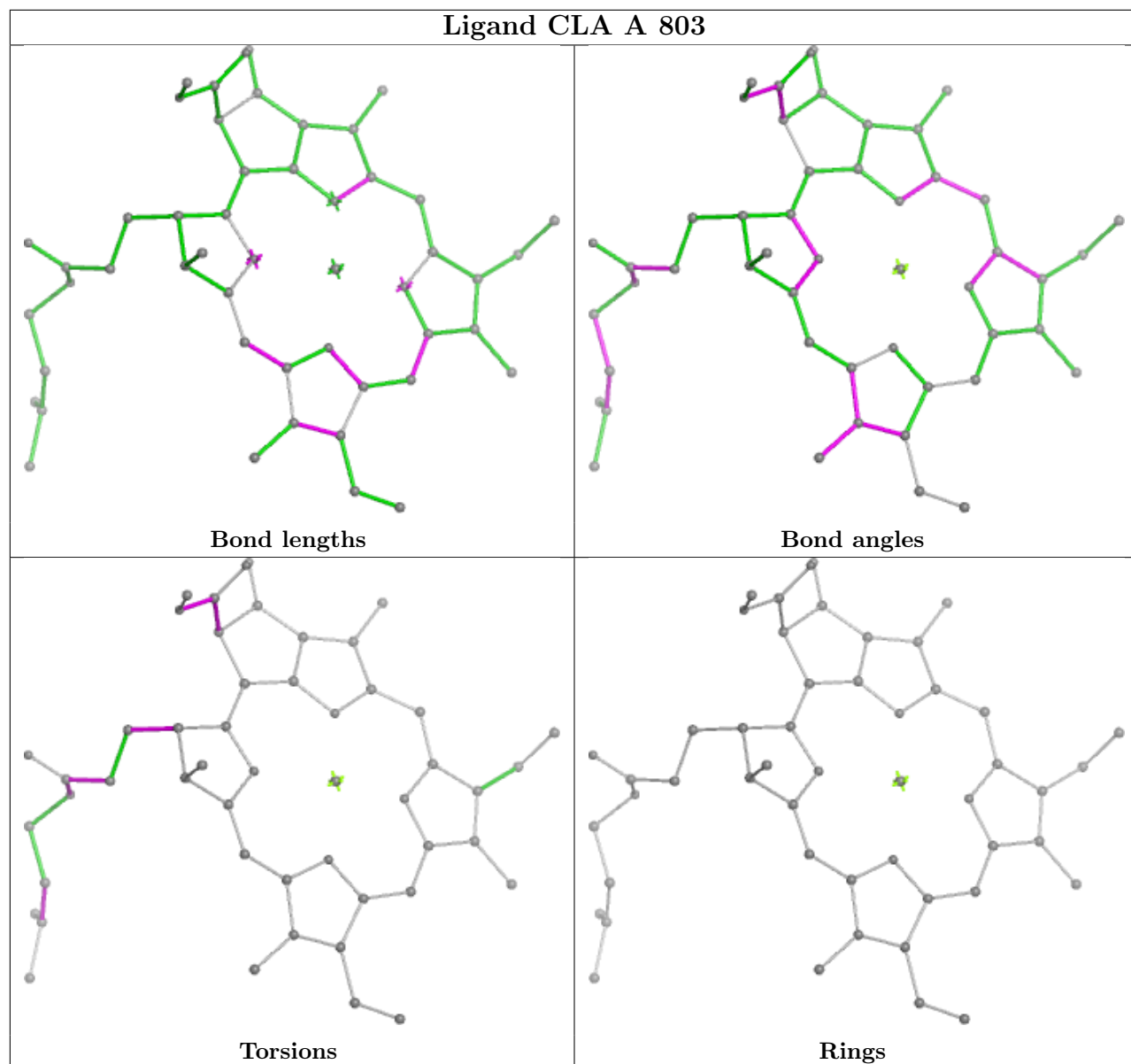
Ligand CLA 1 310

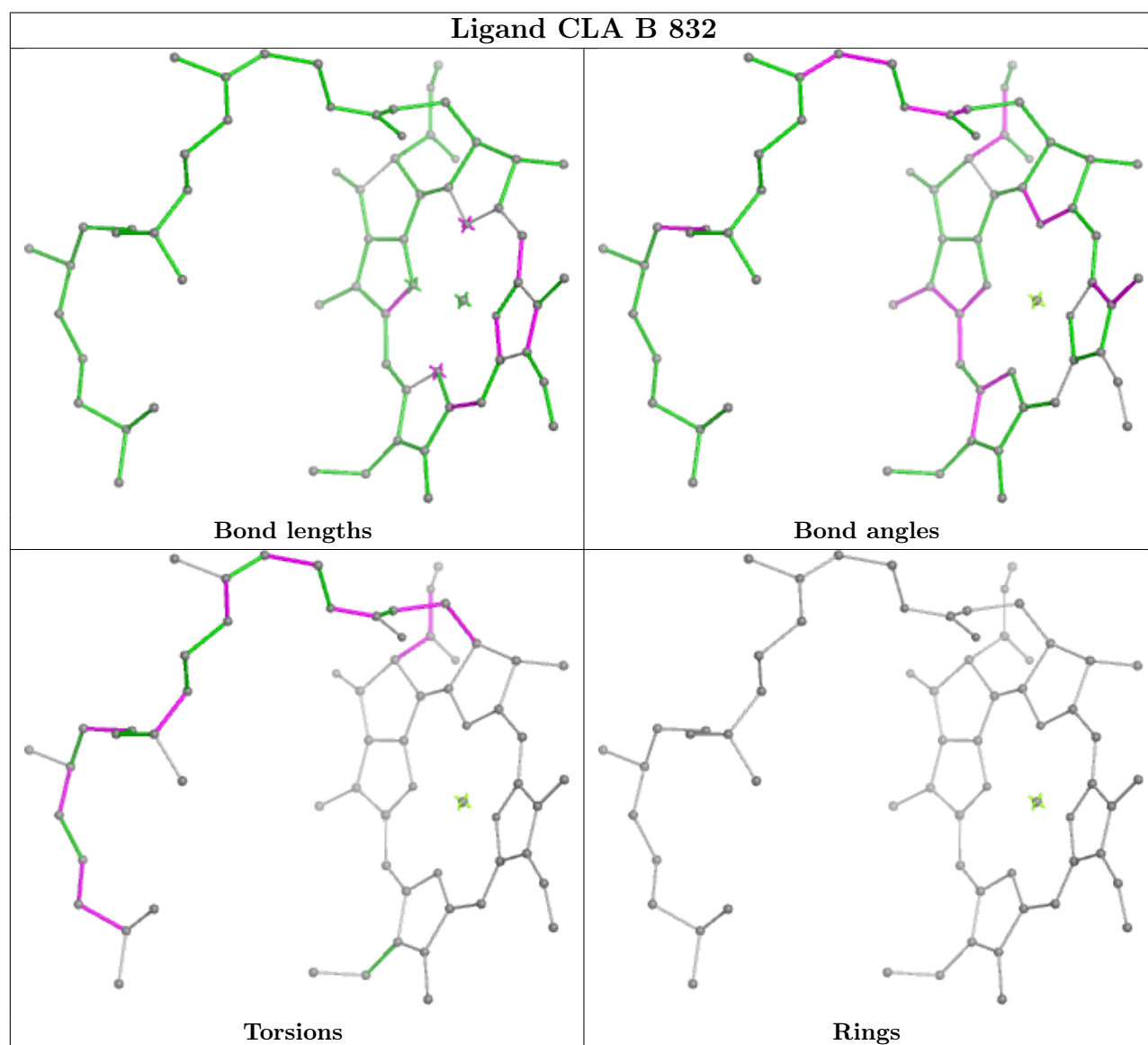
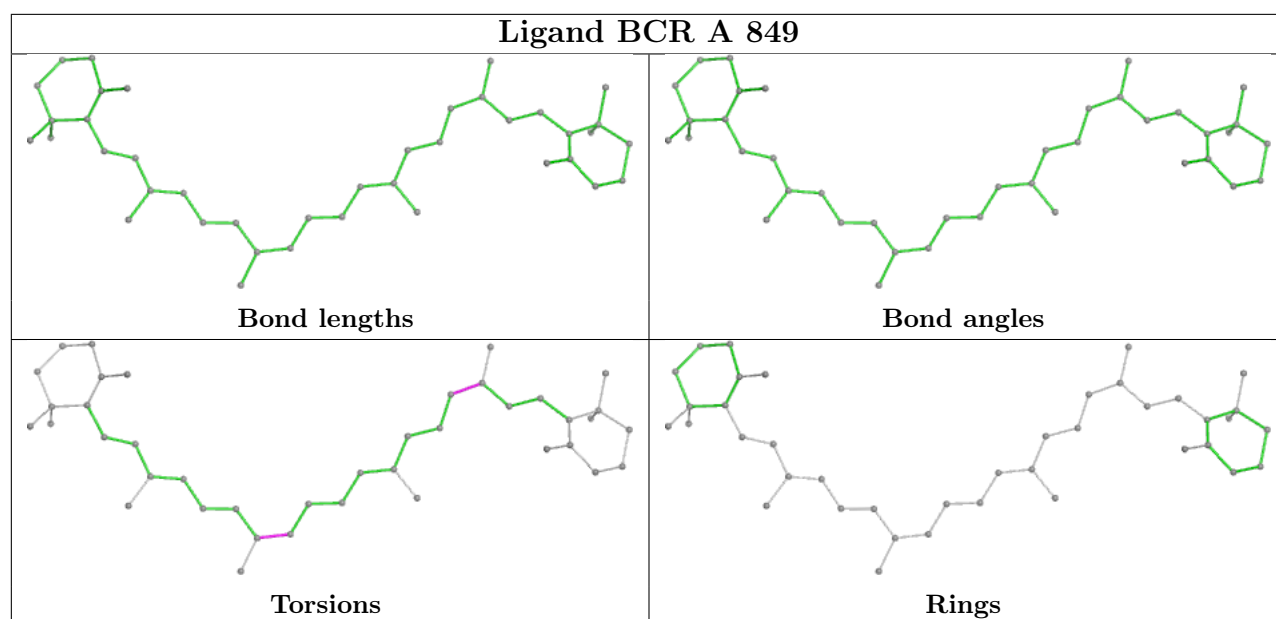


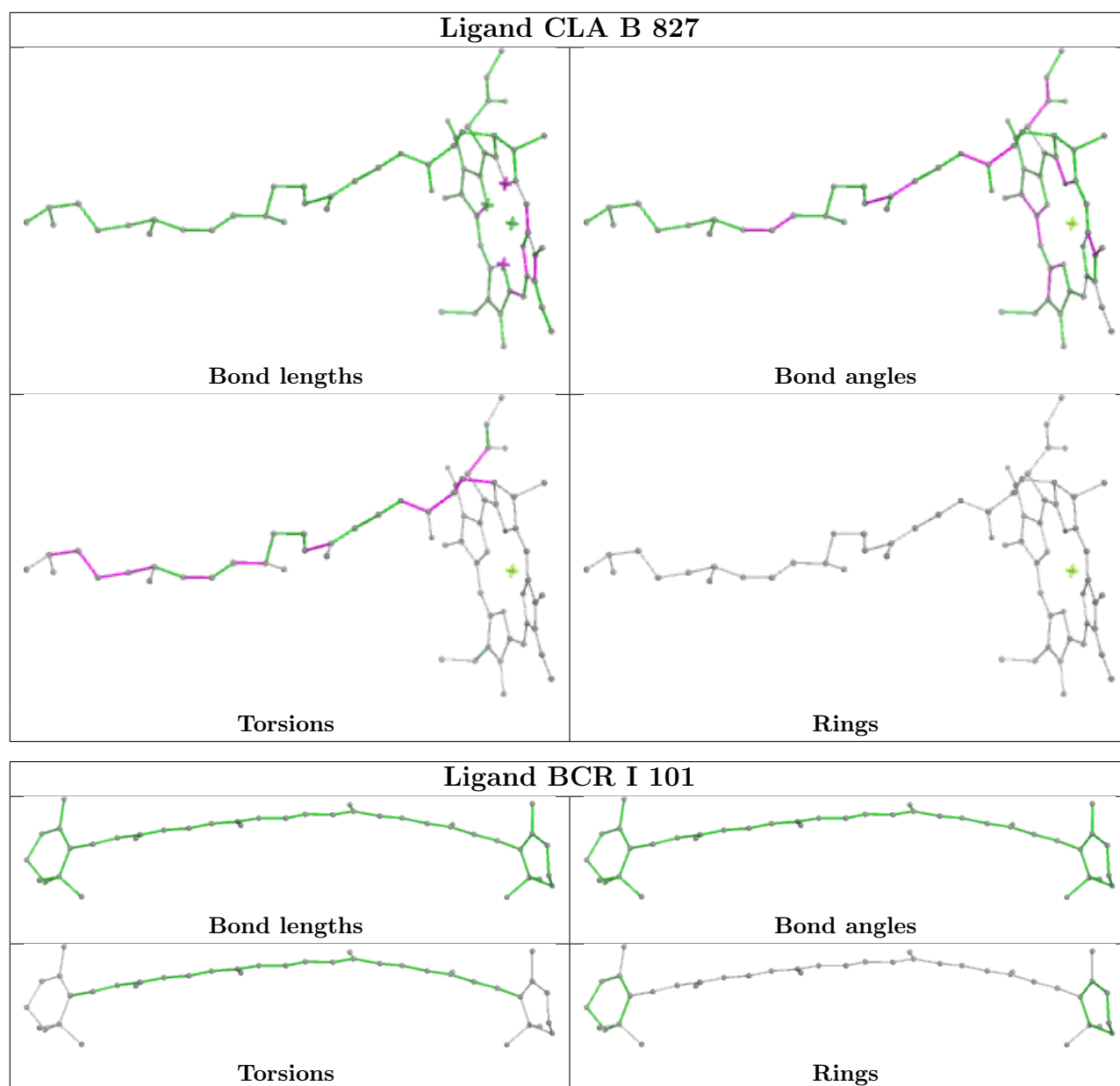
Ligand CLA 3 304



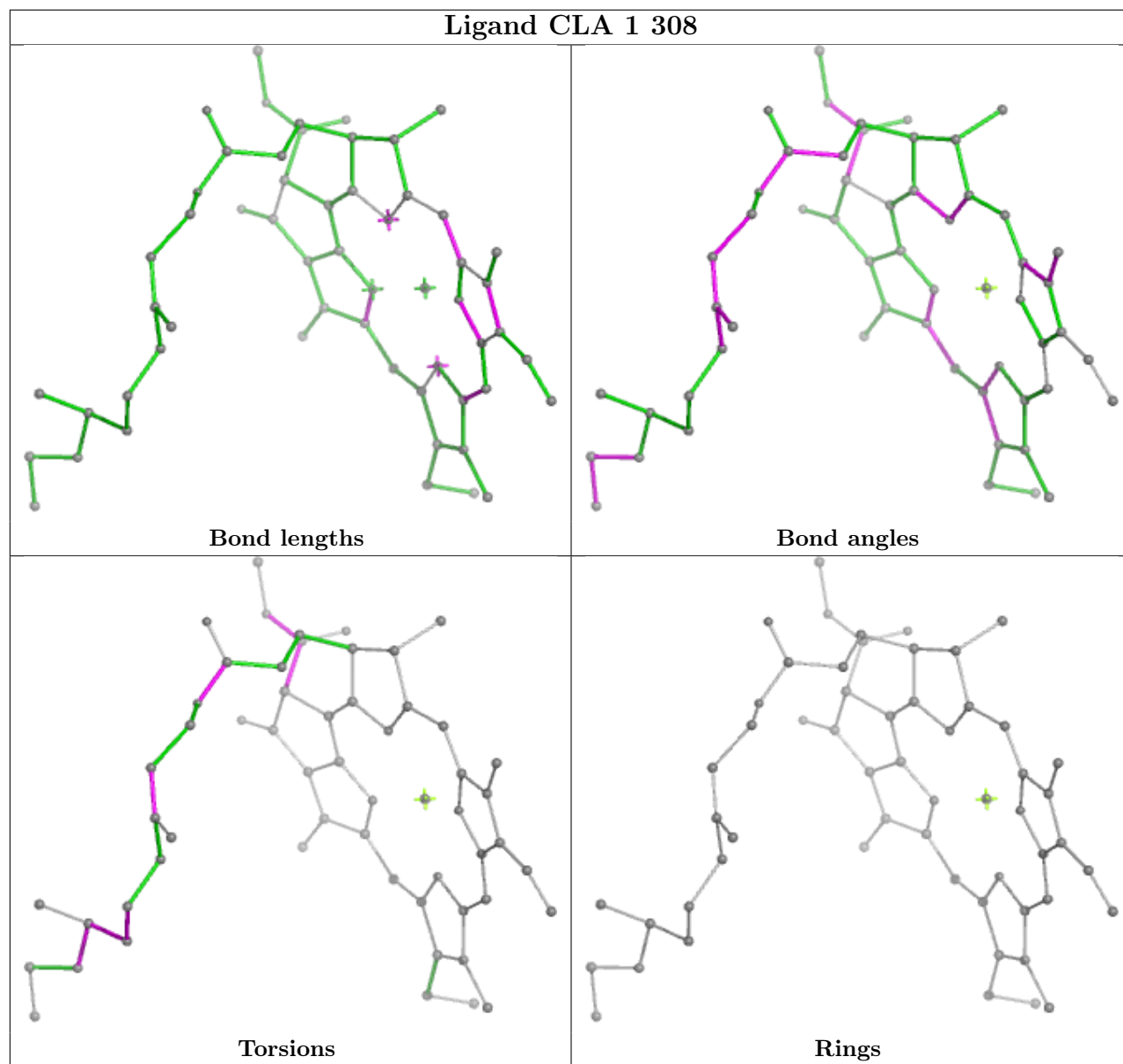
Ligand CLA A 803

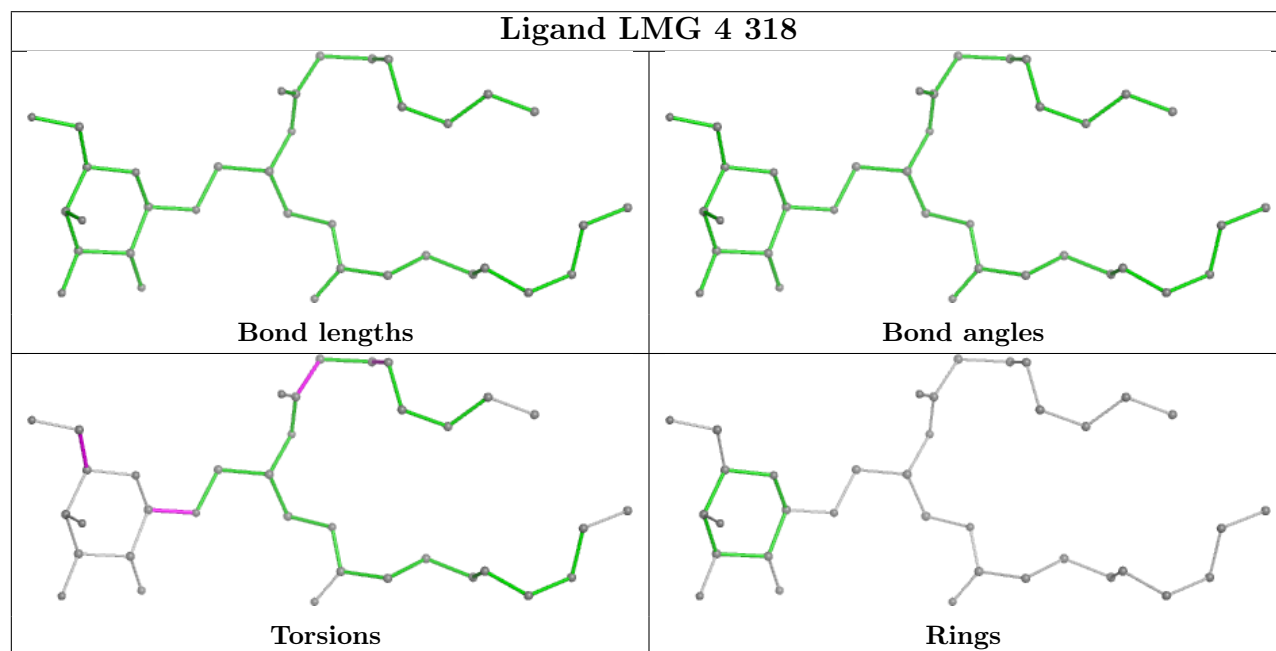
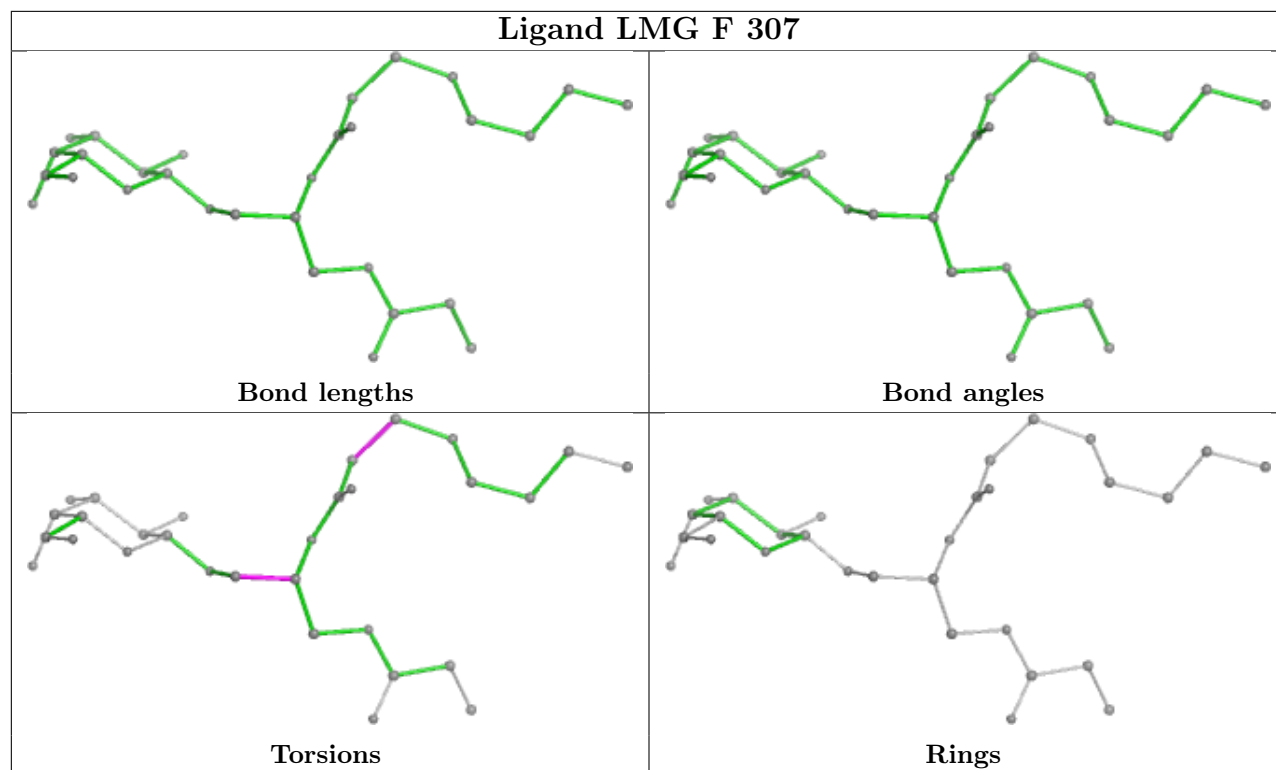


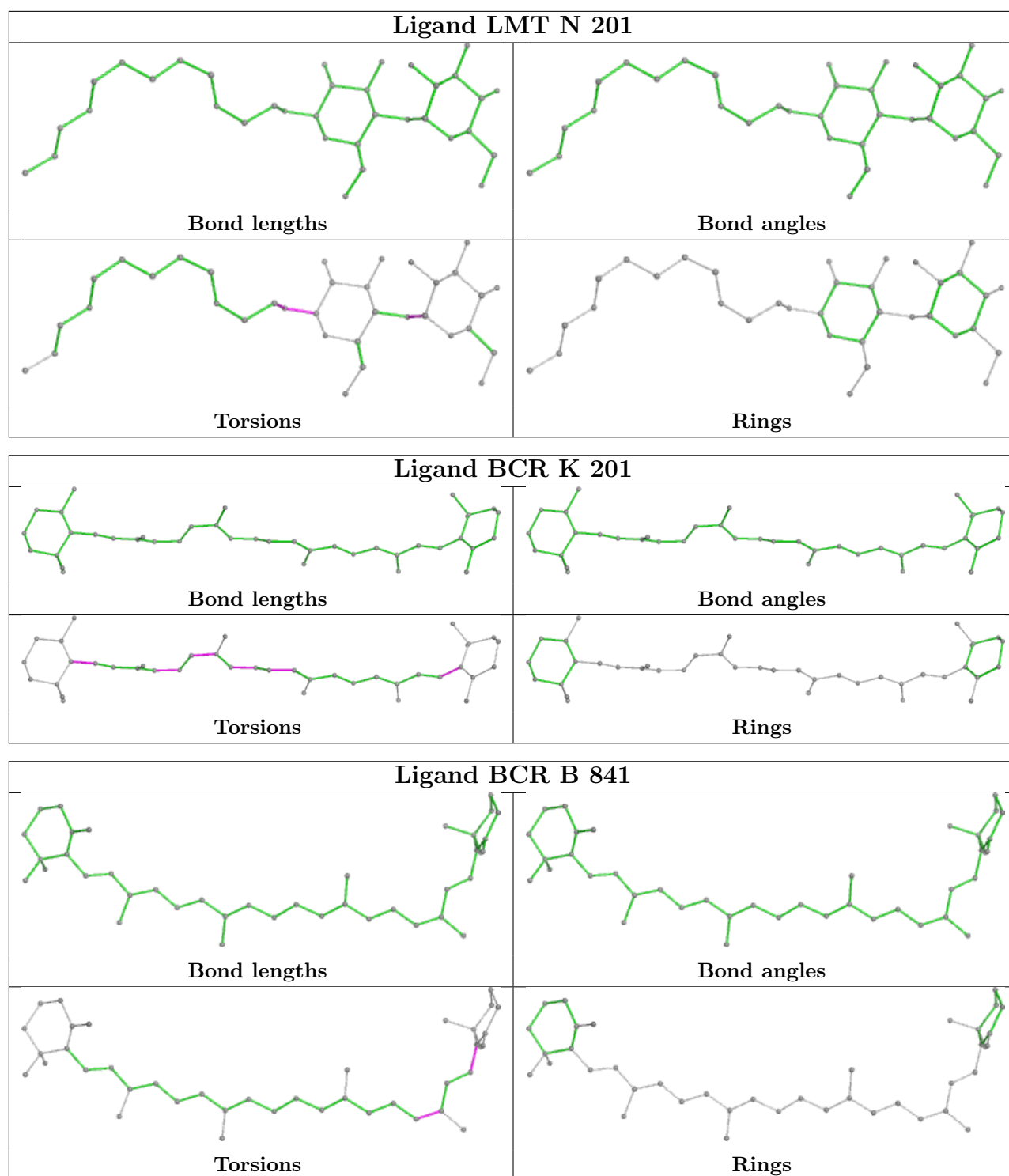




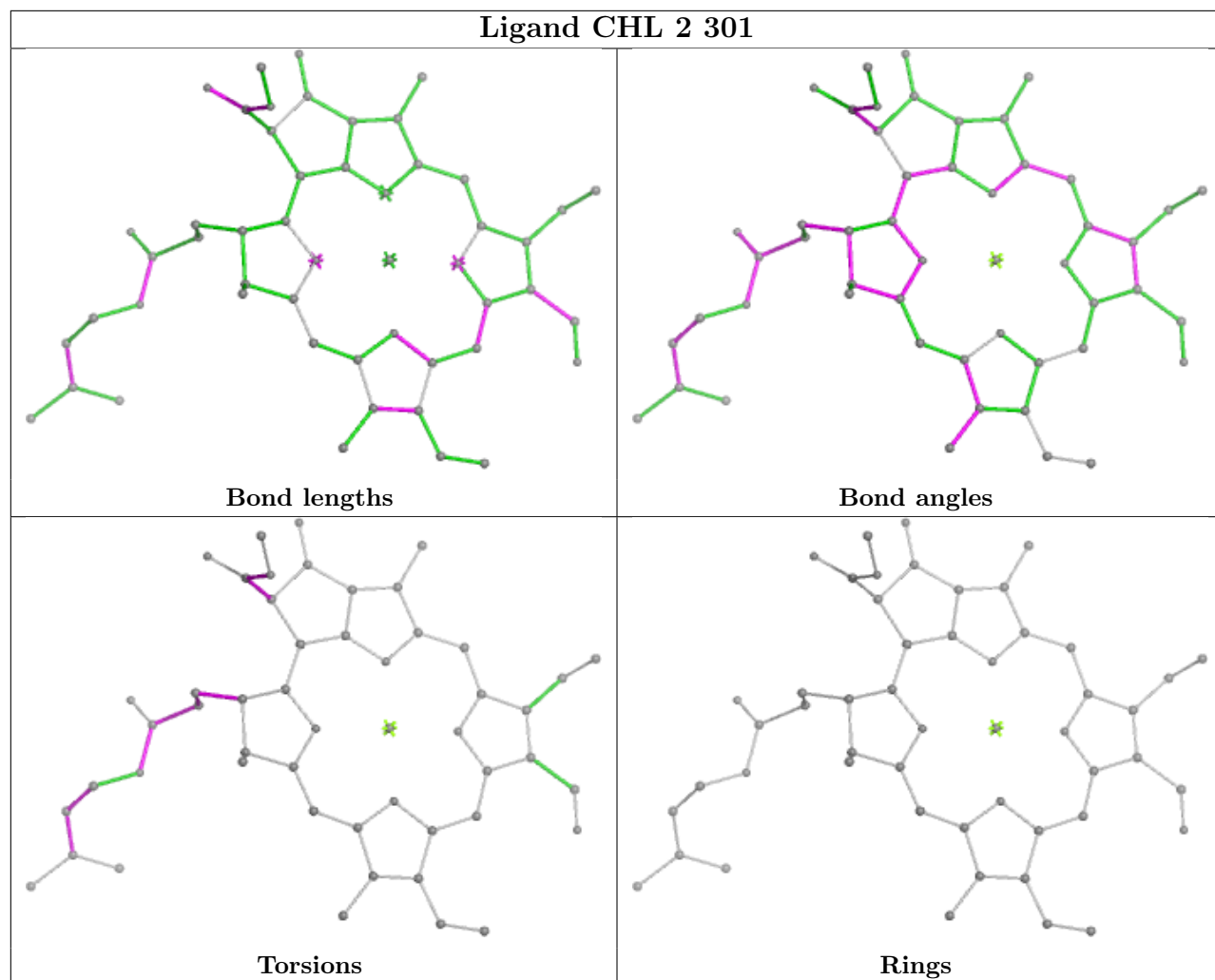
Ligand CLA 1 308

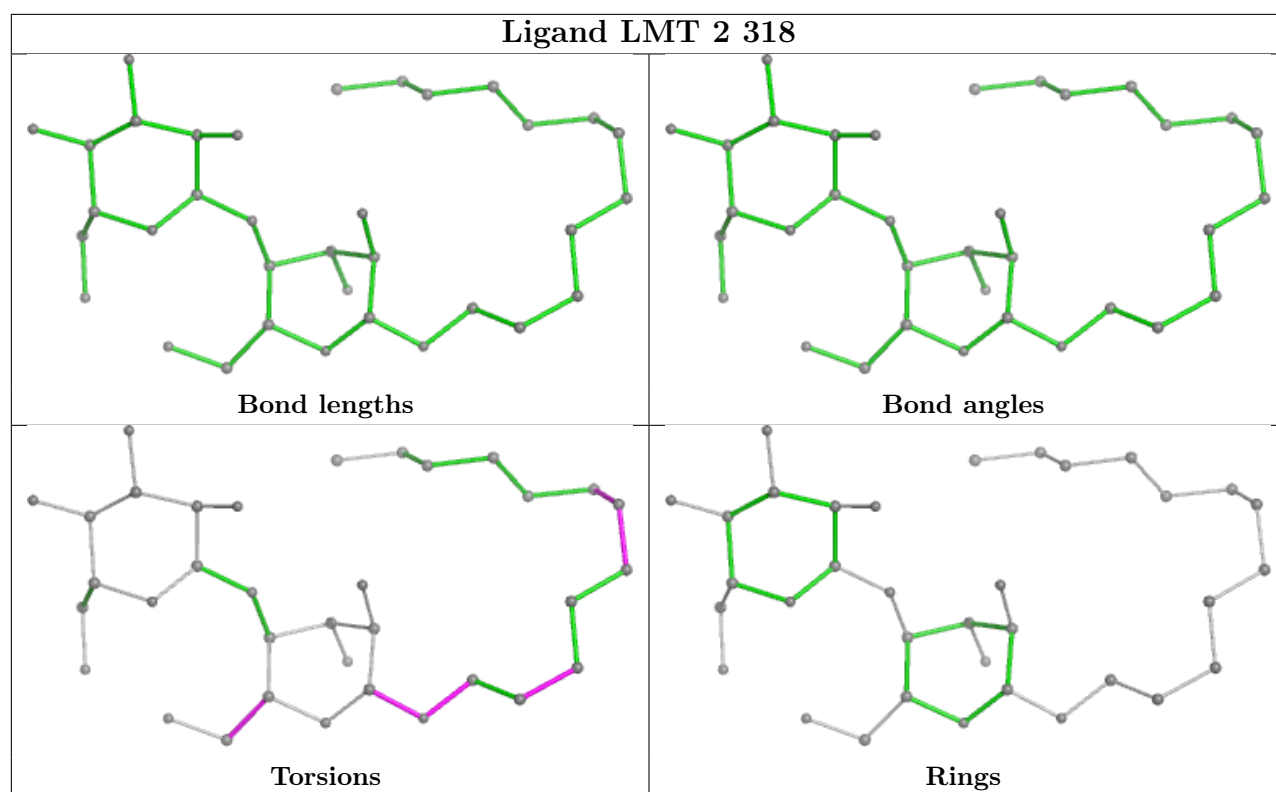




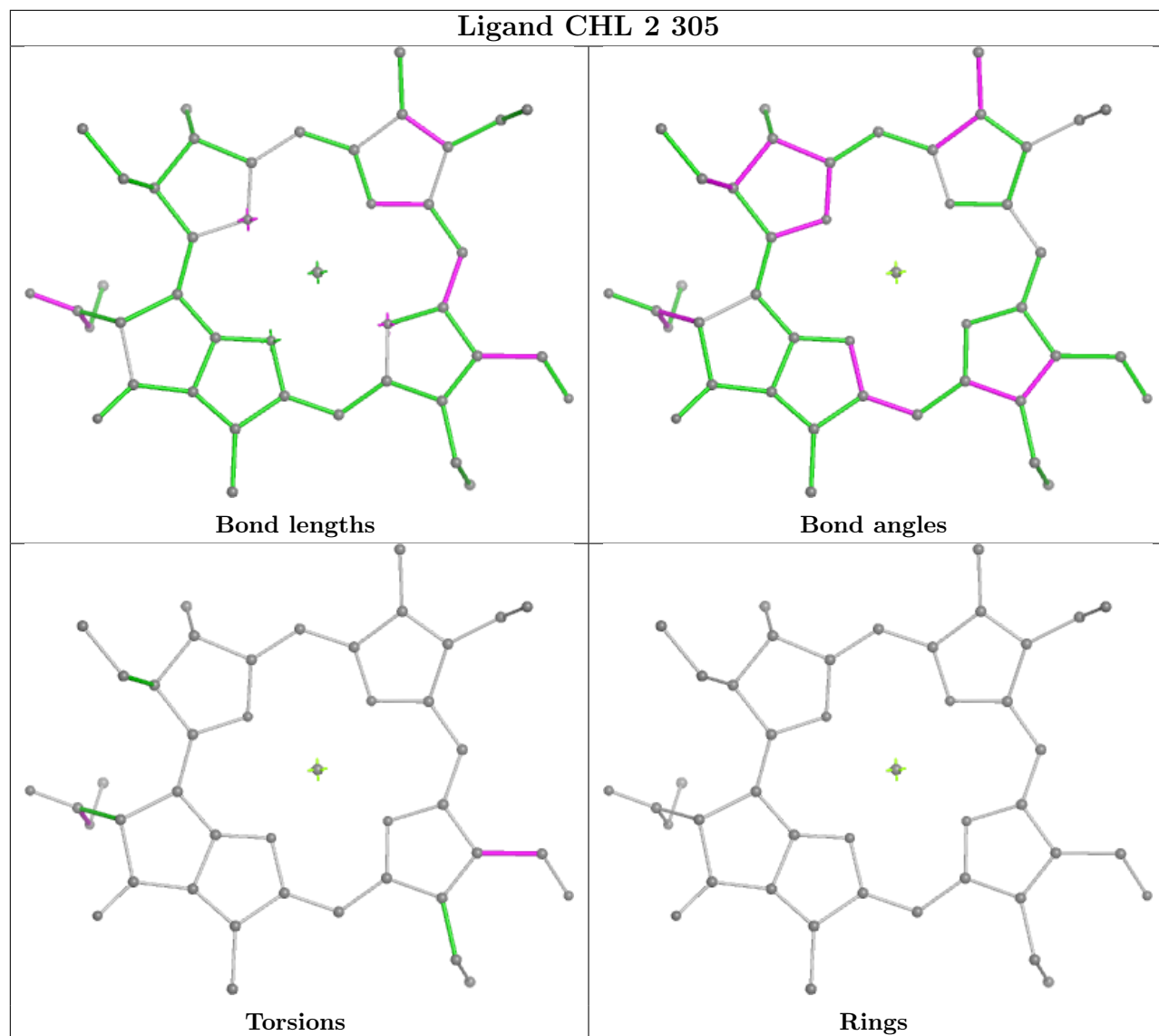


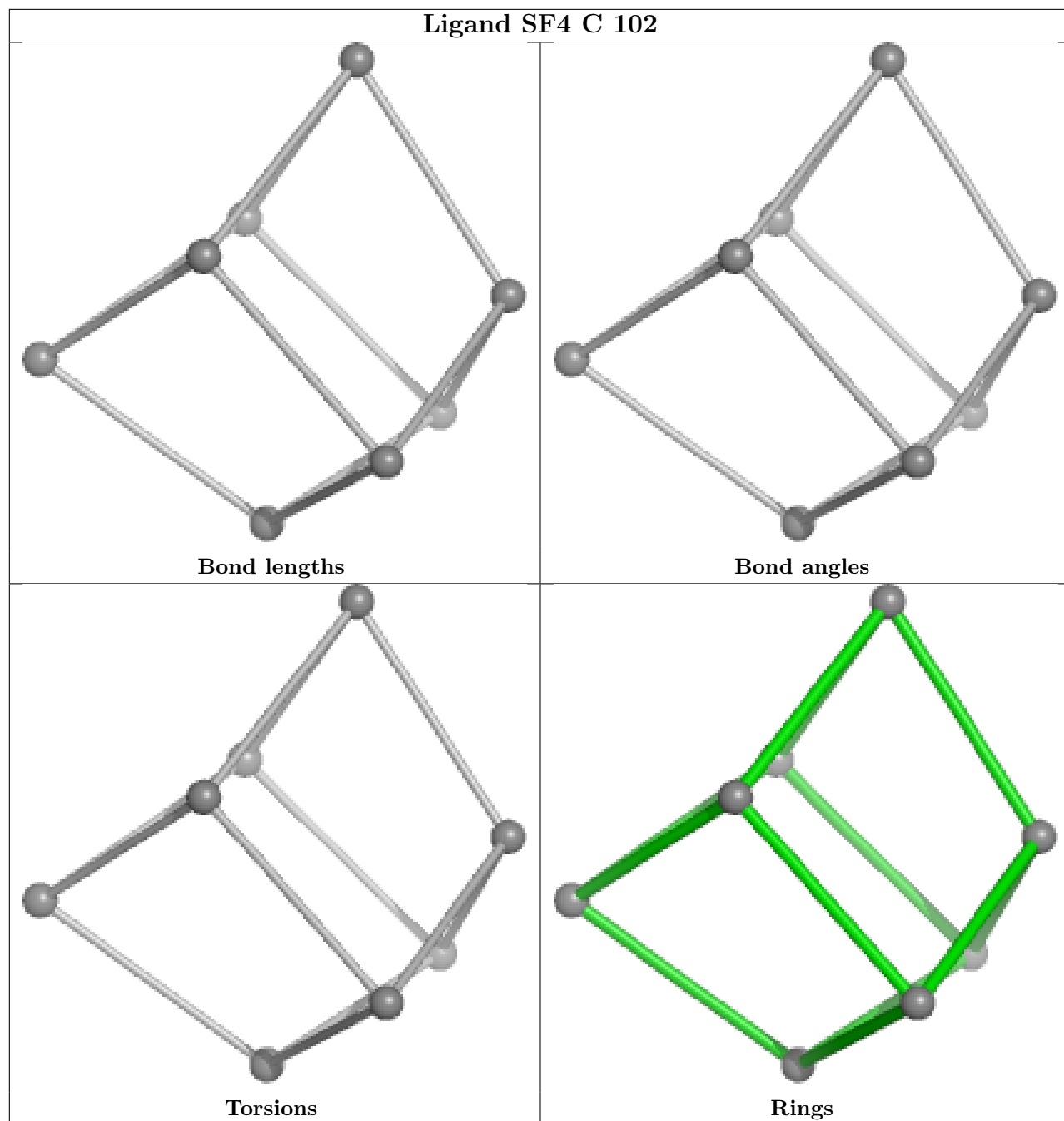
Ligand CHL 2 301



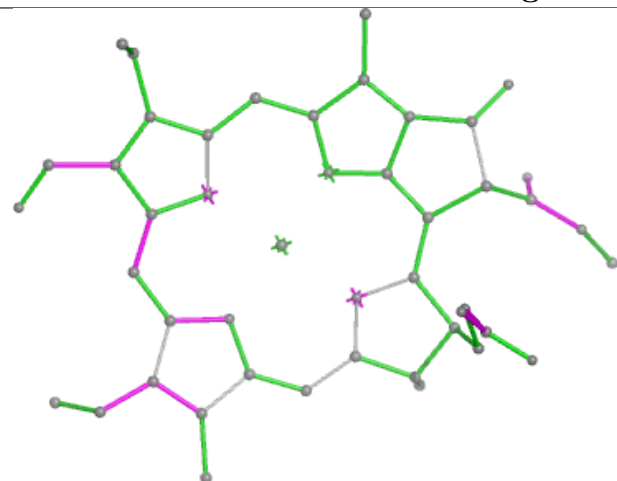


Ligand CHL 2 305

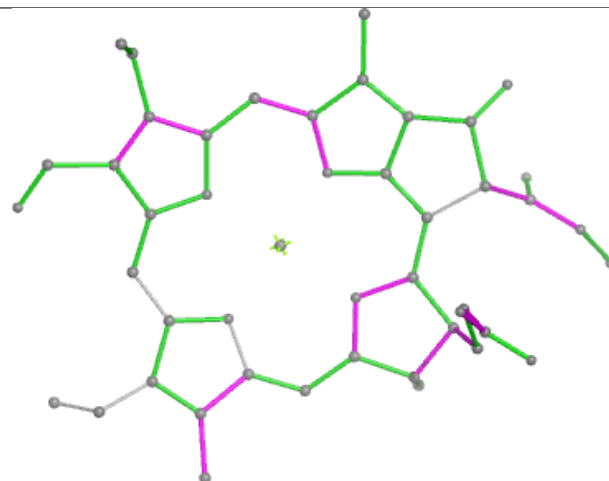




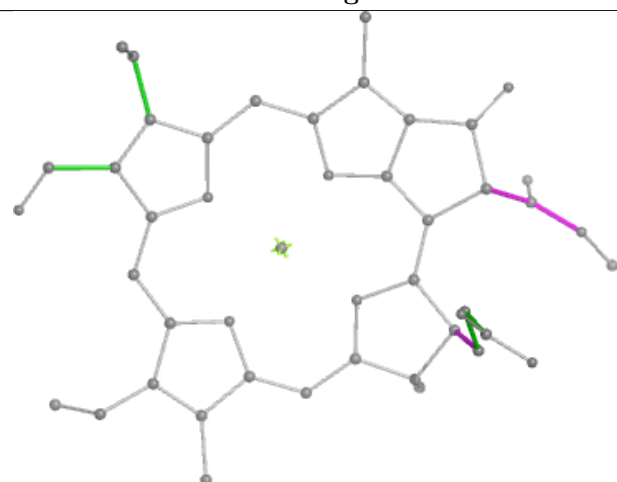
Ligand CHL 2 307



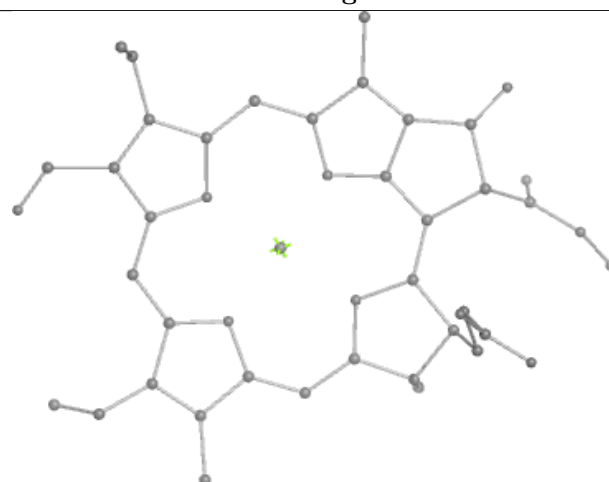
Bond lengths



Bond angles

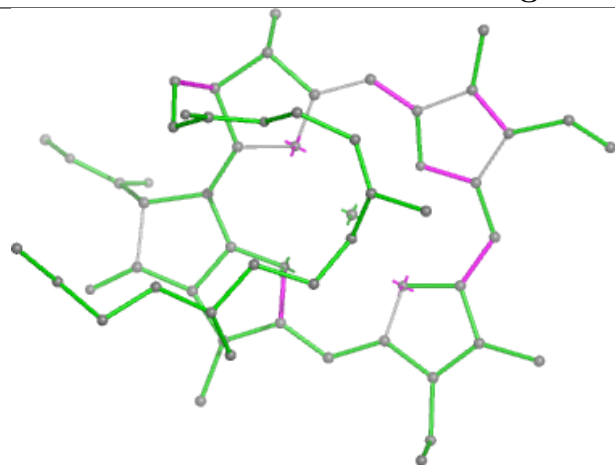


Torsions

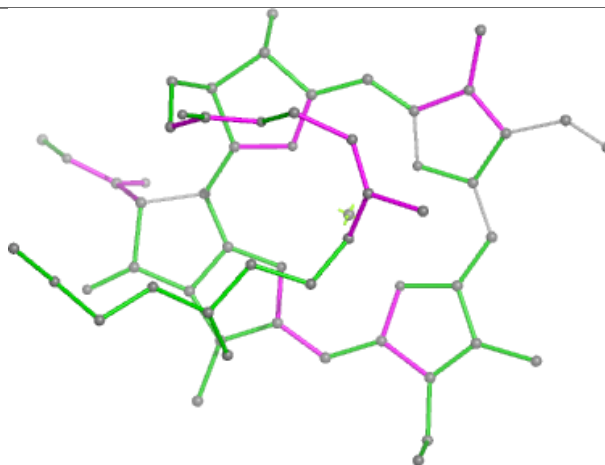


Rings

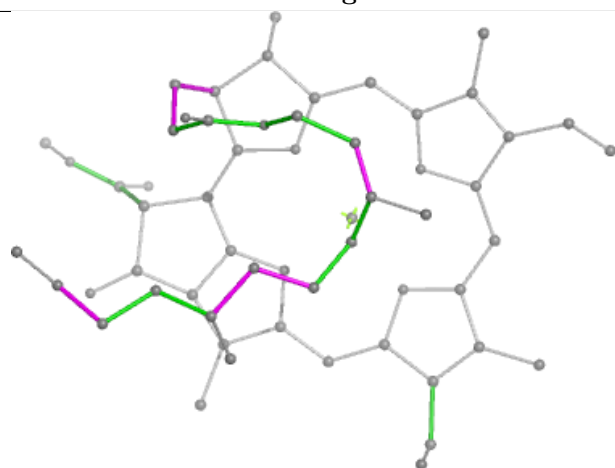
Ligand CLA 2 313



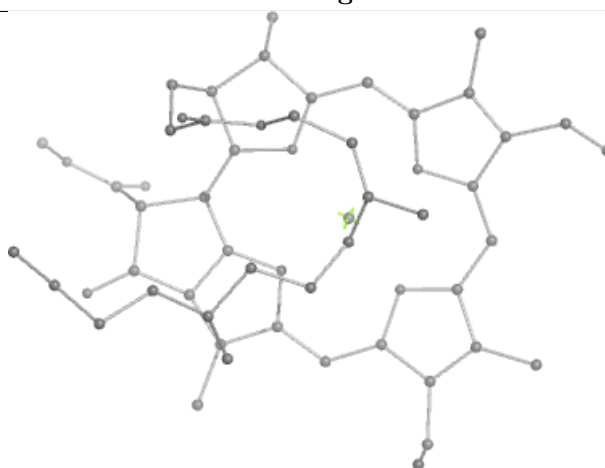
Bond lengths



Bond angles

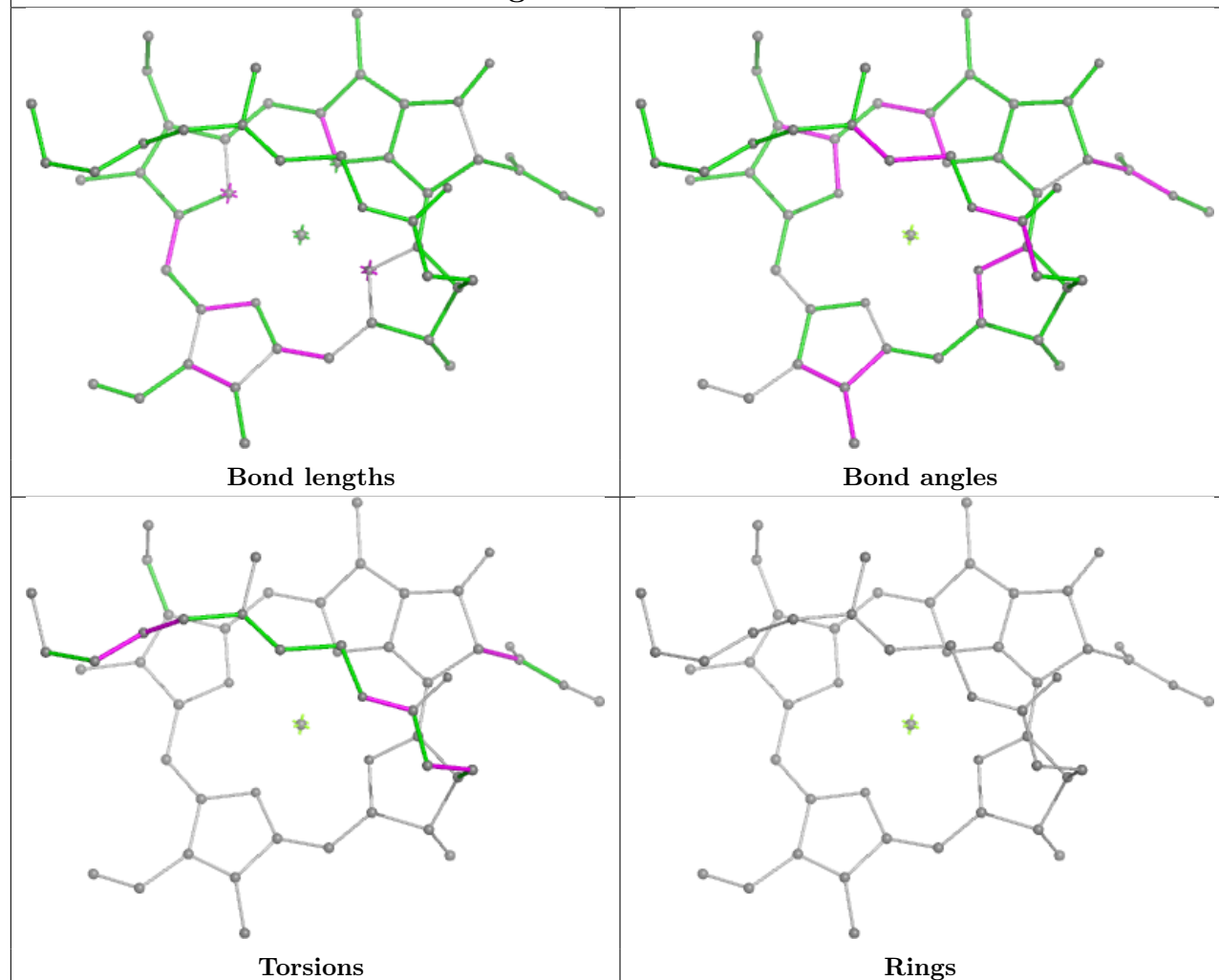


Torsions

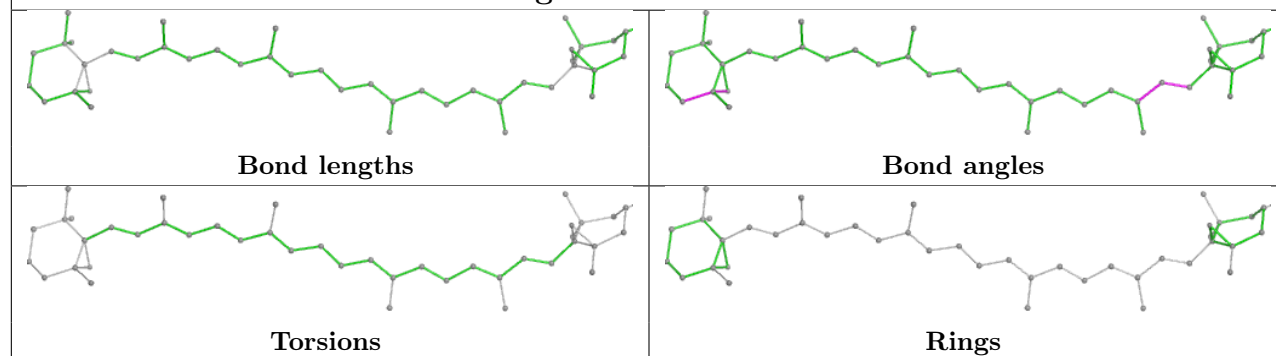


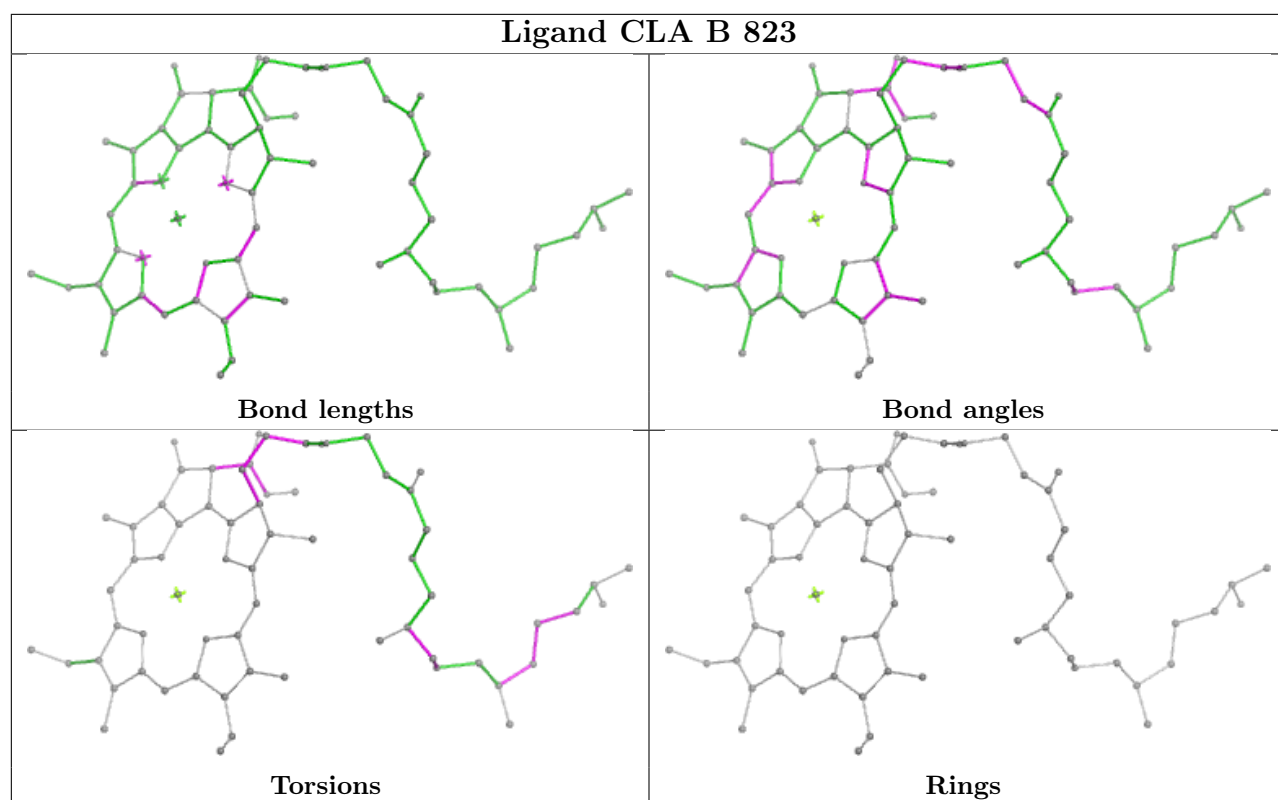
Rings

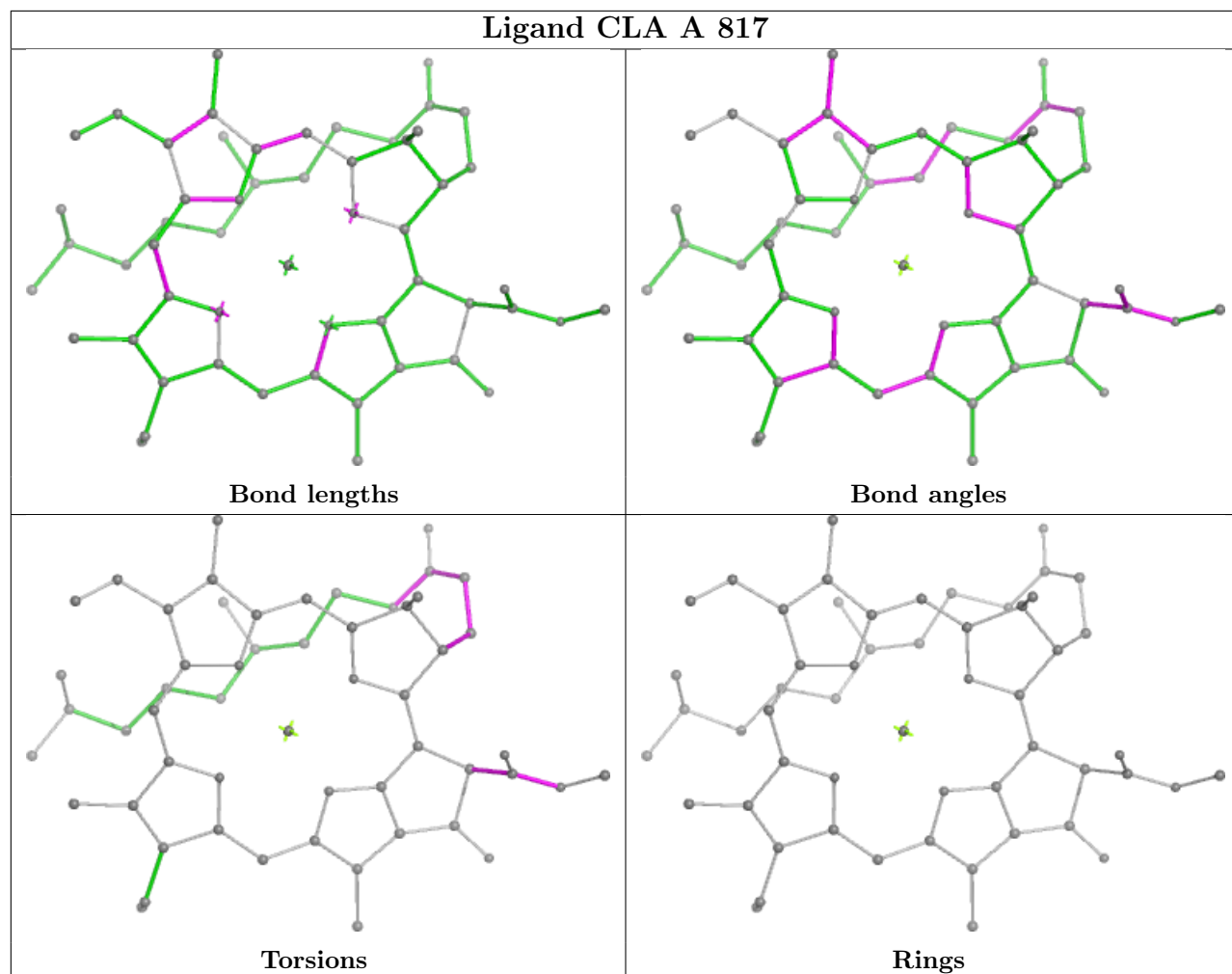
Ligand CLA B 806

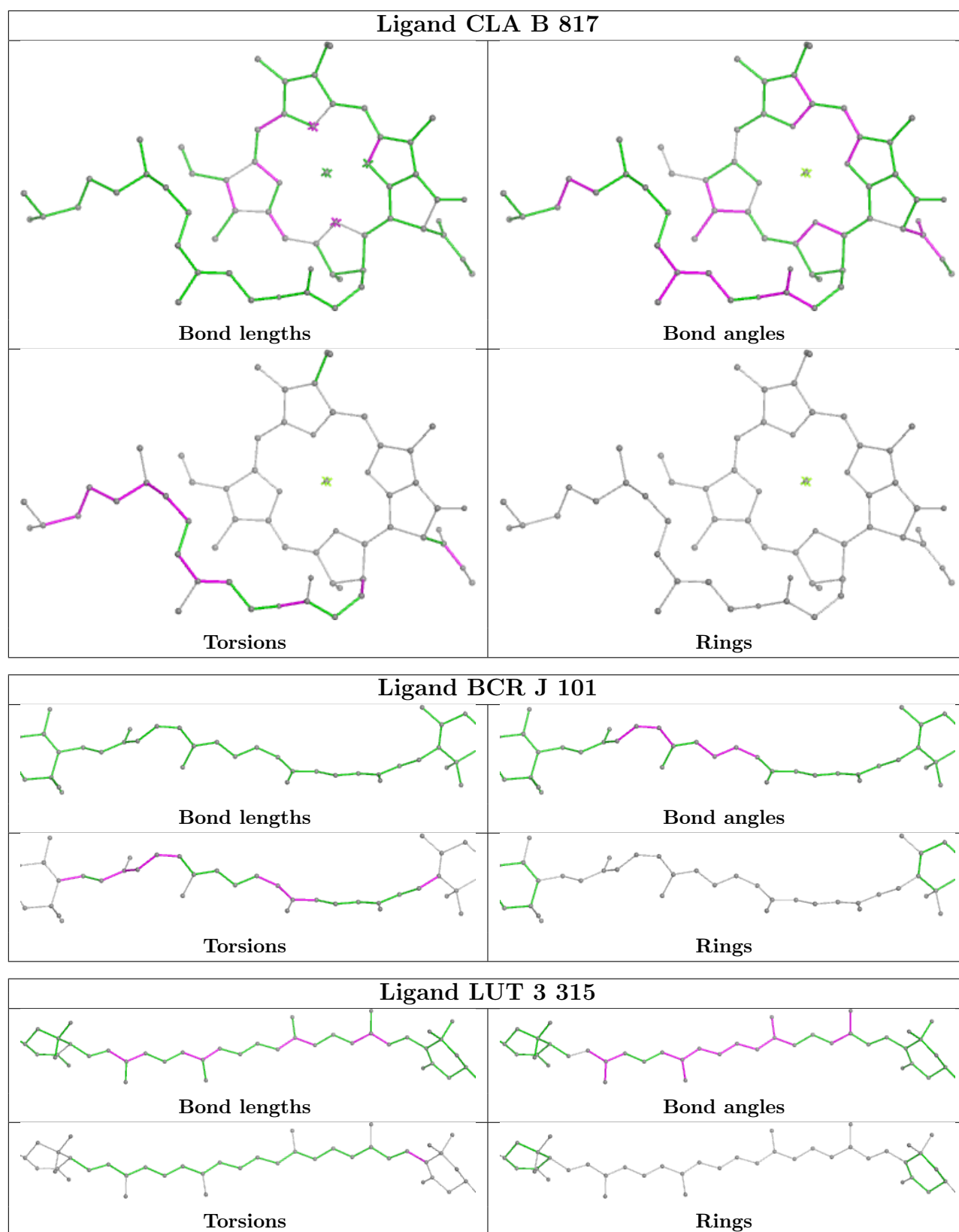


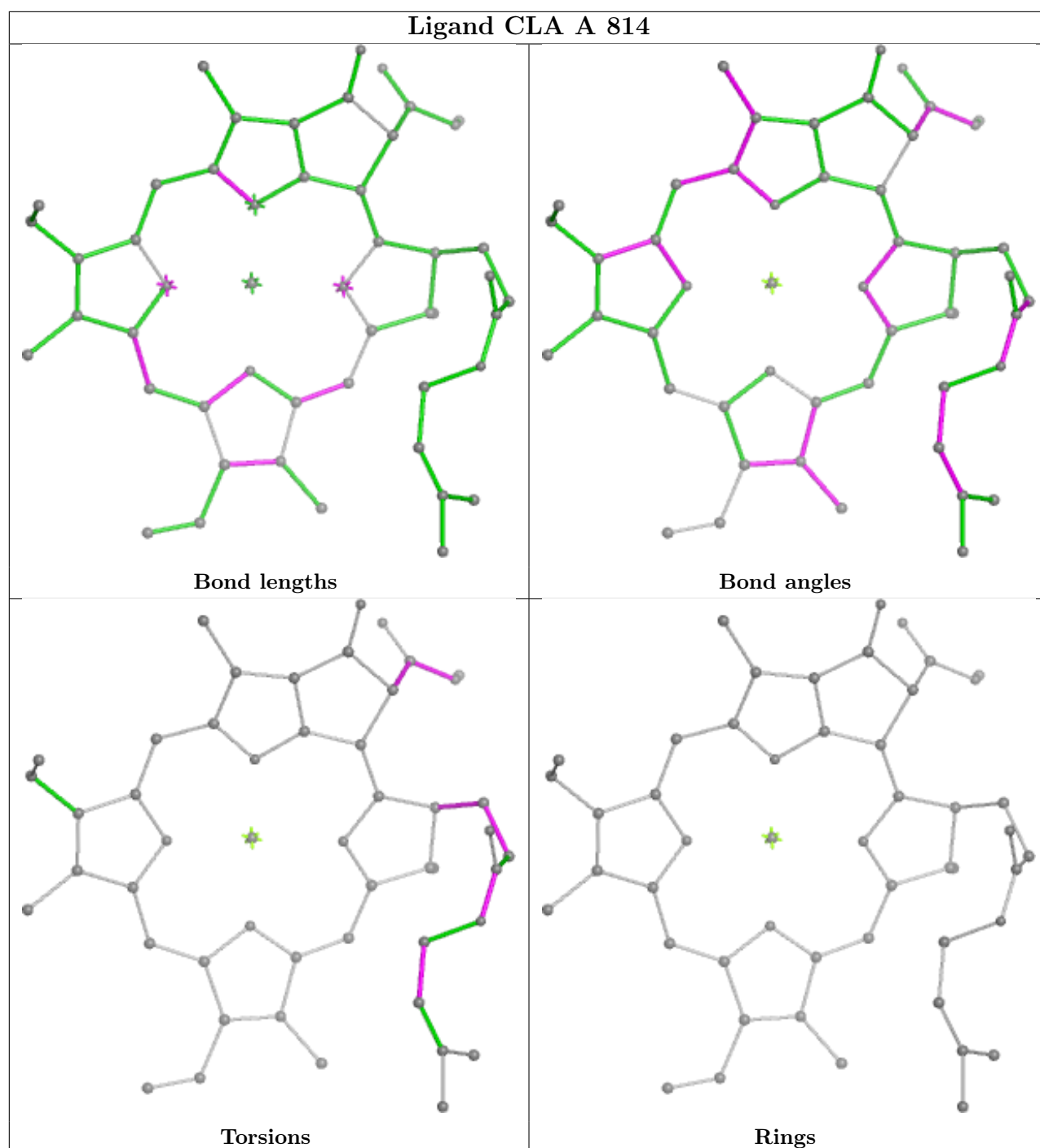
Ligand XAT 3 316



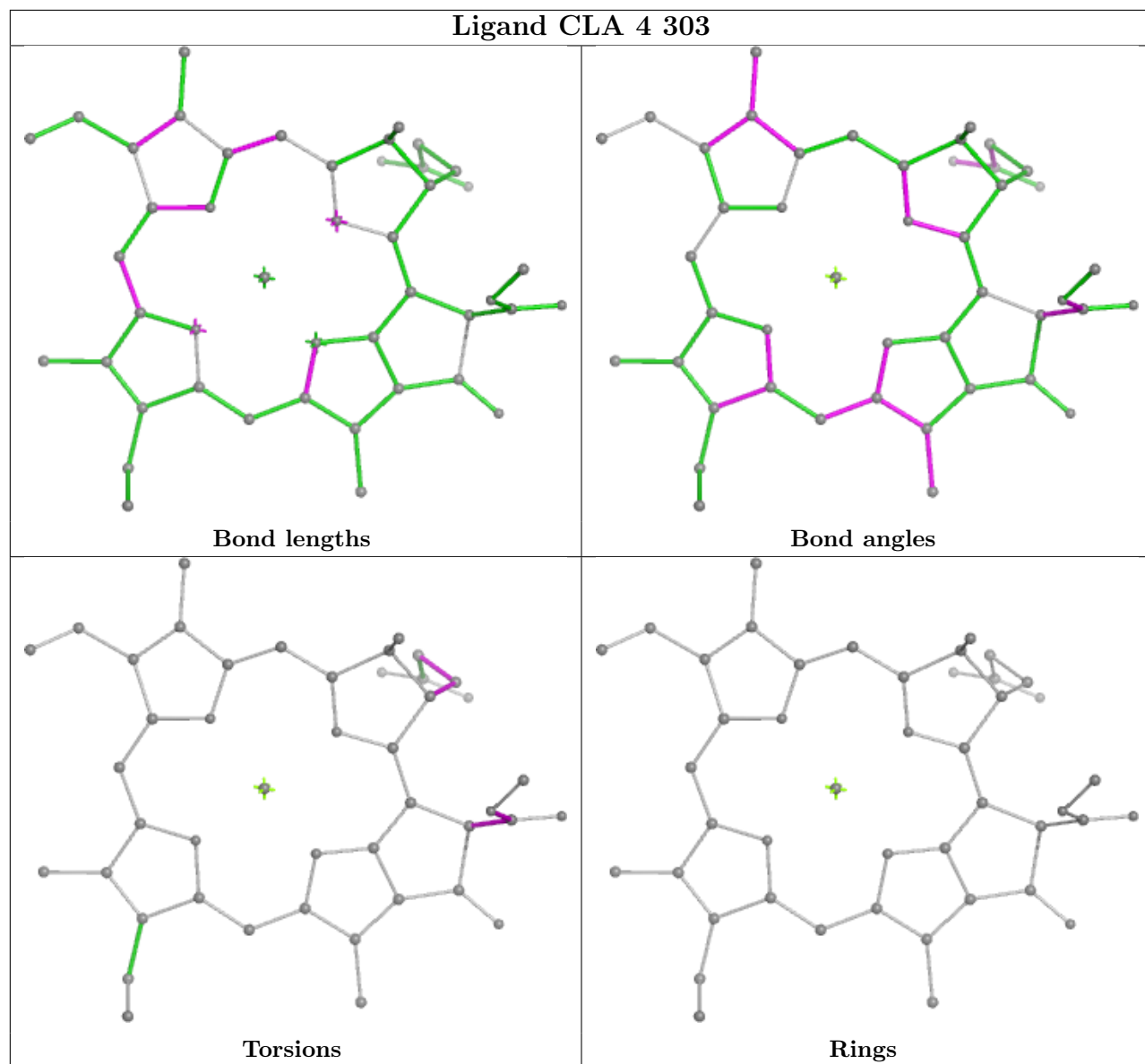


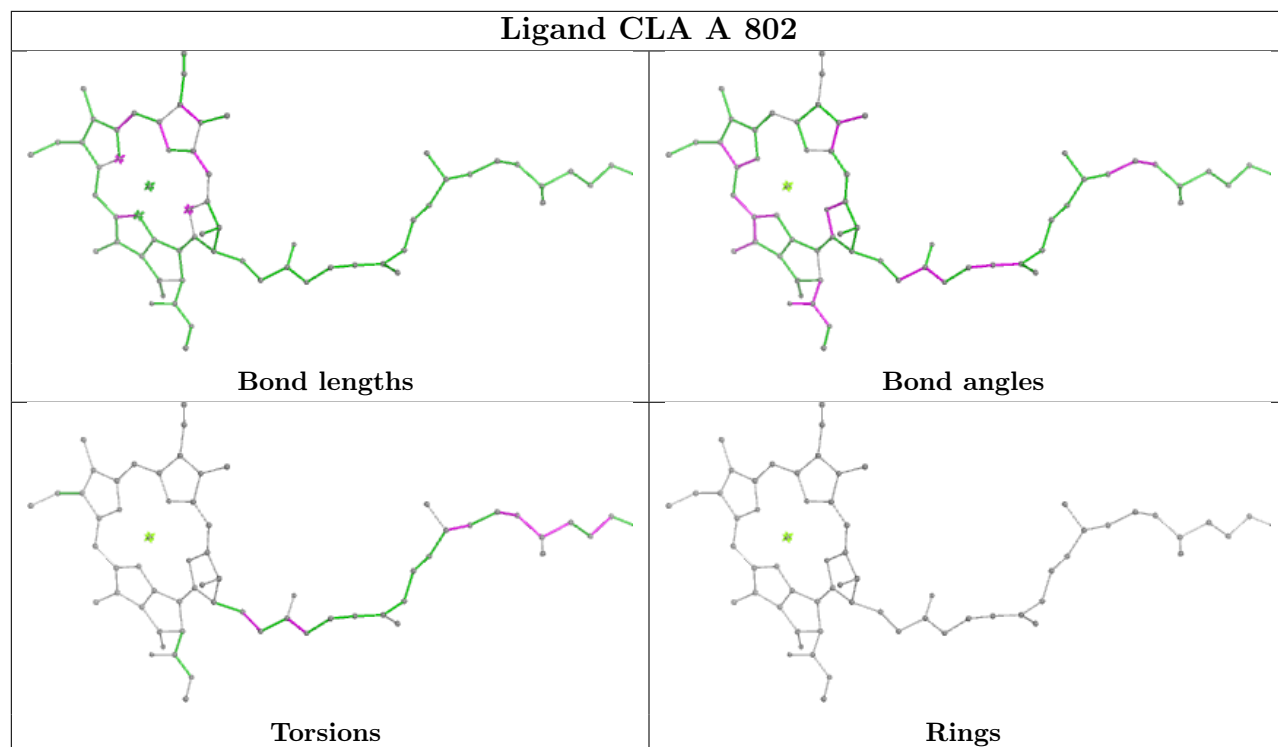
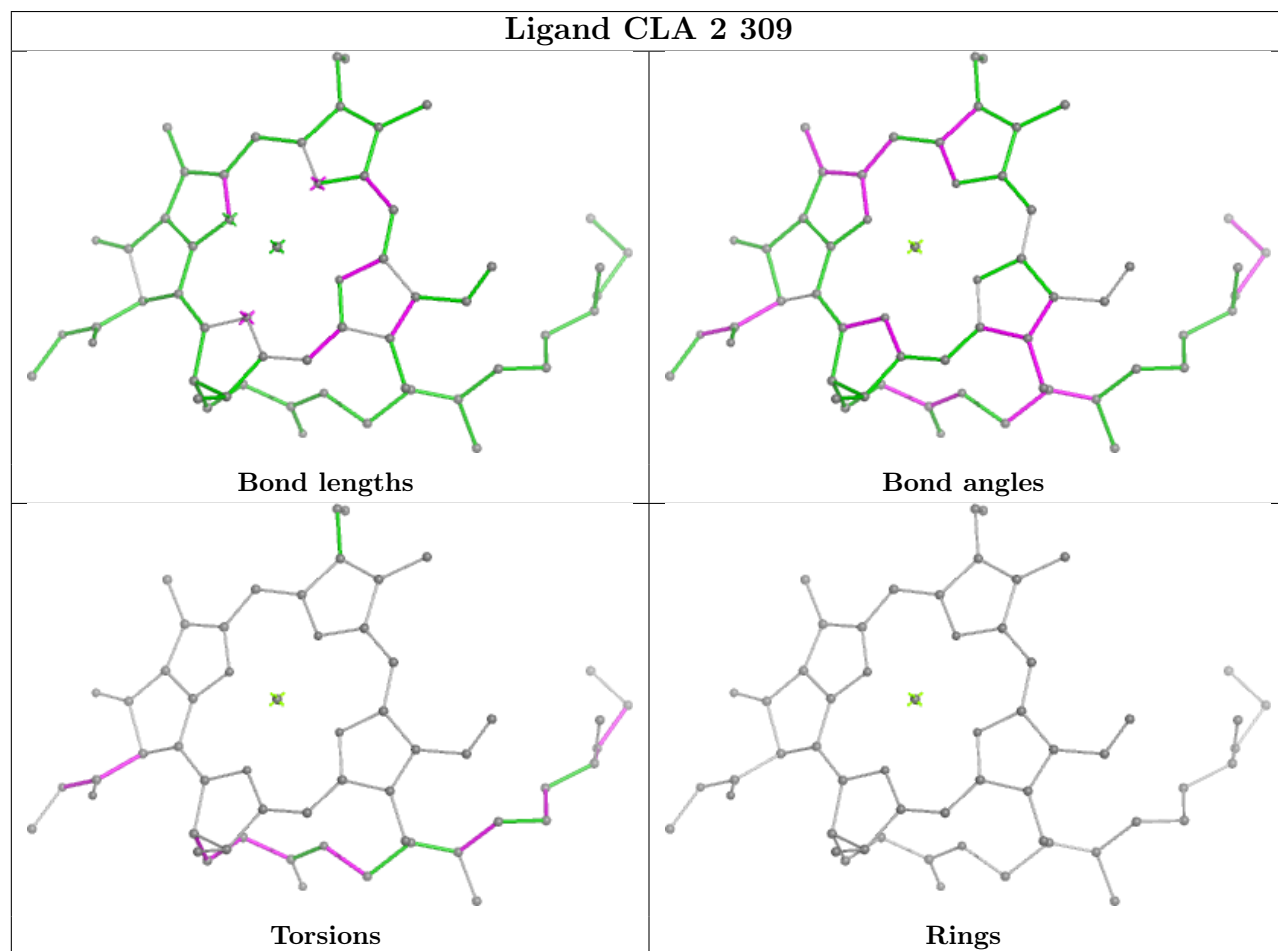


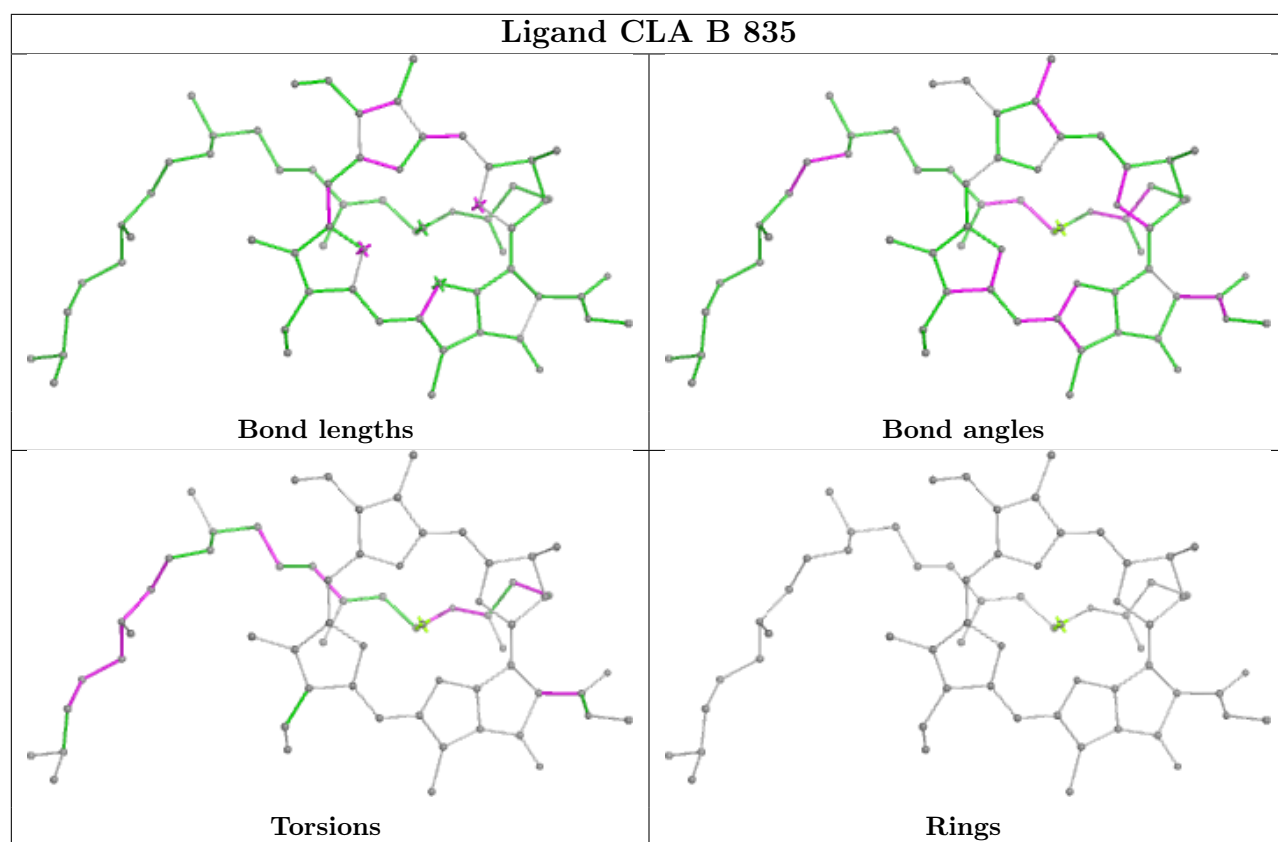




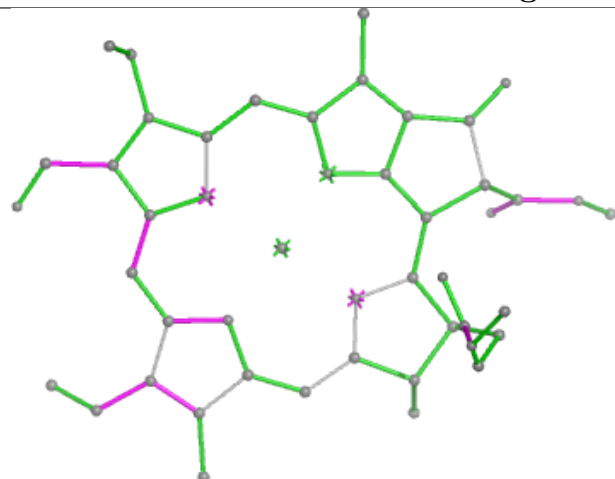
Ligand CLA 4 303



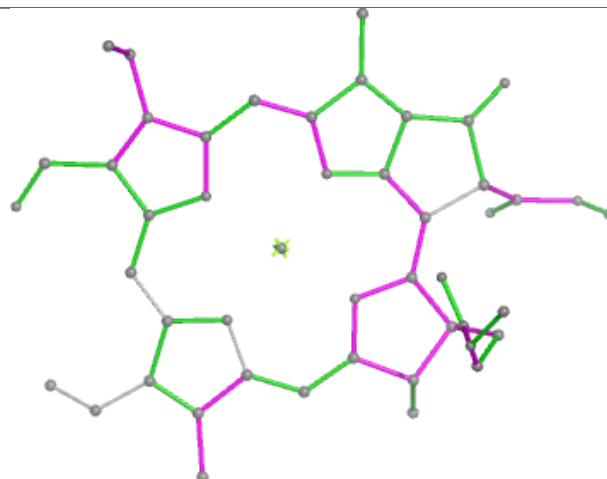
Ligand CLA A 802**Ligand CLA 2 309**



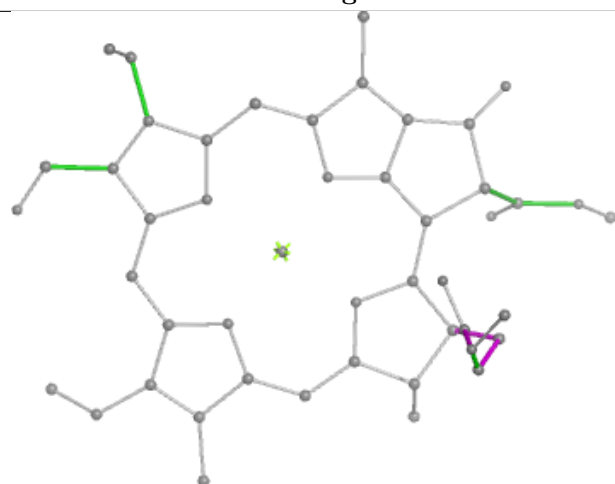
Ligand CHL 3 307



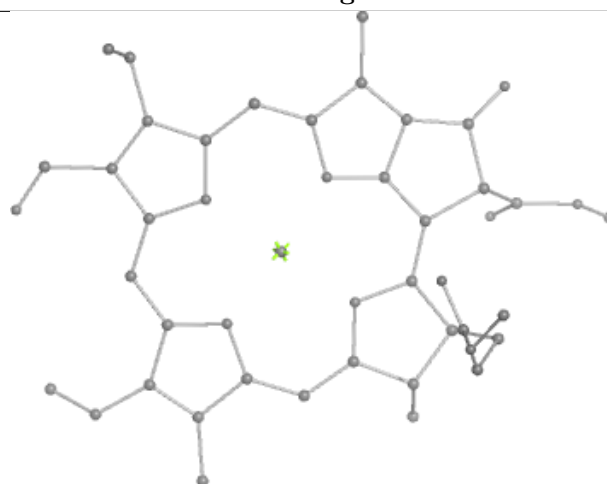
Bond lengths



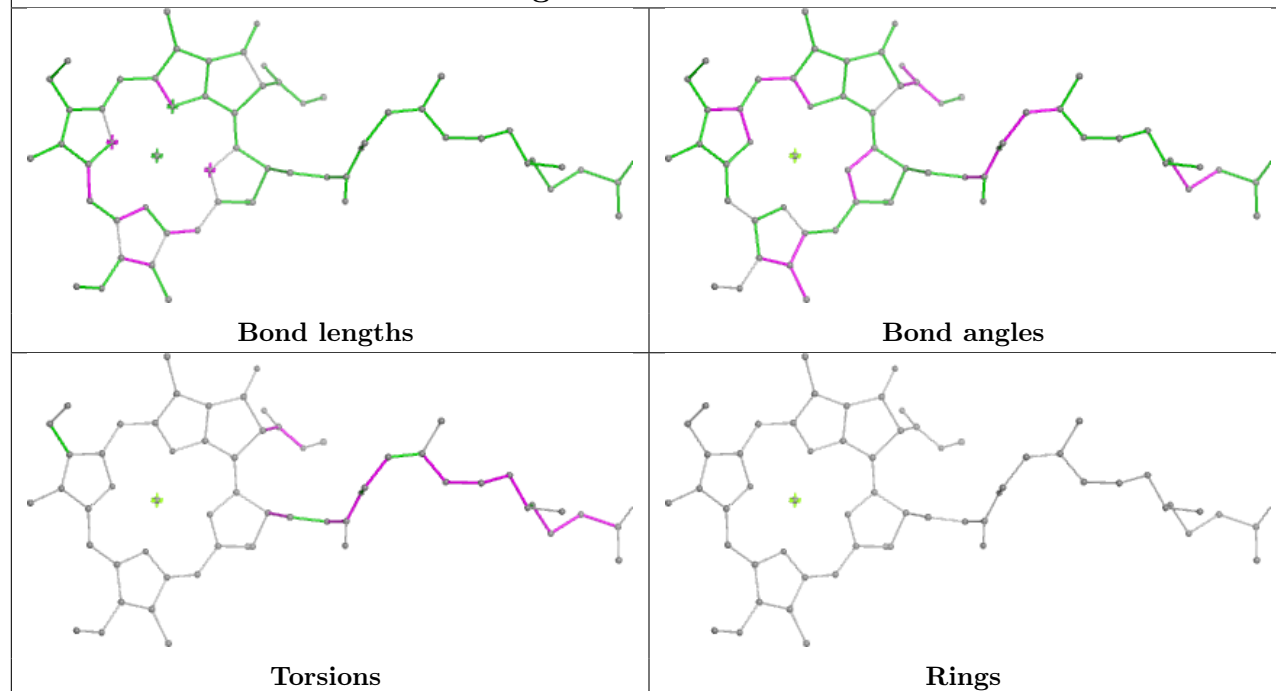
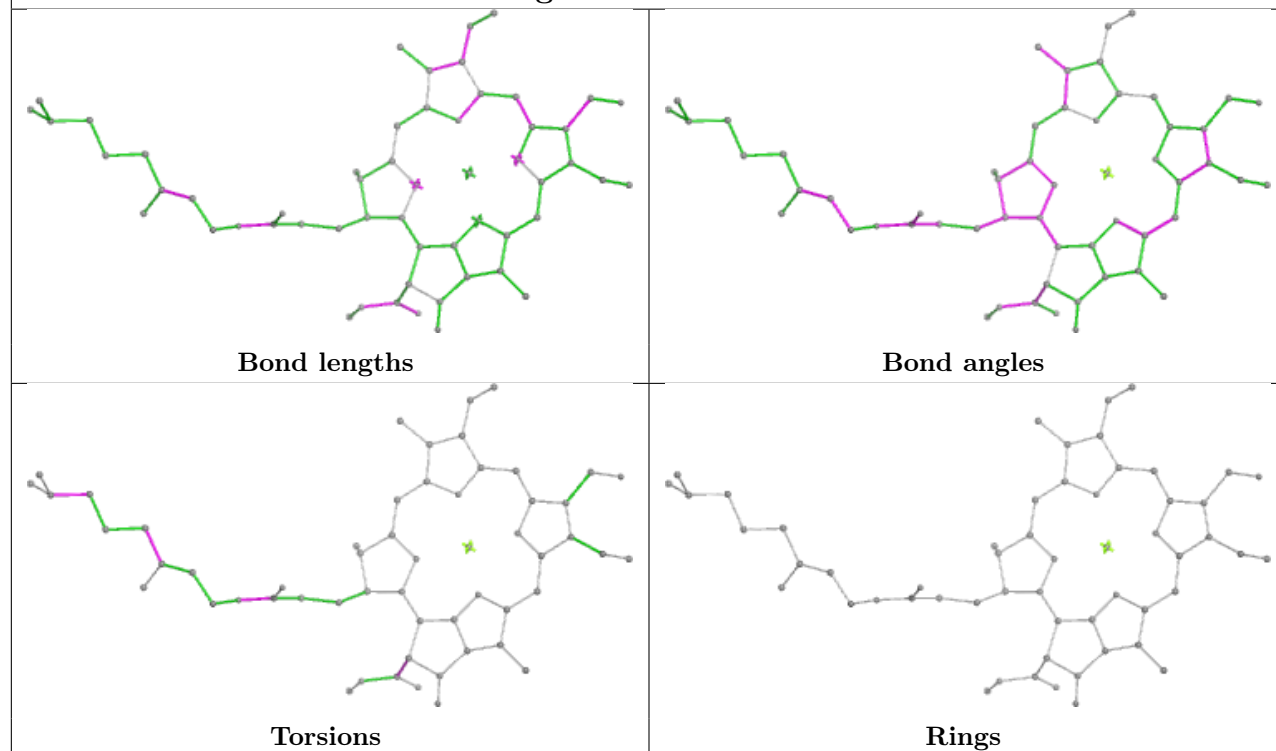
Bond angles

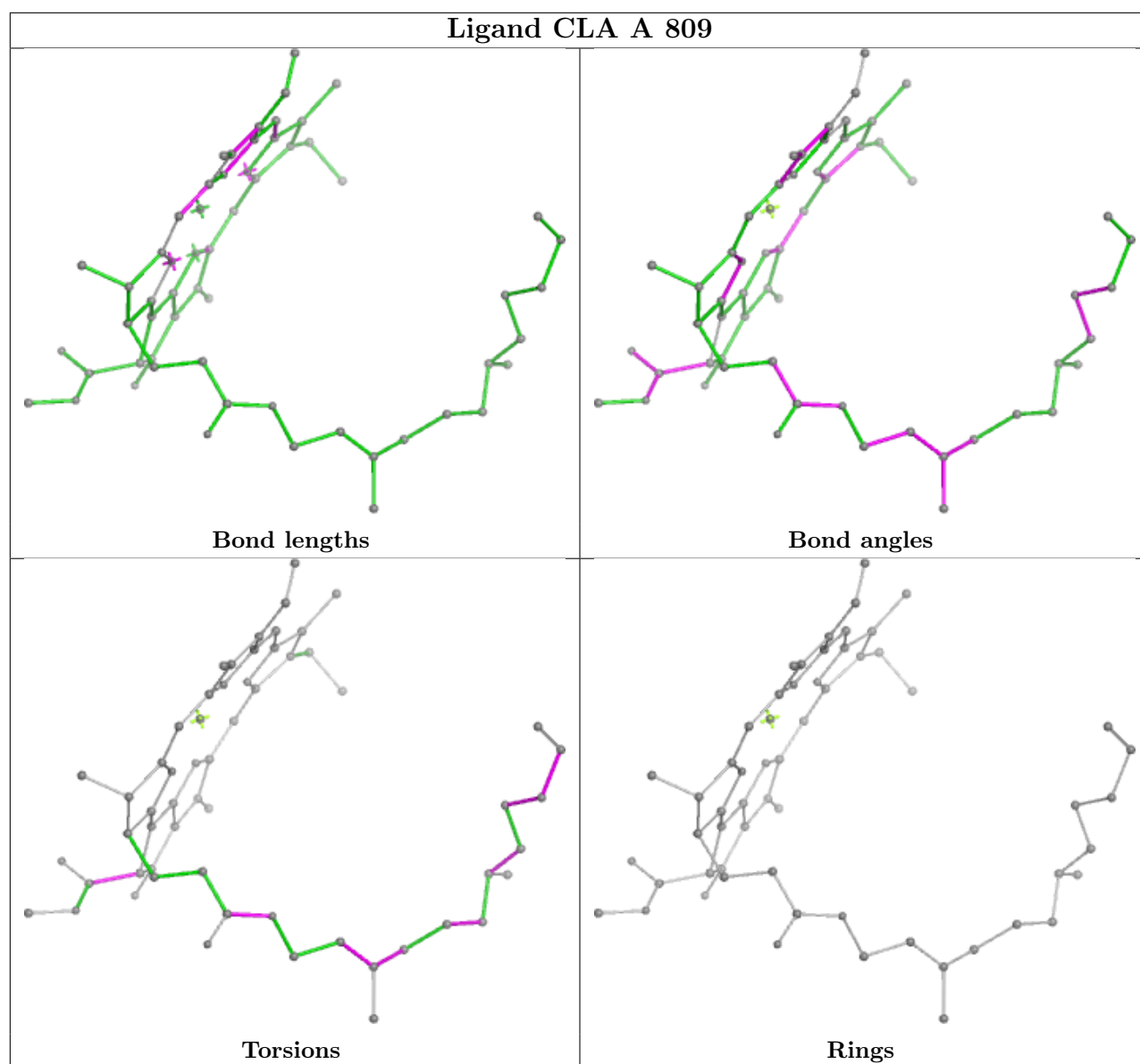


Torsions

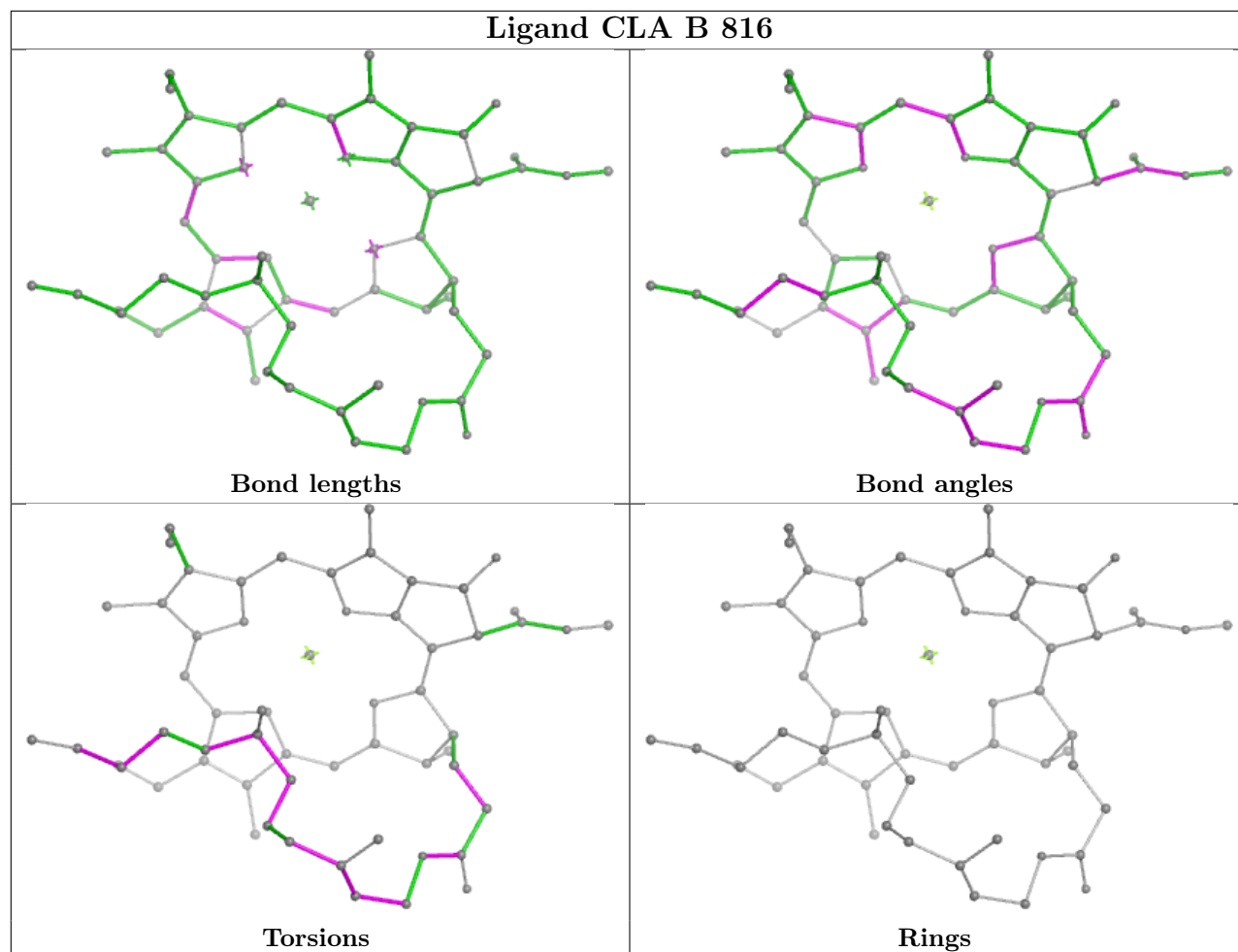


Rings

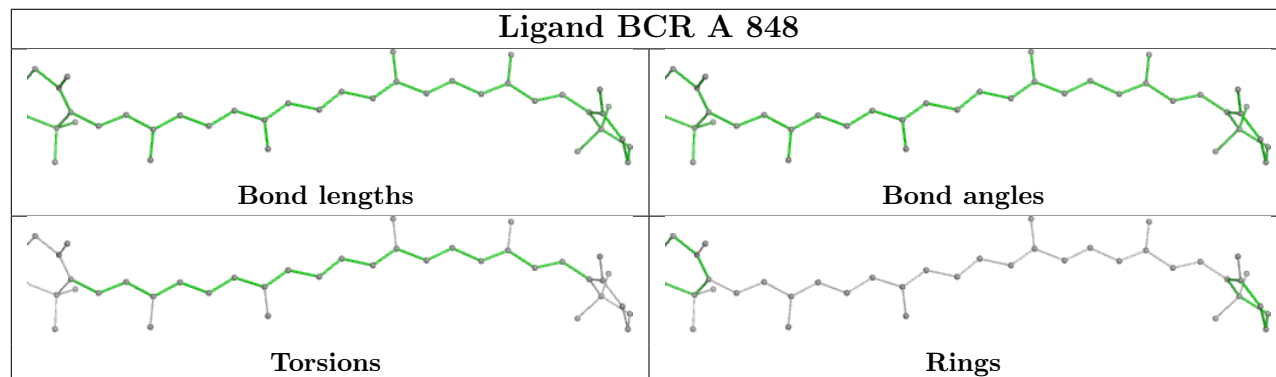
Ligand CLA B 822**Ligand CHL 4 304**

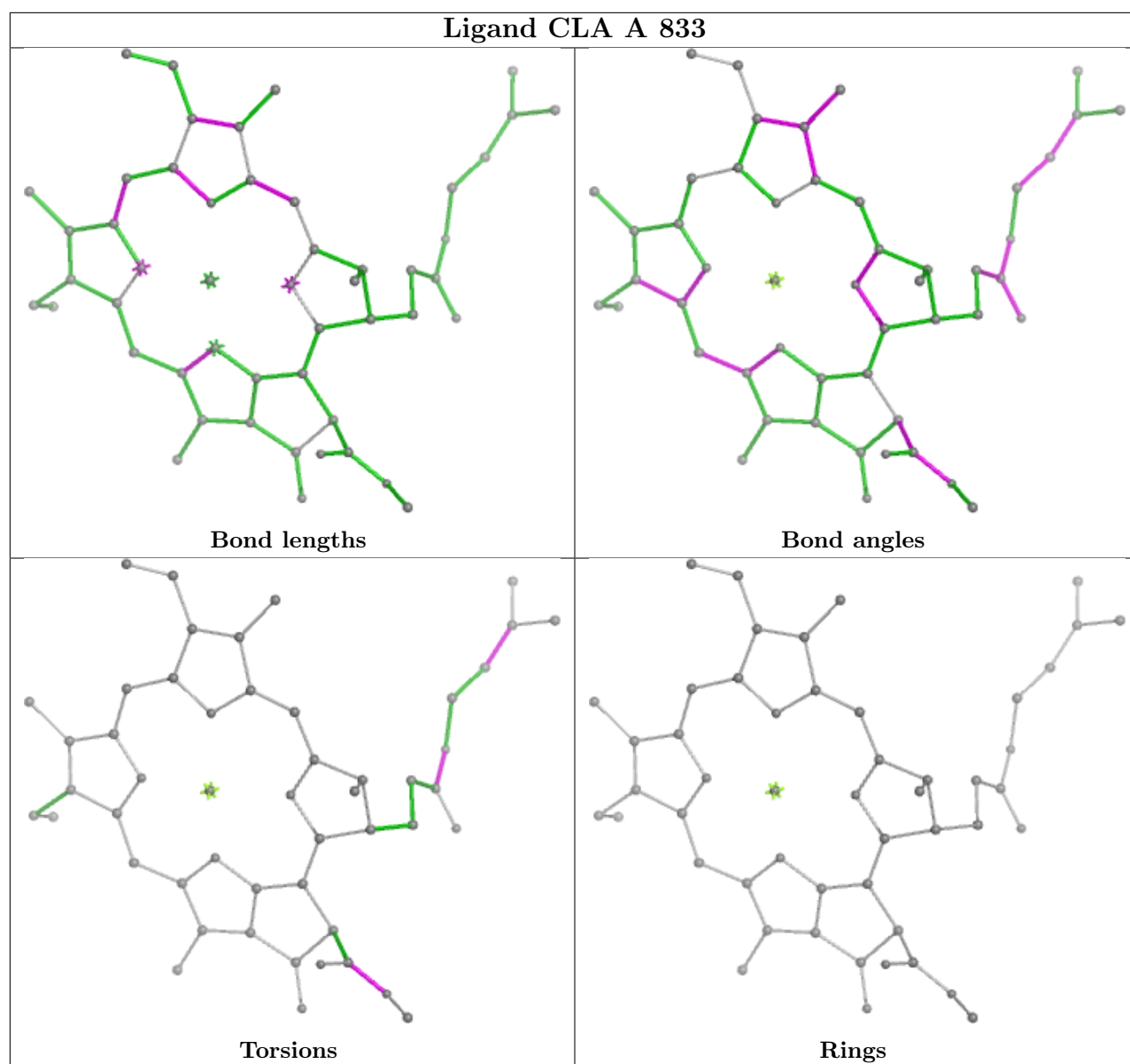


Ligand CLA B 816

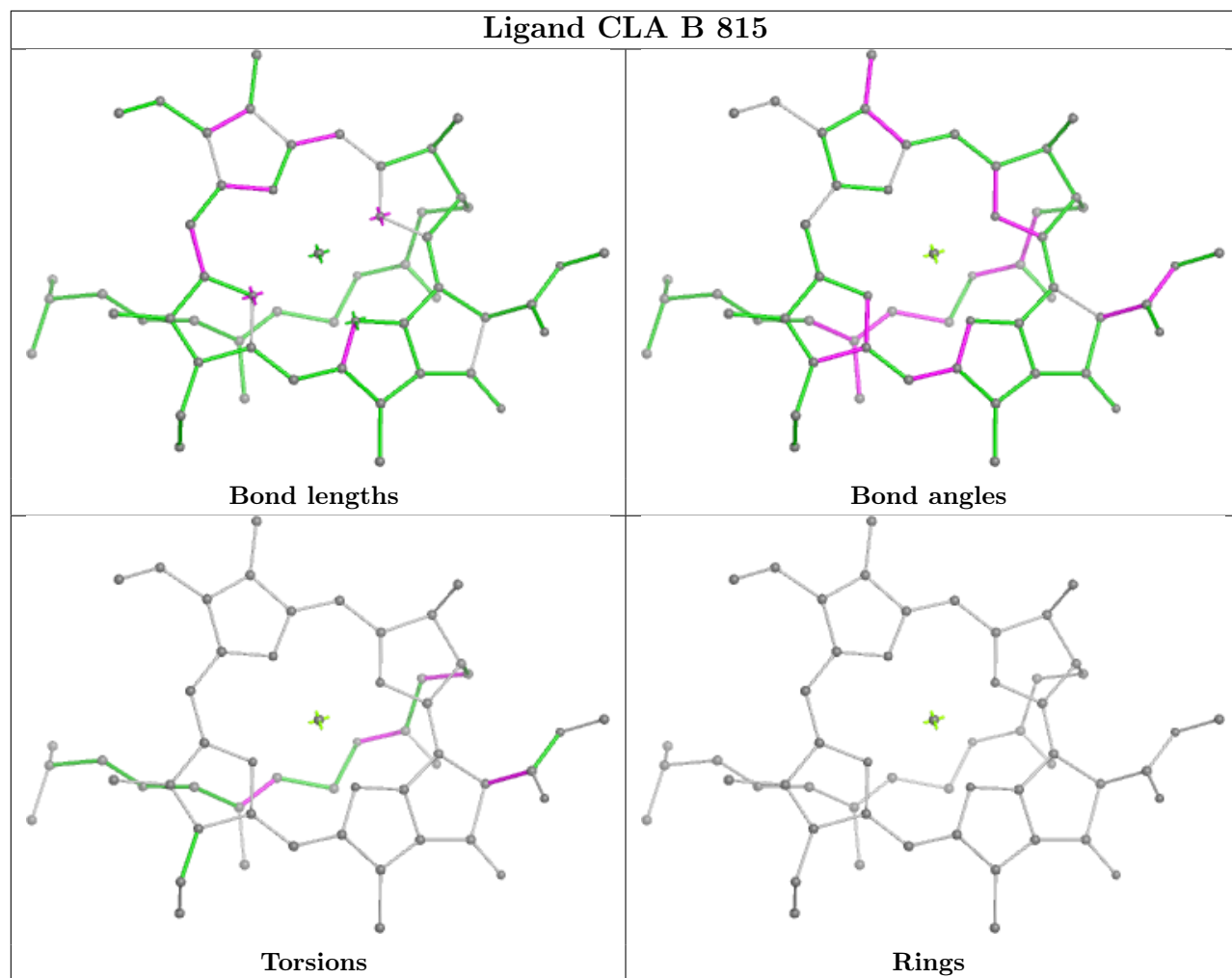


Ligand BCR A 848

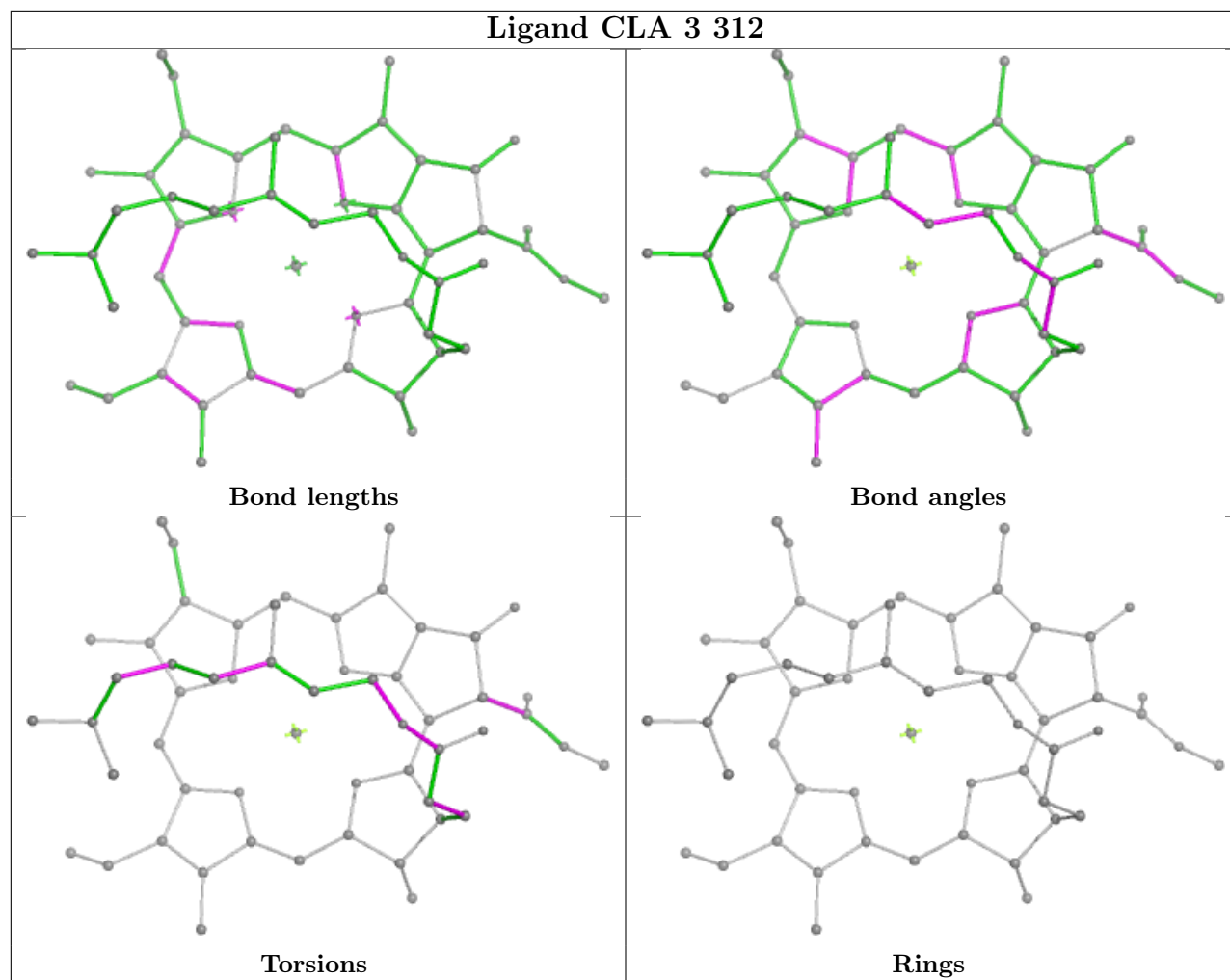




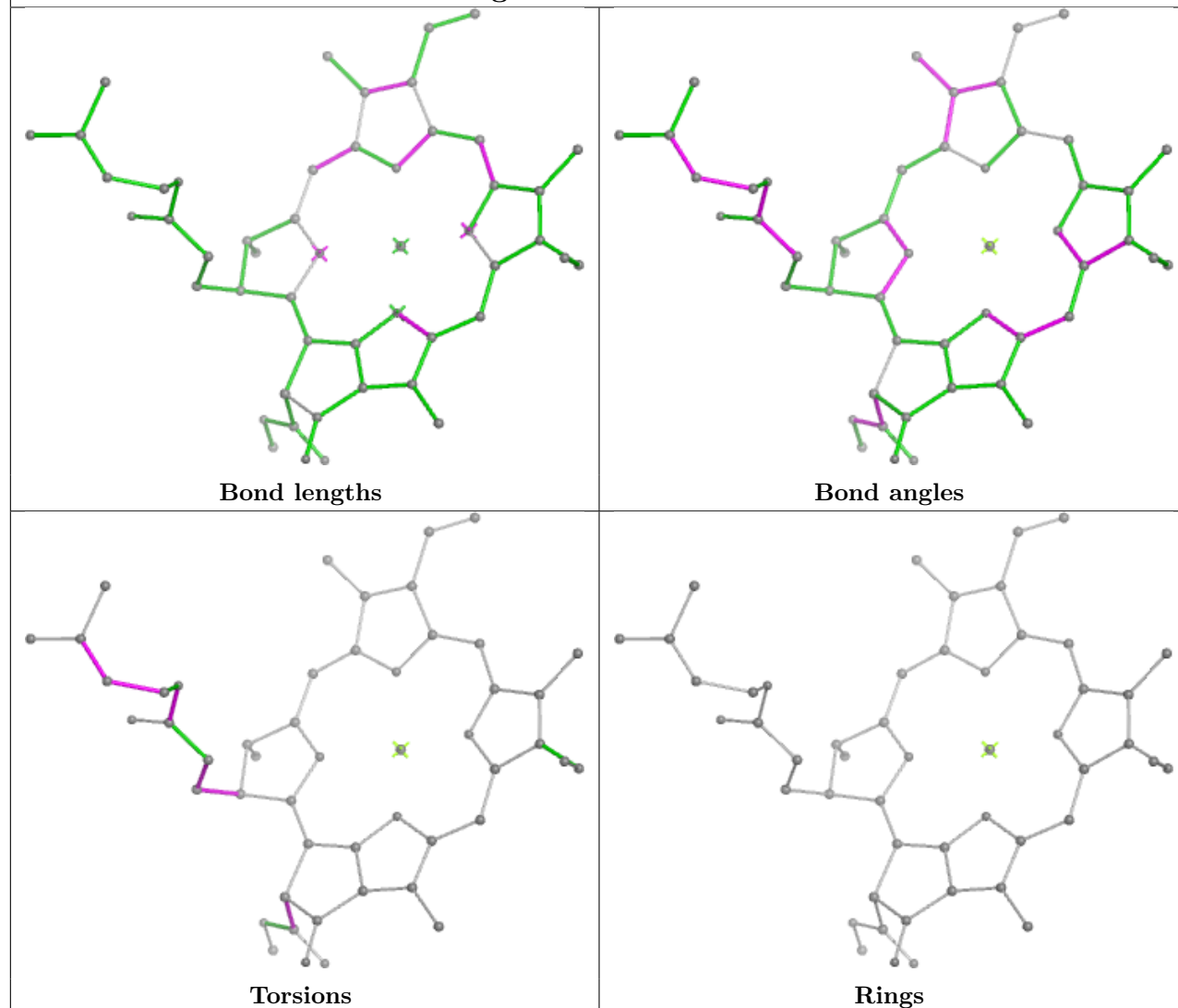
Ligand CLA B 815



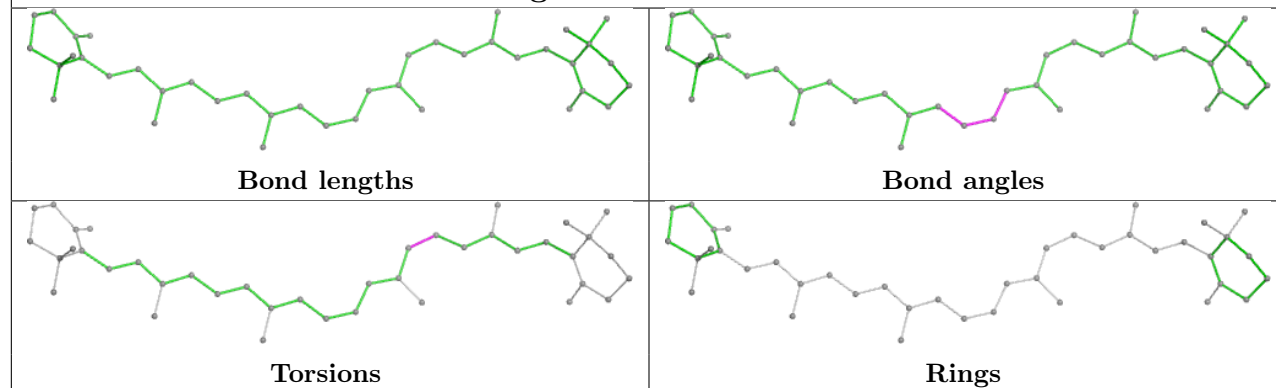
Ligand CLA 3 312

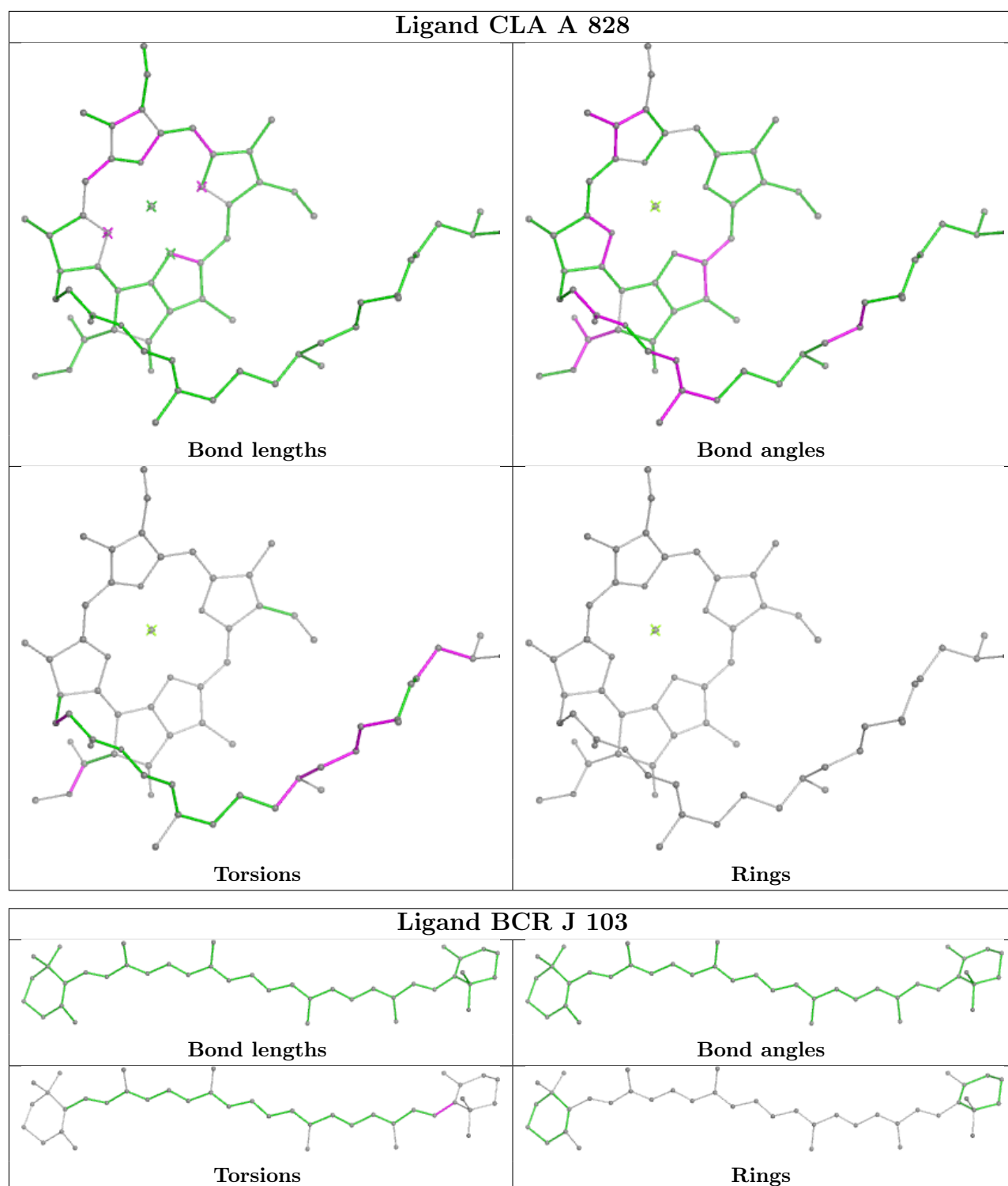


Ligand CLA B 819

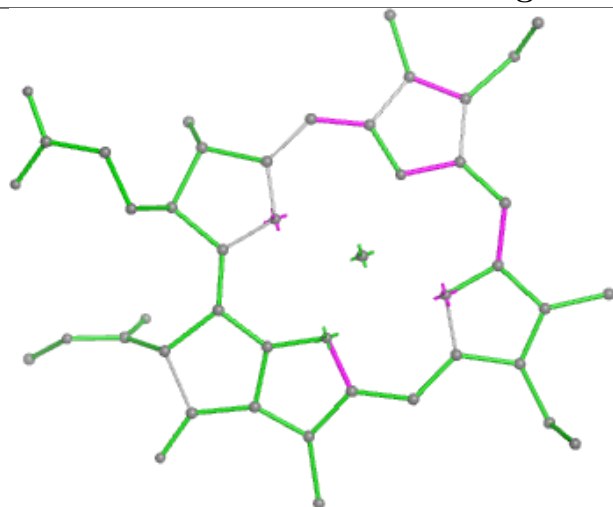


Ligand BCR A 844

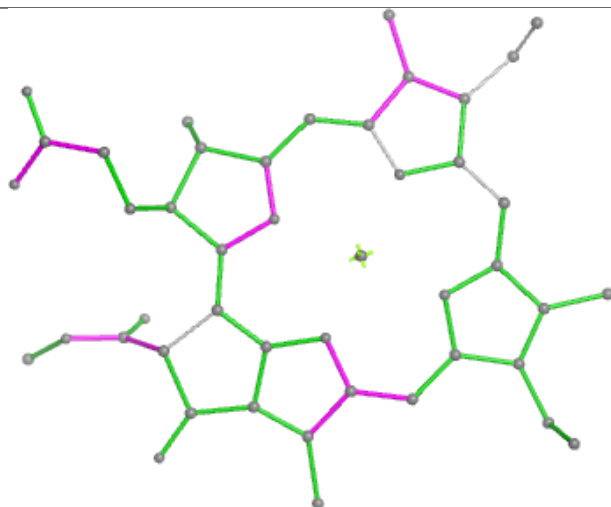




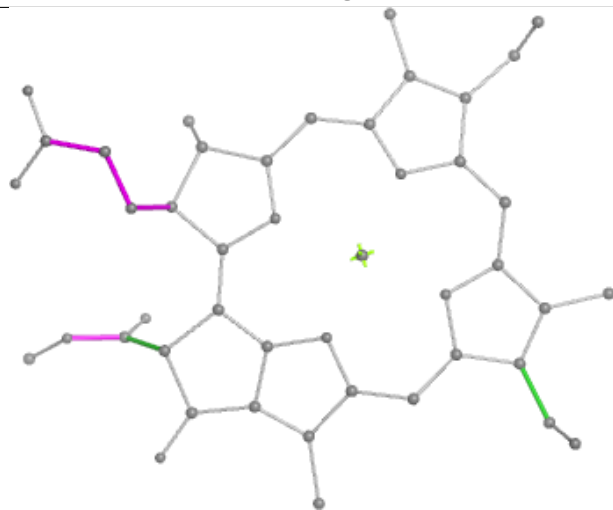
Ligand CLA F 304



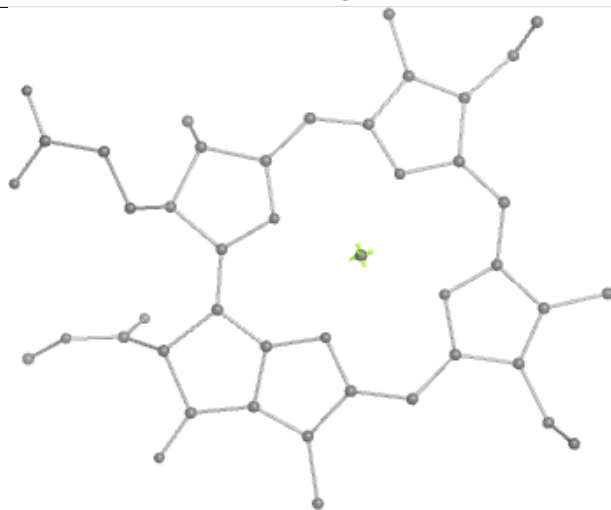
Bond lengths



Bond angles

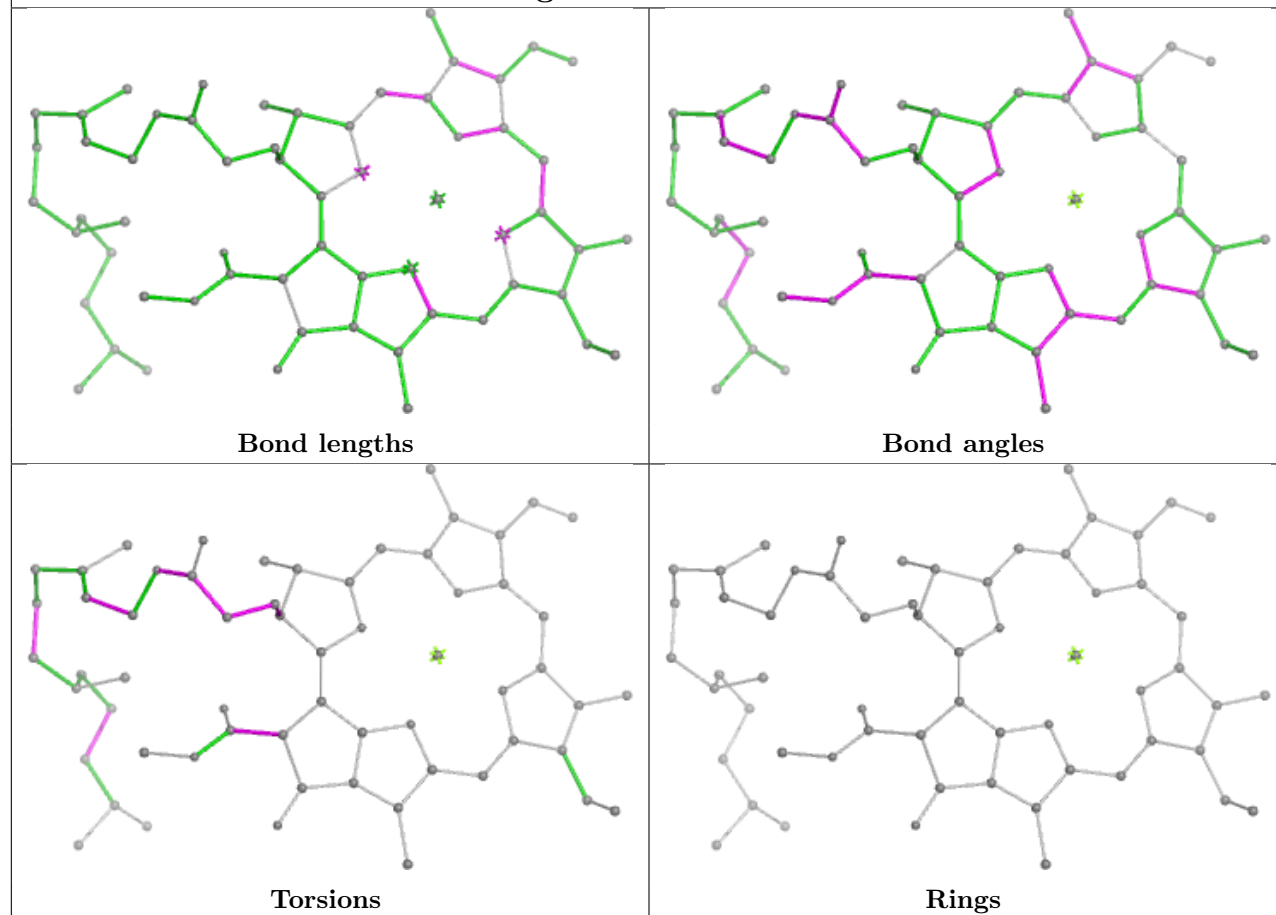


Torsions

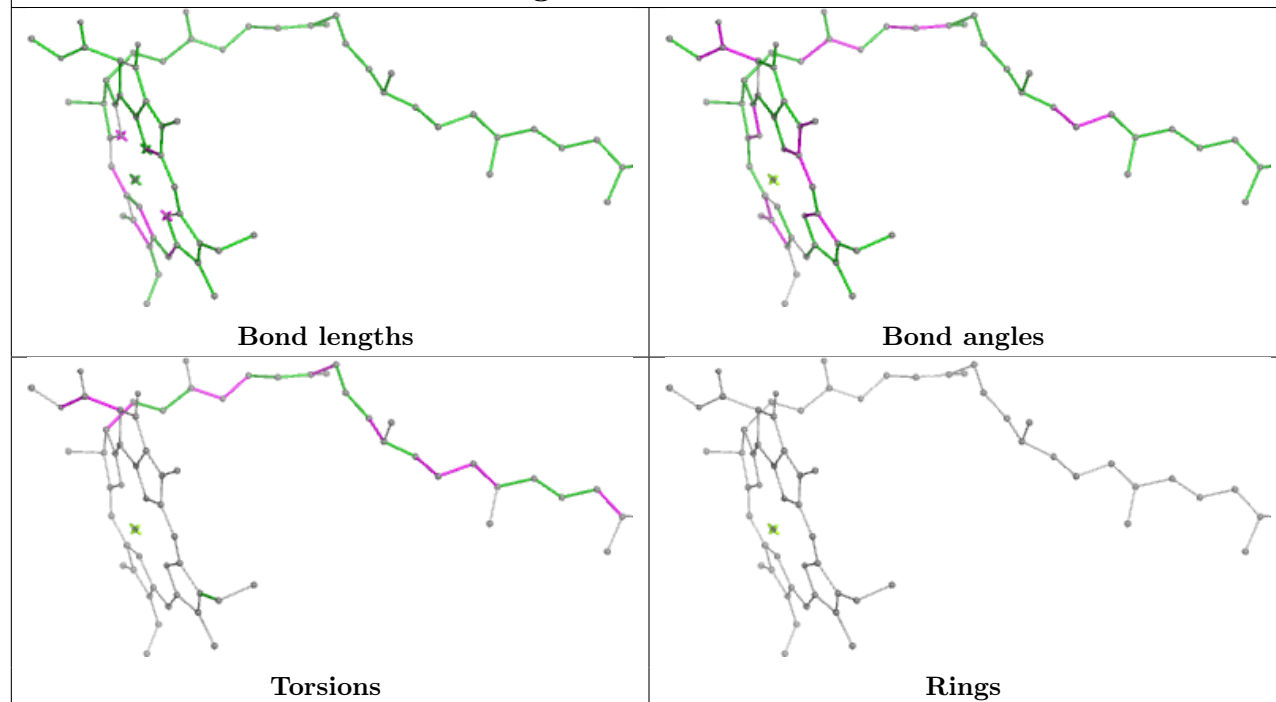


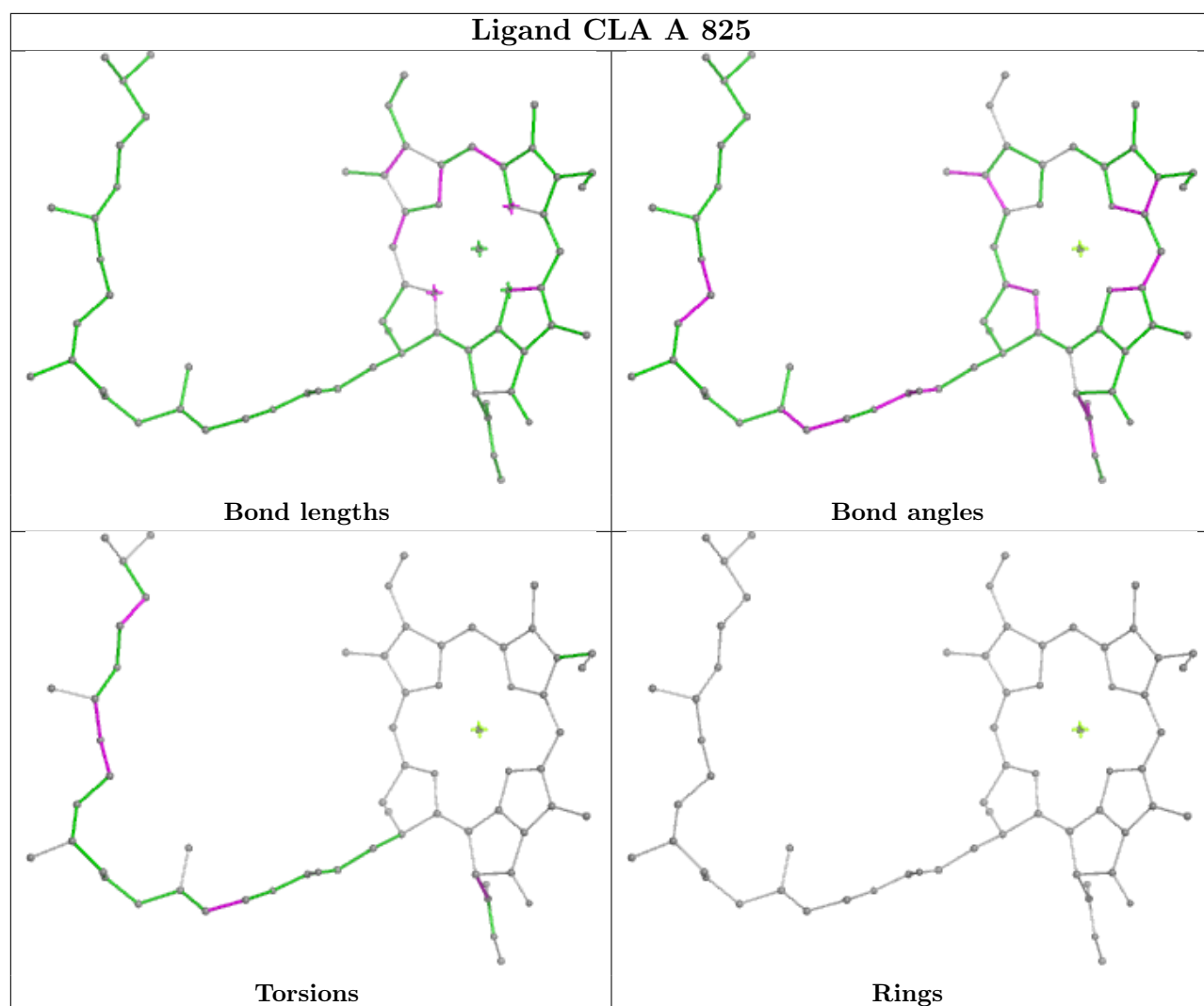
Rings

Ligand CLA 3 302

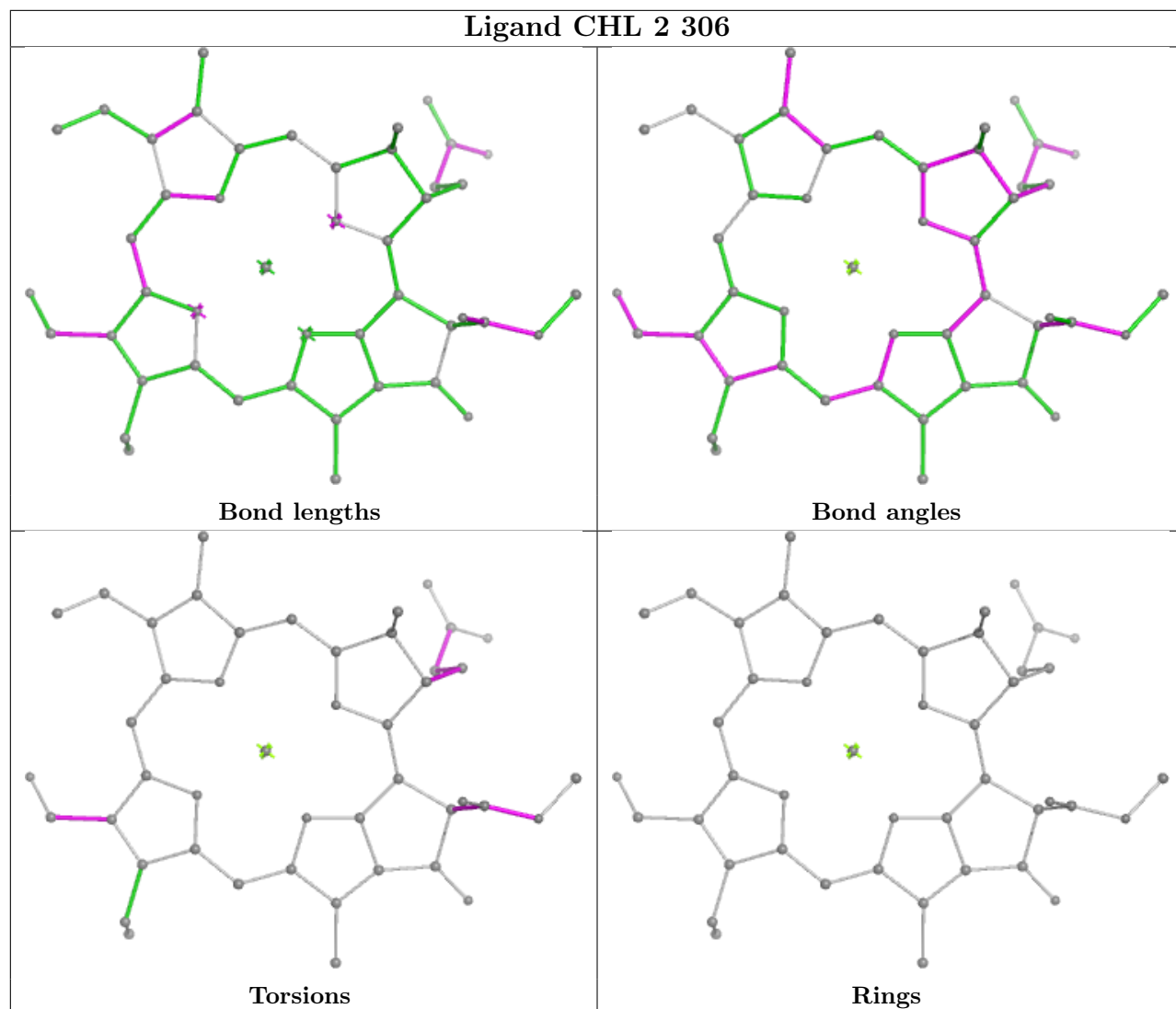


Ligand CLA B 828

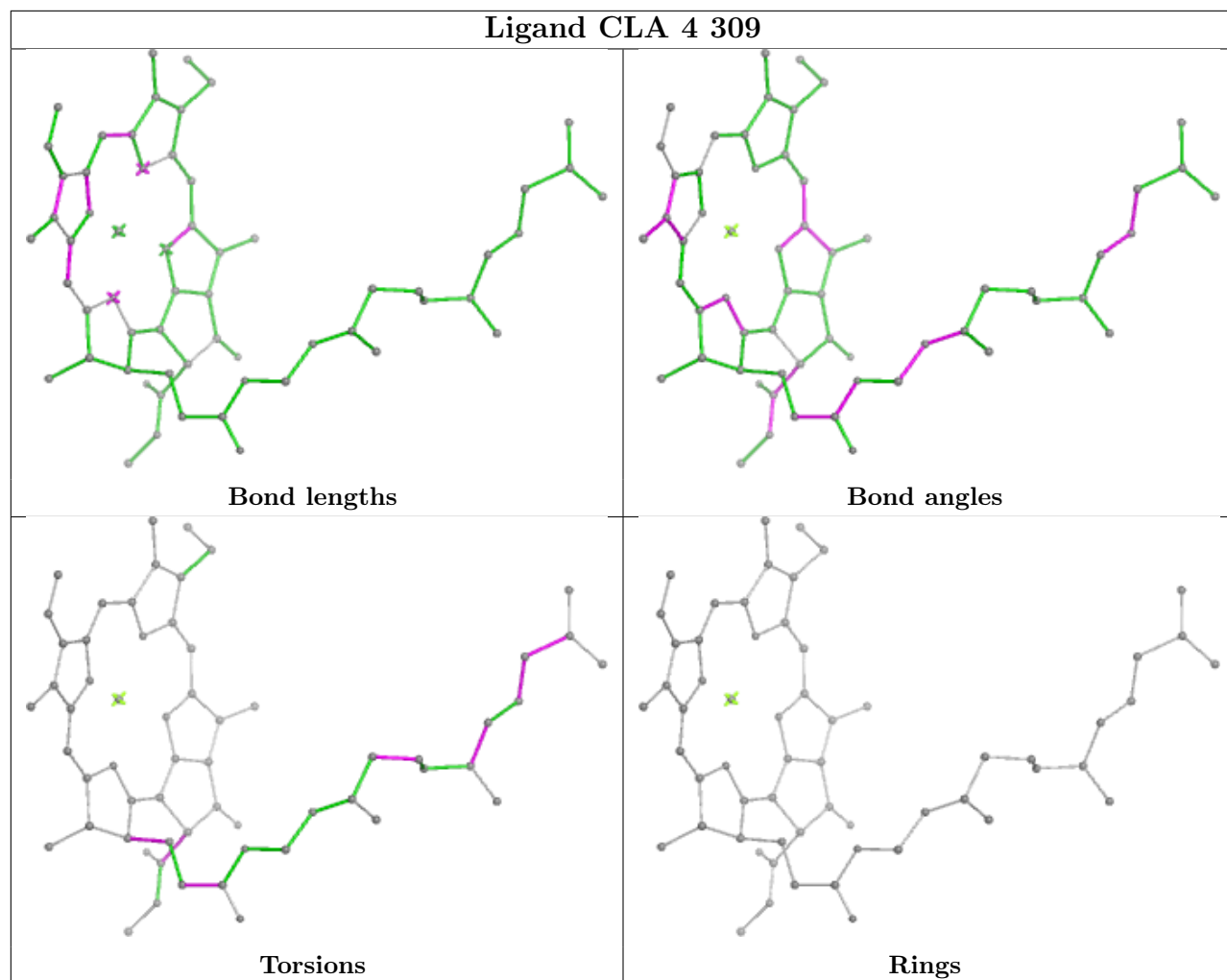




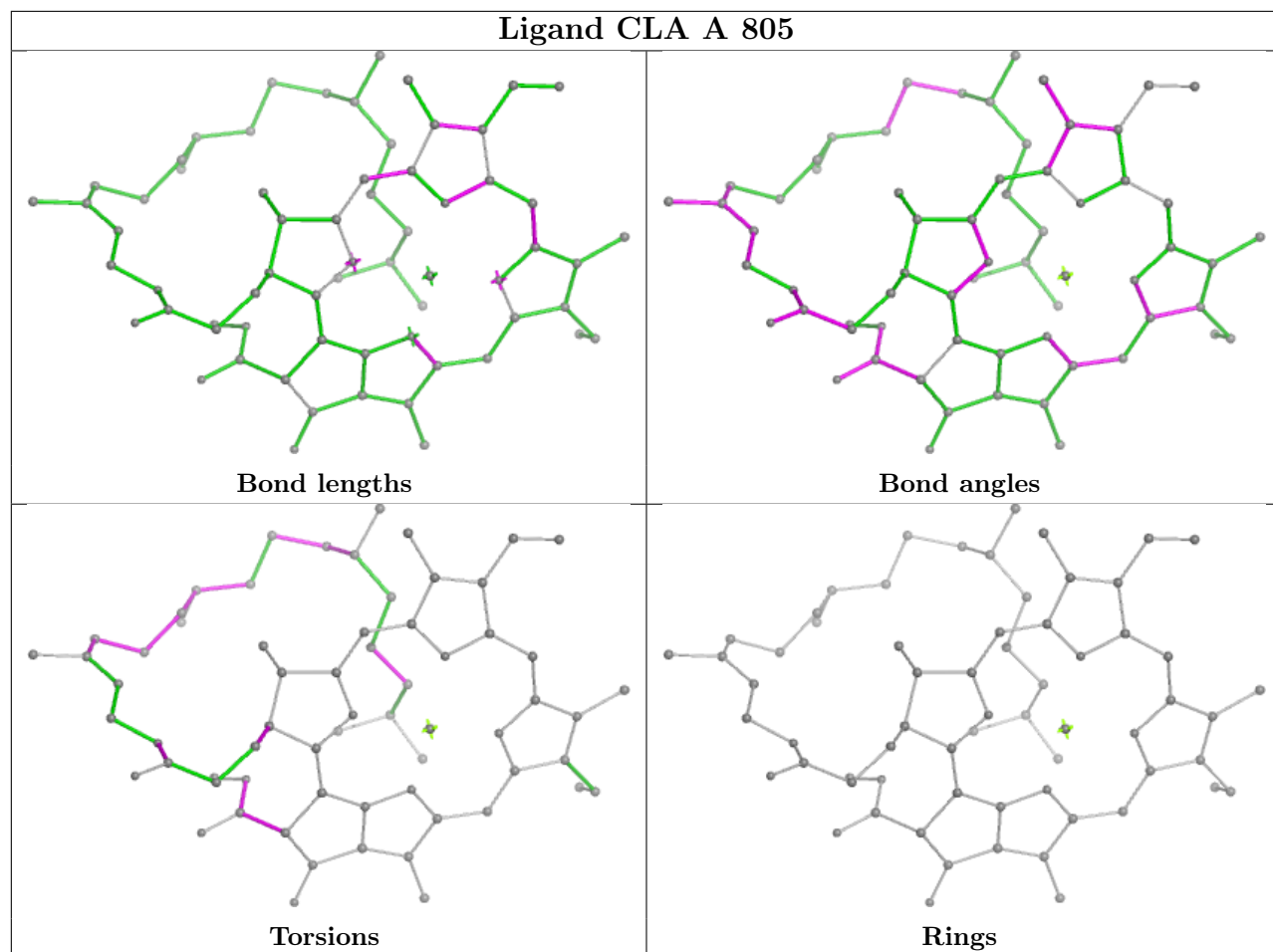
Ligand CHL 2 306



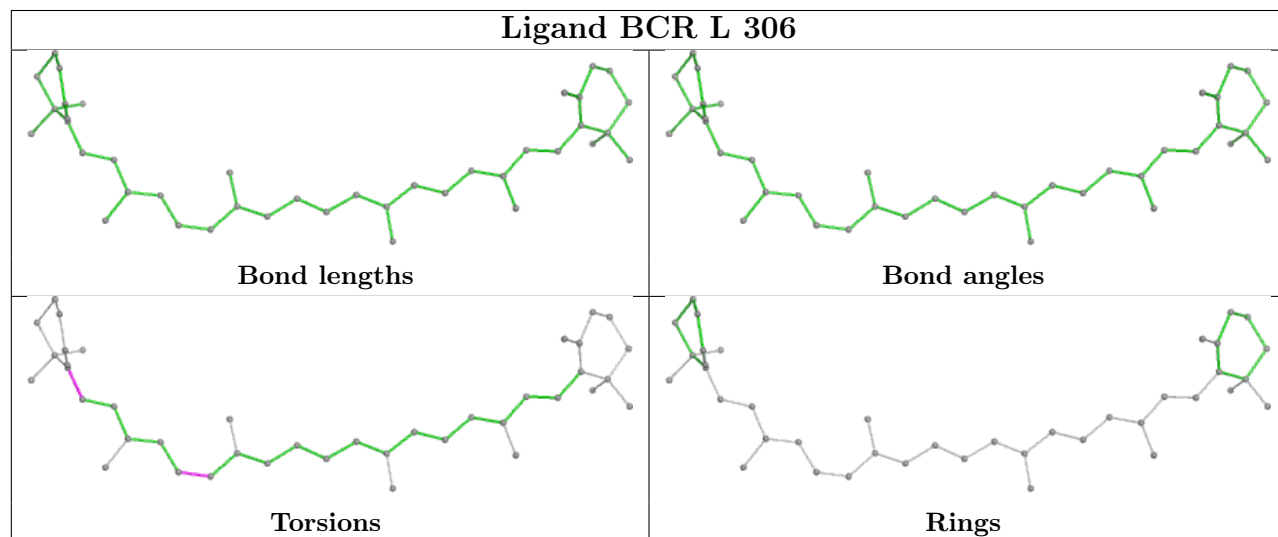
Ligand CLA 4 309

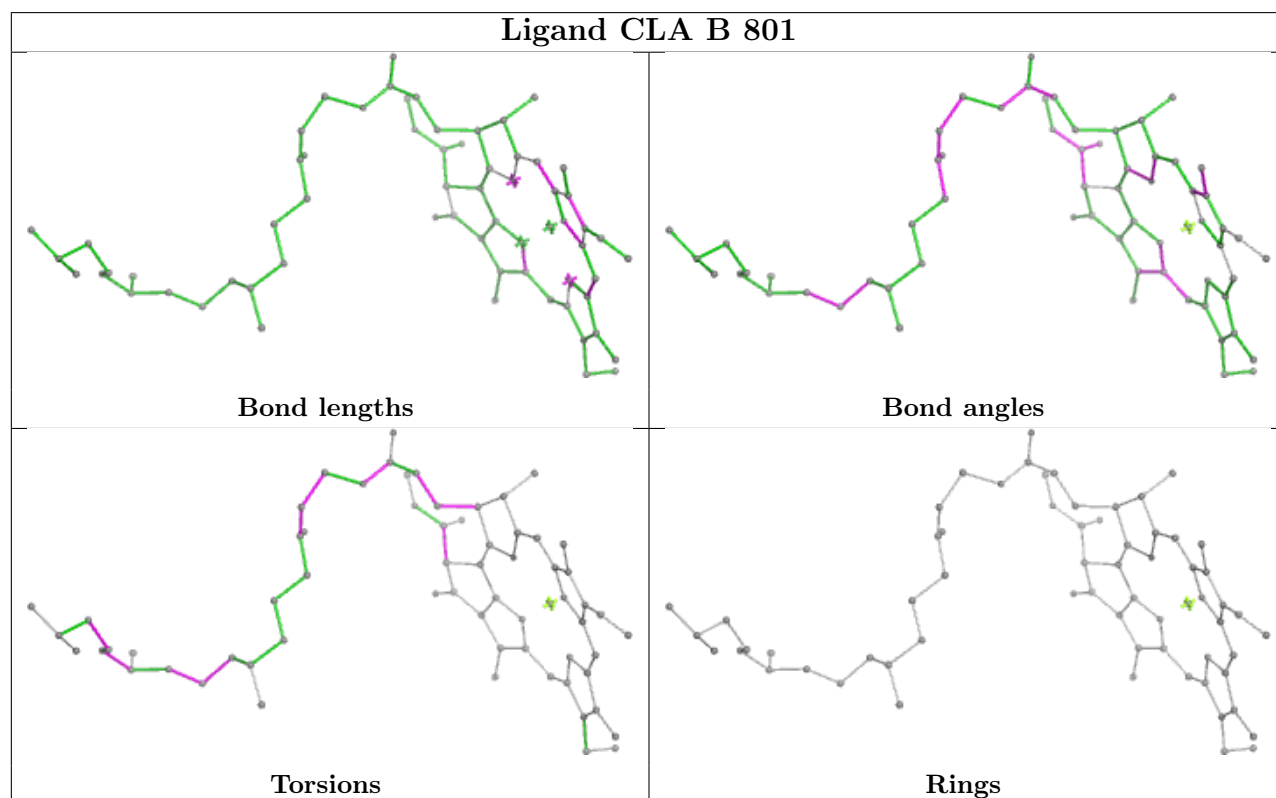
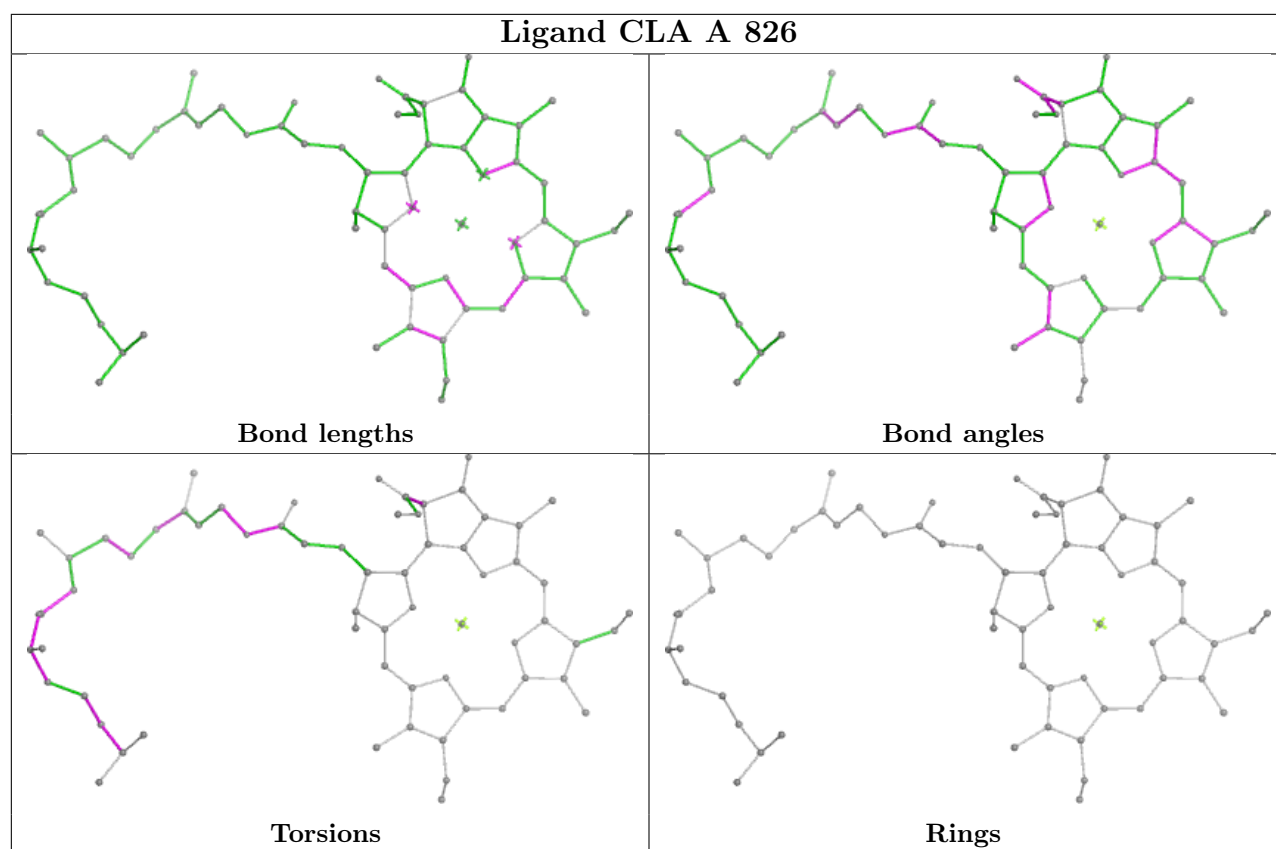


Ligand CLA A 805

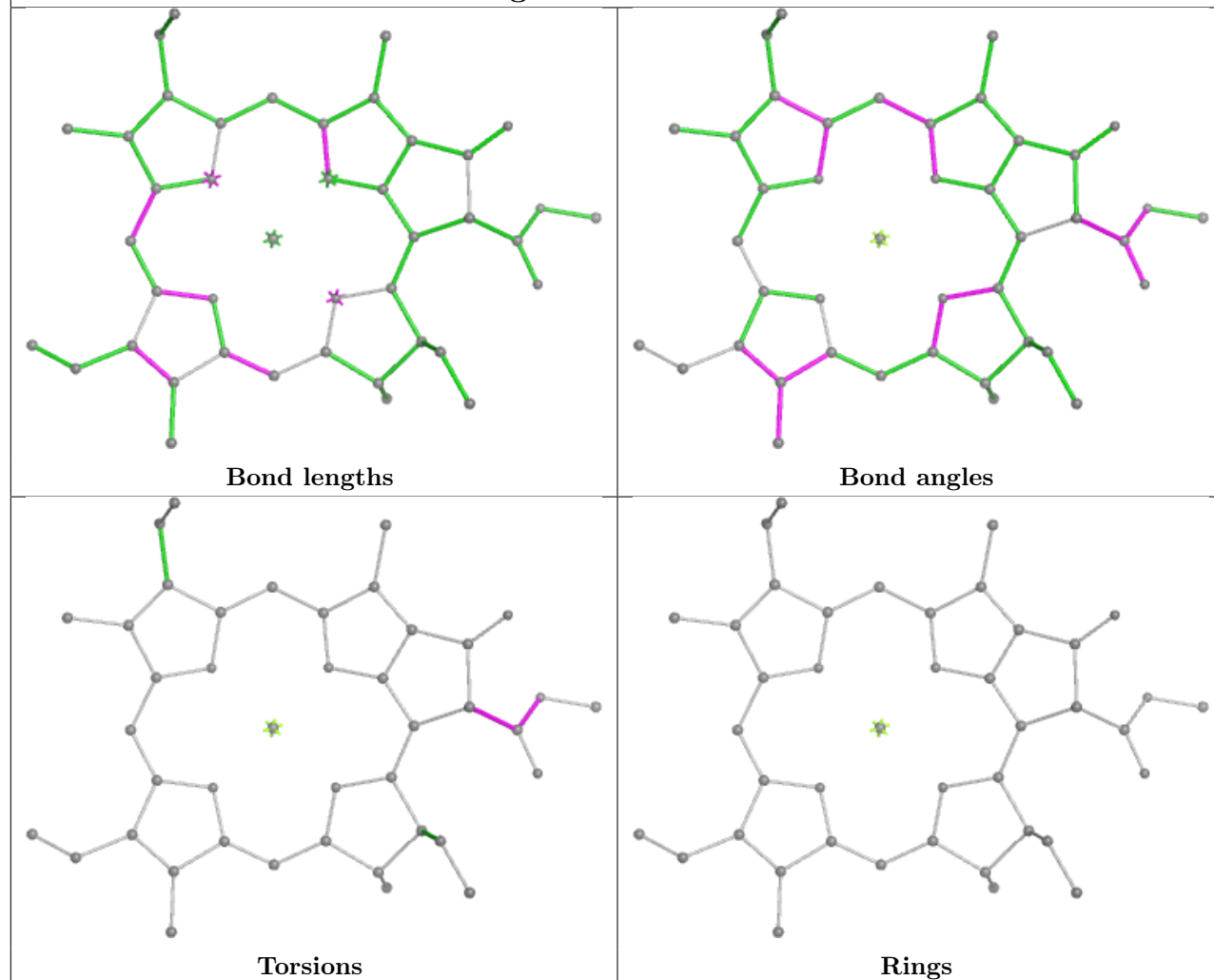


Ligand BCR L 306

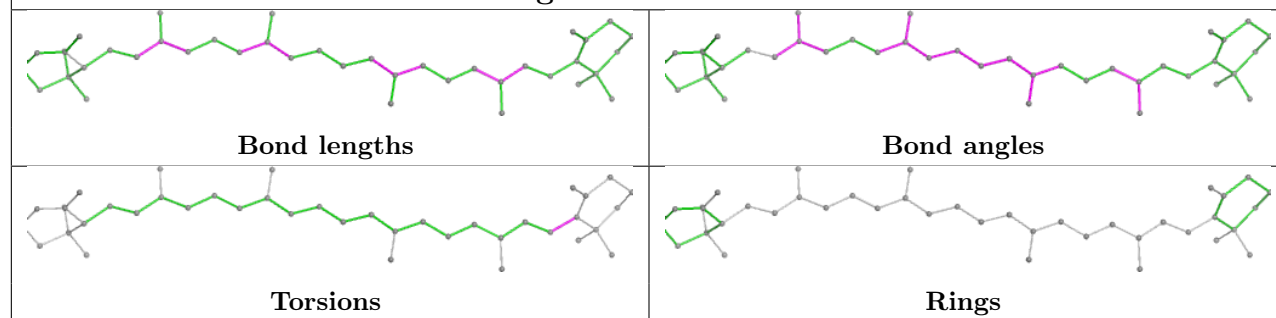


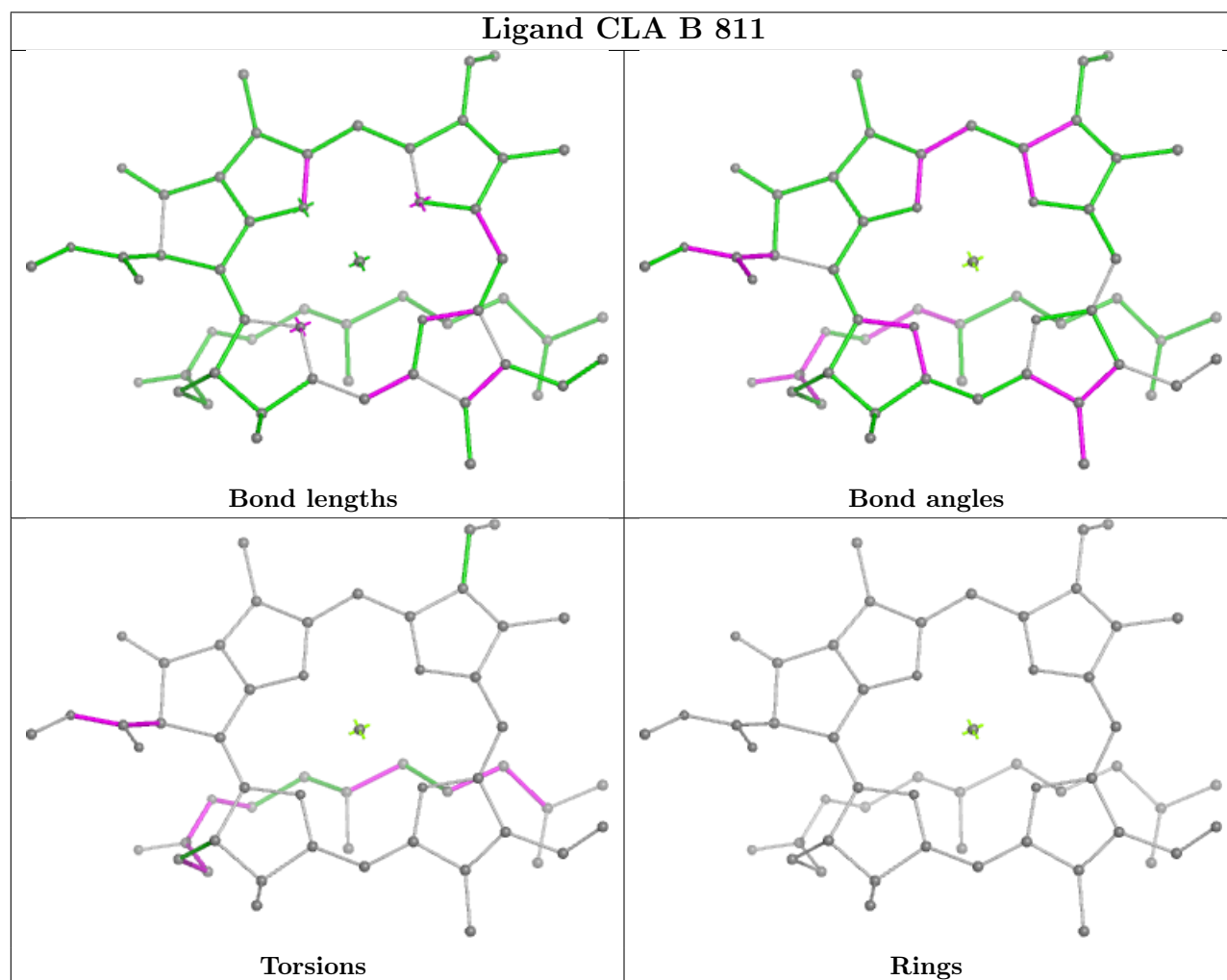
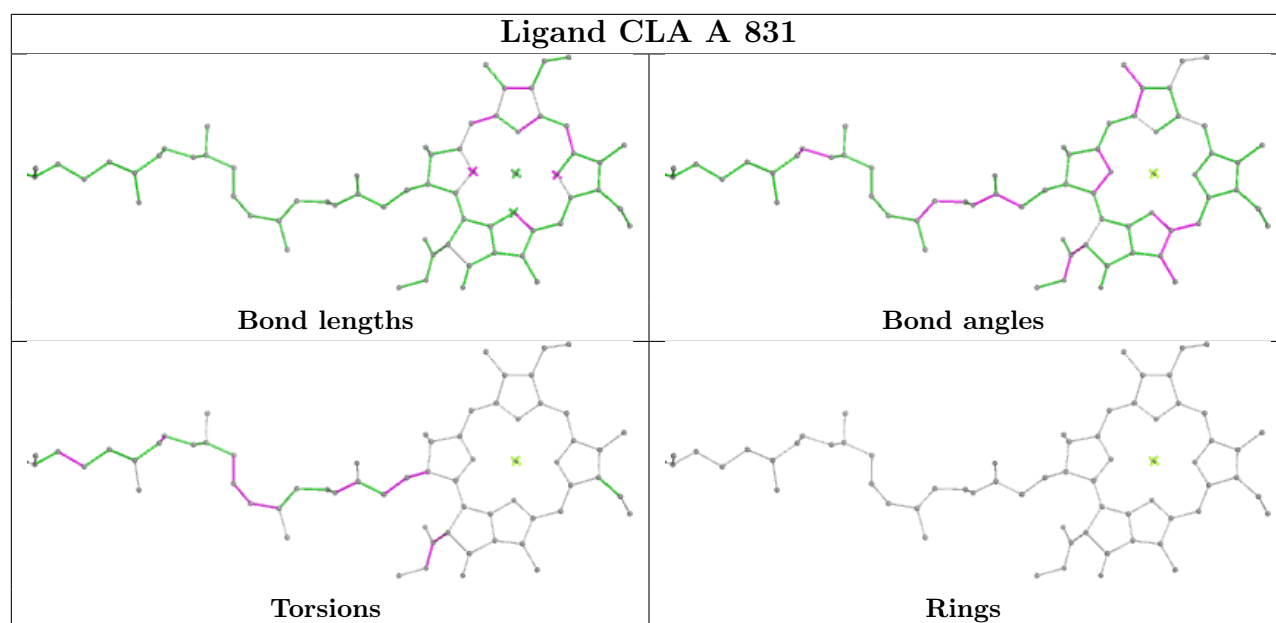


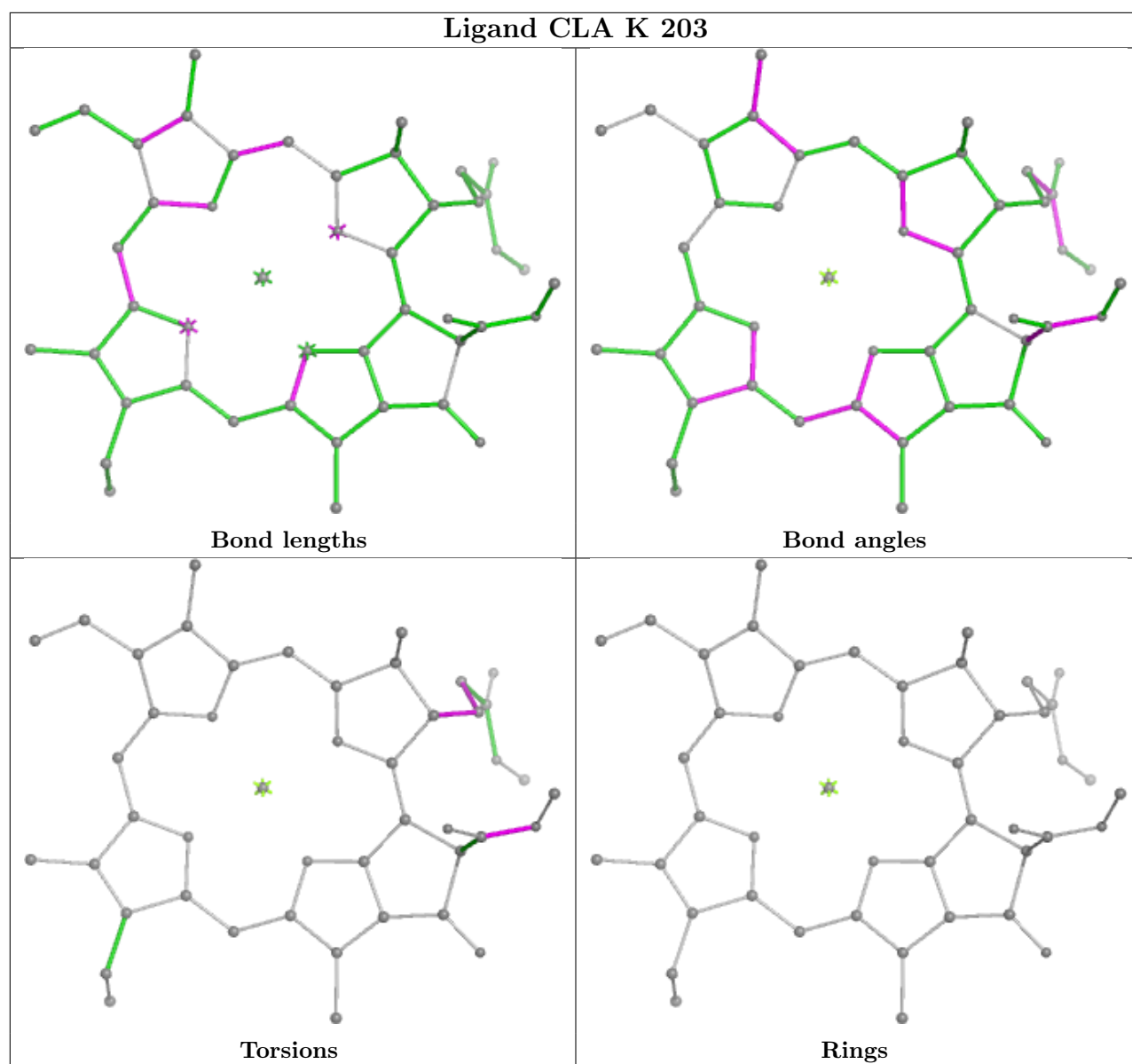
Ligand CLA J 102



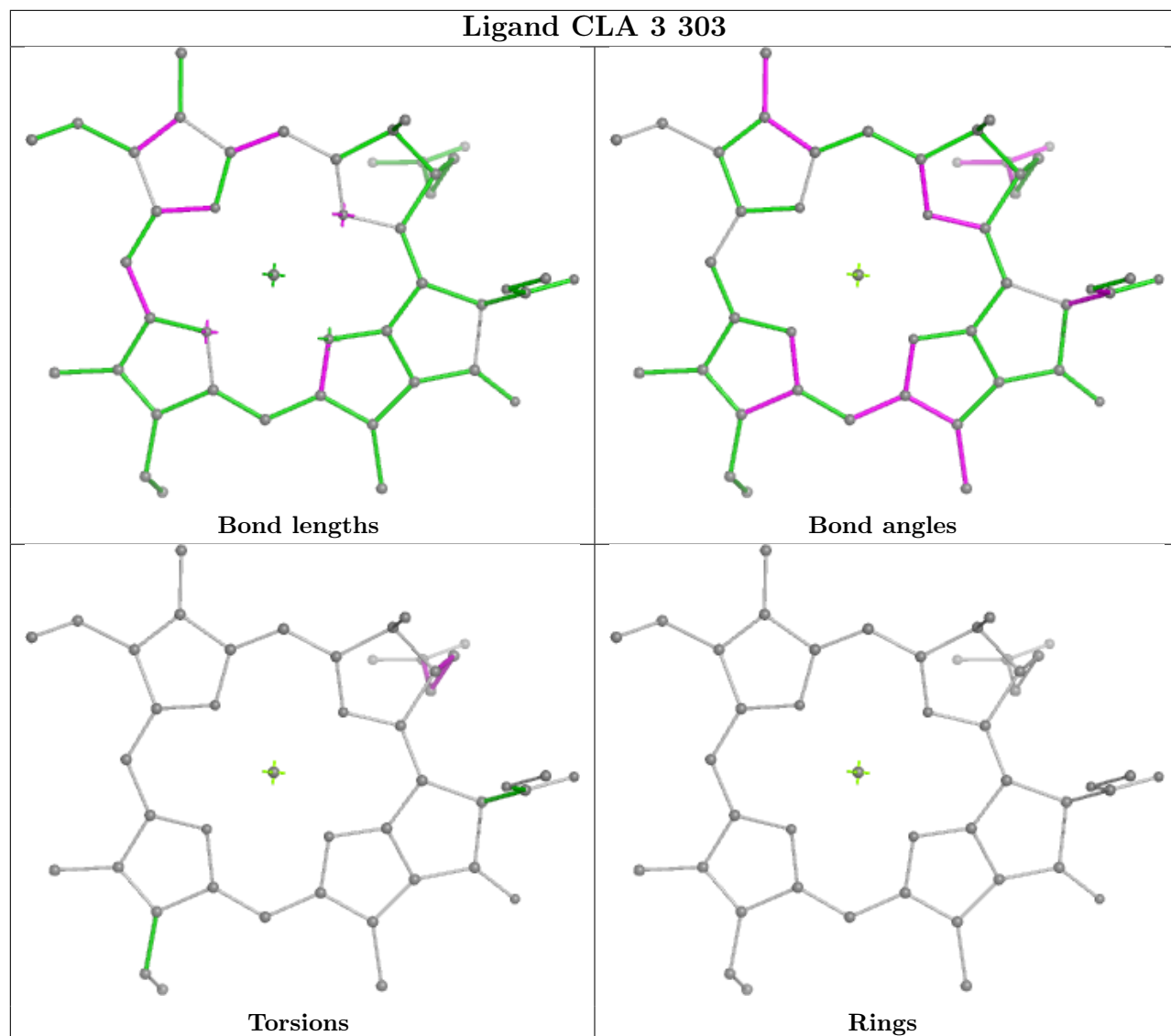
Ligand LUT 4 315

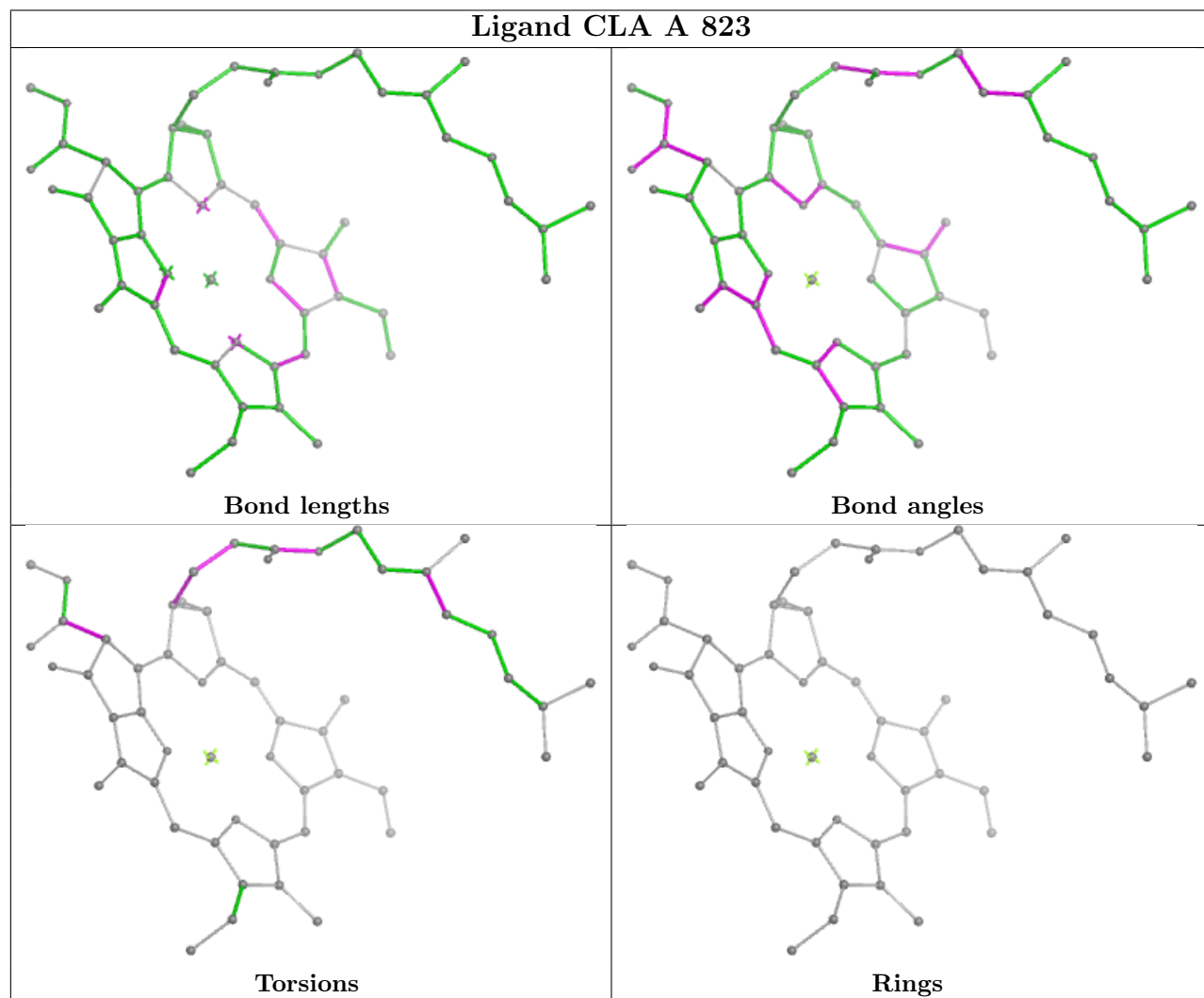
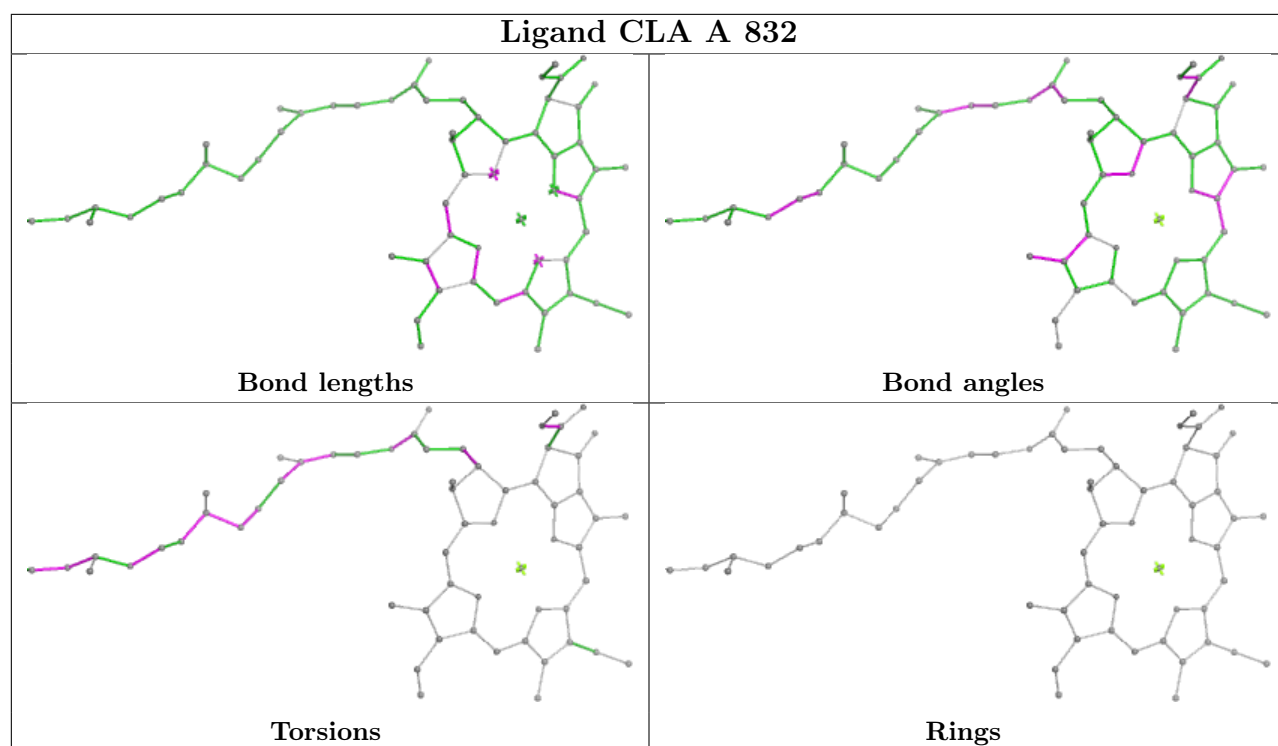




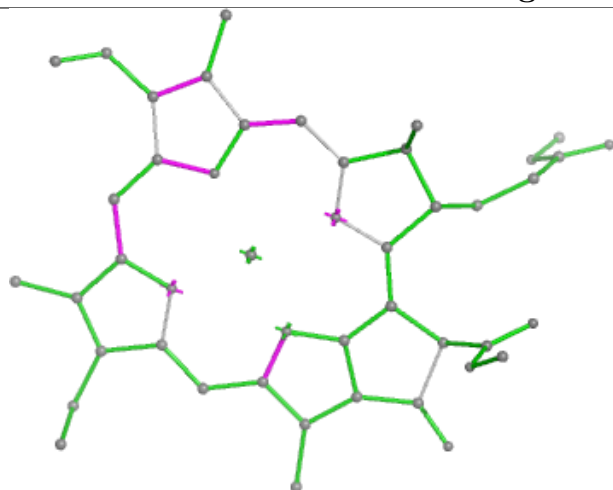


Ligand CLA 3 303

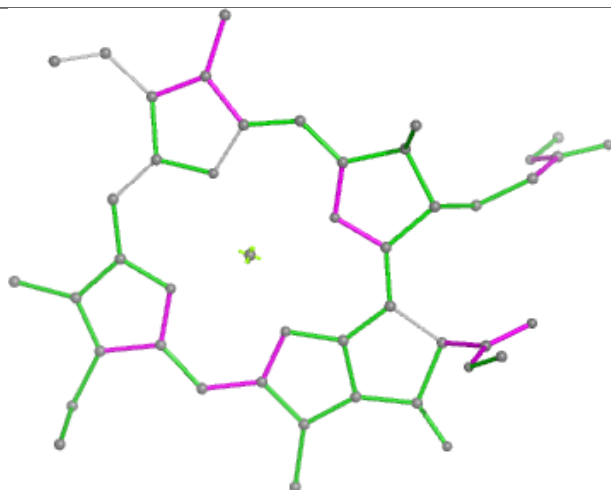




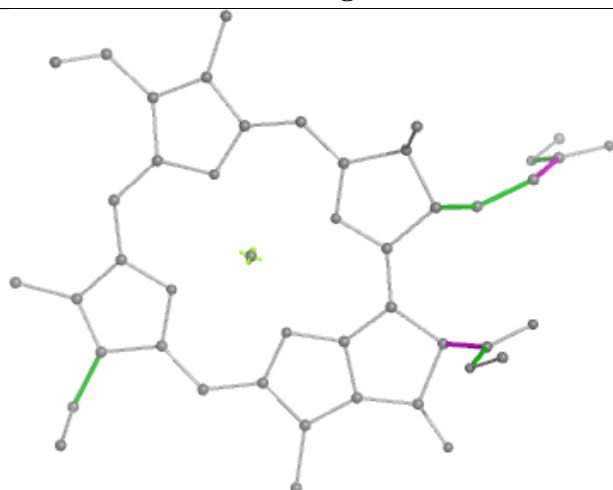
Ligand CLA 2 320



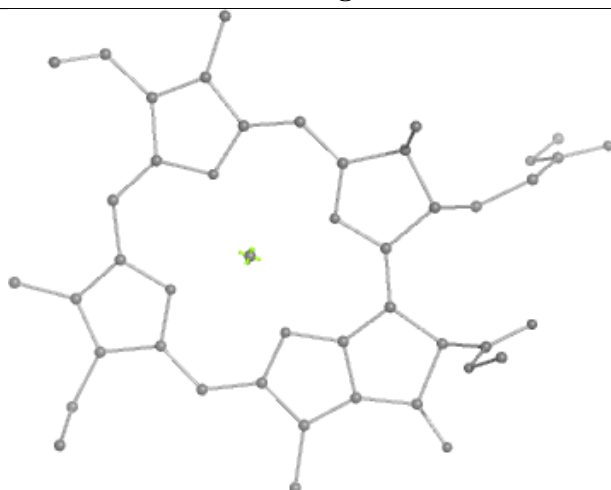
Bond lengths



Bond angles

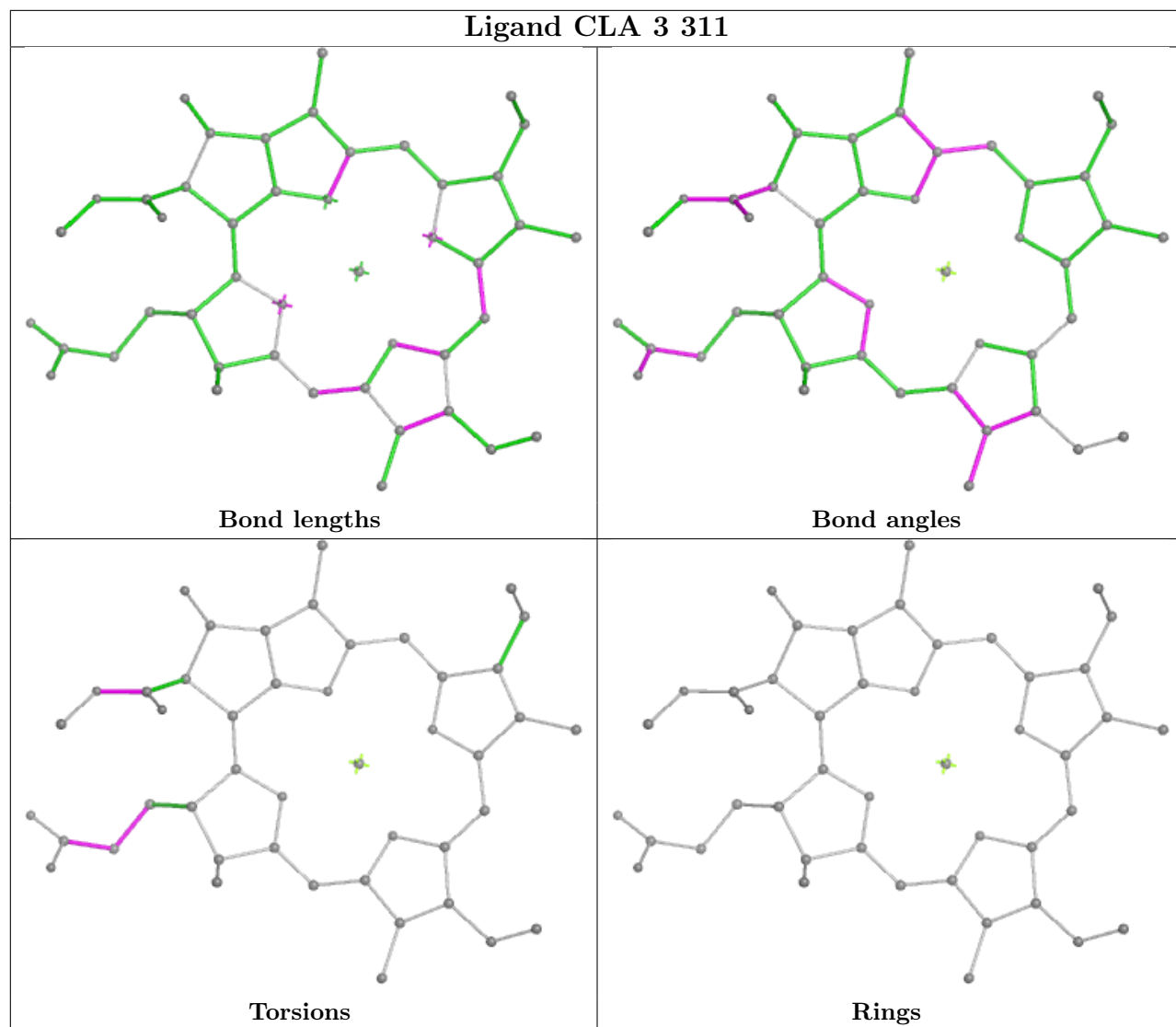


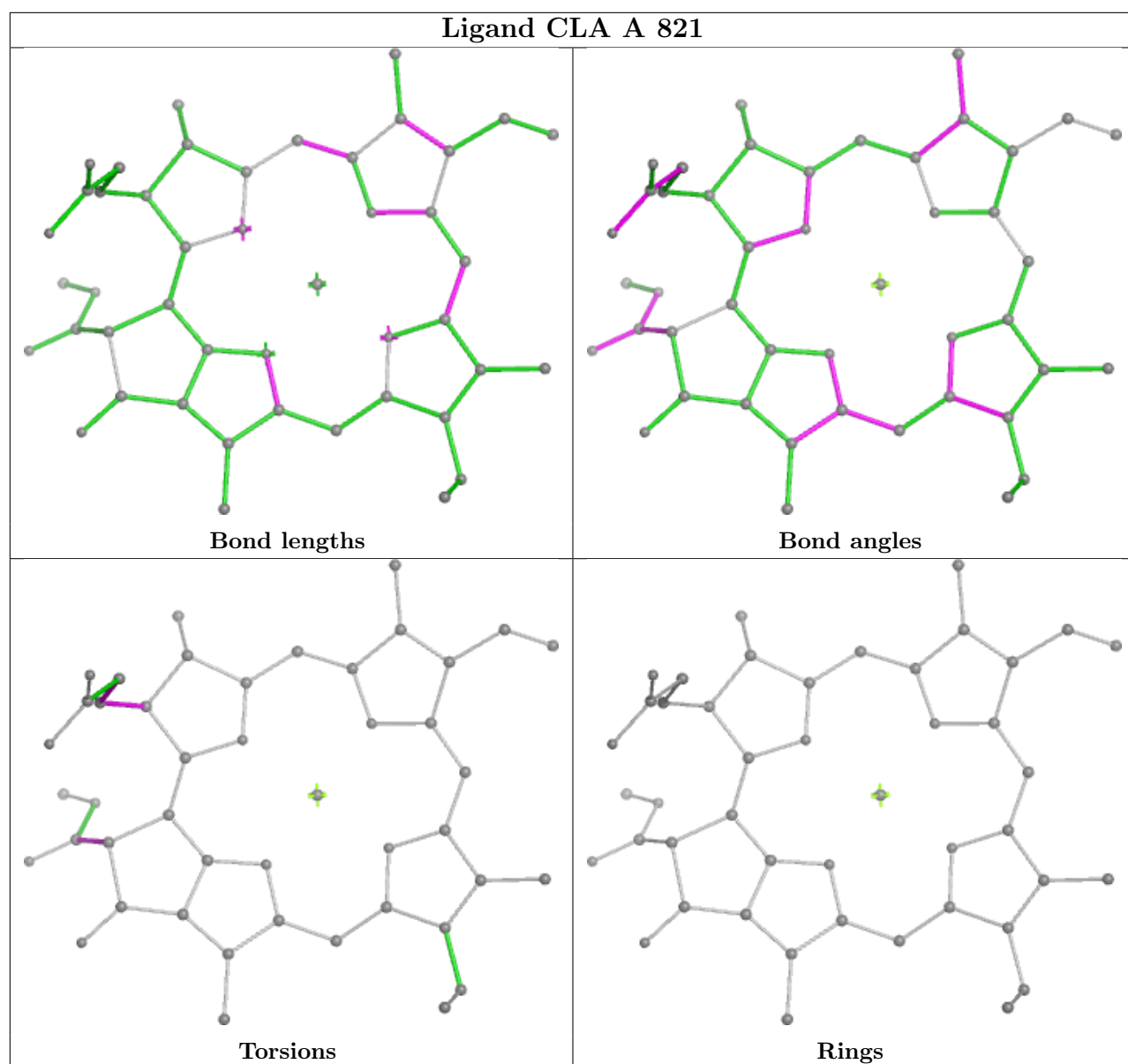
Torsions



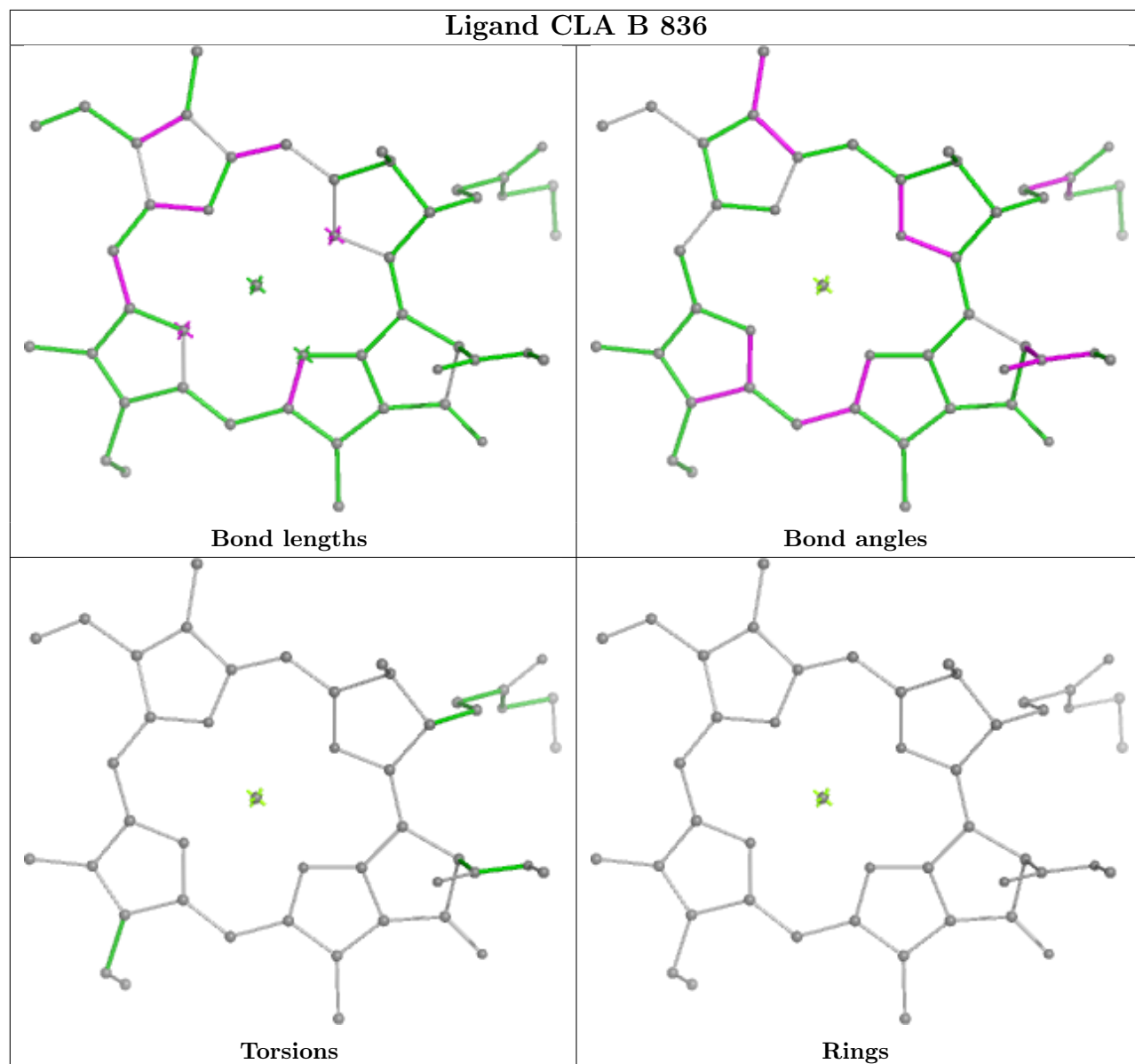
Rings

Ligand CLA 3 311

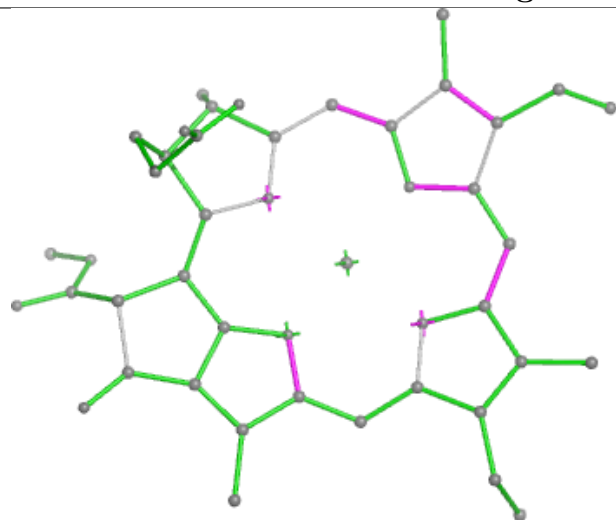




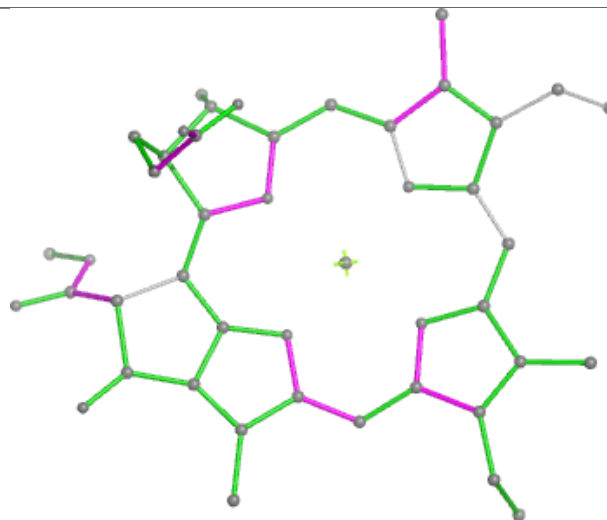
Ligand CLA B 836



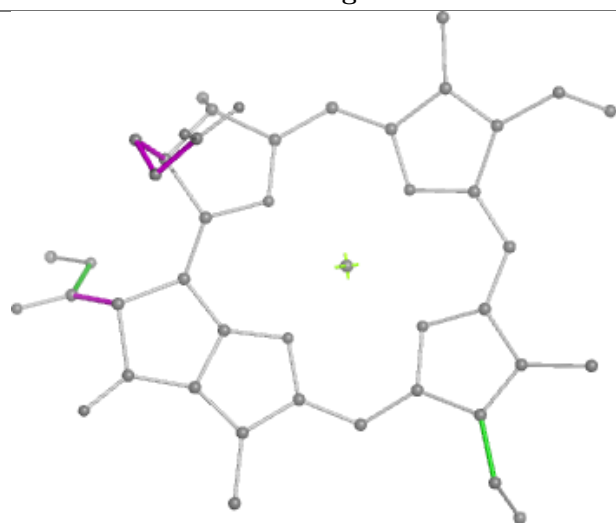
Ligand CLA B 803



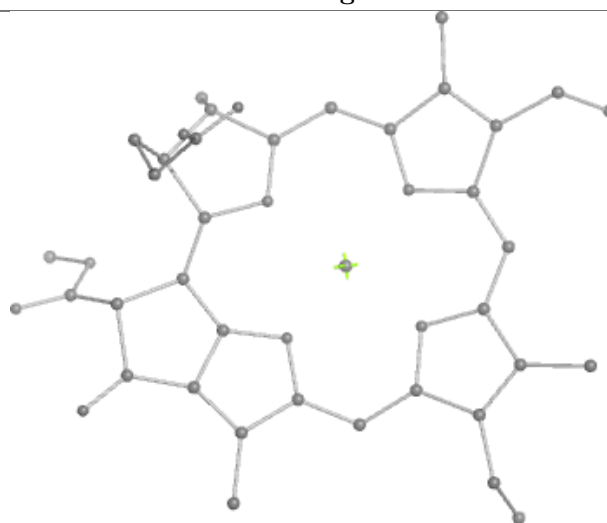
Bond lengths



Bond angles

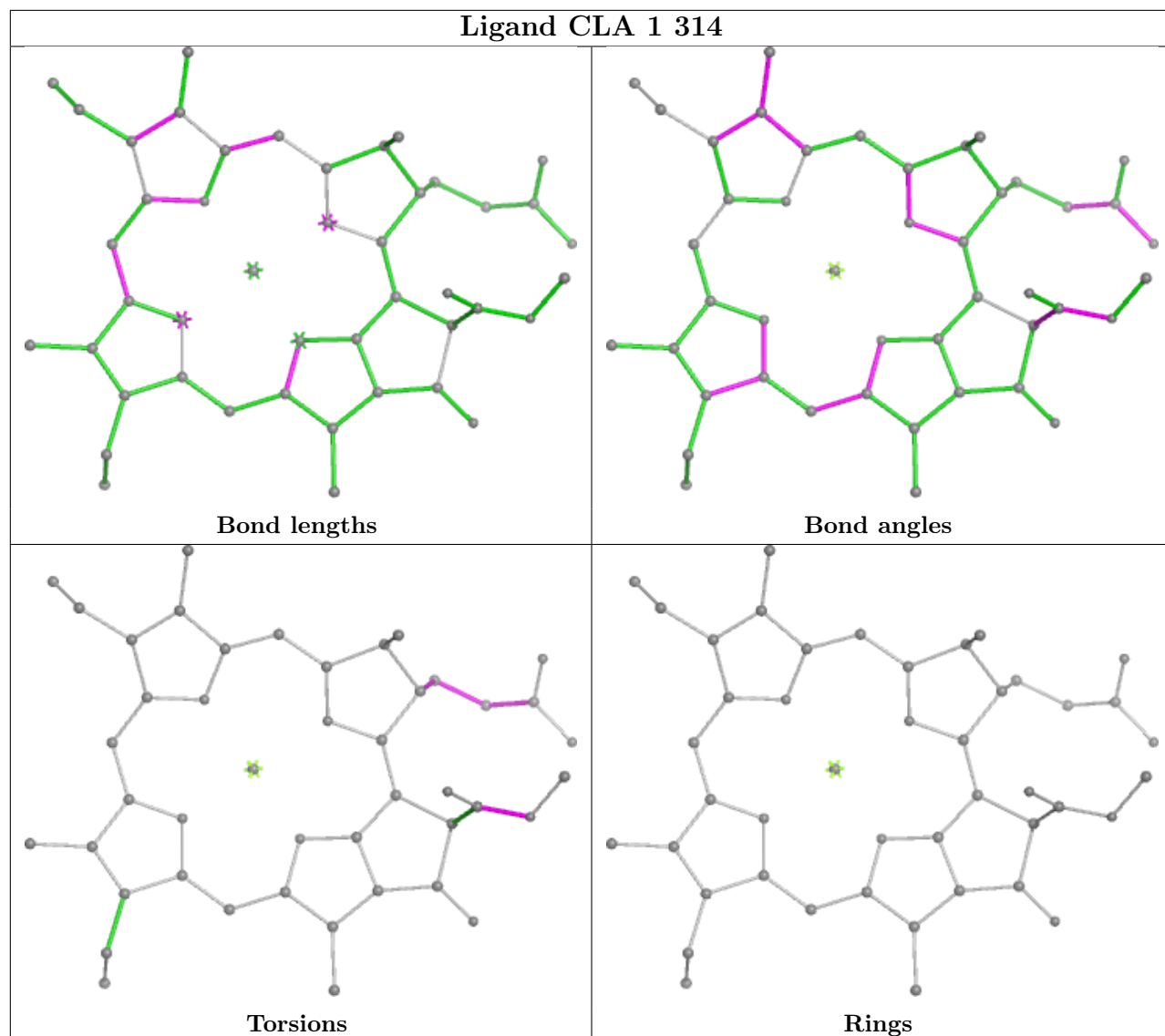


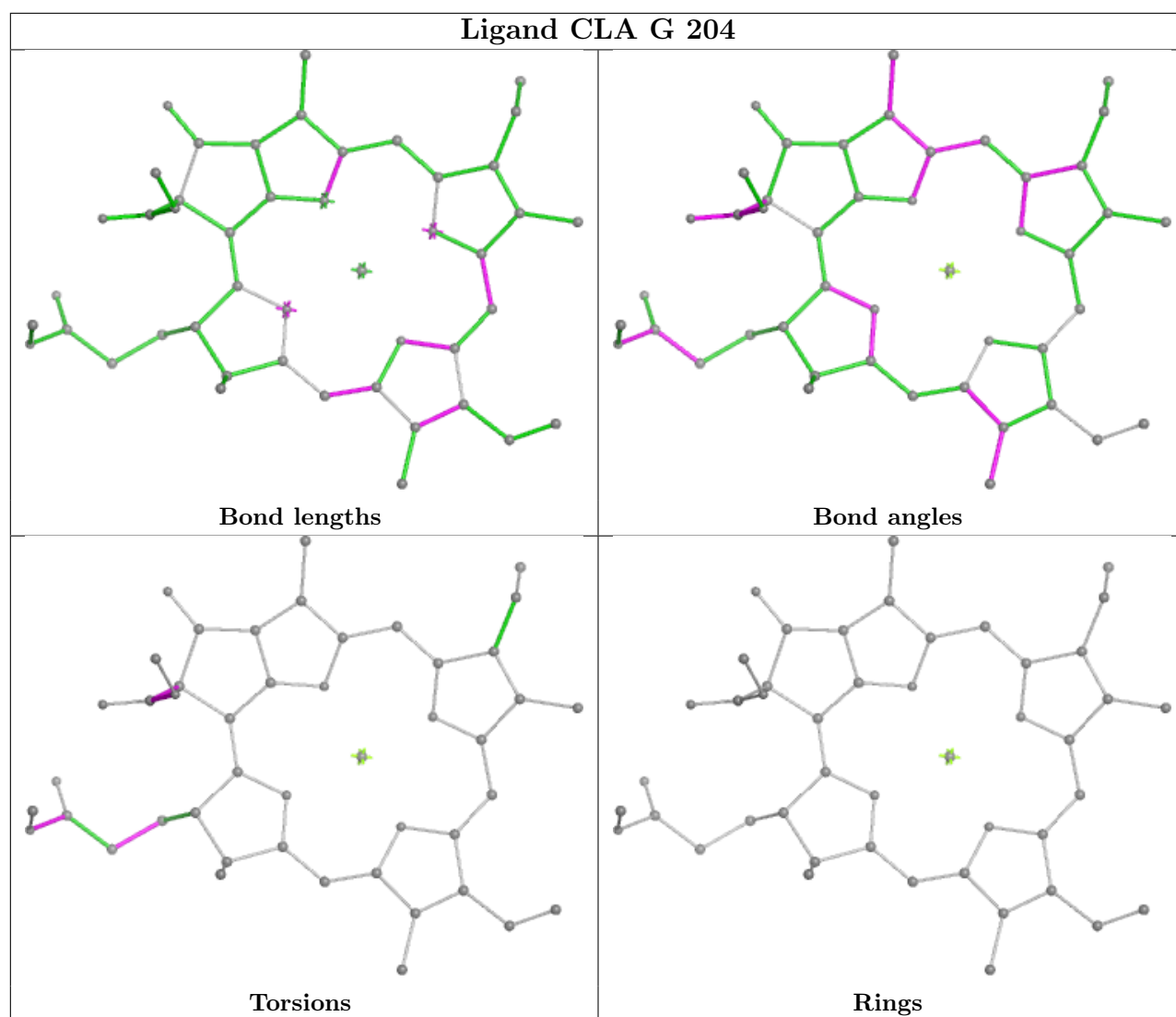
Torsions

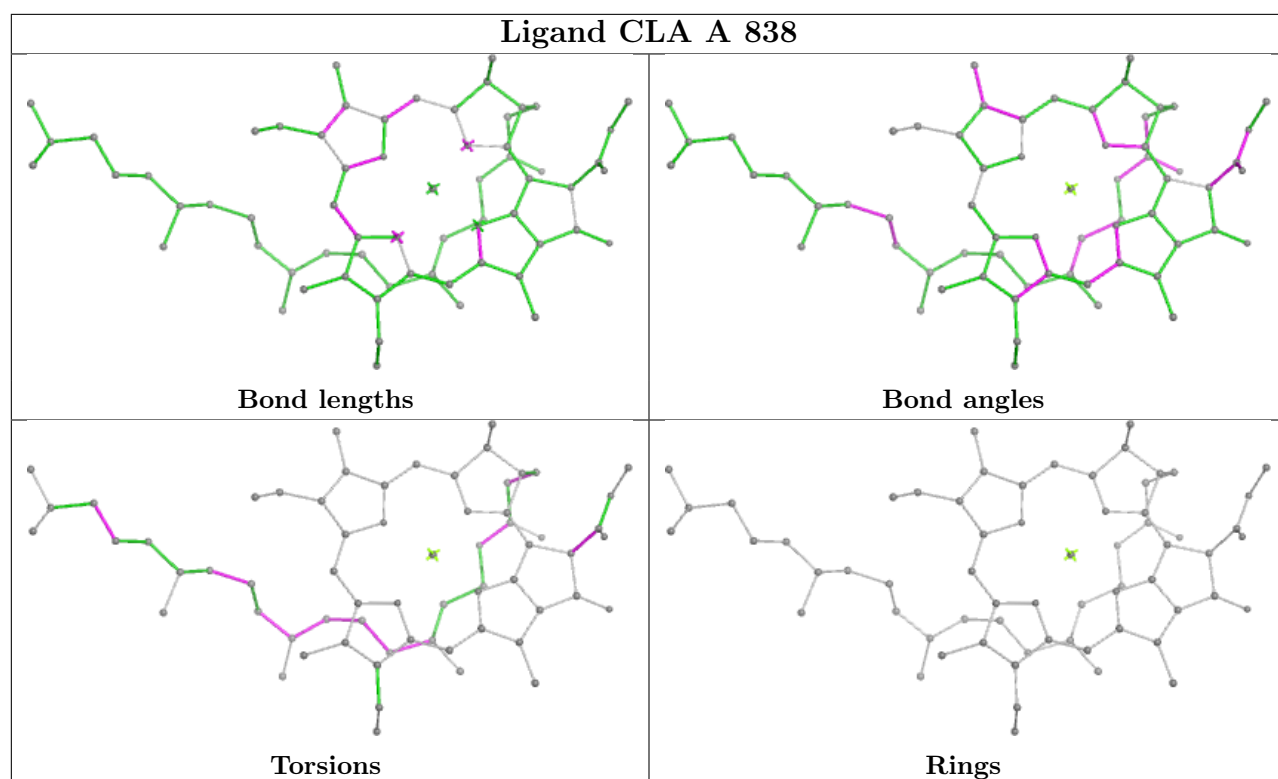


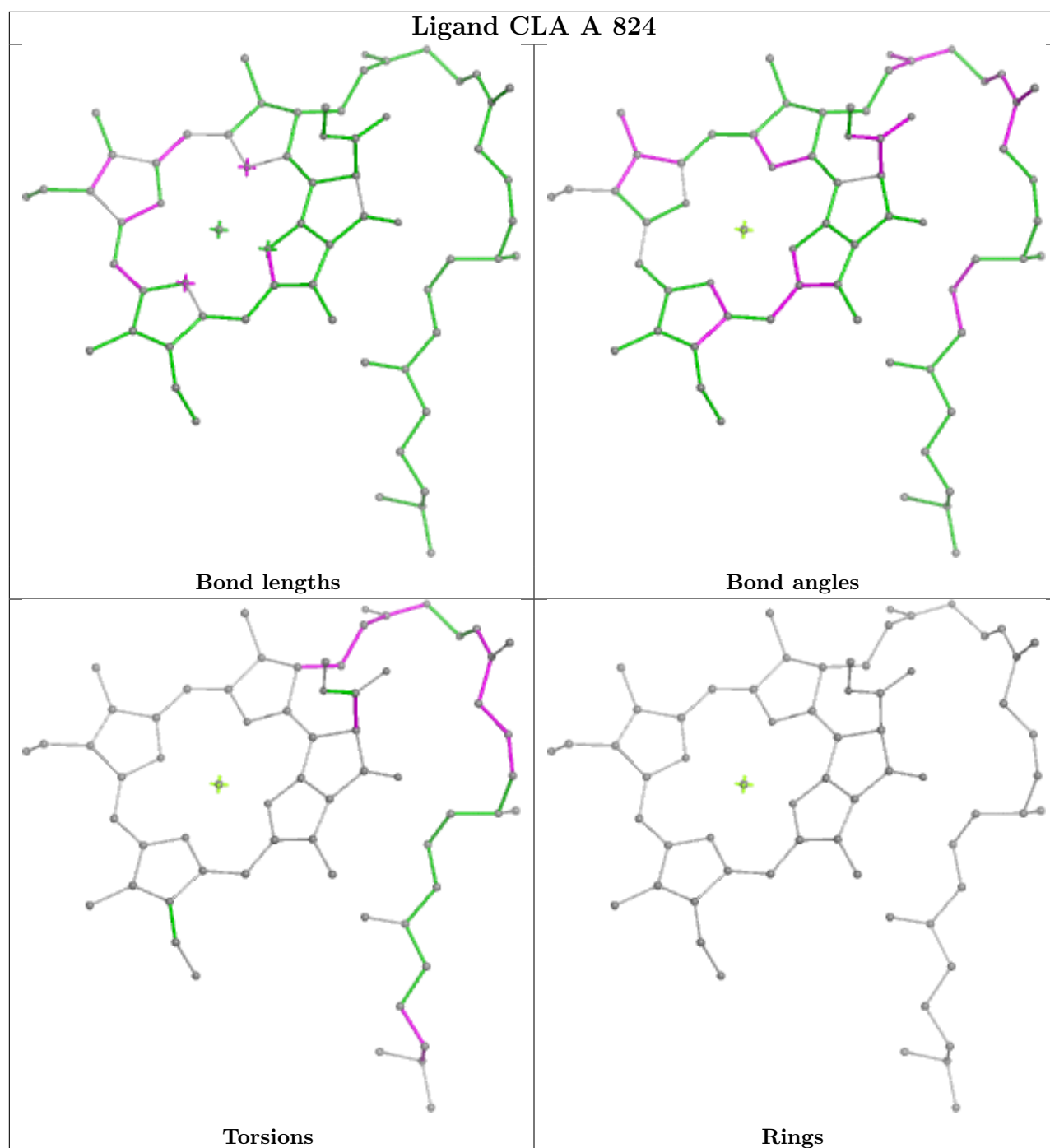
Rings

Ligand CLA 1 314

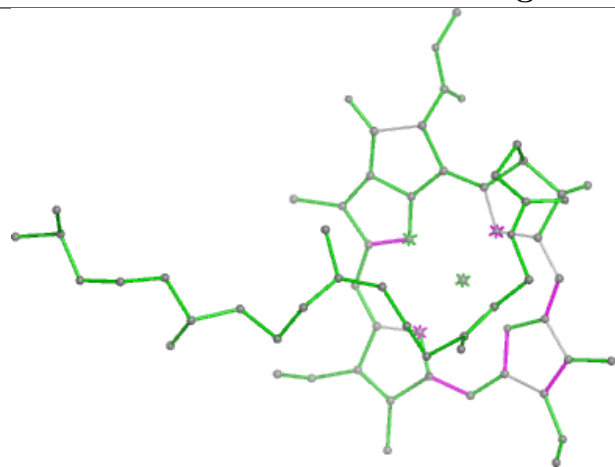




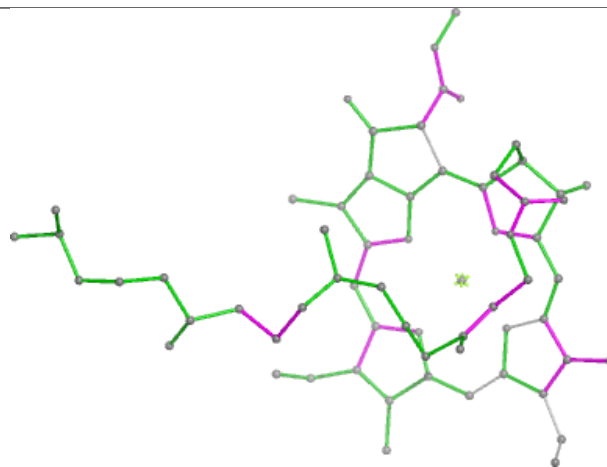




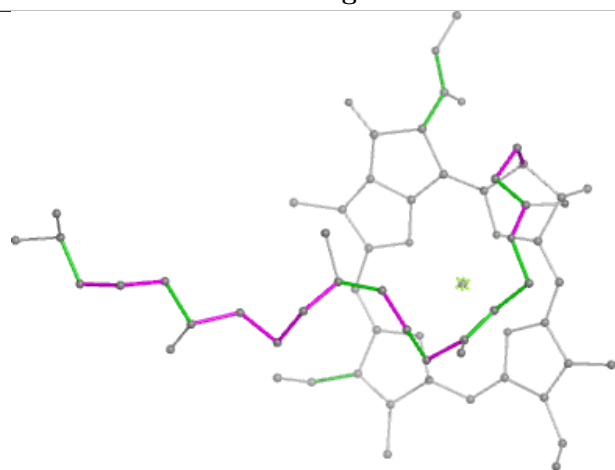
Ligand CLA B 826



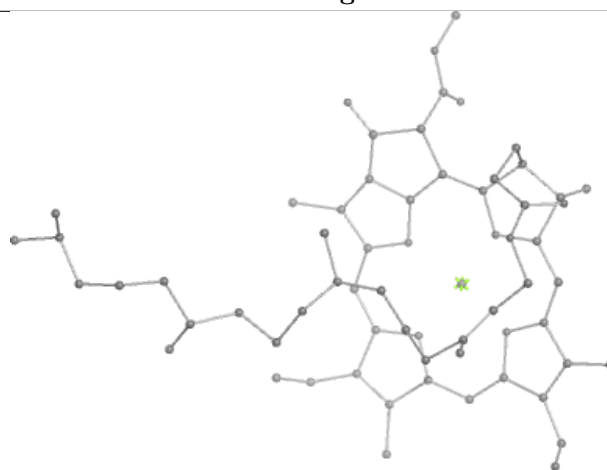
Bond lengths



Bond angles

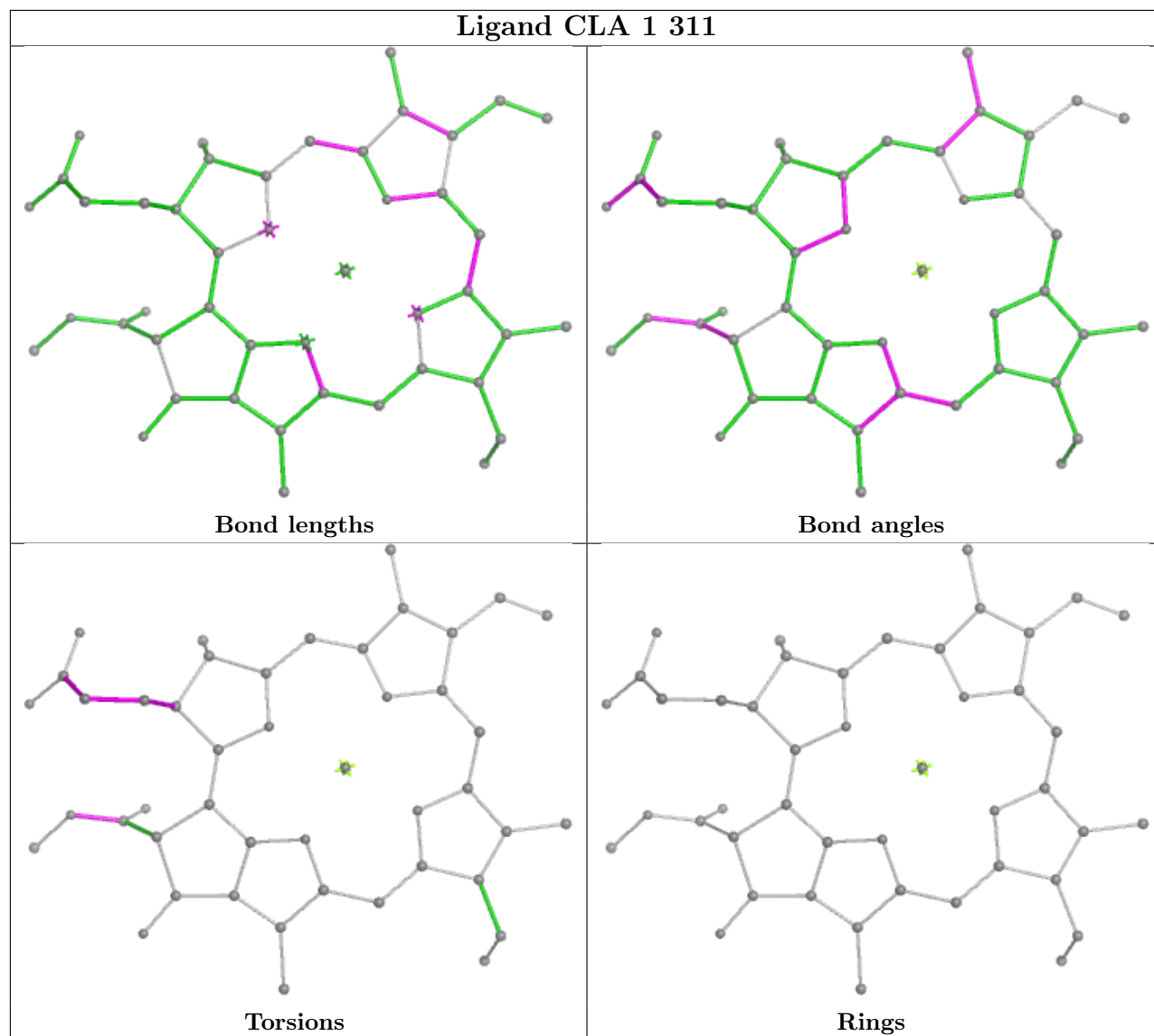


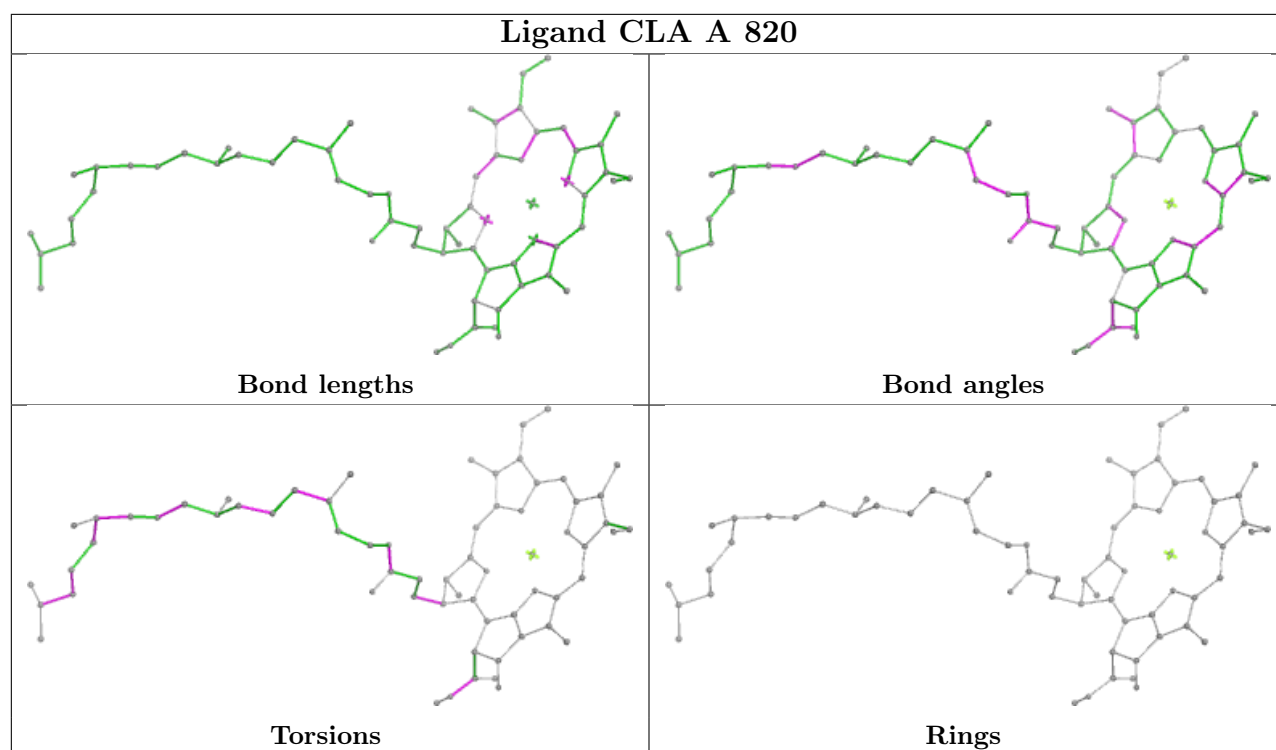
Torsions

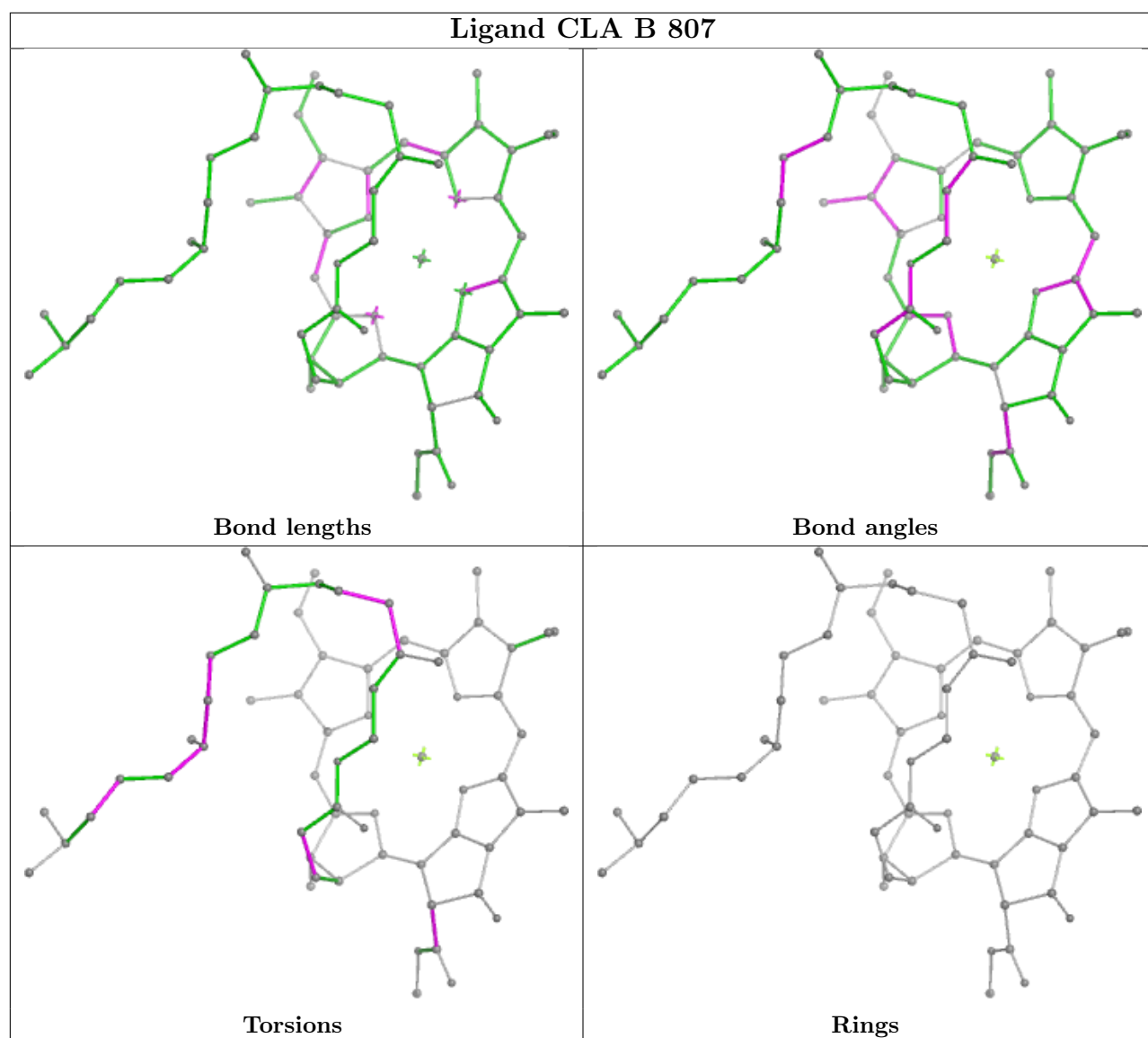


Rings

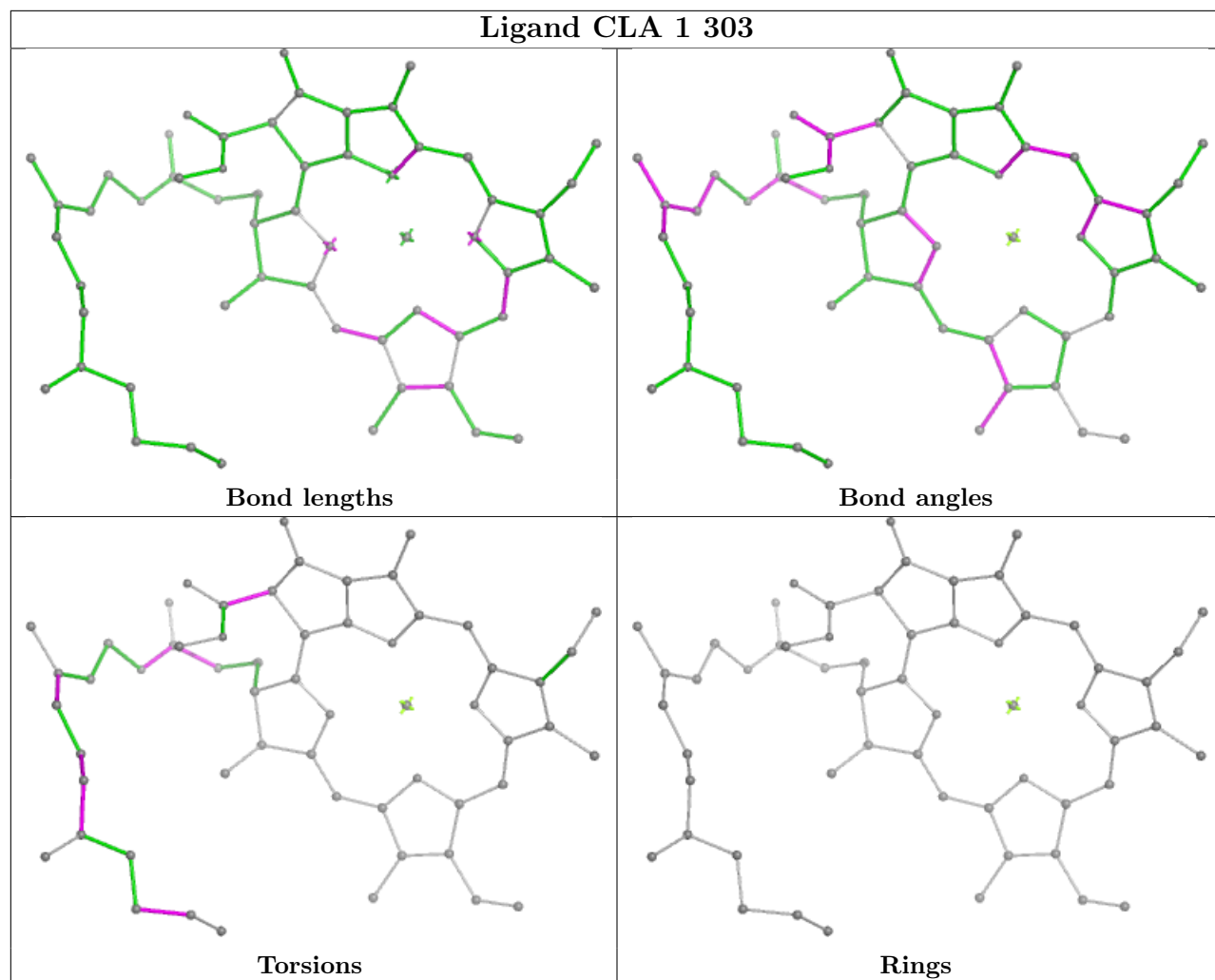
Ligand CLA 1 311

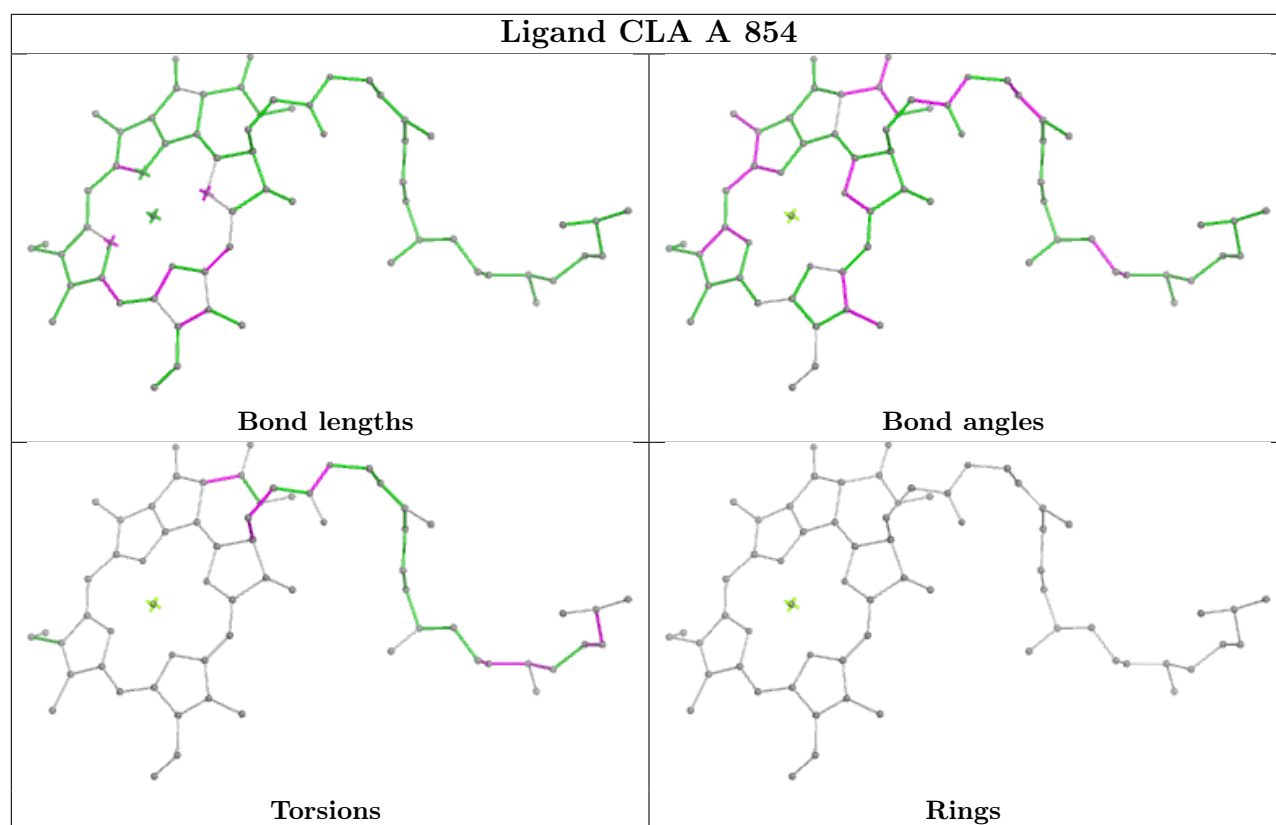




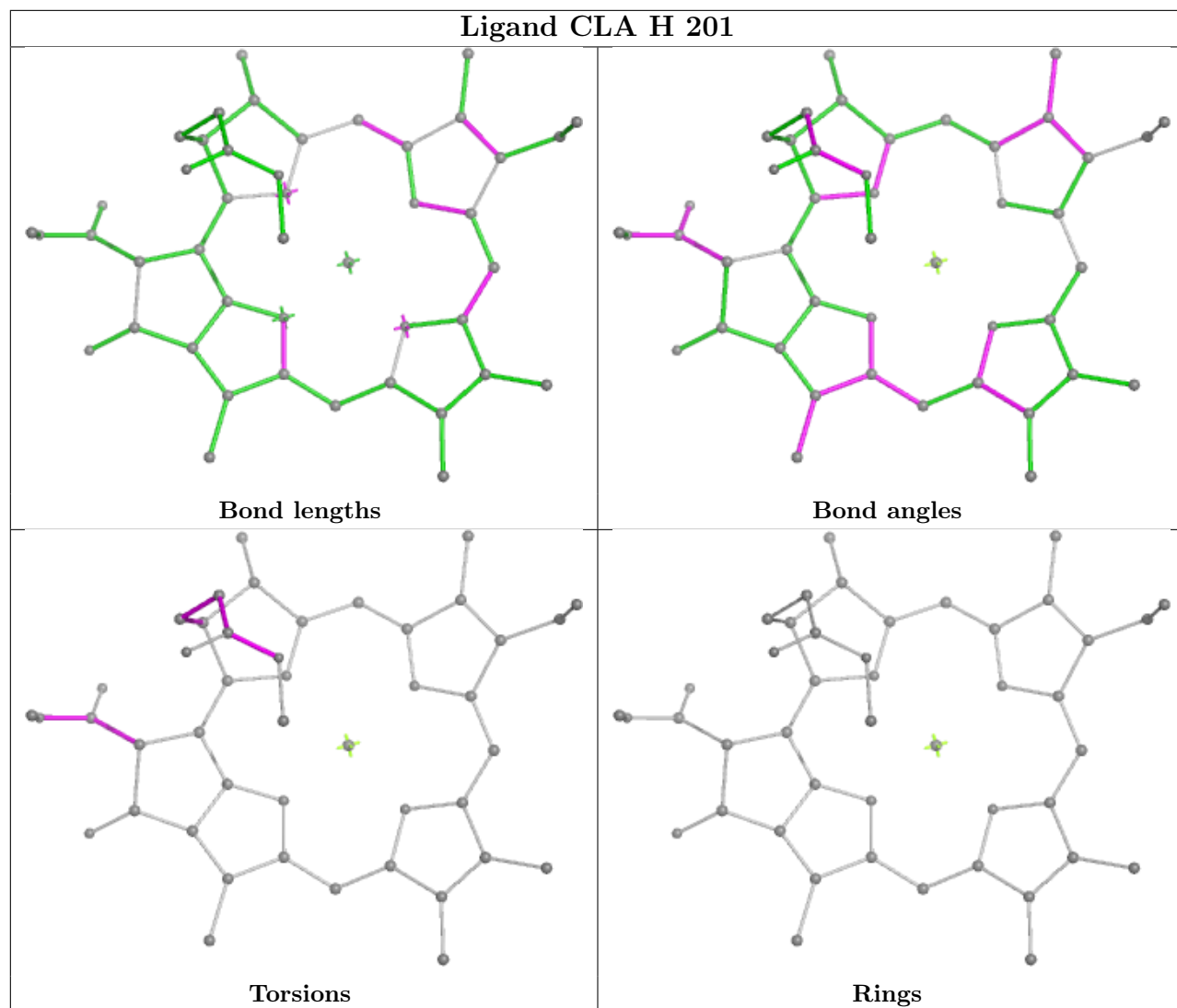


Ligand CLA 1 303

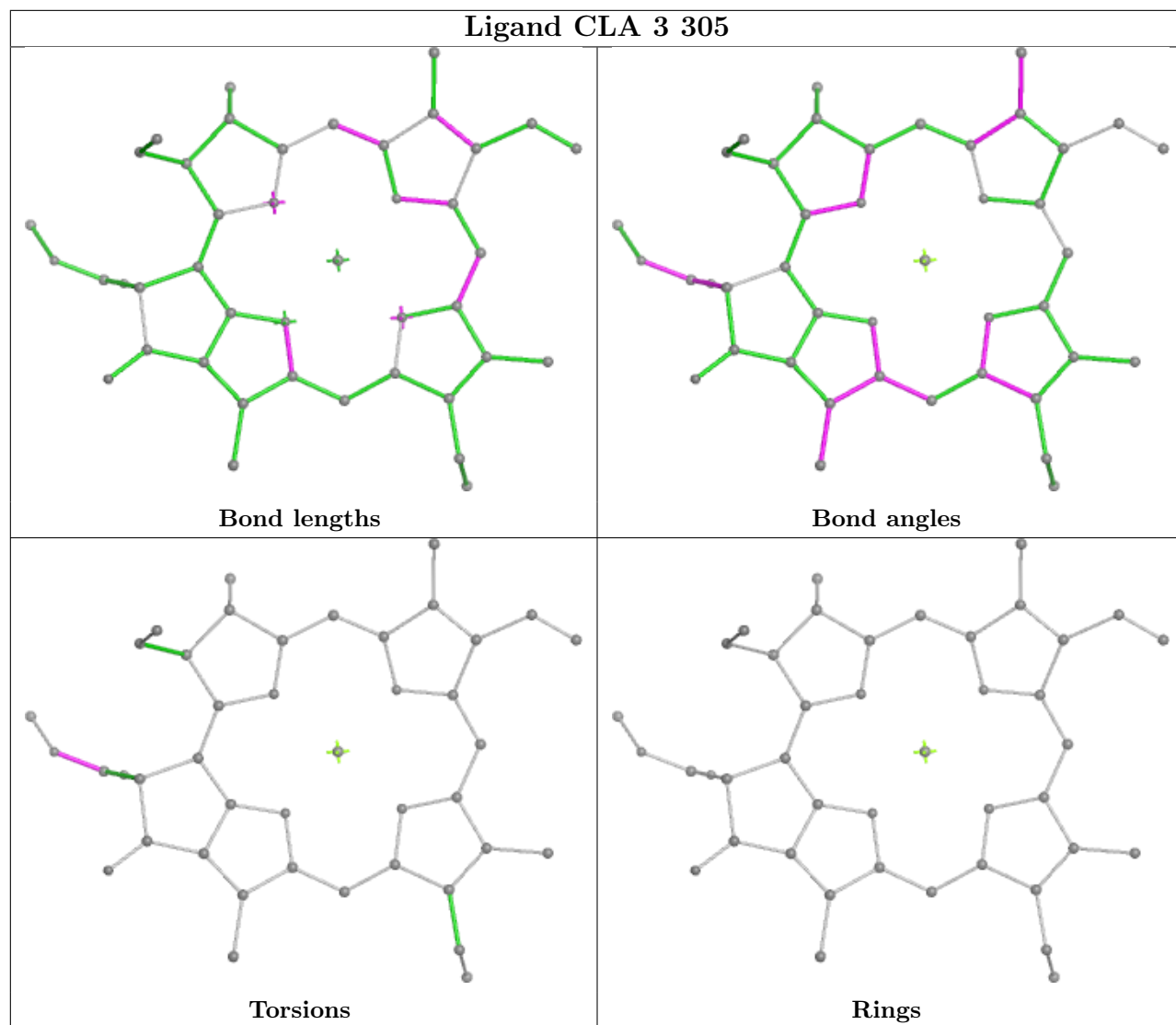




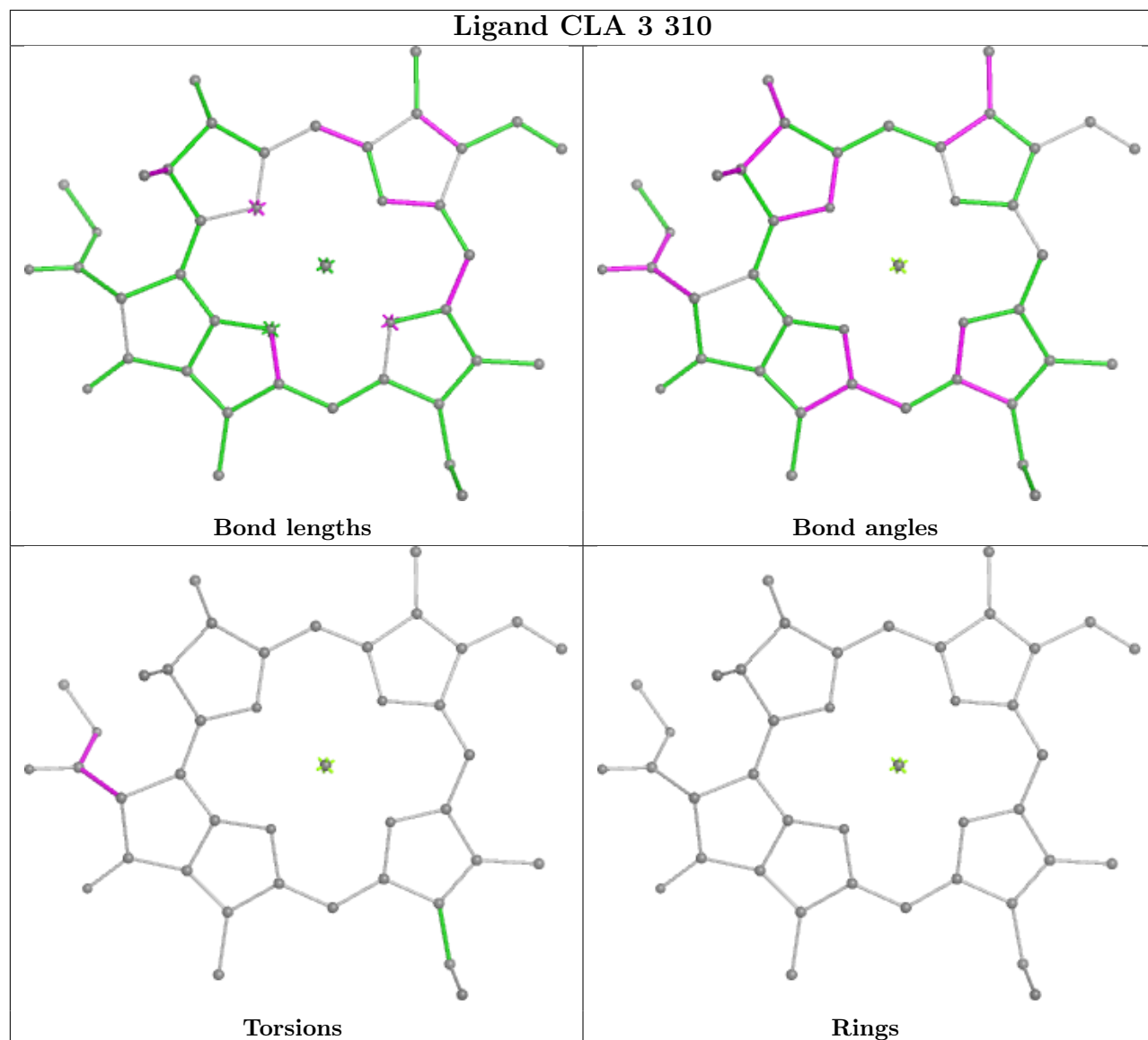
Ligand CLA H 201



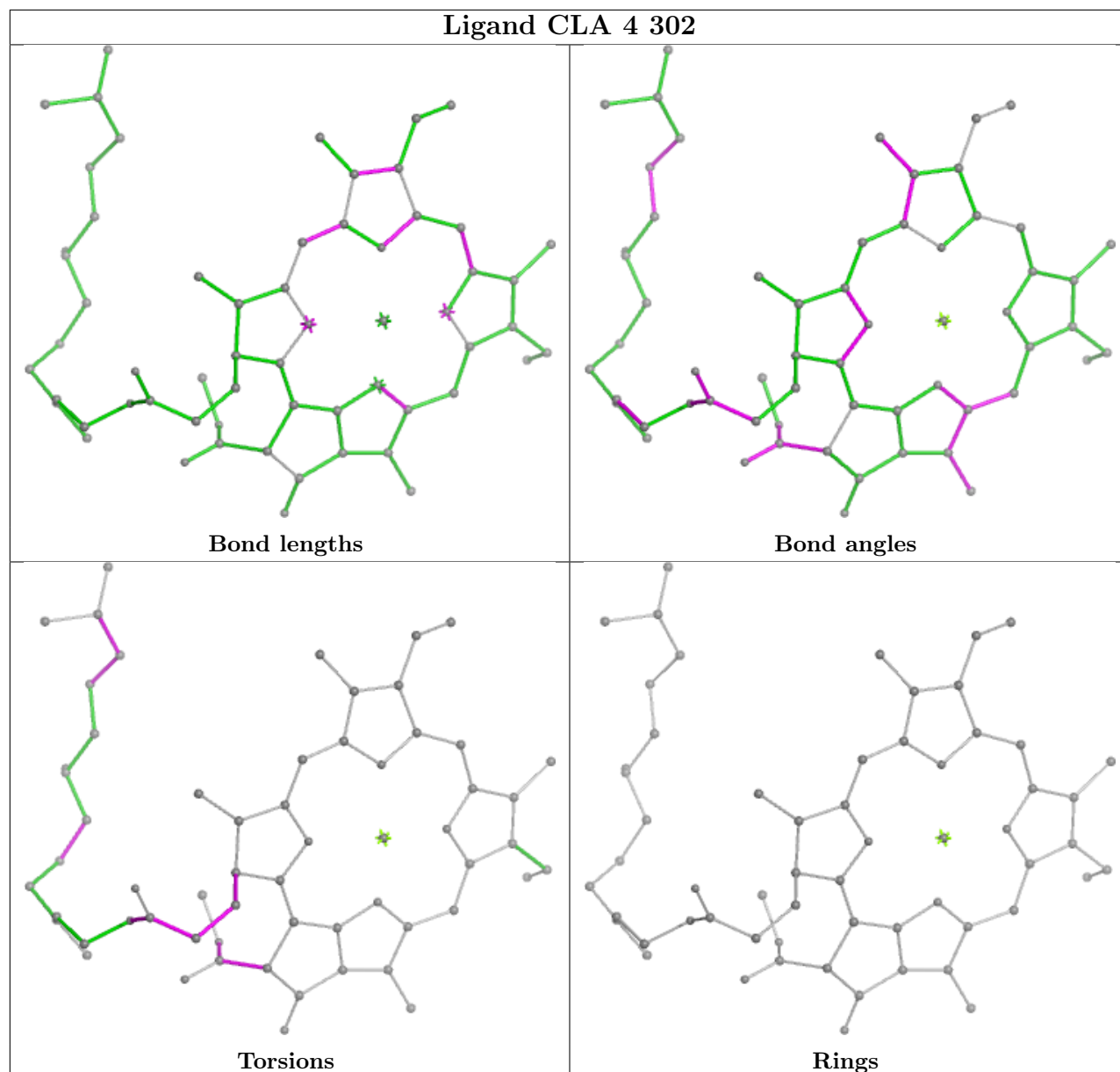
Ligand CLA 3 305



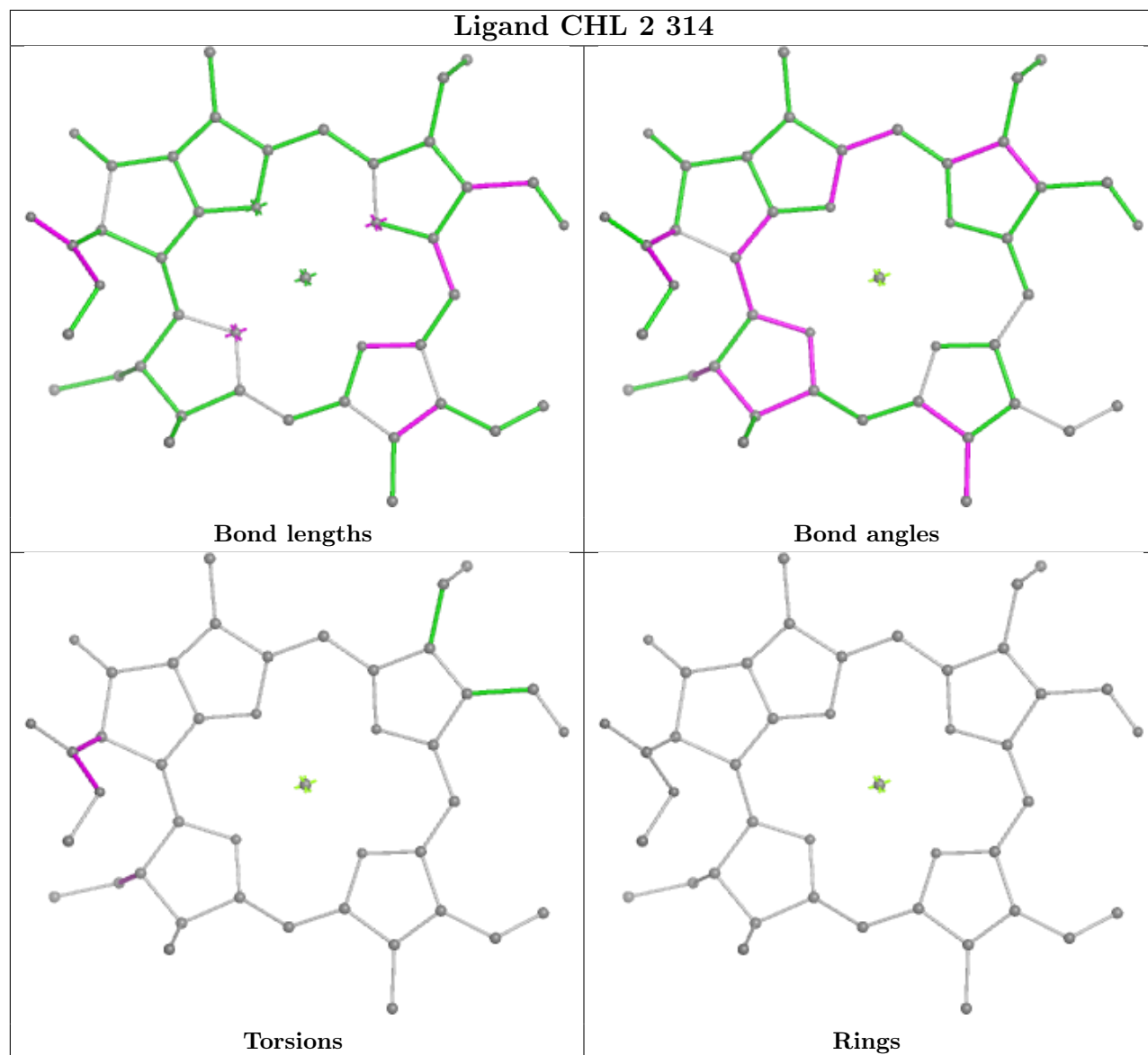
Ligand CLA 3 310



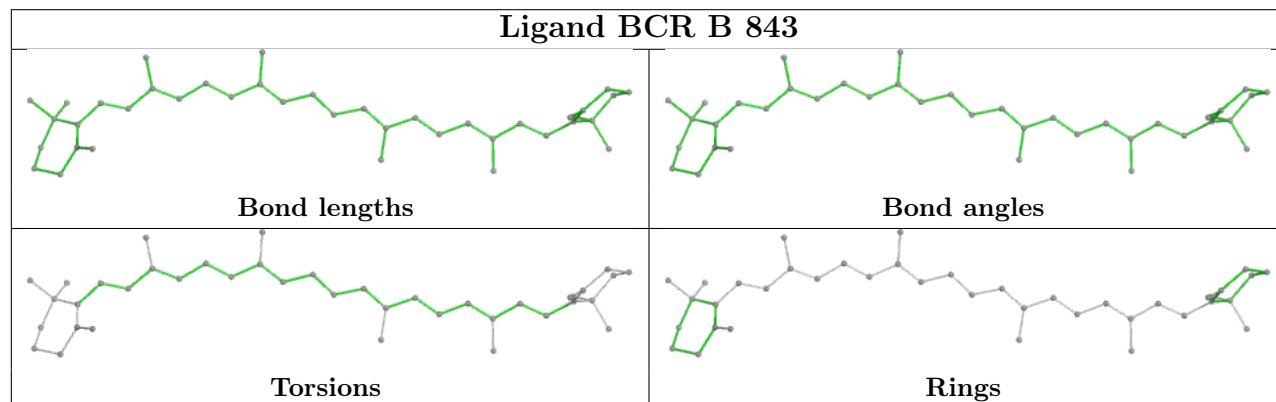
Ligand CLA 4 302

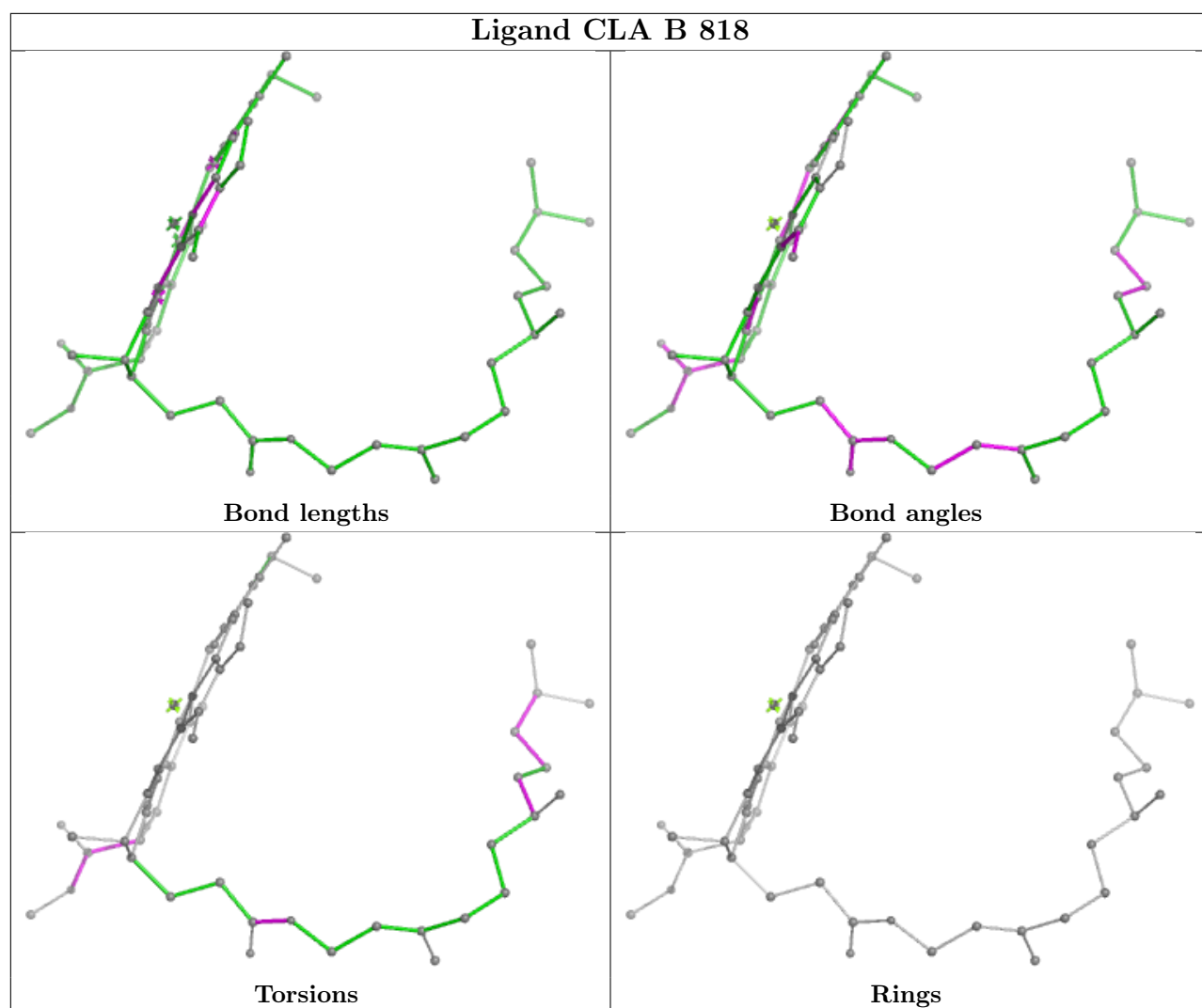


Ligand CHL 2 314

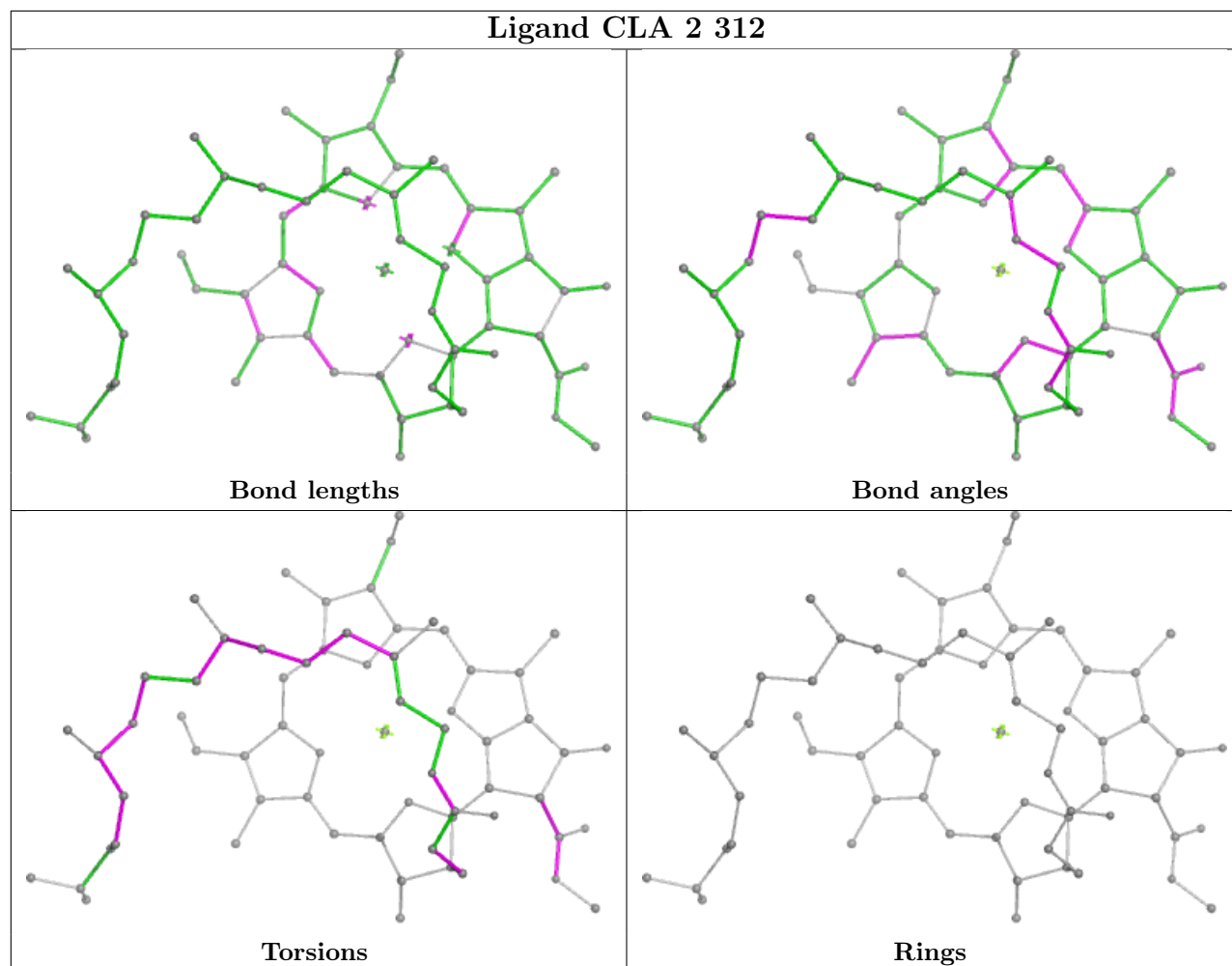


Ligand BCR B 843

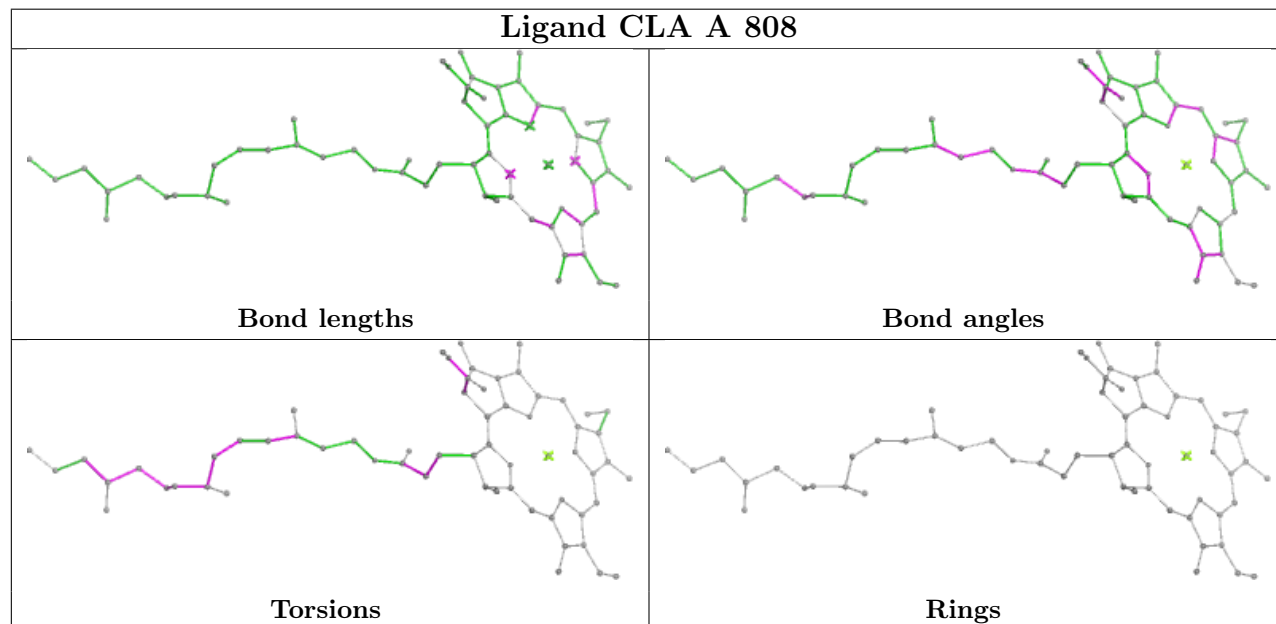


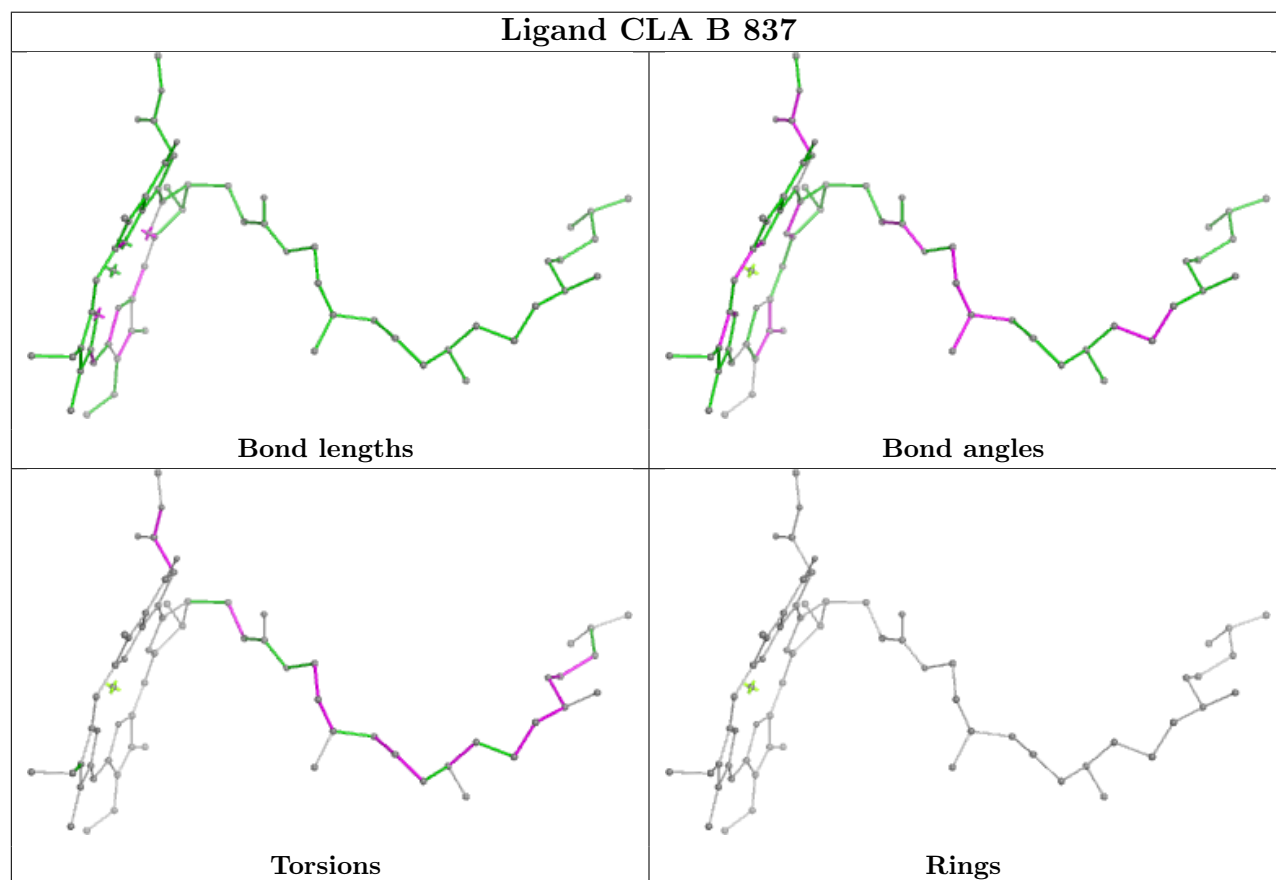
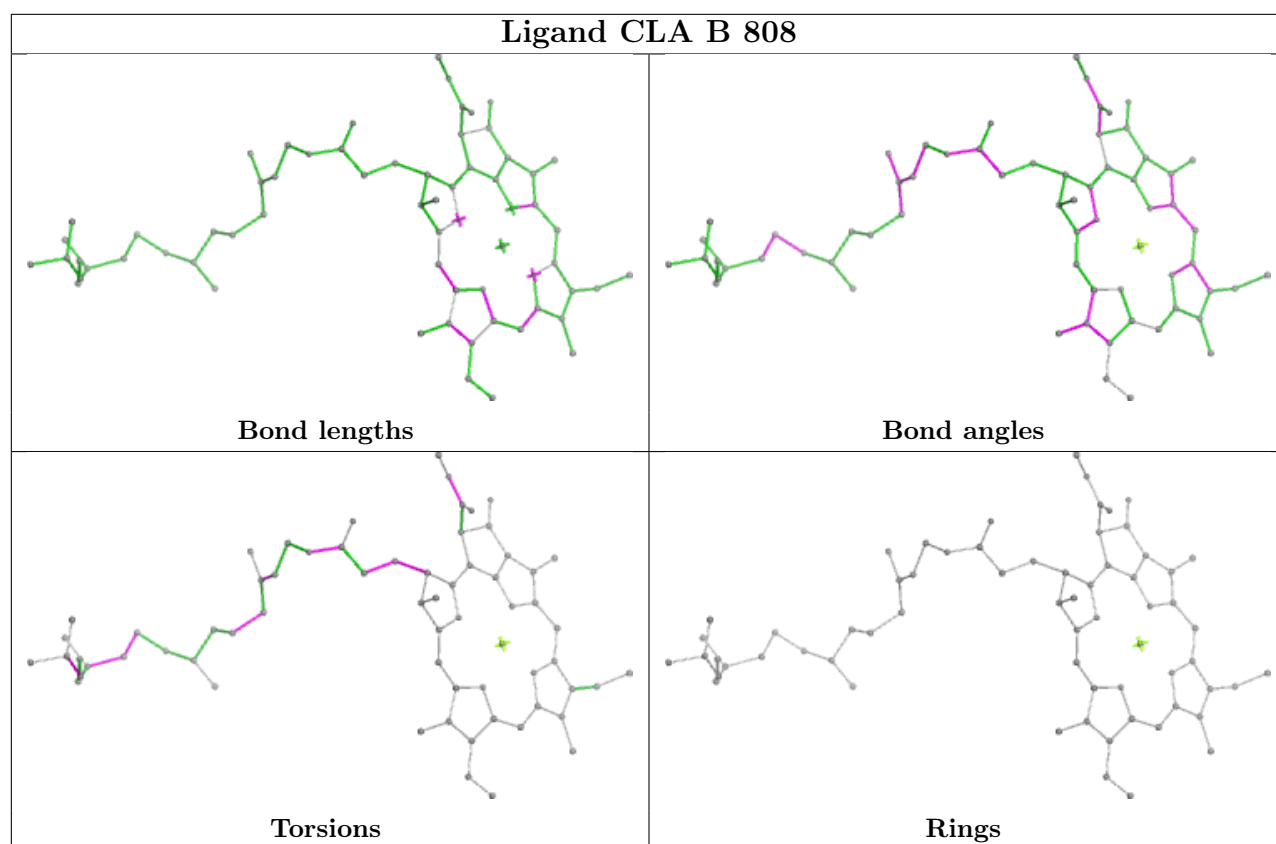


Ligand CLA 2 312

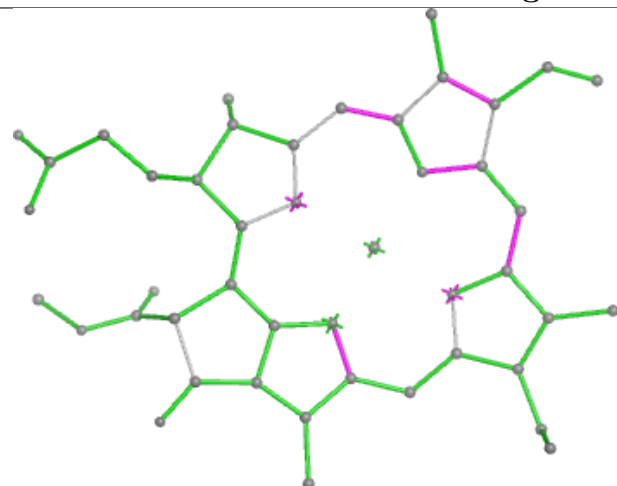


Ligand CLA A 808

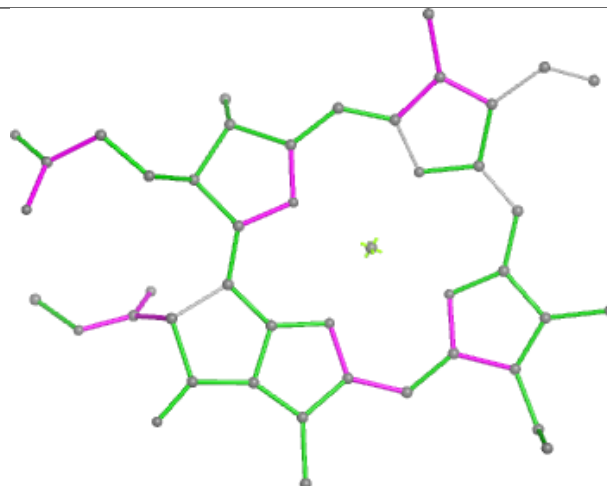




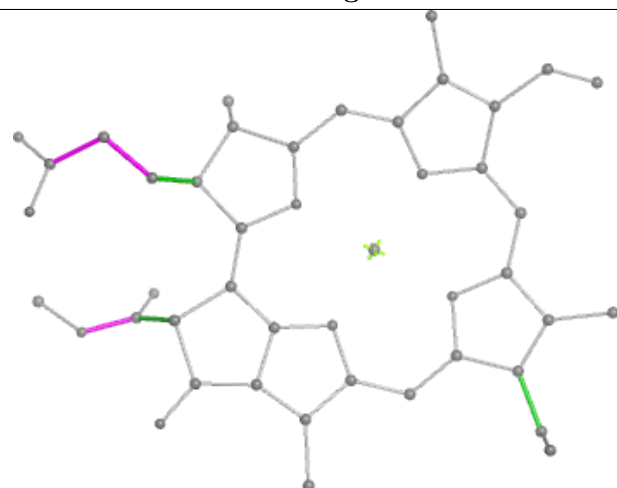
Ligand CLA 3 313



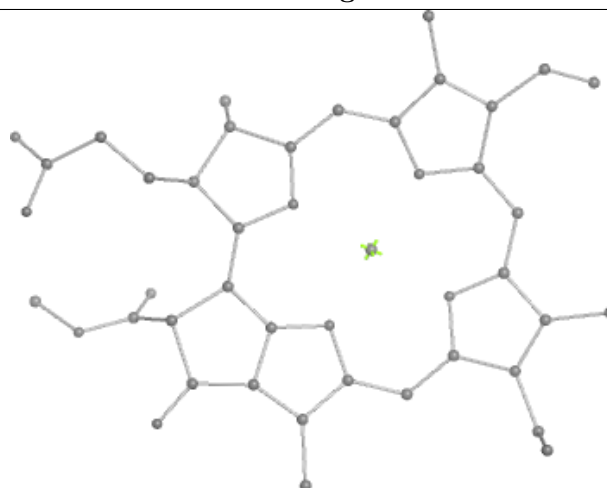
Bond lengths



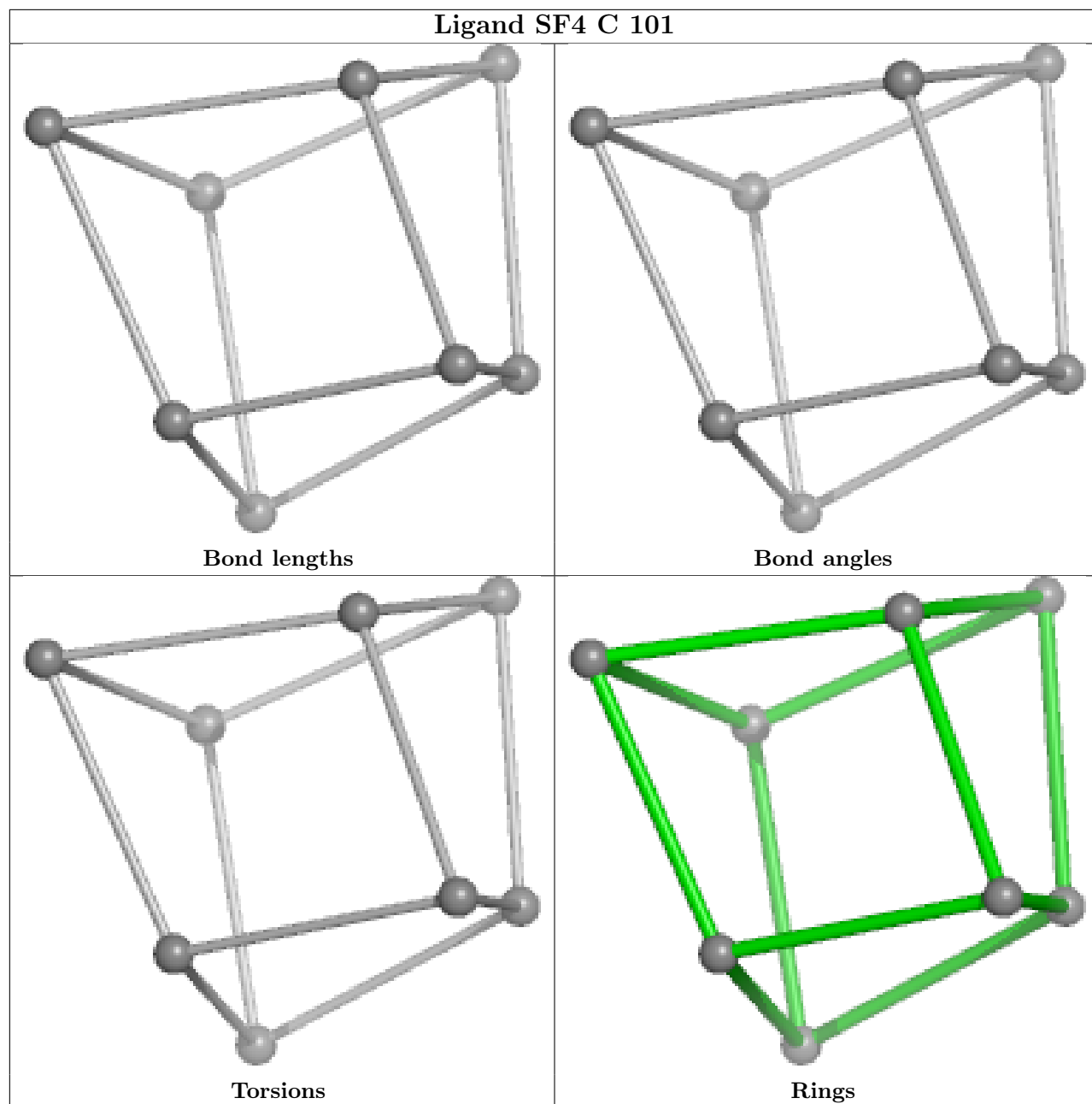
Bond angles

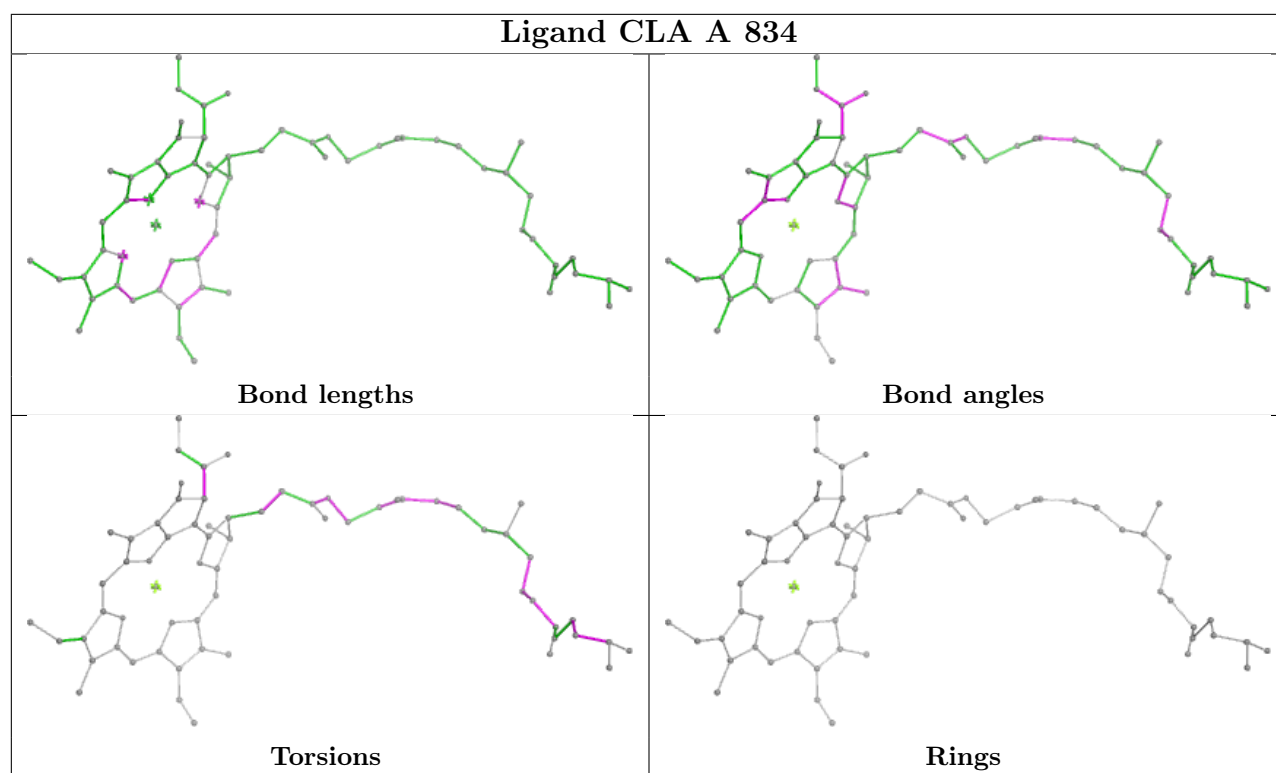


Torsions

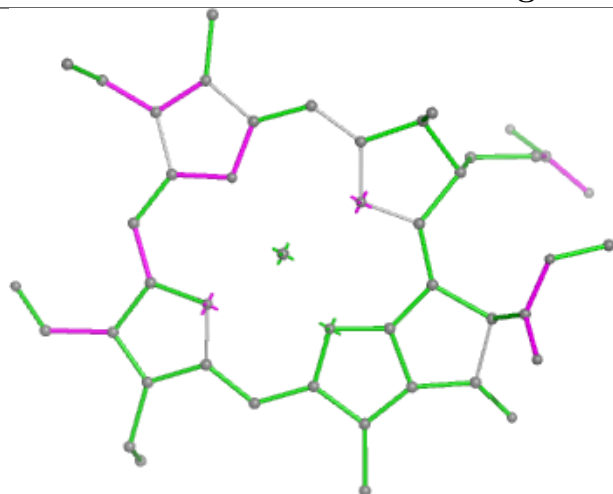


Rings

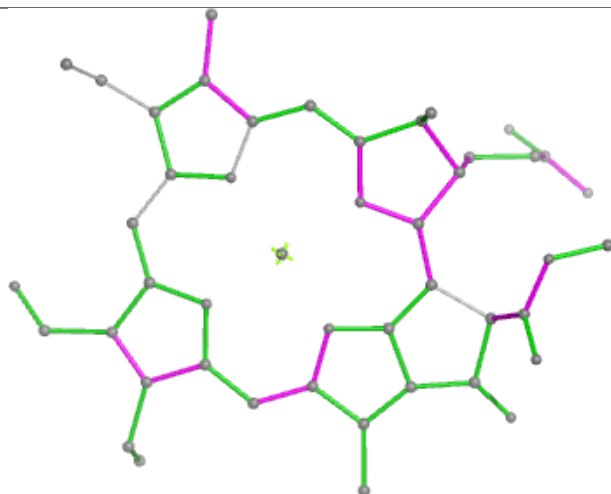




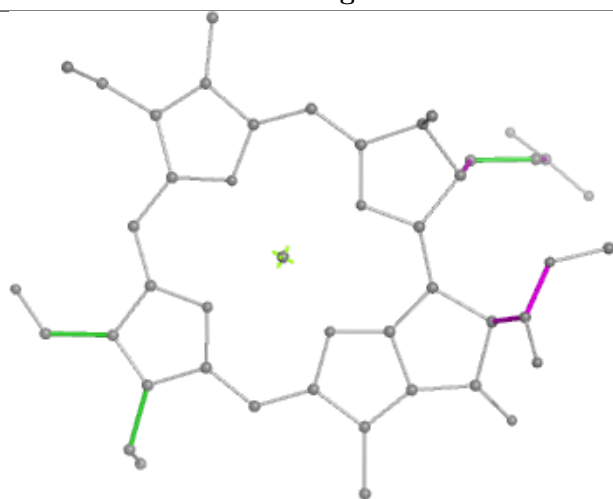
Ligand CHL 4 305



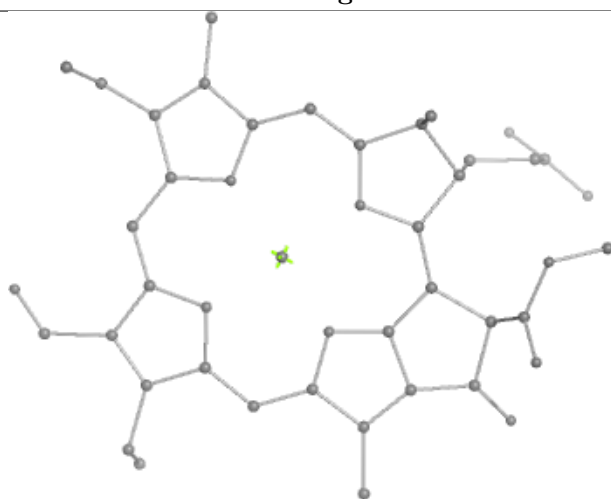
Bond lengths



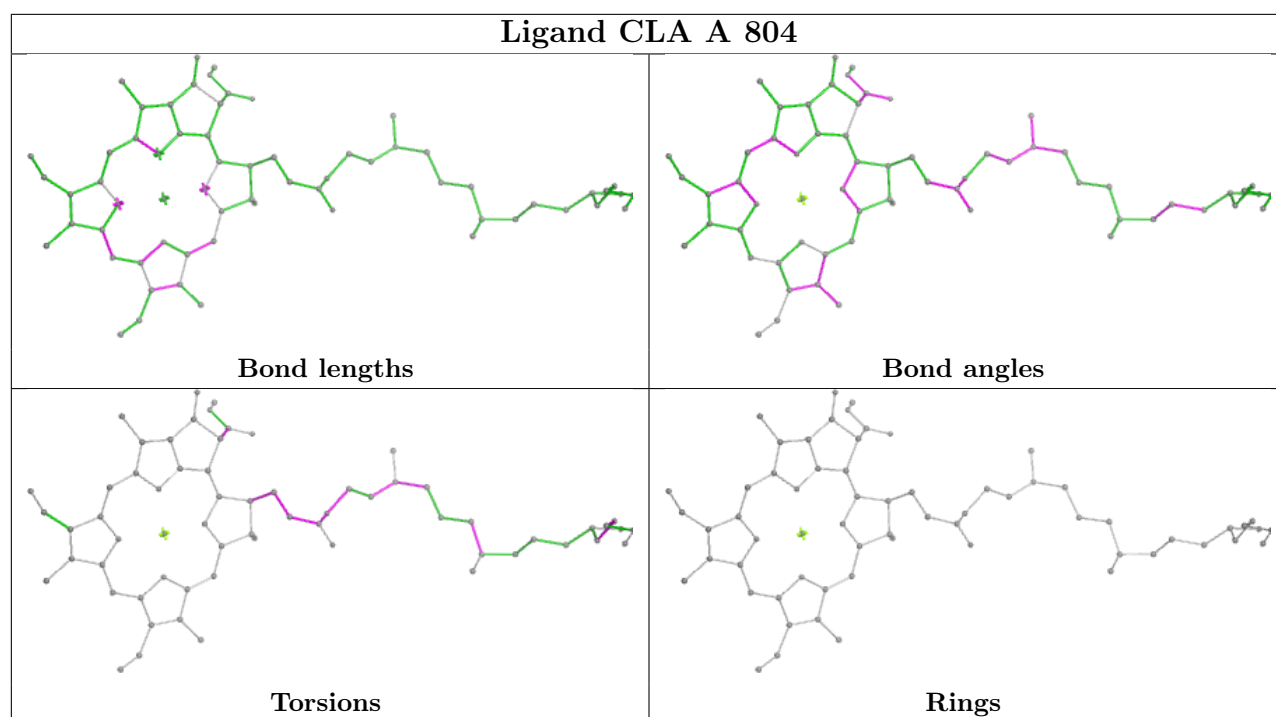
Bond angles



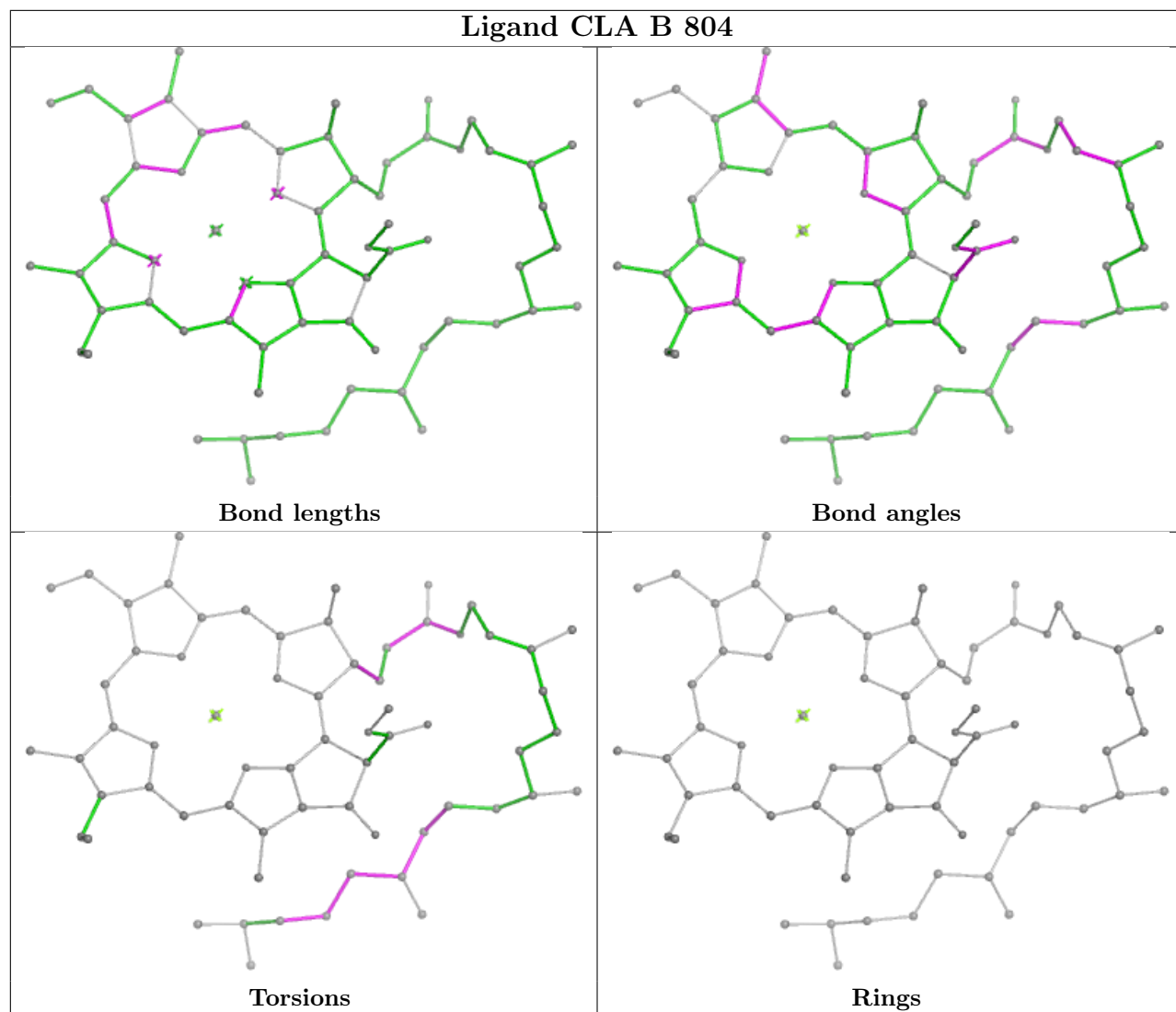
Torsions



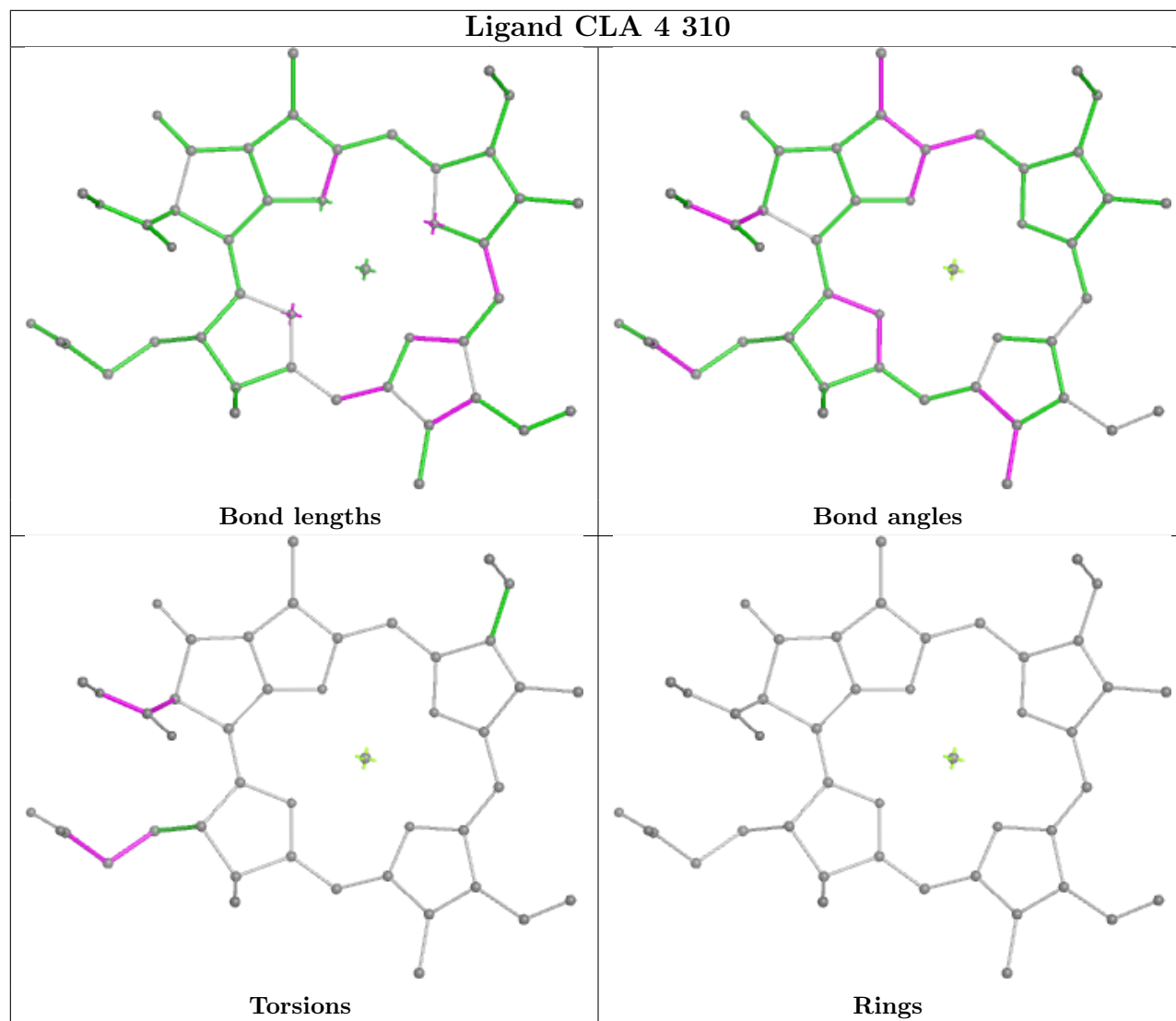
Rings



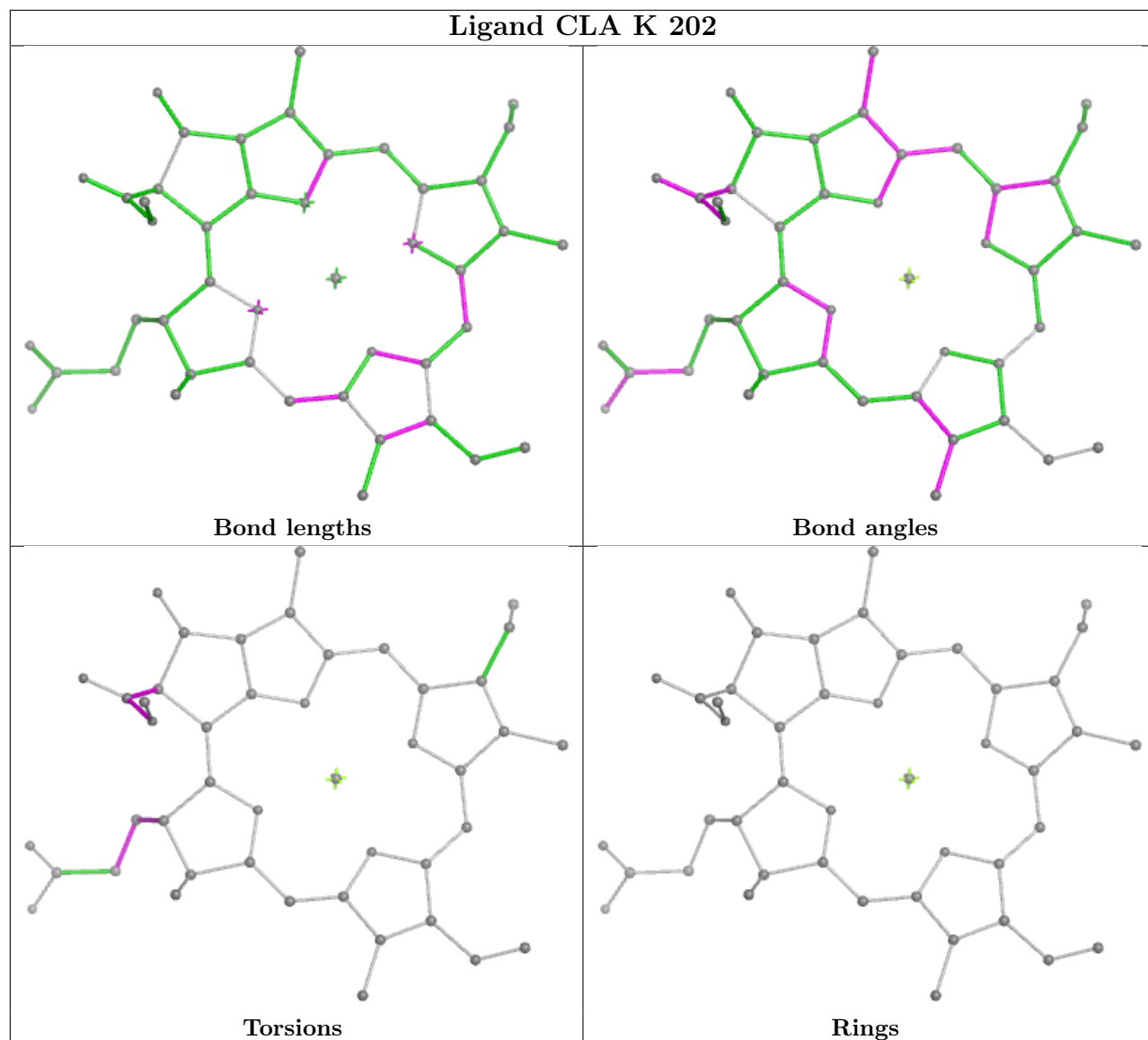
Ligand CLA B 804



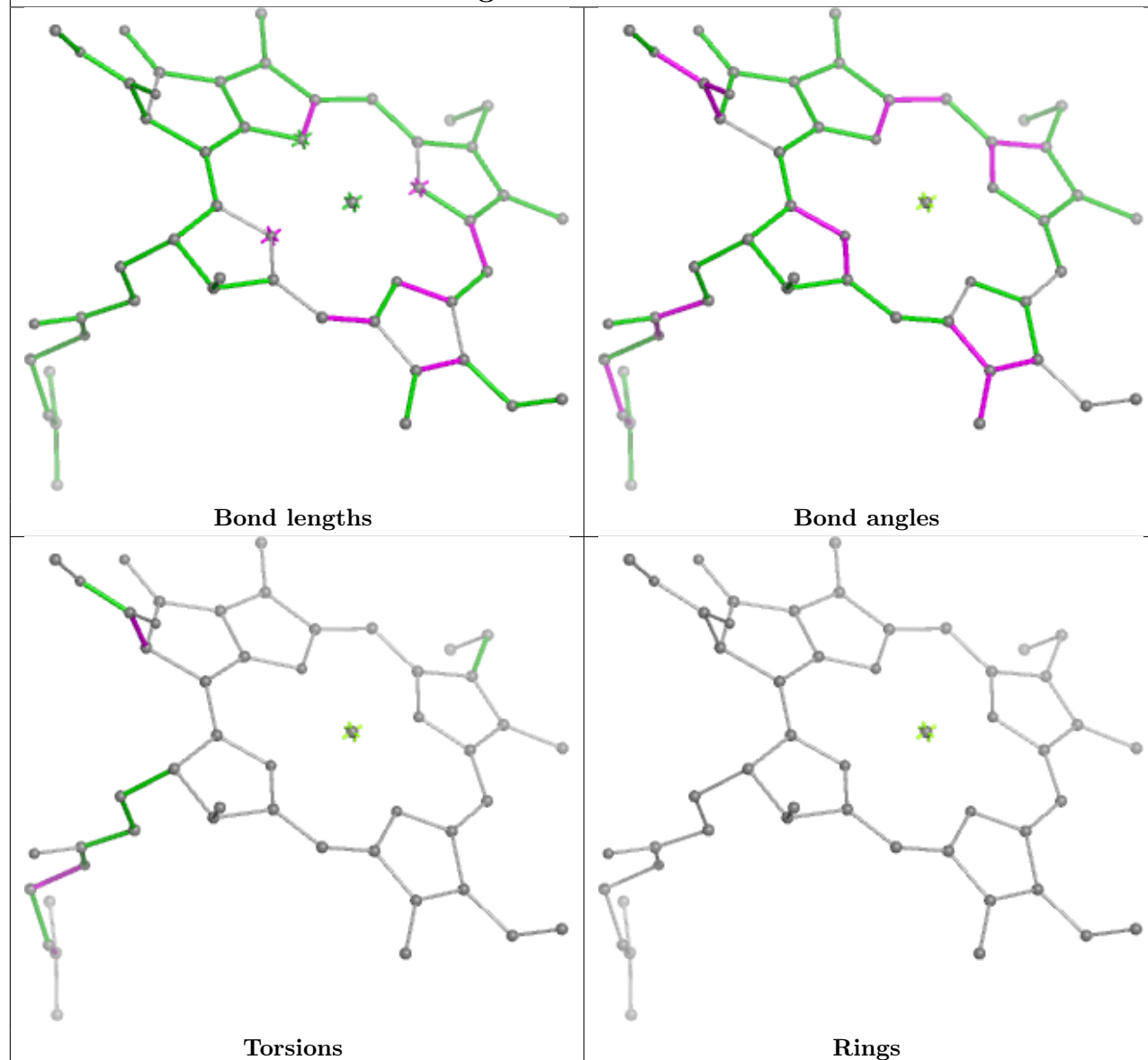
Ligand CLA 4 310

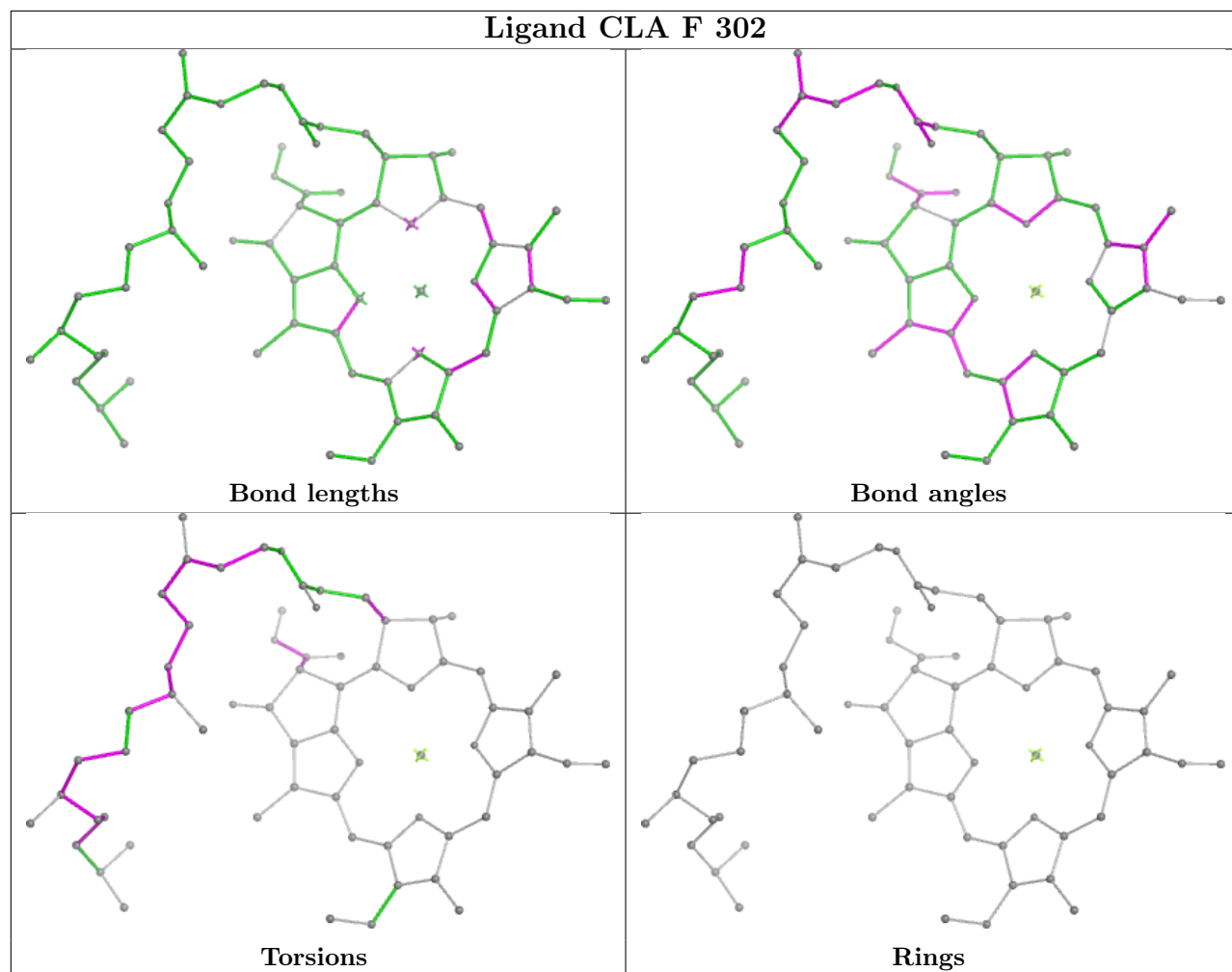


Ligand CLA K 202

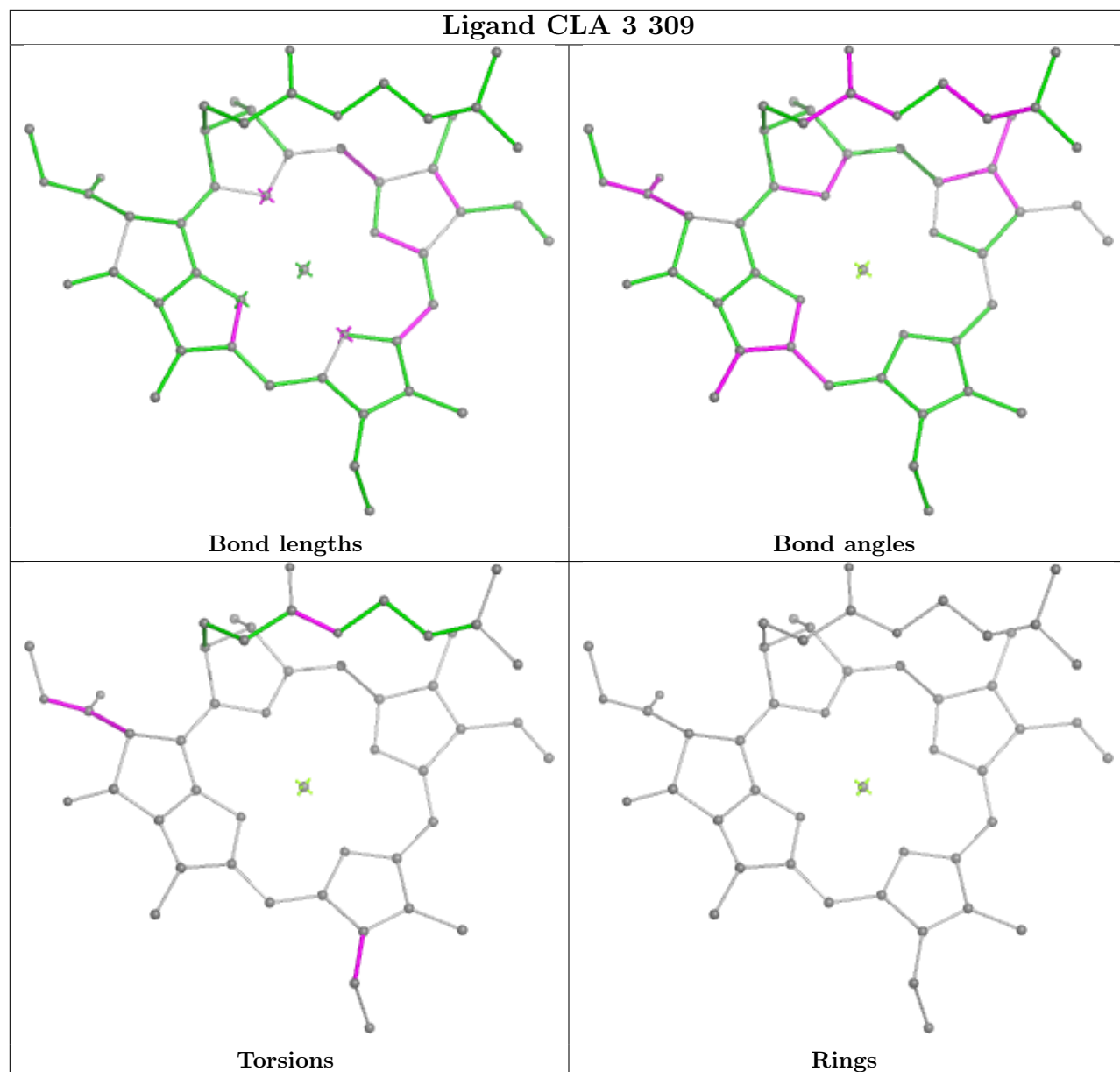


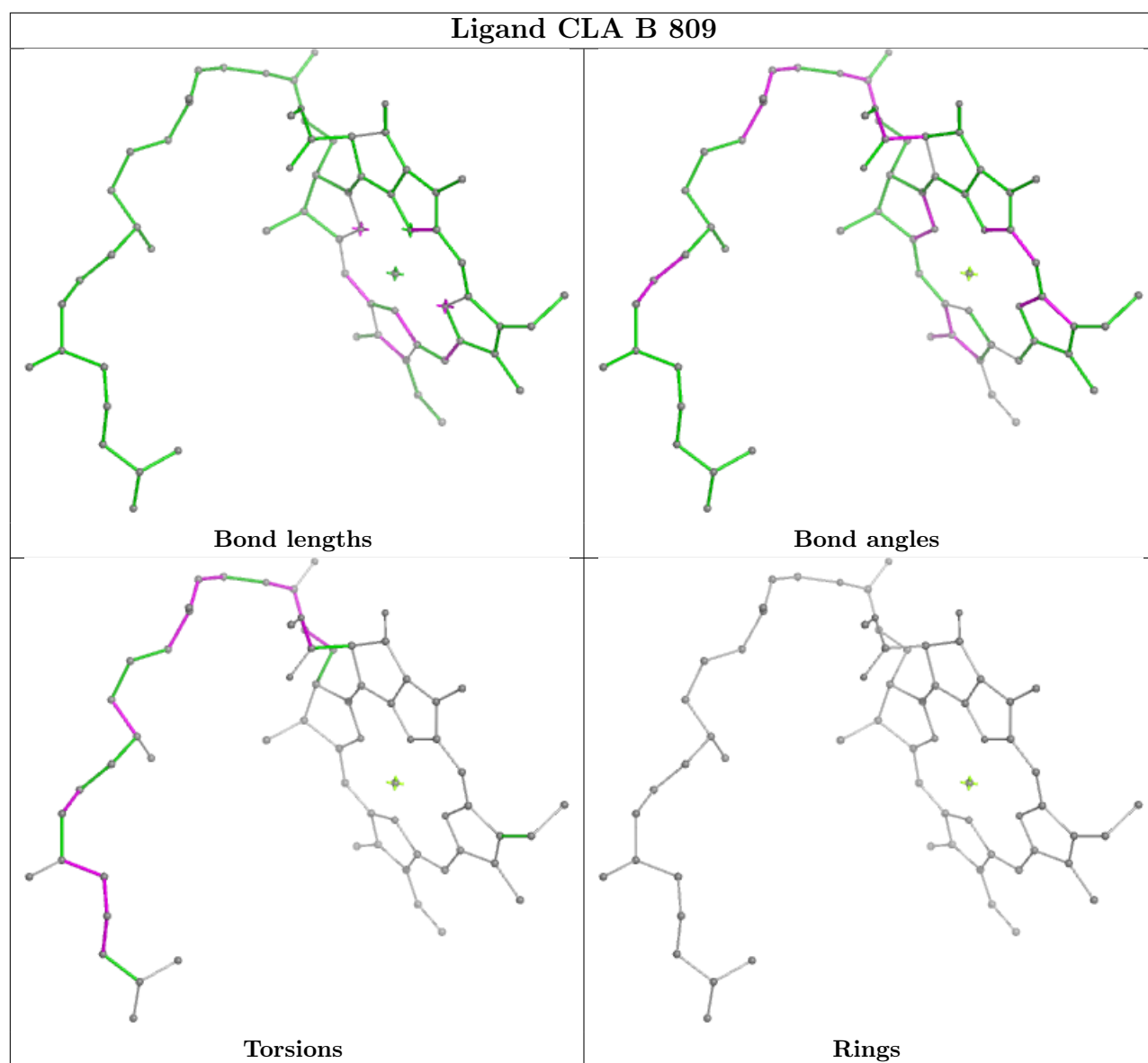
Ligand CLA A 806

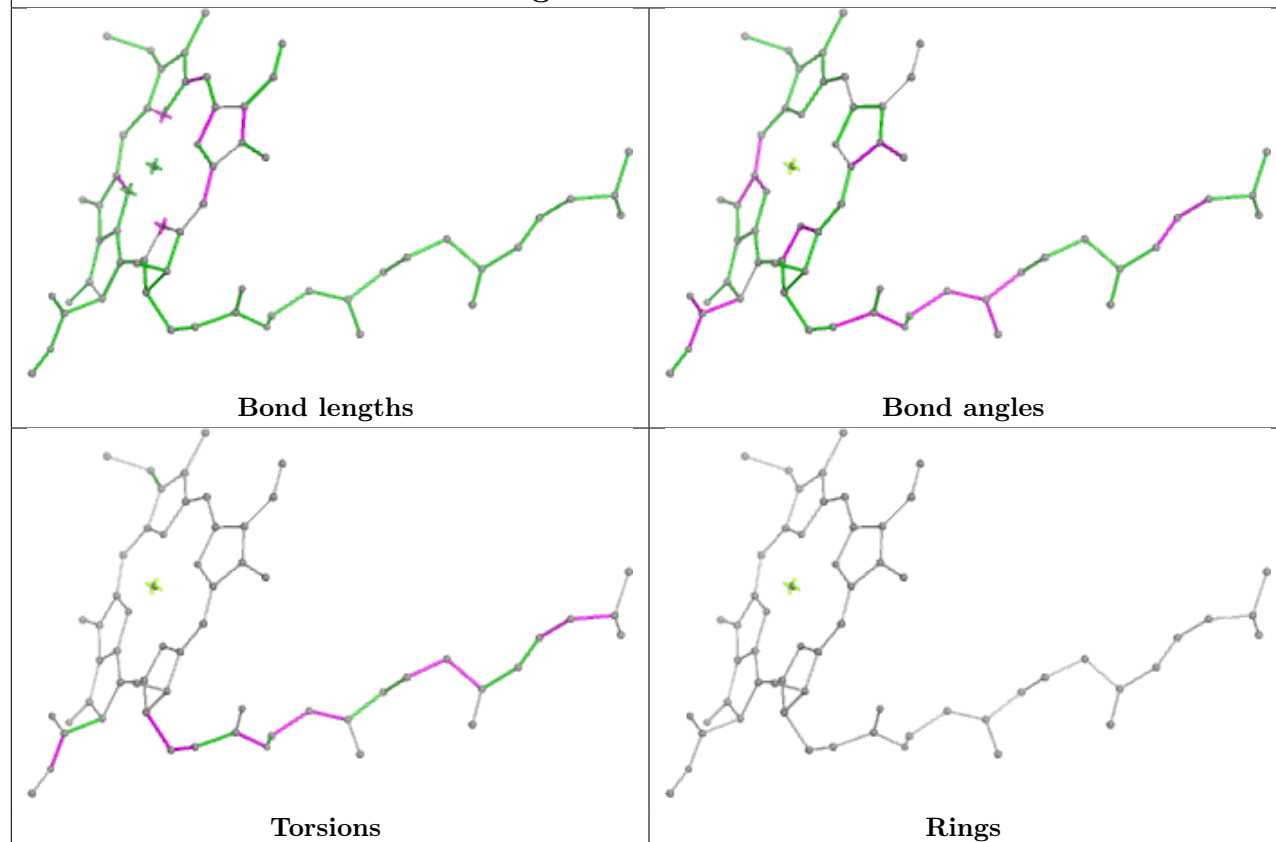
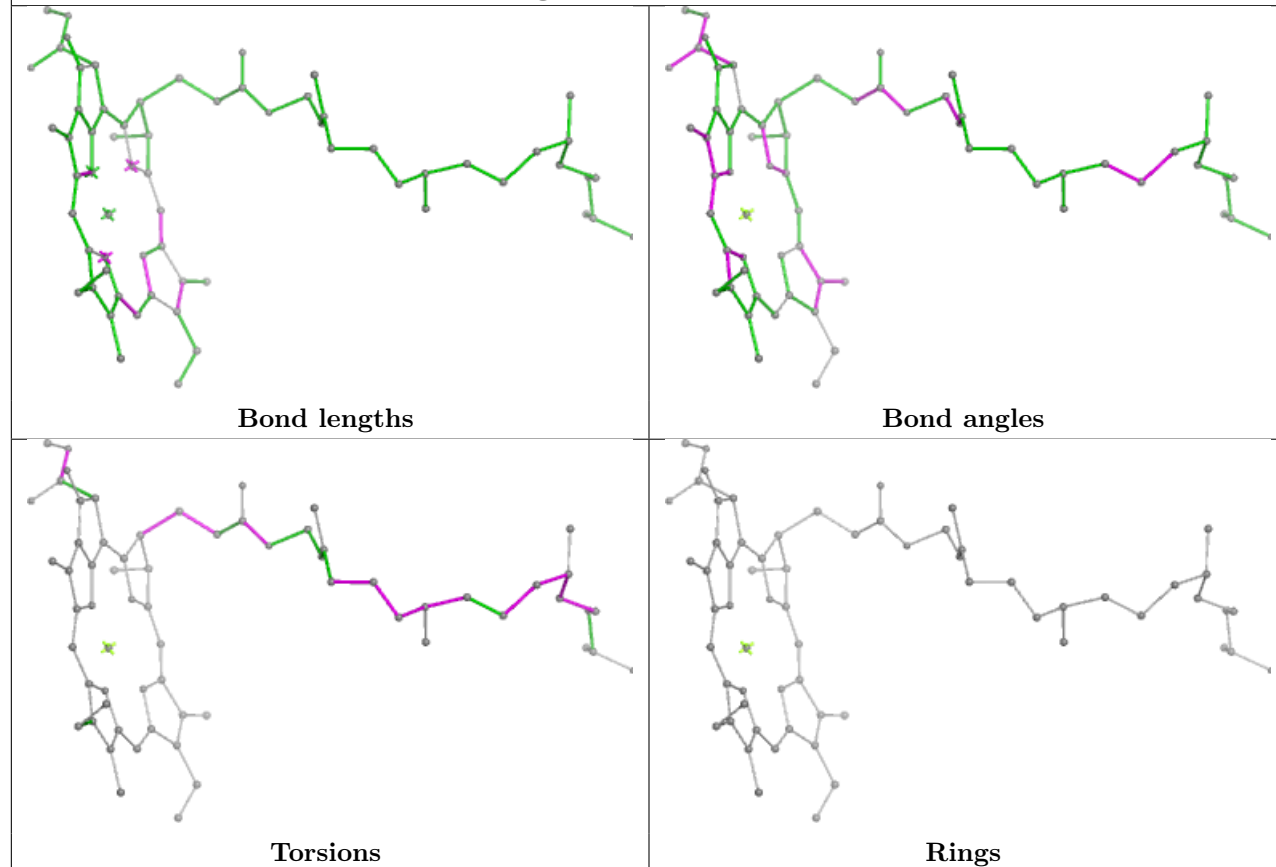


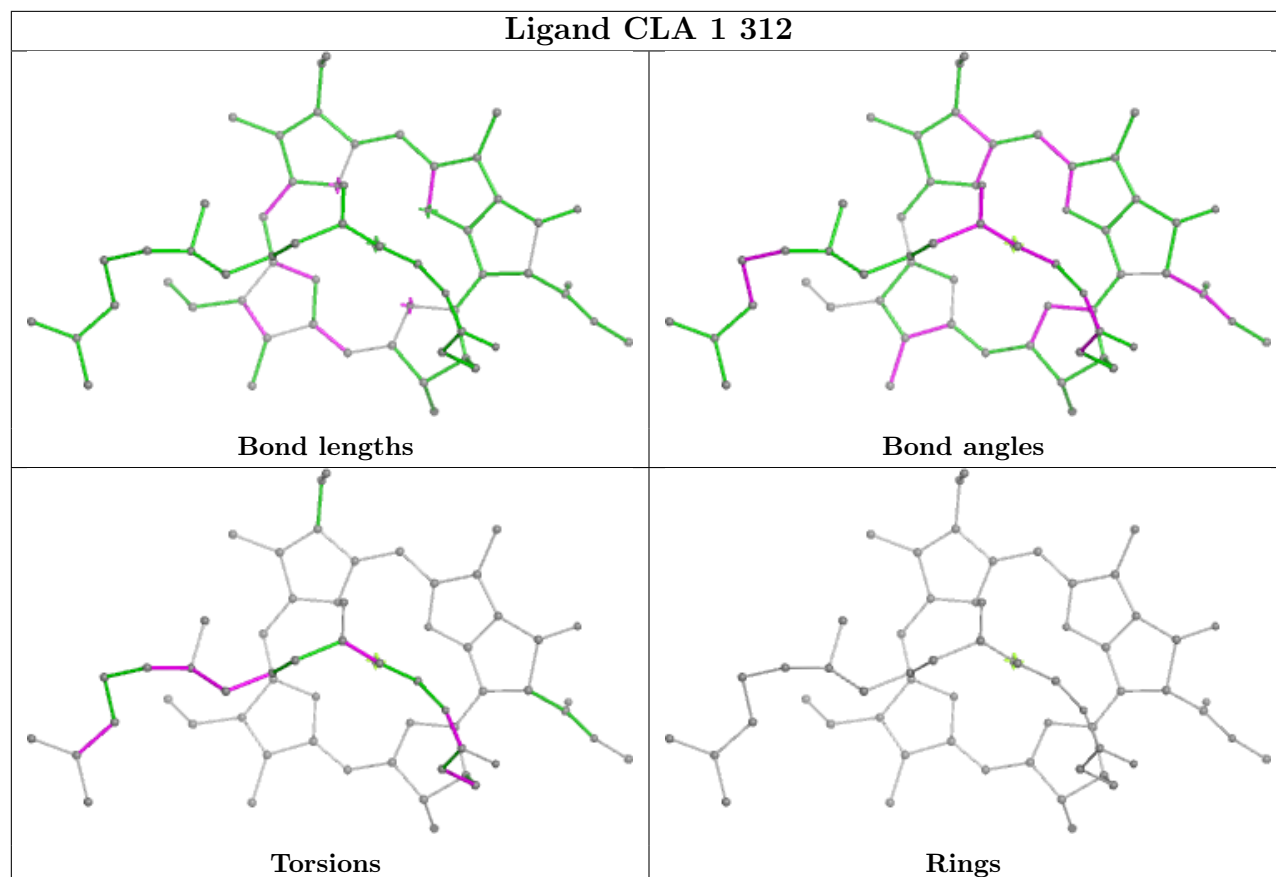
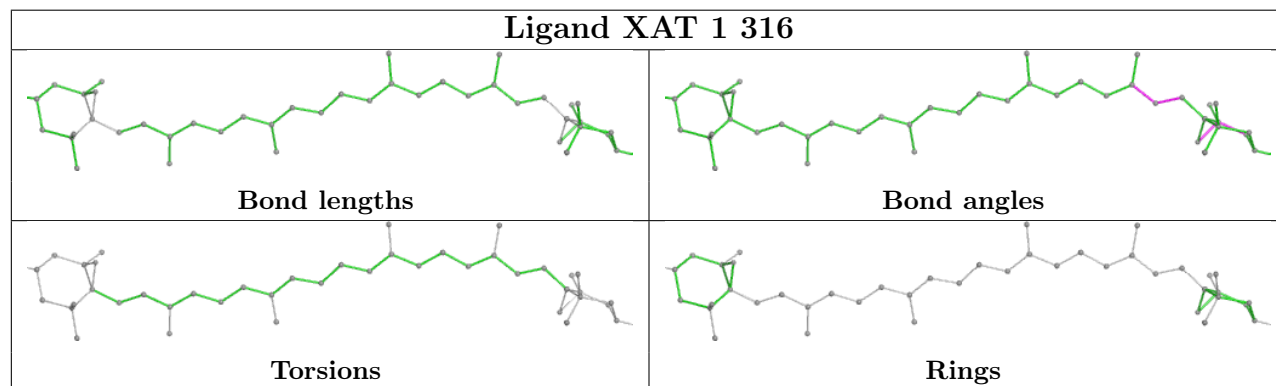
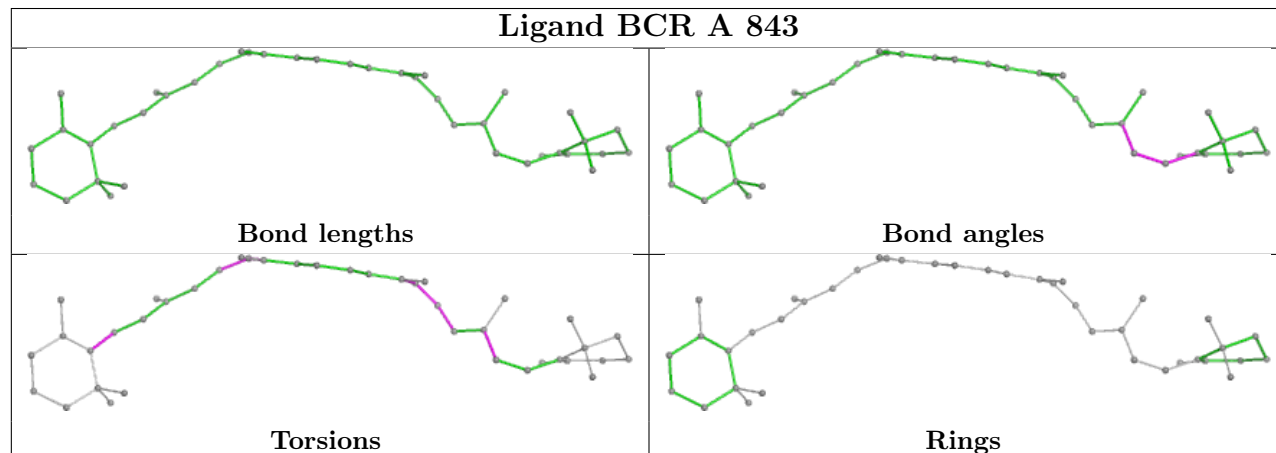


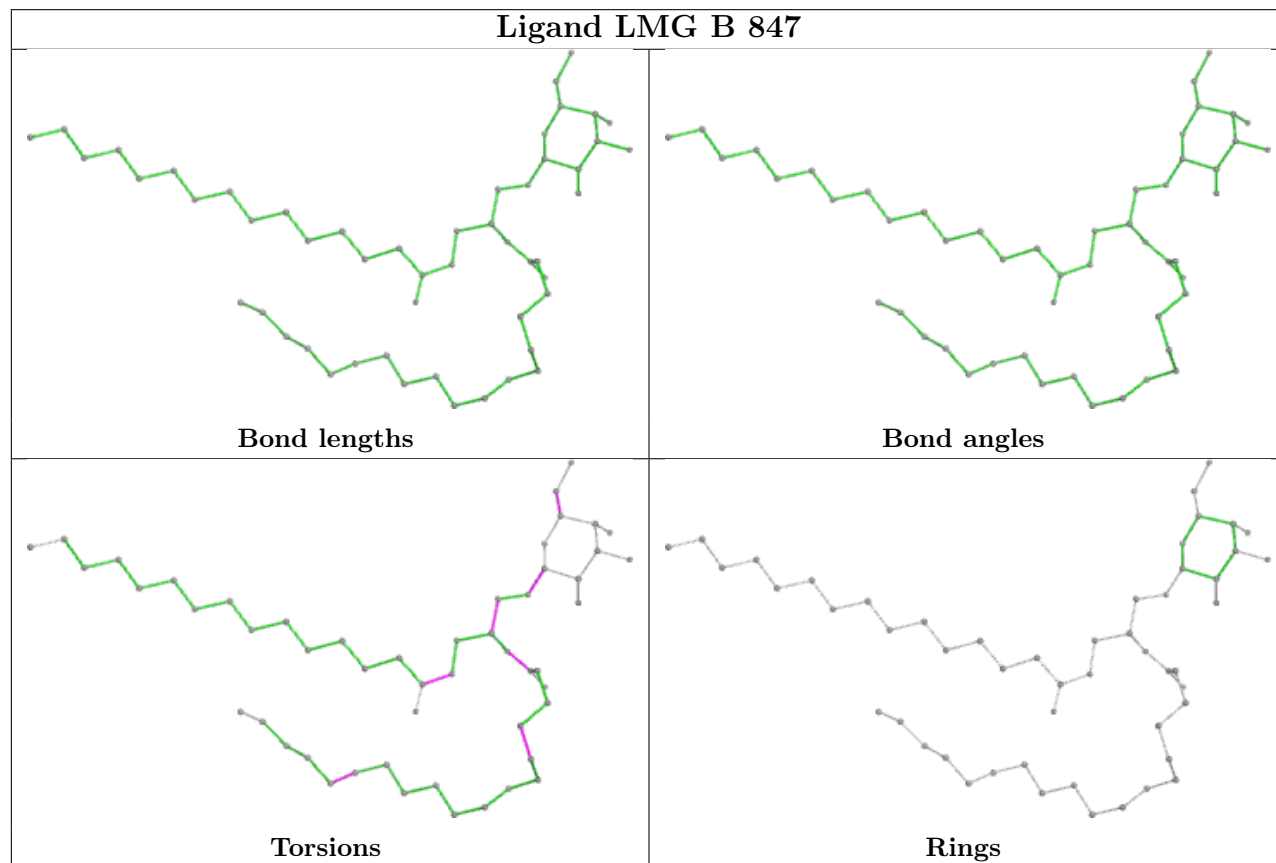
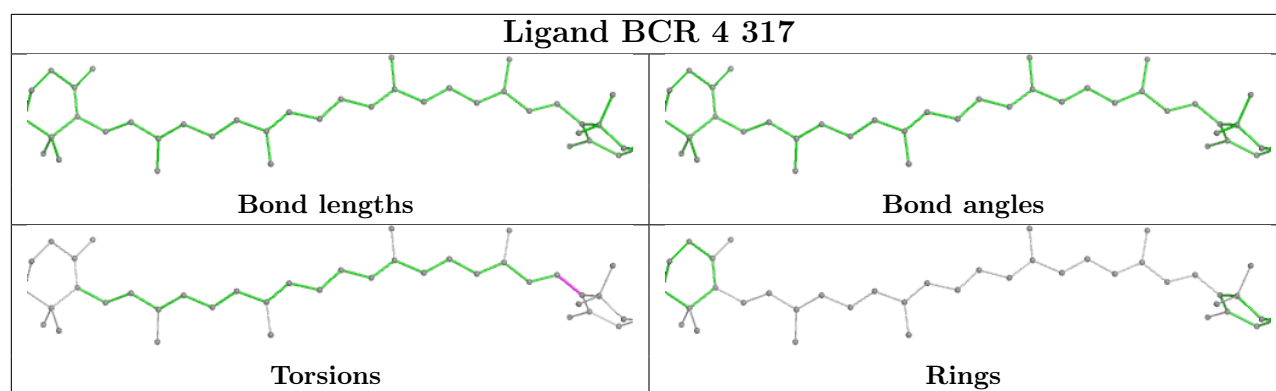
Ligand CLA 3 309



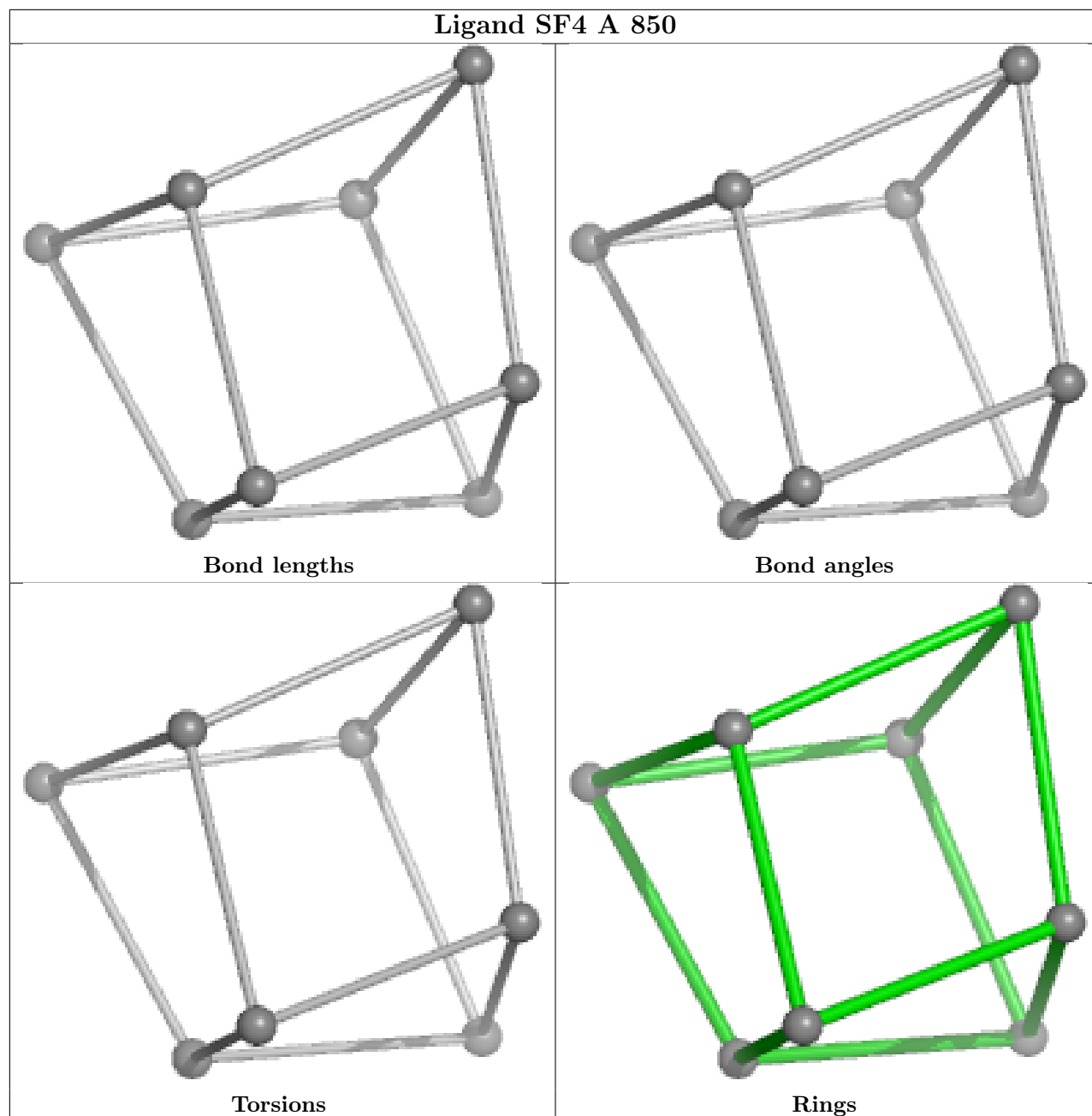


Ligand CLA B 830**Ligand CLA L 302**

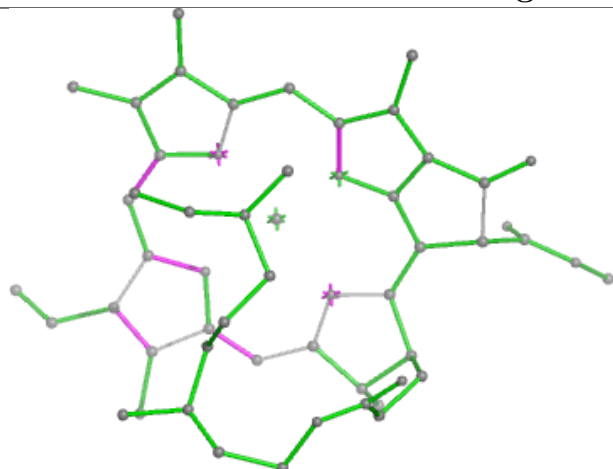
Ligand CLA 1 312**Ligand XAT 1 316****Ligand BCR A 843**



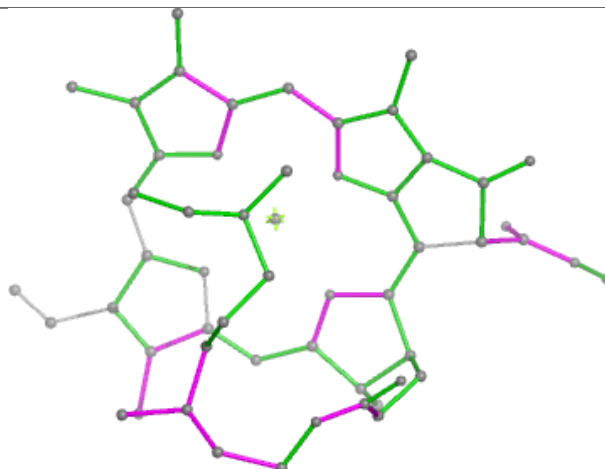
Ligand SF4 A 850



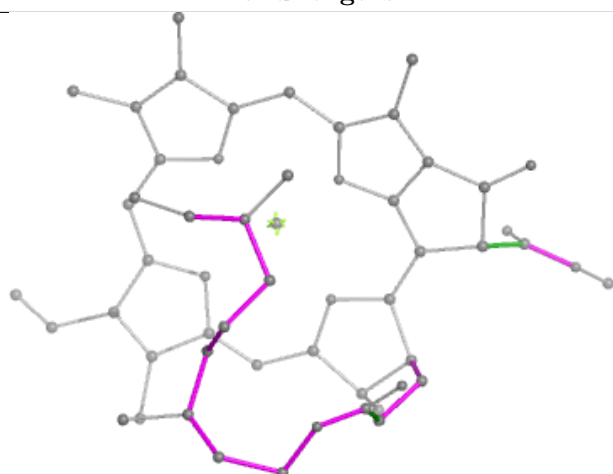
Ligand CLA L 301



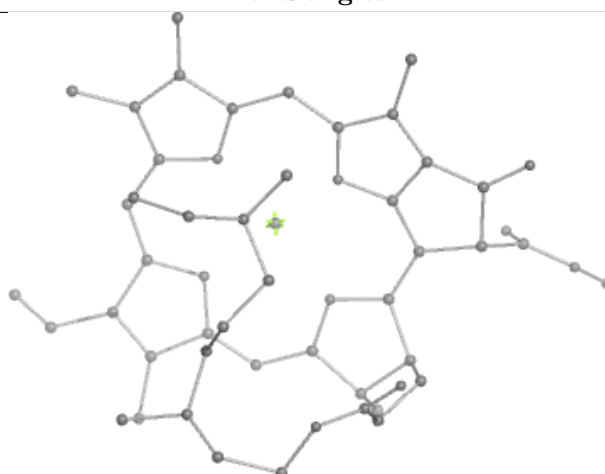
Bond lengths



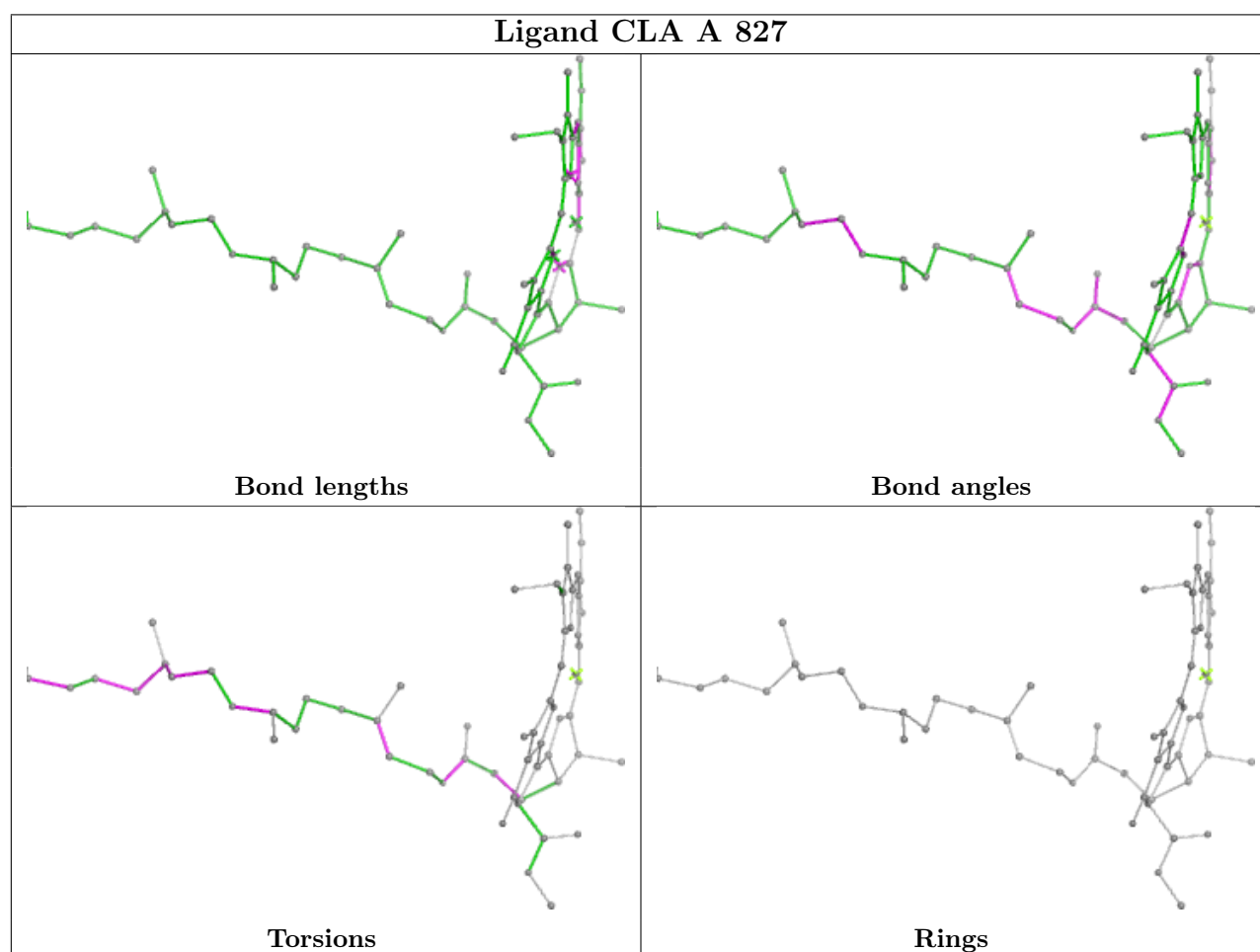
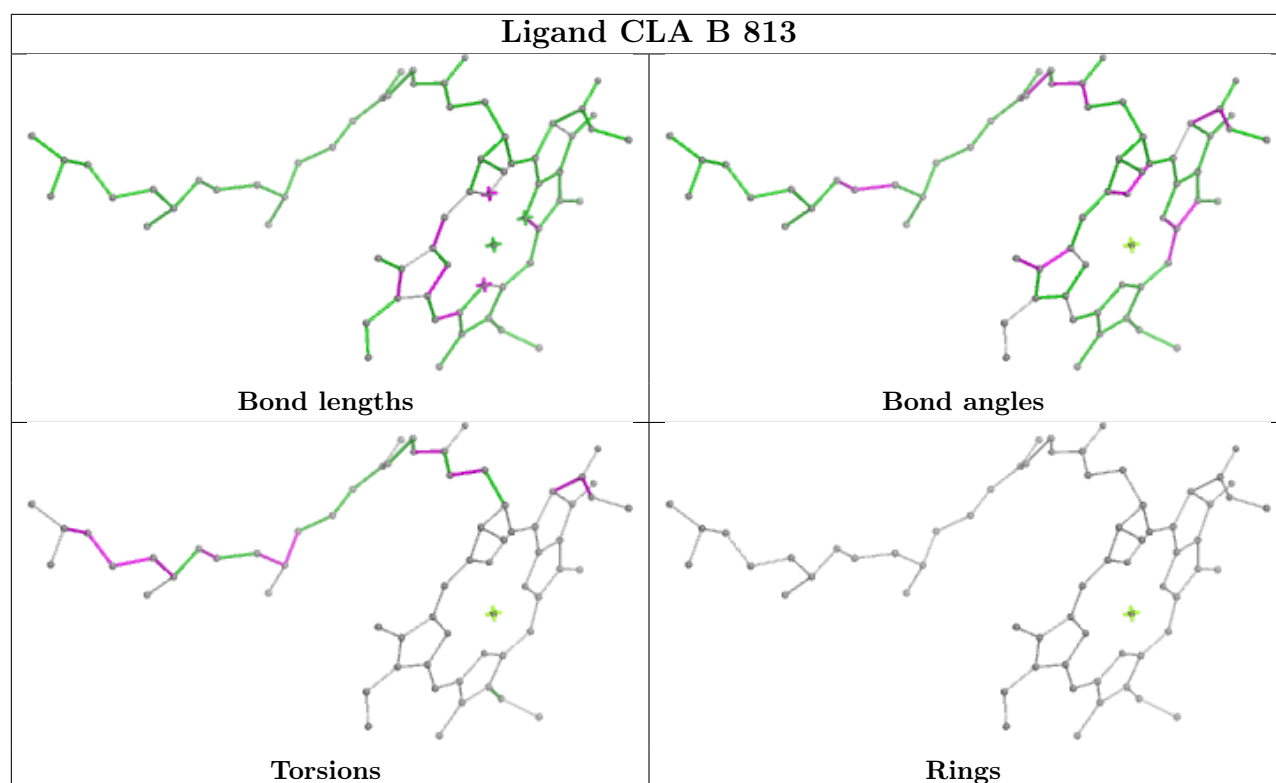
Bond angles

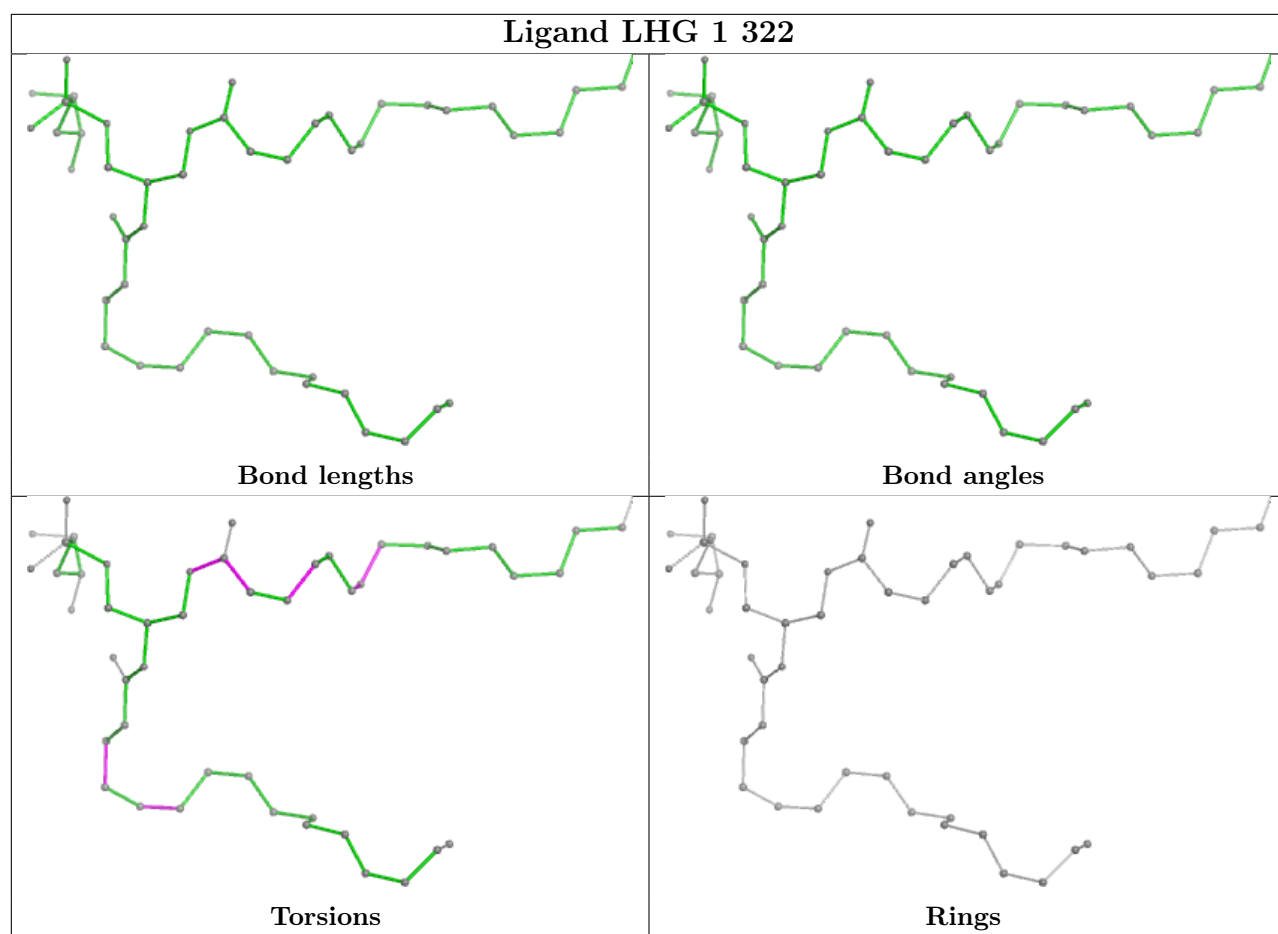


Torsions

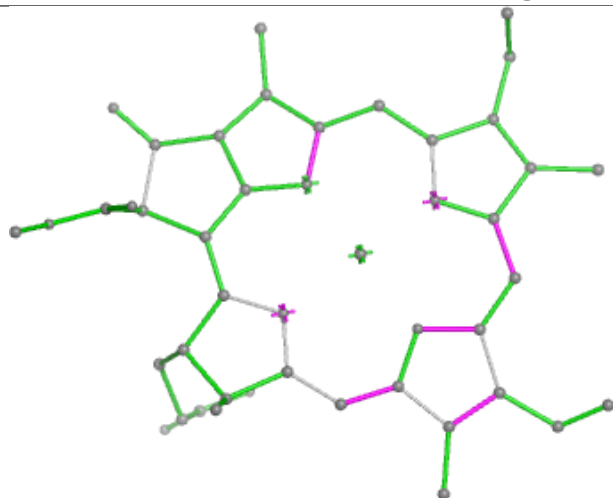


Rings

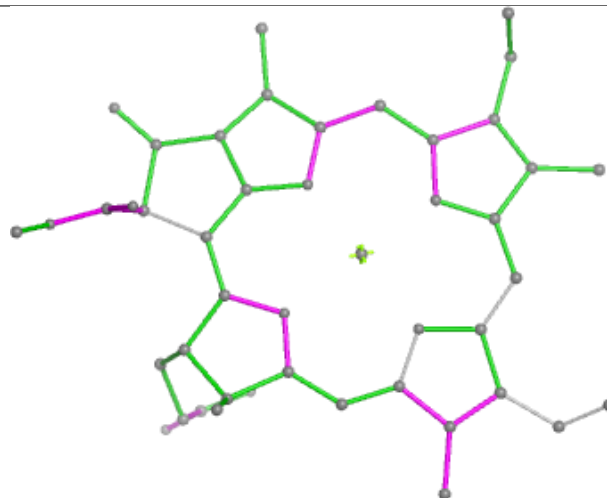




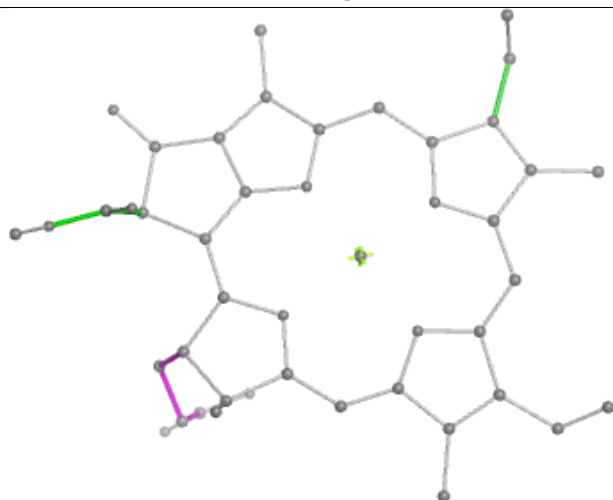
Ligand CLA 3 306



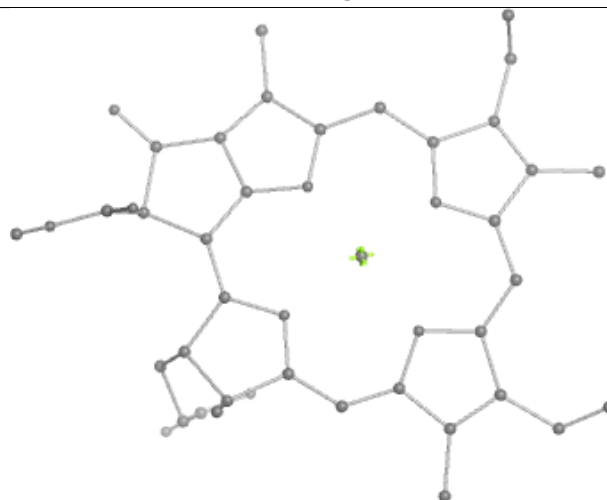
Bond lengths



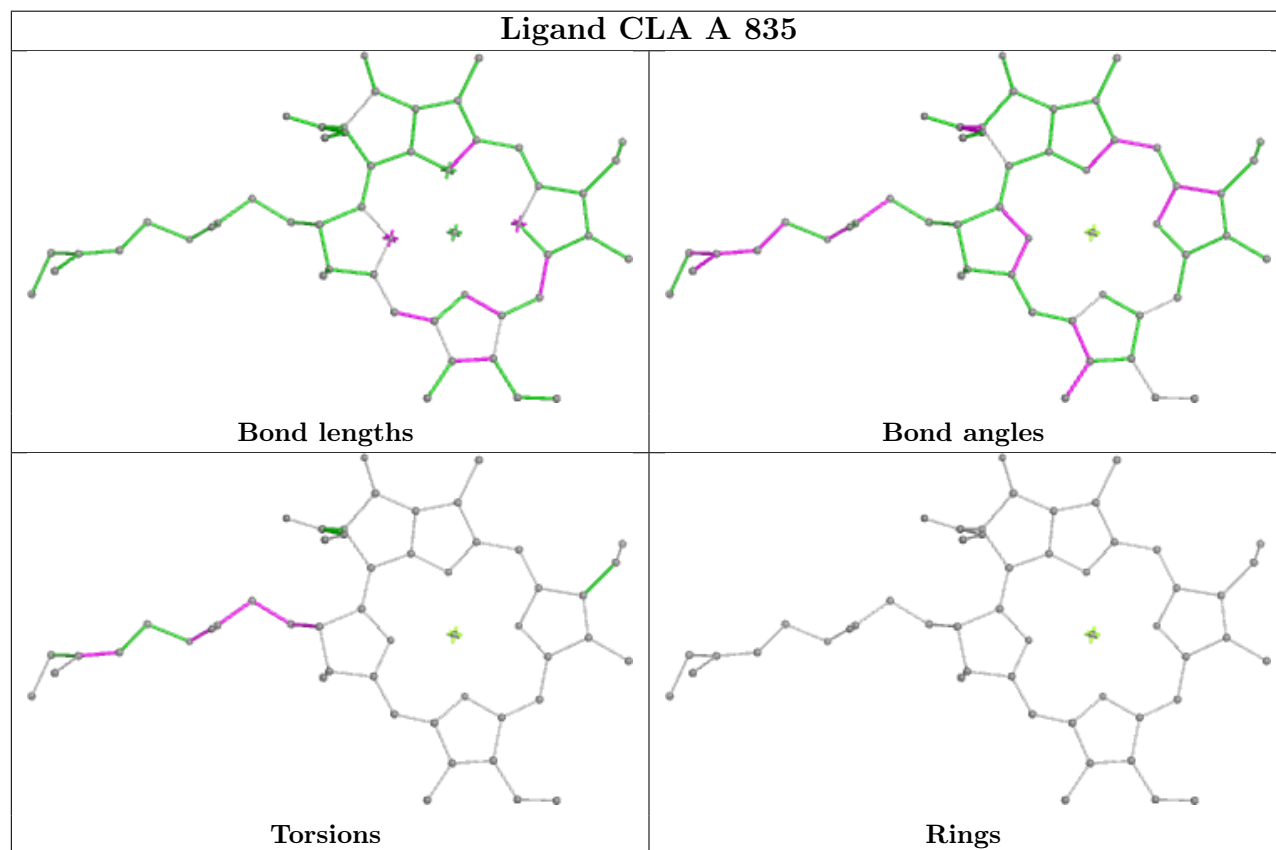
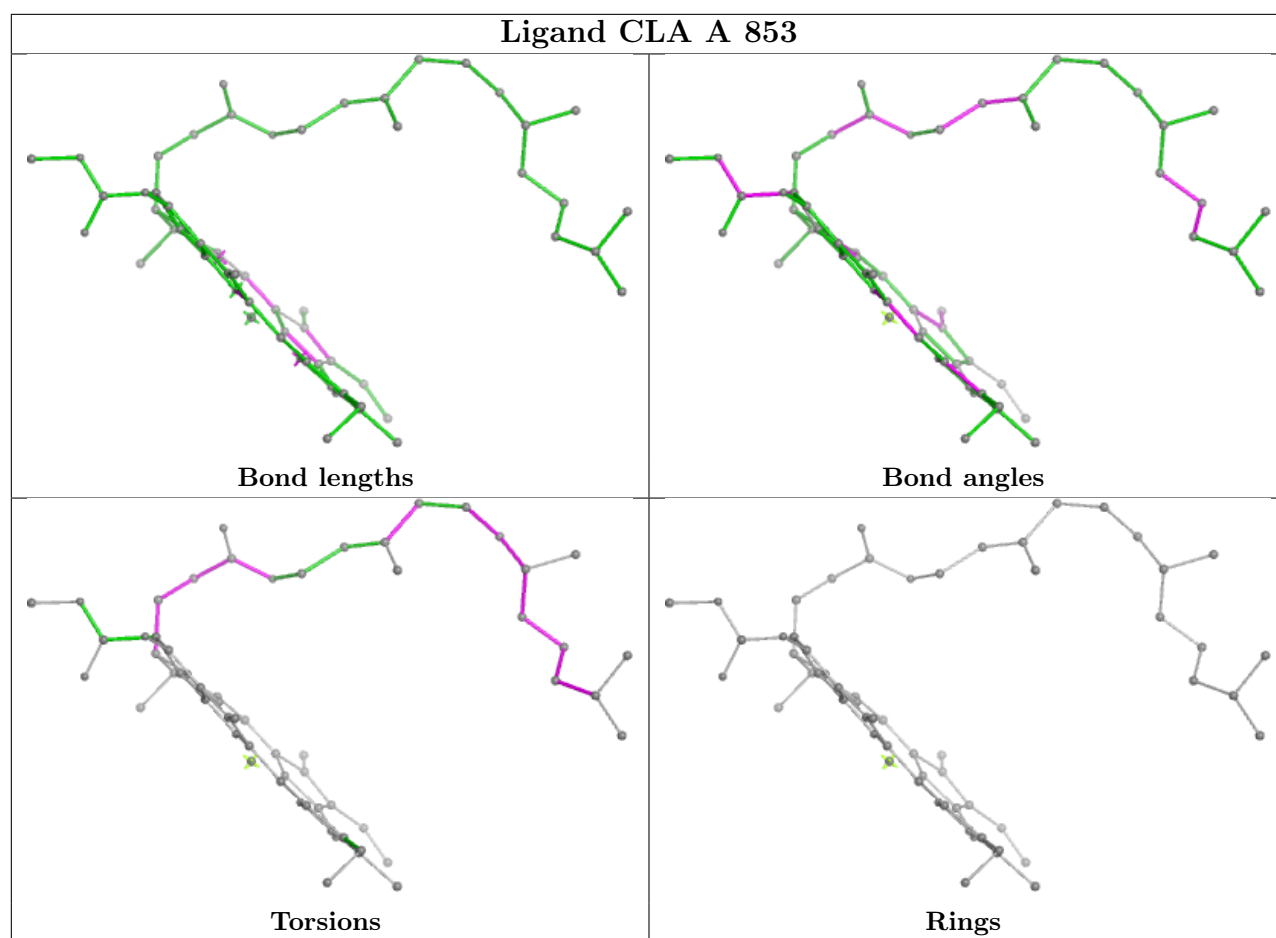
Bond angles



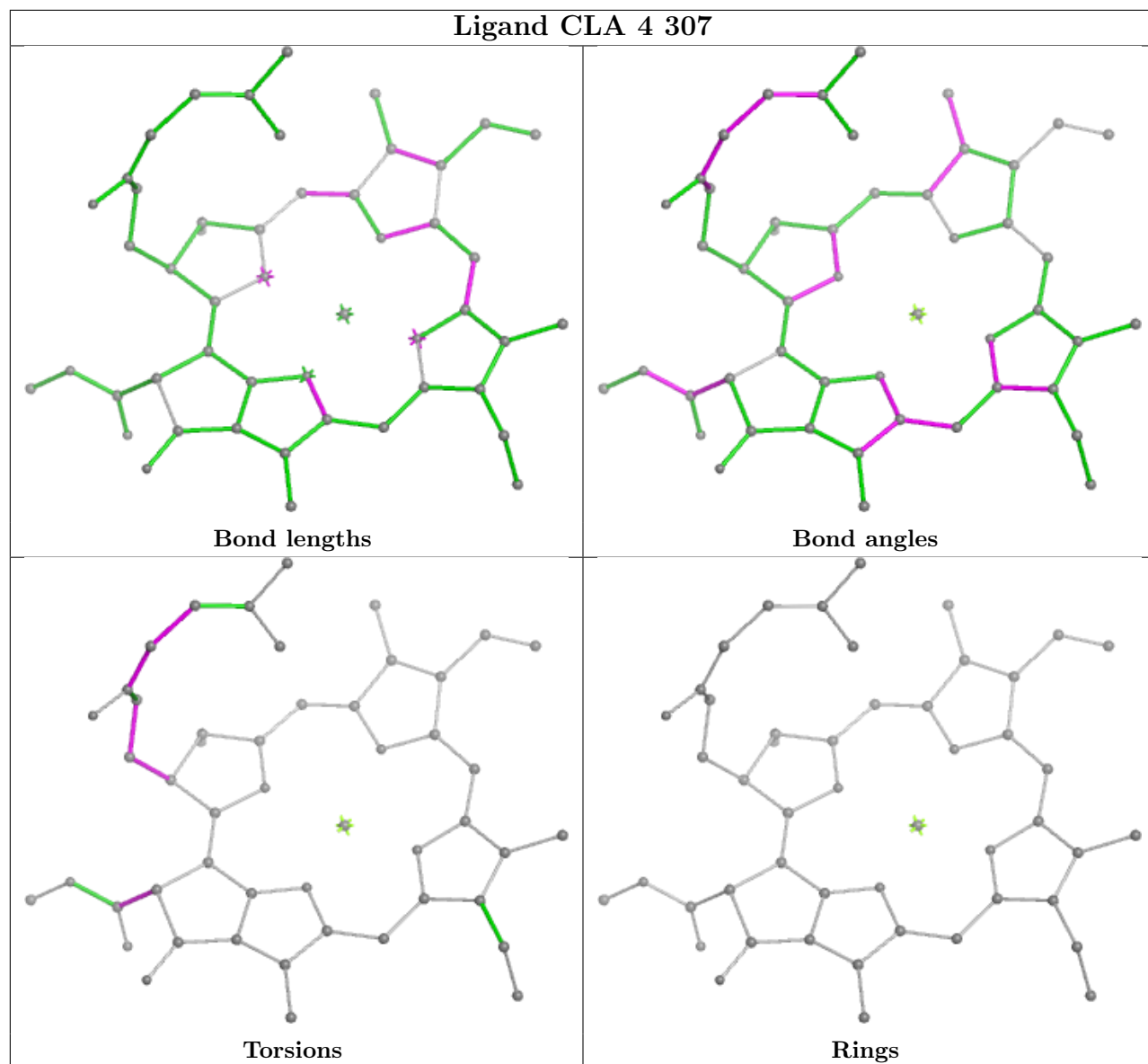
Torsions

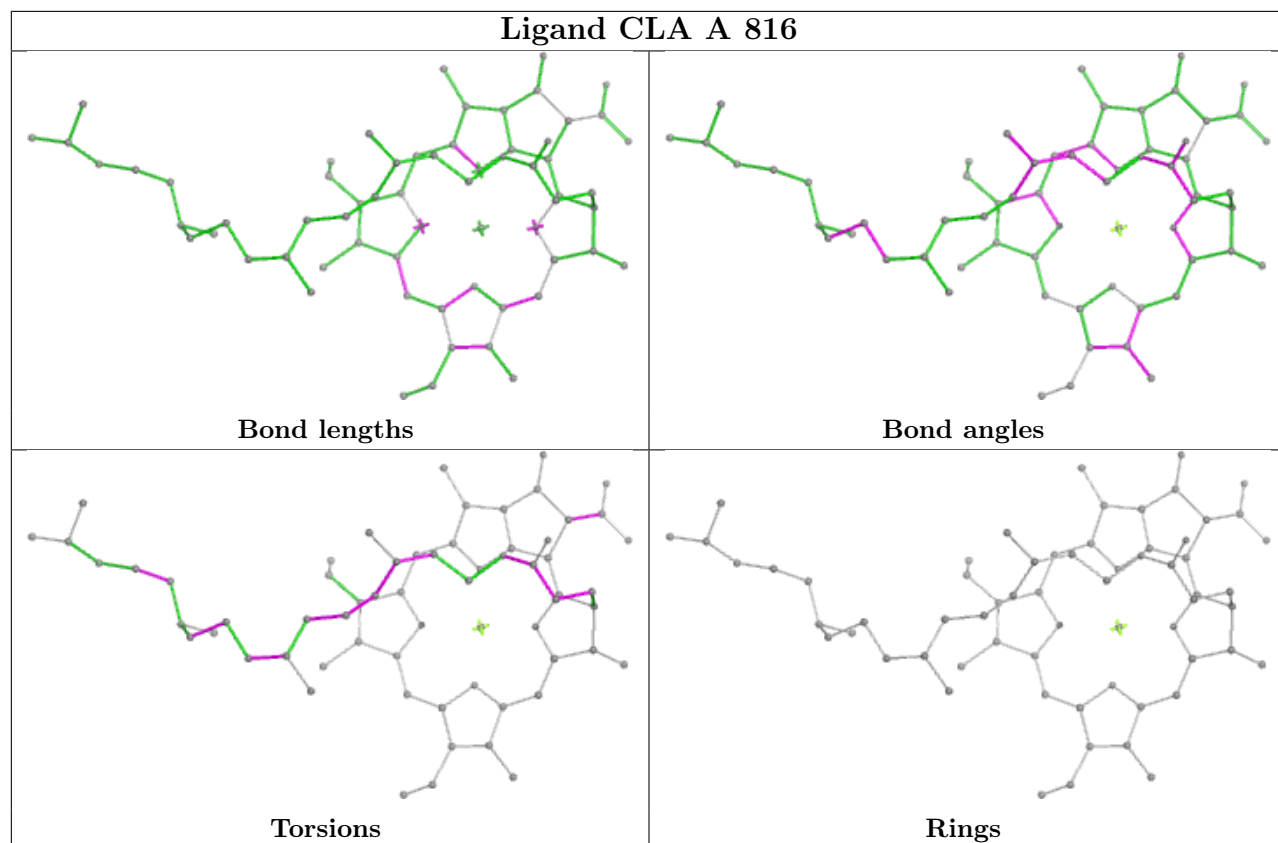


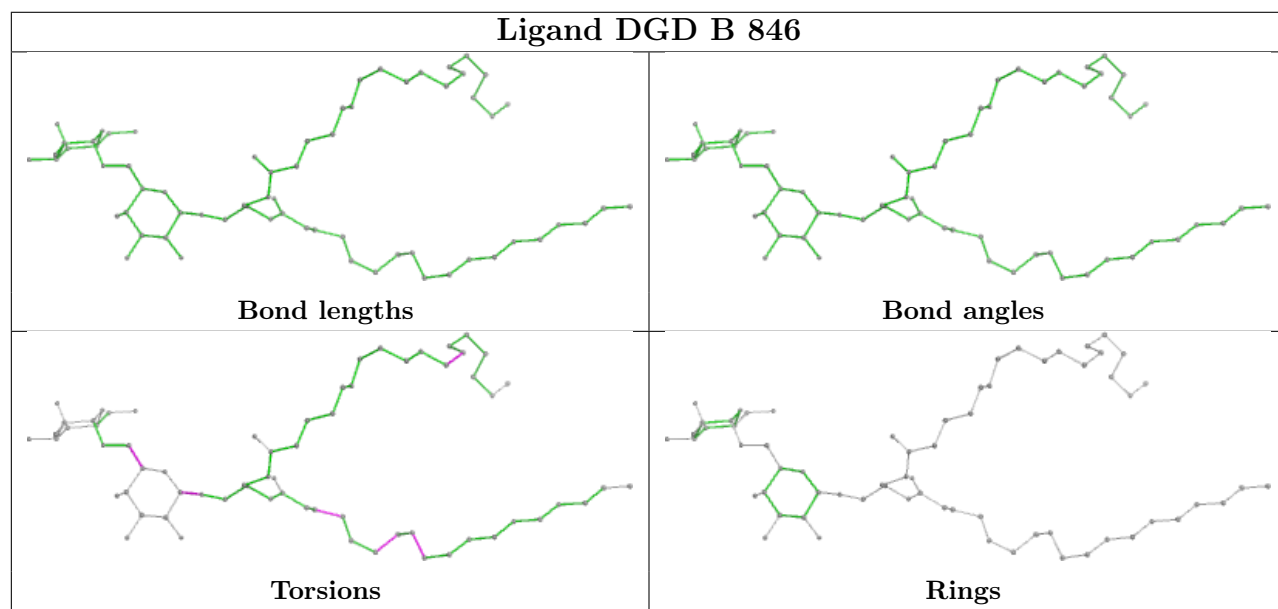
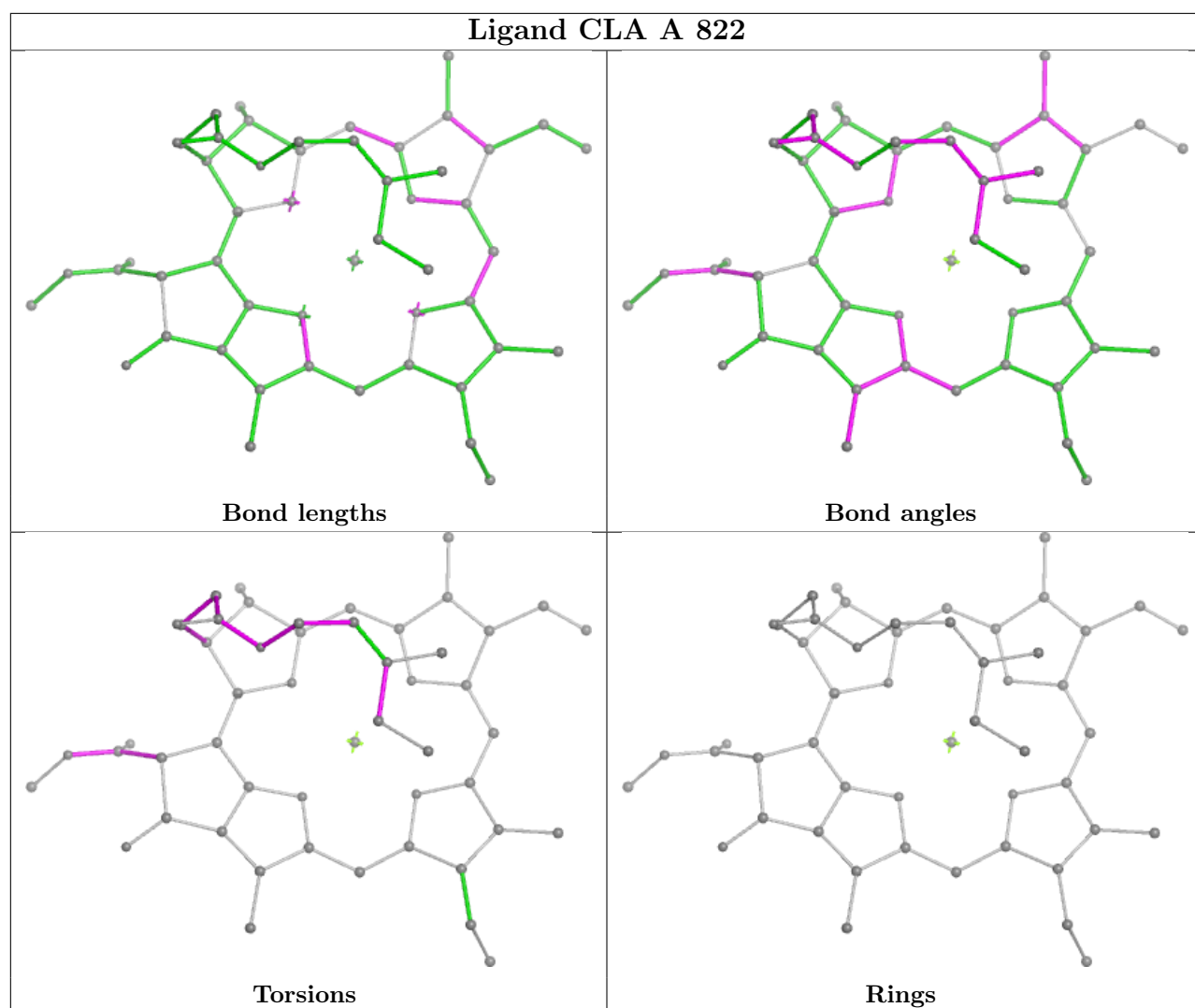
Rings

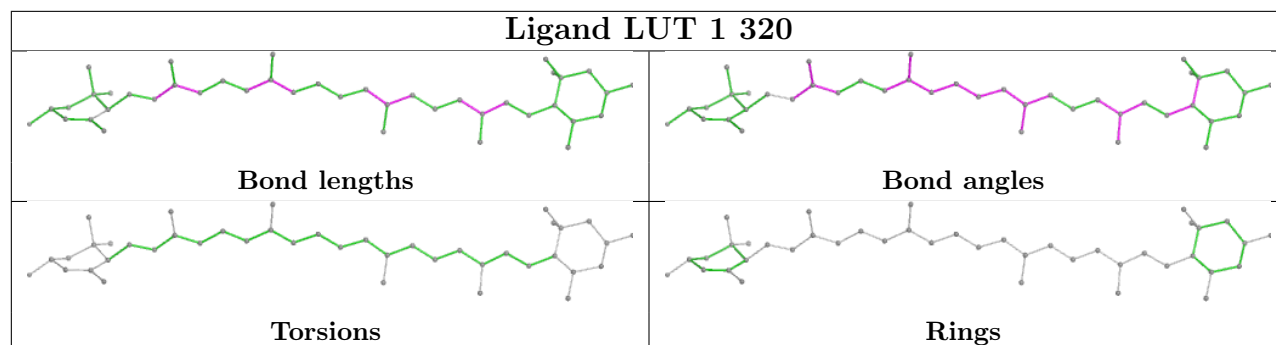
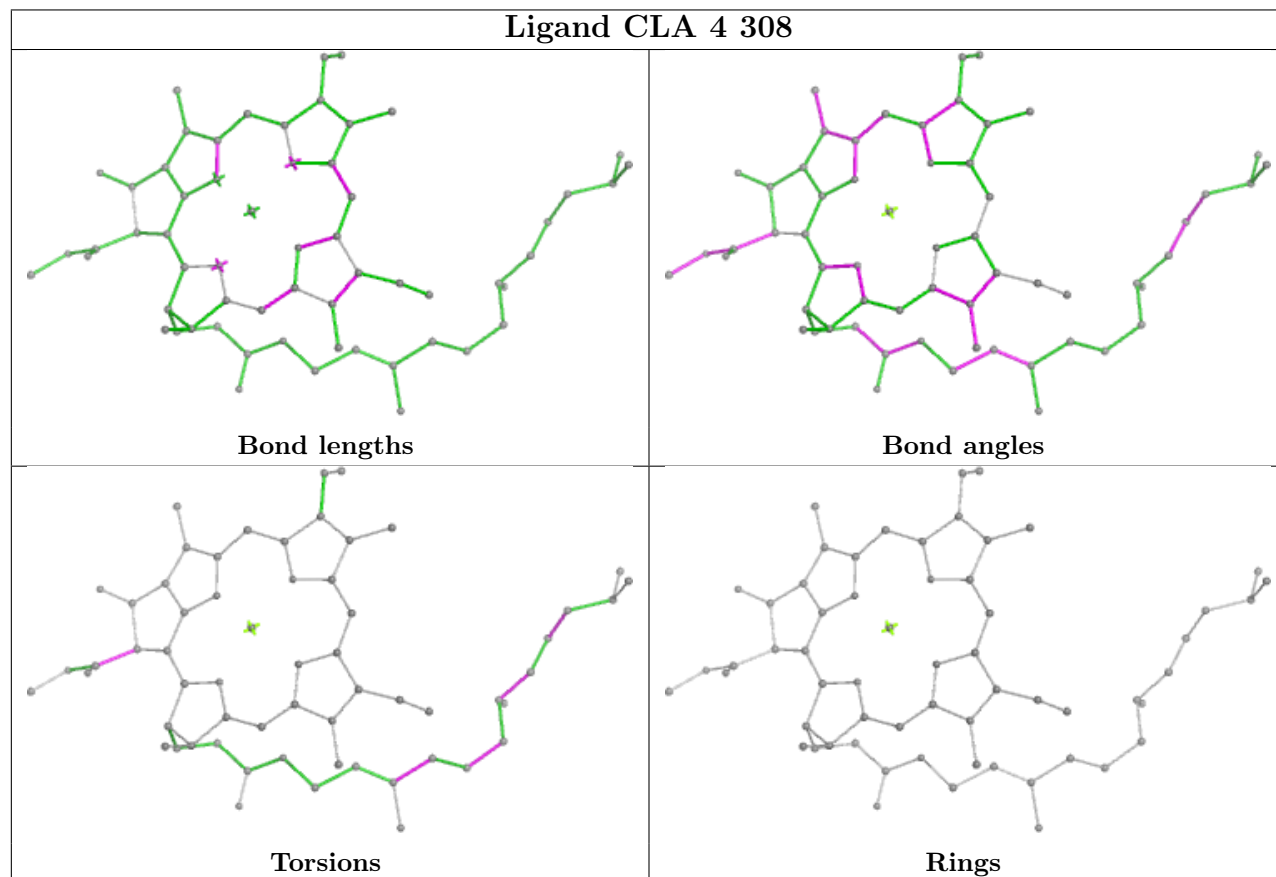


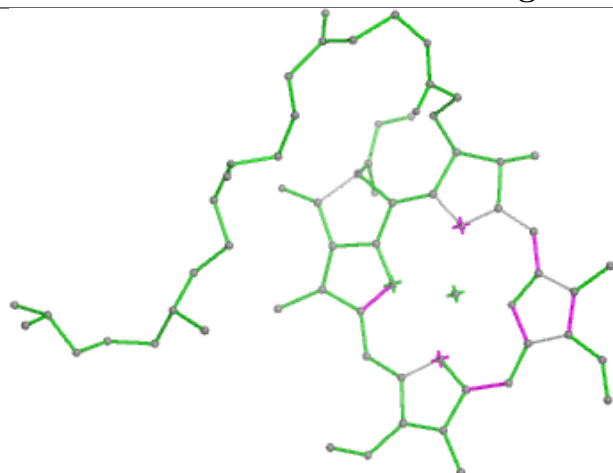
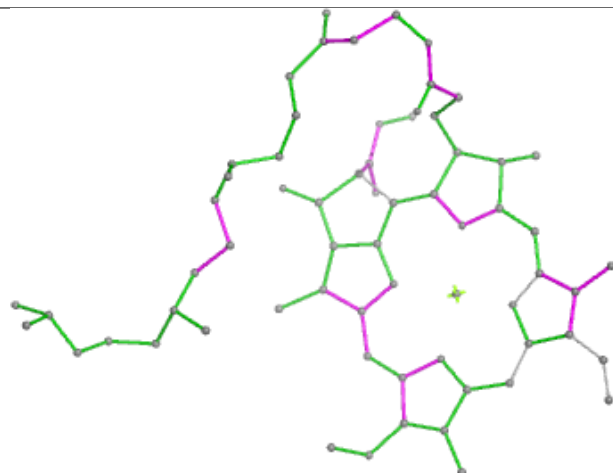
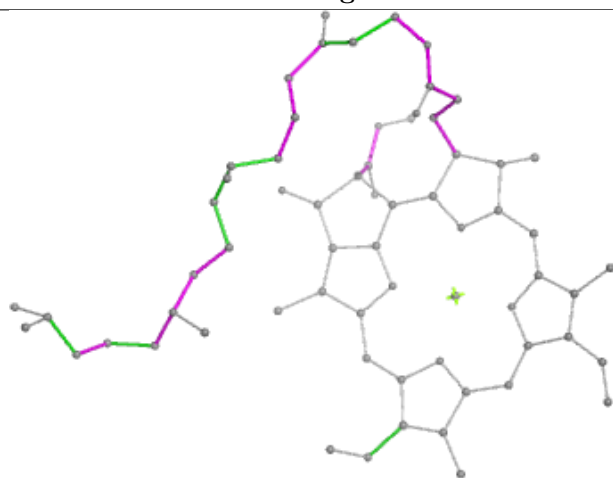
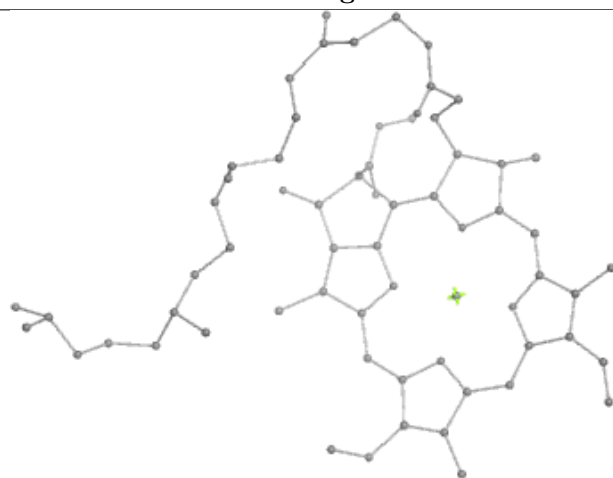
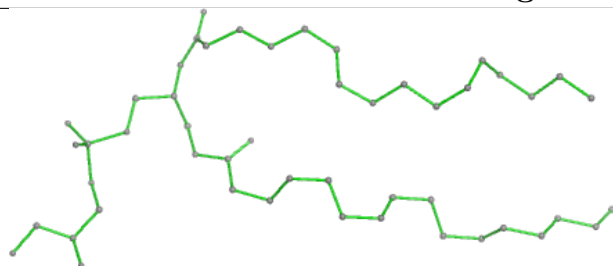
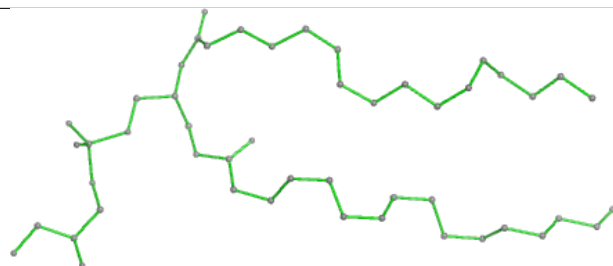
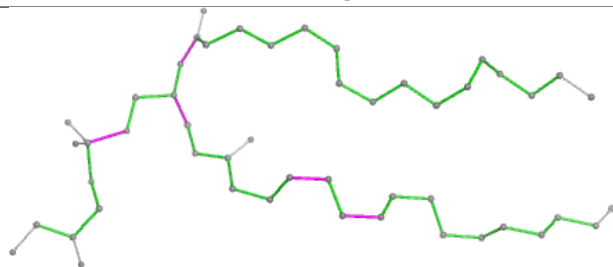
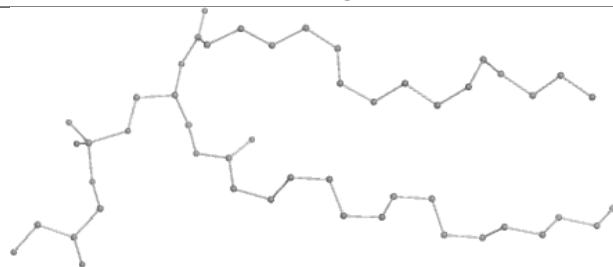
Ligand CLA 4 307

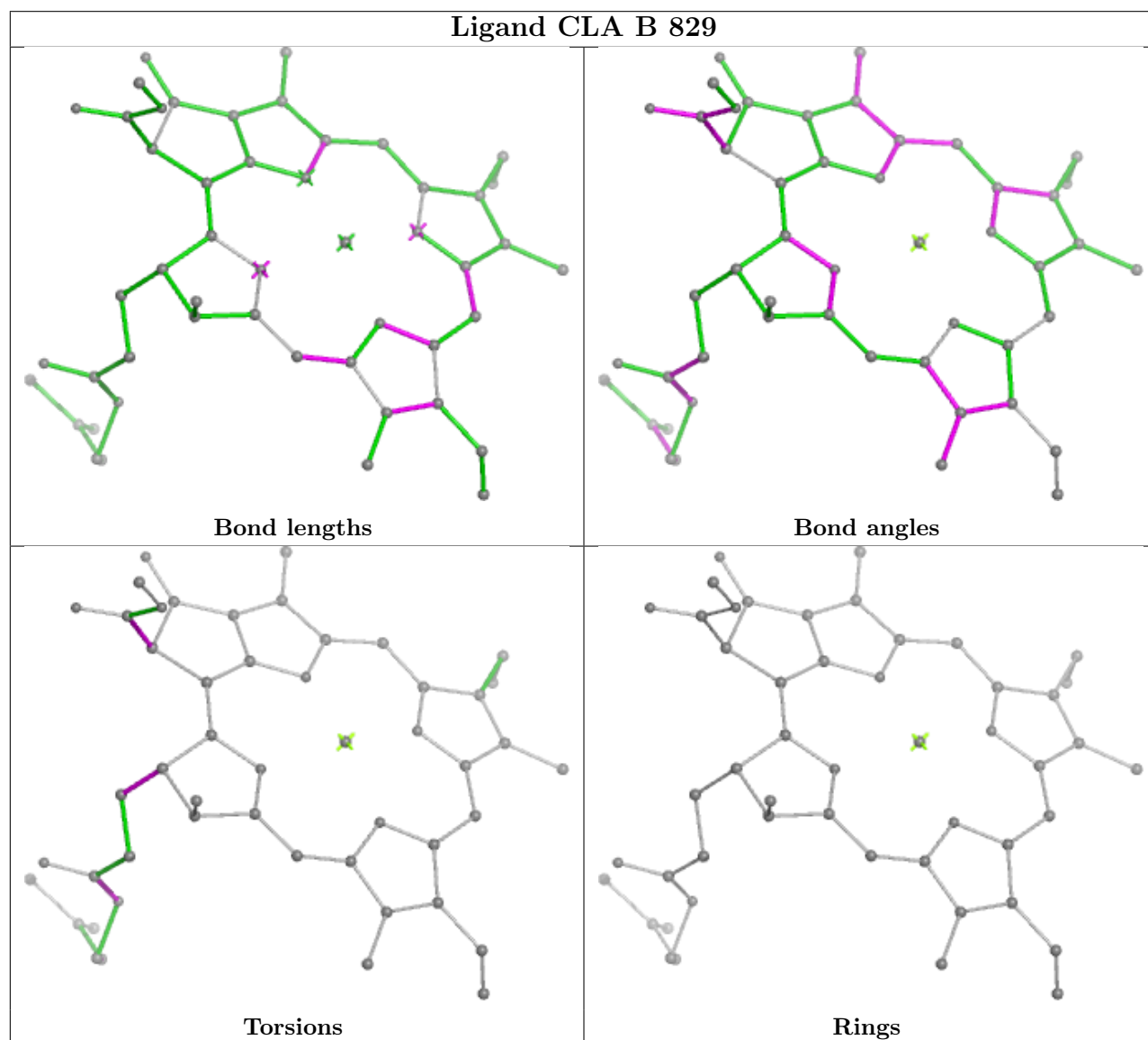
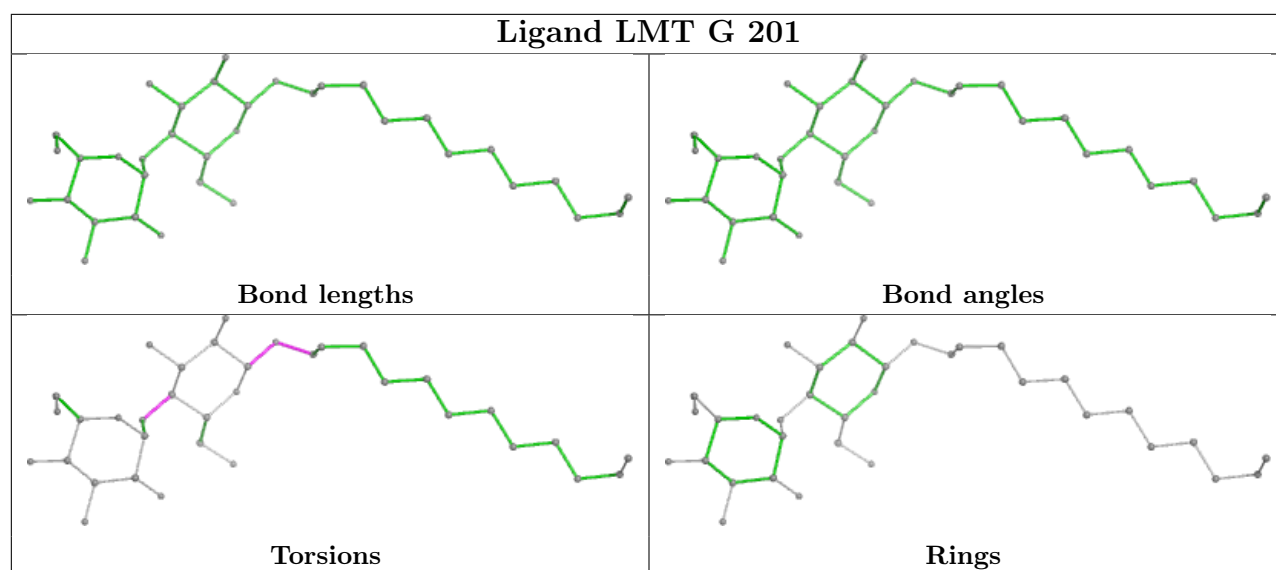


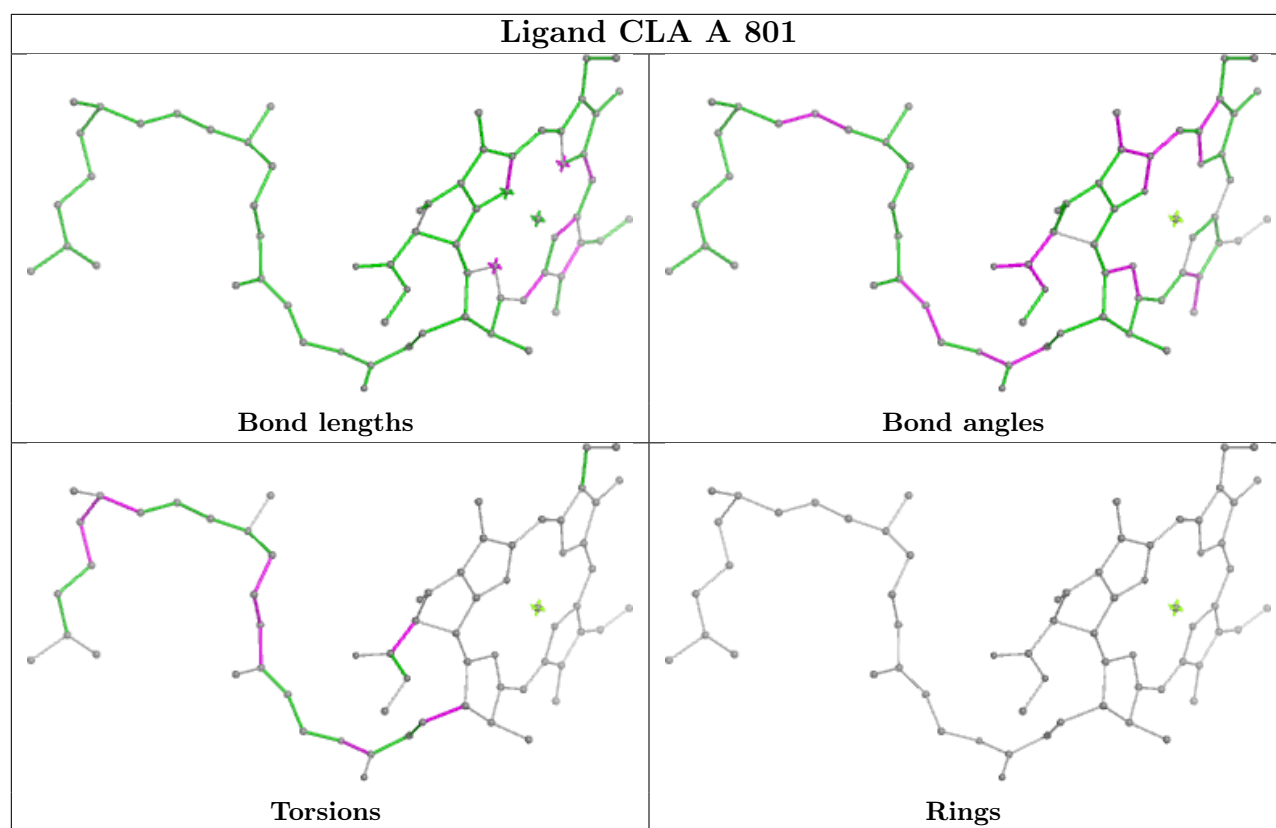




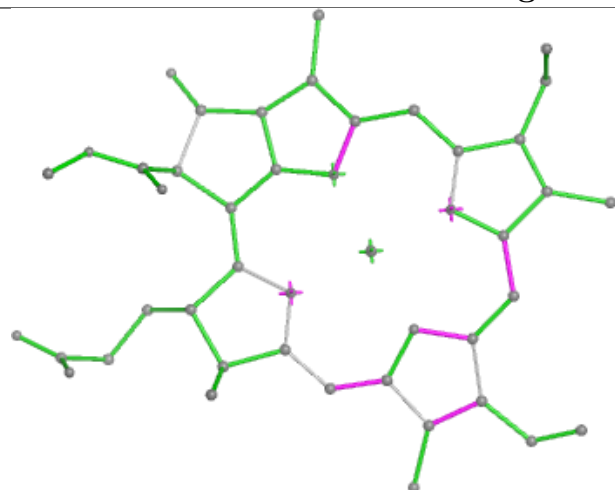
Ligand LUT 1 320**Ligand CLA 4 308**

Ligand CLA 4 313**Bond lengths****Bond angles****Torsions****Rings****Ligand LHG 1 317****Bond lengths****Bond angles****Torsions****Rings**

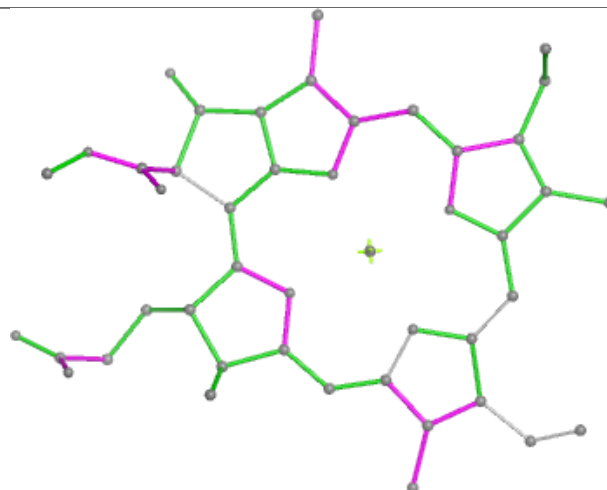




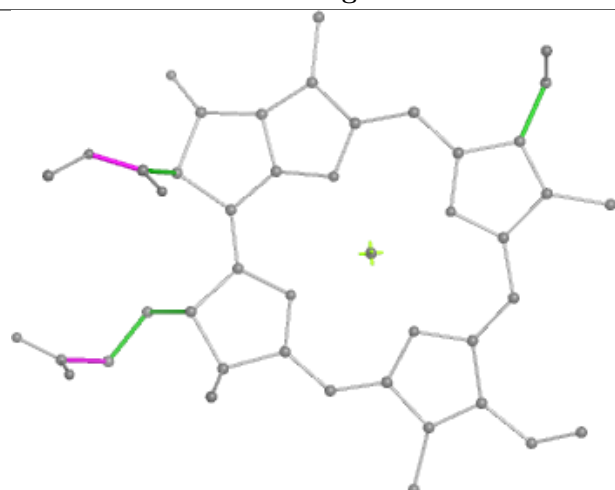
Ligand CLA F 303



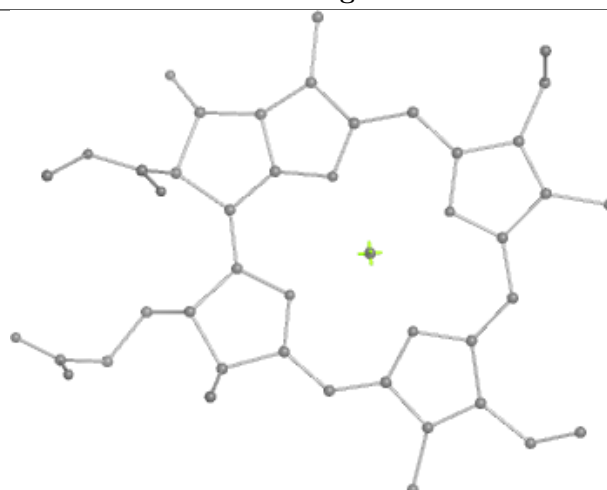
Bond lengths



Bond angles

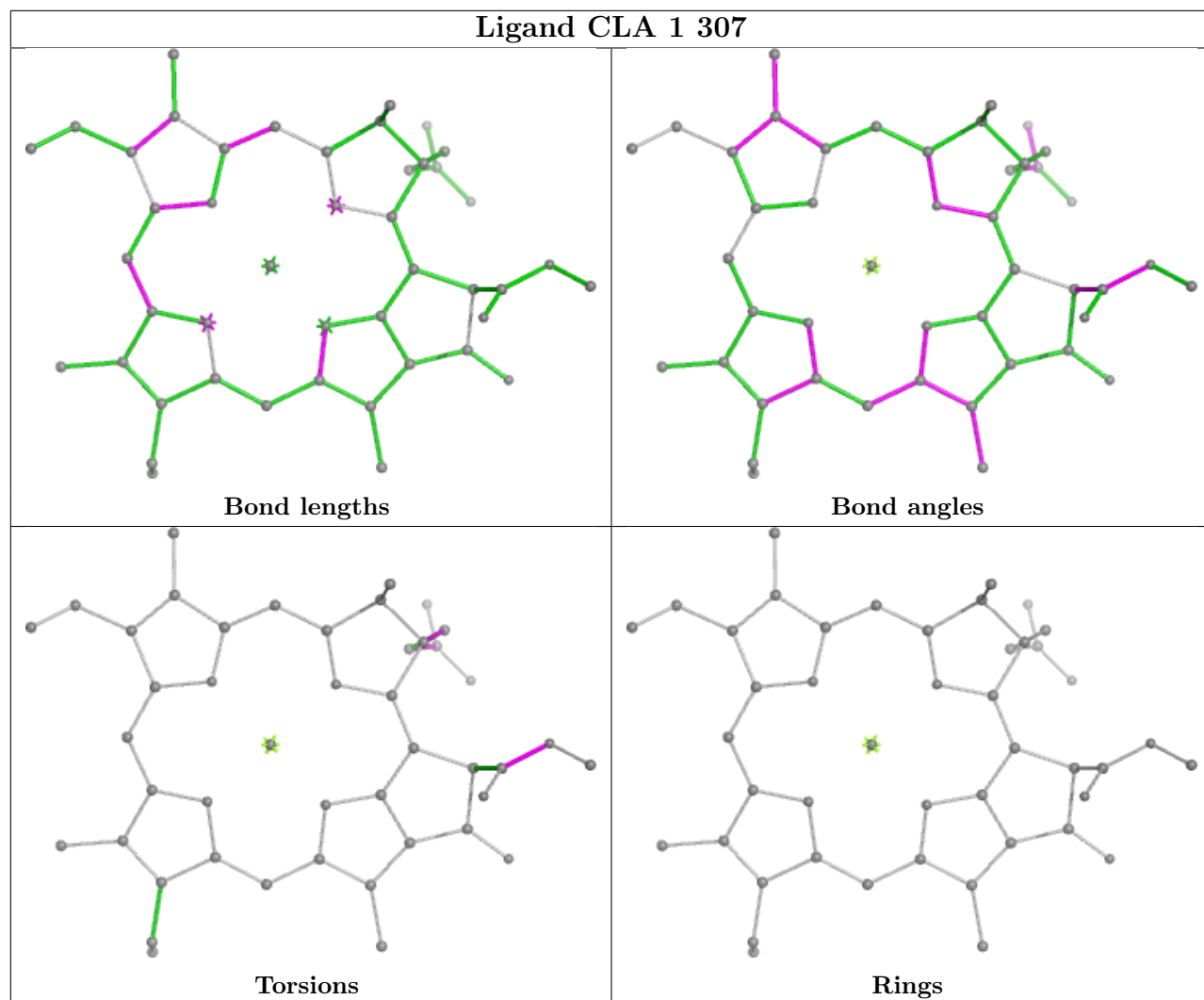


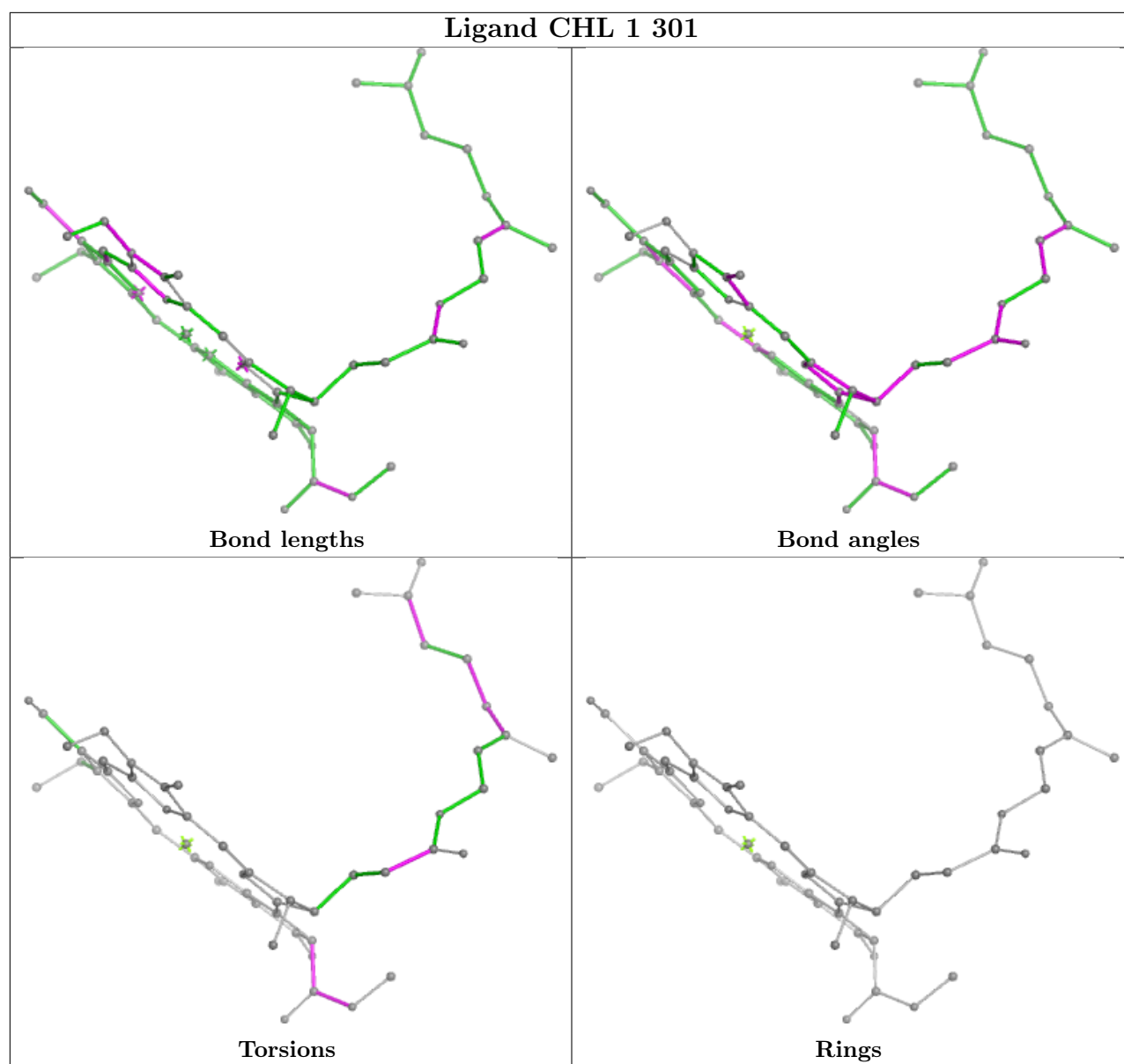
Torsions

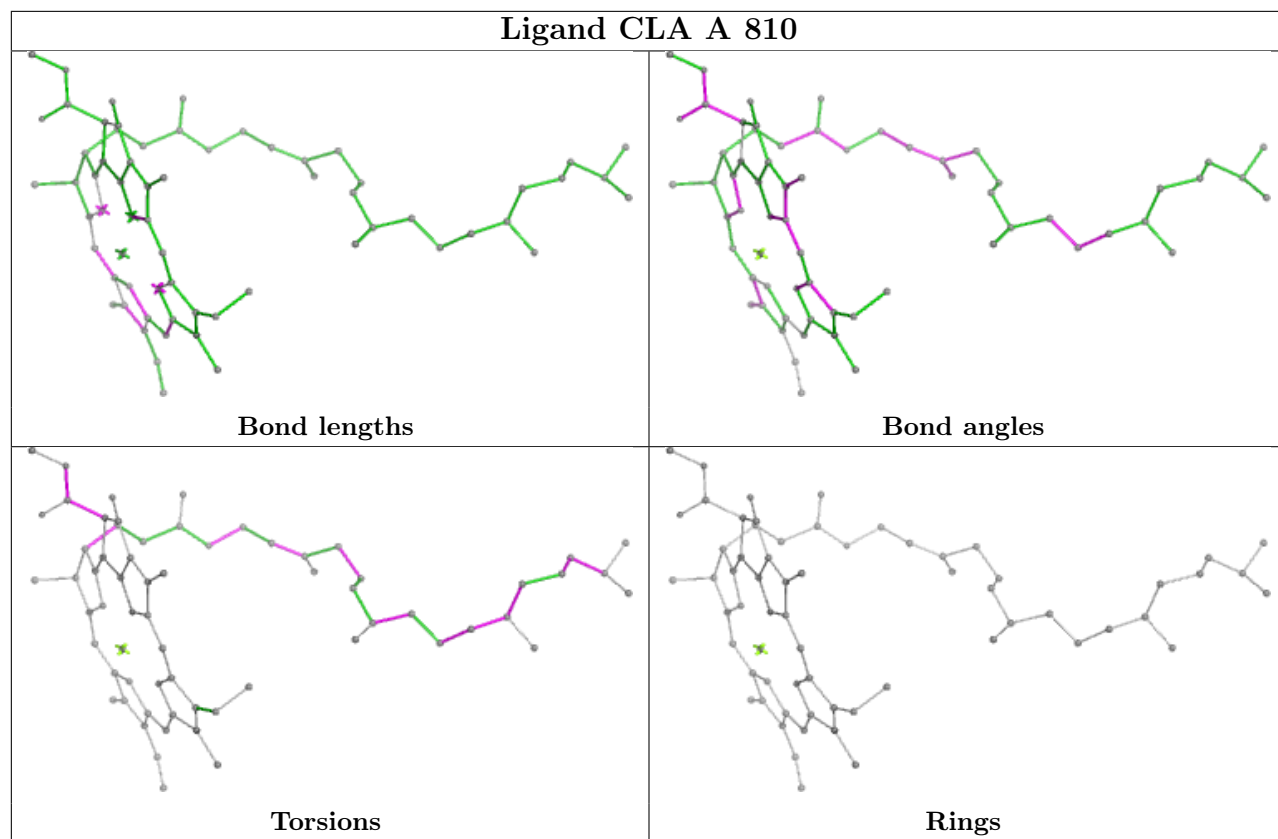


Rings

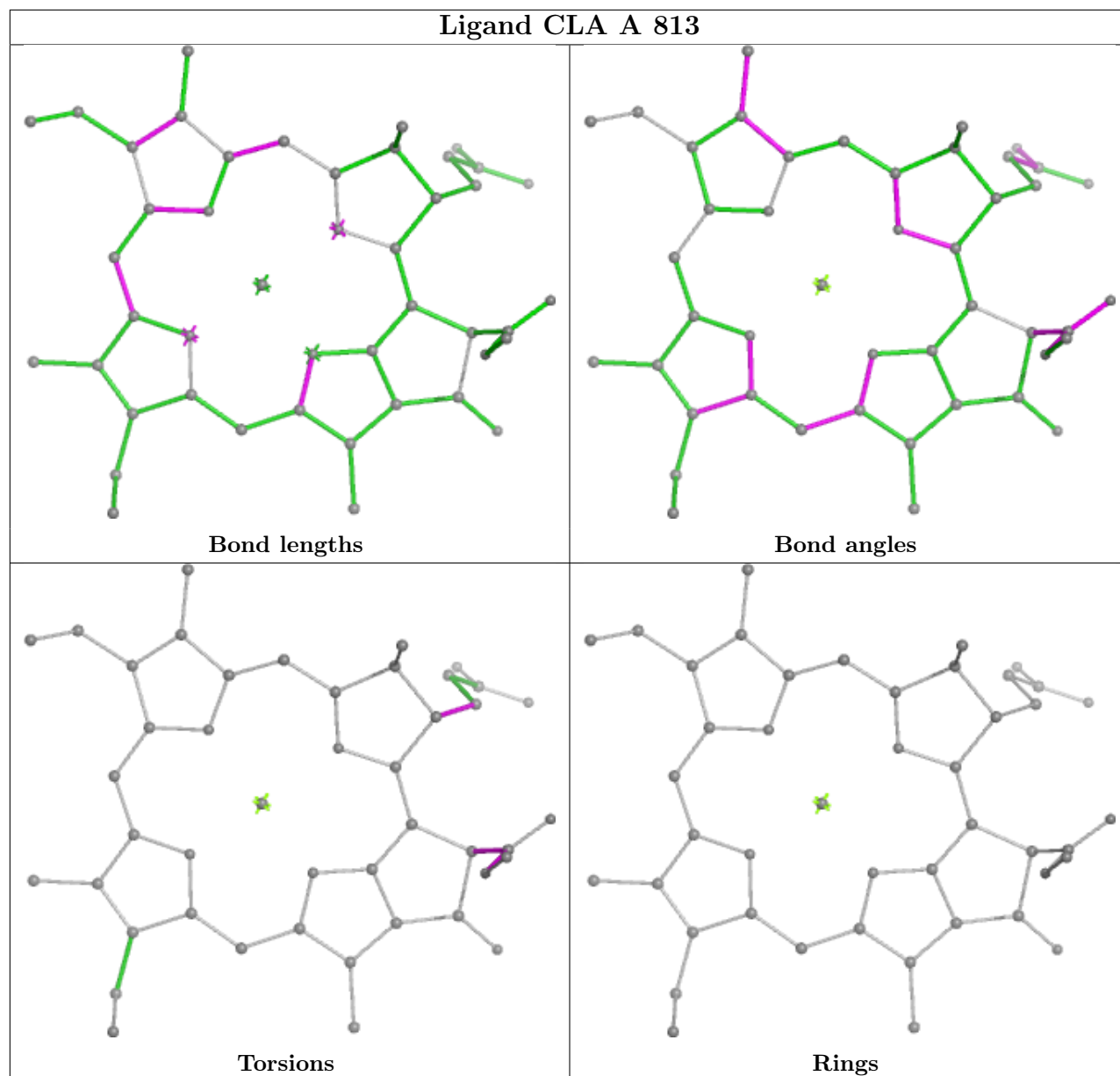
Ligand CLA 1 307



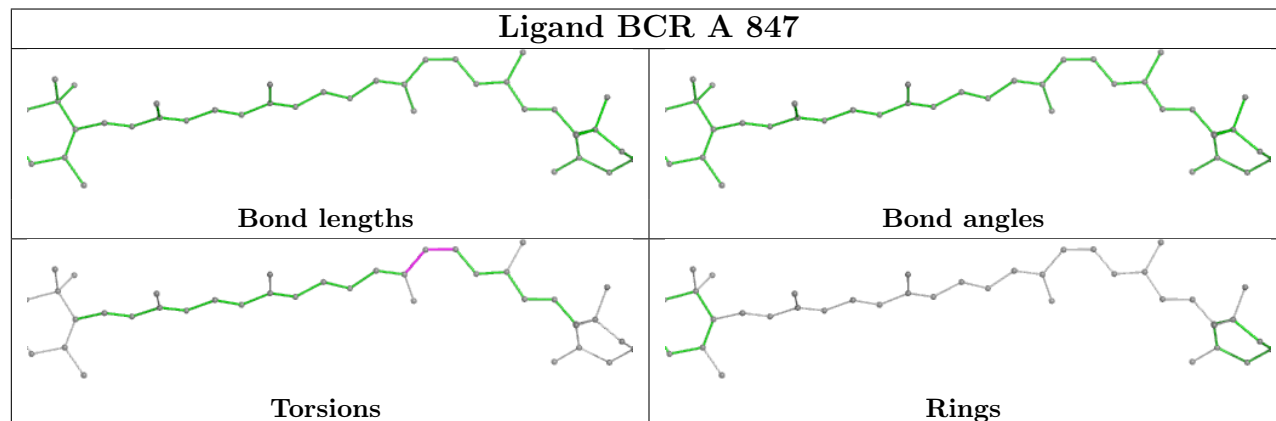


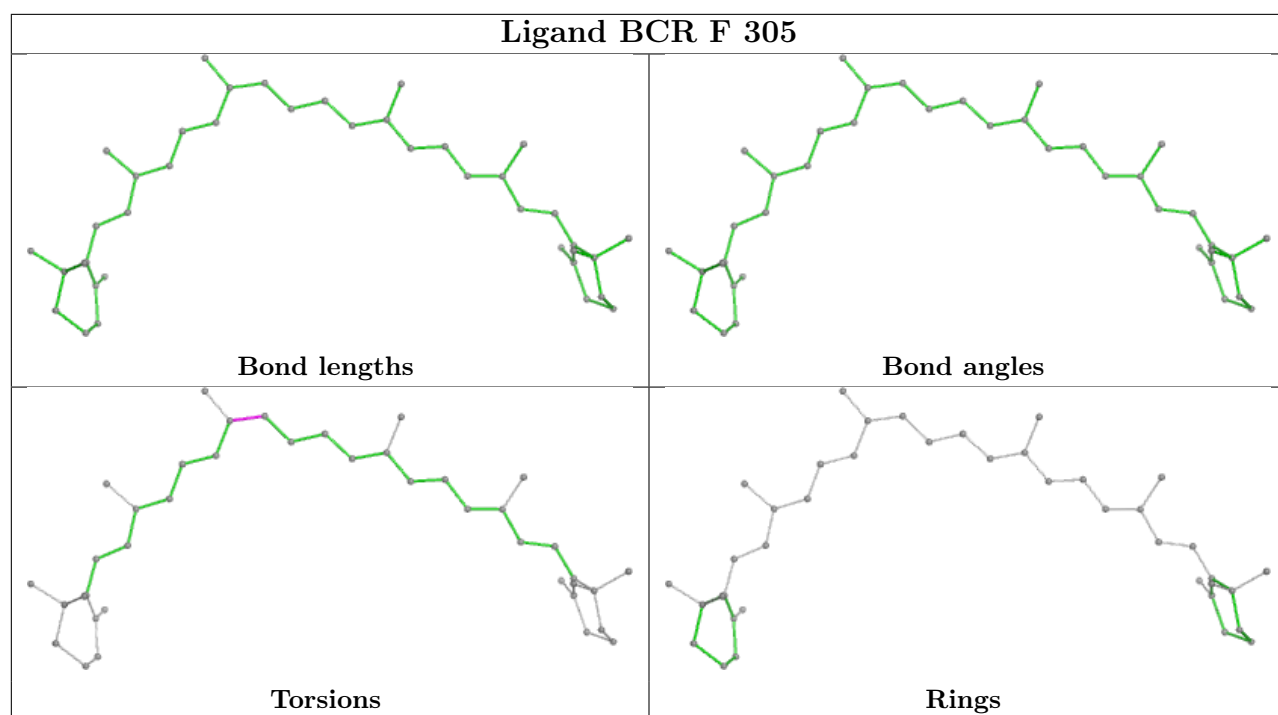


Ligand CLA A 813

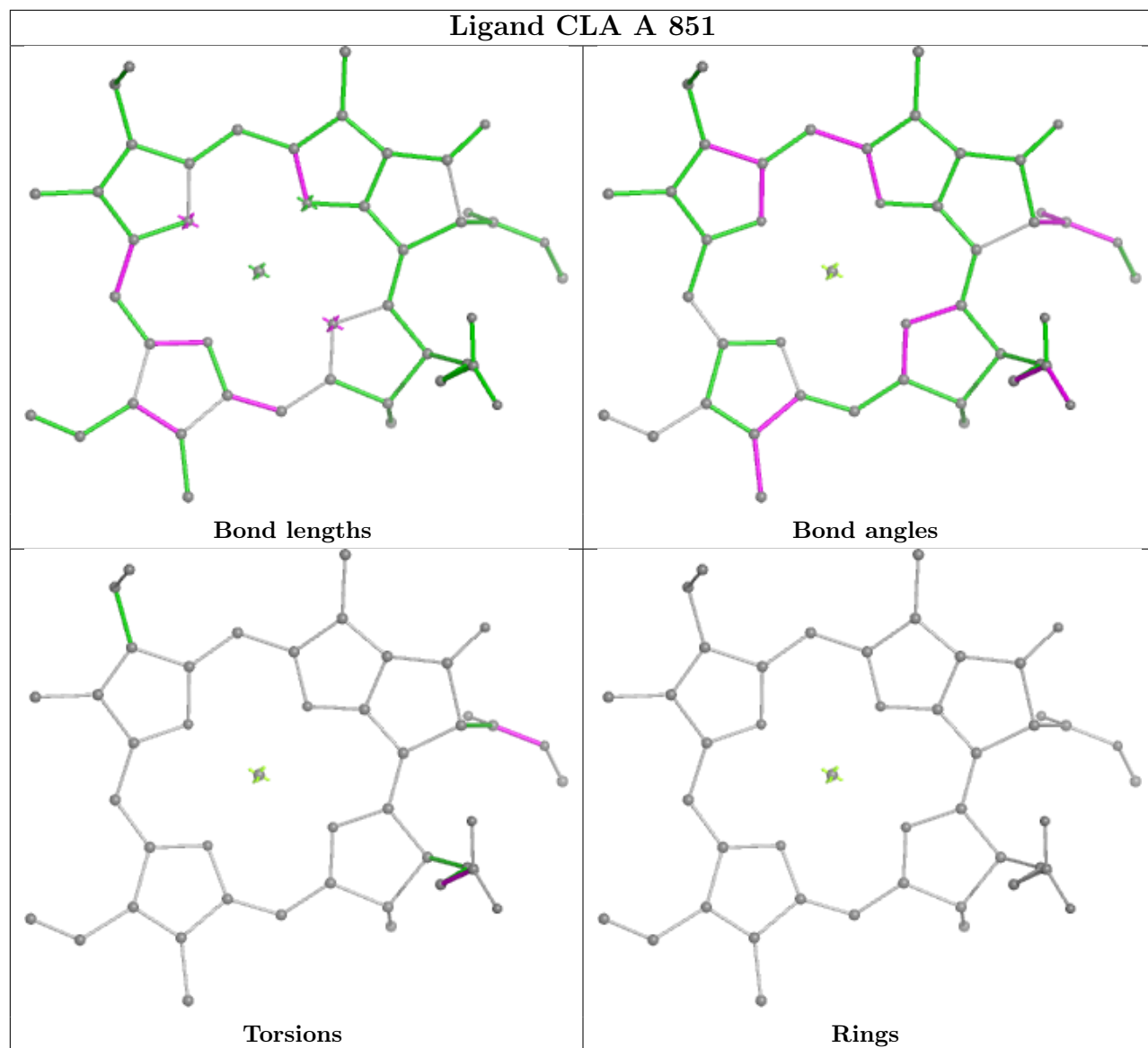


Ligand BCR A 847

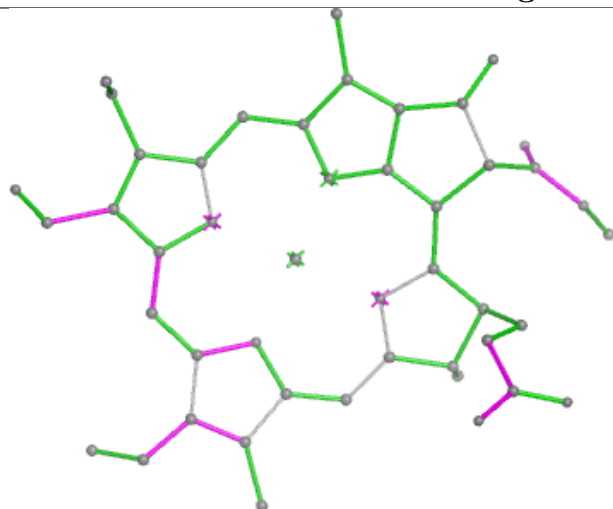




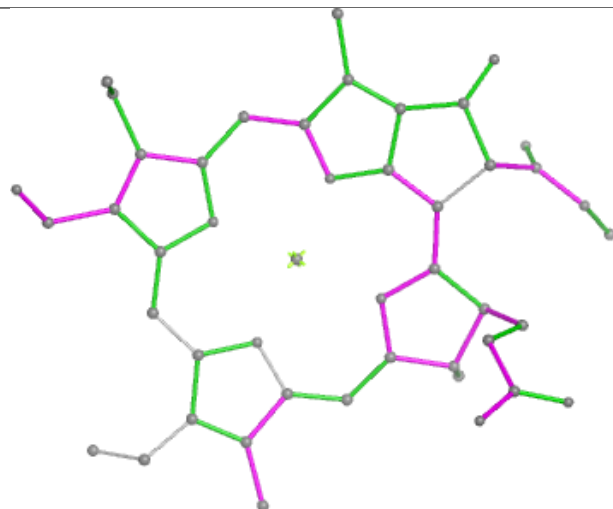
Ligand CLA A 851



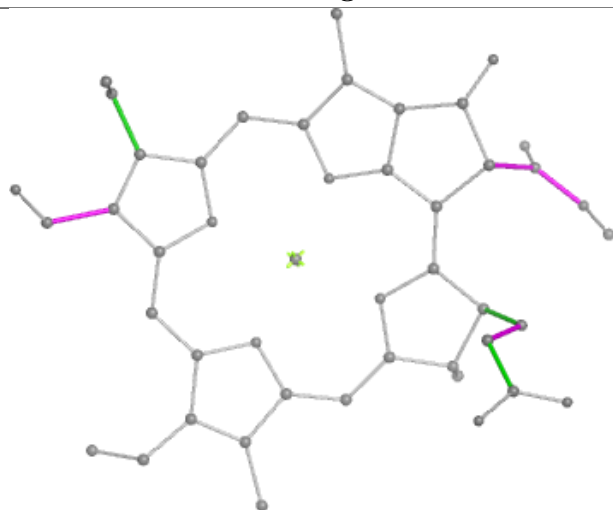
Ligand CHL 1 306



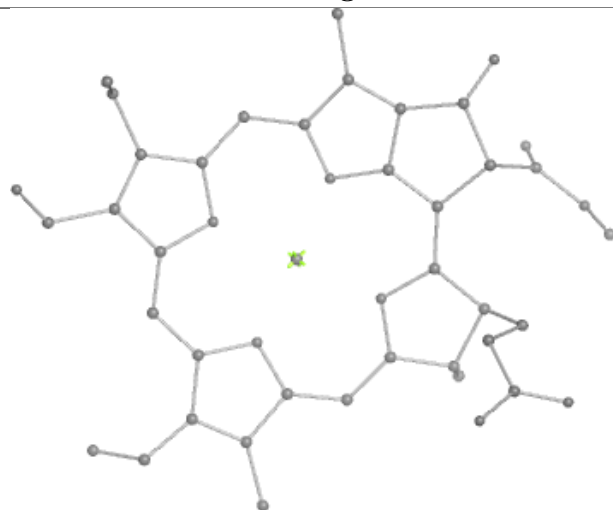
Bond lengths



Bond angles

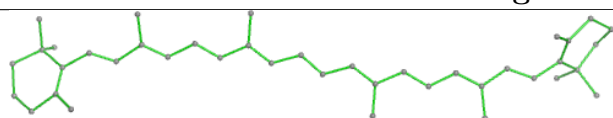


Torsions

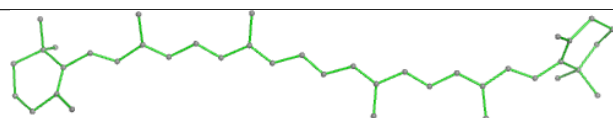


Rings

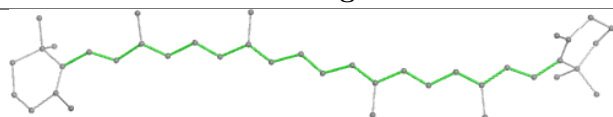
Ligand BCR B 840



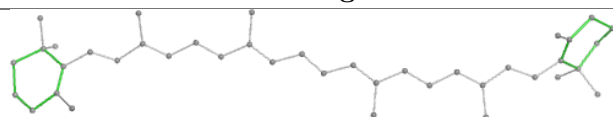
Bond lengths



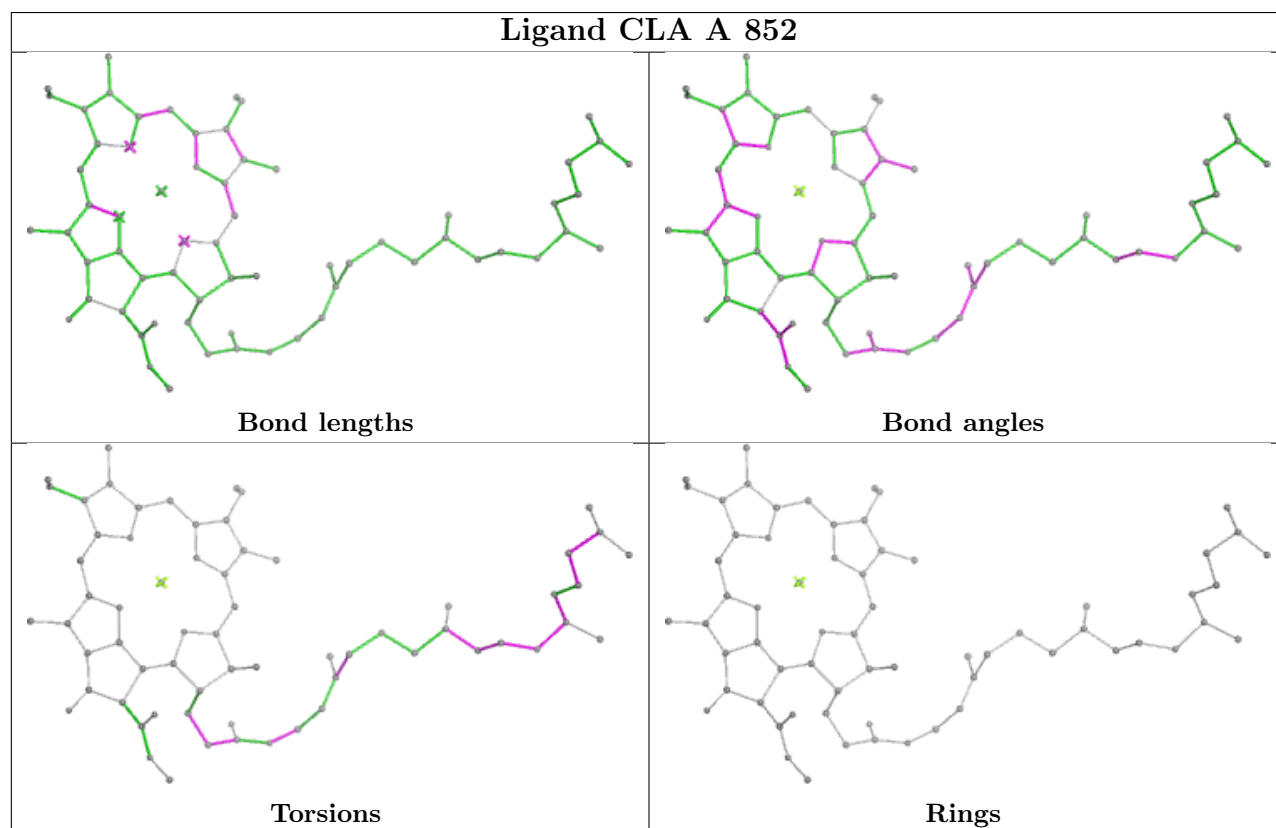
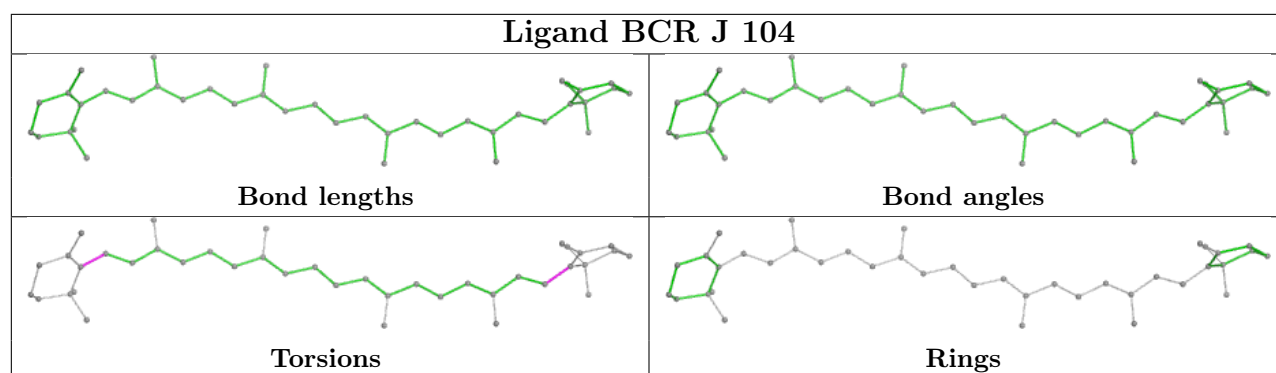
Bond angles



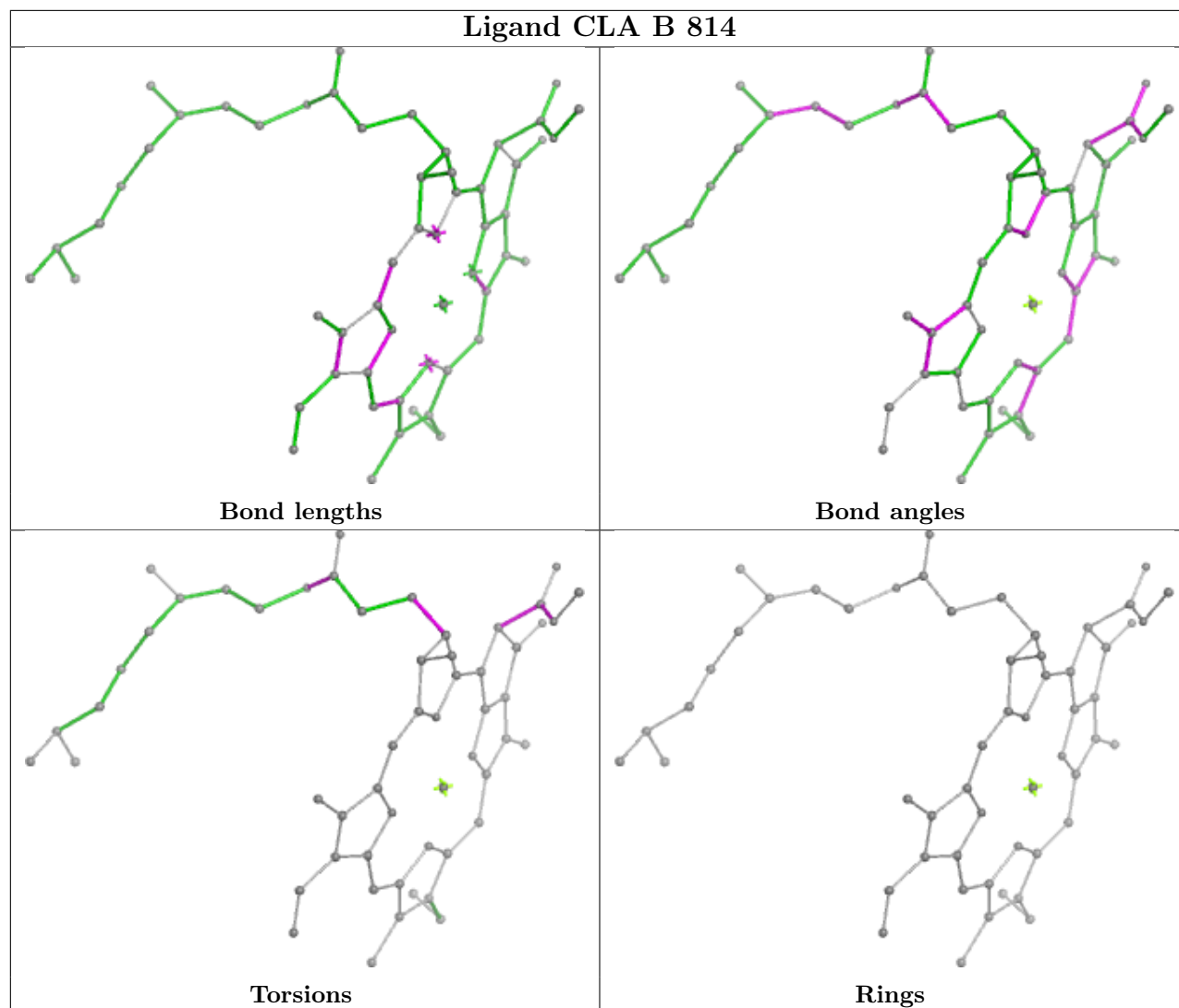
Torsions



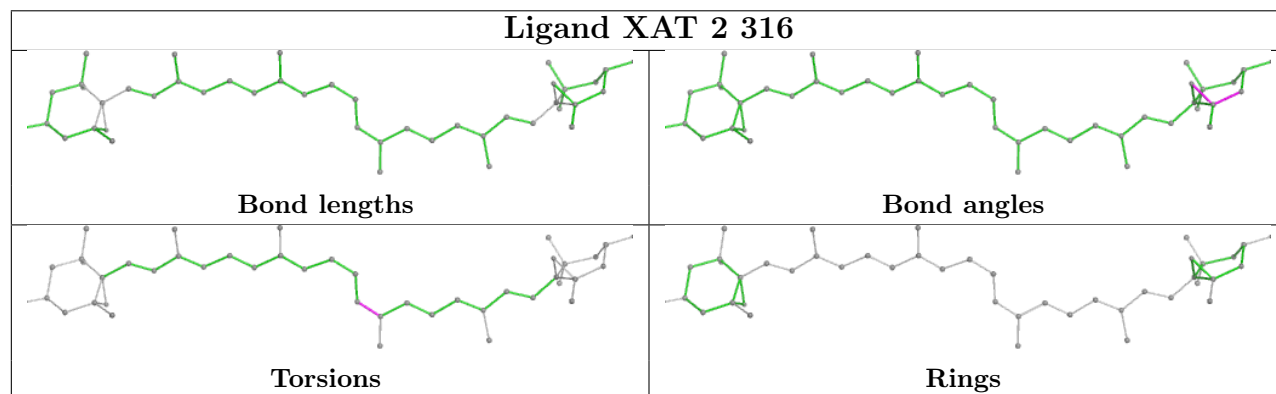
Rings



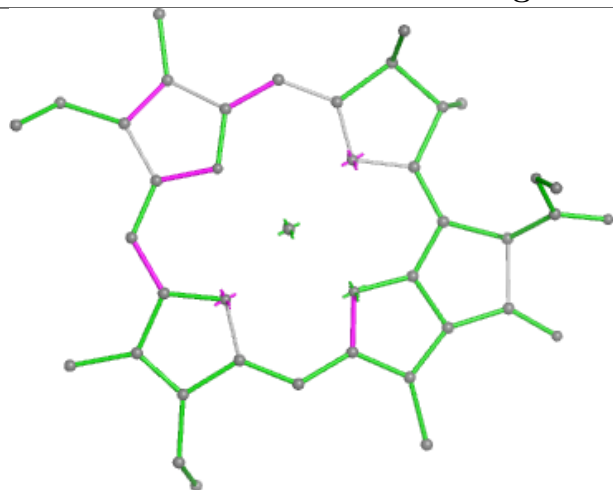
Ligand CLA B 814



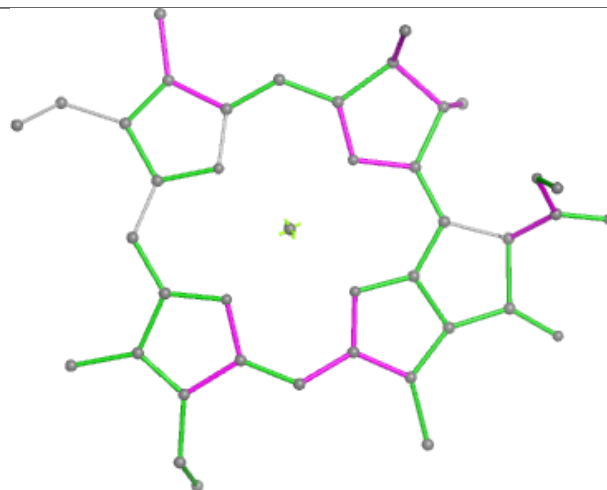
Ligand XAT 2 316



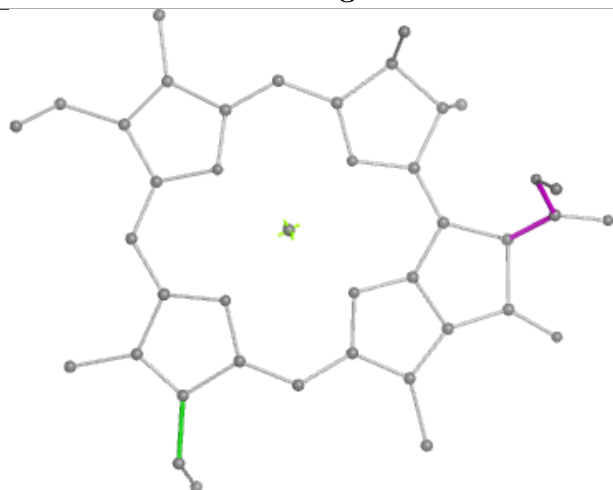
Ligand CLA G 202



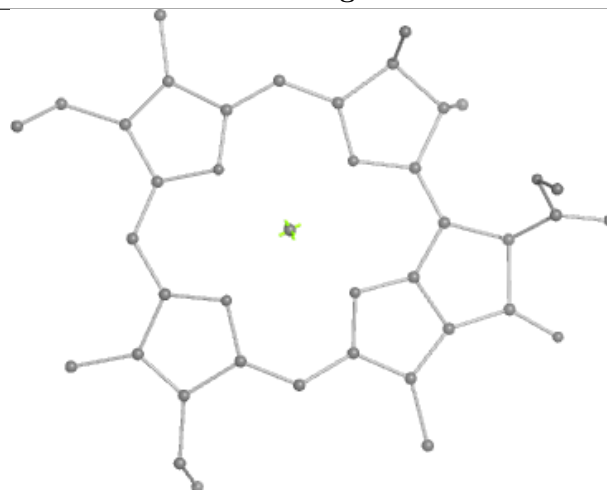
Bond lengths



Bond angles

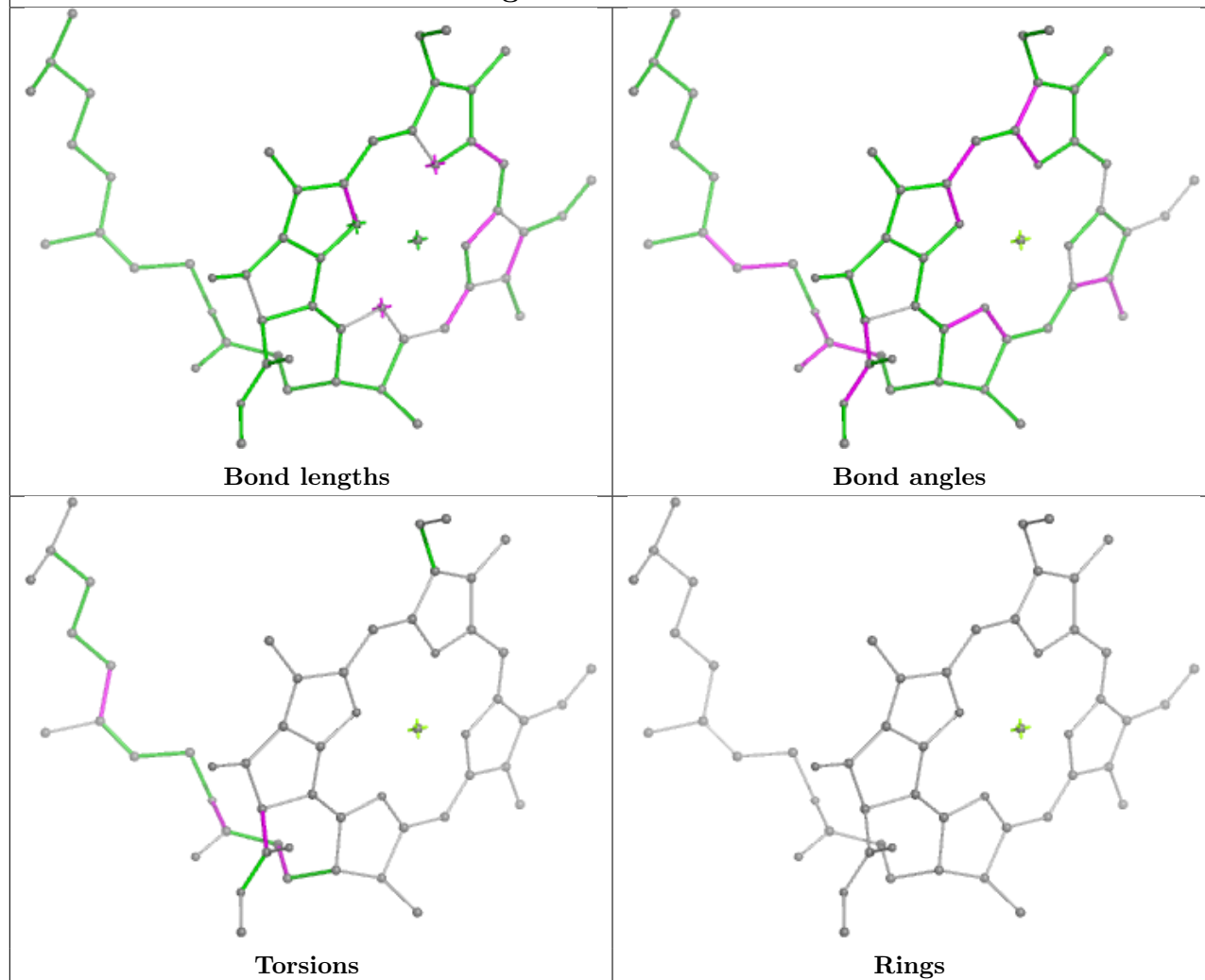


Torsions

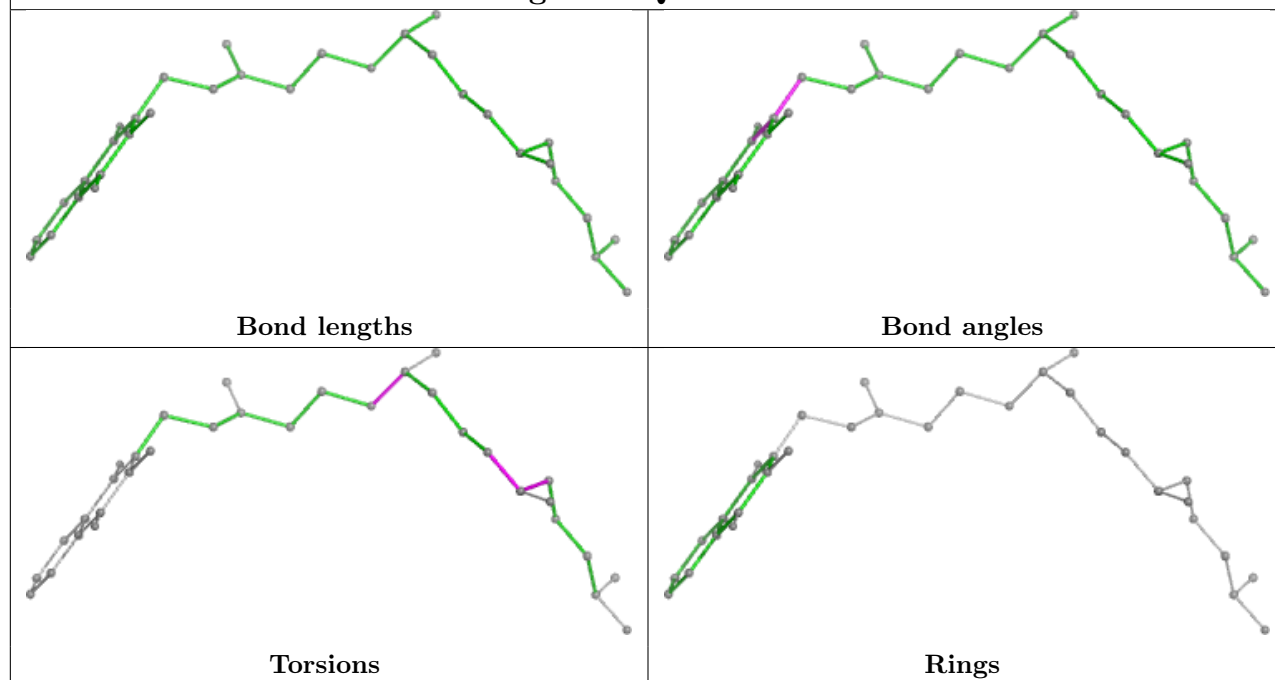


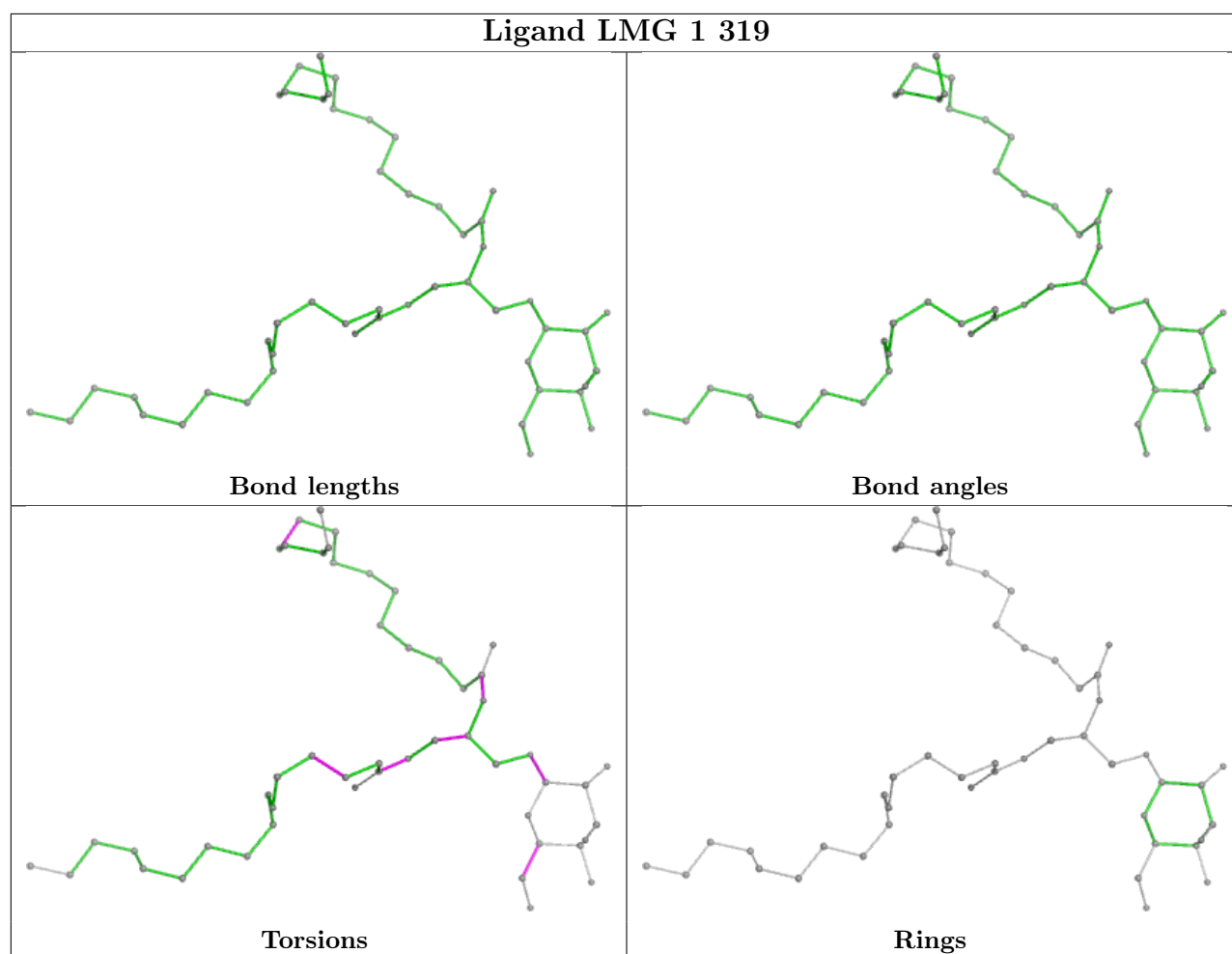
Rings

Ligand CLA B 821

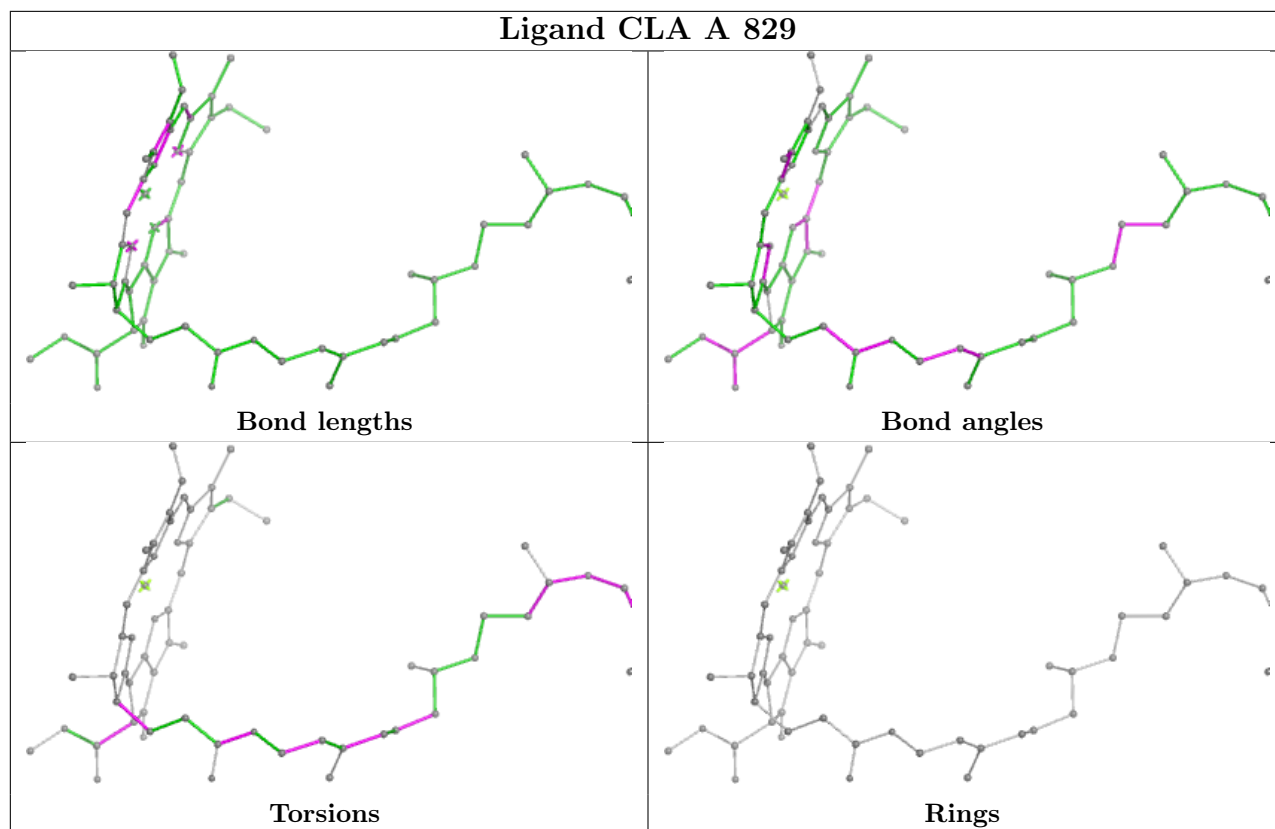


Ligand PQN B 839

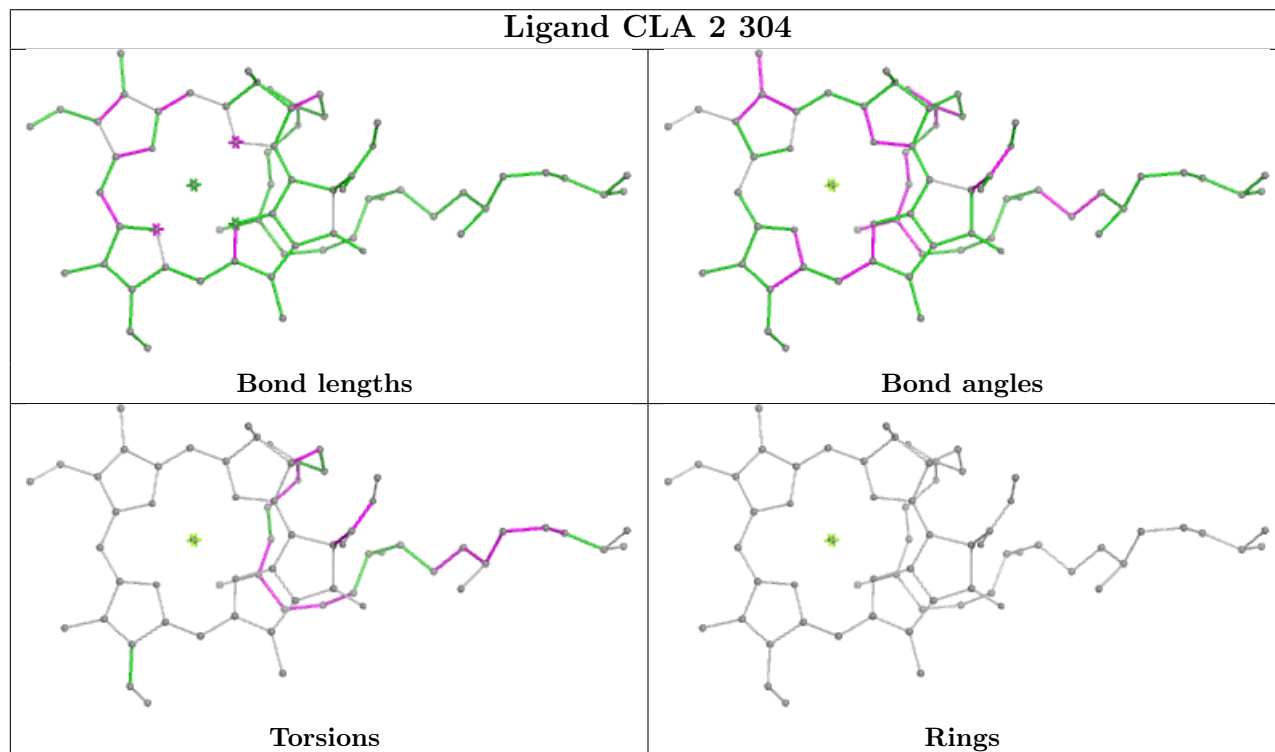


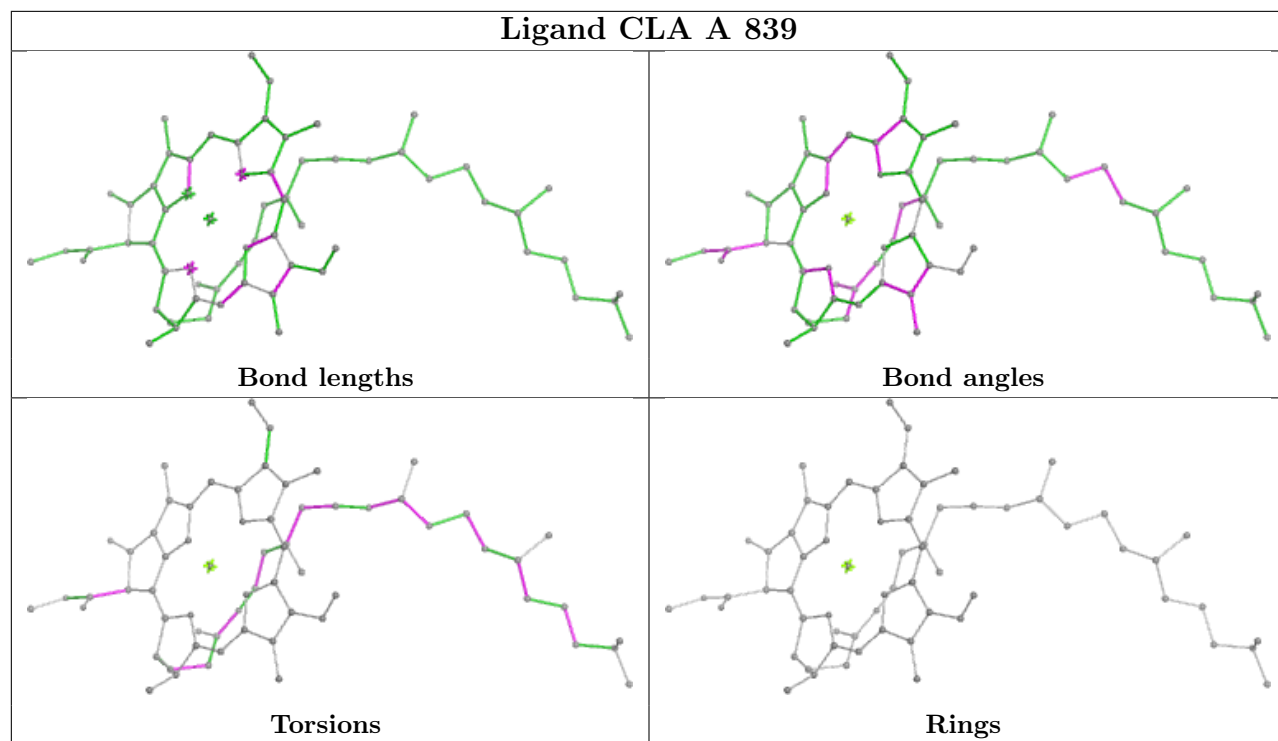


Ligand CLA A 829

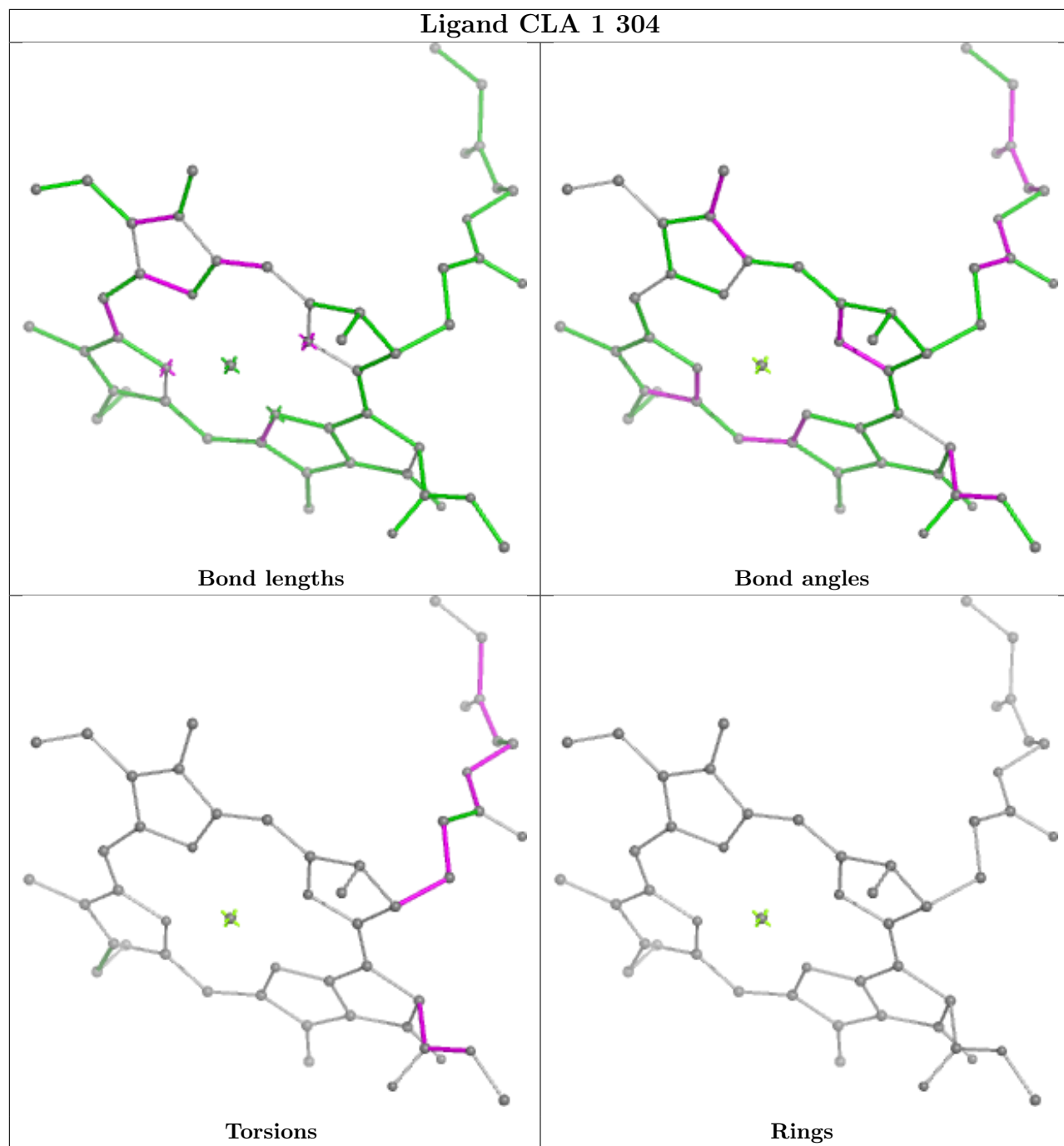


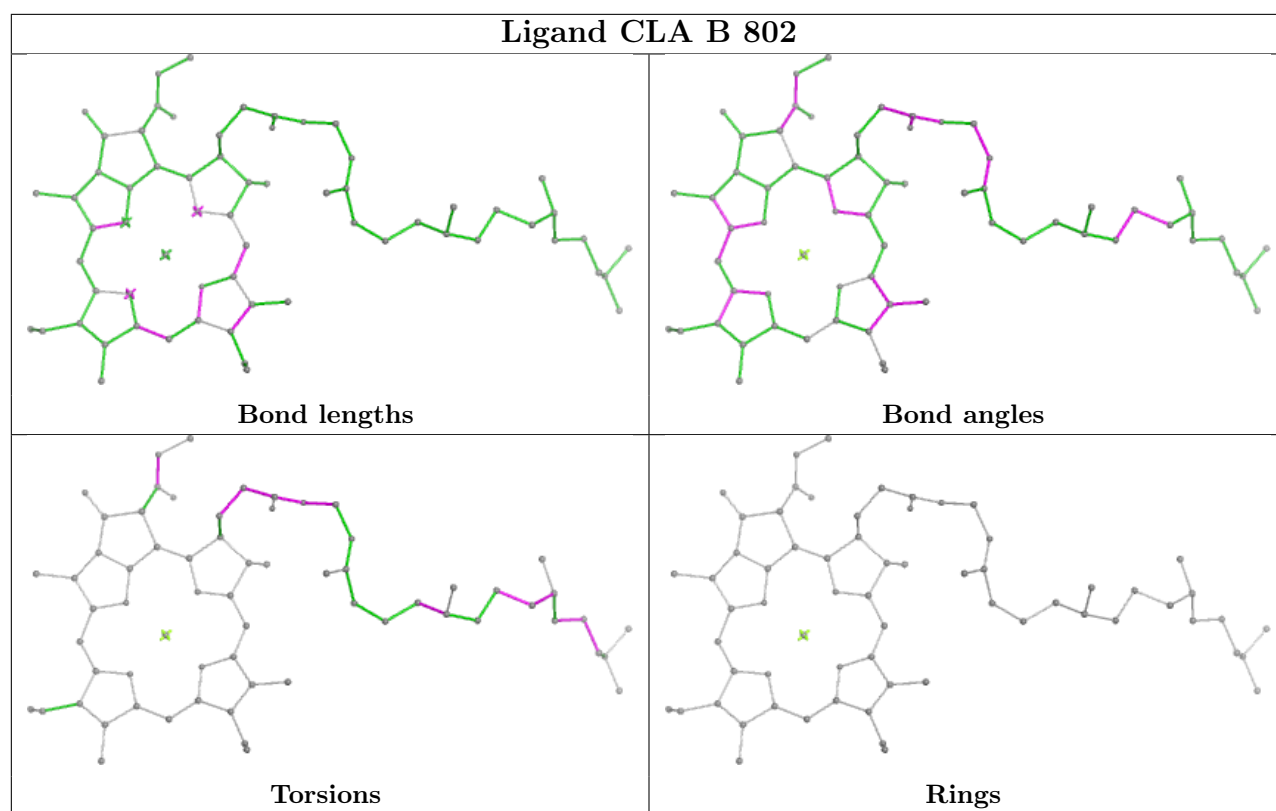
Ligand CLA 2 304



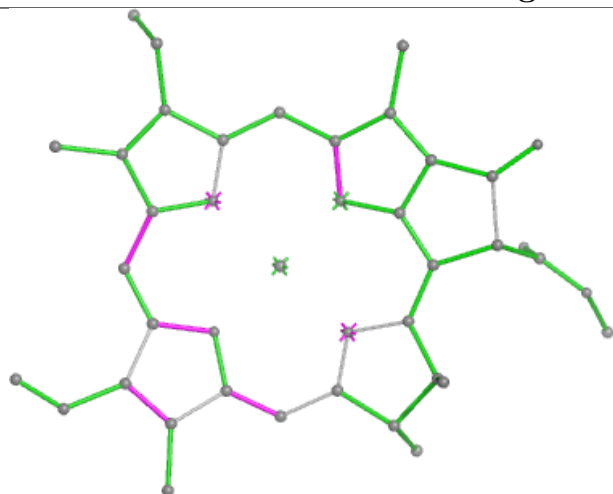


Ligand CLA 1 304

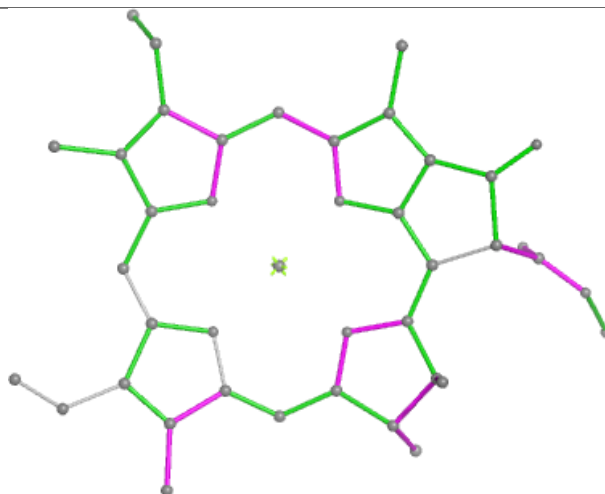




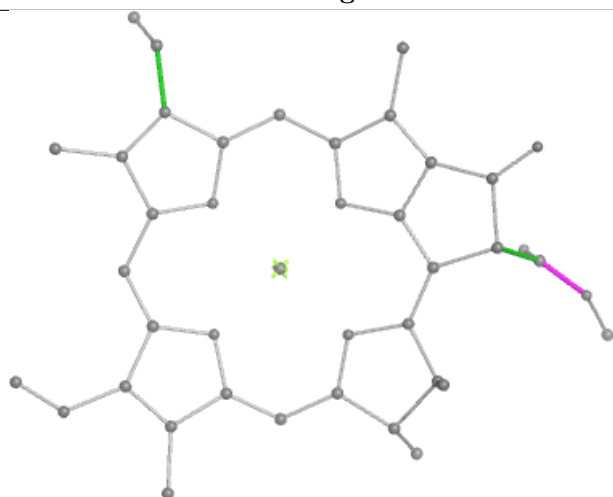
Ligand CLA 2 310



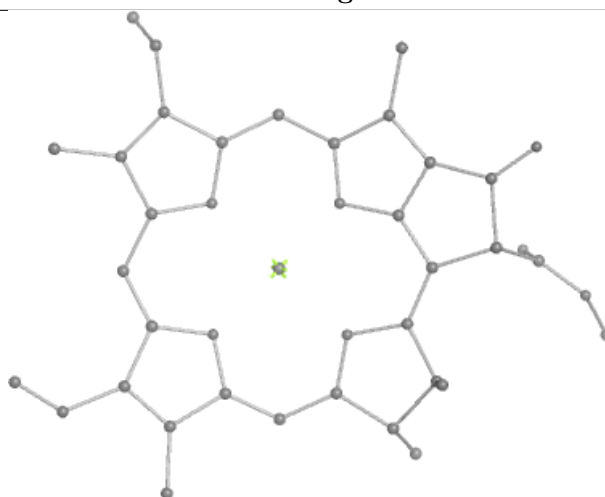
Bond lengths



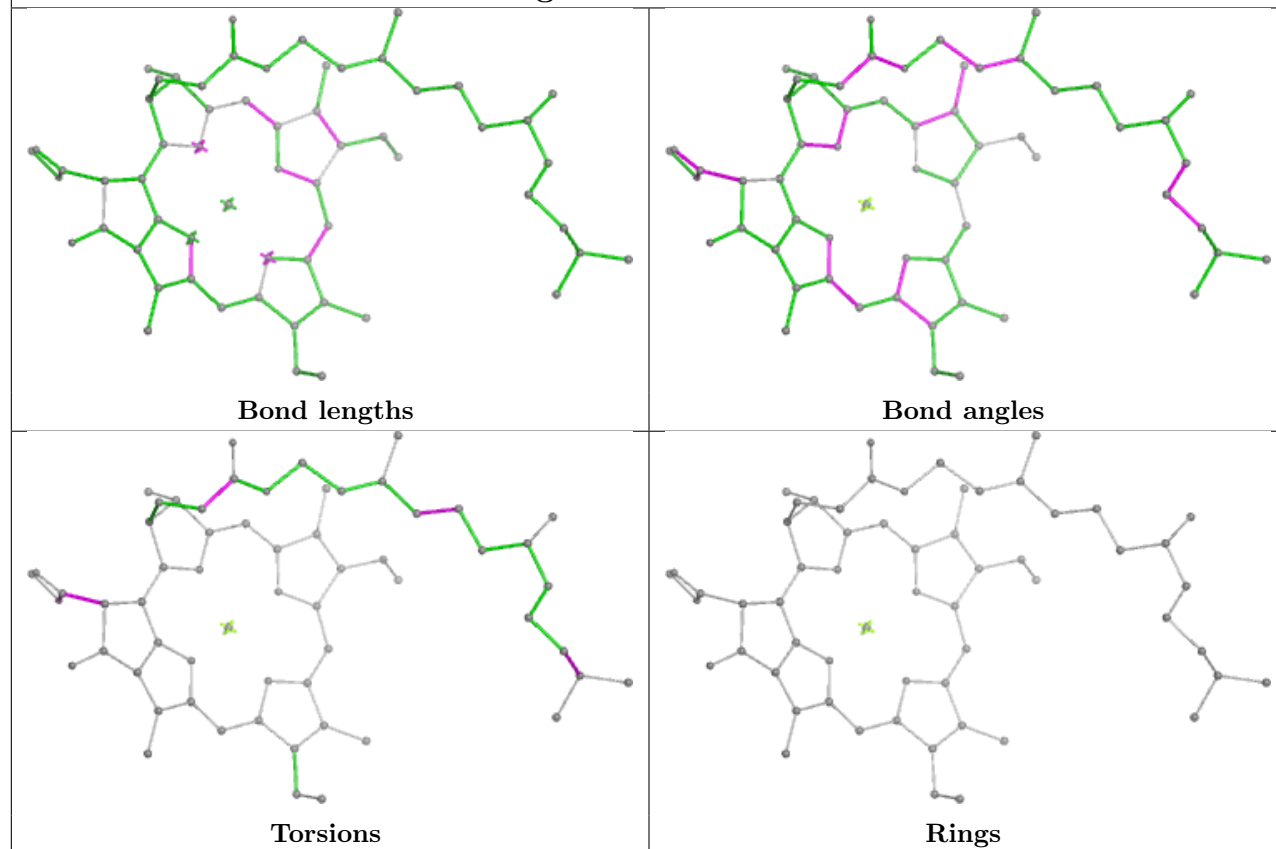
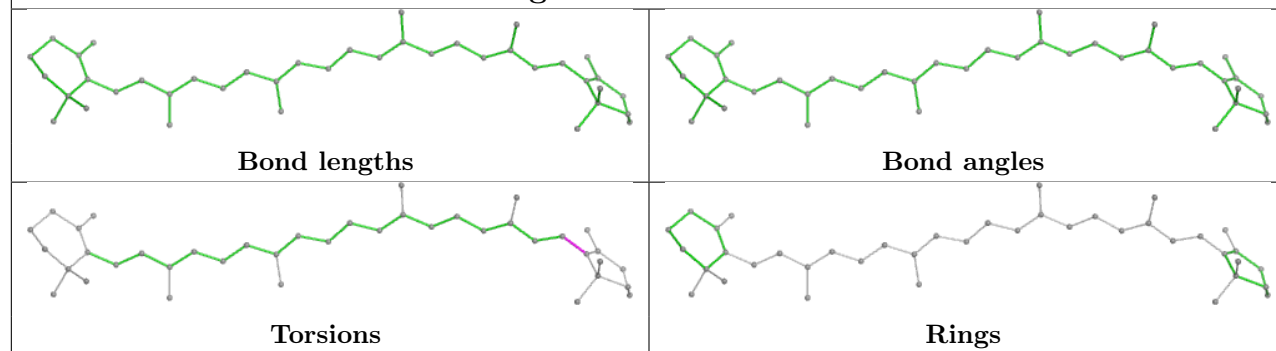
Bond angles

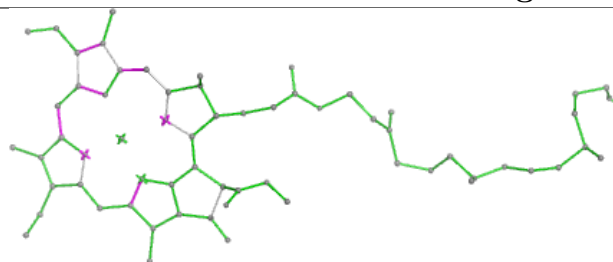
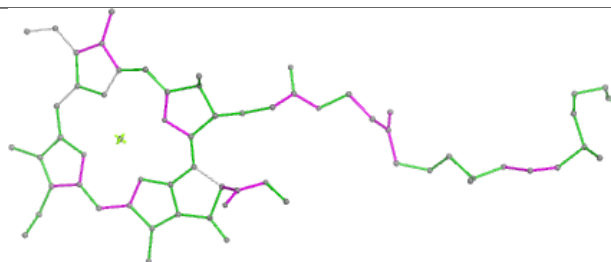
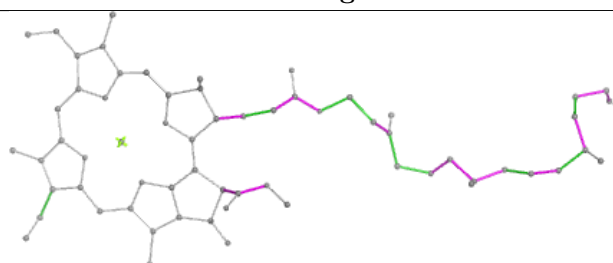
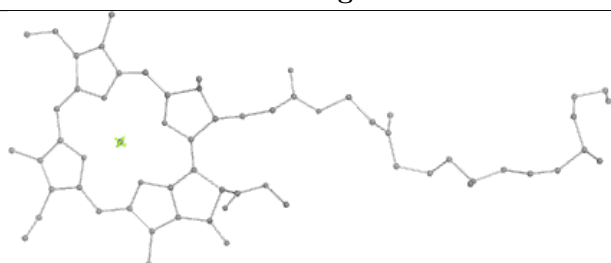
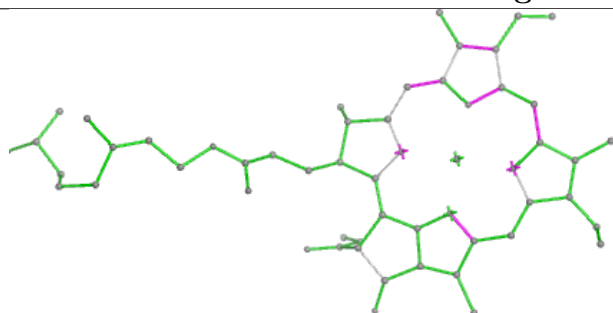
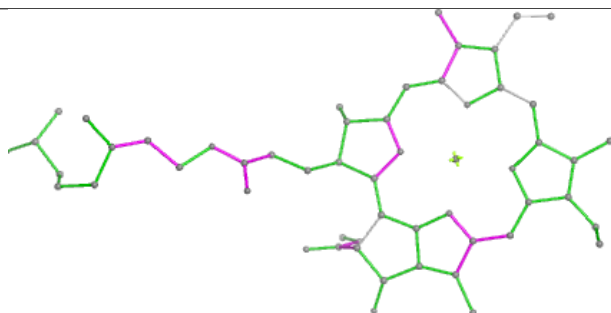
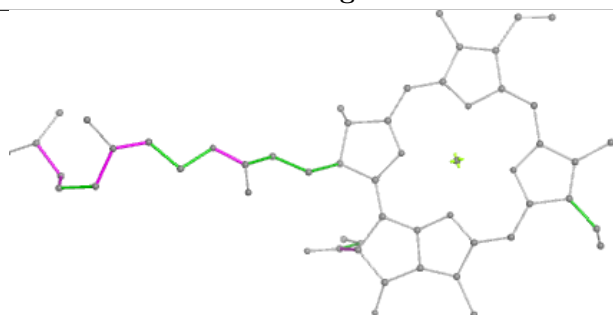
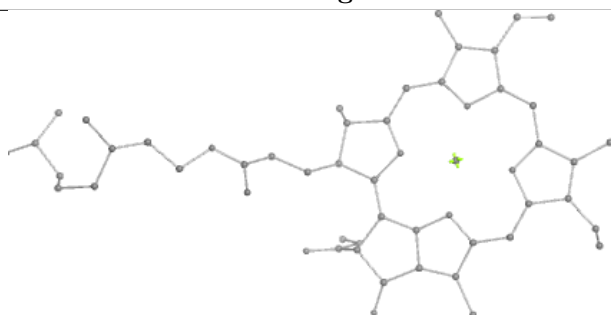


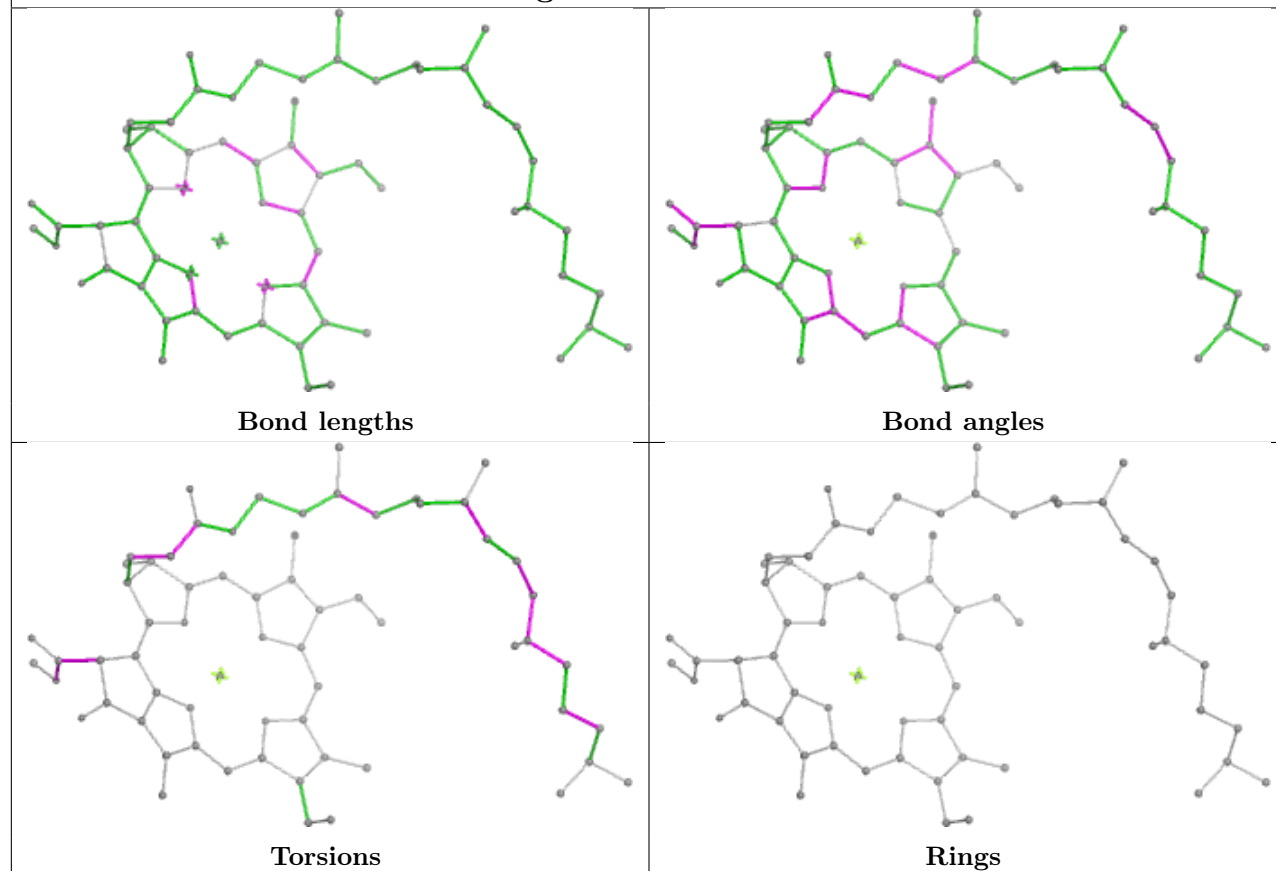
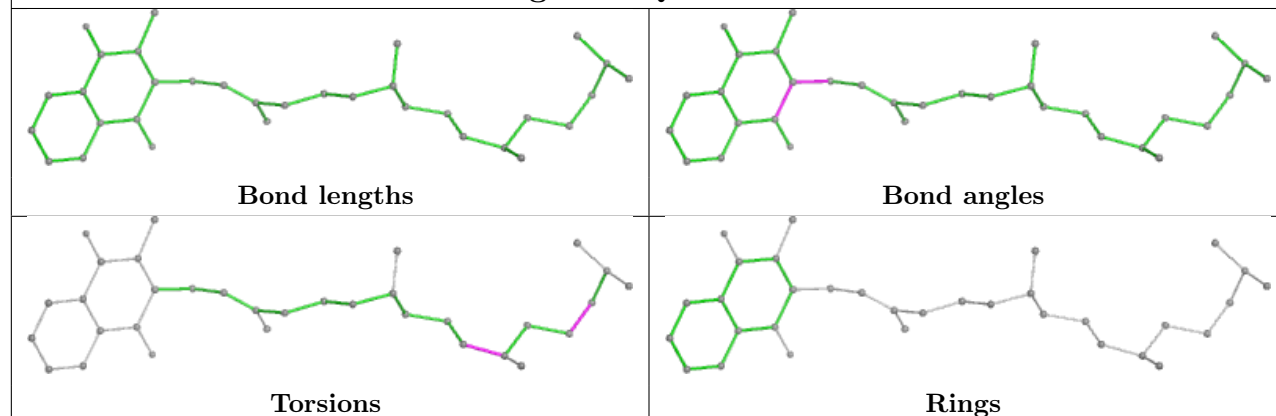
Torsions



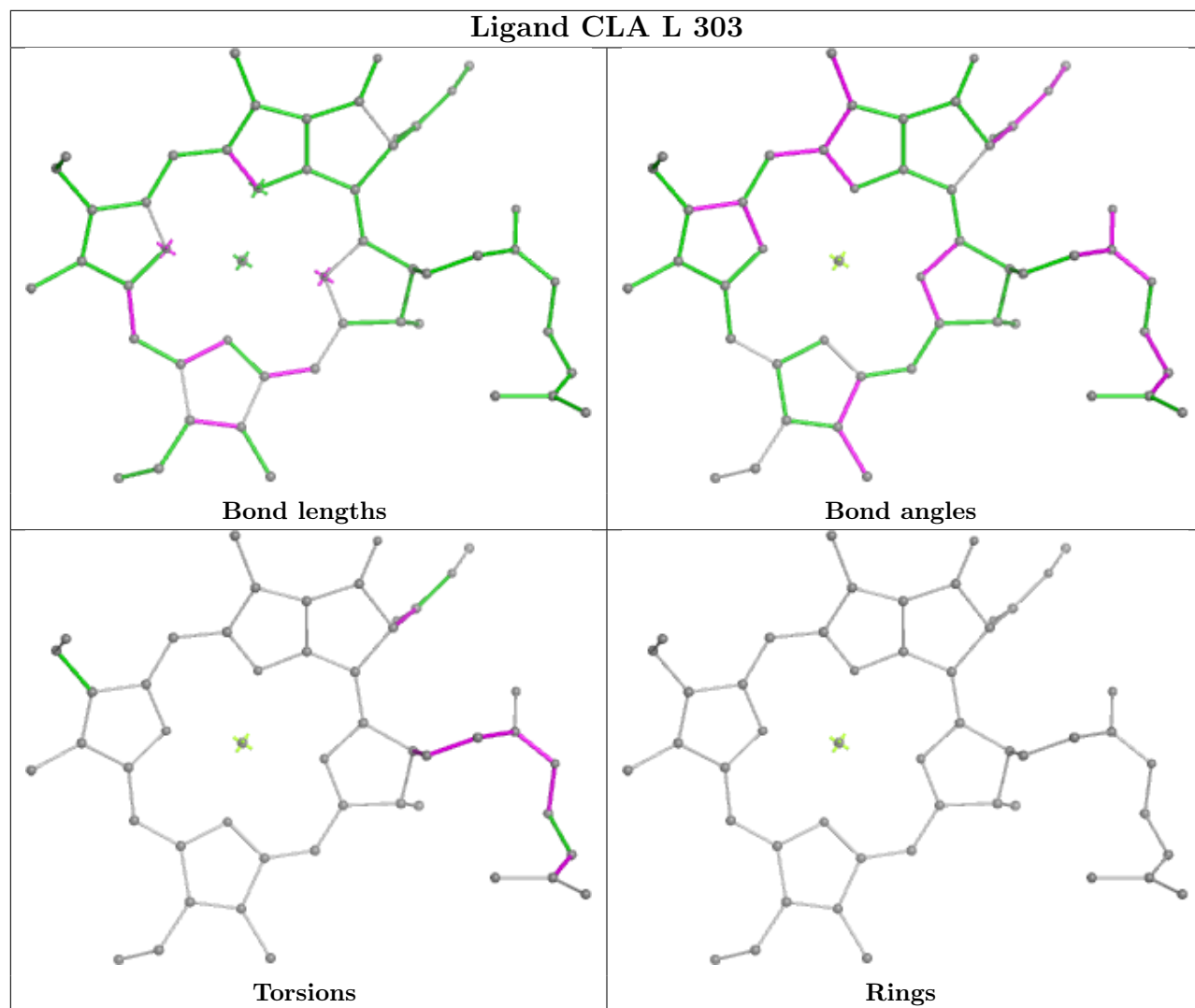
Rings

Ligand CLA 4 301**Ligand BCR G 205**

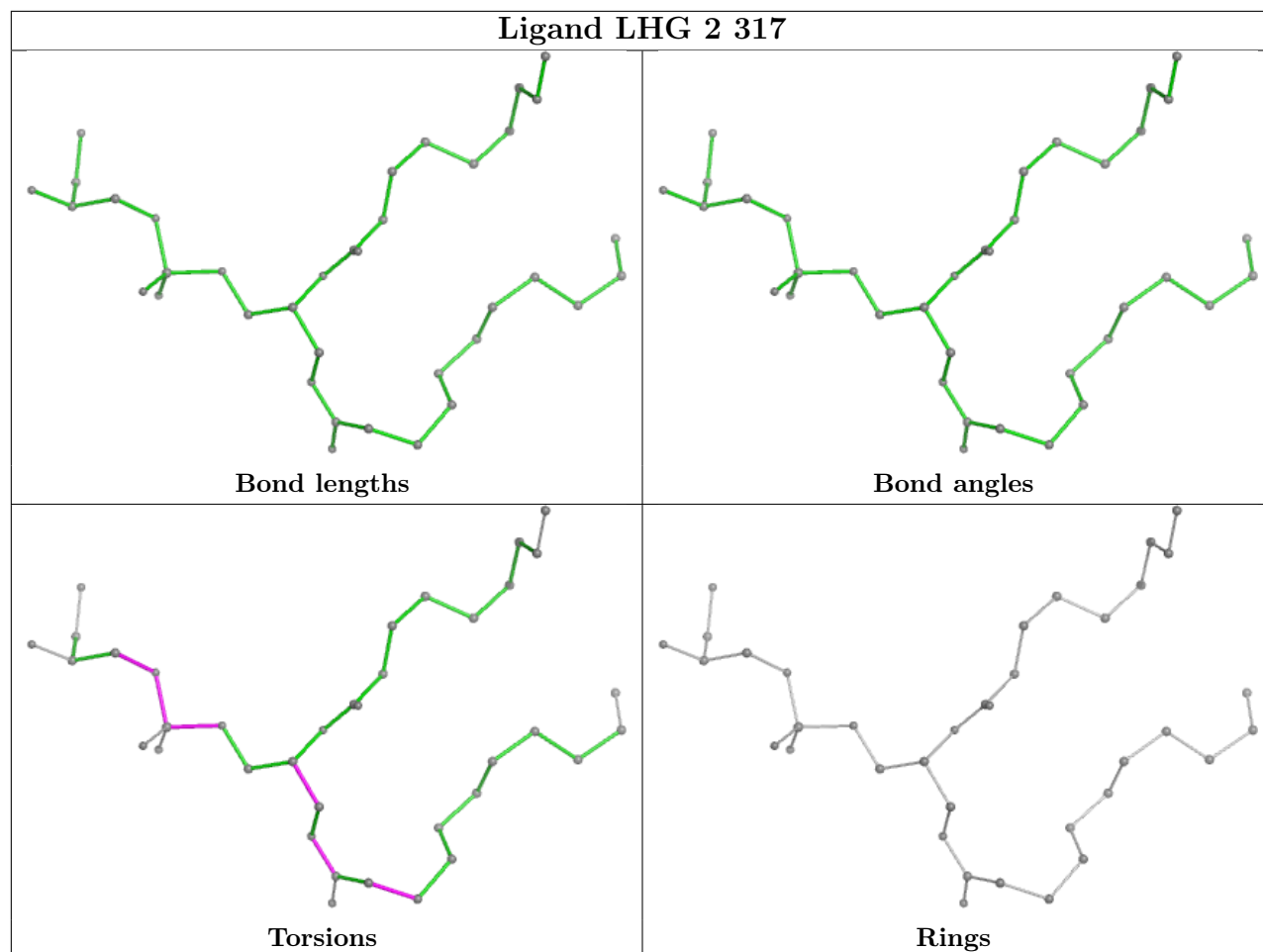
Ligand CLA F 301**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 834****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA 2 302**Ligand PQN A 841**

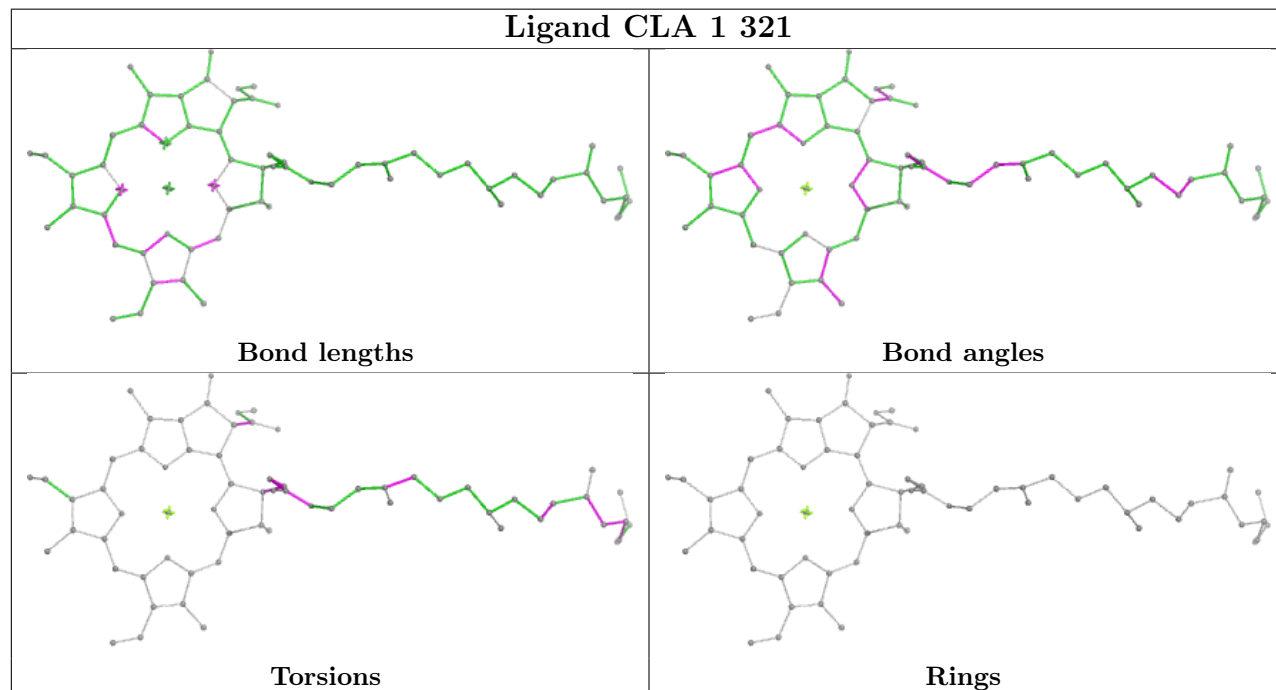
Ligand CLA L 303

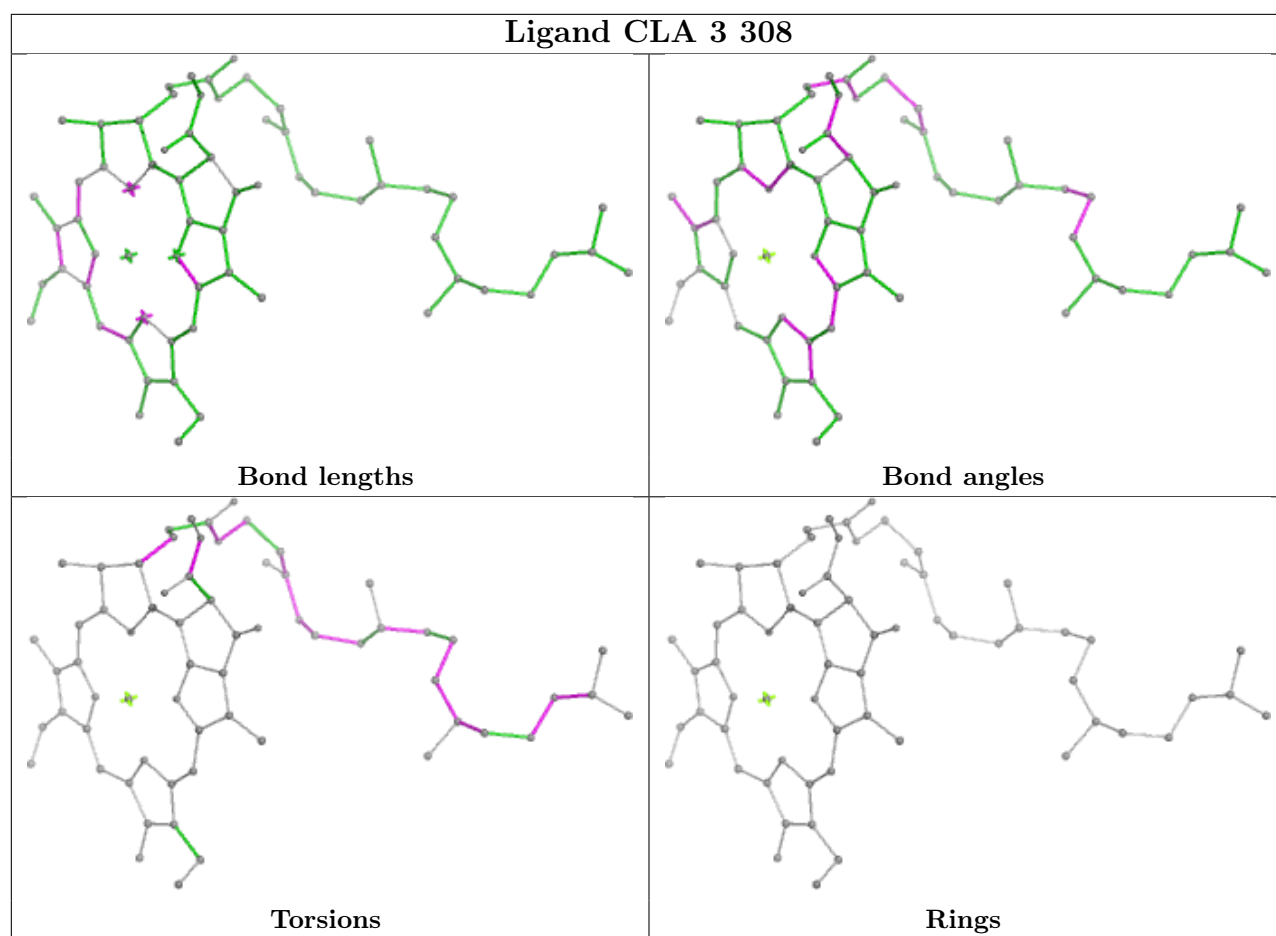


Ligand LHG 2 317

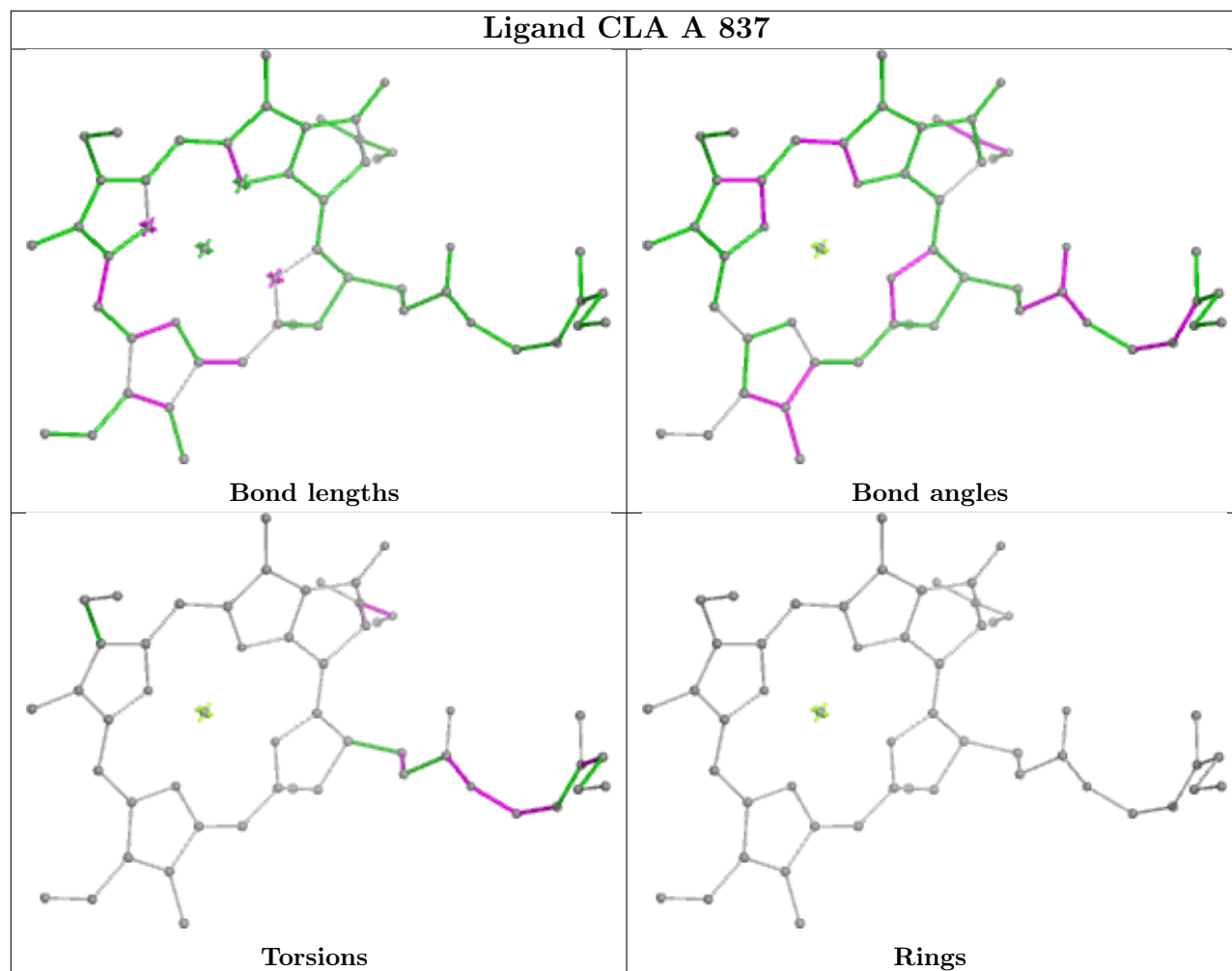


Ligand CLA 1 321

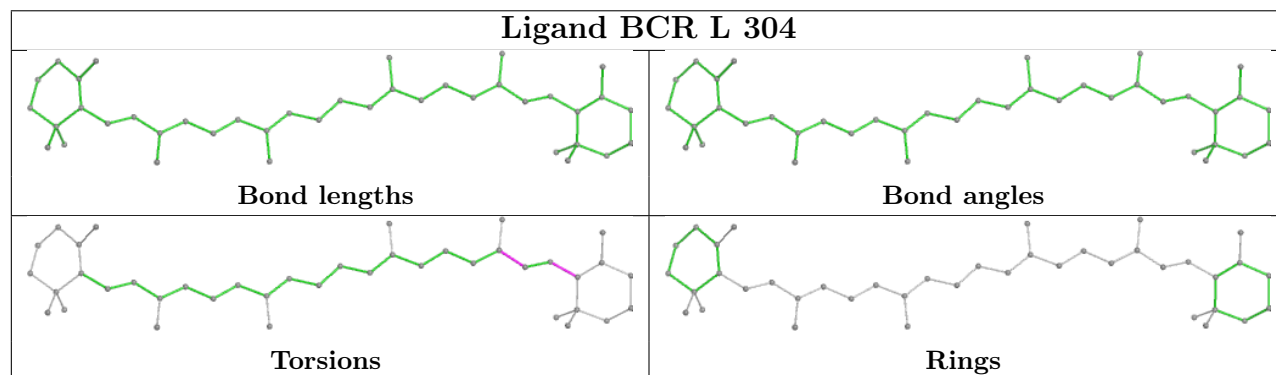




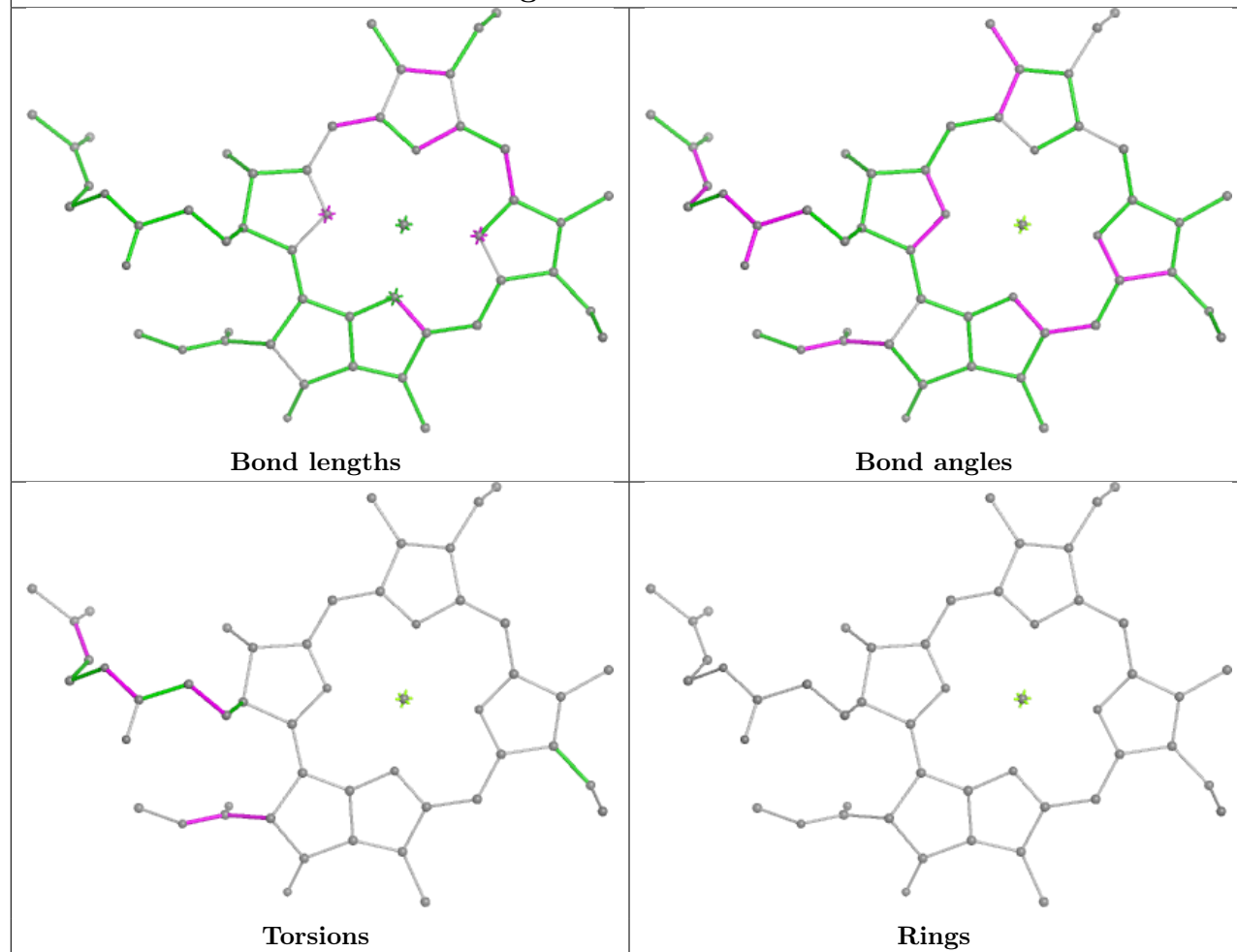
Ligand CLA A 837



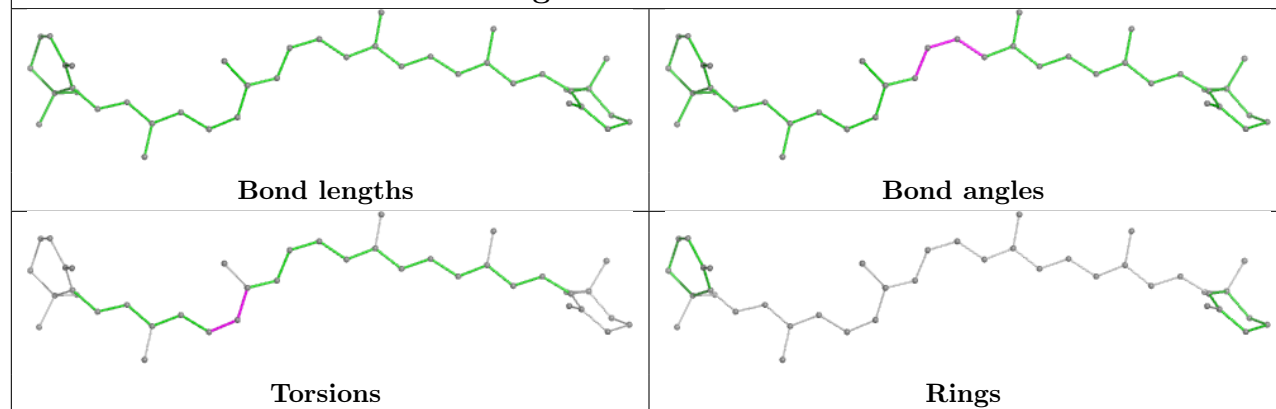
Ligand BCR L 304



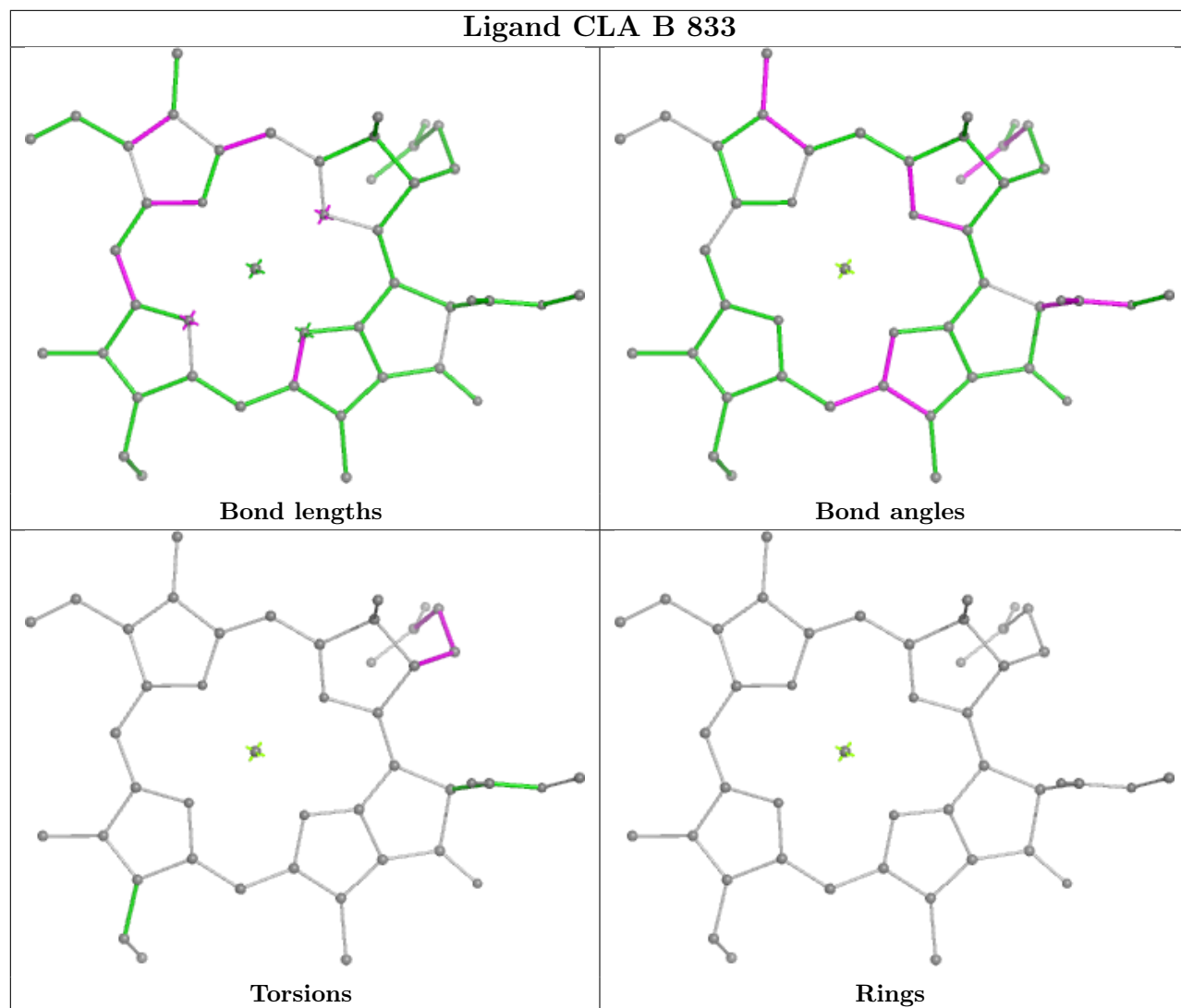
Ligand CLA 2 303

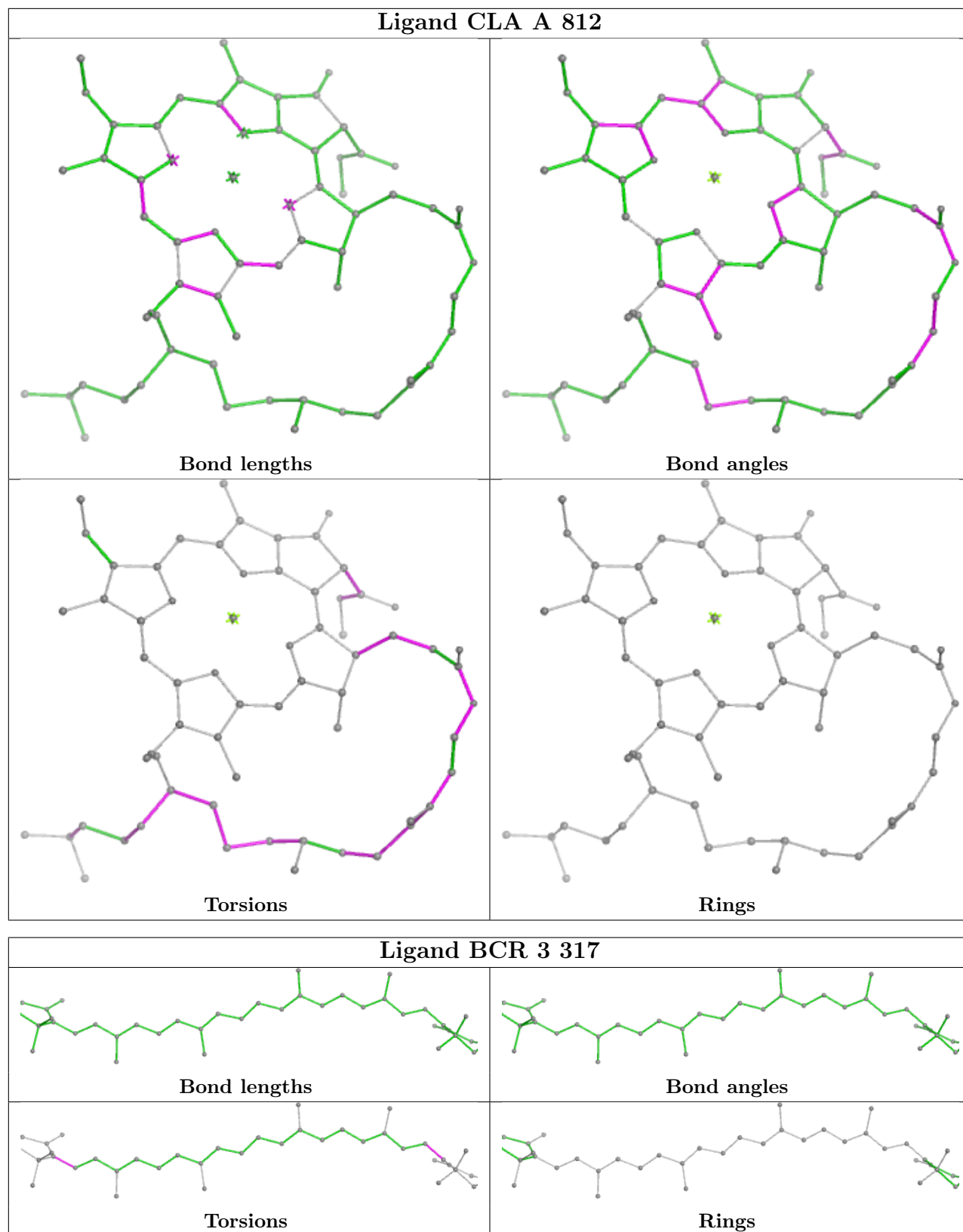


Ligand BCR L 305

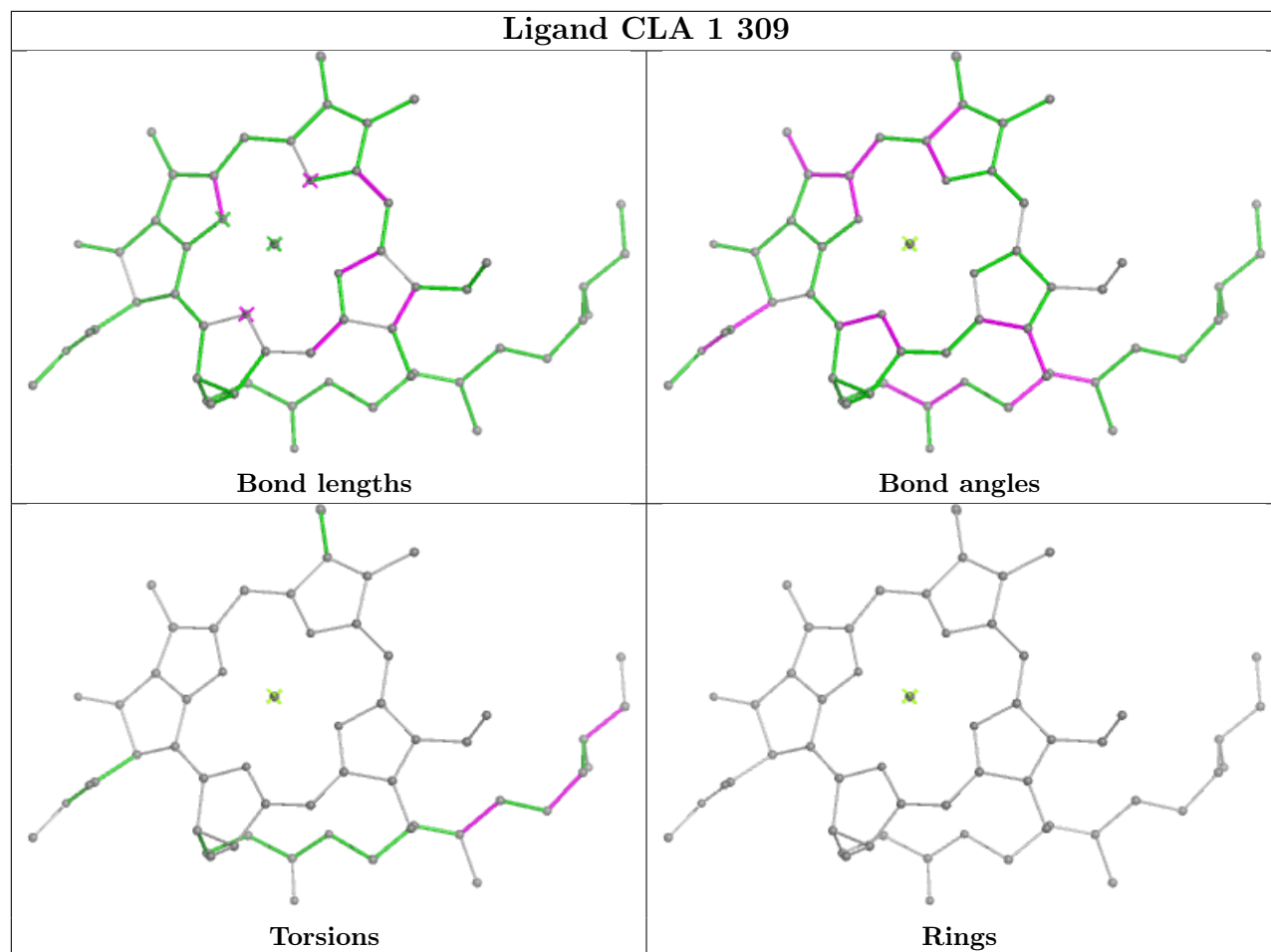


Ligand CLA B 833

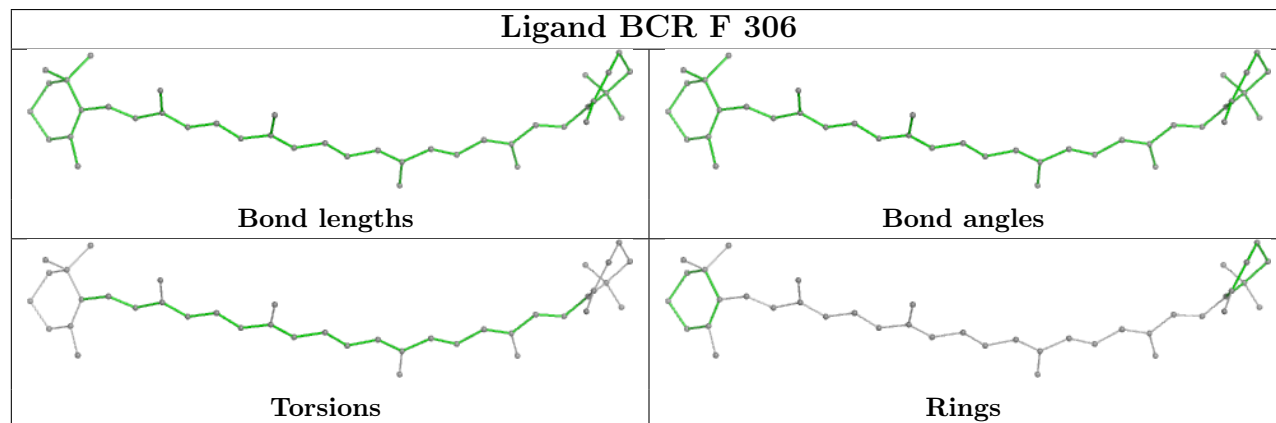


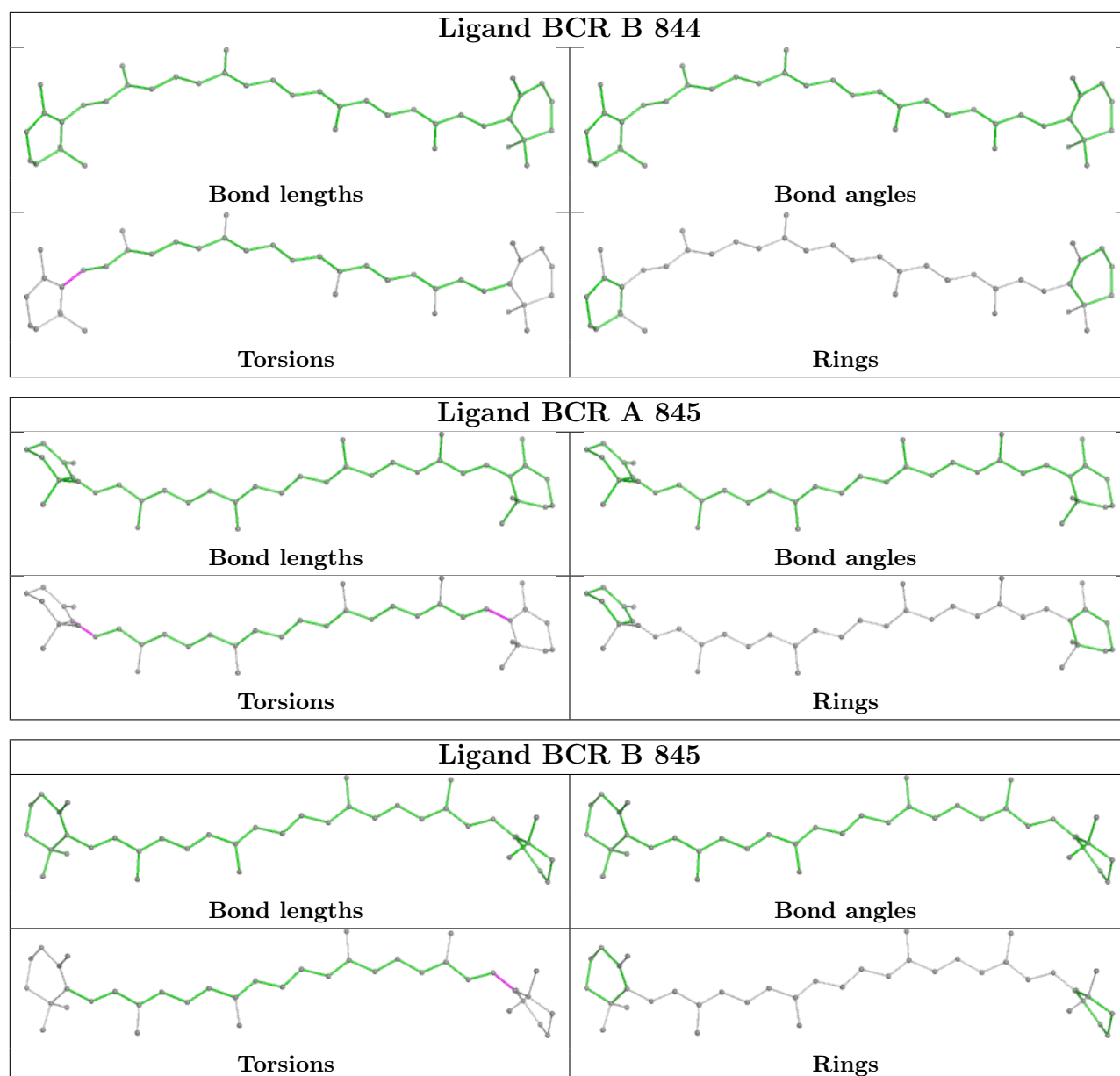


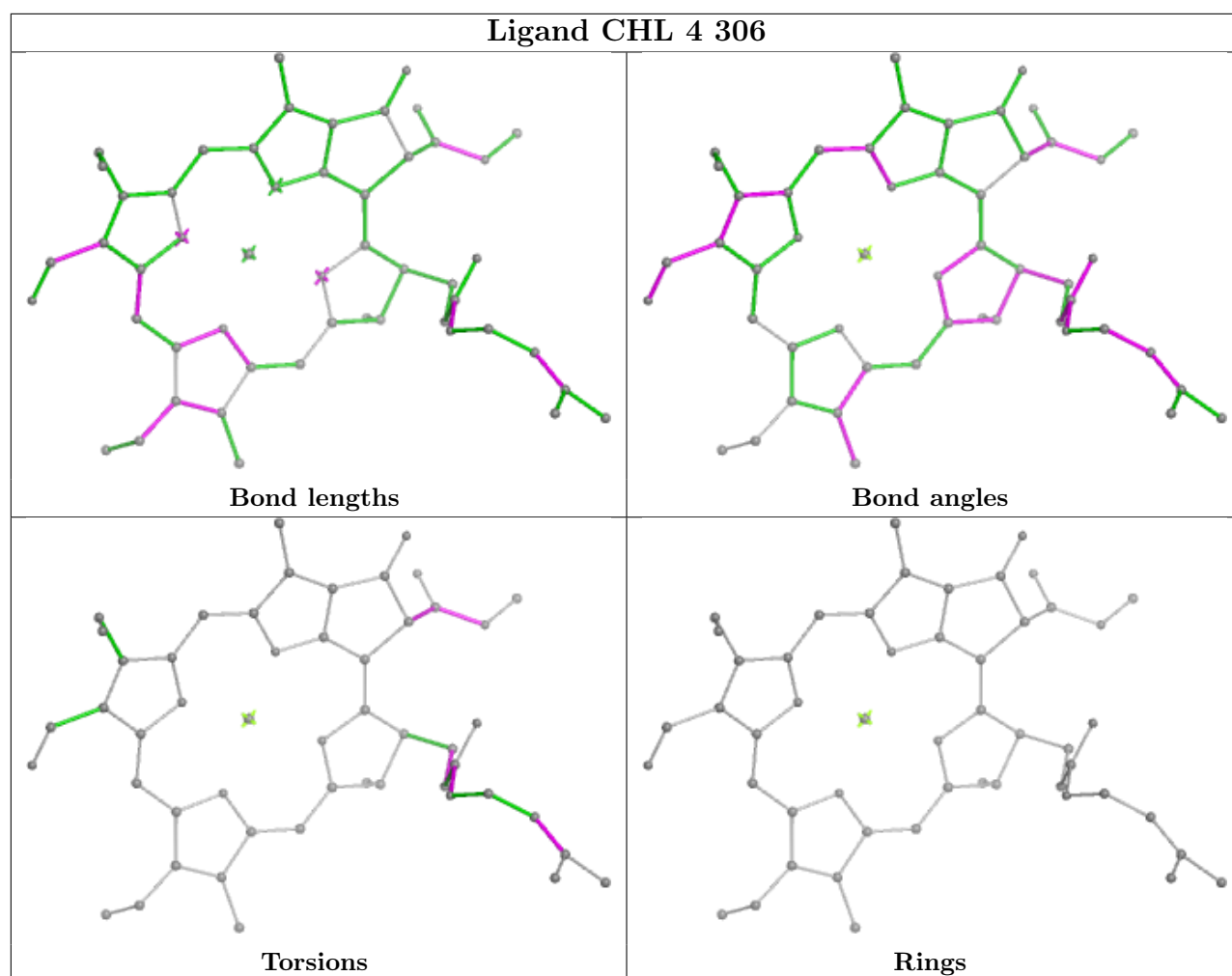
Ligand CLA 1 309



Ligand BCR F 306







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.

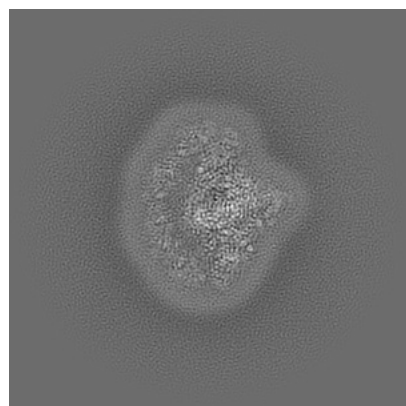
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51219. These allow visual inspection of the internal detail of the map and identification of artifacts.

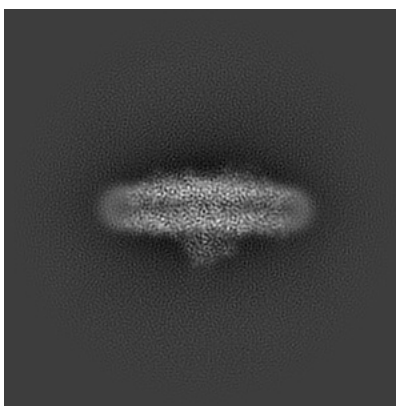
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

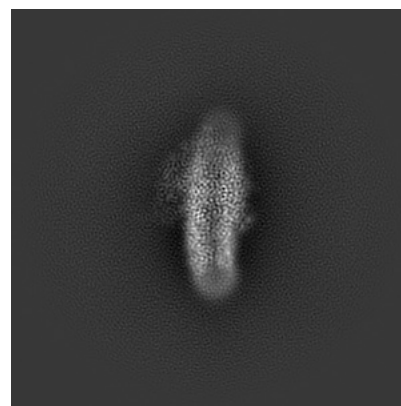
6.1.1 Primary map



X

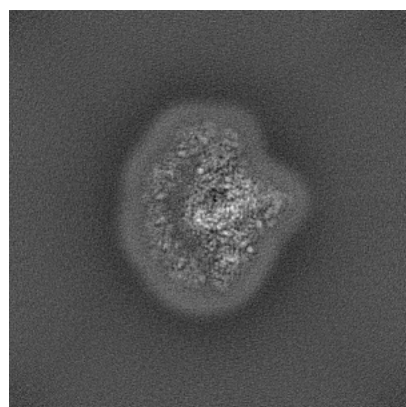


Y

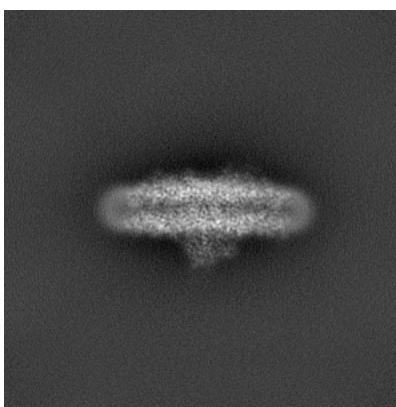


Z

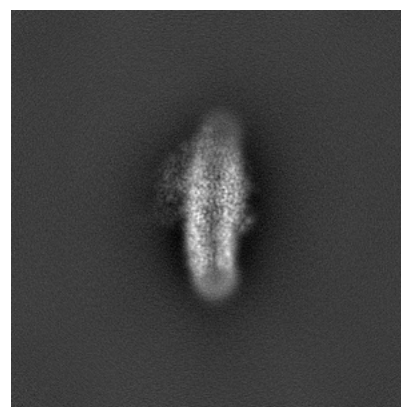
6.1.2 Raw map



X



Y

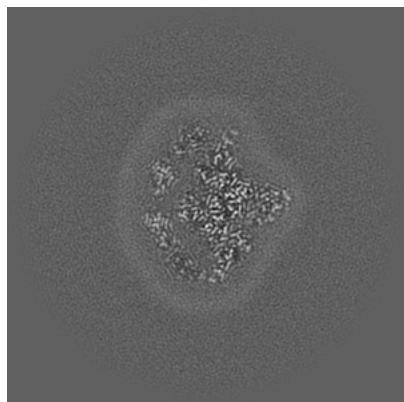


Z

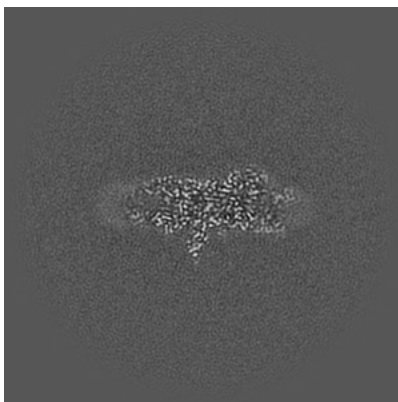
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

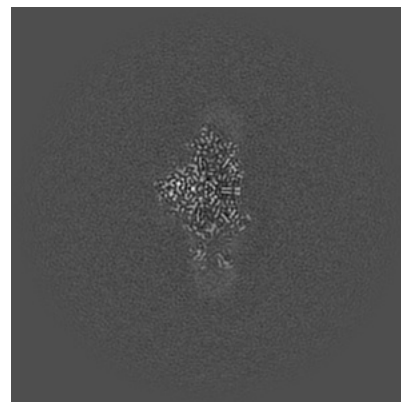
6.2.1 Primary map



X Index: 224

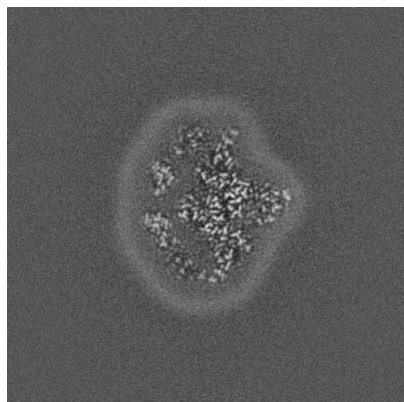


Y Index: 224

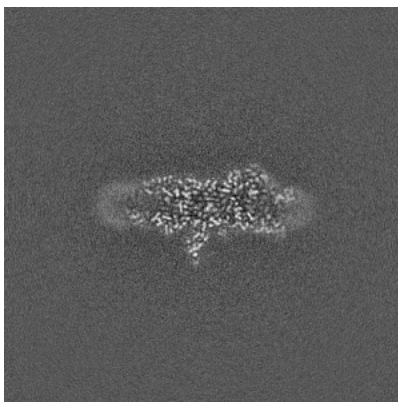


Z Index: 224

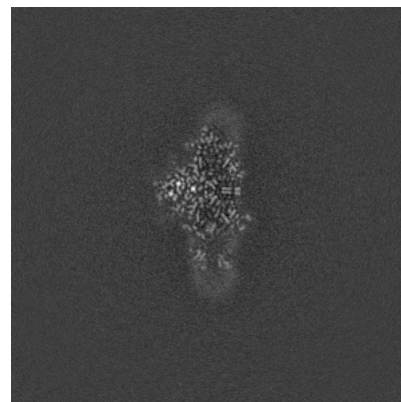
6.2.2 Raw map



X Index: 224



Y Index: 224

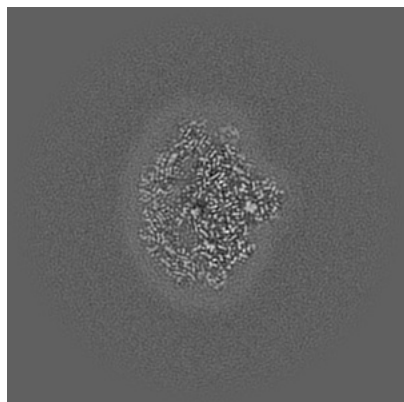


Z Index: 224

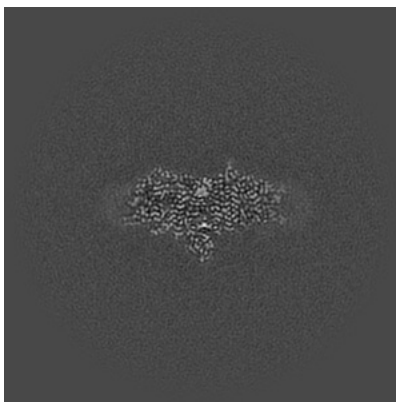
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

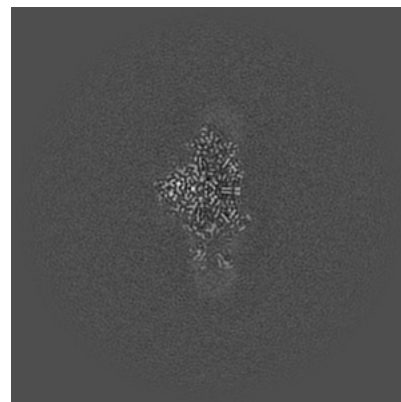
6.3.1 Primary map



X Index: 212

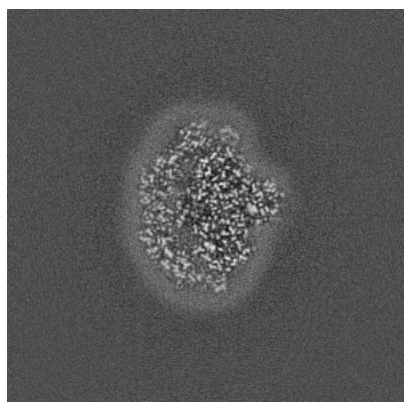


Y Index: 244

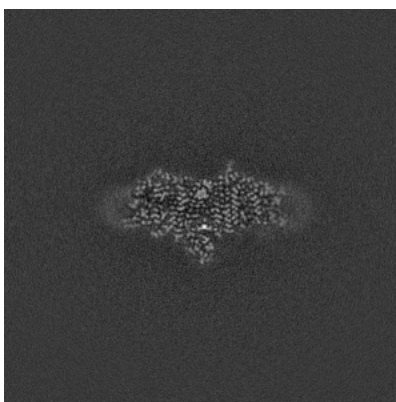


Z Index: 224

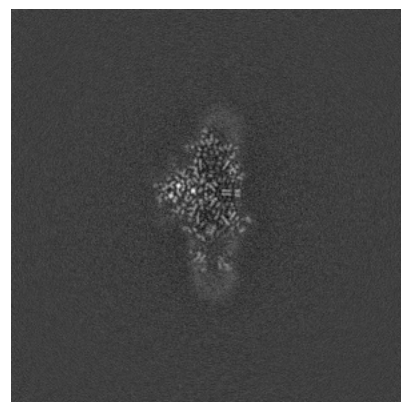
6.3.2 Raw map



X Index: 211



Y Index: 244

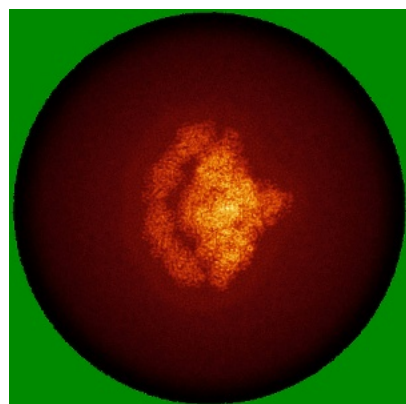


Z Index: 224

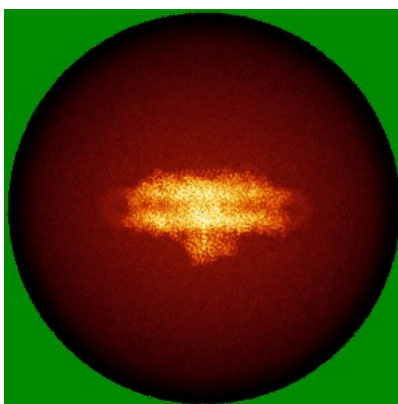
The images above show the largest variance slices of the map in three orthogonal directions.

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

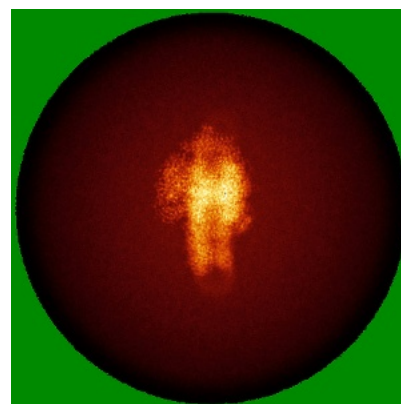
6.4.1 Primary map



X

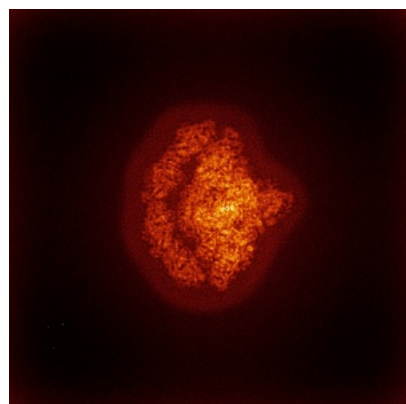


Y

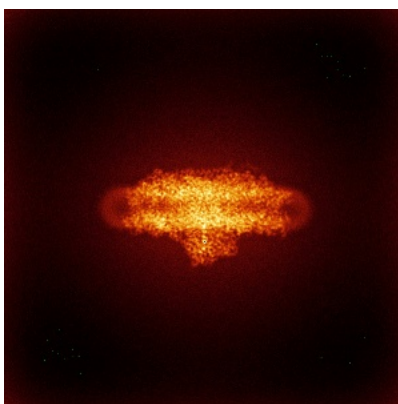


Z

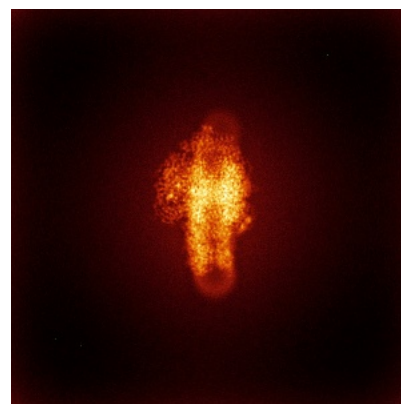
6.4.2 Raw map



X



Y

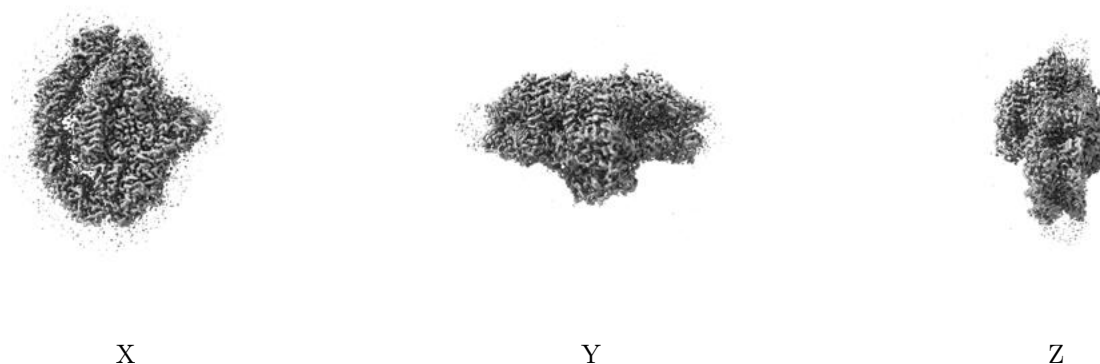


Z

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.

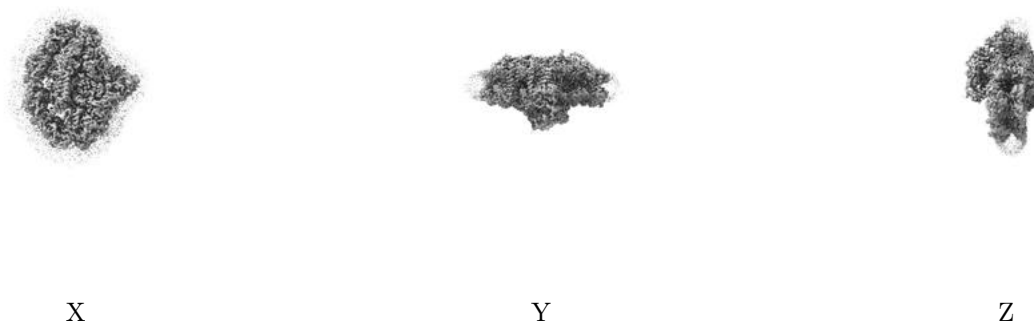
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

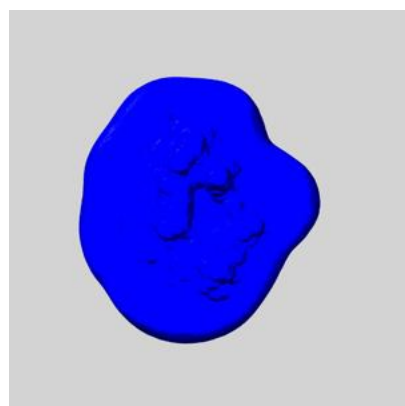
6.6 Mask visualisation [i](#)

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

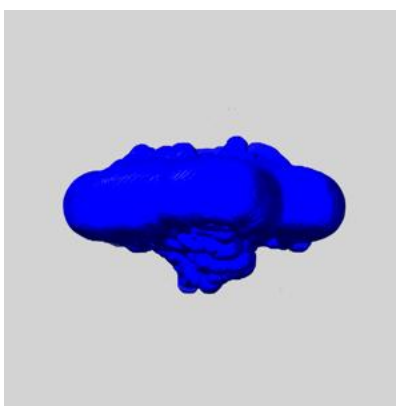
A mask typically either:

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

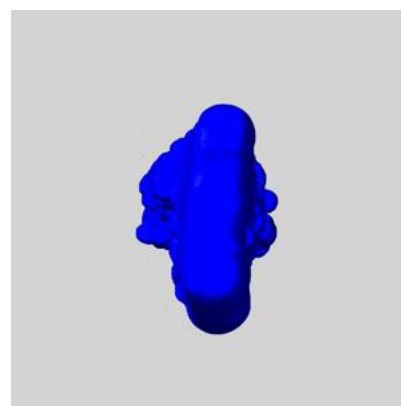
6.6.1 emd_51219_msk_1.map [i](#)



X



Y

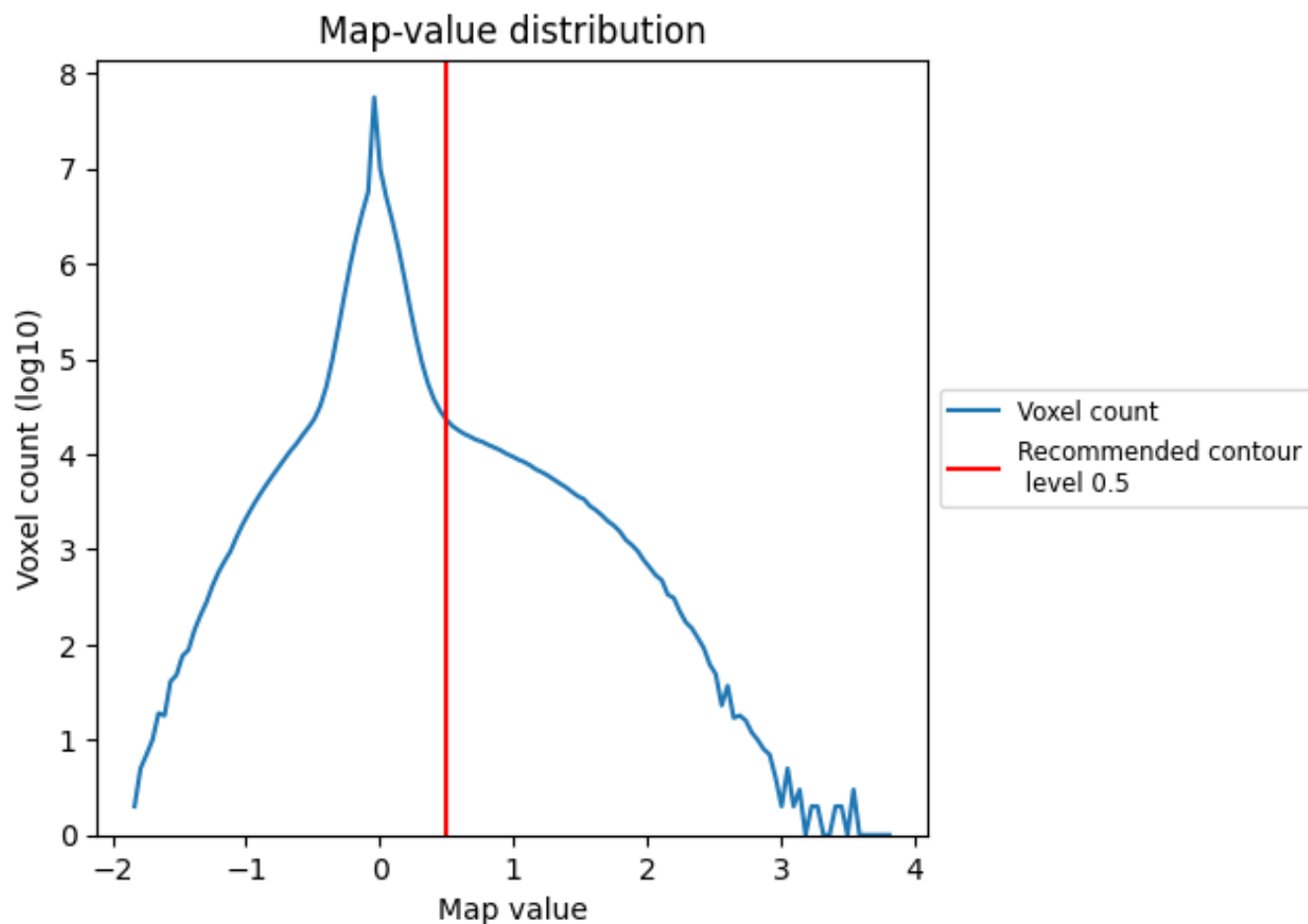


Z

7 Map analysis [i](#)

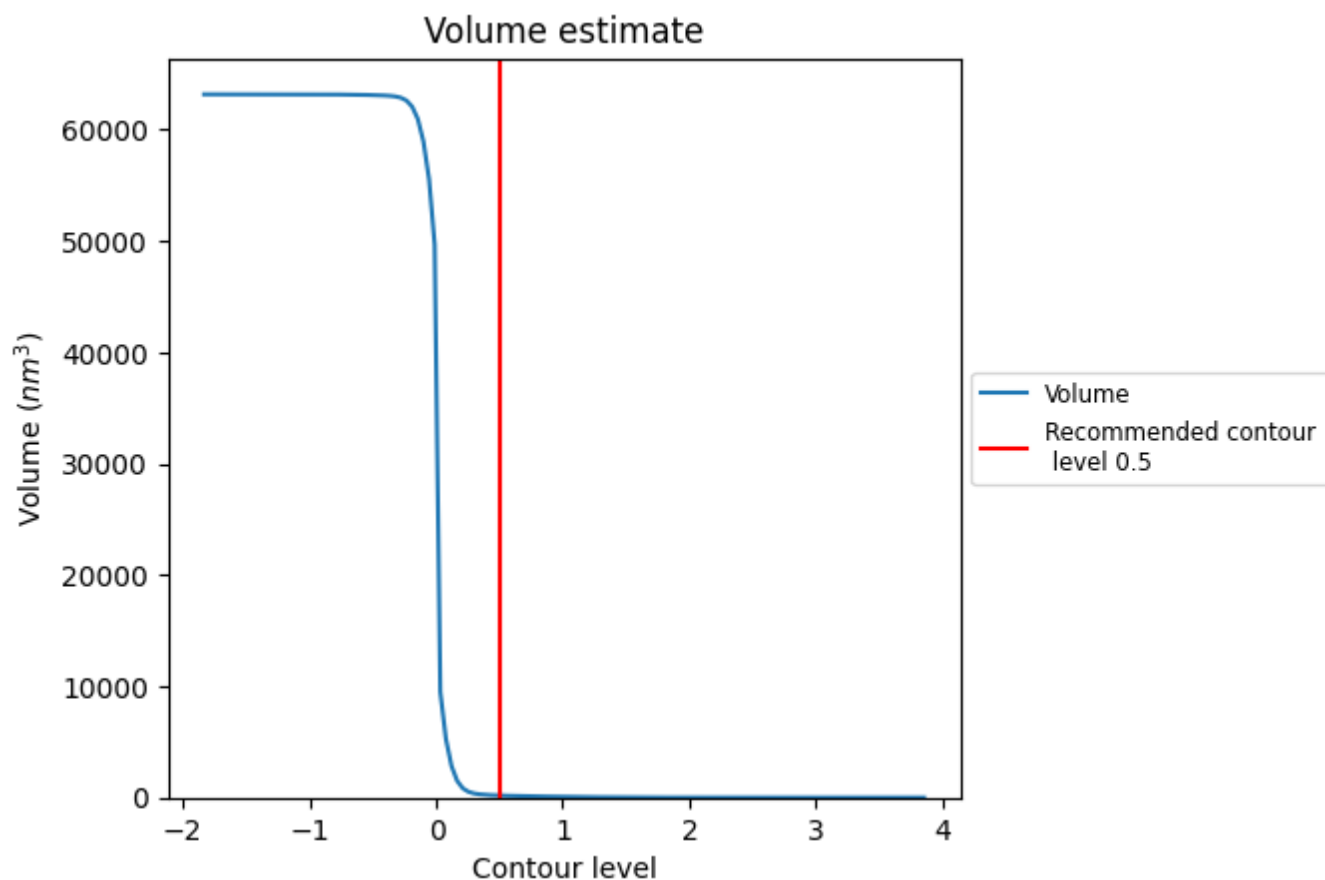
This section contains the results of statistical analysis of the map.

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.

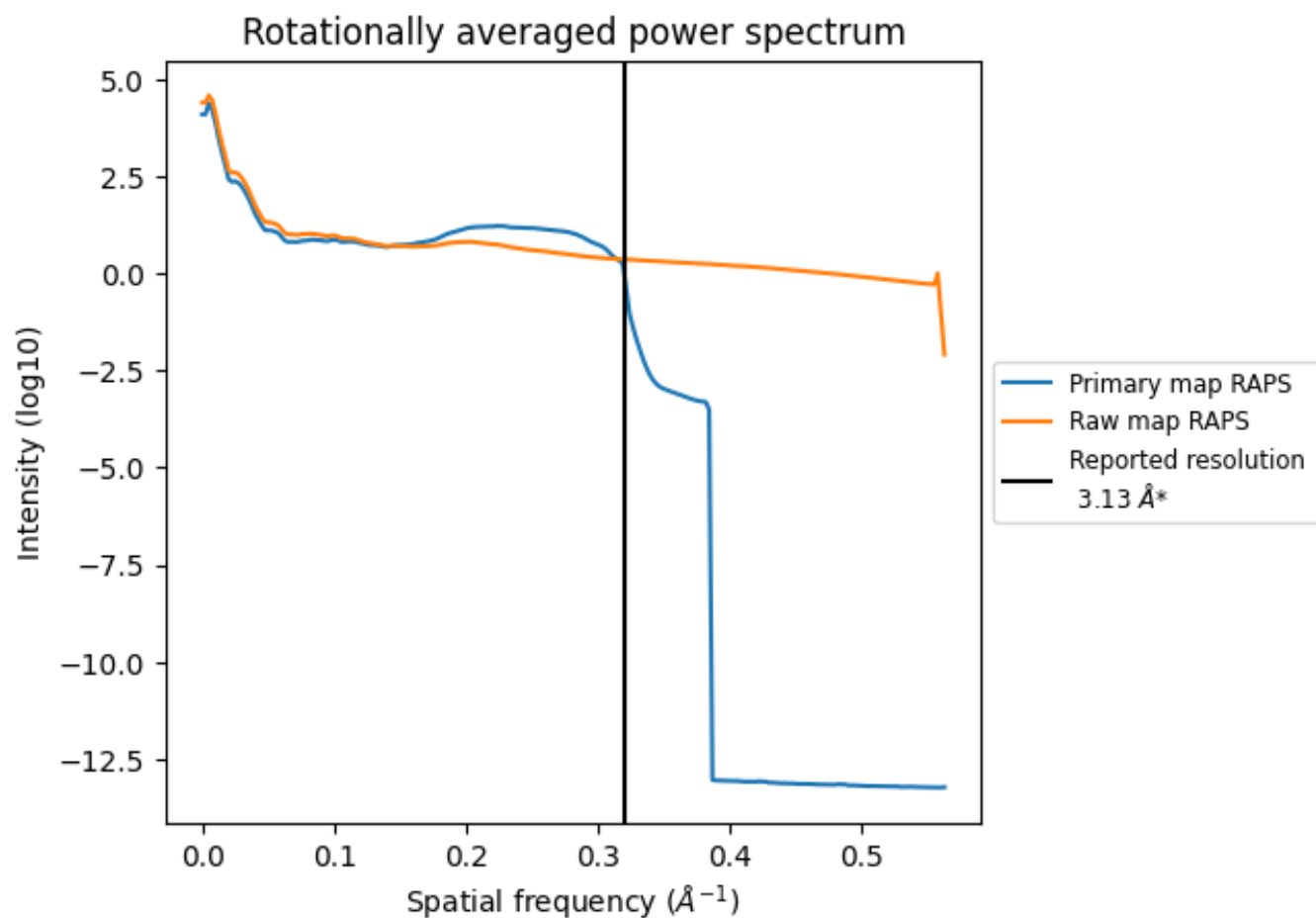
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm^3 ; this corresponds to an approximate mass of 167 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 ⓘ

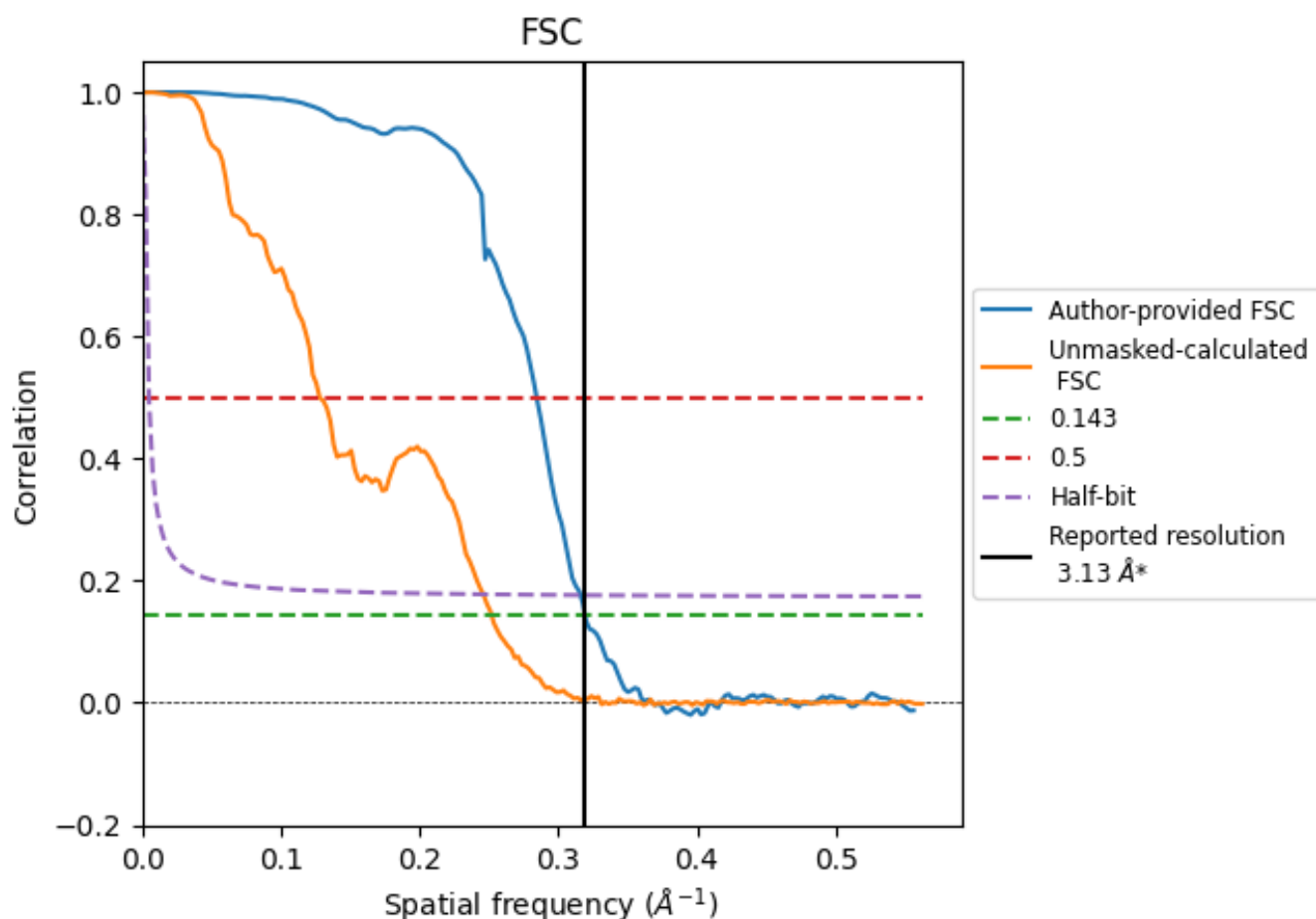


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.319 \AA^{-1}

8.2 Resolution estimates [i](#)

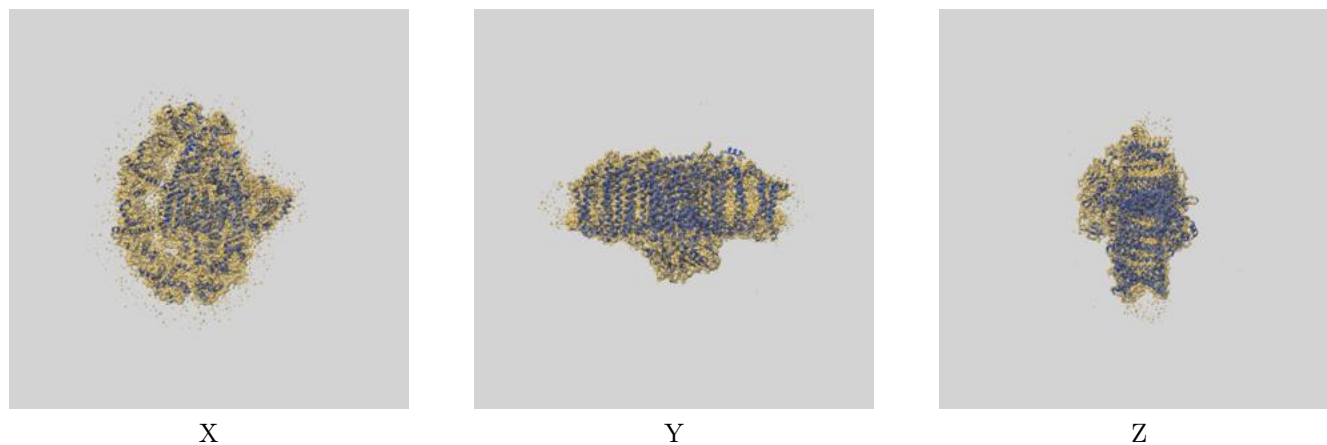
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.52	3.16
Unmasked-calculated*	3.97	7.82	4.07

*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 3.97 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

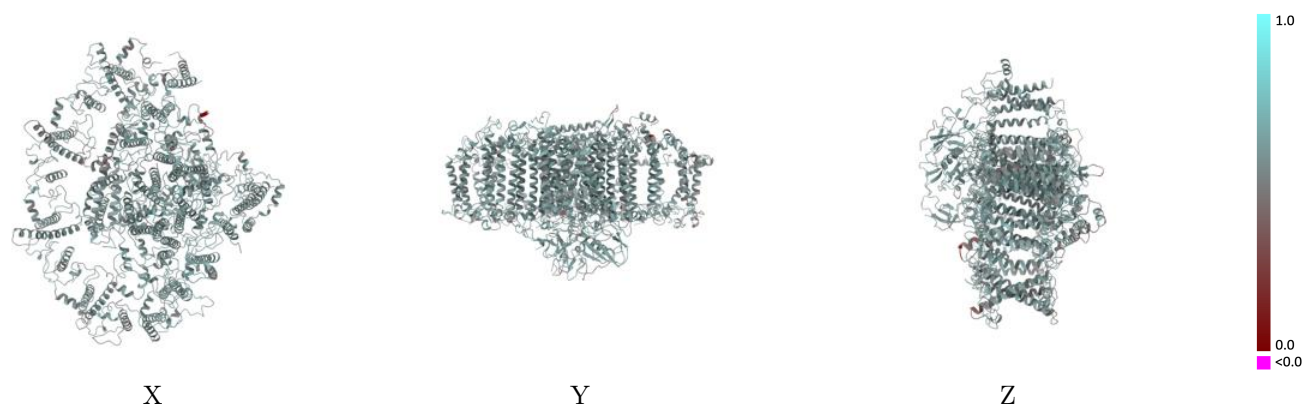
This section contains information regarding the fit between EMDB map EMD-51219 and PDB model 9GBI. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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](#)



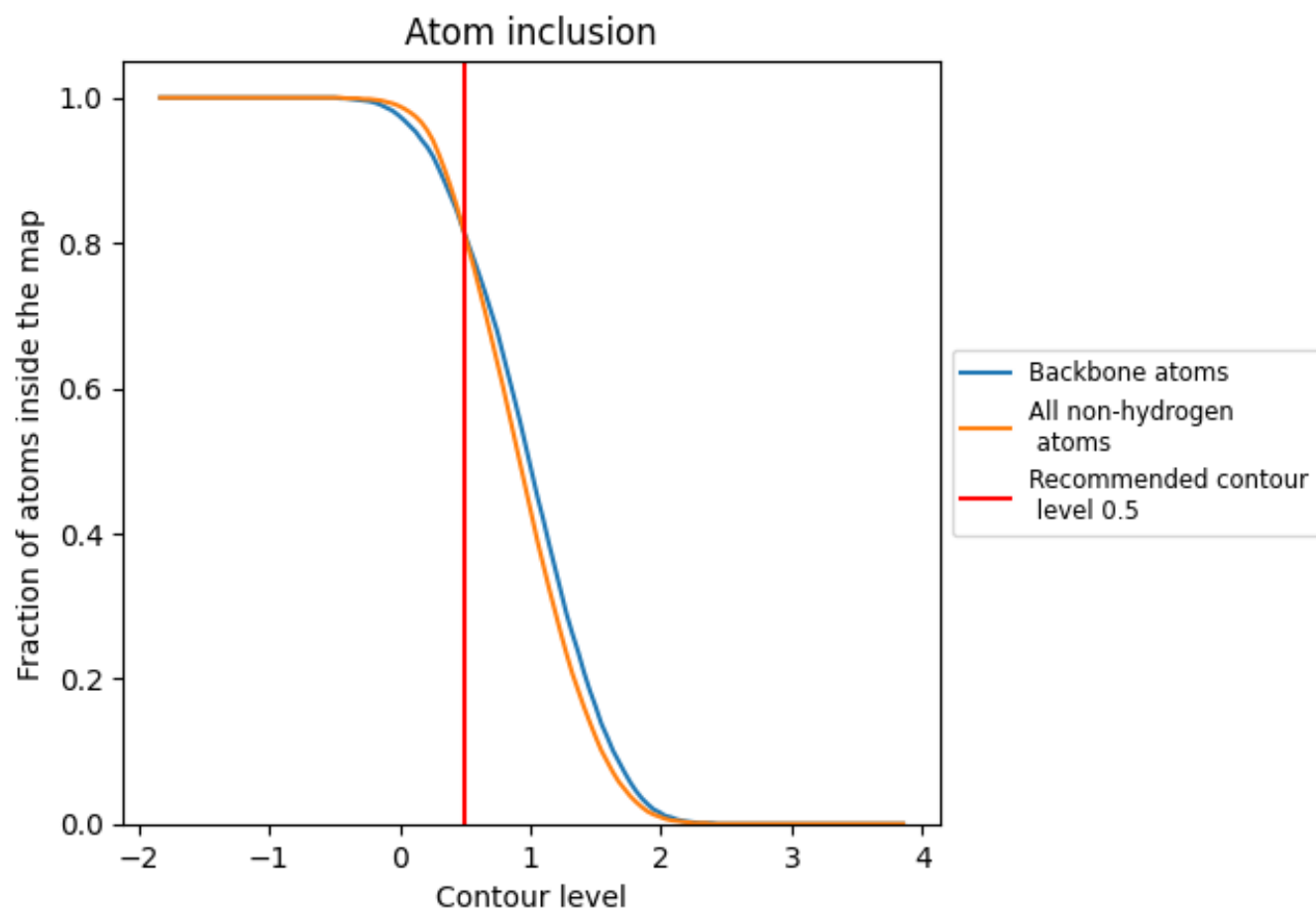
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8100	<div></div> 0.5720
1	<div></div> 0.7480	<div></div> 0.5530
2	<div></div> 0.7420	<div></div> 0.5490
3	<div></div> 0.7740	<div></div> 0.5550
4	<div></div> 0.7570	<div></div> 0.5570
A	<div></div> 0.8570	<div></div> 0.5870
B	<div></div> 0.8660	<div></div> 0.5900
C	<div></div> 0.8880	<div></div> 0.5820
D	<div></div> 0.8120	<div></div> 0.5720
E	<div></div> 0.7580	<div></div> 0.5670
F	<div></div> 0.8020	<div></div> 0.5720
G	<div></div> 0.7750	<div></div> 0.5630
H	<div></div> 0.7410	<div></div> 0.5500
I	<div></div> 0.8190	<div></div> 0.5630
J	<div></div> 0.7680	<div></div> 0.5590
K	<div></div> 0.6570	<div></div> 0.5110
L	<div></div> 0.8080	<div></div> 0.5620
N	<div></div> 0.4300	<div></div> 0.5010

1.0

0.0

<0.0